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

Palladium-Catalyzed Asymmetric Allylic Amination of Racemic Butadiene Monoxide with Isatin Dericatives

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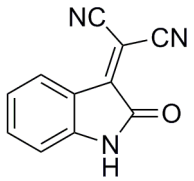
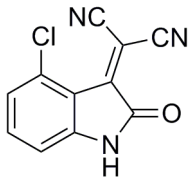
Supporting Information

General consideration: All solvents were purified by conventional methods, distilled before use. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AV 400 at ambient temperature with $CDCl_3$ and DMSO-d_6 as solvent and TMS as internal standard. Chemical shifts (δ) were given in ppm, referenced to the residual proton resonance of TMS (0), to the carbon resonance of the $CDCl_3$ (77.23) and DMSO-d_6 (40.45). Coupling constants (*J*) were given in Hertz (Hz). Optical rotations were measured with PerkinElmer 341 polarimeter. Flash column chromatography was performed on silica gel (200-300 mesh). All solvents were purified by conventional methods, distilled before use. Commercially available reagents were used without further purification.

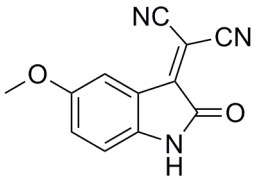
Typical procedure for the synthesis of substrate 1a: A mixture of isatin (5.0 mmol), malononitrile (0.302 g, 5.5 mmol) and piperidine (0.05 mL) in EtOH (10 mL) was stirred at room temperature for 4 h. After filtration and removal of the solvents, the residue was recrystallized from ethanol to give the pure substrate.



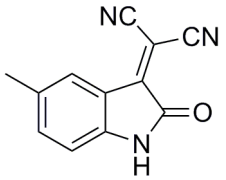
2-(2-oxoindolin-3-ylidene)malononitrile (1a)[1]: ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.21 (s, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.57 (dd, *J* = 8.0, 7.6 Hz, 1H), 7.14 (dd, *J* = 8.0, 7.6 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.7, 151.5, 147.4, 138.7, 126.7, 123.8, 119.6, 114.0, 112.5, 112.4, 81.5.



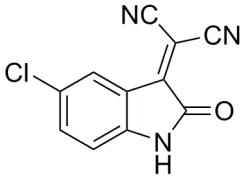
2-(4-chloro-2-oxoindolin-3-ylidene)malononitrile (1b)[1]**:** ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.46 (s, 1H), 7.54 (dd, J = 8.0, 8.0 Hz, 1H), 7.12 (d, J = 8.0 Hz, 1H), 6.87 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 163.7, 148.2, 148.1, 138.6, 132.8, 124.4, 116.7, 114.1, 112.9, 110.3, 83.9.



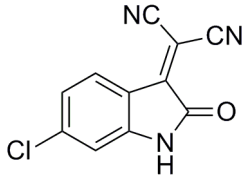
2-(5-methoxy-2-oxoindolin-3-ylidene)malononitrile (1c)[2]**:** ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.99 (s, 1H), 7.31 (d, J = 2.4 Hz, 1H), 7.17 (dd, J = 8.4, 2.4 Hz, 1H), 6.82 (d, J = 8.4 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.6, 155.7, 151.5, 141.5, 125.0, 119.8, 113.8, 113.4, 1112.3, 111.0, 81.6, 56.5.



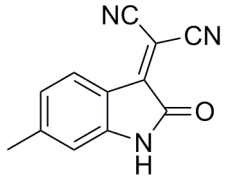
2-(5-methyl-2-oxoindolin-3-ylidene)malononitrile (1d)[3]**:** ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.10 (s, 1H), 7.66 (s, 1H), 7.40 (d, J = 8.0 Hz, 1H), 6.84 (d, J = 8.0 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.7, 151.5, 145.4, 139.5, 132.9, 126.6, 119.6, 114.0, 112.5, 112.5, 81.2, 21.4.



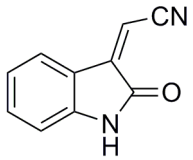
2-(5-chloro-2-oxoindolin-3-ylidene)malononitrile (1e)[4]**:** ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.36 (s, 1H), 7.77 (s, 1H), 7.63 (d, J = 7.6 Hz, 1H), 6.97 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.4, 150.6, 146.1, 137.8, 127.4, 125.7, 120.9, 114.2, 113.7, 112.1, 82.9.



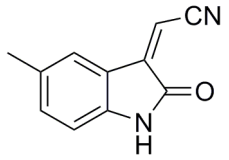
2-(6-chloro-2-oxoindolin-3-ylidene)malononitrile (1f)[5]**:** ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.39 (s, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.22 (dd, J = 8.4, 1.6 Hz, 1H), 6.98 (d, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.7, 150.4, 148.5, 142.8, 128.1, 123.9, 118.5, 113.9, 112.6, 112.3, 81.9.



2-(6-methyl-2-oxoindolin-3-ylidene)malononitrile (1g) [6]**:** Purple solid; mp. 296-298 °C; IR (film) 3273, 1723, 1631, 1596 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.17 (s, 1H), 7.75 (d, J = 8.0 Hz, 1H), 6.95 (d, J = 8.0 Hz, 1H), 6.76 (s, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 164.1, 150.3, 150.0, 146.9, 125.8, 123.8, 116.2, 113.3, 112.1, 111.7, 78.9, 22.3; HRMS (ESI): Calcd. for $C_{12}H_7ON_3Na$ (M+Na): 232.0481; Found: 232.0484.



(*Z*)-2-(2-oxoindolin-3-ylidene)acetonitrile (1h)[7]**:** ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.89 (s, 1H), 7.86 (d, J = 7.6 Hz, 1H), 7.42 (dd, J = 7.6, 7.6 Hz, 1H), 7.10 (dd, J = 7.6, 7.6 Hz, 1H), 6.92 (d, J = 8.0 Hz, 1H), 6.53 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 145.6, 144.7, 134.8, 124.9, 123.3, 120.3, 117.8, 111.9, 98.6.



(*Z*)-2-(5-methyl-2-oxoindolin-3-ylidene)acetonitrile (1i)[8]: Red solid; mp. 167-169 °C; IR (film) 3237, 2213, 1731, 1720 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.87 (s, 1H), 7.61(brs, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 6.27 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 144.1, 140.9, 134.6, 133.3, 125.9, 120.1, 116.3, 110.7, 97.5, 21.2; HRMS (ESI): Calcd. for $C_{11}H_8ON_2Na$ (M+Na): 207.0529; Found: 207.0532.

References

[1] H. Fayez and A. Fatma, *Tetrahedron*, 2000, **56**, 1863-1871.

[2] C. Yu and Y. Cai, *RSC Advances*, 2013, **3**, 18857-18862.

[3] A. Dandia, H. Taneja, R. Gupta and S. Paul, *Synth. Commun.* 1999, **29**, 2323-2335.

[4] P. B. Thakur and H. M. Meshram, *Tetrahedron*, 2013, **69**, 6415-6423.

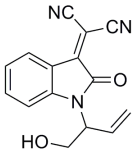
[5] L. Liu, D. Wu, X. Li, S. Wang, H. Li, J. Li and W. Wang, *Chem. Commun*. 2012, **48**, 1692-1694.

[6] Y. B. Lan, H. Zhao and X. Wang, *Org. Lett*., 2011, **13**, 4866-4869.

[7] E. Samahy, A. Fatma and F. Osman, *Tetrahedron*, 2000, **56**, 1863-1867.

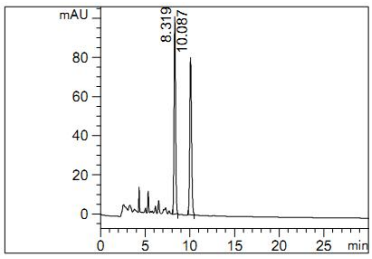
The chromatography for the determination of enantiomeric excess

Table 2, entry 1



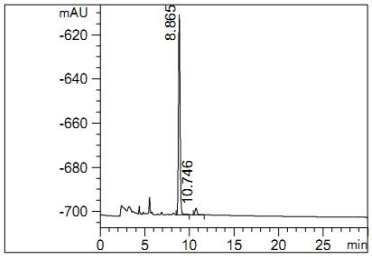
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (80/20); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



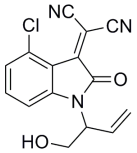
Peak #	RT [min]	Area %	Area
1	8.319	50.187	1.177e3
2	10.087	49.813	1.168e3

Chiral



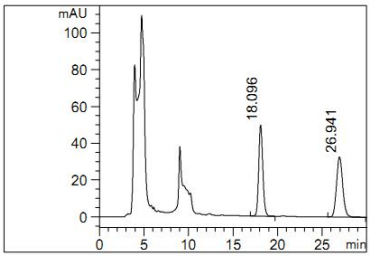
Peak #	RT [min]	Area %	Area
1	8.865	96.068	1.112e3
2	10.746	3.932	45.518

Table 2, entry 2



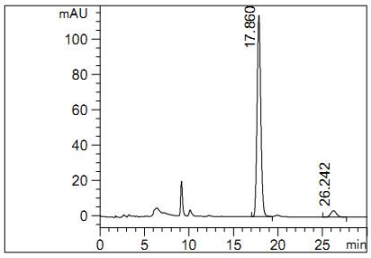
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (80/20); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



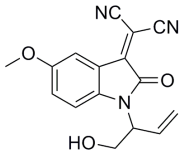
Peak #	RT [min]	Area %	Area
1	18.096	50.192	1.593e3
2	26.941	49.808	1.580e3

Chiral



Peak #	RT [min]	Area %	Area
1	17.860	95.310	3.303e3
2	26.242	4.690	162.554

Table 2, entry 3



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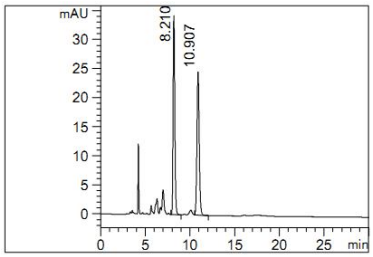
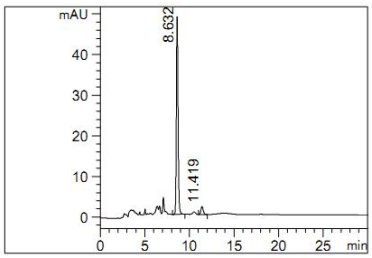
Racemic



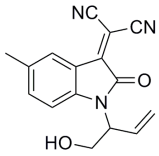
Peak #	RT [min]	Area %	Area
1	8.210	50.388	450.765
2	10.907	49.612	443.815

Chiral



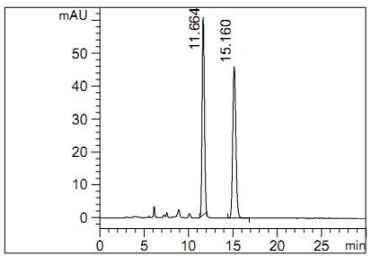
Peak #	RT [min]	Area %	Area
1	8.632	94.861	647.224
2	11.419	5.139	35.062

Table 2, entry 4



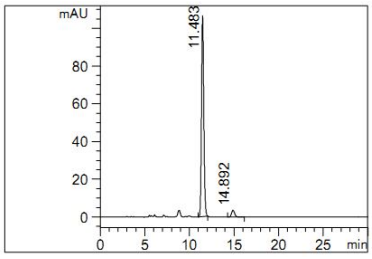
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (80/20); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



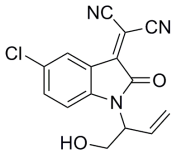
Peak #	RT [min]	Area %	Area
1	11.664	48.791	1.078e3
2	15.160	51.209	1.131e3

Chiral



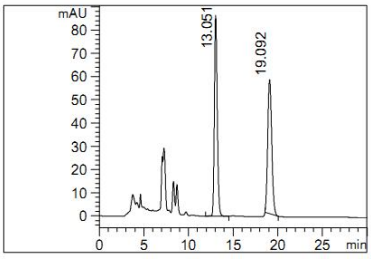
Peak #	RT [min]	Area %	Area
1	11.483	95.582	1.924e3
2	14.892	4.418	88.914

Table 2, entry 5



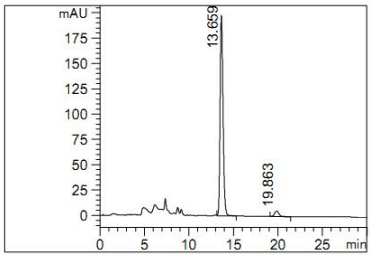
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (80/20); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



Peak #	RT [min]	Area %	Area
1	13.051	51.612	1.942e3
2	19.092	48.388	1.821e3

Chiral



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2	19.863	3.918	184.503

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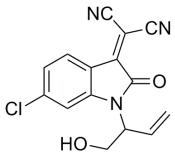
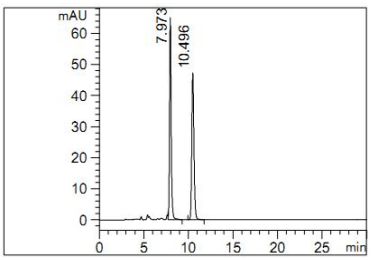


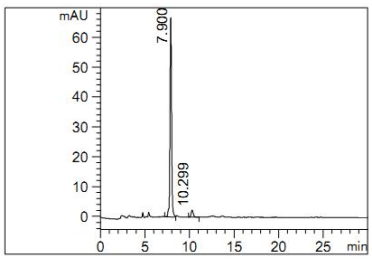
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (80/20); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



Peak #	RT [min]	Area %	Area
1	7.973	50.910	844.195
2	10.496	49.090	814.004

Chiral



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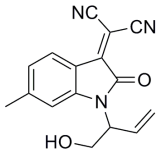
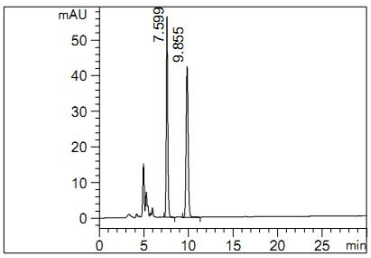
1	7.900	95.500	826.043
2	10.299	4.500	38.925

Table 2, entry 7



HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (80/20); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



Peak #	RT [min]	Area %	Area
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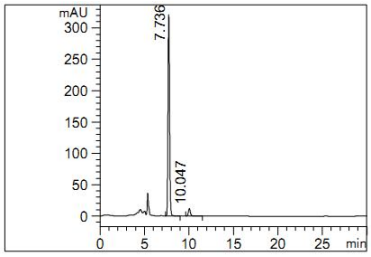
2	9.855	49.977	666.225

Chiral



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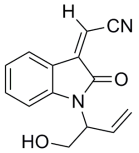
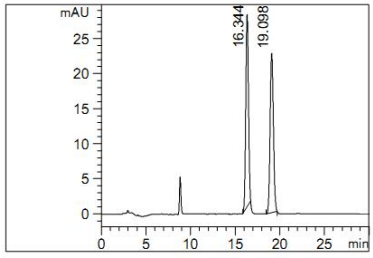
1	7.736	95.301	3.884e3
2	10.047	4.699	191.540

Table 2, entry 8



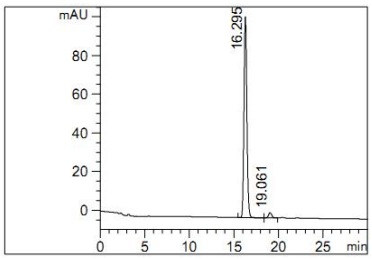
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



Peak #	RT [min]	Area %	Area
1	16.344	49.712	575.863
2	19.098	50.288	582.547

Chiral



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2	19.061	2.966	71.516

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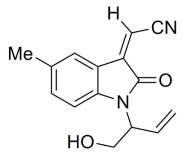
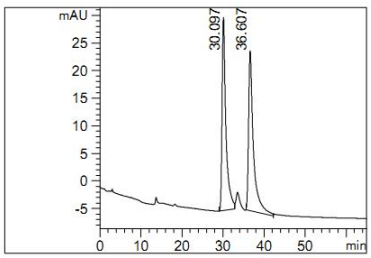


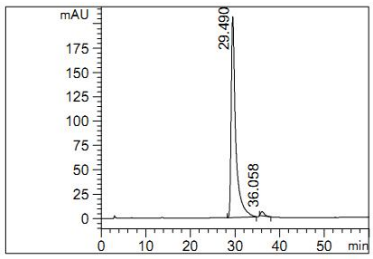
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



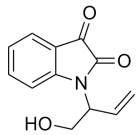
Peak #	RT [min]	Area %	Area
1	30.097	49.019	2.278e3
2	36.607	50.981	2.369e3

Chiral



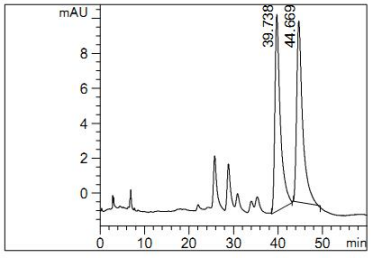
Peak #	RT [min]	Area %	Area
1	29.490	98.307	1.467e4
2	36.058	1.693	252.537

Table 2, entry 10



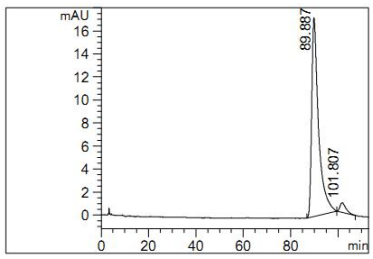
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



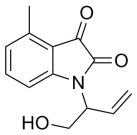
Peak #	RT [min]	Area %	Area
1	39.738	49.541	953.067
2	44.669	50.459	970.728

Chiral



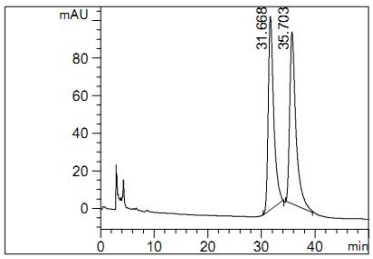
Peak #	RT [min]	Area %	Area
1	39.735	96.592	1.129e4
2	44.617	3.408	398.423

Table 2, entry 11



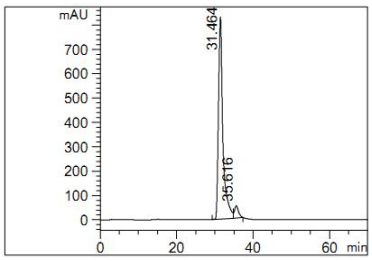
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



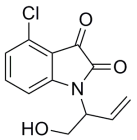
Peak #	RT [min]	Area %	Area
1	31.668	49.582	7.276e3
2	35.703	50.418	7.398e3

Chiral



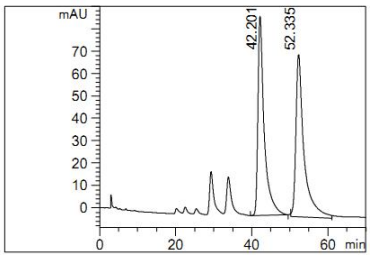
Peak #	RT [min]	Area %	Area
1	31.464	94.626	6.678e4
2	35.616	5.374	3.793e3

Table 2, entry 12



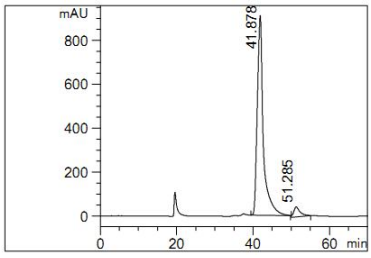
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



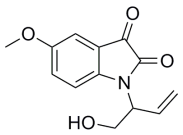
Peak #	RT [min]	Area %	Area
1	42.201	48.966	1.025e4
2	52.335	51.034	1.068e4

Chiral



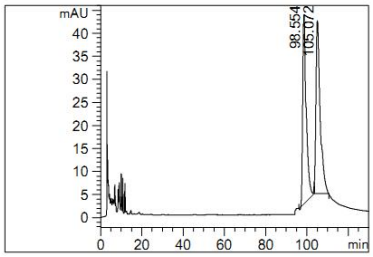
Peak #	RT [min]	Area %	Area
1	41.878	94.982	9.872e4
2	51.285	5.018	5.215e3

