

## 제 출 문

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본 보고서를 “산업별 수입대체 생물자원 근연종 발굴 (I) - 자생 식물자원의  
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# 요 약 문

## 1. 제 목

산업별 수입대체 생물자원 근연종 발굴 (I) - 자생 식물자원의 아로마 물질 탐색 및 발굴

## 2. 용역사업 배경(필요성) 및 목적

산업별(한약재, 원예, 향장, 식용 등)로 활용되는 식물자원의 상당량을 수입에 의존하는 실정이며, 향신료의 수입단가 증가폭(수입량 대비 수입금액 증가 변화폭)은 점차 확대되는 추세이다. 또한 ABS 나고야의정서 발효 이후 생물자원 수입 단가 상승에 대비하고, 국내 관련 산업 지원을 위해 수입대체 식물의 자생 근연종 발굴이 필요하다.

13년도 ‘자생 식물자원 유용성 탐색·발굴을 위한 기반 연구’사업(약용, 식용, 건강기능성 식물대상 유용성 등급평가)의 후속조치 사업으로 추진하고자 한다.

본 연구용역의 목적은

첫째, 향신료의 국제현황 및 국내외 시장 현황 분석을 통하여 자생 아로마 식물자원의 탐색·발굴 추진 중장기 계획 수립

둘째, 1) 자생식물의 아로마 성분 분석을 위한 시료채취 및 분석법 표준화, 2) 시료의 상태(생체시료/건조시료)에 대한 아로마 물질 비교분석, 3) 지역 및 개체에 따른 아로마 물질 분석, 4) 수입 대체 가능한 아로마 식물자원 후보종을 대상으로 시범분석을 통하여 아로마 성분 분석을 위한 조건 확립 및 후보종 대상으로 시범 분석을 시행하고자 한다.

## 3. 연구내용 및 방법

첫째, 수입 향신료 대체 물질로 이용 가능한 자생 아로마 식물자원 후보 목록 구축한다. 이는 국내 수입되는 대표 향신료 및 허브(herbs) 식물의 수입 현황 조사 및 목록화하며, 기존 통계자료를 기초로 분석한다. 또한

둘째, 아로마 성분 분석을 위한 조건 확립 및 후보종 대상으로 시범 분석을 시행한다. 수입 대체 가능한 아로마 식물자원 후보종(충충이꽃, 긴병꽃풀, 벌깨덩굴)을 대상으로 건체-생체, 채집부위, 지역에 따라 향성분을 시범분석하며, 자생식물의 아로마 성분 분석을 위한 분석법에 대하여 SPME와 Steam Distillation을 이용하여 표준 방법을 개발한다.

## 4. 연구결과

향신료의 수입은 점진적으로 증가하고 있으며, 수입중량 대비 수입가격을 볼 경우 수입단가가 지속적으로 증가되고 있다. 계피의 경우 수입단가의 상승으로 수입량이 감소하고 있어 가격 결정력이 매우 높다는 것을 알 수 있다. 다만 한-인도 CEPA협약에 의하여 회향과 심황의 경우 단가의 하락이 발생하였다.

향신료 중 꿀풀과 식물이 정유성분을 확인하였으며, 국내 자생하는 꿀풀과를 중심으로 근연종의 정유 성분을 목록화 하였다.

분석법 중 SPME와 Steam Distillation을 비교하여 Steam Distillation에서 보다 많은 정유 성분이 검출되는 것을 확인하였으며, 생체보다 건체에서 정유성분을 분석하는 것이 효율 적임을 확인하여, 층층이꽃, 긴병꽃풀, 벌깨덩굴에 대하여 지역별, 채집부위별 정유의 성 분을 분석하였다.

## 5. 결 론

국내에 수입되고 있는 향신료는 2007년 이후 수입증량은 일정하게 증가하고 있으나 수 입 단가의 변화와 국제 시장의 변화로 수입금액의 영향을 많이 받는다. 여러 환경적, 경 제적 국제협약으로 인하여 향신료 시장의 변화가 예상되며, 다각적이고, 지속적인 수입대 체 자생종의 연구가 필요하다.

자생식물자원의 아로마 물질을 탐색하기 위한 실험방법으로 SPME 보다 Steam Distillation 을 사용하는 것이 효과적임을 확인하였으며, 또한 채집, 건조, 추출, 분석에 대한 기준을 제시하였다. 현재 사용한 추출 용매 및 시간의 경우 시료의 한정성으로 인하여 기존의 참 고문헌을 토대로 수행하였다. 앞으로 다양한 추출용매 (ethyl acetate, hexane, ethyl ether 등) 및 추출시간 (1, 3, 5, 7 시간) 의 최적화가 필요하다. GC-MS의 분리 조건은 가장 분 리능이 좋은 조건으로 설정하여 수행하였다.

생체와 건체 벌깨덩굴에 함유되어 있는 휘발성 성분은 GC/MS의 TIC로부터 각 피이크 면적으로 비교하였을 때, 건체 상태에서 휘발성 성분의 양이 생체상태보다 상대적으로 높 게 함유되어 있는 것을 확인되었다. 벌깨덩굴과 층층이꽃에서 나타난 대부분의 성분들은 구조적으로 alkane chain을 가지는 화합물들이 나타났다. 긴병꽃풀의 주성분은 eucalyptol 과 o-thymol 로 나타났다. 이외에도  $\gamma$ -terpinene, camphor,  $\beta$ -copaene 이 검출되었으며, phenyl alcohol류, monoterpene류와 같은 휘발성 정유성분도 검출되었다. 타임(thyme)의 경우 국내 근연종으로 백리향과 섬백리향이 있으나, 본 연구를 통하여 긴병꽃풀에도 o-thymol을 확인하였으므로 향신료의 대체가 가능할 것으로 판단된다.

향후 산지별, 시기별 구분하기에는 각 시료 군에 포함된 시료의 개수가 적어 현재의 자 료로는 불가능 할 듯하지만, 적절한 시간을 통하여 다량의 산지, 시료를 채집하여 자생식 물의 대표적인 지표성분을 선정하여 군집분석을 수행할 수 있을 것으로 사료된다.

## 6. 기대효과(또는 활용방안)

산업별 수입대체 생물자원 근연종 발굴을 위한 방법을 제시하였다. 특히, 경제성 검토 와 가능성 검토를 면밀히 시행한 후 대상종 선정과 표준화된 분석법으로 대체가능한 자생 종을 발굴하고 Bioactivity에 대한 연구를 통하여 산업화 단계를 추진하여야 한다. 2단계 사업을 추진하여 국내 자생종에 대한 연구범위를 확대할 수 있을 것이다.

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## Abstract

### Exploring for an Alternative Imported Spices from Biological Resources (I)

#### – Search and Development of the Aroma Material from the Native Plant Resources in Korea

Since 2007 the amount of imported spices to the Korean Markets has been increasing consistently. However the total costs for imported species are heavily influenced by the two factors, i.e. the unit cost of import and the changes of international markets. Various environmental changes and international economic conventions (e.g., 'ABS Nagoya Protocol') could bring about the spices market change internationally. It is therefore badly needed continually to search for an alternative natural resources, especially from native plants.

The purpose of this study is to prepare the list of the status of imported spices, to define the aroma and its use, and finally make up the list of the native plants (in particular Lamiaceae, mint family) which are possibly useful for an alternative spices in the future.

The import amount of mustard (*Brassica* taxa) is consistent, but its import cost has been increasing. Concerning the Cinnamon (*Cinnamomum zeylanicum* Blume), the import amount has decreased, while the import price is increased. The case of the pepper (*Piper* taxa), the import amount proportionate to the GNI (Gross National Income). The Ginger (*Zingiber officinale*) is the price-sensitive item depending on the production and import prices. The import amounts of thyme and bay leaves are also consistent as like mustard, but import price has been increasing because of increasing the IUP (import Unit Price). Since 2012, the IUP of clove (*Syringa velutina*) has been up sharply. The import amount of seeds of coriander (*Coriandrum sativum*) is also constant, because of jumping the IUP. Beginning in 2012, the import prices of both fennel (*Foeniculum vulgare*) and turmeric (*Curcuma longa*) has decreased. It is considered that the signing the CEPA (Communications, Education and Public Awareness – the equivalent to a Free Trade Agreement, FTA) with India which is the trading partner for the coriander import.

Main compositions of the essential oil from four selected representative spices, namely thyme (*Thymus vulgaris* L.), Rosemary (*Rosmarinus officinalis* L.), Mint–Peppermint (*Mentha* × *piperita*), and Spearmint (*Mentha spicata* L.) are selected and listed.

Based on the literatures, the analysed essential oils of all known Lamiaceae taxa in Korea and their related taxa are listed. It is confirmed that there are no information available concerning the essential oil analysis for three taxa, e.g., *Lagopsis* Bunge ex Benth., *Meehania* Britton, and *Tripura* P. D. Cantino.

Steam distillation method was more effective than solid phase microextraction (SPME) method in the extraction of aroma components from the native plant resources. In addition, sample processing steps including collection, drying, extraction, and analysis were optimized on the basis of previous literatures.



Due to tight the time schedule of this project and limited sampling, the extraction solvent and period conditions were selected on the basis of previous literatures. When a large amount of sample could be obtained in next project, various solvents (ethyl acetate, hexane, ethyl ether etc.) and extraction period (1, 3, 5, 7 hr/hrs) examine and test to find the optimum conditions in extraction of aroma components from target plants.

Interestingly, the amounts of aroma components in dried *Meehania urticifolia* (Miq.) Makino were shown to be relatively more than those in raw *Meehania urticifolia*, when the amounts of aroma compounds in raw and dried *Meehania urticifolia*, respectively, were compared by total peak area of aroma compounds obtained from their corresponding GC/MS total ion chromatograms (TIC).

Eight characteristic compounds such as 4-methyloctane, 3,3,6-trimethylheptane, 2,7,10-trimethyldodecane, 2,3,5-trimethyldecane, 2,6,11,15-tetramethyl hexadecane, dihydroactinidioide, 7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene- 2,8-dione, and butylphthalate were observed in flower part of *Meehania urticifolia*. Whereas they were not observed in stem part.

Chemical structures of most of the aroma components observed in both *Meehania urticifolia*. and *Clinopodium chinense* var. *parviflorum* (Kudo) H. Hara contain alkane chain.

The analysis of floral parts in both *Clinopodium chinense* var. *parviflorum* and *Meehania urticifolia* composed of similar chemical components, but some characteristic components such as o-guaiacol, p-ethylphenol, p-creosol, p-ethylguaiacol, p-vinylguaiacol, and syringol were observed in *Clinopodium chinense* var. *parviflorum*, especially for No 3 sample.

For *Glechoma longituba* (Nakai) Kuprian., eucalyptol and o-thymol were observed as major aroma compounds. Besides these compounds,  $\gamma$ -terpinene, camphor,  $\beta$ -copaene, phenyl alcohols, and monoterpenes were also detected.

Thyme (*Thymus vulgaris* L.) as spice was known to be characteristic component in related Korean taxa, *Thymus quinquecostatus* Celak. and *Thymus magnus* (Nakai) Nakai. In accordance with finding new spice, o-thymol that was observed as major component of *Glechoma longituba* through this study is expected to be promising alternative compound.

In future, cluster analysis could discriminate the geographic origins and finding harvest period by the selection of marker compounds of the native plants through statistical chemometric analysis such as principal component analysis (PCA) and hierarchical cluster analysis (HCA), if large volume of samples could be obtained and time schedule of the project is appropriate.

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# I. 서 론

## 1. 연구목적 및 배경

가. 산업별(한약재, 원예, 향장, 식용 등)로 활용되는 식물자원의 상당량을 수입에 의존하는 실정

1) '14년도에는 '자생 식물자원의 아로마 물질 탐색 및 발굴'을 위한 향료 식물 자원 분야에 대한 기반 마련

2) ABS 나고야의정서 발효 이후 생물자원 수입 단가 상승에 대비하고, 국내 관련 산업 지원을 위해 수입대체 식물의 자생 근연종 발굴이 필요함.

- 예: 2013년 기준 정향(17,215원/Kg)이 가장 높으며, 향신료의 수입단가 증가폭(수입량 대비 수입금액 증가 변화폭)은 점차 확대되는 추세임.

※'13년도 '자생 식물자원 유용성 탐색·발굴을 위한 기반 연구'사업(약용, 식용, 건강 기능성 식물대상 유용성 등급평가)의 후속조치 사업으로 추진

나. 아로마 성분 분석을 위한 조건 확립 및 후보종 대상으로 시범 분석

1) 자생식물의 아로마 성분 분석을 위한 시료채취 및 분석법 표준화

※ 고상미세추출법(SPME), 수증기 증류법(Steam distillation) 등을 이용한 아로마 추출법 비교분석 등

2) 시료의 상태(생체시료/건조시료)에 대한 아로마 물질 비교분석

3) 지역 및 개체에 따른 아로마 물질 분석

4) 수입 대체 가능한 아로마 식물자원 후보종을 대상으로 시범분석

다. 자생 아로마 식물자원의 탐색·발굴 추진 중장기 계획 수립

1) ABS 나고야 의정서 등 국제현황 및 국내외 시장 현황 분석

2) 자생식물 대량 증식 및 계통 확보 전략 제시 등

## 2. 2014년도 연구 목표

### 가. 향신료의 정의

향신료라 함은 주로 열대, 아열대지방에서 생산되는 ‘스파이스(SPICES)’와 온대지방에서 생육하는 ‘허브(HERBS)’의 총칭으로 spices의 어원은 라틴어의 ‘*species aromatacea*’에서 유래했는데, “땅의 과일”이라는 의미이다. 이것을 줄여서 ‘spieces’라고 했으며, 후에 스파이스는 ‘spice’로 변화됐다. 즉, 허브는 “온대지방에서 자라는 식물로서 음식의 맛과 향을 내는데 사용하는 초본성식물”로 정의할 수 있고, 반면에 스파이스는 “음식의 맛, 향, 그리고 색깔을 내기위해 온대 및 열대에서 생산되어 건조한 채 이용되는 모든 식물성재료”로 표현할 수 있다. 최근 미국향신료 무역협회에서는 “부엌의 조미료 선반에서 다루는 모든 식용 가능한 물질을 스파이스라고 명명한다. 여기에는 허브와 역사적으로 조미료라고 부르는 조미료종자, 조미혼합물 그리고 건조채소를 포함한다”라고 하고 있다.

또한, 향신료라는 것은 “특유의 향과 맛으로 식품의 향과 맛을 돋워주며 아름다운 색을 더하여 식욕을 증진시키고, 소화기능을 도와주는 작용이 있는 것”으로 정의하고 있지만, 나라와 지역 그리고 각각의 식생활의 방법에 따라 섭취하는 향신료의 종류와 이용방법이 다르다. 이와 같이 향신료는 식생활의 변천에 따라 그 인식도 지속적으로 변화하고 있다. 20세기 초 합성과학이 발달하면서 화학적 향신제 및 인공조미료의 발전으로 천연향과 자연향신료에 타격을 주었으나, 2차 세계대전 후 삶의 질이 높아지면서 화학약품보다는 생약에 대한 관심이 증가되고 특히 보건의식료에 대한 관심이 제고되면서, 생태적인 농업의 발전과 함께 향신료의 소비가 늘고, 유럽의 가정원예에서도 향신채가 중요한 역할을 담당하게 되었다.

### 나. 향신료의 작용과 이용

향신료는 미각, 후각, 시각, 통각 등, 여러 감각신경을 자극하여 음식의 맛을 향상시키거나 음식의 향미에 변화를 주어 식욕을 증진시키는 중요한 역할을 한다. 또한, 향신료는 질병예방과 건강유지에 도움이 되는 것으로 인식되어 왔는데, 비타민과 미네랄이 풍부하고 각종 약리성분이 함유되어서 곡물류, 채소 및 과일류와는 다른 기능을 가지고 있다.

향신료가 식품에 이용될 때는 직접적이고 다양한 효과 즉, 기능을 나타내는데, 색, 향기, 맛(매운맛, 쓴맛, 단맛) 등 식품에 직접적인 효과를 나타내는 기능과 그 효과를 나타내어 저장성 증진, 방부제, 착색제 등의 효과를 주는 기능과 생체 내에 여러 가지 생리활성을 나타내는 기능 등이 있다.

향신료는 영양적 가치는 적으나, 다양한 맛과 향으로 식욕을 좋게 할 뿐 만 아니라, 매운맛 향신료(고추, 후추, 생강, 겨자 등)는 교감신경계의 활동을 높여주고, adrenalin분비 noadrenalin 분비를 촉진하고 항 스트레스 작용과 함께 지방대사, 에너지대사, 체열 생산 등의 이화작용을 촉진 하는 것으로 밝혀지고 있다.

향신료는 특성에 따라 이용 방법을 나누어 볼 수 있다 . ① 매운맛을 내는 향신료로써 후추, 고추, 겨자, 고추냉이 등이 사용되고, ② 향과 맛을 겸한 향신료로써 생강, 계피, 산초, 아니스, 페닐 등이 사용되며 ③ 향기가 강한 향신료로써 월계수, 세이보리, 고수, 등 ④ 색소를 이용하는 향신료로써 사프란(적등색, 노란색, 오렌지색), 심황(노란색, 오렌지색), 커레이 (노란색), 파프리카 (적색, 노란색) 등이 있다.

#### 다. 세계 향신료 수출-수입동향 (2004년 이후 일부 데이터 기준)

향신료의 1970년대부터 2004년까지의 34년간 수출 추세를 보면 전 세계적으로 9배에 가까운 수출 성장을 볼 수 있다(Fig. 1; Tables 1-2). 즉 1970년대 의 주요수출입 국가들을 살펴보면 불과 1억 5천만 달러였던 향신료의 수출이 1980년대까지는 10년 사이에 약 4배가 증가되었고, 1980년대에서 1990년대 사이에는 증가세가 1.4배로 잠시 둔화되었다가 다시 1990년에서 2000년 사이에는 약 2배로 성장하였다. 2000년대부터 2004년도에는 불과 4년 사이에 3배로 증가하였다. 이런 결과를 종합해보면, 지난 34년간 약 8.2배가 증가되었다. 주요 수출국으로는 1970년대와 1980년도까지는 인도와 싱가포르가 전체 수출의 절반 이상을 차지하였으나, 1990년 이후에는 인도네시아 싱가포르가 2004년에는 중국과 말레이시아가 수출 1위국을 지키고 있다. 이는 향신료의 사용이 많은 동남아시아 국가의 생산량이 매우 큰 것을 알 수 있다.

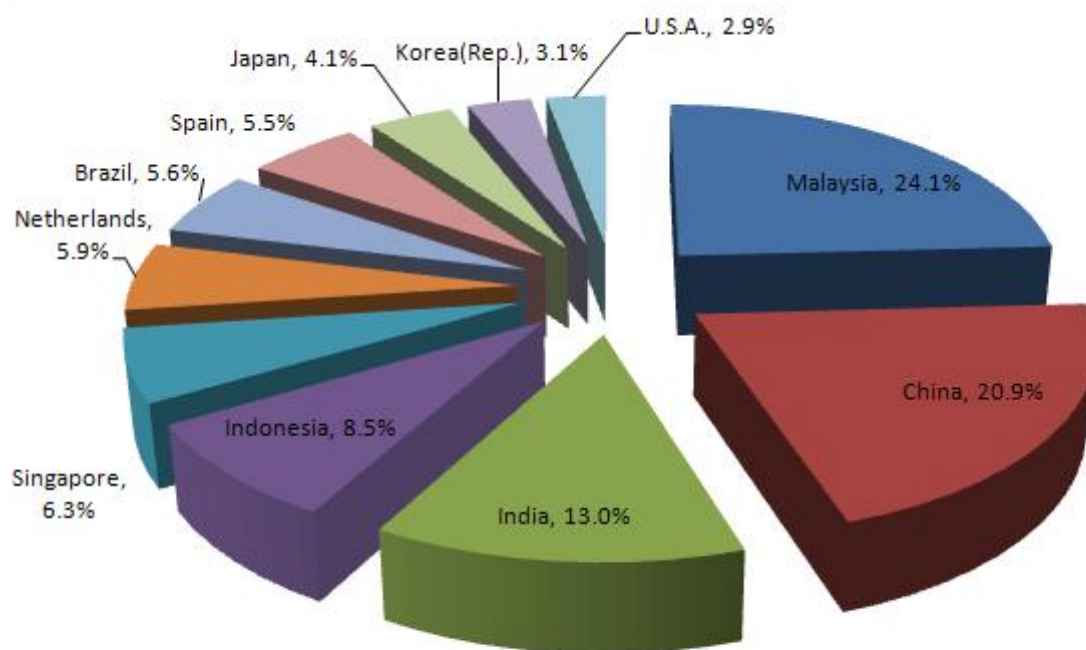


Fig. 1. Main export countries of spices in 2004.

Table 1. Export of spice in main countries.

(unit : Million dollars)

| country     | year | 1970 <sup>z</sup> | 1980 <sup>z</sup> | 1990 <sup>z</sup> | 2000 <sup>z</sup> | 2004 <sup>Y</sup> |
|-------------|------|-------------------|-------------------|-------------------|-------------------|-------------------|
| Malaysia    |      | 20.4              | 52.4              | 51                | 117.6             | 470.9             |
| China       |      | 4.2               | 13                | 91.1              | 146.4             | 408.2             |
| India       |      | 52                | 188.9             | 111               | 238.2             | 254.1             |
| Indonesia   |      | 9.3               | 75                | 152.4             | 263.9             | 165.2             |
| Singapore   |      | 41.2              | 117.9             | 137.3             | 255.1             | 123.9             |
| Netherlands |      | 2.1               | 12.2              | 44.3              | 94.6              | 114.3             |
| Brazil      |      | 8.2               | 57.7              | 50.7              | 84.1              | 109.6             |
| Spain       |      | 8.7               | 46.8              | 67.9              | 79.1              | 107.3             |
| Japan       |      | 0.9               | 0.7               | 1.4               | 6.4               | 80.9              |
| Korea(Rep.) |      | 0                 | 3.2               | 2.9               | 7.3               | 60.6              |
| U.S.A.      |      | 6.1               | 24.9              | 35.1              | 70.1              | 57.1              |

Source : Modified data from z: UNCTAD COMTRADE, Y: UNCTAD/WTO

향신료 주요 수입국은 미국, 일본, 독일, 등 선진 국가들이 주류를 이루고 있다. 수입 대비 수출이 가장 많은 나라는 말레이시아와 중국으로 약 수입량의 70%를 수출하고 있고, 수출대비 수입이 많은 나라는 미국과 일본 등이 있다(cf. Fig. 2, Tables 2, 3).

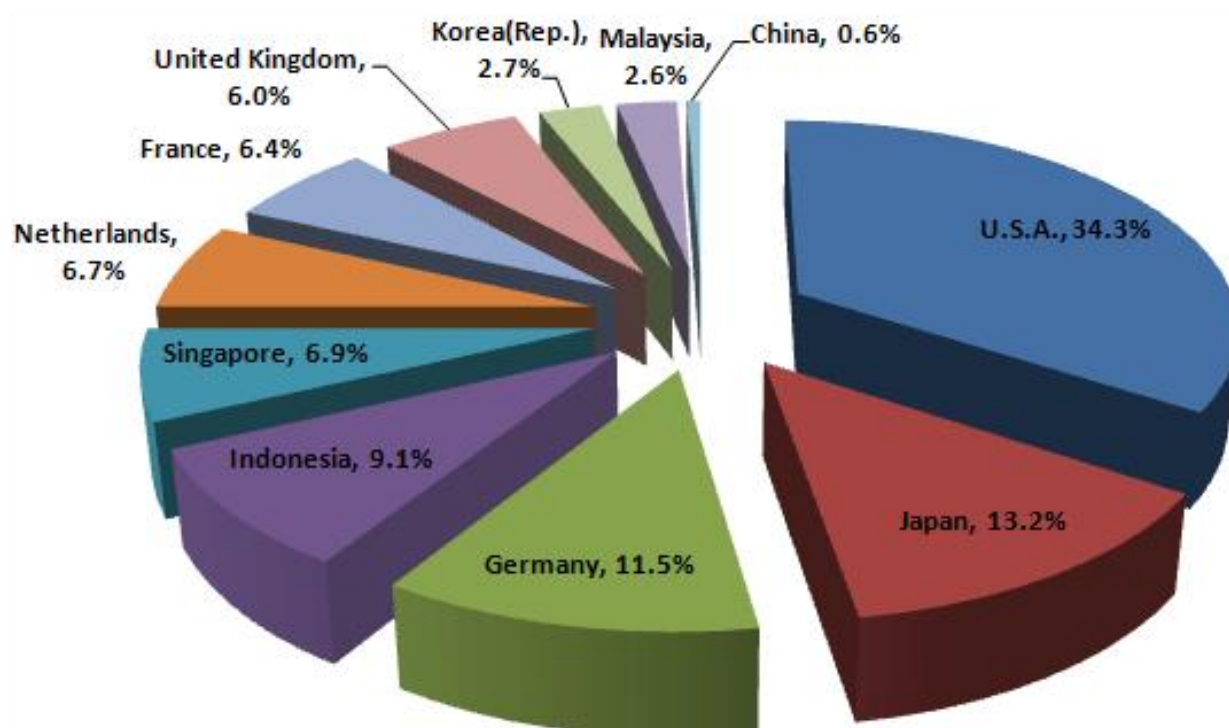


Fig. 2 . Main import countries of spices in 2004.

Table 2. Top importing countries or areas in 2010

| Country or area           | Value<br>(million US\$) | Avg.<br>Growth<br>(%)<br>06-10 | Growth<br>(%)<br>09-10 | World share % |      |
|---------------------------|-------------------------|--------------------------------|------------------------|---------------|------|
|                           |                         |                                |                        |               | Cum. |
| World.....                | 5770.2                  | 14.9                           | 22.5                   | 100.0         |      |
| USA.....                  | 843.1                   | 11.7                           | 23.0                   | 14.6          | 14.6 |
| Germany.....              | 377.2                   | 13.0                           | 27.3                   | 6.5           | 21.1 |
| Japan.....                | 275.8                   | 9.7                            | 21.3                   | 4.8           | 25.9 |
| Saudi Arabia.....         | 270.4                   | 25.5                           | 54.3                   | 4.7           | 30.6 |
| United Arab Emirates..... | 244.7                   | 24.6                           | 55.2                   | 4.2           | 34.9 |
| Malaysia.....             | 243.9                   | 17.7                           | 35.6                   | 4.2           | 39.1 |
| Netherlands.....          | 235.4                   | 18.8                           | 34.9                   | 4.1           | 43.2 |
| United Kingdom.....       | 228.5                   | 16.8                           | 25.4                   | 4.0           | 47.1 |
| Spain.....                | 184.6                   | 14.9                           | -6.8                   | 3.2           | 50.3 |
| France.....               | 175.5                   | 13.3                           | 13.2                   | 3.0           | 53.4 |
| India.....                | 150.8                   | 4.9                            | -11.4                  | 2.6           | 56.0 |
| Singapore.....            | 145.5                   | 3.5                            | -4.2                   | 2.5           | 58.5 |
| Bangladesh.....           | 142.4                   | 30.3                           | 81.8                   | 2.5           | 61.0 |
| Nigeria.....              | 123.5                   | 105.7                          | 969.9                  | 2.1           | 63.1 |
| Mexico.....               | 121.2                   | 9.5                            | -0.6                   | 2.1           | 65.2 |

Table 3. Import of spice in main countries.

(unit : Million dollars)

| country        | year | 1970 <sup>z</sup> | 1980 <sup>z</sup> | 1990 <sup>z</sup> | 2000 <sup>z</sup> | 2004 <sup>y</sup> |
|----------------|------|-------------------|-------------------|-------------------|-------------------|-------------------|
| U.S.A.         |      | 58.1              | 142.0             | 256.8             | 530.4             | 625.2             |
| Japan          |      | 11.9              | 47.8              | 96.1              | 193.0             | 240.4             |
| Germany        |      | 19.6              | 80.3              | 124.2             | 162.3             | 208.8             |
| Indonesia      |      | 26.1              | 62.0              | 5.5               | 62.7              | 165.2             |
| Singapore      |      | 48.2              | 80.4              | 128.6             | 175.8             | 126.6             |
| Netherlands    |      | 3.8               | 18.9              | 59.8              | 133.5             | 122.3             |
| France         |      | 11.3              | 48.1              | 66.7              | 93.5              | 117.2             |
| United Kingdom |      | 10.0              | 28.3              | 48.1              | 86.6              | 110.0             |
| Korea(Rep.)    |      | 2.4               | 12.0              | 11.5              | 33.5              | 49.4              |
| Malaysia       |      | 3.4               | 14.8              | 24.6              | 61.1              | 47.9              |
| China          |      | 0.9               | 6.3               | 2.6               | 27.9              | 10.2              |

## 라. 식물정유의 정의와 분석법개발

### 1) 식물정유 (에센셜 오일 - essential oils in plants) 정의 및 생리적 활성

#### 가) 식물정유 (에센셜 오일) 정의

에센셜 오일(essential oil-식물정유)은 다양한 화학 성분을 지닌 방향성 식물의 각 부위에서 추출한 향과 휘발성을 가진 물질이다. 오래 전부터 정서적 안정을 위해 또는 민간요법이나 종교의식에서 사용되어 왔으며, 현대 향료의 성분 및 효능 등이 과학적으로 입증되면서 스트레스와 질병에 대한 면역력을 향상시킨다는 결과를 나타내고 있다. 또한 근래에 들어서는 정유들이 지니는 독특한 향기를 활용하기 위한 목적 이외에도 기능성 식품, 기능성 향장품, 아로마테라피, 환경개선용 방향제 등으로 용도가 확대되고 있을 뿐만 아니라 정유를 구성하고 있는 각종 구성성분들의 생리활성 구명을 위한 연구도 많이 수행되고 있다.

유럽, 특히 프랑스를 중심으로, 고품질의 풍부한 방향식물 원료 확보와 정유생산설비의 발달로 향장품 향 및 식품 향으로 사용되는 정유를 대량생산하고 있다. 방향성 식물은 향료, 화장품, 의약의 원료로 광범위하게 사용되고 있는 천연물 유래의 생물신소재로 고기능성 제품 개발 및 산업화에 대한 활용도가 매우 높다. 건강지향 신시대에 있는 세계는 천연물에서 유래한 생체조절 및 노화억제와 관련한 생물신소재 발굴 및 개발에 열중하고 있으며 이와 관련한 특허 및 제품들이 산업적으로 매우 중요한 비중을 차지하고 있다.

허브관련 시장점유율은 미국 36%, 유럽 31%, 일본 15% 등 선진국 중심으로 발달하였으며, 미국의 경우 기능성 식품 중 허브가 차지하는 비율은 30% 정도로 상업적 이용 허브

는 400종 이상이며 대규모 허브생산 주 목적은 식용, 의료, 대체치료용으로 광범위하게 활용되고 있다. 유럽의 경우 상업적 이용 허브는 2,000종으로 화장품, 살균, 살충, 방향제 등 향 관련 가공산업 발달 등으로 주 재배종은 140여종을 차지하고 있다.

국내 향료시장은 약 3,500억 원 정도로 매년 5~6%씩 증가하고 있으나 조향 원료는 전량 수입되고 있어 국산화가 시급하다. 전국 허브향료 재배면적은 272ha(2007년, 전남농기원 시험보고서)로 국내의 웰빙 수요가 점차 늘어가고 있는 시점에서 일부 재배 농가를 제외하고는 아직까지 대부분의 허브 관련 산업은 영세한 환경을 벗어나지 못하고 있는 실정이다.

허브식물은 생활밀착형 복합산업으로 관상, 식용, 약용 등 인간생활과 밀접한 다양한 볼거리, 먹거리 제공하고 있다. 허브나 향료작물의 용도로는 조미료, 양념, 차, 화장품, 약품, 음료, 생활용품, 공예품 등 다양하게 이용되고 있어 국내에서도 허브향료작물을 이용한 다양성 있는 개발이 필요하다.

국내의 허브산업은 초보단계로 면적과 생산량 자체가 농림부의 통계연보에도 없는 상황에서 국내 재배되고 있는 허브향료작물의 종묘, 종자, 향 관련 가공품 대부분은 수입 의존하고 있으며 정유생산 및 자체상품 개발과 거리가 먼 관광산업에 만 치중되고 있다. 국내산 자생식물을 이용하여 향장품을 개발 하려는 시도는 여러 번 있었으나 가장 큰 문제점으로 정유를 대량으로 추출할 수 있는 시스템 개발이 없어 산업화에는 실패한 상태이다. 또한 국내 정유시장은 급성장 분야로 블루오션 품목으로 부각되고 있으며 아로마테라피 샵, 피부관리 및 피부미용실 등의 성장과 함께 1997년 IMF 이후 경기침체가 계속되었음에도 불구하고 2001년부터 다양한 형태로 아로마오일 및 허브판매점이 계속 증가 추세에 있다. 웰빙, 건강을 추구하는 국내의 분위기를 힘입어 정유를 포함한 향료 시장은 점점 크게 확장되고 있으나 정유 수입의존율 98% 이상으로 수입량은 해마다 5~6% 이상 꾸준히 증가 추세에 있으며 수입액으로 국내 정유시장을 가늠해 보면 약 1,500억원 이상이 추정되며 2003년을 제외하고는 매년 평균 8%씩 수입액 증가추세에 있다.

이러한 국내 천연정유 시장 성장세를 감안할 때 방향성 정유를 얻을 수 있는 자연향 자생자원식물 확보를 위한 탐색과 재배기술 개발이 시급하다.

에센셜 오일의 종류는 다양하여 500여종 이상이 있는 것으로 알려져 있으나 이 중 50여종의 에센셜 오일이 가장 보편적으로 사용되고 있으며, 피부나 흡입 등을 통해 인체에 흡수되면 심리적, 생리적 효과를 나타내게 된다. 일상생활에서 사용하는 향수는 화학구조를 인위적으로 모방해 만든 인공 향으로 타인에게 좋은 냄새를 풍겨주는데 목적이 있는 반면, 아로마테라피에 사용되는 에센셜 오일은 100% 순수자연식물에서 추출, 정제한 것으로 수십에서 수백 종에 이르는 화학 성분으로 이루어진 복합체이다.



## 나) 식물 정유의 생리적 활성 (Activity of Essential oils)

최근 가장 보편적으로 사용되고 있는 에센셜 오일은 약 50여종으로 화학구조를 보면 C<sub>10</sub>H<sub>16</sub>의 불포화 탄화수소인 terpene계에 속하며, 비교적 분자량이 작은 탄화수소(hydrocarbon), 알코올(alcohol), 알데하이드(aldehyde), 케톤(ketone), 에스테르(ester), 옥사이드(oxide) 등의 간단한 물질로 이루어져 있으며 이러한 화학적 성분들이 치료적인 효과를 나타내고 있다(Fig. 3). 즉, 탄화수소계는 항균, 진통 및 피부를 따뜻하게 해주며 박테리아나 곰팡이를 퇴치함과 동시에 바이러스도 살균하는 작용을 가지고 있으며 알코올계는 항염, 항균, 면역강화작용을 나타낸다. 페놀계는 강력한 살균작용이 있어 박테리아나 곰팡이를 제거해 주며 면역계 강화작용이 우수하고 알데하이드계는 항염증 작용, 진정효과, 혈압강화, 해열작용이 있으며 에스테르계는 진정, 항염증 작용을 나타낸다(Table 4).

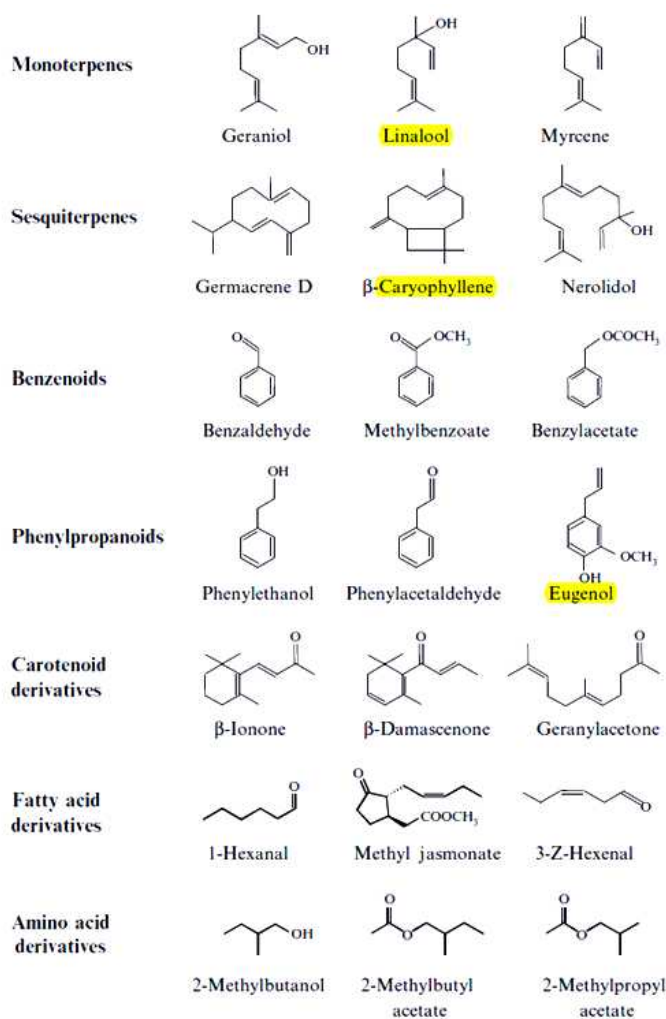


Fig. 3. Representative volatile compounds found in floral scents and fruit aromas.

Table 4. Action of herbs.

| Action            | Name of herbs                                                                                                                                                    |
|-------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Alterative        | Echinacea, Garlic, Red Clover, Yellow Dock                                                                                                                       |
| Analgenic         | Hops, Red Poppy, St John's Wort, Valerian                                                                                                                        |
| Anthelmintic      | Aloe, Garlic, Tansy, Wormwood, Rue                                                                                                                               |
| Anti-Bilious      | Dandelion, Mugwort, Wild Yam, Wormwood                                                                                                                           |
| Anti-Catarrhal    | Echinacea, Garlic, Hyssop, Peppermint, Sage, Thyme, Yarrow                                                                                                       |
| Anti-Emetic       | Balm, Black Horehound, Cloves, Dill, Fennel, Lavender                                                                                                            |
| Anti-Inflammatory | Chamomile, Marigold, St John's Wort                                                                                                                              |
| Anti-Lithic       | Corn Silk, Parsley, Wild Carrot                                                                                                                                  |
| Anti-Microbial    | Aniseed, Caraway oil, Cayenne, Clove, Coriander, Echinacea, Garlic, Gentian, Juniper, Marigold, Majoram, Myrrh, Peppermint, Rosemary, Rue, Sage, Thyme, Wormwood |
| Anti-Spasmodic    | Chamomile, Thyme, Valerian, Wild Lettuce, Wild Yam                                                                                                               |
| Aromatic          | Angelica, Aniseed, Balm, Caraway, Celery, Chamomile, Cinnamon, Cloves, Coriander, Dill, Fennel, Hyssop, Ginger, Pennyroyal, Peppermint, Rosemary, Valerian       |
| Astringent        | Agrimony, Red Sage, Rhubarb Root, Rosemary, Yarrow                                                                                                               |
| Carminative       | Angelica, Aniseed, Caraway, Cinnamon, Chamomile, Coriander, Dill, Fennel, Garlic, Ginger, Hyssop, Juniper, Peppermint, Sage, Thyme, Valerian                     |
| Demulcent         | Comfrey, Corn Silk, Irish Moss                                                                                                                                   |

## 2) 식물의 아로마 성분 분석의 최근 연구 동향

식물의 향 특성을 규명하기 위해서는 휘발성 성분의 조성을 분석하는 분석기술적인 면이 중요하다. 분석의 목표가 되는 시료에서 향기성분을 제대로 추출하는 과정은 매우 중요한 단계로써, 식물의 향 특성을 가장 잘 발현할 수 있는 휘발성 성분을 분리하기 위해 많은 분리방법이 개발되어 왔는데, 그 중 식물로부터 essential oil을 추출하는 방법으로 수증기 증류법(steam distillation), SPME (solid phase micro extraction) 등 비교적 자주 사용되는 방법들이 있다.

가장 일반적으로 행해지고 있는 수증기증류법은, 대량의 시료를 처리하는데 적합하다. 이 방법은 유성의 시료에서 향기성분을 채취할 때도 적용되나, 시료가 수증기와 접촉할 때 향기성분이 변성되거나 2차 생성물이 혼입될 우려가 있다. 감압증류법의 경우, 시료의 열 손상이 적어 대량의 시료를 처리할 수 있는 장점이 있지만 수용성 시료에 한하여 사용되며, 감압 시 낮은 비점의 성분이 제거될 가능성도 있다.

SPME의 경우 사용이 간편하여 식물에서부터 환경오염물질까지 넓은 분야에서 이용되어 지고 있으며 특히 ppt 단위의 극미량의 분석대상물질을 추출해 낼 수 있는 장점 때문에 다양한 환경시료에서 극미량의 오염물질과 다양한 식물에서 휘발성 정유 성분을 분석하는데 널리 사용되고 있다. 또한 유기용매를 사용하지 않고 적은 양의 시료로도 간단하게 전처리 할 수 있는 장점을 가지고 있다. 아래의 표에 최근 발표된 논문 중 식물에서의 essential oil의 추출 및 성분확인을 위한 분석법의 전반적인 내용을 요약 정리하였다.

#### 가) 식물에서의 essential oil 분석법 국외연구현황

| Sample                        | Compound                                | Pretreatment method                                                                                                                                                                                                            | Reference                                        |
|-------------------------------|-----------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------|
| Pine nut shell                | Pine nut shell essential oil            | <ul style="list-style-type: none"> <li>▶Extraction of Essential Oil ; -steam distillation for 3 h.</li> <li>▶Dewatering procedure</li> <li>▶0.45-<math>\mu</math>m filtering, stored at 4°C prior to GC-MS analysis</li> </ul> | Food Anal. Methods (2012) 5:435-440              |
| Rosemary<br>Lavender<br>Basil | Rosemary, Lavender, Basil essential oil | <ul style="list-style-type: none"> <li>▶Steam distillation</li> <li>-T = 366.65K ; -P = 1.01 bar ; -Steam flow = 3.4 mL/min.</li> </ul>                                                                                        | Industrial crops and products 29(2009)171-176    |
| <i>Nepeta</i> species         | <i>Nepeta</i> species essential oil     | <ul style="list-style-type: none"> <li>▶Steam distillation ; -1.5h</li> <li>▶SFE</li> </ul>                                                                                                                                    | Food and bioproducts processing 88 (2010)227-232 |
| <i>N. crispa</i>              | <i>N. crispa</i> essential oil          | <ul style="list-style-type: none"> <li>▶Hydrodistillation ; -3.5 h</li> <li>▶SPME ; -100<math>\mu</math>m PDMS fiber, 65<math>\mu</math>m PDMS/DVB fiber, 85<math>\mu</math>m CAR/PDMS fiber</li> </ul>                        | Acta Chromatographica 24(2012)1, 75-84           |

#### - Food Anal. Methods (2012) 435-440

해당 연구는 GC-MS를 이용하여 pine nut shell의 성분을 분석하였다. 시료는 steam distillation으로 추출하여 gas chromatography로 분석하였다. pine nut shell에 있는  $\alpha$ -Pinene,  $\beta$ -pinene, 3-carene, 1-methy-4-(1-methylethenyl)-(S)-cyclohexene, and n-hexadecanoic acid등 48가지 휘발성 성분이 검출되었다. steam distillation으로 추출한 Essential oil은  $\alpha$ -Pinene,  $\beta$ -pinene, 3-carene과 45개의 다른 성분들을 포함하고 있었으며 mass data를 통하여 규명했다.

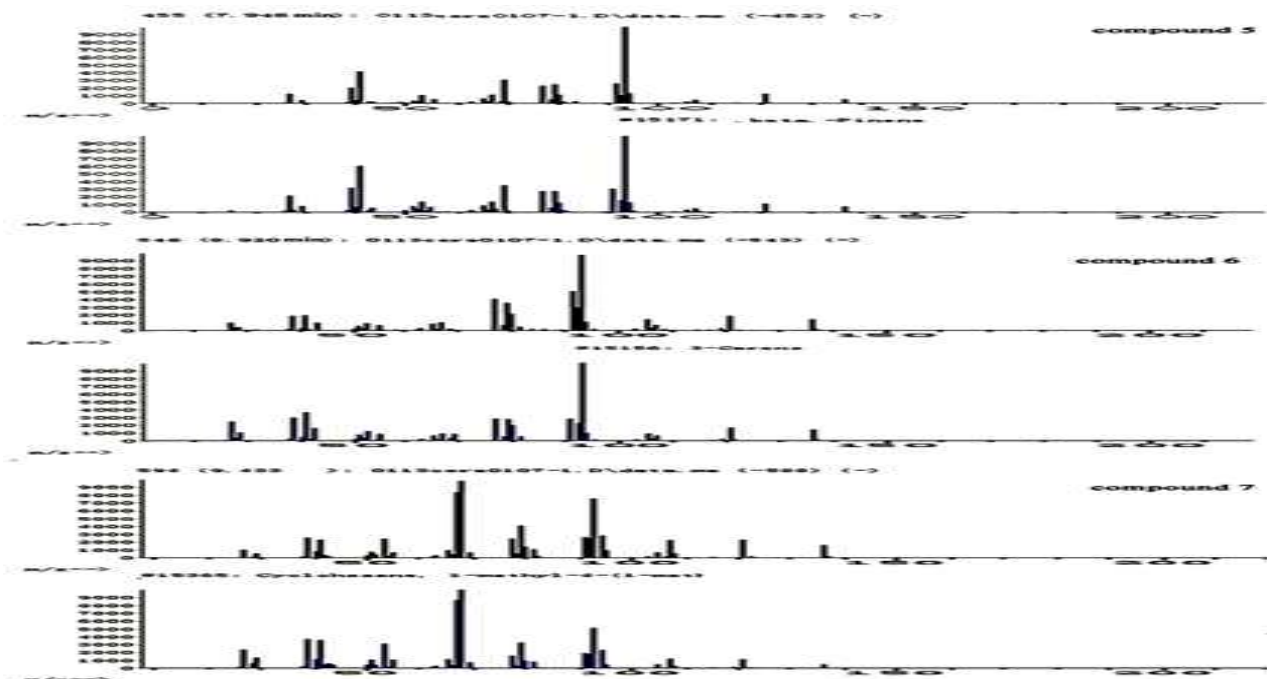


Fig. 4. The mass spectra of pine nut shells essential oil

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해당 연구의 시료는 steam distillation으로 온도 366.6K, 압력 1.01bar, flow 3.4ml/min 조건으로 추출하였다. 로즈마리는 0.51%(w/w), 바질은 0.38%(w/w), 라벤더는 0.32%(w/w)의 수율로 얻었으며 GC/MS, GC/FID를 이용하여 로즈마리, 바질, 라벤더의 성분을 분석하였다.

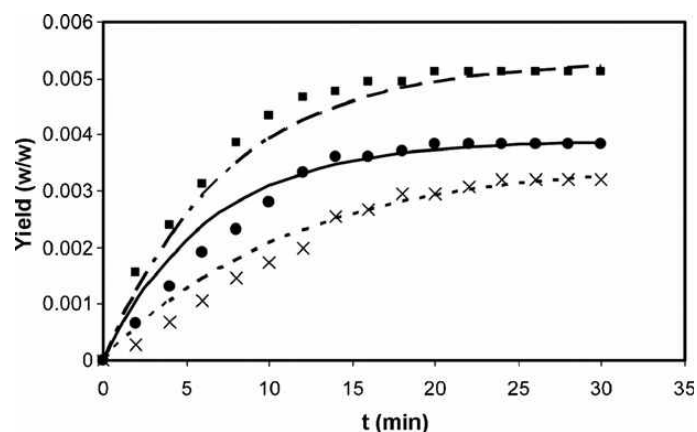


Fig. 5. Steam distillation yield extraction curves vs. time: mathematical model (— rosemary, — basil, and — — — lavender) and experimental data (■ rosemary, ● basil, and X lavender).

| t  | Rosemary |      | Basil |      | Lavender |      |
|----|----------|------|-------|------|----------|------|
|    | m        | e    | m     | e    | m        | e    |
| 0  | 0.00     | 0.00 | 0.00  | 0.00 | 0.00     | 0.00 |
| 2  | 0.37     | 0.30 | 0.14  | 0.17 | 0.08     | 0.08 |
| 4  | 0.55     | 0.45 | 0.28  | 0.34 | 0.21     | 0.19 |
| 6  | 0.71     | 0.59 | 0.41  | 0.49 | 0.33     | 0.30 |
| 8  | 0.87     | 0.72 | 0.49  | 0.59 | 0.46     | 0.42 |
| 10 | 0.98     | 0.81 | 0.60  | 0.72 | 0.54     | 0.49 |
| 12 | 1.06     | 0.88 | 0.71  | 0.86 | 0.63     | 0.57 |
| 14 | 1.08     | 0.89 | 0.77  | 0.93 | 0.80     | 0.72 |
| 16 | 1.12     | 0.93 | 0.77  | 0.93 | 0.84     | 0.76 |
| 18 | 1.12     | 0.93 | 0.79  | 0.95 | 0.92     | 0.84 |
| 20 | 1.16     | 0.96 | 0.81  | 0.98 | 0.92     | 0.84 |
| 22 | 1.16     | 0.96 | 0.81  | 0.98 | 0.96     | 0.88 |
| 24 | 1.16     | 0.96 | 0.81  | 0.98 | 1.00     | 0.91 |
| 26 | 1.16     | 0.96 | 0.81  | 0.98 | 1.00     | 0.91 |
| 28 | 1.16     | 0.96 | 0.81  | 0.98 | 1.00     | 0.91 |
| 30 | 1.16     | 0.96 | 0.81  | 0.98 | 1.00     | 0.91 |

t: time (min); m: extracted mass (g); e: extraction degree (w/w).

Fig. 6. Data used in the mathematical simulation as a function of time

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해당 연구는 이란에서 재배된 *Nepeta persica*의 에센셜 오일을 분석하였다. 시료는 steam distillation과 Supercritical fluid extraction로 전처리 하였다. steam distillation은 1.5 시간동안 0.08 (v/w)수율로 추출하였으며, Supercritical fluid extraction는 0.22~8.90% (w/w)의 수율로 얻었다, GC-MS의 분석 결과 4 $\alpha$  $\beta$ ,7 $\alpha$ ,7 $\alpha\alpha$ -nepetalactone이 주요 성분으로 검출되었다.

| No. | T (°C) | P (MPa) | t <sub>d</sub> (min) | t <sub>e</sub> (min) | M%  | Extraction yield (w/w) |
|-----|--------|---------|----------------------|----------------------|-----|------------------------|
| 1   | 35     | 10.1    | 10                   | 15                   | 0   | 1.20                   |
| 2   | 45     | 35.5    | 10                   | 20                   | 3   | 2.30                   |
| 3   | 55     | 20.3    | 40                   | 15                   | 3   | 6.44                   |
| 4   | 45     | 10.1    | 20                   | 25                   | 4.5 | 6.76                   |
| 5   | 75     | 10.1    | 40                   | 20                   | 6   | 0.36                   |
| 6   | 35     | 25.3    | 30                   | 25                   | 3   | 7.31                   |
| 7   | 55     | 35.5    | 20                   | 30                   | 0   | 4.67                   |
| 8   | 75     | 35.5    | 30                   | 15                   | 4.5 | 3.89                   |
| 9   | 75     | 30.4    | 20                   | 35                   | 3   | 2.88                   |
| 10  | 45     | 25.3    | 40                   | 35                   | 0   | 5.03                   |
| 11  | 45     | 30.4    | 50                   | 15                   | 1.5 | 7.70                   |
| 12  | 45     | 20.3    | 30                   | 30                   | 6   | 7.96                   |
| 13  | 75     | 25.3    | 10                   | 30                   | 1.5 | 7.16                   |
| 14  | 35     | 30.4    | 40                   | 30                   | 4.5 | 4.35                   |
| 15  | 35     | 35.5    | 50                   | 30                   | 6   | 8.90                   |
| 16  | 65     | 25.3    | 20                   | 15                   | 6   | 3.42                   |
| 17  | 65     | 20.3    | 10                   | 35                   | 4.5 | 2.03                   |
| 18  | 55     | 10.1    | 30                   | 35                   | 1.5 | 0.03                   |
| 19  | 55     | 30.4    | 10                   | 25                   | 6   | 3.23                   |
| 20  | 65     | 10.1    | 50                   | 30                   | 3   | 0.22                   |
| 21  | 75     | 20.3    | 50                   | 25                   | 0   | 6.20                   |
| 22  | 35     | 20.3    | 20                   | 20                   | 1.5 | 6.16                   |
| 23  | 65     | 30.4    | 30                   | 20                   | 0   | 4.67                   |
| 24  | 55     | 25.3    | 50                   | 20                   | 4.5 | 3.46                   |
| 25  | 65     | 35.5    | 40                   | 25                   | 1.5 | 3.62                   |

Fig. 7. SFE experimental conditions and extraction yields for *Nepeta persica*

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MD-SPME와 종래의 방법인 HS-SPME를 사용하여 전처리를 한 후 두 가지 방법을 비교하였다. MD-SPME는 HS-SPME에 비해 간단하고 빠르며 용매가 필요없고 효율적이었다. MD-SPME로 전처리를 한 후 GC-MS로 분석한 결과 1,8-cineol (35.2%),  $\beta$ -bourbonene (14.2%),  $\alpha$ -terpineol (9.5%),  $\beta$ -pinene(6.9%), and cis-sabinenehydrate (6.5%)이 주요성분으로 검출되었으며 기타 성분들을 포함하여 26개의 성분이 검출되었다.

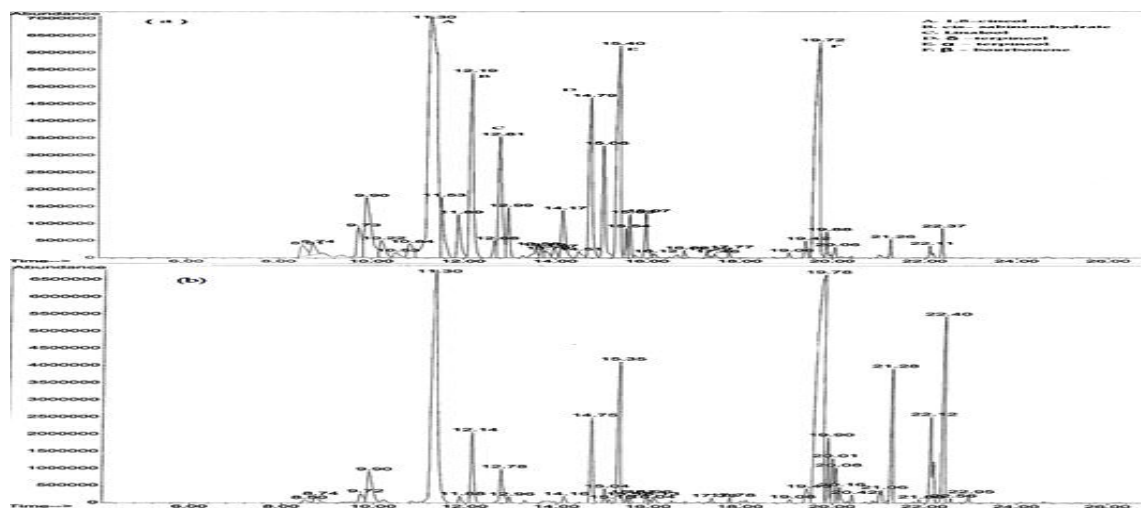
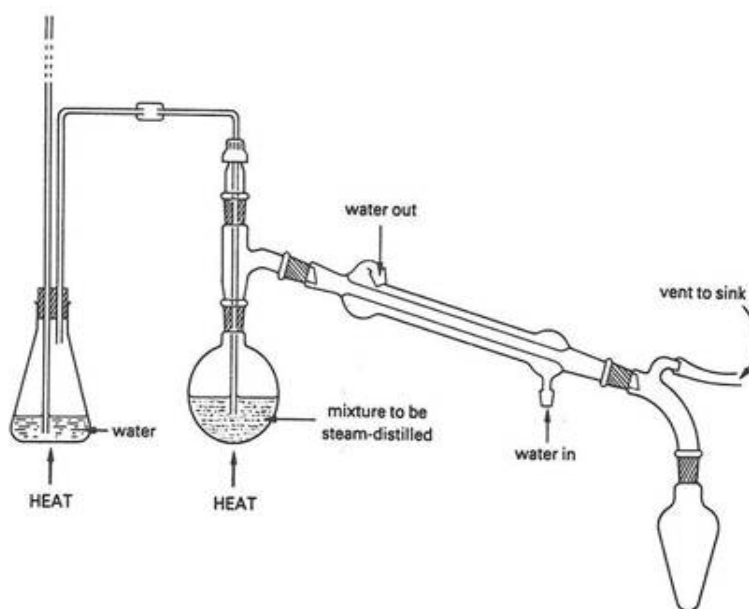


Fig. 8. The GC-MS total ion chromatograms of volatile compounds in *Nepeta crispa* obtained by (a) MD-SPME and (b) HS-SPME

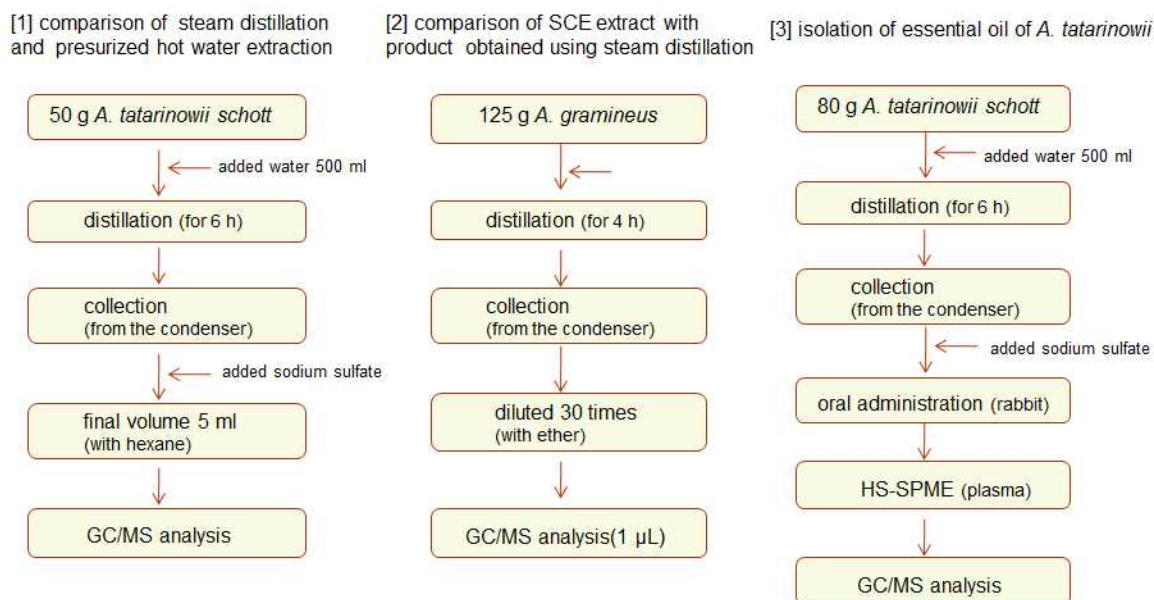
나) essential oil에 가장 많이 사용되는 추출방법

① steam distillation



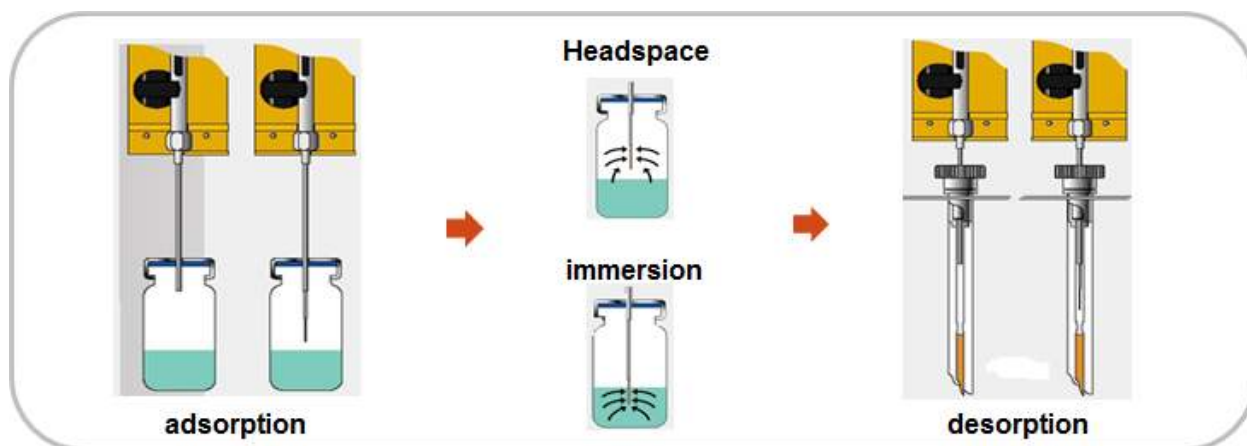


- 물을 가열하여 얻은 수증기에 의해 시료를 가열키고, 증발된 정유와 증기를 같이 냉각시켜 모은 뒤 물층과 유기성분층을 간단하게 분리하는 방법이다. 이 방법은 증기를 이용하므로 증기압이 이용되어 정유성분의 끓는점보다 낮은 온도에서 추출할 수 있어서 열에 민감한 성분을 추출하는데 용이하다.



- steam distillation은 이전엔 정유를 추출하여 그 정유 성분을 회석하여 분석하는 과정을 거쳐 단순히 정유의 추출을 위해 사용되어졌지만 최근에는 다른 추출방법과 적용하여 사용되기도 하고 있다. 위의 그림은 다양한 전처리 방법을 steam distillation과 결합하여 목적 정유성분의 추출과 분리를 하는 방법을 나타내었다. 보통 많은 양의 시료가 사용되어 지기 때문에 효율성이 떨어진다.

## ② Solid phase micro extraction (SPME)



- solid phase micro extraction (SPME)는 바이알내에서 시료의 휘발성 성분들이 휘발되어 막힌 바이알알의 위의 공간인 헤드스페이스내에 분석하고자 하는 물질(휘발성성분)

이 분포하게 된다. 분석물이 분포된 헤드스페이스에 SPME fiber를 노출시켜 시료와 헤드스페이스 그리고 fiber에 분석물질이 상호작용하게 되며 이러한 과정으로 fiber에 분석물질을 흡착시켜 추출하는 원리를 가진다. 소량의 시료와 용매를 사용하지 않으면서 빠르고 간편하게 낮은 농도의 휘발성 성분까지 손실 없이 추출할 수 있으며 ppt단위의 성분들까지도 검출이 가능하다.

## ▪ SPME parameter

- Selection of appropriate SPME fiber
- Temperature and time (adsorption /desorption) (40~90°C).
- Headspace volume (30% or minimize) – headspace
- Agitation or stir - liquid
- Added NaCl and then adjustment of pH

## ▪ selection of fiber

| SPME fibers     | (A)    | (B)    | (C)    | (D)              | Polarity | Use     | present fiber |
|-----------------|--------|--------|--------|------------------|----------|---------|---------------|
| PDMS            | 100 μm | 100 μm | 100 μm | 30 μm,<br>100 μm | low      | GC/HPLC | 100 μm        |
| PDMS / DVB      | 65 μm  | 65 μm  | 65 μm  |                  | low      | GC      | 65 μm         |
| CAR / PDMS      | 75 μm  | 75 μm  | 75 μm  |                  | medium   | GC      | 75 μm         |
| DVB / CAR/ PDMS |        |        |        |                  | medium   | GC      | 50/30 μm      |
| CW / DVB        | 65 μm  | 65 μm  | 65 μm  |                  | high     | GC      |               |
| PA              |        | 85 μm  |        |                  | high     | GC/HPLC |               |

– SPME를 통한 휘발성 성분의 추출에 대하여 고려할 부분은 위의 그림과 같다. 주로 극성과 비극성 및 휘발성 성분의 특성에 따라 SPME fiber 선택이 고려되어지며, 이 외에도 흡착온도와 시간, 노출시간, 탈착온도와 시간 등 다양한 parameter들이 존재한다.

이에 따라 본 연구는 ①‘14년도에는 ‘자생 식물자원의 아로마 물질 탐색 및 발굴’을 위한 향료 식물자원 분야에 대한 기반 마련 ② 아로마 성분 분석을 위한 조건 확립 및 후보 종을 대상으로 시범 분석 ③ 자생 아로마 식물자원의 탐색·발굴 추진 중장기 계획 수립을 하고자 한다.



## II. 연구내용 및 방법

### 1. 수입 향신료 대체 물질로 이용 가능한 자생 아로마 식물자원 후보 목록 구축

⇒ 국내 수입 향신료 및 허브(herbs) 식물의 현황 조사 및 목록화

– 관세청 및 통계청의 최근 데이터 자료분석 및 통계처리 – 수입현황 조사

⇒ <아로마의 정의 및 이용 가능한 자생 아로마 식물자원의 목록화>

– 국내 자생식물 분류군중 정유(essential oils) 성분을 함유하고 있고, 다양한 방향성분이 풍부하고 향료작물로서의 개발 가능 잠재력을 가진 후보 식물자원을 연구문헌 및 자료분석을 통해 목록화 작업을 한다.

– 아래 ‘표’에 제시된 약 18개 과 (family rank)의 현화식물의 분류군내에서 보다 더 광범위한 database를 검토하여, 그 가운데 향신료로 가장 많이 활용되는 꿀풀과 (Lamiaceae-특히 한반도 자생식물분류군)에 대한 구체적인 목록화 작업을 한다.

– 제안된 자생 아로마 식물자원 후보 목록 가운데, 연차적으로 유용성이 큰 식물 분류군을 선별하여 보다 더 정밀한 정유 성분 분석을 수행한다.

| Essential Oils from Plant Sources                                      |  |
|------------------------------------------------------------------------|--|
| (정유포함 가능성 - 현화식물: Hong, <i>Unpublished Data</i> )                      |  |
| 1. Apiaceae (산형과)                                                      |  |
| 2. Araliaceae (두릅나무과)                                                  |  |
| 3. Asteraceae (국화과)                                                    |  |
| 4. Boraginaceae (지치과)                                                  |  |
| 5. Crucifae (Brassicaceae) (십자화과)                                      |  |
| 6. Cucurbitaceae Juss. (박과)                                            |  |
| 7. Ericaceae Juss. (Vacciniaceae S. F. Gray) (진달래과)                    |  |
| 8. Euphorbiaceae (대극과)                                                 |  |
| 9. Lamiaceae (꿀풀과)                                                     |  |
| 10. Leguminosae (콩과)                                                   |  |
| 11. Malvaceae (아욱과)                                                    |  |
| 12. Onagraceae (바늘꽃과)                                                  |  |
| 13. Ranunculaceae Juss. ( <i>incl.</i> Paeoniaceae Rudolphi) (미나리아재비과) |  |
| 14. Rhamnaceae Juss (대추나무과)                                            |  |
| 15. Rosaceae Juss. (장미과)                                               |  |
| 16. Rutaceae Juss. (운향과)                                               |  |
| 17. Salicaceae Mirb. (버드나무과)                                           |  |
| 18. Solanaceae (가지과)                                                   |  |
| © S-P HONG                                                             |  |

## 2. 아로마 성분 분석을 위한 조건 확립 및 후보종 대상으로 시범 분석

가. 수입 대체 가능한 아로마 식물자원 후보종을 대상으로 시범분석

### 1) 분석 대상 자생식물 분류군

\* 한반도에 자생하는 꿀풀과 분류군 중 식물계통분류학적 관점에서 아로마 식물자원으로 활용의 잠재성을 지닌 식물들을 선별한다.

\* 이들 예비검토 대상의 식물들 혹은 근연분류군들의 국내 혹은 해외에서 분석된 자료를 바탕으로 본 과업에서 보다 더 상세하게 분석할 분류군을 최종 선발한다.

\* Lamiaceae (꿀풀과)의 한반도의 대표적인 꿀풀과 분류군 (20속, 77 samples)에 대한 cpDNA (*trnH-psbA* regions)을 분석한 계통수(Fig. 9) 등을 바탕으로 한반도에 자생하는 분류군들 중, 가장 본 과업의 시범분석에 적합한 식물군, 3개의 최종 분류군을 선별한다. 선별된 분류군에 대하여 상세한 분석조사를 시행한다.

\* 현재 예비검검에 의해 제안하는 3분류군의 식물들은 아래의 Table 12와 같다.

Table 12. 연구수행에서 예비적으로 검토할 꿀풀과 내의 대상 자생식물 분류군

#### 꿀풀과 내의 연구 대상 자생식물 분류군

1. *Clinopodium chinense* var. *parviflorum* (Kudo) H. Hara J. Jap. Bot. 12: 41, 1936 층층이꽃
2. *Glechoma longituba* (Nakai) Kuprian. Bot. Zhurn. S.S.S.R. 33: 236, 1948 긴병꽃풀
3. *Meehaniania urticifolia* (Miq.) Makino Bot. Mag. (Tokyo) 13: 159, 1899 벌깨덩굴

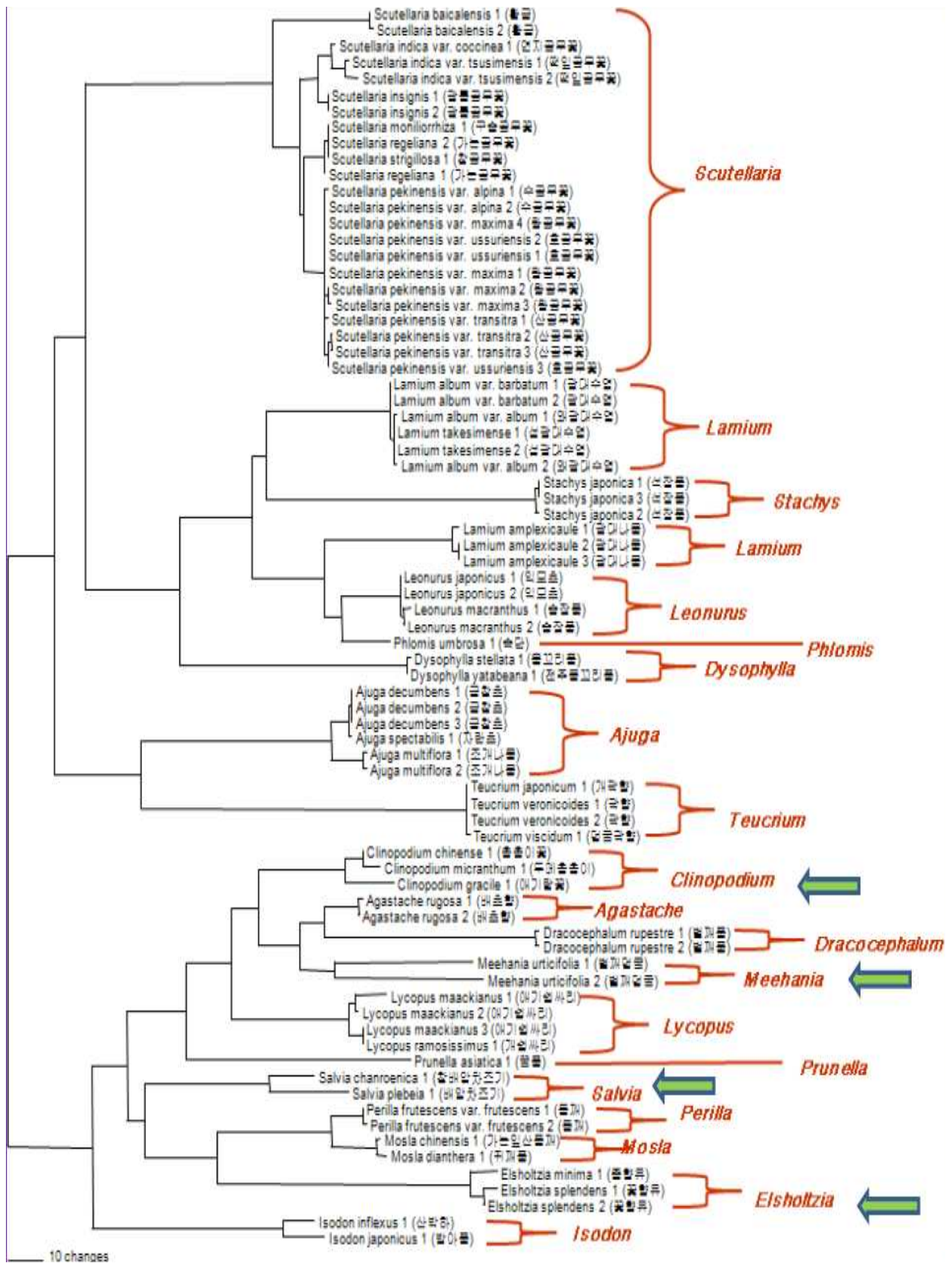


Fig. 9. 한반도의 대표적인 꿀풀과 분류군 (20속, 77 samples)에 대한 cpDNA (*trnH-psbA* regions)을 분석한 계통수

## 2) 꿀풀과 내의 연구 대상 자생식물 분류군

### 가) *Clinopodium chinense* var. *parviflorum* (Kudo) H. Hara 층층이꽃

층층이꽃은 다년생 초본, 키는 15–40cm, 전체에 짧은 털이 있고, 원줄기는 네모지며, 곧게 선다. 잎은 대생이고, 난형 혹은 긴 난형, 끝이 뾰족하고, 밑은 원형, 길이 2–4cm, 가장자리에 톱니가 있으며, 잎자루가 있다. 꽃은 분홍색, 길이 8–12mm, 줄기나 가지 끝에 밀생하여 층층으로 달리고, 포는 선형, 긴털이 있음. 꽃받침은 5갈래, 붉은 빛이 돌고, 털이 있으며, 이강웅예, 열매는 소견과, 둥근모양이다.

– 개화기: 7–8월, 결실기: 8–10월, 분포: 한국(전역), 일본

### \*\* 대조 분류군– *Clinopodium vulgare* L.



Chemical composition *C. vulgare* essential oil (%)

| No.   | K.I. <sup>a</sup> | Components                       | Composition (%) |
|-------|-------------------|----------------------------------|-----------------|
| 1     | 890               | $\alpha$ -Thujene                | 1.4             |
| 2     | 897               | $\alpha$ -Pinene                 | 3.4             |
| 3     | 911               | Camphene                         | 0.2             |
| 4     | 935               | Sabinene                         | tr <sup>b</sup> |
| 5     | 937               | $\beta$ -Pinene                  | 3.1             |
| 6     | 953               | $\beta$ -Myrcene                 | 2.3             |
| 7     | 966               | $\alpha$ -Phelladrene            | 0.4             |
| 8     | 972               | <i>p</i> -Mentha-1(7),8-diene    | 0.1             |
| 9     | 979               | $\alpha$ -Terpinene              | 3.7             |
| 10    | 989               | <i>p</i> -Cymene                 | 9.1             |
| 11    | 1005              | ( <i>Z</i> )- $\beta$ -Ocimene   | 0.1             |
| 12    | 1016              | ( <i>E</i> )- $\beta$ -Ocimene   | 0.2             |
| 13    | 1026              | $\gamma$ -Terpinene              | 29.6            |
| 14    | 1040              | <i>cis</i> -Sabinene hydrate     | tr              |
| 15    | 1062              | Terpinolene                      | 0.2             |
| 16    | 1075              | <i>trans</i> -Sabinene hydrate   | tr              |
| 17    | 1155              | Borneol                          | 0.2             |
| 18    | 1168              | Terpinen-4-ol                    | 0.3             |
| 19    | 1187              | $\alpha$ -Terpineol              | tr              |
| 20    | 1242              | Pulegone                         | tr              |
| 21    | 1247              | Carvacrol methyl ether           | 0.2             |
| 22    | 1260              | <i>cis</i> -Piperitone epoxide   | 0.1             |
| 23    | 1267              | isopulegone                      | 0.1             |
| 24    | 1273              | <i>trans</i> -Piperitone epoxide | 0.2             |
| 25    | 1311              | Thymol                           | 38.9            |
| 26    | 1330              | Carvacrol                        | 4.2             |
| 27    | 1369              | Piperitenone                     | 0.1             |
| 28    | 1377              | Thymol acetate                   | 0.2             |
| 29    | 1393              | Piperitenone oxide               | 0.1             |
| 30    | 1448              | $\beta$ -Caryophyllene           | 0.6             |
| 31    | 1459              | $\beta$ -Copaene                 | tr              |
| 32    | 1470              | Aromadendrene                    | tr              |
| 33    | 1486              | $\alpha$ -Caryophyllene          | tr              |
| 34    | 1511              | $\gamma$ -Murolene               | tr              |
| 35    | 1515              | Germacrene D                     | 0.1             |
| 36    | 1530              | Bicyclogermacrene                | 0.1             |
| 37    | 1544              | $\beta$ -Bisabolene              | 0.2             |
| 38    | 1551              | $\gamma$ -Cadinene               | tr              |
| 39    | 1560              | $\delta$ -Cadinene               | tr              |
| 40    | 1619              | Spathulenol                      | tr              |
| Total |                   |                                  | 99.4            |

<sup>a</sup> K.I. = Kovats Index on HP-5 ms column in reference to *n*-alkanes.

<sup>b</sup> Trace(tr)  $\leq$  0.07%.



나) *Glechoma longituba* (Nakai) Kuprian. 긴병꽃풀

긴병꽃풀은 다년생 초본으로, 식물체는 5-20cm 크고, 줄기는 사각으로 모가지고, 곧게 자라거나 옆으로 50cm정도 뻗는다. 잎은 대생, 신장상 원형, 엽두는 둥근 모양, 엽저는 심장형, 길이 1.5-2.5 cm, 엽연에 둔한 톱니가 있다. 꽃은 연한 자주색, 1-3개씩 줄기의 마디에 액생한다. 꽃받침 갈래는 뽕죽하며, 화관은 길이가 15-25mm, 입술모양으로, 상순꽃잎은 끝이 오목하고, 하순꽃잎은 3갈래로 상순꽃잎의 약 2배 정도 길이 이다. 안쪽에 짙은 자주색 반점이 있고, 수술은 이강웅예. 열매는 소견과, 타원형으로 꽃받침 속에 들어있다.  
- 개화기: 4-5월, 결실기: 5-6월, 분포: 한국을 포함한 동북아시아 (중국, 일본, 아무르지역)



\*\* 대조 분류군 3-1 *Glechoma hederacea* L.

