

# Analysis of Chemical Constituents of Volatiles and Petroleum Ether Extract from the Branch of *Zanthoxylum bungeanum* by GC-MS

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The essential volatiles were extracted by water steam distillation and the petroleum ether extract was extracted with alcohol and then petroleum ether from the branch of <i>Zanthoxylum bungeanum</i> . The chemical constituents of essential volatiles and petroleum ether extract were analyzed by GC-MS and their relative contents were calculated by area normalization method. 45 peaks were obtained and 34						

60 peaks were obtained and 50 components were identified and the major components were organic acids, esters and alkanes.

Keywords: Zanthoxylum bungeanum, Volatiles, Petroleum ether, GC-MS.

## INTRODUCTION

The genus Zanthoxy lum L. consists of about 250 species<sup>1</sup>, which are mainly distributed in tropical and subtropical areas situated in Asia, America, Africa and Oceania<sup>2-6</sup>. In China, 45 species and 13 varieties are mainly distributed in south of the Yangtze river and southwest Provinces. Among them, 18 species are used as traditional Chinese medicine. The fruits, roots, branches, leaves of Zanthoxy lum L. are all medicine, which has been widely used for analgesia, anesthesia, antibacterial, pesticides and anti-tumor<sup>7,8</sup>. The plants of this genus are well known for containing several types of compounds, including volatile oil, alkaloids, amides, lignans, coumarins, fatty acids, flavones, terpenes, sterols and hydrocarbons<sup>9-13</sup>. Although many studies have shown the chemical constituents of Zanthoxy lum L extracted from the fruits or roots, there is little research on the compositions of branches. So the purpose of this study was to identify these compounds in the branches of Zanthoxy lum L. The gas chromatography-mass spectrometry (GC-MS) and computer spectrum search technique were used to identify the chemical composition of Zanthoxylum bungeanum. This study can provide test basis for the rational development and utilization of Zanthoxylum resources.

#### EXPERIMENTAL

The branches of *Zanthoxylum bungeanum* were collected from Hancheng city in the northwest of Shaanxi province in

September, 2011 in China. The fresh branches were dried in the shade at room temperature.

**Sample preparation:** Dried branches of *Zanthoxylum bungeanum* were cut into pieces. The volatile was extracted from the branches of *Zanthoxylum* (0.75 kg) by water steam distillation, then dried to pale yellow liquid using Na<sub>2</sub>SO<sub>4</sub>. 1 mL volatile was diluted to 5 mL with ethanol. Furthermore, the branches of Zanthoxylum (0.75 kg) were extracted with alcohol and then petroleum ether to get the petroleum ether extract. 20 mg of petroleum ether extract was dissolved in 10 mL of petroleum ether. All the solutions were filtered through a 0.45 µm filter.

**Apparatus and GC-MS condition:** The compositions were analyzed by an ISQ 110953 GC-MS system (Thermo Fisher Corp, USA). The condition was shown in the Table-1. Retention times were utilized as primary criterion for the peaks identification. Using the mass spectrometer as chromatographic detector offered additional data (P/N: 274, 102, 74 Thermo Data system) for the identification of the separated compounds. The identification method was reference standard compounds and compared the compositions isolated with the recorded spectra in MS library.

#### **RESULTS AND DISCUSSION**

Total gas chromatograms of volatiles and petroleum ether extract from branches of *Zanthoxylum bungeanum* were shown in Figs. 1 and 2. The relative contents of chemical constituents

TABLE-1 SELECTED PAPAMETERS OF CC MS CONDITION			
Parameter	5111CTT	Description	
Capillary column	CSPD 5MS (20 m	2 0 22 mm 0 22 um film 0 25 um) poly (5 % dinhanyl 05 % dimathyl siloyona)	
Capitally column	USDF-SIVIS (50 III	$\times$ 0.52 min, 0.52 µm min, 0.25 µm), pory (5 % diphenyi, 95 % dimetnyi shoxate).	
Carrier gas	Hellum		
Injection mode	Split		
Column flow	A: 2.1 mL/min	B: 1.4 mL/min	
Split ratio	A: 50:1	B: 10:1	
Injection temperature	250 °C		
Oven temperature progarm	A: Initial temperate	ure was 80 °C (hold time 1 min) then ramped at 10 °C/min to 280 °C (hold time 2 min).	
	B: Initial temperature was 80 °C then ramped at 3 °C/min to 260 °C (hold time 3 min), Again with ramped at		
	20 °C /min to 280 °C (hold time 3 min).		
Ionization energy	70 eV		
Scan range	A: 20-800 amu	B: 35-400 amu	
Event time	A: 0.5 s	B: 0.2 s	
Ionization source temperature	A: 200 °C	B: 260 °C	
Transmission line temperature	A: 250 °C	B: 280 °C	

<sup>a</sup>The GC-MS condition of the volatiles, <sup>b</sup>The GC-MS condition of the petroleum ether extract









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TABLE-2 MASS DATA OF 36 COMPOUNDS IDENTIFIED FROM VOLATILES					
Peak No.	Compounds	T <sub>R</sub> (min)	m.f.	m.w.	Area (%)
1	α-Pinene	4.717	C <sub>10</sub> H <sub>16</sub>	136	4.81
2	β-Pinene	5.575	$C_{10}H_{16}$	136	0.22
3	β-Myrcene	5.985	$C_{10}H_{16}$	136	6.74
4	Cymene	6.642	$C_{10}H_{14}$	134	0.18
5	β-Phellandrene	6.808	$C_{10}H_{16}$	136	2.91
6	1,5-Cyclooctadiene	6.858	$C_{10}H_{16}$	136	1.61
7	β- <i>trans</i> -Ocimene	7.092	$C_{10}H_{16}$	136	14.4
8	β- <i>cis</i> -Ocimene	7.375	$C_{10}H_{16}$	136	5.98
9	γ-Terpinene	7.608	$C_{10}H_{16}$	136	0.18
10	Linalyl alcohol	8.709	$C_{10}H_{18}$	138	0.46
11	Terpinene-4-ol	10.717	$C_{10}H_{18}$	138	0.46
12	Acetic acid, bornyl ester	13.675	$C_{12}H_{20}O_2$	196	0.24
13	Methyl nonyl ketone	13.983	$C_{11}H_{22}$	154	0.80
14	(-)-β-Elemene	16.800	$C_{15}H_{24}$	204	0.22
15	Caryophyllene	17.475	$C_{15}H_{24}$	204	12.4
16	α-Caryophyllene	18.308	$C_{15}H_{24}$	204	3.28
17	γ-Muurolene	18.892	$C_{15}H_{24}$	204	0.20
18	Tridecan-2-one	19.308	$C_{13}H_{26}$	182	0.61
19	(-)-α-Muurolene	19.500	$C_{15}H_{24}$	204	0.36
20	γ-Muurolene	19.792	$C_{15}H_{24}$	204	0.35
21	δ-Cadinene	20.042	$C_{15}H_{24}$	204	1.55
22	Germacra-1(10),4,7(11)-triene	20.808	$C_{15}H_{24}$	204	0.17
23	(-)-Spathulenol	21.175	$C_{15}H_{24}$	204	2.07
24	(-)-Caryophyllene oxide	21.258	$C_{15}H_{24}$	204	7.51
25	(-)-Globulol	21.408	$C_{15}H_{26}O$	222	0.41
26	Viridiflorol	21.575	$C_{15}H_{26}O$	222	0.40
27	Bicyclo[2.2.2]oct-2-ene,1,2,3,6-tetramethyl	21.633	$C_{12}H_{20}$	164	0.21
28	(-)-Caryophyllene oxide	21.858	$C_{15}H_{24}O$	220	1.64
29	4,7-Octadecadiynoic acid, methyl ester	22.008	$C_{19}H_{30}$	360	0.36
30	Widdrol	22.133	$C_{15}H_{26}O$	222	0.54
31	Torreyol	22.717	$C_{15}H_{26}O$	222	6.69
32	α-Copaene	22.783	$C_{15}H_{24}$	204	1.16
33	α-Cadinol	22.992	$C_{15}H_{26}O$	222	12.1
34	4-Bromo-1-naphthylamine	23.650	C <sub>15</sub> H <sub>24</sub> O	220	0.60
35	Sandaracopimaradiene	29.717	$C_{20}H_{32}$	272	0.24
36	Hexadecanoic acid	30.017	$C_{16}H_{32}O_{2}$	256	0.60

