Supporting Information

Structure-Based Optimization of Potent and Selective Inhibitors of the Tyrosine Kinase EphB4

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Table of contents

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Table S1. Local selectivity of compound **66**. These IC_{50} values were measured at the University of Dundee.

Kinases	Percentage of kinase activity compared to a 100% DMSO control	
	54[a]	**66**[b]
MKK1	70	70
ERK1	97	96
ERK2	91	93
JNK1	106	96
JNK2	93	94
p38a MAPK	87	97
p38b MAPK	93	83
p38g MAPK	92	84
p38d MAPK	94	86
ERK8	109	97
RSK1	83	88
RSK2	105	104
PDK1	109	103
PKBa	97	98
PKBb	104	104
SGK1	124	78
S6K1	98	77
PKA	92	96
ROCK 2	94	77
PRK2	95	93
PKCa	97	92
PKCz	98	95
PKD1	100	92
MSK1	95	95
MNK1	93	94
MNK2	85	74
MAPKAP-K2	96	90
PRAK	87	81
CAMKKb	101	104
CAMK1	93	100
SmMLCK	91	87
PHK	92	95

CHK1	93	95
CHK2	99	90
GSK3b	102	89
CDK2-Cyclin A	97	90
PLK1	89	93
Aurora B	104	93
AMPK	92	86
MARK3	111	96
BRSK2	81	82
MELK	89	80
CK1	108	93
CK2	85	80
DYRK1A	99	99
DYRK2	94	86
DYRK3	103	96
NEK2a	102	123
NEK6	103	89
IKKb	92	86
PIM1	96	88
PIM2	115	93
PIM3	111	81
SRPK1	78	94
MST2	95	111
EF2K	93	96
HIPK2	114	98
PAK4	93	102
PAK5	94	94
PAK6	90	92
Src	12	9
Lck	3	0
CSK	72	31
FGF-R1	90	62
IRR	110	100
EPHA2	10	7
MST4	83	78
SYK	94	94
YES1	6	3

IGF-1R	106	94
VEG-FR	106	77
BTK	52	33
IR-HIS	103	104
EPHB3	28	3
TBK1	79	89
IKKe	101	85
GCK	109	22
IRAK4	93	82
NUAK1	140	133
MLK1	85	45
MINK1	101	102
MLK3	136	101
LKB1	89	75
HER4	45	32
TTK	99	98

[a] Percentage of activity @ 3μM concentration of compound **54**
[b] Percentage of activity @ 1μM concentration of compound **66**

Table S2. Selectivity of compound **66** on kinases predicted to have a small gatekeeper. These IC_{50} values were measured at Ambit Biosciences Corporation.

Kinases	Percentage of kinase remaining bound to the beads, relative to a 100% DMSO control[a]
ABL1-phosphorylated	0.15
ABL2	0.75
ALK	99
BLK	0.6
BMPR1A	51
BMPR1B	0.9
BMX	55
BRK	12
DDR1	1.4
DDR2	21
EGFR	8.6
EPHA6	40
EPHB4	1.2
EPHB6	32
ERBB2	27
ERBB3	78
FGFR2	94
FGFR3	89
FGFR4	100
FLT4	93
FRK	0.3
FYN	0.25
GAK	49
GCN2(Kin.Dom.2,S808G)	100
HCK	0.6
KIT	88
LIMK1	83
LIMK2	78
LYN	0.4
NEK11	67
NLK	83
PDGFRA	84
PDGFRB	53

QSK	32
RAF1	14
RET	79
RIPK2	2.9
RSK3(Kin.Dom.2-C-terminal)	84
RSK4(Kin.Dom.2-C-terminal)	5.8
SIK	41
SRMS	18
TEC	100
TESK1	9.8
TGFBR1	3.6
TGFBR2	2.4
VEGFR2	96
YANK1	80
YANK2	89
YANK3	100
ZAK	15

[a] Percentage of activity @ 1μM concentration of compound **66**

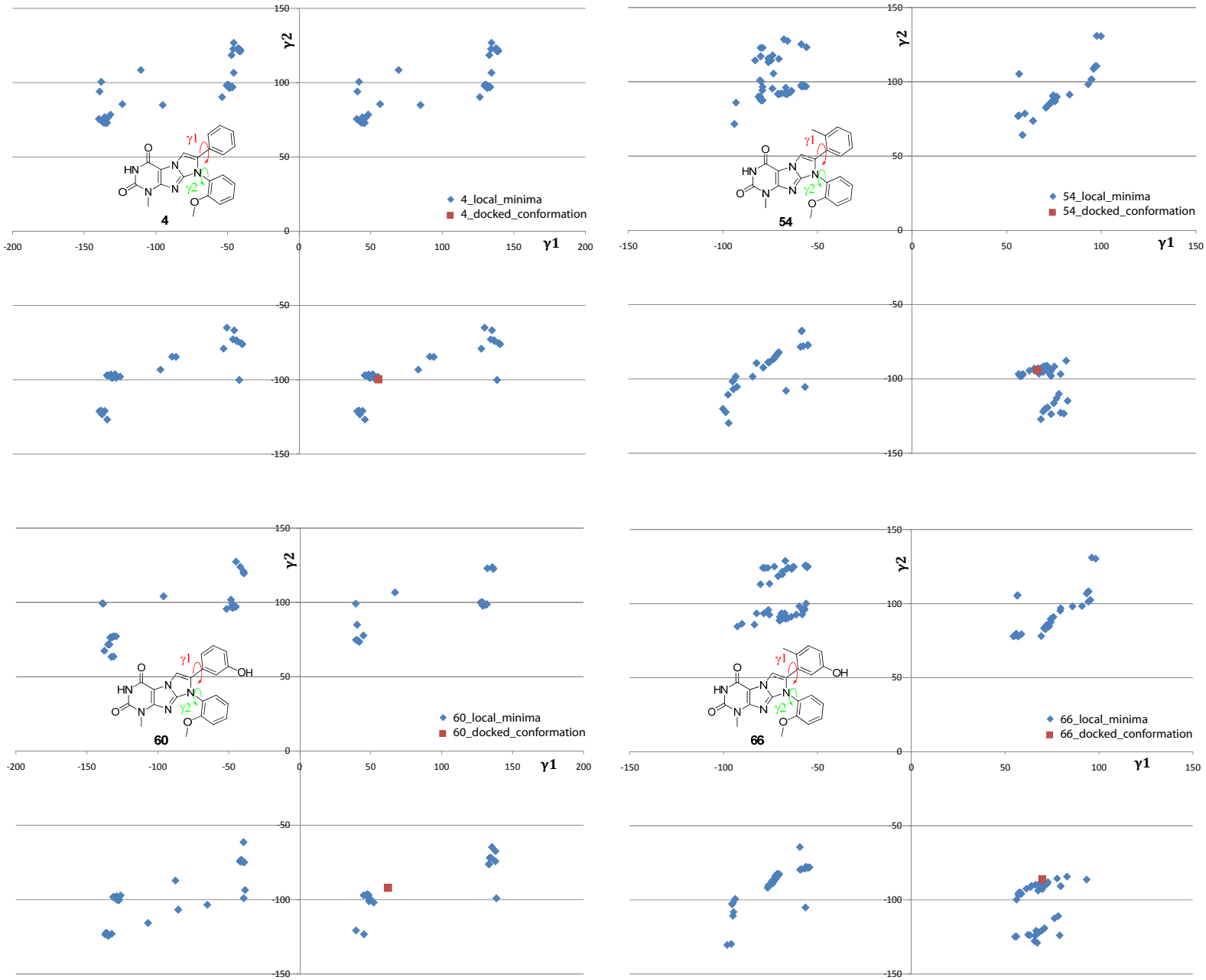


Figure S1. Conformational analysis on **4**, **54**, **60**, **66**. The local minima obtained by ab initio minimization of each rotameric state are plotted against the dihedral angles γ1 and γ2 (blue). The global minima are indicated in red.

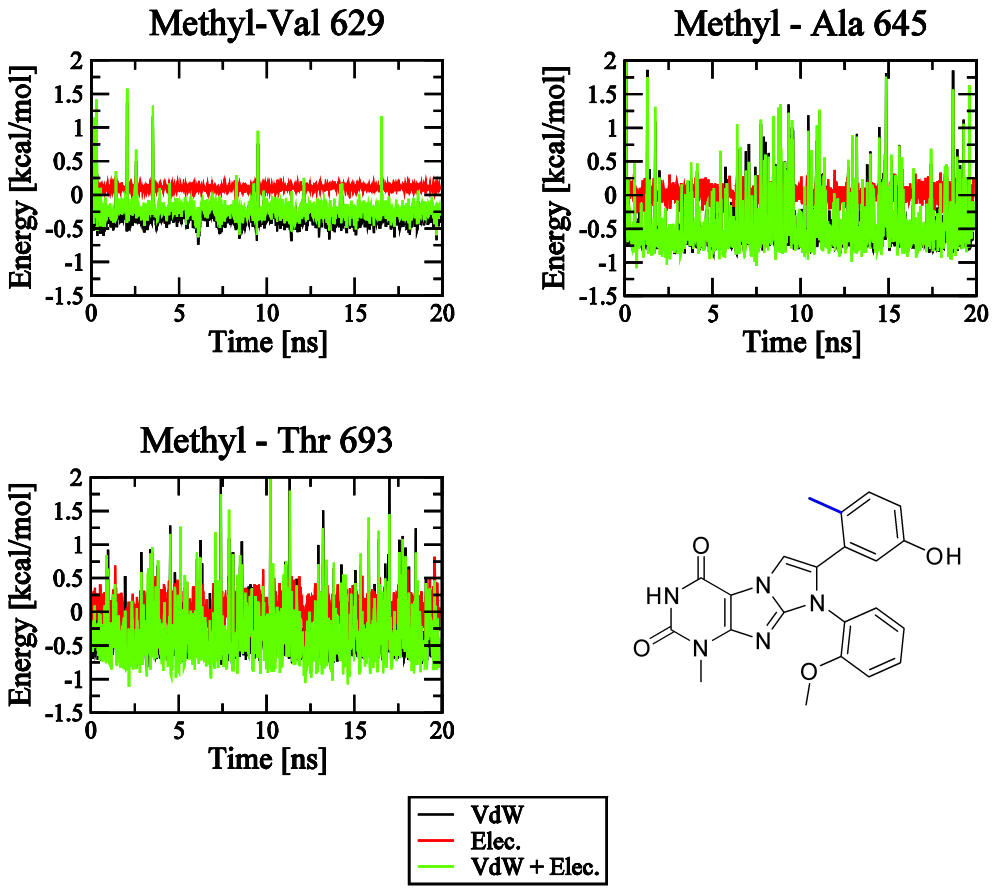
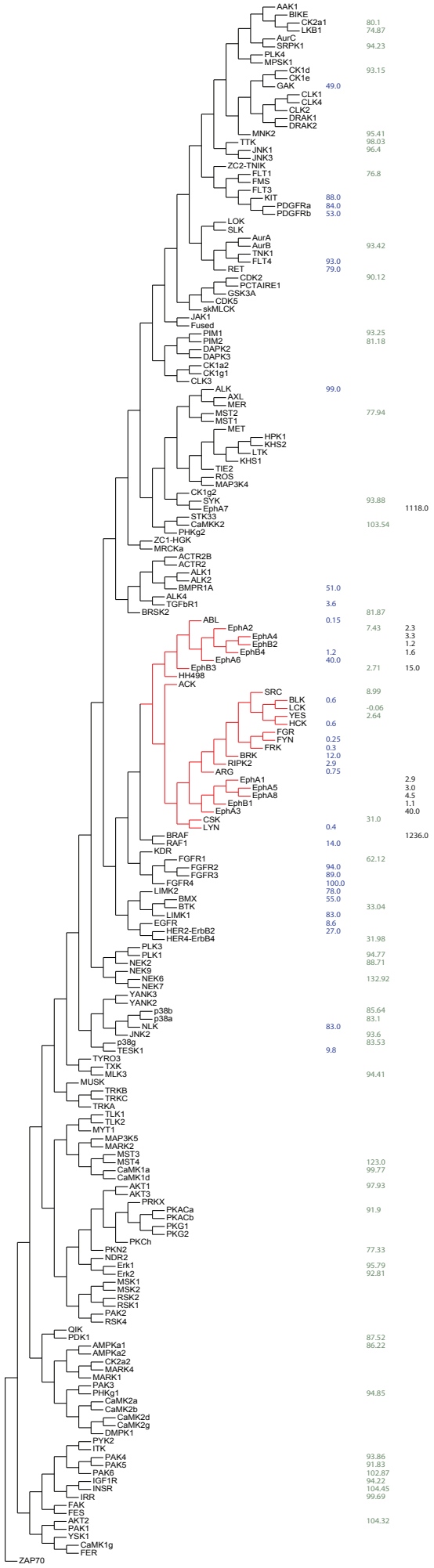


Figure S2. Time series of the van der Waals and electrostatic interaction energies between the methyl of compound **66** and the side chains of Val629, Ala645 and Thr693.



Pourcentage of kinase activity compared to a 100% DMSO control. These values were measured at Reaction Biology Corporation (black), at the University of Dundee (green) and at Ambit Biosciences Corporation (blue).

Figure S3. SAR-based dendrogram.

6-Amino-1-methyl-2,4(1H,3H)-pyrimidinedione (5)

A mixture of methylurea (22.4 g, 302 mmol), 2-cyanoacetic acid (38.0 g, 447 mmol) and Ac_2O (74 mL) was heated to 60 °C for 2.5 h. After cooling to room temperature, water (74 mL) was added, and the suspension was stirred for 1 h. The solid intermediate was filtered, suspended in NaOH (20%, 150 mL), and heated to 90 °C for 1 h. The reaction mixture was then cooled to 20 °C, acidified with concentrated HCl, and the precipitate was collected by filtration (27.2 g, 64% yield) as a light yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.43 (s, 1H), 6.88 (s, 2H), 4.61 (s, 1H), 3.18 (s, 3H); IR (film): $\tilde{\upsilon}$ = 3344, 3183, 3101, 3046, 1660, 1618, 1548, 1276, 1161, 827 cm^{-1}; MS (ESI): *m/z*: calcd for $C_5H_7N_3NaO_2$: 164.0, found: 164.0 $[M + Na]^+$.

6-Amino-1-(phenylmethyl)-2,4(1H,3H)-pyrimidinedione (6)

A mixture of benzylurea (5.0 g, 33.3 mmol), 2-cyanoacetic acid (2.6 g, 36.63 mmol) and Ac_2O (20 mL) was heated at 80 °C for 2 h. After cooling to room temperature, Et_2O (30 mL) was added, and the resultant suspension was stirred for 1 h. The solid intermediate was filtered, suspended in a mixture of water (30 mL) and ethanol (15 mL) and heated at 85 °C. NaOH (10%, 5 mL) were slowly added. After 1 h, the reaction mixture was concentrated, acidified with concentrated HCl, and the precipitate collected by filtration. If necessary, the solid was washed with acetone to afford a light yellow solid (3.5 g, 49% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.44 (s, 1H), 7.19-7.36 (m, 5H), 6.75 (s, 2H), 5.02 (s, 2H), 4.59 (d, J = 2.0 Hz, 1H); ^{13}C NMR (75 MHz, DMSO-d_6): δ = 162.3, 155.7, 151.4, 136.6, 128.4, 127.1, 126.2, 75.5, 43.5; IR (film): $\tilde{\upsilon}$ = 3470, 3327, 3250, 3217, 3070, 2968, 2766, 1694, 1630, 1575, 1494, 1384, 1278, 895, 821, 728 cm^{-1}; MS (ESI): *m/z*: calcd for $C_{11}H_{11}N_3NaO_2$: 240.1, found: 240.1 $[M + Na]^+$.

General procedure for the preparation of 1-alkyl-5-nitroso-4-aminouracil (7, 8)

To a stirred mixture containing 1-alkyl-6-aminouracil (1 eq) in water (0.45 M) and acetic acid (8.2 M) at -5 ºC, $NaNO_2$ (1.1 eq) was added in small portions. A deep purple color, characteristic of the nitroso derivative appeared immediately, and stirring was continued at room temperature

for 19 h. The solid was filtered off, washed with cold water, and dried under high vacuum to obtain the corresponding products in pure form.

6-Amino-1-methyl-5-nitroso-2,4(1H,3H)-pyrimidinedione (7)

Yield: 77%; ^{1}H NMR (300 MHz, DMSO-d_6): δ = 13.02 (s, 1H), 11.51 (s, 1H), 9.14 (s, 1H), 3.19 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 160.2, 148.7, 147.5, 138.6, 27.8; IR (film): $\tilde{\upsilon}$ = 3270, 3225, 3080, 3025, 1700, 1568, 1510, 1427, 1395, 1233, 1107, 1021, 866, 702 cm^{-1}; MS (ESI): *m/z*: calcd for $C_5H_6N_4NaO_3$: 193.0, found: 193.0 $[M + Na]^+$.

6-Amino-5-nitroso-1-(phenylmethyl)-2,4(1H,3H)-pyrimidinedione (8)

Yield: 93%; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 13.33 (s, 1H), 11.66 (s, 1H), 9.12 (s, 1H), 7.24-7.36 (m, 5H), 5.08 (s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): δ = 160.4, 148.9, 146.9, 138.6, 134.6, 128.6, 127.4, 126.3, 43.3; IR (film): $\tilde{\upsilon}$ = 3145, 2969, 2773, 1729, 1691, 1636, 1509, 1448, 1410, 1247, 1161, 725 cm^{-1}; MS (ESI): *m/z*: calcd for $C_{11}H_{10}N_4NaO_3$: 269.1, found: 269.0 $[M + Na]^+$.

General procedure for the preparation of 1-alkyl-5,6-diaminouracil (9, 10)

To a stirred mixture containing 1-alkyl-5-nitroso-4-aminouracil (1 eq) in aqueous ammonia (25%, 0.6 M), sodium dithionite (3.5 eq) was added in small portions. The temperature raised to 35 °C and the purple color disappeared gradually. When no more temperature increase was observed, the reaction mixture was stirred at 60 °C for an additional hour and then 17 h at room temperature in order to complete the reaction (total disappearance of the purple color). The solid was filtered off, thoroughly washed with cold water, and dried under high vacuum to obtain the corresponding products in pure form.

5,6-Diamino-1-methyl-2,4(1H,3H)-pyrimidinedione (9)

Yield: 78%; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.53 (s, 1H), 6.12 (s, 2H), 3.21 (s, 3H), 2.95 (s, 2H); IR (film): $\tilde{\upsilon}$ = 3351, 3313, 3148, 1667, 1636, 1579, 1509, 962, 712 cm^{-1}; MS (ESI): *m/z*: calcd for $C_5H_9N_4O_2$: 157.1, found: 157.0 $[M + H]^+$.

5,6-Diamino-1-(phenylmethyl)-2,4(1H,3H)-pyrimidinedione (10)

Yield: 90%; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.88 (s, 1H), 7.19-7.35 (m, 5H), 6.09 (s, 2H), 5.07 (s, 2H), 2.92 (s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): δ = 159.6, 149.6, 145.3, 136.8, 128.3, 127.0, 126.4, 96.4, 43.9; IR (film): $\tilde{\upsilon}$ = 3406, 3305, 3183, 2968, 2776, 1686, 1628, 1574, 1496, 1402, 942, 717 cm^{-1}; MS (ESI): *m/z*: calcd for $C_{11}H_{12}N_4NaO_2$: 255.1, found: 255.1 $[M + Na]^+$.

3,9-Dihydro-3-methyl-1H-purine-2,6-dione (11)

A solution of 1-methyl-5,6-diaminouracil (18.8 g, 120 mmol) in formic acid (6.2 mL) and water (140 mL) was heated to reflux for 3 h. After cooling to 20 °C, NaOH (9.6 g, 240 mmol) in water (12 mL) was added, and the mixture was heated to reflux for 1 h. After cooling to 0 °C, the mixture was acidified by addition of acetic acid. The precipitate was filtered, washed with water, and dried to afford **11** as a light yellow solid (15.5 g, 78% yield). ^{1}H NMR (300 MHz, DMSO-d_6): δ = 11.09 (s, 1H), 8.04 (s, 1H), 3.37 (s, 3H), N_7H not observed; ^{13}C NMR (100 MHz, DMSO-d_6): δ = 154.6, 151.1, 149.2, 140.2, 106.9, 28.8; IR (film): $\tilde{\upsilon}$ = 3371, 3102, 3011, 1689, 1401, 1164, 827, 742 cm^{-1}; MS (ESI): *m/z*: calcd for $C_6H_7N_4O_2$: 167.1, found: 167.0 $[M + H]^+$.

3,9-Dihydro-3-(phenylmethyl)-1H-purine-2,6-dione (12)

A solution of 1-benzyl-5,6-diaminouracil (761 mg, 3.28 mmol) in formic acid (15 mL) was heated to reflux for 1 h and then the formic acid was evaporated under reduced pressure. The residue was dissolved in aqueous NaOH (10%, 15 mL) and ethanol (5 mL). The mixture was heated to reflux for 1 h, and then concentrated. After cooling to 0 °C, the mixture was acidified by addition of concentrated HCl. The precipitate was filtered, washed with water, and dried to afford **12** as a light yellow solid (714 mg, 90% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 13.54

(s, 1H), 11.18 (s, 1H), 8.01 (s, 1H), 7.23-7.32 (m, 5H), 5.11 (s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): δ = 154.6, 150.9, 149.1, 140.6, 137.0, 128.3, 127.4, 127.1, 107.0, 44.9; IR (film): $\tilde{\upsilon}$ = 3145, 2986, 2906, 1662, 1551, 1414, 1260, 1065, 730 cm^{-1}; MS (ESI): *m/z*: calcd for $C_{12}H_{10}N_4NaO_2$: 265.1, found: 265.0 $[M + Na]^+$.

General procedure for the bromination of 3-alkylxanthines (13, 14)

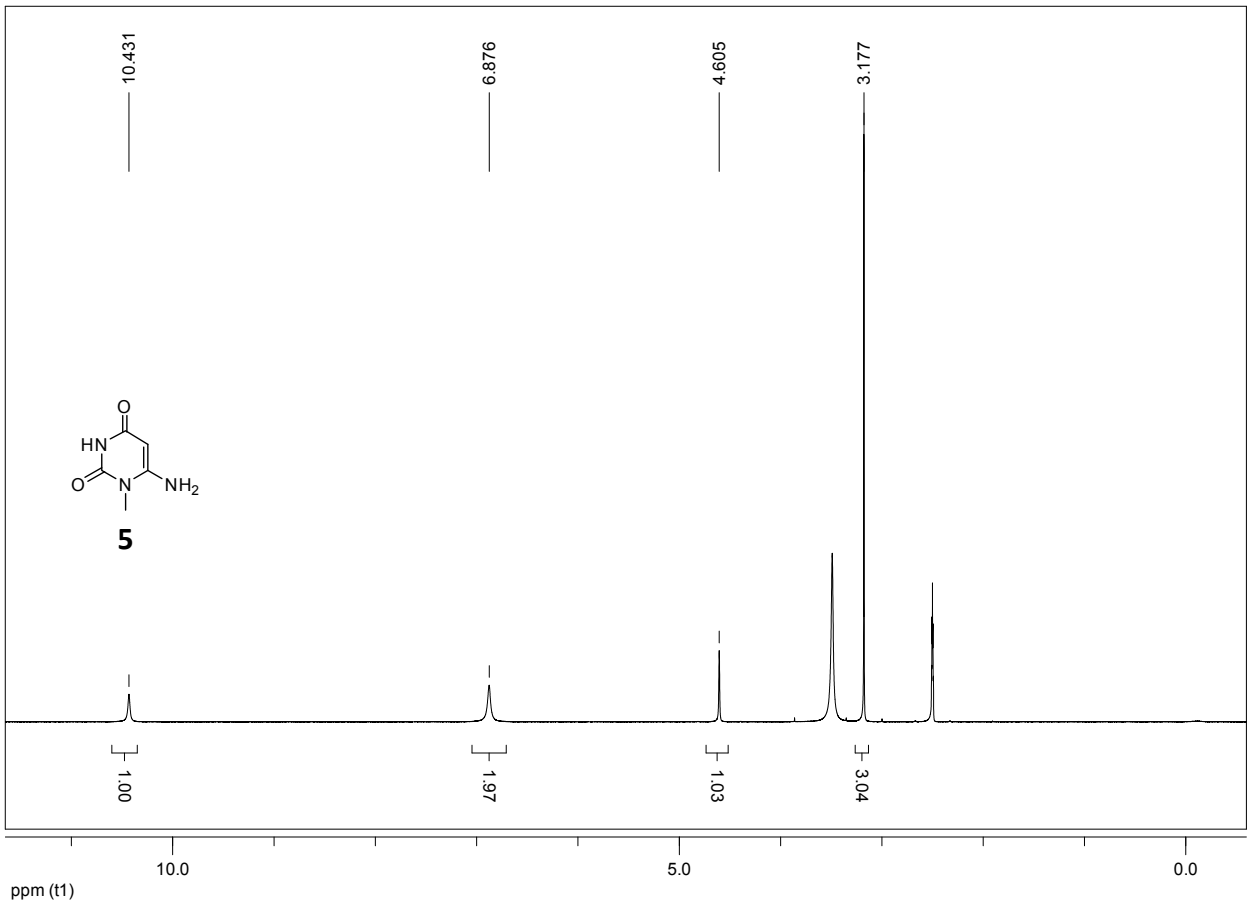
To a stirring suspension of 3-alkylxanthine (1 eq) and sodium acetate (2 eq) in glacial acetic acid (0.39 M) was added bromine dropwise (1.2 eq). The mixture was stirred at 65 °C for 2 h. After cooling to room temperature the precipitate was filtered, washed with acetic acid, water, and dried under vacuum to give the corresponding 3-alkyl-8-bromoxanthine as beige powders in pure form.

8-Bromo-3,9-dihydro-3-methyl-1H-purine-2,6-dione (13)

Yield: 84%; ^{1}H NMR (300 MHz, DMSO-d_6): δ = 11.14 (s, 1H), 3.31 (s, 3H), N_7H not observed; ^{13}C NMR (75 MHz, DMSO-d_6): δ = 153.6, 150.7, 149.4, 124.1, 109.7, 28.8; IR (film): $\tilde{\upsilon}$ = 3577, 3362, 3029, 2968, 2832, 1667, 1468, 1268, 861, 748 cm^{-1}; MS (ESI): *m/z*: calcd for $C_6H_6BrN_4O_2$: 244.9, found: 244.8 $[M + H]^+$.

8-Bromo-3,9-dihydro-3-(phenylmethyl)-1H-purine-2,6-dione (14)

Yield: 73%; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 11.23 (s, 1H), 7.23-7.34 (m, 5H), 5.06 (s, 2H), N_7H not observed; ^{13}C NMR (100 MHz, DMSO-d_6): δ = 153.8, 150.6, 149.2, 136.8, 128.4, 127.3, 127.2, 124.7, 110.1, 45.1; IR (film): $\tilde{\upsilon}$ = 3027, 2850, 2817, 1702, 1667, 1541, 1460, 1368, 1340, 739 cm^{-1}; MS (ESI): *m/z*: calcd for $C_{12}H_{10}BrN_4O_2$: 320.9, found: 321.1 $[M + H]^+$.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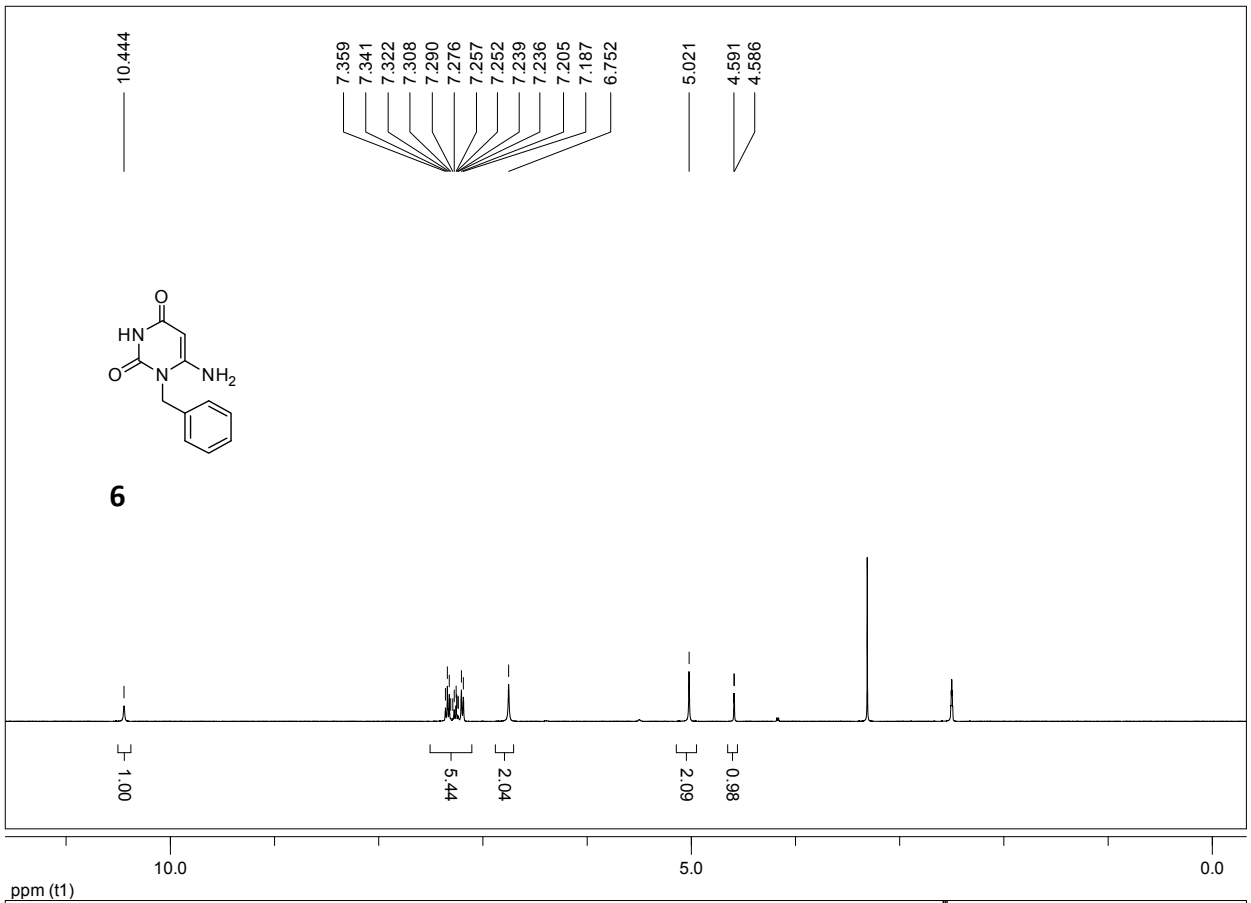
ppm (t1)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5.021
4.591
4.586
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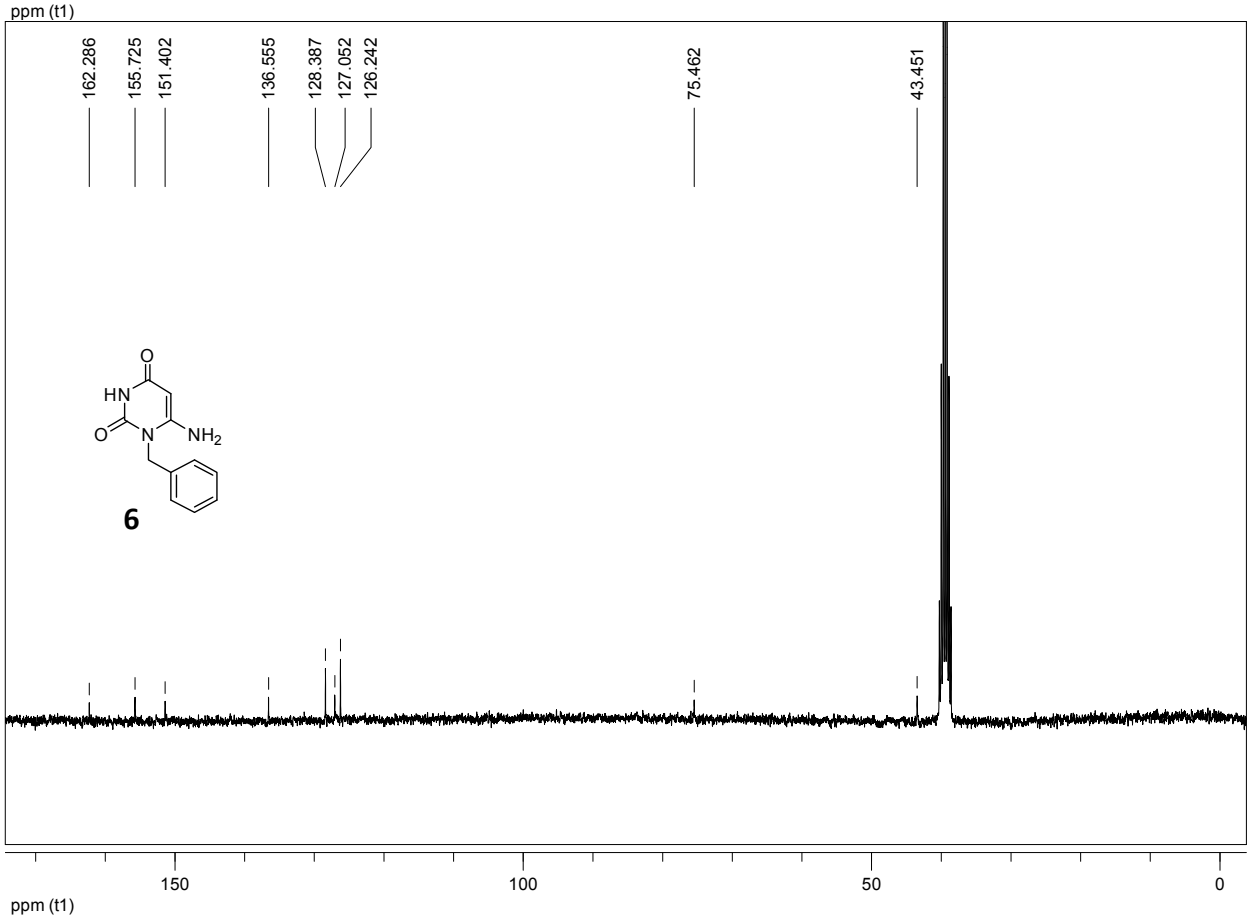
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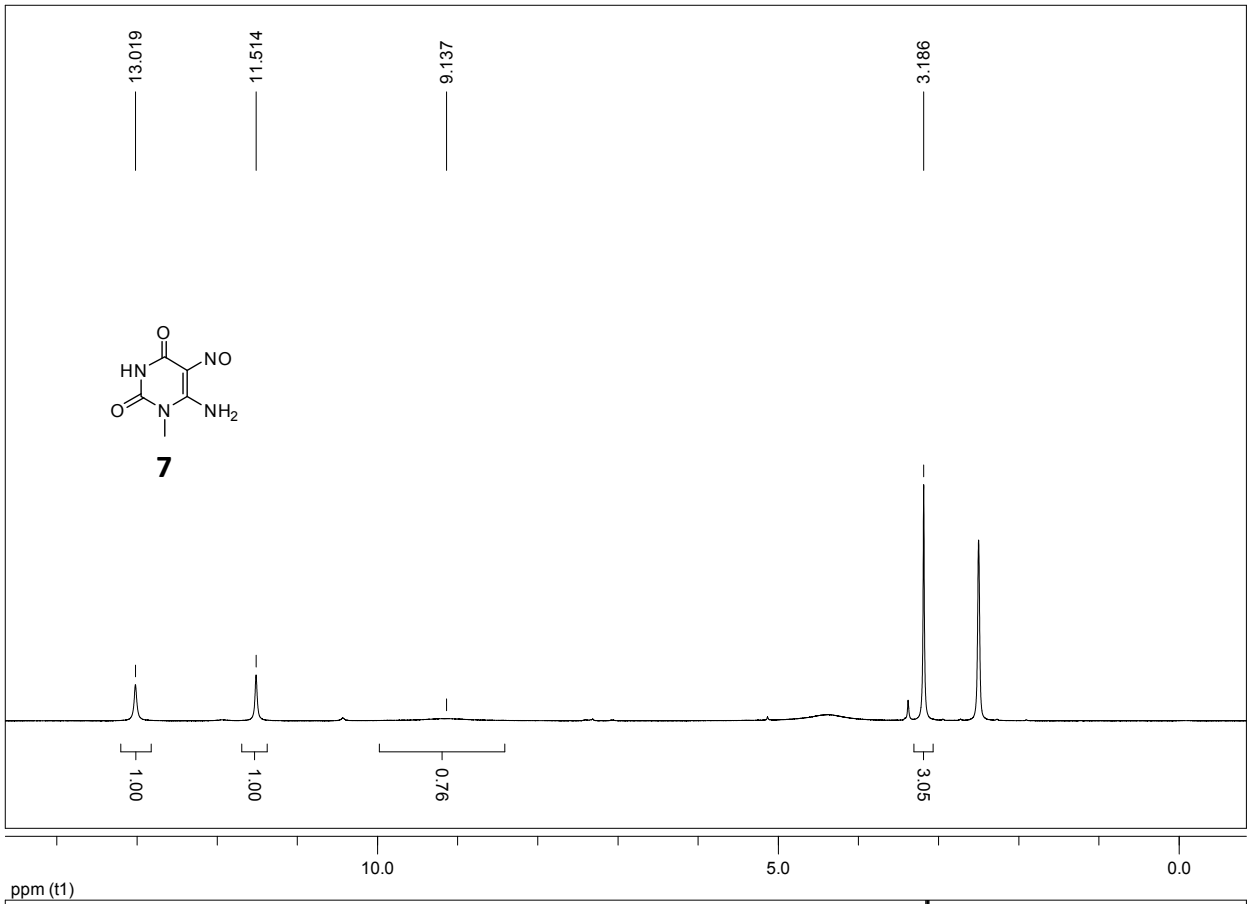
50
0
ppm (t1)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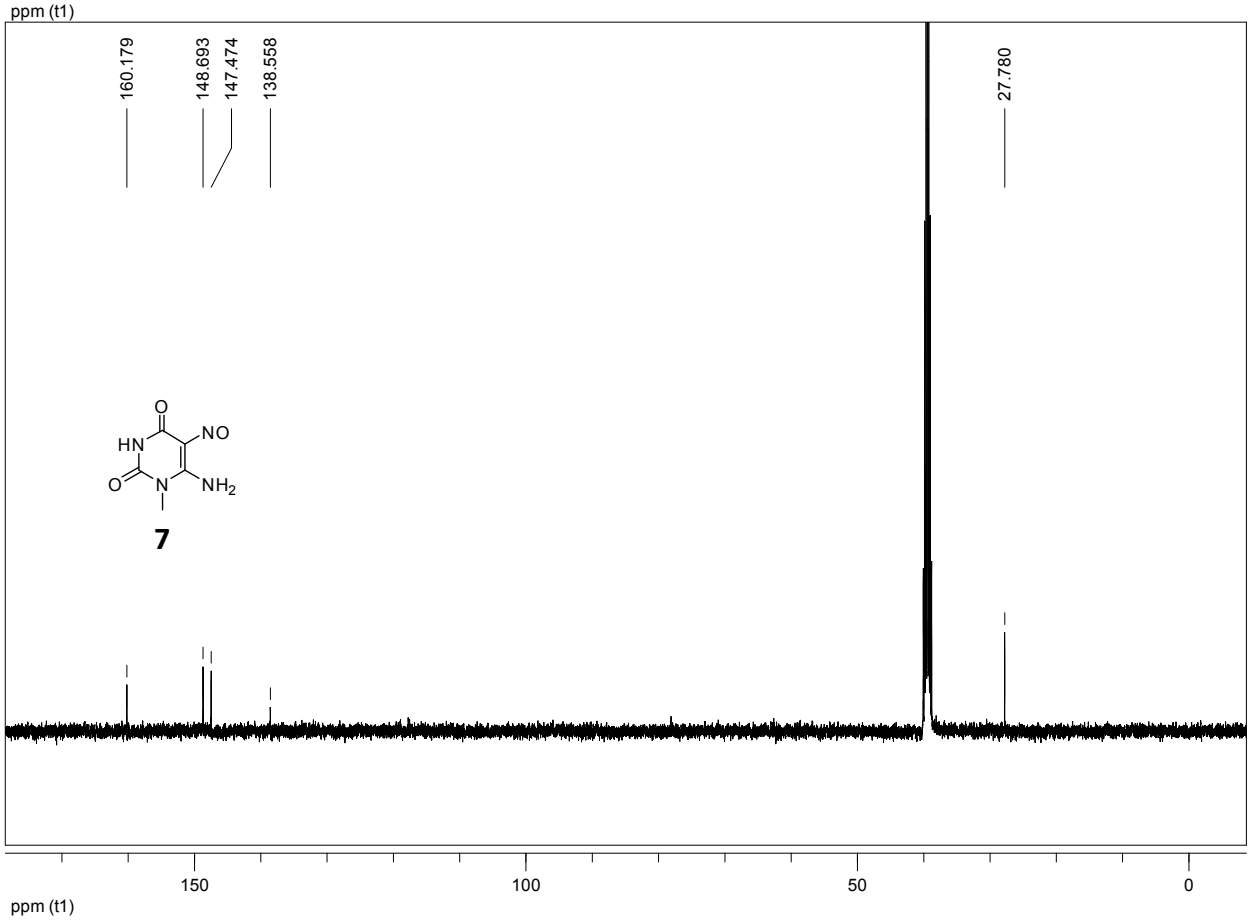
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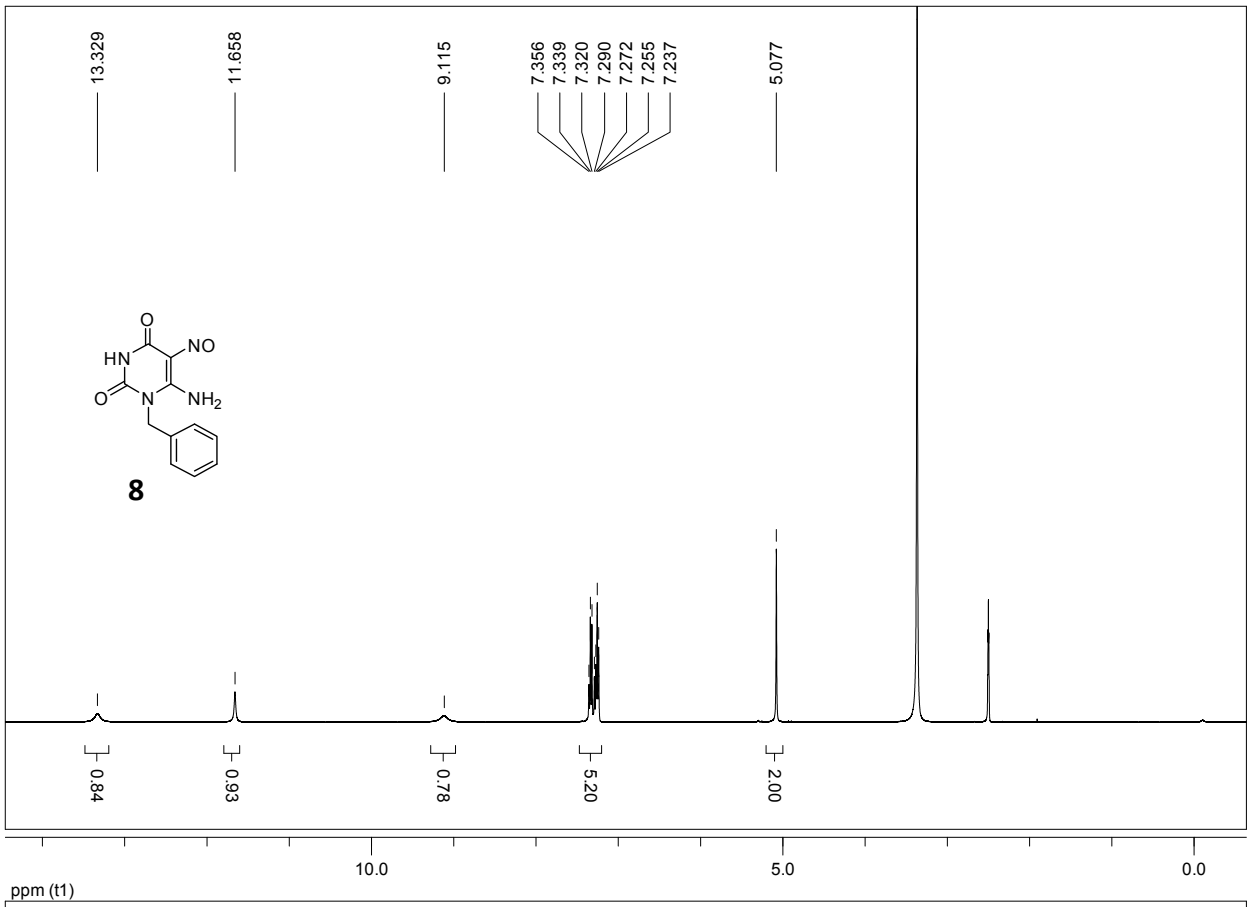
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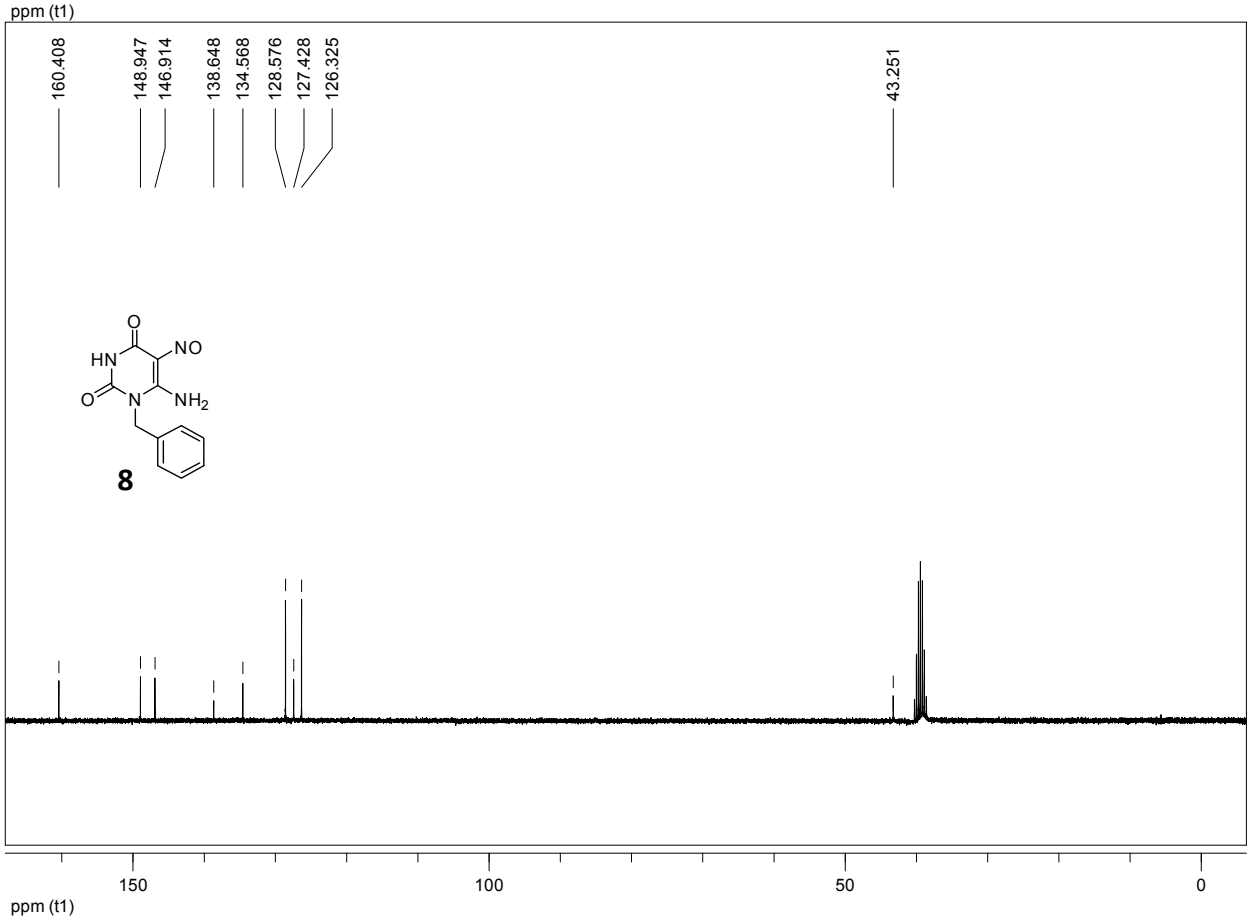
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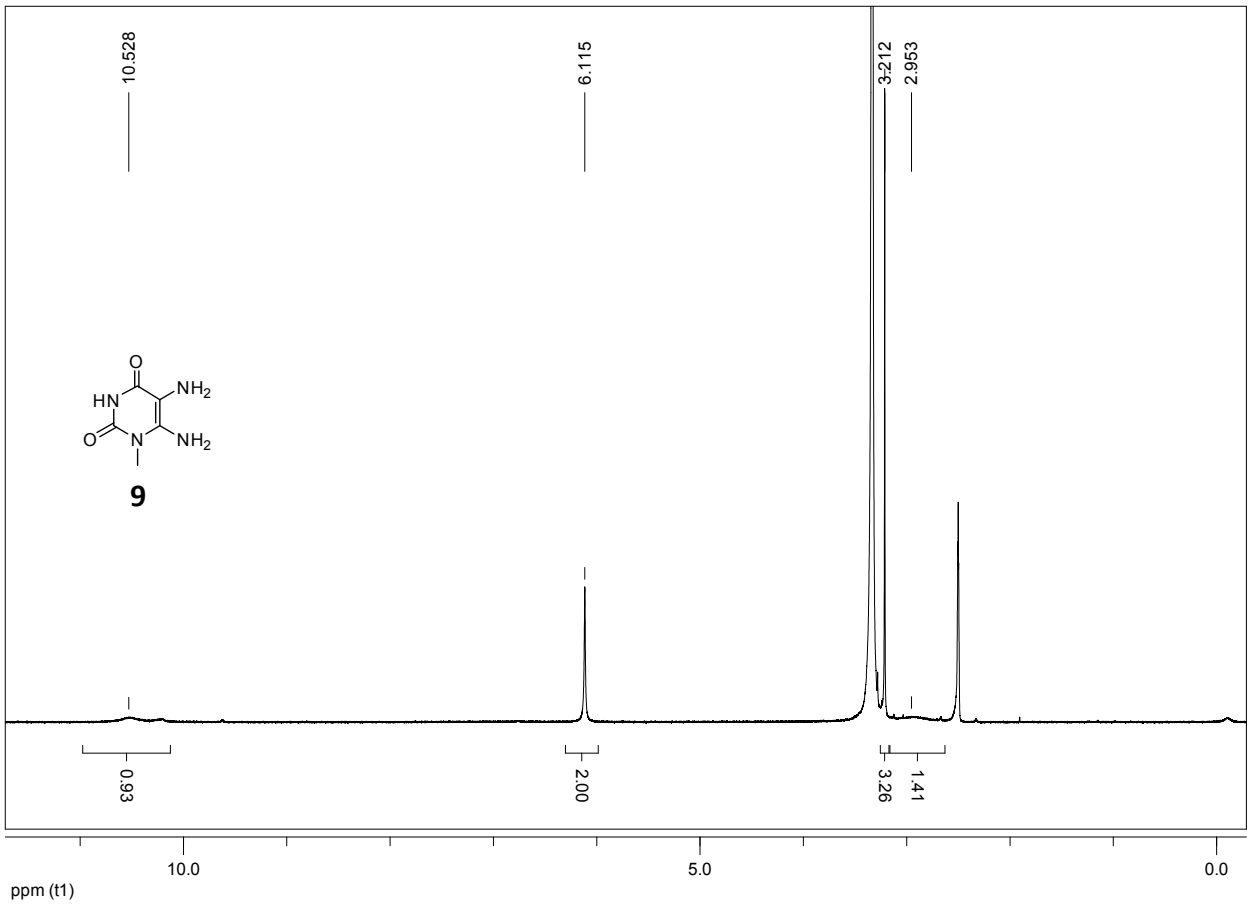
ppm (t1)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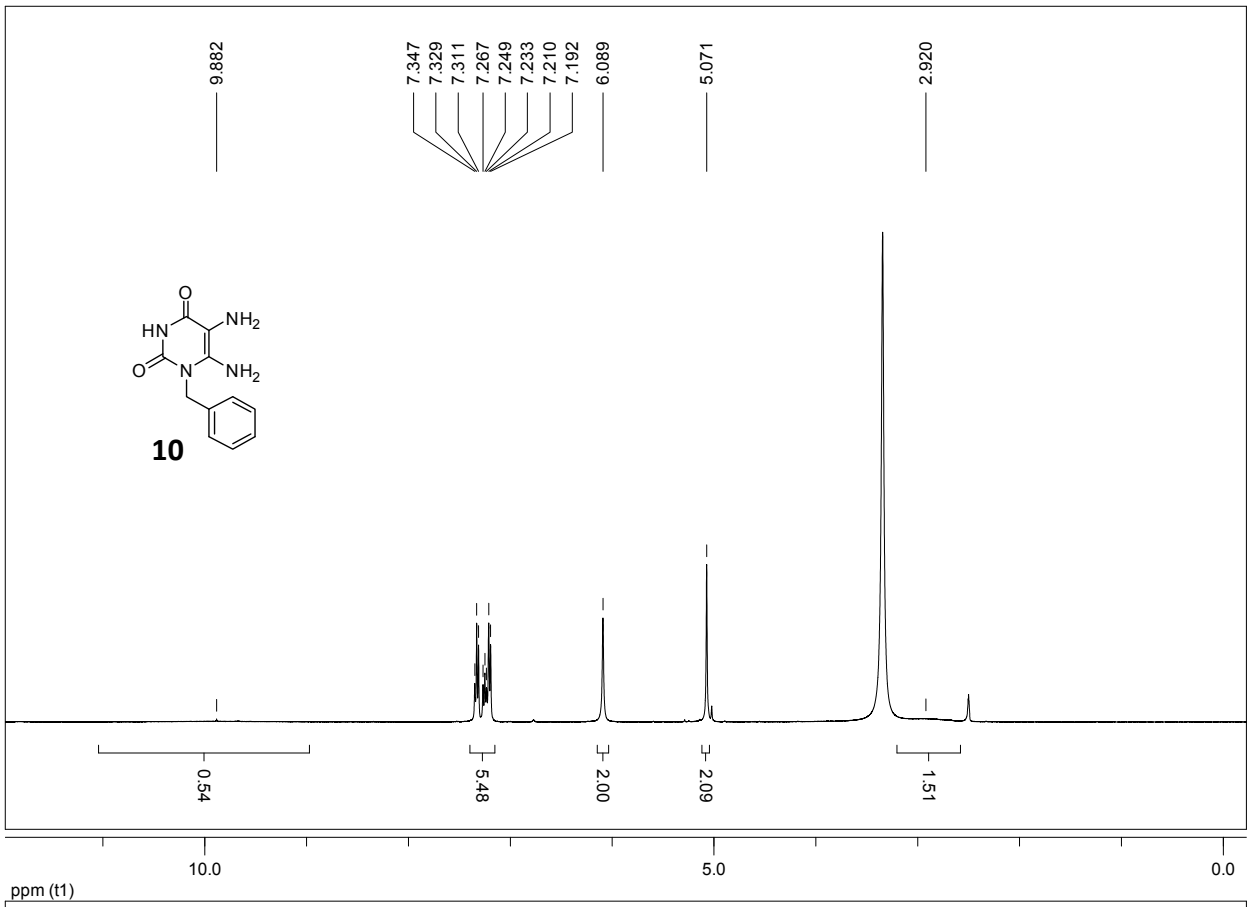
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O
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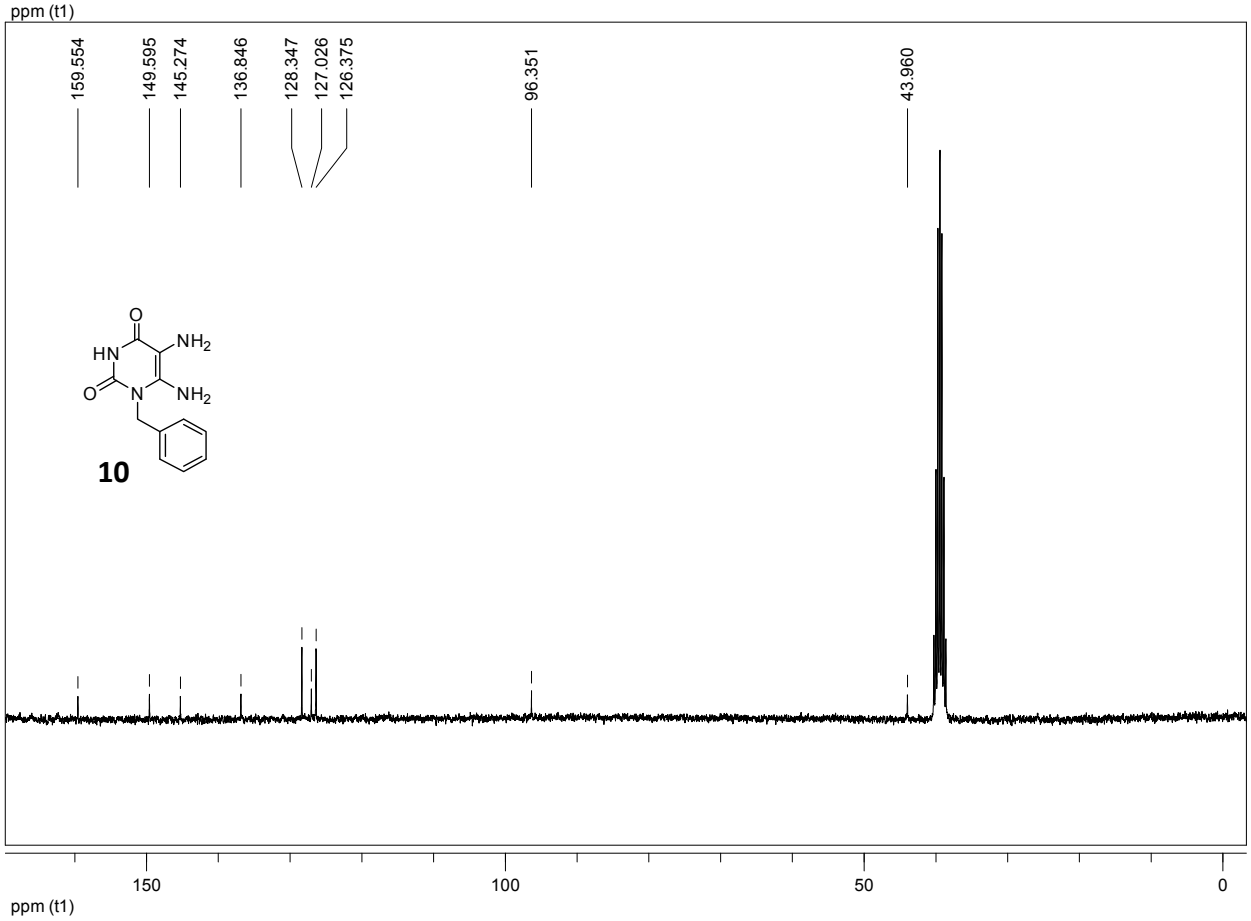
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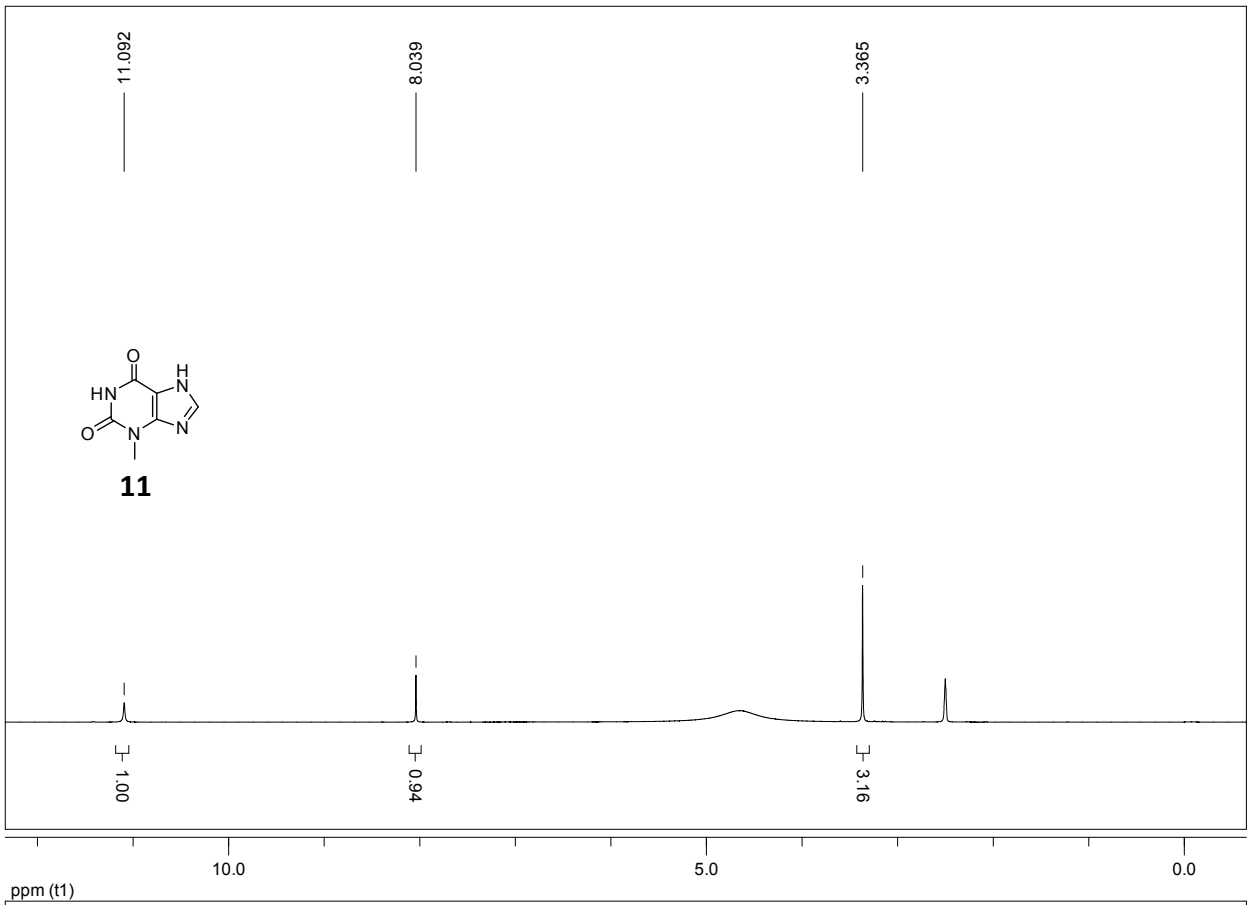
ppm (t1)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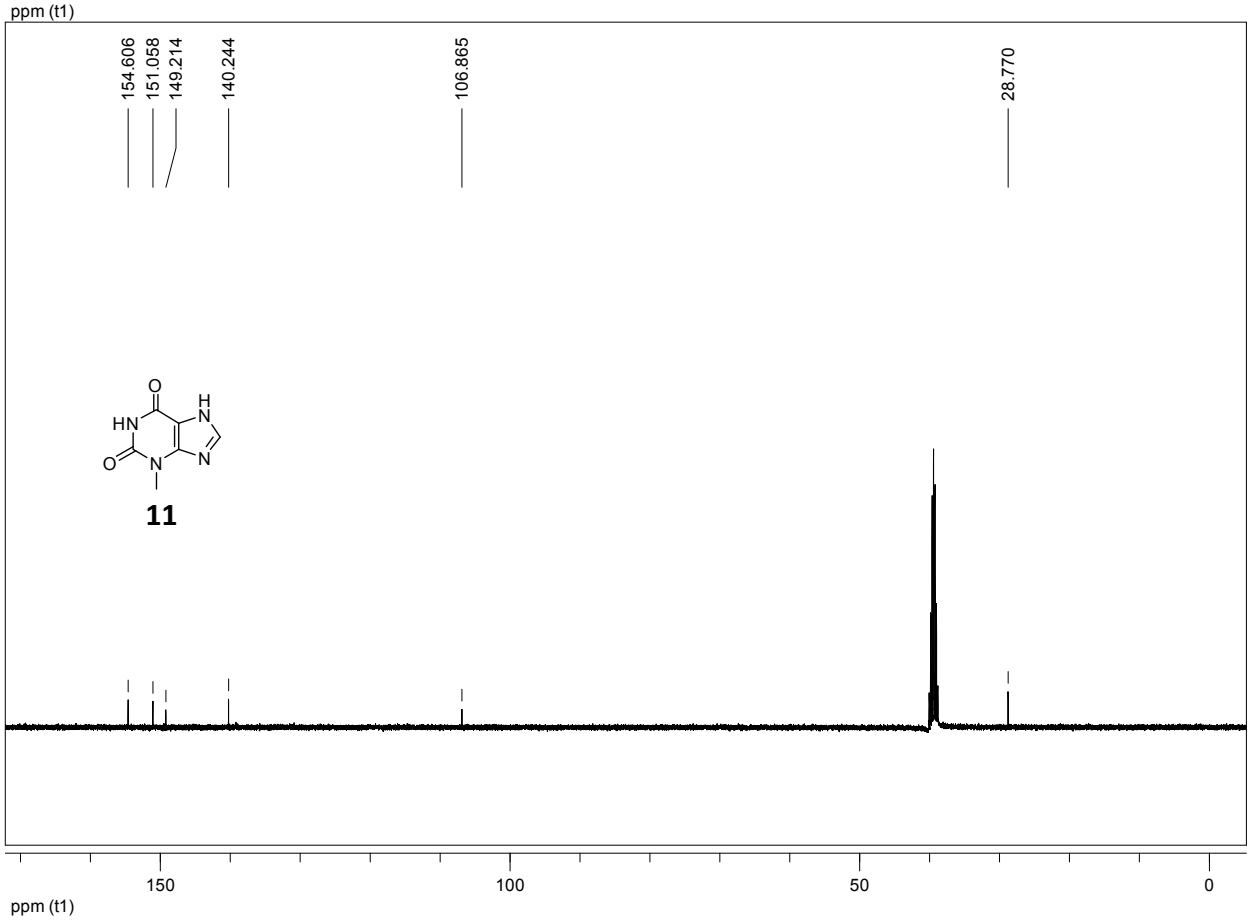
ppm (t1)

