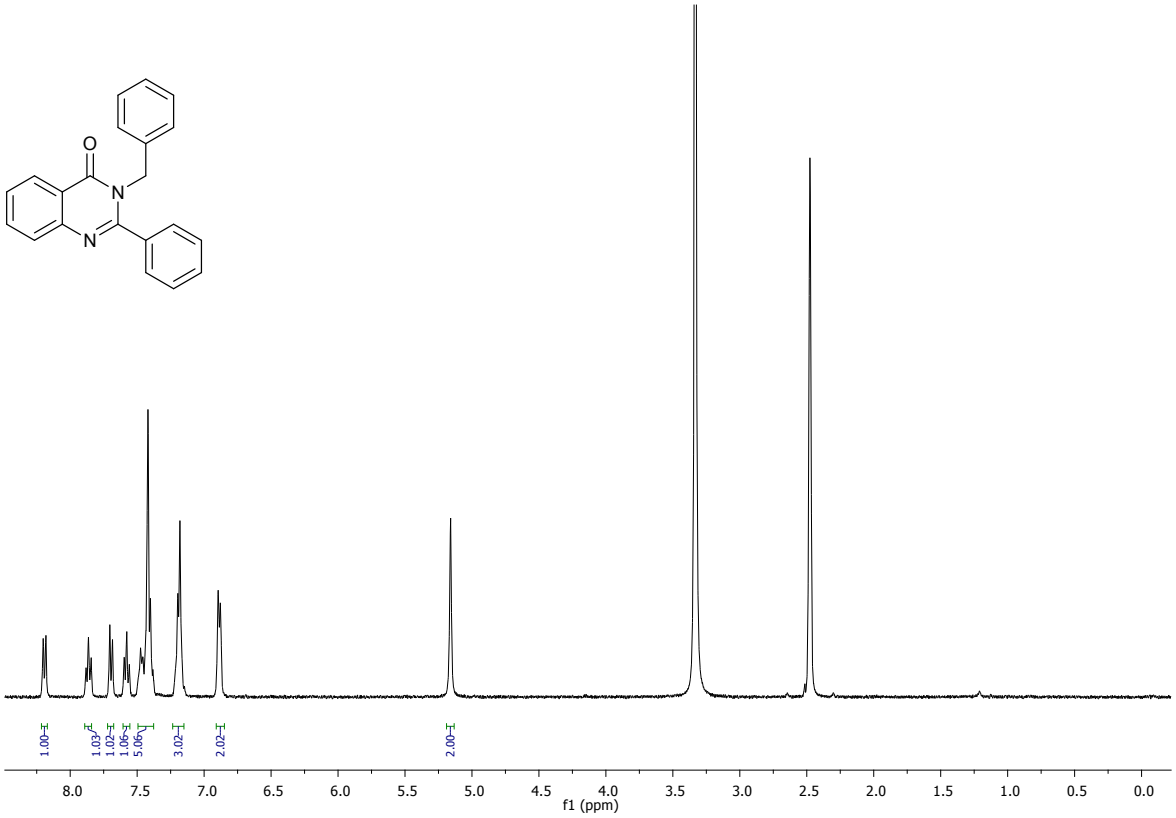
Cu-Catalysed Quinazolinones Synthesis Using CSP3-H Functionalisation/Cyclisation Strategy

Aniket V. A. Gholap,[a] Soham Maity,[b] Carola Schulzke,[c] Debabrata Maiti,[b,*] Anant R. Kapdi[a,*]

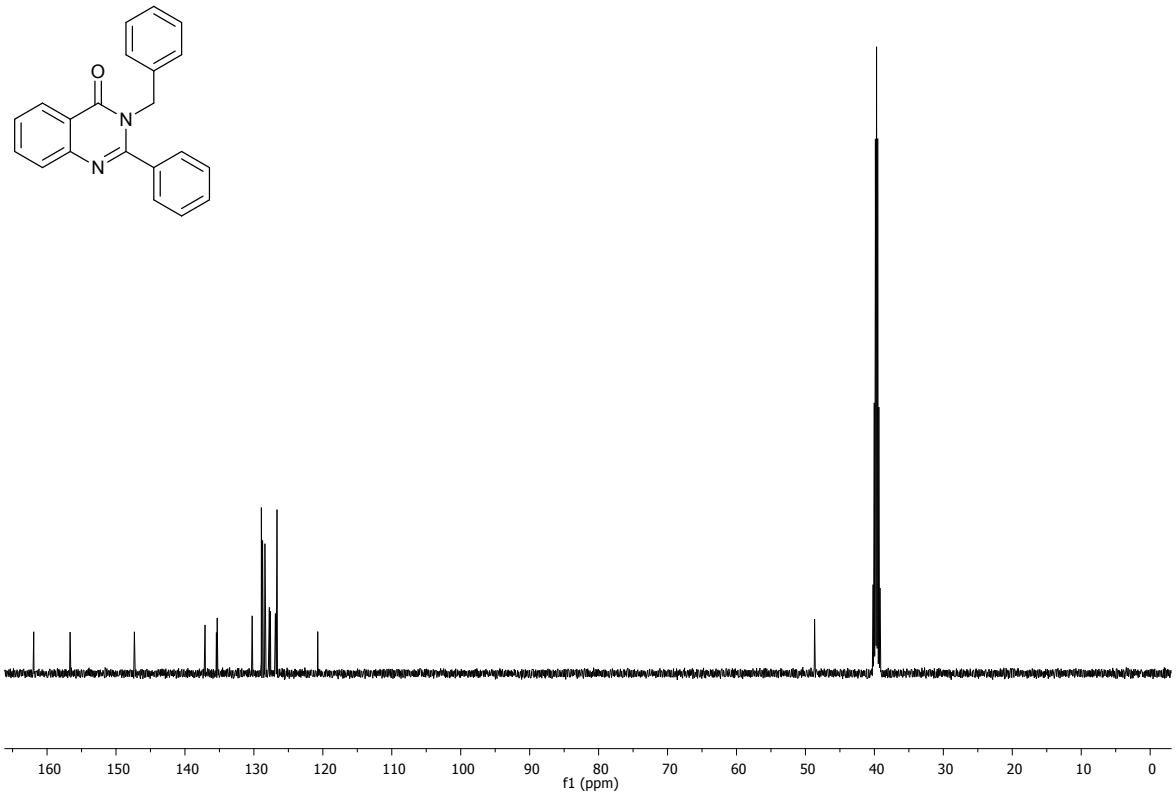
[a.] *Department of Chemistry, Institute of Chemical Technology, Matunga, Mumbai-400019, India. Email id: ar.kapdi@ictmumbai.edu.in*
[b.] *Department of Chemistry, Indian Institute of Technology, Bombay, Powai, Mumbai-400076, India. dmaiti@chem.iitb.ac.in*
[c.] *Institute fur Biochemie, Ernst-Moritz-Arndt Universität Greifswald, Felix-Hausdorff- Straße 4, D-17487 Greifswald, Germany*

Supporting Information

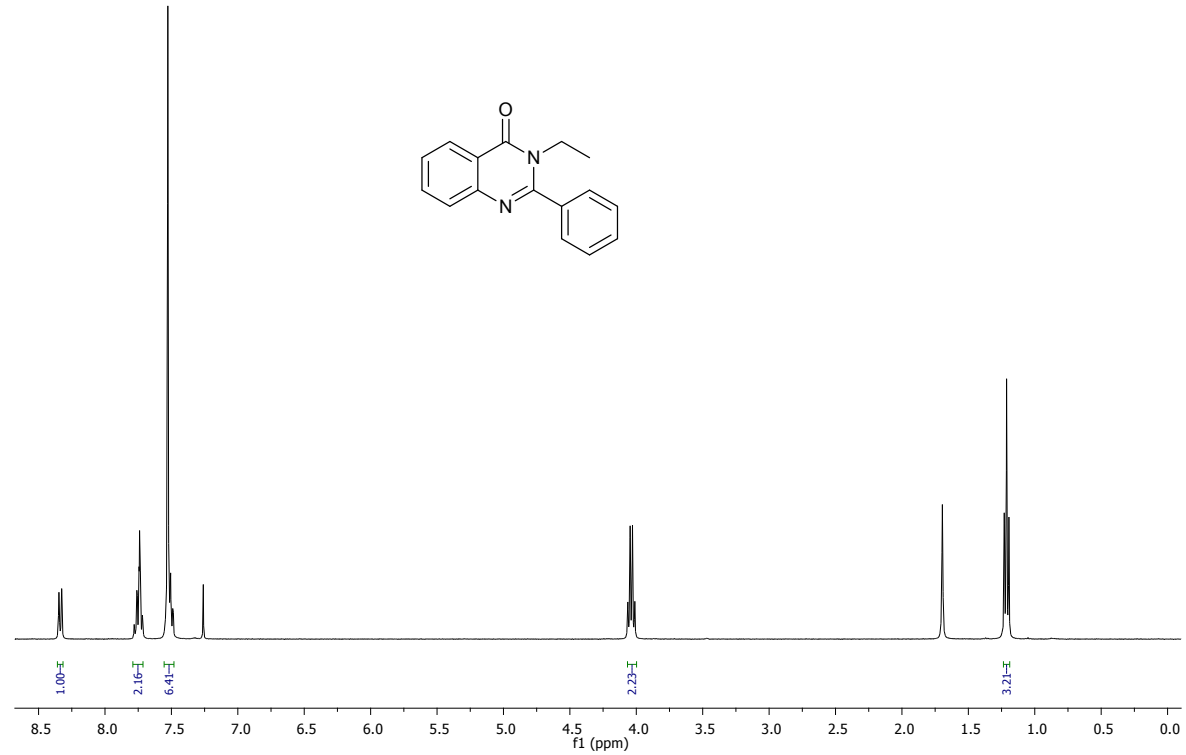
2a

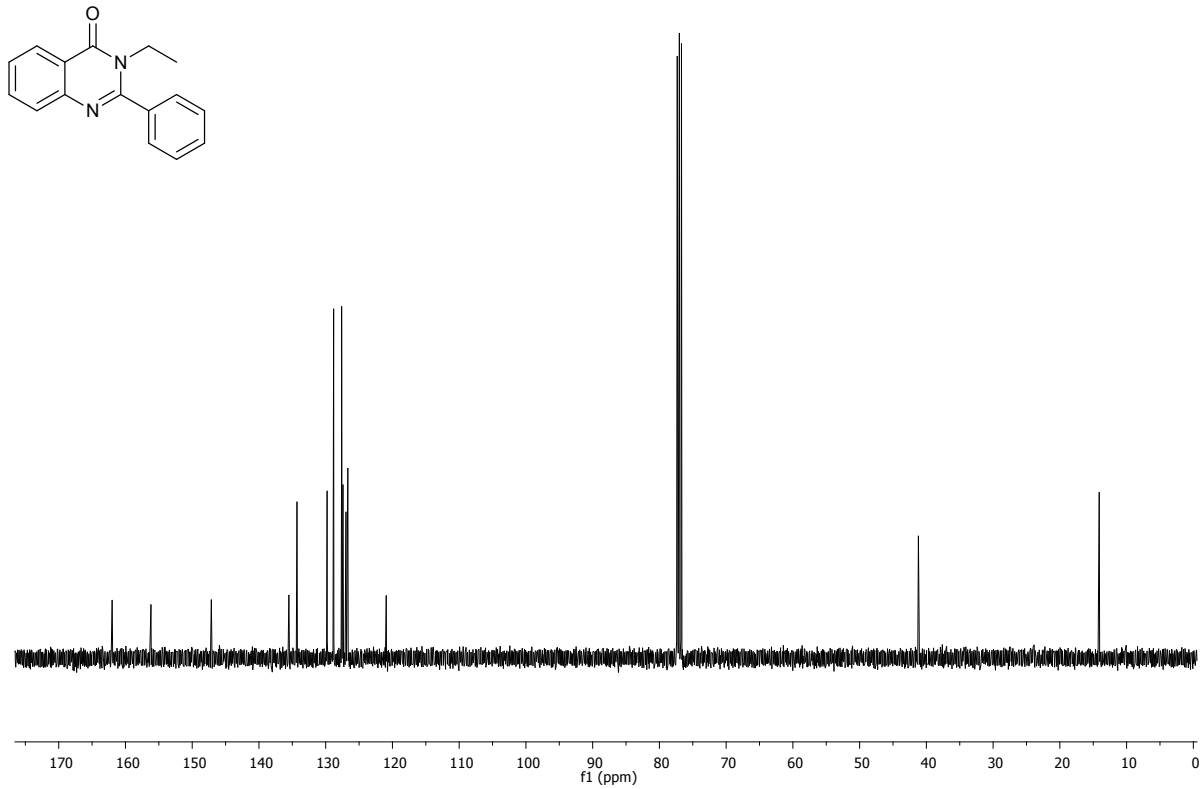

O
N
N
1.00
1.03
1.02
1.06
5.06
3.02
2.02
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

