Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Copper Catalyzed Synthesis of 3-Hydroxyisoindolin-1-one and Benzopyridoindolone Derivatives from 2-Iodobenzamide and Benzylcyanide

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Crystal Data

Crystal Structure of Compound 3aa (ORTEP VIEW 30% probability)

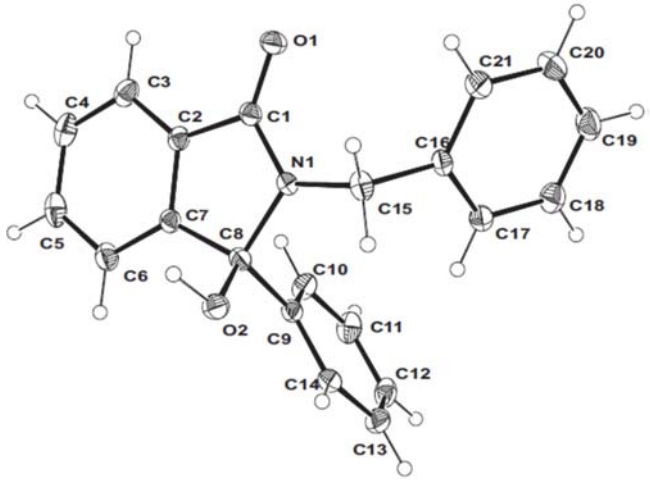


Table S1. Crystal data and structure refinement for 3aa. (CCDC Number- 1945018)

Identification code	ch15498	
Empirical formula	$C_{21}\ H_{17}\ N\ O_2$	
Formula weight	315.36	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.7191(17) Å	α= 61.607(6)°.
	b = 10.2939(19) Å	β= 63.029(5)°.
	c = 10.630(2) Å	γ = 87.604(6)°.
Volume	813.1(3) $Å^3$	
Z	2	
Density (calculated)	1.288 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	332	

Crystal size	0.31 x 0.25 x 0.06 mm^3
Theta range for data collection	2.38 to 25.07°.
Index ranges	-11<=h<=11, -11<=k<=12, -12<=l<=12
Reflections collected	7092
Independent reflections	2860 [R(int) = 0.0384]
Completeness to theta = 25.07°	98.7 %
Absorption correction	multi-scan
Max. and min. transmission	0.9950 and 0.9748
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2860 / 0 / 217
Goodness-of-fit on F^2	1.067
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1208
R indices (all data)	R1 = 0.0879, wR2 = 0.1546
Largest diff. peak and hole	0.223 and -0.236 $e.Å^{-3}$

Crystal Structure of Compound 3ae (ORTEP VIEW 30% probability)

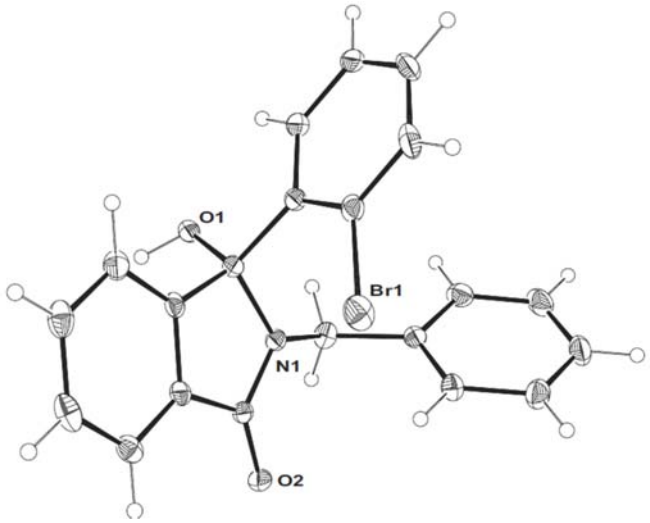


Table S 2. Crystal data and structure refinement for 3ae. (CCDC Number 1945019)

Identification code	ch16057

Empirical formula	$C_{21}H_{16}BrNO_2$	
Formula weight	394.26	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.9170(9) Å	α= 73.236(5)°.
	b = 10.2917(9) Å	β= 67.643(5)°.
	c = 11.1275(8) Å	γ = 65.564(6)°.
Volume	849.34(13) $Å^3$	
Z	2	
Density (calculated)	1.542 Mg/m^3	
Absorption coefficient	2.434 mm^{-1}	
F(000)	400	
Crystal size	0.58 x 0.39 x 0.25 mm^3	
Theta range for data collection	2.20 to 25.07°.	
Index ranges	-10<=h<=10, -12<=k<=12, -12<=l<=13	
Reflections collected	6699	
Independent reflections	2972 [R(int) = 0.0356]	
Completeness to theta = 25.07°	98.1 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.5813 and 0.3326	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2972 / 0 / 226	
Goodness-of-fit on F^2	1.113	
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0986	
R indices (all data)	R1 = 0.0466, wR2 = 0.1128	

Largest diff. peak and hole	0.369 and -0.499 e.Å^{-3}

Crystal Structure of Compound 3mn (ORTEP VIEW 30% probability)

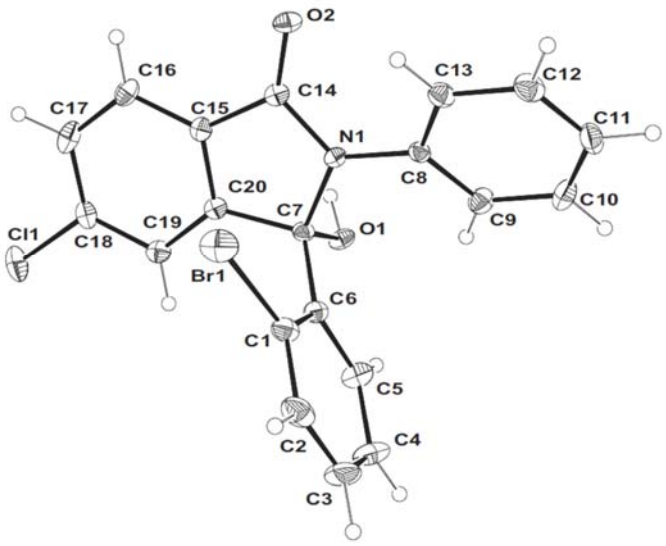


Table S3. Crystal data and structure refinement for 3mn. (CCDC Number 1945020)

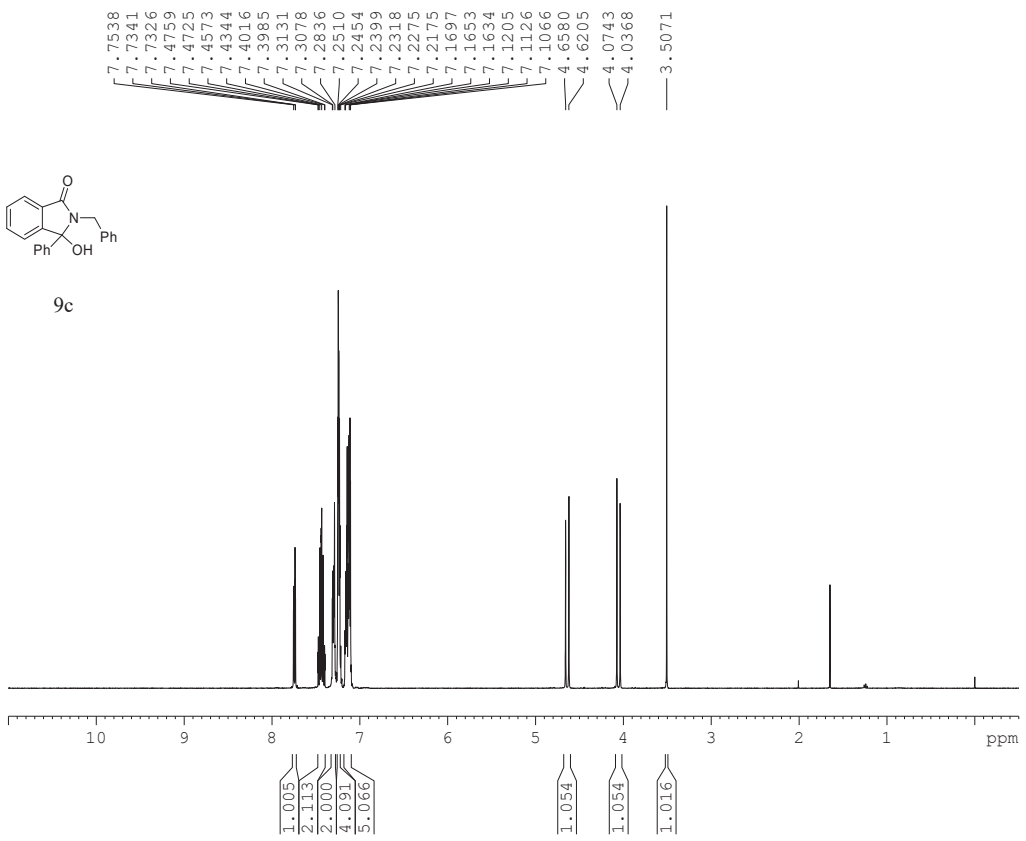
Identification code	a15070	
Empirical formula	C_{20} H_{13} Br Cl N O_2	
Formula weight	414.67	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 25.659(3) Å	α= 90°.
	b = 8.0570(7) Å	β= 114.978(4)°.
	c = 18.4834(17) Å	γ = 90°.
Volume	3463.7(6) Å^3	
Z	8	
Density (calculated)	1.590 Mg/m^3	

Absorption coefficient	2.541 mm^{-1}
F(000)	1664
Crystal size	0.42 x 0.36 x 0.15 mm^3
Theta range for data collection	2.32 to 25.11°.
Index ranges	-30<=h<=24, -9<=k<=7, -22<=l<=21
Reflections collected	9036
Independent reflections	3052 [R(int) = 0.0413]
Completeness to theta = 25.11°	99.1 %
Absorption correction	multi-scan
Max. and min. transmission	0.7018 and 0.4150
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3052 / 0 / 226
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0409, wR2 = 0.0874
R indices (all data)	R1 = 0.0650, wR2 = 0.0965
Largest diff. peak and hole	0.320 and -0.686 e.$Å^{-3}$

Spectra Copies

2-Benzyl-3-hydroxy-3-phenylisoindolin-1-one (3aa)

1H of benzyl final

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Current Data Parameters
NAME          20131019
EXPNO                3
PROCNO               1

F2 - Acquisition Parameters
Date_        20131019
Time             15.20
INSTRUM          SPECT
PROBHD   5 mm PABBO BB/
PULPROG          zg30
TD              32768
SOLVENT          CDCl3
NS                  16
DS                   0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                78.51
DW                69.333 usec
DE                10.52 usec
TE                298.6 K
D1            2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                1H
P1                12.80 usec
PLW1        15.00000000 W

F2 - Processing parameters
SI                  16384
SF          400.1300132 MHz
WDW                 EM
SSB      0
LB       0 Hz
GB       0
PC                1.00
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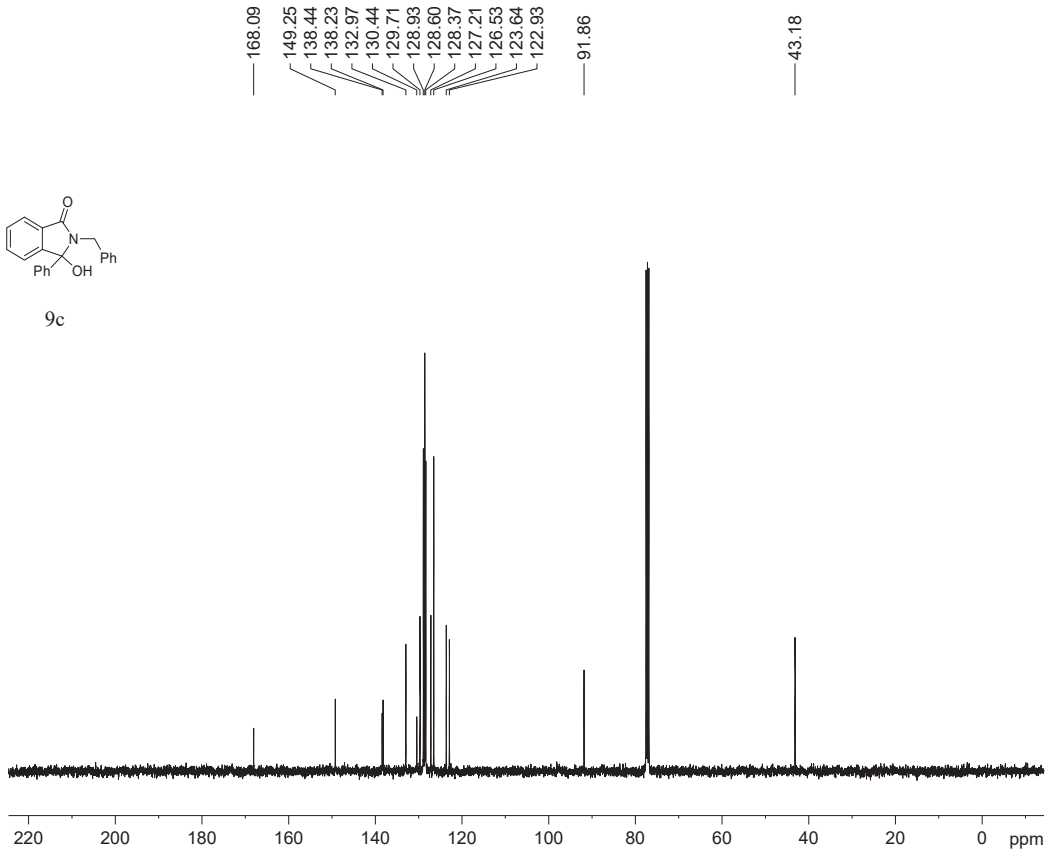
2-Benzyl-3-hydroxy-3-phenylisoindolin-1-one (3aa)

13C of benzyl final

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EXPNO                4
PROCNO               1

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Date_        20131019
Time             15.25
INSTRUM          SPECT
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD              32768
SOLVENT          CDCl3
NS                 171
DS                   0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW                20.800 usec
DE                6.50 usec
TE                299.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6233324 MHz
NUC1                13C
P1                10.00 usec
PLW1        46.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        15.00000000 W
PLW12        0.34252000 W
PLW13        0.27744001 W

F2 - Processing parameters
SI                  32768
SF          100.6127491 MHz
WDW                 EM
SSB      0
LB                2.00 Hz
GB       0
PC                1.00
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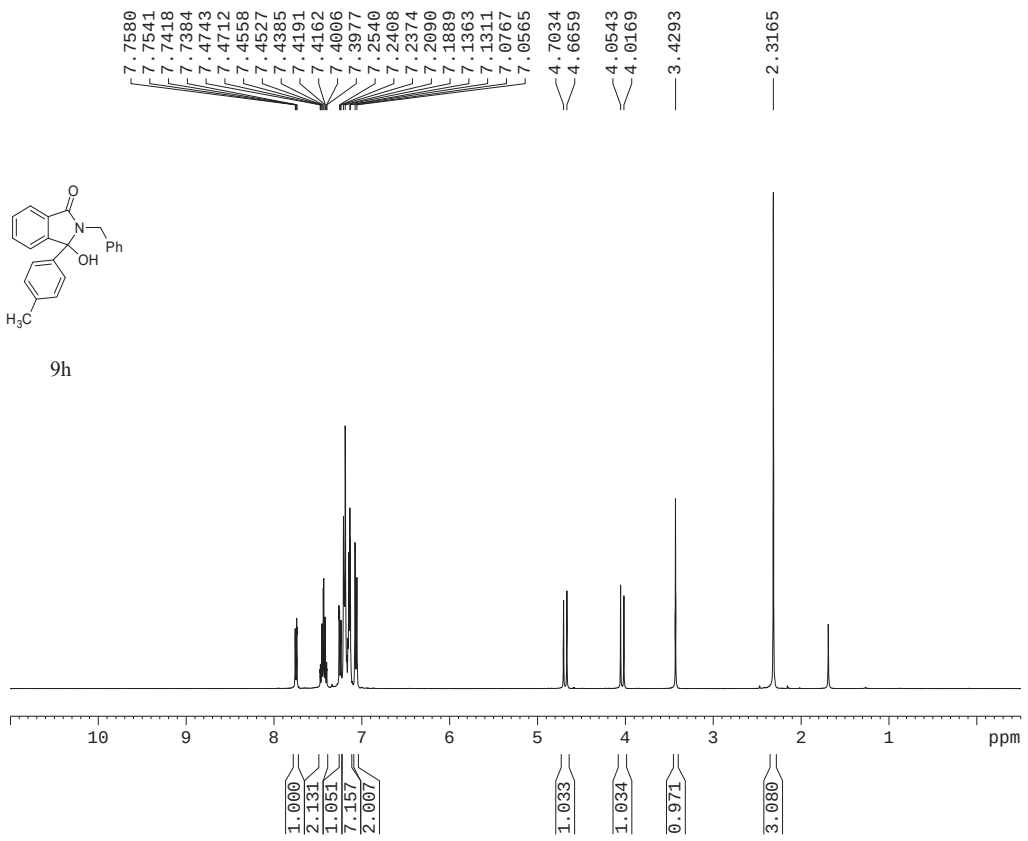
2-Benzyl-3-hydroxy-3-(p-tolyl)isoindolin-1-one (3ab)

1H of 4-CH3 BnCN final product



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NAME 20140419
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140419
Time 18.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 71.42
DW 69.333 usec
DE 10.52 usec
TE 298.6 K
D1 2.00000000 sec
TD0 1

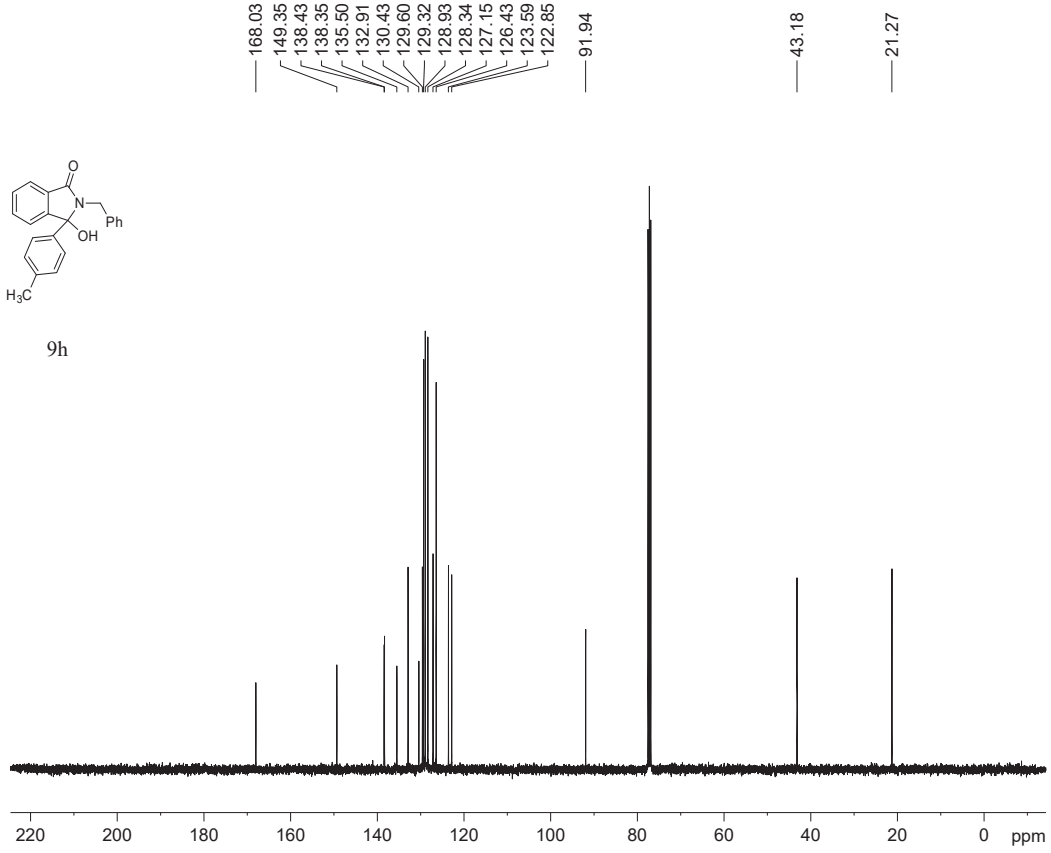
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

2-Benzyl-3-hydroxy-3-(p-tolyl)isoindolin-1-one (3ab)

2

13C of CH3 BnCN final product



Current Data Parameters
NAME 20140418
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140419
Time 0.20
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

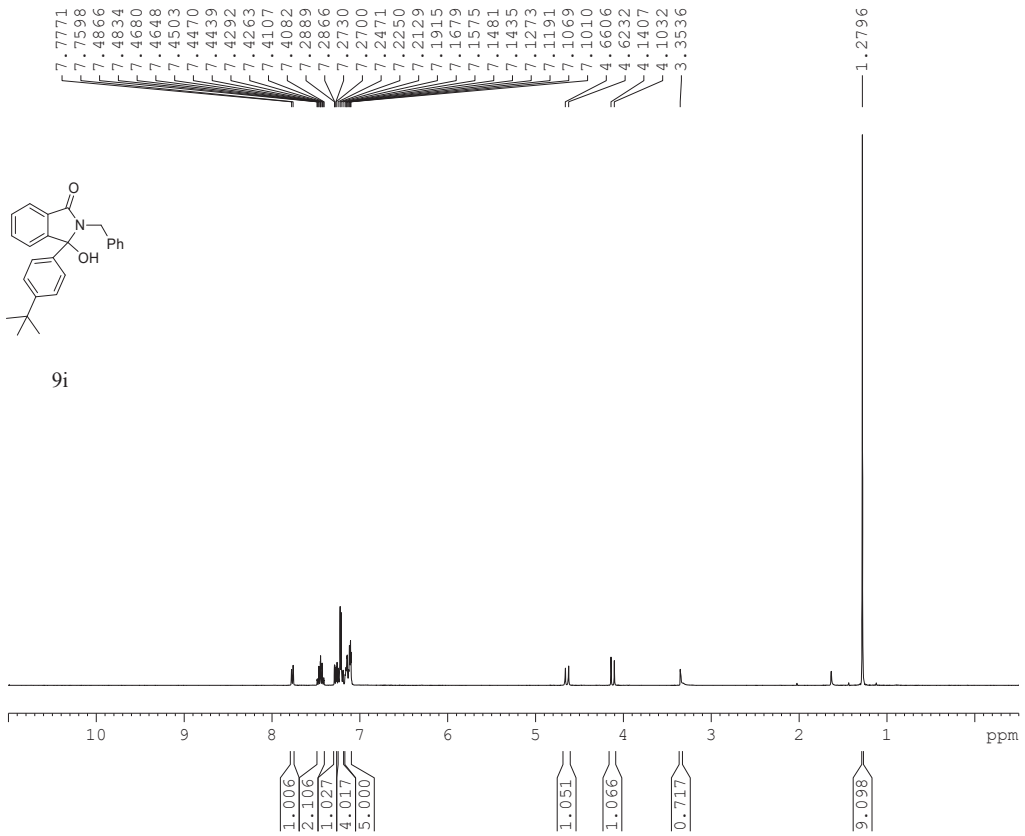
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127499 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

2-Benzyl-3-(4-(tert-butyl)phenyl)-3-hydroxyisoindolin-1-one (3ac)

1H of t-Bu BnCN final product



9i

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Current Data Parameters
NAME          20140418
EXPNO               13
PROCNO               1

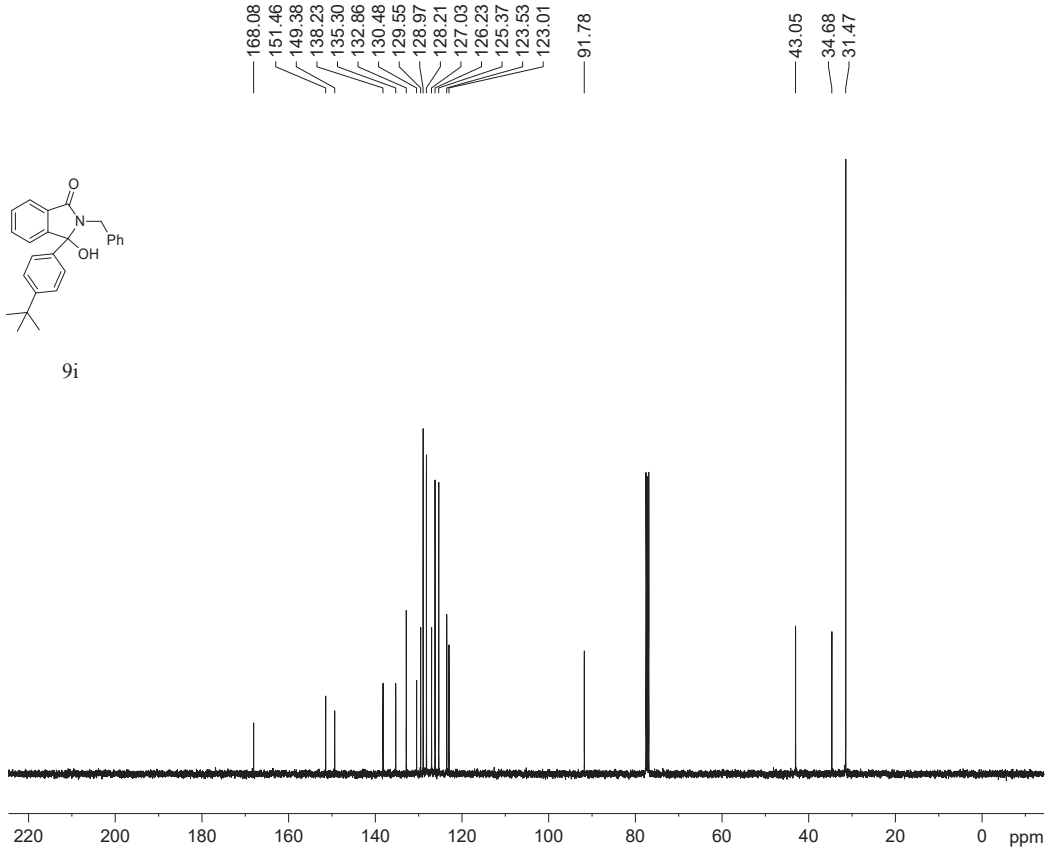
F2 - Acquisition Parameters
Date_         20140418
Time              22.05
INSTRUM           spect
PROBHD   5 mm SEI 1H-13
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   0
SWH          7246.377 Hz
FIDRES       0.221142 Hz
AQ           2.2609921 sec
RG                 114
DW              69.000 usec
DE               6.50 usec
TE               299.6 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1              11.00 usec
PL1             -4.20 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                  16384
SF          400.1300091 MHz
WDW                    EM
SSB      0
LB       0 Hz
GB       0
PC               1.00
```

2-Benzyl-3-(4-(tert-butyl)phenyl)-3-hydroxyisoindolin-1-one (3ac)

13C of t-Bu BnCN final product



9i

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Current Data Parameters
NAME          20140418
EXPNO               17
PROCNO               1

F2 - Acquisition Parameters
Date_         20140418
Time              22.57
INSTRUM           spect
PROBHD   5 mm SEI 1H-13
PULPROG          zgpg30
TD               32768
SOLVENT          CDCl3
NS                 736
DS                   0
SWH         24038.461 Hz
FIDRES       0.733596 Hz
AQ           0.6815744 sec
RG                2048
DW              20.800 usec
DE               6.50 usec
TE               299.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

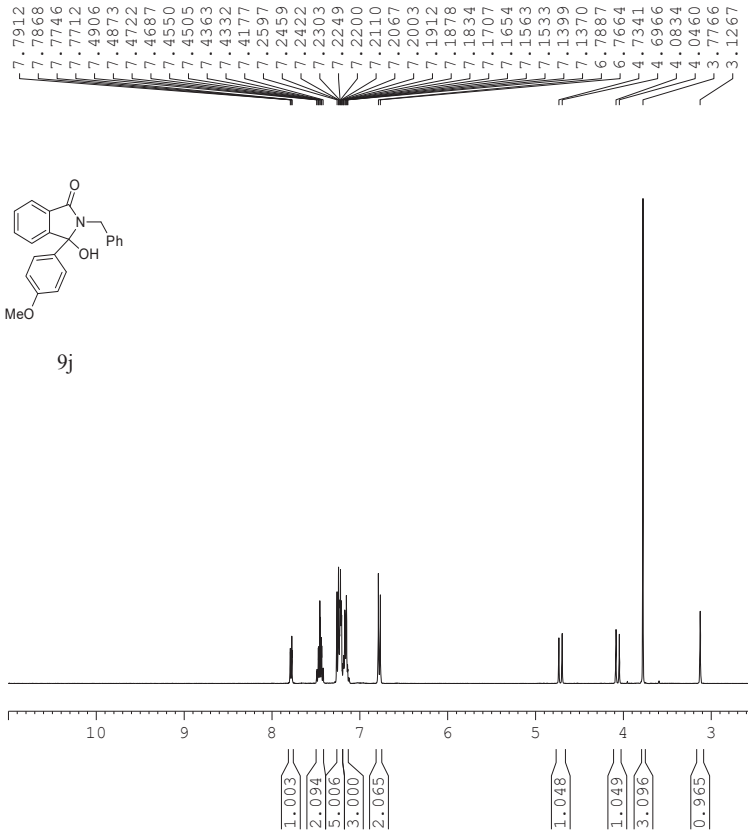
======== CHANNEL f1 ========
NUC1               13C
P1              15.50 usec
PL1              7.30 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2           90.00 usec
PL2             -4.20 dB
PL12             13.10 dB
PL13             16.10 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6127500 MHz
WDW                    EM
SSB      0
LB              1.00 Hz
GB       0
PC               1.00
```