11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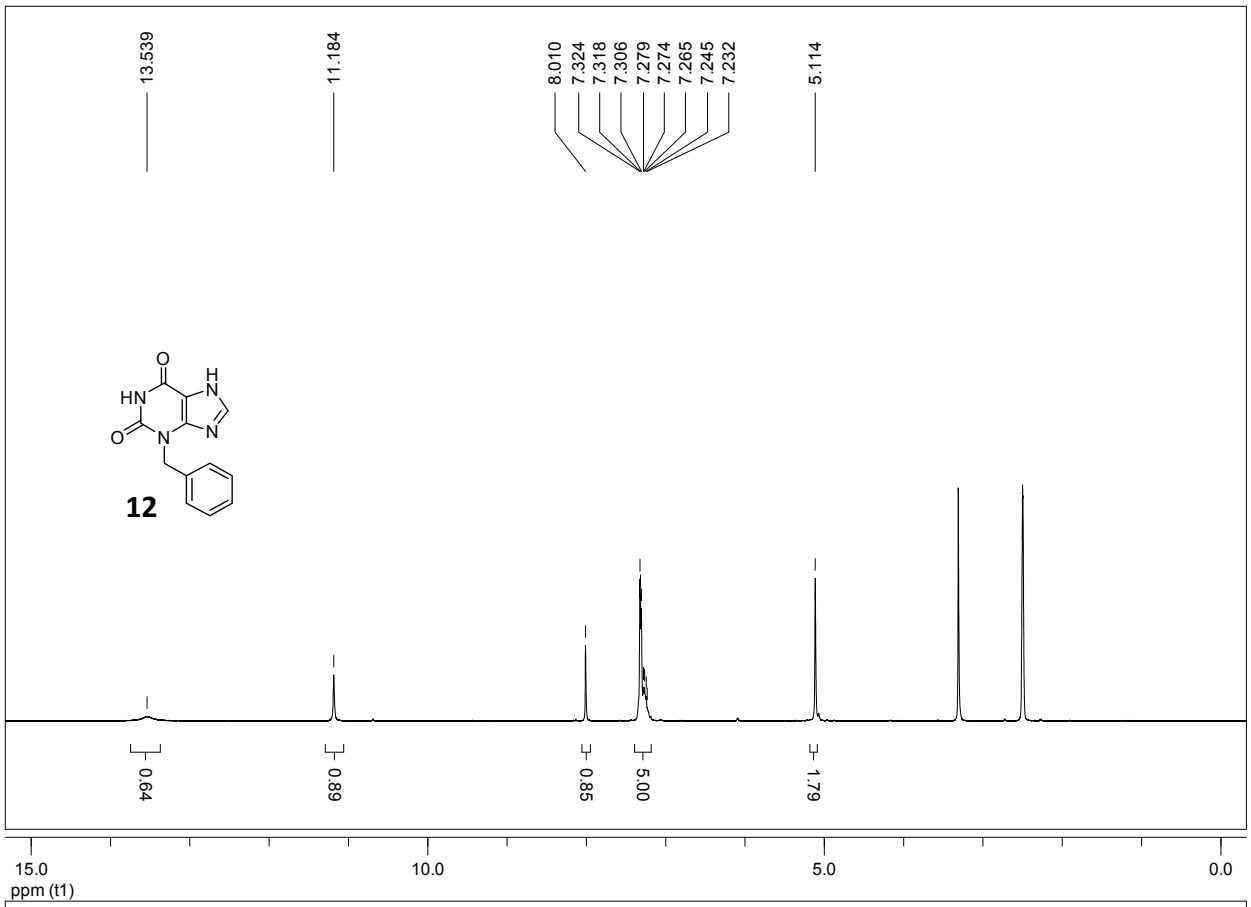
150
100
50
0
ppm (t1)

11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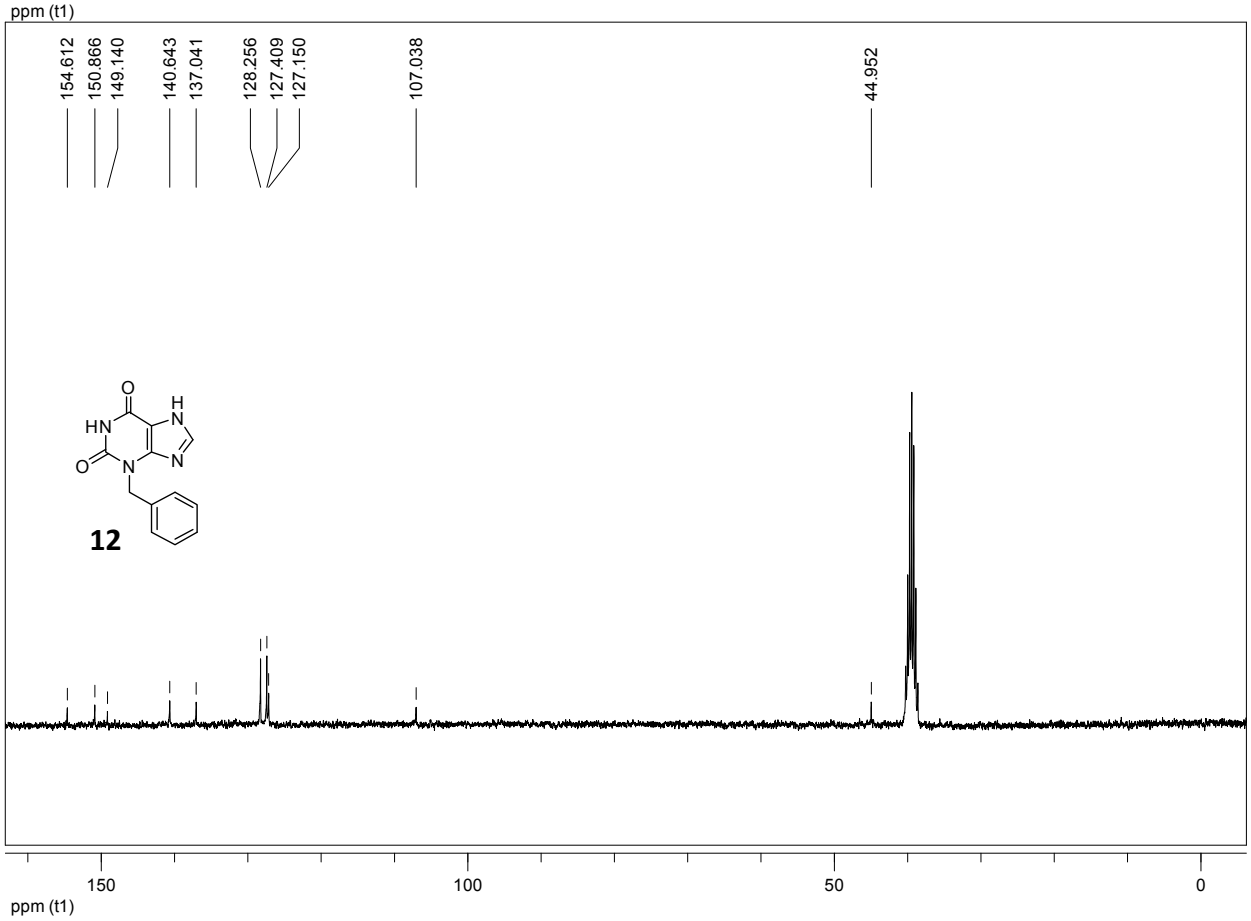
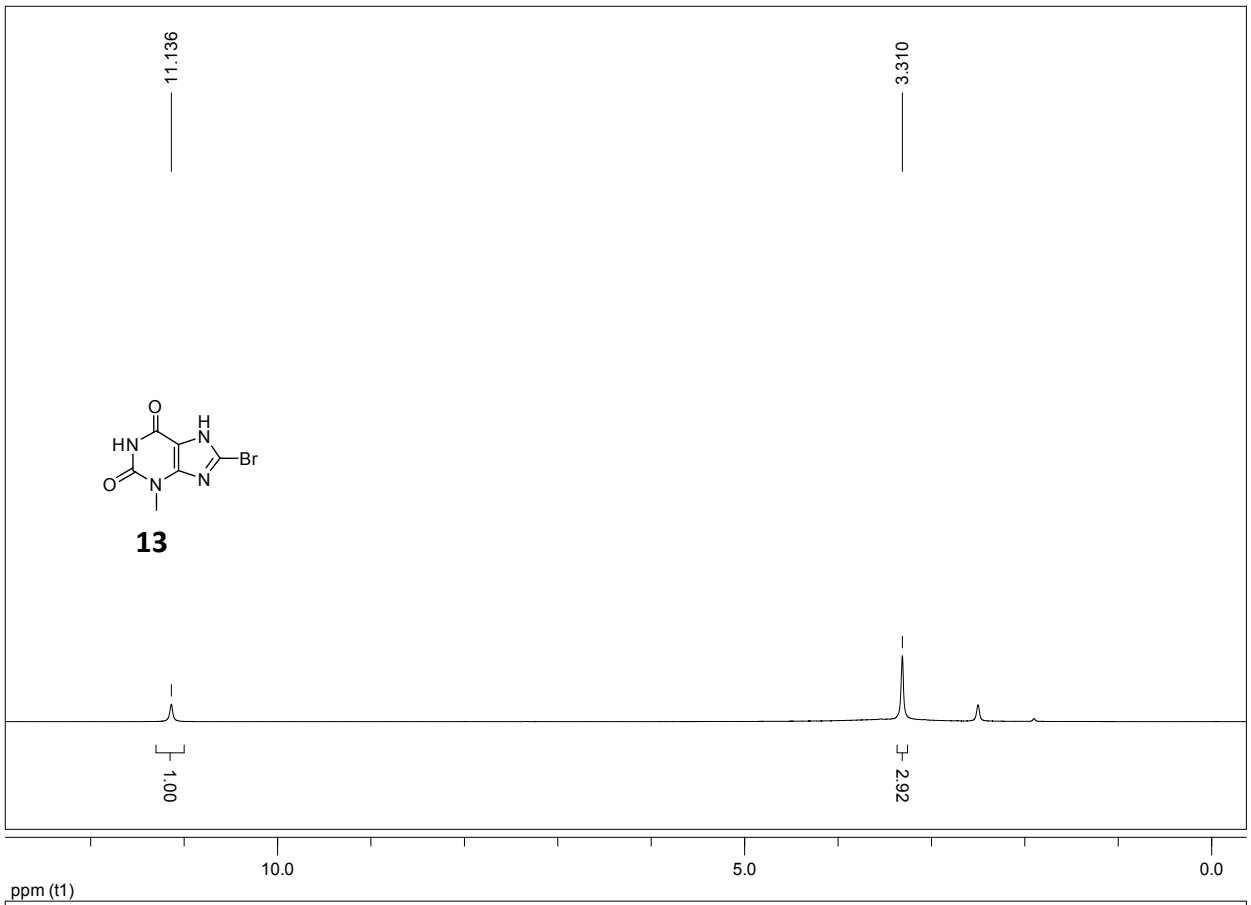
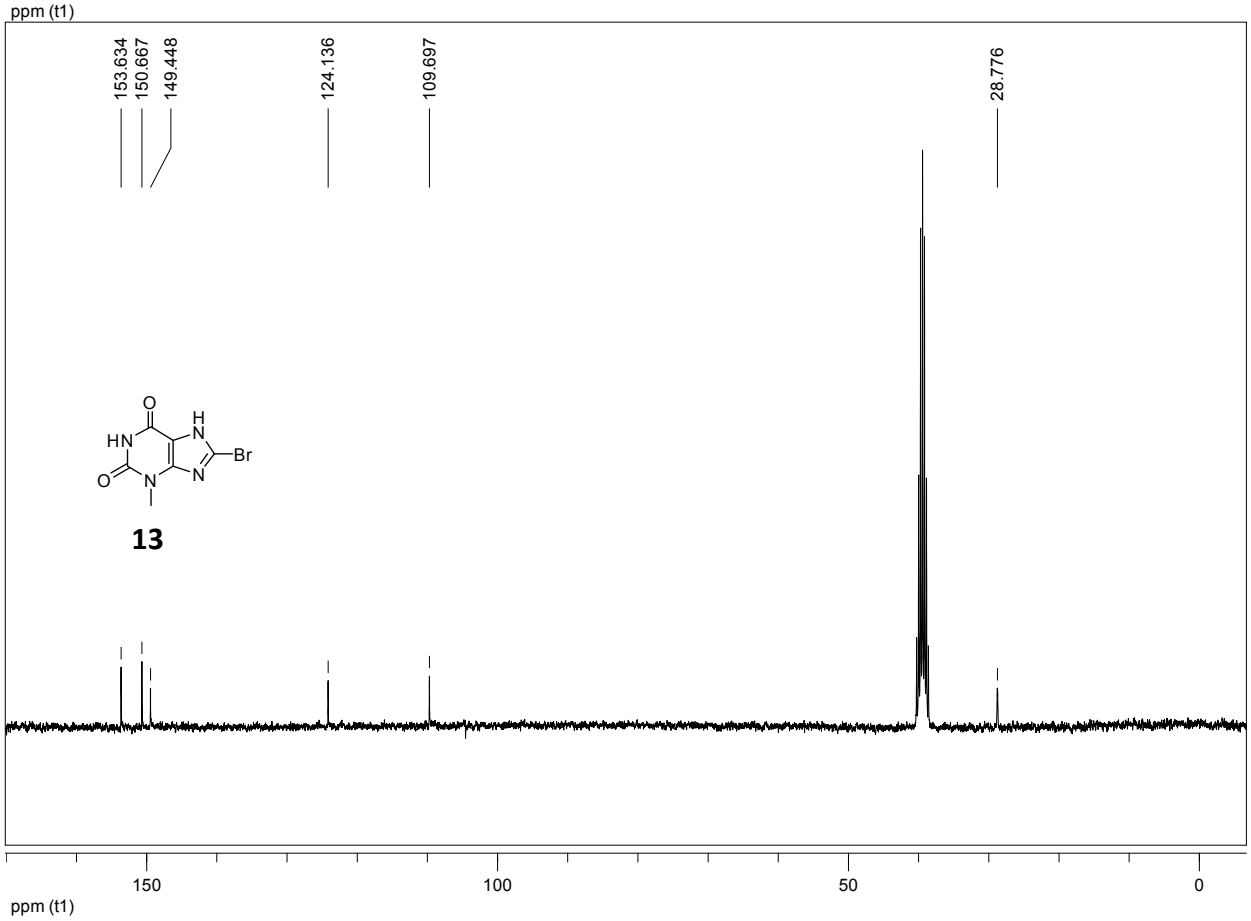
7.245
7.232
5.114
12
0.64
0.89
0.85
5.00
1.79
15.0
10.0
5.0
0.0
ppm (t1)

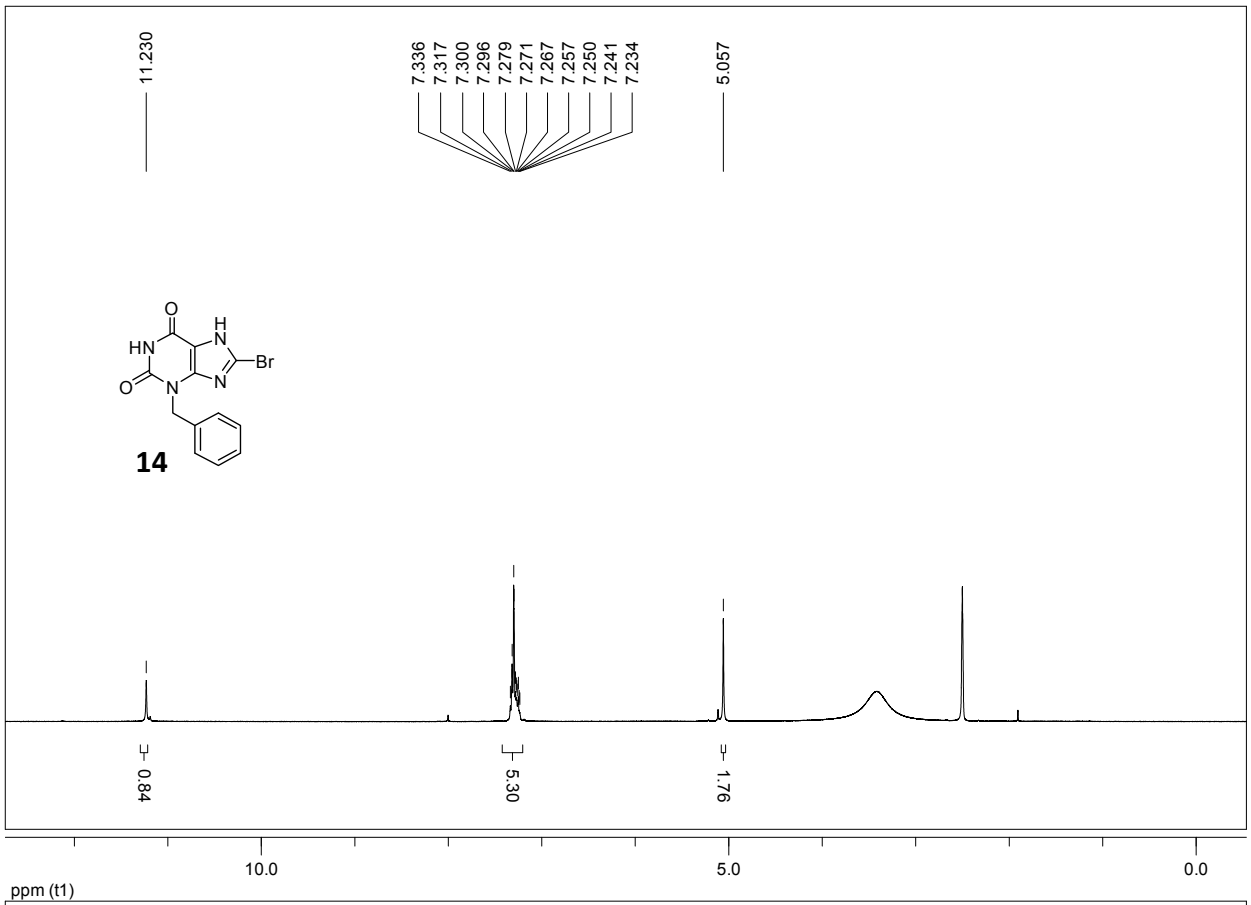

154.612
150.866
149.140
140.643
137.041
128.256
127.409
127.150
107.038
44.952
12
150
100
50
0
ppm (t1)

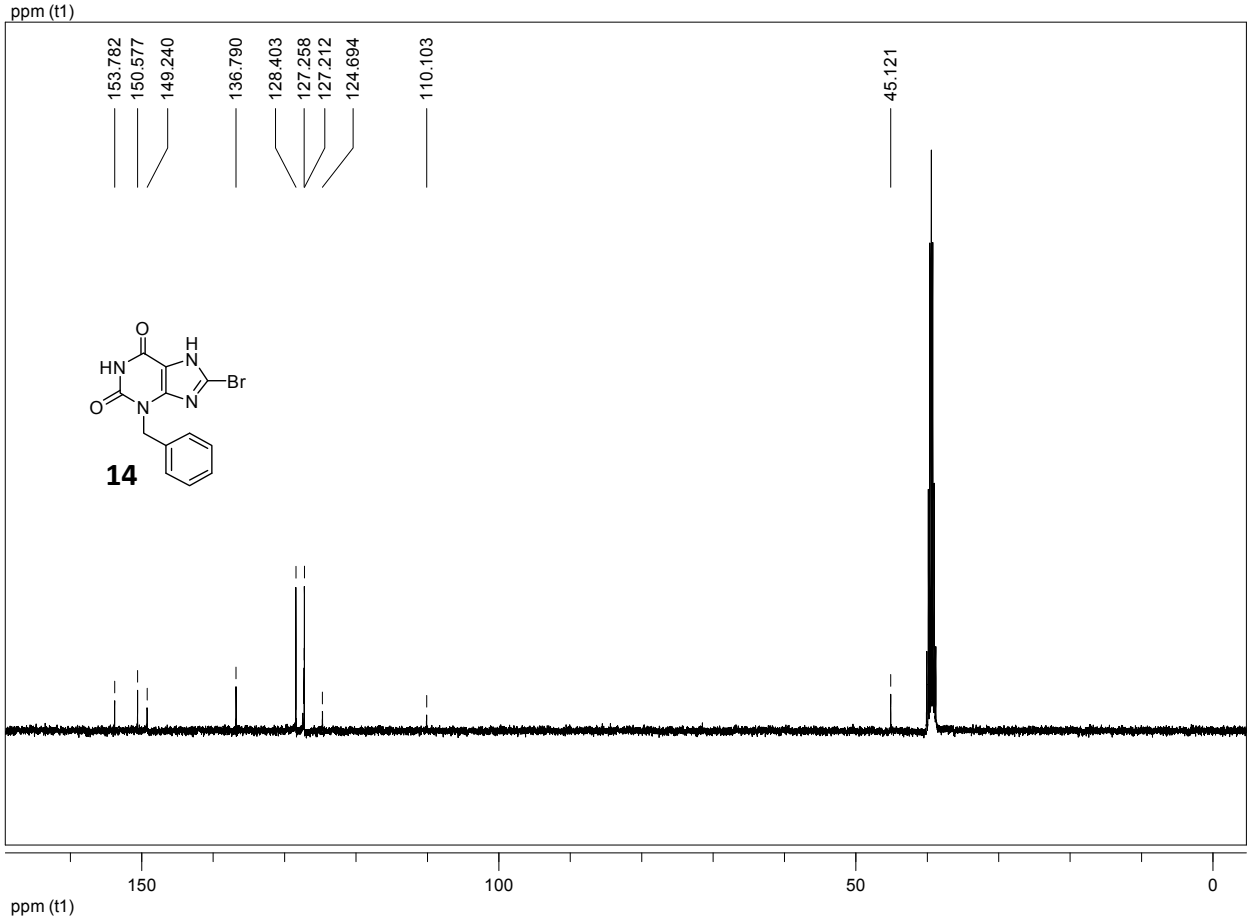

11.136
3.310
O
H
HN
N
Br
O
N
1.00
2.92
10.0
5.0
0.0
ppm (t1)

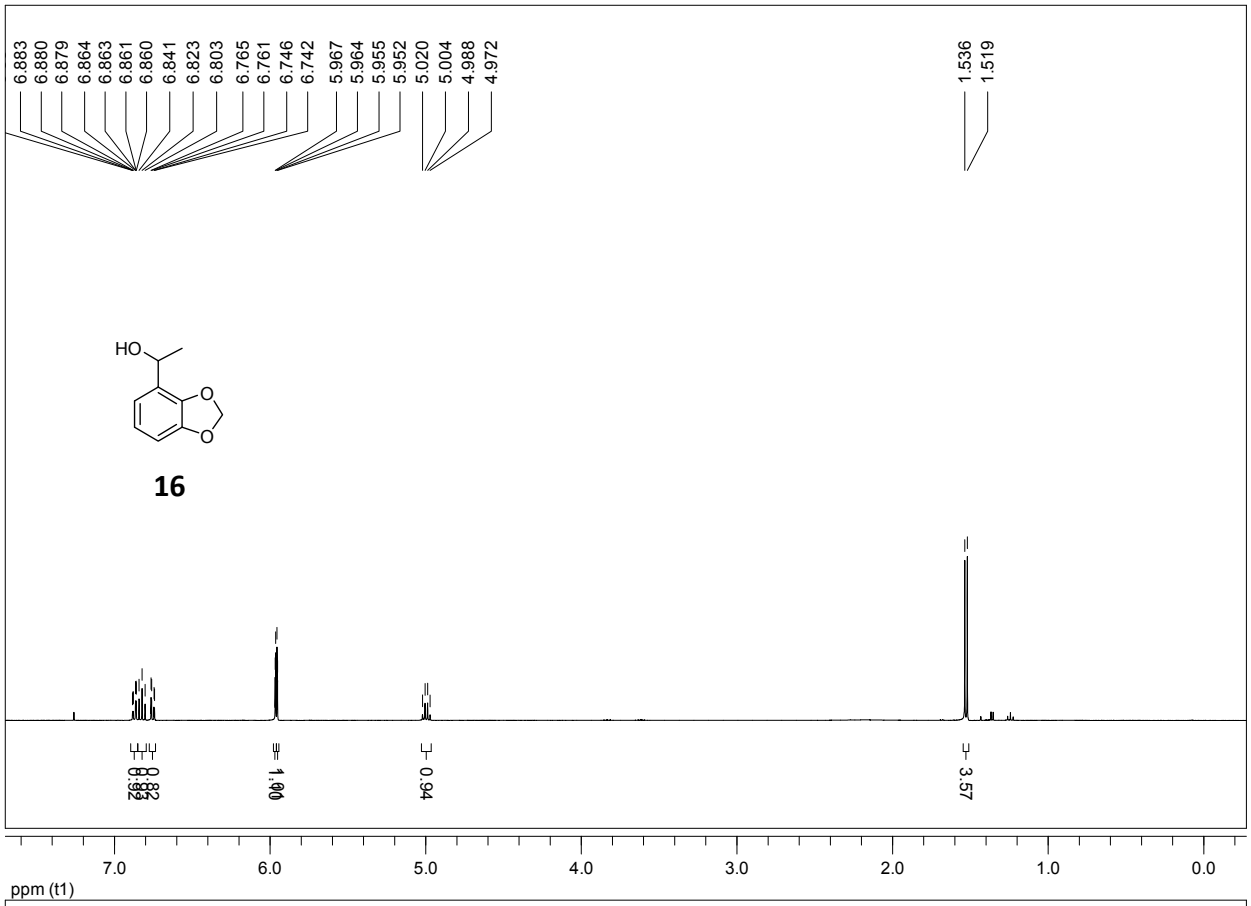
13

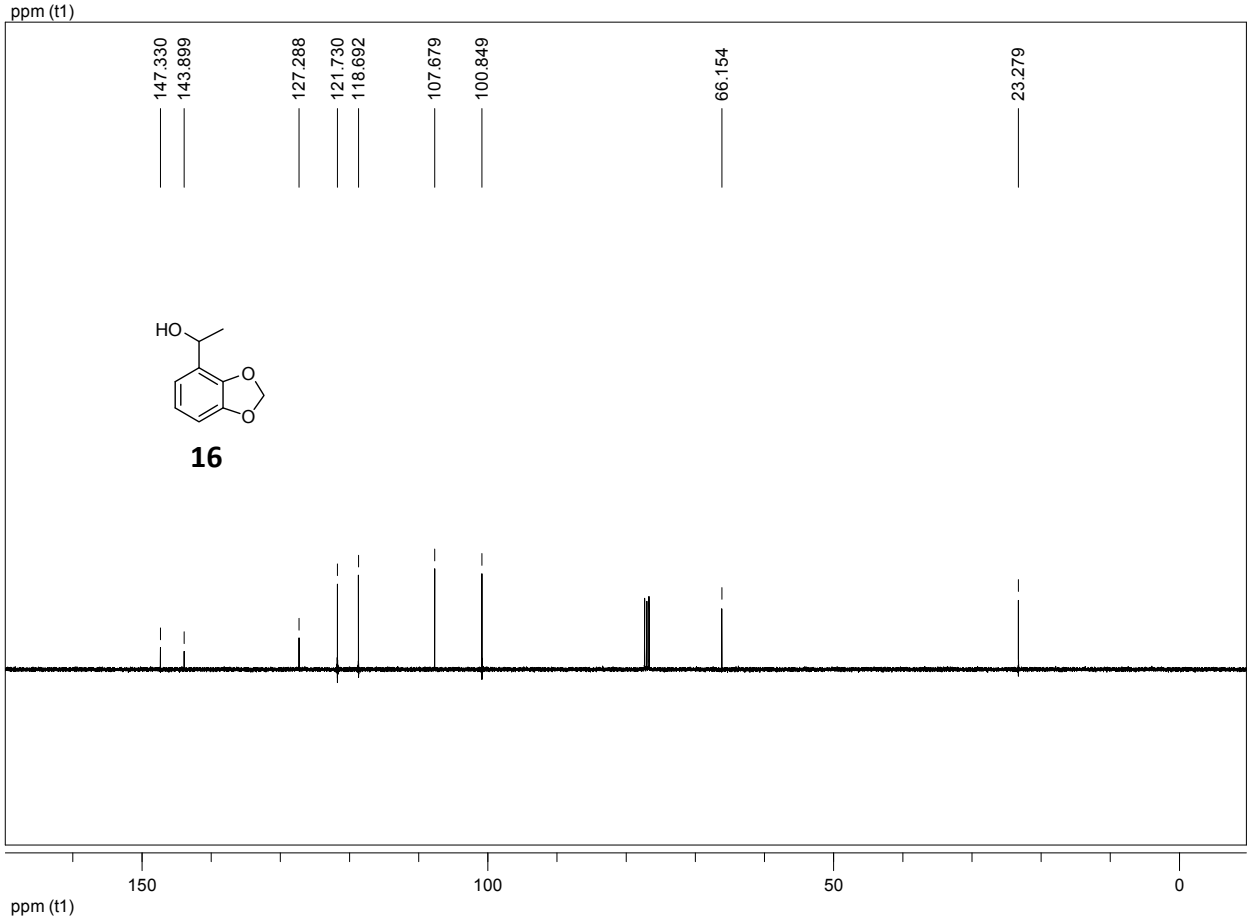

153.634
150.667
149.448
124.136
109.697
28.776
O
H
HN
N
Br
O
N
150
100
50
0
ppm (t1)

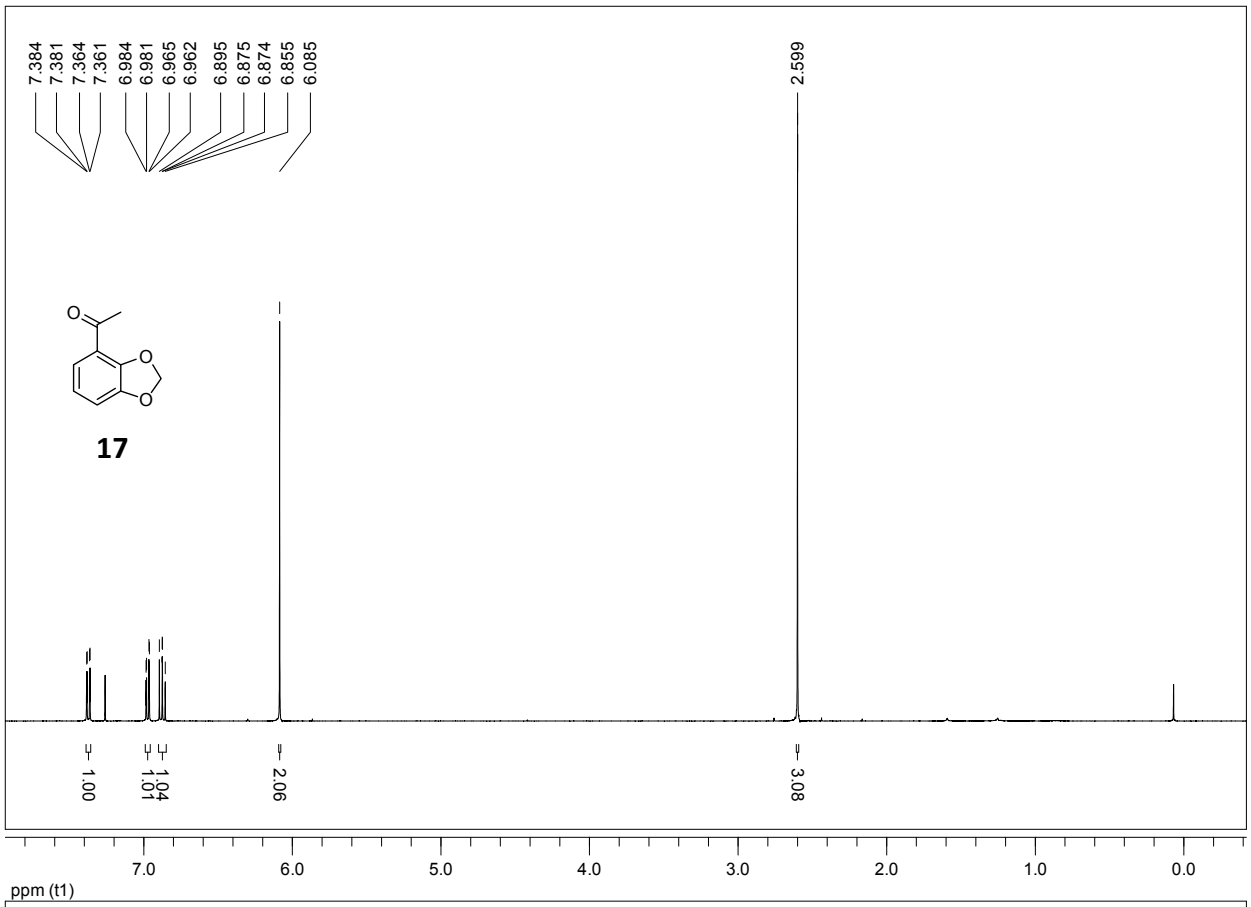
13


11.230
7.336
7.317
7.300
7.296
7.279
7.271
7.267
7.257
7.250
7.241
7.234
5.057
14
0.84
5.30
1.76
10.0
5.0
0.0
ppm (t1)

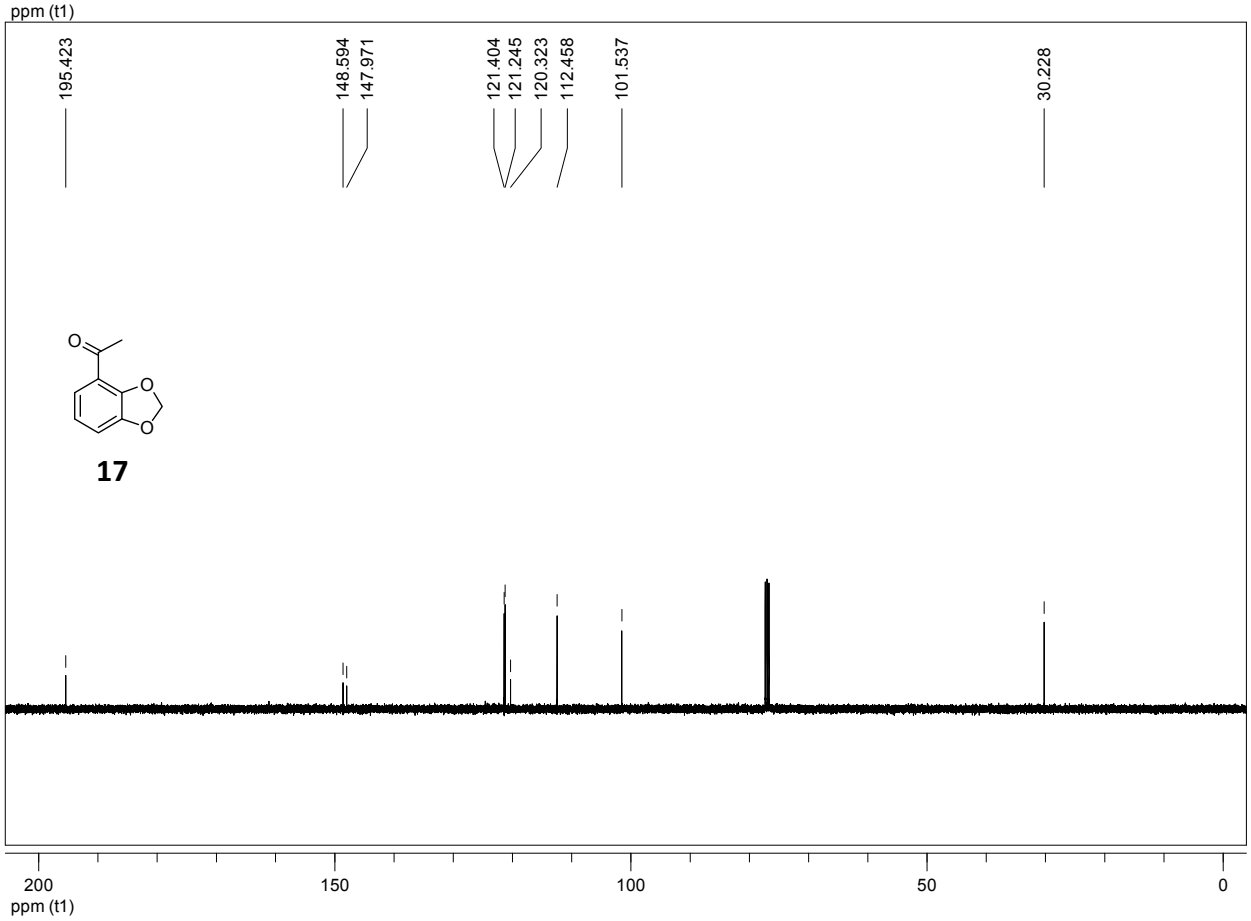

153.782
150.577
149.240
136.790
128.403
127.258
127.212
124.694
110.103
45.121
14
150
100
50
0
ppm (t1)


6.883
6.880
6.879
6.864
6.863
6.861
6.860
6.841
6.823
6.803
6.765
6.761
6.746
6.742
5.967
5.964
5.955
5.952
5.020
5.004
4.988
4.972
1.536
1.519
HO
O
O
16
1.00
0.94
3.57
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

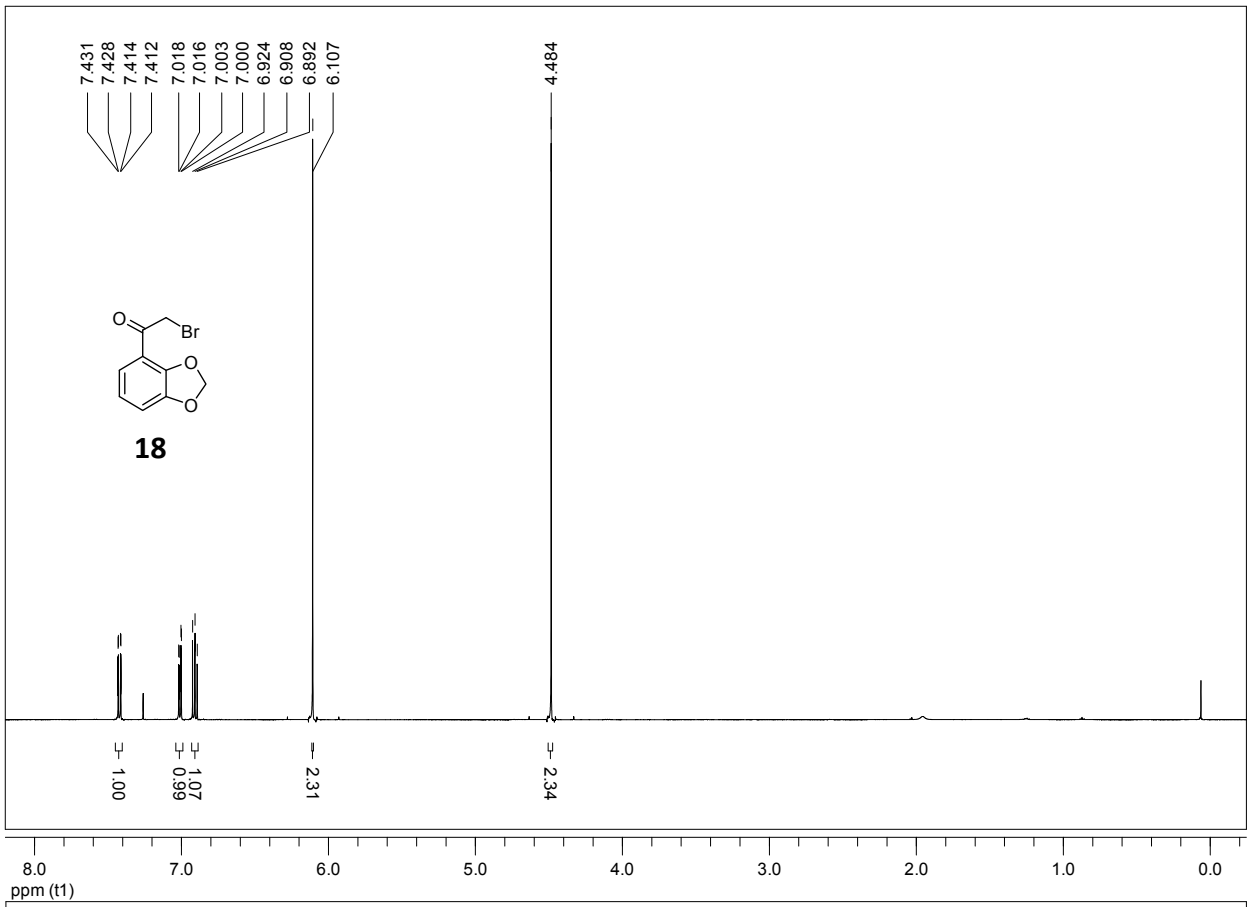

147.330
143.899
127.288
121.730
118.692
107.679
100.849
66.154
23.279
HO
O
O
16
150
100
50
0
ppm (t1)

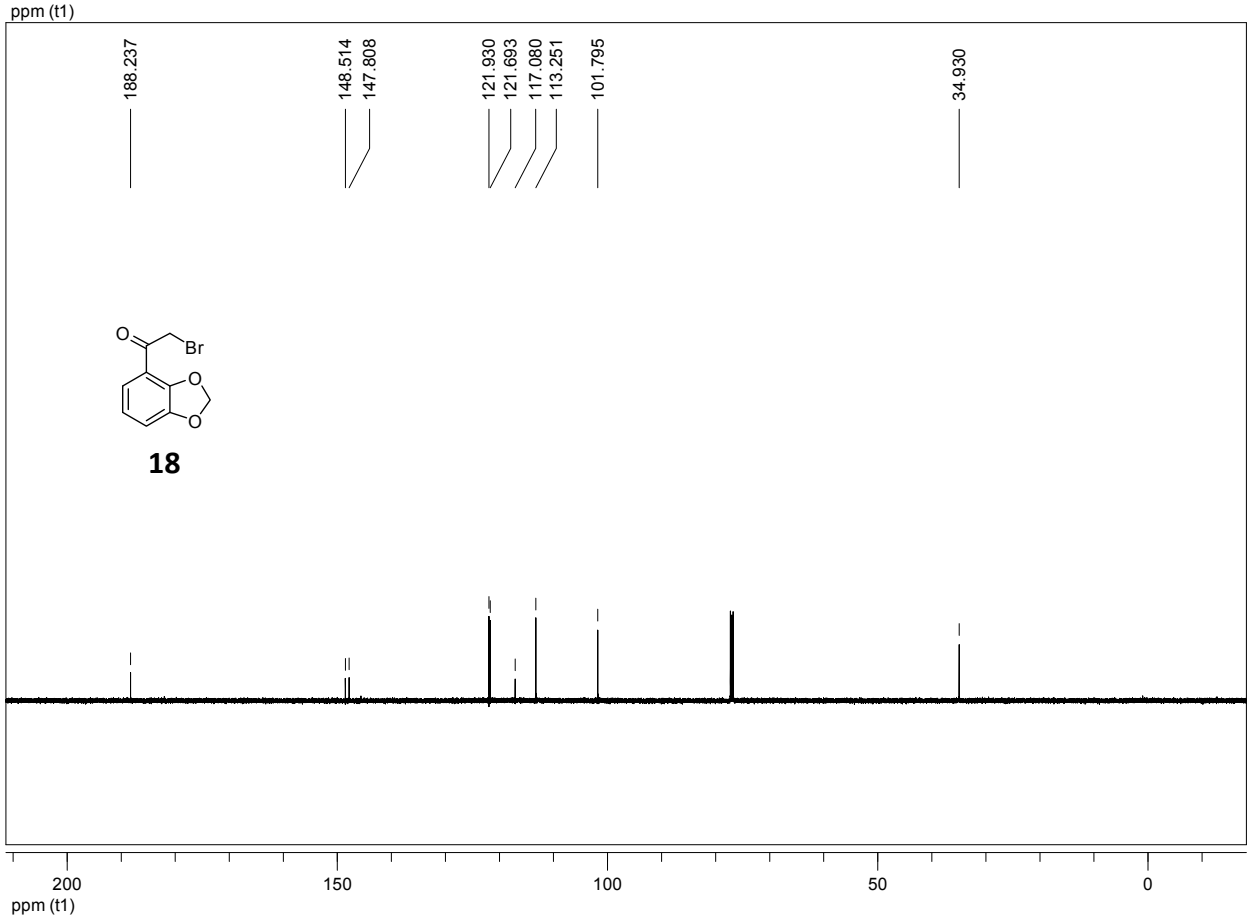

7.384
7.381
7.364
7.361
6.984
6.981
6.965
6.962
6.895
6.875
6.874
6.855
6.085
2.599
1.00
1.04
1.01
2.06
3.08
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

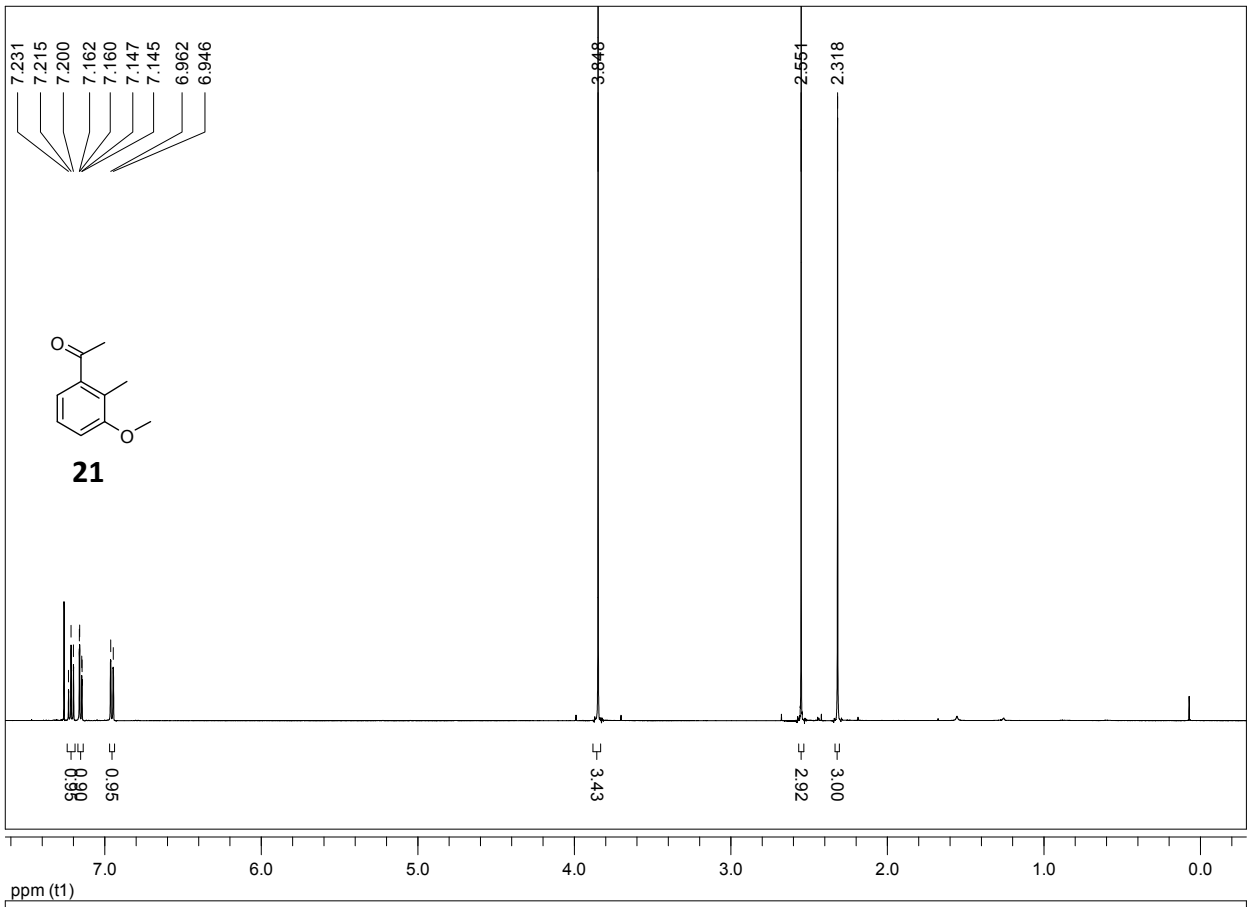
17

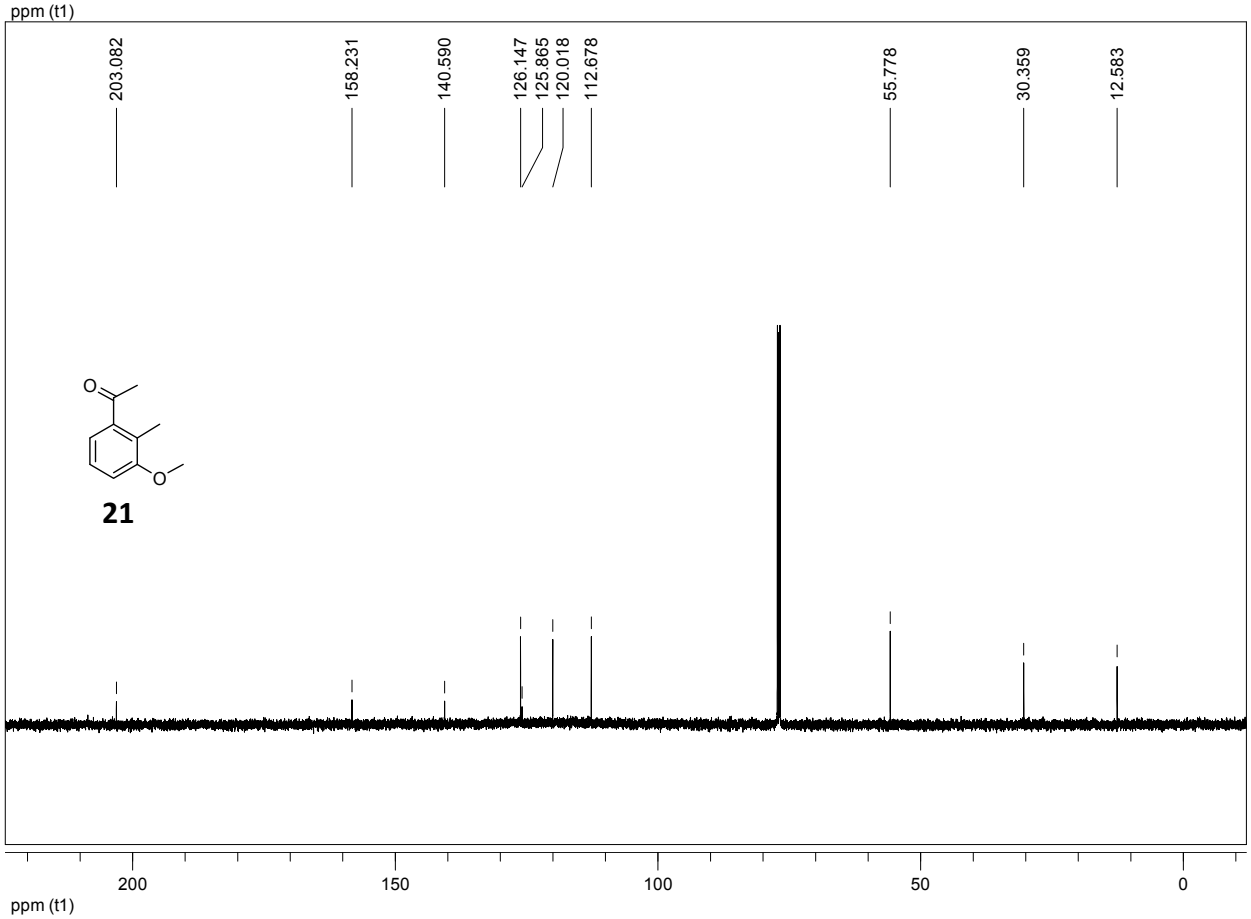

195.423
148.594
147.971
121.404
121.245
120.323
112.458
101.537
30.228
200
150
100
50
0
ppm (t1)

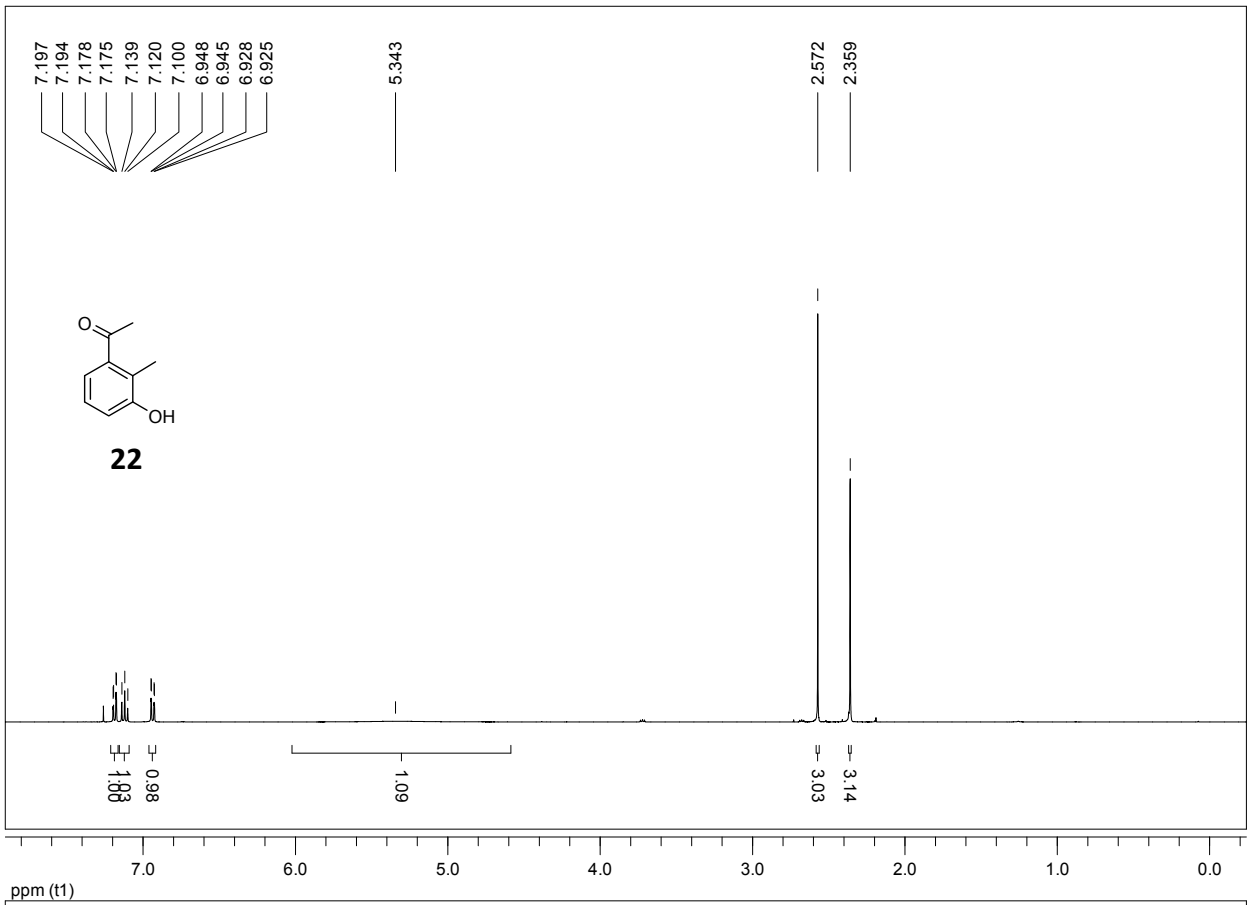
17

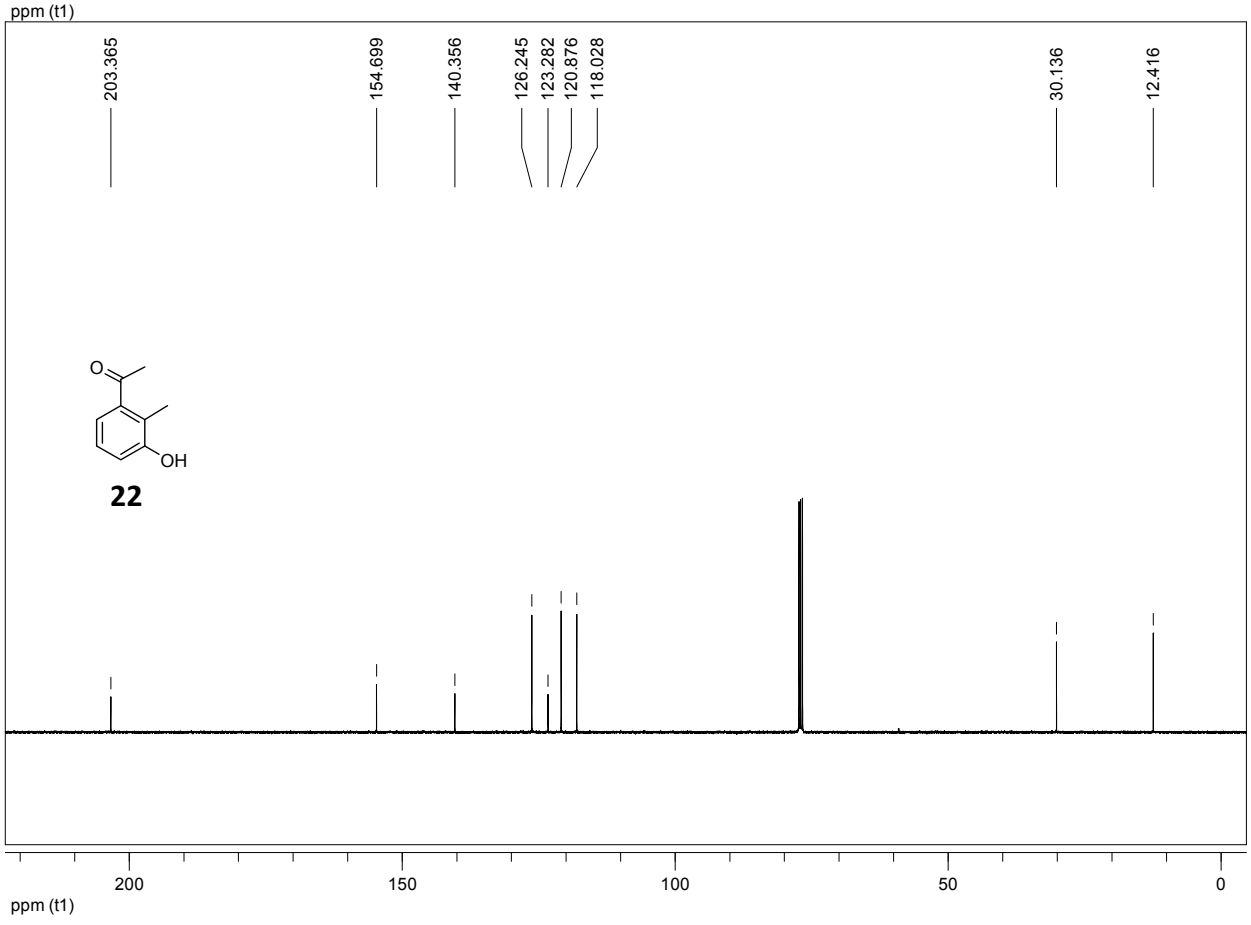

7.431
7.428
7.414
7.412
7.018
7.016
7.003
7.000
6.924
6.908
6.892
6.107
4.484
O
Br
O
O
18
1.00
0.99
1.07
2.31
2.34
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

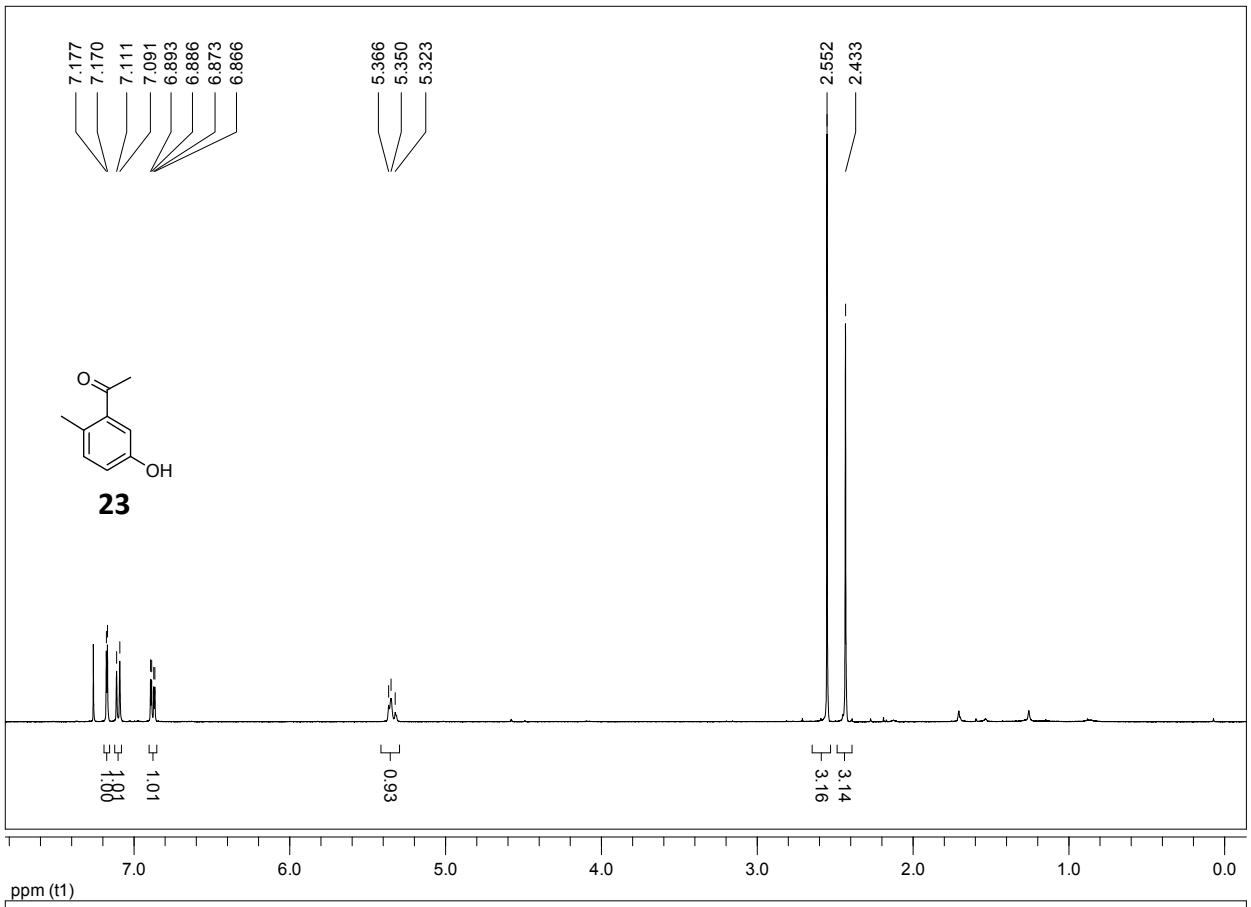

188.237
148.514
147.808
121.930
121.693
117.080
113.251
101.795
34.930
O
Br
O
O
18
200
150
100
50
0
ppm (t1)

