

**A highly efficient and eco-friendly method for synthesis of
1,3-indandione ring-fused 3-oxindoles bearing two contiguous
quaternary stereocenters via Aldol reaction in aqueous media**

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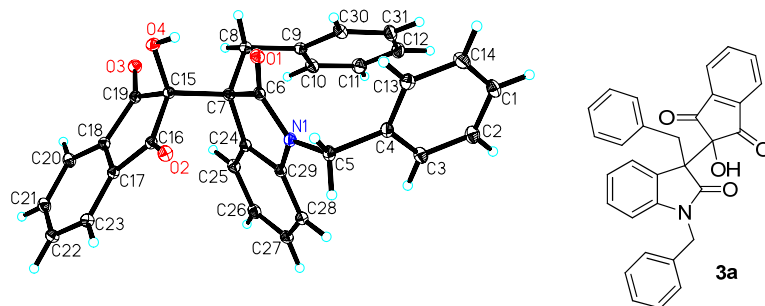
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1. X-Ray Crystal Datas for Compounds 3a



Crystal data for mo_3a: C₃₁H₂₃NO₄, $M = 473.50$, orthorhombic, $a = 10.516(3) \text{ \AA}$, $b = 16.680(4) \text{ \AA}$, $c = 27.091(6) \text{ \AA}$, $\alpha = 90.00^\circ$, $\beta = 90.00^\circ$, $\gamma = 90.00^\circ$, $V = 4752.2(19) \text{ \AA}^3$, $T = 100(2) \text{ K}$, space group $Pbca$, $Z = 8$, $\mu(\text{MoK}\alpha) = 0.088 \text{ mm}^{-1}$, 45752 reflections measured, 6304 independent reflections ($R_{int} = 0.0862$). The final R_1 values were 0.0513 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1302 ($I > 2\sigma(I)$). The final R_1 values were 0.0753 (all data). The final $wR(F^2)$ values were 0.1470 (all data). The goodness of fit on F^2 was 1.048.

Table 1. Crystal data and structure refinement for 3a.

Identification code	mo_3a_0m
Empirical formula	C ₃₁ H ₂₃ N O ₄
Formula weight	473.50
Temperature	100(2) K
Wavelength	0.71073 \AA
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 10.516(3) \AA alpha = 90 deg. b = 16.680(4) \AA beta = 90 deg. c = 27.091(6) \AA gamma = 90 deg.
Volume	4752.2(19) \AA ³
Z, Calculated density	8, 1.324 Mg/m ³
Absorption coefficient	0.088 mm ⁻¹
F(000)	1984
Crystal size	0.55 x 0.22 x 0.18 mm
Theta range for data collection	2.41 to 29.04 deg.
Limiting indices	-14<=h<=14, -22<=k<=22, -36<=l<=36
Reflections collected / unique	45752 / 6304 [R(int) = 0.0862]
Completeness to theta = 29.04	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9844 and 0.9534

Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6304 / 0 / 326
Goodness-of-fit on F ²	1.048
Final R indices [I>2σ(I)]	R1 = 0.0513, wR2 = 0.1302
R indices (all data)	R1 = 0.0753, wR2 = 0.1470
Largest diff. peak and hole	0.368 and -0.305 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **3a**.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	6656(1)	-937(1)	6072(1)	21(1)
O(2)	3892(1)	-1359(1)	5646(1)	22(1)
O(3)	3100(1)	-1138(1)	7368(1)	22(1)
O(4)	4855(1)	-1819(1)	6638(1)	21(1)
N(1)	5609(1)	184(1)	5775(1)	18(1)
C(1)	9654(2)	1834(1)	5563(1)	27(1)
C(2)	8448(2)	2172(1)	5525(1)	26(1)
C(3)	7388(2)	1682(1)	5454(1)	23(1)
C(4)	7532(2)	846(1)	5423(1)	20(1)
C(5)	6392(2)	305(1)	5332(1)	21(1)
C(6)	5827(1)	-418(1)	6106(1)	17(1)
C(7)	4850(1)	-344(1)	6532(1)	16(1)
C(8)	5575(2)	-212(1)	7025(1)	19(1)
C(9)	6328(2)	562(1)	7040(1)	19(1)
C(10)	5826(2)	1234(1)	7280(1)	24(1)
C(11)	6505(2)	1948(1)	7307(1)	29(1)
C(12)	7690(2)	2011(1)	7086(1)	30(1)
C(13)	8744(2)	516(1)	5466(1)	25(1)
C(14)	9804(2)	1007(1)	5536(1)	28(1)
C(15)	4069(1)	-1143(1)	6538(1)	17(1)
C(16)	3359(1)	-1257(1)	6041(1)	18(1)
C(17)	1973(2)	-1277(1)	6138(1)	17(1)
C(18)	1753(2)	-1255(1)	6649(1)	18(1)
C(19)	2966(2)	-1165(1)	6921(1)	18(1)
C(20)	523(2)	-1338(1)	6837(1)	22(1)
C(21)	-473(2)	-1420(1)	6502(1)	24(1)
C(22)	-246(2)	-1430(1)	5991(1)	23(1)
C(23)	979(2)	-1364(1)	5801(1)	21(1)
C(24)	4062(1)	369(1)	6366(1)	18(1)
C(25)	3041(2)	759(1)	6588(1)	22(1)

C(26)	2497(2)	1420(1)	6345(1)	25(1)
C(27)	2977(2)	1678(1)	5893(1)	26(1)
C(28)	4019(2)	1304(1)	5672(1)	23(1)
C(29)	4553(1)	655(1)	5918(1)	18(1)
C(30)	7529(2)	628(1)	6820(1)	24(1)
C(31)	8197(2)	1352(1)	6838(1)	29(1)

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

O(1)-C(6)	1.2317(19)
O(2)-C(16)	1.2212(19)
O(3)-C(19)	1.2217(19)
O(4)-C(15)	1.4243(18)
O(4)-H(4)	0.8400
N(1)-C(6)	1.366(2)
N(1)-C(29)	1.415(2)
N(1)-C(5)	1.470(2)
C(1)-C(14)	1.390(3)
C(1)-C(2)	1.392(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.396(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.405(2)
C(3)-H(3)	0.9500
C(4)-C(13)	1.393(2)
C(4)-C(5)	1.520(2)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.549(2)
C(7)-C(24)	1.517(2)
C(7)-C(8)	1.555(2)
C(7)-C(15)	1.565(2)
C(8)-C(9)	1.515(2)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.398(2)
C(9)-C(30)	1.400(2)
C(10)-C(11)	1.391(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.386(3)
C(11)-H(11)	0.9500
C(12)-C(31)	1.394(3)
C(12)-H(12)	0.9500

C(13)-C(14)	1.396(2)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(16)	1.552(2)
C(15)-C(19)	1.555(2)
C(16)-C(17)	1.482(2)
C(17)-C(23)	1.396(2)
C(17)-C(18)	1.402(2)
C(18)-C(20)	1.398(2)
C(18)-C(19)	1.481(2)
C(20)-C(21)	1.393(2)
C(20)-H(20)	0.9500
C(21)-C(22)	1.405(2)
C(21)-H(21)	0.9500
C(22)-C(23)	1.391(2)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-C(25)	1.392(2)
C(24)-C(29)	1.404(2)
C(25)-C(26)	1.405(2)
C(25)-H(25)	0.9500
C(26)-C(27)	1.394(3)
C(26)-H(26)	0.9500
C(27)-C(28)	1.395(2)
C(27)-H(27)	0.9500
C(28)-C(29)	1.390(2)
C(28)-H(28)	0.9500
C(30)-C(31)	1.399(2)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
C(15)-O(4)-H(4)	109.5
C(6)-N(1)-C(29)	111.10(13)
C(6)-N(1)-C(5)	122.95(13)
C(29)-N(1)-C(5)	125.95(13)
C(14)-C(1)-C(2)	120.10(16)
C(14)-C(1)-H(1)	119.9
C(2)-C(1)-H(1)	119.9
C(1)-C(2)-C(3)	120.02(16)
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	120.27(16)
C(2)-C(3)-H(3)	119.9
C(4)-C(3)-H(3)	119.9
C(13)-C(4)-C(3)	118.99(15)

C(13)-C(4)-C(5)	120.07(15)
C(3)-C(4)-C(5)	120.93(15)
N(1)-C(5)-C(4)	112.98(13)
N(1)-C(5)-H(5A)	109.0
C(4)-C(5)-H(5A)	109.0
N(1)-C(5)-H(5B)	109.0
C(4)-C(5)-H(5B)	109.0
H(5A)-C(5)-H(5B)	107.8
O(1)-C(6)-N(1)	125.88(15)
O(1)-C(6)-C(7)	125.49(14)
N(1)-C(6)-C(7)	108.62(13)
C(24)-C(7)-C(6)	101.82(12)
C(24)-C(7)-C(8)	114.16(13)
C(6)-C(7)-C(8)	109.02(12)
C(24)-C(7)-C(15)	112.64(12)
C(6)-C(7)-C(15)	106.81(12)
C(8)-C(7)-C(15)	111.61(12)
C(9)-C(8)-C(7)	113.63(13)
C(9)-C(8)-H(8A)	108.8
C(7)-C(8)-H(8A)	108.8
C(9)-C(8)-H(8B)	108.8
C(7)-C(8)-H(8B)	108.8
H(8A)-C(8)-H(8B)	107.7
C(10)-C(9)-C(30)	118.40(15)
C(10)-C(9)-C(8)	119.80(14)
C(30)-C(9)-C(8)	121.81(15)
C(11)-C(10)-C(9)	121.10(16)
C(11)-C(10)-H(10)	119.5
C(9)-C(10)-H(10)	119.5
C(12)-C(11)-C(10)	120.21(17)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(31)	119.53(16)
C(11)-C(12)-H(12)	120.2
C(31)-C(12)-H(12)	120.2
C(4)-C(13)-C(14)	120.75(16)
C(4)-C(13)-H(13)	119.6
C(14)-C(13)-H(13)	119.6
C(1)-C(14)-C(13)	119.85(16)
C(1)-C(14)-H(14)	120.1
C(13)-C(14)-H(14)	120.1
O(4)-C(15)-C(16)	110.25(12)
O(4)-C(15)-C(19)	106.79(12)
C(16)-C(15)-C(19)	102.50(12)

O(4)-C(15)-C(7)	111.83(12)
C(16)-C(15)-C(7)	110.25(12)
C(19)-C(15)-C(7)	114.78(12)
O(2)-C(16)-C(17)	127.17(14)
O(2)-C(16)-C(15)	123.94(14)
C(17)-C(16)-C(15)	108.76(13)
C(23)-C(17)-C(18)	121.66(15)
C(23)-C(17)-C(16)	128.50(14)
C(18)-C(17)-C(16)	109.68(13)
C(20)-C(18)-C(17)	120.70(15)
C(20)-C(18)-C(19)	128.72(15)
C(17)-C(18)-C(19)	110.55(14)
O(3)-C(19)-C(18)	126.64(15)
O(3)-C(19)-C(15)	125.03(14)
C(18)-C(19)-C(15)	108.29(13)
C(21)-C(20)-C(18)	117.85(16)
C(21)-C(20)-H(20)	121.1
C(18)-C(20)-H(20)	121.1
C(20)-C(21)-C(22)	121.04(15)
C(20)-C(21)-H(21)	119.5
C(22)-C(21)-H(21)	119.5
C(23)-C(22)-C(21)	121.42(15)
C(23)-C(22)-H(22)	119.3
C(21)-C(22)-H(22)	119.3
C(22)-C(23)-C(17)	117.31(15)
C(22)-C(23)-H(23)	121.3
C(17)-C(23)-H(23)	121.3
C(25)-C(24)-C(29)	119.85(15)
C(25)-C(24)-C(7)	131.36(15)
C(29)-C(24)-C(7)	108.75(13)
C(24)-C(25)-C(26)	118.65(16)
C(24)-C(25)-H(25)	120.7
C(26)-C(25)-H(25)	120.7
C(27)-C(26)-C(25)	120.37(16)
C(27)-C(26)-H(26)	119.8
C(25)-C(26)-H(26)	119.8
C(26)-C(27)-C(28)	121.68(16)
C(26)-C(27)-H(27)	119.2
C(28)-C(27)-H(27)	119.2
C(29)-C(28)-C(27)	117.26(16)
C(29)-C(28)-H(28)	121.4
C(27)-C(28)-H(28)	121.4
C(28)-C(29)-C(24)	122.13(15)
C(28)-C(29)-N(1)	128.20(15)

C(24)-C(29)-N(1)	109.67(13)
C(31)-C(30)-C(9)	120.40(16)
C(31)-C(30)-H(30)	119.8
C(9)-C(30)-H(30)	119.8
C(12)-C(31)-C(30)	120.33(17)
C(12)-C(31)-H(31)	119.8
C(30)-C(31)-H(31)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **3a**.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U11 + \dots + 2 h k a^* b^* U12]$$

	U11	U22	U33	U23	U13	U12
O(1)	17(1)	20(1)	26(1)	-1(1)	0(1)	2(1)
O(2)	21(1)	24(1)	20(1)	-2(1)	2(1)	-1(1)
O(3)	23(1)	26(1)	18(1)	1(1)	0(1)	-2(1)
O(4)	18(1)	18(1)	27(1)	4(1)	1(1)	3(1)
N(1)	17(1)	18(1)	21(1)	1(1)	1(1)	-2(1)
C(1)	21(1)	30(1)	29(1)	-4(1)	-2(1)	-7(1)
C(2)	28(1)	20(1)	31(1)	-4(1)	0(1)	-4(1)
C(3)	19(1)	22(1)	28(1)	-4(1)	2(1)	-1(1)
C(4)	20(1)	21(1)	18(1)	0(1)	1(1)	-4(1)
C(5)	20(1)	23(1)	19(1)	0(1)	2(1)	-6(1)
C(6)	15(1)	17(1)	20(1)	-1(1)	-2(1)	-2(1)
C(7)	15(1)	16(1)	19(1)	0(1)	0(1)	0(1)
C(8)	19(1)	20(1)	19(1)	1(1)	-2(1)	-1(1)
C(9)	19(1)	21(1)	17(1)	1(1)	-3(1)	-1(1)
C(10)	20(1)	24(1)	28(1)	-4(1)	0(1)	-2(1)
C(11)	32(1)	22(1)	35(1)	-5(1)	-5(1)	-1(1)
C(12)	33(1)	27(1)	30(1)	4(1)	-8(1)	-11(1)
C(13)	25(1)	22(1)	27(1)	1(1)	-2(1)	-1(1)
C(14)	20(1)	30(1)	35(1)	-1(1)	-3(1)	0(1)
C(15)	15(1)	15(1)	20(1)	1(1)	0(1)	1(1)
C(16)	17(1)	14(1)	22(1)	2(1)	-1(1)	0(1)
C(17)	18(1)	15(1)	19(1)	0(1)	0(1)	-1(1)
C(18)	18(1)	16(1)	21(1)	0(1)	1(1)	-1(1)
C(19)	18(1)	15(1)	20(1)	1(1)	0(1)	-1(1)
C(20)	18(1)	24(1)	24(1)	-2(1)	3(1)	-1(1)
C(21)	17(1)	25(1)	29(1)	-1(1)	2(1)	-2(1)
C(22)	19(1)	22(1)	28(1)	1(1)	-5(1)	-1(1)
C(23)	21(1)	21(1)	22(1)	1(1)	-2(1)	0(1)

C(24)	16(1)	16(1)	22(1)	0(1)	-2(1)	-1(1)
C(25)	19(1)	20(1)	27(1)	-3(1)	0(1)	-1(1)
C(26)	18(1)	20(1)	38(1)	-4(1)	-2(1)	2(1)
C(27)	21(1)	18(1)	40(1)	4(1)	-9(1)	0(1)
C(28)	20(1)	20(1)	28(1)	4(1)	-4(1)	-3(1)
C(29)	17(1)	16(1)	22(1)	-1(1)	-2(1)	-2(1)
C(30)	19(1)	28(1)	23(1)	-4(1)	-2(1)	-2(1)
C(31)	23(1)	38(1)	25(1)	2(1)	-2(1)	-11(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**.

	x	y	z	U(eq)
H(4)	5521	-1790	6467	31
H(1)	10376	2169	5608	32
H(2)	8347	2737	5547	32
H(3)	6567	1914	5427	28
H(5A)	5859	544	5069	25
H(5B)	6696	-222	5212	25
H(8A)	4954	-210	7299	23
H(8B)	6163	-667	7078	23
H(10)	5008	1201	7427	29
H(11)	6156	2394	7477	35
H(12)	8153	2499	7104	36
H(13)	8850	-48	5447	30
H(14)	10627	776	5565	34
H(20)	371	-1340	7183	26
H(21)	-1320	-1470	6621	29
H(22)	-943	-1483	5771	28
H(23)	1132	-1377	5455	26
H(25)	2719	583	6897	26
H(26)	1798	1693	6491	30
H(27)	2585	2118	5731	32
H(28)	4350	1487	5365	27
H(30)	7892	178	6658	28
H(31)	9001	1396	6680	34

Table 6. Torsion angles [deg] for **3a**.

