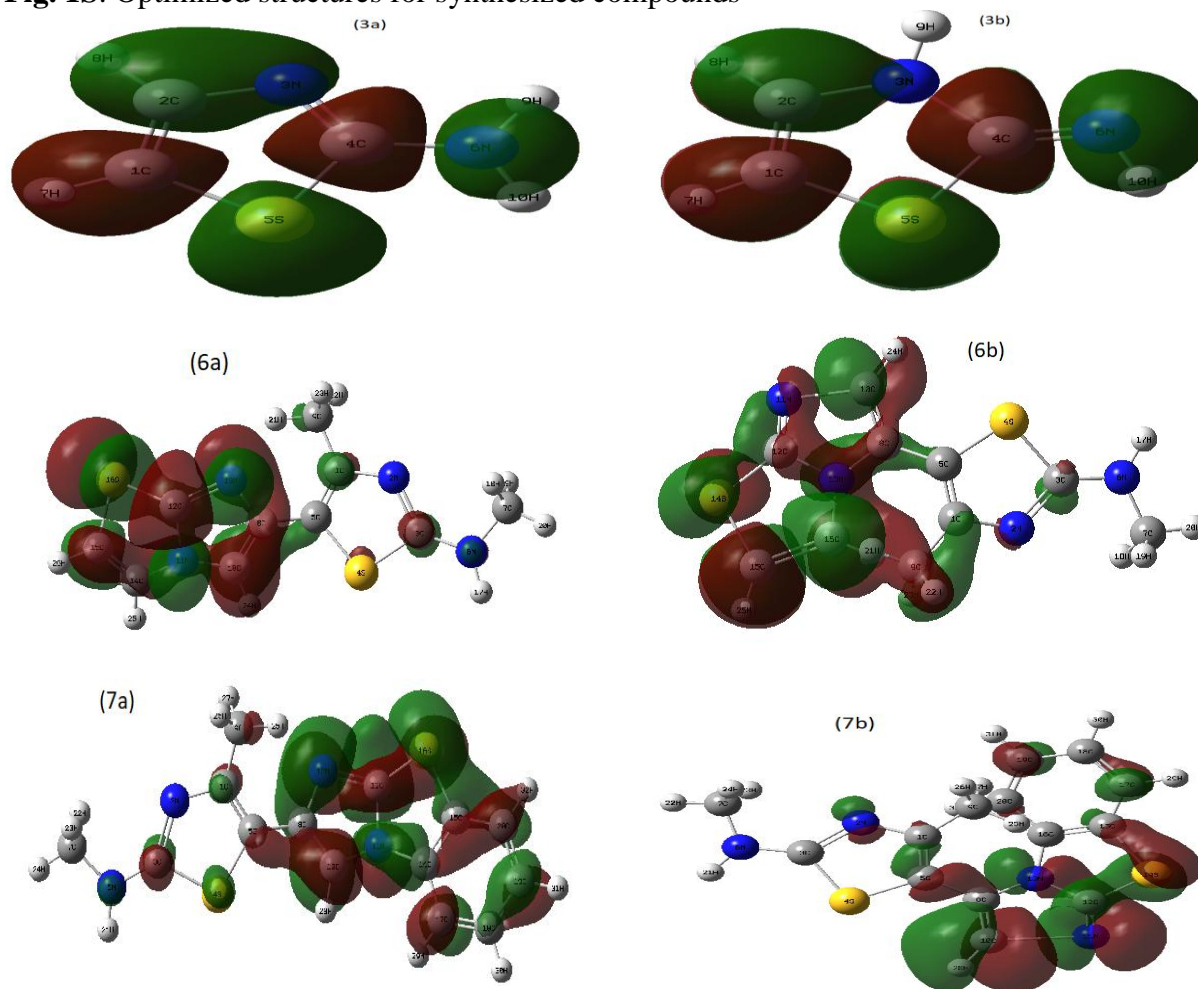


Fig. 1S. Optimized structures for synthesized compounds



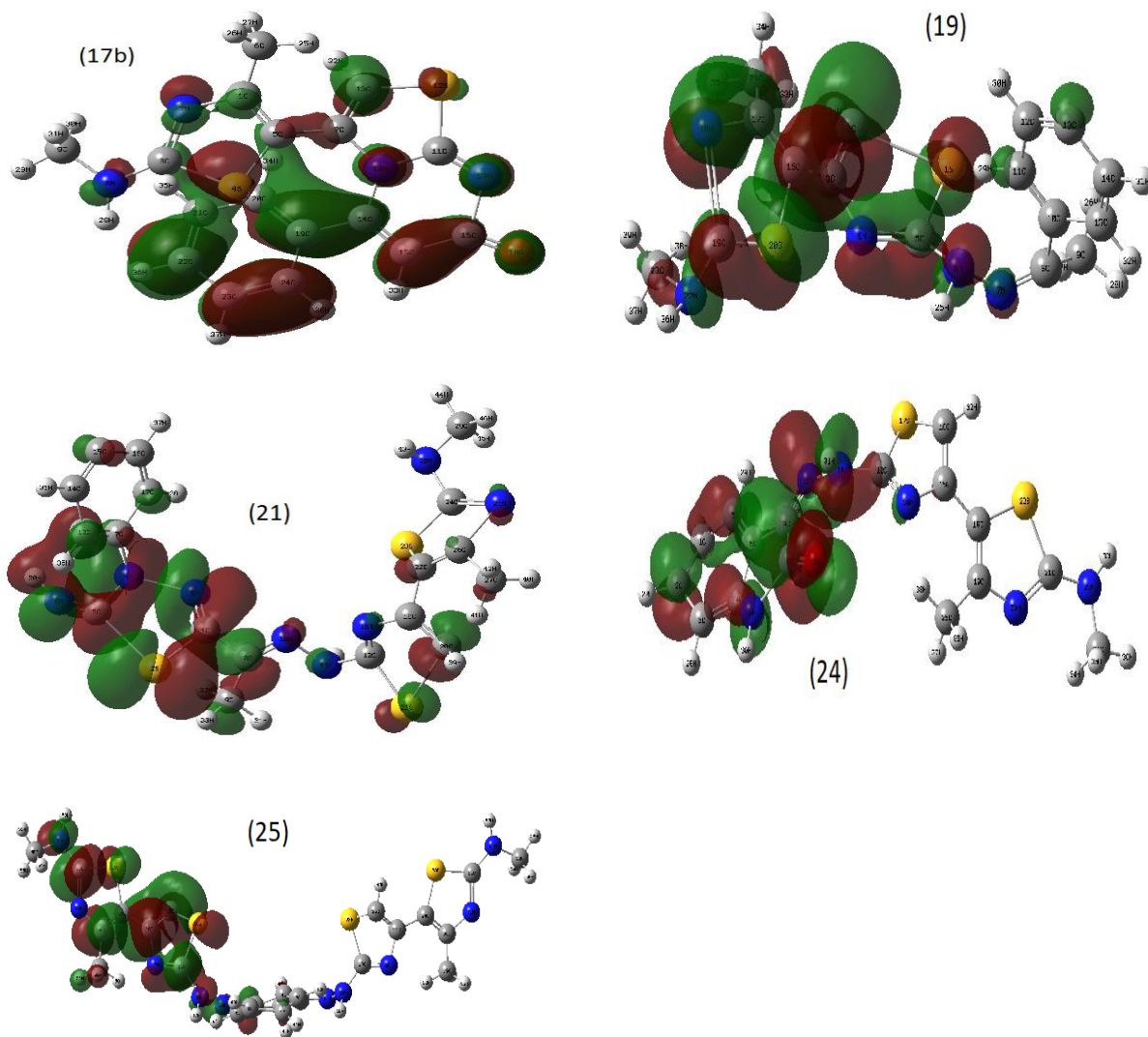
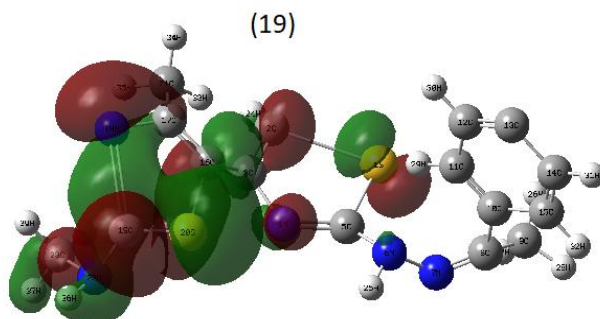
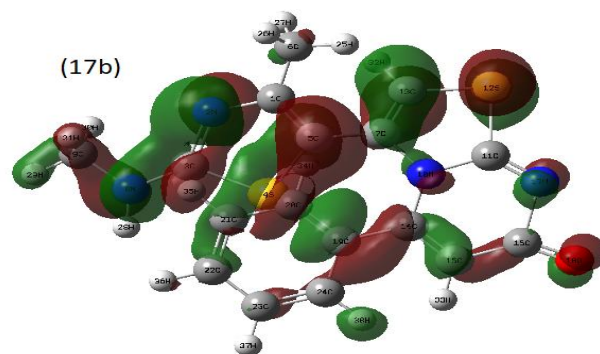
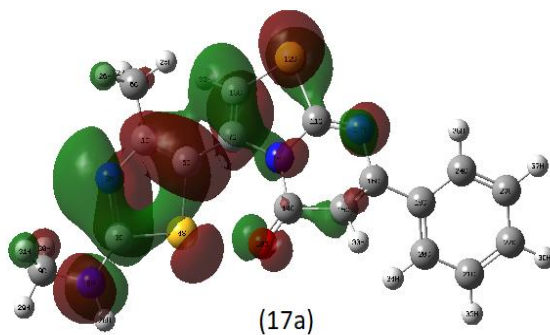
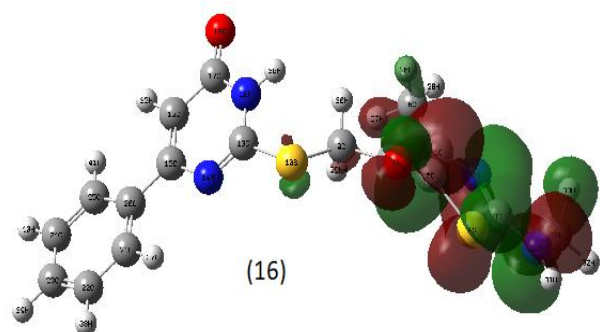
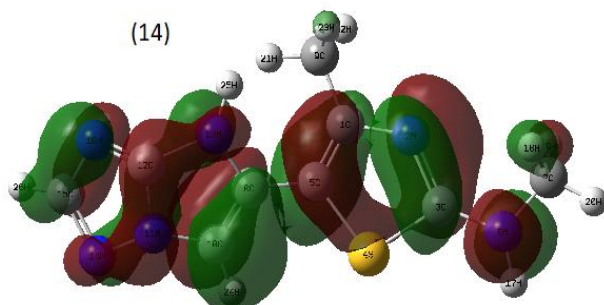
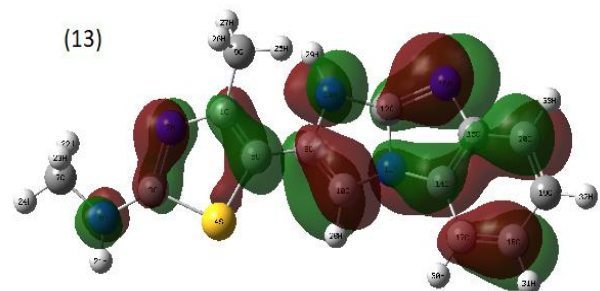
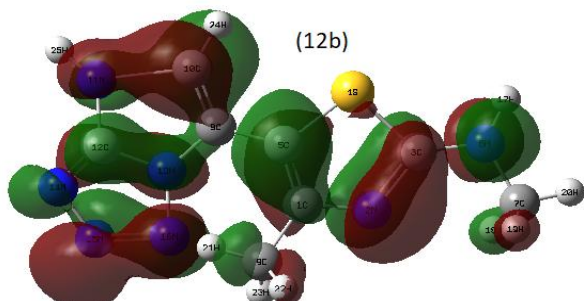
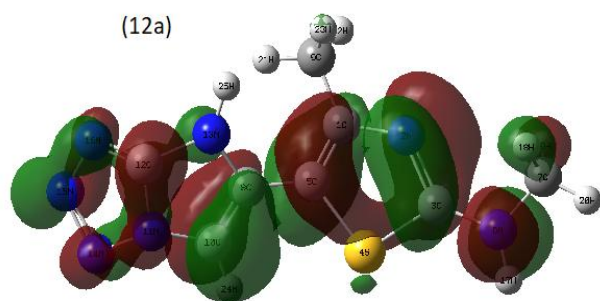


Fig. 2S. LUMO images of optimized structures



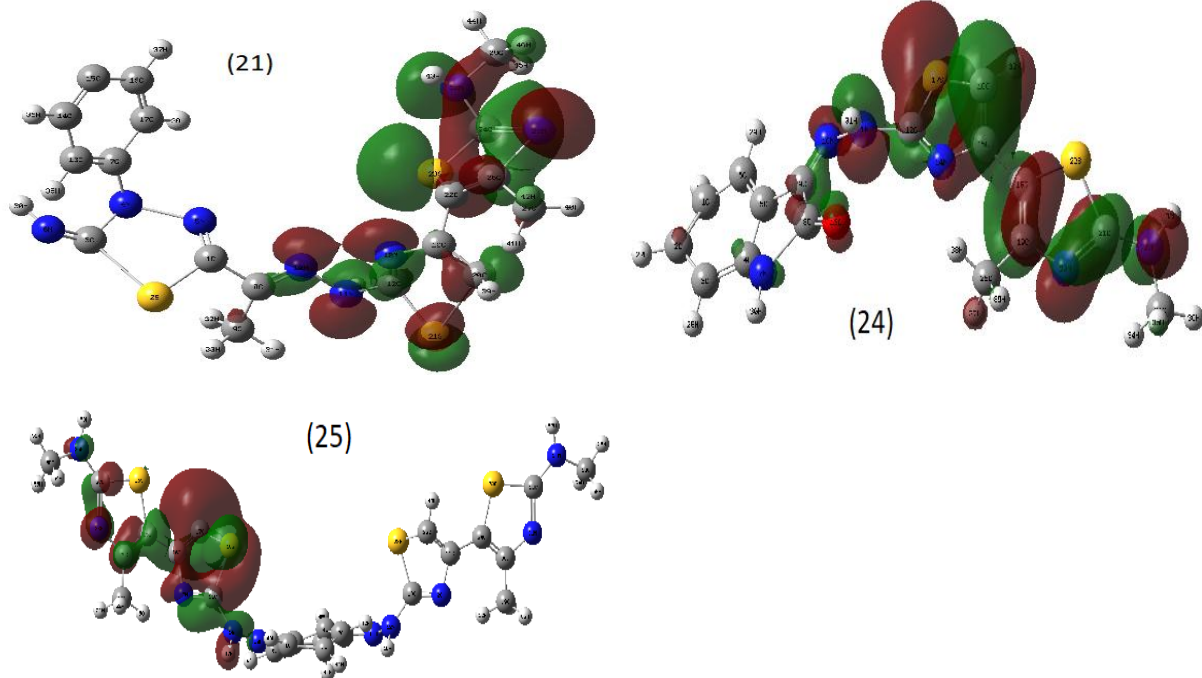
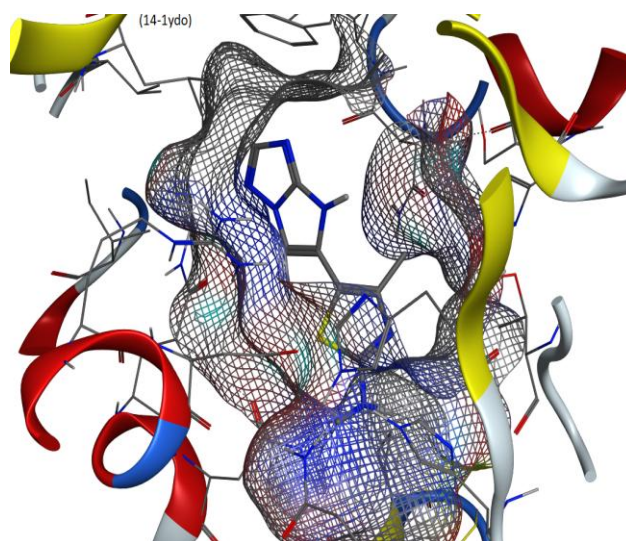
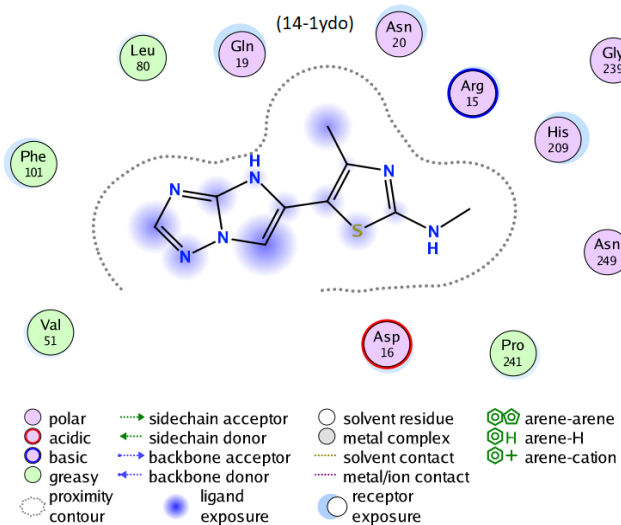
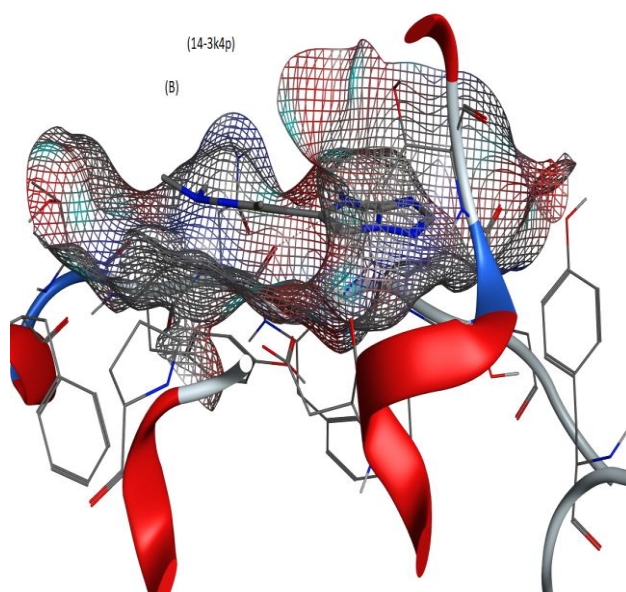
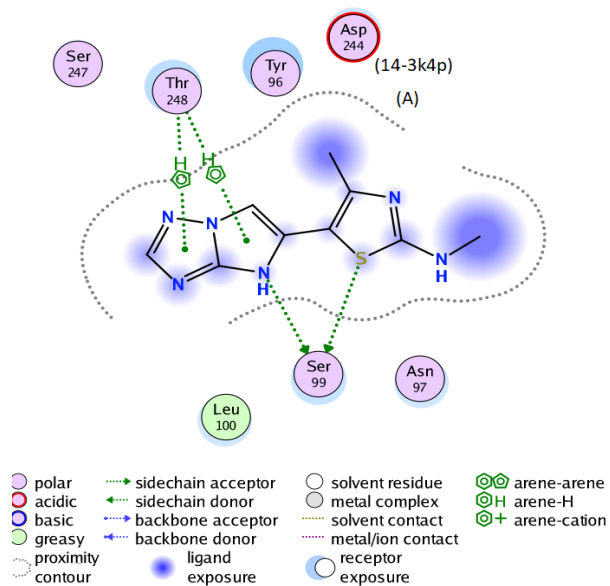
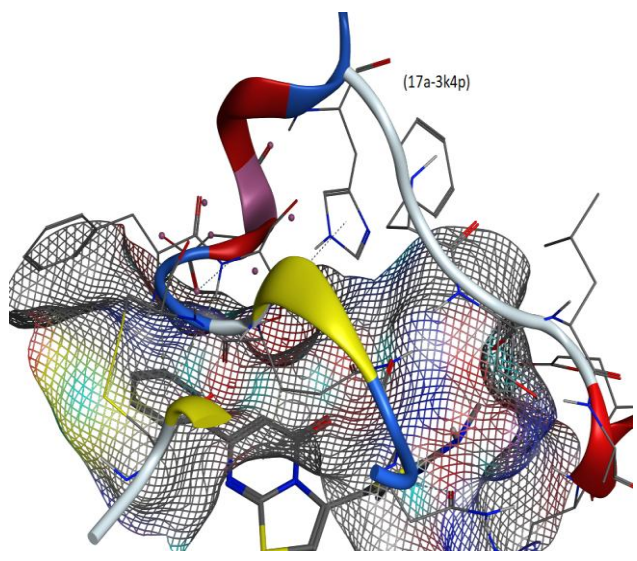
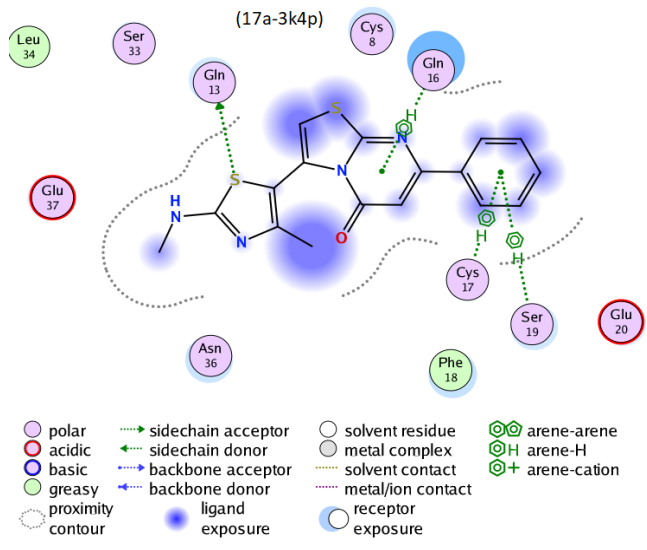
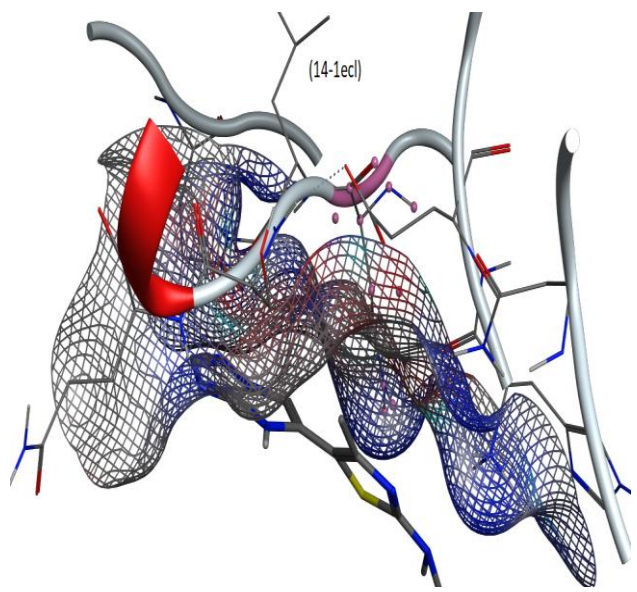
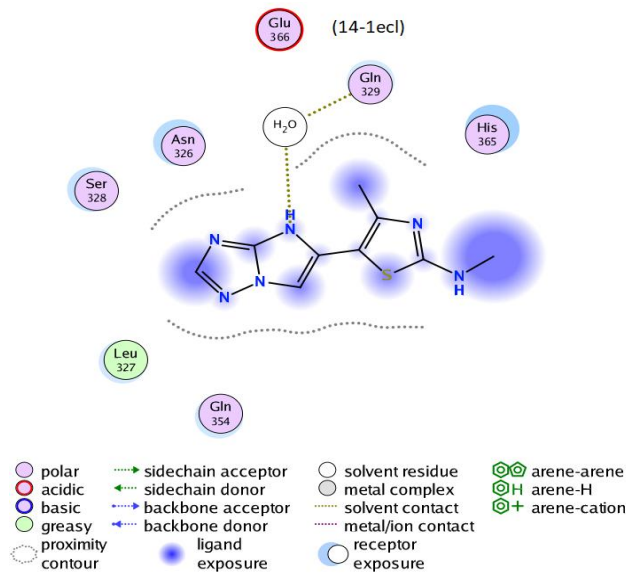
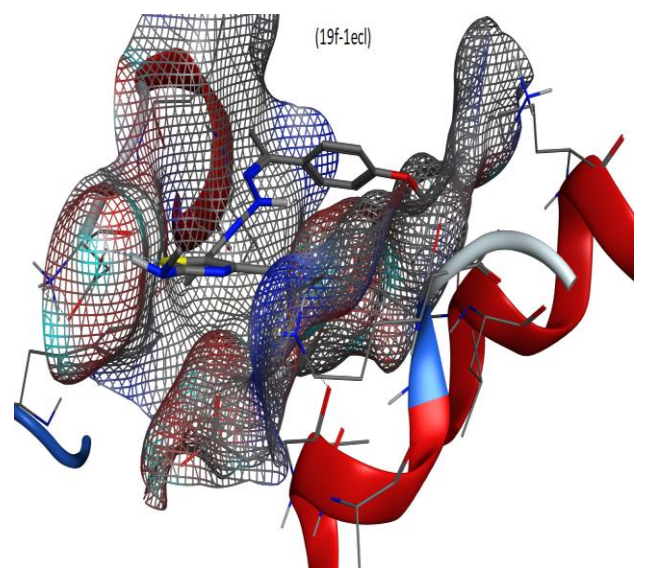
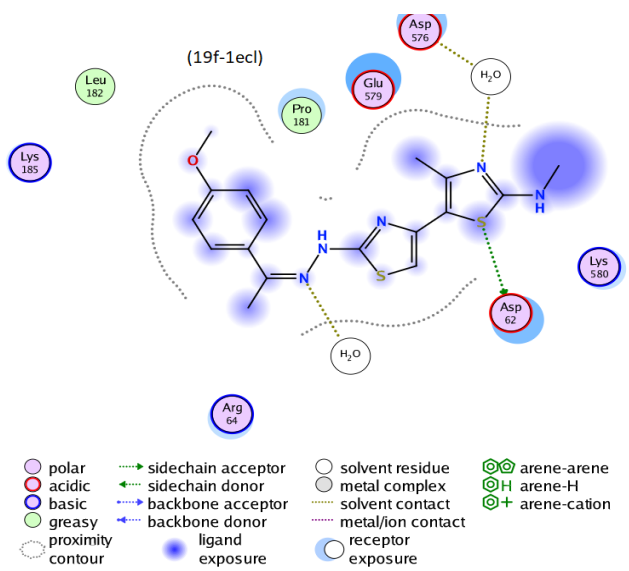
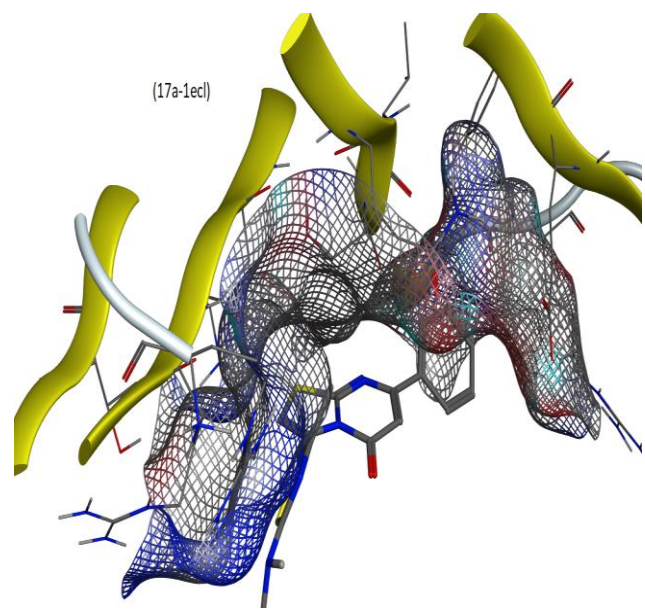
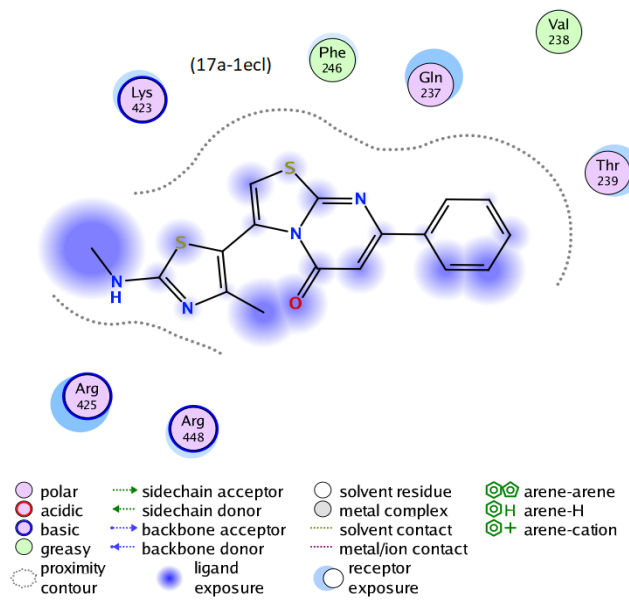


