Supporting information

EXPERIMENTAL

Melting points were determined in an open capillary and are uncorrected. IR spectra were recorded on a Perkin-Elmer spectrum II spectrometer on KBr disks. ^{1}H and ^{13}C NMR spectra were recorded at 300 and 75 MHz respectively in $CDCl_3$ (chemical shift in δ) with TMS as internal standard. Mass spectra were recorded on a TOF MASS ES+ instrument respectively. Silica gel [(60-120 mesh), spectrochem, India] was used for chromatographic separation. Silica gel G [E-Merck (India)] was used for TLC. Petroleum ether refers to the fraction boiling between 60 °C-80 °C.

GENERAL PROCEDURE

A mixture of 2-bromobenzaldehyde (1mmol), CuI (2 mol%) and $Pd(PPh_3)_2Cl_2$ (2 mol%) in DMF (5 mL) was degassed for 5 min under N_2 atmosphere. Then the corresponding alkyne (1.5 equiv) along with 2 mL of triethylamine was added to this mixture and allowed to stir at room temperature under N_2 atmosphere for 2 h. After completion of the reaction indicated by TLC, 5,6-diamino-1,3-dimetyluracil hydrate (1 mmol) and additional (2 mol%) of CuI was added to this mixture in the same reaction vessel. Then the mixture was allowed to reflux for 3-4 h at 120 °C in open air and progress of the reaction was monitored by TLC. After completion of the reaction, solvent was removed under reduced pressure. The organic layer extracted with EtOAc (3X10 mL) and washed with brine water, dried over Na_2SO_4. The organic extract was concentrated under reduced pressure. The crude product was purified by column chromatography with EtOAc: petroleum ether (3:7) as eluent to get the desired compound.

3a. Yield: 85%, mp 180 °C, IR (KBr): 1663, 1703 cm^{-1}, ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 3.26 (s, 3H), 3.79 (s, 3H), 7.19 (s, 1H), 7.46-7.56 (m, 5H), 7.68-7.73 (m, 2H), 7.78-7.81 (m, 1H), 8.72 (t,1H, *J* = 9Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 28.62, 30.13, 104.83, 116.24, 121.16, 124.78, 126.81, 127.44, 128.15, 128.24, 129.21, 130.57, 131.54, 136.58, 137.73, 147.92, 151.33, 151.82. MS *m/z* = 379 (M^+ + Na), Anal. Calcd for $C_{21}H_{16}N_4O_2$: C, 70.77; H, 4.53; N, 15.72. Found: C, 70.78; H, 4.51; N, 15.80.

3b. Yield: 89%, mp 258 °C, IR (KBr): 1665, 1701 cm^{-1}, ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 2.47 (s, 3H), 3.27 (s, 3H), 3.78 (s, 3H), 7.15 (s, 1H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.46 (d, *J* = 8.1 Hz, 2H), 7.66-7.73 (m, 2H), 7.77-7.94 (m, 1H), 8.71 (t, *J* = 9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ:

21.65, 28.64, 30.12, 116.18, 121.08, 124.77, 126.76, 127.15, 128.09, 128.89, 130.52, 131.66, 133.85, 137.92, 139.05, 148.02, 151.36, 151.88, 153.16. MS *m/z* = 393 (M^++ Na), Anal. Calcd for $C_{22}H_{18}N_4O_2$: C, 71.34; H, 4.90; N, 15.13. Found: C, 71.33; H, 4.82; N, 15.22.

3c. Yield: 86%, mp 276 °C, IR (KBr): 1667, 1702 cm^{-1}, ^1H NMR ($CDCl_3$, 300 MHz) δ: 1.34 (t, *J* = 7.5 Hz, 3H), 2.75 (q, *J* = 7.5 Hz, 2H), 3.26 (s, 3H), 3.78 (s, 3H), 7.16 (s, 1H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.45 (d, *J* = 7.8 Hz, 2H), 7.66-7.73 (m, 2H), 7.76- 7.79 (m, 1H), 8.72 (t, *J* = 9 Hz, 1H); ^{13}CNMR ($CDCl_3$,75 MHz) δ: 15.27, 28.80, 28.81, 30.11, 116.19, 121.10, 124.76, 126.76, 127.22, 127.63, 128.08, 130.51, 131.67, 137.96, 145.27, 148.02, 151.36, 151.90. MS *m/z* = 407 (M^++ Na), Anal. Calcd for $C_{23}H_{20}N_4O_2$: C, 71.86; H, 5.25; N, 14.57. Found: C, 71.89; H, 5.16; N, 14.65.

3d. Yield: 90%, mp 252 °C, IR (KBr): 1666, 1702 cm^{-1}, ^1H NMR ($CDCl_3$, 300 MHz) δ: 1.41 (s, 9H), 3.25 (s, 3H), 3.79 (s, 3H), 7.48 (s, 4H), 7.17 (s, 1H), 7.68-7.71 (m, 2H), 7.76-7.79 (m, 1H), 8.72 (t, *J* = 9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 28.46, 30.07, 31.30, 34.81, 104.88, 116.12, 121.08, 124.71, 125.0, 126.73, 126.96, 128.03, 130.45, 131.63, 133.68, 137.91, 147.94, 151.28, 151.90, 152.13, 152.97. MS *m/z* = 435 (M^++ Na), Anal. Calcd for $C_{25}H_{24}N_4O_2$: C, 72.80; H, 5.86; N, 13.58. Found: 72.77; H, 5.81; N, 13.61.

3e. Yield: 95%, mp 120 °C, IR (KBr): 1710, 1725 cm^{-1}, ^1H NMR ($CDCl_3$, 300 MHz) δ: 0.85 (t, *J* = 6.9 Hz, 3H), 1.25 (m, 4H), 1.40-1.47 (m, 2H), 1.62-1.78 (m, 2H), 3.49 (s, 3H), 3.68 (t, *J* = 7.2 Hz, 2H), 3.76 (s, 3H), 7.01 (s, 1H), 7.58-7.71 (m, 3H), 8.62 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 14.16, 22.65, 28.65, 29.01, 29.13, 30.23, 31.82, 34.78, 105.34, 113.0, 120.87, 124.96, 125.92, 130.50, 131.81, 140.44, 148.20, 151.46, 151.64, 154.15. MS *m/z* = 387 (M^+ + Na), Anal. Calcd for $C_{21}H_{24}N_4O_2$: C, 69.21; H, 6.64; N, 15.37. Found: C, 69.17; H, 6.55; N, 15.45.

3f. Yield: 92%, mp 182 °C, IR (KBr): 1648, 1691cm^{-1}, ^1H NMR ($CDCl_3$, 300 MHz) δ: 1.00 (t, *J* = 7.2 Hz, 3H), 1.66 (q, *J* = 7.5 Hz, 2H), 3.49 (s, 3H), 3.63 (t, *J* = 7.5 Hz, 2H), 3.75 (s, 3H), 7.00 (s, 1H) 7.57-7.70 (m, 3H), 8.61 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$,75 MHz) δ: 14.06, 22.59, 25.23, 29.18, 30.11, 31.53, 115.51, 123.47, 124.27, 132.93, 133.85, 150.08, 150.89, 153.79, 155.87, 159.68, 165.20. MS *m/z* = 345 (M^++ Na), Anal. Calcd for $C_{18}H_{18}N_4O_2$: C, 67.07; H, 5.63; N, 17.38. Found: C, 67.01; H, 5.72; N, 17.42.

3g. Yield : 94%, mp 234 °C, IR (KBr): 1638, 1701 cm^{-1}, ^1H NMR ($CDCl_3$, 300 MHz) δ: 3.28 (s, 3H), 3.79 (s, 3H), 3.90 (s, 3H), 7.01 (d, *J* = 8.7 Hz, 2H), 7.14 (s, 1H), 7.50 (d, 2H, *J* = 8.7 Hz),