C(14)-C(1)-C(2)-C(3)	-0.7(3)
C(1)-C(2)-C(3)-C(4)	0.2(3)
C(2)-C(3)-C(4)-C(13)	0.3(2)
C(2)-C(3)-C(4)-C(5)	-178.27(15)
C(6)-N(1)-C(5)-C(4)	-88.88(18)
C(29)-N(1)-C(5)-C(4)	91.20(18)
C(13)-C(4)-C(5)-N(1)	104.18(17)
C(3)-C(4)-C(5)-N(1)	-77.31(19)
C(29)-N(1)-C(6)-O(1)	177.76(14)
C(5)-N(1)-C(6)-O(1)	-2.2(2)
C(29)-N(1)-C(6)-C(7)	-1.91(17)
C(5)-N(1)-C(6)-C(7)	178.16(13)
O(1)-C(6)-C(7)-C(24)	-177.97(14)
N(1)-C(6)-C(7)-C(24)	1.71(15)
O(1)-C(6)-C(7)-C(8)	61.06(19)
N(1)-C(6)-C(7)-C(8)	-119.26(13)
O(1)-C(6)-C(7)-C(15)	-59.67(19)
N(1)-C(6)-C(7)-C(15)	120.00(13)
C(24)-C(7)-C(8)-C(9)	-49.85(18)
C(6)-C(7)-C(8)-C(9)	63.24(16)
C(15)-C(7)-C(8)-C(9)	-179.01(12)
C(7)-C(8)-C(9)-C(10)	99.41(18)
C(7)-C(8)-C(9)-C(30)	-80.89(19)
C(30)-C(9)-C(10)-C(11)	-0.8(2)
C(8)-C(9)-C(10)-C(11)	178.89(15)
C(9)-C(10)-C(11)-C(12)	1.2(3)
C(10)-C(11)-C(12)-C(31)	-0.1(3)
C(3)-C(4)-C(13)-C(14)	-0.3(3)
C(5)-C(4)-C(13)-C(14)	178.21(15)
C(2)-C(1)-C(14)-C(13)	0.6(3)
C(4)-C(13)-C(14)-C(1)	-0.1(3)
C(24)-C(7)-C(15)-O(4)	173.12(12)
C(6)-C(7)-C(15)-O(4)	62.15(15)
C(8)-C(7)-C(15)-O(4)	-56.92(16)
C(24)-C(7)-C(15)-C(16)	50.08(16)
C(6)-C(7)-C(15)-C(16)	-60.89(15)
C(8)-C(7)-C(15)-C(16)	-179.96(12)
C(24)-C(7)-C(15)-C(19)	-65.03(17)
C(6)-C(7)-C(15)-C(19)	-176.00(12)
C(8)-C(7)-C(15)-C(19)	64.93(16)
O(4)-C(15)-C(16)-O(2)	-58.67(19)

C(19)-C(15)-C(16)-O(2)	-172.07(14)
C(7)-C(15)-C(16)-O(2)	65.29(18)
O(4)-C(15)-C(16)-C(17)	117.40(13)
C(19)-C(15)-C(16)-C(17)	4.00(15)
C(7)-C(15)-C(16)-C(17)	-118.63(13)
O(2)-C(16)-C(17)-C(23)	-4.5(3)
C(15)-C(16)-C(17)-C(23)	179.61(15)
O(2)-C(16)-C(17)-C(18)	170.95(15)
C(15)-C(16)-C(17)-C(18)	-4.97(17)
C(23)-C(17)-C(18)-C(20)	1.5(2)
C(16)-C(17)-C(18)-C(20)	-174.33(14)
C(23)-C(17)-C(18)-C(19)	179.58(14)
C(16)-C(17)-C(18)-C(19)	3.78(17)
C(20)-C(18)-C(19)-O(3)	-0.9(3)
C(17)-C(18)-C(19)-O(3)	-178.86(15)
C(20)-C(18)-C(19)-C(15)	176.81(16)
C(17)-C(18)-C(19)-C(15)	-1.11(17)
O(4)-C(15)-C(19)-O(3)	60.05(19)
C(16)-C(15)-C(19)-O(3)	175.98(15)
C(7)-C(15)-C(19)-O(3)	-64.50(19)
O(4)-C(15)-C(19)-C(18)	-117.74(13)
C(16)-C(15)-C(19)-C(18)	-1.82(15)
C(7)-C(15)-C(19)-C(18)	117.70(14)
C(17)-C(18)-C(20)-C(21)	-1.8(2)
C(19)-C(18)-C(20)-C(21)	-179.56(15)
C(18)-C(20)-C(21)-C(22)	0.9(2)
C(20)-C(21)-C(22)-C(23)	0.4(3)
C(21)-C(22)-C(23)-C(17)	-0.8(2)
C(18)-C(17)-C(23)-C(22)	-0.1(2)
C(16)-C(17)-C(23)-C(22)	174.81(15)
C(6)-C(7)-C(24)-C(25)	-178.52(16)
C(8)-C(7)-C(24)-C(25)	-61.2(2)
C(15)-C(7)-C(24)-C(25)	67.4(2)
C(6)-C(7)-C(24)-C(29)	-0.93(15)
C(8)-C(7)-C(24)-C(29)	116.39(15)
C(15)-C(7)-C(24)-C(29)	-114.97(14)
C(29)-C(24)-C(25)-C(26)	2.2(2)
C(7)-C(24)-C(25)-C(26)	179.53(16)
C(24)-C(25)-C(26)-C(27)	-0.2(2)
C(25)-C(26)-C(27)-C(28)	-1.3(3)
C(26)-C(27)-C(28)-C(29)	0.9(2)
C(27)-C(28)-C(29)-C(24)	1.2(2)
C(27)-C(28)-C(29)-N(1)	-179.43(15)
C(25)-C(24)-C(29)-C(28)	-2.7(2)

C(7)-C(24)-C(29)-C(28)	179.39(14)
C(25)-C(24)-C(29)-N(1)	177.79(14)
C(7)-C(24)-C(29)-N(1)	-0.12(17)
C(6)-N(1)-C(29)-C(28)	-178.16(15)
C(5)-N(1)-C(29)-C(28)	1.8(3)
C(6)-N(1)-C(29)-C(24)	1.32(17)
C(5)-N(1)-C(29)-C(24)	-178.76(14)
C(10)-C(9)-C(30)-C(31)	-0.6(2)
C(8)-C(9)-C(30)-C(31)	179.65(15)
C(11)-C(12)-C(31)-C(30)	-1.3(3)
C(9)-C(30)-C(31)-C(12)	1.7(3)

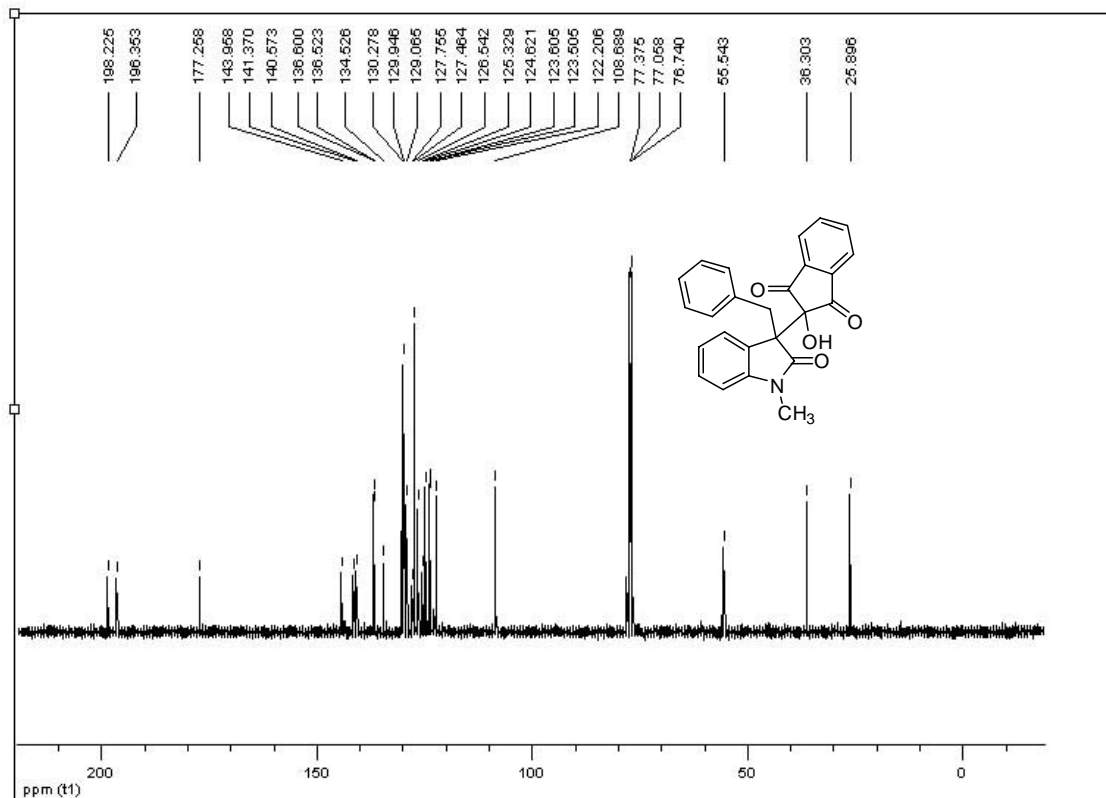
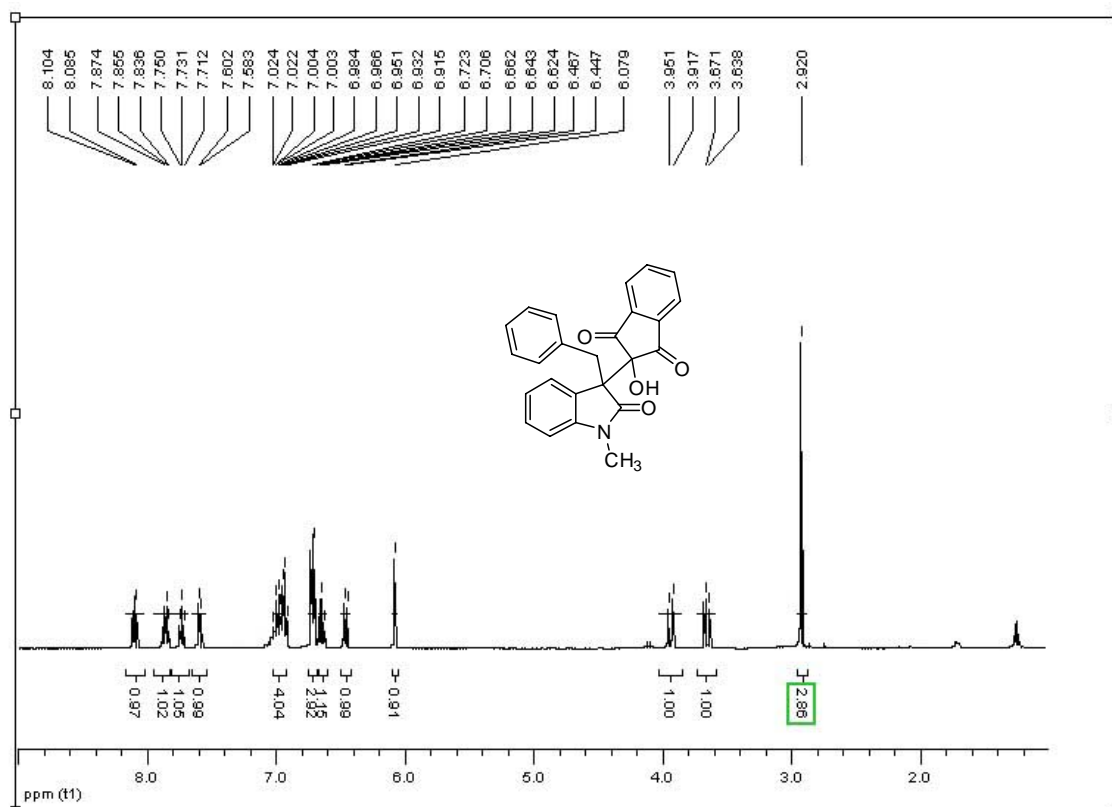
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **3a** [Å and deg.].

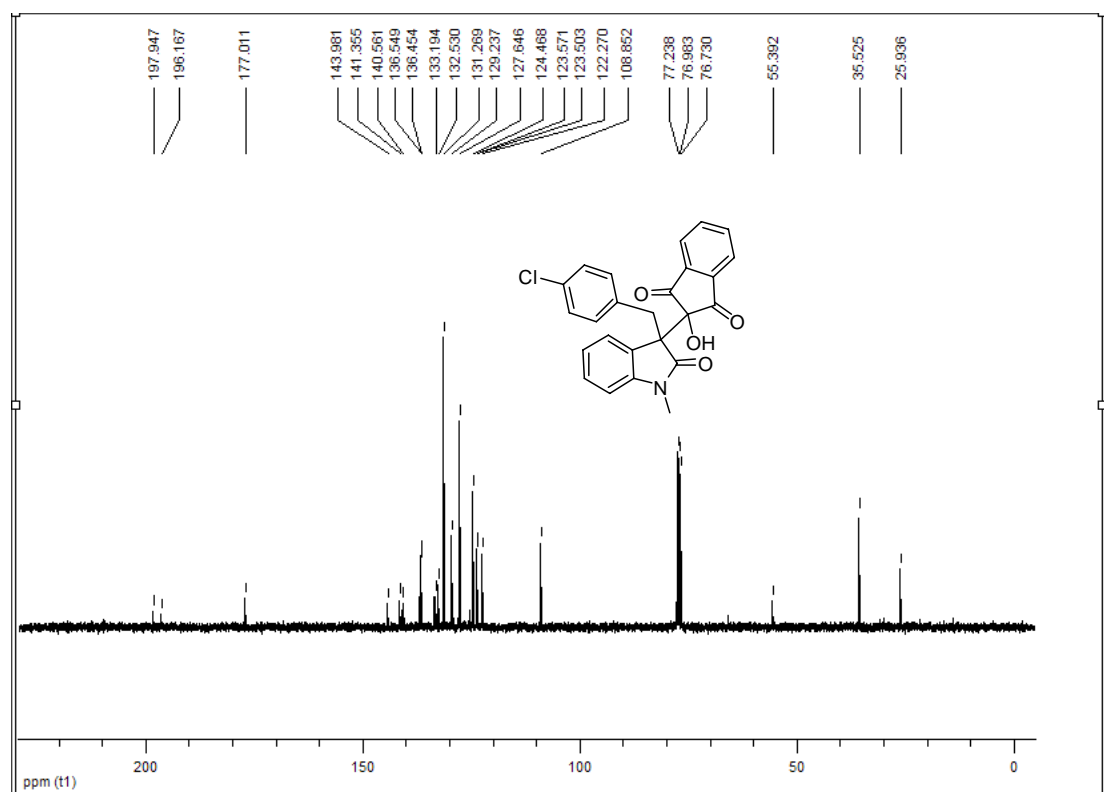
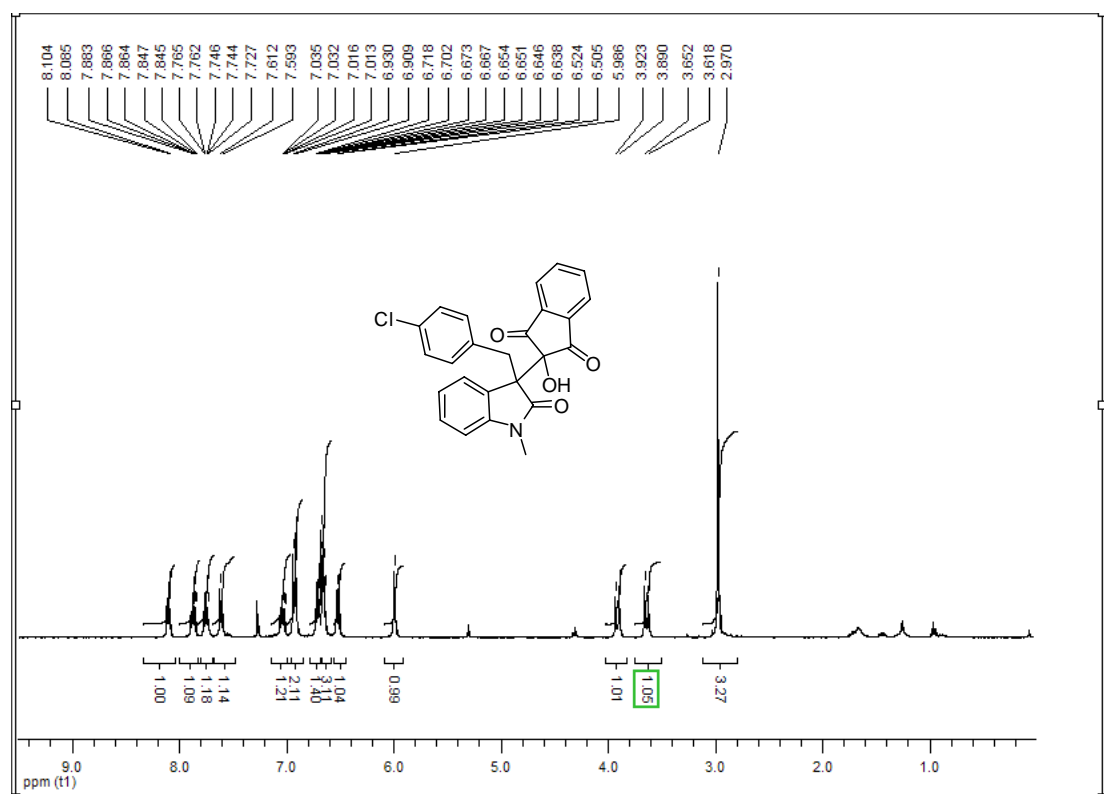
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4)...O(1)	0.84	2.14	2.8460(16)	141.0

Symmetry transformations used to generate equivalent atoms:

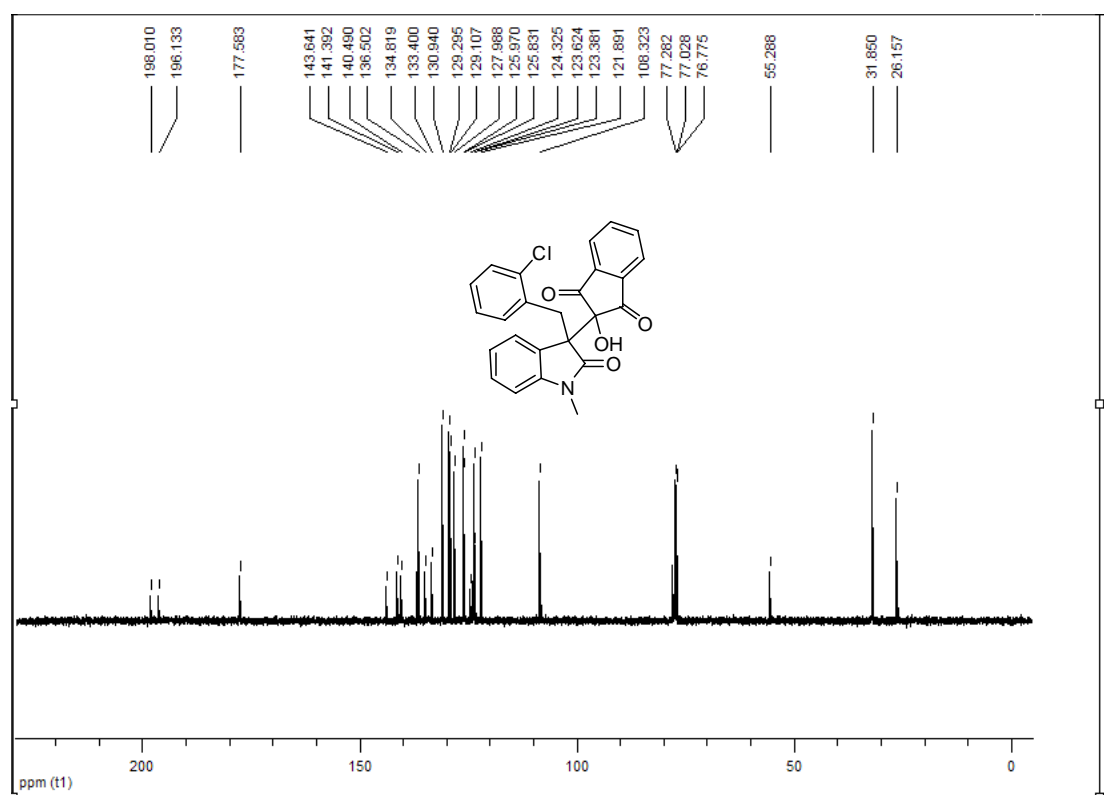
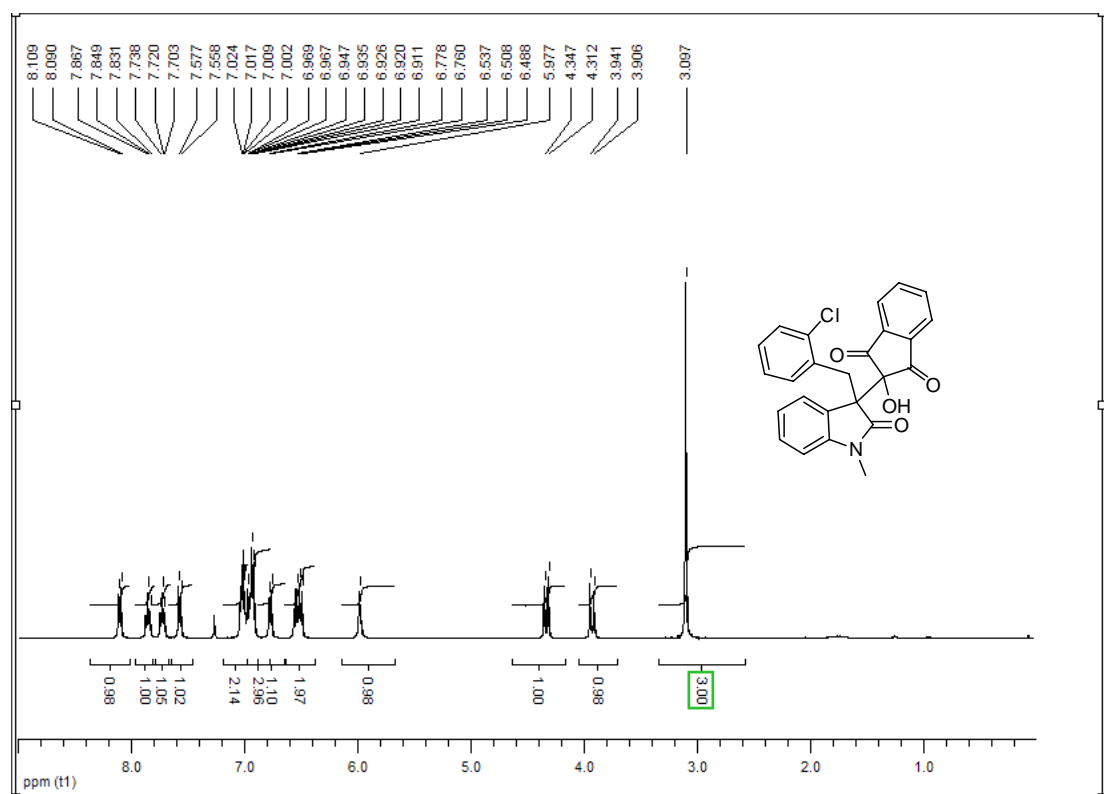
¹H and ¹³C NMR of 3b



