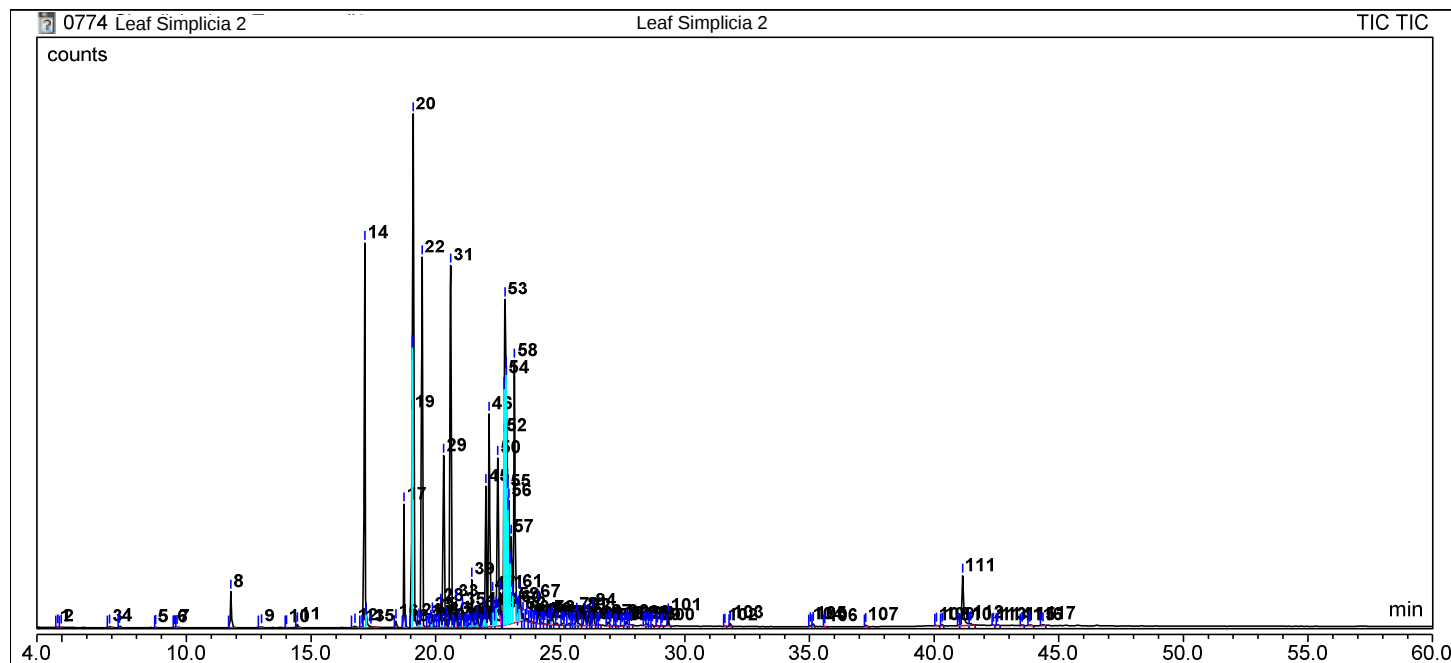




KROMATOGRAM GCMS
LABORATORIUM PENELITIAN DAN PENGUJIAN TERPADU
UNIVERSITAS GADJAH MADA



No.	Ret. Time min	Hit# 1	Chemical Formula	Mol. Weight	SI Hit#1	Hit# 2 min	Chemical Formula	Mol. Weight	SI Hit#2	Hit# 3 counts*min	Chemical Formula
1	4.84	1,3,3-Trimethoxybutane	C7H16O3	148	670	1,3,5-Pentanetriol, 3-methyl-	C6H14O3	134	630	2-Hydroxyisocaproic acid, methyl ether, m	C8H16O3
2	4.97	Acetic acid, 2,2'-[oxybis(2,1-ethanedioxy)]bis-	C8H14O7	222	622	1,3-Dioxolane-4-methanol, 2-ethyl-	C6H12O3	132	621	2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3
3	6.92	α -Pinene	C10H16	136	714	1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	C10H16	136	703	3,5-Methanocyclopentapyrazole, 3,3a,4,5,4a	C10H16N2
4	7.32	Camphene	C10H16	136	830	Bicyclo[2.2.1]heptane, 2,2-dimethyl-	C10H16	136	803	Bicyclo[4.1.0]heptane, 7-(1-methylethylidene	C10H16
5	8.76	Octadecane, 3-ethyl-5-(2-ethylbutyl)-	C26H54	366	547	Decane	C10H22	142	540	2(1H)-Pyrimidinone, 5-chloro-4,6-diphenyl	C16H11ClN2O
6	9.52	α -Cymene	C10H14	134	720	trans-3-Carene-2-ol	C10H16O	152	702	1,3,5-Cycloheptatriene, 3,7,7-trimethyl-	C10H14
7	9.63	Cyclohexane, 1-methylene-4-(1-methylethenyl)-	C10H16	136	697	Cyclohexene, 1-methyl-5-(1-methylethylidene	C10H16	136	686	α -Pinene	C10H16
8	11.79	Linalool	C10H18O	154	930	Linalyl acetate	C12H20O2	196	821	Cyclohexanol, 1-methyl-4-(1-methylethenyl)-	C10H18O
9	13.01	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	C10H16O	152	752	Camphor	C10H16O	152	730	(+)-2-Bornanone	C10H16O
10	14.02	Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, cis-	C10H18O	154	651	5-Isopropyl-2-methylbicyclo[3.1.0]heptan-2-ol	C10H18O	154	649	1,7-Octadien-3-ol, 2,6-dimethyl-	C10H18O
11	14.45	Terpineol	C10H18O	154	886	α -Terpineol	C10H18O	154	861	L- α -Terpineol	C10H18O
12	16.76	Phenol, 4-(2-propenyl)-	C9H10O	134	721	Phenol, 4-(2-propenyl)-, acetate	C11H12O2	176	693	3-(1-Cyclopentenyl)furan	C9H10O
13	17.05	2H-Pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-, acetate	C12H20O3	212	702	Cyclohexanol, 2-methyl-3-(1-methylethylidene	C12H20O2	196	659	2,6-Octadiene-1,8-diol, 2,6-dimethyl-	C10H18O2
14	17.17	Safrole	C10H10O2	162	926	Benzene, 1,2-(methylenedioxy)-4-propenyl-, (E)-	C10H10O2	162	921	1,3-Benzodioxole, 5-(1-propenyl)-, (Z)-	C10H10O2
15	17.40	Benzene, 1,2-(methylenedioxy)-4-propenyl-, (E)-	C10H10O2	162	731	1,3-Benzodioxole, 5-(1-propenyl)-, (Z)-	C10H10O2	162	727	Safrole	C10H10O2
16	18.41	Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethylidene)-	C15H24	204	846	Elemene isomer	C15H24	204	841	Cyclohexane, 1-ethenyl-1-methyl-2-(1-methylethylidene)-	C15H24