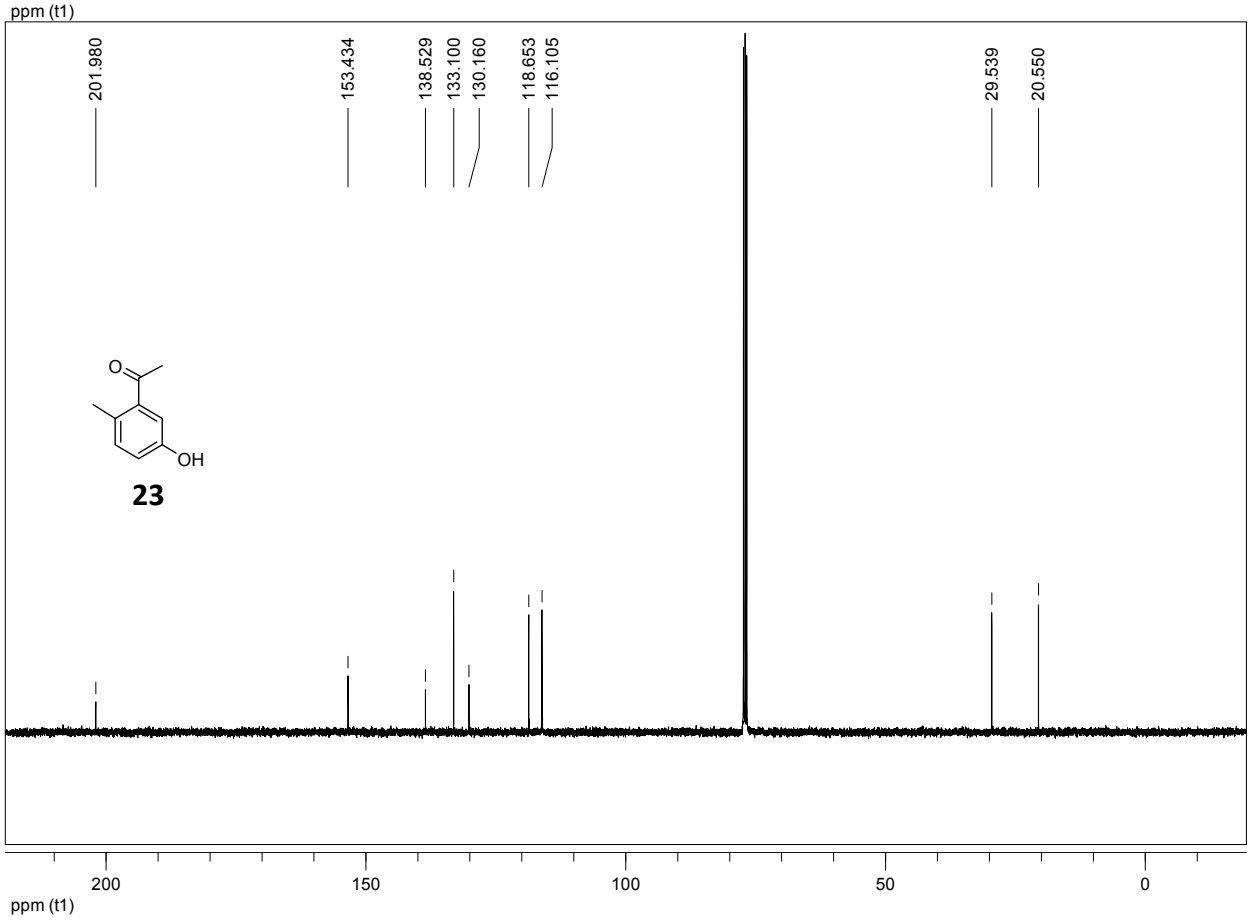

7.231
7.215
7.200
7.162
7.160
7.147
7.145
6.962
6.946
3.848
2.551
2.318
O
O
21
0.95
3.43
2.92
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

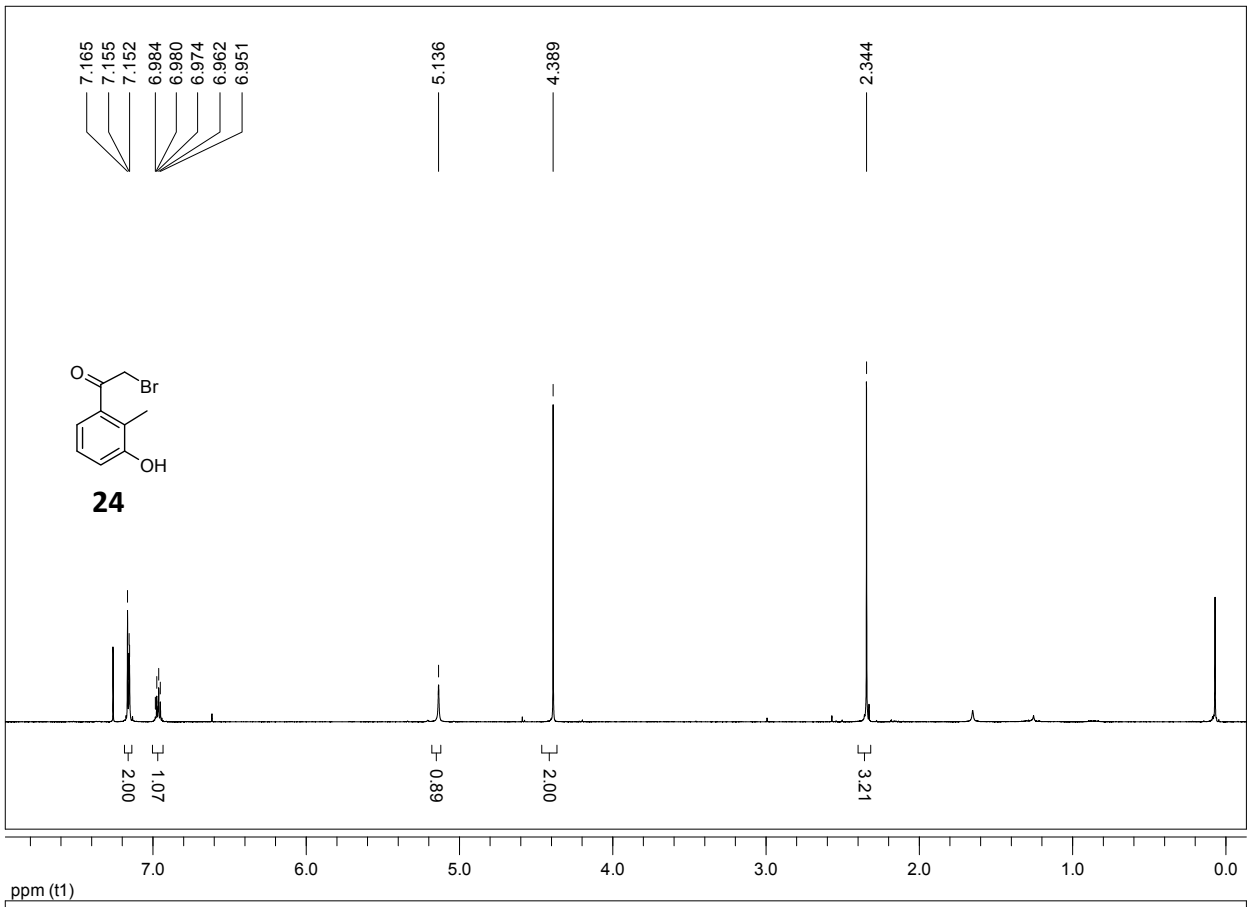

203.082
158.231
140.590
126.147
125.865
120.018
112.678
55.778
30.359
12.583
O
O
21
200
150
100
50
0
ppm (t1)

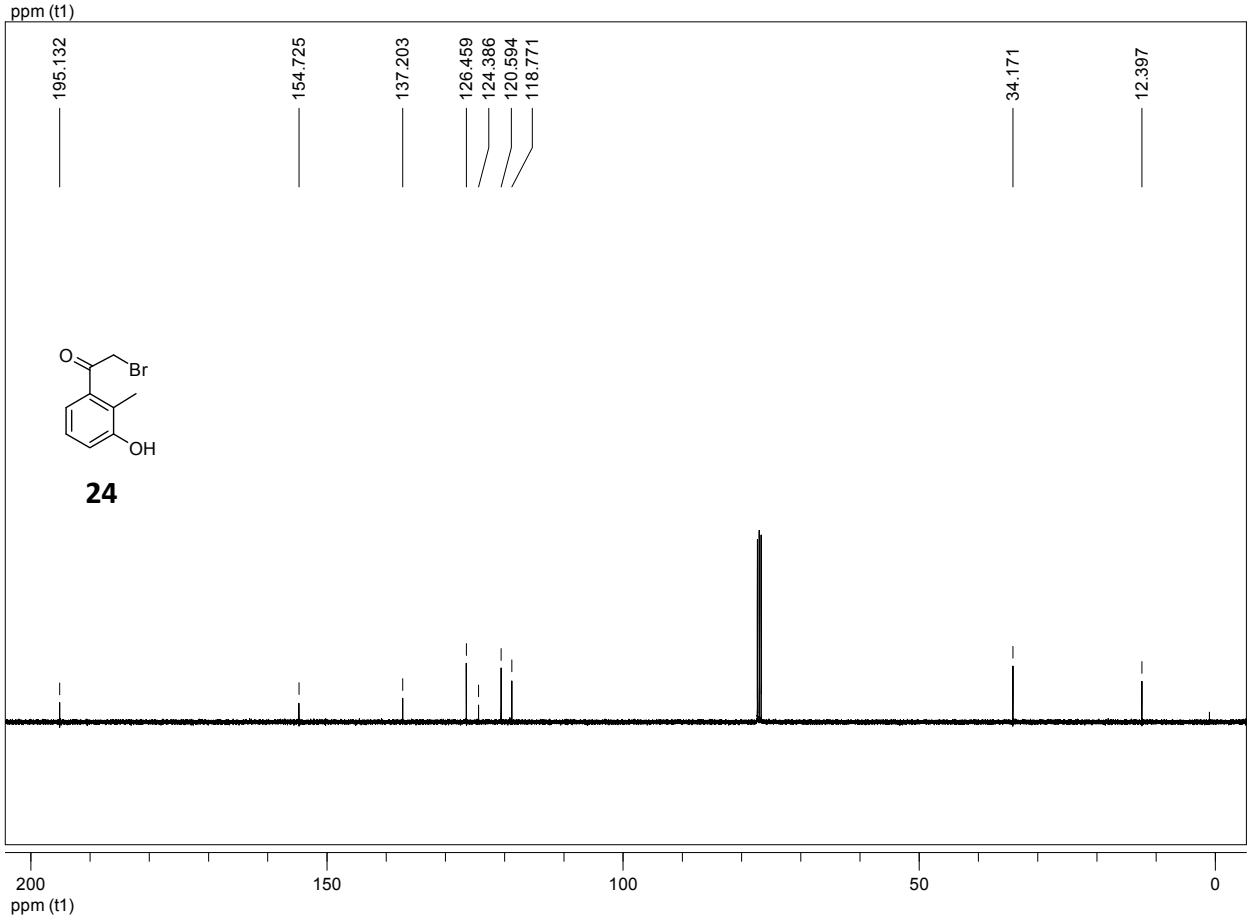

7.197
7.194
7.178
7.175
7.139
7.120
7.100
6.948
6.945
6.928
6.925
5.343
2.572
2.359
O
OH
22
1.00
1.03
0.98
1.09
3.03
3.14
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

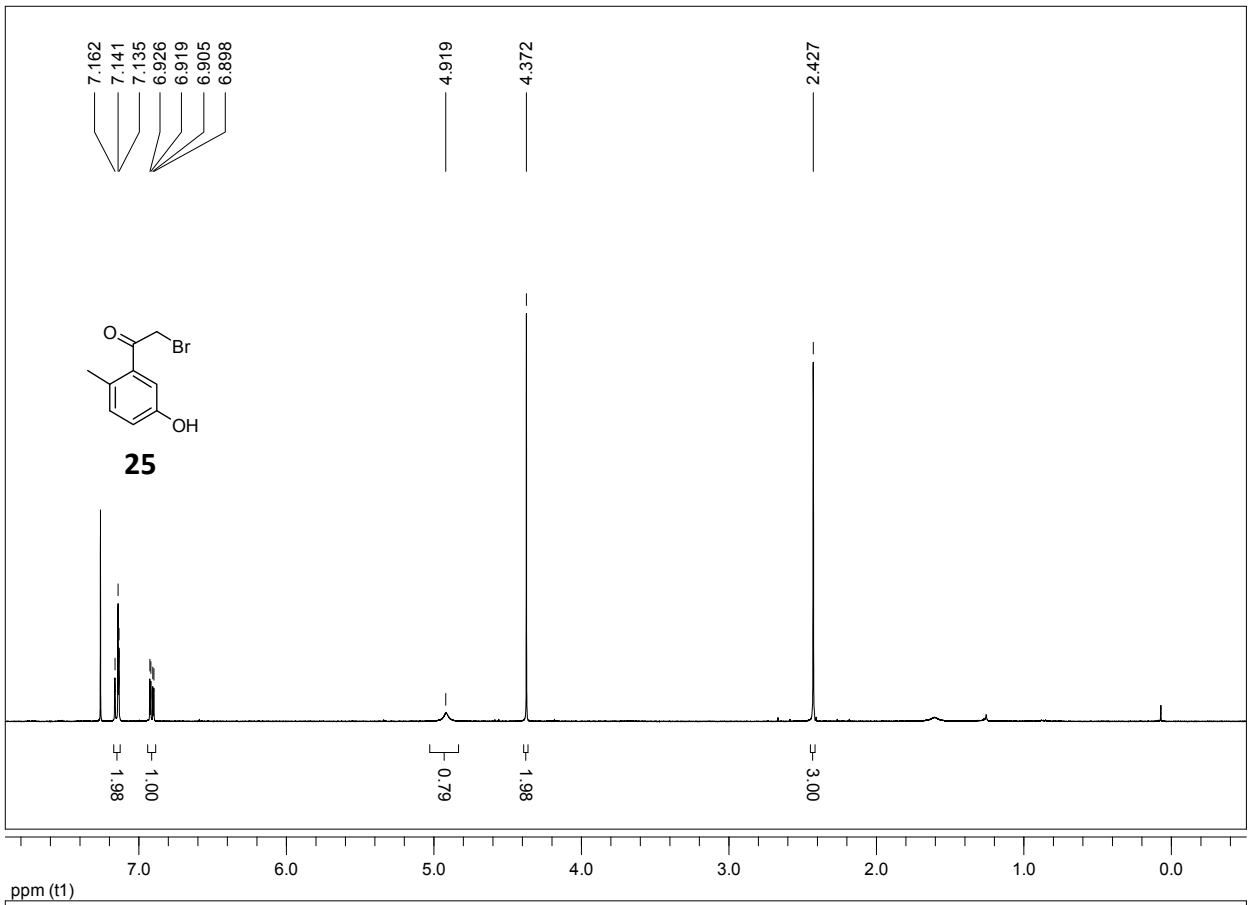

203.365
154.699
140.356
126.245
123.282
120.876
118.028
30.136
12.416
O
OH
22
200
150
100
50
0
ppm (t1)

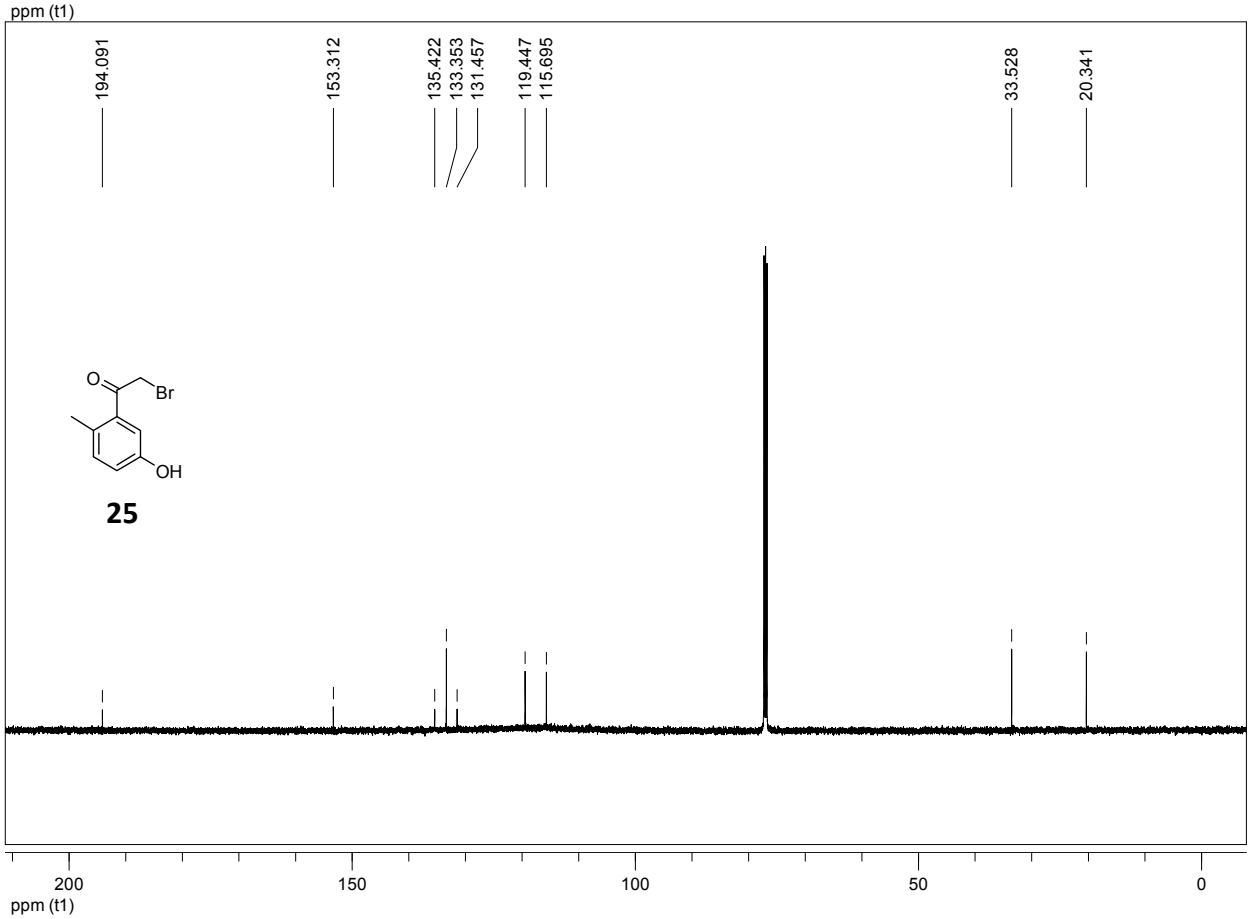

7.177
7.170
7.111
7.091
6.893
6.886
6.873
6.866
5.366
5.350
5.323
2.552
2.433
O
OH
23
1.00
1.01
0.93
3.16
3.14
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

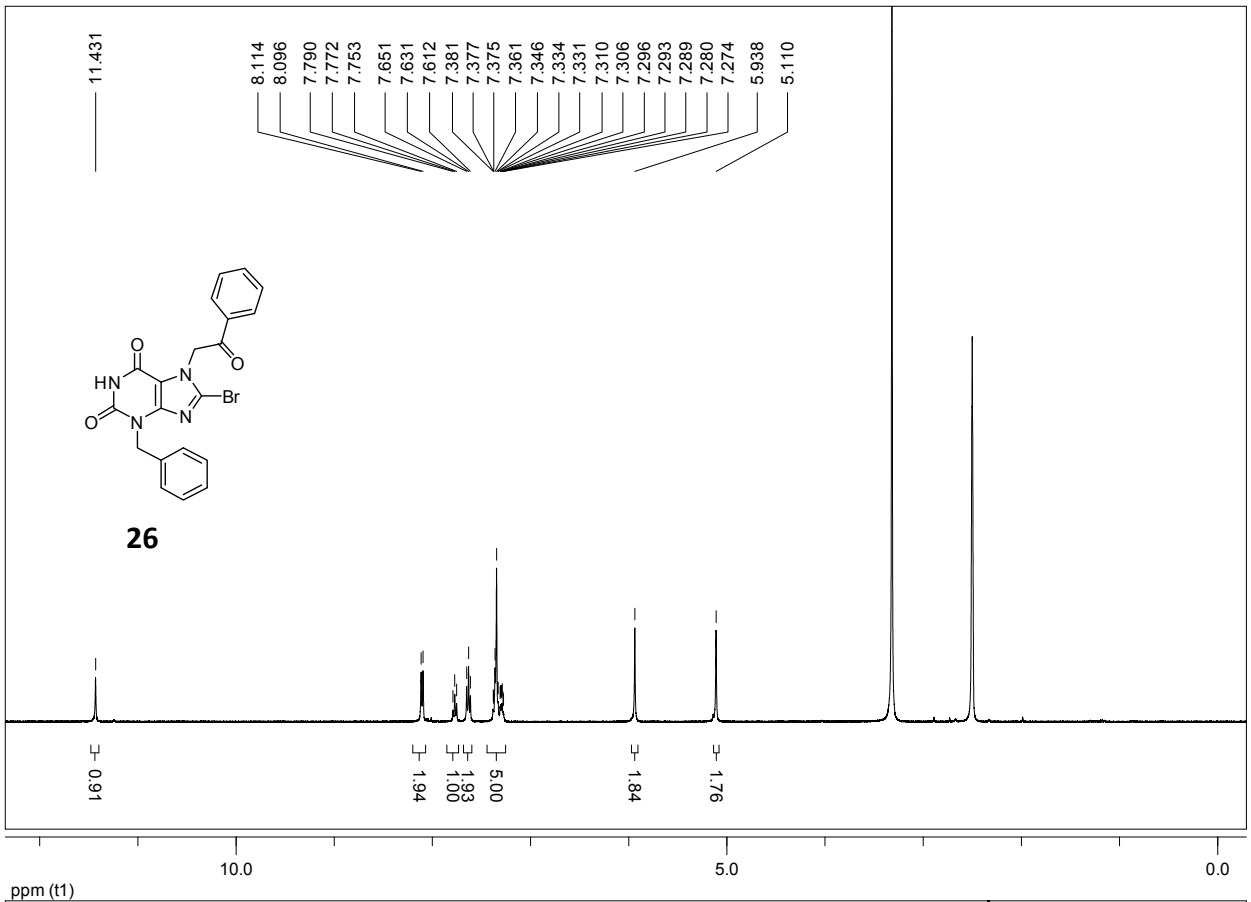

201.980
153.434
138.529
133.100
130.160
118.653
116.105
29.539
20.550
O
OH
23
200
150
100
50
0
ppm (t1)

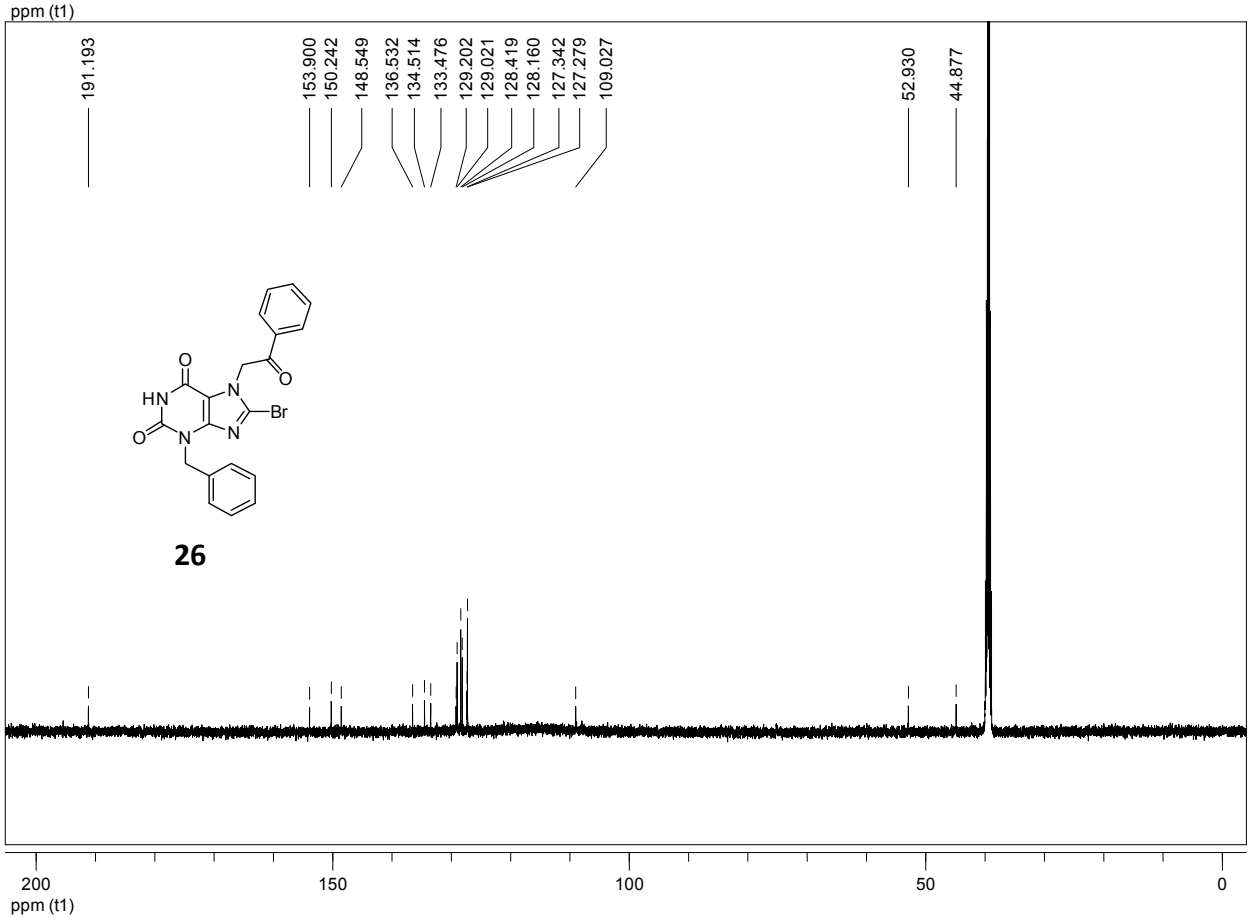

7.165
7.155
7.152
6.984
6.980
6.974
6.962
6.951
5.136
4.389
2.344
O
Br
OH
24
2.00
1.07
0.89
2.00
3.21
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

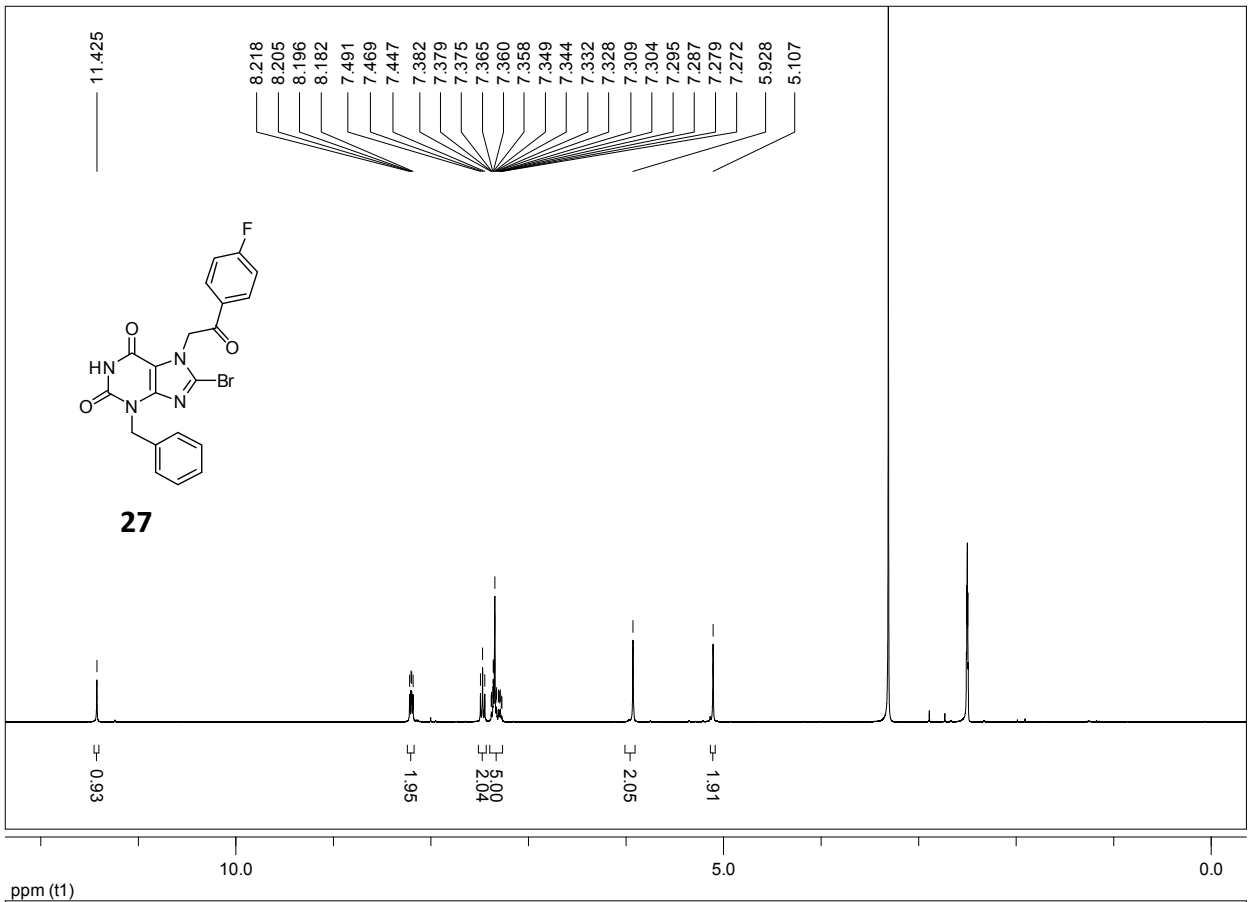

195.132
154.725
137.203
126.459
124.386
120.594
118.771
34.171
12.397
O
Br
OH
24
200
150
100
50
0
ppm (t1)


7.162
7.141
7.135
6.926
6.919
6.905
6.898
4.919
4.372
2.427
O
Br
OH
25
1.98
1.00
0.79
1.98
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

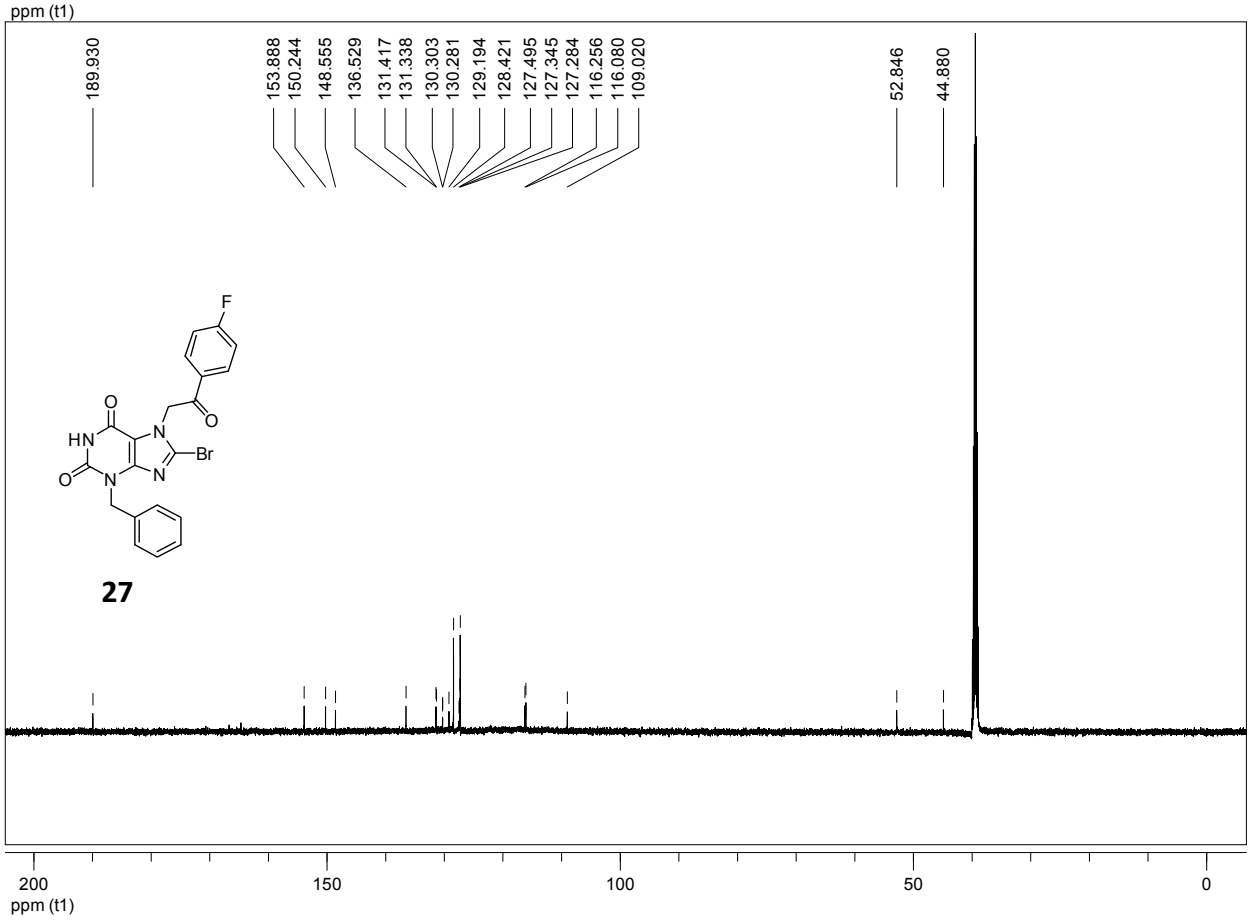

194.091
153.312
135.422
133.353
131.457
119.447
115.695
33.528
20.341
O
Br
OH
25
200
150
100
50
0
ppm (t1)


11.431
8.114
8.096
7.790
7.772
7.753
7.651
7.631
7.612
7.381
7.377
7.375
7.361
7.346
7.334
7.331
7.310
7.306
7.296
7.293
7.289
7.280
7.274
5.938
5.110
HN
O
N
Br
26
0.91
1.94
1.00
1.03
5.00
1.84
1.76
10.0
5.0
0.0
ppm (t1)

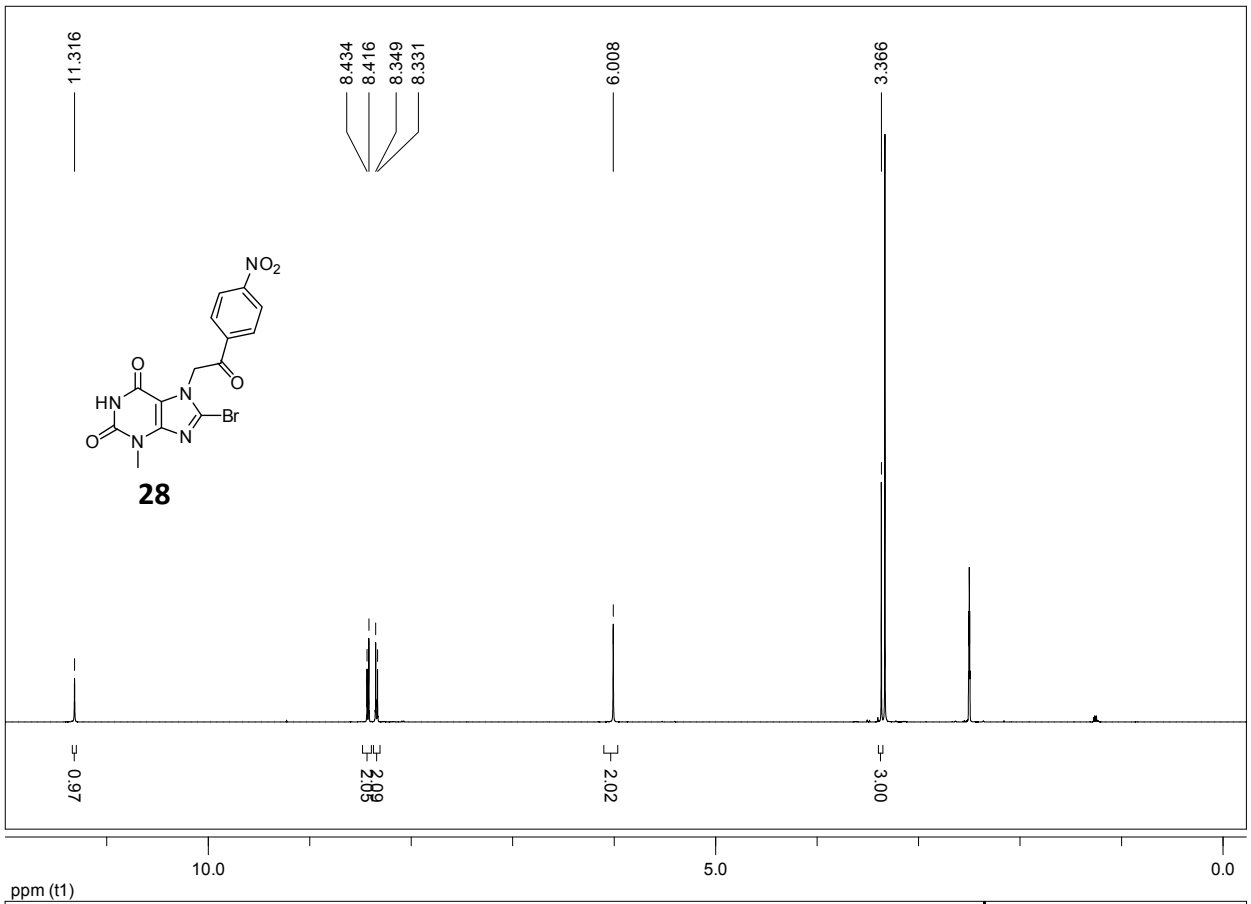

191.193
153.900
150.242
148.549
136.532
134.514
133.476
129.202
129.021
128.419
128.160
127.342
127.279
109.027
52.930
44.877
HN
O
N
Br
26
200
150
100
50
0
ppm (t1)

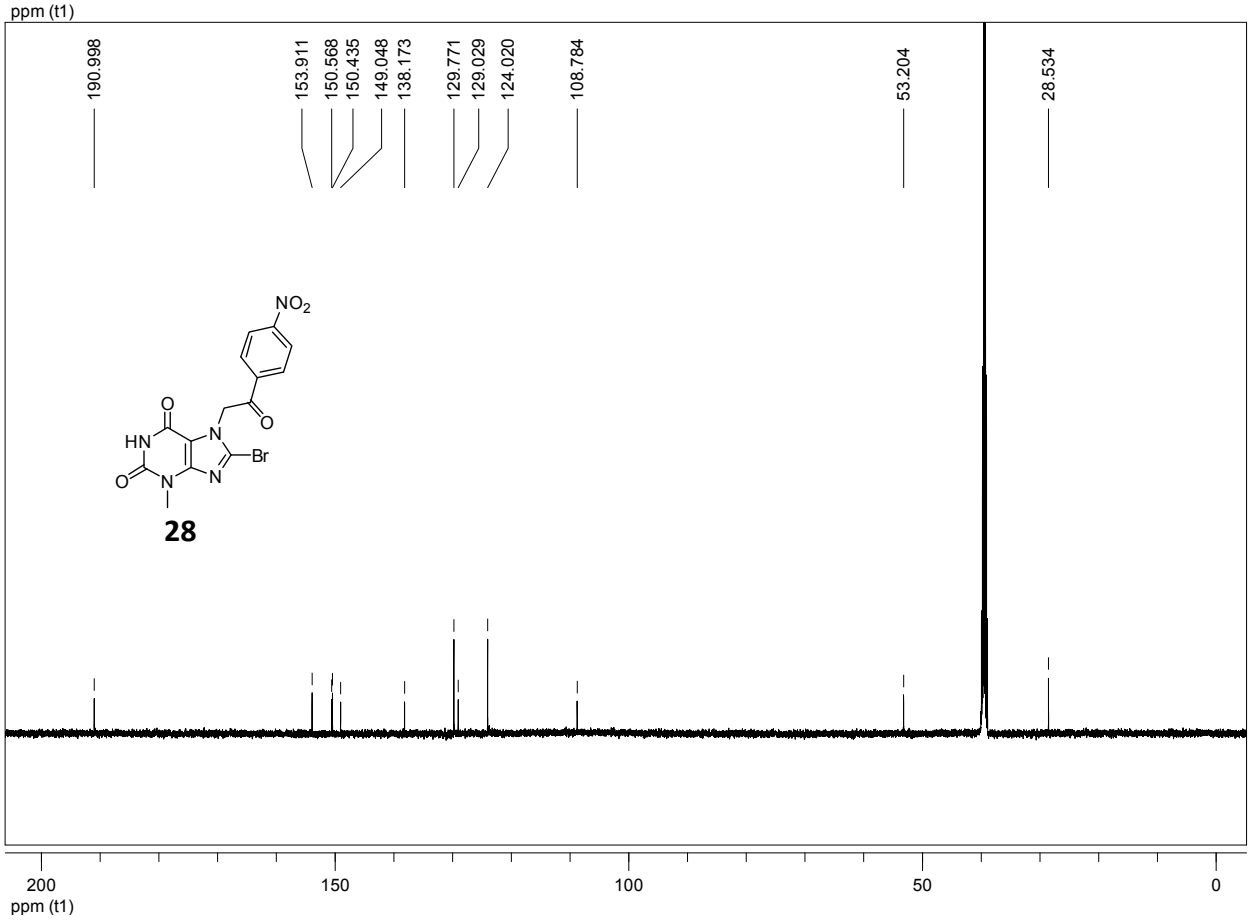

11.425
8.218
8.205
8.196
8.182
7.491
7.469
7.447
7.382
7.379
7.375
7.365
7.360
7.358
7.349
7.344
7.332
7.328
7.309
7.304
7.295
7.287
7.279
7.272
5.928
5.107
F
O
HN
O
N
N
Br
N
O
0.93
1.95
2.04
2.00
2.05
1.91
10.0
5.0
0.0
ppm (t1)

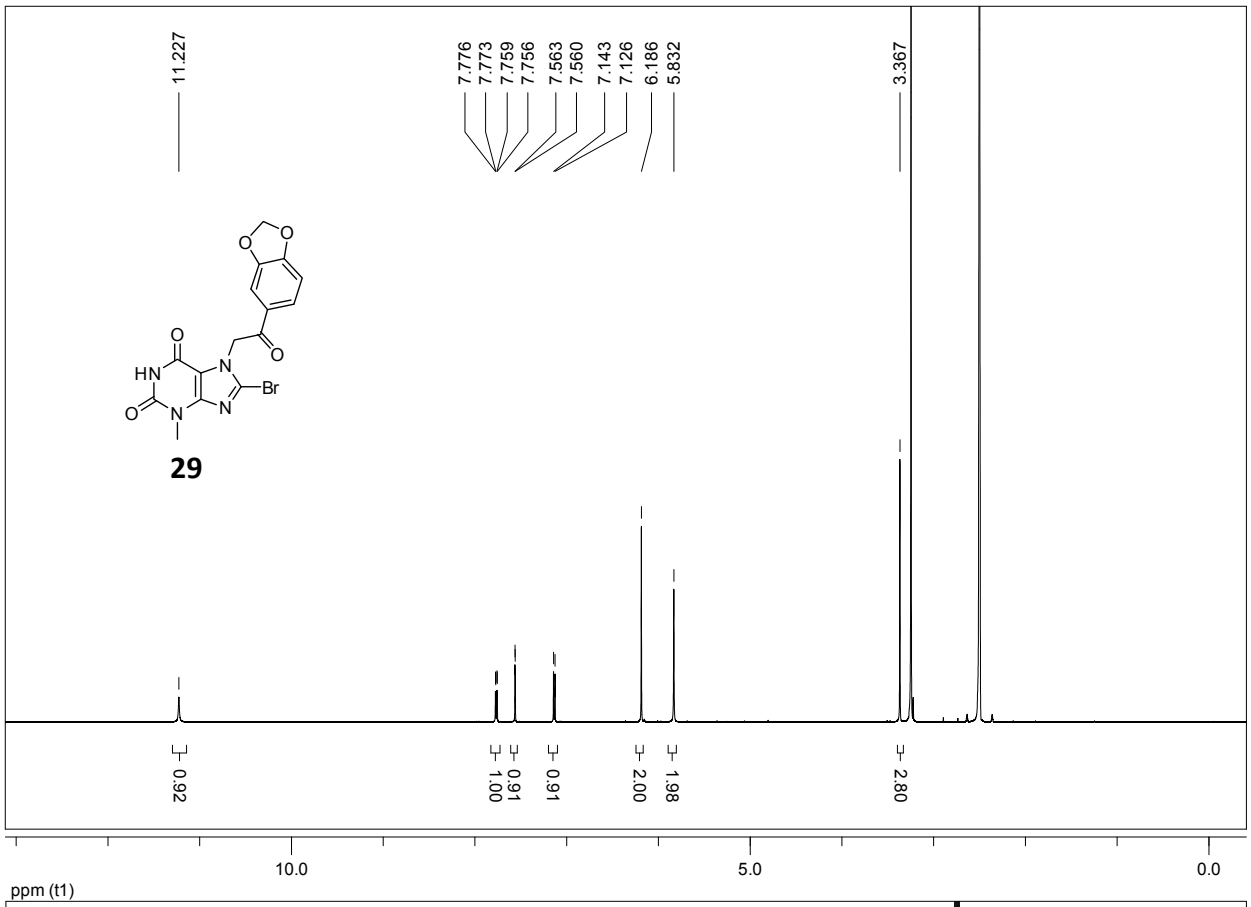
27


189.930
153.888
150.244
148.555
136.529
131.417
131.338
130.303
130.281
129.194
128.421
127.495
127.345
127.284
116.256
116.080
109.020
52.846
44.880
F
O
HN
O
N
N
Br
N
O
200
150
100
50
0
ppm (t1)

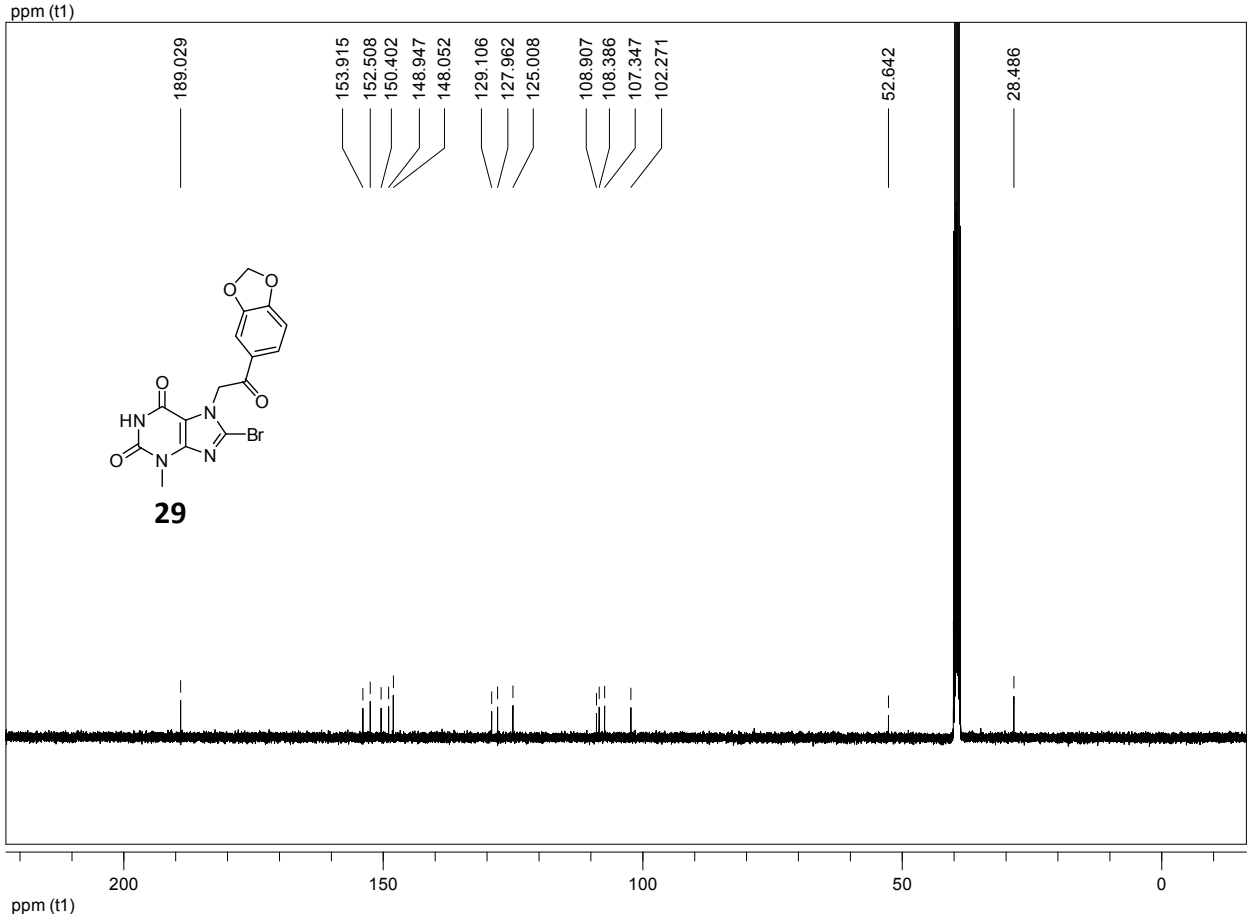
27


11.316
8.434
8.416
8.349
8.331
6.008
3.366
NO2
O
HN
O
N
Br
N
N
O
28
0.97
2.05
2.02
3.00
10.0
5.0
0.0
ppm (t1)

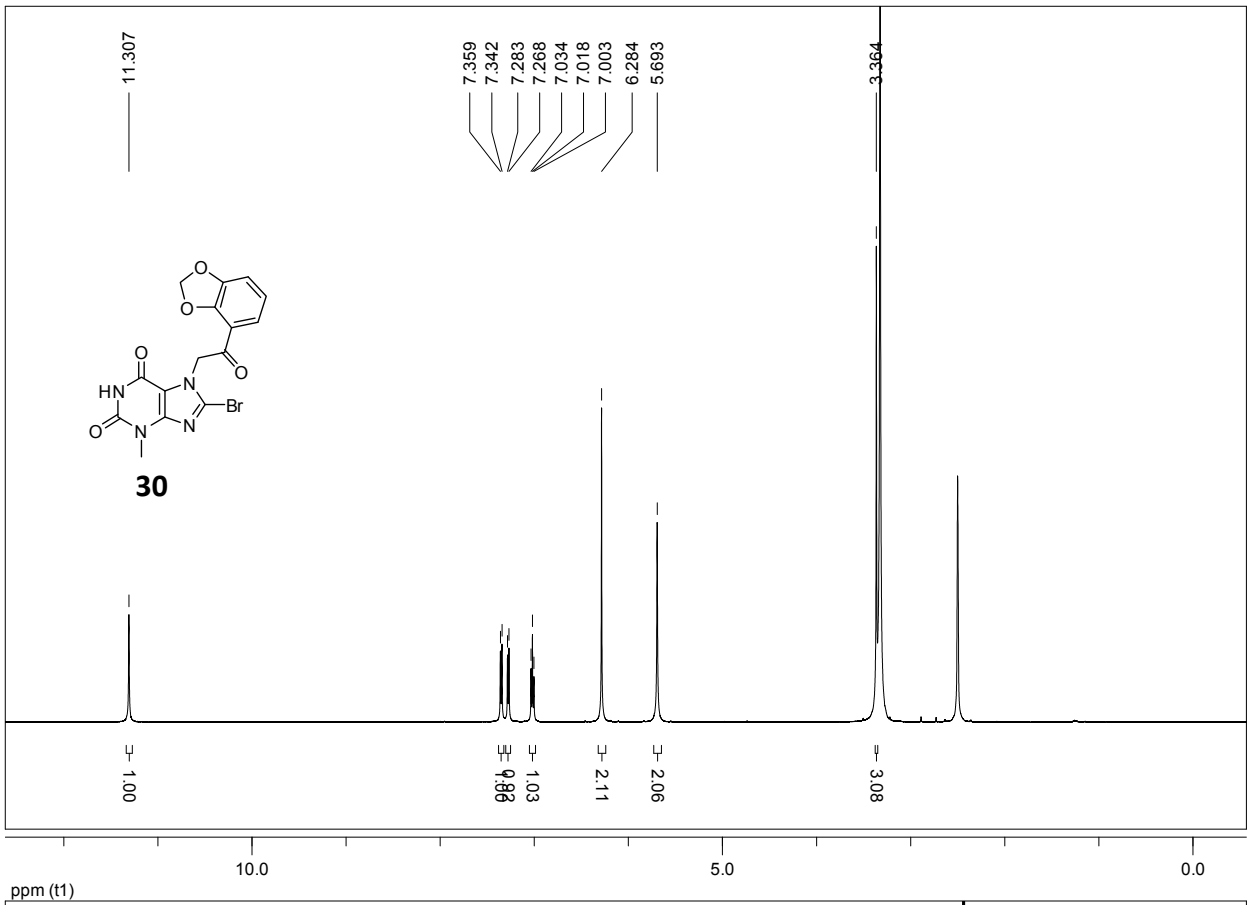

190.998
153.911
150.568
150.435
149.048
138.173
129.771
129.029
124.020
108.784
53.204
28.534
NO2
O
HN
O
N
Br
N
N
O
28
200
150
100
50
0
ppm (t1)

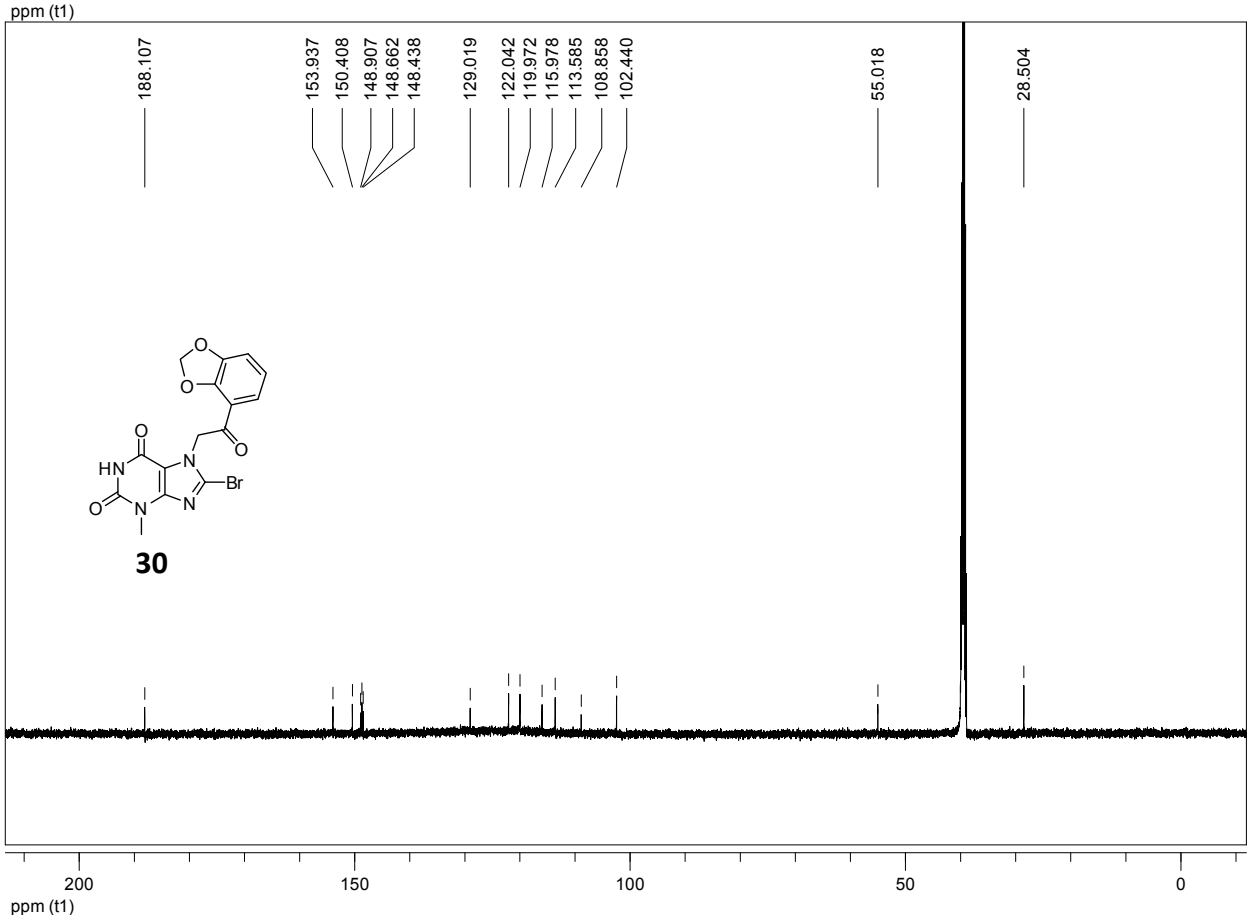

11.227
7.776
7.773
7.759
7.756
7.563
7.560
7.143
7.126
6.186
5.832
3.367
0.92
1.00
0.91
0.91
2.00
1.98
2.80
10.0
5.0
0.0
ppm (t1)

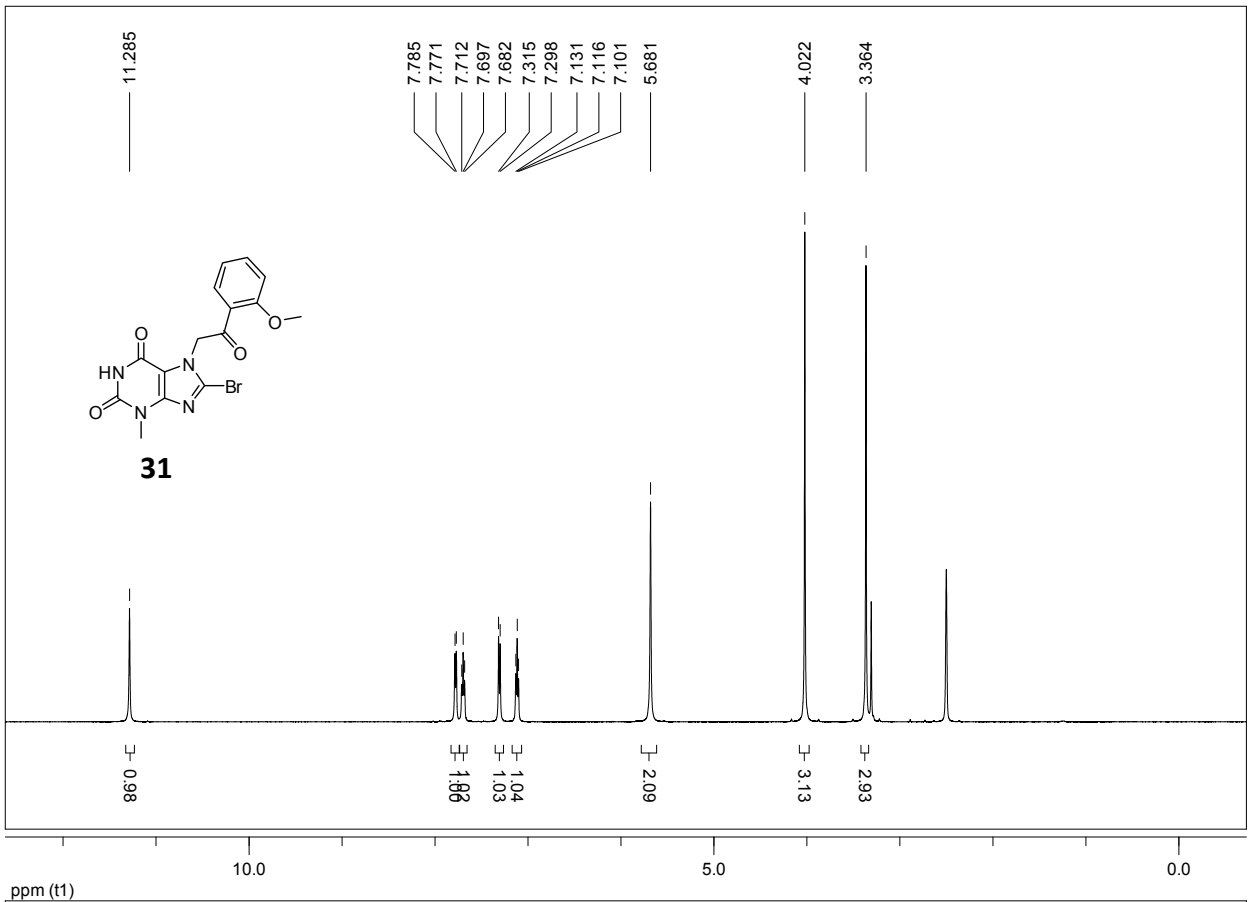
29


189.029
153.915
152.508
150.402
148.947
148.052
129.106
127.962
125.008
108.907
108.386
107.347
102.271
52.642
28.486
200
150
100
50
0
ppm (t1)