were calculated by area normalization method and the results were summarized in Tables 2 and 3.

Forty five peaks were obtained and 34 components were identified from the branches of *Zanthoxylum* by steam distillation, accounting for 95 % of the total of the volatiles (Fig. 1). According to the percentage contents of comparison, the main constituents were  $\beta$ -*trans*-ocimene(14.4 %), caryophyllene (12.4 %),  $\alpha$ -cadinol (12.1 %), (-) -caryophyllene oxide (7.51 %),  $\beta$ -myrcene (6.74 %) and torreyol (6.69 %). The major compositions of the petroleum ether were the terpenes, including 21 kinds of chemical constituents, accounting for 66.1 % of the total compounds. The alcohols included 8 kinds of compositions, accounting for 23.2 %. Furthermore, the fats, ketones and silane acids were also detected in the volatiles (Table-2).

Sixty peaks were obtained and 50 components were identified from petroleum ether extract, accounting for 93.7 % of the total petroleum ether extract (Fig. 2). According to the percentage content of comparison, the main constituents were doconexent (15.5 %), *cis*-5,8,11,14,17-eicosapentaenoic acid (7.30%), hexadecanoic acid, ethyl ester (6.95%), methyl 5,9octad ecadienoate (6.06%) and *n*-hexadecanoic acid (5.84%). The major constituents of the petroleum ether extract were the organic acids, including 6 kinds of components, accounting for 34.5% of the total. The constituents of esters, including 11 kinds of components, accounting for 24.2%. In addition, the petroleum ether extract also contained 18 kinds of alkanes, accounting for 21.3%, ketones and phenols (Table-3).

## Conclusion

Previous experiments have discovered the physiological activity of the volatile oil. Such as, cadinol has anti-diarrheal effect and can inhibit intestinal fluid accumulation of cholera toxin-induced mice<sup>14</sup>. Caryophyllene can modulate immune function by increasing NK cell activity in tumor-bearing mice<sup>15</sup>. Pinene has obviously contact toxicity to aphis gossypii glover. Ocimene and caryophyllene are used to synthesize the spices<sup>16</sup>. All of these constituents of volatiles mentioned above can be extracted from the branches of *Zanthoxylum bungeanum* and have high contents. As for petroleum ether extract, this kind

