Characterization of the chemical composition of Adenostemma lavenia (L.) Kuntze and Adenostemma platyphyllum Cass

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Abstract. The purpose of this study was to characterize the chemical compounds of Adenostemma lavenia (L.) Kuntze (Al) and Adenostemma platyphyllum Cass (Ap) using Pyrolysis-gas chromatography/mass spectrometry (Py-GCMS) and proximate analysis. Two species of Adenostemma samples (roots, stem and leaves) about 1 mg was pyrolyzed directly at the optimum temperature of 600°C. Py-GCMS was relatively fast, easy to use and without samples preparation and identification of the chemical compounds was carried out by comparison of the mass spectra obtained with those stored in Wiley 7th libraries. The data of proximate analysis were statistically analysed using Friedman test followed and hierarchical cluster analysis (HCA) for data of Py-GCMS. The result of proximate analysis showed that A. lavenia (L.) Kuntze (Al) and A. platyphyllum Cass (Ap) contained 8.27% (Al) and 9.18% (Ap) of water, 11.52% (Al) and 17.84% (Ap) of protein, 5.67% (Al) and 6.33% (Ap) of fat, and 17.32% (Al) and 19.94 (Ap) of ash. Amines, aldehydes, fatty acids, terpenoids-steroids, alkaloids, aromatic and aliphatic hydrocarbons, phenolic, and oligopeptides as part of 125 chemical compounds of each species are identified by Py-GCMS analysis. Hierarchical cluster analysis of pyrolysis products indicate not similitary of major chemical compounds of two Adenostemma species.

Keywords : Adenostemma lavenia, Adenostemma platyphyllum, Py-GCMS, Friedman test, hierarchical cluster analysis

1. Introduction
The study of Adenostemma biology and ecology has been receiving growing attention worldwide [1-7], but study of identification basic ecological relationships and chemical compounds is low. Recent studies have found 11-hydroxilated kauranic acids [8], kaurane [9, 10], α-cubebene, caryophyllene [10], flavanoids and alkaloids [11]. The chemical composition of Adenostemma differs depending on species, growth environment and season [12-16, 18], age and plant parts [17], physiological variations, environmental conditions, geographic variations, genetic factors and evolution [19].

So far, several methods have been developed to analyze the chemical compounds of Adenostemma. Phytochemical analysis [11], spectrographic [7, 8], high performance liquid chromatography (HPLC) [8, 9] were used to investigate the chemical compounds of Adenostemma. However, troublesome pretreatments are necessary for all the above methods prior to the final analysis such as solvent extraction, purification, and derivatization. Most of the studies were limited to some components of interest, particularly the flavonoids, lacking of a whole chemical composition analysis. Therefore, it is meaningful to develop a simple, rapid and sensitive method for characterization of the whole chemical composition in Adenostemma.

Recently, py-GCMS has been used extensively in the characterization of both low and high molecular components in various natural products. This technique yields a pyrogram consisting of the characteristic peaks of constituents in the given natural product without any pretreatment. Py-GCMS has been
performed for accurate determination of terpenoids, alcohols in volatile constituents in *Houttuynia cordata* Thunb [16], phenolic compounds in origanum heracleoticum [17], and terpenic acids, aleuritic acid, fatty acids in natural resin shelleac [18]. Organic compounds in plants are divided into two main groups, nitrogen-containing (alkaloids, non-protein amino acids, amines, cyanogenic glycosides, glucosinolates, alkamides, lectins, peptides, polypeptides) and without nitrogen (terpenoids, flavonoids, tannins, phenylpropanoids, lignin, coumarins, lignans, Polycetylenes, fatty acids, waxes, Polyketides, Carbohydrates, organic acids) [20].

In this study, Py–GCMS was first applied to analysis of chemical composition in *Adenostemma* without any cumbersome pretreatment. Furthermore, two species samples obtained from The northern slope of Dieng plateau were also compared, based on the chemical compound of *Adenostemma*. The aim of this paper is to analyze and compare the chemical compositions of two *Adenostemma* species using destructive analytical methods.