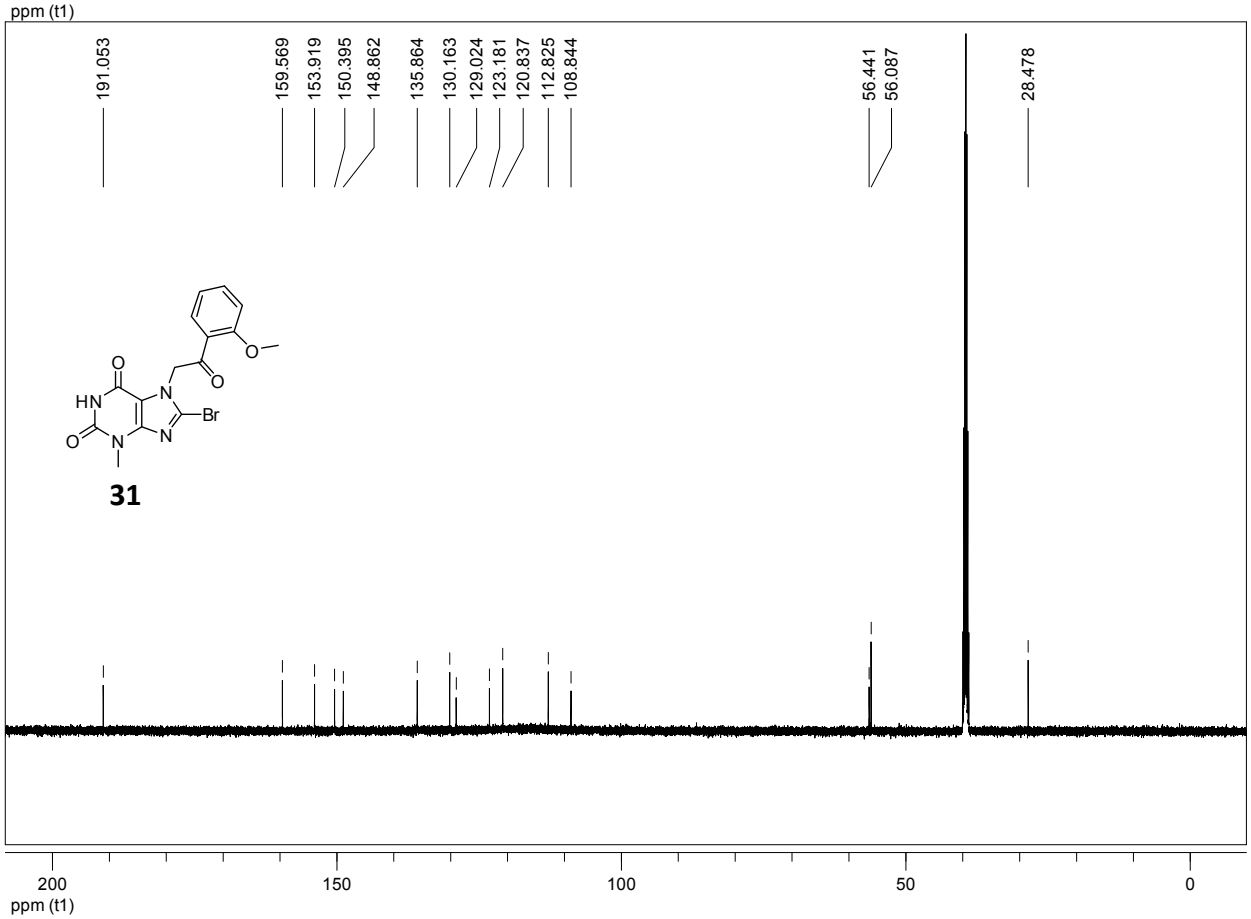
29


11.307
7.359
7.342
7.283
7.268
7.034
7.018
7.003
6.284
5.693
3.364
1.00
0.98
0.92
1.03
2.11
2.06
3.08
10.0
5.0
0.0
ppm (t1)
30

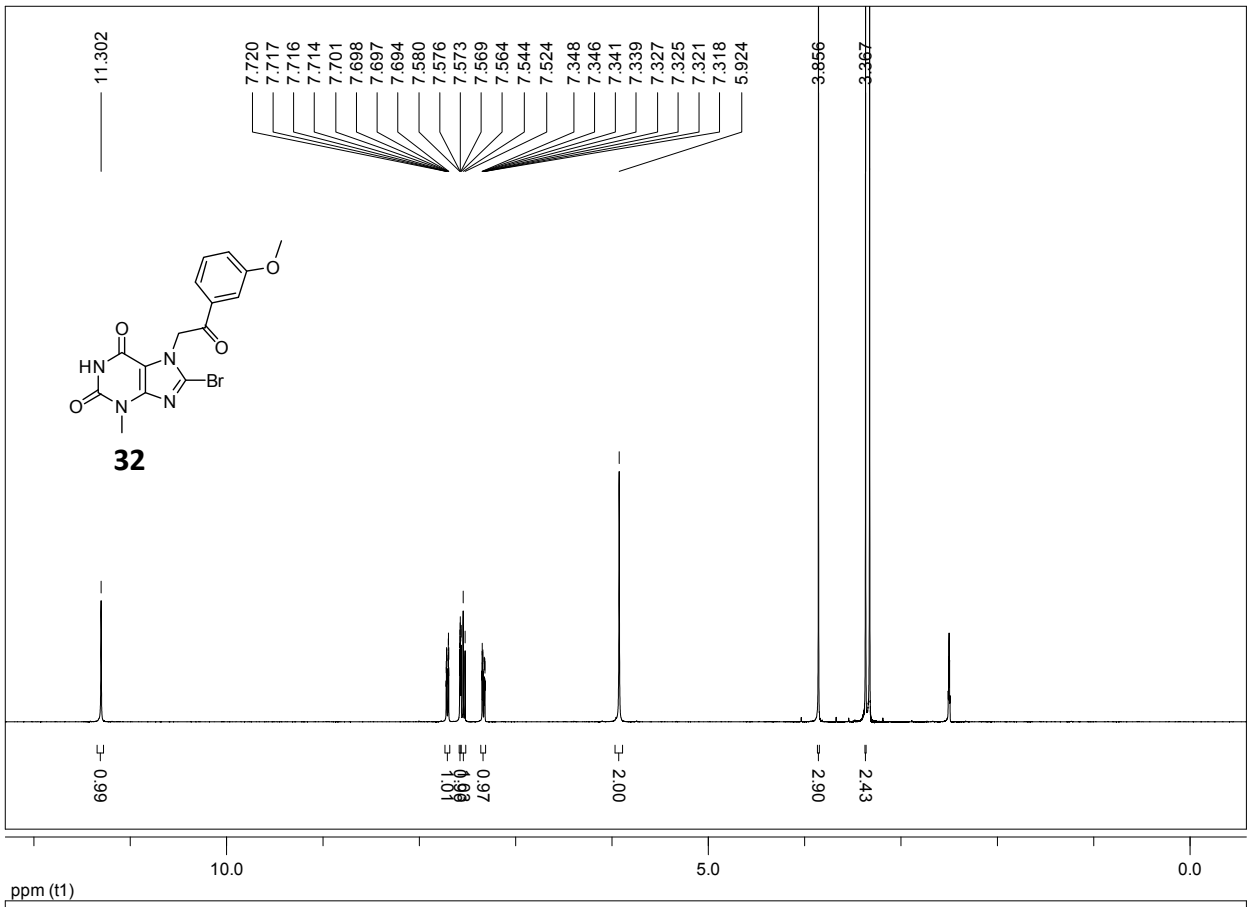

188.107
153.937
150.408
148.907
148.662
148.438
129.019
122.042
119.972
115.978
113.585
108.858
102.440
55.018
28.504
200
150
100
50
0
ppm (t1)
30


11.285
7.785
7.771
7.712
7.697
7.682
7.315
7.298
7.131
7.116
7.101
5.681
4.022
3.364
0.98
1.00
1.03
1.04
2.09
3.13
2.63
10.0
5.0
0.0
ppm (t1)

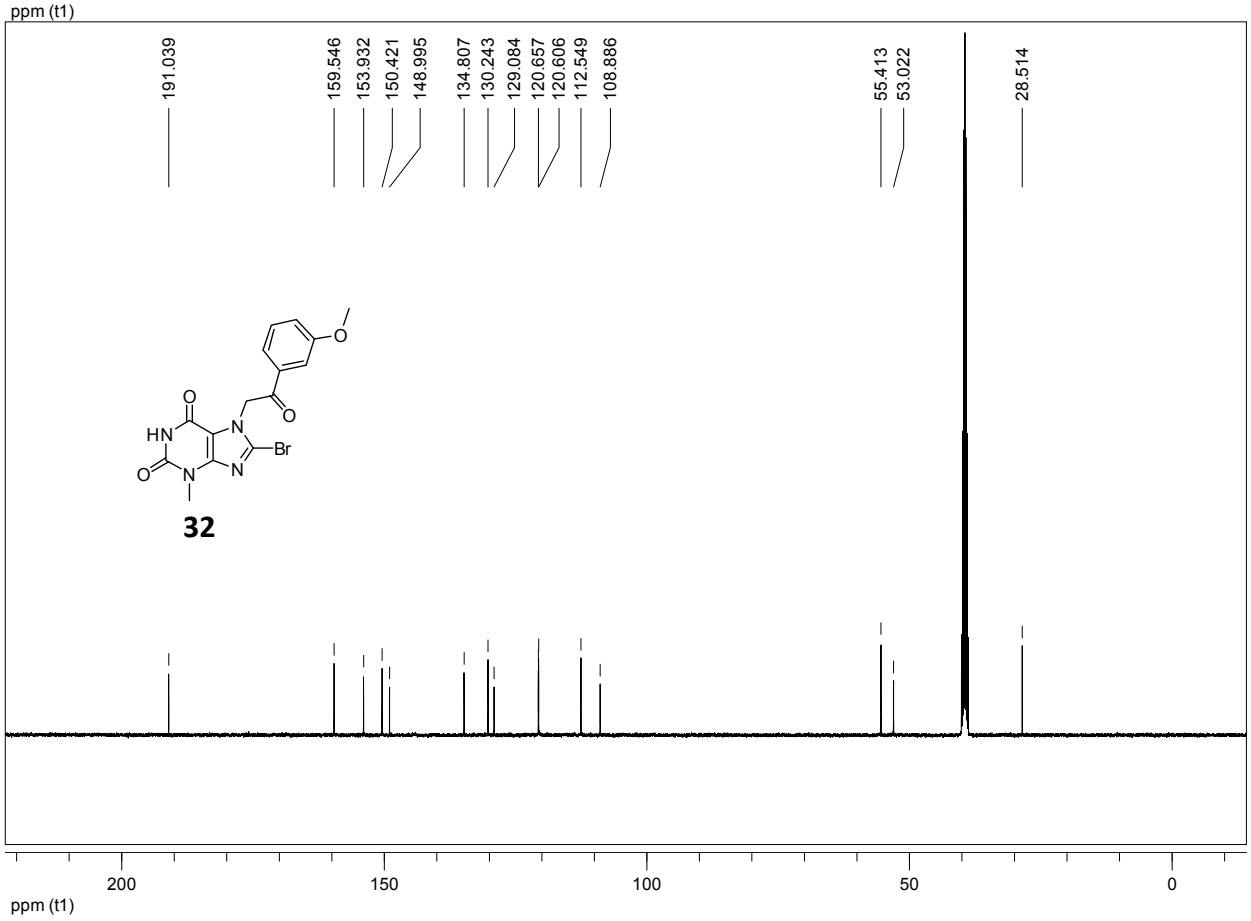
31


191.053
159.569
153.919
150.395
148.862
135.864
130.163
129.024
123.181
120.837
112.825
108.844
56.441
56.087
28.478
200
150
100
50
0
ppm (t1)

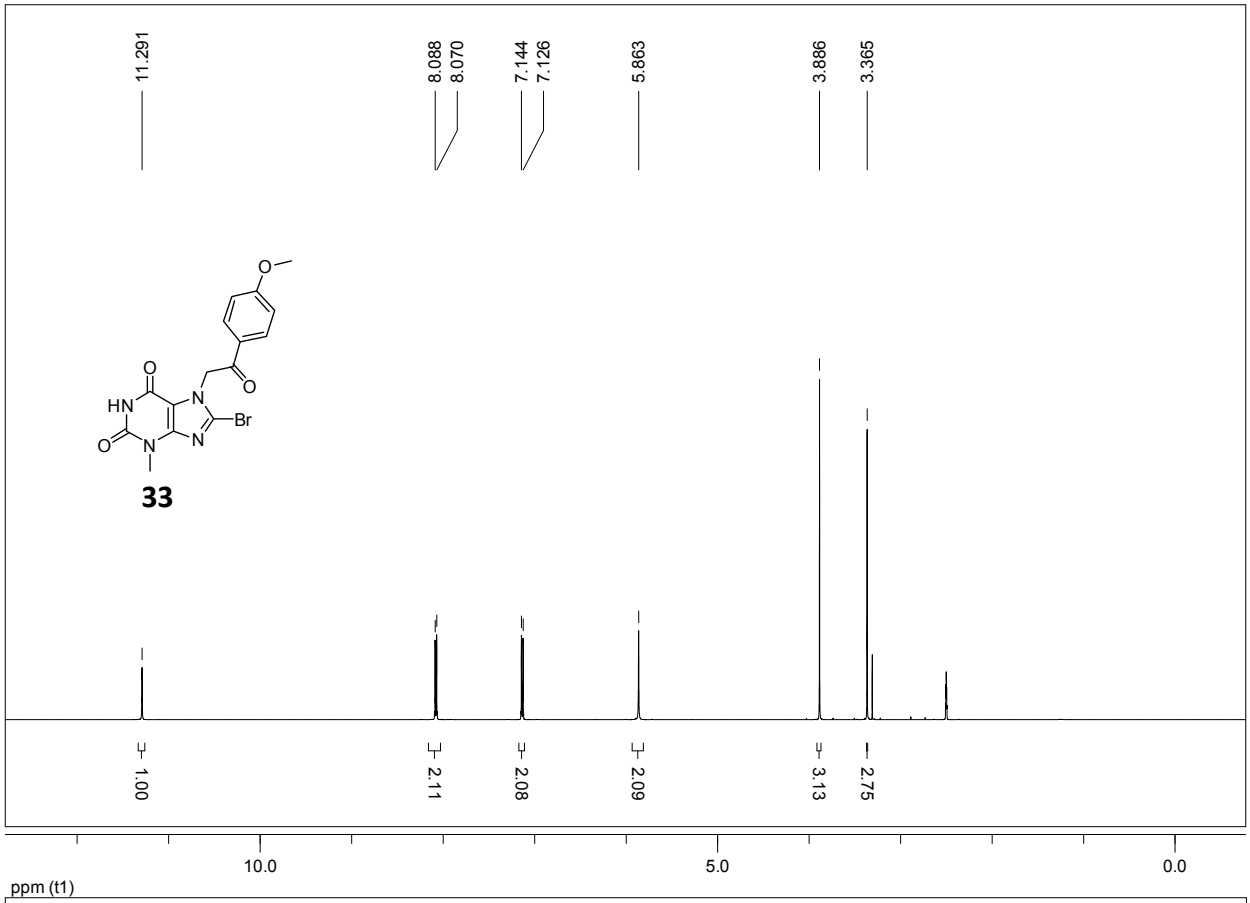
31


11.302
7.720
7.717
7.716
7.714
7.701
7.698
7.697
7.694
7.580
7.576
7.573
7.569
7.564
7.544
7.524
7.348
7.346
7.341
7.339
7.327
7.325
7.321
7.318
5.924
3.856
3.367
0.99
1.01
0.97
2.00
2.90
2.43
10.0
5.0
0.0
ppm (t1)

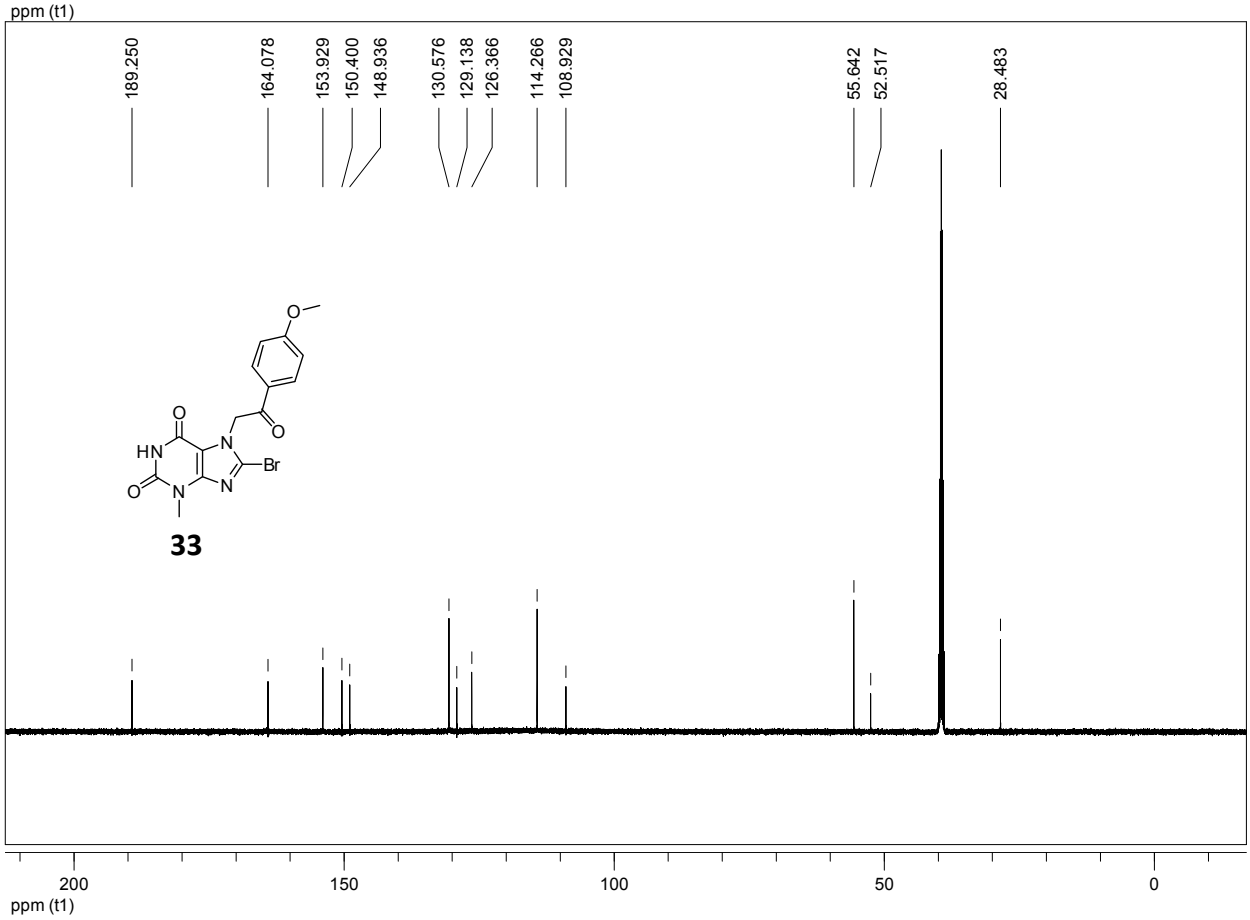
32


191.039
159.546
153.932
150.421
148.995
134.807
130.243
129.084
120.657
120.606
112.549
108.886
55.413
53.022
28.514
200
150
100
50
0
ppm (t1)

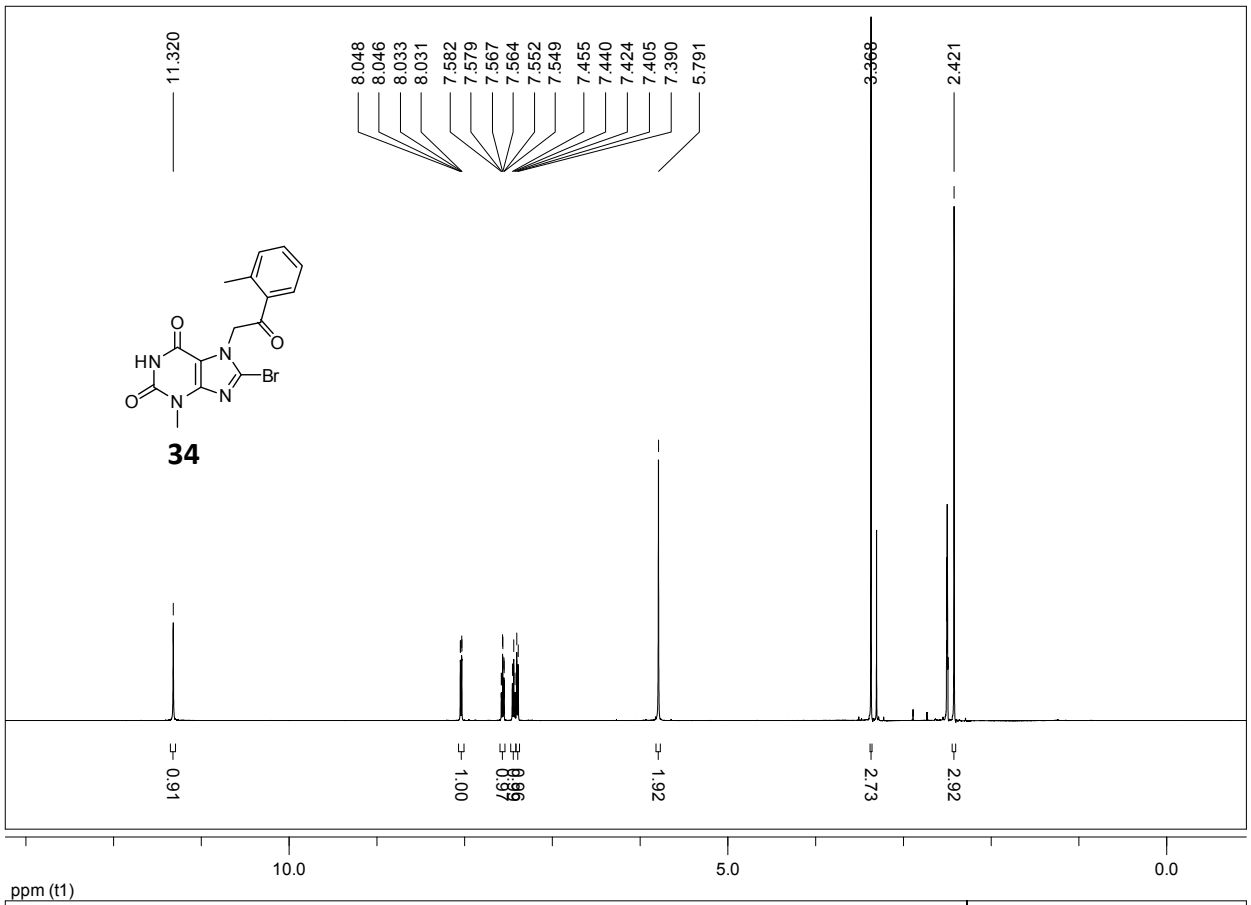
32

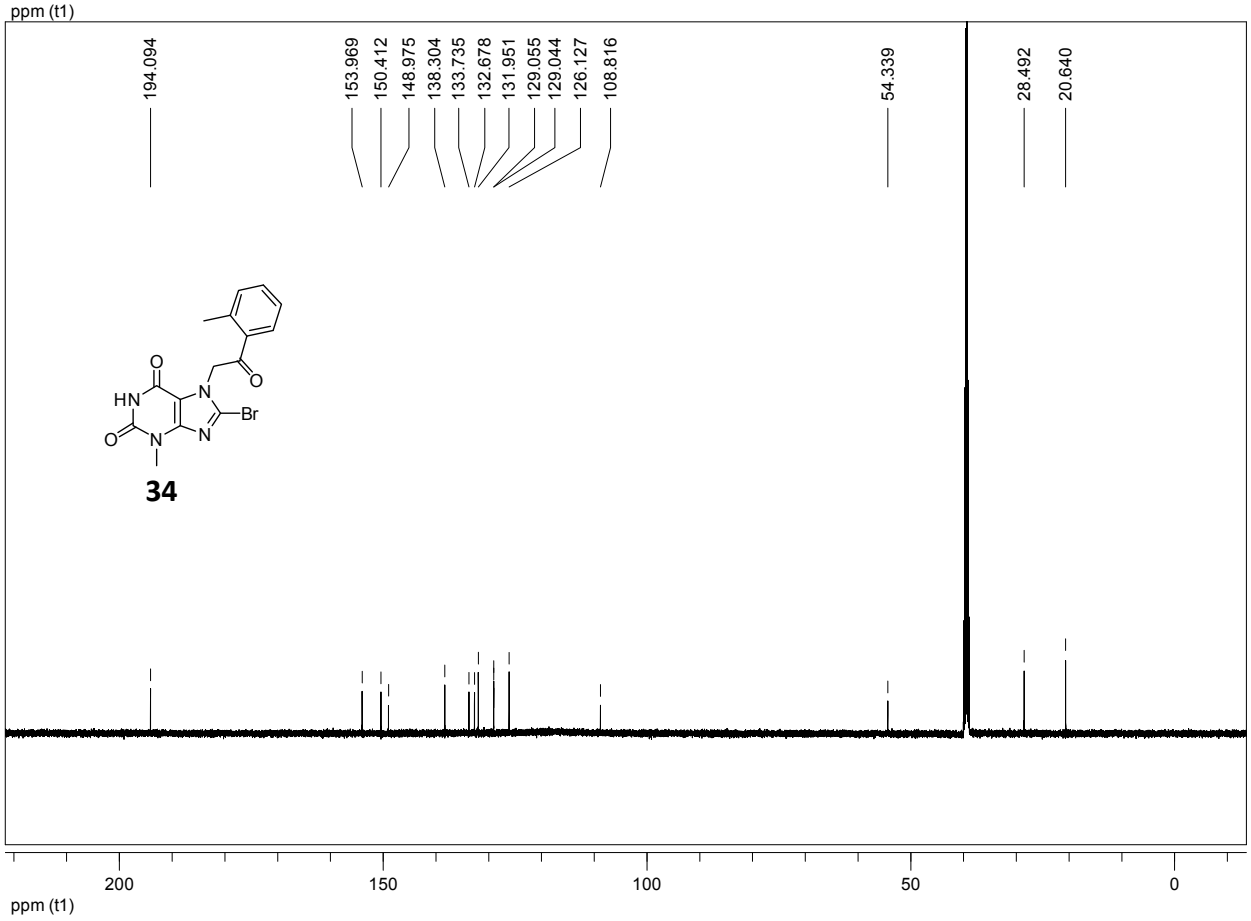

11.291
8.088
8.070
7.144
7.126
5.863
3.886
3.365
1.00
2.11
2.08
2.09
3.13
2.75
10.0
5.0
0.0
ppm (t1)

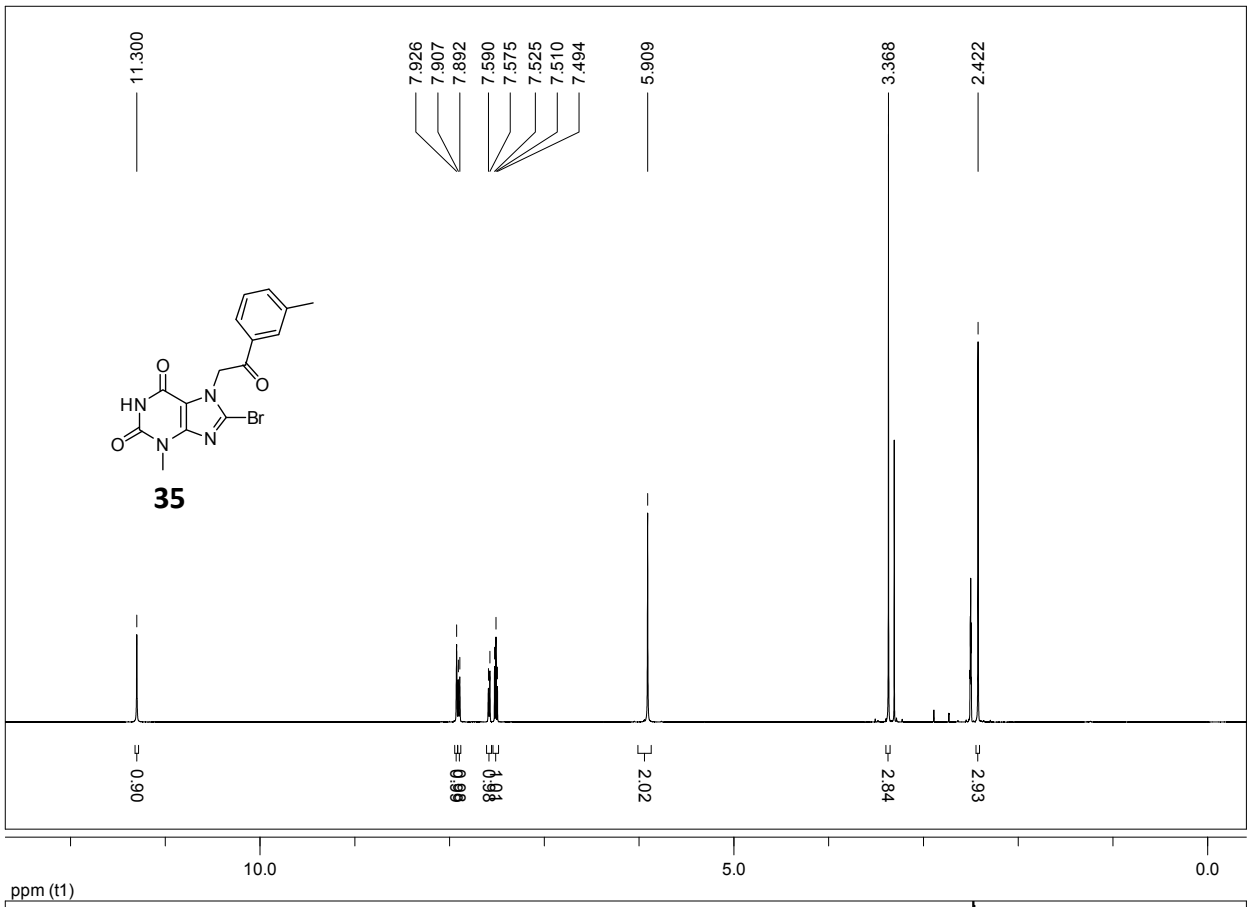
33

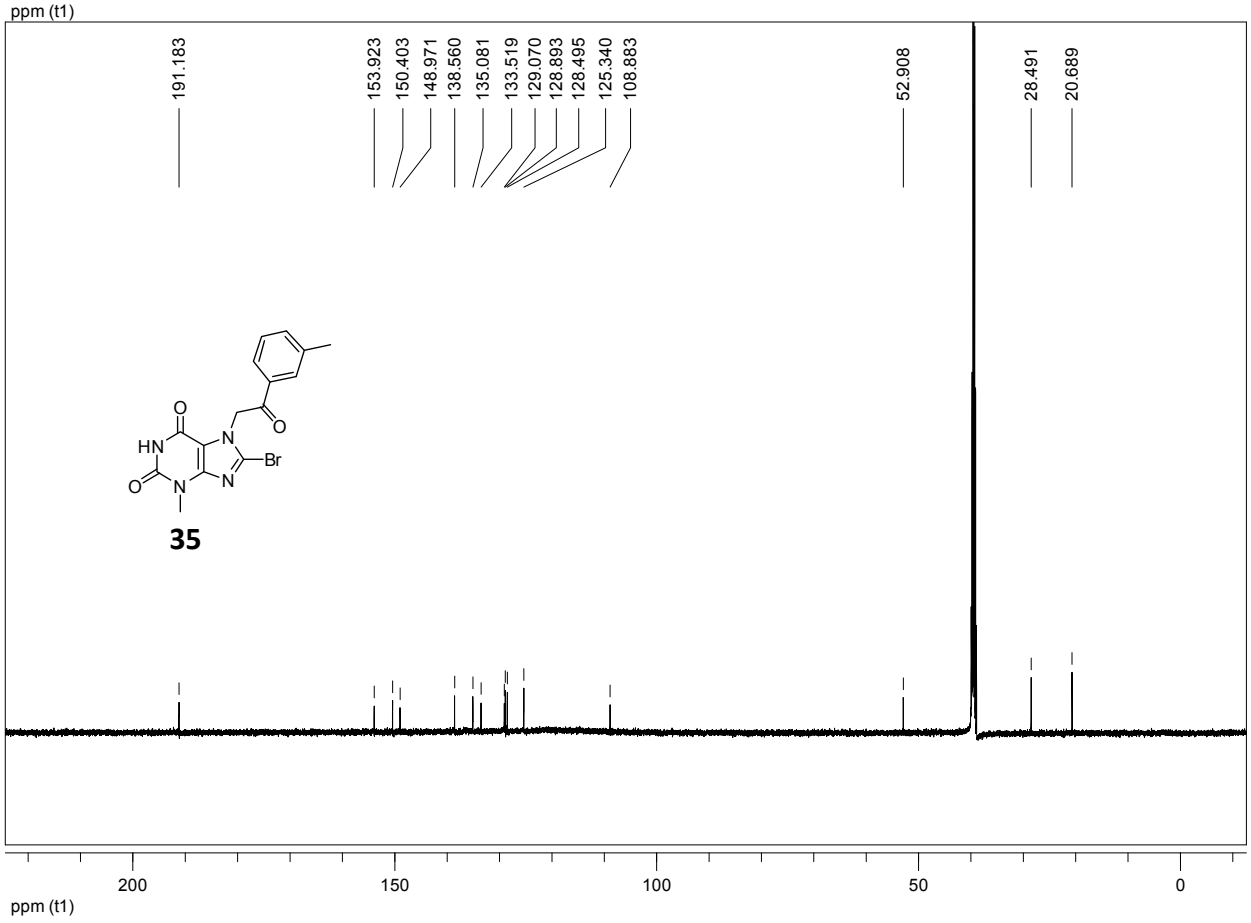

189.250
164.078
153.929
150.400
148.936
130.576
129.138
126.366
114.266
108.929
55.642
52.517
28.483
200
150
100
50
0
ppm (t1)

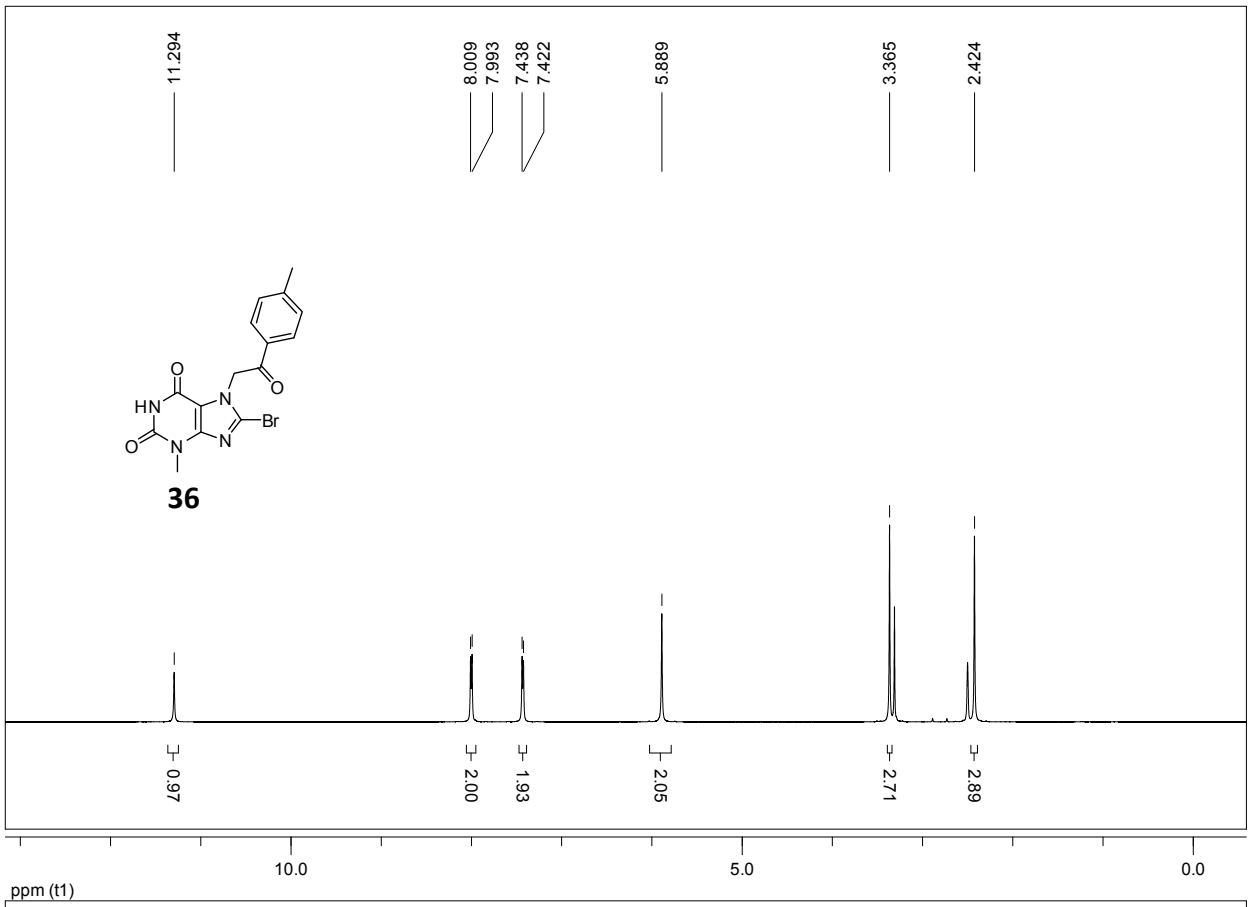
33


11.320
8.048
8.046
8.033
8.031
7.582
7.579
7.567
7.564
7.552
7.549
7.455
7.440
7.424
7.405
7.390
5.791
3.368
2.421
0.91
1.00
1.92
2.73
2.92
10.0
5.0
0.0
ppm (t1)
34


194.094
153.969
150.412
148.975
138.304
133.735
132.678
131.951
129.055
129.044
126.127
108.816
54.339
28.492
20.640
200
150
100
50
0
ppm (t1)
34

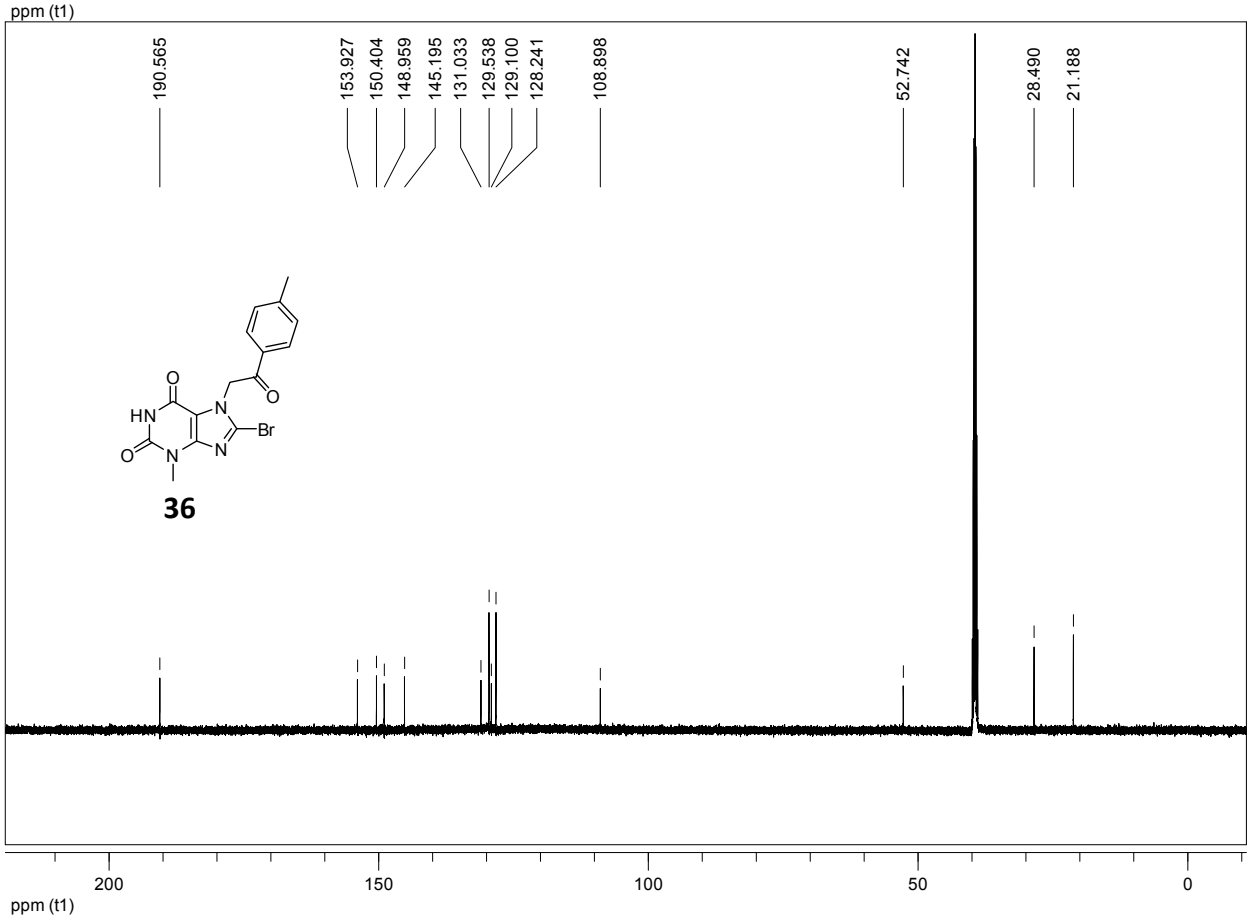

11.300
7.926
7.907
7.892
7.590
7.575
7.525
7.510
7.494
5.909
3.368
2.422
0.90
2.02
2.84
2.93
10.0
5.0
0.0
ppm (t1)
35


191.183
153.923
150.403
148.971
138.560
135.081
133.519
129.070
128.893
128.495
125.340
108.883
52.908
28.491
20.689
200
150
100
50
0
ppm (t1)
35


11.294
8.009
7.993
7.438
7.422
5.889
3.365
2.424
0.97
2.00
1.93
2.05
2.71
2.89
10.0
5.0
0.0
ppm (t1)

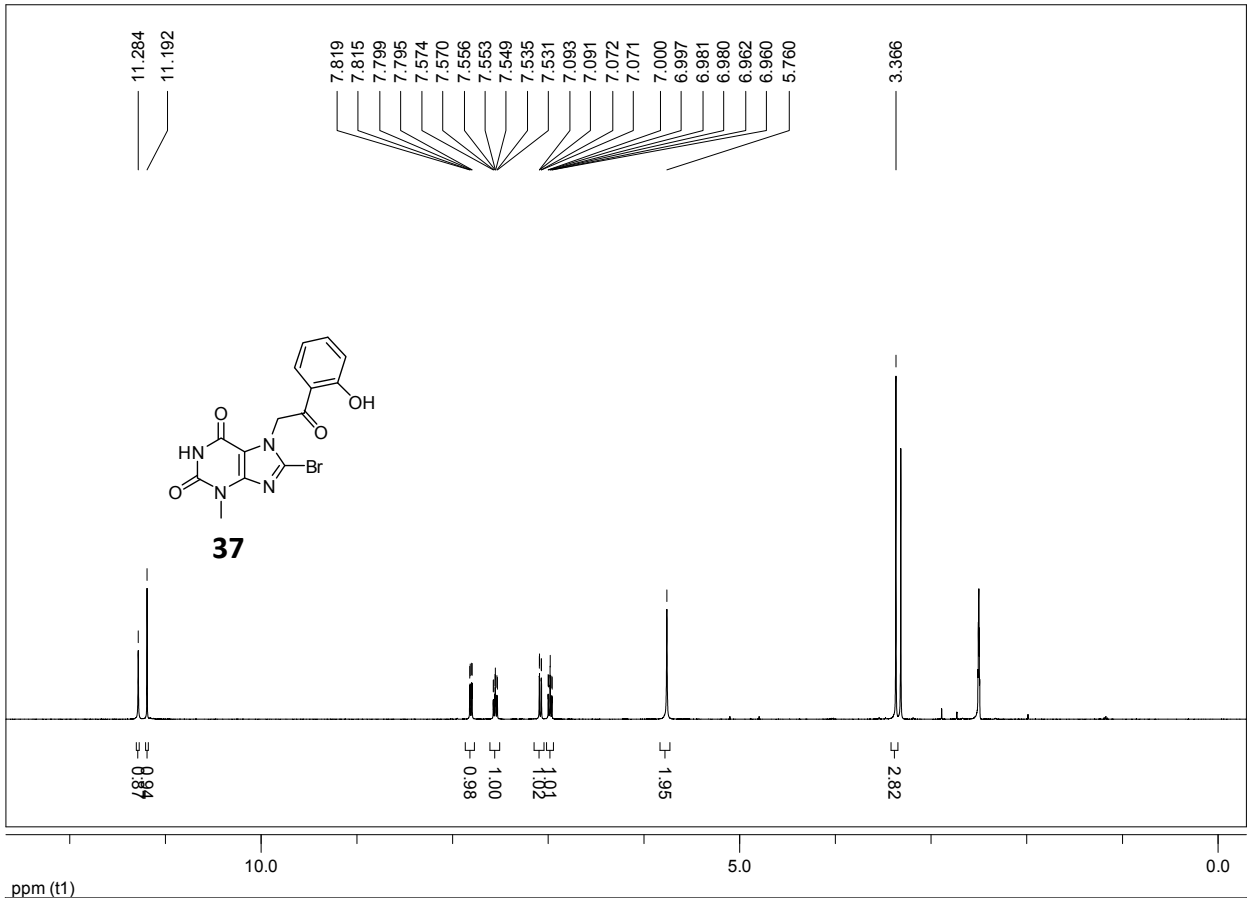
O
HN
O
N
N
Br
N
O
O

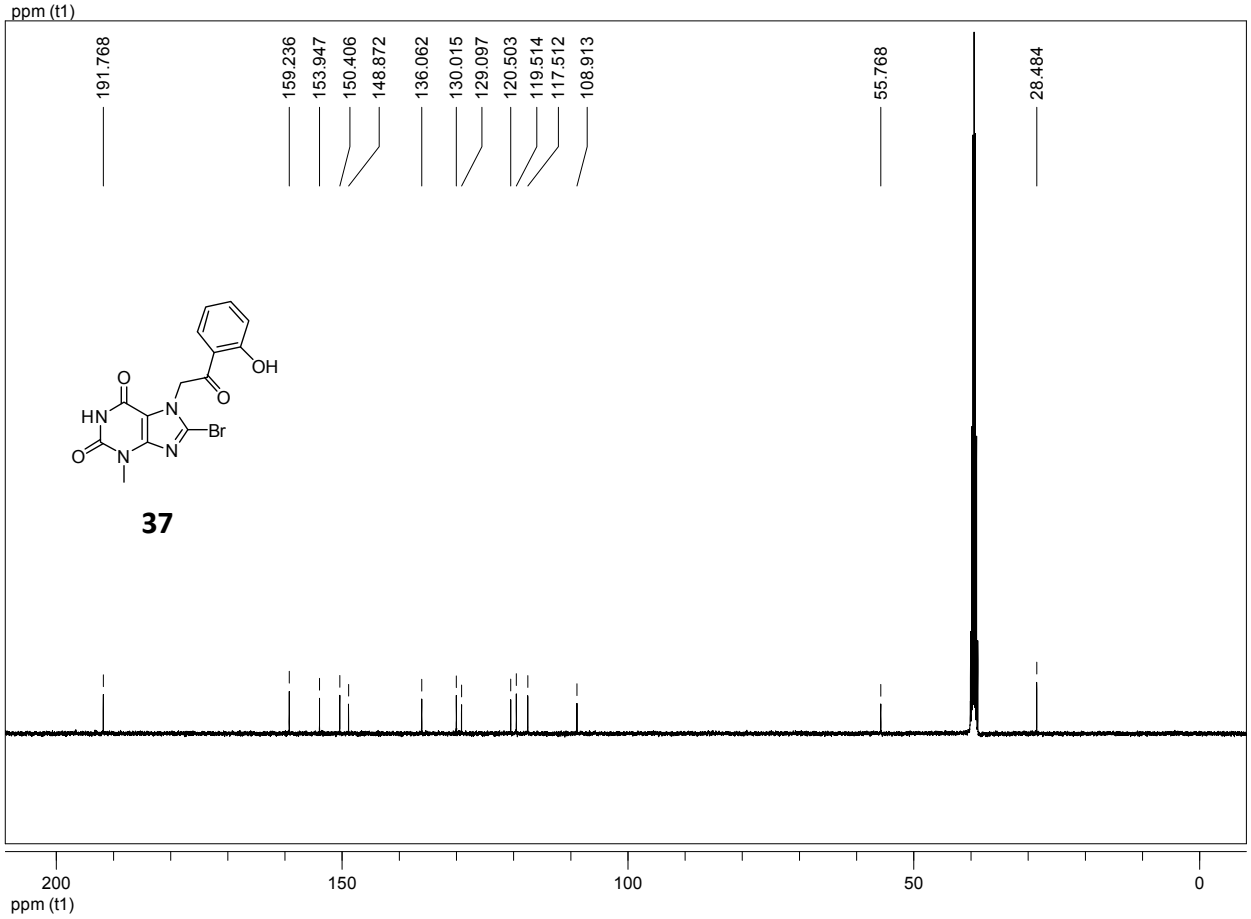
36

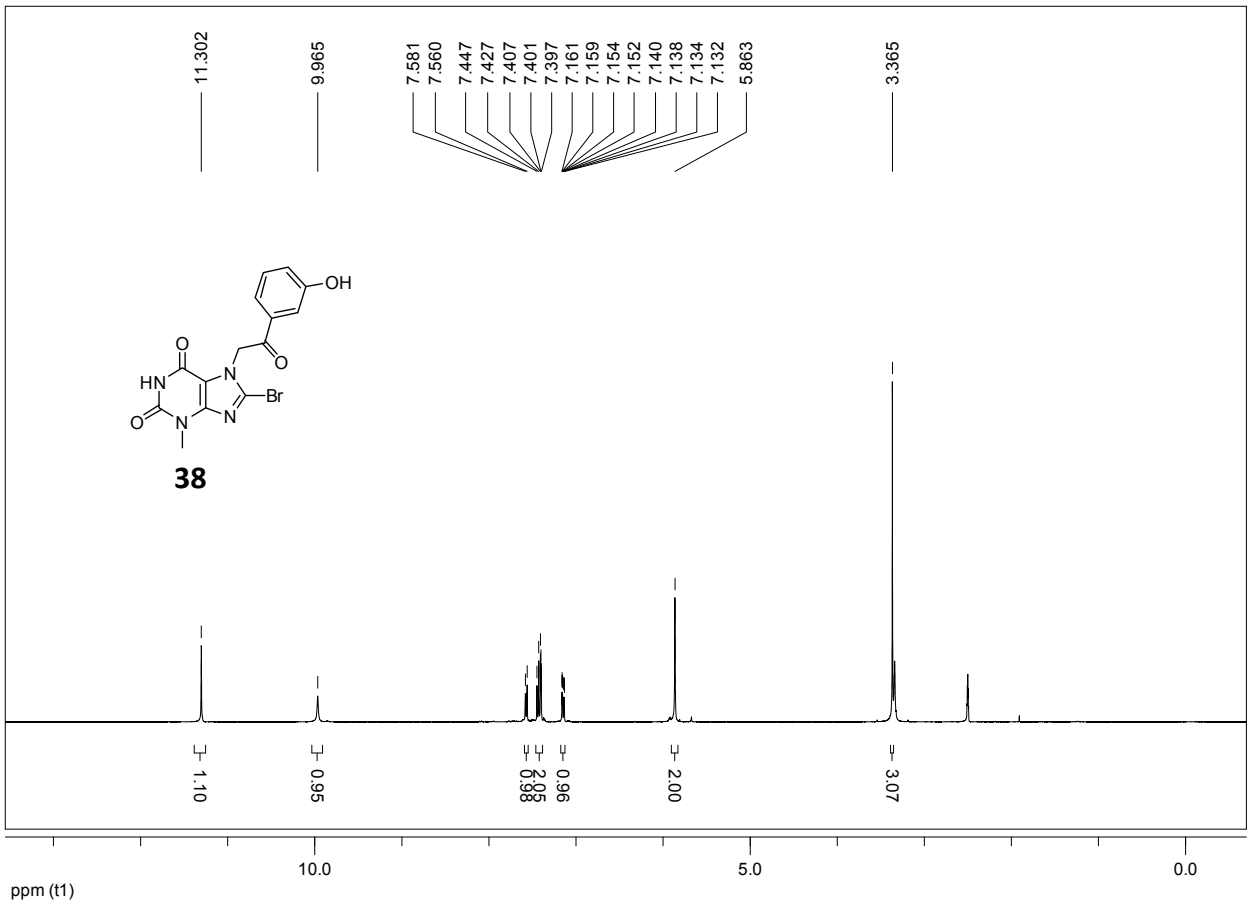

190.565
153.927
150.404
148.959
145.195
131.033
129.538
129.100
128.241
108.898
52.742
28.490
21.188
200
150
100
50
0
ppm (t1)

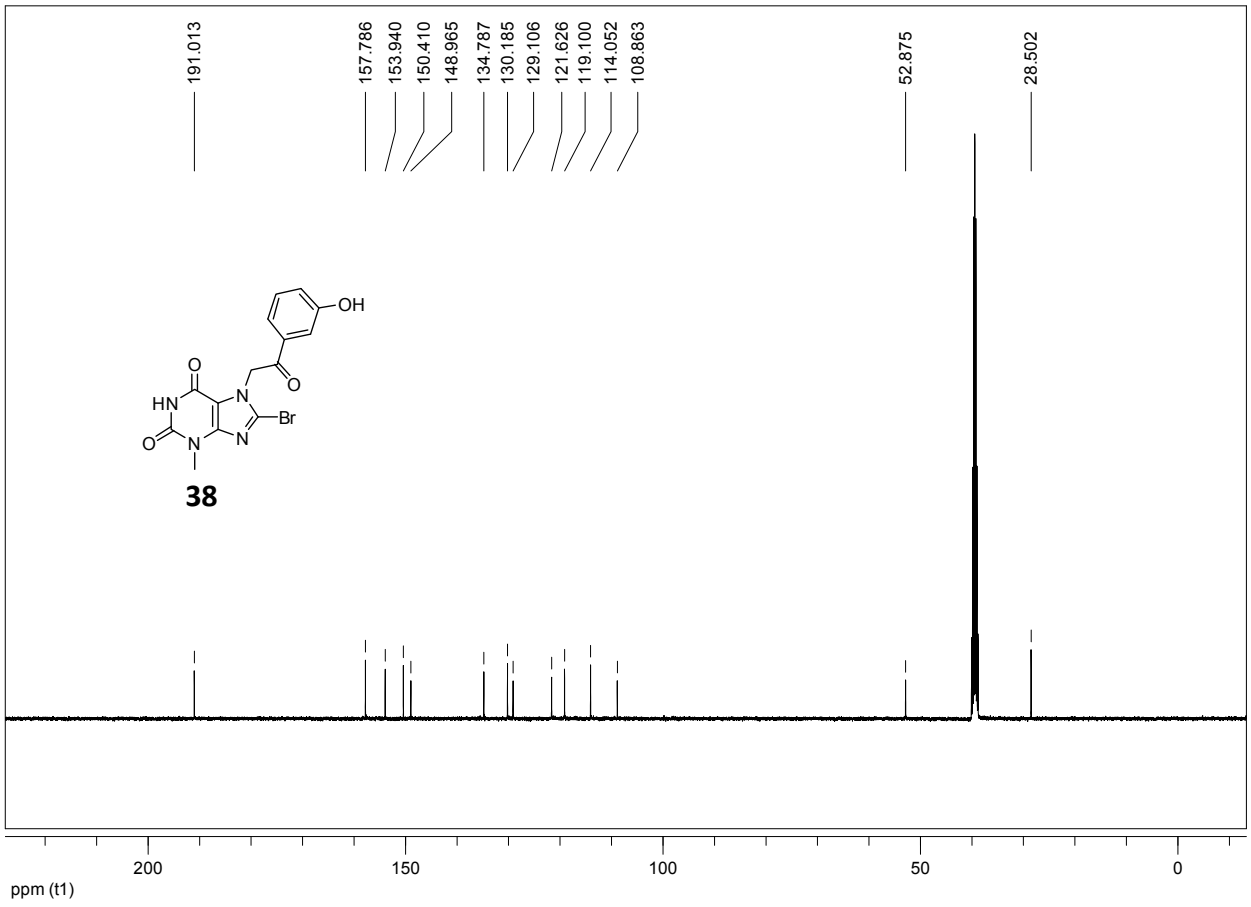
O
HN
O
N
N
Br
N
O
O

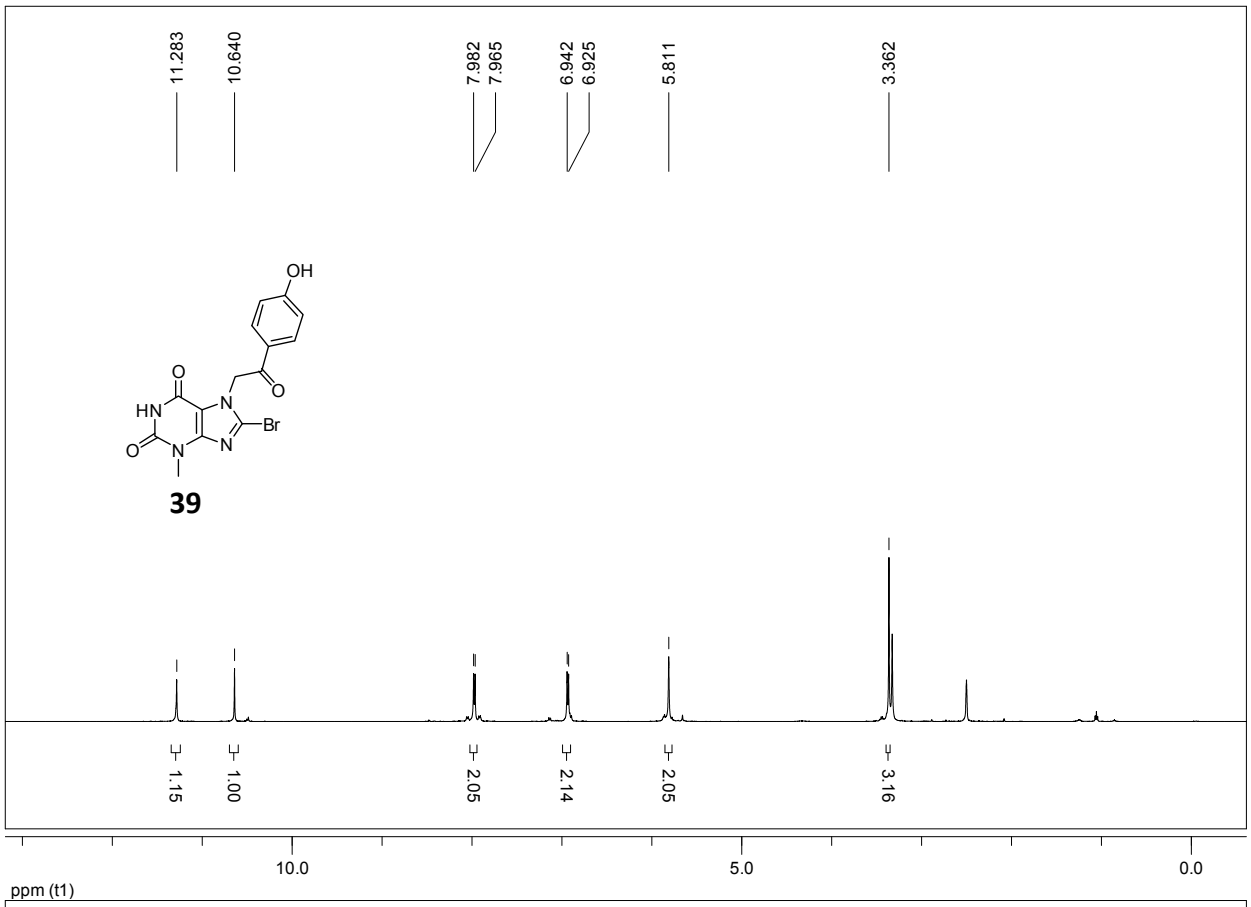
36

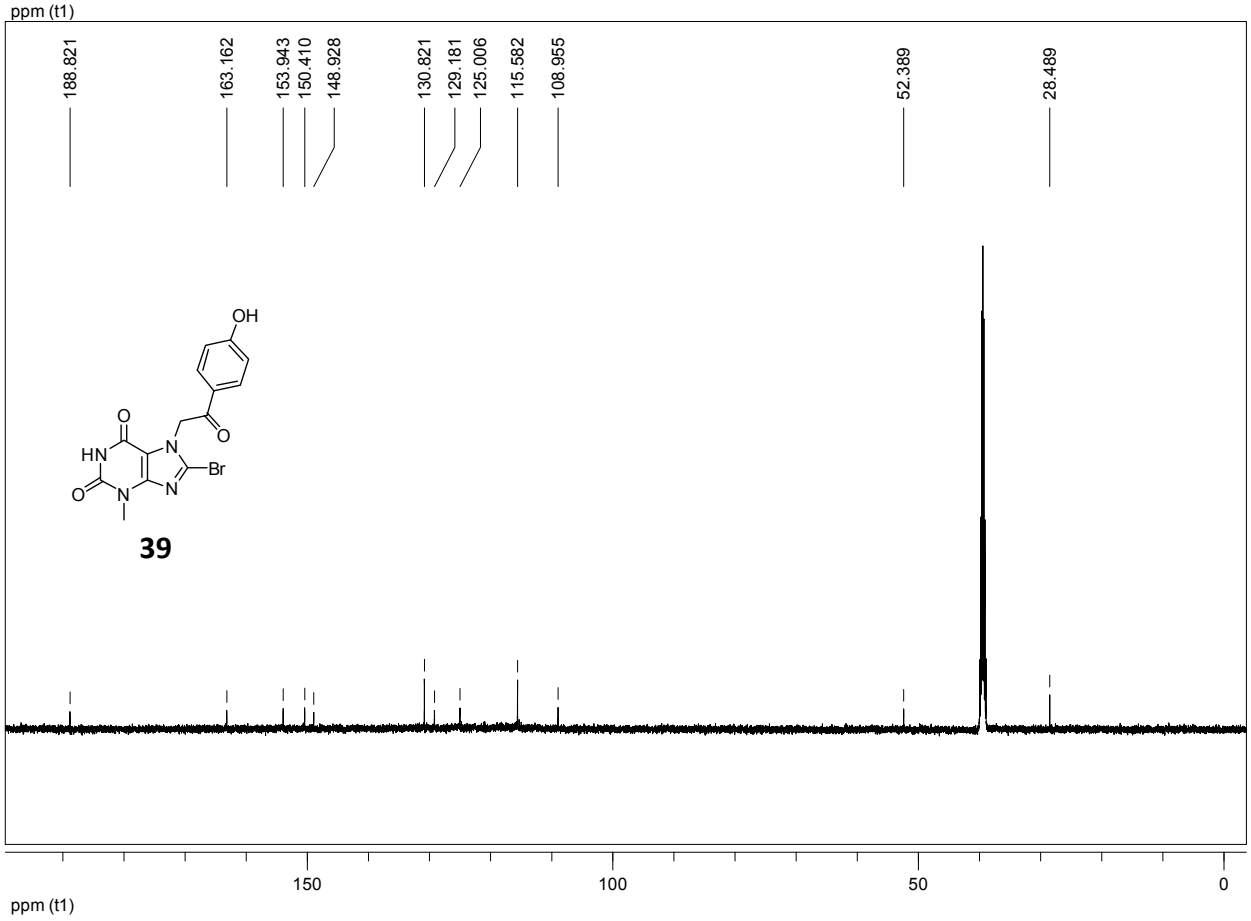

11.284
11.192
7.819
7.815
7.799
7.795
7.574
7.570
7.556
7.553
7.549
7.535
7.531
7.093
7.091
7.072
7.071
7.000
6.997
6.981
6.980
6.962
6.960
5.760
3.366
OH
O
HN
N
Br
O
N
N
O
37
0.84
0.98
1.00
1.02
1.01
1.95
2.82
10.0
5.0
0.0
ppm (t1)