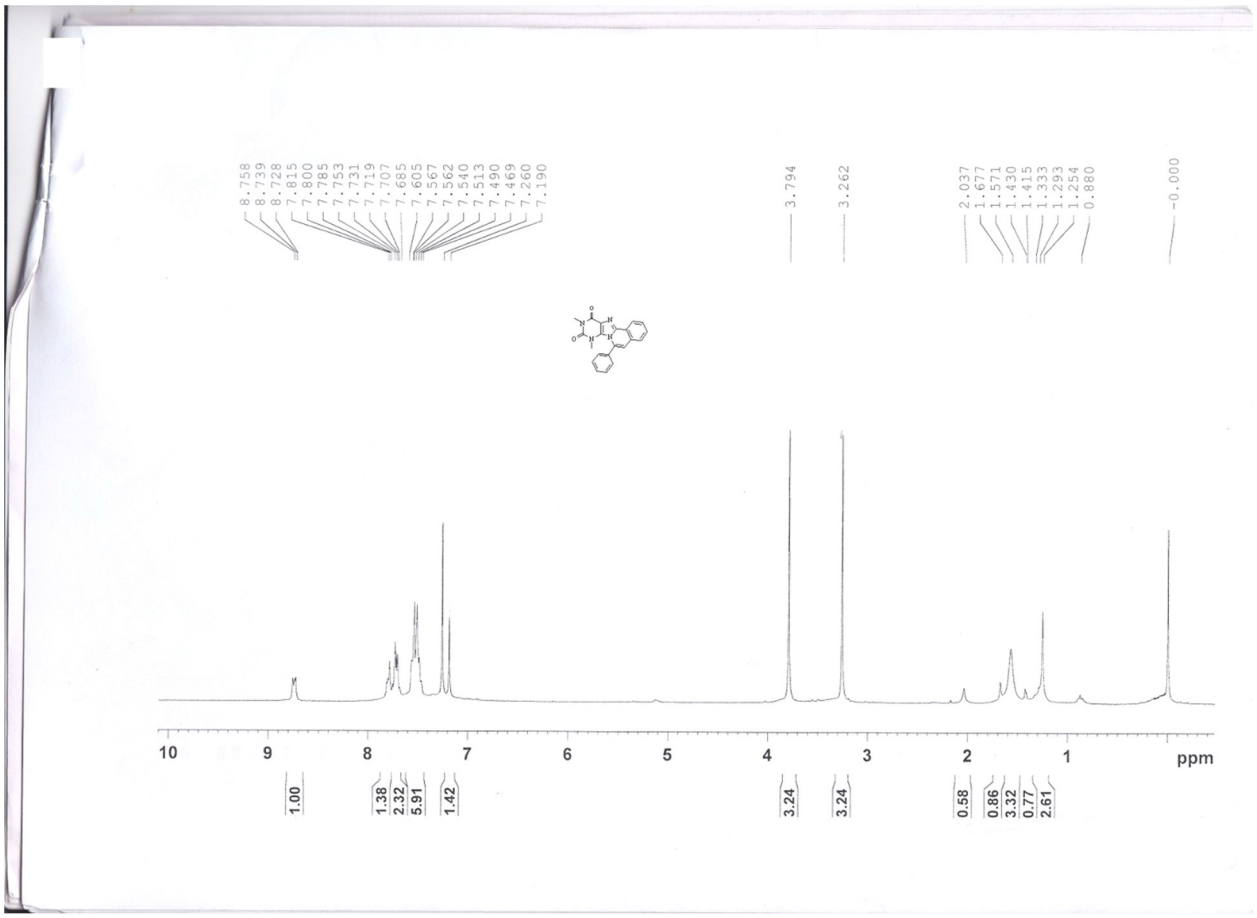
7.65-7.79 (m, 3H), 8.73 (d, 1H, *J* = 9.3 Hz); ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 22.62, 28.61, 30.09, 31.55, 55.24, 104.88, 113.50, 115.98, 121.01, 124.76, 126.67, 127.99, 128.68, 129.22, 130.50, 131.70, 137.73, 148.07, 151.38, 151.85, 153.13, 160.19. MS *m/z* = 387 (M^++ H), Anal. Calcd for $C_{22}H_{18}N_4O_3$: C, 68.38; H, 4.70; N, 14.50 Found: C, 68.32; H, 4.78; N, 14.62.

4a. Yield: 47%, mp 278 °C, IR (KBr): 1708, 1649 cm^{-1}, ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 3.59 (s, 3H), 3.80 (s, 3H), 7.23 (s, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.26 (m, 3H), 7.80 (m, 2H), 7.92 (d, *J* = 8.4 Hz, 1H), 9.92 (s, 1H), MS *m/z* = 356 (M^+), Anal. Calcd for $C_{21}H_{16}N_4O_2$: C, 70.77; H, 4.53; N, 15.72. Found: C, 70.65; H, 4.61; N, 15.63.

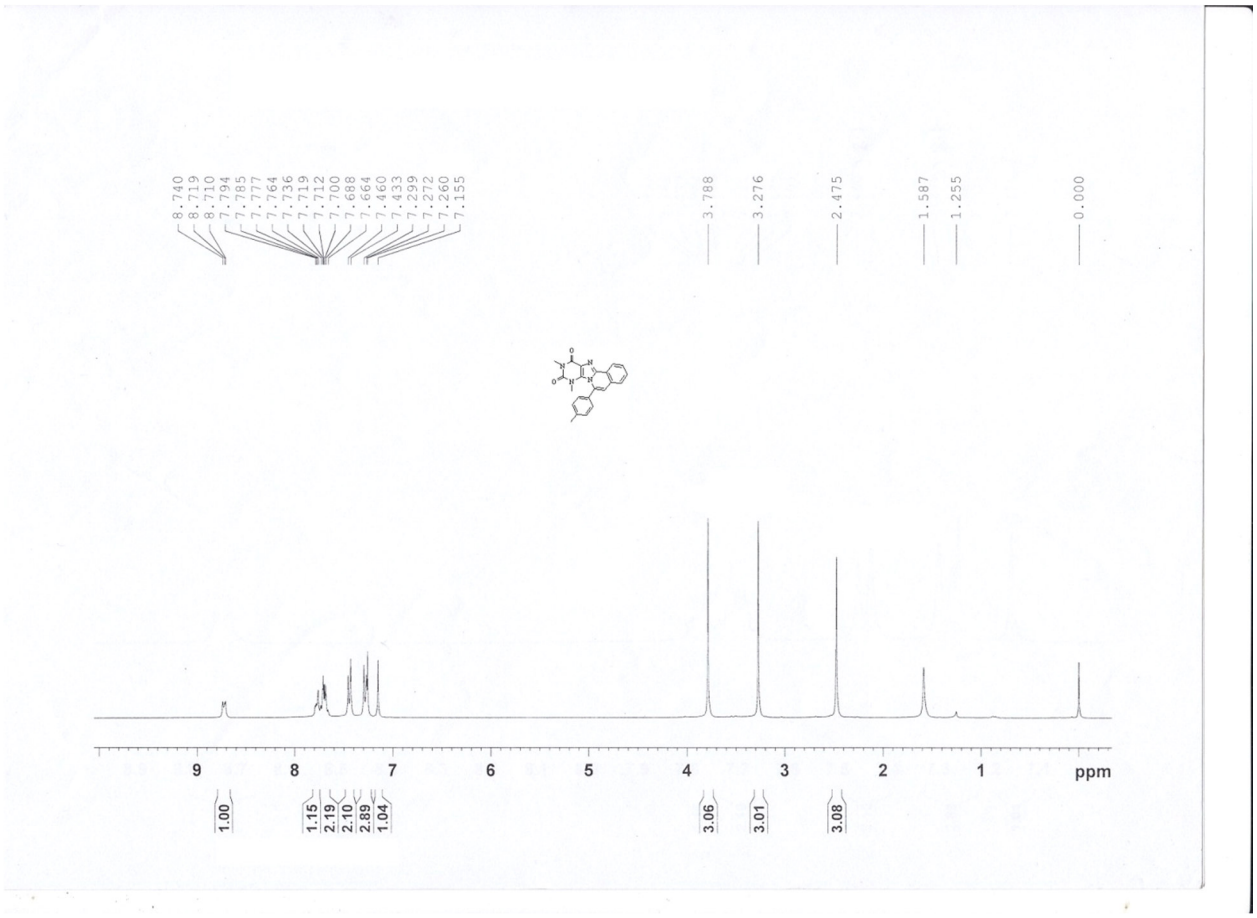
4b. Yield: 45%, mp 274 °C, IR (KBr): 1651, 1648 cm^{-1}, ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 2.53 (s, 3H), 3.57 (s, 3H), 3.78 (s, 3H), 7.23 (m, 1H), 7.41 (m, 3H), 7.60 (d, *J* = 8.8 Hz, 1H), 7.71 (d, *J* = 8 Hz, 2H), 7.89 (d, *J* = 8.4 Hz, 1H), 9.87 (s, 1H), MS *m/z* = 370 (M^+), Anal. Calcd for $C_{22}H_{18}N_4O_2$: C, 71.34; H, 4.90; N, 15.13. Found: C, 71.26; H, 4.85; N, 15.26.

4c. Yield: 60%, mp 280°C, IR (KBr): 1699, 1641 cm^{-1}, ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.14 (s, 9H), 3.58 (s, 3H), 3.80 (s, 3H), 7.27 (m, 1H), 7.42 (m, 1H), 7.61 (m, 3H), 7.77 (q, 2H), 7.91 (d, *J* = 8 Hz, 1H), 9.91 (s, 1H), MS *m/z* = 412 (M^+), Anal. Calcd for $C_{25}H_{24}N_4O_2$: C, 72.80; H, 5.86; N, 13.58. Found: C, 72.89; H, 5.81; N, 13.65.