2a

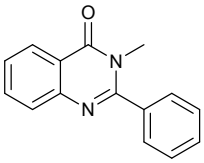

O
N
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

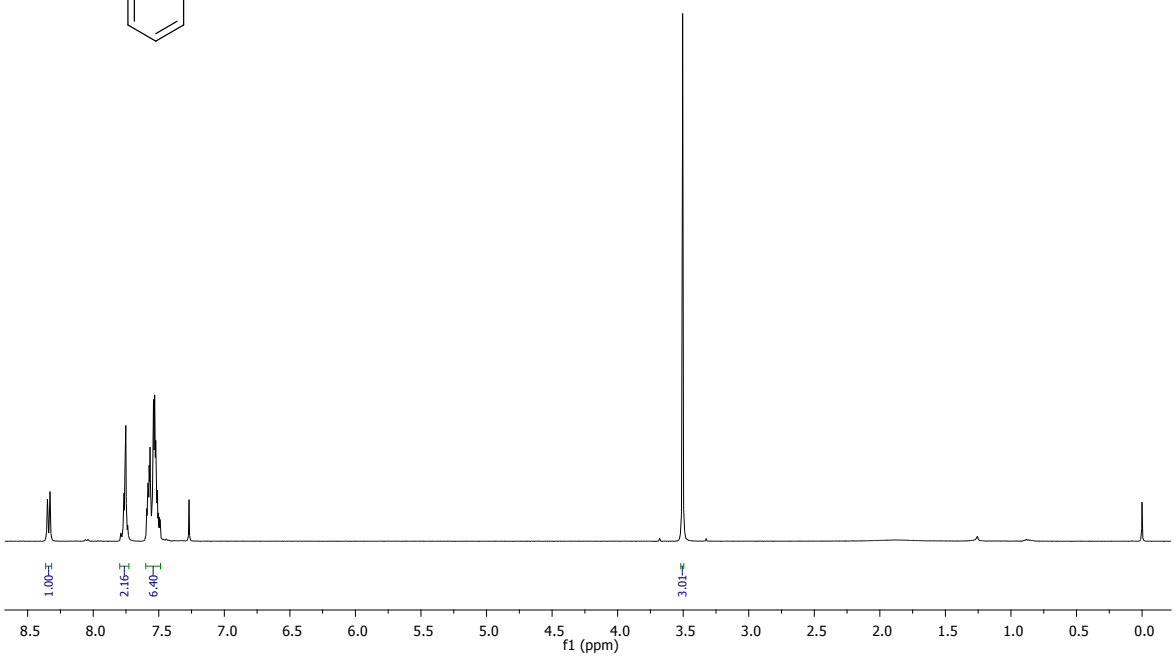
2b

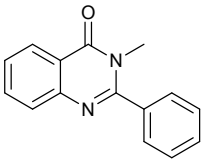

O
N
N
1.00
2.16
6.41
2.23
3.21
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
N
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2c

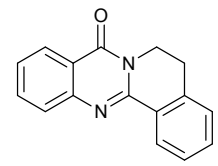

O
N
N


1.00
2.16
6.40
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

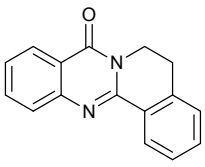

O
N
N

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2d

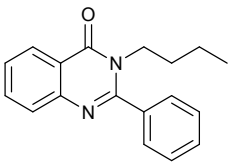

O
N
N

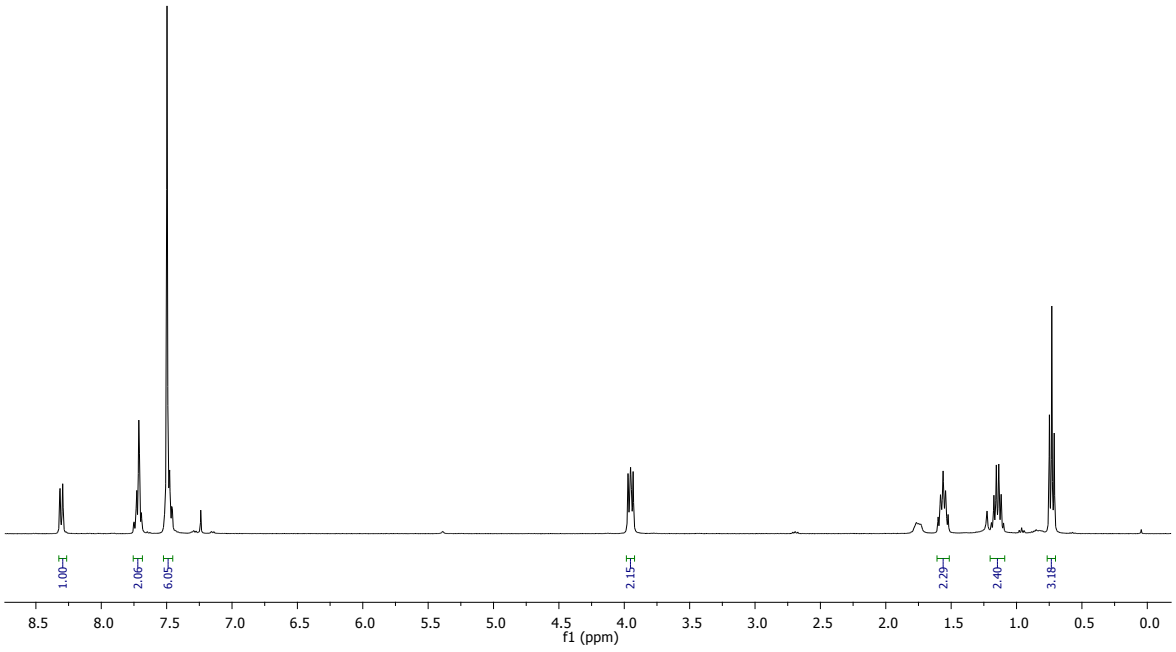
1.00
1.00
1.03
1.03
4.06
2.00
2.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

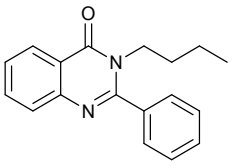

O
N
N

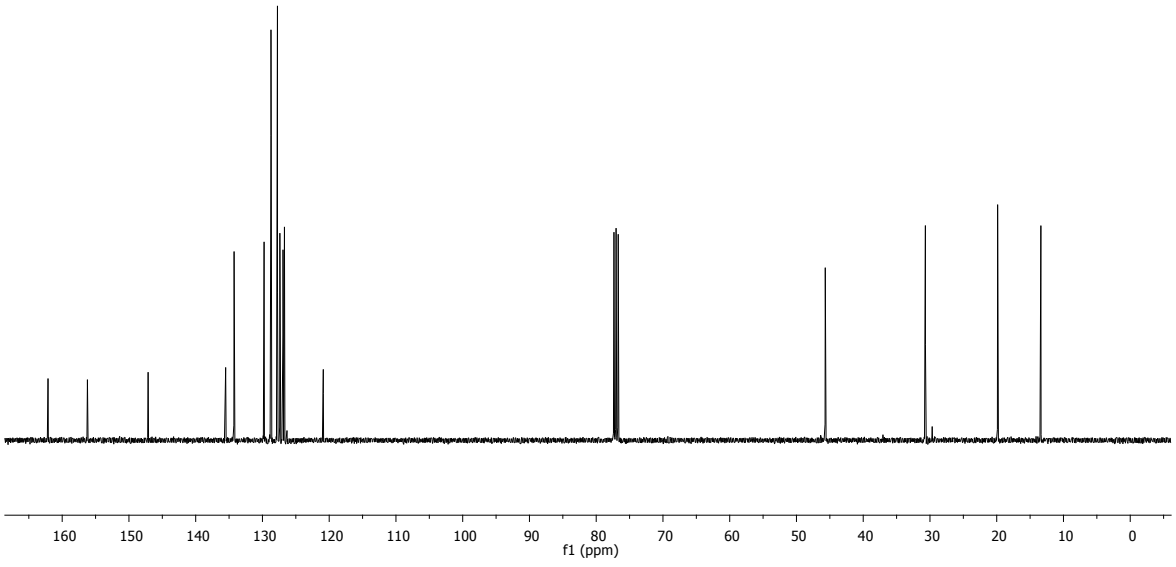
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2e

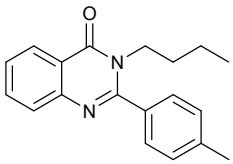

O
N
N

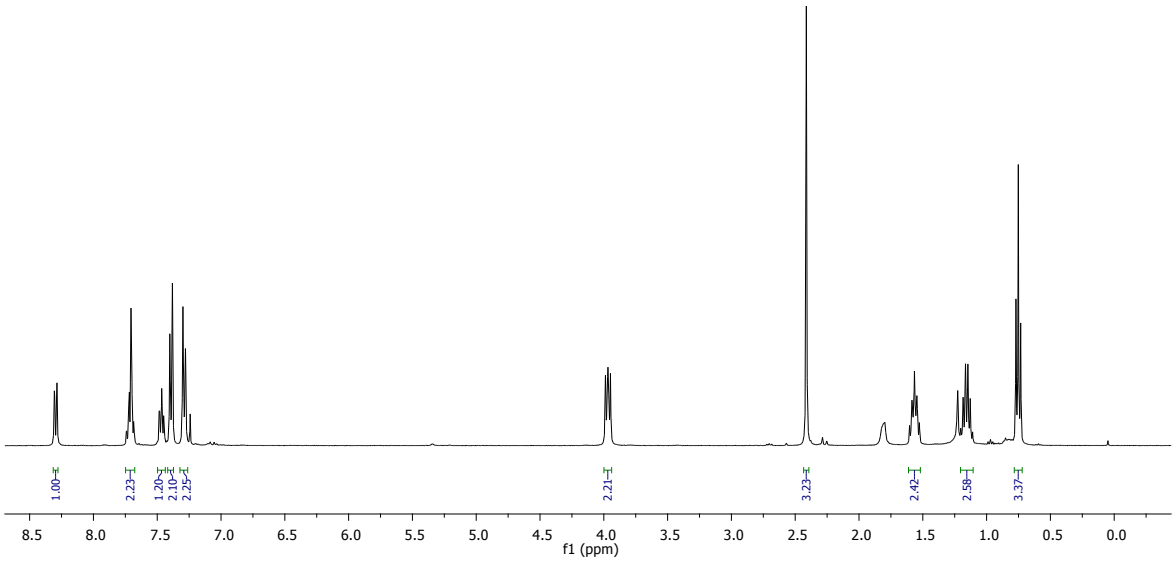

1.00
2.06
6.05
2.15
2.29
2.40
3.18
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

