(1)

(3)

(5)

(7A,a)

(7A,b)

(7A,c)

(7A,d)

(7A,e)

(7A,f) (7B,a) (7B,b) (7B,c) (7B,d) (7B,e) (7B,f) (7C,a)

(7C,b)　　　　　　　　(7C,c)

(7C,d)　　　　　　　　(7C,e)

(7C,f)　　　　　　　　(9a)

(9b)　　　　　　　　(9c)

Fig. 1S. Optimized structures of dithiazole synthesis & conformers
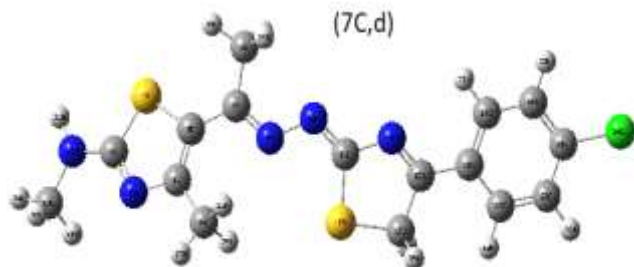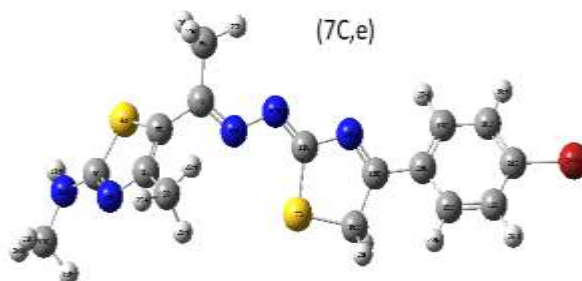
(7A,b)

(7A,c)

(7A,d)

(7A,e)
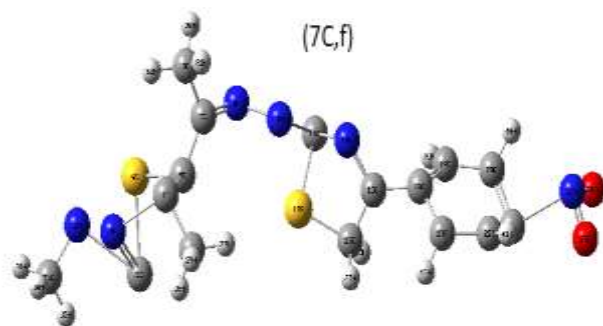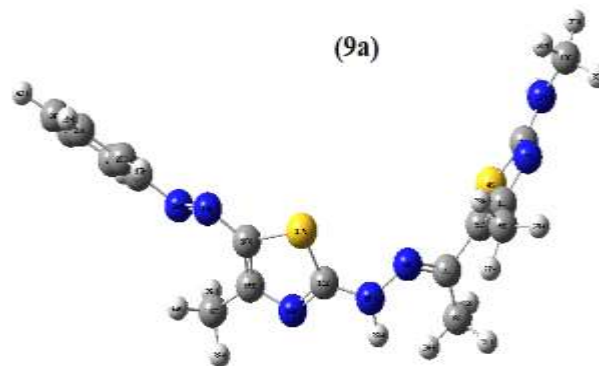
(7A,f)

(7B,a)

(7B,b)

(7B,c)

(7B,d)

(7B,e)

(7B,f)

(7C,a)

(7C,b)

(7C,c)

(7C,d)

(7C,e)

(7C,f)

(9a)

(9b)

(9c)
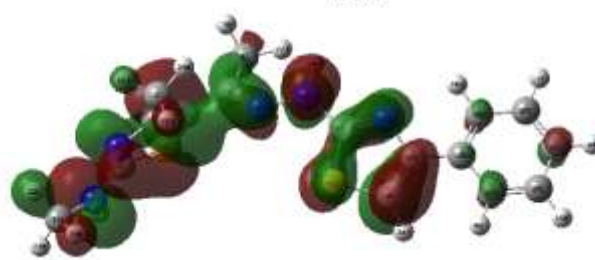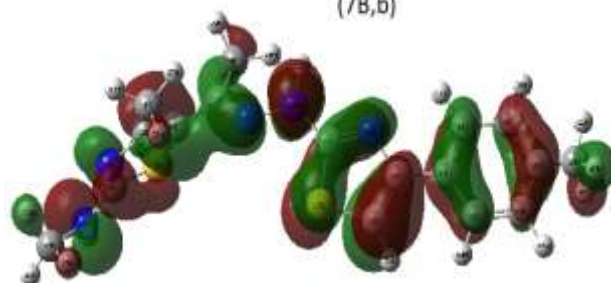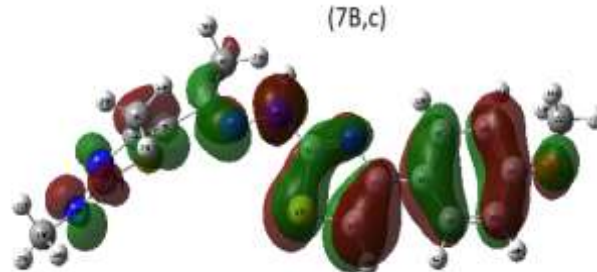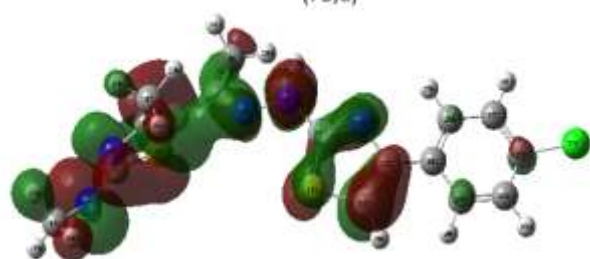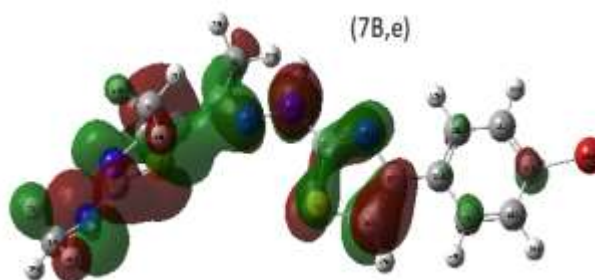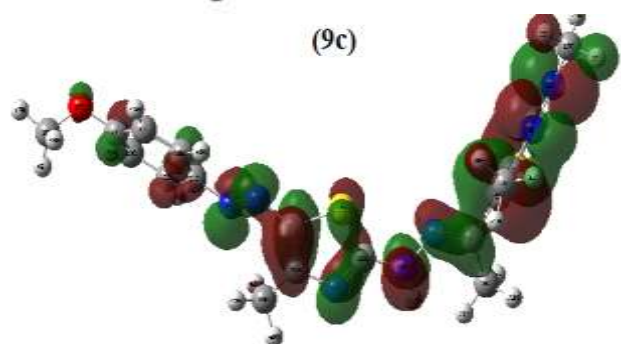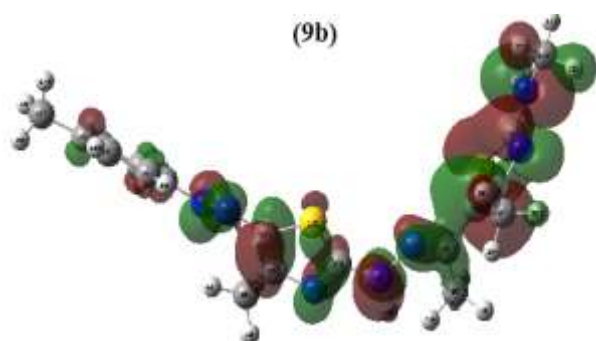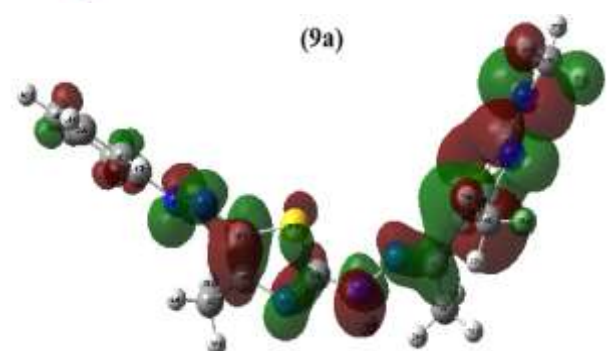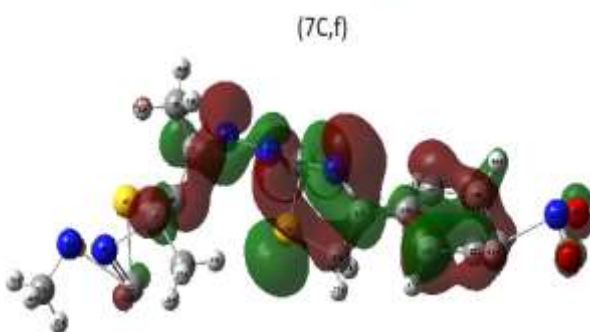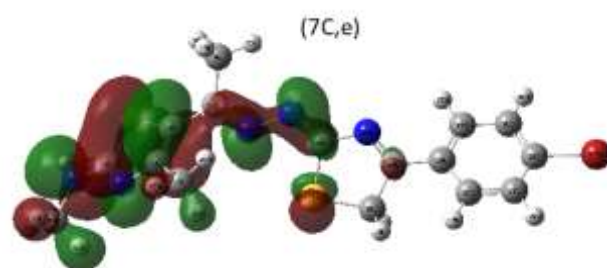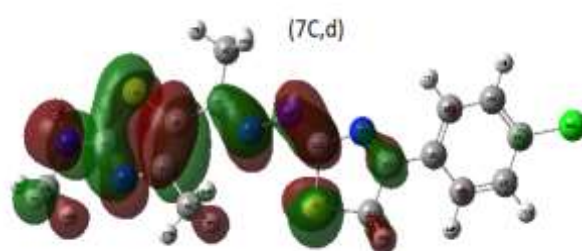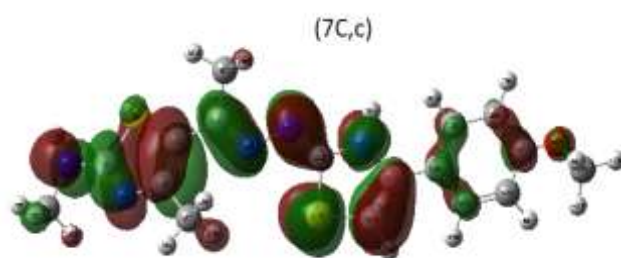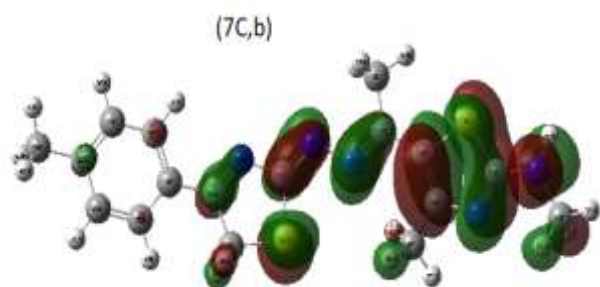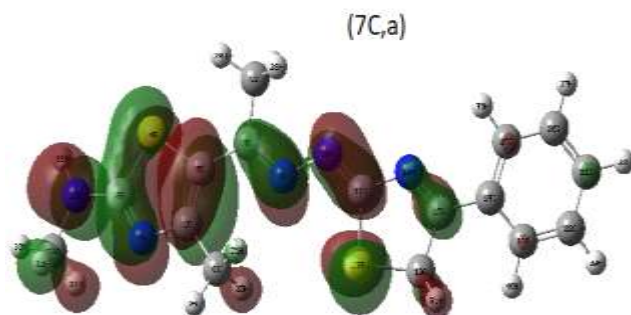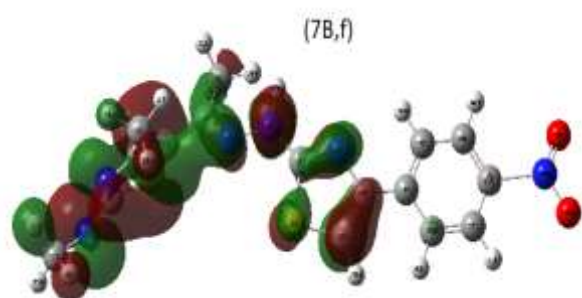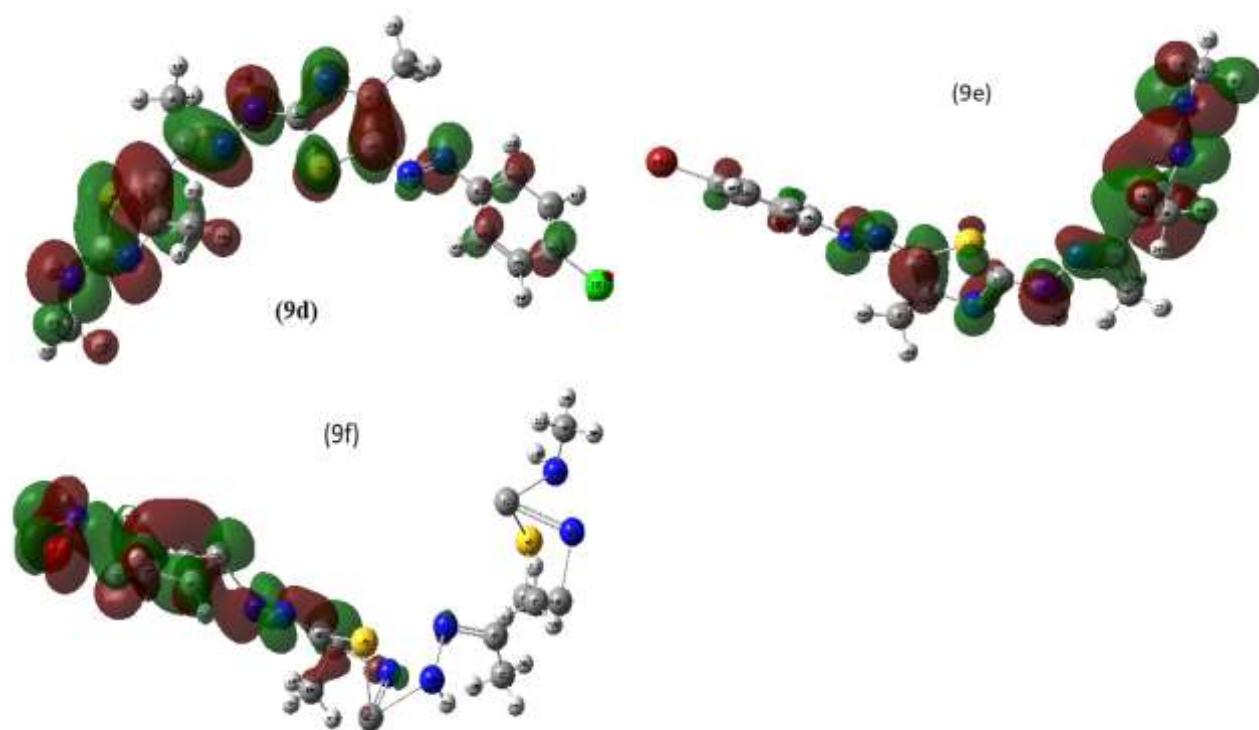
Fig. 2S. HOMO images of dithiazole synthesis & conformers

(7A,b)   (7A,c)

