Electronic Supplementary Information

Regioselective Construction of 1,3-Diaryl Tetrahydroindazolones *via* Three-component Reaction of 1,3-Cyclohexanediones, *β*-Nitrostyrenes and Arylhydrazines

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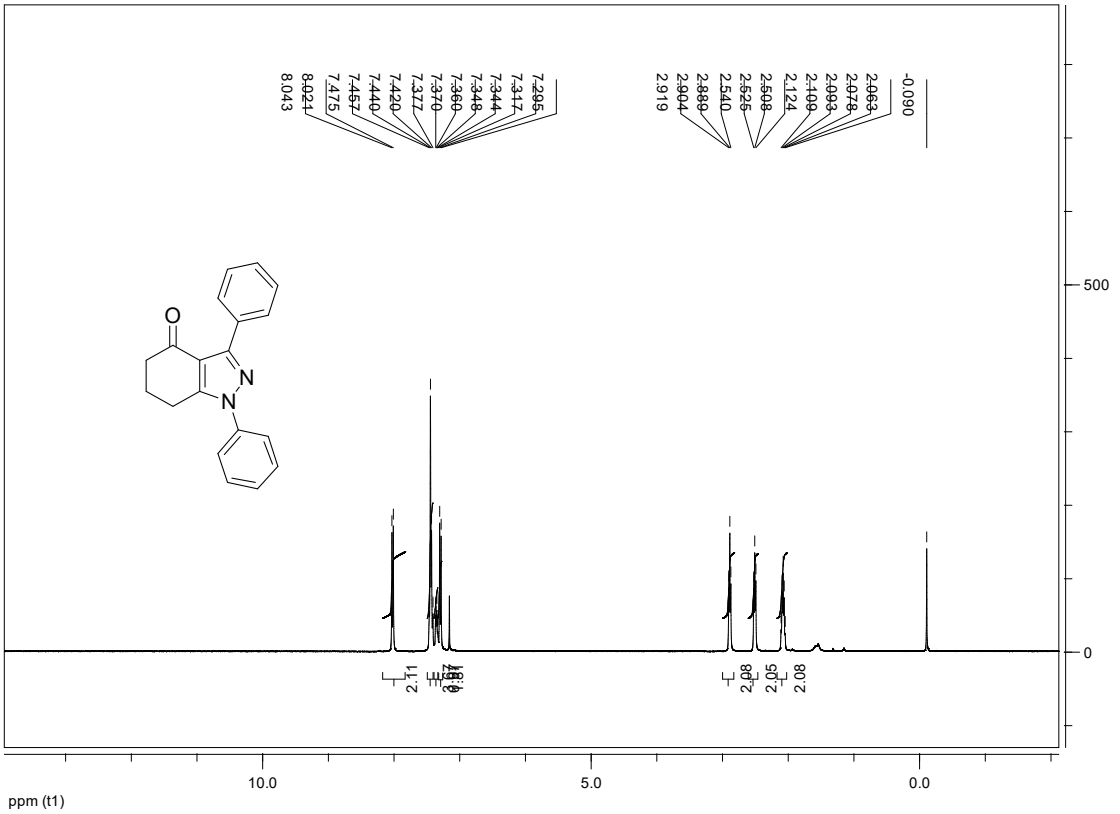
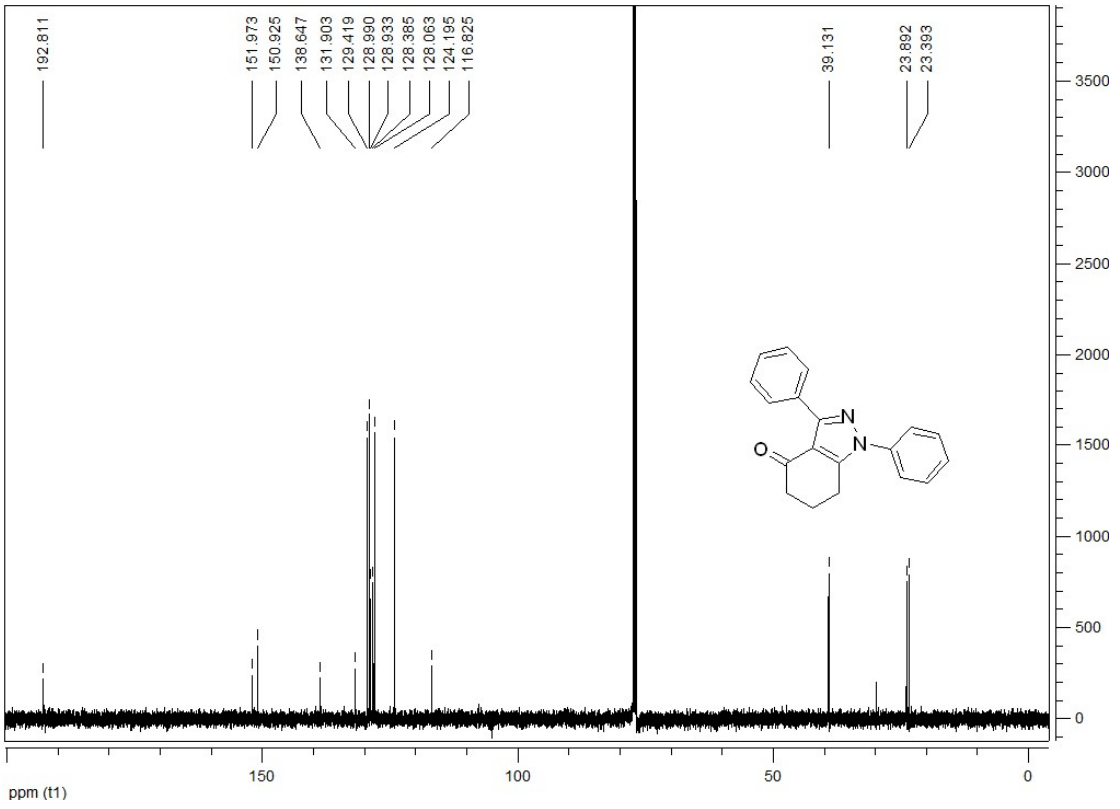
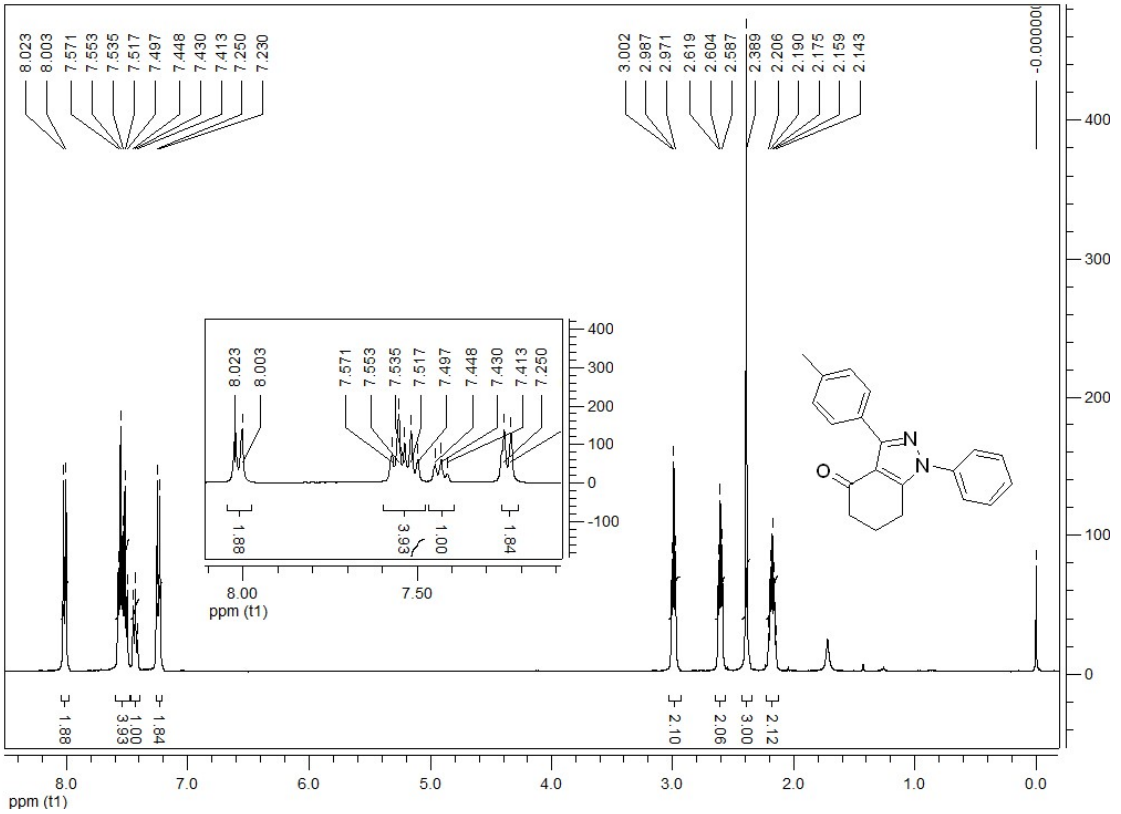
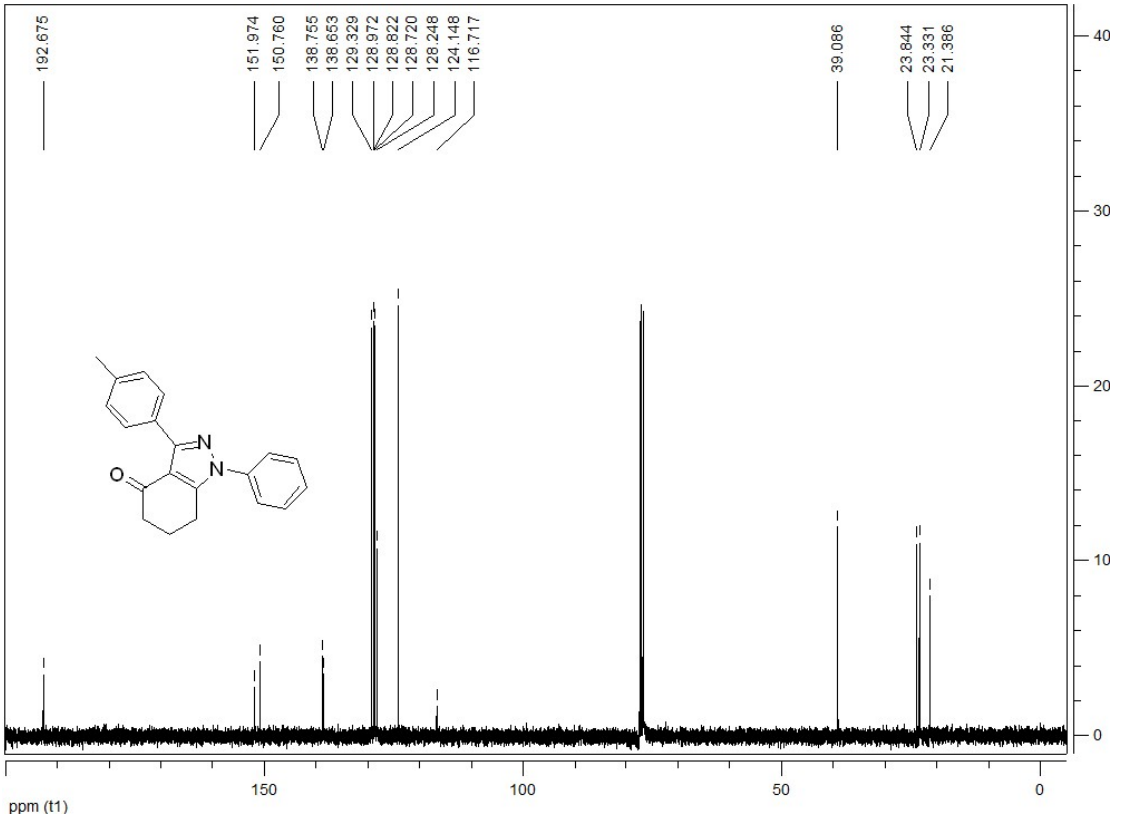
1,3-Diphenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4a**)



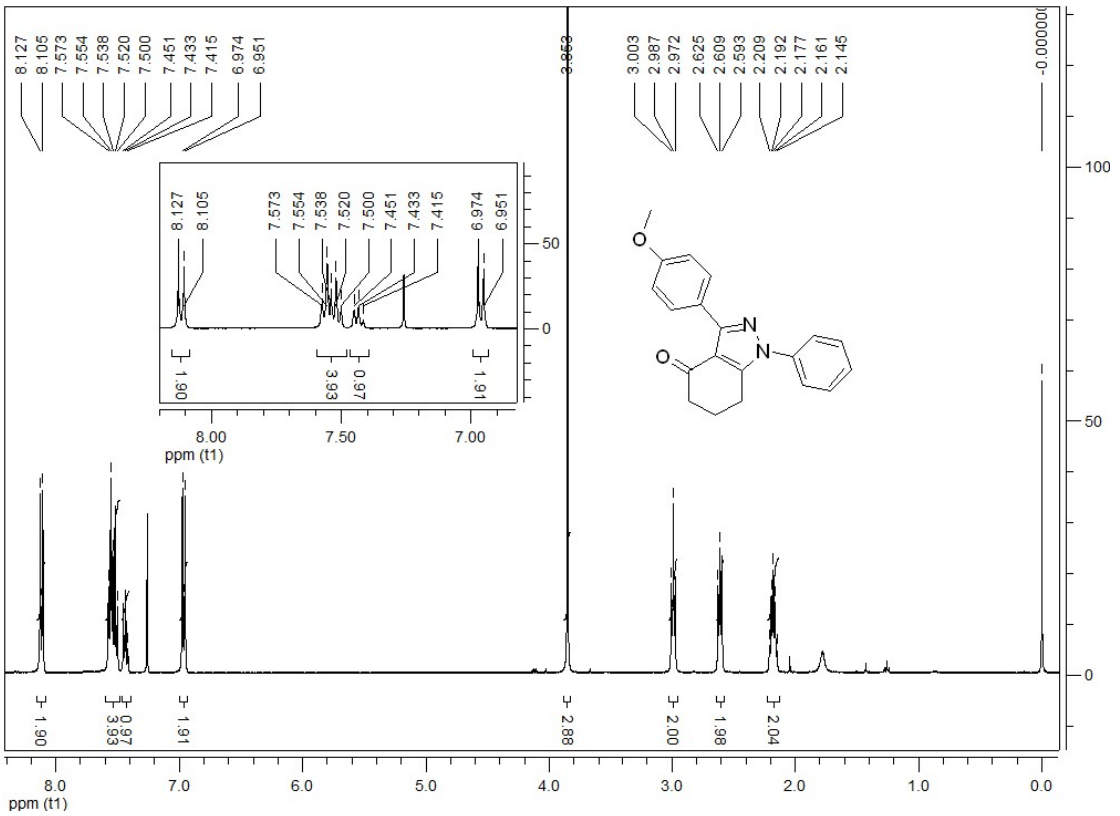


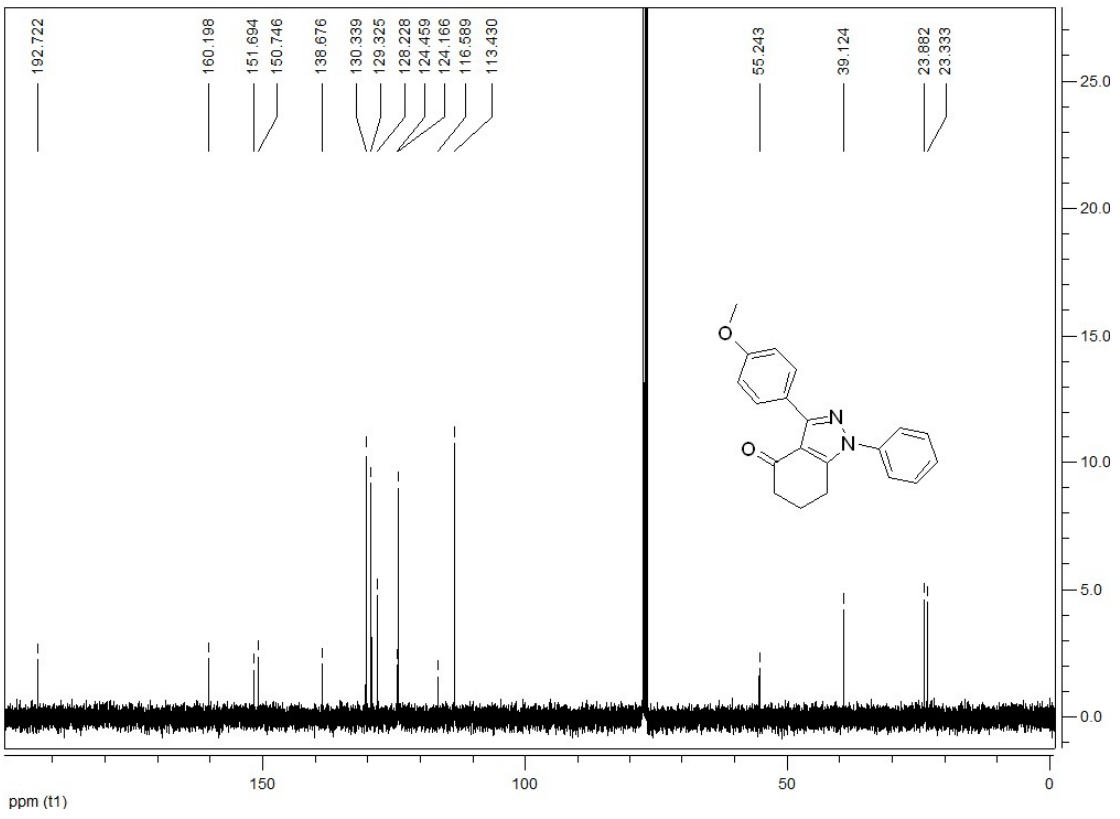
1-Phenyl-3-(p-tolyl)-1,5,6,7-tetrahydro-4H-indazol-4-one (**4b**)