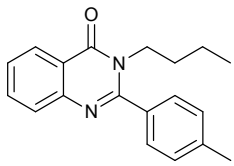

O
N
N

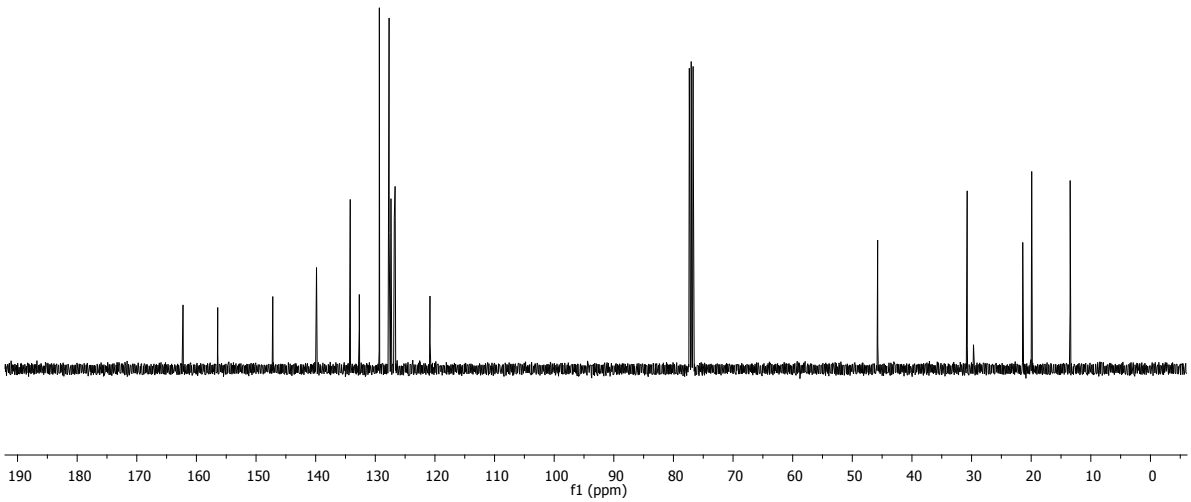

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2f

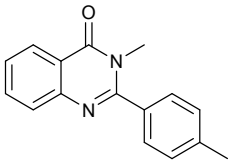

O
N
N

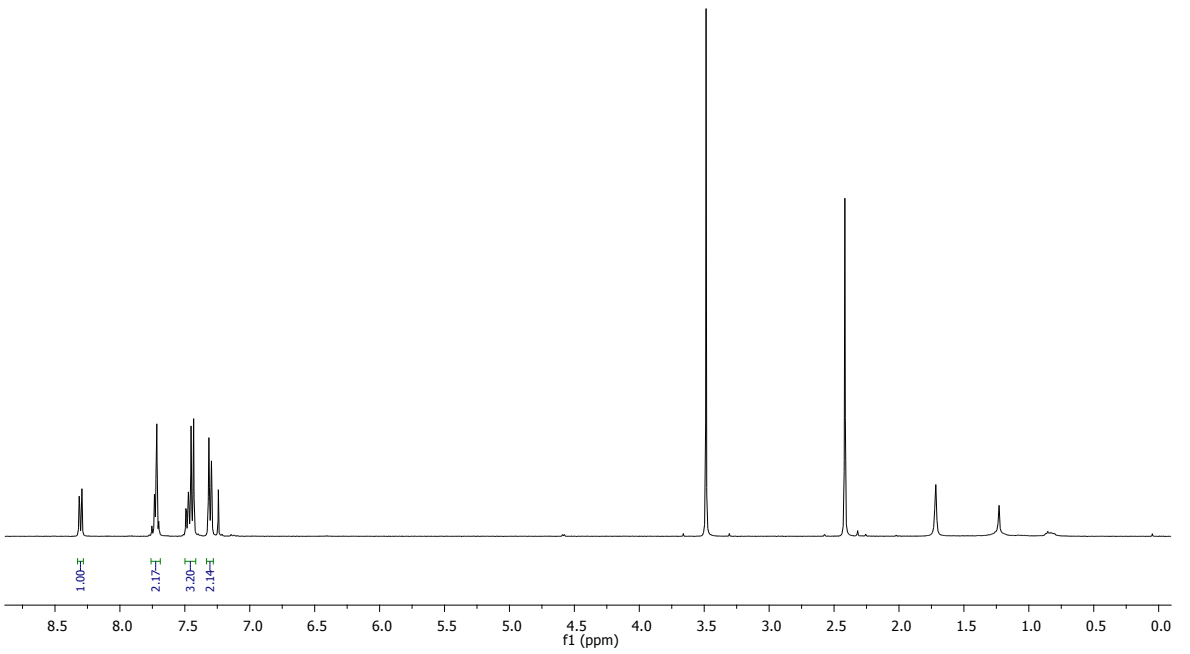

1.00
2.23
1.20
2.10
2.25
2.21
3.23
2.42
2.58
3.37
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

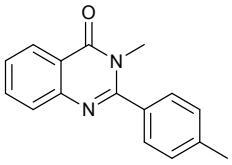

O
N
N

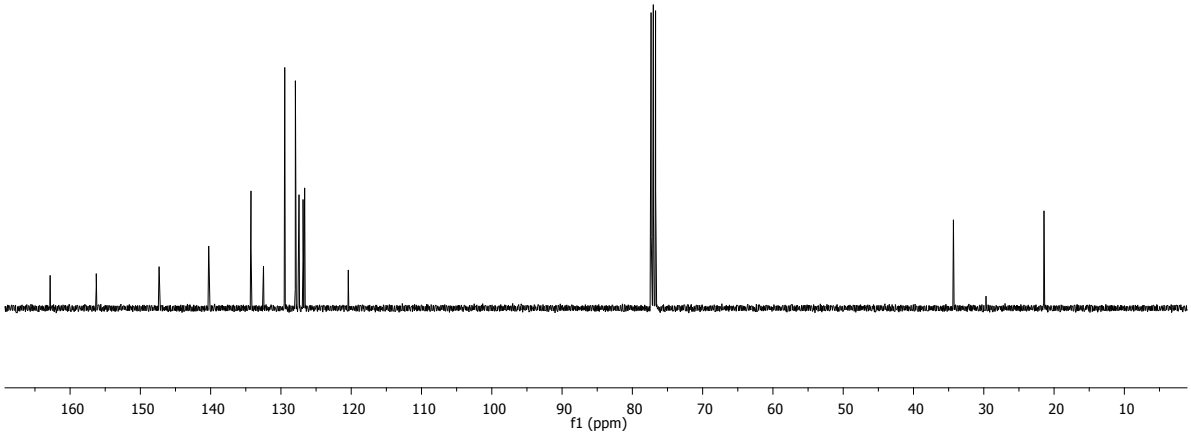

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2g

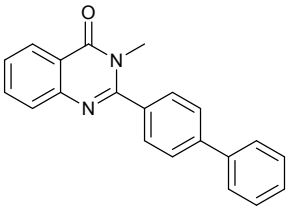


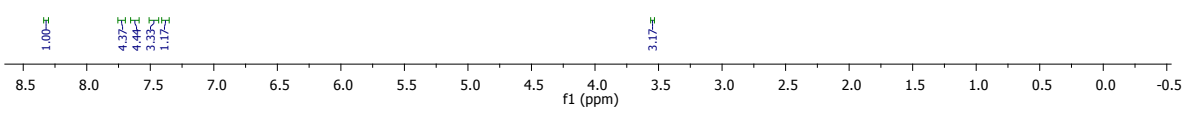

1.00
2.17
3.20
2.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

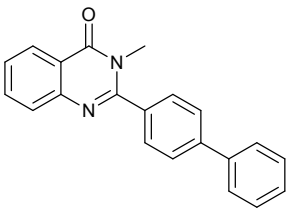



160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

2h

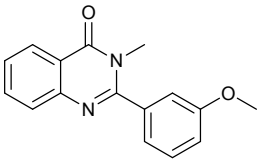

O
N
N


1.00
4.37
4.44
3.33
1.17
3.17
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

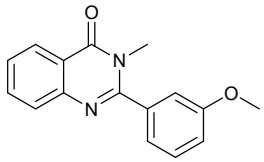

O
N
N

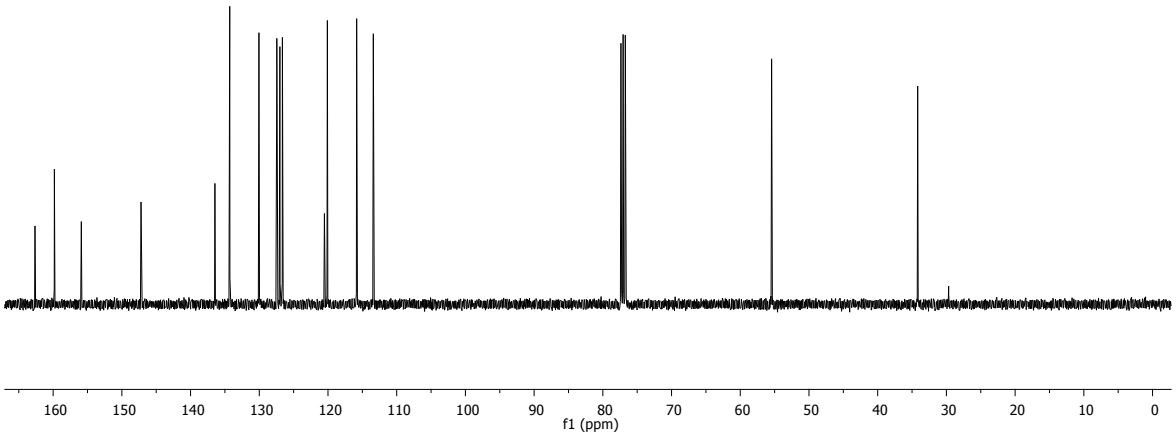
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