Figure 3S HOMO images of optimized structures







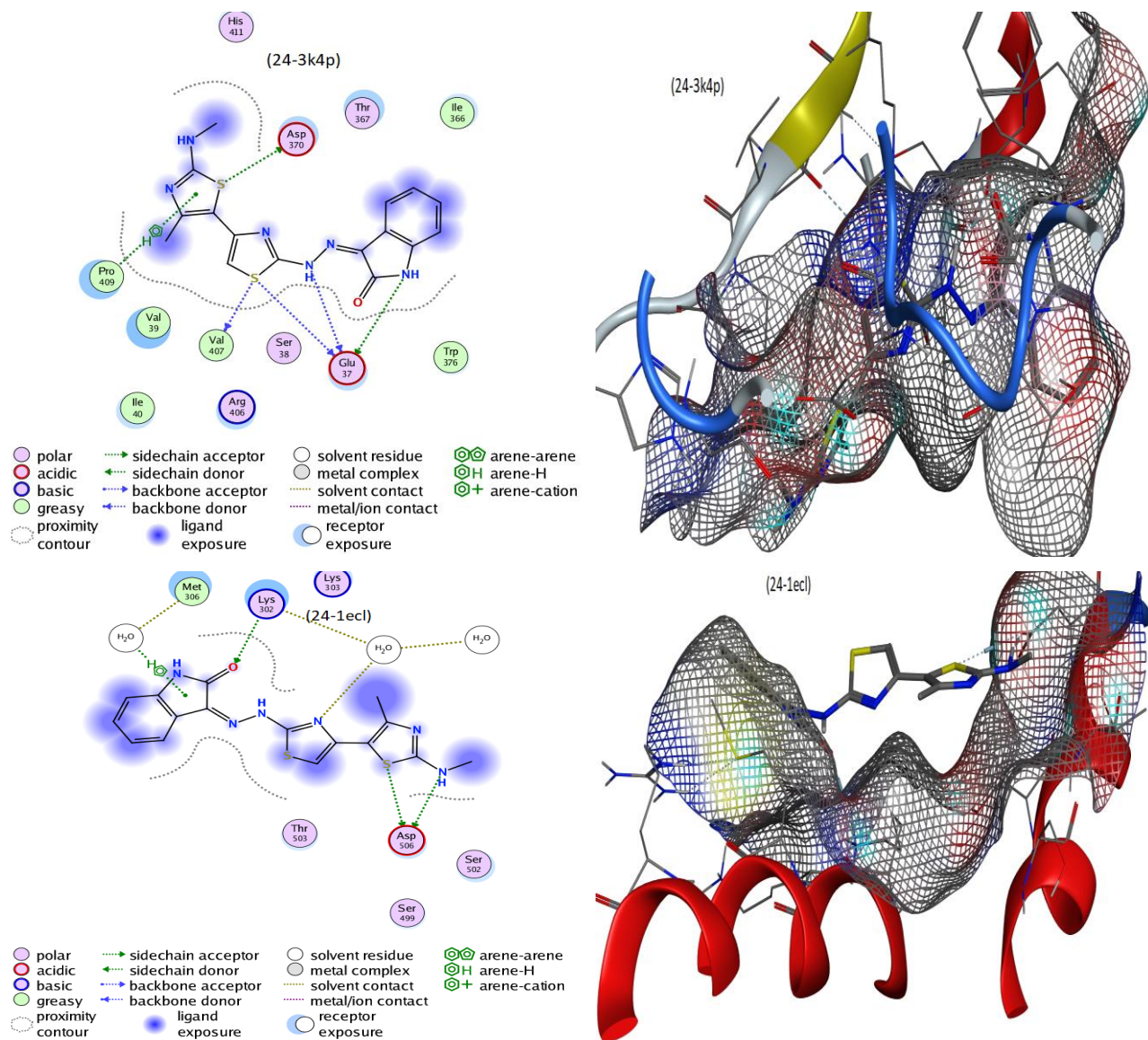
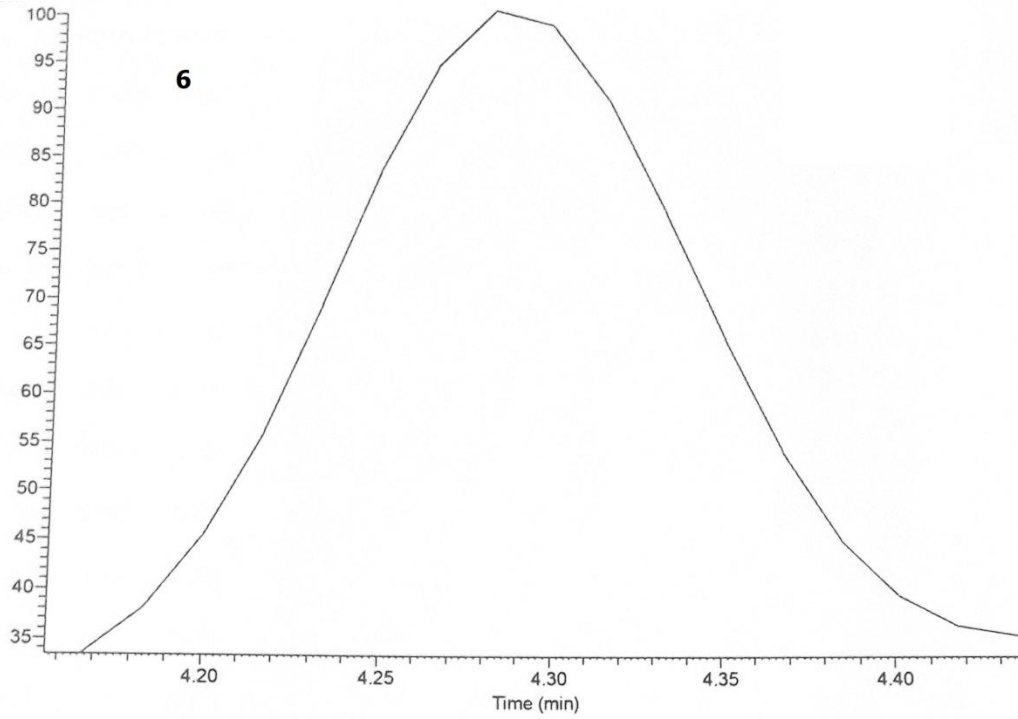
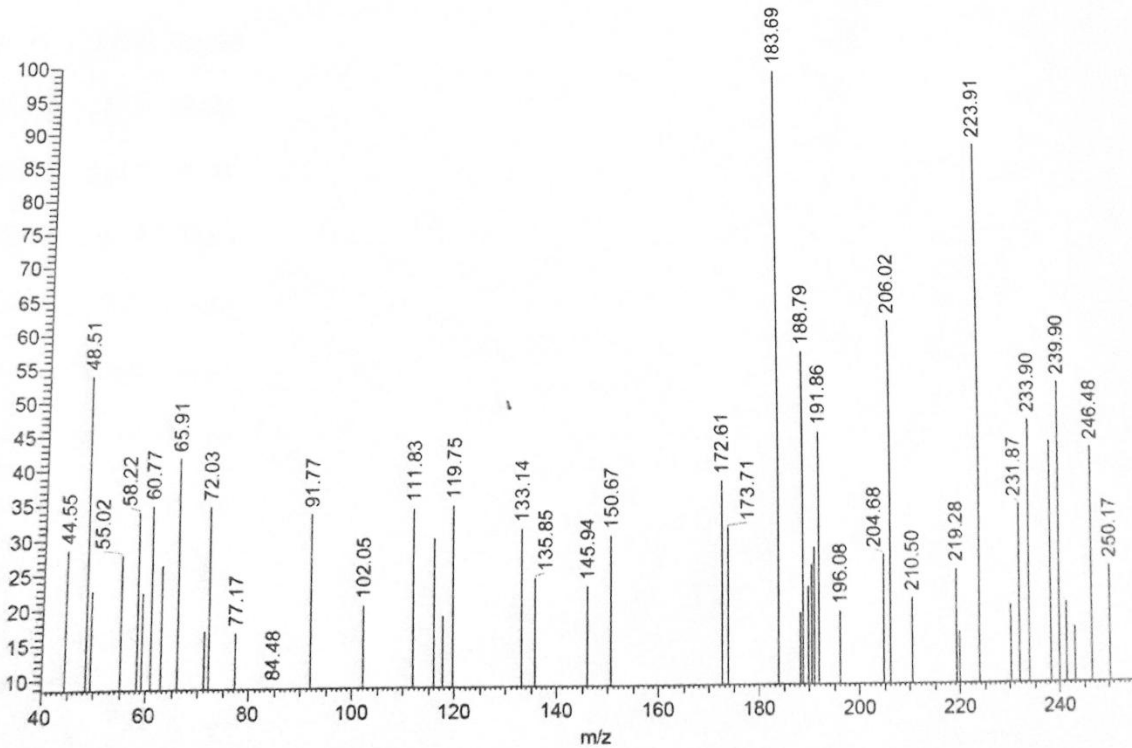
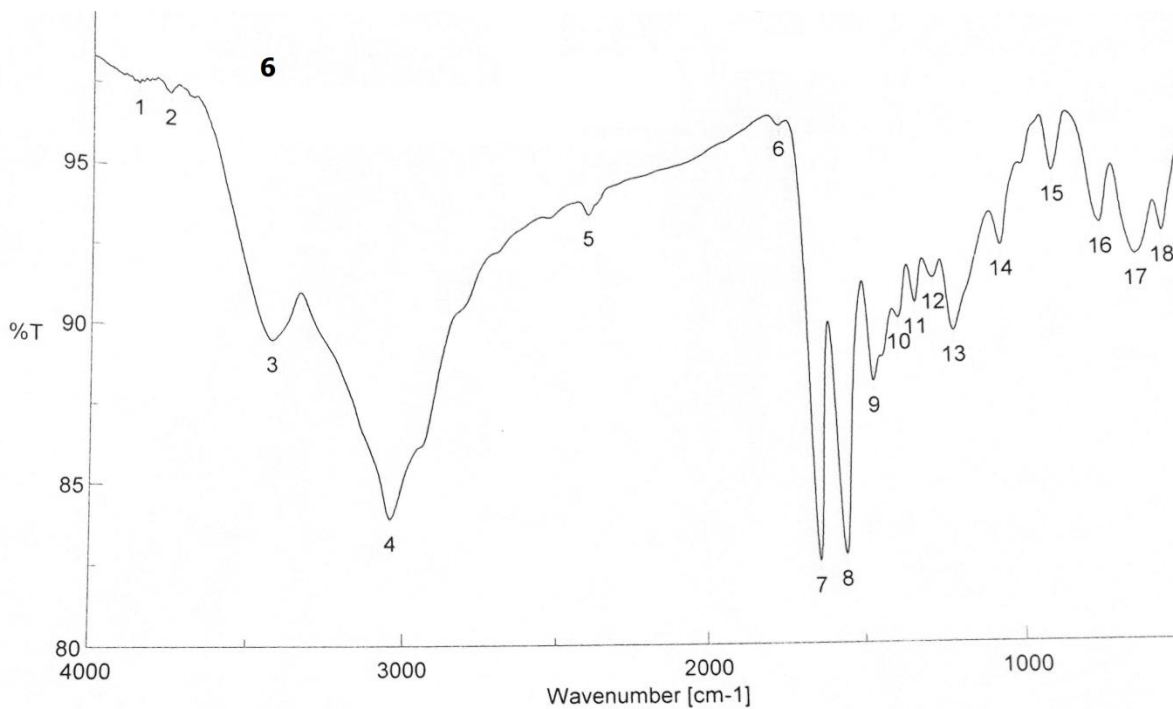


Fig. 4S. Remaining docking interactions (A) and surfaces maps (B) against, 3k4p, 1ydo & 1ecl



5H3 #171 RT: 2.88 AV: 1 NL: 3.79E2
 T: (0.0) + c EI Full ms [40.00-1000.00]