Table 2, entry 13



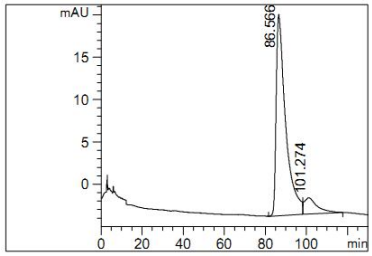
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (99/1); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



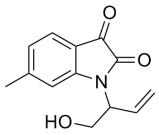
Peak #	RT [min]	Area %	Area
1	98.553	49.989	5.060e3
2	105.077	50.011	5.062e3

Chiral



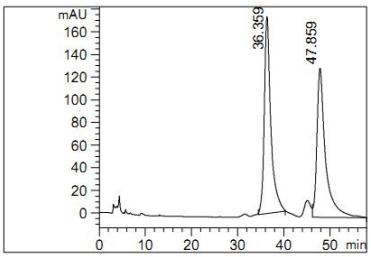
Peak #	RT [min]	Area %	Area
1	86.566	89.861	7.615e3
2	101.274	10.139	859.209

Table 2, entry 14



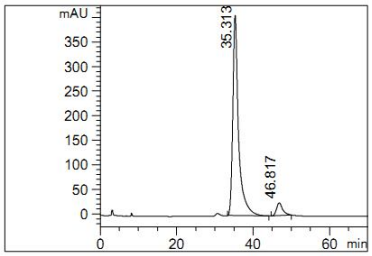
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



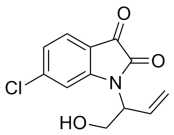
Peak #	RT [min]	Area %	Area
1	36.359	50.127	1.718e4
2	47.859	49.873	1.709e4

Chiral



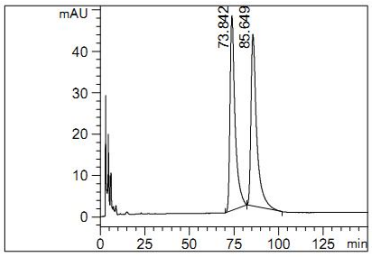
Peak #	RT [min]	Area %	Area
1	35.313	93.631	4.260e4
2	46.817	6.369	2.898e3

Table 2, entry 15



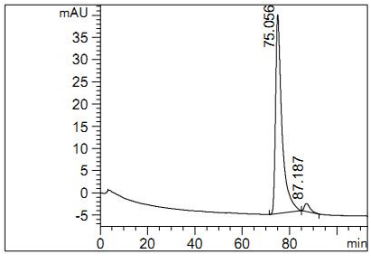
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic

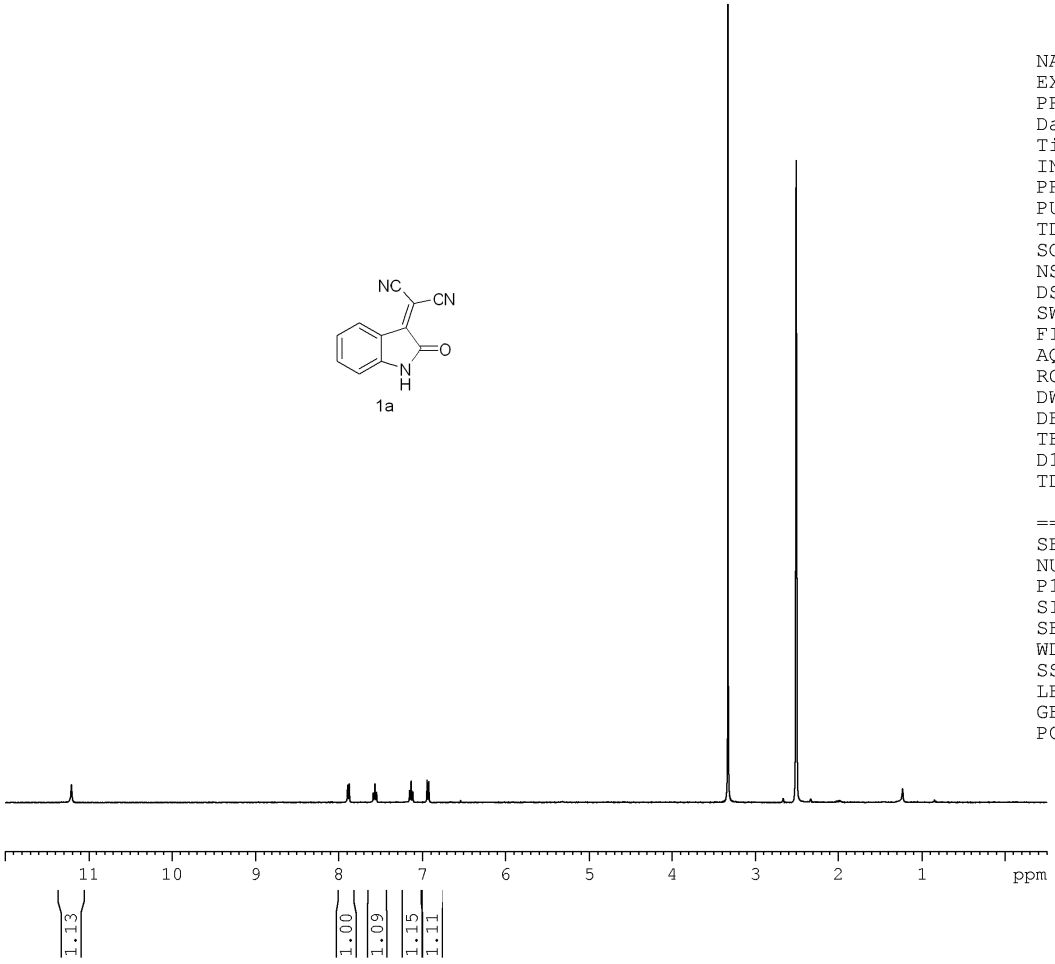


Peak #	RT [min]	Area %	Area
1	73.842	50.179	9.348e3
2	85.649	49.821	9.281e3

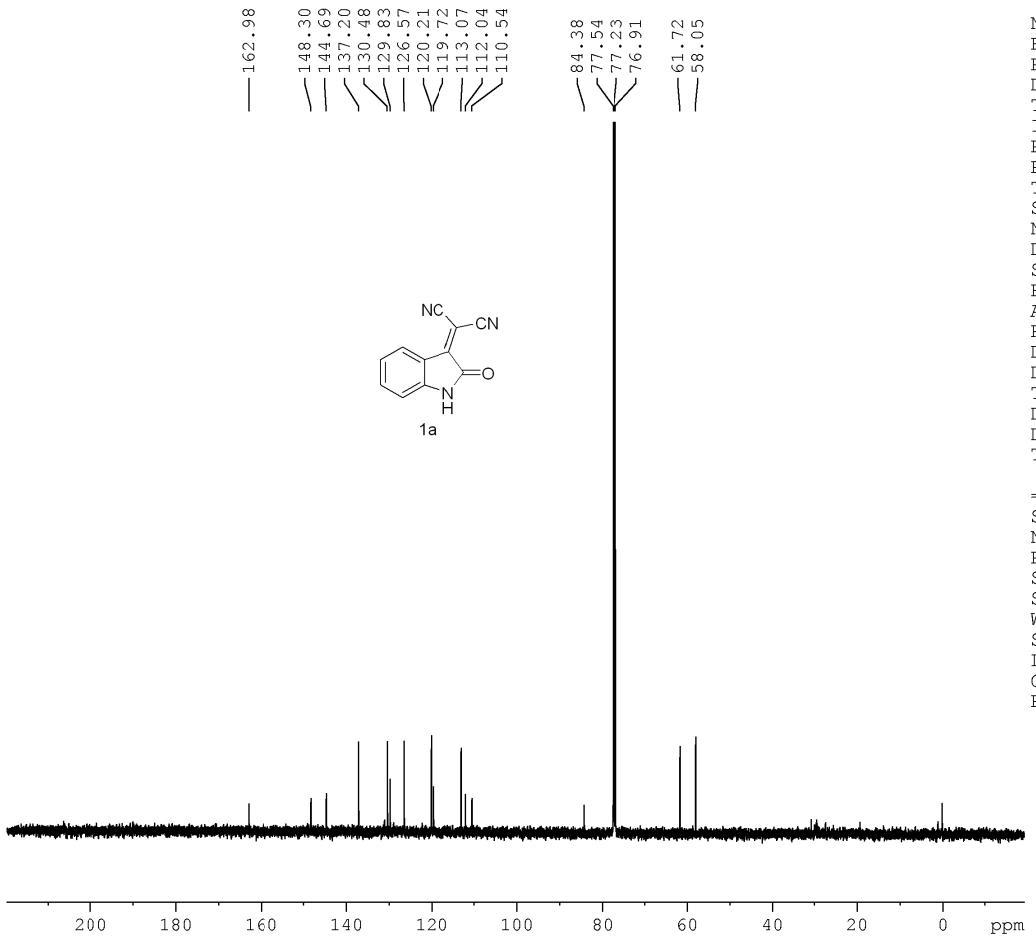
Chiral



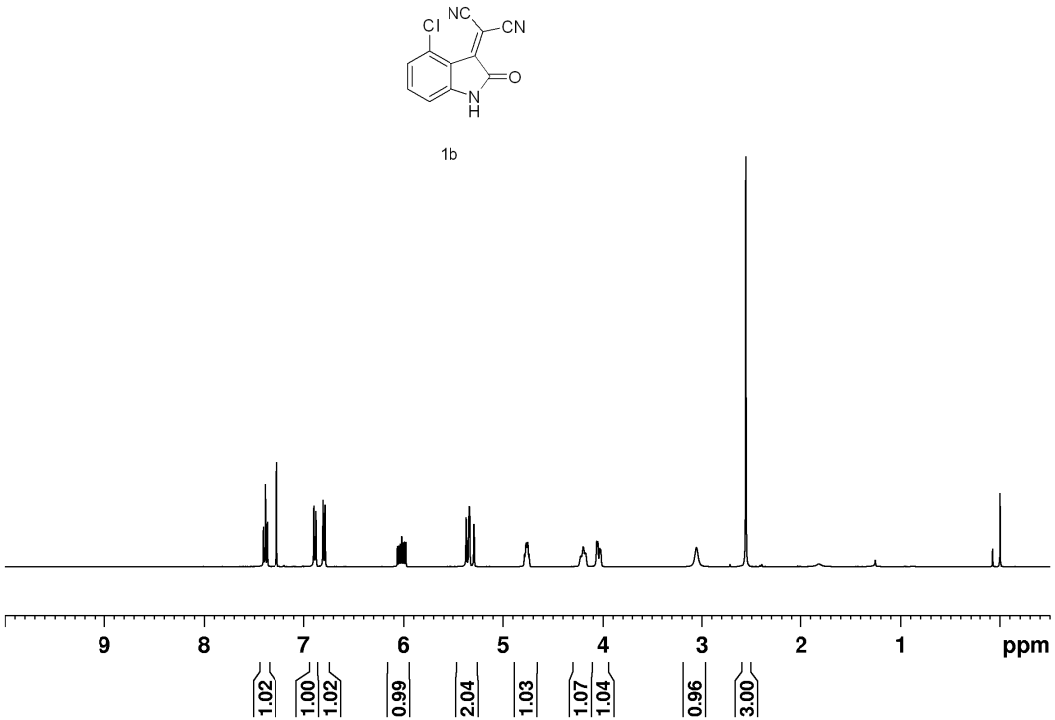
Peak #	RT [min]	Area %	Area
1	75.056	96.400	8.440e3
2	87.187	3.600	315.207



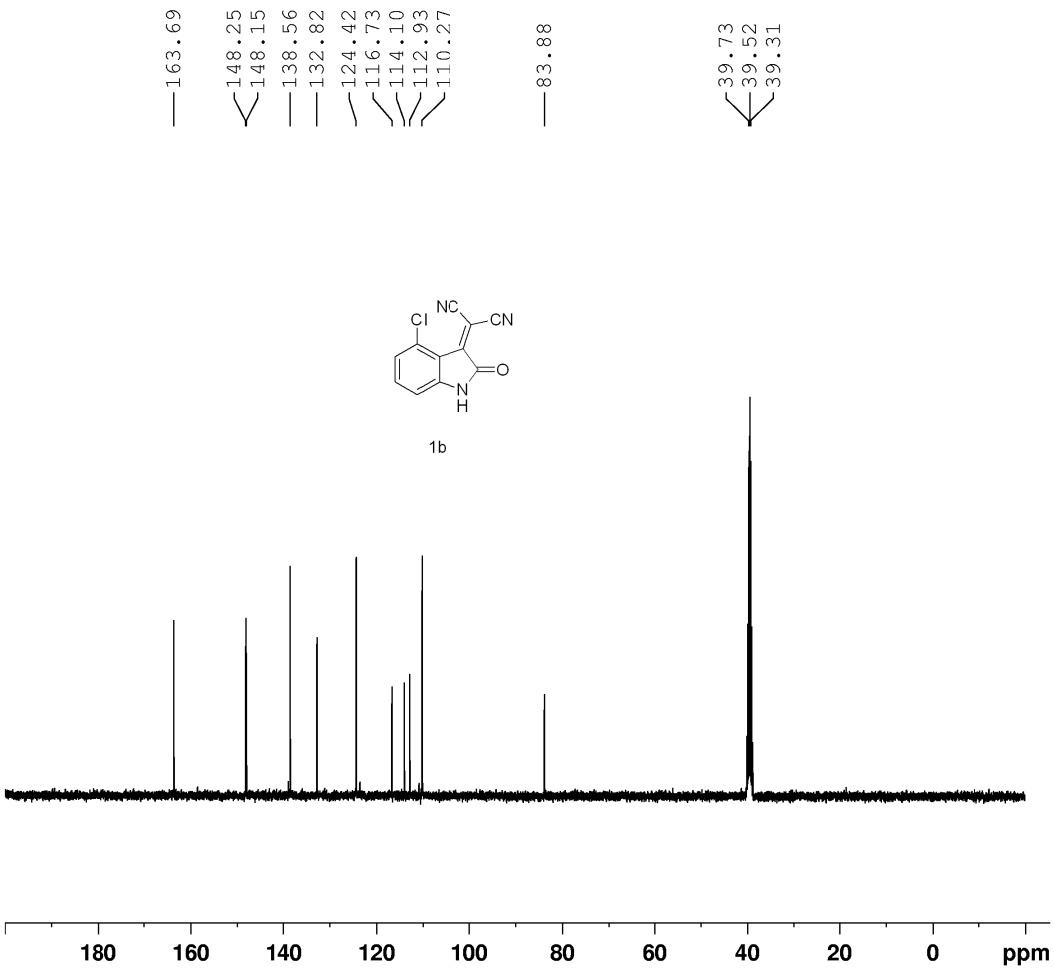

```
NAME                LG-xin
EXPNO                  86
PROCNO                  1
Date_           20140516
Time                 2.56
INSTRUM              spec
PROBHD    5 mm PADUL 13C
PULPROG              zg30
TD                  32768
SOLVENT              DMSO
NS                      9
DS                      0
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                    203
DW                 41.600 usec
DE                  6.50 usec
TE                 300.0 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1320007 MHz
NUC1                1H
P1                 12.60 usec
SI                 65536
SF           400.1300033 MHz
WDW                  EM
SSB                   0
LB                 0.50 Hz
GB                    0
PC                 1.00
```



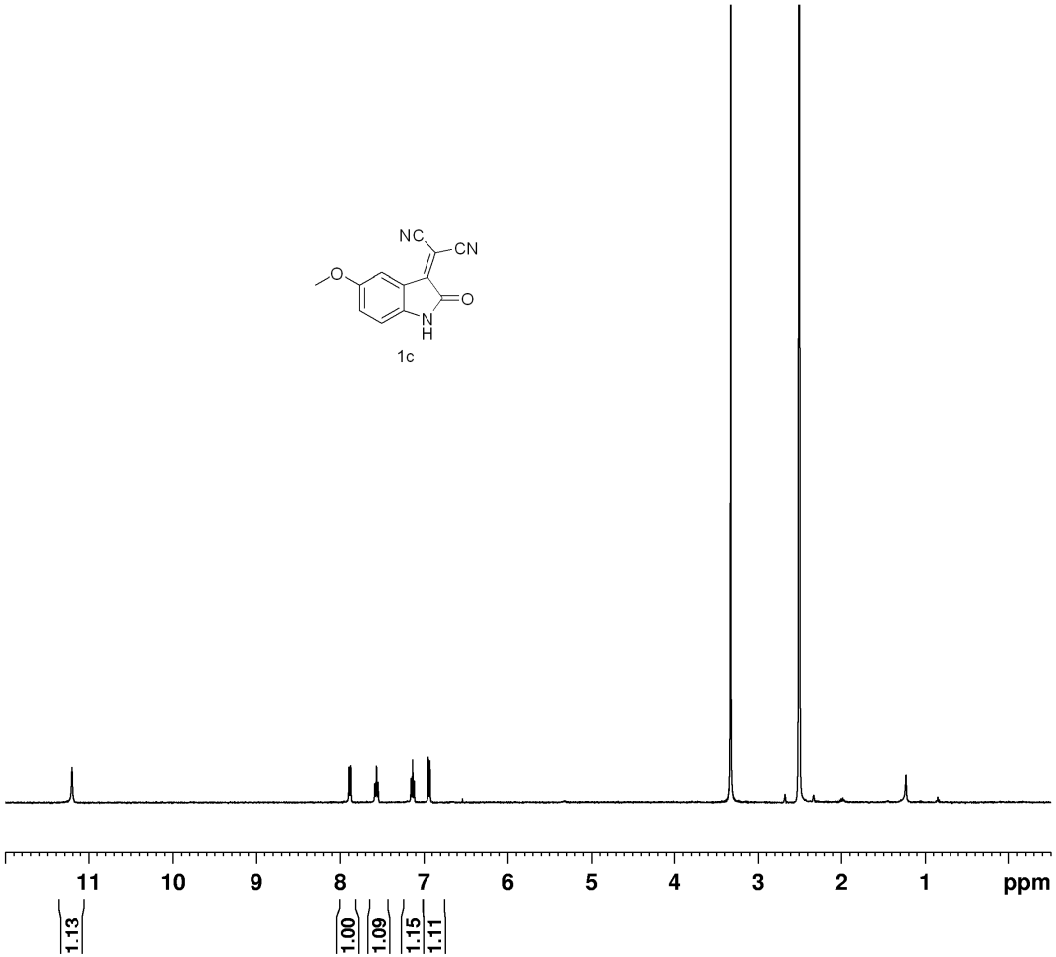
NAME	LG-xin
EXPNO	65
PROCNO	1
Date_	20140508
Time	3.03
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	802
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127493 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