2i

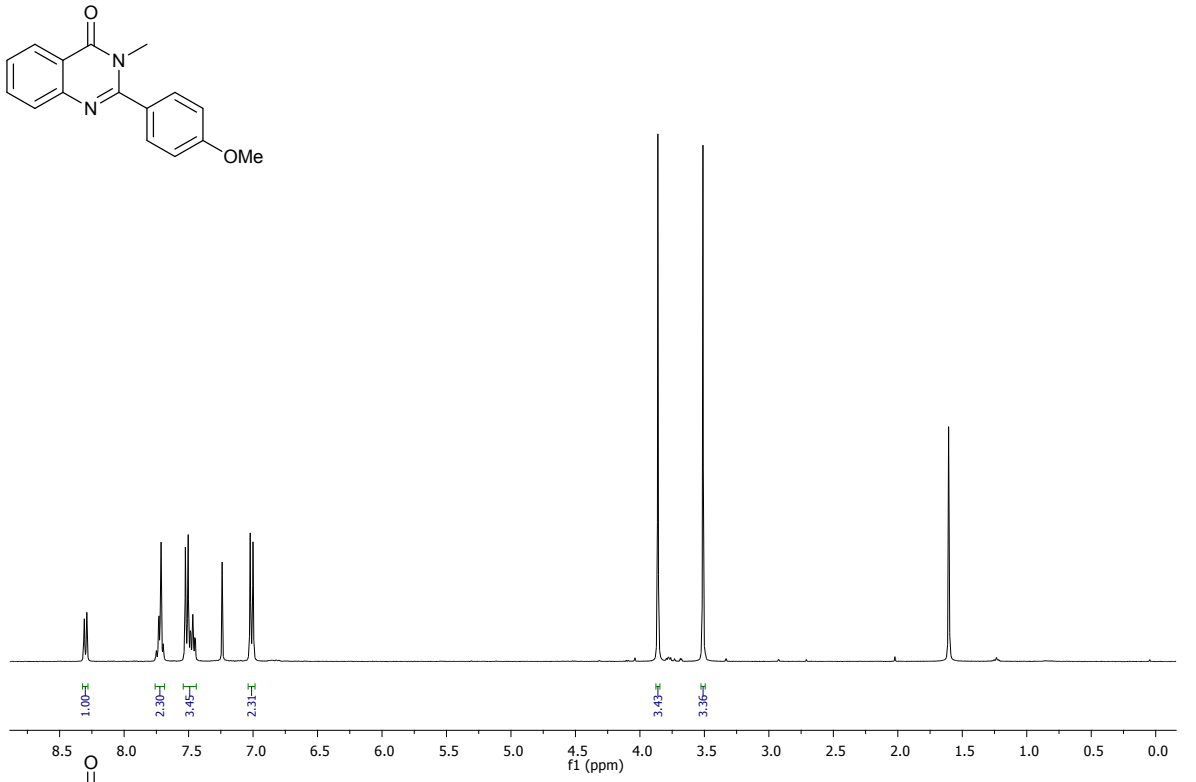

O
N
N
O

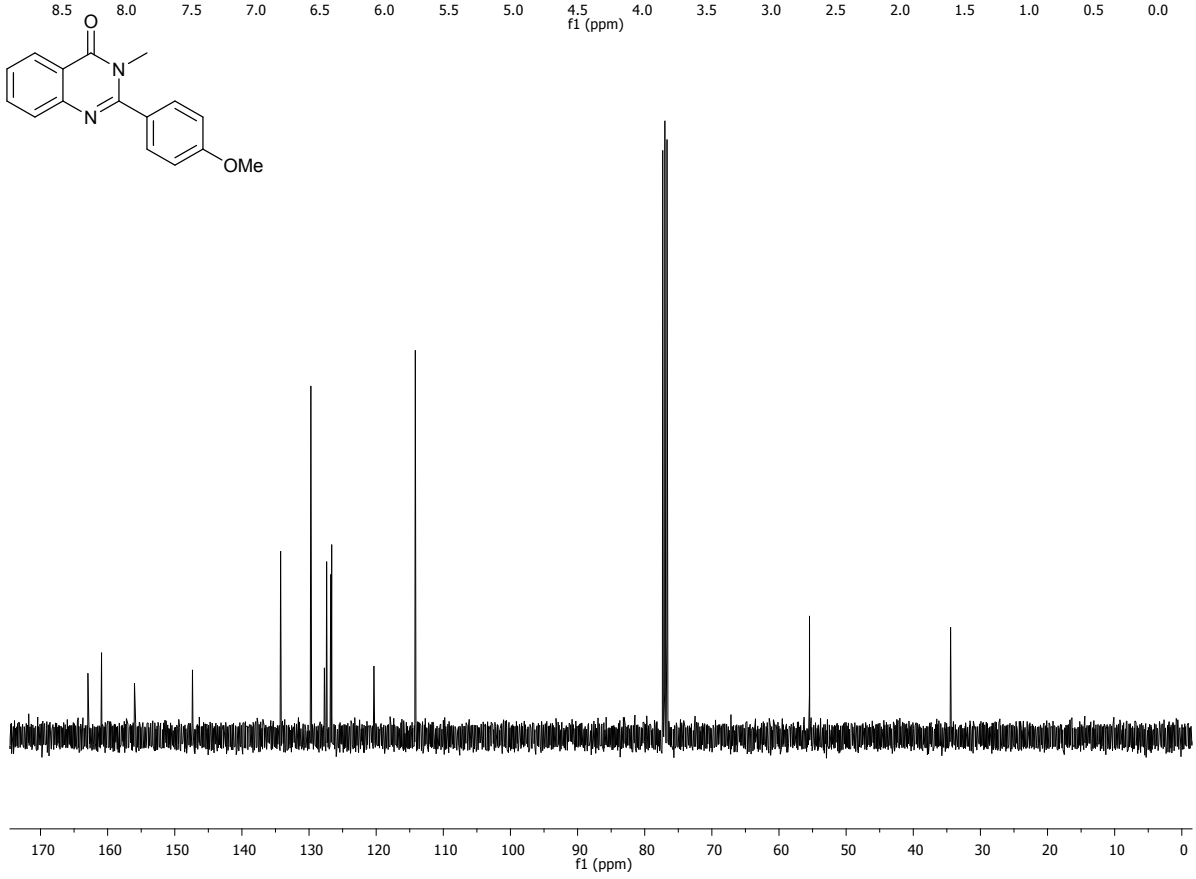
1.00
2.24
1.15
1.14
3.29
3.10
3.25
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


O
N
N
O

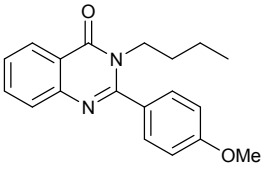

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

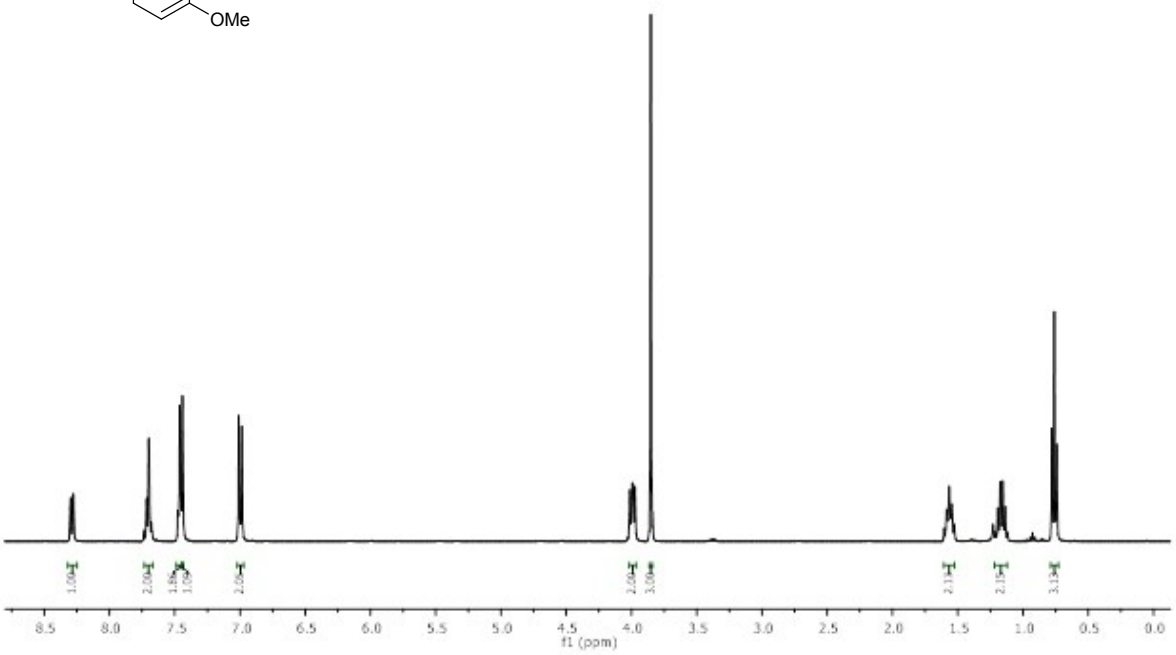
2j

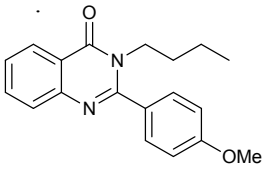

O
N
N
OMe
1.00
2.30
3.45
2.31
3.43
3.36
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