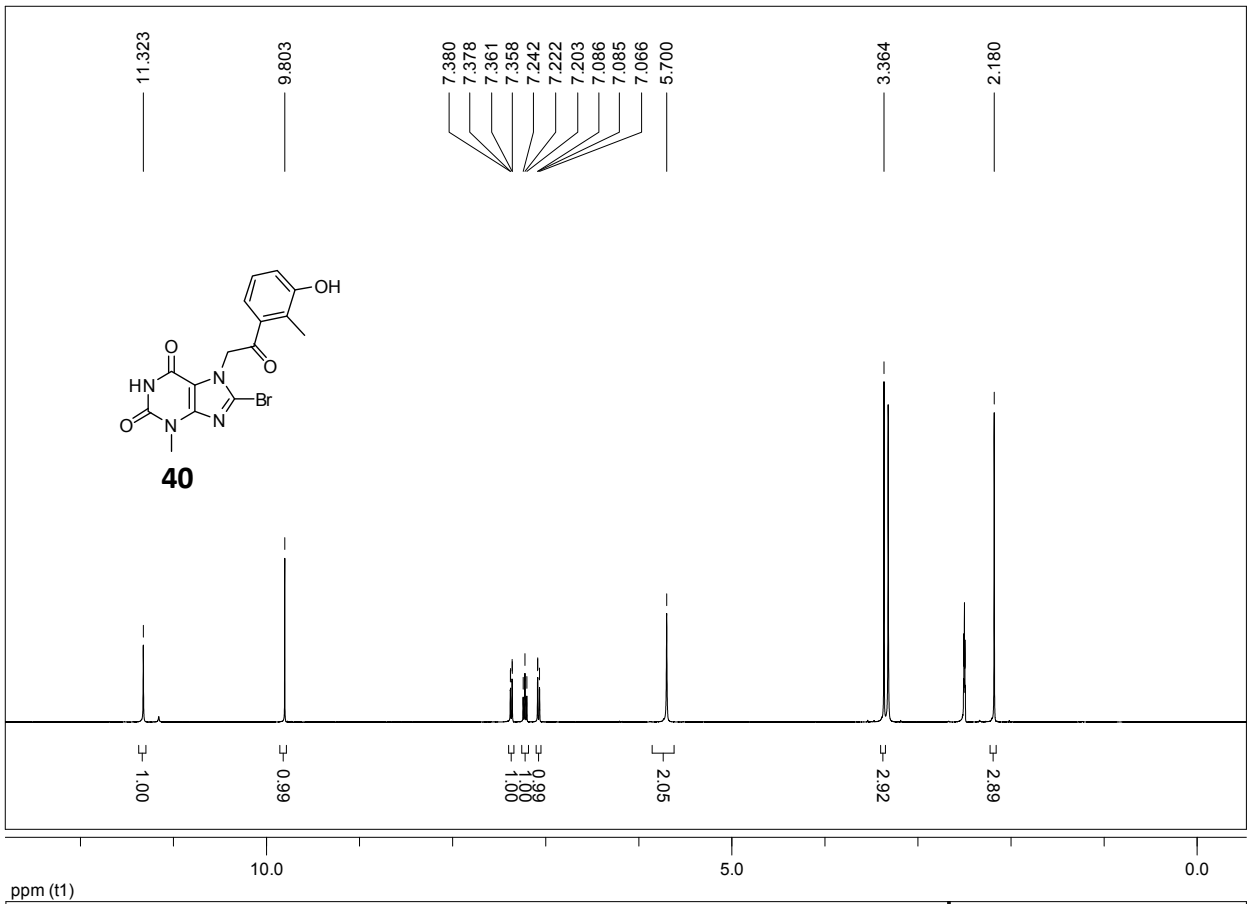

191.768
159.236
153.947
150.406
148.872
136.062
130.015
129.097
120.503
119.514
117.512
108.913
55.768
28.484
OH
O
HN
N
Br
O
N
N
O
37
200
150
100
50
0
ppm (t1)

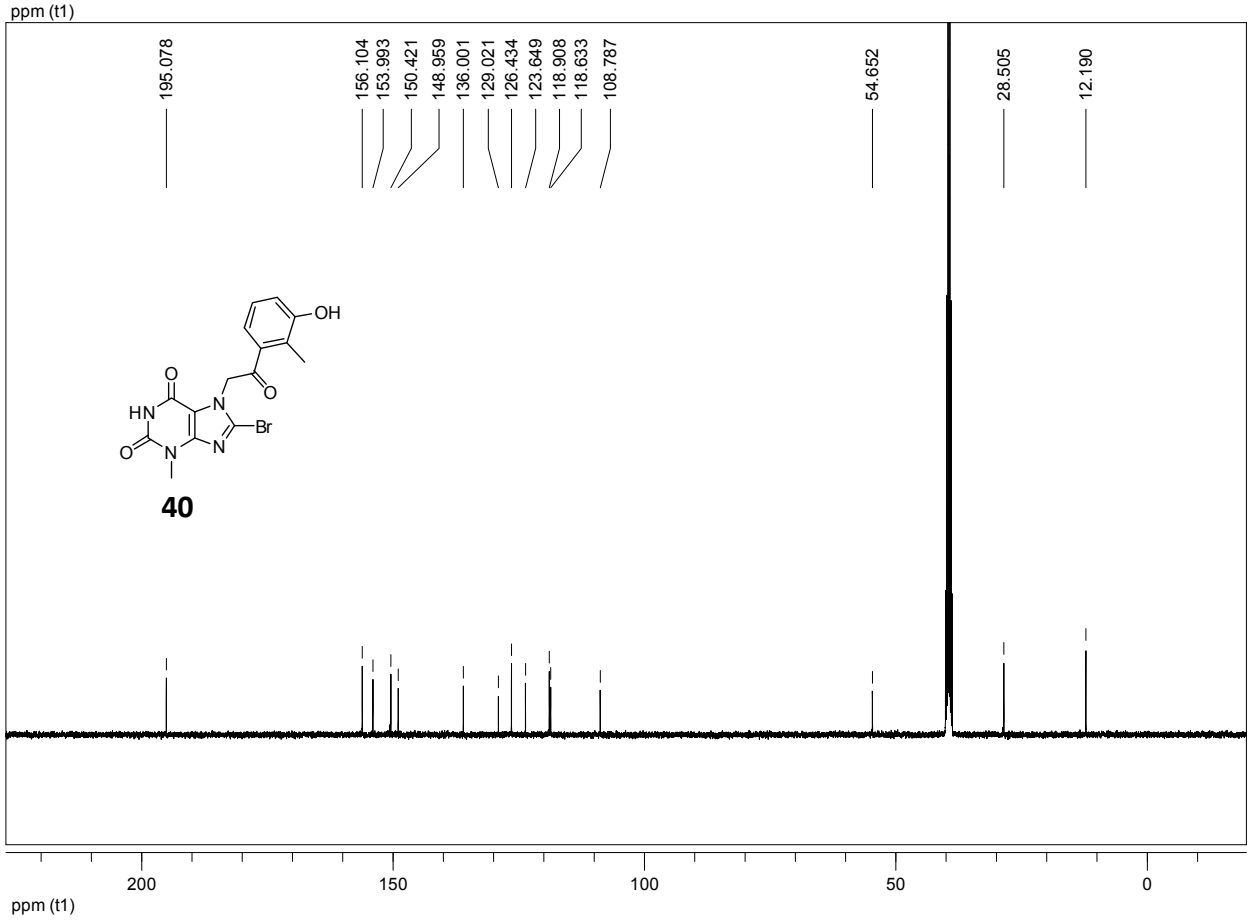

11.302
9.965
7.581
7.560
7.447
7.427
7.407
7.401
7.397
7.161
7.159
7.154
7.152
7.140
7.138
7.134
7.132
5.863
3.365
OH
O
HN
O
N
N
Br
N
O
38
1.10
0.95
2.05
0.98
0.96
2.00
3.07
10.0
5.0
0.0
ppm (t1)

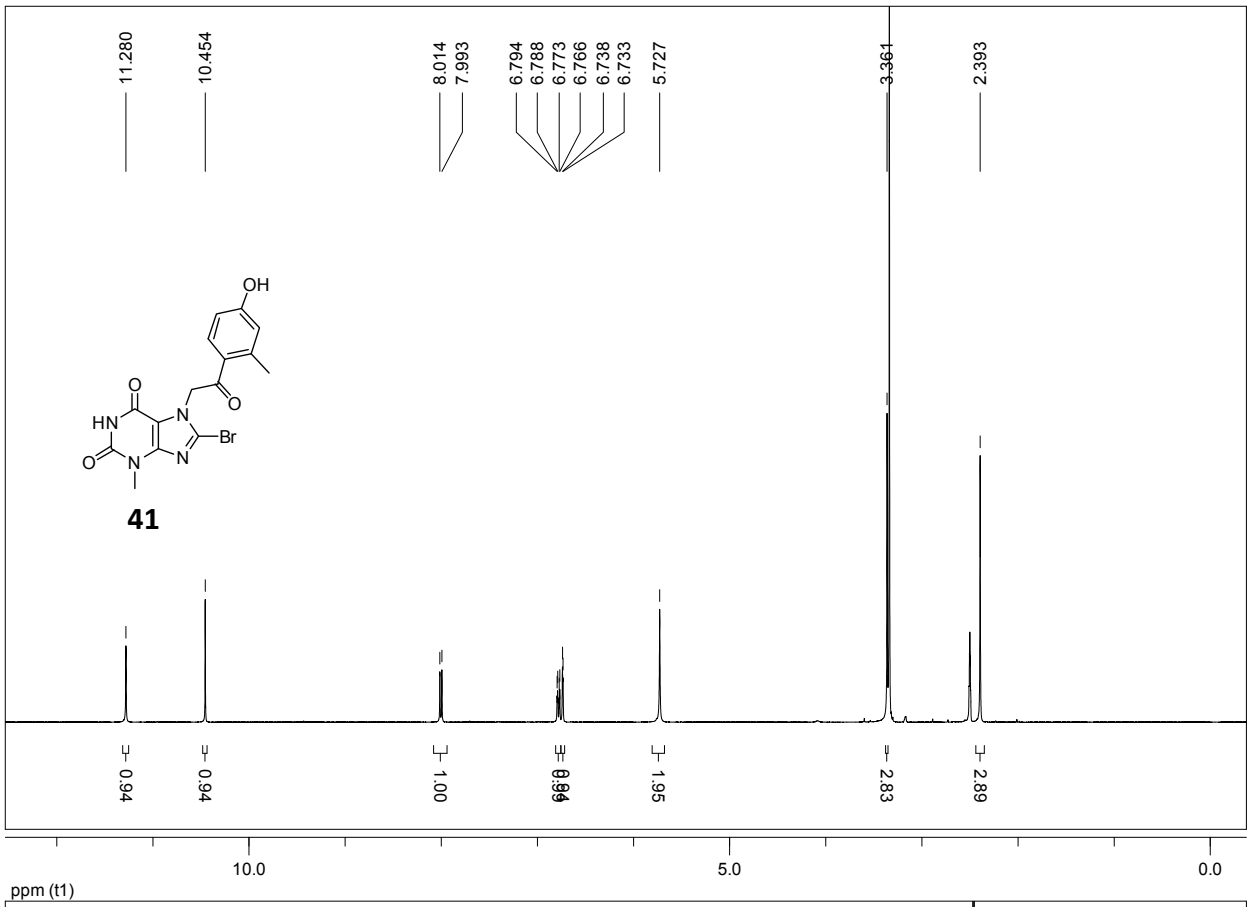

191.013
157.786
153.940
150.410
148.965
134.787
130.185
129.106
121.626
119.100
114.052
108.863
52.875
28.502
OH
O
HN
O
N
N
Br
N
O
38
200
150
100
50
0
ppm (t1)

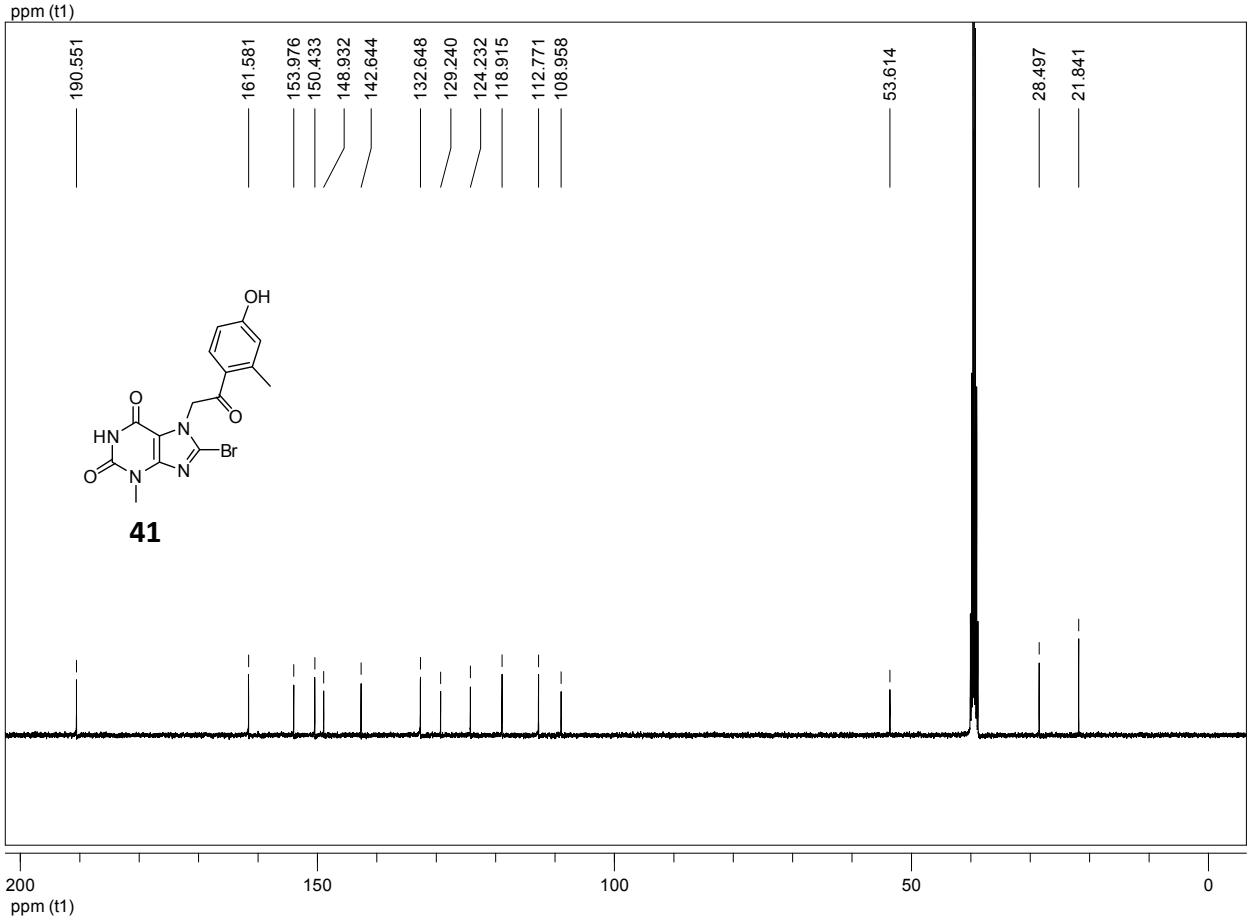

11.283
10.640
7.982
7.965
6.942
6.925
5.811
3.362
OH
O
HN
N
Br
O
N
N
O
39
1.15
1.00
2.05
2.14
2.05
3.16
10.0
5.0
0.0
ppm (t1)

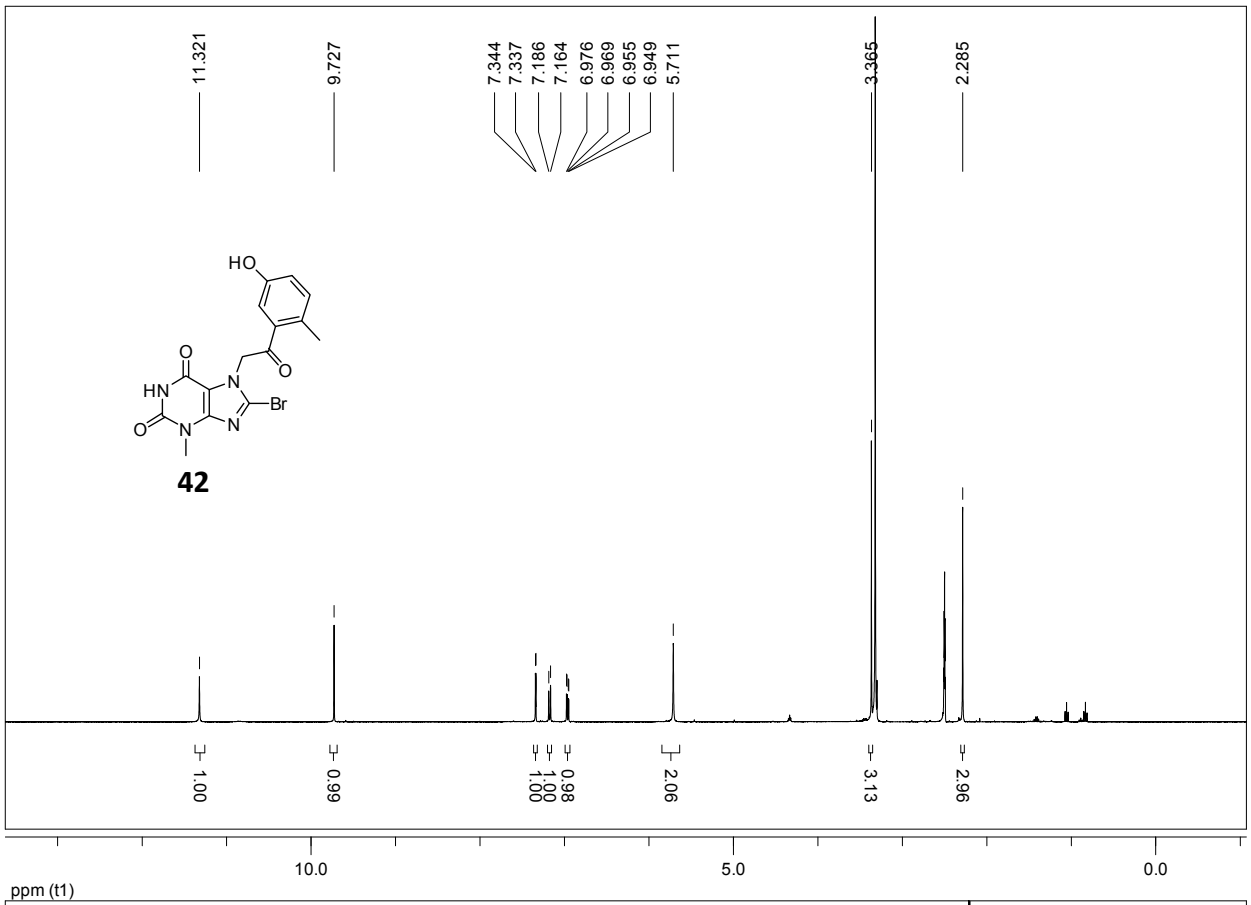

188.821
163.162
153.943
150.410
148.928
130.821
129.181
125.006
115.582
108.955
52.389
28.489
OH
O
HN
N
Br
O
N
N
O
39
150
100
50
0
ppm (t1)

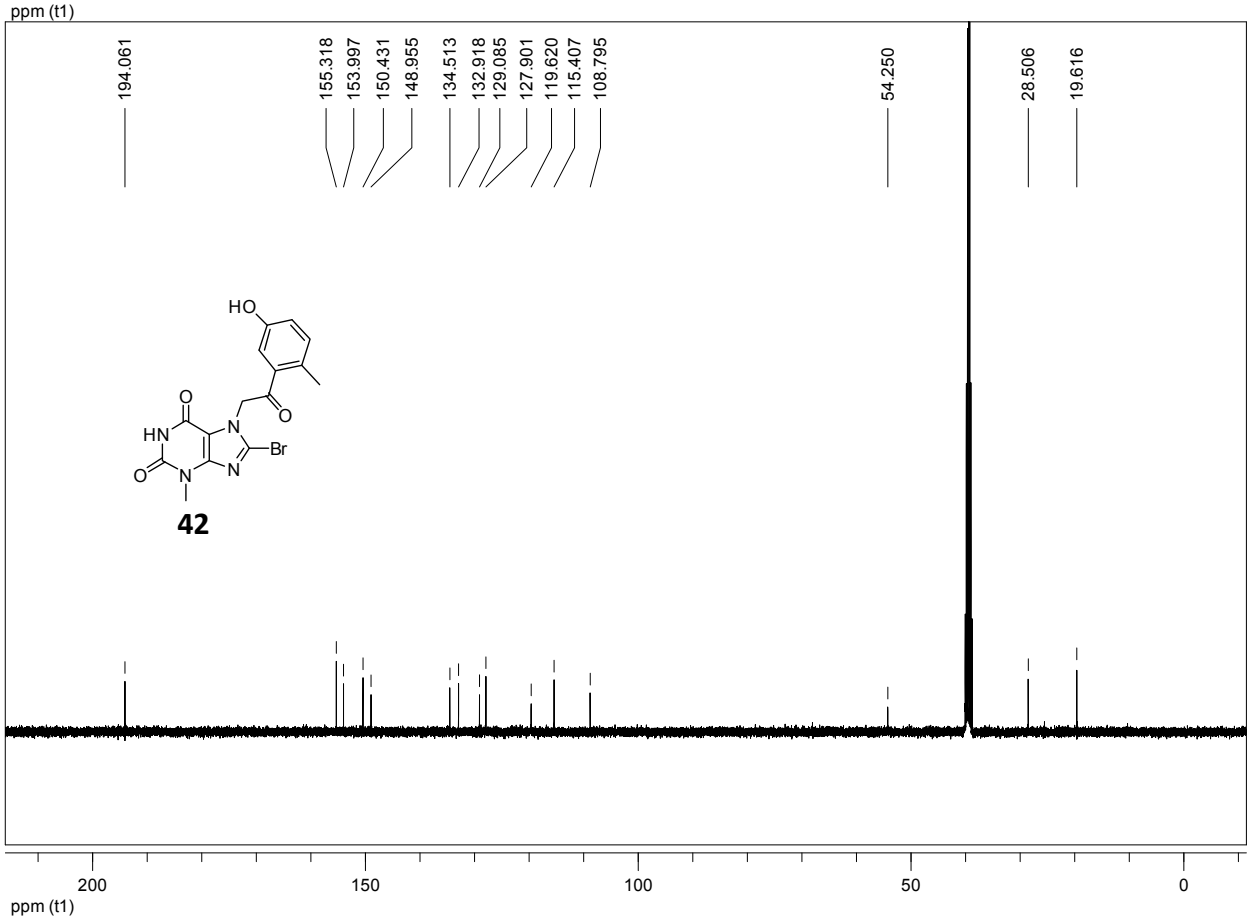

11.323
9.803
7.380
7.378
7.361
7.358
7.242
7.222
7.203
7.086
7.085
7.066
5.700
3.364
2.180
OH
O
HN
N
Br
O
N
O
40
1.00
0.99
1.00
1.00
0.99
2.05
2.92
2.89
10.0
5.0
0.0
ppm (t1)

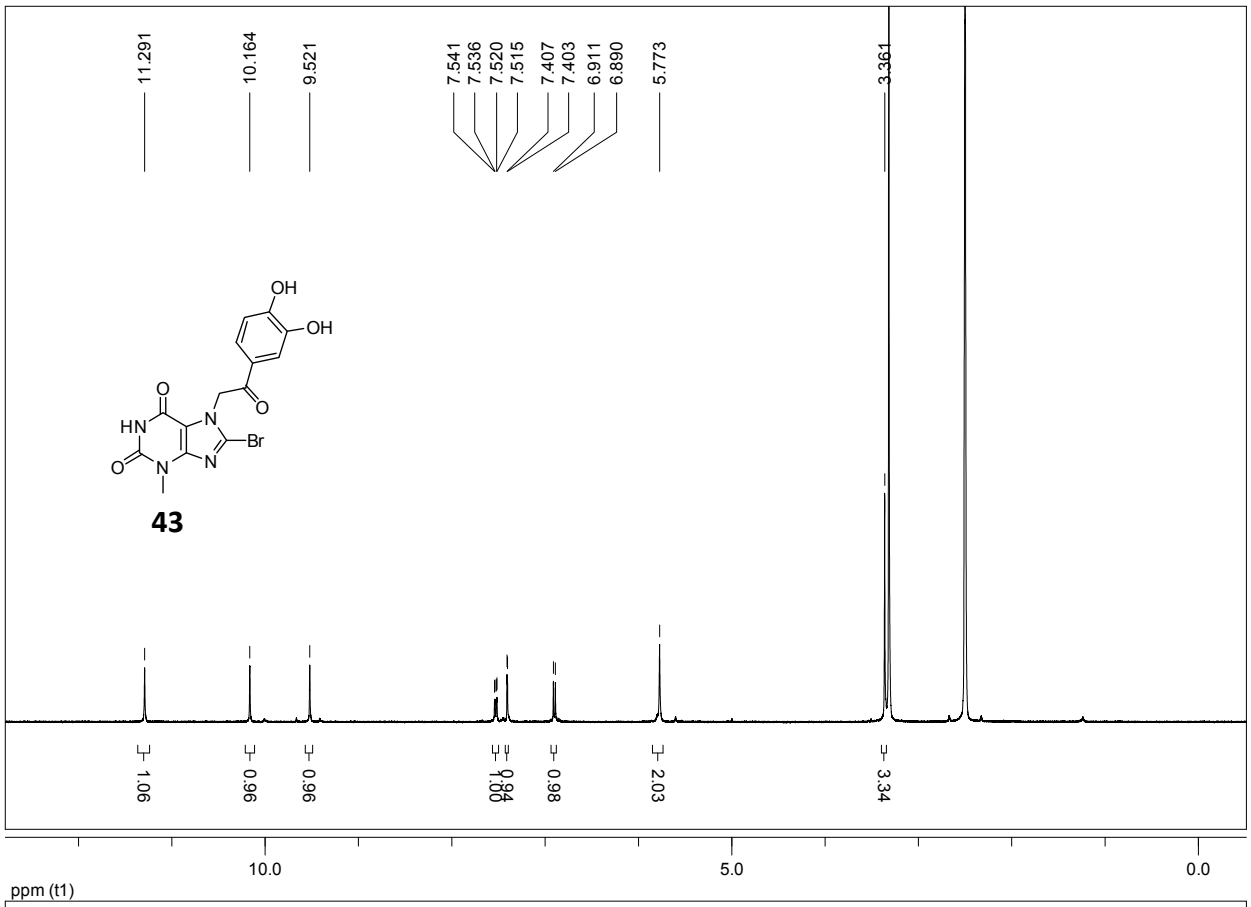

195.078
156.104
153.993
150.421
148.959
136.001
129.021
126.434
123.649
118.908
118.633
108.787
54.652
28.505
12.190
OH
O
HN
N
Br
O
N
O
40
200
150
100
50
0
ppm (t1)

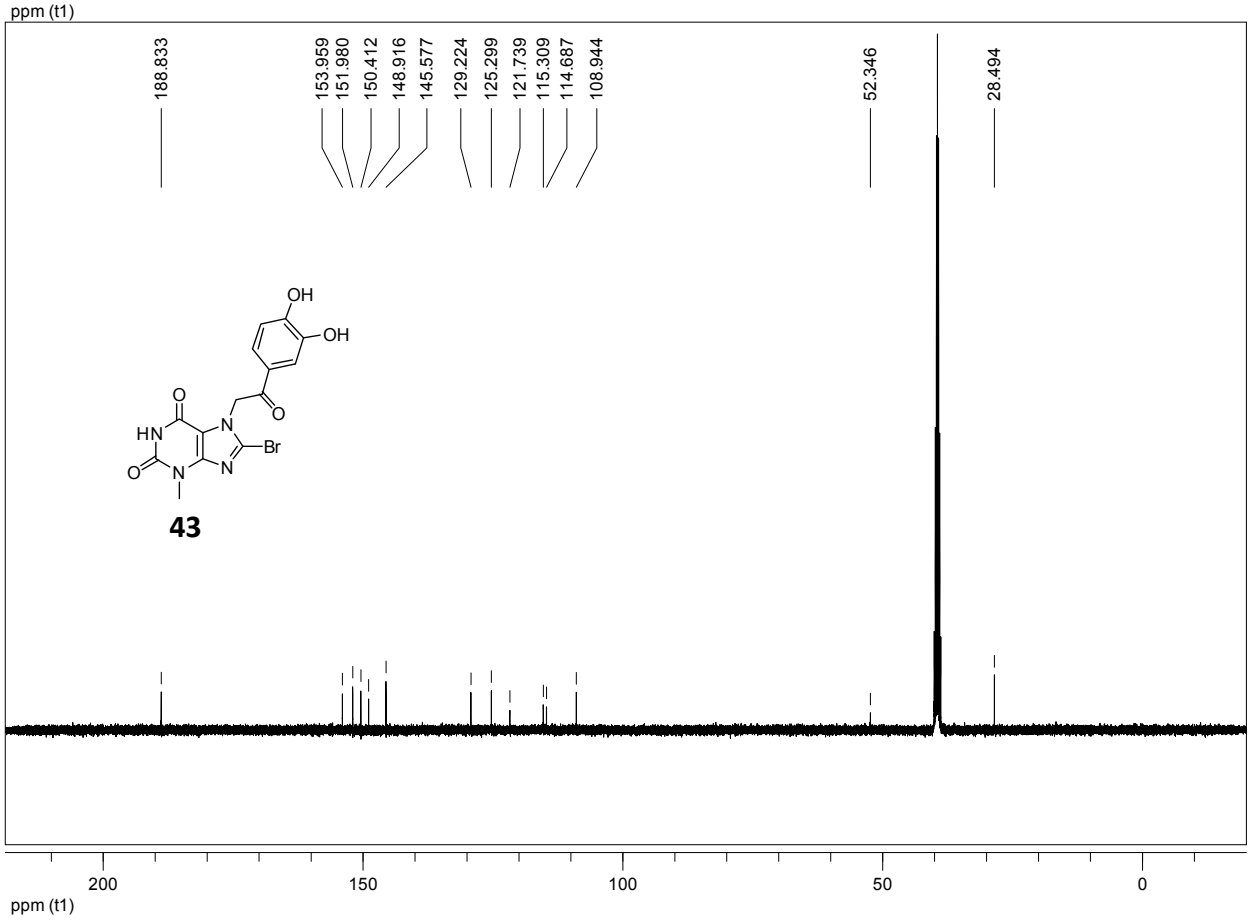

11.280
10.454
8.014
7.993
6.794
6.788
6.773
6.766
6.738
6.733
5.727
3.361
2.393
OH
O
HN
O
N
N
Br
O
O
N
41
0.94
0.94
1.00
0.96
0.96
1.95
2.83
2.89
10.0
5.0
0.0
ppm (t1)

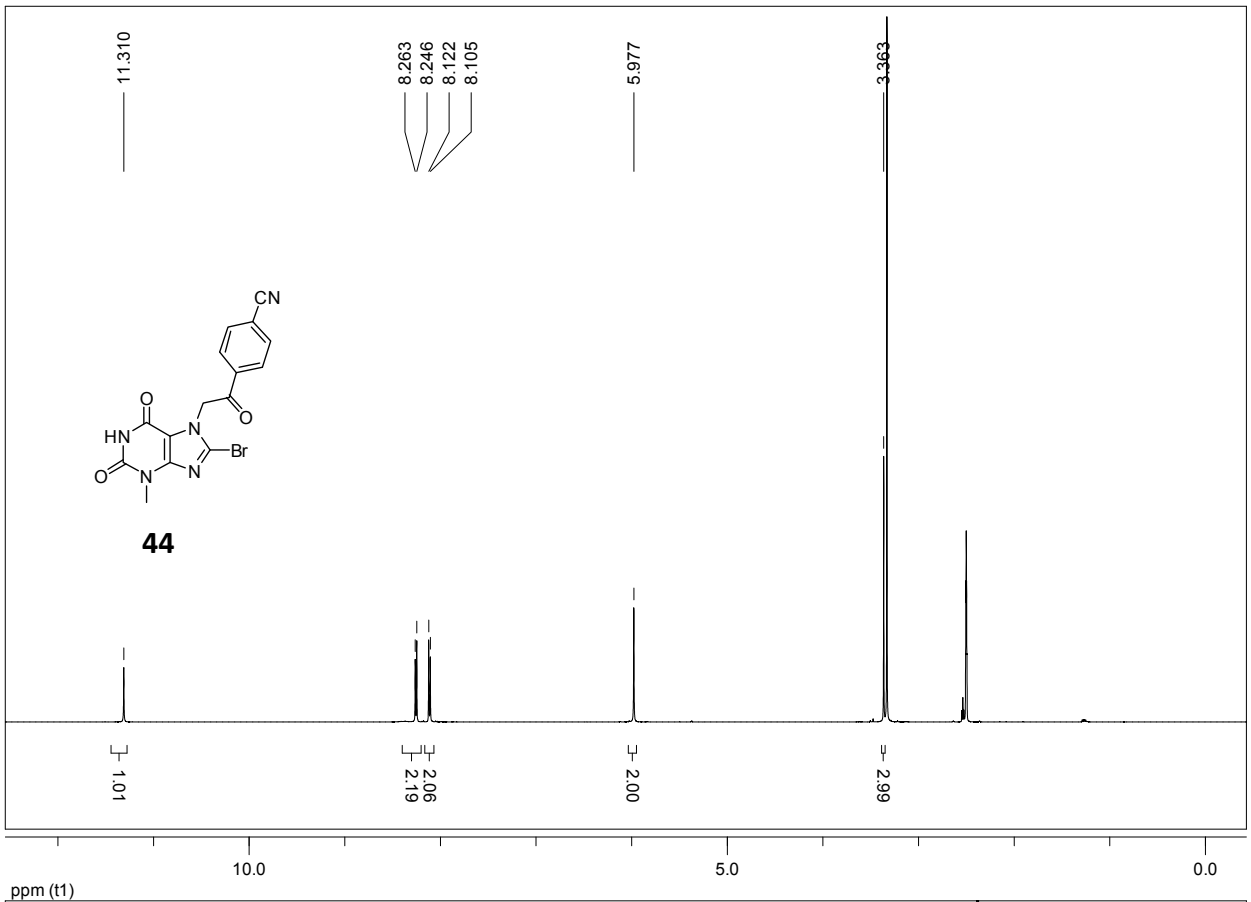

190.551
161.581
153.976
150.433
148.932
142.644
132.648
129.240
124.232
118.915
112.771
108.958
53.614
28.497
21.841
OH
O
HN
O
N
N
Br
O
O
N
41
200
150
100
50
0
ppm (t1)

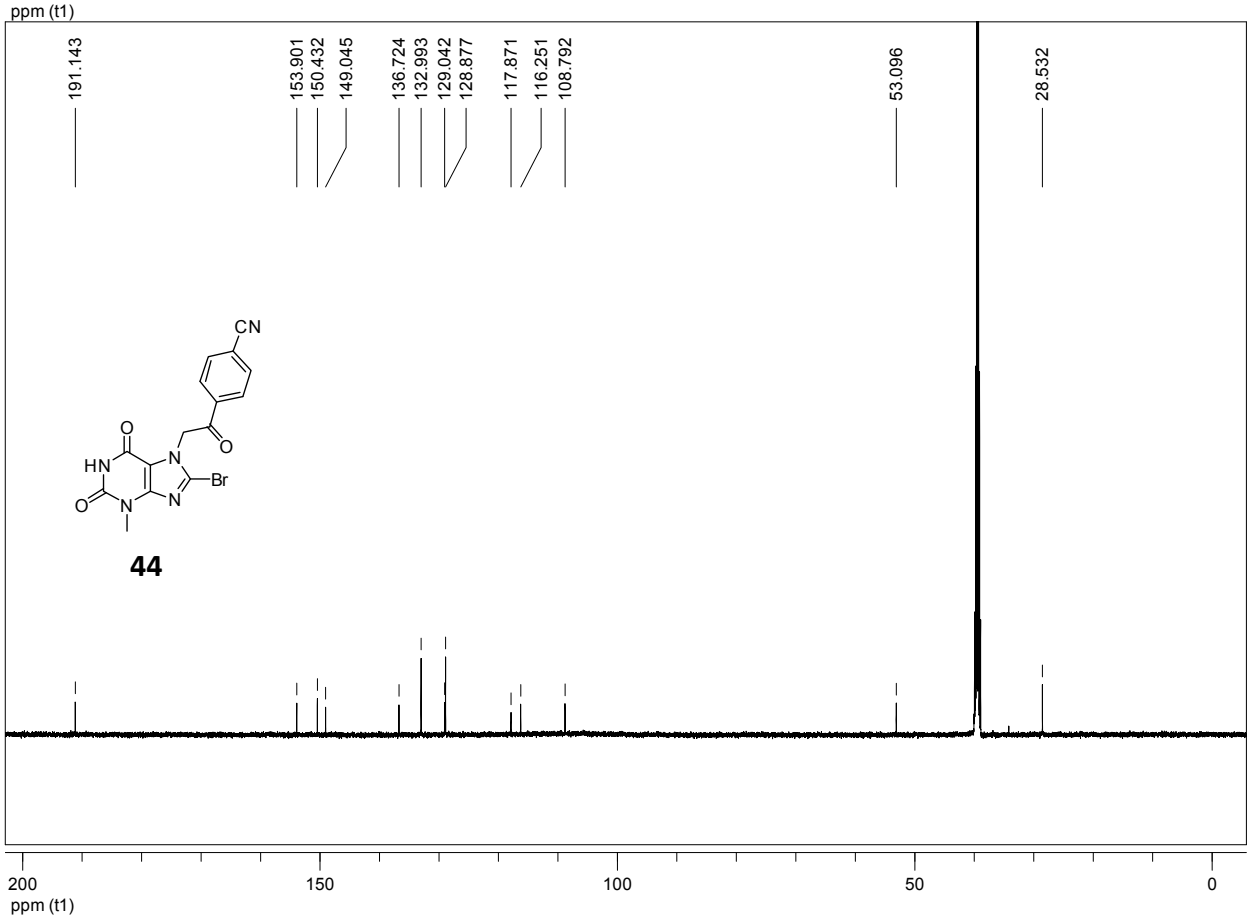

11.321
9.727
7.344
7.337
7.186
7.164
6.976
6.969
6.955
6.949
5.711
3.365
2.285
HO
O
HN
N
Br
O
N
O
42
1.00
0.99
1.00
1.00
0.98
2.06
3.13
2.96
10.0
5.0
0.0
ppm (t1)

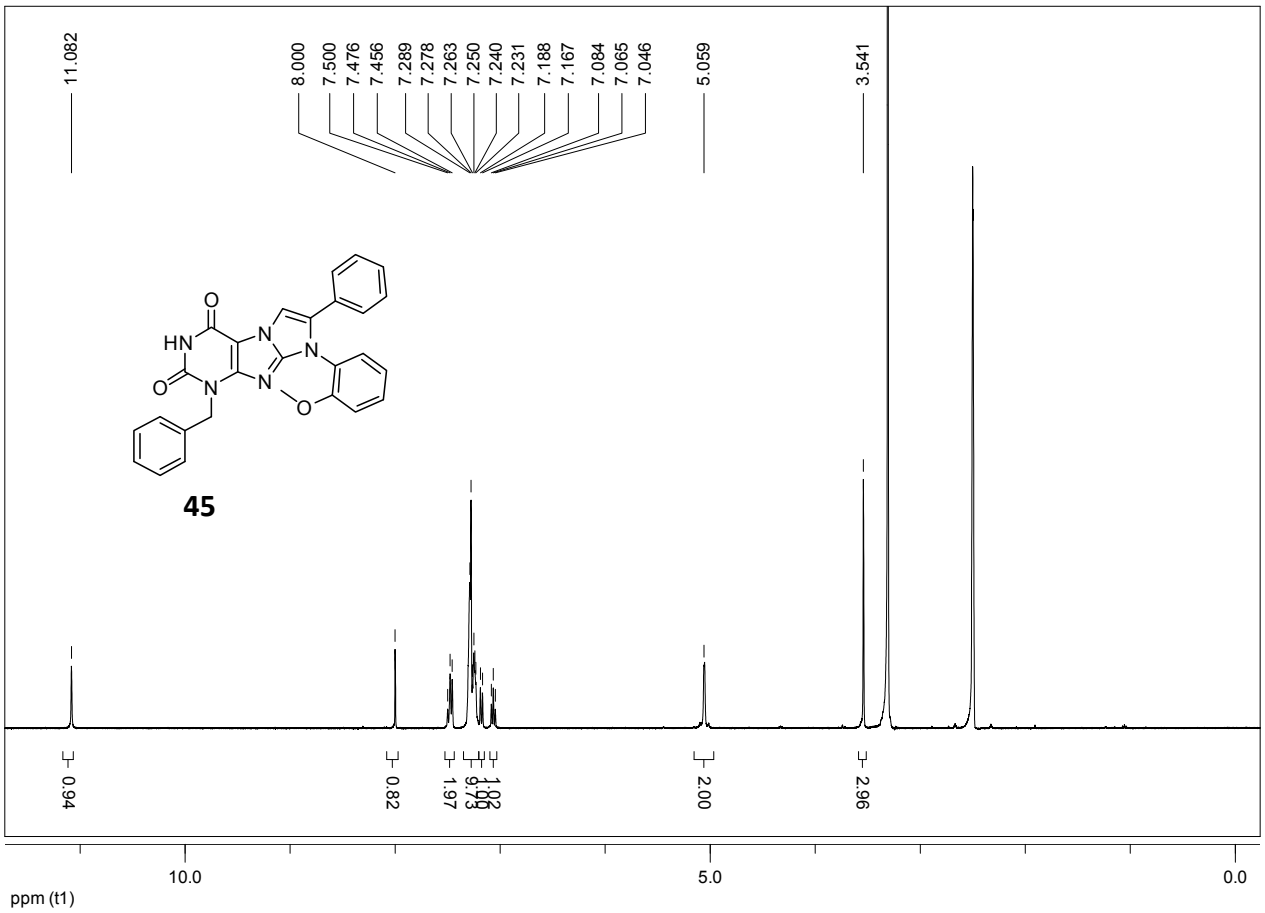

194.061
155.318
153.997
150.431
148.955
134.513
132.918
129.085
127.901
119.620
115.407
108.795
54.250
28.506
19.616
HO
O
HN
N
Br
O
N
O
42
200
150
100
50
0
ppm (t1)


11.291
10.164
9.521
7.541
7.536
7.520
7.515
7.407
7.403
6.911
6.890
5.773
3.361
OH
OH
O
HN
O
N
Br
N
N
O
O
43
1.06
0.96
0.96
1.00
0.98
2.03
3.34
10.0
5.0
0.0
ppm (t1)

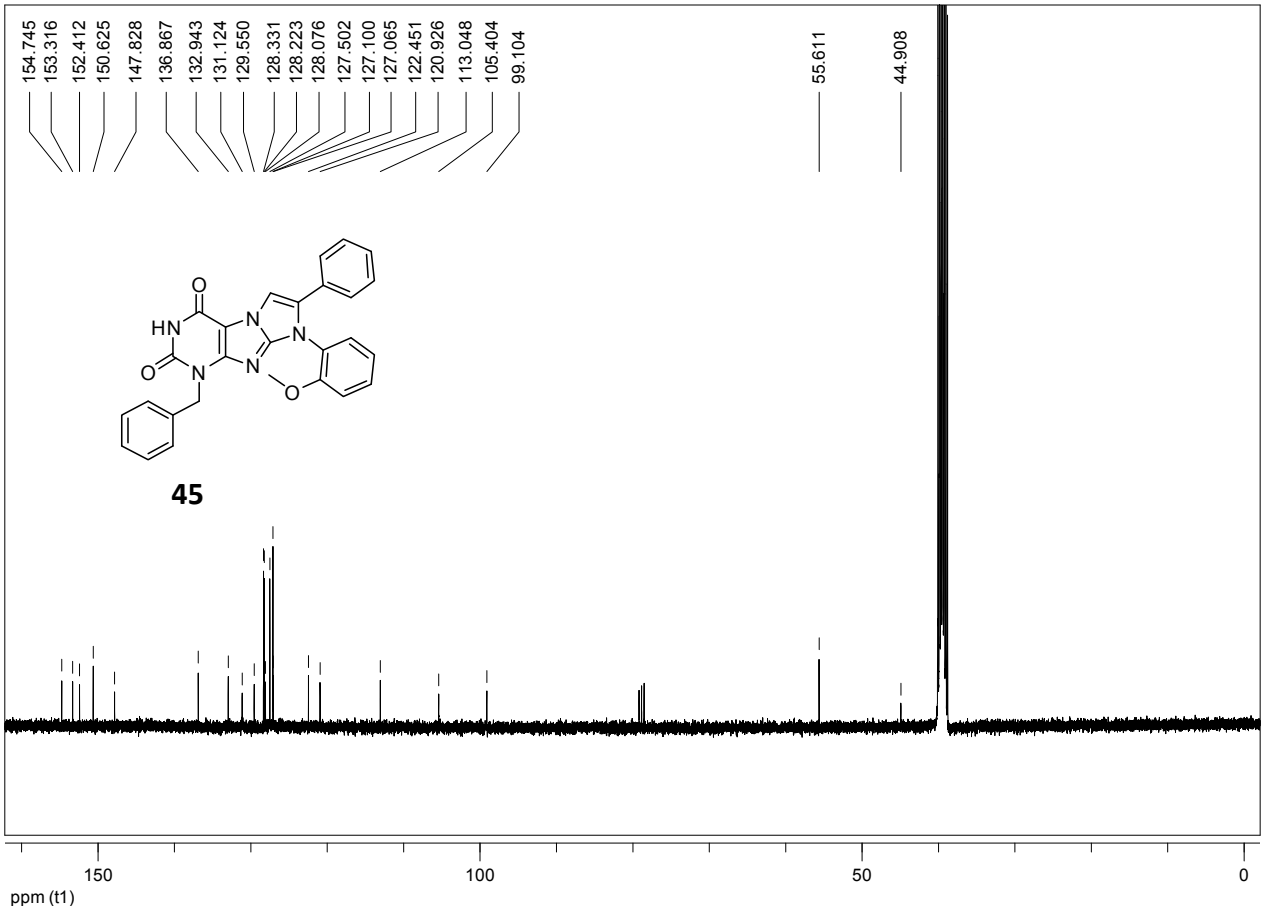

188.833
153.959
151.980
150.412
148.916
145.577
129.224
125.299
121.739
115.309
114.687
108.944
52.346
28.494
OH
OH
O
HN
O
N
Br
N
N
O
O
43
200
150
100
50
0
ppm (t1)


11.310
8.263
8.246
8.122
8.105
5.977
3.363
CN
O
HN
O
N
N
Br
N
O
O
44
1.01
2.19
2.06
2.00
2.99
10.0
5.0
0.0
ppm (t1)

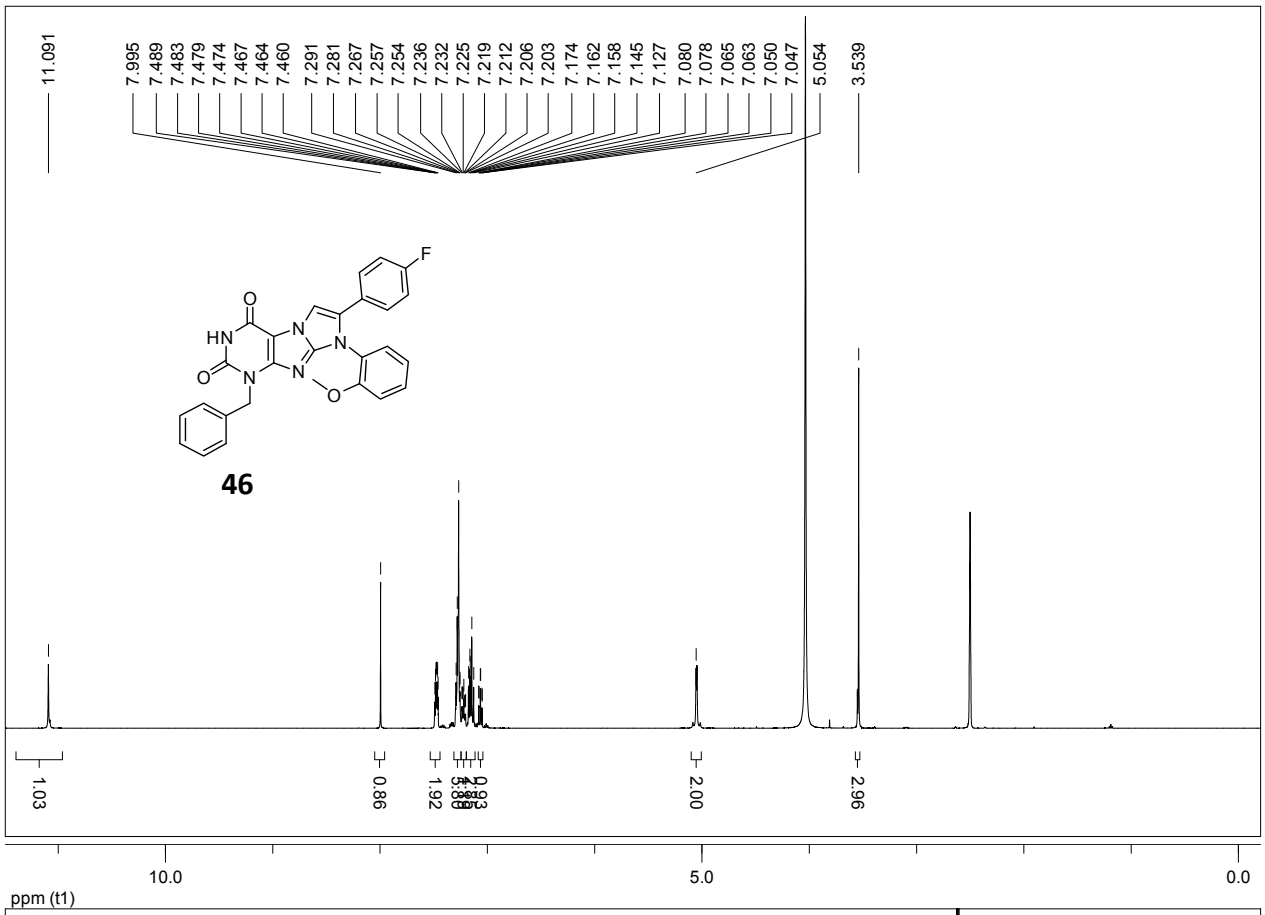

191.143
153.901
150.432
149.045
136.724
132.993
129.042
128.877
117.871
116.251
108.792
53.096
28.532
CN
O
HN
O
N
N
Br
N
O
O
44
200
150
100
50
0
ppm (t1)

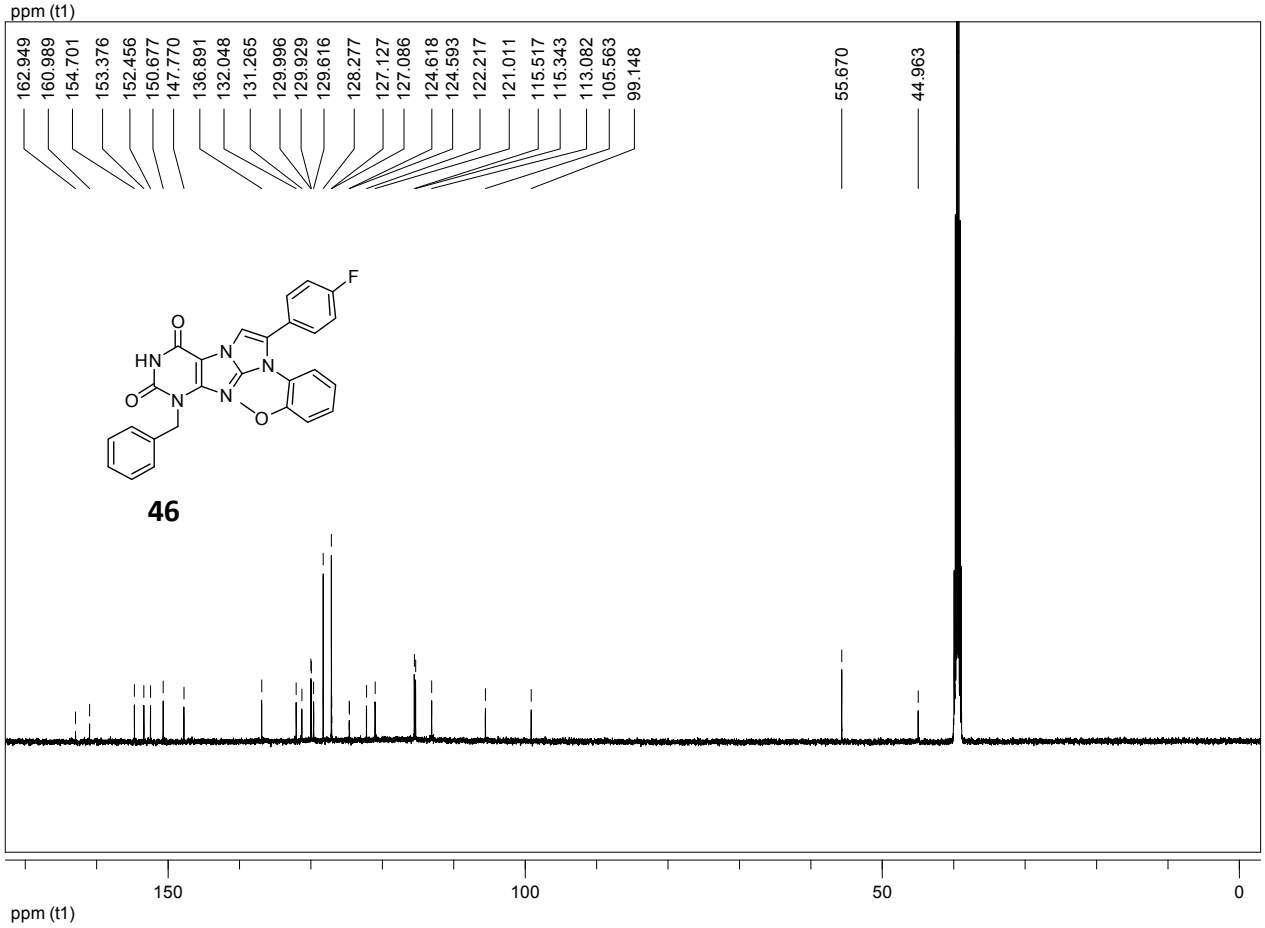

11.082
8.000
7.500
7.476
7.456
7.289
7.278
7.263
7.250
7.240
7.231
7.188
7.167
7.084
7.065
7.046
5.059
3.541
0.94
0.82
1.97
2.00
2.96
10.0
5.0
0.0
ppm (t1)

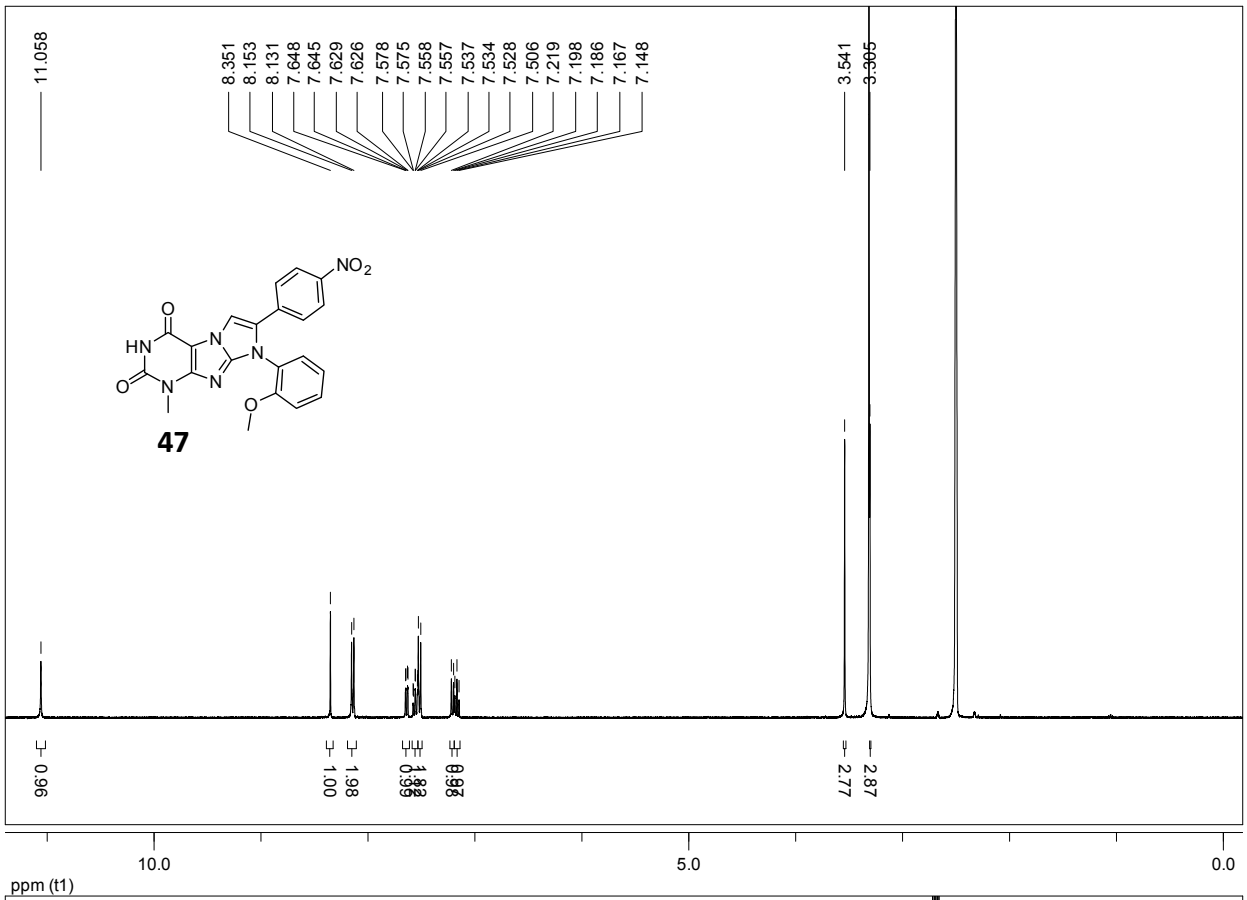
45

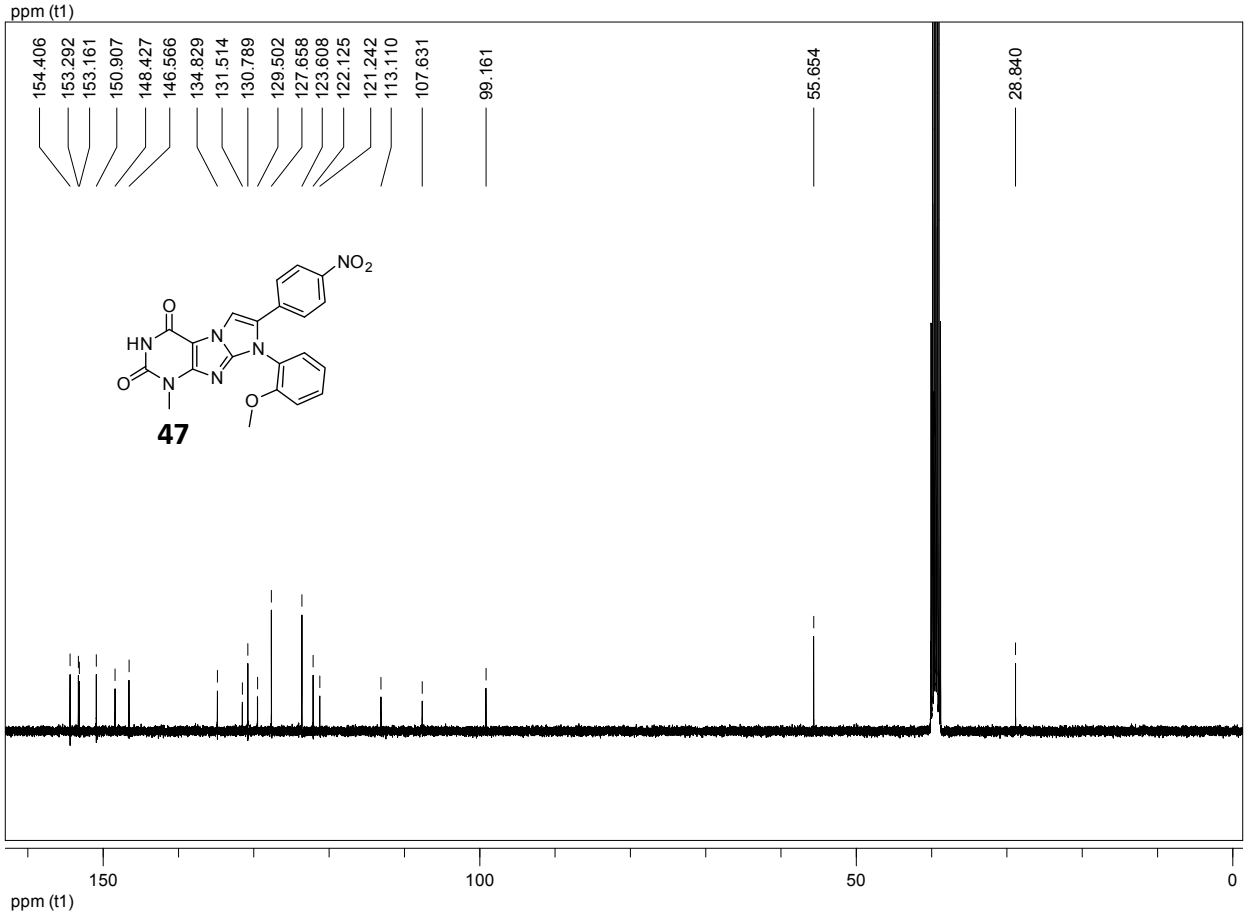

154.745
153.316
152.412
150.625
147.828
136.867
132.943
131.124
129.550
128.331
128.223
128.076
127.502
127.100
127.065
122.451
120.926
113.048
105.404
99.104
55.611
44.908
150
100
50
0
ppm (t1)

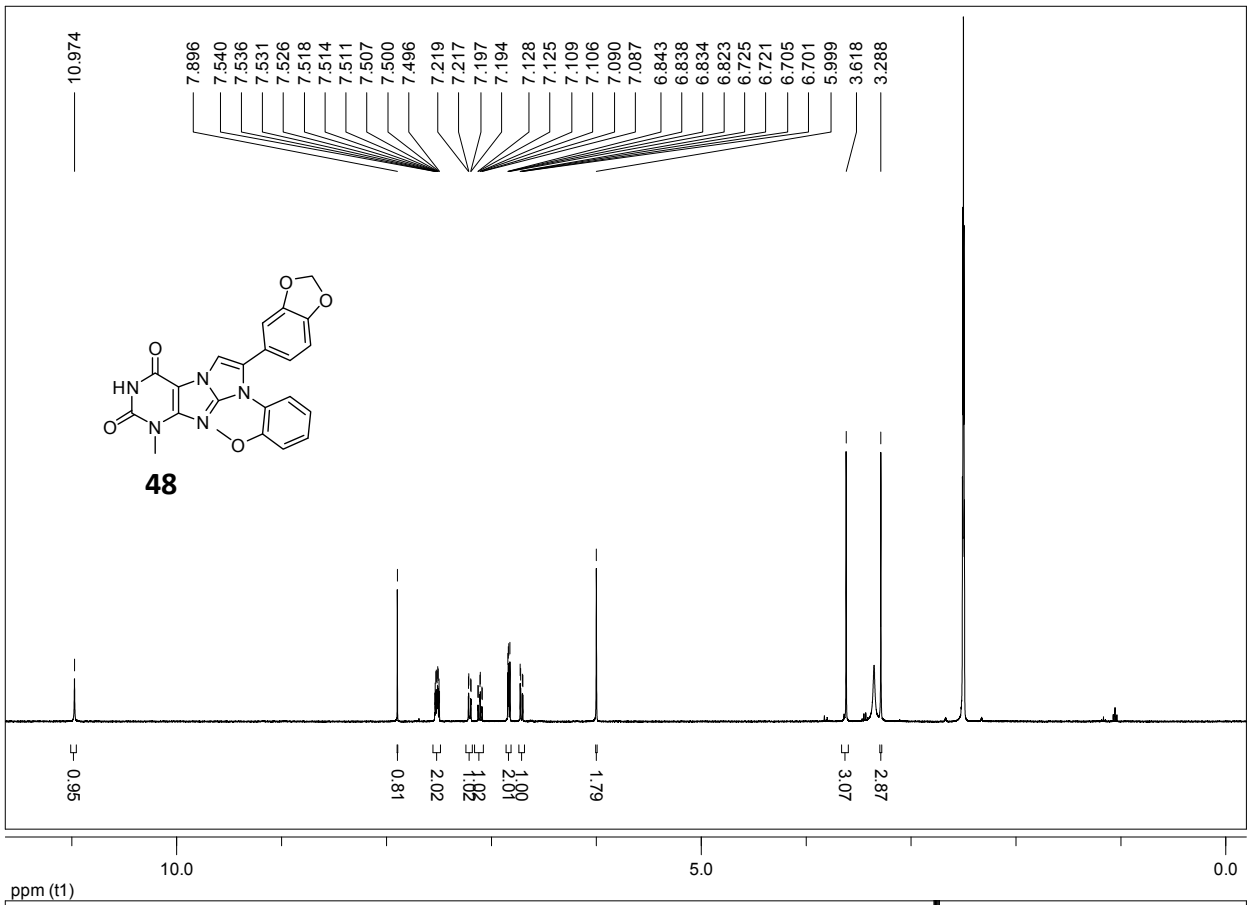
45


11.091
7.995
7.489
7.483
7.479
7.474
7.467
7.464
7.460
7.291
7.281
7.267
7.257
7.254
7.236
7.232
7.225
7.219
7.212
7.206
7.203
7.174
7.162
7.158
7.145
7.127
7.080
7.078
7.065
7.063
7.050
7.047
5.054
3.539
F
O
HN
O
N
N
N
N
O
46
1.03
0.86
1.92
2.00
2.96
10.0
5.0
0.0
ppm (t1)