(7A,d)   (7A,e)
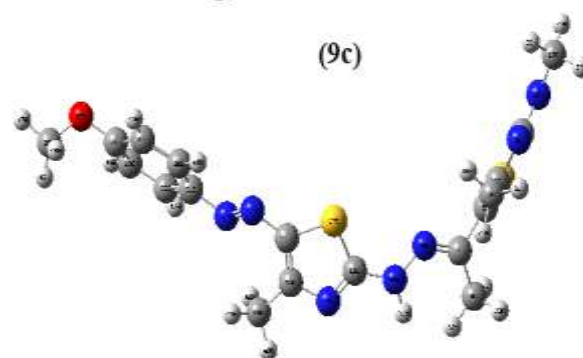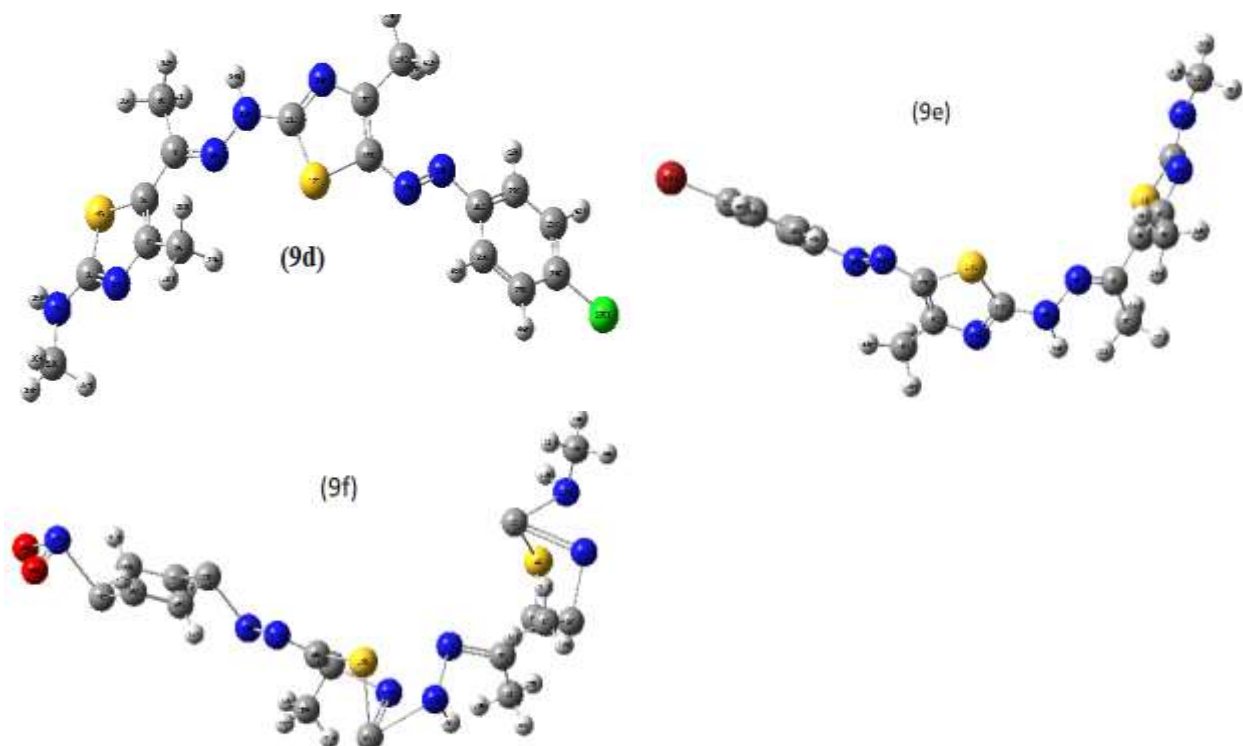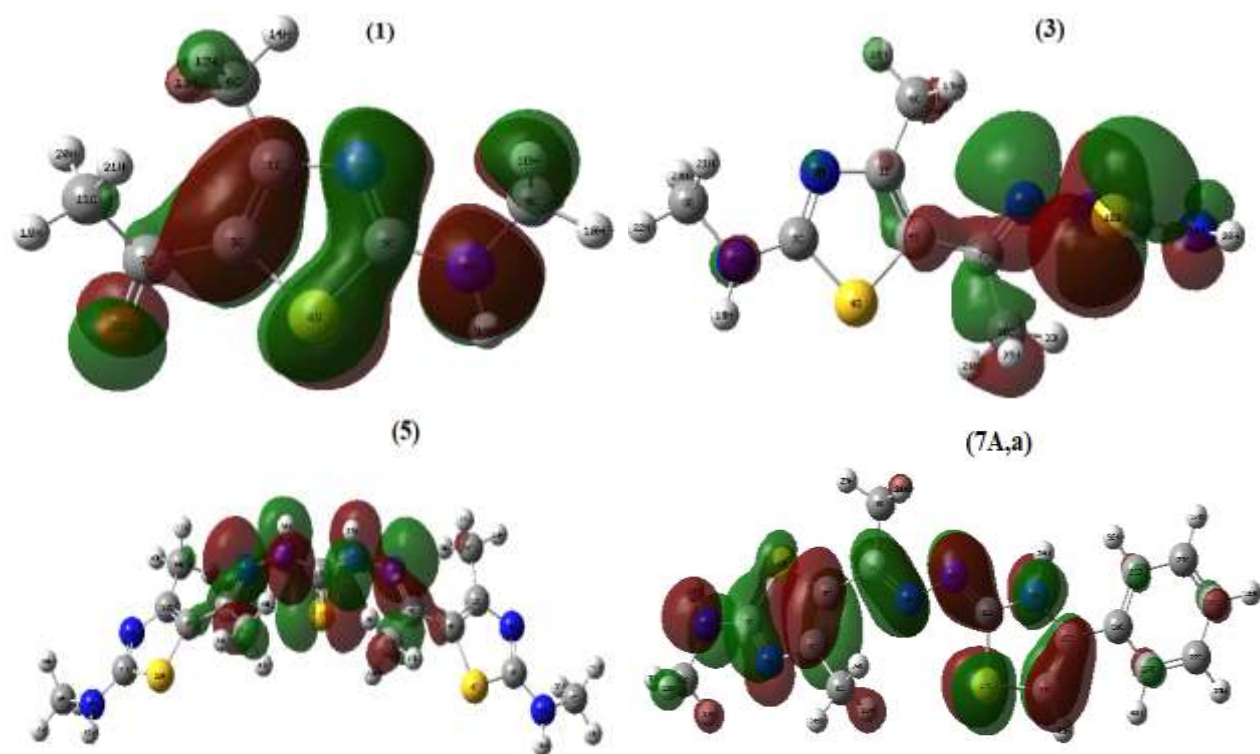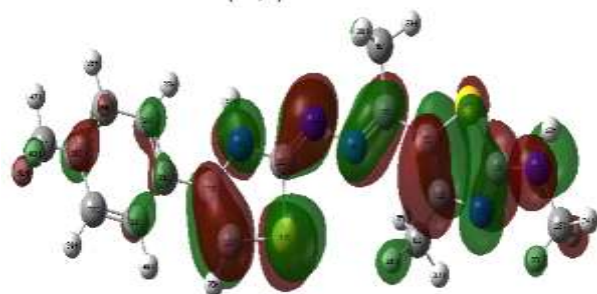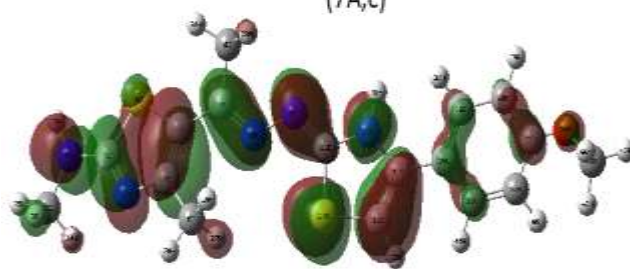
(7A,f)   (7B,a)
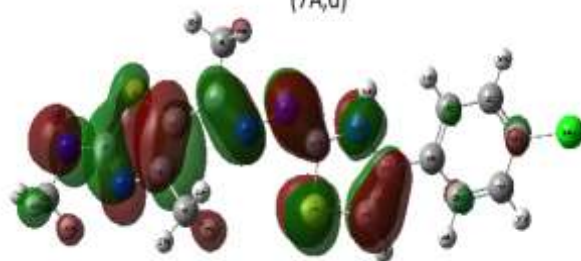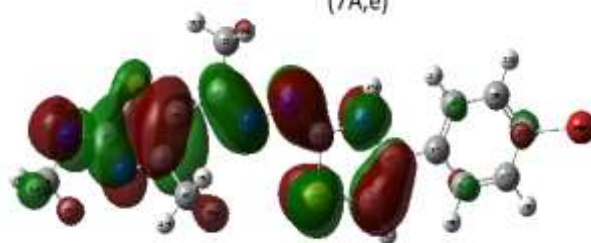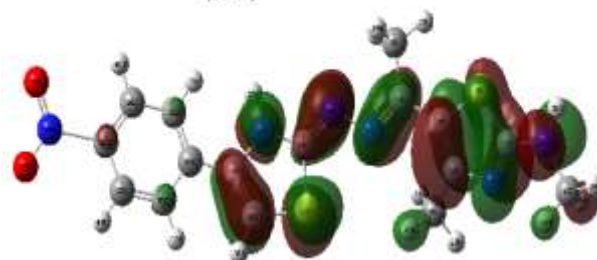
(7B,b)   (7B,c)

(7B,d)

(7B,e)

(7B,f)

(7C,a)

(7C,b)

(7C,c)

(7C,d)

(7C,e)
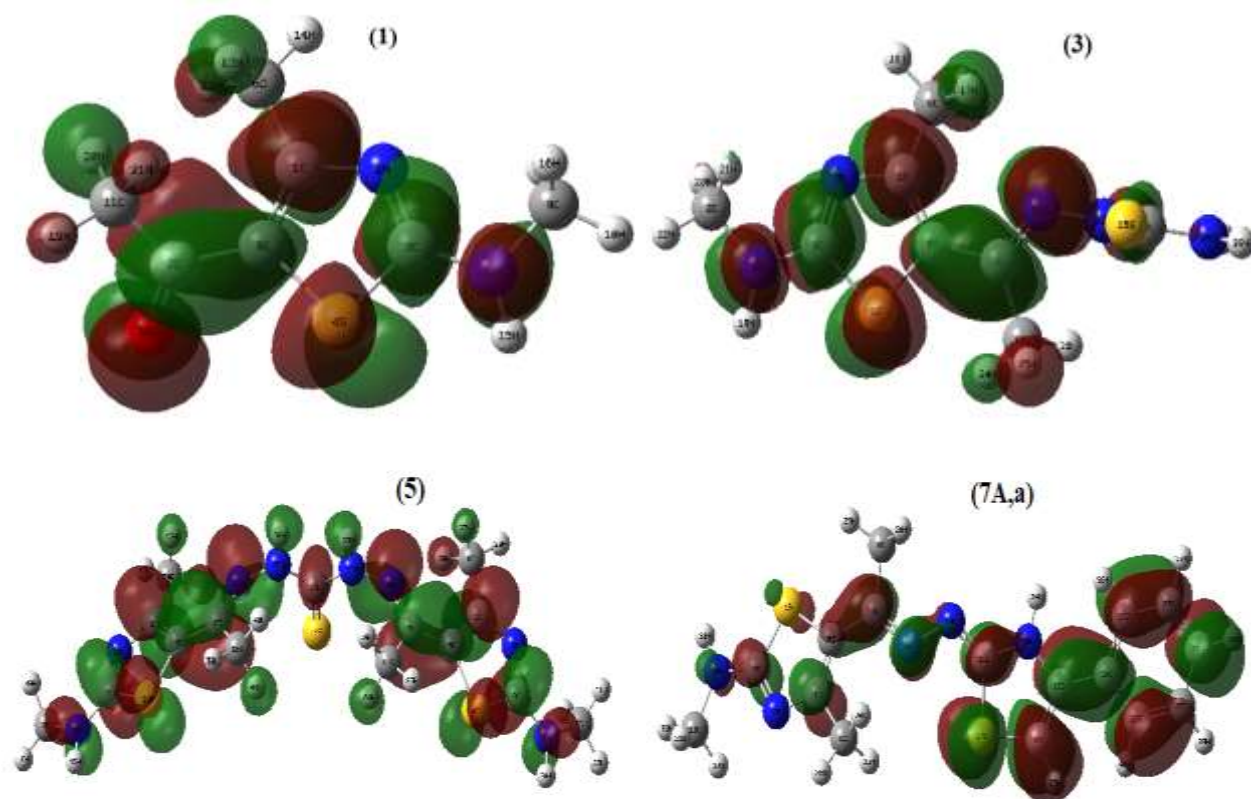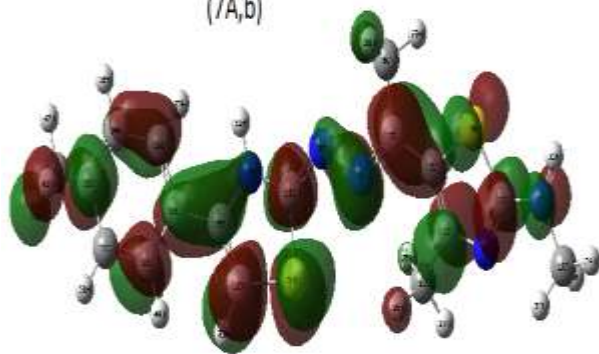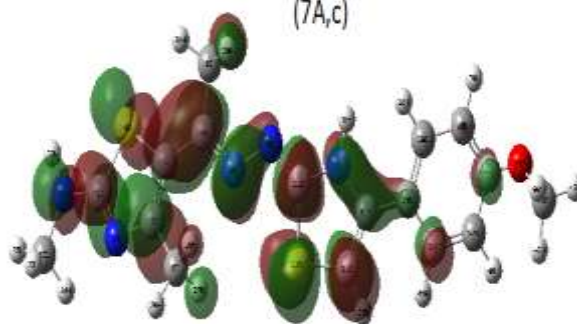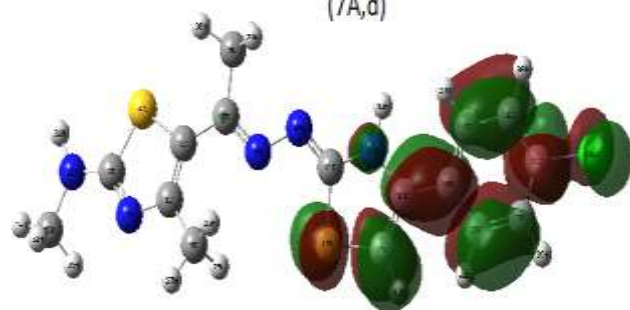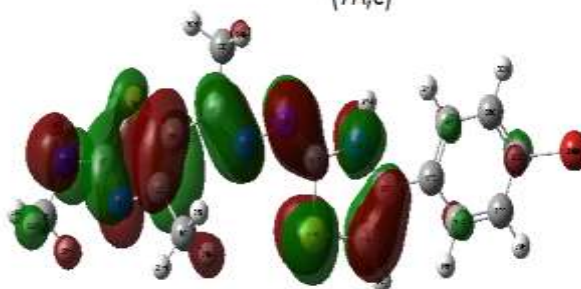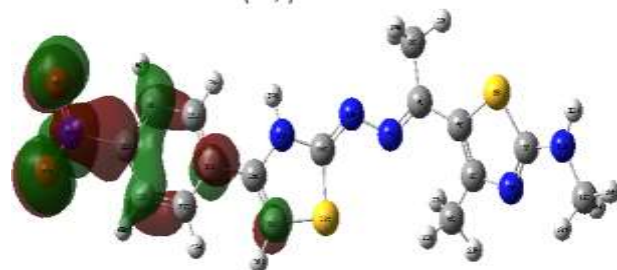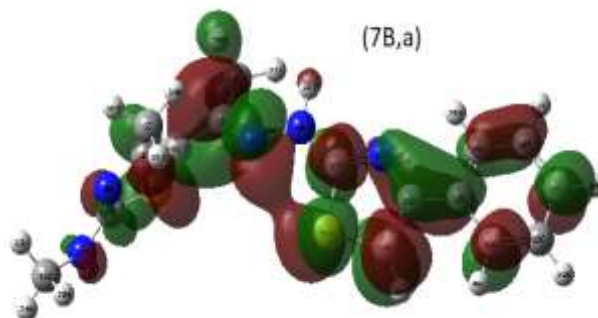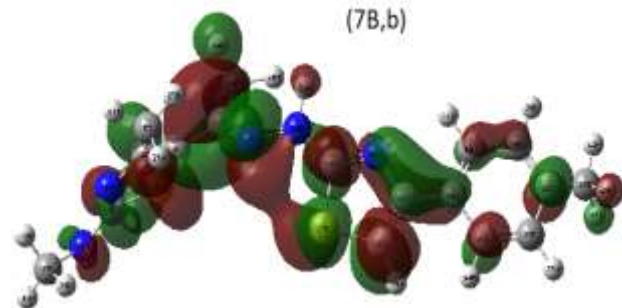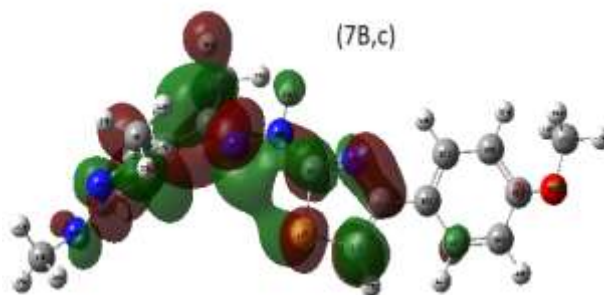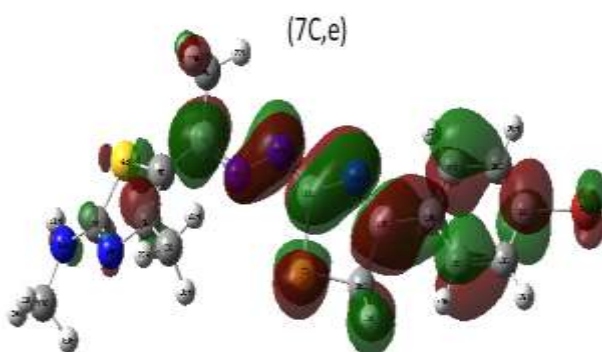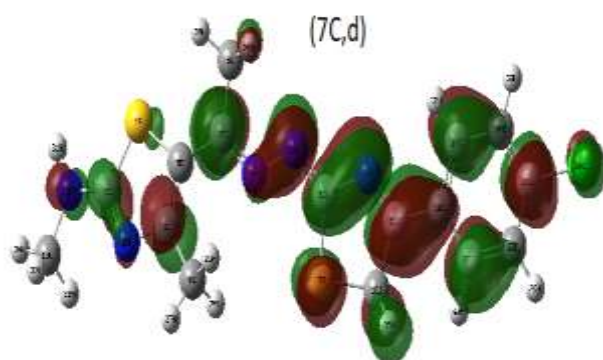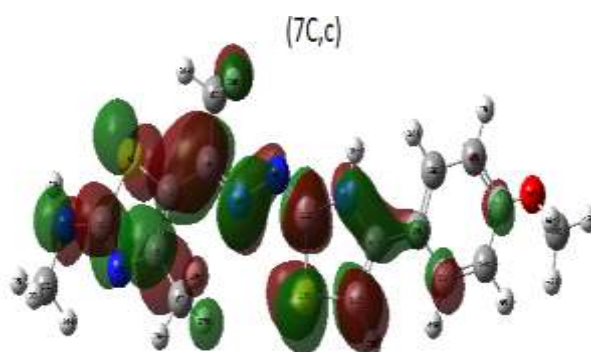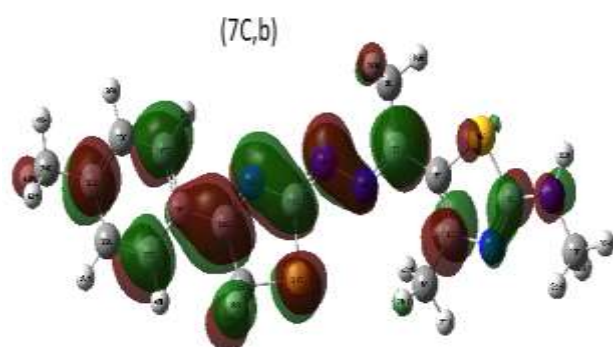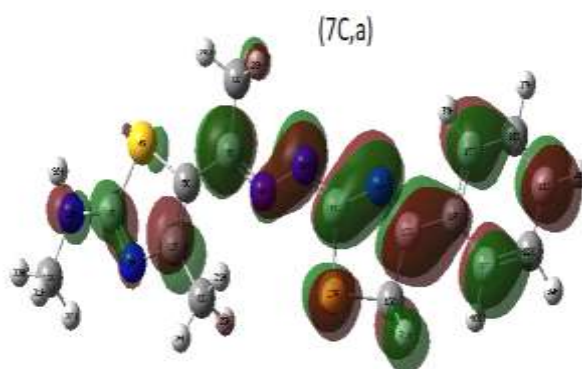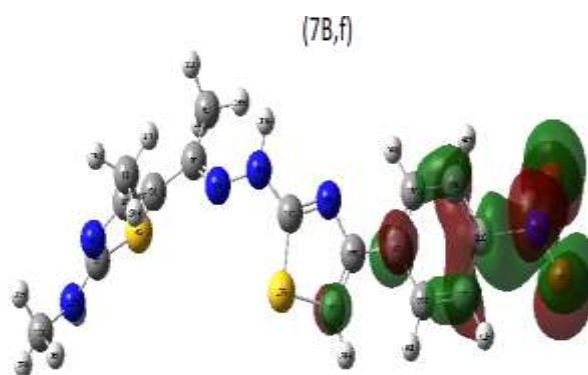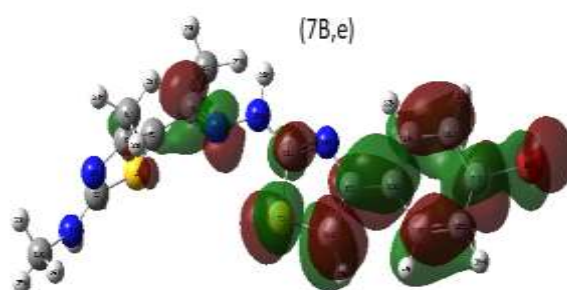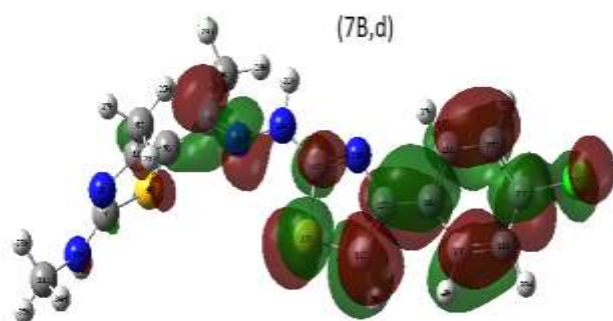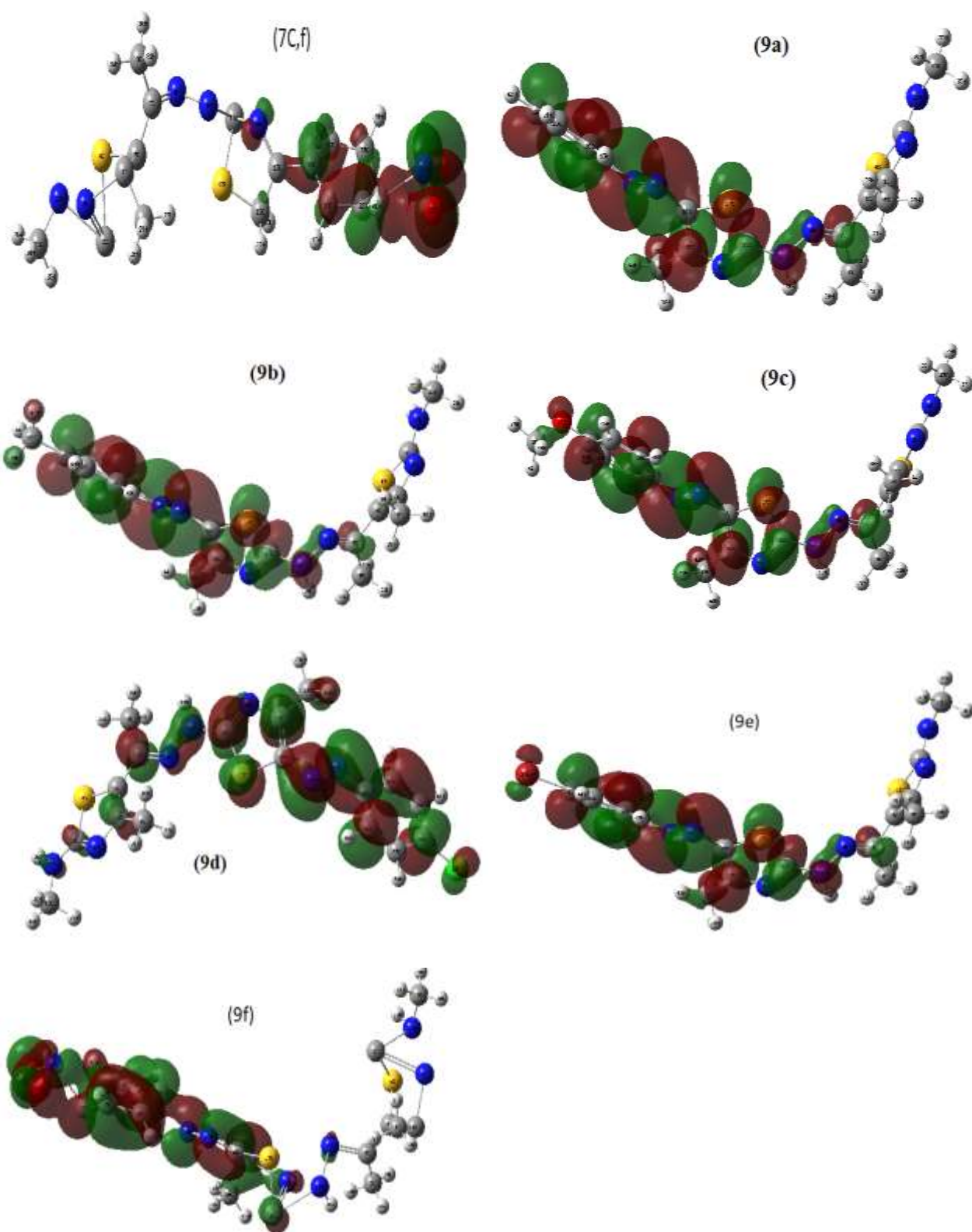
Fig. 3S. LUMO images of dithiazole synthesis & conformers