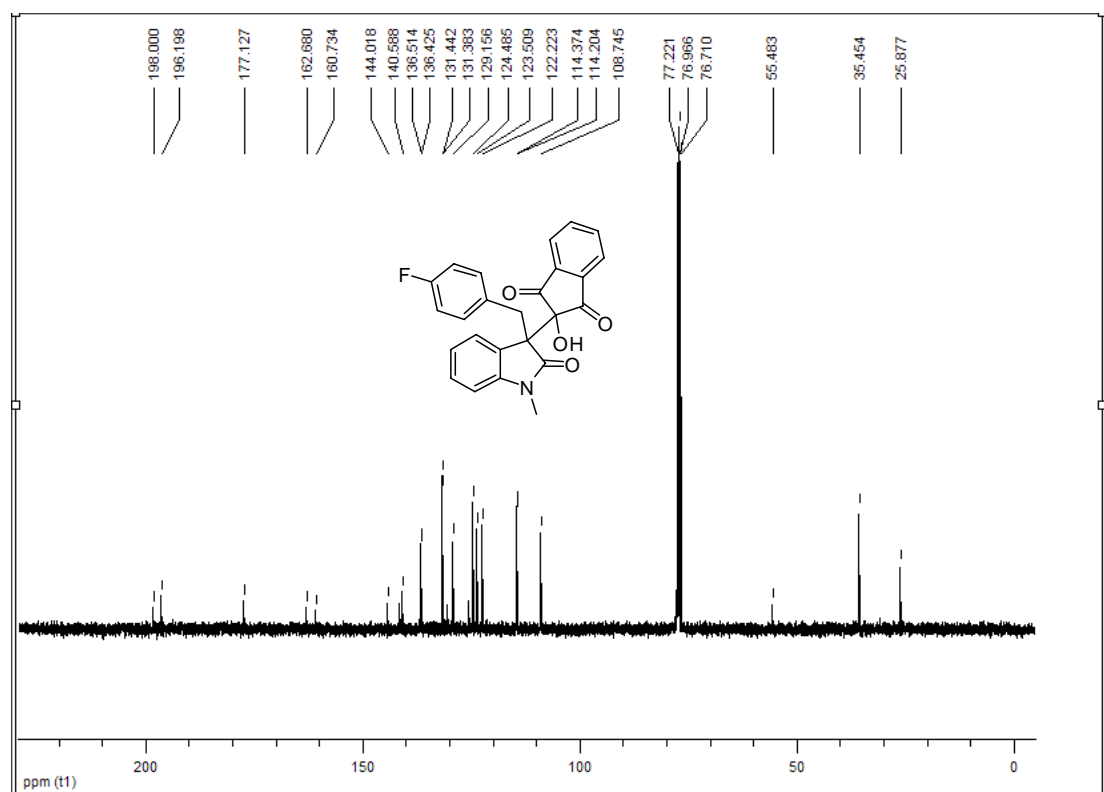
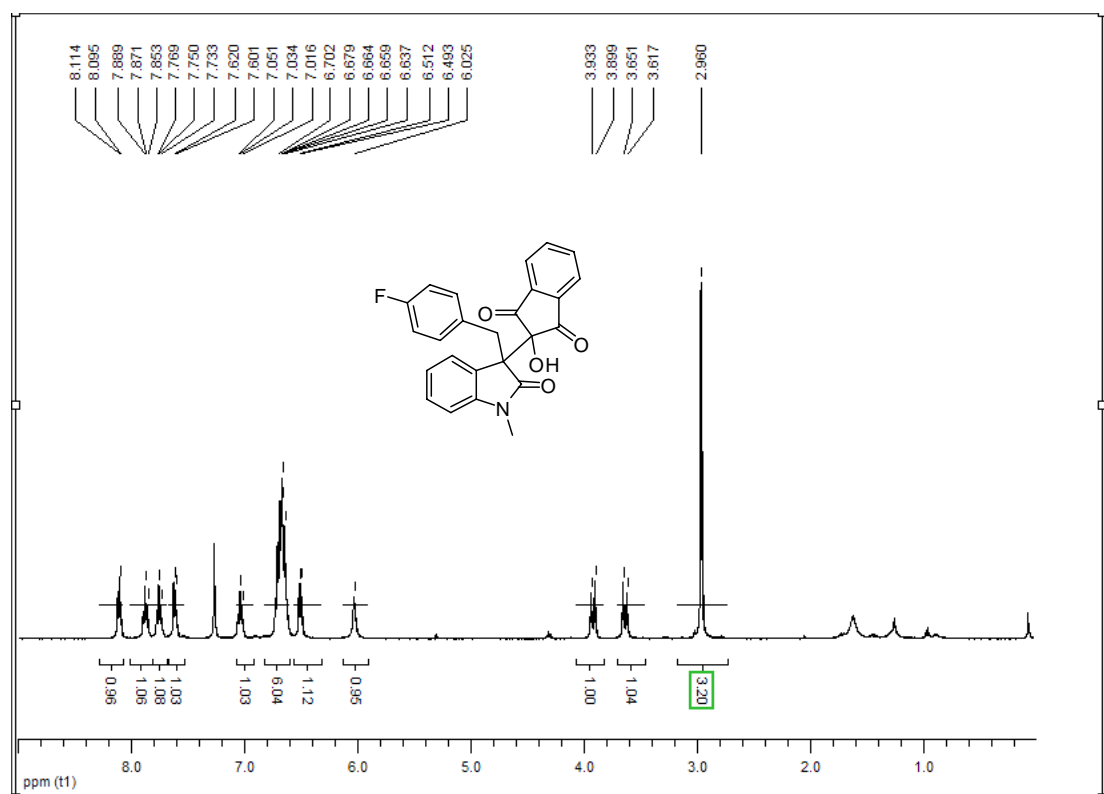
¹H and ¹³C NMR of 3e



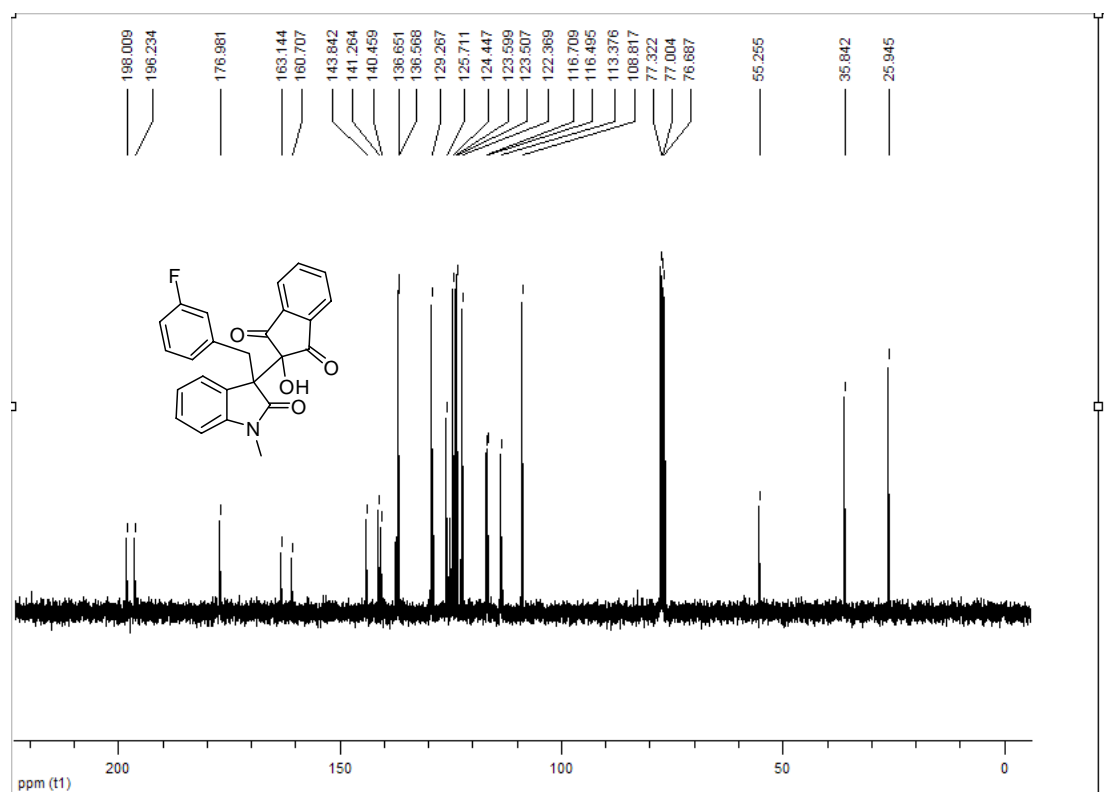
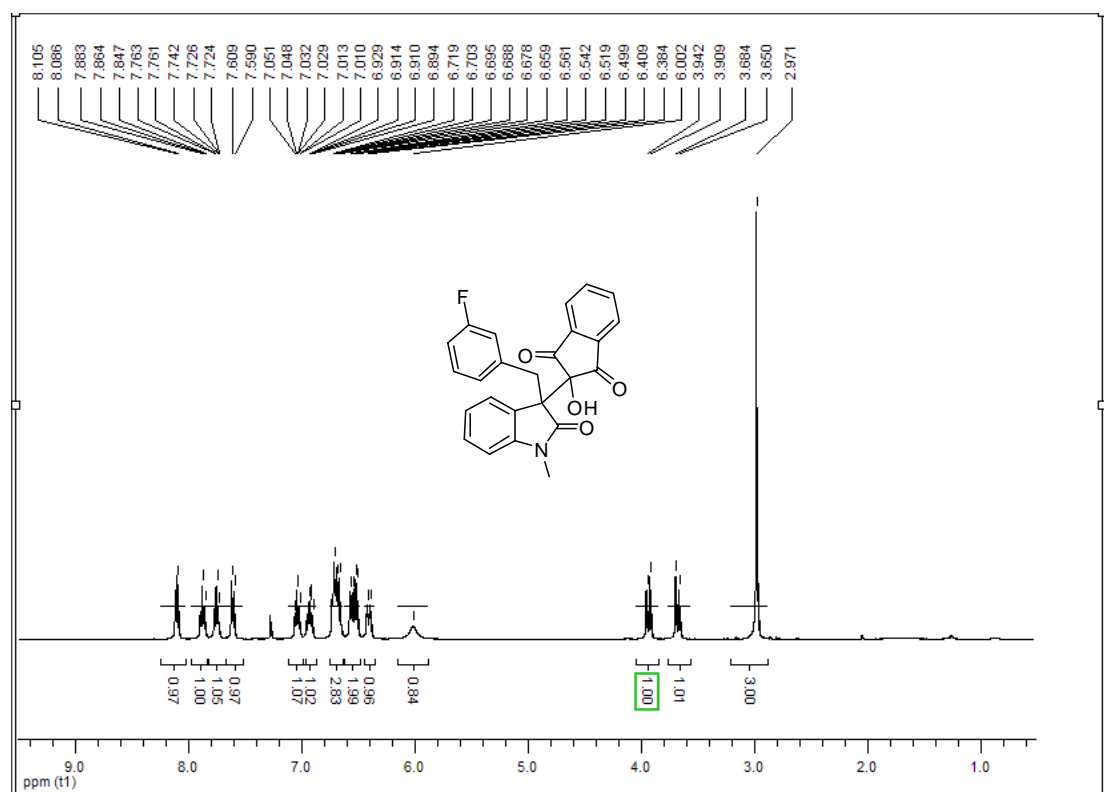
^1H and ^{13}C NMR of 3f



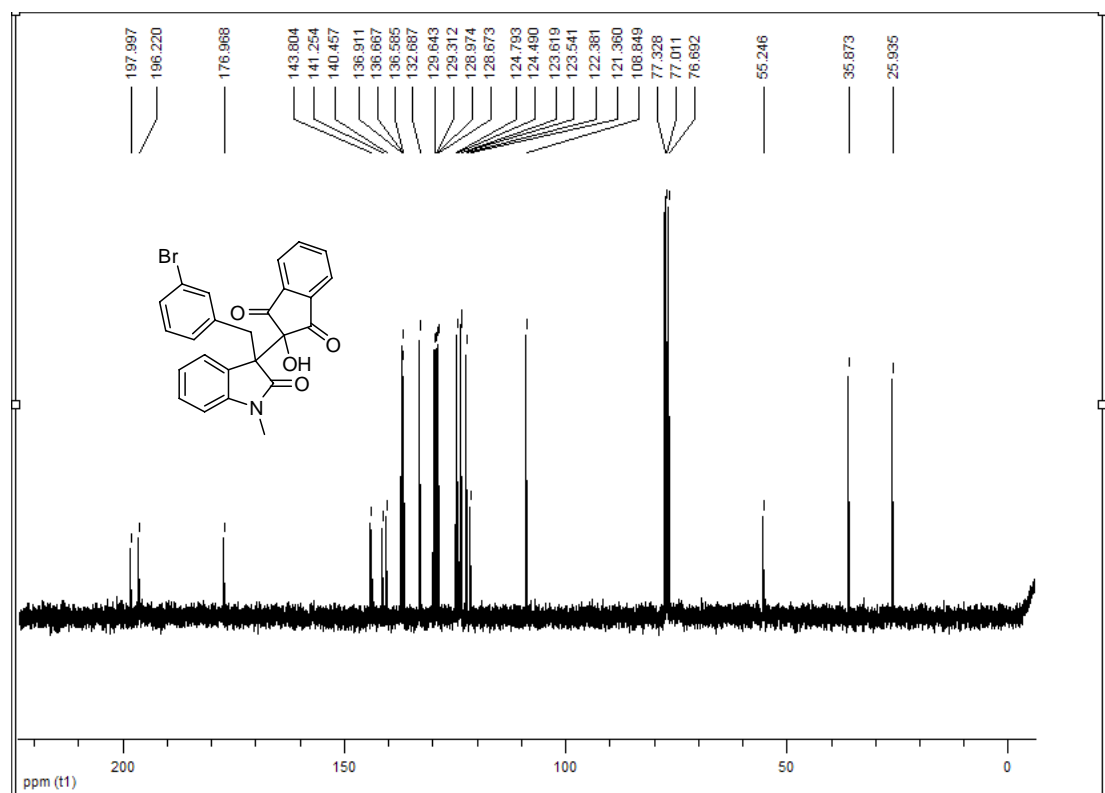
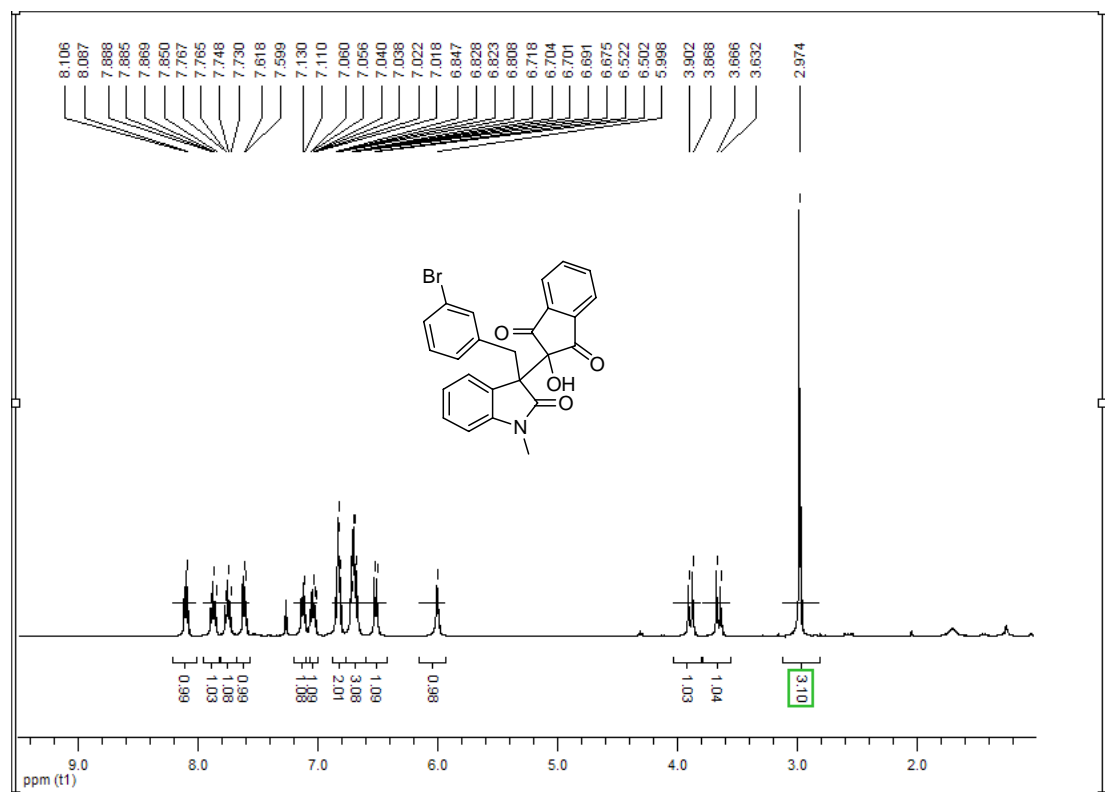
¹H and ¹³C NMR of 3g