2-Benzyl-3-hydroxy-3-(4-methoxyphenyl)isoindolin-1-one (3ad)

1H of 4-OMe BnCN final product



9j

Current Data Parameters
NAME 20140425
EXPNO 4
PROCNO 1

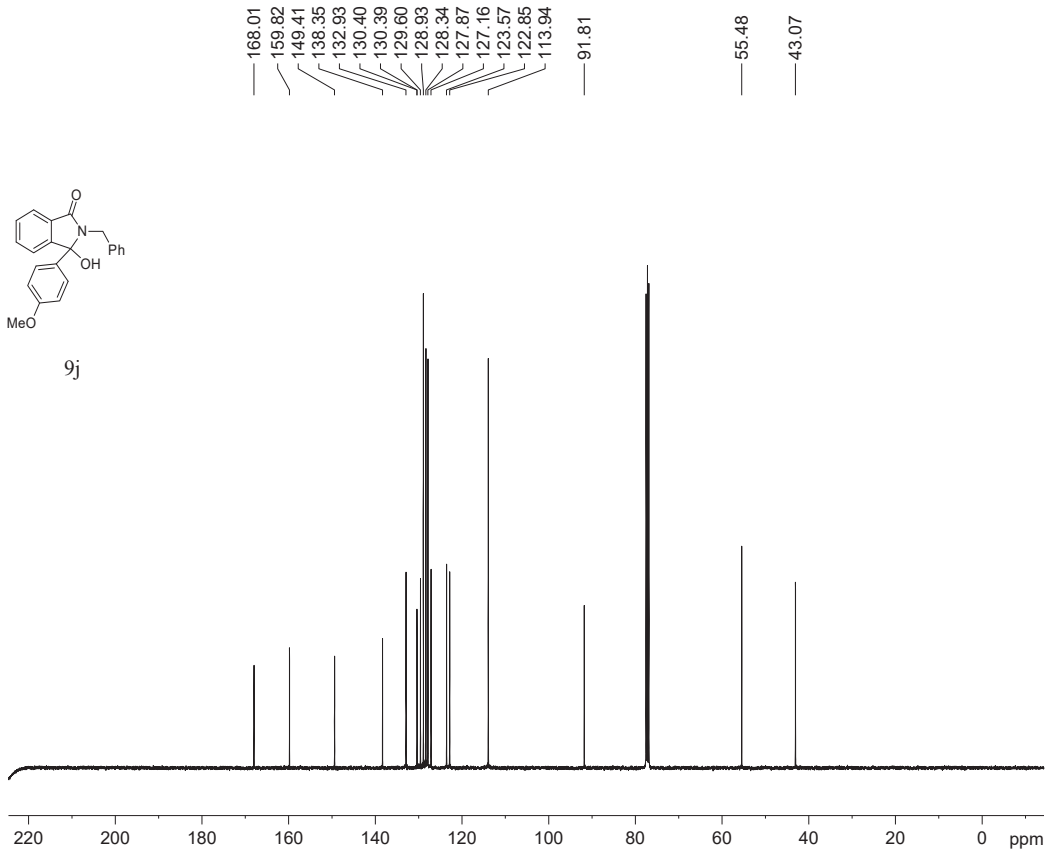
F2 - Acquisition Parameters
Date_ 20140425
Time 22.13
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300089 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

2-Benzyl-3-hydroxy-3-(4-methoxyphenyl)isoindolin-1-one (3ad)

13C of 4-OMe BnCN final product



9j

Current Data Parameters
NAME 20140425
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140425
Time 22.40
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 12318
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

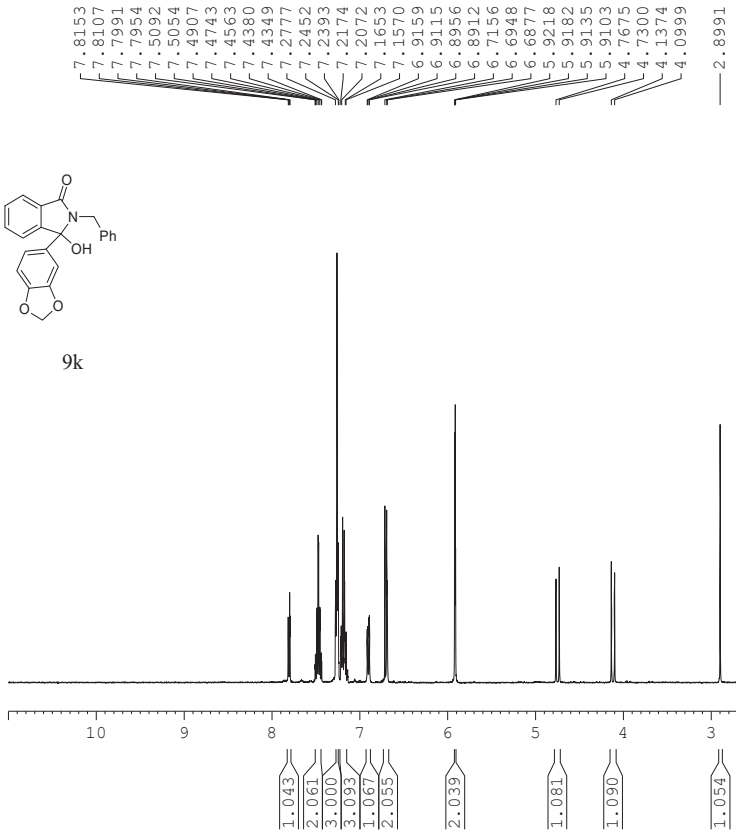
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127492 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

3-(Benzo[d][1,3]dioxol-5-yl)-2-benzyl-3-hydroxyisoindolin-1-one (3ae)

1H of methylenedioxy BnCN final product



Current Data Parameters
NAME 20131116
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131116
Time 15.55
INSTRUM SPECT
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 198.09
DW 69.333 usec
DE 10.52 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

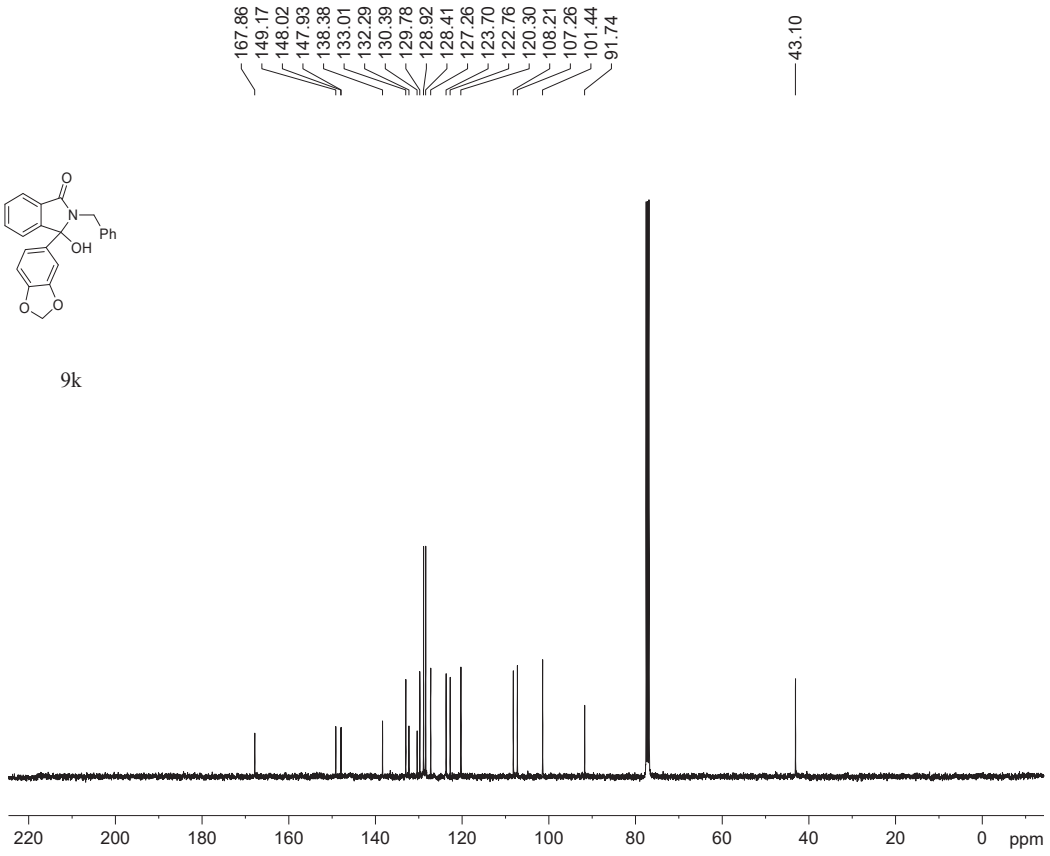
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

3-(Benzo[d][1,3]dioxol-5-yl)-2-benzyl-3-hydroxyisoindolin-1-one (3ae)

3

13C of methylenedioxy BnCN final product



Current Data Parameters
NAME 20131116
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131116
Time 14.40
INSTRUM SPECT
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 779
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

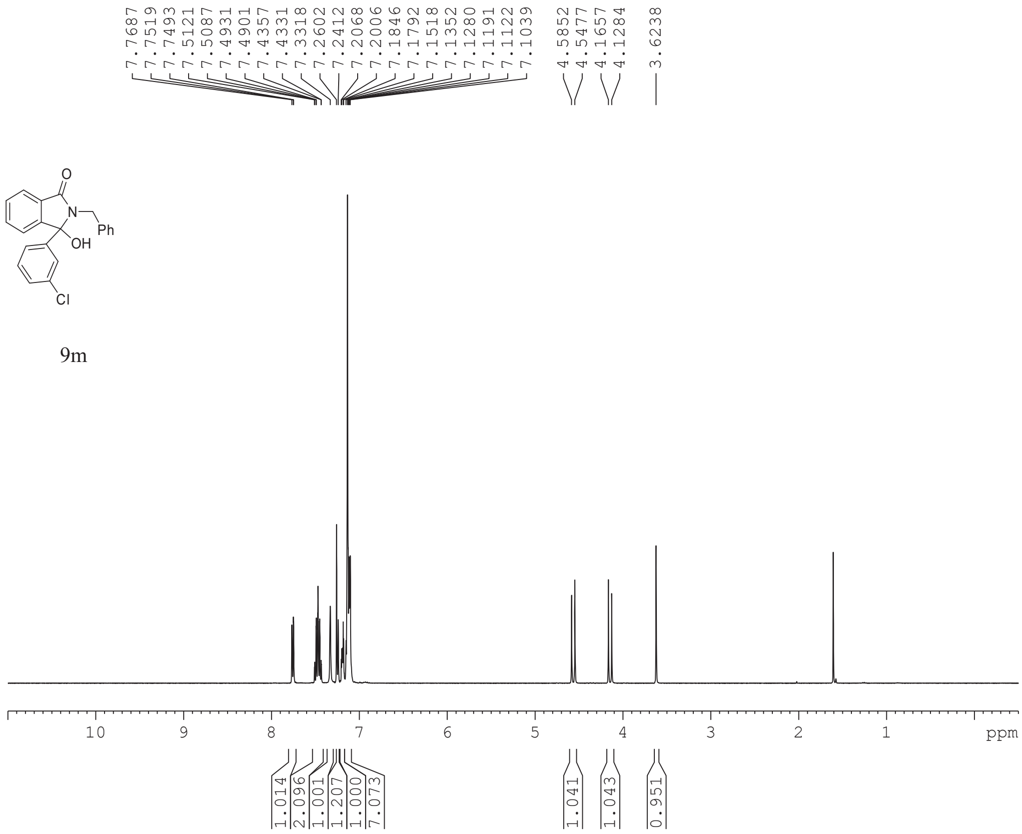
======== CHANNEL f1 ========
SFO1 100.6233324 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127462 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

2-Benzyl-3-(3-chlorophenyl)-3-hydroxyisoindolin-1-one (3af)

1H of 3-Cl BnCN final product



Current Data Parameters
NAME 20140418
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140418
Time 15.14
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
TD0 1

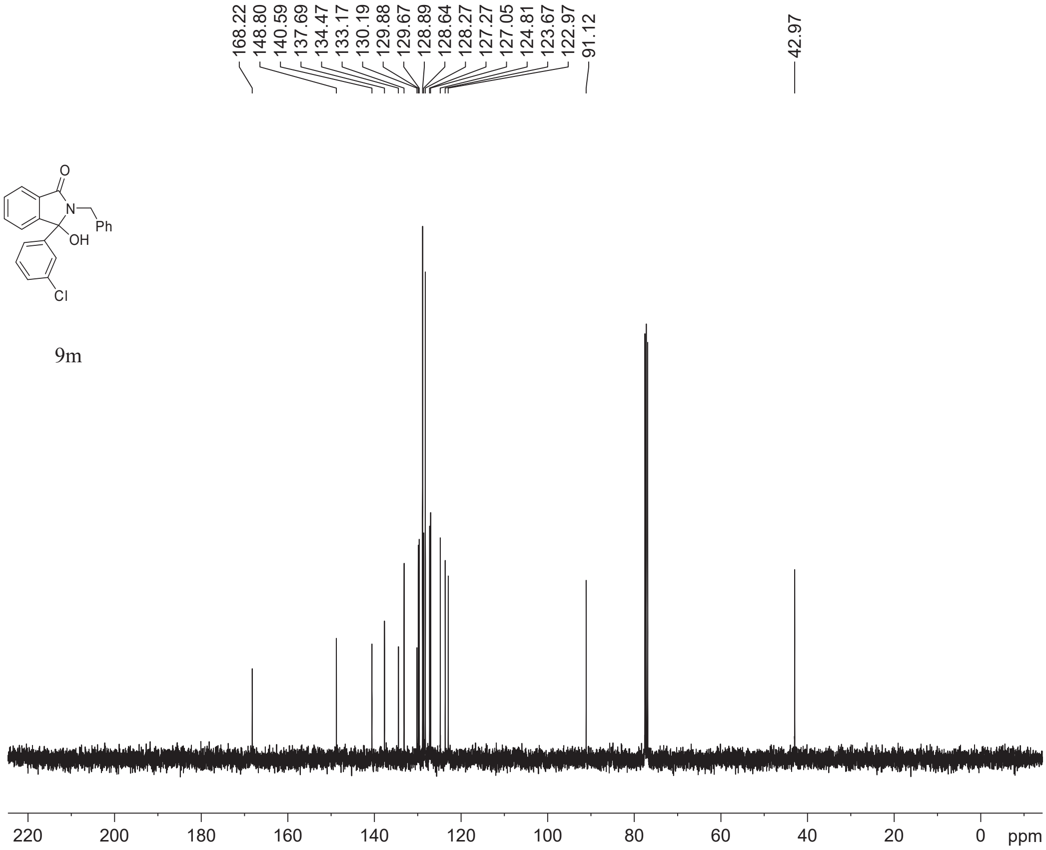
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

2-Benzyl-3-(3-chlorophenyl)-3-hydroxyisoindolin-1-one (3af)

2

13C of 3-Cl BnCN final product



Current Data Parameters
NAME 20140418
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140418
Time 15.36
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 116
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2048
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

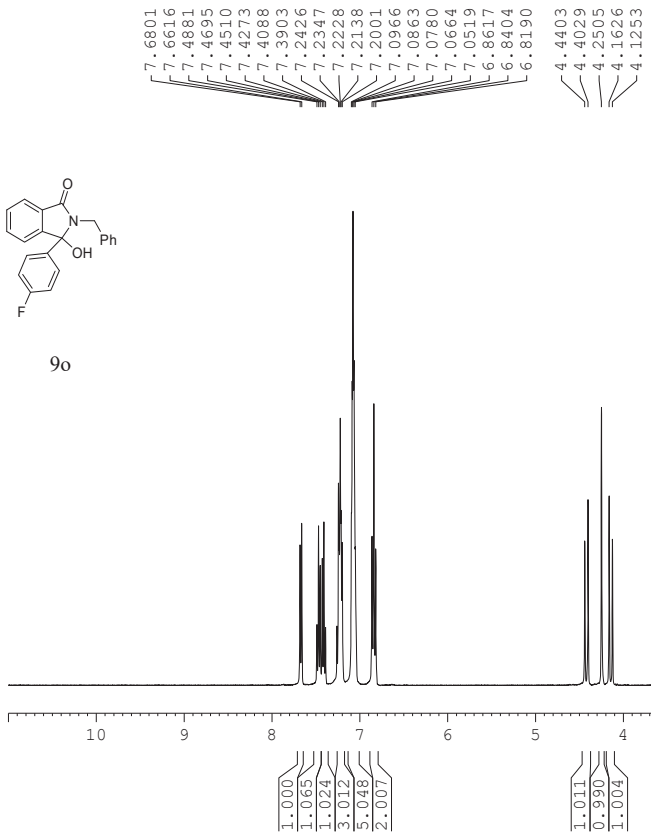
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127506 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

2-Benzyl-3-(4-fluorophenyl)-3-hydroxyisoindolin-1-one (3ag)

1H of 4-F BnCN final product



Current Data Parameters
NAME 20140415
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140415
Time 21.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
TD0 1

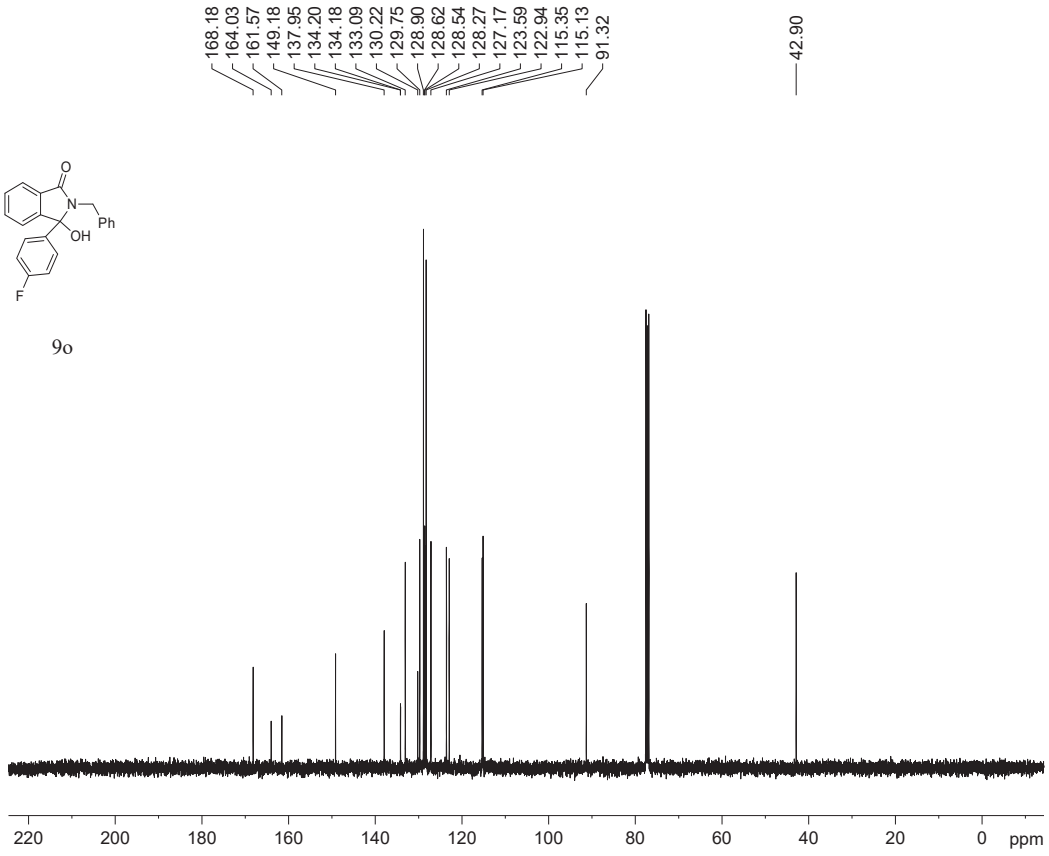
======== CHANNEL f1 ========
NUC1 1H
P1 14.35 usec
PL1 -2.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

2-Benzyl-3-(4-fluorophenyl)-3-hydroxyisoindolin-1-one (3ag)

2

13C of 4-F BnCN final product



Current Data Parameters
NAME 20140415
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140415
Time 21.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 134
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

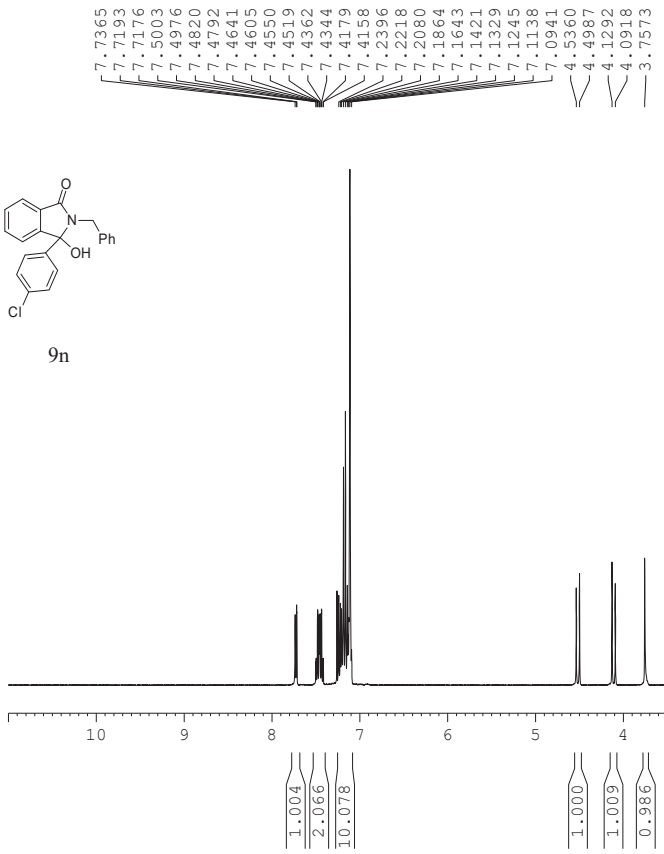
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 13.95 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127506 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

2-Benzyl-3-(4-chlorophenyl)-3-hydroxyisoindolin-1-one (3ah)

1H of 4-Cl BnCN final product



9n

Current Data Parameters
NAME 20131206
EXPNO 5
PROCNO 1

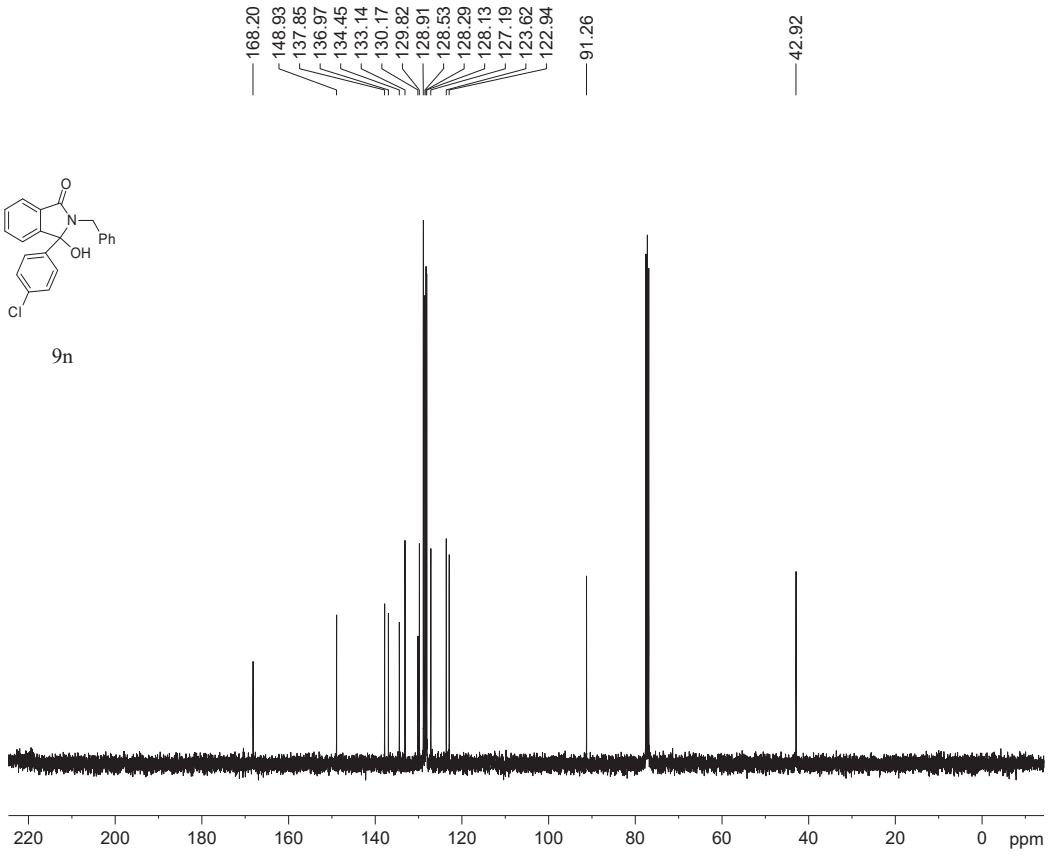
F2 - Acquisition Parameters
Date_ 20131206
Time 10.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

2-Benzyl-3-(4-chlorophenyl)-3-hydroxyisoindolin-1-one (3ah)