(-7.632e-2)

(1)

(7.632e-2]

(-9.394e-2)

(3)

(9.394e-2)

(-9.513e-2)

(5)

(9.513e-2)

(-7.223e-2)

(7A,a)

(7.223e-2)

(-7.221e-2)

(7A,b)

(7.221e-2)

(-7.315e-2)

(7A,c)

(7.315e-2)

(-7.511e-2)

(7A,d)

(7.511e-2)

(-7.366e-2)

(7A,e)

(7.366e-2)

(-8.532e-2)

(7A,f)

(8.532e-2)

(-7.488e-2)

(7B,a)

(7.488e-2)

(-7.325e-2)

(7B,b)

(7.325e-2)

(-7.205e-2)

(7B,c)

(7.205e-2)

(-7.591e-2)

(7B,d)

(7.591e-2)

(-7.552e-2)

(7B,e)

(7.552e-2)

(-7.774e-2)

(7B,f)

(7.774e-2)

(-8.344e-2)

(7C,a)

(8.344e-2)

(-8.580e-2)

(7C,b)

(8.580e-2)

(-7.315e-2)

(7C,c)

(7.315e-2)

(-7.740e-2)

(7C,d)

(7.740e-2)

(-7.768e-2)

(7C,e)

(7.768e-2)
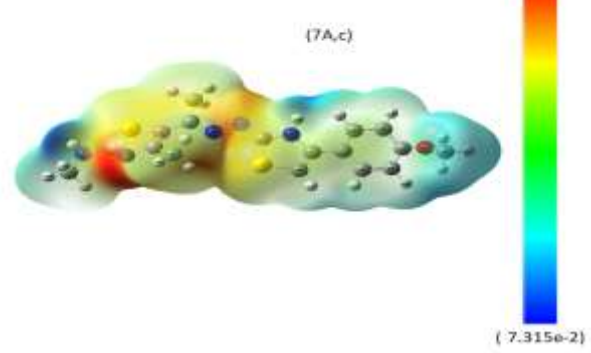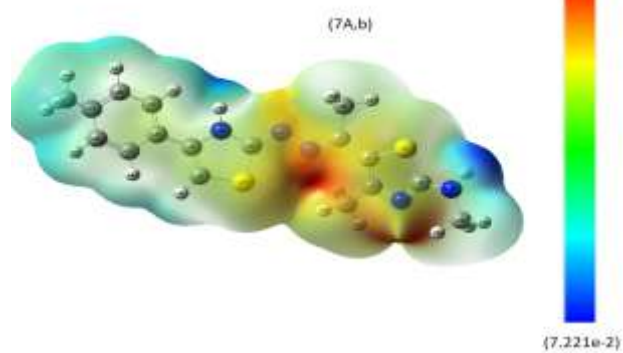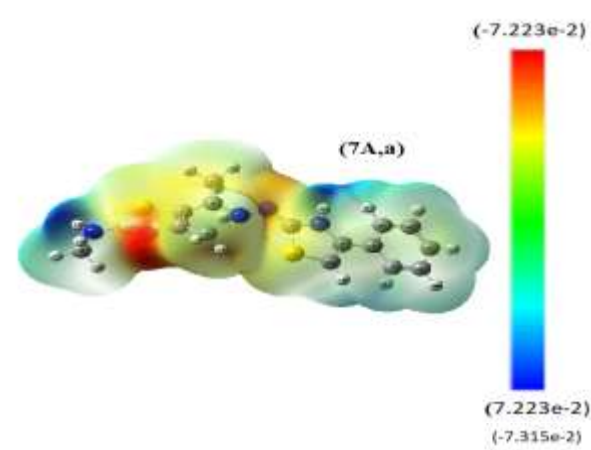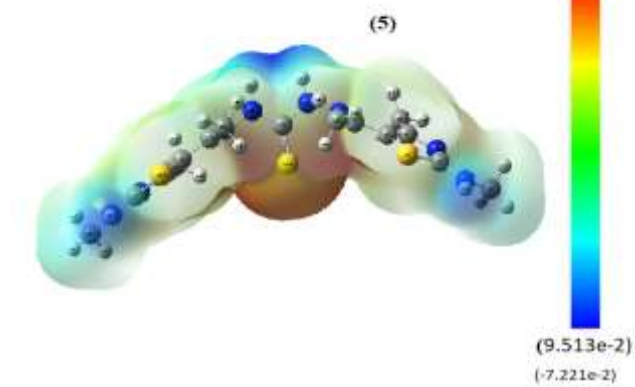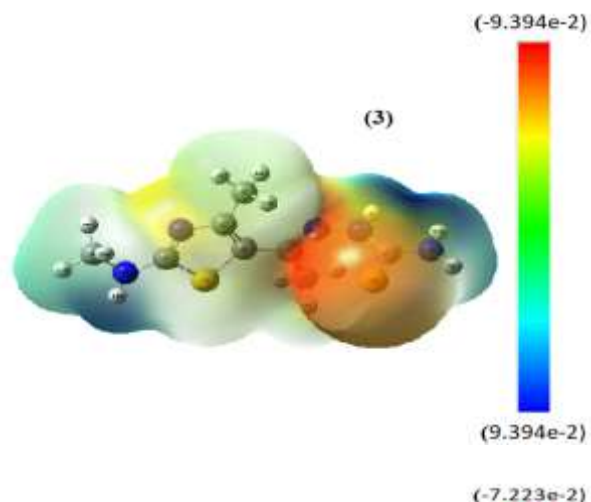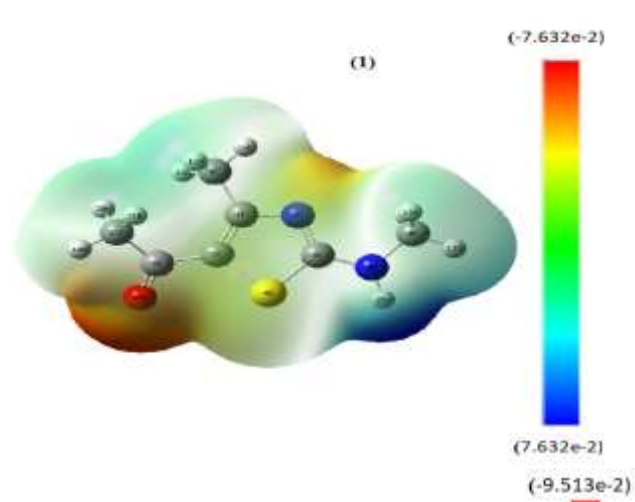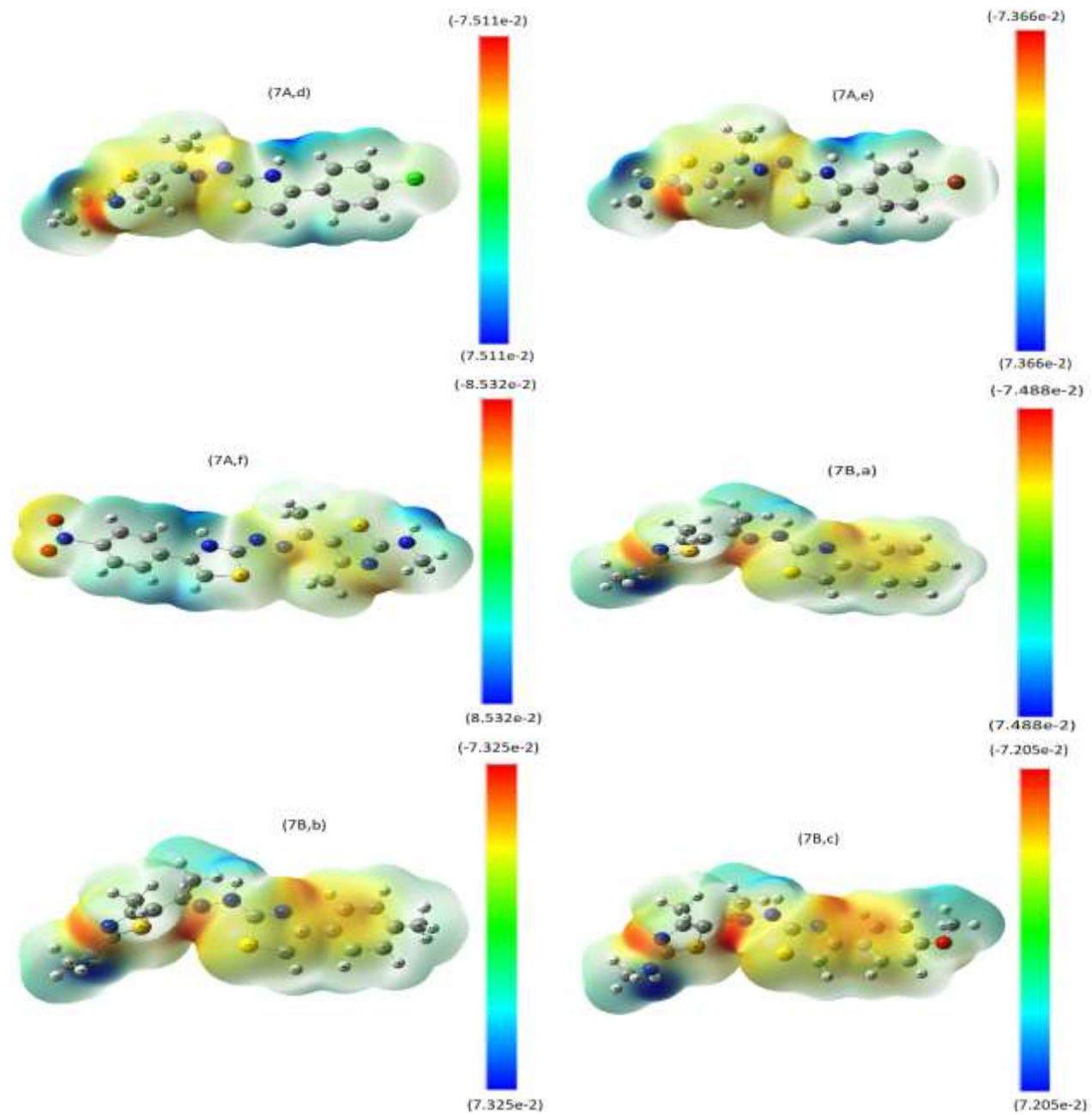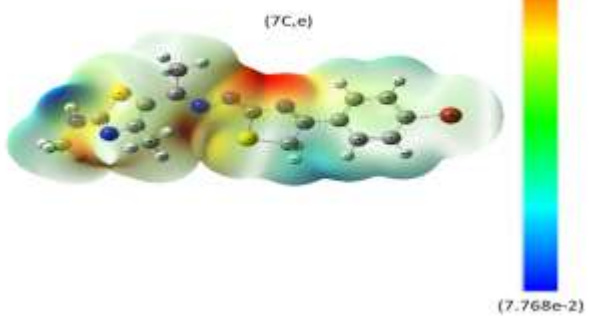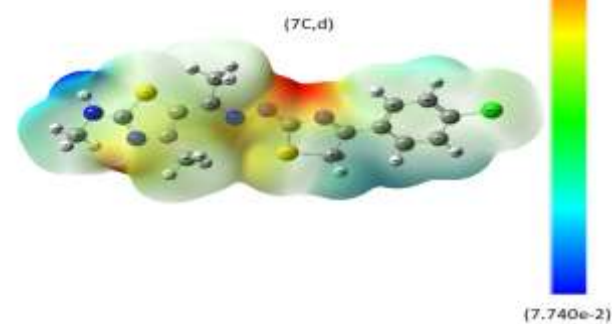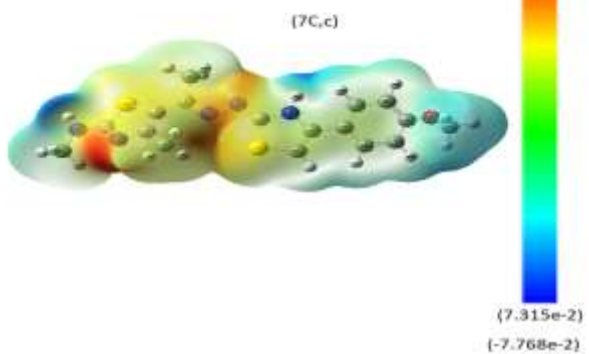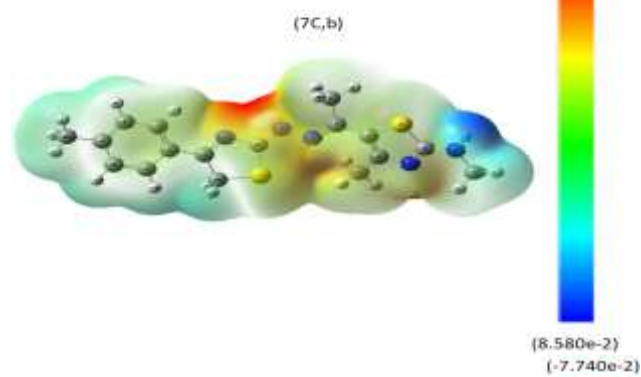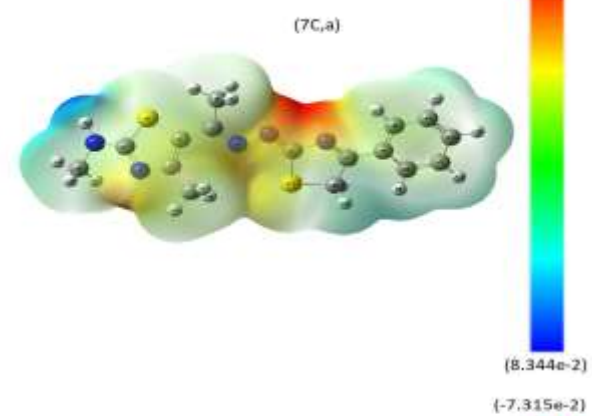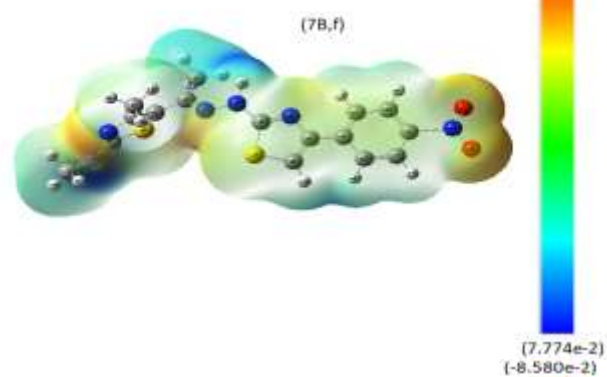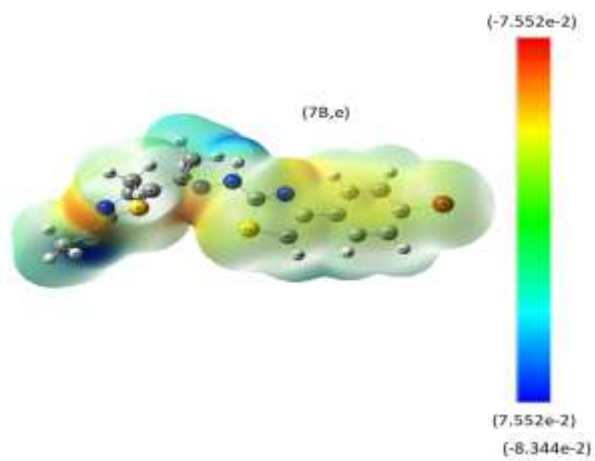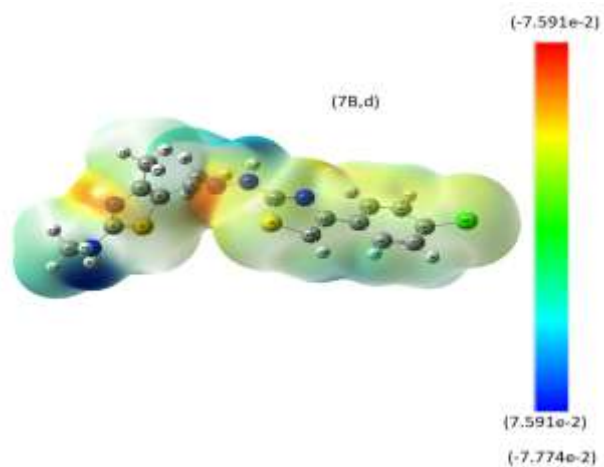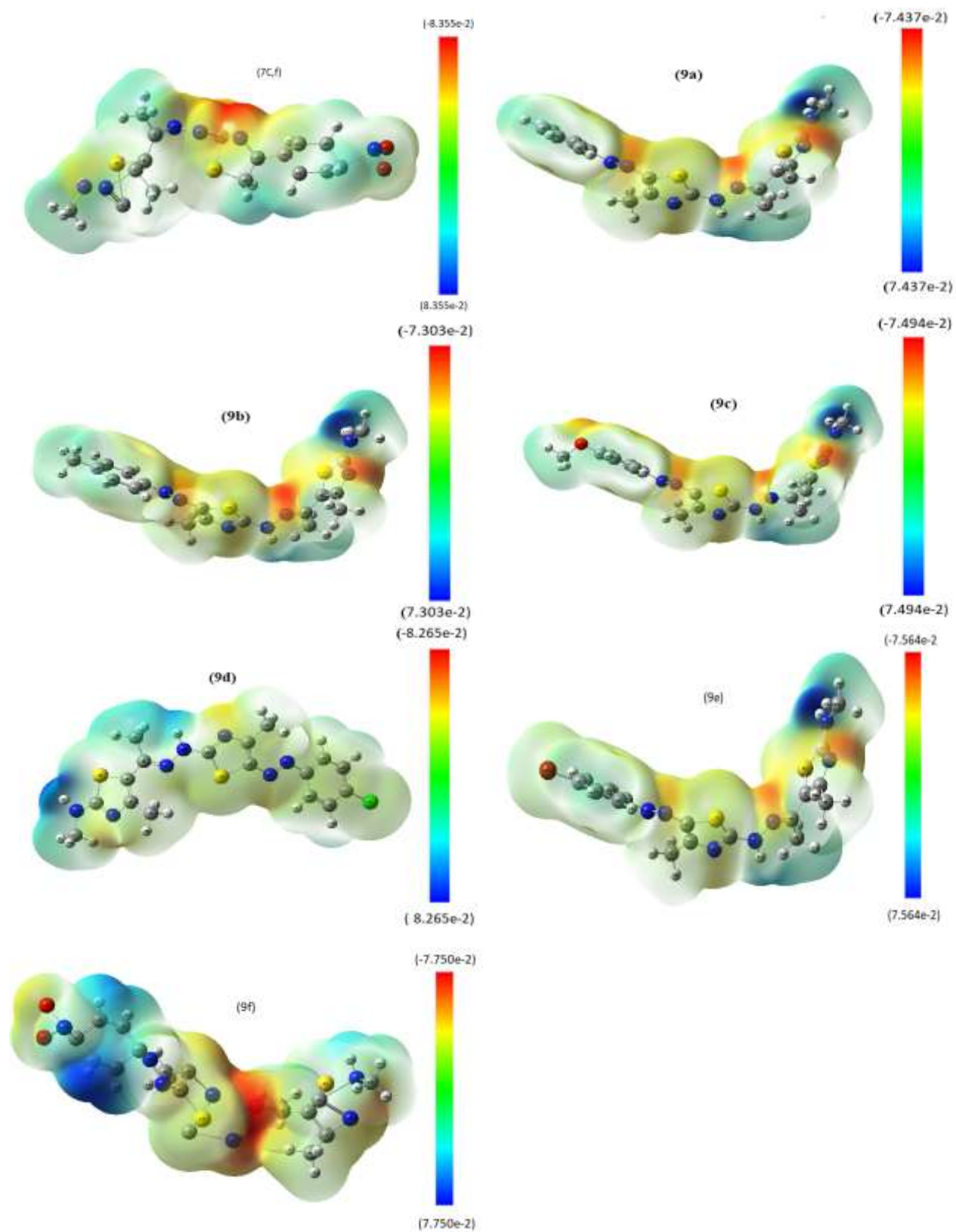
