Supporting Information

Catalyst-Free Coupling of Peroxypyrroloindolenines with Amines to Afford Stable Peroxyindolenines

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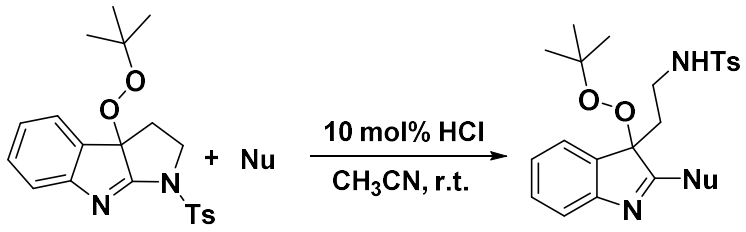
1. General Information

All reactions were performed under a designated atmosphere in flame-dried round bottom flasks, magnetically stirred, unless otherwise noted. All reactions were performed at room temperature (r.t., approximately 25 ^{o}C) unless otherwise noted. Preparative column chromatography was performed using silica gel 60, particle size 0.063–0.200 mm (70–230 mesh, flash). Analytical TLC was carried out employing silica gel 60 F254 plates (Merck, Darmstadt). Visualization of the developed chromatograms was performed with detection by UV (254 nm and 365 nm).^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectrum were recorded on a JEOL-500 (^{1}H, 500 MHz; ^{13}C, 126 MHz; ^{19}F 471 MHz) spectrometer. Chemical shifts for protons are reported in parts per million and are references to the NMR solvent peak ($CDCl_3$: δ 7.26; DMSO-d_6: 2.50). Chemical shifts for carbons are reported in parts per million and are referenced to the carbon resonances of the NMR solvent ($CDCl_3$: δ 77.16; DMSO-d_6: 39.52). Signals are listed in ppm, and multiplicity identified as s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Chemical shifts were expressed in ppm, and J values were given in Hz. High resolution mass Spectrum (HRMS) were obtained from Thermo Fisher Scientific Exactive Plus mass spectrometer by using ESI (Electrospray ionization). X-ray crystal structure data were obtained from Buker D8Venture. The melting point was determined using the X-4A melting point apparatus (Shanghai Yidian Co., Ltd.) and uncorrected. Concentration under reduced pressure was performed by rotary evaporation at 25–35 °C at appropriate pressure. Purified compounds were further dried under high vacuum (0.01-0.10 Torr). Yields refer to purified and spectroscopically pure compounds unless otherwise noted. All commercially available starting materials and solvents were reagent grade and used without further purification.

Abbreviations used: EtOAc = ethyl acetate; THF = tetrahydrofuran; DCE = 1,2-dichloroethane; Et_3N = triethylamine; Nu = Nucleophile; PE = petroleum ether; TLC = thin layer chromatography.

2. Optimization of Reaction Conditions

Table S1. Optimization of Nucleophiles

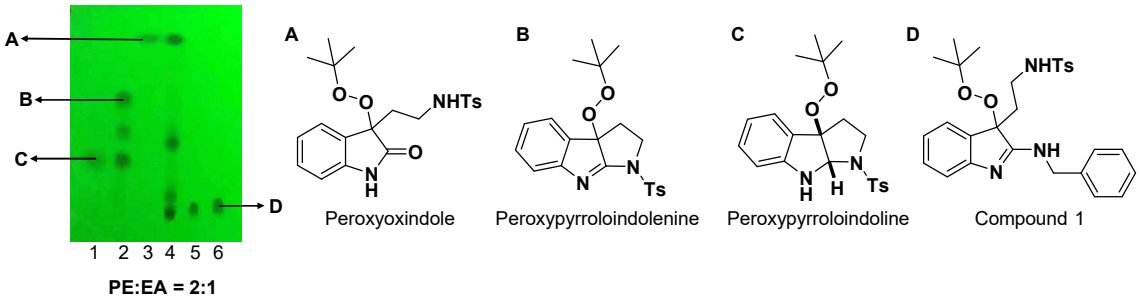


Entry[a]	Nucleophile	Yield[b]	Entry[a]	Nucleophile	Yield[b]
1	Indole	trace	8	Pyrrole	trace
2	Phenol	trace	9	Diethyl malonate	trace
3	Aniline	trace	10	Diethylamine	trace
4	Styrene	trace	11	Salicylaldehyde	trace
5	Phenylacetylene	trace	12	Trimethylsilyl cyanide	trace
6	Isoprene	trace	13	Benzylamine	88%
7	Benzoic acid	trace	14	1-Methylimidazole	trace

[a]Unless otherwise noted, all the reactions were performed using pyrroloindoline (0.1 mmol) and Nucleophile (0.11 mmol) in 1 mL of CH_3CN at room temperature overnight. [b]Conversion to the desired product by analysis of ^1H NMR spectra of unpurified reaction mixture.

