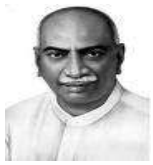
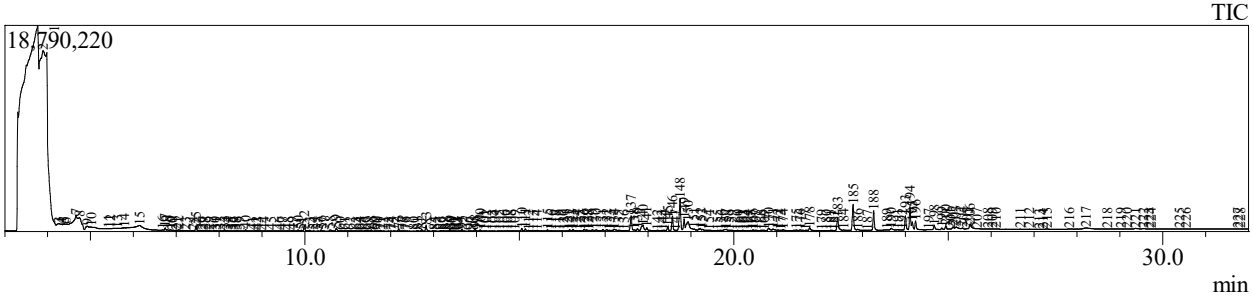
Madurai Kamaraj University
School of Biological Sciences
Gas Chromatography Mass Spectrometry Facility
DST-FIST Facility



Sample Information

Analyzed by	: Admin
Analyzed	: 6/3/2022 5:55:17 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: TP - 36
Sample ID	:
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 4
Injection Volume	: 0.50

Chromatogram TP - 36 E:\SBS\M.Sc students\Dr. J. Rajendran\TP - 36_1_03-06-2022_8.qgd



Peak Report TIC

Peak#	Name	R.Time	Area	Area%	Similarity	Base m/z
1	PYRIDINE	3.768	456616263	57.86	93	79.05
2	PYRIDINE	3.893	226017162	28.64	95	79.05
3	PYRIDINE	4.263	783787	0.10	97	79.05
4	PYRIDINE	4.320	435938	0.06	93	79.05
5	PYRIDINE	4.384	589401	0.07	94	79.05
6	PYRIDINE	4.430	1132826	0.14	91	79.05
7	PYRIDINE	4.662	8301224	1.05	98	79.05
8	PYRIDINE	4.740	5743175	0.73	98	79.05
9	ACETIC ACID, TRIFLUORO-	4.919	1930704	0.24	83	45.00
10	ACETIC ACID, TRIFLUORO-	5.020	2358570	0.30	85	45.00
11		5.420	1144409	0.15	0	51.00
12		5.460	430519	0.05	0	45.00
13		5.625	1313619	0.17	0	57.10
14	Dimethyl sulfone	5.784	1200433	0.15	83	79.00
15	ACETIC ACID, TRIFLUORO-	6.142	7634224	0.97	95	45.00
16	HEXANOIC ACID	6.683	110232	0.01	95	60.00
17	Phenol	6.738	378226	0.05	98	94.05
18	METHYL 2-HYDROXYETHYL SULFOXIDE	6.793	93511	0.01	86	45.00
19	2-(ACETYLOXY)ETHYL ACETATE	6.859	120421	0.02	85	86.05
20	Butanoic acid, butyl ester	6.905	56734	0.01	87	71.05
21		6.993	59751	0.01	0	205.00
22	ETHANOL, 2-(2-ETHOXYETHOXY)-	7.056	139256	0.02	95	45.05
23	2-Propanol, 1-(2-methoxypropoxy)-	7.224	20657	0.00	86	59.05
24		7.390	12325	0.00	0	99.05
25	1-HEXANOL, 2-ETHYL-	7.458	772855	0.10	98	57.05
26	1-HEPTANOL, 4-METHYL-	7.572	34352	0.00	86	69.05
27	Benzyl alcohol	7.624	26090	0.00	91	79.05
28	3-UNDECENE, 5-METHYL-, CIS/TRANS	7.679	24068	0.00	84	55.05
29	3-METHYLBUTYL BENZENEACETATE	7.770	38006	0.00	74	91.05
30	5-(HYDROXYMETHYL)DIHYDRO-2(3H)-FURANONE	7.890	60389	0.01	78	85.05
31		7.930	33961	0.00	0	119.10
32	S-Methyl methanethiosulphonate	8.016	31330	0.00	83	81.00
33	ETHANONE, 1-PHENYL-	8.124	184690	0.02	87	105.05
34	p-Cresol	8.185	93235	0.01	90	107.05
35	BENZENE, 1,2,3,4-TETRAMETHYL-	8.265	5935	0.00	80	119.05
36	2-Butoxyethyl acetate	8.320	14210	0.00	75	57.05
37	BENZENE, METHYL(1-METHYLETHYL)-	8.361	16982	0.00	82	119.10
38	1-(4-FLUOROPHENYL)-3-{[2-(4-METHOXYPHENYL)ETHYL]AMINO}-1H-PYRROLE	8.407	45878	0.01	71	121.10
39	GLUTARALDEHYDIC ACID, ETHYL ESTER, 5-(DIETHYL ACETAL)	8.472	28126	0.00	73	85.10