1H NMR Data: Compound **3a**



Compound **3b:**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7.664
7.460
7.433
7.299
7.272
7.260
7.155
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1.587
1.255
0.000
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8
7
6
5
4
3
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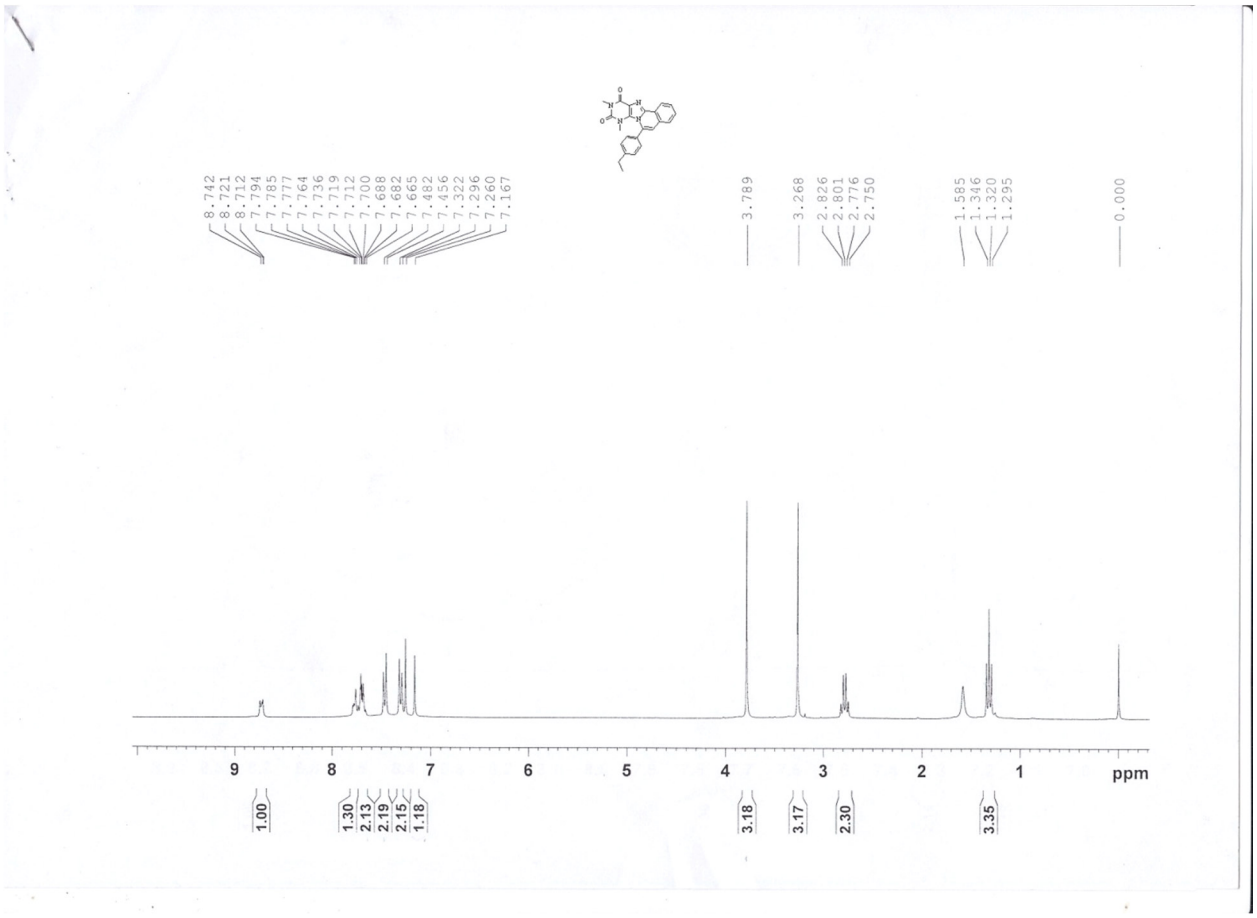
3.06
3.01
3.08

Compound **3c:**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7.682
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7.482
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3.268
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2.776
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1.295
0.000
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8
7
6
5
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3
2
1
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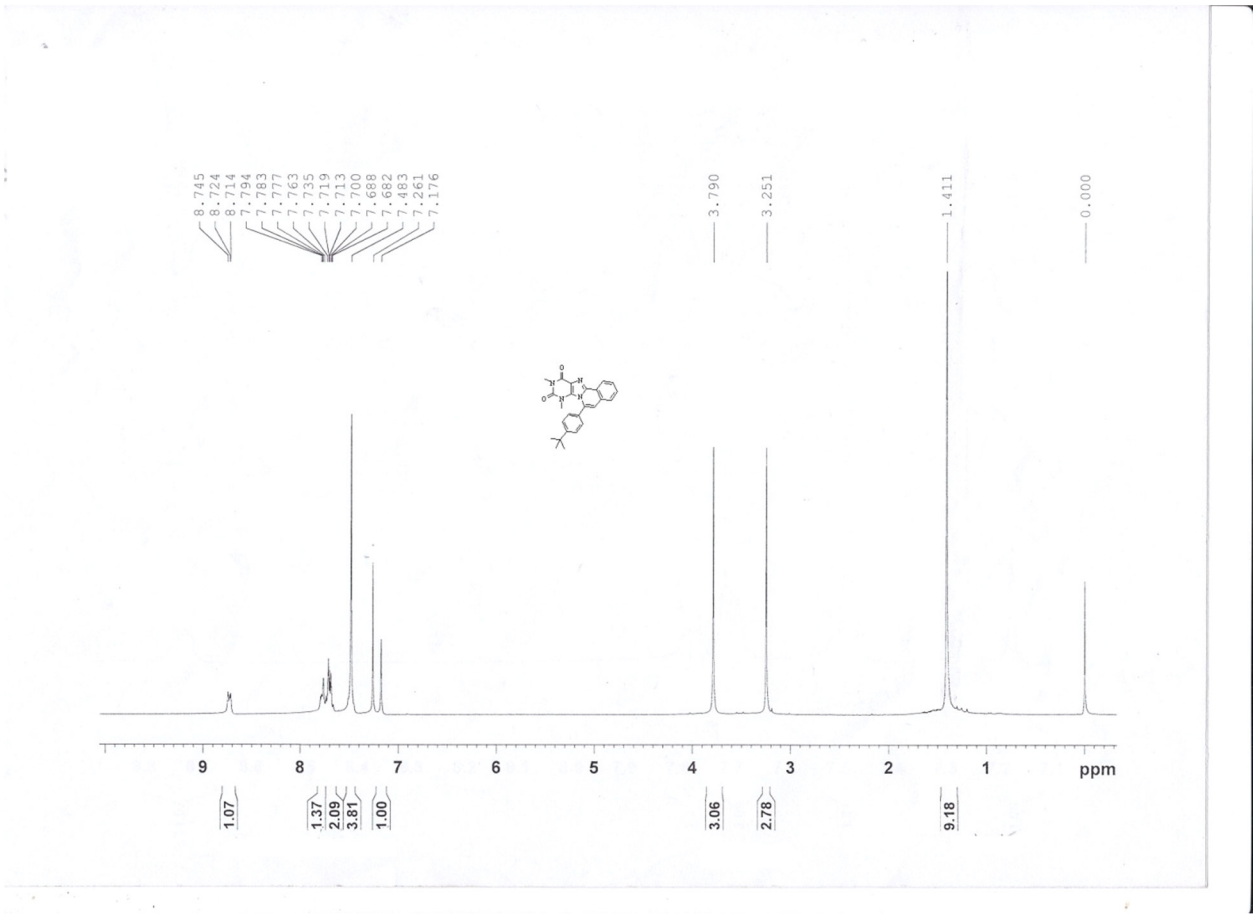
3.17
2.30
3.35

Compound **3d**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7.688
7.682
7.483
7.261
7.176
3.790
3.251
1.411
0.000
9
8
7
6
5
4
3
2
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3.06
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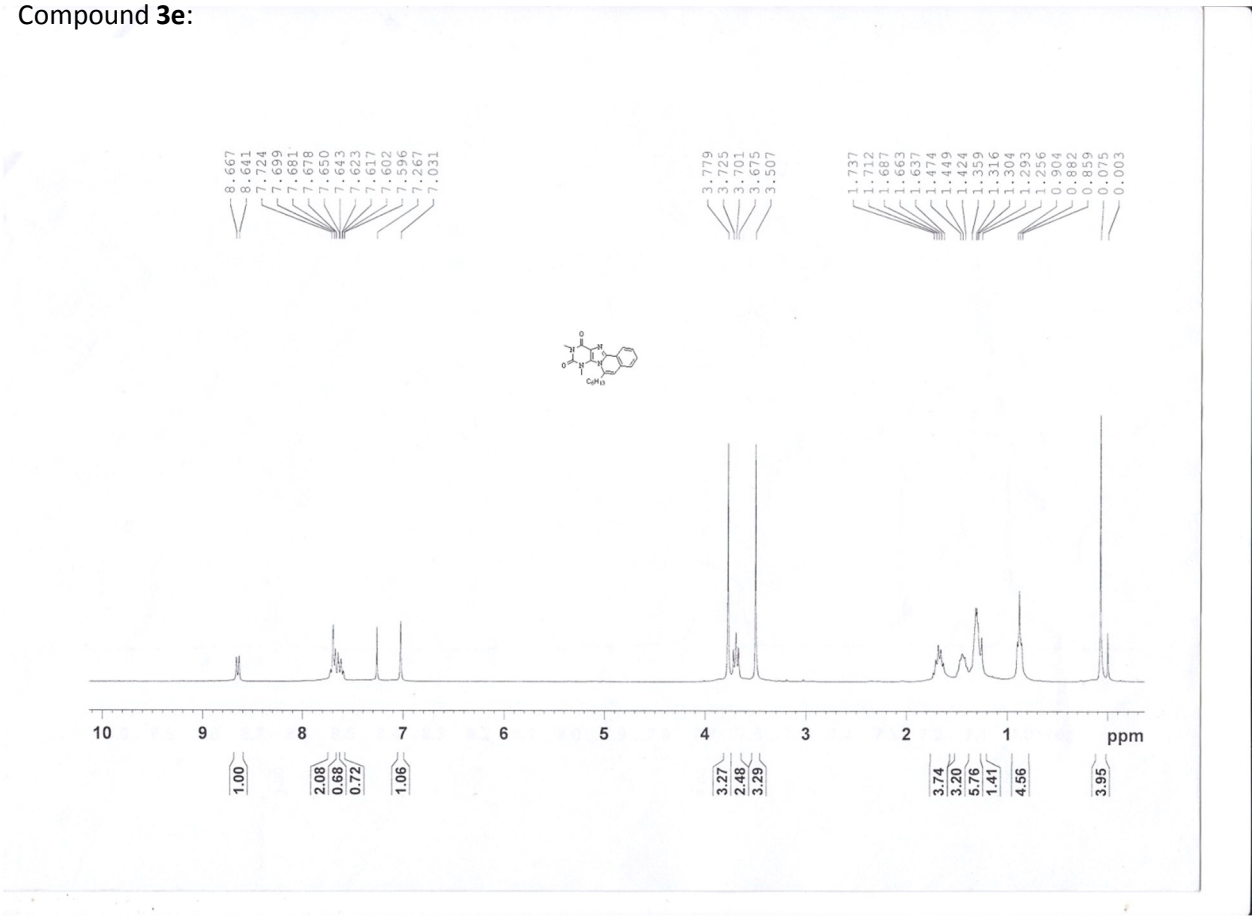
9.18