$\begin{array}{c c c c c c c c c c c c c c c c c c c $	MASS DATA OF 36 COMPOUNDS IDENTIFIED FROM PETROLEUM ETHER EXTRACT PART					
$  \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Peak No.	Compounds	T <sub>R</sub> (min)	m.f.	m.w.	Area (%)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1	Hexadecane	11.02	$C_{16}H_{34}$	226	0.71
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2	2-Butanone,1-[ (1,1-dimethylethyl)amino]-3,3-dimethyl	15.23	$C_{10}H_{21}NO$	171	0.75
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	Tetradecane	15.38	$C_{14}H_{30}$	198	0.94
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	4	2,6,10,15-Tetramethylheptadecane	17.72	$C_{21}H_{44}$	296	0.89
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	5	11-Pentan-3-ylhenicosane	18.99	$C_{26}H_{54}$	366	3.50
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			26.67			
6       2.6.10-Trimethyltertadecane       19.14       C,H,o.       240       1.95         7       2.4.bi/scrz-butylphenol       19.56       C,H,a.       366       1.04         9       3.Fib/J-5.2-ct-tylbylphenol       24.15       C,H,a.       366       0.09         10       Paromonycin       24.62       C,H,a.       324       0.66         12       Filesoane       25.73       C,H,a.       292       1.41         13       Hencicosane       28.32       C,H,a.       296       1.44         14       5.8-Dicthyldodecane       29.92       C,H,a.       226       0.69         15       9-Hexylheptaldecane       30.24       C,H,a.       324       1.14         46       7.8-Fpoxylanostan-11-0, 3-acetoxy-       31.39       C,H,Q,       376       0.96         17       Phthaliacid butyl undecyl ester       35.37       C,H,Q,       362       0.24       0.44,0,       376         10       1.2-Fenzenoticiarboylic acid, butyl octyl ester       35.37       C,H,Q,       334       0.49         2.4-Dimethylicosane       35.51       C,H,Q,       384       0.51       0.32         2.4-Dimethylicosanic acid       35.25       C,H,Q,			26.80			
7       2.4-Di-tert-hulyphenol       19.56       C, H, Q.       206       2.54         8       5.14-Dibutyloctadecane       22.86       C, H, Q.       366       1.94         9       3-Ehpl-5.72-ethylbutyljoctadecane       24.62       C, H, Q.       322       1.16         11       9-Hexylheptadecane       25.73       C, H, Q.       324       0.66         12       Eicosane       26.46       C, H, Q.       324       0.66         13       Hencicosane       28.32       -       -       -         14       5.8-Diethyldodecane       30.24       C, H, Q.       324       1.44         5.8-Diethyldodecane       30.24       C, H, Q.       502       0.55         7       Pituliaciaci butyl indecyl ester       33.01       C, H, Q.       376       0.96         9       2.4-Dimethylicosane       33.62       C, H, Q.       374       0.49         2       Fully 1-investylicosane       35.51       C, H, Q.       284       0.49         2       Puly 14-methylicosane       35.52       C, H, Q.       284       0.49         2       Ethyl 9-hexadecanota       35.53       C, H, Q.       284       0.55         2 <td>6</td> <td>2,6,10-Trimethyltetradecane</td> <td>19.14</td> <td><math>C_{17}H_{36}</math></td> <td>240</td> <td>1.95</td>	6	2,6,10-Trimethyltetradecane	19.14	$C_{17}H_{36}$	240	1.95
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	7	2,4-Di- <i>tert</i> -butylphenol	19.56	$C_{14}H_{22}O$	206	2.54
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	8	5,14-Dibutyloctadecane	22.86	$C_{26}H_{54}$	366	1.94
	9	3-Ethyl-5-(2-ethylbutyl)octadecane	24.15	$C_{26}H_{54}$	366	0.69
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	10	Paromomycin	24.62	$C_{15}H_{26}O$	222	1.16
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	11	9-Hexylheptadecane	25.73	$C_{23}H_{48}$	324	0.66
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	12	Eicosane	26.46	$C_{20}H_{42}$	282	1.81
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	13	Heneicosane	28.32	$C_{21}H_{44}$	296	1.44
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			33.23			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	14	5,8-Diethyldodecane	29.92	$C_{16}H_{34}$	226	0.69
42.3         16       7.8-Epoxylanostan-11-ol, 3-acetoxy-       31.39 $C_{a}H_{a}O_{a}$ 502       0.55         17       Phthalicacid butyl undecyl ester       32.04 $C_{a}H_{a}O_{a}$ 376       0.96         18       7.9-Di-terr-butyl-1-oxaspiro(4.5) deca-6.9-diene-2.8-Dione       33.07 $C_{a}H_{a}O_{a}$ 216       0.86         19       2.4-Dimethylicosane       33.97 $C_{a}H_{a}O_{a}$ 334       0.49         20       1.2-Benzenedicarboxylic acid, butyl octyl ester       35.07 $C_{a}H_{a}O_{a}$ 234       0.49         21 <i>n</i> -Hexadecanoic acid       35.53 $C_{a}H_{a}O_{a}$ 284       6.95         22       Ethyl 9-hexadecanoate       38.071 $C_{a}H_{a}O_{a}$ 284       6.95         23       Hexadecanoic acid, ethyl ester       36.07 $C_{a}H_{a}O_{a}$ 298       0.81         24       Envici acid       38.071 $C_{a}H_{a}O_{a}$ 298       0.81         25       Ethyl 14-methyl-hexadecanoate       39.47 $C_{a}H_{a}O_{a}$ 328       3.55         26       1.1-Didodecoxyhexadecane       39.77 $C_{a}H_{a}$ $O_{a}H_{a}O_{a}$ 3.66         29       (3Z.7E, 10E)-	15	9-Hexylheptadecane	30.24	$C_{23}H_{48}$	324	1.14