Peak#	Name	R.Time	Area	Area%	Similarity	Base m/z
40	NONANAL	8.614	167205	0.02	97	57.05
41	HEXANOIC ACID, 2-ETHYL-	8.777	24746	0.00	89	73.05
42	BENZENE, 1,2,3,4-TETRAMETHYL-	8.861	58324	0.01	93	119.05
43	BENZENE, 1,2,3,4-TETRAMETHYL-	8.917	48770	0.01	96	119.10
44	Pentanedioic acid, dimethyl ester	9.040	16003	0.00	74	59.05
45		9.210	37360	0.00	0	70.05
46	Benzene, 1,2,3,4-tetramethyl-	9.398	92426	0.01	88	119.10
47	2-NONENAL	9.463	38288	0.00	86	55.05
48	9,12,15-OCTADECATRIENOIC ACID, (2-PHENYL-1,3-DIOXOLAN-4-YL)METHYL ES	9.599	57761	0.01	71	105.05
49	ETHANONE, 1-(4-METHYLPHENYL)-	9.704	90875	0.01	71	119.05
50	Ethanol, 1-(2-butoxyethoxy)-	9.837	168152	0.02	96	57.05
51	ETHANONE, 1-(4-METHYLPHENYL)-	9.917	110467	0.01	94	119.05
52	NAPHTHALENE	9.982	955422	0.12	97	128.05
53	DECANAL	10.112	109635	0.01	97	57.05
54		10.191	37257	0.00	0	133.10
55	Pinocarvone	10.296	12475	0.00	72	81.05
56	BENZALDEHYDE, 3,4-DIMETHYL-	10.376	196788	0.02	90	133.05
57		10.435	28423	0.00	0	112.05
58	Benzothiazole	10.587	344233	0.04	90	135.00
59		10.727	546011	0.07	0	192.05
60		10.820	22441	0.00	0	57.05
61	2-DECENAL, (E)-	10.920	31196	0.00	78	70.05
62	OCTADECANOIC ACID	11.046	87470	0.01	84	57.05
63	3(2H)-BENZOFURANONE, 7-METHYL-	11.192	31302	0.00	73	119.05
64		11.255	15176	0.00	0	59.05
65		11.306	42488	0.01	0	58.05
66	TRIDECANE	11.400	74555	0.01	95	57.05
67	1H-INDOLE	11.455	106296	0.01	94	117.05
68	NAPHTHALENE, 2-METHYL-	11.546	202741	0.03	95	142.10
69	BENZENEACETIC ACID, .ALPHA.-HYDROXY-	11.615	11928	0.00	70	107.05
70	TETRADECANE	11.684	18337	0.00	85	71.10
71	NAPHTHALENE, 2-METHYL-	11.766	72277	0.01	93	142.10
72		11.826	22865	0.00	0	71.05
73	4-(DIMETHOXYMETHYL)-1,2-DIMETHYLBENZENE	11.949	27752	0.00	77	149.05
74		12.007	15814	0.00	0	84.00
75	1-CHLOROOCTADECANE	12.065	28290	0.00	75	57.05
76	Ethanol, 2-(2-butoxyethoxy)-, acetate	12.181	278924	0.04	96	57.05
77	2(3H)-FURANONE, 5-HEPTYLDIHYDRO-	12.283	44265	0.01	89	85.00
78	TETRADECANE, 2-METHYL-	12.338	9207	0.00	77	57.05
79	1-Undecanol	12.383	16709	0.00	77	55.05
80	2-AMYL-4-METHYL-1,3-DIOXOLANE	12.535	14862	0.00	84	87.05
81	1-TRIDECANOL	12.619	119653	0.02	85	55.05
82	Tetradecane	12.718	246118	0.03	97	57.05
83	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	12.822	1053210	0.13	94	109.10
84	NAPHTHALENE, 1,8-DIMETHYL-	13.001	82642	0.01	83	156.05
85	BENZOIC ACID, 2-METHYLPROPYL ESTER	13.045	32161	0.00	86	105.05
86		13.166	103162	0.01	0	107.05
87		13.228	72851	0.01	0	156.10
88	Diphenylmethane	13.278	9361	0.00	78	167.10
89	QUINOLINE, 1,2-DIHYDRO-2,2,4-TRIMETHYL-	13.379	212102	0.03	88	158.10