Compound **3e**: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3.701
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0.859
0.075
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8
7
6
5
4
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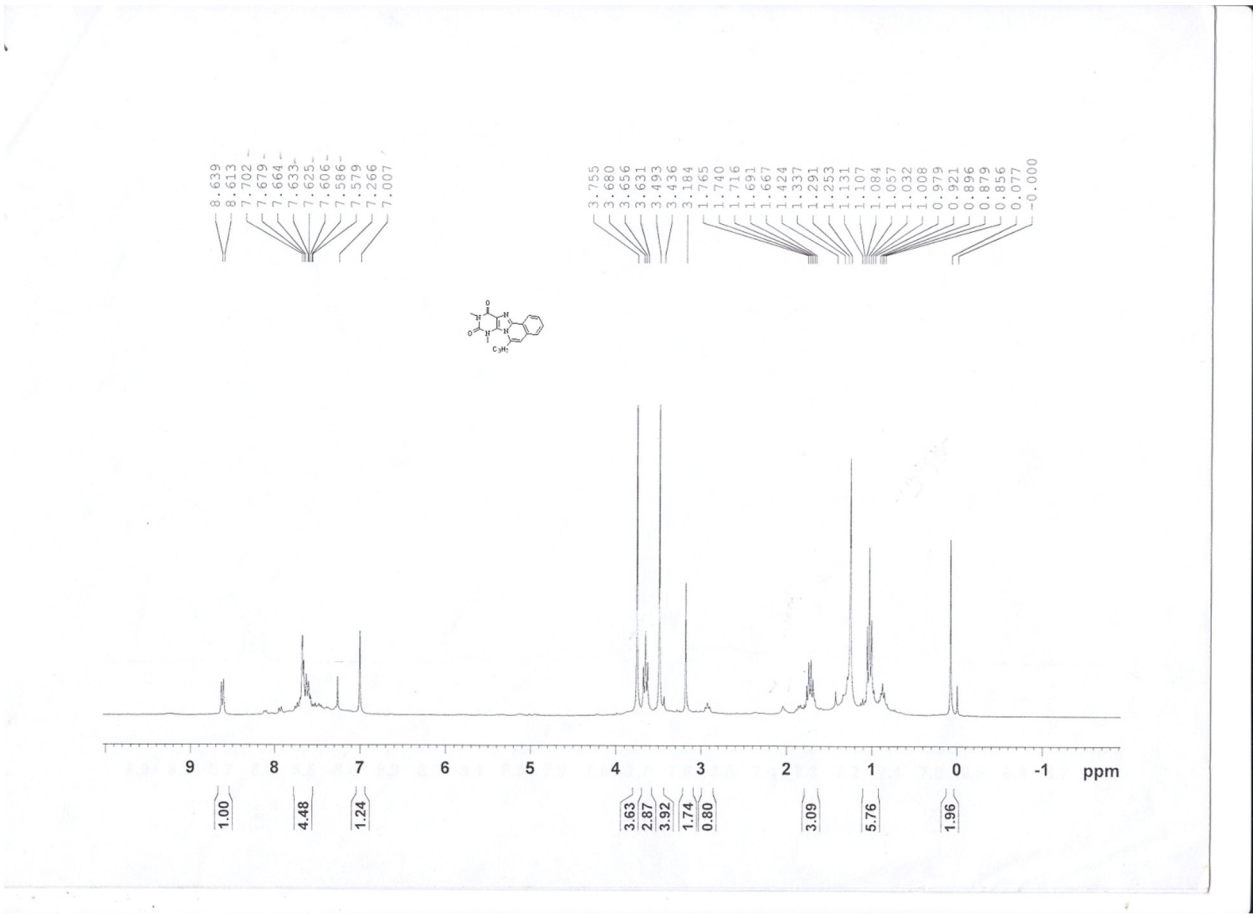
Compound **3f**: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3.656
3.631
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3.436
3.184
1.765
1.740
1.716
1.691
1.667
1.424
1.337
1.291
1.253
1.131
1.107
1.084
1.057
1.032
1.008
0.979
0.921
0.896
0.879
0.856
0.077
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9
8
7
6
5
4
3
2
1
0
-1
ppm
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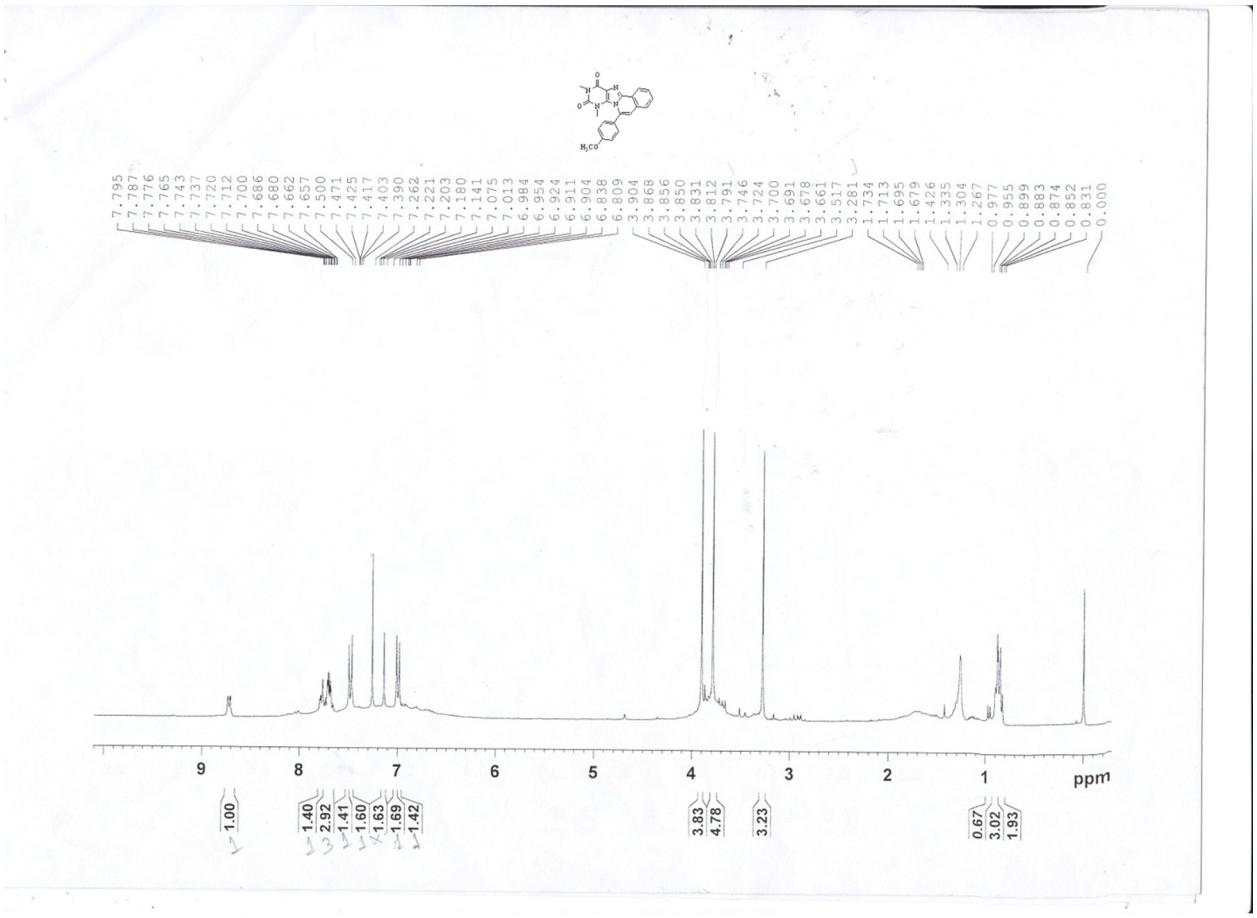
3.09
5.76
1.96