3. Stability study

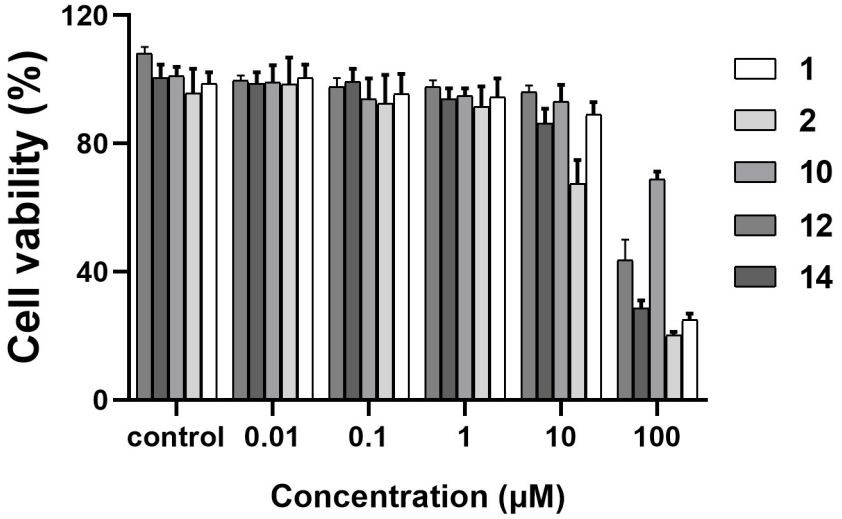
Peroxypyrroloindolenine, peroxypyrroloindoline and compound 1 are treated with 0.1 eq of HCl, respectively. Then, the reaction was monitored by TLC analysis.

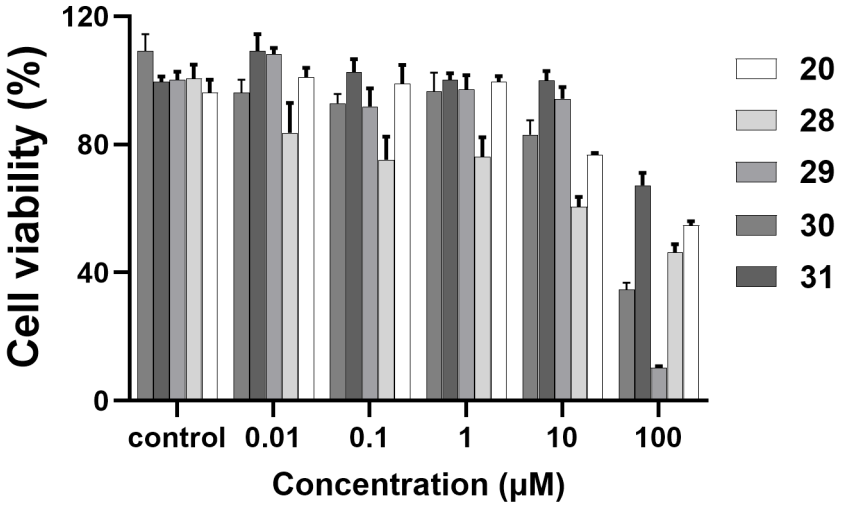


TLC under UV (PE/EtOAc = 2:1, line 1: peroxyoxindole; line 2: Peroxypyrroloindolenine (4 mg, 0.01 mmol) was added 0.1 eq of HCl; line 3: peroxypyrroloindoline; line 4: peroxypyrroloindoline (4 mg, 0.01 mmol) was added 0.1 eq of HCl; line 5: compound 1; line 6: compound 1 (5 mg, 0.01 mmol) was added 0.1 eq of HCl).