90		13.430	29042	0.00	0	105.00
91		13.474	11313	0.00	0	55.05
92		13.512	27278	0.00	0	57.05
93	NAPHTHALENE, 1-METHOXY-	13.560	10787	0.00	76	158.05
94	3,11-DIMETHYL-NONACOSANE	13.607	46658	0.01	71	57.05
95	1-DODECANOL	13.659	308513	0.04	96	55.05
96	HENEICOSANE	13.822	31040	0.00	82	71.10
97		13.864	21488	0.00	0	69.05
98	HEXADECANE	13.960	328799	0.04	90	57.05
99		14.011	12178	0.00	0	91.05
100	2,4-Di-tert-butylphenol	14.084	206162	0.03	86	191.10
101		14.175	45638	0.01	0	161.05
102		14.225	30989	0.00	0	155.10
103	EICOSANE	14.367	41680	0.01	74	57.05
104		14.416	9589	0.00	0	168.05
105	4,5-DIPROPYLOCTANE	14.529	44536	0.01	72	57.10
106	Pentadecane, 4-methyl-	14.645	17479	0.00	83	71.10
107	HEXADECANE, 2,6,10,14-TETRAMETHYL-	14.713	74351	0.01	77	57.05
108	PENTADECANE, 3-METHYL-	14.800	52697	0.01	85	57.05
109	CYCLOHEXANONE, 5-METHYL-2-(1-METHYLETHYL)-, CIS-	14.884	25100	0.00	71	69.00
110	1,2-Benzenedicarboxylic acid, diundecyl ester	15.055	305956	0.04	76	149.00
111	HEXADECANE	15.137	270163	0.03	97	57.05
112	Acetic acid n-octadecyl ester	15.213	77198	0.01	72	97.10
113	1-METHYL-2,4-(1H,3H)PYRIMIDINDIONE	15.315	77897	0.01	71	126.05
114	Dodecanoic acid, 1-methylethyl ester	15.409	69595	0.01	79	60.00
115	METHANONE, DIPHENYL-	15.655	196665	0.02	90	105.05
116	2,5-PIPERAZINEDIONE, 3-ISOPROPYL-6-METHYL-, (3S,6S)-	15.738	79661	0.01	83	128.05
117	Tetradecane, 1-chloro-	15.853	36931	0.00	74	57.05
118	Benzene, 1,1'-(1,3-propanediyl)bis-	15.895	5634	0.00	79	92.05
119	PENTADECANE, 8-HEXYL-	15.934	15656	0.00	84	57.05
120	1-HEXADECANOL	16.023	35524	0.00	89	57.05

Peak#	Name	R.Time	Area	Area%	Similarity	Base m/z
121		16.120	23076	0.00	0	236.10
122	1-HEXADECANOL	16.170	206271	0.03	85	55.05
123	Heptadecane	16.250	217310	0.03	96	57.05
124	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	16.334	25001	0.00	79	207.10
125	2H-PYRROLE, 5-ETHYL-3,4-DIHYDRO-2-METHYL-4,4-DIPHENYL-	16.417	59179	0.01	77	208.10
126	1H-PURINE-2,6,8(3H)-TRIONE, 7,9-DIHYDRO-	16.508	322919	0.04	77	70.05
127	3-(1-METHOXY-1-METHYLETHOXY)-2-METHYLPROPYL BENZOATE	16.569	183259	0.02	83	105.05
128	[(2E)-4-PHENYL-2-BUTENYL]BENZENE #	16.620	89111	0.01	74	91.05
129		16.704	240284	0.03	0	59.05
130		16.790	282395	0.04	0	70.05
131	BENZENE, 1,1'-(1,2-CYCLOBUTANEDIYL)BIS-, TRANS-	16.946	293427	0.04	78	104.05
132	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-	17.032	213192	0.03	72	111.05
133		17.095	68116	0.01	0	114.00
134		17.208	427246	0.05	0	209.10
135	Hexadecane	17.314	84769	0.01	90	57.05