13C of 4-Cl BnCN final product



9n

Current Data Parameters
NAME 20131206
EXPNO 11
PROCNO 1

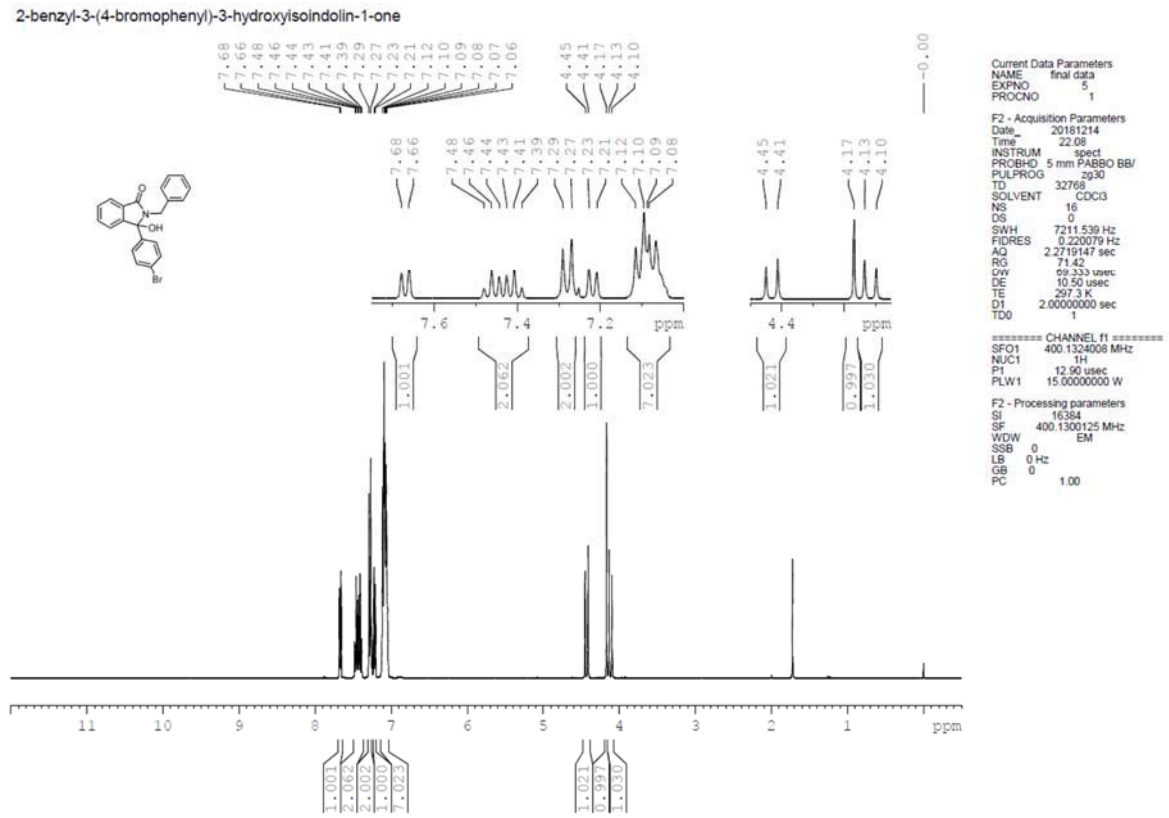
F2 - Acquisition Parameters
Date_ 20131206
Time 11.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 105
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

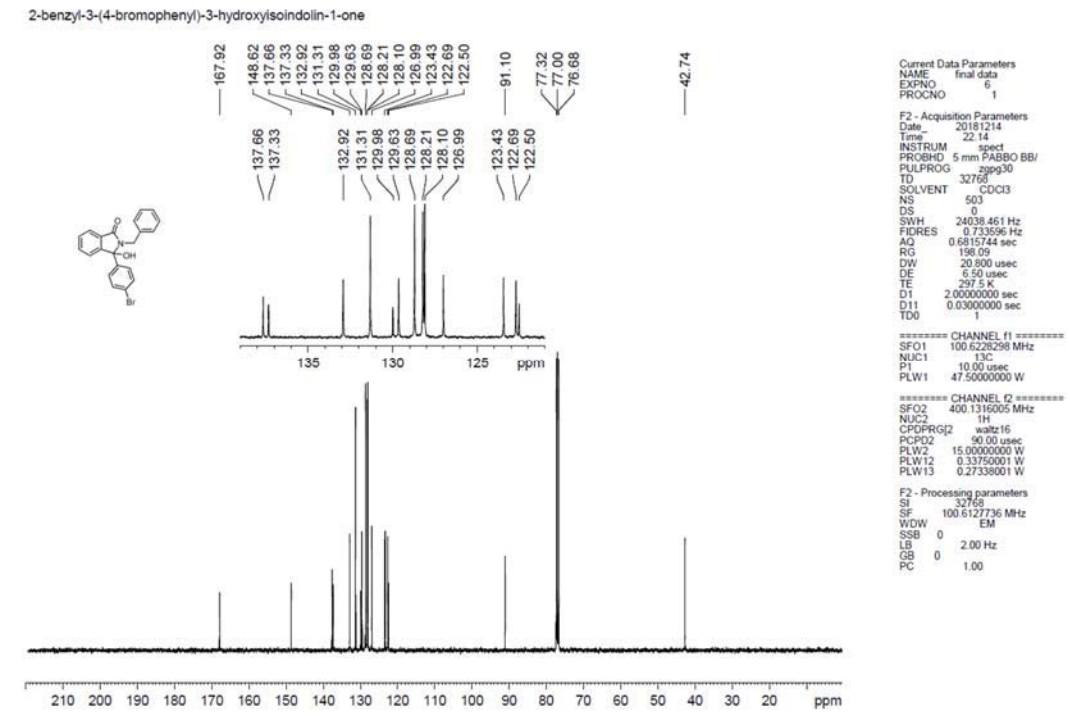
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

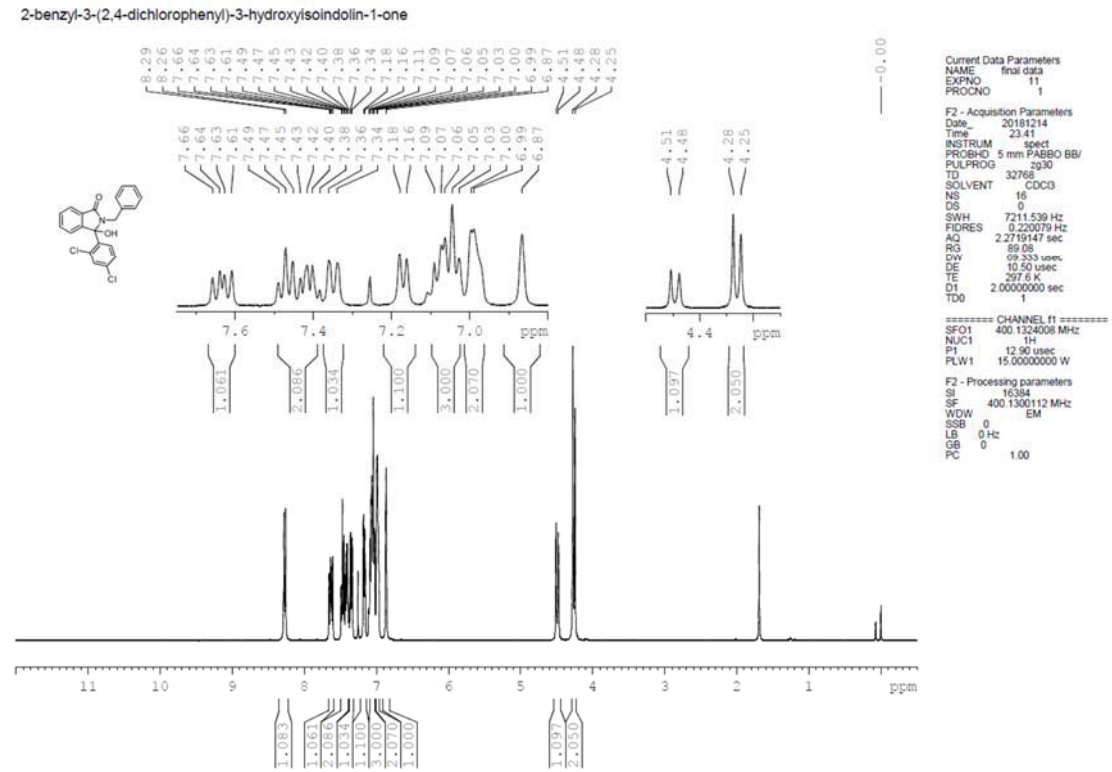
^{1}H NMR spectra of 2-Benzyl-3-(4-bromophenyl)-3-hydroxyisoindolin-1-one (**3ai**)



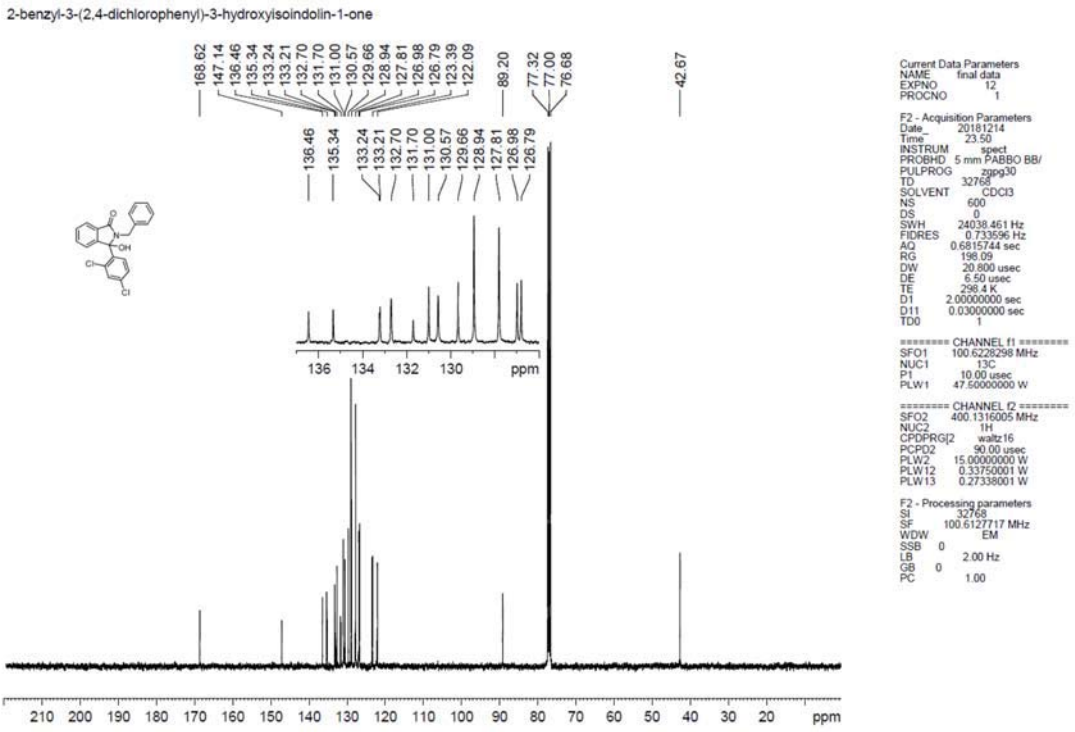
^{13}C NMR spectra of 2-Benzyl-3-(4-bromophenyl)-3-hydroxyisoindolin-1-one (**3ai**)



^{1}H NMR spectra of 2-Benzyl-3-(2,4-dichlorophenyl)-3-hydroxyisoindolin-1-one (**3aj**)

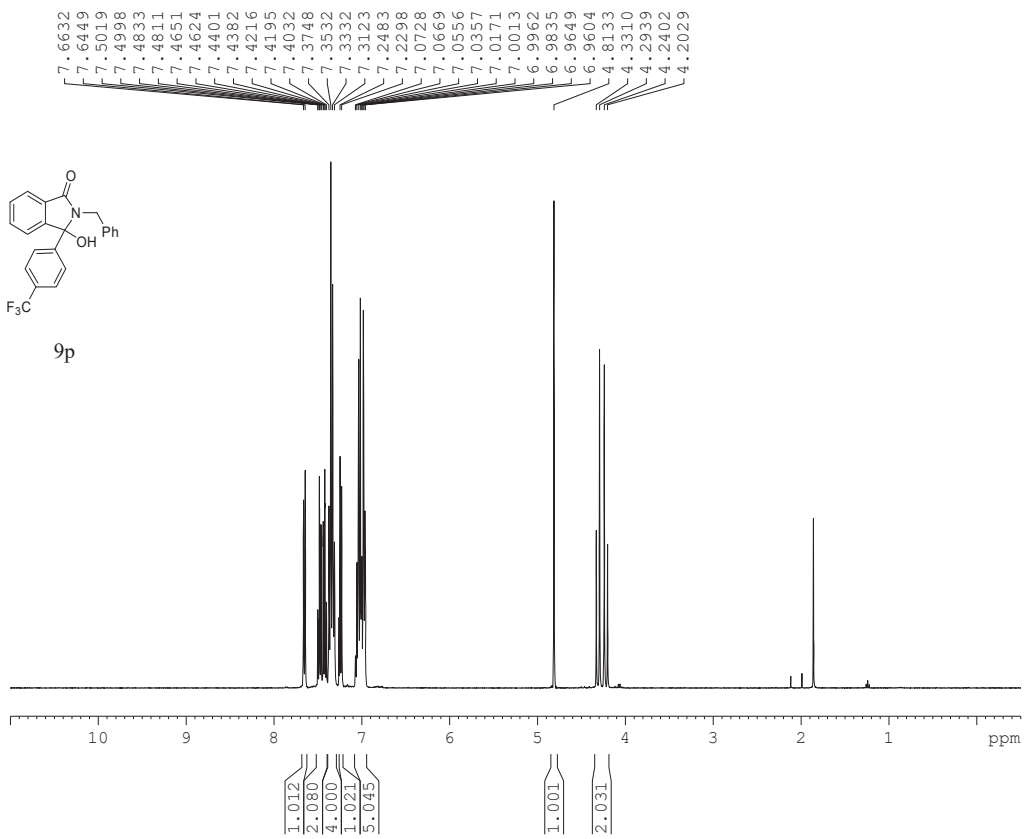


^{13}C NMR spectra of 2-Benzyl-3-(2,4-dichlorophenyl)-3-hydroxyisoindolin-1-one (**3aj**)



2-Benzyl-3-hydroxy-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (3ak)

1H of CF3 BnCN final product



Current Data Parameters
NAME 20140418
EXPNO 3
PROCNO 1

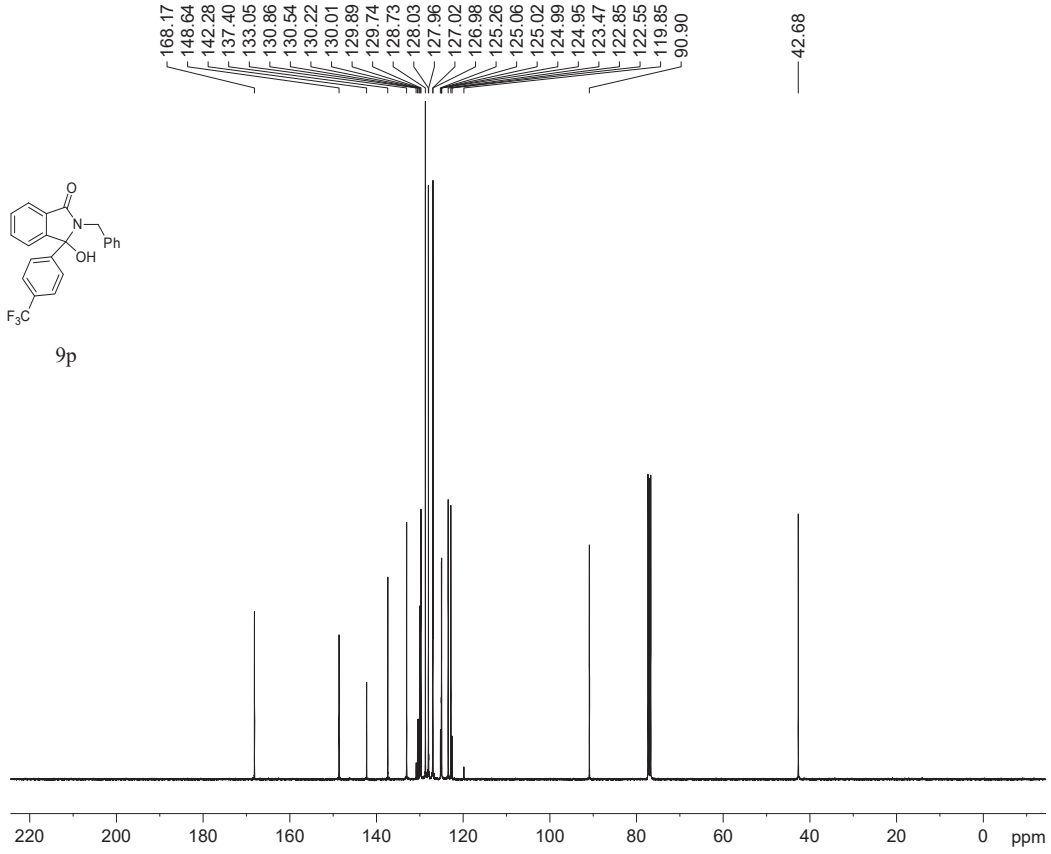
F2 - Acquisition Parameters
Date_ 20140418
Time 13.47
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 45.3
DW 69.000 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300087 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

2-Benzyl-3-hydroxy-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (3ak)

13C of CF3 BnCN final product



Current Data Parameters
NAME 20140418
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140419
Time 0.39
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 10620
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2048
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

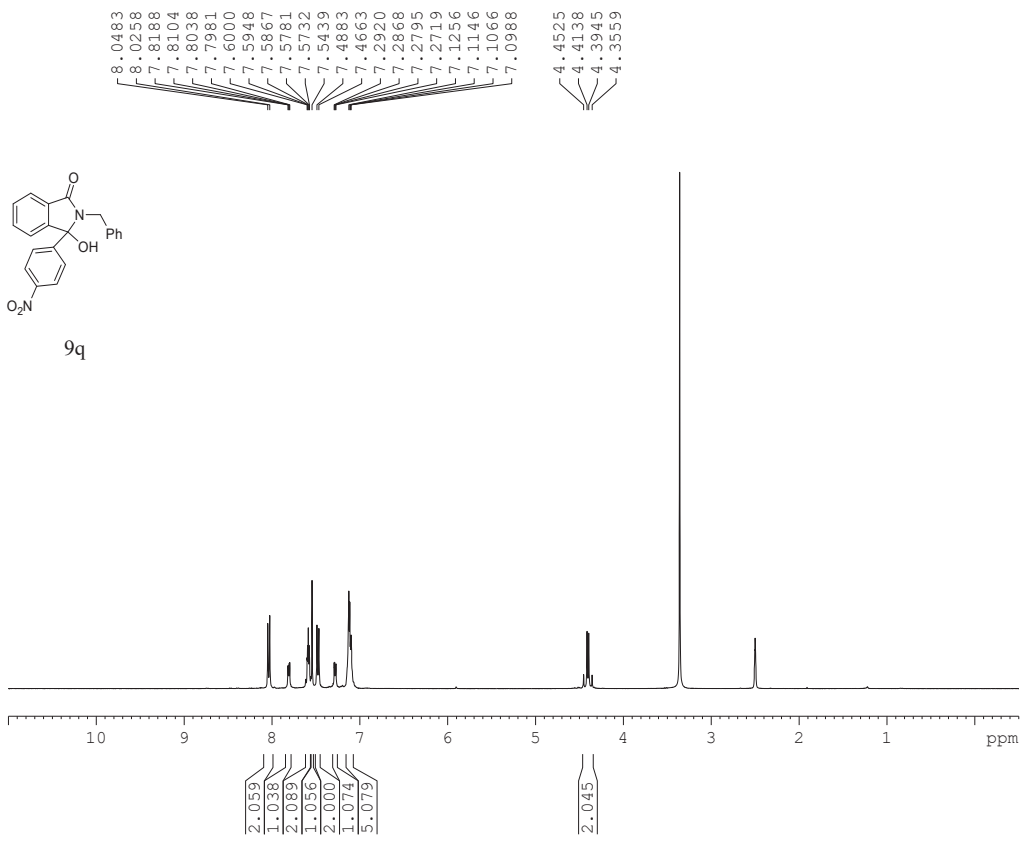
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

2-Benzyl-3-hydroxy-3-(4-nitrophenyl)isoindolin-1-one (3al)

1H of 4-NO2 BnCN final product



Current Data Parameters
NAME 20140430
EXPNO 1
PROCNO 1

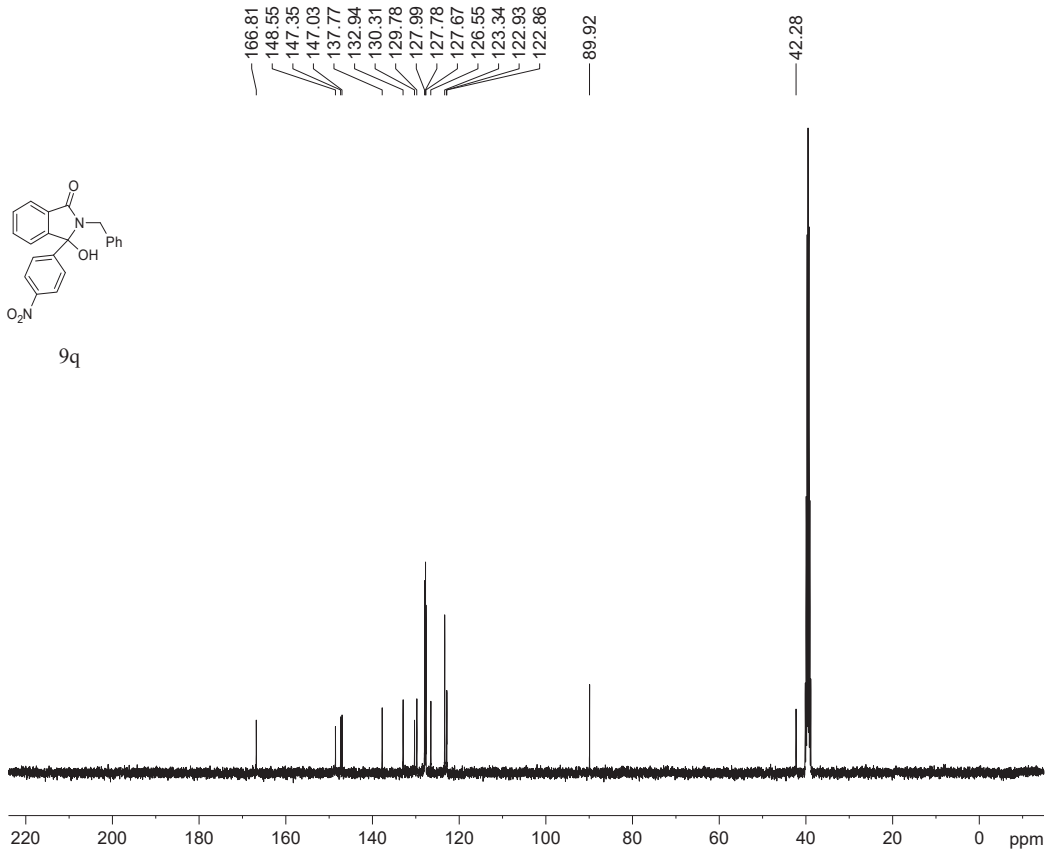
F2 - Acquisition Parameters
Date_ 20140430
Time 20.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 71.42
DW 69.333 usec
DE 10.52 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

2-Benzyl-3-hydroxy-3-(4-nitrophenyl)isoindolin-1-one (3al)

13C of 4-NO2 BnCN final product



Current Data Parameters
NAME 20140502
EXPNO 2
PROCNO 1

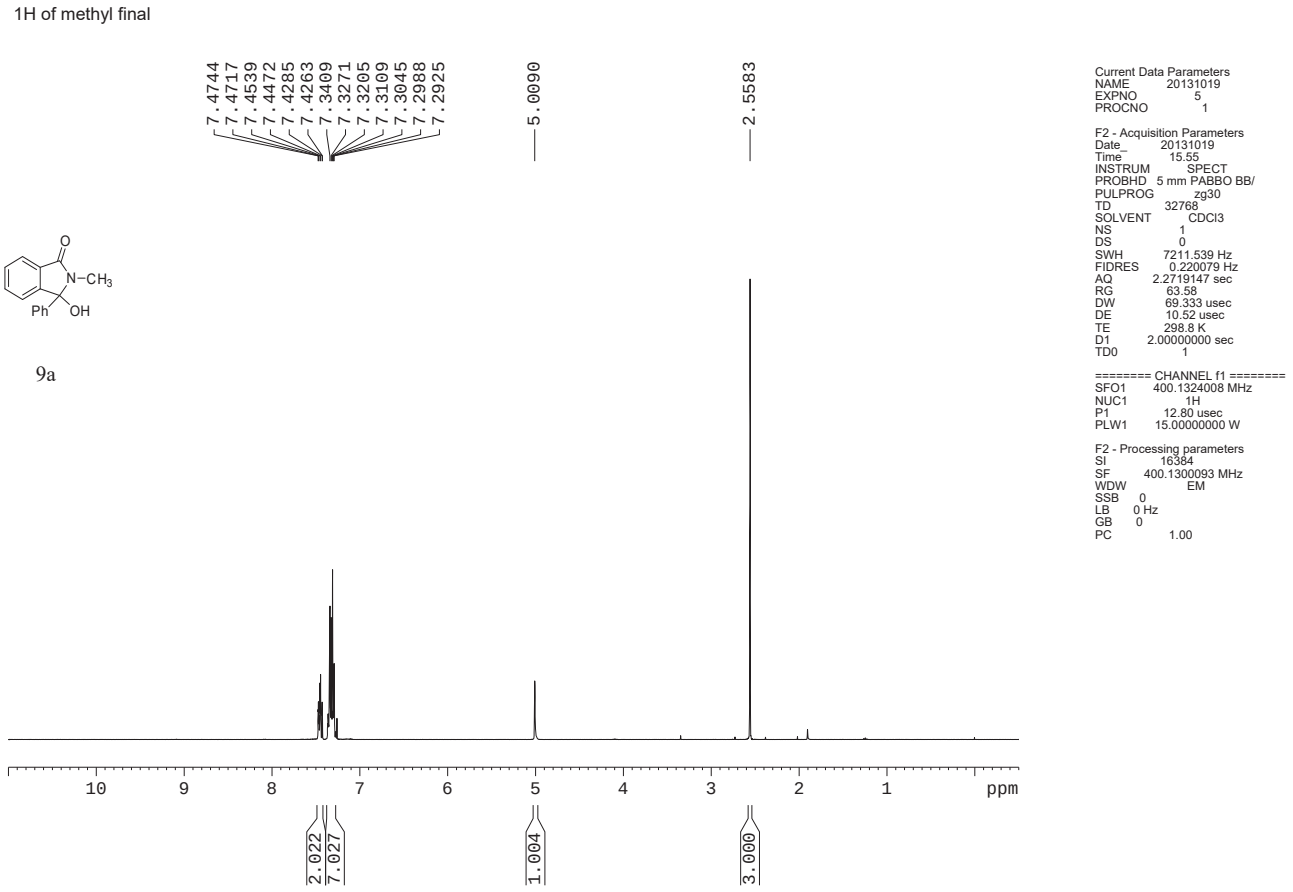
F2 - Acquisition Parameters
Date_ 20140502
Time 16.52
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 499
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128154 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 3-Hydroxy-2-methyl-3-phenylisoindolin-1-one (3ba)