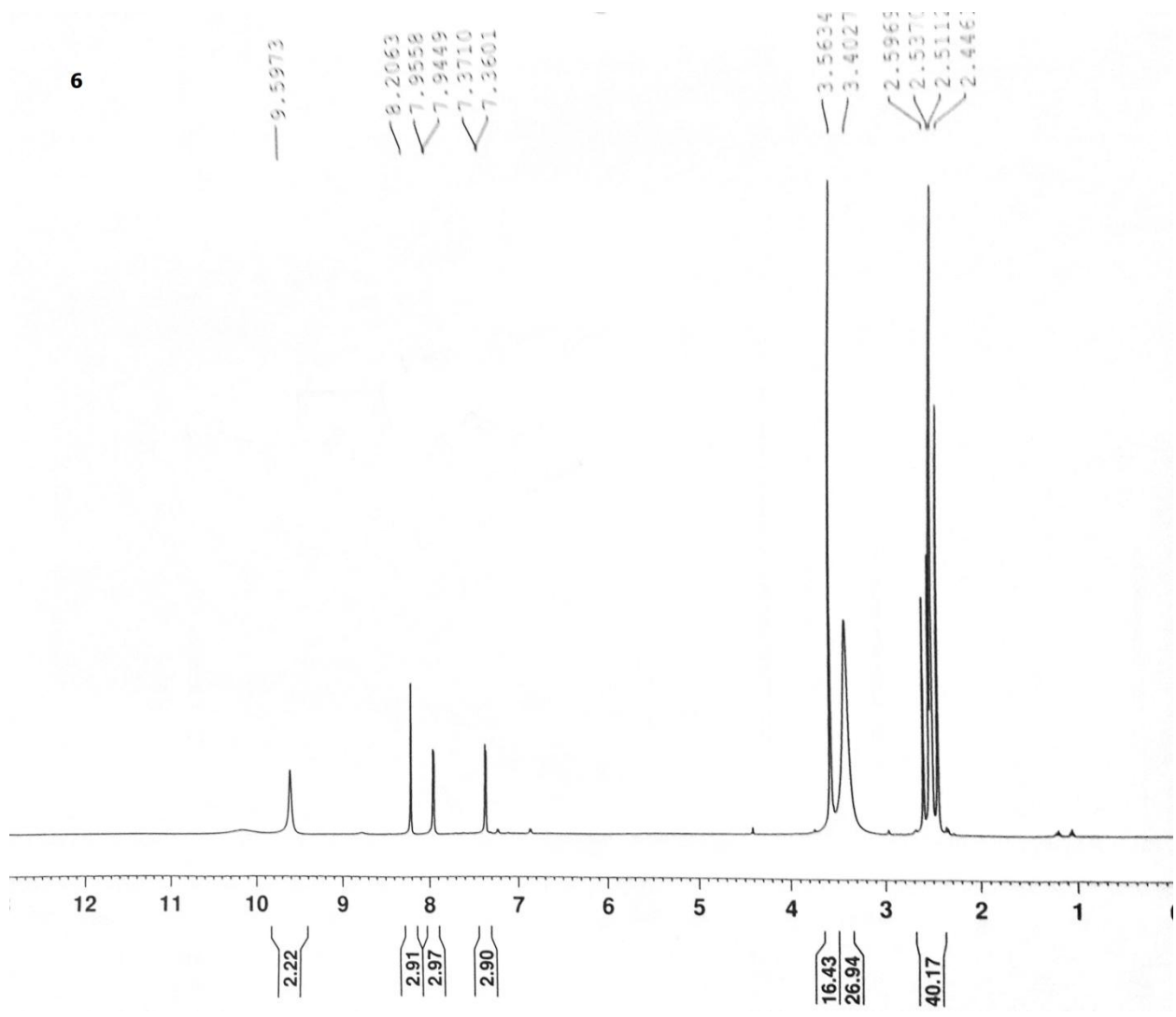
[Comments]

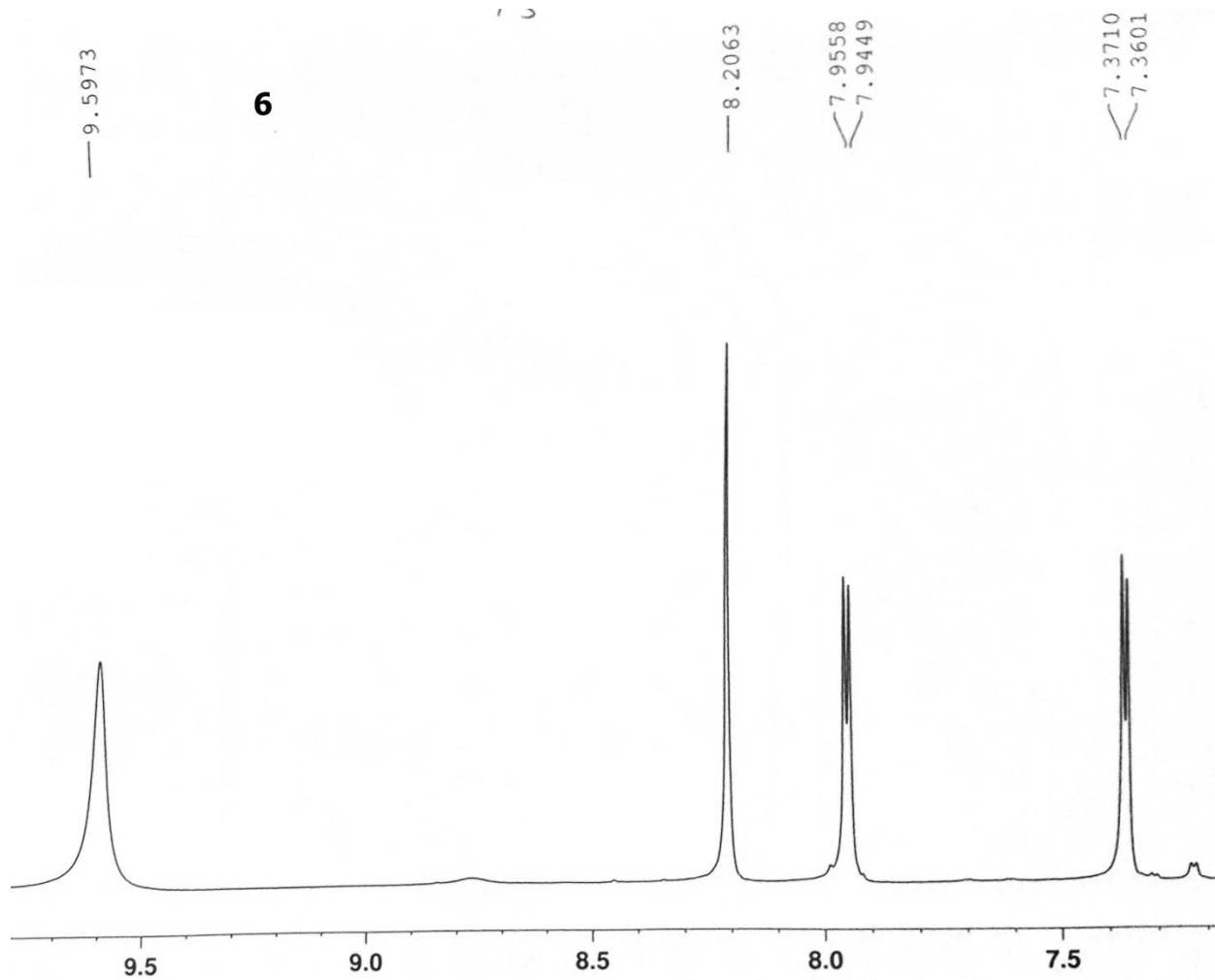
Sample name SH 3
 Comment 6/2018
 User IR
 Division IR
 Company MAC

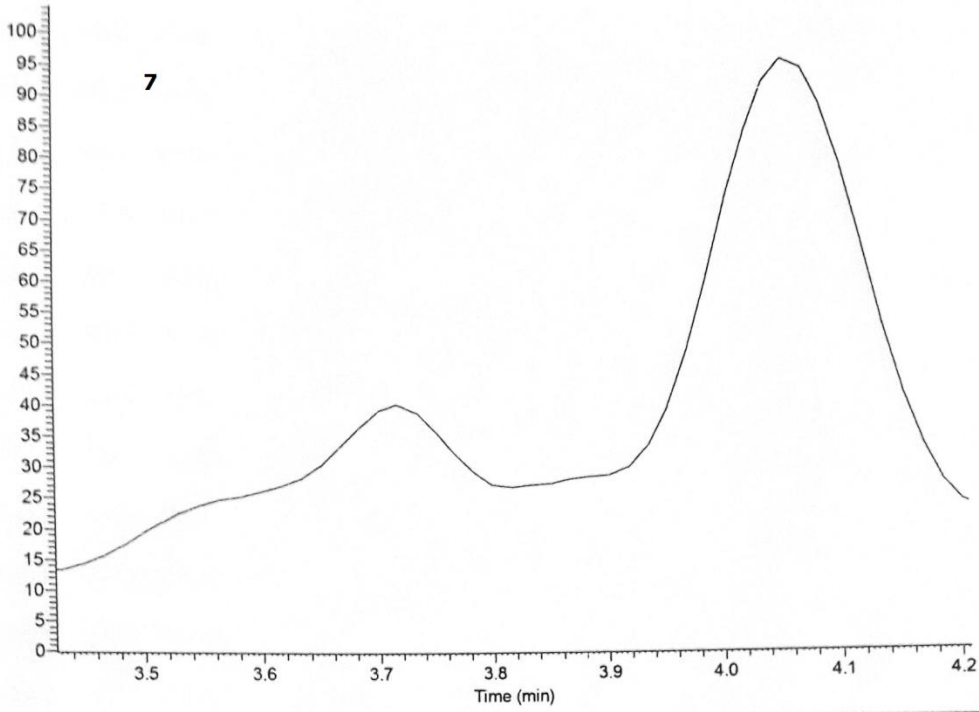
[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3855.01	97.5896	2	3752.8	97.3519	3	3417.24	89.564
4	3038.3	83.9486	5	2372.98	93.5806	6	1738.51	96.2254
7	1634.38	82.5251	8	1551.45	82.7093	9	1454.06	88.0556
10	1371.14	89.9974	11	1316.18	90.4638	12	1257.36	91.2128
13	1196.61	89.552	14	1036.55	92.1737	15	864.917	94.4247
16	717.39	92.7528	17	608.431	91.7391	18	523.579	92.4123
19	423.298	95.1315						

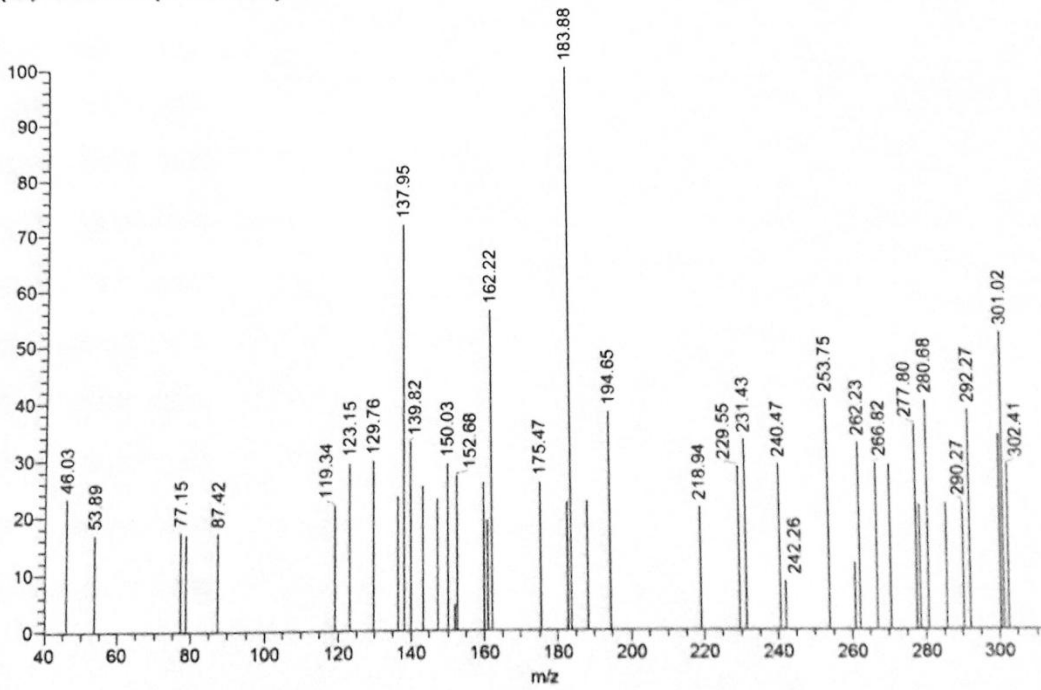
6

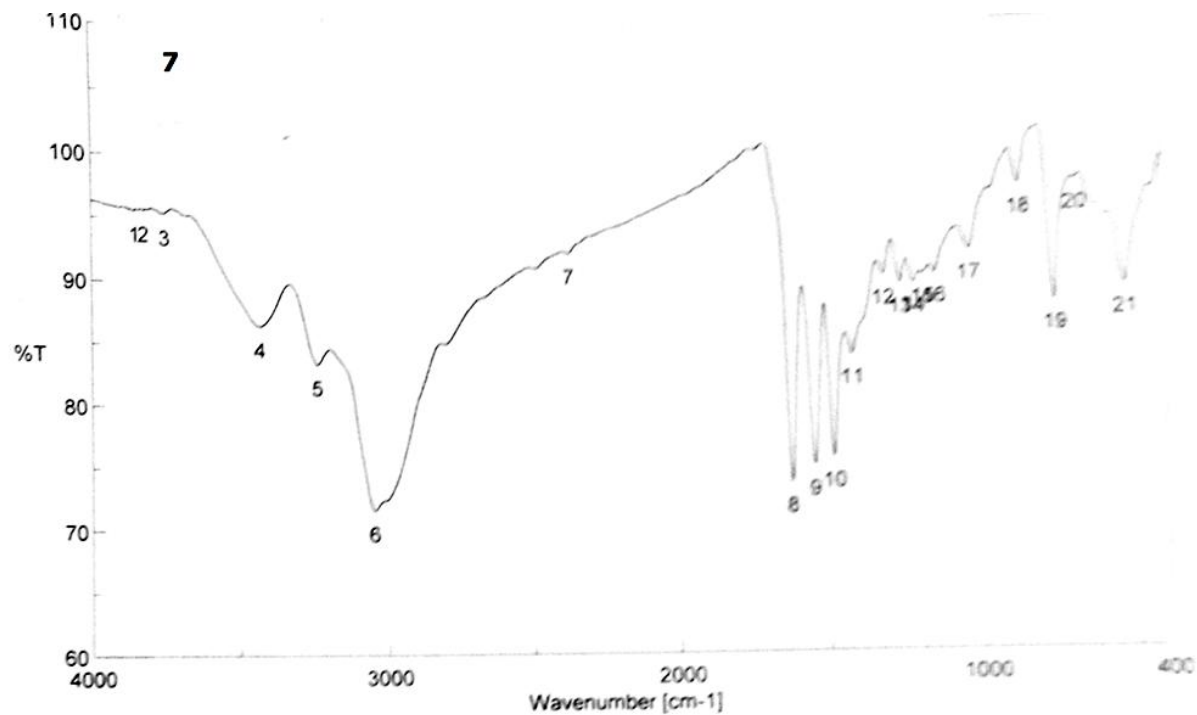






5h4 #157 RT: 2.64 AV: 1 NL: 4.04E2
 T: (0.0) + c EI Full ms [40.00-1000.00]



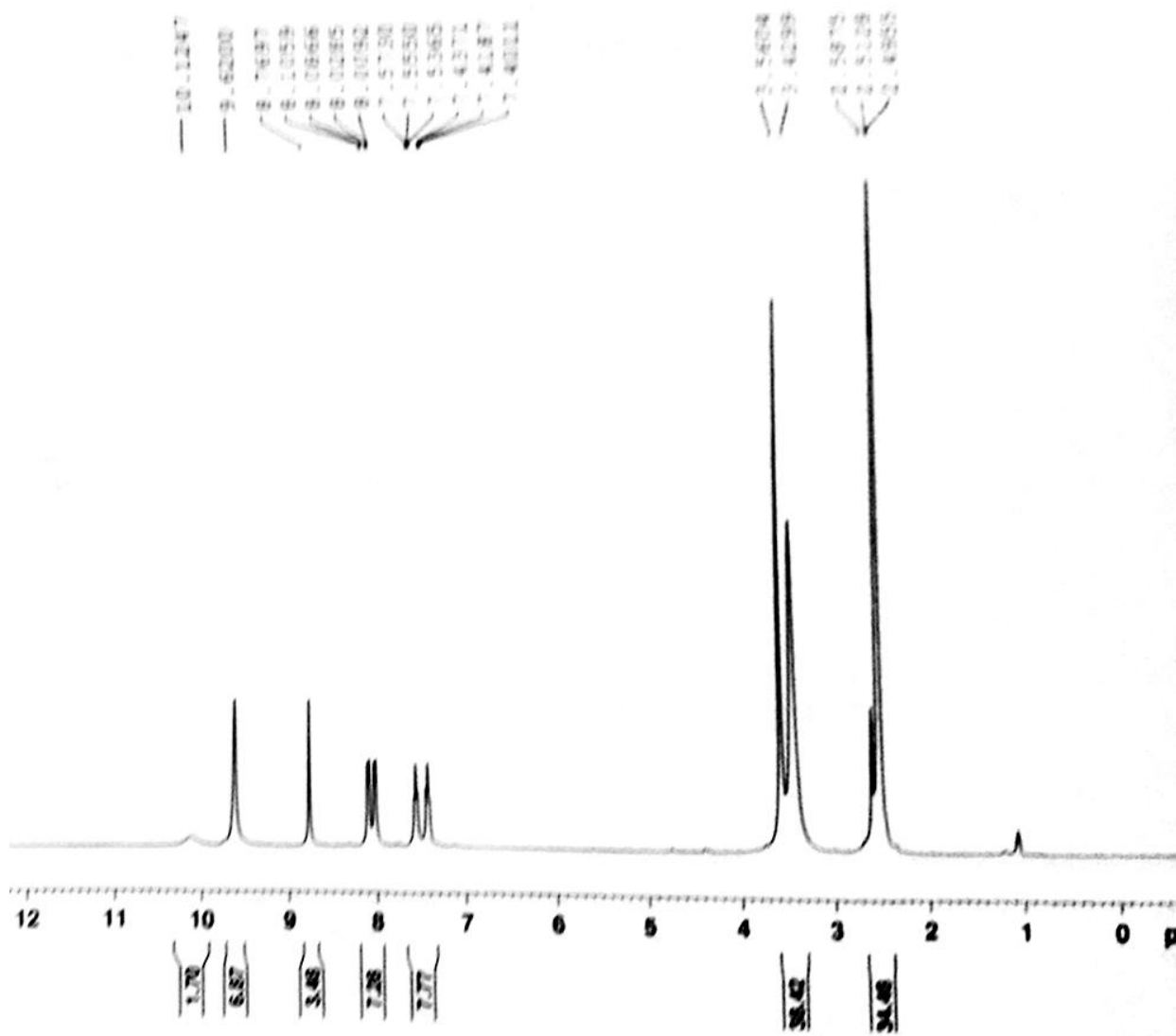


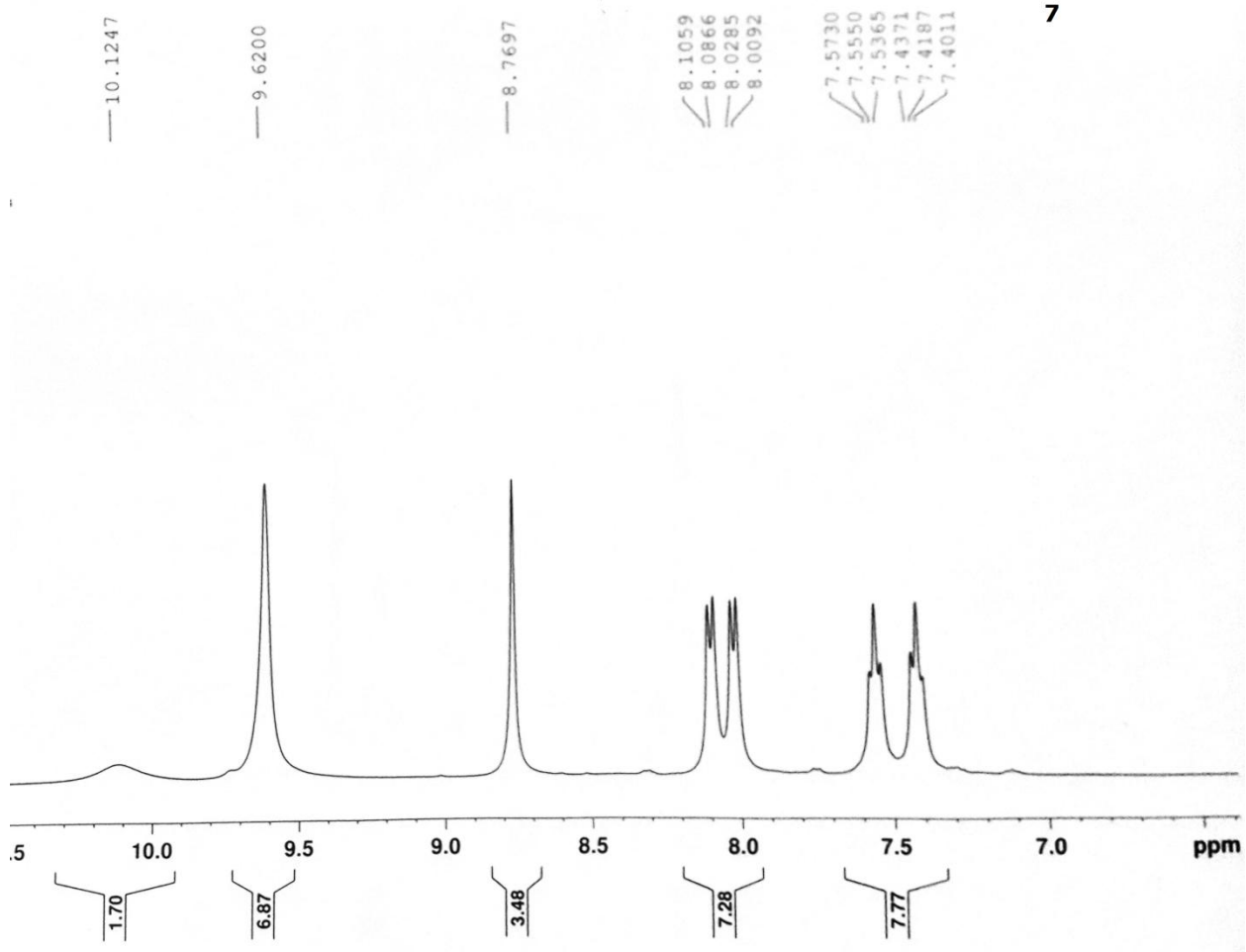
[Comments]
 Sample name SH 4
 Comment 6/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