136		17.438	33756	0.00	0	178.05
137	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	17.606	3177960	0.40	81	154.05
138		17.675	167903	0.02	0	156.10
139	2,4-Diphenyl-4-methyl-2(E)-pentene	17.750	347333	0.04	84	143.10
140	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	17.882	1954503	0.25	83	154.05
141	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	17.969	485062	0.06	92	149.00
142	Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-	18.217	130402	0.02	73	152.05
143		18.320	57521	0.01	0	57.05
144		18.374	122828	0.02	0	236.10
145	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	18.460	699901	0.09	89	205.05
146	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	18.567	2701722	0.34	86	154.05
147		18.635	8714	0.00	0	119.10
148	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	18.746	6802021	0.86	85	154.05
149	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	18.839	2128921	0.27	89	154.05
150		18.932	4342901	0.55	0	167.00
151	1,2-Benzenedicarboxylic acid, butyl octyl ester	19.076	266201	0.03	90	149.00
152		19.218	471000	0.06	0	118.05
153	BENZALDEHYDE, 4-HYDROXY-3-METHOXY-	19.269	164896	0.02	78	152.05
154	9,10-ANTHRACENEDIONE, 2-METHYL-	19.427	36879	0.00	71	222.10
155		19.627	15284	0.00	0	143.05
156	2-CYCLOHEXYL-5-HYDROXY-4-METHOXY-3(2H)-PYRIDAZINONE #	19.706	23311	0.00	70	143.10
157		19.822	392032	0.05	0	118.05
158		19.875	21327	0.00	0	191.05
159		19.945	16114	0.00	0	57.05
160		20.087	20857	0.00	0	105.05
161		20.145	7822	0.00	0	120.05
162	TRICOSANE	20.206	36433	0.00	78	57.10
163	SULFUR, MOL. (S8)	20.235	8965	0.00	85	63.95
164	2(3H)-Furanone, 5-dodecyldihydro-	20.305	13531	0.00	72	85.05
165		20.394	32286	0.00	0	221.10
166		20.446	119184	0.02	0	74.05
167		20.502	114830	0.01	0	91.05
168		20.636	62807	0.01	0	131.10
169		20.700	42294	0.01	0	157.10
170	3-BENZYL-6-METHYL-2,5-PIPERAZINEDIONE #	20.808	620869	0.08	91	91.05
171	3,6-DIISOBUTYL-2,5-PIPERAZINEDIONE #	20.911	392660	0.05	84	170.05
172	HEPTADECANOIC ACID, 15-METHYL-, ETHYL ESTER	21.026	39443	0.00	75	88.05
173	BENZENE, (2,3-DIMETHYLDECYL)-	21.085	45088	0.01	73	91.05
174	2-Pentadecanol	21.150	138430	0.02	85	70.10
175		21.455	187528	0.02	0	91.05
176	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	21.546	105263	0.01	71	154.05
177	3-ISOBUTYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	21.679	45578	0.01	73	154.05
178	3-BENZYL-6-ISOPROPYL-2,5-PIPERAZINEDIONE #	21.766	623262	0.08	88	91.05
179		22.050	23442	0.00	0	144.00
180	CYCLONONASILOXANE, OCTADECAMETHYL-	22.152	13966	0.00	70	281.05