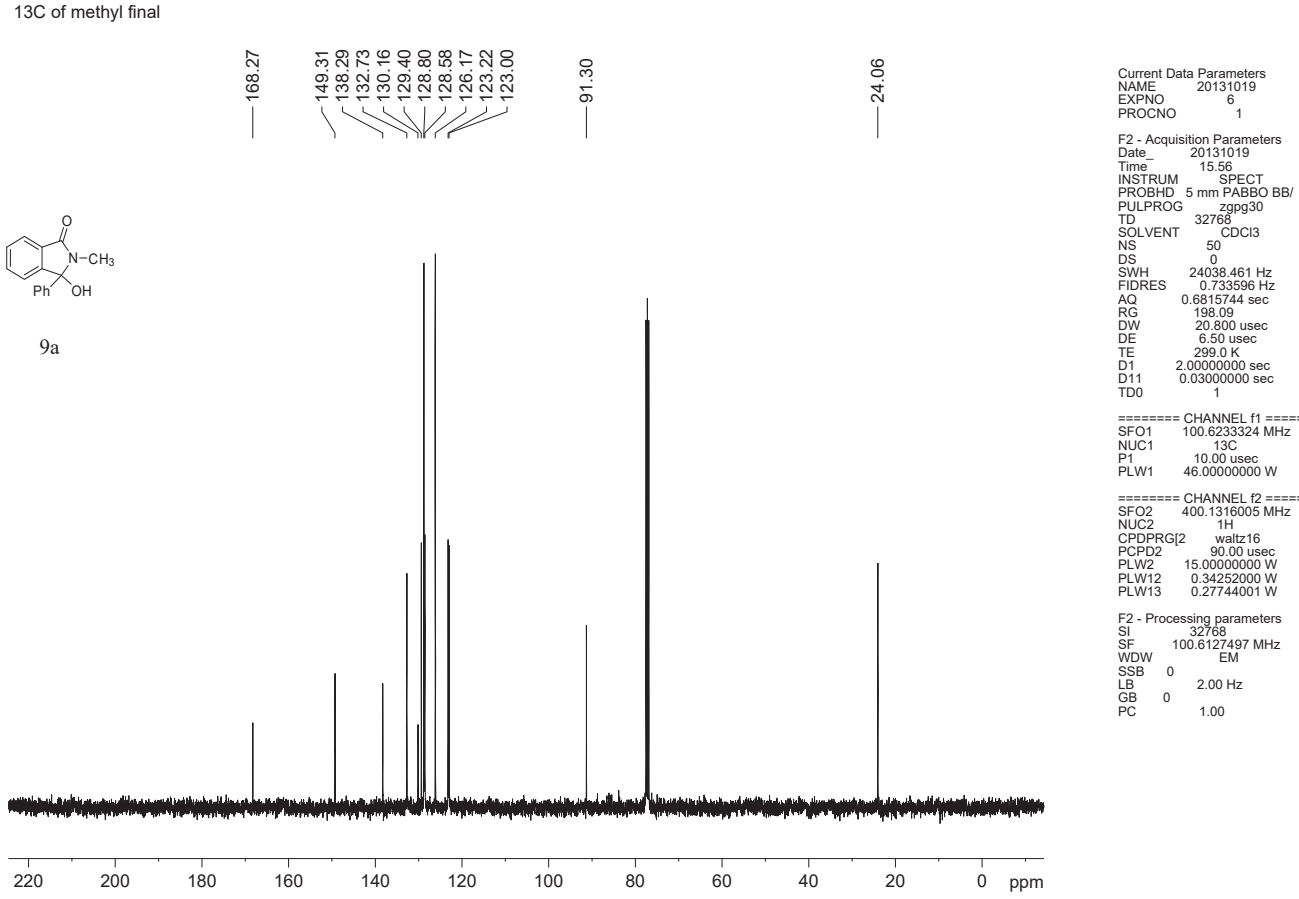
Current Data Parameters
NAME 20131019
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131019
Time 15.55
INSTRUM SPECT
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 63.58
DW 69.333 usec
DE 10.52 usec
TE 298.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 3-Hydroxy-2-methyl-3-phenylisoindolin-1-one (3ba)



Current Data Parameters
NAME 20131019
EXPNO 6
PROCNO 1

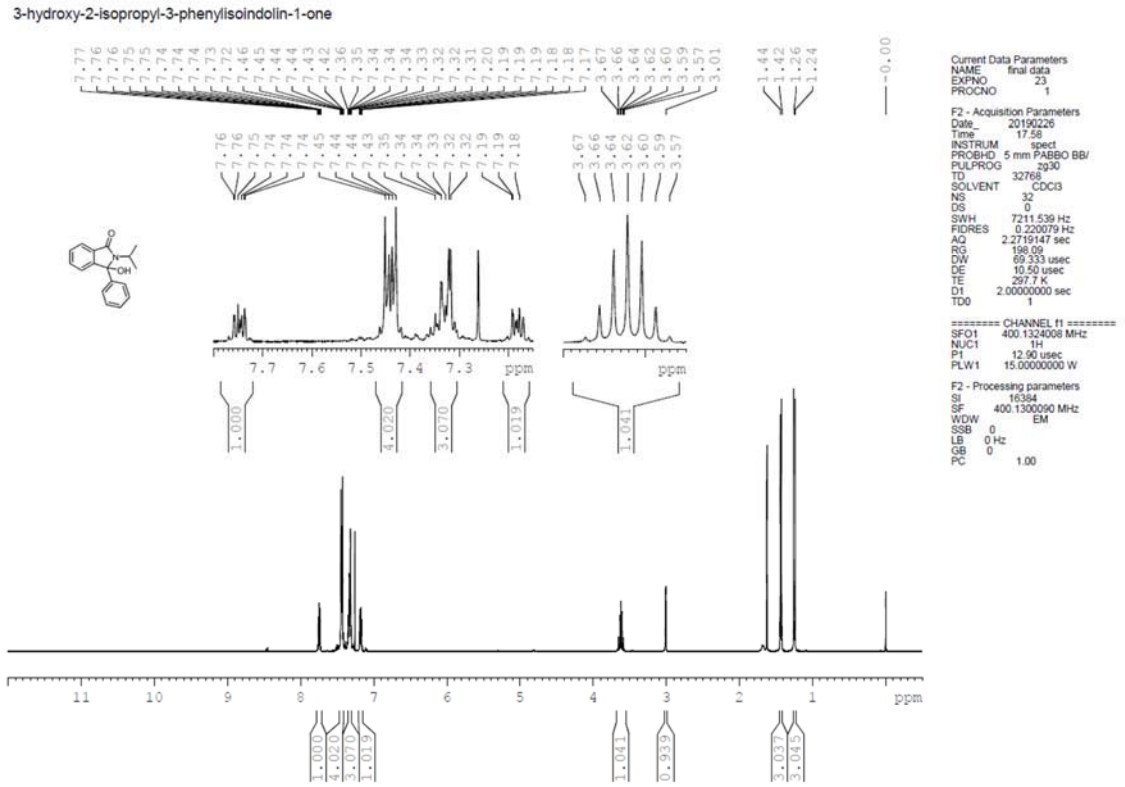
F2 - Acquisition Parameters
Date_ 20131019
Time 15.56
INSTRUM SPECT
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 50
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233324 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

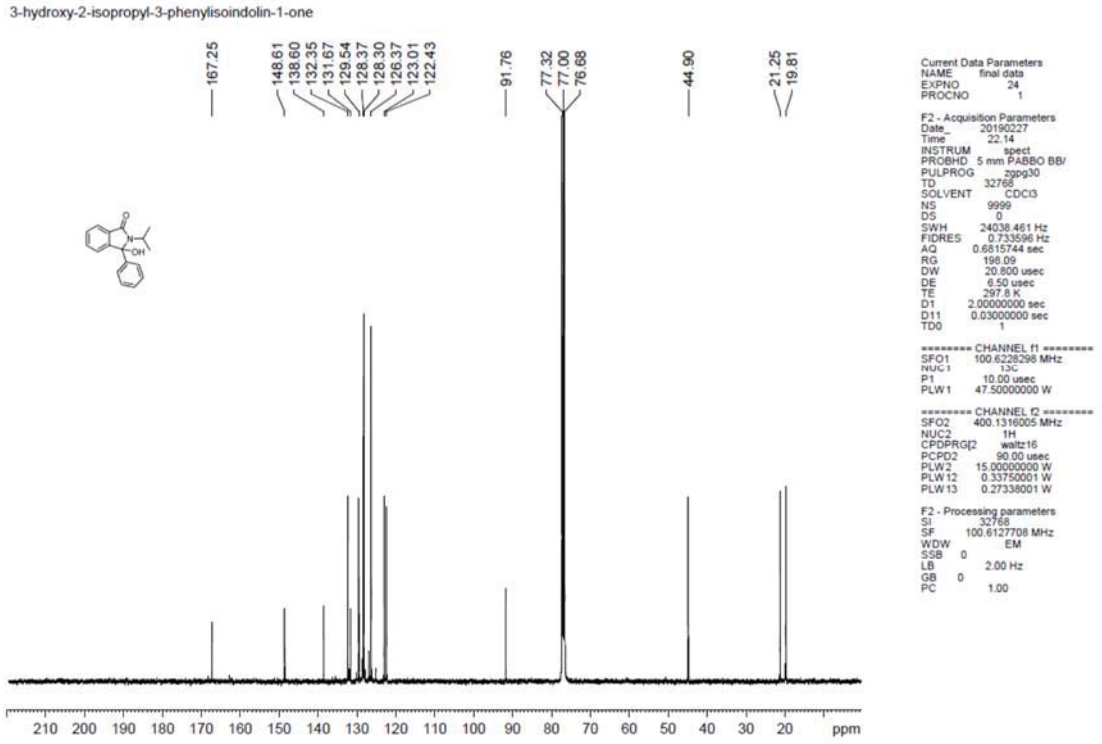
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127497 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

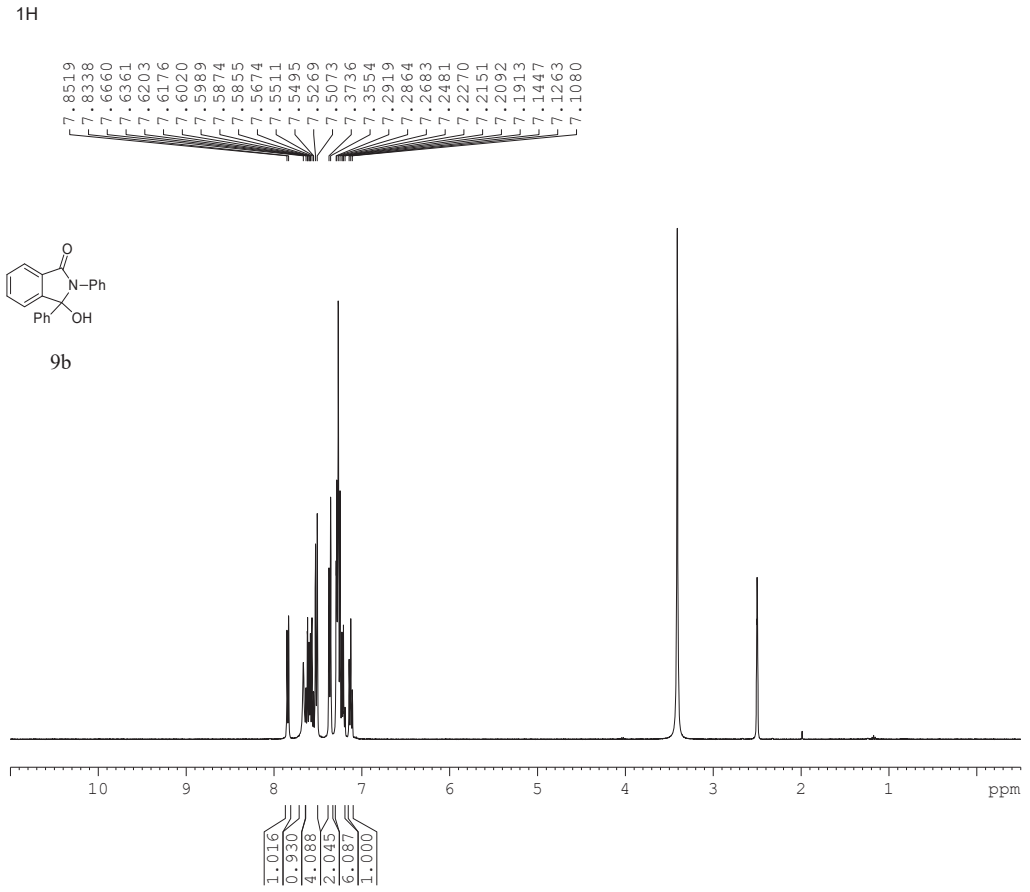
^{1}H NMR spectra of 3-hydroxy-2-isopropyl-3-phenylisoindolin-1-one (**3ca**)



^{13}C NMR spectra of 3-hydroxy-2-isopropyl-3-phenylisoindolin-1-one (**3ca**)



1H NMR of 3-Hydroxy-2,3-diphenylisoindolin-1-one (3da)



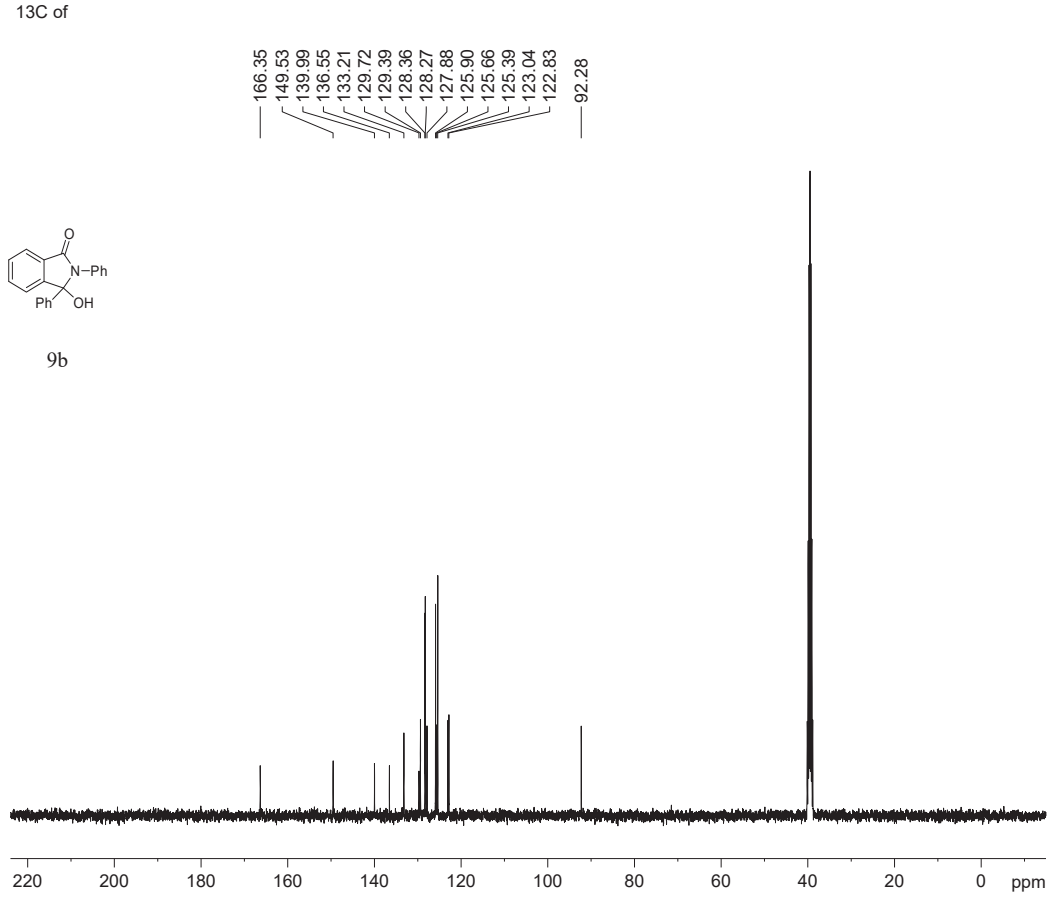
Current Data Parameters
NAME 20140106
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140106
Time 14.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 4
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 71.42
DW 69.333 usec
DE 10.52 usec
TE 297.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 3-Hydroxy-2,3-diphenylisoindolin-1-one (3da)



Current Data Parameters
NAME 20140106
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140106
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 66
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

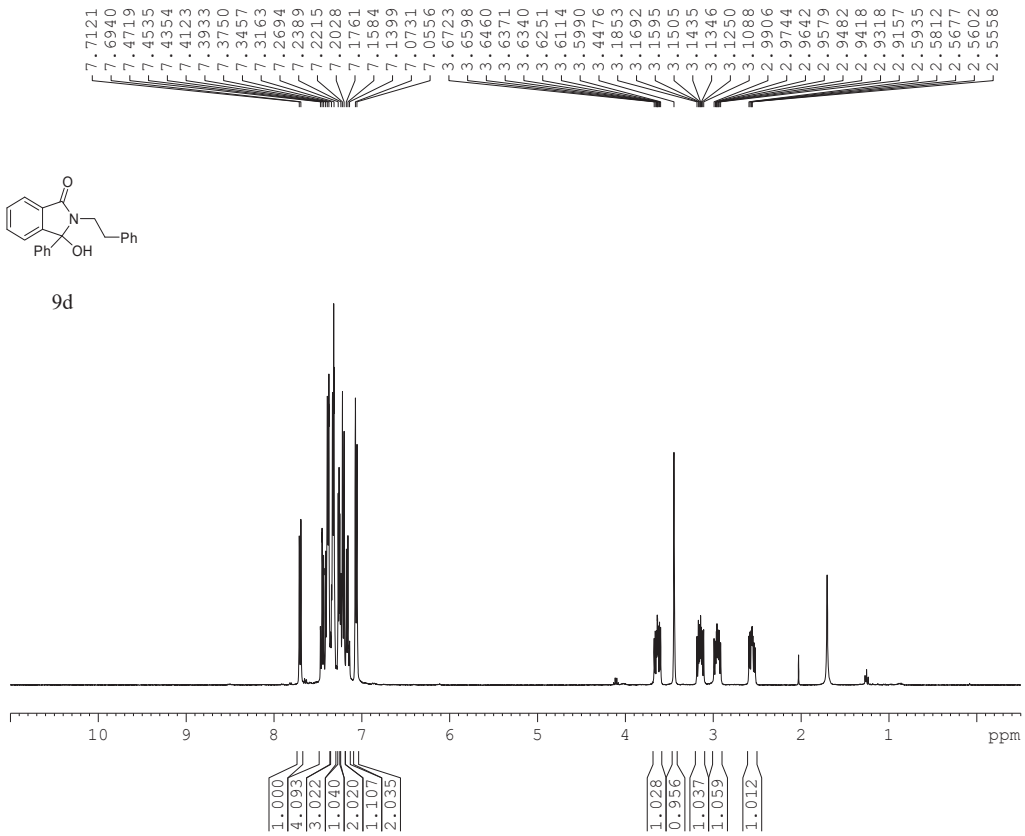
======== CHANNEL f1 ========
SFO1 100.6233324 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6128170 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

3-Hydroxy-2-phenethyl-3-phenylisoindolin-1-one (3ea)

1H of N-ethylphenyl final product



9d

```
Current Data Parameters
NAME          20140418
EXPNO             14
PROCNO             1

F2 - Acquisition Parameters
Date_         20140418
Time              22.10
INSTRUM           spect
PROBHD   5 mm SEI 1H-13
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                  16
DS                   0
SWH           7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2609921 sec
RG                 114
DW              69.000 usec
DE               6.50 usec
TE              299.6 K
D1            2.00000000 sec
TD0                 1

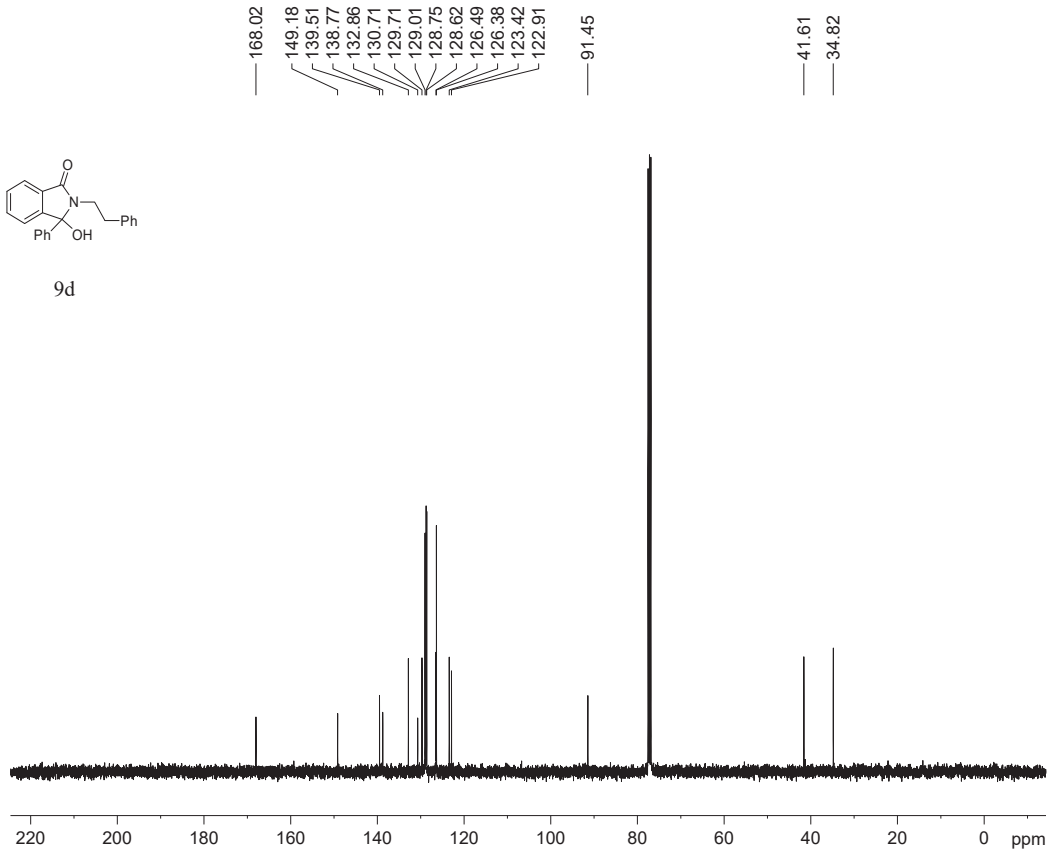
======== CHANNEL f1 ========
NUC1               1H
P1              11.00 usec
PL1             -4.20 dB
SFO1       400.1324008 MHz

F2 - Processing parameters
SI                16384
SF         400.1300091 MHz
WDW                EM
SSB       0
LB      0 Hz
GB        0
PC              1.00
```

3-Hydroxy-2-phenethyl-3-phenylisoindolin-1-one (3ea)

3-hydroxy-2-phenethyl-3-phenylisoindolin-1-e

13C of N-ethylphenyl final product



9d

```
Current Data Parameters
NAME          20140418
EXPNO             15
PROCNO             1

F2 - Acquisition Parameters
Date_         20140418
Time              22.13
INSTRUM           spect
PROBHD   5 mm SEI 1H-13
PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
NS                 500
DS                   0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                4096
DW              20.800 usec
DE               6.50 usec
TE              299.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                 1

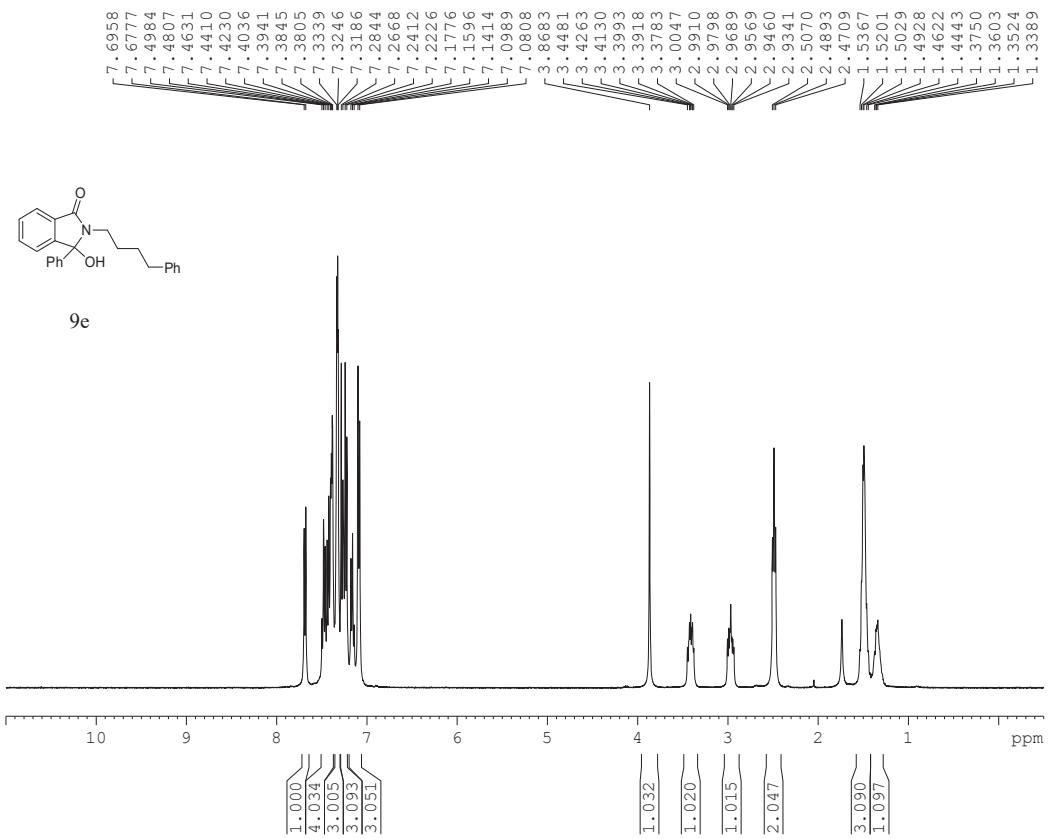
======== CHANNEL f1 ========
NUC1              13C
P1              15.50 usec
PL1              7.30 dB
SFO1       100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2           90.00 usec
PL2             -4.20 dB
PL12             13.10 dB
PL13             16.10 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127484 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.00
```

3-Hydroxy-3-phenyl-2-(4-phenylbutyl)isoindolin-1-one (3fa)

1H of butyl phenyl final




```
Current Data Parameters
NAME          20131112
EXPNO                3
PROCNO               1

F2 - Acquisition Parameters
Date_        20131112
Time             21.40
INSTRUM          SPECT
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                71.42
DW               69.333 usec
DE               10.52 usec
TE               298.6 K
D1            2.00000000 sec
TD0                  1

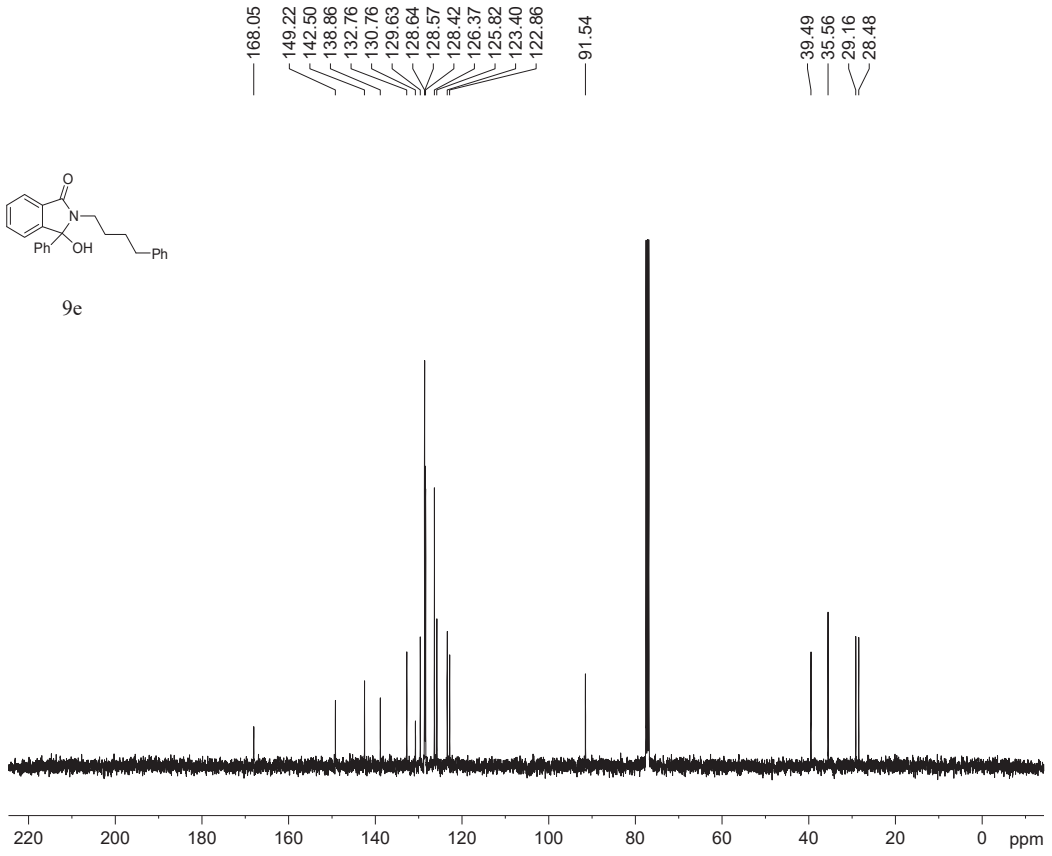
======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                1H
P1                12.80 usec
PLW1        15.00000000 W

F2 - Processing parameters
SI                  16384
SF          400.1300000 MHz
WDW                 EM
SSB     0
LB      0 Hz
GB      0
PC                1.00
```