16       7.8-Epoxylanostan-11-0, 3-acetoxy-       31.39       C <sub>2</sub> ,H <sub>2</sub> O <sub>4</sub> 502       0.55         17       Phthalicacid buyl undcyl seter       32.04       C <sub>2</sub> ,H <sub>4</sub> O,       376       0.96         18       7.9-Di- <i>tert</i> -buyl-1-oxaspiro(4,5) deca-6.9-diene-2,8-Dione       33.62       C <sub>17</sub> H <sub>4</sub> O,       276       0.86         19       2.4-Dimethylicosane       33.07       C <sub>2</sub> H <sub>4</sub> O,       234       0.997         20       1.2-Berzzenciarboxylic acid, buyl octyl ester       35.07       C <sub>2</sub> H <sub>4</sub> O,       284       6.95         21 <i>n</i> -Hexadecanoic acid       35.53       C <sub>10</sub> H <sub>4</sub> O,       284       6.95         23       Hexadecanoic acid, ethyl ester       36.25       C <sub>4</sub> H <sub>4</sub> O,       284       6.95         24       Erucic acid       38.07       C <sub>2</sub> H <sub>4</sub> O,       288       0.71         25       Ethyl 14-methyl-hexadecanoate       38.45       C <sub>4</sub> H <sub>4</sub> O,       282       0.70         27       1,3-5 Trimethyl-2-octadecylcyclobexane       39.45       C <sub>4</sub> H <sub>4</sub> O,       352       366         26       1,1-Didodecoxyhexadecanoate       41.01       C <sub>1</sub> H <sub>4</sub> O,       312       0.48         2       3.5Dirdytoxypropyl (97,12/52)       12,15-Octadecatienoate       41.20       C <sub>2</sub> H <sub>4</sub> O,			42.37			
17       Phthalicacid butyl undecyl ester       32.04 $C_{\mu}H_{u}O_{\nu}$ 376       0.96         18       7.9-Di-terr-butyl-1-oxaspiro(4.5) deca-6.9-diene-2,8-Dione       33.62 $C_{\nu}H_{u}O_{\nu}$ 276       0.86         19       2.4-Dimethylicosane       33.97 $C_{\nu}H_{u}O_{\nu}$ 334       0.49         1.2-Benzenedicarboxylic acid, butyl octyl ester       35.05 $C_{\nu}H_{u}O_{\nu}$ 282       0.30         21 <i>n</i> -Hexadecanoic acid, ethyl ester       36.25 $C_{\nu}H_{u}O_{\nu}$ 284       6.95         22       Ethyl 14-methyl-hexadecanoate       38.07 $C_{\nu}H_{u}O_{\nu}$ 284       6.95         24       Erucic acid       38.07 $C_{\nu}H_{u}O_{\nu}$ 298       0.81         25       Ethyl 14-methyl-hexadecanoate       39.45 $C_{\nu}H_{u}O_{\nu}$ 298       0.81         26       1,1-Didodecoxyhexadecane       39.77 $C_{\nu}H_{u}O_{\nu}$ 352       3.66         29       (37,TE,10F)-trideca-3,7,10,12-tetraenoic acid       40.54 $C_{\mu}H_{u}O_{\nu}$ 352       3.66         20       (37,TE,10F)-trideca-3,7,10,12-tetraenoic acid       41.40 $C_{\mu}H_{u}O_{\nu}$ 302       7.30         31 <i>cis</i> -58,11,1,4,17-Eicosapentaenoic	16	7,8-Epoxylanostan-11-ol, 3-acetoxy-	31.39	$C_{32}H_{54}O_{4}$	502	0.55
18       7,9-Diterr-butyl-1-oxaspirol(4,5) deca-6,9-diene-2,8-Dione       33,62       C,H,g,O,       276       0.86         19       2.4-Dimethylicosane       33,97       C,Hg,O,       334       0.49         20       1.2-Benzenedicarboxylic acid, butyl octyl ester       35,07       C,Hg,O,       286       5.84         21       n-Hexadecenoic acid       35,25       C,Hg,O,       282       0.30         23       Hexadecenoic acid, ethyl ester       36,25       C,Hg,O,       284       6.95         24       Erucic acid       38,07       C,Hg,O,       284       6.95         24       Erucic acid       38,44       C,Hg,O,       284       6.95         25       Ethyl 14-methyl-hexadecanoate       39,45       C,Hg,O,       282       3.36         26       1.1-Didodecoxyhexadecane       39,45       C,Hg,O,       352       3.66         29       (3Z,TE,10F)-trideca-3,7.10,12-tetraenoic acid Methyl ester       41.01       C,Hg,O,       322       3.66         29       (3Z,TE,10F)-trideca-3,7.10,12-tetraenoic acid       41.40       C,Hg,O,       312       0.48         31       cis-5,8.11,14,17-Eicospentaenoic acid       41.85       C,Hg,O,       322       7.30	17	Phthalicacid butyl undecyl ester	32.04	$C_{23}H_{36}O_{4}$	376	0.96
19       2,4-Dimethylicosane       33,97       C,H <sub>u</sub> 310       0,97         20       1,2-Benzenedicarboxylic acid, butyl octyl ester       35,07       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 354       0,49         21       n-Hexadecenoic acid       35,25       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 282       0,30         23       Hexadecenoic acid, ethyl ester       36,25       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 284       6.95         24       Erucic acid       38,07       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 284       0,49         25       Ethyl 1+ methyl-hexadecanoate       38,44       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 298       0,81         26       1,1-Didodecoxybroxplexadecane       39,45       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 294       0,70         27       1,3,5-Trimethyl-2-octadecylcyclohexane       39,47       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 352       3,66         29       (3Z,7E,10E)-trideca-3,7,10,12-tetraenoic acid Methyl ester       41.01       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 302       7,30         31 <i>cir.</i> 5,8,11,14,17-Eicosapentaenoic acid       41.40       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 302       7,30         32       Minaprine       41.61       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 308       4,78         33       Doconexent       41.85       C <sub>u</sub> H <sub>u</sub> O <sub>s</sub> 308       1,75	18	7,9-Di- <i>tert</i> -butyl-1-oxaspiro(4,5) deca-6,9-diene-2,8-Dione	33.62	$C_{17}H_{24}O_3$	276	0.86
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	19	2,4-Dimethylicosane	33.97	$C_{22}H_{46}$	310	0.97