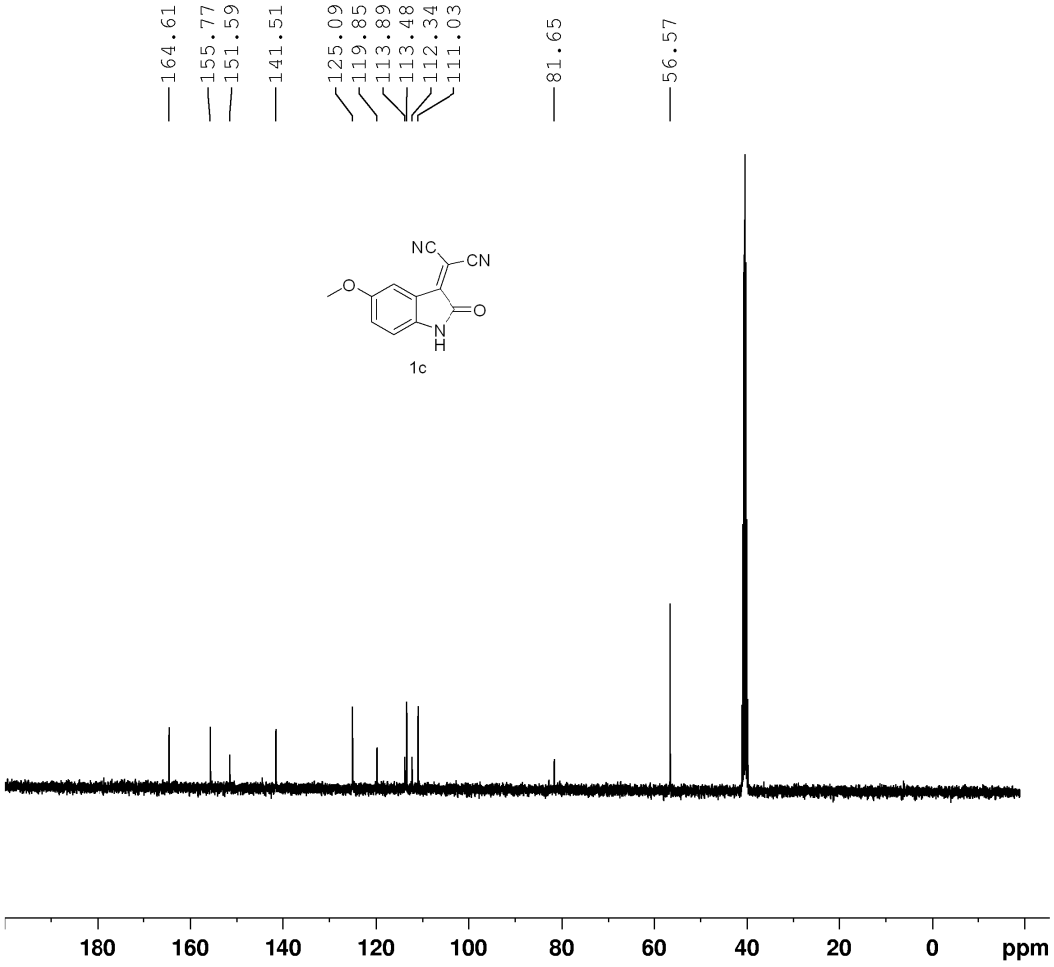
NAME	LG-xin
EXPNO	54
PROCNO	1
Date_	20140416
Time	7.48
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	6
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	101
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300043 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00



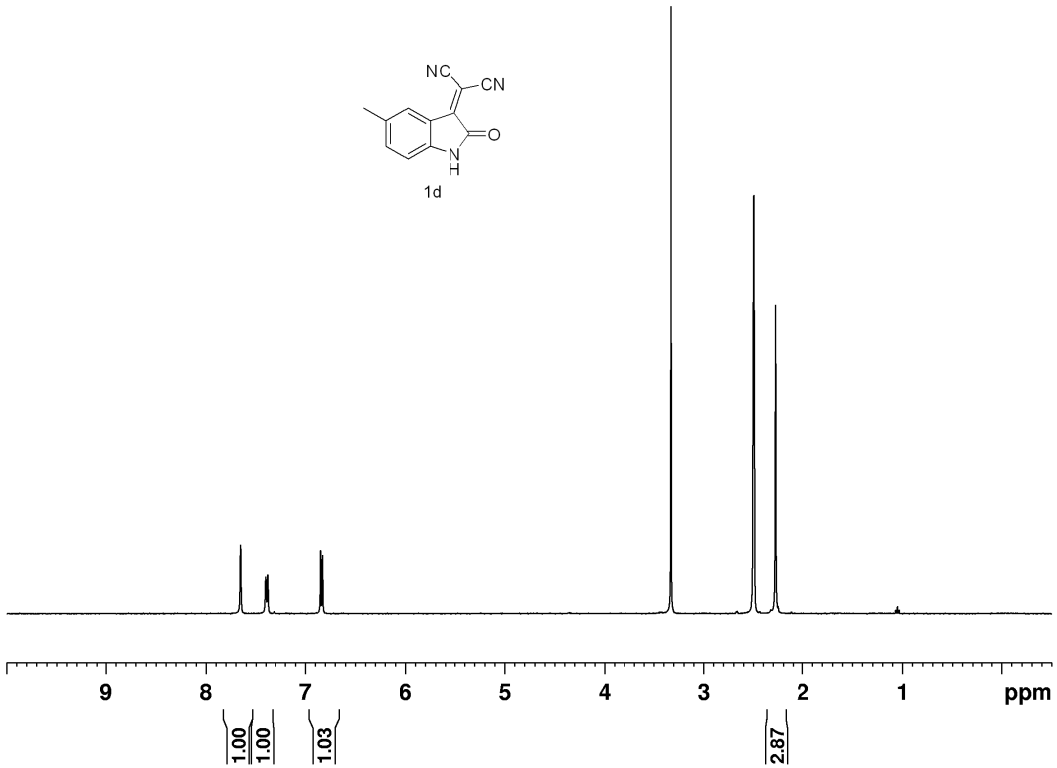

```
NAME                lgx
EXPNO                97
PROCNO                1
Date_          20141210
Time              23.34
INSTRUM           spect
PROBHD    5 mm PADUL 13C
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                    62
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1                13C
P1                 9.40 usec
SI                32768
SF          100.6128116 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



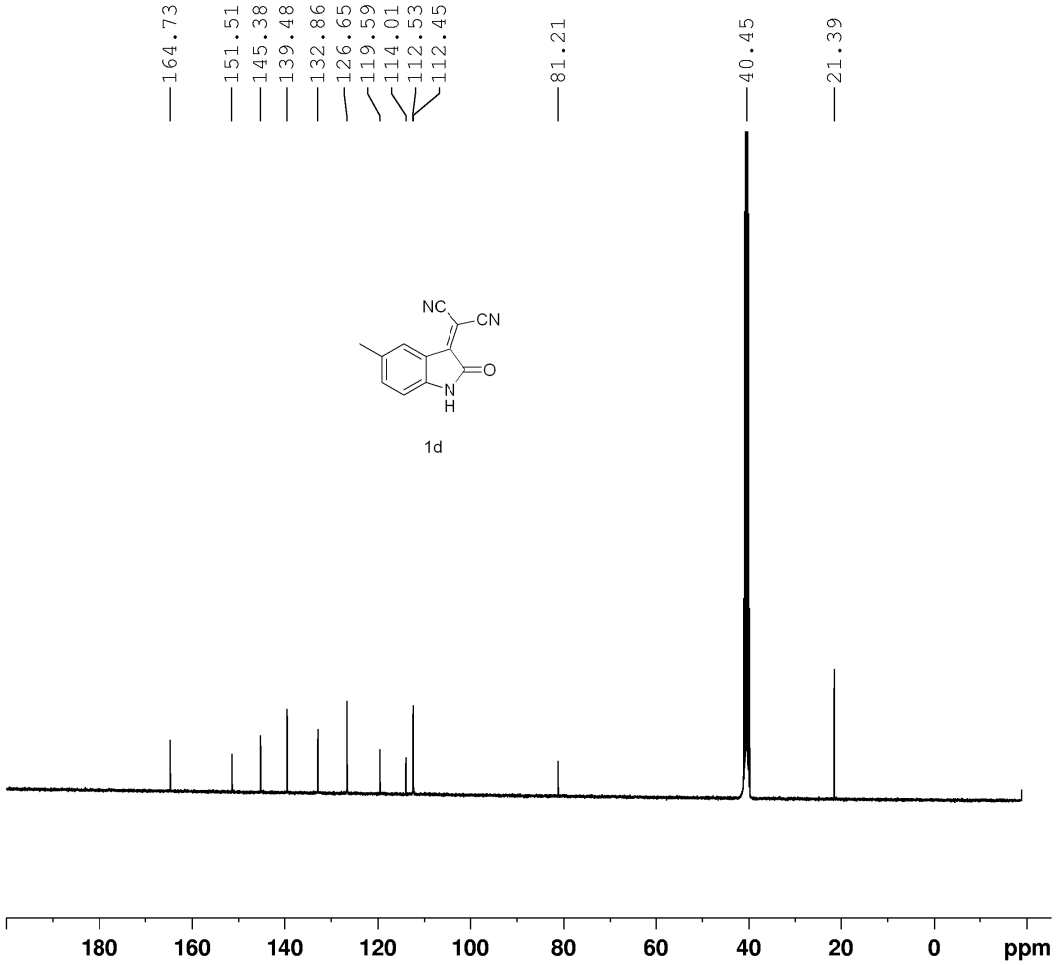
NAME	LG-xin
EXPNO	86
PROCNO	1
Date_	20140516
Time	2.56
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	9
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300033 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00



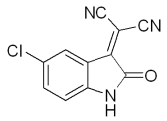
NAME	LG-xin
EXPNO	85
PROCNO	1
Date_	20140514
Time	3.03
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	DMSC
NS	96
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127196 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



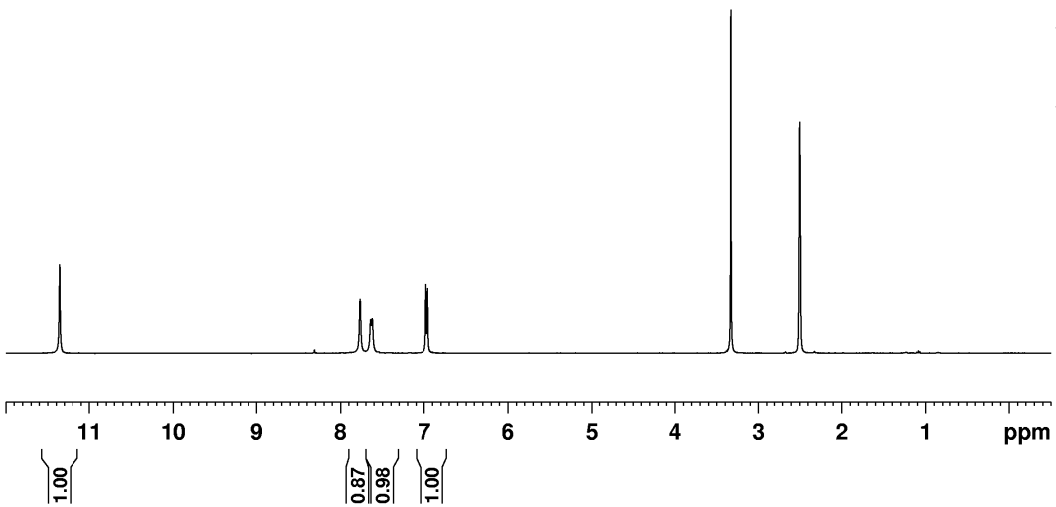
NAME	LG-xin
EXPNO	75
PROCNO	1
Date_	20140511
Time	6.21
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	6
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300032 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00



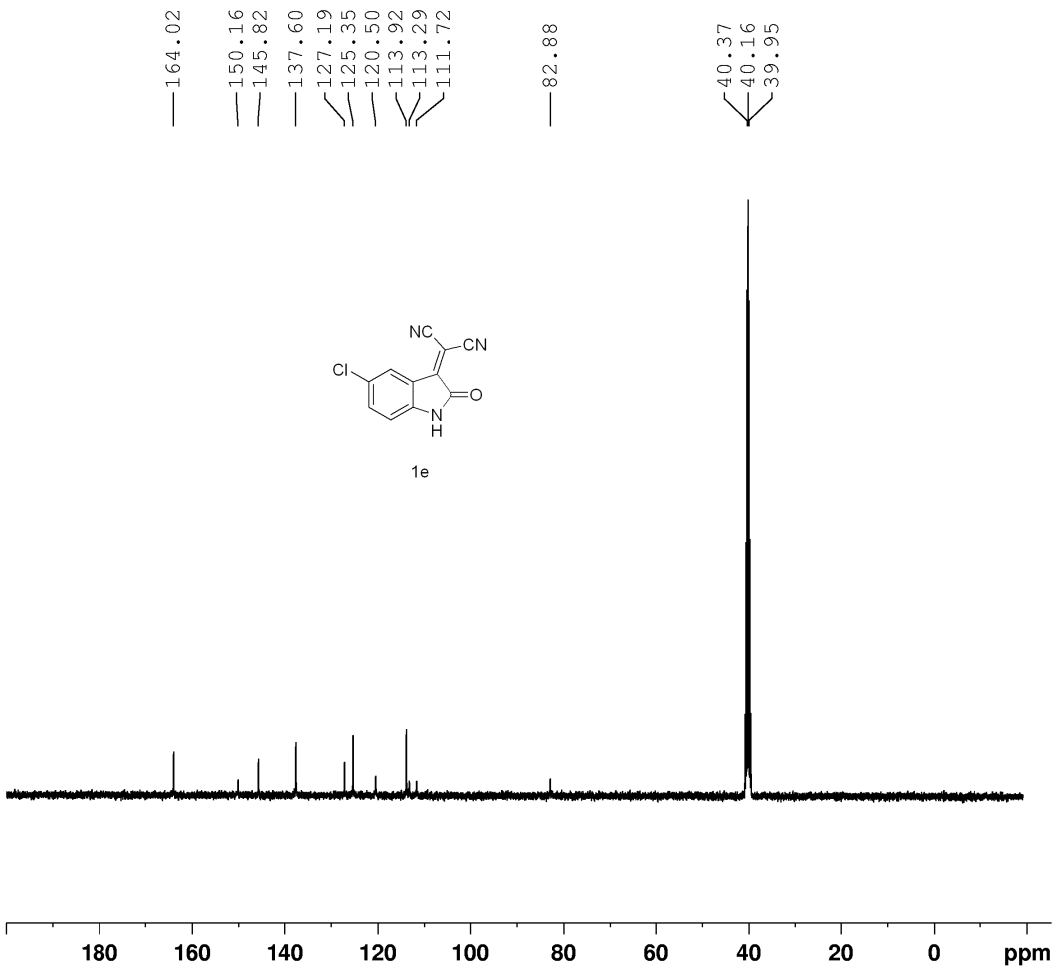
NAME	lgx
EXPNO	76
PROCNO	1
Date_	20140514
Time	23.15
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	10563
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127211 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



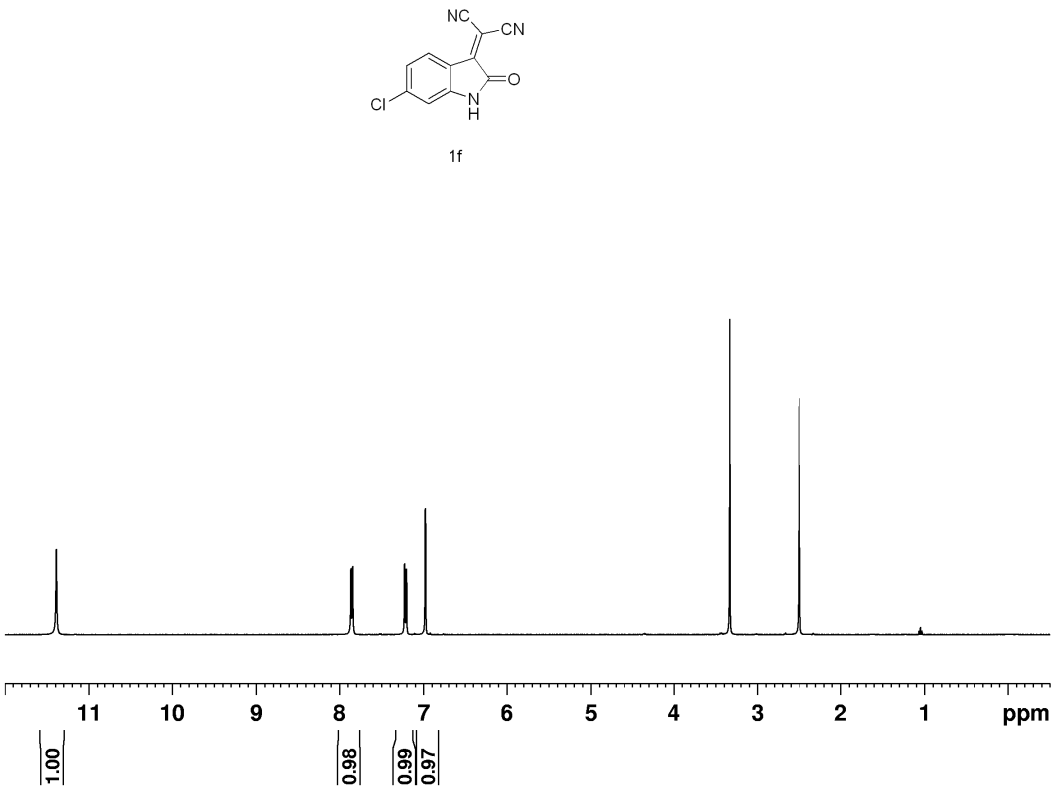
1e



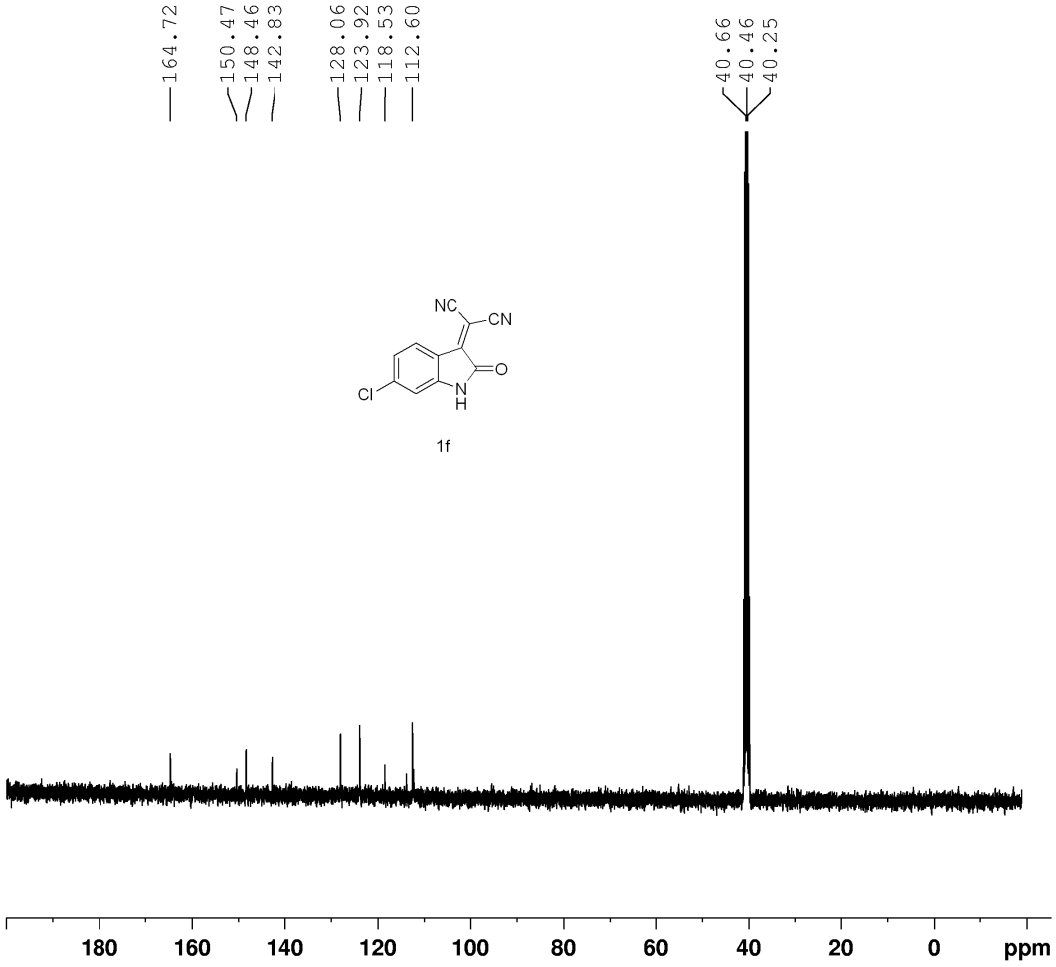
NAME	LG-xin
EXPNO	72
PROCNO	1
Date_	20140511
Time	5.53
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	9
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300032 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00



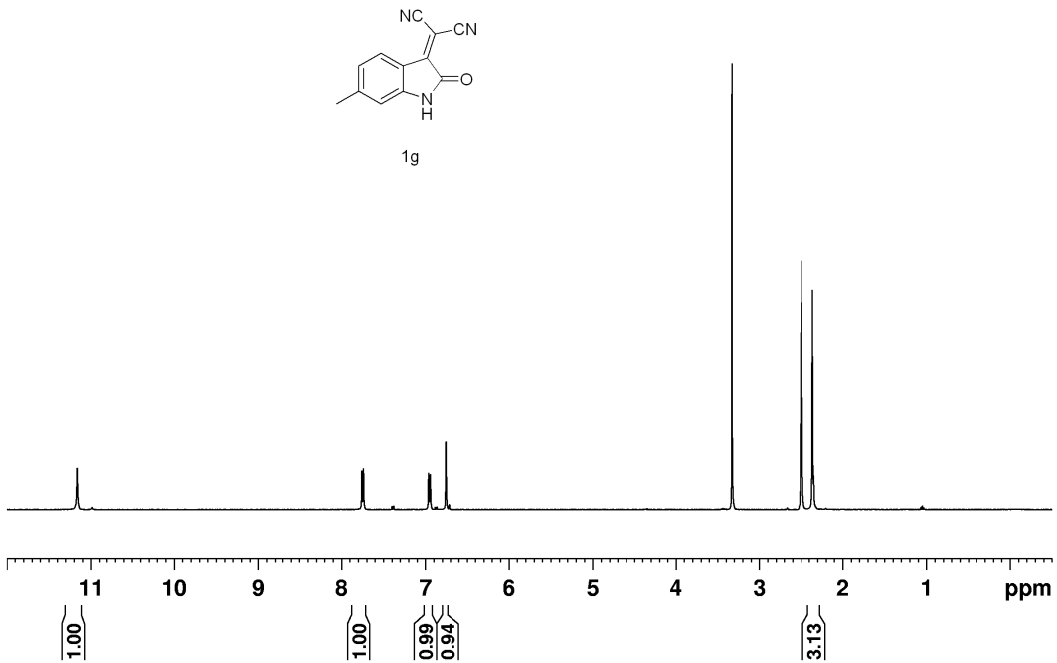
NAME	lgx
EXPNO	96
PROCNO	1
Date_	20141210
Time	9.12
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	288
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127507 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



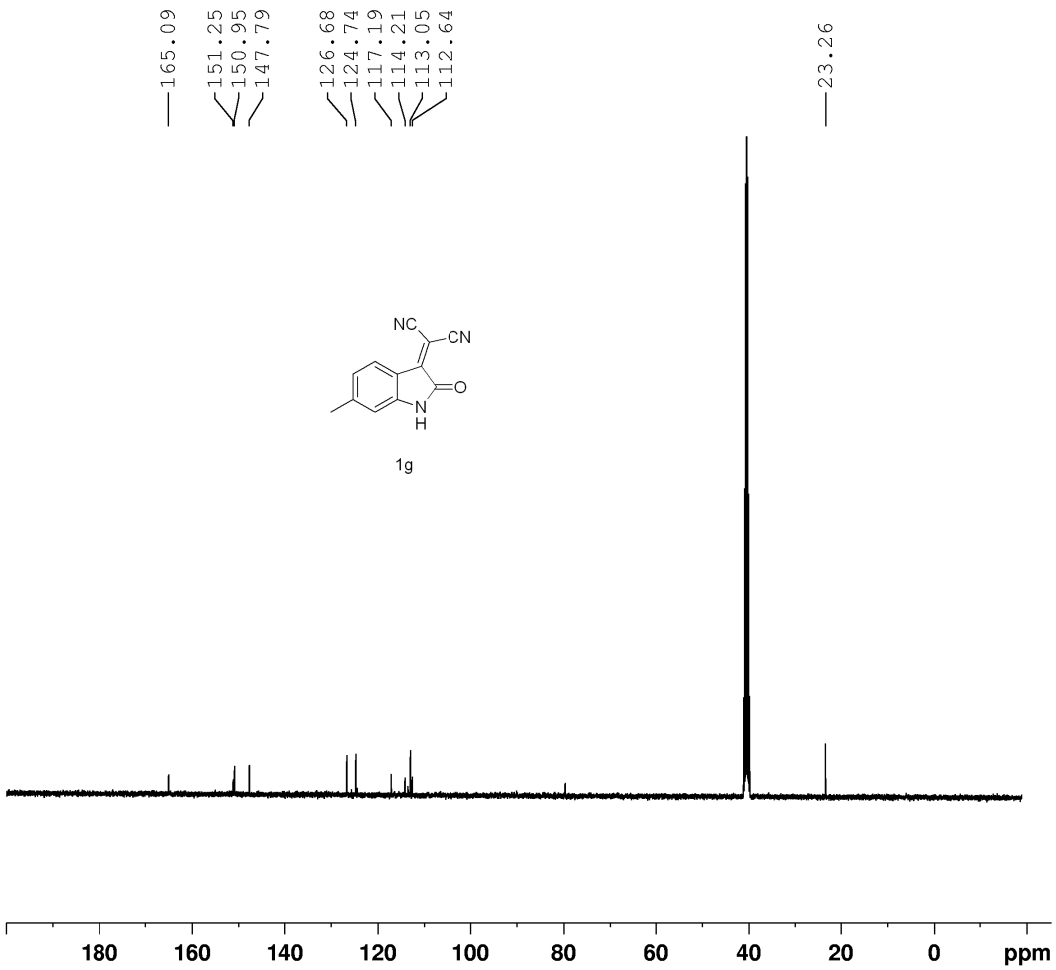
NAME	LG-xin
EXPNO	73
PROCNO	1
Date_	20140511
Time	6.03
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	5
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300032 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00



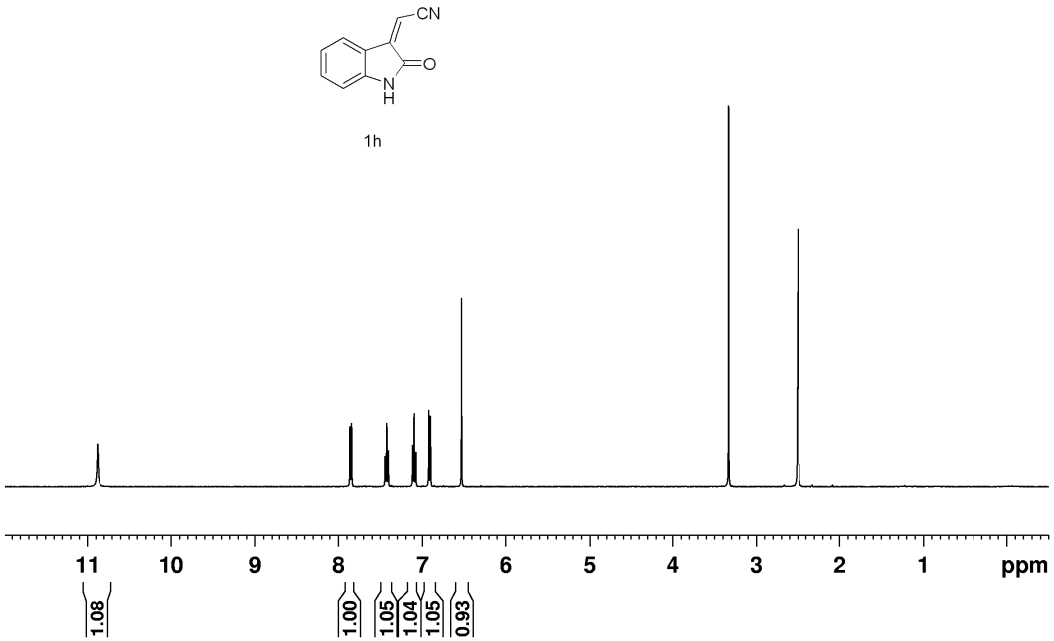