### 2. Material and Method

#### 2.1 Adenostemma sampling

Fresh *Adenostemma* material from two species was collected in the growing season of 2016 in north slope Dieng plateau (07°3’20.29” - 7°10’25.09” N; 109°40’21.33” – 109°36’20.09” E; 200 – 1,000 m amsl) in tropical rain forest (Java, Indonesia). Only living material with green leaves and fresh flower without signs of decomposition was collected. Samples were identified at Center for Plant Conservation Botanic Garden – Indonesian Institute of Science as *Adenostemma platyphyllum* Cass. and *Adenostemma lavenia* (L.) Kuntze.

#### 2.2 Sample preparation

The approximate amount of collected adenostemma material was 50 g dry weight species. The samples was cleaned. The roots, stems and leaves were cut out from some plants; others were kept intact. Afterwards, the roots (Ap1 and A11), stems (Ap2 and Al2), leaves (Ap3 and Al3) and entire plants (Ap and Al) were oven-dried separately at 40°C until dry weight was constant and were stored at 5°C in air-tight containers before analysis. Samples for proximate analysis and Py-GCMS analysis were dried, ground with a grinder and sieved through a 40 mesh [21].

#### 2.3 Proximate Analysis

The proximate analysis (water, proteins, crude fats, ash, carbohydrates and total dietary fiber) of all the samples carried out in triplicate [22]. The water and ash were determined using gravimetric method. The nitrogen value was determined by micro-Kjeldahl method described by [23] involving digestions, distillation and finally titration of the sample. The nitrogen value was converted to protein by multiplying a factor of 6.25. The crude fat was determined by soxhlet extraction method, employing a n-hexane extraction. Carbohydrate was determined by difference method. Carbohydrate was determined when the sum of the percentages of water, ash, crude protein, and crude fat were subtracted from 100. All the proximate values were reported in percentage [22].

#### 2.4 The Pyrolysis GCMS Analysis

The chemical compounds in sample were identified by a Pyrolysis GCMS (Shimadzu GCMS-QP2010; Shimadzu Corporation, Kyoto, Japan). One milligram ±0.05 mg of powdered sample was introduced into a pyrolyzer (PY-2020iS). Pyrolysis was performed at a temperature of 600°C with a ramp rate of 20°C/ms with a hold time of 10 s. The pyrolyzer was directly interfaced with a GCMS. A capillary column (RTX-5MS) with 60 m length, 0.25 mm internal diameter and a 0.25 μm stationary phase film was used. The volatiles were trapped on adsorbent trap before being desorbed at 280 °C onto a heated transfer line which was held at 280°C. The purge flow of helium UHP to remove any oxygen from the sample, prior to pyrolysis, was set to 3 ml/min and a split ratio 1:50. The injector temperature was set at 280ºC, ion source 200°C. The identification of the chemical compounds was carried out by comparison of the mass spectra obtained with those stored in Wiley 7th libraries [24].

#### 2.5 Data Analysis

The data of proximate analysis were statistically analysed using Friedman test followed with Post Hoc test using Wilcoxon Signed Rank test, and hierarchical cluster analysis (HCA) was used to identify relatively homogeneous clusters of samples based on their similarity [25] in chemical compound *Adenostemma*’s. Cluster analysis is technique for grouping object into clusters so that object in same cluster. A cluster are more like one another than they are like object in other cluster [26]. Cluster analysis involves at least two step. The first is the measurement of some form of similarity to determine how many groups really exist in the sample [26, 27]. The second step is to profile the variable to determine their composition [28]. Beginning with N clusters consisting exactly of two entities, the similarity matrix is searched for the most
similar pair of clusters and the number of clusters is reduced by one by merging the most similar pair of clusters with the minimum increase in the total within group error sum of squares [21]. The analysis was performed using IBM SPSS Statistics 23 version software.

| Table 1. List of studied Adenostemma species with codes and their growth conditions |
|--------------------|-----------------|
| Species            | Code            |
| A. platyphyllum    | Ap              |
| roots              | A0              |
| stems              | A1              |
| leaves             | A2              |
| A. lavenia         | A1              |
| roots              | A1              |
| stems              | A2              |
| leaves             | A3              |
| Apl. platyphyllum  | A1              |
| roots              | A1              |
| stems              | A2              |
| leaves             | A3              |