21 $n$ -Hexadecanoic acid35.25 $C_nH_nO_2$ 2565.8422Ethyl 9-hexadecanoita35.53 $C_nH_nO_2$ 2820.3023Hexadecanoic acid, ethyl ester36.25 $C_nH_nO_2$ 2846.9524Erucic acid38.07 $C_{2n}H_nO_2$ 3380.7125Ethyl 14-methyl-hexadecanoate39.45 $C_nH_nO_2$ 5940.70261,1-Didodecox/hexadecane39.45 $C_nH_nO_2$ 5940.70271,3.5-Tirimethyl-2-octadecylcyclohexane39.77 $C_{2n}H_nO_2$ 3523.6629(3Z-TE,10E)-trideca-37,10,12-tetraenoic acid Methyl ester41.01 $C_nH_nO_2$ 2203.4130Methyl 5.9-octadecadienoate41.21 $C_nH_nO_2$ 2046.0631 $cis-5,8,11.14,17-Eicosapentaenoic acid41.140C_nH_nO_23027.3032Minaprine41.61C_nH_nO_232815.534Nalpha-cbz-L-arginine42.23C_{1H_nN}N_03084.7835Eicosanoic acid42.23C_{2n}H_nN_03420.5036Pentacosane45.17C_{2n}H_nN_03521.0637Ethyl ibo-allocholate40.52C_{2n}H_nN_03521.06369-Oximino-2,7-diethoxyflorene48.19C_{1H_nN}N_02830.5541Tetratetracontae50.47C_{n}H_nO_03680.79422-Butyryl-3-[[2-(5-methoxy-2-methyl-1H-indol-3-y])ethyl]amino]-2-51.5$	20	1,2-Benzenedicarboxylic acid, butyl octyl ester	35.07	$C_{20}H_{30}O_4$	334	0.49
22       Ethyl 9-hexadecenoite $35.53$ $C_{\mu}H_{\nu}O_{\tau}$ $282$ $0.30$ 23       Hexadecanoic acid, ethyl ester $36.25$ $C_{\mu}H_{\nu}O_{\tau}$ $284$ $6.95$ 24       Erucic acid $38.07$ $C_{\mu}H_{\nu}O_{\tau}$ $284$ $6.95$ 24       Erucic acid $38.07$ $C_{\mu}H_{\nu}O_{\tau}$ $284$ $6.95$ 25       Ethyl 14-methyl-hexadecanoate $38.44$ $C_{\mu}H_{\nu}O_{\tau}$ $298$ $0.81$ 26       1,1-Didodecoxyhexadecane $39.45$ $C_{\mu}H_{\nu}O_{\tau}$ $378$ $0.49$ 28       2,3-Dihydroxypropyl (9Z,12Z,15Z)- 9,12,15-Octadecatrienoate $40.54$ $C_{2}H_{\nu}O_{\tau}$ $352$ $3.66$ 29 $(3Z,7E,10E)$ -trideca- $3.7,10,12$ -tetraenoic acid Methyl ester $41.01$ $C_{\mu}H_{\nu}O_{\tau}$ $294$ $6.06$ 31 $cis-5.8,11,14,17$ -Eicosapentaenoic acid $41.40$ $C_{\mu}H_{\nu}NO_{\tau}$ $328$ $15.5$ 34       Malpha-cbcz-Larginine $42.03$ $C_{\mu}H_{\nu}NO_{\tau}$ $328$ $15.5$ 35       Eicosanoic acid $42.23$ $C_{2}H_{u}O_{\tau}$ $328$ $15.5$ 36 <td< td=""><td>21</td><td><i>n</i>-Hexadecanoic acid</td><td>35.25</td><td><math>C_{16}H_{32}O_{2}</math></td><td>256</td><td>5.84</td></td<>	21	<i>n</i> -Hexadecanoic acid	35.25	$C_{16}H_{32}O_{2}$	256	5.84
23Hexadecanoic acid, ethyl ester36.25C $_{\rm 2}H_{\rm 4}O_{\rm 2}$ 2846.9524Erucic acid38.07C $_{\rm 2}L_{\rm 4}O_{\rm 2}$ 3380.7125Ethyl 14-methyl-hexadecanoate38.44C $_{\rm 0}H_{\rm 4}O_{\rm 2}$ 2980.81261,1-Didodecoxyhexadecane39.45C $_{\rm a}H_{\rm 4}O_{\rm 2}$ 5940.70271,3.5-Trimethyl-2-octadecylcyclohexane39.77C $_{\rm 2}H_{\rm 4}$ 3780.49282,3-Dihydroxypropyl (9Z,12Z,15Z)- 9.12,15-Octadecatrienoate40.54C $_{\rm 2}H_{\rm 4}O_{\rm 2}$ 2203.4130Methyl 5,9-octadecadienoate41.21C $_{\rm 0}H_{\rm 4}O_{\rm 2}$ 2046.0631 <i>cis</i> -58,8,11,14,17-Eicosapentaenoic acid41.40C $_{\rm 2}H_{\rm 4}O_{\rm 2}$ 3027.3032Minaprine41.61C $_{\rm 0}H_{\rm 4}O_{\rm 2}$ 32815.534Nalpha-cbz-L-arginine42.03C $_{\rm 2}H_{\rm 4}N_{\rm 2}O_{\rm 2}$ 3084.7835Eicosanoic acid42.23C $_{\rm 2}H_{\rm 4}N_{\rm 2}O_{\rm 3}$ 3084.7836Pentacosane45.17C $_{\rm 3}H_{\rm 4}N_{\rm 2}$ 3521.0637Ethyl iso-allocholate46.52C $_{\rm 2}H_{\rm 4}N_{\rm 3}$ 240.5036Pentacosane45.17C $_{\rm 3}H_{\rm 4}N_{\rm 3}$ 0.67380.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86C $_{\rm 9}H_{\rm 8}N_{\rm 3}$ 0.6734Malpha-cbz-l-arginine50.47C $_{\rm 4}H_{\rm 6}$ 6180.7942 <t< td=""><td>22</td><td>Ethyl 9-hexadecenoate</td><td>35.53</td><td><math>C_{18}H_{34}O_{2}</math></td><td>282</td><td>0.30</td></t<>	22	Ethyl 9-hexadecenoate	35.53	$C_{18}H_{34}O_{2}$	282	0.30
24Erucic acid38.07C. 2, H <sub>2</sub> O <sub>2</sub> 33.80.7125Ethyl 14-methyl-hexadecanoate38.44C. 9H <sub>8</sub> O <sub>2</sub> 2980.81261.1-Didodecoxyhexadecane39.45C. 9H <sub>8</sub> O <sub>2</sub> 5940.70271,3,5-Trimethyl-2-octadecylcyclohexane39.77C. 7H <sub>4</sub> 3780.49282,3-Dihydroxypropyl (9Z,12Z,15Z) - 9,12,15-Octadecatrienoate40.54C. 9H <sub>8</sub> O <sub>2</sub> 2203.4130Methyl 5,9-octadecadienoate41.01C. 9H <sub>9</sub> O <sub>2</sub> 2946.0631cis.58,11,14,17-Eicosapentaenoic acid41.40C. 9H <sub>8</sub> O <sub>2</sub> 3027.3032Minaprine41.61C. 9H <sub>8</sub> O <sub>2</sub> 3027.3033Doconexent41.85C. 2H <sub>9</sub> O <sub>2</sub> 32815.534Nalpha-cbz-L-arginine42.03C. 14H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> 3084.7835Eicosanoic acid42.23C. 3H <sub>8</sub> 3240.5036Pentacosane45.17C. 3H <sub>4</sub> O <sub>2</sub> 4360.67382,4,6-Tri-(rer-butyl)benzonitrile46.86C. 9H <sub>8</sub> N2712.1949Heneicosane47.87C. 3H <sub>4</sub> O <sub>2</sub> 3680.67382,4,6-Tri-(rer-butyl)benzonitrile50.47C. 3H <sub>4</sub> O <sub>2</sub> 3680.5941Tetratetracontane50.47C. 3H <sub>4</sub> O <sub>2</sub> 3680.59422-Buttyryl-3-[(2-G-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino]-2-51.55C. 3H <sub>8</sub> O <sub>2</sub> 3680.5944Ethyl tetracosanoate57.66C. 9H <sub>6</sub> O <sub>2</sub>	23	Hexadecanoic acid, ethyl ester	36.25	$C_{18}H_{36}O_{2}$	284	6.95
25Ethyl 14-methyl-hexadecanoate38.44C, H, Q, C, H, Q, 2980.81261,1-Didodecoxyhexadecane39.45C, H, Q, C, H, X, 3780.49271,3.5-Timethyl-2-octadecylcyclohexane39.77C, H, Q, C, H, X, 3523.6629(3Z, TE, 10E)-trideca-3,7,10,12-tetraenoic acid Methyl ester41.01C, H, Q, 2002203.4130Methyl 5.9-octadecadienoate41.21C, H, Q, S, 81,114,17-Eicosapentaenoic acid41.40C, H, Q, S, 81,114,17-Eicosapentaenoic acid41.61C, H, Q, S, 80,03027.3032Minaprine41.61C, H, Q, S, 80,03027.3032815.534Nalpha-cbz-L-arginine42.03C, H, Q, S, 80,03084.7835Eicosanoic acid42.23C, H, Q, S, 40,03084.7836Pentacosane45.17C, H, Q, S, 40,03521.0637Ethyl iso-allocholate46.52C, H, Q, S, 40,03521.06382,4,6-Tiri-(tert-butyl)benzonitrile46.52C, H, Q, S, 4330.55409-Oximino-2,7-diethoxyfluorene48.19C, H, Q, S, 3680.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino]-2- cyclohecen-1-one51.55C, H, Q, S, 3683680.7943Docosanoic acid, ethyl ester57.66C, H, Q, S, 3683680.7944Ethyl tetracosanoat61.53C, H, Q, S, 4643541.42 <t< td=""><td>24</td><td>Erucic acid</td><td>38.07</td><td><math>C_{22}H_{42}O_{2}</math></td><td>338</td><td>0.71</td></t<>	24	Erucic acid	38.07	$C_{22}H_{42}O_{2}$	338	0.71