```
NAME                LG-xin
EXPNO                   74
PROCNO                   1
Date_             20140511
Time                  6.04
INSTRUM              spect
PROBHD    5 mm PADUL 13C
PULPROG            zgpg30
TD                   65536
SOLVENT                DMSO
NS                       254
DS                         4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                       203
DW                  20.800 usec
DE                   6.50 usec
TE                  300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6228293 MHz
NUC1                   13C
P1                    9.40 usec
SI                   32768
SF             100.6127209 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



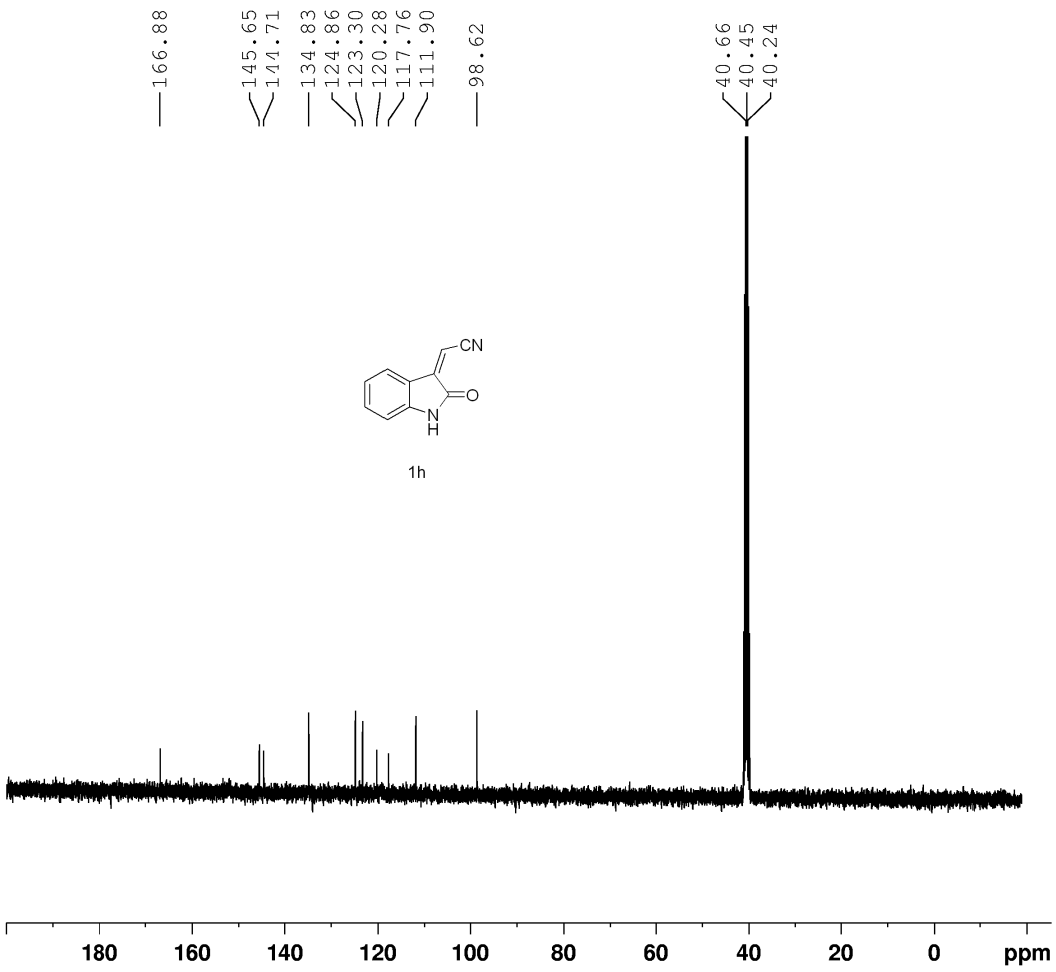
NAME	LG-xin
EXPNO	81
PROCNO	1
Date_	20140511
Time	6.54
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	4
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300032 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00



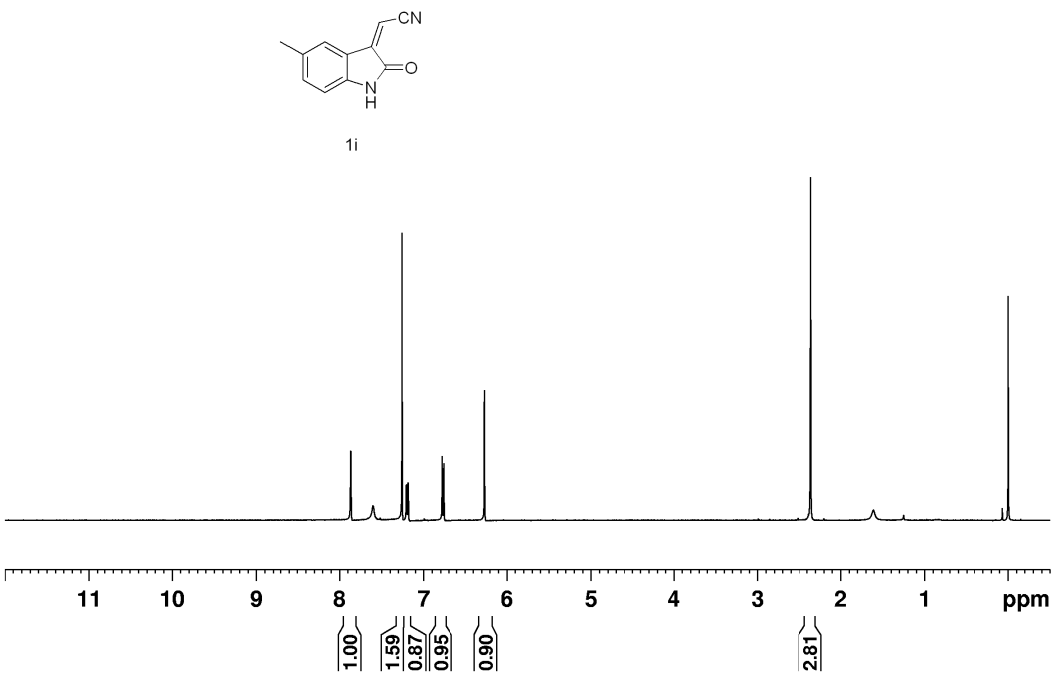
NAME	lgx
EXPNO	82
PROCNO	1
Date_	20140513
Time	12.51
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	700
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127216 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



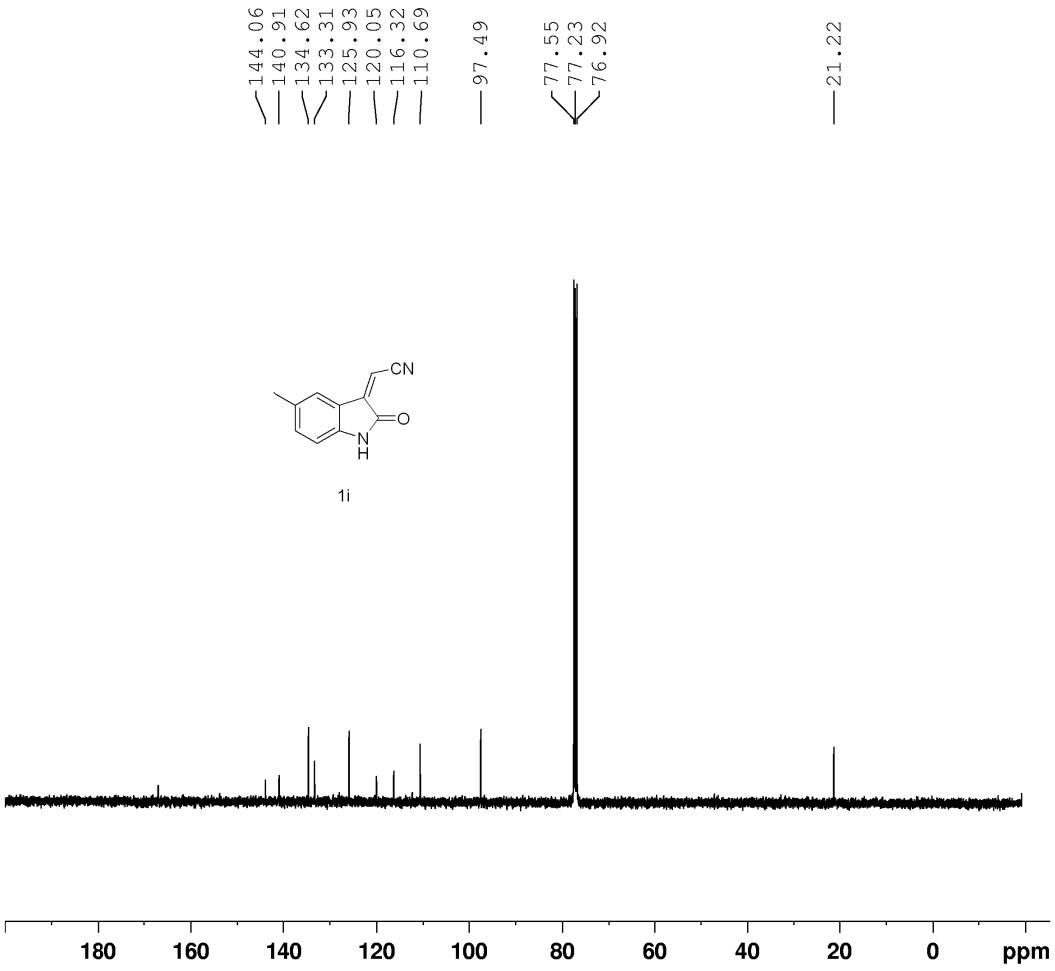
NAME	LG-xin
EXPNO	79
PROCNO	1
Date_	20140511
Time	6.42
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	3
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300032 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00



NAME	LG-xin
EXPNO	80
PROCNO	1
Date_	20140511
Time	6.44
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	151
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127210 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40




```
NAME              LG-xin
EXPNO                 29
PROCNO                 1
Date_           20140315
Time                3.05
INSTRUM            spect
PROBHD    5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH           12019.230 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   203
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1320007 MHz
NUC1                   1H
P1                 12.60 usec
SI                 65536
SF          400.1300093 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```



NAME	LG-xin
EXPNO	30
PROCNO	1
Date_	20140319
Time	11.58
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	665
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

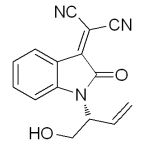
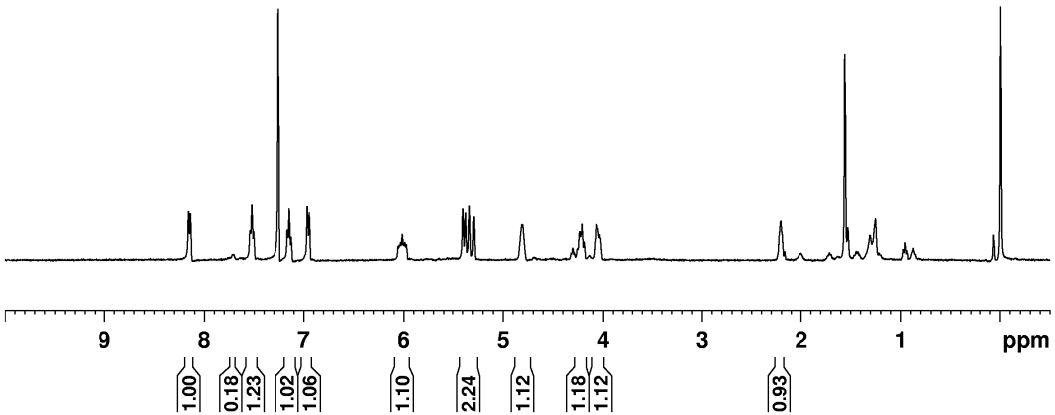


Table 2, entry 1




```
NAME                  LG
EXPNO                112
PROCNO                 1
Date_           20121103
Time                6.30
INSTRUM            spect
PROBHD    5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH           12019.230 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   203
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.60 usec
SI                 65536
SF          400.1300187 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```