Compound **3g**: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7.657
7.500
7.471
7.425
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7.180
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7.013
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6.954
6.924
6.911
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6.838
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3.724
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0.831
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4
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2
1
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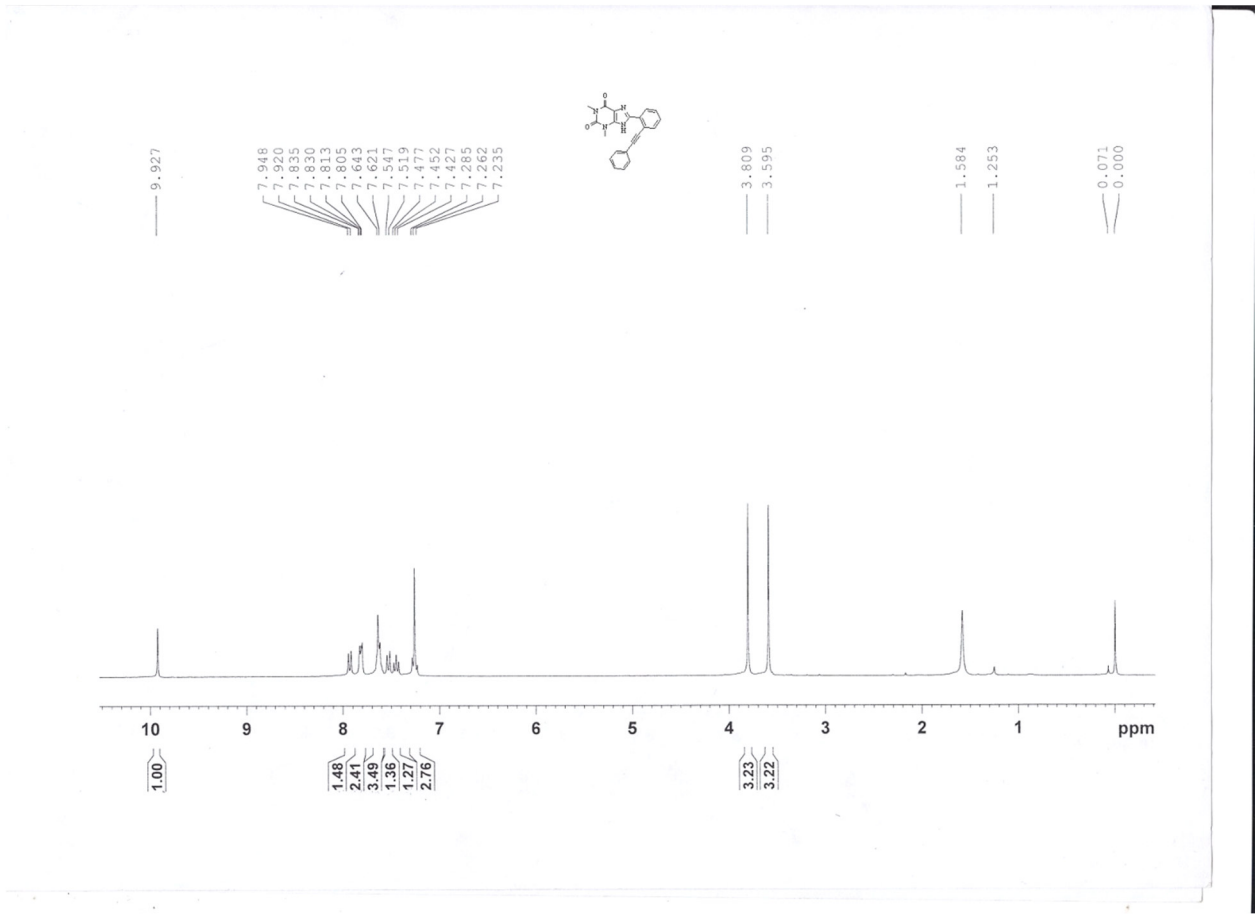
Compound **4a**: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7.285
7.262
7.235
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3.595
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1.253
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9
8
7
6
5
4
3
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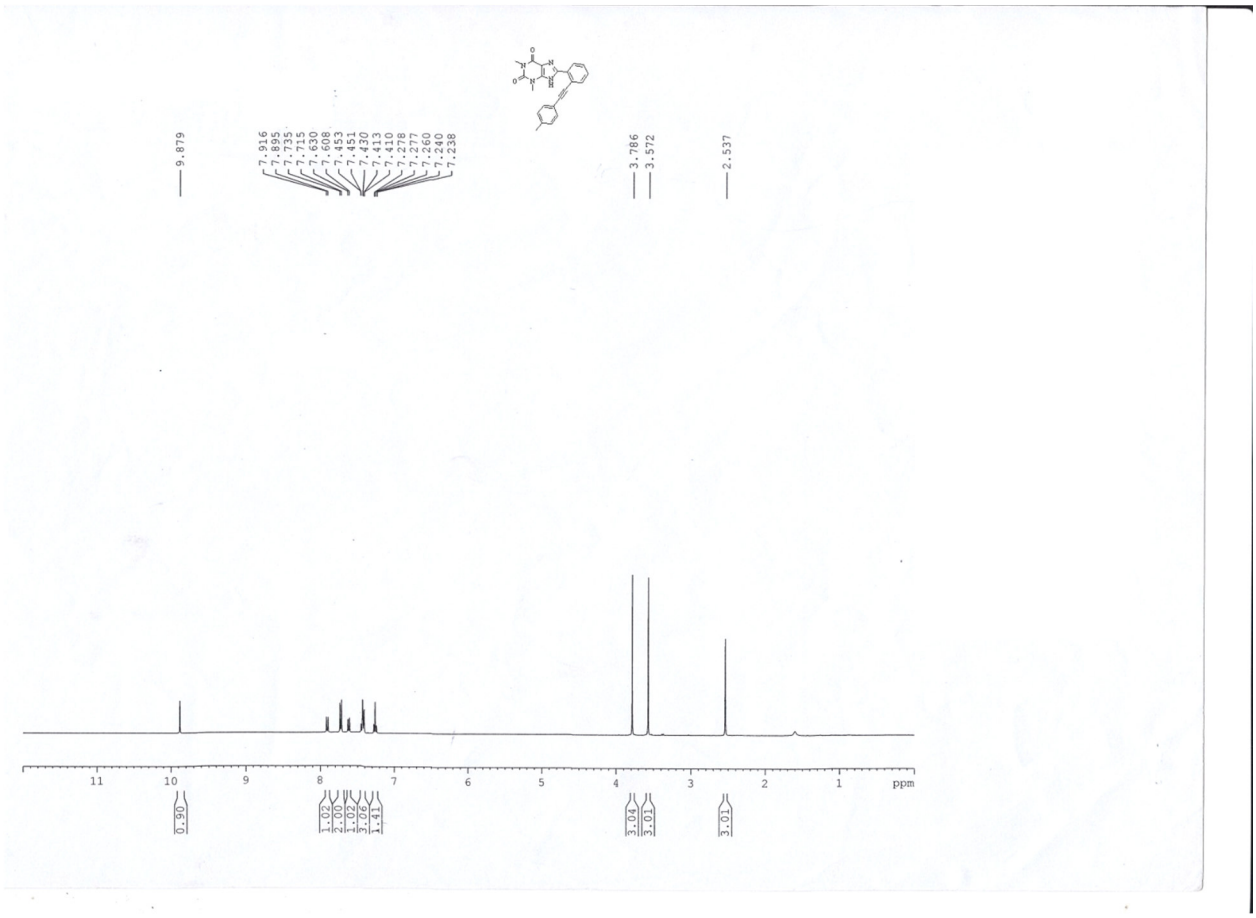
Compound **4b:**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7.240
7.238
3.786
3.572
2.537
11
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9
8
7
6
5
4
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ppm
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3.04
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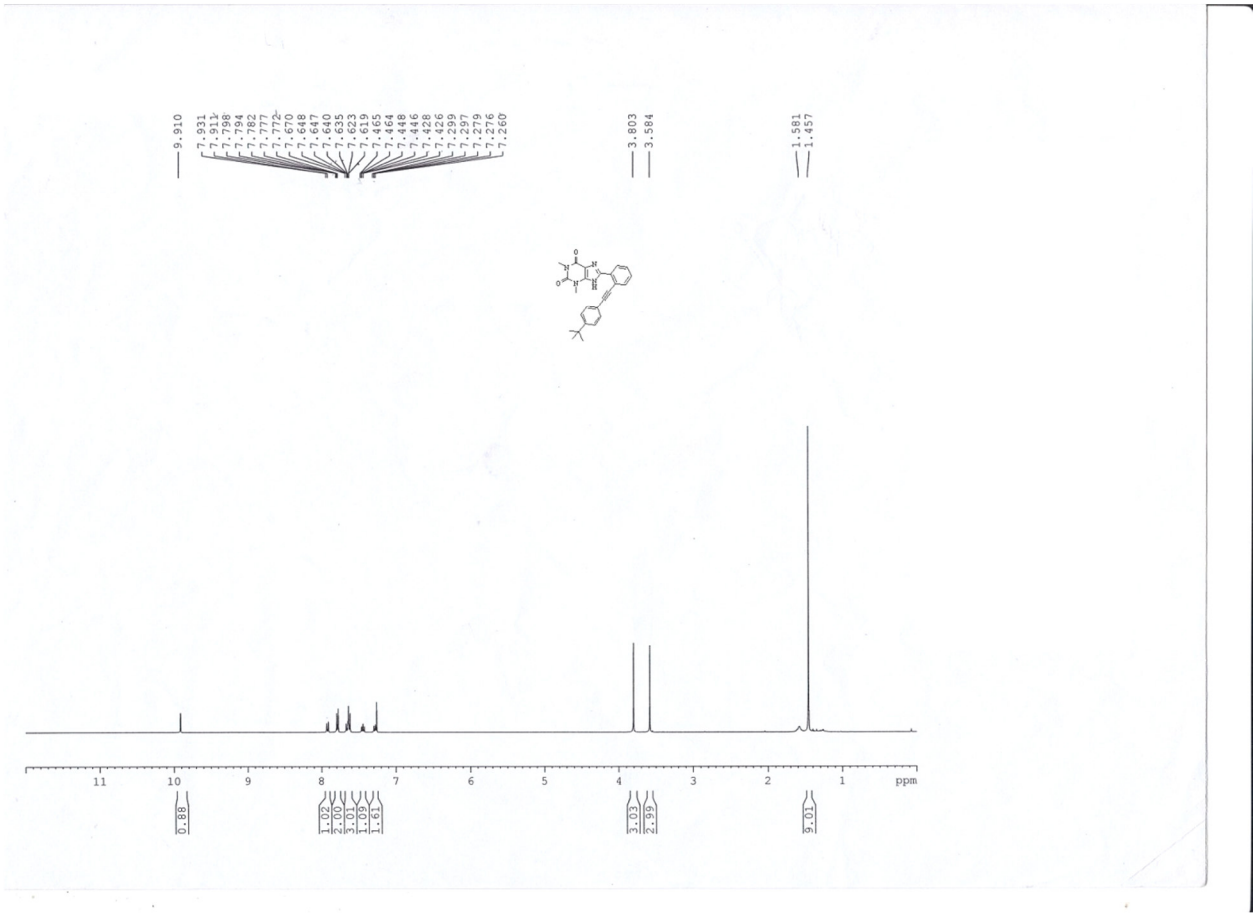
3.01

