



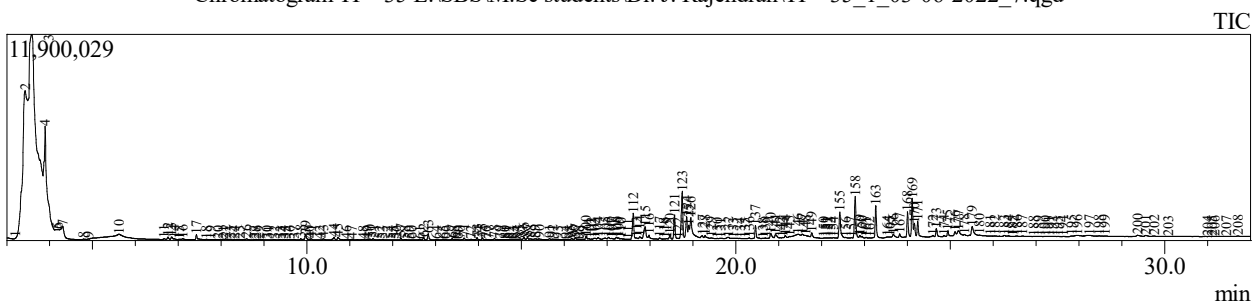
Madurai Kamaraj University
School of Biological Sciences
Gas Chromatography Mass Spectrometry Facility
DST-FIST Facility



Sample Information

Analyzed by : Admin
Analyzed : 6/3/2022 5:13:25 PM
Sample Type : Unknown
Level # : 1
Sample Name : TP - 35
Sample ID :
Sample Amount : 1
Dilution Factor : 1
Vial # : 3
Injection Volume : 0.50

Chromatogram TP - 35 E:\SBS\M.Sc students\Dr. J. Rajendran\TP - 35_1_03-06-2022_7.qgd



Peak Report TIC

Peak#	Name	R.Time	Area	Area%	Similarity	Base m/z
1	BOROXIN, TRIMETHOXY-	3.037	34665	0.01	74	73.05
2	PYRIDINE	3.429	66850459	18.48	97	79.05
3	PYRIDINE	3.583	156411043	43.23	95	79.05
4	PYRIDINE	3.895	42439473	11.73	97	79.05
5		4.164	43509	0.01	0	51.05
6	PYRIDINE	4.200	35880	0.01	87	79.05
7	PYRIDINE	4.305	4862334	1.34	97	79.05
8	Butanoic acid, 3-methyl-	4.790	78906	0.02	95	60.00
9	BUTANOIC ACID, 2-METHYL-	4.905	62542	0.02	92	74.05
10	Trifluoroacetic acid	5.614	5537035	1.53	95	45.00
11	HEXANOIC ACID	6.669	98215	0.03	94	60.00
12	Phenol	6.757	272882	0.08	98	94.05
13	METHYL 2-HYDROXYETHYL SULFOXIDE	6.842	329209	0.09	85	45.00
14	2-(ACETYLOXY)ETHYL ACETATE	6.902	77989	0.02	92	86.05
15		7.028	40025	0.01	0	110.00
16	Ethanol, 2-(2-ethoxyethoxy)-	7.100	124466	0.03	96	45.05
17	1-HEXANOL, 2-ETHYL-	7.421	720030	0.20	97	57.10
18	L-Glutamine, N2-[(phenylmethoxy)carbonyl]-	7.656	42008	0.01	80	79.05
19		7.749	30989	0.01	0	91.10
20	2(3H)-FURANONE, 5-ETHYLDIHYDRO-	7.924	55465	0.02	81	85.05
21	S-Methyl methanethiosulphonate	8.051	43780	0.01	83	81.00
22	Acetophenone	8.102	70563	0.02	94	105.05
23	p-Cresol	8.206	49788	0.01	90	107.05
24	BENZENE, 1-METHYL-3-(1-METHYLETHYL)-	8.311	27168	0.01	76	119.10
25	PHENOL, 3-(1-METHYLETHYL)-	8.438	49140	0.01	70	121.10
26	NONANAL	8.588	151567	0.04	97	57.05
27	HEXANOIC ACID, 2-ETHYL-	8.773	37275	0.01	84	88.05
28	Benzene, 1,2,3,4-tetramethyl-	8.820	31760	0.01	85	119.10
29	BENZENE, 1,2,3,4-TETRAMETHYL-	8.880	57041	0.02	93	119.10
30	Pentanedioic acid, dimethyl ester	9.064	13150	0.00	77	100.05
31		9.105	4872	0.00	0	55.05
32	Hexanoic acid, 2-methylpropyl ester	9.236	32138	0.01	71	99.05
33	BENZENE, 1-ETHYL-2,3-DIMETHYL-	9.380	38797	0.01	78	119.10
34	6-NONENAL, (Z)-	9.448	19615	0.01	86	55.05
35	Acetic acid, phenylmethyl ester	9.506	11934	0.00	83	108.10
36	(2-HEXYLCYCLOPROPYL)ACETIC ACID #	9.593	43921	0.01	74	60.00
37	Phenol, 2,6-dichloro-	9.697	51416	0.01	80	161.95
38	Ethanol, 2-(2-butoxyethoxy)-	9.853	133610	0.04	95	57.10
39	NAPHTHALENE	9.968	761834	0.21	98	128.05