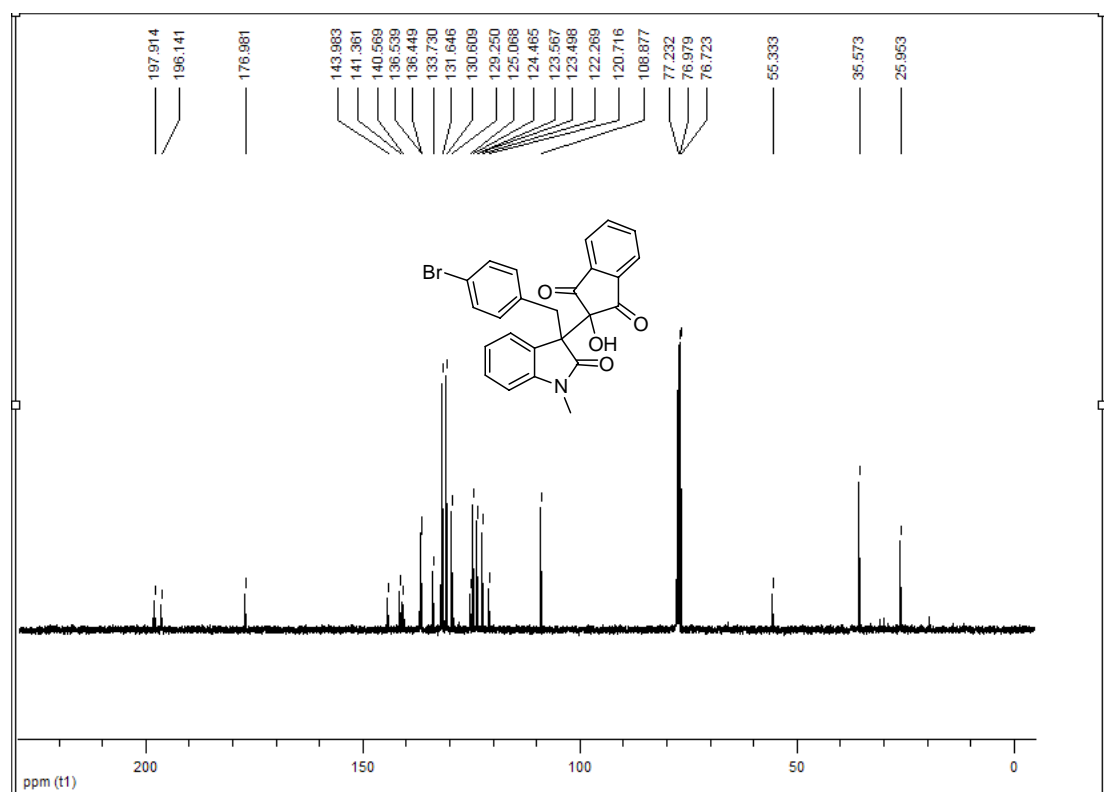
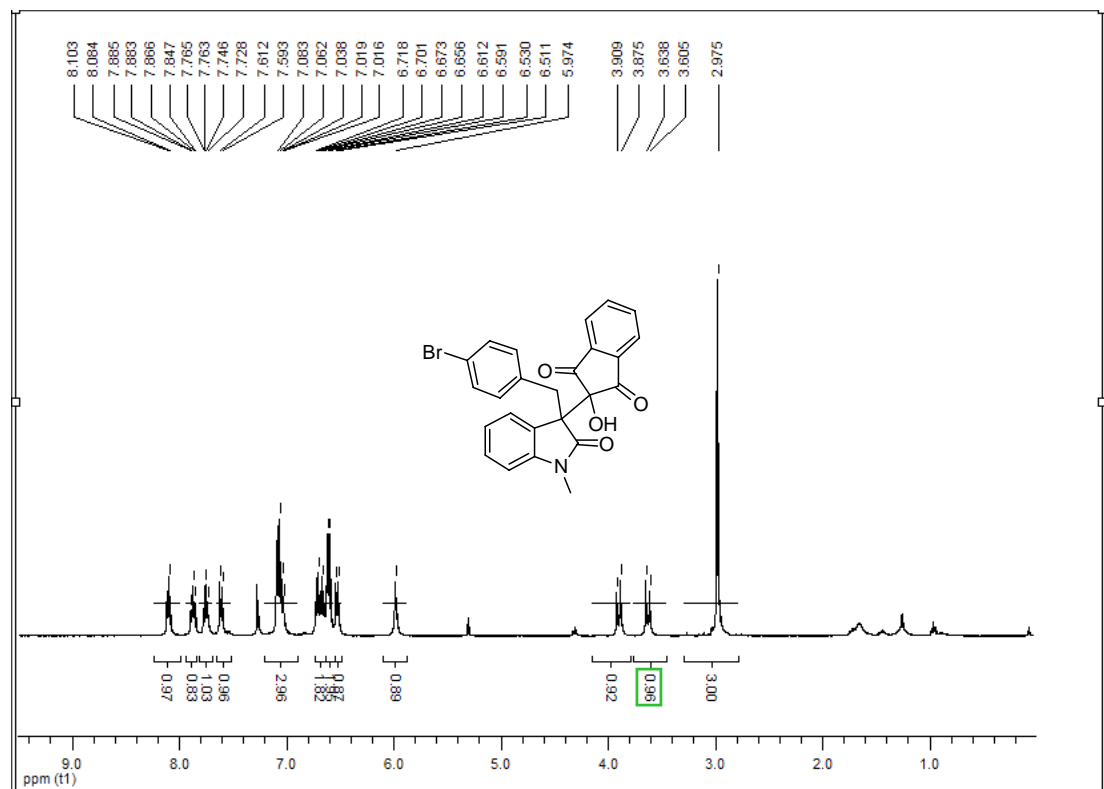
¹H and ¹³C NMR of 3h



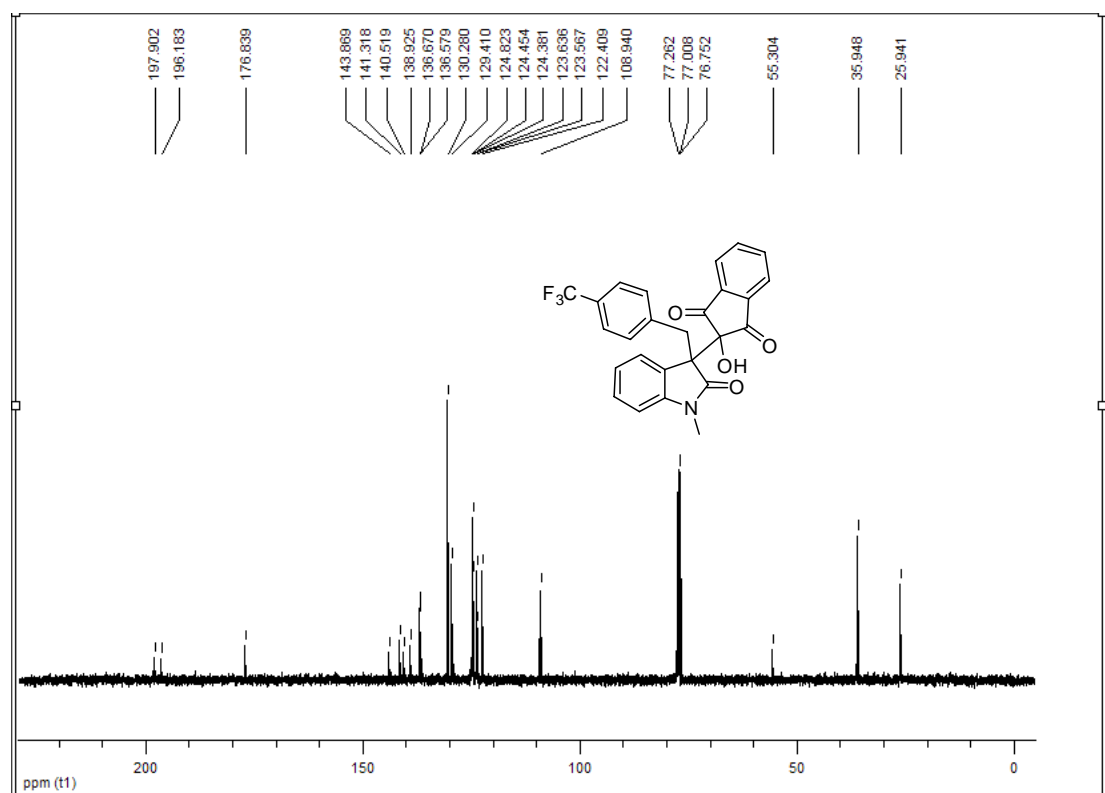
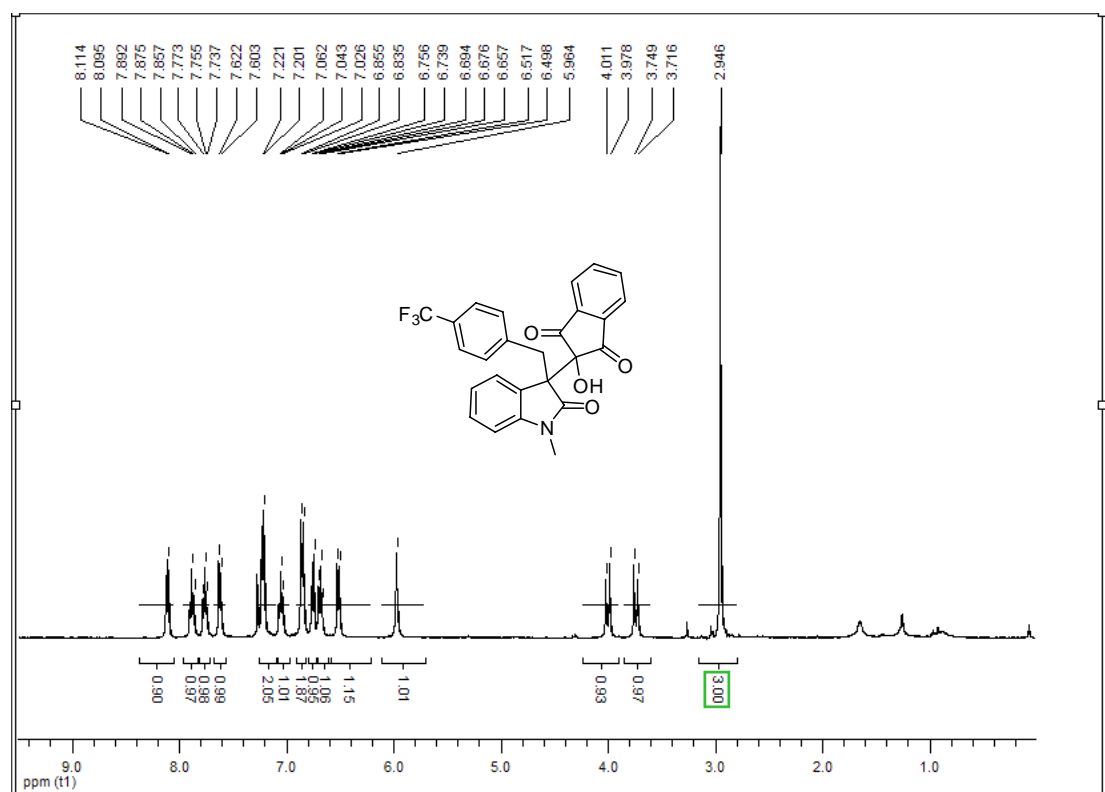
^1H and ^{13}C NMR of 3j



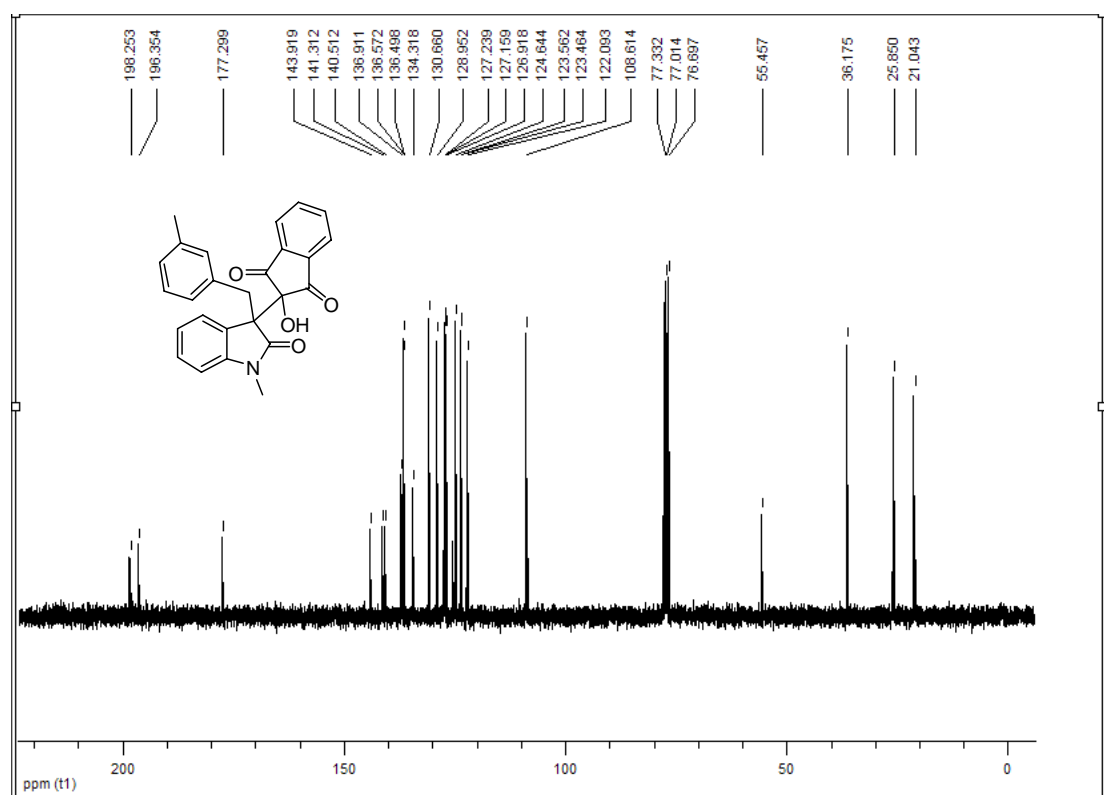
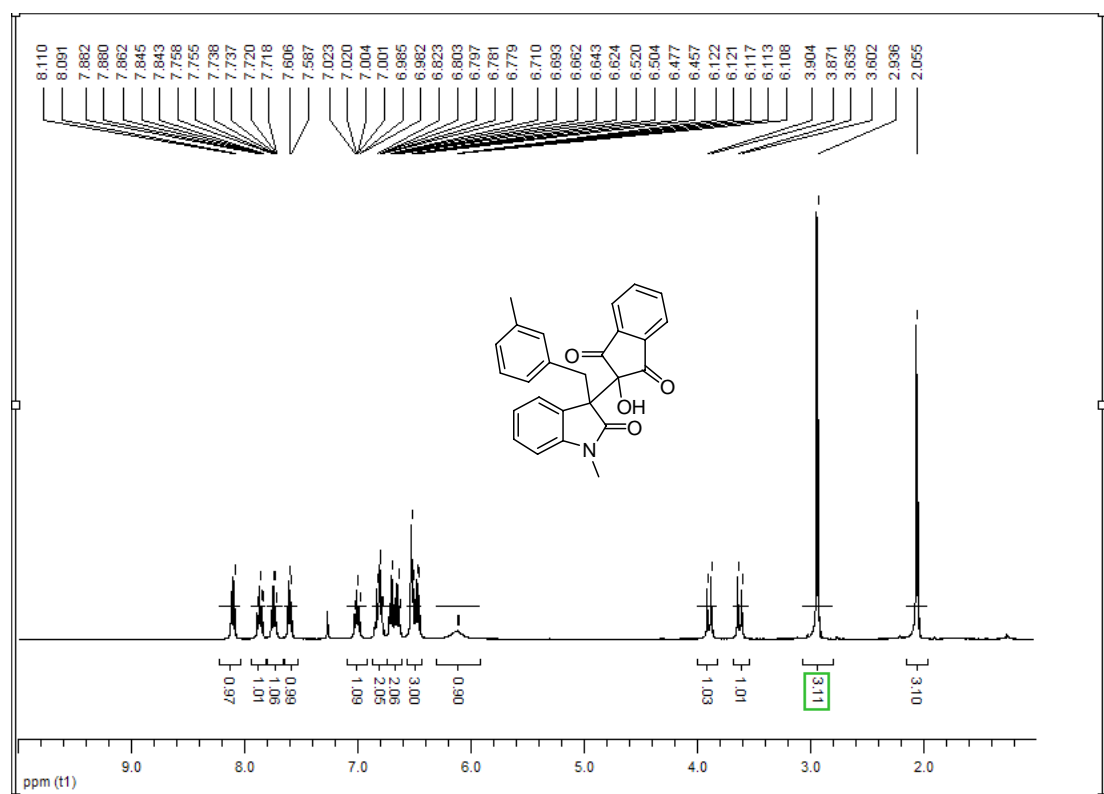
¹H and ¹³C NMR of 3k



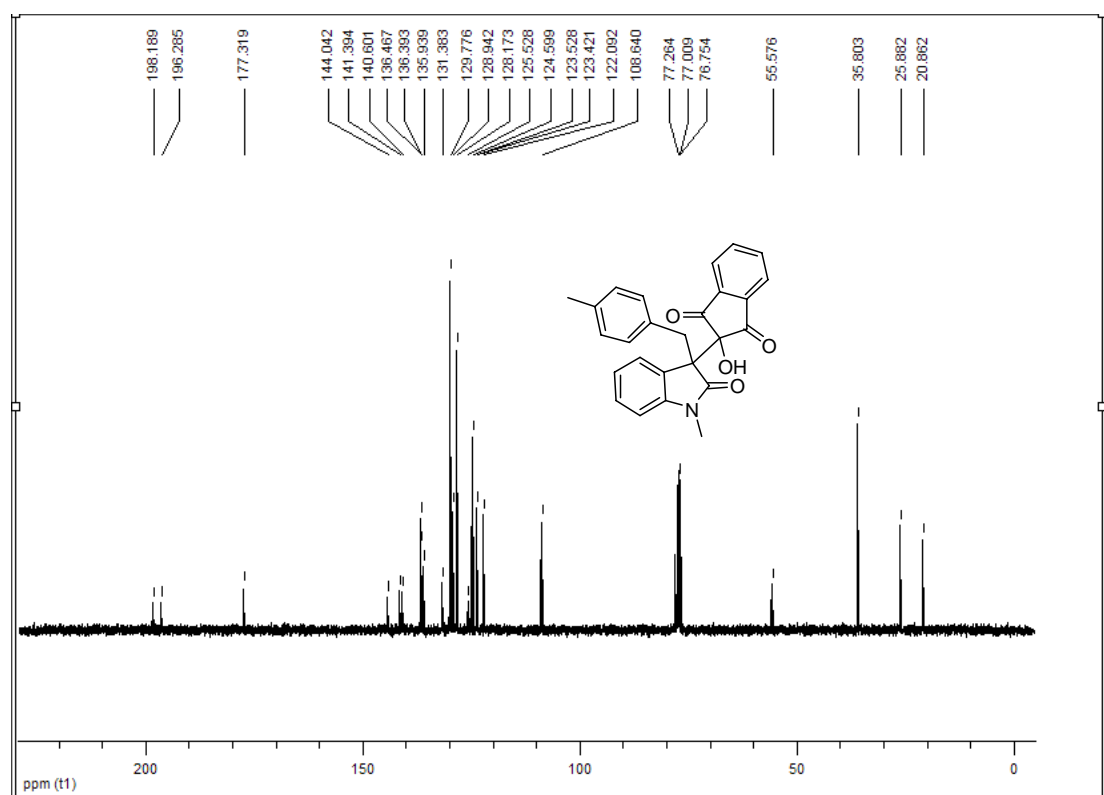
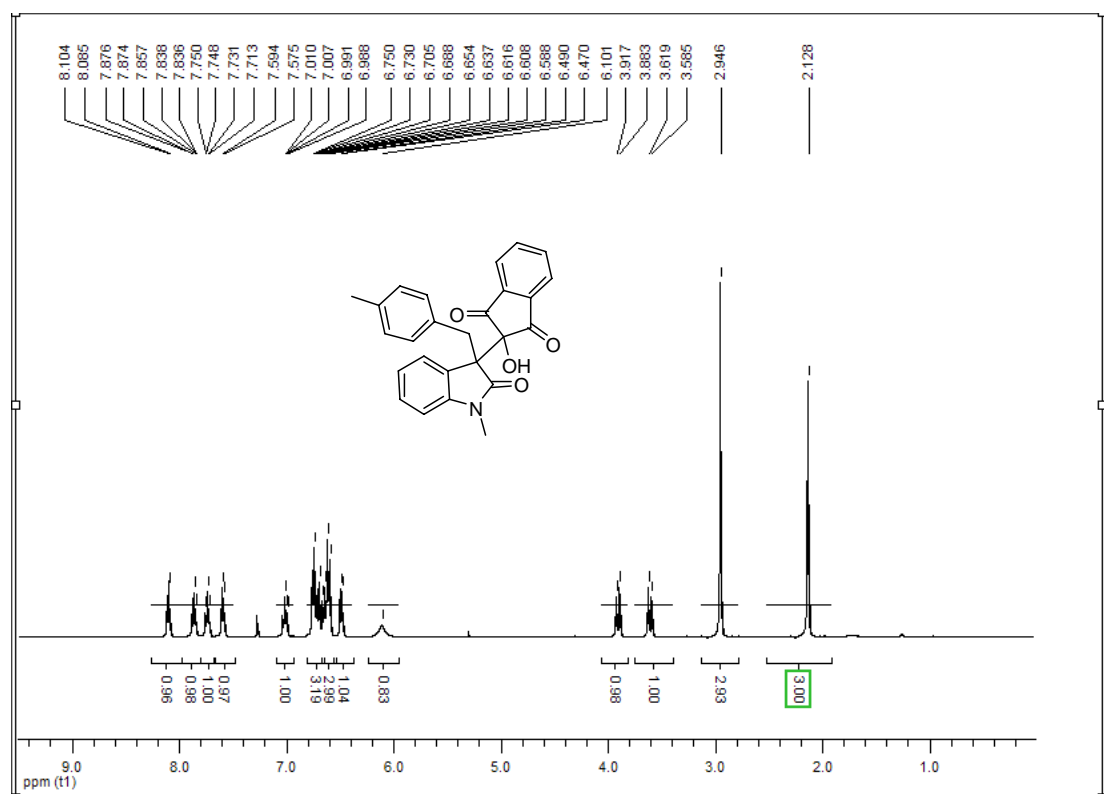
^1H and ^{13}C NMR of 31