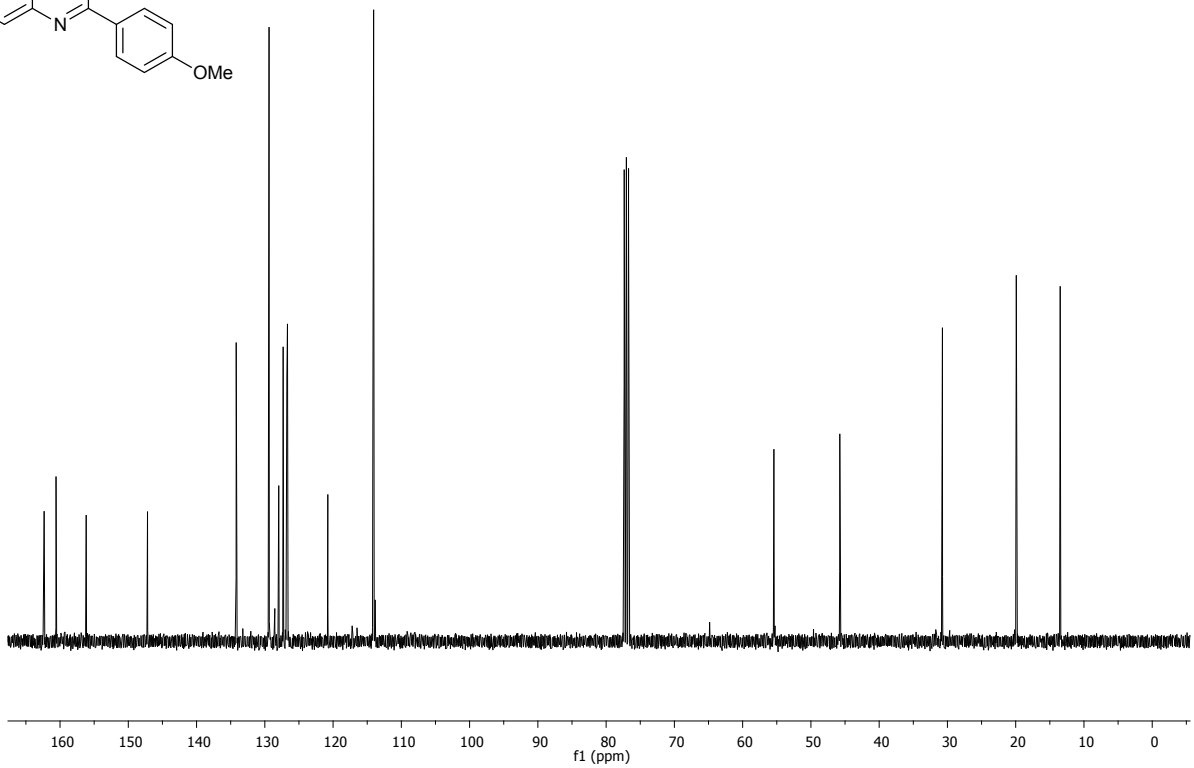

O
N
N
OMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2k

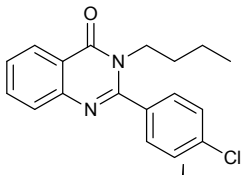

O
N
N
OMe

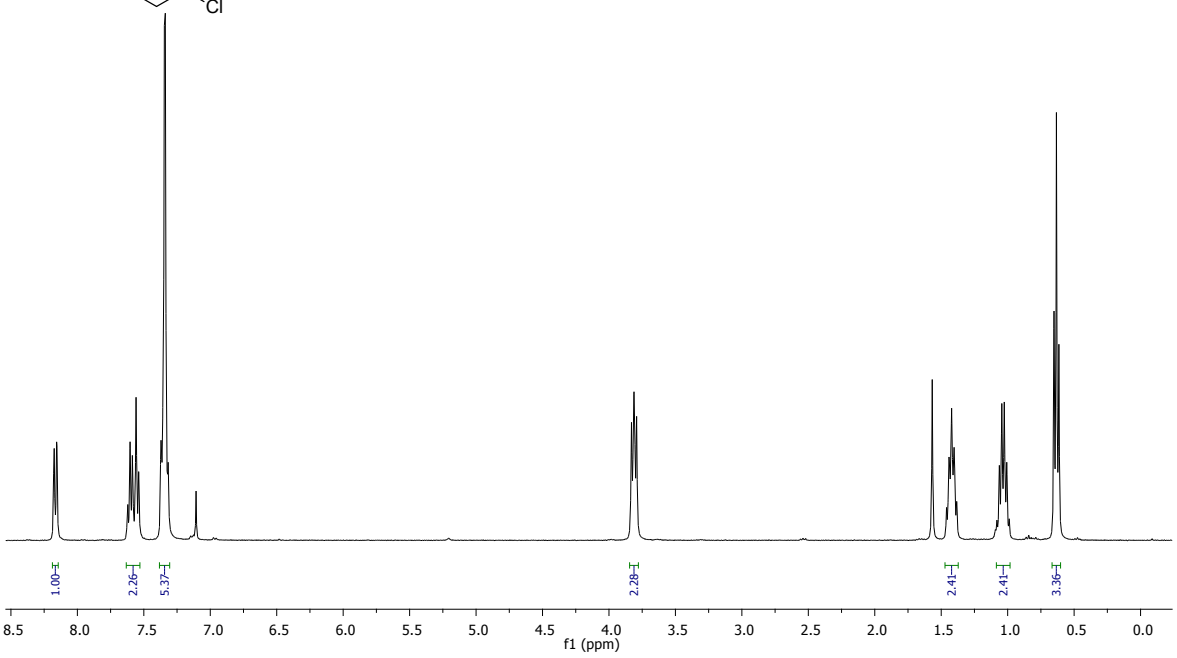

8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

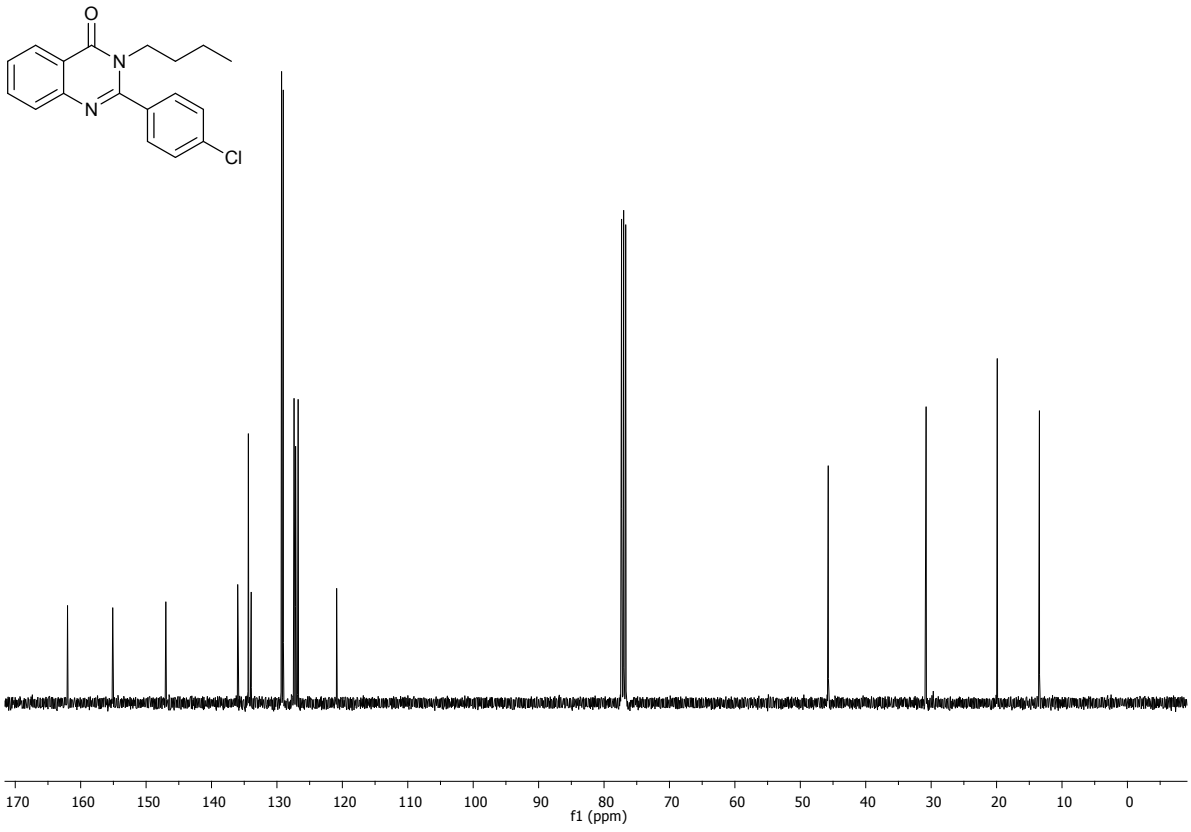

O
N
N
OMe


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

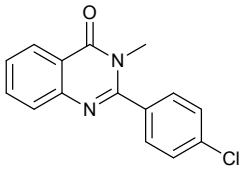
2l

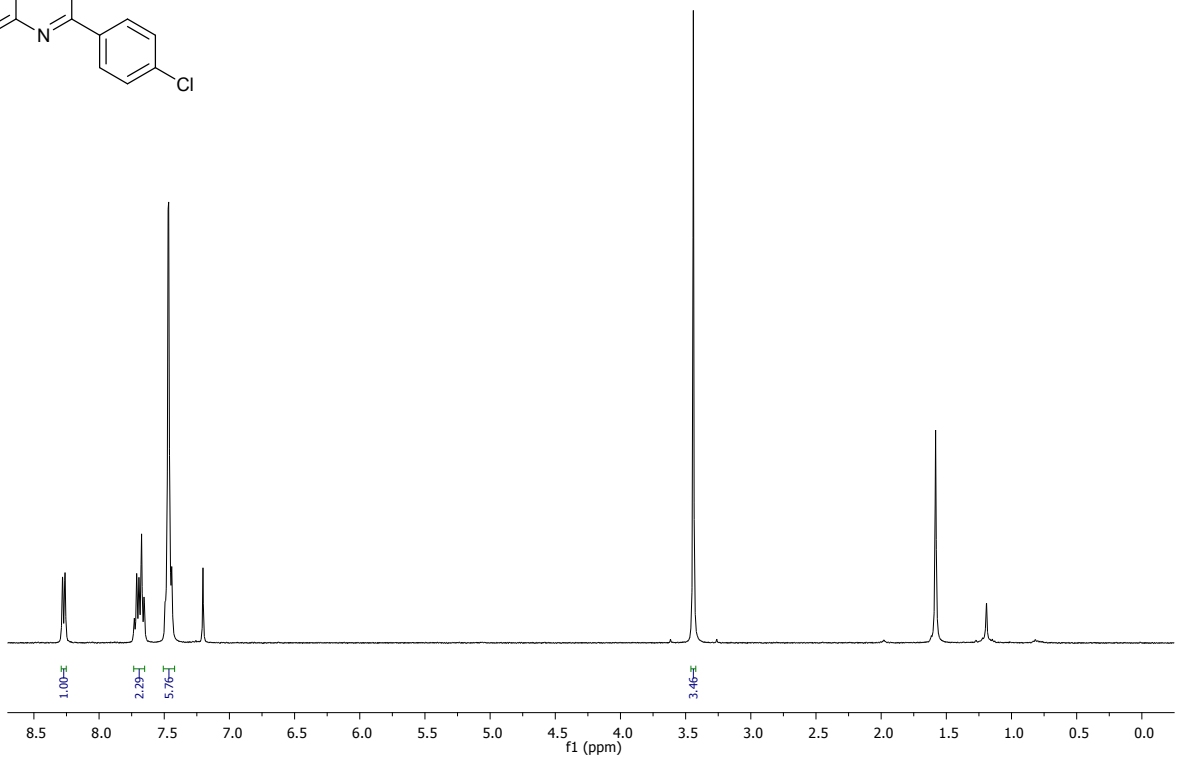

O
N
N
Cl

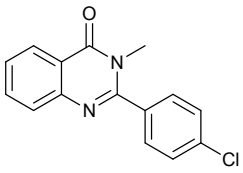

1.00
2.26
5.37
2.28
2.41
2.41
3.36
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

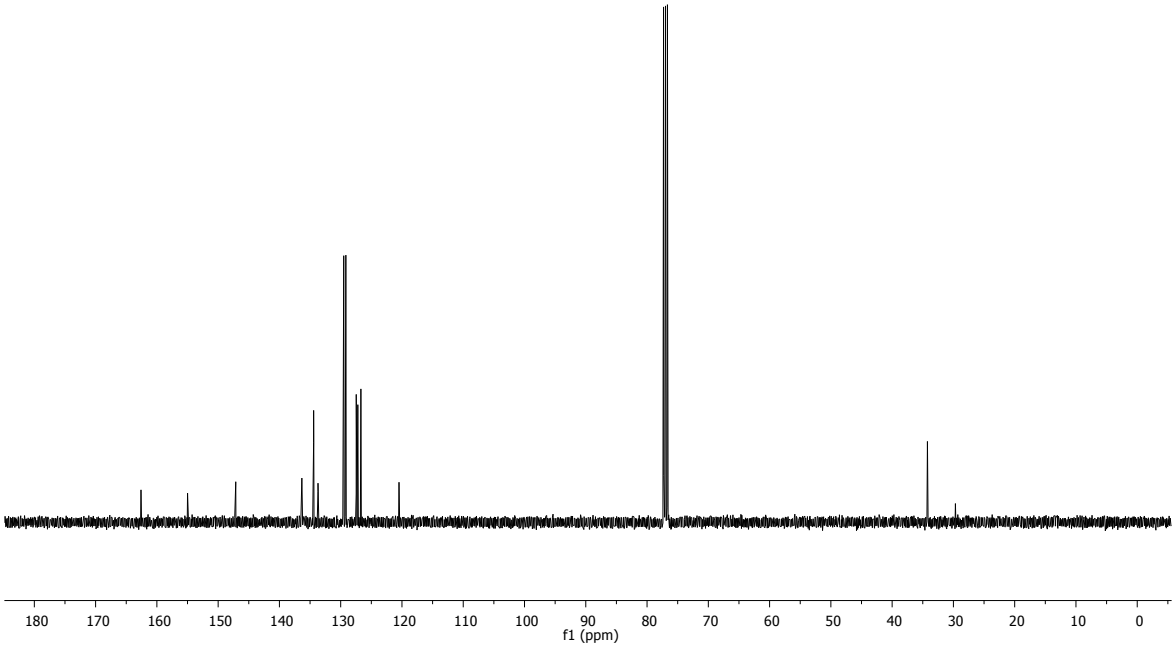

O
N
N
Cl
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2m

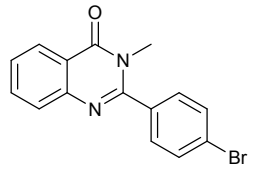

O
N
N
Cl

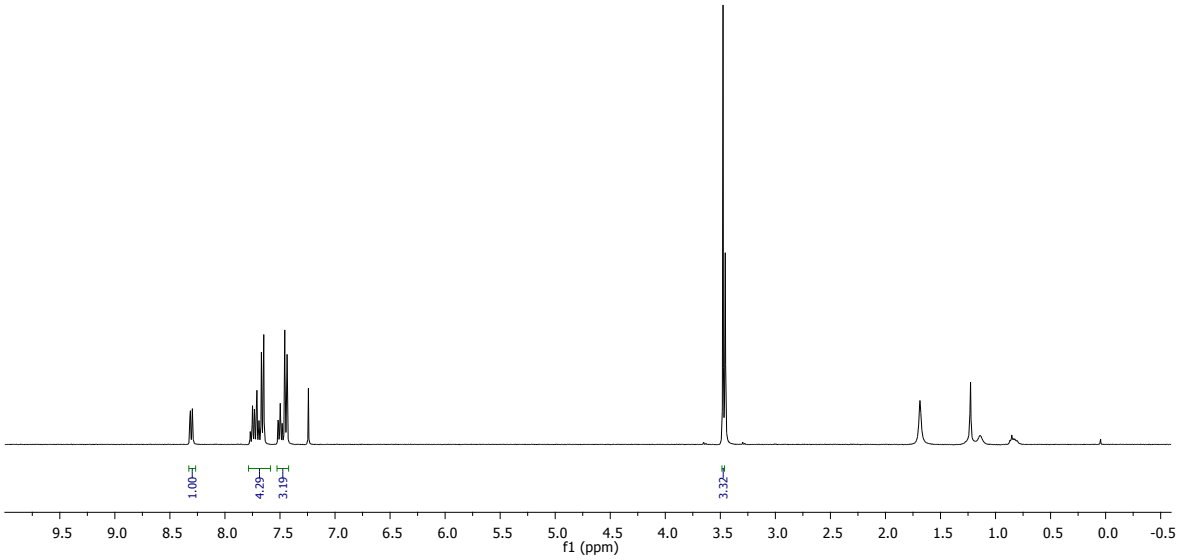

1.00
2.29
5.76
3.46
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

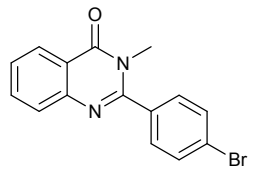

O
N
N
Cl

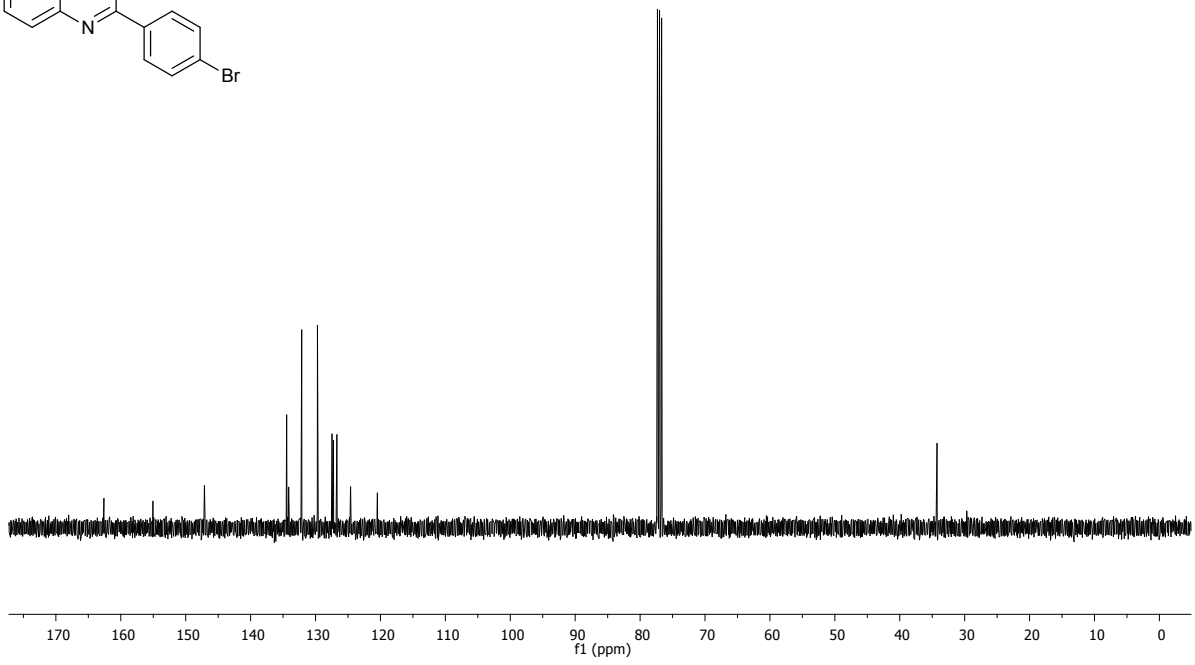

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2n


O
N
N
Br

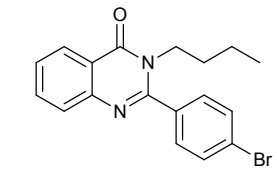

1.00
4.29
3.19
3.32
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

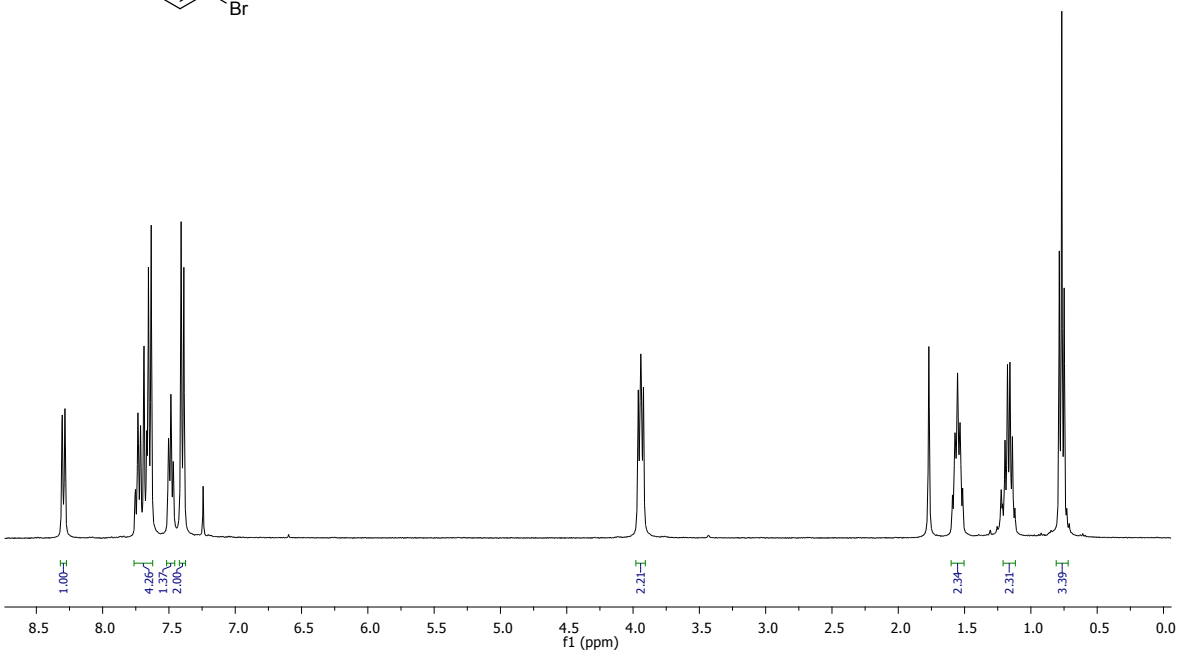

O
N
N
Br

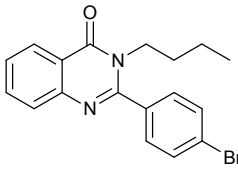

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

.

2o

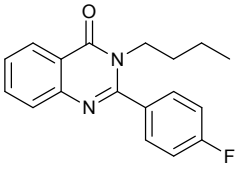

O
N
N
Br


1.00
4.26
1.37
2.06
2.21
2.34
2.31
3.39
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