3. Results and discussion

3.1 Proximate analysis

The result of proximate analysis shows variant concentration of chemical compounds (water, protein, fat, ash, carbohydrate and total dietary fiber). Based on Friedman test analysis, the water contents of samples are different. The water contents of whole A. platyphyllum were higher than A. lavenia. Considering the overall percentage of water composition, it was highest in A. platyphyllum stems followed by A. platyphyllum roots, A. platyphyllum leaves and A. lavenia leaves while other had comparatively lesser composition (Table 2). However, the water in dry powder of stems and roots of A. lavenia are the highest.

| Code | Fresh Water | Powder Water | Protein* | Fat* | Ash* | Carbohydrate* | Fiber, total dietary* |
|------|-------------|--------------|----------|------|------|---------------|-----------------------|
| Ap   | 89.54 b     | 9.18 d       | 17.84 f  | 6.33 d | 19.94 | 55.89 b       | 2.41 b                |
| Ap1  | 90.66 d     | 7.45 b       | 8.85 a   | 3.61 b | 16.47 | 71.07 d       | 6.27 f                |
| Ap2  | 91.73 e     | 9.39 f       | 12.49 c  | 7.31 f | 21.24 | 58.96 c       | 2.36 a                |
| Ap3  | 89.64 c     | 7.17 a       | 18.38 g  | 10.50 g | 21.00 | 50.12 a       | 2.62 c                |
| A1   | 88.56 a     | 8.27 c       | 11.52 e  | 5.67 c | 17.32 | 68.41 c       | 2.62 c                |
| A11  | 89.35 b     | 9.58 g       | 11.52 b  | 6.71 e | 15.05 | 67.64 d       | 6.75 g                |
| A12  | 90.61 c     | 10.36 h      | 10.60 b  | 2.75 a | 17.32 | 68.41 c       | 3.40 d                |
| A13  | 88.82 a     | 9.34 e       | 13.37 d  | 10.93 h | 16.92 | 58.79 d       | 3.72 e                |

Friedman test

Chi-Square 15.667
Df 7
Asymp. Sig 0.028a

Note: Data are means from three samples. *: dry basis; ns: non-significant, s: significant at P 0.05 Friedman test.

The protein contents of each species and organs are different. Considering the overall percentage of protein composition, it was highest in A. platyphyllum leaves by whole of A. platyphyllum. Whole of A. lavenia, and A. lavenia leaves while other had comparatively lesser composition (Table 2). Considering the result crude fat A. lavenia leaves and A. platyphyllum leaves had prominent levels compared to other plant organs. Considering the resulted achieved from ash analysis. The ash contents of each species are not different. While analyzing the carbohydrate contents in the samples. The results showed that A. platyphyllum roots. Whole of A. lavenia, A. lavenia roots and A. lavenia stems had highest concentration of carbohydrate to other plant organs (Table 2).

Based on the proximate analysis it is known that two species of Adenostemma exhibit different characteristics, except ash content. Different concentrations of chemical compounds are caused by differences in species, plant organs and growing places of each samples [20]. The sample of this study was
obtained from wild forests that have different ecology, macro and microclimates (temperature, water, humidity, sunlight intensity).

3.2 Pyrolysis GCMS Analysis

Py-GCMS is a suitable method for the quantitative and qualitative analysis of complex mixtures with high efficiency, precision, and simplicity [30, 31]. In a merbau extractives pyrolysis study, flash pyrolysis-GCMS used in structure analysis provided information at the presence of phenolic forms [24]. Pyrolysis-gas chromatography/mass spectrometry was used to characterize the chemical composition of *A. platyphyllum* and *A. lavenia*. The result of Py-GCMS analysis to those sample found 125 chemical compounds. Among all, the 5 compounds dominant were: epoxycyclododecane, 4-allyl-2,6-dimethoxyphenol, Cis,Cis,Cis-8,11,14 eicosatrienoic acid, tetradecahydroanthracene, and levoglucosan. The chemical compounds in the studied two species *Adenostemma* can be seen in Appendix 1. GCMS analysis revealed the presence of terpenoids, phenolic compounds, alkaloids and fatty acids.