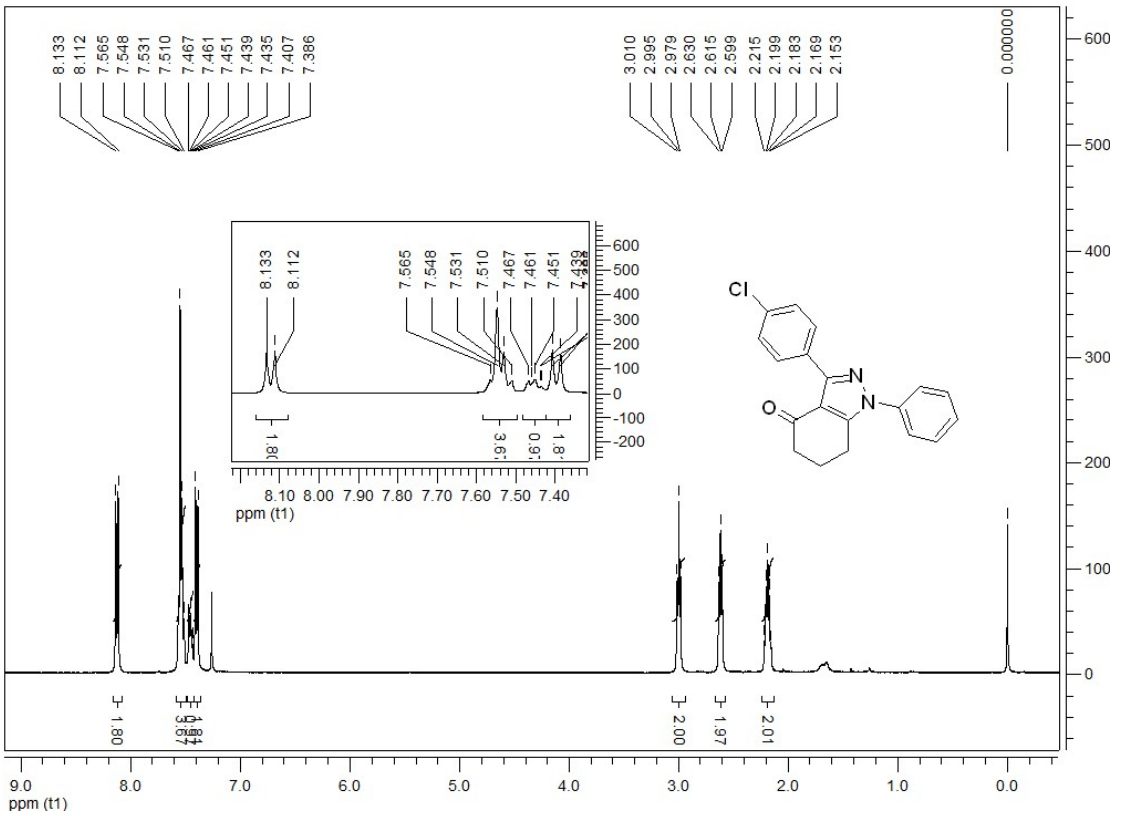


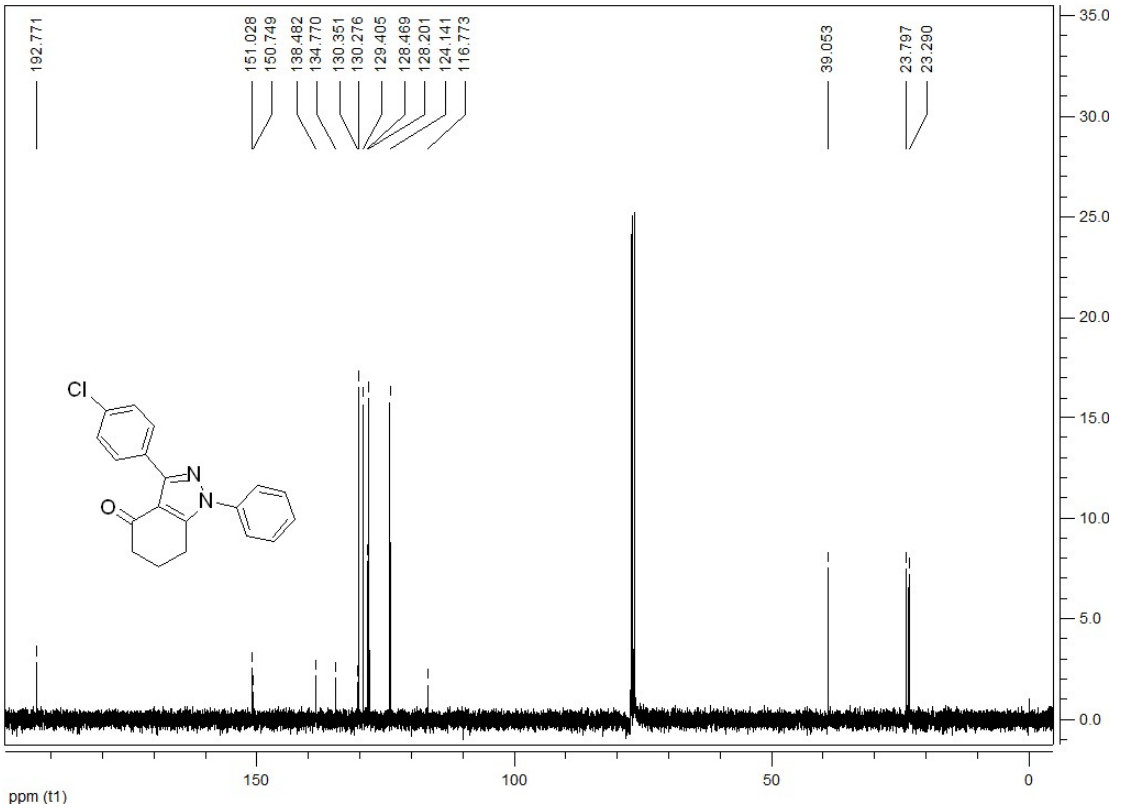
2-(4-Methoxyphenyl)-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4c**)



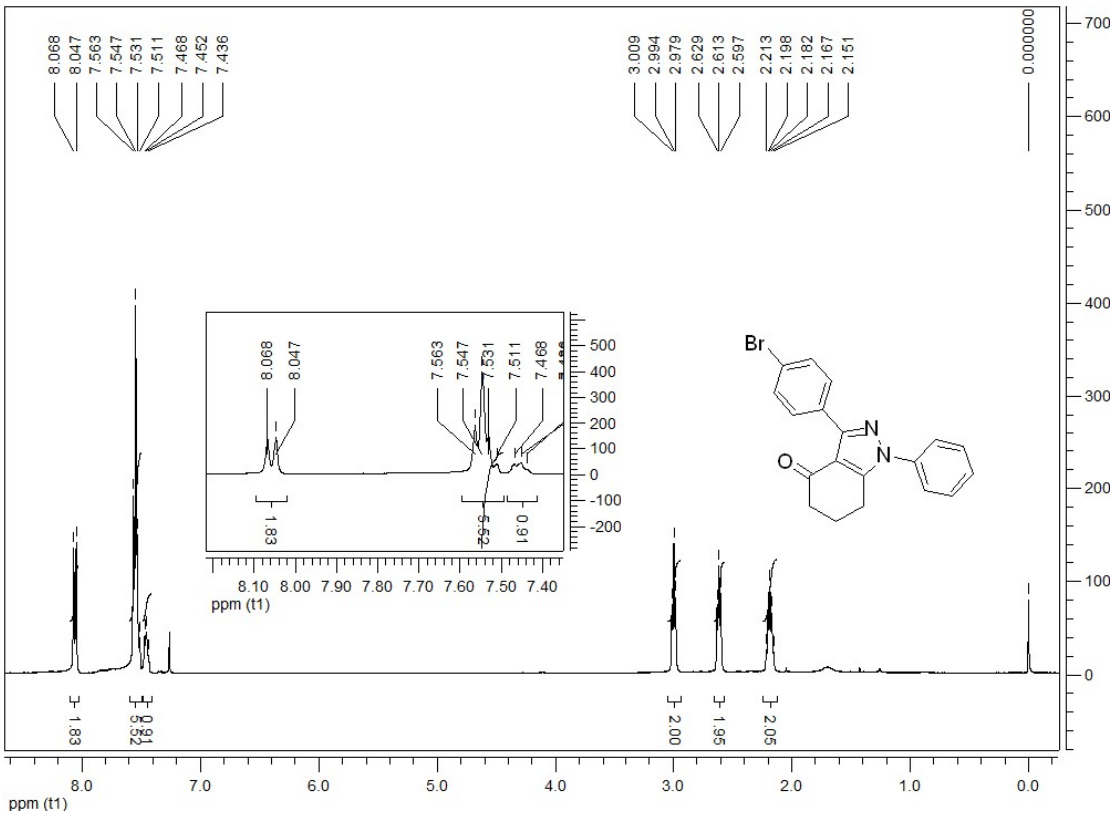


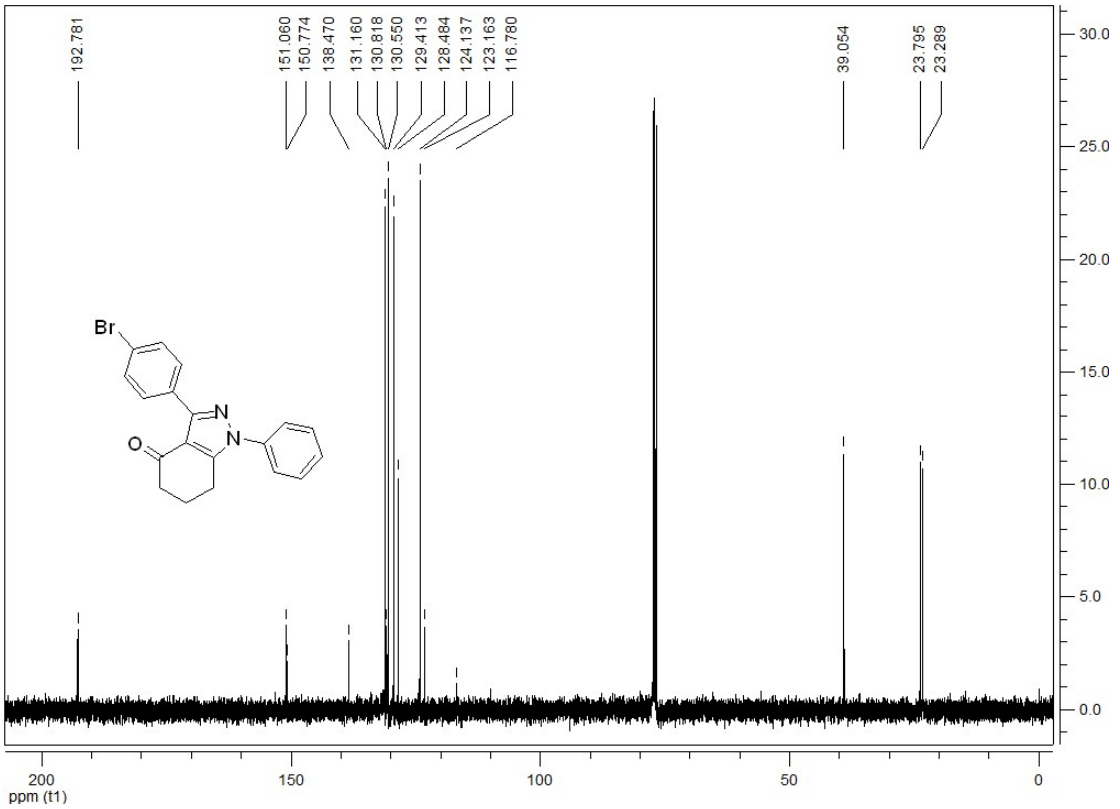
3-(4-Chlorophenyl)-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4d**)



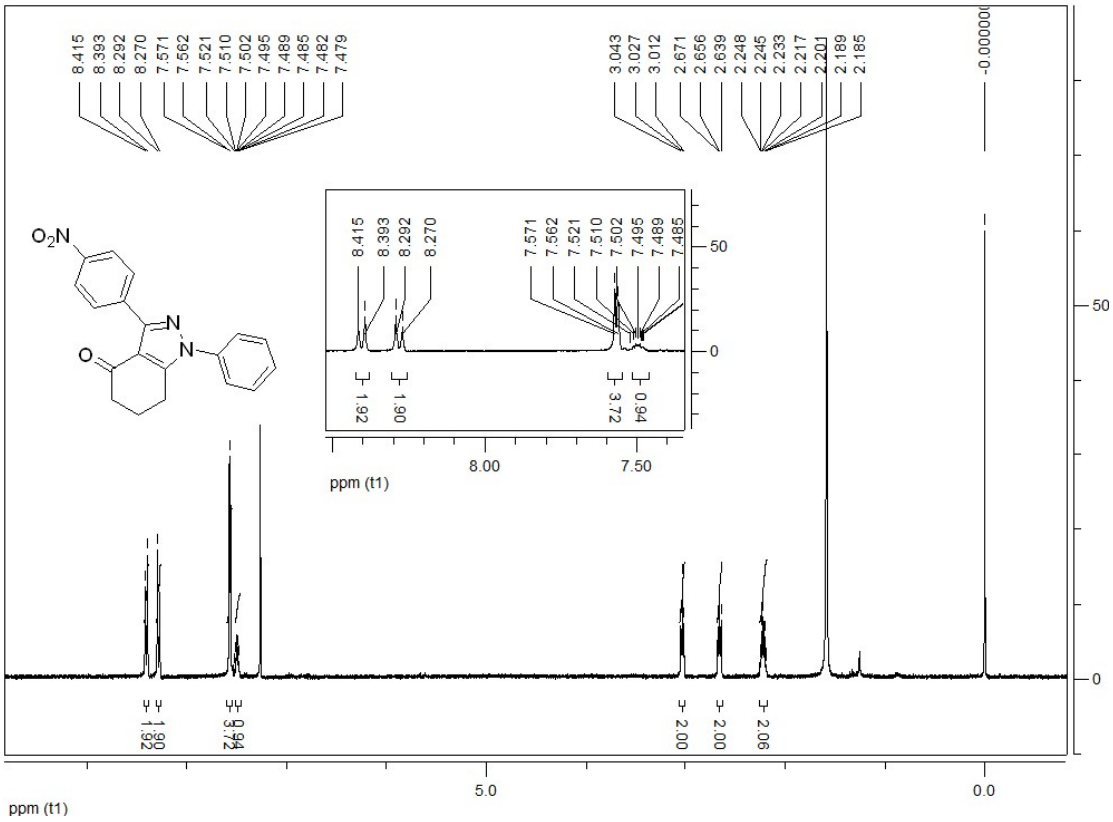


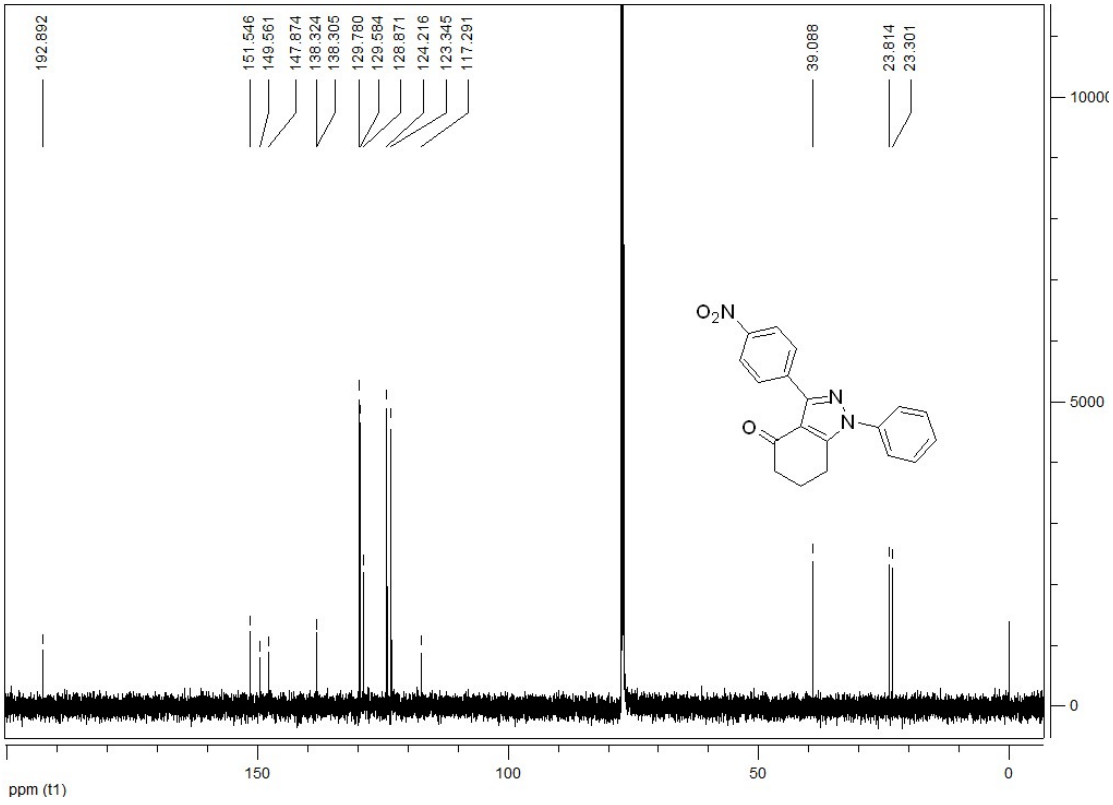
4-(4-Bromophenyl)-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4e**)