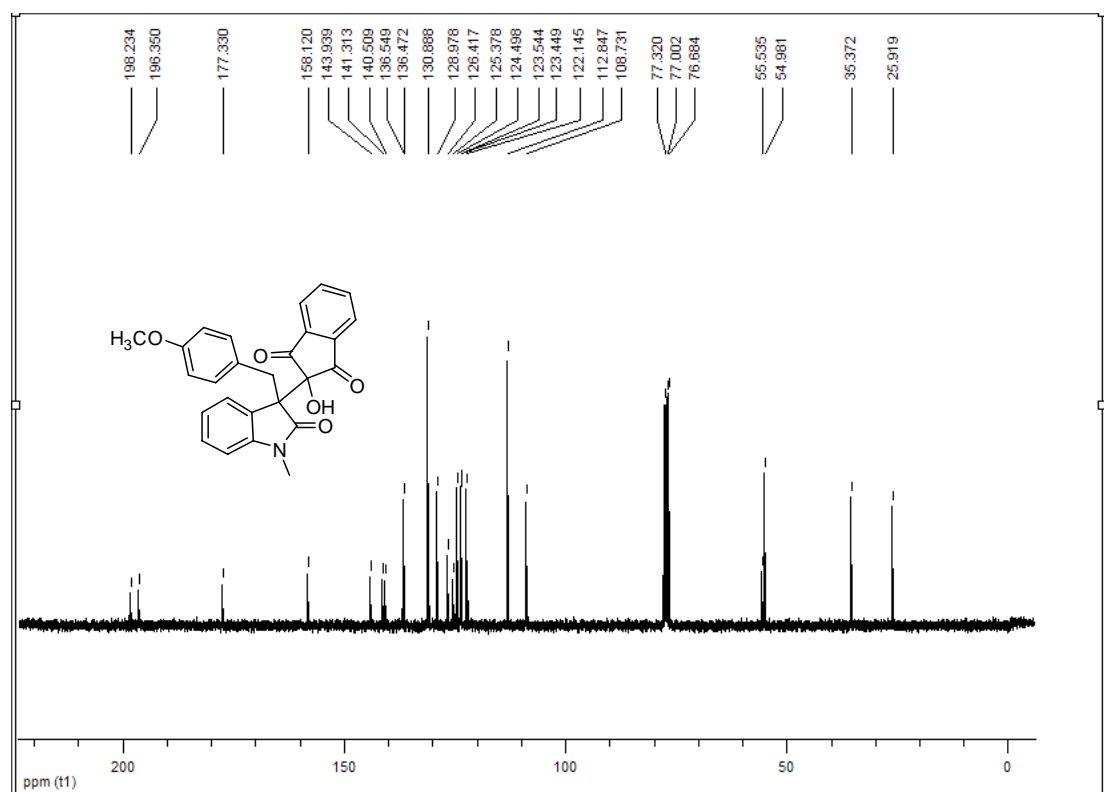
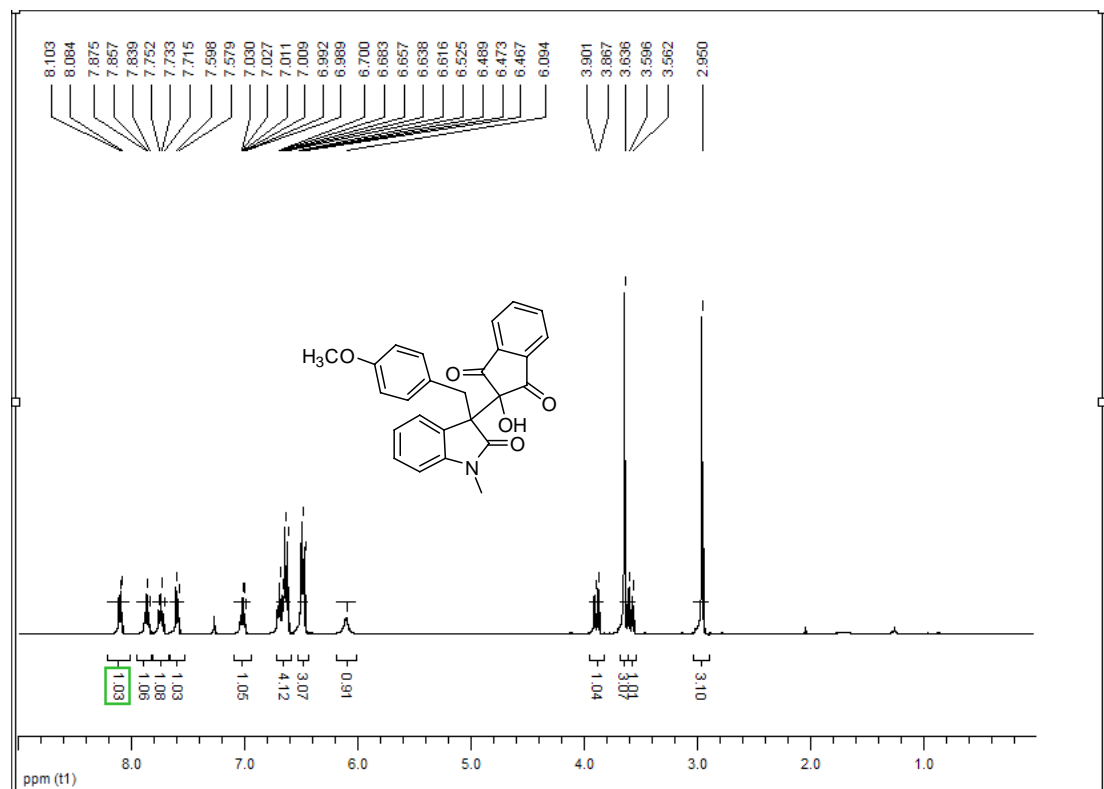
^1H and ^{13}C NMR of 3n



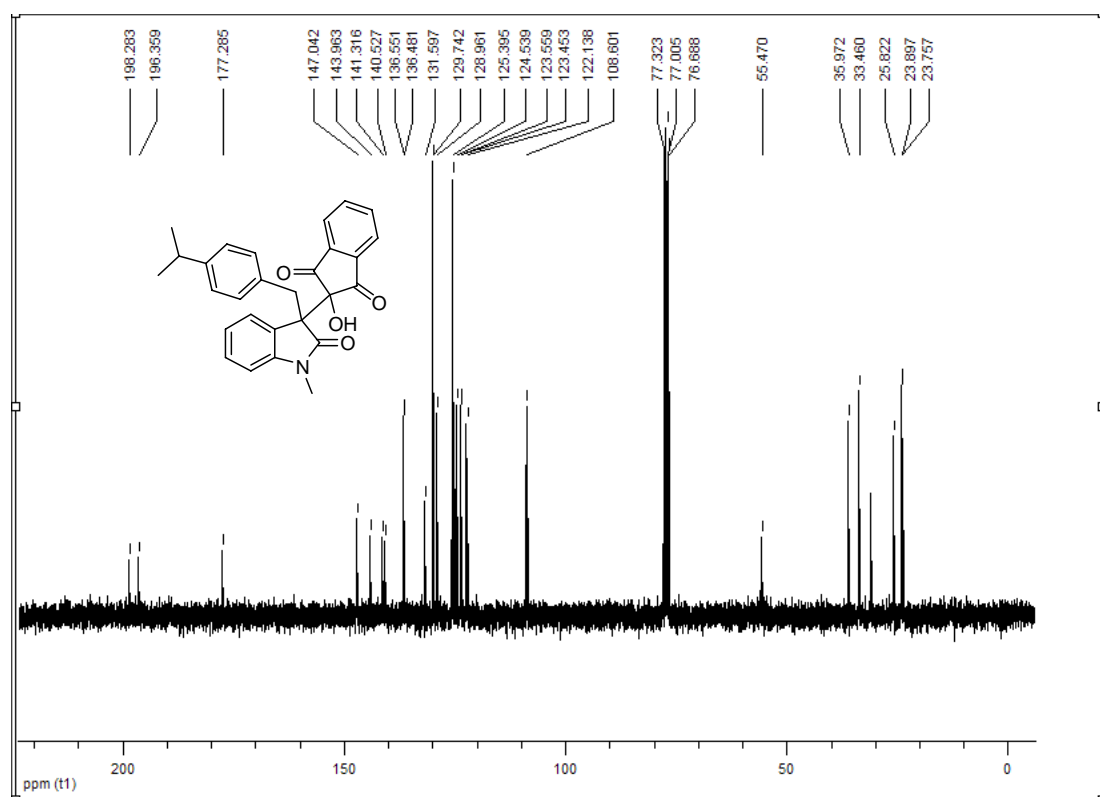
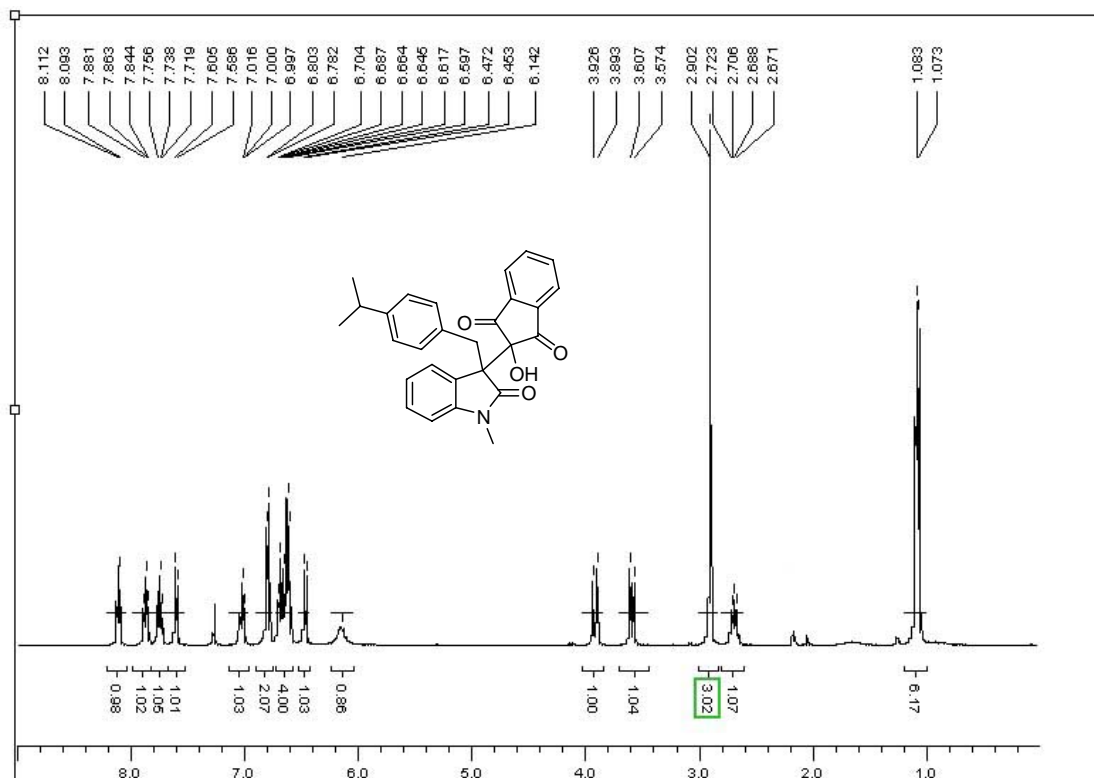
^1H and ^{13}C NMR of 3o



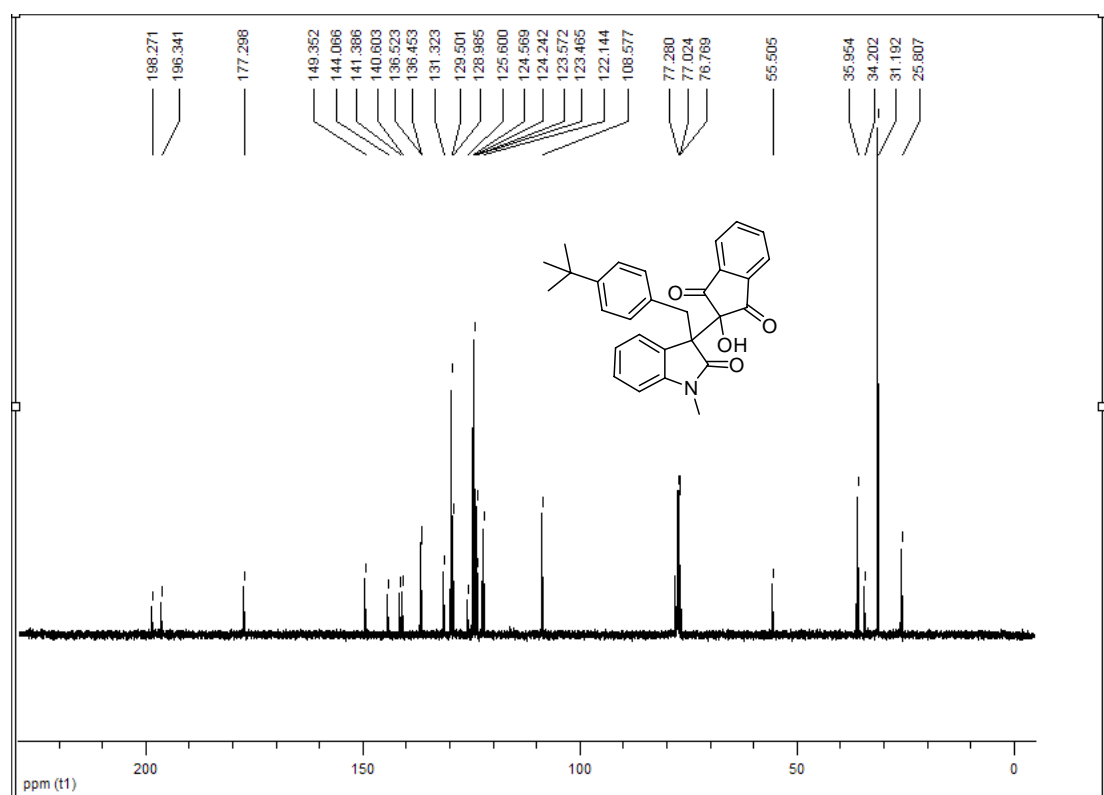
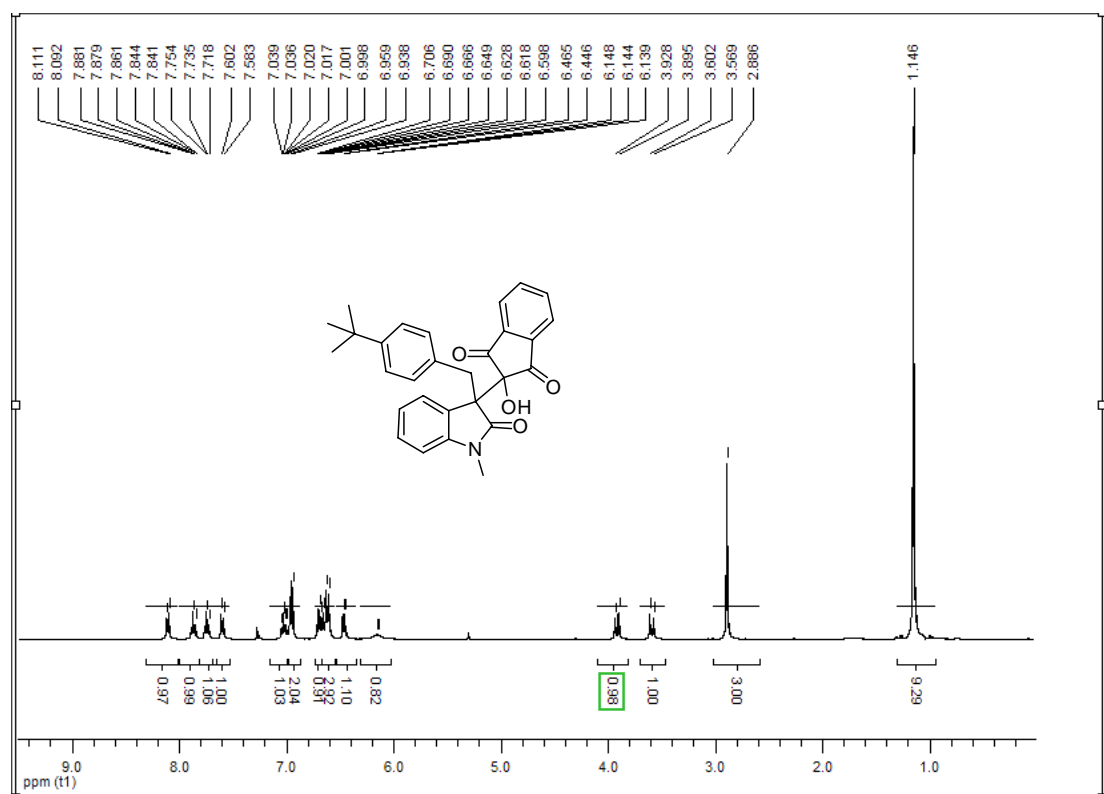
^1H and ^{13}C NMR of 3p