Fig. 4S. Electrostatic maps of dithiazole compounds & conformers
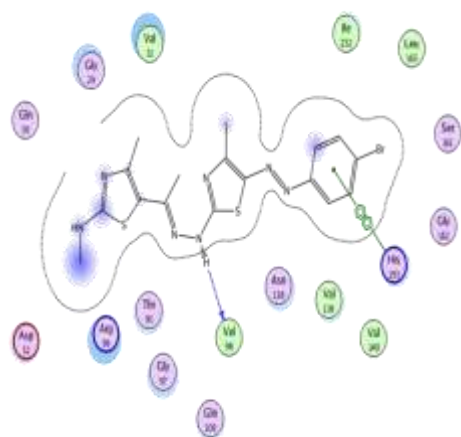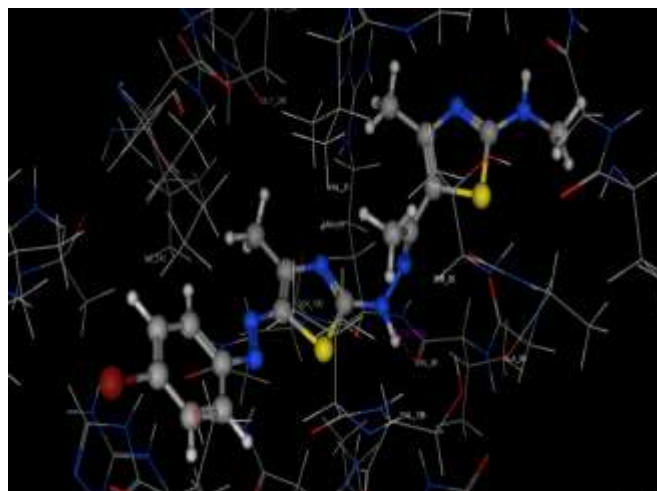
A   B

Figure 5S: The proposed binding mode of the **9e** docked in the active site of LDH-5; A and B showing 2D and 3D ligand-receptor interactions
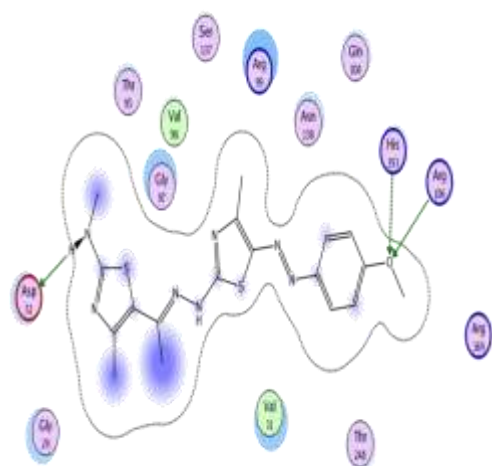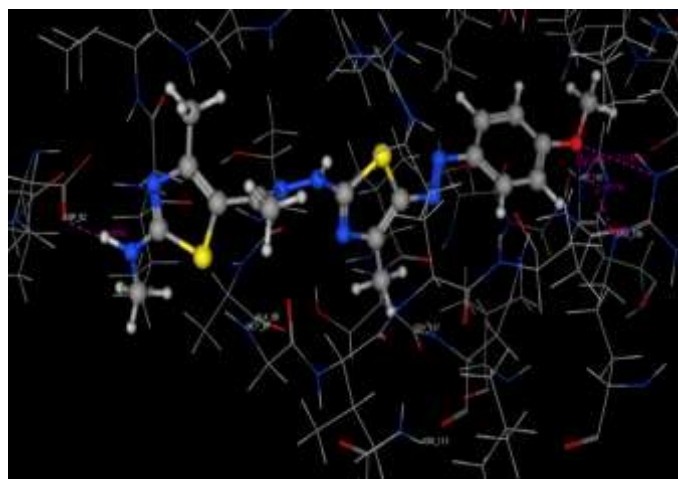
A   B

Figure 6S: The proposed binding mode of the **9c** docked in the active site of LDH-5; A and B showing 2D and 3D ligand-receptor interactions

Peak Find - Memory-90
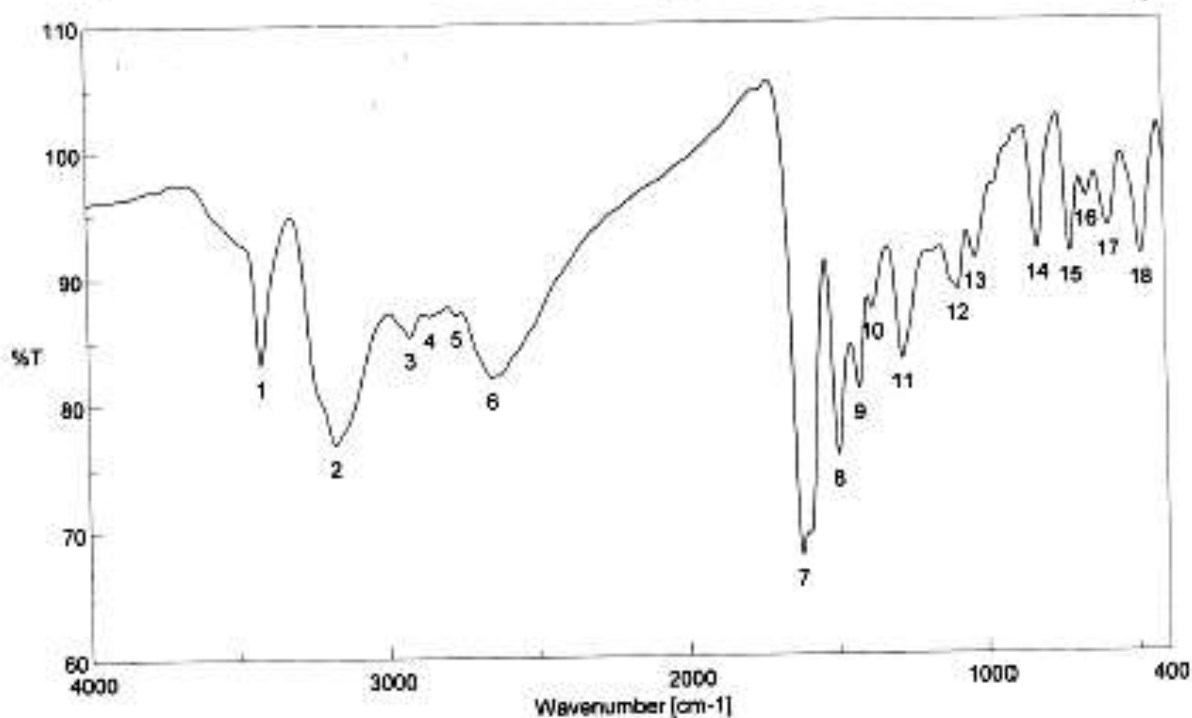
[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3423.03	83.2412	2	3177.15	76.85	3	2925.48	85.3475
4	2859.92	86.9167	5	2770.24	87.0068	6	2650.68	82.0628
7	1620.88	67.8441	8	1495.53	75.6668	9	1424.17	80.8497
10	1377.89	87.2187	11	1278.54	83.2181	12	1090.55	88.6135
13	1030.77	91.0792	14	829.241	91.7458	15	716.425	91.4859
16	662.426	95.8962	17	588.182	93.4936	18	479.224	91.2237