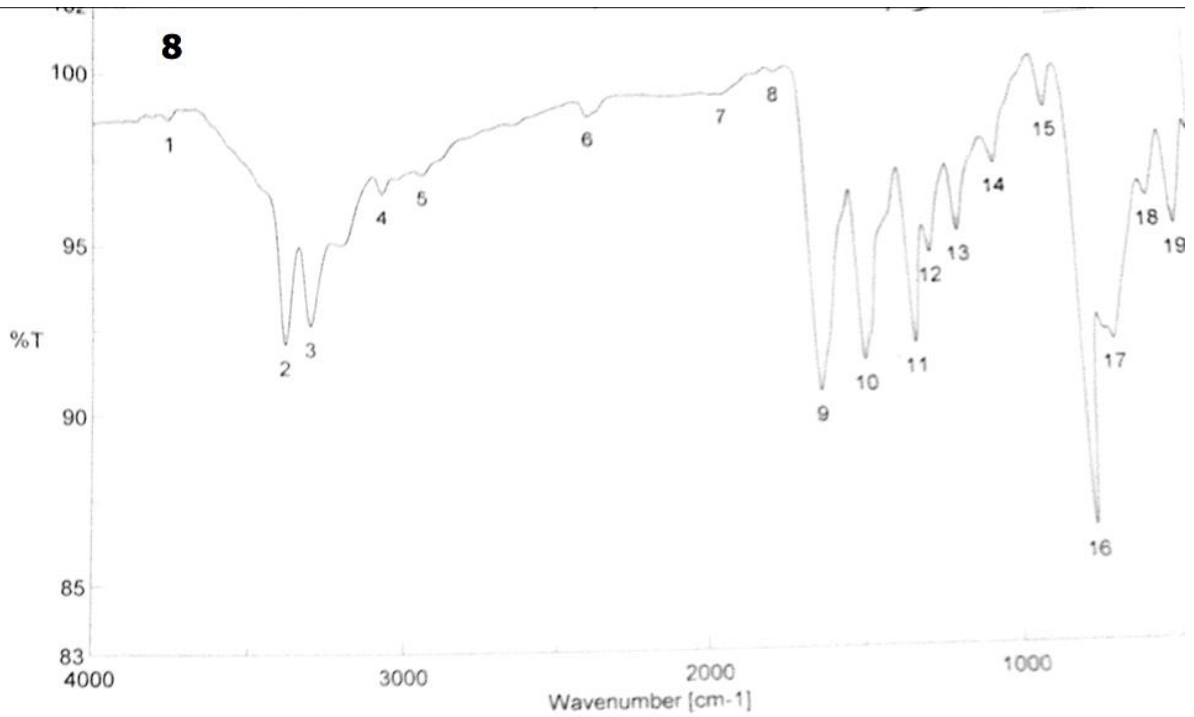
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3855.01	95.5399	2	3823.19	95.5808	3	3753.76	95.2994
4	3432.67	86.4814	5	3238.86	83.4322	6	3047.94	71.651
7	2377.8	92.2107	8	1623.77	73.4401	9	1549.52	74.7523
10	1486.85	75.3384	11	1424.17	83.4751	12	1318.11	89.7044
13	1262.18	89.0024	14	1219.76	88.9877	15	1188.9	89.6694
16	1149.37	89.7399	17	1034.62	91.5184	18	864.917	96.6301
19	752.102	87.3453	20	679.785	96.8004	21	522.615	88.4527

7





7



[Comments]

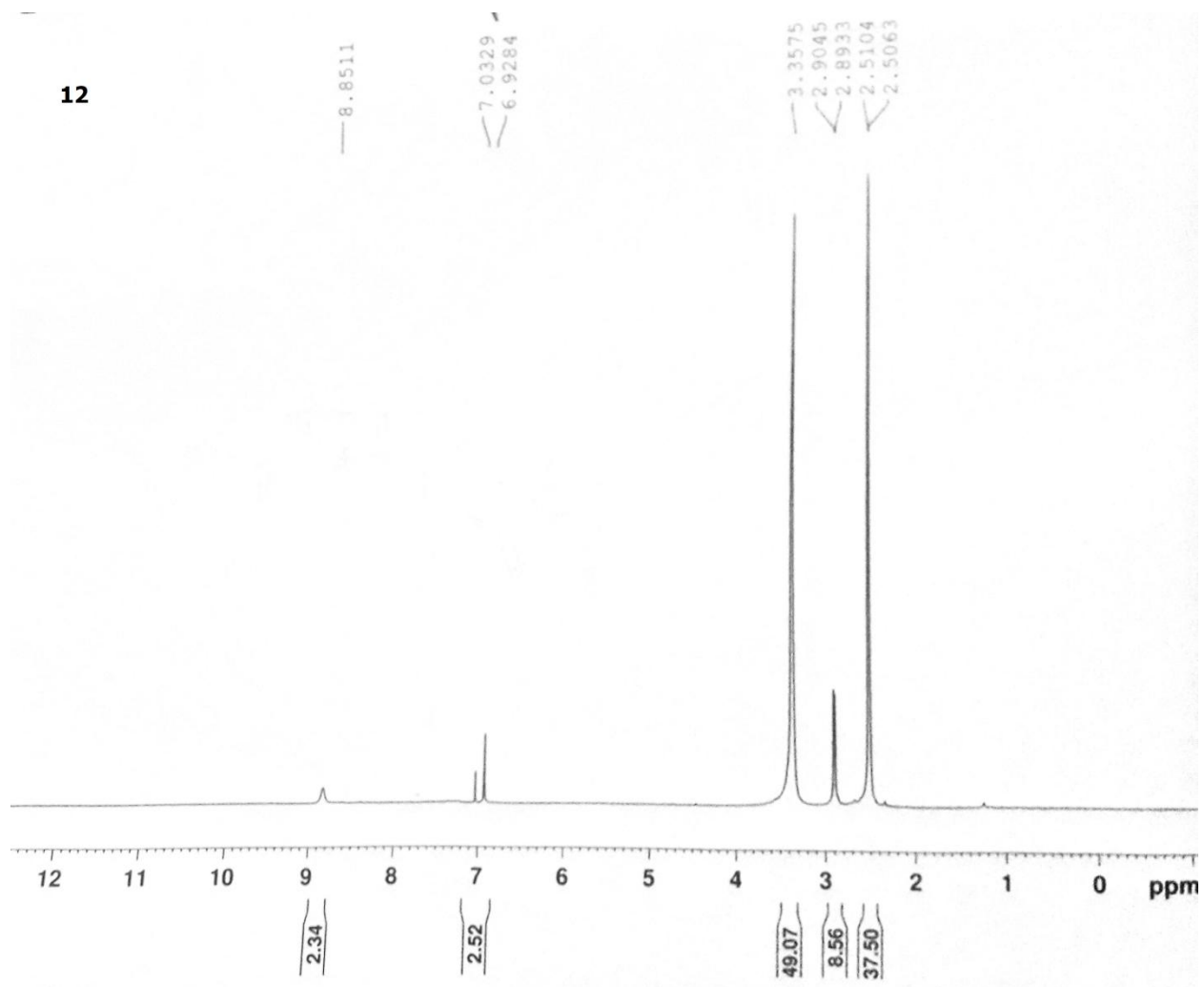
Sample name SH20
 Comment 9/2018
 User IR
 Division IR
 Company MAC

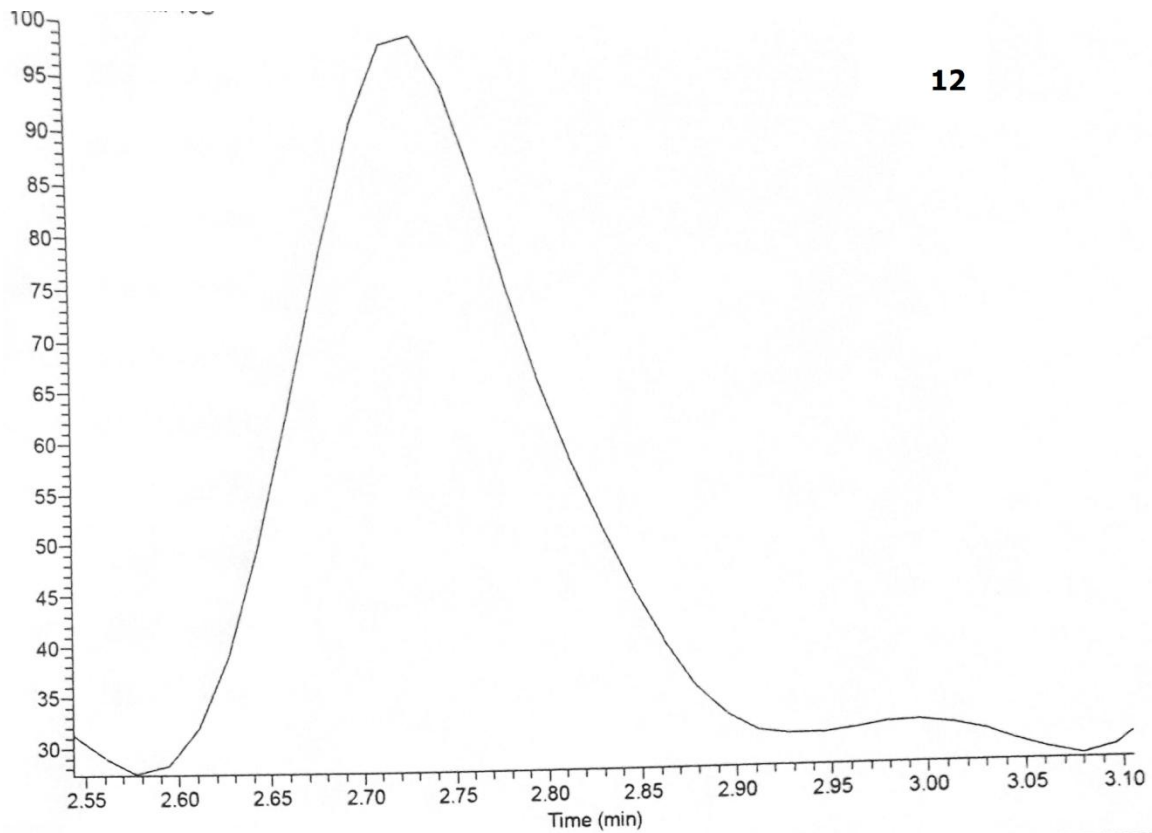
[Result of Peak Picking]

No	Position	Intensity	No	Position	Intensity	No	Position	Intensity
1	3755.69	98.9028	2	3374.82	92.2544	3	3293.82	92.832
4	3059.51	96.9929	5	2926.45	97.6254	6	2365.26	99.5368
7	1912.07	100.128	8	1735.62	100.759	9	1612.2	90.618
10	1466.6	91.5195	11	1300.75	92.0103	12	1243.86	94.7822
13	1151.29	95.4065	14	1024.98	97.4375	15	853.347	99.0744
16	749.209	86.3346	17	665.321	91.8759	18	540.935	96.1316
19	458.011	95.2293						

Handwritten signature
 P. Ananthan

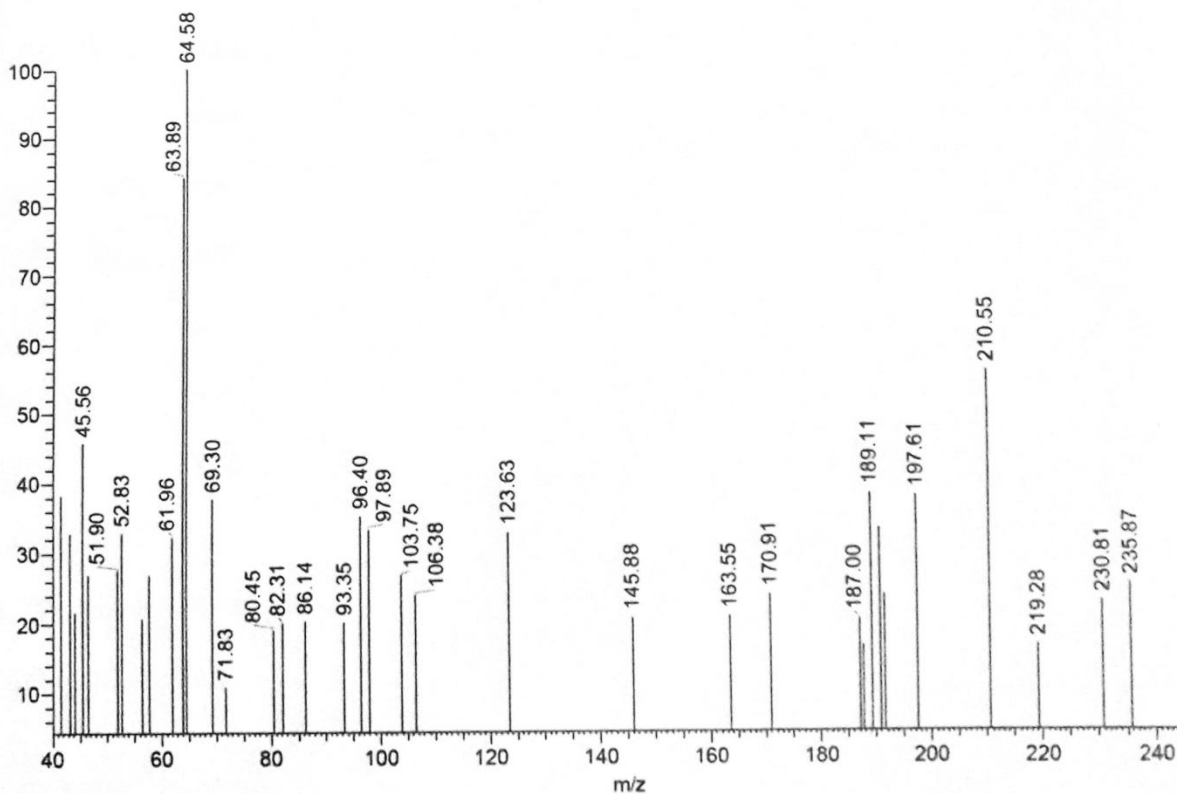
12

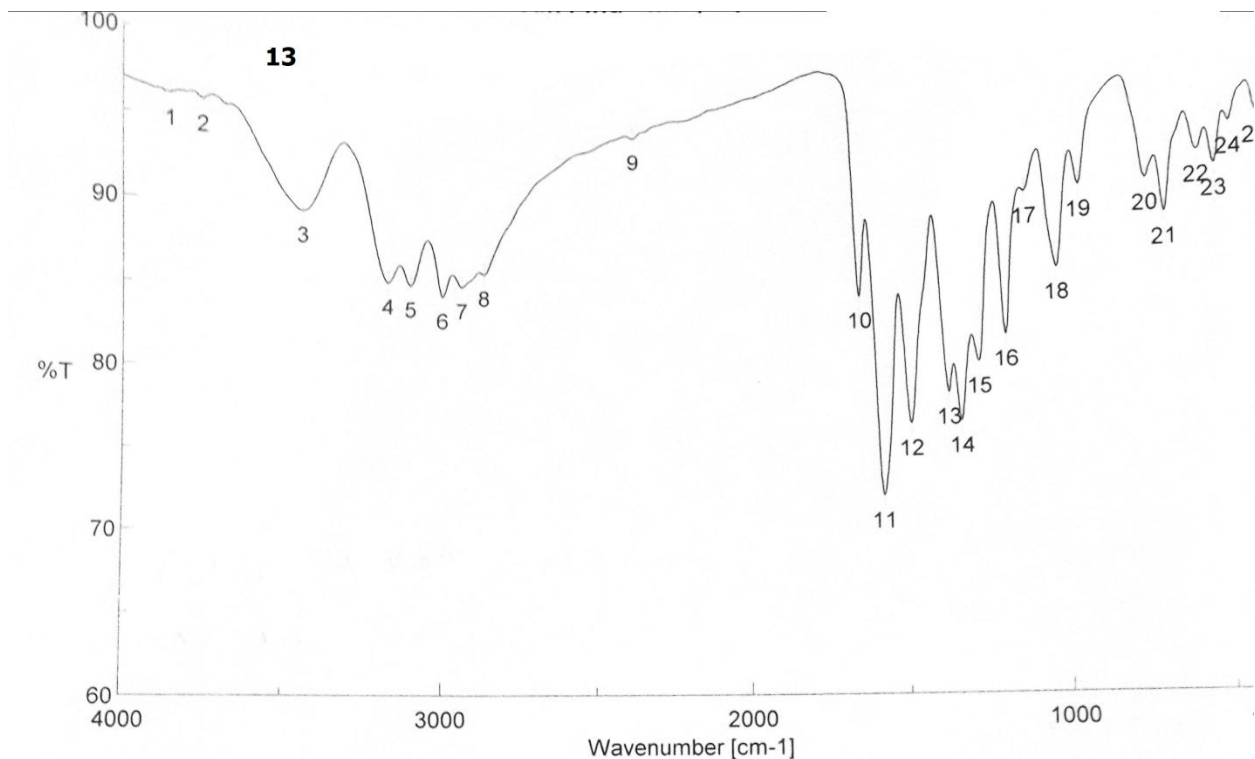




12

sh6 #256 RT: 4.30 AV: 1 NL: 4.11E2
 F: (0,0) + c EI Full ms [40.00-1000.00]

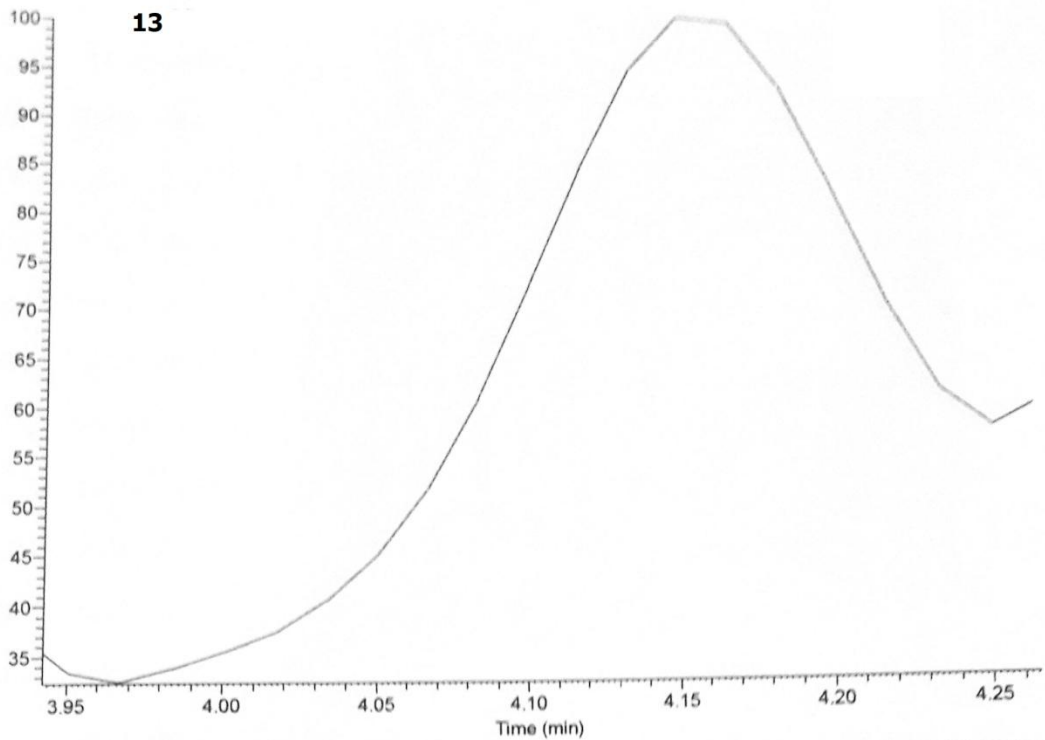




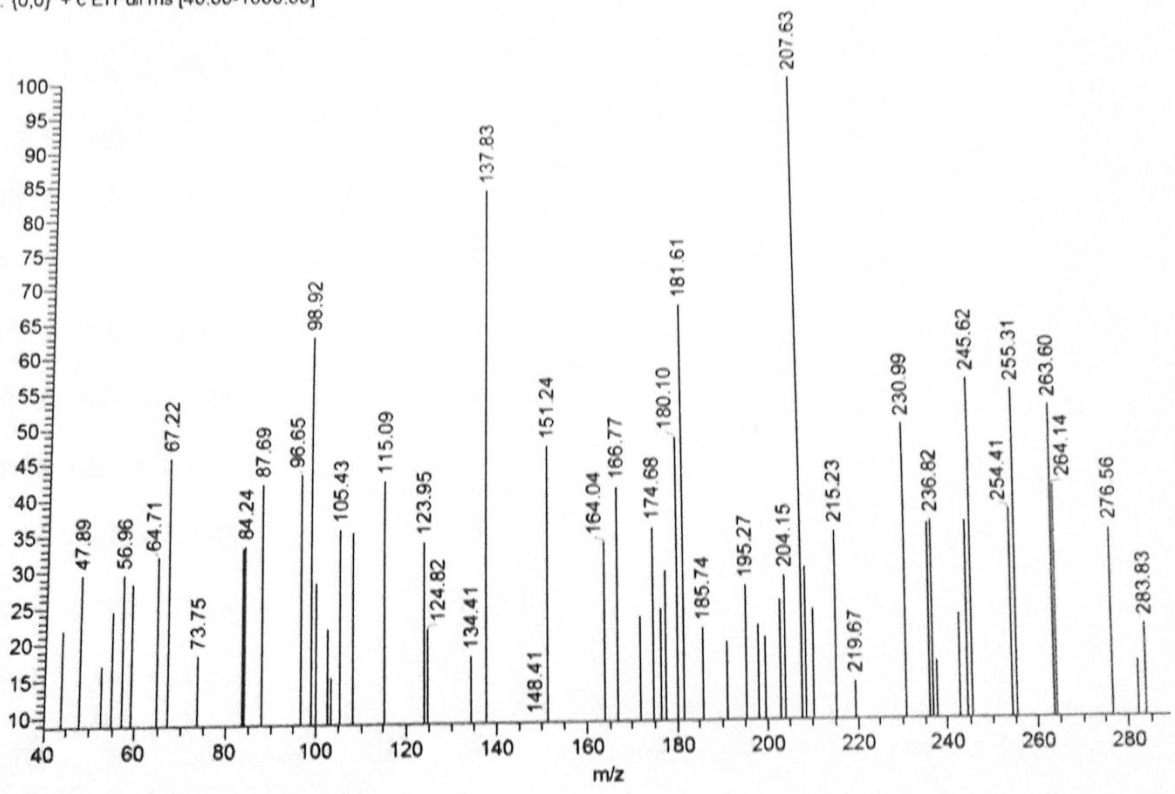
[Comments]
 Sample name SH 6
 Comment 6/2018
 User IR
 Division IR
 Company MAC

