Catalyst-Free Synthesis of Fused 1,2,3-Triazole and Isoindoline Derivatives via Intramolecular Azide-Alkene Cascade Reaction

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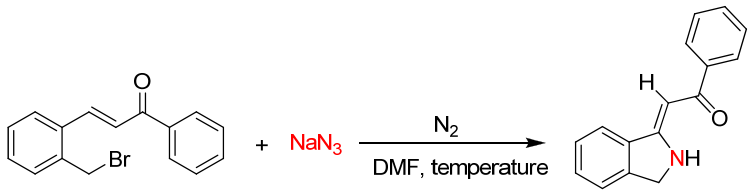
Table of Contents

Table S1 Optimization of reaction conditions for isoindoline derivative **3a**[a]



1a **3a**

Entry	**1a**:NaN_3 (by mole)	T_1, 3 h	T_2, 1 h	Yield of **3a** (%)[b]
1	1.0/2.0	10 °C	60 °C	0
2	1.0/2.0	10 °C	60 °C	0
3	1.0/1.2	10 °C	60 °C	0
4	**1.0/1.0**	**10 °C**	**60 °C**	**74**
5	1.0/0.9	10 °C	60 °C	69
6	1.0/1.0	10 °C	80 °C	41
7	1.0/1.0	10 °C	100 °C	0

[a] Reactions conditions: **1a** (1 mmol), NaN_3 (2, 1.2, 1 and 0.9 mmol), DMF (2 mL), N_2, 10 °C for 3 h then rise to 60, 80,100 °C for 1 h. [b] Isolated yield of pure product based on **1a**. Entry in bold highlights optimized reaction conditions.

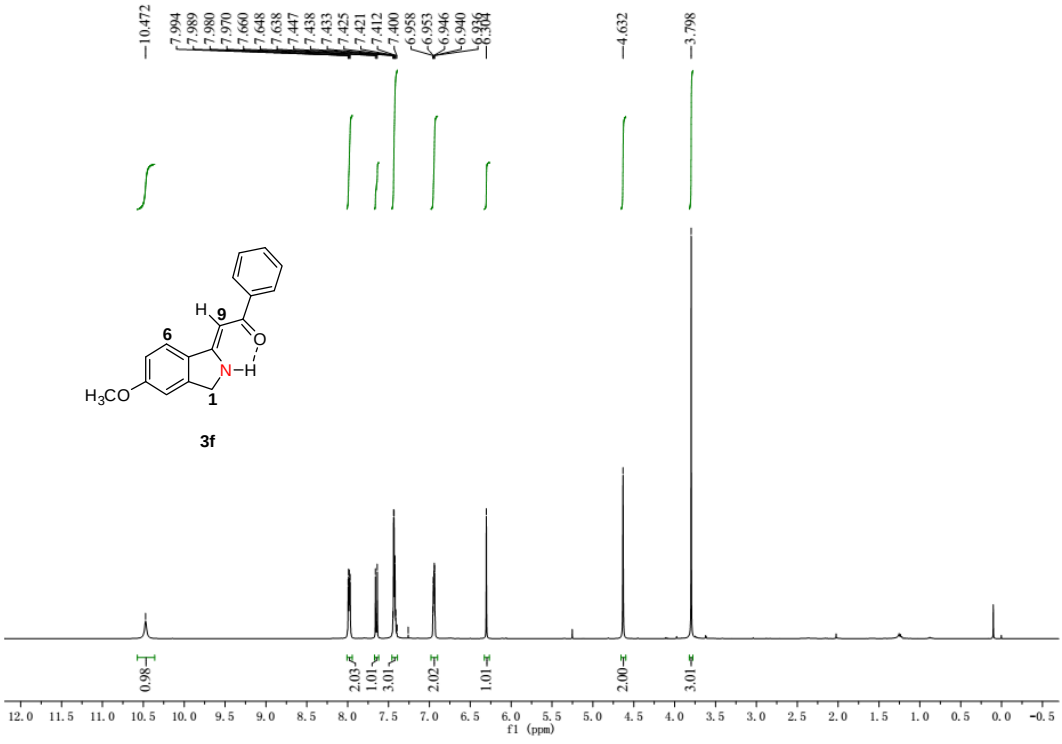


Figure S1 The ^1H NMR spectrum of **3f** in $CDCl_3$

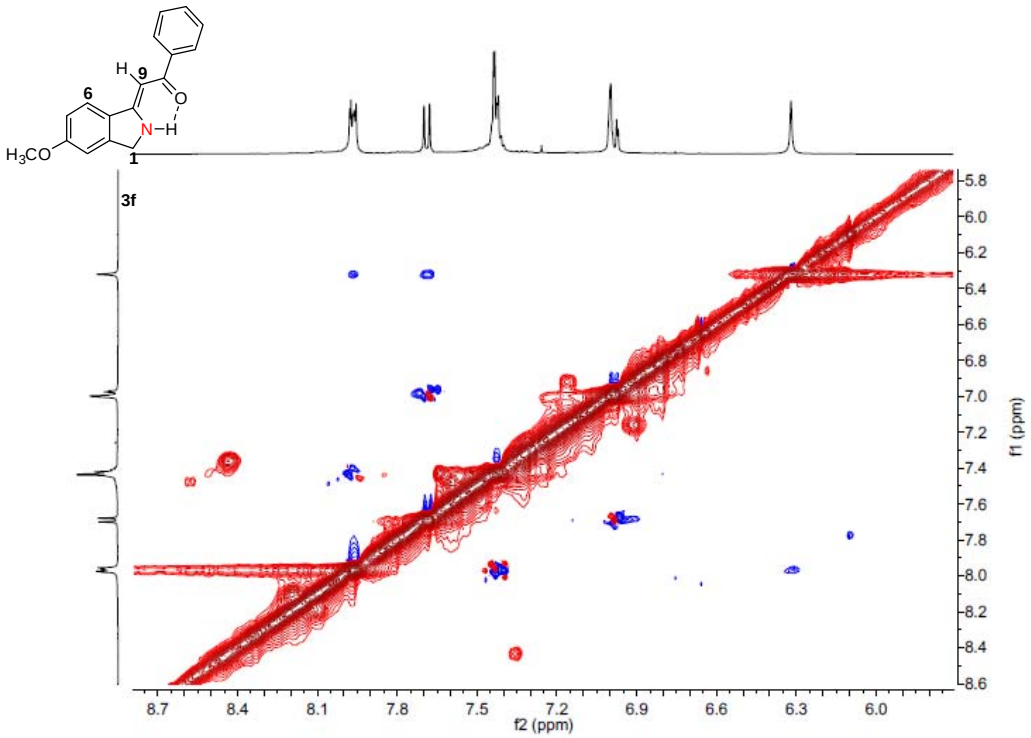
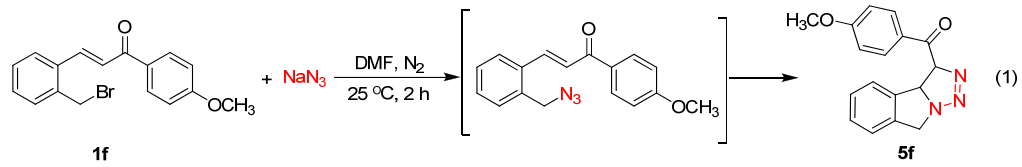
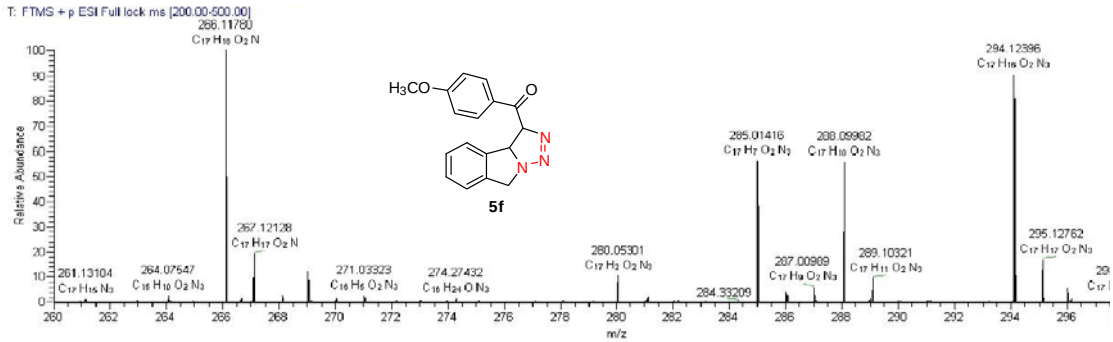


Figure S2 The NOESY spectrum of **3f** in $CDCl_3$

ESI/MS experiments:

Under the atmosphere of nitrogen, a mixture of **1f** (0.5 mmol) and sodium azide (0.5 mmol) in DMF (2.0 mL) was reacted at 10 °C for 3 h and 50 μL of the mixture was used for the ESI analysis in CH_3OH.

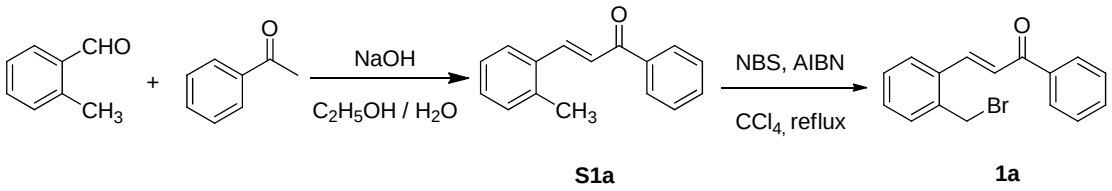




Experimental

General methods and materials. Proton nuclear magnetic resonance spectra (^{1}H NMR) and carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 400 MHz and 100 MHz or 500 MHz and 125 MHz, respectively, using $CDCl_3$ as reference standard (δ 7.26 ppm) for ^{1}H NMR and (δ 77.04 ppm) for ^{13}C NMR. HRMS (ion trap) were recorded using APCI or ESI. Melting points were uncorrected. Precoated silica gel plates F-254 were used for analytical thin-layer chromatography. Column chromatography was performed on silica gel (300-400 mesh). Starting materials were readily prepared according to literature procedures. Unless otherwise noted, all reagents were obtained commercially and used without further purification.

Procedure of synthesis of starting materials 1:



S1a **1a**

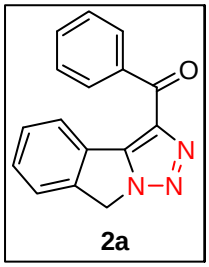
(i) NaOH (160 mg, 4.0 mmol) was added to a solution of aldehydes (2.0 mmol) in MeOH (20 mL) at rt. Then ketones (2.05 mmol) was added to the reaction mixture. The reaction mixture was stirred at reflux for 6 h. The reaction mixture was concentrated to yield the residue. The residue was extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product. Purification on silica gel afforded chalcones **S1a**.

(ii) Chalcone **S1a** (2.0 mmol) were dissolved in 30 ml of CCl_4 and N-bromosuccinimide (2.2 mmol) was added while stirring. Then catalytic amounts of dibenzoylperoxide were added and the solution was refluxed for 4-6 h. The resulting solution was cooled and evaporated under reduced pressure. The target product **1a** was purified by column chromatography on silica gel using a mixture of ethyl acetate and petroleum ether.

General procedure for the synthesis of fused 1,2,3-triazole 2. To the mixture of **1** (1.0 equiv, 0.5 mmol) and sodium azide (1.2 equiv., 0.6 mmol), and 2.0 mL DMF at 25 ^{o}C for 6 h in the air. The progress of the reaction was monitored by thin-layer chromatography. Upon completion, the reaction mixture was diluted with H_2O (10 mL), extracted with ethyl acetate (3 × 10 mL). The organic extract was washed with H_2O (3 × 5 mL), dried over anhydrous magnesium sulfate. After filtration, the mixture was evaporated under reduced pressure, and the residue was separated by column chromatography to give the pure product **2**.

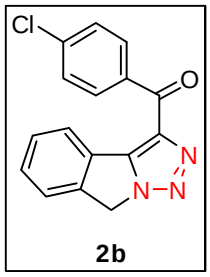
General procedure for the synthesis of Isoindoline Derivatives 3. To a Schlenk tube equipped with a stir bar was added **1** (1.0 equiv., 0.5 mmol), NaN_3 (1.0 equiv., 0.5 mmol), and a balloon filled with N_2 was connected to the Schlenk tube through the side arm and purged one time. Then, DMF (2.0 mL) were injected in the reaction tube with magnetic stirring. The reaction mixture was allowed to stir vigorously at 10 ^{o}C for 3 h. Thereafter the reaction mixture was stirred at 60 °C for 1 h. Upon completion, the reaction mixture was diluted with H_2O (10 mL), extracted with ethyl acetate (3 × 10 mL). The organic extract was washed with H_2O (3 × 5 mL), dried over anhydrous magnesium sulfate. After filtration, the mixture was evaporated under reduced pressure, and the resulting crude product **3** was separated on a silica gel column with petroleum ether and ethyl acetate as eluent.

Spectral data of all compounds



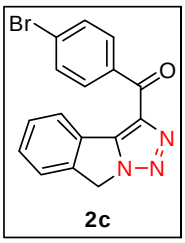
2a

(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(phenyl)methanone (2a) White solid, m.p. 162-164 °C; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.54–8.51 (m, 3H), 7.65–7.60 (m, 1H), 7.56–7.53 (m, 4H), 7.52–7.48 (m, 1H), 5.39 (s, 2H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 186.3, 148.1, 142.4, 139.7, 137.2, 133.4, 130.9, 130.4, 129.5, 128.7, 127.6, 125.5, 124.0, 51.8 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{12}N_3O$ 262.0980 [M+H$^+$]; found 262.0973.



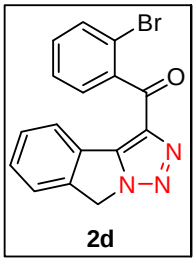
2b

(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(4-chlorophenyl)methanone (2b) Light yellow solid, m.p. 154-156 °C; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.49 (d, *J* = 1.8 Hz, 1H), 8.48–8.44 (m, 2H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.49 (s, 1H), 7.47 (dt, *J* = 8.9, 1.7 Hz, 3H), 5.34 (s, 2H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 184.6, 148.1, 142.4, 139.8, 139.4, 135.3, 134.5, 132.4, 130.5, 129.4, 128.9, 127.4, 125.5, 123.9, 123.7, 51.8 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{11}N_3O$ 296.0591 [M+H$^+$]; found 296.0575.



2c

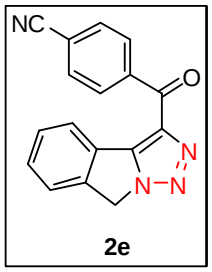
(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(4-bromophenyl)methanone (2c) White solid, m.p. 173-175 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.54 (d, *J* = 7.6 Hz, 1H), 8.45 (d, *J* = 7.8 Hz, 2H), 7.68 (d, *J* = 7.9 Hz, 2H), 7.60–7.52 (m, 3H), 5.41 (s, 2H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 186.3, 148.1, 142.4, 139.7, 137.2, 133.4, 130.9, 130.4, 129.5, 128.7, 127.6, 125.5, 123.9, 51.8 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{11}BrN_3O$ 340.0085, 342.0065 [M+H$^+$]; found 340.0074, 342.0051.



2d

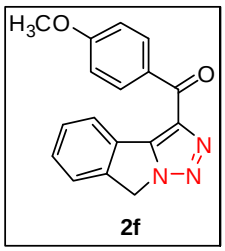
(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(2-bromophenyl)methanone (2d) White solid, m.p. 153-156 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.0 Hz, 1H), 7.65 (dd, *J* = 5.6, 2.0 Hz, 2H), 7.55–7.47 (m, 3H), 7.45–7.39 (m, 1H), 7.34 (dd, *J* = 10.1, 4.5 Hz, 1H), 5.36 (d, *J* = 3.0 Hz, 2H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$) δ 188.2, 147.3, 142.5, 139.6, 138.6, 133.7, 131.9, 130.6, 130.4, 129.4, 127.3, 126.9, 125.2, 124.1,

120.2, 51.9 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{11}BrN_3O$ 340.0085, 342.0065 [M+H$^+$]; found 340.0092, 342.0070.



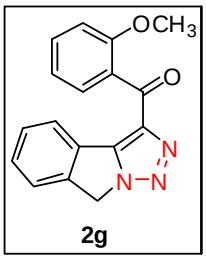
2e

4-(8*H*-[1,2,3]triazolo[5,1-a]isoindole-3-carbonyl)benzonitrile (2e) Light yellow solid, m.p. 226-228 °C; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.64–8.60 (m, 2H), 8.55–8.50 (m, 1H), 7.84–7.80 (m, 2H), 7.60–7.53 (m, 3H), 5.43 (s, 2H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 184.5, 148.6, 142.5, 140.3, 139.1, 132.4, 131.3, 130.9, 129.7, 127.2, 125.6, 124.1, 118.5, 116.4, 51.9 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{11}N_4O$ 287.0933 [M+H$^+$]; found 287.0926.



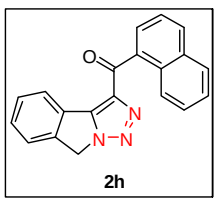
2f

(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(4-methoxyphenyl)methanone (2f) White solid, m.p. 202-204 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.66–8.59 (m, 2H), 8.56 (dd, *J* = 6.6, 2.2 Hz, 1H), 7.60–7.48 (m, 3H), 7.06–7.00 (m, 2H), 5.41 (s, 2H), 3.91 (s, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 184.3, 163.7, 147.6, 141.9, 139.8, 133.1, 129.9, 129.7, 129.2, 127.4, 125.3, 123.6, 113.7, 55.5, 51.4 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{14}N_3O_2$ 292.1086 [M+H$^+$]; found 292.1074.



2g

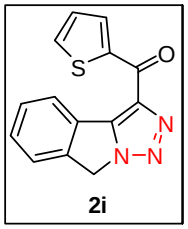
(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(2-methoxyphenyl)methanone (2g) Light yellow solid, m.p. 174-176 °C; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.43 (dd, *J* = 7.2, 1.5 Hz, 1H), 7.68 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.55–7.47 (m, 4H), 7.09–7.03 (m, 2H), 5.38 (s, 2H), 3.82 (s, 3H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 188.3, 158.0, 146.5, 142.0, 139.6, 132.6, 130.4, 130.0, 129.1, 128.0, 127.1, 125.1, 123.6, 120.3, 111.8, 55.8, 51.5 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{14}N_3O_2$ 292.1086 [M+H$^+$]; found 292.1077.



2h

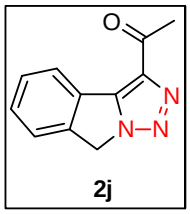
(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(naphthalen-1-yl)methanone (2h) White solid, m.p. 208-210 °C; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.54 (d, *J* = 7.4 Hz, 1H), 8.49 (dd, *J* = 8.2, 0.9 Hz, 1H),

8.26 (dd, *J* = 7.1, 1.2 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.95–7.90 (m, 1H), 7.62–7.52 (m, 6H), 5.42 (s, 2H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 189.1, 147.5, 142.1, 139.9, 134.4, 133.9, 132.4, 130.9, 130.3, 130.2, 129.2, 128.5, 127.5, 127.2, 126.2, 125.4, 125.2, 124.4, 123.7, 51.6 ppm. **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{14}N_3O$ 312.1137 [$M+H^+$]; found 312.1128.



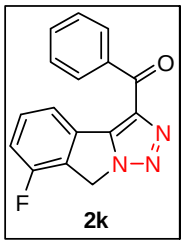
2i

(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(thiophen-2-yl)methanone (2i) Light yellow solid, m.p. 184-186 °C; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.80 (d, *J* = 3.3 Hz, 1H), 8.47 (t, *J* = 7.3 Hz, 1H), 7.74 (dd, *J* = 4.9, 1.0 Hz, 1H), 7.52–7.42 (m, 3H), 7.24–7.21 (m, 1H), 5.36 (s, 2H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 177.5, 147.2, 142.5, 141.9, 138.7, 135.9, 134.7, 134.2, 132.6, 130.1, 129.1, 128.4, 127.1, 125.3, 123.6, 123.3, 51.5 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{14}H_{10}N_3OS$ 268.0545 [$M+H^+$]; found 268.0531.



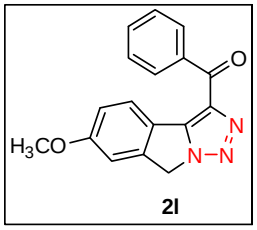
2j

1-(8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)ethanone (2j) Light yellow solid, m.p. 164-167 °C; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.24–8.03 (m, 1H), 7.44–7.40 (m, 1H), 7.40–7.35 (m, 2H), 5.20 (s, 2H), 2.61 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ 192.9, 144.9, 142.2, 139.3, 130.1, 129.2, 126.9, 124.8, 123.8, 51.6, 27.1 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{11}H_{10}N_3O$ 200.0824 [$M+H^+$]; found 200.0817.

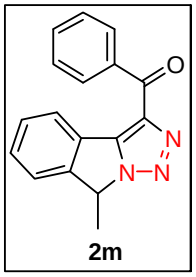


2k

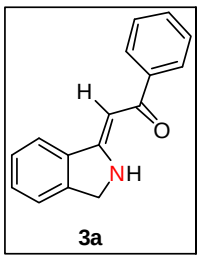
(7-fluoro-8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(phenyl)methanone (2k) White solid, m.p. 187-189 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.54–8.47 (m, 2H), 8.31 (d, *J* = 7.6 Hz, 1H), 7.61 (dd, *J* = 10.5, 4.2 Hz, 1H), 7.56–7.51 (m, 3H), 7.20 (t, *J* = 8.8 Hz, 1H), 5.44 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ 185.6, 157.3 (d, $^1J_{CF}$ = 250.0 Hz), 147.1, 147.0, 139.5, 136.5, 133.2, 131.5 (d, $^3J_{CF}$ = 7.5 Hz), 130.6, 128.3, 121.2, 121.1, 117.1 (d, $^2J_{CF}$ = 18.8 Hz), 48.9 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{11}FN_3O$ 280.0886 [$M+H^+$]; found 280.0875.



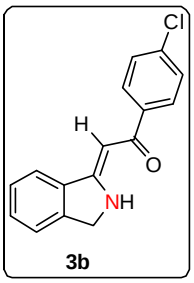
(6-methoxy-8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(phenyl)methanone (2l) Light yellow solid, m.p. 147-150 °C; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.49 (d, *J* = 7.5 Hz, 2H), 8.31 (d, *J* = 8.8 Hz, 1H), 7.63–7.56 (m, 1H), 7.50 (t, *J* = 7.2 Hz, 2H), 6.94 (d, *J* = 6.4 Hz, 2H), 5.24 (s, 2H), 3.77 (s, 3H) ppm; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 185.9, 161.7, 148.0, 144.6, 138.7, 137.2, 133.1, 130.8, 128.5, 126.5, 120.1, 114.6, 110.0, 55.9, 51.6 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{14}N_3O_2$ 292.1086 [M+H$^+$]; found 292.1080.



(8-methyl-8*H*-[1,2,3]triazolo[5,1-a]isoindol-3-yl)(phenyl)methanone (2m) White solid, m.p. 115-117 °C; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.52 (dd, *J* = 7.1, 1.3 Hz, 2H), 8.50–8.42 (m, 1H), 7.62–7.58 (m, 1H), 7.54–7.44 (m, 5H), 5.49 (qd, *J* = 6.8, 3.1 Hz, 1H), 1.86 (dd, *J* = 6.9, 3.0 Hz, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 185.9, 147.9, 145.9, 139.4, 136.7, 132.9, 130.5, 130.0, 129.0, 128.2, 126.0, 124.9, 122.8, 59.2, 18.9 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{14}N_3O$ 276.1137 [M+H$^+$]; found 276.1131.