Peak Find - Memory-86
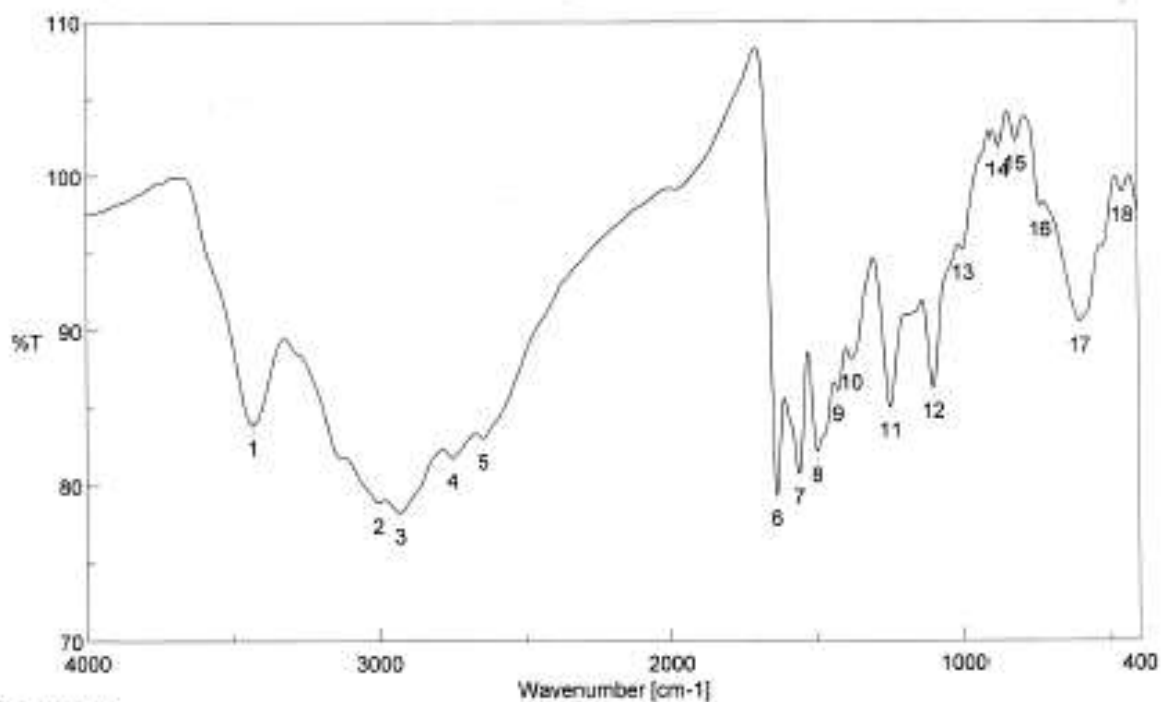
[Comments]
Sample name **Compound 5**
Comment 6/2018
User IR
Division IR
Company MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3428.81	83.928	2	3001.66	78.9073	3	2927.41	78.2705
4	2748.07	81.8189	5	2643.93	83.0612	6	1636.3	79.3552
7	1560.13	80.756	8	1498.42	82.1682	9	1426.1	86.1045
10	1380.78	86.143	11	1248.68	85.0351	12	1100.19	86.2835
13	996.053	95.2217	14	878.417	101.882	15	821.527	102.286
16	735.71	97.997	17	602.646	90.5132	18	452.225	98.9232

Compound 5
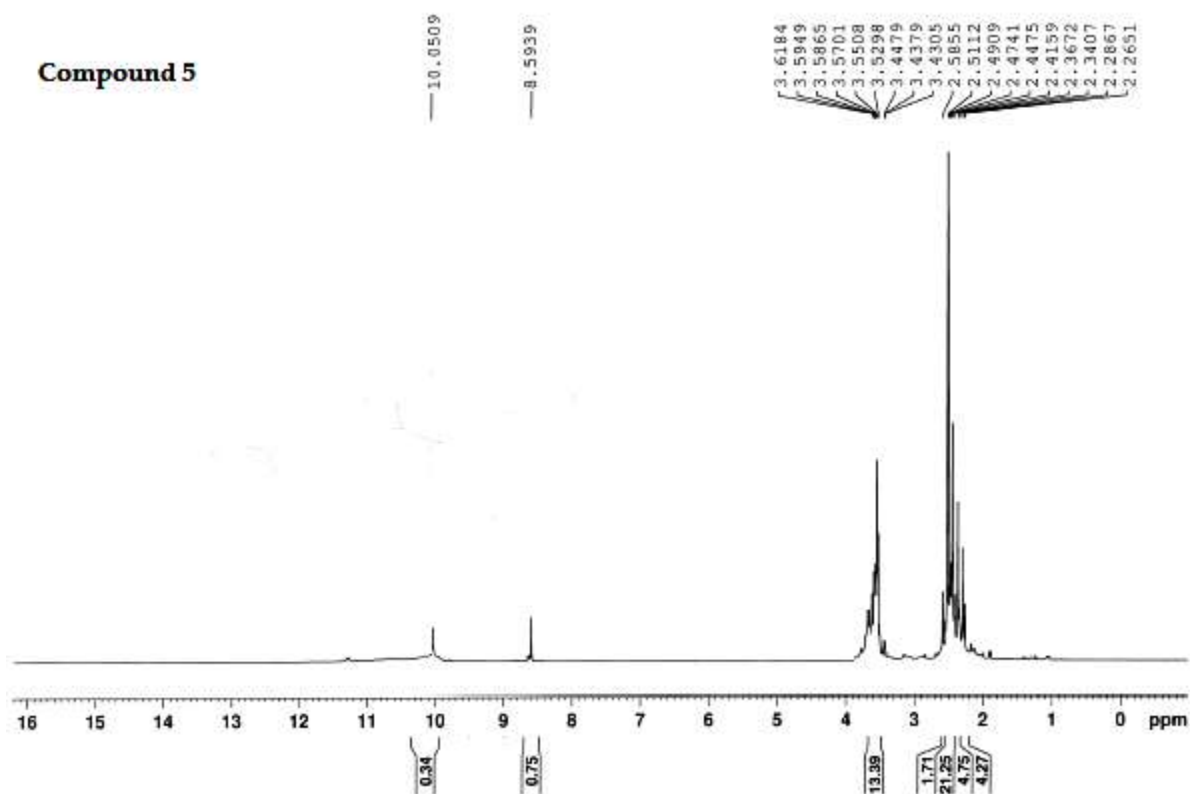
Peaks labeled: 10.0509, 8.5939, 3.6184, 3.5949, 3.5865, 3.5701, 3.5508, 3.5298, 3.4479, 3.4379, 3.4305, 2.5855, 2.5112, 2.4909, 2.4741, 2.4475, 2.4159, 2.3672, 2.3407, 2.2867, 2.2651
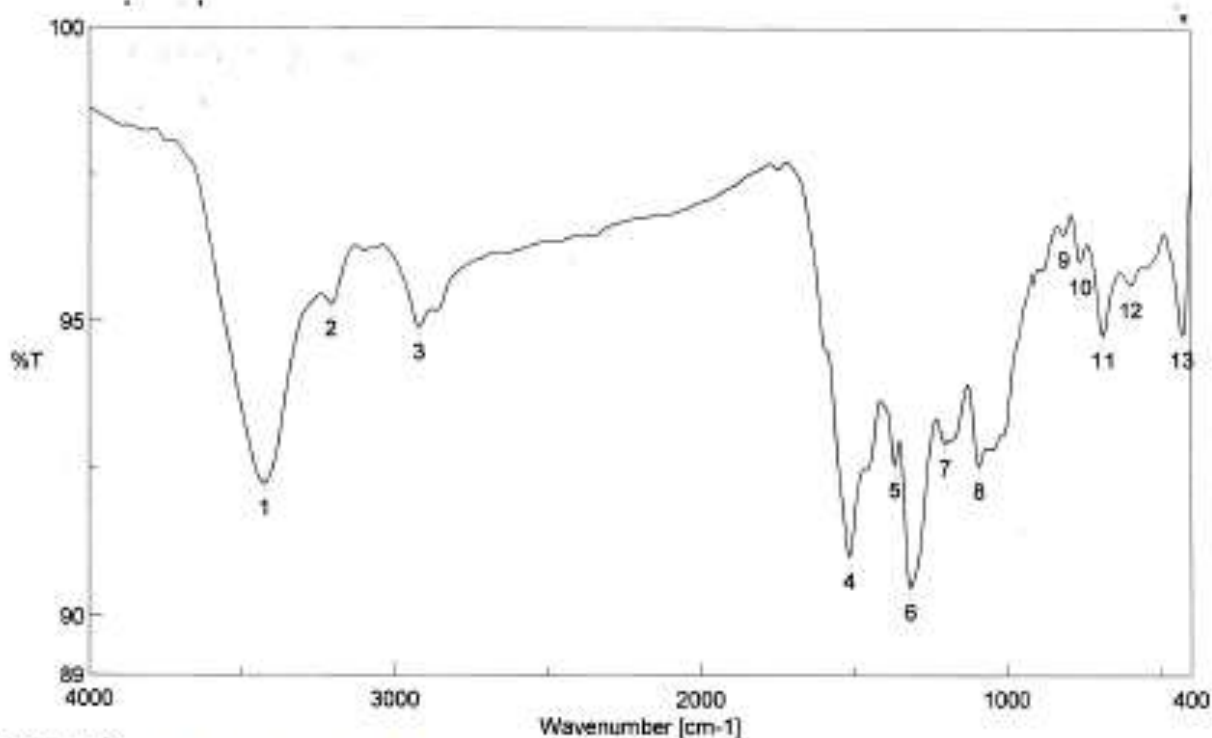
Integrations: 0.34, 0.75, 13.39, 1.71, 21.25, 4.75, 4.27

x-axis: 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

Peak Find - Memory-114

Compound 7a

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3424.96	92.2504	2	3208	95.2979	3	2920.66	94.9039
4	1514.81	91.0288	5	1366.32	92.5672	6	1316.18	90.4977
7	1202.4	92.9342	8	1090.55	92.5501	9	818.634	96.484
10	762.709	96.0171	11	688.463	94.7678	12	597.825	95.6226
13	429.084	94.7818						

Compound 7b
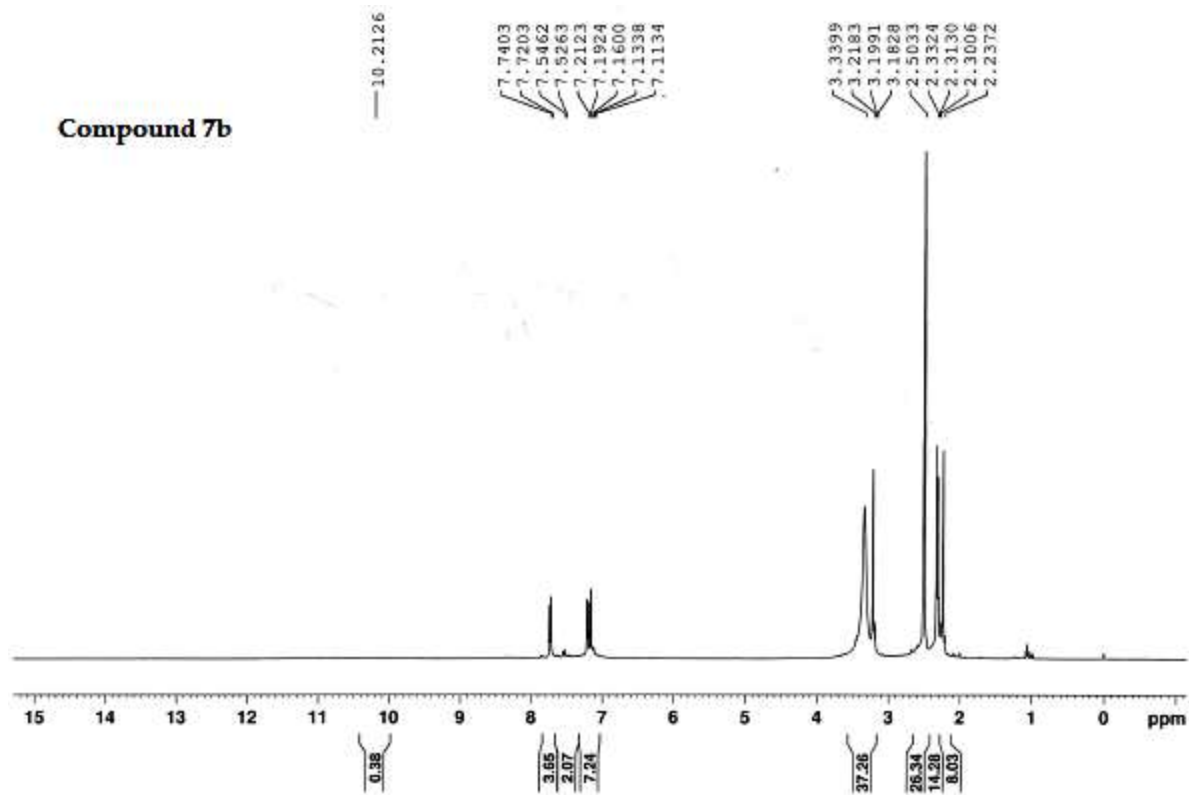
Peaks (ppm): 10.2126; 7.7403, 7.7203, 7.5462, 7.5263, 7.2123, 7.1924, 7.1600, 7.1338, 7.1134; 3.3399, 3.2183, 3.1991, 3.1828, 2.5033, 2.3324, 2.3130, 2.3006, 2.2372
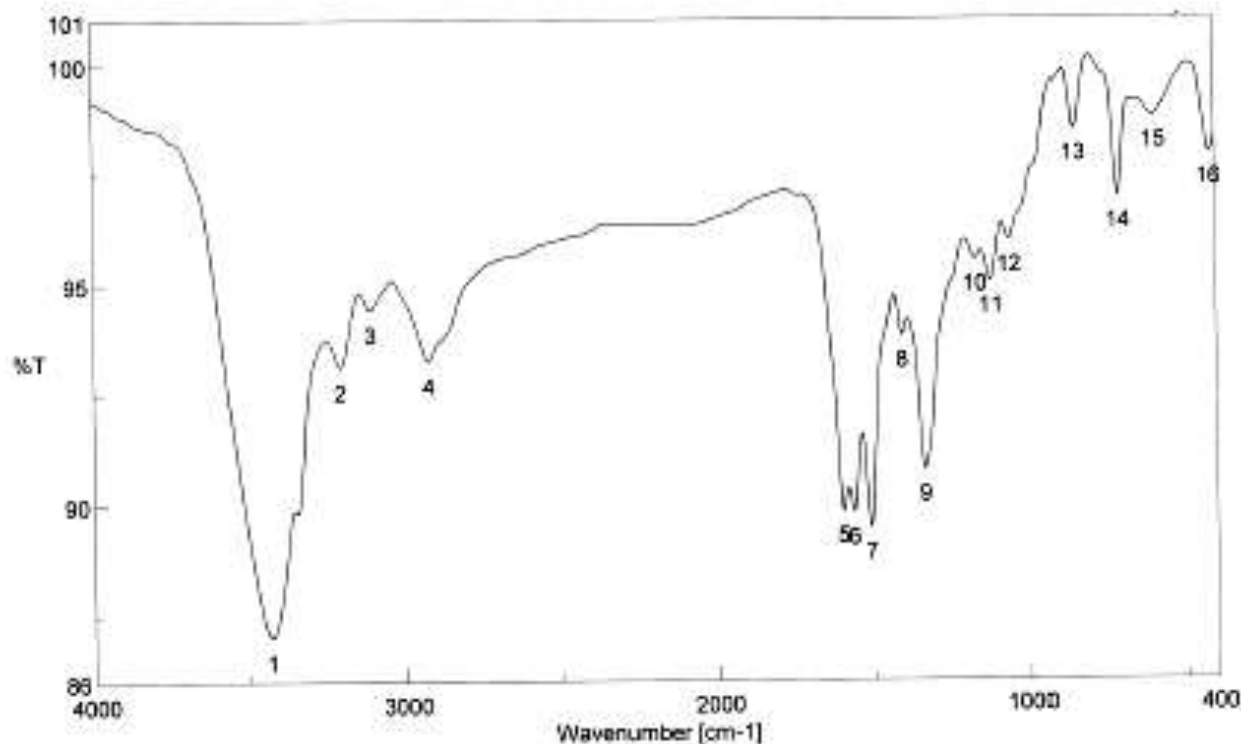
Integrations: 0.38 | 3.65, 2.07, 7.24 | 37.26 | 26.34, 14.28, 8.03

%T vs Wavenumber [cm-1]