![Root of *A. platyphyllum*](image1)

![Root of *A. lavenia*](image2)

![Stem of *A. platyphyllum*](image3)

![Stem of *A. lavenia*](image4)

![Leaves of *A. platyphyllum*](image5)

![Leaves of *A. lavenia*](image6)

**Fig. 1.** Chromatogram py-GCMS of *Adenostemma platyphyllum* and *Adenostemma lavenia*

The presence of dominant product groups from each *Adenostemma* species is illustrated in Table 3. The pyrolysates of the studied *Adenostemma* species were dominated by phenolic compounds, lipid orginated compounds and N-bearing compounds. The dominant compounds in *A. platyphyllum* were phenolic compounds and originated lipids (fatty acid). The dominant compounds in *A. lavenia* were N-bearing compounds, alkaloid, aromatic compounds, and terpenoid-steroid. Abundant aromatic compounds products (phenol and derivate) confirm the importance of phenol in the structural make-up of *Adenostemma*. As one of the main products, *A. lavenia* species contained more terpenoid-steroid and alkaloid in comparison with *A. platyphyllum* species. *A. lavenia* species has a higher alkaloid compounds than *A. platyphyllum*.

4- Allyl-2,6-Dimethoxyphenol (C11H14O3), coniferyl alcohol (C10H12O3), and linoleic acid (C18H32O2) were the dominant phenolics found in *Adenostemma* species. 4-Allyl-2,6-Dimethoxyphenol was phenol detected in the largest quantity (14.2%). 4-O-[3-Acetyl-1-(Trimethylsilyl)-1h-Indolyl]-1h-Indolyl]-D-Glucose (C35H45N2O9; 2.14%) and 5h-1-Pyrindine (C8H7N; 5.07%) were the alkaloid found in the leaf tissue of *A. lavenia*. 3-methylindole (C9H9N; 0.93%) and 1-cyano-3-methylisoquinoline (C11H8N2; 1.83%) were the alkaloid found in the stem tissue of *A. lavenia*. 6,7-Dihydro-3-Nitro-5h-Cyclopenta[1B]Pyridin-2(1h)-One (C8H9N2O7; 2.94%) and 5,10-Diethoxy-2,3,7,8-Tetrahydro-1h,6h-Dipyrrrolo[1,2-A;1',2'-D] Pyrazine (C14H22N2O2; 4.0%) were found in the root tissue of *A. lavenia*. The alkaloids were detected in *A. platyphyllum* only two substance i.e. 3-Methylindole (1.62%) and 2-O-[3-Acetyl-1-(Trimethylsilyl)-1h-Indolyl]-D-Glucose (C35H45N2O9; 1.38%).
Table 3. Relative abundance (%) of the main groups of pyrolysis products of *Adenostemma*.

| Metabolite Group | N   | Alk  | MA  | C   | Al  | Alc | Ar  | Ph  | Lp  | TS  |
|------------------|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|
| Al1              | 13.39 | 6.94 | 6.11 | 5.44 | 0   | 2.61 | 3.68 | 44.84 | 11.9 | 5.08 |
| Al2              | 27.97 | 2.76 | 0   | 0   | 0   | 3.93 | 10.71 | 0   | 44.22 | 10.41 |
| Al3              | 11.88 | 11.24 | 3.93 | 1.51 | 1.41 | 0   | 12.59 | 4.37 | 29.62 | 23.46 |
| Ap1              | 2.55  | 1.08 | 4.69 | 2.01 | 0   | 2.37 | 72.45 | 14.88 | 0   |      |
| Ap2              | 3.1   | 0    | 0   | 0   | 5.25 | 8.66 | 0   | 62.74 | 18.51 | 1.73 |
| Ap3              | 12.06 | 4.27 | 1.63 | 1.41 | 7.21 | 17.22 | 13.72 | 7.42 | 18.23 | 16.82 |

Note: Code of studied species as in Table 1. N, N-bearing compounds (except alkaloids); Alk, Alkaloids; MA, multi-origin aliphatic compounds with C≤6; C, furan originated from carbohydrates, pyran and cyclopentene derivatives; Al, aliphatic compounds with C>6; Alc, Alcohol; Ar, aromatic compounds (except phenolic compounds); Ph, phenolic compounds; Lp, compounds originated from lipids (except terpenoid, steroid); TS, terpenoid-steroid.