3-Hydroxy-3-phenyl-2-(4-phenylbutyl)isoindolin-1-one (3fa)

3-hydroxy-3-phenyl-2-(4-phenylbutyl)isoindolin-1-one

13C of butyl phenyl final




```
Current Data Parameters
NAME          20131112
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_        20131112
Time             21.42
INSTRUM          SPECT
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD               32768
SOLVENT          CDCl3
NS                 100
DS                   0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
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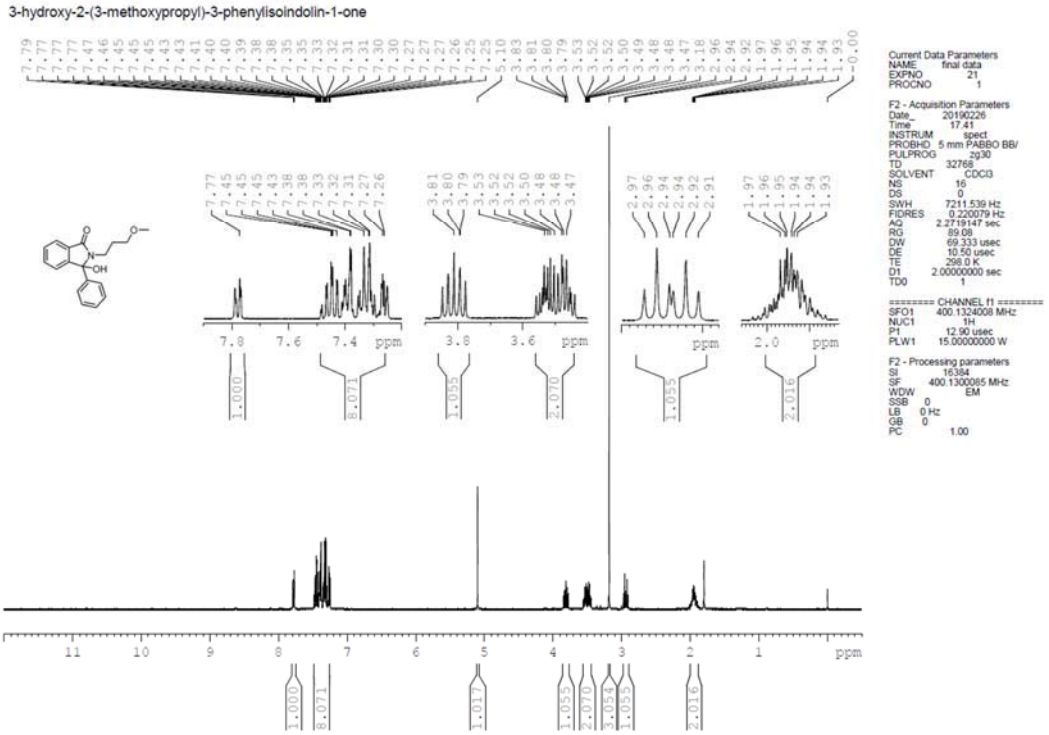
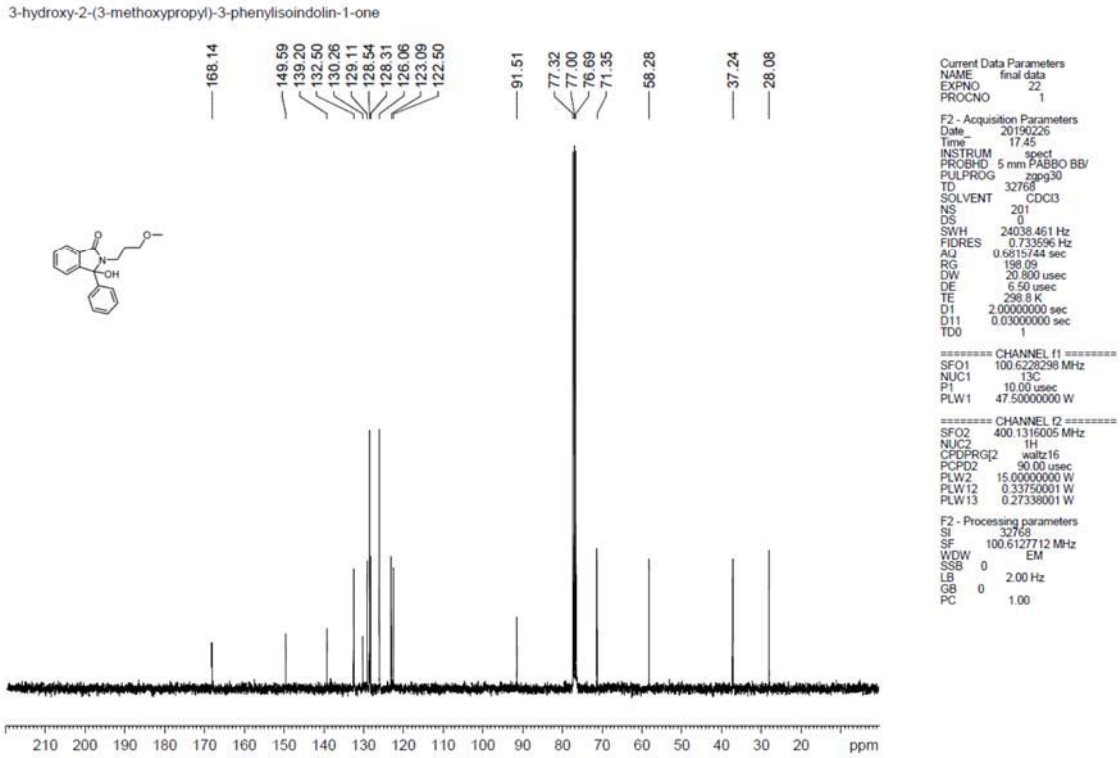
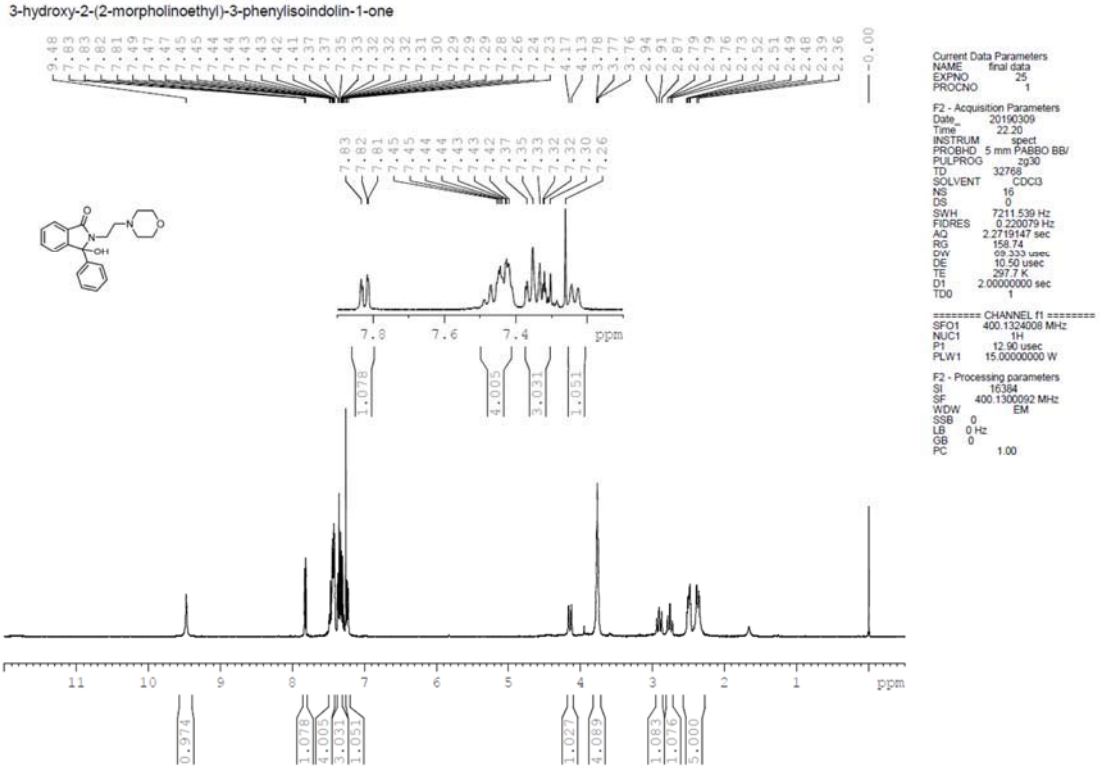
^{1}H NMR spectra of 3-hydroxy-2-(3-methoxypropyl)-3-phenylisoindolin-1-one (**3ga**)



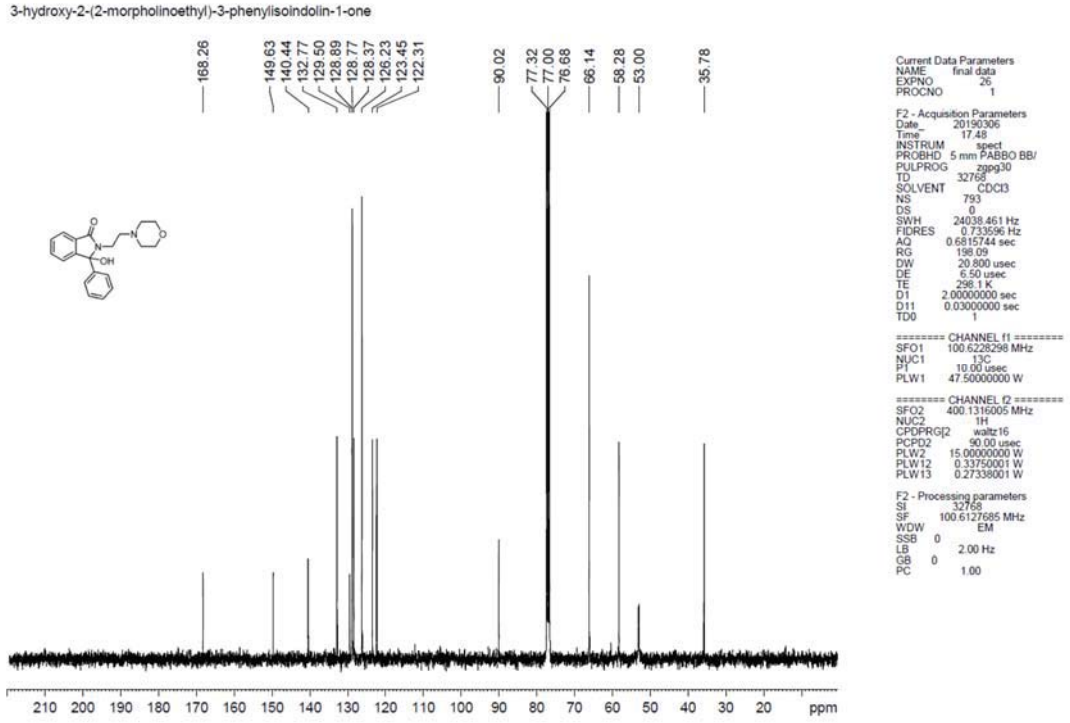
^{13}C NMR spectra of 3-hydroxy-2-(3-methoxypropyl)-3-phenylisoindolin-1-one (**3ga**)



^{1}H NMR spectra of 3-hydroxy-2-(2-morpholinoethyl)-3-phenylisoindolin-1-one (**3ha**)



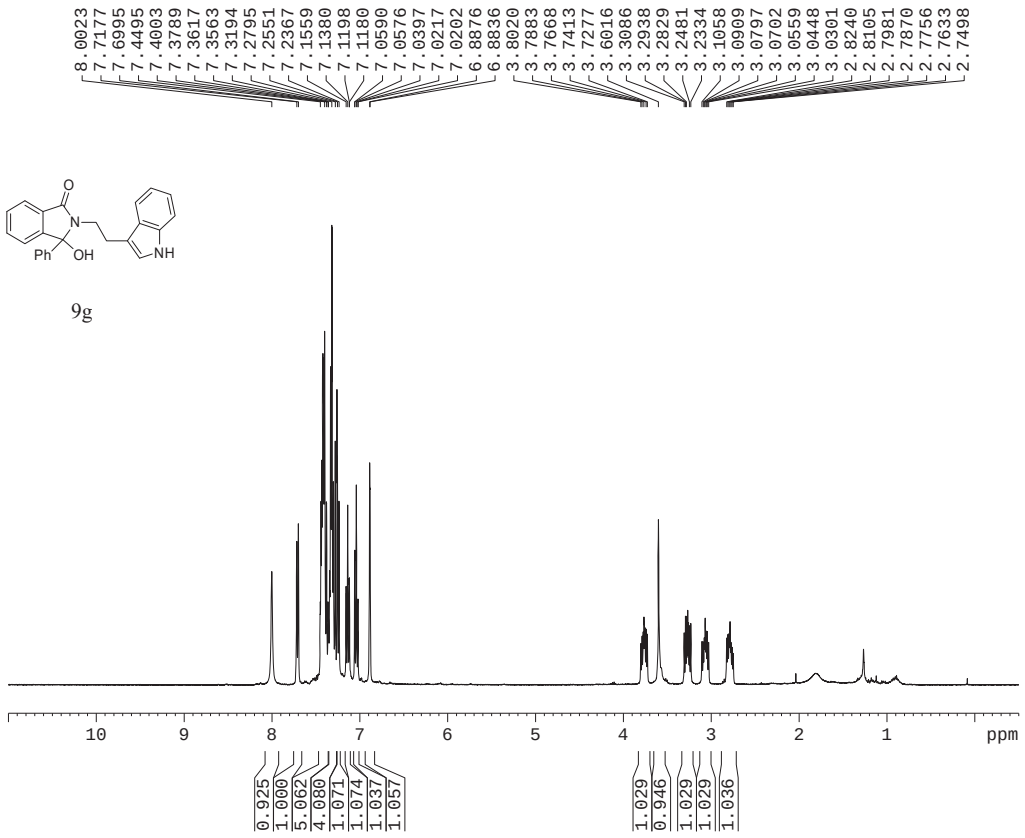
^{13}C NMR spectra of 3-hydroxy-2-(2-morpholinoethyl)-3-phenylisoindolin-1-one (**3ha**)



2-(2-(1H-Indol-3-yl)ethyl)-3-hydroxy-3-phenylisoindolin-1-one (3ia)

2-(2-(1H-indol-3-yl)ethyl)-3-hydroxy-3-phenylisoindolin-1-one

1H of N-c2h4indole final



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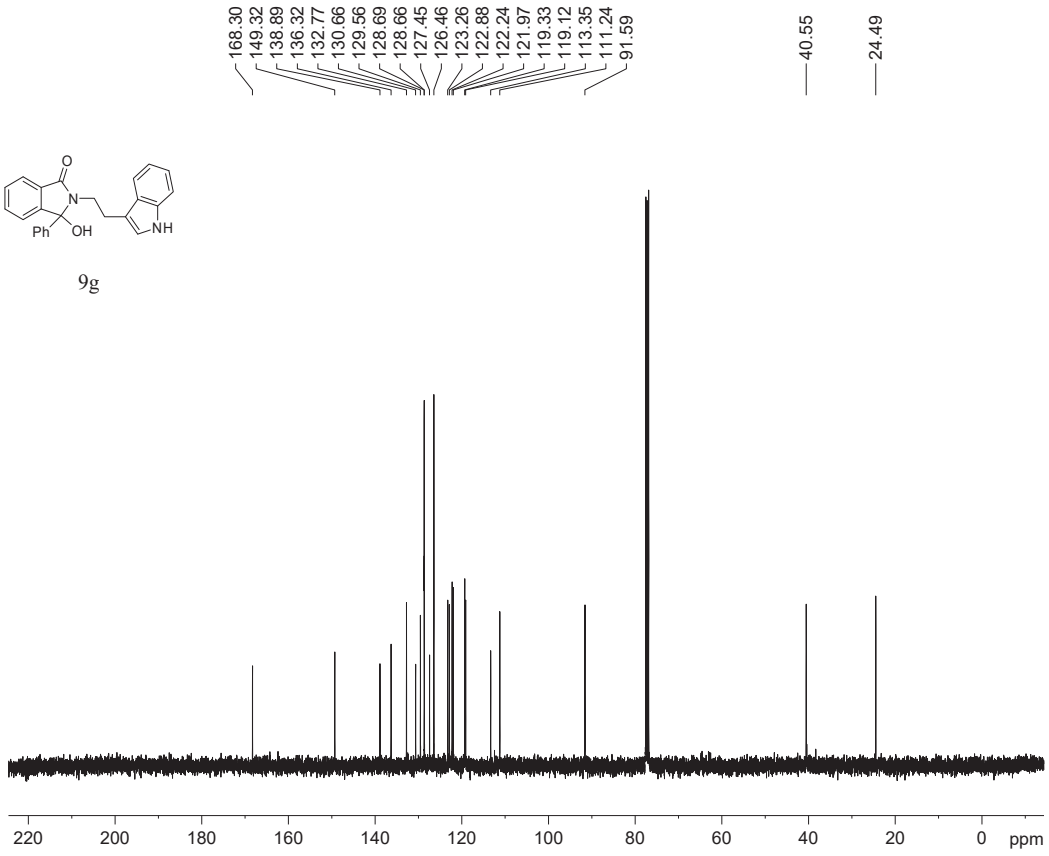
2-(2-(1H-Indol-3-yl)ethyl)-3-hydroxy-3-phenylisoindolin-1-one (3ia)

2-(2-(1H-indol-3-yl)ethyl)-3-hydroxy-3-phenylisoindolin-1-one

13C of N-c2h4indole final product



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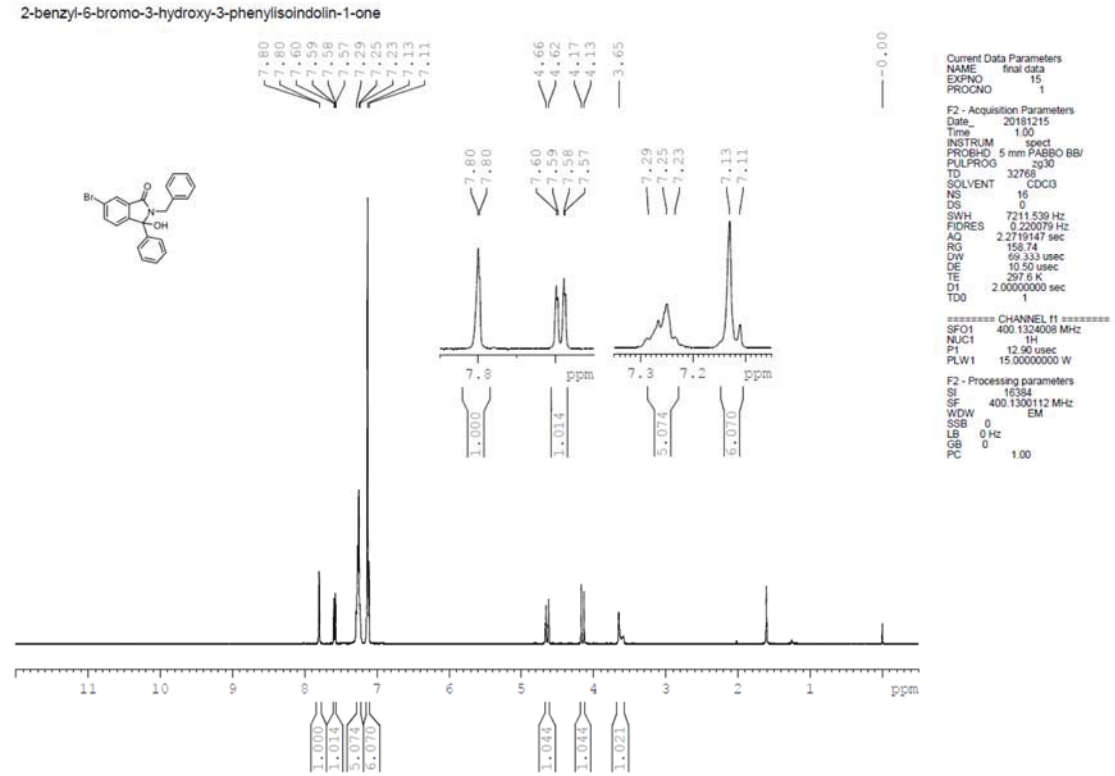
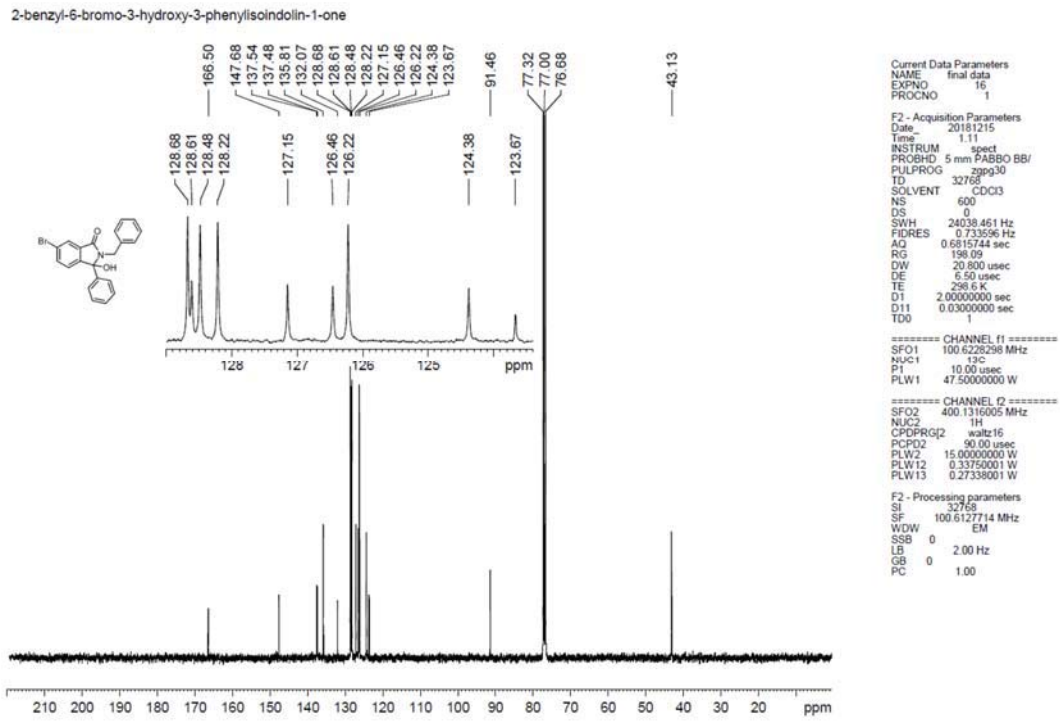