[Comments]
Sample name **Compound 7c**
Comment   6/2018
User   IR
Division   IR
Company   MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3431.71	87.0209	2	3208	93.113	3	3110.62	94.4106
4	2925.48	93.244	5	1596.77	89.827	6	1563.99	89.7965
7	1509.03	89.4465	8	1405.85	93.7974	9	1334.5	90.7615
10	1168.65	95.5139	11	1118.51	95.0186	12	1067.76	95.9433
13	854.311	96.4714	14	712.569	96.9257	15	595.896	98.7525
16	418.477	87.9128						
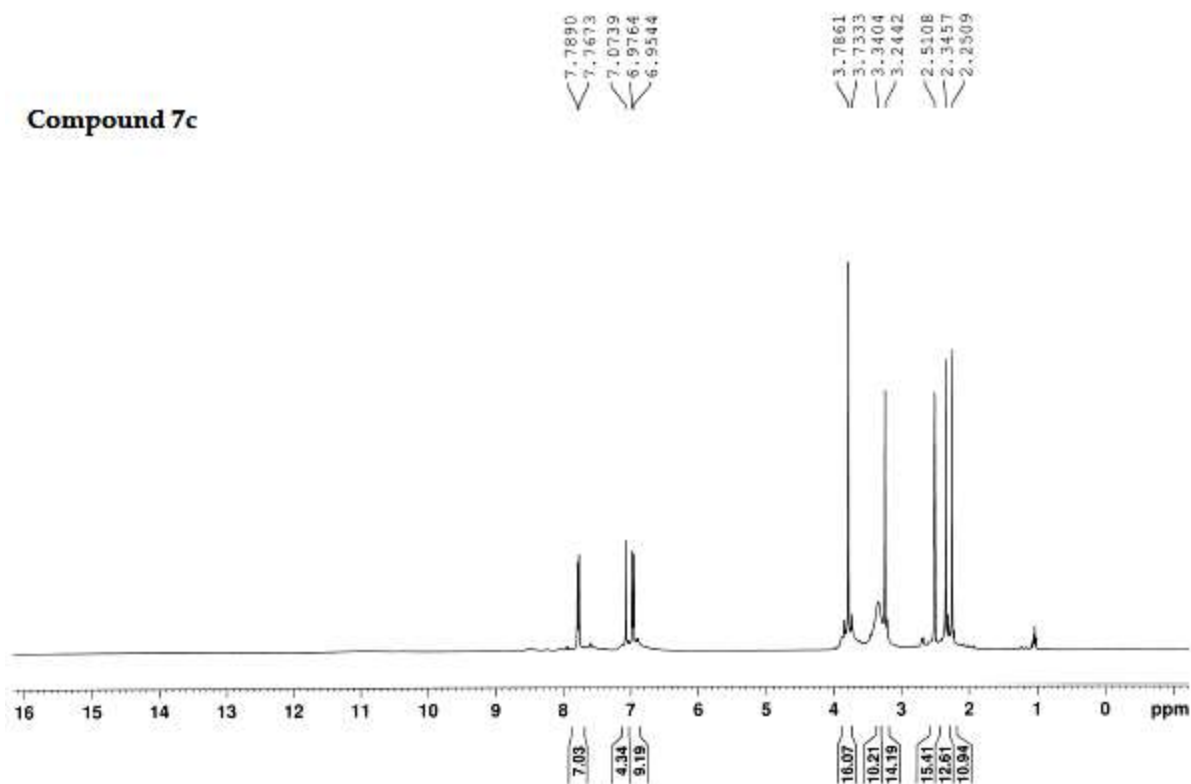
Compound 7c

Compound 7c

Compound 7e
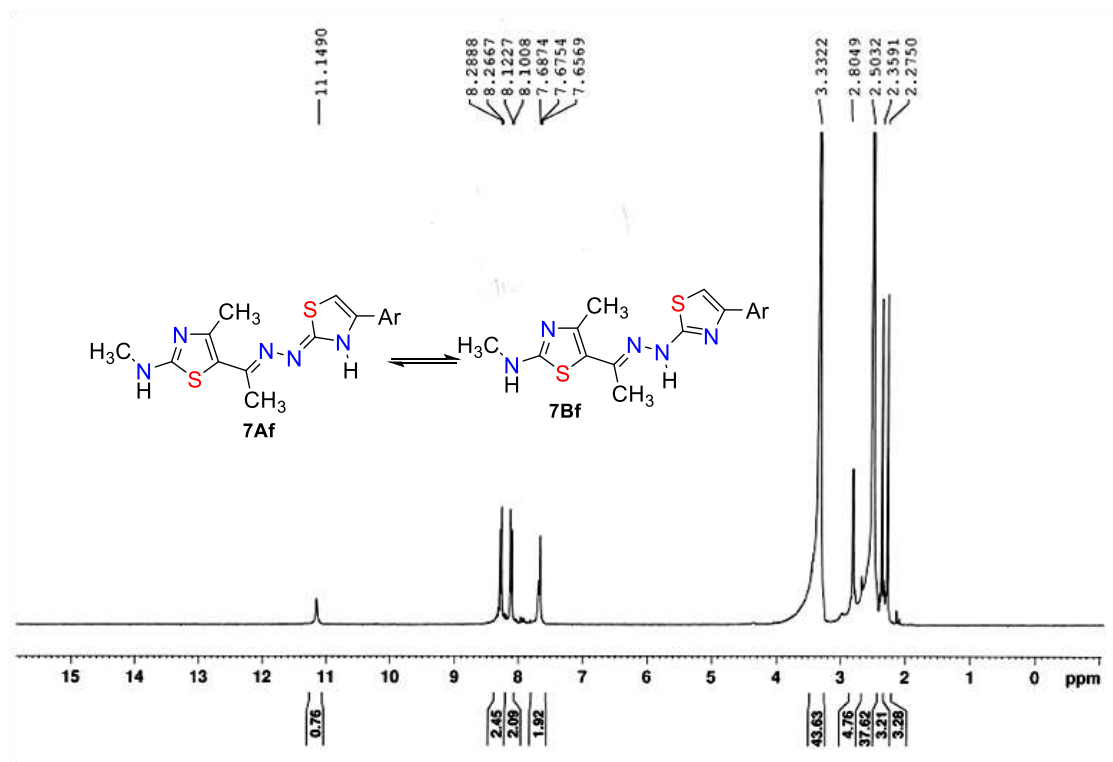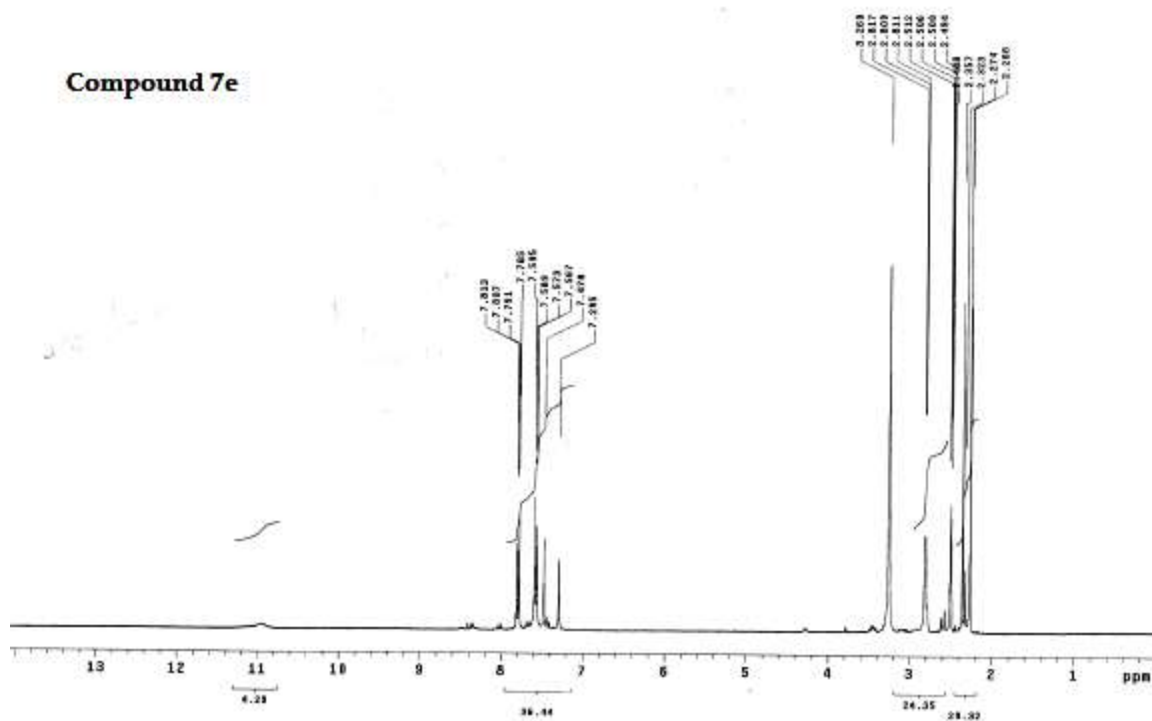
Compound 7f
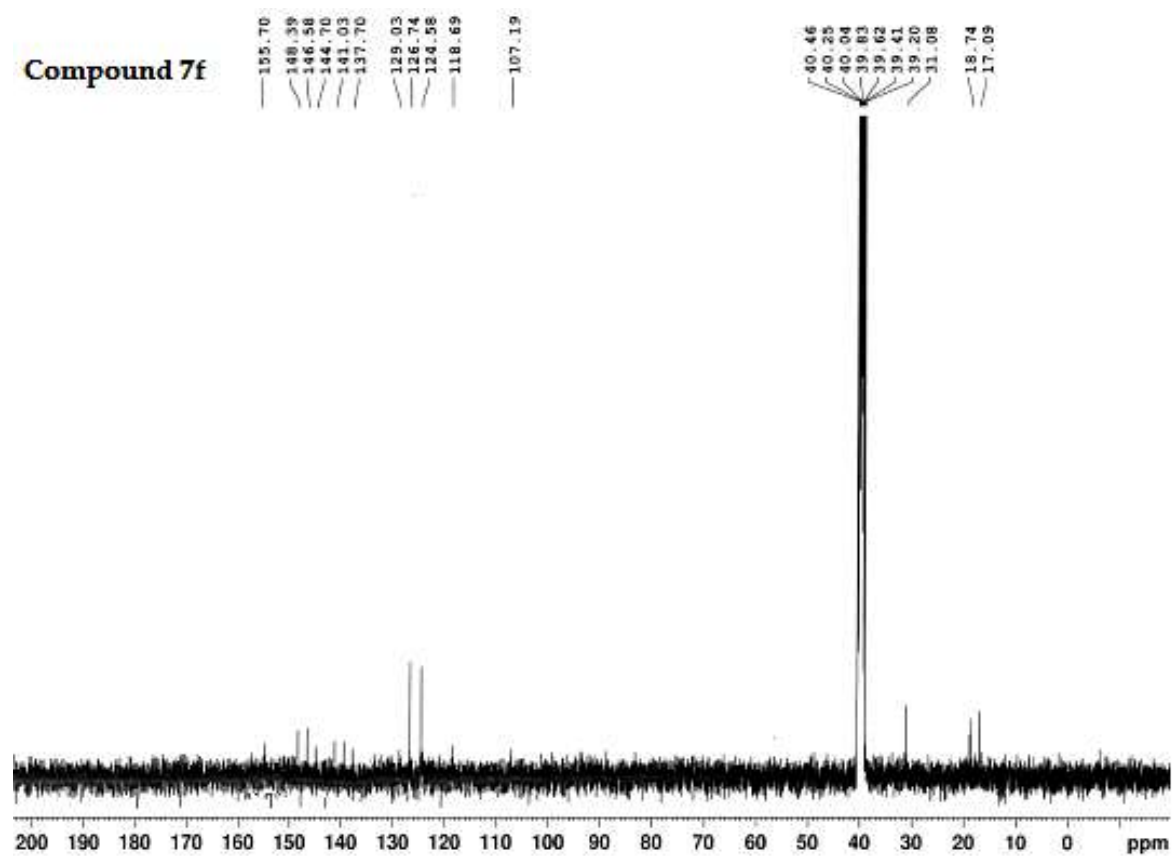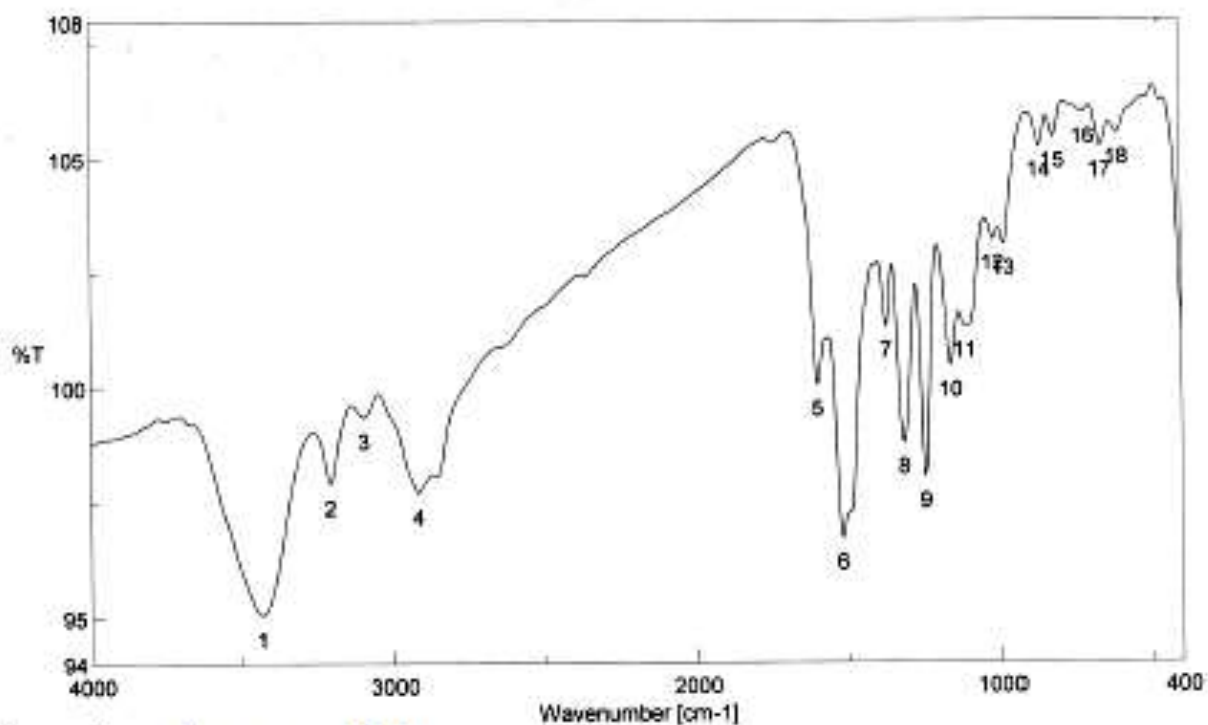
155.70
148.39
146.58
144.70
141.03
137.70
129.03
126.74
124.58
118.69
107.19
40.46
40.25
40.04
39.83
39.62
39.41
39.20
31.08
18.74
17.09

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

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

Compound 9a

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3436.53	96.0585	2	3209.93	97.9074	3	3098.06	99.351
4	2920.66	97.7048	5	1598.7	100.04	6	1518.67	96.7069
7	1372.1	101.311	8	1315.21	96.7738	9	1244.83	98.0352
10	1160.94	100.451	11	1112.73	101.309	12	1018.23	103.2
13	983.518	103.092	14	869.739	105.244	15	823.455	105.447
16	722.211	105.974	17	666.285	105.243	18	610.36	105.52

Compound 9a
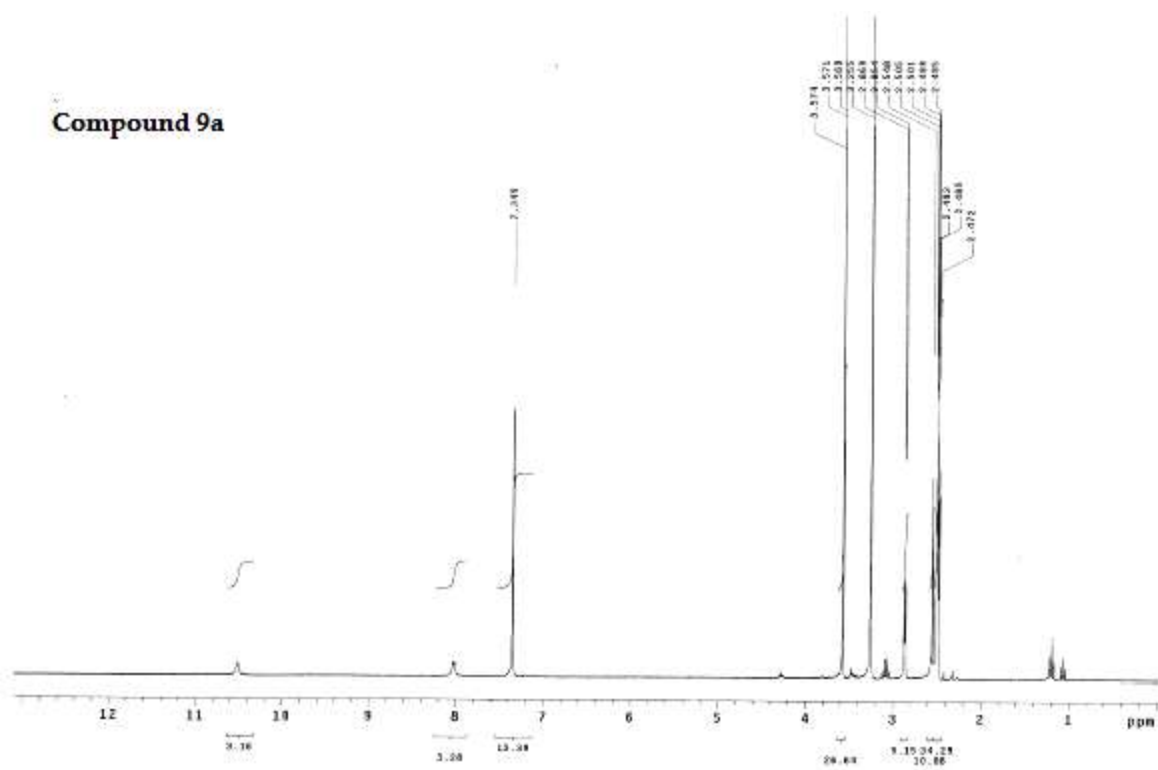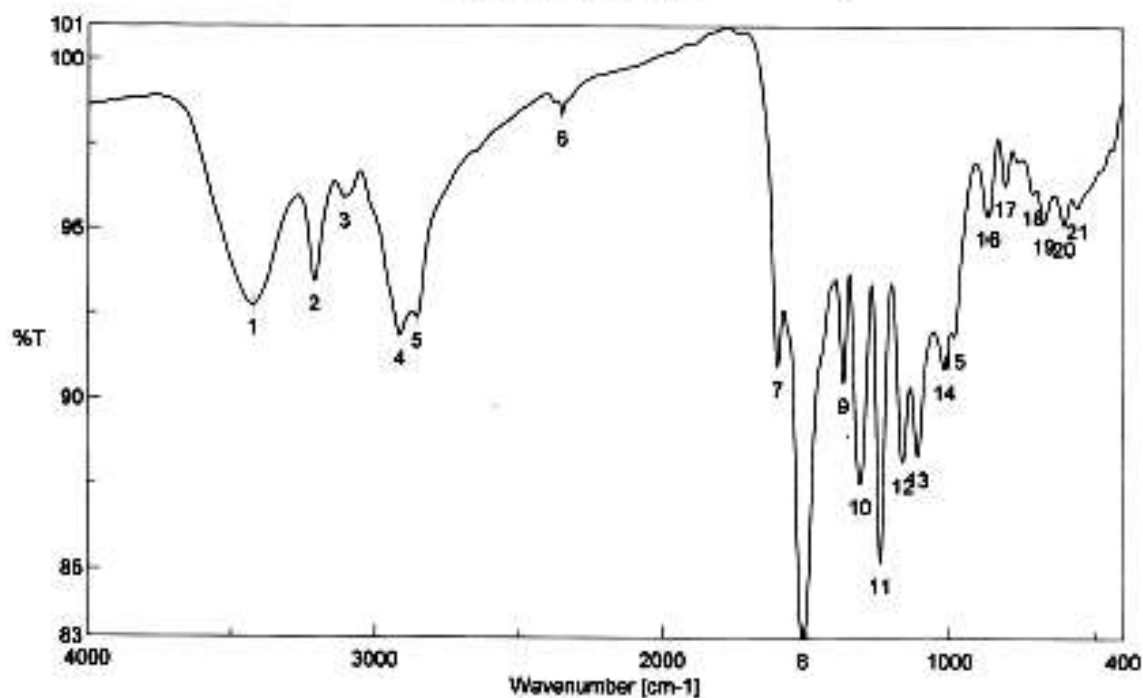
[Comments]
Sample name   **Compound 9b**
Comment   11/2018
User   IR
Division   IR
Company   MAC