17	18.73	α -Cubebene	C15H24	204	907	α -Copaene	C15H24	204	905	(1S,4aR,8aS)-1-Isopropyl-7-methyl-4-methyl-	C15H24

18	18.81	8,11-Octadecadiynoic acid, methyl ester	C19H30O2	290	709	Methyl 10,12-pentacosadiynoate	C26H44O2	388	702	2,5-Octadecadiynoic acid, methyl ester	C19H30O2
19	19.05	Phenol, 2-methoxy-3-(2-propenyl)-	C10H12O2	164	946	Eugenol	C10H12O2	164	936	3-Allyl-6-methoxyphenol	C10H12O2
20	19.10	Phenol, 2-methoxy-3-(2-propenyl)-	C10H12O2	164	931	Eugenol	C10H12O2	164	927	3-Allyl-6-methoxyphenol	C10H12O2
21	19.33	α -ylangene	C15H24	204	849	β -ylangene	C15H24	204	838	α .lfa.-Copaene	C15H24
22	19.46	α .lfa.-Copaene	C15H24	204	922	γ langene	C15H24	204	906	Copaene	C15H24
23	19.71	α -ylangene	C15H24	204	752	β -ylangene	C15H24	204	748	β -copaene	C15H24
24	19.81	β -ylangene	C15H24	204	879	β -copaene	C15H24	204	876	(15,4aR,8a5)-1-Isopropyl-7-methyl-4-meth	C15H24
25	19.87	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-	C15H24	204	901	Cyclohexane, 1-ethenyl-1-methyl-2,4	C15H24	204	886	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-	C15H24
26	19.96	α -ylangene	C15H24	204	798	α .lfa.-Copaene	C15H24	204	797	β -ylangene	C15H24
27	20.12	Cyclohexene, 1,5,5-trimethyl-6-acetylmethyl-	C12H20O	180	673	Spiro[4.4]non-3-en-2-one, 4-methyl	C10H12N4O2	220	668	10-Heptadecen-8-ynoic acid, methyl ester	C18H30O2
28	20.20	Benzene, 1,2-dimethoxy-4-propenyl-, (Z)-	C11H14O2	178	846	Methyleugenol	C11H14O2	178	825	2-Allyl-1,4-dimethoxybenzene	C11H14O2
29	20.33	(1R,3a5,8a5)-7-Isopropyl-1,4-dimethyl-1,2,3,3a,6,8a-hexahydro	C15H24	204	894	1H-Cycloprop[e]azulene, 1a,2,3,4,4a,	C15H24	204	892	1H-Cyclopropa[a]naphthalene, 1a,2,3,3a,4	C15H24
30	20.44	Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl	C15H24	204	853	Di-epi- α -cedrene	C15H24	204	851	α -ylangene	C15H24
31	20.60	Caryophyllene	C15H24	204	956	Bicyclo[7.2.0]undec-4-ene, 4,11,11-tri	C15H24	204	926	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-t	C15H24
32	20.68	1R,3Z,9s-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-en	C15H24	204	774	(1R,9R,E)-4,11,11-Trimethyl-8-methyle	C15H24	204	770	Caryophyllene	C15H24
33	20.82	(1R,2S,6S,7S,8S)-8-Isopropyl-1-methyl-3-methylenetricyclo[4.4,	C15H24	204	920	1H-Cyclopenta[1,3]cyclopropa[1,2]be	C15H24	204	900	Germacrene D	C15H24
34	20.95	Bicyclo[3.1.1]hept-2-ene, 2,6-dimethyl-6-(4-methyl-3-pentenyl	C15H24	204	847	1,3,6,10-Dodecatetraene, 3,7,11-trime	C15H24	204	836	cis- α -Bergamotene	C15H24
35	21.08	1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methyle	C15H24	204	903	(1R,9R,E)-4,11,11-Trimethyl-8-methyle	C15H24	204	901	Alloaromadendrene	C15H24
36	21.18	(15,4aR,7R)-1,4a-Dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-c	C15H24	204	792	β -Longipinene	C15H24	204	779	α -Bulnesene	C15H24