Compound **4c:**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7.465
7.464
7.448
7.446
7.428
7.426
7.299
7.297
7.279
7.276
7.260
3.803
3.584
1.581
1.457
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10
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8
7
6
5
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3.03
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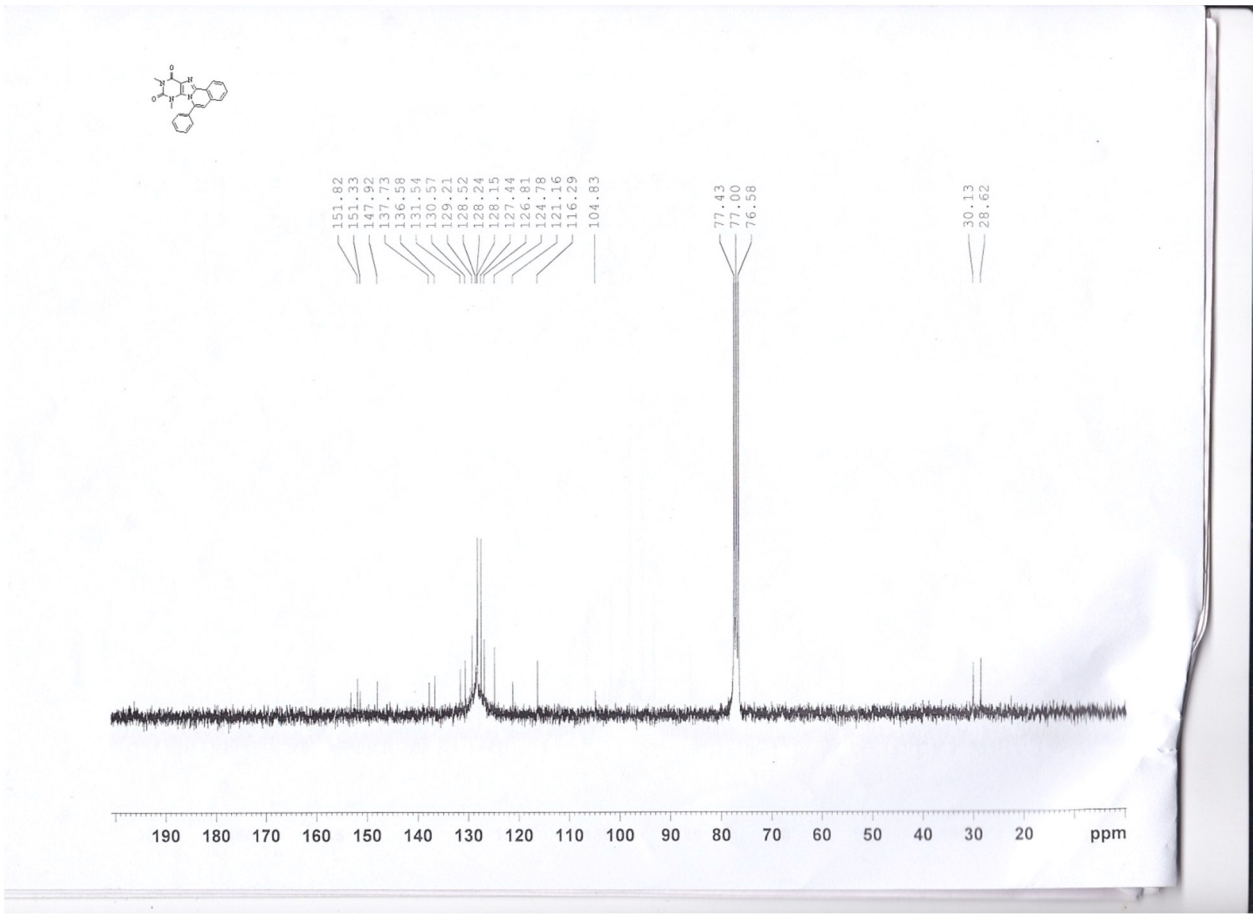
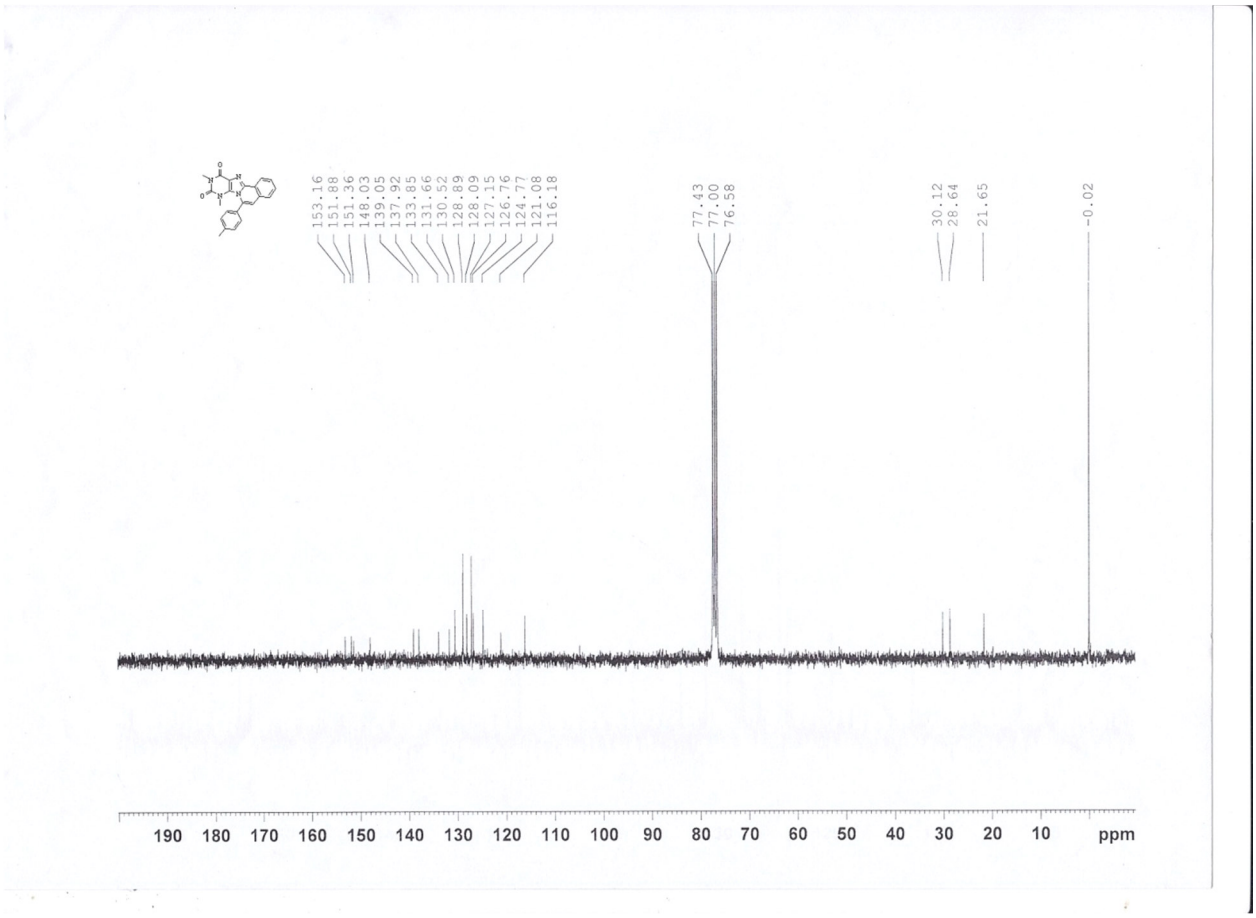
13C NMR data: Compound 3a