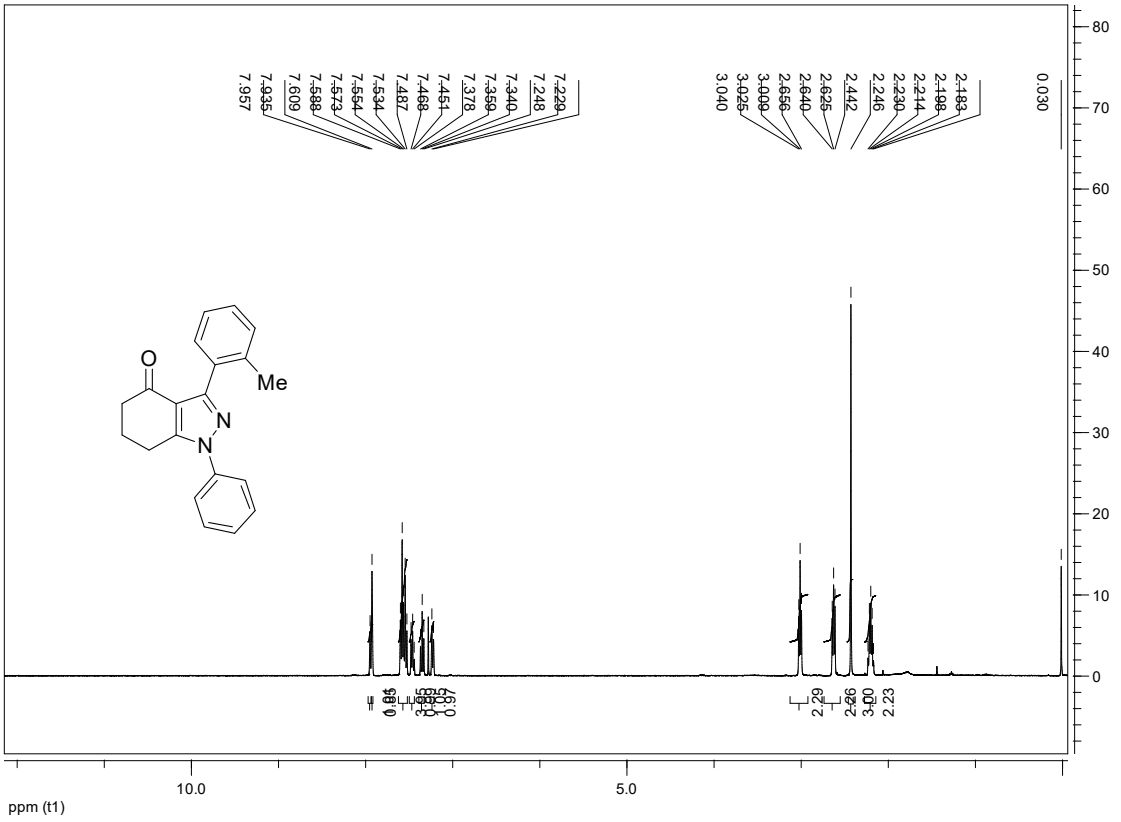


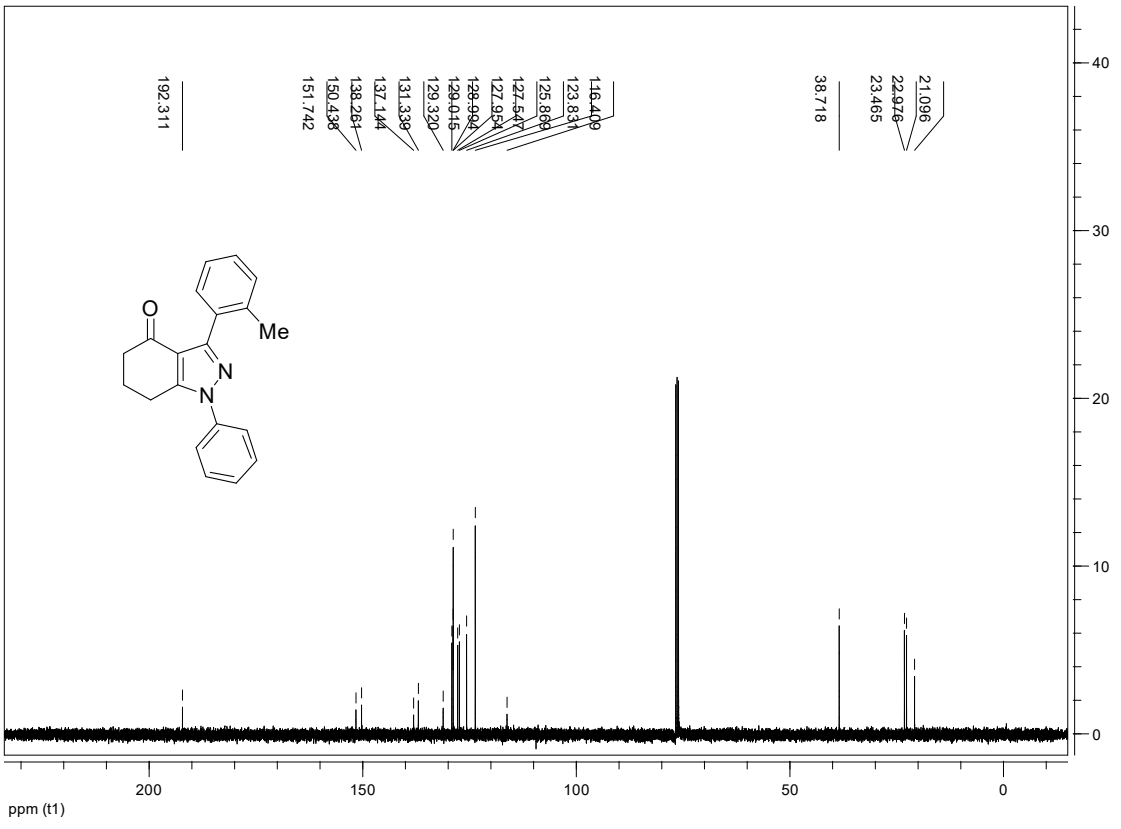
3-(4-Nitrophenyl)-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4f**)



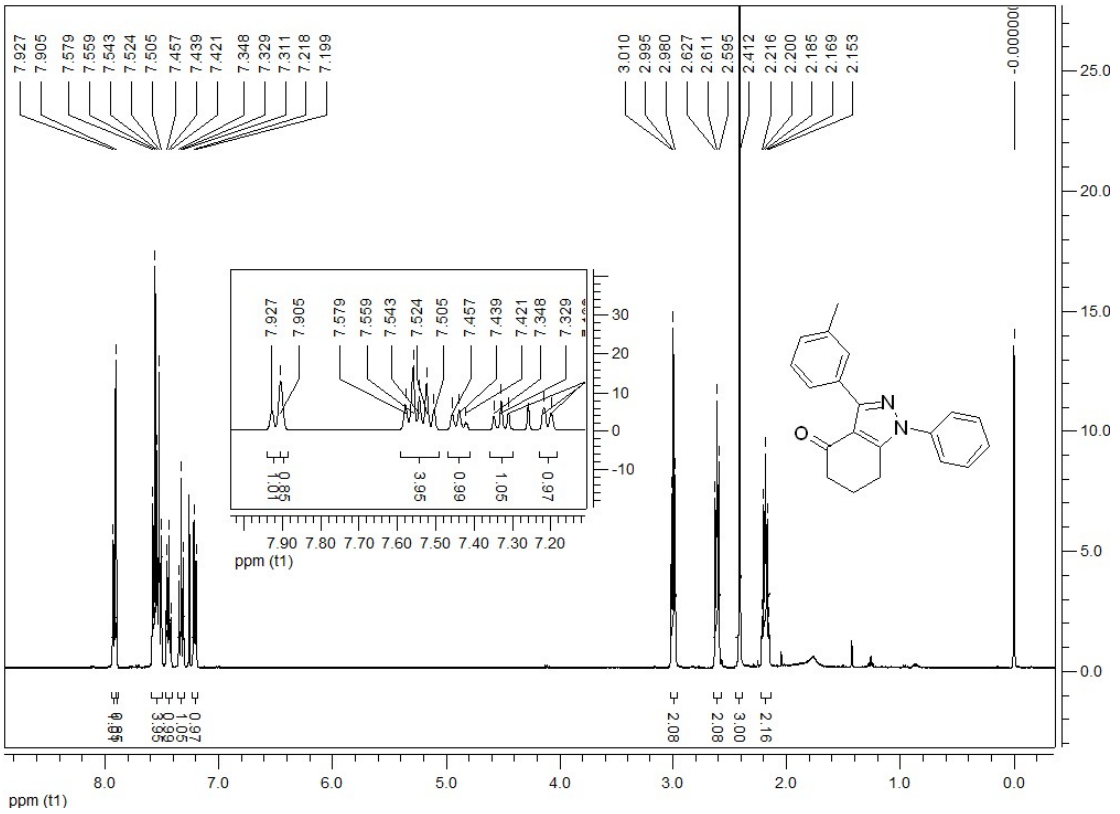


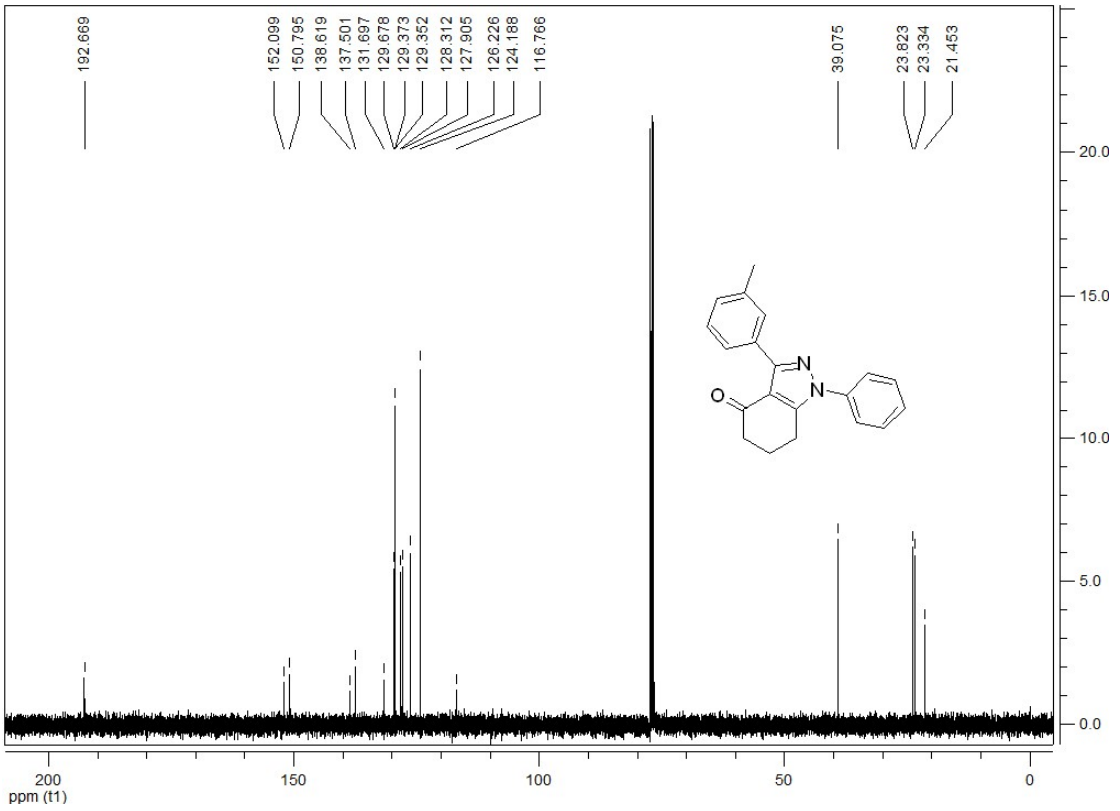
1-Phenyl-3-(o-tolyl)-1,5,6,7-tetrahydro-4H-indazol-4-one (**4g**)



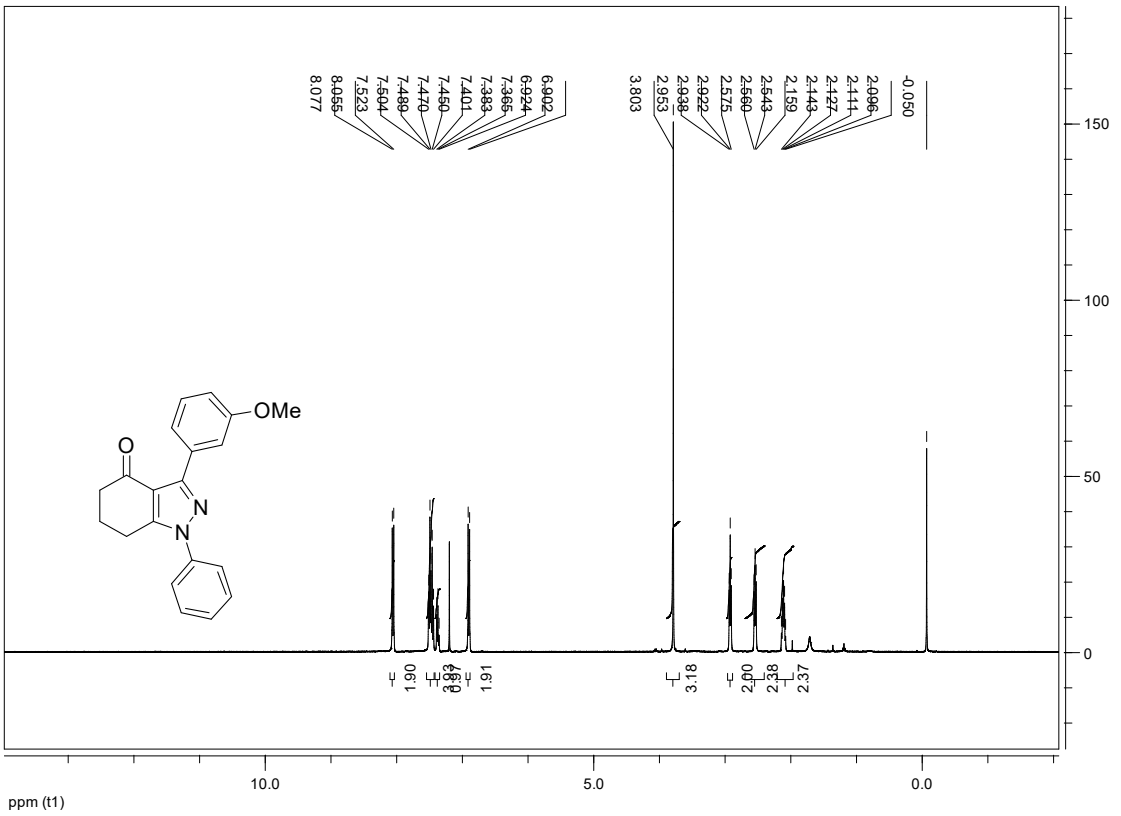


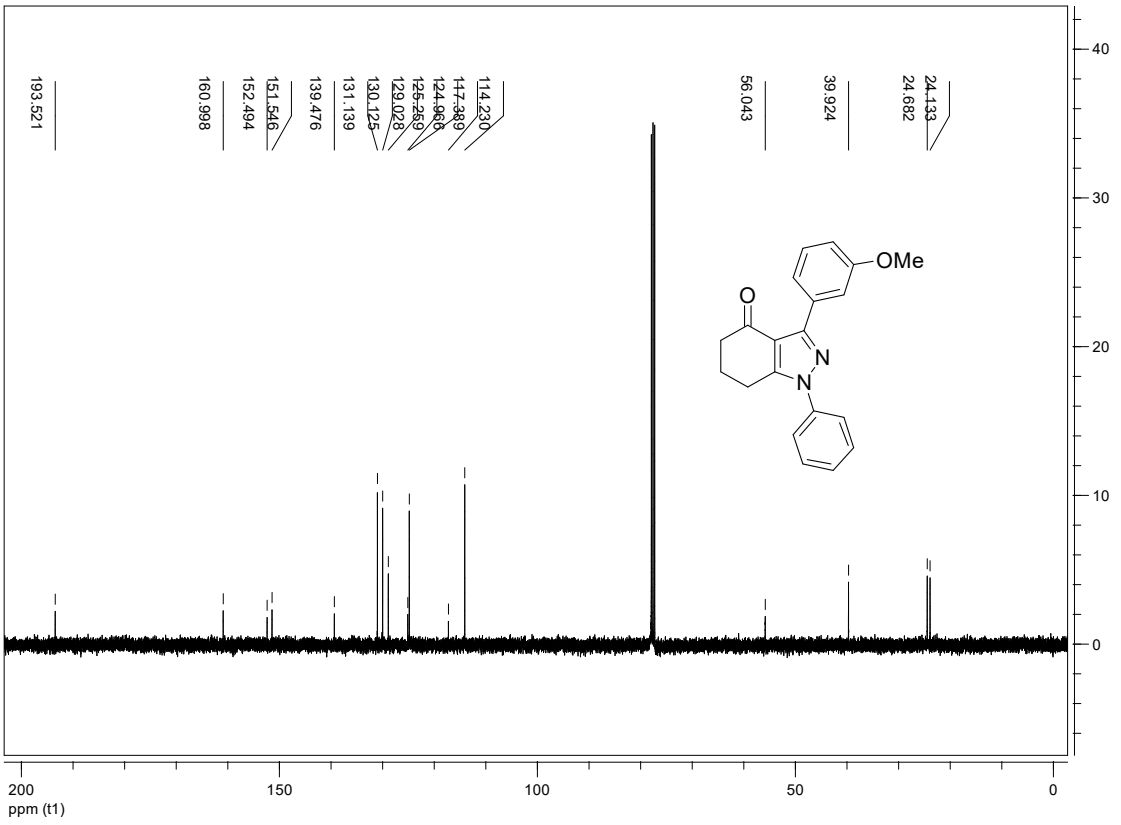
1-Phenyl-3-(m-tolyl)-1,5,6,7-tetrahydro-4H-indazol-4-one (**4h**)