Those compounds support the healing of wound or infection, antioxidant and also act as antibacterial agents. Naturally occurring phenolic compounds have been shown to scavenge active oxygen species and to effectively prevent oxidative cell damage [32]. Inhibitory effects of phenolic compounds containing allyl groups were similar to those of flavonoids [33]. 2,6-diphenyl-piperidine, and 5,10-dioxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo[1,2- a;1 -d] pyrazine (a member of alkaloids) also acts as antifungal agent [34]. A considerable amount of 3-methylpyridine is used as a starting material for pharmaceuticals and agrochemicals [42] and 4-cyano-3-methylisoquinoline as potential antimalarial agents [35].

Fig. 2. Cluster analysis of amounts of pyrolysis products of *Adenostemma*.

Note: Ap1: root of *A. platyphyllum*; Ap2: stem of *A. platyphyllum*; Ap3: leaves of *A. platyphyllum*; Al1: root of *A. lavenia*; Ap2: stem of *A. lavenia*; Ap3: leaves of *A. lavenia*.

3.3 Cluster Analysis

Cluster analysis of pyrolysis products indicates not similitary of major chemical compounds of the studied *Adenostemma* species (Fig. 2). For example, despite the evident similarity in plants organs composition, the *A. platyphyllum* species were grouped together. For example, despite the evident similarity in plants organs composition, the *A. platyphyllum* species were grouped together. The decisiveness of this classification is reflected in the dendrogram (fig. 2). The initial splitting of the tree forms to two clusters. The top contains *A. platyphyllum*. The bottom contains *A. lavenia*. The *A. platyphyllum* roots and *A. platyphyllum* stems are each more similar than the *A. platyphyllum* leaves. The chemical compounds in chemical taxonomy of *Adenostemma* can be seen in Appendix 1.

4. Conclusions

The chemical compounds *A. lavenia* and *A. platyphyllum* are significantly different. Pyrolysis GCMS showed that the major compound of *A. platyphyllum* is aromatic compounds (phenolic) with a concentration of 26.4% and *A. lavenia* is originated lipids and terpenoid steroid with a concentration of...
29.7% and 15.8%. Chemical compounds of *A. platyphyllum* and *A. lavenia* as potential antimicrobial, antioxidant and anti-inflammation agent.

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Appendix 1. Peak assignments and relative abundance (%) of pyrolysis products of Adenostemma.