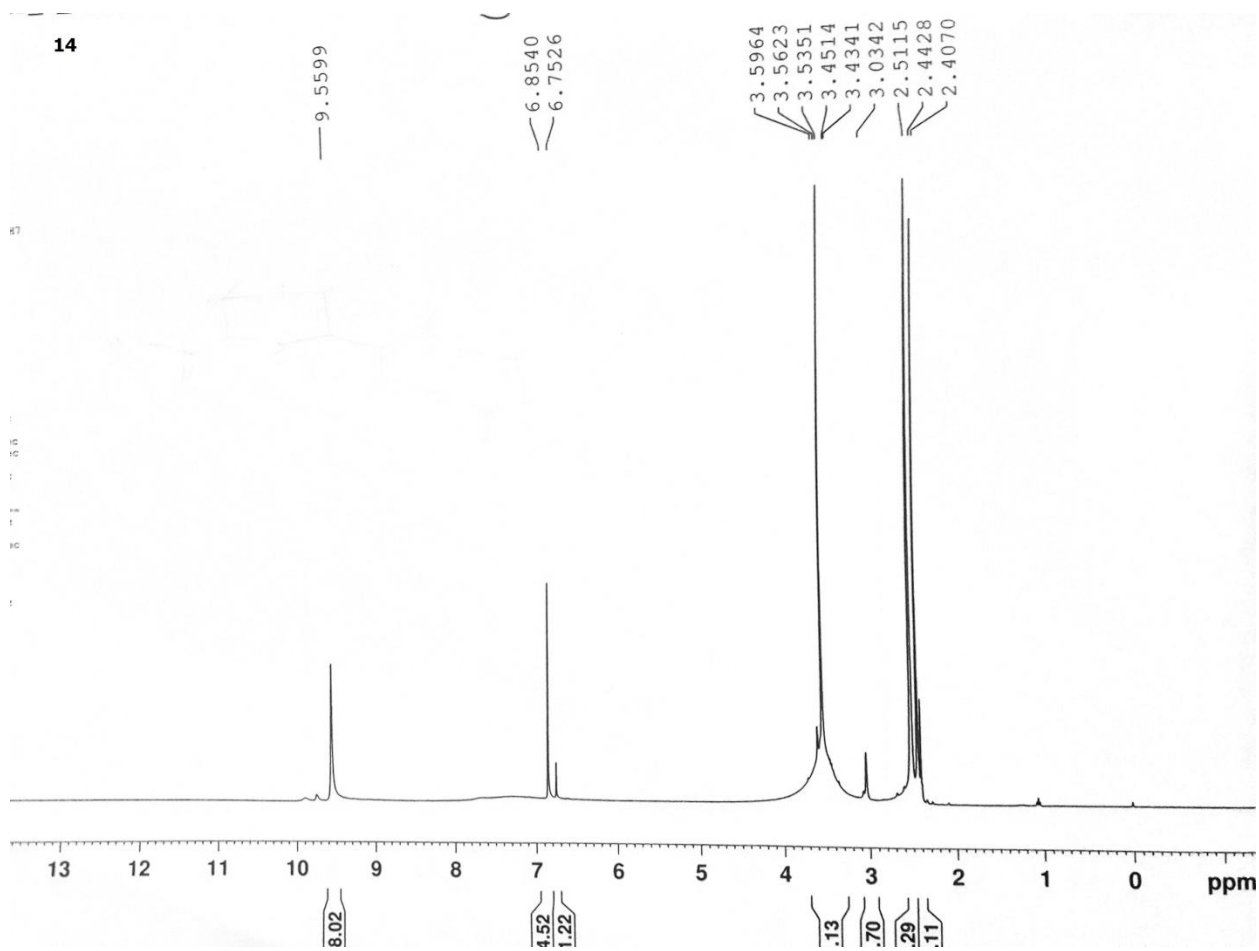
[Result of Peak Picking]

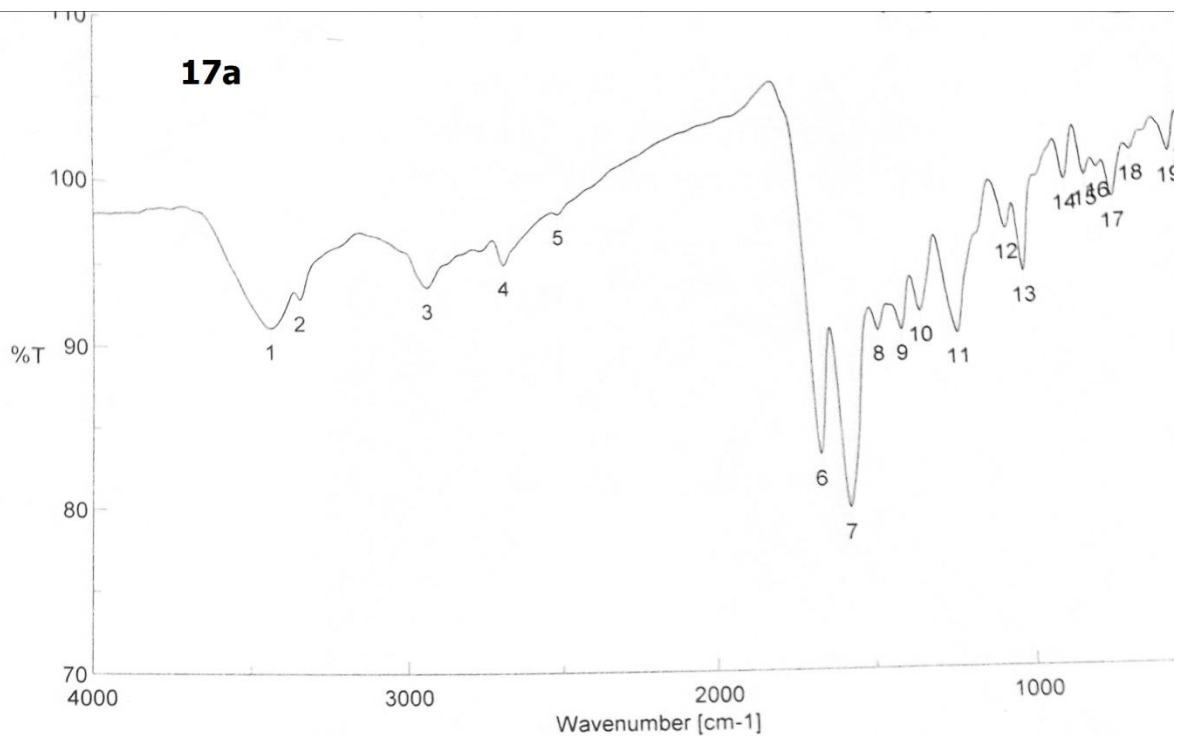
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3855.01	96.2807	2	3752.8	96.1058	3	3438.46	89.6872
1	3165.58	85.267	5	3094.23	85.0812	6	2991.05	84.3754
1	2929.34	84.9898	8	2858.95	85.8038	9	2375.87	94.5437
0	1649.8	84.2043	11	1579.41	71.9408	12	1491.67	76.2948
3	1372.1	78.1473	14	1333.53	76.4006	15	1275.68	79.9921
6	1189.86	81.6008	17	1126.22	90.2535	18	1027.87	85.5647
9	957.484	90.4577	20	751.138	90.5705	21	693.284	88.4892
2	593.968	92.0406	23	541.899	91.1604	24	496.58	93.5907
5	414.62	94.1162						



5h5 #282 RT: 4.74 AV: 1 NL: 3.44E2
 T: (0,0) + c EI Full ms [40.00-1000.00]



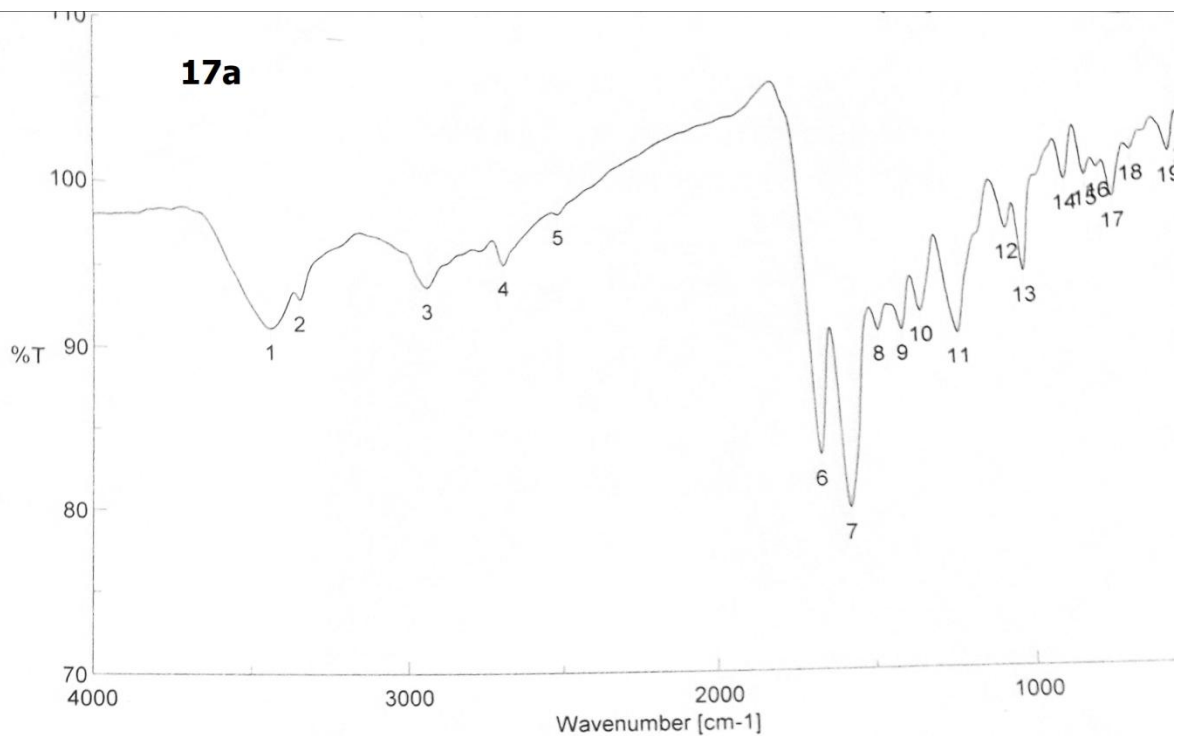




[Comments]
 Sample name SH 17
 Comment 6/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3433.64	91.427	2	3338.18	93.2701	3	2926.45	94.1149
4	2674.78	95.6015	5	2491.58	98.9628	6	1653.66	83.1979
7	1564.95	79.8526	8	1455.99	90.9884	9	1380.78	91.0034
10	1319.07	92.1345	11	1201.43	90.6785	12	1033.66	97.1217
13	983.518	94.3792	14	842.74	99.9796	15	778.136	100.131
16	737.639	100.543	17	695.212	98.623	18	632.537	101.463
19	514.901	101.163	20	458.011	102.308			

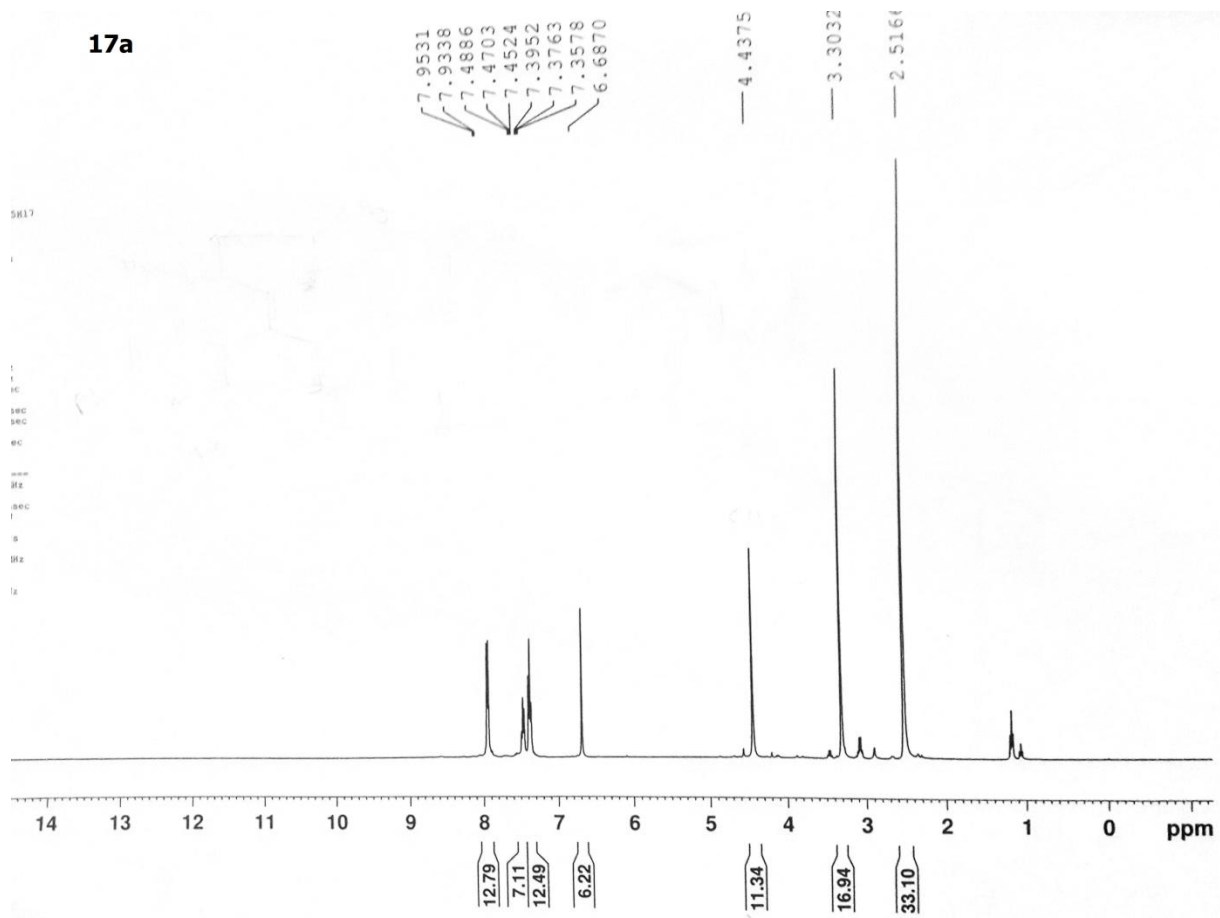


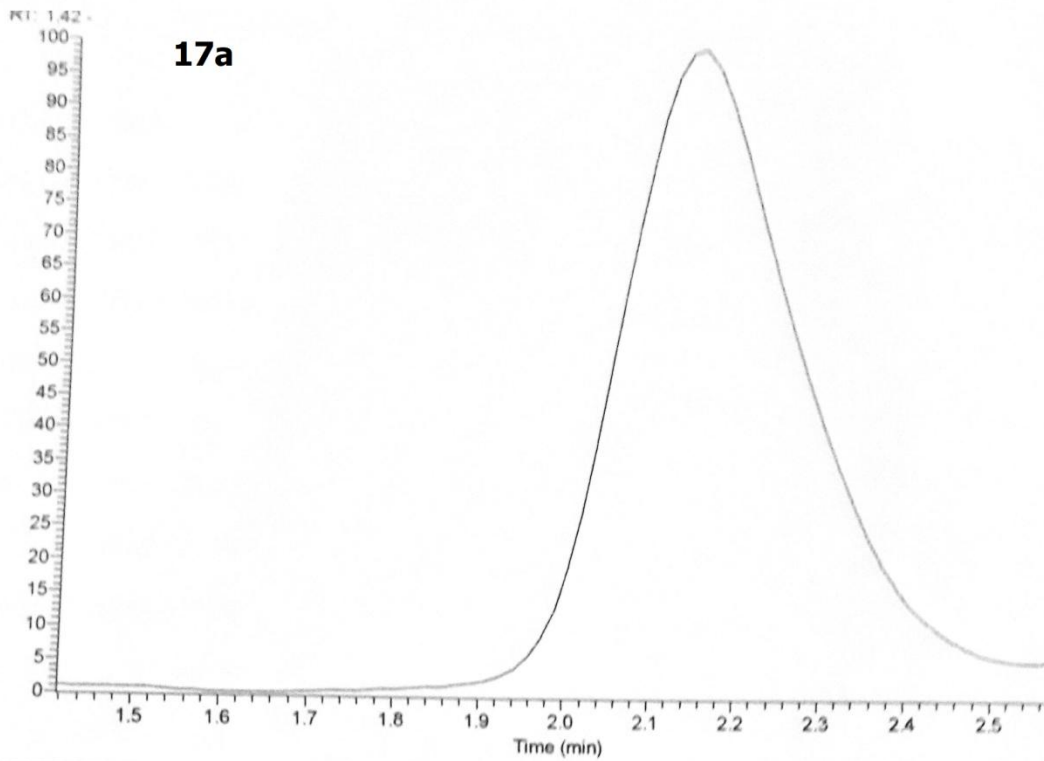
[Comments]
 Sample name SH 17
 Comment 6/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

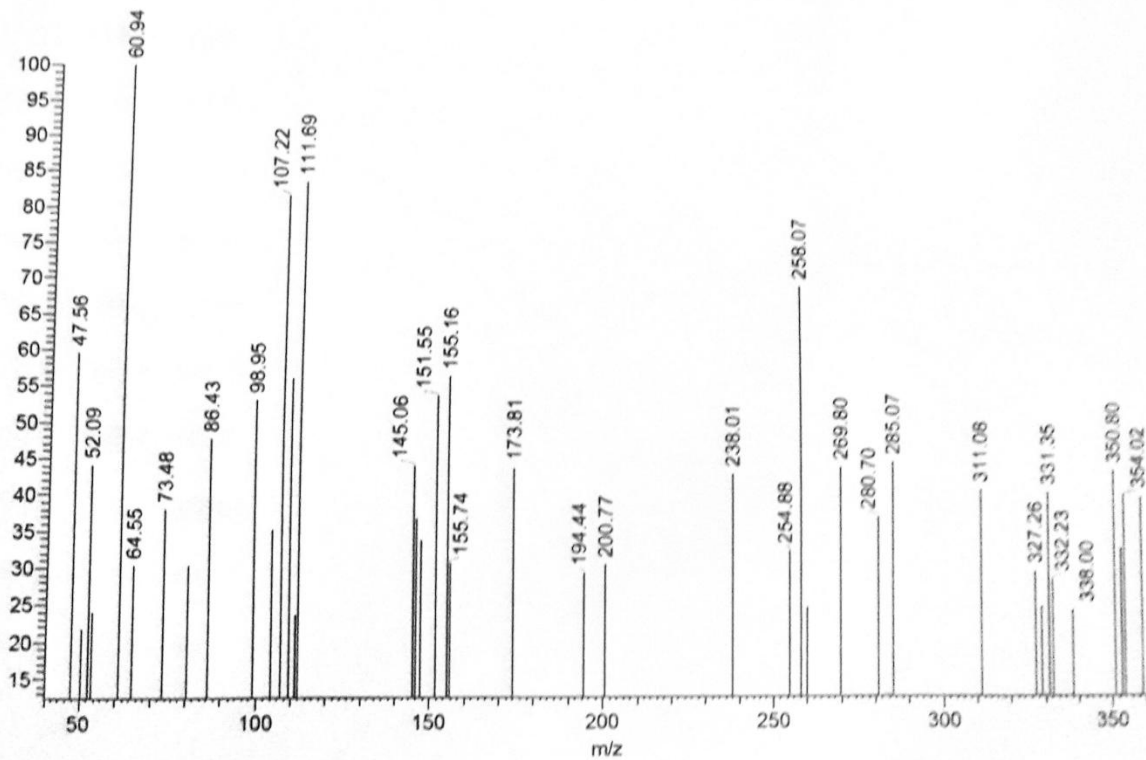
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3433.64	91.427	2	3338.18	93.2701	3	2926.45	94.1149
4	2674.78	95.6015	5	2491.58	98.9628	6	1653.66	83.1979
7	1564.95	79.8526	8	1455.99	90.9884	9	1380.78	91.0034
10	1319.07	92.1345	11	1201.43	90.6785	12	1033.66	97.1217
13	983.518	94.3792	14	842.74	99.9796	15	778.136	100.131
16	737.639	100.543	17	695.212	98.623	18	632.537	101.463
19	514.901	101.163	20	458.011	102.308			