37	21.25	β -copaene	C15H24	204	753	α .lfa.-Copaene	C15H24	204	742	α -ylangene	C15H24
38	21.35	α .lfa.-Copaene	C15H24	204	853	β -copaene	C15H24	204	845	Copaene	C15H24
39	21.45	Humulene	C15H24	204	879	1,4,7,-Cycloundecatriene, 1,5,9,9-tetr	C15H24	204	864	cis- α -Bisabolene	C15H24
40	21.53	β -Longipinene	C15H24	204	812	(1R,9R,E)-4,11,11-Trimethyl-8-methyle	C15H24	204	809	Alloaromadendrene	C15H24
41	21.62	(1R,9R,E)-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-4-e	C15H24	204	839	β -Longipinene	C15H24	204	838	Alloaromadendrene	C15H24
42	21.68	cis-Murola-4(15),5-diene	C15H24	204	901	(1R,2S,6S,7S,8S)-8-Isopropyl-1-methy	C15H24	204	885	1H-Cyclopenta[1,3]cyclopropa[1,2]benzene	C15H24
43	21.83	4,5-di-epi-aristolochene	C15H24	204	723	α -ylangene	C15H24	204	713	β -ylangene	C15H24
44	21.92	β -copaene	C15H24	204	859	α .lfa.-Copaene	C15H24	204	858	(1R,3a5,8a5)-7-Isopropyl-1,4-dimethyl-1,2,3	C15H24
45	22.02	?-Murolene	C15H24	204	912	(5,1Z,6Z)-8-Isopropyl-1-methyl-5-me	C15H24	204	911	(15,4aR,8a5)-1-Isopropyl-7-methyl-4-meth	C15H24
46	22.15	Germacrene D	C15H24	204	899	(1R,2S,6S,7S,8S)-8-Isopropyl-1-methy	C15H24	204	882	1H-Cyclopenta[1,3]cyclopropa[1,2]benzene	C15H24
47	22.28	Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methyl	C15H24	204	896	Bicyclo[5.3.0]decane, 2-methylene-5	C15H24	204	886	Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,6	C15H24
48	22.33	Alloaromadendrene	C15H24	204	858	Guaiac-1(10),11-diene	C15H24	204	855	1H-Cycloprop[e]azulene, decahydro-1,1,7-e	C15H24
49	22.40	1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, octahydro-7-meth	C15H24	204	882	(1R,2S,6S,7S,8S)-8-Isopropyl-1-methy	C15H24	204	878	β -copaene	C15H24
50	22.50	Guaiac-1(10),11-diene	C15H24	204	882	Naphthalene, 1,2,3,5,6,7,8,8a-octahy	C15H24	204	867	Longifolene-(V4)	C15H24
51	22.59	(1R,4a5,8aR)-1-Isopropyl-4,7-dimethyl-1,2,4a,5,6,8a-hexahydro	C15H24	204	894	Naphthalene, 1,2,4a,5,6,8a-hexahyd	C15H24	204	894	α -Murolene	C15H24
52	22.74	4-Chromanol	C9H10O2	150	707	Benzoic acid, 2,5-dimethyl-	C9H10O2	150	700	Benzoic acid, 3,5-dimethyl-	C9H10O2
53	22.78	Benzoic acid, 2,5-dimethyl-	C9H10O2	150	713	4-Chromanol	C9H10O2	150	713	Benzoic acid, 2,3-dimethyl-	C9H10O2
54	22.83	Benzoic acid, 2,5-dimethyl-	C9H10O2	150	725	4-Chromanol	C9H10O2	150	715	Benzoic acid, 2,3-dimethyl-	C9H10O2
55	22.89	Benzoic acid, 2,5-dimethyl-	C9H10O2	150	721	4-Chromanol	C9H10O2	150	712	Benzoic acid, 2,6-dimethyl-	C9H10O2
56	22.93	(2R,3R,3aR,6R,8a5)-3,7,7-Trimethyl-8-methyleneoctahydro-1H	C15H24O	220	687	4-Chromanol	C9H10O2	150	674	Methyl 4,6-tetradecadiynoate	C15H22O2