Compound **3b:**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131.66
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128.09
127.15
126.76
124.77
121.08
116.18
77.43
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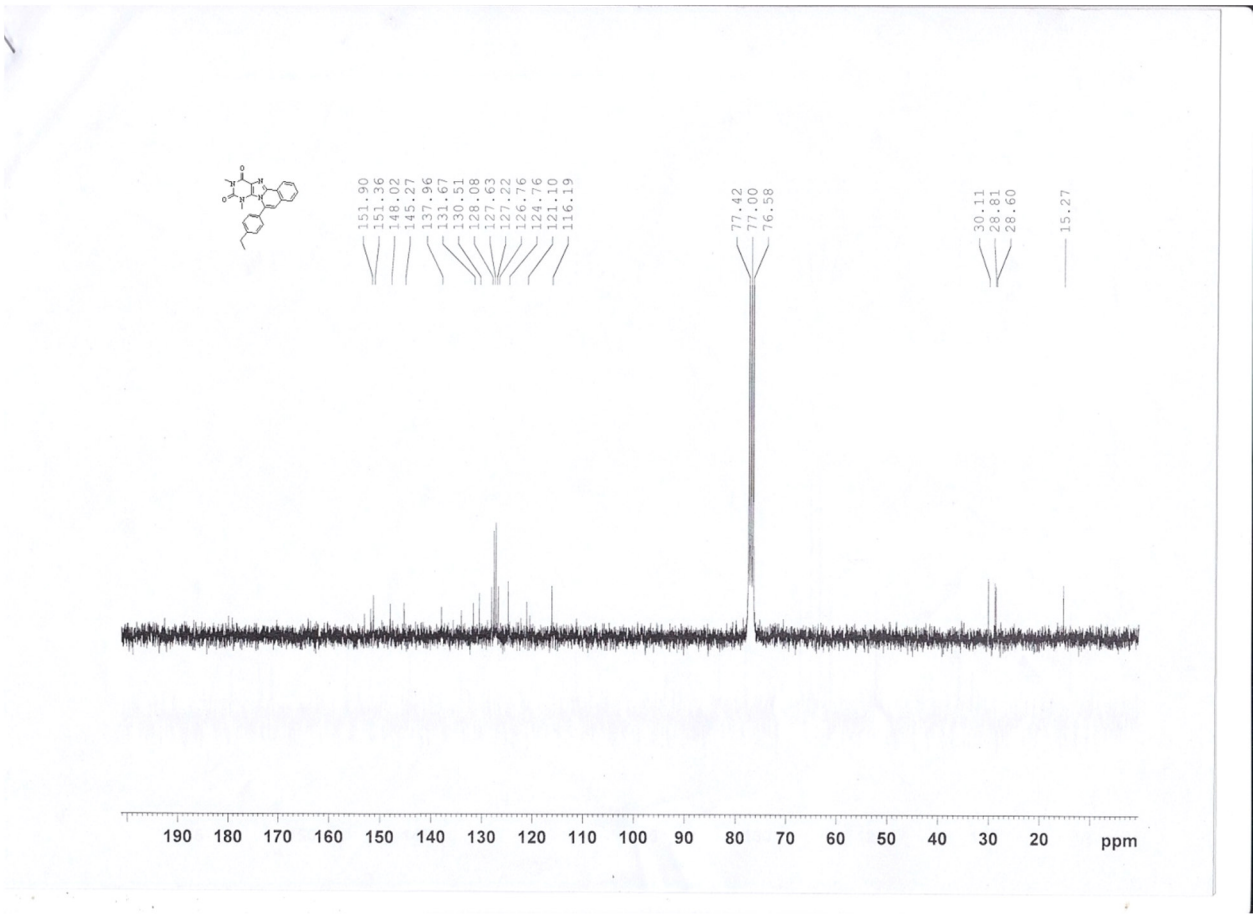
Compound 3c: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127.63
127.22
126.76
124.76
121.10
116.19
77.42
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28.81
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15.27
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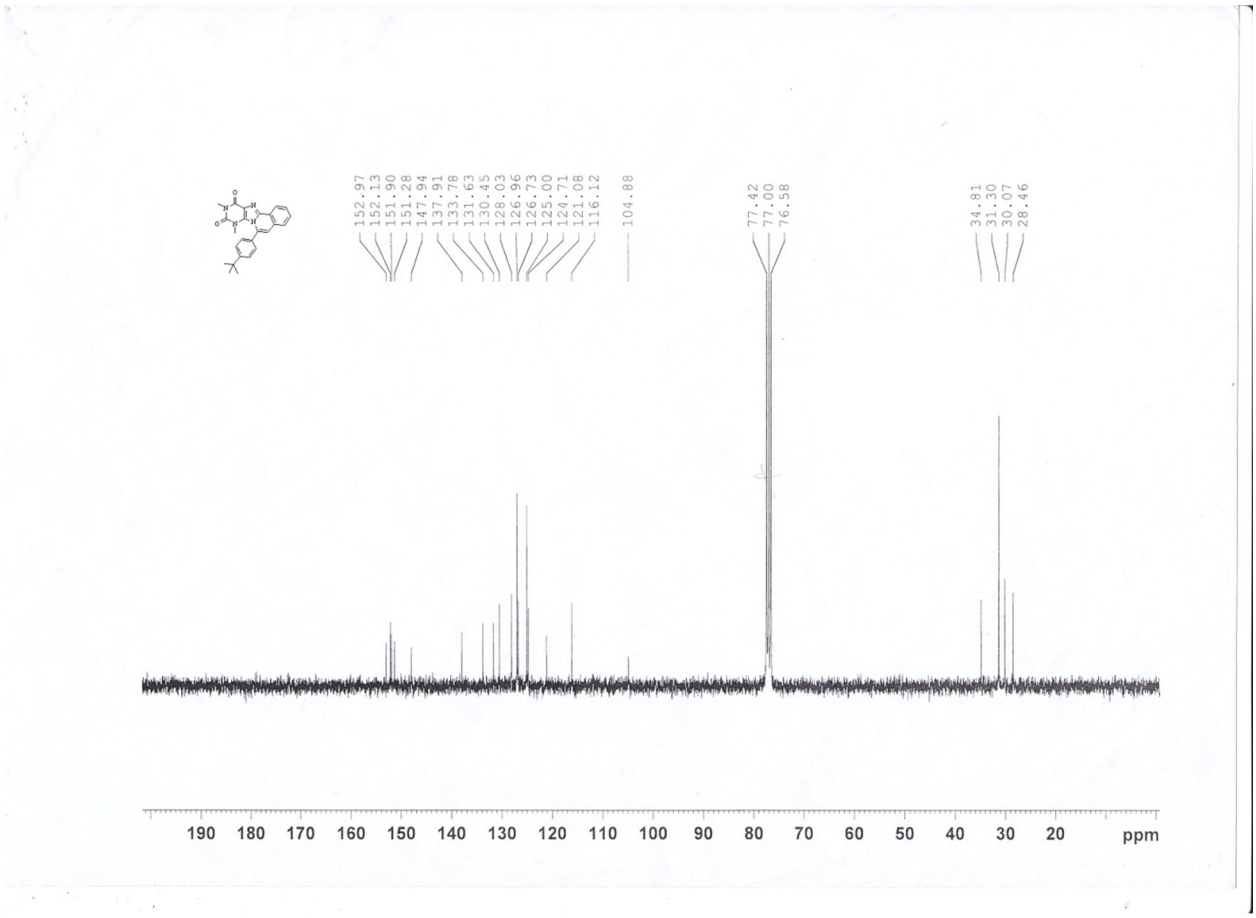
Compound **3d**: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131.63
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126.96
126.73
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124.71
121.08
116.12
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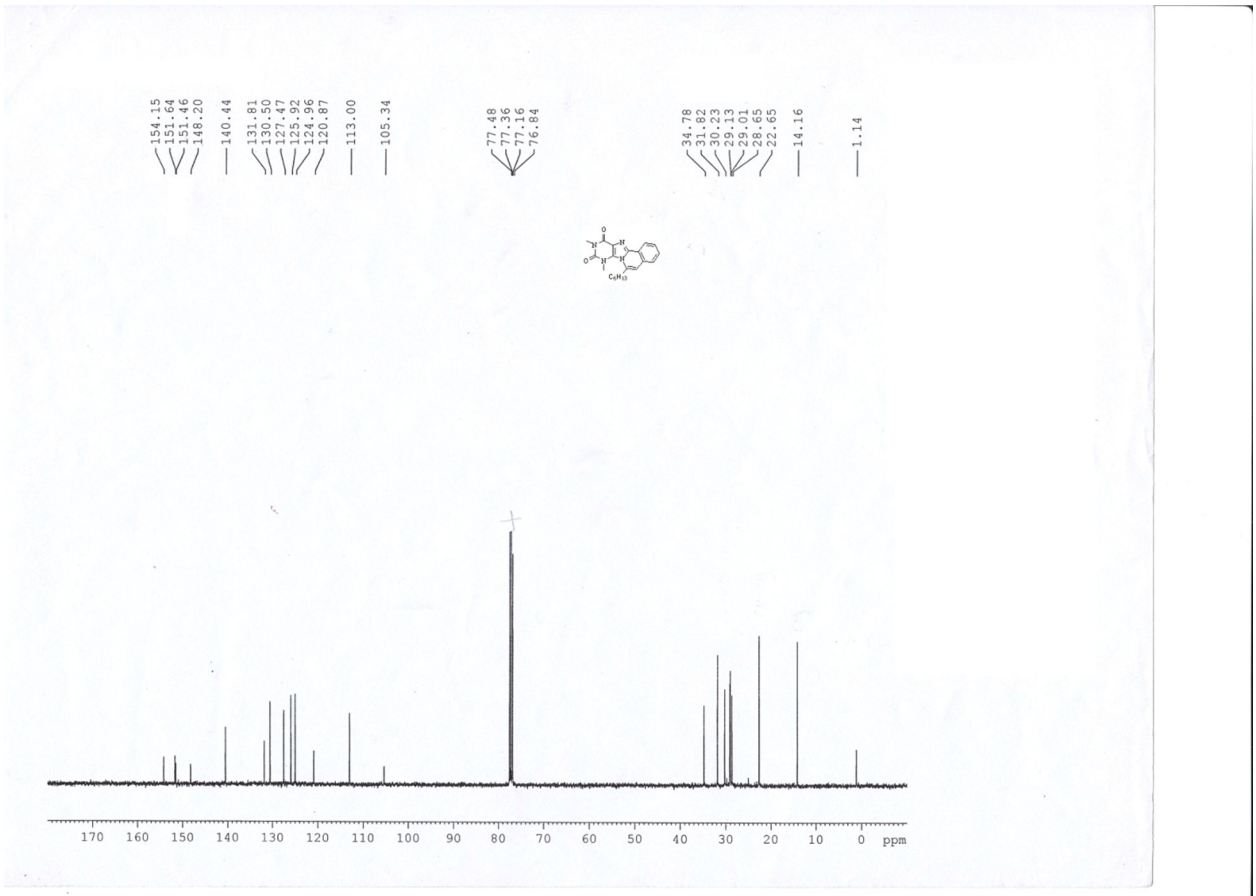