261,1-Didodecoxybexadecane39,45C <sub>u</sub> ,H <sub>u</sub> ,O <sub>2</sub> 5940.70271,3,5-Trimethyl-2-octadecylcyclohexane39,77C <sub>u</sub> ,H <sub>u</sub> ,O <sub>1</sub> 3780.49282,3-Dihydroxypropi (9Z,12Z,15Z)- 9,12,15-Octadecatrienoate40.54C <sub>21</sub> H <sub>u</sub> ,O <sub>1</sub> 3523.6629(3Z,7E,10E)-trideca-3,7,10,12-tetraenoic acid Methyl ester41.01C <sub>u</sub> ,H <sub>u</sub> ,O <sub>2</sub> 2946.0631 <i>cis</i> -5,8,11,14,17-Eicosapentaenoic acid41.40C <sub>u</sub> ,H <sub>u</sub> ,O <sub>2</sub> 3027.3032Minaprine41.61C <sub>u</sub> ,H <sub>u</sub> ,O <sub>1</sub> 3120.4833Doconexent41.85C <sub>u</sub> ,H <sub>u</sub> ,O <sub>1</sub> 32815.534Nalpha-cbz-L-arginine42.03C <sub>u</sub> ,H <sub>u</sub> ,M <sub>2</sub> O <sub>4</sub> 3084.7835Eicosanoic acid42.23C <sub>u</sub> ,H <sub>u</sub> 3240.5036Pentacosane45.17C <sub>24</sub> H <sub>32</sub> 3521.0637Ethyl iso-allocholate46.52C <sub>u</sub> ,H <sub>u</sub> O,4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86C <sub>10</sub> ,H <sub>u</sub> O,3281.5541Tetrateracontane50.47C <sub>u</sub> ,H <sub>u</sub> O,3680.79422-Butyr)l-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl]ethyl]amino]-2-51.55C <sub>u</sub> ,H <sub>u</sub> O,3680.7943Docosanoic acid, ethyl ester52.89C <sub>24</sub> H <sub>40</sub> O,3680.5944Ethyl terlocasanae57.66C <sub>28</sub> H <sub>40</sub> O,3680.594524α-Methylcholesterol61.53C <sub>48</sub> H <sub>6</sub> O,4420.4446Stig	25	Ethyl 14-methyl-hexadecanoate	38.44	$C_{19}H_{38}O_2$	298	0.81
271.3.5-Trimethyl-2-octadecylcylohexane39.77C $_2$ H $_4$ 3780.49282.3-Dihydroxyproyl (92,122,152)-9,12,15-Octadecatrienoate40.54C $_{21}$ H $_{40}$ O3523.6629(3Z.7E,10E)-trideca-3.7,10,12-tetraenoic acid Methyl ester41.01C $_{10}$ H $_{20}$ O2203.4130Methyl 5,9-octadecadienoate41.21C $_{10}$ H $_{40}$ O2946.0631cix-5,8,11,14,17-Eicosapentaenoic acid41.40C $_{20}$ H $_{30}$ O3027.3032Minaprine41.61C $_{10}$ H $_{20}$ O3027.3033Doconexent41.85C $_{24}$ H $_{22}$ O32815.534Nalpha-cbz-L-arginine42.03C $_{14}$ H $_{20}$ O3084.7835Eicosanoic acid42.23C $_{23}$ H $_{48}$ 3240.5036Pentacosane45.17C $_{23}$ H $_{40}$ 3460.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86C $_{10}$ H $_{10}$ N2712.1949Heneicosane47.87C $_{21}$ H $_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19C $_{17}$ H $_{10}$ NO <sub>3</sub> 2830.5541Tetratetracontane50.47C $_{44}$ H $_{00}$ 6180.79422-Butyryl-3-{12-12-methyl-1H-indol-3-yl)ethyl]amino)-2-51.55C $_{24}$ H $_{40}$ O3680.5944Ethyl tetracosanoate57.66C $_{34}$ H $_{40}$ O3680.5945246-Methylcholesterol61.53C $_{94}$ H $_{40}$ O <t< td=""><td>26</td><td>1,1-Didodecoxyhexadecane</td><td>39.45</td><td><math>C_{40}H_{82}O_{2}</math></td><td>594</td><td>0.70</td></t<>	26	1,1-Didodecoxyhexadecane	39.45	$C_{40}H_{82}O_{2}$	594	0.70
282,3-Dihydroxypropyl (9Z,12Z,15Z) - 9,12,15-Octadecatrienoate40,54 $C_{21}H_{30}O_{1}$ 3523.6629(3Z,7E,10E)-trideca-3,7,10,12-tetraenoic acid Methyl ester41.01 $C_{41}H_{30}O_{2}$ 2203.4130Methyl 5,9-octadecadienoate41.21 $C_{10}H_{30}O_{2}$ 2946.0631 $cis-5.8,11,14,17$ -Eicosapentaenoic acid41.40 $C_{31}H_{30}O_{2}$ 3027.3032Minaprine41.61 $C_{10}H_{30}O_{2}$ 3120.4833Doconexent41.85 $C_{21}H_{30}O_{2}$ 32815.534Nalpha-cbz-L-arginine42.03 $C_{41}H_{30}O_{4}$ 3084.7835Eicosanoic acid42.23 $C_{22}H_{43}$ 3240.5036Pentacosane45.17 $C_{21}H_{22}$ 3521.0637Ethyl iso-allocholate46.52 $C_{20}H_{41}O_{5}$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{11}H_{10}N_{13}$ 2830.55409-Oximino-2,7-diethoxyfluorene47.87 $C_{21}H_{40}O_{5}$ 3680.67422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-y])ethyl]amino}-2-51.55 $C_{21}H_{30}O_{5}$ 3680.7943Docosanoic acid, ethyl ester52.89 $C_{21}H_{40}O_{5}$ 3680.5944Ethyl tetracosanoate57.66 $C_{3}H_{30}O_{5}$ 3680.594524α-Methylcholesterol61.53 $C_{3}H_{30}O_{5}$ 4420.4446Stigmasta-5,22-dien-	27	1,3,5-Trimethyl-2-octadecylcyclohexane	39.77	$C_{27}H_{54}$	378	0.49
29 $(3Z,7E,10E)$ -trideca-3,7,10,12-tetraenoic acid Methyl ester41.01 $C_{14}H_{10}O_{2}$ 2203.4130Methyl 5,9-octadecadienoate41.21 $C_{19}H_{40}O_{2}$ 2946.0631 $cis$ -5,8,11,14,17-Eicosapentaenoic acid41.40 $C_{20}H_{40}O_{2}$ 3027.3032Minaprine41.61 $C_{19}H_{20}O_{2}$ 32815.534Nalpha-cbz-L-arginine42.03 $C_{14}H_{20}N_{2}$ 3084.7835Eicosanoic acid42.23 $C_{23}H_{28}$ 3240.5036Pentacosane45.17 $C_{23}H_{28}$ 3221.0637Ethyl iso-allocholate46.52 $C_{28}H_4O_5$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{29}N$ 2712.1949Hencicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_3$ 2830.5541Tetrateracontane50.47 $C_{44}H_{60}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino]-2- cyclohexen-1-one51.55 $C_{22}H_{20}O_3$ 3680.5944Ethyl tetracosanoate57.66 $C_{20}H_{20}O_3$ 3680.594524α-Methylcholesterol61.53 $C_{30}H_{6}O_3$ 3541.554524a-Methylcholesterol61.53 $C_{30}H_{6}O_3$ 3541.5546Stigmasta-5,22-dien-3 β-o163.81 $C_{11}H_{6}O_3$ 35	28	2,3-Dihydroxypropyl (9Z,12Z,15Z)- 9,12,15-Octadecatrienoate	40.54	$C_{21}H_{36}O_4$	352	3.66