57	23.03	(3S,3aR,3bR,4S,7R,7aR)-4-Isopropyl-3,7-dimethyloctahydro-1H	C15H26O	222	740	(3R,3aR,3bR,4S,7R,7aR)-4-Isopropyl-	C15H26O	222	725	Methyl 4,6-tetradecadiynoate	C15H22O2
58	23.16	1-Isopropyl-4,7-dimethyl-1,2,3,5,6,8a-hexahydronaphthalene	C15H24	204	817	α .lfa.-Copaene	C15H24	204	790	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-c	C15H24
59	23.23	Methyl 4,6-tetradecadiynoate	C15H22O2	234	687	Methyl 5,7-hexadecadiynoate	C17H26O2	262	674	Ethyl 9,9-diformylnona-2,4,6,8-tetraenoat	C13H14O4
60	23.33	2-Isopropylidene-3-methylhexa-3,5-dienal	C10H14O	150	719	3,5-Heptadienal, 2-ethylidene-6-me	C10H14O	150	708	5-Isopropenyl-2-methylcyclopent-1-enecar	C10H14O
61	23.38	α .lfa.-Copaene	C15H24	204	794	α -ylangene	C15H24	204	791	Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-d	C15H24
62	23.50	Methyl 4,6-tetradecadiynoate	C15H22O2	234	721	(2R,3R,3aR,6R,8a5)-3,7,7-Trimethyl-	C15H24O	220	704	4,5-di-epi-aristolochene	C15H24
63	23.65	1,1-Cyclopropanedimethanol, 2-methyl- α -phenyl-	C12H16O2	192	612	2,3-Diazabicyclo[2.2.1]hept-2-ene, 7	C13H16N2	200	607	α -Calacorene	C15H20
64	23.81	Ethyl 9,9-diformylnona-2,4,6,8-tetraenoate	C13H14O4	234	641	Benzenepropanoic acid, octyl ester	C17H26O2	262	634	4-Chromanol	C9H10O2
65	23.87	Benzenepropanoic acid, octyl ester	C17H26O2	262	647	Ethyl 9,9-diformylnona-2,4,6,8-tetra	C13H14O4	234	638	4-Chromanol	C9H10O2
66	23.97	(2R,3R,3aR,6R,8a5)-3,7,7-Trimethyl-8-methyleneoctahydro-1H	C15H24O	220	683	Benzenemethanol, 2,4,5-trimethyl-	C10H14O	150	644	4-Chromanol	C9H10O2

67	24.11	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	C15H26O	222	829	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	C15H26O	222	826	Nerolidol	C15H26O
68	24.27	(2R,3R,3aR,6R,8aS)-3,7,7-Trimethyl-8-methylenooctahydro-1H-indene	C15H24O	220	666	Ethyl 9,9-diformylnona-2,4,6,8-tetraenoate	C13H14O4	234	637	Myrtenoic acid, ethyl ester	C12H18O2
69	24.38	Methyl 5,7-hexadecadiynoate	C17H26O2	262	701	(2R,3R,3aR,6R,8aS)-3,7,7-Trimethyl-8-methylenooctahydro-1H-indene	C15H24O	220	701	Ethyl 9,9-diformylnona-2,4,6,8-tetraenoate	C13H14O4
70	24.53	(-)-Spathulenol	C15H24O	220	770	(2R,3R,3aR,6R,8aS)-3,7,7-Trimethyl-8-methylenooctahydro-1H-indene	C15H24O	220	757	2,5-Octadecadienoic acid, methyl ester	C19H30O2
71	24.63	Caryophyllene oxide	C15H24O	220	742	Methyl 4,6-tetradecadiynoate	C15H22O2	234	740	2,5-Octadecadienoic acid, methyl ester	C19H30O2
72	24.68	(-)-Globulol	C15H26O	222	815	Globulol	C15H26O	222	808	Epiglobulol	C15H26O
73	24.87	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	704	1H-3a,7-Methanoazulen-5-ol, octahydro-	C15H24O	220	699	2,2,6-Trimethyl-1-(3-methylbuta-1,3-dienyl)-4-methylenecyclohexane	C14H22O2