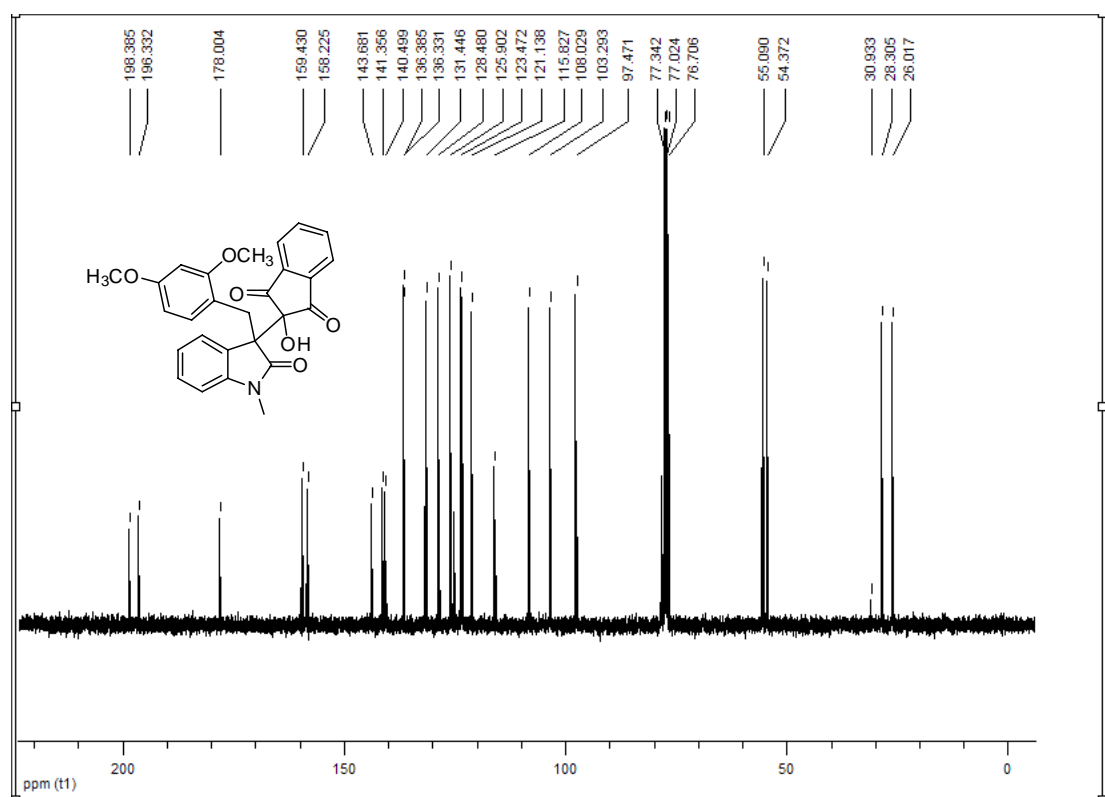
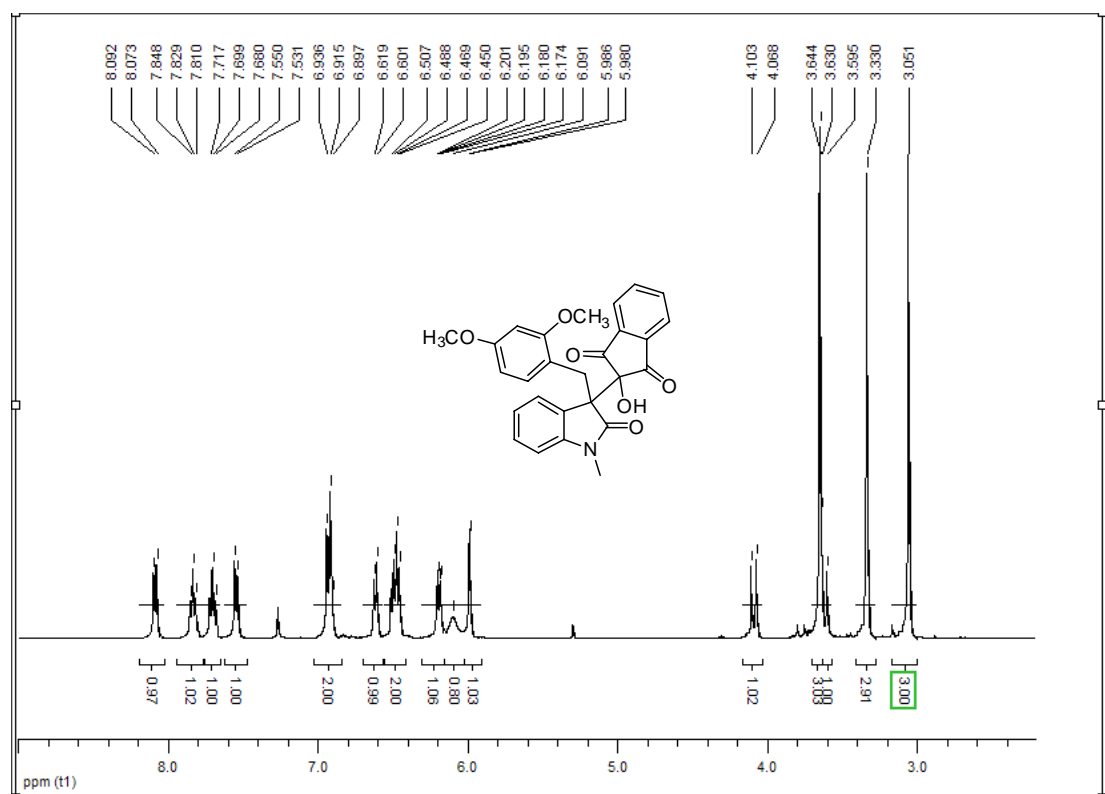
^1H and ^{13}C NMR of 3r



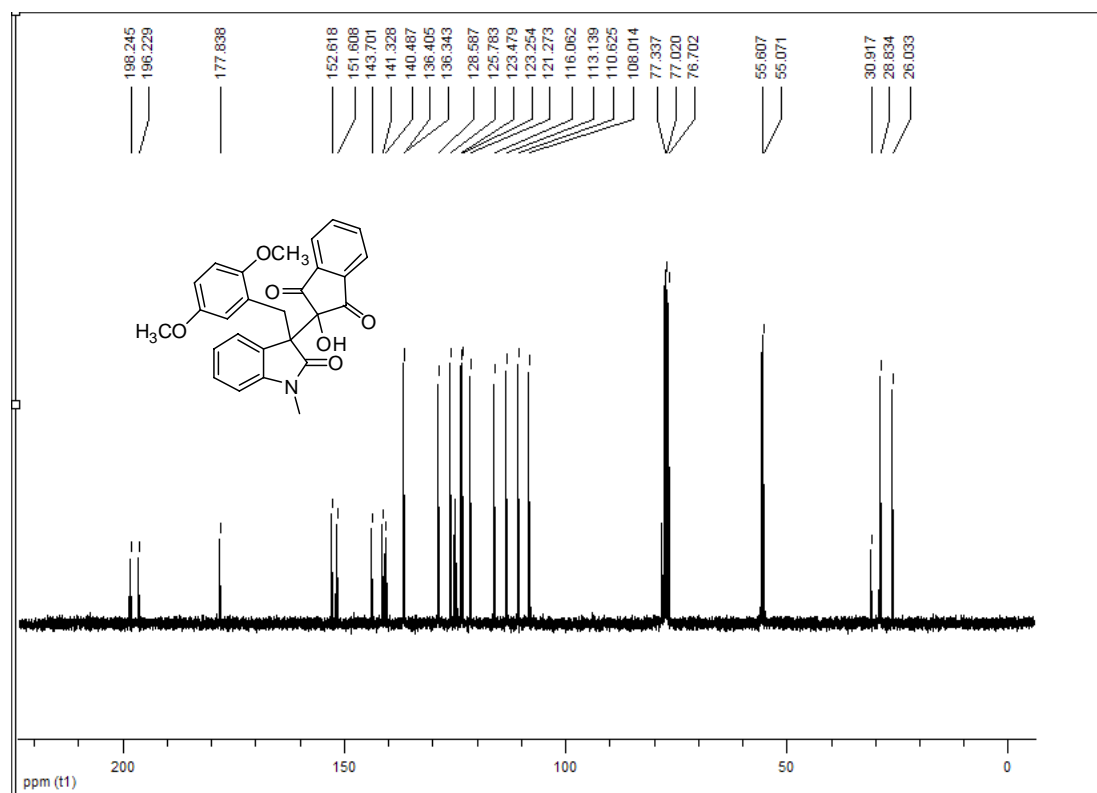
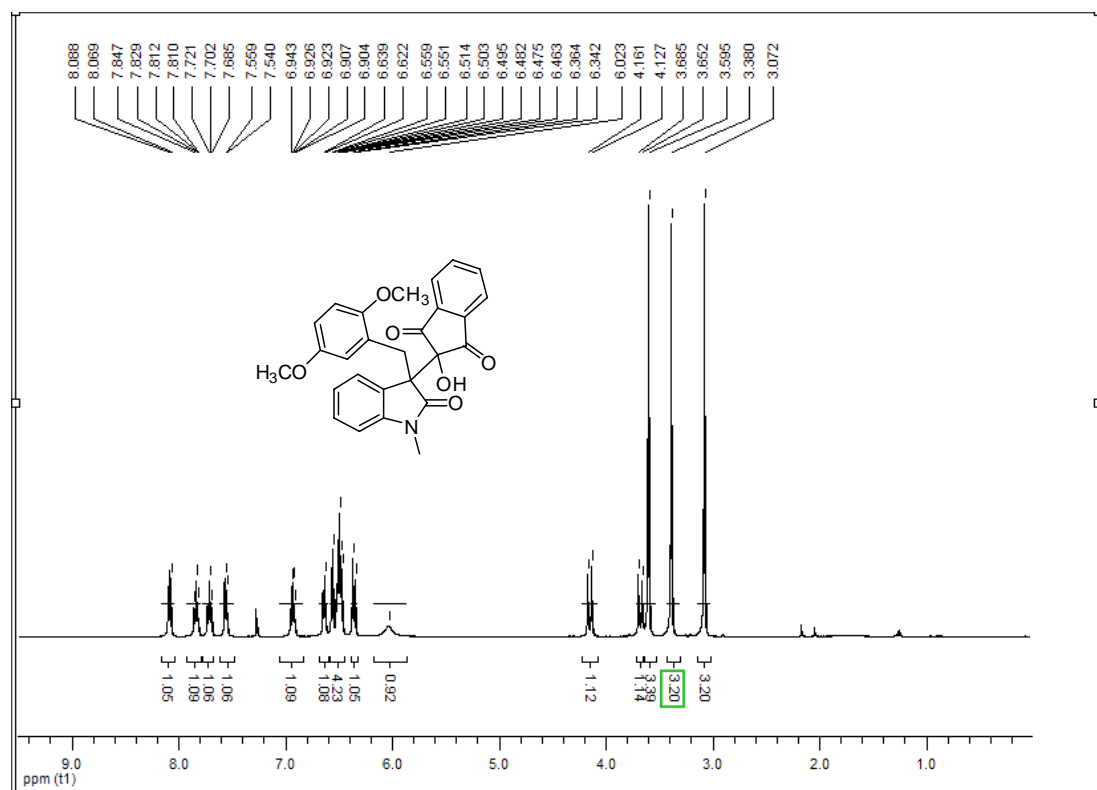
¹H and ¹³C NMR of 3s



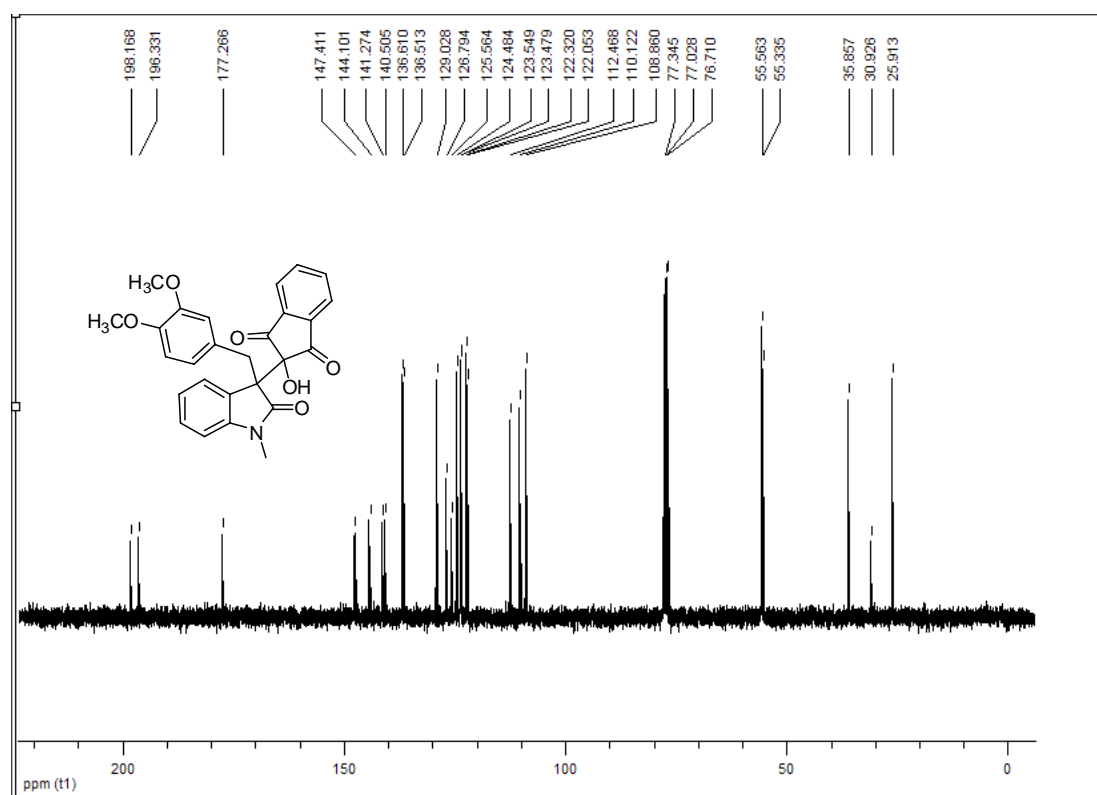
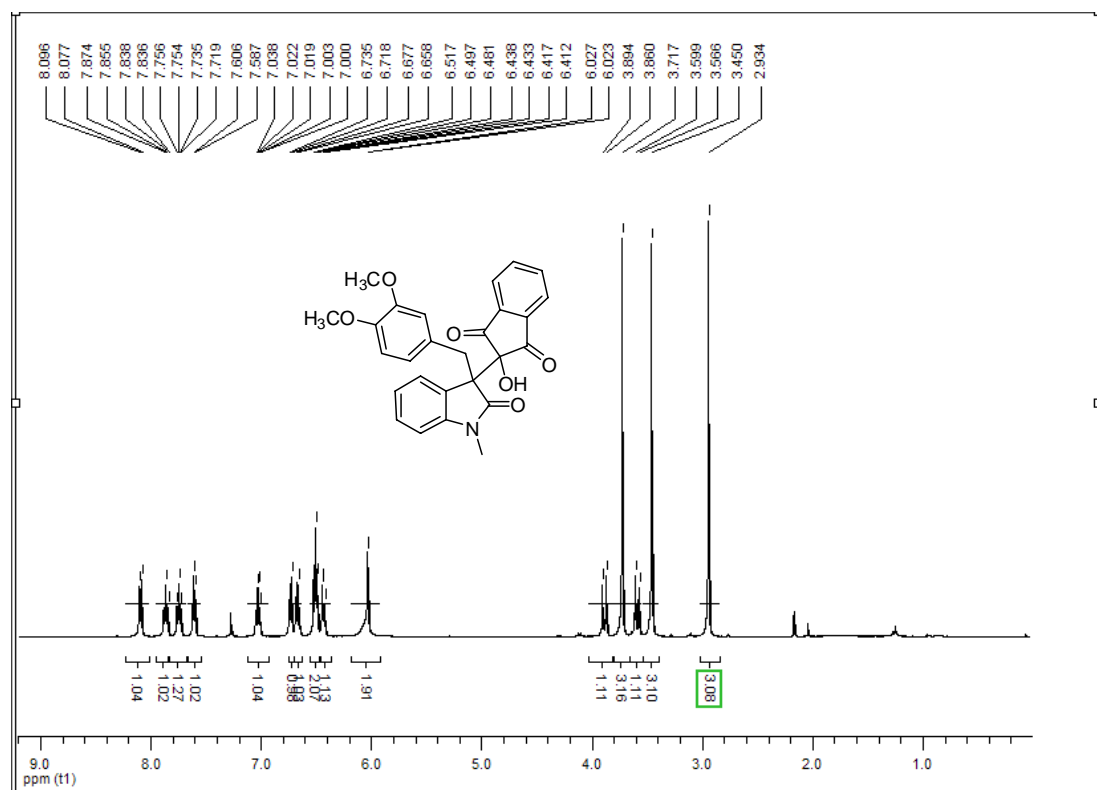
^1H and ^{13}C NMR of 3t



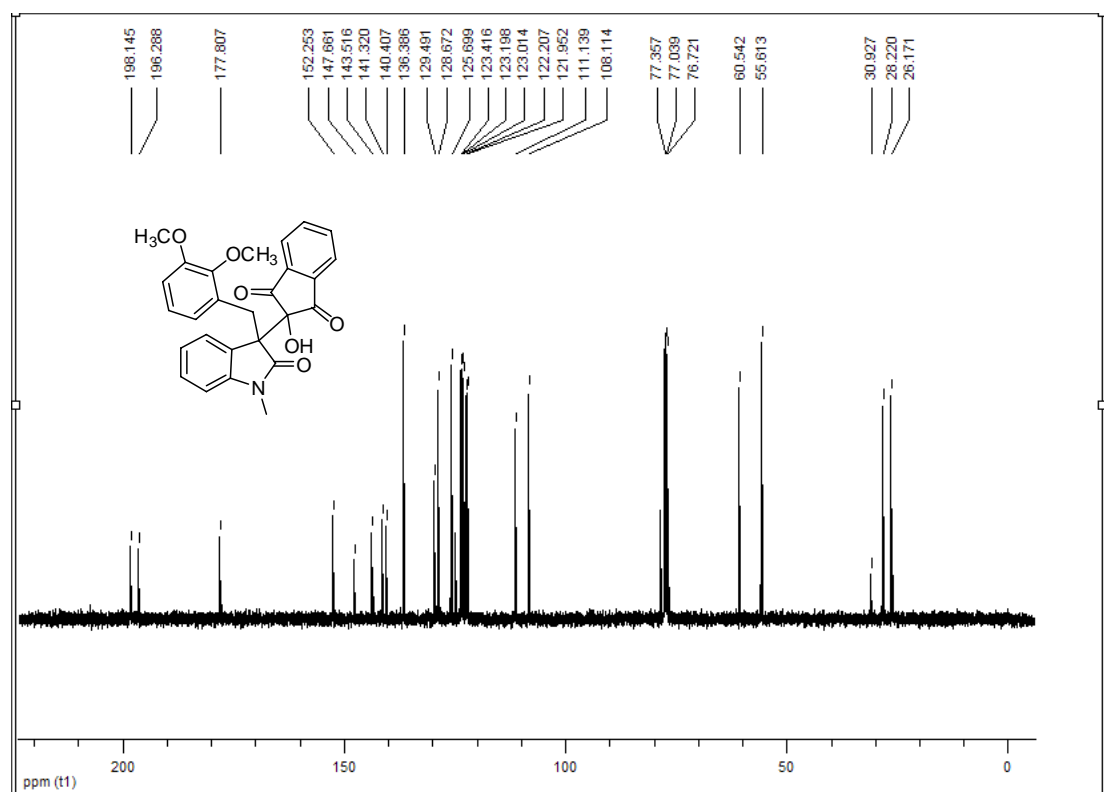
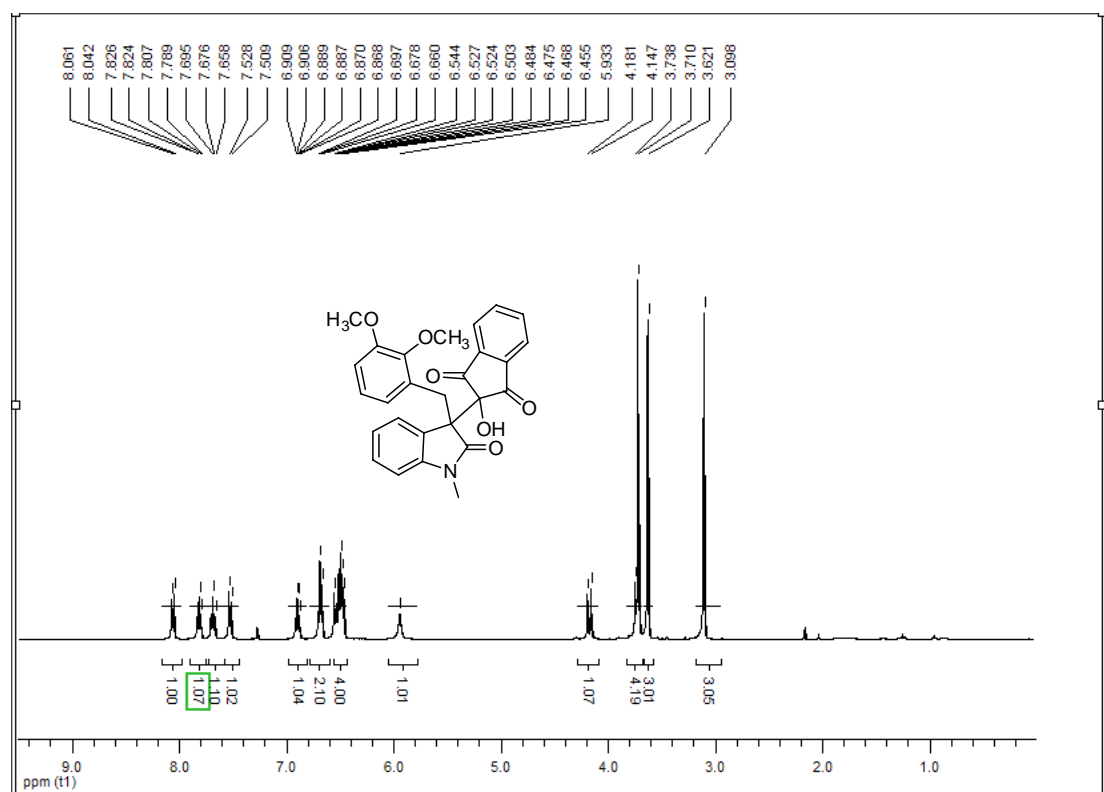
¹H and ¹³C NMR of 3u