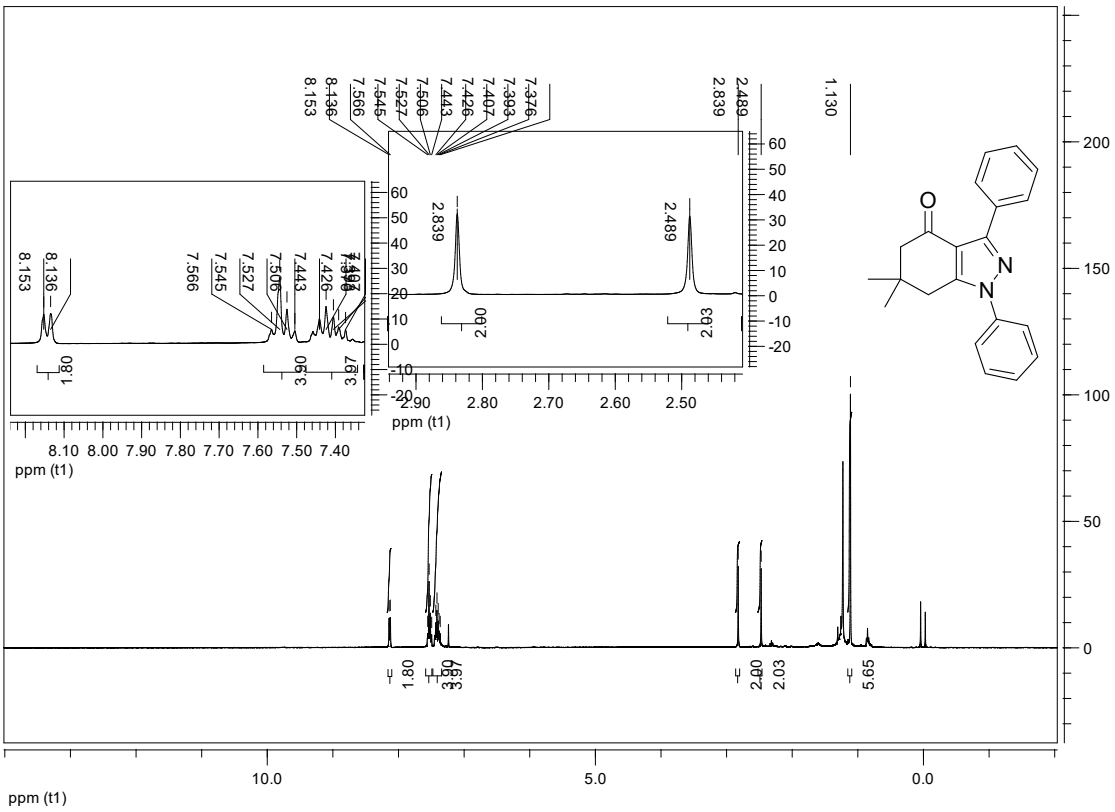


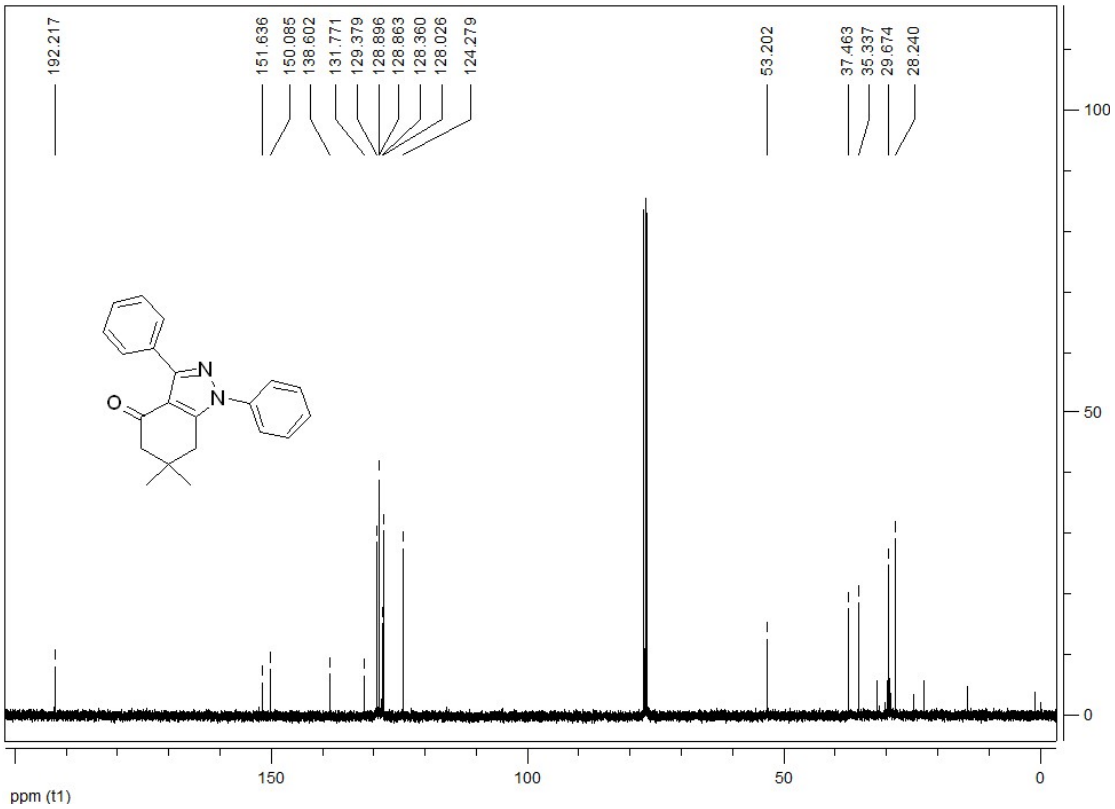
3-(3-Methoxyphenyl)-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4i**)



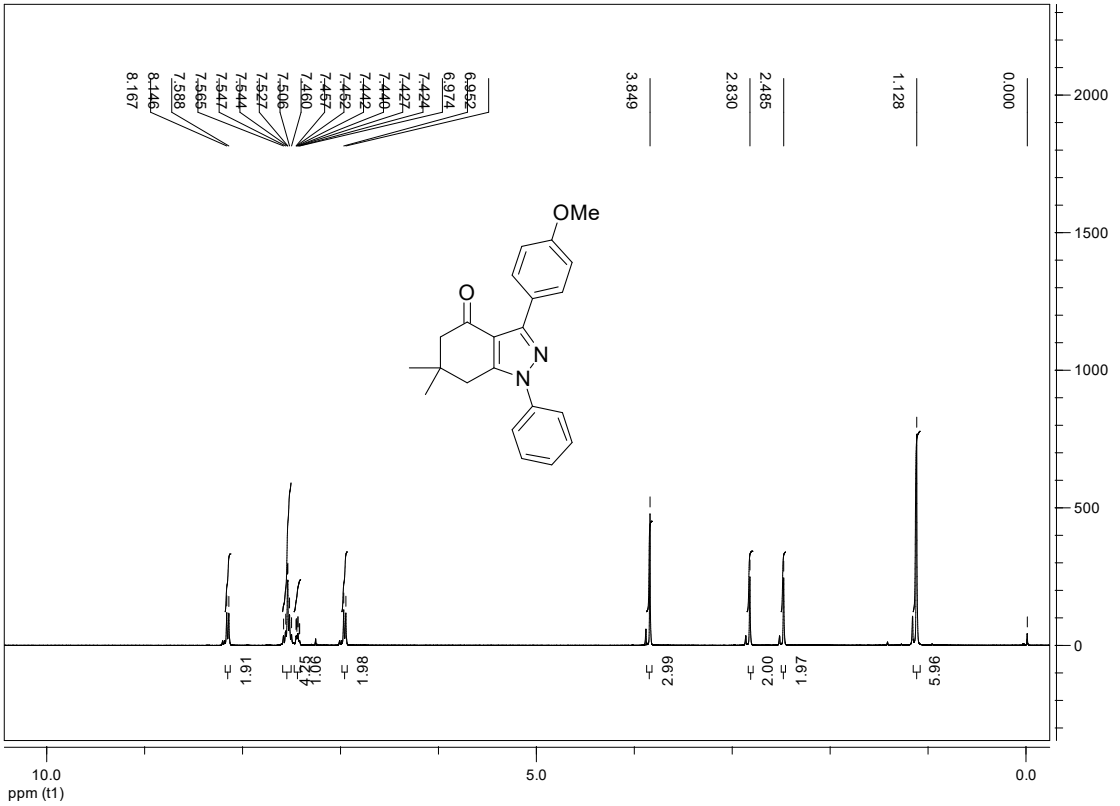


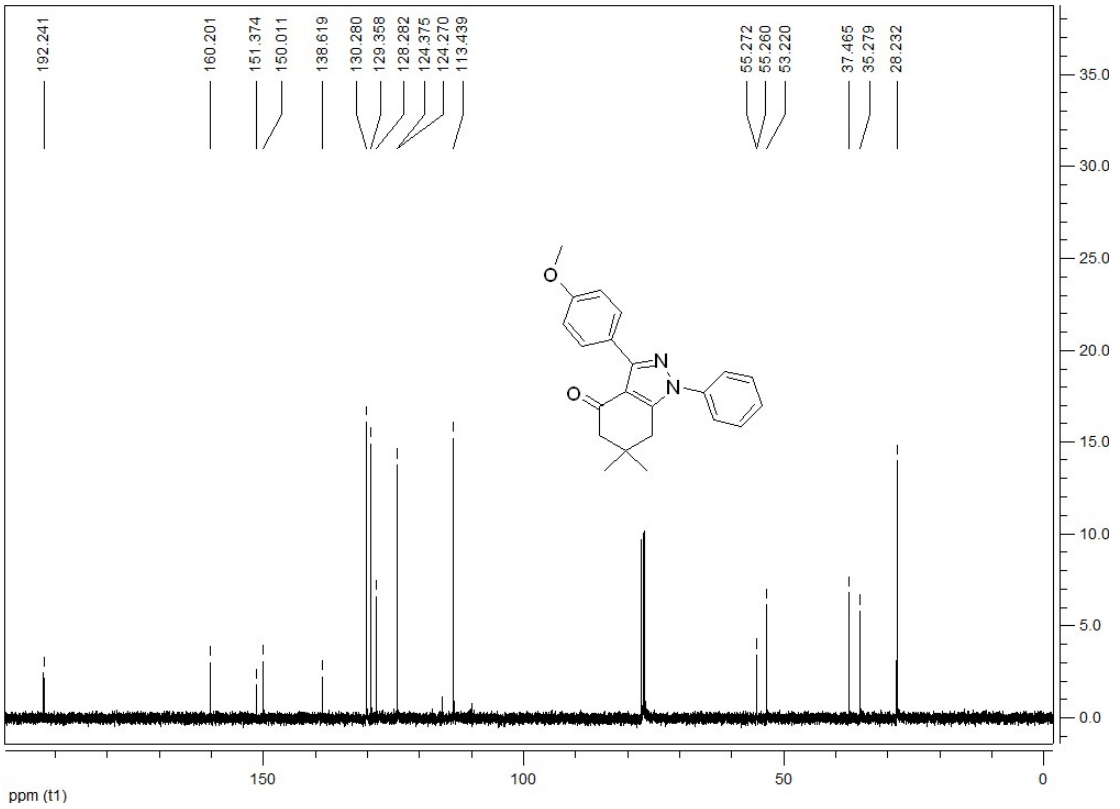
6,6-Dimethyl-1,3-diphenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4j**)



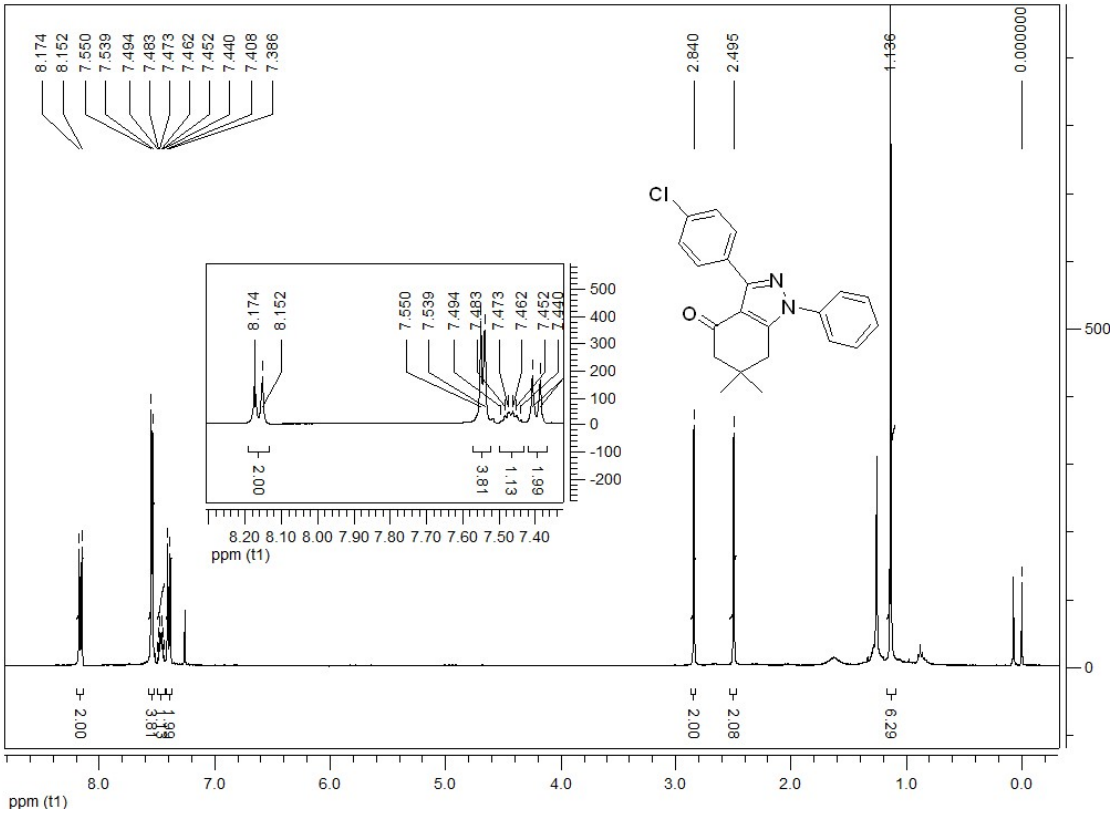


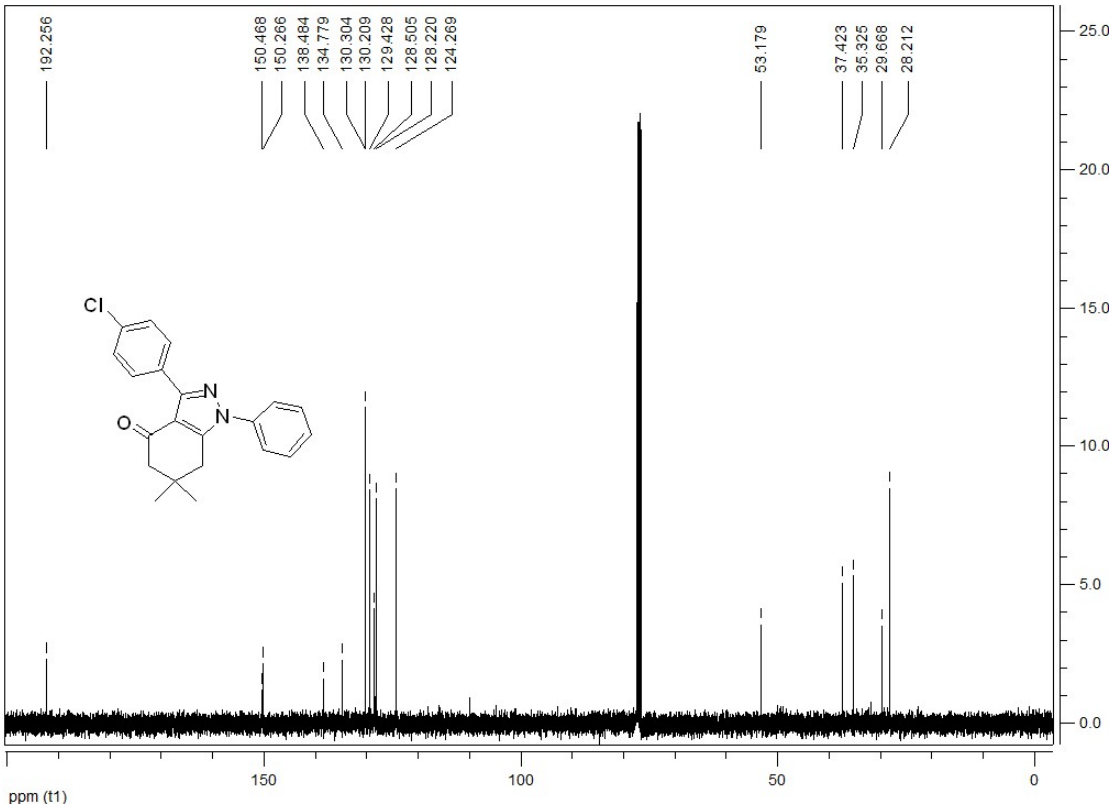
3-(4-Methoxyphenyl)-6,6-dimethyl-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4k**)