Peak#	Name	R.Time	Area	Area%	Similarity	Base m/z
40	L-.alpha.-Terpineol	10.050	24039	0.01	73	59.05
41	DECANAL	10.103	65318	0.02	96	57.05
42		10.295	11358	0.00	0	81.05
43	BENZALDEHYDE, 3,4-DIMETHYL-	10.376	146898	0.04	90	133.05
44	2-Coumaranone	10.629	372172	0.10	90	134.05
45		10.718	415515	0.11	0	192.10
46	2-DECENAL, (E)-	10.915	39255	0.01	72	130.05
47	ETHANOL, 2-(DODECYLOXY)-	11.050	54216	0.01	82	57.10
48		11.310	54709	0.02	0	58.05
49	TETRADECANE	11.399	56083	0.02	92	57.10
50	1H-INDOLE	11.464	82856	0.02	95	117.05
51	NAPHTHALENE, 2-METHYL-	11.542	151240	0.04	91	142.10
52	Hexane, 3,3-dimethyl-	11.691	18389	0.01	85	71.10
53	NAPHTHALENE, 1-METHYL-	11.764	40298	0.01	88	142.10
54	1,2-BENZENEDICARBOXYLIC ACID, DIISONONYL ESTER	11.946	18156	0.01	71	149.10
55	2-CYCLOHEXEN-1-OL, 4,4,6-TRIMETHYL-	12.017	8822	0.00	72	84.05
56	3-TERT-BUTYL-6-OCTEN-1-OL	12.074	40357	0.01	72	57.05
57	Ethanol, 2-(2-butoxyethoxy)-, acetate	12.188	181583	0.05	96	57.10
58	.gamma.-Dodecalactone	12.288	31188	0.01	86	85.05
59	1-DODECENE	12.387	11758	0.00	74	75.10
60	PROPANOIC ACID, 2-METHYL-, 3-HYDROXY-2,4,4-TRIMETHYLPENTYL ESTER	12.441	13605	0.00	80	71.10
61	1-TRIDECENE	12.622	76429	0.02	86	69.05
62	Tetradecane	12.719	251425	0.07	89	57.10
63	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	12.826	775252	0.21	93	109.10
64	Naphthalene, 2,3-dimethyl-	13.011	29516	0.01	78	156.10
65		13.170	77861	0.02	0	105.05
66		13.232	42773	0.01	0	156.10
67	QUINOLINE, 1,2-DIHYDRO-2,2,4-TRIMETHYL-	13.383	127742	0.04	85	158.10
68		13.435	18409	0.01	0	105.05
69		13.516	25982	0.01	0	57.05
70		13.565	3974	0.00	0	158.05
71	1-DODECANOL	13.664	238701	0.07	96	55.05
72	HEXADECANE, 2,6,10,14-TETRAMETHYL-	13.827	62375	0.02	86	71.10
73	HEXADECANE	13.965	197094	0.05	92	57.10
74		14.013	12428	0.00	0	147.10
75	2,4-Di-tert-butylphenol	14.088	198142	0.05	91	191.15
76	Propanoic acid, 2,2-dimethyl-, 2-phenylethyl ester	14.175	41961	0.01	72	104.05
77		14.235	23650	0.01	0	57.10
78		14.369	153597	0.04	0	120.05
79	NONADECANE	14.497	30488	0.01	86	71.10
80		14.606	8567	0.00	0	71.10
81	NONAHEXACONTANOIC ACID	14.650	8542	0.00	79	57.10
82	EICOSANE	14.720	67006	0.02	76	57.10
83	PENTADECANE, 8-HEXYL-	14.806	39691	0.01	82	57.10
84		14.888	14362	0.00	0	92.10
85	8-QUINOLINOL	14.968	40704	0.01	85	145.05
86	1,2-Benzenedicarboxylic acid, diundecyl ester	15.059	213931	0.06	77	149.00
87	HEXADECANE	15.142	168962	0.05	97	57.05
88		15.212	33634	0.01	0	105.05
89	1H-AZONINE, OCTAHYDRO-1-NITROSO-	15.317	56952	0.02	77	126.00
90	Dodecanoic acid, 1-methylethyl ester	15.412	57162	0.02	82	60.05
91	Benzophenone	15.660	112812	0.03	87	105.05
92	2,5-PIPERAZINEDIONE, 3-ISOPROPYL-6-METHYL-, (3S,6S)-	15.726	103053	0.03	91	128.05
93	Octadecane, 1-chloro-	15.855	33349	0.01	74	57.10
94	1-NONADECENE	16.030	29760	0.01	87	57.05
95		16.125	19716	0.01	0	236.10
96	1-HEXADECANOL	16.174	120393	0.03	86	55.05
97	Heptadecane	16.257	186926	0.05	95	57.10
98	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	16.341	30356	0.01	74	207.10
99		16.430	32069	0.01	0	105.05
100	1H-PURINE-2,6,8(3H)-TRIONE, 7,9-DIHYDRO-	16.505	392449	0.11	78	70.05
101	3-(1-METHOXY-1-METHYLETHOXY)-2-METHYLPROPYL BENZOATE	16.575	84018	0.02	85	105.05
102		16.629	16055	0.00	0	91.05
103		16.708	249457	0.07	0	59.05
104		16.789	313740	0.09	0	70.10
105		16.951	294081	0.08	0	104.05
106	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-	17.033	254343	0.07	82	111.05
107		17.105	82395	0.02	0	114.05
108		17.215	222936	0.06	0	209.10
109		17.262	129210	0.04	0	70.10
110	Dodecane, 2-methyl-	17.321	48220	0.01	88	57.05
111		17.485	54027	0.01	0	100.10
112	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	17.608	3569989	0.99	81	154.10
113		17.682	239124	0.07	0	156.10
114	2,4-Diphenyl-4-methyl-2(E)-pentene	17.757	449410	0.12	79	143.10
115	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	17.884	2692996	0.74	83	154.10
116	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	17.974	665945	0.18	94	149.00
117	Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-	18.222	188639	0.05	75	152.05
118		18.323	15404	0.00	0	129.05
119		18.384	50435	0.01	0	236.10
120	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	18.464	517923	0.14	89	205.10