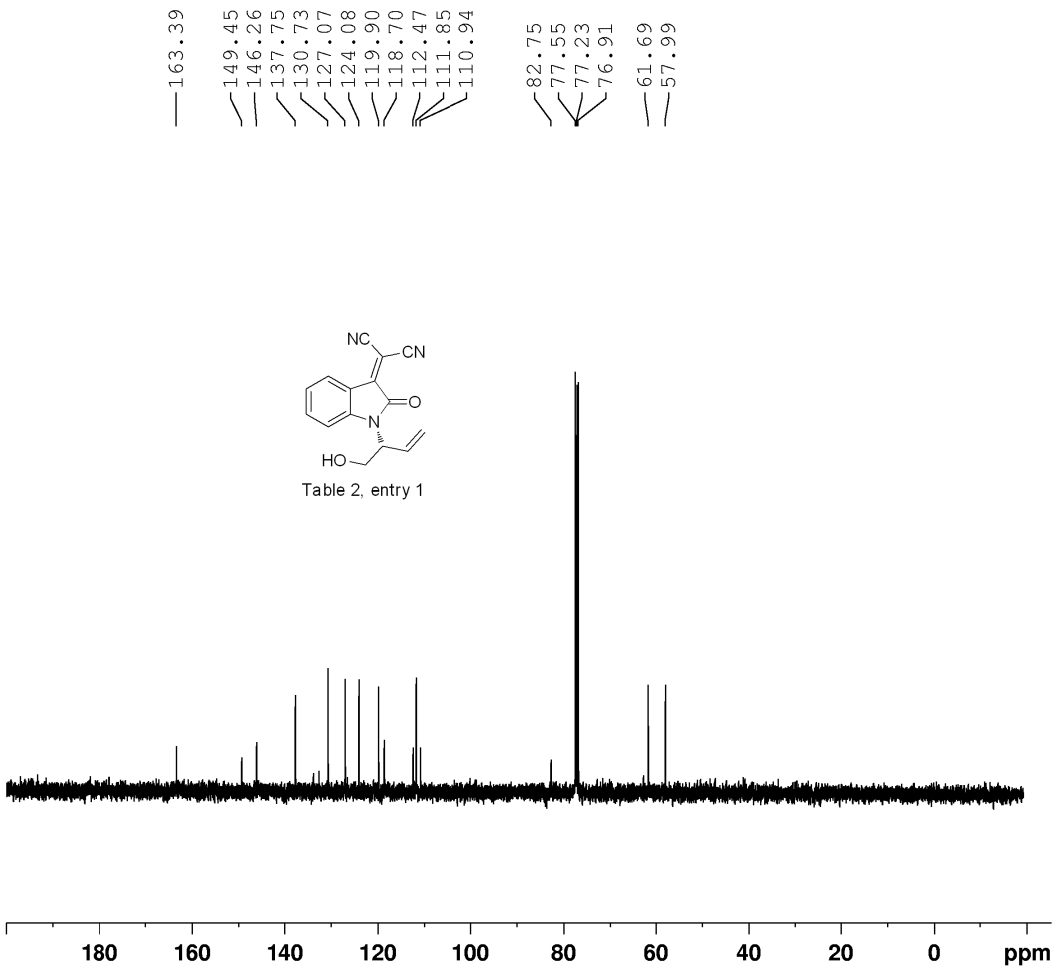


Table 2, entry 1

NAME	LG-xin
EXPNO	63
PROCNO	1
Date_	20140508
Time	1.58
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	75
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127521 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

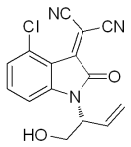
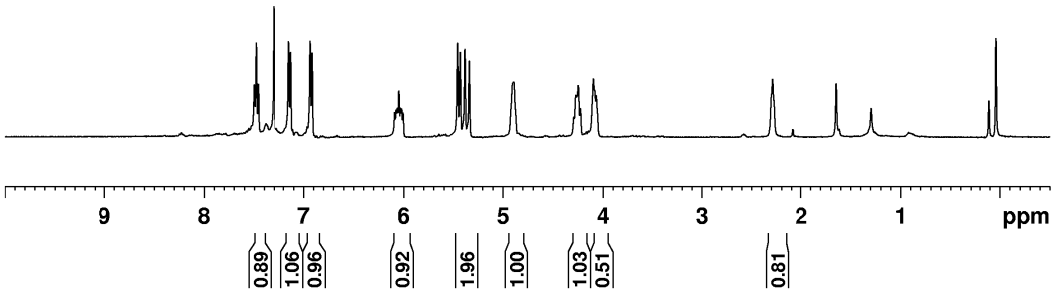


Table 2, entry 2



NAME	LG
EXPNO	203
PROCNO	1
Date_	20121129
Time	12.29
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

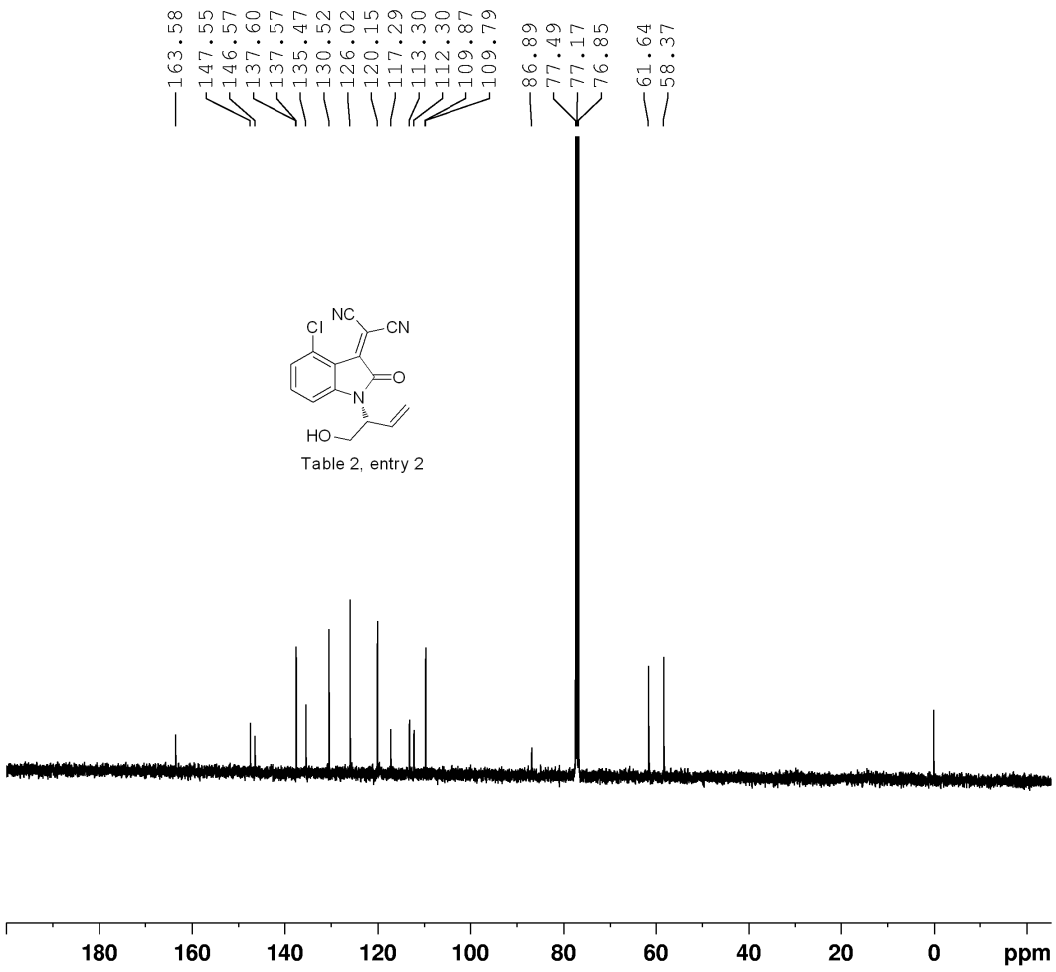


Table 2, entry 2

NAME	LG	
EXPNO	199	
PROCNO	1	
Date_	20140508	
Time	23.39	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	19245	
DS	0	
SWH	25252.525	Hz
FIDRES	0.770646	Hz
AQ	0.6488564	sec
RG	203	
DW	19.800	usec
DE	6.50	usec
TE	300.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.40	usec
SI	32768	
SF	100.6127550	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

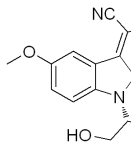
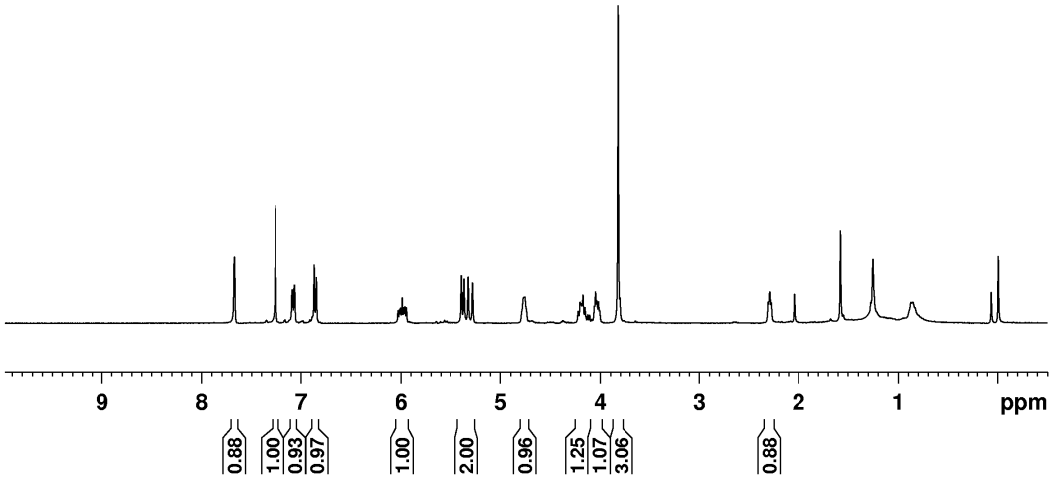


Table 2, entry 3



NAME	LG
EXPNO	156
PROCNO	1
Date_	20121116
Time	8.57
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300184 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

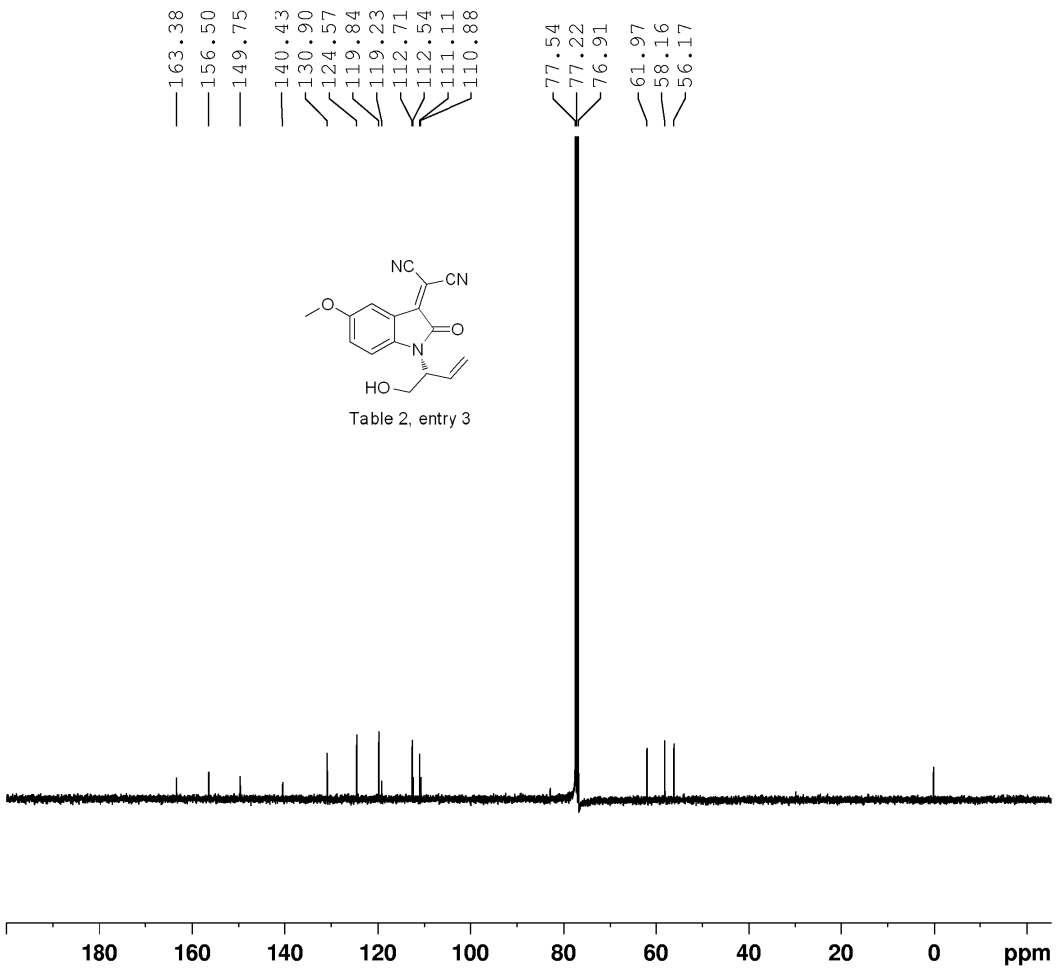


Table 2, entry 3

NAME	LG
EXPNO	157
PROCNO	1
Date_	20140510
Time	6.09
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	7072
DS	0
SWH	25252.525 Hz
FIDRES	0.770646 Hz
AQ	0.6488564 sec
RG	203
DW	19.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127495 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

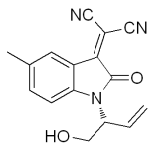
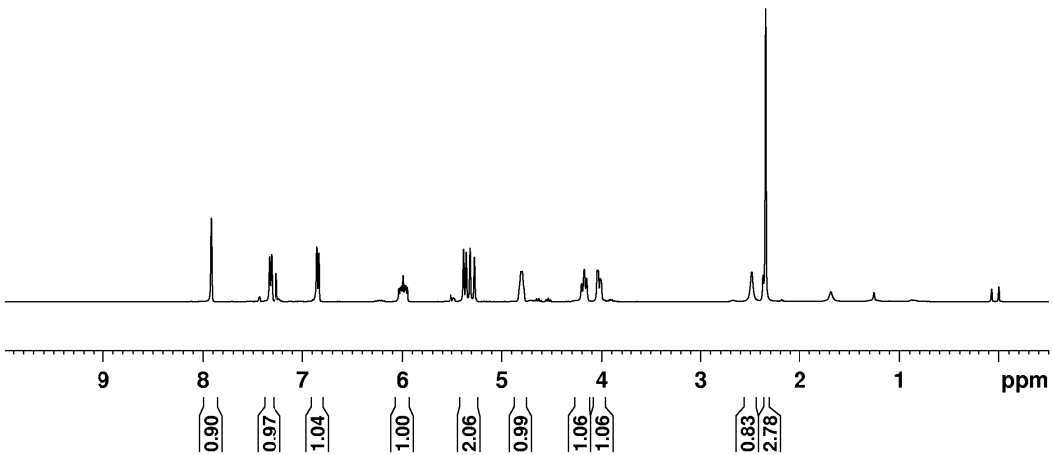


Table 2, entry 4



NAME	lgx
EXPNO	189
PROCNO	1
Date_	20121124
Time	9.27
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	181
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300159 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

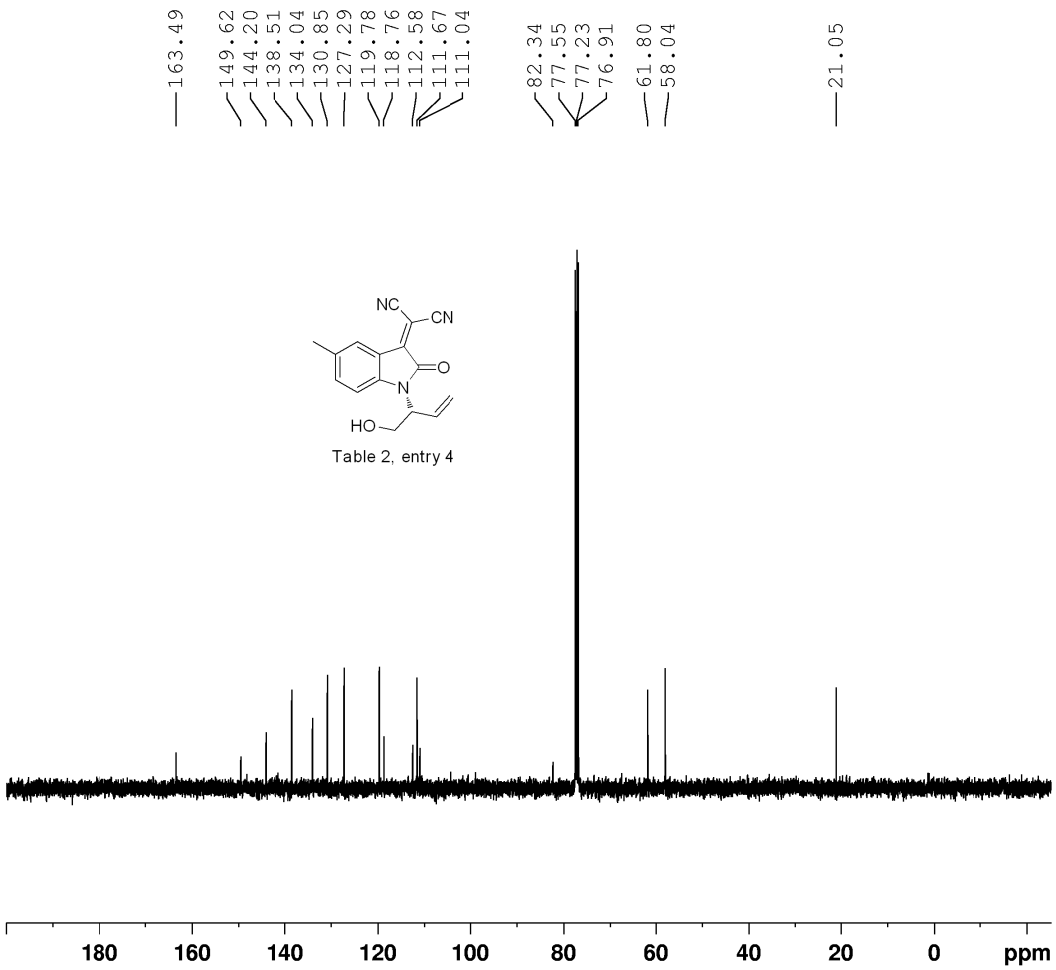


Table 2, entry 4

NAME	LG	
EXPNO	190	
PROCNO	1	
Date_	20121124	
Time	9.30	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	90	
DS	0	
SWH	25252.525	Hz
FIDRES	0.770646	Hz
AQ	0.6488564	sec
RG	203	
DW	19.800	usec
DE	6.50	usec
TE	300.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.40	usec
SI	32768	
SF	100.6127525	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

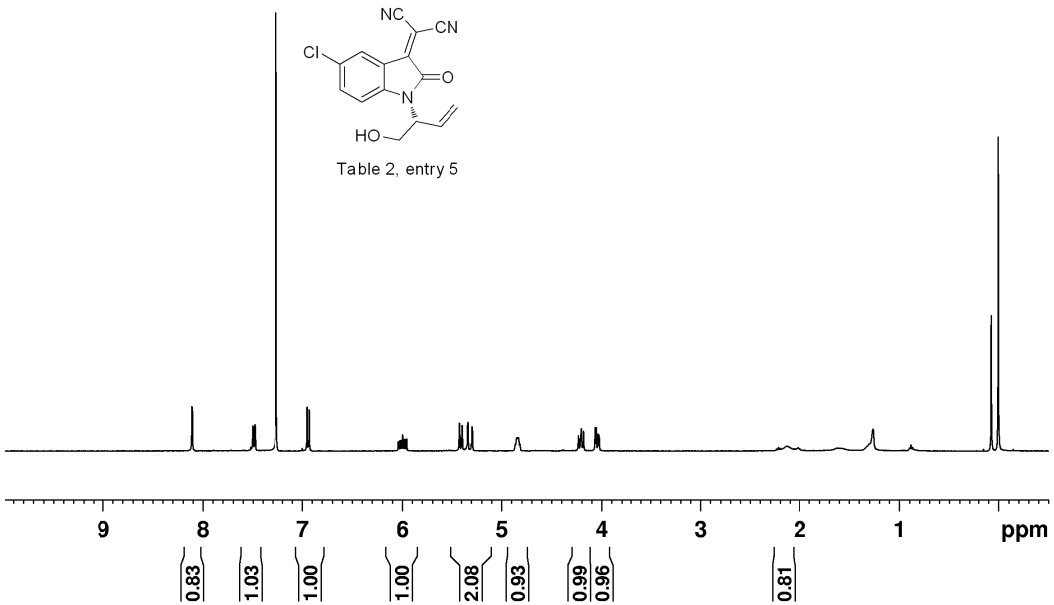


Table 2, entry 5

NAME	LG-xin
EXPNO	20
PROCNO	1
Date_	20140302
Time	6.13
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300070 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