| Result of Peak Picking |

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3426.89	92.7543	2	3210.9	93.4446	3	3106.8	95.9259
4	2916.81	91.8534	5	2857.02	92.3829	6	2348.87	98.375
7	1600.63	90.9643	8	1511.92	83.0263	9	1372.1	90.4938
10	1315.21	87.5435	11	1243.86	85.2285	12	1164.79	88.1517
13	1113.69	88.3474	14	1019.19	90.9008	15	965.447	91.8334
16	869.739	95.4384	17	814.777	96.3259	18	716.425	96.067
19	677.856	95.2327	20	608.431	95.1486	21	561.184	95.8603
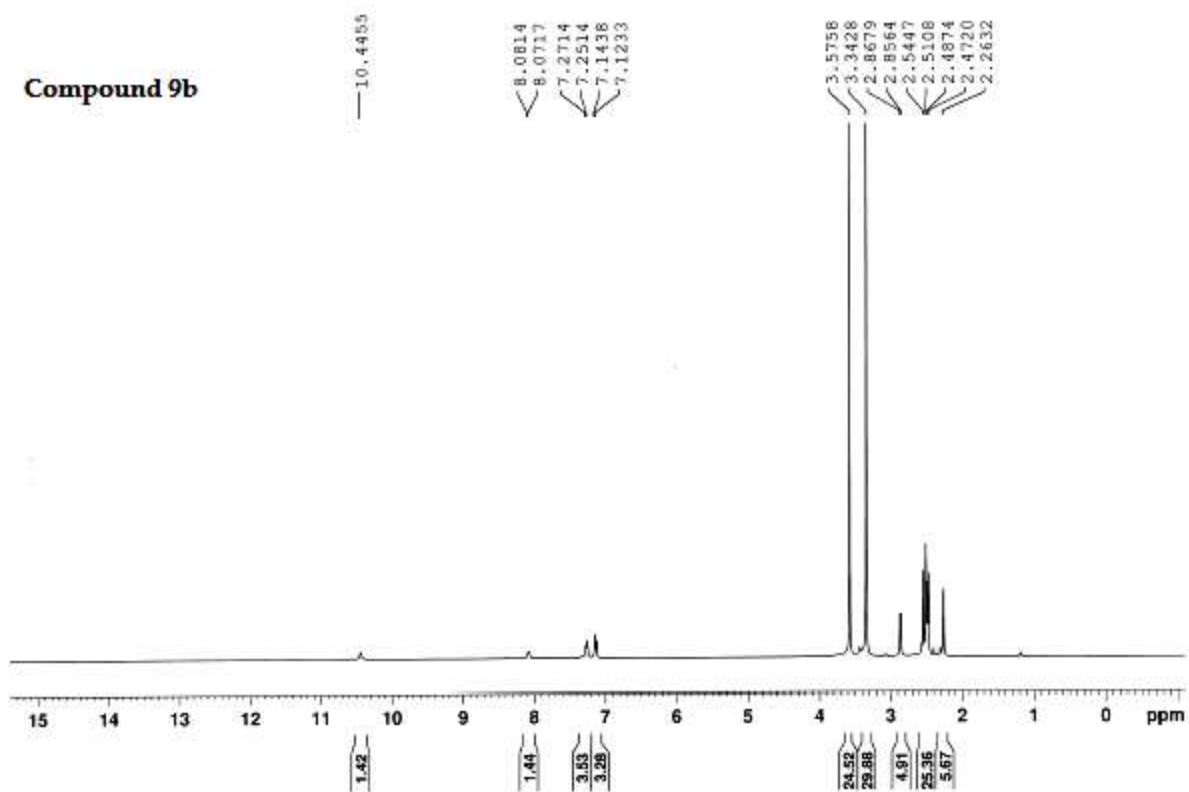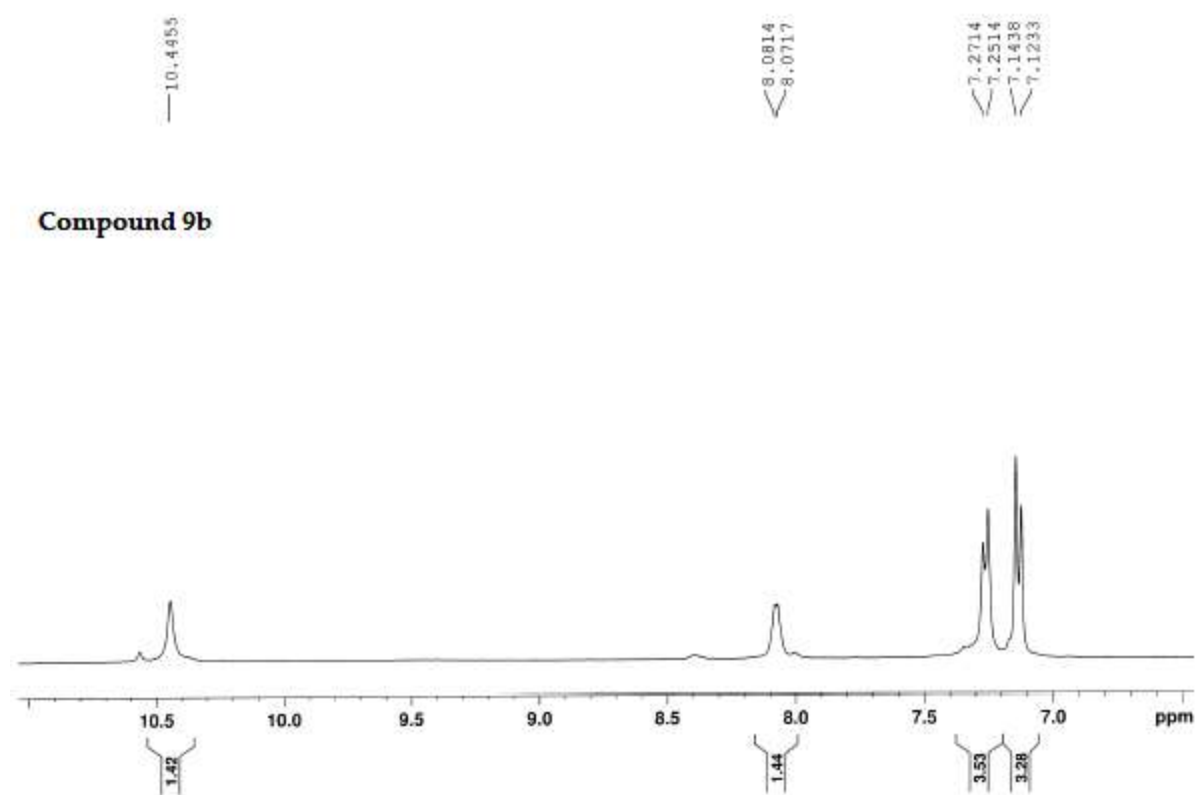
Compound 9b

Compound 9b

Peak Find - Memory-47

Compound 9c

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3905.15	97.9017	2	3752.8	97.8199	3	3430.74	90.3983
4	3210.9	93.0697	5	3107.72	95.0024	6	2823.56	92.6616
7	1595.81	93.9024	8	1500.35	86.5089	9	1372.1	94.7812
10	1313.29	91.5088	11	1236.15	88.4153	12	1167.69	90.6702
13	1109.83	93.0927	14	1023.05	95.001	15	864.917	99.9623
16	820.563	99.2196	17	715.461	99.7485	18	673.035	99.9496
19	603.61	99.4827	20	558.291	100.206	21	517.793	100.348
22	464.761	100.924						

Compound 9d

Peak labels (ppm): 10.5919, 8.1947, 7.3599, 3.5759, 3.3505, 2.8768, 2.8658, 2.5553, 2.5108, 2.5003, 2.4800
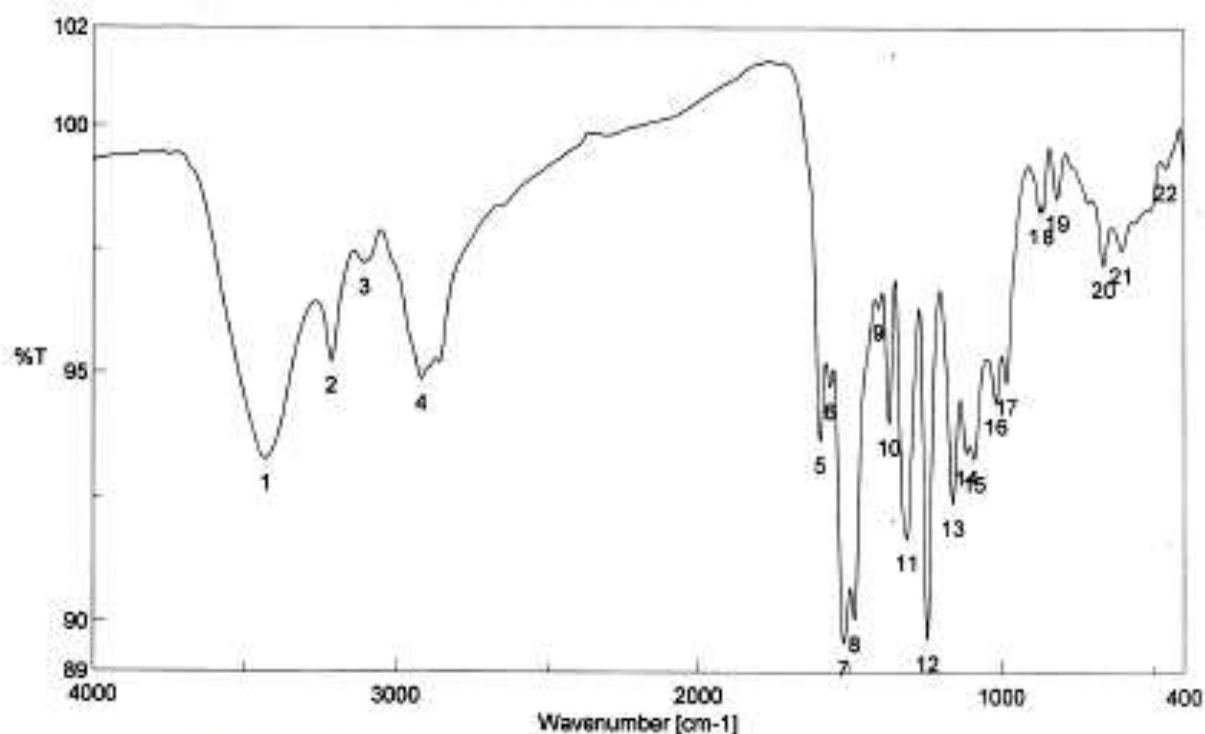
Integration values: 1.76, 1.47, 6.66, 19.80, 35.92, 5.18, 29.21

ppm scale: 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0

Peak Find - Memory-10

Wavenumber [cm-1]

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

Compound 9d

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3427.85	93.2727	2	3210.9	95.2372	3	3103.87	97.2411
4	2915.84	94.887	5	1598.7	93.6494	6	1564.95	94.731
7	1521.56	89.5833	8	1466.85	90.0616	9	1405.85	96.3344
10	1372.1	94.0145	11	1313.29	91.6946	12	1245.79	89.6696
13	1160.94	92.3946	14	1115.62	93.4127	15	1090.55	93.2673
16	1018.23	94.4377	17	984.482	94.8284	18	869.739	96.2874
19	821.527	96.5535	20	667.25	97.213	21	608.431	97.4962
22	459.939	99.1687						

Peak Find - Memory-57
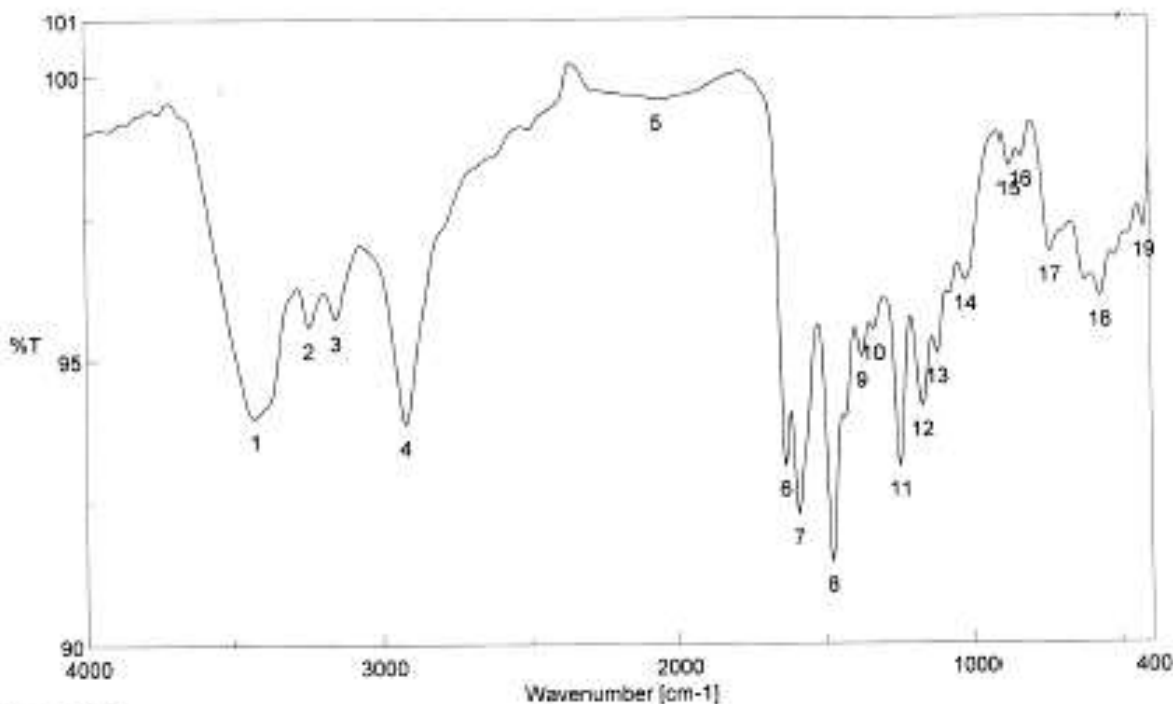
[Comments]
Sample name   **Compound 9e**
Comment   6/2018
User   IR
Division   IR
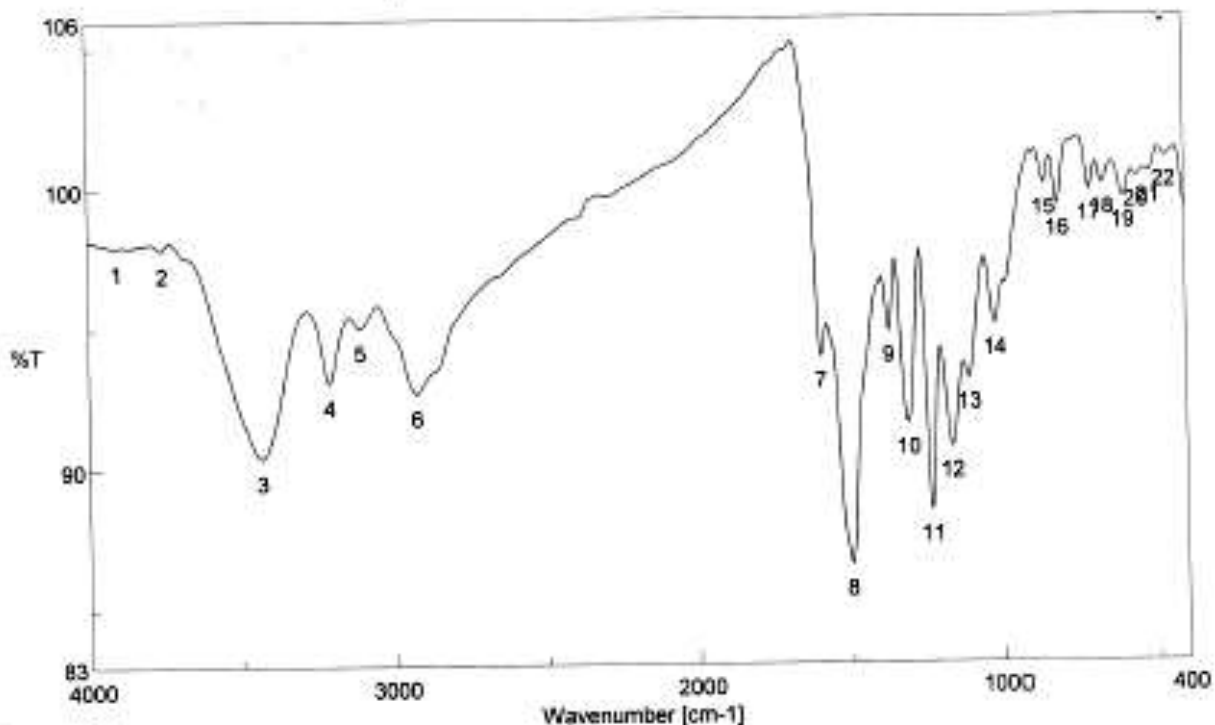Company   MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3425.92	93.9871	2	3244.65	95.5777	3	3155.94	95.709
4	2920.66	93.8701	5	2061.53	99.5736	6	1636.3	93.1242
7	1592.91	92.2744	8	1480.1	91.4512	9	1375.96	96.0254
10	1336.43	95.4947	11	1248.68	93.1117	12	1171.54	94.1572
13	1120.44	95.0879	14	1022.09	96.356	15	877.452	98.3678
16	837.919	98.5354	17	741.496	96.8545	18	572.755	96.0636
19	421.37	97.2842						