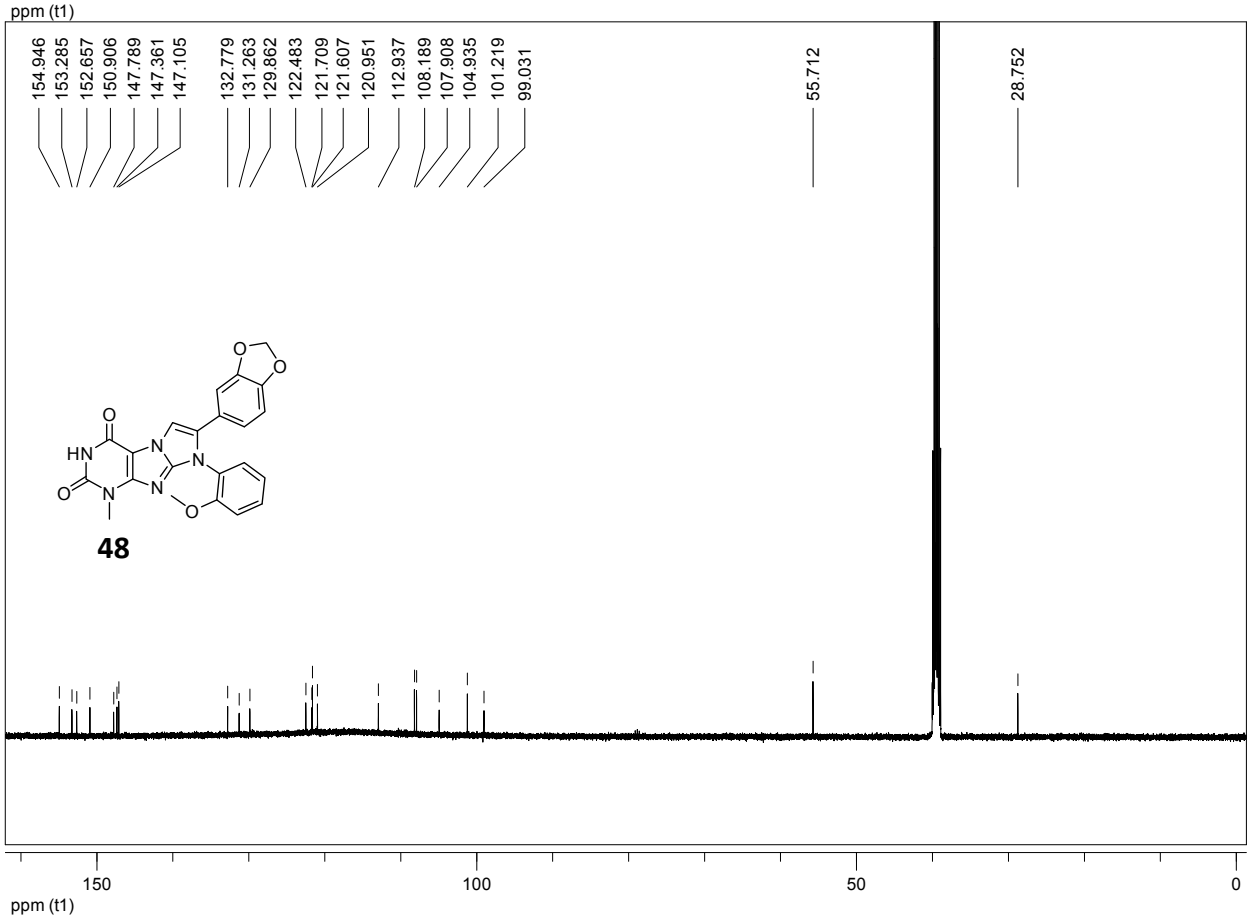

162.949
160.989
154.701
153.376
152.456
150.677
147.770
136.891
132.048
131.265
129.996
129.929
129.616
128.277
127.127
127.086
124.618
124.593
122.217
121.011
115.517
115.343
113.082
105.563
99.148
55.670
44.963
F
O
HN
O
N
N
N
N
O
46
150
100
50
0
ppm (t1)


11.058
8.351
8.153
8.131
7.648
7.645
7.629
7.626
7.578
7.575
7.558
7.557
7.537
7.534
7.528
7.506
7.219
7.198
7.186
7.167
7.148
3.541
3.305
NO2
O
HN
O
N
N
N
N
O
47
0.96
1.00
1.98
2.77
2.87
10.0
5.0
0.0
ppm (t1)

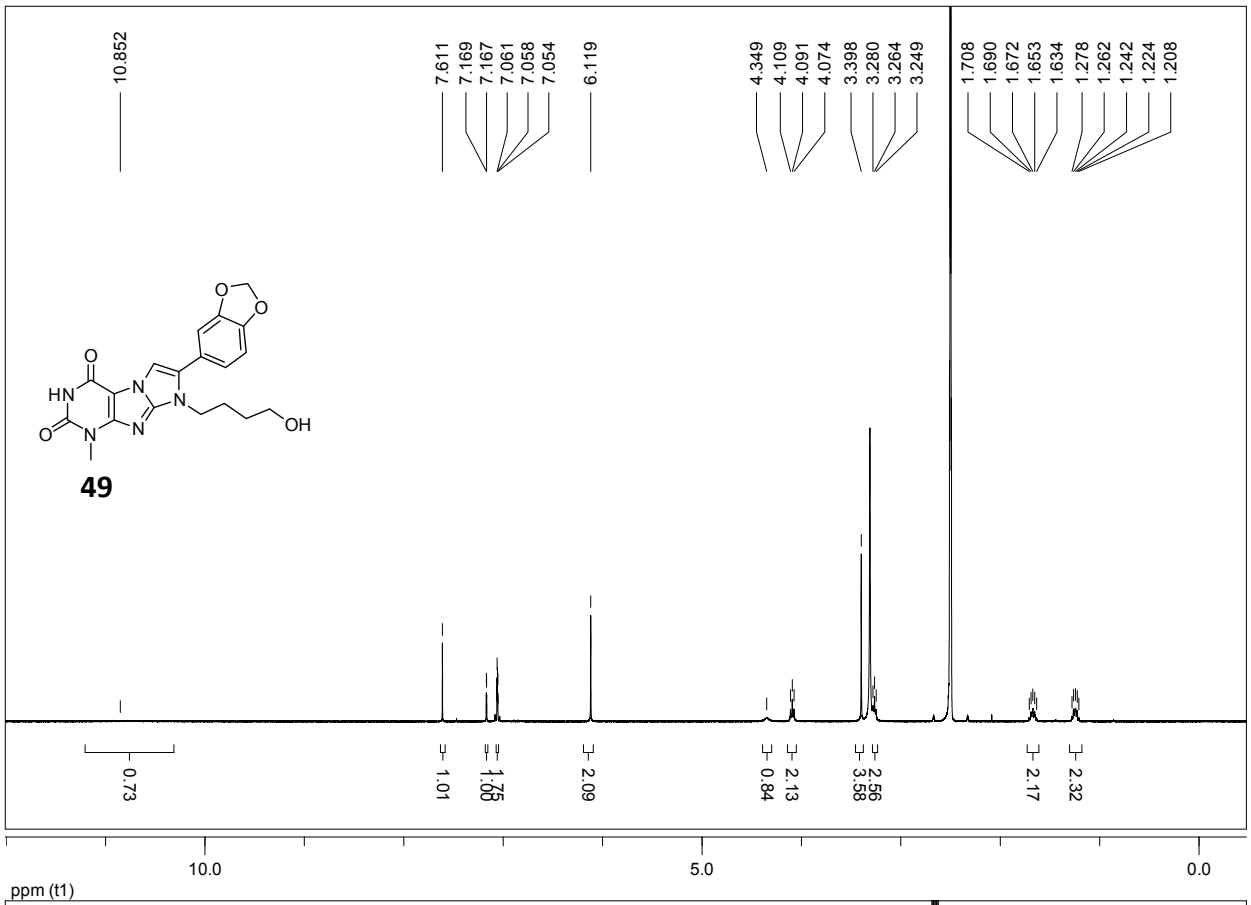

154.406
153.292
153.161
150.907
148.427
146.566
134.829
131.514
130.789
129.502
127.658
123.608
122.125
121.242
113.110
107.631
99.161
55.654
28.840
NO2
O
HN
O
N
N
N
N
O
47
150
100
50
0
ppm (t1)


10.974
7.896
7.540
7.536
7.531
7.526
7.518
7.514
7.511
7.507
7.500
7.496
7.219
7.217
7.197
7.194
7.128
7.125
7.109
7.106
7.090
7.087
6.843
6.838
6.834
6.823
6.725
6.721
6.705
6.701
5.999
3.618
3.288
0.95
0.81
2.02
1.02
1.02
2.01
1.00
1.79
3.07
2.87
10.0
5.0
0.0
ppm (t1)

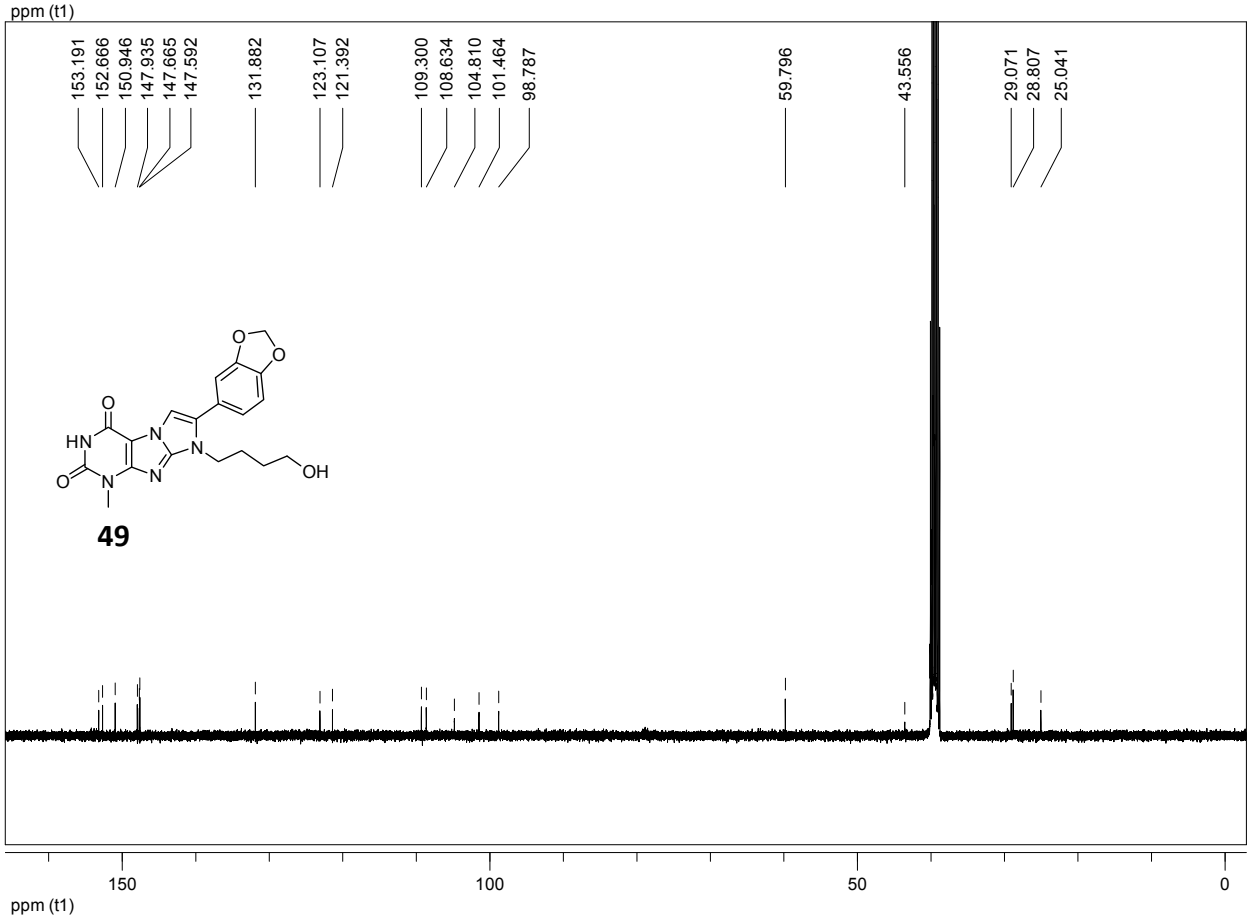
48


154.946
153.285
152.657
150.906
147.789
147.361
147.105
132.779
131.263
129.862
122.483
121.709
121.607
120.951
112.937
108.189
107.908
104.935
101.219
99.031
55.712
28.752
150
100
50
0
ppm (t1)

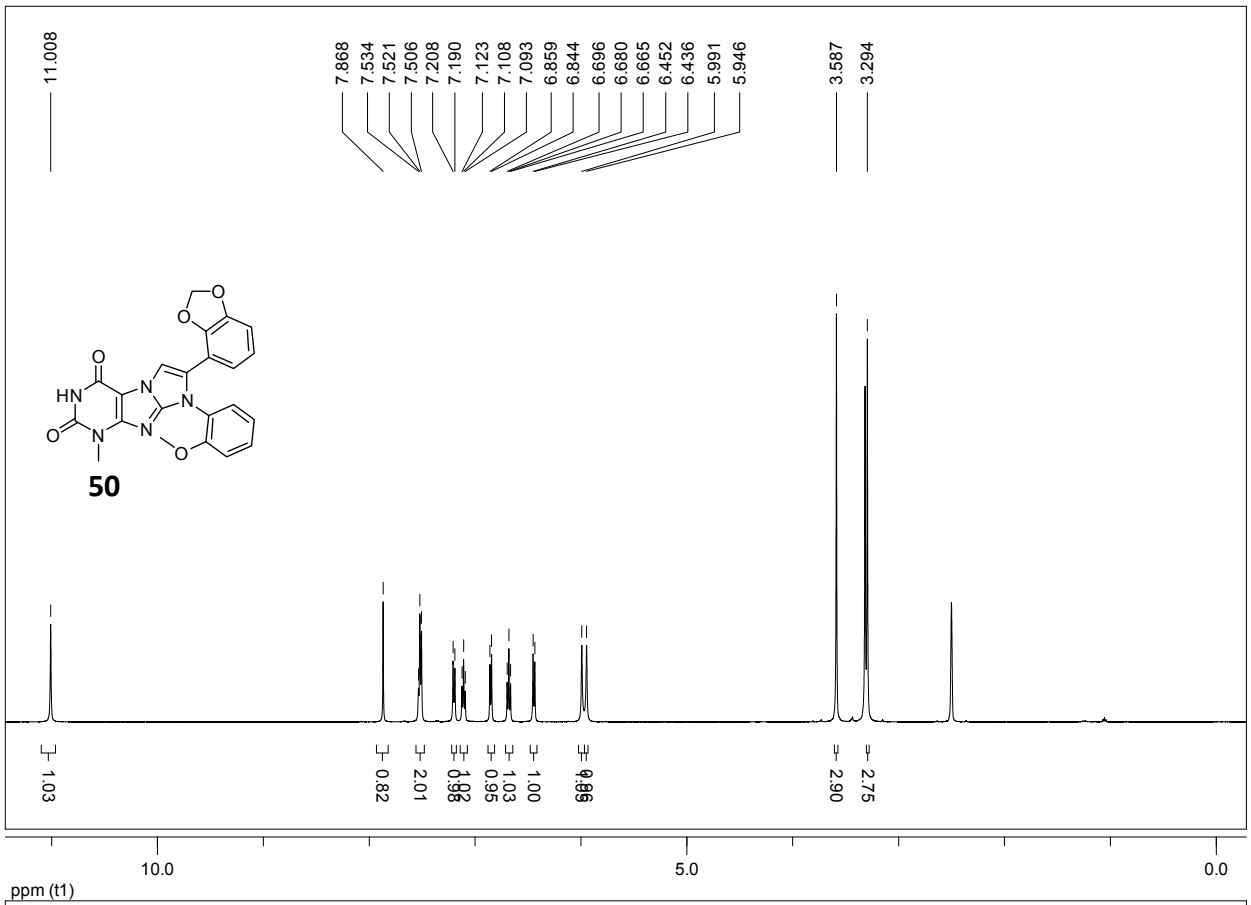
48


10.852
7.611
7.169
7.167
7.061
7.058
7.054
6.119
4.349
4.109
4.091
4.074
3.398
3.280
3.264
3.249
1.708
1.690
1.672
1.653
1.634
1.278
1.262
1.242
1.224
1.208
0.73
1.01
1.00
1.75
2.09
0.84
2.13
3.58
2.56
2.17
2.32
10.0
5.0
0.0
ppm (t1)

49


153.191
152.666
150.946
147.935
147.665
147.592
131.882
123.107
121.392
109.300
108.634
104.810
101.464
98.787
59.796
43.556
29.071
28.807
25.041
150
100
50
0
ppm (t1)

49


11.008
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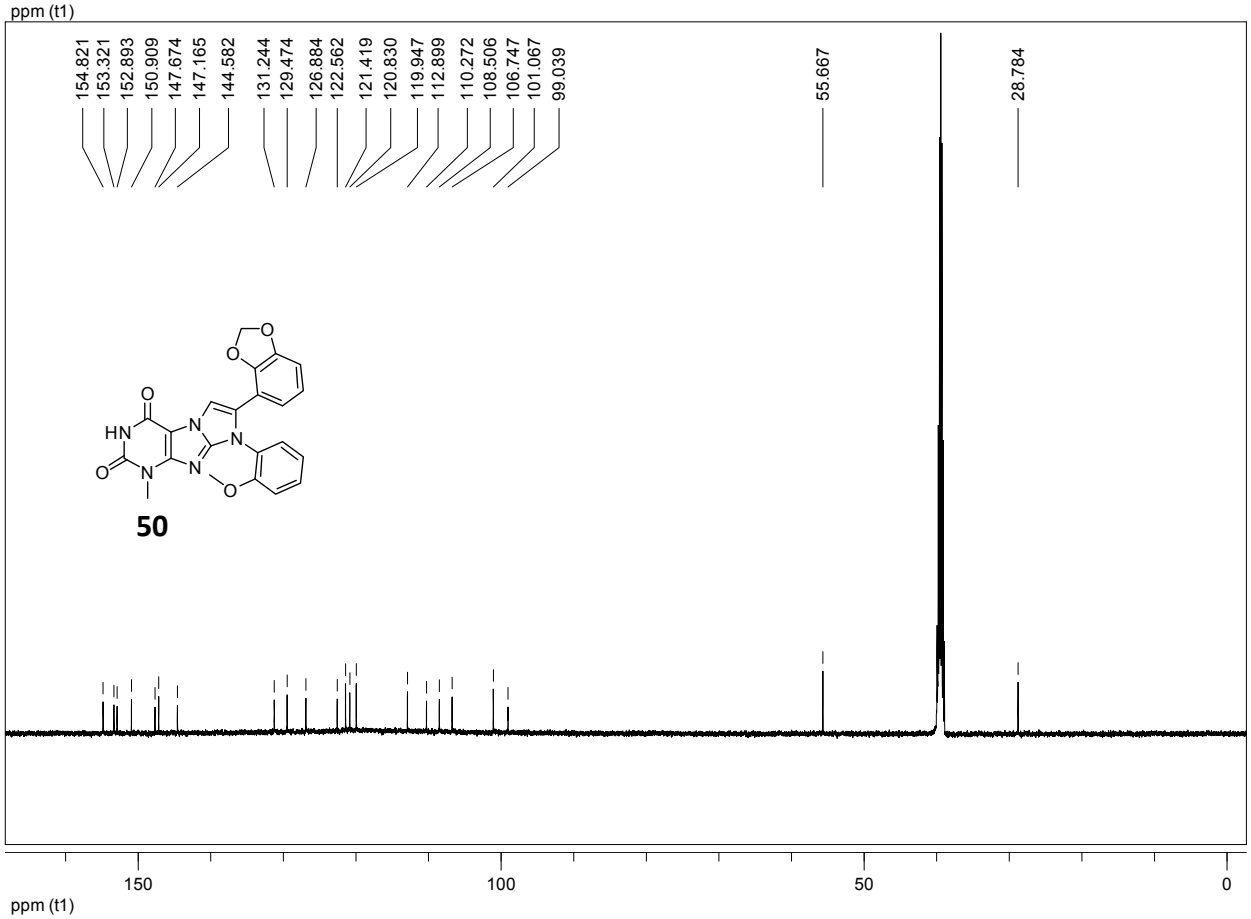
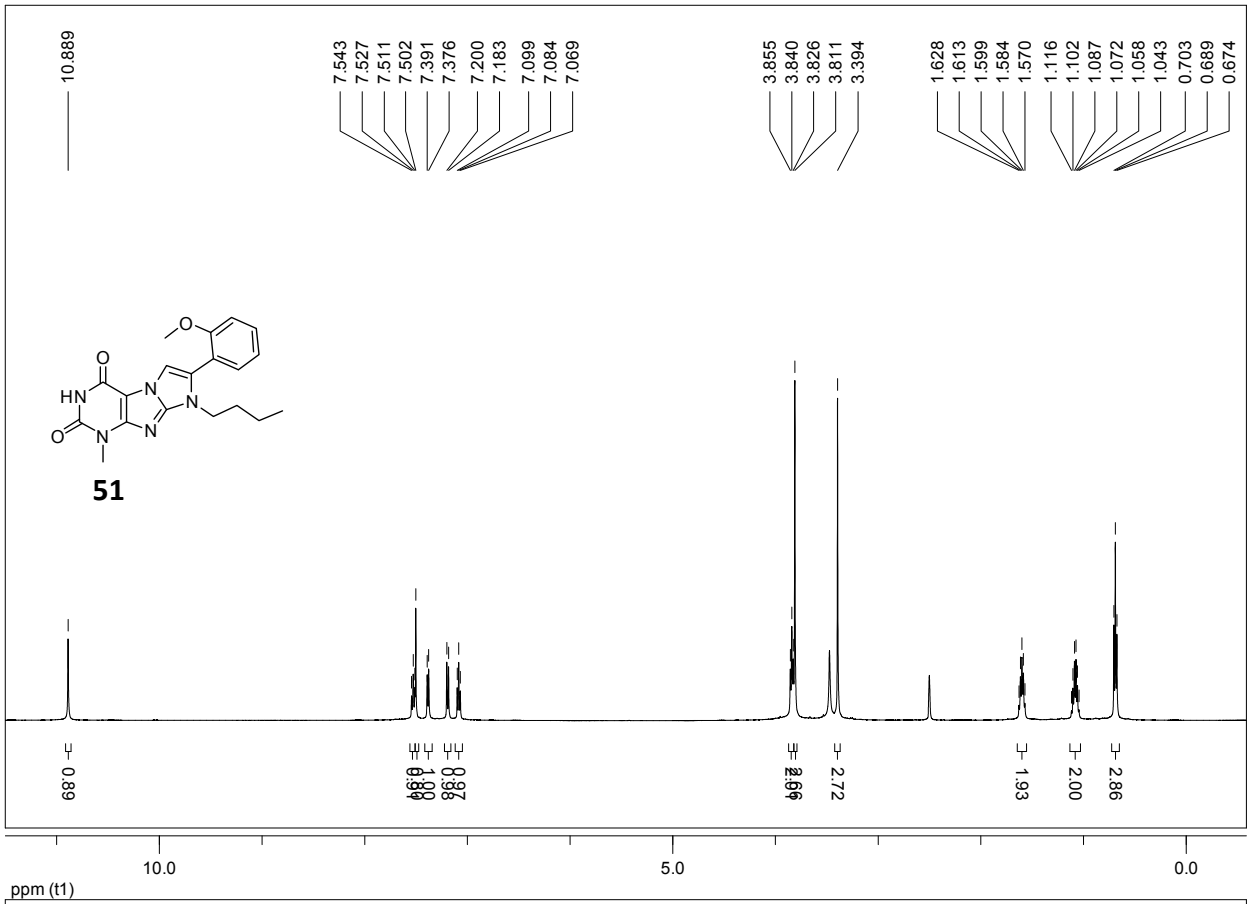
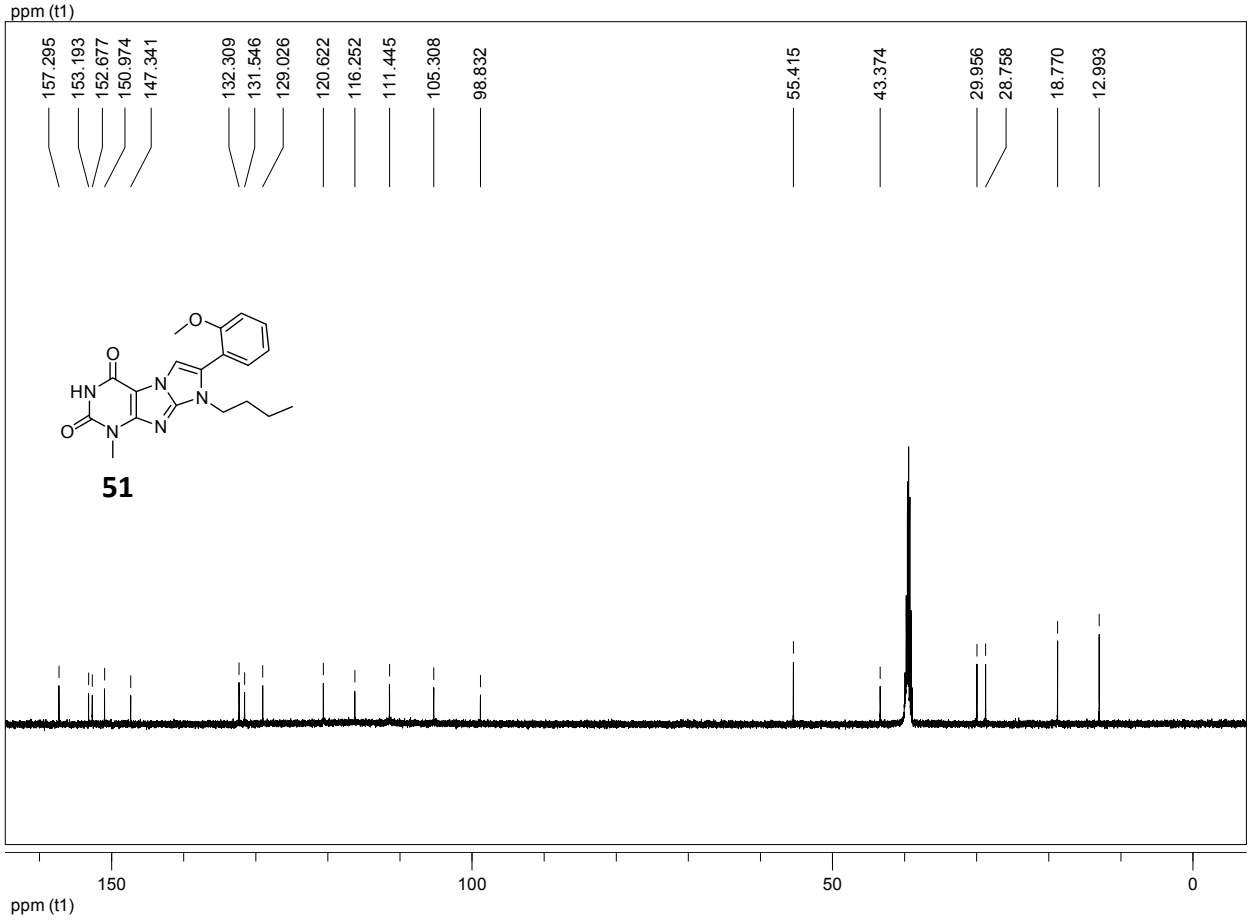
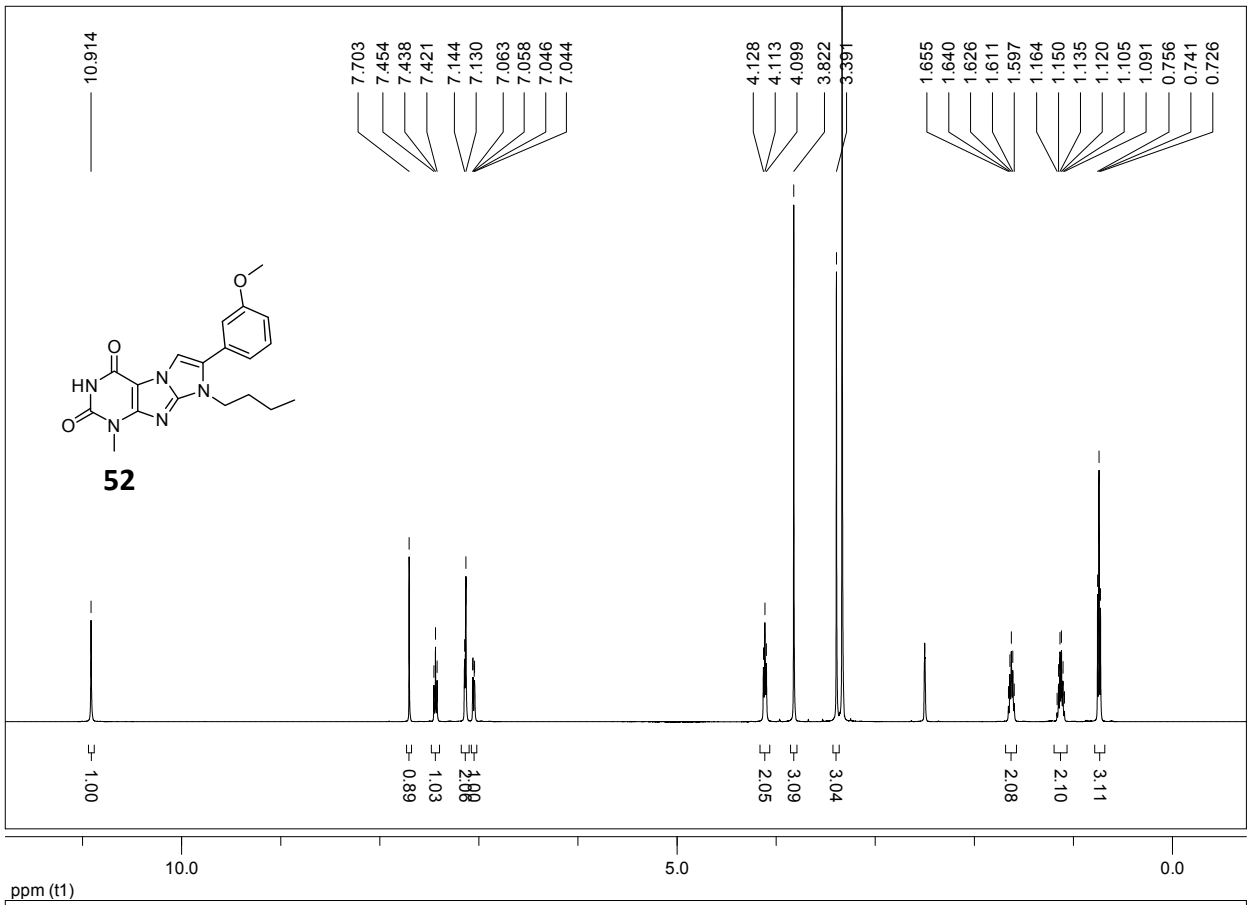
7.534
7.521
7.506
7.208
7.190
7.123
7.108
7.093
6.859
6.844
6.696
6.680
6.665
6.452
6.436
5.991
5.946
3.587
3.294
50
1.03
0.82
2.01
1.03
1.00
2.90
2.75
10.0
5.0
0.0
ppm (t1)

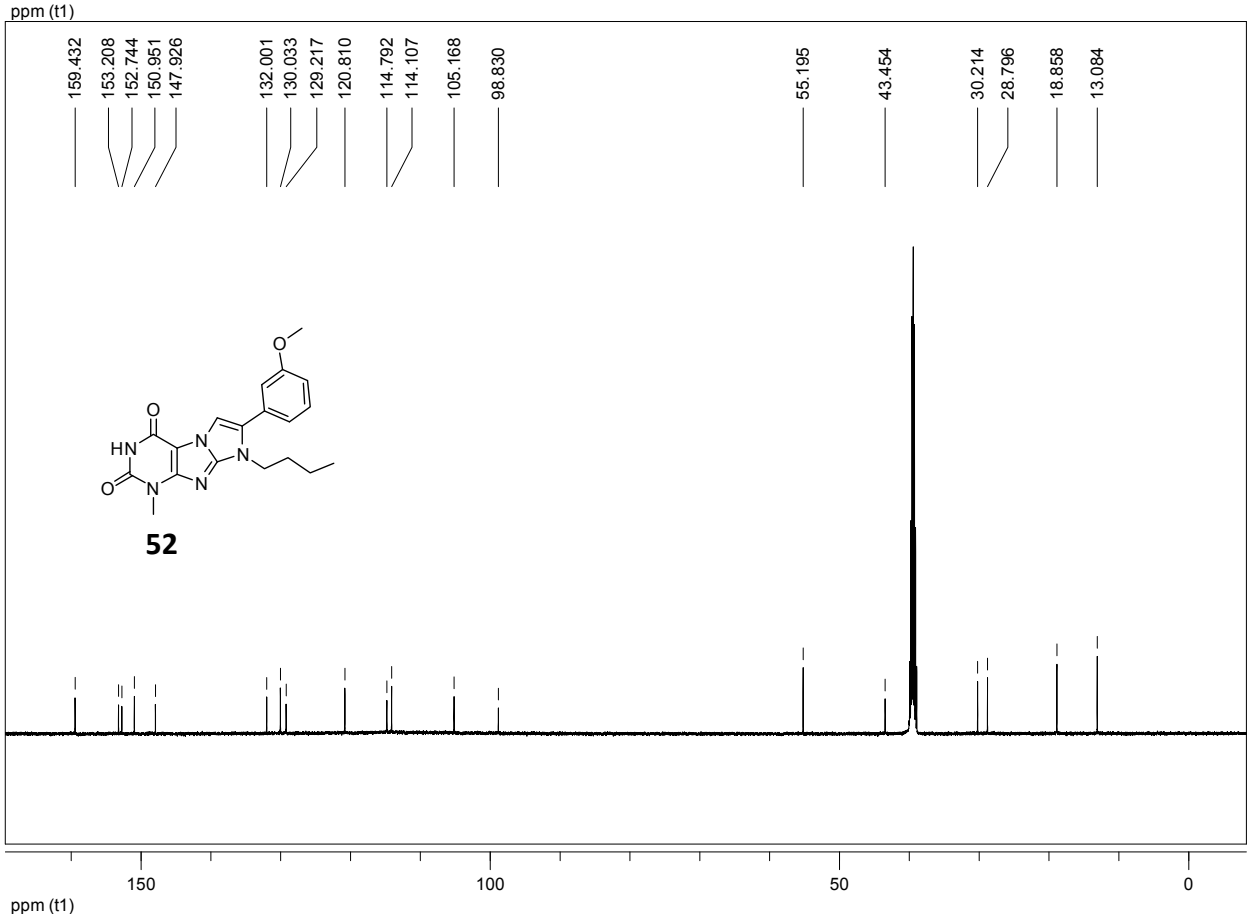

154.821
153.321
152.893
150.909
147.674
147.165
144.582
131.244
129.474
126.884
122.562
121.419
120.830
119.947
112.899
110.272
108.506
106.747
101.067
99.039
55.667
28.784
50
150
100
50
0
ppm (t1)


10.889
7.543
7.527
7.511
7.502
7.391
7.376
7.200
7.183
7.099
7.084
7.069
3.855
3.840
3.826
3.811
3.394
1.628
1.613
1.599
1.584
1.570
1.116
1.102
1.087
1.072
1.058
1.043
0.703
0.689
0.674
51
0.89
1.00
0.98
0.97
2.72
1.93
2.00
2.89
10.0
5.0
0.0
ppm (t1)

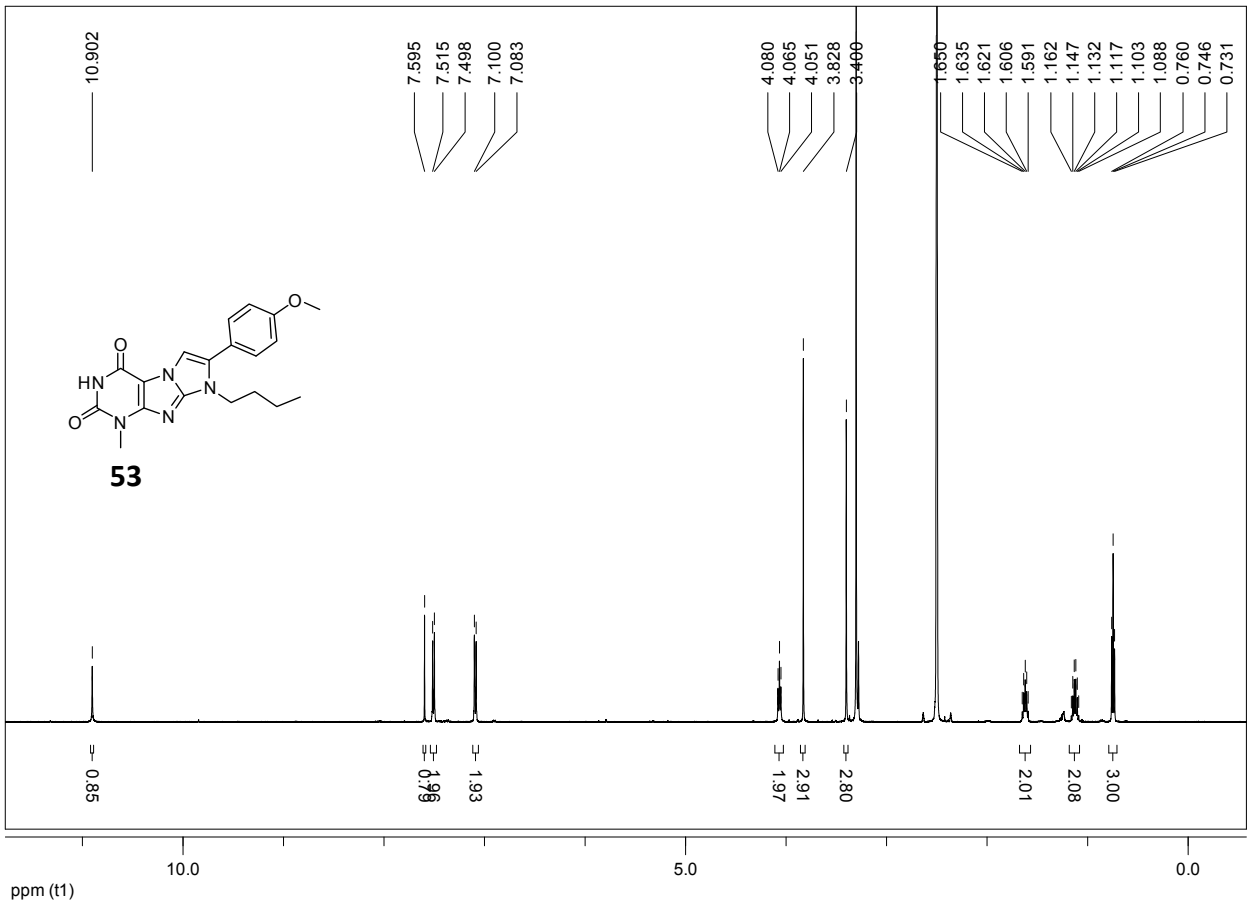

157.295
153.193
152.677
150.974
147.341
132.309
131.546
129.026
120.622
116.252
111.445
105.308
98.832
55.415
43.374
29.956
28.758
18.770
12.993
51
150
100
50
0
ppm (t1)

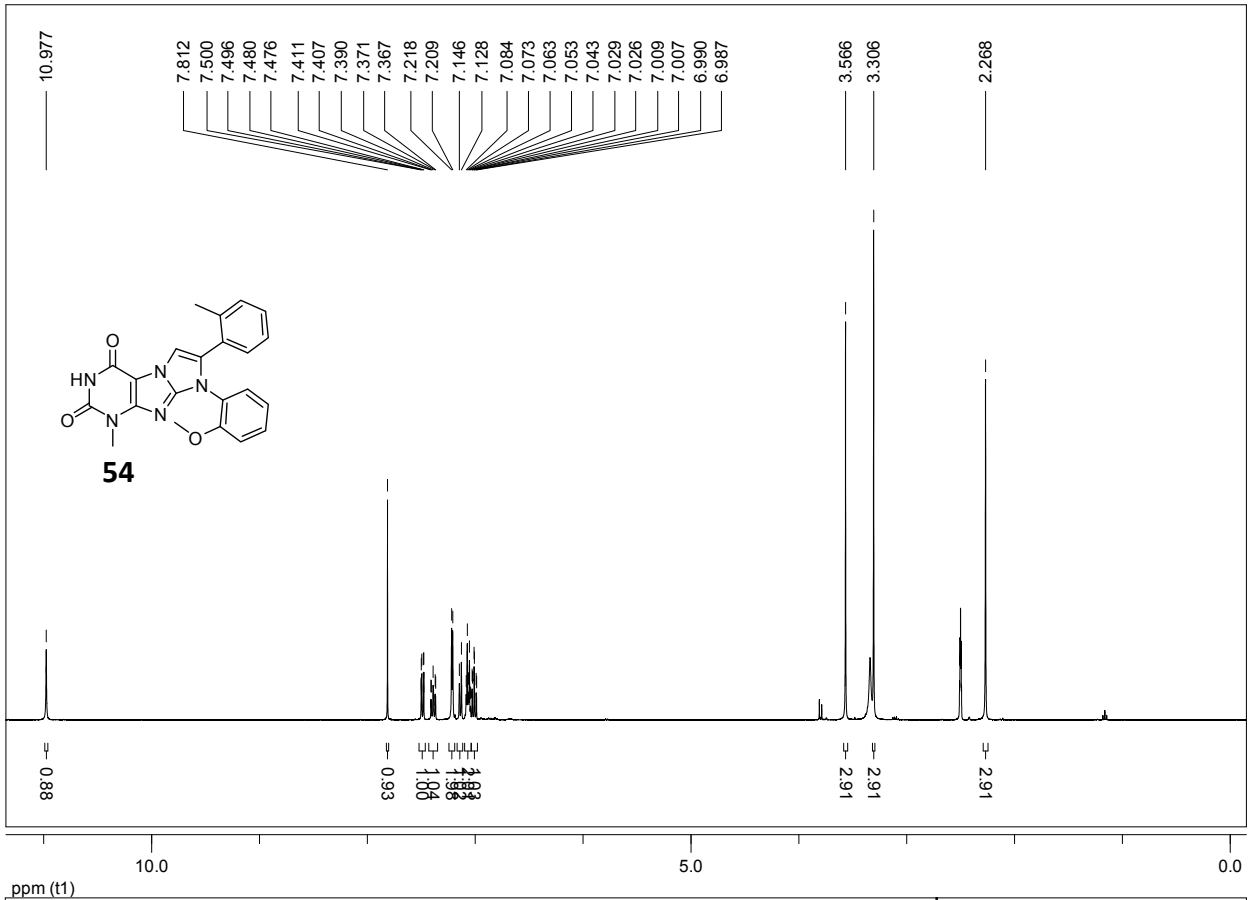

10.914
7.703
7.454
7.438
7.421
7.144
7.130
7.063
7.058
7.046
7.044
4.128
4.113
4.099
3.822
3.391
1.655
1.640
1.626
1.611
1.597
1.164
1.150
1.135
1.120
1.105
1.091
0.756
0.741
0.726
1.00
0.89
1.03
2.05
3.09
3.04
2.08
2.10
3.11
10.0
5.0
0.0
ppm (t1)

52

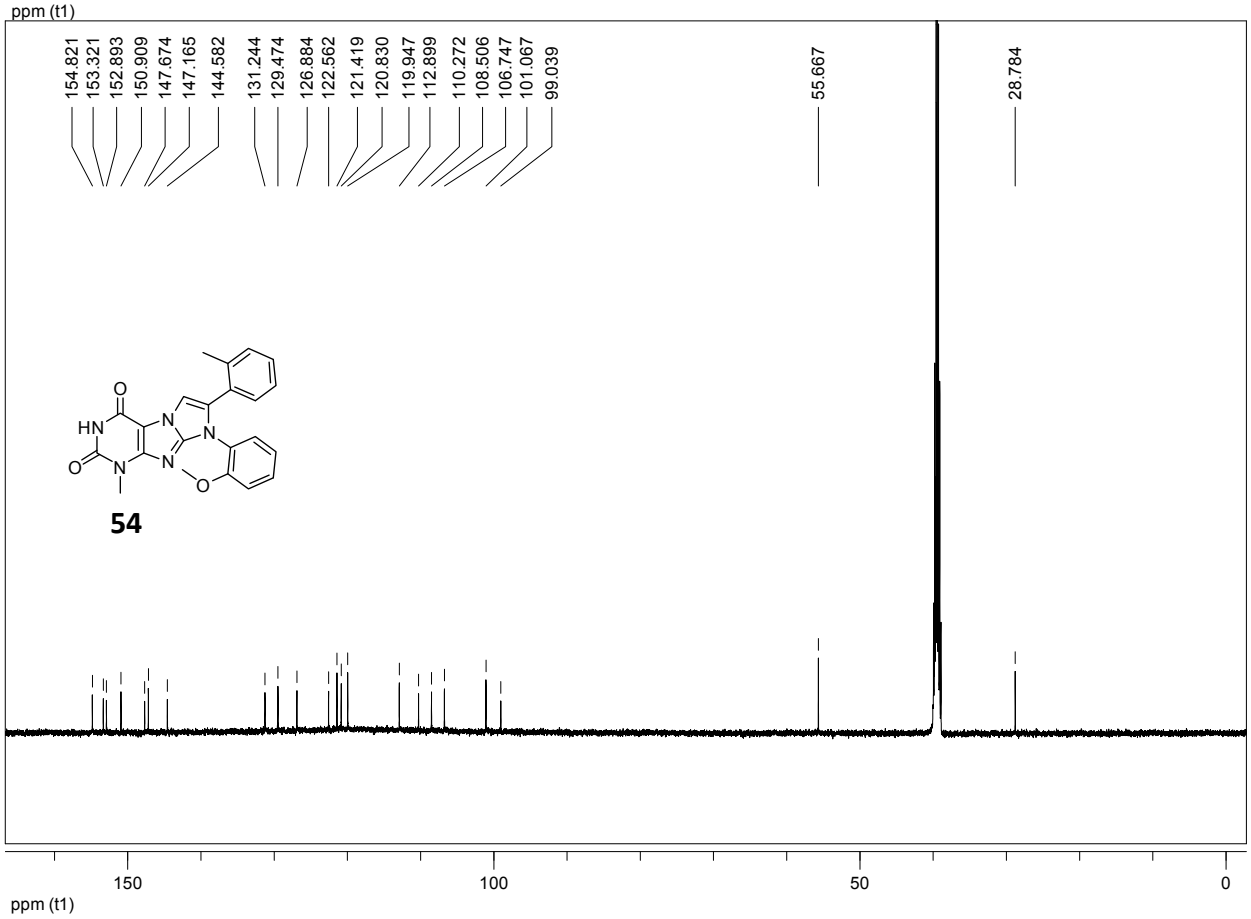

159.432
153.208
152.744
150.951
147.926
132.001
130.033
129.217
120.810
114.792
114.107
105.168
98.830
55.195
43.454
30.214
28.796
18.858
13.084
150
100
50
0
ppm (t1)

52

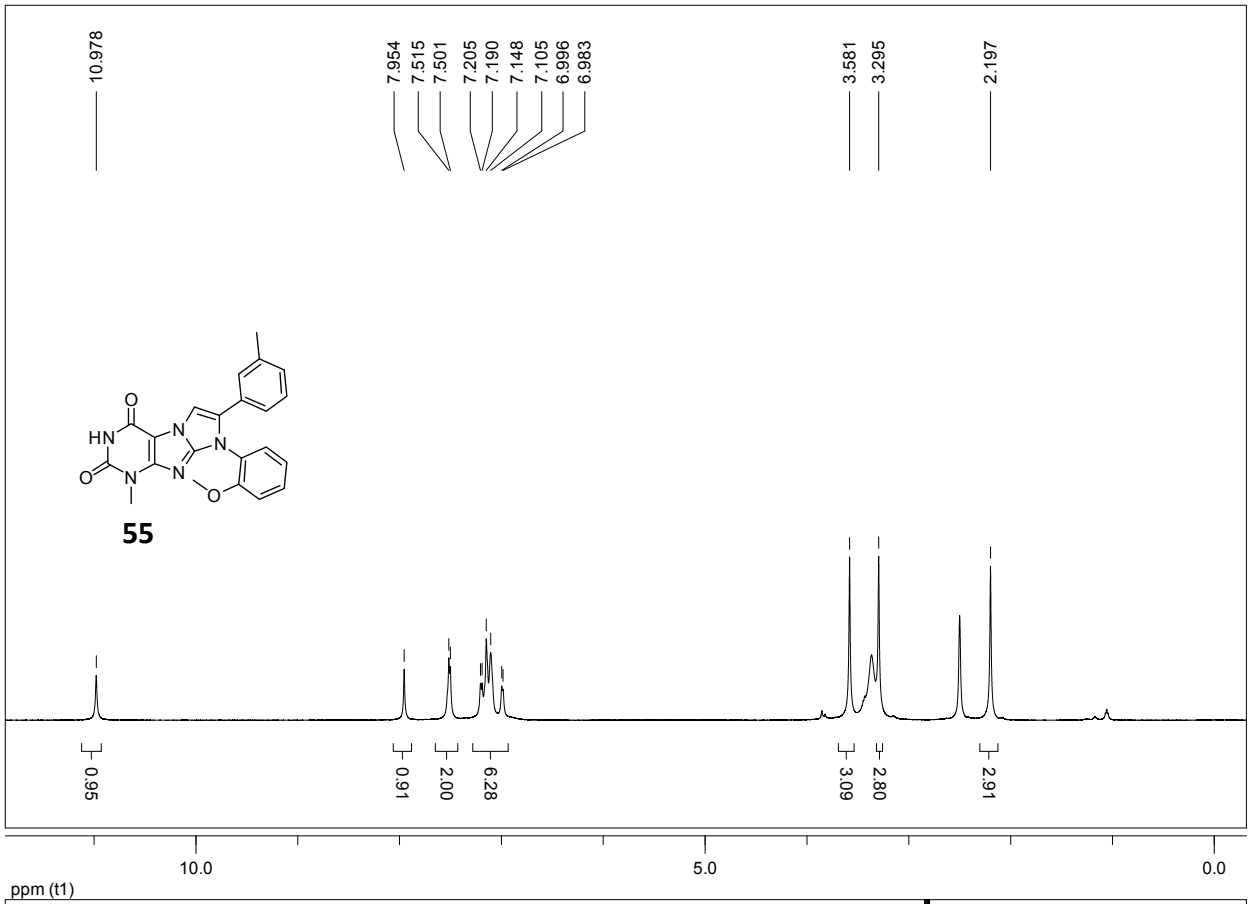

10.902
7.595
7.515
7.498
7.100
7.083
4.080
4.065
4.051
3.828
3.400
1.650
1.635
1.621
1.606
1.591
1.162
1.147
1.132
1.117
1.103
1.088
0.760
0.746
0.731
HN
O
O
N
N
N
O
53
0.85
1.96
1.93
1.97
2.91
2.80
2.01
2.08
3.00
10.0
5.0
0.0
ppm (t1)

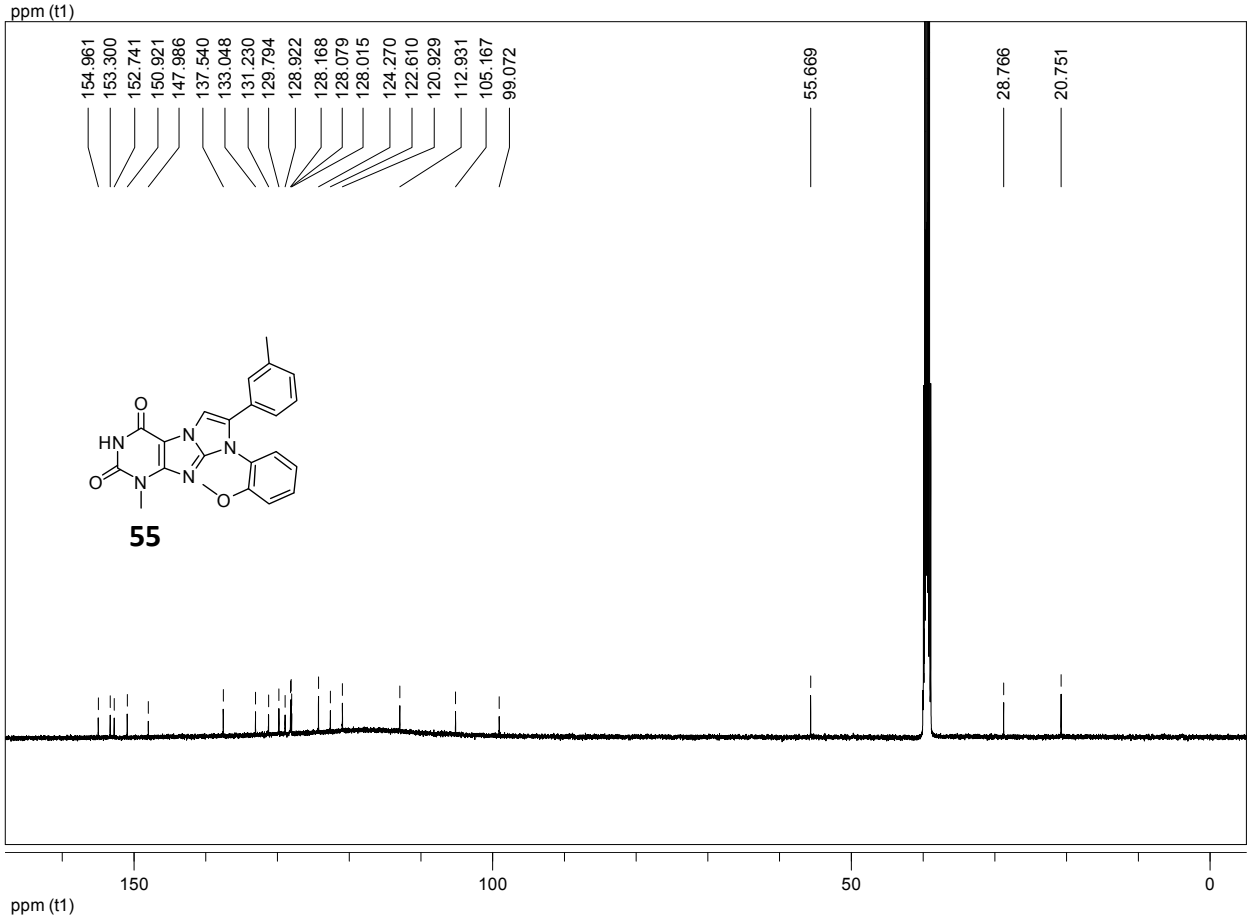

10.977
7.812
7.500
7.496
7.480
7.476
7.411
7.407
7.390
7.371
7.367
7.218
7.209
7.146
7.128
7.084
7.073
7.063
7.053
7.043
7.029
7.026
7.009
7.007
6.990
6.987
3.566
3.306
2.268
0.88
0.93
2.91
2.91
2.91
10.0
5.0
0.0
ppm (t1)

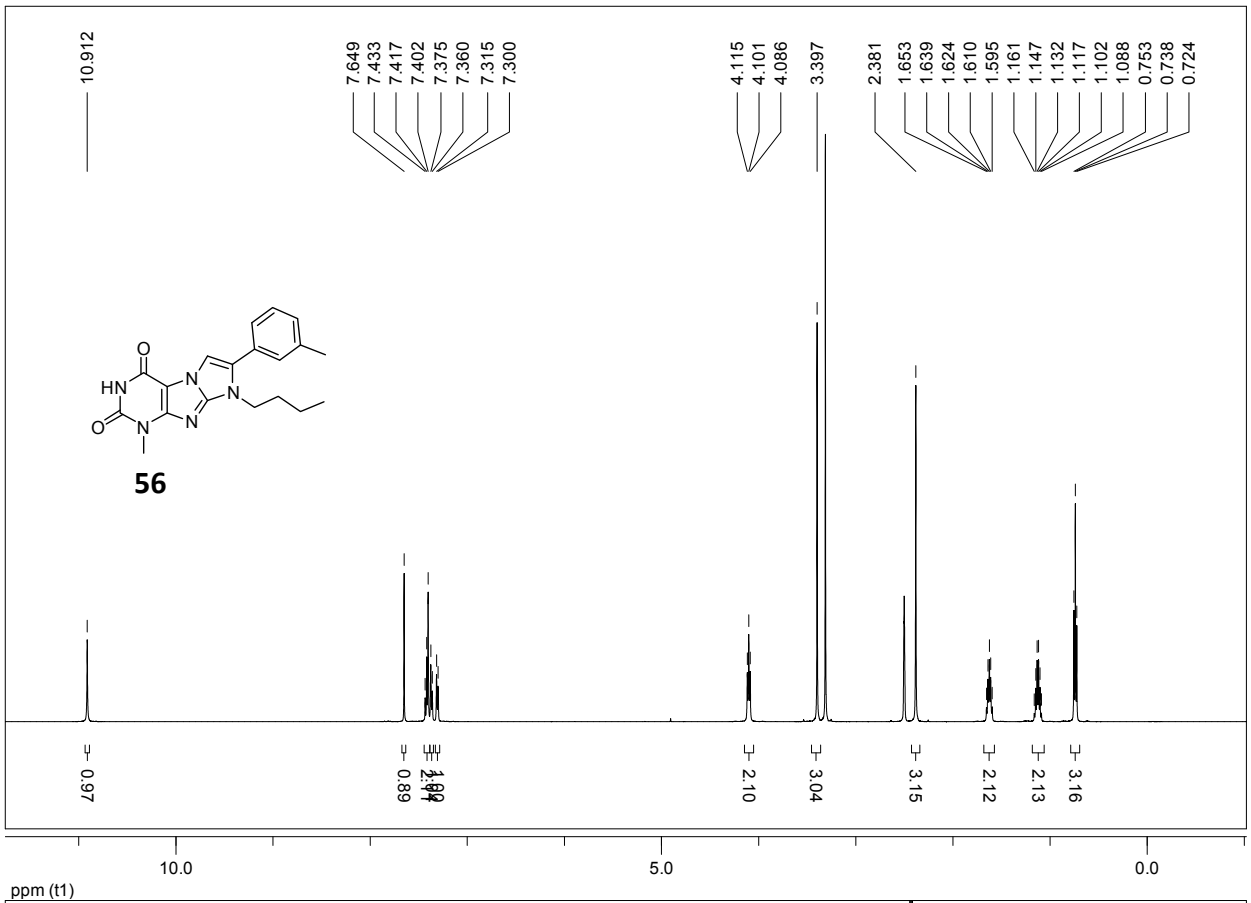
54

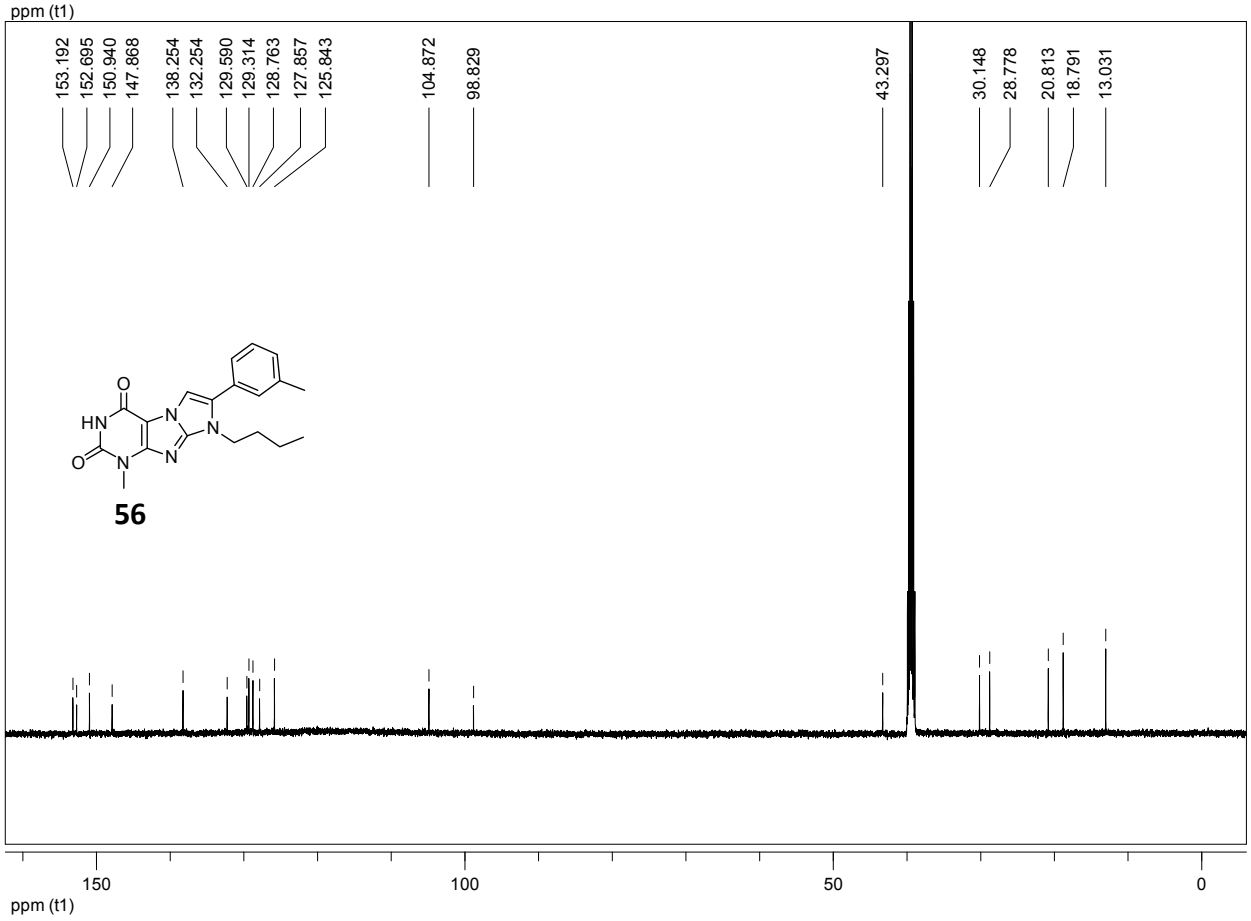

154.821
153.321
152.893
150.909
147.674
147.165
144.582
131.244
129.474
126.884
122.562
121.419
120.830
119.947
112.899
110.272
108.506
106.747
101.067
99.039
55.667
28.784
150
100
50
0
ppm (t1)