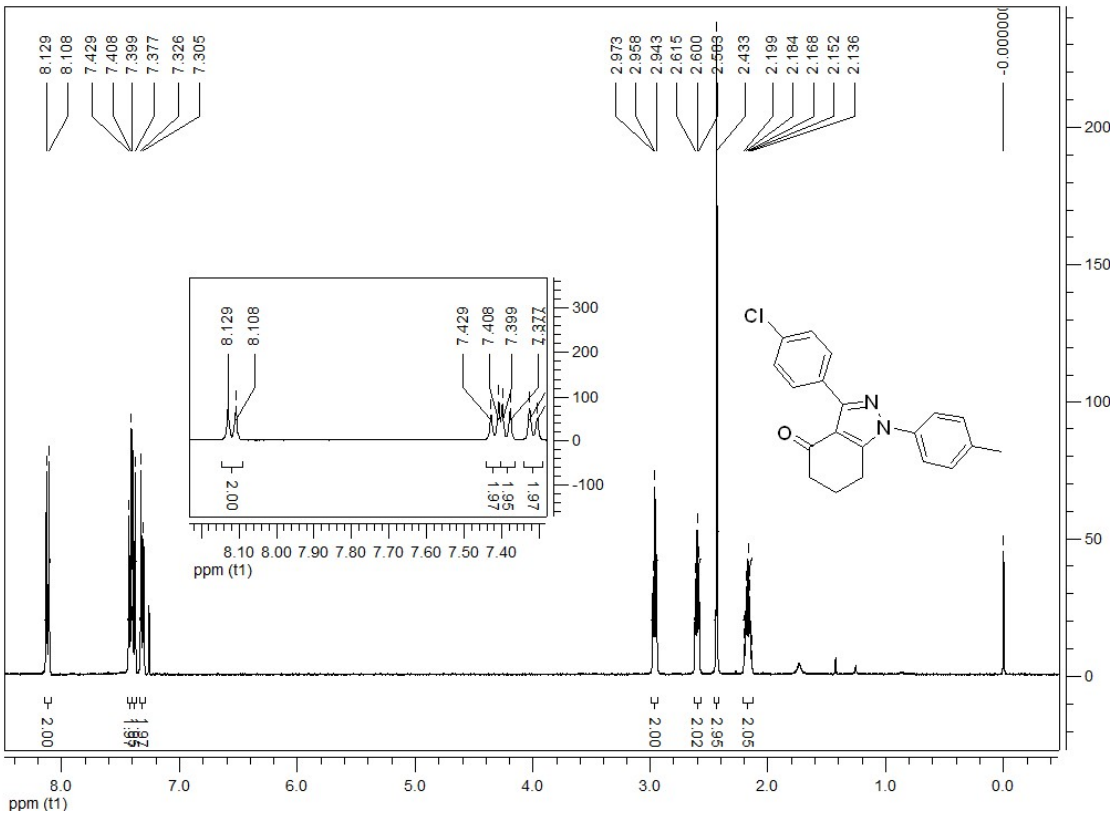


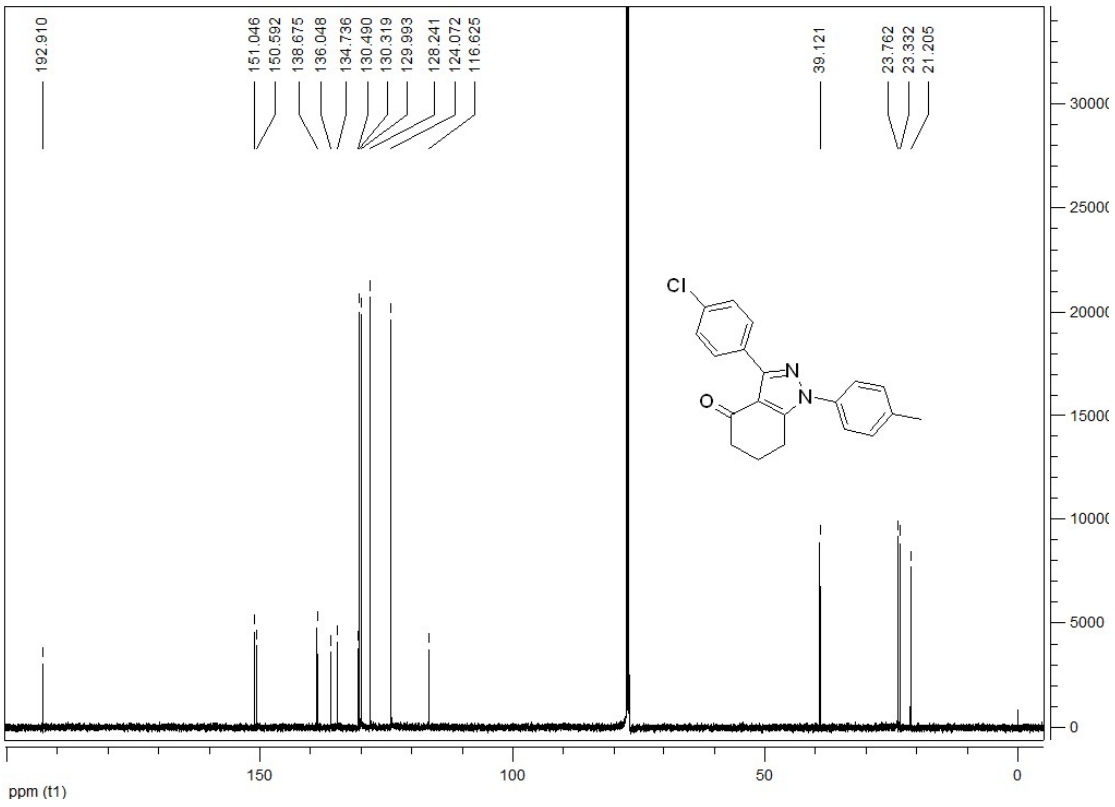
1-(4-Chlorophenyl)-6,6-dimethyl-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4l**)



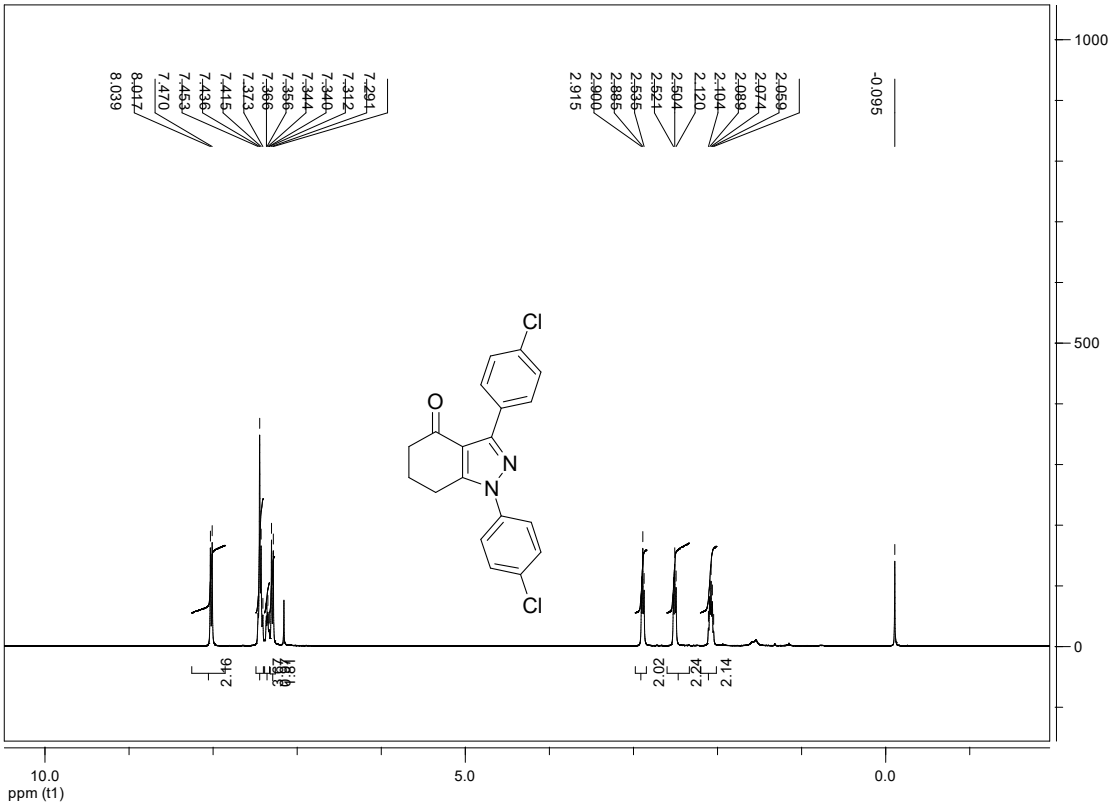


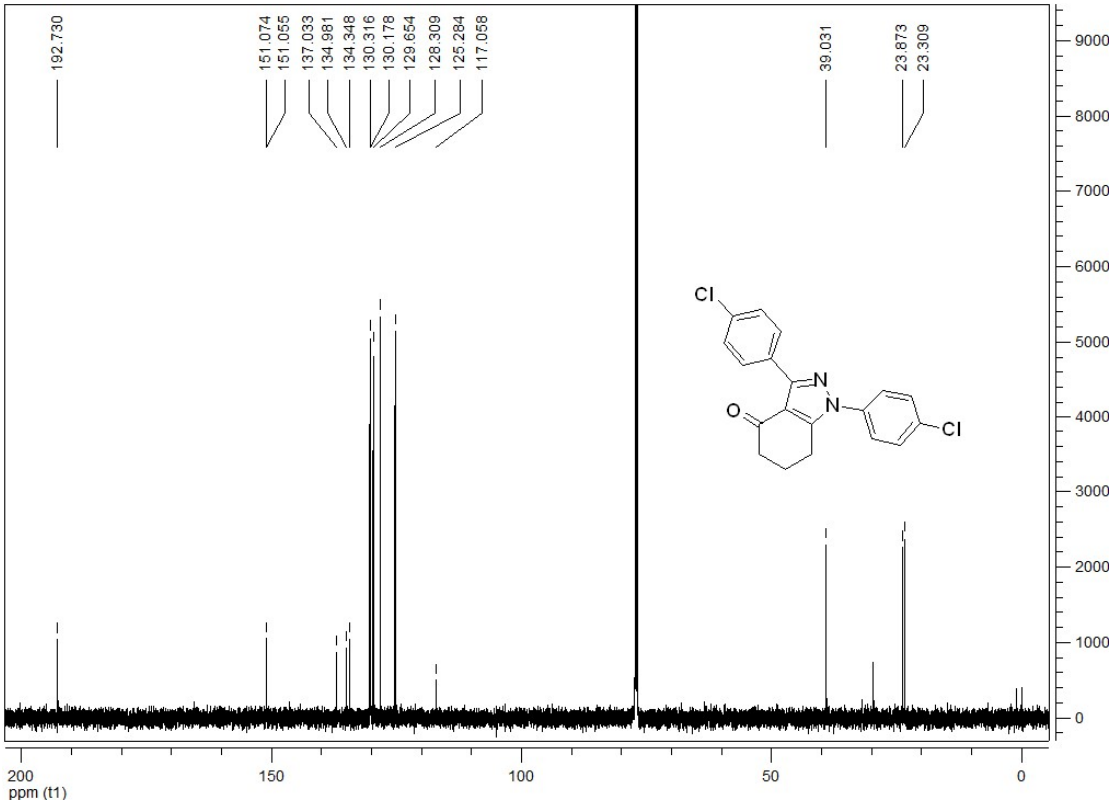
2-(4-Chlorophenyl)-1-(p-tolyl)-1,5,6,7-tetrahydro-4H-indazol-4-one (**4m**)



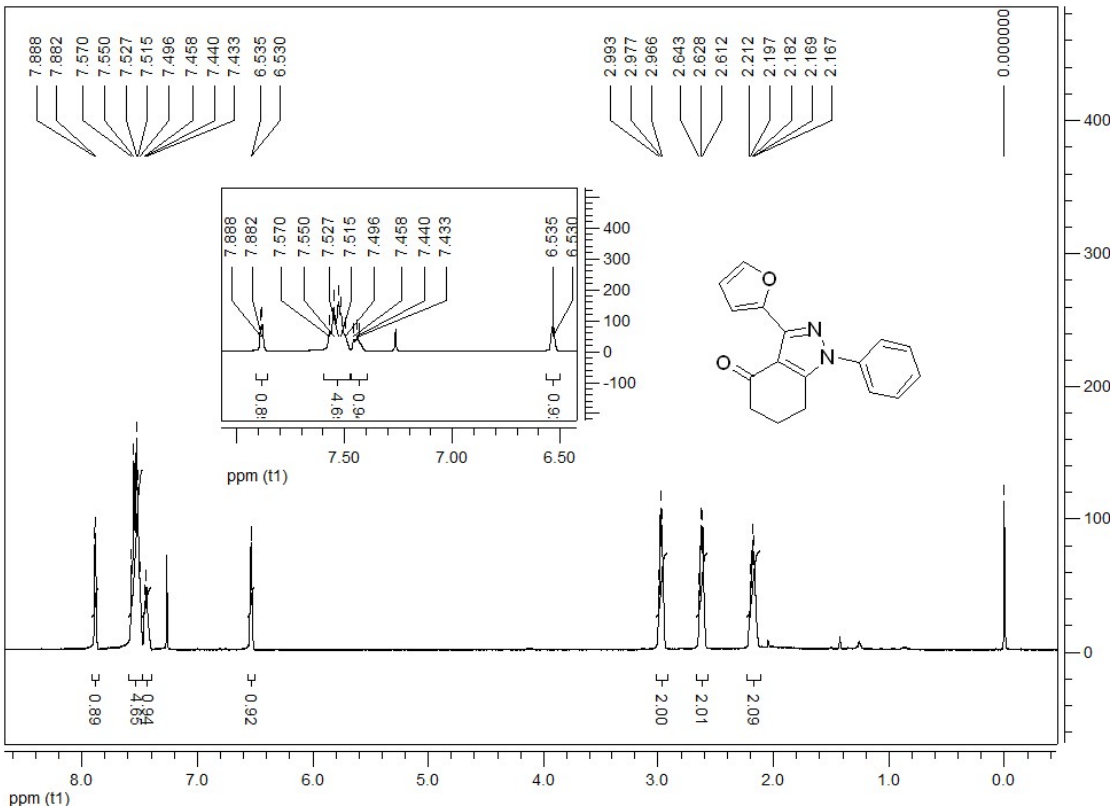


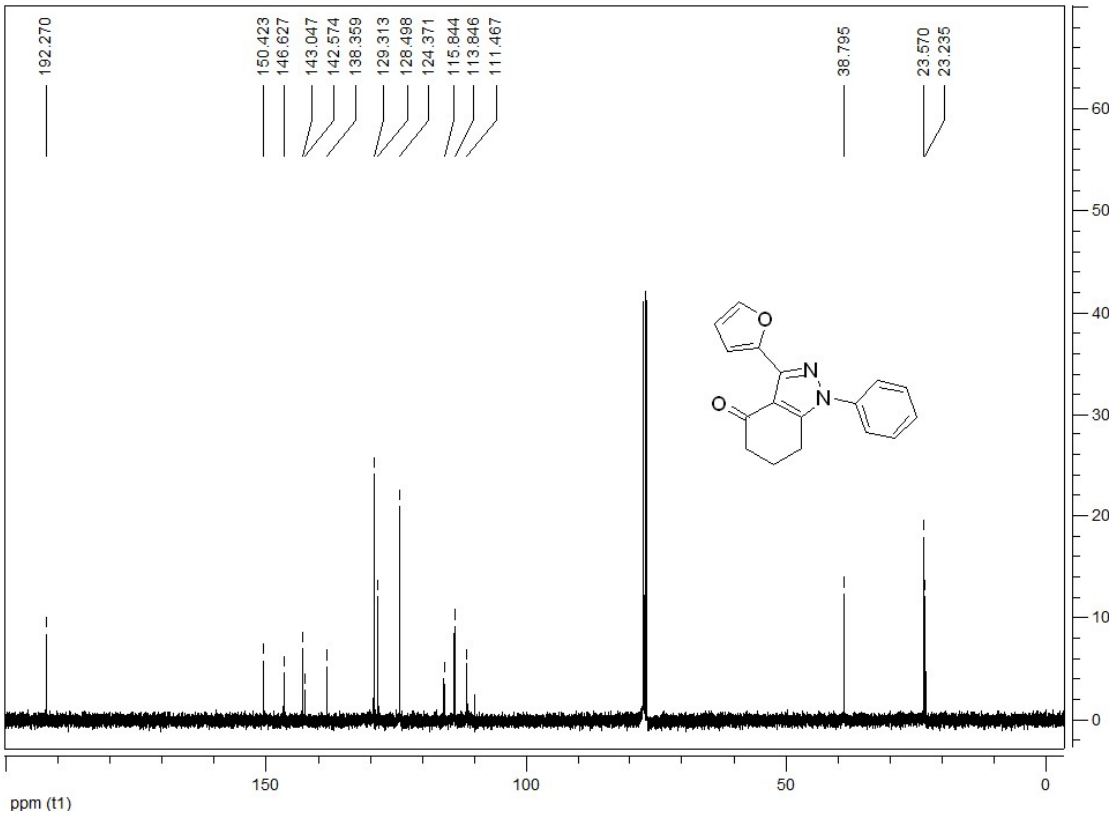
1,3-Bis(4-chlorophenyl)-1,5,6,7-tetrahydro-4H-indazol-4-one (**4n**)