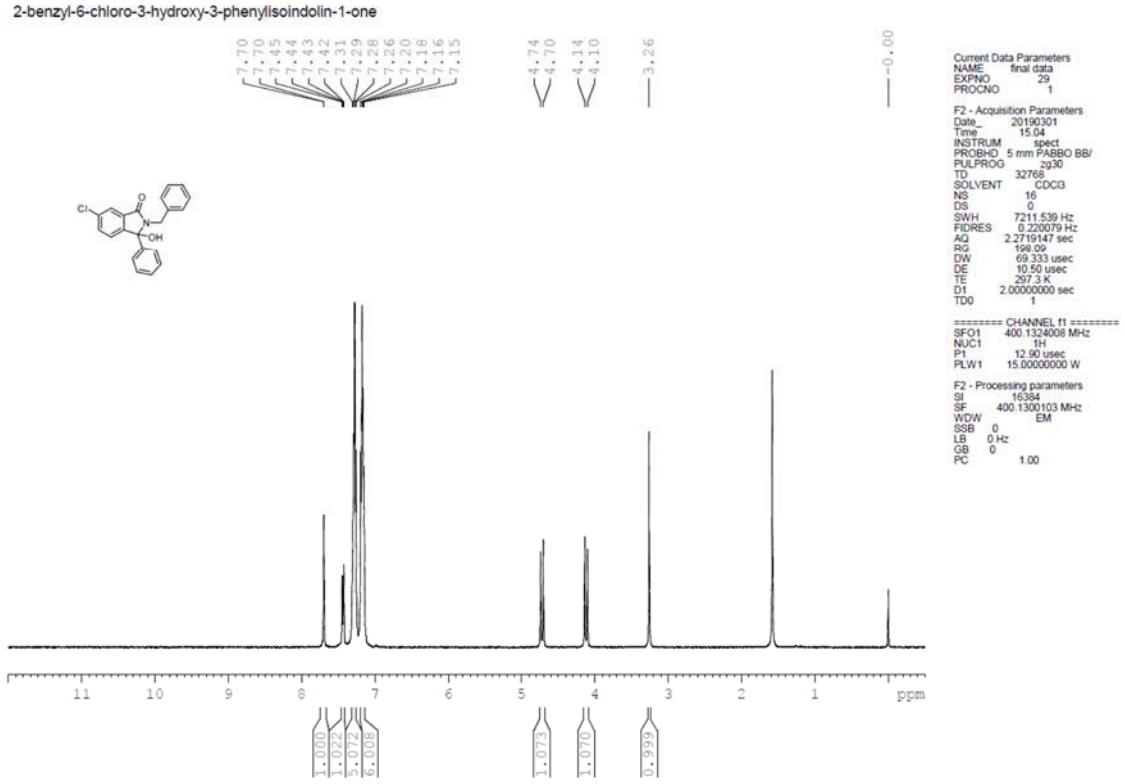
^{1}H NMR spectra of 2-Benzyl-6-bromo-3-hydroxy-3-phenylisoindolin-1-one (**3ja**)



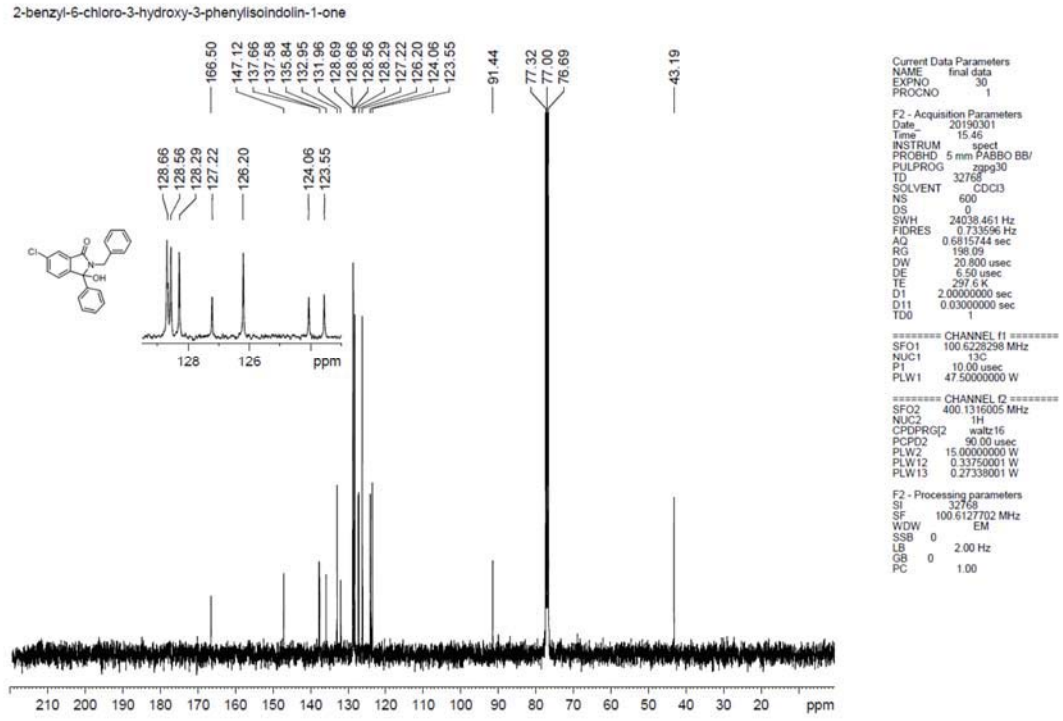
^{13}C NMR spectra of 2-Benzyl-6-bromo-3-hydroxy-3-phenylisoindolin-1-one (**3ja**)



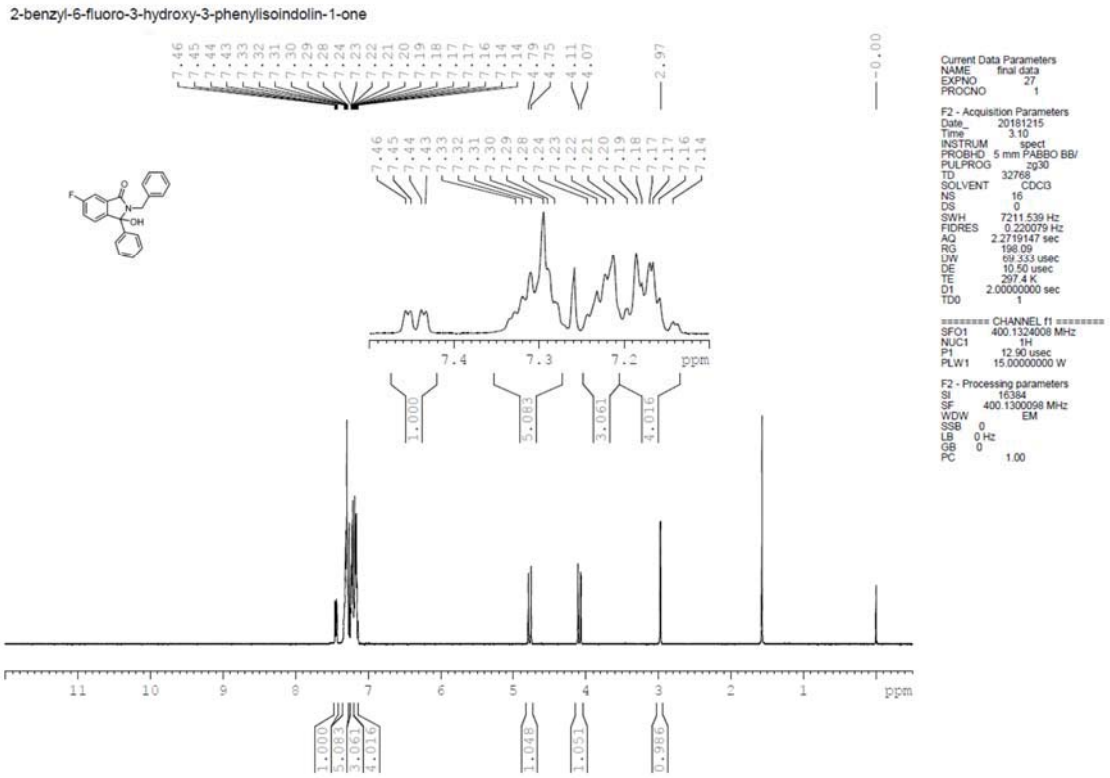
^{1}H NMR spectra of 2-Benzyl-6-chloro-3-hydroxy-3-phenylisoindolin-1-one (**3ka**)



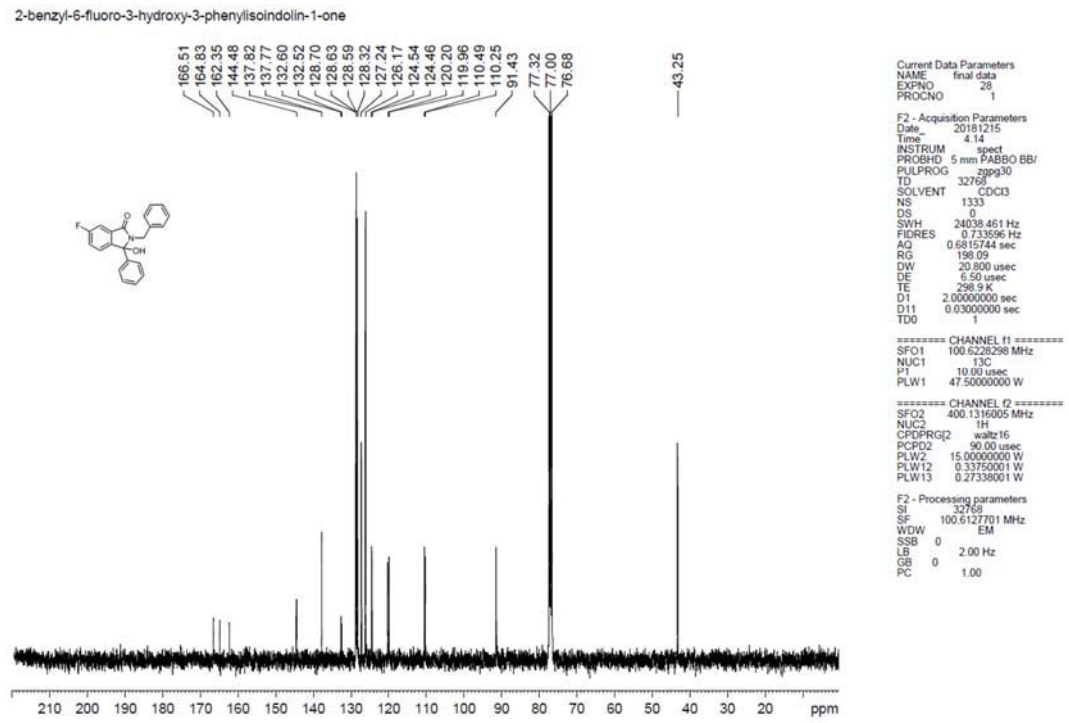
^{13}C NMR spectra of 2-Benzyl-6-chloro-3-hydroxy-3-phenylisoindolin-1-one (**3ka**)



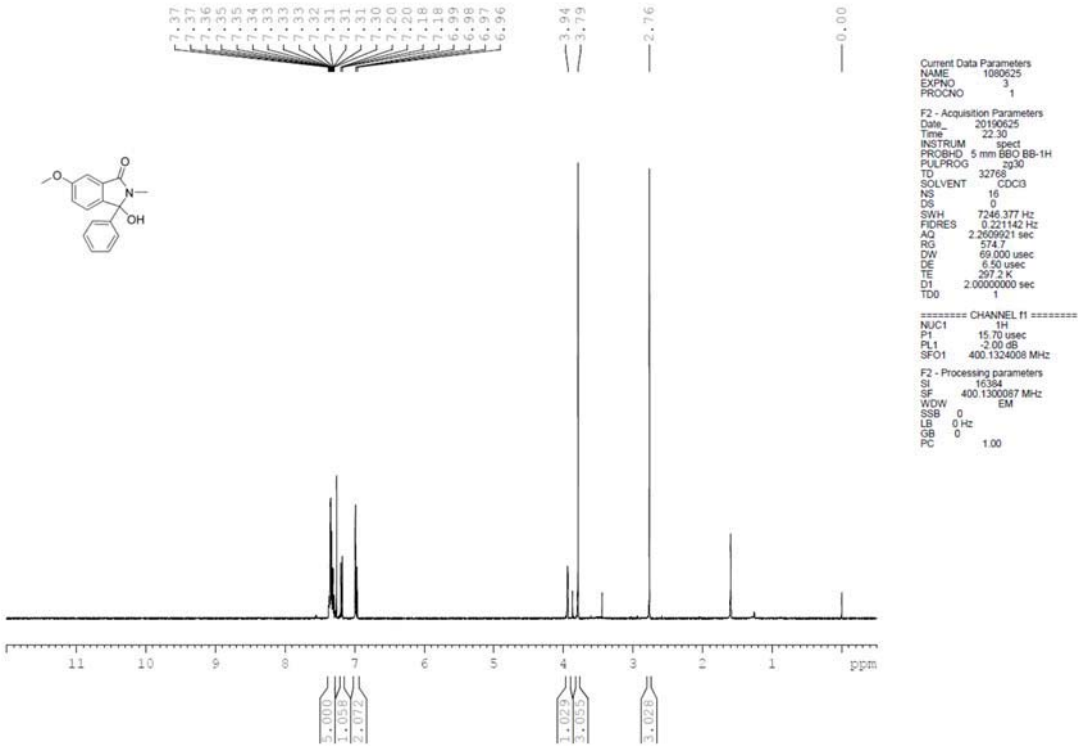
^{1}H NMR spectra of 2-Benzyl-6-fluoro-3-hydroxy-3-phenylisoindolin-1-one (**3la**)



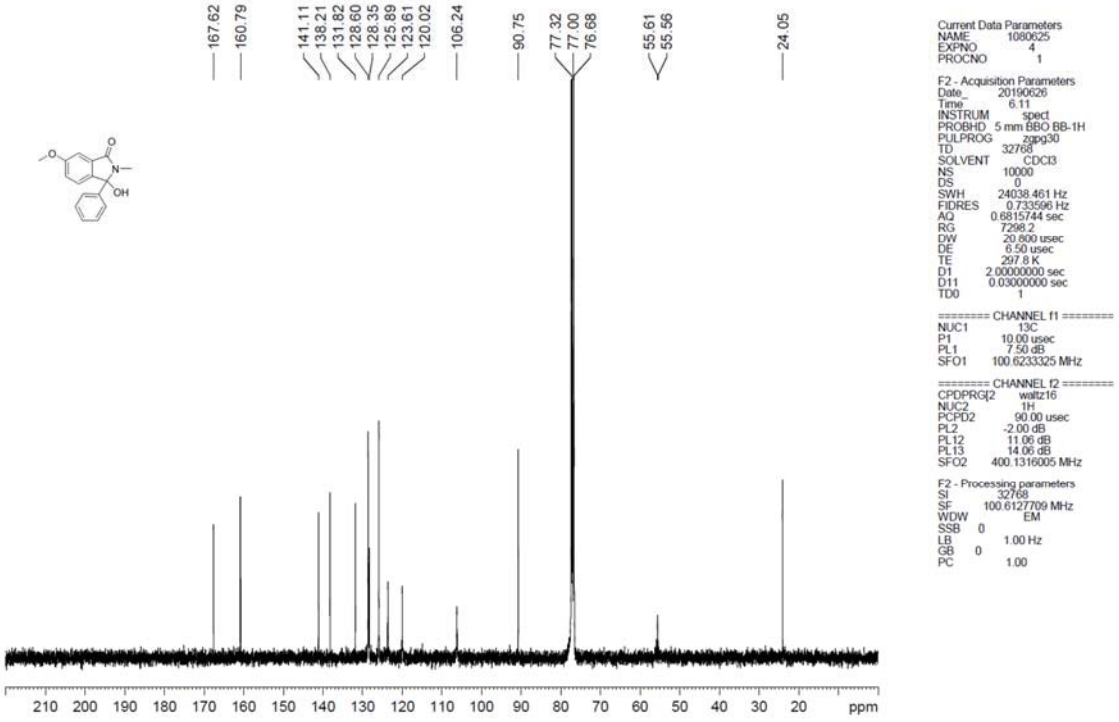
^{13}C NMR spectra of 2-Benzyl-6-fluoro-3-hydroxy-3-phenylisoindolin-1-one (**3la**)



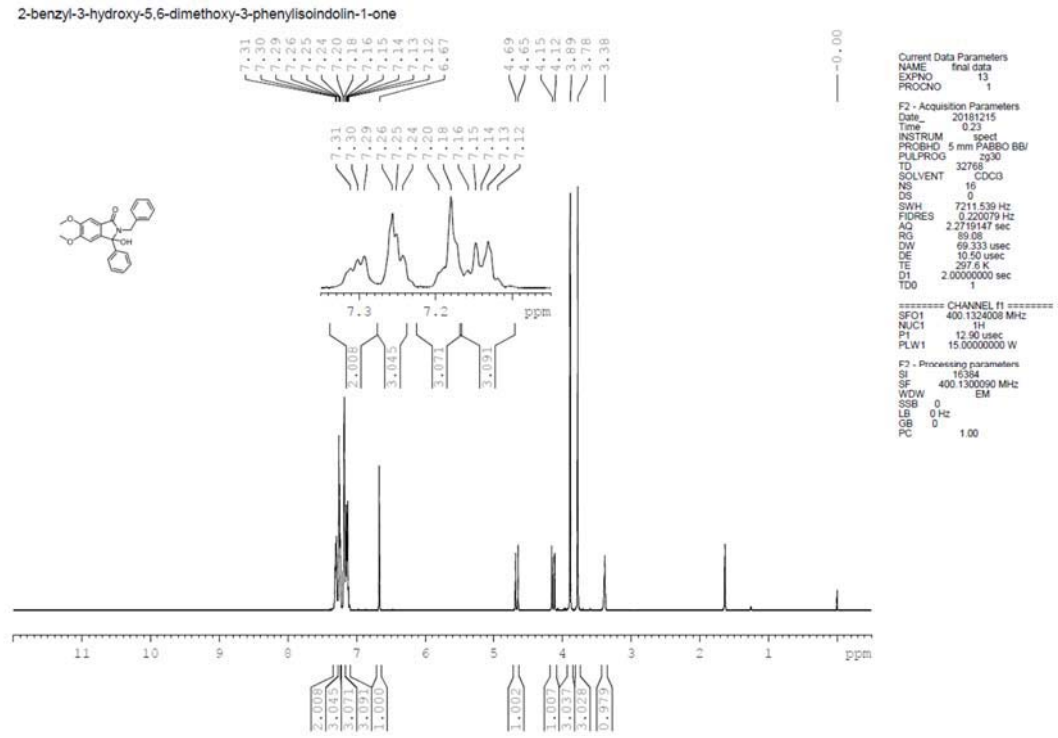
3-Hydroxy-6-methoxy-2-methyl-3-phenylisoindolin-1-one (3ma):



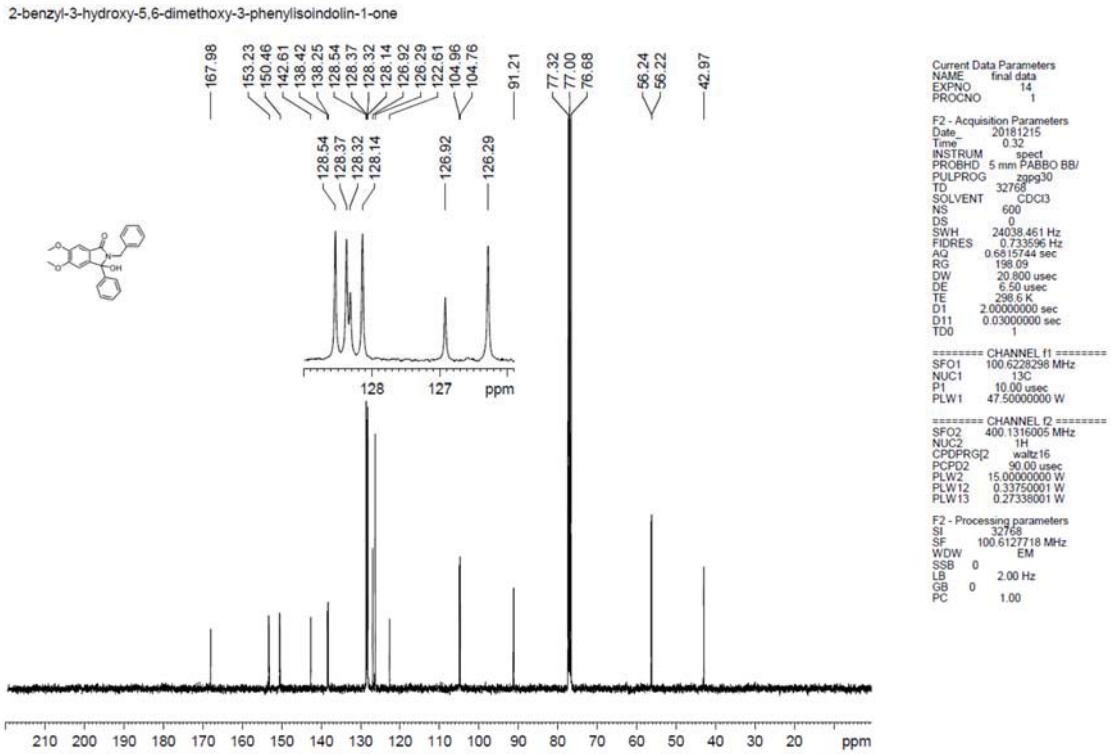
3-Hydroxy-6-methoxy-2-methyl-3-phenylisoindolin-1-one (3ma):



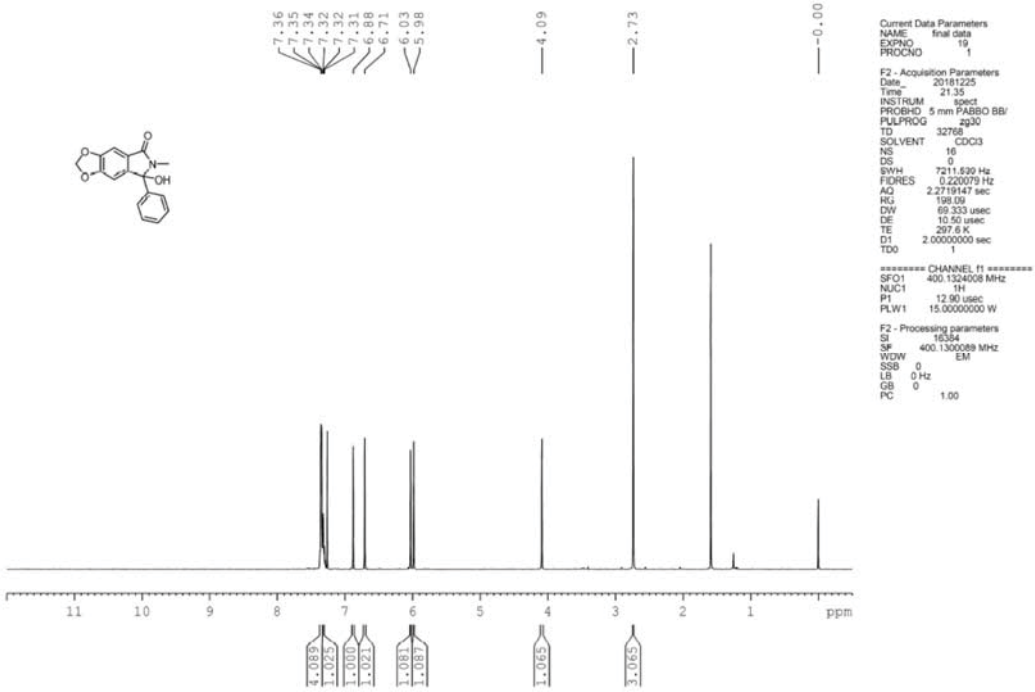
^{1}H NMR spectra of 6-Benzyl-7-hydroxy-7-phenyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]isoindol-5-one (**3na**)



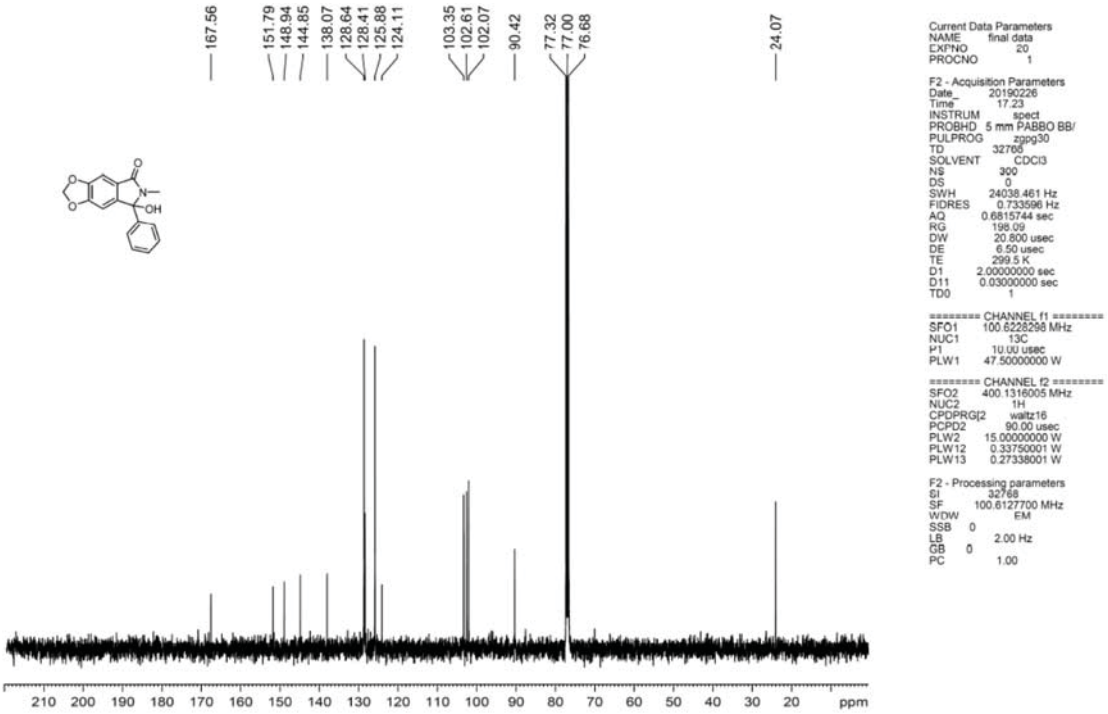
^{13}C NMR spectra of 6-Benzyl-7-hydroxy-7-phenyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]isoindol-5-one (**3na**)



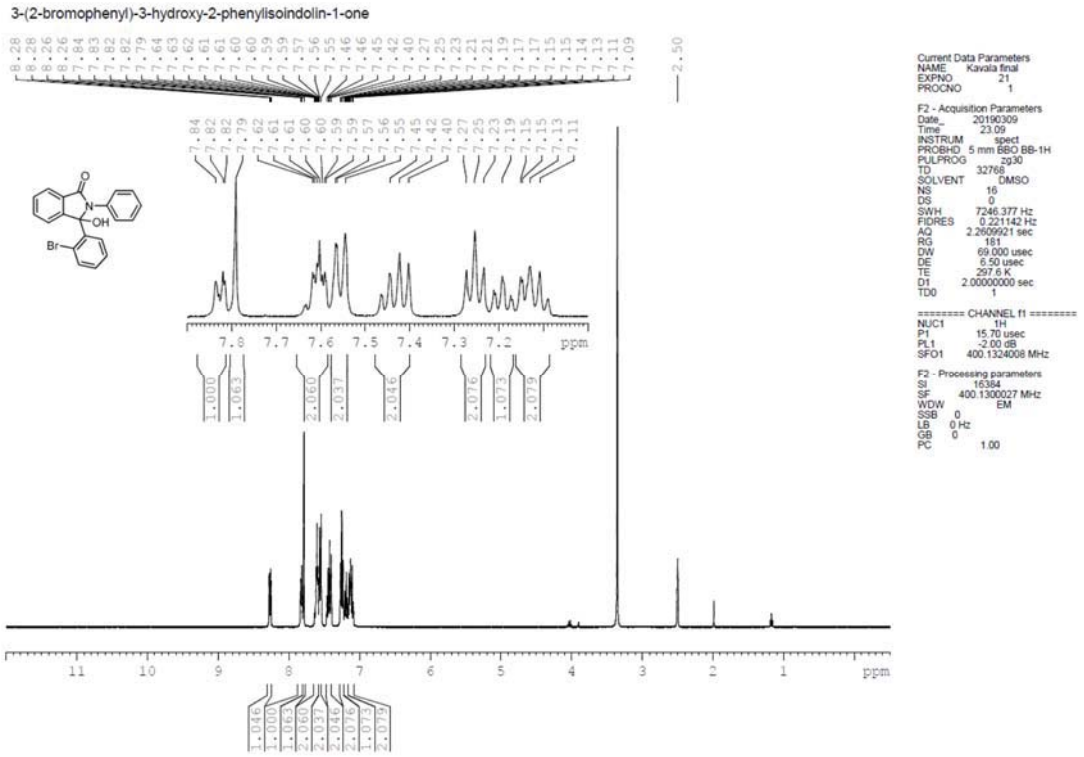
7-Hydroxy-6-methyl-7-phenyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]isoindol-5-one (3oa):



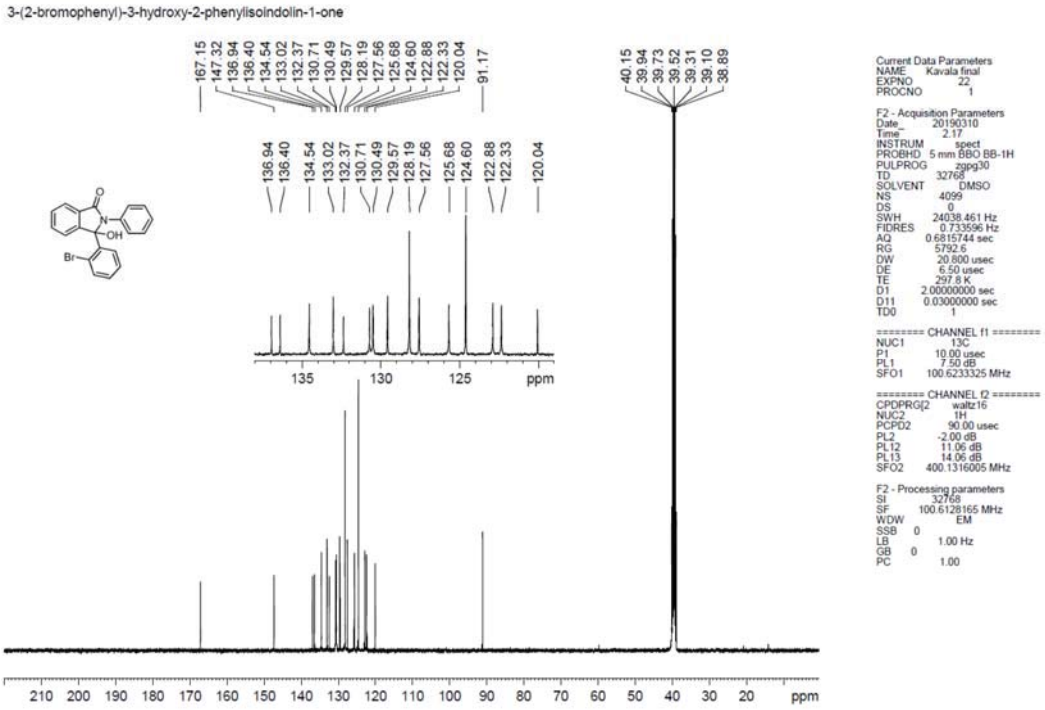
7-Hydroxy-6-methyl-7-phenyl-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]isoindol-5-one (3oa):



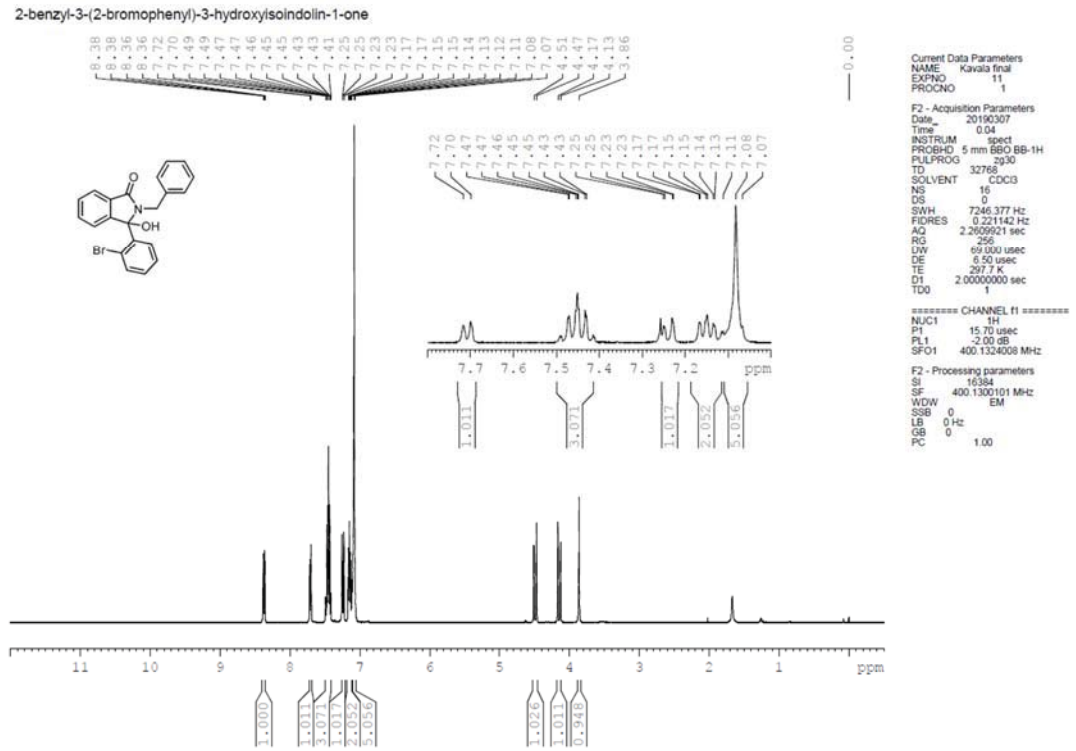