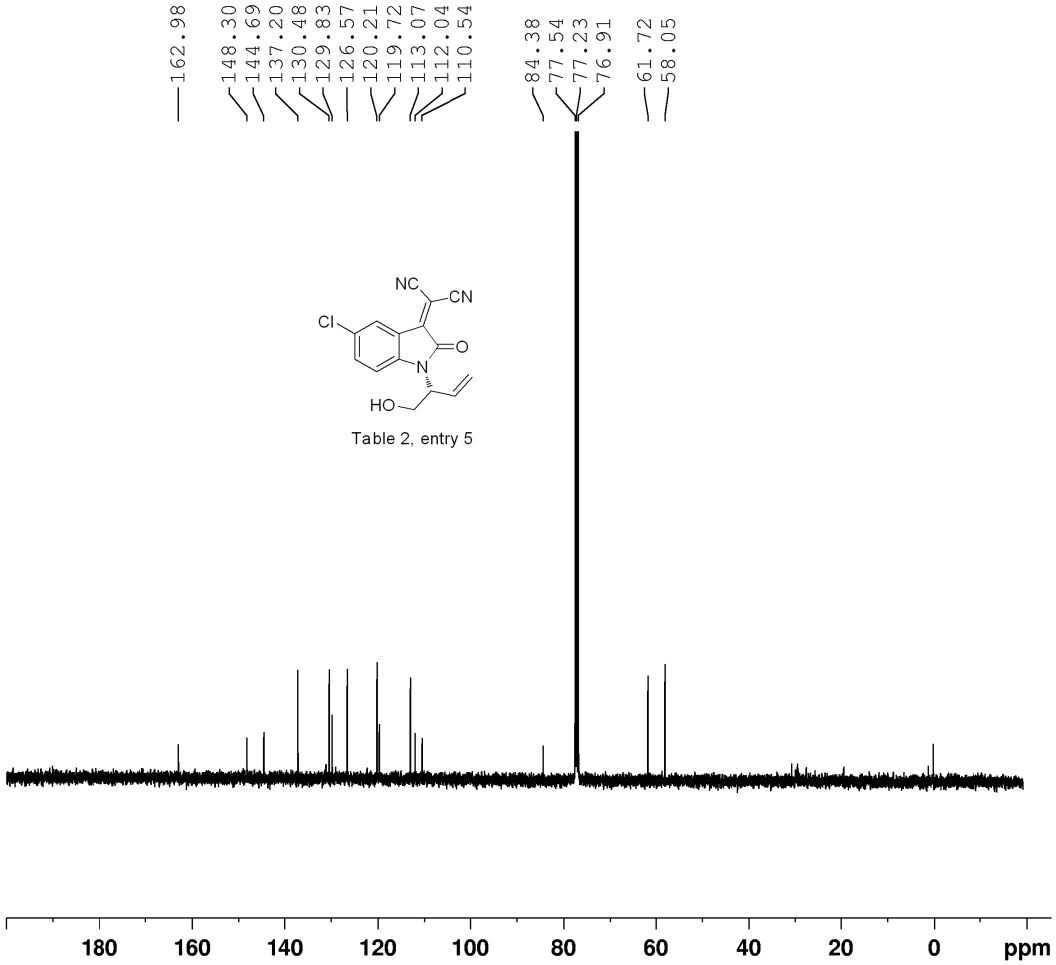


Table 2, entry 5

NAME	LG-xin
EXPNO	65
PROCNO	1
Date_	20140508
Time	3.03
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	802
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127493 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

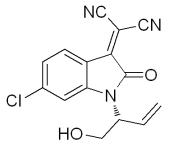
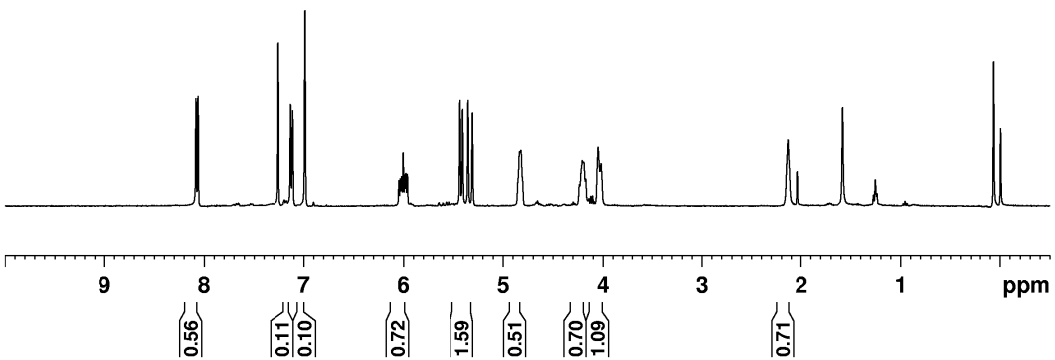


Table 2, entry 6




```
NAME                  LG
EXPNO                186
PROCNO                 1
Date_           20121123
Time                9.05
INSTRUM            spect
PROBHD    5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH           12019.230 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   203
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.60 usec
SI                 65536
SF          400.1300182 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```

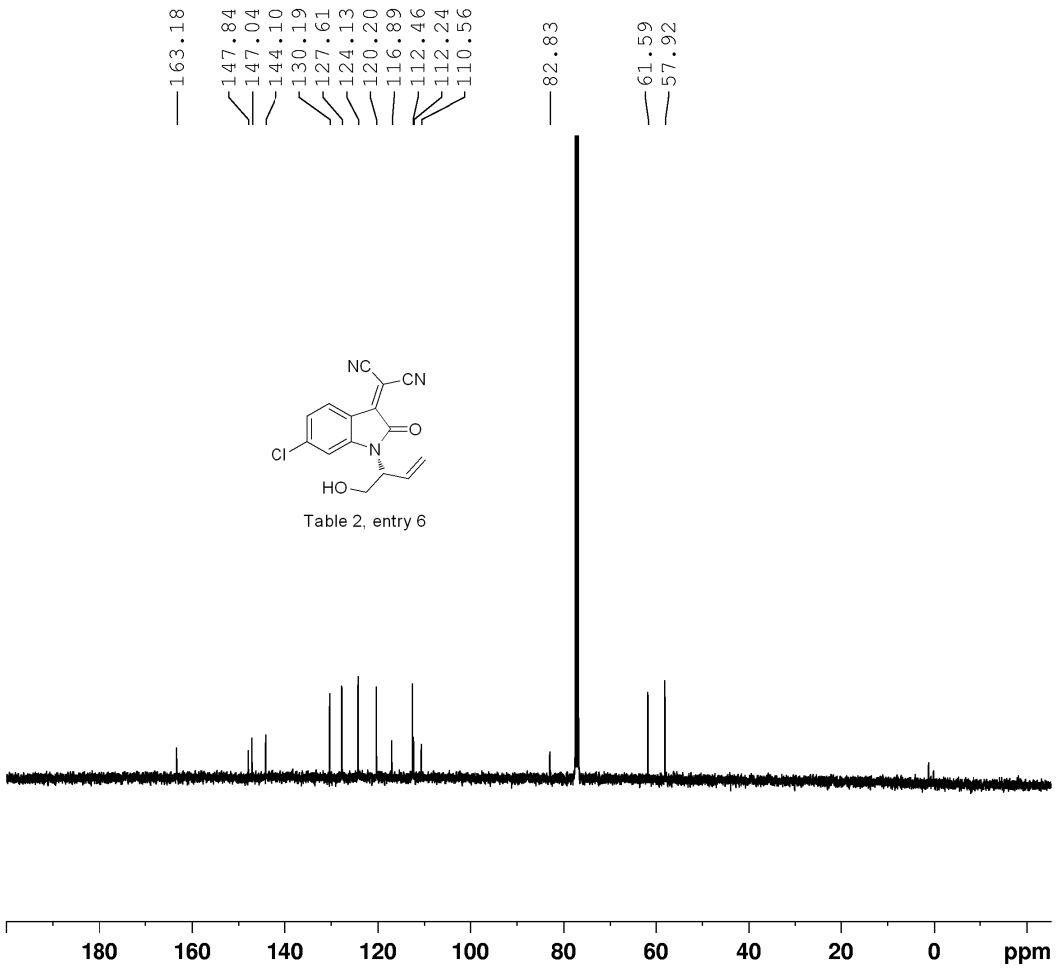


Table 2, entry 6

NAME	LG
EXPNO	187
PROCNO	1
Date_	20121123
Time	13.19
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	3729
DS	0
SWH	25252.525 Hz
FIDRES	0.770646 Hz
AQ	0.6488564 sec
RG	203
DW	19.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127494 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

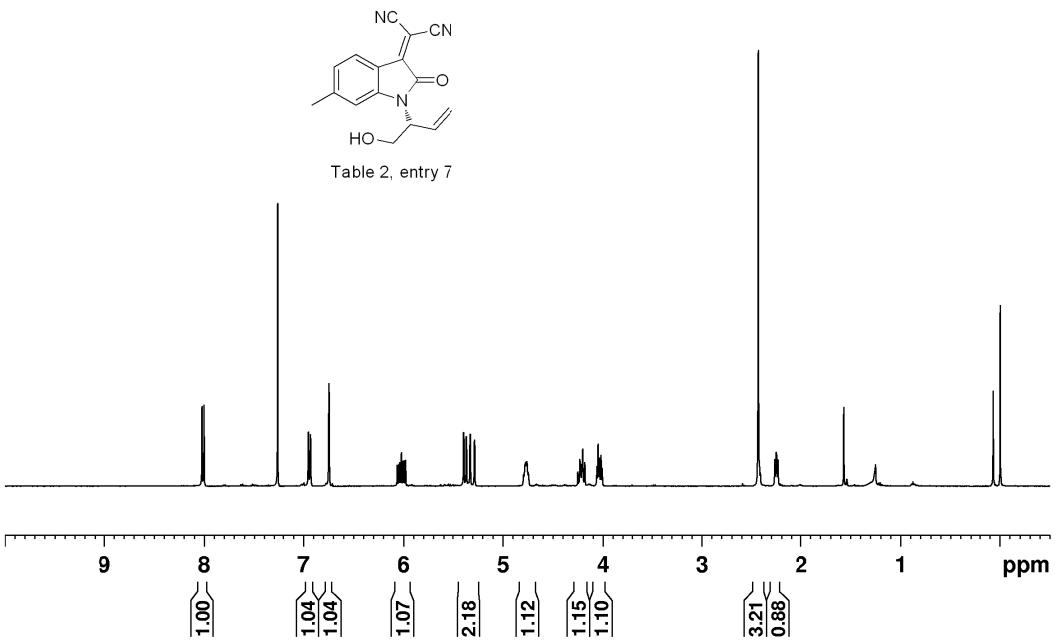


Table 2, entry 7

NAME	LG-xin
EXPNO	26
PROCNO	1
Date_	20140313
Time	4.20
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

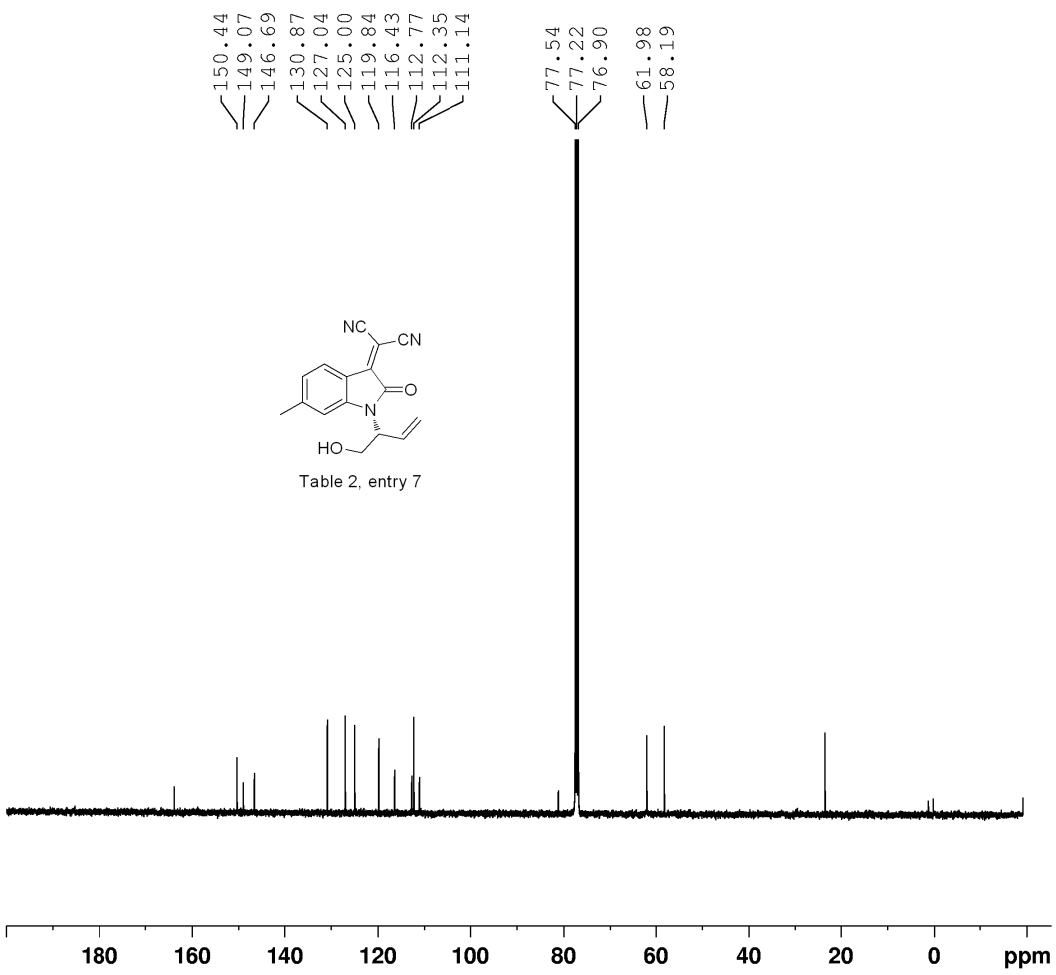


Table 2, entry 7

NAME	LG-xin
EXPNO	27
PROCNO	1
Date_	20140313
Time	14.50
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	5791
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

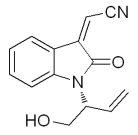
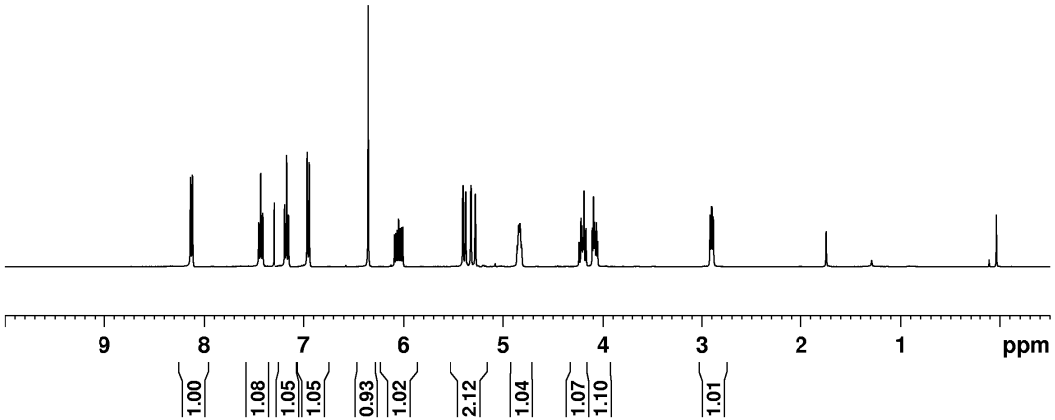


Table 2, entry 8



NAME	LG
EXPNO	207
PROCNO	1
Date_	20121202
Time	6.05
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	181
DW	41.600 usec
DE	6.50 usec
TE	293.3 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

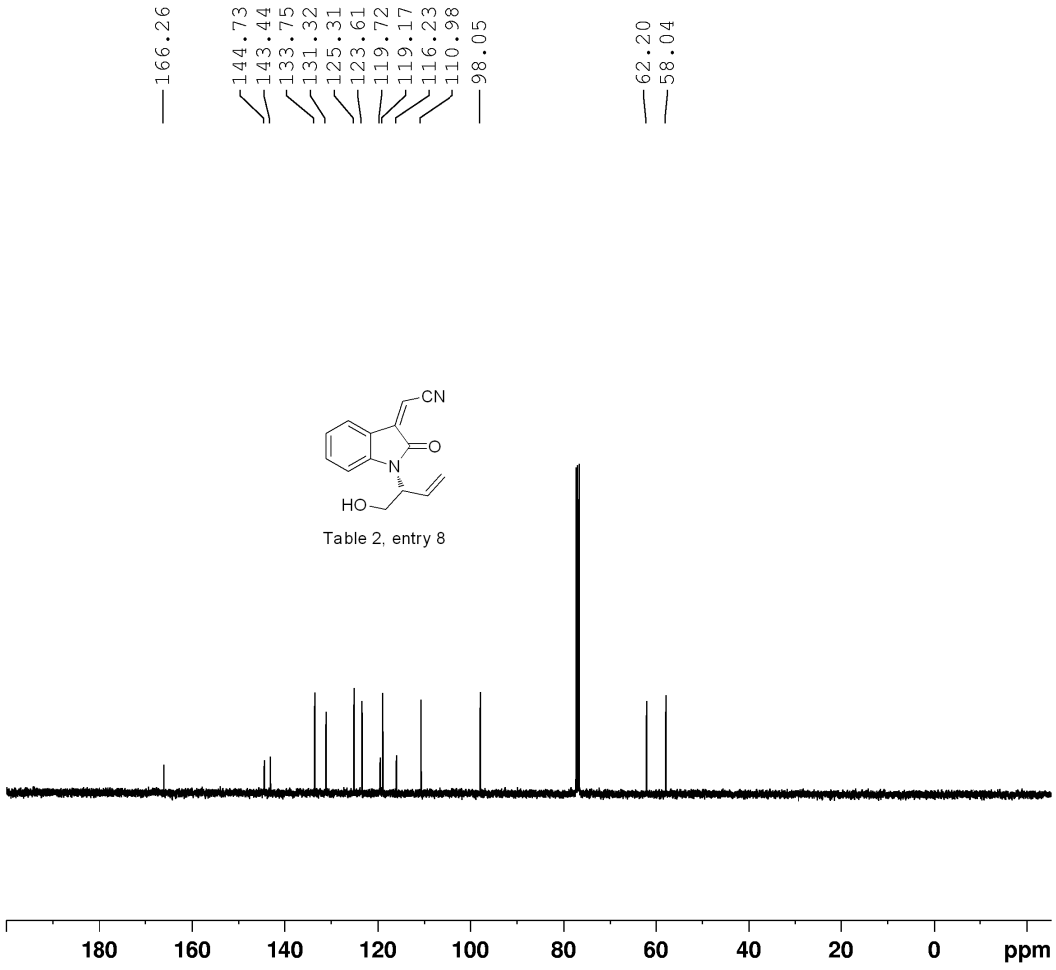


Table 2, entry 8

NAME	LG	
EXPNO	208	
PROCNO	1	
Date_	20121202	
Time	6.08	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	118	
DS	0	
SWH	25252.525	Hz
FIDRES	0.770646	Hz
AQ	0.6488564	sec
RG	203	
DW	19.800	usec
DE	6.50	usec
TE	294.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.40	usec
SI	32768	
SF	100.6127690	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

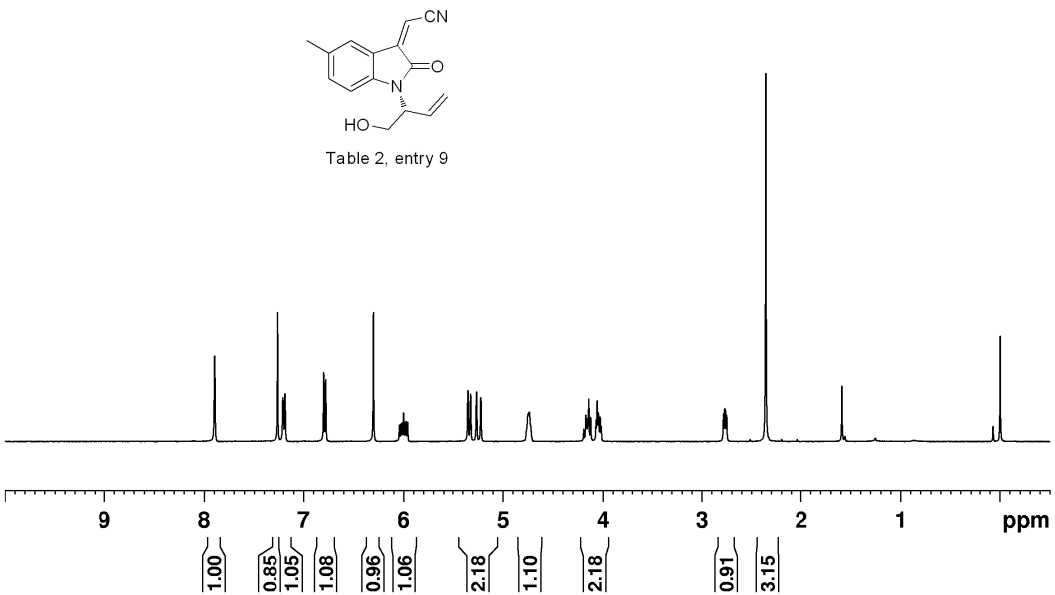


Table 2, entry 9

NAME	LG-xin
EXPNO	33
PROCNO	1
Date_	20140318
Time	2.43
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	7
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300088 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

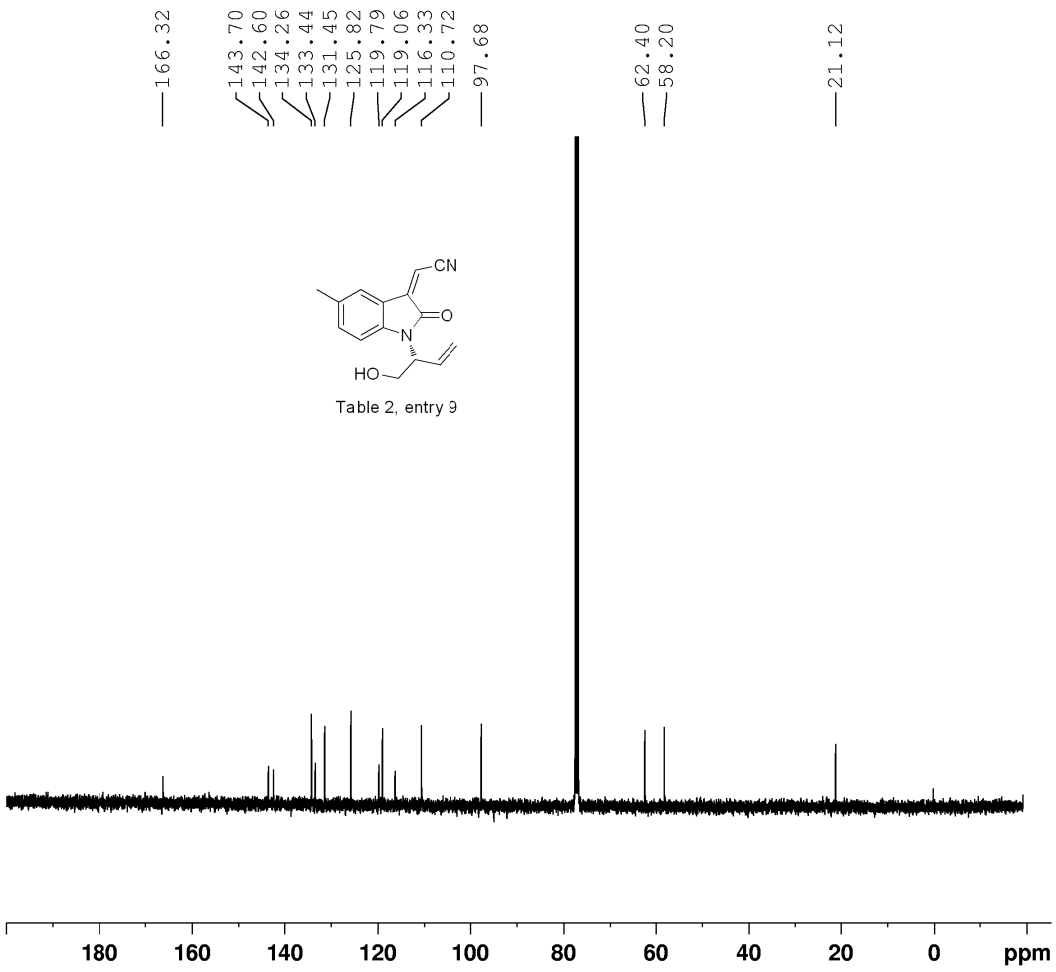


Table 2, entry 9

NAME	LG-xin
EXPNO	34
PROCNO	1
Date_	20140318
Time	2.44
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	513
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228293 MHz
NUC1	13C
P1	9.40 usec
SI	32768
SF	100.6127485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

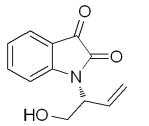
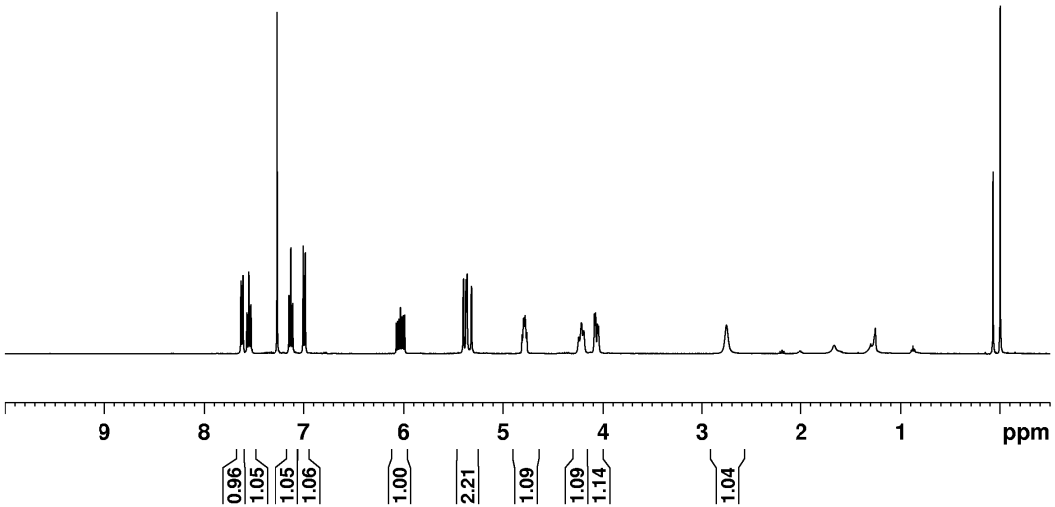


Table 2, entry 10



NAME	LG-xin
EXPNO	48
PROCNO	1
Date_	20140410
Time	3.17
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300069 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

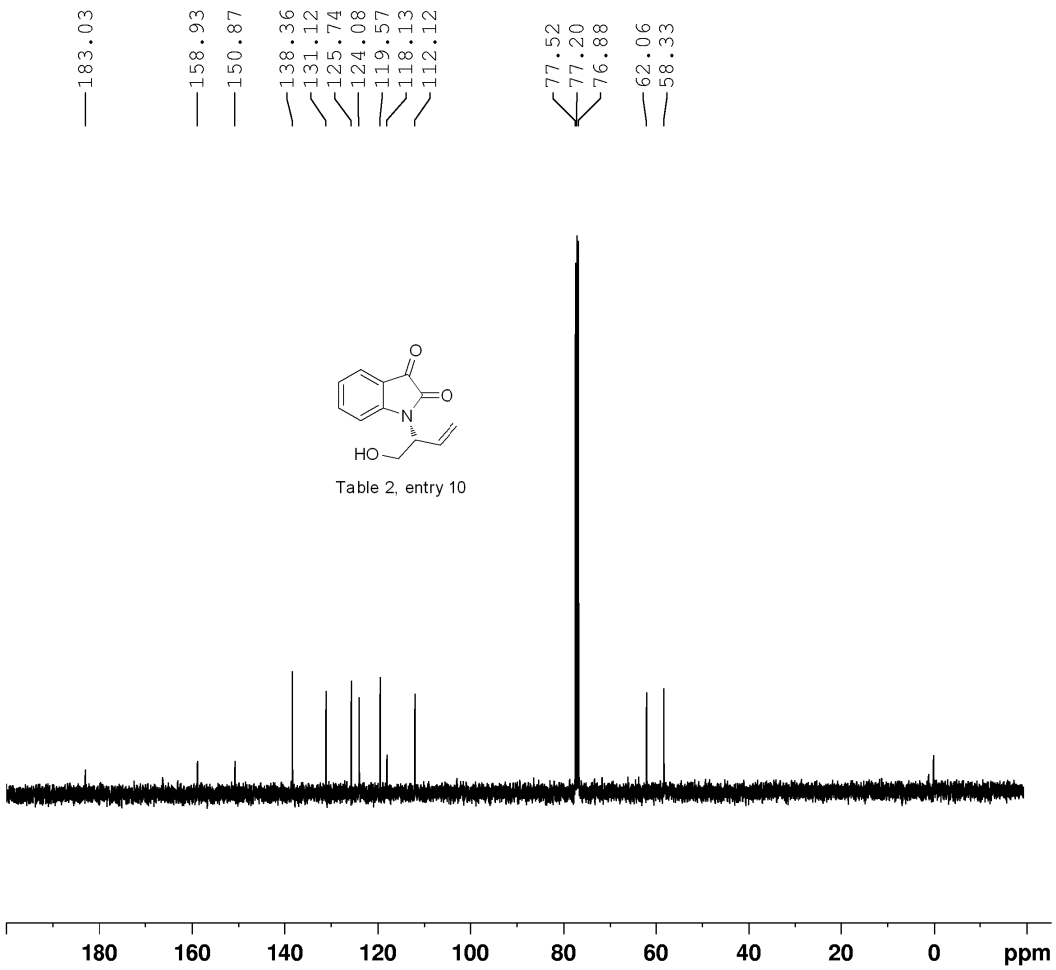


Table 2, entry 10

NAME	LG-xin	
EXPNO	47	
PROCNO	1	
Date_	20140410	
Time	3.19	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	108	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	300.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
SFO1	100.6228293	MHz
NUC1	13C	
P1	9.40	usec
SI	32768	
SF	100.6127519	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

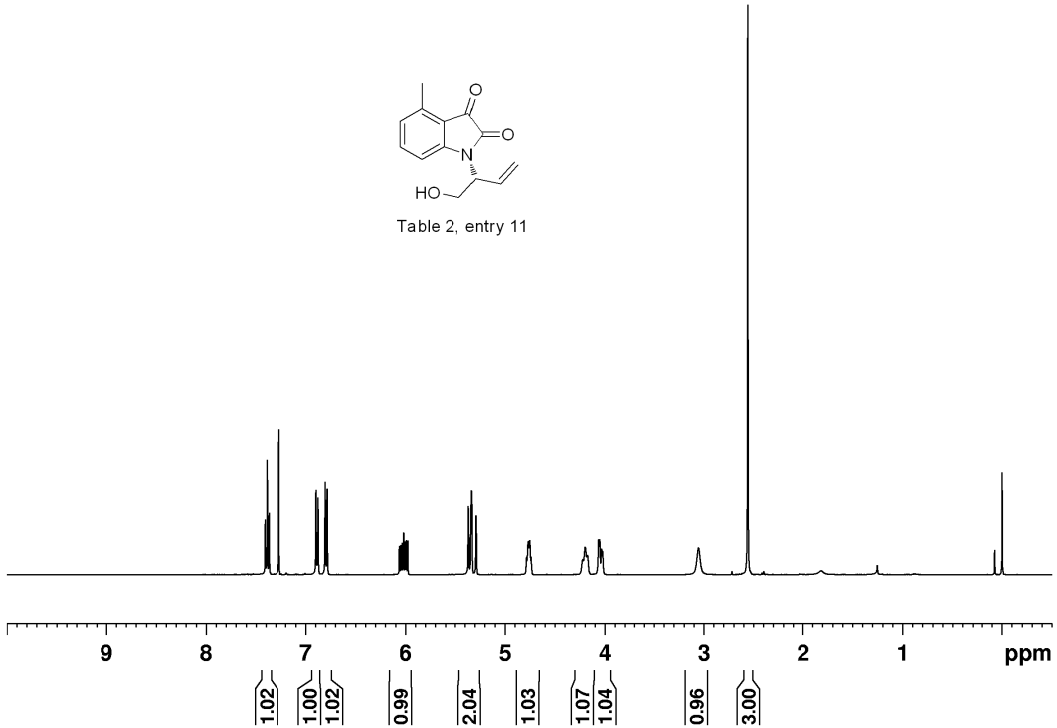


Table 2, entry 11