17a

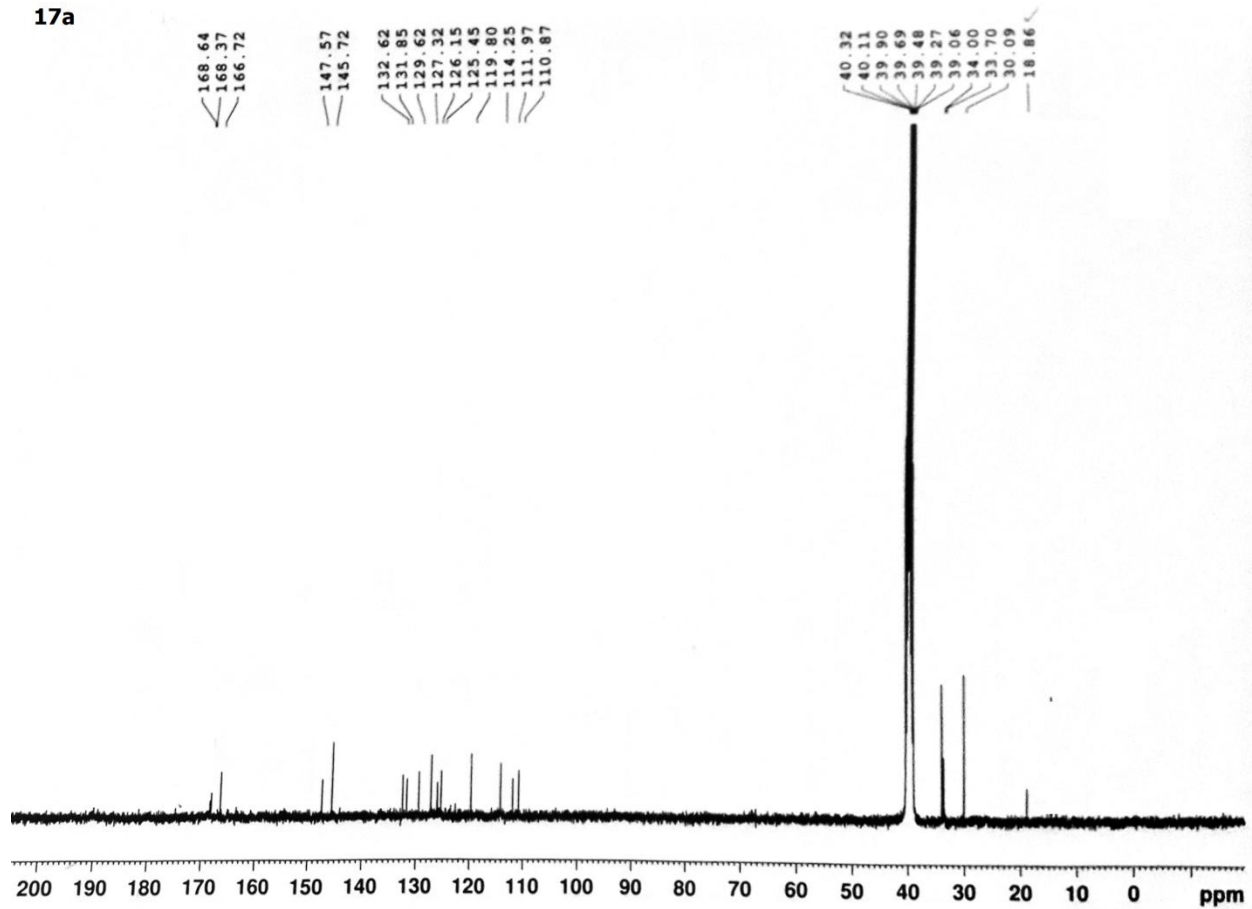


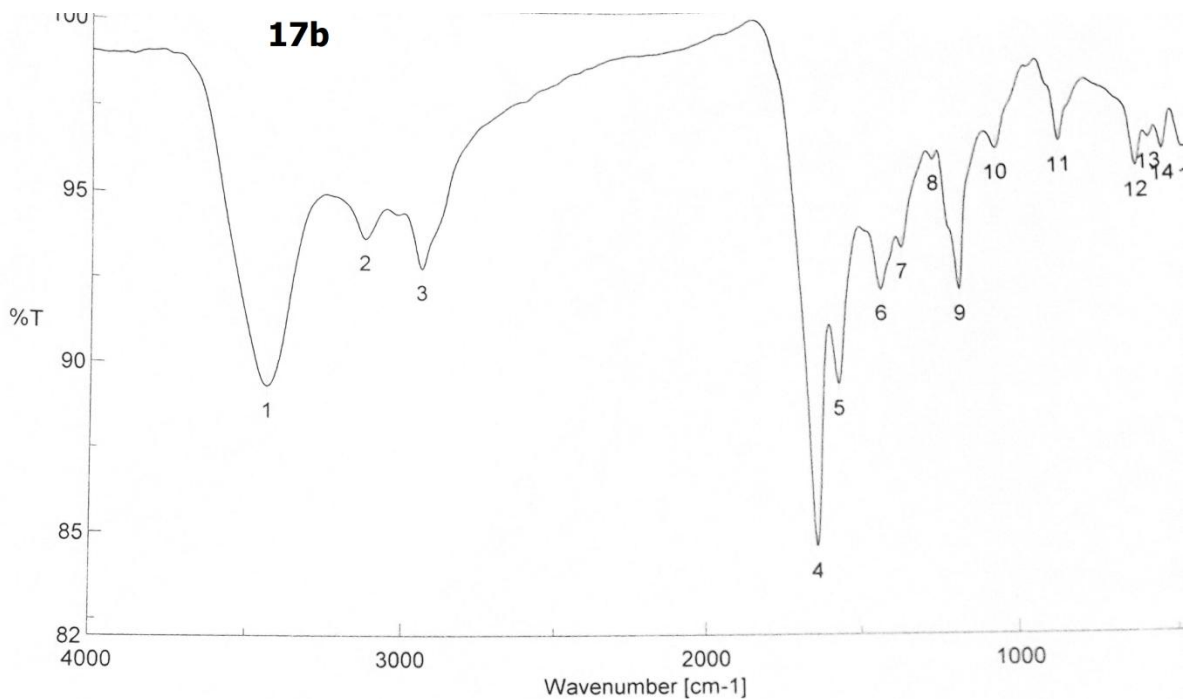


5h17 #192 RT: 3.23 AV: 1 NL: 2.77E2
 T: (0,0) + c EI Full ms [40.00-1000.00]



17a



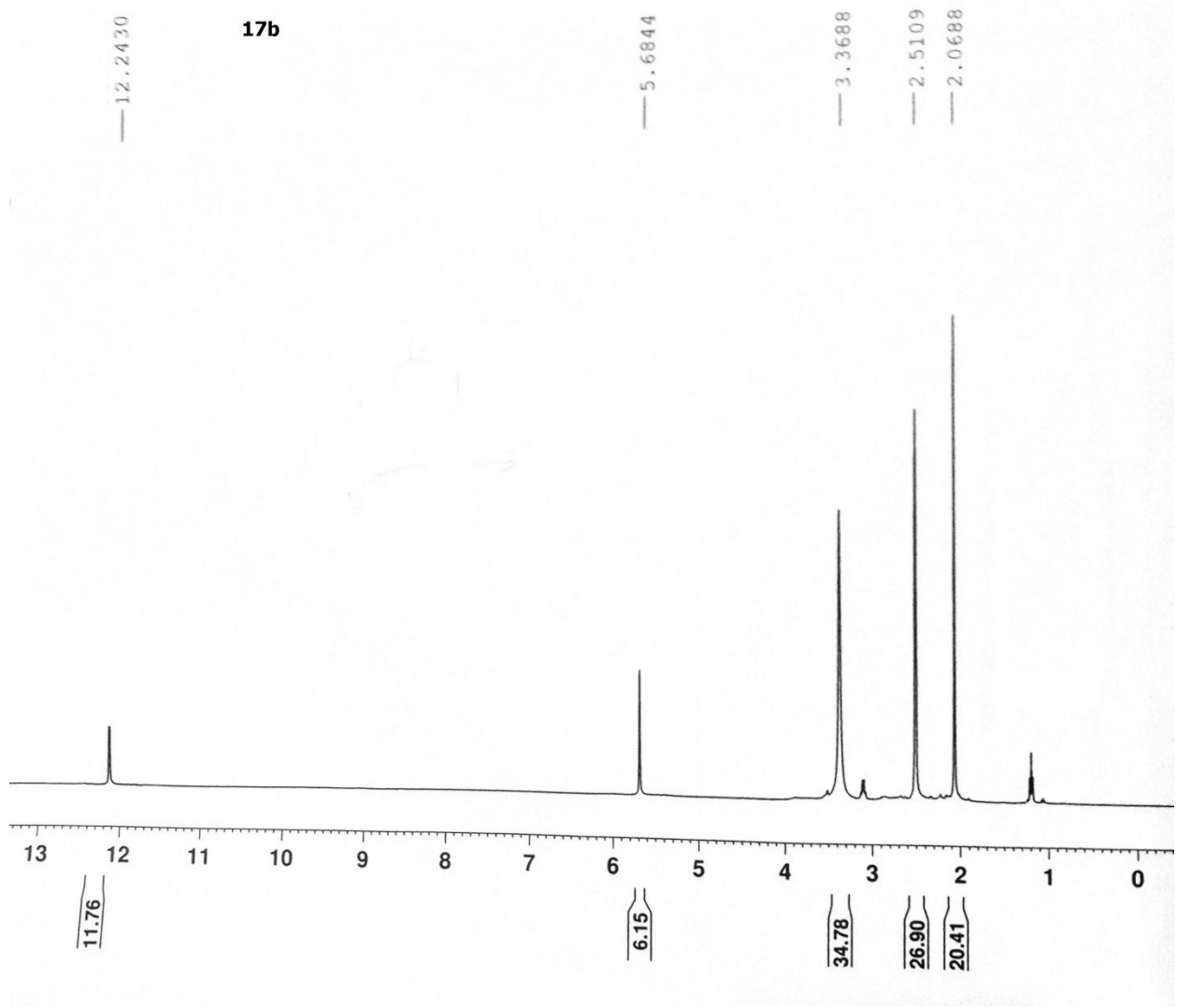


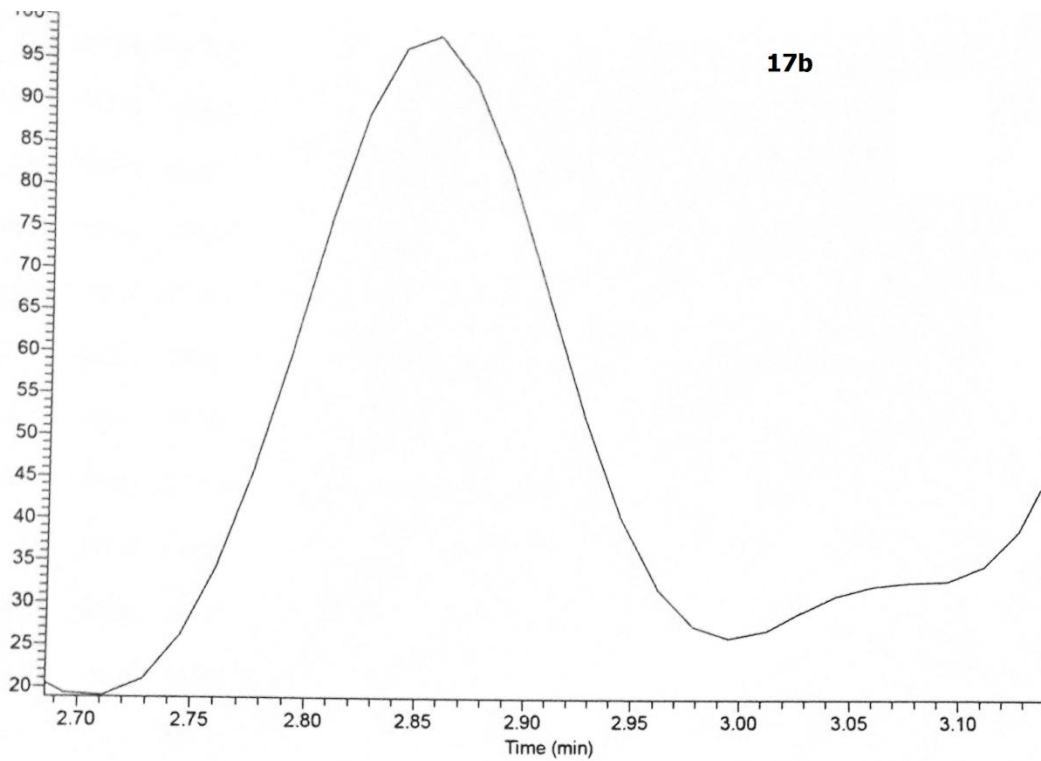
[Comments]

Sample name SH 18
 Comment 6/2018
 User IR
 Division IR
 Company MAC

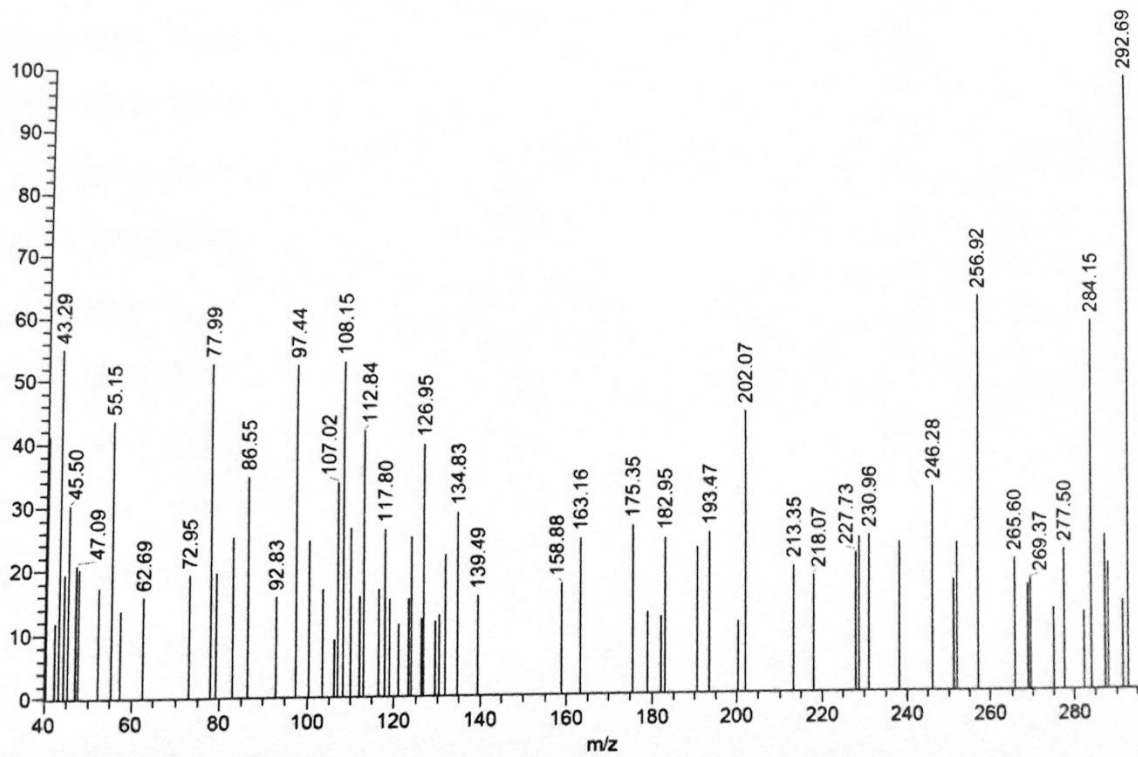
[Result of Peak Picking]

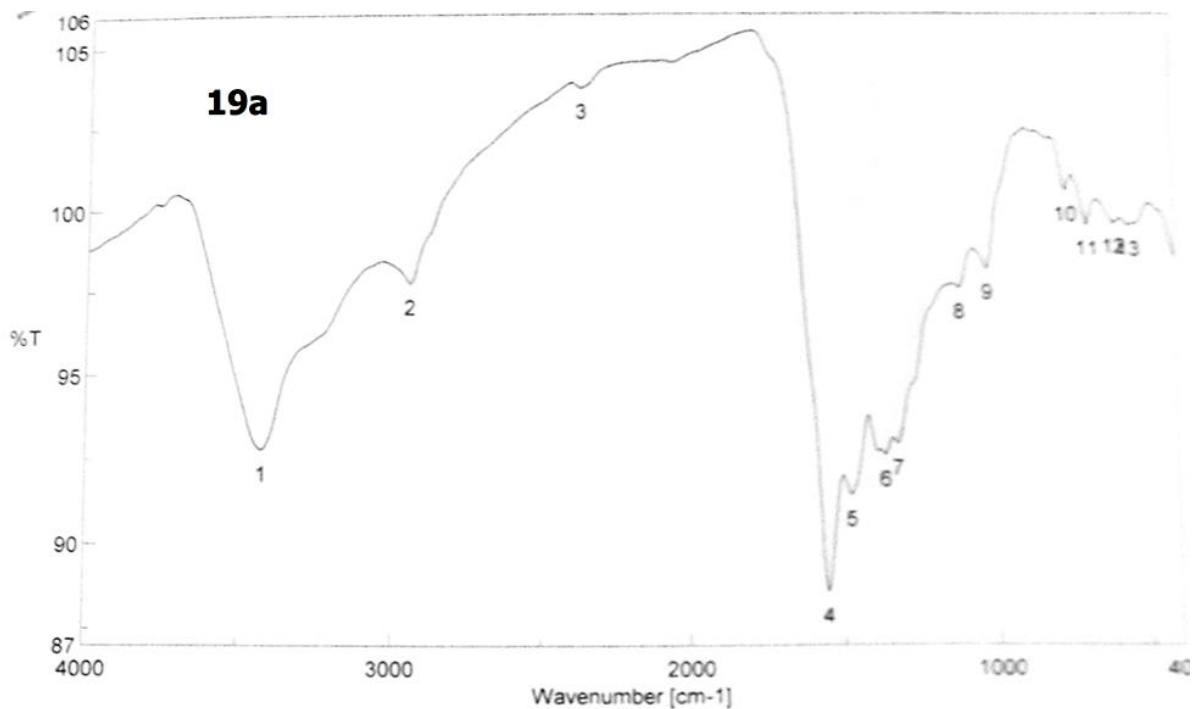
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3430.74	89.348	2	3114.47	93.8009	3	2928.38	92.9064
4	1636.3	84.5798	5	1560.13	89.3871	6	1417.42	92.2107
7	1347.03	93.4573	8	1240	96.0959	9	1163.83	92.1475
10	1037.52	96.3368	11	835.026	96.4471	12	593.968	95.5555
13	552.506	96.3766	14	511.044	96.0017	15	422.334	95.8984





5h18 #193 RT: 3.25 AV: 1 NL: 4.85E2
 T: (0,0) + c EI Full ms [40.00-1000.00]

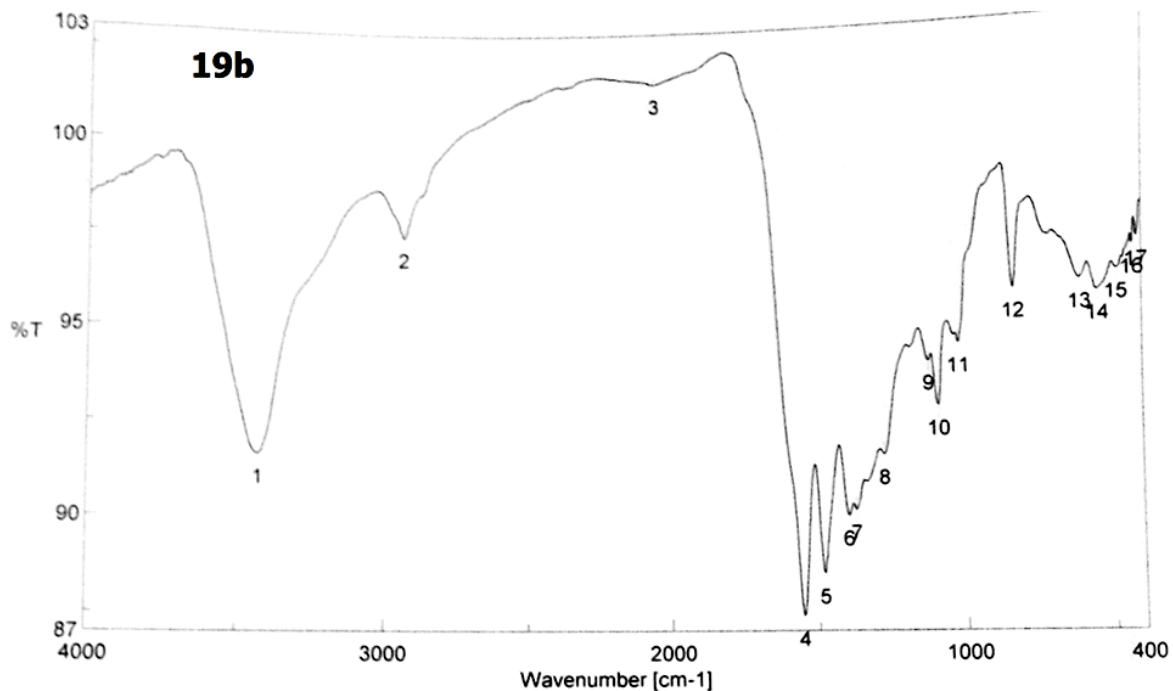




[Comments]
 Sample name SH 11
 Comment 6/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