[1]HNMR spectra of 3-(2-bromophenyl)-3-hydroxy-2-phenylisoindolin-1-one (3an)



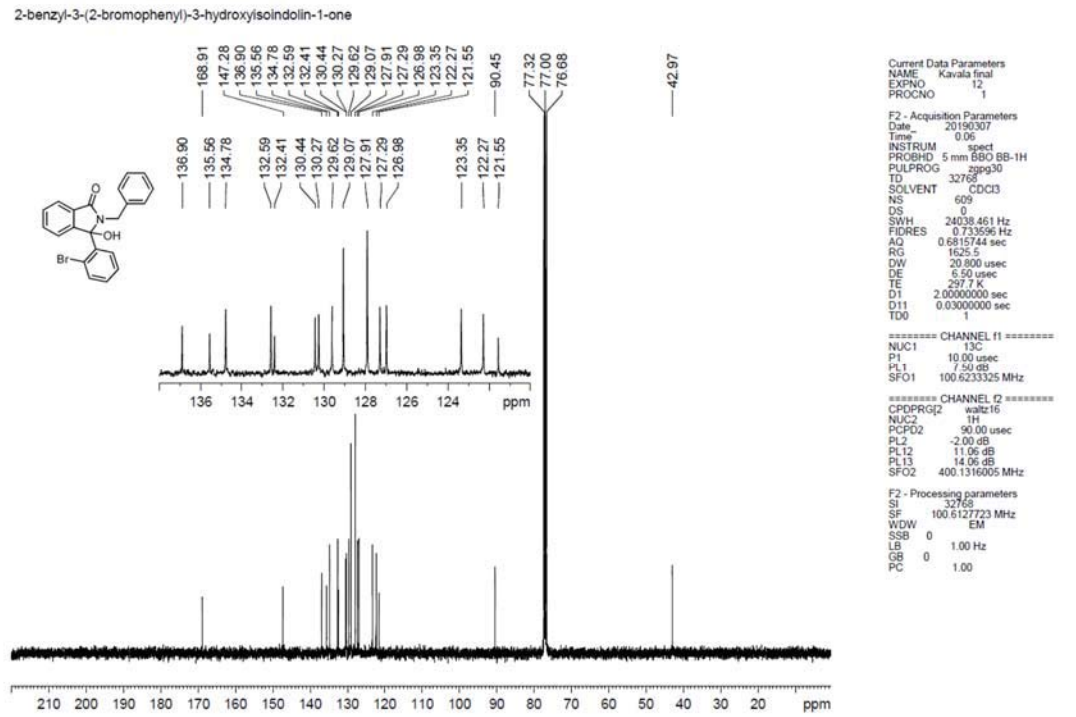
[13]C NMR spectra of 3-(2-bromophenyl)-3-hydroxy-2-phenylisoindolin-1-one (**3an**)



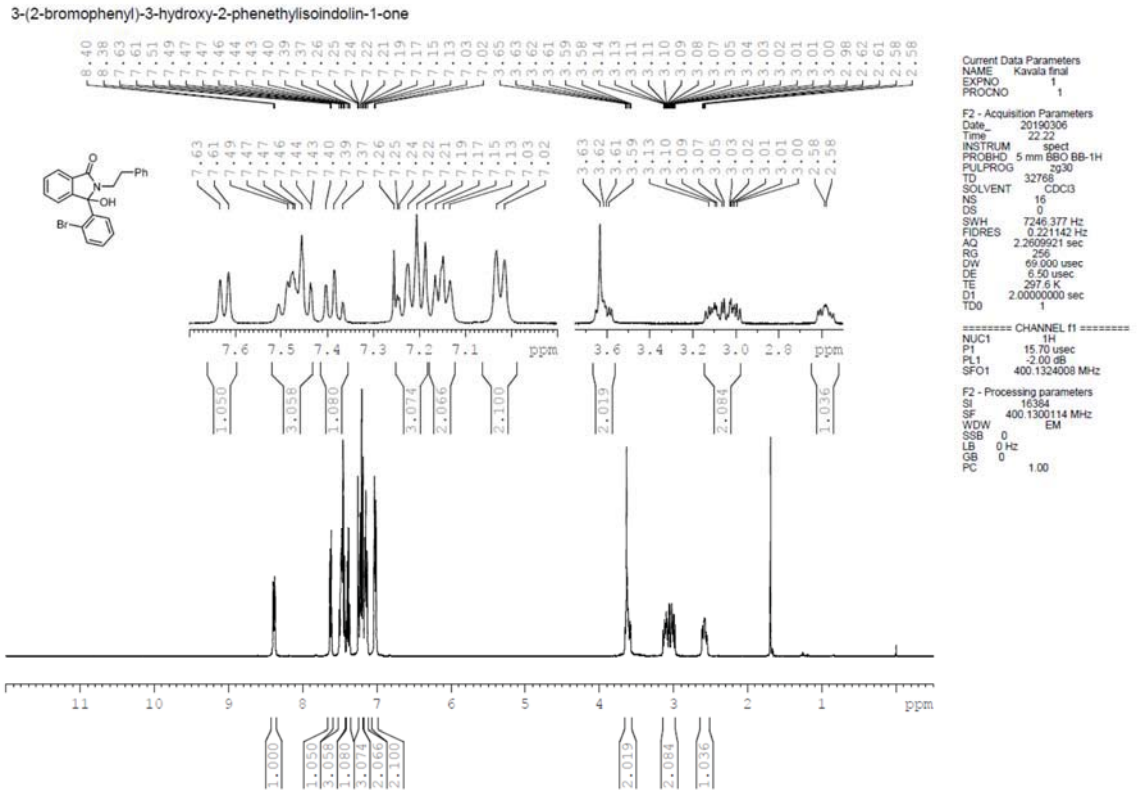
[1]HNMR spectra of 2-Benzyl-3-(2-bromophenyl)-3-hydroxyisoindolin-1-one (3en)



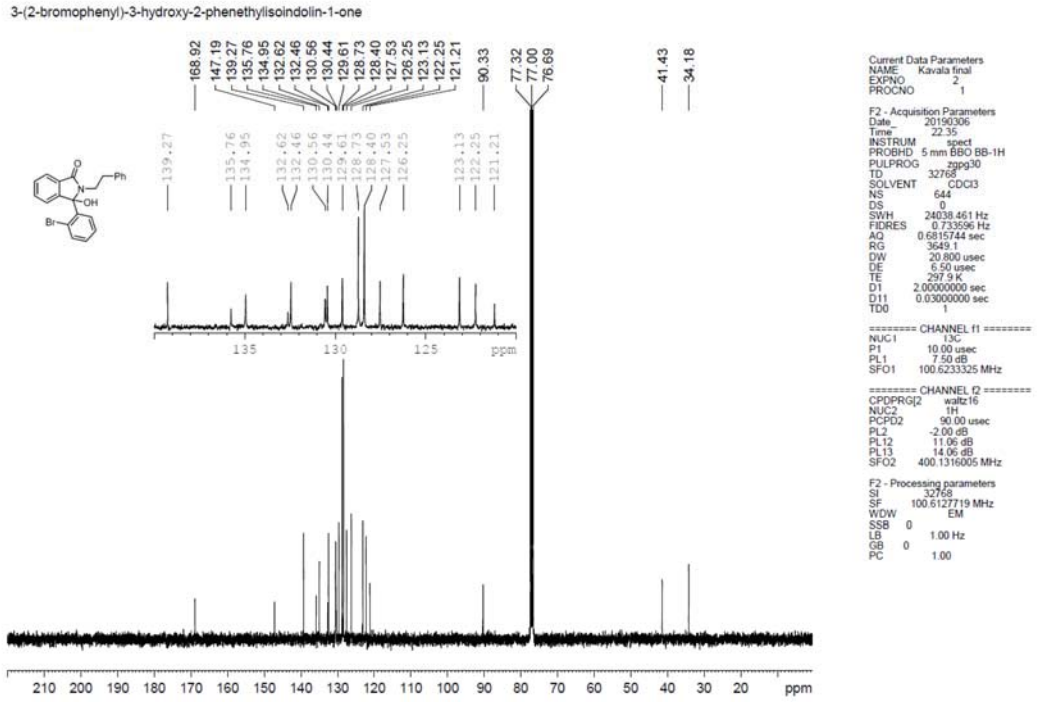
[13]C NMR spectra of 2-Benzyl-3-(2-bromophenyl)-3-hydroxyisoindolin-1-one (**3en**)



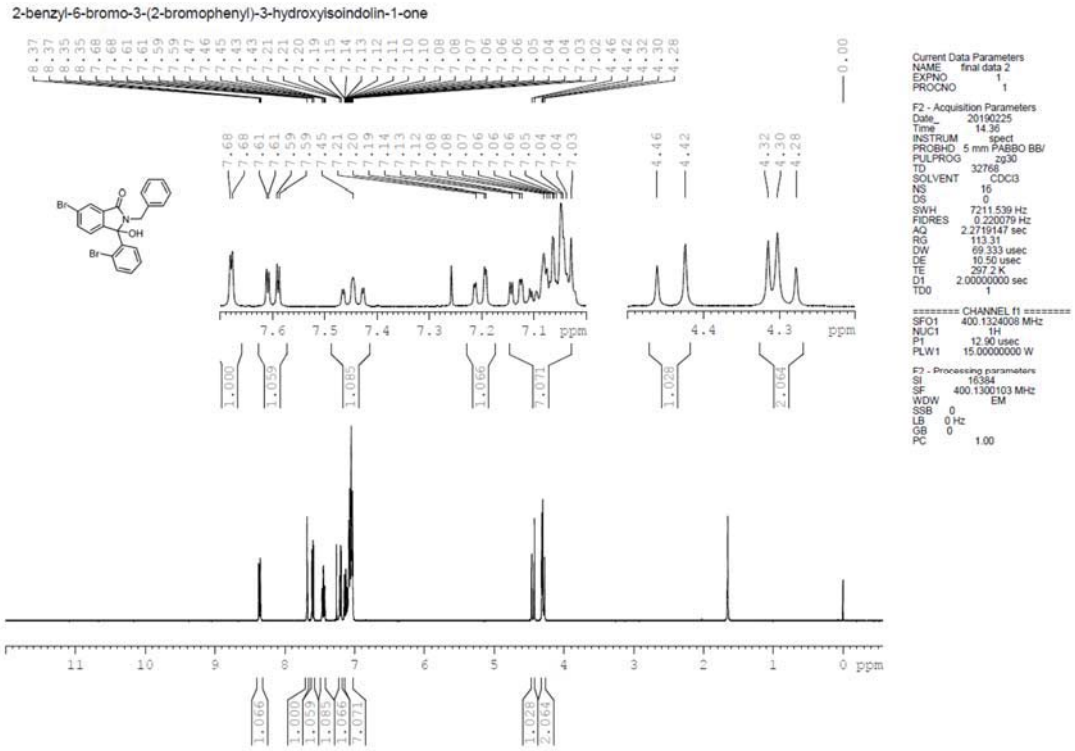
[1]HNMR spectra of 3-(2-bromophenyl)-3-hydroxy-2-phenethylisoindolin-1-one (**3fn**)



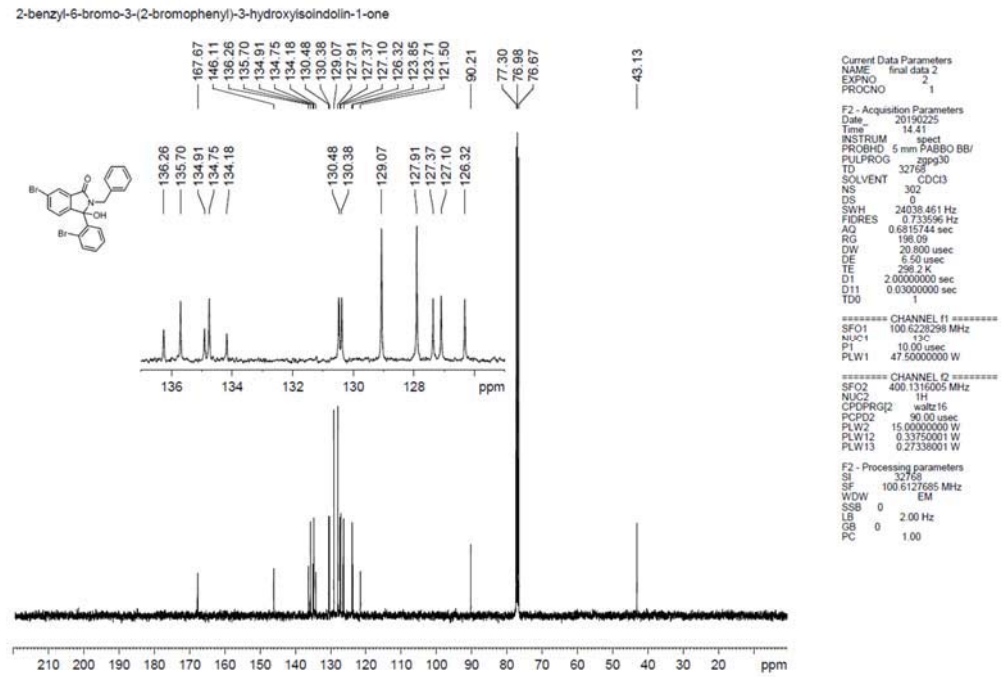
[13]C NMR spectra of 3-(2-bromophenyl)-3-hydroxy-2-phenethylisoindolin-1-one (**3fn**)



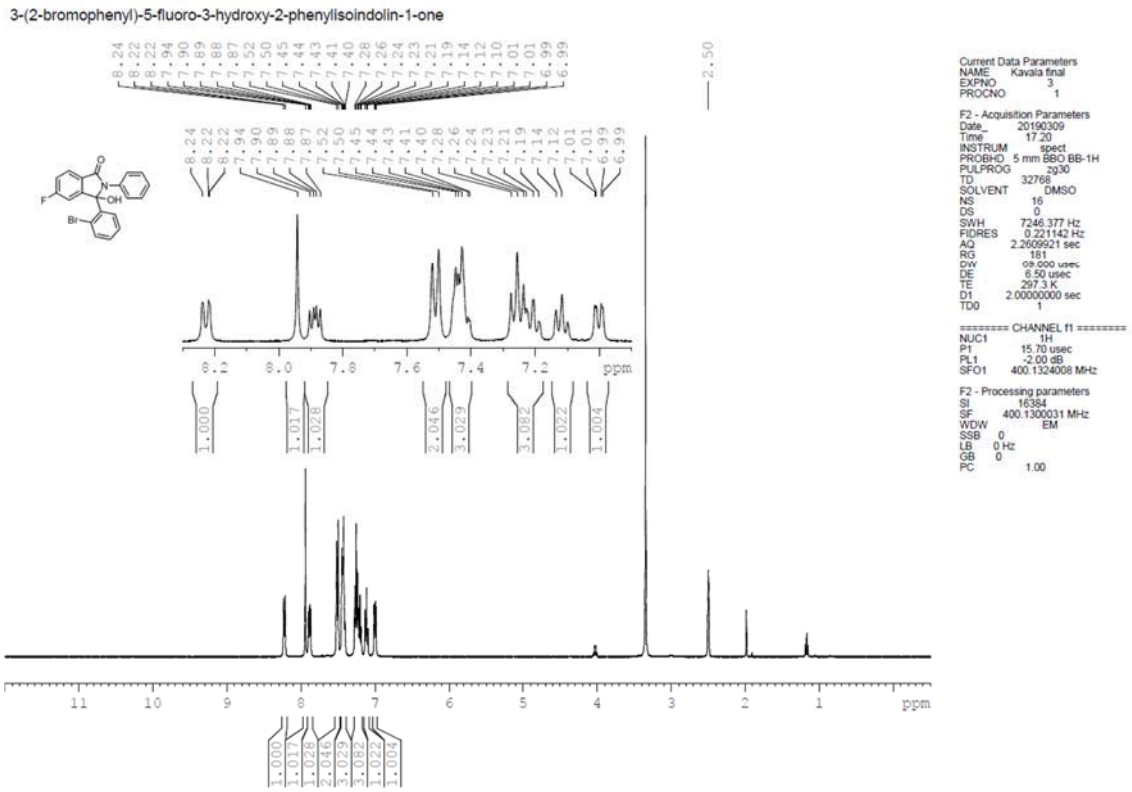
[1]HNMR spectra of 2-benzyl-6-bromo-3-(2-bromophenyl)-3-hydroxyisoindolin-1-one (**3kn**)



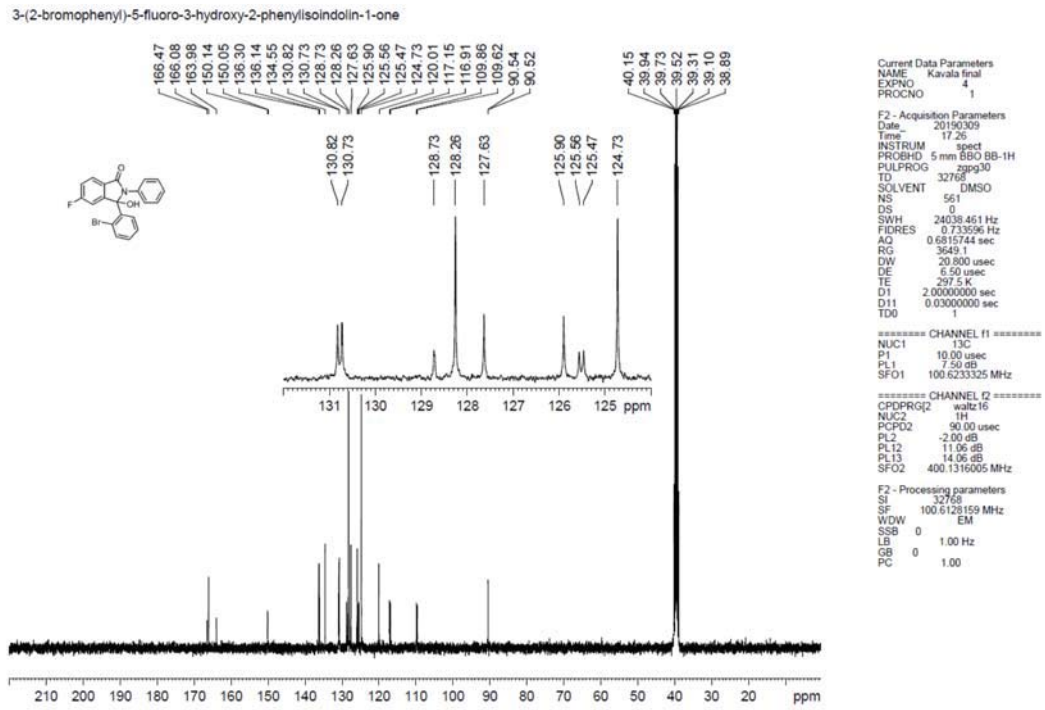
[13]C NMR spectra of 2-benzyl-6-bromo-3-(2-bromophenyl)-3-hydroxyisoindolin-1-one (**3kn**)



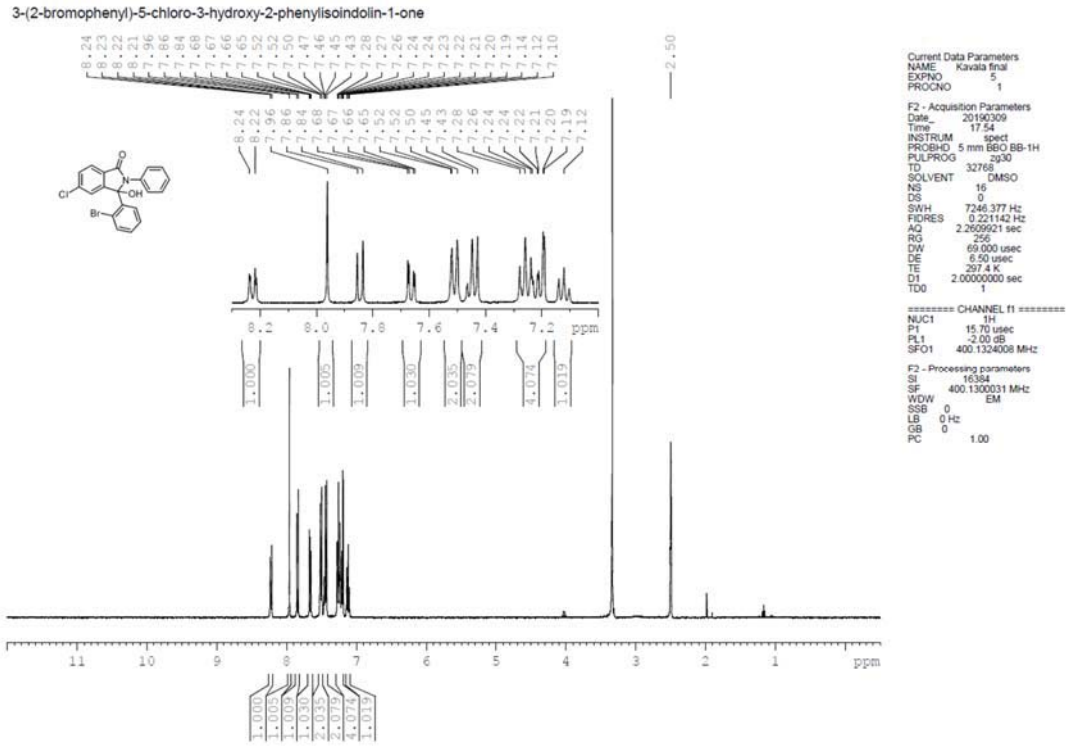
[1]HNMR spectra of 3-(2-bromophenyl)-5-fluoro-3-hydroxy-2-phenylisoindolin-1-one (3ln)



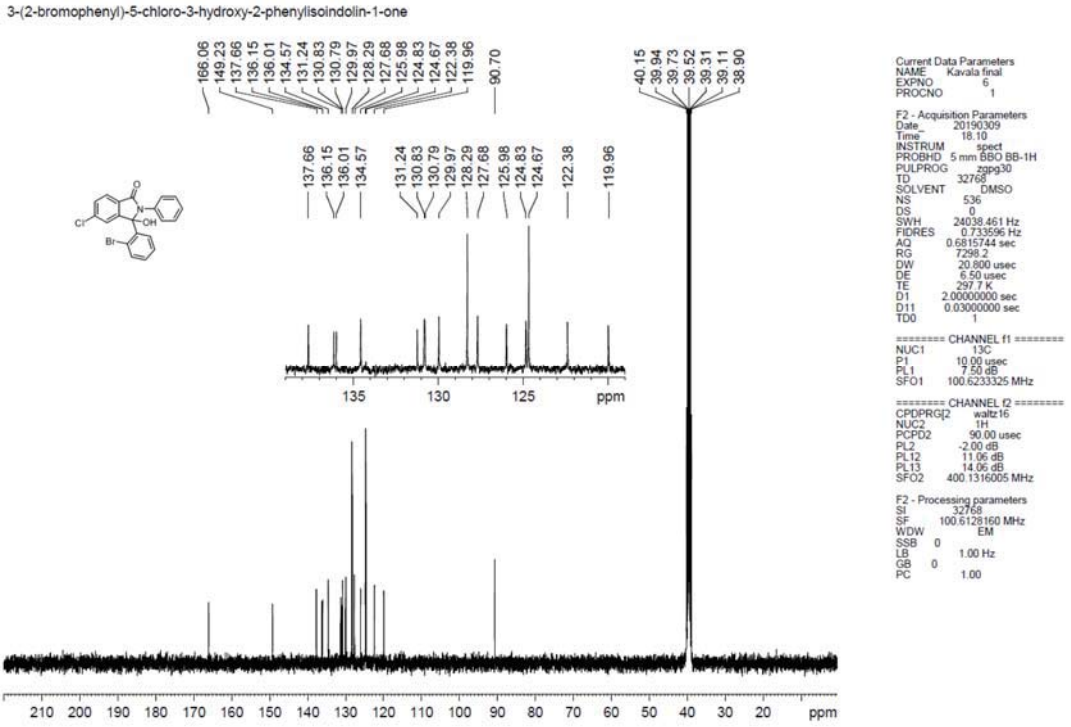
[13]C NMR spectra of 3-(2-bromophenyl)-5-fluoro-3-hydroxy-2-phenylisoindolin-1-one (**3ln**)



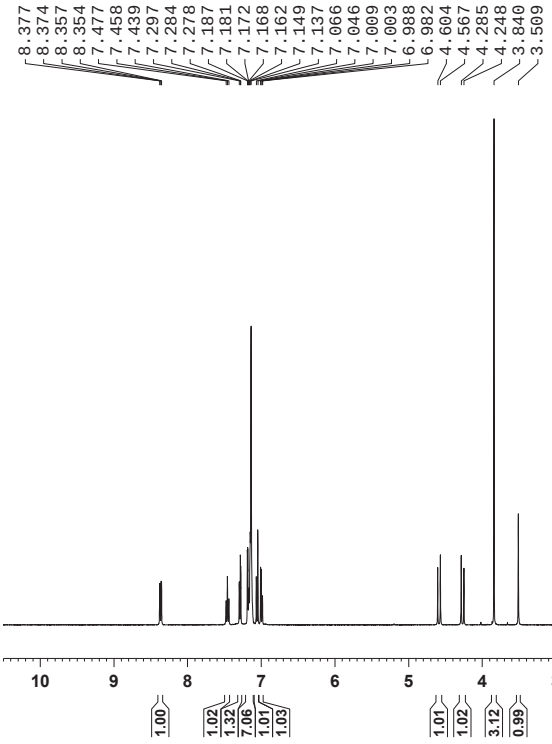
[1]HNMR spectra of 3-(2-bromophenyl)-5- chloro-3-hydroxy-2-phenylisoindolin-1-one (3mn)



[13]C NMR spectra of 3-(2-bromophenyl)-5-chloro-3-hydroxy-2-phenylisoindolin-1-one (3mn)



^{1}H NMR of 2-Benzyl-3-(2-bromophenyl)-3-hydroxy-6-methoxyisoindolin-1-one (3nn)

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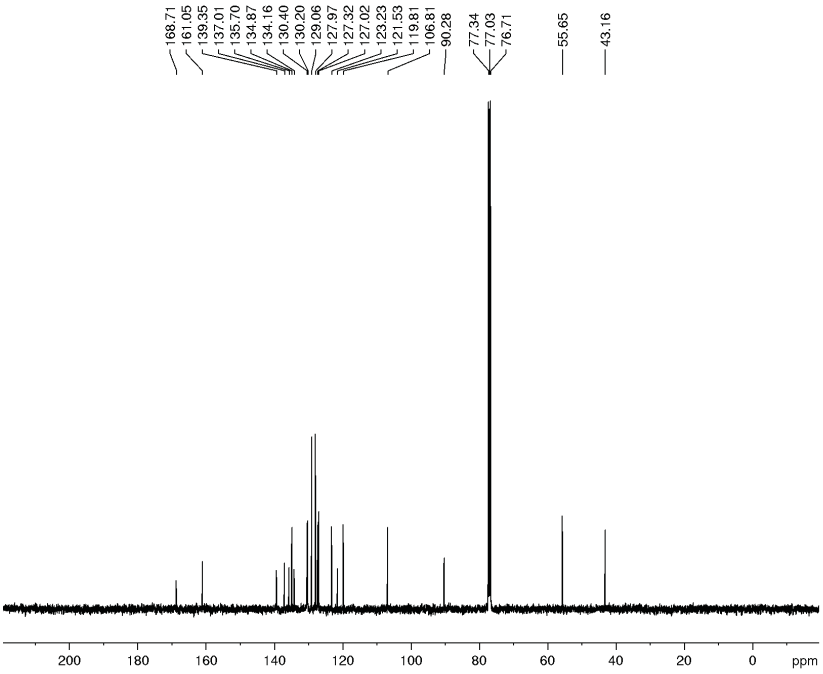