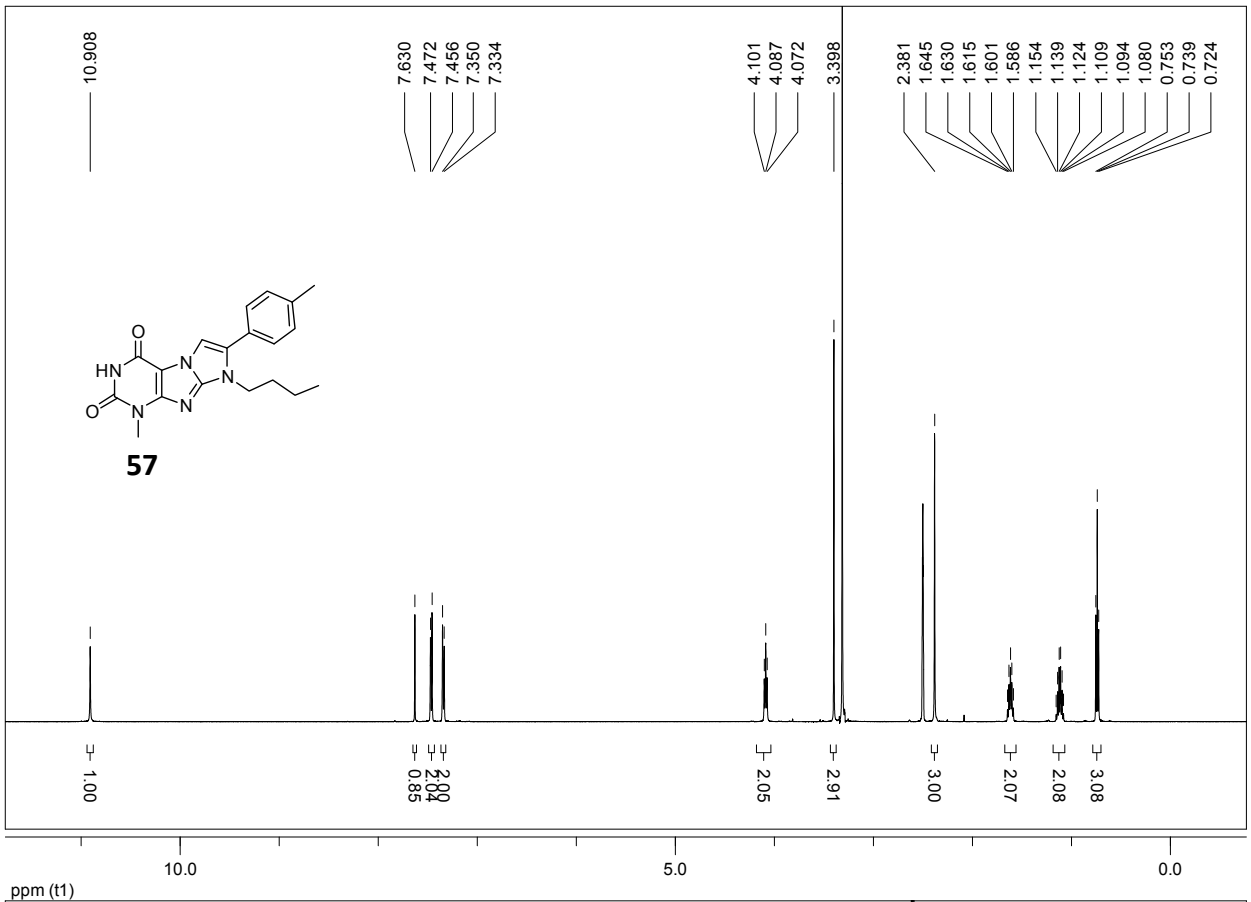
54

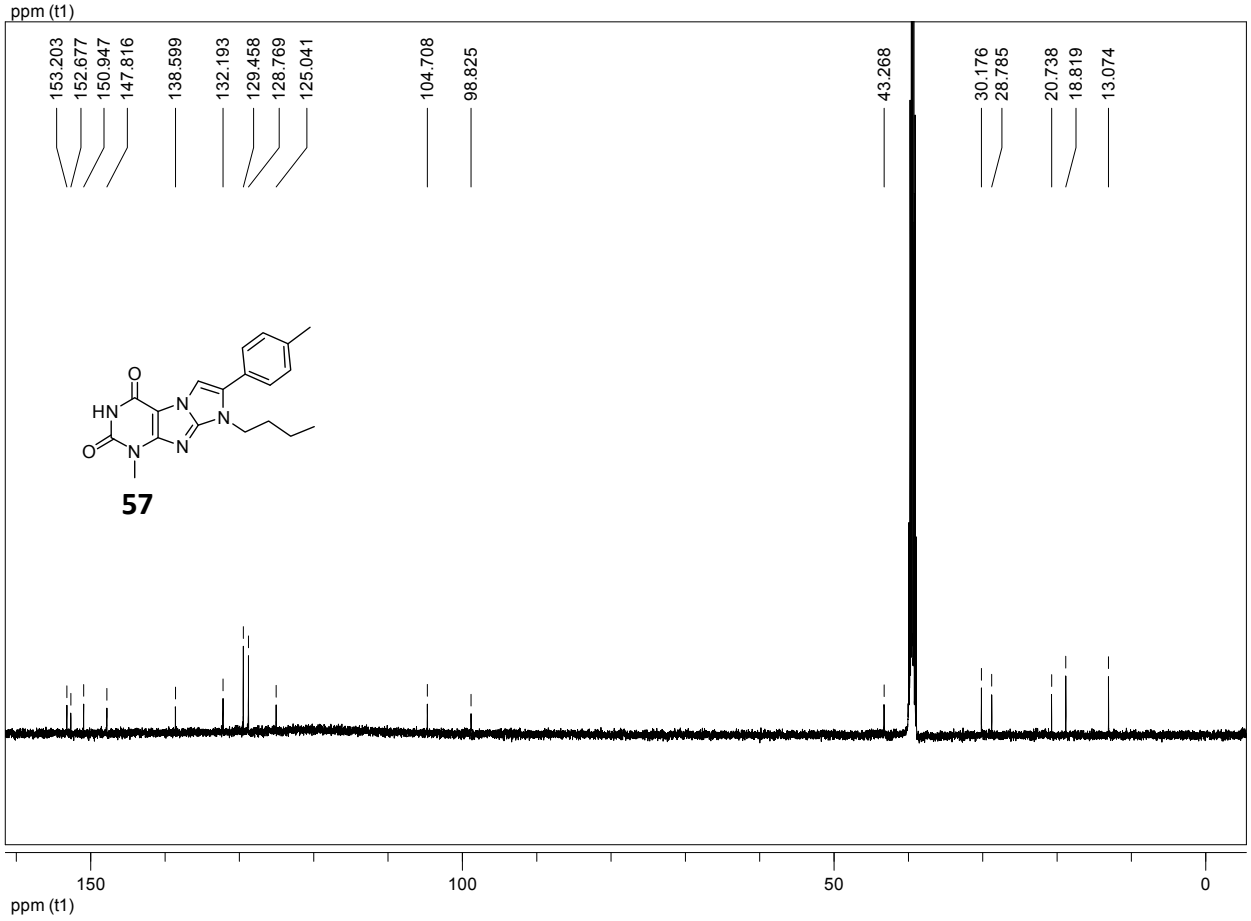

10.978
7.954
7.515
7.501
7.205
7.190
7.148
7.105
6.996
6.983
3.581
3.295
2.197
55
0.95
0.91
2.00
6.28
3.09
2.80
2.91
10.0
5.0
0.0
ppm (t1)


154.961
153.300
152.741
150.921
147.986
137.540
133.048
131.230
129.794
128.922
128.168
128.079
128.015
124.270
122.610
120.929
112.931
105.167
99.072
55.669
28.766
20.751
55
150
100
50
0
ppm (t1)


10.912
7.649
7.433
7.417
7.402
7.375
7.360
7.315
7.300
4.115
4.101
4.086
3.397
2.381
1.653
1.639
1.624
1.610
1.595
1.161
1.147
1.132
1.117
1.102
1.088
0.753
0.738
0.724
0.97
0.89
2.10
3.04
3.15
2.12
2.13
3.16
10.0
5.0
0.0
ppm (t1)
56


153.192
152.695
150.940
147.868
138.254
132.254
129.590
129.314
128.763
127.857
125.843
104.872
98.829
43.297
30.148
28.778
20.813
18.791
13.031
150
100
50
0
ppm (t1)
56


10.908
7.630
7.472
7.456
7.350
7.334
4.101
4.087
4.072
3.398
2.381
1.645
1.630
1.615
1.601
1.586
1.154
1.139
1.124
1.109
1.094
1.080
0.753
0.739
0.724
1.00
0.85
2.00
2.04
2.05
2.91
3.00
2.07
2.08
3.08
10.0
5.0
0.0
ppm (t1)
57


153.203
152.677
150.947
147.816
138.599
132.193
129.458
128.769
125.041
104.708
98.825
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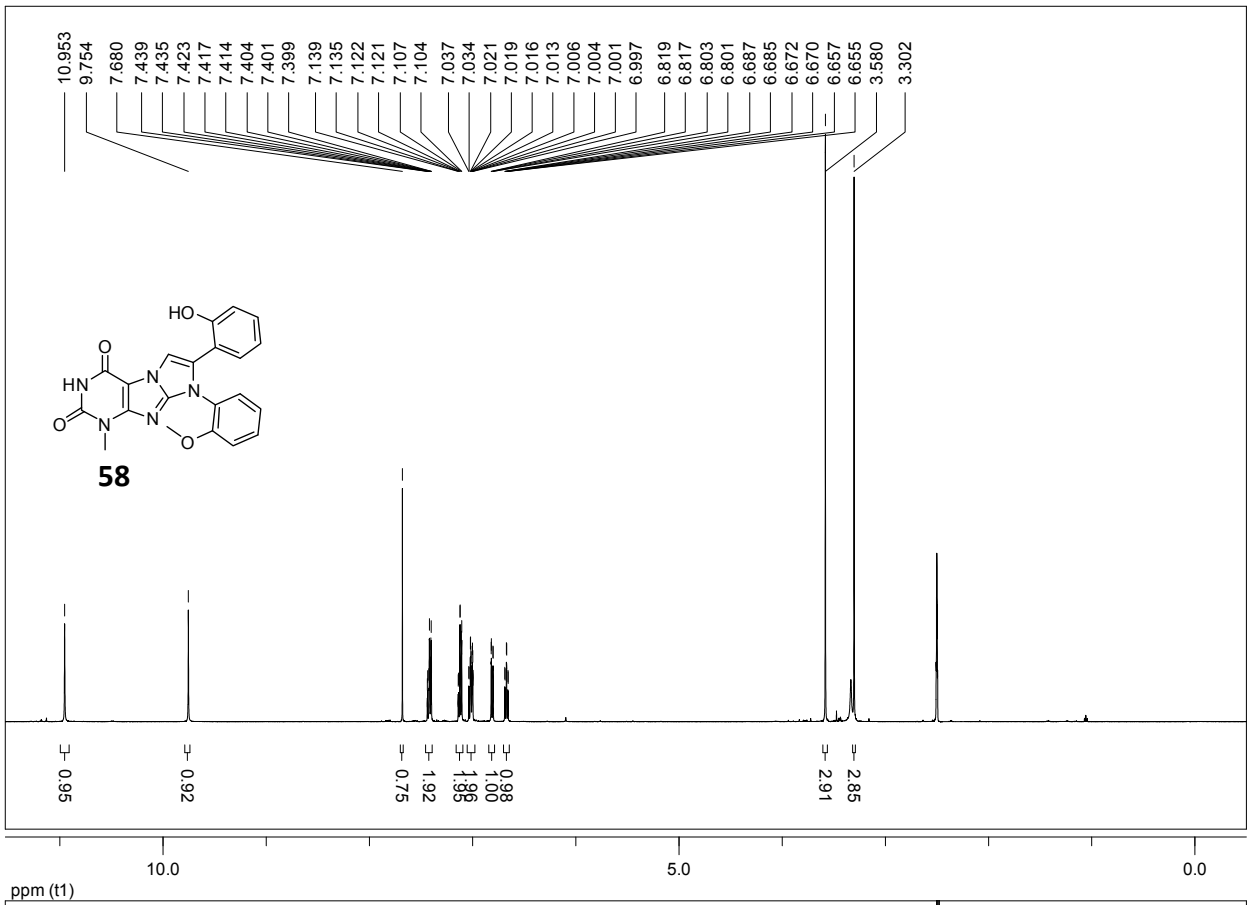
30.176
28.785
20.738
18.819
13.074
150
100
50
0
ppm (t1)
57


10.953
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7.439
7.435
7.423
7.417
7.414
7.404
7.401
7.399
7.139
7.135
7.122
7.121
7.107
7.104
7.037
7.034
7.021
7.019
7.016
7.013
7.006
7.004
7.001
6.997
6.819
6.817
6.803
6.801
6.687
6.685
6.672
6.670
6.657
6.655
3.580
3.302
HO
O
HN
O
N
N
N
N
O
58
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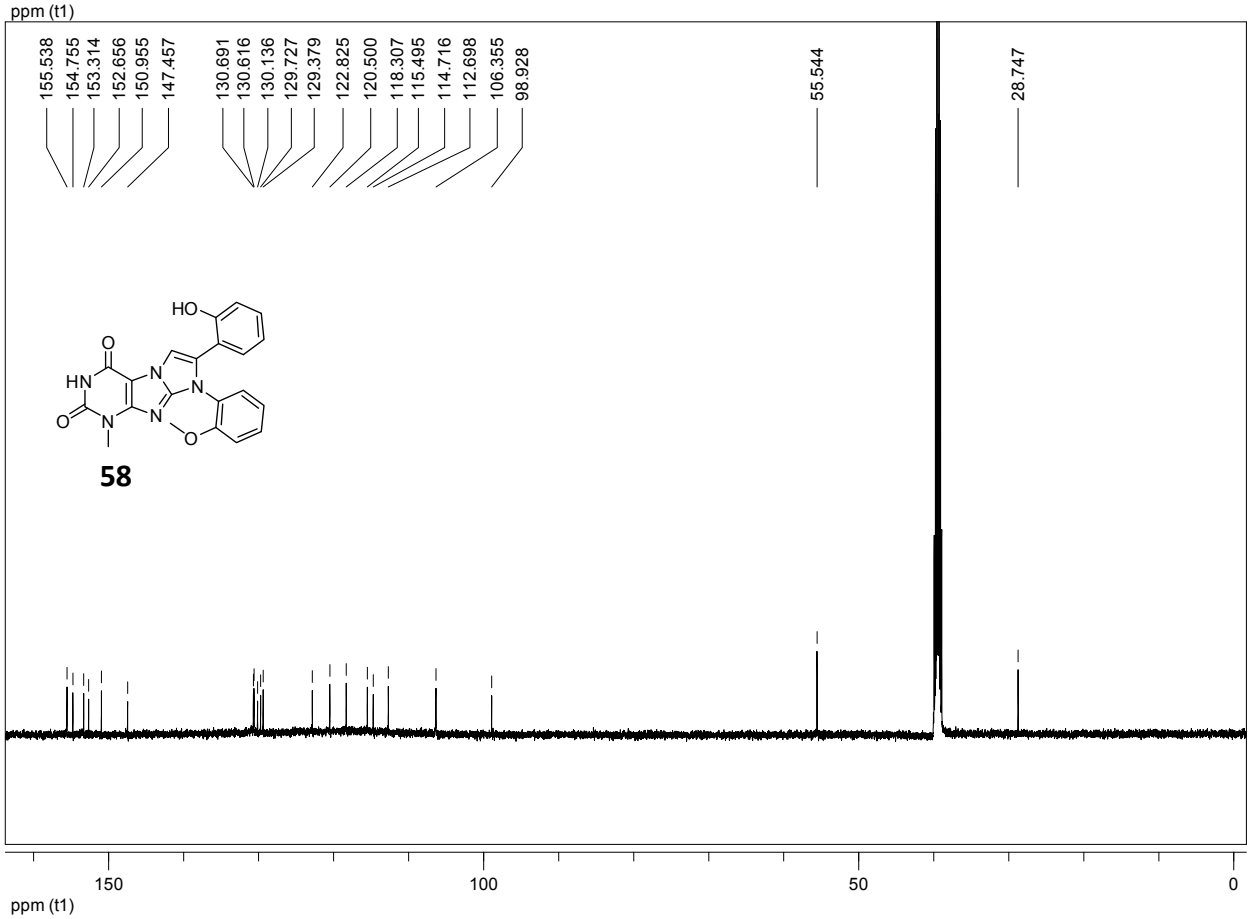
1.92
1.00
0.98
2.91
2.85
10.0
5.0
0.0
ppm (t1)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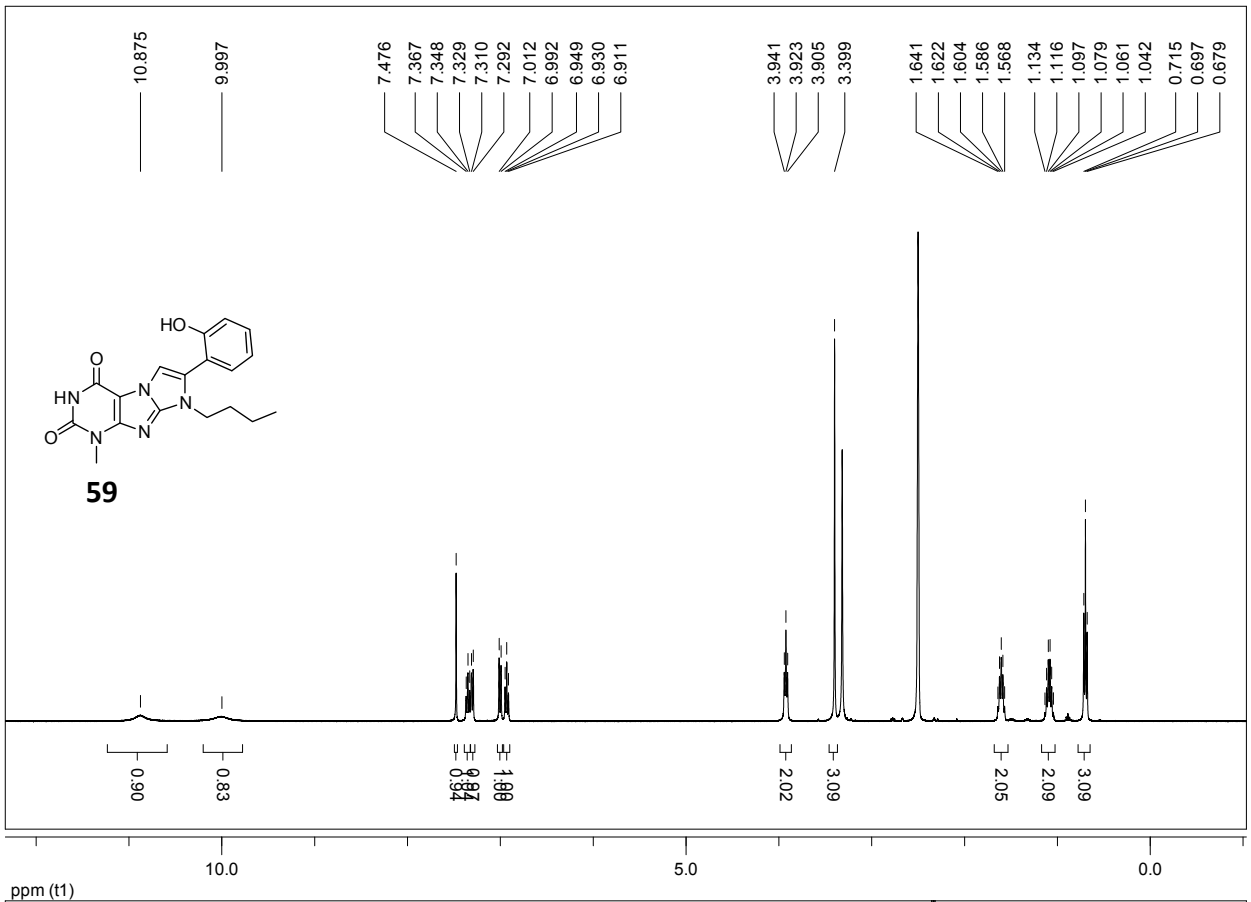
153.314
152.656
150.955
147.457
130.691
130.616
130.136
129.727
129.379
122.825
120.500
118.307
115.495
114.716
112.698
106.355
98.928
55.544
28.747
HO
O
HN
O
N
N
N
N
O
58
150
100
50
0
ppm (t1)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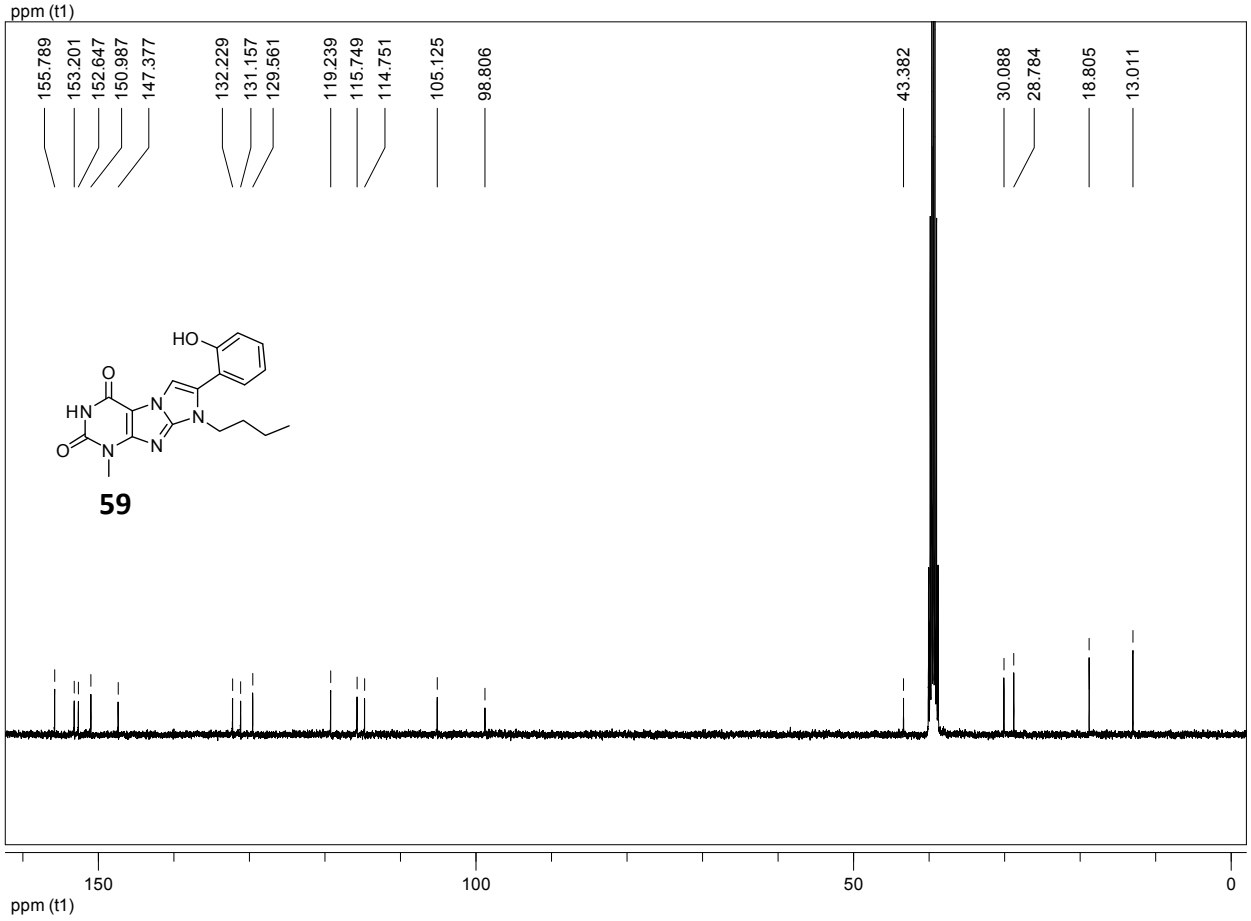
7.367
7.348
7.329
7.310
7.292
7.012
6.992
6.949
6.930
6.911
3.941
3.923
3.905
3.399
1.641
1.622
1.604
1.586
1.568
1.134
1.116
1.097
1.079
1.061
1.042
0.715
0.697
0.679
HO
O
HN
O
N
N
N
59
0.90
0.83
2.02
3.09
2.05
2.09
3.09
10.0
5.0
0.0
ppm (t1)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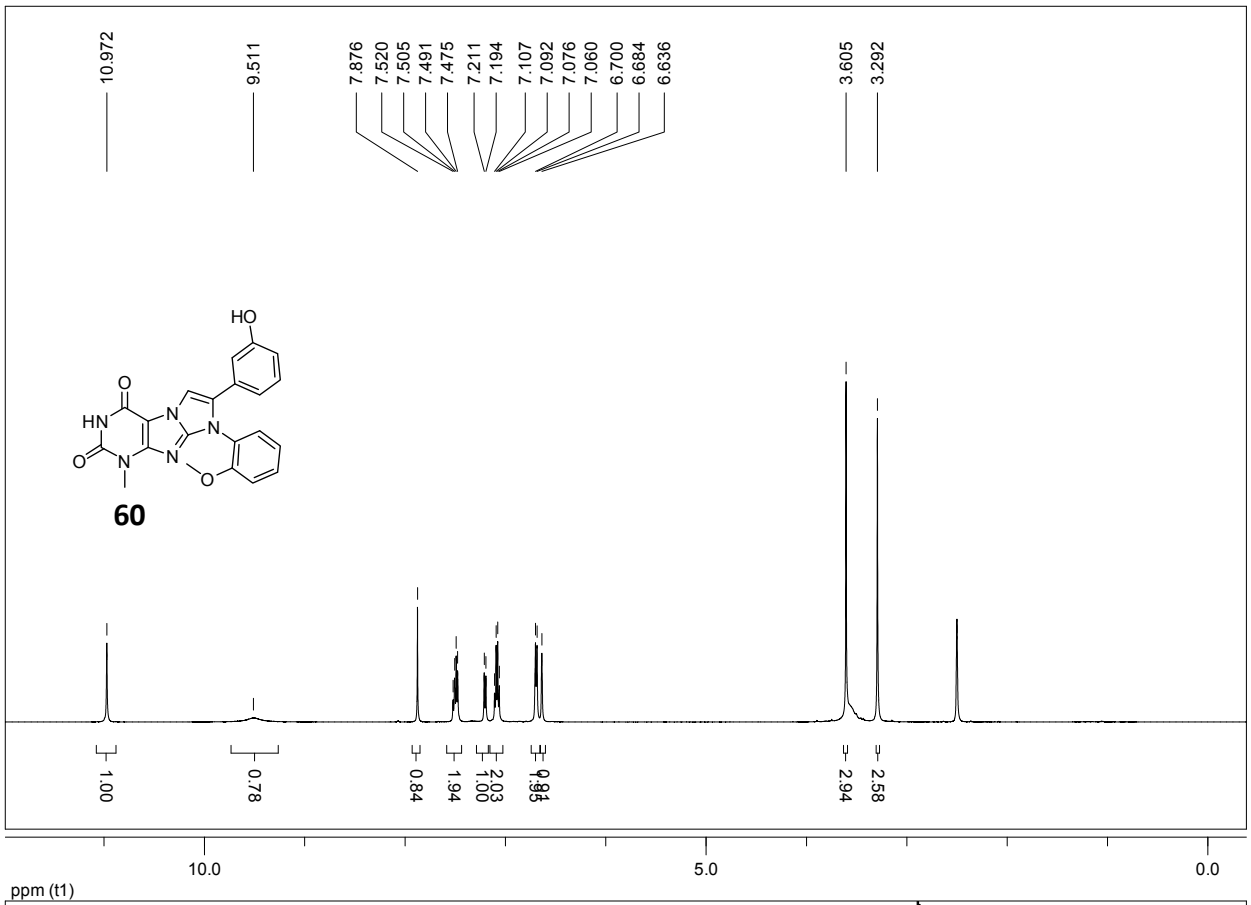
152.647
150.987
147.377
132.229
131.157
129.561
119.239
115.749
114.751
105.125
98.806
43.382
30.088
28.784
18.805
13.011
HO
O
HN
O
N
N
N
59
150
100
50
0
ppm (t1)


10.972
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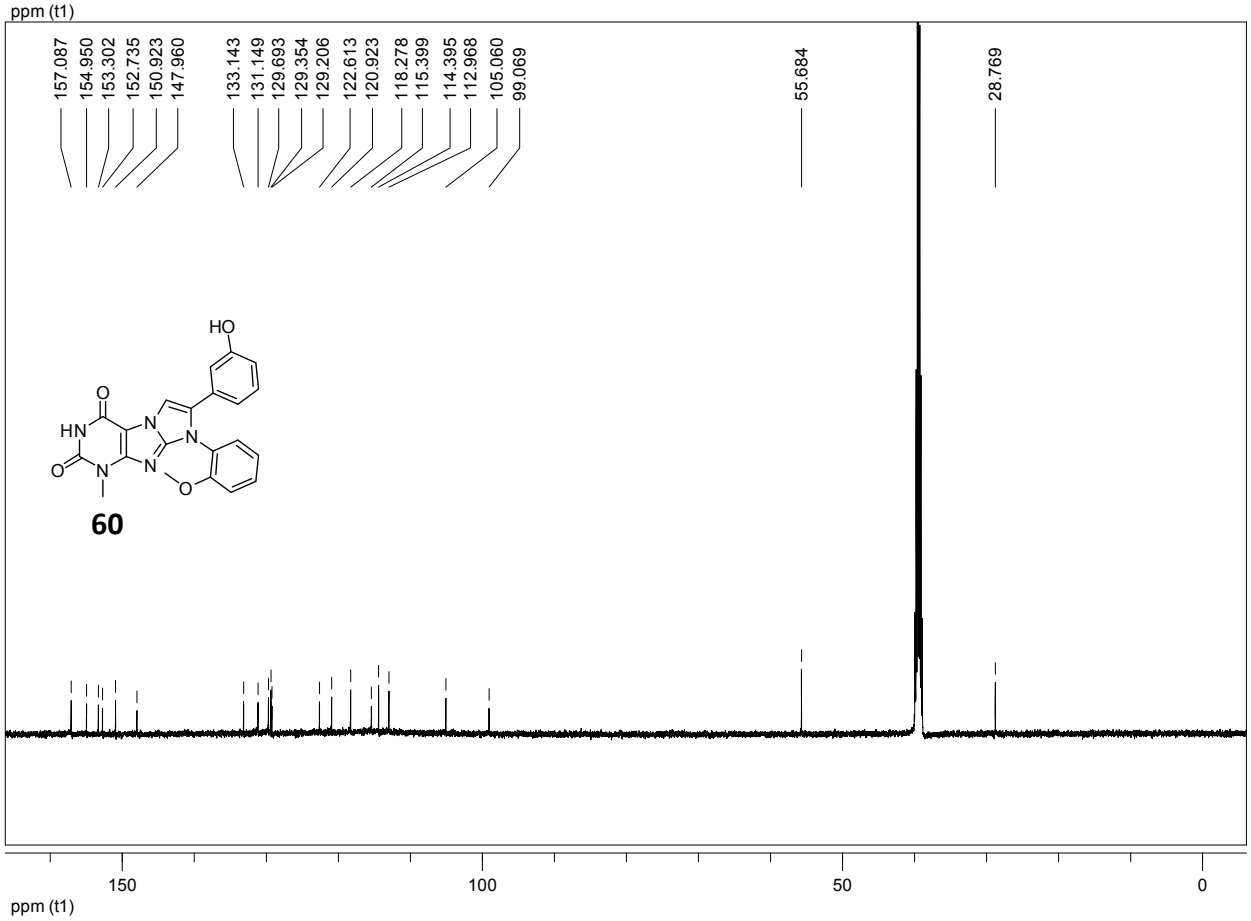
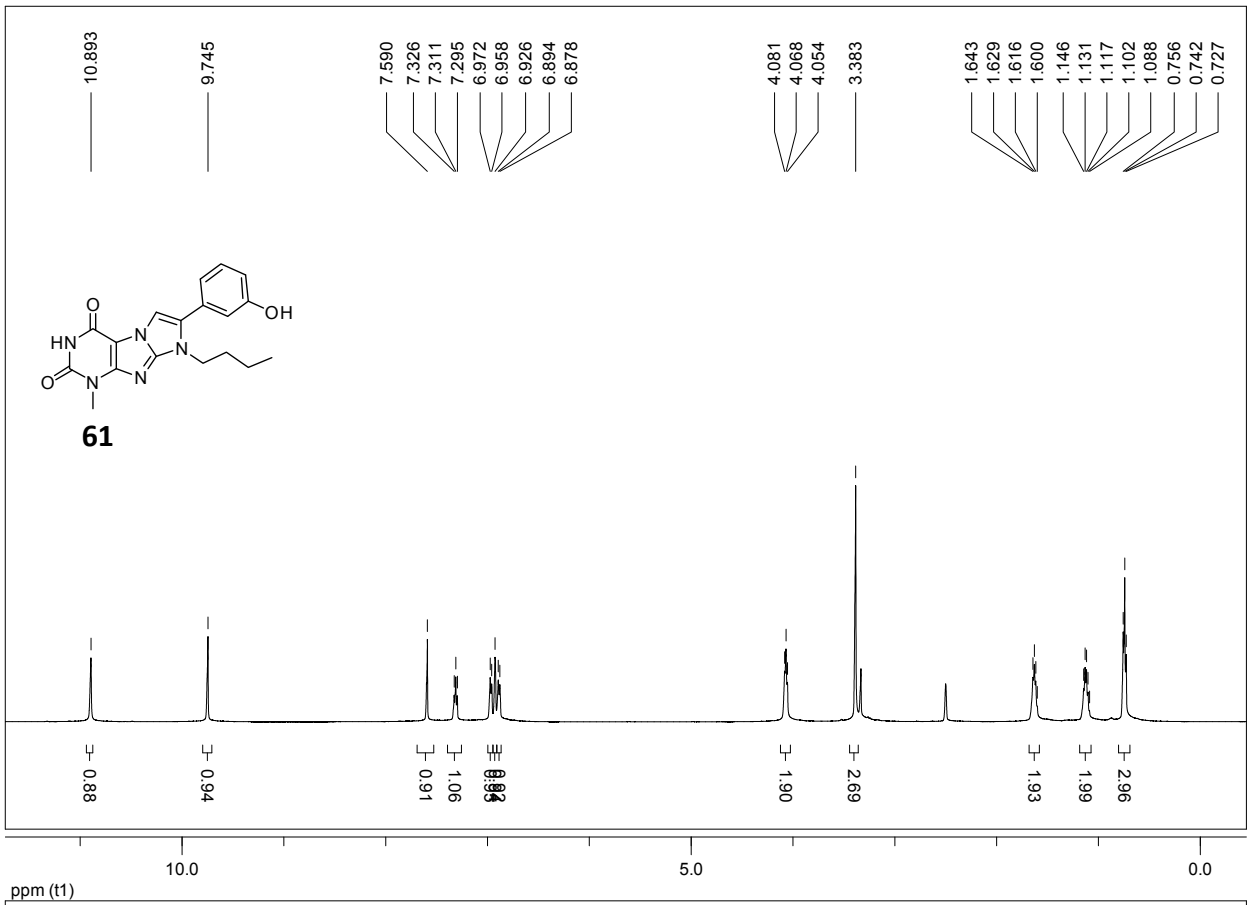
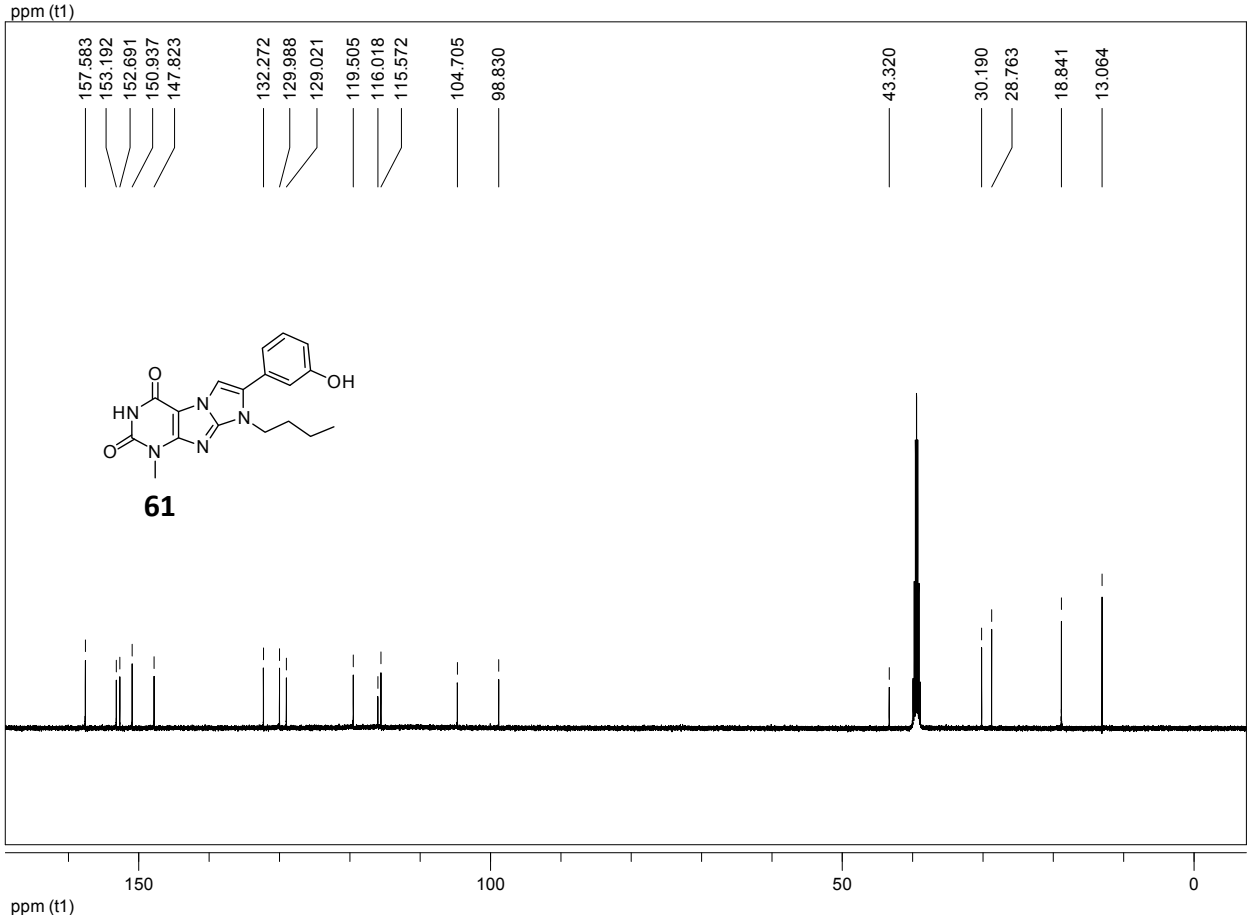
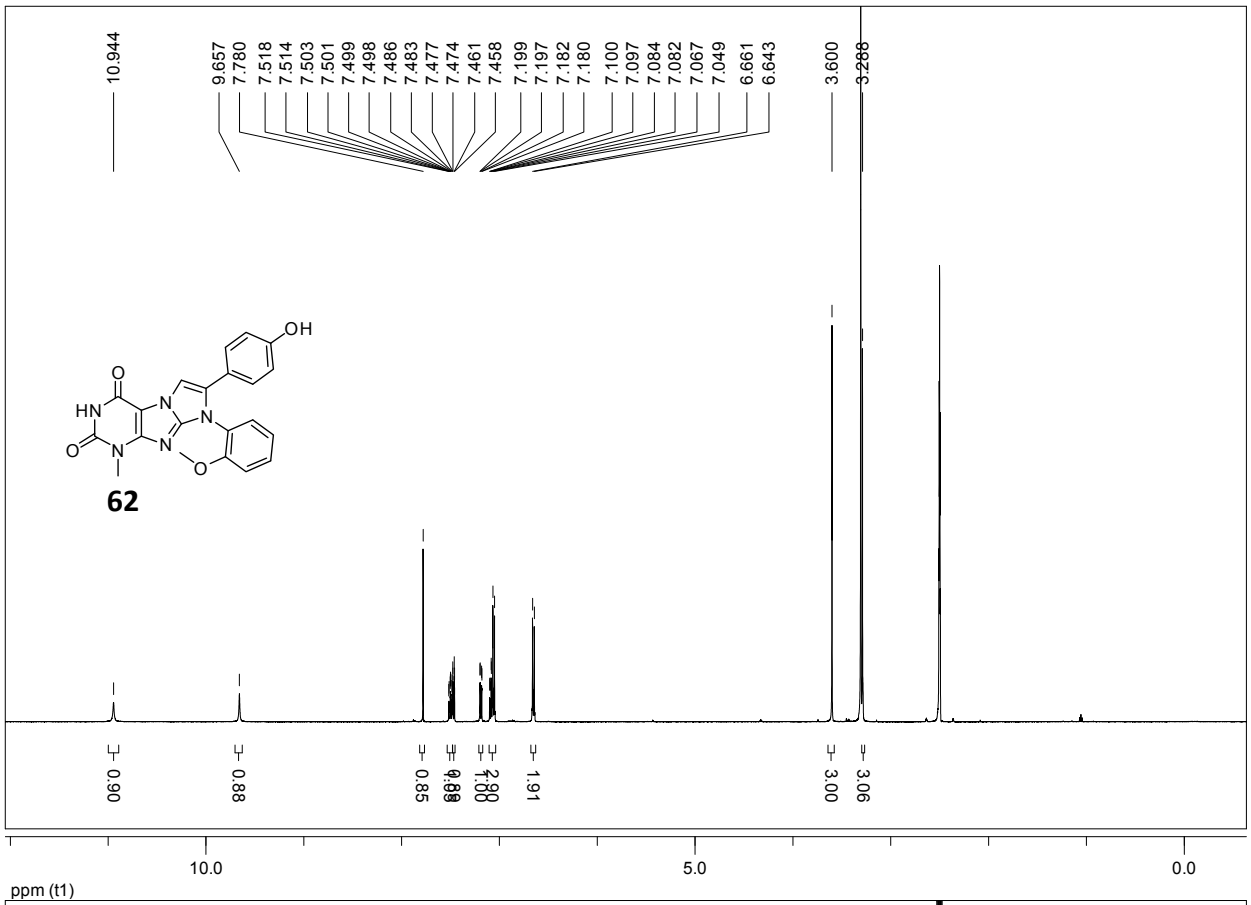
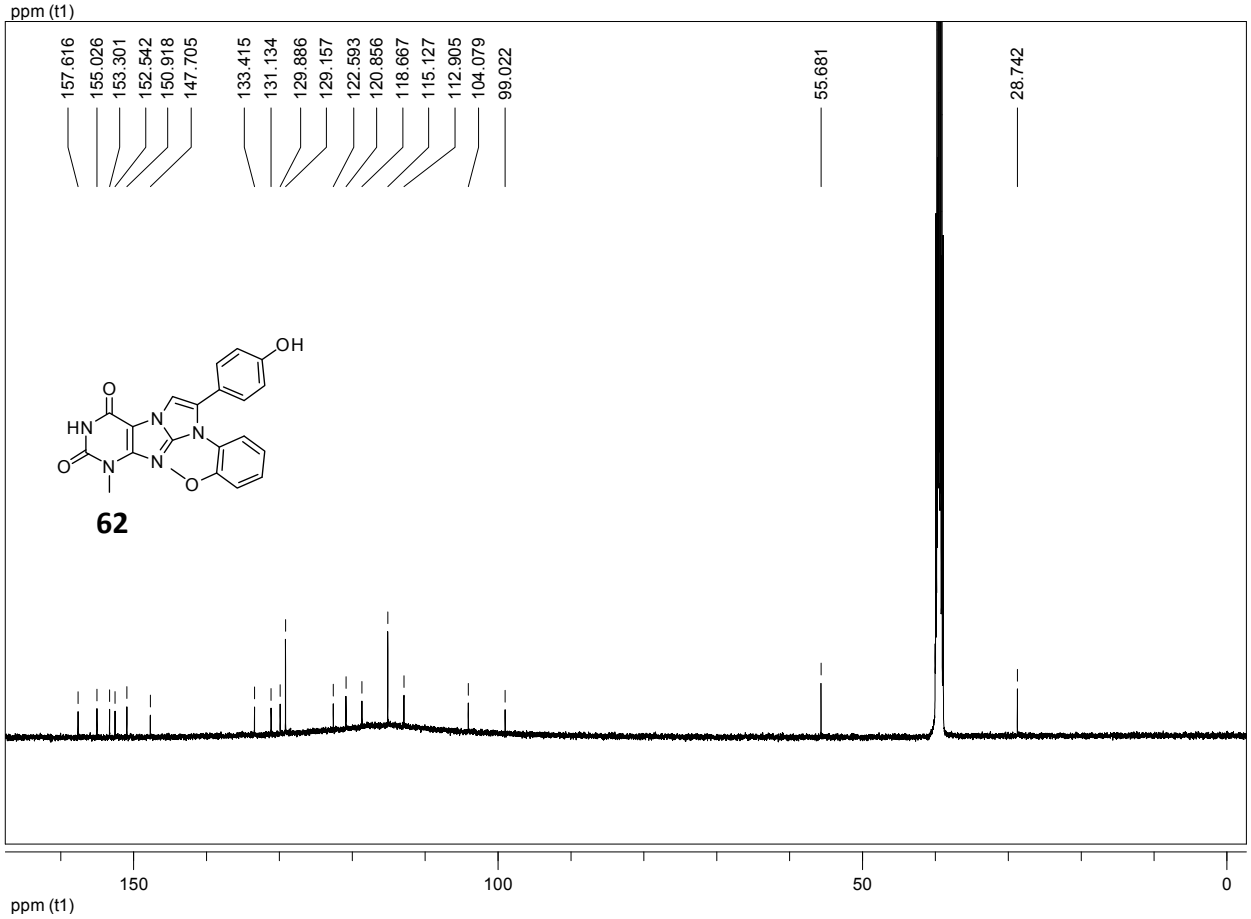
7.520
7.505
7.491
7.475
7.211
7.194
7.107
7.092
7.076
7.060
6.700
6.684
6.636
3.605
3.292
HO
O
HN
N
O
N
N
O
60
1.00
0.78
0.84
1.94
1.00
2.03
2.94
2.58
10.0
5.0
0.0
ppm (t1)

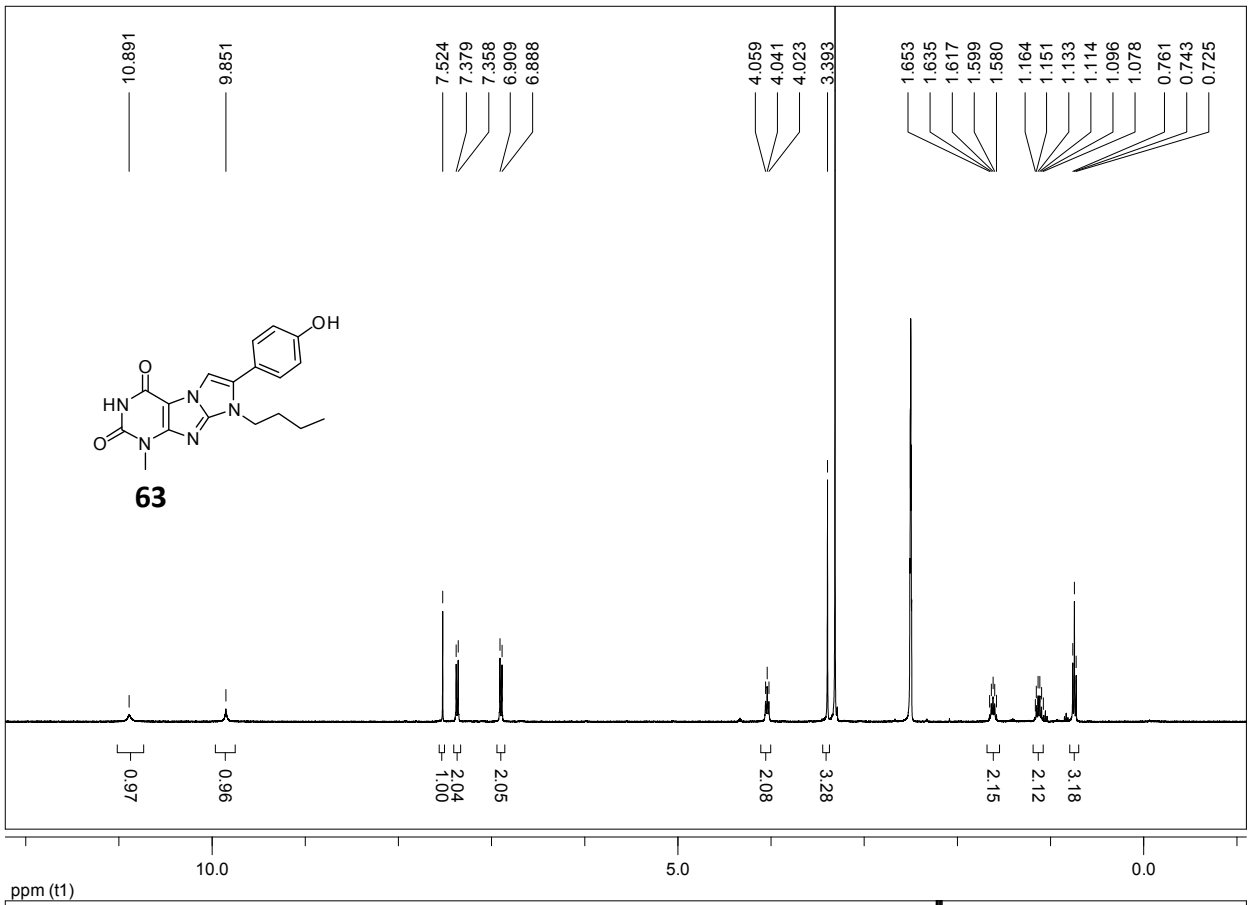

157.087
154.950
153.302
152.735
150.923
147.960
133.143
131.149
129.693
129.354
129.206
122.613
120.923
118.278
115.399
114.395
112.968
105.060
99.069
55.684
28.769
HO
O
HN
N
O
N
N
O
60
150
100
50
0
ppm (t1)

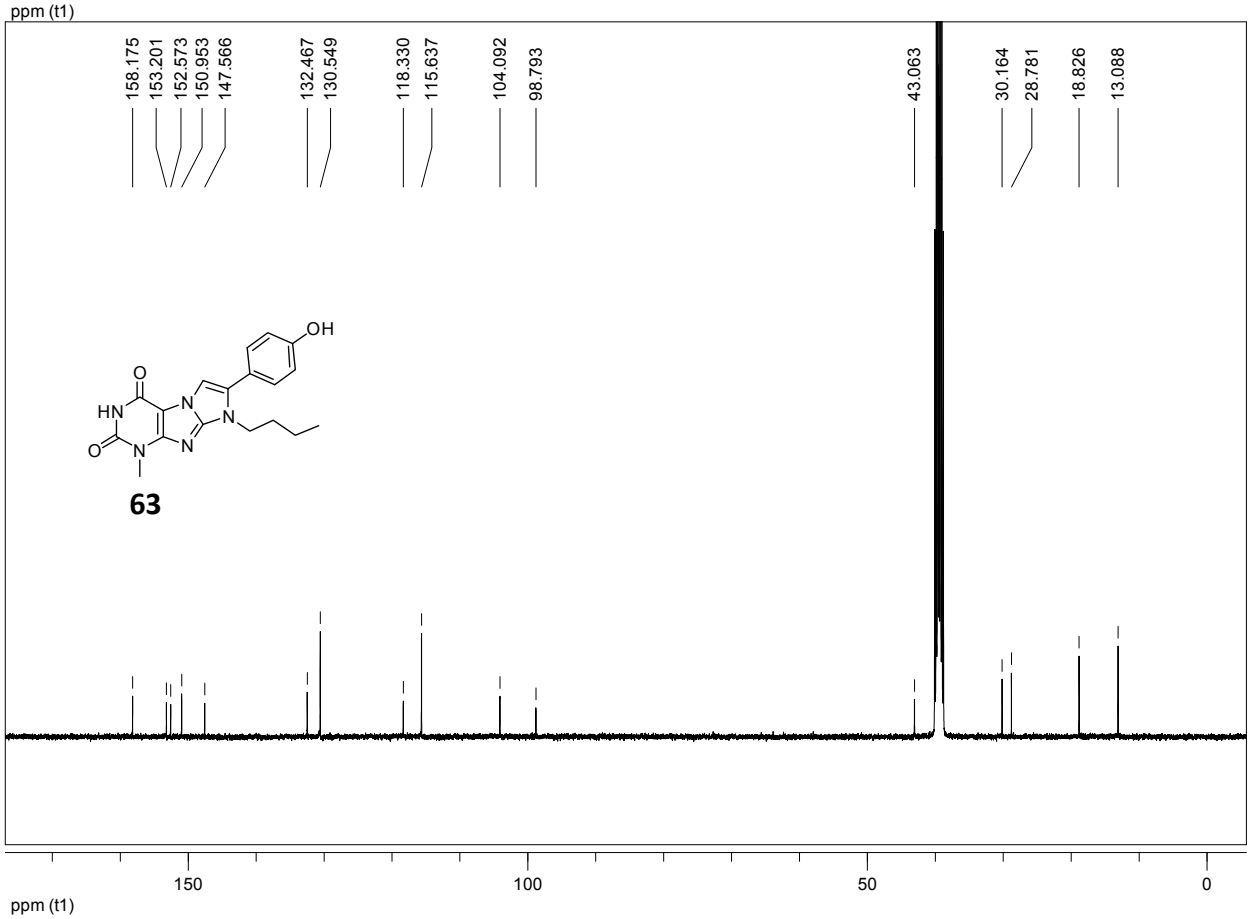

10.893
9.745
7.590
7.326
7.311
7.295
6.972
6.958
6.926
6.894
6.878
4.081
4.068
4.054
3.383
1.643
1.629
1.616
1.600
1.146
1.131
1.117
1.102
1.088
0.756
0.742
0.727
OH
HN
O
N
61
0.88
0.94
0.91
1.06
1.90
2.69
1.93
1.99
2.96
10.0
5.0
0.0
ppm (t1)

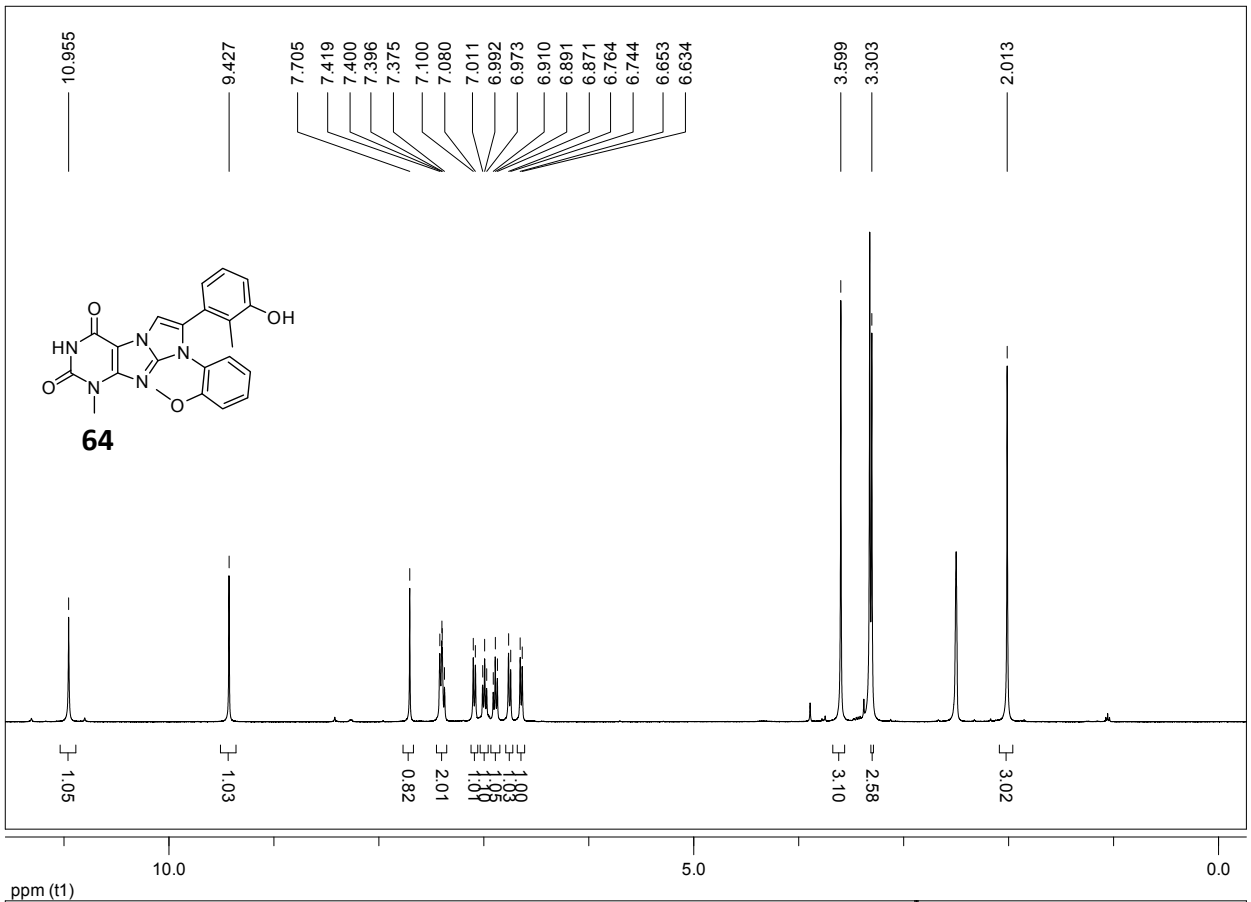

157.583
153.192
152.691
150.937
147.823
132.272
129.988
129.021
119.505
116.018
115.572
104.705
98.830
43.320
30.190
28.763
18.841
13.064
OH
HN
O
N
61
150
100
50
0
ppm (t1)


10.944
9.657
7.780
7.518
7.514
7.503
7.501
7.499
7.498
7.486
7.483
7.477
7.474
7.461
7.458
7.199
7.197
7.182
7.180
7.100
7.097
7.084
7.082
7.067
7.049
6.661
6.643
3.600
3.288
0.90
0.88
0.85
1.91
3.00
3.06
10.0
5.0
0.0
ppm (t1)
OH
HN
O
N
O
62

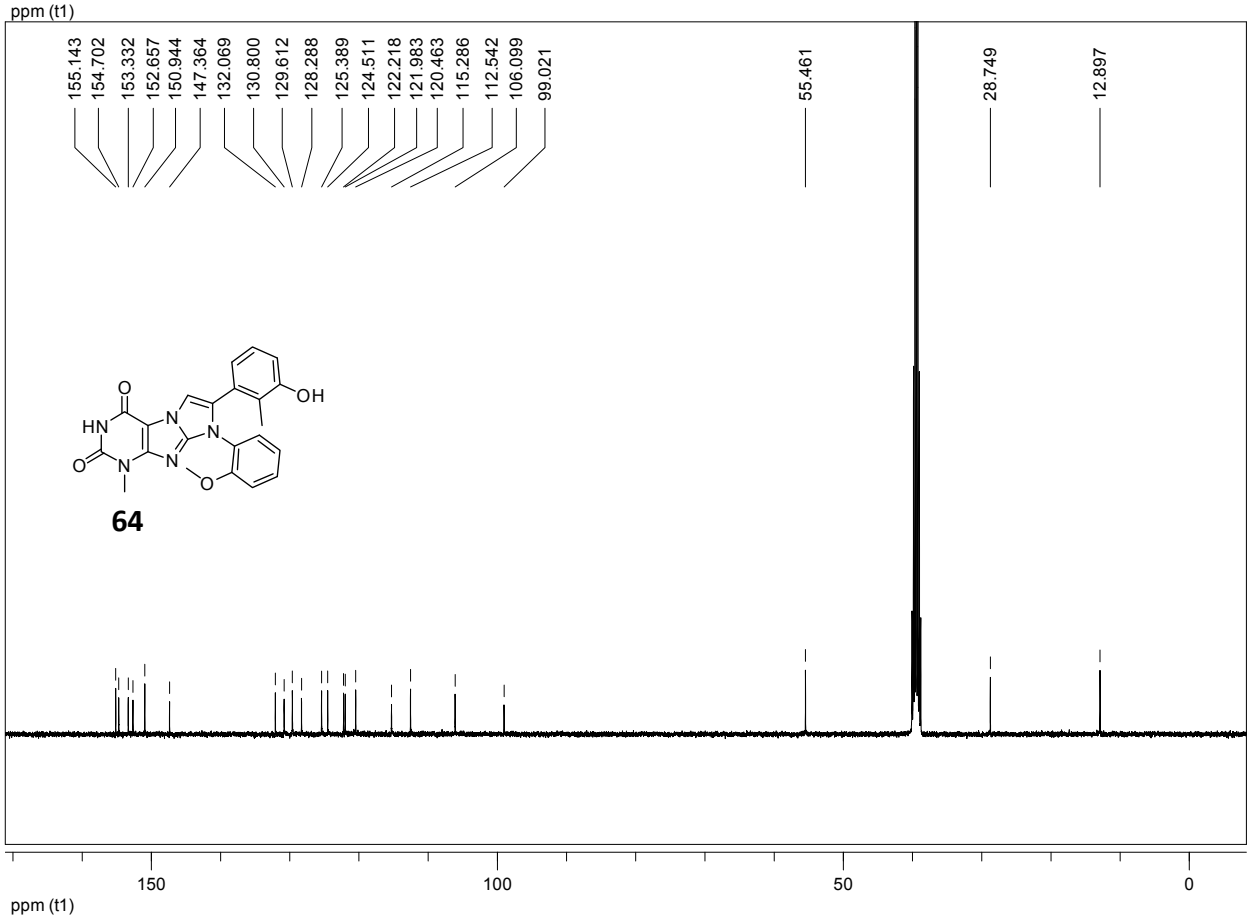

157.616
155.026
153.301
152.542
150.918
147.705
133.415
131.134
129.886
129.157
122.593
120.856
118.667
115.127
112.905
104.079
99.022
55.681
28.742
150
100
50
0
ppm (t1)
OH
HN
O
N
O
62


10.891
9.851
7.524
7.379
7.358
6.909
6.888
4.059
4.041
4.023
3.393
1.653
1.635
1.617
1.599
1.580
1.164
1.151
1.133
1.114
1.096
1.078
0.761
0.743
0.725
OH
HN
O
N
63
0.97
0.96
2.04
1.00
2.05
2.08
3.28
2.15
2.12
3.18
10.0
5.0
0.0
ppm (t1)