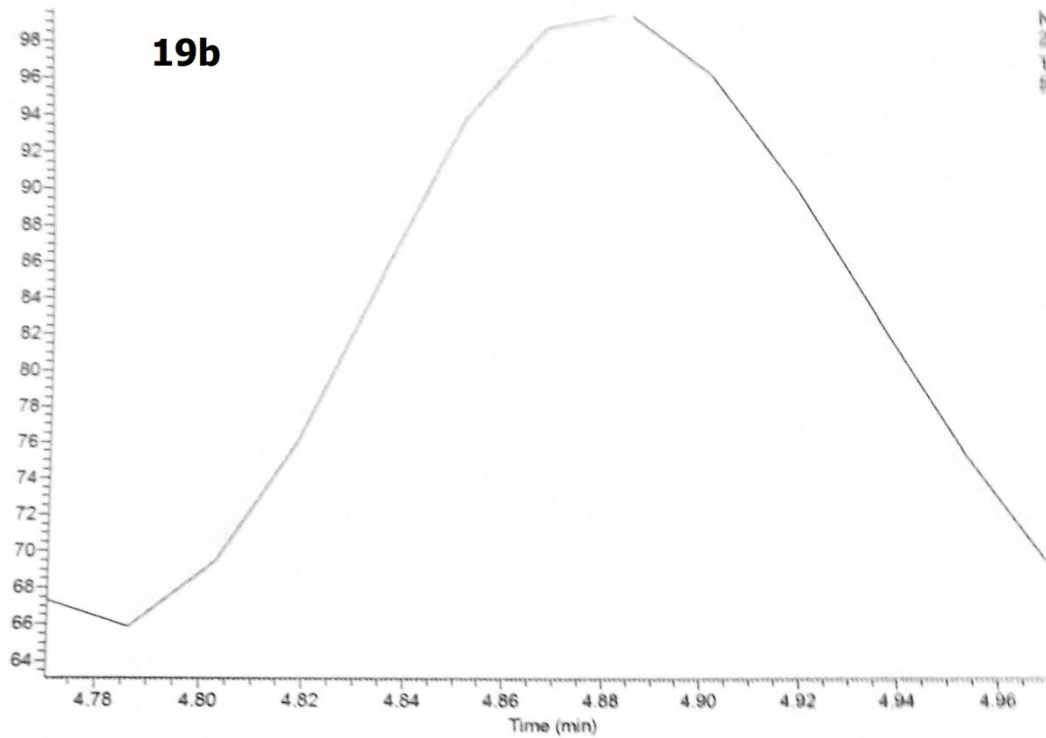
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3419.17	92.7854	2	2929.34	97.7475	3	2362.37	103.713
4	1554.34	88.5783	5	1480.1	91.4049	6	1370.18	92.566
7	1330.64	92.905	8	1124.3	97.5709	9	1029.8	98.1671
10	760.78	100.58	11	691.355	99.5347	12	601.682	99.6101
13	553.47	99.5343						



[Comments]
 Sample name SH 13
 Comment 6/2018
 User IR
 Division IR
 Company MAC

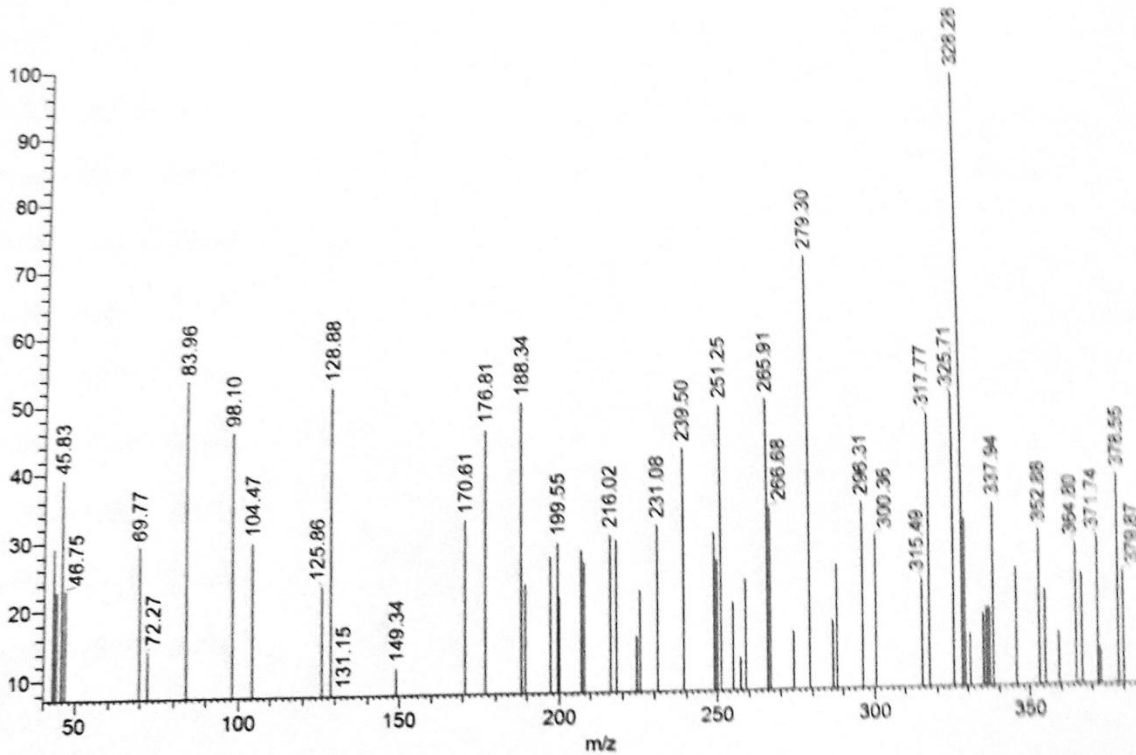
[Result of Peak Picking]

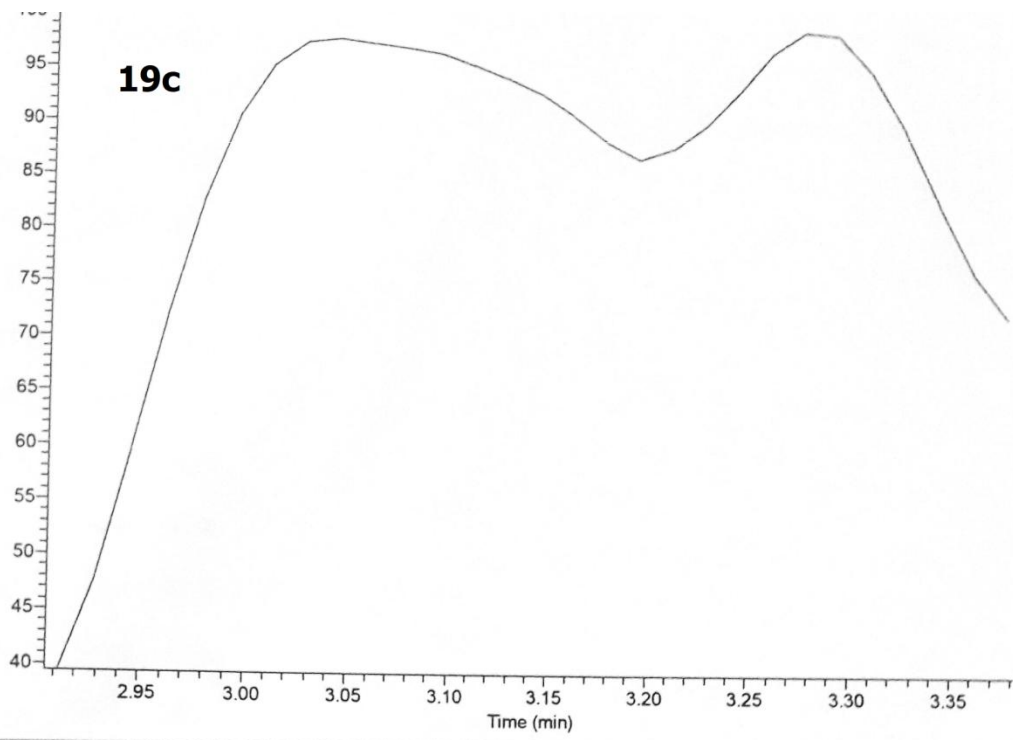
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3423.99	91.6275	2	2925.48	97.3724	3	2049.96	101.615
4	1552.42	87.3904	5	1482.03	88.4942	6	1398.14	90.0004
7	1373.07	90.1508	8	1275.68	91.599	9	1121.4	94.0569
10	1089.58	92.8718	11	1018.23	94.5151	12	827.312	95.9205
13	604.574	96.105	14	545.756	95.7886	15	484.045	96.3221
16	431.012	96.9329	17	416.549	97.127			



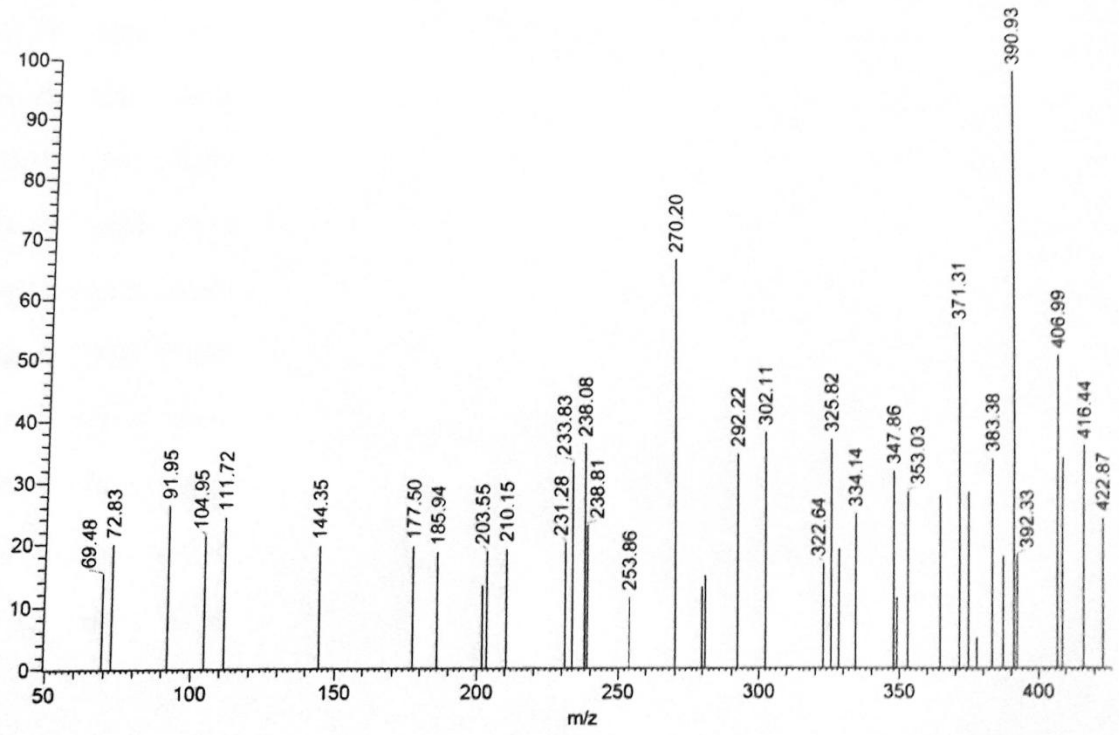
NL:
2.23E4
TK: MS
5H13

5H13 #281 RT: 4.72 AV: 1 NL: 4.36E2
T: (0.0) + c EI Full ms [40.00-1000.00]

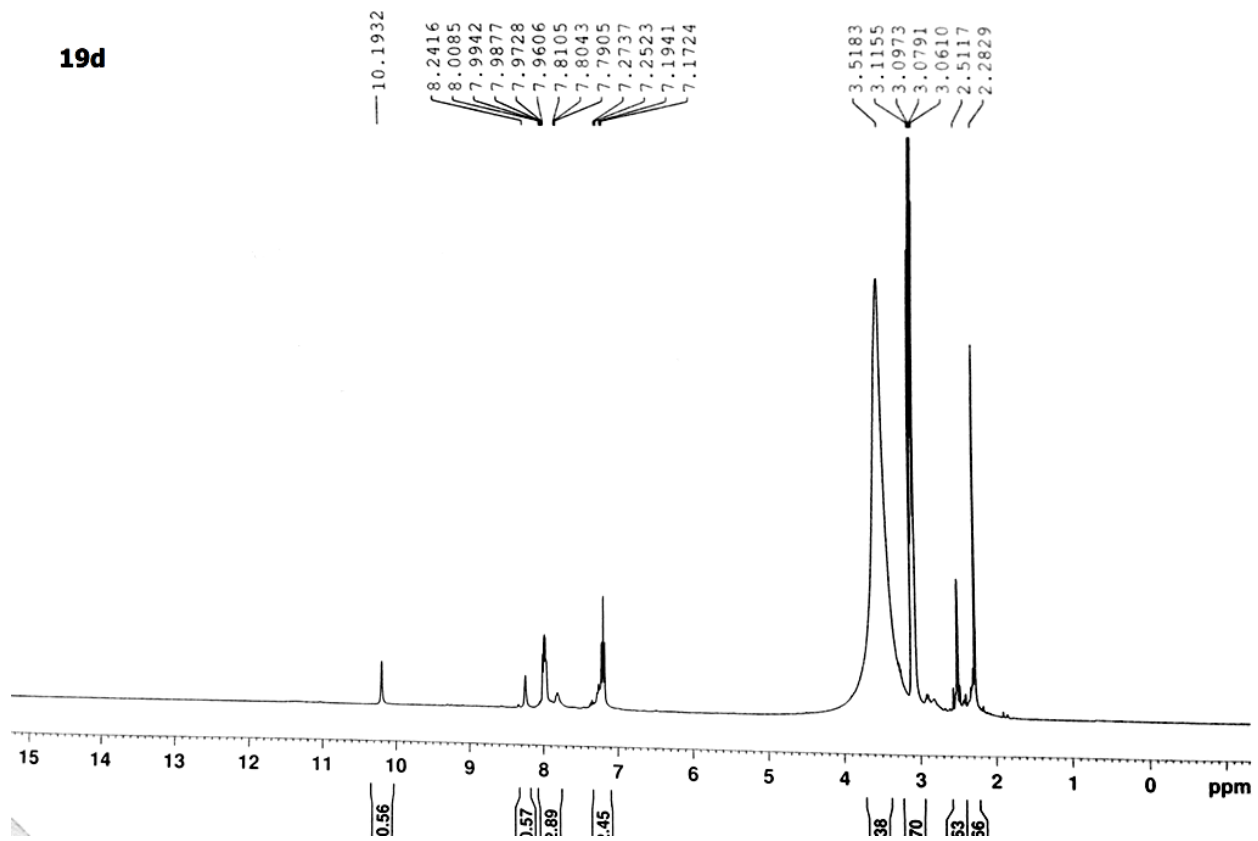


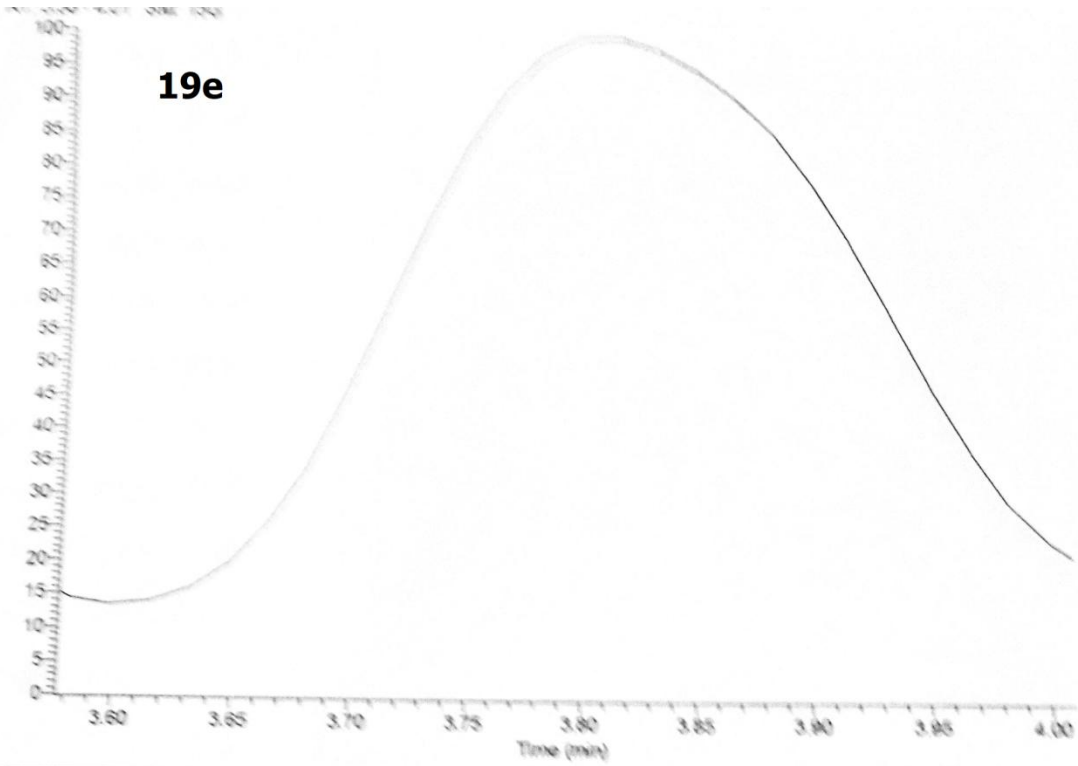


5h14 #192 RT: 3.23 AV: 1 NL: 4.99E2
 T: (0,0) + c EI Full ms [40.00-1000.00]

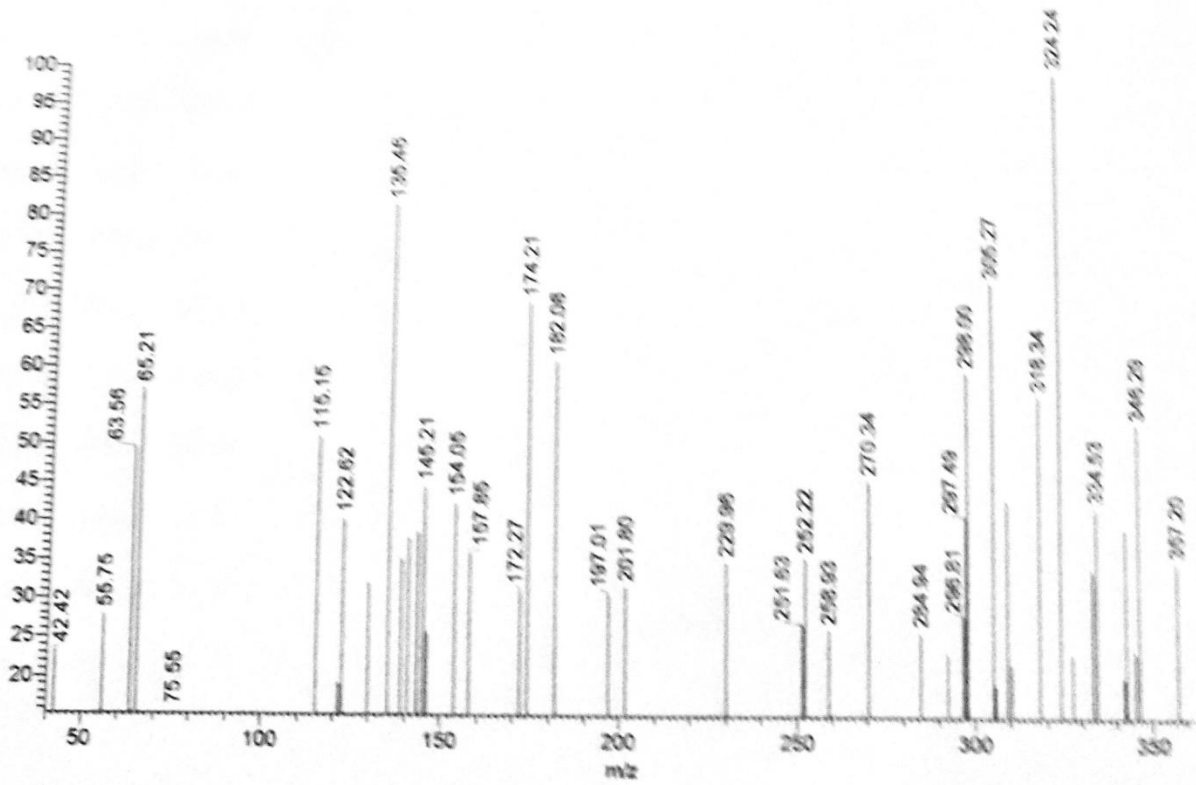


19d



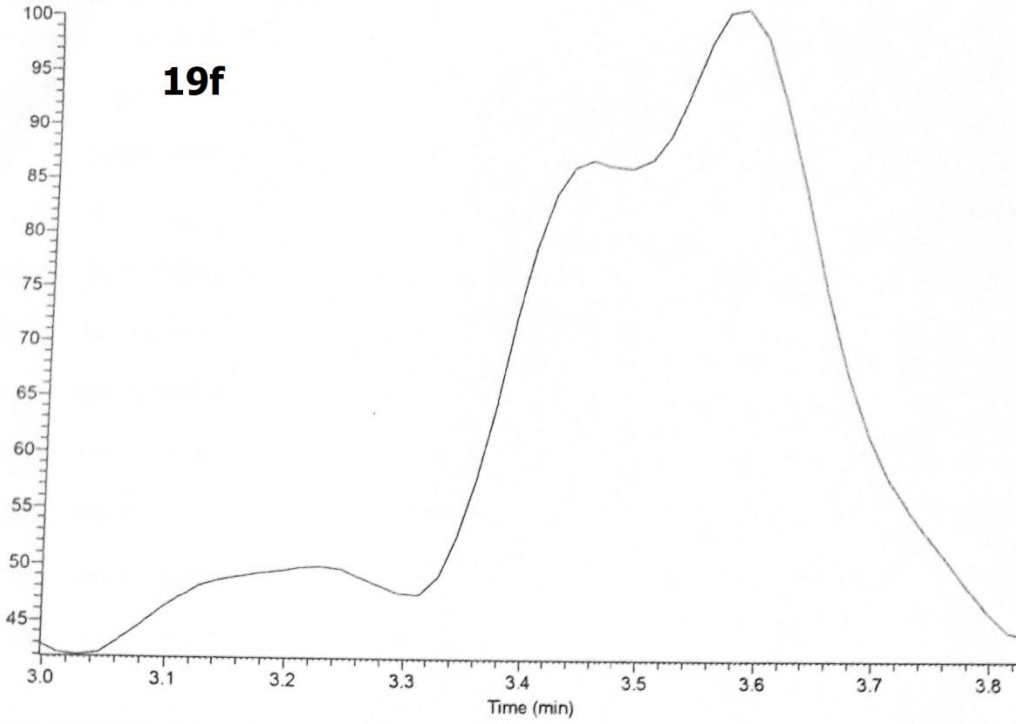


5h12#194 RT: 3.26 AV: 1 NL: 3.24E2
 T: (0.0) + c EI Full m/z [40.00-1000.00]