30Methyl 5.9-octadecadienoate41.21 $C_{19}H_{41}O_{2}$ 2946.0631 $cis$ -5,8,11,14,17-Eicosapentaenoic acid41.40 $C_{21}H_{40}O_{2}$ 3027.3032Minaprine41.61 $C_{19}H_{40}O_{3}$ 3120.4833Doconexent41.85 $C_{21}H_{20}O_{3}$ 32815.534Nalpha-cbz-L-arginine42.03 $C_{14}H_{20}N_{40}A_{3}$ 3084.7835Eicosanoic acid42.23 $C_{23}H_{48}$ 3240.5036Pentacosane45.17 $C_{23}H_{42}$ 3521.0637Ethyl iso-allocholate46.52 $C_{28}H_{40}O_{3}$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{90}N_{1}$ 2712.1949Hencicosane47.87 $C_{21}H_{41}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_{3}$ 2830.5541Tetratetracontane50.47 $C_{44}H_{60}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-y])ethyl]amino}-2- cyclohexen-1-one51.55 $C_{22}H_{20}N_{2}O_{3}$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{2}O_{2}$ 3960.544524α-Methylcholesterol61.53 $C_{20}H_{8}O_{6}$ 3541.4246Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{6}O_{6}$ 3541.52481,4-bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{2$	29	(3Z,7E,10E)-trideca-3,7,10,12-tetraenoic acid Methyl ester	41.01	$C_{14}H_{20}O_{2}$	220	3.41
31 $cis$ -5,8,11,14,17-Eicosapentaenoic acid41.40 $C_{2i}H_{30}O_2$ 3027.3032Minaprine41.61 $C_{ij}H_{3i}O_3$ 3120.4833Doconexent41.85 $C_{2i}H_{30}O_2$ 32815.534Nalpha-cbz-L-arginine42.03 $C_{ii}H_{3i}O_1O_2$ 3084.7835Eicosanoic acid42.23 $C_{2i}H_{4i}$ 3240.5036Pentacosane45.17 $C_{2i}H_{4i}$ 3521.0637Ethyl iso-allocholate46.52 $C_{2i}H_{4i}O_5$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{1i}H_{2i}N$ 2712.1949Heneicosane47.87 $C_{3i}H_{4i}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{1i}H_{2i}NO_3$ 2830.5541Tetratetracontane50.47 $C_{4i}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2-51.55 $C_{2i}H_{3i}N_2O_3$ 3680.5944Ethyl tetracosanoate57.66 $C_{3i}H_{30}O_2$ 4420.444524α-Methylcholesterol61.53 $C_{3i}H_{30}O_2$ 4541.4247Sesamin63.81 $C_{3i}H_{30}O_2$ 4541.4247Sesamin64.80 $C_{2i}H_{10}O_3$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{2i}H_{10}O_3$ 3541.5249Campesterol66	30	Methyl 5,9-octadecadienoate	41.21	$C_{19}H_{34}O_{2}$	294	6.06
32Minaprine41.61 $C_{19}H_{36}O_{3}$ 3120.4833Doconexent41.85 $C_{21}H_{30}O_{3}$ 3120.4834Nalpha-cbz-L-arginine42.03 $C_{14}H_{30}N_{4}O_{4}$ 3084.7835Eicosanoic acid42.23 $C_{23}H_{48}$ 3240.5036Pentacosane45.17 $C_{23}H_{42}$ 3521.0637Ethyl iso-allocholate46.52 $C_{26}H_{4}O_{5}$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{29}N$ 2712.1949Heneicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_{3}$ 2830.5541Tetratetracontane50.47 $C_{44}H_{40}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one51.55 $C_{20}H_{30}O_{3}$ 3680.5944Ethyl tetracosanoate57.66 $C_{20}H_{20}O_{3}$ 3680.594524\alpha-Methylcholesterol61.53 $C_{30}H_{6}O_{3}$ 4420.4446Stigmasta-5,22-dien-3 $\beta$ -ol63.81 $C_{31}H_{6}O_{3}$ 3541.4247Sesamin64.80 $C_{30}H_{18}O_{3}$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{20}H_{18}O_{3}$ 3541.2249Campesterol67.99 $C_{29}H_{8}O_{3}$ 4143.01 </td <td>31</td> <td>cis-5,8,11,14,17-Eicosapentaenoic acid</td> <td>41.40</td> <td><math>C_{20}H_{30}O_{2}</math></td> <td>302</td> <td>7.30</td>	31	cis-5,8,11,14,17-Eicosapentaenoic acid	41.40	$C_{20}H_{30}O_{2}$	302	7.30
33Doconexent41.85 $C_{22}H_{32}O_2$ 32815.534Nalpha-cbz-L-arginine42.03 $C_{14}H_{30}N_{3}O_{4}$ 3084.7835Eicosanoic acid42.23 $C_{31}H_{48}$ 3240.5036Pentacosane45.17 $C_{23}H_{32}$ 3521.0637Ethyl iso-allocholate46.52 $C_{24}H_{41}O_5$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{29}N$ 2712.1949Heneicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{19}H_{17}NO_3$ 2830.5541Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one51.55 $C_{24}H_{45}O_2$ 3680.5943Docosanoic acid, ethyl ester52.89 $C_{24}H_{45}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{24}H_{52}O_2$ 3960.544524\alpha-Methylcholesterol61.53 $C_{34}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 $\beta$ -ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{29}H_{18}O_6$ 3541.55481.4- <i>Bis</i> (1,3-benzodioxole-5-yl)tetrahydro-1 <i>H</i> ,3 <i>H</i> -furo[3,4-c]furan64.904002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{8}O$ 4143.01	32	Minaprine	41.61	$C_{19}H_{36}O_{3}$	312	0.48
34Nalpha-cbz-L-arginine42.03 $C_{14}H_{20}N_4O_4$ 3084.7835Eicosanoic acid42.23 $C_{23}H_{48}$ 3240.5036Pentacosane45.17 $C_{23}H_{52}$ 3521.0637Ethyl iso-allocholate46.52 $C_{26}H_{4}O_5$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{29}N$ 2712.1949Heneicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_3$ 2830.5541Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one51.55 $C_{22}H_{48}O_3$ 3680.5943Docosanoic acid, ethyl ester52.89 $C_{24}H_{48}O_3$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524 $\alpha$ -Methylcholesterol61.53 $C_{30}H_{8}O_2$ 4541.4246Stigmasta-5,22-dien-3 $\beta$ -ol63.81 $C_{31}H_{8}O_2$ 4541.4247Sesamin64.80 $C_{29}H_{18}O_6$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{29}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{40}O$ 4143.01 <td>33</td> <td>Doconexent</td> <td>41.85</td> <td><math>C_{22}H_{32}O_2</math></td> <td>328</td> <td>15.5</td>	33	Doconexent	41.85	$C_{22}H_{32}O_2$	328	15.5
35Eicosanoic acid42.23 $C_{23}H_{48}$ 3240.5036Pentacosane45.17 $C_{23}H_{52}$ 3521.0637Ethyl iso-allocholate46.52 $C_{26}H_{44}O_5$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{29}N$ 2712.1949Heneicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_3$ 2830.5541Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one52.89 $C_{24}H_{48}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750β-Sitosterol67.99 $C_{29}H_{40}O$ 4143.01	34	Nalpha-cbz-L-arginine	42.03	$C_{14}H_{20}N_4O_4$	308	4.78