74	25.10	3-Buten-2-one, 4-(3-hydroxy-6,6-dimethyl-2-methylenecyclohexyl)-	C13H20O2	208	663	1-Butyn-3-one, 1-(6,6-dimethyl-1,2-epoxycyclohexyl)-	C12H16O2	192	658	2,11-Dioxatetracyclo[4.3.1.1(3,10).0(6,9)]undecane	C13H18O2
75	25.17	Ethyl 9,9-diformylnona-2,4,6,8-tetraenoate	C13H14O4	234	645	4-(2,2-Dimethyl-6-methylenecyclohexyl)-1,3-butadiene	C13H22O	194	633	3-Buten-2-ol, 4-(2,6,6-trimethyl-1-cyclohexyl)-	C13H22O
76	25.37	α -acorenol	C15H26O	222	711	Cubenol	C15H26O	222	709	Isoaromadendrene epoxide	C15H24O
77	25.46	1,1-Diphenyl-4-phenylthiobut-3-en-1-ol	C22H20O5	332	682	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	671	4-(2,2-Dimethyl-6-methylenecyclohexyl)-1,3-butadiene	C12H22O
78	25.55	Methyl 3,5-tetradecadiynoate	C15H22O2	234	706	1H-Indene, 1-ethylideneoctahydro-7H-	C12H20	164	698	2,5-Octadecadienoic acid, methyl ester	C19H30O2
79	25.66	Di-epi-1,10-cubenol	C15H26O	222	833	Cubenol	C15H26O	222	829	Epicubenol	C15H26O
80	25.77	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	717	4,7-Octadecadienoic acid, methyl ester	C19H30O2	290	703	Cubenol	C15H26O
81	25.99	α -Cadinol	C15H26O	222	829	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-	C15H26O	222	826	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-	C15H26O
82	26.11	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methyl-4,6-tetradecadiynoate)	C15H26O	222	844	1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-	C15H26O	222	822	α -ylangene	C15H24
83	26.24	Methyl 4,6-tetradecadiynoate	C15H22O2	234	704	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	699	4,7-Octadecadienoic acid, methyl ester	C19H30O2
84	26.32	α -Cadinol	C15H26O	222	853	α -Cadinol	C15H26O	222	829	Selin-6-en-4a-ol	C15H26O
85	26.48	10-12-Pentacosadienoic acid	C25H42O2	374	614	1,1-Diphenyl-4-phenylthiobut-3-en-1-ol	C22H20O5	332	614	Cedren-13-ol, 8-epi-	C15H24O
86	26.57	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	669	4,7-Octadecadienoic acid, methyl ester	C19H30O2	290	659	Methyl 4,6-tetradecadiynoate	C15H22O2
87	26.94	β -copaene	C15H24	204	796	α -ylangene	C15H24	204	784	α -Copaene	C15H24
88	27.02	4,7-Octadecadienoic acid, methyl ester	C19H30O2	290	698	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	692	Methyl 5,7-hexadecadiynoate	C17H26O2
89	27.19	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	652	1,1-Diphenyl-4-phenylthiobut-3-en-1-ol	C22H20O5	332	641	5-Benzofuranacetic acid, 6-ethenyl-2,4,5,6-tetrahydro-	C16H20O4
90	27.27	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	612	Methyl 4,6-tetradecadiynoate	C15H22O2	234	609	1,1-Diphenyl-4-phenylthiobut-3-en-1-ol	C22H20O5
91	27.48	Methyl 4,6-tetradecadiynoate	C15H22O2	234	665	4,7-Octadecadienoic acid, methyl ester	C19H30O2	290	665	2,5-Octadecadienoic acid, methyl ester	C19H30O2