Peak#	Name	R.Time	Area	Area%	Similarity	Base m/z
121	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	18.570	2883251	0.80	87	154.10
122		18.646	19486	0.01	0	154.10
123	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	18.749	6653545	1.84	87	154.10
124	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	18.851	3002484	0.83	89	154.10
125	PROLYLLEUCYL ANHYDRIDE	18.900	1667219	0.46	79	154.10
126	n-Hexadecanoic acid	18.948	4767957	1.32	93	73.05
127		19.218	529370	0.15	0	152.05
128	BENZALDEHYDE, 4-HYDROXY-3-METHOXY-	19.280	455016	0.13	79	152.05
129		19.429	59395	0.02	0	222.10
130	CYCLOPENTANE, 1,1'-[3-(2-CYCLOPENTYLETHYL)-1,5-PENTANEDIYL]BIS-	19.565	11826	0.00	71	69.05
131	2,6,10,10-TETRAMETHYL-1-OXASPIRO[4.5]DECAN-6-OL	19.648	72134	0.02	76	85.10
132		19.823	253814	0.07	0	118.10
133		19.941	85542	0.02	0	45.05
134	1-HEXADECANOL	20.093	26849	0.01	71	105.05
135		20.211	12289	0.00	0	105.05
136	2(3H)-Furanone, 5-dodecyldihydro-	20.308	100561	0.03	89	85.05
137	Triclosan	20.456	1607753	0.44	88	218.00
138		20.635	39954	0.01	0	85.05
139		20.688	47570	0.01	0	69.05
140	3-BENZYL-6-METHYL-2,5-PIPERAZINEDIONE #	20.813	803164	0.22	89	91.05
141	3,6-DIISOBUTYL-2,5-PIPERAZINEDIONE #	20.921	692074	0.19	87	170.05
142	Octadecanoic acid, ethyl ester	21.030	36121	0.01	76	88.10
143	2,5-Piperazinedione, 3-(phenylmethyl)-	21.090	58651	0.02	86	91.05
144	Behenic alcohol	21.152	334176	0.09	79	85.10
145	1,2,3,5-TETRAISOPROPYLCYCLOHEXANE	21.253	305039	0.08	74	85.10
146		21.447	2036386	0.56	0	441.30
147	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	21.547	1152266	0.32	75	154.10
148		21.625	726252	0.20	0	441.30
149	2,5-PIPERAZINEDIONE, 3-(1-METHYLETHYL)-6-(PHENYLMETHYL)-, (3S-CIS)-	21.770	773809	0.21	87	91.05
150		22.051	16767	0.00	0	144.00
151		22.096	15743	0.00	0	69.05
152	2(3H)-FURANONE, 5-HEPTYLDIHYDRO-	22.137	11476	0.00	73	85.05
153	2-BUTOXYSULFONYLHEXADECANE	22.201	23558	0.01	73	85.10
154		22.275	86203	0.02	0	129.05
155	3-BENZYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	22.422	3957850	1.09	91	153.05
156	2,5-PIPERAZINEDIONE, 3-(2-METHYLPROPYL)-6-(PHENYLMETHYL)-, (3S-CIS)-	22.560	113378	0.03	76	204.10
157		22.695	41395	0.01	0	59.05
158	3-BENZYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	22.782	5680517	1.57	91	153.05
159		22.889	339192	0.09	0	151.05
160	14-.BETA.-H-PREGNA	22.941	198244	0.05	73	85.10
161	14-.BETA.-H-PREGNA	23.035	76084	0.02	76	85.10
162	OCTADECANOIC ACID, 2-HYDROXYETHYL ESTER	23.118	21411	0.01	71	98.05