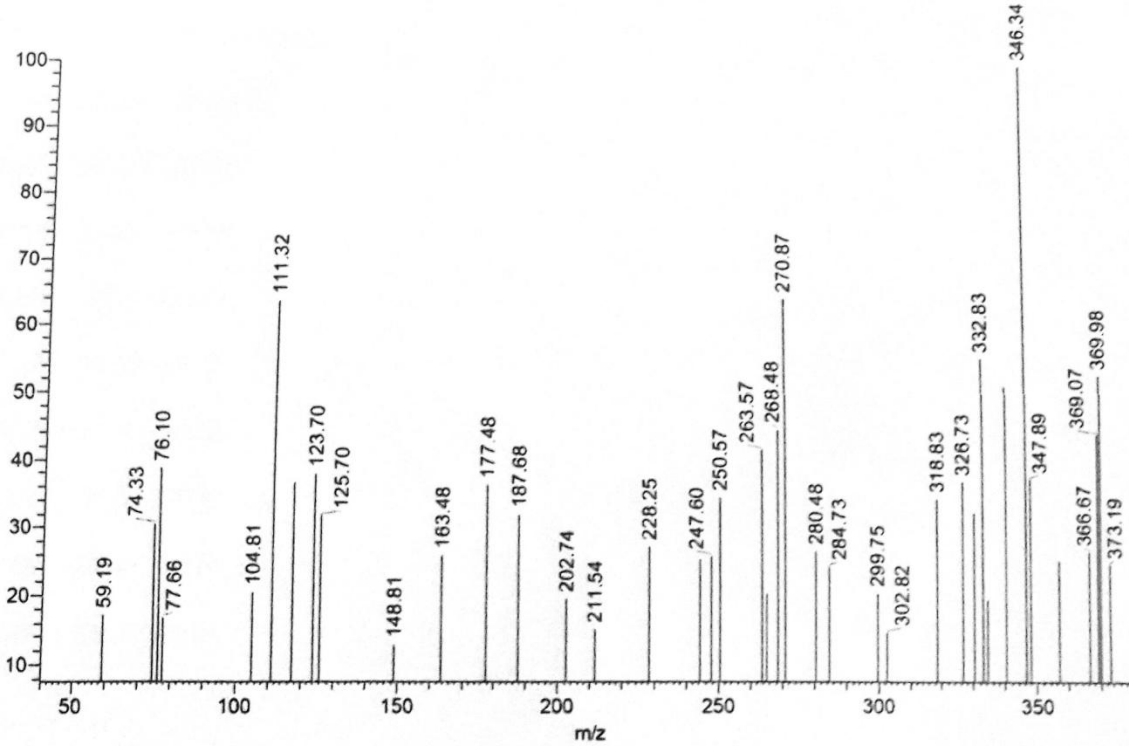


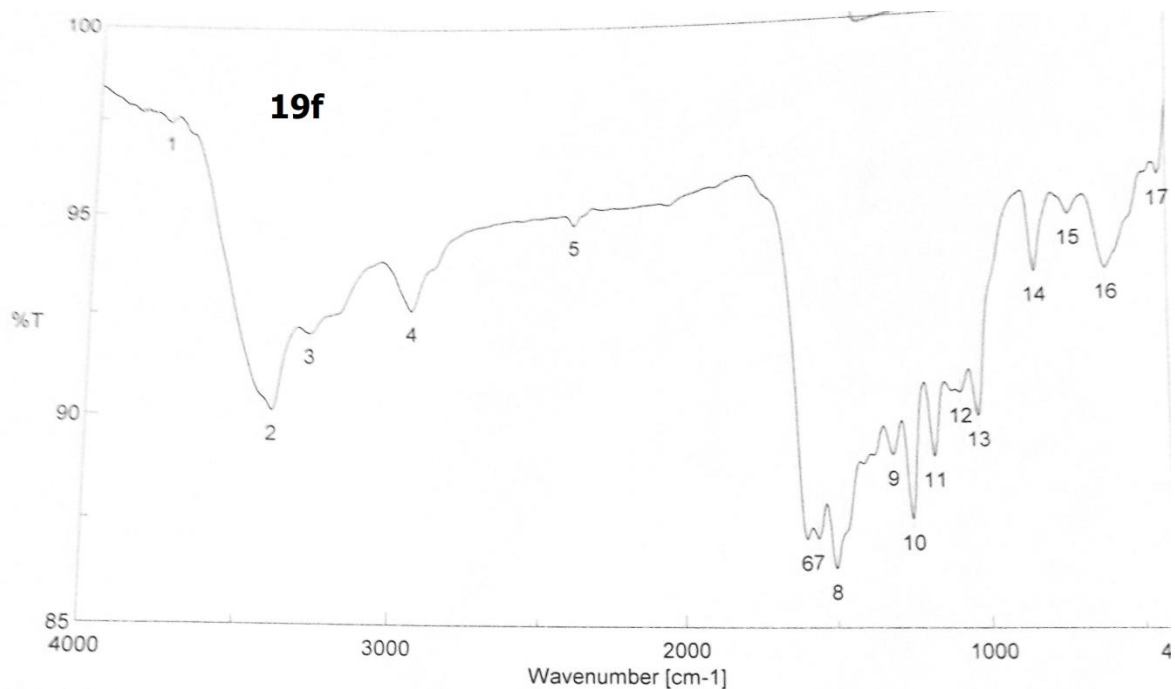
RT: 3.00-3.83 SM: 156

19f



h16 #233 RT: 3.92 AV: 1 NL: 3.74E2
: (0,0) + c EIFull ms [40.00-1000.00]



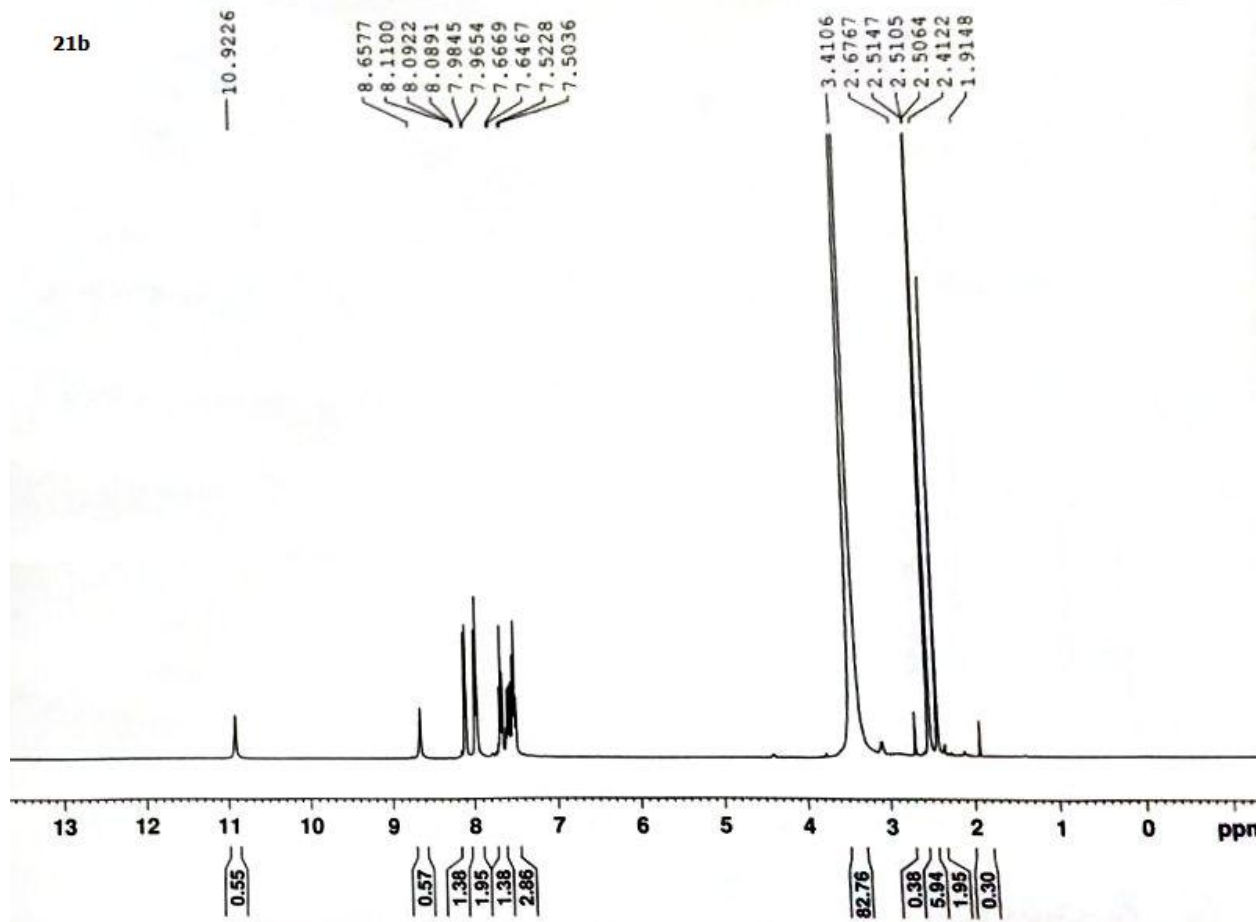


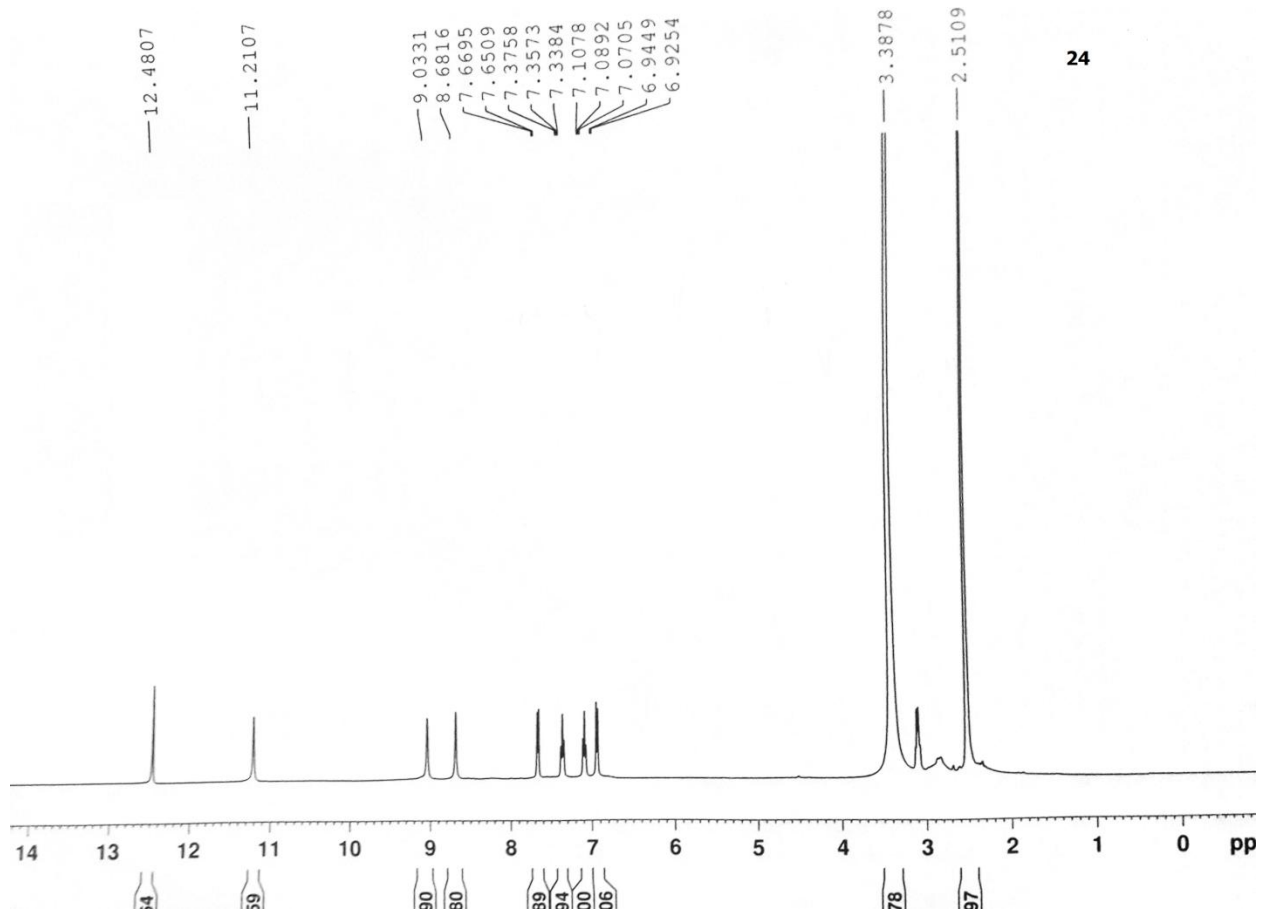
[Comments]
 Sample name SH 16
 Comment 6/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

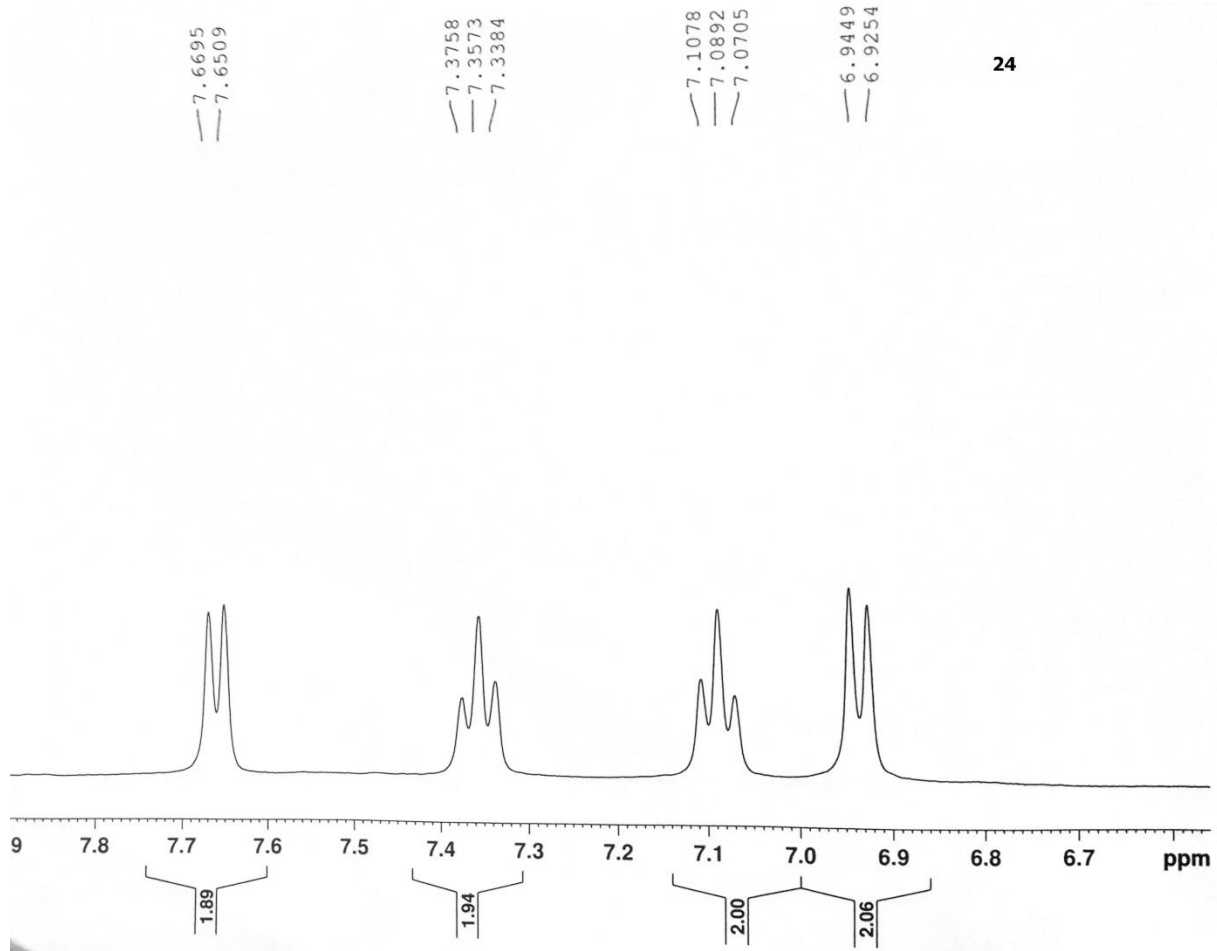
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3752.8	97.4128	2	3386.39	90.152	3	3265.86	92.0557
4	2926.45	92.6479	5	2374.91	94.8463	6	1597.73	87.1141
7	1560.13	87.1277	8	1502.28	86.4138	9	1311.36	89.1524
10	1249.65	87.6011	11	1175.4	89.1103	12	1086.69	90.6569
13	1028.84	90.0818	14	832.133	93.5772	15	717.39	94.9346
16	597.825	93.6022	17	427.155	95.7834			

21b

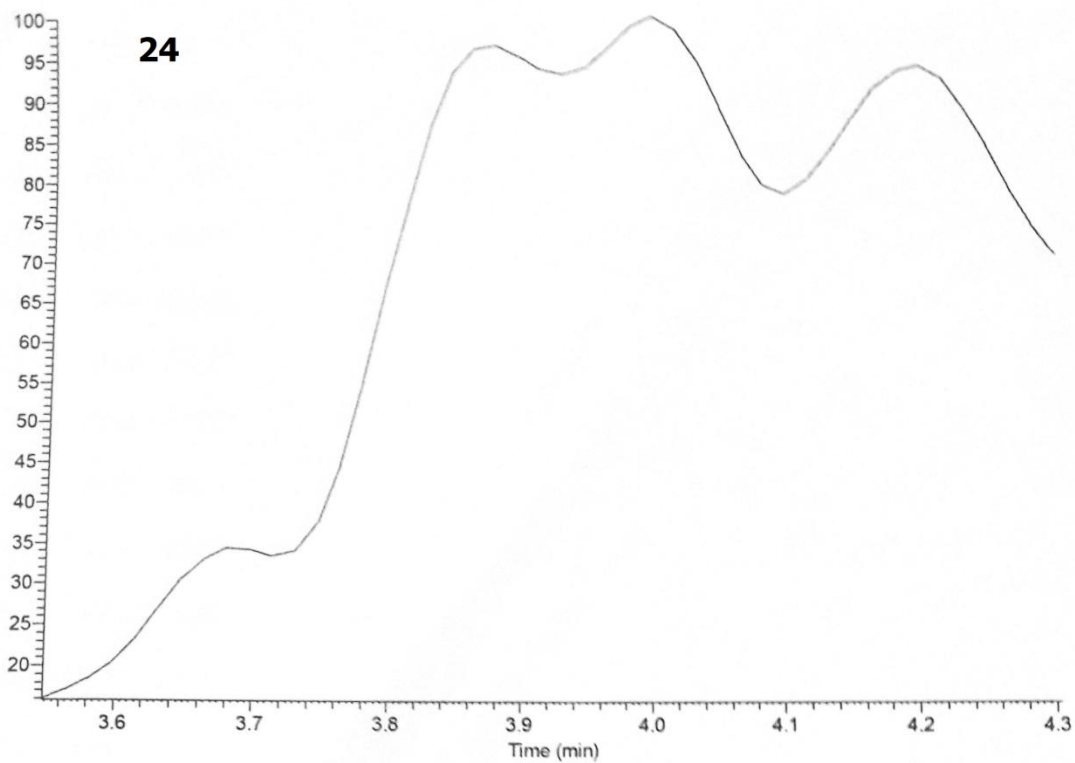




24



24



5h22 #250 RT: 4.20 AV: 1 NL: 5.19E2
 T: {0.0} + c EI Full ms [40.00-1000.00]