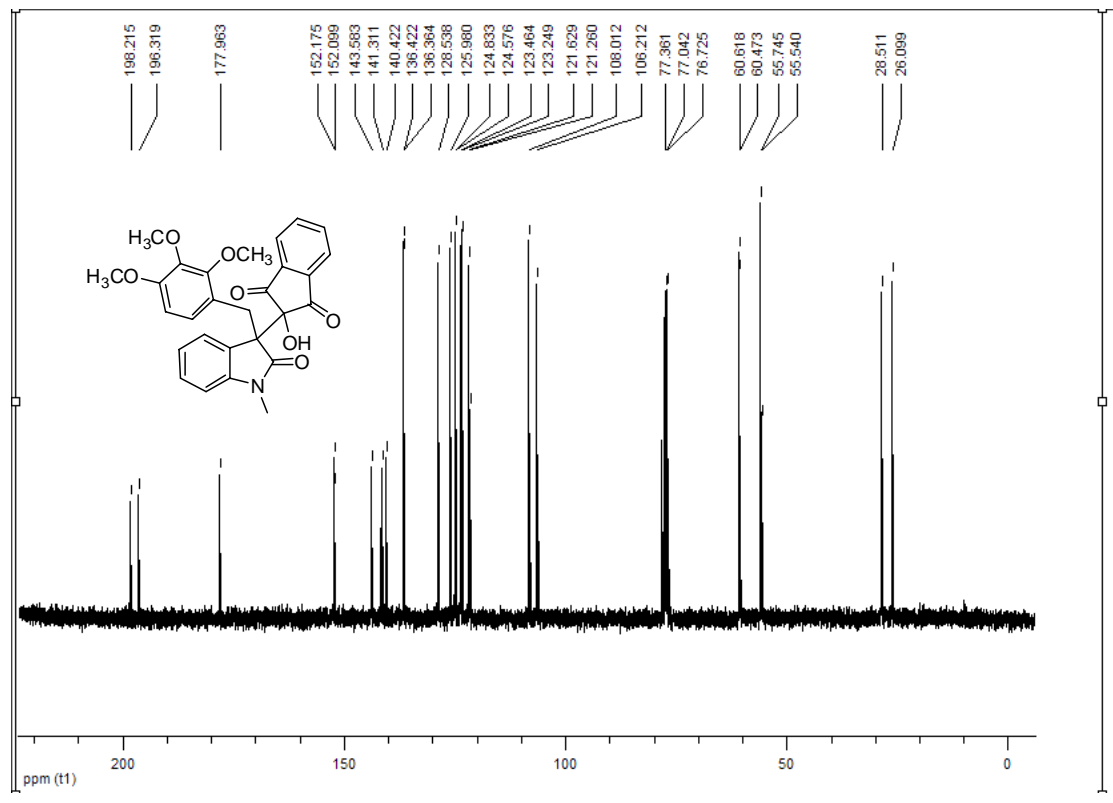
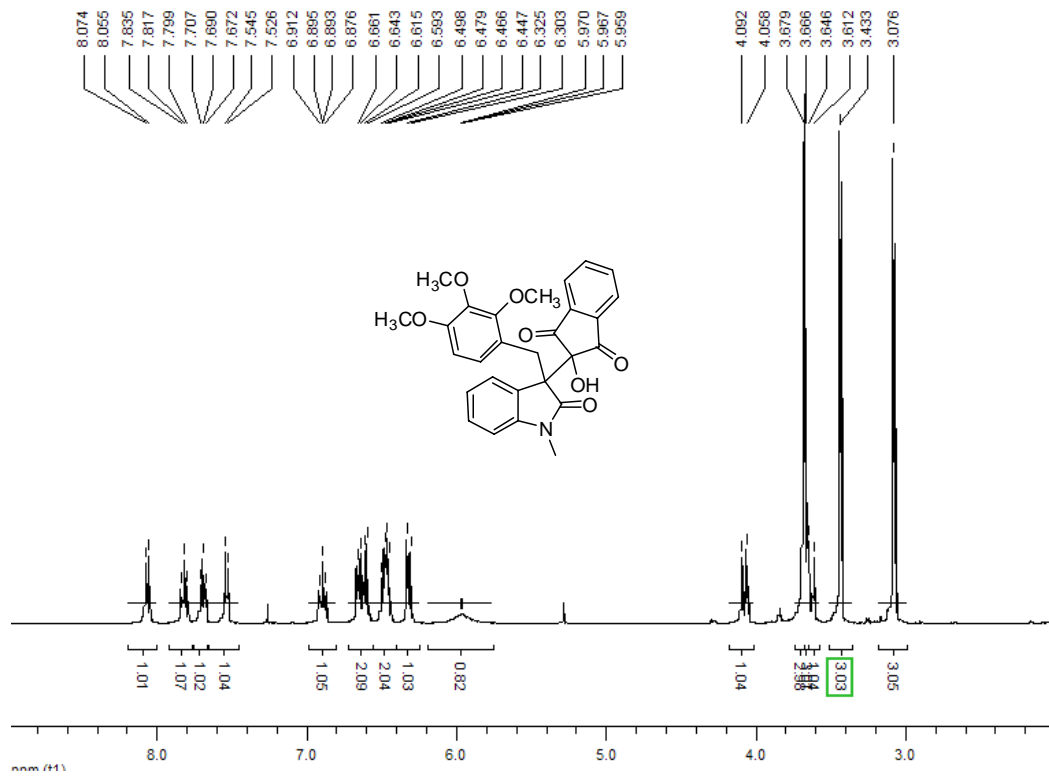
¹H and ¹³C NMR of 3v



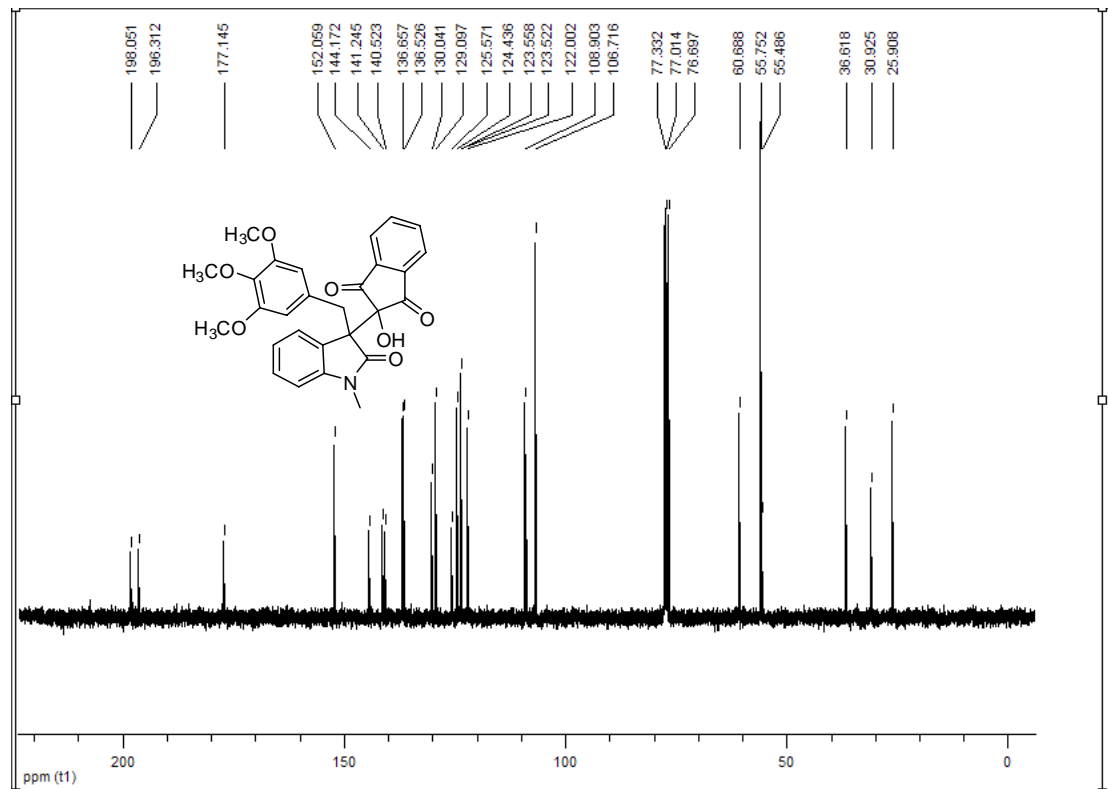
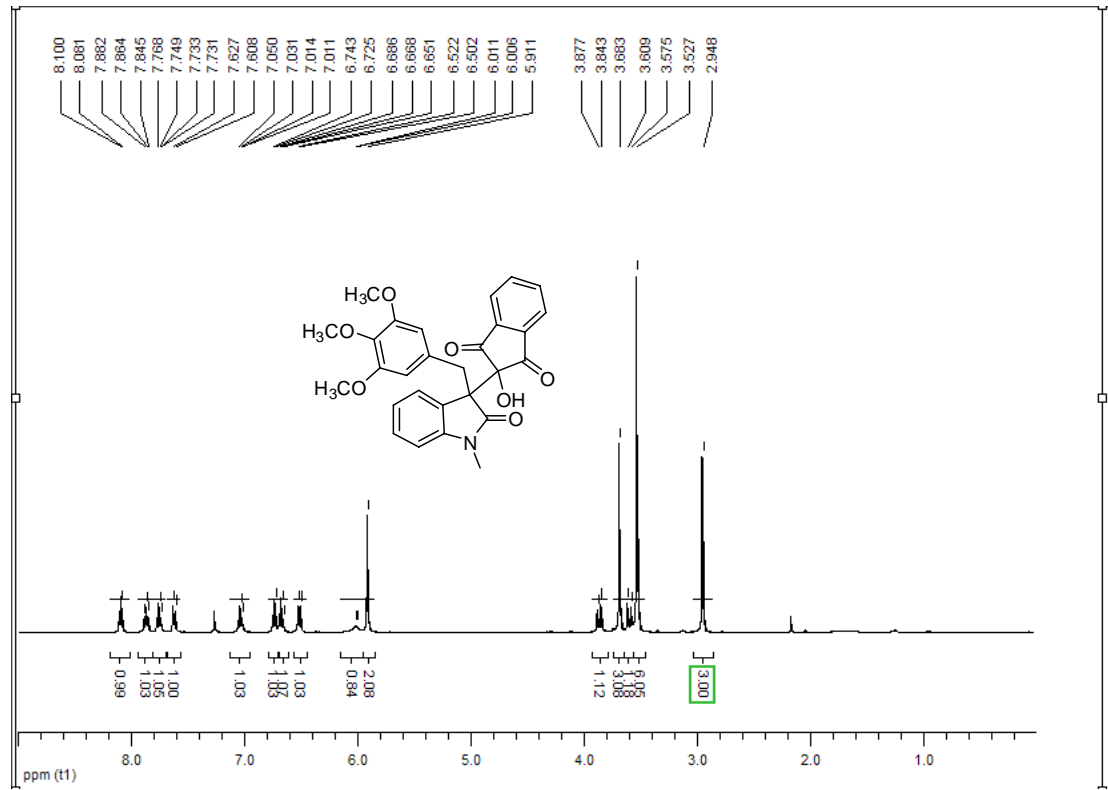
^1H and ^{13}C NMR of 3w



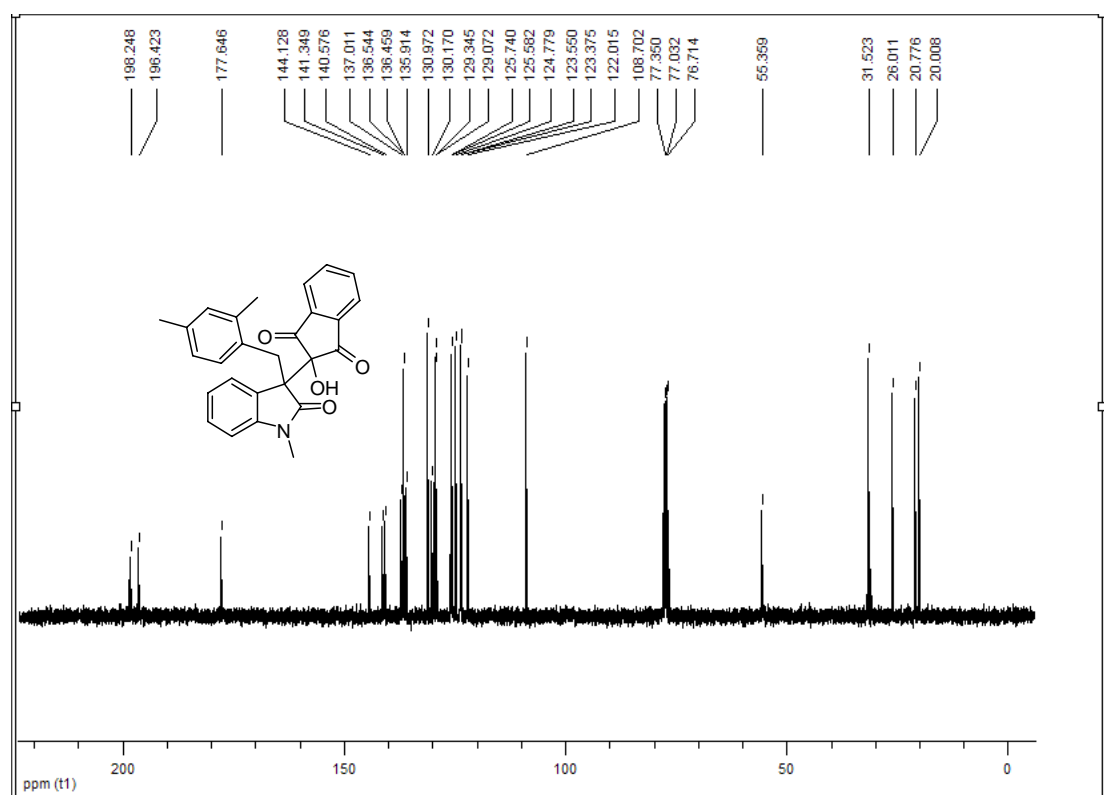
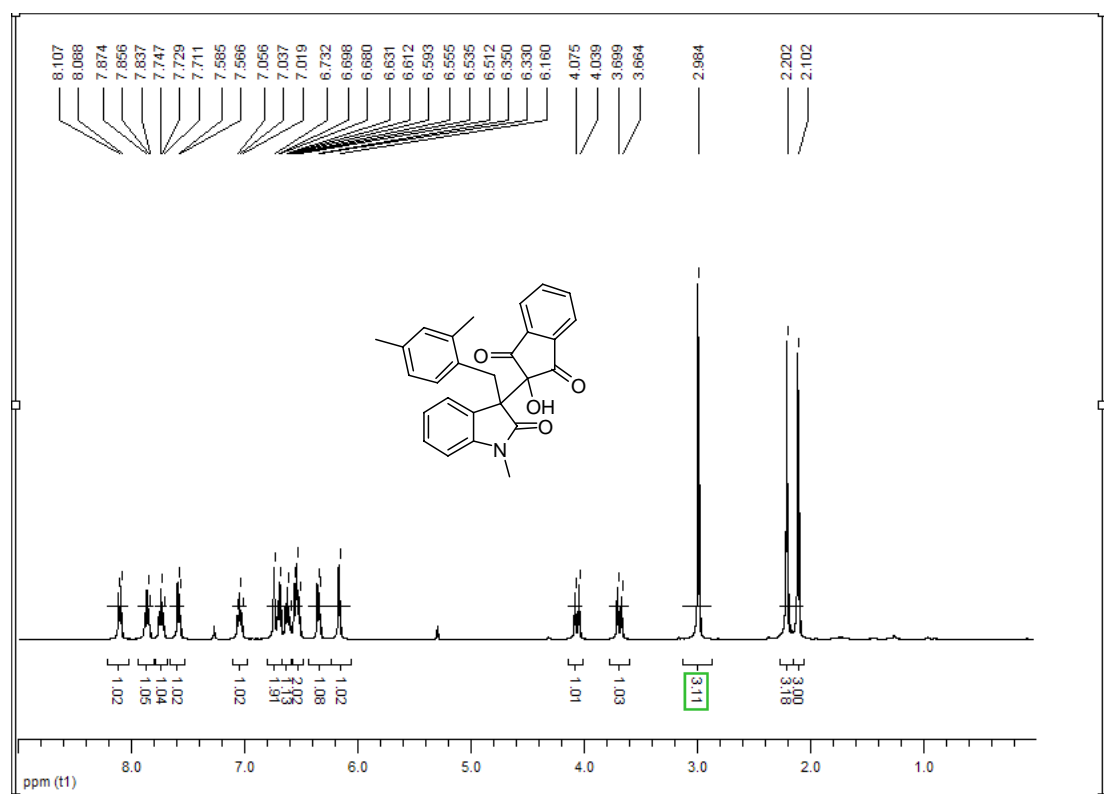
^1H and ^{13}C NMR of 3x



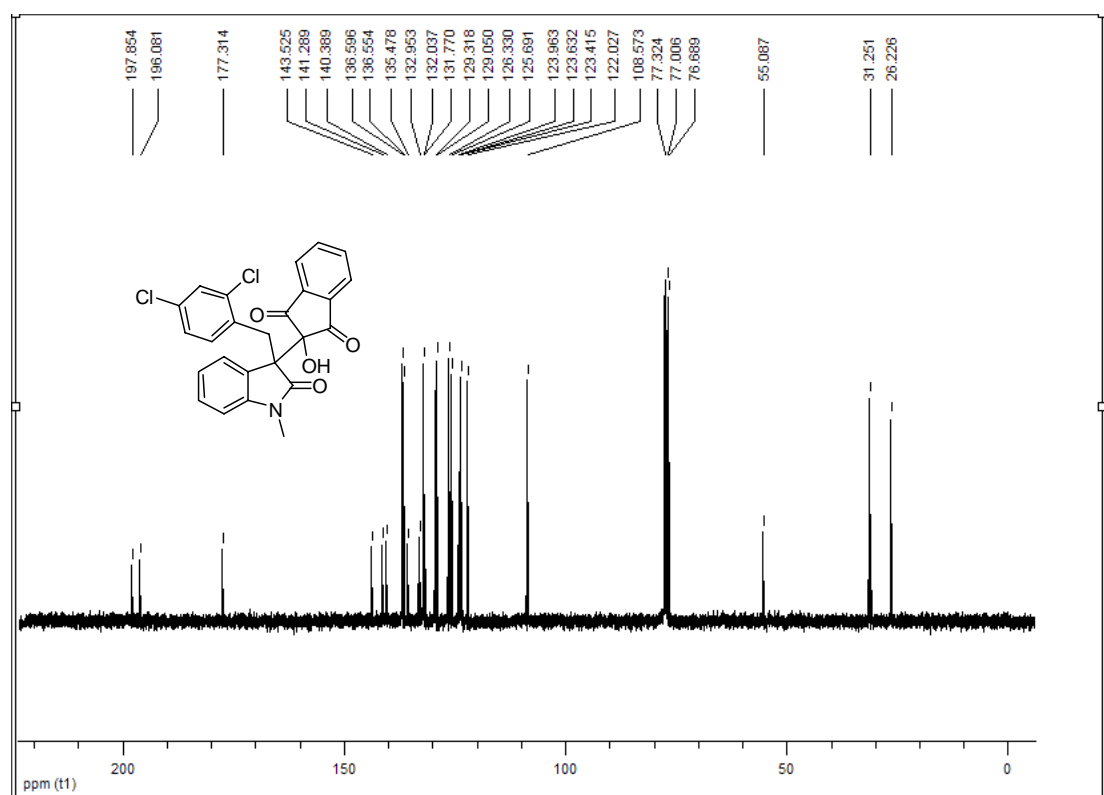
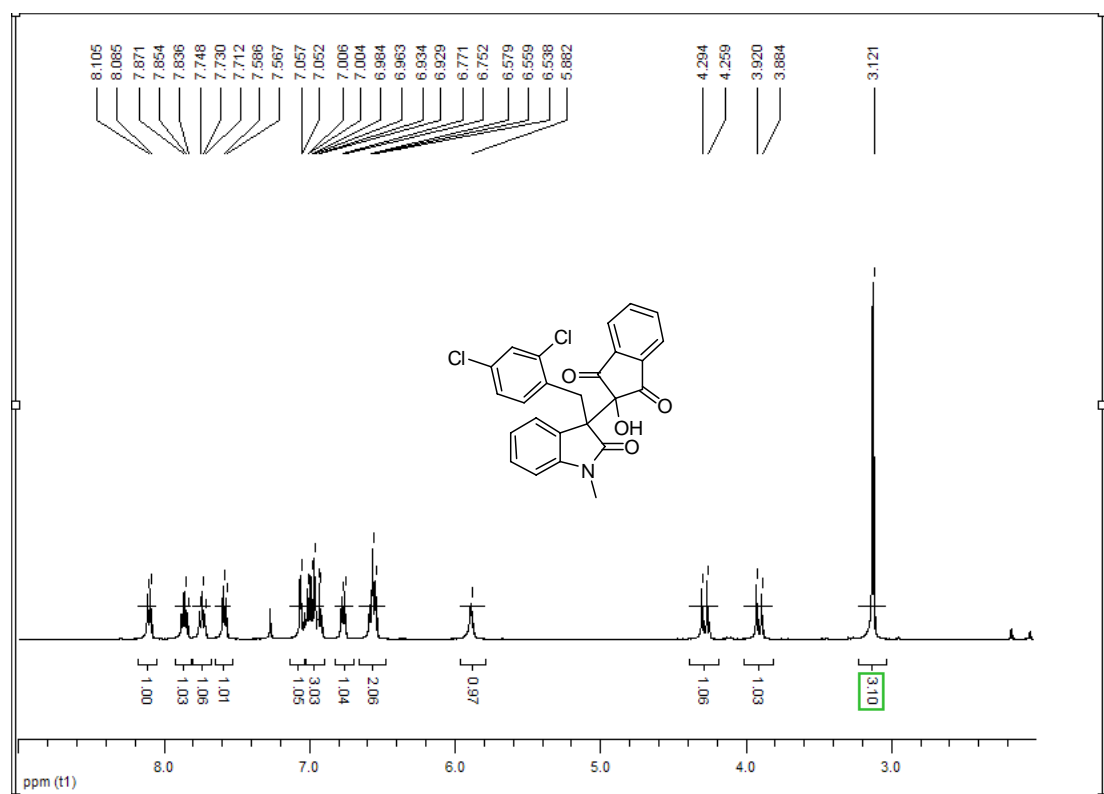
¹H and ¹³C NMR of 3z