| R.Time | Name                                      | MG | WM | Formula          | Area1 | Area2 | Area3 | Area4 | Area5 | Area6 | Area7 | Area8 | Area9 | Area10 |
|--------|------------------------------------------|----|----|------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|
| 18.645 | 2-Methyl-4-Pyrrole-Indole               | Al |     | C6H5N          | 1,69  |       |       |       |       |       |       |       |       |        |
| 21.225 | 4,5-Norflavone (Cas)                    | Al |     | C9H6           | 5,25  |       |       |       |       |       |       |       |       |        |
| 21.333 | Cyclomuscene                            | Al | 152 | C11H12O         | 1,41  |       |       |       |       |       |       |       |       |        |
| 22.758 | 1-Chloromethyl-1-Yne                    | Al |     | C9H12C1        | 1,82  |       |       |       |       |       |       |       |       |        |
| 22.903 | Cyclomuscene, 3-Methylene-4-1,2-Propiolanyl | Al | C9H12           | 1,34  |       |       |       |       |       |       |       |       |        |
| 14.064 | N-Heptan                                 | Al |     | C7H14O         | 2,01  |       |       |       |       |       |       |       |       |        |
| 18.285 | N-Octanol                                | Al |     | C9H18O         | 2,16  |       |       |       |       |       |       |       |       |        |
| 3.322  | 3,5-Diethylphenol                       | Al |     | C9H18O         | 2,77  | 4,69  |       |       |       |       |       |       |       |        |
| 14.782 | 5,8-Heptadione-2-OH, 2,6-Dimethyl-       | Al |     | C9H18O         | 1,83  |       |       |       |       |       |       |       |       |        |
| 16.396 | Hexa-2,4-Diyne-1-Oxyl                    | Al | C8H16O         | 1,52  |       |       |       |       |       |       |       |       |       |        |
| 19.438 | 3-Nonyl-2-01(Cas)                       | Al |     | C9H18O         | 1,93  |       |       |       |       |       |       |       |       |        |
| 20.086 | Cy-8-Octadecene-1-01                    | Al |     | C10H20O        | 3,86  |       |       |       |       |       |       |       |       |        |
| 20.358 | Oxolin                                   | Al |     | C9H18O         | 5,89  |       |       |       |       |       |       |       |       |        |
| 20.395 | Phyto                                    | Al |     | C20H16O        | 3,77  |       |       |       |       |       |       |       |       |        |
| 21.229 | Z-D8-Pentalone-1-01                     | Al | 226 | C10H80         | 2,61  |       |       |       |       |       |       |       |       |        |
| 24.076 | N-Isoumarone                             | Al | 298 | C12H20O        | 2,1   |       |       |       |       |       |       |       |       |        |
| 18.875 | Dodica-7-OI                             | Al |     | C12H20O        | 1,45  |       |       |       |       |       |       |       |       |        |
| 16.196 | 8h-1-Prusline                            | Alk | 117 | C9H7N         | 5,07  |       |       |       |       |       |       |       |       |        |
| 17.017 | 3-Methylphenol                          | Alk | 131 | C9H9N         | 0,93  |       |       |       |       |       |       |       |       |        |
| 17.064 | D-Glucose-4,6-[(3-Acetyl-1-Thymolyl)-1-b-Indoly]- | Alk | 126 | C32H62N2O7Si5 | 2,14  |       |       |       |       |       |       |       |        |
| 17.859 | D-Glucose-2,4-[(3-Acetyl-1-Thymolyl)-1-b-Indoly]- | Alk | 126 | C32H62N2O7    | 1,38  |       |       |       |       |       |       |       |        |
| 18.364 | 5,7-Dihydo-3-Nitro-3b-Cyclopenta(B)Pyridol(2)-8h-One | Alk | 180 | C9H8N2O2       | 2,94  |       |       |       |       |       |       |       |       |        |
| 21.523 | 5,10-Diethoxyl-2,3,7,8-Tetraldehyde-8h-Bdiperox(1,2)-2h-Di     | Alk | 250 | C14H22O2        | 4,00  |       |       |       |       |       |       |       |       |        |
| 22.245 | 1-Cyano-4methylisoquinoline             | Alk | 168 | C11H18N2       | 1,83  |       |       |       |       |       |       |       |       |        |
| 23.466 | 4-Benzyl-3-Methyl-6,7-Dihydro-b-Isoumarole| Alk | 14H8N2O2      | 1,27  |       |       |       |       |       |       |       |       |        |
| 14.55  | 3-Cyclohexol                            | Ar  |     | C9H16O         | 1,88  |       |       |       |       |       |       |       |       |        |
| 15.444 | Acyrtinin                               | Ar  |     | C9H18O         | 1,83  |       |       |       |       |       |       |       |       |        |
| 15.465 | O-Tolualdehyde                          | Ar  |     | C9H18O         | 0,66  |       |       |       |       |       |       |       |       |        |
| 16.413 | 4-Formylcysteine                        | Ar  |     | C7H14O         | 1,71  |       |       |       |       |       |       |       |       |        |
| 19.923 | Mesterf 1-Methylulide-4,Alpha-Methyl-   | Ar  |     | C12H14C5H11O10  | 2,08  |       |       |       |       |       |       |       |       |        |
| 21.215 | Biphenyl-3,4-Diethyl                   | Ar  | 166 | C12H22        | 7,54  | 3,41  |       |       |       |       |       |       |       |        |
| 21.829 | 5-Buta-2,3-Epoxy-3,6,8-Tetraldehyde-9h-2-Benzopyrro- | Ar  | 150 | C9H6O2        | 8,13  |       |       |       |       |       |       |       |        |
| 22.297 | Spirocyclobutene-1,12(2h)-Phenanthrene- | Ar  | 240 | C14H24        | 2,54  |       |       |       |       |       |       |       |        |
| 22.396 | 5-Nitro-2-benzanthracene                | Ar  | 206 | C14H14        | 3,17  |       |       |       |       |       |       |       |       |        |
| 22.451 | Anthracene-9,10-Diethoxy-(Cas)          | Ar  | 206 | C14H14        | 4,95  |       |       |       |       |       |       |       |       |        |
| 23.184 | 1-Iodo-4-Phenylbutyric2                 | Ar  | 312 | C14H17I        | 1,69  |       |       |       |       |       |       |       |       |        |
| 9.38   | Cyclopentone                            | C   |     | C5H8O       | 0,66  |       |       |       |       |       |       |       |       |        |
| 12.934 | Corylynn                                | C   | 112 | C6H8O2         | 5,44  | 2,43  |       |       |       |       |       |       |       |        |
| 12,936 | 2,5-Methans-2h-Fum(3,2-B)-4,1-One, Hexalhydro- | C   | 154 | C8H10O3       | 1,51  |       |       |       |       |       |       |       |        |
aliphatic compounds with C≤6; C, furan originated from carbohydrates. pyran and cyclopentene derivatives; Al. Alavenia
17-Acetoxy-19 kauranal
Cis,Cis,Cis-8,11,14-eicosatrienoic Acid
N-Hexatriacontane
Mannit, 5-Phenylpent-1-Yl-
Methyl Linolenate
Myristic Acid
Aceteugenol
Carvacrol
2,5-Dimethoxytoluene
M-Ethylphenol
O-Ethylphenol
Phenol, 4-Methoxy- (Cas)
1,4-Diaza-2,5-Dioxo-3-Isobutyl Bicyclo[4,3,0]Nonane
1-Cyclopentene-1-Carboxamide
1-Methyl-2-Cyanobenzene
2-Imidazolidinone, 1,3-Diethenyl-
2,3-Epoxybutane
Cyclohexyleicosane
2-Octenoic Acid (Cas)
Epoxycyclododecane
Palmitic Acid
Adacene 12
N-Dodecane
Oleic Acid
Carbazic Acid, 3-Pentylidene-, Ethyl Ester
13,308