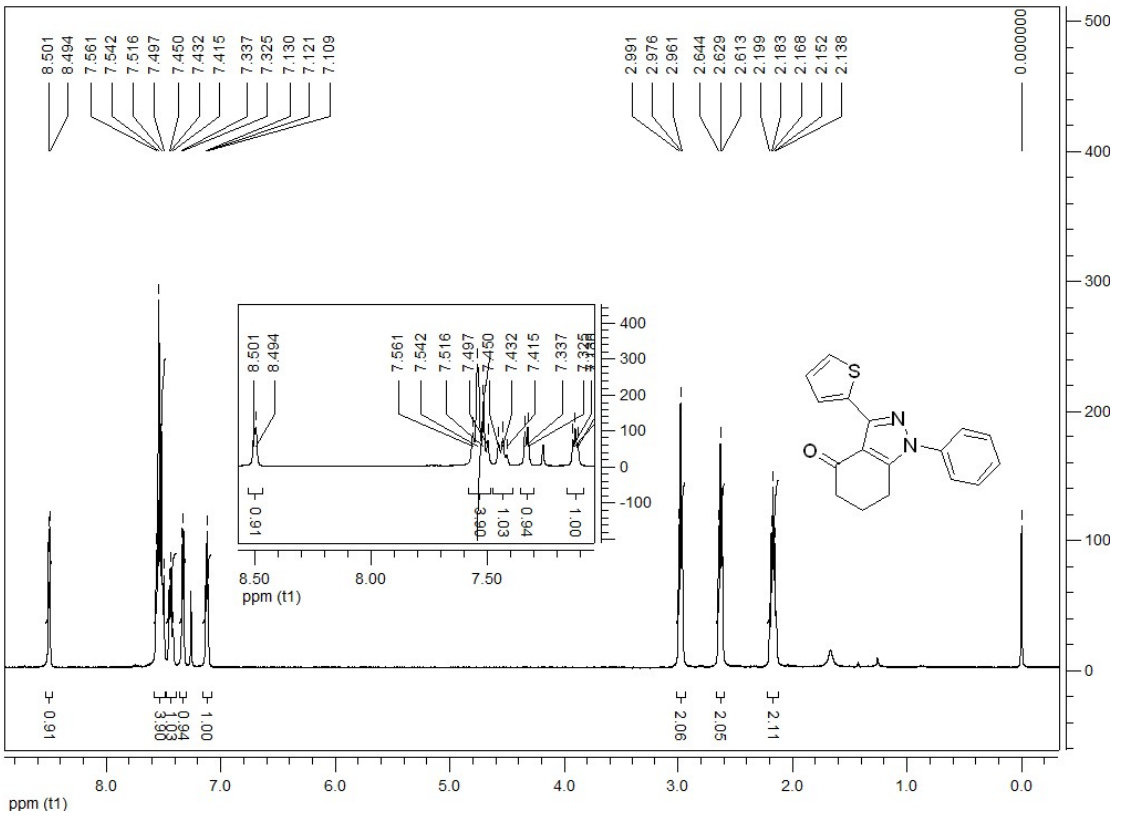


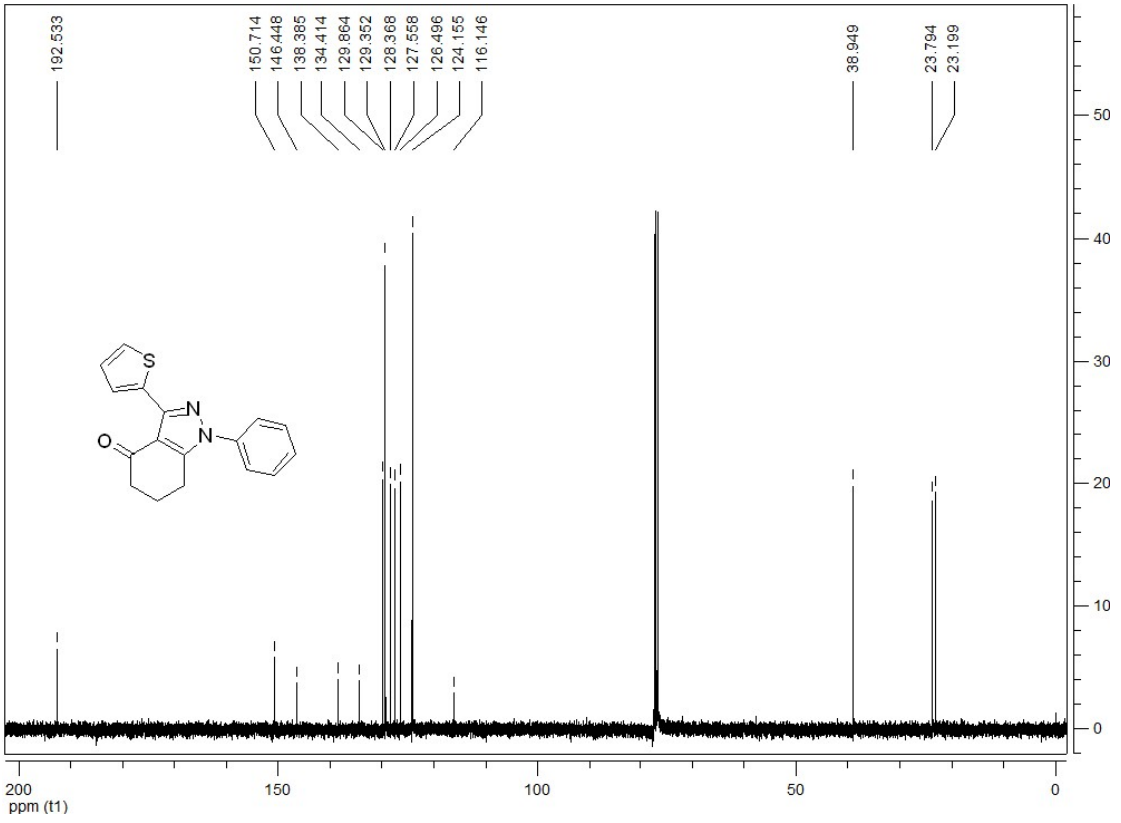
3-(Furan-2-yl)-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4o**)



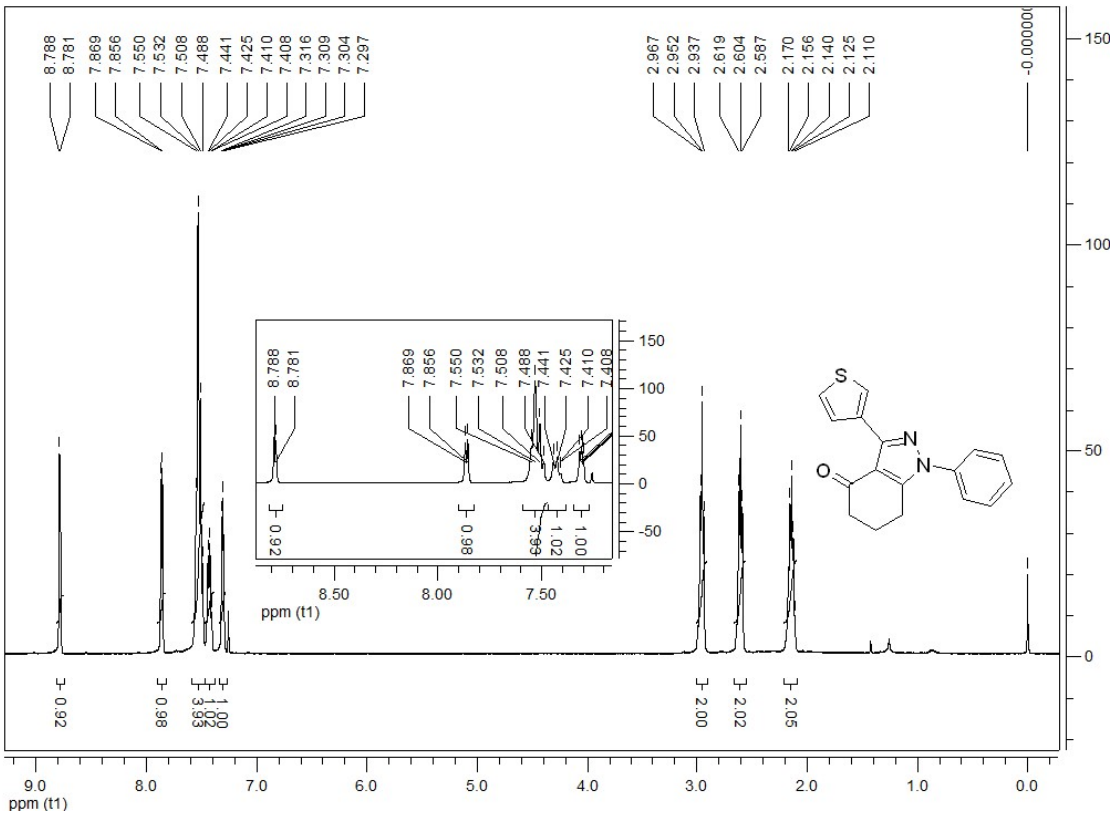


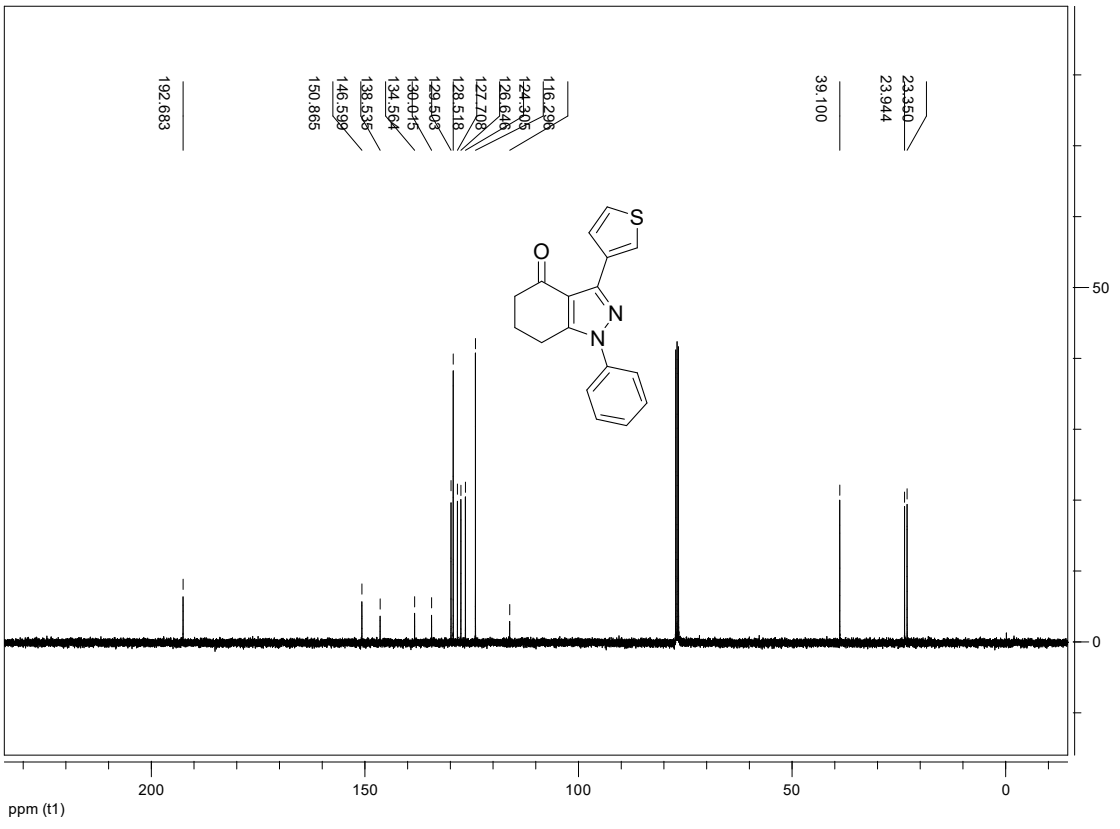
1-Phenyl-3-(thiophen-2-yl)-1,5,6,7-tetrahydro-4H-indazol-4-one (**4p**)



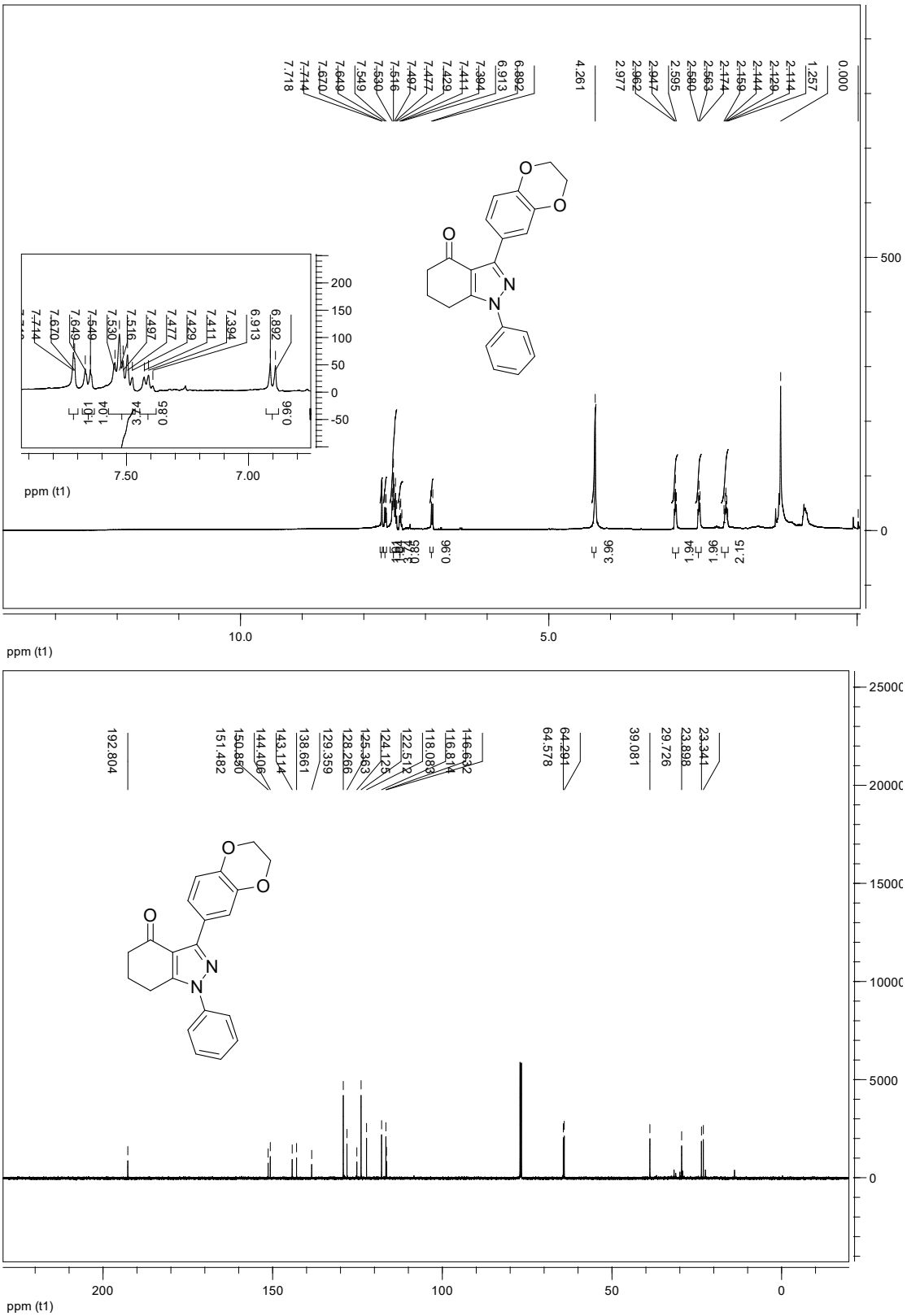


1-Phenyl-3-(thiophen-3-yl)-1,5,6,7-tetrahydro-4H-indazol-4-one (**4q**)





2-(2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)-1-phenyl-1,5,6,7-tetrahydro-4H-indazol-4-one (**4r**)



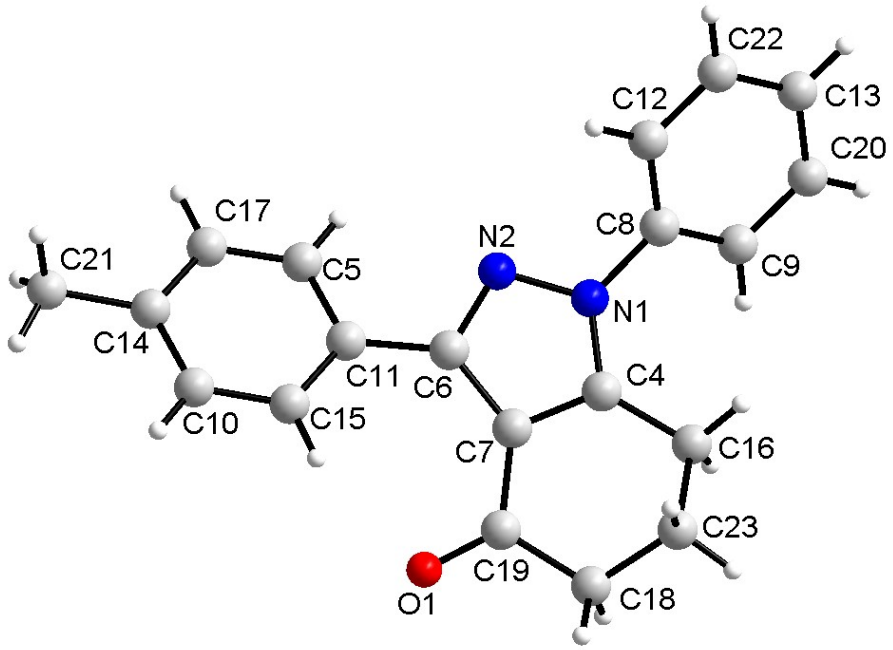


Table S1. Crystal data and structure refinement for 4b.