Table. Chemical composition (%) of essential oils of *Glechoma hederacea* L. collected in Vilnius district (2005).

| Compound                          | RI   | A    | B    | C    | D    |
|-----------------------------------|------|------|------|------|------|
| 1,3-trans, 5-cis-Octatriene       | 920  | 0.3  | t    | 0.5  | t    |
| $\alpha$ -Pinene                  | 939  | t    | 0.1  | 0.2  | t    |
| $\beta$ -Pinene                   | 979  | 0.3  | 0.2  | 0.7  | 1.7  |
| 3-Octanone                        | 984  | 0.6  | 0.3  | 0.5  | 1.0  |
| Myrcene                           | 991  | 0.6  | 0.4  | 1.3  | 1.7  |
| 1,8-Cineole                       | 1033 | 2.0  | 1.9  | 2.4  | 3.5  |
| Z- $\beta$ -Ocimene               | 1037 | 2.5  | 1.9  | 4.7  | 5.6  |
| E- $\beta$ -Ocimene               | 1050 | 1.5  | 0.7  | 0.9  | 0.7  |
| p-Mentha-2,4(8)-diene             | 1088 | t    |      | 0.1  | t    |
| n-Nonanal                         | 1101 | 0.5  | 0.2  | 0.2  | 0.2  |
| 1-Octen-3-yl acetate              | 1113 | t    | 0.1  | 0.4  | 0.6  |
| allo-Ocimene                      | 1132 | 1.2  | 0.8  | 2.4  | 2.5  |
| dihydro-Pinocarvone               | 1160 |      | 1.2  | 1.6  | 8.5  |
| Myrtenal                          | 1196 |      | t    | 0.1  | 0.4  |
| n-Decanal                         | 1202 | 0.2  | t    | 0.1  | 0.3  |
| $\delta$ -Elemene                 | 1338 | 2.4  | 2.1  | 1.9  | 2.2  |
| Eugenol                           | 1359 | t    |      |      | t    |
| $\alpha$ -Copaene                 | 1377 | 0.5  | 0.6  | 0.9  | 0.2  |
| $\beta$ -Bourbonene               | 1388 | 2.0  | 1.6  | 1.5  | 1.7  |
| $\beta$ -Elemene                  | 1391 | 10.2 | 9.8  | 10.2 | 11.1 |
| $\beta$ -Ylangene                 | 1421 | 3.9  | 3.6  | 3.9  | 2.7  |
| $\beta$ -Gurjunene                | 1434 | 1.2  | 1.2  | 2.0  | 1.0  |
| $\gamma$ -Elemene                 | 1437 | 16.0 | 16.0 | 10.3 | 9.7  |
| Aromadendrene                     | 1441 | 1.5  |      | 1.1  | 0.8  |
| $\alpha$ -Humulene                | 1455 | 0.2  | 1.6  | 1.9  | 1.5  |
| $\gamma$ -Murolene                | 1480 | 0.6  | 0.5  | 0.6  | t    |
| Germacrene D                      | 1485 | 17.2 | 17.8 | 18.8 | 15.6 |
| $\alpha$ -Zingiberene             | 1494 |      | t    |      | 3.4  |
| Bicyclgermacrene                  | 1500 | 2.0  | 2.5  | 2.0  | t    |
| (E,E)- $\alpha$ -Farnesene        | 1506 | 1.8  | 1.0  | 1.3  | 1.9  |
| $\gamma$ -Cadinene                | 1514 | 0.6  | 0.4  | 0.6  | t    |
| d-Cadinene                        | 1523 | 1.1  | 1.3  | 1.0  | 0.8  |
| trans-Cadina-1(2),4-diene         | 1535 |      |      | 0.5  |      |
| $\alpha$ -Cadinene                | 1539 | 1.1  | t    |      |      |
| cis-Sesquibabine hydrate          | 1544 | t    |      | 0.5  |      |
| Germacrene B                      | 1561 | 3.9  | 3.4  | 2.9  | 2.4  |
| Germacrene D-4-ol                 | 1576 | 1.8  | 2.0  | 1.8  | 1.4  |
| $\gamma$ -Eudesmol                | 1632 | 0.6  |      |      | t    |
| Cubenol                           | 1647 |      | 1.0  |      | t    |
| $\alpha$ -Cadinol                 | 1654 | 1.2  | 1.3  | 2.3  | 1.1  |
| 6,10,14-trimethyl-2-Pentadecanone | 1860 | 1.0  | 2.9  | 0.7  | t    |
| iso-Phytol + Phytol               | 1945 | 10.0 | 15.6 | 4.7  | 5.9  |
| Total                             |      | 90.5 | 94.0 | 87.5 | 90.1 |
| Monoterpene hydrocarbons          |      | 6.4  | 4.1  | 10.8 | 12.2 |
| Oxygenated monoterpenes           |      | 2.0  | 3.1  | 4.1  | 12.4 |
| Sesquiterpene hydrocarbons        |      | 66.2 | 63.4 | 61.4 | 55.0 |
| Oxygenated sesquiterpenes         |      | 3.6  | 4.3  | 4.6  | 2.5  |
| Germacrene skeleton               |      | 22.9 | 23.2 | 23.5 | 19.4 |
| Elemene skeleton                  |      | 28.6 | 27.9 | 22.4 | 23.0 |

RI- Retention index on nonpolar column CP-Sil 8CB, t-traces.

다) *Meehanian urticifolia* (Miq.) Makino 벌깨덩굴

벌깨덩굴은 다년생 초본으로, 줄기는 사각으로 네모지고, 길이는 15-30cm, 5쌍 정도의 잎이 붙으며, 긴 흰색 털이 나있고, 옆으로 뻗으며, 마디에서 뿌리가 뻗어내려 나간다. 아래부분의 잎은 대생, 잎자루가 있고, 심장형, 약간 세모지고, 가장자리에 둔한톱니가 있으며 길이는 2-5 x 2-3.5 cm 정도이다. 덩굴줄기의 잎은 잎자루가 거의 없다. 꽃은 보라색, 커다란 입술모양, 줄기의 위쪽 잎겨드랑이에 한쪽을 향하여 4개 정도씩 핀다. 꽃받침은 짧은 통모양으로 끝은 5갈래, 길이는 약 1cm 정도, 화관통은 길이가 4-5cm, 하순꽃잎은 특히 크고, 옆의 꽃잎 갈래와 함께 짙은 자주색 점과 긴 흰색 털이 있음. 수술은 이강웅예. 열매는 소견과, 도란형, 길이 3mm 정도, 잔털이 나있다.

개화기: 5월, 결실기: 7-8월, 분포: 한국 (전역), 일본, 중국 (우수리).

**\*\* 대조 분류군- *Agastache rugosa* (Fisch. & C. A. Mey.) Kuntze 배초향**

Composition of essential oil isolated from leaves or flowers of *Agastache rugosa*.



| Peak no | RT (min) | Components                     | Peak area(%) |         |
|---------|----------|--------------------------------|--------------|---------|
|         |          |                                | Leaves       | Flowers |
| 1       | 3.76     | $\alpha$ -Pinene               | < 0.1        | —       |
| 2       | 4.07     | Camphene                       | 0.2          | 0.1     |
| 3       | 4.38     | $\beta$ -Pinene                | 0.3          | —       |
| 4       | 5.08     | Myrcene                        | 0.1          | —       |
| 5       | 5.56     | $\alpha$ -Terpinene            | 0.1          | —       |
| 6       | 6.18     | Limonene                       | 1.7          | 0.5     |
| 7       | 6.41     | $\beta$ -Phellandrene          | < 0.1        | —       |
| 8       | 6.79     | $\alpha$ -Phellandrene         | 0.2          | —       |
| 9       | 7.19     | $\gamma$ -Terpinene            | < 0.1        | 0.2     |
| 10      | 7.28     | trans-2-Hexenal                | 2.4          | —       |
| 11      | 8.20     | 3-Octanone                     | 0.4          | < 0.1   |
| 12      | 8.40     | p-Cymene                       | < 0.1        | —       |
| 13      | 9.98     | 1-Octen-3-one                  | 0.2          | < 0.1   |
| 14      | 12.34    | n-Hexanol                      | 0.2          | 0.1     |
| 15      | 13.16    | 3-Ethyl-2-methyl-1-penten-3-ol | 0.5          | 0.1     |
| 16      | 13.77    | cis-3-Hexen-1-ol               | 0.8          | 0.2     |
| 17      | 14.18    | 3-Octanol                      | 0.2          | 0.1     |
| 18      | 17.02    | 1-Octen-3-ol                   | 1.9          | 0.8     |
| 19      | 17.97    | 2,4-Heptadienal                | 0.1          | —       |
| 20      | 18.28    | $\alpha$ -Copaene              | 0.2          | < 0.1   |
| 21      | 18.86    | 2,4-Heptadienal                | < 0.1        | 0.3     |
| 22      | 19.51    | Linalool                       | 0.4          | < 0.1   |
| 23      | 20.92    | $\beta$ -Ylangene              | 0.1          | < 0.1   |
| 24      | 22.26    | Linalyl acetate                | 0.4          | < 0.1   |
| 25      | 22.93    | $\beta$ -Caryophyllene         | 2.7          | 1.9     |
| 26      | 24.70    | Limonene epoxide               | 0.1          | —       |
| 27      | 26.50    | $\alpha$ -Humulene             | 0.3          | 0.2     |
| 28      | 27.30    | Valeric acid                   | 0.9          | —       |
| 29      | 28.64    | Methyl chavicol                | 64.4         | 78.4    |
| 30      | 29.08    | Sesquiterpene(MW 204)          | 0.7          | 0.3     |
| 31      | 30.31    | $\delta$ -Cadinene             | 0.6          | 0.1     |
| 32      | 31.56    | $\beta$ -Bisabolene            | 0.3          | 0.2     |
| 33      | 32.86    | $\beta$ -Sesquiphellandrene    | 0.1          | —       |
| 34      | 33.12    | Methyl salicylate              | 0.2          | 0.1     |
| 35      | 34.28    | n-Octadecane                   | 0.1          | —       |
| 36      | 36.06    | $\beta$ -Damascenone           | 0.5          | —       |
| 37      | 37.74    | Caproic acid                   | 0.1          | —       |
| 38      | 38.16    | Geranylacetone                 | 0.1          | < 0.1   |
| 39      | 38.54    | Carvone                        | < 0.1        | —       |
| 40      | 40.30    | Benzyl alcohol                 | 0.6          | 0.3     |
| 41      | 41.92    | 2-Phenylethyl alcohol          | 0.4          | 0.4     |
| 42      | 43.58    | Jasmone                        | 0.3          | 1.5     |
| 43      | 42.28    | $\beta$ -Ionone                | 0.2          | 0.1     |
| 44      | 45.24    | Cadina-1,4-dien-4-ol           | < 0.1        | —       |
| 45      | 45.56    | Caryophyllene epoxide          | 0.9          | 0.1     |
| 46      | 46.92    | Methyl eugenol                 | 0.3          | 0.3     |
| 47      | 47.85    | Anisaldehyde                   | 0.1          | 0.2     |

## 나. 자생식물의 아로마 성분 분석을 위한 분석법 개발

### 1) 시료 채취

– 분석을 위한 시료채취는 3 집단 이상 채취한다. 채취는 한 집단별로 생체-건조 할 수 있는 양으로 100g이상 채취한다. 채취시기는 꽃이 피기 전과 꽃이 있는 시기를 구분하여 채취한다.

### 2) 시료 준비

– 생체시료의 경우 20g을 1cm이하의 크기로 자른다.  
– 건조시료의 경우 생체를 상온(35℃)에서 8시간 건조한다. 건조한 시료는 5g을 잘게 자른다.

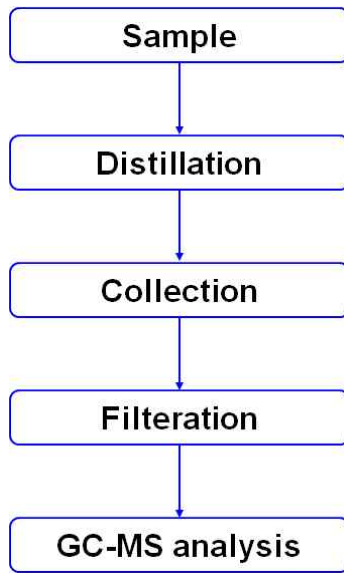
### 3) 표준용액 (standard preparation) 조제

– 본 실험에서 사용될 모든 용매는 HPLC 등급으로 사용한다. 자생식물의 성분 중 대표적인 성분 몇 가지를 추려내어 표준물질을 구입한다. 모든 표준용액과 내부표준물질은 HPLC 등급으로 희석하며, 용액 제조 후 -4℃에서 냉동 보관한다.

### 4) 시료 전처리

– 자생식물시료(생체시료/건조시료)를 바탕으로 실험을 진행할 것이며, 건조된 시료는 분쇄하여 분말화한 뒤, 분말화한 시료는 30mesh의 체를 통해 균일화하여 사용한다. 건조되지 않은 생체 시료는 즉시 추출을 진행하며, 남은 시료는 유리 바이알에 담아 냉동 보관한다. 모든 시료는 SPME와 steam distillation 두 가지 방법을 이용하여 추출을 진행한다.

# ① Steam distillation



Steam distillation을 통한 essential oil의 추출과정은 다음과 같다. Essential oil의 손실을 줄이기 위하여 dichloromethane을 receiving flask에 넣어 놓은 뒤 시료를 3시간 동안 증류 추출을 진행한다. 증류된 용매는 냉각관에 의해 응축되어 receiving flask에 있는 dichloromethane에 모아지게 될 것이다 essential oil은 dichloromethane 층에 녹아나게 됨으로 dichloromethane층을 확보한다. 확보된 dichloromethane층은  $\text{Na}_2\text{SO}_4$ 를 통과하여 수분을 제거하고 0.45 $\mu\text{m}$  멤브레인 필터에 여과한 뒤 GC-MS로 분석하기 전 4 $^{\circ}\text{C}$ 에 냉장 보관한다. 동일과정을 3회 반복수행하여 재현성을 확인한다.



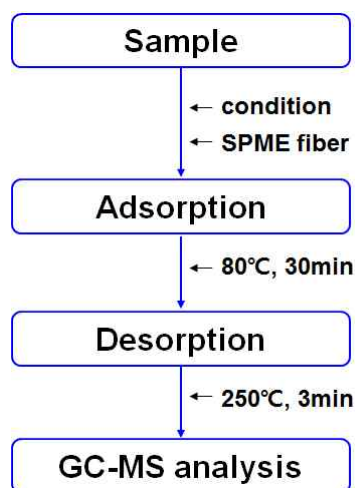
Fig. 10 증류수 400mL에 준비된 시료



Fig. 11 증류준비 완료



## ② Solid phase micro extraction (SPME)



SPME 추출을 위한 과정은 위와 같다. 일정량의 시료를 10 ml screw-top vial에 넣고 teflon/silicon septum cap을 닫은 후, heating block을 사용하여 시료가 든 vial을 가열한다. 그 후 SPME fiber는 80°C에서 30분간 headspace 내에 노출시킨 뒤, 곧바로 GC 주입구에서 250°C에서 3분간 노출하여 fiber에 추출된 성분을 탈착시킨다. GC 주입구에서는 20:1의 split ratio를 사용하고, 각 시료마다 동일과정을 3회 반복수행하여 재현성을 확인한다.

SPME 실험에서 휘발성 성분의 추출은 volatile한 성분들이 headspace안에서 시료와 분석물질의 평형과 분석물질과 fiber의 평형이 적절하게 이루어 졌을 때 가장 큰 추출효율을 나타내며 이는 추출시의 온도와 추출시간에 따라 달라지게된다. 시료를 담은 vial을 60 ~ 90°C의 온도조건에서 휘발성 성분의 추출효율을 비교하며, 10 ~ 40min의 추출시간을 검토하여 가장 적합한 추출시간을 선정하도록 한다. 또한 같은 방법으로 추출시간 및 탈착 온도와 시간을 최적화하여 분석하도록 한다.

## ③ 기기분석조건

자생식물의 아로마 성분 분리와 정량분석을 위한 기기로는 gas chromatography-mass spectrometry(GC-MS)는 agilent 6890N gas chromatography와 Agilent-5973 mass selective detector, agilent injector가 사용한다. 분석용 컬럼은 DB-5MS 컬럼 (30m×0.25m×0.25 $\mu$ m film)을 사용하며, GC 분리관 온도는 80°C(3 min)에서 90°C까지 5°C/min 씩 승온시킨 후, 90°C에서 140°C까지 10°C/min씩 승온시키며 140°C에서 280°C(3min)지 20°C/min씩 승온하여 총 20분 안에 빠른 용리가 일어날 수 있도록 진행한다. MS 조건 이온화는 전자 이온화 방식을 사용하는 electron ionization (EI)방식을 사용하며 그에 따른 이온화 에너지는 70 eV로 고정하여 진행한다. 이때 사용된 분리관은 사중극자로서 위와 같은 조건하에서 각 아로마 성분들의 질량 스펙트럼과 Total Ion Chromatogram (TIC)를 얻는다(Table 5).

Table 5. GC–MS experimental conditions

|                    |                                                                     |
|--------------------|---------------------------------------------------------------------|
| Column             | DB–5MS (30m × 0.32m × 0.25 $\mu$ m Film)                            |
| Flow rate          | 1.0 ml/min                                                          |
| Carrier gas        | Helium                                                              |
| Injection vol.     | 1.0 $\mu$ l                                                         |
| Split ratio        | 20:1                                                                |
| Injection temp.    | 270 °C                                                              |
| Oven temp.         | 80(3min)→(5°C/min)→90°C→(10°C/min)→140°C→(20°C/min)→280°C<br>(3min) |
| Interface temp.    | 280 °C                                                              |
| Scanning range     | 40–400 amu                                                          |
| Ionization voltage | 70 eV                                                               |
| Analyzer           | Quadrupole                                                          |

### Ⅲ. 연구결과 및 고찰

#### 1. 향신료의 수입동향

전 세계적으로 교역이 이루어지고 있는 여러 품목 중에 향신료는 매우 중요한 교역 품목이다. 향신료의 주요 수출국가를 볼 경우 아시아 국가가 80%를 차지하고 있으며, 이중 말레이시아, 중국, 인도에서 수출되는 비중이 58%로 절반 이상을 차지하고 있다.

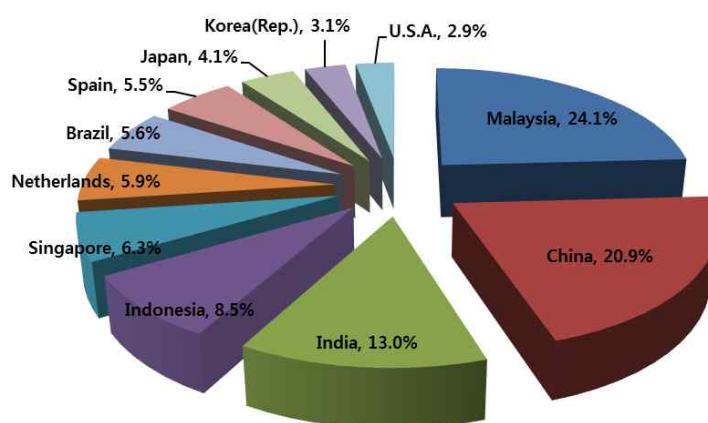


Fig. 12. 향신료 주요 수출국가

향신료의 수입은 항목별로 차이가 있으나 캡시컴, 후추, 생강 등 대부분의 향신료를 수입하는 국가도 중국, 베트남, 인도와 같은 아시아 국가들이다. 향신료는 국가나 민족의 고유한 식자재에 첨가하는 품목으로 국가별 집중도 또한 매우 다르다. 중국의 경우 캡시컴의 98%, 생강의 99.9%를 수입하며, 터키의 경우 월계수잎을 90.58% 수입하고 있다.

Table 6. 2013년 향신료 수입 상위국

|       | 1위     |       |        | 2위    |       |        |
|-------|--------|-------|--------|-------|-------|--------|
|       | 국가     | 중량(톤) | 비중(%)  | 국가    | 중량(톤) | 비중(%)  |
| 캡시컴   | 중국     | 5,386 | (98.4) | 인도    | 36    | (0.7)  |
| 후추    | 베트남    | 2,707 | (62.5) | 말레이시아 | 1,355 | (31.3) |
| 생강    | 중국     | 7,570 | (99.9) | 베트남   | 3     | (0.0)  |
| 심황    | 인도     | 496   | (79.9) | 인도네시아 | 69    | (11.1) |
| 계피    | 베트남    | 2,127 | (77.9) | 중국    | 49    | (15.7) |
| 월계수잎  | 터키     | 108   | (90.8) | 미국    | 4     | (3.7)  |
| 코리앤더씨 | 모로코    | 309   | (77.5) | 인도    | 54    | (13.5) |
| 회향씨   | 인도     | 160   | (58.8) | 중국    | 55    | (20.0) |
| 커민씨   | 이란     | 118   | (53.9) | 인도    | 63    | (28.8) |
| 정향    | 마다카스카르 | 43    | (52.6) | 인도네시아 | 31    | (38.1) |

Table 7. 국내 수입되는 향신료와 허브의 종류 (in part)

| 한글품명  | 영문품명                  | 국명        | 학명                                        | 과명             | 부위           | 참고                                                                                                            |
|-------|-----------------------|-----------|-------------------------------------------|----------------|--------------|---------------------------------------------------------------------------------------------------------------|
| 겨자    | Mustard               | 겨자        | genera <i>Brassica</i> and <i>Sinapis</i> | Brassicaceae   | seed         | <a href="http://en.wikipedia.org/wiki/Mustard_plant">http://en.wikipedia.org/wiki/Mustard_plant</a>           |
| 계피    | Cinnamon              | 계피        | genus <i>Cinnamomum</i>                   | Lauraceae      | inner bark   | <a href="http://en.wikipedia.org/wiki/Cinnamon">http://en.wikipedia.org/wiki/Cinnamon</a>                     |
| 고수    | Coriander             | 고수        | <i>Coriandrum sativum</i>                 | Apiaceae       | seed / leaf  | <a href="http://en.wikipedia.org/wiki/Coriander">http://en.wikipedia.org/wiki/Coriander</a>                   |
| 고추    | Chili pepper          | 고추        | genus <i>Capsicum</i>                     | Solanaceae     | fruit        | <a href="http://en.wikipedia.org/wiki/Chili_pepper">http://en.wikipedia.org/wiki/Chili_pepper</a>             |
| 고추냉이  | Wasabi                | 고추냉이      | <i>Wasabia japonica</i>                   | Brassicaceae   | root         | <a href="http://en.wikipedia.org/wiki/Wasabi">http://en.wikipedia.org/wiki/Wasabi</a>                         |
| 대회향   | Badian                | 팔각        | <i>Illicium verum</i>                     | Schisandraceae | fruit        | <a href="http://en.wikipedia.org/wiki/Illicium_verum">http://en.wikipedia.org/wiki/Illicium_verum</a>         |
| 딜     | Dill                  | 딜         | <i>Anethum graveolens</i>                 | Apiaceae       | leaf         | <a href="http://en.wikipedia.org/wiki/Dill">http://en.wikipedia.org/wiki/Dill</a>                             |
| 러버지   | Lovage                | 오피키날레비스티움 | <i>Levisticum officinale</i>              | Apiaceae       | seed / leaf  | <a href="http://en.wikipedia.org/wiki/Lovage">http://en.wikipedia.org/wiki/Lovage</a> / 국가표준식물목록              |
| 로즈마리  | Rosemary              | 로즈마리      | <i>Rosmarinus officinalis</i>             | Lamiaceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Rosemary">http://en.wikipedia.org/wiki/Rosemary</a>                     |
| 마늘    | Garlic                | 마늘        | <i>Allium sativum</i>                     | Amaryllidaceae | stem         | <a href="http://en.wikipedia.org/wiki/Garlic">http://en.wikipedia.org/wiki/Garlic</a>                         |
| 산초    | Sichuan pepper        | 산초        | genus <i>Zanthoxylum</i>                  | Rutaceae       | seed / leaf  | <a href="http://en.wikipedia.org/wiki/Sichuan_pepper">http://en.wikipedia.org/wiki/Sichuan_pepper</a>         |
| 생강    | Ginger                | 생강        | <i>Zingiber officinale</i>                | Zingiberaceae  | root         | <a href="http://en.wikipedia.org/wiki/Ginger">http://en.wikipedia.org/wiki/Ginger</a>                         |
| 카르다몸  | Cardamoms             | 소두구       | genera <i>Elettaria</i> and <i>Amomum</i> | Zingiberaceae  | fruit        | <a href="http://en.wikipedia.org/wiki/Cardamom">http://en.wikipedia.org/wiki/Cardamom</a>                     |
| 정향    | Clove                 | 정향        | <i>Syzygium aromaticum</i>                | Myrtaceae      | flower buds  | <a href="http://en.wikipedia.org/wiki/Clove">http://en.wikipedia.org/wiki/Clove</a>                           |
| 차조기   | Shiso                 | 소엽        | <i>Perilla frutescens</i>                 | Lamiaceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Perilla_frutescens">http://en.wikipedia.org/wiki/Perilla_frutescens</a> |
| 회향    | Fennel                | 회향        | <i>Foeniculum vulgare</i>                 | Apiaceae       | seed         | <a href="http://en.wikipedia.org/wiki/Fennel">http://en.wikipedia.org/wiki/Fennel</a>                         |
| 후추    | Pepper                | 후추        | <i>Piper nigrum</i>                       | Piperaceae     | fruit / seed | <a href="http://en.wikipedia.org/wiki/Black_pepper">http://en.wikipedia.org/wiki/Black_pepper</a>             |
| 아니스   | Anise                 | 아니스       | <i>Pimpinella anisum</i>                  | Apiaceae       | seed         | <a href="http://en.wikipedia.org/wiki/Anise">http://en.wikipedia.org/wiki/Anise</a>                           |
| 바질    | Basil                 | 바질        | <i>Ocimum basilicum</i>                   | Lamiaceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Basil">http://en.wikipedia.org/wiki/Basil</a>                           |
| 캐러웨이  | Caraway               | 캐러웨이      | <i>Carum carvi</i>                        | Apiaceae       | fruit        | <a href="http://en.wikipedia.org/wiki/Caraway">http://en.wikipedia.org/wiki/Caraway</a>                       |
| 커민    | Cumin                 | 커민        | <i>Cuminum cyminum</i>                    | Apiaceae       | seed         | <a href="http://en.wikipedia.org/wiki/Cumin">http://en.wikipedia.org/wiki/Cumin</a>                           |
| 타라곤   | Tarragon              | 드라쿤쿨루스속   | <i>Artemisia dracunculus</i>              | Asteraceae     | leaf         | <a href="http://en.wikipedia.org/wiki/Tarragon">http://en.wikipedia.org/wiki/Tarragon</a> / 국가표준식물목록          |
| 호로파   | Fenugreek             | 호로파       | <i>Trigonella foenum-graecum</i>          | Fabaceae       | seed / leaf  | <a href="http://en.wikipedia.org/wiki/Fenugreek">http://en.wikipedia.org/wiki/Fenugreek</a>                   |
| 마조람   | Marjoram              | 마조람       | <i>Origanum majorana</i>                  | Lamiaceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Marjoram">http://en.wikipedia.org/wiki/Marjoram</a> / 국가표준식물목록          |
| 세이지   | Sage                  | 살비아       | <i>Salvia officinalis</i>                 | Lamiaceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Salvia_officialis">http://en.wikipedia.org/wiki/Salvia_officialis</a>   |
| 타임    | Thyme                 | 타임        | genus <i>Thymus</i>                       | Lamiaceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Thymus_(plant)">http://en.wikipedia.org/wiki/Thymus_(plant)</a>         |
| 바닐라   | Vanilla               | 바닐라       | <i>Vanilla planifolia</i>                 | Orchidaceae    | seed         | <a href="http://en.wikipedia.org/wiki/Vanilla_planifolia">http://en.wikipedia.org/wiki/Vanilla_planifolia</a> |
| 월계수   | bay                   | 월계수       | <i>Laurus nobilis</i>                     | Lauraceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Laurus_nobilis">http://en.wikipedia.org/wiki/Laurus_nobilis</a>         |
| 육두구   | Nutmeg                | 육두구       | genus <i>Myristica</i>                    | Myristicaceae  | seed         | <a href="http://en.wikipedia.org/wiki/Nutmeg">http://en.wikipedia.org/wiki/Nutmeg</a>                         |
| 메이스   | Mace                  | 메이스       | genus <i>Myristica</i>                    | Myristicaceae  | aril         | <a href="http://en.wikipedia.org/wiki/Nutmeg">http://en.wikipedia.org/wiki/Nutmeg</a>                         |
| 오레가노  | Oregano               | 불가레오레가노   | <i>Origanum vulgare</i>                   | Lamiaceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Oregano">http://en.wikipedia.org/wiki/Oregano</a>                       |
| 주니퍼   | Juniper               | 주니퍼       | genus <i>Juniperus</i>                    | Cupressaceae   | fruit        | <a href="http://en.wikipedia.org/wiki/Juniper">http://en.wikipedia.org/wiki/Juniper</a>                       |
| 사프란   | Saffron               | 사프란       | <i>Crocus sativus</i>                     | Iridaceae      | stigmas      | <a href="http://en.wikipedia.org/wiki/Crocus_sativus">http://en.wikipedia.org/wiki/Crocus_sativus</a>         |
| 강황    | Turmeric              | 강황        | <i>Curcuma longa</i>                      | Zingiberaceae  | root         | <a href="http://en.wikipedia.org/wiki/Turmeric">http://en.wikipedia.org/wiki/Turmeric</a>                     |
| 올스파이스 | Allspice              | 올스파이스     | <i>Pimenta dioica</i>                     | Myrtaceae      | fruit        | <a href="http://en.wikipedia.org/wiki/Allspice">http://en.wikipedia.org/wiki/Allspice</a>                     |
| 꼭할    | Wrinkled Giant Hyssop | 배조할       | <i>Agastache rugosa</i>                   | Lamiaceae      | leaf         | <a href="http://en.wikipedia.org/wiki/Agastache_rugosa">http://en.wikipedia.org/wiki/Agastache_rugosa</a>     |

국내에도 다양한 향신료가 수입되고 있으며 수입량도 지속적으로 증가 하고 있다. 1998년도부터 2008년도까지 통계청의 최근 11년 간의 수입 통계(Table 7.)를 토대로 국내 향신료 수입량 변화를 분석하였다.

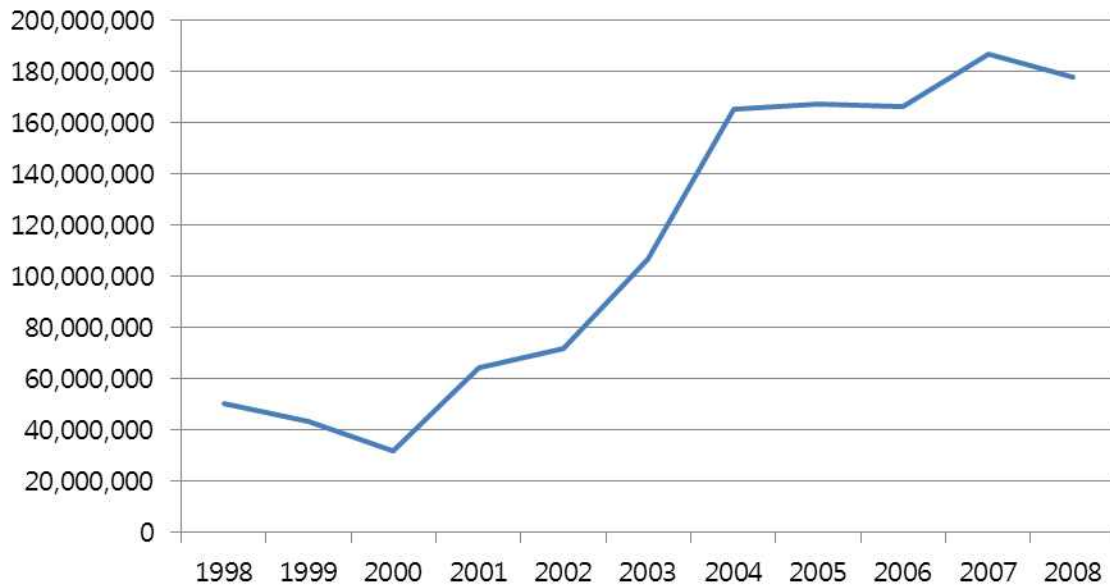


Fig. 13 국내 향신료 수입량 변화(단위: Kg)

2008년에는 1998년에 비해 4배 가까이 되는 향신료가 수입되었다. Fig. 13에서 확인 한 것과 마찬가지로 꾸준히 향신료의 수요가 증가하고 있음을 알 수 있다.

140여 가지의 향신료 품목 중 대표적인 향신료 선정하여 최근 11년(1998~2008)간 수입량 변화를 비교 분석하였다. 같은 품목이라도 건조●냉장●냉동 등 다양한 가공을 거쳐 다른 항목으로 수입되기 때문에 중량이나 가격으로 수입량을 비교하는 것은 적절치 않다고 판단되어 건조된 물품의 중량을 기준으로 수입량을 비교하였다.

가. 겨자씨와 분말(Mustard flour)

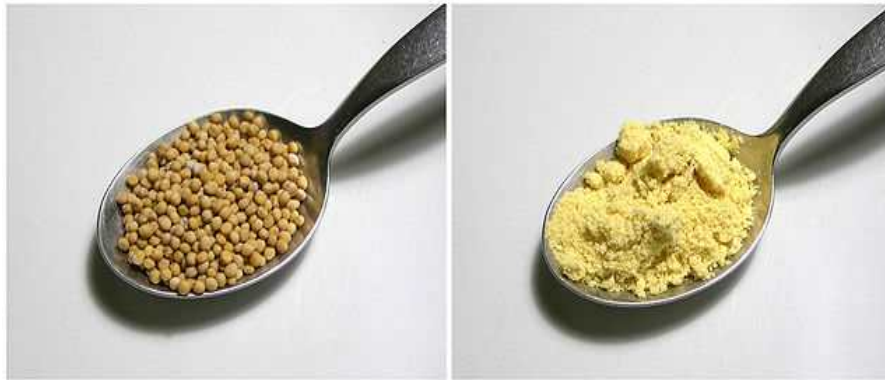


Fig. 14 겨자씨와 분말 (<http://ko.wikipedia.org/wiki/겨자>)

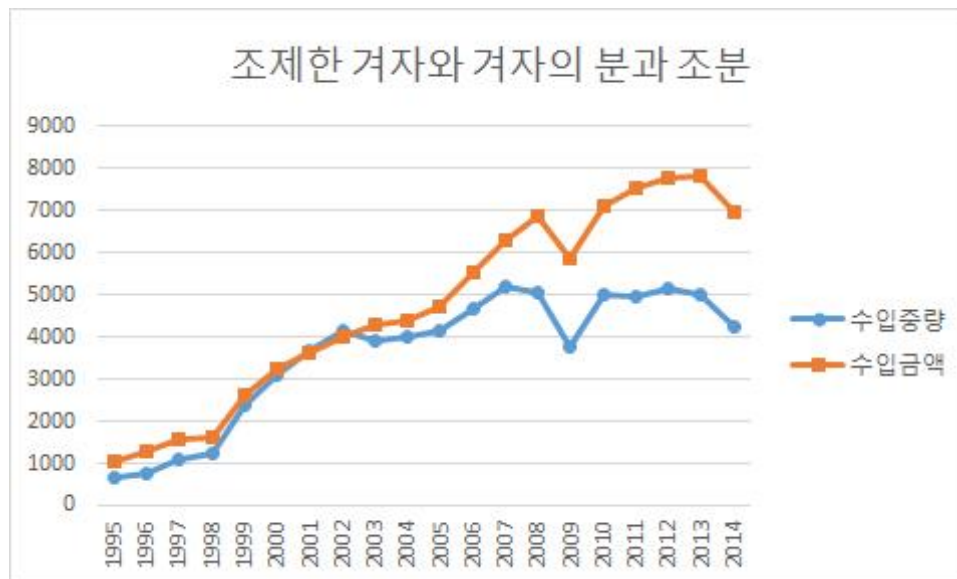


Fig. 15. 조제한 겨자와 겨자의 조분의 수입증량과 수입 금액

건조 겨자씨의 경우 1995년부터 꾸준히 일정한 량이 수입되고 있다(fig. 15). 그러나 수입량에 비하여 수입금액은 지속적으로 차이가 발생하고 있어 겨자의 수입 단가가 지속적으로 오르고 있음을 알 수 있다.



나. 계피와 계피나무의 꽃[Cinnamon and cinnamon-tree flowers ; *Cinnamomum zeylanicum* Blume]



Fig. 16. 실론 계피와 인도네시아 계피 (<http://en.wikipedia.org/wiki/Cinnamon>)

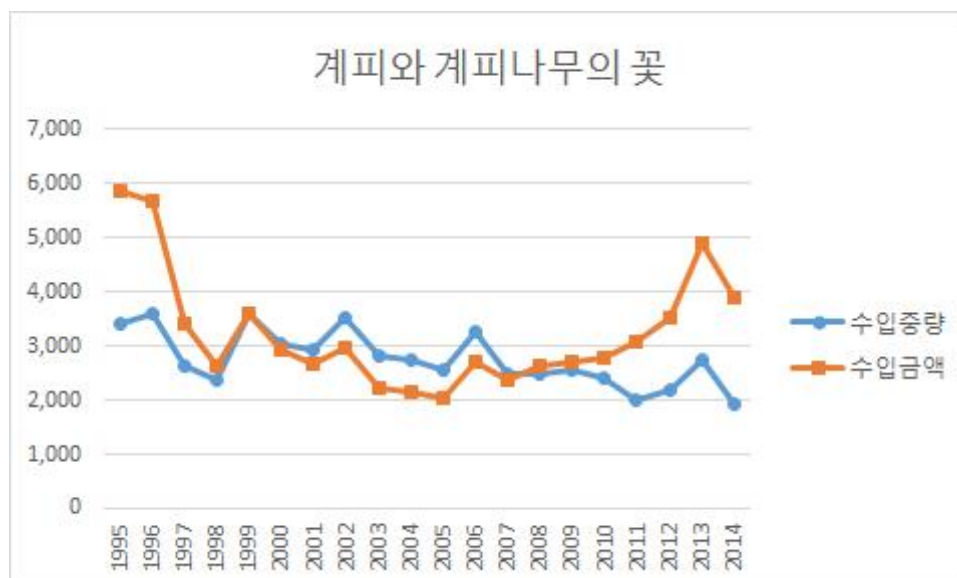


Fig. 17. 계피와 계피나무의 꽃 수입증량과 수입 금액



스리랑카 베트남에서 많이 재배되고 열대 각지에서 폭넓게 재배된다. 인류의 가장 오래 된 향신료 중 하나이며 중국에서는 약 4천 년 전부터 약재로 사용하였고 이집트인들은 B·C 2천 년 전부터 시신을 방부처리하고 미라로 만들 때 계피를 사용하였다.

계피의 수입중량은 점차 증가하다가 2014년을 기점으로 다소 감소했으며 수입가격은 5 년 사이 10%가량 꾸준히 증가하는 것을 볼 수 있다.

건조 계피의 경우에는 수입량이 일정하지는 않지만, 건조된 향신료의 특성상 유통기한이 길기 때문에, 수입량이 많은 해의 다음 년도에는 적게 수입하는 것으로 보인다(fig. 17). 수입량은 지속적인 감소 추세를 보이지만 단가의 상승으로 수입금액은 수입량에 비하여 증가되고 있다.

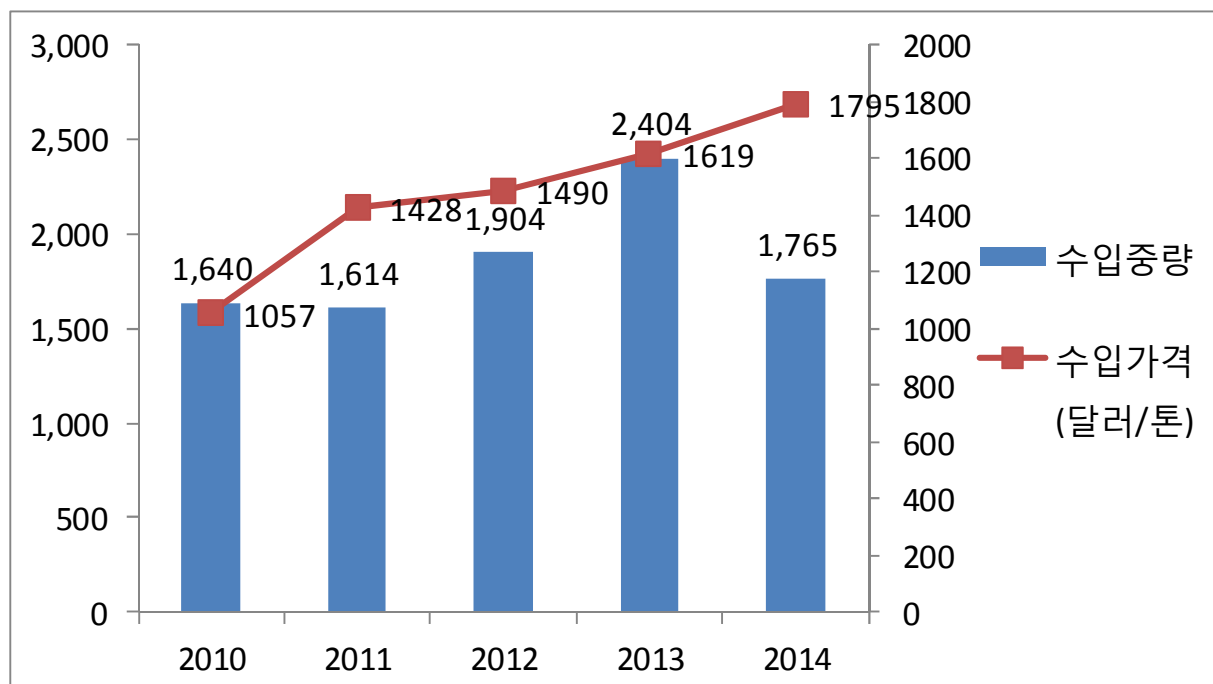


Fig. 18. 계피의 수입동향 - 계피의 수입중량은 점차 증가하다가 2014년을 기점으로 감소했으며, 수입가격은 계속 증가하고 있는 추세이다.

#### 다. 후추 및 유사 향신료 (*Piper*)

후추는 세계에서 가장 많이 사용하고 있는 향신료로 유럽에서는 이미 기원전에 알려져 있었고 해열제로서 사용되어 왔으며 후추에 함유되어 있는 피페린은 소화를 돕고 침과 위액 속에 들어 있는 박테리아를 죽인다.



후추 역시 다른 향신료와 비슷하게 약 20년간 수입량이 꾸준히 증가하는 추세를 보이고 있다. 다만 1997년과 2007년 에 후추의 수입중량이 급격히 감소하였는데 이것은 1인당 국민총소득과 연관 지어 설명할 수 있다. Fig. 21을 보면 1인당 국민총소득과 수입량은 매우 유사한 변화를 보인다. 차이가 있다면 후추의 수입량은 2007년부터 감소하기 시작한 반면에 1인당 국민총소득은 2008년부터 감소했다는 것인데, 이것은 2007년 세계경제붕괴 당시 이 사건이 한국의 GNI에는 즉각적인 영향을 미치지 않았지만 경제의 위기감을 주었기 때문에 후추의 수입중량은 2007년부터 이미 낮아진 것이라고 생각해 볼 수 있다. 따라서 후추의 수입량은 경제와 밀접한 연관성을 갖는다고 할 수 있는데 이것은 후추가 가지는 특성 때문이다. 후추는 조미료로서 음식에 필수적으로 들어가는 요소는 아니지만 음식의 맛을 돋우어 주는 식품이며 특정 음식이 아닌 여러 가지 음식에 걸쳐 광범위하게 사용되는 식품이라는 것이다. 따라서 경제상황이 좋을 때에는 음식에 대한 만족감을 높이기 위해 후추를 사용하는 빈도가 높아지지만 경제상황이 나빠지게 되면 음식의 맛과 향을 위하기보다는 당장의 경제상황을 생각하여 사용빈도가 낮아지기 때문에 이로 인하여 후추의 소비가 감소한 것이라고 생각할 수 있다.

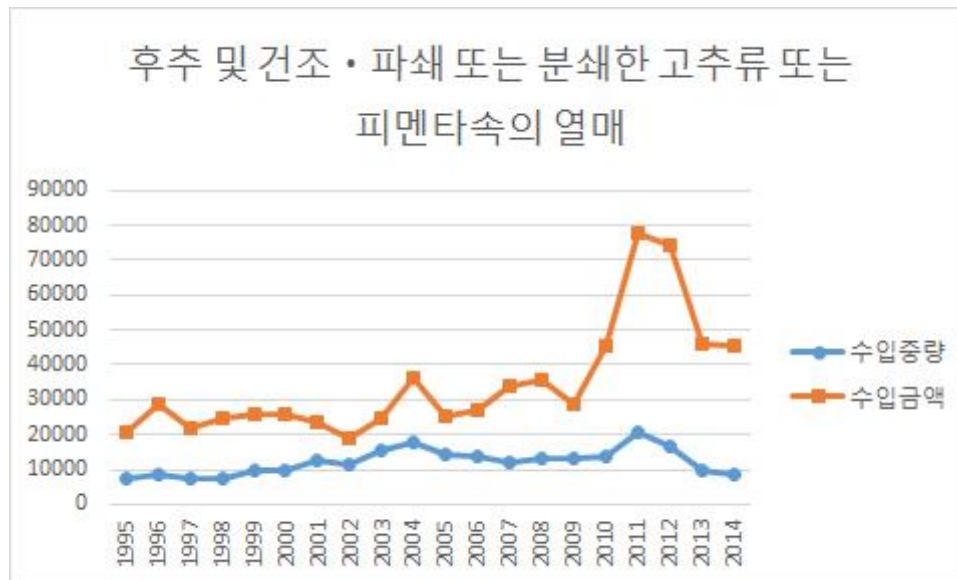


Fig. 19 후추 및 건조·파쇄 또는 분쇄한 고추류 또는 피멘타속의 열매

흑후추의 경우 점차 수입량이 증가하는 모습을 보이고 있다. 90년대 후반에는 후추 / 건조 항목으로 많이 수입되었으나, 향신료의 이해가 높아진 최근에 들어서 흰후추와 흑후추 각각의 항목으로도 많이 수입되고 있다(fig.19).

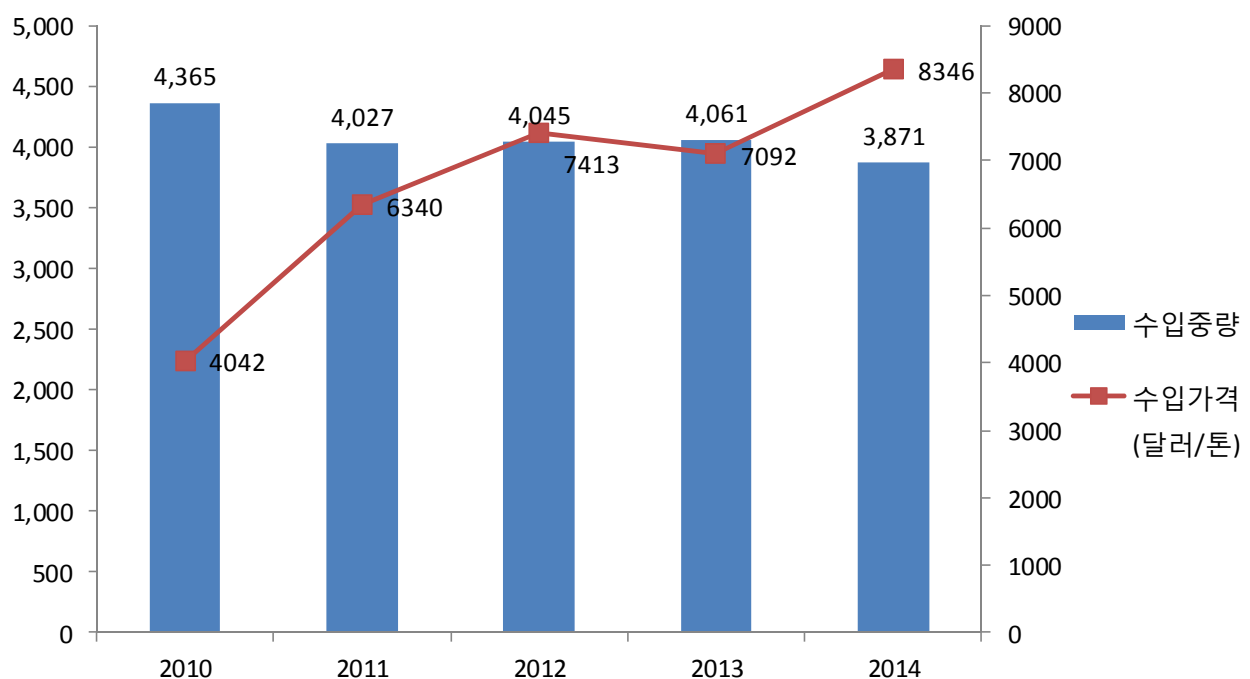


Fig. 20. 후추 (2010~2014년) 수입량과 수입가격

– 후추의 수입증량은 조금씩 감소하는 반면에 수입가격은 2010년 후추 1톤당 수입 가격

이 4,042달러에서 2014년 1톤당 수입 가격이 8,346달러로 5년 사이 수입가격이 2배 이상 증가하였다.



Fig. 21. 1인당 국민총소득(GNI)과 후추의 수입증량의 변화 비교.

#### 라. 생강 (Ginger)



생강은 옛날부터 열대 아시아 지역에서 재배되었으며 원산지는 인도 또는 중국의 사천성이라 추측되고 있다. 생강이 유럽으로 전해진 것은 1세기경으로 처음에는 약용이었으나 9세기경에 향신료로 프랑스와 독일 등에 소개되었다고 한다.

진저론은 생강 매운맛의 한 성분으로 항산화 역할을 한다. 진저론은 트롬복산의 형성을 방해하여 혈소판 기능을 억제하며 항염증 작용을 하며 콜레스테롤을 제거한다.

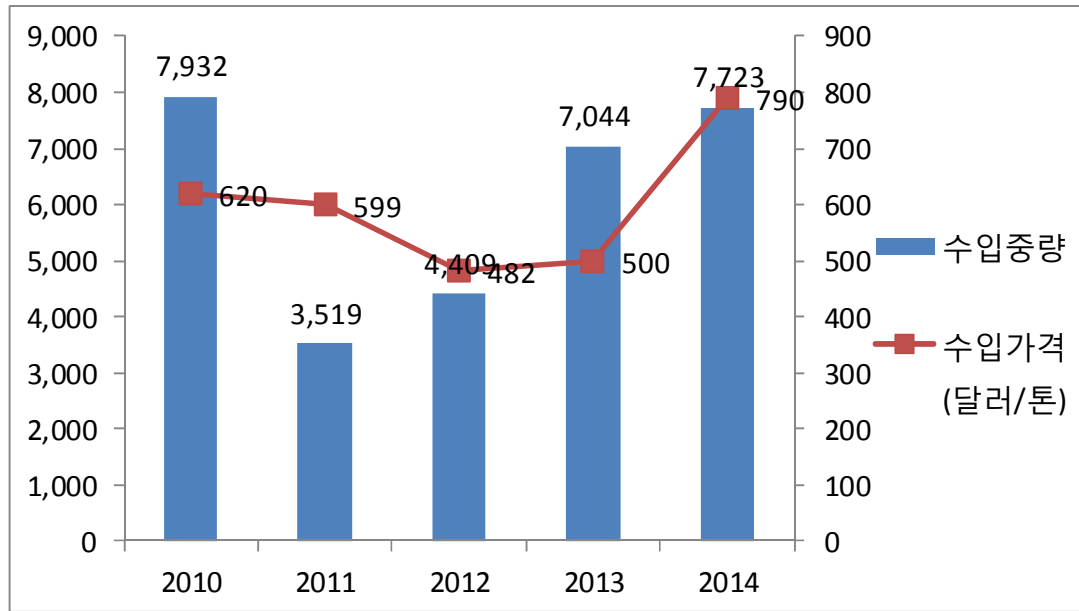


Fig. 22. 생강의 수입동향 - 생강의 수입 중량은 2011년에 절반수준으로 급락했다가 그 후 꾸준히 수입량이 증가하고 있고 수입가격은 2010년부터 2012년까지 하락하다가 2014년 급등하였다.

생강의 수입 중량은 2009년부터 2012년까지 큰 폭으로 하락하고 있는 것을 볼 수 있다. 반면 생강의 수입가격은 5년 사이 55%가량 급증했다.

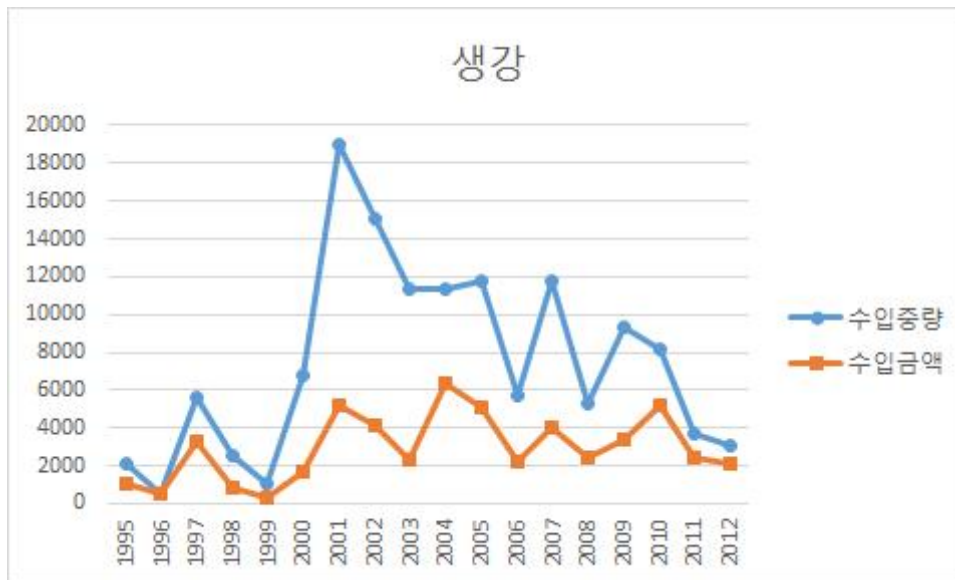


Fig. 23. 생강의 수입중량 및 수입금액

생강의 주요 수입국은 중국으로 중국의 경제상황과도 밀접한 관계가 있다. 또한 생강의 경우 국내 재배가 이루어지고 있는 품목으로 국내 농가의 생산량도 수입량에 영향이 있다. 수입중량 대비 수입금액은 수입원가로 해석할 수 있는데 국내 수입되는 생강은 수입 원가에 대한 의존도가 높다는 것을 확인할 수 있다.

#### 마. 타임 및 월계수 잎 (Thyme; bay leaves)



타임의 원산지는 남부유럽의 지중해연안으로 서아시아, 북아프리카 등에 분포하고 있다. 타임은 프랑스의 달팽이 요리에 첨가되며 추출한 정유의 주성분은 치약이나 파스 등에 첨가된다.

월계수 잎의 원산지는 남부유럽의 지중해 연안으로 월계수 잎은 향신료로 쓰이며 프랑스, 유고연방, 그리스, 터키, 멕시코를 중심으로 자생한다. 월계수 잎은 생잎을 그대로 건조하여 향신료로 사용하고 생잎은 약간 쓴맛이 있지만, 건조하면 단맛과 함께 향긋한 향이 난다.

월계수 잎에 함유되어있는 Cineol은 향긋한 향과 시원한 맛을 가지고 있고 유칼립투스 에 식물성 방향유로 90% 이상 포함되어 있다. 부드럽고 달콤한 향과 맛 때문에 향신료, 향수, 화장품으로 이용되며 입 냄새를 없애는 양치질 물약과 기침억제제 제조 원료로도 사용한다. 또한 만성 폐색성 폐질환과 천식의 치료제로 가치가 있으며, 염증과 고통을 경감시키는 데 효과가 있다. 또한, 백혈구 안에서 사이토카인 생산을 자극하고 항염증효과를 나타내게 된다.

타임과 월계수 잎은 주로 프랑스, 이탈리아 요리에 많이 이용된다. 전통적으로 한국에서 쓰던 향신료가 아니기 때문에 이 전의 다른 향신료보다 수입중량이 현저하게 적은 것을 볼 수 있다. 하지만 이 향신료도 5년 사이 수입량이 약 37% 증가하는 것으로 보아 점점 이 향신료의 쓰임이 많아지고 프랑스, 이탈리아 요리가 국내에서도 많이 만들어지고 있다는 것을 알 수 있다.

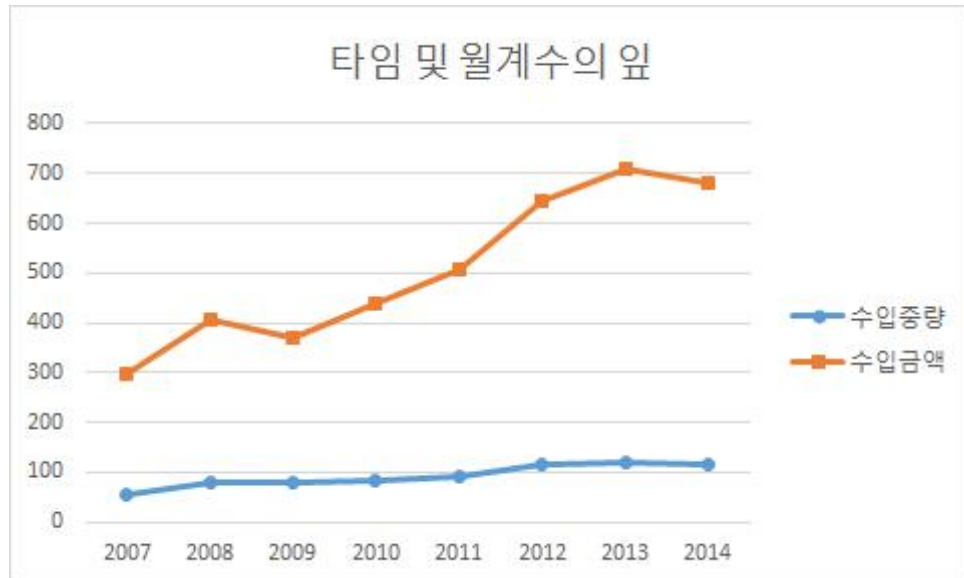


Fig. 24. 타임 및 월계수 잎의 수입중량 및 수입금액

타임 및 월계수 잎의 수입동향 - 2012년까지 수입중량이 증가하다가 2012년 이후 변화 없이 지속되고 있으며 수입가격은 증가와 하락을 반복하지만 전체적으로는 수입가격이 증가하고 있는 추세를 보이고 있다.



바. 정향 (Cloves; *Syringa velutina*)



정향의 원산지는 몰루카섬이지만, 오늘날에는 서인도, 잔지바와 마다가스카르를 포함한 몇몇 곳에서 재배된다. 정향은 향신료 중 방부 효과와 살균력이 가장 강력해서 중국에서는 약재로 사용된다. 화장품, 치약, 약품이나 향수의 재료로도 쓰이며 치통이 있을 때 정향을 물고 있으면 응급진통제 역할을 한다.

양식에서는 햄을 구울 때나 채소 피클을 담글 때 주로 사용한다. 카레, 육수, 전채요리, 소스, 편치, 사과요리, 마른 과일 설탕 절임, 케이크, 빵, 다진 고기와 마른 과일 디저트의 향을 내는 데 사용하고 육류요리를 위한 소스에도 사용한다.

정향은 한국에서 많이 사용하지 않는 향신료로서 연 평균 수입량이 60톤 정도이며, 정향의 수입가격은 2010년부터 2012년까지 급증하여 5년 동안 3배 가까이 가격이 상승하였다.

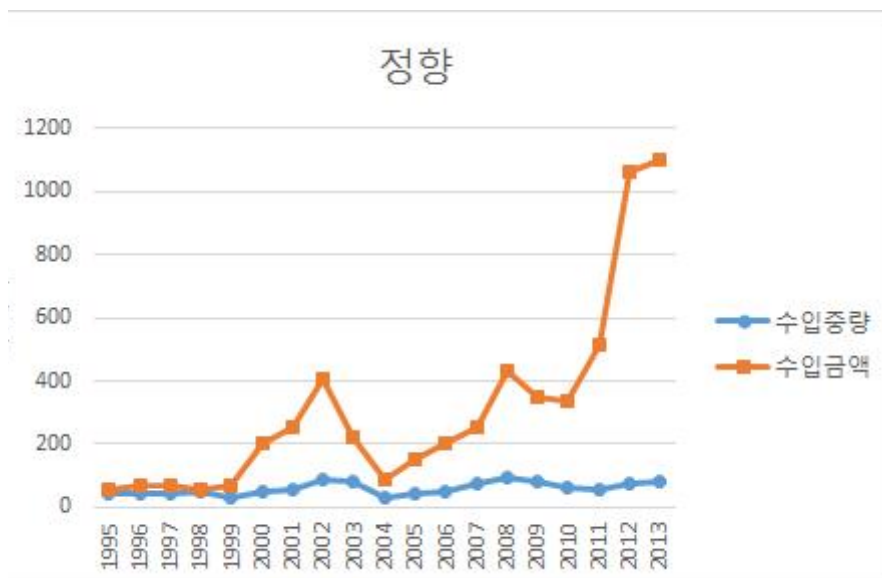


Fig. 25. 정향의 수입증량 및 수입금액

정향의 수입동향 - 정향의 수입량은 증가와 하락을 반복하고 있고 수입가격은 5년 사이 크게 상승하였다.

사. 코리앤더 씨(Seeds of coriander; *Coriandrum sativum*)



코리앤더의 원산지는 동부 지중해 연안으로 그 씨를 얻기 위해 재배하는 품종이 매우 다양하다. 성경에도 등장하고, 이집트의 고고학 발굴에서 코리앤더 깍지가 발견되는 것으로 보아, 오래 전부터 코리앤더를 재배해 왔음을 알 수 있다. 유럽과 아프리카의 코리앤더는 둥글고 살짝 물결무늬로 패여 있지만, 인도의 코리앤더는 더 매끄럽고 모양도 타원형이다.

원산지인 지중해 근처는 물론 인도의 혼합 향신료, 유럽의 소시지, 아메리카의 콘비프, 아시아의 커리 등 코리앤더씨를 사용하는 음식은 매우 다양하다.

코리앤더씨의 수입량과 수입가격은 5년간 조금 씩 감소하는 추세였으나 2014년 들어 수입가격이 증가하였다.

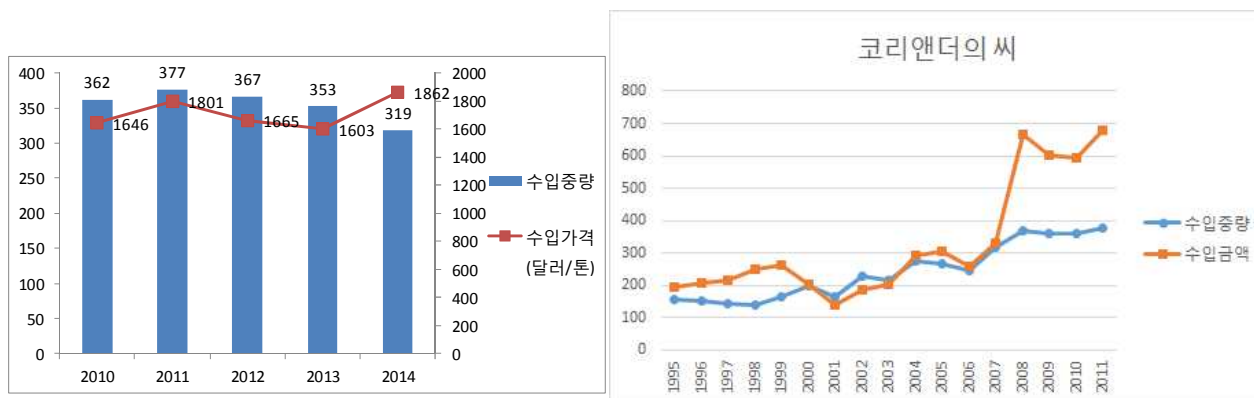


Fig. 26. 코리앤더 씨의 수입중량 및 수입금액

코리앤더씨의 수입동향 - 코리앤더씨의 수입량은 2011년 들어 점점 감소하는 추세를 보이고 있고 수입가격은 증감을 반복하고 있다. 2008년을 기준으로 볼 경우 수입금액이 두배이상 증가된 것을 알 수 있으며, 수입원가의 폭등으로 인하여 수입량은 증가되지 않고 있다.

아. 회향 씨(Seeds of fennel; *Foeniculum vulgare*)



회향 씨는 지중해 연안이 원산지이며 달콤하고 상큼한 맛이다. 생선의 비린내, 육류의 느끼함과 누린내를 없애고 맛을 돋운다. 회향에는 대회향과 소회향이 있는데, 우리나라에서 생산되는 것은 소회향이다. 회향은 장의 연동운동을 원활하게 하고 헛배가 불러 속이 더부룩한 것을 풀어주며 위를 튼튼하게 하여 소화가 잘 되게 도와주는 작용을 한다.

회향은 이탈리아 요리에서 가장 많이 등장하는 재료 중 하나이며 샐러드, 파스타 등 주요 요리에는 꼭 등장하고 빵을 만들 때 반죽에 넣어서 향을 더하기도 한다.

회향씨의 수입량은 증감을 반복하지만 점차 증가하고 있는 추세이고 수입가격은 2012년과 2013년에 걸쳐 크게 하락했다.

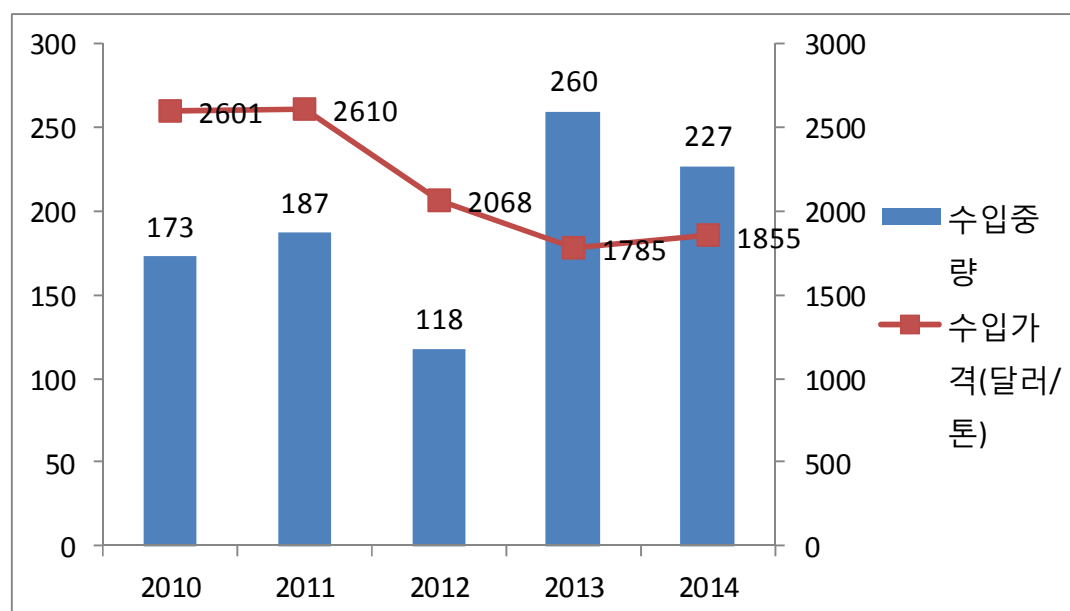


Fig. 27. 회향의 수입중량 및 수입금액

회향씨의 수입동향 - 회향씨의 수입량은 2013년에 2배 넘게 증가하였으나 수입가격은 하락하고 있는 추세이다.

자. 커민 씨(Seeds of cumin; *Cuminum cyminum*)



커민씨는 이집트가 원산지인 한해살이풀로 맵고 다른 냄새를 모두 감출 정도로 향이 강하다. 구미날이라는 성분이 있어 타는 듯 매운맛을 내는 성분을 포함하며 특 쏘는 쓴맛이 난다.

고대 로마인들은 이것을 지금 우리가 검은 후추를 쓰는 것처럼 양념에 이용했다. 지금은 그리스, 터키, 아랍 요리에서 빠져서는 안 될 향신료로 쓰이고 있다. 칠리 파우더나 가람 마살라 혼합 향신료의 재료 중 하나이며, 모로코의 케밥, 중동과 북아프리카 전통요리인 쿠스쿠스, 인도의 카레요리나 탄두리 치킨, 그 외 고기요리에 쓰이고, 네덜란드 에담 치즈와 독일 뮌스터 치즈에 맛을 더하는데 쓰인다. 스페인과 포르투갈에서는 소시지의 향을 내는데 쓰인다.

커민씨는 2011년을 기점으로 수입량이 줄어들고 가격은 높아졌지만 곧 회복되어 2010년의 상태를 유지하고 있다.

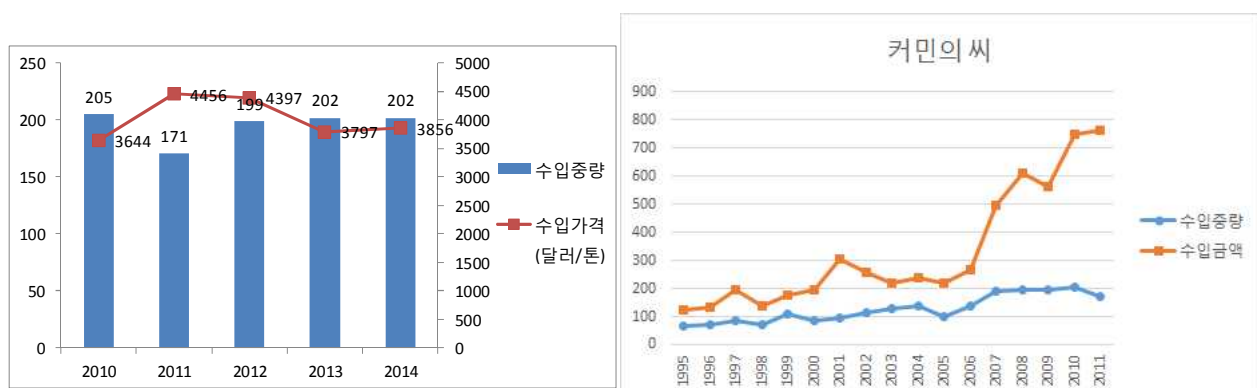


Fig. 28. 커민 씨의 수입증량 및 수입금액

커민 씨의 수입동향 - 커민 씨의 수입량은 큰 차이 없이 비슷한 값을 지속하고 있으며 2007년부터 수입량에 비하여 수입금액이 급격하게 증가되었다. 그 후 수입가격은 2011년과 2012년에 높아졌다가 다시 하락하였다.

차. 심황(Turmeric; *Curcuma longa*)



말레이시아와 인도가 원산지로 생강과에 속하며 심황에서 만들어지는 노란 색소는 카레 등에 이용된다.

심황에 들어있는 커큐민은 항종양, 항산화, 항아밀로이드와 항염증작용을 가지고 있다. 항염증작용은 이코사노이드 생합성의 억제에 의해서 기능을 수행한다. 커큐민은 산화에 의한 DNA 손상과 지질과산화를 억제하고, 항산화 작용을 한다

심황의 수입 중량은 5년 사이 31% 증가한 것을 볼 수 있다. 반면 심황의 수입 가격은 2012년을 기점으로 심황의 수입가격이 절반 수준으로 떨어진 것을 볼 수 있다. 이것은 한국에서는 심황의 약 80%를 인도에서 수입하는데 2012년에 루피의 약세화가 나타났으며 한국과 인도의 CEPA 체결로 인한 관세인하의 영향으로 심황의 수입가격이 하락한 것이라 생각된다.

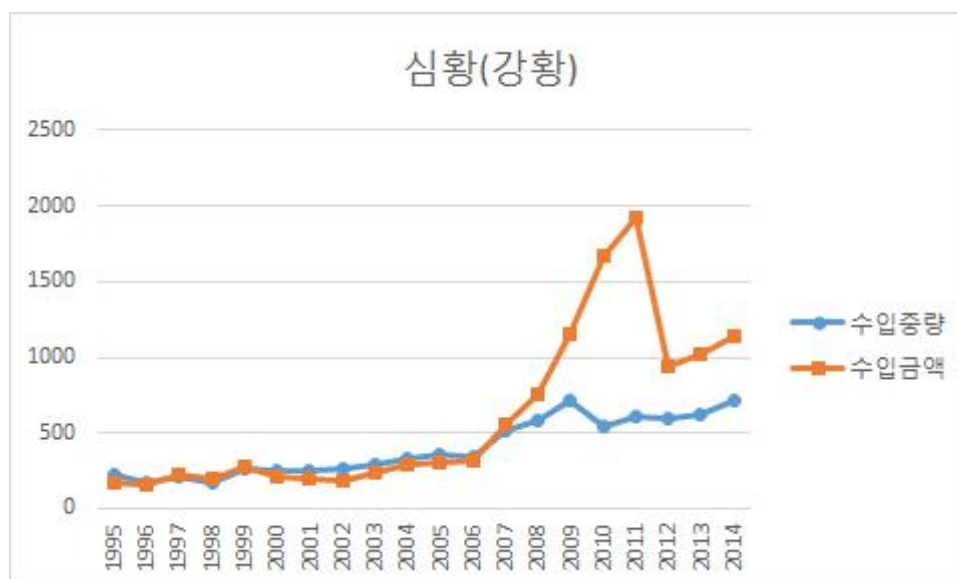


Fig. 29. 심황의 수입중량 및 수입금액



## 2. 향신료 중 꿀풀과 식물의 정유성분

### 가. 타임 (Thyme; *Thymus vulgaris* L.)

EO (essential oil-많은 순서) - Brazil: thymol, P-cymene,  $\gamma$ -terpinene

EO - from New Zealand: thymol, carvacrol, P-cymene

EO- from spice material: Thymol, p-Cymene, Linalool

EO - from Moroco: camphor, camphene,  $\alpha$ -pinene, 1, 8-cineole, borneol,  $\beta$ -pinene

EO - from Spain: 1,8-cineole, terpenyl acetate, borneol, linalool, pinene, terpineol, camphor

근연종 (*Thymus glandulosus* Lag. ex H. del Villar)

EO:  $\gamma$ -terpinene, p-cymene, thymol, carvacrol

Table 8. Chemical composition of the essential oil from leaves of *Thymus vulgaris* L. from Rio de Janeiro State, Brazil

| Compound                       | Content, % |
|--------------------------------|------------|
| 1,3-Octadiene                  | 0.3        |
| 1,7-Octadiene                  | 0.1        |
| 2,4-Dimethyl-2,4-heptadiene    | 1.5        |
| $\alpha$ -Pinene               | 0.8        |
| Camphene                       | 0.3        |
| Sabinene                       | 0.1        |
| <i>para</i> -Menthene-1        | 1.8        |
| <i>para</i> -Menthene-3        | 0.1        |
| Myrcene                        | 2.4        |
| $\alpha$ -Phellandrene         | 0.3        |
| $\alpha$ -Terpinene            | 1.8        |
| <i>p</i> -Cymene               | 18.6       |
| Limonene                       | 0.8        |
| ( <i>Z</i> )- $\beta$ -Ocimene | 0.1        |
| ( <i>E</i> )- $\beta$ -Ocimene | 0.1        |
| $\gamma$ -Terpinene            | 16.5       |
| Mentha-3,8-diene               | 0.4        |
| $\alpha$ -Terpinolene          | 0.2        |
| <i>p</i> -Cimenene             | 0.1        |
| Borneol                        | 0.5        |
| <i>trans</i> -Dihydrocarvone   | 0.2        |
| Thymol methyl ether            | 0.1        |
| Thymol                         | 44.7       |
| Carvacrol                      | 2.4        |
| Carvacrol acetate              | < 0.1      |
| $\beta$ -Caryophyllene         | 0.8        |
| Calamenene                     | < 0.1      |
| $\delta$ -Cadinene             | 0.1        |
| Total                          | 95.1       |

#### 나. 로즈마리 (Rosemary; *Rosmarinus officinalis* L.)

EO (essential oil-맑은 순서) – from Poland:  $\alpha$ -pinene, bornyl acetate, camphene and 1,8-cineole

EO – from South Africa: Hydrodistillation method (HD):  $\alpha$ -pinene, camphene, 1,8 cineole, camphor, borneol, bornyl acetate, verbenone – Solvent free microwave extraction method (SFME): borneol, camphor, terpene-4-ol, linalool,  $\alpha$ -terpeneol

EO – from China (commercial sources): 1,8-cineole,  $\alpha$ -pinene, camphor, camphene,  $\beta$ -pinene

EO – from Spain:  $\alpha$ -pinene, 1,8-cineole, camphor; from France:  $\alpha$ -pinene, 1,8-cineole, bornyl acetate

EO – from Turkey: p-cymene, linalool, g-terpinene, thymol,  $\beta$ -pinene,  $\alpha$ -pinene, eucalyptol

Composition percentage of *Rosmarinus officinalis* L. essential oil

| No. | RT    | Compounds               | Molecular formula                              | MW  | Relative percentage |
|-----|-------|-------------------------|------------------------------------------------|-----|---------------------|
| 1   | 5.75  | $\alpha$ -Thujene       | C <sub>10</sub> H <sub>16</sub>                | 136 | 0.43                |
| 2   | 5.99  | $\alpha$ -Pinene        | C <sub>10</sub> H <sub>16</sub>                | 136 | 19.43               |
| 3   | 6.39  | Camphene                | C <sub>10</sub> H <sub>16</sub>                | 136 | 11.52               |
| 4   | 7.24  | $\beta$ -Pinene         | C <sub>10</sub> H <sub>16</sub>                | 136 | 6.71                |
| 5   | 7.81  | $\beta$ -Phellandrene   | C <sub>10</sub> H <sub>16</sub>                | 136 | 1.23                |
| 6   | 8.03  | $\alpha$ -Terpinene     | C <sub>10</sub> H <sub>16</sub>                | 136 | 0.41                |
| 7   | 8.23  | p-Cymene                | C <sub>10</sub> H <sub>14</sub>                | 134 | 1.67                |
| 8   | 8.36  | Limonene                | C <sub>10</sub> H <sub>16</sub>                | 136 | 1.95                |
| 9   | 8.48  | 1,8-Cineole             | C <sub>10</sub> H <sub>18</sub> O              | 154 | 27.23               |
| 10  | 9.14  | Linalool                | C <sub>10</sub> H <sub>18</sub> O              | 154 | 0.25                |
| 11  | 10.26 | Isopulegol 2            | C <sub>10</sub> H <sub>18</sub> O              | 154 | 1.19                |
| 12  | 11.80 | Camphor                 | C <sub>10</sub> H <sub>16</sub> O              | 152 | 14.26               |
| 13  | 12.5  | Borneol                 | C <sub>10</sub> H <sub>18</sub> O              | 154 | 3.17                |
| 14  | 12.72 | Terpinene 4-ol          | C <sub>10</sub> H <sub>18</sub> O              | 154 | 0.53                |
| 15  | 13.14 | $\alpha$ -Terpineol     | C <sub>10</sub> H <sub>18</sub> O              | 154 | 2.11                |
| 16  | 13.53 | Verbenone               | C <sub>10</sub> H <sub>14</sub> O              | 150 | 1.48                |
| 17  | 15.75 | Bornyl acetate          | C <sub>12</sub> H <sub>20</sub> O <sub>2</sub> | 196 | 1.13                |
| 18  | 19.65 | $\beta$ -Caryophyllene  | C <sub>15</sub> H <sub>24</sub>                | 204 | 2.41                |
| 19  | 20.65 | $\alpha$ -Caryophyllene | C <sub>15</sub> H <sub>24</sub>                | 204 | 0.86                |

Compounds, identified on the basis of comparison with MS database spectra, retention indices and pure reference chemicals, are listed in order of elution from a DB-5MS column. RT: retention time; MW: molecular weight.