```
NAME              LG-xin
EXPNO                 54
PROCNO                 1
Date_           20140416
Time                7.48
INSTRUM            spect
PROBHD    5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     6
DS                     0
SWH           12019.230 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   101
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1320007 MHz
NUC1                   1H
P1                 12.60 usec
SI                 65536
SF          400.1300043 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```

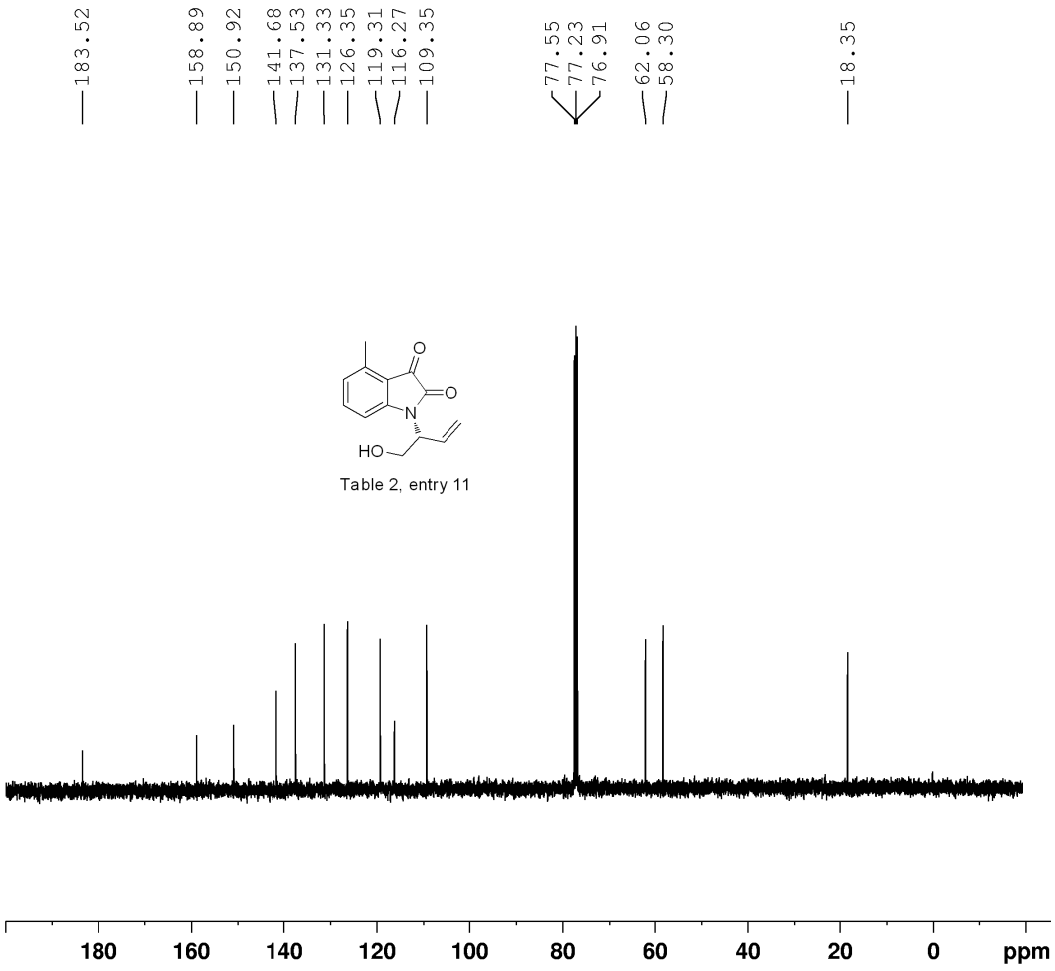


Table 2, entry 11

NAME	LG-xin	
EXPNO	55	
PROCNO	1	
Date_	20140416	
Time	7.50	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	77	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	300.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
SFO1	100.6228293	MHz
NUC1	13C	
P1	9.40	usec
SI	32768	
SF	100.6127516	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

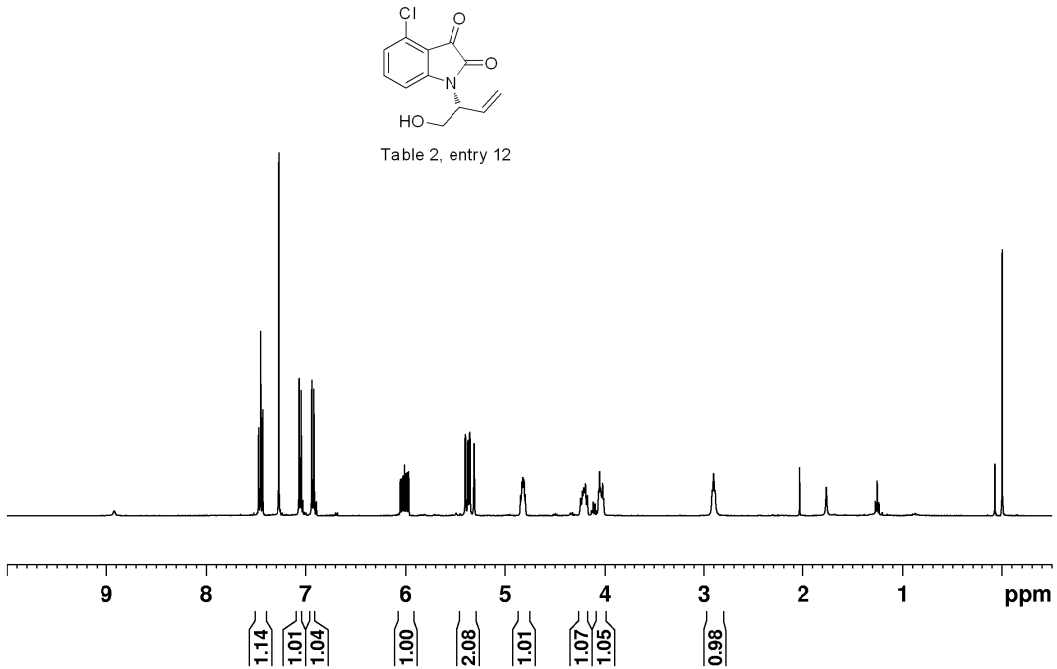


Table 2, entry 12

```
NAME              LG-xin
EXPNO                 56
PROCNO                 1
Date_           20140416
Time                7.55
INSTRUM            spect
PROBHD    5 mm PADUL 13C
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     5
DS                     0
SWH           12019.230 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   203
DW                41.600 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1320007 MHz
NUC1                   1H
P1                 12.60 usec
SI                 65536
SF          400.1300058 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.00
```