Identification code	4b
Empirical formula	C20 H18 N2 O
Formula weight	302.36
Temperature	296 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 11.586(3) A alpha = 90 deg. b = 15.822(3) A beta = 97.997(8) deg. c = 8.7845(18) A gamma = 90 deg.
Volume	1594.6(6) A^3
Z, Calculated density	4, 1.259 Mg/m^3
Absorption coefficient	0.078 mm^-1
F(000)	640

Crystal size	0.35 x 0.33 x 0.3 mm
Theta range for data collection	2.19 to 27.45 deg.
Limiting indices	-14<=h<=15, -20<=k<=16, -11<=l<=11
Reflections collected / unique	16142 / 3632 [R(int) = 0.0821]
Completeness to theta = 27.45	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3644 / 0 / 209
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0683, wR2 = 0.1135
R indices (all data)	R1 = 0.1739, wR2 = 0.1401
Largest diff. peak and hole	0.148 and -0.231 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 4b.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	7258(2)	10357(1)	-1019(2)	44(1)
N(2)	7756(2)	10217(1)	467(2)	48(1)
O(1)	5089(1)	8272(1)	784(2)	74(1)
C(4)	6370(2)	9820(1)	-1468(3)	42(1)
C(5)	8135(2)	9882(1)	3586(3)	55(1)
C(6)	7146(2)	9589(1)	977(3)	44(1)
C(7)	6258(2)	9314(1)	-208(2)	42(1)
C(8)	7785(2)	10967(1)	-1905(2)	43(1)
C(9)	7103(2)	11460(1)	-2962(3)	53(1)
C(10)	7672(2)	8311(2)	4635(3)	60(1)
C(11)	7486(2)	9330(1)	2583(3)	45(1)
C(12)	8985(2)	11042(1)	-1702(3)	52(1)
C(13)	8824(3)	12069(2)	-3705(3)	68(1)
C(14)	8325(2)	8855(2)	5630(3)	55(1)
C(15)	7249(2)	8539(1)	3145(3)	54(1)
C(16)	5684(2)	9750(1)	-3011(3)	53(1)
C(17)	8543(2)	9648(2)	5072(3)	58(1)
C(18)	4625(2)	8572(1)	-1875(3)	60(1)
C(19)	5327(2)	8681(1)	-312(3)	49(1)
C(20)	7630(2)	12007(1)	-3879(3)	63(1)
C(21)	8795(3)	8614(2)	7252(3)	77(1)
C(22)	9499(2)	11596(1)	-2609(3)	63(1)
C(23)	5225(2)	8849(1)	-3213(3)	63(1)

Table S3. Bond lengths [A] and angles [deg] for 4b.

N(1)-C(4)	1.349(3)
N(1)-N(2)	1.371(2)
N(1)-C(8)	1.429(3)
N(2)-C(6)	1.333(2)
O(1)-C(19)	1.222(3)
C(4)-C(7)	1.387(3)
C(4)-C(16)	1.478(3)
C(5)-C(17)	1.376(3)
C(5)-C(11)	1.385(3)
C(6)-C(7)	1.426(3)
C(6)-C(11)	1.470(3)
C(7)-C(19)	1.466(3)
C(8)-C(9)	1.375(3)
C(8)-C(12)	1.382(3)
C(9)-C(20)	1.380(3)
C(10)-C(14)	1.376(3)
C(10)-C(15)	1.380(3)
C(11)-C(15)	1.387(3)
C(12)-C(22)	1.375(3)
C(13)-C(20)	1.374(3)
C(13)-C(22)	1.376(3)
C(14)-C(17)	1.383(3)
C(14)-C(21)	1.502(3)
C(16)-C(23)	1.523(3)
C(18)-C(19)	1.506(3)
C(18)-C(23)	1.511(3)
C(4)-N(1)-N(2)	112.30(16)
C(4)-N(1)-C(8)	129.22(19)
N(2)-N(1)-C(8)	118.19(17)
C(6)-N(2)-N(1)	105.52(17)
N(1)-C(4)-C(7)	106.45(19)
N(1)-C(4)-C(16)	127.32(19)
C(7)-C(4)-C(16)	126.16(19)
C(17)-C(5)-C(11)	121.3(2)
N(2)-C(6)-C(7)	110.18(18)
N(2)-C(6)-C(11)	116.53(19)
C(7)-C(6)-C(11)	133.29(19)
C(4)-C(7)-C(6)	105.53(18)

C(4)-C(7)-C(19)	119.7(2)
C(6)-C(7)-C(19)	134.7(2)
C(9)-C(8)-C(12)	120.8(2)
C(9)-C(8)-N(1)	120.1(2)
C(12)-C(8)-N(1)	119.04(19)
C(8)-C(9)-C(20)	119.4(2)
C(14)-C(10)-C(15)	122.0(2)
C(5)-C(11)-C(15)	117.3(2)
C(5)-C(11)-C(6)	118.95(19)
C(15)-C(11)-C(6)	123.6(2)
C(22)-C(12)-C(8)	119.2(2)
C(20)-C(13)-C(22)	120.3(2)
C(10)-C(14)-C(17)	117.0(2)
C(10)-C(14)-C(21)	122.5(2)
C(17)-C(14)-C(21)	120.4(2)
C(10)-C(15)-C(11)	120.7(2)
C(4)-C(16)-C(23)	108.19(19)
C(5)-C(17)-C(14)	121.6(2)
C(19)-C(18)-C(23)	115.3(2)
O(1)-C(19)-C(7)	123.9(2)
O(1)-C(19)-C(18)	120.4(2)
C(7)-C(19)-C(18)	115.7(2)
C(13)-C(20)-C(9)	120.0(2)
C(12)-C(22)-C(13)	120.2(2)
C(18)-C(23)-C(16)	111.8(2)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 4b.
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
N(1)	46(1)	39(1)	49(1)	2(1)	10(1)	-5(1)
N(2)	53(1)	45(1)	47(1)	2(1)	10(1)	-4(1)
O(1)	63(1)	77(1)	85(1)	20(1)	17(1)	-23(1)
C(4)	38(1)	37(1)	53(2)	-1(1)	11(1)	-1(1)
C(5)	62(2)	48(1)	57(2)	2(1)	13(1)	-2(1)
C(6)	45(1)	36(1)	54(2)	1(1)	17(1)	1(1)
C(7)	39(1)	36(1)	54(1)	-1(1)	14(1)	0(1)
C(8)	46(2)	35(1)	50(1)	-1(1)	15(1)	-4(1)
C(9)	53(2)	42(1)	66(2)	4(1)	13(1)	1(1)
C(10)	75(2)	49(1)	60(2)	10(1)	20(2)	8(1)
C(11)	46(1)	42(1)	51(1)	1(1)	16(1)	3(1)
C(12)	51(2)	43(1)	62(2)	1(1)	9(1)	-6(1)
C(13)	80(2)	54(2)	77(2)	11(1)	31(2)	-12(2)
C(14)	59(2)	55(2)	53(2)	4(1)	16(1)	13(1)
C(15)	61(2)	45(1)	58(2)	0(1)	16(1)	-2(1)
C(16)	48(2)	54(1)	58(2)	2(1)	6(1)	-4(1)
C(17)	63(2)	59(2)	52(2)	-7(1)	11(1)	0(1)
C(18)	52(2)	51(1)	78(2)	-4(1)	10(1)	-12(1)
C(19)	41(1)	41(1)	69(2)	1(1)	19(1)	0(1)
C(20)	70(2)	49(1)	71(2)	12(1)	17(1)	0(1)
C(21)	95(2)	74(2)	62(2)	10(2)	9(2)	19(2)
C(22)	52(2)	55(1)	86(2)	0(2)	21(2)	-13(1)
C(23)	66(2)	59(2)	63(2)	-6(1)	6(1)	-15(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 4b.

	x	y	z	U(eq)
H(5)	8298	10420	3249	66
H(9)	6295	11426	-3059	64
H(10)	7510	7773	4977	72
H(12)	9439	10720	-960	63
H(13)	9177	12434	-4332	82
H(15)	6800	8157	2511	65
H(16A)	6170	9879	-3794	64
H(16B)	5039	10146	-3110	64
H(17)	8977	10033	5718	69
H(18A)	3907	8890	-1903	72
H(18B)	4418	7980	-2012	72
H(20)	7177	12333	-4615	75
H(21A)	8572	9033	7946	116
H(21B)	9630	8580	7358	116
H(21C)	8483	8075	7488	116
H(22)	10306	11651	-2481	76
H(23A)	4680	8812	-4154	76
H(23B)	5869	8469	-3308	76

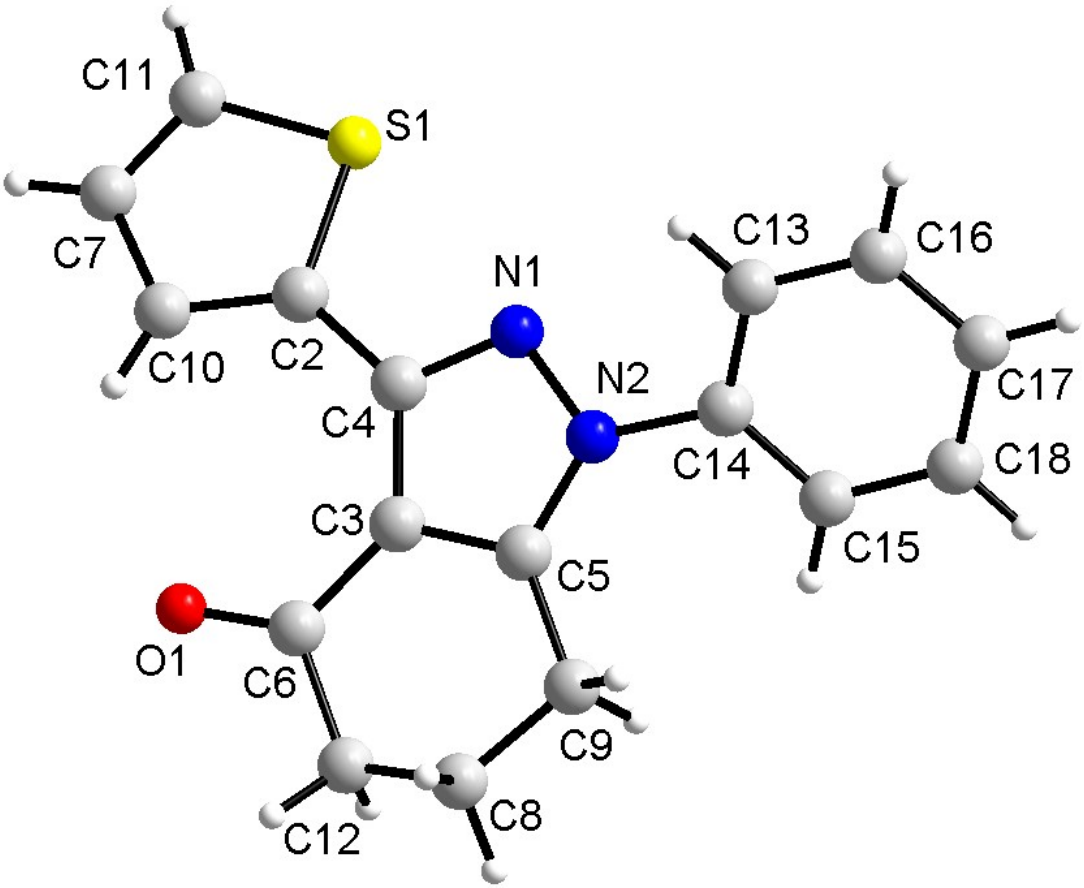


Table S6. Crystal data and structure refinement for 4q.

Identification code	4q
Empirical formula	C17 H14 N2 O S
Formula weight	294.36
Temperature	296 K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 31.267(8) A alpha = 90 deg. b = 8.132(3) A beta = 90 deg. c = 22.702(6) A gamma = 90 deg.
Volume	5773(3) A^3
Z, Calculated density	16, 1.355 Mg/m^3

Absorption coefficient	0.224 mm^-1
F(000)	2464
Crystal size	0.35 x 0.33 x 0.3 mm
Theta range for data collection	1.30 to 27.42 deg.
Limiting indices	-33<=h<=40, -10<=k<=10, -29<=l<=23
Reflections collected / unique	27936 / 6584 [R(int) = 0.1114]
Completeness to theta = 27.42	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6568 / 0 / 379
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0799, wR2 = 0.1818
R indices (all data)	R1 = 0.2036, wR2 = 0.2381
Largest diff. peak and hole	0.392 and -0.496 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 4q.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	1202(1)	8566(2)	379(1)	60(1)
N(1)	301(1)	7791(4)	603(1)	39(1)
O(1)	125(1)	8507(4)	-1295(1)	60(1)
N(2)	-105(1)	7138(4)	628(1)	39(1)
C(2)	792(1)	8764(5)	-122(2)	40(1)
C(3)	0(1)	7720(5)	-306(1)	35(1)
C(4)	369(1)	8138(5)	38(2)	38(1)
C(5)	-289(1)	7067(5)	90(1)	36(1)
C(6)	-102(1)	7844(5)	-930(2)	45(1)
C(13)	-157(1)	7629(5)	1682(2)	46(1)
C(7)	1369(2)	10001(7)	-577(2)	68(1)
C(14)	-270(1)	6686(5)	1195(2)	39(1)
C(15)	-526(1)	5320(6)	1258(2)	49(1)
C(8)	-847(2)	6923(8)	-659(2)	79(2)
C(9)	-724(1)	6443(6)	-54(2)	51(1)
C(10)	926(1)	9564(5)	-636(2)	48(1)
C(16)	-290(1)	7142(6)	2230(2)	56(1)
C(17)	-541(1)	5778(6)	2304(2)	61(1)
C(18)	-665(1)	4880(6)	1813(2)	58(1)
C(11)	1549(1)	9545(6)	-72(2)	63(1)
C(12)	-515(1)	7075(7)	-1099(2)	72(2)
S(2)	1255(1)	5683(2)	2850(1)	65(1)
N(3)	2173(1)	5912(4)	3066(1)	44(1)
C(19)	2799(1)	5657(5)	3668(2)	40(1)
N(4)	2610(1)	5870(4)	3100(1)	43(1)
C(39)	2084(1)	6205(5)	2505(2)	43(1)
C(28)	2793(1)	6118(5)	2567(2)	41(1)
C(29)	1631(1)	6278(5)	2342(2)	40(1)
O(2)	2287(1)	6939(6)	1178(1)	100(1)
C(31)	2467(1)	6343(5)	2166(2)	44(1)
C(20)	3158(1)	4693(5)	3740(2)	50(1)

C(21)	2610(1)	6410(6)	4149(2)	53(1)
C(22)	3325(1)	4491(6)	4299(2)	59(1)
C(36)	988(1)	6664(6)	1862(2)	61(1)
C(23)	2776(1)	6165(7)	4704(2)	63(1)
C(32)	1443(1)	6766(5)	1809(2)	49(1)
C(24)	3134(1)	5194(7)	4775(2)	67(1)
C(37)	853(1)	6110(6)	2379(2)	58(1)
C(33)	2557(2)	6631(7)	1547(2)	66(1)
C(34)	3327(2)	6896(7)	1835(2)	78(2)
C(35)	3261(1)	6173(6)	2435(2)	57(1)
C(38)	3016(2)	6431(8)	1381(2)	93(2)

Table S8. Bond lengths [A] and angles [deg] for 4q.

S(1)-C(11)	1.690(5)
S(1)-C(2)	1.721(4)
N(1)-C(4)	1.329(4)
N(1)-N(2)	1.378(4)
O(1)-C(6)	1.216(4)
N(2)-C(5)	1.350(4)
N(2)-C(14)	1.434(4)
C(2)-C(10)	1.399(5)
C(2)-C(4)	1.463(5)
C(3)-C(5)	1.381(5)
C(3)-C(4)	1.434(5)
C(3)-C(6)	1.456(5)
C(5)-C(9)	1.490(5)
C(6)-C(12)	1.485(6)
C(13)-C(16)	1.370(5)
C(13)-C(14)	1.391(5)
C(7)-C(11)	1.330(6)
C(7)-C(10)	1.436(6)
C(14)-C(15)	1.378(6)
C(15)-C(18)	1.379(5)
C(8)-C(12)	1.447(6)
C(8)-C(9)	1.478(6)
C(16)-C(17)	1.368(6)
C(17)-C(18)	1.389(6)
S(2)-C(37)	1.686(4)
S(2)-C(29)	1.715(4)
N(3)-C(39)	1.326(5)
N(3)-N(4)	1.371(4)
C(19)-C(20)	1.377(5)
C(19)-C(21)	1.384(5)
C(19)-N(4)	1.431(4)
N(4)-C(28)	1.351(4)
C(39)-C(31)	1.428(5)
C(39)-C(29)	1.466(5)
C(28)-C(31)	1.378(5)
C(28)-C(35)	1.497(5)
C(29)-C(32)	1.403(5)
O(2)-C(33)	1.216(5)
C(31)-C(33)	1.452(5)

C(20)-C(22)	1.382(5)
C(21)-C(23)	1.375(5)
C(22)-C(24)	1.360(6)
C(36)-C(37)	1.327(6)
C(36)-C(32)	1.430(6)
C(23)-C(24)	1.381(6)
C(33)-C(38)	1.492(6)
C(34)-C(38)	1.466(6)
C(34)-C(35)	1.498(6)

C(11)-S(1)-C(2)	91.9(2)
C(4)-N(1)-N(2)	105.6(3)
C(5)-N(2)-N(1)	111.8(3)
C(5)-N(2)-C(14)	130.3(3)
N(1)-N(2)-C(14)	117.9(3)
C(10)-C(2)-C(4)	129.8(3)
C(10)-C(2)-S(1)	111.7(3)
C(4)-C(2)-S(1)	118.4(3)
C(5)-C(3)-C(4)	105.1(3)
C(5)-C(3)-C(6)	121.2(3)
C(4)-C(3)-C(6)	133.6(3)
N(1)-C(4)-C(3)	110.3(3)
N(1)-C(4)-C(2)	117.3(3)
C(3)-C(4)-C(2)	132.3(3)
N(2)-C(5)-C(3)	107.1(3)
N(2)-C(5)-C(9)	127.0(3)
C(3)-C(5)-C(9)	125.8(3)
O(1)-C(6)-C(3)	124.5(4)
O(1)-C(6)-C(12)	121.2(3)
C(3)-C(6)-C(12)	114.3(3)
C(16)-C(13)-C(14)	119.0(4)
C(11)-C(7)-C(10)	114.7(4)
C(15)-C(14)-C(13)	120.6(3)
C(15)-C(14)-N(2)	120.6(3)
C(13)-C(14)-N(2)	118.7(3)
C(14)-C(15)-C(18)	119.2(4)
C(12)-C(8)-C(9)	118.6(4)
C(8)-C(9)-C(5)	110.6(3)
C(2)-C(10)-C(7)	109.1(3)
C(17)-C(16)-C(13)	121.4(4)
C(16)-C(17)-C(18)	119.2(4)
C(15)-C(18)-C(17)	120.6(4)
C(7)-C(11)-S(1)	112.5(3)
C(8)-C(12)-C(6)	118.8(4)