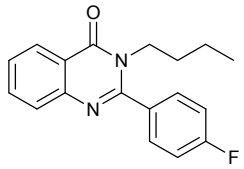

O
N
N
Br

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2p

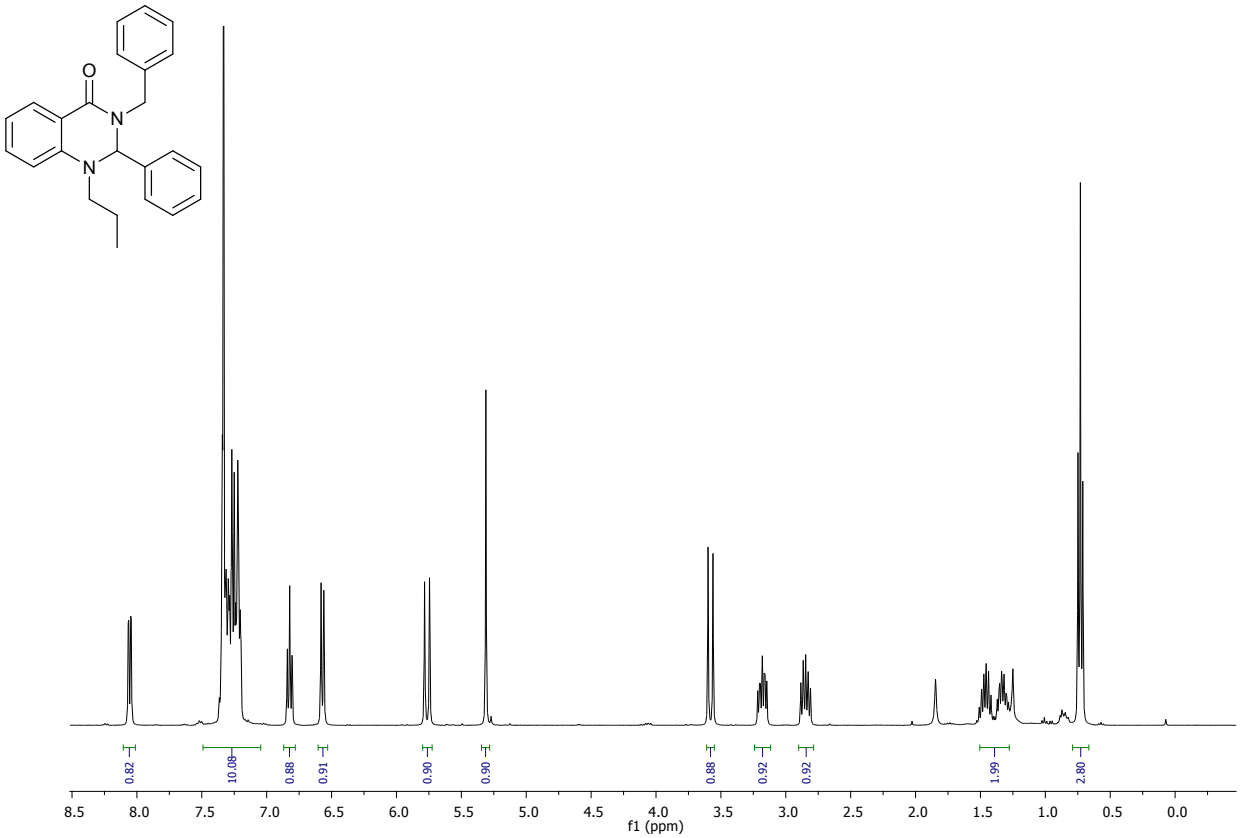

O
N
N
F

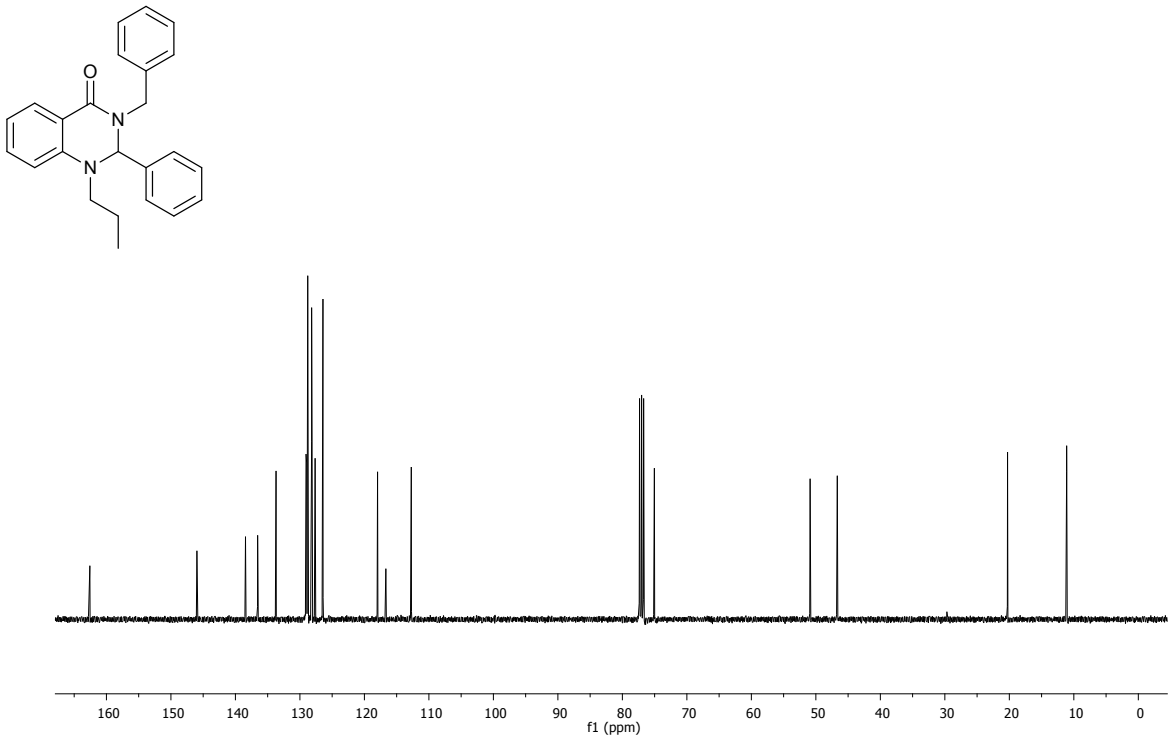
1.00
2.22
3.25
2.16
2.27
2.38
2.33
3.33
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


O
N
N
F

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4a


O
N
N
0.82
10.08
0.88
0.91
0.90
0.90
0.88
0.92
0.92
1.99
2.80
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


O
N
N
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

X-ray Data Collection.

Table 1. Crystal data and structure refinement for 3-benzyl-2-phenylquinazolin-4(3H)-one (**2a**).

Identification code	shelx
Empirical formula	C_{21} H_{16} N_2 O
Formula weight	312.36
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 9.933(2) A alpha = 90 deg.
	b = 29.454(6) A beta = 112.40(3) deg.
	c = 11.470(2) A gamma = 90 deg.
Volume	3102.5(12) A^3
Z, Calculated density	8, 1.337 Mg/m^3
Absorption coefficient	0.083 mm^-1
F(000)	1312
Crystal size	0.292 x 0.081 x 0.060 mm
Theta range for data collection	3.109 to 20.818 deg.
Limiting indices	-9<=h<=9, -29<=k<=29, -11<=l<=11
Reflections collected / unique	10622 / 3231 [R(int) = 0.1280]
Completeness to theta = 25.242	57.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3231 / 0 / 433
Goodness-of-fit on F^2	0.794
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.0723
R indices (all data)	R1 = 0.1464, wR2 = 0.0960
Extinction coefficient	n/a
Largest diff. peak and hole	0.159 and -0.202 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	5941(7)	924(2)	453(5)	24(2)
C(2)	6877(7)	1173(2)	2646(6)	30(2)
C(3)	8017(6)	836(2)	2850(6)	25(2)
C(4)	9124(7)	787(2)	4027(6)	33(2)
C(5)	10177(7)	465(2)	4198(6)	37(2)
C(6)	10115(7)	183(2)	3207(6)	35(2)
C(7)	9039(7)	230(2)	2036(6)	31(2)
C(8)	7977(7)	560(2)	1846(5)	27(2)
C(9)	4889(7)	1002(2)	-860(5)	27(2)
C(10)	3494(7)	825(2)	-1310(6)	36(2)
C(11)	2577(7)	905(2)	-2540(6)	41(2)
C(12)	3034(8)	1152(2)	-3336(6)	40(2)
C(13)	4439(7)	1320(2)	-2904(5)	38(2)
C(14)	5368(6)	1247(2)	-1664(5)	33(2)
C(15)	4634(6)	1532(2)	1159(6)	29(2)
C(16)	4938(6)	1992(2)	737(6)	29(2)
C(17)	4293(6)	2117(2)	-514(5)	34(2)
C(18)	4549(6)	2541(2)	-901(6)	37(2)
C(19)	5446(7)	2844(2)	-51(6)	37(2)
C(20)	6079(6)	2727(2)	1208(6)	39(2)
C(21)	5833(6)	2303(2)	1609(5)	36(2)
C(22)	933(7)	907(2)	510(6)	27(2)
C(23)	2080(7)	1132(2)	2701(6)	28(2)

C(24)	3137(7)	781(2)	2813(6)	25(2)
C(25)	4327(7)	714(2)	3943(6)	34(2)
C(26)	5322(7)	383(2)	4007(6)	34(2)
C(27)	5151(7)	116(2)	2965(6)	33(2)
C(28)	3973(7)	178(2)	1844(6)	32(2)
C(29)	2955(6)	516(2)	1764(5)	24(2)
C(30)	-195(7)	999(2)	-794(5)	26(2)
C(31)	-66(6)	1381(2)	-1439(5)	34(2)
C(32)	-1000(7)	1442(2)	-2684(6)	41(2)
C(33)	-2067(7)	1121(2)	-3262(6)	38(2)
C(34)	-2197(7)	745(2)	-2605(6)	40(2)
C(35)	-1256(6)	680(2)	-1364(5)	31(2)
C(36)	-186(6)	1515(2)	1359(6)	28(2)
C(37)	15(7)	1975(2)	881(5)	28(2)
C(38)	-1206(7)	2224(2)	173(5)	39(2)
C(39)	-1049(7)	2646(2)	-303(6)	46(2)
C(40)	305(9)	2818(2)	-103(6)	45(2)
C(41)	1527(7)	2570(2)	621(6)	45(2)
C(42)	1372(6)	2154(2)	1116(5)	38(2)
N(1)	6922(5)	614(2)	634(4)	28(1)
N(2)	5861(5)	1197(2)	1415(4)	24(1)
O(1)	6805(5)	1424(2)	3473(4)	42(1)
N(4)	1811(5)	575(2)	602(4)	30(1)
N(5)	973(5)	1186(2)	1501(4)	26(1)
O(2)	2099(4)	1383(1)	3560(4)	38(1)

Table 3. Bond lengths [A] and angles [deg] for **2a**.

C(1)-N(1)	1.294(7)
C(1)-N(2)	1.392(7)
C(1)-C(9)	1.487(8)
C(2)-O(1)	1.226(7)
C(2)-N(2)	1.389(8)
C(2)-C(3)	1.456(8)
C(3)-C(4)	1.387(9)
C(3)-C(8)	1.397(8)
C(4)-C(5)	1.369(8)
C(4)-H(4)	0.9500
C(5)-C(6)	1.389(8)
C(5)-H(5)	0.9500
C(6)-C(7)	1.368(9)
C(6)-H(6)	0.9500
C(7)-C(8)	1.390(8)
C(7)-H(7)	0.9500
C(8)-N(1)	1.396(7)
C(9)-C(10)	1.384(8)
C(9)-C(14)	1.390(8)
C(10)-C(11)	1.378(8)
C(10)-H(10)	0.9500
C(11)-C(12)	1.373(8)
C(11)-H(11)	0.9500
C(12)-C(13)	1.383(8)
C(12)-H(12)	0.9500
C(13)-C(14)	1.386(8)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500

C(15)-N(2)	1.507(7)
C(15)-C(16)	1.507(8)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.380(7)
C(16)-C(21)	1.398(8)
C(17)-C(18)	1.381(7)
C(17)-H(17)	0.9500
C(18)-C(19)	1.370(8)
C(18)-H(18)	0.9500
C(19)-C(20)	1.380(7)
C(19)-H(19)	0.9500
C(20)-C(21)	1.384(7)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-N(4)	1.288(7)
C(22)-N(5)	1.390(7)
C(22)-C(30)	1.513(9)
C(23)-O(2)	1.227(7)
C(23)-N(5)	1.405(8)
C(23)-C(24)	1.445(8)
C(24)-C(29)	1.387(8)
C(24)-C(25)	1.396(9)
C(25)-C(26)	1.371(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.387(8)
C(26)-H(26)	0.9500
C(27)-C(28)	1.382(9)
C(27)-H(27)	0.9500
C(28)-C(29)	1.397(8)
C(28)-H(28)	0.9500

C(29)-N(4)	1.393(7)
C(30)-C(35)	1.378(8)
C(30)-C(31)	1.379(8)
C(31)-C(32)	1.387(8)
C(31)-H(31)	0.9500
C(32)-C(33)	1.386(8)
C(32)-H(32)	0.9500
C(33)-C(34)	1.374(8)
C(33)-H(33)	0.9500
C(34)-C(35)	1.386(8)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(36)-N(5)	1.467(7)
C(36)-C(37)	1.503(8)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(42)	1.376(7)
C(37)-C(38)	1.386(8)
C(38)-C(39)	1.389(8)
C(38)-H(38)	0.9500
C(39)-C(40)	1.372(8)
C(39)-H(39)	0.9500
C(40)-C(41)	1.387(8)
C(40)-H(40)	0.9500
C(41)-C(42)	1.383(8)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500

N(1)-C(1)-N(2)	123.2(5)
N(1)-C(1)-C(9)	117.8(5)
N(2)-C(1)-C(9)	118.9(6)