163	1,2-PROPANEDIOL, 3-(PHENYLMETHOXY)-, DIACETATE	23.262	3944550	1.09	75	91.05
164		23.525	157950	0.04	0	113.05
165		23.585	197484	0.05	0	85.10
166	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	23.670	628502	0.17	87	98.10
167	Bis(2-ethylhexyl) phthalate	23.819	405939	0.11	95	149.00
168	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	24.001	3029359	0.84	81	91.05
169	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	24.108	4628927	1.28	81	91.05
170	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	24.162	1671647	0.46	81	91.05
171	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	24.239	1971729	0.54	81	91.10
172	14-.BETA.-H-PREGNA	24.593	265786	0.07	70	85.10
173	1,3,5-TRIPHENYLPENTAN-1-ONE	24.672	1077957	0.30	70	105.05
174		24.852	149938	0.04	0	331.20
175		24.940	691483	0.19	0	91.05
176		25.109	874935	0.24	0	170.10
177	4(1H)-Pyrimidinone, 6-amino-2-methyl-5-nitroso-	25.184	1503088	0.42	72	154.10
178	NAPHTHALENE, 1,2,3,4-TETRAHYDRO-1-PHENYL-	25.329	220321	0.06	84	208.10
179	2-THIOPHENECARBOXAMIDE, N-[2-(4-ETHYLPHENOXY)ETHYL]-	25.508	1960169	0.54	74	154.10
180	13-Docosenamide, (Z)-	25.675	40480	0.01	72	59.00
181		25.932	23151	0.01	0	69.05
182	2,5-PIPERAZINEDIONE, 3,6-BIS(PHENYLMETHYL)-	26.033	66549	0.02	83	91.05
183	14-.BETA.-H-PREGNA	26.257	137458	0.04	74	85.10
184	14-.BETA.-H-PREGNA	26.354	47633	0.01	72	85.10
185		26.450	6367	0.00	0	208.00
186		26.552	47640	0.01	0	85.10
187	CHOLESTA-4,6-DIEN-3-OL, (3.BETA.)-	26.679	96084	0.03	80	135.10
188		26.947	14529	0.00	0	69.10
189		27.057	48811	0.01	0	207.00
190		27.215	15993	0.00	0	207.00
191		27.290	9087	0.00	0	371.25
192		27.381	14669	0.00	0	207.00
193		27.517	14147	0.00	0	207.00
194		27.627	11142	0.00	0	207.00
195		27.825	111689	0.03	0	489.30
196		27.960	587898	0.16	0	57.05
197		28.239	599032	0.17	0	316.25
198	14-.BETA.-H-PREGNA	28.469	65453	0.02	74	85.10
199		28.601	50211	0.01	0	85.10
200	1H-INDENE, 2,3-DIHYDRO-	29.366	354657	0.10	71	91.05
201	1H-INDENE, 2,3-DIHYDRO-	29.553	210354	0.06	71	91.05

Peak#	Name	R.Time	Area	Area%	Similarity	Base m/z
202		29.760	53922	0.01	0	130.05
203		30.079	18943	0.01	0	207.00
204		31.000	19241	0.01	0	209.00
205		31.100	6847	0.00	0	207.00
206		31.165	12551	0.00	0	207.00
207		31.435	33650	0.01	0	208.00
208		31.708	33439	0.01	0	85.10
			361838012	100.00		

***Kindly Acknowledge GC-MS/MS, DST-FIST Facility, School of Biological Sciences,
Madurai Kamaraj University while publishing the results in journals, dissertation, thesis, etc.***