181		22.272	80541	0.01	0	129.05
182		22.340	5993	0.00	0	45.05
183	3-BENZYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	22.417	3063593	0.39	90	153.05
184	2,5-PIPERAZINEDIONE, 3-(2-METHYLPROPYL)-6-(PHENYLMETHYL)-, (3S-CIS)-	22.560	29225	0.00	78	91.05
185	3-BENZYLHEXAHYDROPYRROLO[1,2-A]PYRAZINE-1,4-DIONE #	22.780	5703367	0.72	91	153.05
186		22.887	313254	0.04	0	151.05
187	OCTADECANOIC ACID, 2-HYDROXYETHYL ESTER	23.108	46828	0.01	83	98.10
188	1,2-PROPANEDIOL, 3-(PHENYLMETHOXY)-, DIACETATE	23.258	3647838	0.46	75	91.05
189		23.574	268720	0.03	0	117.00
190	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	23.666	666797	0.08	86	98.05
191	1,2-BENZENEDICARBOXYLIC ACID	23.815	131860	0.02	90	149.00
192		23.930	9537	0.00	0	205.05
193	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	23.997	2678948	0.34	82	91.05
194	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	24.105	4375348	0.55	82	91.05
195	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	24.159	1467911	0.19	81	91.05
196	1-PROPEN, 3-(2-CYCLOPENTENYL)-2-METHYL-1,1-DIPHENYL-	24.235	1928529	0.24	81	91.05
197		24.542	122100	0.02	0	156.10
198	1,3,5-Triphenyl-1,5-pentanedione	24.670	1031753	0.13	73	105.05
199	4-TERT-BUTYL-2-(4-METHOXY-PHENYL)-6-P-TOLYL-PYRIDINE	24.847	283176	0.04	75	331.20
200		24.937	687731	0.09	0	91.05
201		25.040	110315	0.01	0	117.00

Peak#	Name	R.Time	Area	Area%	Similarity	Base m/z
202		25.106	693797	0.09	0	91.05
203	4(1H)-Pyrimidinone, 6-amino-2-methyl-5-nitroso-	25.180	988042	0.13	73	154.05
204	NAPHTHALENE, 1,2,3,4-TETRAHYDRO-1-PHENYL-	25.327	248838	0.03	84	208.05
205	NAPHTHALENE, 1,2,3,4-TETRAHYDRO-1-PHENYL-	25.441	83028	0.01	82	208.05
206	4,6-DIHYDROFURO[3,4-B]FURAN-3-CARBOXYLIC ACID	25.507	1675067	0.21	71	154.05
207		25.670	5354	0.00	0	207.00
208		25.927	22130	0.00	0	69.05
209	2,5-PIPERAZINEDIONE, 3,6-BIS(PHENYLMETHYL)-	26.031	58366	0.01	79	91.05
210		26.111	45195	0.01	0	281.05
211		26.674	53819	0.01	0	207.00
212		26.889	67577	0.01	0	221.05
213		27.120	14202	0.00	0	177.00
214		27.205	4128	0.00	0	207.00
215		27.299	33029	0.00	0	371.20
216		27.816	102235	0.01	0	489.25
217		28.205	1002079	0.13	0	316.25
218		28.706	29115	0.00	0	207.00
219		29.030	16742	0.00	0	208.00
220		29.165	9881	0.00	0	57.05
221	1H-INDENE, 2,3-DIHYDRO-	29.365	260345	0.03	70	91.05
222		29.546	161396	0.02	0	91.05
223		29.675	5688	0.00	0	207.00
224		29.725	15714	0.00	0	130.05
225		30.394	7292	0.00	0	207.00
226		30.542	40316	0.01	0	208.00
227		31.750	7151	0.00	0	281.05
228		31.834	19514	0.00	0	207.00
			789148436	100.00		