N, N-bearing compounds (except alkaloids); Alk, Alkaloids; MA, multi-origin

14,897

N-Bentionic acid, 1,3-Dienes-

13,308

3-Methanol
N

13,179

Ammonium Carbamate

16,152

7-Cyclopent-9a-Cyclopentatriene

16,176

1-Methyl-2-Cyclohexene

15,375

2-Amino-4,5-Dihydroxyalcohol

19,806

N-Phenyl-N-Paraldehyde Hydrate

19,819

1-Cyclopentene-1-Carboxamide

16,208

1,8-Octadienamide

16,602

Palmitonitrile

15,335

1,4-Diazaoctane-2,5-Diols-3-Isobutyryl Bicyclo[4,3,0]Nonane

22,478

2,4-Diisocyanate

13,434

N,N-Diisopropylacetamide

14,682

2,3-Dihydrofuran

14,897

2-Methyl-4-Methylphenol

16,738

2,5-Dihydroxyacetone

16,161

Carvacrol

16,483

2,6-Dimethoxyphenol

16,625

2-Pyrrolidonitrile

17,363

2,3,6-Trimethoxybenzene

17,391

2,5-Dimethoxyphenyl Alcohol

17,458

Atractogen

18,028

Toluene, 3,4,5-Trimethoxy-

18,272

16-Acetyl-2,6-Di-Glucopyranosyl-L-Asparaginase

18,229

1,4-Hydroxy-2-Methoxy-

18,369

Methyl 2,4-Dimethoxybenzyl Acetate

18,657

4-Acetyl-2,6-Dimethoxyphenol

19,709

Myristic Acid

19,763

Acetylsaliclylate

19,866

3,4,5-Trimesitylbenzylalcohol

19,905

Cyclohexene, (Z)-

21,257

1,12-Tridecadiene

21,316

Amylbutyrolactone

21,457

Stearic acid-1,12-Undecanoyl(Al)Amphoropea(E)Cyclohexene-11-One, 12,15-Di-

21,707

12,15-Dihydroxytetradecane-4,7,10-Triene

22,417

Tricalciumhydronitrate

22,483

Methyl Linolenate

22,525

3-Methyl-2,4-Pentadiyne-1-Yl-

22,556

N-Hexanoic acid

12,668

L-Limonene

20,195

3,9-Dehydro-1,12,3,4,5,9-Hexahydroxy-Cyclopept

20,551

Isopropyl Biphenyl

21,803

N-Phenylacetamide

21,851

Cineole,Cis-8,11-4,4-noriostecinninic Acid

24,211

Spiro(Am87,3-En8,17-1,7-Cyclooctatetra-2,-one),3-hydroxy

25,720

7-Acetoxy-19-kauranol

38,938

Stigmaster-5,22-Dienone