36Pentacosane45.17 $C_{28}H_{52}$ 3521.0637Ethyl iso-allocholate46.52 $C_{28}H_{44}O_5$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{29}N$ 2712.1949Heneicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{19}H_{19}NO_3$ 2830.5541Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one51.55 $C_{22}H_{28}N_2O_3$ 3680.5943Docosanoic acid, ethyl ester52.89 $C_{24}H_{30}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{28}H_{53}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{31}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{51}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{29}H_{18}O_6$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{29}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{40}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	35	Eicosanoic acid	42.23	$C_{23}H_{48}$	324	0.50
37Ethyl iso-allocholate46.52 $C_{26}H_{44}O_5$ 4360.67382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{29}N$ 2712.1949Heneicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_3$ 2830.5541Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2-51.55 $C_{22}H_{28}N_2O_3$ 3680.5943Docosanoic acid, ethyl ester52.89 $C_{24}H_{48}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{40}O$ 4143.01	36	Pentacosane	45.17	$C_{25}H_{52}$	352	1.06
382,4,6-Tri-( <i>tert</i> -butyl)benzonitrile46.86 $C_{19}H_{29}N$ 2712.1949Heneicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_3$ 2830.5541Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2-51.55 $C_{22}H_{28}N_2O_3$ 3680.7943Docosanoic acid, ethyl ester52.89 $C_{24}H_{48}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4- <i>Bis</i> (1,3-benzodioxole-5-yl)tetrahydro-1 <i>H</i> ,3 <i>H</i> -furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	37	Ethyl iso-allocholate	46.52	$C_{26}H_{44}O_5$	436	0.67
49Heneicosane47.87 $C_{21}H_{44}$ 2960.88409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_3$ 2830.5541Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one51.55 $C_{22}H_{28}N_2O_3$ 3680.7943Docosanoic acid, ethyl ester52.89 $C_{24}H_{48}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	38	2,4,6-Tri-( <i>tert</i> -butyl)benzonitrile	46.86	$C_{19}H_{29}N$	271	2.19
409-Oximino-2,7-diethoxyfluorene48.19 $C_{17}H_{17}NO_3$ 2830.5541Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one51.55 $C_{22}H_{28}N_2O_3$ 3680.7943Docosanoic acid, ethyl ester52.89 $C_{24}H_{48}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4- <i>Bis</i> (1,3-benzodioxole-5-yl)tetrahydro-1 <i>H</i> ,3 <i>H</i> -furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	49	Heneicosane	47.87	$C_{21}H_{44}$	296	0.88
41Tetratetracontane50.47 $C_{44}H_{90}$ 6180.79422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one51.55 $C_{22}H_{28}N_2O_3$ 3680.7943Docosanoic acid, ethyl ester52.89 $C_{24}H_{48}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4- <i>Bis</i> (1,3-benzodioxole-5-yl)tetrahydro-1 <i>H</i> ,3 <i>H</i> -furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	40	9-Oximino-2,7-diethoxyfluorene	48.19	$C_{17}H_{17}NO_3$	283	0.55
422-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one51.55 $C_{22}H_{28}N_2O_3$ 3680.7943Docosanoic acid, ethyl ester52.89 $C_{24}H_{48}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4- <i>Bis</i> (1,3-benzodioxole-5-yl)tetrahydro-1 <i>H</i> ,3 <i>H</i> -furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	41	Tetratetracontane	50.47	$C_{44}H_{90}$	618	0.79
43Docosanoic acid, ethyl ester52.89 $C_{24}H_{48}O_2$ 3680.5944Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4- <i>Bis</i> (1,3-benzodioxole-5-yl)tetrahydro-1 <i>H</i> ,3 <i>H</i> -furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750 $\beta$ -Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	42	2-Butyryl-3-{[2-(5-methoxy-2-methyl-1H-indol-3-yl)ethyl]amino}-2- cyclohexen-1-one	51.55	$C_{22}H_{28}N_2O_3$	368	0.79
44Ethyl tetracosanoate57.66 $C_{26}H_{52}O_2$ 3960.544524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4- <i>Bis</i> (1,3-benzodioxole-5-yl)tetrahydro-1 <i>H</i> ,3 <i>H</i> -furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750β-Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	43	Docosanoic acid, ethyl ester	52.89	$C_{24}H_{48}O_2$	368	0.59
4524α-Methylcholesterol61.53 $C_{30}H_{50}O_2$ 4420.4446Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750β-Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	44	Ethyl tetracosanoate	57.66	$C_{26}H_{52}O_{2}$	396	0.54
46Stigmasta-5,22-dien-3 β-ol63.81 $C_{31}H_{50}O_2$ 4541.4247Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750β-Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	45	24α-Methylcholesterol	61.53	$C_{30}H_{50}O_{2}$	442	0.44
47Sesamin64.80 $C_{20}H_{18}O_6$ 3541.55481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750β-Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	46	Stigmasta-5,22-dien-3 β-ol	63.81	$C_{31}H_{50}O_2$	454	1.42
481,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan64.97 $C_{20}H_{18}O_6$ 3541.2249Campesterol66.23 $C_{28}H_{48}O$ 4002.2750β-Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	47	Sesamin	64.80	$C_{20}H_{18}O_{6}$	354	1.55
49Campesterol66.23 $C_{28}H_{48}O$ 4002.2750β-Sitosterol67.99 $C_{29}H_{50}O$ 4143.01	48	1,4-Bis(1,3-benzodioxole-5-yl)tetrahydro-1H,3H-furo[3,4-c]furan	64.97	$C_{20}H_{18}O_{6}$	354	1.22
50 $\beta$ -Sitosterol 67.99 C <sub>29</sub> H <sub>50</sub> O 414 3.01	49	Campesterol	66.23	C <sub>28</sub> H <sub>48</sub> O	400	2.27
	50	β-Sitosterol	67.99	$C_{29}H_{50}O$	414	3.01

TABLE-3

of chemical constituent is often applied to chemical production. Such as, hexadecanoic acid ethyl ester is used in lubricant. Erucic acid is used to manufacture the artificial fiber<sup>17</sup>. The identification of the chemical constituents of volatiles and petroleum ether extract from the branch of Zanthoxylum bungeanu would contribute to making full use of herb resource.

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