92	27.64	1,2-Diphenyl-1-isocyanoethane	C15H13N	207	660	(3-Methyl-1,4-diphenylbicyclo[2.2.0]hex-5-en-2-ylidene)-1,1-diphenyl-4-phenylthiobut-3-en-1-ol	C20H22O	278	657	3-(2-Carboxy-1-methyl-ethoxy)-5-phenyl-1,1-diphenyl-4-phenylthiobut-3-en-1-ol	C17H24O5
93	27.72	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	667	1,1-Diphenyl-4-phenylthiobut-3-en-1-ol	C22H20O5	332	666	Panaxydol	C17H24O2
94	27.85	Methyl 4,6-tetradecadiynoate	C15H22O2	234	701	2,5-Octadecadienoic acid, methyl ester	C19H30O2	290	693	1,1-Diphenyl-4-phenylthiobut-3-en-1-ol	C22H20O5
95	28.39	β -copaene	C15H24	204	728	β -Guaiene	C15H24	204	723	Tau-Cadinol acetate	C17H28O2
96	28.47	Phenol, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, (R)-	C15H22O	218	674	Phenol, 2-methyl-5-(1,2,2-trimethylcyclohexyl)-	C15H22O	218	673	Bicyclo[4.1.0]heptan-2-one, 3,4,4-trimethyl-	C15H22O
97	28.58	β -copaene	C15H24	204	711	β -Guaiene	C15H24	204	711	α -ylangene	C15H24
98	28.69	1,1,4a-Trimethyl-5,6-dimethylenedecahydronaphthalene	C15H24	204	685	5-Benzofuranacetic acid, 6-ethenyl-	C16H20O4	276	685	β -Guaiene	C15H24
99	28.90	4,7-Octadecadienoic acid, methyl ester	C19H30O2	290	662	5-Benzofuranacetic acid, 6-ethenyl-	C16H20O4	276	656	Methyl 4,6-tetradecadiynoate	C15H22O2
100	29.09	4,7-Octadecadienoic acid, methyl ester	C19H30O2	290	663	5-Benzofuranacetic acid, 6-ethenyl-	C16H20O4	276	653	Methyl 4,6-tetradecadiynoate	C15H22O2
101	29.34	Tau-Cadinol acetate	C17H28O2	264	862	α -Cadinol	C15H26O	222	825	β -copaene	C15H24
102	31.60	4,7-Octadecadienoic acid, methyl ester	C19H30O2	290	641	2-[4-methyl-6-(2,6,6-trimethylcyclohexyl)-2-methoxy]-1,3-dioxane	C23H32O	324	628	2,5-Octadecadienoic acid, methyl ester	C19H30O2
103	31.83	Pentadecanoic acid, 13-methyl-, methyl ester	C17H34O2	270	704	Hexadecanoic acid, methyl ester	C17H34O2	270	693	Cyclopropanebutanoic acid, 2-[[2-[(2-oxo-1,3-dioxol-5-ylidene)-2-methoxy]-2-oxoethyl]-2-oxoethyl]-	C25H42O2
104	35.04	7,10-Octadecadienoic acid, methyl ester	C19H34O2	294	718	9,12-Octadecadienoic acid, methyl ester	C19H34O2	294	718	8,11-Octadecadienoic acid, methyl ester	C19H34O2
105	35.15	11-Octadecenoic acid, methyl ester	C19H36O2	296	711	10-Octadecenoic acid, methyl ester	C19H36O2	296	710	16-Octadecenoic acid, methyl ester	C19H36O2
106	35.62	Ethyl iso-allochololate	C26H44O5	436	644	(5S)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-oxa-4-oxa-2-ylidene)-2-methoxy]-	C28H43NO6	489	609	3-Pyridinecarboxylic acid, 2,7,10-tris(acetyloxy)-	C32H39NO10
107	37.25	Ethyl iso-allochololate	C26H44O5	436	662	(5S)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-oxa-4-oxa-2-ylidene)-2-methoxy]-	C28H43NO6	489	647	Milbemycin B, 6,28-anhydro-15-chloro-25-epoxy-	C33H47ClO7