^{13}C NMR of 2-Benzyl-3-(2-bromophenyl)-3-hydroxy-6-methoxyisoindolin-1-one (3nn)

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RG              198.09
DW              20.800 usec
DE               6.50 usec
TE               298.4 K
D1          2.00000000 sec
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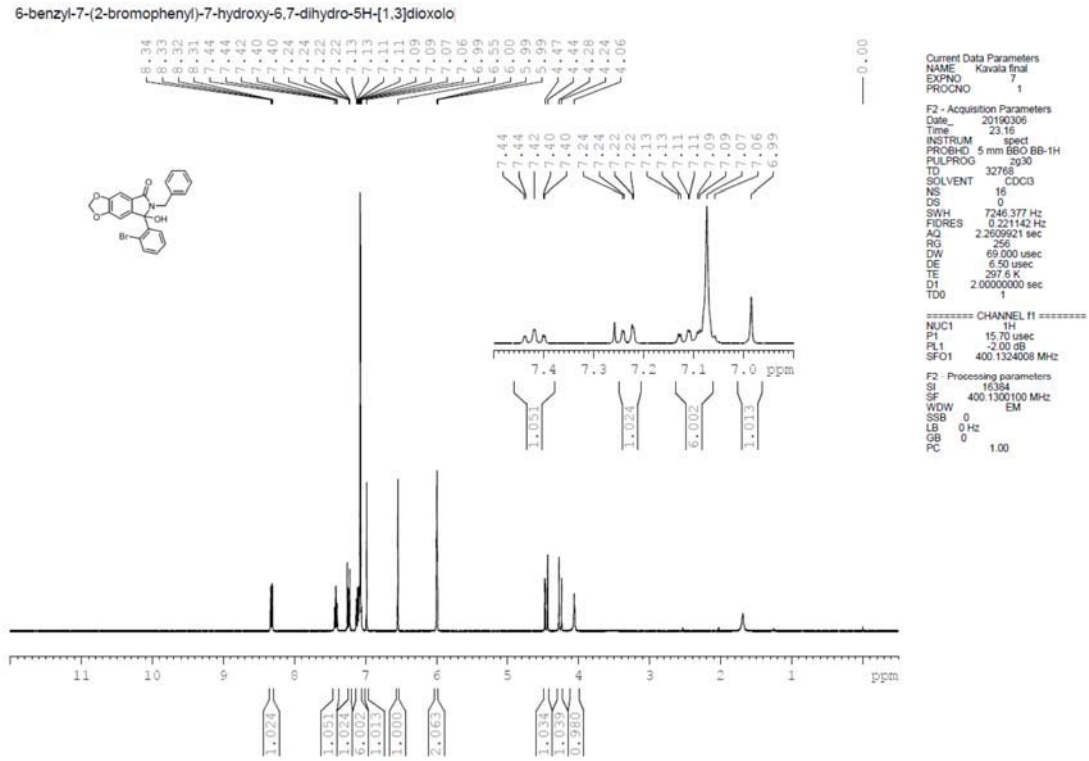
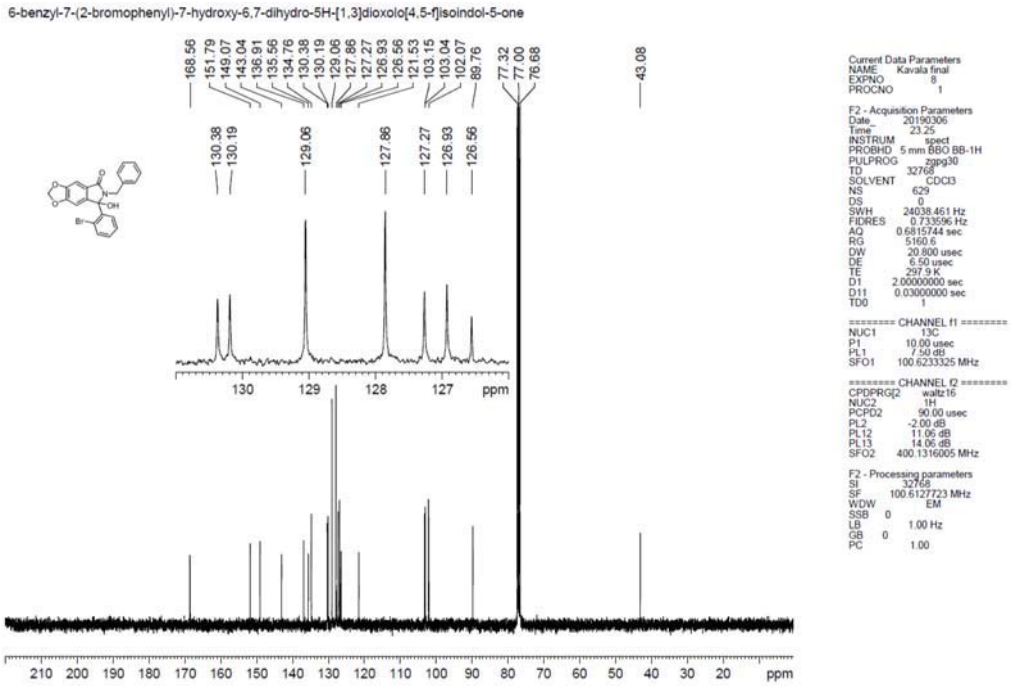
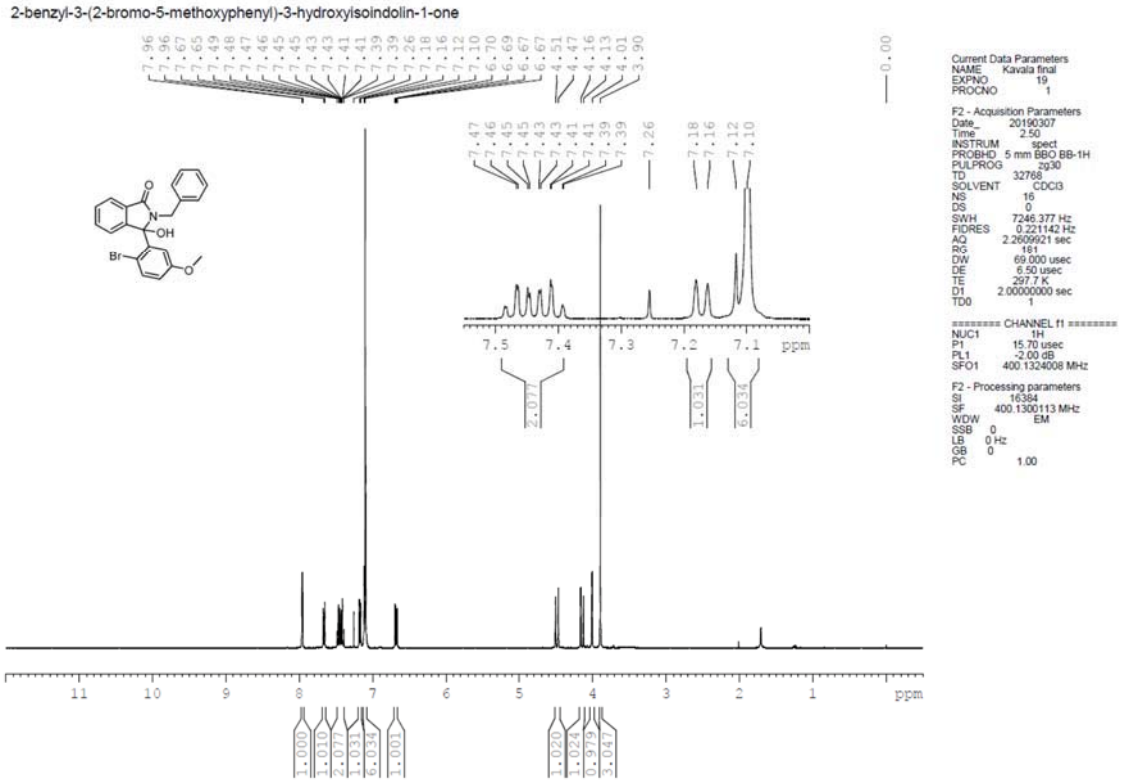
[1]HNMR spectra of 6-benzyl-7-(2-bromophenyl)-7-hydroxy-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]isoindol-5-one (**3pn**)



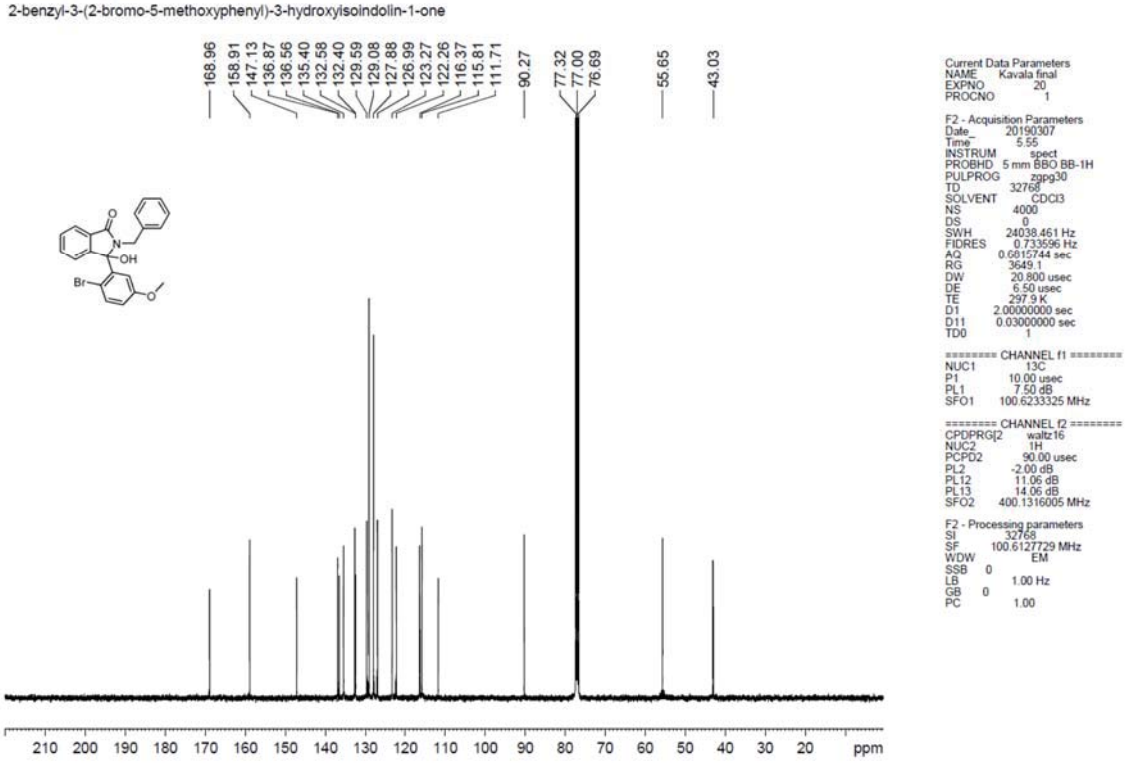
[13]C NMR spectra of 6-benzyl-7-(2-bromophenyl)-7-hydroxy-6,7-dihydro-5H-[1,3]dioxolo[4,5-f]isoindol-5-one (**3pn**)



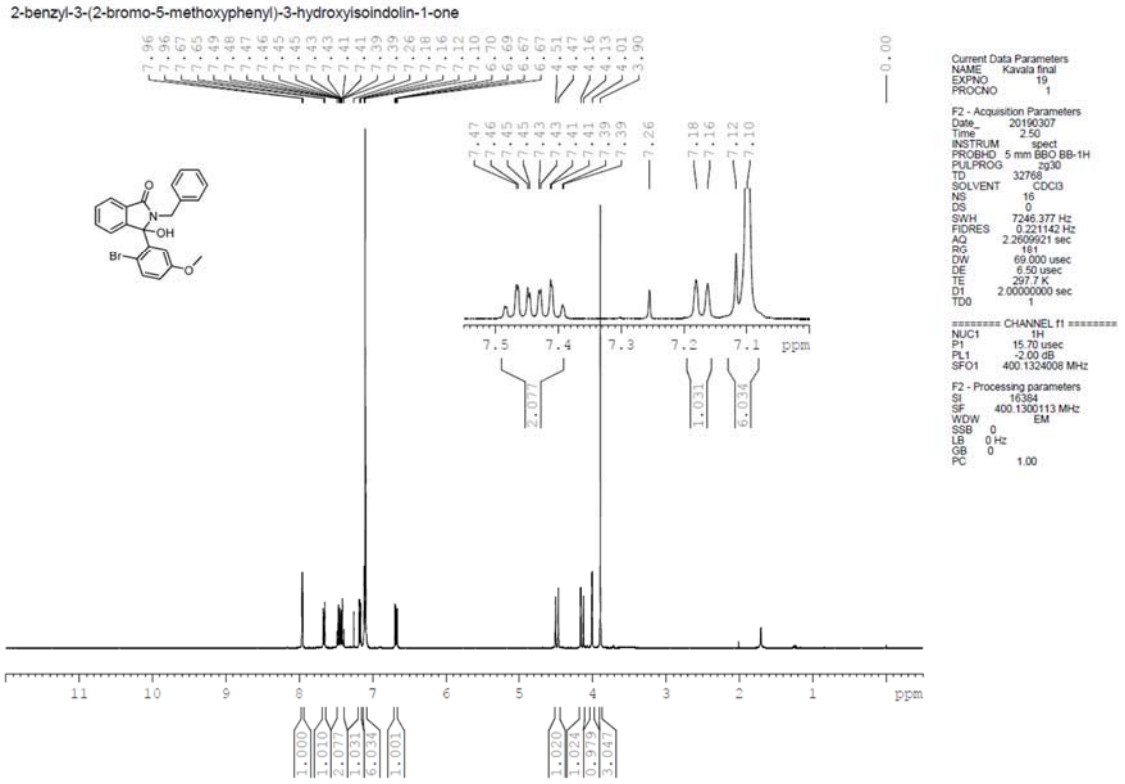
[1]HNMR spectra of 2-Benzyl-3-(2-bromo-5-methoxyphenyl)-3-hydroxyisoindolin-1-one (**3ao**)



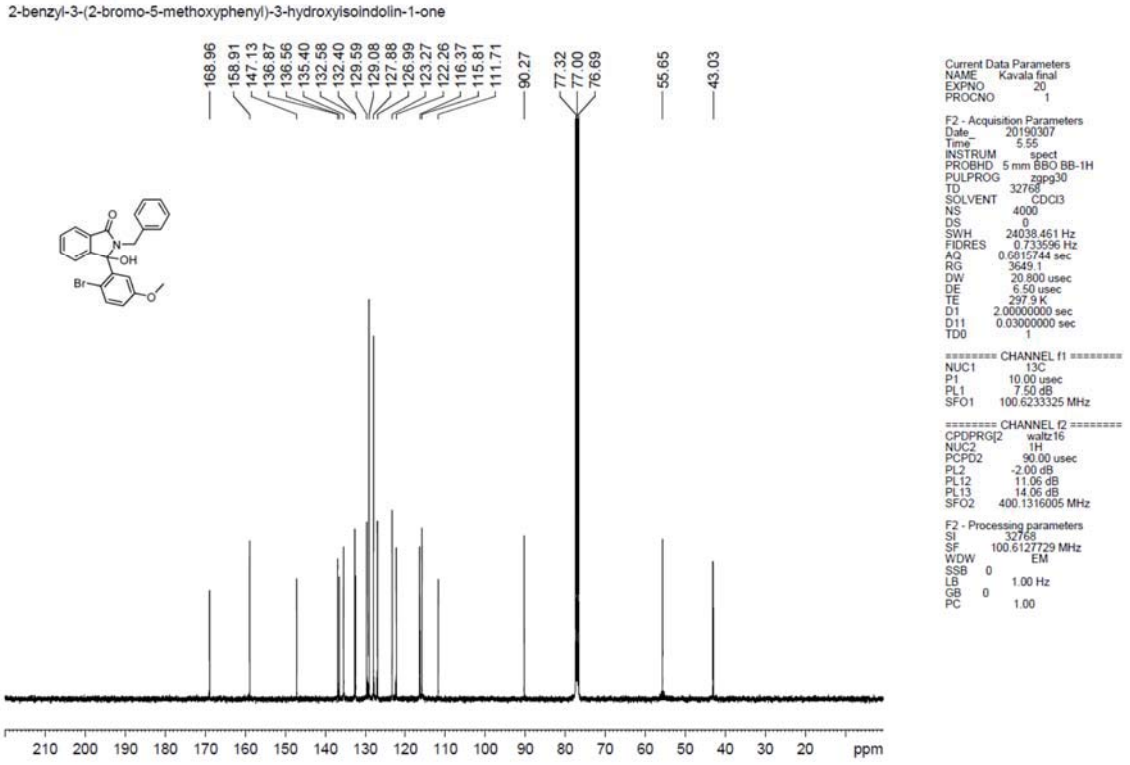
[13]C NMR spectra of 2-Benzyl-3-(2-bromo-5-methoxyphenyl)-3-hydroxyisoindolin-1-one (3ao)



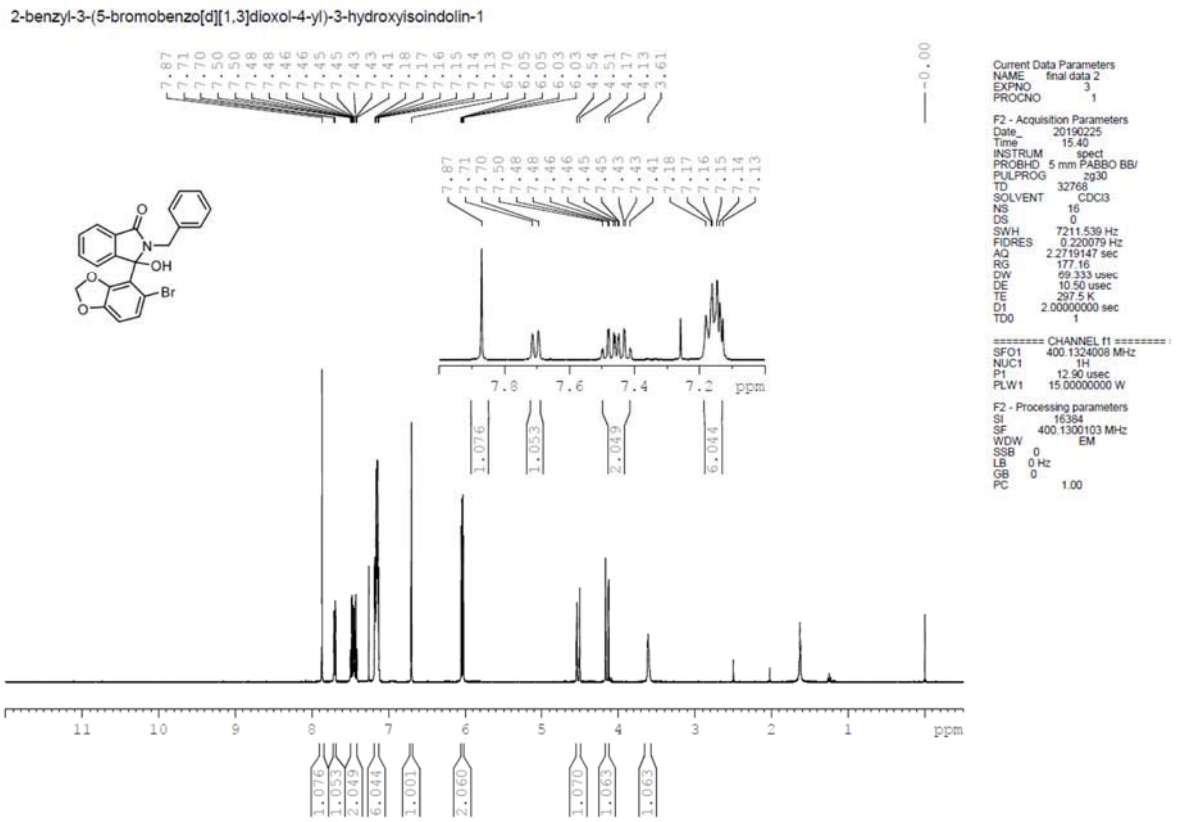
[1]HNMR spectra of 2-Benzyl-3-(2-bromo-4,5-dimethoxyphenyl)-3-hydroxyisoindolin-1-one (**3ap**)



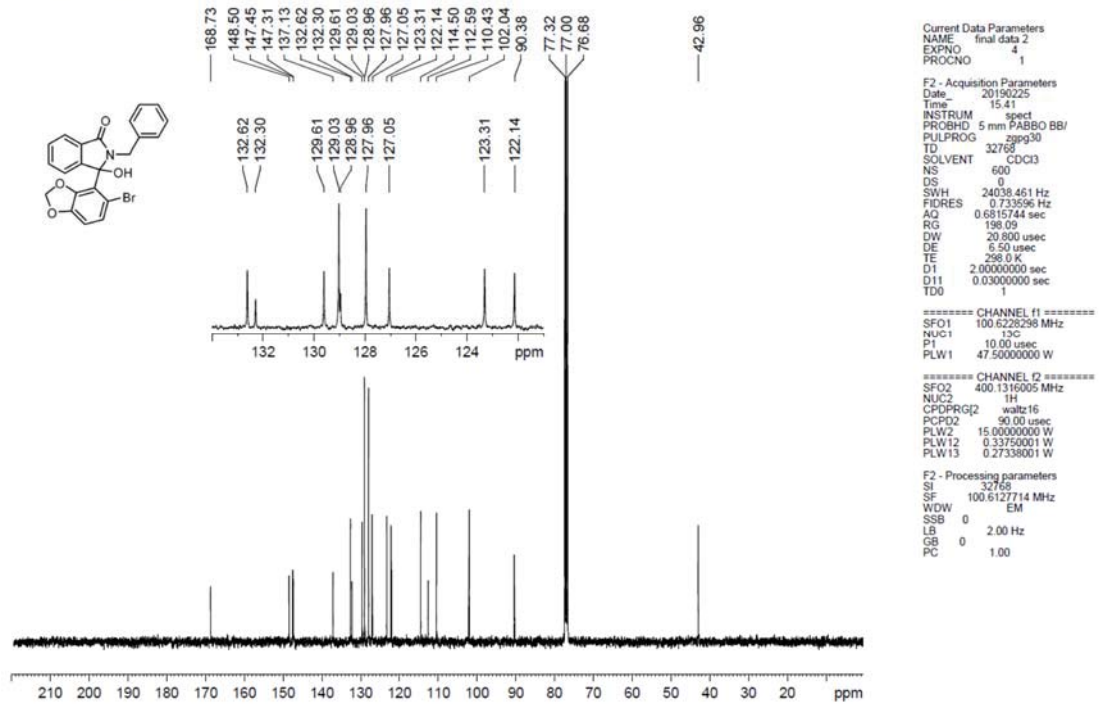
[13]C NMR spectra of 2-Benzyl-3-(2-bromo-4,5-dimethoxyphenyl)-3-hydroxyisoindolin-1-one (**3ap**)



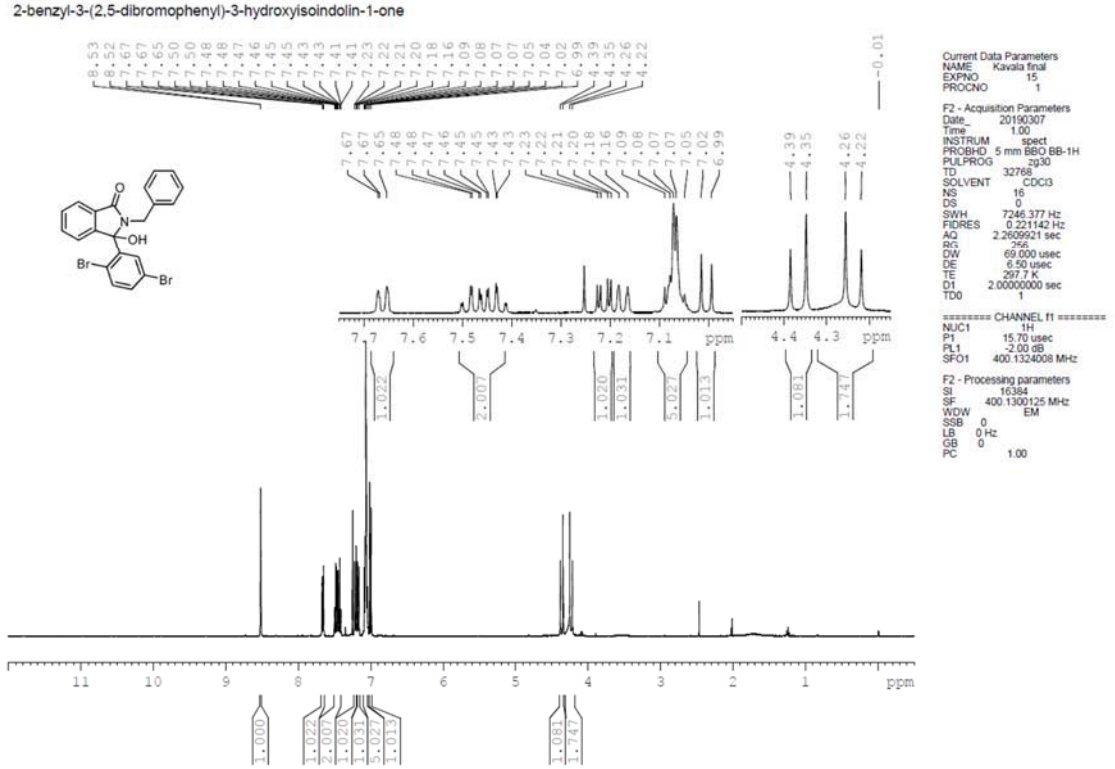
[1]HNMR spectra of 2-Benzyl-3-(6-bromobenzo[d][1,3]dioxol-5-yl)-3-hydroxyisoindolin-1-one (**3aq**)



[13]C NMR spectra of 2-Benzyl-3-(6-bromobenzo[d][1,3]dioxol-5-yl)-3-hydroxyisoindolin-1-one (**3aq**)



[1]HNMR spectra of 2-Benzyl-3-(2,5-dibromophenyl)-3-hydroxyisoindolin-1-one (**3ar**)



[13]C NMR spectra of 2-Benzyl-3-(2,5-dibromophenyl)-3-hydroxyisoindolin-1-one (**3ar**)