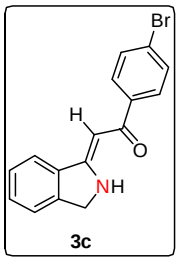


(*Z*)-2-(isoindolin-1-ylidene)-1-phenylethanone (3a) Colorless liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.57 (s, 1H), 8.02–7.98 (m, 2H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.52 (d, *J* = 4.2 Hz, 2H), 7.48–7.42 (m, 4H), 6.44 (s, 1H), 4.75 (s, 2H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 189.2, 162.9, 141.7, 140.4, 135.5, 130.8, 130.6, 128.2, 127.7, 127.0, 122.9, 121.9, 84.0, 51.7 ppm; **HRMS** (*m/z*) (APCI): calcd for $C_{16}H_{14}NO$ 236.1075 [M+H$^+$]; found 236.1066.

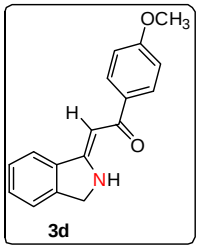


(*Z*)-1-(4-chlorophenyl)-2-(isoindolin-1-ylidene)ethanone (3b) Light yellow liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.57 (s, 1H), 7.93 (d, *J* = 8.5 Hz, 2H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 4.0 Hz, 2H), 7.49–7.44 (m, 1H), 7.40 (d, *J* = 8.5 Hz, 2H), 6.37 (s, 1H), 4.76

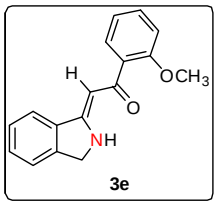
(s, 2H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 187.6, 163.3, 141.7, 138.8, 136.7, 135.3, 130.9, 128.5, 128.4, 127.8, 122.9, 122.0, 83.7, 51.7 ppm; **HRMS** (*m/z*) (APCI): calcd for $C_{16}H_{13}ClNO$ 270.0686 [M+H$^+$]; found 270.0686.



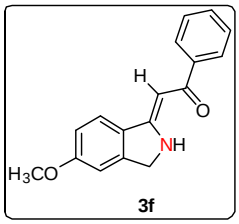
(*Z*)-1-(4-bromophenyl)-2-(isoindolin-1-ylidene)ethanone (3c)
Colorless liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.57 (s, 1H), 7.87–7.83 (m, 2H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.57–7.50 (m, 4H), 7.47–7.43 (m, 1H), 6.36 (s, 1H), 4.73 (s, 2H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 187.6, 163.3, 141.6, 139.2, 135.2, 131.3, 130.9, 128.7, 127.8, 125.2, 122.9, 121.9, 83.7, 51.7 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{16}H_{13}BrNO$ 314.0181, 316.0160 [M+H$^+$]; found 314.0176, 316.0156.



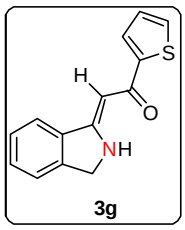
(*Z*)-2-(isoindolin-1-ylidene)-1-(4-methoxyphenyl)ethanone (3d)
Colorless liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.45 (s, 1H), 7.98 (d, *J* = 8.7 Hz, 2H), 7.78 (d, *J* = 7.5 Hz, 1H), 7.49–7.40 (m, 3H), 6.93 (d, *J* = 8.6 Hz, 2H), 6.39 (s, 1H), 4.70 (s, 2H), 3.83 (s, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 188.2, 162.4, 161.6, 141.5, 135.5, 133.0, 130.5, 128.8, 127.6, 122.8, 121.8, 113.3, 83.5, 55.2, 51.5 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{16}NO_2$ 266.1181 [M+H$^+$]; found 266.1179.



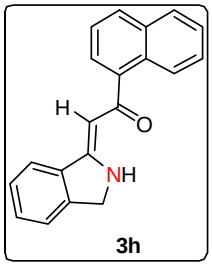
(*Z*)-2-(isoindolin-1-ylidene)-1-(2-methoxyphenyl)ethanone (3e)
Light yellow liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.48 (s, 1H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.69 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.54–7.50 (m, 2H), 7.46–7.43 (m, 1H), 7.39–7.35 (m, 1H), 7.01 (td, *J* = 7.5, 0.9 Hz, 1H), 6.97 (d, *J* = 8.3 Hz, 1H), 6.36 (s, 1H), 4.76 (s, 2H), 3.90 (s, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 189.9, 162.3, 157.1, 141.7, 135.6, 131.4, 130.9, 130.7, 129.6, 127.7, 122.8, 122.1, 120.5, 111.4, 88.9, 55.7, 51.7 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{16}NO_2$ 266.1181 [M+H$^+$]; found 266.1180.



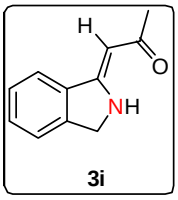
(*Z*)-2-(5-methoxyisoindolin-1-ylidene)-1-phenylethanone (3f) Light yellow liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.47 (s, 1H), 7.98 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.67–7.62 (m, 1H), 7.46–7.39 (m, 3H), 6.98–6.90 (m, 2H), 6.30 (s, 1H), 4.63 (s, 2H), 3.80 (s, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 188.46, 163.00, 162.11, 143.95, 140.45, 130.37, 128.03, 127.86, 126.87, 123.04, 114.61, 107.27, 83.29, 55.42, 51.44 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{17}H_{16}NO_2$ 266.1181 [M+H$^+$]; found 266.1179.



(*Z*)-2-(isoindolin-1-ylidene)-1-(thiophen-2-yl)ethanone (3g) Light yellow liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.30 (s, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.68 (dd, *J* = 3.7, 1.0 Hz, 1H), 7.54 (d, *J* = 4.0 Hz, 2H), 7.51–7.43 (m, 2H), 7.11 (dd, *J* = 4.9, 3.7 Hz, 1H), 6.30 (s, 1H), 4.77 (s, 2H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 182.0, 162.7, 147.3, 141.7, 135.3, 130.9, 129.9, 127.8, 127.7, 127.6, 122.9, 122.1, 83.8, 51.8 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{14}H_{12}NOS$ 242.0640 [M+H$^+$]; found 242.0632.



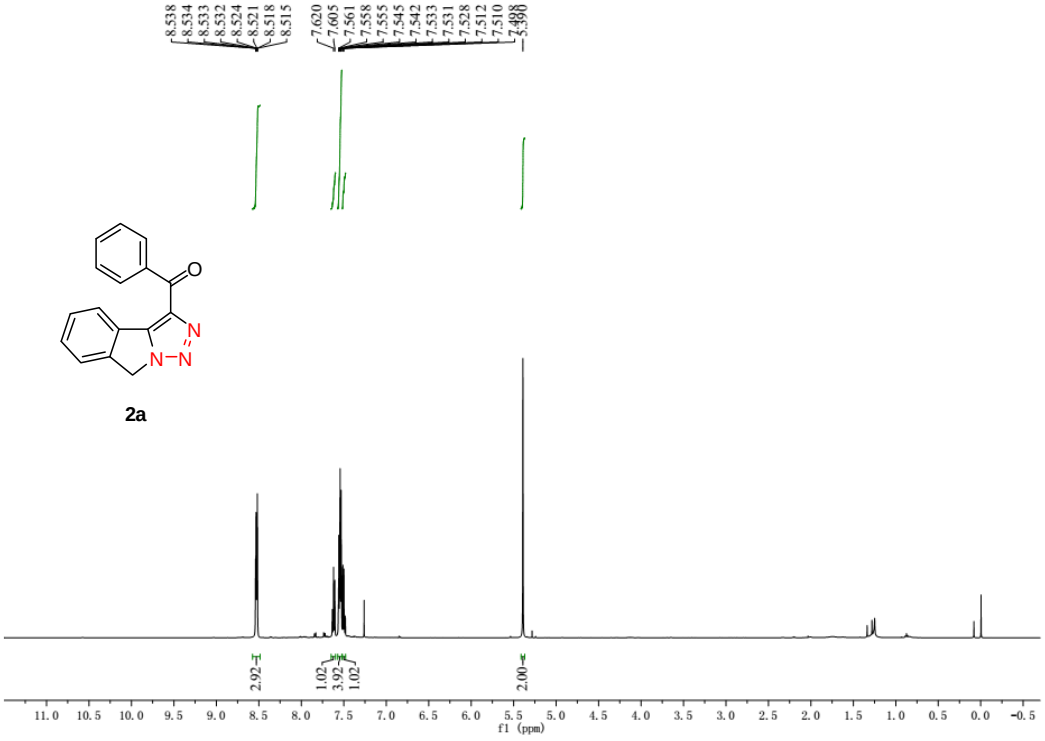
(*Z*)-2-(isoindolin-1-ylidene)-1-(naphthalen-1-yl)ethanone (3h) Light yellow liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.65 (s, 1H), 8.54 (dd, *J* = 10.0, 8.4 Hz, 1H), 7.89 (dd, *J* = 9.9, 5.1 Hz, 2H), 7.77 (d, *J* = 7.0 Hz, 1H), 7.72 (d, *J* = 7.7 Hz, 1H), 7.56–7.48 (m, 5H), 7.46–7.41 (m, 1H), 6.24 (s, 1H), 4.80 (s, 2H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ 193.3, 162.6, 141.7, 140.6, 135.3, 133.7, 130.9, 130.3, 129.6, 128.1, 127.8, 126.4, 126.1, 125.8, 125.1, 124.9, 122.9, 122.1, 88.9, 51.7 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{20}H_{16}NO$ 286.1232 [M+H$^+$]; found 286.1225.

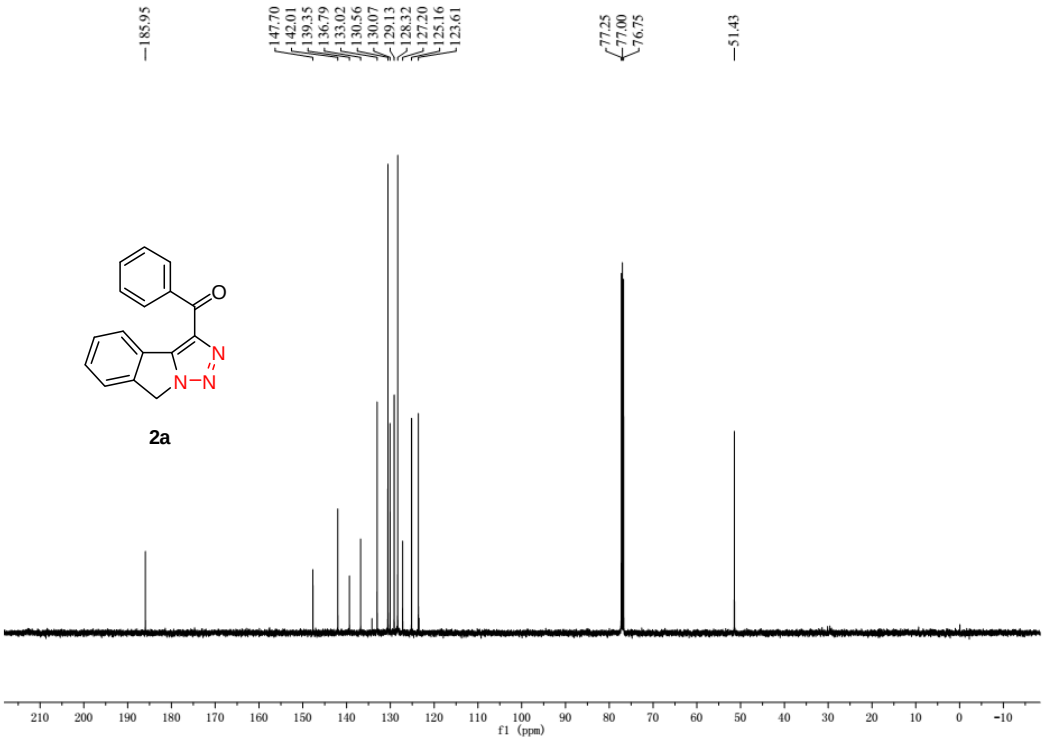


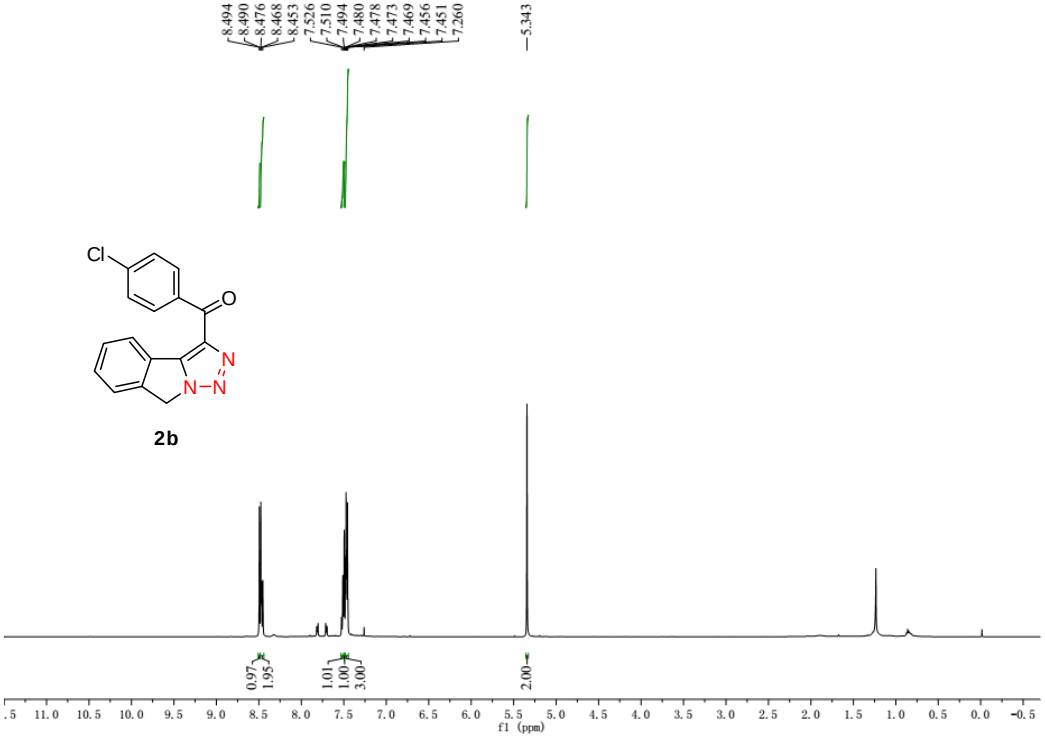
(*Z*)-1-(isoindolin-1-ylidene)propan-2-one (3i) Colorless liquid, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 10.08 (s, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 6.2 Hz, 2H), 7.41 (dt, *J* = 7.9, 4.1 Hz, 1H), 5.73 (s, 1H), 4.67 (s, 2H), 2.17 (s, 3H) ppm; **^{13}C NMR** (100 MHz, $CDCl_3$): δ

196.20, 161.28, 141.63, 135.19, 130.60, 127.65, 122.79, 121.82, 87.25, 77.32, 77.00, 76.68, 51.47, 29.08 ppm; **HRMS** (*m/z*) (ESI): calcd for $C_{11}H_{12}NO$ 174.0919 [$M+H^+$]; found 174.0913.

Copies of ^{1}H NMR and ^{13}C NMR Spectra of all compounds



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8.468
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7.526
7.510
7.494
7.480
7.478
7.473
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7.456
7.451
7.260
5.343
Cl
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N
N–N
2b
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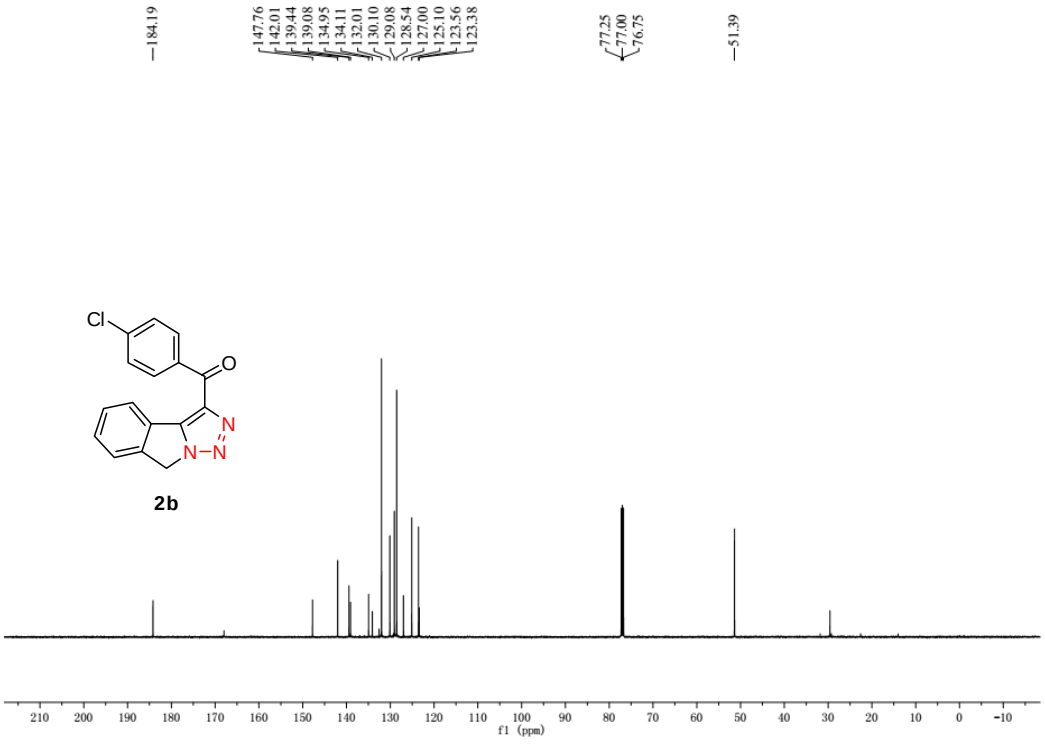
1.01
1.00
3.00
2.00
f1 (ppm)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132.01
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129.08
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127.00
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77.00
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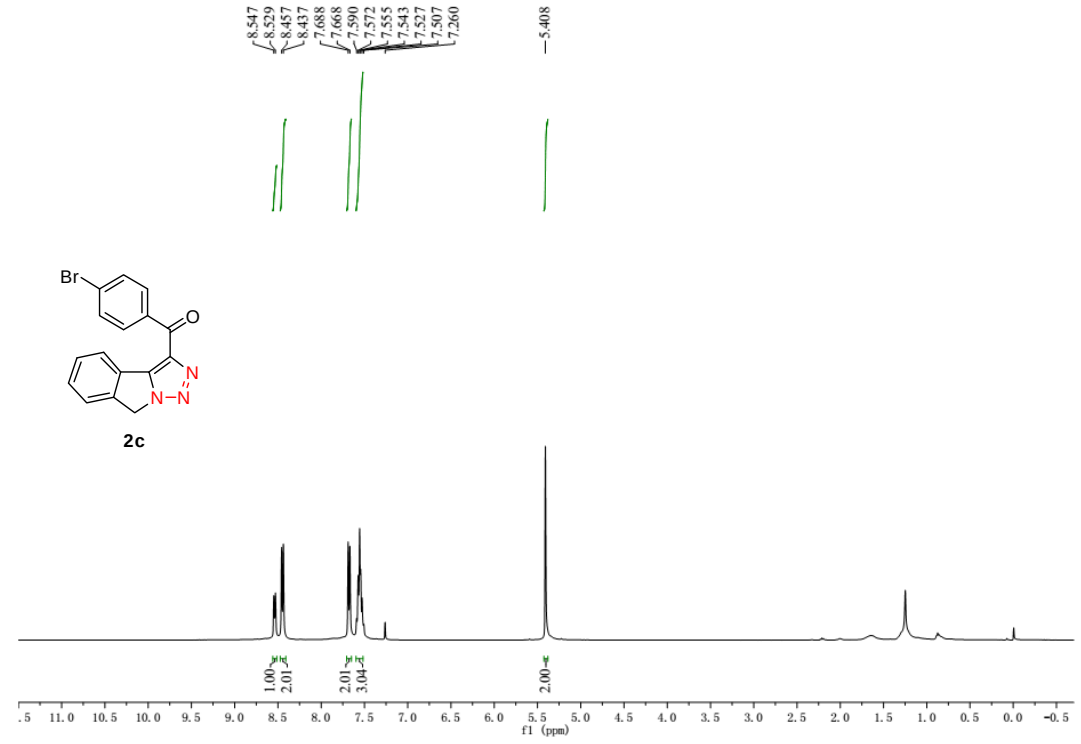
51.39
Cl
O
N
N–N
2b
f1 (ppm)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8.437
7.688
7.668
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7.572
7.555
7.543
7.527
7.507
7.260
5.408
Br
O
N
N–N
2c
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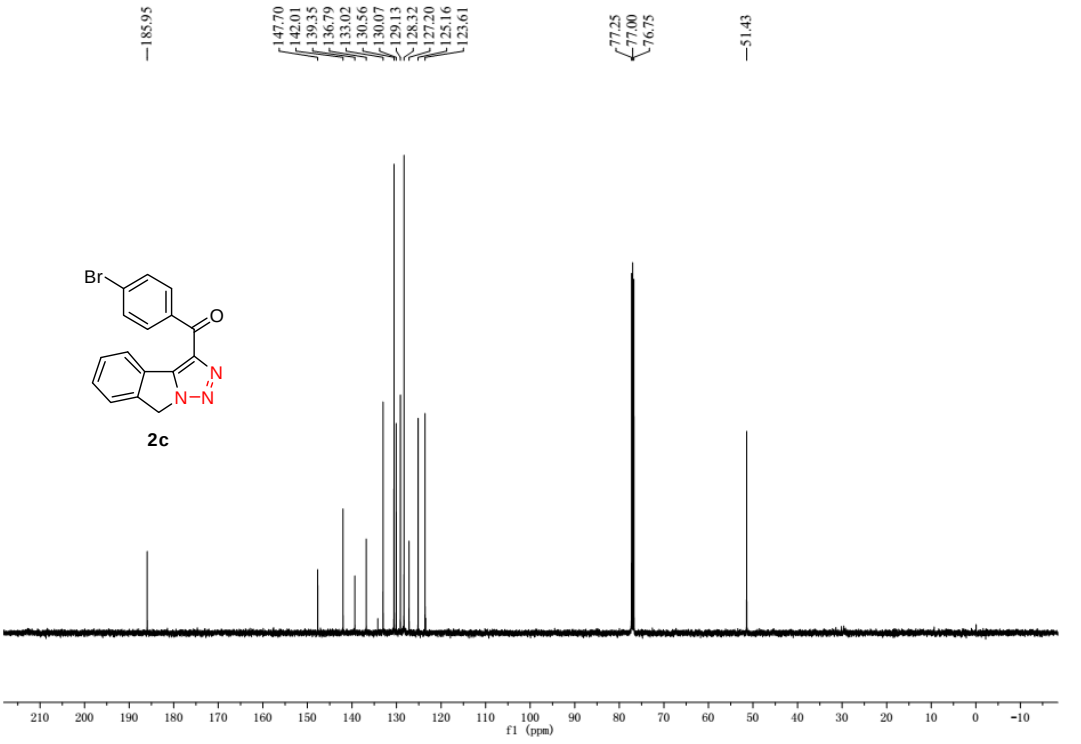
2.01
2.01
3.04
2.00
f1 (ppm)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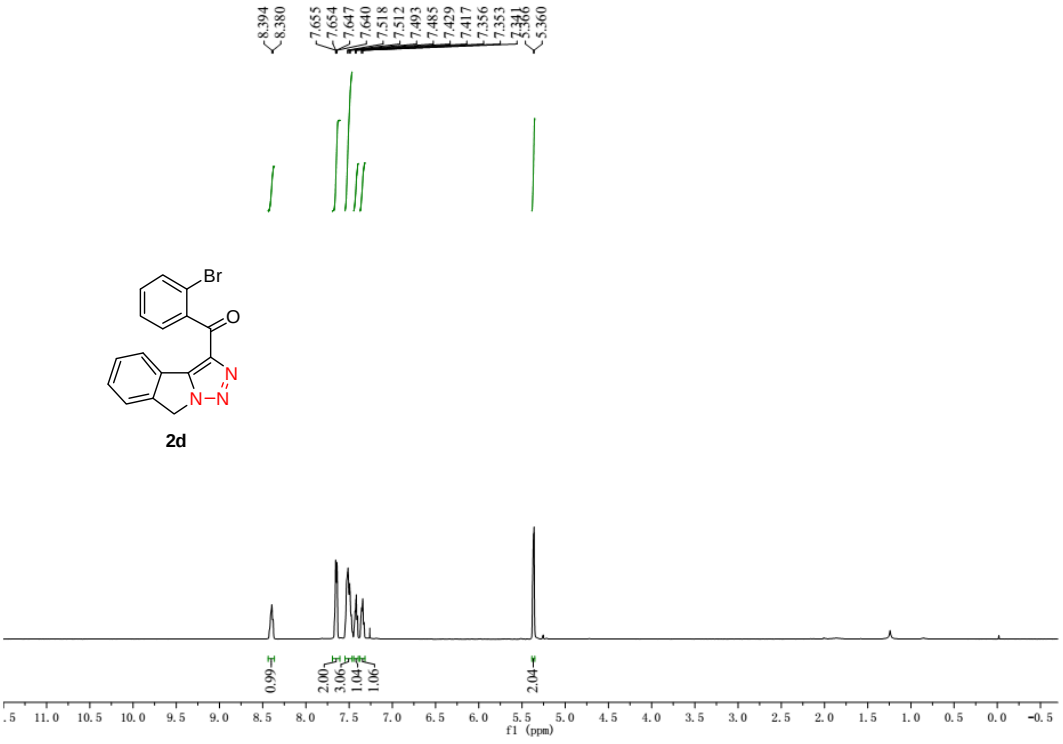
139.35
136.79
133.02
130.56
130.07
129.13
128.32
127.20
125.16
123.61
77.25
77.00
76.75
51.43
Br
O
N
N–N
2c
f1 (ppm)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7.647
7.640
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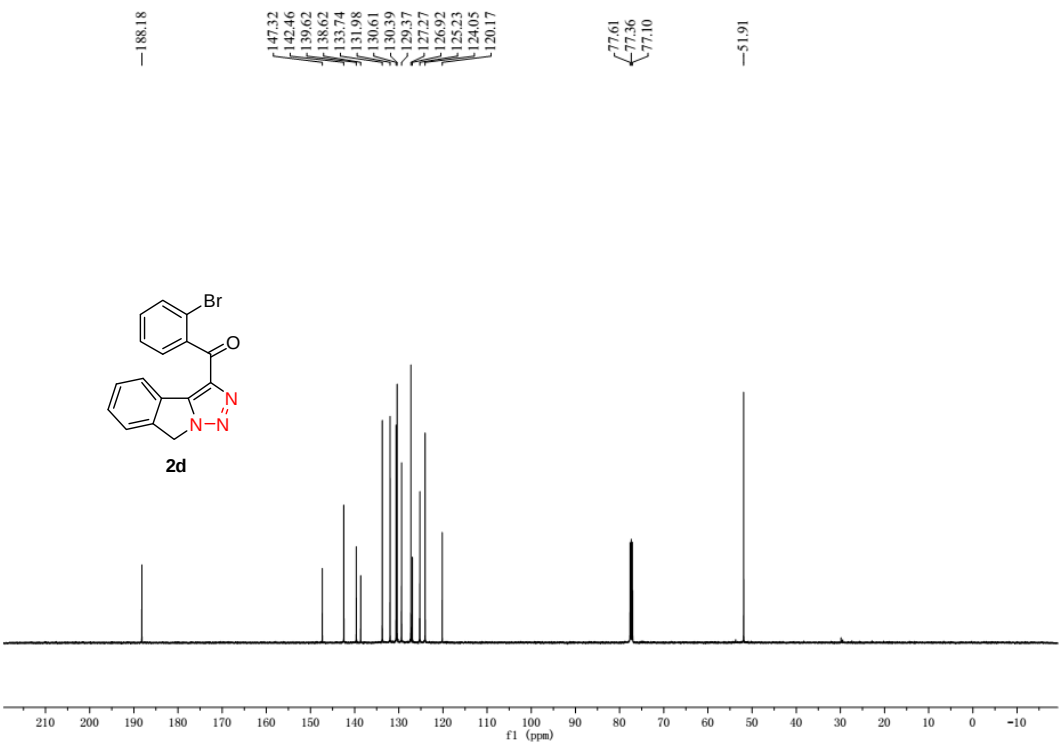
7.512
7.493
7.485
7.429
7.417
7.356
7.353
5.360
Br
O
N
N–N
0.99
2.00
3.06
1.04
1.06
2.04
f1 (ppm)

2d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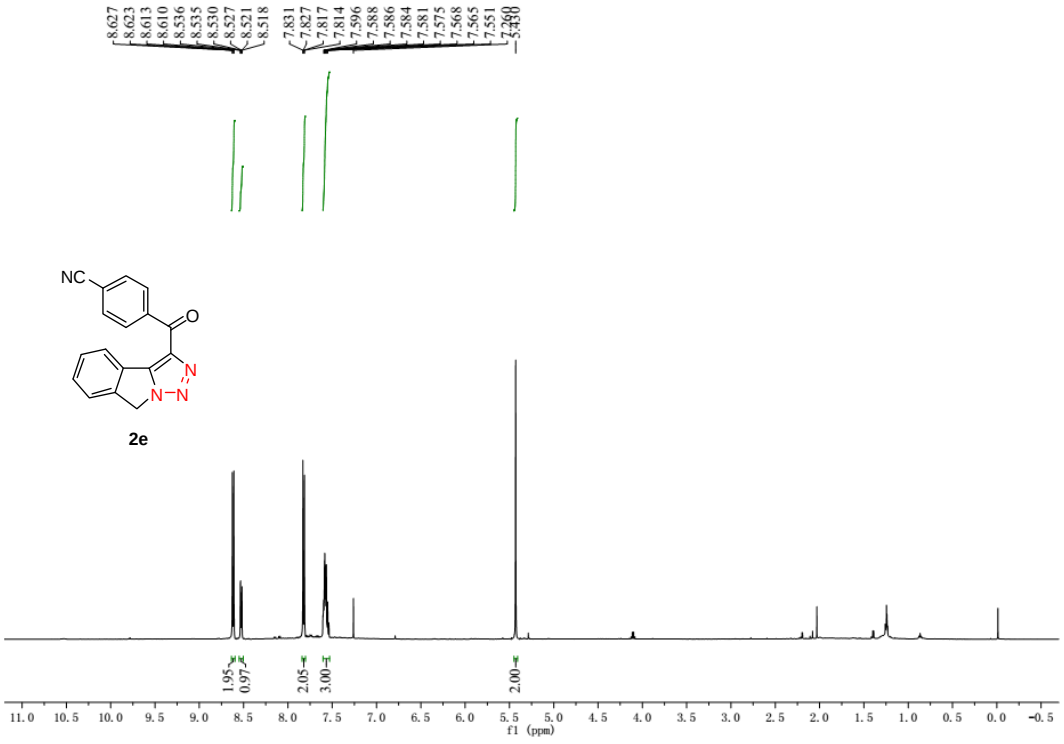
120.17
77.61
77.36
77.10
51.91
Br
O
N
N–N
f1 (ppm)

2d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8.535
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8.527
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8.518
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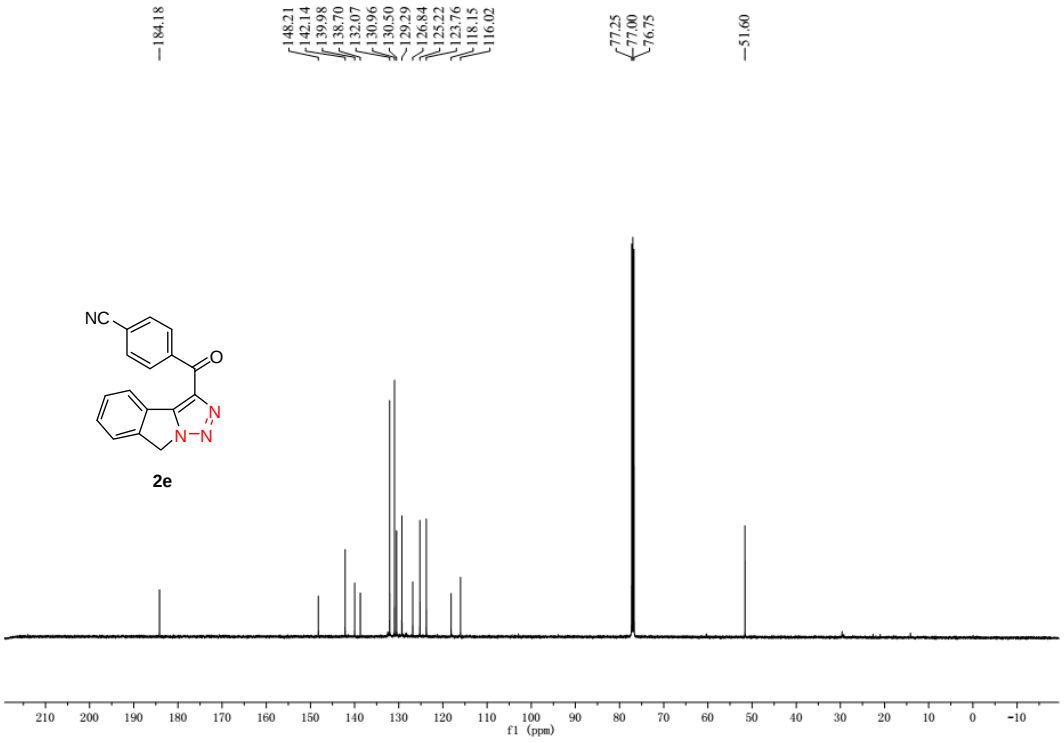
7.814
7.596
7.588
7.586
7.584
7.581
7.575
7.568
7.565
7.551
7.250
7.250
NC
O
N
N–N
2e
1.95
0.97
2.05
3.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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148.21
142.14
139.98
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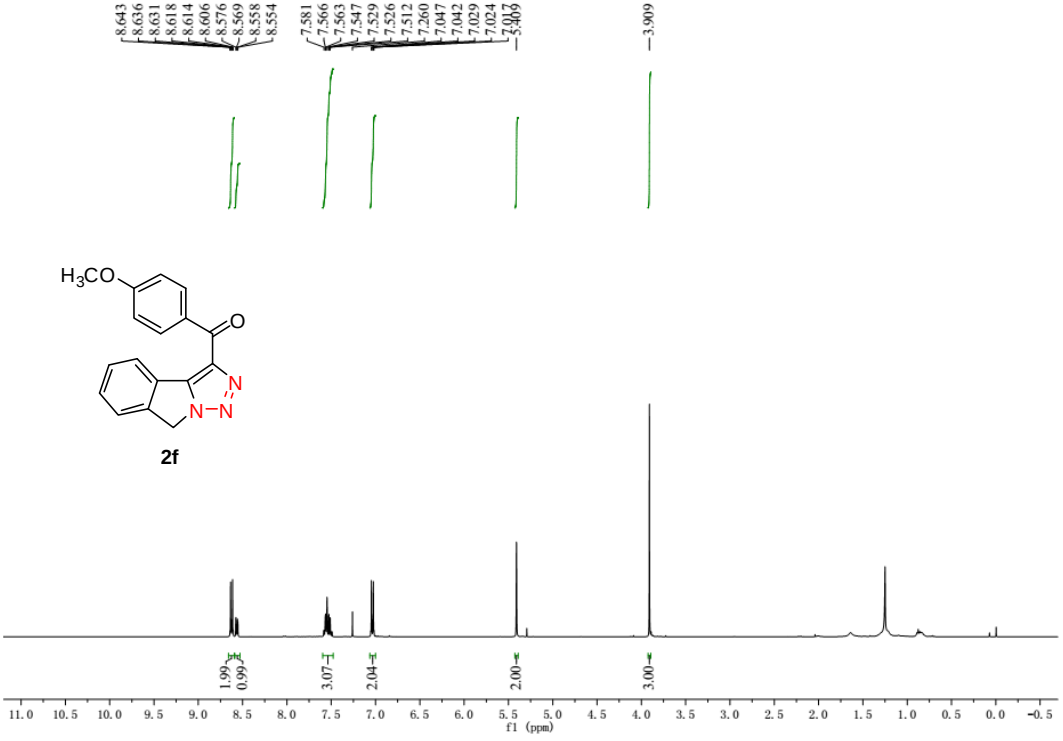
132.07
130.96
130.50
129.29
126.84
125.22
123.76
118.15
116.02
77.25
77.00
76.75
51.60
NC
O
N
N–N
2e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.554
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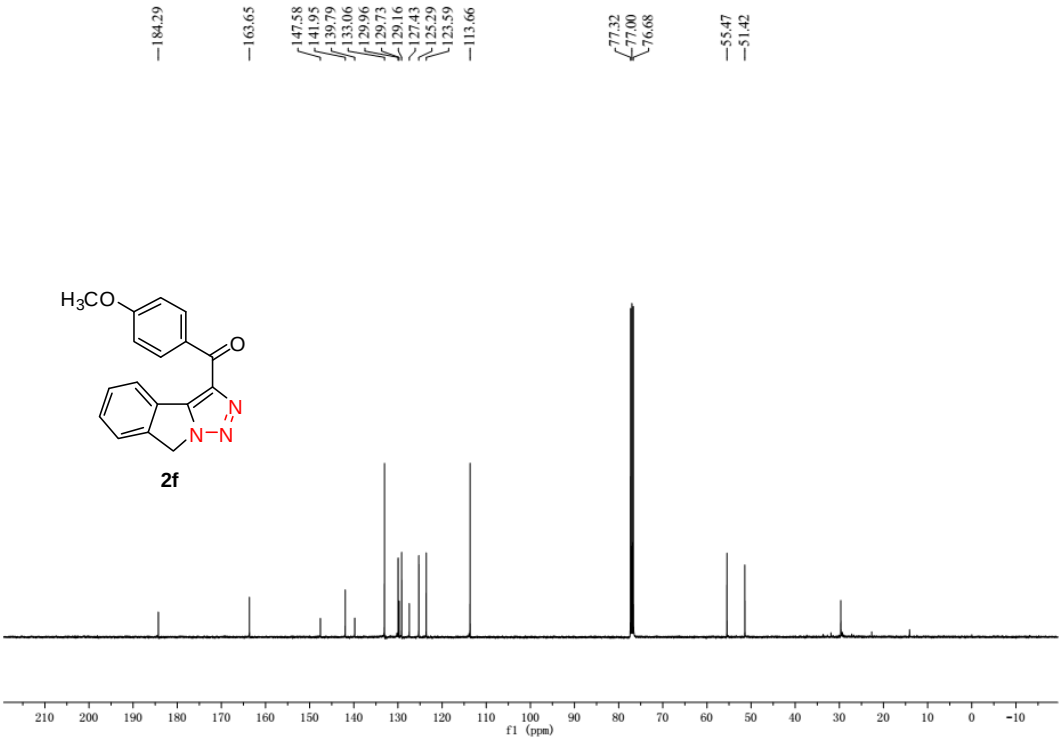
7.563
7.547
7.529
7.526
7.512
7.260
7.047
7.042
7.029
7.024
7.017
7.009
3.909
H3CO
O
N
N–N
2f
1.99
0.99
3.07
2.04
2.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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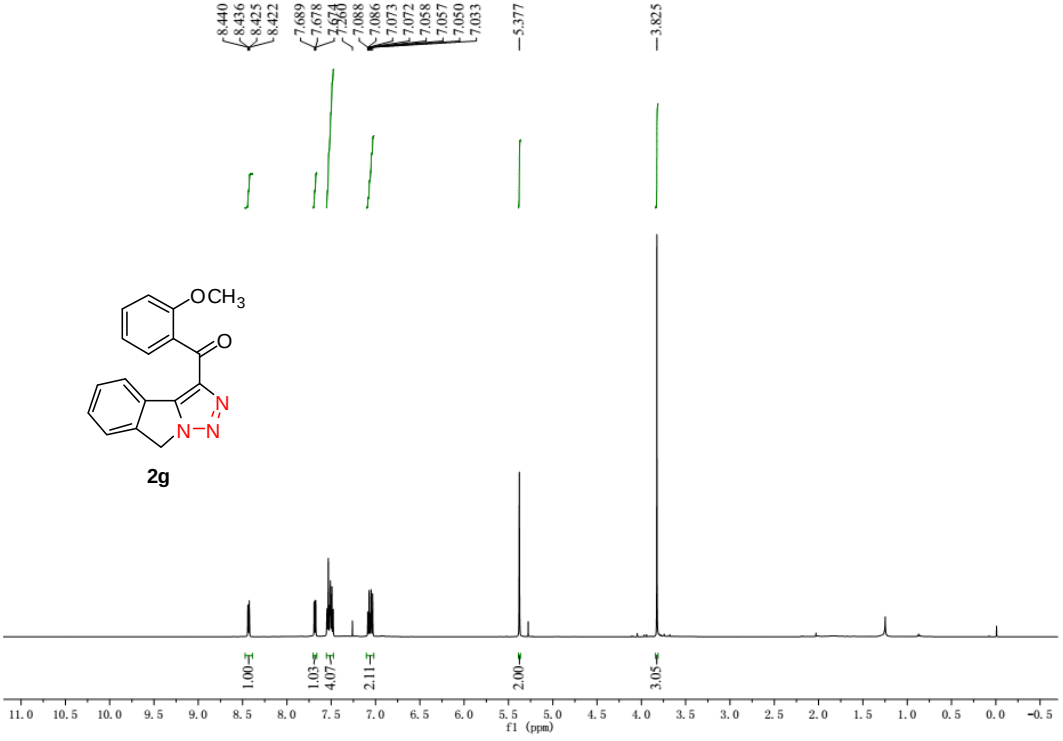
147.58
141.95
139.79
133.06
129.96
129.73
129.16
127.43
125.29
123.59
113.66
77.32
77.00
76.68
55.47
51.42
H3CO
O
N
N–N
2f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.086
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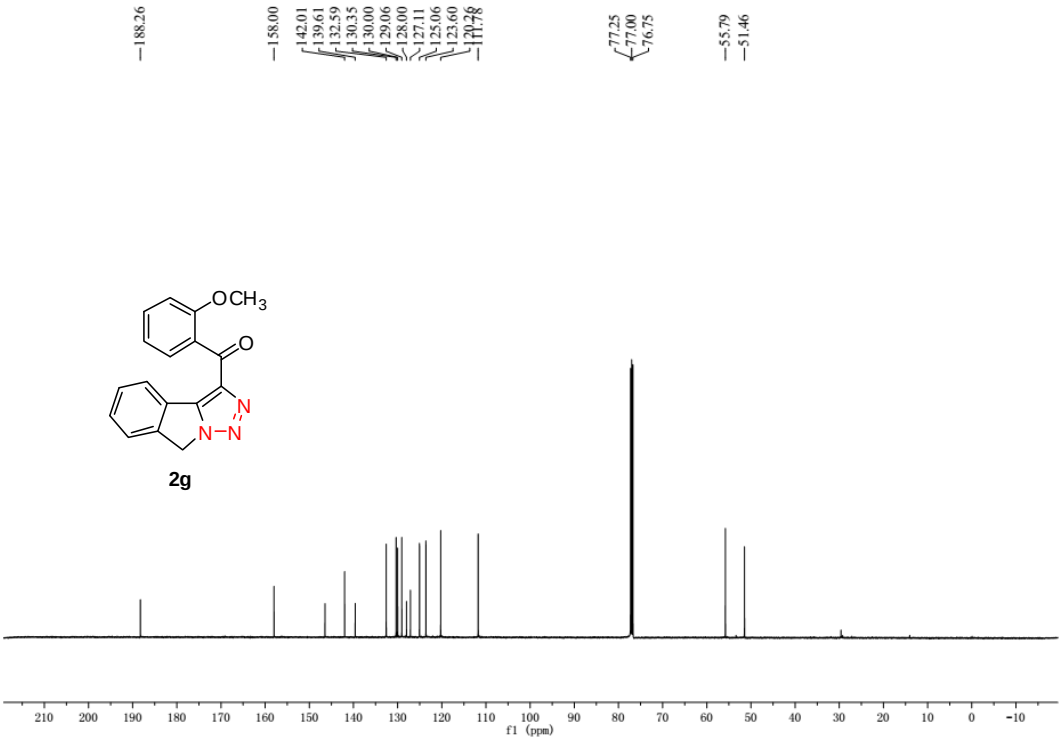
7.058
7.057
7.050
7.033
5.377
3.825
OCH3
O
N
N–N
2g
1.00
1.03
4.07
2.11
2.00
3.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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111.78
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77.00
76.75
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N–N
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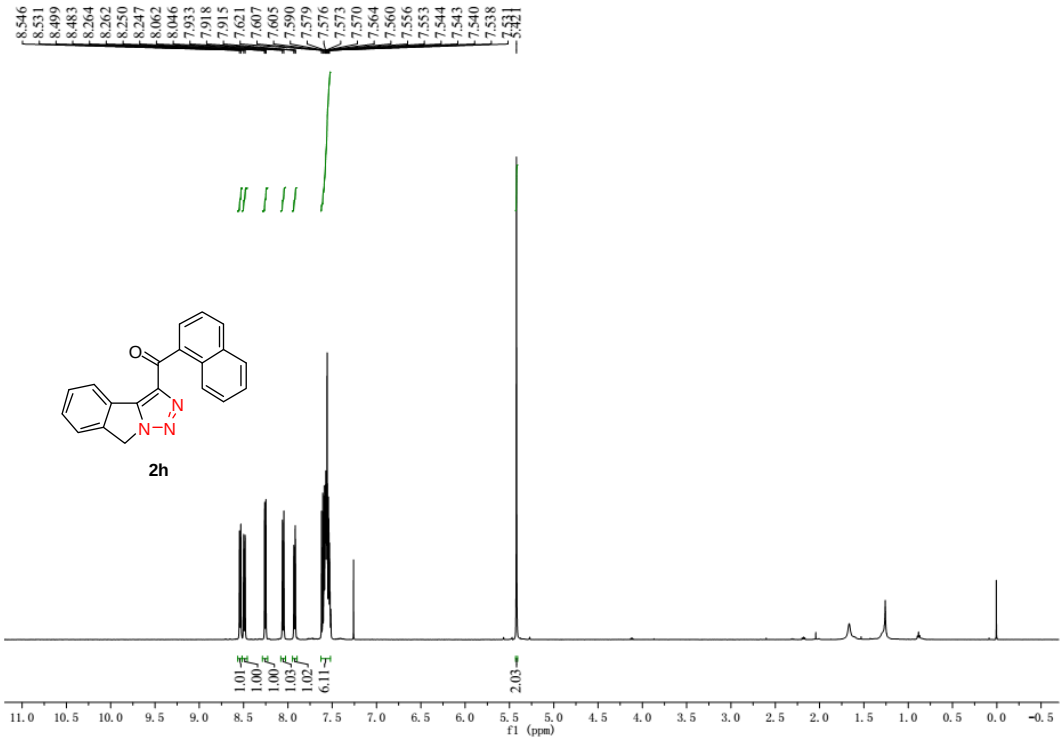
f1 (ppm)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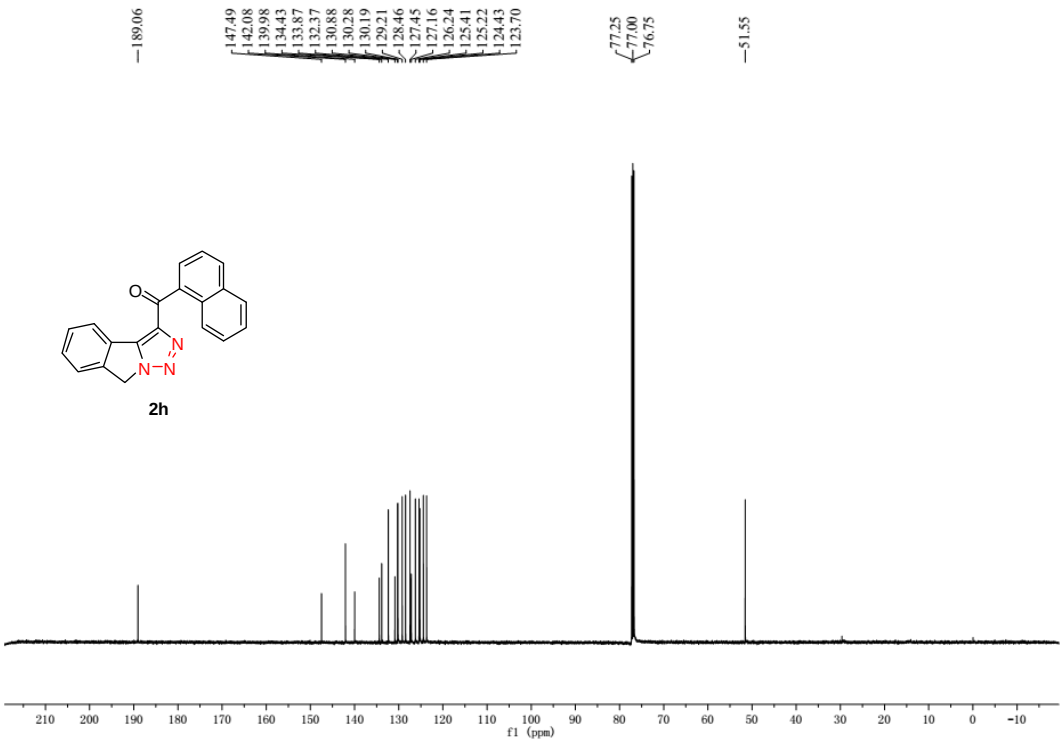
7.576
7.573
7.570
7.564
7.560
7.556
7.553
7.544
7.543
7.540
7.538
5.421
O
N
N–N
2h
1.01
1.00
1.00
1.03
1.02
6.11
2.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


189.06
147.49
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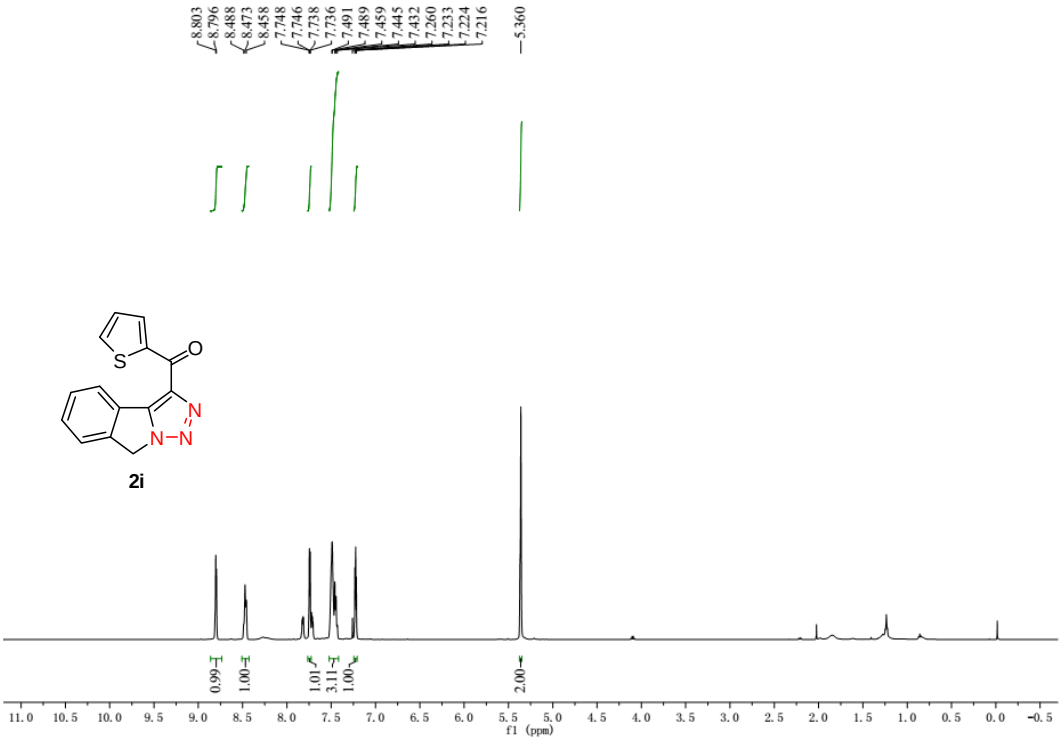
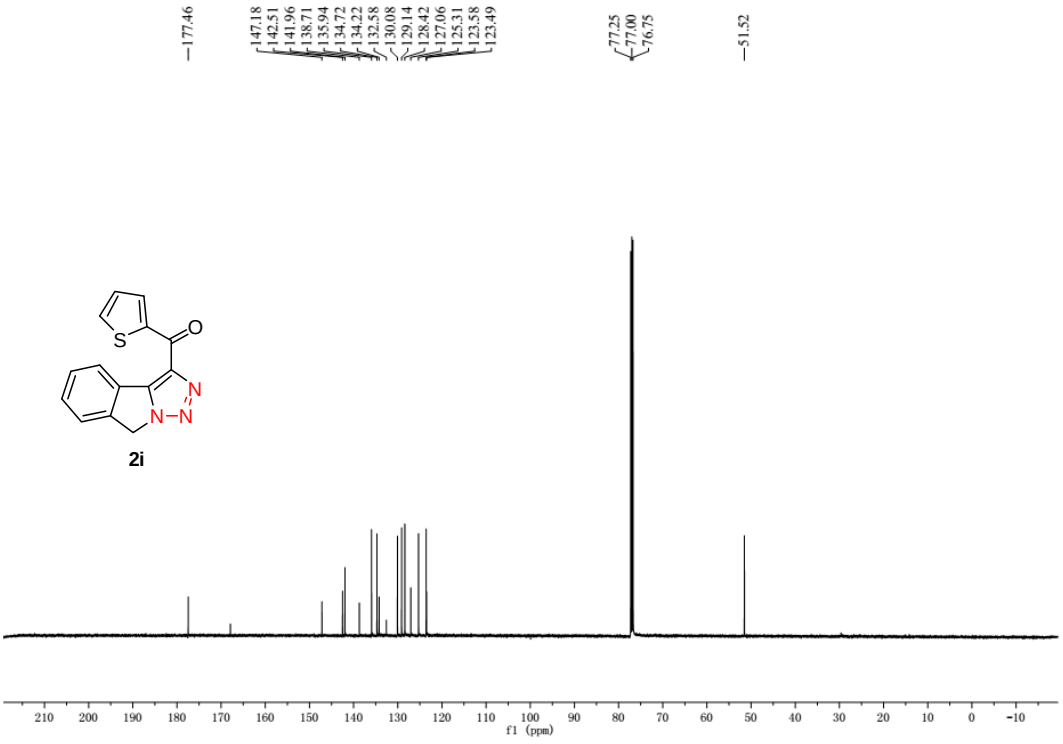
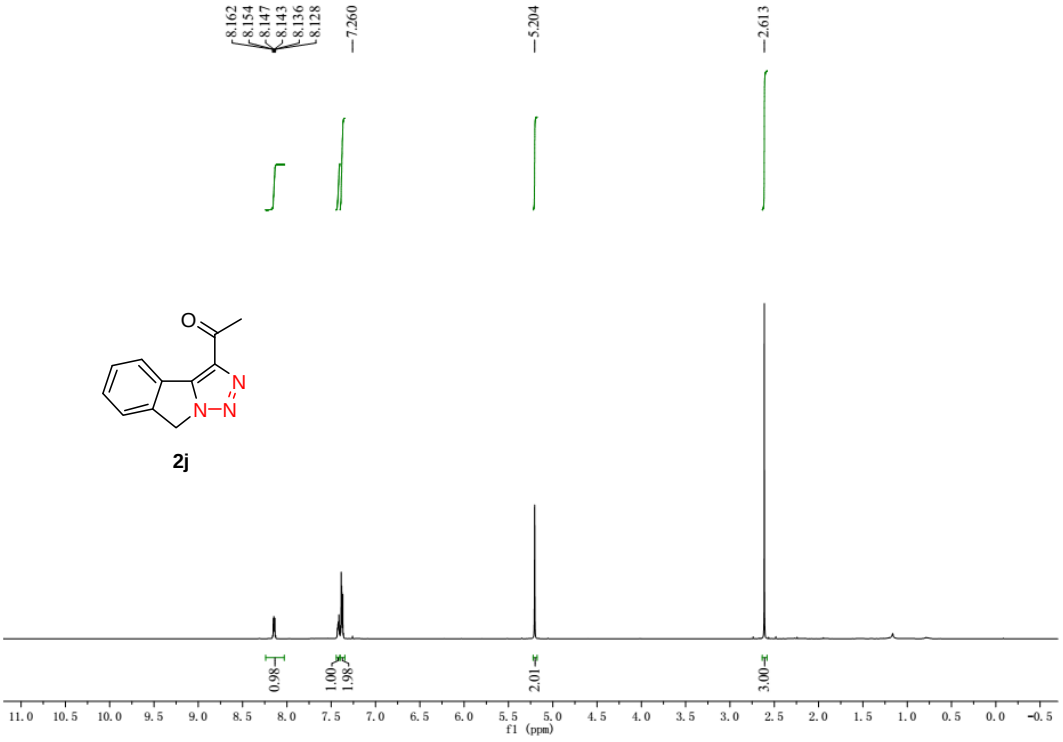
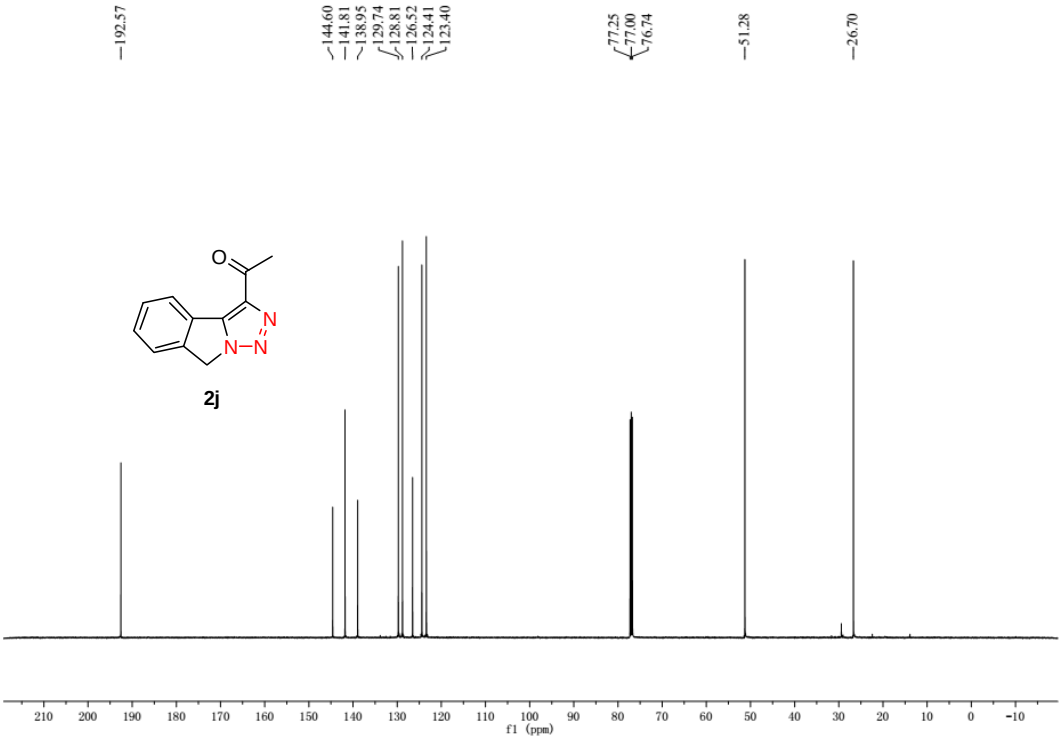
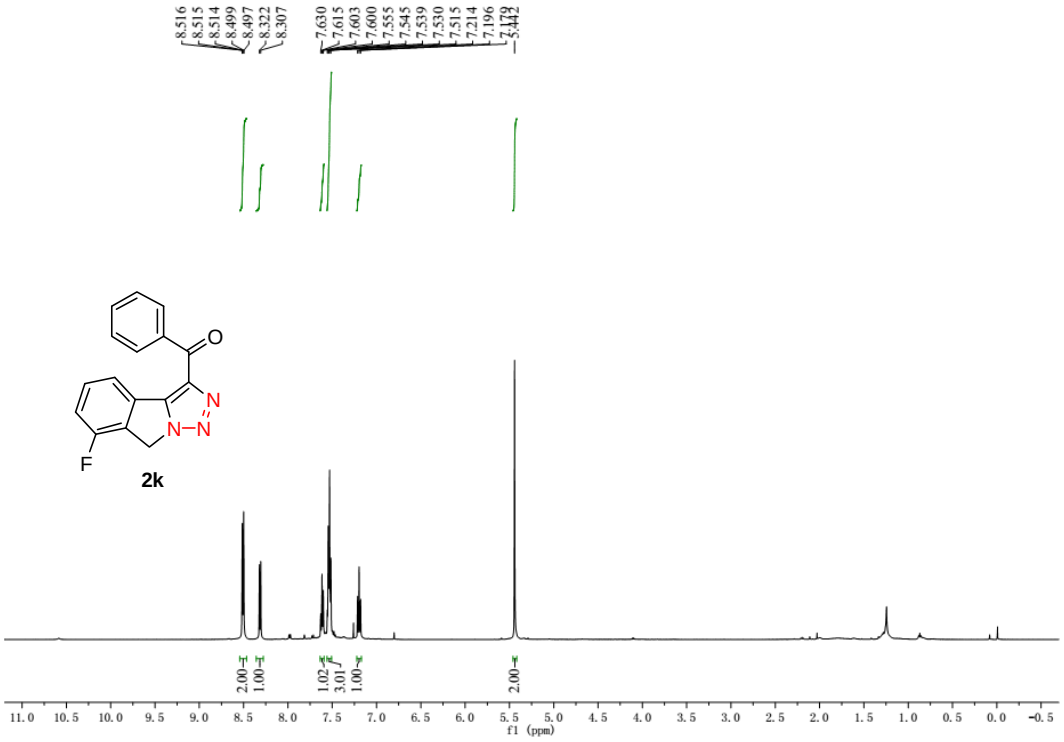
134.43
133.87
132.37
130.88
130.28
130.19
129.21
128.46
127.45
127.16
126.24
125.41
125.22
124.43
123.70
77.25
77.00
76.75
51.55
O
N
N–N
2h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

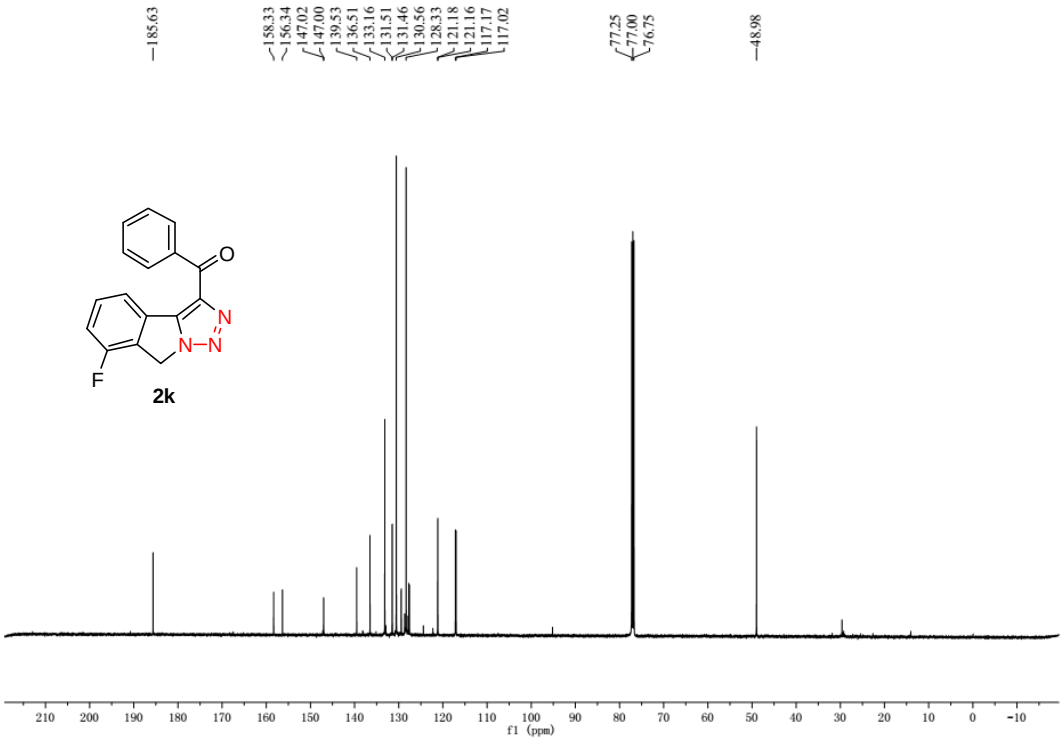

8.803
8.796
8.488
8.473
8.458
7.748
7.746
7.738
7.736
7.491
7.489
7.459
7.445
7.432
7.260
7.233
7.224
7.216
5.360
O
S
N
N–N
2i
0.99
1.00
1.01
3.11
1.00
2.00
f1 (ppm)

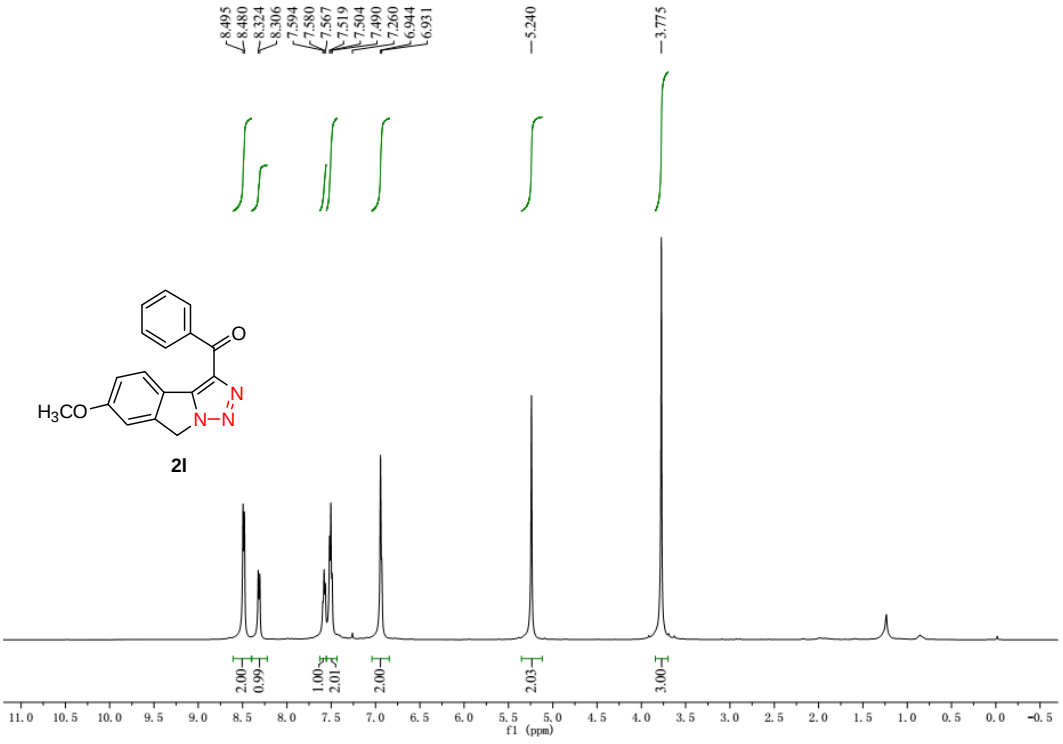

177.46
147.18
142.51
141.96
138.71
135.94
134.72
134.22
132.58
130.08
129.14
128.42
127.06
125.31
123.58
123.49
77.25
77.00
76.75
51.52
O
S
N
N–N
2i
f1 (ppm)


8.162
8.154
8.147
8.143
8.136
8.128
7.260
5.204
2.613
O
N
N–N
2j
0.98
1.00
1.98
2.01
3.00
f1 (ppm)

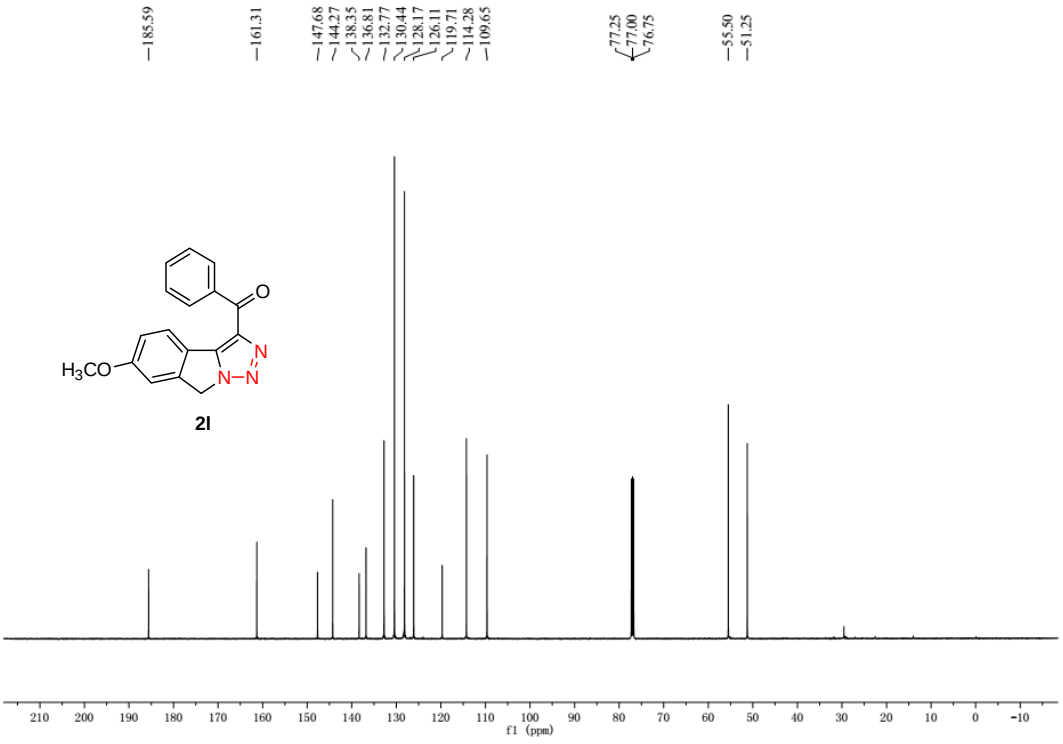

192.57
144.60
141.81
138.95
129.74
128.81
126.52
124.41
123.40
77.25
77.00
76.74
51.28
26.70
O
N
N–N
2j
f1 (ppm)


8.516
8.515
8.514
8.499
8.497
8.322
8.307
7.630
7.615
7.603
7.600
7.555
7.545
7.539
7.530
7.515
7.214
7.196
5.442
O
N
N–N
F
2k
2.00
1.00
1.02
3.01
1.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

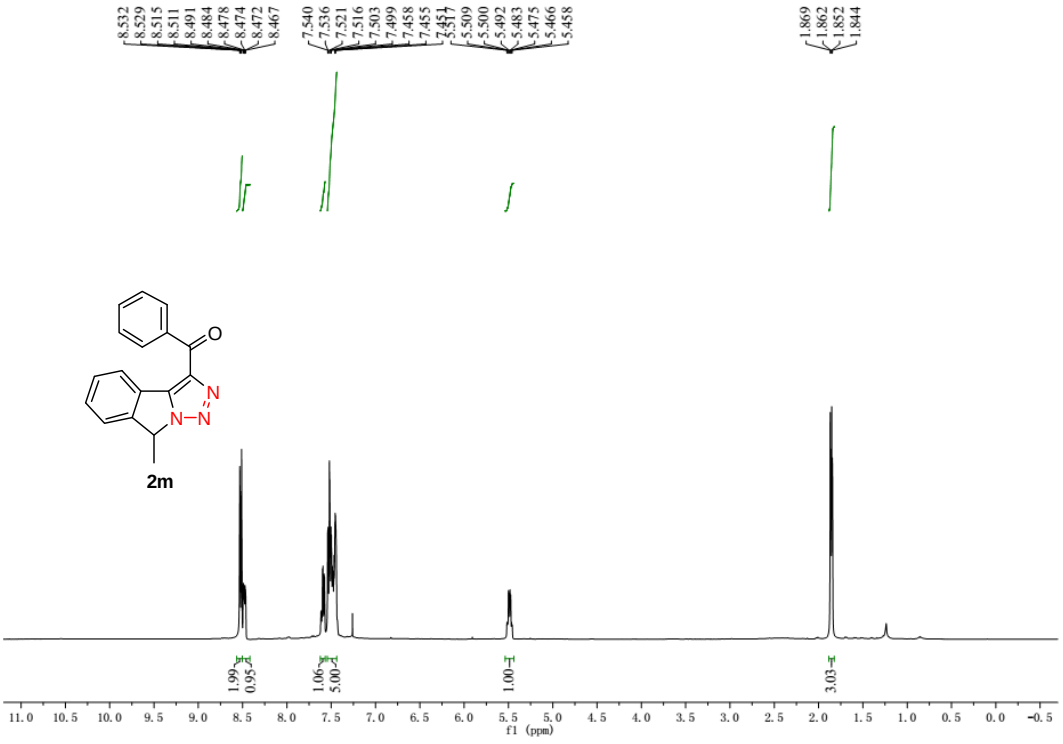

185.63
158.33
156.34
147.02
147.00
139.53
136.51
133.16
131.51
131.46
130.56
128.33
121.18
121.16
117.17
117.02
77.25
77.00
76.75
48.98
O
N
N–N
F
2k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

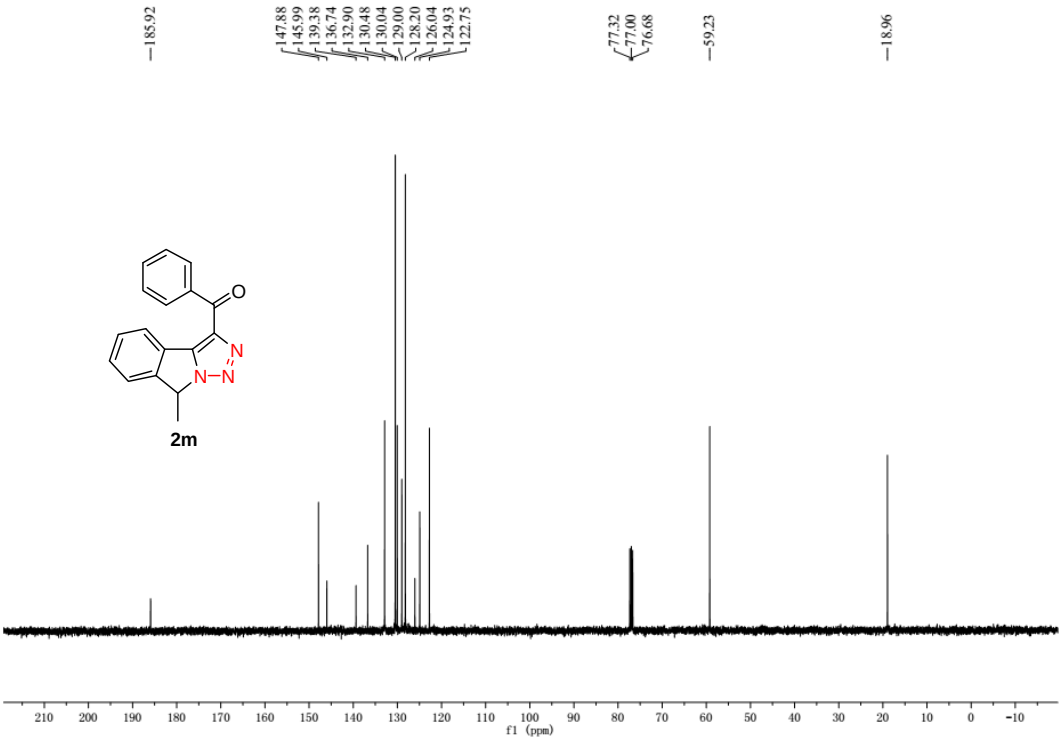

8.495
8.480
8.324
8.306
7.594
7.580
7.567
7.519
7.504
7.490
7.260
6.944
6.931
5.240
3.775
O
N
N–N
H3CO
2.00
0.99
1.00
2.01
2.00
2.03
3.00
f1 (ppm)

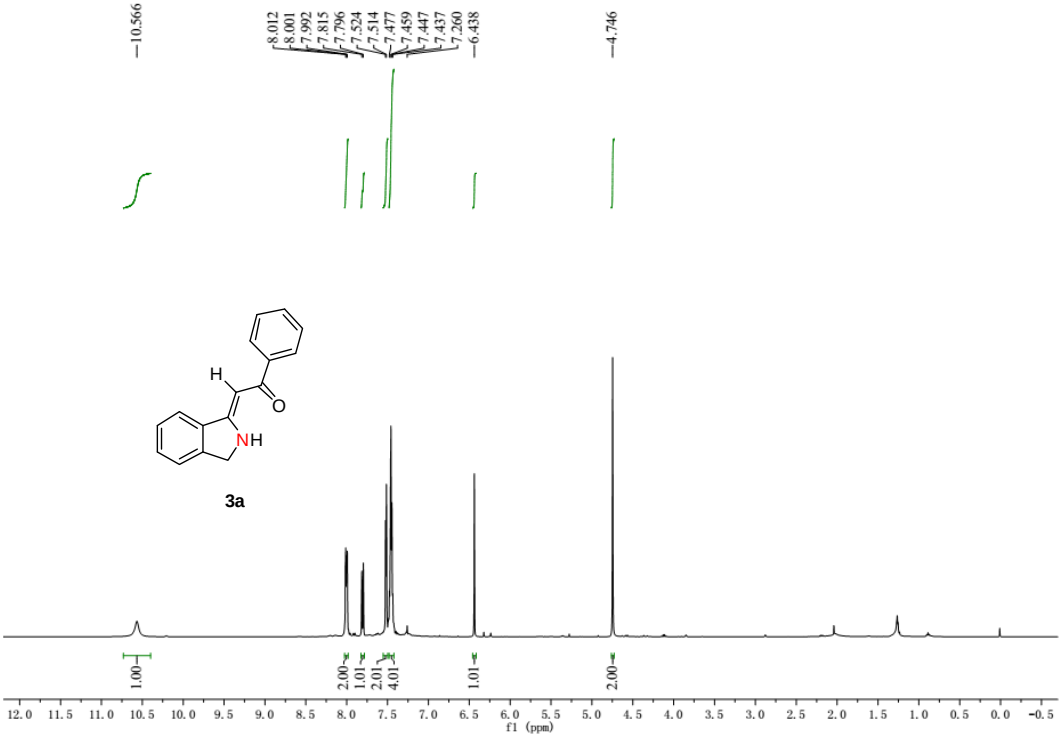
2l

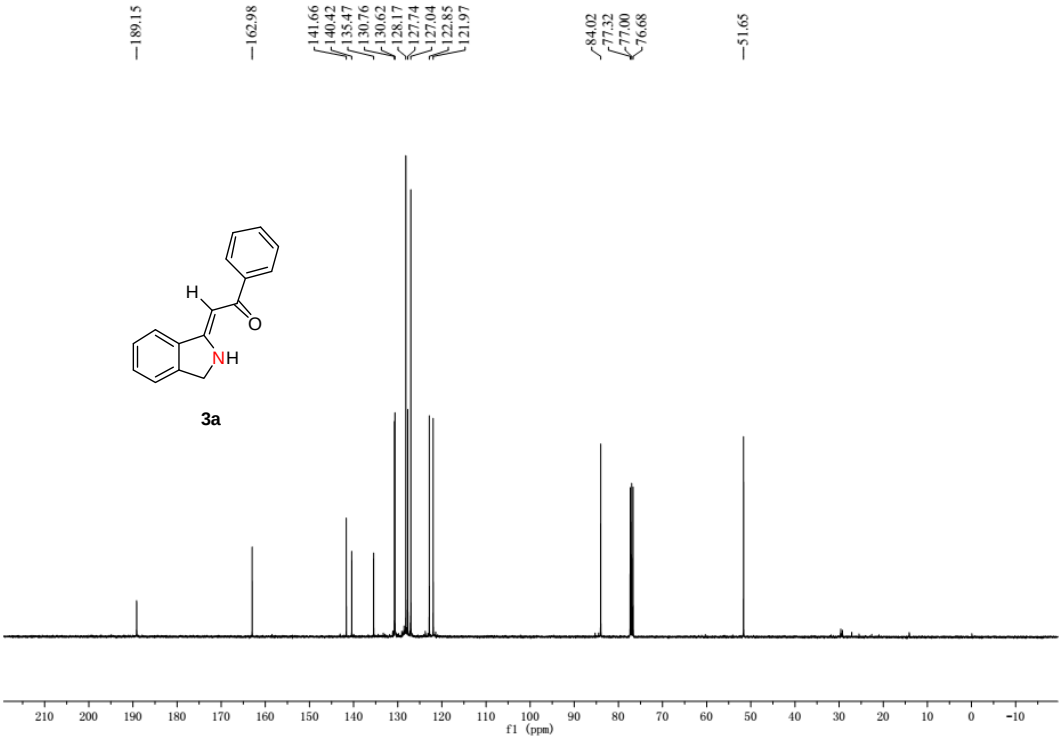

185.59
161.31
147.68
144.27
138.35
136.81
132.77
130.44
128.17
126.11
119.71
114.28
109.65
77.25
77.00
76.75
55.50
51.25
O
N
N–N
H3CO
f1 (ppm)

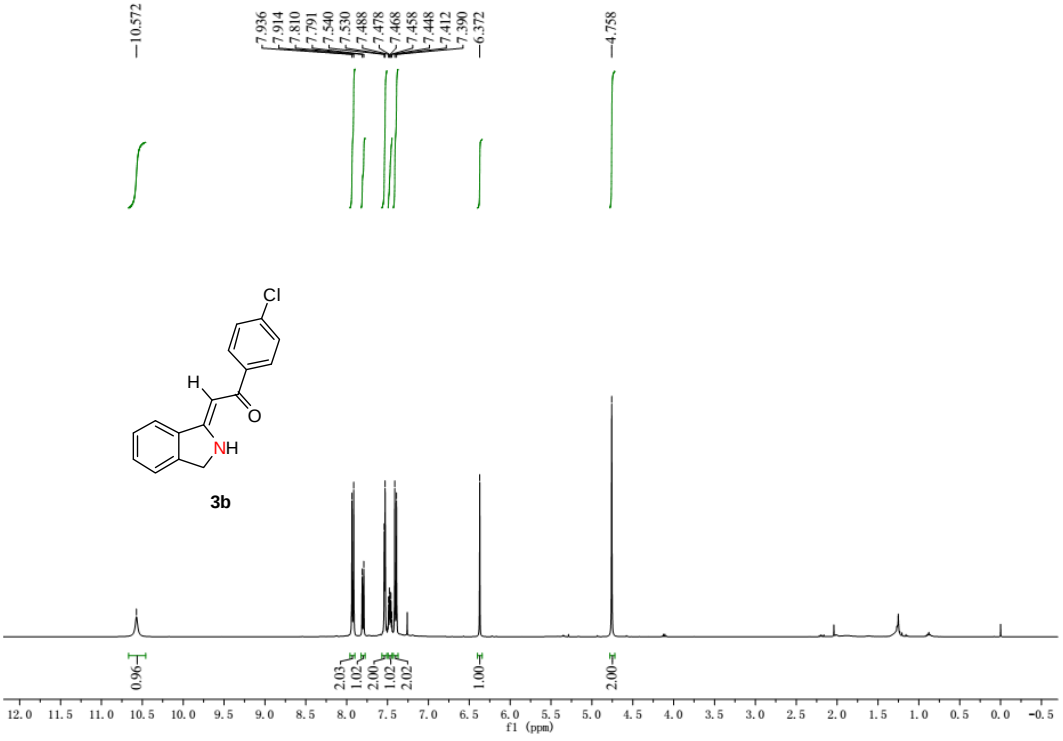
2l

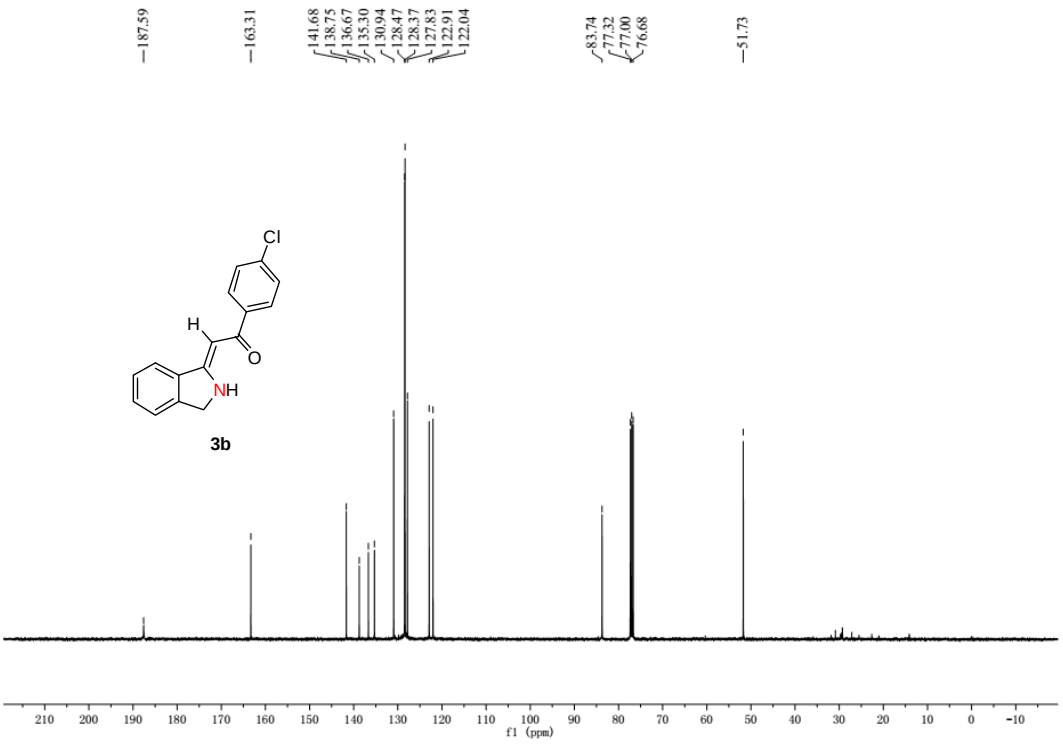

8.532
8.529
8.515
8.511
8.491
8.484
8.478
8.474
8.472
8.467
7.540
7.536
7.521
7.516
7.503
7.499
7.458
7.455
7.451
5.511
5.509
5.500
5.492
5.483
5.475
5.466
5.458
1.869
1.862
1.852
1.844
O
N
N–N
2m
1.99
0.95
1.06
5.00
1.00
3.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

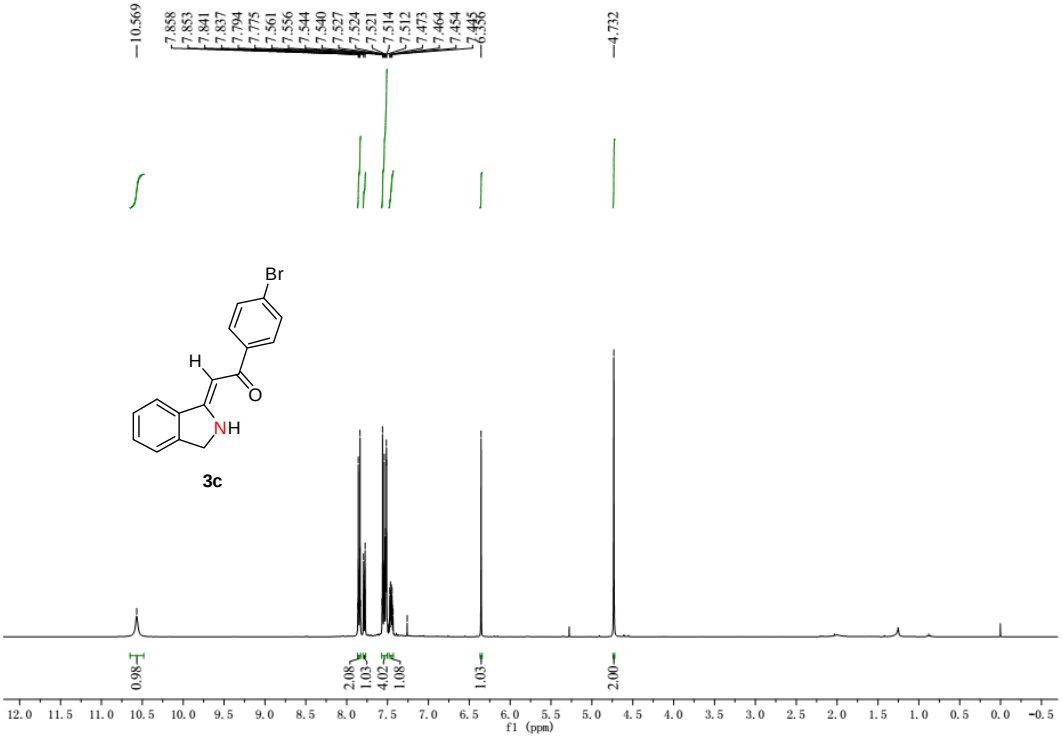

185.92
147.88
145.99
139.38
136.74
132.90
130.48
130.04
129.00
128.20
126.04
124.93
122.75
77.32
77.00
76.68
59.23
18.96
O
N
N–N
2m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

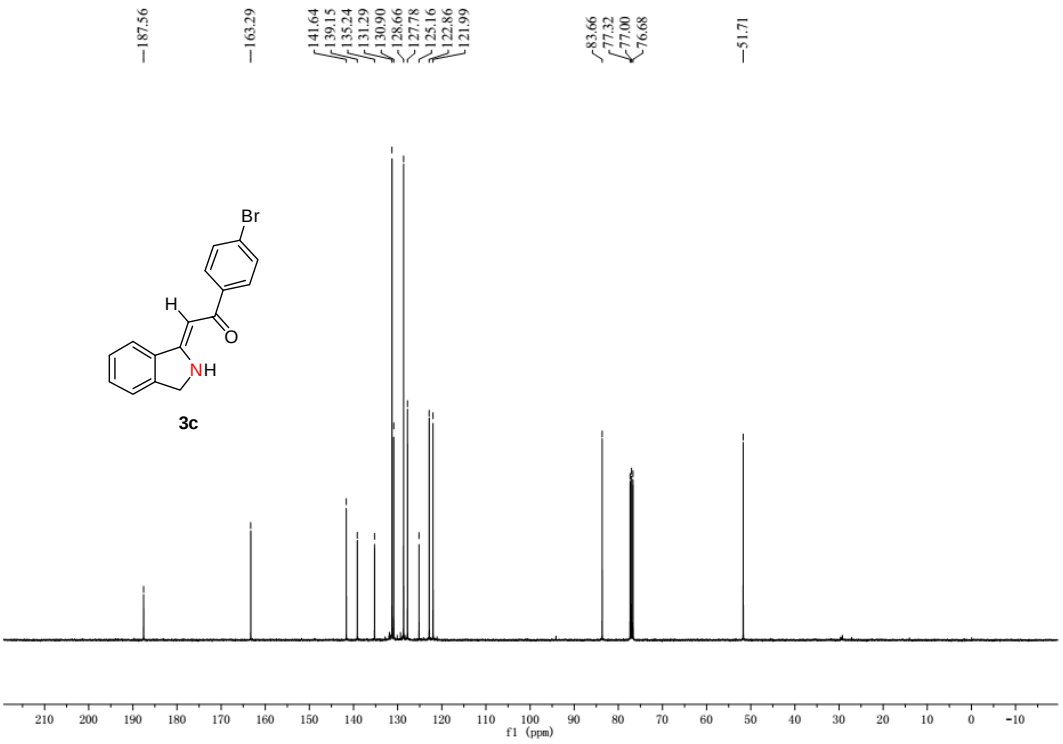

10.566
8.012
8.001
7.992
7.815
7.796
7.524
7.514
7.477
7.459
7.447
7.437
7.260
6.438
4.746
H
O
NH
3a
1.00
2.00
1.01
2.01
4.01
1.01
2.00
f1 (ppm)

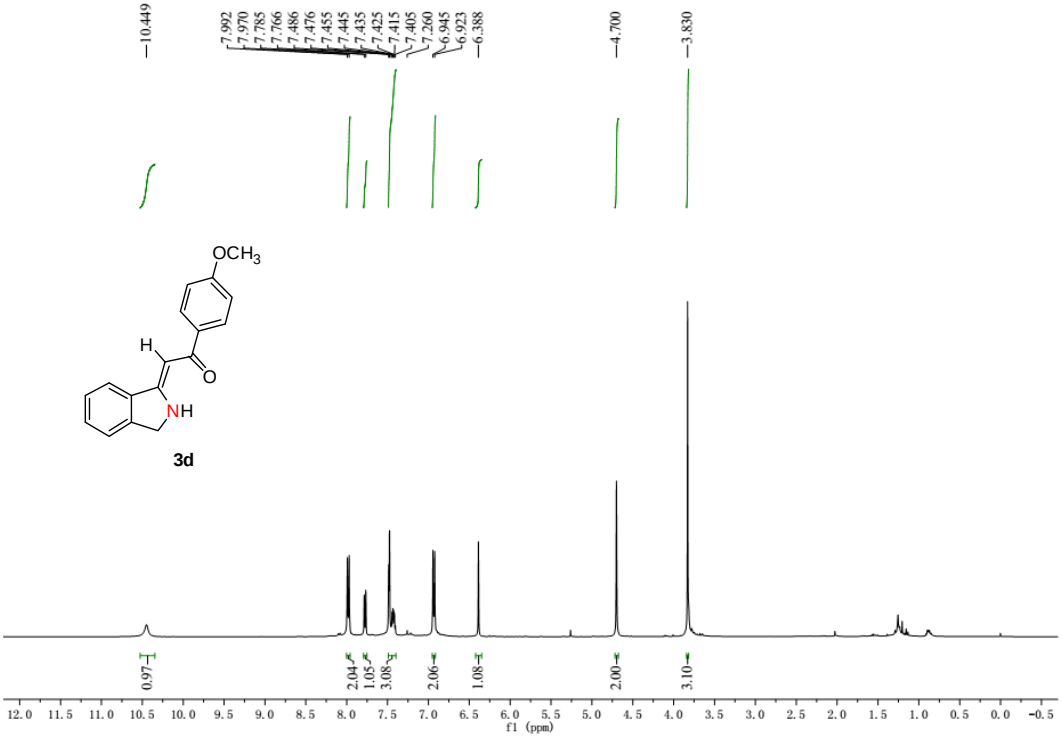

189.15
162.98
141.66
140.42
135.47
130.76
130.62
128.17
127.74
127.04
122.85
121.97
84.02
77.32
77.00
76.68
51.65
H
O
NH
3a
f1 (ppm)

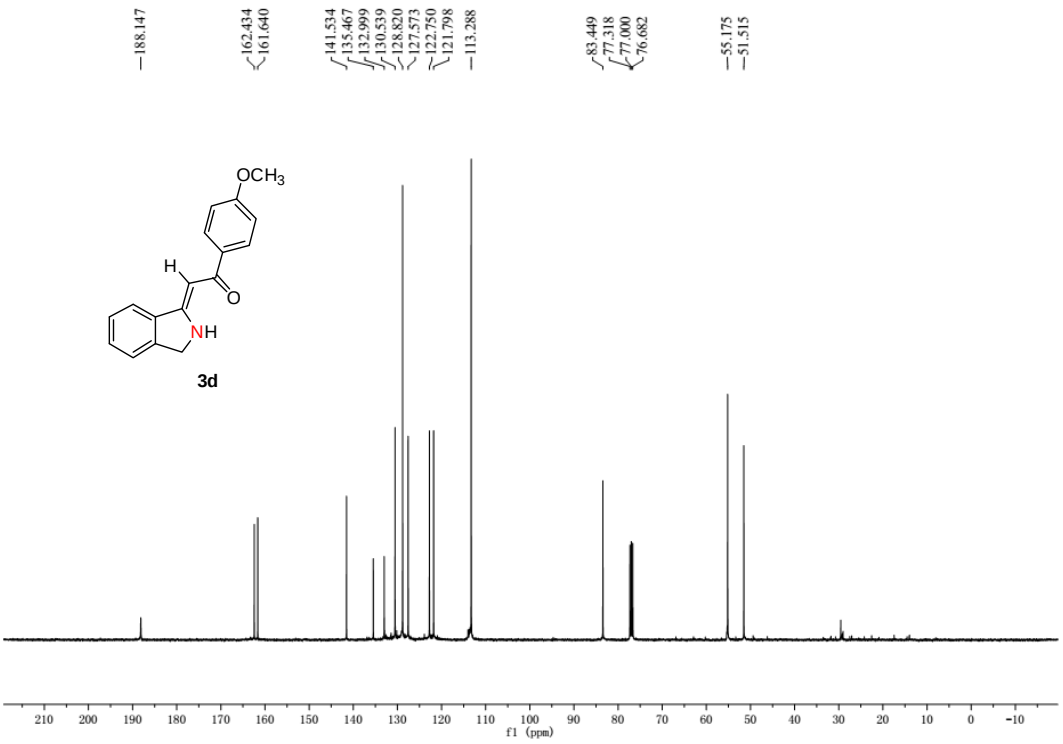

10.572
7.936
7.914
7.810
7.791
7.540
7.530
7.488
7.478
7.468
7.458
7.448
7.412
7.390
6.372
4.758
Cl
H
O
NH
3b
0.96
2.03
1.02
2.00
1.02
2.02
1.00
2.00
f1 (ppm)

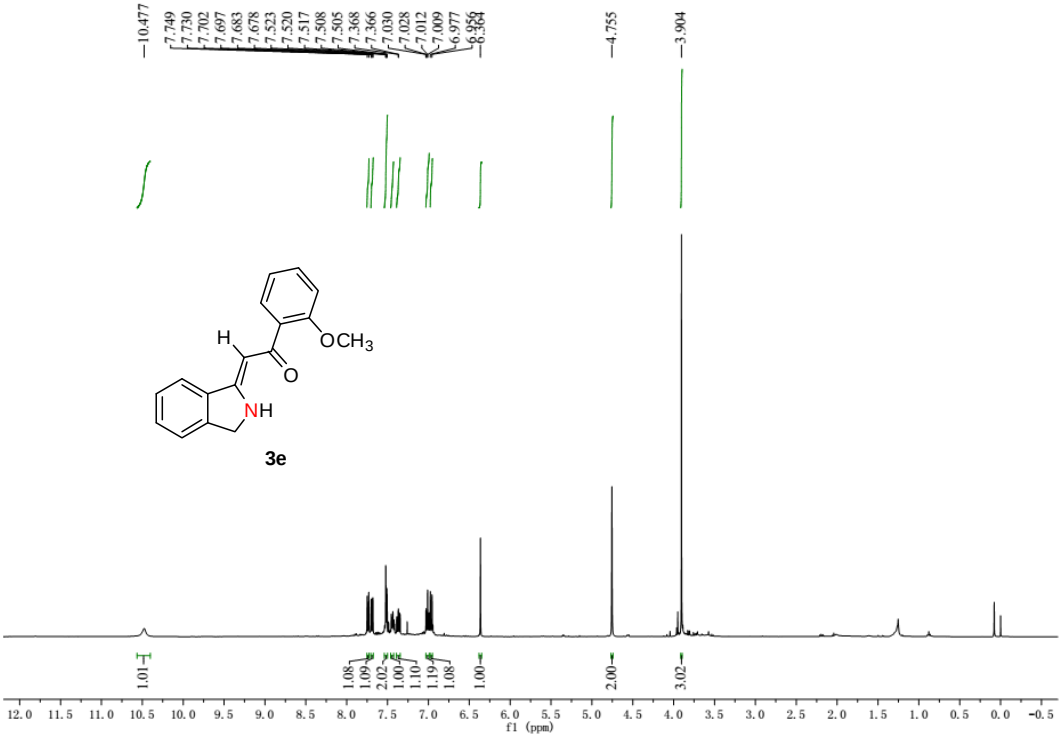

187.59
163.31
141.68
138.75
136.67
135.30
130.94
128.47
128.37
127.83
122.91
122.04
83.74
77.32
77.00
76.68
51.73
Cl
H
O
NH
3b
f1 (ppm)

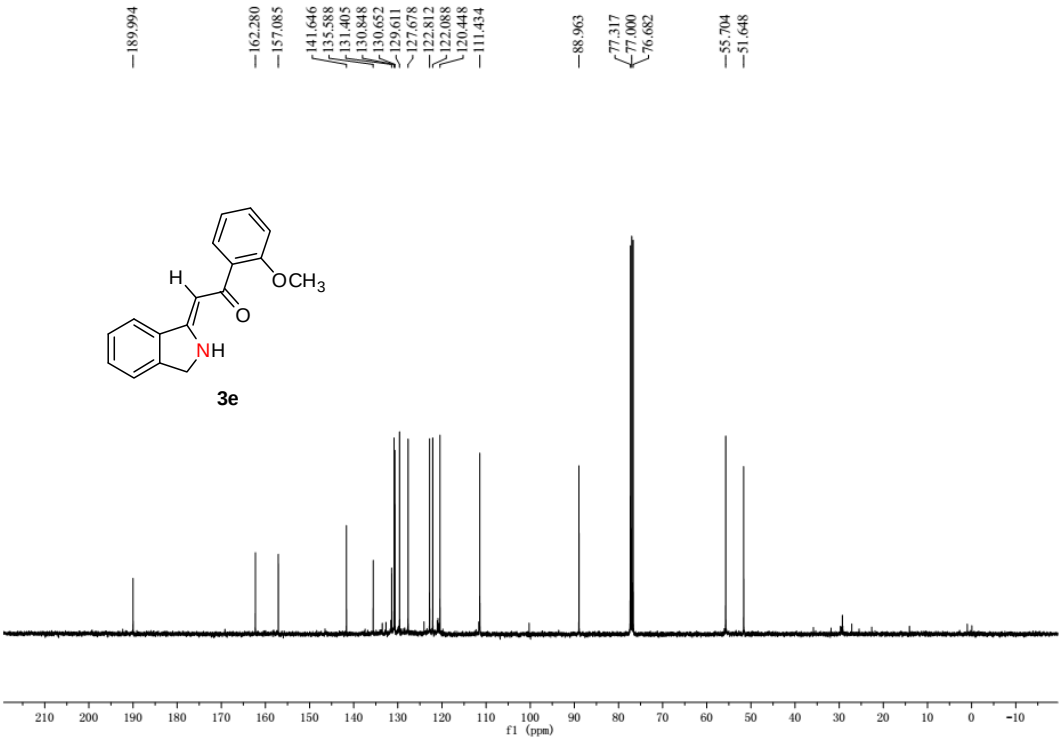

10.569
7.858
7.853
7.841
7.837
7.794
7.775
7.561
7.556
7.544
7.540
7.527
7.524
7.521
7.514
7.512
7.473
7.464
7.454
7.445
6.356
4.732
Br
H
O
NH
3c
0.98
2.08
1.03
4.02
1.08
1.03
2.00
f1 (ppm)

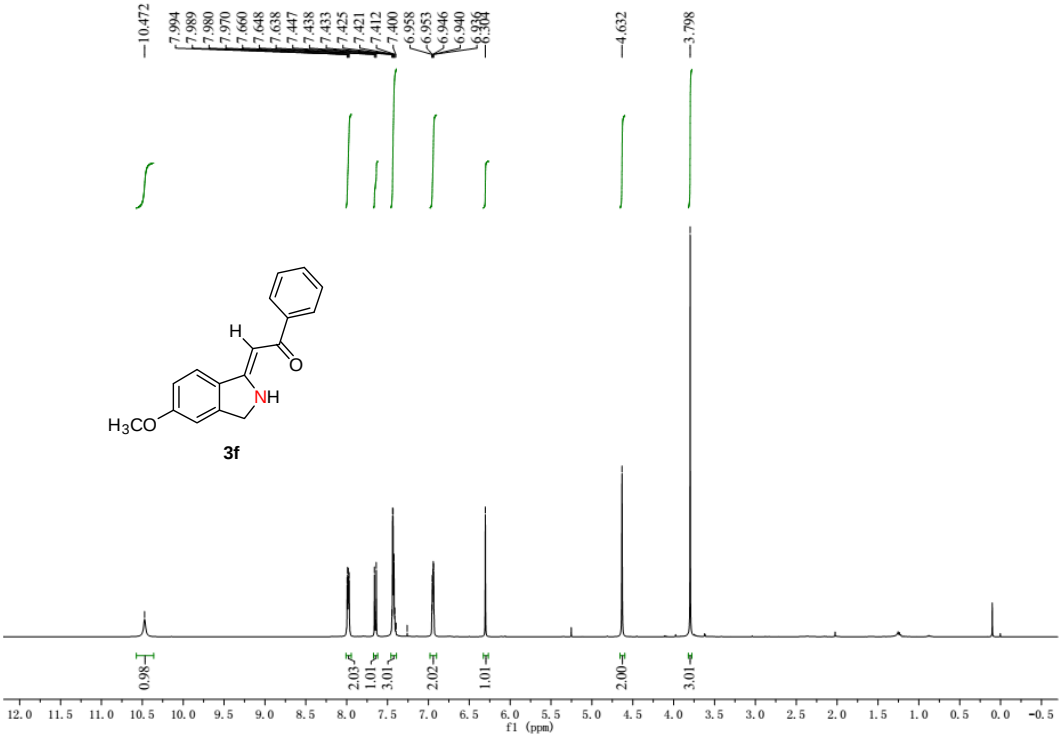

187.56
163.29
141.64
139.15
135.24
131.29
130.90
128.66
127.78
125.16
122.86
121.99
83.66
77.32
77.00
76.68
51.71
Br
H
O
NH
3c
f1 (ppm)

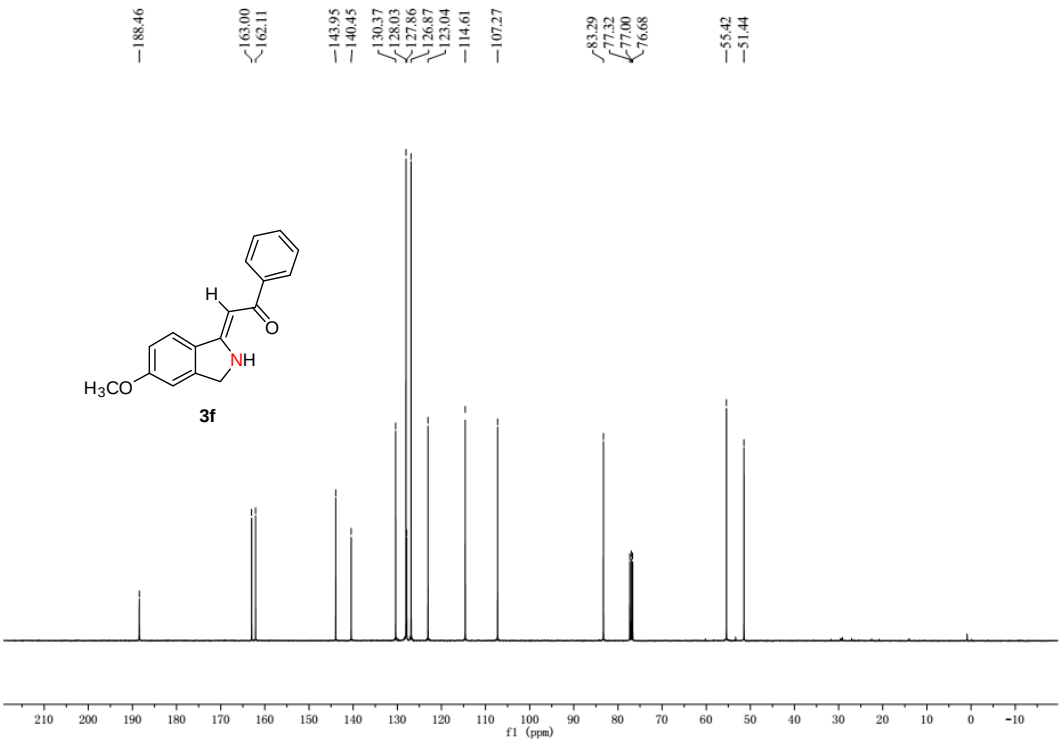

10.449
7.992
7.970
7.785
7.766
7.486
7.476
7.455
7.445
7.435
7.425
7.415
7.405
7.260
6.945
6.923
6.388
4.700
3.830
OCH3
H
O
NH
3d
0.97
2.04
1.05
3.08
2.06
1.08
2.00
3.10
f1 (ppm)

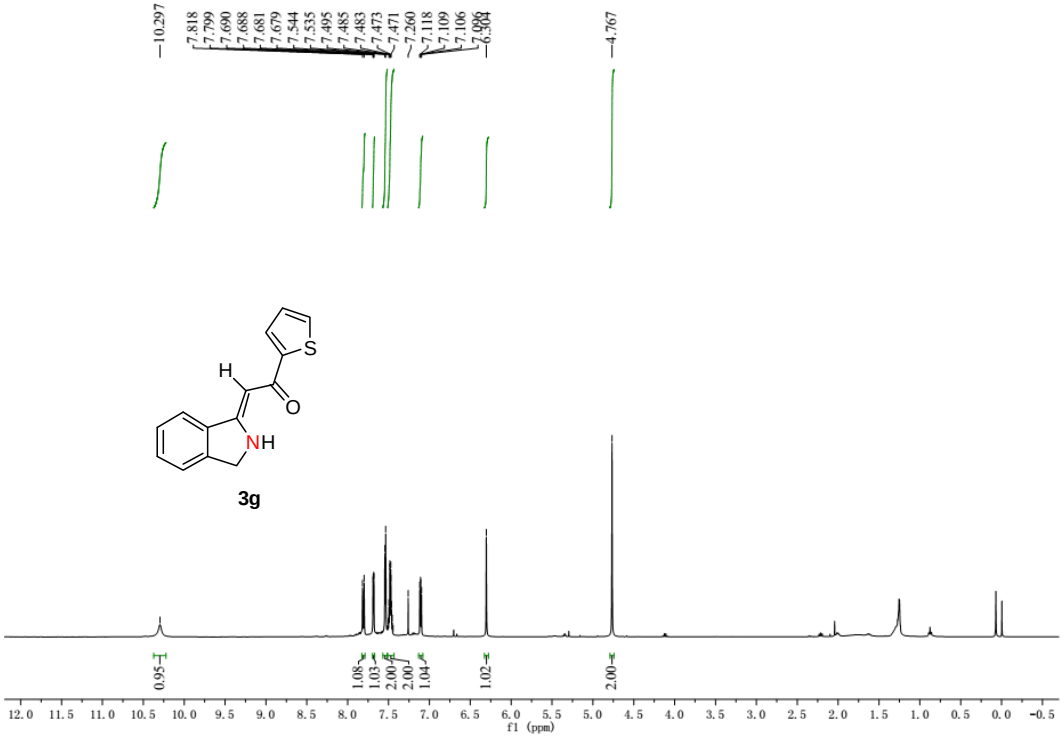

188.147
162.434
161.640
141.534
135.467
132.999
130.539
128.820
127.573
122.750
121.798
113.288
83.449
77.318
77.000
76.682
55.175
51.515
OCH3
H
O
NH
3d
f1 (ppm)


10.477
7.749
7.730
7.702
7.697
7.683
7.678
7.523
7.520
7.517
7.508
7.505
7.368
7.366
7.030
7.028
7.012
7.009
6.977
6.956
6.954
4.755
3.904
H
OCH3
O
NH
3e
1.01
1.08
1.09
2.02
1.00
1.10
1.19
1.08
1.00
2.00
3.02
f1 (ppm)

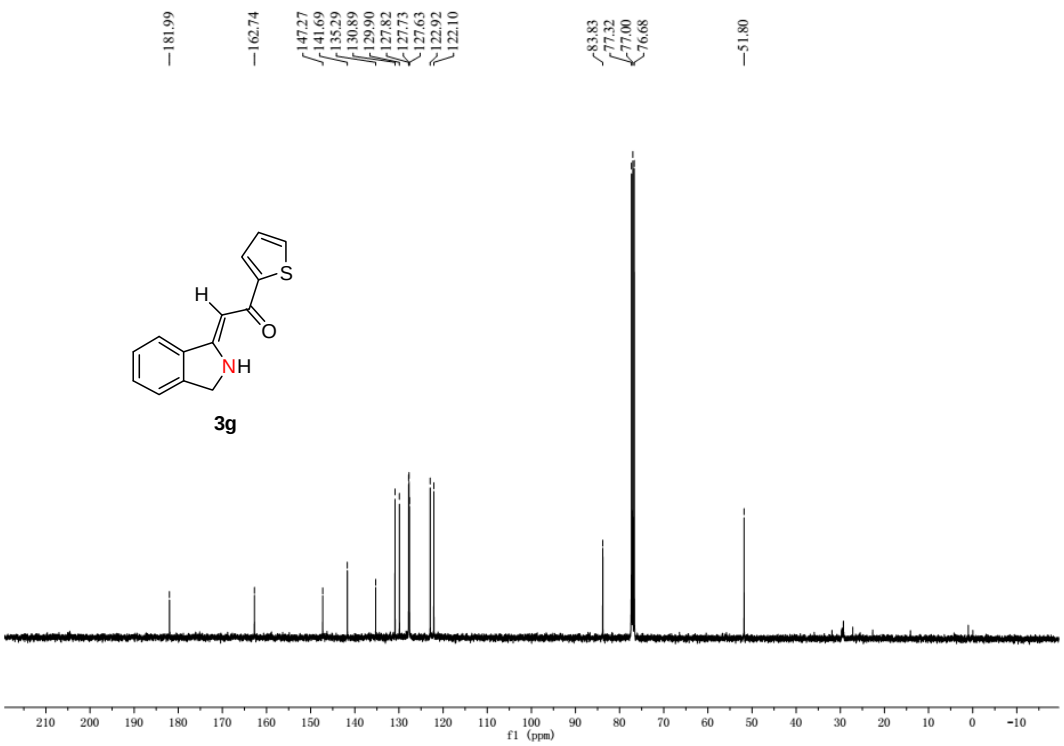

189.994
162.280
157.085
141.646
135.588
131.405
130.848
130.652
129.611
127.678
122.812
122.088
120.448
111.434
88.963
77.317
77.000
76.682
55.704
51.648
H
OCH3
O
NH
3e
f1 (ppm)


10.472
7.994
7.989
7.980
7.970
7.660
7.648
7.638
7.447
7.438
7.433
7.425
7.421
7.412
7.400
6.958
6.953
6.946
6.940
4.632
3.798
H
O
NH
H3CO
3f
0.98
2.03
1.01
3.01
2.02
1.01
2.00
3.01
f1 (ppm)

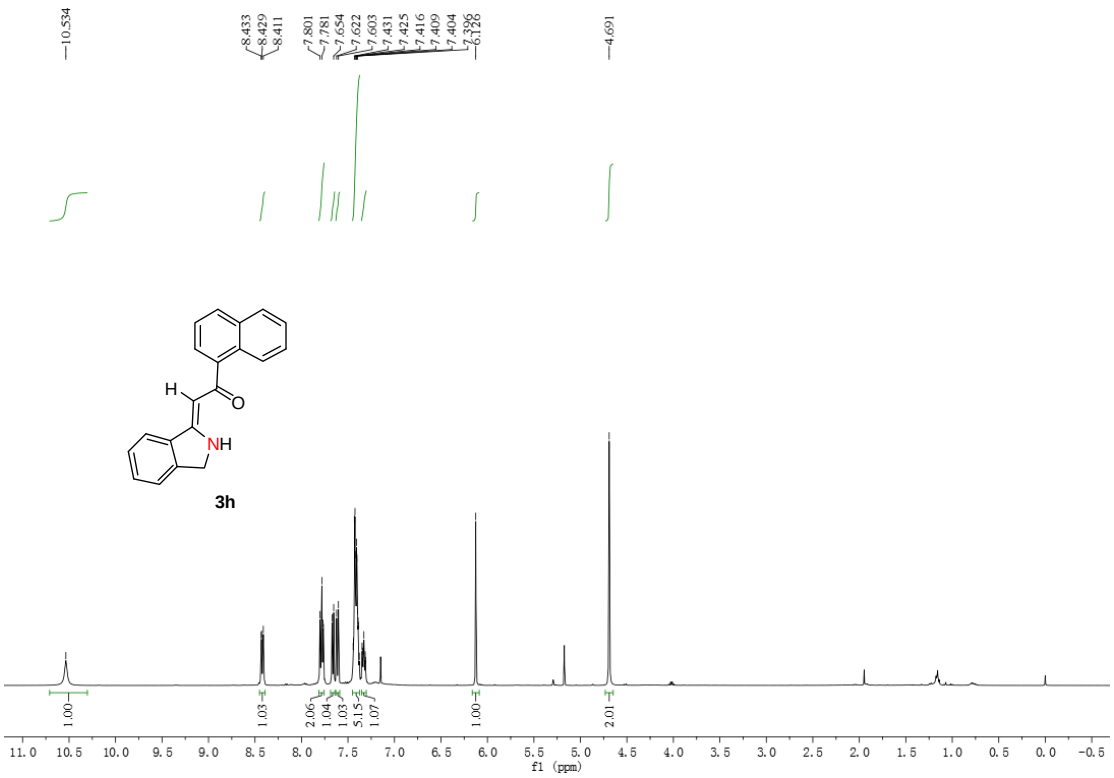

188.46
163.00
162.11
143.95
140.45
130.37
128.03
127.86
126.87
123.04
114.61
107.27
83.29
77.32
77.00
76.68
55.42
51.44
H
O
NH
H3CO
3f
f1 (ppm)


10.297
7.818
7.799
7.690
7.688
7.681
7.679
7.544
7.535
7.495
7.485
7.483
7.473
7.471
7.260
7.118
7.109
7.106
6.304
4.767
S
H
O
NH
0.95
1.08
1.03
2.00
2.00
1.04
1.02
2.00
f1 (ppm)

3g


181.99
162.74
147.27
141.69
135.29
130.89
129.90
127.82
127.73
127.63
122.92
122.10
83.83
77.32
77.00
76.68
51.80
S
H
O
NH
f1 (ppm)

3g


10.534
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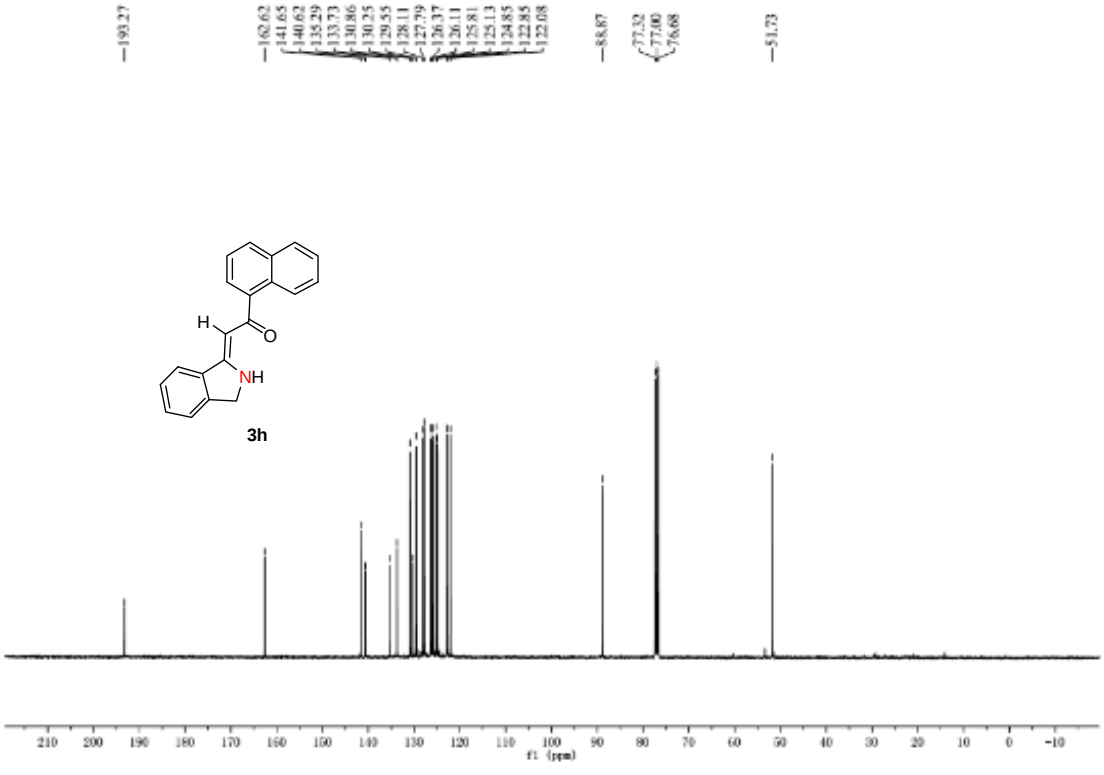
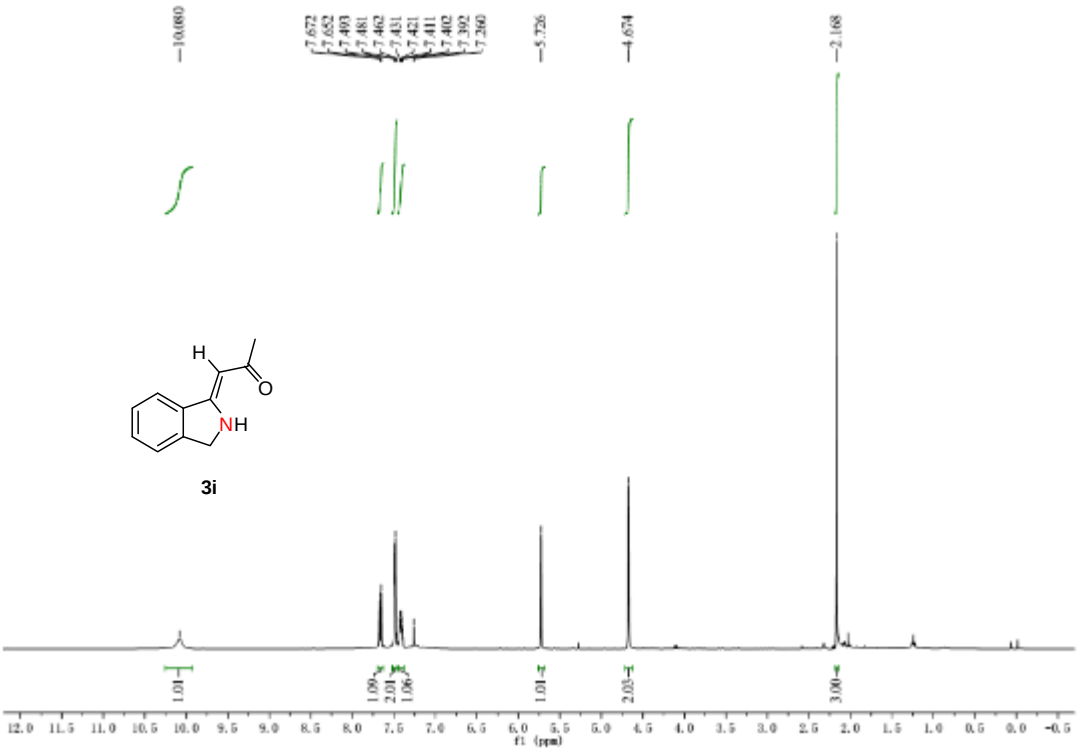
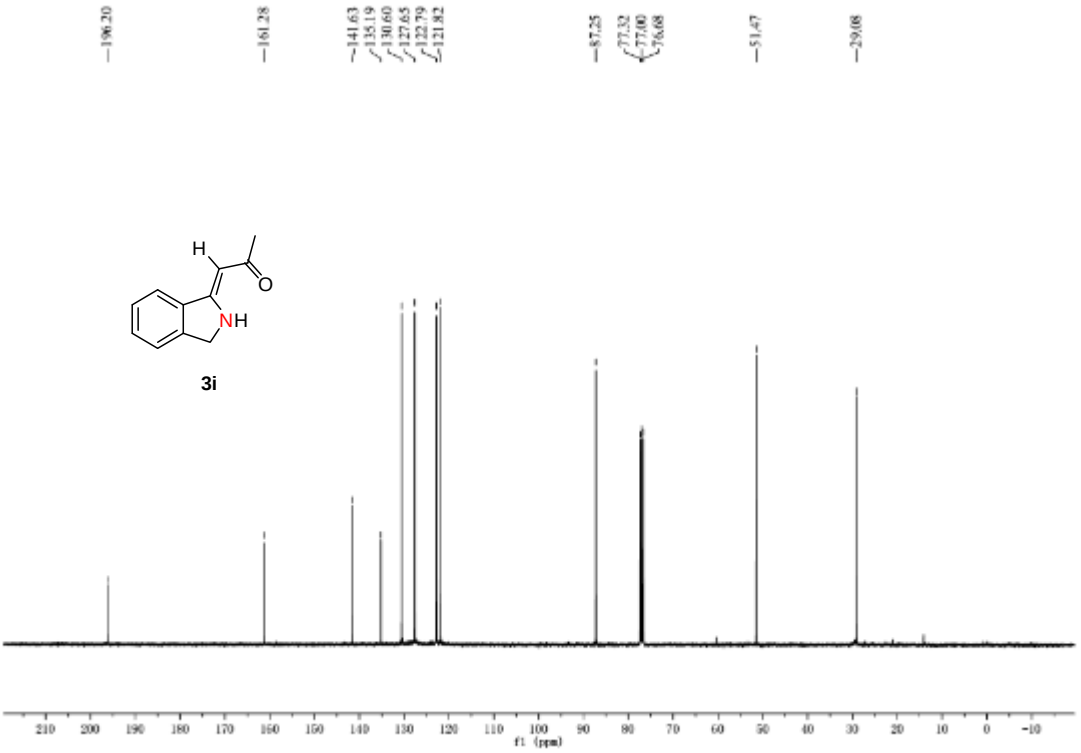
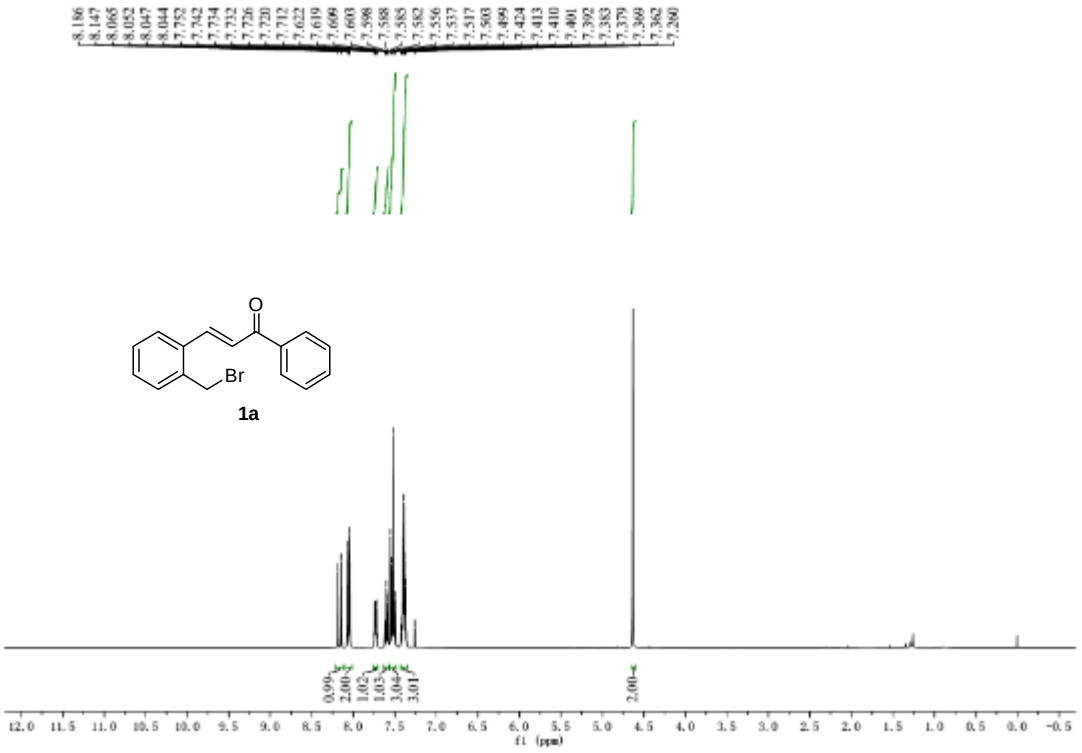
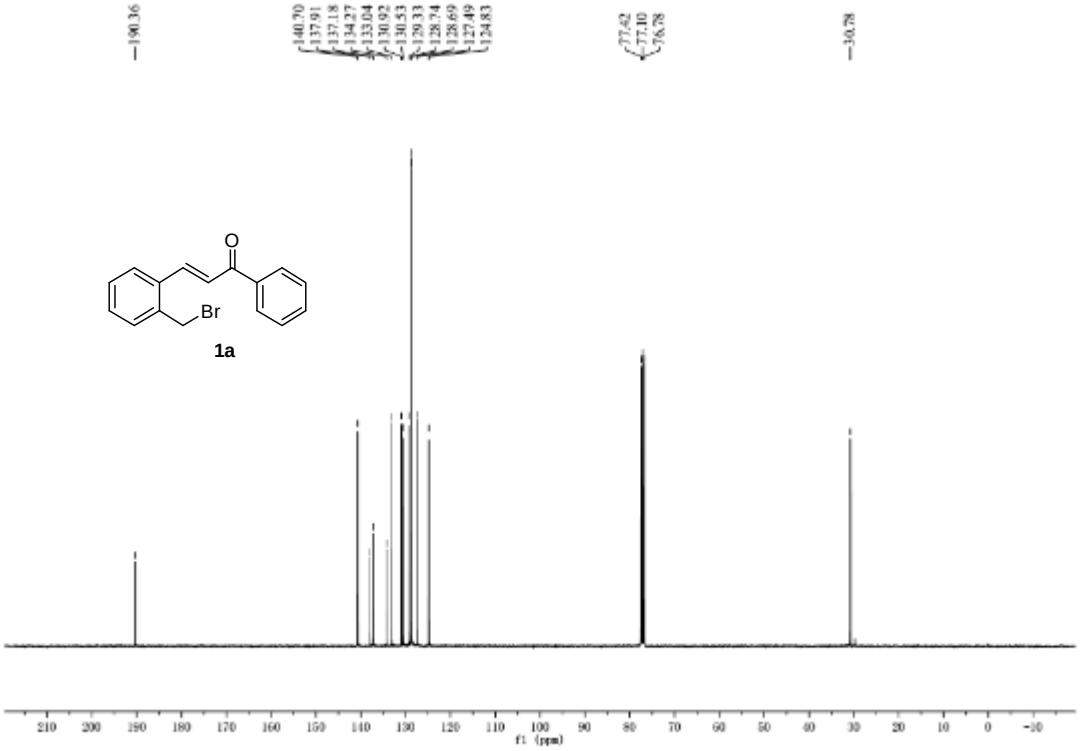
8.429
8.411
7.801
7.781
7.654
7.622
7.603
7.431
7.425
7.416
7.409
7.404
7.396
7.126
4.691
H
O
NH
3h
1.00
1.03
2.06
1.04
1.03
5.15
1.07
1.00
2.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


193.27
162.62
141.65
140.62
135.29
133.73
130.86
130.35
129.55
128.11
127.79
126.37
126.11
125.81
125.13
124.85
122.85
122.08
58.87
77.32
77.00
76.68
51.73
H
O
NH
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

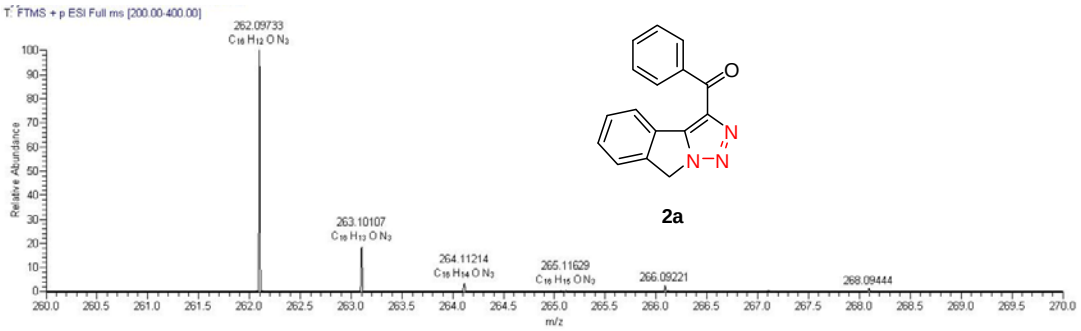

10.080
7.672
7.652
7.493
7.481
7.462
7.431
7.421
7.411
7.402
7.392
7.260
5.726
4.674
2.168
H
O
NH
3i
1.01
1.09
2.01
1.06
1.01
2.03
3.00
f1 (ppm)


196.20
161.28
141.63
135.19
130.60
127.65
122.79
121.82
87.25
77.32
77.00
76.68
51.47
29.08
H
O
NH
3i
f1 (ppm)

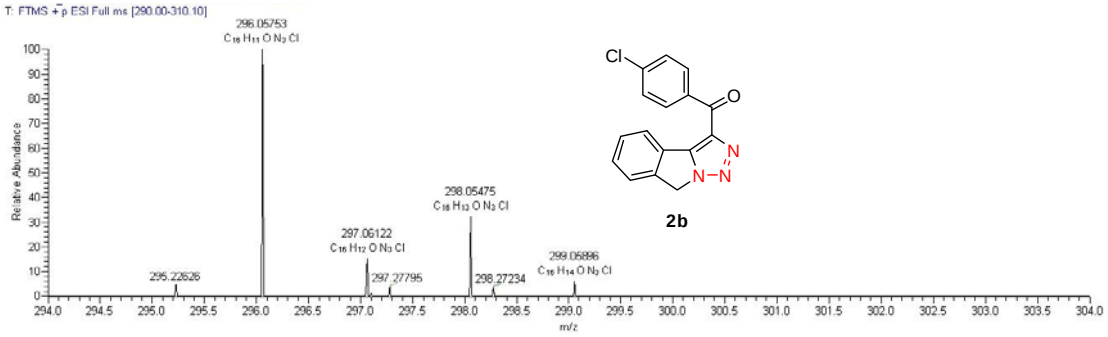

8.186
8.147
8.065
8.052
8.047
8.044
7.752
7.742
7.734
7.732
7.726
7.720
7.712
7.622
7.619
7.609
7.603
7.598
7.588
7.585
7.582
7.556
7.537
7.517
7.503
7.499
7.424
7.413
7.410
7.401
7.392
7.383
7.379
7.369
7.362
7.280
O
Br
1a
0.99
2.00
1.02
1.03
3.04
3.01
2.00
f1 (ppm)


190.36
140.70
137.91
137.18
134.27
133.04
130.92
130.53
129.33
128.74
128.69
127.49
124.83
77.62
77.10
76.78
30.78
O
Br
1a
f1 (ppm)

Copies of HRMS Spectra of all compounds



2a



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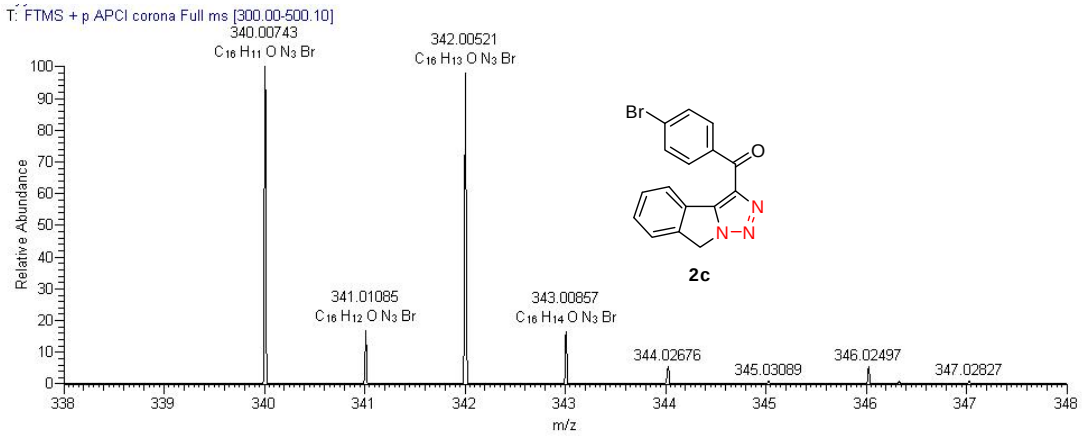

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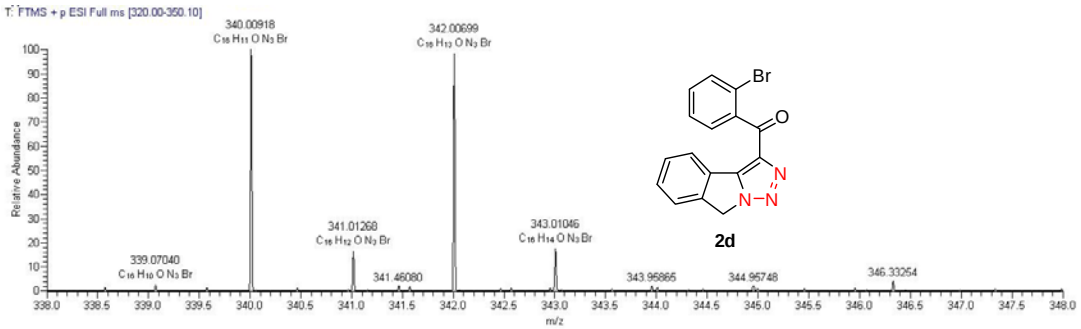
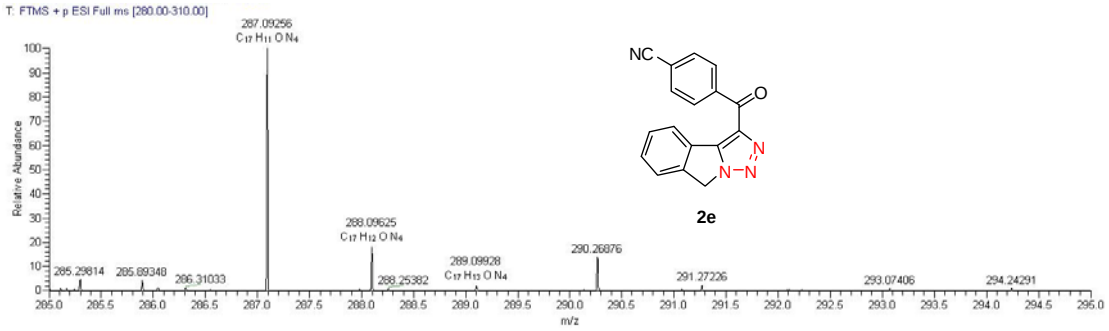
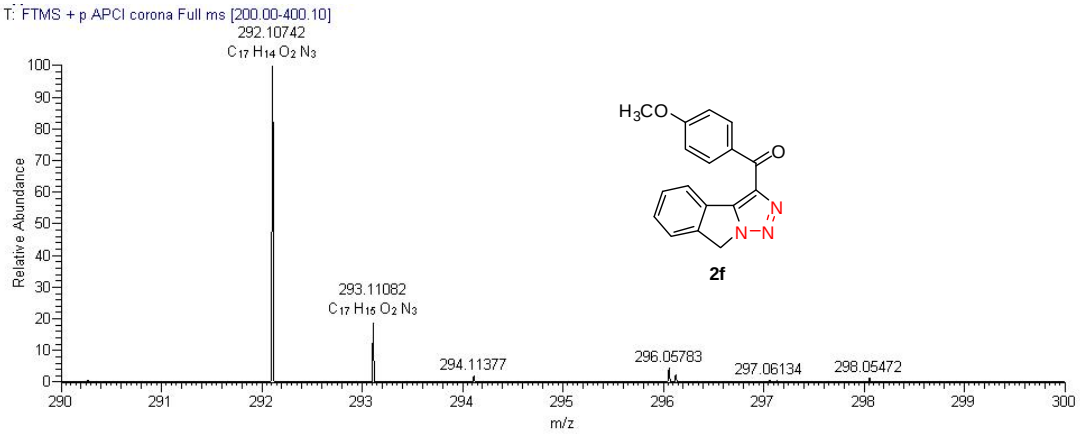


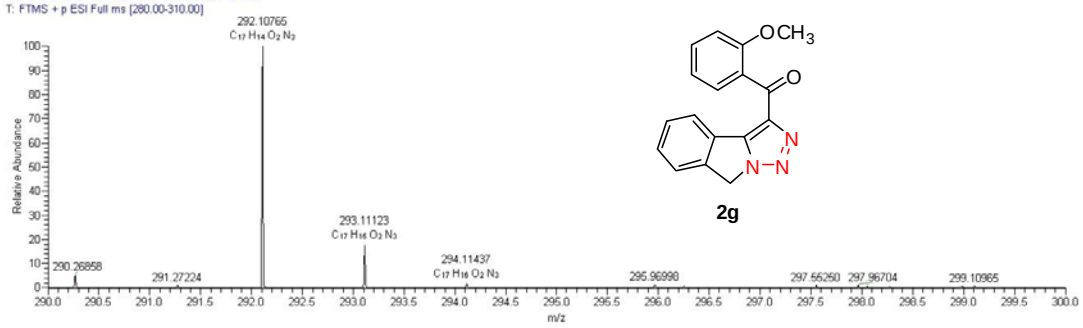
2d


T: FTMS + p ESI Full ms [280.00-310.00]
287.09256
C17 H11 O N4
288.09625
C17 H12 O N4
289.09928
C17 H13 O N4
285.29814
285.89348
286.31033
288.25382
290.26876
291.27226
293.07406
294.24291
Relative Abundance
m/z
NC
O
N
N–N

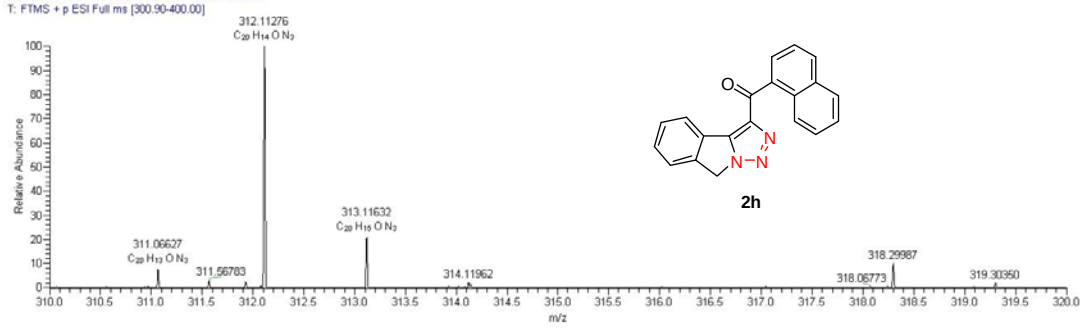
2e


T: FTMS + p APCI corona Full ms [200.00-400.10]
292.10742
C17 H14 O2 N3
293.11082
C17 H15 O2 N3
294.11377
296.05783
297.06134
298.05472
Relative Abundance
m/z
H3CO
O
N
N–N

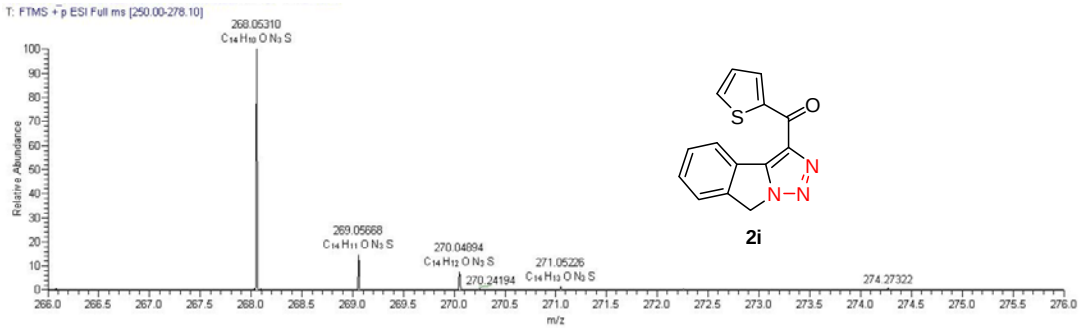
2f


T: FTMS + p ESI Full ms [280.00-310.00]
292.10765
C17 H14 O2 N3
293.11123
C17 H15 O2 N3
294.11437
C17 H16 O2 N3
290.26858
291.27224
295.96998
297.55250
297.96704
299.10965
Relative Abundance
m/z
OCH3
O
N
N–N

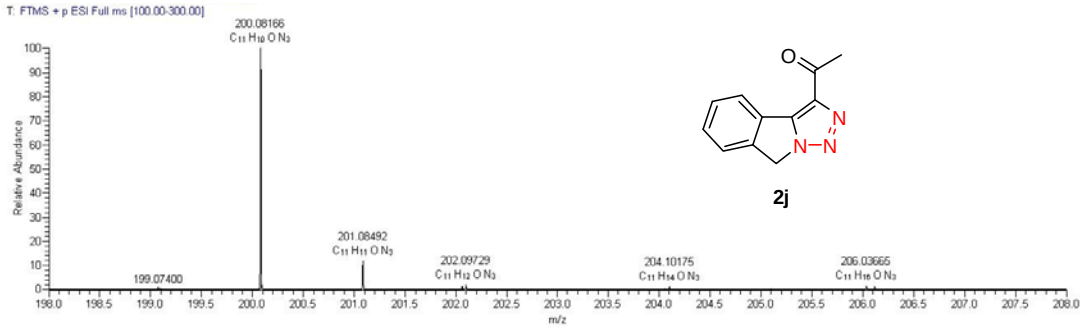
2g


T: FTMS + p ESI Full ms [300.90-400.00]
312.11276
C20 H14 O N3
313.11632
C20 H15 O N3
311.09627
C20 H13 O N3
311.56783
314.11962
318.06773
318.29987
319.30350
Relative Abundance
m/z
O
N
N–N

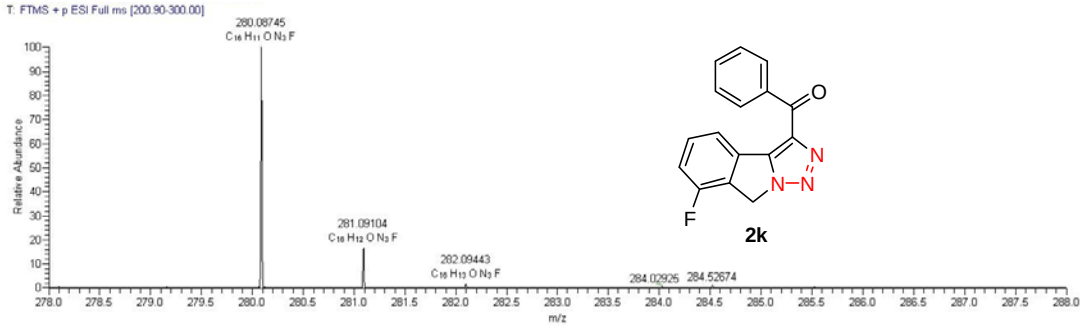
2h


T: FTMS + p ESI Full ms [250.00-278.10]
268.05310
C14 H10 O N3 S
269.05668
C14 H11 O N3 S
270.04894
C14 H12 O N3 S
270.24194
271.05226
C14 H13 O N3 S
274.27322
Relative Abundance
m/z
O
S
N
N–N

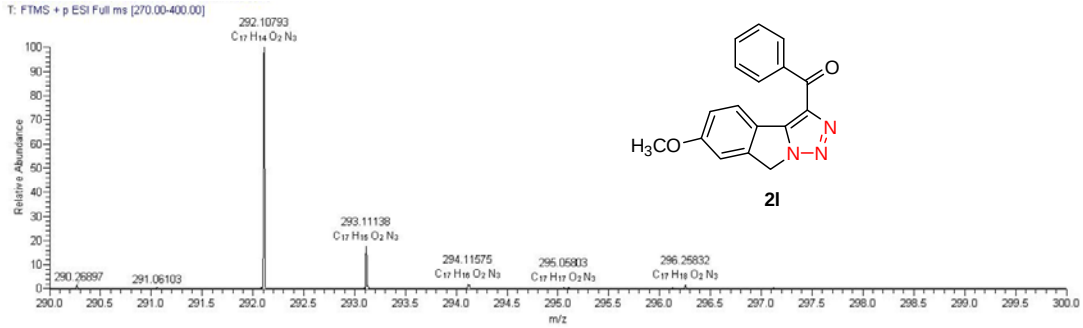
2i


T: FTMS + p ESI Full ms [100.00-300.00]
200.08166
C11 H10 O N3
201.08492
C11 H11 O N3
199.07400
202.09729
C11 H12 O N3
204.10175
C11 H14 O N3
206.03665
C11 H8 O N3
Relative Abundance
m/z
O
N
N–N

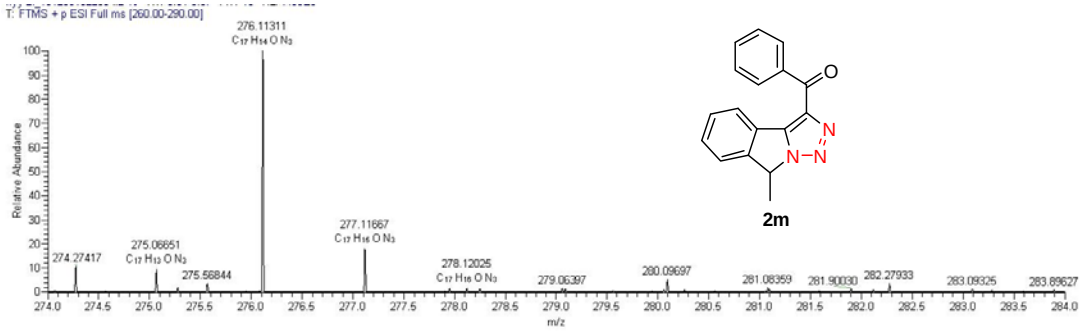
2j

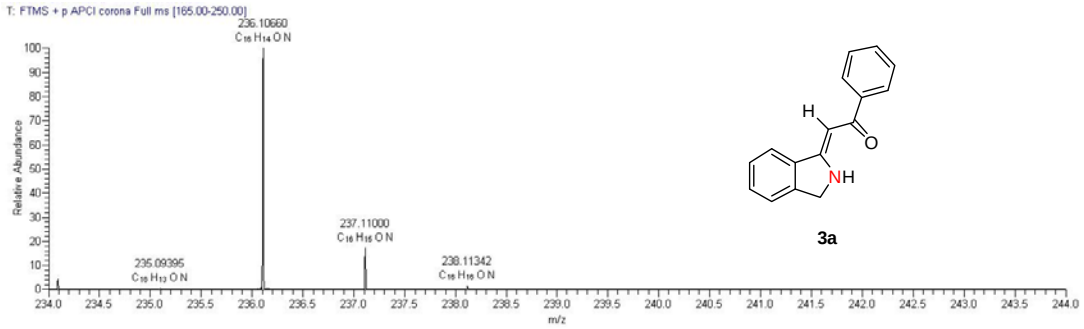

T: FTMS + p ESI Full ms [200.90-300.00]
280.08745
C16 H11 O N3 F
281.09104
C16 H12 O N3 F
282.09443
C16 H13 O N3 F
284.02925
284.52674
Relative Abundance
m/z
O
N
N–N
F

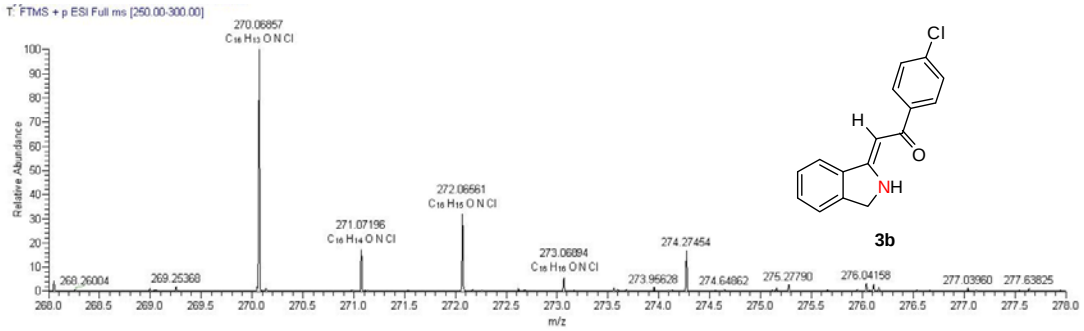
2k

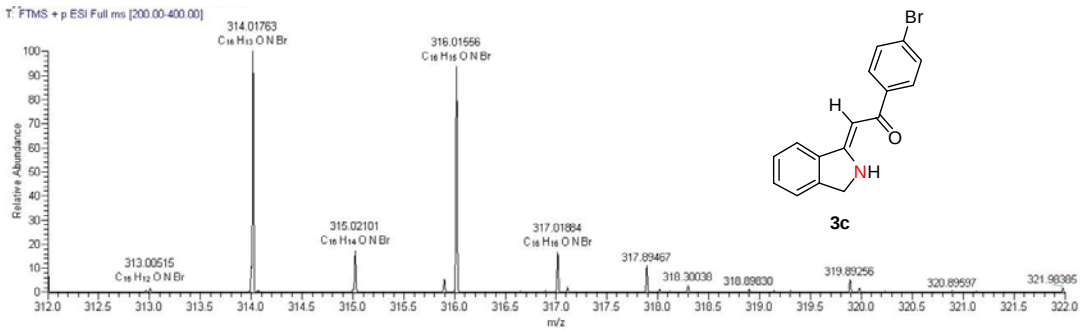

T: FTMS + p ESI Full ms [270.00-400.00]
292.10793
C17 H14 O2 N3
293.11138
C17 H15 O2 N3
290.26897
291.06103
294.11575
C17 H16 O2 N3
295.05803
C17 H17 O2 N3
296.25832
C17 H18 O2 N3
Relative Abundance
m/z
O
H3CO
N
N–N

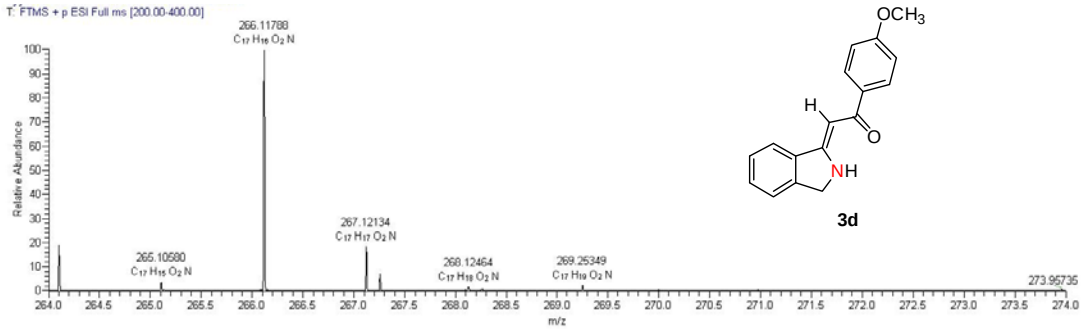
2l

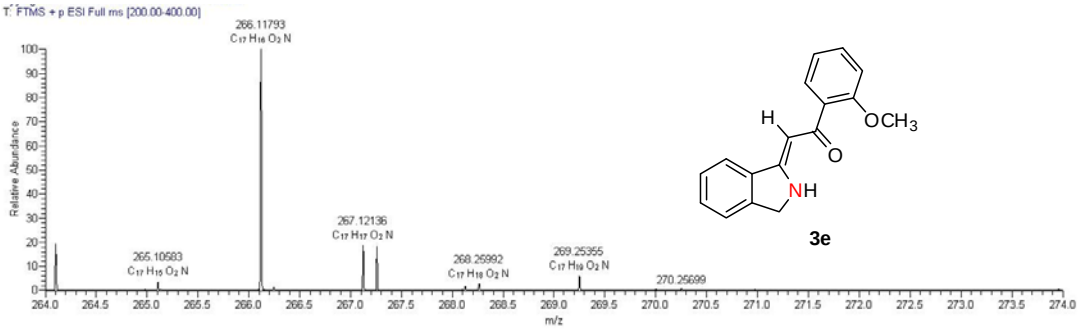

T: FTMS + p ESI Full ms [260.00-290.00]
276.11311
C17 H14 O N3
277.11667
C17 H16 O N3
275.06851
C17 H13 O N3
274.27417
275.56844
278.12025
C17 H18 O N3
279.06397
280.09697
281.08359
281.90030
282.27933
283.09325
283.89627
Relative Abundance
m/z
O
N
N–N
2m

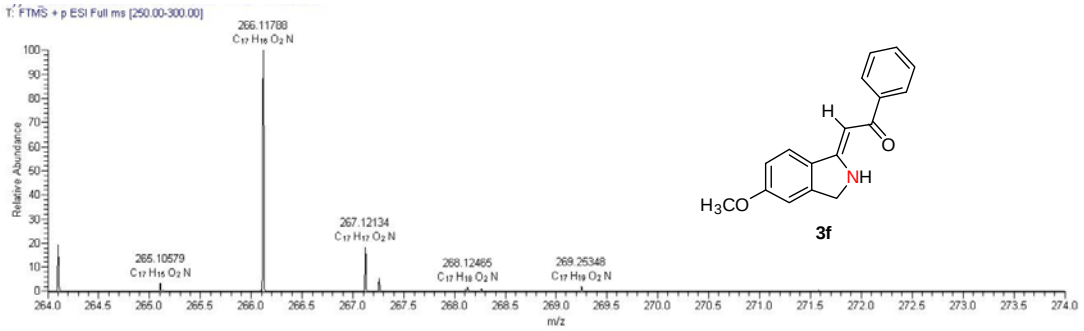

T: FTMS + p APCI corona Full ms [165.00-250.00]
236.10660
C16 H14 O N
237.11000
C16 H15 O N
235.09395
C15 H13 O N
238.11342
C15 H16 O N
Relative Abundance
m/z
H
O
NH
3a

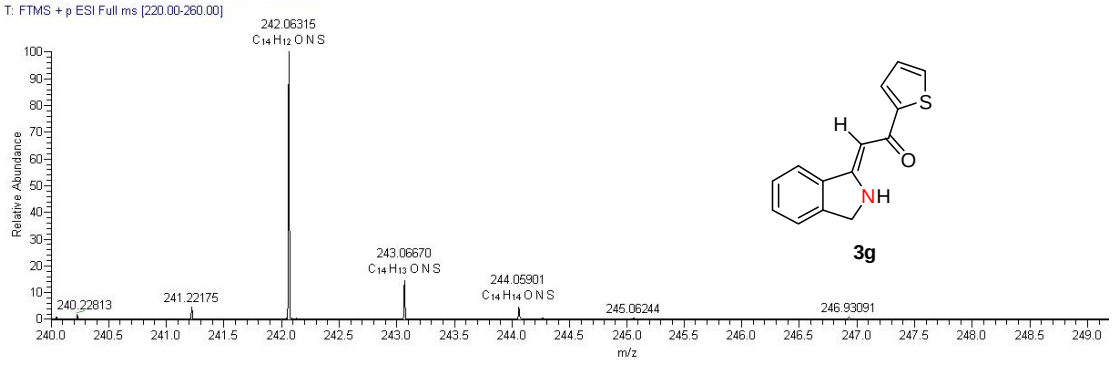

T: FTMS + p ESI Full ms [250.00-300.00]
270.06857
C16 H13 O N Cl
272.06561
C16 H15 O N Cl
271.07196
C16 H14 O N Cl
273.06894
C16 H16 O N Cl
274.27454
268.26004
269.25368
273.95628
274.64862
275.27790
276.04158
277.03960
277.63825
Relative Abundance
m/z
Cl
H
O
NH
3b

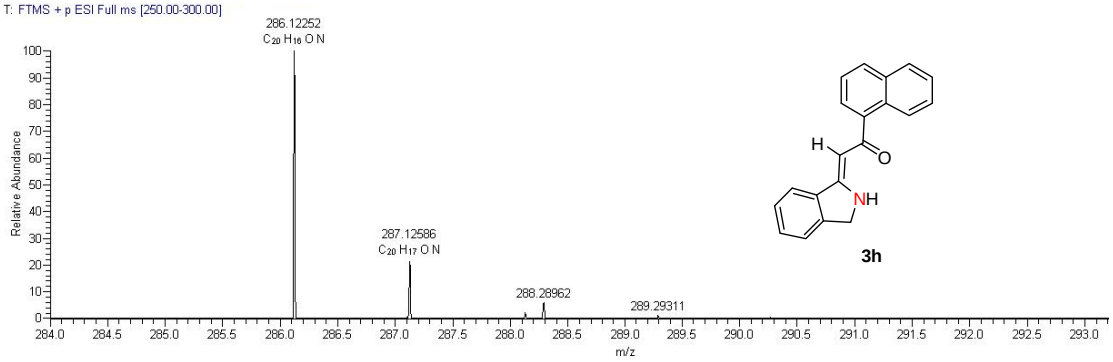

T: FTMS + p ESI Full ms [200.00-400.00]
314.01763
C16 H13 O N Br
316.01556
C16 H15 O N Br
315.02101
C16 H14 O N Br
317.01884
C16 H16 O N Br
313.00515
C15 H12 O N Br
317.89467
318.30038
318.89830
319.89256
320.89597
321.98395
Relative Abundance
m/z
Br
H
O
NH
3c

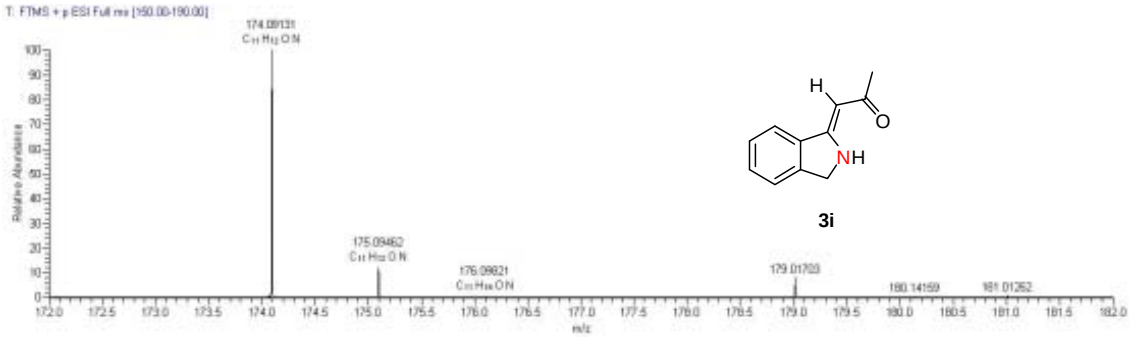

T: FTMS + p ESI Full ms [200.00-400.00]
266.11788
C17 H16 O2 N
267.12134
C17 H17 O2 N
265.10580
C17 H15 O2 N
268.12464
C17 H18 O2 N
269.25349
C17 H19 O2 N
273.95735
Relative Abundance
m/z
OCH3
H
O
NH
3d


T: FTMS + p ESI Full ms [200.00-400.00]
266.11793
C17 H16 O3 N
267.12136
C17 H17 O2 N
265.10583
C17 H15 O2 N
268.25992
C17 H18 O2 N
269.25355
C17 H19 O2 N
270.25699
Relative Abundance
m/z
H
OCH3
O
NH
3e


T: FTMS + p ESI Full ms [250.00-300.00]
266.11788
C17 H16 O2 N
267.12134
C17 H17 O2 N
265.10579
C17 H15 O2 N
268.12465
C17 H18 O2 N
269.25348
C17 H19 O2 N
Relative Abundance
m/z
H
O
NH
H3CO
3f


T: FTMS + p ESI Full ms [220.00-260.00]
242.06315
C14 H12 O N S
243.06670
C14 H13 O N S
244.05901
C14 H14 O N S
240.22813
241.22175
245.06244
246.93091
Relative Abundance
m/z
H
S
O
NH
3g


T: FTMS + p ESI Full ms [250.00-300.00]
286.12252
C20 H16 O N
287.12586
C20 H17 O N
288.28962
289.29311
Relative Abundance
m/z
H
O
NH
3h


T: FTMS + p ESI Full ms [150.00-190.00]
174.09131
C11 H12 O N
175.09462
C11 H13 O N
176.09821
C11 H14 O N
179.01703
180.14159
181.01262
Relative Abundance
m/z
H
O
NH
3i