C(37)-S(2)-C(29)	91.5(2)
C(39)-N(3)-N(4)	105.4(3)
C(20)-C(19)-C(21)	120.4(3)
C(20)-C(19)-N(4)	120.7(3)
C(21)-C(19)-N(4)	118.9(3)
C(28)-N(4)-N(3)	111.6(3)
C(28)-N(4)-C(19)	130.7(3)
N(3)-N(4)-C(19)	117.7(3)
N(3)-C(39)-C(31)	110.9(3)
N(3)-C(39)-C(29)	116.8(3)
C(31)-C(39)-C(29)	132.3(3)
N(4)-C(28)-C(31)	107.5(3)
N(4)-C(28)-C(35)	126.7(3)
C(31)-C(28)-C(35)	125.9(3)
C(32)-C(29)-C(39)	129.2(3)
C(32)-C(29)-S(2)	112.0(3)
C(39)-C(29)-S(2)	118.8(3)
C(28)-C(31)-C(39)	104.6(3)
C(28)-C(31)-C(33)	121.2(3)
C(39)-C(31)-C(33)	134.2(4)
C(19)-C(20)-C(22)	118.8(4)
C(23)-C(21)-C(19)	119.8(4)
C(24)-C(22)-C(20)	121.0(4)
C(37)-C(36)-C(32)	114.4(4)
C(21)-C(23)-C(24)	119.7(4)
C(29)-C(32)-C(36)	109.0(4)
C(22)-C(24)-C(23)	120.2(4)
C(36)-C(37)-S(2)	113.1(3)
O(2)-C(33)-C(31)	124.4(4)
O(2)-C(33)-C(38)	121.1(4)
C(31)-C(33)-C(38)	114.4(4)
C(38)-C(34)-C(35)	116.5(4)
C(28)-C(35)-C(34)	109.2(3)
C(34)-C(38)-C(33)	115.6(4)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for 4q.
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
S(1)	47(1)	86(1)	47(1)	-6(1)	0(1)	2(1)
N(1)	37(2)	50(2)	32(2)	-1(2)	0(1)	4(2)
O(1)	76(2)	70(2)	34(2)	9(2)	-5(2)	-3(2)
N(2)	32(2)	53(2)	31(2)	4(2)	1(1)	2(2)
C(2)	37(2)	46(3)	36(2)	-13(2)	6(2)	0(2)
C(3)	37(2)	35(2)	32(2)	-5(2)	-1(2)	10(2)
C(4)	43(2)	38(2)	32(2)	-2(2)	3(2)	10(2)
C(5)	39(2)	43(2)	27(2)	-1(2)	-5(2)	7(2)
C(6)	51(2)	52(3)	33(2)	2(2)	-1(2)	8(2)
C(13)	51(2)	51(3)	36(2)	1(2)	-1(2)	1(2)
C(7)	66(3)	83(4)	55(3)	-4(3)	22(2)	-18(3)
C(14)	33(2)	51(3)	31(2)	5(2)	1(2)	9(2)
C(15)	49(2)	59(3)	39(2)	2(2)	1(2)	0(2)
C(8)	62(3)	128(5)	46(3)	12(3)	-19(2)	-22(3)
C(9)	42(2)	67(3)	43(2)	-4(2)	-6(2)	-4(2)
C(10)	42(2)	59(3)	44(2)	2(2)	10(2)	-6(2)
C(16)	55(3)	81(4)	32(2)	-6(2)	4(2)	1(3)
C(17)	56(3)	87(4)	39(2)	13(2)	14(2)	4(3)
C(18)	55(3)	60(3)	57(3)	14(2)	6(2)	-4(2)
C(11)	43(2)	88(4)	58(3)	-24(3)	8(2)	-2(2)
C(12)	53(3)	132(5)	31(2)	2(3)	-14(2)	-4(3)
S(2)	47(1)	96(1)	54(1)	5(1)	-2(1)	9(1)
N(3)	32(2)	64(2)	36(2)	2(2)	-3(1)	7(2)
C(19)	34(2)	47(3)	40(2)	6(2)	-6(2)	-3(2)
N(4)	32(2)	61(2)	37(2)	1(2)	0(1)	5(2)
C(39)	43(2)	48(3)	37(2)	-1(2)	-3(2)	6(2)
C(28)	42(2)	41(3)	41(2)	0(2)	7(2)	0(2)
C(29)	43(2)	42(3)	35(2)	-4(2)	-6(2)	4(2)
O(2)	82(2)	176(4)	42(2)	19(2)	2(2)	6(3)
C(31)	46(2)	49(3)	36(2)	0(2)	1(2)	-2(2)

C(20)	36(2)	58(3)	56(3)	7(2)	0(2)	1(2)
C(21)	44(2)	71(3)	45(2)	5(2)	-6(2)	12(2)
C(22)	37(2)	77(4)	64(3)	24(3)	-15(2)	-2(2)
C(36)	65(3)	57(3)	61(3)	-3(2)	-32(2)	-1(2)
C(23)	52(3)	92(4)	44(2)	-3(2)	-8(2)	-1(3)
C(32)	43(2)	50(3)	53(2)	0(2)	-18(2)	0(2)
C(24)	52(3)	97(4)	52(3)	17(3)	-23(2)	-13(3)
C(37)	44(2)	70(3)	60(3)	-7(3)	-10(2)	3(2)
C(33)	61(3)	96(4)	40(2)	5(2)	3(2)	0(3)
C(34)	61(3)	107(5)	66(3)	13(3)	21(3)	-10(3)
C(35)	43(2)	73(3)	56(3)	0(2)	10(2)	-5(2)
C(38)	80(4)	151(6)	48(3)	7(3)	18(3)	-4(4)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 4q.

	x	y	z	U(eq)
H(13)	7	8576	1636	55
H(7)	1519	10558	-870	82
H(15)	-605	4702	931	59
H(8A)	-1052	6122	-800	94
H(8B)	-994	7971	-635	94
H(9A)	-729	5254	-19	61
H(9B)	-929	6889	224	61
H(10)	756	9779	-962	58
H(16)	-208	7751	2558	67
H(17)	-626	5457	2679	73
H(18)	-844	3975	1859	69
H(11)	1833	9743	23	75
H(12A)	-631	7702	-1425	86
H(12B)	-453	5981	-1247	86
H(20)	3285	4186	3417	60
H(21)	2372	7080	4098	64
H(22)	3571	3865	4350	71
H(36)	803	6960	1560	73
H(23)	2647	6650	5029	76
H(32)	1591	7101	1474	58
H(24)	3246	5020	5149	80
H(37)	565	5973	2473	70
H(34A)	3325	8084	1872	94
H(34B)	3610	6581	1699	94
H(35A)	3380	5071	2449	69
H(35B)	3407	6837	2728	69
H(38A)	3065	5290	1277	112
H(38B)	3071	7087	1033	112

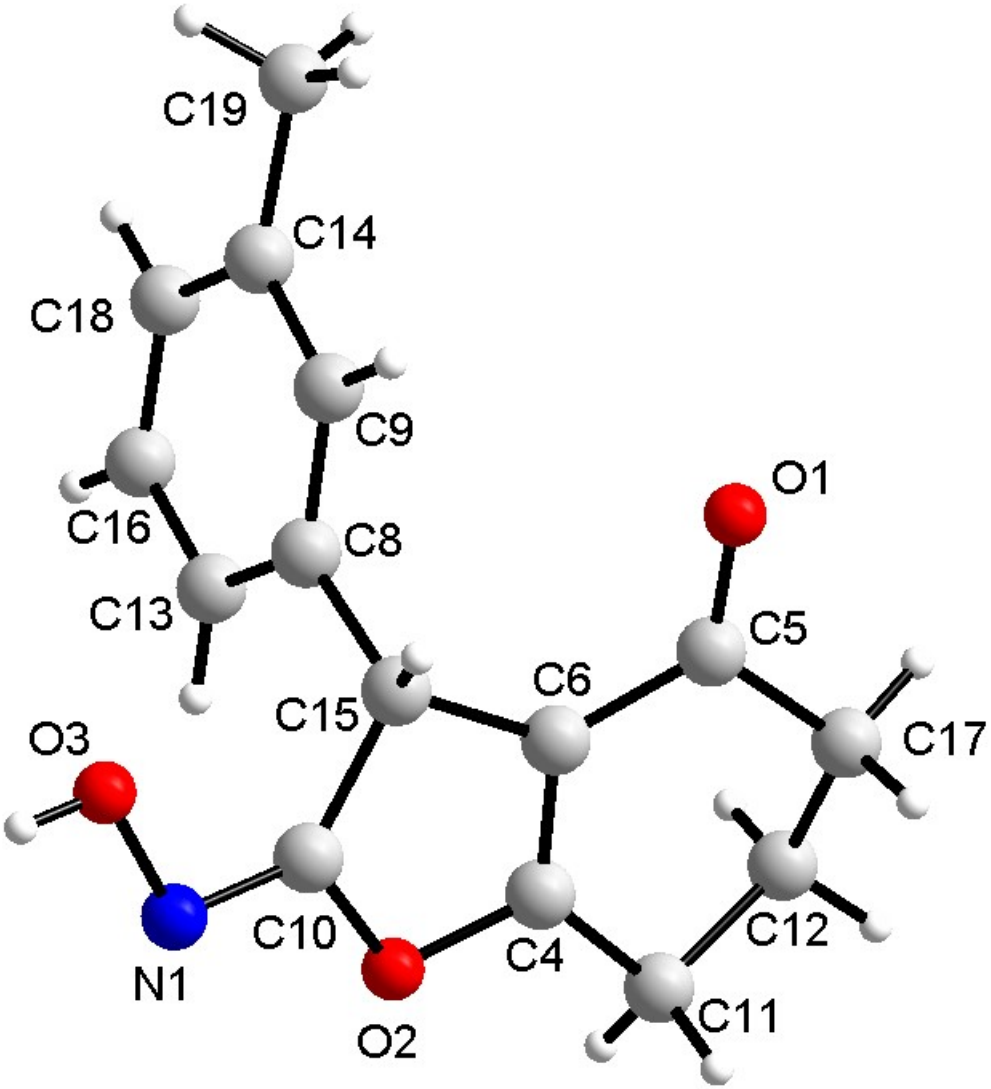


Table S11. Crystal data and structure refinement for 4h^{o}.

Identification code	4h^{o}
Empirical formula	C15 H15 N O3
Formula weight	257.28
Temperature	296 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.836(7) A alpha = 90 deg.

	b = 8.234(3) A beta = 117.679(17) deg. c = 13.790(10) A gamma = 90 deg.
Volume	1290.7(12) A^3
Z, Calculated density	4, 1.324 Mg/m^3
Absorption coefficient	0.093 mm^-1
F(000)	544
Crystal size	0.35 x 0.33 x 0.3 mm
Theta range for data collection	1.79 to 25.00 deg.
Limiting indices	-15<=h<=10, -8<=k<=9, -11<=l<=16
Reflections collected / unique	5381 / 2271 [R(int) = 0.0285]
Completeness to theta = 25.00	94.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2154 / 1 / 174
Goodness-of-fit on F^2	1.082
Final R indices [I>2sigma(I)]	R1 = 0.0595, wR2 = 0.1671
R indices (all data)	R1 = 0.0896, wR2 = 0.1884
Largest diff. peak and hole	0.597 and -0.255 e.A^-3

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 4h^{o}.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	3407(2)	-397(3)	1432(2)	55(1)
O(2)	3528(2)	-850(3)	4816(2)	58(1)
O(3)	2796(2)	3173(3)	4725(2)	67(1)
C(4)	3648(3)	-1620(4)	3992(2)	43(1)
C(5)	3574(2)	-1250(4)	2222(2)	40(1)
C(6)	3369(2)	-677(4)	3111(2)	38(1)
N(1)	3149(3)	1657(4)	5195(2)	60(1)
C(8)	1593(3)	1129(3)	2483(2)	40(1)
C(9)	1231(3)	1947(4)	1500(2)	47(1)
C(10)	3175(3)	710(4)	4460(2)	50(1)
C(11)	4049(3)	-3319(4)	4160(3)	53(1)
C(12)	3748(3)	-4055(4)	3051(3)	59(1)
C(13)	754(3)	392(4)	2697(3)	53(1)
C(14)	39(3)	2014(4)	723(2)	53(1)
C(15)	2905(3)	931(4)	3271(2)	42(1)
C(16)	-424(3)	473(5)	1945(3)	67(1)
C(17)	4083(3)	-2929(4)	2361(3)	56(1)
C(18)	-766(3)	1272(5)	975(3)	62(1)
C(19)	-347(4)	2813(6)	-381(3)	84(1)

Table S13. Bond lengths [A] and angles [deg] for 4h^{o}.

O(1)-C(5)	1.228(3)
O(2)-C(4)	1.371(4)
O(2)-C(10)	1.374(4)
O(3)-N(1)	1.383(4)
C(4)-C(6)	1.343(4)
C(4)-C(11)	1.471(5)
C(5)-C(6)	1.447(4)
C(5)-C(17)	1.503(4)
C(6)-C(15)	1.510(4)
N(1)-C(10)	1.292(4)
C(8)-C(13)	1.382(4)
C(8)-C(9)	1.386(4)
C(8)-C(15)	1.531(4)
C(9)-C(14)	1.403(4)
C(10)-C(15)	1.521(4)
C(11)-C(12)	1.519(5)
C(12)-C(17)	1.526(5)
C(13)-C(16)	1.382(5)
C(14)-C(18)	1.377(5)
C(14)-C(19)	1.515(5)
C(16)-C(18)	1.366(5)

C(4)-O(2)-C(10)	106.3(2)
C(6)-C(4)-O(2)	113.4(3)
C(6)-C(4)-C(11)	128.2(3)
O(2)-C(4)-C(11)	118.4(2)
O(1)-C(5)-C(6)	122.6(3)
O(1)-C(5)-C(17)	121.7(3)
C(6)-C(5)-C(17)	115.5(2)
C(4)-C(6)-C(5)	120.1(3)
C(4)-C(6)-C(15)	109.4(2)
C(5)-C(6)-C(15)	130.5(3)
C(10)-N(1)-O(3)	107.4(3)
C(13)-C(8)-C(9)	118.8(3)
C(13)-C(8)-C(15)	120.7(3)
C(9)-C(8)-C(15)	120.3(3)
C(8)-C(9)-C(14)	121.2(3)
N(1)-C(10)-O(2)	114.1(3)
N(1)-C(10)-C(15)	134.2(3)

O(2)-C(10)-C(15)	111.7(3)
C(4)-C(11)-C(12)	108.3(3)
C(11)-C(12)-C(17)	111.8(3)
C(8)-C(13)-C(16)	120.5(3)
C(18)-C(14)-C(9)	118.0(3)
C(18)-C(14)-C(19)	120.9(3)
C(9)-C(14)-C(19)	121.1(3)
C(6)-C(15)-C(10)	98.3(2)
C(6)-C(15)-C(8)	111.6(2)
C(10)-C(15)-C(8)	113.8(2)
C(18)-C(16)-C(13)	120.0(3)
C(5)-C(17)-C(12)	114.0(3)
C(16)-C(18)-C(14)	121.5(3)

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters (A^2 x 10^3) for 4h^{o}.
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
O(1)	70(2)	58(2)	41(1)	13(1)	31(1)	7(1)
O(2)	84(2)	58(2)	34(1)	5(1)	30(1)	12(1)
O(3)	85(2)	56(2)	56(2)	-7(1)	28(1)	3(1)
C(4)	52(2)	46(2)	32(2)	0(1)	21(1)	1(1)
C(5)	44(2)	45(2)	31(2)	3(1)	17(1)	0(1)
C(6)	46(2)	36(2)	34(2)	0(1)	19(1)	1(1)
N(1)	71(2)	53(2)	53(2)	-5(1)	27(1)	8(1)
C(8)	51(2)	30(2)	39(2)	-4(1)	21(1)	3(1)
C(9)	59(2)	39(2)	48(2)	-4(1)	29(2)	0(1)
C(10)	52(2)	57(2)	38(2)	-7(1)	17(1)	-3(2)
C(11)	65(2)	48(2)	50(2)	17(2)	31(2)	9(2)
C(12)	76(2)	36(2)	65(2)	2(2)	32(2)	6(2)
C(13)	57(2)	53(2)	48(2)	2(2)	25(2)	-5(2)
C(14)	67(2)	42(2)	43(2)	-4(1)	20(2)	8(2)
C(15)	48(2)	34(2)	43(2)	-3(1)	20(1)	-1(1)
C(16)	55(2)	77(3)	68(2)	-4(2)	29(2)	-13(2)
C(17)	80(2)	52(2)	42(2)	1(2)	33(2)	15(2)
C(18)	47(2)	69(3)	58(2)	-10(2)	15(2)	1(2)
C(19)	95(3)	82(3)	56(2)	10(2)	18(2)	12(2)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 4h^{o}.

	x	y	z	U(eq)
H(3)	2792	3807	5181	101
H(9)	1787	2461	1354	57
H(11A)	3663	-3922	4506	63
H(11B)	4892	-3365	4631	63
H(12A)	2910	-4276	2662	71
H(12B)	4160	-5079	3156	71
H(13)	984	-164	3352	63
H(15)	3359	1835	3196	51
H(16)	-984	-16	2098	80
H(17A)	4933	-2846	2701	68
H(17B)	3819	-3412	1643	68
H(18)	-1561	1315	475	74
H(19A)	-662	2005	-947	126
H(19B)	316	3330	-395	126
H(19C)	-941	3610	-501	126