108	40.09	(5S)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-oxa-4-oxa-2-ylidene)-2-methoxy]-	C28H43NO6	489	598	5 α -Pregn-16-en-20-one, 3 β ,12 α -dihydroxy-	C25H36O5	416	553	Pregnan-20-one, 3-(acetyloxy)-5,6,16,17-tetrahydro-	C23H32O5
109	40.32	(5S)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-oxa-4-oxa-2-ylidene)-2-methoxy]-	C28H43NO6	489	605	Acetic acid, 17-acetoxy-4,4,10,13-tetramethyl-	C25H36O5	416	598	(22S)-21-Acetoxy-6 α ,11 β -dihydroxy-16 α ,17 α -tetramethyl-	C27H36O8
110	41.00	(5S)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-oxa-4-oxa-2-ylidene)-2-methoxy]-	C28H43NO6	489	589	Methyl glycocholate, 3TMS derivative	C36H69NO6Si3	695	558	Acetic acid, 17-acetoxy-4,4,10,13-tetramethyl-	C25H36O5
111	41.15	(2,3-Diphenylcyclopropyl)methyl phenyl sulfoxide, trans-	C22H20O5	332	619	benzene, 1,1',1''-[5-methyl-1-pentene-1,1,1'-triyl]-	C24H24	312	610	Ni-Benzyl-N2(benzylidenyl-benzylamino)-1,1'-bis(2-oxo-1,3-dioxol-5-ylidene)-2,2'-bis(methoxy)-	C28H25N3
112	41.47	5 α -Pregn-16-en-20-one, 3 β ,12 α -dihydroxy-, diacetate	C25H36O5	416	566	Pregnan-20-one, 3,5-dihydroxy-6-methoxy-	C22H36O3	348	544	Benzenepropanoic acid, 4-[(2,4-dinitrophenyl)-2-methoxy]-	C18H18N4O6
113	42.37	(5S)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-oxa-4-oxa-2-ylidene)-2-methoxy]-	C28H43NO6	489	584	Methyl glycocholate, 3TMS derivative	C36H69NO6Si3	695	554	5 α -Pregn-16-en-20-one, 3 β ,12 α -dihydroxy-	C25H36O5
114	42.55	(5S)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-oxa-4-oxa-2-ylidene)-2-methoxy]-	C28H43NO6	489	592	5 α -Pregn-16-en-20-one, 3 β ,12 α -dihydroxy-	C25H36O5	416	565	Acetic acid, 17-acetoxy-4,4,10,13-tetramethyl-	C25H36O5
115	43.53	(5S)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-oxa-4-oxa-2-ylidene)-2-methoxy]-	C28H43NO6	489	597	(22S)-21-Acetoxy-6 α ,11 β -dihydroxy-16 α ,17 α -tetramethyl-	C27H36O8	488	583	5H-Cyclopropa[3,4]benz[1,2-e]azulen-5-ol	C24H32O9

116	43.84	(5 β)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-ox α -4- α	C28H43NO6	489	593	Acetic acid, 17-acetoxy-4,4,10,13-tetr	C25H36O5	416	576	5 α -Pregn-16-en-20-one, 3 β ,12 α -dihydroxy	C25H36O5
117	44.37	(5 β)Pregnane-3,20 β -diol, 14 α ,18 α -[4-methyl-3-oxo-(1-ox α -4- α	C28H43NO6	489	607	5H-Cyclopropa[3,4]benz[1,2-e]azul	C24H32O9	464	591	(22 S)-6 α ,11 β ,21-Trihydroxy-16 α ,17 α -propyl	C25H34O7
Total:											

Mol. Weight	SI Hit#3 counts*min	Rel.Area %	Area counts*min
160	622	0.03	195820.971
190	615	0.02	132823.722
164	703	0.03	253114.636
136	800	0.04	321691.580
282	538	0.01	89352.080
134	695	0.01	97632.310
136	679	0.03	216693.661
154	817	0.83	6305645.418
152	708	0.04	278680.879