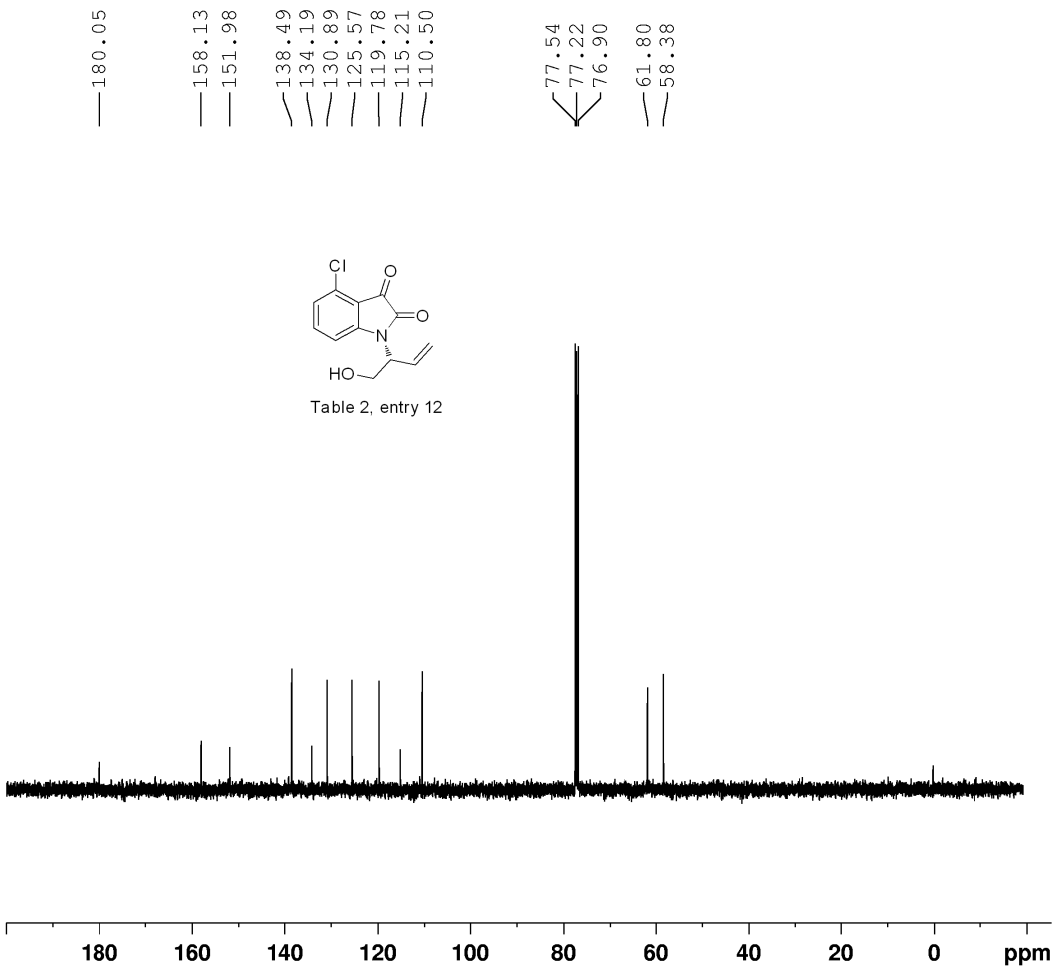


Table 2, entry 12

```
NAME                LG-xin
EXPNO                   57
PROCNO                   1
Date_             20140416
Time                  7.58
INSTRUM              spect
PROBHD    5 mm PADUL 13C
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     100
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     203
DW                  20.800 usec
DE                   6.50 usec
TE                  300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                  13C
P1                   9.40 usec
SI                  32768
SF            100.6127513 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

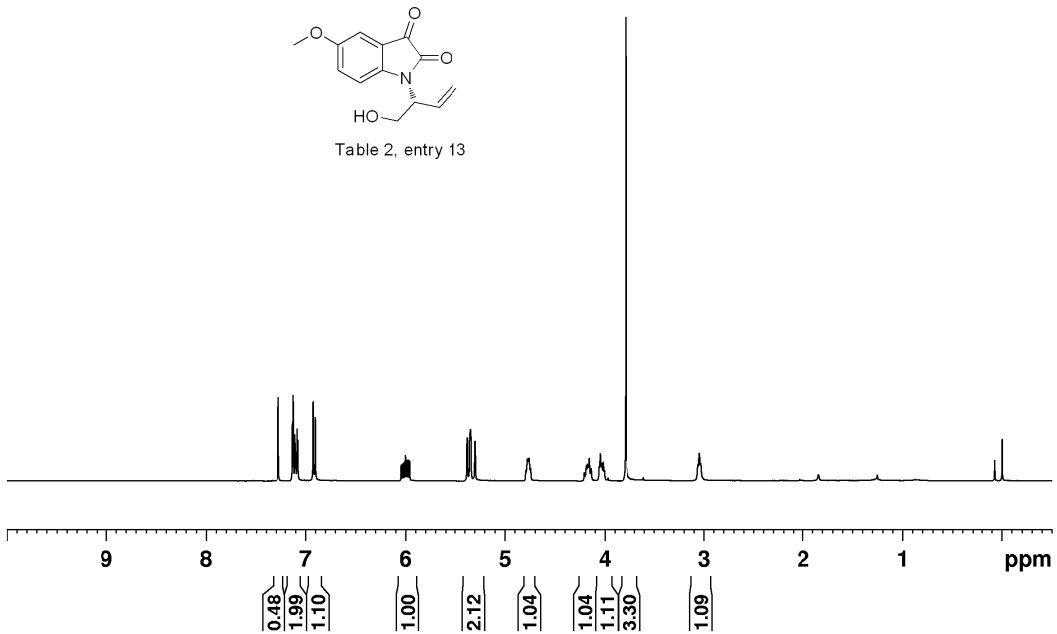


Table 2, entry 13

NAME	LG-xin
EXPNO	45
PROCNO	1
Date_	20140410
Time	3.10
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	128
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300027 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

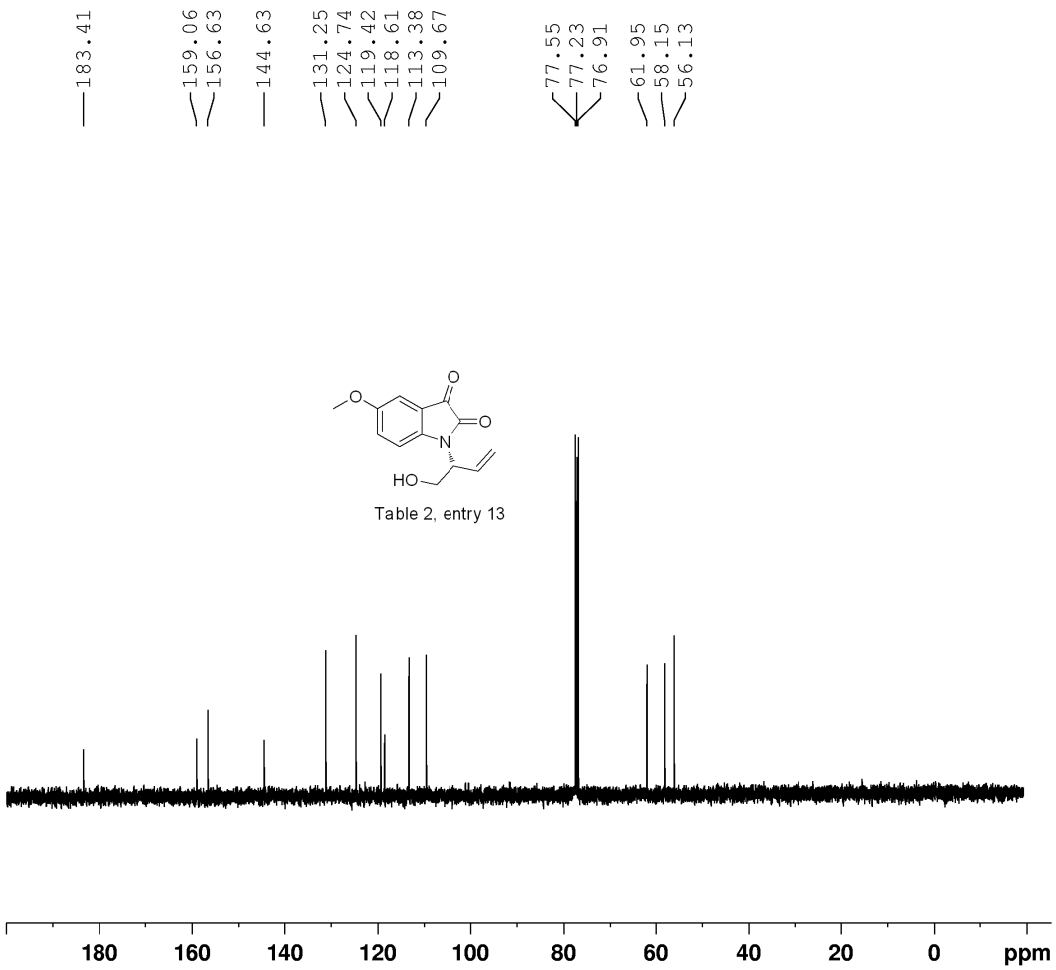


Table 2, entry 13

```
NAME                LG-xin
EXPNO                   46
PROCNO                   1
Date_             20140410
Time                  3.12
INSTRUM              spect
PROBHD    5 mm PADUL 13C
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                      39
DS                       4
SWH             24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                     203
DW                20.800 usec
DE                 6.50 usec
TE                 300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                  13C
P1                  9.40 usec
SI                 32768
SF            100.6127519 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

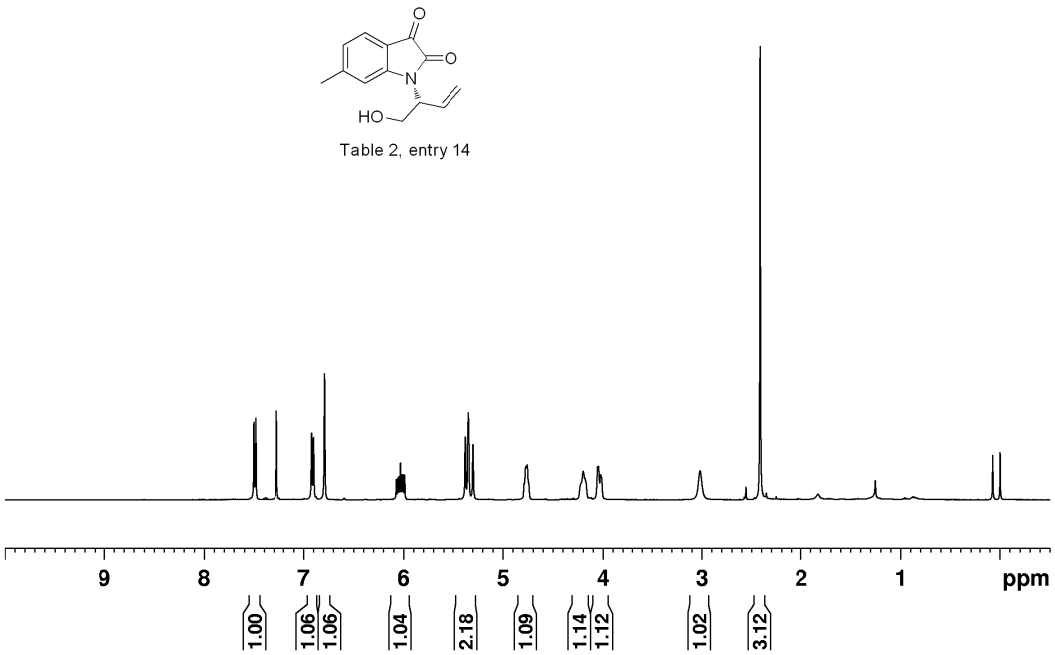


Table 2, entry 14

NAME	LG-xin
EXPNO	41
PROCNO	1
Date_	20140409
Time	6.13
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	9
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	128
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300035 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

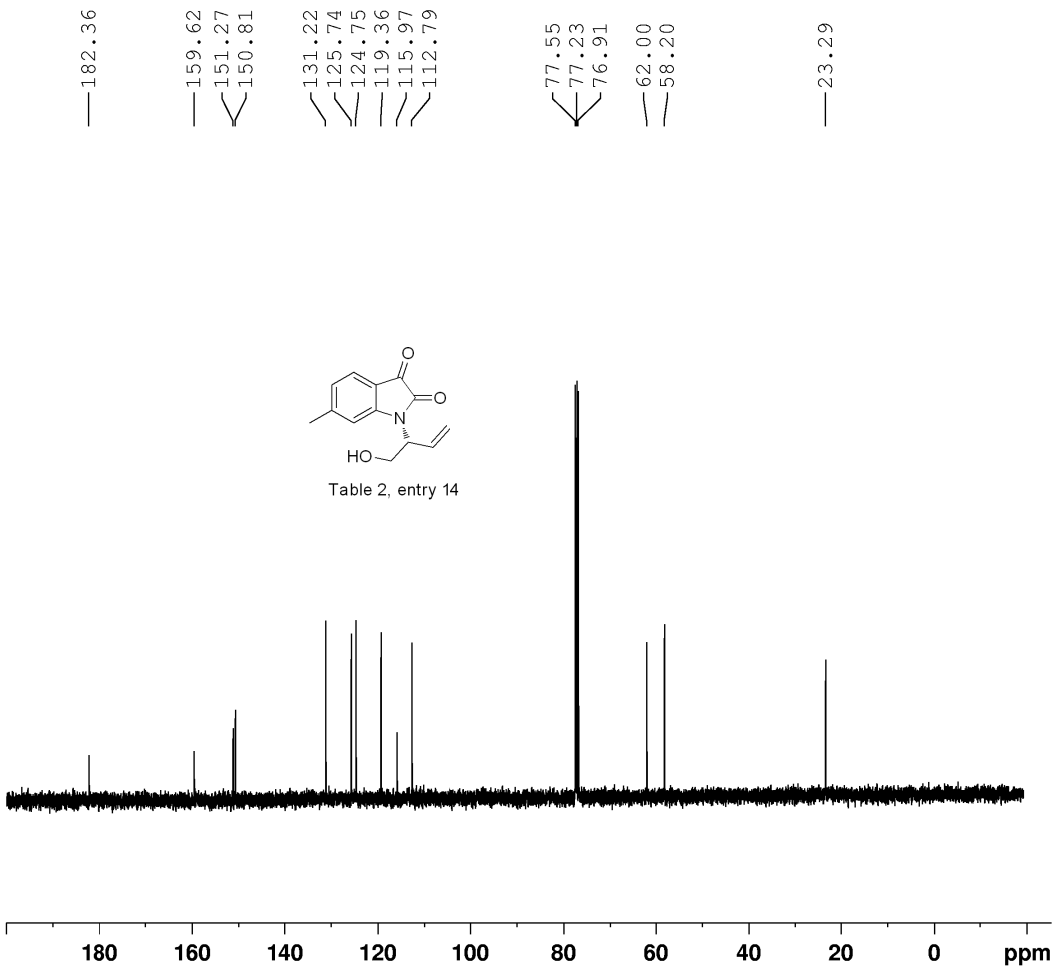


Table 2, entry 14

NAME	LG-xin	
EXPNO	42	
PROCNO	1	
Date_	20140409	
Time	6.16	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	85	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	300.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
SFO1	100.6228293	MHz
NUC1	13C	
P1	9.40	usec
SI	32768	
SF	100.6127516	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

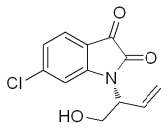
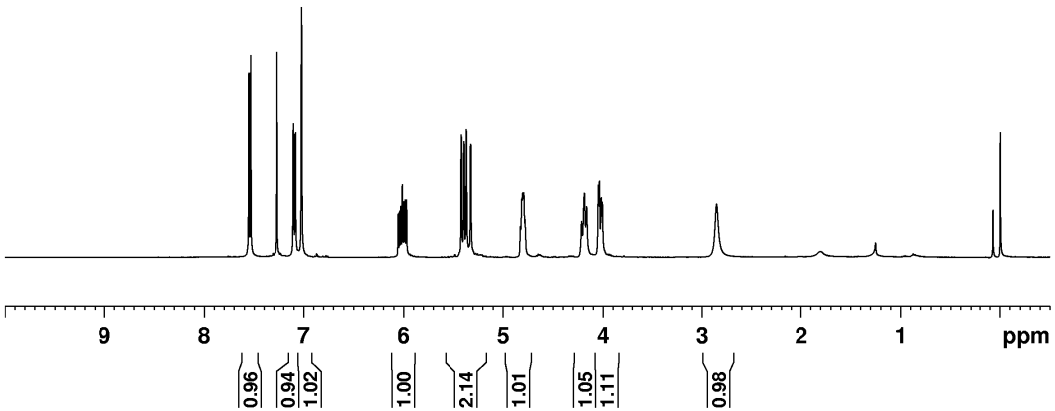


Table 2, entry 15



NAME	LG-xin
EXPNO	49
PROCNO	1
Date_	20140412
Time	4.45
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	9
DS	0
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	41.600 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1320007 MHz
NUC1	1H
P1	12.60 usec
SI	65536
SF	400.1300052 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

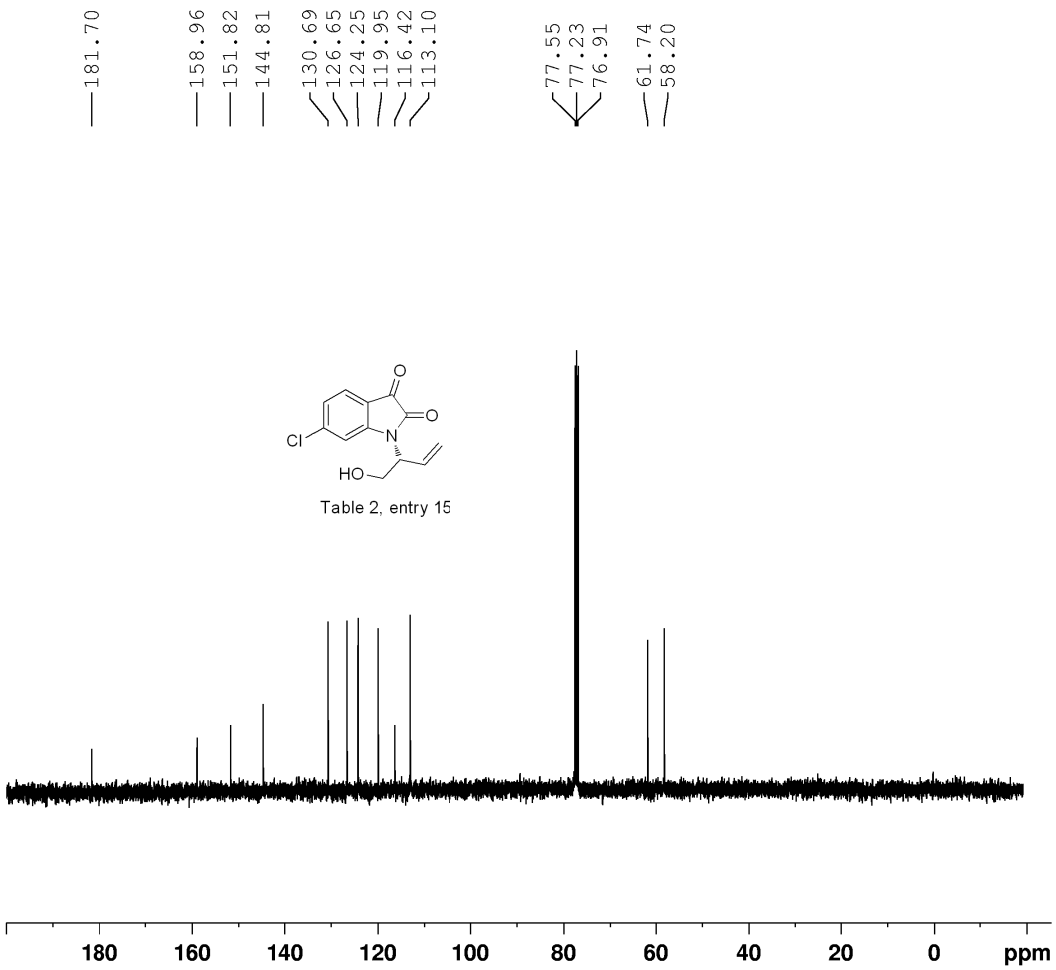


Table 2, entry 15

NAME	LG-xin	
EXPNO	50	
PROCNO	1	
Date_	20140412	
Time	4.46	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	71	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	203	
DW	20.800	usec
DE	6.50	usec
TE	300.0	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
SFO1	100.6228293	MHz
NUC1	13C	
P1	9.40	usec
SI	32768	
SF	100.6127513	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	