Compound **3e:**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127.47
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120.87
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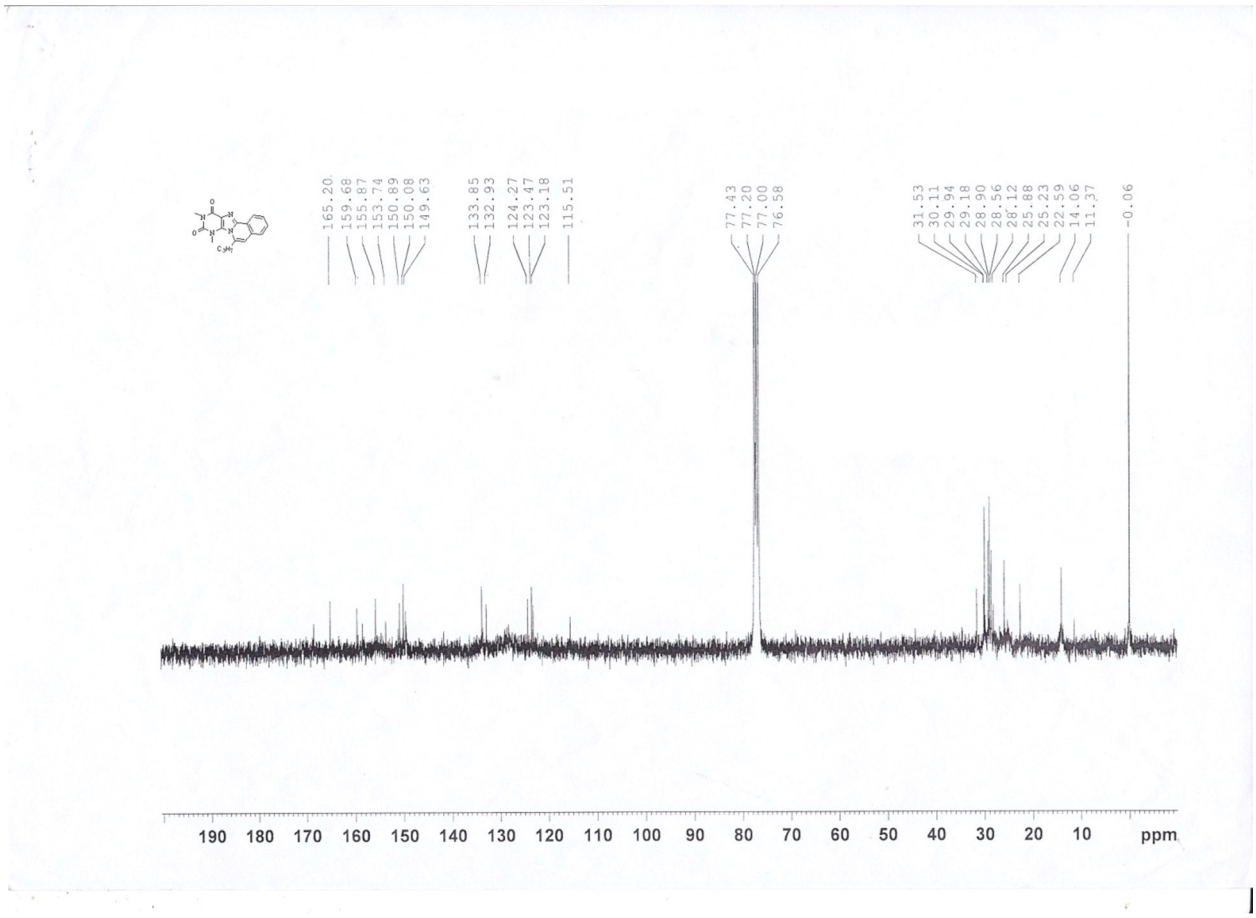
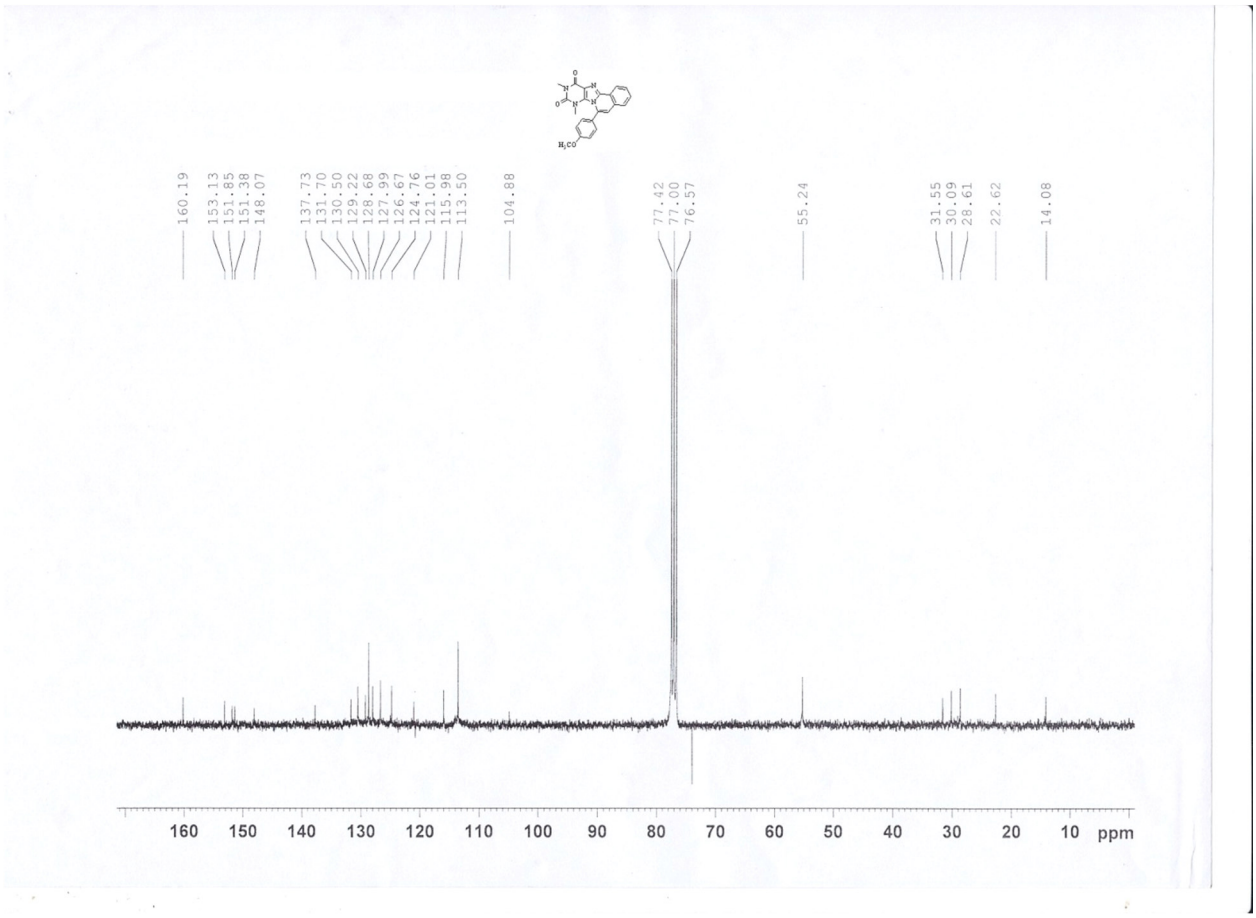
77.48
77.36
77.16
76.84
34.78
31.82
30.23
29.13
29.01
28.65
22.65
14.16
1.14
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Compound **3f:**


165.20
159.68
155.87
153.74
150.89
150.08
149.63
133.85
132.93
124.27
123.47
123.18
115.51
77.43
77.20
77.00
76.58
31.53
30.11
29.94
29.18
28.90
28.56
28.12
25.88
25.23
22.59
14.06
11.37
-0.06
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Compound **3g:**


160.19
153.13
151.85
151.38
148.07
137.73
131.70
130.50
129.22
128.68
127.99
126.67
124.76
121.01
115.98
113.50
104.88
77.42
77.00
76.57
55.24
31.55
30.09
28.61
22.62
14.08
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm