Electronic Supplementary Material (ESI) for Green Chemistry

Supporting Information

An Eco-benign and Highly Efficient Access to 3-Heterocyclic-Substituted Isoindolinones in Ammonia Water

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Table of Contents

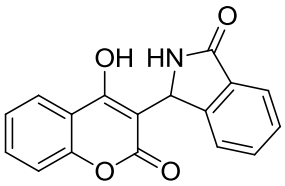
1. General experimental methods:

Unless stated otherwise, reactions were performed in sealed tubes. All of the commercial reagents and solvents were used as received. Flash column chromatography was performed using silica gel (300-400 mesh). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230-400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Organic solutions were concentrated on rotary evaporators at ~20 Torr (house vacuum) at 40-45^{o}C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale.

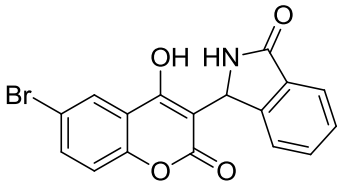
2. Typical experimental procedure for the synthesis of 3-subsititued isoindolinones.

A mixture of 4-hydroxycoumarins **1** (or indoles **4**) (0.3 mmol, 1.0equiv) and 2-formylbenzoid acids **2** (0.45 mmol, 1.5 equiv) in $NH_3{\cdot}H_2O$ (2.0 mL) was stirred in a sealed tube at 80 ^{o}C for 24h. After that the reaction mixture was added by toluene and then removed the solvent on the rotary evaporator. The residue was purified by flash column chromatography on silica gel to give the corresponding products **3** (or **5**).

3. Spectral data of the compounds:

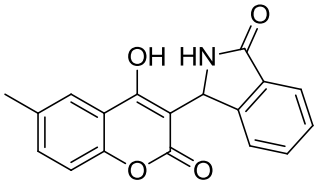


3-(4-hydroxy-2-oxo-2H-chromen-3-yl)isoindolin-1-one (3a): 83mg (light yellow solid), 94% yield. ^{1}H NMR (500MHz, DMSO-D^{6}): δ(ppm) 8.45(s, 1H), 8.00(d, *J*=7.1Hz, 1H), 7.65(d, *J*=7.4Hz, 1H), 7.59(t, *J*=7.1Hz, 7.3Hz, 1H), 7.48(t, *J*=7.1Hz, 7.3Hz, 1H), 7.43(t, *J*=7.3Hz, 7.2Hz, 1H), 7.33-7.30(m, 3H), 6.09(s,1H). ^{13}C NMR (125MHz, DMSO-D^{6}): δ(ppm) 170.5, 165.5, 161.2, 153.2, 148.1, 132.5, 131.5, 127.6, 124.3, 123.9, 122.8, 122.6, 118.0, 116.6, 100.1, 52.0. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{17}H_{11}NO_4Na^{+}$: 316.0580, Found: 316.0599.

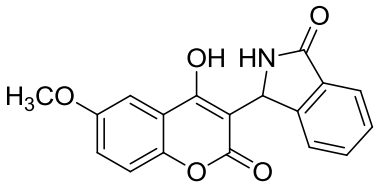


3-(6-bromo-4-hydroxy-2-oxo-2H-chromen-3-yl)isoindolin-1-one (3b): 66.6mg (light yellow solid), 60% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 8.16(s, 1H), 7.93(d, *J*=2.8Hz, 1H), 7.58(d, *J*=7.8Hz, 1H), 7.58(d, *J*=7.8Hz, 1H), 7.52(dd, *J*=8.7Hz, 2.8Hz, 1H), 7.40(t, *J*=7.2Hz, 6.8Hz, 1H), 7.35(t, *J*=7.3Hz, 7.2Hz, 1H), 7.18(d, *J*=7.4Hz, 1H), 7.06(d, *J*=8.3Hz, 1H), 6.12(s, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 171.2, 170.0, 161.7, 152.9, 150.1, 133.7, 132.4, 130.5, 127.1, 126.3, 125.0, 122.0, 118.1, 113.8, 93.0, 52.4. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{17}H_{10}BrNO_4Na^{+}$:

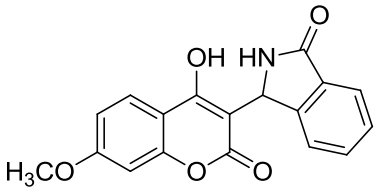
393.9685, Found: 393.9670.



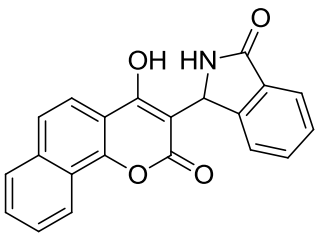
3-(4-hydroxy-6-methyl-2-oxo-2H-chromen-3-yl)isoindolin-1-one (3c): 87.6mg (yellow solid), 95% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 8.46(s, 1H), 7.81(s, 1H), 7.65(d, *J*=7.3Hz, 1H), 7.47-7.38(m, 3H), 7.30(d, *J*=7.3Hz, 1H), 7.20(d, *J*=8.3Hz, 1H), 6.12(s, 1H), 2.40(s, 3H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 170.1, 165.7, 160.9, 151.0, 147.9, 133.5, 132.8, 132.5, 131.1, 127.2, 123.7, 122.4, 122.2, 117.5, 116.0, 99.3, 51.6, 20.5. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{18}H_{13}NO_4Na^{+}$: 330.0737, Found: 330.0732.



3-(4-hydroxy-6-methoxy-2-oxo-2H-chromen-3-yl)isoindolin-1-one (3d): 71mg (yellow solid), 73% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 8.41(s,1H), 7.64(d, *J*=7.4Hz, 1H), 7.51-7.40(m, 3H), 7.30(d, *J*=7.3Hz, 1H), 7.23(d, *J*=9.2Hz, 1H), 7.16(d, *J*=8.0Hz, 3.2Hz, 1H), 6.11(s, 1H), 3.78(s, 3H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 170.1, 161.3, 155.0, 148.2, 147.3, 133.5, 131.0, 127.0, 122.3, 122.2, 119.2, 117.3, 106.5, 98.7, 55.7, 51.8. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{18}H_{13}NO_5Na^{+}$: 346.0686, Found: 346.0681.

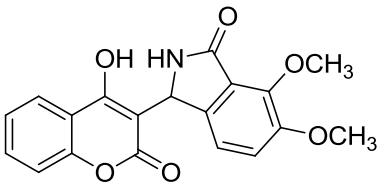


3-(4-hydroxy-7-methoxy-2-oxo-2H-chromen-3-yl)isoindolin-1-one (3e): 78.6mg (yellow solid), 81% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 8.38(s,1H), 7.90(d, *J*=9.2Hz, 1H), 7.63(d, *J*=7.3Hz, 1H), 7.47-7.39(m, 2H), 7.29(d, *J*=7.8Hz, 1H), 6.88-6.83(m, 2H), 6.10(s, 1H), 3.82(s, 3H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 170.1, 167.4, 162.2, 161.5, 154.8, 148.5, 133.5, 131.0, 127.0, 125.4,, 122.3, 122.2, 112.1, 111.0, 100.1, 95.9, 55.8, 51.8. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{18}H_{13}NO_5Na^{+}$: 346.0686, Found: 346.0663.

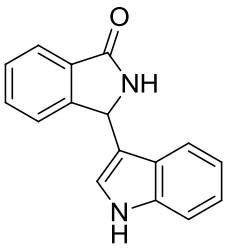


3-(4-hydroxy-2-oxo-2H-benzo[h]chromen-3-yl)isoindolin-1-one (3f): 80.5mg (yellow solid), 78%

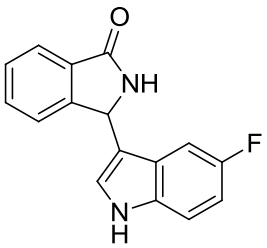
yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 8.46(s, 1H), 9.32(d, *J*=7.6Hz, 1H), 8.03-7.99(m, 2H), 7.79(d, *J*=8.7Hz, 1H), 7.68-7.65(m, 3H), 7.49-7.42(m, 2H), 7.35(d, *J*=7.8Hz, 1H), 6.17(s, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 170.1, 167.4, 160.9, 149.7, 148.1, 134.4, 133.6, 131.0, 128.3, 127.9, 127.1, 127.0, 122.7, 122.4, 122.3(3), 122.2(7), 121.7, 120.4, 113.8, 98.2, 51.8. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{21}H_{13}NO_4Na^{+}$: 366.0737, Found: 366.0716.



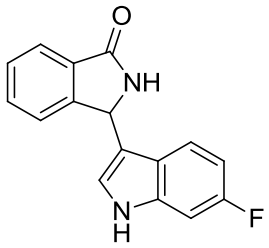
3-(4-hydroxy-2-oxo-2H-chromen-3-yl)-6,7-dimethoxyisoindolin-1-one (3g): 66mg (brown solid), 62% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 7.93(s, 1H), 7.87(d, *J*=7.3Hz, 1H), 7.35(t, *J*=8.1Hz, 6.8Hz, 1H), 7.11-7.03(m, 3H), 6.81(d, *J*=8.2Hz, 1H), 6.04(s, 1H), 3.89(s, 3H), 3.77(s, 3H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 172.6, 168.5, 162.1, 153.9, 150.6, 145.8, 144.2, 129.9, 125.7, 124.9, 123.0, 121.6, 116.9, 116.2, 115.4, 93.4, 61.6, 56.4, 51.3. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{19}H_{15}NO_6Na^{+}$: 376.0792, Found: 346.0786.



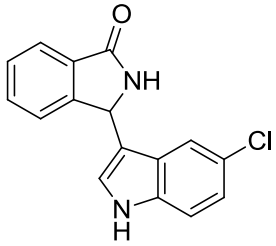
3-(1H-indol-3-yl)isoindolin-1-one (5a): 63.6mg (light yellow solid), 85% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 11.06(s, 1H), 8.96(s, 1H), 7.77(d, *J*=6.4Hz, 1H), 7.52-7.46(m, 3H), 7.37-7.29(m, 2H), 7.05(t, *J*=6.8Hz, 7.8Hz, 1H), 6.89-6.82(m, 2H), 5.97(s, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 148.4, 136.8, 132.2, 131.7, 128.0, 125.0, 124.4, 123.5, 122.7, 121.3, 118.7, 118.5, 111.8, 53.8. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{16}H_{12}N_2ONa^{+}$: 271.0842, Found: 271.0812.



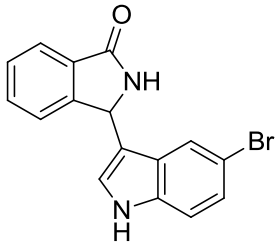
3-(5-fluoro-1H-indol-3-yl)isoindolin-1-one (5b): 71mg (yellow solid), 89% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 11.22(s, 1H), 8.98(s, 1H), 7.78(d, *J*=6.9Hz, 1H), 7.58-7.49(m, 3H), 7.39-7.31(m, 2H), 6.92(t, *J*=9.6Hz, 8.7Hz, 1H), 6.60(d, *J*=10.1Hz, 1H), 5.97(s, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 156.5(d, *J*=230.5Hz), 148.0, 133.4, 132.1, 128.1, 126.4, 125.2(d, *J*=10.0Hz), 123.5, 122.8, 112.9(d, *J*=10.0Hz), 112.1(d, *J*=4.9Hz), 109.5(d, *J*=26.6Hz), 103.0(d, *J*=23.4Hz), 53.5. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{16}H_{11}FN_2ONa^{+}$: 289.0748, Found: 289.0750.



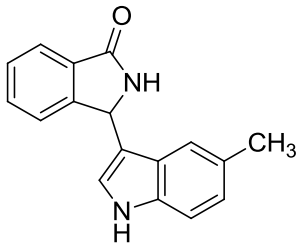
3-(6-fluoro-1H-indol-3-yl)isoindolin-1-one (5c): 65mg (yellow solid), 81% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 11.17(s, 1H), 8.97(s, 1H), 7.77(d, *J*=6.9Hz, 1H), 7.53-7.47(m, 3H), 7.31(d, *J*=6.8Hz, 1H), 7.16(dd, *J*=10.1Hz, 2.32Hz, 1H), 6.86-6.83(m, 1H), 6.74-6.72(m, 1H), 5.96(s, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 158.8(d, *J*=233.4Hz), 148.2, 136.7(d, *J*=12.6Hz), 132.1, 131.7, 128.0, 125.1(d, *J*=3.8Hz), 123.5, 122.7, 121.9, 119.4(d, *J*=10.5Hz), 112.1, 107.3(d, *J*=24.5Hz), 97.8(d, *J*=25.4Hz), 53.6. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{16}H_{11}FN_2ONa^{+}$: 289.0748, Found: 289.0745.



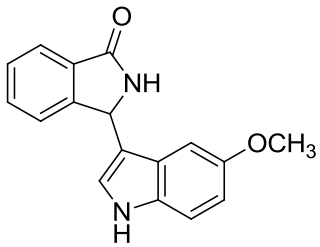
3-(5-chloro-1H-indol-3-yl)isoindolin-1-one (5d): 77.2mg (yellow solid), 91% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 11.32(s, 1H), 8.99(s, 1H), 7.78(d, *J*=6.4Hz, 1H), 7.54-7.51(m, 3H), 7.40(d, *J*=8.7Hz, 1H), 7.32(d, *J*=6.4Hz, 1H), 7.06(dd, *J*=8.7Hz, 1.8Hz, 1H), 6.89(d, *J*=1.4Hz, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 148.0, 135.2, 132.0, 131.8, 128.1, 126.3, 126.2, 123.5, 123.3, 122.8, 121.3, 117.6, 113.4, 111.8, 53.4. HRMS (EI, 70eV): *m/z* [M+Na]$^{+}$ calcd for $C_{16}H_{11}ClN_2ONa^{+}$: 305.0452, Found: 305.0454.



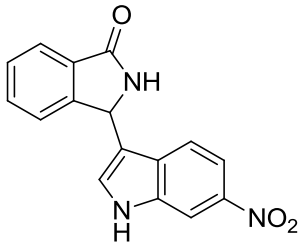
3-(5-bromo-1H-indol-3-yl)isoindolin-1-one (5e): 77mg (yellow solid), 78% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 11.32(s, 1H), 8.98(s, 1H), 7.83(s, 1H), 7.78(d, *J*=6.9Hz, 1H), 7.55(t, *J*=6.0Hz, 7.3Hz, 2H), 7.35-7.30(m, 2H), 7.17(dd, *J*=8.7Hz, 1.8Hz, 1H), 7.05(s, 1H), 5.97(s, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 148.0, 135.5, 132.0, 131.8, 128.1, 126.9, 126.1, 123.8, 123.5, 122.8, 120.7, 113.9, 111.7, 111.3, 53.4. HRMS (EI, 70eV): *m/z* [M+H]$^{+}$ calcd for $C_{16}H_{12}BrN_2O^{+}$: 327.0128, Found: 327.0113.



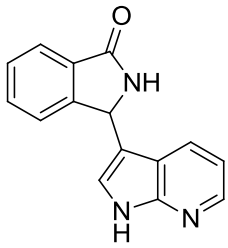
3-(5-methyl-1H-indol-3-yl)isoindolin-1-one (5f): 63.1mg (yellow solid), 80% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 10.95(s, 1H), 8.92(s, 1H), 7.76(d, *J*=7.4Hz, 1H), 7.52-7.49(m, 2H), 7.37(d, *J*=2.3Hz, 1H), 7.31(d, *J*=7.3Hz, 1H), 7.25(d, *J*=8.2Hz, 1H), 6.87(d, *J*=8.2Hz, 1H), 6.72(s, 1H), 2.20(s, 3H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 148.4, 135.2, 132.1, 131.6, 127.9, 127.0, 125.4, 124.3, 123.4, 122.9, 122.7, 118.1, 111.5, 111.2, 53.8, 21.3. HRMS (EI, 70eV): *m/z* $[M+Na]^{+}$ calcd for $C_{17}H_{14}N_2ONa^{+}$: 285.0998, Found: 285.0990.



3-(5-methoxy-1H-indol-3-yl)isoindolin-1-one (5g): 79.6mg (yellow solid), 95% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 10.92(s, 1H), 8.92(s, 1H), 7.77(d, *J*=6.9Hz, 1H), 7.55-7.48(m, 2H), 7.34(t, *J*=1.8Hz, 6.8Hz, 1H), 7.26(d, *J*=9.2Hz, 1H), 6.72(dd, *J*=9.2Hz, 2.3Hz, 1H), 6.42(d, *J*=2.3Hz, 1H), 5.95(s, 1H), 3.56(s, 3H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 152.9, 148.2, 132.2, 131.9, 131.6, 127.9, 125.6, 124.8, 123.6, 122.6, 112.3, 111.5, 111.0, 100.8, 55.1, 53.6. HRMS (EI, 70eV): *m/z* $[M+H]^{+}$ calcd for $C_{17}H_{15}N_2O_2^{+}$: 279.1128, Found: 279.1128.

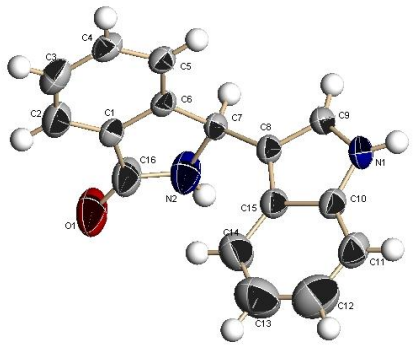


3-(6-nitro-1H-indol-3-yl)isoindolin-1-one (5h): 52mg (yellow solid), 59% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 11.82(s, 1H), 9.00(s, 1H), 8.30(d, *J*=2.3Hz, 1H), 7.86(d, *J*=2.3Hz, 1H), 7.75-7.73(m, 2H), 7.50-7.48(m, 2H), 7.29(t, *J*=1.8Hz, 6.0Hz, 1H), 7.10(d, *J*=9.2Hz, 1H), 6.03(s, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 147.8, 142.1, 135.2, 131.9(7), 131.8(6), 131.2, 129.9, 128.2, 123.4, 122.9, 118.6, 114.0, 113.5, 108.6, 53.0. HRMS (EI, 70eV): *m/z* $[M+Na]^{+}$ calcd for $C_{16}H_{11}N_3O_3Na^{+}$: 316.0693, Found: 316.0707.



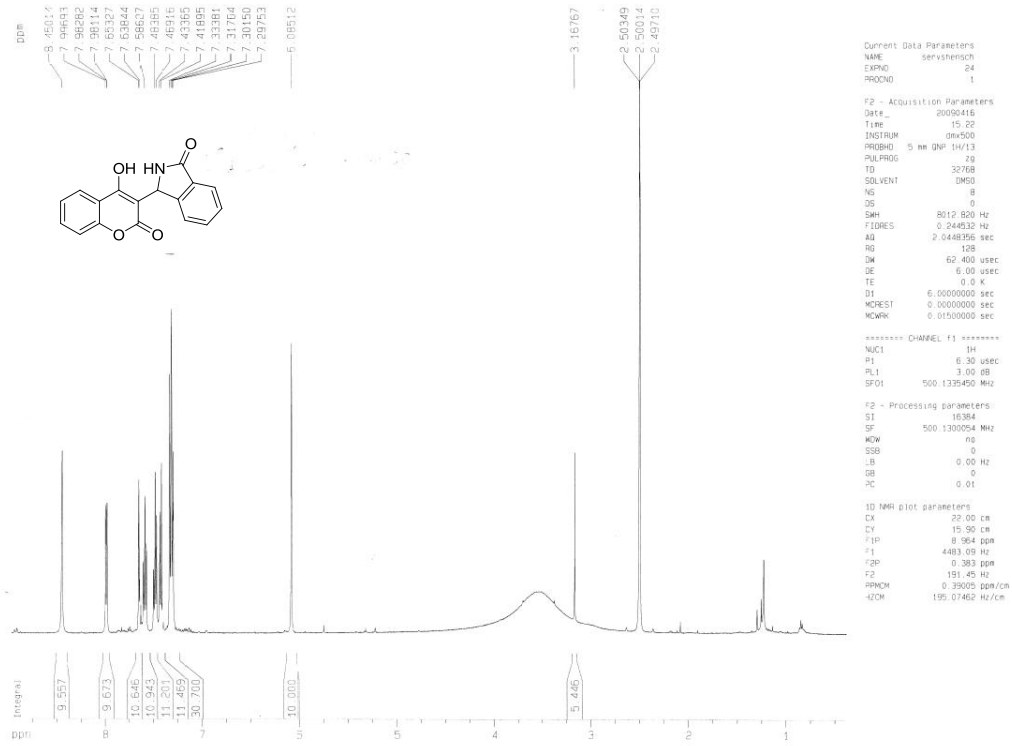
3-(1H-pyrrolo[2,3-b]pyridin-3-yl)isoindolin-1-one (5i): 62.9mg (yellow solid), 84% yield. ^{1}H NMR (400MHz, DMSO-D^{6}): δ(ppm) 11.65(s, 1H), 9.00(s, 1H), 8.16(d, *J*=4.6Hz, 1H), 7.78(d, *J*=6.9Hz, 1H), 7.61(d, *J*=2.3Hz, 1H), 7.55-7.49(m, 2H), 7.33(d, *J*=6.8Hz, 1H), 7.24(d, *J*=7.8Hz, 1H), 6.91(dd, *J*=7.8Hz, 4.6Hz, 1H), 5.96(s, 1H). ^{13}C NMR (100MHz, DMSO-D^{6}): δ(ppm) 169.3, 147.8, 142.1, 135.2, 131.9(132.0), 131.2, 129.9, 128.2, 123.4, 122.9, 118.6, 114.0, 113.5, 108.6, 53.0. HRMS (EI, 70eV): *m/z* $[M+H]^{+}$ calcd for $C_{15}H_{12}N_{3}O^{+}$: 250.0975, Found: 250.0971.

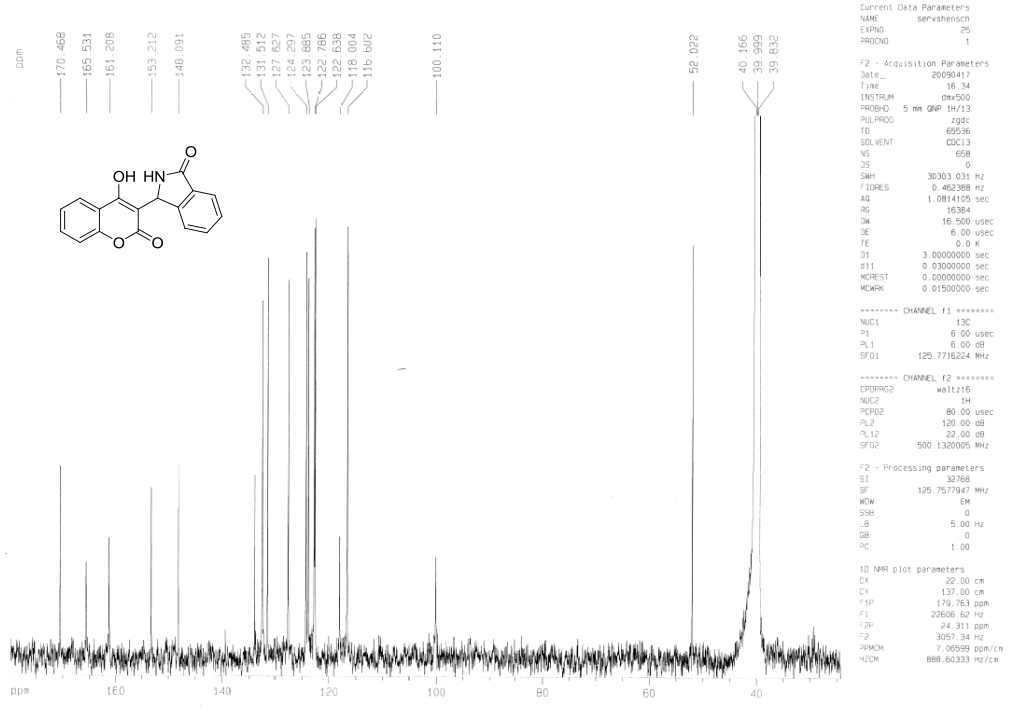
X-Ray crystallographic data for 5a ($C_{16}H_{12}N_2O$, CCDC 918177):



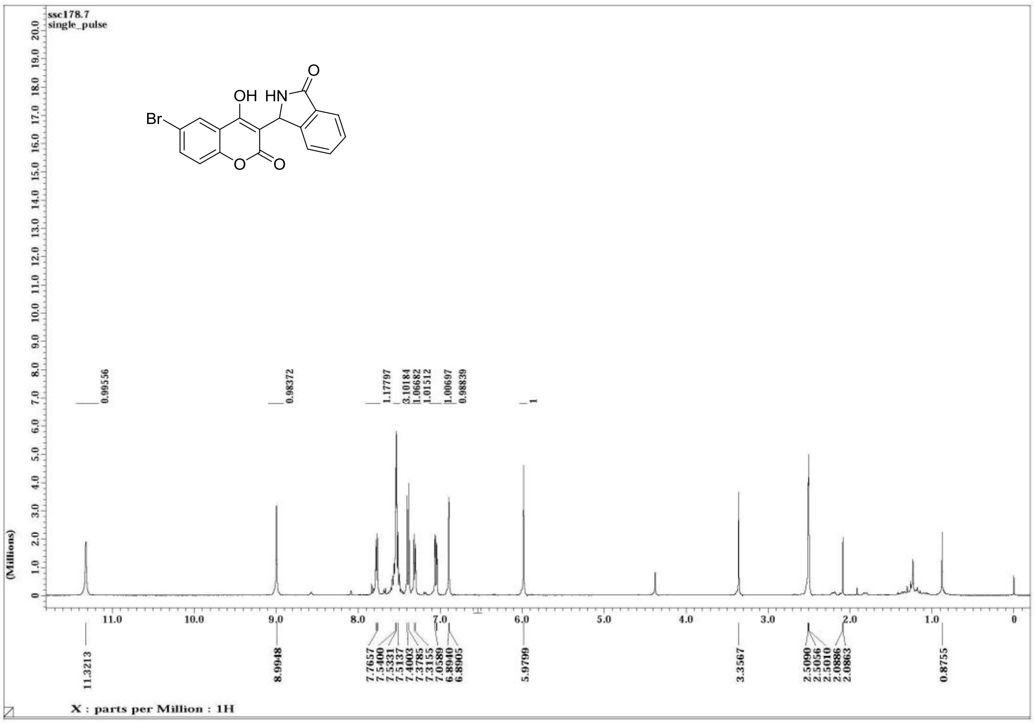
Empirical formula	$C_{16}H_{12}N_2O$
Formula weight	248.28
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 9.5564(13) Å alpha = 90 º.
	b = 16.830(2) Å beta = 98.5320(10) º.
	c = 7.9596(10) Å gamma = 90 º.
Volume	1266.0(3) Å ^3
Z, Calculated density	4, 1.303 mg/m^3
Absorption coefficient	0.083 mm^{-1}
F(000)	520
Crystal size	0.35 x 0.22 x 0.20 mm
Theta range for data collection	2.15 to 26.51 º.
Limiting indices	-11<=h<=7, -21<=k<=21, -9<=l<=9
Reflections collected / unique	7029 / 2611 [R_{int} = 0.0266]
Completeness to theta = 26.51	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9836 and 0.9715
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2611 / 0 / 173
Goodness-of-fit on F^2	1.031
Final R indices [*I*>2sigma(*I*)]	R_1 = 0.0399, wR_2 = 0.0983
R indices (all data)	R_1 = 0.0560, wR_2 = 0.1100
Extinction coefficient	0.011(2)
Largest diff. peak and hole	0.172 and -0.158 e. Å $^{-3}$

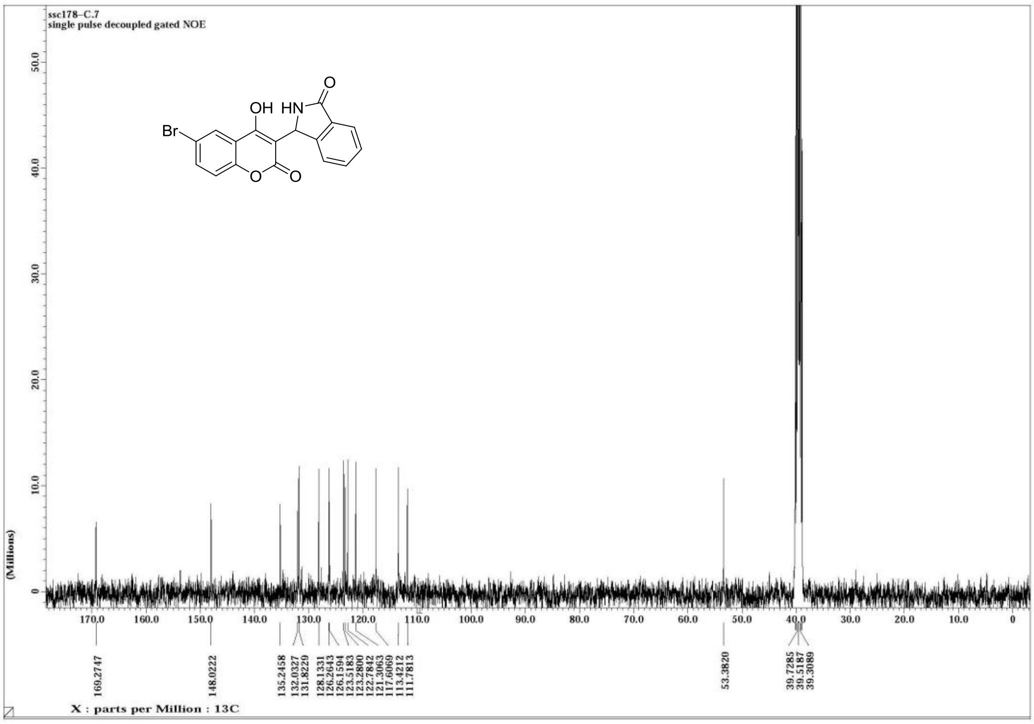
3a


OH HN
O
O
ppm
Integral
9.557
9.673
10.646
10.943
11.201
11.469
30.700
10.000
5.446

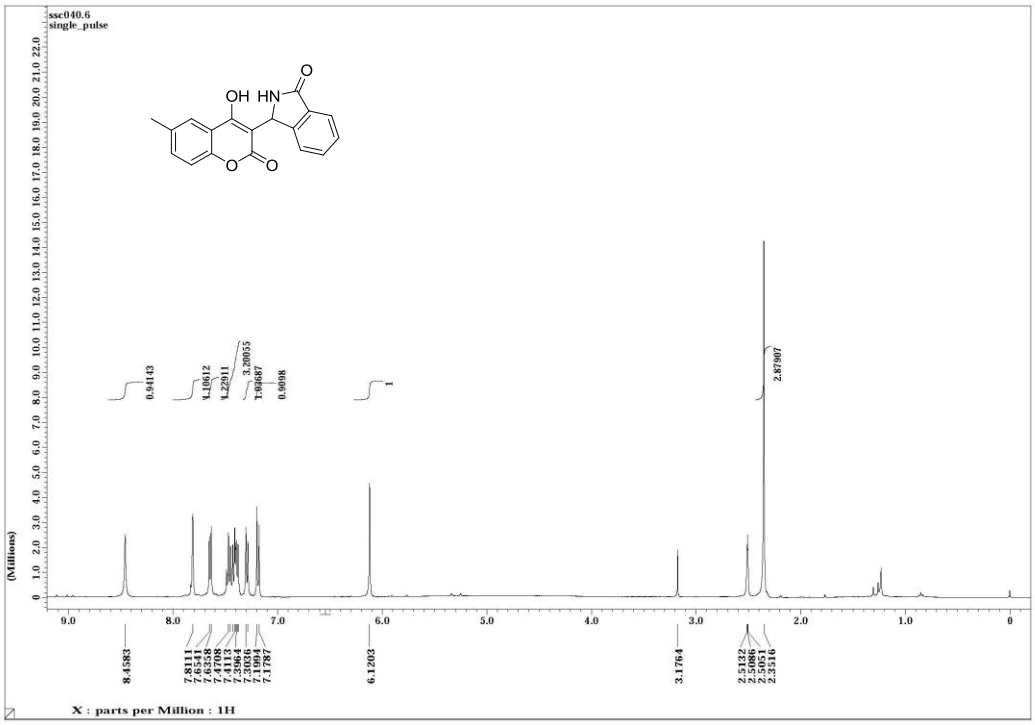

OH HN
O
O
ppm
170.468
165.531
161.208
153.212
148.091
132.485
131.512
127.627
124.297
123.885
122.786
122.638
118.004
116.602
100.110
52.022
40.166
39.999
39.832

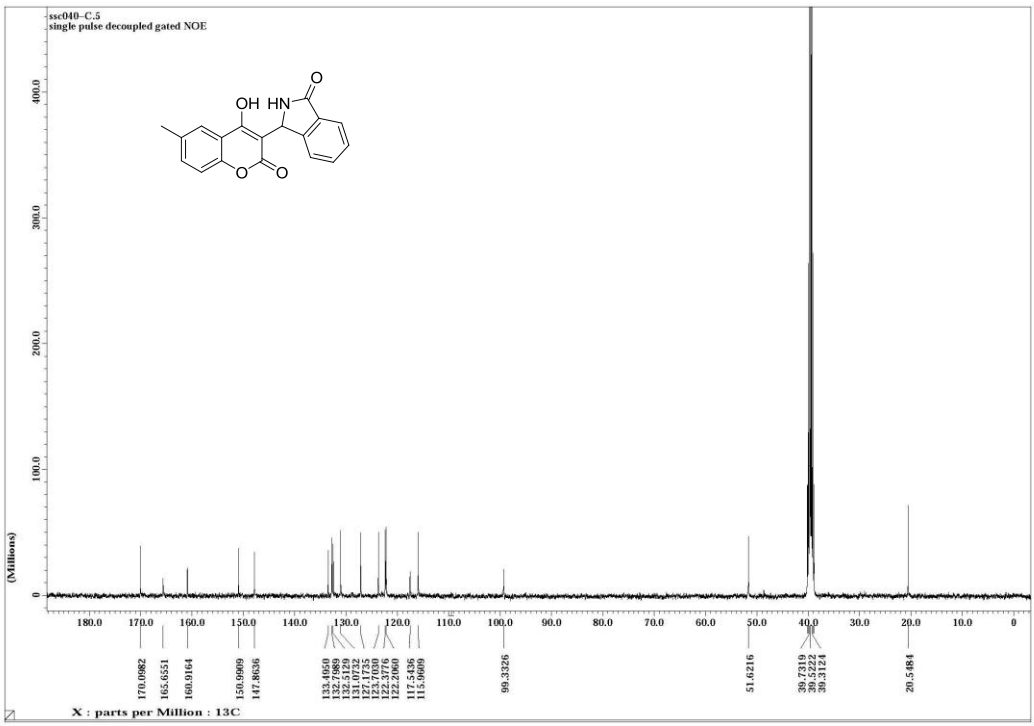
3b


ssc178.7
single_pulse
X : parts per Million : 1H
(Millions)
11.3213
8.9948
5.9799
3.3567
0.8755

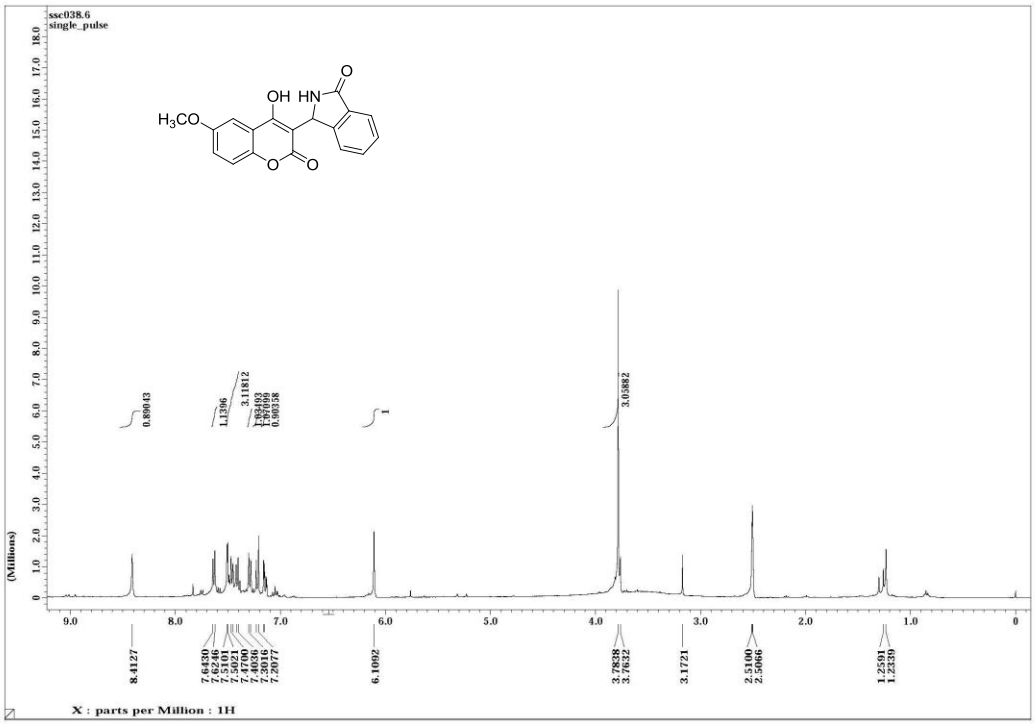

ssc178-C.7
single pulse decoupled gated NOE
X : parts per Million : 13C
(Millions)
169.2747
148.0222
53.3820

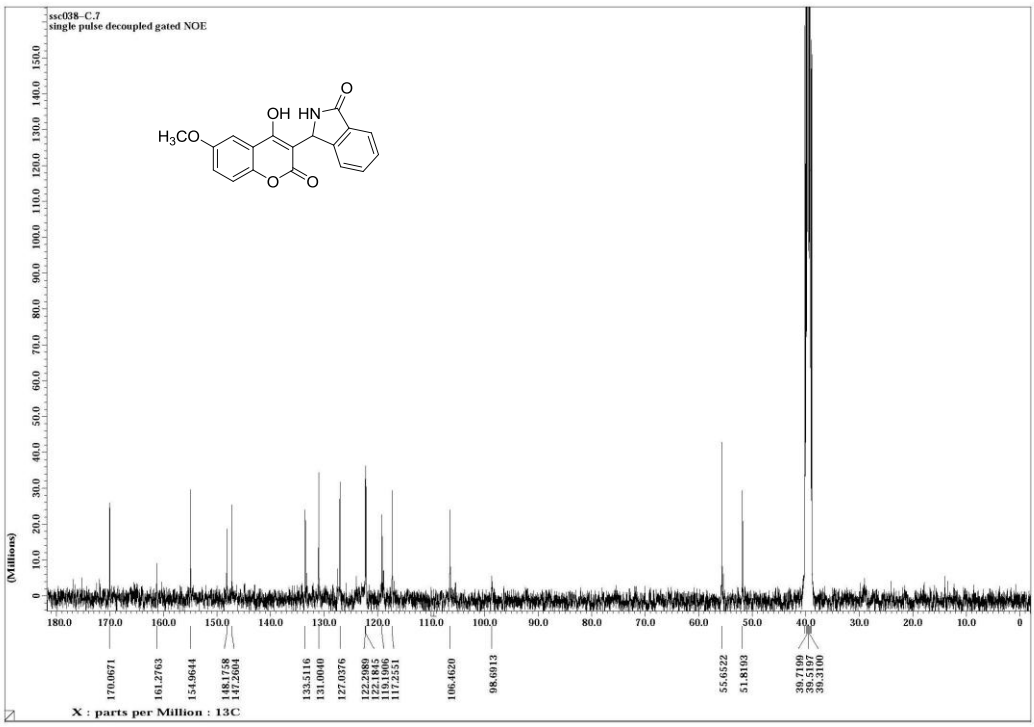
3c


ssc040.6
single_pulse
OH HN
O
O
O
(Millions)
0.94143
1.18612
1.22911
2.20055
1.93087
0.9098
1
2.87907
8.4583
7.8111
7.6541
7.6358
7.4708
7.4113
7.3964
7.3816
7.1994
7.1787
6.1203
3.1764
2.5132
2.5066
2.5051
2.3516
X : parts per Million : 1H


ssc040-C.5
single pulse decoupled gated NOE
OH HN
O
O
O
(Millions)
170.0982
165.6551
160.9164
150.9909
147.8636
133.4950
132.7989
132.1529
131.0172
127.1735
123.7030
122.7376
122.2060
117.5436
115.9609
99.3326
51.6216
39.7319
39.5222
39.3124
20.5484
X : parts per Million : 13C

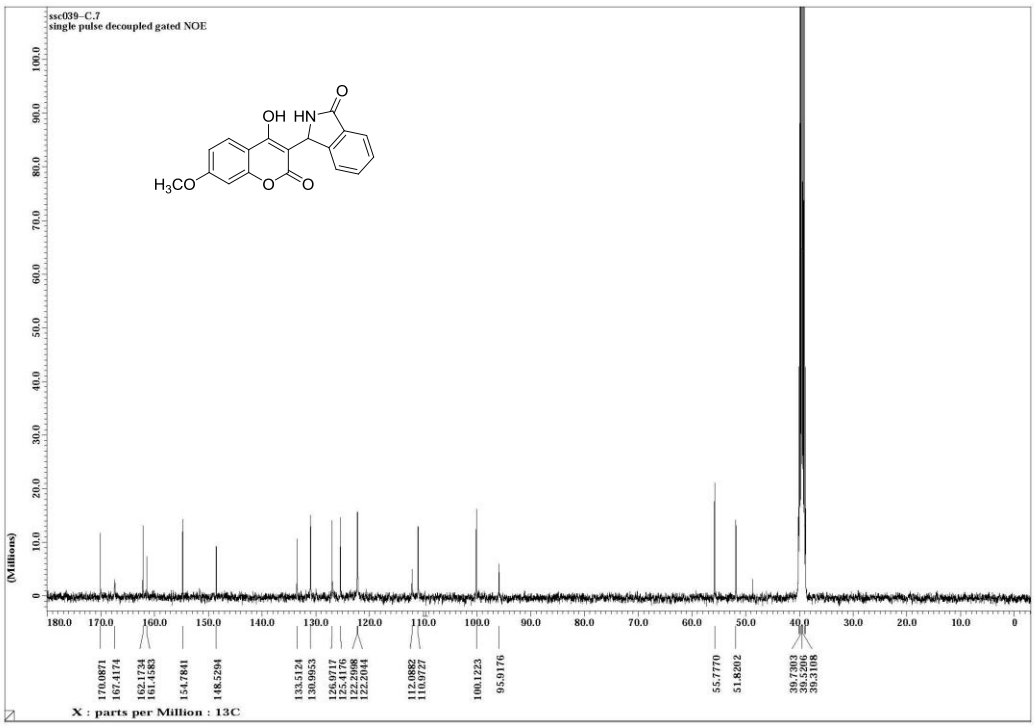
3d


ssc038.6
single_pulse
OH HN
O
H3CO
O
O
(Millions)
0.89043
1.1396
3.11812
1.93493
1.87699
0.90038
1
3.03882
8.4127
7.6430
7.6246
7.5101
7.4761
7.4700
7.4036
7.3016
7.2977
6.1092
3.7838
3.7632
3.1721
2.5100
2.5066
1.2591
1.2339
X : parts per Million : 1H

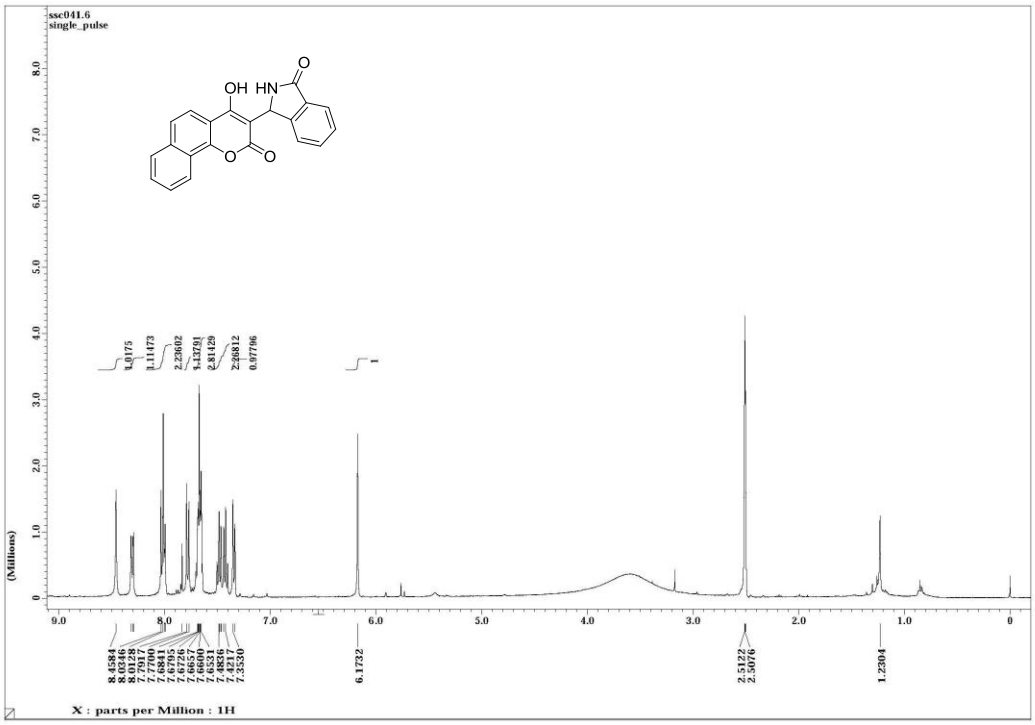

ssc038–C.7
single pulse decoupled gated NOE
OH HN
O
H3CO
O
O
(Millions)
170.0671
161.2763
154.9644
148.1738
147.2684
133.5116
131.0040
127.0376
122.2989
122.1845
119.1096
117.2251
106.4620
98.6913
55.6522
51.8193
39.7199
39.5197
39.3100
X : parts per Million : 13C

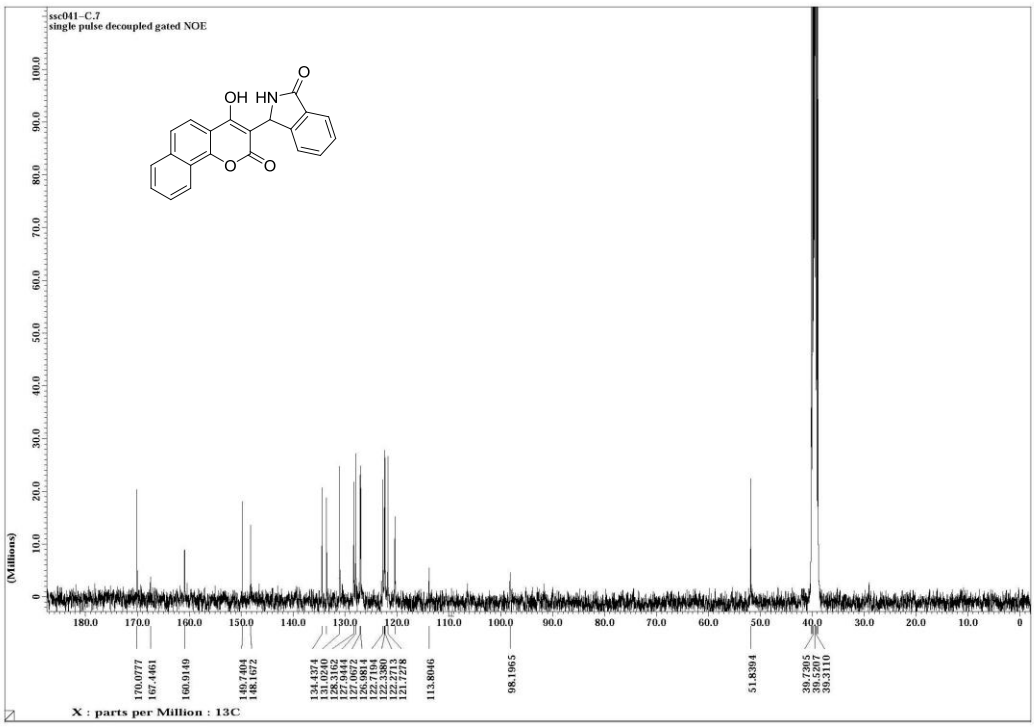
3e


ssc039.6
single_pulse
OH HN
O
H3CO
O
O
(Millions)
30.0
20.0
10.0
0
1.00986
1.02205
1.03694
2.24172
1.01870
2.01785
1
2.99734
8.3815
7.8993
7.8764
7.6369
7.6156
7.4651
7.4617
7.3941
7.2910
7.2715
6.8523
6.8328
6.8271
6.0963
3.8190
3.7640
3.7354
3.6976
3.1741
2.5086
2.5040
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : 1H

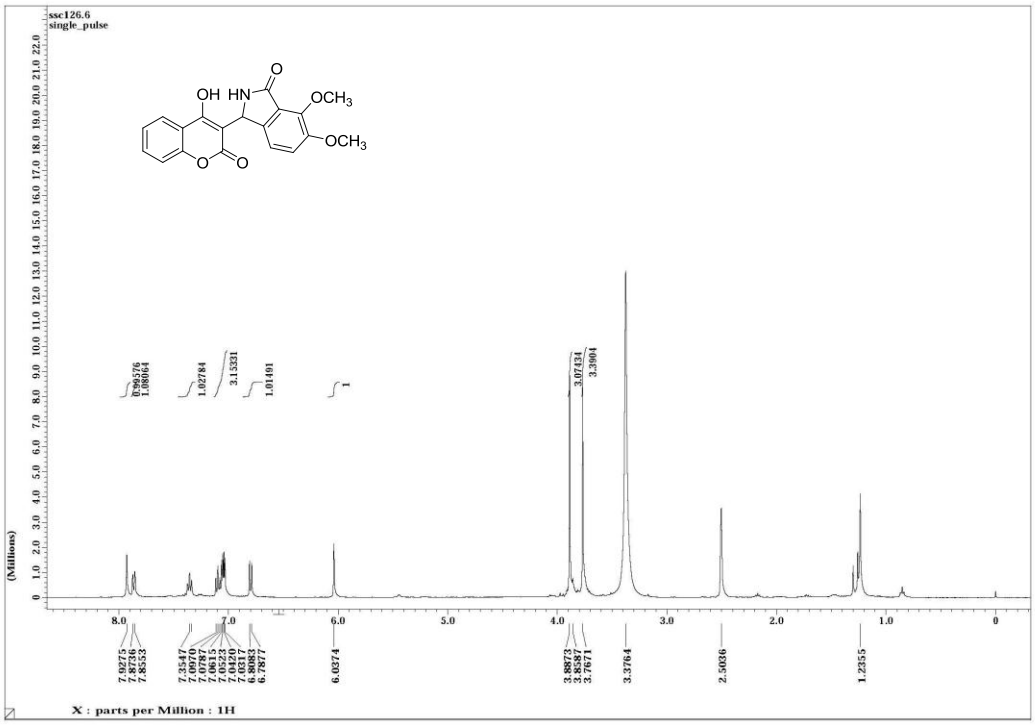

ssc039–C.7
single pulse decoupled gated NOE
OH HN
O
H3CO
O
O
(Millions)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
170.0871
167.4174
162.1734
161.4583
154.7841
148.5294
133.5124
130.9953
126.9717
125.4176
122.2098
122.2044
112.0882
110.0727
100.1223
95.9176
55.7770
51.8202
39.7303
39.5206
39.3108
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : 13C

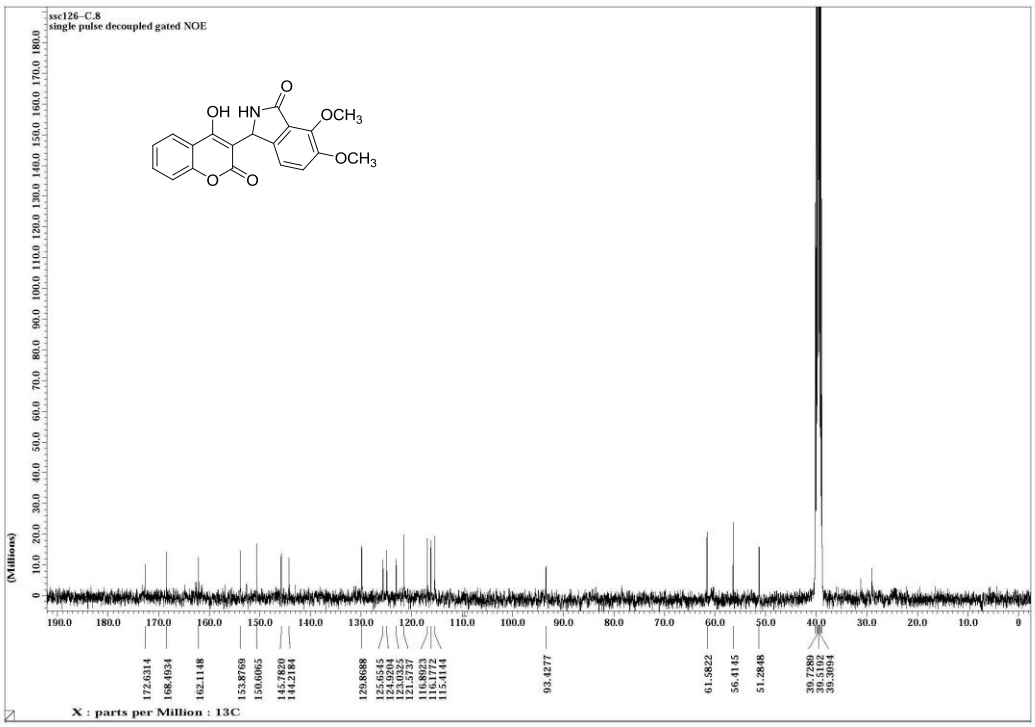
3f


ssc041.6
single_pulse
OH HN
O
O
O
(Millions)
X : parts per Million : 1H

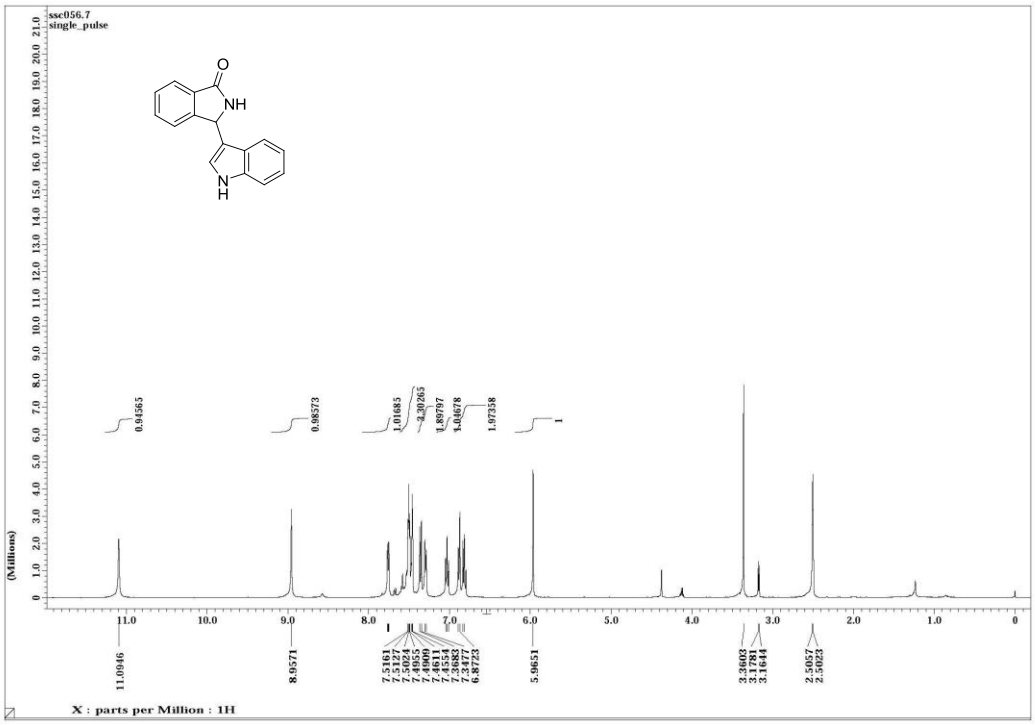

ssc041-C.7
single pulse decoupled gated NOE
OH HN
O
O
O
(Millions)
X : parts per Million : 13C

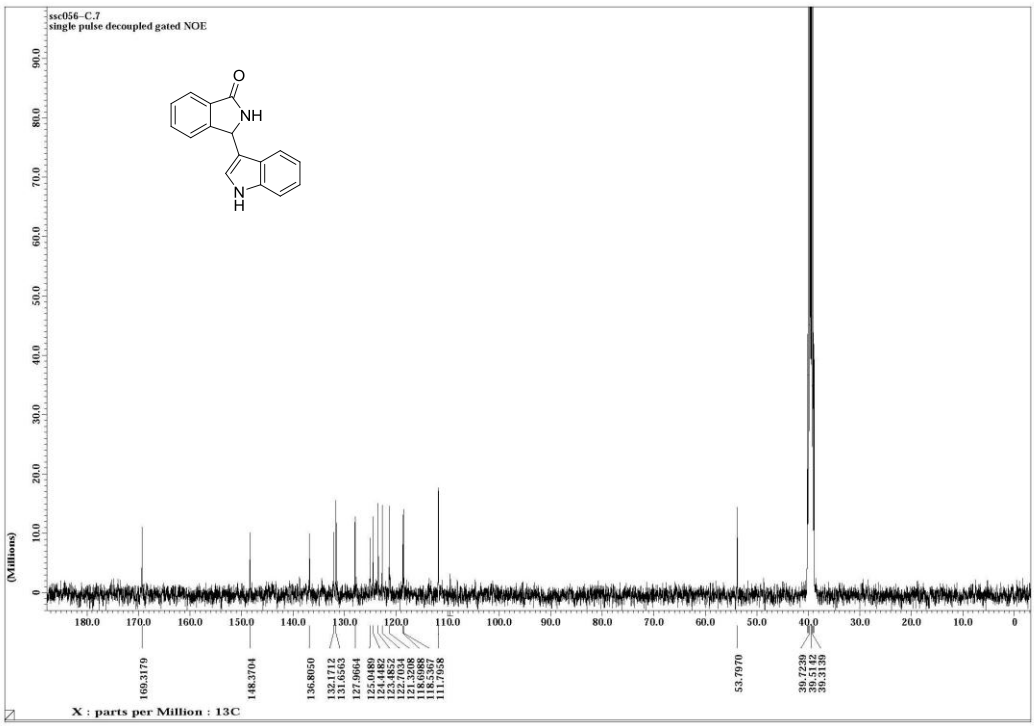
3g


ssc126.6
single_pulse
OH HN
O
OCH3
OCH3
O
O
(Millions)
X : parts per Million : 1H

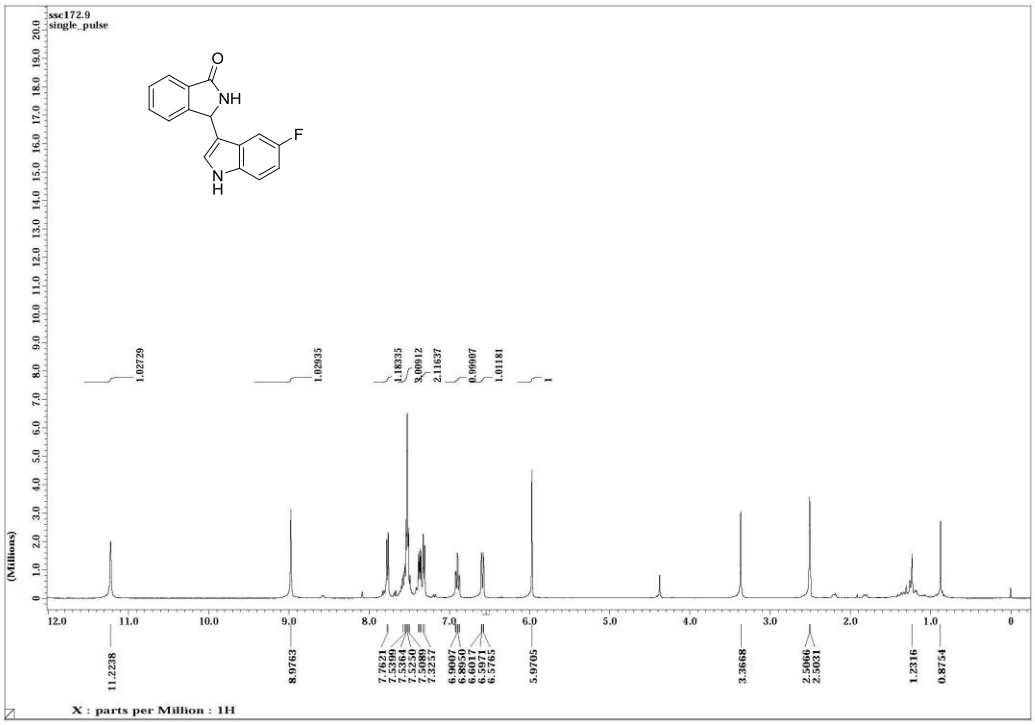

ssc126-C.8
single pulse decoupled gated NOE
OH HN
O
OCH3
OCH3
O
O
(Millions)
X : parts per Million : 13C

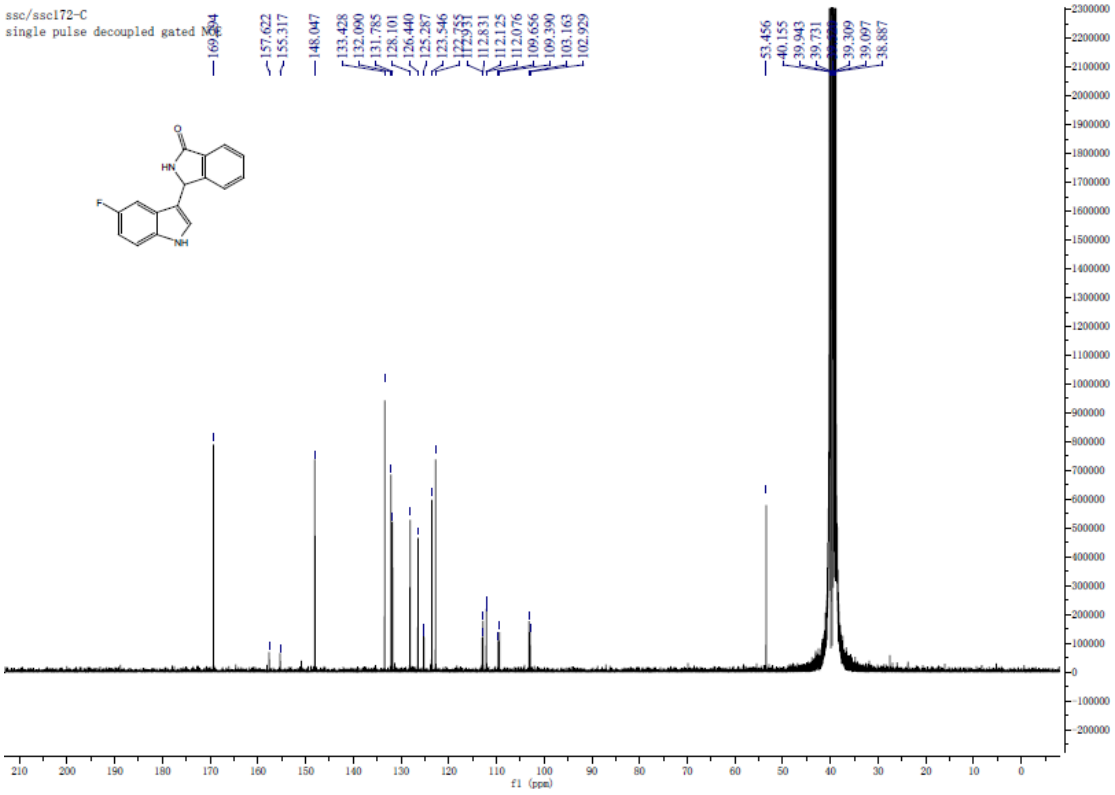
5a


ssc056.7
single_pulse
O
NH
N
H
(Millions)
0.94565
0.98573
1.01685
4.30265
1.89797
1.04678
1.97358
1
11.0946
8.9571
7.5161
7.5127
7.5024
7.4965
7.4906
7.4611
7.4554
7.3965
7.3477
6.8723
5.9651
3.3603
3.1781
3.1644
2.5057
2.5023
X : parts per Million : 1H

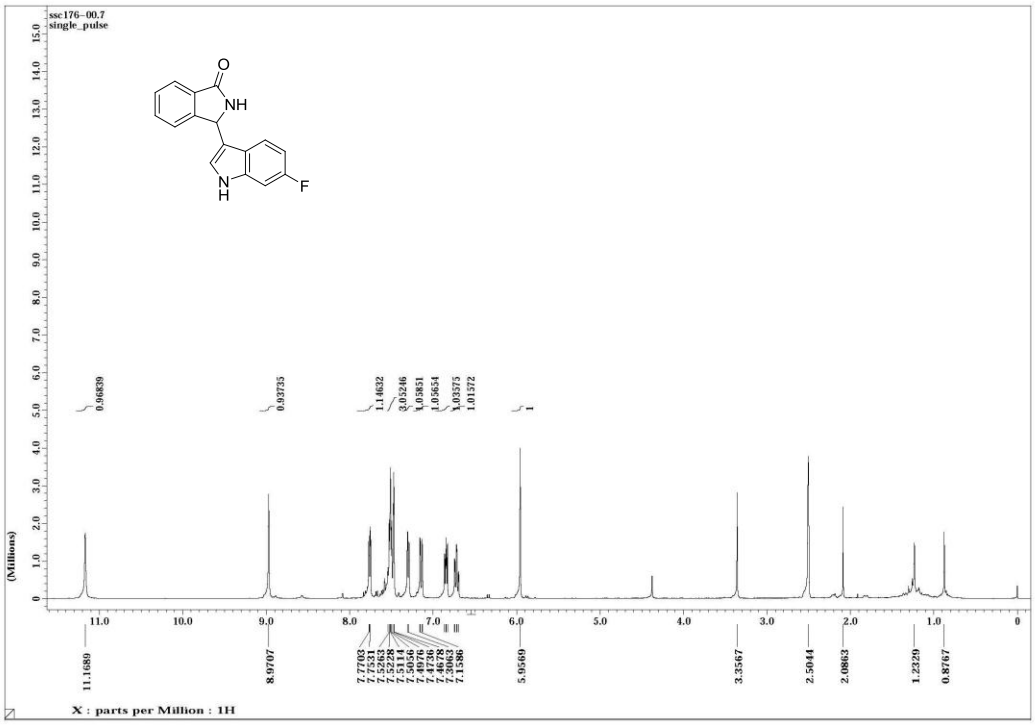

ssc056–C.7
single pulse decoupled gated NOE
O
NH
N
H
(Millions)
169.3179
148.3704
136.8050
132.1712
131.6563
127.9664
125.0489
124.4482
123.4852
122.7014
121.3208
118.6988
118.5387
111.7958
53.7970
39.7239
39.5142
39.3139
X : parts per Million : 13C

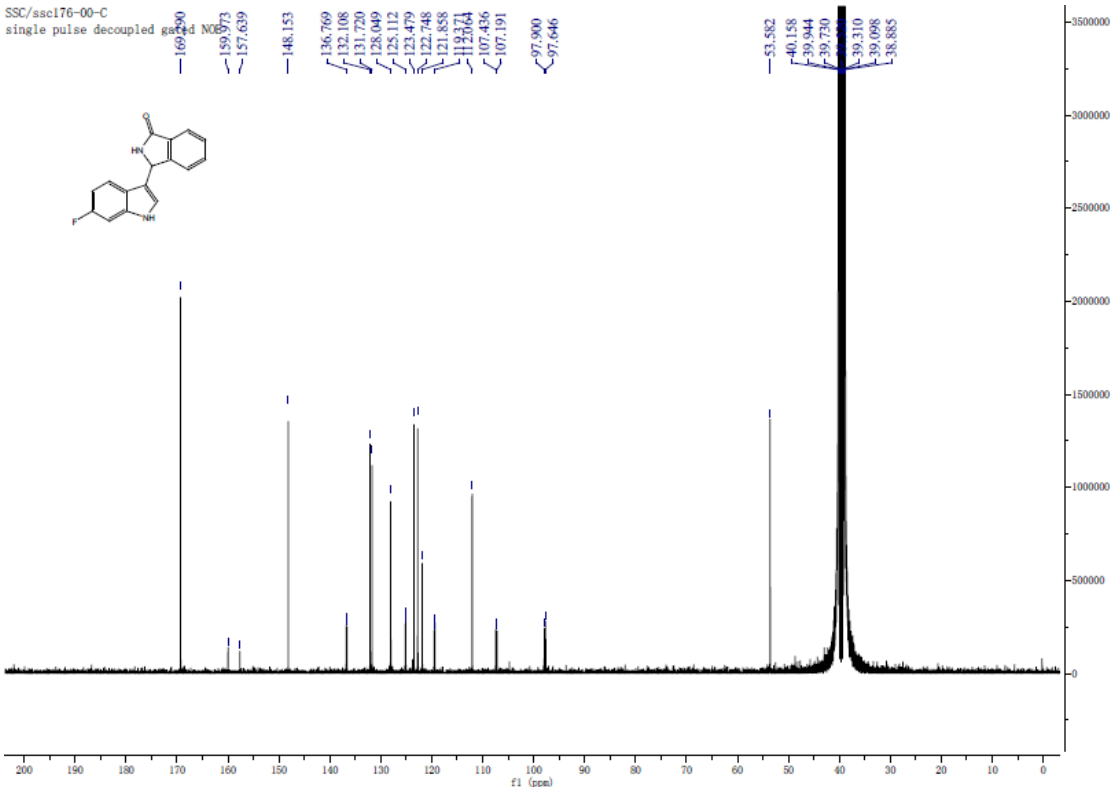
5b


ssc172.9
single_pulse
O
NH
F
N
H
(Millions)
X : parts per Million : 1H

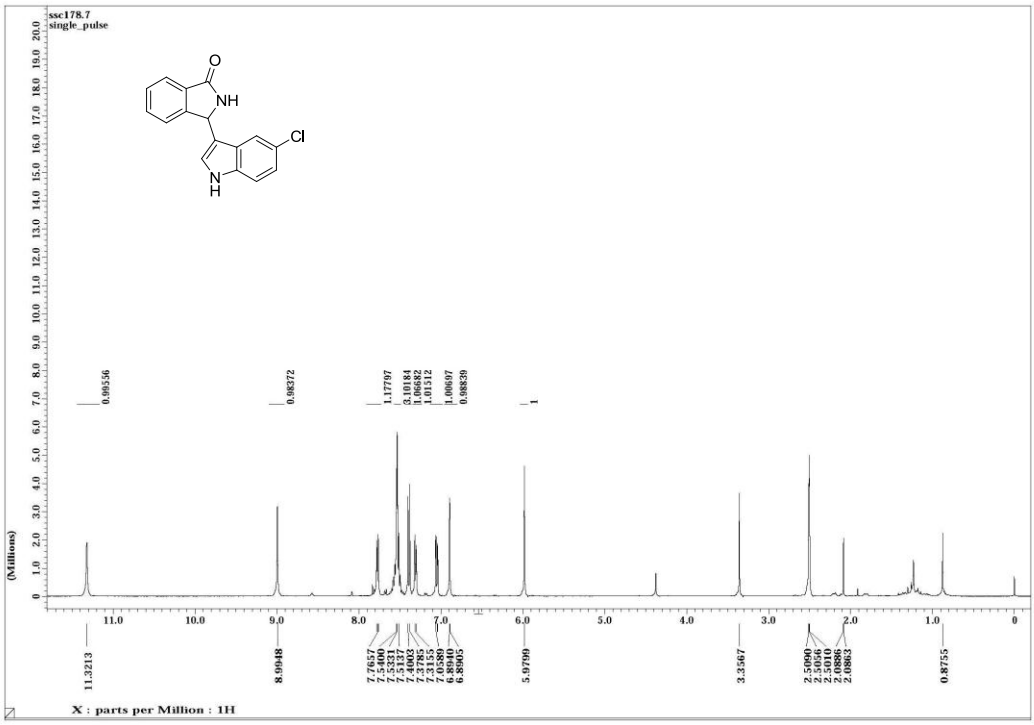

ssc/ssc172-C
single pulse decoupled gated NOE
O
HN
F
NH
f1 (ppm)

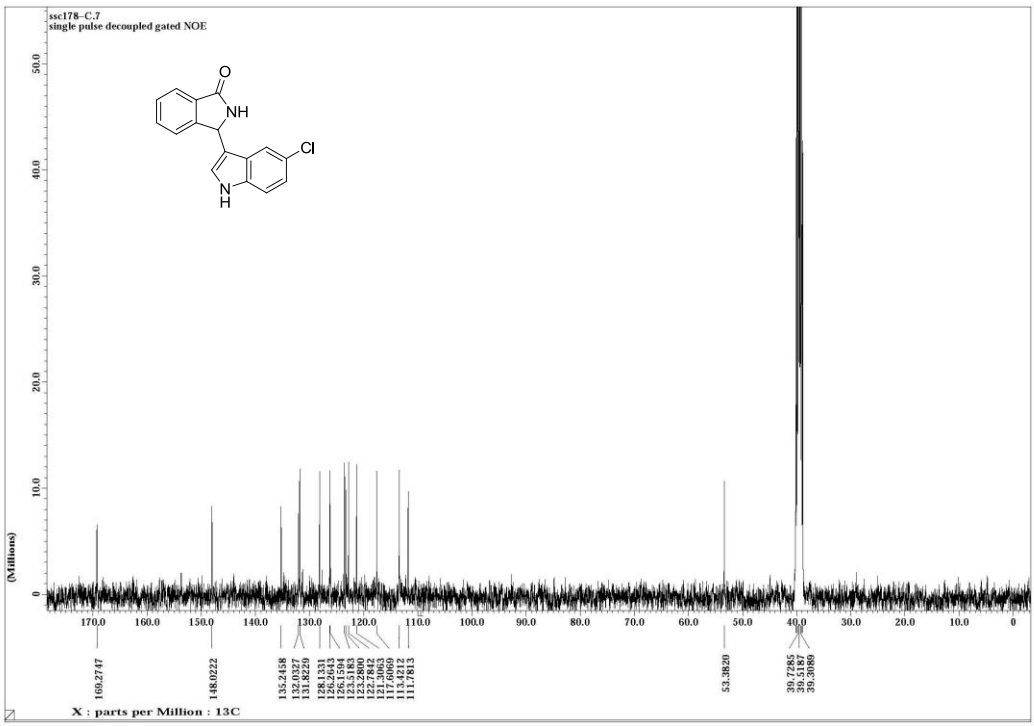
5c


ssc176-00.7
single_pulse
O
NH
N
H
F
(Millions)
X : parts per Million : 1H

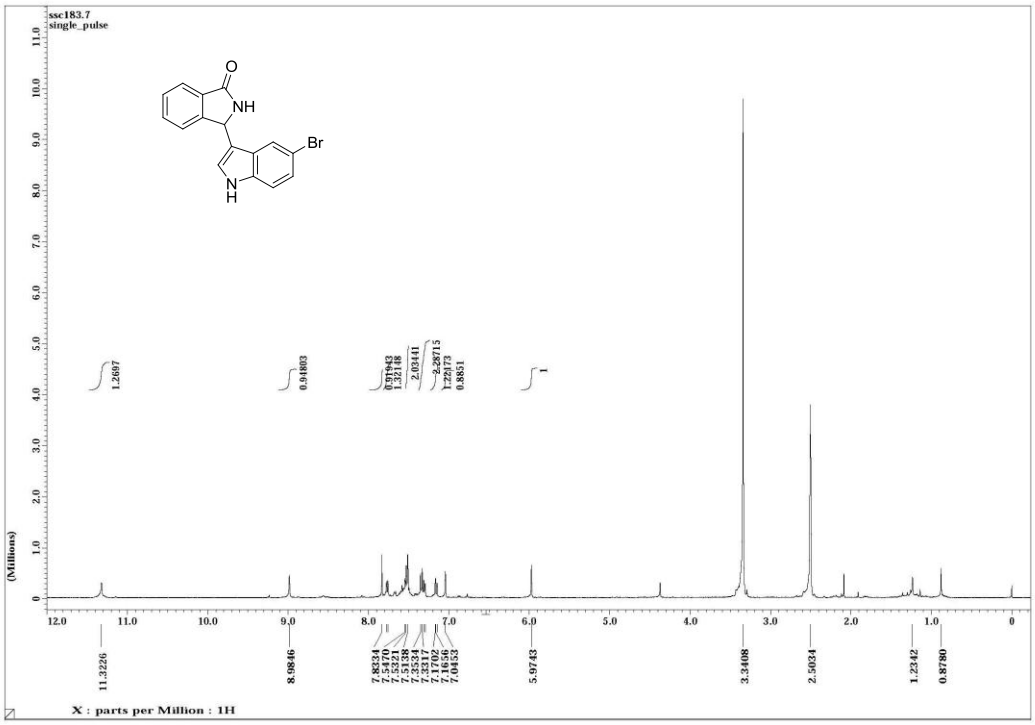

SSC/ssc176-00-C
single pulse decoupled gated NOE
f1 (ppm)

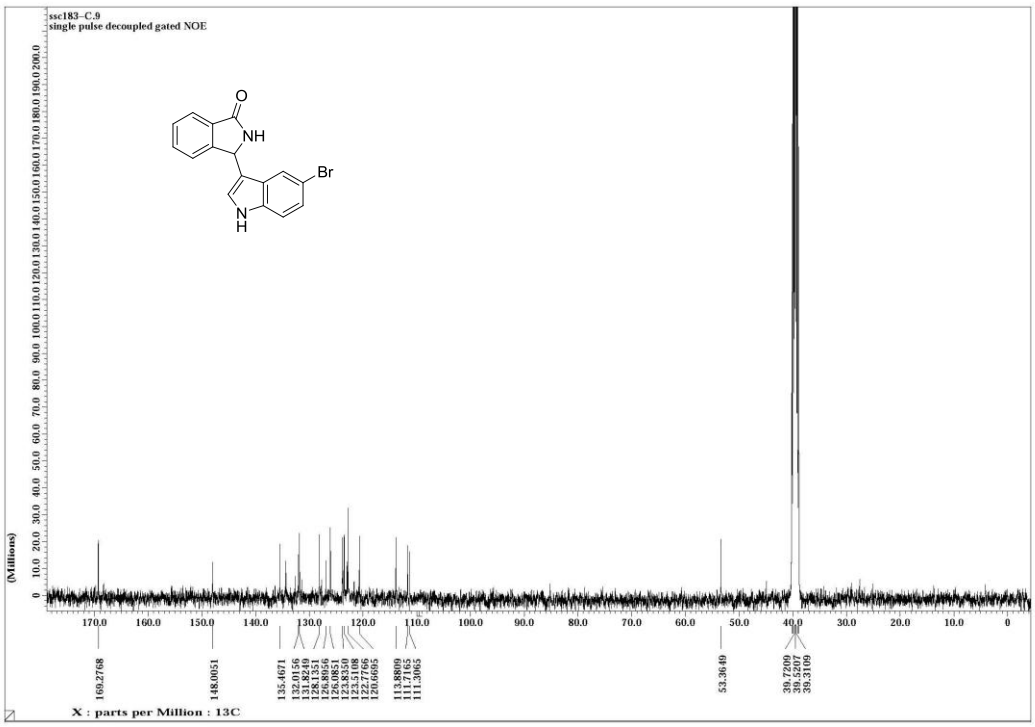
5d


ssc178.7
single_pulse
O
NH
Cl
N
H
(Millions)
X : parts per Million : 1H

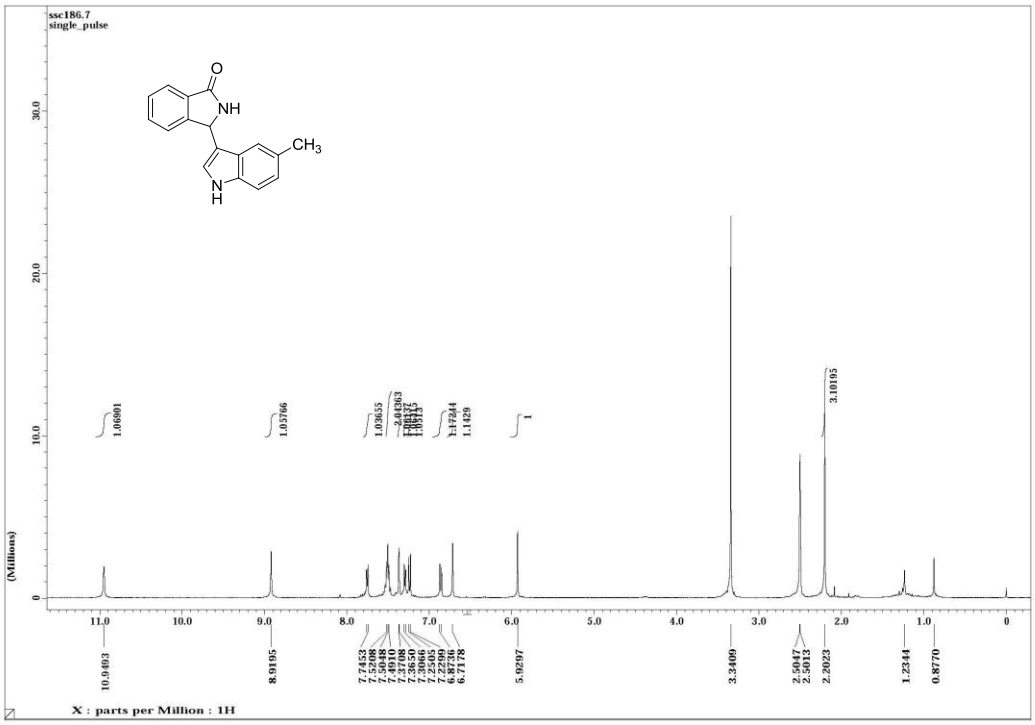

ssc178–C.7
single pulse decoupled gated NOE
O
NH
Cl
N
H
(Millions)
X : parts per Million : 13C

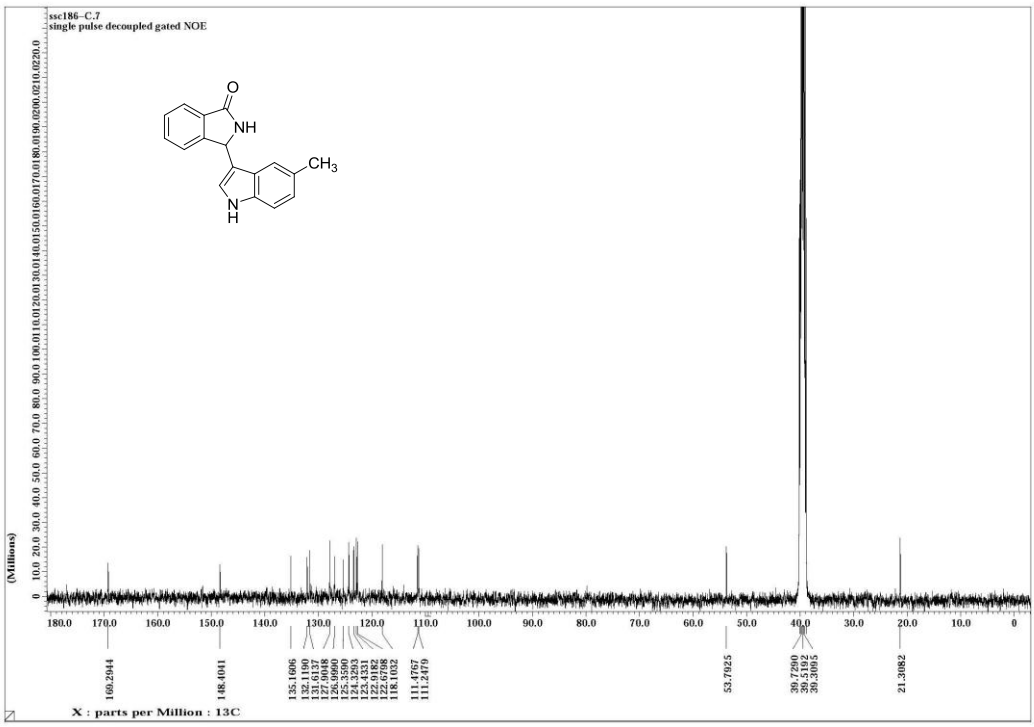
5e


ssc183.7
single_pulse
O
NH
Br
N
H
(Millions)
X : parts per Million : 1H

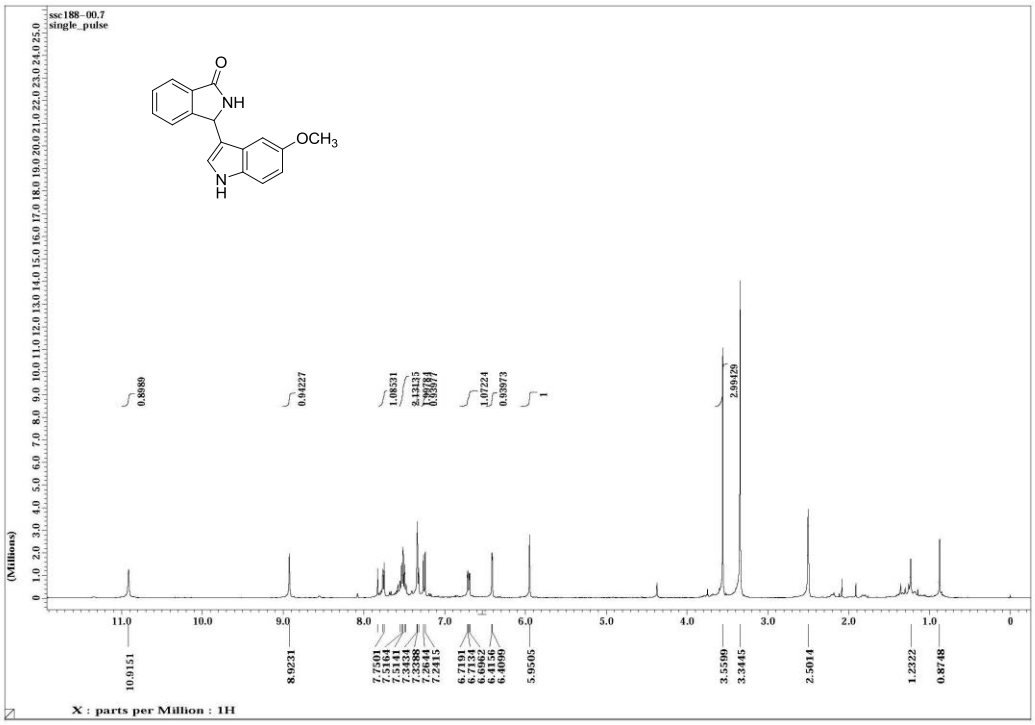

ssc183–C.9
single pulse decoupled gated NOE
O
NH
Br
N
H
(Millions)
X : parts per Million : 13C

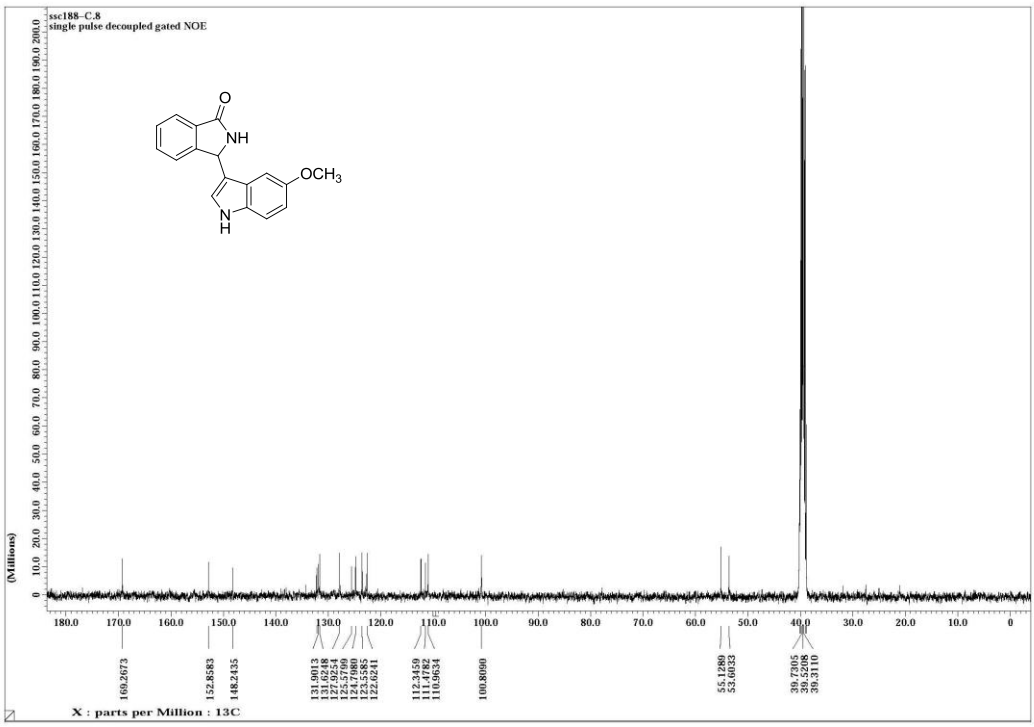
5f


ssc186.7
single_pulse
O
NH
CH3
N
H
(Millions)
X : parts per Million : 1H

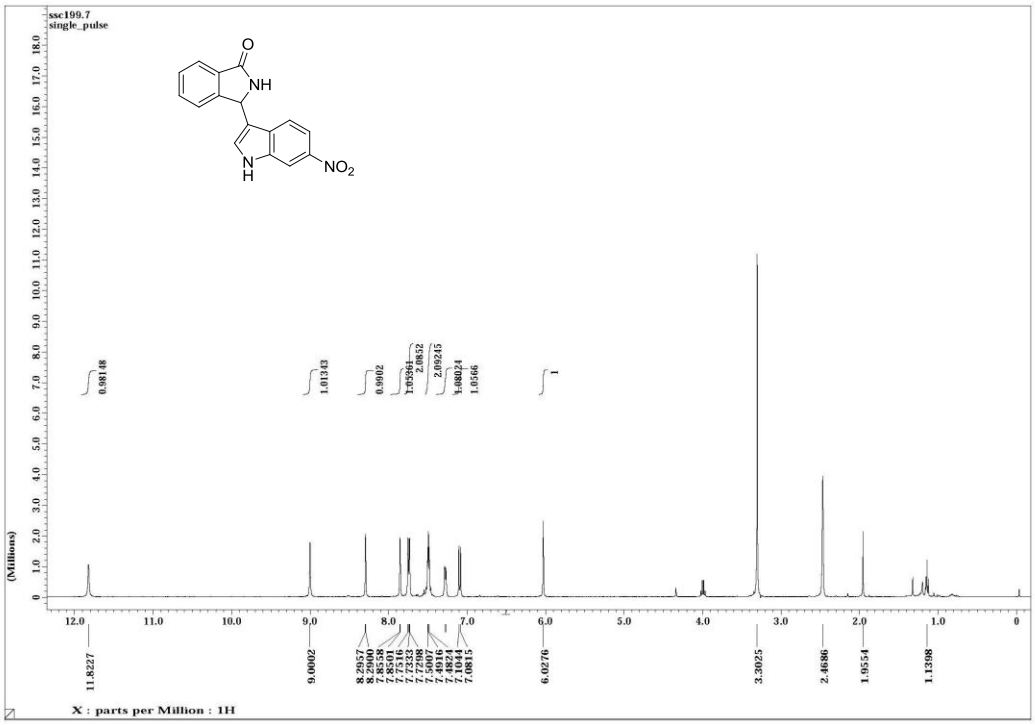

ssc186-C.7
single pulse decoupled gated NOE
O
NH
CH3
N
H
(Millions)
X : parts per Million : 13C

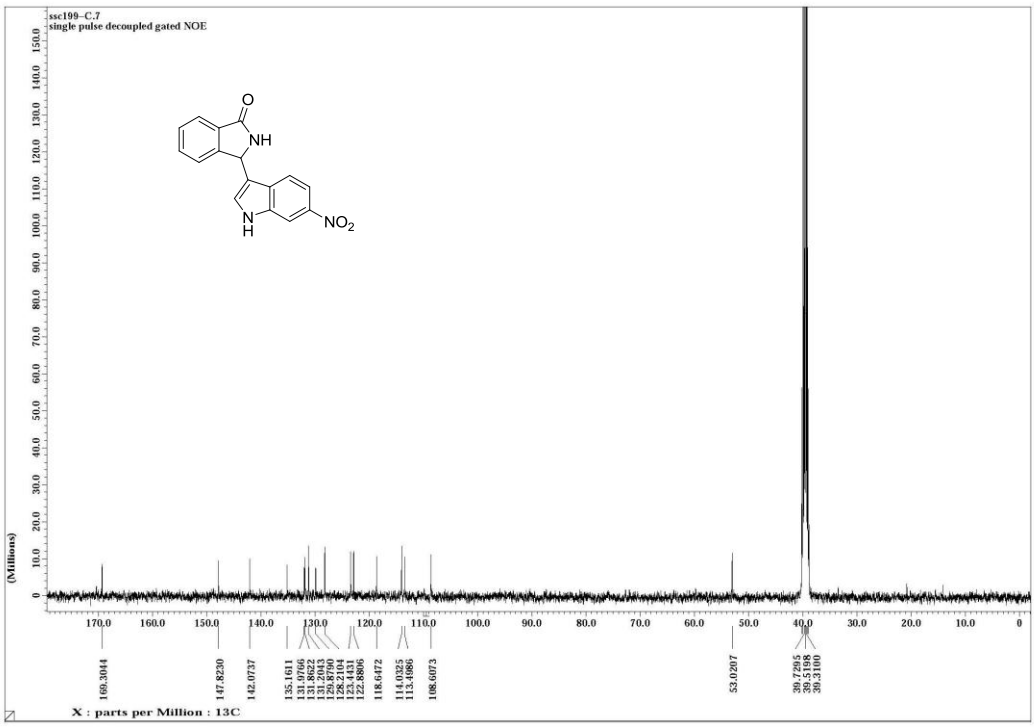
5g


ssc188-00.7
single_pulse
O
NH
OCH3
N
H
(Millions)
X : parts per Million : 1H

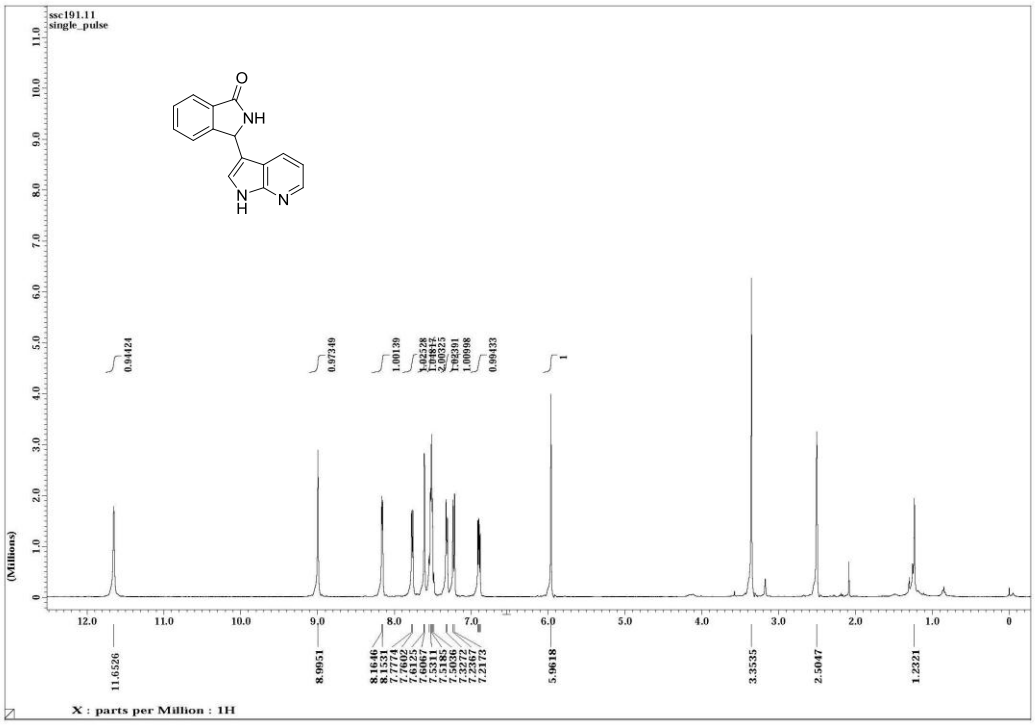

ssc188-C.8
single pulse decoupled gated NOE
O
NH
OCH3
N
H
(Millions)
X : parts per Million : 13C

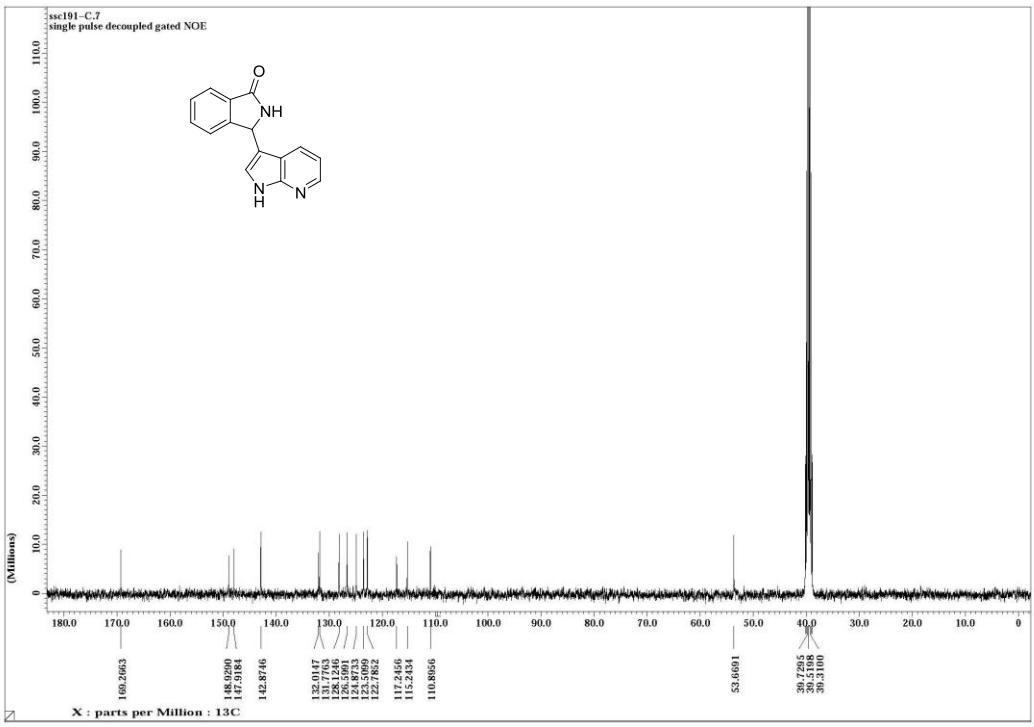
5h


ssc199.7
single_pulse
O
NH
N
H
NO2
(Millions)
X : parts per Million : 1H


ssc199–C.7
single pulse decoupled gated NOE
O
NH
N
H
NO2
(Millions)
X : parts per Million : 13C

5i


ssc191.11
single_pulse
O
NH
N
H
N
(Millions)
X : parts per Million : 1H


ssc191-C.7
single pulse decoupled gated NOE
O
NH
N
H
N
(Millions)
X : parts per Million : 13C