154	637	0.01	86759.677
154	822	0.08	637818.203
134	673	0.09	703619.806
170	658	0.02	189382.926
162	916	8.16	61810975.636
162	694	0.33	2476648.822
204	829	0.11	870363.835
204	893	2.16	16349455.796

290	702	0.02	143605.462
164	925	2.94	22280081.273
164	917	11.35	85999746.108
204	835	0.24	1816746.621
204	900	7.02	53171261.597
204	727	0.03	258873.911
204	874	0.11	834477.540
204	874	0.25	1928271.224
204	794	0.04	329514.850
278	653	0.03	216425.322
178	815	0.46	3476228.232
204	881	3.14	23762192.340
204	845	0.16	1227843.861
204	915	7.08	53656360.638
204	766	0.03	223063.358
204	899	0.51	3867720.790
204	825	0.12	885453.627
204	891	0.38	2899093.338
204	776	0.04	298703.216
204	739	0.04	307607.741
204	832	0.10	737157.064
204	851	0.93	7084550.137
204	807	0.05	396585.062
204	838	0.08	635173.479
204	878	0.19	1465207.760
204	698	0.01	80780.973
204	853	0.44	3300401.969
204	909	2.78	21073053.209
204	879	4.23	32070345.813
204	882	0.64	4815638.030
204	854	0.32	2389143.162
204	876	0.27	2029764.909
204	866	5.07	38384405.242
204	881	0.42	3168197.180
150	681	2.43	18429723.896
150	686	9.89	74980903.769
150	699	5.08	38506572.055
150	687	1.16	8800262.112
234	669	3.78	28680244.820
234	701	2.92	22141183.143
204	789	6.07	46015681.703
234	661	0.31	2332584.061
150	693	0.33	2527484.224
204	785	0.75	5712655.732
204	699	0.14	1065093.155
200	599	0.07	543053.437
150	631	0.04	313303.696
150	636	0.02	171793.356
150	640	0.02	149885.879

222	825	0.43	3294481.211
194	616	0.03	223140.656
234	664	0.04	276183.734
290	756	0.10	739448.276
290	735	0.05	360896.866
222	787	0.16	1236488.587
222	695	0.07	553338.831
206	621	0.06	447860.815
194	630	0.02	171053.948
220	694	0.05	408849.915
194	659	0.02	185285.480
290	694	0.05	380462.865
222	822	0.26	2004271.789
222	692	0.07	550069.276
222	819	0.36	2728826.009
204	807	0.20	1478908.027
290	683	0.02	119149.486
222	800	0.39	2966188.139
220	612	0.02	130585.772
234	658	0.03	262533.366
204	781	0.10	773161.925
262	683	0.03	235301.328
276	641	0.01	69746.048
332	602	0.01	112982.579
290	655	0.02	148359.759
308	653	0.10	794811.406
260	638	0.03	238305.835
332	691	0.03	244351.809
264	705	0.05	371125.115
218	657	0.06	489744.254
204	701	0.04	284296.353
204	684	0.03	253104.441
234	643	0.01	109512.982
234	649	0.01	88865.644
204	824	0.21	1575503.910
290	625	0.01	95117.457
374	669	0.07	503640.407
294	717	0.05	358314.826
296	706	0.06	432675.956
597	605	0.01	95576.787
590	625	0.04	308808.611
388	540	0.03	258237.583
488	593	0.03	224595.317
416	547	0.02	185023.168
403	603	1.63	12376207.621
386	541	0.10	760324.072
416	550	0.02	131365.001
416	564	0.03	211261.726
464	578	0.03	241420.858

416	571	0.04	278600.942
446	590	0.06	417619.089
757786565.887			