Compound 9f
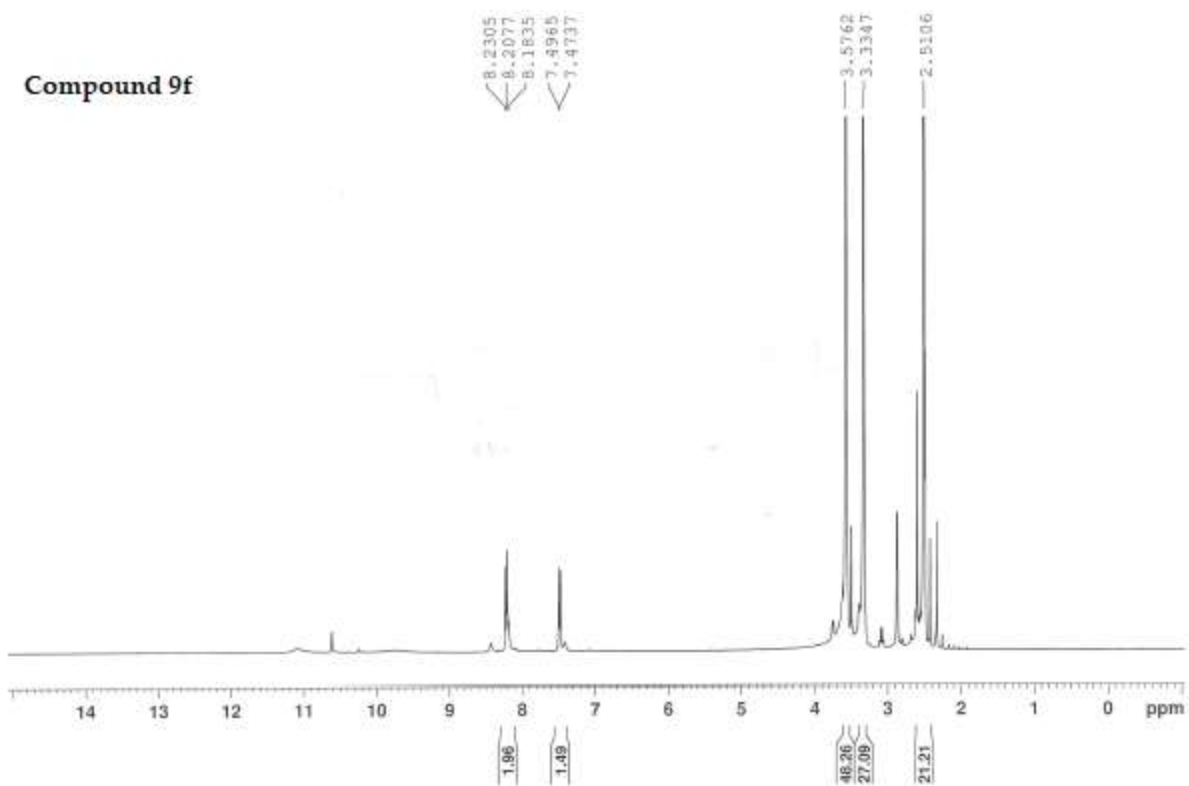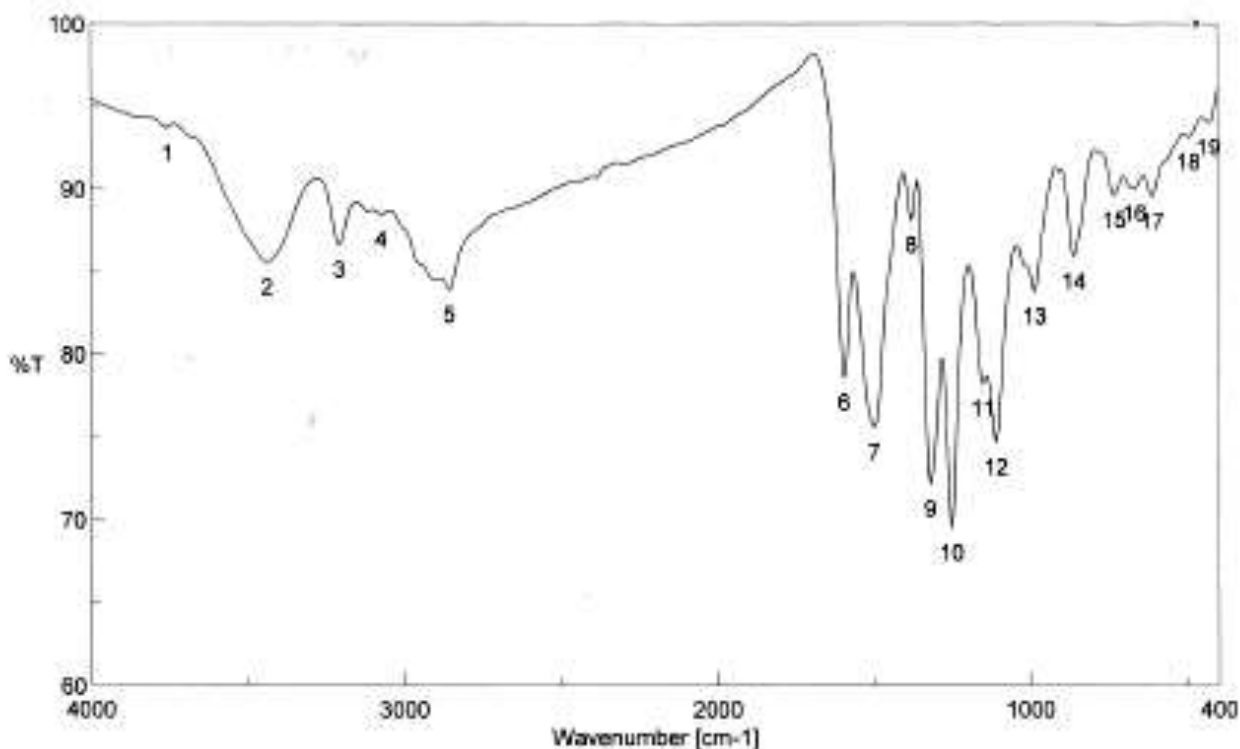
8.2305
8.2077
8.1835
7.4965
7.4737

3.5762
3.3347

2.5106

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.96   1.49   48.26 21.21
                        27.09

[Comments]
Sample name   **Compound 9f**
Comment   6/2018
User   IR
Division   IR
Company   MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3753.76	93.6764	2	3432.67	85.5676	3	3204.15	86.5943
4	3070.12	88.4359	5	2853.17	83.8747	6	1593.88	78.5774
7	1497.45	75.5644	8	1375.96	88.1027	9	1319.07	72.1368
10	1251.56	69.4994	11	1150.33	78.2065	12	1107.9	74.545
13	982.554	83.7813	14	862.989	85.89	15	733.782	89.5946
16	668.214	89.986	17	612.288	89.5261	18	494.652	93.1383
19	429.084	94.0449						

Compound 3

NL:
1.95E4
TC MS 1h

1hF201 RT: 3.35 AV: 1 NL: 3.27E2
T: (0,0) + c EI Full ms [40.00-1000.00]

Compound 5

RT: 2.85 - 3.33 SM: 15G
NL:
2.00E6
TIC MS 2h
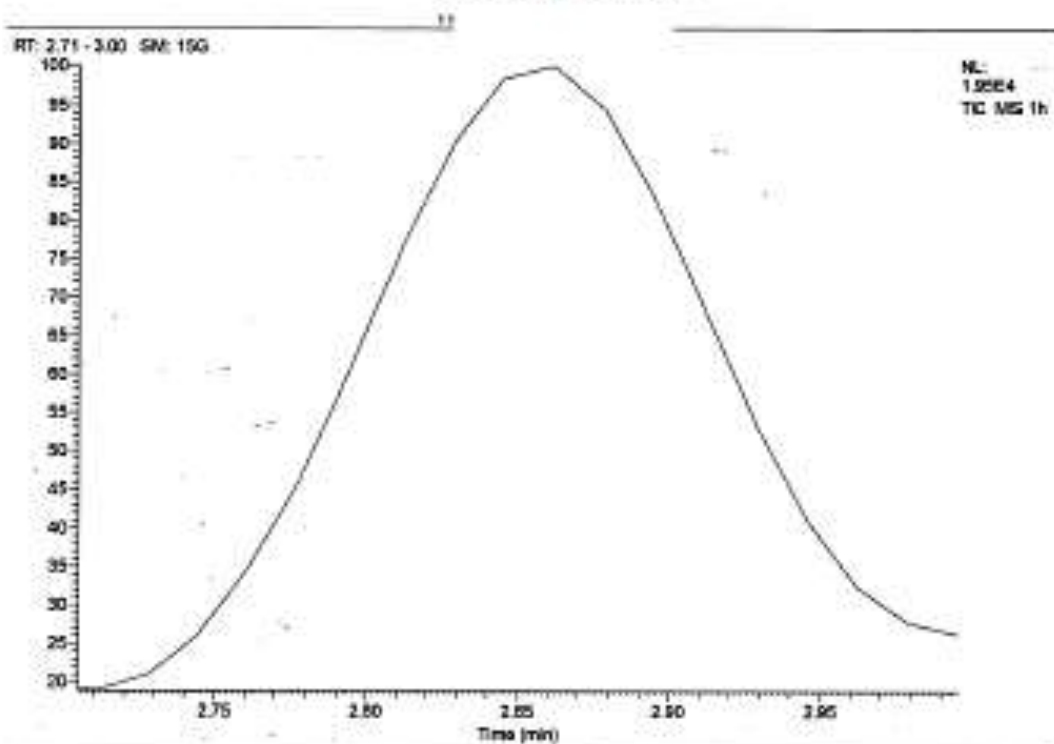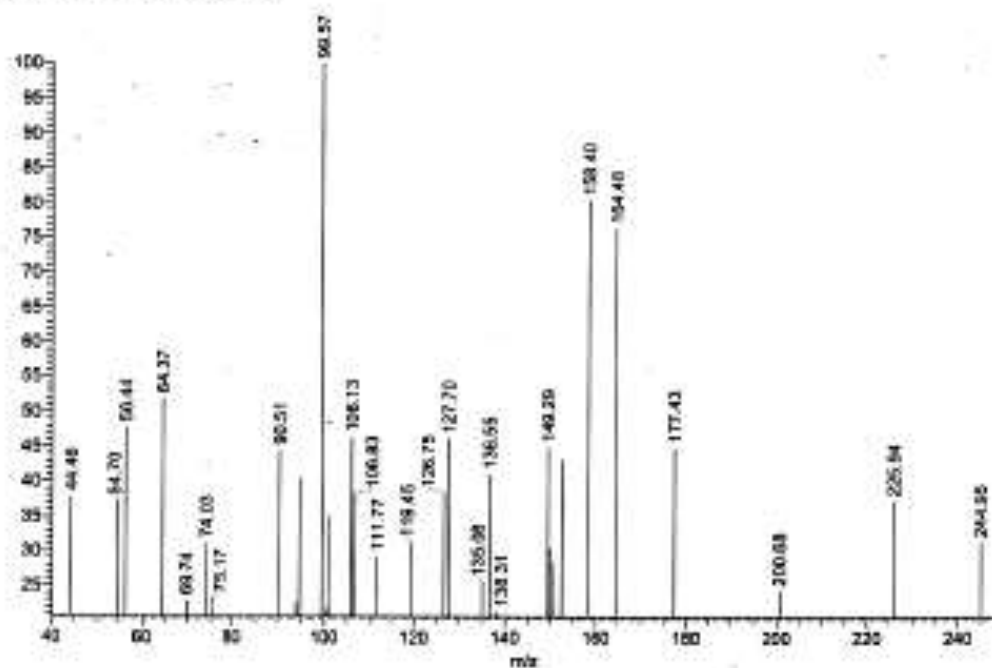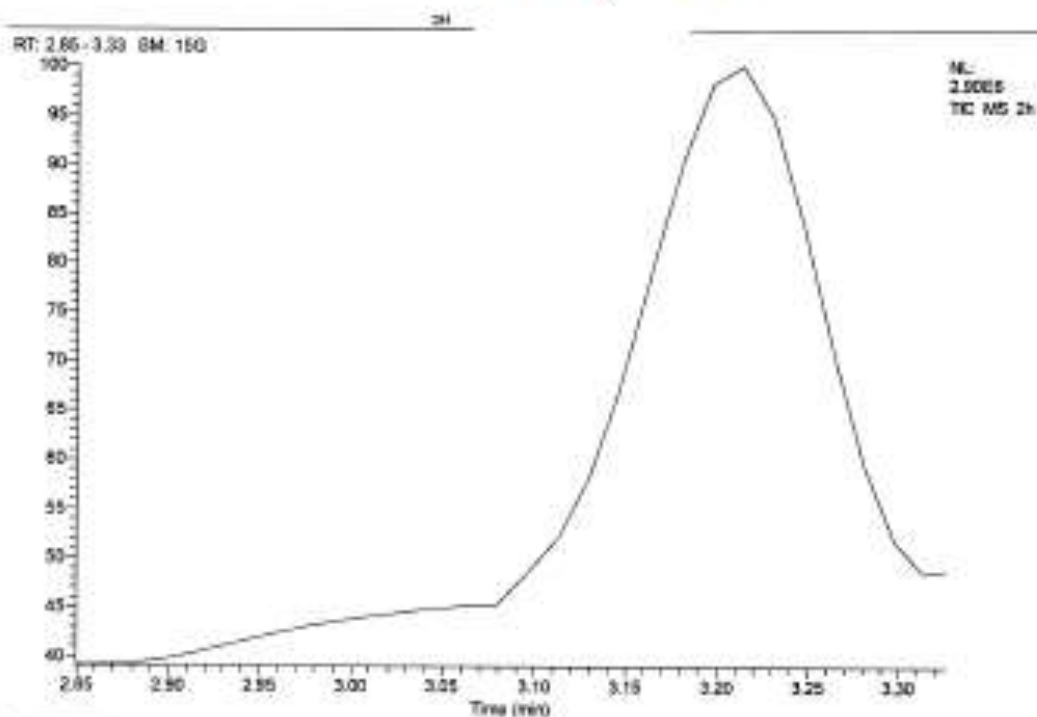
2h#50 RT: 1.36 AV: 1 SB: 10 1.31-1.41 , 1.42-1.46 NL: 1.07E3
T: (0,0) + c EI Full ms [40.00-1000.00]

Compound 7a

1H7

Time (min)

m/z

Compound 7b

Compound 7d

NL:
1.70E4
TIC MS
1h2

Time (min)

1h2 #151   RT: 2.54   AV: 1   NL: 8.67E2
T: {0,0} + c EI Full ms [40.00-1000.00]

m/z

Compound 7f

NL:
7.40E9
TIC MS
1h9

Time (min)

1h9 #231   RT: 3.85   AV: 1   NL: 7.02E2
T: {0,0} + c EI Full ms [40.00-1000.00]

m/z

Compound 9b

NL:
3.37E5
TIC MS
1h11

1h11 #190 RT: 3.29 AV: 1 NL: 1.42E3
T: (0,0) + c EI Full ms [40.00-1000.00]

compound 9d

Compound 9e

Time (min)

m/z

Compound 9f

NL:
1.73E9
TIC MS
1H5

1H5 #234   RT: 3.93   AV: 1   SB: 14 3.80-3.87 , 3.77-3.90   NL: 2.54E3
T: {0,0} + c EI Full ms [40.00-1000.00]