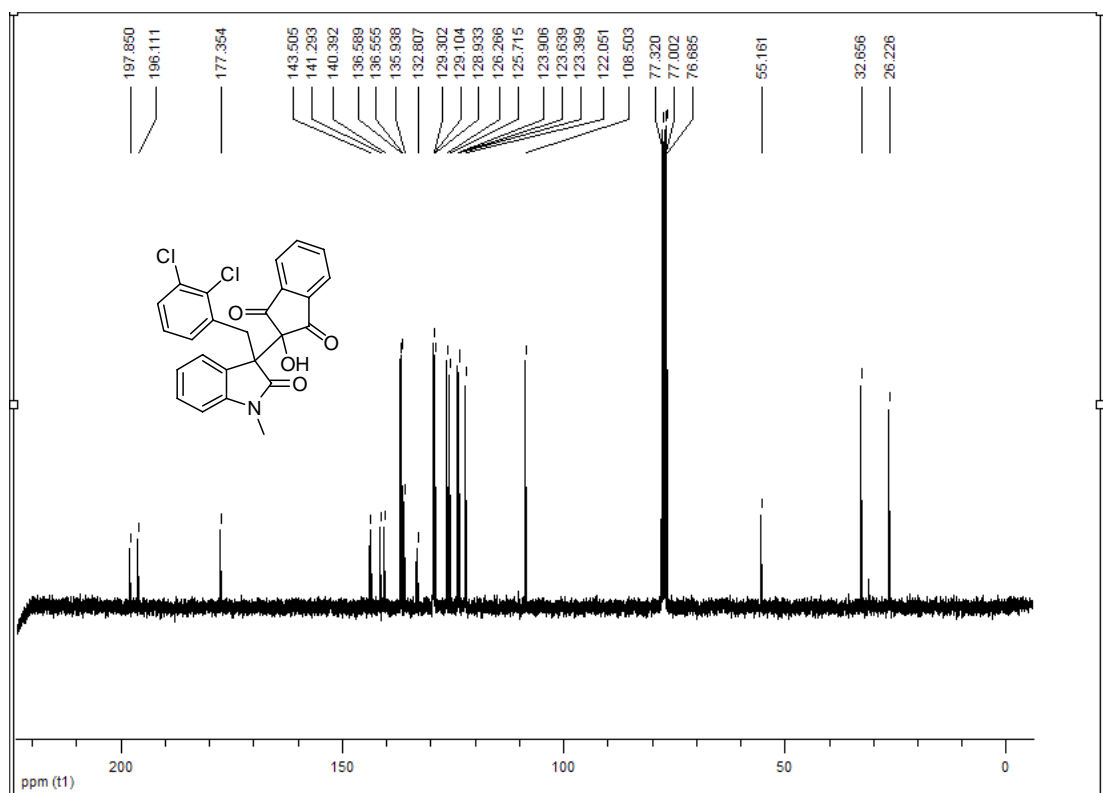
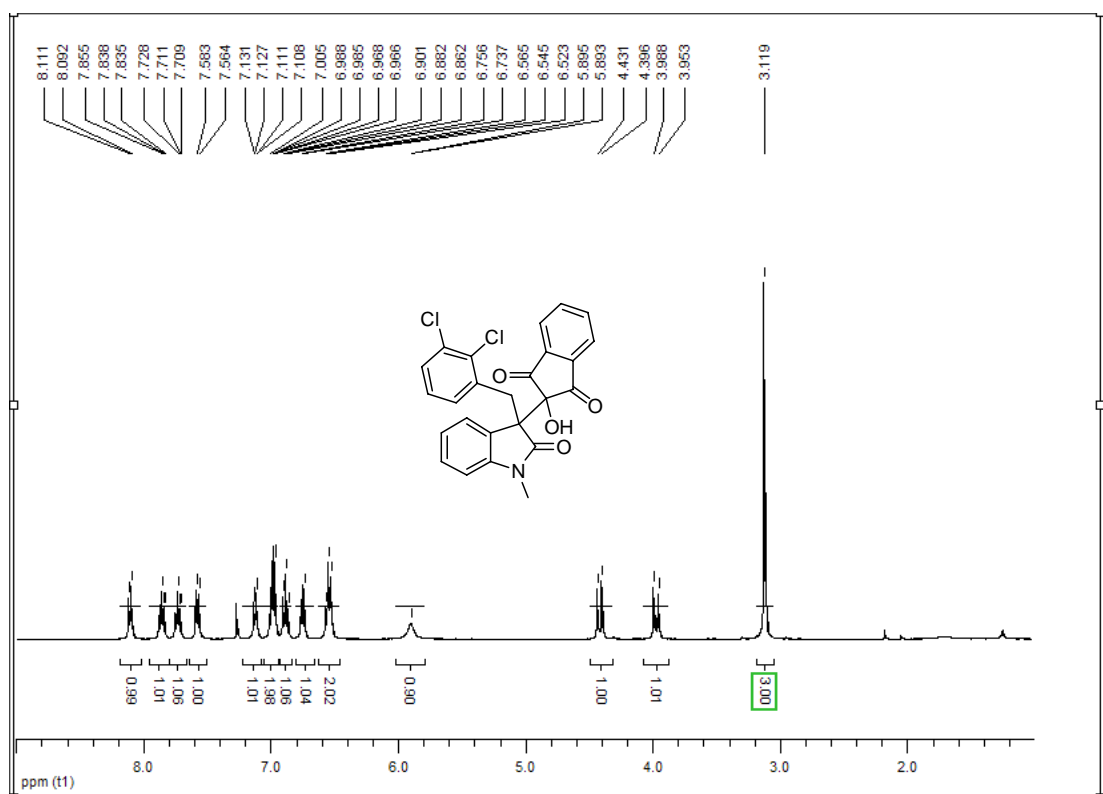
^1H and ^{13}C NMR of 3a'



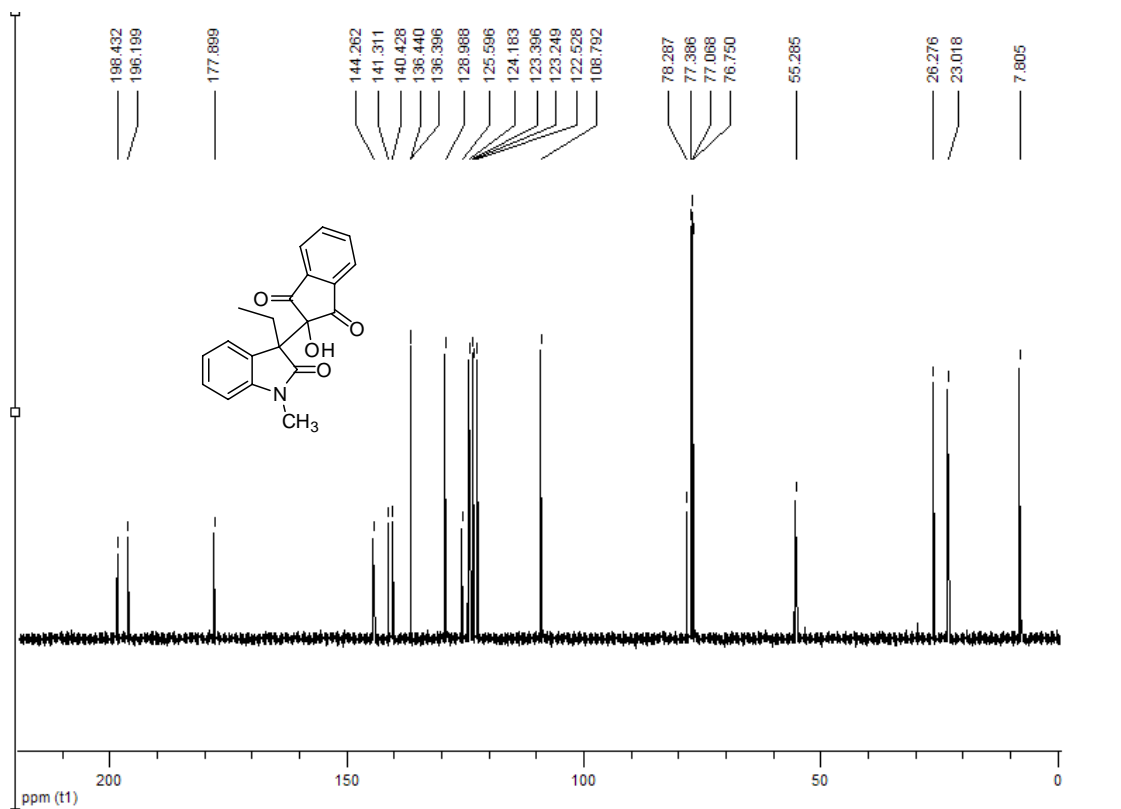
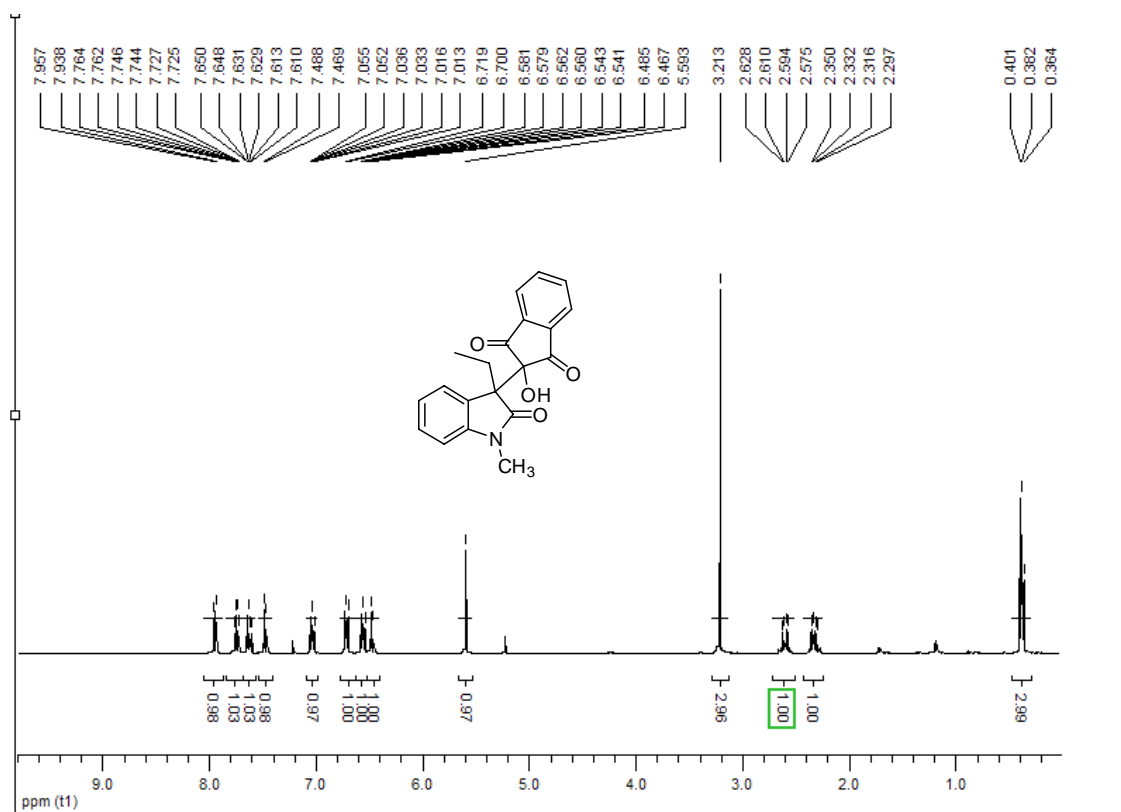
¹H and ¹³C NMR of 3b'



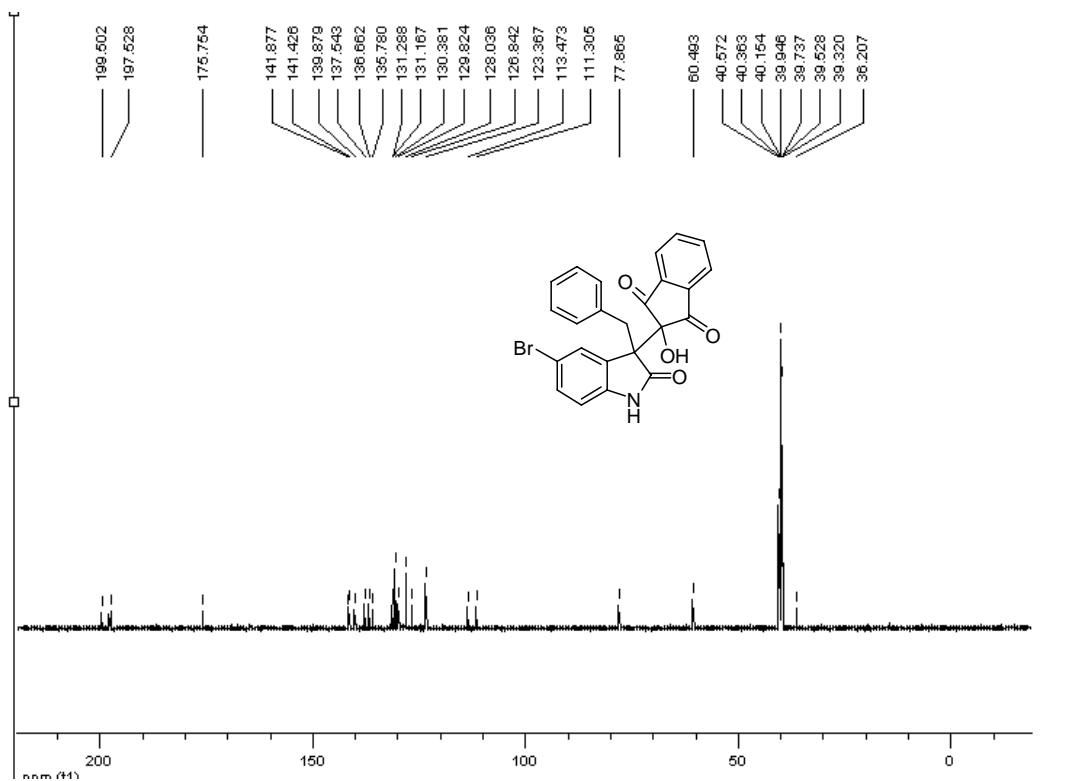
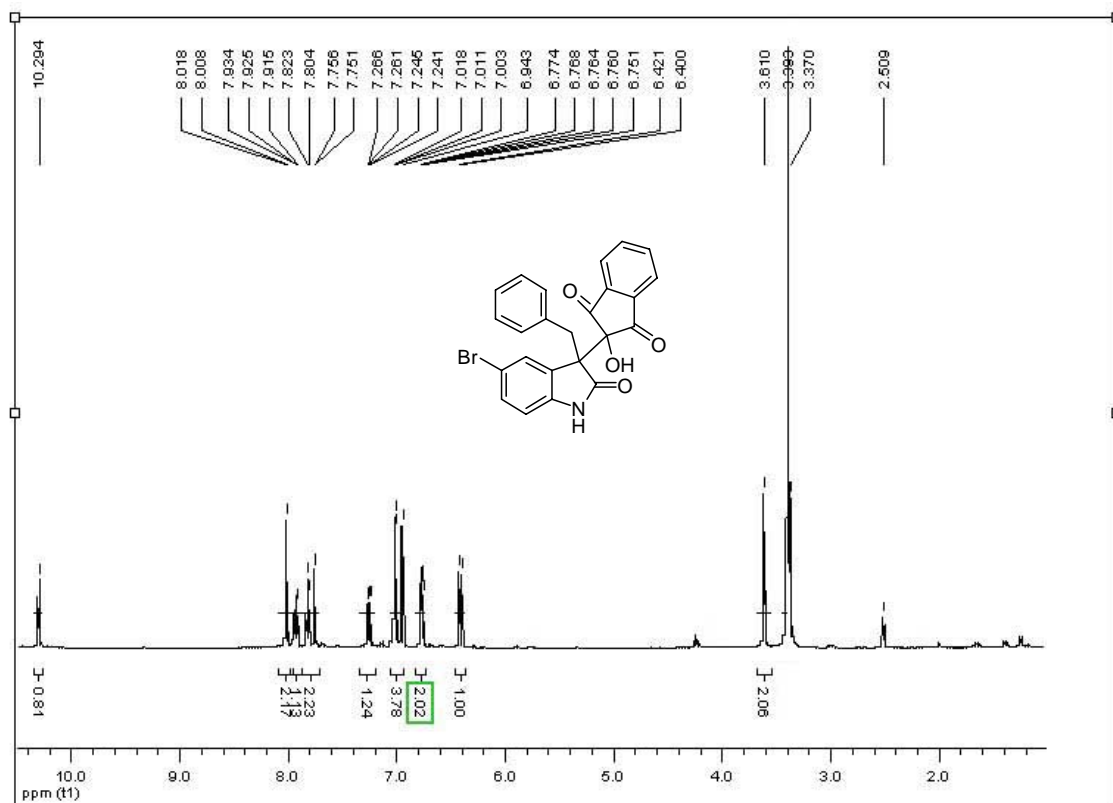
^1H and ^{13}C NMR of 3c'



¹H and ¹³C NMR of 3d'



^1H and ^{13}C NMR of 3e'



^1H and ^{13}C NMR of 3g'