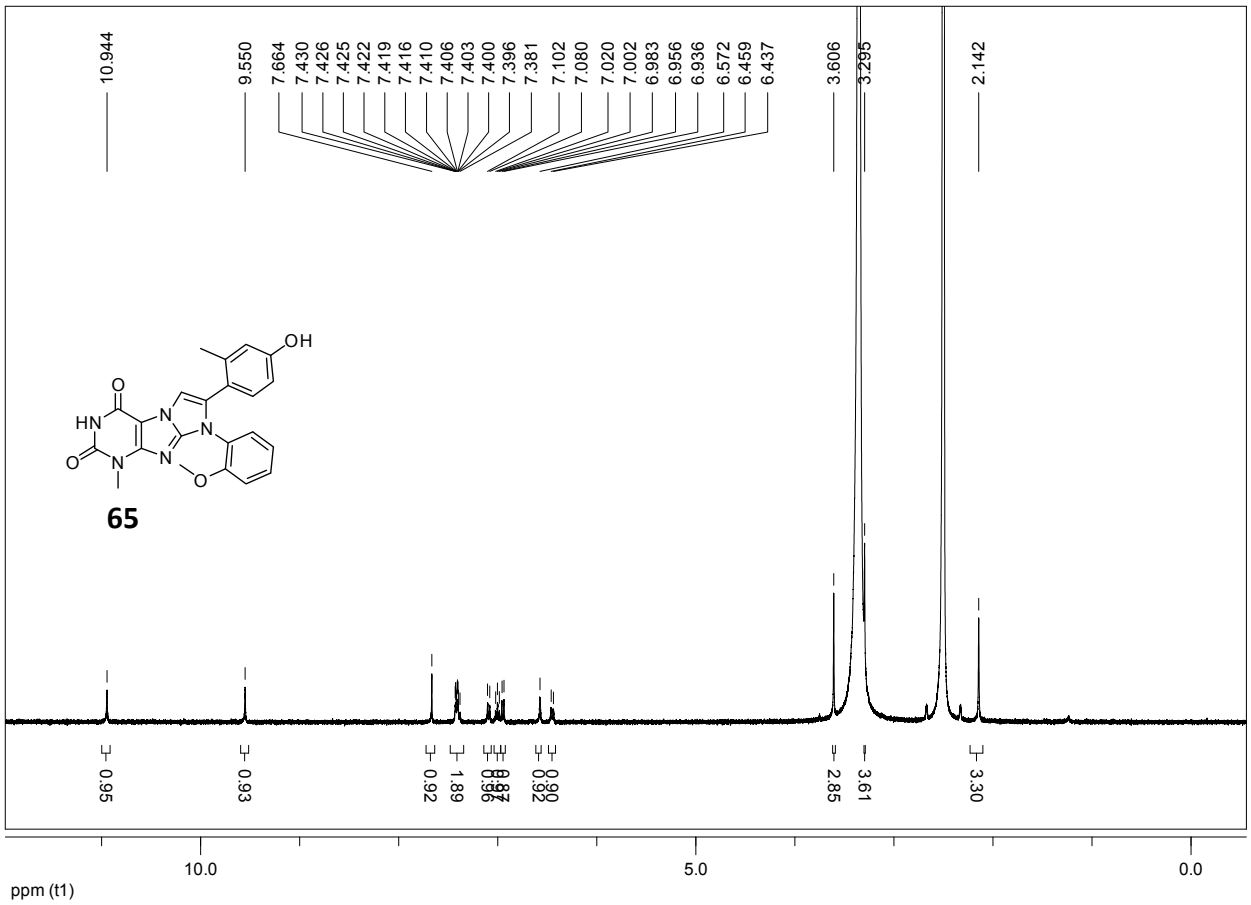

158.175
153.201
152.573
150.953
147.566
132.467
130.549
118.330
115.637
104.092
98.793
43.063
30.164
28.781
18.826
13.088
OH
HN
O
N
63
150
100
50
0
ppm (t1)


10.955
9.427
7.705
7.419
7.400
7.396
7.375
7.100
7.080
7.011
6.992
6.973
6.910
6.891
6.871
6.764
6.744
6.653
6.634
3.599
3.303
2.013
1.05
1.03
0.82
2.01
3.10
2.58
3.02
10.0
5.0
0.0
ppm (t1)

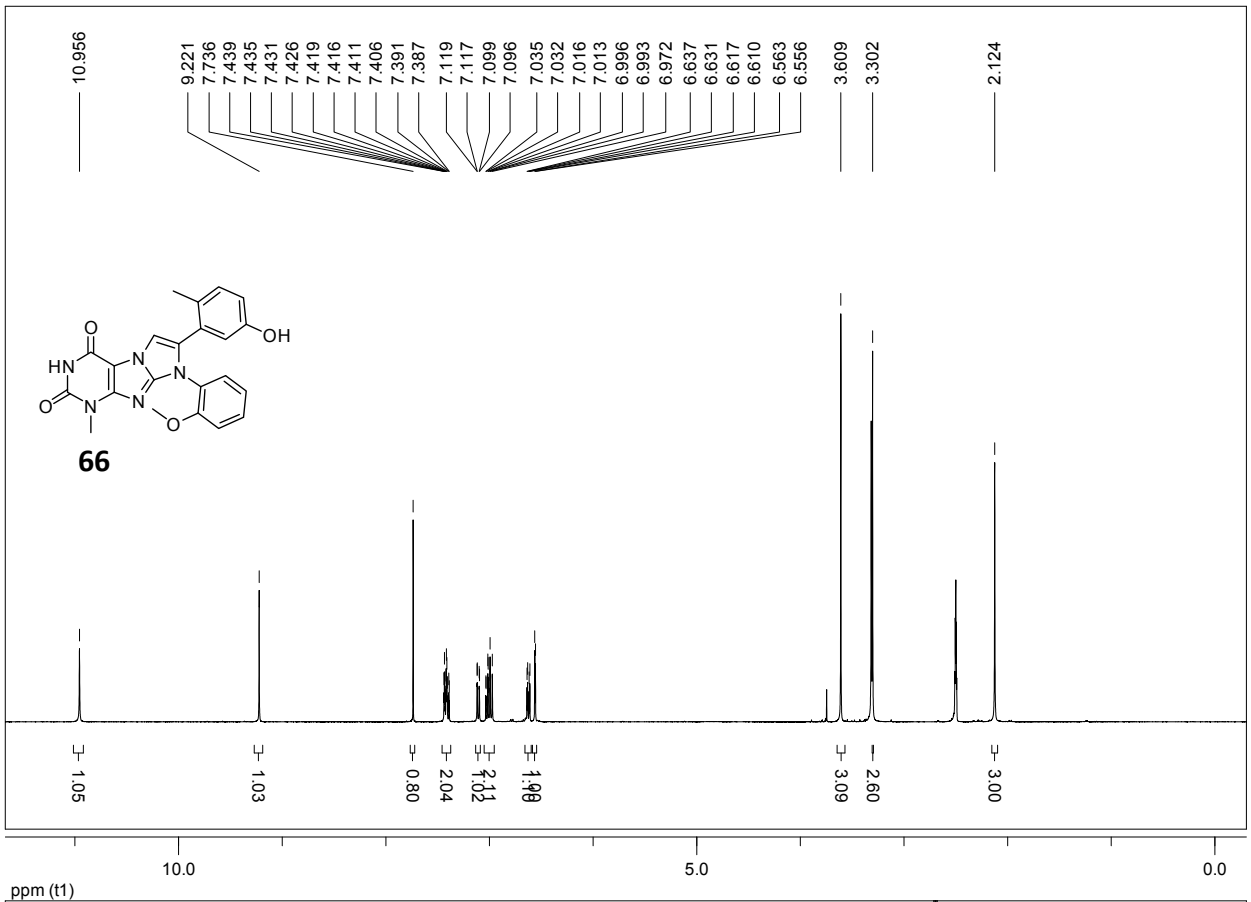
64

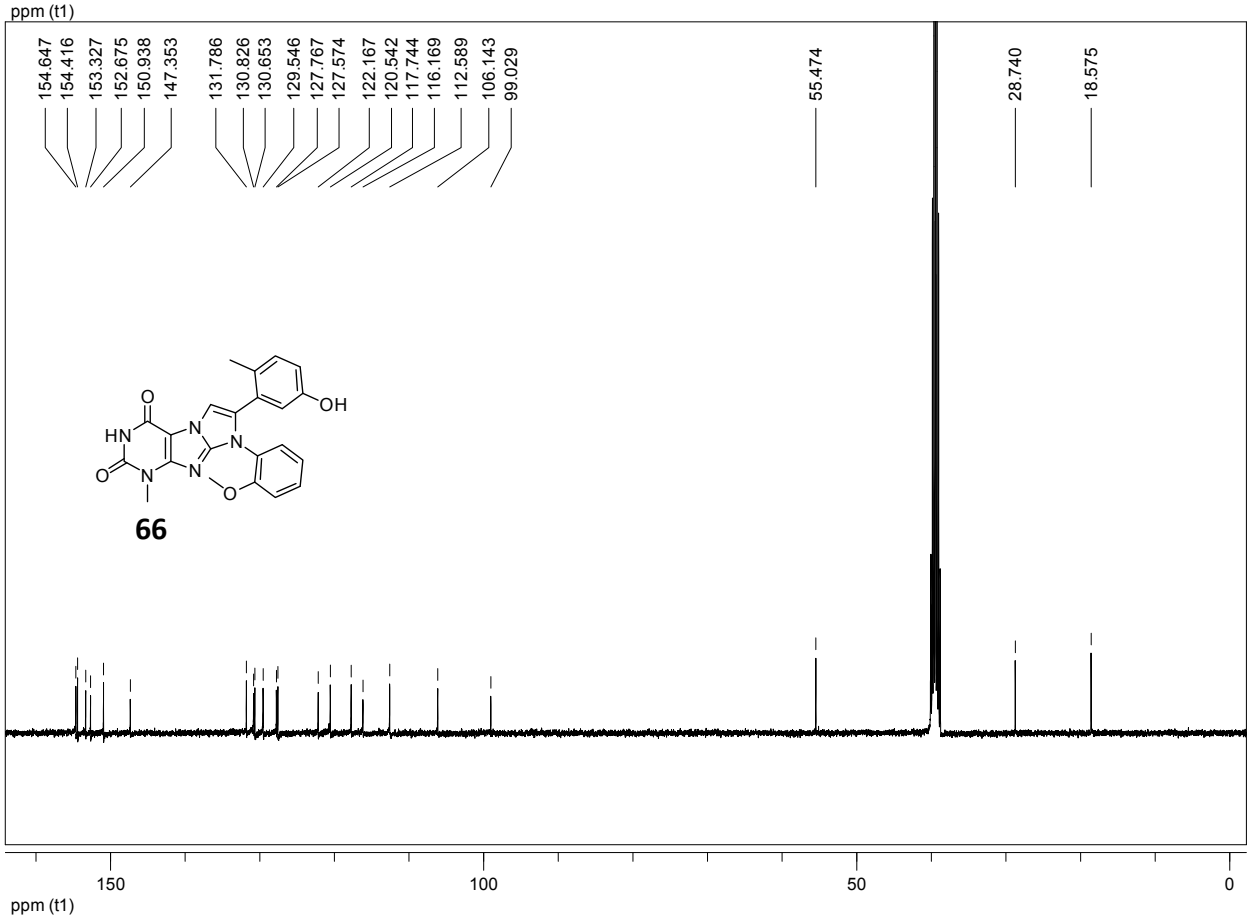

155.143
154.702
153.332
152.657
150.944
147.364
132.069
130.800
129.612
128.288
125.389
124.511
122.218
121.983
120.463
115.286
112.542
106.099
99.021
55.461
28.749
12.897
150
100
50
0
ppm (t1)

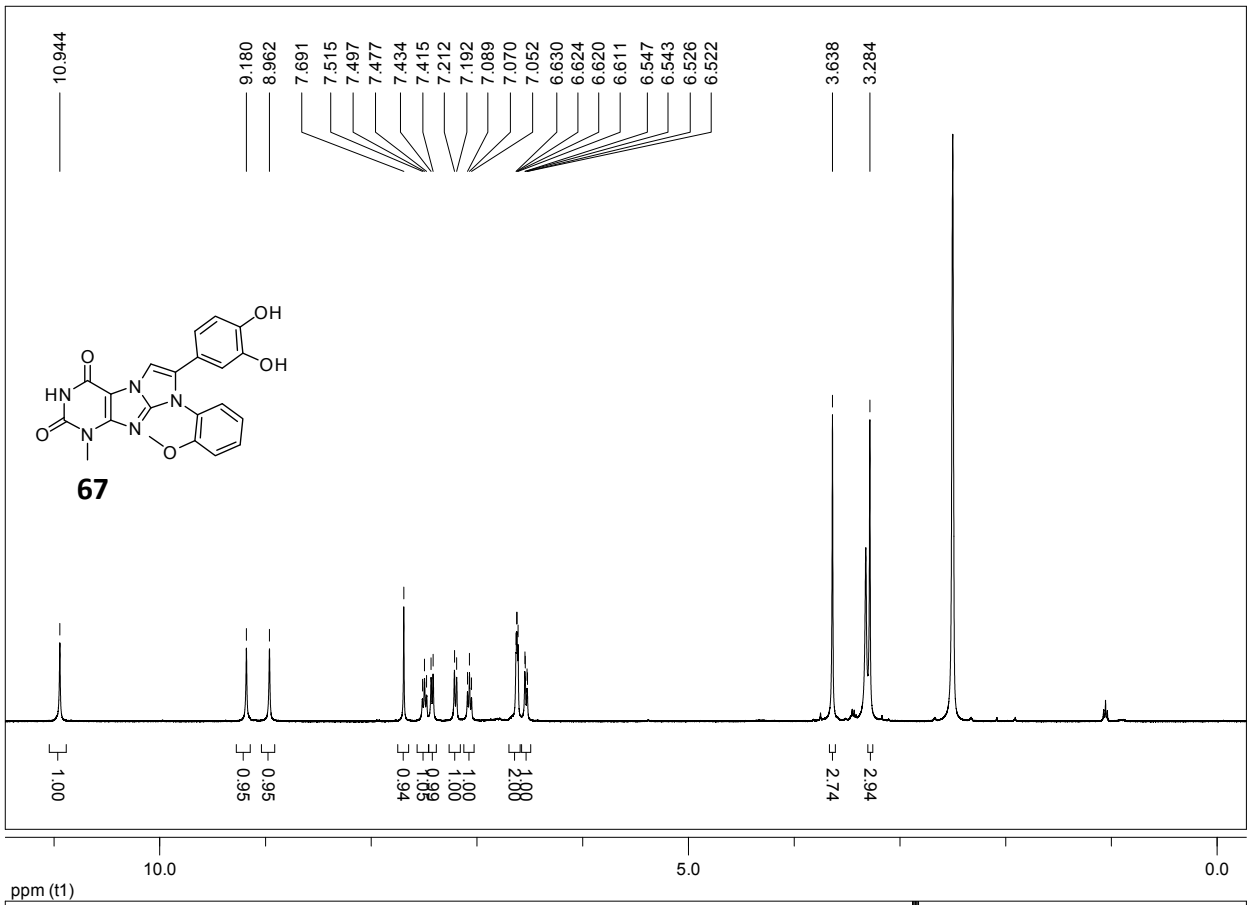
64


10.944
9.550
7.664
7.430
7.426
7.425
7.422
7.419
7.416
7.410
7.406
7.403
7.400
7.396
7.381
7.102
7.080
7.020
7.002
6.983
6.956
6.936
6.572
6.459
6.437
3.606
3.295
2.142
OH
HN
O
N
O
0.95
0.93
0.92
1.89
0.90
2.85
3.61
3.30
10.0
5.0
0.0
ppm (t1)

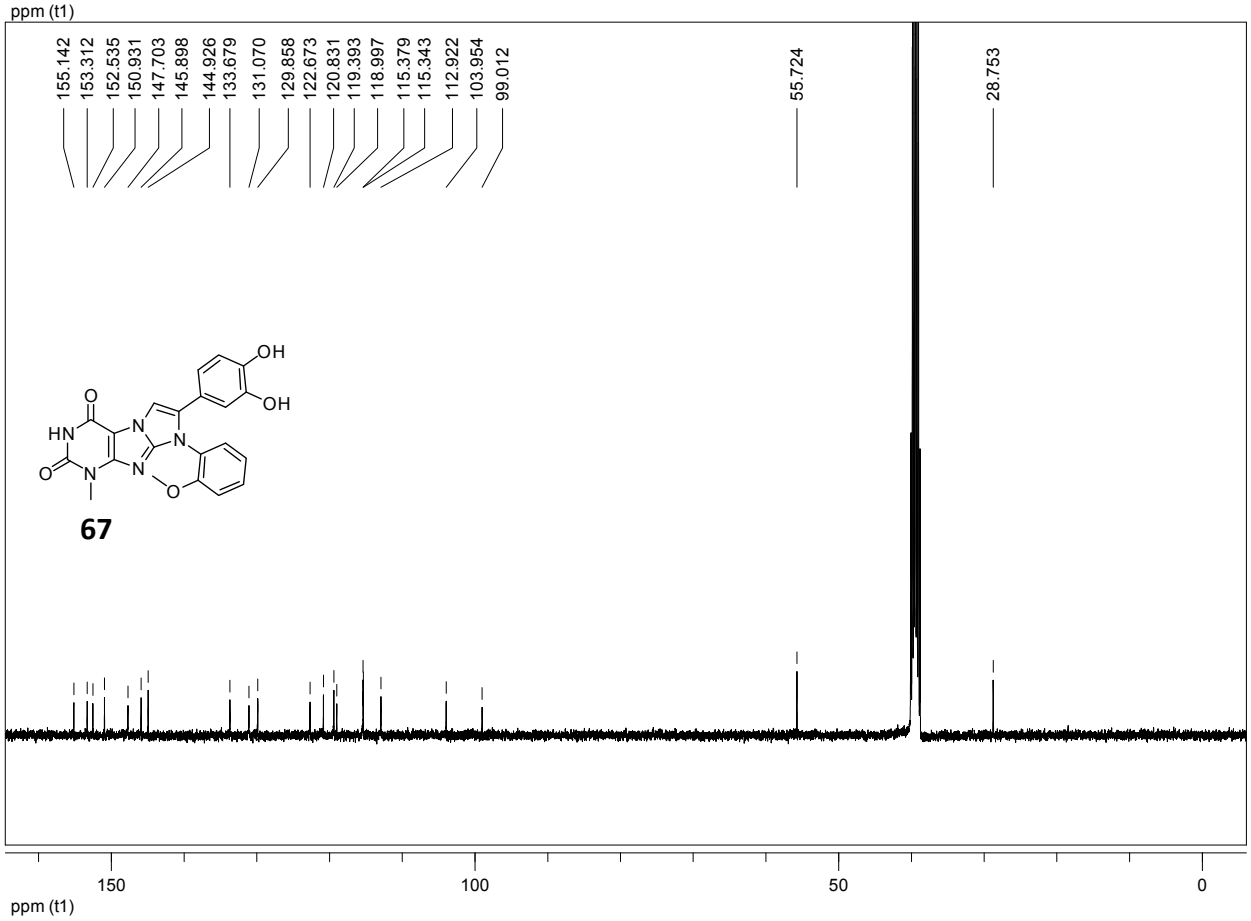
65


10.956
9.221
7.736
7.439
7.435
7.431
7.426
7.419
7.416
7.411
7.406
7.391
7.387
7.119
7.117
7.099
7.096
7.035
7.032
7.016
7.013
6.996
6.993
6.972
6.637
6.631
6.617
6.610
6.563
6.556
3.609
3.302
2.124
OH
HN
O
N
66
1.05
1.03
0.80
2.04
1.02
3.09
2.60
3.00
10.0
5.0
0.0
ppm (t1)

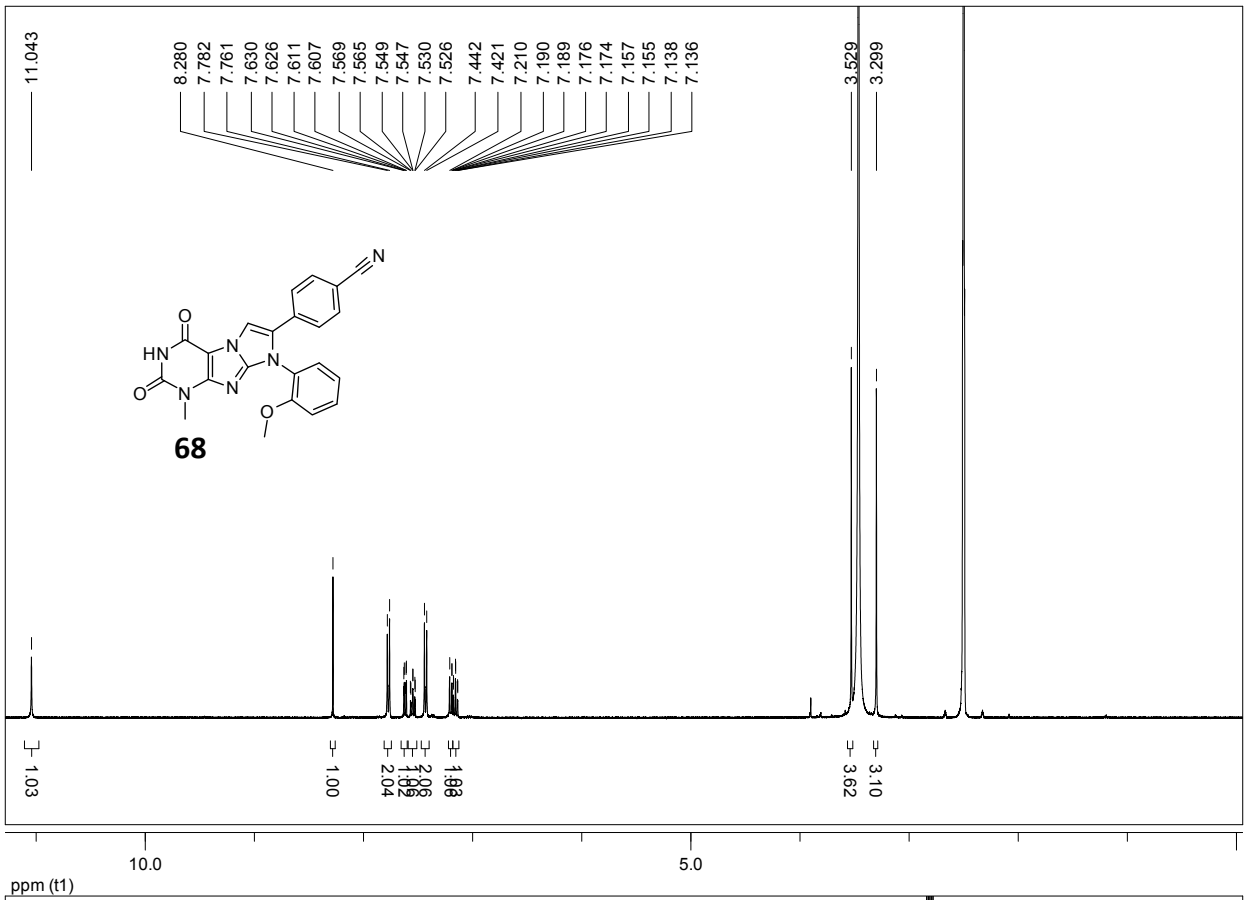

154.647
154.416
153.327
152.675
150.938
147.353
131.786
130.826
130.653
129.546
127.767
127.574
122.167
120.542
117.744
116.169
112.589
106.143
99.029
55.474
28.740
18.575
OH
HN
O
N
66
150
100
50
0
ppm (t1)

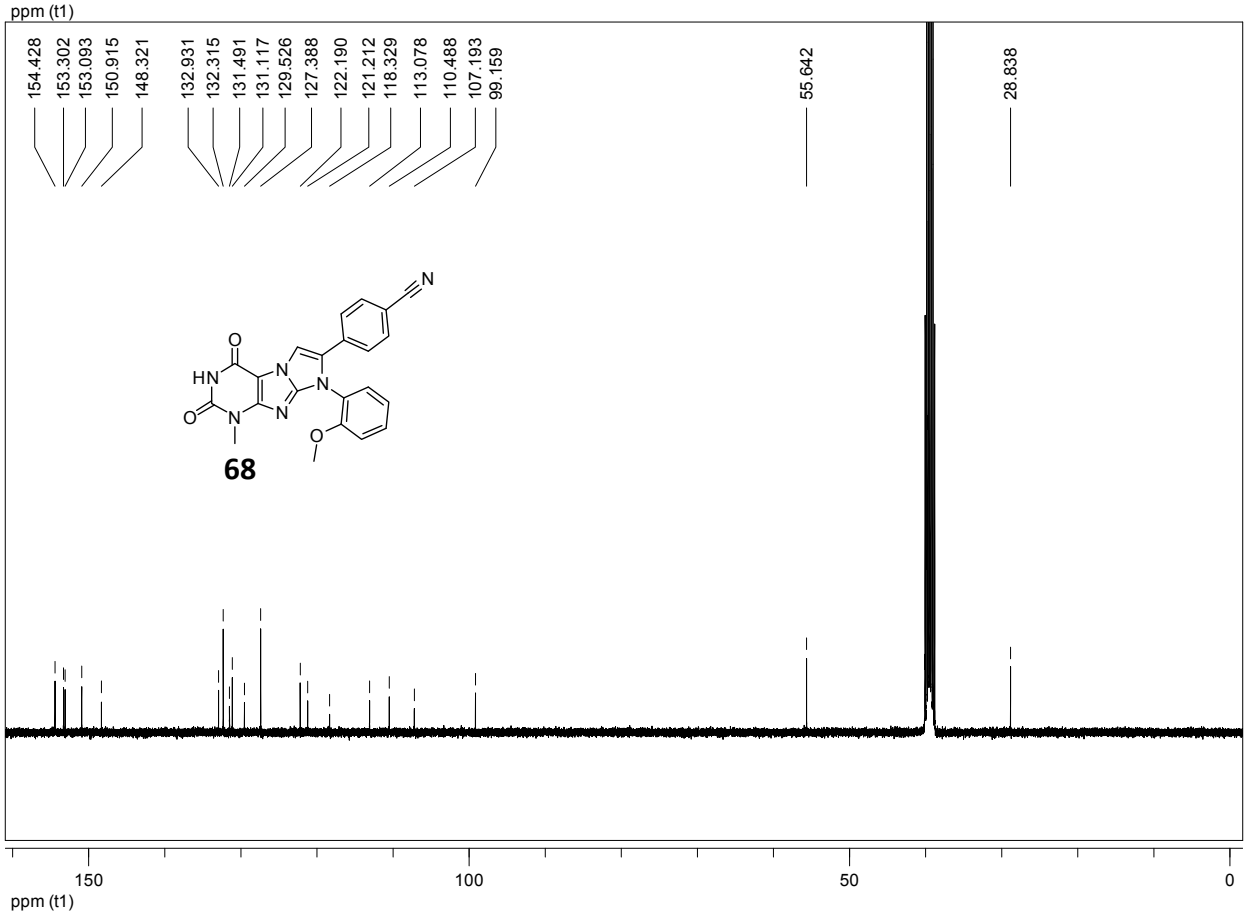

10.944
9.180
8.962
7.691
7.515
7.497
7.477
7.434
7.415
7.212
7.192
7.089
7.070
7.052
6.630
6.624
6.620
6.611
6.547
6.543
6.526
6.522
3.638
3.284
OH
OH
HN
O
N
O
1.00
0.95
0.95
0.94
1.00
1.00
2.00
2.74
2.94
10.0
5.0
0.0
ppm (t1)

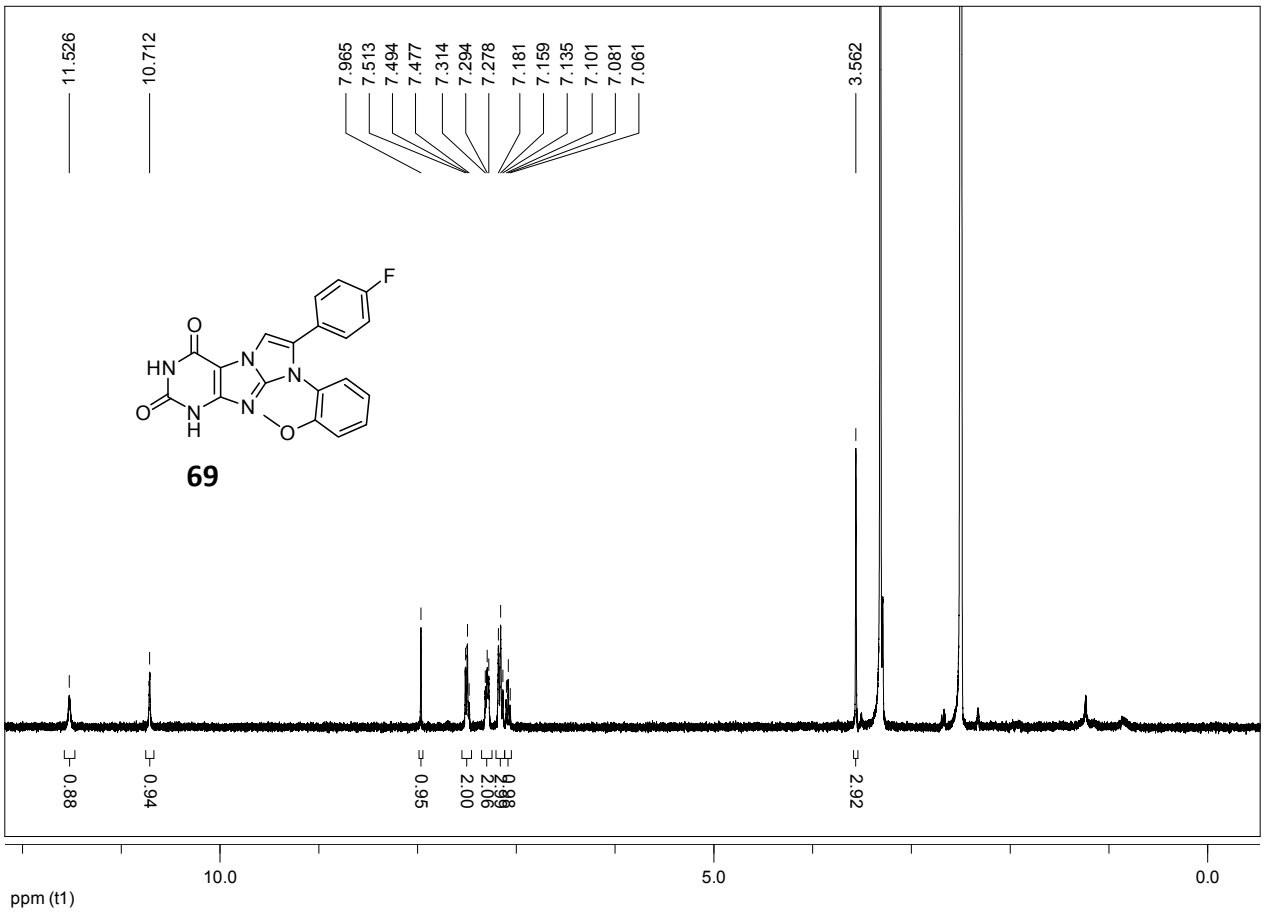
67

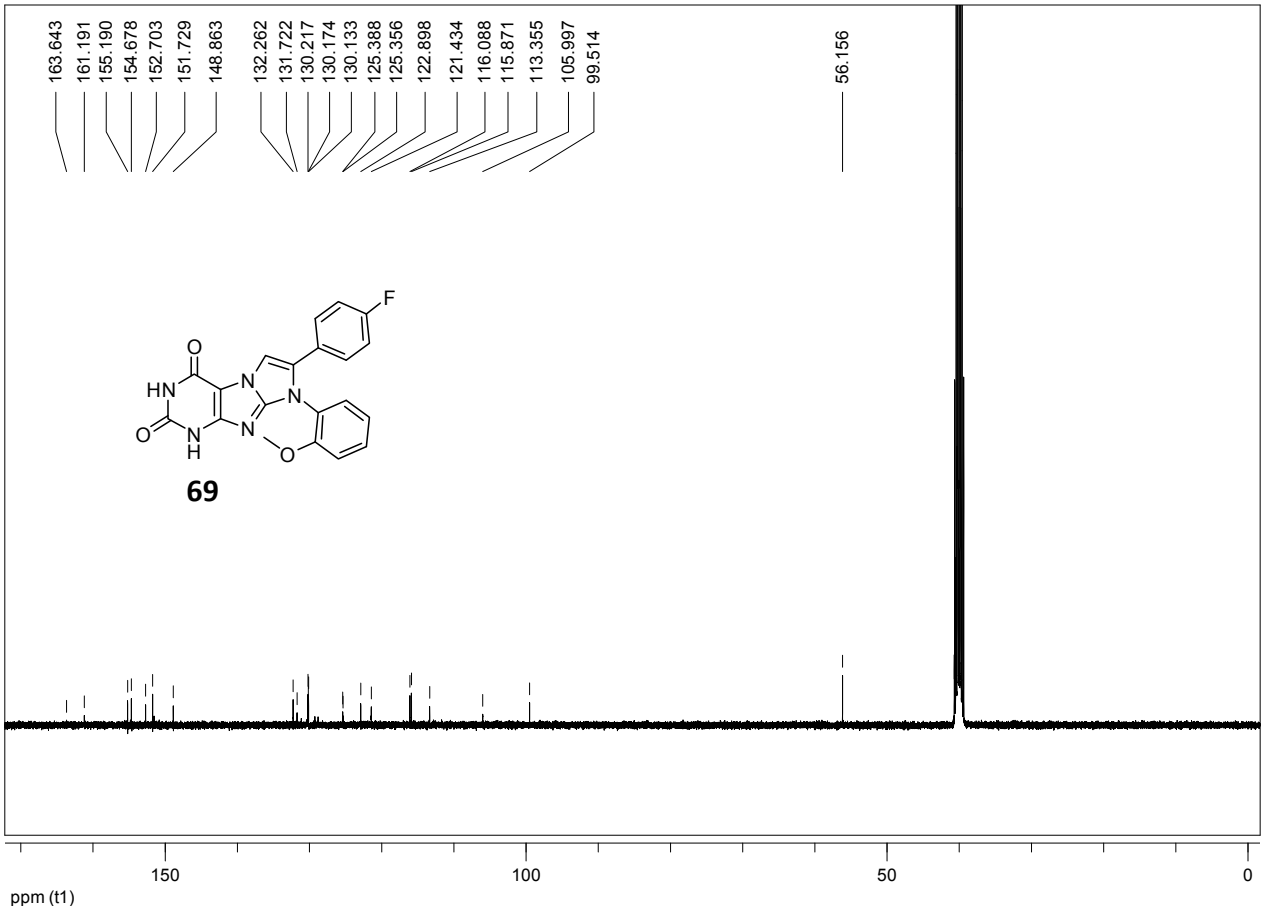

155.142
153.312
152.535
150.931
147.703
145.898
144.926
133.679
131.070
129.858
122.673
120.831
119.393
118.997
115.379
115.343
112.922
103.954
99.012
55.724
28.753
OH
OH
HN
O
N
O
150
100
50
0
ppm (t1)

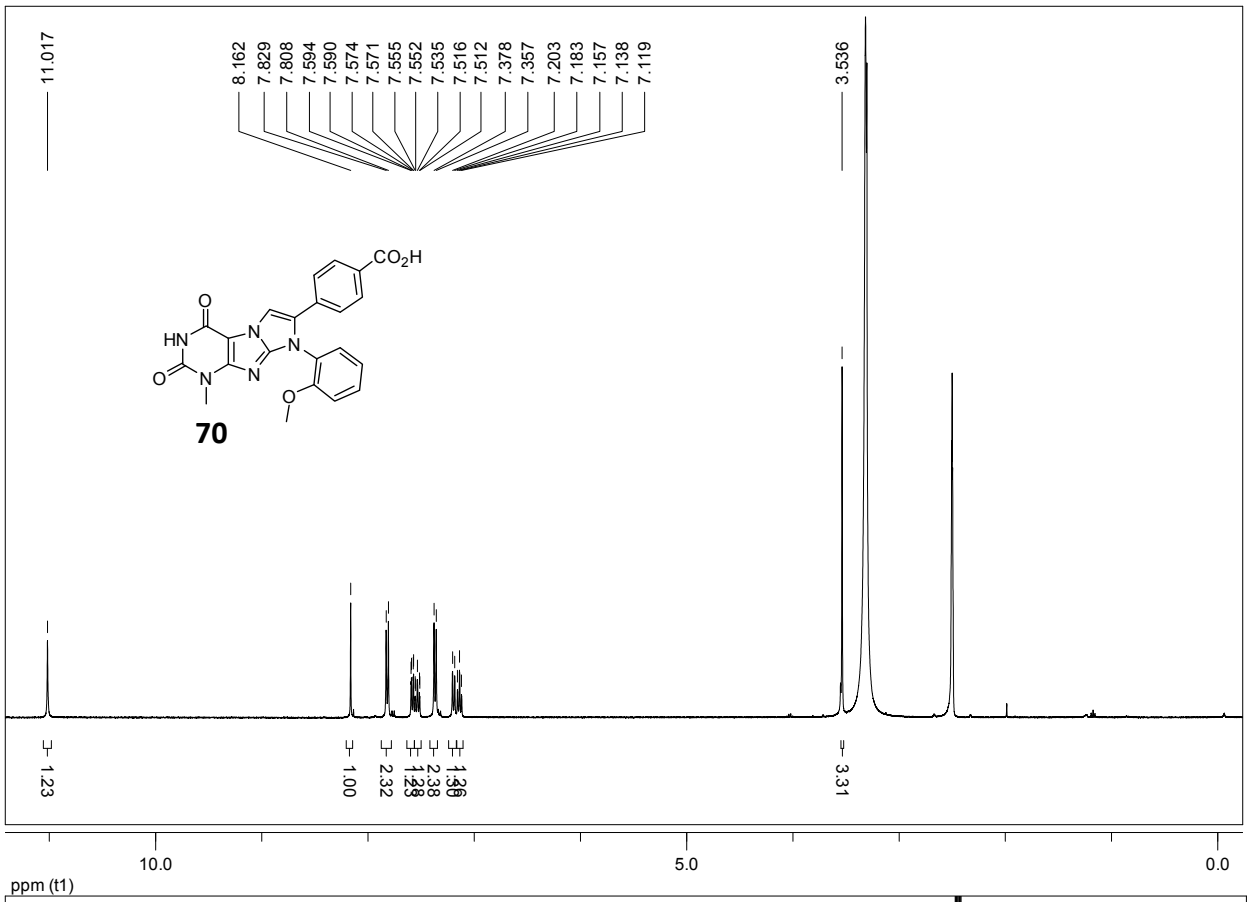
67

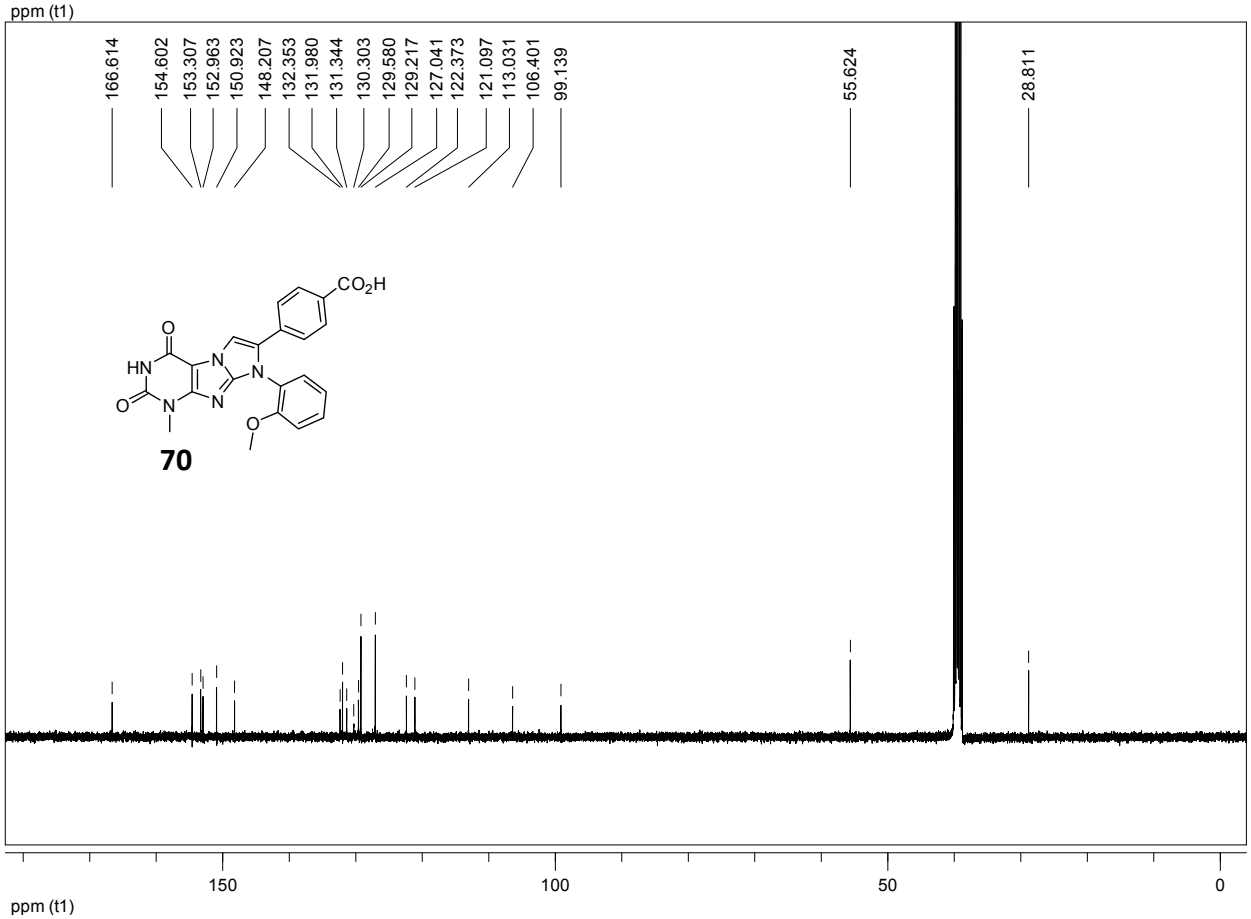

11.043
8.280
7.782
7.761
7.630
7.626
7.611
7.607
7.569
7.565
7.549
7.547
7.530
7.526
7.442
7.421
7.210
7.190
7.189
7.176
7.174
7.157
7.155
7.138
7.136
3.529
3.299
68
1.03
1.00
2.04
3.62
3.10
10.0
5.0
ppm (t1)

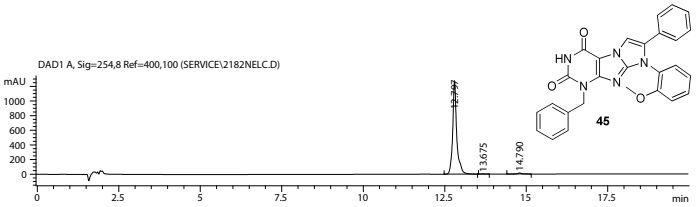

154.428
153.302
153.093
150.915
148.321
132.931
132.315
131.491
131.117
129.526
127.388
122.190
121.212
118.329
113.078
110.488
107.193
99.159
55.642
28.838
68
150
100
50
0
ppm (t1)


11.526
10.712
7.965
7.513
7.494
7.477
7.314
7.294
7.278
7.181
7.159
7.135
7.101
7.081
7.061
3.562
F
O
HN
N
N
O
N
H
N
O
69
0.88
0.94
0.95
2.00
2.92
10.0
5.0
0.0
ppm (t1)


163.643
161.191
155.190
154.678
152.703
151.729
148.863
132.262
131.722
130.217
130.174
130.133
125.388
125.356
122.898
121.434
116.088
115.871
113.355
105.997
99.514
56.156
F
O
HN
N
N
O
N
H
N
O
69
150
100
50
0
ppm (t1)


11.017
8.162
7.829
7.808
7.594
7.590
7.574
7.571
7.555
7.552
7.535
7.516
7.512
7.378
7.357
7.203
7.183
7.157
7.138
7.119
3.536
CO2H
HN
O
N
O
70
1.23
1.00
2.32
3.31
10.0
5.0
0.0
ppm (t1)


166.614
154.602
153.307
152.963
150.923
148.207
132.353
131.980
131.344
130.303
129.580
129.217
127.041
122.373
121.097
113.031
106.401
99.139
55.624
28.811
CO2H
HN
O
N
O
70
150
100
50
0
ppm (t1)

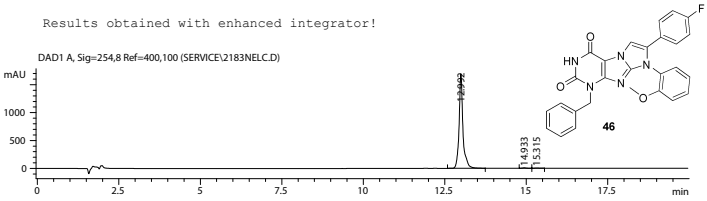


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.797	PB	0.1248	1.10298e4	1276.96851	98.3752
2	13.675	BB	0.1491	45.46704	4.30844	0.4055
3	14.790	BP	0.1271	136.70268	15.46290	1.2193

Totals : 1.12120e4 1296.73985

Results obtained with enhanced integrator!

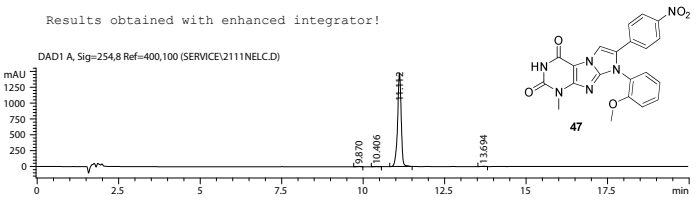


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.992	BB	0.1208	1.40679e4	1695.99756	99.2969
2	14.933	BV	0.1175	67.43863	8.41861	0.4760
3	15.315	VB	0.1172	32.17053	4.02817	0.2271

Totals : 1.41675e4 1708.44434

Results obtained with enhanced integrator!

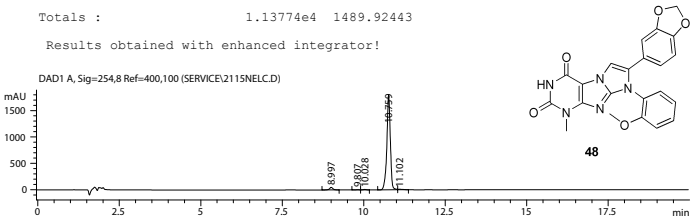


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.870	MM	0.1175	25.79613	3.65922	0.2267
2	10.406	MM	0.1312	23.97427	3.04527	0.2107
3	11.112	MM	0.1273	1.12961e4	1478.62524	99.2858
4	13.694	MM	0.1142	31.48430	4.59470	0.2767

Totals : 1.13774e4 1489.92443

Results obtained with enhanced integrator!

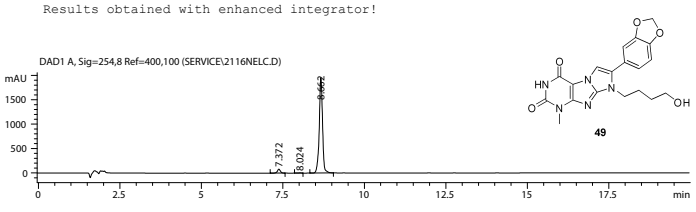


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.997	MM	0.1245	365.03687	48.85506	2.6020
2	9.807	MF	0.1540	47.37795	5.12762	0.3377
3	10.028	FM	0.1270	69.68505	9.14234	0.4967
4	10.759	MF	0.1240	1.34124e4	1803.15283	95.6047
5	11.102	FM	0.1922	134.51891	11.66585	0.9589

Totals : 1.40290e4 1877.94371

Results obtained with enhanced integrator!

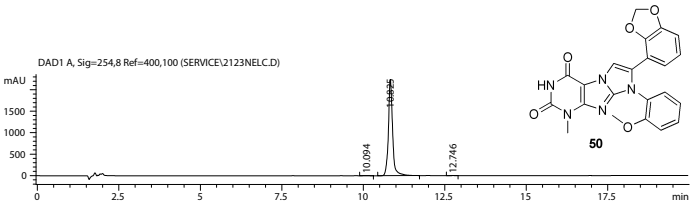


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.372	MM	0.1060	517.74554	81.43184	3.6379
2	8.024	MM	0.1224	29.69349	4.04195	0.2086
3	8.662	MM	0.1164	1.36846e4	1959.62842	96.1535

Totals : 1.42320e4 2045.10221

Results obtained with enhanced integrator!



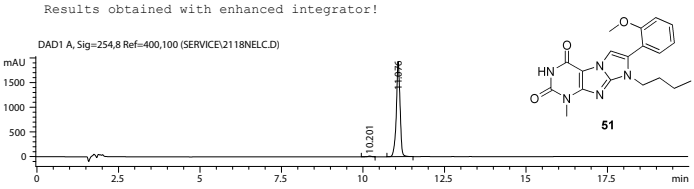
50

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.094	MM	0.1940	43.73960	3.75803	0.2176
2	10.825	MM	0.1487	2.00344e4	2246.17871	99.6705
3	12.746	MM	0.1566	22.49511	2.39463	0.1119

Totals : 2.01006e4 2252.33137

Results obtained with enhanced integrator!



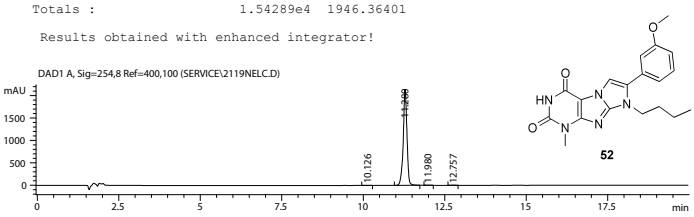
51

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.201	MM	0.1267	111.57723	14.67663	0.7232
2	11.076	MM	0.1322	1.53173e4	1931.68738	99.2768

Totals : 1.54289e4 1946.36401

Results obtained with enhanced integrator!



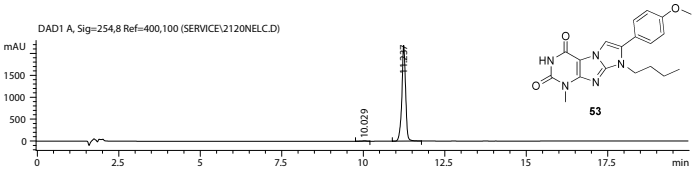
52

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.126	MM	0.1237	17.37408	2.34133	0.1018
2	11.280	MM	0.1327	1.70207e4	2137.00659	99.7444
3	11.980	MM	0.1211	13.62705	1.87581	0.0799
4	12.757	MM	0.1344	12.61421	1.56463	0.0739

Totals : 1.70644e4 2142.78836

Results obtained with enhanced integrator!



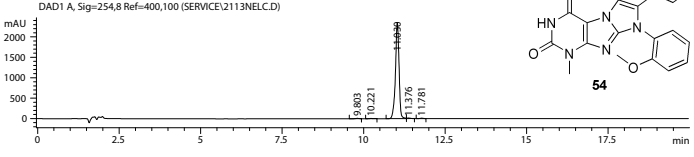
53

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.029	MM	0.1192	76.10860	10.64413	0.4344
2	11.237	MM	0.1328	1.74434e4	2189.52124	99.5656

Totals : 1.75195e4 2200.16537

Results obtained with enhanced integrator!



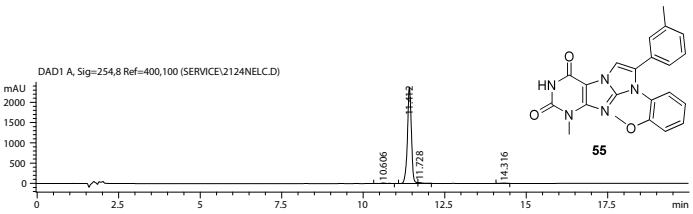
54

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.803	MM	0.1229	73.87368	10.01421	0.4015
2	10.221	MM	0.1528	74.93574	8.17328	0.4073
3	11.030	MF	0.1279	1.80571e4	2352.78564	98.1513
4	11.376	FM	0.1215	103.95795	14.25452	0.5651
5	11.781	MM	0.1266	87.33304	11.49384	0.4747

Totals : 1.83972e4 2396.72150

Results obtained with enhanced integrator!



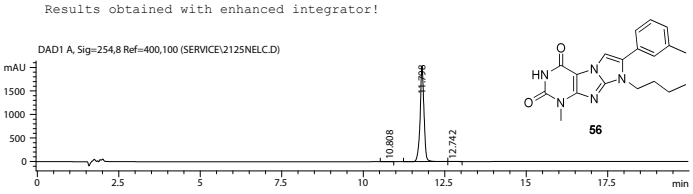
55

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.606	MM	0.2148	204.42885	15.86199	1.0054
2	11.412	MF	0.1390	1.98586e4	2380.76709	97.6648
3	11.728	FM	0.1754	217.98387	20.71004	1.0720
4	14.316	MM	0.1347	52.40693	6.48435	0.2577

Totals : 2.03334e4 2423.82348

Results obtained with enhanced integrator!



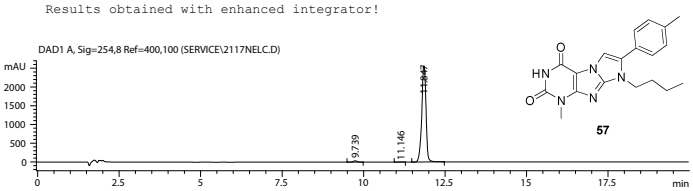
56

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.808	MF	0.1668	13.18572	1.31732	0.0787
2	11.798	MF	0.1367	1.67153e4	2037.58545	99.7264
3	12.742	FM	0.2300	32.66756	2.36725	0.1949

Totals : 1.67611e4 2041.27003

Results obtained with enhanced integrator!



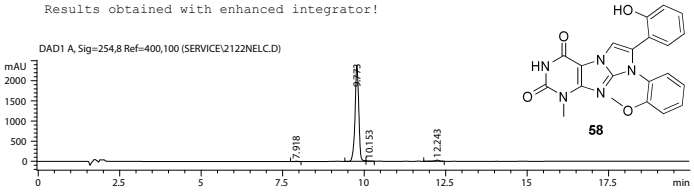
57

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.201	MM	0.1267	111.57723	14.67663	0.7232
2	11.076	MM	0.1322	1.53173e4	1931.68738	99.2768

Totals : 1.54289e4 1946.36401

Results obtained with enhanced integrator!



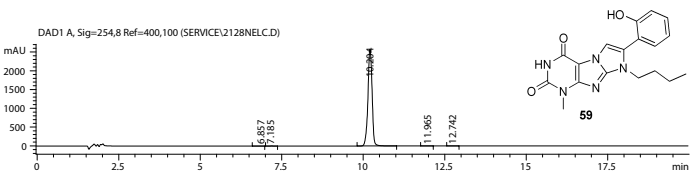
58

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.918	MM	0.1740	75.24974	7.20904	0.3917
2	9.773	MF	0.1307	1.87471e4	2391.36938	97.5843
3	10.153	FM	0.1634	93.26763	9.51487	0.4855
4	12.243	MM	0.1658	295.55783	29.71509	1.5385

Totals : 1.92111e4 2437.80838

Results obtained with enhanced integrator!



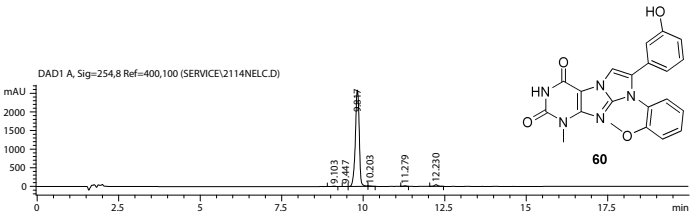
59

Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.857	MM	0.1342	26.07518	3.23900	0.1133
2	7.185	MM	0.1342	31.55520	3.91949	0.1371
3	10.204	MM	0.1480	2.29106e4	2580.79053	99.5636
4	11.965	MM	0.1659	23.60228	2.37142	0.1026
5	12.742	MM	0.1755	19.17964	1.82131	0.0833

Totals : 2.30110e4 2592.14175

Results obtained with enhanced integrator!

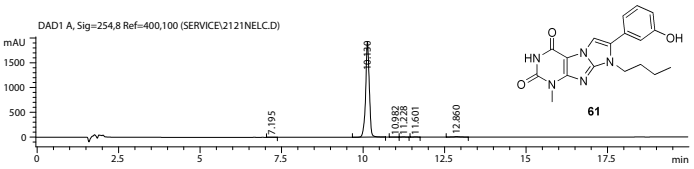


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.103	MM	0.1118	70.24006	10.47079	0.3193
2	9.447	MM	0.0846	16.68053	3.28499	0.0758
3	9.817	MF	0.1380	2.14358e4	2588.07349	97.4434
4	10.203	FM	0.1222	79.49773	10.84007	0.3614
5	11.279	MM	0.0952	74.81622	13.10363	0.3401
6	12.230	MM	0.1194	321.17963	44.81770	1.4600

Totals : 2.19983e4 2670.59068

Results obtained with enhanced integrator!

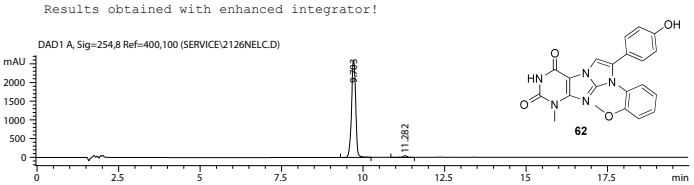


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.195	MM	0.1391	23.98127	2.87387	0.1578
2	10.130	MM	0.1289	1.49298e4	1929.99719	98.2180
3	10.982	MM	0.1375	15.29320	1.85433	0.1006
4	11.228	MM	0.1402	39.58162	4.70694	0.2604
5	11.601	MM	0.1242	38.70705	5.19376	0.2546
6	12.860	MM	0.2227	153.32024	11.47576	1.0086

Totals : 1.52007e4 1956.10184

Results obtained with enhanced integrator!

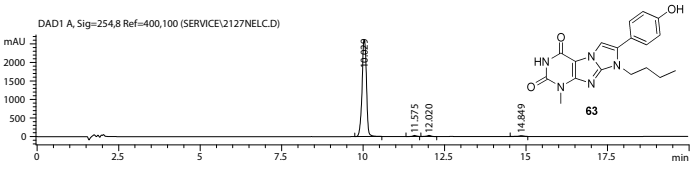


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.703	MM	0.1481	2.30244e4	2590.73120	97.7303
2	11.282	MM	0.1827	534.71448	48.76721	2.2697

Totals : 2.35591e4 2639.49841

Results obtained with enhanced integrator!

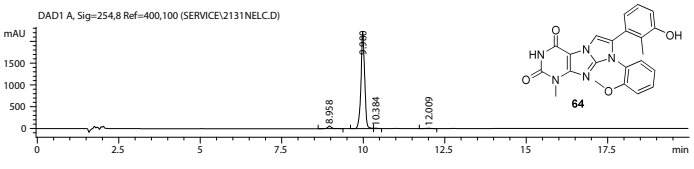


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.029	MM	0.1555	2.43647e4	2611.37354	96.9998
2	11.575	MM	0.1356	241.77534	29.71087	0.9625
3	12.020	MM	0.1514	283.01013	31.16286	1.1267
4	14.849	MM	0.1666	228.81995	22.88530	0.9110

Totals : 2.51183e4 2695.13256

Results obtained with enhanced integrator!

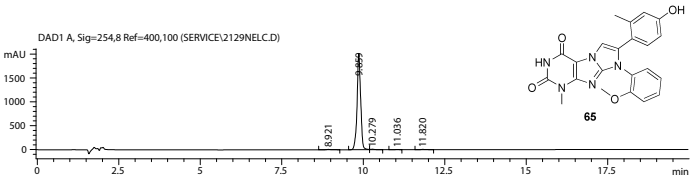


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.958	MM	0.1460	533.52417	60.88585	2.9225
2	9.980	MF	0.1316	1.74874e4	2215.40356	95.7901
3	10.384	FM	0.1489	88.33442	9.89022	0.4839
4	12.009	MM	0.2668	146.70917	9.16612	0.8036

Totals : 1.82560e4 2295.34576

Results obtained with enhanced integrator!

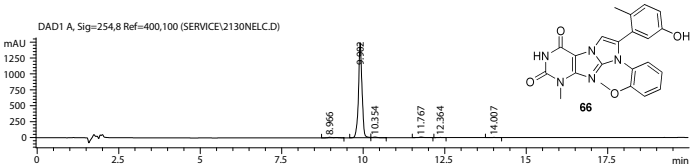


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.921	MM	0.1999	101.07433	8.42708	0.6430
2	9.859	MF	0.1275	1.53868e4	2011.61133	97.8851
3	10.279	FM	0.1719	112.27142	10.88832	0.7142
4	11.036	MM	0.1330	36.10246	4.52356	0.2297
5	11.820	MM	0.2016	82.99743	6.86162	0.5280

Totals : 1.57192e4 2042.31190

Results obtained with enhanced integrator!

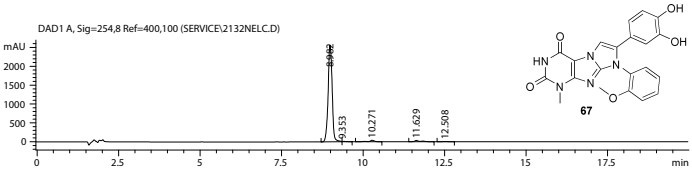


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.966	MM	0.2361	128.96809	9.10297	1.1015
2	9.902	MF	0.1253	1.12371e4	1494.13733	95.9766
3	10.354	FM	0.1763	126.24681	11.93596	1.0783
4	11.767	MM	0.2062	134.32549	10.85975	1.1473
5	12.364	MM	0.1572	30.51100	3.23468	0.2606
6	14.007	MM	0.2541	51.00922	3.34590	0.4357

Totals : 1.17081e4 1532.61658

Results obtained with enhanced integrator!

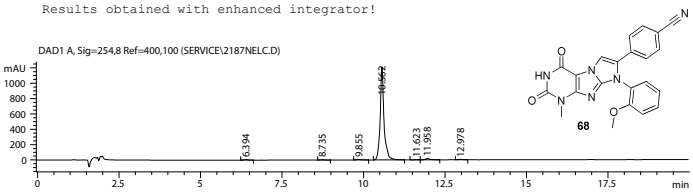


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.982	MM	0.1442	2.22129e4	2567.81519	94.7668
2	9.353	FM	0.1626	103.62782	10.62265	0.4421
3	10.271	MM	0.2064	516.68903	41.72570	2.2043
4	11.629	MM	0.2281	464.24408	33.92147	1.9806
5	12.508	MM	0.2558	142.06587	9.25592	0.6061

Totals : 2.34395e4 2663.34092

Results obtained with enhanced integrator!

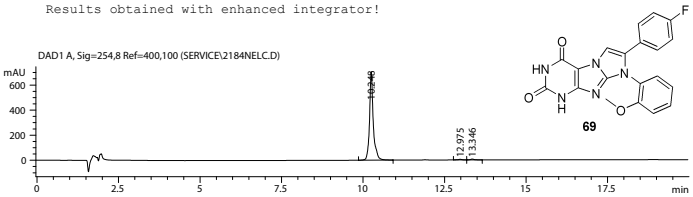


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.394	PB	0.1265	57.81351	7.29481	0.5549
2	8.735	BB	0.1129	43.03243	5.52182	0.4130
3	9.855	BB	0.1190	53.27367	6.41040	0.5113
4	10.562	BB	0.1178	9972.16406	1214.57849	95.7149
5	11.623	BV	0.1521	31.61758	2.83508	0.3035
6	11.958	VB	0.1367	191.63791	19.49966	1.8394
7	12.978	VV	0.1331	69.06989	7.25406	0.6629

Totals : 1.04186e4 1263.39431

Results obtained with enhanced integrator!

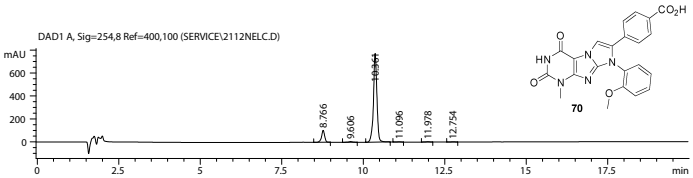


Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.248	BB	0.1157	5675.17529	706.35577	98.0475
2	12.975	VV	0.1385	53.75838	5.38432	0.9288
3	13.346	VP	0.1242	59.25332	6.90132	1.0237

Totals : 5788.18699 718.64141

Results obtained with enhanced integrator!



Signal 1: DAD1 A, Sig=254,8 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.766	MM	0.1087	681.62402	104.54838	10.5335
2	9.606	MM	0.1229	43.43242	5.89087	0.6712
3	10.361	MM	0.1226	5690.32275	773.36554	87.9355
4	11.096	MM	0.1180	18.34534	2.59204	0.2835
5	11.978	MM	0.1435	25.17184	2.92326	0.3890
6	12.754	MM	0.1205	12.12391	1.67696	0.1874
Totals :				6471.02029	890.99703	

Results obtained with enhanced integrator!