#### 다. 박하 (Mint-Peppermint; *Mentha × piperita* = *M. balsamea* Willd.)

EO – from Norway: 1,8-cineole, menthol, menthone, limonene,  $\beta$ -pinene,  $\alpha$ -pinene, menthofuran, isomenthone, neomenthol,  $\beta$ -caryophyllene

#### 라. 스피아민트 (Spearment; *Mentha spicata* L.)

EO – from the North-West Himalayan region of India: 1,8-cineole, trans-carveol, carvone, limonene

EO – from Crete, Greece: C-2 substituted p-methane, carvone, Trans- and cis-dihydrocarvone, dihydrocarveol, trans- and cis-carveol



### 3. 꿀풀과 식물의 향성분 목록

(정유포함 가능성 – 현화식물: Hong, *Unpublished Data*)

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1. Apiaceae (산형과)
2. Araliaceae (두릅나무과)
3. Asteraceae (국화과)
4. Boraginaceae (지치과)
5. Cruciferae (Brassicaceae) (십자화과)
6. Cucurbitaceae Juss. (박과)
7. Ericaceae Juss. (Vacciniaceae S. F. Gray) (진달래과)
8. Euphorbiaceae (대극과)

#### 9. Lamiaceae (꿀풀과) ◀

10. Leguminosae (콩과)
11. Malvaceae (아욱과)
12. Onagraceae (바늘꽃과)
13. Ranunculaceae Juss. (*incl.* Paeoniaceae Rudolphi) (미나리아재비과)
14. Rhamnaceae Juss (대추나무과)
15. Rosaceae Juss. (장미과)
16. Rutaceae Juss. (운향과)
17. Salicaceae Mirb. (버드나무과)
18. Solanaceae (가지과)

Table 9. Twenty-seven Lamiaceae genera in Korea

|                                         |                                   |                           |
|-----------------------------------------|-----------------------------------|---------------------------|
| <i>Agastache</i> Clayton ex Gronov.     | <i>Lamium</i> L.                  | <i>Prunella</i> L.        |
| <i>Ajuga</i> L.                         | <i>Leonurus</i> Mill.             | <i>Salvia</i> L.          |
| <i>Amethystea</i> L.                    | <i>Lycopus</i> L.                 | <i>Scutellaria</i> Baumg. |
| <i>Clinopodium</i> L.                   | <i>Meehania</i> Britton*          | <i>Stachys</i> L.         |
| <i>Dracocephalum</i> L.                 | <i>Mentha</i> L.                  | <i>Teucrium</i> L.        |
| <i>Elsholtzia</i> Willd.                | <i>Mosla</i> Buch.-Ham. ex Maxim. | <i>Thymus</i> L.          |
| <i>Galeopsis</i> Moench                 | <i>Nepeta</i> L.                  | <i>Tripura</i> *          |
| <i>Glechoma</i> L.                      | <i>Perilla</i> L.                 |                           |
| <i>Isodon</i> Schrad. ex Benth. & Spach | <i>Phlomis</i> L.                 |                           |
| <i>Lagopsis</i> Bunge ex Benth. *       | <i>Pogostemon</i> Desf.           |                           |

\* : No information available

## LAMIACEAE

### *Agastache* Clayton ex Gronov.

*Agastache rugosa* (Fisch. & C.A.Mey.) Kuntze, Revis. Gen. Pl. 2: 511 (1891) Nat; N Korea, SKorea 배초향

- EO: Methyl chavicol (90%), anisaldehyde and p-methoxy cinnamaldehyde (ca. 10%)
- EO: Methyl chavicol (92.0% and 75.9% in the leaf and flower oils, respectively).

### *Ajuga* L.

*Ajuga decumbens* Thunb., Fl. Jap. (Thunberg) 243 (1784) Nat; S Korea 금창초

*Ajuga multiflora* Bunge, Enum. Pl. Chin. Bor. 51 (1833) Nat; N Korea, S Korea 조개나물

*Ajuga spectabilis* Nakai, Bot. Mag. (Tokyo) 30: 290 (1916) Nat; S Korea, Endemic 자란초

- *Ajuga chamaepitys* subsp. *chia* var. *chia* and var. *ciliata* – EO:  $\beta$ -pinene (20.8%) and germacrene D (12.6%) – EO: germacrene D (14.6%) and  $\beta$ -pinene (14.0%)
- *Ajuga chamaepitys* (L.) Schreb. – EO: monoterpene hydrocarbons (65.6%) –  $\alpha$ -pinene (16.1%) and P-pinene (34.3%). EO: sesquiterpene (18.0%) – germacrene D (5.6%).

### *Amethystea* L.

*Amethystea caerulea* L., Sp. Pl. 21 (1753) Nat; N Korea, S Korea 개차즈기

- *Amethystea caerulea* L. – EO: morrilol (25.1%), 4-vinylguaiacol (14.3%) and acetoanisole (14.3%), linalool (6.6%), eugenol (5.8%) and  $\alpha$ -caryophyllene (5.2%).

### *Clinopodium* L.

*Clinopodium chinense* (Benth.) Kuntze var. *grandiflorum* (Maxim.) H.Hara, J. Jap. Bot. 12:39 (1936) Nat; N Korea, S Korea 꽃층층이꽃

*Clinopodium chinense* (Benth.) Kuntze var. *parviflorum* (Kudô) H.Hara, J. Jap. Bot. 12: 41(1936) Nat; N Korea, S Korea 층층이꽃

*Clinopodium chinense* (Benth.) Kuntze var. *shibetchense* (H.Lév.) Koidz., Bot. Mag. (Tokyo) 43: 387 (1929) Nat; N Korea, S Korea 산층층이

*Clinopodium fauriei* (H.Lév. & Vaniot) H.Hara, J. Jap. Bot. 11: 106 (1935) Nat; S Korea 개탑꽃

*Clinopodium gracile* (Benth.) Kuntze, Revis. Gen. Pl. 2: 514 (1891) Nat; S Korea 애기탑꽃

*Clinopodium micranthum* (Regel) H.Hara, J. Jap. Bot. 16: 156 (1940) Nat; N Korea, S Korea 두메층층이

*Clinopodium multicaule* (Maxim.) Kuntze, Revis. Gen. Pl. 2: 515 (1891) Nat; N Korea, SKorea 탐꽃

- *Clinopodium* (Benth.) Matsum. – EO: sesquiterpenoids (70.49 %), monoterpenoids (12.21 %), germacrene D (20.59 %), nootkatone (8.22 %), morillol (7.74 %),  $\beta$ -elemene (7.38 %),  $\alpha$ -bergamotene (6.08 %), cis- $\beta$ -farnesene (5.47 %) and caryophyllene (5.17 %).

### ***Dracocephalum* L.**

*Dracocephalum argunense* Fisch. ex Link, Enum. Hort. Berol. Alt. 2: 118 (1822) Nat; N Korea, S Korea 용머리

*Dracocephalum rupestre* Hance, J. Bot. 7: 166 (1869) Nat; N Korea 별개풀

- *Dracocephalum ruyschiana* L. – EO: pinocamphone and isopinocamphone and sesquiterpenes ( $\beta$ -caryophyllene, caryophyllene oxide,  $\beta$ -cubebene, germacrene-D and elemol),  $\beta$ -pinene, myrcene, limonene, p-cymene, methyl chavicol.
- *Dracocephalum grandiflorum* L. sesquiterpenes (aromadendrene,  $\beta$ -caryophyllene, caryophyllene oxide,  $\beta$ -cubebene and  $\beta$ -bourbonene), carvacrol,  $\beta$ -asarone and methyl chavicol.

### ***Elsholtzia* Willd.**

*Elsholtzia ciliata* (Thunb.) Hyl., Bot. Not. 1941: 129 (1941) Nat; N Korea, S Korea 향유

*Elsholtzia splendens* Nakai ex F.Maek., Bot. Mag. (Tokyo) 48: 50 (1934) Nat; N Korea, S Korea 꽃향유

- *Elsholtzia stauntonii* Benth. EO: rosefuran (41.73 $\pm$ 0.62%) and rosefuran epoxide (40.36 $\pm$ 0.89%).
- *Elsholtzia pilosa* – EO: 1,8-cineol (50%).
- *Elsholtzia cristata* Willd. – EO: 88% dehydroelsholtzia ketone, acylfuran derivatives.
- *Elsholtzia polystachya* – EO: 1,8-cineol (37.3%), perillene (61.2%).
- *Elsholtzia ciliata* (Thunb.) Hyland. – EO: neral(15.2-20.5%), geranial (19.5-26.5%), limonene (10.9-14.2%) and (Z)- $\beta$ -farnesene (10.8-11.7%). – linalool, nerol, neral, geranial, geraniol, neryl and geranyl formates and acetates, (Z)-methyl geranate and (Z)-nerolidol.
- *Elsholtzia argyi* – EO: caryophyllene (55.02%).
- *Elsholtzia eriostachya* var. *pusilla* – EO: gerania (53%), 39% neral (39%), 19 other terpenoid constituents.

### ***Galeopsis* Moench**

*Galeopsis bifida* Boenn., Prodr. Fl. Monast. Westphal. 178 (1824) Nat; N Korea 털향유

- *G. bifida* - EO: sesquiterpenes (77.8% identified), caryophyllene (22.0%), spatulenol (12.1%), caryophyllene oxide (11.0%), and germacreneD (10.6%).
- *G. pubescens* and *G. tetrahit* - EO: sesquiterpenes (88.9 and 90.4%, respectively), germacrene D, bicyclogermacrene, aryophyllene and farnesene.

### ***Glechoma* L.**

*Glechoma longituba* (Nakai) Kuprian., Bot. Zhurn. (Moscow & Leningrad) 33: 236 (1948) Nat; N Korea 긴병꽃풀

- *G. longituba* - EO:  $\alpha$ -cadinol, germacrene B, germacrene D-4-ol, and  $\alpha$ -caryophyllene

### ***Isodon* Schrad. ex Benth. & Spach**

*Isodon excisus* (Maxim.) Kudô, Mem. Fac. Sci. Taihoku Imp. Univ. 2: 133 (1929) Nat; N Korea, S Korea 오리방풀

*Isodon inflexus* (Thunb.) Kudô, Mem. Fac. Sci. Taihoku Imp. Univ. 2: 127 (1929) Nat; N Korea, S Korea 털산박하

*Isodon japonicus* (Burm.) H.Hara, Enum. Spermatophytarum Japon. 1: 206 (1948) Nat; N Korea, S Korea 방아풀

*Isodon serra* (Maxim.) Kudô, Mem. Fac. Sci. Taihoku Imp. Univ. 2: 125 (1929) Nat; N Korea, S Korea 자주방아풀

- *Isodon henryi* (Hemsl.) Kudo - EO: monoterpenoids, sesquiterpenoids and diterpenoids.

### ***Lagopsis* Bunge ex Benth.**

*Lagopsis supina* (Stephan) Ikonn.-Gal., Bot. Mater. Gerb. Bot. Inst. Komarova Akad. Nauk S.S.S.R. 7: 45 (1937) Nat; N Korea 자주방아풀

- No information available

### ***Lamium* L.**

*Lamium album* L., Sp. Pl. 2: 579 (1753) Nat; N Korea, S Korea 왜광대수염

*Lamium album* L. var. *album*

*Lamium album* L. subsp. *barbatum* (Siebold & Zucc.) Mennema, Leiden Bot. Ser. 11: 70 (1989) Nat; N Korea, S Korea 광대수염

*Lamium amplexicaule* L., Sp. Pl. 579 (1753) Nat; N Korea, S Korea 광대나물

*Lamium purpureum* L., Sp. Pl. 579 (1753) Int 자주광대나물

- *Laminum purpureum* (germacrene D-35.4%), *L. hybridum* (germacrene D-39.0%) and *L. bifidum* (germacrene D-34.9%).

### ***Leonurus* Mill.**

*Leonurus japonicus* Houtt., Nat. Hist. (Houttuyn) 9: 366 (1778) Nat; N Korea, S Korea 익모초

*Leonurus macranthus* Maxim., Mem. Acad. Imp. Sci. St.-Petersbourg Divers Savans 9: 476 (1859) Nat; N Korea, S Korea 송장풀

- *Leonurus cardiaca* L. - EO: Caryophyllene (39.8%), ahumulene (34.8%),  $\alpha$ -pinene(5.6%),  $\beta$ -pinene(0.5%), linolool (0.7%), limonene (0.4%)

### ***Lycopus* L.**

*Lycopus coreanus* H.Lév., Repert. Spec. Nov. Regni Veg. 8: 423 (1910) Nat; N Korea, S Korea 개쑥싸리

*Lycopus lucidus* Turcz. ex Benth., Prodr. (DC.) 12: 179 (1848) Nat; N Korea, S Korea 쑥싸리

*Lycopus lucidus* Turcz. ex Benth. var. *lucidus*

*Lycopus lucidus* Turcz. ex Benth. var. *maackianus* Maxim. ex Herder, Bull. Soc. Imp. Naturalistes Moscou 2: 12 (1884) Nat; N Korea, S Korea 애기쑥싸리

*Lycopus uniflorus* Michx., Fl. Bor.-Amer. (Michaux) 1: 14 (1803) Nat; N Korea, S Korea 털쑥싸리

- *Lycopus europaeus* L. - EO:  $\alpha$ -pinene camphene, limonene,  $\gamma$ -terpinene, p-eymene, and terpinolene
- *L. lucidus* Turcz. var. *hirtus* Regel - EO:  $\alpha$ -Humulene (15.97%),  $\beta$ -caryophyllene (10.69%) and humulene epoxide II (10.51%), caryophyllene oxide (8.91%), myrcene (8.65%) and  $\gamma$ -cymene(4.13%).

### ***Meehania* Britton**

*Meehania urticifolia* (Miq.) Makino, Bot. Mag. (Tokyo) 13: 159 (1899) Nat; N Korea, S Korea 벌깨덩굴

- No information available (New EO data are provided in the present work-2014, and will be reported in 2015)

### ***Mentha* L.**

*Mentha arvensis* L. var. *piperascens* Malinv. ex Holmes, Pharm. J. Trans. III, 13: 381 (1882) Nat; N Korea, S Korea 박하

- *Mentha arvensis* – EO: menthol (71.40%), *p* –menthone (8.04%), iso–menthone (5.42%) and neo –menthol (3.18%).
- *Mentha arvensis* L. f. *piperascens* Malinvaud ex. Holmes – EO: Menthol (77.5–89.3%), menthone, isomenthone, *p*–cymene, isopulegol and decanol,
- *Mentha x piperita* L. – EO: menthol (40%), *p*–menthane group (isomenthone, menthyl acetate, and menthofuran), monoterpenes, limonene and 1,8–cineole

### ***Mosla* Buch.–Ham. ex Maxim.**

*Mosla chinensis* Maxim., Bull. Acad. Imp. Sci. Saint–Pétersbourg 29: 177 (1883) Nat; S Korea 가는잎산들개

*Mosla dianthera* (Buch.–Ham. ex Roxb.) Maxim., Bull. Acad. Imp. Sci. Saint–Pétersbourg 10: 457 (1865) Nat; N Korea, S Korea 쥐깨풀

*Mosla japonica* (Benth.) Maxim., Bull. Acad. Imp. Sci. Saint–Pétersbourg 20: 461 (1875) Nat; N Korea, S Korea 산들개

*Mosla scabra* (Thunb.) C.Y.Wu & H.W.Li, Acta Phytotax. Sin. 12: 230 (1974) Nat; N Korea, S Korea 들깨풀

- *Mosla chinensis* Maxim. – EO: carvacrol (57.08%), *p*–cymene (13.61%), thymol acetate (12.68%), thymol (6.67%), and  $\gamma$ –terpinene (2.46%).
- *Mosla chinensis* Maxim, *M. hangchowensis* Matsuda and *M. scabra* (Thunb.) C. Y. Wu et H. W. Li – EO: carvacrol (50%) (with a small amount of thymol) and other mono–terpenes, methyleugenols, cineoles, monoterpenes, and sesquiterpenes.
- *Mosla dianthera* – EO: elemicin (16.51%), thymol (14.77%),  $\beta$ –caryophyllene (14.49%), iso–elemicin (9.22%), asarone (6.09%) and  $\alpha$ –caryophyllene (5.26%)

### ***Nepeta* L.**

*Nepeta cataria* L., Sp. Pl. 570 (1753) Nat; N Korea, S Korea 개박하

*Nepeta multifida* L., Sp. Pl. 572 (1753) Nat; N Korea 개형개

*Nepeta stewartiana* Diels, Notes Roy. Bot. Gard. Edinburgh 5: 237 (1912) Nat; N Korea 잔장풀

*Nepeta tenuifolia* Benth., Labiat. Gen. Spec. 468 (1834) Int 형개

- *Nepeta caesarea* Boiss. – *N. cataria* L. – *N. cadmea* Boiss. – *N. pilinux* P. H. Davis – *N. racemosa* Lam. – EO: 4aa–7a–7aa–nepetalactone, caryophyllene oxide, 1,8–Cineole / linalool,  $\beta$ –Pinene,  $\alpha$ –terpineol, germacrene–D, and spathulenol
- *Nepeta cataria* L. – EO: 4aa, 7a, 7aa–nepetalactone; 3,4 $\beta$ –dihydro–4aa, 7a, 7aa–nepetalactone; 4aa, 7a, 7a $\beta$ –nepetalactone,  $\beta$ –caryophyllene, dimethyl–3,7 oxa–1 bicyclo [3,3,0] oct–2–ene, piperitone, thymol methyl ether, hexenyl benzoate and humulene oxide.

### *Perilla* L.

*Perilla frutescens* (L.) Britton, Mem. Torrey Bot. Club 5: 277 (1894) Int 들깨

*Perilla frutescens* (L.) Britton var. *frutescens*

*Perilla frutescens* (L.) Britton var. *crispa* (Thunb.) H.Deane, Rhodora 25: 40 (1923) Int 소엽

- *Perilla frutescens* (L.) Britton – EO: perillaketone (35.6%) and isoegomaketone (35.1%)
- *Perilla frutescens* var. *crispa* (vegetable crop form), *P. frutescens* var. *frutescens* (oil crop form), *Perilla citriodora*, *Perilla hirtella* and *Perilla setoyensis* – EO: Egomaketone, asaron, methyleugenol and 4,6–dimethoxy– or 4,7 – dimethoxy – 5 – (2–propenyl) – 1,3 – dioxaindan.
- *Perilla frutescens* – EO: piperitenone (36.3%) and limonene (23.7%).

### *Phlomis* L.

*Phlomis koraiensis* Nakai, Rep. Veg. Mt. Waigalbon 37 (1916) Nat; N Korea 산속단

*Phlomis maximowiczii* Regel, Trudy Imp. S.–Peterburgsk. Bot. Sada 9: 696 (1884) Nat; N Korea, S Korea 큰속단

- *Phlomis herbaventi* L. – EO: germacrene D (33.9%), hexadecanoic acid (12.9%) and  $\alpha$ –pinene (9.4%). – The major constituents of the flower – EO: hexadecanoic acid (33.1%), 6,10,14–trimethylpentadecan–2–one (16.2%), 3–methyltetradecane (6.7%) and germacrene D (6.7%).
- *Phlomis fruticosa* L. – EO (in flower): germacrene D (17.8%),  $\gamma$ –bisabolene (12.6%),  $\alpha$ –pinene (8.9%),  $\beta$ –caryophyllene (8.7%).
- *Phlomis umbrosa* Turcz., *Phlomis megalantha* Diels and *Phlomis szechuanensis* C.Y. Wu – EO: hexadecanoic acid (7.1–52.1%), *trans*–phytol (5.7–50.8%) and 9,12,15–octadecatrien–1–ol (2.2–24.8%).
- *Phlomis bruguieri* Desf. – EO: germacrene D (23.6%), 4–hydroxy–4–methyl–2–pentanone (15.0%),  $\alpha$ –pinene (6.8%) and  $\beta$ –caryophyllene (6.7%).



- *Phlomis leucophracta*, *Phlomis chimerae* and *Phlomis grandiflora* var. *grandiflora* – EO:  $\beta$ -caryophyllene (20.2%),  $\alpha$ -pinene (19.2%) and limonene (11.0%), 15-isopimaradiene, manoyl oxide and *epi*-13-manoyl oxide.
- *Phlomis olivieri* Benth. – EO: germacrene D (28.1%),  $\beta$ -caryophyllene (16.1%),  $\alpha$ -pinene (11.7%) and  $\beta$ -selinene (10.2%).
- *Phlomis fruticosa*, *P. cretica* and *P. samia* – EO:  $\alpha$ -pinene, limonene,  $\beta$ -caryophyllene, linalool, (*E*)- $\beta$ -farnesene, germacrene D, (*Z*)- $\gamma$ -bisabolene and *cis*- $\beta$ -ocimene

### ***Pogostemon* Desf.**

*Pogostemon stellatus* (Lour.) Kuntze, Revis. Gen. Pl. 2: 429 (1891) Nat; S Korea 물꼬리풀  
*Pogostemon yatabeanus* (Makino) Press, Bull. Brit. Mus. (Nat. Hist.), Bot. 10: 74 (1982) Nat;  
 S Korea 전주물꼬리풀

- *Pogostemon cablin* – EO:  $\alpha$ -guaiene (20.62%),  $\alpha$ -bulnesene (16.18%),  $\beta$ -patchoulene (12.12%), and Patchouli alcohol (11.12%),  $\beta$ -pinene (1.00%),  $\beta$ -elemene (1.23%),  $\beta$ -caryophyllene (3.89%),  $\alpha$ -patchoulene (10.52%),  $\beta$ -cubebene (1.34%) and  $\alpha$ -selinene (4.17%)

### ***Prunella* L.**

*Prunella vulgaris* L. subsp. *asiatica* (Nakai) H.Hara, Enum. Spermatophytarum Japon. 1: 220 (1948) Nat; N Korea, S Korea 꿀풀

- *Prunella vulgaris* L., *P. asiatica* Nakai and *P. hispida* Benth. – EO: hexadecanoic acid  $\text{CH}_3(\text{CH}_2)_{14}\text{COOH}$  17.16%, 51.52% and 34.85% respectively.

### ***Salvia* L.**

*Salvia japonica* Thunb., Nova Acta Regiae Soc. Sci. Upsal. 4: 40 (1783) Nat; S Korea 둥근 배암차즈기

*Salvia maximowicziana* Hemsl., J. Linn. Soc., Bot. 26: 285 (1890) Nat; S Korea, Endemic 참 배암차즈기

*Salvia miltiorrhiza* Bunge, Enum. Pl. Chin. Bor. 50 (1835) Int 단삼

*Salvia officinalis* L., Sp. Pl. 23 (1753) Int 살비아

*Salvia splendens* Sellow ex Schult., Mant. 1 (Schultes) 1: 185 (1822) Int 깨꽃

- *Salvia officinalis* – EO:  $\alpha$ - and  $\beta$ -thujones and camphor
- *Salvia lavandulaefolia* – EO: Camphor, 1,8-Cineole,  $\alpha$ -Pinene,  $\beta$ -Pinene, Thujone, Bornyl acetate, Borneol, Geraniol

- *Salvia tomentosa* – EO: 1,8-cineol 17%, caryophyllene 11%, cyclofenchene 10%. And cadinene 6%
- *Salvia miltiorrhiza* Bge. – EO:  $\beta$ -caryophyllene (12.2–31.7%),  $\beta$ -caryophyllene oxide (1.4–11.6%),  $\alpha$ -caryophyllene (4.8–10.6%), cadinadiene (7.4–29.3%), and hexadecanoic acid (3.9–18.8%)
- *Salvia virgata* Jacq. – EO:  $\beta$ -caryophyllene (46.6%), germacrene B (13.9%),  $\beta$ -caryophyllene epoxide (13.2%), spathulenol (6.4%) and germacrene D (5.7%)
- *Salvia syriaca* L. – EO: germacrene-B (34.8%), germacrene-D (29.2%),  $\alpha$ -ylangene (3.6%) and spathulenol (3.4%)
- *Salvia albicaulis* Benth. – EO: sesquiterpenes (47%), viridiflorol (25%), 1,8-cineole (9%) and limonene (9%)
- *Salvia dolomitica* – EO: monoterpenes (72%), geraniol (20%), linalyl acetate (20%) and linalool (17%)
- *Salvia caespitosa* Montbret et Aucher ex Benth. – EO: Camphor (20.71%), 1,8-cineole (16.10%) and  $\beta$ -pinene (13.54%)
- *Salvia aucheri* Benth. var. Boiss. & Heldr. – EO: 1,8-cineole (32.3%, 28.6%), camphor (18.9%, 22.8%), borneol (8.2%, 8.9%),  $\alpha$ -pinene (6.3%, 9.0%) and  $\beta$ -pinene (5.3%, 6.2%)
- *Salvia aucheri* var. *aucheri* – EO: camphor (21.1%), 1,8-cineole (20.3%), borneol (7.8%), spathulenol (6.3%) and camphene (5.3%)
- *Salvia aucheri* var. *canescens* – EO: 1,8-cineole (25.2%), camphor (17.9%), borneol (10.6%),  $\alpha$ -pinene (5.4%) and camphene (5.3%)
- *Salvia S. canariensis* L., *S. confertiflora* Pohl, *S. cfr. mexicana* L., *S. microphylla* H.B.K. (syn. *S. grahamii* Benth.) and *S. somaliensis* Vatke. – EO:  $\alpha$ -pinene,  $\beta$ -pinene, camphene, 8-3-carene and limonene (monoterpene hydrocarbons); 1,8-cineole, camphor, borneol and bornyl acetate (oxygenated monoterpenes);  $\beta$ -caryophyllene,  $\gamma$ -muurolene, germacrene B and  $\alpha$ -copaene (sesquiterpene hydrocarbons).
- *Salvia cryptantha* – EO: Camphor (19.1%), 1,8-cineole (16.4%), borneol (11.9%), viridiflorol (11.5%) and bornyl acetate (2.4%)
- *Salvia heldreichiana* – EO: linalool (9.4%),  $\alpha$ -pinene (5.6%), 1,8-cineole (5.6%), borneol (5.6%), cryptone (5.3%), linalyl acetate (4.9%),  $\alpha$ -terpineol (4.4%), camphor (3.9%), terpinen-4-ol (3.3%), trans-linalool oxide (Furanoid) (2.9%), trans-verbenol (2.2%), geranyl acetate (2.2%) and cis-linalool oxide (Furanoid) (2.1%).
- *Salvia blepharochlaena*, *S. caespitosa*, *S. divaricata*, *S. hypargeia*, *S. longipedicellata* and *S. pilifera* – EO:  $\alpha$ -Pinene,  $\beta$ -pinene, 1,8-cineole, thymol, caryophyllene oxide,  $\alpha$

–thujone

- *Salvia fruticosa* – EO: 1,8–cineole (22.7 – 64.2% of total oil),  $\alpha$ –thujone (1.0 – 19.2%)  $\beta$ –thujone (0.9 – 25.6%) and camphor (0.8 – 30.3%)
- *Salvia officinalis* L. – Cuba populations – EO: manool (14.74%), viridiflorol (13.46%),  $\alpha$ –thujone (12.95%),  $\beta$ –thujone (10.89%) and camphor (10.36%)
- *Salvia bracteata* – EO:  $\alpha$ –pinene, limonene, myrecene and  $\beta$ –pinene
- *Salvia verticillata* – EO:  $\beta$ –pinene (30.7%), *p*–cymene (23.0%) and isopropyl ester of lauric acid (16.8%)
- *Salvia verbenaca* – EO:  $\beta$ –phellandrene (30.3%), (*E*)–caryophyllene (16.1%), methyl ester of 6–octadecenoic acid (15.0%)
- *Salvia glutinosa* – EO: butyl butyryl lactate (26.7%)
- *Salvia candidissima* – EO:  $\alpha$ –pinene (11.2%) and 1,8–cineole (9.89%)

### ***Scutellaria* Baumg.**

*Scutellaria baicalensis* Georgi, Reise Russ. Reich. 1: 223 (1775) Int 황금

*Scutellaria dependens* Maxim., Mem. Acad. Imp. Sci. St.–Petersbourg Divers Savans 9: 217 (1859) Nat; N Korea, S Korea 애기골무꽃

*Scutellaria fauriei* H.Lév. & Vaniot, Repert. Spec. Nov. Regni Veg. 8: 401 (1910) Nat; N Korea, S Korea 그늘골무꽃

*Scutellaria indica* L., Sp. Pl. 600 (1753) Nat; S Korea 골무꽃

*Scutellaria insignis* Nakai, Bot. Mag. (Tokyo) 29: 2 (1915) Nat; S Korea, Endemic 광릉골무꽃

*Scutellaria laeteviolacea* Koidz., Fl. Austro–Higoensis 50 (1931) Nat; S Korea 들깨잎골무꽃

*Scutellaria moniliorhiza* Kom., Trudy Imp. S.–Peterburgsk. Bot. Sada 25: 346 (1907) Nat; N Korea 구슬골무꽃

*Scutellaria pekinensis* Maxim., Mem. Acad. Imp. Sci. St.–Petersbourg Divers Savans 9: 476 (1859) Nat; N Korea, S Korea 산골무꽃

*Scutellaria regeliana* Nakai, Bot. Mag. (Tokyo) 35: 197 (1921) Nat; N Korea 가는골무꽃

*Scutellaria strigillosa* Hemsl., J. Linn. Soc., Bot. 26: 297 (1890) Nat; N Korea, S Korea 참골무꽃

- *Scutellaria albida* ssp. *albida* – EO: linalool(52.63%)and–nerolidol(9.03%)
- *Scutellaria barbata* – EO: hexahydrofarnesylacetone (11.0%), 3,7,11,15–tetramethyl–2–hexadecen–1–ol (7.8%), menthol (7.7%) and 1–octen–3–ol (7.1%)
- *Scutellaria lateriflora* L. – EO: sesquiterpenes (78.3%)– $\beta$ –cadinene (27%), calamenene

- (15.2%),  $\beta$ -elemene (9.2%),  $\alpha$ -cubebene (4.2%), and  $\alpha$ -humulene (4.2%)
- *Scutellaria sieberia* Benth. – EO: Linalool (22.7%),  $\beta$ -caryophyllene (14.2%), (2R, 5E)-caryophyll-5-en-12-al (6.3%) and (2S, 5E)-caryophyll-5-en-12-al (14.1%)
  - *Scutellaria rupestris* Boiss. et Heldr. ssp. *adenotricha* (Boiss. et Heldr.) Greuter et Burdet – EO: linalool (38.8%), geraniol (8.1%) and  $\alpha$ -terpineol (7.1%)
  - *Scutellaria albida* L. (including four subspecies) – EO: Linalool (20% and 29%), hexadecanoic acid (13%),  $\beta$ -Caryophyllene (20%)
  - *Scutellaria californica* A. Gray – EO:  $\beta$ -Caryophyllene (56.6%), germacrene D (6.9%), methyl 2-methylbutyrate (4.9%),  $\beta$ -bourbonene (4.5%),  $\alpha$ -humulene (2.8%), methyl butyrate (2.7%), and  $\alpha$ -copaene (1.5%)
  - *Scutellaria orientalis* L. ssp. *alpina* (Boiss.) O. Schwarz – EO: sesquiterpenes (41.2%), sesquiterpene hydrocarbons (31.7%), hexahydrofarnesylacetone (11.7%), hexadecanoic acid (7.6%), caryophyllene (7.4%), caryophyllene oxide (6.8%), 4-vinylguaiacol (5.4%) and germacrene D (5.4%).
  - *Scutellaria utriculata* – EO: monoterpenes (42.2%), particularly oxygen containing monoterpenes (39.9%), linalool (20.1%), 4-vinyl guaiacol (15.5%),  $\alpha$ -terpineol (8.9%), (E)-nerolidol (8.9%) and geraniol (8.2%).
  - *Scutellaria baicalensis* Georgi – EO:  $\beta$ -Caryophyllene (22.3 – 41.5 %), germacrene D (12.4 – 27.5 %),  $\delta$ -cadinene (3.1 – 5.4 %),  $\gamma$ -muurolene (1.9 – 3.4 %),  $\gamma$ -cadinene (1.6 – 3.1 %),  $\alpha$ -humulene (1.6 – 2.6 %),  $\alpha$ -copaene (1.4 – 2.3 %),  $\alpha$ -muurolene (1.0 – 2.6 %), bicyclogermacrene (1.1 – 2.1 %) and 3-octanone (0.9 – 3.0 %), 2-(methylamino) benzaldehyde
  - *Scutellaria laeteviolacea* – EO: 1-octen-3-ol (27.72 %), germacrene D (21.67 %), and  $\beta$ -caryophyllene (9.18 %)
  - *Scutellaria diffusa* – EO: hexadecanoic acid (30%) and caryophyllene oxide (9%)
  - *Scutellaria heterophylla* – EO: Germacrene D (21%), hexadecanoic acid (16%) and  $\beta$ -caryophyllene (13%)
  - *Scutellaria salviifolia* – EO: germacrene D (40%), bicyclogermacrene (14%) and  $\beta$ -caryophyllene (11%)
  - *Scutellaria grossa* Wall ex Benth. – EO: Linalool (37.0%) and 1-octen-3-ol (32.0%)
  - *Scutellaria hastifolia* L. – EO: sesquiterpenes hydrocarbons (44.9%), caryophyllene (12.9%), germacrene D (7.7%), caryophyllene oxide (6.9%), hexadecanoic acid (6.3%) and hexahydrofarnesylacetone (5.6%)
  - *Scutellaria volubilis* – EO: sesquiterpene hydrocarbons: germacrene D (20.4%),

b-caryophyllene (17.5%),  $\alpha$ -humulene (14.7%) and b-bisabolene (5.8%)

### ***Stachys* L.**

*Stachys oblongifolia* Benth., Pl. Asiat. Rar. 1: 64 (1830) Nat; N Korea 우단석잠풀

*Stachys riederi* Cham. var. *japonica* (Miq.) H.Hara, Bot. Mag. (Tokyo) 51: 144 (1937) Nat;  
N Korea, S Korea 석잠풀

The main components (%) quantified in the essential oils of *Stachys* species with the respective percentages and the plant origine are listed in Tables 1 and 2 (sesquiterpenes and monoterpenes), respectively.

- sesquiterpene hydrocarbons (69.1%) as the main fraction
- Germacrane, cadinane and cadinane-related sesquiterpenoids, and caryophyllanes represent the most abundant skeleton types.
- *Stachys lavandulifolia* - EO: sesquiterpene hydrocarbons (31.8-66.4%), myrcene (0.0-26.2%), limonene (0.0-24.5%), germacrene D (4.2-19.3%), bicyclogermacrene (1.6-18.0%), d-cadinene (6.5-16.0%), pulegone (0.0-15.1%), (Z)-hex-3-enyl tiglate (0.0-15.1%), (E)-caryophyllene (0.0-12.9%),  $\alpha$ -zingiberene (0.2-12.2%), and spathulenol (1.6-11.1%).
- *Stachys sylvatica* - EO:  $\alpha$ -pinene,  $\beta$ -pinene and germacrene D
- *Stachys palustris* - EO: caryophyllene oxide, hexahydrofarnesyl acetone, hexadecanoic acid, (Z,Z,Z)-9,12,15-octadecatrienoic acid, (Z)-phytol, thymol, p-ethoxyacetophenone, 4-vinylguaiacole, tetradecanoic acid, (E)-caryophyllene, b-ionone and b-damascenone.
- *Stachys acerosa* - EO: cis-chrysanthenyl acetate (33.4%), 1,8-cineole (10.2%), apinene (10.1%), and linalool (9.6%)

### ***Teucrium* L.**

*Teucrium japonicum* Houtt., Nat. Hist. (Houttuyn) 9: 282 (1778) Nat; N Korea, S Korea 개곽향

*Teucrium veronicoides* Maxim., Bull. Acad. Imp. Sci. Saint-Petersbourg 23: 388 (1877) Nat;  
N Korea, S Korea 곱향

*Teucrium viscidum* Blume, Bijdr. Fl. Ned. Ind. 14: 827 (1826) Nat; S Korea 섬곱향

*Teucrium viscidum* Blume var. *miquelianum* (Maxim.) H.Hara, Bot. Mag. (Tokyo) 51: 145 (1937) Nat; S Korea 덩굴곱향

Mainly monoterpene and sesquiterpene hydrocarbons and oxygenated sesquiterpenes

- *Teucrium leucocladum* Boiss. - EO: patchouli alcohol (31.24%),  $\beta$ -pinene (12.66%),  $\alpha$

- pinene (10.99%),  $\alpha$ -cadinol (9.27%), viridiflorol (5.36%) and myrcene (5.35%)
- *Teucrium marum* subsp. *marum* – EO: Isocaryophyllene (20.24%), bisabolene (14.73%), sesquiphellandrene (11.27%), santalene (10.97%), dolichodial (9.38%) and, caryophyllene (7.18%)
- *Teucrium montanum* – EO:  $\delta$ -cadinene (17.19%),  $\beta$ -selinene (8.16%)  $\alpha$ -calacorene (4.97%), 1,6-dimethyl-4-(1-methylethyl)-naphthalene (4.91%), caryophyllene (4.35%), copaene (4.23%), torreyol (3.91%), 4-terpineol (3.90%), cadina-1,4-diene (3.39%),  $\beta$ -sesquiphellandrene (3.34%),  $\tau$ -cadinol (3.12%) and  $\gamma$ -curcumene (3.18%).
- *Teucrium parviflorum* L. – EO:  $\beta$ -caryophyllene (18.6%), germacrene D (9.2%), caryophyllene oxide (8.8%) and bicyclogermacrene (6%)
- *Teucrium polium* subsp. *capitatum* – EO:  $\alpha$ -pinene (28.8%), –pinene (7.2%) and –cymene (7.0%)
- *Teucrium polium* ssp. *aurasiacum* – EO:  $\alpha$ -cadinol (46.8%), 3 $\beta$ -hydroxy- $\alpha$ -muurolene (22.5%),  $\alpha$ -pinene (9.5%) and  $\beta$ -pinene (8.3%)
- *Teucrium polium* L. (Jordan) – EO:
- *Teucrium polium* L. subsp. *valentinum* (Schreber) Borja – EO:  $\alpha$ -pinene (15.8%), sabinene (7.2%),  $\beta$ -pinene (11.7%), trans-pinocarveol (4.3%), terpinen-4-ol (4.5%) and  $\beta$ -bisabolene (2.5%)
- *Teucrium gnaphalodes* L'Hér. – EO: sabinene (8.8%),  $\beta$ -pinene (7.1%), trans-pinocarveol(7.8%), p-cymen-8-ol(4.5%), myrtenal(5.7%)and  $\beta$ -caryophyllene(12.1%).
- Seven *Teucrium* species (*T. arduini* L., *T. botrys* L., *T. chamaedrys* L., *T. flavum* L., *T. montanum* L., *T. polium* L., *T. scordium* L.) – *T. arduini* and *T. chamaedrys* – EO:  $\beta$ -caryophyllene (24.5%; 26.9%) and germacrene D (21.9%; 22.8%) – *T. botrys* – EO:  $\beta$ -caryophyllene (20.4%),  $\alpha$ -humulene (13.9%) and (E)- $\beta$ -farnesene (17.7%). – *T. flavum* – EO:  $\alpha$ -pinene (17.5%),  $\beta$ -pinene (11.5) and  $\beta$ -bisabolene (35.0%). – *T. scordium* – EO:  $\alpha$ -pinene (17.7%) and  $\beta$ -pinene (10.0 %). – *T. montanum* – EO:  $\alpha$ -pinene (12.4%), germacrene D (15.0%) and  $\beta$ -eudesmol (10.1%). – *T. polium* – EO:  $\beta$ -pinene (19.8%), and germacrene D (11.9%)

### ***Thymus* L.**

*Thymus quinquecostatus* Celak., Oesterr. Bot. Z. 39: 263 (1889) Nat; N Korea, S Korea 백리향

- 1960 to 1989 more than 80 *Thymus* taxa from 27 different countries all over the world have been investigated for the composition of their essential oils. About 200 different compounds, mostly terpenes, have been identified. (ref. Stahl-Biskup, E. (1991). The chemical composition of Thymus oils: a review of the literature 1960–1989. *Journal of Essential Oil Research*, 3(2), 61–82.)
- The terpene phenols thymol and carvacrol represent the most important compounds in

the genus, followed by linalool, p-cymene,  $\gamma$ -terpinene, borneol, terpinen-4-ol and 1, 8-cineole.

- *Thymus quinquecostatus* (Korea) - EO: P-cymen-3ol (50.41%), P-cymen-2ol (24.06%), cymene (19.04%),  $\beta$ -linalool (1.73%), camphene (0.62%),  $\alpha$ -terpineol (0.60%), limonene (0.48%), caryophyllene oxide (0.46%),  $\gamma$ -terpinene (0.45%).
- *Thymus quinquecostatus* (Ningxia Guyuan, China) - EO: carvacrol (28.54%), 1-methyl-3-(1-methylethyl)-benzene(22.77%), thymol (11.45%) and 1-methyl-4-(1-methylethyl)-1,4-cyclohexadiene(9.78%).
- *Thymus pulegioides* - EO: carvacrol (50.5–62.6 %),  $\gamma$ -terpinene (9.8–9.9 %) and p-cymene (5.8–7.1 %).
- *Thymus glabrescens* - EO: geraniol (55.5 %), neryl acetate (11.1 %) and  $\beta$ -bisabolene (6.7 %).

### *Tripora*

*Tripora divaricata* (Maxim.) P.D.Cantino, Syst. Bot. 23: 382 (1998) Nat; N Korea, S Korea  
누린내풀

- No information available so far.



## 4. 향 시료 표준화 방법

### 가. 연구개발 내용 및 방법

#### 1) 시약

○ 추출, 분리 및 정성분석에 사용한 hexane과 diethyl ether는 HPLC grade 용으로 J. T. Baker (Phillipsburg, NJ, USA)로부터 구입하여 사용하였으며 사용된 모든 증류수는 Millipore PURE-UP (chem-science, USA)를 이용하여 필터 처리된 18 MΩ 이상의 순수한 증류수를 사용하였다. Na<sub>2</sub>SO<sub>4</sub> (Junsei, Tokyo, Japan)는 고온의 vacuum oven에서 72시간 이상 방치하여 수분을 제거하여 사용하였다.

○ 사용된 표준품은 α-pinene, camphene, caryophyllene을 sigma aldrich (purity ≥ 98%, USA)에서 구입하여 사용하였으며, 이외의 성분들은 NIST 14 MS search library에서 matching percent 85% 이상으로 나타나는 것을 확인하였다.

#### 2) 실험 기구 및 분석기기

##### ○ 추출기구

- Steam distillator : Behr KOL steam distillation unit (Clevanger type)
- Funnel shaker : 창신과학 shaker C-SKR

##### ○ GC-MS 분석법

- GC : Agilent 6890 gas chromatograph (Palo Alto, CA, USA)
- MS : Agilent 5973 mass spectrometer (Palo Alto, CA, USA)

#### 3) 자생식물의 추출

##### ① 시료의 조제

- 시료는 자생지에서 채집하였다. 생체시료는 4℃의 냉장조건에서 3일 이내 보관한 시

료를 20 g 사용하였으며, 건체시료의 경우 5 g을 분말화하여 순수하게 정제된 증류수 400 mL을 가하여 3시간 동안 추출하였다.

## ② 추출조건

－ 본 실험과정은 기존문헌을 참고하여 수행하였다 (Bull. Chem. Soc. Ethiop. 24 (2010) 67–76, J. Essent. Oil Res. 19 (2007) 449–451, Chemija 16 (2005) 47–50). 증류수를 가하여 조제된 시료는 3시간 동안 끓여서 hydrodistillator를 통하여 추출하였다. 증류 추출된 시료는 분획깔때기로 옮겨 담아 hexane 과 diethyl ether (1 : 1) 용액 100 mL을 가한 뒤 funnel shaker에서 10분 동안 300 rpm으로 분획하였다. 약 10분간 방치 후 유기용매 층을 따내어 둥근 플라스크에 옮겨 담았다. 본 과정을 2 회 반복 수행한 뒤, 둥근 플라스크에 모여진 유기용매를 rotary vaccum evaporator로 농축시켰다. 약 10 mL 정도 되었을 때  $\text{Na}_2\text{SO}_4$ 를 첨가한 뒤, 상층액을 바이알에 옮겨 담아  $-18^\circ\text{C}$ 에서 보관하였다. 전반적인 실험 과정은 Fig. 30에 나타내었다.

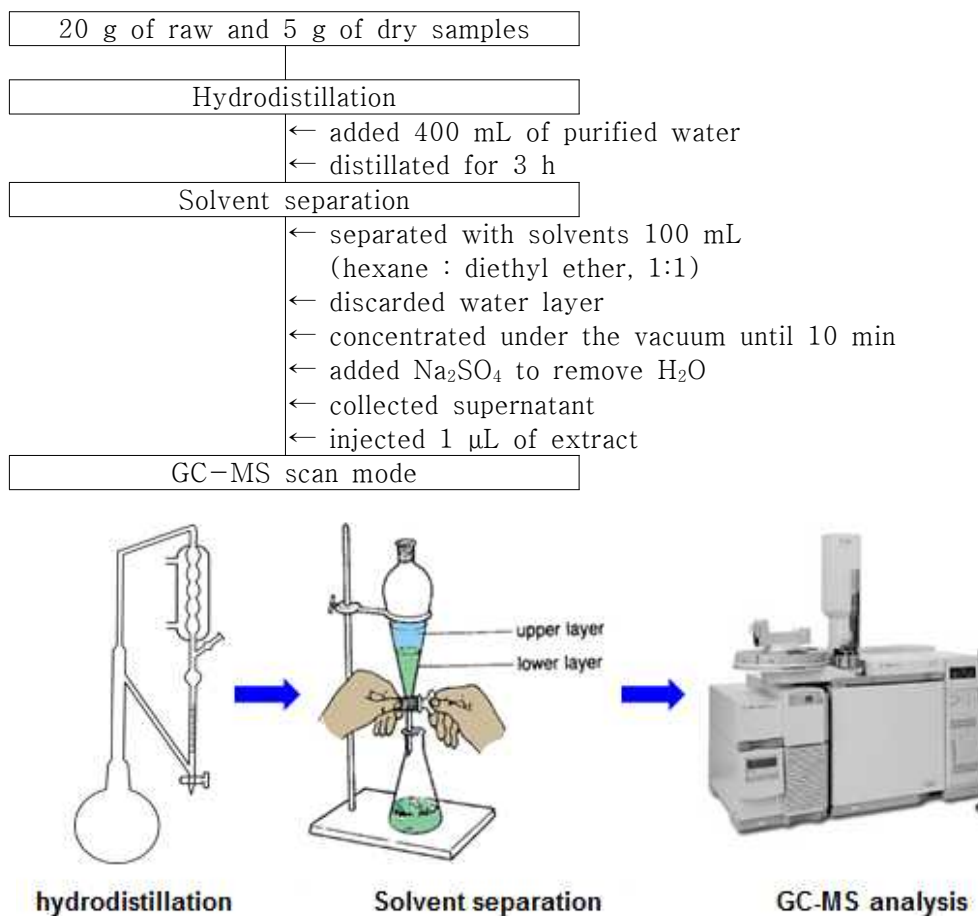


Fig. 30. Overall analytical procedure of extracts from *Pinellia* species

#### 4) GC-MS 분석법 개발

##### ① 분석조건

– 식물의 아로마 성분 정성 분리를 위한 기기로는 GC (Palo Alto, CA, USA)로서, mass spectrometry (MS) 검출기를 사용하였다. 컬럼은 5% phenyl dimethylpolysiloxane fused-silica capillary column (DB-5MS, 30 m × 0.32 mm i.d., film thickness 0.25 µm, J&W Scientific, Folsom, CA, USA)을 사용하여 분리하였으며, 시료 주입방식은 분할방식 (split mode, 10:1)을 사용하여 주입구(injection port) 온도는 270°C에서 1 µL 정하였다. 주입된 성분들은 헬륨을 이동상 기체로 하여 컬럼 내로 이동하였으며, 이동한 다 양한 성분들은 컬럼과 상호작용 및 오븐의 온도프로그래밍에 의해 분리하였다.

– 컬럼의 온도 프로그래밍은 50°C에서 3분 간의 등온조건에서 120°C까지 분당 10°C씩 상온 후에 2분 간 등온하였으며, 120°C에서 150°C까지 분당 10°C씩 상온 후 4분간 등온하였다. 150°C에서 290°C까지 10°C씩 상온하였다. 마지막으로 post oven 온도는 290°C에서 1분간 실시하였다.

– Mass detector는 Agilent 5973 mass selective detector를 사용하였으며, 이온화 방식은 electron ionization (EI)을 70 eV로 고정하고 사중극자 분리관 (quadrupole analyzer)를 거쳐 total ion chromatogram (TIC)과 mass spectrum을 얻었다. 질량조사 범위(mass scan range)는 40–450 amu로 설정하였다. 또한 ion source와 interface 온도는 각 230°C와 290°C로 설정하였다. 아로마성분을 분석하기 위한 GC/MS 조건은 Table 10에 실었다.

Table 10. GC-MS experimental conditions for the analysis of aroma components

| Gas chromatograph  |                                                                                  |
|--------------------|----------------------------------------------------------------------------------|
| Column             | DB-5MS (30 m × 0.32 mm × 0.25 µm Film)                                           |
| Flow rate          | 1.0 mL/min                                                                       |
| Injection vol.     | 1.0 µL                                                                           |
| Split ratio        | 10:1                                                                             |
| Injection temp.    | 270°C                                                                            |
| Oven temp.         | 50°C (3 min)→(10 °C/min)→120°C (2 min)→(10°C/min)→150°C (4 min)→(10°C/min)→290°C |
| Post oven temp.    | 290°C (1 min)                                                                    |
| Mass spectrometer  |                                                                                  |
| Interface temp.    | 290°C                                                                            |
| Scan range         | 40-450                                                                           |
| Ionization voltage | 70 eV                                                                            |
| Analyzer           | Quadrupole                                                                       |

## 나. 대상식물의 성분분석 결과

### 1) 자생식물의 추출

○ 자생식물로부터 아로마 성분들을 추출하기 위하여 steam distillator를 사용하여 수증기 증류 추출을 하였다. 생체시료의 경우 500 mL 부피 플라스크에 절반 이상 차오르는 양으로 사용하고자 하였으며, 그 양이 약 20 g 정도였다. 건체시료의 경우 생체시료와의 휘발성 성분 비교를 위하여 20 g 을 정밀하게 재어 건조시켰을 때의 양을 사용하였으며, 그 양은 약 5 g정도로 나타났다. 따라서 생체시료의 경우 20 g, 건체시료의 경우 5 g을 사용하여 추출하였다.

○ 용매 추출 시간과 분획 용매는 기존의 문헌들을 토대로 선정하였으며, 용매 추출 시간은 증류수가 끓을 때부터 3시간 동안 수행하였으며, 아로마 성분을 추출하기 위한 유기용매는 hexane과 diethyl ether (1:1) 용매를 사용하였다. Funnel shaker는 300 rpm으로 10 분간 2회 수행하였다. 얻어진 유기층은 rotary evaporator를 이용하여 약 10 mL까지 농축하였다. 주의할 사항은 처음 농축을 진행할 때 용매 안에 녹여있는 휘발성 성분을 응축시키기 위하여, 진공을 켜 상태로 압은 잡지 않고 5분 동안 30 rpm으로 방치하였다. 농축을 완료 한 뒤, 고온의 vacuum oven에서 수분을 제거한 무수 Na<sub>2</sub>SO<sub>4</sub>를 넣어 유기용매에 잔

존해 있는 수분을 제거하였다.

## 2) 벌깨덩굴의 아로마 성분 확인

○ 벌깨덩굴 (*Meehania urticifolia* (Miq.) Makino Bot. Mag.)의 줄기부분은 강원 북주산 (Site A, B, C)에서 수집하여 각각 생체와 건체로 만들어서 사용하였다. 벌깨덩굴의 꽃 부분은 경기도 축령산 (Site D, E), 경기도 과천 청계산 (Site F), 경상남도 창원시 진동면 (Site G)에서 수집하여 건조한 형태로 사용하였다.

### ① 생체 벌깨덩굴 줄기 추출물의 아로마 성분 확인

○ 생체 벌깨덩굴의 줄기 추출물을 확립된 GC-MS 분석방법에 적용하여 분석한 결과는 Fig. 31에 나타났다. 함량을 육안으로 쉽게 확인하기 위하여 y축의 abundance를 통일시켰다. Fig. 31의 total ion chromatograms (TICs)에서 보이듯이 Site A, B, C의 구성 성분은 큰 차이가 없이 비슷한 패턴으로 나오는 것을 확인할 수 있다. 약 21-25가지의 휘발성 성분들이 생체 벌깨덩굴 줄기 추출물에서 검출되었으며, 이들 화합물들은 NIST/Wiley MS spectra library와 대조하였을 때 85%이상의 일치율을 나타내는 것으로 명명하였다.

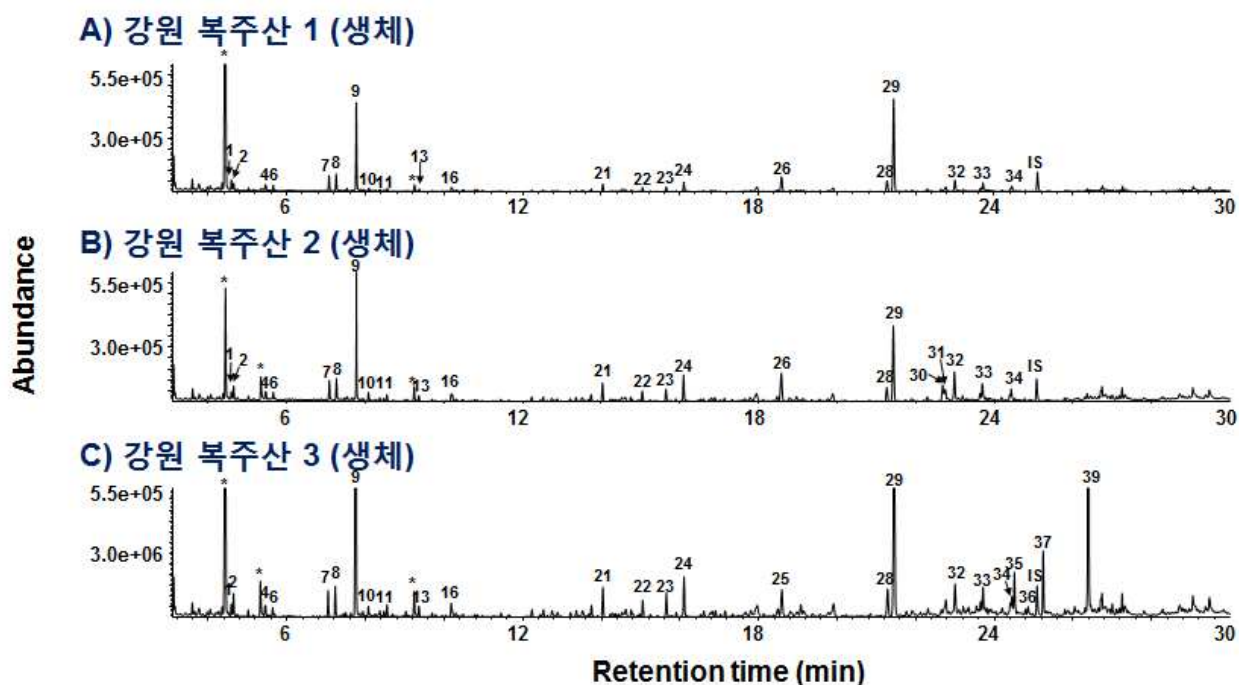


Fig. 31. Total ion chromatograms of raw *M. urticifolia* extracts

Peak identified follow as : 1.2-ethoxy butane, 2.2,4-dimethyl heptane, 3.2,4-dimethyl-1-heptane, 4.unknown1, 5.4-methyl octane, 6.2-ethoxy-3-chlorobutane, 7.1-ethylbutyl hydroperoxide, 8.methylpen tyl hydroxide, 9.1-octen-3-ol, 10.3-octanol, 11.2-methyl-5-ethyl hetane, 12.3,3,6-trimethyl hept ane, 13.2,6,10-trimethyl dodecane, 14.2-octanol acetate, 15.4,7-dimethyl undecane, 16.β-linalool, 17.2-octyl acetate, 18.ethyl octanoate, 19.2,7,10-trimethyl dodecane, 20.2,3,5-trimethyl decane, 21.2,6,10,15-tetramethyl heptadecane, 22.4,6-dimethyl dodecane, 23.1-(2-hydroxy-1-methyl ethyl)-2,2-dimethyl propyl-2-methyl propanoate, 24.3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate, 25.2,6,11,15-tetramethylhexadecane, 26.β-copaene, 27.dihydroactinidioide, 28.spathulenol, 29.1-isobutyl-4-isopropyl-3-isopropyl- 2,2-dimethyl succinate, 30.α-copaen-11-ol, 31.α-cadinol, 32.tau-muurolol, 33.2,6,10-trimethyl tetradecane, 34.2,6,10,15-tetramethyl heptadecane, 35.1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-7-oxabicyclo [4.1.0]heptane, 36.unknown2, 37.tetrakis(1-methylethylidene)-cyclobutane, 38.2-methyl-4- (2,6,6-trimethyl-1-cyclohexene-1-yl)-2-butanal, 39.unknown3, 40.7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, 41.butyl phthalate, \*. solvent peaks.

○ 강원 복주산에서 채집한 생체시료 A와 B 시료를 비교하였을 때, B 시료에서 추가로 3개의 peak이 검출되었다. peak 30과 31번은 각각  $\alpha$ -copaen-11-ol과 31. $\alpha$ -cadinol 성분인 것으로 확인하였다. 이와 더불어 강원 복주산에 채집한 C의 경우 다른 복주산 시료와 비교하였을 때 peak 25, 35, 36, 37, 39이 추가로 검출되었으며, peak 39의 경우 C시료에서 높은 함량을 나타내는 것으로 확인하였다. 각 peak들은 순서대로 25번 2,6,11,15-tetramethylhexadecane, 35번 1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-7-oxabicyclo [4.1.0]heptane, 36번 unknown2, 37번 tetrakis (1-methylethylidene)-cyclobutane, 39번 unknown3으로 확인하였다.

○ 주요성분으로는 peak 9번의 1-octen-3-ol, 26번의  $\beta$ -copaene, 28번의 spathulenol 29번의 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate가 나타나는 것을 확인할 수 있었다.

## ② 건체 벌깨덩굴 줄기 추출물의 아로마 성분 확인

○ 건체 벌깨덩굴의 줄기 추출물을 GC-MS 분석방법에 적용하여 분석한 결과를 Fig. 32에 나타냈다. 생체 벌깨덩굴 추출물과 마찬가지로, 함량을 육안으로 쉽게 확인하기 위하여 y축의 abundance를 통일시켰다. Fig. 32의 TICs에서 보이듯이 건체 Site A, B, C의 구성 성분은 큰 차이가 없이 비슷한 패턴으로 나오는 것을 확인할 수 있다. 생체시료에 비해 전체적으로 양이 줄어든 것으로 보여졌으며, 약 22-23가지의 휘발성 성분들이 건체 벌깨덩굴 줄기 추출물에서 검출되었으며, 이들 화합물들은 NIST/Wiley MS spectra library와 대조하였을 때 85%이상의 일치율을 나타내는 것으로 명명하였다.

○ 생체시료를 건조시킨 시료의 경우 생체시료에 비하여 상대적으로 abundance가 높아졌다. A와 B를 비교하였을 때, B 시료에서 ethyl octanoate이 추가로 검출되었다. 이와 더불어 시료 C의 경우 다른 건체시료와 비교하였을 때 peak 40이 추가로 검출되었으며, MS library를 토대로 7,9-ditertbutyl -1-oxaspiro (4,5) deca-6,9-diene-2,8-dione로 확인하였다. 생체에서 높은 함량을 나타내었던 39번의 경우 다른 성분들의 함량이 높아짐에 따라 상대적으로 작게 나타나는 것으로 보여졌다.

○ 주요성분으로는 peak 29번의 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate가 나타나는 것을 확인할 수 있었다.

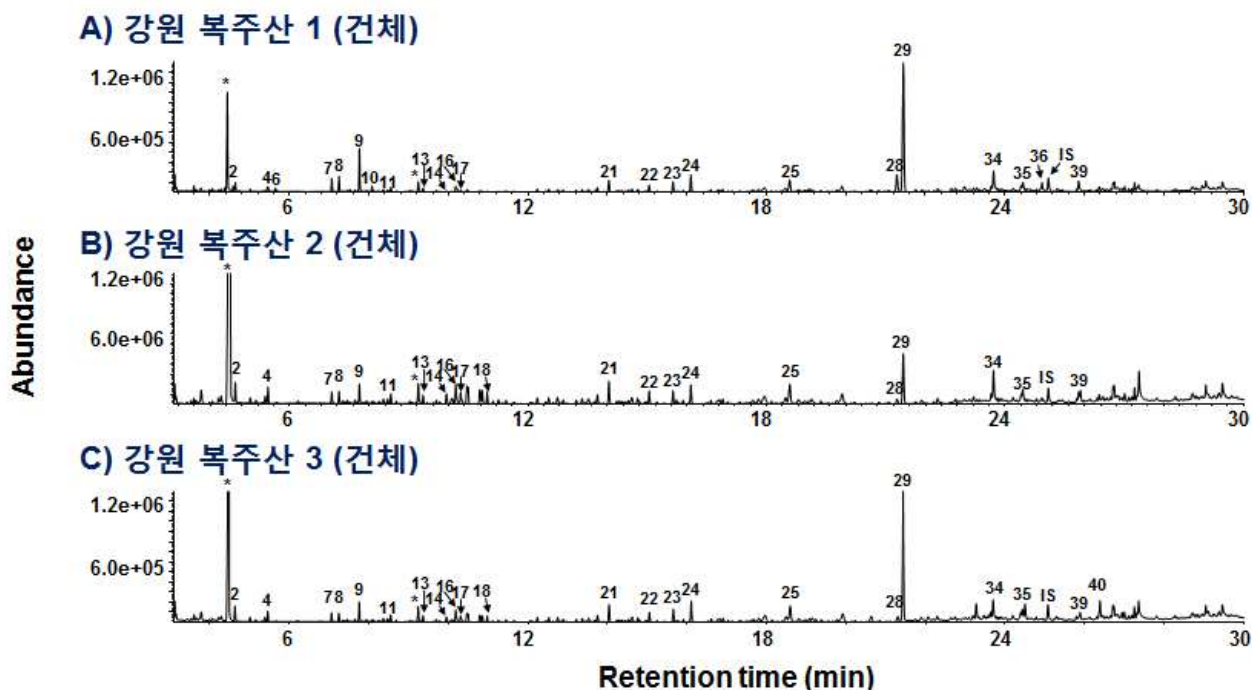


Fig. 32. Total ion chromatograms of dry *M. urticifolia* extracts

Peak identified follow as : 1.2-ethoxy butane, 2.2,4-dimethyl heptane, 3.2,4-dimethyl-1-heptane, 4.unknown1, 5.4-methyl octane, 6.2-ethoxy-3-chlorobutane, 7.1-ethylbutyl hydroperoxide, 8.methylpentyl hydroxide, 9.1-octen-3-ol, 10.3-octanol, 11.2-methyl-5-ethyl hetane, 12.3,3,6-trimethyl heptane, 13.2,6,10-trimethyl dodecane, 14.2-octanol acetate, 15.4,7-dimethyl undecane, 16.β-linalool, 17.2-octyl acetate, 18.ethyl octanoate, 19.2,7,10-trimethyl dodecane, 20.2,3,5-trimethyl decane, 21.2,6,10,15-tetramethyl heptadecane, 22.4,6-dimethyl dodecane, 23.1-(2-hydroxy-1-methyl ethyl)-2,2-dimethylpropyl-2-methyl propanoate, 24.3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate, 25.2,6,11,15-tetramethylhexadecane, 26.β-copaene, 27.dihydroactinidioid, 28.spathulenol, 29.1-isobutyl-4-isopropyl-3-isopropyl- 2,2-dimethyl succinate, 30.α-copaen-11-ol, 31.α-cadinol, 32.τ-murolol, 33.2,6,10-trimethyl tetradecane, 34.2,6,10,15-tetramethyl heptadecane, 35.1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-7-oxabicyclo [4.1.0]heptane, 36.unknown2, 37.tetrakis(1-methylethylidene)-cyclobutane, 38.2-methyl-4- (2,6,6-trimethyl-1-cyclohexene-1-yl)-2-butanol, 39.unknown3, 40.7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, 41.butyl phthalate, \*. solvent peaks.

### ③ 건체 벌개데굴 꽃 추출물의 아로마 성분 확인

○ 벌개데굴의 꽃 부분을 건조시킨 추출물을 확립된 GC-MS 분석방법에 적용하여 분석한 결과를 Fig. 33에 나타냈다. 함량을 육안으로 쉽게 확인하기 위하여 y축의 abundance를 통일시켰다. Fig. 33의 TICs에서 보이듯이 Site D, E, F, G의 구성 성분은 큰 차이가 없이 비슷한 패턴으로 나오는 것을 확인할 수 있다. 약 26가지의 휘발성 성분들이 건체 벌개데굴 꽃 추출물에서 검출되었으며, 화합물들은 NIST MS spectra library와 대조하였을 때 85%이상의 일치율을 나타내는 것으로 명명하였다.



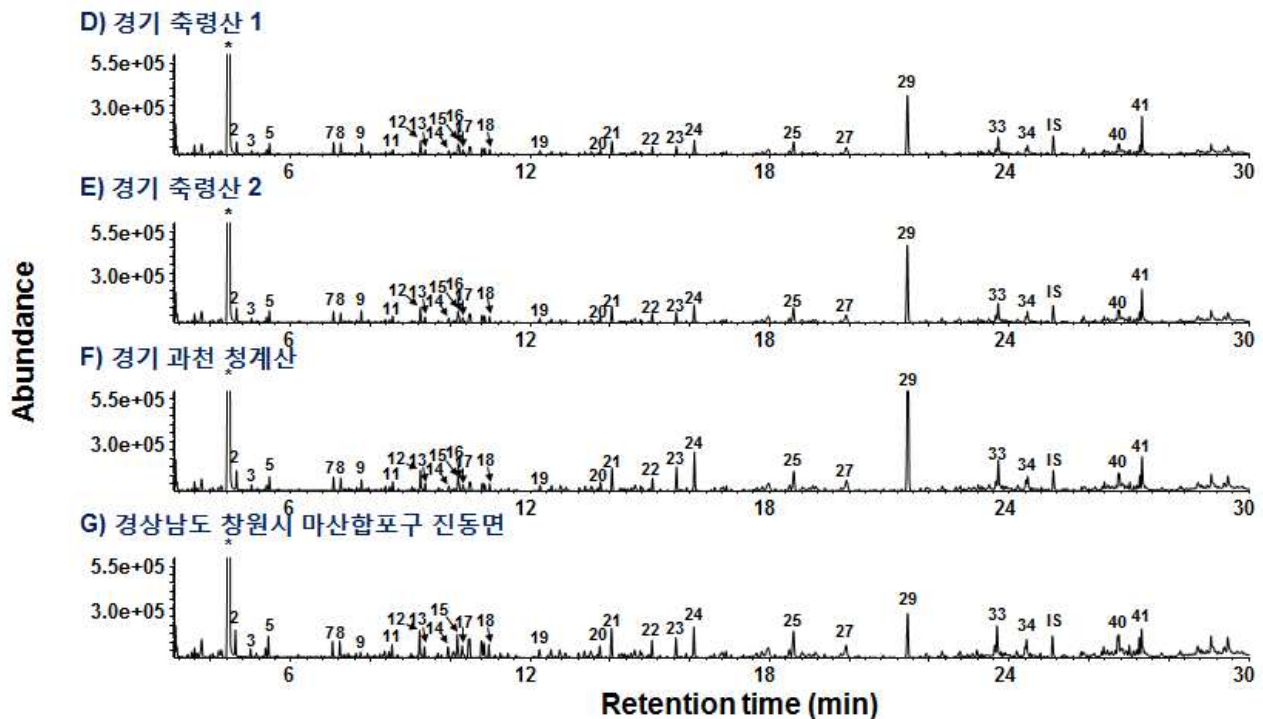


Fig. 33. Total ion chromatograms of *M. urticifolia* dry flower extracts

Peak identified follow as : 1.2-ethoxy butane, 2.2,4-dimethyl heptane, 3.2,4-dimethyl-1-heptane, 4.unknown1, 5.4-methyl octane, 6.2-ethoxy-3-chlorobutane, 7.1-ethylbutyl hydroperoxide, 8.methylpentyl hydroxide, 9.1-octen-3-ol, 10.3-octanol, 11.2-methyl-5-ethyl hetane, 12.3,3,6-trimethyl heptane, 13.2,6,10-trimethyl dodecane, 14.2-octanol acetate, 15.4,7-dimethyl undecane, 16.β-linalool, 17.2-octyl acetate, 18.ethyl octanoate, 19.2,7,10-trimethyl dodecane, 20.2,3,5-trimethyl decane, 21.2,6,10,15-tetramethyl heptadecane, 22.4,6-dimethyl dodecane, 23.1-(2-hydroxy-1-methyl ethyl)-2,2-dimethyl propyl-2-methyl propanoate, 24.3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate, 25.2,6,11,15-tetramethylhexadecane, 26.β-copaene, 27.dihydroactinidioides, 28.spathulenol, 29.1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate, 30.α-copaen-11-ol, 31.α-cadinol, 32.τ-murolol, 33.2,6,10-trimethyl tetradecane, 34.2,6,10,15-tetramethyl heptadecane, 35.1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-7-oxabicyclo [4.1.0]heptane, 36.unknown2, 37.tetrakis(1-methylethylidene)-cyclobutane, 38.2-methyl-4-(2,6,6-trimethyl-1-cyclohexene-1-yl)-2-butanal, 39.unknown3, 40.7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, 41.butyl phthalate, \*. solvent peaks.

○ 경기 축령산에서 채집하여 건조시킨 건체시료의 경우 줄기 부분과 비교하였을 때, 4 가지 성분이 추가로 검출되었다. 각각의 성분들은 MS library를 토대로 19번 2,7,10-trimethyl dodecane, 27번 dihydroactinidioides, 33. 2,6,10-trimethyl tetradecane, 41 번 butyl phthalate 인 것으로 확인하였다. 대부분의 화합물들이 alkane류 인 것으로 보여 졌다. 주성분은 줄기부분과 마찬가지로 29번 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate인 것으로 나타났다.

#### ④ 벌깨덩굴 추출물의 비교

○ 생체 및 전체 벌깨덩굴 줄기 추출물과 전체 벌깨덩굴 꽃 추출물에서 검출된 Total ion chromatograms를 비교한 결과를 Fig. 34 에 수록하였다. 총 41가지의 성분들이 GC-MS scan mode에서 관측되었다. 검출된 화합물은 saturated alkane, alcohol류, terpene 류 등이 나타나는 것을 확인하였으며, MS library와 mass spectra를 대조하여 확인하였다. 벌깨덩굴 추출물로부터 검출된 다양한 화학적 구성성분들의 머무름 시간과 특성이온을 Table 2에 나타내었다.

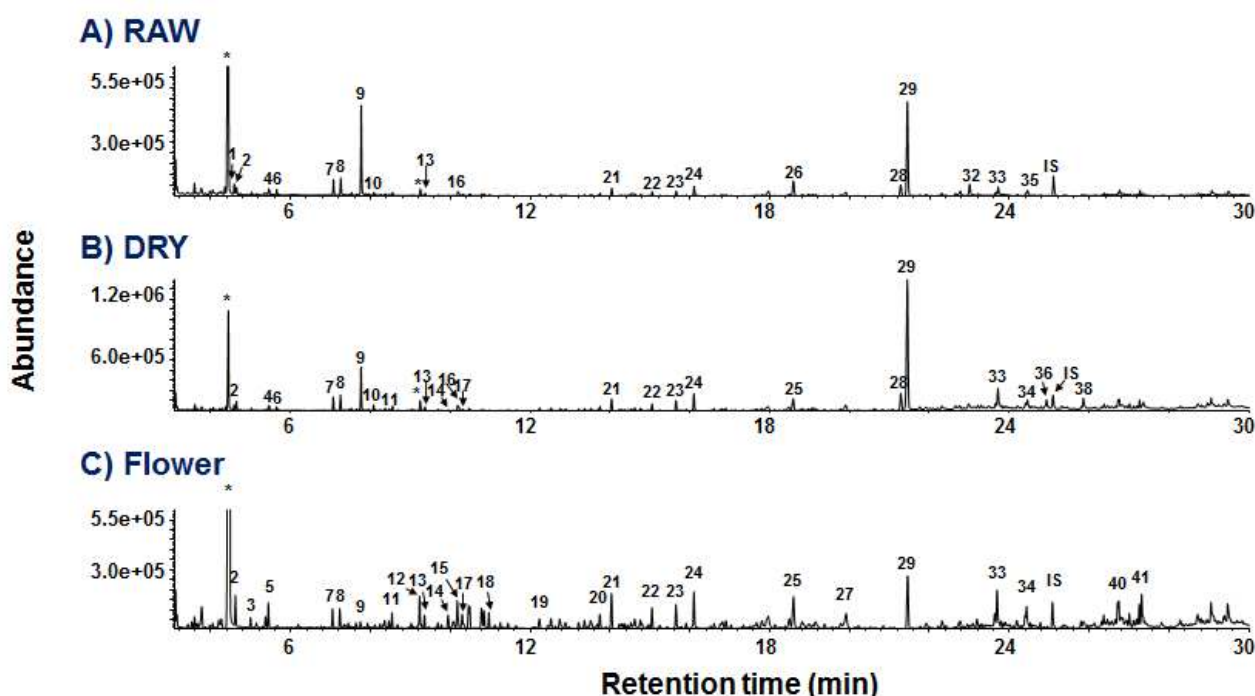


Fig. 34. Comparison of *M. urticifolia* extracts

Peak identified follow as : 1.2-ethoxy butane, 2.2,4-dimethyl heptane, 3.2,4-dimethyl-1-heptane, 4.unknown1, 5.4-methyl octane, 6.2-ethoxy-3-chlorobutane, 7.1-ethylbutyl hydroperoxide, 8.methylpentyl hydroxide, 9.1-octen-3-ol, 10.3-octanol, 11.2-methyl-5-ethyl hetane, 12.3,3,6-trimethyl heptane, 13.2,6,10-trimethyl dodecane, 14.2-octanol acetate, 15.4,7-dimethyl undecane, 16.β-linalool, 17.2-octyl acetate, 18.ethyl octanoate, 19.2,7,10-trimethyl dodecane, 20.2,3,5-trimethyl decane, 21.2,6,10,15-tetramethyl heptadecane, 22.4,6-dimethyl dodecane, 23.1-(2-hydroxy-1-methyl ethyl)-2,2-dimethyl propyl-2-methyl propanoate, 24.3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate, 25.2,6,11,15-tetramethylhexadecane, 26.β-copaene, 27.dihydroactinidioides, 28.spathulenol, 29.1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate, 30.α-copaen-11-ol, 31.α-cadinol, 32.tau-murolol, 33.2,6,10-trimethyl tetradecane, 34.2,6,10,15-tetramethyl heptadecane, 35.1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-7-oxabicyclo [4.1.0]heptane, 36.unknown2, 37.tetrakis(1-methylethylidene)-cyclobutane, 38.2-methyl-4-(2,6,6-trimethyl-1-cyclohexene-1-yl)-2-butanal, 39.unknown3, 40.7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, 41.butyl phthalate, \*. solvent peaks.

Table 11.. Retention time and characteristic ions of *M. urticifolia* extracts

| No. | R.T.  | compound                   | M.W. | Characteristic ion, <i>m/z</i> (relative abundance,%)                                         | R..I. | Detection |     |      |
|-----|-------|----------------------------|------|-----------------------------------------------------------------------------------------------|-------|-----------|-----|------|
|     |       |                            |      |                                                                                               |       | raw       | dry | flo. |
| 1   | 4.57  | 2-ethoxy butane            | 102  | 45(100), 73(63), 57(7), 89(2)                                                                 | 821   | ○         |     |      |
| 2   | 4.63  | 2,4-dimethyl heptane       | 128  | 43(100), 85(76), 57(42), 71(39), 128(3)                                                       | 825   | ○         | ●   | ◎    |
| 3   | 5.01  | 2,4-dimethyl-1-heptene     | 126  | 70(100), 43(99), 55(59), 83(31), 126(21),                                                     | 846   |           |     | ◎    |
| 4   | 5.44  | unknown1                   | –    | 73(100), 45(97), 55(7), 91(4), 84(2)                                                          | 868   | ○         | ●   |      |
| 5   | 5.46  | 4-methyl octane            | 128  | 43(100), 85(52), 71(49), 57(35), 128(6), 98(5)                                                | 869   |           |     | ◎    |
| 6   | 5.64  | 2-ethoxy-3-chlorobutane    | 136  | 73(100), 45(99), 55(8), 43(10), 90(3)                                                         | 877   | ○         | ●   |      |
| 7   | 7.07  | 1-ethylbutyl hydroperoxide | 118  | 43(100), 57(37), 41(34), 85(33), 73(15)                                                       | 950   | ○         | ●   | ◎    |
| 8   | 7.25  | methylpentyl hydroxide     | 118  | 43(100) 85(35), 57(21), 69(8), 100(1)                                                         | 959   | ○         | ●   | ◎    |
| 9   | 7.76  | 1-octen-3-ol               | 128  | 57(100), 43(19), 72(16), 55(11), 85(9), 99(5), 68(5), 81(5)                                   | 984   | ○         | ●   | ◎    |
| 10  | 8.07  | 3-octanol                  | 130  | 59(100), 55(62), 83(59), 41(35), 101(28)                                                      | 998   | ○         | ●   |      |
| 11  | 8.55  | 2-methyl-5-ethyl hetane    | 142  | 71(100), 43(78), 57(71), 85(18), 113(17), 97(3)                                               | 1023  | ○         | ●   | ◎    |
| 12  | 9.24  | 3,3,6-trimethyl heptane    | 142  | 71(100), 43(93), 57(86), 85(68), 113(17), 127(17), 99(7)                                      | 1057  |           |     | ◎    |
| 13  | 9.36  | 2,6,10-trimethyl dodecane  | 212  | 71(100), 57(89), 43(83), 85(53), 113(14), 127(8), 99(4)                                       | 1063  | ○         | ●   | ◎    |
| 14  | 9.95  | 2-octanol acetate          | 172  | 43(100), 87(51), 55(22), 112(14), 55(22), 69(10), 100(3)                                      | 1089  |           | ●   | ◎    |
| 15  | 10.18 | 4,7-dimethyl undecane      | 184  | 43(100), 57(76), 85(45), 70(27), 113(13), 127(9), 99(7)                                       | 1099  |           |     | ◎    |
| 16  | 10.21 | β-linalool                 | 154  | 93(100), 71(94), 41(74), 43(70), 55(68), 69(53), 67(34),<br>80(44), 121(31), 109(11), 105(10) | 1101  | ○         | ●   | ◎    |
| 17  | 10.31 | 2-octyl acetate            | 172  | 43(100), 72(40), 87(40), 57(28), 112(16), 97(4), 127(4)                                       | 1106  |           | ●   | ◎    |
| 18  | 10.98 | ethyl octanoate            | 172  | 88(100), 115(27), 127(24), 57(24), 70(24), 43(24), 101(3)                                     | 1141  |           | ●   | ◎    |

R.T. : retention time, M.W. : molecular weight, R.I. : retention index

Table 11. Continued

| No. | R.T.  | compound                                                                    | M.W. | Characteristic ion, $m/z$ (relative abundance,%)                                                          | R..I. | Detection |     |      |
|-----|-------|-----------------------------------------------------------------------------|------|-----------------------------------------------------------------------------------------------------------|-------|-----------|-----|------|
|     |       |                                                                             |      |                                                                                                           |       | raw       | dry | flo. |
| 19  | 12.24 | 2,7,10-trimethyl dodecane                                                   | 212  | 57(100), 43(67), 71(62), 85(46), 99(15), 121(14), 136(14),                                                | 1200  |           |     | ☉    |
| 20  | 13.75 | 2,3,5-trimethyl decane                                                      | 184  | 43(100), 85(99), 57(76), 71(68), 99(21), 141(14), 113(11),<br>155(10), 127(7)                             | 1266  |           |     | ☉    |
| 21  | 14.04 | 2,6,10,15-tetramethyl heptadecane                                           | 296  | 71(100), 57(91), 85(73), 43(68), 113(14), 99(13), 127(11),<br>155(6), 169(2),                             | 1277  | ○         | ●   | ☉    |
| 22  | 15.05 | 4,6-dimethyl dodecane                                                       | 198  | 71(100), 57(93), 43(67), 85(66), 127(16), 99(15), 113(13),<br>155(8), 141(3)                              | 1322  | ○         | ●   | ☉    |
| 23  | 15.65 | 1-(2-hydroxy-1-methyl<br>ethyl)-2,2-dimethyl propyl<br>-2-methyl propanoate | 216  | 71(100), 43(64), 83(39), 56(30), 98(26), 143(6), 173(6),<br>111(5), 127(2)                                | 1353  | ○         | ●   | ☉    |
| 24  | 16.1  | 3-hydro-2,4,4-trimethyl pentyl<br>2-methylpropanoate                        | 216  | 71(100), 89(74), 56(70), 43(55), 173(16), 143(9), 161(2),                                                 | 1376  | ○         | ●   | ☉    |
| 25  | 18.58 | 2,6,11,15-tetramethylhexadecane                                             | 282  | 71(100), 57(93), 85(80), 43(63), 99(26), 113(21), 127(11),<br>155(11), 141(4), 169(4), 197(2)             | 1485  |           | ●   | ☉    |
| 26  | 18.6  | $\beta$ -copaene                                                            | 204  | 161(100), 105(57), 91(49), 81(34), 119(31), 41(26),<br>133(16), 204(15), 55(14), 67(13), 147(6), 189(2)   | 1584  | ○         |     |      |
| 27  | 19.91 | dihydroactinidioidide                                                       | 180  | 71(100), 57(83), 43(72), 85(64), 111(40), 99(23), 169(14),<br>137(14), 127(13), 155(10), 180(9)           | 1536  |           |     | ☉    |
| 28  | 21.29 | spathulenol                                                                 | 220  | 91(100), 105(81), 159(81), 43(78), 119(73), 79(61),<br>131(61), 205(58), 147(44), 67(39), 187(30), 55(28) | 1592  | ○         | ●   |      |
| 29  | 21.44 | 1-isobutyl-4-isopropyl-3-isopropyl<br>1-2,2-dimethyl succinate              | 286  | 71(100), 43(38), 111(7), 159(7), 55(7), 243(5), 83(5),<br>93(5), 173(3), 121(2), 143(2)                   | 1589  | ○         | ●   | ☉    |
| 30  | 22.67 | $\alpha$ -copaen-11-ol                                                      | 220  | 59(100), 91(68), 162(65), 147(62), 105(52), 43(49), 79(45),<br>119(33), 133(25)                           | 1647  | ○         |     |      |

R.T. : retention time, M.W. : molecular weight, R.I. : retention index

Table 11. Continued

| No. | R.T.  | compound                                                                    | M.W. | Characteristic ion, $m/z$ (relative abundance,%)                                                                                              | R..I. | Detection |     |      |
|-----|-------|-----------------------------------------------------------------------------|------|-----------------------------------------------------------------------------------------------------------------------------------------------|-------|-----------|-----|------|
|     |       |                                                                             |      |                                                                                                                                               |       | raw       | dry | flo. |
| 31  | 22.76 | $\alpha$ -cadinol                                                           | 222  | 57(100), 95(79), 71(63), 121(58), 204(50), 43(45), 164(39), 85(26), 109(18), 179(11), 222(8)                                                  | 1651  | ○         |     |      |
| 32  | 23    | tau-muurolol                                                                | 222  | 95(100), 121(83), 16(62), 43(59), 204(51), 105(45), 79(35), 91(95), 109(35), 164(30), 71(24), 55(19), 137(17), 189(9), 149(7), 179(3), 222(3) | 1666  | ○         |     |      |
| 33  | 23.71 | 2,6,10-trimethyl tetradecane                                                | 240  | 71(100), 57(81), 85(73), 43(62), 99(30), 113(25), 127(16), 167(11), 155(9), 141(7), 177(3), 197(3), 211(2)                                    | 1697  | ○         | ●   | ◎    |
| 34  | 24.45 | 2,6,10,15-tetramethyl heptadecane                                           | 296  | 71(100), 57(72), 43(68), 85(61), 99(39), 113(35), 127(18), 155(16), 169(12), 144(7), 197(7), 211(4)                                           | 1745  | ○         | ●   | ◎    |
| 35  | 24.51 | 1-(1,3-dimethyl-1,3-butadienyl)-2, 2,6-trimethyl-7-oxabicyclo[4.1.0]heptane | 220  | 137(100), 110(52), 95(36), 41(31), 55(18), 82(18), 67(17), 123(8), 220(7), 149(4), 177(3), 205(3) 163(1)                                      | 1748  | ○         |     |      |
| 36  | 24.99 | unknown2                                                                    | –    | 81(100), 95(60), 41(35), 123(44), 55(39), 147(33), 137(32), 67(31), 109(29), 193(26), 190(17), 175(13)                                        | 1779  | ○         | ●   |      |
| 37  | 25.25 | tetrakis(1-methylethylidene)-cyclobutane                                    | 216  | 216(100), 201(66), 159(45), 173(40), 145(31), 91(29), 115(22), 128(20), 77(19), 105(18), 41(11), 65(8), 187(9), 53(6)                         | 1795  | ○         |     |      |
| 38  | 25.85 | 2-methyl-4-(2,6,6-trimethyl-1-cyclohexene-1-yl)-2-butanal                   | 206  | 191(100), 123(96), 41(95), 79(88), 91(83), 151(83), 55(69), 107(59), 163(54), 131(40), 121(45), 145(37), 139(30), 173(19), 176(11), 208(3)    | 1844  |           | ●   |      |
| 39  | 26.41 | unknown3                                                                    | –    | 165(100), 109(48), 137(32), 55(24), 41(17), 67(12), 95(11), 82(8), 125(2)                                                                     | 1882  | ○         | ●   |      |
| 40  | 26.72 | 7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione                   | 276  | 71(100), 85(78), 43(61), 57(59), 99(35), 113(26), 127(16), 155(16), 141(10), 169(7), 197(4), 211(3), 183(2), 239(2)                           | 1906  |           |     | ◎    |
| 41  | 27.31 | butyl phthalate                                                             | 278  | 149(100), 223(5), 104(4), 205(4), 41(4), 76(3), 93(3), 121(2), 278(1)                                                                         | 1957  |           |     | ◎    |

R.T. : retention time, M.W. : molecular weight, R.I. : retention index

○ 생체 및 건체 벌개똥굴 줄기와 건조된 꽃 추출물에서 TICs에 검출된 화합물은 총 41가지가 나타난 것으로 확인하였다. 주로 alkane류, terpene류, alcohol류의 화합물들이 나타났다. TICs에서 검출된 성분들을 토대로 벌개똥굴에서 주요 성분 몇 가지 화합물에 한하여 질량 스펙트럼을 수록하였다(Fig. 35).

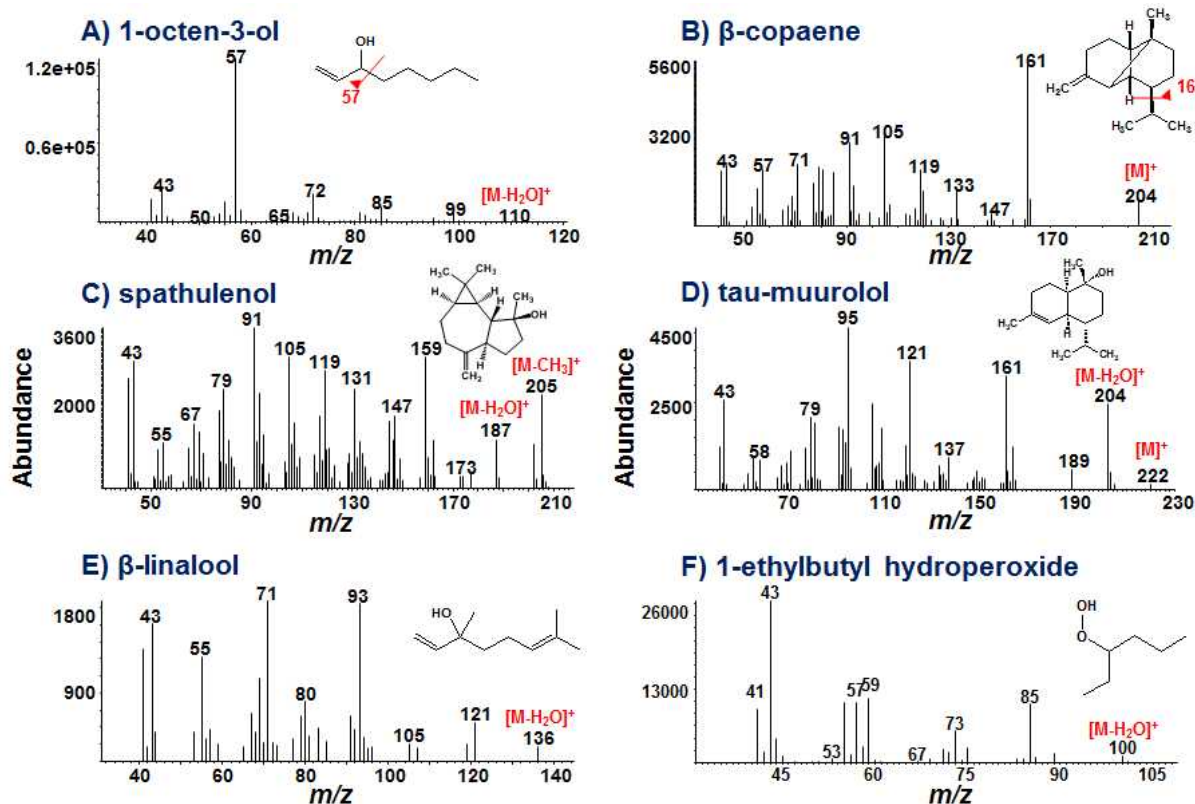


Fig. 35. Mass spectra of major compounds in *M. urticifolia* extracts

○ 벌개똥굴 추출물에서 검출된 성분들의 함량을 확인하기 위해, phenanthrene d-10을 내부표준물질로 사용하여 area ratio로 계산하였다. 결과는 Fig. 36에 막대그래프로 나타내었다.

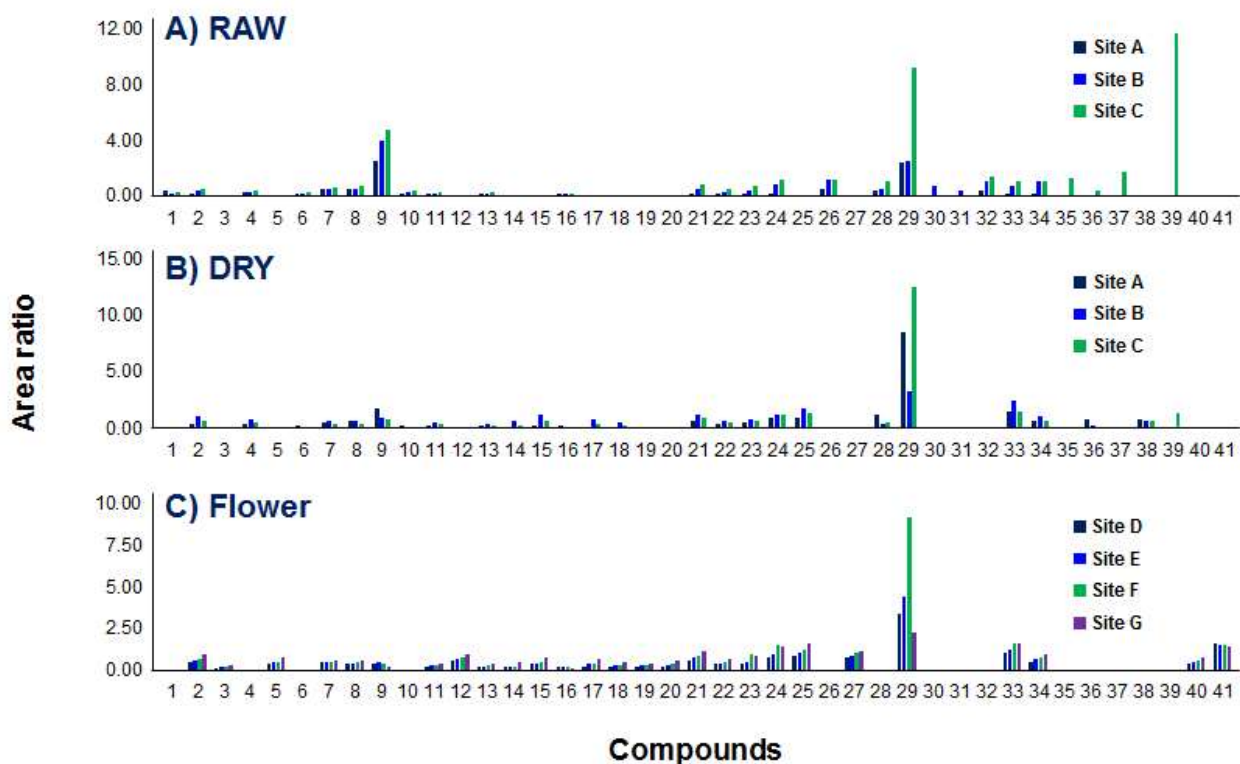


Fig. 36. Peak area ratio of compounds in *M. urticifolia* detected by GC-MS

Peak identified follow as : 1.2-ethoxy butane, 2.2,4-dimethyl heptane, 3.2,4-dimethyl-1-heptane, 4.unknown1, 5.4-methyl octane, 6.2-ethoxy-3-chlorobutane, 7.1-ethylbutyl hydroperoxide, 8.methylpentyl hydroxide, 9.1-octen-3-ol, 10.3-octanol, 11.2-methyl-5-ethyl hetane, 12.3,3,6-trimethyl heptane, 13.2,6,10-trimethyl dodecane, 14.2-octanol acetate, 15.4,7-dimethyl undecane, 16.β-linalool, 17.2-octyl acetate, 18.ethyl octanoate, 19.2,7,10-trimethyl dodecane, 20.2,3,5-trimethyl decane, 21.2,6,10,15-tetramethyl heptadecane, 22.4,6-dimethyl dodecane, 23.1-(2-hydroxy-1-methyl ethyl)-2,2-dimethyl propyl-2-methyl propanoate, 24.3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate, 25.2,6,11,15-tetramethylhexadecane, 26.β-copaene, 27.dihydroactinidioid, 28.spathulenol, 29.1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate, 30.α-copaen-11-ol, 31.α-cadinol, 32.tau-muurolool, 33.2,6,10-trimethyl tetradecane, 34.2,6,10,15-tetramethyl heptadecane, 35.1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-7-oxabicyclo [4.1.0]heptane, 36.unknown2, 37.tetrakis(1-methylethylidene)-cyclobutane, 38.2-methyl-4-(2,6,6-trimethyl-1-cyclohexene-1-yl)-2-butanal, 39.unknown3, 40.7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, 41.butyl phthalate, \*. solvent peaks.

○ 생체 줄기 시료의 경우 세 가지 다른 산지 시료에서 9번 1-octen-3-ol, 26번 β-copaene, 29. 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate, 32번 tau-muurolool 33번 2,6,10-trimethyl tetradecane과 같은 성분들이 공통적으로 검출되는 것을 확인할 수 있었다. 그 중 특히 site C에서 모든 성분들의 함량이 높게 나타나는 것을



확인하였다. 39번 unknown3 시료의 경우 C시료에서만 높은 함량을 나타내는 것으로 확인하였다.

○ 전체 줄기 시료의 경우 생체 줄기 시료의 주성분으로 나타났던, 9번 1-octen-3-ol과 29. 1-isobutyl-4-isopropyl- 3-isopropyl-2,2-dimethyl succinate의 경우 그 함량이 줄어들었으며, 26번  $\beta$ -copaene, 32번 tau-muurolol은 검출되지 않았다. 두 성분은 휘발성 성분으로써 미량으로 함유되어 있는 것으로 보여지며, 건조과정에서 소실되었을 것이라 사료된다. 생체 시료 C에서 가장 많은 함량을 가지는 것으로 나타났던 unknown3의 경우도 건조과정을 거치니 급격히 적어든 것을 확인할 수 있었다.

○ 벌깨덩굴의 꽃부분을 건조시킨 시료에서는 산지별 차이가 나타나지 않았다. 또한 생체 및 전체 줄기 시료와 마찬가지로 29. 1-isobutyl-4-isopropyl- 3-isopropyl-2,2-dimethyl succinate가 높은 함량을 가지는 것으로 나타났으며, 특히 site F의 경우 본 화합물의 함량이 가장 많이 함유되어있는 것을 확인할 수 있다. 생체 및 전체 벌깨덩굴의 줄기 부분에서는 검출되지 않았던 40번 7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione과 41번 butyl phthalate 화합물은 전체 꽃 부분에서만 나타났다.

○ TIC에서 검출된 화합물들을 토대로 대표적인 성분들을 선정하여 화합물의 % 함량을 구하였다. % 함량을 구할 때 사용하였던 식은 아래에 나타내었으며 결과는 Table 12에 기재하였다.

$$\% \text{ 함량} = \frac{\text{Compounds of peak area}}{\text{Sum of total compounds peak area}} \times 100$$



Table 12. Amounts of volatile compounds in *M. urticifolia*

| No. | compounds                                                 | % [compounds of area/ sum of total compounds x 100] |             |             |             |             |             |             |             |             |             |
|-----|-----------------------------------------------------------|-----------------------------------------------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|     |                                                           | Raw                                                 |             |             | Dry         |             |             | Flower      |             |             |             |
|     |                                                           | A                                                   | B           | C           | A           | B           | C           | D           | E           | F           | G           |
| 1   | 1-ethylbutyl hydroperoxide                                | 4.93                                                | 2.81        | 1.50        | 2.58        | 2.66        | 1.68        | 2.86        | 2.48        | 1.70        | 2.72        |
| 2   | 1-octen-3-ol                                              | 27.37                                               | 23.67       | 11.29       | 7.96        | 4.07        | 3.35        | 2.65        | 2.66        | 1.42        | 0.99        |
| 3   | 4,6-dimethyl dodecane                                     | 0.89                                                | 1.68        | 1.10        | 1.54        | 3.18        | 1.99        | 2.21        | 2.22        | 1.89        | 3.00        |
| 4   | $\beta$ -copaene                                          | <b>5.29</b>                                         | <b>6.84</b> | <b>2.77</b> | -           | -           | -           | -           | -           | -           | -           |
| 5   | dihydroactinid ioide                                      | -                                                   | -           | -           | -           | -           | -           | <b>4.98</b> | <b>4.68</b> | <b>4.10</b> | <b>5.29</b> |
| 6   | spathulenol                                               | <b>4.85</b>                                         | <b>3.04</b> | <b>2.62</b> | <b>5.57</b> | <b>1.87</b> | <b>2.00</b> | -           | -           | -           | -           |
| 7   | 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate | 27.01                                               | 15.02       | 21.99       | 39.77       | 15.51       | 50.88       | 21.52       | 23.58       | 35.64       | 10.21       |
| 8   | tau-murolol 2,6,10,15-tetra                               | 4.80                                                | 6.25        | 3.39        | 7.09        | 11.14       | 5.74        | 6.75        | 6.40        | 6.14        | 7.27        |
| 9   | methyl heptadecane                                        | <b>1.36</b>                                         | <b>6.25</b> | <b>2.50</b> | -           | -           | -           | -           | -           | -           | -           |

○ 굵게 표시한 부분들은 부위별 및 상태별에 따른 차이를 구분 지을 수 있는 화합물로 선정할 수 있다. 화합물  $\beta$ -copaene와 2,6,10,15-tetramethyl heptadecane의 경우 전체 줄기 및 꽃 추출물을 제외한 생체 벌깨덩굴 줄기 시료에서만 검출된 것으로 보아 건조과정중 휘발되어 소실되었을 거라 사료된다.

○ Spathulenol의 경우 생체 및 전체 줄기 시료에서는 검출되었으나 전체 꽃 추출에서는 검출되지 않은 것으로 보아 줄기 부분에만 함유되어 있는 것으로 보여진다.

○ 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate은 모든 벌깨덩굴 시료에서 가장 많은 함량을 가지는 것으로 나타났다.

### 3) 층층이꽃의 아로마 성분 확인

○ 층층이꽃은 가평 명지산 (Site A, B)와 강원 가리산 (Site C)에서 수집하여 각 생체 및 전체 형태로 만들어서 사용하였다.

#### ① 층층이꽃 추출물의 아로마 성분 확인

○ 층층이꽃 추출물을 확립된 GC-MS 분석방법에 적용하여 분석한 결과는 Fig. 8에 나타냈다. 함량을 육안으로 쉽게 확인하기 위하여 y축의 abundance를 통일시켰다. Fig. 8의 total ion chromatograms (TICs)에서 보이듯이 Site A, B, C의 구성 성분은 큰 차이가 없이 비슷한 패턴으로 나오는 것을 확인할 수 있다. 화합물들의 확인은 NIST MS spectra library와 대조하였을 때 85%이상의 일치율을 나타내는 것과 기존 문헌을 토대로 명명하였다.

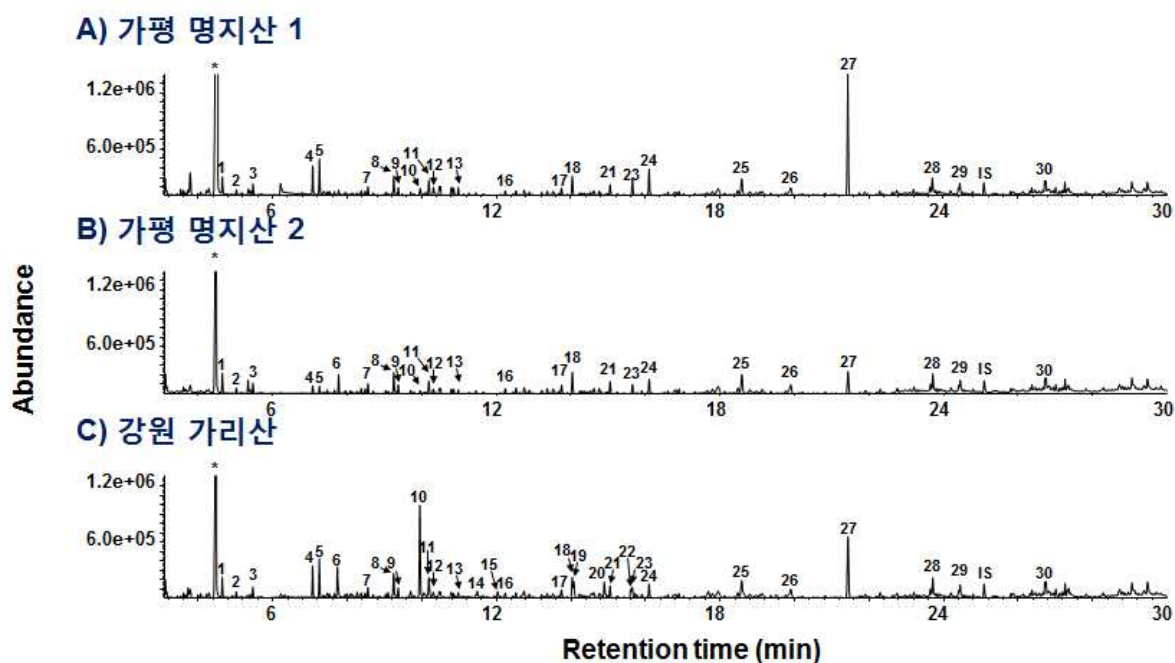


Fig. 37. Total ion chromatograms of *C. chinense* var. *parviflorum* extracts

Peak identified follow as : 1.2,4-dimethyl heptane, 2.2,4-dimethyl-1-heptene, 3.4-methyl octane, 4.1-ethylbutyl hydroperoxide, 5.methylpentyl hydroxide, 6.1-octen-3-ol, 7.2-methyl-5-ethyl hetane, 8.3,3,6-trimethyl heptane, 9.2,6,10-trimethyl dodecane, 10.o-guaiacol, 11.4,7-dimethyl undecane, 12.2-octyl acetate, 13. ethyl octanoate, 14.p-ethyl phenol, 15.p-creosol, 16.2,7,10-trimethyl dodecane, 17.2,3,5-trimethyl decane, 18.2,6,10,15-tetramethyl heptadecane, 19.p-ethylguaiaicol, 20.p-vinylguaiaicol, 21.4,6-dimethyl dodecane, 22.syringol, 23.1-(2-hydroxy-1-methyl ethyl)-2,2-dimethyl lpropyl-2-methyl propanoate, 24.3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate, 25.2,6,11,15-tetramethyl hexadecane, 26.dihydroactinidioide, 27.1-isobutyl-4-isopropyl-3-isopropyl-2,2- dimethyl succinate, 28.2,6,10-trimethyl tetradecane, 29.2,6,10,15-tetramethyl heptadecane, 30.7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, \*. solvent peaks.

○ 생체 및 건체 층층이꽃 추출물에서 검출된 Total ion chromatograms를 비교한 결과를 Fig. 37에 수록하였다. 총 30가지의 성분들이 GC-MS scan mode에서 관측되었다. 검출된 화합물은 벌깨덩굴과 비슷하게도 saturated alkane, phenyl alcohol류 등이 나타나는 것을 확인하였으며, MS library mass spectra를 대조하여 확인하였다. 층층이꽃 추출물로부터 검출된 다양한 화학적 구성성분들의 머무름 시간과 특성이온을 Table 13에 나타내었다.

Table 13. Retention time and characteristic ions of *C. chinense* var. *parviflorum* extracts

| Peak No. | R.T.  | compound                   | M.W. | Characteristic ion, $m/z$ (relative abundance,%)            | R.I. |
|----------|-------|----------------------------|------|-------------------------------------------------------------|------|
| 1        | 4.63  | 2,4-dimethyl heptane       | 128  | 43(100), 85(76), 57(42), 71(39), 128(3)                     | 825  |
| 2        | 5.01  | 2,4-dimethyl-1-heptane     | 126  | 70(100), 43(99), 55(59), 83(31), 126(21),                   | 846  |
| 3        | 5.46  | 4-methyl octane            | 128  | 43(100), 85(52), 71(49), 57(35), 128(6), 98(5)              | 869  |
| 4        | 7.07  | 1-ethylbutyl hydroperoxide | 118  | 43(100), 57(37), 41(34), 85(33), 73(15)                     | 950  |
| 5        | 7.25  | methylpentyl hydroxide     | 118  | 43(100) 85(35), 57(21), 69(8), 100(1)                       | 959  |
| 6        | 7.76  | 1-octen-3-ol               | 128  | 57(100), 43(19), 72(16), 55(11), 85(9), 99(5), 68(5), 81(5) | 984  |
| 7        | 8.55  | 2-methyl-5-ethyl heptane   | 142  | 71(100), 43(78), 57(71), 85(18), 113(17), 97(3)             | 1023 |
| 8        | 9.24  | 3,3,6-trimethyl heptane    | 142  | 71(100), 43(93), 57(86), 85(68), 113(17), 127(17), 99(7)    | 1057 |
| 9        | 9.36  | 2,6,10-trimethyl dodecane  | 212  | 71(100), 57(89), 43(83), 85(53), 113(14), 127(8), 99(4)     | 1063 |
| 10       | 9.94  | o-guaiacol                 | 124  | 109(100), 124(88), 81(54), 53(13), 65(4), 95(2)             | 1089 |
| 11       | 10.18 | 4,7-dimethyl undecane      | 184  | 43(100), 57(76), 85(45), 70(27), 113(13), 127(9), 99(7)     | 1099 |
| 12       | 10.31 | 2-octyl acetate            | 172  | 43(100), 72(40), 87(40), 57(28), 112(16), 97(4), 127(4)     | 1106 |
| 13       | 10.98 | ethyl octanoate            | 172  | 88(100), 115(27), 127(24), 57(24), 70(24), 43(24), 101(3)   | 1141 |
| 14       | 11.49 | p-ethyl phenol             | 122  | 107(100), 122(33), 77(13), 91(4), 65(3), 51(2)              | 1166 |
| 15       | 12.03 | p-creosol                  | 138  | 138(100), 123(91), 95(25), 67(15), 77(14), 55(8), 41(5)     | 1191 |
| 16       | 12.24 | 2,7,10-trimethyl dodecane  | 212  | 57(100), 43(67), 71(62), 85(46), 99(15), 121(14), 136(14),  | 1200 |

R.T. : retention time, M.W. : molecular weight, R.I. : retention index

Table 13. Continued

| Peak No. | R.T.  | compound                                                              | M.W. | Characteristic ion, $m/z$ (relative abundance,%)                                                                    | R.I. |
|----------|-------|-----------------------------------------------------------------------|------|---------------------------------------------------------------------------------------------------------------------|------|
| 17       | 13.75 | 2,3,5-trimethyl decane                                                | 184  | 43(100), 85(99), 57(76), 71(68), 99(21), 141(14), 113(11), 155(10), 127(7)                                          | 1266 |
| 18       | 14.04 | 2,6,10,15-tetramethyl heptadecane                                     | 296  | 71(100), 57(91), 85(73), 43(68), 113(14), 99(13), 127(11), 155(6), 169(2),                                          | 1277 |
| 19       | 14.08 | p-ethylguaiacol                                                       | 152  | 137(100), 152(39), 122(9), 91(6), 77(5), 65(4), 109(2), 53(2)                                                       | 1279 |
| 20       | 14.9  | p-vinylguaiacol                                                       | 150  | 150(100), 135(76), 107(27), 77(25), 63(5)                                                                           | 1315 |
| 21       | 15.05 | 4,6-dimethyl dodecane                                                 | 198  | 71(100), 57(93), 43(67), 85(66), 127(16), 99(15), 113(13), 155(8), 141(3)                                           | 1322 |
| 22       | 15.6  | syringol                                                              | 154  | 154(100), 139(74), 96(47), 93(45), 111(39), 65(20), 51(22), 81(22), 79(20)                                          | 1351 |
| 23       | 15.65 | 1-(2-hydroxy-1-methyl ethyl)-2,2-dimethyl propyl -2-methyl propanoate | 216  | 71(100), 43(64), 83(39), 56(30), 98(26), 143(6), 173(6), 111(5), 127(2)                                             | 1353 |
| 24       | 16.1  | 3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate                     | 216  | 71(100), 89(74), 56(70), 43(55), 173(16), 143(9), 161(2),                                                           | 1376 |
| 25       | 18.58 | 2,6,11,15-tetramethylhexadecane                                       | 282  | 71(100), 57(93), 85(80), 43(63), 99(26), 113(21), 127(11), 155(11), 141(4), 169(4), 197(2)                          | 1485 |
| 26       | 19.91 | dihydroactinidioides                                                  | 180  | 71(100), 57(83), 43(72), 85(64), 111(40), 99(23), 169(14), 137(14), 127(13), 155(10), 180(9)                        | 1536 |
| 27       | 21.44 | 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate             | 286  | 71(100), 43(38), 111(7), 159(7), 55(7), 243(5), 83(5), 93(5), 173(3), 121(2), 143(2)                                | 1589 |
| 28       | 23.71 | 2,6,10-trimethyl tetradecane                                          | 240  | 71(100), 57(81), 85(73), 43(62), 99(30), 113(25), 127(16), 167(11), 155(9), 141(7), 177(3), 197(3), 211(2)          | 1697 |
| 29       | 24.45 | 2,6,10,15-tetramethyl heptadecane                                     | 296  | 71(100), 57(72), 43(68), 85(61), 99(39), 113(35), 127(18), 155(16), 169(12), 144(7), 197(7), 211(4)                 | 1745 |
| 30       | 26.72 | 7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione             | 276  | 71(100), 85(78), 43(61), 57(59), 99(35), 113(26), 127(16), 155(16), 141(10), 169(7), 197(4), 211(3), 183(2), 239(2) | 1906 |

R.T. : retention time, M.W. : molecular weight, R.I. : retention index

○ 층층이꽃 추출물에서 TICs에 검출된 화합물은 중 주로 saturated alkane, phenyl alcohol류의 화합물들이 나타났다. TICs에서 검출된 성분들을 토대로 층층이꽃에서 주요 성분 몇 가지 화합물에 한하여 질량 스펙트럼을 수록하였다(Fig. 38).

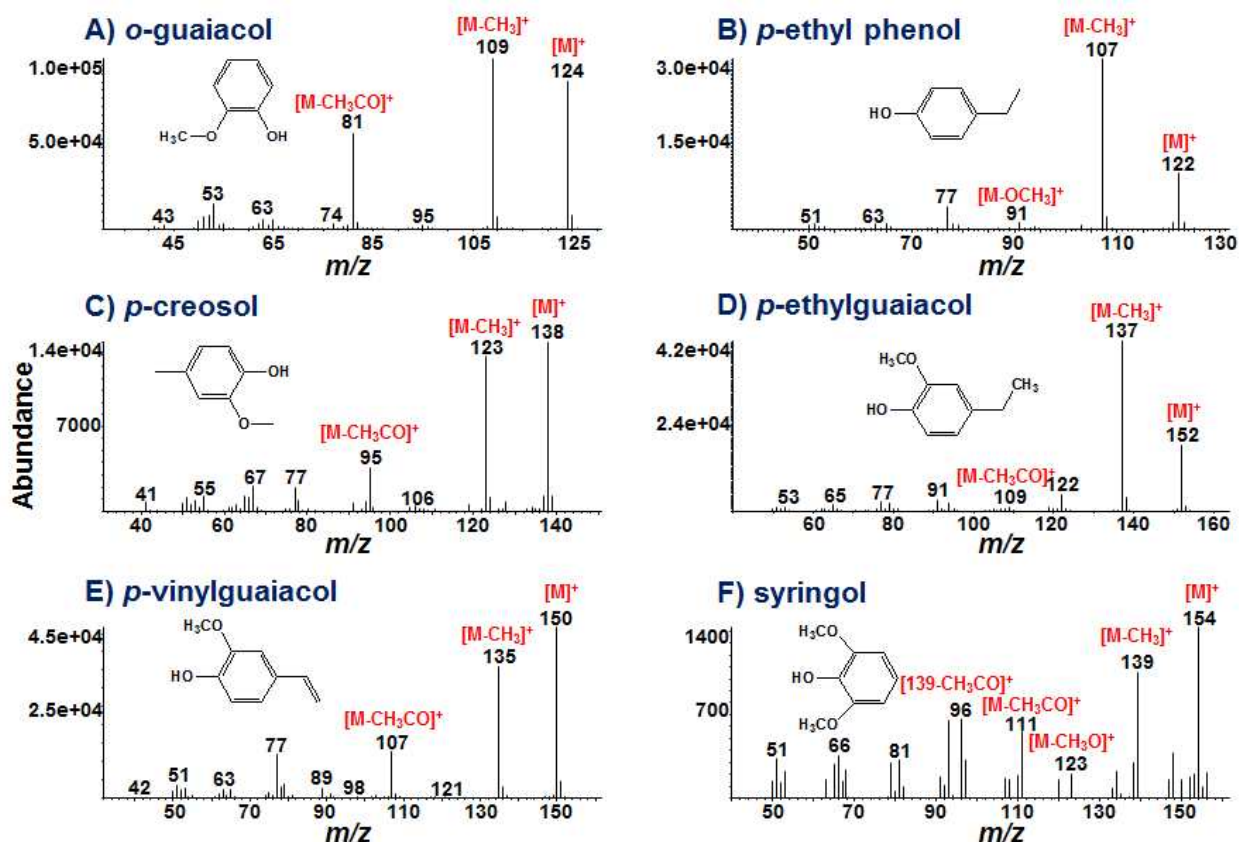


Fig. 38. Mass spectra of major compounds in *C. chinense* var. *parviflorum*.

○ 층층이꽃 추출물에서 검출된 성분들의 함량을 확인하기 위해, phenanthrene d-10을 내부표준물질로 사용하여 area ratio로 계산하였다. 결과는 Fig. 39에 막대그래프로 나타내었다.

○ 층층이꽃 추출물의 경우, 총 30가지 성분 중 25가지 성분이 모든 층층이꽃 시료에서 공통적으로 검출되었다. 가평 명지산에서 채집된 A와 B시료는 포함되어 있는 구성 화합물의 종류에는 차이가 없었으나, 함량에서 차이를 나타내었다. 특히 1-ethylbutyl hydroperoxide, 5-methylpentyl hydroxide, 27번 1-isobutyl-4-isopropyl-3-isopropyl-2, 2-dimethyl succinate 화합물의 경우 시료 A의 함량이 우세한 것으로 나타났다.

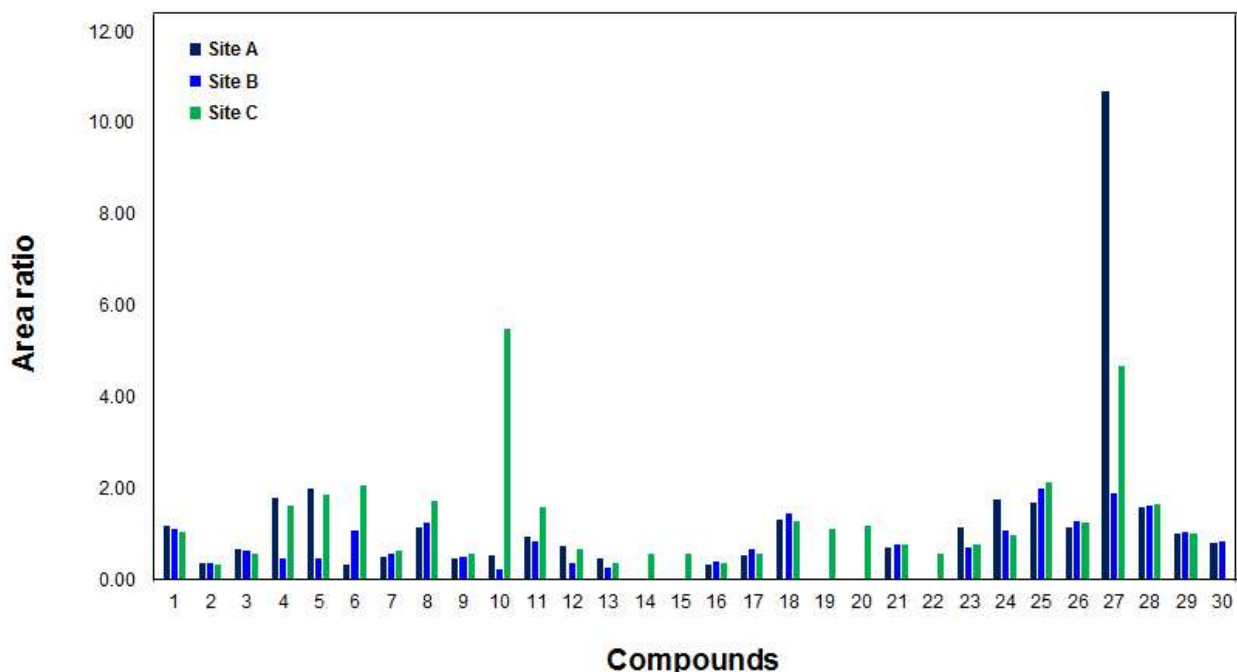


Fig. 39. Peak area ratio of compounds in *C. chinense* var. *parviflorum* detected by GC-MS

Peak identified follow as : 1.2,4-dimethyl heptane, 2.2,4-dimethyl-1-heptene, 3.4-methyl octane, 4.1-ethylbutyl hydroperoxide, 5.methylpentyl hydroxide, 6.1-octen-3-ol, 7.2-methyl-5-ethyl hetane, 8.3,3,6-trimethyl heptane, 9.2,6,10-trimethyl dodecane, 10.o-guaiacol, 11.4,7-dimethyl undecane, 12.2-octyl acetate, 13. ethyl octanoate, 14.p-ethyl phenol, 15.p-creosol, 16.2,7,10-trimethyl dodecane, 17.2,3,5-trimethyl decane, 18.2,6,10,15-tetramethyl heptadecane, 19.p-ethylguaiacol, 20.p-vinylguaiacol, 21.4,6-dimethyl dodecane, 22.syringol, 23.1-(2-hydroxy-1-methyl ethyl)-2,2-dimethy lpropyl-2-methyl propanoate, 24.3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate, 25.2,6,11,15-tetramethyl hexadecane, 26.dihydroactinidioidide, 27.1-isobutyl-4-isopropyl-3-isopropyl-2,2- dimethyl succinate, 28.2,6,10-trimethyl tetradecane, 29.2,6,10,15-tetramethyl heptadecane, 30.7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, \*. solvent peaks.

○ 강원 가리산에서 채집된 층층이꽃의 경우, 가평 명지산에서 채집된 시료 추출물에 비하여 육안으로 확인하였을 때 추출물의 색과 향이 달랐다. 14번 p-ethyl phenol, 15번 p-creosol, 19번 p-ethylguaiacol, 20번 p-vinylguaiacol, 22번 syringol과 같은 phenyl alcohol 류 성분들이 추가로 검출되었다. 또한 10번 o-guaiacol의 경우 시료 A와 B에 비하여 함량이 높게 나타났다.

○ TIC에서 검출된 화합물들을 토대로 대표적인 성분들을 선정하여 화합물의 % 함량을 구하였다. % 함량을 구할 때 사용하였던 식은 아래에 나타내었으며 결과는 Table 14에 기재하였다.

$$\% \text{ 함량} = \frac{\text{Compounds of peak area}}{\text{Sum of total compounds peak area}} \times 100$$

Table 14. Amounts of volatile compounds in *C. chinense* var. *parviflorum* extracts

| No. | compounds                                                 | % [compounds of area/ sum of total compounds x 100] |      |       |
|-----|-----------------------------------------------------------|-----------------------------------------------------|------|-------|
|     |                                                           | Raw                                                 |      |       |
|     |                                                           | A                                                   | B    | C     |
| 1   | 1-octen-3-ol                                              | 1.01                                                | 4.98 | 5.30  |
| 2   | o-guaiacol                                                | 1.56                                                | 1.02 | 14.21 |
| 3   | p-ethyl phenol                                            | -                                                   | -    | 1.45  |
| 4   | p-cresol                                                  | -                                                   | -    | 1.42  |
| 5   | p-ethylguaiacol                                           | -                                                   | -    | 2.90  |
| 6   | p-vinylguaiacol                                           | -                                                   | -    | 3.06  |
| 7   | syringol                                                  | -                                                   | -    | 1.41  |
| 8   | 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate | 31.73                                               | 8.74 | 12.08 |

○ 시료 C의 경우 시료 A, B와 비교하였을 때, phenyl alcohol류가 더 많이 검출되었으며, p-ethyl phenol, p-cresol, p-ethylguaiacol, p-vinylguaiacol, syringol과 같은 화합물이 특징적으로 검출되었다.

○ 1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate은 벌깨덩굴과 마찬가지로 층층이꽃에서 가장 많은 함량을 가지는 것으로 나타났다.

#### 4) 긴병꽃풀의 아로마 성분 확인

○ 수집된 긴병꽃풀 시료들은 경희대학교 홍석표 교수팀으로부터 제공받았다. 긴병꽃풀은 경기도 과천 청계산의 Site A와 Site B에서 수집하여 생체 상태로 사용하였다.

##### ① 긴병꽃풀 추출물의 아로마 성분 확인

○ 긴병꽃풀 (*Glechoma hederacea*) 줄기 추출물을 확립된 GC-MS 분석방법에 적용하여 분석한 결과는 Fig. 40에 나타났다. 함량을 육안으로 쉽게 확인하기 위하여 y축의



abundance를 통일시켰다. Fig. 40의 total ion chromatograms (TICs)에서 보이듯이 Site A, B, C의 구성 성분은 큰 차이가 없이 비슷한 패턴으로 나오는 것을 확인할 수 있다. 화합물들의 확인은 NIST/Wiley MS spectra library와 대조하였을 때 85%이상의 일치율을 나타내는 것과 기존 문헌을 토대로 명명하였다.

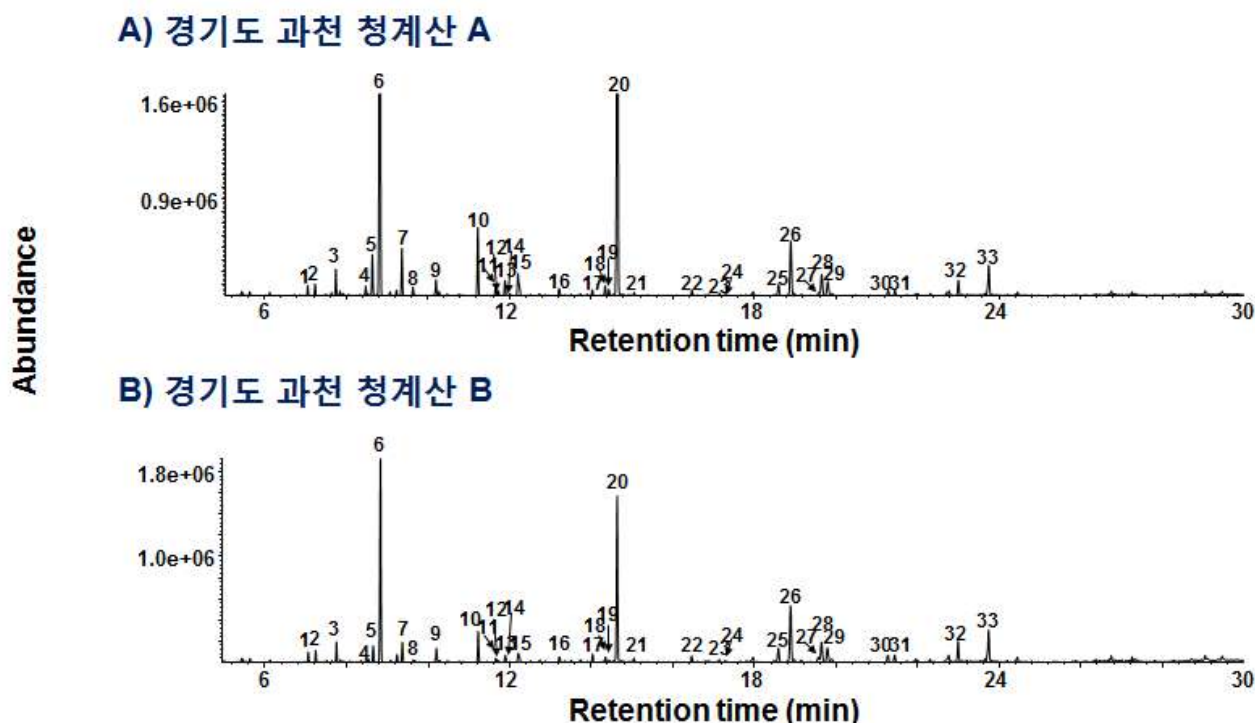


Fig. 40. Total ion chromatograms of *G. hederacea* extracts

Peak identified follow as : 1.2,4-dimethyl heptane, 2.2,4-dimethyl-1-heptene, 3.4-methyl octane, 4.1-ethylbutyl hydroperoxide, 5.methylpentyl hydroxide, 6.1-octen-3-ol, 7.2-methyl-5-ethyl hetane, 8.3,3,6-trimethyl heptane, 9.2,6,10-trimethyl dodecane, 10.o-guaiacol, 11.4,7-dimethyl undecane, 12.2-octyl acetate, 13. ethyl octanoate, 14.p-ethyl phenol, 15.p-creosol, 16.2,7,10-trimethyl dodecane, 17.2,3,5-trimethyl decane, 18.2,6,10,15-tetramethyl heptadecane, 19.p-ethylguaiacol, 20.p-vinylguaiacol, 21.4,6-dimethyl dodecane, 22.syringol, 23.1-(2-hydroxy-1-methyl ethyl)-2,2-dimethylpropyl-2-methyl propanoate, 24.3-hydro-2,4,4-trimethyl pentyl 2-methylpropanoate, 25.2,6,11,15-tetramethyl hexadecane, 26.dihydroactinidioidide, 27.1-isobutyl-4-isopropyl-3-isopropyl-2,2-dimethyl succinate, 28.2,6,10-trimethyl tetradecane, 29.2,6,10,15-tetramethyl heptadecane, 30.7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, \*. solvent peaks.

○ 생체 긴병꽃풀 추출물에서 검출된 Total ion chromatograms를 비교한 결과를 Fig. 11에 수록하였다. 총 33가지의 성분들이 GC-MS scan mode에서 관측되었다. 검출된 화합물은 phenyl alcohol류, terpene류 등이 나타나는 것을 확인하였으며, MS library mass spectra와 기존문헌을 참고하여 확인하였다. 생체 긴병꽃풀 줄기 추출물로부터 검출된 다양한 화학적 구성성분들의 머무름 시간과 특성이온을 Table 15에 나타내었다.



Table 15. Retention time and characteristic ions of *G. hederacea* extracts

| Peak No. | R.T.  | compound                | M.W. | Characteristic ion, <i>m/z</i> (relative abundance,%)                                      | R.I. |
|----------|-------|-------------------------|------|--------------------------------------------------------------------------------------------|------|
| 1        | 7.07  | 3-hexyl hydroperoxide   | 118  | 43(100), 85(36), 57(33), 73(12), 100(3)                                                    | 950  |
| 2        | 7.25  | 2-hexyl hydroperoxide   | 118  | 43(100), 85(38), 57(20), 61(10) 69(9), 100(2)                                              | 959  |
| 3        | 7.76  | 1-octen-3-ol            | 128  | 57(100), 43(20), 72(17), 85(9), 99(5)                                                      | 984  |
| 4        | 8.50  | $\alpha$ -terpinene     | 136  | 121(100), 93(81), 136(53), 77(31), 105(23), 41(12), 65(9), 53(7)                           | 1020 |
| 5        | 8.66  | $\rho$ -cymene          | 134  | 119(100), 134(26), 91(21), 77(7), 65(5), 103(4), 41(3), 53(1)                              | 1029 |
| 6        | 8.84  | eucalyptol(=1,8cineole) | 154  | 43(100), 81(74), 108(59), 71(56), 84(51), 111(51), 154(45), 93(43),139(41), 55(35), 125(8) | 1038 |
| 7        | 9.37  | $\gamma$ -terpinene     | 136  | 93(100), 77(34),136(29), 121(29), 43(14),105(11), 65(7), 51(5),                            | 1063 |
| 8        | 9.65  | cis-sabinene hydrate    | 154  | 71(100), 43(91), 93(90), 81(58), 111(58), 121(46), 55(36), 139(28), 136(23), 154(9)        | 1076 |
| 9        | 10.21 | $\beta$ -linalool       | 154  | 71(100), 93(88), 41(57), 55(53), 80(37),121(26), 107(8), 136(8)                            | 1101 |
| 10       | 11.24 | camphor                 | 152  | 95(100), 81(64), 41(39), 108(64), 69(32), 152( 28), 55(27), 137(3), 123(1)                 | 1154 |
| 11       | 11.67 | $\alpha$ -terpineol     | 154  | 59(100), 81(60), 93(35), 43(28), 136(22), 96(19), 67(17), 54(11), 121(4), 107(1)           | 1174 |
| 12       | 11.74 | endo-borneol            | 154  | 95(100), 110(18), 41(11), 55(8), 69(8),139(8), 121(7), 83(5)                               | 1178 |
| 13       | 11.90 | terpinen-4-ol           | 154  | 71(100), 93(58), 111(57), 43(38), 55(24), 56(24), 67(22), 154(17), 136(13), 121(5)         | 1185 |
| 14       | 12.02 | $\rho$ -cymen-8-ol      | 150  | 43(100), 135(98), 91(32), 65(12), 150(12),119(11), 77(10), 207(7), 105(6), 55(3)           | 1190 |
| 15       | 12.22 | unknown1                | —    | 59(100), 93(64), 121(58), 136(51), 81(39), 43(25), 67(17),55(10)                           | 1199 |
| 16       | 13.23 | isothymol methyl ester  | 164  | 149(100), 164(38), 91(19), 117(10), 134(10), 77(9), 57(9), 43(7), 105(6), 65(3)            | 1244 |
| 17       | 14.04 | unknown2                | 226  | 71(100), 57(90), 43(77), 85(68), 99(16), 113(13), 127(13), 155(7), 169(2)                  | 1277 |
| 18       | 14.35 | bornyl acetate          | 196  | 95(100), 43(52), 121(41), 136(37), 108(19), 55(15), 80(14), 69(13), 154(9), 196(1)         | 1289 |
| 19       | 14.45 | <i>m</i> -thymol        | 150  | 135(100), 150(30), 91(19), 115(15), 77(6),107(5), 65(4), 51(3), 121(2)                     | 1293 |

R.T. : retention time, M.W. : molecular weight, R.I. : retention index

Table 15. continued

| Peak No. | R.T.  | compound        | M.W. | Characteristic ion, <i>m/z</i> (relative abundance,%)                                                                        | R.I. |
|----------|-------|-----------------|------|------------------------------------------------------------------------------------------------------------------------------|------|
| 20       | 14.65 | o-thymol        | 150  | 135(100), 150(34), 91(17), 77(9), 107(9), 115(9), 51(3), 65(3), 41(2), 121(3)                                                | 1301 |
| 21       | 15.05 | unknown3        | –    | 71(100), 57(81), 43(72), 85(64), 99(13), 127(13), 113(12), 155(9), 169(5), 141(3)                                            | 1322 |
| 22       | 16.47 | β-elemene       | 205  | 93(100), 81(98), 67(78), 107(68), 41(58), 147(52), 121(50), 55(37), 161(35), 133(35), 189(30), 175(8)                        | 1393 |
| 23       | 17.15 | caryophyllene   | 204  | 133(100), 93(95), 69(92), 79(64), 41(60), 107(51), 55(38), 147(35), 119(33), 161(19), 189(19), 175(14), 204(11)              | 1424 |
| 24       | 17.29 | γ-elemene       | 204  | 121(100), 93(79), 107(49), 79(38), 67(38), 41(32), 133(26), 161(26), 189(26), 53(23), 204(13), 147(12)                       | 1430 |
| 25       | 18.60 | β-copaene       | 204  | 71(100), 161(95), 57(94), 43(86), 85(74), 105(56), 91(54), 119(36), 133(17), 204(14), 147(6)                                 | 1486 |
| 26       | 18.89 | curzerene       | 216  | 108(100), 148(29), 79(14), 91(13), 216(10), 133(9), 201(7), 41(6), 119(5), 159(5), 53(4), 65(4), 173(4), 187(2)              | 1497 |
| 27       | 19.57 | δ-cadinene      | 204  | 161(100), 134(79), 105(62), 91(54), 119(54), 204(50), 78(30), 147(27), 71(24), 57(2)                                         | 1523 |
| 28       | 19.65 | 6-epi-shyobunol | 222  | 81(100), 93(72), 121(69), 41(61), 55(54), 69(52), 109(48), 136(34), 161(25), 179(7), 189(7), 149(6), 207(3), 222(2)          | 1526 |
| 29       | 19.80 | 6-epi-shyobunol | 222  | 81(100), 93(81), 109(79), 41(67), 67(57), 55(56), 123(50), 161(35), 136(34), 189(8), 149(7), 179(7), 207(5)                  | 1532 |
| 30       | 21.28 | 4-epi-cubedol   | 222  | 81(100), 43(40), 161(32), 105(29), 123(20), 93(20), 55(16), 67(16), 207(10), 147(4), 189(4)                                  | 1584 |
| 31       | 21.45 | unknown4        | –    | 71(100), 43(44), 56(10), 111(8), 159(7), 83(4), 243(4), 97(3), 173(3), 143(2), 207(2)                                        | 1590 |
| 32       | 23.00 | tau-muurolol    | 222  | 95(100), 121(88), 43(67), 161(50), 204(47), 79(41), 105(38), 71(30), 55(21), 137(20), 69(19), 189(9), 149(9), 179(5), 222(3) | 1663 |
| 33       | 23.75 | carotol         | 222  | 84(100), 41(57), 71(56), 55(50), 109(36), 121(30), 161(27), 93(28), 137(14), 204(7), 189(5), 222(4)                          | 1699 |

R.T. : retention time, M.W. : molecular weight, R.I. : retention index

○ 긴병꽃풀 줄기 추출물에서 TICs에 검출된 화합물은 중 주로 phenyl alcohol류, terpen류와 같은 정유성분의 화합물들이 나타났다. TICs에서 검출된 성분들을 토대로 긴병꽃풀 줄기에서 주요 성분 몇 가지 화합물에 한하여 질량 스펙트럼을 수록하였다(Fig. 41).

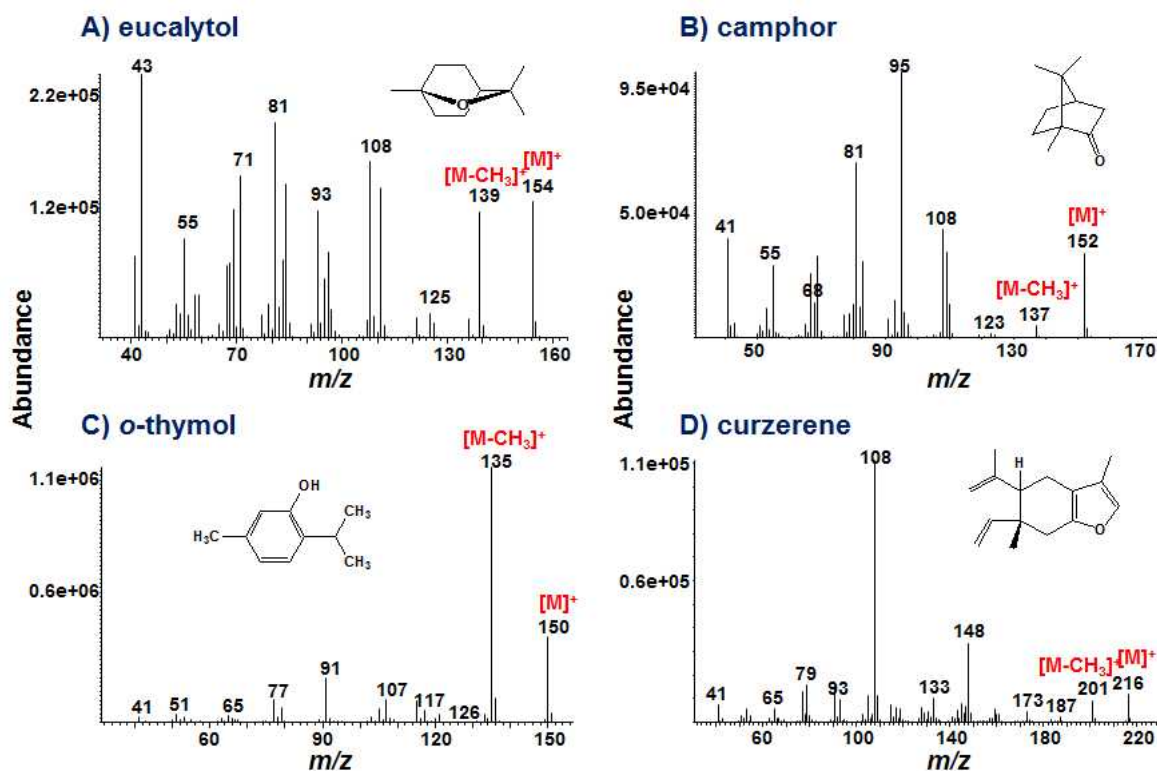


Fig. 41. Mass spectra of major compounds in *G. hederacea*

○ 긴병꽃풀 추출물에서 검출된 성분들의 함량을 확인하기 위해, phenanthrene d-10을 내부표준물질로 사용하여 area ratio로 계산하였다. 결과는 Fig. 42에 막대그래프로 나타내었다.

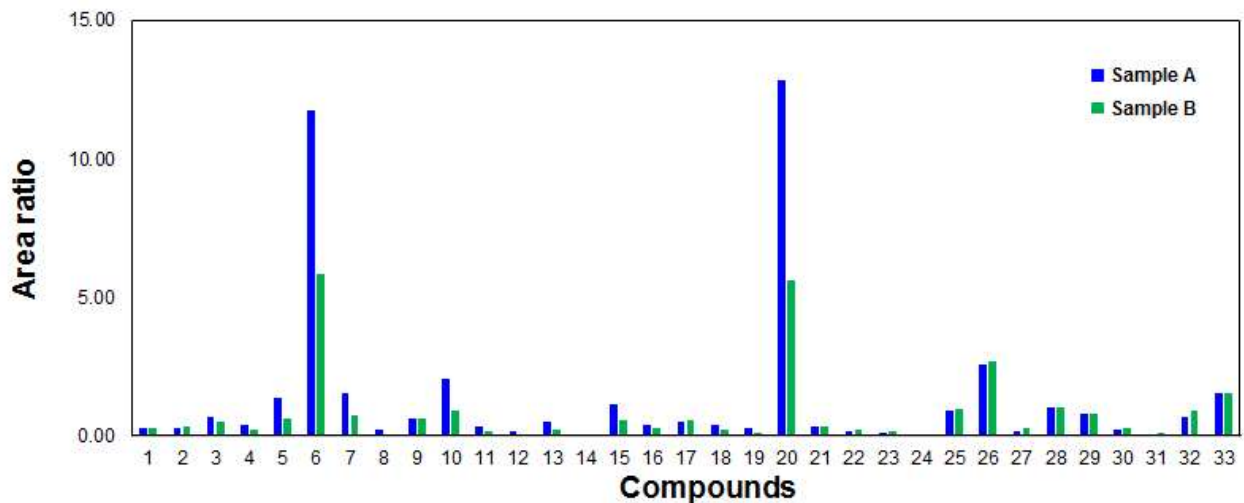


Fig. 42. Peak area ratio of compounds in *G. hederacea* detected by GC-MS

Peak identified follow as : 1.3-hexyl hydroperoxide; 2.2-hexyl hydroperoxide; 3.1-octen-3-ol; 4.α-terpinene; 5.p-cymene; 6.eucalyptol(=1,8-cineole); 7.γ-terpinene; 8.cis-sabinene hydrate; 9.β-linalool; 10.camphor; 11.α-terpineol; 12.endo-borneol; 13.terpinen-4-ol; 14.p-cymen-8-ol; 15.unknown1; 16.isothymol methyl ester; 17.unknown2; 18.bornyl acetate; 19.m-thymol; 20.o-thymol; 21.unknown3; 22.β-elemene; 23.caryophyllene; 24.γ-elemene; 25.β-copaene; 26.curzerene; 27.δ-cadinene; 28.6-epi-shyobunol; 29.6-epi-shyobunol; 30.4-epi-cubedol; 31.unknown4; 32.tau-muurolool; 33.carotol

○ 긴병꽃풀에서 주로 포함되어 있는 성분은 eucalyptol과 o-thymol인 것으로 나타났다. 이외에도 γ-terpinene, camphor, β-copaene과 같은 화합물이 나타났으며, 이러한 화합물은 phenyl alcoho류, monoterpene류와 같은 휘발성 정유성분이 검출되었다.

○ TIC에서 검출된 화합물들을 토대로 대표적인 성분들을 선정하여 화합물의 % 함량을 구하였다. % 함량을 구할 때 사용하였던 식은 아래에 나타내었으며 결과는 Table 16에 기재하였다.

$$\% \text{ 함량} = \frac{\text{Compounds of peak area}}{\text{Sum of total compounds peak area}} \times 100$$

Table 16. Amounts of volatile compounds in *G. hederacea* extracts

| No. | compounds           | % [compounds of area/ sum of total compounds x 100] |       |
|-----|---------------------|-----------------------------------------------------|-------|
|     |                     | A                                                   | B     |
| 1   | eucalyptol          | 26.17                                               | 21.10 |
| 2   | $\gamma$ -terpinene | 3.42                                                | 2.74  |
| 3   | camphor             | 4.65                                                | 3.42  |
| 4   | o-thymol            | 28.64                                               | 20.26 |
| 5   | $\beta$ -copaene    | 2.06                                                | 3.64  |
| 6   | curzerene           | 5.79                                                | 9.76  |
| 7   | carotol             | 3.47                                                | 5.64  |

○ 산지별 휘발성 성분의 차이는 산지 A에서 수집된 긴병꽃풀 시료에서 eucalyptol과 o-thymol이 area ratio의 함량이 산지 B보다 2배 이상 높은 것으로 나타났다. 하지만 %함량에서는 큰 차이가 나타나지 않는 것으로 보아 각 산지별 긴병꽃풀에 구성된 휘발성 성분은 비슷한 조성을 가지는 것으로 보여진다.

## ② 기존 문헌과의 비교

○ 긴병꽃풀은 다른 식물에 비하여 정유성분이 연구가 된 바가 있다. 따라서 본 연구 결과를 기존 문헌과 대조하여 함유된 성분을 확인하였다.

1) Bull. Chem. Soc. Ethiop. 24 (2010) 67-76

2) J. Essent. Oil Res. 19 (2007) 449-451

3) Chemija 16 (2005) 47-50

### Matching 14 compounds of 256

|     |                                |
|-----|--------------------------------|
| 27  | 1-Octen-3-ol                   |
| 38  | p-Cymene                       |
| 40  | 1,8-Cineole                    |
| 45  | $\gamma$ -Terpinene=eucalyptol |
| 52  | Linalool                       |
| 81  | Terpinen-4-ol                  |
| 83  | p-Cymen-8-ol                   |
| 86  | $\alpha$ -Terpineol            |
| 97  | Thymol methylether             |
| 113 | Thymol                         |
| 137 | $\beta$ -Elemene               |
| 148 | $\gamma$ -Elemene              |
| 153 | $\beta$ -Copaene               |
| 177 | $\delta$ -Cadinene             |

| Compound                   |
|----------------------------|
| 1,3-(E), 5(Z)-octatriene   |
| $\alpha$ -pinene           |
| $\beta$ -pinene            |
| 3-octanone                 |
| myrcene                    |
| 1,8-cineole                |
| (Z)- $\beta$ -ocimene      |
| (E)- $\beta$ -ocimene      |
| p-mentha-2,4(8)-diene      |
| nonanal                    |
| 1-octen-3-yl acetate       |
| allo-ocimene*              |
| dihydriopinocarvone        |
| methyl salicylate          |
| myrtanal                   |
| decanal                    |
| $\delta$ -elemene          |
| eugenol                    |
| $\alpha$ -copaene          |
| $\beta$ -bourbonene        |
| $\beta$ -elemene           |
| $\beta$ -ylangene          |
| -gurjunene                 |
| $\gamma$ -elemene          |
| aromadendrene              |
| $\alpha$ -humulene         |
| $\gamma$ -muurolene        |
| germacrene D               |
| zingiberene                |
| bicyclogermacrene          |
| (E,E)- $\alpha$ -farnesene |
| $\gamma$ -cadinene         |
| $\delta$ -cadinene         |
| trans-cadina-1(2),4-diene  |
| $\alpha$ -cadinene         |
| cis-sesquibabinene hydrate |
| germacrene B               |
| germacrene D-4-ol          |
| $\gamma$ -eudesmol         |
| cubenol                    |
| $\alpha$ -cadinol          |
| 6,10,14-trimethyl-2-       |

1,8-cineole  
(=eucalyptol)

| Compound                    |
|-----------------------------|
| 1,3-trans, 5-cis-Octatriene |
| $\alpha$ -Pinene            |
| $\beta$ -Pinene             |
| 3-Octanone                  |
| Myrcene                     |
| 1,8-Cineole                 |
| Z- $\beta$ -Ocimene         |
| E- $\beta$ -Ocimene         |
| p-Mentha-2,4(8)-diene       |
| n-Nonanal                   |
| 1-Octen-3-yl acetate        |
| allo-Octimene               |
| dihydro-Pinocarvone         |
| Myrtanal                    |
| n-Decanal                   |
| $\delta$ -Elemene           |
| Eugenol                     |
| $\alpha$ -Copaene           |
| $\beta$ -Bourbonene         |
| $\beta$ -Elemene            |
| $\beta$ -Ylangene           |
| $\beta$ -Gurjunene          |
| $\gamma$ -Elemene           |
| Aromadendrene               |
| $\alpha$ -Humulene          |
| $\gamma$ -Murolene          |
| Germacrene D                |
| $\alpha$ -Zingiberene       |
| Bicyclogermacrene           |
| (E,E)- $\alpha$ -Farnesene  |
| $\gamma$ -Cadinene          |
| d-Cadinene                  |
| trans-Cadina-1(2),4-diene   |
| $\alpha$ -Cadinene          |
| cis-Sesquibabinene hydrate  |
| Germacrene B                |
| Germacrene D-4-ol           |
| $\gamma$ -Eudesmol          |
| Cubenol                     |
| $\alpha$ -Cadinol           |

1,8-cineole  
(=eucalyptol)

Fig. 43. Comparison of previous literatures

○ 첫 번째 논문(Bull. Chem. Soc. Ethiop. 24 (2010) 67-76)은 *Glechoma* L. 종에 속해있는 *G. hederacea* L., *G. hirsuta* Waldst. & Kit., *G. serbica* Halácsy & Wettst.에서 나타난 휘발성 성분을 나타내었다. 본 연구에서는 총 세가지 *Glechoma* L. 종을 clevenger type hydrodistillation 방법에 의하여 추출하였으며, GC-MS와 GC-FID를 통하여 256가지의 휘발성 성분을 확인을 하였다. 기존문헌에서 나타난 성분을 본 연구에서 검출된 성분들과 대조하였을 때 14가지의 성분이 겹치는 것을 확인할 수 있었다.

○ 두 번째 논문과 세 번째 논문 (J. Essent. Oil Res. 19 (2007) 449-451, Chemija 16 (2005) 47-50)에서는 hydrodistillation 방법을 이용하여 추출하였으며 각각 42개, 44개의 휘발성 정유성분을 확인하였다. 본 연구에서 검출된 성분들을 위의 기존문헌에 보고된 성분들과 대조하였을 때 1,8-cineole (=eucalyptol)이 겹치는 것을 확인할 수 있었다.

## IV. 결 론

○ 국내에 수입되고 있는 향신료는 2007년 이후 수입중량은 일정하게 증가하고 있으나 수입 단가의 변화와 국제 시장의 변화로 수입금액의 영향을 많이 받는다. 여러 환경적, 경제적 국제협약으로 인하여 향신료 시장의 변화가 예상되며, 다각적이고, 지속적인 수입 대체 자생종의 연구가 필요하다. 본 연구용역의 목적은 국내 수입 향신료의 현황 조사 및 목록화 및 아로마의 정의 및 차후에 이용 가능한 한반도 자생 아로마 식물자원 (특히 꿀풀과)의 목록화를 수행함에 있다.

○ 겨자는 수입량이 일정하지만 수입금액은 상승하고 있고,계피의 경우 수입량은 감소되며, 수입금액은 증가된다. 후추는 한국 GNI와 연계하였을 경우 그 수입양이 비례하고 있다. 생강은 국내 재배량, 수입원가에 민감하게 반응하는 품목이다. 타임 및 월계수는 겨자와 마찬가지로 수입량이 일정한 반면, 수입단가의 상승으로 수입금액은 상승하였다. 정향은 2012년부터 수입단가가 급등하였다. 코리앤더 씨는 정향과 마찬가지로 수입원가의 폭등으로 수입량이 일정하다. 회향과 심황은 2012년을 기점으로 수입가격이 하락되었는데 이는 한국과 인도의 포괄적경제동반자협정(CEPA) 체결로 관세인하의 영향으로 수입가격이 하락한 것이라 사료된다.

○ 향신료로 사용되는 꿀풀과의 4종류(타임, 로즈마리, 박하, 스피아민트)에 대한 분석된 주요 향 성분(정유)을 정리하여 제시하였다.

○ 국내에 자생하는 꿀풀과와 근연종에 대한 향성분을 목록화 하였고, 자주방아풀속 (*Lagopsis* Bunge ex Benth.), 벌개덩굴속 (*Meehanian* Britton), 누린내풀속 (*Tripura* P. D. Cantino)의 분류군은 향성분에 대한 연구 결과가 없음을 확인하였다.

○ 자생식물자원의 아로마 물질을 탐색하기 위한 실험방법으로 SPME 보다 Steam Distillation을 사용하는 것이 아로마 물질을 분석하는데 효과적임을 확인하였으며, 또한 채집, 건조, 추출, 분석에 대한 기준을 제시하였다.

○ 현재 사용한 추출 용매 및 시간의 경우 시료의 한정성으로 인하여 기존의 참고문헌

을 토대로 수행하였다. 추후 시료가 확보가 된다면, 다양한 추출용매 (ethyl acetate, hexane, ethyl ether 등) 및 추출시간 (1, 3, 5, 7 시간) 의 최적화를 수행할 것이다. GC-MS의 분리 조건은 가장 분리능이 좋은 조건으로 설정하여 수행하였다.

○ 생체와 건체 벌개데굴에 함유되어 있는 휘발성 성분은 GC/MS의 TIC로부터 각 피크 면적으로 비교하였을 때, 건체 상태에서 휘발성 성분의 양이 생체상태보다 상대적으로 높게 함유되어 있는 것을 확인되었다.

○ 벌개데굴의 꽃 부분에서는 줄기부분에서 검출되지 않은 4-methyl octane, 3,3,6-trimethyl heptane, 2,7,10-trimethyl dodecane, 2,3,5-trimethyl decane, 2,6,11,15-tetramethylhexadecane, dihydroactinidioid, 7,9-ditertbutyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione, butyl phthalate 와 같은 8가지 성분들이 검출되었다.

○ 벌개데굴과 층층이꽃에서 나타난 대부분의 성분들은 구조적으로 alkane chain을 가지는 화합물들이 나타났다.

○ 층층이꽃은 벌개데굴의 꽃 부분과 유사한 화학적 성분 구성을 나타냈다. 하지만 3번 시료의 경우 o-guaiacol, p-ethyl phenol, p-creosol, p-ethylguaiacol, p-vinylguaiacol, syringol 성분들이 벌개데굴과는 다르게 층층이꽃에서 검출되었다.

○ 긴병꽃풀의 주성분은 eucalyptol과 o-thymol 로 나타났다. 이외에도  $\gamma$ -terpinene, camphor,  $\beta$ -copaene 이 검출되었으며, phenyl alcoho류, monoterpene류와 같은 휘발성 정유성분도 검출되었다.

○ 타임(thyme)의 경우 국내 근연종으로 백리향과 섬백리향이 있으나 본 연구를 통하여 긴병꽃풀에도 o-thymol을 확인하였으므로 향신료의 대체가 가능할 것으로 판단된다.

○ 향후 산지별, 시기별 구분하기에는 각 시료 군에 포함된 시료의 개수가 적어 현재의 자료로는 불가능 할 듯하지만, 적절한 시간을 통하여 다량의 산지, 시료를 채집하여 자생 식물의 대표적인 지표성분을 선정하여 군집분석을 수행할 수 있을 것으로 사료된다.



## V. 기대성과(활용방안) 또는 향후계획

### 1. 산업별 수입대체 생물자원 근연종 발굴을 위한 방법

산업별 수입대체 생물자원 근연종 발굴에 근거한 자생식물자원의 아로마 물질 탐색 및 발굴은 국가 간의 무역이나 산업 개발에 매우 중요한 연구자료이다. 본 연구과정에 따라 자생식물자원의 아로마 물질 탐색 및 발굴에 대한 과정을 제시하고자 한다.

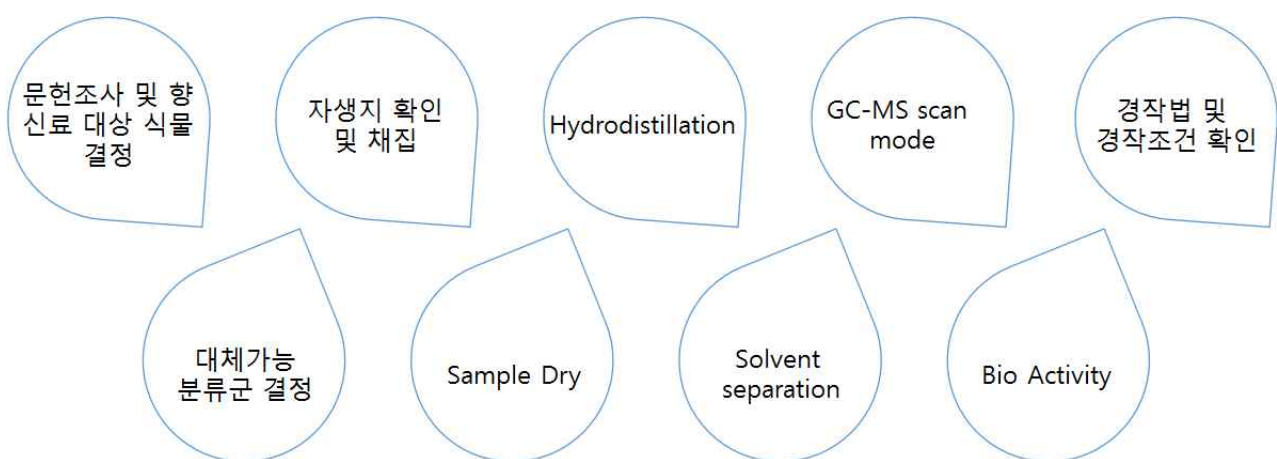


Fig. 44 자생식물자원의 아로마 물질 탐색 및 발굴에 대한 과정

#### 가. 문헌조사 및 향신료 대상 식물 결정

##### 1) 경제성 검토: 수입량과 수입단가를 고려하여 향신료 식물 결정

수입을 대체하고자 하는 향신료에 대하여 심황이나 회향같이 한-인도간 CEPA의 체결로 단가의 하락이 발생한다면 수입대체로 인한 경제적 가치는 감소된다. 국제무역동향과 국내 시장 동향을 면밀히 검토하여 경제적 가치가 높은 대상에 대한 경제성 검토를 시행한다.

##### 2) 가능성 검토: 기존 향신료 및 근연분류군에 대한 성분 분석

경제적 가치가 충족되더라도 기존 향신료를 대체할 수 있는 식물에 대한 사전 검토를 시행한다. 향신료는 개인이나 민족의 성향이 중요하기 때문에 비슷하다 하더라도 대체가 불가능한 향신료가 있으므로 가능성 검토를 시행한다.

## 나. 대체가능 분류군 결정

### 1) 대상 분류군 검토: 자생종 중 대체가능한 분류군 탐색

자생종 중 희귀한 식물이거나 보호종의 경우 수입 대체식물로 적합하지 않을 수 있다. 또한 유사한 기존 재배작물이 있는지 검토를 시행한다.

### 2) 대상 분류군 선정

근연종이나 기존 연구를 통한 유사 향 성분이 있는 대상에 대하여 연구 분류군을 선정

## 다. 자생지 확인 및 채집

### 1) 국내 자생지 확인: 국내 자생하는 집단에 대한 사전 조사

### 2) 군집 및 개체군별로 시료 채집:

3곳 이상의 군집을 선택하며, 각 군집에서는 개체군 조사를 위하여 3 sample 이상을 채집한다. 채집된 시료는 voucher를 제작한다.

## 라. Sample Dry

1) 채집된 시료는 향이 휘발되는 시간을 최대한 단축하여 건조시킨다. 시료 건조는 상온 (35℃)에서 8시간을 건조한다.

2) 건조된 시료는 향이 오염되지 않도록 유리병에 분말로 보관한다.

## 마. Hydrodistillation

1) Steam Distillation 방법으로 시료 추출하며, 400ml의 증류수에 5g의 건조시료를 넣은 후 3시간 동안 추출한다.

2) 추출된 용액은 냉장보관하며 48시간 이내에 Solvent separation을 시행한다.

## 바. Solvent separation

1) Hexan : diethyl ether(1:1)용액 100mL을 가한 후 funnel shake에서 10분동안 300rpm으로 분획 후, 10분후에 유기용매층을 옮기는 과정을 총 3회시행한다.

2) 모여진 유기용매를 농축하여 10mL을 만든후 Na<sub>2</sub>SO<sub>4</sub>를 첨가한 뒤, 상층액을 바이알에 옮겨 담아 -18℃에서 보관한다.

## 사. GC/MS scan mode

- 1) GC column은 DB-5MS를 사용하며, 헬륨을 이동상 기체로 사용한다.
- 2) mass spectrometer 의 interface 온도는 각 290℃, Scan range는 40-450amu로 설정한다.

## 아. Bio Activity

대체물질 탐색이 이루어진 분류군에 대하여 Bio Activity를 조사하는데 이는 별도의 연구자의 협조를 통하여 다양한 분석이 필요하다.

## 자. 경작법 및 경작조건 확인

Bio Activity까지 연구가 끝난 수입대체 근연종에 대하여는 재배법과 증식, 채취, 및 산업화 과정을 통하여 산업화를 시행하며, 이는 관계기관의 긴밀한 협조가 요구된다.

# 2. 단계별 추진계획 시행

|                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |      |                                          |      |                                          |      |                                     |      |                                     |      |                                                       |    |
|--------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|------------------------------------------|------|------------------------------------------|------|-------------------------------------|------|-------------------------------------|------|-------------------------------------------------------|----|
| 1 단계<br>(14'년)     | <ul style="list-style-type: none"> <li>- 수입대체 생물자원 발굴 및 탐색</li> <li>- Essential Oil Analysis: 정유 분석</li> <li>- 분석방법 및 데이터 분석결과를 통한 2단계 과업수행을 위한 지침과 토대마련</li> <li>- Lamiaceae I (꿀풀과 I) 가운데 3개의 선별된 분류군 대상</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                     | 완료   |                                          |      |                                          |      |                                     |      |                                     |      |                                                       |    |
| 2 단계<br>(‘15~’19년) | <ul style="list-style-type: none"> <li>- 수입대체 생물자원 후보종의 물질 추출 및 분석</li> <li>- 연차별로 중요 식물분류군 선별 - 분석수행 추진</li> </ul> <table border="1"> <tr> <td>2015</td> <td>Lamiaceae II (꿀풀과 II)-Apiaceae I (산형과 I)</td> </tr> <tr> <td>2016</td> <td>Apiaceae II (산형과 II) -Rosaceae I (장미과 I)</td> </tr> <tr> <td>2017</td> <td>Rosaceae II (장미과 II)-Rutaceae (운향과)</td> </tr> <tr> <td>2018</td> <td>Asteraceae (국화과)-Araliaceae (두릅나무과)</td> </tr> <tr> <td>2019</td> <td>Solanaceae (가지과)<br/>-Gymnosperms/Monocots(나자식물/단자엽식물)</td> </tr> </table> <ul style="list-style-type: none"> <li>- 유효성분의 정량분석</li> </ul> | 2015 | Lamiaceae II (꿀풀과 II)-Apiaceae I (산형과 I) | 2016 | Apiaceae II (산형과 II) -Rosaceae I (장미과 I) | 2017 | Rosaceae II (장미과 II)-Rutaceae (운향과) | 2018 | Asteraceae (국화과)-Araliaceae (두릅나무과) | 2019 | Solanaceae (가지과)<br>-Gymnosperms/Monocots(나자식물/단자엽식물) | 추진 |
| 2015               | Lamiaceae II (꿀풀과 II)-Apiaceae I (산형과 I)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |      |                                          |      |                                          |      |                                     |      |                                     |      |                                                       |    |
| 2016               | Apiaceae II (산형과 II) -Rosaceae I (장미과 I)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |      |                                          |      |                                          |      |                                     |      |                                     |      |                                                       |    |
| 2017               | Rosaceae II (장미과 II)-Rutaceae (운향과)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |      |                                          |      |                                          |      |                                     |      |                                     |      |                                                       |    |
| 2018               | Asteraceae (국화과)-Araliaceae (두릅나무과)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |      |                                          |      |                                          |      |                                     |      |                                     |      |                                                       |    |
| 2019               | Solanaceae (가지과)<br>-Gymnosperms/Monocots(나자식물/단자엽식물)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |      |                                          |      |                                          |      |                                     |      |                                     |      |                                                       |    |
| 3 단계<br>(‘20~’22년) | <ul style="list-style-type: none"> <li>- 수입대체 생물자원의 제품화/실용화 단계 추진</li> <li>- 선별된 우수 후보 자생식물 분류군에 대한 증식기술 연구</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 예정   |                                          |      |                                          |      |                                     |      |                                     |      |                                                       |    |

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## VII. 부 록

### 1. GC-MS Library Search Report

#### 가. 건채 벌깨덩굴 A

No Name Entered Library Search Report

Data Path : C:\msdchem\1\data\LJY\2014\herbal biology\141030\dry bulggae\  
Data File : dry\_bulggae\_A\_1.D  
Acq On : 30 Oct 2014 2:32  
Operator : LJY  
Sample : dry\_bulggae\_A\_1  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 0

Unknown Spectrum: Apex  
Integration Events: ChemStation Integrator - autoint1.e

| Pk# | RT    | Area% | Library/ID                        | Ref#                   | CAS#              | Qual |
|-----|-------|-------|-----------------------------------|------------------------|-------------------|------|
| 1   | 3.592 | 0.37  | C:\Database\WILEY275.L            |                        |                   |      |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$  | 2                      | 11032 003404-78-2 | 91   |
|     |       |       | ,5-Dimethyl-2-hexene              |                        |                   |      |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$  | 2                      | 11034 003404-78-2 | 91   |
|     |       |       | ,5-Dimethyl-2-hexene              |                        |                   |      |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$  | 2                      | 11031 003404-78-2 | 91   |
|     |       |       | ,5-Dimethyl-2-hexene              |                        |                   |      |
| 2   | 3.644 | 0.16  | C:\Database\WILEY275.L            |                        |                   |      |
|     |       |       | Heptane, 2-methyl- (CAS) \$       | 2-Meth                 | 12449 000592-27-8 | 58   |
|     |       |       | ylheptane \$                      | Methylheptane \$       | (CH3)2CH(CH2)4CH3 |      |
|     |       |       | Heptane, 2-methyl- (CAS) \$       | 2-Meth                 | 12451 000592-27-8 | 58   |
|     |       |       | ylheptane \$                      | Methylheptane \$       | (CH3)2CH(CH2)4CH3 |      |
|     |       |       | Hexane, 2,5-dimethyl- (CAS) \$    | 2,5                    | 12475 000592-13-2 | 53   |
|     |       |       | -Dimethylhexane \$                | Biisobutyl             |                   |      |
| 3   | 3.768 | 0.43  | C:\Database\WILEY275.L            |                        |                   |      |
|     |       |       | Hexane, 3-ethyl- (CAS) \$         | 3-Ethylh               | 12462 000619-99-8 | 72   |
|     |       |       | exane                             |                        |                   |      |
|     |       |       | Hexane, 2,3,3-trimethyl- (CAS) \$ |                        | 19863 016747-28-7 | 72   |
|     |       |       | 2,3,3-Trimethylhexane \$          | 2,3,3-Trimethylheptane |                   |      |
|     |       |       | Heptane, 3-methyl- (CAS) \$       | 3-Meth                 | 12454 000589-81-1 | 70   |
|     |       |       | ylheptane \$                      | 2-Ethylhexane          |                   |      |
| 4   | 3.977 | 0.13  | C:\Database\WILEY275.L            |                        |                   |      |
|     |       |       | 3-Hexanone (CAS) \$               | Hexan-3-one \$         | 6693 000589-38-8  | 83   |
|     |       |       | Ethyl propyl ketone \$            | n-C3H7COC2             |                   |      |
|     |       |       | H5 \$                             | Hexanone-(3) \$        | Aethylpropylketon |      |
|     |       |       | 3-Hexanone (CAS) \$               | Hexan-3-one \$         | 6695 000589-38-8  | 83   |
|     |       |       | Ethyl propyl ketone \$            | n-C3H7COC2             |                   |      |



H5 \$\$ Hexanone-(3) \$\$ Aethylpropylketon  
3-Hexanone (CAS) \$\$ Hexan-3-one \$\$ 6689 000589-38-8 80  
Ethyl propyl ketone \$\$ n-C3H7COC2  
H5 \$\$ Hexanone-(3) \$\$ Aethylpropylketon

5 4.053 0.20 C:\Database\WILEY275.L  
Hexanal (CAS) \$\$ n-Hexanal \$\$ Hexa 6643 000066-25-1 80  
ldehyde \$\$ Caproaldehyde \$\$ Capron  
aldehyde \$\$ n-Caproaldehyde \$\$ Cap  
roic aldehyde \$\$ Hexylaldehyde \$\$  
n-Capronaldehyde \$\$ cyclohexanol \$\$ 1-hexanal \$\$ n-C5H11CHO \$\$ n-Hex  
aldehyde \$\$ n-Caproylaldehyde \$\$ Aldehyde C-6 \$\$ Ka  
2-Hexanone (CAS) \$\$ Hexan-2-one \$\$ 6673 000591-78-6 72  
MBK \$\$ Methyl n-butyl ketone \$\$ 2  
-Oxohexane \$\$ Butyl methyl ketone  
\$\$ Methyl butyl ketone \$\$ n-Butyl  
methyl ketone \$\$ n-C4H9COCH3 \$\$ He  
xanone-2 \$\$ Ketone, butyl methyl \$\$ Mnbk  
2-Hexanone (CAS) \$\$ Hexan-2-one \$\$ 6672 000591-78-6 72  
MBK \$\$ Methyl n-butyl ketone \$\$ 2  
-Oxohexane \$\$ Butyl methyl ketone  
\$\$ Methyl butyl ketone \$\$ n-Butyl  
methyl ketone \$\$ n-C4H9COCH3 \$\$ Hexanone-2 \$\$ Ketone, butyl methyl \$\$ Mnbk

6 4.206 0.11 C:\Database\WILEY275.L  
3-Hexanol (CAS) \$\$ Hexan-3-ol \$\$ C 7756 000623-37-0 72  
2H5CH(OH)C3H7 \$\$ Ethylpropylcarbinol \$\$ Hexanol-(3)  
3-Hexanol (CAS) \$\$ Hexan-3-ol \$\$ C 7767 000623-37-0 72  
2H5CH(OH)C3H7 \$\$ Ethylpropylcarbinol \$\$ Hexanol-(3)  
3-Hexanol (CAS) \$\$ Hexan-3-ol \$\$ C 7766 000623-37-0 64  
2H5CH(OH)C3H7 \$\$ Ethylpropylcarbinol \$\$ Hexanol-(3)

7 4.277 0.19 C:\Database\WILEY275.L  
2-Pentanol, 4-methyl- (CAS) \$\$ 4-M 7805 000108-11-2 59  
ethyl-2-pentanol \$\$ MIC \$\$ MAOH \$\$  
MIBC \$\$ 3-MIC \$\$ 2-Methyl-4-penta  
nol \$\$ Isobutylmethylethanol \$\$ I  
sobutylmethylcarbinol \$\$ Methyliso  
butyl carbinol \$\$ 4-Methyl-2-penty  
l alcohol \$\$ 1,3-Dimethyl-1-butanol \$\$ 4-methyl 2-p  
2-Hexanol (CAS) \$\$ n-C4H9CH(OH)CH3 7750 000626-93-7 59  
\$\$ n-Butylmethylcarbinol \$\$ Hexanol-(2) \$\$ sec-Hexyl alcohol  
2-Pentanol, 4-methyl- (CAS) \$\$ 4-M 7804 000108-11-2 59  
ethyl-2-pentanol \$\$ MIC \$\$ MAOH \$\$  
MIBC \$\$ 3-MIC \$\$ 2-Methyl-4-penta  
nol \$\$ Isobutylmethylethanol \$\$ I  
sobutylmethylcarbinol \$\$ Methyliso  
butyl carbinol \$\$ 4-Methyl-2-penty  
l alcohol \$\$ 1,3-Dimethyl-1-butanol \$\$ 4-methyl 2-p

8 4.363 0.26 C:\Database\WILEY275.L  
Butane, 2-ethoxy- (CAS) \$\$ Ethyl s 7866 002679-87-0 72  
ec-butyl ether \$\$ ETHER, 2-BUTYL E  
THYL \$\$ sec-Butyl ethyl ether \$\$ E  
ther, sec-butyl ethyl \$\$ sec-C4H9OC2H5  
Butane, 2-ethoxy- (CAS) \$\$ Ethyl s 7865 002679-87-0 56

ec-butyl ether \$\$ ETHER, 2-BUTYL E  
 THYL \$\$ sec-Butyl ethyl ether \$\$ E  
 ther, sec-butyl ethyl \$\$ sec-C<sub>4</sub>H<sub>9</sub>OC<sub>2</sub>H<sub>5</sub>  
 2-METHYL-5-TRIDEUTEROMETHYLTETRAZO 5465 026087-53-6 45LE

9 4.434 6.47 C:\Database\WILEY275.L  
 2-Butanol, 3-methyl- (CAS) \$\$ 3-Me 4107 000598-75-4 38  
 thyl-2-butanol \$\$ sec-Isoamyl alco  
 hol \$\$ Methylisopropylcarbinol \$\$  
 (CH<sub>3</sub>)<sub>2</sub>CHCH(OH)CH<sub>3</sub> \$\$ (+)-3-Methyl-2-butanol  
 (2S)-3-methyl-2-butanol \$\$ 2-Butan 4129 001517-66-4 38  
 ol, 3-methyl-, (S)- \$\$ (S)-(+)-3-M  
 ethyl-2-butanol \$\$ (+)-3-Methyl-2-  
 butanol \$\$ (S)-3-Methyl-2-butanol  
 \$\$ (+)-(S)-3-Methyl-2-butanol \$\$ (  
 S)-1-Isopropylethanol \$\$ S-(+)-3-Methylbutan-2-ol  
 Ethane, 1,1-diethoxy- (CAS) \$\$ 1,1 14160 000105-57-7 36  
 -Diethoxyethane \$\$ Acetal \$\$ Dieth  
 yl acetal \$\$ Ethylidene diethyl et  
 her \$\$ Acetaldehyde diethyl acetal  
 \$\$ Acetaldehyde, diethyl acetal \$  
 \$ CH<sub>3</sub>CH(OC<sub>2</sub>H<sub>5</sub>)<sub>2</sub> \$\$ Acetal diethyli  
 que \$\$ Diaethylacetal \$\$ 1,1-Diaethoxy-aethan \$\$ 1,

10 4.496 0.17 C:\Database\WILEY275.L  
 Hexane, 2,3,5-trimethyl- (CAS) \$\$ 19868 001069-53-0 14  
 2,3,5-Trimethylhexane  
 Pyrrolidine, 3-methyl- (CAS) \$\$ 3- 3076 034375-89-8 14  
 Methylpyrrolidine  
 Hexane, 2,3,5-trimethyl- (CAS) \$\$ 19867 001069-53-0 14  
 2,3,5-Trimethylhexane

11 4.577 0.36 C:\Database\WILEY275.L  
 Butane, 2-ethoxy- (CAS) \$\$ Ethyl s 7866 002679-87-0 50  
 ec-butyl ether \$\$ ETHER, 2-BUTYL E  
 THYL \$\$ sec-Butyl ethyl ether \$\$ E  
 ther, sec-butyl ethyl \$\$ sec-C<sub>4</sub>H<sub>9</sub>OC<sub>2</sub>H<sub>5</sub>  
 2-METHYL-5-TRIDEUTEROMETHYLTETRAZO 5465 026087-53-6 45LE  
 Formic acid, 1-methylpropyl ester 7500 000589-40-2 39  
 (CAS) \$\$ sec-Butyl formate \$\$ 1-ME  
 THYLPROPYL FORMATE \$\$ Formic acid,  
 sec-butyl ester \$\$ sec-Butyl methanoate \$\$ s-Butyl formate

12 4.634 0.59 C:\Database\WILEY275.L  
 Heptane, 2,4-dimethyl- (CAS) \$\$ 2, 19825 002213-23-2 91  
 4-Dimethylheptane  
 Octane (CAS) \$\$ n-Octane \$\$ Octane 12440 000111-65-9 72  
 (DOT) \$\$ Isooctane \$\$ n-C<sub>8</sub>H<sub>18</sub> \$\$  
 Oktan \$\$ Oktanen \$\$ Ottani \$\$ UN 1262  
 Heptane, 2,4-dimethyl- (CAS) \$\$ 2, 19823 002213-23-2 64  
 4-Dimethylheptane

13 5.011 0.15 C:\Database\WILEY275.L  
 2,4-Dimethyl-1-heptene 18332 019549-87-2 76  
 1-Heptene, 5-methyl- (CAS) \$\$ 5-Me 10978 013151-04-7 53  
 thyl-1-heptene

- Cyclopentane, 1,3-dimethyl- \$\$ 1,3 6015 002453-00-1 50-Dimethylcyclopentane
- 14 5.453 0.45 C:\Database\WILEY275.L  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19808 002216-34-4 64  
 loctane \$\$ Isononane  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19809 002216-34-4 64  
 loctane \$\$ Isononane  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19810 002216-34-4 52  
 loctane \$\$ Isononane
- 15 5.639 0.18 C:\Database\WILEY275.L  
 Isoxazolidine (CAS) \$\$ 1,2-Oxazoli 1577 000504-72-3 50  
 dine \$\$ Isoxazole, tetrahydro- \$\$  
 1-Oxa-2-azacyclopentane \$\$ isoxazolidin  
 2-Propanol, 1-propoxy- (CAS) \$\$ 1- 14119 001569-01-3 40  
 Propoxy-2-propanol \$\$ 1-PROPOXYISO  
 PROPANOL \$\$ Propasol solvent P \$\$  
 Propylene glycol n-propyl ether  
 2-Heptanol (CAS) \$\$ 2-Hydroxyhepta 13457 000543-49-7 33  
 ne \$\$ s-Heptyl alcohol \$\$ 2-Heptyl  
 alcohol \$\$ Amyl methyl carbinol \$  
 \$ Methyl amyl carbinol \$\$ 1-Methyl  
 hexanol \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>4</sub>CHOHCH<sub>3</sub> \$\$ Heptanol-2
- 16 7.063 0.86 C:\Database\WILEY275.L  
 3-BUTENYL HEXYL ETHER \$\$ Hexane, 1 42546 107995-55-1 38  
 -(3-butenyloxy)-  
 Ethanone, 1-(3-ethyloxiranyl)- (CA 11797 017257-81-7 38  
 S) \$\$ 3,4-EPOXY-2-HEXANONE \$\$ 2-He  
 xanone, 3,4-epoxy- \$\$ 1-Acetyl-2-ethyloxirane  
 Oxirane, 2-methyl-3-propyl-, cis- 6921 006124-90-9 37  
 (CAS) \$\$ Hexane, 2,3-epoxy-, cis-
- 17 7.244 1.01 C:\Database\WILEY275.L  
 Ethanone, 1-(3-butyloxiranyl)- (CA 29471 017257-80-6 38  
 S) \$\$ 2-Octanone, 3,4-epoxy- \$\$ 1-Acetyl-2-butyloxirane  
 2-Pentanone, 3-ethyl-3-methyl- \$\$ 19761 019780-65-5 38  
 3-Ethyl-3-methyl-2-pentanone  
 Hexane, 2,3,5-trimethyl- (CAS) \$\$ 19869 001069-53-0 37  
 2,3,5-Trimethylhexane
- 18 7.454 0.09 C:\Database\WILEY275.L  
 Nonane, 2-methyl- (CAS) \$\$ 2-Methy 30027 000871-83-0 64  
 Inonane \$\$ 2-Methyl-nonane  
 Nonane, 2-methyl- (CAS) \$\$ 2-Methy 30025 000871-83-0 59  
 Inonane \$\$ 2-Methyl-nonane  
 Undecane (CAS) \$\$ n-Undecane \$\$ He 42752 001120-21-4 50  
 ndecane \$\$ n-C<sub>11</sub>H<sub>24</sub> \$\$ UN 2330
- 19 7.515 0.17 C:\Database\WILEY275.L  
 Cyclohexane, azido- (CAS) \$\$ CYCLO 17164 019573-22-9 47  
 HEXYL AZIDE \$\$ Cyclohexyl azide \$\$ Azidocyclohexane  
 2-Pentene, 4,4-dimethyl-, (E)- (CA 6057 000690-08-4 47  
 S) \$\$ 4,4-Dimethyl-trans-2-pentene  
 \$\$ (E)-4,4-Dimethyl-2-pentene \$\$  
 trans-4,4-Dimethyl-2-pentene \$\$ (E)-(CH<sub>3</sub>)<sub>2</sub>C=CHCH<sub>3</sub>

trans-4,4-Dimethyl-2-hexene \$\$ 2-H 11203 019550-83-5 38  
 exene, 4,4-dimethyl-, (E)- \$\$ 4,4-Dimethyl-trans-2-hexene

20 7.649 0.10 C:\Database\WILEY275.L  
 Hexane, 2,4-dimethyl- (CAS) \$\$ 2,4 12470 000589-43-5 50  
 -Dimethylhexane  
 Hexane, 2,4-dimethyl- (CAS) \$\$ 2,4 12472 000589-43-5 50  
 -Dimethylhexane  
 Hexane, 2,4-dimethyl- (CAS) \$\$ 2,4 12471 000589-43-5 50  
 -Dimethylhexane

21 7.758 2.72 C:\Database\WILEY275.L  
 1 OCTEN 3 OL 19694 003391-86-4 90  
 1-OCTEN-3-OL 19692 053907-72-5 86  
 1-Octen-3-ol (CAS) \$\$ Oct-1-en-3-o 19569 003391-86-4 86  
 l \$\$ 3-Hydroxy-1-octene \$\$ Amyl vi  
 nyl carbinol \$\$ Vinyl amyl carbino  
 l \$\$ n-Oct-1-en-3-ol \$\$ Octan-3-on  
 e \$\$ (Z)-Oct-5-en-3-ol \$\$ octen-3-ol \$\$ Matsutake alcohol \$\$ 1-Okten-3-ol

22 7.939 0.10 C:\Database\WILEY275.L  
 Heptane, 2,2,4,6,6-pentamethyl- (C 55986 013475-82-6 53  
 AS) \$\$ 2,2,4,6,6-Pentamethylheptan  
 Octane, 2,5,6-trimethyl- (CAS) 42800 062016-14-2 50  
 Heptane, 2,2,4-trimethyl- (CAS) \$\$ 30078 014720-74-2 47  
 2,2,4-Trimethylheptane

23 8.073 0.27 C:\Database\WILEY275.L  
 3-Octanol (CAS) \$\$ n-Octan-3-ol \$\$ 21076 000589-98-0 86  
 Ethylamylcarbinol \$\$ Octan-3-ol \$  
 \$ Amylethylcarbinol \$\$ Ethyl-n-amy  
 lcarbinol \$\$ Octanol-3 \$\$ D-n-Octanol  
 ETHYL AMYL CARBINOL \$\$ 3 OCTANOL 21217 000589-98-0 80  
 3-Octanol (CAS) \$\$ n-Octan-3-ol \$\$ 21079 000589-98-0 80  
 Ethylamylcarbinol \$\$ Octan-3-ol \$  
 \$ Amylethylcarbinol \$\$ Ethyl-n-amy  
 lcarbinol \$\$ Octanol-3 \$\$ D-n-Octanol

24 8.363 0.22 C:\Database\WILEY275.L  
 Nonane, 2,5-dimethyl- (CAS) \$\$ 2,5 42787 017302-27-1 52  
 -Dimethylnonane  
 Heptane, 4,4-dimethyl- (CAS) \$\$ 4, 19841 001068-19-5 52  
 4-Dimethylheptane  
 4,4-Dimethylcyclooctene 26889 000000-00-0 47

25 8.473 0.15 C:\Database\WILEY275.L  
 Nonane, 2,5-dimethyl- (CAS) \$\$ 2,5 42787 017302-27-1 64  
 -Dimethylnonane  
 Hexane, 2,2,3,3-tetramethyl- (CAS) 30095 013475-81-5 53  
 \$\$ 2,2,3,3-Tetramethylhexane  
 Hexane, 2,2,3,3-tetramethyl- (CAS) 30094 013475-81-5 53  
 \$\$ 2,2,3,3-Tetramethylhexane

26 8.549 0.32 C:\Database\WILEY275.L  
 Decane, 4-methyl- (CAS) \$\$ 4-Methy 42779 002847-72-5 90ldecane  
 Nonane, 2,6-dimethyl- (CAS) \$\$ 2,6 42788 017302-28-2 90-Dimethylnonane

Decane, 4-methyl- (CAS) \$\$ 4-Methy 42781 002847-72-5 87ldecane

- 27 9.030 0.15 C:\Database\WILEY275.L  
 Cyclohexanone, 3,3,5-trimethyl- (C 28088 000873-94-9 74  
 AS) \$\$ 3,3,5-Trimethylcyclohexanone \$\$ Dihydroisophorone  
 Cyclohexanone, 3,3,5-trimethyl- (C 28089 000873-94-9 72  
 AS) \$\$ 3,3,5-Trimethylcyclohexanone \$\$ Dihydroisophorone  
 Cyclohexanone, 3,3,5-trimethyl- (C 28084 000873-94-9 68  
 AS) \$\$ 3,3,5-Trimethylcyclohexanone \$\$ Dihydroisophorone
- 28 9.239 0.79 C:\Database\WILEY275.L  
 3,6-Dimethyldecane \$\$ Decane, 3,6- 55972 017312-53-7 62  
 dimethyl-  
 Decane, 2,3,7-trimethyl- (CAS) 69525 062238-13-5 59  
 (R,R)-3,8-Dimethyldecane 55973 000000-00-0 53
- 29 9.363 0.28 C:\Database\WILEY275.L  
 Dodecane, 2,6,10-trimethyl- (CAS) 98330 003891-98-3 72  
 \$\$ Farnesane \$\$ Farnesan \$\$ 2,6,10-Trimethyldodecane  
 Octane, 6-ethyl-2-methyl- (CAS) 42794 062016-19-7 64  
 Nonane, 3-methyl-5-propyl- (CAS) 69544 031081-18-2 64
- 30 9.696 0.11 C:\Database\WILEY275.L  
 1-methyl-2-ethylcyclopentane isome 11183 000000-00-0 38r 1  
 Cyclohexane, 1,2,4-trimethyl- (CAS 18319 002234-75-5 35  
 ) \$\$ 1,2,4-TRIMETHYLCYCLOHEXANE, (CIS PLUS TRANS) \$\$ 1,2,4-Trimethyl  
 cyclohexane  
 4-Methyl-2-heptene \$\$ 2-Heptene, 4 11196 003404-56-6 30-methyl-
- 31 10.182 0.66 C:\Database\WILEY275.L  
 Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12480 000563-16-6 53-Dimethylhexane  
 Heptane, 2,5,5-trimethyl- (CAS) \$\$ 30083 001189-99-7 50 2,5,5-Trimethylheptane  
 Pentane, 2,3,3-trimethyl- (CAS) \$\$ 12497 000560-21-4 50  
 2,3,3-Trimethylpentane \$\$ C2H5C(CH3)2CH(CH3)2
- 32 10.301 0.21 C:\Database\WILEY275.L  
 Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12481 000563-16-6 47  
 -Dimethylhexane  
 Tetradecane, 4-methyl- (CAS) 98321 025117-24-2 47  
 3,6-Dimethyldecane \$\$ Decane, 3,6- 55972 017312-53-7 43  
 dimethyl-
- 33 10.468 0.29 C:\Database\WILEY275.L  
 1-Iodo-2-methylnonane 150962 000000-00-0 38  
 2-METHOXYCYCLOHEXANONE 19319 000000-00-0 35  
 Triacontane (CAS) \$\$ n-Triacontane 242803 000638-68-6 35
- 34 11.449 0.16 C:\Database\WILEY275.L  
 Hexadecane, 7,9-dimethyl- (CAS) \$\$ 139421 021164-95-4 58  
 7,9-Dimethylhexadecane  
 Pentadecane, 2-methyl- (CAS) \$\$ 14 112861 001560-93-6 58  
 -METHYLPENTADECANE \$\$ 2-Methylpentadecane  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 53  
 \$ Octadecan
- 35 12.235 0.30 C:\Database\WILEY275.L

Heptadecane (CAS) \$\$ n-Heptadecane 126477 000629-78-7 72  
 \$\$ Normal-heptadecane  
 10-Methylnonadecane 163906 000000-00-0 64  
 Decane, 2,4,6-trimethyl- (CAS) 69527 062108-27-4 59

36 12.525 0.27 C:\Database\WILEY275.L  
 Undecane, 2,6-dimethyl- (CAS) \$\$ 2 69488 017301-23-4 72  
 ,6-Dimethylundecane \$\$ 2,6-Dimethylundecene  
 Dodecane, 6-methyl- (CAS) \$\$ 6-Met 69473 006044-71-9 72  
 hylldodecane  
 Undecane, 2,5-dimethyl- (CAS) \$\$ 2 69484 017301-22-3 59  
 ,5-Dimethylundecane

37 12.749 0.33 C:\Database\WILEY275.L  
 2,3-DIMETHYLBENZALDEHYDE \$\$ Benzal 23118 005779-93-1 43  
 dehyde, 2,3-dimethyl- (CAS) \$\$ Hemellitaldehyde  
 Undecane, 4,8-dimethyl- (CAS) 69504 017301-33-6 35  
 Benzaldehyde, ethyl- (CAS) \$\$ AR-E 23117 053951-50-1 30  
 THYLBENZALDEHYDE \$\$ P-ETHYLBENZALD  
 EHYDE \$\$ Ethylbenzaldehyde

38 12.887 0.20 C:\Database\WILEY275.L  
 3,3,3-d(3)-exo-2-Norbornyl chlorid 20657 000000-00-0 38  
 4-Heptenal (CAS) 10676 062238-34-0 38  
 Cyclopentane, heneicosyl- (CAS) \$\$ 219250 006703-82-8 37  
 Heneicosane, 1-cyclopentyl- \$\$ n-Heneicosylcyclopentane

39 13.216 0.17 C:\Database\WILEY275.L  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260489 000630-06-8 80  
 acontane \$\$ NOR-HEXATRIACONTANE  
 Nonadecane (CAS) \$\$ n-Nonadecane 151986 000629-92-5 74  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 72  
 \$ Octadecan

40 13.363 0.22 C:\Database\WILEY275.L  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139441 000593-45-3 90  
 \$ Octadecan  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260489 000630-06-8 90  
 acontane \$\$ NOR-HEXATRIACONTANE  
 10-Methylnonadecane 163906 000000-00-0 80

41 13.520 0.28 C:\Database\WILEY275.L  
 Dodecane, 4,6-dimethyl- (CAS) 83566 061141-72-8 86  
 Dodecane, 4,6-dimethyl- (CAS) 83567 061141-72-8 78  
 1-Decene, 4-methyl- (CAS) 40862 013151-29-6 50

42 13.744 0.37 C:\Database\WILEY275.L  
 Undecane, 2,4-dimethyl- (CAS) \$\$ 2 69481 017312-80-0 72  
 ,4-Dimethylundecane  
 Dodecane, 3-methyl- (CAS) \$\$ 3-Met 69468 017312-57-1 64  
 hylldodecane  
 Triacontane (CAS) \$\$ n-Triacontane 242809 000638-68-6 53

43 14.035 0.99 C:\Database\WILEY275.L  
 Pentadecane (CAS) \$\$ n-Pentadecane 98307 000629-62-9 72  
 \$\$ CH3(CH2)13CH3

Dodecane, 4,6-dimethyl- (CAS) 83566 061141-72-8 72  
Nonane, 2-methyl-5-propyl- (CAS) 69543 031081-17-1 72

44 14.235 0.14 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151985 000629-92-5 64  
Dodecane (CAS) \$\$ n-Dodecane \$\$ Ba 55928 000112-40-3 64  
51-090453 \$\$ Adakane 12 \$\$ Isododecane \$\$ CH3(CH2)10CH3 \$\$ Bihexyl  
\$\$ Dihexyl \$\$ n-Dodecane min \$\$ N-Dodecan \$\$ Duodecane  
Pentadecane (CAS) \$\$ n-Pentadecane 98310 000629-62-9 53  
\$\$ CH3(CH2)13CH3

45 14.301 0.15 C:\Database\WILEY275.L  
Pentadecane (CAS) \$\$ n-Pentadecane 98301 000629-62-9 50  
\$\$ CH3(CH2)13CH3  
Undecane, 3,7-dimethyl- (CAS) 69497 017301-29-0 50  
Tetradecane (CAS) \$\$ n-Tetradecane 83535 000629-59-4 50  
\$\$ Isotetradecane

46 14.525 0.23 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 43  
\$ Octadecan  
N-TETRADECANE 83576 000000-00-0 38  
Undecane, 2,3-dimethyl- (CAS) \$\$ 2 69480 017312-77-5 38  
,3-Dimethylundecane

47 14.616 0.41 C:\Database\WILEY275.L  
2-Hexyl-1-octanol 100077 000000-00-0 72  
Ethanol, 2-(octyloxy)- (CAS) \$\$ 2- 59033 010020-43-6 50  
(X-OCTYLOXY)ETHANOL \$\$ 2-Octyloxye  
thanol \$\$ 2-(Octyloxy)ethanol \$\$ 1  
-(2-Hydroxyethoxy)octane \$\$ Ethyle  
ne glycol mono-n-octyl ether \$\$ Et  
hylene glycol mono-octyl ether \$\$ n-Octyl-mono-oxyethylene  
1-Hexadecanol (CAS) \$\$ Cetal \$\$ Et 128171 036653-82-4 47  
hal \$\$ Ethol \$\$ Cetanol \$\$ Cetylol  
\$\$ Adol 52 \$\$ Lanol C \$\$ Adol 54  
\$\$ Lorol 24 \$\$ Alfol 16 \$\$ Aldol 5  
4 \$\$ Atalco C \$\$ Cetaffine \$\$ Loxa  
nol K \$\$ Adol 52NF \$\$ Elfacos C \$\$  
Crodacol C \$\$ Hyfatol 16 \$\$ Cetanol CA \$\$ Siponol

48 14.754 0.13 C:\Database\WILEY275.L  
Undecane, 2,4-dimethyl- (CAS) \$\$ 2 69481 017312-80-0 58  
,4-Dimethylundecane  
Heptane, 2,4-dimethyl- (CAS) \$\$ 2, 19824 002213-23-2 50  
4-Dimethylheptane  
Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12480 000563-16-6 50  
-Dimethylhexane

49 15.054 0.53 C:\Database\WILEY275.L  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112856 000544-76-3 78  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
Decane, 2,3,6-trimethyl- (CAS) 69524 062238-12-4 72  
Dodecane, 1-iodo- (CAS) \$\$ n-Dodec 174485 004292-19-7 64  
yl iodide \$\$ Dodecyl iodide \$\$ Lauryl iodide \$\$ 1-Iodododecane

50 15.654 0.78 C:\Database\WILEY275.L  
 Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(2-hydroxy-1-methylethyl)propyl ester (CAS) \$\$ 2,2-Dimethyl-1-(2-hydroxy-1-isopropyl)propyl ester of isobutanoic acid  
 Butanoic acid, 2-methylpropyl ester (CAS) \$\$ isobutyl butanoate \$\$ Isobutyl butyrate \$\$ Isobutyl n-butylate \$\$ 2-Methylpropyl butyrate \$  
 \$ Butyric acid, isobutyl ester \$\$  
 Isobutyl ester of butanoic acid \$\$  
 n-Butyric acid isobutyl ester \$\$ 2-Methylpropyl butanoic acid, hexyl ester (CAS) \$ 57350 002639-63-6 40  
 \$ Hexyl butanoate \$\$ HEXYL ESTER OF BUTYRIC ACID \$  
 n-HEXYL BUTYRATE \$  
 Hexyl butyrate \$  
 n-HEXYL BUTYRATE \$  
 Hexyl butanoate \$  
 Butyric acid, hexyl ester \$  
 HEXYL-N-BUTANOATE \$  
 n-HEXYL N-BUTANOATE

51 15.906 0.12 C:\Database\WILEY275.L  
 Tridecane, 2-methyl- (CAS) \$\$ 2-Methyltridecane \$\$ 2-Methyl-n-tridecane  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112843 000544-76-3 64  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
 Tetracosane (CAS) \$\$ n-Tetracosane 204922 000646-31-1 64

52 16.101 1.37 C:\Database\WILEY275.L  
 Butanoic acid, butyl ester (CAS) \$ 31035 000109-21-7 91  
 \$ n-Butyl n-butylate \$\$ Butyl butylate \$\$ Butyl butanoate \$\$ 1-Butyl butylate \$\$ n-Butyl butylate \$\$ n-Butyl butanoate  
 \$\$ Butyric acid, butyl ester \$  
 Butyl ester of butanoic acid \$  
 Butyl n-butylate \$  
 Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester (CAS) \$ 101383 074367-34-3 83  
 \$ 3-Hydroxy-2,2,4-trimethylpentyl ester of isobutanoic acid  
 Butanoic acid, butyl ester (CAS) \$ 31034 000109-21-7 83  
 \$ n-Butyl n-butylate \$\$ Butyl butylate \$\$ Butyl butanoate \$\$ 1-Butyl butylate \$\$ n-Butyl butylate \$\$ n-Butyl butanoate  
 \$\$ Butyric acid, butyl ester \$  
 Butyl ester of butanoic acid \$  
 Butyl n-butylate \$

53 16.606 0.22 C:\Database\WILEY275.L  
 Tetradecane (CAS) \$\$ n-Tetradecane 83536 000629-59-4 80  
 \$\$ Isotetradecane  
 TRIDECANE 69549 000000-00-0 80  
 Tridecane (CAS) \$\$ n-Tridecane \$ 69456 000629-50-5 80  
 Tridecane, n-

54 16.763 0.17 C:\Database\WILEY275.L  
 Hexadecane, 7,9-dimethyl- (CAS) \$\$ 139421 021164-95-4 58  
 7,9-Dimethylhexadecane



|    |        |      |                                       |                            |
|----|--------|------|---------------------------------------|----------------------------|
|    |        |      | pentadecane                           | 98340 000629-62-9 53       |
|    |        |      | TRIDECANE                             | 69549 000000-00-0 52       |
| 55 | 16.816 | 0.26 | C:\Database\WILEY275.L                |                            |
|    |        |      | Pentacosane (CAS) \$\$ n-Pentacosane  | 212920 000629-99-2 80      |
|    |        |      | Nonadecane (CAS) \$\$ n-Nonadecane    | 151981 000629-92-5 80      |
|    |        |      | NONADECANE                            | 152008 000000-00-0 80      |
| 56 | 16.901 | 0.25 | C:\Database\WILEY275.L                |                            |
|    |        |      | Heneicosane (CAS) \$\$ n-Heneicosane  | 175419 000629-94-7 74      |
|    |        |      | Heptadecane (CAS) \$\$ n-Heptadecane  | 126473 000629-78-7 72      |
|    |        |      | \$\$ Normal-heptadecane               |                            |
|    |        |      | Octadecane (CAS) \$\$ n-Octadecane \$ | 139439 000593-45-3 72      |
|    |        |      | \$ Octadecan                          |                            |
| 57 | 17.663 | 0.31 | C:\Database\WILEY275.L                |                            |
|    |        |      | Pentadecane (CAS) \$\$ n-Pentadecane  | 98310 000629-62-9 72       |
|    |        |      | \$\$ CH3(CH2)13CH3                    |                            |
|    |        |      | Pentadecane (CAS) \$\$ n-Pentadecane  | 98301 000629-62-9 72       |
|    |        |      | \$\$ CH3(CH2)13CH3                    |                            |
|    |        |      | Tetradecane (CAS) \$\$ n-Tetradecane  | 83536 000629-59-4 64       |
|    |        |      | \$\$ Isotetradecane                   |                            |
| 58 | 17.797 | 0.40 | C:\Database\WILEY275.L                |                            |
|    |        |      | Docosane (CAS) \$\$ n-Docosane \$     | 186056 000629-97-0 80      |
|    |        |      | 2H46 STANDARD \$ Normal-docosane      |                            |
|    |        |      | Nonadecane (CAS) \$\$ n-Nonadecane    | 151982 000629-92-5 80      |
|    |        |      | Heptadecane (CAS) \$\$ n-Heptadecane  | 126473 000629-78-7 74      |
|    |        |      | \$\$ Normal-heptadecane               |                            |
| 59 | 17.954 | 0.95 | C:\Database\WILEY275.L                |                            |
|    |        |      | Eicosane (CAS) \$\$ n-Eicosane        | 163881 000112-95-8 86      |
|    |        |      | Eicosane (CAS) \$\$ n-Eicosane        | 163880 000112-95-8 78      |
|    |        |      | Eicosane (CAS) \$\$ n-Eicosane        | 163886 000112-95-8 55      |
| 60 | 18.368 | 0.14 | C:\Database\WILEY275.L                |                            |
|    |        |      | Undecane, 3,9-dimethyl- (CAS)         | 69499 017301-31-4 38       |
|    |        |      | Nonadecane (CAS) \$\$ n-Nonadecane    | 151982 000629-92-5 35      |
|    |        |      | Iron, tricarbonyl[N-(phenyl-2-pyri    | 233784 074764-11-7 35      |
|    |        |      | dinylmethylene)benzenamine-N,N']-     |                            |
| 61 | 18.477 | 0.58 | C:\Database\WILEY275.L                |                            |
|    |        |      | Octadecane (CAS) \$\$ n-Octadecane \$ | 139440 000593-45-3 80      |
|    |        |      | \$ Octadecan                          |                            |
|    |        |      | Dodecane, 3-methyl- (CAS) \$          | 3-Met 69468 017312-57-1 72 |
|    |        |      | hyldodecane                           |                            |
|    |        |      | Eicosane (CAS) \$\$ n-Eicosane        | 163885 000112-95-8 58      |
| 62 | 18.587 | 1.41 | C:\Database\WILEY275.L                |                            |
|    |        |      | Docosane (CAS) \$\$ n-Docosane \$     | 186056 000629-97-0 87      |
|    |        |      | 2H46 STANDARD \$ Normal-docosane      |                            |
|    |        |      | Octadecane (CAS) \$\$ n-Octadecane \$ | 139440 000593-45-3 83      |
|    |        |      | \$ Octadecan                          |                            |
|    |        |      | Triacontane (CAS) \$\$ n-Triacontane  | 242802 000638-68-6 80      |
| 63 | 18.801 | 0.36 | C:\Database\WILEY275.L                |                            |

Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 80  
 \$\$ Normal-heptadecane  
 Pentadecane (CAS) \$\$ n-Pentadecane 98301 000629-62-9 80  
 \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>13</sub>CH<sub>3</sub>  
 Dodecane (CAS) \$\$ n-Dodecane \$\$ Ba 55935 000112-40-3 72  
 51-090453 \$\$ Adakane 12 \$\$ Isododecane  
 ecane \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>10</sub>CH<sub>3</sub> \$\$ Bihexyl  
 \$\$ Dihexyl \$\$ n-Dodecane min \$\$ N-Dodecan \$\$ Duodecane

64 18.973 0.31 C:\Database\WILEY275.L  
 Tetradecane (CAS) \$\$ n-Tetradecane 83544 000629-59-4 80  
 \$\$ Isotetradecane  
 Heptadecane (CAS) \$\$ n-Heptadecane 126477 000629-78-7 80  
 \$\$ Normal-heptadecane  
 Heptadecane (CAS) \$\$ n-Heptadecane 126478 000629-78-7 80  
 \$\$ Normal-heptadecane

65 19.068 0.35 C:\Database\WILEY275.L  
 BHT \$\$ Butylated hydroxytoluene 105989 000128-37-0 96  
 Phenol, 2,6-bis(1,1-dimethylethyl) 105779 000128-37-0 94  
 -4-methyl- (CAS) \$\$ 4-Methyl-2,6-di-  
 i-tert-butylphenol \$\$ BHT \$\$ P 21  
 \$\$ CAO 3 \$\$ AO 29 \$\$ CAO 1 \$\$ AO 4  
 K \$\$ DBPC \$\$ P 21 \$ \$\$ 2,6-DI-TERT  
 -4-METHYLPHENOL \$\$ Buks \$\$ Ional \$  
 \$ Ionole \$\$ Deenax \$\$ Dalpac \$\$ Stavox \$\$ Vianol \$\$  
 Phenol, 2,6-bis(1,1-dimethylethyl) 105772 000128-37-0 93  
 -4-methyl- (CAS) \$\$ 4-Methyl-2,6-di-  
 i-tert-butylphenol \$\$ BHT \$\$ P 21  
 \$\$ CAO 3 \$\$ AO 29 \$\$ CAO 1 \$\$ AO 4  
 K \$\$ DBPC \$\$ P 21 \$ \$\$ 2,6-DI-TERT  
 -4-METHYLPHENOL \$\$ Buks \$\$ Ional \$  
 \$ Ionole \$\$ Deenax \$\$ Dalpac \$\$ Stavox \$\$ Vianol \$\$

66 19.144 0.45 C:\Database\WILEY275.L  
 Phenol, 2,4-bis(1,1-dimethylethyl) 91570 000096-76-4 64  
 - (CAS) \$\$ 2,4-Di-tert-butylphenol  
 \$\$ 2,4-BIS(TERT-BUTYL)-PHENOL \$\$  
 2,4-Di-t-butylphenol \$\$ Phenol, 2,  
 4-di-tert-butyl- \$\$ 2,4-Bis(1,1-di-  
 methylethyl)phenol \$\$ 2,4-Di-tert-  
 butyl-phenol \$\$ 4-(1,5-Dimethylhex-4-enyl)cyclohex-  
 Phenol, 2,4-bis(1,1-dimethylethyl) 91572 000096-76-4 58  
 - (CAS) \$\$ 2,4-Di-tert-butylphenol  
 \$\$ 2,4-BIS(TERT-BUTYL)-PHENOL \$\$  
 2,4-Di-t-butylphenol \$\$ Phenol, 2,  
 4-di-tert-butyl- \$\$ 2,4-Bis(1,1-di-  
 methylethyl)phenol \$\$ 2,4-Di-tert-  
 butyl-phenol \$\$ 4-(1,5-Dimethylhex-4-enyl)cyclohex-  
 Phenol, 2,5-bis(1,1-dimethylethyl) 91579 005875-45-6 58  
 - (CAS) \$\$ 2,5-Di-tert-butylphenol  
 \$\$ Phenol, 2,5-di-tert-butyl- \$\$  
 2,5-Di-tert-butylhydroxybenzene

67 19.363 0.20 C:\Database\WILEY275.L  
 Decane (CAS) \$\$ n-Decane \$\$ Isodec 30015 000124-18-5 38

ane \$\$ n-C10H22 \$\$ UN 2247  
 1-Octanol, 2-butyl- (CAS) \$\$ 2-But 71293 003913-02-8 38  
 yl-1-octanol \$\$ 2-Butyloctanol \$\$  
 2-Butyloctyl alcohol \$\$ 5-(Hydroxymethyl)undecane  
 pentadecane 98340 000629-62-9 27

68 19.773 0.27 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 72  
 Undecane, 4,7-dimethyl- (CAS) 69503 017301-32-5 64  
 Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 64

69 19.901 1.08 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
 2H46 STANDARD \$\$ Normal-docosane  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 72  
 Dodecane, 1-iodo- (CAS) \$\$ n-Dodec 174485 004292-19-7 64  
 yl iodide \$\$ Dodecyl iodide \$\$ Lauryl iodide \$\$ 1-Iodododecane

70 20.616 0.41 C:\Database\WILEY275.L  
 Spiro[4.5]dec-6-ene (CAS) \$\$ SPIRO 25140 000697-28-9 38  
 (4,5)DEC-6-ENE \$\$ Spiro[4,5]dec-6-ene  
 (-)-Caryophyllene oxide \$\$ (-)-5-O 105971 001139-30-6 35  
 xatricyclo[8.2.0.0(4,6)]dodecane,,  
 12-trimethyl-9-methylene-, [1R-(1R  
 \*,4R\*,6R\*,10S\*)]- (CAS) \$\$ (-)-.be  
 ta.-Caryophyllene epoxide \$\$ caryo  
 phyllene oxide \$\$ (-)caryophyllene  
 oxide \$\$ 5-Oxatricyclo[8.2.0.0(4,6)-]dodecane, 4,1  
 3-Tetradecen-5-yne, (E)- (CAS) 76729 074744-44-8 27

71 21.087 0.23 C:\Database\WILEY275.L  
 2-ethoxycarbonylbenzothiazole \$\$ 2 92170 032137-76-1 50  
 -Benzothiazolecarboxylic acid, eth  
 yl ester \$\$ Ethyl 2-benzothiazolecarboxylate  
 1-Azido-1-(p-methoxyphenyl)ethane 61251 091633-30-6 22  
 Benzenemethanol, 4-(1-methylethyl) 35755 000536-60-7 14  
 - (CAS) \$\$ P-CYMEN-.ALPHA.-OL \$\$ 1  
 -HYDROXYMETHYL-4-ISOPROPYLBENZENE  
 \$\$ Cuminol \$\$ p-Cymen-7-ol \$\$ Cumi  
 c alcohol \$\$ Cumyl alcohol \$\$ Cumi  
 nyl alcohol \$\$ Cuminic alcohol \$\$  
 p-Isopropylbenzyl alcohol \$\$ CUMINYL ALCOHOL (20 EV

72 21.287 1.88 C:\Database\WILEY275.L  
 (+) spathulenol 105983 077171-55-2 99  
 Spathulenol \$\$ 1H-Cycloprop[e]azul 105942 006750-60-3 98  
 en-7-ol, decahydro-1,1,7-trimethyl  
 -4-methylene-, [1ar-(1a.alpha.,4a.  
 alpha.,7.beta.,7a.beta.,7b.alpha.)  
 ]- \$\$ 1H-Cycloprop[e]azulen-7-ol,  
 decahydro-1,1,7-trimethyl-4-methyl  
 ene- \$\$ Espatulenol \$\$ (+)-Spathulenol  
 (-)-Spathulenol (CAS) \$\$ 1H-Cyclop 105982 077171-55-2 94  
 rop[e]azulen-7-ol, decahydro-1,1,7  
 -trimethyl-4-methylene-, [1aS-(1a.  
 alpha.,4a.alpha.,7.beta. \$\$ ent-Spa

thulenol \$\$ 1H-Cycloprop[e]azulen-  
7-ol, decahydro-1,1,7-trimethyl-4-  
methylene-, [1aS-(1a.alpha.,4a.alpha.,7.beta.)] \$\$

- 73 21.444 13.75 C:\Database\WILEY275.L  
PENTAN-1,3-DIOLDIISOBUTYRATE, 2,2, 166858 000000-00-0 64  
4-TRIMETHYL- \$\$ 1,3-Di(isobutoxyca  
rbonyl)-2,4,4-trimethylpentane  
Propanoic acid, 2-methyl-, 1-(1,1- 166859 074381-40-1 56  
dimethylethyl)-2-methyl-1,3-propanediyl ester (CAS)  
Butanoic acid, 2-butoxy-1-methyl-2 101132 007492-70-8 53  
-oxoethyl ester (CAS) \$\$ Butyl but  
yryllactate \$\$ Butyric acid, ester  
with butyl lactate \$\$ Butyl butyr  
yl lactate \$\$ Butyl butyrolactate  
\$\$ Lactic acid, butyl ester, butyrate
- 74 21.758 0.29 C:\Database\WILEY275.L  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112855 000544-76-3 95  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112845 000544-76-3 94  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112856 000544-76-3 81  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane
- 75 21.906 0.25 C:\Database\WILEY275.L  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 83  
\$\$ Normal-heptadecane  
9-methylnonadecane 163903 000000-00-0 80  
10-Methylnonadecane 163906 000000-00-0 80
- 76 22.206 0.11 C:\Database\WILEY275.L  
t-(4,7)-E-(7,8)-8-exo-ethenyl-8-ex 118125 069855-24-9 72  
o-methyl-4-methylene-7-endo-propen-2'-yl-2-oxabicyclo[4.3.0]non-3-on  
1-deoxy-8-epiivangustin 118139 097605-47-5 72  
t-(4,7)-E-(7,8)-8-endo-ethenyl-8-e 118124 069855-24-9 72  
ndo-methyl-4-methylene-7-exo-prope  
n-2'-yl-2-oxabicyclo[4.3.0]non-3-one
- 77 22.306 0.24 C:\Database\WILEY275.L  
Octadecane, 9-ethyl-9-heptyl- (CAS 226681 055282-27-4 43  
) \$\$ 9-Ethyl-9-n-heptyloctadecane  
Eicosane, 9-octyl- (CAS) \$\$ 9-n-Oc 232584 013475-77-9 43  
tyleicosane  
Hexadecane, 8-hexyl-8-pentyl- (CAS 226679 055282-29-6 43  
) \$\$ 8-N-PENTYL-8-N-HEXYLHEXADECAN
- 78 22.649 0.47 C:\Database\WILEY275.L  
1,4-Methanobenzocyclodecene, 1,2,3 87303 074708-73-9 45  
,4,4a,5,8,9,12,12a-decahydro- (CAS  
) \$\$ TRICYCLO[10.2.1.0(2,11)]PENTADEC-4,8-DIENE  
Tricyclopentadeca-3,7-dien[8.4.0.1 87339 000000-00-0 45  
(11,14)]  
exo-Octahydro-4,7-methano-1H-inden 25274 002825-82-3 30  
e \$\$ 4,7-Methano-1H-indene, octahy  
dro-, (3a.alpha.,4.beta.,7.beta.,7

a.alpha.)- (CAS) \$\$ JP 10 \$\$ 4,7-M  
ethanoindan, hexahydro-, exo- \$\$ e  
xo-3,4,8,9-Tetrahydrodicyclopentad  
iene \$\$ exo-Tricyclo[5.2.1.0(2,6)]decane \$\$ exo-Tet

- 79 22.706 0.19 C:\Database\WILEY275.L  
Octadecane, 3-ethyl-5-(2-ethylbutyl 220178 055282-12-7 58  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Undecane (CAS) \$\$ n-Undecane \$\$ He 42750 001120-21-4 58  
ndecane \$\$ n-C11H24 \$\$ UN 2330  
Undecane (CAS) \$\$ n-Undecane \$\$ He 42752 001120-21-4 58  
ndecane \$\$ n-C11H24 \$\$ UN 2330
- 80 22.758 0.38 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151982 000629-92-5 80  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 80  
PENTADECANE, 2,6,10-TRIMETHYL- \$\$ 139453 000000-00-0 80  
NOR-PRISTAN
- 81 22.844 0.14 C:\Database\WILEY275.L  
Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 50  
tane \$\$ Bicetyl \$\$ Tris(trimethyls  
ilyl)ether, methyl ester of ethyl  
anthranilate azo pigment(.alpha.z)  
of bilivubin-1x.alpha. 2-O-acyl glucuronide  
10-Methylnonadecane 163906 000000-00-0 49  
Tetracosane (CAS) \$\$ n-Tetracosane 204917 000646-31-1 47
- 82 22.978 0.83 C:\Database\WILEY275.L  
Octadecane, 1-bromo- (CAS) \$\$ Stea 200817 000112-89-0 38  
ryl bromide \$\$ Octadecyl bromide \$  
\$ 1-Bromooctadecane \$\$ n-Octadecyl  
bromide \$\$ 1-BROMO OCTADECANE (DOMIPHEN BR ART.)  
spathulanol 108426 000000-00-0 25  
Tritriacontane (CAS) \$\$ n-Tritriac 253566 000630-05-7 25  
ontane
- 83 23.116 0.41 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 64  
2H46 STANDARD \$\$ Normal-docosane  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 58  
Eicosane (CAS) \$\$ n-Eicosane 163886 000112-95-8 58
- 84 23.206 0.41 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 87  
N-NONADECANE 152007 000629-92-5 86  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
2H46 STANDARD \$\$ Normal-docosane
- 85 23.292 0.39 C:\Database\WILEY275.L  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 49  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 46  
Octadecane (CAS) \$\$ n-Octadecane \$ 139441 000593-45-3 46  
\$ Octadecan
- 86 23.358 0.23 C:\Database\WILEY275.L

Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 68  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 68  
Heptadecane, 2,6,10,15-tetramethyl 175423 054833-48-6 64  
- (CAS) \$\$ 2,6,10,15-TETRAMETHYLHEPTADECANE

87 23.482 0.45 C:\Database\WILEY275.L  
Silane, trichlorooctadecyl- (CAS) 228772 000112-04-9 38  
\$\$ Octadecyltrichlorosilane \$\$ Sil  
ane, octadecyltrichloro- \$\$ Trichlorooctadecylsilane \$\$ UN 1800  
Octadecane, 1-chloro- (CAS) \$\$ 1-C 168748 003386-33-2 30  
hlorooctadecane \$\$ Octadecyl chlor  
ide \$\$ n-Octadecyl chloride \$\$ Chlorooctadecane  
Tetradecane (CAS) \$\$ n-Tetradecane 83544 000629-59-4 27  
\$\$ Isotetradecane

88 23.654 0.46 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 91  
2H46 STANDARD \$\$ Normal-docosane  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 91  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 91

89 23.711 2.22 C:\Database\WILEY275.L  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 80  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 72  
2H46 STANDARD \$\$ Normal-docosane  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 72

90 23.806 0.23 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 86  
2H46 STANDARD \$\$ Normal-docosane  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 83  
Hexadecane, 2,6,10,14-tetramethyl- 163891 000638-36-8 83  
(CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane \$\$ Phytan

91 23.868 0.12 C:\Database\WILEY275.L  
Octadecane, 3-ethyl-5-(2-ethylbuty 220178 055282-12-7 87  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Octadecane, 3-ethyl-5-(2-ethylbuty 220176 055282-12-7 86  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 83  
ane \$\$ n-Hentriacontane

92 23.916 0.16 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 87  
2H46 STANDARD \$\$ Normal-docosane  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 86  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 86

93 24.201 0.37 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151984 000629-92-5 53  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 49  
2H46 STANDARD \$\$ Normal-docosane  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69461 000629-50-5 47  
Tridecane, n-

94 24.406 0.56 C:\Database\WILEY275.L

Iron, tricarbonyl[N-(phenyl-2-pyridylmethylene)benzenamine-N,N']- 233784 074764-11-7 80  
 Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 80  
 Tetratriacontane (CAS) \$\$ n-Tetra- 256280 014167-59-0 80  
 riacontane

95 24.449 0.96 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 90  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87  
 Docosane (CAS) \$\$ n-Docosane \$ C2 186056 000629-97-0 87  
 2H46 STANDARD \$\$ Normal-docosane

96 24.539 0.23 C:\Database\WILEY275.L  
 Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 62  
 OCTACOSANE 232594 000000-00-0 62  
 Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 58

97 24.625 0.38 C:\Database\WILEY275.L  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 47  
 \$ Octadecan  
 Undecane, 3,9-dimethyl- (CAS) 69499 017301-31-4 46  
 Octacosane (CAS) \$\$ n-Octacosane 232589 000630-02-4 43

98 24.792 0.24 C:\Database\WILEY275.L  
 Heptadecane, 2-methyl- (CAS) \$\$ 2- 139419 001560-89-0 72  
 Methylheptadecane \$ 16-Methylheptadecane  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 64  
 Heptadecane (CAS) \$\$ n-Heptadecane 126476 000629-78-7 64  
 \$\$ Normal-heptadecane

99 24.925 1.06 C:\Database\WILEY275.L  
 1H-Pyrrole, 1-butyl- (CAS) \$\$ N-Bu 16258 000589-33-3 25  
 tylpyrrole \$\$ 1-Butylpyrrole \$\$ Py  
 rrole, 1-butyl- \$\$ N-N-BUTYLPYRROL  
 E \$\$ BUTYLPYRROLE,1- \$ 1-n-Butylpyrrole  
 1H-Pyrrole, 1-butyl- (CAS) \$\$ N-Bu 16261 000589-33-3 25  
 tylpyrrole \$\$ 1-Butylpyrrole \$\$ Py  
 rrole, 1-butyl- \$\$ N-N-BUTYLPYRROL  
 E \$\$ BUTYLPYRROLE,1- \$ 1-n-Butylpyrrole  
 2-Octyne (CAS) \$\$ n-C5H11C\$.CCH3 9915 002809-67-8 25  
 \$\$ Methylpentylacetylene

100 24.973 0.22 C:\Database\WILEY275.L  
 BISTRIMETHYLSILYL N-ACETYL EICOSAS 261044 000000-00-0 32  
 PHINGA-4,11-DIENINE  
 1,1,1,5,7,7,7-Heptamethyl-3,3-bis( 248666 038147-00-1 25  
 trimethylsiloxy)tetrasiloxane  
 Cholest-5-en-3-ol (3.beta.)-, 9-oc 271182 000303-43-5 18  
 tadecenoate, (Z)- \$ Cholesterol,  
 oleate \$ Cholesteryl-oleate \$ C  
 holesteryl cis-9-octadecenoate \$  
 Cholesteryl oleate \$ Oleoylcholesterol

101 25.087 1.52 C:\Database\WILEY275.L  
 Anthracene-D10 63087 000000-00-0 97  
 Anthracene-d10- 63091 001719-06-8 95

DECADEUTEROPHENANTHRENE \$\$ Phenant 63089 001517-22-2 94  
hrene-d10

- 102 25.301 0.39 C:\Database\WILEY275.L  
6-METHYLPROTOADAMANTANE \$\$ 2,5-Met 36275 052719-64-9 43  
hano-1H-indene, octahydro-5-methyl- (CAS)  
1-ethylidene-2-methylenecyclopenta 9341 121013-07-8 25  
ne \$\$ Cyclopentane, 1-ethylidene-2-methylene-, (E)-  
spathulanol 108426 000000-00-0 22
- 103 25.382 0.23 C:\Database\WILEY275.L  
10-Methylnonadecane 163906 000000-00-0 60  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 58  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 58
- 104 25.449 0.26 C:\Database\WILEY275.L  
6-ACETYL-8-METHOXY-2,2-DIMETHYL-2H 132954 061670-29-9 72  
-CHROMEN-5-OL \$\$ Ethanone, 1-(5-hy  
droxy-8-methoxy-2,2-dimethyl-2H-1-benzopyran-6-yl)- (CAS)  
2-Morpholino-3-methylbenzo[b]thiop 118677 066902-25-8 25  
hene  
1,2,3,3a-Tetrahydro-9-nitropyrrolo 118551 084831-78-7 22  
[1,2-a]quinoxalin-4-one \$\$ Pyrrolo  
[1,2-a]quinoxalin-4(5H)-one, 1,2,3,3a-tetrahydro-9-nitro- (CAS)
- 105 25.801 0.17 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 74  
2H46 STANDARD \$\$ Normal-docosane  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 72  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 72
- 106 25.849 1.12 C:\Database\WILEY275.L  
1,4,4,8-tetramethyl-2-oxatricyclo[ 120134 000000-00-0 64  
6.3.1.0(3,7)]undec-3(7)en-5-one  
Isocurcumenol \$\$ 6H-3a,6-Epoxyazul 120028 024063-71-6 55  
en-6-ol, octahydro-3-methyl-8-meth  
ylene-5-(1-methylethylidene)-, [3S  
-(3.alpha.,3a.alpha.,6.alpha.,8a.b  
eta.)]- \$\$ 5.beta.-Guaia-7(11),10(  
14)-dien-8.alpha.-ol, 5,8-epoxy-,  
(+)- \$\$ (+)-Isocurcumenol \$\$ Isocurcumenol, (+)-  
3-Methyltricyclo[5.3.1.0(3,8)]unde 76314 130877-11-1 50  
cane-2,6-dione \$\$ 1,6-Methanonapht  
halene-4,9(1H)-dione, octahydro-8a-methyl-, (.+-.)-
- 107 26.139 0.16 C:\Database\WILEY275.L  
Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 64  
OCTACOSANE 232594 000000-00-0 64  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 64  
2H46 STANDARD \$\$ Normal-docosane
- 108 26.320 0.22 C:\Database\WILEY275.L  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87  
Octadecane (CAS) \$\$ n-Octadecane \$ 139434 000593-45-3 86  
\$ Octadecan  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 83



109 26.373 0.42 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 91  
 2H46 STANDARD \$\$ Normal-docosane  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 90  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 90  
 Decyldocosane \$\$ 11-NOR-DECYLDOSANE

110 26.463 0.38 C:\Database\WILEY275.L  
 Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 80  
 ane \$\$ n-Hentriacontane  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 80  
 Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 74

111 26.568 0.33 C:\Database\WILEY275.L  
 Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 87  
 Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 83  
 ane \$\$ n-Hentriacontane  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 83

112 26.663 0.30 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 87  
 2H46 STANDARD \$\$ Normal-docosane  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 86  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 86

113 26.720 0.60 C:\Database\WILEY275.L  
 7,9-di-tert-butyl-1-oxaspiro[4.5]d 158640 000000-00-0 99  
 eca-6,9-diene-2,8-dione  
 Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 15  
 2,5-bis[(E)-2,2-dimethylpropyliden 106100 115592-12-6 15  
 e]cyclopentanone \$\$ Cyclopentanone  
 , 2,5-bis(2,2-dimethylpropylidene)-, (E,E)-

114 26.749 0.74 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 90  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 90  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 90

115 26.820 0.79 C:\Database\WILEY275.L  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87  
 Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 87  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 87

116 26.939 0.26 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 86  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 80  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80

117 27.006 0.45 C:\Database\WILEY275.L  
 METHYL-3-(3,5-DITERTBUTYL-4-HYDROX 171951 000000-00-0 95  
 YPHENYL) PROPIONATE \$\$ Methyl este  
 r of 3-(3,5-di-tert-butyl-4-hydrox  
 yphenyl)-propionic acid  
 3,4-dihydro-7,12-dihydroxy-7,12-di 172165 000000-00-0 90  
 methylbenz[a]anthracene

Evodione \$\$ Ethanone, 1-(5,7,8-tri 171655 000482-07-5 38  
 methoxy-2,2-dimethyl-2H-1-benzopyr  
 an-6-yl)- (CAS) \$\$ Ketone, methyl  
 5,7,8-trimethoxy-2,2-dimethyl-2H-1-benzopyran-6-yl

118 27.111 0.27 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 80  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 72  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE  
 Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 72  
 ane \$\$ n-Hentriacontane

119 27.192 0.27 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 87  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 86  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 83

120 27.254 0.63 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 91  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 90  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 90

121 27.354 0.80 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 53  
 Pentatriacontane (CAS) \$\$ n-Pentat 258572 000630-07-9 53  
 riacontane  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 53

122 27.392 0.40 C:\Database\WILEY275.L  
 Triacontane (CAS) \$\$ n-Triacontane 242803 000638-68-6 62  
 Nonadecane (CAS) \$\$ n-Nonadecane 151984 000629-92-5 53  
 Tritetracontane (CAS) \$\$ N-TRIATET 269077 007098-21-7 53  
 RACONTANE

123 27.816 0.26 C:\Database\WILEY275.L  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 74  
 riacontane  
 Heptadecane, 9-octyl- (CAS) \$\$ 9-N 212918 007225-64-1 74  
 -OCTYLHEPTADECANE  
 Eicosane, 7-hexyl- (CAS) \$\$ 7-n-He 220184 055333-99-8 72  
 xyleicosane

124 28.244 0.11 C:\Database\WILEY275.L  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 72  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 72

125 28.282 0.21 C:\Database\WILEY275.L  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 80  
 riacontane  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 80

126 28.716 0.57 C:\Database\WILEY275.L  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 91  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 90

Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87

127 28.797 0.25 C:\Database\WILEY275.L  
 Heptadecane, 3-methyl- (CAS) \$\$ 3- 139429 006418-44-6 80  
 Methylheptadecane \$\$ 15-Methylheptadecane  
 Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 74  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 74

128 28.854 0.17 C:\Database\WILEY275.L  
 N-EICOSANE 163902 000112-95-8 97  
 EICOSANE 163904 000000-00-0 95  
 Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 95

129 28.954 0.64 C:\Database\WILEY275.L  
 Nonadecane (CAS) \$\$ n-Nonadecane 151984 000629-92-5 83  
 Tetratetracontane (CAS) \$\$ n-Tetra 269825 007098-22-8 74  
 tetracontane  
 Pentatriacontane (CAS) \$\$ n-Pentat 258572 000630-07-9 74  
 riacontane

130 29.044 1.26 C:\Database\WILEY275.L  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 80  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 80

131 29.240 0.30 C:\Database\WILEY275.L  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 74  
 \$ Octadecan  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 64  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 64

132 29.378 0.41 C:\Database\WILEY275.L  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 83  
 riacontane  
 Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 80  
 Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 80  
 tane \$\$ Bicetyl \$\$ Tris(trimethyls  
 ilyl)ether, methyl ester of ethyl  
 anthranilate azo pigment(.alpha.z)  
 of bilivubin-1x.alpha. 2-O-acyl glucuronide

133 29.463 0.93 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 90  
 N-EICOSANE 163902 000112-95-8 87  
 Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 87

134 30.320 0.10 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163884 000112-95-8 90  
 N-EICOSANE 163902 000112-95-8 86  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 72

135 30.501 0.09 C:\Database\WILEY275.L  
 Pentatriacontane (CAS) \$\$ n-Pentat 258572 000630-07-9 76  
 riacontane  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 72

Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 68  
 acontane \$\$ NOR-HEXATRIACONTANE

136 30.692 0.65 C:\Database\WILEY275.L  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 83  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 83  
 NONADECANE 152008 000000-00-0 80

137 30.735 0.26 C:\Database\WILEY275.L  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 87  
 acontane \$\$ NOR-HEXATRIACONTANE  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 83  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 83

138 30.892 0.16 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 83  
 3-Methylheneicosane \$\$ Heneicosane 186065 006418-47-9 83  
 , 3-methyl-  
 Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 80  
 tane \$\$ Bicetyl \$\$ Tris(trimethyls  
 ilyl)ether, methyl ester of ethyl  
 anthranilate azo pigment(.alpha.z) of bilivubin-1x.alpha. 2-O-acyl glucuronide

139 30.940 0.33 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 97  
 Eicosane (CAS) \$\$ n-Eicosane 163879 000112-95-8 78  
 Eicosane (CAS) \$\$ n-Eicosane 163884 000112-95-8 70

140 30.992 1.14 C:\Database\WILEY275.L  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 62  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 58  
 OCTACOSANE 232594 000000-00-0 58

141 31.149 4.16 C:\Database\WILEY275.L  
 4,5.alpha.-Epoxy-3-methoxy-17-meth 248045 085454-97-3 78  
 yl-7.alpha.-(4-phenyl-1,3-butadien  
 yl)-6.beta.,7.beta.-(oxymethylene)morphinan  
 1-Methyl-2,5-diphenyl-3,4-bispheny 248044 000000-00-0 40  
 lazopyrrole  
 methyl 7-(n-octylamino)-2-n-heptyl 248029 116350-49-3 40  
 pyrrolo[2,3-e]benzoxazole-5-carboxylate

142 31.216 1.24 C:\Database\WILEY275.L  
 4,5.alpha.-Epoxy-3-methoxy-17-meth 248045 085454-97-3 83  
 yl-7.alpha.-(4-phenyl-1,3-butadien  
 yl)-6.beta.,7.beta.-(oxymethylene)morphinan  
 methyl 7-(n-octylamino)-2-n-heptyl 248029 116350-49-3 50  
 pyrrolo[2,3-e]benzoxazole-5-carboxylate  
 1-Methyl-2,5-diphenyl-3,4-bispheny 248044 000000-00-0 40  
 lazopyrrole

143 31.278 1.25 C:\Database\WILEY275.L  
 Tridecane (CAS) \$\$ n-Tridecane \$\$ 69452 000629-50-5 35  
 Tridecane, n-

Pentatriacontane (CAS) \$\$ n-Pentat 258572 000630-07-9 35  
riacontane  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69451 000629-50-5 35  
Tridecane, n-

144 31.344 1.69 C:\Database\WILEY275.L  
N-EICOSANE 163902 000112-95-8 58  
OCTACOSANE 232594 000000-00-0 58  
Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 58

145 31.711 0.16 C:\Database\WILEY275.L  
4-Benzylamino-1-methyl-3-phenyl-qu 206082 083609-76-1 70  
inolin-2(1H)-one \$\$ 2(1H)-Quinolin  
one, 1-methyl-3-phenyl-4-[(phenylmethyl)amino]- (CAS)  
Phenol, 2,2'-methylenebis[6-(1,1-d 206103 000119-47-1 50  
imethylethyl)-4-methyl- (CAS) \$\$ 2  
,2'-Methylenebis(4-methyl-6-tert-b  
utylphenol) \$\$ BKF \$\$ AO 1 \$\$ S 67  
\$\$ CAO 5 \$\$ CAO 14 \$\$ CAO-14 \$\$ A  
O 2246 \$\$ A-22-46 \$\$ NG 2246 \$\$ A  
22-46 \$\$ MBP 5 \$\$ 2,2'-METHYLENE-BIS(6-T-BUTYL-P-CR  
2-(4'-NITRO-3'-THIENYL)PYRIMIDINE 92106 065868-26-0 50  
\$\$ Pyrimidine, 2-(4-nitro-3-thienyl)- (CAS)

146 32.025 0.24 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151982 000629-92-5 90  
N-EICOSANE 163902 000112-95-8 89  
N-NONADECANE 152007 000629-92-5 86

147 32.106 0.31 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163884 000112-95-8 83  
Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 78  
Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 58  
tane \$\$ Bicetyl \$\$ Tris(trimethyls  
ilyl)ether, methyl ester of ethyl  
anthranilate azo pigment(.alpha.z)  
of bilivubin-1x.alpha. 2-O-acyl glucuronide

148 32.201 2.55 C:\Database\WILEY275.L  
1H-Indole, 3-methyl- (CAS) \$\$ 3-Me 21502 000083-34-1 37  
thylindole \$\$ Skatol \$\$ Scatole \$\$  
Skatole \$\$ Indole, 3-methyl- \$\$ .  
beta.-Methylindole \$\$ 3-MI \$\$ 3-Methyl-1H-indole  
3-Cyanobenzaldehyde \$\$ Benzonitril 21464 024964-64-5 37  
e, 3-formyl-  
Thiophene, 2-(methylthio)- (CAS) \$ 20347 005780-36-9 27  
\$ 2-METHYLTHIOTHIOPHENE \$\$ 2-(Methylthio)thiophene

149 32.344 0.90 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 15  
PENTADECANE, 2,6,10-TRIMETHYL- \$\$ 139453 000000-00-0 14  
NOR-PRISTAN  
OCTACOSANE 232594 000000-00-0 11

150 32.425 1.21 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 64

|     |        |                                                         |        |             |             |
|-----|--------|---------------------------------------------------------|--------|-------------|-------------|
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163884 | 000112-95-8 | 60          |
|     |        | Tetratriacontane (CAS) \$\$ n-Tetratriacontane          | 256280 | 014167-59-0 | 52          |
| 151 | 32.521 | 1.32 C:\Database\WILEY275.L                             |        |             |             |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163881 | 000112-95-8 | 87          |
|     |        | Hexadecane, 2,6,10,14-tetramethyl-                      | 163894 | 000638-36-8 | 80          |
|     |        | (CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane |        |             |             |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163884 | 000112-95-8 | 78          |
| 152 | 32.616 | 0.37 C:\Database\WILEY275.L                             |        |             |             |
|     |        | EICOSANE                                                | 163904 | 000000-00-0 | 93          |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163884 | 000112-95-8 | 93          |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163882 | 000112-95-8 | 92          |
| 153 | 32.701 | 1.62 C:\Database\WILEY275.L                             |        |             |             |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163881 | 000112-95-8 | 91          |
|     |        | Heptacosane (CAS) \$\$ n-Heptacosane                    | 226684 | 000593-49-7 | 87          |
|     |        | Docosane, 11-decyl- (CAS) \$\$ 11-n-                    | 250412 | 055401-55-3 | 83          |
|     |        | Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE                 |        |             |             |
| 154 | 32.959 | 0.61 C:\Database\WILEY275.L                             |        |             |             |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163884 | 000112-95-8 | 93          |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163881 | 000112-95-8 | 91          |
|     |        | Docosane, 11-decyl- (CAS) \$\$ 11-n-                    | 250412 | 055401-55-3 | 68          |
|     |        | Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE                 |        |             |             |
| 155 | 33.030 | 0.56 C:\Database\WILEY275.L                             |        |             |             |
|     |        | Heptacosane (CAS) \$\$ n-Heptacosane                    | 226684 | 000593-49-7 | 86          |
|     |        | Docosane, 11-decyl- (CAS) \$\$ 11-n-                    | 250412 | 055401-55-3 | 80          |
|     |        | Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE                 |        |             |             |
|     |        | Tetracosane, 11-decyl- (CAS) \$\$ 11                    | 256278 | 055429-84-0 | 74          |
|     |        | -n-Decyltetracosane                                     |        |             |             |
| 156 | 33.768 | 1.23 C:\Database\WILEY275.L                             |        |             |             |
|     |        | 1-ethoxy-2-aminocarbonyl-1-aza-cyc                      | 20371  | 000000-00-0 | 35lopropane |
|     |        | Thiophene, 3-(methylthio)- (CAS) \$                     | 20349  | 020731-74-2 | 27          |
|     |        | \$ 3-(1-THIAETHYL)THIOPHENE \$\$ METH                   |        |             |             |
|     |        | YL 3-THIENYL SULFIDE \$\$ 3-(Methylt                    |        |             |             |
|     |        | hio)thiophene \$\$ 3-(methylthio)-thiophene             |        |             |             |
|     |        | Octadecanoic acid, 4-oxo-, methyl                       | 187308 | 002380-19-0 | 16          |
|     |        | ester (CAS) \$\$ METHYL 4-OXOOCTADECANOATE              |        |             |             |
| 157 | 33.887 | 0.10 C:\Database\WILEY275.L                             |        |             |             |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163884 | 000112-95-8 | 25          |
|     |        | Nonacosane (CAS) \$\$ n-Nonacosane \$                   | 237994 | 000630-03-5 | 15          |
|     |        | \$ Celidoniol, deoxy-                                   |        |             |             |
|     |        | Nonadecane (CAS) \$\$ n-Nonadecane                      | 151987 | 000629-92-5 | 15          |
| 158 | 33.940 | 0.10 C:\Database\WILEY275.L                             |        |             |             |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163881 | 000112-95-8 | 95          |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                          | 163880 | 000112-95-8 | 95          |
|     |        | Nonadecane (CAS) \$\$ n-Nonadecane                      | 151981 | 000629-92-5 | 90          |

# 충충이꽃 A

No Name Entered Library Search Report

Data Path : C:\msdchem\1\data\LJY\2014\herbal biology\141030\flower\_chengcheng\  
 Data File : flower\_chengcheng\_1.D  
 Acq On : 30 Oct 2014 22:02  
 Operator : LJY  
 Sample : flower\_chengcheng\_1  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 0

Unknown Spectrum: Apex  
 Integration Events: ChemStation Integrator - autoint1.e

| Pk# | RT    | Area% | Library/ID                                              | Ref#        | CAS#        | Qual |
|-----|-------|-------|---------------------------------------------------------|-------------|-------------|------|
| 1   | 3.425 | 0.08  | C:\Database\WILEY275.L                                  |             |             |      |
|     |       |       | Hexane, 3-methyl- (CAS) \$\$ 3-Methy                    | 7073        | 000589-34-4 | 43   |
|     |       |       | lhexane \$\$ 2-Ethylpentane                             |             |             |      |
|     |       |       | Hexane, 3-methyl- (CAS) \$\$ 3-Methy                    | 7074        | 000589-34-4 | 43   |
|     |       |       | lhexane \$\$ 2-Ethylpentane                             |             |             |      |
|     |       |       | 3-METHYLHEXANE                                          | 7099        | 000000-00-0 | 43   |
| 2   | 3.520 | 0.21  | C:\Database\WILEY275.L                                  |             |             |      |
|     |       |       | Acetic acid, 1-methylpropyl ester 13078                 | 000105-46-4 | 83          |      |
|     |       |       | (CAS) \$\$ 2-Butyl acetate \$\$ sec-Bu                  |             |             |      |
|     |       |       | tyl acetate \$\$ sec-Butyl alcohol a                    |             |             |      |
|     |       |       | cetate \$\$ Acetic acid, sec-butyl e                    |             |             |      |
|     |       |       | ster \$\$ CH3COOCH(CH3)C2H5 \$\$ Aceti                  |             |             |      |
|     |       |       | c acid, 2-butoxy ester \$\$ dl-sec-B                    |             |             |      |
|     |       |       | utyl acetate \$\$ sec-Butyl ethanoate \$\$ Acetate de b |             |             |      |
|     |       |       | Acetic acid, 1-methylpropyl ester 13076                 | 000105-46-4 | 74          |      |
|     |       |       | (CAS) \$\$ 2-Butyl acetate \$\$ sec-Bu                  |             |             |      |
|     |       |       | tyl acetate \$\$ sec-Butyl alcohol a                    |             |             |      |
|     |       |       | cetate \$\$ Acetic acid, sec-butyl e                    |             |             |      |
|     |       |       | ster \$\$ CH3COOCH(CH3)C2H5 \$\$ Aceti                  |             |             |      |
|     |       |       | c acid, 2-butoxy ester \$\$ dl-sec-B                    |             |             |      |
|     |       |       | utyl acetate \$\$ sec-Butyl ethanoate \$\$ Acetate de b |             |             |      |
|     |       |       | Acetic acid, 1-methylpropyl ester 13077                 | 000105-46-4 | 74          |      |
|     |       |       | (CAS) \$\$ 2-Butyl acetate \$\$ sec-Bu                  |             |             |      |
|     |       |       | tyl acetate \$\$ sec-Butyl alcohol a                    |             |             |      |
|     |       |       | cetate \$\$ Acetic acid, sec-butyl e                    |             |             |      |
|     |       |       | ster \$\$ CH3COOCH(CH3)C2H5 \$\$ Aceti                  |             |             |      |
|     |       |       | c acid, 2-butoxy ester \$\$ dl-sec-B                    |             |             |      |
|     |       |       | utyl acetate \$\$ sec-Butyl ethanoate \$\$ Acetate de b |             |             |      |
| 3   | 3.591 | 0.17  | C:\Database\WILEY275.L                                  |             |             |      |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$\$ 2                    | 11031       | 003404-78-2 | 91   |
|     |       |       | ,5-Dimethyl-2-hexene                                    |             |             |      |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$\$ 2                    | 11034       | 003404-78-2 | 91   |
|     |       |       | ,5-Dimethyl-2-hexene                                    |             |             |      |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$\$ 2                    | 11029       | 003404-78-2 | 91   |
|     |       |       | ,5-Dimethyl-2-hexene                                    |             |             |      |

4 3.644 0.14 C:\Database\WILEY275.L  
 Heptane, 2-methyl- (CAS) \$\$ 2-Meth 12450 000592-27-8 58  
 ylheptane \$\$ Methylheptane \$\$ (CH3)2CH(CH2)4CH3  
 Heptane, 2-methyl- (CAS) \$\$ 2-Meth 12449 000592-27-8 58  
 ylheptane \$\$ Methylheptane \$\$ (CH3)2CH(CH2)4CH3  
 Nonane, 4-methyl- (CAS) \$\$ 4-Methy 30039 017301-94-9 53  
 Inonane \$\$ 4-n-Methylnonane \$\$ n-C3H7CH(CH3)(CH2)4CH3

5 3.715 0.18 C:\Database\WILEY275.L  
 Toluene 4599 000108-88-3 90  
 Benzene, methyl- (CAS) \$\$ Toluene 4560 000108-88-3 90  
 \$\$ CP 25 \$\$ Methylbenzene \$\$ Toluo  
 l \$\$ Methacide \$\$ Antisal 1a \$\$ Me  
 thylbenzol \$\$ Phenylmethane \$\$ MET  
 HYL BENZENE(TOLUENE) \$\$ Benzene, me  
 thyl \$\$ Methane, phenyl- \$\$ NCI-C0  
 7272 \$\$ Tolueen \$\$ Toluen \$\$ Toluolo \$\$ Rcra waste  
 Benzene, methyl- (CAS) \$\$ Toluene 4557 000108-88-3 87  
 \$\$ CP 25 \$\$ Methylbenzene \$\$ Toluo  
 l \$\$ Methacide \$\$ Antisal 1a \$\$ Me  
 thylbenzol \$\$ Phenylmethane \$\$ MET  
 HYL BENZENE(TOLUENE) \$\$ Benzene, me  
 thyl \$\$ Methane, phenyl- \$\$ NCI-C0  
 7272 \$\$ Tolueen \$\$ Toluen \$\$ Toluolo \$\$ Rcra waste

6 3.772 1.00 C:\Database\WILEY275.L  
 Pentane, 3-ethyl-2,4-dimethyl- (CA 19884 001068-87-7 72  
 S) \$\$ 2,4-Dimethyl-3-ethylpentane \$\$ 3-Ethyl-2,4-dimethylpentane  
 Nonane, 5-methyl- (CAS) \$\$ 5-Methy 30042 015869-85-9 64  
 Inonane  
 Hexane, 3-ethyl- (CAS) \$\$ 3-Ethylh 12462 000619-99-8 64  
 exane

7 3.863 0.03 C:\Database\WILEY275.L  
 Cyclohexane, 1,3-dimethyl-, trans- 11156 002207-03-6 55  
 (CAS) \$\$ trans-1,3-Dimethylcycloh  
 exane \$\$ CYCLOHEXANE, 1,3-DIMETHYL  
 -, (E)- \$\$ 1,trans-3-Dimethylcyclohexane  
 Thiophene, 2-ethyl- (CAS) \$\$ 2-Eth 10559 000872-55-9 46ylthiophene  
 Cyclohexane, 1,4-dimethyl-, cis- ( 11159 000624-29-3 46  
 CAS) \$\$ 1,cis-4-Dimethylcyclohexan  
 e \$\$ cis-1,4-Dimethylcyclohexane \$\$ 1,4-Dimethylcyclohexane, cis-

8 3.977 0.09 C:\Database\WILEY275.L  
 3-Hexanone (CAS) \$\$ Hexan-3-one \$\$ 6694 000589-38-8 90  
 Ethyl propyl ketone \$\$ n-C3H7COC2  
 H5 \$\$ Hexanone-(3) \$\$ Aethylpropylketon  
 3-Hexanone (CAS) \$\$ Hexan-3-one \$\$ 6693 000589-38-8 83  
 Ethyl propyl ketone \$\$ n-C3H7COC2  
 H5 \$\$ Hexanone-(3) \$\$ Aethylpropylketon  
 3-Hexanone (CAS) \$\$ Hexan-3-one \$\$ 6695 000589-38-8 74  
 Ethyl propyl ketone \$\$ n-C3H7COC2  
 H5 \$\$ Hexanone-(3) \$\$ Aethylpropylketon

9 4.053 0.15 C:\Database\WILEY275.L



2-Hexanone (CAS) \$\$ Hexan-2-one \$\$ 6678 000591-78-6 83  
 MBK \$\$ Methyl n-butyl ketone \$\$ 2  
 -Oxohexane \$\$ Butyl methyl ketone  
 \$\$ Methyl butyl ketone \$\$ n-Butyl  
 methyl ketone \$\$ n-C4H9COCH3 \$\$ He  
 xanone-2 \$\$ Ketone, butyl methyl \$\$ Mnbk  
 2-Hexanone (CAS) \$\$ Hexan-2-one \$\$ 6672 000591-78-6 80  
 MBK \$\$ Methyl n-butyl ketone \$\$ 2  
 -Oxohexane \$\$ Butyl methyl ketone  
 \$\$ Methyl butyl ketone \$\$ n-Butyl  
 methyl ketone \$\$ n-C4H9COCH3 \$\$ He  
 xanone-2 \$\$ Ketone, butyl methyl \$\$ Mnbk  
 Hexanal (CAS) \$\$ n-Hexanal \$\$ Hexa 6643 000066-25-1 80  
 ldehyde \$\$ Caproaldehyde \$\$ Capron  
 aldehyde \$\$ n-Caproaldehyde \$\$ Cap  
 roic aldehyde \$\$ Hexylaldehyde \$\$  
 n-Capronaldehyde \$\$ cyclohexanol \$  
 \$ 1-hexanal \$\$ n-C5H11CHO \$\$ n-Hex  
 aldehyde \$\$ n-Caproylaldehyde \$\$ Aldehyde C-6 \$\$ Ka

- 10 4.125 0.05 C:\Database\WILEY275.L  
 1-Hexanol, 2-ethyl- (CAS) \$\$ 2-Eth 21138 000104-76-7 35  
 ylhexanol \$\$ 2-Ethyl-1-hexanol \$\$  
 Ethylhexanol \$\$ 2-Ethylhexan-1-ol  
 \$\$ 2-Ethylhexyl alcohol \$\$ 2-Ethyl  
 -hexanol-1 \$\$ Ethylhexyl alcohol \$\$ Octyl alcohol \$\$ 2-Ethylhexanol-  
 Aziridinone, 1,3-bis(1,1-dimethyle 54307 014387-89-4 22  
 thyl)- (CAS) \$\$ 1,3-Di-tert-butyla  
 ziridinone \$\$ 2-Aziridinone, 1,3-di-tert-butyl-  
 1-Hexanol, 2-ethyl- (CAS) \$\$ 2-Eth 21135 000104-76-7 22  
 ylhexanol \$\$ 2-Ethyl-1-hexanol \$\$  
 Ethylhexanol \$\$ 2-Ethylhexan-1-ol  
 \$\$ 2-Ethylhexyl alcohol \$\$ 2-Ethyl  
 -hexanol-1 \$\$ Ethylhexyl alcohol \$\$ Octyl alcohol \$\$ 2-Ethylhexanol-
- 11 4.206 0.18 C:\Database\WILEY275.L  
 3-HEXANOL 7893 000000-00-0 83  
 3-Hexanol (CAS) \$\$ Hexan-3-ol \$\$ C 7757 000623-37-0 83  
 2H5CH(OH)C3H7 \$\$ Ethylpropylcarbinol \$\$ Hexanol-(3)  
 3-Hexanol (CAS) \$\$ Hexan-3-ol \$\$ C 7761 000623-37-0 83  
 2H5CH(OH)C3H7 \$\$ Ethylpropylcarbinol \$\$ Hexanol-(3)
- 12 4.272 0.43 C:\Database\WILEY275.L  
 2-Octanol (CAS) \$\$ n-Octan-2-ol \$\$ 21065 000123-96-6 53  
 Capryl alcohol \$\$ s-Octyl alcohol  
 \$\$ 1-Methyl-1-heptanol \$\$ Methylh  
 exylcarbinol \$\$ Hexylmethylcarbino  
 l \$\$ sec-Caprylic alcohol \$\$ .beta  
 .-Octyl alcohol \$\$ 1-Methylheptyl  
 alcohol \$\$ 2-Octyl alcohol iamine \$\$ sec-Octyl Alco  
 2-Hexanol (CAS) \$\$ n-C4H9CH(OH)CH3 7753 000626-93-7 53  
 \$\$ n-Butylmethylcarbinol \$\$ Hexanol-(2) \$\$ sec-Hexyl alcohol  
 2-Octanol (CAS) \$\$ n-Octan-2-ol \$\$ 21063 000123-96-6 53  
 Capryl alcohol \$\$ s-Octyl alcohol  
 \$\$ 1-Methyl-1-heptanol \$\$ Methylh  
 exylcarbinol \$\$ Hexylmethylcarbino

1 \$\$ sec-Caprylic alcohol \$\$ .beta  
 .-Octyl alcohol \$\$ 1-Methylheptyl  
 alcohol \$\$ 2-Octyl alcohol iamine \$\$ sec-Octyl Alco

- 13 4.501 27.73 C:\Database\WILEY275.L  
 (2S,4S)-(+)-Pentanediol 8271 072345-23-4 28  
 Acetaldehyde, methoxy- (CAS) \$\$ Me 1709 010312-83-1 9  
 thoxyacetaldehyde \$\$ Acetaldehyde,  
 2-methoxy- \$\$ .alpha.-Methoxyacet  
 aldehyde \$\$ 2-Methoxyacetaldehyde \$\$ Methoxyethanal  
 Acetic acid, fluoro- (CAS) \$\$ Fluo 2089 000144-49-0 9  
 roacetic acid \$\$ HFA \$\$ Cymonic ac  
 id \$\$ Gifblaar poison \$\$ Fluoroeth  
 anoic acid \$\$ Monofluoroacetic aci  
 d \$\$ CH2FCOOH \$\$ Acide-monofluorac  
 etique \$\$ Acido monofluoroaceticio \$  
 \$ FAA \$\$ Fluoroacetate \$\$ 2-Fluoroacetic acid \$\$ MF
- 14 4.634 0.68 C:\Database\WILEY275.L  
 Heptane, 2,4-dimethyl- (CAS) \$\$ 2, 19825 002213-23-2 87  
 4-Dimethylheptane  
 Heptane, 2,4-dimethyl- (CAS) \$\$ 2, 19824 002213-23-2 72  
 4-Dimethylheptane  
 Heptane, 2,4-dimethyl- (CAS) \$\$ 2, 19823 002213-23-2 64  
 4-Dimethylheptane
- 15 5.011 0.20 C:\Database\WILEY275.L  
 2,4-Dimethyl-1-heptene 18332 019549-87-2 81  
 Undecane, 3-methylene- (CAS) \$\$ 1- 53837 071138-64-2 53  
 DECENE, 2-ETHYL-  
 Cyclopentane, 1,2,3-trimethyl-, (1 11123 002613-69-6 47  
 .alpha.,2.alpha.,3.alpha.)- (CAS)  
 \$\$ 1,CIS-2,CIS-3-TRIMETHYLCYCLOPEN  
 TANE \$\$ Cyclopentane, 1,2,3-trimet  
 hyl-, cis-1,2,cis-1,3- \$\$ CYCLOPEN  
 TANE, 1,2,3-TRIMETHYL-, ALL-CIS \$\$ cis,cis,cis-1,2,3-Trimethylcyclopentane
- 16 5.158 0.21 C:\Database\WILEY275.L  
 1-Butanol, 2-methyl-, acetate (CAS 20827 000624-41-9 43  
 ) \$\$ 2-Methylbutyl acetate \$\$ 2-ME  
 THYL-1-ACETOXYBUTANE \$\$ 2-Methyl-1  
 -butyl acetate \$\$ 2-METHYL BUTYL A  
 CETATE \$\$ Acetic acid 2-methylbutyl ester  
 2-PENTYL ACETATE 20966 000000-00-0 38  
 2-Pentanol, acetate (CAS) \$\$ 2-Pen 20823 000626-38-0 38  
 tyl acetate \$\$ 2-Acetoxypentane \$\$  
 1-Methylbutyl acetate \$\$ Acetic a  
 cid, 2-pentyl ester \$\$ sec-Amyl ac  
 etate \$\$ sek.Amylester kyseliny octove \$\$ 2-Amylester kyseliny octove \$\$ UN 1104
- 17 5.330 0.26 C:\Database\WILEY275.L  
 CIS-3-HEXENOL 6975 000928-96-1 96  
 3-Hexen-1-ol, (Z)- (CAS) \$\$ cis-3- 6776 000928-96-1 93  
 Hexene-1-ol \$\$ Z-3-Hexenol \$\$ Leaf  
 alcohol \$\$ 3-(Z)-Hexenol \$\$ cis-3  
 -Hexenol \$\$ Blatteralkohol \$\$ cis-

3-Hexen-1-ol \$\$ (Z)-Hex-3-en-1-ol  
 \$\$ Blatteralkohol (German) \$\$ .bet  
 a,,gamma.-Hexenol \$\$ HEXEN-30L-1 \$\$ 3-Hexen-1-ol \$  
 3-Hexen-1-ol, (Z)- (CAS) \$\$ cis-3- 6779 000928-96-1 90  
 Hexene-1-ol \$\$ Z-3-Hexenol \$\$ Leaf  
 alcohol \$\$ 3-(Z)-Hexenol \$\$ cis-3  
 -Hexenol \$\$ Blatteralkohol \$\$ cis-  
 3-Hexen-1-ol \$\$ (Z)-Hex-3-en-1-ol  
 \$\$ Blatteralkohol (German) \$\$ .bet  
 a,,gamma.-Hexenol \$\$ HEXEN-30L-1 \$\$ 3-Hexen-1-ol \$

18 5.387 0.19 C:\Database\WILEY275.L  
 Heptane, 4-ethyl- (CAS) \$\$ 4-Ethyl 19814 002216-32-2 76heptane  
 Heptane, 4-ethyl- (CAS) \$\$ 4-Ethyl 19815 002216-32-2 68heptane  
 Heptane, 4-ethyl- (CAS) \$\$ 4-Ethyl 19817 002216-32-2 64heptane

19 5.458 0.39 C:\Database\WILEY275.L  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19808 002216-34-4 91octane \$\$ Isononane  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19806 002216-34-4 91octane \$\$ Isononane  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19807 002216-34-4 90octane \$\$ Isononane

20 5.687 0.10 C:\Database\WILEY275.L  
 2-Buten-1-ol, (E)- (CAS) \$\$ trans- 1380 000504-61-0 18  
 2-Butenol \$\$ trans-BUT-2-ENOL \$\$ t  
 rans-2-Buten-1-ol \$\$ 2-(E)-Buten-1  
 -olral \$\$ trans-Crotyl alcohol \$\$  
 trans-Crotonyl alcohol \$\$ trans-2-  
 Butenyl alcohol \$\$ 2-(E)-Buten-1-ol \$\$ (E)-CH<sub>3</sub>CH=C(CH<sub>3</sub>)OH  
 2-Propen-1-ol, 2-methyl- (CAS) \$\$ 1412 000513-42-8 18  
 Methallyl alcohol \$\$ Isopropenyl c  
 arbinol \$\$ 2-Methylallyl alcohol \$  
 \$ 3-Hydroxy-2-methylpropene \$\$ CH<sub>2</sub>  
 =C(CH<sub>3</sub>)CH<sub>2</sub>OH \$\$ 2-Methyl-2-propen-  
 1-ol \$\$ .beta.-Methallyl alcohol \$\$ 2-Methyl-2-propene-1-ol \$\$ UN 2614  
 2-Buten-1-ol, (E)- (CAS) \$\$ trans- 1391 000504-61-0 14  
 2-Butenol \$\$ trans-BUT-2-ENOL \$\$ t  
 rans-2-Buten-1-ol \$\$ 2-(E)-Buten-1  
 -olral \$\$ trans-Crotyl alcohol \$\$  
 trans-Crotonyl alcohol \$\$ trans-2-  
 Butenyl alcohol \$\$ 2-(E)-Buten-1-ol \$\$ (E)-CH<sub>3</sub>CH=C(CH<sub>3</sub>)OH

21 6.201 0.81 C:\Database\WILEY275.L  
 1,1,3,3,5,5,7,7,9,9,11,11,13,13-TE 260039 000000-00-0 46  
 TRADECAMETHYL-HEPTASILOXANE  
 3,3-Diethoxy-1,1,1,5,5,5-hexamethy 174413 000000-00-0 40ltrisiloxane  
 1,2-Bis(trimethylsilyl)benzene 107559 017151-09-6 27

22 6.330 0.27 C:\Database\WILEY275.L  
 1,1,1,3,5,5,5-Heptamethyltrisiloxa 106885 001873-88-7 49  
 ne \$\$ Bis(trimethylsiloxy)methylsi  
 lane \$\$ Hydromethylsiloxane \$\$ Tri  
 siloxane, 1,1,1,3,5,5,5-heptamethyl-  
 Tetrasiloxane, decamethyl- (CAS) \$ 185153 000141-62-8 43  
 \$ Decamethyltetrasiloxane \$\$ [(CH<sub>3</sub>)<sub>3</sub>SiOSi(CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub>O \$\$ KF 96L1.5  
 Arsenous acid, tris(trimethylsilyl 206537 055429-29-3 43  
 ) ester (CAS) \$\$ TRIMETHYLSILYL ARSINATE

23 6.411 0.30 C:\Database\WILEY275.L  
1,1,3,3,5,5,7,7,9,9,11,11,13,13-TE 260039 000000-00-0 53  
TRADECAMETHYL-HEPTASILOXANE  
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15 267298 000000-00-0 47  
,15-HEXADECAMETHYL-OCTASILOXANE  
1,1,1,3,5,5,5-Heptamethyltrisiloxa 106885 001873-88-7 43  
ne \$\$ Bis(trimethylsiloxy)methylsi  
lane \$\$ Hydromethylsiloxane \$\$ Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-

24 6.511 0.06 C:\Database\WILEY275.L  
1,1,3,3,5,5,7,7,9,9,11,11,13,13-TE 260039 000000-00-0 72  
TRADECAMETHYL-HEPTASILOXANE  
1,1,1,3,5,5,5-Heptamethyltrisiloxa 106885 001873-88-7 43  
ne \$\$ Bis(trimethylsiloxy)methylsi  
lane \$\$ Hydromethylsiloxane \$\$ Tri  
siloxane, 1,1,1,3,5,5,5-heptamethyl-  
CIS-4-ETHOXY-B-METHYL-B-NITROSTYRE 92299 000000-00-0 43NE

25 6.549 0.16 C:\Database\WILEY275.L  
1,1,1,3,5,7,7,7-Octamethyltetrasil 162851 000000-00-0 47oxane  
CIS-4-ETHOXY-B-METHYL-B-NITROSTYRE 92299 000000-00-0 46NE  
3,3-Diisopropoxy-1,1,1,5,5,5-hexam 195153 018082-56-9 37ethyltrisiloxane

26 6.692 0.17 C:\Database\WILEY275.L  
1,1,1,3,5,5,5-Heptamethyltrisiloxa 106885 001873-88-7 38  
ne \$\$ Bis(trimethylsiloxy)methylsi  
lane \$\$ Hydromethylsiloxane \$\$ Tri  
siloxane, 1,1,1,3,5,5,5-heptamethyl-  
1,1,1,3,5,7,7,7-Octamethyltetrasil 162851 000000-00-0 37oxane  
CIS-4-ETHOXY-B-METHYL-B-NITROSTYRE 92299 000000-00-0 35NE

27 6.772 0.17 C:\Database\WILEY275.L  
Tetrasiloxane, decamethyl- (CAS) \$ 185153 000141-62-8 37  
\$ Decamethyltetrasiloxane \$\$ [(CH3)3SiOSi(CH3)2]2O \$\$ KF 96L1.5  
1-(3,4-METHYLENEDIOXYPHENYL)-2-PRO 92303 000000-00-0 27  
PANONE OXIME METHYL ETHER  
Cyclotrisiloxane, hexamethyl- (CAS 106848 000541-05-9 27  
) \$\$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH  
EXASILOXANE \$\$ Hexamethylcyclotris  
iloxane \$\$ HEXAMETHYL-CYCLOTTRISILO  
XANE \$\$ Dimethylsiloxane cyclic trimer

28 6.853 0.08 C:\Database\WILEY275.L  
1,1,1,3,5,7,7,7-Octamethyltetrasil 162851 000000-00-0 40oxane  
Propiophenone, 2'-(trimethylsiloxy 107526 033342-87-9 38  
)-(CAS) \$\$ TRIMETHYLSILOXYL ETHER  
OF O-HYDROXYPROPIOPHENONE \$\$ Trime  
thylsilyl ether of o-hydroxypropiophenone  
Cyclotrisiloxane, hexamethyl- (CAS 106849 000541-05-9 38  
) \$\$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH  
EXASILOXANE \$\$ Hexamethylcyclotris  
iloxane \$\$ HEXAMETHYL-CYCLOTTRISILO  
XANE \$\$ Dimethylsiloxane cyclic trimer

29 7.063 1.05 C:\Database\WILEY275.L

Ethanone, 1-(3-ethyloxiranyl)- (CA 11797 017257-81-7 43  
 S) \$\$ 3,4-EPOXY-2-HEXANONE \$\$ 2-He  
 xanone, 3,4-epoxy- \$\$ 1-Acetyl-2-ethyloxirane  
 Ethanone, 1-(3-ethyloxiranyl)- (CA 11796 017257-81-7 43  
 S) \$\$ 3,4-EPOXY-2-HEXANONE \$\$ 2-He  
 xanone, 3,4-epoxy- \$\$ 1-Acetyl-2-ethyloxirane  
 2-Nonanone, 9-[(tetrahydro-2H-pyra 127783 054699-41-1 38  
 n-2-yl)oxy]- (CAS)

30 7.244 1.18 C:\Database\WILEY275.L  
 Ethanone, 1-(3-ethyloxiranyl)- (CA 11796 017257-81-7 38  
 S) \$\$ 3,4-EPOXY-2-HEXANONE \$\$ 2-He  
 xanone, 3,4-epoxy- \$\$ 1-Acetyl-2-ethyloxirane  
 Ethanone, 1-(3-butyloxiranyl)- (CA 29471 017257-80-6 38  
 S) \$\$ 2-Octanone, 3,4-epoxy- \$\$ 1-Acetyl-2-butyloxirane  
 Ethanone, 1-(3-ethyloxiranyl)- (CA 11797 017257-81-7 38  
 S) \$\$ 3,4-EPOXY-2-HEXANONE \$\$ 2-He  
 xanone, 3,4-epoxy- \$\$ 1-Acetyl-2-ethyloxirane

31 7.349 0.12 C:\Database\WILEY275.L  
 Piperidine (CAS) \$\$ Cypentil \$\$ Az 3090 000110-89-4 64  
 acyclohexane \$\$ Cyclopentimine \$\$  
 Hexazane \$\$ Hexahydropyridine \$\$ P  
 entamethylenimine \$\$ Pyridine, hex  
 ahydro- \$\$ Perhydropyridine \$\$ Pen  
 tamethyleneimine \$\$ Piperidin \$\$ UN 2401  
 Piperidine (CAS) \$\$ Cypentil \$\$ Az 3086 000110-89-4 59  
 acyclohexane \$\$ Cyclopentimine \$\$  
 Hexazane \$\$ Hexahydropyridine \$\$ P  
 entamethylenimine \$\$ Pyridine, hex  
 ahydro- \$\$ Perhydropyridine \$\$ Pen  
 tamethyleneimine \$\$ Piperidin \$\$ UN 2401  
 Piperidine (CAS) \$\$ Cypentil \$\$ Az 3083 000110-89-4 59  
 acyclohexane \$\$ Cyclopentimine \$\$  
 Hexazane \$\$ Hexahydropyridine \$\$ P  
 entamethylenimine \$\$ Pyridine, hex  
 ahydro- \$\$ Perhydropyridine \$\$ Pen  
 tamethyleneimine \$\$ Piperidin \$\$ UN 2401

32 7.382 0.15 C:\Database\WILEY275.L  
 Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55976 001636-43-7 38  
 -Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
 Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55977 001636-43-7 32  
 -Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
 1-Heptanol, 2,4-dimethyl-, (2S,4R) 31452 018450-74-3 32  
 -(-)- (CAS) \$\$ 2L,4D-DIMETHYLHEPTANOL

33 7.453 0.12 C:\Database\WILEY275.L  
 Nonane, 2-methyl- (CAS) \$\$ 2-Methy 30025 000871-83-0 59  
 Inonane \$\$ 2-Methyl-nonane  
 Nonane, 2-methyl- (CAS) \$\$ 2-Methy 30027 000871-83-0 59  
 Inonane \$\$ 2-Methyl-nonane  
 Dodecane, 3-methyl- (CAS) \$\$ 3-Met 69468 017312-57-1 47  
 hyldodecane

34 7.515 0.16 C:\Database\WILEY275.L

Cyclohexane, azido- (CAS) \$\$ CYCLO 17164 019573-22-9 53  
 HEXYL AZIDE \$\$ Cyclohexyl azide \$\$ Azidocyclohexane  
 Cyclohexane, bromo- (CAS) \$\$ Bromo 46669 000108-85-0 53  
 cyclohexane \$\$ BROMO-CYCLOHEXANE \$  
 \$ Cyclohexyl bromide \$\$ 1-Bromocyclohexane  
 Cyclohexane, bromo- (CAS) \$\$ Bromo 46670 000108-85-0 53  
 cyclohexane \$\$ BROMO-CYCLOHEXANE \$  
 \$ Cyclohexyl bromide \$\$ 1-Bromocyclohexane

35 7.587 0.05 C:\Database\WILEY275.L  
 N-Cyano-N',N',N'',N''-tetramethyl- 92124 074150-88-2 35  
 1,3,5-triazinetriamine  
 N-Cyano-N',N',N'',N''-tetramethyl- 92123 074150-88-2 35  
 1,3,5-triazinetriamine  
 1,1,1,3,5,7,7,7-Octamethyltetrasil 162851 000000-00-0 32  
 oxane

36 7.649 0.14 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163887 000112-95-8 53  
 Hexane, 2,4-dimethyl- (CAS) \$\$ 2,4 12472 000589-43-5 50  
 -Dimethylhexane  
 2,2-Dimethyl-3-heptanone 29988 019078-97-8 50

37 7.763 0.20 C:\Database\WILEY275.L  
 1-OCTEN-3-OL 19692 053907-72-5 49  
 1 OCTEN 3 OL 19694 003391-86-4 49  
 1-OCTEN-3-OL 19698 003391-86-4 47

38 7.939 0.15 C:\Database\WILEY275.L  
 Decane, 2,2,6-trimethyl- (CAS) 69518 062237-97-2 47  
 Decane, 2,2,8-trimethyl- (CAS) 69520 062238-01-1 47  
 Heptane, 2,2,4,6,6-pentamethyl- (C 55987 013475-82-6 47  
 AS) \$\$ 2,2,4,6,6-Pentamethylheptan

39 8.125 0.16 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163884 000112-95-8 46  
 Decane (CAS) \$\$ n-Decane \$\$ Isodec 30008 000124-18-5 45  
 ane \$\$ n-C10H22 \$\$ UN 2247  
 Decane (CAS) \$\$ n-Decane \$\$ Isodec 30009 000124-18-5 45  
 ane \$\$ n-C10H22 \$\$ UN 2247

40 8.249 0.11 C:\Database\WILEY275.L  
 Tetradecane, 4-methyl- (CAS) 98321 025117-24-2 43  
 Decane, 5-ethyl-5-methyl- (CAS) \$\$ 69512 017312-74-2 43  
 5-METHYL-5-ETHYLDECANE  
 Dodecane, 2,7,10-trimethyl- (CAS) 98336 074645-98-0 43

41 8.334 0.07 C:\Database\WILEY275.L  
 Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12480 000563-16-6 49  
 -Dimethylhexane  
 Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12481 000563-16-6 47  
 -Dimethylhexane  
 Tetradecane, 4-methyl- (CAS) 98321 025117-24-2 47

42 8.368 0.16 C:\Database\WILEY275.L  
 4,4-Dimethylcyclooctene 26889 000000-00-0 59

Heptane, 4,4-dimethyl- (CAS) \$\$ 4, 19841 001068-19-5 58  
 4-Dimethylheptane  
 Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12481 000563-16-6 50  
 -Dimethylhexane

43 8.420 0.03 C:\Database\WILEY275.L  
 N-Cyano-N',N',N'',N'''-tetramethyl- 92124 074150-88-2 38  
 1,3,5-triazinetriamine  
 N-Cyano-N',N',N'',N'''-tetramethyl- 92123 074150-88-2 38  
 1,3,5-triazinetriamine  
 8-Methylisothiazolo[4,5-c]-2,1,3-b 92115 074801-78-8 35  
 enzothiadiazole \$\$ Isothiazolo[3,4  
 -e]-2,1,3-benzothiadiazole, 4-methyl- (CAS)

44 8.473 0.15 C:\Database\WILEY275.L  
 Decane, 5-methyl- (CAS) \$\$ 5-Methy 42785 013151-35-4 81  
 ldecane  
 Nonane, 2,5-dimethyl- (CAS) \$\$ 2,5 42787 017302-27-1 60  
 -Dimethylnonane  
 Undecane (CAS) \$\$ n-Undecane \$\$ He 42751 001120-21-4 53  
 ndecane \$\$ n-C11H24 \$\$ UN 2330

45 8.549 0.30 C:\Database\WILEY275.L  
 Decane, 4-methyl- (CAS) \$\$ 4-Methy 42778 002847-72-5 80  
 ldecane  
 Nonane, 2,6-dimethyl- (CAS) \$\$ 2,6 42788 017302-28-2 78  
 -Dimethylnonane  
 Nonane, 5-propyl- (CAS) 55979 000998-35-6 64

46 8.687 0.11 C:\Database\WILEY275.L  
 1-Hexanol, 2-ethyl- (CAS) \$\$ 2-Eth 21129 000104-76-7 80  
 ylhexanol \$\$ 2-Ethyl-1-hexanol \$\$  
 Ethylhexanol \$\$ 2-Ethylhexan-1-ol  
 \$\$ 2-Ethylhexyl alcohol \$\$ 2-Ethyl  
 -hexanol-1 \$\$ Ethylhexyl alcohol \$\$ Octyl alcohol \$\$ 2-Ethylhexanol-  
 1-Hexanol, 2-ethyl- (CAS) \$\$ 2-Eth 21138 000104-76-7 80  
 ylhexanol \$\$ 2-Ethyl-1-hexanol \$\$  
 Ethylhexanol \$\$ 2-Ethylhexan-1-ol  
 \$\$ 2-Ethylhexyl alcohol \$\$ 2-Ethyl  
 -hexanol-1 \$\$ Ethylhexyl alcohol \$\$ Octyl alcohol \$\$ 2-Ethylhexanol-  
 1-Hexanol, 2-ethyl- (CAS) \$\$ 2-Eth 21134 000104-76-7 80  
 ylhexanol \$\$ 2-Ethyl-1-hexanol \$\$  
 Ethylhexanol \$\$ 2-Ethylhexan-1-ol  
 \$\$ 2-Ethylhexyl alcohol \$\$ 2-Ethyl  
 -hexanol-1 \$\$ Ethylhexyl alcohol \$\$ Octyl alcohol \$\$ 2-Ethylhexanol-

47 8.982 0.03 C:\Database\WILEY275.L  
 Pentane, 2-cyclopropyl- \$\$ 1-Methy 11211 005458-16-2 38  
 lbutylcyclopropane  
 N-OCTANOL 21215 000111-87-5 38  
 Cyclopropane, pentyl- (CAS) \$\$ 1,2 11095 002511-91-3 38  
 -METHYLENEHEPTANE \$\$ Pentylcyclopr  
 opane \$\$ 1-Cyclopropylpentane \$\$ Pentane, 1-cyclopropyl-

48 9.030 0.13 C:\Database\WILEY275.L  
 Cyclohexanone, 3,3,5-trimethyl- (C 28088 000873-94-9 93

AS) \$\$ 3,3,5-Trimethylcyclohexanon  
e \$\$ Dihydroisophorone  
Cyclohexanone, 3,3,5-trimethyl- (C 28085 000873-94-9 87  
AS) \$\$ 3,3,5-Trimethylcyclohexanone \$\$ Dihydroisophorone  
Cyclohexanone, 3,3,5-trimethyl- (C 28084 000873-94-9 81  
AS) \$\$ 3,3,5-Trimethylcyclohexanone \$\$ Dihydroisophorone

49 9.092 0.09 C:\Database\WILEY275.L  
EICOSANE 163904 000000-00-0 27  
Hexadecane, 2,6,10,14-tetramethyl- 163893 000638-36-8 27  
(CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane \$\$ Phytan  
Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 27

50 9.192 0.08 C:\Database\WILEY275.L  
D,L-2,3-BUTANDIOL DIACETATE 58607 000000-00-0 50  
MESO-2,3-BUTANDIOL DIACETATE 58606 000000-00-0 50  
2-Butanol, 3-methyl-, acetate (CAS 20852 005343-96-4 12  
) \$\$ 1,2-Dimethylpropyl acetate \$\$  
3-Methyl-2-butyl acetate \$\$ CH3C(  
O)OCH(CH3)CH(CH3)2 \$\$ 1,2-Dimethylpropyl ethanoate

51 9.239 0.75 C:\Database\WILEY275.L  
Decane, 2,3,6-trimethyl- (CAS) 69524 062238-12-4 64  
4-Octanone (CAS) \$\$ Butyl propyl k 19494 000589-63-9 58  
etone \$\$ n-C4H9COCH2CH2CH3 \$\$ Propyl n-butyl ketone \$\$ 4-Oxoctane  
Decane, 2,3,7-trimethyl- (CAS) 69525 062238-13-5 50

52 9.363 0.27 C:\Database\WILEY275.L  
pentadecane 98340 000629-62-9 72  
Hexadecane, 7,9-dimethyl- (CAS) \$\$ 139421 021164-95-4 72  
7,9-Dimethylhexadecane  
Decane, 2,6,7-trimethyl- (CAS) 69531 062108-25-2 64

53 9.473 0.06 C:\Database\WILEY275.L  
MESO-2,3-BUTANDIOL DIACETATE 58606 000000-00-0 27  
D,L-2,3-BUTANDIOL DIACETATE 58607 000000-00-0 12  
Ethanol, 2-[2-(2-methoxyethoxy)eth 90646 003610-27-3 10  
oxy]-, acetate (CAS) \$\$ Methoxytri  
glycol acetate \$\$ Triethylene glyc  
ol monomethyl ether acetate \$\$ Ace  
tic acid, 2-(2-(2-methoxyethoxy)et  
hoxy)ethyl ester \$\$ 2-(2-(2-Methox  
yethoxy)ethoxy)ethylester kyseliny octove \$\$ 2-(2-(

54 9.701 0.11 C:\Database\WILEY275.L  
3-Heptene, 4-methyl- (CAS) \$\$ 4-Me 10992 004485-16-9 38  
thyl-3-heptene  
1-methyl-3-(hydroxyethyl)propadien 5900 005689-23-6 35  
e \$\$ 1-methyl-3-(hydroxyethyl)allene \$\$ 3,4-Hexadien-1-ol  
2-Heptene, 4-methyl-, (E)- \$\$ tran 11194 066225-17-0 30  
s-4-Methyl-2-heptene \$\$ 4-Methyl-trans-2-heptene

55 9.787 0.07 C:\Database\WILEY275.L  
1,3-Propanediol, 2-butyl-2-ethyl- 45446 000115-84-4 38  
(CAS) \$\$ 2-Butyl-2-ethyl-1,3-propa  
nediol \$\$ BEP \$\$ 2-Ethyl-2-butylpr



opanediol-1,3 \$\$ 2-n-Butyl-2-ethyl  
 -1,3-propanediol \$\$ 2-Ethyl-2-buty  
 l-1,3-propandiol \$\$ 3,3-Bis(hydro  
 xymethyl)heptane \$\$ 2-Ethyl-2-butyl-1,3-propanediol  
 2-Propenoic acid, 6-methylheptyl e 68895 054774-91-3 27  
 ster (CAS) \$\$ 6-METHYLHEPTYL ACRYLATE  
 2-ethyl butanol 7887 000000-00-0 27

56 9.953 0.31 C:\Database\WILEY275.L  
 2-Butanol, 3-methyl-, acetate (CAS 20851 005343-96-4 17  
 ) \$\$ 1,2-Dimethylpropyl acetate \$\$  
 3-Methyl-2-butyl acetate \$\$ CH3C(  
 O)OCH(CH3)CH(CH3)2 \$\$ 1,2-Dimethylpropyl ethanoate  
 Acetic acid, sec-octyl ester (CAS) 57387 054515-77-4 17  
 \$\$ sec-Octyl acetate \$\$ 2-Methylheptyl acetate  
 1,3-Dioxolane, 2,2-dimethyl- (CAS) 7546 002916-31-6 16  
 \$\$ Acetone, cyclic ethylene aceta  
 l \$\$ 2,2-Dimethyl-1,3-dioxolane \$\$  
 Acetone glycol \$\$ Acetone ethylene ketal

57 10.039 0.05 C:\Database\WILEY275.L  
 Decane, 2,4,6-trimethyl- (CAS) 69527 062108-27-4 50  
 Pentacosane (CAS) \$\$ n-Pentacosane 212921 000629-99-2 47  
 Tetradecane, 4-ethyl- (CAS) \$\$ 4-E 112871 055045-14-2 47  
 thyltetradecane

58 10.077 0.09 C:\Database\WILEY275.L  
 Hexanal, 3,3-dimethyl- (CAS) 19456 055320-57-5 53  
 Hexanal, 3,3-dimethyl- (CAS) 19457 055320-57-5 53  
 Piperidine (CAS) \$\$ Cypentil \$\$ Az 3089 000110-89-4 50  
 acyclohexane \$\$ Cyclopentimine \$\$  
 Hexazane \$\$ Hexahydropyridine \$\$ P  
 entamethylenimine \$\$ Pyridine, hex  
 ahydro- \$\$ Perhydropyridine \$\$ Pen  
 tamethyleneimine \$\$ Piperidin \$\$ UN 2401

59 10.101 0.09 C:\Database\WILEY275.L  
 Piperidine (CAS) \$\$ Cypentil \$\$ Az 3080 000110-89-4 52  
 acyclohexane \$\$ Cyclopentimine \$\$  
 Hexazane \$\$ Hexahydropyridine \$\$ P  
 entamethylenimine \$\$ Pyridine, hex  
 ahydro- \$\$ Perhydropyridine \$\$ Pen  
 tamethyleneimine \$\$ Piperidin \$\$ UN 2401  
 Piperidine (CAS) \$\$ Cypentil \$\$ Az 3082 000110-89-4 50  
 acyclohexane \$\$ Cyclopentimine \$\$  
 Hexazane \$\$ Hexahydropyridine \$\$ P  
 entamethylenimine \$\$ Pyridine, hex  
 ahydro- \$\$ Perhydropyridine \$\$ Pen  
 tamethyleneimine \$\$ Piperidin \$\$ UN 2401  
 Piperidine (CAS) \$\$ Cypentil \$\$ Az 3087 000110-89-4 50  
 acyclohexane \$\$ Cyclopentimine \$\$  
 Hexazane \$\$ Hexahydropyridine \$\$ P  
 entamethylenimine \$\$ Pyridine, hex  
 ahydro- \$\$ Perhydropyridine \$\$ Pen  
 tamethyleneimine \$\$ Piperidin \$\$ UN 2401

60 10.182 0.56 C:\Database\WILEY275.L  
Hexane, 2,3,4-trimethyl- (CAS) \$\$ 19865 000921-47-1 49  
2,3,4-Trimethylhexane \$\$ 3-Ethyl-2-methylhexane  
Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12480 000563-16-6 47  
-Dimethylhexane  
Heneicosane, 11-(1-ethylpropyl)- ( 220175 055282-11-6 47  
CAS) \$\$ 11-(3-PENTYL)HENEICOSANE \$  
\$ 11-(1-Ethylpropyl)heneicosane \$\$ 11-(3'-n-Pentyl)heneicosane

61 10.306 0.44 C:\Database\WILEY275.L  
2-Butanol, 3-methyl-, acetate (CAS 20852 005343-96-4 38  
) \$\$ 1,2-Dimethylpropyl acetate \$\$  
3-Methyl-2-butyl acetate \$\$ CH3C(  
O)OCH(CH3)CH(CH3)2 \$\$ 1,2-Dimethylpropyl ethanoate  
2-PENTYL ACETATE 20966 000000-00-0 25  
2-Pentanol, acetate (CAS) \$\$ 2-Pen 20823 000626-38-0 25  
tyl acetate \$\$ 2-Acetoxy-pentane \$\$  
1-Methylbutyl acetate \$\$ Acetic a  
cid, 2-pentyl ester \$\$ sec-Amyl ac  
etate \$\$ sek.Amylester kyseliny oc  
tove \$\$ 2-Amylester kyseliny octove \$\$ UN 1104

62 10.463 0.31 C:\Database\WILEY275.L  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55976 001636-43-7 87  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55977 001636-43-7 83  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55978 001636-43-7 83  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE

63 10.496 0.32 C:\Database\WILEY275.L  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55977 001636-43-7 83  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55976 001636-43-7 83  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55978 001636-43-7 83  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE

64 10.792 0.42 C:\Database\WILEY275.L  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55976 001636-43-7 50  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
Hexanal, 3,3-dimethyl- (CAS) 19456 055320-57-5 38  
Piperidine (CAS) \$\$ Cypentil \$\$ Az 3082 000110-89-4 38  
acyclohexane \$\$ Cyclopentimine \$\$  
Hexazane \$\$ Hexahydropyridine \$\$ P  
entamethylenimine \$\$ Pyridine, hex  
ahydro- \$\$ Perhydropyridine \$\$ Pen  
tamethyleneimine \$\$ Piperidin \$\$ UN 2401

65 10.853 0.28 C:\Database\WILEY275.L  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55976 001636-43-7 64  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
Piperidine (CAS) \$\$ Cypentil \$\$ Az 3088 000110-89-4 52  
acyclohexane \$\$ Cyclopentimine \$\$  
Hexazane \$\$ Hexahydropyridine \$\$ P  
entamethylenimine \$\$ Pyridine, hex

ahydro- \$\$ Perhydropyridine \$\$ Pen  
 tamethyleneimine \$\$ Piperidin \$\$ UN 2401  
 Hexanal, 3,3-dimethyl- (CAS) 19457 055320-57-5 50

- 66 10.973 0.27 C:\Database\WILEY275.L  
 ETHYL OCTANOATE 57531 000000-00-0 64  
 Octanoic acid, ethyl ester (CAS) \$ 57304 000106-32-1 64  
 \$ Ethyl caprylate \$\$ Ethyl octanoa  
 te \$\$ Ethyl octoate \$\$ Ethyl n-oct  
 anoate \$\$ Caprylic acid ethyl este  
 r \$\$ n-Caprylic acid ethyl ester \$\$ Ethyl octylate  
 Heptanoic acid, ethyl ester (CAS) 43883 000106-30-9 50  
 \$\$ Ethyl heptanoate \$\$ Wine oil \$\$  
 Grape oil \$\$ Cognac oil \$\$ Ethyl  
 enanthate \$\$ Oenanthic ether \$\$ Et  
 hyl heptylate \$\$ Enanthylic ether  
 \$\$ Ethyl oenanthate \$\$ Ethyl n-hep  
 tanoate \$\$ Aether oenanthicus \$\$ Ethyl oenanthylate
- 67 11.125 0.05 C:\Database\WILEY275.L  
 3-Ethyl-3-methylheptane \$\$ Heptane 30105 017302-01-1 50  
 , 3-ethyl-3-methyl- \$\$ 3-Methyl-3-ethylheptane  
 Decane, 3-bromo- (CAS) 104896 030571-71-2 47  
 Tridecane, 7-propyl- (CAS) \$\$ 7-n- 112877 055045-09-5 46  
 Propyltridecane
- 68 11.258 0.11 C:\Database\WILEY275.L  
 Undecane, 5-methyl- (CAS) \$\$ 5-Met 55961 001632-70-8 80  
 hylundecane \$\$ Methylundecane  
 Nonadecane (CAS) \$\$ n-Nonadecane 151986 000629-92-5 58  
 Undecane, 2,7-dimethyl- (CAS) 69489 017301-24-5 53
- 69 11.344 0.03 C:\Database\WILEY275.L  
 Decane, 3-methyl- (CAS) \$\$ 3-Methy 42777 013151-34-3 53  
 ldecane \$\$ 2-Ethylnonane  
 Undecane, 4-methyl- (CAS) \$\$ 4-Met 55955 002980-69-0 53  
 hylundecane  
 Undecane, 4-methyl- (CAS) \$\$ 4-Met 55956 002980-69-0 53  
 hylundecane
- 70 11.449 0.10 C:\Database\WILEY275.L  
 Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 72  
 Octacosane (CAS) \$\$ n-Octacosane 232589 000630-02-4 64  
 Eicosane (CAS) \$\$ n-Eicosane 163886 000112-95-8 64
- 71 11.653 0.09 C:\Database\WILEY275.L  
 Tridecane, 3-methyl- (CAS) \$\$ 3-Me 83556 006418-41-3 59  
 thyltridecane \$\$ 3-METHYL-TRIDECAN  
 Decane, 2,6,8-trimethyl- (CAS) 69532 062108-26-3 53  
 PENTADECANE, 2,6,10-TRIMETHYL- \$\$ 139453 000000-00-0 53  
 NOR-PRISTAN
- 72 12.106 0.08 C:\Database\WILEY275.L  
 Hydroxylamine, O-decyl- (CAS) \$\$ O 58133 029812-79-1 43  
 -Decylhydroxylamine \$\$ Decyloxyamine  
 Dodecane, 2,6,10-trimethyl- (CAS) 98330 003891-98-3 38

\$\$ Farnesane \$\$ Farnesan \$\$ 2,6,10-Trimethyldodecane  
 Undecane (CAS) \$\$ n-Undecane \$\$ He 42753 001120-21-4 35  
 ndecane \$\$ n-C11H24 \$\$ UN 2330

- 73 12.239 0.19 C:\Database\WILEY275.L  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139441 000593-45-3 83  
 \$ Octadecan  
 Tetracosane (CAS) \$\$ n-Tetracosane 204917 000646-31-1 83  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139436 000593-45-3 83  
 \$ Octadecan
- 74 12.444 0.08 C:\Database\WILEY275.L  
 Undecane, 2,4-dimethyl- (CAS) \$\$ 2 69482 017312-80-0 59  
 ,4-Dimethylundecane  
 Undecane, 2,4-dimethyl- (CAS) \$\$ 2 69483 017312-80-0 53  
 ,4-Dimethylundecane  
 Decane, 1-iodo- (CAS) \$\$ Decyl iod 150960 002050-77-3 47  
 ide \$\$ 1-Iododecane \$\$ 1-Iododecan  
 e \$\$ n-Decyl iodide \$\$ 1-Decyl iodide
- 75 12.525 0.23 C:\Database\WILEY275.L  
 Undecane, 2,5-dimethyl- (CAS) \$\$ 2 69484 017301-22-3 81  
 ,5-Dimethylundecane  
 Undecane, 2,6-dimethyl- (CAS) \$\$ 2 69487 017301-23-4 81  
 ,6-Dimethylundecane \$\$ 2,6-Dimethylundecene  
 Undecane, 2,6-dimethyl- (CAS) \$\$ 2 69488 017301-23-4 70  
 ,6-Dimethylundecane \$\$ 2,6-Dimethylundecene
- 76 12.630 0.07 C:\Database\WILEY275.L  
 Dodecane, 5-methyl- (CAS) \$\$ 5-Met 69472 017453-93-9 47  
 hylundecane  
 Undecane, 3-methyl- (CAS) \$\$ 3-Met 55950 001002-43-3 47  
 hylundecane  
 3-BROMODECANE 104901 000000-00-0 43
- 77 12.744 0.31 C:\Database\WILEY275.L  
 Benzaldehyde, ethyl- (CAS) \$\$ AR-E 23117 053951-50-1 60  
 THYLBENZALDEHYDE \$\$ P-ETHYLBENZALD  
 EHYDE \$\$ Ethylbenzaldehyde  
 4-ETHYLBENZALDEHYDE 23079 000000-00-0 53  
 Benzaldehyde, ethyl- (CAS) \$\$ AR-E 23116 053951-50-1 53  
 THYLBENZALDEHYDE \$\$ P-ETHYLBENZALD  
 EHYDE \$\$ Ethylbenzaldehyde
- 78 12.887 0.20 C:\Database\WILEY275.L  
 3,3,3-d(3)-exo-2-Norbornyl chlorid 20657 000000-00-0 27  
 (S)-(-)-Ipsenol \$\$ 7-Octen-4-ol, 2 40074 035628-05-8 23  
 -methyl-6-methylene-, (S)- (CAS) \$  
 \$ Ipsenol \$\$ 7-Octen-4-ol, 2-methy  
 l-6-methylene-, (-)- \$\$ 2-Methyl-6  
 -methylene-7-octen-4-ol \$\$ (-)-Ipsenol  
 2-Propenal, 3-(2-ethyl-1,3,2-dioxa 39336 074807-48-0 23  
 borolan-4-yl)-, (E)- (CAS) \$\$ 1,3,  
 2-DIOXABOROLANE, 2-ETHYL-4-(2-FORMYL-1-ETHENYL-TRANS)-
- 79 12.982 0.05 C:\Database\WILEY275.L

Hexadecane, 7,9-dimethyl- (CAS) \$\$ 139421 021164-95-4 38  
7,9-Dimethylhexadecane  
Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12480 000563-16-6 35  
-Dimethylhexane  
Heptadecane, 2,6,10,14-tetramethyl 175424 018344-37-1 35  
- (CAS) \$\$ 2,6,10,14-Tetramethylheptadecane

80 13.215 0.16 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 86  
\$ Octadecan  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69455 000629-50-5 78  
Tridecane, n-  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69459 000629-50-5 72  
Tridecane, n-

81 13.363 0.19 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 87  
Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 80  
\$ Octadecan  
Decane, 2,4,6-trimethyl- (CAS) 69527 062108-27-4 80

82 13.444 0.04 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151986 000629-92-5 49  
Pentadecane (CAS) \$\$ n-Pentadecane 98301 000629-62-9 47  
\$\$ CH3(CH2)13CH3  
Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 47

83 13.520 0.26 C:\Database\WILEY275.L  
Dodecane, 4,6-dimethyl- (CAS) 83566 061141-72-8 86  
Pentadecane, 2,6,10,14-tetramethyl 151993 001921-70-6 72  
- (CAS) \$\$ Pristane \$\$ PRISTANE (F  
IELD ION) \$\$ 2,6,10,14-Tetramethyl  
pentadecane \$\$ Pristan \$\$ Norphyta  
n \$\$ Norphytane \$\$ Bute hydrocarbo  
n \$\$ 2,6,10,14-TETRAMETHYL PENTADECANE  
Undecane, 4,6-dimethyl- (CAS) 69502 017312-82-2 64

84 13.682 0.11 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 72  
\$ Octadecan  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 72  
Tetradecane, 4-methyl- (CAS) 98321 025117-24-2 64

85 13.749 0.33 C:\Database\WILEY275.L  
Dodecane, 5-methyl- (CAS) \$\$ 5-Met 69472 017453-93-9 58  
hyldodecane  
Undecane, 2,9-dimethyl- (CAS) 69491 017301-26-7 53  
Decane, 3-ethyl-3-methyl- (CAS) 69511 017312-66-2 50

86 13.901 0.06 C:\Database\WILEY275.L  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 50  
\$\$ Normal-heptadecane  
Heptadecane, 9-octyl- (CAS) \$\$ 9-N 212918 007225-64-1 50  
-OCTYLHEPTADECANE  
Iron, tricarbonyl[N-(phenyl-2-pyri 233784 074764-11-7 50  
dinylmethylene)benzenamine-N,N']-

87 14.039 0.78 C:\Database\WILEY275.L  
Dodecane, 4,6-dimethyl- (CAS) 83566 061141-72-8 72  
Decane, 2,3,6-trimethyl- (CAS) 69524 062238-12-4 64  
Heptadecane (CAS) \$\$ n-Heptadecane 126477 000629-78-7 59  
\$\$ Normal-heptadecane

88 14.234 0.12 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 74  
\$ Octadecan  
Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 72  
\$ Octadecan  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 72

89 14.301 0.12 C:\Database\WILEY275.L  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 64  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 64  
Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 59  
\$ Octadecan

90 14.363 0.09 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175420 000629-94-7 64  
Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 64  
\$ Octadecan  
OCTADECANE 139454 000593-45-3 64

91 14.435 0.08 C:\Database\WILEY275.L  
Dodecane, 4,6-dimethyl- (CAS) 83566 061141-72-8 59  
Pentadecane, 2,6,10,14-tetramethyl 151993 001921-70-6 58  
- (CAS) \$\$ Pristane \$\$ PRISTANE (F  
IELD ION) \$\$ 2,6,10,14-Tetramethyl  
pentadecane \$\$ Pristan \$\$ Norphyta  
n \$\$ Norphytane \$\$ Bute hydrocarbo  
n \$\$ 2,6,10,14-TETRAMETHYL PENTADECANE  
Undecane, 4,6-dimethyl- (CAS) 69502 017312-82-2 58

92 14.525 0.18 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 62  
\$ Octadecan  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 58  
2H46 STANDARD \$\$ Normal-docosane  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112855 000544-76-3 58  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane

93 14.620 0.33 C:\Database\WILEY275.L  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69459 000629-50-5 38  
Tridecane, n-  
1-Iodo-2-methylnonane 150962 000000-00-0 38  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69462 000629-50-5 38  
Tridecane, n-

94 14.758 0.17 C:\Database\WILEY275.L  
3-BROMODECANE 104901 000000-00-0 64  
Undecane, 2,4-dimethyl- (CAS) \$\$ 2 69481 017312-80-0 64  
,4-Dimethylundecane  
Decane (CAS) \$\$ n-Decane \$\$ Isodec 30015 000124-18-5 59

ane \$\$ n-C10H22 \$\$ UN 2247

- 95 14.801 0.11 C:\Database\WILEY275.L  
Cyclohexane, 1,2,3-trimethyl-, (1. 18310 007667-55-2 43  
alpha.,2.alpha.,3.beta.)- (CAS) \$\$  
1,TRANS-2,CIS-3-TRIMETHYLCYCLOHEX  
ANE \$\$ Cyclohexane, 1,2,3-trimethy  
l-, cis,trans- \$\$ Cyclohexane, 1,2  
,3-trimethyl-, cis-1,2,trans-1,3-  
\$\$ 1,cis-2,trans-3-Trimethylcyclohexane \$\$ cis,cis,  
1,2,3-trimethylcyclohexane (1r,2t, 18336 001678-81-5 433c)  
(s)-3-ethyl-4-methylpentanol-1 \$\$ 21220 100431-87-6 35  
1-Pentanol, 3-ethyl-4-methyl-, (S)
- 96 14.930 0.06 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 50  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 50  
Heptadecane (CAS) \$\$ n-Heptadecane 126478 000629-78-7 50  
\$\$ Normal-heptadecane
- 97 14.973 0.08 C:\Database\WILEY275.L  
Octane, 4-methyl- (CAS) \$\$ 4-Methy 19808 002216-34-4 35  
loctane \$\$ Isononane  
Hexane, 2,3,4-trimethyl- (CAS) \$\$ 19866 000921-47-1 35  
2,3,4-Trimethylhexane \$\$ 3-Ethyl-2-methylhexane  
Octane, 4-methyl- (CAS) \$\$ 4-Methy 19809 002216-34-4 35  
loctane \$\$ Isononane
- 98 15.054 0.42 C:\Database\WILEY275.L  
Octane, 5-ethyl-2-methyl- (CAS) 42793 062016-18-6 83  
pentadecane 98339 000629-62-9 80  
Nonadecane (CAS) \$\$ n-Nonadecane 151979 000629-92-5 72
- 99 15.244 0.11 C:\Database\WILEY275.L  
Decane, 2,3,6-trimethyl- (CAS) 69524 062238-12-4 53  
Hexadecane, 2,6,10,14-tetramethyl- 163891 000638-36-8 50  
(CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane \$\$ Phytan  
Decane (CAS) \$\$ n-Decane \$\$ Isodec 30015 000124-18-5 49  
ane \$\$ n-C10H22 \$\$ UN 2247
- 100 15.430 0.07 C:\Database\WILEY275.L  
Undecane, 4,7-dimethyl- (CAS) 69503 017301-32-5 53  
Nonane, 3-methyl-5-propyl- (CAS) 69544 031081-18-2 50  
pentadecane 98339 000629-62-9 50
- 101 15.654 0.68 C:\Database\WILEY275.L  
Propanoic acid, 2-methyl-, 2,2-dim 101386 074367-33-2 59  
ethyl-1-(2-hydroxy-1-methylethyl)p  
ropyl ester (CAS) \$\$ 2,2-Dimethyl-  
1-(2-hydroxy-1-isopropyl)propyl ester of isobutanoic acid  
Butanoic acid, 2-methylpropyl este 31039 000539-90-2 50  
r (CAS) \$\$ isobutyl butanoate \$\$ I  
sobutyl butyrate \$\$ Isobutyl n-but  
yrate \$\$ 2-Methylpropyl butyrate \$  
\$ Butyric acid, isobutyl ester \$\$  
Isobutyl ester of butanoic acid \$\$

n-Butyric acid isobutyl ester \$\$  
 2-Methylpropyl bu  
 Butanoic acid, butyl ester (CAS) \$ 31030 000109-21-7 43  
 \$ n-Butyl n-butyrate \$\$ Butyl buty  
 late \$\$ Butyl butyrate \$\$ Butyl bu  
 tanoate \$\$ 1-Butyl butyrate \$\$ n-B  
 utyl butyrate \$\$ n-Butyl butanoate  
 \$\$ Butyric acid, butyl ester \$\$ B  
 utyl ester of butanoic acid \$\$ Butyl n-butyrate \$\$

102 15.792 0.07 C:\Database\WILEY275.L  
 Tetracosane, 2,6,10,15,19,23-hexam 242815 000111-01-3 38  
 ethyl- (CAS) \$\$ Squalane \$\$ Robane  
 \$\$ Squalan \$\$ Cosbiol \$\$ Spinacan  
 e \$\$ Vitabiosol \$\$ Perhydrosqualen  
 e \$\$ Dodecahydrosqualene \$\$ 2,6,10  
 ,15,19,23-Hexamethyltetracosane \$\$ Hexamethyltetracosane  
 Hexadecane, 7-methyl- (CAS) 126482 026730-20-1 38  
 Hexadecane, 2,6,10,14-tetramethyl- 163891 000638-36-8 38  
 (CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane \$\$ Phytan

103 15.906 0.10 C:\Database\WILEY275.L  
 Eicosane, 10-methyl- (CAS) \$\$ 10-M 175412 054833-23-7 80  
 ETHYLEICOSANE  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 74  
 Eicosane (CAS) \$\$ n-Eicosane 163880 000112-95-8 72

104 16.101 0.95 C:\Database\WILEY275.L  
 Butanoic acid, butyl ester (CAS) \$ 31035 000109-21-7 87  
 \$ n-Butyl n-butyrate \$\$ Butyl buty  
 late \$\$ Butyl butyrate \$\$ Butyl bu  
 tanoate \$\$ 1-Butyl butyrate \$\$ n-B  
 utyl butyrate \$\$ n-Butyl butanoate  
 \$\$ Butyric acid, butyl ester \$\$ B  
 utyl ester of butanoic acid \$\$ Butyl n-butyrate \$\$  
 Butanoic acid, butyl ester (CAS) \$ 31036 000109-21-7 78  
 \$ n-Butyl n-butyrate \$\$ Butyl buty  
 late \$\$ Butyl butyrate \$\$ Butyl bu  
 tanoate \$\$ 1-Butyl butyrate \$\$ n-B  
 utyl butyrate \$\$ n-Butyl butanoate  
 \$\$ Butyric acid, butyl ester \$\$ B  
 utyl ester of butanoic acid \$\$ Butyl n-butyrate \$\$  
 Butanoic acid, butyl ester (CAS) \$ 31033 000109-21-7 78  
 \$ n-Butyl n-butyrate \$\$ Butyl buty  
 late \$\$ Butyl butyrate \$\$ Butyl bu  
 tanoate \$\$ 1-Butyl butyrate \$\$ n-B  
 utyl butyrate \$\$ n-Butyl butanoate  
 \$\$ Butyric acid, butyl ester \$\$ B  
 utyl ester of butanoic acid \$\$ Butyl n-butyrate \$\$

105 16.515 0.06 C:\Database\WILEY275.L  
 N-NONADECANE 152007 000629-92-5 58  
 pentadecane 98340 000629-62-9 53  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 53  
 \$ Octadecan



106 16.606 0.15 C:\Database\WILEY275.L  
Tetradecane (CAS) \$\$ n-Tetradecane 83536 000629-59-4 96  
\$\$ Isotetradecane  
Tetradecane (CAS) \$\$ n-Tetradecane 83545 000629-59-4 95  
\$\$ Isotetradecane  
Tetradecane (CAS) \$\$ n-Tetradecane 83548 000629-59-4 93  
\$\$ Isotetradecane

107 16.763 0.13 C:\Database\WILEY275.L  
Hexadecane, 7,9-dimethyl- (CAS) \$\$ 139421 021164-95-4 64  
7,9-Dimethylhexadecane  
Nonadecane (CAS) \$\$ n-Nonadecane 151985 000629-92-5 53  
Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 52  
\$ Octadecan

108 16.815 0.20 C:\Database\WILEY275.L  
Heptadecane (CAS) \$\$ n-Heptadecane 126476 000629-78-7 87  
\$\$ Normal-heptadecane  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112852 000544-76-3 87  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
Octadecane (CAS) \$\$ n-Octadecane \$ 139434 000593-45-3 86  
\$ Octadecan

109 16.901 0.18 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 87  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 80  
2H46 STANDARD \$\$ Normal-docosane  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 80

110 17.030 0.07 C:\Database\WILEY275.L  
Tetradecane, 4-methyl- (CAS) 98321 025117-24-2 80  
Heptadecane, 4-methyl- (CAS) \$\$ 4- 139425 026429-11-8 59  
Methylheptadecane  
Undecane, 2,8-dimethyl- (CAS) 69490 017301-25-6 53

111 17.296 0.04 C:\Database\WILEY275.L  
1-Heptadecanamine (CAS) \$\$ n-Hepta 140020 004200-95-7 43  
decylamine \$\$ Margarylamine \$\$ Heptadecylamine \$\$ 1-Aminoheptadecane  
1-Heptadecanamine (CAS) \$\$ n-Hepta 140018 004200-95-7 43  
decylamine \$\$ Margarylamine \$\$ Heptadecylamine \$\$ 1-Aminoheptadecane  
Octadecane, 3-ethyl-5-(2-ethylbuty 220178 055282-12-7 43  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane

112 17.344 0.08 C:\Database\WILEY275.L  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69461 000629-50-5 58  
Tridecane, n-  
Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 58  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 58  
2H46 STANDARD \$\$ Normal-docosane

113 17.482 0.05 C:\Database\WILEY275.L  
Octadecane, 3-ethyl-5-(2-ethylbuty 220176 055282-12-7 53  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Pentadecane (CAS) \$\$ n-Pentadecane 98302 000629-62-9 50  
\$\$ CH3(CH2)13CH3  
Undecane, 4,7-dimethyl- (CAS) 69503 017301-32-5 50

114 17.558 0.07 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 64  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112843 000544-76-3 64  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 64

115 17.668 0.23 C:\Database\WILEY275.L  
Decane, 2,4-dimethyl- (CAS) \$\$ 2,4 55967 002801-84-5 59  
-Dimethyldecane  
PENTADECANE, 2,6,10-TRIMETHYL- \$\$ 139453 000000-00-0 59  
NOR-PRISTAN  
Octadecane (CAS) \$\$ n-Octadecane \$ 139441 000593-45-3 50  
\$ Octadecan

116 17.715 0.05 C:\Database\WILEY275.L  
Octadecane, 5-methyl- (CAS) \$\$ 5-M 151973 025117-35-5 47  
ETHYL OCTADECANE  
Dotriacontane (CAS) \$\$ n-Dotriacon 250416 000544-85-4 43  
tane \$\$ Bicetyl \$\$ Tris(trimethyls  
ilyl)ether, methyl ester of ethyl  
anthranilate azo pigment(.alpha.z)  
of bilivubin-1x.alpha. 2-O-acyl glucuronide  
Decane, 2,4,6-trimethyl- (CAS) 69527 062108-27-4 43

117 17.801 0.31 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 86  
Octadecane (CAS) \$\$ n-Octadecane \$ 139436 000593-45-3 80  
\$ Octadecan  
Nonadecane (CAS) \$\$ n-Nonadecane 151982 000629-92-5 80

118 17.958 0.71 C:\Database\WILEY275.L  
3-Methylheneicosane \$\$ Heneicosane 186066 006418-47-9 43  
, 3-methyl-  
Octadecane, 3-ethyl-5-(2-ethylbuty 220177 055282-12-7 40  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Hexadecane, 8-hexyl-8-pentyl- (CAS 226679 055282-29-6 40  
) \$\$ 8-N-PENTYL-8-N-HEXYLHEXADECAN

119 18.130 0.14 C:\Database\WILEY275.L  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112843 000544-76-3 64  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
pentadecane 98339 000629-62-9 59  
Nonadecane (CAS) \$\$ n-Nonadecane 151979 000629-92-5 59

120 18.377 0.07 C:\Database\WILEY275.L  
Hexadecane, 2,6,11,15-tetramethyl- 163897 000504-44-9 58  
(CAS) \$\$ 2,6,11,15-Tetramethylhexadecane \$\$ Crocetane  
Hexadecane, 2,6,10,14-tetramethyl- 163888 000638-36-8 53  
(CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane \$\$ Phytan  
pentadecane 98338 000629-62-9 50

121 18.487 0.34 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 53  
Undecane, 2,4-dimethyl- (CAS) \$\$ 2 69483 017312-80-0 53  
,4-Dimethylundecane

Undecane, 3,9-dimethyl- (CAS) 69499 017301-31-4 52

122 18.592 1.01 C:\Database\WILEY275.L  
Dodecane, 3-methyl- (CAS) \$\$ 3-Met 69468 017312-57-1 86  
hyldodecane  
Nonadecane (CAS) \$\$ n-Nonadecane 151987 000629-92-5 86  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 80

123 18.801 0.22 C:\Database\WILEY275.L  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 80  
\$\$ Normal-heptadecane  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 52  
Eicosane, 2,4-dimethyl- 186068 075163-98-3 52

124 18.849 0.10 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 72  
2H46 STANDARD \$\$ Normal-docosane  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112845 000544-76-3 64  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 64

125 18.973 0.27 C:\Database\WILEY275.L  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 83  
\$\$ Normal-heptadecane  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112855 000544-76-3 80  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
pentadecane 98340 000629-62-9 80

126 19.073 0.20 C:\Database\WILEY275.L  
Phenol, 2,6-bis(1,1-dimethylethyl) 105777 000128-37-0 96  
-4-methyl- (CAS) \$\$ 4-Methyl-2,6-d  
i-tert-butylphenol \$\$ BHT \$\$ P 21  
\$\$ CAO 3 \$\$ AO 29 \$\$ CAO 1 \$\$ AO 4  
K \$\$ DBPC \$\$ P 21 \$ \$\$ 2,6-DI-TERT  
-4-METHYLPHENOL \$\$ Buks \$\$ Ional \$  
\$ Ionole \$\$ Deenax \$\$ Dalpac \$\$ Stavox \$\$ Vianol \$\$  
Phenol, 2,6-bis(1,1-dimethylethyl) 105783 000128-37-0 95  
-4-methyl- (CAS) \$\$ 4-Methyl-2,6-d  
i-tert-butylphenol \$\$ BHT \$\$ P 21  
\$\$ CAO 3 \$\$ AO 29 \$\$ CAO 1 \$\$ AO 4  
K \$\$ DBPC \$\$ P 21 \$ \$\$ 2,6-DI-TERT  
-4-METHYLPHENOL \$\$ Buks \$\$ Ional \$  
\$ Ionole \$\$ Deenax \$\$ Dalpac \$\$ Stavox \$\$ Vianol \$\$  
Phenol, 2,6-bis(1,1-dimethylethyl) 105779 000128-37-0 95  
-4-methyl- (CAS) \$\$ 4-Methyl-2,6-d  
i-tert-butylphenol \$\$ BHT \$\$ P 21  
\$\$ CAO 3 \$\$ AO 29 \$\$ CAO 1 \$\$ AO 4  
K \$\$ DBPC \$\$ P 21 \$ \$\$ 2,6-DI-TERT  
-4-METHYLPHENOL \$\$ Buks \$\$ Ional \$  
\$ Ionole \$\$ Deenax \$\$ Dalpac \$\$ Stavox \$\$ Vianol \$\$

127 19.139 0.36 C:\Database\WILEY275.L  
Phenol, 2,4-bis(1,1-dimethylethyl) 91574 000096-76-4 93  
- (CAS) \$\$ 2,4-Di-tert-butylphenol  
\$\$ 2,4-BIS(TERT-BUTYL)-PHENOL \$\$  
2,4-Di-t-butylphenol \$\$ Phenol, 2,

4-di-tert-butyl- \$\$ 2,4-Bis(1,1-di  
 methylethyl)phenol \$\$ 2,4-Di-tert-  
 butyl-phenol \$\$ 4-(1,5-Dimethylhex-4-enyl)cyclohex-  
 Phenol, 2,4-bis(1,1-dimethylethyl) 91572 000096-76-4 89  
 - (CAS) \$\$ 2,4-Di-tert-butylphenol  
 \$\$ 2,4-BIS(TERT-BUTYL)-PHENOL \$\$  
 2,4-Di-t-butylphenol \$\$ Phenol, 2,  
 4-di-tert-butyl- \$\$ 2,4-Bis(1,1-di  
 methylethyl)phenol \$\$ 2,4-Di-tert-  
 butyl-phenol \$\$ 4-(1,5-Dimethylhex-4-enyl)cyclohex-  
 Phenol, 2,4-bis(1,1-dimethylethyl) 91571 000096-76-4 76  
 - (CAS) \$\$ 2,4-Di-tert-butylphenol  
 \$\$ 2,4-BIS(TERT-BUTYL)-PHENOL \$\$  
 2,4-Di-t-butylphenol \$\$ Phenol, 2,  
 4-di-tert-butyl- \$\$ 2,4-Bis(1,1-di  
 methylethyl)phenol \$\$ 2,4-Di-tert-  
 butyl-phenol \$\$ 4-(1,5-Dimethylhex-4-enyl)cyclohex-

128 19.368 0.14 C:\Database\WILEY275.L  
 Cyclohexane, 1,2,4-trimethyl- (CAS 18320 002234-75-5 42  
 ) \$\$ 1,2,4-TRIMETHYLCYCLOHEXANE, (  
 CIS PLUS TRANS) \$\$ 1,2,4-Trimethylcyclohexane  
 Decanedioic acid, didecyl ester \$\$ 256920 002432-89-5 38  
 Didecyl sebacate  
 Cyclohexane, 1,2,4-trimethyl- (CAS 18319 002234-75-5 30  
 ) \$\$ 1,2,4-TRIMETHYLCYCLOHEXANE, (  
 CIS PLUS TRANS) \$\$ 1,2,4-Trimethylcyclohexane

129 19.558 0.07 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163879 000112-95-8 86  
 Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 70  
 N-EICOSANE 163902 000112-95-8 70

130 19.654 0.05 C:\Database\WILEY275.L  
 Ethanol, 2-(hexadecyloxy)- (CAS) \$ 167142 002136-71-2 38  
 \$ 2-Hexadecyloxyethanol \$\$ 2-Hexad  
 ecoxyethanol \$\$ 2-HEXADECYLOXY-ETH  
 ANOL \$\$ Ethylene glycol monohexadecyl ether  
 Octadecane, 3-ethyl-5-(2-ethylbuty 220178 055282-12-7 35  
 l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
 Tritriacontane (CAS) \$\$ n-Tritriac 253566 000630-05-7 35  
 ontane

131 19.773 0.19 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 80  
 N-NONADECANE 152007 000629-92-5 72  
 Nonadecane (CAS) \$\$ n-Nonadecane 151987 000629-92-5 72

132 19.901 0.68 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 86  
 2H46 STANDARD \$\$ Normal-docosane  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 72  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 72

133 20.120 0.03 C:\Database\WILEY275.L  
 Hexadecane, 2,6,10,14-tetramethyl- 163893 000638-36-8 38

(CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane \$\$ Phytan  
3-Ethyl-3-methylheptane \$\$ Heptane 30105 017302-01-1 38  
, 3-ethyl-3-methyl- \$\$ 3-Methyl-3-ethylheptane  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69452 000629-50-5 35  
Tridecane, n-

134 20.225 0.10 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 52  
2H46 STANDARD \$\$ Normal-docosane  
Tetradecane (CAS) \$\$ n-Tetradecane 83542 000629-59-4 52  
\$\$ Isotetradecane  
Nonadecane (CAS) \$\$ n-Nonadecane 151986 000629-92-5 50

135 20.511 0.06 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175421 000629-94-7 58  
Octadecane, 3-ethyl-5-(2-ethylbuty 220176 055282-12-7 50  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Nonadecane (CAS) \$\$ n-Nonadecane 151984 000629-92-5 50

136 20.835 0.15 C:\Database\WILEY275.L  
Eicosane, 2-methyl- (CAS) \$\$ 2-Met 175409 001560-84-5 74  
hyleicosane \$\$ 19-Methyleicosane  
Tetracosane (CAS) \$\$ n-Tetracosane 204922 000646-31-1 74  
Pentadecane, 2-methyl- (CAS) \$\$ 14 112861 001560-93-6 72  
-METHYLPENTADECANE \$\$ 2-Methylpentadecane

137 21.020 0.06 C:\Database\WILEY275.L  
Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 52  
riacontane  
Heptadecane (CAS) \$\$ n-Heptadecane 126476 000629-78-7 47  
\$\$ Normal-heptadecane  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 47

138 21.101 0.07 C:\Database\WILEY275.L  
1-Oxa-3-aza-2-silacyclopentan-5-on 92202 057954-43-5 43  
e, 2,2-dimethyl-3-phenyl- (CAS)  
1-Azido-1-(p-methoxyphenyl)ethane 61251 091633-30-6 38  
(5-deuterio)=tetracyclo[4.4.0.0(2, 23500 098675-23-1 35  
4).0(3,7)]decane

139 21.449 6.37 C:\Database\WILEY275.L  
ALLYL BUTYRATE \$\$ PROPENYL BUTYRAT 19278 002051-78-7 53  
PENTAN-1,3-DIOLDIISOBUTYRATE, 2,2, 166858 000000-00-0 50  
4-TRIMETHYL- \$\$ 1,3-Di(isobutoxyca  
rbonyl)-2,4,4-trimethylpentane  
BUTYL BUTYRYL LACTATE 101150 007492-70-8 45

140 21.592 0.07 C:\Database\WILEY275.L  
PHYTOL ISOMER 175378 000000-00-0 37  
5-Hepten-3-one, 5-ethyl-2-methyl- 39987 049833-97-8 35  
(CAS) \$\$ 5-ETHYL-2-METHYL-5-HEPTEN-3-ONE  
2-Hexadecen-1-ol, 3,7,11,15-tetram 175363 000150-86-7 32  
ethyl-, [R-[R\*,R\*-(E)]]- (CAS) \$\$  
Phytol \$\$ trans-Phytol \$\$ (E)-(7R,  
11R)-3,7,11,15-tetramethyl-2-hexad  
ecen-1-ol \$\$ 2-Hexadecen-1-ol, 3,7

,11,15-tetramethyl-, [R-[R@,R@-(E)  
 ]]- \$\$ 3,7,11,15-Tetramethyl-2-hexadecen-1-ol \$\$ (E

- 141 21.763 0.18 C:\Database\WILEY275.L  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112843 000544-76-3 95  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112855 000544-76-3 95  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112852 000544-76-3 94  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane
- 142 21.911 0.26 C:\Database\WILEY275.L  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 87  
 \$ Octadecan  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 87  
 acontane \$\$ NOR-HEXATRIACONTANE  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139436 000593-45-3 87  
 \$ Octadecan
- 143 21.992 0.08 C:\Database\WILEY275.L  
 Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 43  
 \$\$ Normal-heptadecane  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 43  
 Nonadecane (CAS) \$\$ n-Nonadecane 151984 000629-92-5 43
- 144 22.211 0.09 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 41  
 2H46 STANDARD \$\$ Normal-docosane  
 Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 38  
 Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 38
- 145 22.306 0.29 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163880 000112-95-8 87  
 EICOSANE 163904 000000-00-0 70  
 N-EICOSANE 163902 000112-95-8 70
- 146 22.397 0.11 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 83  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 81  
 riacontane  
 Nonacosane (CAS) \$\$ n-Nonacosane \$ 237993 000630-03-5 80  
 \$ Celidoniol, deoxy-
- 147 22.649 0.20 C:\Database\WILEY275.L  
 exo-Octahydro-4,7-methano-1H-inden 25274 002825-82-3 38  
 e \$\$ 4,7-Methano-1H-indene, octahy  
 dro-, (3a.alpha.,4.beta.,7.beta.,7  
 a.alpha.)- (CAS) \$\$ JP 10 \$\$ 4,7-M  
 ethanoindan, hexahydro-, exo- \$\$ e  
 xo-3,4,8,9-Tetrahydrodicyclopentad  
 iene \$\$ exo-Tricyclo[5.2.1.0(2,6)]decane \$\$ exo-Tet  
 2-methyl propenylpyrazine (propeny 23015 000000-00-0 27  
 l 1 or 2, Z or E and 5 or 6 on the pyrazine)  
 4,7-Methano-1H-indene, octahydro- 25301 006004-38-2 27  
 (CAS) \$\$ Tricyclo[5.2.1.0(2,6)]dec  
 ane \$\$ Tricyclo[5.2.1.0(sup2,6)]de

cane \$\$ Octahydro-4,7-methano inde  
 ne \$\$ Tetracyclo[5.2.1.0<2,6>]-dec  
 ane \$\$ Tricyclo[5.1.0-2.6]decane \$  
 \$ Tetrahydrodicyclopentadiene \$\$ Tcd-hydrocarbon A

- 148 22.763 0.40 C:\Database\WILEY275.L  
 Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 83  
 PENTADECANE, 2,6,10-TRIMETHYL- \$\$ 139453 000000-00-0 80  
 NOR-PRISTAN  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 74
- 149 22.844 0.12 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175421 000629-94-7 58  
 Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 58  
 \$\$ Normal-heptadecane  
 Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 53
- 150 22.892 0.07 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175421 000629-94-7 72  
 Octadecane, 3-ethyl-5-(2-ethylbuty 220178 055282-12-7 72  
 l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
 Octadecane, 3-ethyl-5-(2-ethylbuty 220176 055282-12-7 64  
 l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane
- 151 22.968 0.24 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 58  
 Triacontane (CAS) \$\$ n-Triacontane 242809 000638-68-6 58  
 Octacosane (CAS) \$\$ n-Octacosane 232588 000630-02-4 58
- 152 23.030 0.10 C:\Database\WILEY275.L  
 Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 83  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 74  
 riacontane  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 74  
 \$ Octadecan
- 153 23.106 0.25 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 87  
 2H46 STANDARD \$\$ Normal-docosane  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 83  
 Nonadecane (CAS) \$\$ n-Nonadecane 151987 000629-92-5 80
- 154 23.211 0.36 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 91  
 Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 91  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 91
- 155 23.297 0.15 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 87  
 2H46 STANDARD \$\$ Normal-docosane  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 86  
 Decyldocosane \$\$ 11-NOR-DECYLDOSANE  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 86
- 156 23.358 0.16 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 87

Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
2H46 STANDARD \$\$ Normal-docosane  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 83

157 23.439 0.17 C:\Database\WILEY275.L  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 80  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 74  
2H46 STANDARD \$\$ Normal-docosane  
Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 72

158 23.497 0.12 C:\Database\WILEY275.L  
Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 81  
Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 81  
riacontane  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 74  
\$\$ Normal-heptadecane

159 23.539 0.10 C:\Database\WILEY275.L  
Octadecane, 3-ethyl-5-(2-ethylbuty 220178 055282-12-7 64  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Heneicosane (CAS) \$\$ n-Heneicosane 175421 000629-94-7 58  
Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 58

160 23.597 0.08 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
2H46 STANDARD \$\$ Normal-docosane  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 83  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 80

161 23.654 0.42 C:\Database\WILEY275.L  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 87  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 87  
N-NONADECANE 152007 000629-92-5 86

162 23.711 0.93 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 90  
Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 86  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
2H46 STANDARD \$\$ Normal-docosane

163 23.806 0.23 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 90  
2H46 STANDARD \$\$ Normal-docosane  
Eicosane, 7-hexyl- (CAS) \$\$ 7-n-He 220184 055333-99-8 90  
xyleicosane  
Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 87

164 23.873 0.17 C:\Database\WILEY275.L  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 83  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
2H46 STANDARD \$\$ Normal-docosane  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80

165 23.920 0.25 C:\Database\WILEY275.L  
Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 86  
Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE



Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) 220176 055282-12-7 86  
 1)- (CAS) 3-Ethyl-5-(2'-ethylbutyl)octadecane  
 Eicosane (CAS) n-Eicosane 163883 000112-95-8 83

166 23.982 0.14 C:\Database\WILEY275.L  
 Hentriacontane (CAS) Untriacontane 246864 000630-04-6 72  
 n-Hentriacontane  
 10-Methylnonadecane 163906 000000-00-0 70  
 Heneicosane (CAS) n-Heneicosane 175421 000629-94-7 68

167 24.039 0.10 C:\Database\WILEY275.L  
 Pentadecane (CAS) n-Pentadecane 98305 000629-62-9 70  
 CH<sub>3</sub>(CH<sub>2</sub>)<sub>13</sub>CH<sub>3</sub>  
 Hexacosane (CAS) n-Hexacosane 220199 000630-01-3 68  
 Hentriacontane (CAS) Untriacontane 246864 000630-04-6 68  
 n-Hentriacontane

168 24.120 0.11 C:\Database\WILEY275.L  
 TETRADECANE 83575 000000-00-0 70  
 Tetratetracontane (CAS) n-Tetracontane 269825 007098-22-8 64  
 Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) 220178 055282-12-7 64  
 1)- (CAS) 3-Ethyl-5-(2'-ethylbutyl)octadecane

169 24.201 0.35 C:\Database\WILEY275.L  
 Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) 220176 055282-12-7 72  
 1)- (CAS) 3-Ethyl-5-(2'-ethylbutyl)octadecane  
 Pentadecane (CAS) n-Pentadecane 98301 000629-62-9 60  
 CH<sub>3</sub>(CH<sub>2</sub>)<sub>13</sub>CH<sub>3</sub>  
 Heptacosane (CAS) n-Heptacosane 226684 000593-49-7 59

170 24.292 0.09 C:\Database\WILEY275.L  
 Hexacosane (CAS) n-Hexacosane 220199 000630-01-3 83  
 Nonadecane (CAS) n-Nonadecane 151981 000629-92-5 72  
 Heneicosane (CAS) n-Heneicosane 175422 000629-94-7 72

171 24.363 0.08 C:\Database\WILEY275.L  
 Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) 220178 055282-12-7 64  
 1)- (CAS) 3-Ethyl-5-(2'-ethylbutyl)octadecane  
 Heptadecane (CAS) n-Heptadecane 126476 000629-78-7 59  
 Normal-heptadecane  
 Docosane, 11-decyl- (CAS) 11-n- 250413 055401-55-3 59  
 Decyldocosane 11-NOR-DECYLDOCOSANE

172 24.411 0.27 C:\Database\WILEY275.L  
 N-DOCOSANE 186069 000629-97-0 91  
 Triacontane (CAS) n-Triacontane 242802 000638-68-6 90  
 Pentacosane (CAS) n-Pentacosane 212919 000629-99-2 83

173 24.449 0.61 C:\Database\WILEY275.L  
 Octadecane (CAS) n-Octadecane 139440 000593-45-3 86  
 Octadecane  
 Pentacosane (CAS) n-Pentacosane 212919 000629-99-2 86  
 Docosane (CAS) n-Docosane 186056 000629-97-0 83  
 C<sub>22</sub>H<sub>46</sub> STANDARD Normal-docosane

174 24.539 0.14 C:\Database\WILEY275.L  
N-NONADECANE 152007 000629-92-5 86  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 74  
Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 72

175 24.597 0.09 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 64  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 64  
Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 59

176 24.639 0.09 C:\Database\WILEY275.L  
Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 59  
Heneicosane (CAS) \$\$ n-Heneicosane 175421 000629-94-7 58  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 58  
2H46 STANDARD \$\$ Normal-docosane

177 24.692 0.11 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151984 000629-92-5 38  
Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 38  
acontane \$\$ NOR-HEXATRIACONTANE  
Tritriacontane (CAS) \$\$ n-Tritriac 253566 000630-05-7 35  
ontane

178 24.792 0.19 C:\Database\WILEY275.L  
Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 86  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 83  
Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 83

179 24.897 0.08 C:\Database\WILEY275.L  
Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 62  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 58  
Pentatriacontane (CAS) \$\$ n-Pentat 258572 000630-07-9 58  
riacontane

180 24.973 0.06 C:\Database\WILEY275.L  
1,1,3,3,5,5,7,7,9,9,11,11,13,13-TE 260039 000000-00-0 23  
TRADECAMETHYL-HEPTASILOXANE  
9-epi-19-norambrox 108521 105561-24-8 22  
TETRACOSAMETHYLCYCLODODECASILOXANE 275053 018919-94-3 12  
\$\$ Cyclododecasiloxane, tetracosamethyl- (CAS)

181 25.092 0.60 C:\Database\WILEY275.L  
Anthracene-D10 63087 000000-00-0 95  
Anthracene-d10- 63091 001719-06-8 95  
DECADEUTEROPHENANTHRENE \$\$ Phenant 63089 001517-22-2 91  
hrene-d10

182 25.335 0.07 C:\Database\WILEY275.L  
Eicosane, 7-hexyl- (CAS) \$\$ 7-n-He 220184 055333-99-8 74  
xyleicosane  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 74  
10-Methylnonadecane 163906 000000-00-0 68

183 25.382 0.11 C:\Database\WILEY275.L  
Nonadecane, 9-methyl- (CAS) 163898 013287-24-6 81  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 81

Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 81  
2H46 STANDARD \$\$ Normal-docosane

184 25.439 0.11 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 70  
Eicosane (CAS) \$\$ n-Eicosane 163884 000112-95-8 49  
Eicosane (CAS) \$\$ n-Eicosane 163878 000112-95-8 42

185 25.611 0.07 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 68  
2H46 STANDARD \$\$ Normal-docosane  
Heptadecane, 2-methyl- (CAS) \$\$ 2- 139419 001560-89-0 64  
Methylheptadecane \$\$ 16-Methylheptadecane  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 64

186 25.801 0.17 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 80  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 80  
NONADECANE 152008 000000-00-0 72

187 25.878 0.27 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 70  
Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 70  
\$ Octadecan  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 70

188 25.973 0.09 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 74  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 74  
2H46 STANDARD \$\$ Normal-docosane  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 74

189 26.049 0.08 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 80  
\$ Octadecan  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 74  
Iron, tricarbonyl[N-(phenyl-2-pyridylmethylene)benzenamine-N,N']-

190 26.101 0.12 C:\Database\WILEY275.L  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 76  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 70  
2H46 STANDARD \$\$ Normal-docosane  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 70

191 26.144 0.19 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 81  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 81  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 81  
2H46 STANDARD \$\$ Normal-docosane

192 26.320 0.20 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 90  
Heptadecane, 9-octyl- (CAS) \$\$ 9-N 212918 007225-64-1 90  
-OCTYLHEPTADECANE  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 87

2H46 STANDARD \$\$ Normal-docosane

- 193 26.373 0.34 C:\Database\WILEY275.L  
 Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 86  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 86  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 86
- 194 26.463 0.33 C:\Database\WILEY275.L  
 Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 90  
 tane \$\$ Bicetyl \$\$ Tris(trimethyls  
 ilyl)ether, methyl ester of ethyl  
 anthranilate azo pigment(.alpha.z)  
 of bilivubin-1x.alpha. 2-O-acyl glucuronide  
 pentadecane 98339 000629-62-9 86  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
 2H46 STANDARD \$\$ Normal-docosane
- 195 26.520 0.13 C:\Database\WILEY275.L  
 N-DOCOSANE 186069 000629-97-0 87  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 83  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 83
- 196 26.573 0.25 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 90  
 2H46 STANDARD \$\$ Normal-docosane  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 90  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87
- 197 26.663 0.30 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 86  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 86  
 9-methylnonadecane 163903 000000-00-0 72
- 198 26.716 0.47 C:\Database\WILEY275.L  
 7,9-di-tert-butyl-1-oxaspiro[4.5]d 158640 000000-00-0 98  
 eca-6,9-diene-2,8-dione  
 7,8-dimethoxy-2,2-dimethyl-2H-chro 105325 067015-35-4 38  
 mene \$\$ 2H-1-Benzopyran, 7,8-dimet  
 hoxy-2,2-dimethyl- \$\$ Eupatoriochromene B  
 2-methoxy-6-allyloxy-7-methyl-7H-p 104854 097184-80-0 38  
 urine \$\$ 7H-Purine, 2-methoxy-7-methyl-6-(2-propenyloxy)-
- 199 26.749 0.50 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 91  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139434 000593-45-3 83  
 \$ Octadecan  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 72
- 200 26.825 0.39 C:\Database\WILEY275.L  
 Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 90  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 87  
 2H46 STANDARD \$\$ Normal-docosane  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 80
- 201 26.849 0.22 C:\Database\WILEY275.L  
 Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 80

OCTACOSANE 232594 000000-00-0 80  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 80

202 26.939 0.34 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 87  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 87  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87

203 27.006 0.38 C:\Database\WILEY275.L  
METHYL-3-(3,5-DITERTBUTYL-4-HYDROX 171951 000000-00-0 94  
YPHENYL) PROPIONATE \$\$ Methyl este  
r of 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-propionic acid  
1,2,3,4-Tetrahydro-1,1,4,4,6-penta 171584 000000-00-0 83  
methyl-5,7-dinitronaphthalene  
Evodione \$\$ Ethanone, 1-(5,7,8-tri 171655 000482-07-5 47  
methoxy-2,2-dimethyl-2H-1-benzopyr  
an-6-yl)- (CAS) \$\$ Ketone, methyl  
5,7,8-trimethoxy-2,2-dimethyl-2H-1-benzopyran-6-yl

204 27.116 0.23 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 80  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 72  
ane \$\$ n-Hentriacontane  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 72

205 27.192 0.24 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139434 000593-45-3 80  
\$ Octadecan  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 80  
N-NONADECANE 152007 000629-92-5 72

206 27.258 0.47 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 90  
2H46 STANDARD \$\$ Normal-docosane  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 80  
Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 80  
\$ Octadecan

207 27.325 0.27 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 74  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 74  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 74

208 27.354 0.27 C:\Database\WILEY275.L  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 76  
Heptadecane, 9-octyl- (CAS) \$\$ 9-N 212918 007225-64-1 68  
-OCTYLHEPTADECANE  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 68

209 27.401 0.15 C:\Database\WILEY275.L  
Tetratetracontane (CAS) \$\$ n-Tetra 269825 007098-22-8 76  
tetracontane  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 76  
Eicosane, 9-octyl- (CAS) \$\$ 9-n-Oc 232584 013475-77-9 74  
tyleicosane

210 27.673 0.05 C:\Database\WILEY275.L  
Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 46  
acontane \$\$ NOR-HEXATRIACONTANE  
PENTADECANE, 2,6,10-TRIMETHYL- \$\$ 139453 000000-00-0 43  
NOR-PRISTAN  
Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 43  
Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE

211 27.716 0.05 C:\Database\WILEY275.L  
Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 52  
Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 49  
\$ Octadecan  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 49

212 27.816 0.25 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163887 000112-95-8 97  
EICOSANE 163904 000000-00-0 91  
Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 91

213 28.025 0.02 C:\Database\WILEY275.L  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 58  
ane \$\$ n-Hentriacontane  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 58  
Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 53  
riacontane

214 28.063 0.03 C:\Database\WILEY275.L  
Nonahexacontanoic acid (CAS) \$\$ N- 275385 040710-32-5 52  
NONAHEXACONTANOIC ACID  
Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 49  
acontane \$\$ NOR-HEXATRIACONTANE  
Tritriacontane (CAS) \$\$ n-Tritriac 253566 000630-05-7 46  
ontane

215 28.178 0.06 C:\Database\WILEY275.L  
Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 58  
tane \$\$ Bicetyl \$\$ Tris(trimethyls  
ilyl)ether, methyl ester of ethyl  
anthranilate azo pigment(.alpha.z)  
of bilivubin-1x.alpha. 2-O-acyl glucuronide  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 58  
2H46 STANDARD \$\$ Normal-docosane  
Eicosane, 7-hexyl- (CAS) \$\$ 7-n-He 220184 055333-99-8 58  
xyleicosane

216 28.244 0.11 C:\Database\WILEY275.L  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 87  
ane \$\$ n-Hentriacontane  
Eicosane, 7-hexyl- (CAS) \$\$ 7-n-He 220184 055333-99-8 83  
xyleicosane  
Tetracosane (CAS) \$\$ n-Tetracosane 204922 000646-31-1 83

217 28.282 0.20 C:\Database\WILEY275.L  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 90  
ane \$\$ n-Hentriacontane  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 90

|     |        |                                                  |                       |
|-----|--------|--------------------------------------------------|-----------------------|
|     |        | OCTACOSANE                                       | 232594 000000-00-0 87 |
| 218 | 28.335 | 0.07 C:\Database\WILEY275.L                      |                       |
|     |        | Octacosane (CAS) \$\$ n-Octacosane               | 232590 000630-02-4 74 |
|     |        | Hexacosane (CAS) \$\$ n-Hexacosane               | 220199 000630-01-3 74 |
|     |        | OCTACOSANE                                       | 232594 000000-00-0 74 |
| 219 | 28.411 | 0.14 C:\Database\WILEY275.L                      |                       |
|     |        | Docosane (CAS) \$\$ n-Docosane                   | 186056 000629-97-0 76 |
|     |        | 2H46 STANDARD \$\$ Normal-docosane               |                       |
|     |        | Tetratriacontane (CAS) \$\$ n-Tetratriacontane   | 256280 014167-59-0 76 |
|     |        | Octacosane (CAS) \$\$ n-Octacosane               | 232591 000630-02-4 74 |
| 220 | 28.516 | 0.10 C:\Database\WILEY275.L                      |                       |
|     |        | Pentacosane (CAS) \$\$ n-Pentacosane             | 212919 000629-99-2 81 |
|     |        | Hexacosane (CAS) \$\$ n-Hexacosane               | 220199 000630-01-3 74 |
|     |        | Heptadecane, 9-octyl- (CAS) \$\$ 9-N             | 212918 007225-64-1 74 |
|     |        | -OCTYLHEPTADECANE                                |                       |
| 221 | 28.592 | 0.12 C:\Database\WILEY275.L                      |                       |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                   | 163880 000112-95-8 96 |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                   | 163879 000112-95-8 93 |
|     |        | Eicosane (CAS) \$\$ n-Eicosane                   | 163884 000112-95-8 93 |
| 222 | 28.644 | 0.08 C:\Database\WILEY275.L                      |                       |
|     |        | Tetratetracontane (CAS) \$\$ n-Tetratetracontane | 269825 007098-22-8 74 |
|     |        | Nonacosane (CAS) \$\$ n-Nonacosane               | 237992 000630-03-5 74 |
|     |        | \$ Celidoniol, deoxy-                            |                       |
|     |        | Triacontane (CAS) \$\$ n-Triacontane             | 242803 000638-68-6 74 |
| 223 | 28.716 | 0.52 C:\Database\WILEY275.L                      |                       |
|     |        | Hexadecane, 3-methyl- (CAS) \$\$ 3-M             | 126468 006418-43-5 86 |
|     |        | ethylhexadecane                                  |                       |
|     |        | Heptadecane, 9-octyl- (CAS) \$\$ 9-N             | 212918 007225-64-1 86 |
|     |        | -OCTYLHEPTADECANE                                |                       |
|     |        | Octadecane (CAS) \$\$ n-Octadecane               | 139444 000593-45-3 86 |
|     |        | \$ Octadecan                                     |                       |
| 224 | 28.797 | 0.26 C:\Database\WILEY275.L                      |                       |
|     |        | Heneicosane (CAS) \$\$ n-Heneicosane             | 175419 000629-94-7 91 |
|     |        | Tricosane (CAS) \$\$ n-Tricosane                 | 195910 000638-67-5 91 |
|     |        | Triacontane (CAS) \$\$ n-Triacontane             | 242802 000638-68-6 91 |
| 225 | 28.849 | 0.19 C:\Database\WILEY275.L                      |                       |
|     |        | Octacosane (CAS) \$\$ n-Octacosane               | 232590 000630-02-4 80 |
|     |        | OCTACOSANE                                       | 232594 000000-00-0 80 |
|     |        | Docosane (CAS) \$\$ n-Docosane                   | 186056 000629-97-0 76 |
|     |        | 2H46 STANDARD \$\$ Normal-docosane               |                       |
| 226 | 28.949 | 0.26 C:\Database\WILEY275.L                      |                       |
|     |        | OCTACOSANE                                       | 232594 000000-00-0 80 |
|     |        | Heptacosane (CAS) \$\$ n-Heptacosane             | 226683 000593-49-7 80 |
|     |        | Octacosane (CAS) \$\$ n-Octacosane               | 232590 000630-02-4 80 |

227 28.992 0.10 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
 2H46 STANDARD \$\$ Normal-docosane  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 83  
 riacontane  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 83  
 \$ Octadecan

228 29.049 1.00 C:\Database\WILEY275.L  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 91  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 90  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 90

229 29.163 0.20 C:\Database\WILEY275.L  
 Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 86  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 80  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 80

230 29.239 0.16 C:\Database\WILEY275.L  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 83  
 riacontane  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 83  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 83

231 29.382 0.49 C:\Database\WILEY275.L  
 N-EICOSANE 163902 000112-95-8 95  
 Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 70  
 EICOSANE 163904 000000-00-0 70

232 29.463 0.88 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 90  
 N-EICOSANE 163902 000112-95-8 87  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 83

233 29.582 0.11 C:\Database\WILEY275.L  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 68  
 acontane \$\$ NOR-HEXATRIACONTANE  
 Pentacosane (CAS) \$\$ n-Pentacosane 212923 000629-99-2 64  
 Tetratetracontane (CAS) \$\$ n-Tetra 269825 007098-22-8 64  
 tetracontane

234 29.639 0.08 C:\Database\WILEY275.L  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 58  
 acontane \$\$ NOR-HEXATRIACONTANE  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 46  
 Decanedioic acid, didecyl ester \$\$ 256920 002432-89-5 43  
 Didecyl sebacate

235 29.697 0.27 C:\Database\WILEY275.L  
 Carbamic acid, (2-hydroxy-1-methyl 175762 117828-58-7 43  
 -4,6-tridecadienyl)-, ethyl ester, [S-[R\*,R\*-(E,E)]]-  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 83  
 \$ Octadecan  
 3-Methyl-2-(2-oxopropyl)furan 26213 000000-00-0 35

236 29.830 0.21 C:\Database\WILEY275.L



Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 87  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 87  
 acontane \$\$ NOR-HEXATRIACONTANE  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 87  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE

237 30.125 0.06 C:\Database\WILEY275.L  
 Heptadecane, 9-octyl- (CAS) \$\$ 9-N 212918 007225-64-1 72  
 -OCTYLHEPTADECANE  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 72  
 OCTACOSANE 232594 000000-00-0 64

238 30.159 0.08 C:\Database\WILEY275.L  
 N-EICOSANE 163902 000112-95-8 93  
 Eicosane (CAS) \$\$ n-Eicosane 163878 000112-95-8 93  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 93

239 30.282 0.12 C:\Database\WILEY275.L  
 Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 42  
 \$\$ Normal-heptadecane  
 Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 30  
 OCTACOSANE 232594 000000-00-0 30

240 30.320 0.11 C:\Database\WILEY275.L  
 Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 86  
 tane \$\$ Bicetyl \$\$ Tris(trimethyls  
 ilyl)ether, methyl ester of ethyl  
 anthranilate azo pigment(.alpha.z) of bilivubin-1x.alpha. 2-O-acyl glucuronide  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 86  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 83

241 30.359 0.06 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163884 000112-95-8 94  
 N-EICOSANE 163902 000112-95-8 93  
 EICOSANE 163904 000000-00-0 93

242 30.435 0.07 C:\Database\WILEY275.L  
 Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 68  
 tane \$\$ Bicetyl \$\$ Tris(trimethyls  
 ilyl)ether, methyl ester of ethyl  
 anthranilate azo pigment(.alpha.z) of bilivubin-1x.alpha. 2-O-acyl glucuronide  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 58  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 58  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE

243 30.497 0.12 C:\Database\WILEY275.L  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 81  
 riacontane  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 76  
 acontane \$\$ NOR-HEXATRIACONTANE  
 N-DOCOSANE 186069 000629-97-0 74

244 30.597 0.14 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175421 000629-94-7 76  
 Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 74  
 tane \$\$ Bicetyl \$\$ Tris(trimethyls

ilyl)ether, methyl ester of ethyl  
 anthranilate azo pigment(.alpha.z) of bilivubin-1x.alpha. 2-O-acyl glucuronide  
 Tetratetracontane (CAS) \$\$ n-Tetra 269825 007098-22-8 74  
 tetracontane

245 30.692 0.75 C:\Database\WILEY275.L  
 N-EICOSANE 163902 000112-95-8 87  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 86

246 30.801 0.07 C:\Database\WILEY275.L  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 87  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 83  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 83

247 30.825 0.16 C:\Database\WILEY275.L  
 Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 87  
 tane \$\$ Bicetyl \$\$ Tris(trimethyls  
 ilyl)ether, methyl ester of ethyl  
 anthranilate azo pigment(.alpha.z) of bilivubin-1x.alpha. 2-O-acyl glucuronide  
 Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 83  
 acontane \$\$ NOR-HEXATRIACONTANE  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 83

248 30.892 0.13 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 87  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 87  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 86

249 30.935 0.21 C:\Database\WILEY275.L  
 Tetratetracontane (CAS) \$\$ n-Tetra 269825 007098-22-8 87  
 tetracontane  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 83  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE  
 Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 83  
 ane \$\$ n-Hentriacontane

250 30.987 0.62 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 86  
 2H46 STANDARD \$\$ Normal-docosane  
 HENEICOSANE 175427 000629-94-7 80  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 78

251 31.049 0.40 C:\Database\WILEY275.L  
 HEXACOSANE 220207 000000-00-0 68  
 N-EICOSANE 163902 000112-95-8 68  
 Hexacosane (CAS) \$\$ n-Hexacosane 220198 000630-01-3 68

252 31.154 0.29 C:\Database\WILEY275.L  
 OCTACOSANE 232594 000000-00-0 53  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 53  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE  
 Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 53

253 31.225 0.31 C:\Database\WILEY275.L

|     |        |      |                                                       |        |             |    |
|-----|--------|------|-------------------------------------------------------|--------|-------------|----|
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane                    | 151981 | 000629-92-5 | 60 |
|     |        |      | OCTACOSANE                                            | 232594 | 000000-00-0 | 49 |
|     |        |      | Octacosane (CAS) \$\$ n-Octacosane                    | 232590 | 000630-02-4 | 49 |
| 254 | 31.278 | 0.58 | C:\Database\WILEY275.L                                |        |             |    |
|     |        |      | 9-Octadecenamide, (Z)- (CAS) \$\$ OL                  | 162710 | 000301-02-0 | 59 |
|     |        |      | EOAMIDE \$\$ OELIC ACID AMIDE \$\$ Ole                |        |             |    |
|     |        |      | amide \$\$ Adogen 73 \$\$ Oleylamide \$               |        |             |    |
|     |        |      | \$ Slip-ezeCI) \$\$ Oleic acid amide                  |        |             |    |
|     |        |      | \$\$ Slip-eze \$\$ Armoslip CP \$\$ Crod              |        |             |    |
|     |        |      | amide O \$\$ Crodamide OR \$\$ Amide O                |        |             |    |
|     |        |      | \$\$ Diamide O 200 \$\$ Diamit O 200 \$\$ Oleyl amide |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163884 | 000112-95-8 | 52 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163881 | 000112-95-8 | 46 |
| 255 | 31.344 | 0.62 | C:\Database\WILEY275.L                                |        |             |    |
|     |        |      | Octadecane (CAS) \$\$ n-Octadecane \$                 | 139444 | 000593-45-3 | 83 |
|     |        |      | \$ Octadecan                                          |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163881 | 000112-95-8 | 83 |
|     |        |      | N-EICOSANE                                            | 163902 | 000112-95-8 | 83 |
| 256 | 31.592 | 0.17 | C:\Database\WILEY275.L                                |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163884 | 000112-95-8 | 97 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163882 | 000112-95-8 | 95 |
|     |        |      | EICOSANE                                              | 163904 | 000000-00-0 | 93 |
| 257 | 31.706 | 0.12 | C:\Database\WILEY275.L                                |        |             |    |
|     |        |      | 14-.BETA.-H-PREGNA \$\$ 14-.BETA.-PR                  | 169066 | 000000-00-0 | 42 |
|     |        |      | EGNA \$\$ 14B-PREGNANE                                |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163884 | 000112-95-8 | 38 |
|     |        |      | 14-.BETA.-H-PREGNA \$\$ 14-.BETA.-PR                  | 169067 | 000000-00-0 | 38 |
|     |        |      | EGNA \$\$ 14B-PREGNANE                                |        |             |    |
| 258 | 31.844 | 0.05 | C:\Database\WILEY275.L                                |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163883 | 000112-95-8 | 47 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163877 | 000112-95-8 | 47 |
|     |        |      | Heneicosane (CAS) \$\$ n-Heneicosane                  | 175422 | 000629-94-7 | 46 |
| 259 | 31.916 | 0.11 | C:\Database\WILEY275.L                                |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163884 | 000112-95-8 | 46 |
|     |        |      | Pentatriacontane (CAS) \$\$ n-Pentat                  | 258572 | 000630-07-9 | 41 |
|     |        |      | riacontane                                            |        |             |    |
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane                    | 151984 | 000629-92-5 | 41 |
| 260 | 32.025 | 0.19 | C:\Database\WILEY275.L                                |        |             |    |
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane                    | 151982 | 000629-92-5 | 68 |
|     |        |      | NONADECANE                                            | 152008 | 000000-00-0 | 62 |
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane                    | 151980 | 000629-92-5 | 62 |
| 261 | 32.106 | 0.23 | C:\Database\WILEY275.L                                |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163884 | 000112-95-8 | 83 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                        | 163881 | 000112-95-8 | 78 |
|     |        |      | Tetracosane, 11-decyl- (CAS) \$\$ 11                  | 256278 | 055429-84-0 | 68 |
|     |        |      | -n-Decyltetracosane                                   |        |             |    |
| 262 | 32.201 | 1.49 | C:\Database\WILEY275.L                                |        |             |    |

1H-Indole, 2-methyl- (CAS) \$\$ 2-Me 21487 000095-20-5 37  
 thylindole \$\$ SKATOLE \$\$ Indole, 2-methyl- \$\$ 2-Methyl-1H-indole  
 1H-Indole, 4-methyl- (CAS) \$\$ Indo 21544 016096-32-5 37  
 le, 4-methyl- \$\$ 4-Methylindole \$\$ 4-Methyl-1H-indole  
 Thiophene, 2-(methylthio)- (CAS) \$ 20347 005780-36-9 27  
 \$ 2-METHYLTHIOTHIOPHENE \$\$ 2-(Methylthio)thiophene

263 32.349 0.55 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 56  
 Dotriacontane (CAS) \$\$ n-Dotriacon 250418 000544-85-4 20  
 tane \$\$ Bicetyl \$\$ Tris(trimethyls  
 ilyl)ether, methyl ester of ethyl  
 anthranilate azo pigment(.alpha.z)  
 of bilivubin-1x.alpha. 2-O-acyl glucuronide  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 20

264 32.416 0.95 C:\Database\WILEY275.L  
 Nonadecane (CAS) \$\$ n-Nonadecane 151987 000629-92-5 60  
 Heneicosane, 11-decyl- (CAS) \$\$ 11 246863 055320-06-4 58  
 -n-Decylheneicosane \$\$ 11-Decylheneicosane  
 Tetracosane, 11-decyl- (CAS) \$\$ 11 256278 055429-84-0 58  
 -n-Decyltetracosane

265 32.525 1.41 C:\Database\WILEY275.L  
 HEPTADECANE 126483 000000-00-0 55  
 Nonadecane, 2-methyl- (CAS) \$\$ 2-M 163871 001560-86-7 44  
 ethylnonadecane \$\$ 2-Methylnonadecene  
 CYCLONONANONE 28217 000000-00-0 43

266 32.616 0.32 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163884 000112-95-8 93  
 Tricosane (CAS) \$\$ n-Tricosane 195915 000638-67-5 68  
 Pentacosane (CAS) \$\$ n-Pentacosane 212923 000629-99-2 62

267 32.706 1.25 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 93  
 Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 87  
 ane \$\$ n-Hentriacontane  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 86

268 32.959 0.64 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 86  
 Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 74  
 ane \$\$ n-Hentriacontane  
 Docosane, 11-decyl- (CAS) \$\$ 11-n- 250412 055401-55-3 74  
 Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE

269 33.030 0.49 C:\Database\WILEY275.L  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 83  
 Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 80  
 OCTACOSANE 232594 000000-00-0 80

270 33.087 0.18 C:\Database\WILEY275.L  
 EICOSANE 163904 000000-00-0 92  
 Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 92  
 Eicosane (CAS) \$\$ n-Eicosane 163884 000112-95-8 91

|     |        |      |                                                                        |        |             |    |
|-----|--------|------|------------------------------------------------------------------------|--------|-------------|----|
| 271 | 33.187 | 0.23 | C:\Database\WILEY275.L                                                 |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163881 | 000112-95-8 | 95 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163884 | 000112-95-8 | 93 |
|     |        |      | EICOSANE                                                               | 163904 | 000000-00-0 | 90 |
| 272 | 33.430 | 0.09 | C:\Database\WILEY275.L                                                 |        |             |    |
|     |        |      | Nonahexacontanoic acid (CAS) \$\$ N-                                   | 275385 | 040710-32-5 | 58 |
|     |        |      | NONAHEXACONTANOIC ACID                                                 |        |             |    |
|     |        |      | Tritetracontane (CAS) \$\$ N-TRIATET                                   | 269077 | 007098-21-7 | 58 |
|     |        |      | RACONTANE                                                              |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163884 | 000112-95-8 | 58 |
| 273 | 33.578 | 0.03 | C:\Database\WILEY275.L                                                 |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163884 | 000112-95-8 | 92 |
|     |        |      | EICOSANE                                                               | 163904 | 000000-00-0 | 89 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163882 | 000112-95-8 | 89 |
| 274 | 33.720 | 0.01 | C:\Database\WILEY275.L                                                 |        |             |    |
|     |        |      | N-ethyl-1,3-dithioisindoline \$\$ 1                                    | 92199  | 035373-06-9 | 72 |
|     |        |      | H-Isoindole-1,3(2H)-dithione, 2-ethyl-                                 |        |             |    |
|     |        |      | Docosane, 11-decyl- (CAS) \$\$ 11-n-                                   | 250412 | 055401-55-3 | 68 |
|     |        |      | Decyldocosane \$\$ 11-NOR-DECYLDOCOSANE                                |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163884 | 000112-95-8 | 64 |
| 275 | 33.768 | 1.04 | C:\Database\WILEY275.L                                                 |        |             |    |
|     |        |      | 1-ethoxy-2-aminocarbonyl-1-aza-cyc                                     | 20371  | 000000-00-0 | 35 |
|     |        |      | lopropane                                                              |        |             |    |
|     |        |      | 1H-Indole, 4-methyl- (CAS) \$\$ Indo                                   | 21544  | 016096-32-5 | 32 |
|     |        |      | le, 4-methyl- \$\$ 4-Methylindole \$\$ 4-Methyl-1H-indole              |        |             |    |
|     |        |      | 1H-Indole, 2-methyl- (CAS) \$\$ 2-Me                                   | 21493  | 000095-20-5 | 32 |
|     |        |      | thylindole \$\$ SKATOLE \$\$ Indole, 2-methyl- \$\$ 2-Methyl-1H-indole |        |             |    |
| 276 | 33.887 | 0.09 | C:\Database\WILEY275.L                                                 |        |             |    |
|     |        |      | 1H-Indene, 1-hexadecyl-2,3-dihydro                                     | 207324 | 055334-29-7 | 18 |
|     |        |      | - (CAS) \$\$ 1-N-HEXADECYLINDANE \$\$                                  |        |             |    |
|     |        |      | 1-n-Hexadecylindan \$\$ 1-NOR-HEXADE                                   |        |             |    |
|     |        |      | CYL-(2,3-DIHYDROINDENE) (1-NOR-HEX                                     |        |             |    |
|     |        |      | ADECYLINDAN) \$\$ 1-n-Hexadecyl(2,3-dihydroindene)                     |        |             |    |
|     |        |      | 1H-Indene, 1-hexadecyl-2,3-dihydro                                     | 207326 | 055334-29-7 | 14 |
|     |        |      | - (CAS) \$\$ 1-N-HEXADECYLINDANE \$\$                                  |        |             |    |
|     |        |      | 1-n-Hexadecylindan \$\$ 1-NOR-HEXADE                                   |        |             |    |
|     |        |      | CYL-(2,3-DIHYDROINDENE) (1-NOR-HEX                                     |        |             |    |
|     |        |      | ADECYLINDAN) \$\$ 1-n-Hexadecyl(2,3-dihydroindene)                     |        |             |    |
|     |        |      | 5-Phenyl-6-hepten-1-ol                                                 | 74572  | 023431-45-0 | 14 |
| 277 | 33.940 | 0.10 | C:\Database\WILEY275.L                                                 |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163884 | 000112-95-8 | 84 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163881 | 000112-95-8 | 83 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163887 | 000112-95-8 | 42 |

# 진병꽃풀 A

No Name Entered Library Search Report

Data Path : C:\msdchem\1\data\LJY\2014\herbal biology\ginbyung\_final\

Data File : ginbyung A.D

Acq On : 4 Dec 2014 16:31 (#1); 04 Dec 2014 16:31 (#2)

Operator : lly

Sample : ginbyung A

Misc :

ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 0

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint1.e

| Pk# | RT    | Area% | Library/ID                          | Ref#                       | CAS#            | Qual                |
|-----|-------|-------|-------------------------------------|----------------------------|-----------------|---------------------|
| 1   | 3.573 | 0.05  | C:\Database\WILEY275.L              |                            |                 |                     |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$    | 2                          | 11032           | 003404-78-2 87      |
|     |       |       | ,5-Dimethyl-2-hexene                |                            |                 |                     |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$    | 2                          | 11034           | 003404-78-2 87      |
|     |       |       | ,5-Dimethyl-2-hexene                |                            |                 |                     |
|     |       |       | 2-Hexene, 2,5-dimethyl- (CAS) \$    | 2                          | 11031           | 003404-78-2 87      |
|     |       |       | ,5-Dimethyl-2-hexene                |                            |                 |                     |
| 2   | 3.639 | 0.21  | C:\Database\WILEY275.L              |                            |                 |                     |
|     |       |       | Heptane, 4-methyl- (CAS) \$         | 4-Meth                     | 12460           | 000589-53-7 90      |
|     |       |       | ylheptane \$ (n-C3H7)2CHCH3         |                            |                 |                     |
|     |       |       | Heptane, 4-methyl- (CAS) \$         | 4-Meth                     | 12459           | 000589-53-7 87      |
|     |       |       | ylheptane \$ (n-C3H7)2CHCH3         |                            |                 |                     |
|     |       |       | Heptane, 4-methyl- (CAS) \$         | 4-Meth                     | 12461           | 000589-53-7 87      |
|     |       |       | ylheptane \$ (n-C3H7)2CHCH3         |                            |                 |                     |
| 3   | 3.758 | 0.21  | C:\Database\WILEY275.L              |                            |                 |                     |
|     |       |       | 3,4,5-TRIMETHYL-HEPTANE \$          | Heptane                    | 30091           | 020278-89-1 78      |
|     |       |       | , 3,4,5-trimethyl- \$               | 3,4,5-Trimethylheptane     |                 |                     |
|     |       |       | Nonane, 5-methyl- (CAS) \$          | 5-Methy                    | 30041           | 015869-85-9 78      |
|     |       |       | Inonane                             |                            |                 |                     |
|     |       |       | Pentane, 2,3,3,4-tetramethyl- (CAS) | 19891                      | 016747-38-9 64  |                     |
|     |       |       | ) \$                                | 2,3,3,4-Tetramethylpentane |                 |                     |
| 4   | 3.958 | 0.15  | C:\Database\WILEY275.L              |                            |                 |                     |
|     |       |       | Pentane, 1,5-dimethoxy- (CAS) \$    | 1                          | 21982           | 000111-89-7 64      |
|     |       |       | ,5-Dimethoxypentane \$              | CH3O(CH2)5OCH3             |                 |                     |
|     |       |       | Ethyl 2-propynyl sulfide            | 6565                       | 007310-92-1 59  |                     |
|     |       |       | 3-Hexanone (CAS) \$                 | Hexan-3-one \$             | 6695            | 000589-38-8 50      |
|     |       |       | Ethyl propyl ketone \$              | n-C3H7COC2H5 \$            | Hexanone-(3) \$ | Aethylpropylketon   |
| 5   | 4.035 | 0.17  | C:\Database\WILEY275.L              |                            |                 |                     |
|     |       |       | Hexanal (CAS) \$                    | n-Hexanal \$               | Hexa            | 6643 000066-25-1 74 |
|     |       |       | ldehyde \$                          | Caproaldehyde \$           | Capron          |                     |
|     |       |       | aldehyde \$                         | n-Caproaldehyde \$         | Cap             |                     |
|     |       |       | roic aldehyde \$                    | Hexylaldehyde \$           |                 |                     |
|     |       |       | n-Capronaldehyde \$                 | cyclohexanol \$            |                 |                     |
|     |       |       | \$                                  | 1-hexanal \$               | n-C5H11CHO \$   | n-Hex               |

aldehyde \$\$ n-Caproylaldehyde \$\$ Aldehyde C-6 \$\$ Ka  
 2-HEXANONE 6994 000000-00-0 74  
 2-Hexanone (CAS) \$\$ Hexan-2-one \$\$ 6678 000591-78-6 74  
 MBK \$\$ Methyl n-butyl ketone \$\$ 2  
 -Oxohexane \$\$ Butyl methyl ketone  
 \$\$ Methyl butyl ketone \$\$ n-Butyl  
 methyl ketone \$\$ n-C4H9COCH3 \$\$ He  
 xanone-2 \$\$ Ketone, butyl methyl \$\$ Mnbk

6 4.111 0.13 C:\Database\WILEY275.L  
 2-Hexanol (CAS) \$\$ n-C4H9CH(OH)CH3 7747 000626-93-7 64  
 \$\$ n-Butylmethylcarbinol \$\$ Hexanol-(2) \$\$ sec-Hexyl alcohol  
 2,3-Butanediol (CAS) \$\$ Butane-2,3 4368 000513-85-9 64  
 -diol \$\$ 2,3-BUTANDIOL \$\$ 2,3-Buty  
 lene glycol \$\$ 2,3-Dihydroxybutane  
 \$\$ Dimethylethylene glycol \$\$ D-2  
 ,3-Butane diol \$\$ Dimethylene glycol  
 2,3-Butanediol (CAS) \$\$ Butane-2,3 4370 000513-85-9 64  
 -diol \$\$ 2,3-BUTANDIOL \$\$ 2,3-Buty  
 lene glycol \$\$ 2,3-Dihydroxybutane  
 \$\$ Dimethylethylene glycol \$\$ D-2,3-Butane diol \$\$ Dimethylene glycol

7 4.187 0.07 C:\Database\WILEY275.L  
 3-Hexanol (CAS) \$\$ Hexan-3-ol \$\$ C 7760 000623-37-0 59  
 2H5CH(OH)C3H7 \$\$ Ethylpropylcarbinol \$\$ Hexanol-(3)  
 3-Hexanol (CAS) \$\$ Hexan-3-ol \$\$ C 7764 000623-37-0 59  
 2H5CH(OH)C3H7 \$\$ Ethylpropylcarbinol \$\$ Hexanol-(3)  
 3-HEXANOL 7893 000000-00-0 59

8 4.225 0.06 C:\Database\WILEY275.L  
 Octane (CAS) \$\$ n-Octane \$\$ Octane 12441 000111-65-9 49  
 (DOT) \$\$ Isooctane \$\$ n-C8H18 \$\$ Oktan \$\$ Oktanen \$\$ Ottani \$\$ UN 1262  
 Octane (CAS) \$\$ n-Octane \$\$ Octane 12443 000111-65-9 49  
 (DOT) \$\$ Isooctane \$\$ n-C8H18 \$\$ Oktan \$\$ Oktanen \$\$ Ottani \$\$ UN 1262  
 Octane (CAS) \$\$ n-Octane \$\$ Octane 12440 000111-65-9 47  
 (DOT) \$\$ Isooctane \$\$ n-C8H18 \$\$ Oktan \$\$ Oktanen \$\$ Ottani \$\$ UN 1262

9 4.258 0.10 C:\Database\WILEY275.L  
 2-Pentanol, 4-methyl- (CAS) \$\$ 4-M 7809 000108-11-2 72  
 ethyl-2-pentanol \$\$ MIC \$\$ MAOH \$\$  
 MIBC \$\$ 3-MIC \$\$ 2-Methyl-4-penta  
 nol \$\$ Isobutylmethylethanol \$\$ I  
 sobutylmethylcarbinol \$\$ Methyliso  
 butyl carbinol \$\$ 4-Methyl-2-penty  
 l alcohol \$\$ 1,3-Dimethyl-1-butanol \$\$ 4-methyl 2-p  
 hexan-2-ol 7886 000000-00-0 64  
 2-Pentanol, 4-methyl- (CAS) \$\$ 4-M 7804 000108-11-2 64  
 ethyl-2-pentanol \$\$ MIC \$\$ MAOH \$\$  
 MIBC \$\$ 3-MIC \$\$ 2-Methyl-4-penta  
 nol \$\$ Isobutylmethylethanol \$\$ I  
 sobutylmethylcarbinol \$\$ Methyliso  
 butyl carbinol \$\$ 4-Methyl-2-penty  
 l alcohol \$\$ 1,3-Dimethyl-1-butanol \$\$ 4-methyl 2-p

10 4.349 0.16 C:\Database\WILEY275.L  
 Butane, 2-ethoxy- (CAS) \$\$ Ethyl s 7866 002679-87-0 78

ec-butyl ether \$\$ ETHER, 2-BUTYL E  
 THYL \$\$ sec-Butyl ethyl ether \$\$ E  
 ther, sec-butyl ethyl \$\$ sec-C4H9OC2H5  
 Butane, 2-ethoxy- (CAS) \$\$ Ethyl s 7868 002679-87-0 56  
 ec-butyl ether \$\$ ETHER, 2-BUTYL E  
 THYL \$\$ sec-Butyl ethyl ether \$\$ E  
 ther, sec-butyl ethyl \$\$ sec-C4H9OC2H5  
 Butane, 2-ethoxy- (CAS) \$\$ Ethyl s 7867 002679-87-0 56  
 ec-butyl ether \$\$ ETHER, 2-BUTYL E  
 THYL \$\$ sec-Butyl ethyl ether \$\$ E  
 ther, sec-butyl ethyl \$\$ sec-C4H9OC2H5

11 4.411 2.05 C:\Database\WILEY275.L  
 (2S,4S)-(+) -Pentanediol 8271 072345-23-4 28  
 1,3,5-Trioxane, 2,4,6-trimethyl- ( 21885 000123-63-7 25  
 CAS) \$\$ Paraldehyde \$\$ Pcho \$\$ 2,4  
 ,6-Trimethyl-1,3,5-trioxane \$\$ 2,4  
 ,6-Trimethyl-1,3,5-trioxacyclohexa  
 ne \$\$ Paral \$\$ Elaldehyde \$\$ Parac  
 etaldehyde \$\$ Paraacetaldehyde \$\$  
 Acetaldehyde trimer \$\$ Acetaldehyde, trimer \$\$ 2,4,  
 2-Butanol, 3-methyl- (CAS) \$\$ 3-Me 4106 000598-75-4 9  
 thyl-2-butanol \$\$ sec-Isoamyl alco  
 hol \$\$ Methylisopropylcarbinol \$\$  
 (CH3)2CHCH(OH)CH3 \$\$ (+)-3-Methyl-2-butanol

12 4.482 0.12 C:\Database\WILEY275.L  
 Pyrrolidine, 3-methyl- (CAS) \$\$ 3- 3076 034375-89-8 38  
 Methylpyrrolidine  
 3,4,5-TRIMETHYL-HEPTANE \$\$ Heptane 30091 020278-89-1 38  
 , 3,4,5-trimethyl- \$\$ 3,4,5-Trimethylheptane  
 Hexane, 2,3,3-trimethyl- (CAS) \$\$ 19863 016747-28-7 38  
 2,3,3-Trimethylhexane \$\$ 2,3,3-Trimethylheptane

13 4.558 0.22 C:\Database\WILEY275.L  
 Ethane, 1,1-diethoxy- (CAS) \$\$ 1,1 14166 000105-57-7 56  
 -Diethoxyethane \$\$ Acetal \$\$ Dieth  
 yl acetal \$\$ Ethylidene diethyl et  
 her \$\$ Acetaldehyde diethyl acetal  
 \$\$ Acetaldehyde, diethyl acetal \$  
 \$ CH3CH(OC2H5)2\$\$\$ Acetal diethyli  
 que \$\$ Diaethylacetal \$\$ 1,1-Diaethoxy-aethan \$\$ 1,  
 Butane, 2-ethoxy- (CAS) \$\$ Ethyl s 7866 002679-87-0 56  
 ec-butyl ether \$\$ ETHER, 2-BUTYL E  
 THYL \$\$ sec-Butyl ethyl ether \$\$ E  
 ther, sec-butyl ethyl \$\$ sec-C4H9OC2H5  
 Butane, 2-ethoxy- (CAS) \$\$ Ethyl s 7868 002679-87-0 40  
 ec-butyl ether \$\$ ETHER, 2-BUTYL E  
 THYL \$\$ sec-Butyl ethyl ether \$\$ Ether, sec-butyl ethyl \$\$ sec-C4H9OC2H5

14 4.620 0.61 C:\Database\WILEY275.L  
 Heptane, 2,4-dimethyl- (CAS) \$\$ 2, 19823 002213-23-2 94  
 4-Dimethylheptane  
 Heptane, 2,4-dimethyl- (CAS) \$\$ 2, 19824 002213-23-2 91  
 4-Dimethylheptane  
 Octane (CAS) \$\$ n-Octane \$\$ Octane 12446 000111-65-9 53



(DOT) \$\$ Isooctane \$\$ n-C8H18 \$\$ Oktan \$\$ Oktanen \$\$ Ottani \$\$ UN 1262

- 15 4.716 0.05 C:\Database\WILEY275.L  
 Butanal, 2-ethyl- (CAS) \$\$ 2-Ethyl 6661 000097-96-1 47  
 butanal \$\$ 2-Ethylbutyraldehyde \$\$  
 3-Formylpentane \$\$ Diethylacetalde  
 hyde \$\$ Butyraldehyde, 2-ethyl- \$  
 \$ 2-Ethylbutyric aldehyde \$\$ .alph  
 a.-Ethylbutyraldehyde \$\$ (C2H5)2CH  
 CHO \$\$ Aldehyde 2-ethylbutyrique \$\$ Ethylbutyraldeh  
 2-Buten-1-ol acetate \$\$ 2-Buten-1- 11765 000628-08-0 46  
 ol, acetate \$\$ 2-Butenyl acetate \$  
 \$ Crotyl acetate \$\$ 1-Acetoxy-2-butene \$\$ 2-Buten-1-yl acetate  
 3-METHYL-HEXAN-2-ONE \$\$ 2-Hexanone 12135 002550-21-2 38  
 , 3-methyl- (CAS) \$\$ 3-Methyl-2-hexanone \$\$ CH3(CH2)2CH(CH3)COCH3
- 16 4.997 0.27 C:\Database\WILEY275.L  
 Cyclopentane, 1,2,3-trimethyl-, (1 11122 002613-69-6 53  
 .alpha.,2.alpha.,3.alpha.)- (CAS)  
 \$\$ 1,CIS-2,CIS-3-TRIMETHYLCYCLOPEN  
 TANE \$\$ Cyclopentane, 1,2,3-trimet  
 hyl-, cis-1,2,cis-1,3- \$\$ CYCLOPEN  
 TANE, 1,2,3-TRIMETHYL-, ALL-CIS \$\$ cis,cis,cis-1,2,3-Trimethylcyclopentane  
 Cyclopentane, 1,3-dimethyl- \$\$ 1,3 6015 002453-00-1 53  
 -Dimethylcyclopentane  
 Cyclopentane, 1,2,3-trimethyl-, (1 11124 002613-69-6 53  
 .alpha.,2.alpha.,3.alpha.)- (CAS)  
 \$\$ 1,CIS-2,CIS-3-TRIMETHYLCYCLOPEN  
 TANE \$\$ Cyclopentane, 1,2,3-trimet  
 hyl-, cis-1,2,cis-1,3- \$\$ CYCLOPEN  
 TANE, 1,2,3-TRIMETHYL-, ALL-CIS \$\$ cis,cis,cis-1,2,3-Trimethylcyclopentane
- 17 5.444 0.37 C:\Database\WILEY275.L  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19807 002216-34-4 90  
 loctane \$\$ Isononane  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19808 002216-34-4 90  
 loctane \$\$ Isononane  
 Octane, 4-methyl- (CAS) \$\$ 4-Methy 19809 002216-34-4 76  
 loctane \$\$ Isononane
- 18 5.630 0.14 C:\Database\WILEY275.L  
 Pentane, 1-(1-ethoxyethoxy)- (CAS) 45458 013442-89-2 40  
 \$\$ 1-ETHOXY-1-PENTOXYETHANE \$\$ Acetaldehyde ethyl amyl acetal  
 Methyl 3-Butenyl Ether 3506 000000-00-0 40  
 2-Pentanol, 3-chloro-4-methyl-, (R 24137 074685-47-5 40  
 \*,R\*)-(.+-.)- (CAS) \$\$ 4-PENTANOL,  
 3-CHLORO-(SS)-2-METHYL-(RR)- \$\$ 2  
 -Pentanol, 3-chloro-4-methyl-, (R@  
 ,R@)-(./+-.)- \$\$ 2-Pentanol, 3-chloro-4-methyl-, (R@,R@)-(./+-.)-
- 19 6.120 0.13 C:\Database\WILEY275.L  
 Furan, 2,5-diethyltetrahydro- (CAS 19643 041239-48-9 58  
 ) \$\$ 2,5-Diethyltetrahydrofuran \$\$ 2,5-DIETHYL-TETRAHYDROFURAN  
 Furan, 2,5-diethyltetrahydro- (CAS 19642 041239-48-9 53  
 ) \$\$ 2,5-Diethyltetrahydrofuran \$\$ 2,5-DIETHYL-TETRAHYDROFURAN  
 2,2'-Bioxepane (CAS) \$\$ Oxepane, b 83093 074793-02-5 43mol. deriv.

20 6.725 0.05 C:\Database\WILEY275.L  
.alpha.-Thujene \$\$ Bicyclo[3.1.0]h 25175 002867-05-2 87  
ex-2-ene, 2-methyl-5-(1-methylethy  
l)- (CAS) \$\$ Origanene \$\$ 3-Thujene \$\$ ALPHA-THUJENE \$\$ ALFA-THUJENE  
.alpha.-Thujene \$\$ Bicyclo[3.1.0]h 25174 002867-05-2 83  
ex-2-ene, 2-methyl-5-(1-methylethy  
l)- (CAS) \$\$ Origanene \$\$ 3-Thujene \$\$ ALPHA-THUJENE \$\$ ALFA-THUJENE  
.alpha.-Thujene \$\$ Bicyclo[3.1.0]h 25173 002867-05-2 80  
ex-2-ene, 2-methyl-5-(1-methylethy  
l)- (CAS) \$\$ Origanene \$\$ 3-Thujene \$\$ ALPHA-THUJENE \$\$ ALFA-THUJENE

21 6.882 0.07 C:\Database\WILEY275.L  
.alpha.-pinene \$\$ .alpha.-pinene 25312 000080-56-8 87  
cis-Ocimene \$\$ 1,3,7-Octatriene, 3 24919 006874-10-8 83  
,7-dimethyl-, (E)- \$\$ trans-.alpha.-Ocimene  
.ALPHA.-PINENE, (-)- \$\$ Bicyclo[3. 25198 000080-56-8 83  
1.1]hept-2-ene, 2,6,6-trimethyl- (  
CAS) \$\$ Pinene \$\$ 2-Pinene \$\$ .alp  
ha.-Pinene \$\$ 2,6,6-Trimethylbicyc  
lo[3.1.1]hept-2-ene \$\$ .alpha.-(+)  
-Pinene \$\$ ALPHA-PINENE \$\$ ALFA-PI  
NENE \$\$ Pinene isomer \$\$ PINENE, .alpha. \$\$ 2,6,6-T

22 7.049 0.34 C:\Database\WILEY275.L  
FURAN, TETRAHYDRO-2,2-DIMETHYL- \$\$ 6945 001003-17-4 25  
Tetrahydrofuran, 2,2-dimethyl- \$\$ 2,2-Dimethyltetrahydrofuran  
Oxirane, 2-methyl-3-propyl-, cis- 6921 006124-90-9 25  
(CAS) \$\$ Hexane, 2,3-epoxy-, cis-  
2-Nonanone, 9-[(tetrahydro-2H-pyra 127783 054699-41-1 23  
n-2-yl)oxy]- (CAS)

23 7.230 0.40 C:\Database\WILEY275.L  
Ethanone, 1-(3-butyloxiranyl)- (CA 29471 017257-80-6 38  
S) \$\$ 2-Octanone, 3,4-epoxy- \$\$ 1-Acetyl-2-butyloxirane  
Ethanone, 1-(3-ethyloxiranyl)- (CA 11796 017257-81-7 37  
S) \$\$ 3,4-EPOXY-2-HEXANONE \$\$ 2-He  
xanone, 3,4-epoxy- \$\$ 1-Acetyl-2-ethyloxirane  
Pentanoic acid, 2,2-dimethyl-, eth 42078 044970-05-0 37  
enyl ester (CAS) \$\$ VINYL 2,2-DIMETHYLPENTANOATE

24 7.377 0.05 C:\Database\WILEY275.L  
Nonane, 4-methyl- (CAS) \$\$ 4-Methy 30038 017301-94-9 60  
lnonane \$\$ 4-n-Methylnonane \$\$ n-C3H7CH(CH3)(CH2)4CH3  
Nonane, 4-methyl- (CAS) \$\$ 4-Methy 30037 017301-94-9 53  
lnonane \$\$ 4-n-Methylnonane \$\$ n-C3H7CH(CH3)(CH2)4CH3  
Octane, 2,5-dimethyl- (CAS) \$\$ 2,5 30051 015869-89-3 43-Dimethyloctane

25 7.444 0.09 C:\Database\WILEY275.L  
Dodecane, 2-methyl- (CAS) \$\$ 2-Met 69464 001560-97-0 50  
hyldodecane \$\$ 11-Methyldodecane \$\$ 2-Methyl-dodecane  
1-Iodo-2-methylundecane 174486 073105-67-6 50  
Octadecane, 2-methyl- (CAS) \$\$ 2-M 151970 001560-88-9 50  
ethyloctadecane \$\$ 17-Methyloctadecane

26 7.501 0.06 C:\Database\WILEY275.L

3-BROMO-1,1,2-TRIMETHYL-CYCLOPROPA 46668 000000-00-0 38 NE  
 1-Tridecyn-4-ol (CAS) 81145 074646-37-0 33  
 3-Hexen-2-one (CAS) \$\$ 1-Butenyl m 5669 000763-93-9 33  
 ethyl ketone \$\$ Methyl 1-butenyl ketone

27 7.639 0.17 C:\Database\WILEY275.L  
 Sabinene \$\$ Bicyclo[3.1.0]hexane, 25193 003387-41-5 91  
 4-methylene-1-(1-methylethyl)- (CA  
 S) \$\$ 4(10)-Thujene \$\$ Sabinen \$\$  
 (+)-Sabinene \$\$ THUJENE, 4(10)- \$\$  
 1-Isopropyl-4-methylenebicyclo[3.1.0]hexane  
 sabinene 25337 003387-41-5 91  
 Sabinene \$\$ Bicyclo[3.1.0]hexane, 25186 003387-41-5 90  
 4-methylene-1-(1-methylethyl)- (CA  
 S) \$\$ 4(10)-Thujene \$\$ Sabinen \$\$  
 (+)-Sabinene \$\$ THUJENE, 4(10)- \$\$  
 1-Isopropyl-4-methylenebicyclo[3.1.0]hexane

28 7.749 0.88 C:\Database\WILEY275.L  
 1 OCTEN 3 OL 19694 003391-86-4 72  
 1-OCTEN-3-OL 19692 053907-72-5 72  
 1-Octen-3-ol (CAS) \$\$ Oct-1-en-3-o 19569 003391-86-4 72  
 l \$\$ 3-Hydroxy-1-octene \$\$ Amyl vi  
 nyl carbinol \$\$ Vinyl amyl carbino  
 l \$\$ n-Oct-1-en-3-ol \$\$ Octan-3-on  
 e \$\$ (Z)-Oct-5-en-3-ol \$\$ octen-3-  
 ol \$\$ Matsutake alcohol \$\$ 1-Okten-3-ol

29 7.849 0.20 C:\Database\WILEY275.L  
 3-OCTANONE 19691 000106-68-3 90  
 3-Octanone (CAS) \$\$ EAK \$\$ Octan-3 19485 000106-68-3 81  
 -one \$\$ n-Octanone-3 \$\$ Amyl ethyl  
 ketone \$\$ Ethyl amyl ketone \$\$ Et  
 hyl n-amyl ketone \$\$ Ethyl pentyl ketone \$\$ Ethyl n-pentyl ketone  
 3-Octanone (CAS) \$\$ EAK \$\$ Octan-3 19486 000106-68-3 81  
 -one \$\$ n-Octanone-3 \$\$ Amyl ethyl  
 ketone \$\$ Ethyl amyl ketone \$\$ Et  
 hyl n-amyl ketone \$\$ Ethyl pentyl ketone \$\$ Ethyl n-pentyl ketone

30 7.925 0.37 C:\Database\WILEY275.L  
 Heptane, 2,2,4,6,6-pentamethyl- (C 55984 013475-82-6 59  
 AS) \$\$ 2,2,4,6,6-Pentamethylheptan  
 Heptane, 2,2,4,6,6-pentamethyl- (C 55988 013475-82-6 59  
 AS) \$\$ 2,2,4,6,6-Pentamethylheptan  
 Heptane, 2,2,4,6,6-pentamethyl- (C 55986 013475-82-6 59  
 AS) \$\$ 2,2,4,6,6-Pentamethylheptan

31 8.068 0.06 C:\Database\WILEY275.L  
 3-Heptanol, 6-methyl- (CAS) \$\$ 6-M 21116 018720-66-6 50  
 ethyl-3-heptanol \$\$ 2-Methyl-5-heptanol  
 (+-)-threo-1,2,3,4,6,7,9,10,15b,15 162706 131652-92-1 42  
 c-decahydropyrido[1",2":1',2']pyrazino[4',3':1,2]pyrido[3,4-b]-indol  
 ETHYL AMYL CARBINOL \$\$ 3 OCTANOL 21217 000589-98-0 40

32 8.116 0.08 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163879 000112-95-8 49

Dodecane (CAS) \$\$ n-Dodecane \$\$ Ba 55935 000112-40-3 47  
51-090453 \$\$ Adakane 12 \$\$ Isododecane  
ecane \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>10</sub>CH<sub>3</sub> \$\$ Bihexyl  
\$\$ Dihexyl \$\$ n-Dodecane min \$\$ N-Dodecan \$\$ Duodecane  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69455 000629-50-5 47  
Tridecane, n-

33 8.239 0.11 C:\Database\WILEY275.L  
Undecane, 4,6-dimethyl- (CAS) 69502 017312-82-2 53  
Dodecane, 2,7,10-trimethyl- (CAS) 98336 074645-98-0 50  
Tetradecane, 4-methyl- (CAS) 98321 025117-24-2 50

34 8.320 0.12 C:\Database\WILEY275.L  
.DELTA.3-Carene \$\$ Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl- (CAS) 25250 013466-78-9 68  
\$\$ (+)-3-CARENE \$\$ .delta.-3-carene  
e \$\$ 3-Carene \$\$ .DELTA.(sup3)-Carene  
ene \$\$ CAR-3-ENE \$\$ D-3-carene \$\$  
3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene  
ene \$\$ .delta. 3-carene \$\$ 3,7,7-Trimethylbicyclo  
.DELTA.3-Carene \$\$ Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl- (CAS) 25245 013466-78-9 60  
\$\$ (+)-3-CARENE \$\$ .delta.-3-carene  
e \$\$ 3-Carene \$\$ .DELTA.(sup3)-Carene  
ene \$\$ CAR-3-ENE \$\$ D-3-carene \$\$  
3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene  
ene \$\$ .delta. 3-carene \$\$ 3,7,7-Trimethylbicyclo  
.DELTA.3-Carene \$\$ Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl- (CAS) 25254 013466-78-9 41  
\$\$ (+)-3-CARENE \$\$ .delta.-3-carene  
e \$\$ 3-Carene \$\$ .DELTA.(sup3)-Carene  
ene \$\$ CAR-3-ENE \$\$ D-3-carene \$\$  
3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene  
ene \$\$ .delta. 3-carene \$\$ 3,7,7-Trimethylbicyclo

35 8.354 0.13 C:\Database\WILEY275.L  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 59  
\$\$ Normal-heptadecane  
4,4-Dimethylcyclooctene 26889 000000-00-0 47  
Eicosane (CAS) \$\$ n-Eicosane 163879 000112-95-8 46

36 8.487 0.51 C:\Database\WILEY275.L  
.alpha.-Terpinene \$\$ 1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- (CAS) 24982 000099-86-5 97  
1,3-P-MENTHADIENE \$\$ 1-Methyl-4-isopropyl-1,3-cyclohexadiene  
ne \$\$ Terpinene \$\$ .alpha.-Terpinene  
n \$\$ p-Mentha-1,3-diene \$\$ ALPHA-TERPINENE  
ERPINE \$ \$ 1-Isopropyl-4-methyl-1,3-cyclohexadiene  
.alpha.-terpinene \$ \$ .ALPHA.-TERPINENE 25315 000099-86-5 97  
NENE  
.ALPHA. TERPINENE \$ \$ PARA-MENTHA-1,3-DIENE 25364 000099-86-5 97

37 8.539 0.28 C:\Database\WILEY275.L  
Nonane, 2,6-dimethyl- (CAS) \$ \$ 2,6 42788 017302-28-2 93

-Dimethylnonane  
 Decane, 4-methyl- (CAS) \$\$ 4-Methy 42781 002847-72-5 81  
 ldecane  
 Decane, 4-methyl- (CAS) \$\$ 4-Methy 42778 002847-72-5 80  
 ldecane

38 8.649 1.86 C:\Database\WILEY275.L  
 Benzene, 1-methyl-2-(1-methylethyl 23292 000527-84-4 97  
 )- (CAS) \$\$ 1-Methyl-2-isopropylbe  
 nzene \$\$ o-Cymene \$\$ o-Cymol \$\$ o-  
 Isopropyltoluene \$\$ 2-Isopropyltol  
 uene \$\$ 1-Isopropyl-2-methylbenzen  
 e \$\$ 1-Methyl-2-(1-methylethyl)-benzene \$\$ Cymene, ortho \$\$ UN 2046  
 Benzene, 1-methyl-2-(1-methylethyl 23294 000527-84-4 95  
 )- (CAS) \$\$ 1-Methyl-2-isopropylbe  
 nzene \$\$ o-Cymene \$\$ o-Cymol \$\$ o-  
 Isopropyltoluene \$\$ 2-Isopropyltol  
 uene \$\$ 1-Isopropyl-2-methylbenzen  
 e \$\$ 1-Methyl-2-(1-methylethyl)-benzene \$\$ Cymene, ortho \$\$ UN 2046  
 Benzene, 1-methyl-4-(1-methylethyl 23306 000099-87-6 95  
 )- (CAS) \$\$ p-Cymene \$\$ 1-Methyl-4  
 -isopropylbenzene \$\$ p-Cymol \$\$ p-  
 Cime \$ \$ Camphogen \$ \$ Dolcymene \$  
 \$ 2-p-Tolylpropane \$ \$ p-Isopropylt  
 oluene \$ \$ p-Methylisopropylbenzene  
 \$ \$ 1-Isopropyl-4-methylbenzene \$ \$ 4-Isopropyl-1-me

39 8.749 0.07 C:\Database\WILEY275.L  
 LIMONENE 25366 000138-86-3 98  
 l-Limonene \$ \$ Cyclohexene, 1-methy 25068 005989-54-8 93  
 l-4-(1-methylethenyl)-, (S)- (CAS)  
 \$ \$ \$ (-)-Limonene \$ \$ p-Mentha-1,8  
 -diene, (S)-(-)- \$ \$ (-)-Limonene \$  
 \$ Limonene \$ \$ (-)-(S)-Limonene \$ \$  
 (S)-Limonene \$ \$ .beta.-Limonene \$ \$ (S)-(-)-Limonene  
 LIMONENE 25367 000138-86-3 90

40 8.825 15.85 C:\Database\WILEY275.L  
 1,8-CINEOLE 40554 000470-82-6 98  
 1,8 CINEOLE \$ \$ EUCALYPTOL \$ \$ CAJEP 40592 000470-82-6 98  
 UTOL \$ \$ 1,8-EPOXY-para-MENTHANE  
 1,8-CINEOLE \$ \$ EUCALYPTOL 40619 000470-82-6 98

41 9.078 0.18 C:\Database\WILEY275.L  
 TRANS-.BETA.-OCIMENE 25361 003779-61-1 98  
 1,3,6-Octatriene, 3,7-dimethyl-, ( 24905 003779-61-1 90  
 E)- (CAS) \$ \$ .BETA. OCIMENE Y \$ \$ t  
 rans-.beta.-Ocimene \$ \$ .beta.-tran  
 s-Ocimene \$ \$ Ocimene, trans-.beta.  
 - \$ \$ trans-3,7-Dimethyl-1,3,6-octa  
 triene \$ \$ BETA OCIMENE Y \$ \$ E-.bet  
 a.-ocimene \$ \$ (E)-Ocimene \$ \$ trans-Ocimene \$ \$ (E)-.  
 Z-.beta.-ocimene 25324 000000-00-0 81

42 9.230 0.71 C:\Database\WILEY275.L  
 Dodecane, 4,6-dimethyl- (CAS) 83567 061141-72-8 59

3,6-Dimethyldecane \$\$ Decane, 3,6- 55972 017312-53-7 58  
dimethyl-  
4-Octanone (CAS) \$\$ Butyl propyl k 19494 000589-63-9 52  
etone \$\$ n-C4H9COCH2CH2CH3 \$\$ Propyl n-butyl ketone \$\$ 4-Oxooctane

- 43 9.363 2.05 C:\Database\WILEY275.L  
.gamma.-Terpinene \$\$ 1,4-Cyclohexa 25031 000099-85-4 97  
diene, 1-methyl-4-(1-methylethyl)-  
(CAS) \$\$ 1-ISOPROPYL-4-METHYL-1,4  
-CYCLOHEXADIENE \$\$ Moslene \$\$ Crit  
hmene \$\$ p-Mentha-1,4-diene \$\$ .ga  
mma.-Terpinen \$\$ 4-Isopropyl-1-met  
hyl-1,4-cyclohexadiene \$\$ 1-Methyl-4-isopropyl-1,4-  
.gamma.-Terpinene \$\$ 1,4-Cyclohexa 25027 000099-85-4 97  
diene, 1-methyl-4-(1-methylethyl)-  
(CAS) \$\$ 1-ISOPROPYL-4-METHYL-1,4  
-CYCLOHEXADIENE \$\$ Moslene \$\$ Crit  
hmene \$\$ p-Mentha-1,4-diene \$\$ .ga  
mma.-Terpinen \$\$ 4-Isopropyl-1-met  
hyl-1,4-cyclohexadiene \$\$ 1-Methyl-4-isopropyl-1,4-  
.GAMMA.-TERPINENE 25416 000000-00-0 97
- 44 9.635 0.32 C:\Database\WILEY275.L  
CIS-SABINENEHYDRATE \$\$ Bicyclo[3.1 40331 000546-79-2 95  
.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-  
CIS-SABINENEHYDRATE 40576 015826-82-1 94  
TRANS-SABINENE HYDRATE 40611 017699-16-0 94
- 45 9.687 0.15 C:\Database\WILEY275.L  
Ethanone, 1-cyclopentyl- (CAS) \$\$ 10720 006004-60-0 38  
Cyclopentylethanone \$\$ Cyclopentyl  
methyl ketone \$\$ Ketone, cyclopen  
tyl methyl \$\$ Acetylcyclopentane \$\$ Methyl cyclopentyl ketone  
2-Pentene, 2-methyl- (CAS) \$\$ 2-Me 2920 000625-27-4 25  
thyl-2-pentene \$\$ 4-Methyl-3-pente  
ne \$\$ (CH3)2C=CHC2H5 \$\$ 2-Methyl-pentene-2  
2-Pentene, 3-methyl-, (Z)- (CAS) \$ 2922 000922-62-3 25  
\$ (Z)-3-Methyl-2-pentene \$\$ 3-Meth  
yl-cis-2-pentene \$\$ cis-3-Methyl-2  
-pentene \$\$ (Z)-CH3CH=C(CH3)C2H5
- 46 9.778 0.10 C:\Database\WILEY275.L  
2-UNDECENE, 4,5-DIMETHYL-, CIS-, T 67386 055170-93-9 50  
HREO-  
1-Butanol, 2-ethyl- (CAS) \$\$ 2-Eth 7828 000097-95-0 35  
yl-1-butanol \$\$ 3-Methylolpentane  
\$\$ Pseudohexyl alcohol \$\$ 2-Ethylb  
utyl alcohol \$\$ 2-Ethylbutanol \$\$  
2-Ethylbutanol-1 \$\$ sec-Hexyl alco  
hol \$\$ sec-Pentyl carbinol \$\$ 3-Pe  
ntyl carbinol \$\$ 2-Ethylbutan-1-ol \$\$ Ethylbutanol  
4-Ethyl-1-hexene 11191 000000-00-0 35
- 47 10.025 0.04 C:\Database\WILEY275.L  
Decane, 2,4-dimethyl- (CAS) \$\$ 2,4 55967 002801-84-5 47  
-Dimethyldecane

Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 43  
\$ Octadecan  
Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 43  
\$ Octadecan

48 10.201 0.87 C:\Database\WILEY275.L  
.alpha.-terpinolene \$\$ Cyclohexene 25089 000586-62-9 95  
, 1-methyl-4-(1-methylethylidene)-  
(CAS) \$\$ 1,4(8)-P-MENTHADIENE \$\$  
1-METHYLENE-4-ISOPROPYLENECYCLOHEX  
ANE \$\$ Terpinolene \$\$ .ALPHA.-TERP  
INOLEN \$\$ Terpinolen \$\$ p-Mentha-1  
,4(8)-diene \$\$ UN 2541 \$\$ 4-Isopropylidene-1-methyl  
L-LINALOOL 40556 000078-70-6 91  
LINALOOL 40613 000078-70-6 91

49 10.278 0.26 C:\Database\WILEY275.L  
TRANS-SABINENE HYDRATE 40611 017699-16-0 94  
trans-sabinene hydrate \$\$ TRANS-TH 40341 017699-16-0 86  
UJAN-4-OL  
CIS-SABINENE HYDRATE 40612 015826-82-1 86

50 10.449 0.06 C:\Database\WILEY275.L  
Heptane, 2,3-dimethyl- (CAS) \$\$ 2, 19820 003074-71-3 53  
3-Dimethylheptane  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55977 001636-43-7 43  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE  
Decane, 5,6-dimethyl- (CAS) \$\$ 5,6 55978 001636-43-7 43  
-Dimethyldecane \$\$ 5,6-DIMETHYL-DECANE

51 10.763 0.09 C:\Database\WILEY275.L  
NEO-ALLO-OCIMENE 25384 007216-56-0 30  
2,2-DIMETHYL-BICYCLO(4.2.0)OCT-1(6 25258 060714-18-3 30  
)-ENE \$\$ Bicyclo[4.2.0]oct-1(6)-ene, 2,2-dimethyl- (CAS)  
Bicyclo[3.1.0]hexane, 6-isopropylidene-1-methyl- (CAS) 25183 024524-57-0 27  
dene-1-methyl- (CAS) \$\$ 1-METHYL-6  
-ISOPROPYLIDENEBICYCLO(3.1.0)HEXAN  
E \$\$ Bicyclo[3.1.0]hexane, 1-methyl-  
1-6-(1-methylethylidene)- (CAS) \$\$  
1,METHYL-6-DIMETHYLMETHYLENEYLBI-CYCLO(3.1.0)HEXANE

52 10.839 0.06 C:\Database\WILEY275.L  
Heptane, 2,3-dimethyl- (CAS) \$\$ 2, 19820 003074-71-3 27  
3-Dimethylheptane  
Heptane, 2,3-dimethyl- (CAS) \$\$ 2, 19822 003074-71-3 16  
3-Dimethylheptane  
Hexane, 3-ethyl- (CAS) \$\$ 3-Ethylh 12463 000619-99-8 16  
exane

53 11.225 2.79 C:\Database\WILEY275.L  
CAMPHOR 37940 000076-22-2 98  
camphor 37827 000076-22-2 98  
Camphor \$\$ Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- (CAS) 38372 000076-22-2 98  
\$ NOR  
BORNAN-2-ONE \$\$ BORNAN-2-ONE \$\$ 2-  
Bornanone \$\$ 2-Camphanone \$\$ Root

bark oil \$\$ Camphor--natural \$\$ Sp  
 irit of camphor \$\$ 1,7,7-Trimethyl  
 norcamphor \$\$ 1,7,7-Trimethylbicyclo[2.2.1]-2-hepta

- 54 11.439 0.09 C:\Database\WILEY275.L  
 Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 59  
 \$\$ Normal-heptadecane  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112855 000544-76-3 59  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
 Tetradecane, 2-methyl- (CAS) \$\$ 2- 98316 001560-95-8 59  
 Methyltetradecane
- 55 11.659 0.47 C:\Database\WILEY275.L  
 .delta.-terpineol 40502 000000-00-0 78  
 l-.alpha.-Terpineol \$\$ 3-Cyclohexe 40197 010482-56-1 59  
 ne-1-methanol, .alpha.,.alpha.,4-t  
 rimethyl-, (S)- (CAS) \$\$ (-)-.alph  
 a.-Terpineol \$\$ .alpha.-Terpineol,  
 (-)- \$\$ p-Menth-1-en-8-ol, (S)-(-  
 )- \$\$ CYCL(-)-.alpha.-Terpineol \$\$  
 CYCLOHEXENE, 1-METHYL-4-(2-PROPANOL-2-YL)- \$\$ ALPH  
 Linalyl propionate \$\$ 1,6-Octadien 95762 000144-39-8 56  
 -3-ol, 3,7-dimethyl-, propanoate (  
 CAS) \$\$ linalyl propanoate \$\$ 1,6-  
 Octadien-3-ol, 3,7-dimethyl-, propionate
- 56 11.720 0.22 C:\Database\WILEY275.L  
 (-)-BORNEOL 40558 000464-45-9 90  
 endo-Borneol \$\$ Bicyclo[2.2.1]hept 40396 000507-70-0 86  
 an-2-ol, 1,7,7-trimethyl-, endo- (  
 CAS) \$\$ Borneol (CAS) \$\$ Camphol \$  
 \$ endo-2-Hydroxy-1,7,7-trimethylno  
 rbornane \$\$ Bicyclo[2.2.1]heptan-2  
 -ol, 1,7,7-trimethyl- \$\$ 2-Bornano  
 l, endo- \$\$ Baros camphor \$\$ Bhimsaim camphor \$\$ Bo  
 endo-Borneol \$\$ Bicyclo[2.2.1]hept 40407 000507-70-0 86  
 an-2-ol, 1,7,7-trimethyl-, endo- (  
 CAS) \$\$ Borneol (CAS) \$\$ Camphol \$  
 \$ endo-2-Hydroxy-1,7,7-trimethylno  
 rbornane \$\$ Bicyclo[2.2.1]heptan-2  
 -ol, 1,7,7-trimethyl- \$\$ 2-Bornano  
 l, endo- \$\$ Baros camphor \$\$ Bhimsaim camphor \$\$ Bo
- 57 11.887 0.68 C:\Database\WILEY275.L  
 TERPINEOL-4 40615 000562-74-3 96  
 3-Cyclohexen-1-ol, 4-methyl-1-(1-m 40153 000562-74-3 96  
 ethylethyl)- (CAS) \$\$ 4-Terpineol  
 \$\$ Terpinene-4-ol \$\$ 1-Terpinen-4-  
 ol \$\$ 4-Carvomenthenol \$\$ p-Menth-  
 1-en-4-ol \$\$ TERPINEOL-4 \$\$ Terpin  
 en-4-ol \$\$ 1-Methyl-4-isopropyl-1-  
 cyclohexen-4-ol \$\$ 4-Terpinenol \$\$ Terpene-4-ol \$\$  
 TERPINEN-4-OL 40552 000562-74-3 96
- 58 12.011 0.11 C:\Database\WILEY275.L  
 PARA-CYMEN-8-OL 36059 001197-01-9 64



Benzenemethanol, .alpha...alpha.,4 35775 001197-01-9 59  
 -trimethyl- (CAS) \$\$ p-Cymen-8-ol  
 \$\$ P-CYMENE-8-OL \$\$ 8-Hydroxy-p-cy  
 mene \$\$ 2-(4-Methylphenyl)-2-propa  
 nol \$\$ 1-Methyl-4-(1-hydroxy-1-met  
 hylethyl)benzene \$\$ 1-Methyl-4-(.a  
 lpha.-hydroxyisopropyl)benzene \$\$ P-CYMENE-8-OL \$\$  
 Benzenemethanol, 4-(1-methylethyl) 35755 000536-60-7 58  
 - (CAS) \$\$ P-CYMEN-.ALPHA.-OL \$\$ 1  
 -HYDROXYMETHYL-4-ISOPROPYLBENZENE  
 \$\$ Cuminol \$\$ p-Cymen-7-ol \$\$ Cumi  
 c alcohol \$\$ Cumyl alcohol \$\$ Cumi  
 nyl alcohol \$\$ Cuminic alcohol \$\$  
 p-Isopropylbenzyl alcohol \$\$ CUMINYL ALCOHOL (20 EV

- 59 12.206 1.57 C:\Database\WILEY275.L  
 .ALPHA. TERPINEOL 40595 000098-55-5 91  
 .BETA. FENCHYL ALCOHOL 40589 000470-08-6 90  
 .ALPHA. TERPINENE \$\$ PARA-MENTHA-1 25364 000099-86-5 60  
 ,3-DIENE
- 60 12.430 0.07 C:\Database\WILEY275.L  
 2-N-PROPYL-1-D1-AZIRIDINE 3064 030691-56-6 53  
 Decane, 3,8-dimethyl- (CAS) \$\$ 3,8 55975 017312-55-9 50  
 -Dimethyldecane  
 Dodecane, 5-methyl- (CAS) \$\$ 5-Met 69472 017453-93-9 50  
 hyldodecane
- 61 12.511 0.22 C:\Database\WILEY275.L  
 Undecane, 3,6-dimethyl- (CAS) 69496 017301-28-9 64  
 Undecane, 2,6-dimethyl- (CAS) \$\$ 2 69488 017301-23-4 64  
 ,6-Dimethylundecane \$\$ 2,6-Dimethylundecene  
 Nonane, 3-methyl-5-propyl- (CAS) 69544 031081-18-2 53
- 62 12.616 0.04 C:\Database\WILEY275.L  
 Tetradecane, 4-ethyl- (CAS) \$\$ 4-E 112871 055045-14-2 50  
 thyltetradecane  
 Undecane, 2,7-dimethyl- (CAS) 69489 017301-24-5 50  
 Tetradecane, 2,6,10-trimethyl- (CA 126480 014905-56-7 50  
 S) \$\$ 2,6,10-Trimethyltetradecane
- 63 12.730 0.34 C:\Database\WILEY275.L  
 2,3-DIMETHYLBENZALDEHYDE \$\$ Benzal 23118 005779-93-1 59  
 dehyde, 2,3-dimethyl- (CAS) \$\$ Hemellitaldehyde  
 Benzaldehyde, 4-ethyl- (CAS) \$\$ p- 23115 004748-78-1 52  
 Ethylbenzaldehyde \$\$ 4-Ethylbenzaldehyde  
 Benzaldehyde, 2,4-dimethyl- (CAS) 23119 015764-16-6 52  
 \$\$ 2,4-Dimethylbenzaldehyde \$\$ 2,4-Dimethylbenzenecarboxaldehyde
- 64 12.873 0.20 C:\Database\WILEY275.L  
 1,1-Difluoro-3-methyl-1-silacyclo- 22657 054077-66-6 40  
 3-pentene  
 1,1-Difluoro-3-methyl-1-silacyclo- 22656 054077-66-6 40  
 3-pentene  
 neroloxide \$\$ 2H-Pyran, 3,6-dihydr 37731 001786-08-9 33  
 o-4-methyl-2-(2-methyl-1-propenyl)

- \$\$ Nerol oxide \$\$ 2H-Pyran, 3,6-  
dihydro-4-methyl-2-(2-methylpropenyl)-

- 65 12.968 0.06 C:\Database\WILEY275.L  
Undecane, 4,6-dimethyl- (CAS) 69502 017312-82-2 46  
Decane, 2-methyl- (CAS) \$\$ 2-Methy 42768 006975-98-0 43  
ldecane \$\$ 2-Methyl-decane \$\$ n-C<sub>8</sub>H<sub>17</sub>CH(CH<sub>3</sub>)<sub>2</sub>  
Decane, 2-methyl- (CAS) \$\$ 2-Methy 42766 006975-98-0 43  
ldecane \$\$ 2-Methyl-decane \$\$ n-C<sub>8</sub>H<sub>17</sub>CH(CH<sub>3</sub>)<sub>2</sub>
- 66 13.211 0.52 C:\Database\WILEY275.L  
CARVACROL METHYL ETHER 49398 006379-73-3 93  
1-ISOPROPYL-2-METHOXY-4-METHYLBENZ 49401 000000-00-0 87  
ENE  
METHYL THYMYLEETHER \$\$ Benzene, 2-m 49281 001076-56-8 87  
ethoxy-4-methyl-1-(1-methylethyl)-  
\$\$ Thymol methyl ether \$\$ Anisole  
, 2-isopropyl-5-methyl- \$\$ Thymyl  
methyl ether \$\$ Methyl thymyl ethe  
r \$\$ 3-Methoxy-p-cymene \$\$ 4-Isopr  
opyl-3-methoxytoluene \$\$ 2-Isopropyl-5-methylanisol
- 67 13.349 0.20 C:\Database\WILEY275.L  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 86  
Hexatriacontane (CAS) \$\$ n-Hexatri 260489 000630-06-8 86  
acontane \$\$ NOR-HEXATRIACONTANE  
Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 83
- 68 13.506 0.27 C:\Database\WILEY275.L  
Dodecane, 4,6-dimethyl- (CAS) 83567 061141-72-8 78  
Dodecane, 4,6-dimethyl- (CAS) 83566 061141-72-8 78  
Heptadecane, 2,6-dimethyl- 152005 054105-67-8 72
- 69 13.668 0.11 C:\Database\WILEY275.L  
Tetradecane, 4-methyl- (CAS) 98321 025117-24-2 72  
pentadecane 98339 000629-62-9 59  
Undecane, 3,8-dimethyl- (CAS) 69498 017301-30-3 47
- 70 13.735 0.31 C:\Database\WILEY275.L  
Undecane, 4,4-dimethyl- (CAS) 69500 017312-68-4 53  
Dodecane, 1-iodo- (CAS) \$\$ n-Dodec 174485 004292-19-7 47  
yl iodide \$\$ Dodecyl iodide \$\$ Lau  
ryl iodide \$\$ 1-Iodododecane  
Nonadecane (CAS) \$\$ n-Nonadecane 151987 000629-92-5 46
- 71 13.892 0.12 C:\Database\WILEY275.L  
LINALOOL L 40593 000078-70-6 38  
Heptadecane (CAS) \$\$ n-Heptadecane 126475 000629-78-7 35  
\$\$ Normal-heptadecane  
Docosane (CAS) \$\$ n-Docosane \$\$ C<sub>2</sub> 186059 000629-97-0 35  
2H<sub>46</sub> STANDARD \$\$ Normal-docosane
- 72 14.025 0.72 C:\Database\WILEY275.L  
pentadecane 98339 000629-62-9 80  
Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12480 000563-16-6 72  
-Dimethylhexane

Hexadecane, 2,6,10,14-tetramethyl- 163891 000638-36-8 64  
 (CAS) \$\$ Phytane \$\$ 2,6,10,14-Tet  
 ramethylhexadecane \$\$ Phytan

73 14.220 0.10 C:\Database\WILEY275.L  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112854 000544-76-3 72  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
 Decane, 2,3,6-trimethyl- (CAS) 69524 062238-12-4 64  
 Heneicosane (CAS) \$\$ n-Heneicosane 175421 000629-94-7 64

74 14.287 0.12 C:\Database\WILEY275.L  
 Tetradecane (CAS) \$\$ n-Tetradecane 83540 000629-59-4 64  
 \$\$ Isotetradecane  
 Dodecane (CAS) \$\$ n-Dodecane \$\$ Ba 55927 000112-40-3 64  
 51-090453 \$\$ Adakane 12 \$\$ Isodod  
 ecane \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>10</sub>CH<sub>3</sub> \$\$ Bihexyl  
 \$\$ Dihexyl \$\$ n-Dodecane min \$\$ N-Dodecan \$\$ Duodecane  
 Pentadecane (CAS) \$\$ n-Pentadecane 98302 000629-62-9 64  
 \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>13</sub>CH<sub>3</sub>

75 14.339 0.55 C:\Database\WILEY275.L  
 (-)-BORNYL ACETATE 80882 005655-61-8 99  
 Bicyclo[2.2.1]heptan-2-ol, 1,7,7-t 80812 005655-61-8 98  
 rimethyl-, acetate, (1S-endo)- (CA  
 S) \$\$ l-Bornyl acetate \$\$ (-)-Born  
 yl acetate \$\$ Levo-bornyl acetate  
 \$\$ l-.alpha.-Bornyl acetate \$\$ Bor  
 neol, acetate, (1S,2R,4S)-(-)- \$\$  
 iso-bornyl acetate \$\$ 1S-endo-Bornyl acetate  
 BORNYL ACETATE 80904 000076-49-3 96

76 14.420 0.37 C:\Database\WILEY275.L  
 Phenol, 5-methyl-2-(1-methylethyl) 35717 000089-83-8 94  
 - (CAS) \$\$ Thymol \$\$ m-Thymol \$\$ p  
 -Cymen-3-ol \$\$ Thyme camphor \$\$ 3-  
 Hydroxy-p-cymene \$\$ 6-Isopropyl-m-  
 cresol \$\$ 5-Methyl-2-isopropylphen  
 ol \$\$ 2-Isopropyl-5-methylphenol \$  
 \$ 6-Isopropyl-3-methylphenol \$\$ 3-Methyl-6-isopropy  
 THYMOL 36062 000089-83-8 91  
 Phenol, 5-methyl-2-(1-methylethyl) 35726 000089-83-8 91  
 - (CAS) \$\$ Thymol \$\$ m-Thymol \$\$ p  
 -Cymen-3-ol \$\$ Thyme camphor \$\$ 3-  
 Hydroxy-p-cymene \$\$ 6-Isopropyl-m-  
 cresol \$\$ 5-Methyl-2-isopropylphen  
 ol \$\$ 2-Isopropyl-5-methylphenol \$  
 \$ 6-Isopropyl-3-methylphenol \$\$ 3-Methyl-6-isopropy

77 14.511 0.15 C:\Database\WILEY275.L  
 Hexane, 3,3-dimethyl- (CAS) \$\$ 3,3 12480 000563-16-6 43  
 -Dimethylhexane  
 Decane, 2-methyl- (CAS) \$\$ 2-Methy 42772 006975-98-0 43  
 ldecane \$\$ 2-Methyl-decane \$\$ n-C<sub>8</sub>H<sub>17</sub>CH(CH<sub>3</sub>)<sub>2</sub>  
 Docosane (CAS) \$\$ n-Docosane \$\$ C<sub>2</sub> 186056 000629-97-0 43  
 2H<sub>46</sub> STANDARD \$\$ Normal-docosane

78 14.620 17.34 C:\Database\WILEY275.L  
 Phenol, 2-methyl-5-(1-methylethyl) 35733 000499-75-2 94  
 - (CAS) \$\$ Carvacrol \$\$ 2-HYDROXY-  
 4-ISOPROPYL-1-METHYLBENZENE \$\$ TOL  
 UOL, 2-HYDROXY-4-ISOPROPYL- \$\$ Ant  
 ioxine \$\$ Isothymol \$\$ Karvakrol \$  
 \$ p-Cymen-2-ol \$\$ 2-Hydroxy-p-cyme  
 ne \$\$ 2-Methyl-5-isopropylphenol \$\$ 5-Isopropyl-2-m  
 Phenol, 2-methyl-5-(1-methylethyl) 35734 000499-75-2 94  
 - (CAS) \$\$ Carvacrol \$\$ 2-HYDROXY-  
 4-ISOPROPYL-1-METHYLBENZENE \$\$ TOL  
 UOL, 2-HYDROXY-4-ISOPROPYL- \$\$ Ant  
 ioxine \$\$ Isothymol \$\$ Karvakrol \$  
 \$ p-Cymen-2-ol \$\$ 2-Hydroxy-p-cyme  
 ne \$\$ 2-Methyl-5-isopropylphenol \$\$ 5-Isopropyl-2-m  
 Phenol, 5-methyl-2-(1-methylethyl) 35717 000089-83-8 91  
 - (CAS) \$\$ Thymol \$\$ m-Thymol \$\$ p  
 -Cymen-3-ol \$\$ Thyme camphor \$\$ 3-  
 Hydroxy-p-cymene \$\$ 6-Isopropyl-m-  
 cresol \$\$ 5-Methyl-2-isopropylphen  
 ol \$\$ 2-Isopropyl-5-methylphenol \$  
 \$ 6-Isopropyl-3-methylphenol \$\$ 3-Methyl-6-isopropy

79 14.744 0.25 C:\Database\WILEY275.L  
 Decane (CAS) \$\$ n-Decane \$\$ Isodec 30015 000124-18-5 70  
 ane \$\$ n-C10H22 \$\$ UN 2247  
 Dodecane, 3-methyl- (CAS) \$\$ 3-Met 69468 017312-57-1 52  
 hyl dodecane  
 Undecane, 3-methyl- (CAS) \$\$ 3-Met 55950 001002-43-3 52  
 hyl undecane

80 14.787 0.25 C:\Database\WILEY275.L  
 2-Pentene, 4-methyl-, (Z)- (CAS) \$ 2932 000691-38-3 25  
 \$ 4-METHYL-CIS-PENT-2-ENE \$\$ 4-Met  
 hyl-2-cis-pentene \$\$ (Z)-4-Methyl-  
 2-pentene \$\$ cis-4-Methyl-2-penten  
 e \$\$ (Z)-(CH3)2CHCH=CHCH3 \$\$ 4-Methyl-cis-2-pentene  
 2-Butene, 2,3-dimethyl- (CAS) \$\$ 2 2959 000563-79-1 25  
 ,3-Dimethyl-2-butene \$\$ Tetramethy  
 lethylene \$\$ 2,3-Dimethylbutene-2  
 \$\$ 2,3-Dimethylbut-2-ene \$\$ 1,1,2,  
 2-Tetramethylethylene \$\$ Tetramethylethene \$\$ (CH3)2C=C(CH3)2  
 Cyclohexane, 1,2,4-trimethyl-, (1. 18322 007667-60-9 25  
 alpha.,2.beta.,4.beta.)- (CAS) \$\$  
 1,TRANS-2,TRANS-4-TRIMETHYLCYCLOHE  
 XANE \$\$ trans, cis-1,2,4-Trimethyl  
 cyclohexane \$\$ Cyclohexane, 1,2,4-  
 trimethyl-, trans,cis- \$\$ cis,trans,trans-1,2,4-Trimethylcyclohexane

81 14.916 0.09 C:\Database\WILEY275.L  
 2-Methoxymesitylene 36190 000000-00-0 35  
 4-vinyl-2-methoxy-phenol 35459 000000-00-0 30  
 (Z)-ocimenone \$\$ 2-methyl-6-vinylh 36049 000000-00-0 30  
 eptane-2,5-dien-4-one

82 14.963 0.18 C:\Database\WILEY275.L

Cyclohexane, 1,2,3-trimethyl-, (1. 18310 007667-55-2 41  
 alpha.,2.alpha.,3.beta.)- (CAS) \$\$  
 1,TRANS-2,CIS-3-TRIMETHYLCYCLOHEX  
 ANE \$\$ Cyclohexane, 1,2,3-trimethy  
 l-, cis,trans- \$\$ Cyclohexane, 1,2  
 ,3-trimethyl-, cis-1,2,trans-1,3-  
 \$\$ 1,cis-2,trans-3-Trimethylcyclohexane \$\$ cis,cis,  
 1-ethyl-2,2,6-trimethylcyclohexane 40927 000000-00-0 38  
 \$\$ 2-ETHYL-1,1,3-TRIMETHYLCYCLOHEXANE  
 1-Ethyl-2,2,6-trimethylcyclohexane 40935 000000-00-0 38

83 15.040 0.45 C:\Database\WILEY275.L  
 Decane, 2,3,6-trimethyl- (CAS) 69524 062238-12-4 80  
 Nonadecane (CAS) \$\$ n-Nonadecane 151985 000629-92-5 72  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 72  
 \$ Octadecan

84 15.235 0.10 C:\Database\WILEY275.L  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 52  
 \$ Octadecan  
 Tetradeceane (CAS) \$\$ n-Tetradeceane 83546 000629-59-4 50  
 \$\$ Isotetradeceane  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 50  
 \$ Octadecan

85 15.344 0.04 C:\Database\WILEY275.L  
 Germacrene B (CAS) \$\$ 1,5-Cyclodec 89208 015423-57-1 58  
 adiene, 1,5-dimethyl-8-(1-methylet  
 hydilene)-, (E,E)- \$\$ Germacre-1(1  
 0),4,7(11)-triene \$\$ Germacre-1(10),4,7(11)-triene, (E,E)-  
 Germacrene B (CAS) \$\$ 1,5-Cyclodec 89207 015423-57-1 52  
 adiene, 1,5-dimethyl-8-(1-methylet  
 hydilene)-, (E,E)- \$\$ Germacre-1(1  
 0),4,7(11)-triene \$\$ Germacre-1(10),4,7(11)-triene, (E,E)-  
 bicyclogermacrene \$\$ Bicyclo[8.1.0 89616 100762-46-7 49  
 ]undeca-2,6-diene, 3,7,11,11-tetra  
 methyl-, (1R\*,2Z,6E,10R\*)-(.+-.)- \$\$ (.+-.)-Lepidozene

86 15.416 0.08 C:\Database\WILEY275.L  
 Tetradeceane (CAS) \$\$ n-Tetradeceane 83540 000629-59-4 50  
 \$\$ Isotetradeceane  
 Tetradeceane (CAS) \$\$ n-Tetradeceane 83535 000629-59-4 50  
 \$\$ Isotetradeceane  
 Dodecane (CAS) \$\$ n-Dodecane \$\$ Ba 55927 000112-40-3 47  
 51-090453 \$\$ Adakane 12 \$\$ Isodod  
 ecane \$\$ CH3(CH2)10CH3 \$\$ Bihexyl  
 \$\$ Dihexyl \$\$ n-Dodecane min \$\$ N-Dodecan \$\$ Duodecane

87 15.897 0.07 C:\Database\WILEY275.L  
 Undecane, 5-ethyl- (CAS) 69476 017453-94-0 59  
 1-Decanol, 2,2-dimethyl- (CAS) \$\$ 71288 002370-15-2 53  
 2,2-DIMETHYL-DECANOL-1 \$\$ 1-Hydroxy-2,2-dimethyldecane  
 Pentadecane (CAS) \$\$ n-Pentadecane 98301 000629-62-9 50  
 \$\$ CH3(CH2)13CH3

88 16.459 0.26 C:\Database\WILEY275.L

.BETA. ELEMENE 89661 000515-13-9 87  
 (-)-.beta.-Elemene \$\$ Cyclohexane, 89181 000515-13-9 86  
 1-ethenyl-1-methyl-2,4-bis(1-meth  
 ylethenyl)-, [1S-(1.alpha.,2.beta.  
 ,4.beta.)]- (CAS) \$\$ CIS-1,3-DIISO  
 PROPENYL-TRANS-4-VINYL-4-METHYLCYC  
 LOHEXANE \$\$ .beta.-Elemene, (-)- \$  
 \$ Cyclohexane, 2,4-diisopropenyl-1-methyl-1-vinyl-,  
 (-)-.beta.-Elemene \$\$ Cyclohexane, 89180 000515-13-9 86  
 1-ethenyl-1-methyl-2,4-bis(1-meth  
 ylethenyl)-, [1S-(1.alpha.,2.beta.  
 ,4.beta.)]- (CAS) \$\$ CIS-1,3-DIISO  
 PROPENYL-TRANS-4-VINYL-4-METHYLCYC  
 LOHEXANE \$\$ .beta.-Elemene, (-)- \$  
 \$ Cyclohexane, 2,4-diisopropenyl-1-methyl-1-vinyl-,

89 16.511 0.05 C:\Database\WILEY275.L  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112851 000544-76-3 47  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
 Tetradecane (CAS) \$\$ n-Tetradecane 83546 000629-59-4 47  
 \$\$ Isotetradecane  
 Nonadecane (CAS) \$\$ n-Nonadecane 151979 000629-92-5 47

90 16.597 0.10 C:\Database\WILEY275.L  
 Tetradecane (CAS) \$\$ n-Tetradecane 83548 000629-59-4 81  
 \$\$ Isotetradecane  
 Tetradecane (CAS) \$\$ n-Tetradecane 83544 000629-59-4 81  
 \$\$ Isotetradecane  
 N-TETRADECANE 83576 000000-00-0 64

91 16.754 0.09 C:\Database\WILEY275.L  
 Heptadecane, 8-methyl- (CAS) \$\$ 8- 139431 013287-23-5 59  
 Methylheptadecane  
 Nonane, 5-(1-methylpropyl)- (CAS) 69541 062185-54-0 53  
 Nonadecane (CAS) \$\$ n-Nonadecane 151986 000629-92-5 52

92 16.801 0.16 C:\Database\WILEY275.L  
 Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 83  
 \$\$ Normal-heptadecane  
 pentadecane 98339 000629-62-9 80  
 Heptadecane (CAS) \$\$ n-Heptadecane 126476 000629-78-7 80  
 \$\$ Normal-heptadecane

93 16.892 0.23 C:\Database\WILEY275.L  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 64  
 Nonadecane (CAS) \$\$ n-Nonadecane 151979 000629-92-5 64  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 64

94 17.016 0.06 C:\Database\WILEY275.L  
 Heptadecane, 4-methyl- (CAS) \$\$ 4- 139425 026429-11-8 53  
 Methylheptadecane  
 Undecane, 4,8-dimethyl- (CAS) 69505 017301-33-6 53  
 Tridecane, 4-methyl- (CAS) \$\$ 4-Me 83559 026730-12-1 53  
 thyltridecane

95 17.130 0.18 C:\Database\WILEY275.L

.beta.-CARYOPHYLLENE 89707 000087-44-5 90  
trans-Caryophyllene \$\$ Bicyclo[7.2 89249 000087-44-5 76  
.0]undec-4-ene, 4,11,11-trimethyl-  
8-methylene-, [1R-(1R\*,4E,9S\*)]- (CAS) \$\$ 1-Caryophyllene \$\$ (-)-Car  
yophyllene \$\$ Caryophyllene \$\$ .be  
ta.-Caryophyllen \$\$ .beta.-Caryoph  
yllene \$\$ .beta.-Caryophyllene, (-) \$\$ Bicyclo[7.2.  
trans-Caryophyllene \$\$ Bicyclo[7.2 89254 000087-44-5 72  
.0]undec-4-ene, 4,11,11-trimethyl-  
8-methylene-, [1R-(1R\*,4E,9S\*)]- (CAS) \$\$ 1-Caryophyllene \$\$ (-)-Car  
yophyllene \$\$ Caryophyllene \$\$ .be  
ta.-Caryophyllen \$\$ .beta.-Caryoph  
yllene \$\$ .beta.-Caryophyllene, (-) \$\$ Bicyclo[7.2.

96 17.278 0.11 C:\Database\WILEY275.L  
(1S\*,2S\*,5R\*,6R\*,10R\*)-1,6-dimethy 108041 124780-76-3 53  
l-10-ethoxy-11-oxatricyclo[5.3.0.1(2,5)]undec-6-ene  
bicyclgermacrene \$\$ Bicyclo[8.1.0 89615 100762-46-7 50  
]undeca-2,6-diene, 3,7,11,11-tetra  
methyl-, (1R\*,2Z,6E,10R\*)-(.+-.)- \$\$ (.+-.)-Lepidozene  
.GAMMA.-ELEMENE \$\$ Cyclohexane, 1- 89185 003242-08-8 47  
ethenyl-1-methyl-2-(1-methyletheny  
l)-4-(1-methylethylidene)- (CAS) \$  
\$ Elixene \$\$ o-Menth-8-ene, 4-isop  
ropylidene-1-vinyl- \$\$ GAMMA-ELEMENE

97 17.325 0.07 C:\Database\WILEY275.L  
pentadecane 98340 000629-62-9 53  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 53  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 53

98 17.544 0.05 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 64  
\$ Octadecan  
Heptadecane (CAS) \$\$ n-Heptadecane 126476 000629-78-7 59  
\$\$ Normal-heptadecane  
Tricosane (CAS) \$\$ n-Tricosane 195911 000638-67-5 59

99 17.601 0.06 C:\Database\WILEY275.L  
pentadecane 98339 000629-62-9 53  
Dodecane (CAS) \$\$ n-Dodecane \$\$ Ba 55930 000112-40-3 53  
51-090453 \$\$ Adakane 12 \$\$ Isodod  
ecane \$\$ CH3(CH2)10CH3 \$\$ Bihexyl  
\$\$ Dihexyl \$\$ n-Dodecane min \$\$ N-Dodecan \$\$ Duodecane  
Dodecane (CAS) \$\$ n-Dodecane \$\$ Ba 55933 000112-40-3 50  
51-090453 \$\$ Adakane 12 \$\$ Isodod  
ecane \$\$ CH3(CH2)10CH3 \$\$ Bihexyl  
\$\$ Dihexyl \$\$ n-Dodecane min \$\$ N-Dodecan \$\$ Duodecane

100 17.649 0.12 C:\Database\WILEY275.L  
Undecane, 2,4-dimethyl- (CAS) \$\$ 2 69481 017312-80-0 52  
,4-Dimethylundecane  
Octadecane (CAS) \$\$ n-Octadecane \$ 139436 000593-45-3 50  
\$ Octadecan

|     |        |      |                                                                |                                            |
|-----|--------|------|----------------------------------------------------------------|--------------------------------------------|
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane                             | 151981 000629-92-5 50                      |
| 101 | 17.782 | 0.27 | C:\Database\WILEY275.L<br>NONADECANE                           | 152008 000000-00-0 80                      |
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane                             | 151980 000629-92-5 80                      |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                 | 163880 000112-95-8 72                      |
| 102 | 17.940 | 0.59 | C:\Database\WILEY275.L<br>EICOSANE                             | 163904 000000-00-0 83                      |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                 | 163883 000112-95-8 83                      |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                 | 163886 000112-95-8 83                      |
| 103 | 18.111 | 0.13 | C:\Database\WILEY275.L<br>Tetradecane (CAS) \$\$ n-Tetradecane | 83546 000629-59-4 64                       |
|     |        |      | \$\$ Isotetradecane                                            |                                            |
|     |        |      | Dodecane, 2,6,11-trimethyl- (CAS)                              | 98333 031295-56-4 64                       |
|     |        |      | \$\$ 2,6,11-Trimethyldodecane                                  |                                            |
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane                             | 151984 000629-92-5 59                      |
| 104 | 18.468 | 0.30 | C:\Database\WILEY275.L<br>Octadecane (CAS) \$\$ n-Octadecane   | \$ 139446 000593-45-3 80                   |
|     |        |      | \$ Octadecan                                                   |                                            |
|     |        |      | Octadecane (CAS) \$\$ n-Octadecane                             | \$ 139440 000593-45-3 78                   |
|     |        |      | \$ Octadecan                                                   |                                            |
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane                             | 151981 000629-92-5 72                      |
| 105 | 18.573 | 1.24 | C:\Database\WILEY275.L<br>Heneicosane (CAS) \$\$ n-Heneicosane | 175422 000629-94-7 52                      |
|     |        |      | Triacontane (CAS) \$\$ n-Triacontane                           | 242802 000638-68-6 52                      |
|     |        |      | OCTADECANE                                                     | 139454 000593-45-3 50                      |
| 106 | 18.787 | 0.16 | C:\Database\WILEY275.L<br>Nonadecane (CAS) \$\$ n-Nonadecane   | 151987 000629-92-5 80                      |
|     |        |      | Heneicosane (CAS) \$\$ n-Heneicosane                           | 175419 000629-94-7 74                      |
|     |        |      | Heptadecane (CAS) \$\$ n-Heptadecane                           | 126473 000629-78-7 72                      |
|     |        |      | \$\$ Normal-heptadecane                                        |                                            |
| 107 | 18.873 | 3.50 | C:\Database\WILEY275.L<br>3,6-dimethyl-5-(1-methylethenyl)-6   | 101833 121470-80-2 64                      |
|     |        |      | -ethenyl-4,7-dihydro-benzofuran                                | \$\$                                       |
|     |        |      | Benzofuran, 6-ethenyl-4,5,6,7-tet                              |                                            |
|     |        |      | rahydro-3,6-dimethyl-5-(1-methylethenyl)-, trans-(+.-)-        |                                            |
|     |        |      | ISOSERICENINE \$\$ 5-Benzofuranaceti                           | 144417 019912-86-8 50                      |
|     |        |      | c acid, 6-ethenyl-4,5,6,7-tetrahyd                             |                                            |
|     |        |      | ro-3,6-dimethyl-.alpha.-methylene-                             |                                            |
|     |        |      | , methyl ester (CAS) \$\$ Isosericen                           |                                            |
|     |        |      | in \$\$ p-Mentha-4,8-diene-2-acetic                            |                                            |
|     |        |      | acid, 5,9-epoxy-.alpha.-methylene-1-vinyl-, methyl ester       |                                            |
|     |        |      | ANISOLE                                                        | 9189 000000-00-0 47                        |
| 108 | 18.959 | 0.32 | C:\Database\WILEY275.L<br>.gamma. 1-cadinene                   | 89609 000000-00-0 38                       |
|     |        |      | Germacrene B (CAS) \$\$ 1,5-Cyclodec                           | 89206 015423-57-1 38                       |
|     |        |      | adiene, 1,5-dimethyl-8-(1-methylet                             |                                            |
|     |        |      | hylidene)-, (E,E)-                                             | \$\$ Germacra-1(1                          |
|     |        |      | 0),4,7(11)-triene                                              | \$\$ Germacra-1(10),4,7(11)-triene, (E,E)- |



Heptadecane (CAS) \$\$ n-Heptadecane 126477 000629-78-7 38  
 \$\$ Normal-heptadecane

109 19.121 0.34 C:\Database\WILEY275.L  
 Phenol, 2,5-bis(1,1-dimethylethyl) 91579 005875-45-6 74  
 - (CAS) \$\$ 2,5-Di-tert-butylphenol  
 \$\$ Phenol, 2,5-di-tert-butyl- \$\$ 2,5-Di-tert-butylhydroxybenzene  
 Phenol, 2,4-bis(1,1-dimethylethyl) 91573 000096-76-4 74  
 - (CAS) \$\$ 2,4-Di-tert-butylphenol  
 \$\$ 2,4-BIS(TERT-BUTYL)-PHENOL \$\$  
 2,4-Di-t-butylphenol \$\$ Phenol, 2,  
 4-di-tert-butyl- \$\$ 2,4-Bis(1,1-di  
 methylethyl)phenol \$\$ 2,4-Di-tert-  
 butyl-phenol \$\$ 4-(1,5-Dimethylhex-4-enyl)cyclohex-  
 Phenol, 2,4-bis(1,1-dimethylethyl) 91571 000096-76-4 72  
 - (CAS) \$\$ 2,4-Di-tert-butylphenol  
 \$\$ 2,4-BIS(TERT-BUTYL)-PHENOL \$\$  
 2,4-Di-t-butylphenol \$\$ Phenol, 2,  
 4-di-tert-butyl- \$\$ 2,4-Bis(1,1-di  
 methylethyl)phenol \$\$ 2,4-Di-tert-  
 butyl-phenol \$\$ 4-(1,5-Dimethylhex-4-enyl)cyclohex-

110 19.349 0.13 C:\Database\WILEY275.L  
 Tridecane (CAS) \$\$ n-Tridecane \$\$ 69452 000629-50-5 35  
 Tridecane, n-  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 35  
 \$ Octadecan  
 Cyclohexane, 1,1,2-trimethyl- (CAS 18298 007094-26-0 25  
 ) \$\$ 1,1,2-Trimethylcyclohexane

111 19.549 0.23 C:\Database\WILEY275.L  
 .delta.-cadinene (armoise-Maroc) \$ 89582 000483-76-1 99  
 \$ .DELTA.-CADINENE  
 .delta.-Cadinene \$\$ Naphthalene, 1 89349 000483-76-1 98  
 ,2,3,5,6,8a-hexahydro-4,7-dimethyl  
 -1-(1-methylethyl)-, (1S-cis)- (CA  
 S) \$\$ (+)-.delta.-Cadinene \$\$ Cadi  
 na-1(10),4-diene \$\$ .delta.-Cadinene, (+)- \$\$ DELTA-CADINENE  
 .delta.-Cadinene \$\$ Naphthalene, 1 89354 000483-76-1 98  
 ,2,3,5,6,8a-hexahydro-4,7-dimethyl  
 -1-(1-methylethyl)-, (1S-cis)- (CA  
 S) \$\$ (+)-.delta.-Cadinene \$\$ Cadi  
 na-1(10),4-diene \$\$ .delta.-Cadinene, (+)- \$\$ DELTA-CADINENE

112 19.630 1.42 C:\Database\WILEY275.L  
 Cyclohexanol, 3-ethenyl-3-methyl-2 108214 035727-45-8 99  
 -(1-methylethenyl)-6-(1-methylethy  
 l)-, [1R-(1.alpha.,2.alpha.,3.beta  
 .,6.alpha.)]- (CAS) \$\$ Shyobunol \$  
 \$ 1.beta.-Isopropyl-2.beta.-hydrox  
 y-3.alpha.-isopropenyl-4.alpha.-et  
 henyl-4.beta.-methylcyclohexane  
 Bicyclo[4.1.0]heptane, 7-(1-methyl 25256 053282-47-6 72  
 ethylidene)- (CAS) \$\$ 7-ISOPROPYLENYL BICYCLO(4.1.0(1-6))HEPTANE  
 Camphene \$\$ Bicyclo[2.2.1]heptane, 25161 000079-92-5 66  
 2,2-dimethyl-3-methylene- (CAS) \$

\$ 3,3-Dimethyl-2-methylenenorbornane  
 \$\$ 2,2-Dimethyl-3-methylenenorbornane  
 \$\$ 3,3-Dimethyl-2-methylene norcamphane  
 \$\$ 2,2-Dimethyl-3-methylenebicyclo[2.2.1]heptane  
 \$\$ NA 9011

- 113 19.773 1.07 C:\Database\WILEY275.L  
 Cyclohexanol, 3-ethenyl-3-methyl-2-(1-methylethenyl)-6-(1-methylethyl)-, [1R-(1.alpha.,2.alpha.,3.beta.,6.alpha.)]- (CAS) \$ \$ Shyobunol \$  
 \$ 1.beta.-Isopropyl-2.beta.-hydroxy-3.alpha.-isopropenyl-4.alpha.-ethenyl-4.beta.-methylcyclohexane  
 2,4-DIISOPROPENYL-1-METHYL-1-VINYL 89188 033880-83-0 38  
 -CYCLOHEXANE  
 CIS-ISOPULEGONE 37936 000000-00-0 35
- 114 19.882 0.64 C:\Database\WILEY275.L  
 Tetratriacontane (CAS) \$ \$ n-Tetratriacontane 256280 014167-59-0 80  
 Heptacosane (CAS) \$ \$ n-Heptacosane 226683 000593-49-7 78  
 Triacontane (CAS) \$ \$ n-Triacontane 242802 000638-68-6 72
- 115 20.201 0.12 C:\Database\WILEY275.L  
 Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) \$ \$ 3-Ethyl-5-(2'-ethylbutyl)octadecane 220176 055282-12-7 53  
 Hexadecane, 2,6,10,14-tetramethyl- (CAS) \$ \$ 2,6,10,14-Tetramethylhexadecane 163888 000638-36-8 47  
 (CAS) \$ \$ Phytane \$ \$ 2,6,10,14-Tetramethylhexadecane \$ \$ Phytan  
 Heneicosane (CAS) \$ \$ n-Heneicosane 175422 000629-94-7 47
- 116 20.482 0.08 C:\Database\WILEY275.L  
 Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) \$ \$ 3-Ethyl-5-(2'-ethylbutyl)octadecane 220178 055282-12-7 43  
 Tetratetracontane (CAS) \$ \$ n-Tetratetracontane 269825 007098-22-8 38  
 Dotriacontane (CAS) \$ \$ n-Dotriacontane 250417 000544-85-4 38  
 tane \$ \$ Bicetyl \$ \$ Tris(trimethylsilyl)ether, methyl ester of ethyl anthranilate azo pigment(.alpha.z) of bilivubidin-1x.alpha. 2-O-acyl glucuronide
- 117 20.821 0.10 C:\Database\WILEY275.L  
 Pentadecane, 2-methyl- (CAS) \$ \$ 14 112860 001560-93-6 49  
 -METHYLPENTADECANES \$ \$ 2-Methylpentadecane  
 Eicosane, 7-hexyl- (CAS) \$ \$ 7-n-Hexyl- 220184 055333-99-8 47  
 xyleicosane  
 Hexadecane (CAS) \$ \$ n-Hexadecane \$ 112843 000544-76-3 43  
 \$ Cetane \$ \$ n-Cetane \$ \$ Isohexadecane
- 118 21.259 0.29 C:\Database\WILEY275.L  
 .beta.-cubebene 89691 013744-15-5 56  
 (-)-ISOLEDENE 89790 000000-00-0 50  
 .alpha.-Elemene \$ \$ Cyclohexene, 6-ethenyl-6-methyl-1-(1-methylethyl)-3-(1-methylethylidene)-, (S)- (CAS) \$ \$ o-Menth-2-ene, 4-isopropylidene-1-vinyl-

119 21.744 0.05 C:\Database\WILEY275.L  
10-Methylnonadecane 163906 000000-00-0 49  
Nonadecane (CAS) \$\$ n-Nonadecane 151986 000629-92-5 49  
Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 49  
\$ Octadecan

120 21.906 0.10 C:\Database\WILEY275.L  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 64  
\$\$ Normal-heptadecane  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 64  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112843 000544-76-3 64  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane

121 21.949 0.16 C:\Database\WILEY275.L  
.gamma.-Gurjunene \$\$ Azulene, 1,2, 89274 022567-17-5 86  
3,3a,4,5,6,7-octahydro-1,4-dimethy  
l-7-(1-methylethenyl)-, [1R-(1.alp  
ha.,3a.beta.,4.alpha.,7.beta.)]- (CAS) \$\$ 1.beta.,4.beta.H,10.beta.H  
-Guaia-5,11-diene \$\$ GAMMA-GURJUNE  
NE \$\$ .gamma. gurjunene \$\$ 5,6,11,11-tetramethyltri  
Eremophilene \$\$ Naphthalene, 1,2,3 89361 010219-75-7 70  
,5,6,7,8,8a-octahydro-1,8a-dimethy  
l-7-(1-methylethenyl)-, [1S-(1.alp  
ha.,7.alpha.,8a.alpha.)]- (CAS) \$\$ Eremophila-1(10),11-diene  
Cyclopropa[d]naphthalen-2(4aH)-one 89007 004677-90-1 64  
, 1,1a,5,6,7,8-hexahydro-4a,8,8-tr  
imethyl-, [1aR-(1a.alpha.,4a.beta.  
,8aS\*)]- (CAS) \$\$ Mayurone \$\$ Mayu  
ron \$\$ Cyclopropa[d]naphthalen-2(4  
aH)-one, 1,1a,5,6,7,8-hexahydro-4a  
,8,8-trimethyl-, (1aR,4aS,8aS)-(+)- \$\$ Cyclopropa[d]

122 21.992 0.09 C:\Database\WILEY275.L  
.alpha.-Sinensal \$\$ 2,6,9,11-Dodec 103660 017909-77-2 22  
atetraenal, 2,6,10-trimethyl-, (E,E,E)- (CAS)  
Anthranilic acid, N-methyl-, butyl 92385 015236-34-7 18  
ester (CAS) \$\$ N-BUTYL O-METHYLAMINOBENZOATE  
(-)-campborsulfonimine \$\$ 3H-3a,6- 98546 060886-80-8 14  
Methano-2,1-benzisothiazole, 4,5,6  
,7-tetrahydro-8,8-dimethyl-, 2,2-dioxide, (3aS)-

123 22.292 0.19 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163880 000112-95-8 55  
HEXADECANE 112890 000000-00-0 43  
Hexadecane (CAS) \$\$ n-Hexadecane \$ 112848 000544-76-3 43  
\$ Cetane \$\$ n-Cetane \$\$ Isohexadecane

124 22.382 0.07 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 58  
\$ Octadecan  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 53  
Tridecane (CAS) \$\$ n-Tridecane \$\$ 69461 000629-50-5 53  
Tridecane, n-

125 22.692 0.22 C:\Database\WILEY275.L  
Methyl jasmonate (CAS) \$\$ Cyclopentaneacetic acid, 3-oxo-trans-2-(cis-2-pentenyl), methyl ester \$\$ methyl (1S,2S)-3-oxo-2-[(2'Z)pent-2'-enyl]cyclopentan-1-acetate \$\$ Cyclopentaneacetic acid, 3-oxo-2-(2-pentenyl)-, methyl ester, [1R-[1.alpha.,2.beta.(Z)]]  
METHYL JASMONATE 110223 001211-29-6 87  
methyl epijasmonate 110221 000000-00-0 59

126 22.754 0.37 C:\Database\WILEY275.L  
.alpha.-cadinol 108441 000481-34-5 64  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 25  
2H46 STANDARD \$\$ Normal-docosane  
Octadecane (CAS) \$\$ n-Octadecane \$ 139441 000593-45-3 25  
\$ Octadecan

127 22.982 0.96 C:\Database\WILEY275.L  
T-Cadinol \$\$ 1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1S-(1.alpha.,4.alpha.,4a.alpha.,8a.beta.)]- (CAS) \$\$ Cedrelanol \$\$ 10.beta.H-Cadin-4-en-10-ol \$\$ 10-epi-.alpha.-Cadinol  
.alpha.-cadinol 108441 000481-34-5 87  
T-Muurolol \$\$ 1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1S-(1.alpha.,4.alpha.,4a.alpha.,8a.alpha.)]- (CAS) \$\$ 1.beta.,10.beta.H-Cadin-4-en-10-ol \$\$ (-)-T-Muurolol

128 23.087 0.21 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 72  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 72  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 64

129 23.192 0.29 C:\Database\WILEY275.L  
Tetradecane, 4-ethyl- (CAS) \$\$ 4-Ethyltetradecane 112871 055045-14-2 64  
Undecane, 2,9-dimethyl- (CAS) 69491 017301-26-7 64  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 58

130 23.282 0.12 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
2H46 STANDARD \$\$ Normal-docosane  
Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 80  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80

131 23.344 0.12 C:\Database\WILEY275.L  
Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 59  
Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 59  
\$ Octadecan  
Heptadecane (CAS) \$\$ n-Heptadecane 126476 000629-78-7 53  
\$\$ Normal-heptadecane

132 23.425 0.12 C:\Database\WILEY275.L  
Hexadecane, 2,6,10,14-tetramethyl- 163889 000638-36-8 72  
(CAS) \$\$ Phytane \$\$ 2,6,10,14-Tet  
ramethylhexadecane \$\$ Phytan  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 64  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 64  
2H46 STANDARD \$\$ Normal-docosane

133 23.640 0.43 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163886 000112-95-8 86  
Tricosane (CAS) \$\$ n-Tricosane 195914 000638-67-5 86  
Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 86  
Decyldocosane \$\$ 11-NOR-DECYLDOSANE

134 23.730 2.10 C:\Database\WILEY275.L  
HEXENYL CYCLOPENTANONE 51420 034687-46-2 35  
2-Butenal, 3-methyl- (CAS) \$\$ 3-Me 2713 000107-86-8 30  
thyl-2-butenal \$\$ Prenal \$\$ Seneci  
aldehyde \$\$ Senecioaldehyde \$\$ 3,3  
-Dimethylacrolein \$\$ 3-Methylcroto  
naldehyde \$\$ Crotonaldehyde, 3-met  
hyl- \$\$ .beta.-Methylcrotonaldehyde \$\$ .beta.,.beta.-Dimethylacrolei  
Furan, 2,3-dihydro-4-methyl- (CAS) 2802 034314-83-5 27  
\$\$ 4-METHYL-2,3-DIHYDROFURAN

135 23.792 0.16 C:\Database\WILEY275.L  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 74  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 72  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 72

136 23.859 0.13 C:\Database\WILEY275.L  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80  
Octadecane (CAS) \$\$ n-Octadecane \$ 139438 000593-45-3 72  
\$ Octadecan  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 72  
ane \$\$ n-Hentriacontane

137 23.906 0.18 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 64  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 64  
Heptadecane (CAS) \$\$ n-Heptadecane 126476 000629-78-7 64  
\$\$ Normal-heptadecane

138 24.106 0.08 C:\Database\WILEY275.L  
Octadecane, 3-ethyl-5-(2-ethylbuty 220176 055282-12-7 72  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 58  
\$ Octadecan  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 53  
\$\$ Normal-heptadecane

139 24.187 0.28 C:\Database\WILEY275.L  
Nonahexacontanoic acid (CAS) \$\$ N- 275385 040710-32-5 50  
NONAHEXACONTANOIC ACID  
Octadecane, 3-ethyl-5-(2-ethylbuty 220176 055282-12-7 49  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbu

tyl)octadecane  
 Octadecane, 3-ethyl-5-(2-ethylbutyl) 220178 055282-12-7 47  
 l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane

140 24.282 0.07 C:\Database\WILEY275.L  
 Octadecane, 3-ethyl-5-(2-ethylbutyl) 220176 055282-12-7 80  
 l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
 Hexadecane, 2,6,10,14-tetramethyl- 163889 000638-36-8 59  
 (CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane \$\$ Phytan  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139446 000593-45-3 53  
 \$ Octadecan

141 24.349 0.08 C:\Database\WILEY275.L  
 Octadecane, 3-ethyl-5-(2-ethylbutyl) 220176 055282-12-7 64  
 l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
 Heneicosane (CAS) \$\$ n-Heneicosane 175421 000629-94-7 59  
 Octadecane, 3-ethyl-5-(2-ethylbutyl) 220178 055282-12-7 53  
 l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane

142 24.402 0.23 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 87  
 2H46 STANDARD \$\$ Normal-docosane  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 86  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 83

143 24.435 0.55 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 90  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 90  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 87  
 2H46 STANDARD \$\$ Normal-docosane

144 24.525 0.11 C:\Database\WILEY275.L  
 Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 64  
 OCTACOSANE 232594 000000-00-0 64  
 Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 58

145 24.582 0.08 C:\Database\WILEY275.L  
 Tridecanol, 2-ethyl-2-methyl- 128189 000000-00-0 72  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 72  
 2H46 STANDARD \$\$ Normal-docosane  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 72

146 24.621 0.18 C:\Database\WILEY275.L  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112843 000544-76-3 53  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane  
 pentadecane 98340 000629-62-9 53  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 53  
 \$ Octadecan

147 24.782 0.13 C:\Database\WILEY275.L  
 Nonadecane (CAS) \$\$ n-Nonadecane 151982 000629-92-5 72  
 Tridecanol, 2-ethyl-2-methyl- 128189 000000-00-0 64  
 Tetratetracontane (CAS) \$\$ n-Tetra 269825 007098-22-8 64  
 tetracontane

148 24.963 0.07 C:\Database\WILEY275.L

TETRACOSAMETHYLCYCLODODECASILOXANE 275053 018919-94-3 12  
 \$\$ Cyclododecasiloxane, tetracosamethyl- (CAS)  
 Triacontane (CAS) \$\$ n-Triacontane 242803 000638-68-6 10  
 Dodecane (CAS) \$\$ n-Dodecane \$\$ Ba 55939 000112-40-3 10  
 51-090453 \$\$ Adakane 12 \$\$ Isododecane  
 ecane \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>10</sub>CH<sub>3</sub> \$\$ Bihexyl  
 \$\$ Dihexyl \$\$ n-Dodecane min \$\$ N-Dodecan \$\$ Duodecane

149 25.078 1.33 C:\Database\WILEY275.L  
 Anthracene-D10 63087 000000-00-0 95  
 Anthracene-d10- 63091 001719-06-8 95  
 DECADEUTEROPHENANTHRENE \$\$ Phenant 63088 001517-22-2 90  
 hrene-d10

150 25.325 0.02 C:\Database\WILEY275.L  
 N-NONADECANE 152007 000629-92-5 47  
 OCTADECANE 139454 000593-45-3 47  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 46  
 2H46 STANDARD \$\$ Normal-docosane

151 25.378 0.04 C:\Database\WILEY275.L  
 Hexadecane, 2,6,10,14-tetramethyl- 163891 000638-36-8 35  
 (CAS) \$\$ Phytane \$\$ 2,6,10,14-Tetramethylhexadecane \$\$ Phytan  
 pentadecane 98340 000629-62-9 35  
 Undecane, 2,3-dimethyl- (CAS) \$\$ 2 69480 017312-77-5 35  
 ,3-Dimethylundecane

152 25.792 0.11 C:\Database\WILEY275.L  
 5,5-Dibutylnonane 126484 000000-00-0 64  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 64  
 2H46 STANDARD \$\$ Normal-docosane  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 64

153 25.883 0.14 C:\Database\WILEY275.L  
 Eicosane (CAS) \$\$ n-Eicosane 163886 000112-95-8 96  
 EICOSANE 163904 000000-00-0 96  
 Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 96

154 25.963 0.05 C:\Database\WILEY275.L  
 Nonahexacontanoic acid (CAS) \$\$ N- 275385 040710-32-5 64  
 NONAHEXACONTANOIC ACID  
 Eicosane, 2-methyl- (CAS) \$\$ 2-Met 175409 001560-84-5 58  
 hyleicosane \$\$ 19-Methyleicosane  
 Hexadecane (CAS) \$\$ n-Hexadecane \$ 112843 000544-76-3 53  
 \$ Cetane \$\$ n-Cetane \$\$ Isohexadecane

155 26.130 0.18 C:\Database\WILEY275.L  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 64  
 \$ Octadecan  
 Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) 220176 055282-12-7 64  
 l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
 Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 64  
 \$ Octadecan

156 26.311 0.14 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 86

Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 80  
2H46 STANDARD \$\$ Normal-docosane  
Nonadecane (CAS) \$\$ n-Nonadecane 151987 000629-92-5 72

157 26.359 0.26 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 52  
Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 52  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 50

158 26.449 0.24 C:\Database\WILEY275.L  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 91  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 87  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 87

159 26.506 0.08 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 80  
\$ Octadecan  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 80  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 72  
2H46 STANDARD \$\$ Normal-docosane

160 26.554 0.21 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
2H46 STANDARD \$\$ Normal-docosane  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 83  
Octadecane (CAS) \$\$ n-Octadecane \$ 139440 000593-45-3 80  
\$ Octadecan

161 26.654 0.20 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 81  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80  
HENEICOSANE 175428 000000-00-0 80

162 26.740 0.61 C:\Database\WILEY275.L  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 90  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 80  
2H46 STANDARD \$\$ Normal-docosane  
Tetratetracontane (CAS) \$\$ n-Tetra 269825 007098-22-8 64  
tetracontane

163 26.811 0.29 C:\Database\WILEY275.L  
Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 78  
\$ Octadecan  
Nonadecane (CAS) \$\$ n-Nonadecane 151981 000629-92-5 78  
Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 74  
2H46 STANDARD \$\$ Normal-docosane

164 26.840 0.19 C:\Database\WILEY275.L  
N-EICOSANE 163902 000112-95-8 90  
OCTACOSANE 232594 000000-00-0 86  
Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 86

165 26.930 0.25 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 72  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 72  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 72



166 27.106 0.17 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 64  
Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane 220176 055282-12-7 64  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 64

167 27.183 0.23 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 91  
EICOSANE 163904 000000-00-0 91  
N-EICOSANE 163902 000112-95-8 83

168 27.249 0.45 C:\Database\WILEY275.L  
OCTACOSANE 232594 000000-00-0 90  
Octacosane (CAS) \$\$ n-Octacosane 232590 000630-02-4 90  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 90

169 27.340 0.41 C:\Database\WILEY275.L  
Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 74  
Nonadecane (CAS) \$\$ n-Nonadecane 151980 000629-92-5 72  
Hentriacontane (CAS) \$\$ Untriacontane 246864 000630-04-6 72  
ane \$\$ n-Hentriacontane

170 27.387 0.10 C:\Database\WILEY275.L  
Docosane (CAS) \$\$ n-Docosane \$ C2 186056 000629-97-0 62  
2H46 STANDARD \$\$ Normal-docosane  
Heptadecane, 9-octyl- (CAS) \$\$ 9-N 212918 007225-64-1 59  
-OCTYLHEPTADECANE  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 58

171 27.806 0.12 C:\Database\WILEY275.L  
Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 87  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 87  
Octadecane (CAS) \$\$ n-Octadecane \$ 139439 000593-45-3 81  
\$ Octadecan

172 28.273 0.22 C:\Database\WILEY275.L  
Heneicosane (CAS) \$\$ n-Heneicosane 175419 000629-94-7 83  
Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 80  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 74

173 28.330 0.04 C:\Database\WILEY275.L  
Heptadecane (CAS) \$\$ n-Heptadecane 126473 000629-78-7 47  
\$\$ Normal-heptadecane  
Pentadecane, 2-methyl- (CAS) \$\$ 14 112858 001560-93-6 43  
-METHYLPENTADECANE \$\$ 2-Methylpentadecane  
Dodecane, 2-methyl-6-propyl- (CAS) 112878 055045-08-4 43  
\$\$ 2-METHYL-6-PROPYLDODECANE

174 28.421 0.09 C:\Database\WILEY275.L  
Octadecane, 3-ethyl-5-(2-ethylbutyl)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane 220176 055282-12-7 38  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Tridecanol, 2-ethyl-2-methyl- 128189 000000-00-0 35  
Hexacosane (CAS) \$\$ n-Hexacosane 220198 000630-01-3 35

175 28.502 0.09 C:\Database\WILEY275.L

Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 62  
 Eicosane, 7-hexyl- (CAS) \$\$ 7-n-He 220184 055333-99-8 53  
 xyleicosane  
 Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 52

176 28.706 0.43 C:\Database\WILEY275.L  
 PENTACOSANE 212928 000000-00-0 80  
 Pentacosane (CAS) \$\$ n-Pentacosane 212922 000629-99-2 80  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 72

177 28.783 0.20 C:\Database\WILEY275.L  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 81  
 2H46 STANDARD \$\$ Normal-docosane  
 Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 74  
 Eicosane (CAS) \$\$ n-Eicosane 163885 000112-95-8 74

178 28.844 0.15 C:\Database\WILEY275.L  
 Heneicosane (CAS) \$\$ n-Heneicosane 175422 000629-94-7 83  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 83  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 83

179 28.940 0.20 C:\Database\WILEY275.L  
 Heptacosane (CAS) \$\$ n-Heptacosane 226683 000593-49-7 87  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 80  
 Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80

180 28.973 0.09 C:\Database\WILEY275.L  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 83  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 83  
 2H46 STANDARD \$\$ Normal-docosane  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 83

181 29.035 0.86 C:\Database\WILEY275.L  
 Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 90  
 riacontane  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 90  
 2H46 STANDARD \$\$ Normal-docosane  
 Nonadecane (CAS) \$\$ n-Nonadecane 151980 000629-92-5 90

182 29.154 0.18 C:\Database\WILEY275.L  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 87  
 Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 86  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 86

183 29.230 0.14 C:\Database\WILEY275.L  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 72  
 Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 72  
 ane \$\$ n-Hentriacontane  
 Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 64

184 29.363 0.38 C:\Database\WILEY275.L  
 Heptadecane, 9-octyl- (CAS) \$\$ 9-N 212918 007225-64-1 53  
 -OCTYLHEPTADECANE  
 Tricosane (CAS) \$\$ n-Tricosane 195910 000638-67-5 53  
 Docosane (CAS) \$\$ n-Docosane \$\$ C2 186056 000629-97-0 53  
 2H46 STANDARD \$\$ Normal-docosane

185 29.454 0.73 C:\Database\WILEY275.L  
Eicosane, 3-methyl- (CAS) \$\$ 3-Met 175414 006418-46-8 72  
hyleicosane  
Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 72  
\$ Octadecan  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 64  
ane \$\$ n-Hentriacontane

186 29.683 0.14 C:\Database\WILEY275.L  
Nonahexacontanoic acid (CAS) \$\$ N- 275385 040710-32-5 38  
NONAHEXACONTANOIC ACID  
Nonadecane (CAS) \$\$ n-Nonadecane 151984 000629-92-5 38  
Cyclohexane, 1-(1,5-dimethylhexyl) 162220 056009-20-2 30  
-4-(4-methylpentyl)- (CAS) \$\$ OCTAHYDRO-.ALPHA.-CAMPHORENE

187 29.816 0.17 C:\Database\WILEY275.L  
Octadecane, 3-ethyl-5-(2-ethylbutyl) 220176 055282-12-7 74  
l)- (CAS) \$\$ 3-Ethyl-5-(2'-ethylbutyl)octadecane  
Tetratetracontane (CAS) \$\$ n-Tetra 269825 007098-22-8 64  
tetracontane  
Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 64  
riacontane

188 30.025 0.07 C:\Database\WILEY275.L  
5,6,8,9-TETRAMETHOXY-2-METHYLPEPER 214259 074199-94-3 59  
O(3,4,5-JK)-9,10-DIHYDROPHENANTHRA  
CENE \$\$ 4H-Dibenz[de,g]isoquinolin  
e, 5,6,6a,7-tetrahydro-1,2,9,10-tetramethoxy-5-methyl- (CAS)  
1-(2-trimethylsiloxy-1,1-dideuteri 161523 126210-55-7 32  
oviny)-4-trimethylsiloxy-benzene  
\$\$ Silane, trimethyl[4-[1-[(trimet  
hylsilyl)oxy]ethenyl-2,2-d2]phenoxy]-  
Tetrasiloxane, decamethyl- (CAS) \$ 185152 000141-62-8 14  
\$ Decamethyltetrasiloxane \$\$ [(CH3)3SiOSi(CH3)2]2O \$\$ KF 96L1.5

189 30.111 0.06 C:\Database\WILEY275.L  
Hexatriacontane (CAS) \$\$ n-Hexatri 260486 000630-06-8 68  
acontane \$\$ NOR-HEXATRIACONTANE  
Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 64  
riacontane  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 64

190 30.311 0.18 C:\Database\WILEY275.L  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 80  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 80  
ane \$\$ n-Hentriacontane  
Hexacosane (CAS) \$\$ n-Hexacosane 220199 000630-01-3 80

191 30.492 0.09 C:\Database\WILEY275.L  
Tetratriacontane (CAS) \$\$ n-Tetrat 256280 014167-59-0 72  
riacontane  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 72  
ane \$\$ n-Hentriacontane  
OCTACOSANE 232594 000000-00-0 72

|     |        |      |                                      |        |                |
|-----|--------|------|--------------------------------------|--------|----------------|
| 192 | 30.583 | 0.10 | C:\Database\WILEY275.L               |        |                |
|     |        |      | Tetratetracontane (CAS) \$\$ n-Tetra | 269826 | 007098-22-8 58 |
|     |        |      | tetracontane                         |        |                |
|     |        |      | Tetratriacontane (CAS) \$\$ n-Tetrat | 256280 | 014167-59-0 58 |
|     |        |      | riacontane                           |        |                |
|     |        |      | Tetratetracontane (CAS) \$\$ n-Tetra | 269825 | 007098-22-8 58 |
|     |        |      | tetracontane                         |        |                |
| 193 | 30.678 | 0.55 | C:\Database\WILEY275.L               |        |                |
|     |        |      | Pentacosane (CAS) \$\$ n-Pentacosane | 212919 | 000629-99-2 86 |
|     |        |      | Heptacosane (CAS) \$\$ n-Heptacosane | 226683 | 000593-49-7 83 |
|     |        |      | Eicosane, 2-methyl- (CAS) \$\$ 2-Met | 175409 | 001560-84-5 80 |
|     |        |      | hyleicosane \$\$ 19-Methyleicosane   |        |                |
| 194 | 30.811 | 0.14 | C:\Database\WILEY275.L               |        |                |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163878 | 000112-95-8 70 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163881 | 000112-95-8 70 |
|     |        |      | EICOSANE                             | 163904 | 000000-00-0 70 |
| 195 | 30.840 | 0.07 | C:\Database\WILEY275.L               |        |                |
|     |        |      | N-EICOSANE                           | 163902 | 000112-95-8 92 |
|     |        |      | EICOSANE                             | 163904 | 000000-00-0 91 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163881 | 000112-95-8 83 |
| 196 | 30.878 | 0.10 | C:\Database\WILEY275.L               |        |                |
|     |        |      | Heptadecane, 9-octyl- (CAS) \$\$ 9-N | 212918 | 007225-64-1 72 |
|     |        |      | -OCTYLHEPTADECANE                    |        |                |
|     |        |      | Docosane, 11-decyl- (CAS) \$\$ 11-n- | 250413 | 055401-55-3 72 |
|     |        |      | Decyldocosane \$\$ 11-NOR-DECYLD     |        |                |
|     |        |      | DOCOSANE                             |        |                |
|     |        |      | Hentriacontane (CAS) \$\$ Untriacont | 246864 | 000630-04-6 68 |
|     |        |      | ane \$\$ n-Hentriacontane            |        |                |
| 197 | 30.930 | 0.19 | C:\Database\WILEY275.L               |        |                |
|     |        |      | N-EICOSANE                           | 163902 | 000112-95-8 95 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163881 | 000112-95-8 89 |
|     |        |      | EICOSANE                             | 163904 | 000000-00-0 86 |
| 198 | 30.978 | 0.57 | C:\Database\WILEY275.L               |        |                |
|     |        |      | Tricosane (CAS) \$\$ n-Tricosane     | 195910 | 000638-67-5 87 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163882 | 000112-95-8 86 |
|     |        |      | N-EICOSANE                           | 163902 | 000112-95-8 86 |
| 199 | 31.040 | 0.30 | C:\Database\WILEY275.L               |        |                |
|     |        |      | EICOSANE                             | 163904 | 000000-00-0 91 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163882 | 000112-95-8 91 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163881 | 000112-95-8 83 |
| 200 | 31.225 | 0.22 | C:\Database\WILEY275.L               |        |                |
|     |        |      | N-EICOSANE                           | 163902 | 000112-95-8 90 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163882 | 000112-95-8 90 |
|     |        |      | EICOSANE                             | 163904 | 000000-00-0 90 |
| 201 | 31.268 | 0.34 | C:\Database\WILEY275.L               |        |                |
|     |        |      | N-EICOSANE                           | 163902 | 000112-95-8 93 |
|     |        |      | EICOSANE                             | 163904 | 000000-00-0 91 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163882 | 000112-95-8 91 |

|     |        |      |                                                                        |        |                |
|-----|--------|------|------------------------------------------------------------------------|--------|----------------|
| 202 | 31.335 | 0.49 | C:\Database\WILEY275.L                                                 |        |                |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163881 | 000112-95-8 86 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163882 | 000112-95-8 80 |
|     |        |      | EICOSANE                                                               | 163904 | 000000-00-0 80 |
| 203 | 31.697 | 0.09 | C:\Database\WILEY275.L                                                 |        |                |
|     |        |      | Phenol, 2,2'-methylenebis[6-(1,1-d                                     | 206103 | 000119-47-1 86 |
|     |        |      | imethylethyl)-4-methyl- (CAS) \$\$ 2                                   |        |                |
|     |        |      | ,2'-Methylenebis(4-methyl-6-tert-b                                     |        |                |
|     |        |      | utylphenol) \$\$ BKF \$\$ AO 1 \$\$ S 67                               |        |                |
|     |        |      | \$\$ CAO 5 \$\$ CAO 14 \$\$ CAO-14 \$\$ A                              |        |                |
|     |        |      | O 2246 \$\$ A-22-46 \$\$ NG 2246 \$\$ A                                |        |                |
|     |        |      | 22-46 \$\$ MBP 5 \$\$ 2,2'-METHYLENE-BIS(6-T-BUTYL-P-CR                |        |                |
|     |        |      | 4-Benzylamino-1-methyl-3-phenyl-qu                                     | 206082 | 083609-76-1 83 |
|     |        |      | inolin-2(1H)-one \$\$ 2(1H)-Quinolin                                   |        |                |
|     |        |      | one, 1-methyl-3-phenyl-4-[(phenylmethyl)amino]- (CAS)                  |        |                |
|     |        |      | Bis(3-tert-butyl-2-hydroxy-5-methy                                     | 206108 | 000000-00-0 38 |
|     |        |      | lphenyl)methane                                                        |        |                |
| 204 | 32.040 | 0.10 | C:\Database\WILEY275.L                                                 |        |                |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163884 | 000112-95-8 84 |
|     |        |      | N-EICOSANE                                                             | 163902 | 000112-95-8 42 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163877 | 000112-95-8 42 |
| 205 | 32.097 | 0.15 | C:\Database\WILEY275.L                                                 |        |                |
|     |        |      | EICOSANE                                                               | 163904 | 000000-00-0 55 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163882 | 000112-95-8 55 |
|     |        |      | Octacosane (CAS) \$\$ n-Octacosane                                     | 232590 | 000630-02-4 46 |
| 206 | 32.192 | 0.71 | C:\Database\WILEY275.L                                                 |        |                |
|     |        |      | 1-ethoxy-2-aminocarbonyl-1-aza-cyc                                     | 20371  | 000000-00-0 35 |
|     |        |      | lopropane                                                              |        |                |
|     |        |      | 1H-Indole, 2-methyl- (CAS) \$\$ 2-Me                                   | 21492  | 000095-20-5 32 |
|     |        |      | thylindole \$\$ SKATOLE \$\$ Indole, 2-methyl- \$\$ 2-Methyl-1H-indole |        |                |
|     |        |      | ISOPROPYL 2-BENZYL-2-PROPENYLETHER                                     | 74585  | 000000-00-0 25 |
| 207 | 32.325 | 0.36 | C:\Database\WILEY275.L                                                 |        |                |
|     |        |      | N-Carbomethoxy-4-(hydroxymethyl)in                                     | 92289  | 089875-39-8 43 |
|     |        |      | doline                                                                 |        |                |
|     |        |      | 1,4-DIPHENYL-2-BUTENE                                                  | 94225  | 001142-21-8 35 |
|     |        |      | 5-Phenyl-6-hepten-1-ol                                                 | 74572  | 023431-45-0 22 |
| 208 | 32.425 | 0.59 | C:\Database\WILEY275.L                                                 |        |                |
|     |        |      | Pentacosane (CAS) \$\$ n-Pentacosane                                   | 212919 | 000629-99-2 64 |
|     |        |      | Eicosane, 3-methyl- (CAS) \$\$ 3-Met                                   | 175413 | 006418-46-8 64 |
|     |        |      | hyleicosane                                                            |        |                |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane                                         | 163884 | 000112-95-8 64 |
| 209 | 32.511 | 0.47 | C:\Database\WILEY275.L                                                 |        |                |
|     |        |      | HEPTADECANE                                                            | 126483 | 000000-00-0 81 |
|     |        |      | Heptadecane (CAS) \$\$ n-Heptadecane                                   | 126473 | 000629-78-7 42 |
|     |        |      | \$\$ Normal-heptadecane                                                |        |                |
|     |        |      | Heptadecane (CAS) \$\$ n-Heptadecane                                   | 126472 | 000629-78-7 42 |
|     |        |      | \$\$ Normal-heptadecane                                                |        |                |

210 32.621 0.18 C:\Database\WILEY275.L  
Dotriacontane (CAS) \$\$ n-Dotriacon 250415 000544-85-4 74  
tane \$\$ Bicetyl \$\$ Tris(trimethyls  
ilyl)ether, methyl ester of ethyl  
anthranilate azo pigment(.alpha.z)  
of bilivubin-1x.alpha. 2-O-acyl glucuronide  
Octacosane (CAS) \$\$ n-Octacosane 232591 000630-02-4 74  
Eicosane (CAS) \$\$ n-Eicosane 163883 000112-95-8 68

211 32.697 0.60 C:\Database\WILEY275.L  
Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 86  
N-EICOSANE 163902 000112-95-8 83  
Octadecane (CAS) \$\$ n-Octadecane \$ 139444 000593-45-3 80  
\$ Octadecan

212 32.740 0.36 C:\Database\WILEY275.L  
Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 89  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 76  
ane \$\$ n-Hentriacontane  
N-EICOSANE 163902 000112-95-8 74

213 32.954 0.46 C:\Database\WILEY275.L  
Docosane, 11-decyl- (CAS) \$\$ 11-n- 250413 055401-55-3 68  
Decyldocosane \$\$ 11-NOR-DECYLDOSANE  
Hentriacontane (CAS) \$\$ Untriacont 246864 000630-04-6 64  
ane \$\$ n-Hentriacontane  
Pentacosane (CAS) \$\$ n-Pentacosane 212919 000629-99-2 59

214 33.021 0.40 C:\Database\WILEY275.L  
Heptacosane (CAS) \$\$ n-Heptacosane 226684 000593-49-7 87  
Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 87  
Triacontane (CAS) \$\$ n-Triacontane 242802 000638-68-6 86

215 33.068 0.22 C:\Database\WILEY275.L  
EICOSANE 163904 000000-00-0 90  
Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 90  
Eicosane (CAS) \$\$ n-Eicosane 163881 000112-95-8 90

216 33.345 0.10 C:\Database\WILEY275.L  
2,4-Cyclohexadien-1-one, 3,5-bis(1 107918 054965-43-4 38  
,1-dimethylethyl)-4-hydroxy- (CAS)  
\$\$ 3,5-DI-T-BUTYL-1,2-DIHYDROBENZOQUINONE  
Tetrasiloxane, decamethyl- (CAS) \$ 185153 000141-62-8 38  
\$ Decamethyltetrasiloxane \$\$ [(CH3)3SiOSi(CH3)2]2O \$\$ KF 96L1.5  
2-Propen-1-one, 3-(4-methylphenyl) 108629 004224-87-7 32  
-1-phenyl- (CAS) \$\$ Chalcone, 4-me  
thyl- \$\$ 4-Methylchalcone \$\$ p-Met  
hylchalcone \$\$ Phenyl p-methylstyr  
yl ketone \$\$ (4-Methylbenzylidene)  
acetophenone \$\$ 3-(P-METHYLPHENYL)-1-PHENYLPROPENONE

217 33.711 0.01 C:\Database\WILEY275.L  
EICOSANE 163904 000000-00-0 90  
Eicosane (CAS) \$\$ n-Eicosane 163882 000112-95-8 90  
N-EICOSANE 163902 000112-95-8 89

|     |        |      |                                      |        |             |    |
|-----|--------|------|--------------------------------------|--------|-------------|----|
| 218 | 33.759 | 0.21 | C:\Database\WILEY275.L               |        |             |    |
|     |        |      | Nonadecane (CAS) \$\$ n-Nonadecane   | 151980 | 000629-92-5 | 59 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163881 | 000112-95-8 | 59 |
|     |        |      | NONADECANE                           | 152008 | 000000-00-0 | 59 |
| 219 | 33.873 | 0.05 | C:\Database\WILEY275.L               |        |             |    |
|     |        |      | N-EICOSANE                           | 163902 | 000112-95-8 | 38 |
|     |        |      | Nonahexacontanoic acid (CAS) \$\$ N- | 275385 | 040710-32-5 | 38 |
|     |        |      | NONAHEXACONTANOIC ACID               |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163878 | 000112-95-8 | 35 |
| 220 | 33.935 | 0.03 | C:\Database\WILEY275.L               |        |             |    |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163881 | 000112-95-8 | 89 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163884 | 000112-95-8 | 83 |
|     |        |      | Eicosane (CAS) \$\$ n-Eicosane       | 163879 | 000112-95-8 | 64 |