O(1)-C(2)-N(2)	121.4(6)
O(1)-C(2)-C(3)	123.9(6)
N(2)-C(2)-C(3)	114.7(6)
C(4)-C(3)-C(8)	120.3(6)
C(4)-C(3)-C(2)	120.5(6)
C(8)-C(3)-C(2)	119.2(6)
C(5)-C(4)-C(3)	119.4(6)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.3(6)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(7)-C(6)-C(5)	121.1(6)
C(7)-C(6)-H(6)	119.4
C(5)-C(6)-H(6)	119.4
C(6)-C(7)-C(8)	119.1(6)
C(6)-C(7)-H(7)	120.4
C(8)-C(7)-H(7)	120.4
C(7)-C(8)-N(1)	118.2(5)
C(7)-C(8)-C(3)	119.8(5)
N(1)-C(8)-C(3)	121.9(6)
C(10)-C(9)-C(14)	119.7(5)
C(10)-C(9)-C(1)	122.5(6)
C(14)-C(9)-C(1)	117.7(6)
C(11)-C(10)-C(9)	119.7(6)
C(11)-C(10)-H(10)	120.2
C(9)-C(10)-H(10)	120.2
C(12)-C(11)-C(10)	121.0(6)
C(12)-C(11)-H(11)	119.5
C(10)-C(11)-H(11)	119.5
C(11)-C(12)-C(13)	119.8(6)

C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(12)-C(13)-C(14)	119.9(6)
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1
C(13)-C(14)-C(9)	120.0(6)
C(13)-C(14)-H(14)	120.0
C(9)-C(14)-H(14)	120.0
N(2)-C(15)-C(16)	113.8(5)
N(2)-C(15)-H(15A)	108.8
C(16)-C(15)-H(15A)	108.8
N(2)-C(15)-H(15B)	108.8
C(16)-C(15)-H(15B)	108.8
H(15A)-C(15)-H(15B)	107.7
C(17)-C(16)-C(21)	119.0(5)
C(17)-C(16)-C(15)	120.3(5)
C(21)-C(16)-C(15)	120.6(5)
C(16)-C(17)-C(18)	120.5(6)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(19)-C(18)-C(17)	120.6(6)
C(19)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	119.7(6)
C(18)-C(19)-H(19)	120.2
C(20)-C(19)-H(19)	120.2
C(19)-C(20)-C(21)	120.3(6)
C(19)-C(20)-H(20)	119.8
C(21)-C(20)-H(20)	119.8
C(20)-C(21)-C(16)	119.9(5)
C(20)-C(21)-H(21)	120.1

C(16)-C(21)-H(21)	120.1
N(4)-C(22)-N(5)	125.0(5)
N(4)-C(22)-C(30)	116.2(5)
N(5)-C(22)-C(30)	118.8(5)
O(2)-C(23)-N(5)	119.1(6)
O(2)-C(23)-C(24)	124.9(6)
N(5)-C(23)-C(24)	116.0(5)
C(29)-C(24)-C(25)	120.8(6)
C(29)-C(24)-C(23)	118.4(6)
C(25)-C(24)-C(23)	120.8(6)
C(26)-C(25)-C(24)	119.2(6)
C(26)-C(25)-H(25)	120.4
C(24)-C(25)-H(25)	120.4
C(25)-C(26)-C(27)	120.6(6)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(28)-C(27)-C(26)	120.6(6)
C(28)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7
C(27)-C(28)-C(29)	119.4(6)
C(27)-C(28)-H(28)	120.3
C(29)-C(28)-H(28)	120.3
C(24)-C(29)-N(4)	123.2(6)
C(24)-C(29)-C(28)	119.5(6)
N(4)-C(29)-C(28)	117.3(5)
C(35)-C(30)-C(31)	120.9(6)
C(35)-C(30)-C(22)	119.4(5)
C(31)-C(30)-C(22)	119.4(6)
C(30)-C(31)-C(32)	119.7(6)
C(30)-C(31)-H(31)	120.1
C(32)-C(31)-H(31)	120.1

C(33)-C(32)-C(31)	119.6(6)
C(33)-C(32)-H(32)	120.2
C(31)-C(32)-H(32)	120.2
C(34)-C(33)-C(32)	120.2(6)
C(34)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9
C(33)-C(34)-C(35)	120.5(7)
C(33)-C(34)-H(34)	119.8
C(35)-C(34)-H(34)	119.8
C(30)-C(35)-C(34)	119.2(6)
C(30)-C(35)-H(35)	120.4
C(34)-C(35)-H(35)	120.4
N(5)-C(36)-C(37)	115.4(5)
N(5)-C(36)-H(36A)	108.4
C(37)-C(36)-H(36A)	108.4
N(5)-C(36)-H(36B)	108.4
C(37)-C(36)-H(36B)	108.4
H(36A)-C(36)-H(36B)	107.5
C(42)-C(37)-C(38)	119.0(5)
C(42)-C(37)-C(36)	122.1(6)
C(38)-C(37)-C(36)	118.9(5)
C(37)-C(38)-C(39)	120.0(6)
C(37)-C(38)-H(38)	120.0
C(39)-C(38)-H(38)	120.0
C(40)-C(39)-C(38)	121.0(6)
C(40)-C(39)-H(39)	119.5
C(38)-C(39)-H(39)	119.5
C(39)-C(40)-C(41)	119.0(6)
C(39)-C(40)-H(40)	120.5
C(41)-C(40)-H(40)	120.5
C(42)-C(41)-C(40)	120.1(6)

C(42)-C(41)-H(41)	119.9
C(40)-C(41)-H(41)	119.9
C(37)-C(42)-C(41)	120.9(6)
C(37)-C(42)-H(42)	119.5
C(41)-C(42)-H(42)	119.5
C(1)-N(1)-C(8)	118.3(5)
C(2)-N(2)-C(1)	122.5(5)
C(2)-N(2)-C(15)	116.9(5)
C(1)-N(2)-C(15)	120.6(5)
C(22)-N(4)-C(29)	117.0(5)
C(22)-N(5)-C(23)	120.2(5)
C(22)-N(5)-C(36)	121.5(5)
C(23)-N(5)-C(36)	118.1(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2a**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	29(4)	20(4)	22(4)	-1(3)	10(3)	-11(3)
C(2)	42(5)	24(4)	28(4)	2(3)	17(4)	-3(3)
C(3)	24(4)	30(4)	18(4)	0(3)	5(3)	-4(3)
C(4)	44(4)	23(4)	37(4)	-5(3)	22(4)	-4(4)
C(5)	48(5)	32(4)	24(4)	1(3)	6(3)	-1(4)
C(6)	33(4)	25(4)	42(4)	5(3)	8(4)	10(3)
C(7)	43(4)	25(4)	29(4)	-4(3)	19(4)	-5(4)
C(8)	28(4)	27(4)	23(4)	4(3)	7(3)	0(3)
C(9)	29(4)	28(4)	22(4)	-3(3)	8(3)	-1(3)
C(10)	39(4)	42(4)	32(4)	6(3)	18(3)	0(4)
C(11)	29(4)	54(5)	34(4)	-6(4)	6(4)	-6(3)
C(12)	52(5)	39(5)	27(4)	3(3)	13(4)	13(4)
C(13)	56(5)	34(4)	27(4)	2(3)	18(4)	3(4)
C(14)	33(4)	36(4)	30(4)	-1(3)	11(3)	-1(3)
C(15)	29(4)	35(4)	25(4)	-3(3)	12(3)	-2(3)
C(16)	25(4)	31(4)	35(4)	-1(3)	16(3)	4(3)
C(17)	38(4)	29(4)	31(4)	-1(3)	8(3)	4(3)
C(18)	42(4)	33(4)	37(4)	14(3)	15(3)	7(3)
C(19)	41(4)	24(4)	47(4)	8(4)	17(4)	-2(4)
C(20)	38(4)	22(4)	47(5)	-1(3)	5(3)	-6(3)
C(21)	43(4)	38(4)	27(4)	-2(3)	11(3)	0(3)
C(22)	28(4)	23(4)	28(4)	2(3)	11(3)	-2(4)

C(23)	36(4)	25(4)	20(4)	-3(3)	7(4)	-13(4)
C(24)	36(4)	15(4)	28(4)	6(3)	14(4)	6(3)
C(25)	38(4)	33(4)	23(4)	-3(3)	4(4)	-1(4)
C(26)	36(4)	33(4)	25(4)	3(3)	3(3)	-1(4)
C(27)	35(4)	29(4)	38(4)	2(3)	19(4)	4(3)
C(28)	38(4)	30(4)	27(4)	1(3)	11(4)	3(4)
C(29)	31(4)	16(4)	30(4)	-1(3)	15(4)	-4(3)
C(30)	37(4)	23(4)	25(4)	4(3)	20(3)	9(4)
C(31)	34(4)	28(4)	36(4)	-1(3)	10(3)	4(3)
C(32)	45(4)	40(4)	36(4)	9(3)	12(3)	2(4)
C(33)	24(4)	59(5)	32(4)	-3(4)	12(3)	9(4)
C(34)	45(4)	42(5)	32(4)	-2(3)	13(4)	-8(4)
C(35)	40(4)	35(4)	18(4)	-1(3)	10(3)	-2(3)
C(36)	33(4)	19(4)	37(4)	-2(3)	17(3)	-1(3)
C(37)	35(4)	23(4)	31(4)	-3(3)	18(3)	-2(4)
C(38)	43(4)	32(4)	44(4)	7(3)	17(3)	4(3)
C(39)	46(5)	44(5)	50(4)	11(4)	20(4)	14(4)
C(40)	79(6)	20(4)	48(5)	5(4)	39(4)	2(5)
C(41)	47(5)	35(4)	64(5)	-9(4)	33(4)	-14(4)
C(42)	31(4)	35(4)	48(4)	-2(3)	13(3)	1(3)
N(1)	30(3)	29(3)	29(3)	1(3)	14(3)	7(3)
N(2)	27(3)	24(3)	20(3)	-1(2)	6(3)	-4(3)
O(1)	56(3)	44(3)	26(3)	-6(2)	16(2)	10(2)
N(4)	31(3)	31(3)	22(3)	3(3)	5(3)	-3(3)
N(5)	38(3)	17(3)	27(3)	-3(3)	16(3)	3(3)
O(2)	48(3)	33(3)	28(3)	-7(2)	11(2)	2(2)

Table 5. Hydrogen bonds for **2a** [A and deg.].

Nr	Typ	Res	Donor --- H....Acceptor	[ARU]	D - H	H...A	D...A	D - H...A
1		1	C(10) --H(10) ..N(4)	[1555.02]	0.95	2.45	3.307(9)	151
2		1	C(12) --H(12) ..O(2)	[1554.02]	0.95	2.55	3.389(8)	147
3	Intra	1	C(15) --H(15A) ..O(1)	[ ]	0.99	2.38	2.727(8)	100
4	Intra	1	C(21) --H(21) ..O(1)	[ ]	0.95	2.58	3.261(7)	128
5		2	C(28) --H(28) ..N(1)	[3655.01]	0.95	2.59	3.519(8)	166
6	Intra	2	C(36) --H(36A) ..O(2)	[ ]	0.99	2.33	2.703(8)	101
7		2	C(39) --H(39) ..O(2)	[4454.02]	0.95	2.56	3.381(8)	145
8		2	C(40) --H(40) ..O(1)	[4454.01]	0.95	2.59	3.425(9)	147

Translation of ARU-Code to CIF and Equivalent Position Code

[1554.] =	x,y,-1+z
[4454.] =	-1/2+x,1/2-y,-1/2+z
[3655.] =	1-x,-y,-z