4. MTT assay

The cytotoxicities of compounds were determined by MTT assay. B16/F10 cells were seeded in a 96-well plate at a density of 8000 cells per well and cultured for 24 h. Then cells were treated with compounds at different concentrations. After 48 h incubation, the cells were washed three times with PBS followed by the addition of MTT solution (0.5 μg/mL, 100 μL). The plates were incubated for an additional 4 h at 37°C. After the medium was removed, 100 μL of DMSO was added to the well and the plates were incubated under constant shaking at 37 °C for >10 min until the formazan crystals were fully dissolved. The absorbance of the solution was measured at 570 nm by using a Tecan Infinite™ 200 PRO multimode microplate reader with five replicates at each dose. All IC_{50} values were calculated by GraphPad Prism 9 with nonlinear regression. Experiments were repeated three times with five replications for each dose.

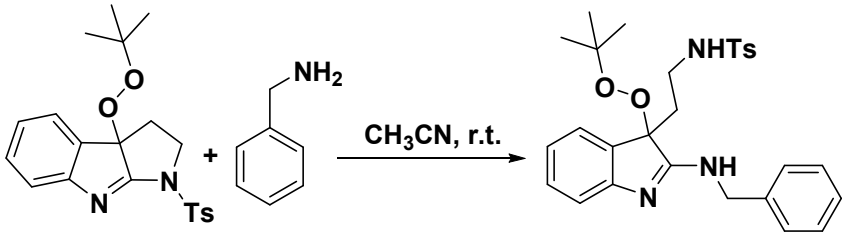




5. General Procedures

Note: All peroxyindolenines were prepared according to ***Org. Lett. 2018, 20, 7937-7941*** and ***Chem. Commun. 2019, 55, 63-66.***

Compound 1



N-(2-(2-(benzylamino)-3-(tert-butylperoxy)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added *phenylmethanamine* (60 µL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 1 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (246 mg, 97%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 83 - 84 °C

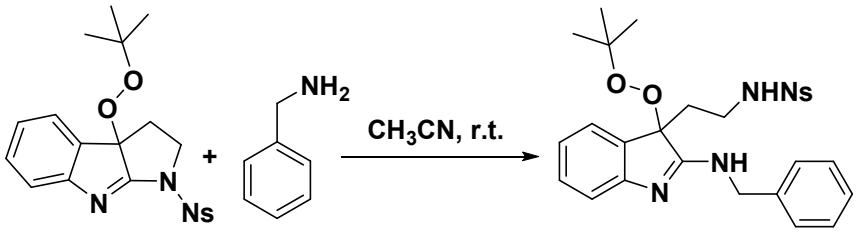
TLC: R_f = 0.42 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, Acetonitrile-d_3) δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 7.0 Hz, 2H), 7.34 (d, *J* = 2.5 Hz, 2H), 7.31 (d, *J* = 7.7 Hz, 2H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.21 – 7.16 (m, 1H), 7.09 (d, *J* = 7.0 Hz, 1H), 6.92 – 6.89 (m, 1H), 6.89 – 6.85 (m, 1H), 6.39 (s, 1H), 5.43 (s, 1H), 4.72 – 4.63 (m, 1H), 4.53 – 4.45 (m, 1H), 2.73 – 2.63 (m, 1H), 2.43 (d, *J* = 5.6 Hz, 1H), 2.40 (s, 3H), 2.20 – 2.12 (m, 1H), 2.01 – 1.95 (m, 1H), 1.11 (s, 9H).

^{13}C NMR (126 MHz, Acetonitrile-d_3) δ172.82, 157.18, 144.59, 140.19, 137.78, 133.96, 130.97, 130.66, 129.28, 128.16, 127.88, 127.78, 123.84, 121.92, 117.24, 90.50, 81.03, 46.23, 38.79, 35.29, 26.63, 21.45.

HRMS (ESI): calcd for $C_{28}H_{34}N_3O_4S$ $[M + H]^+$ m/z: 508.2265, found 508.2272.

Compound 2



N-(2-(2-(benzylamino)-3-(tert-butylperoxy)-3H-indol-3-yl) ethyl)-4-nitrobenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-((4-nitrophenyl) sulfonyl)-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (173 mg, 0.4 mmol) in CH_3CN (4 mL) was added *phenylmethanamine* (48 μL, 0.44 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 2 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether: EtOAc = 2:1) to give the desired product (209 mg, 97%) as a yellow oil.

Physical state: yellow oil.

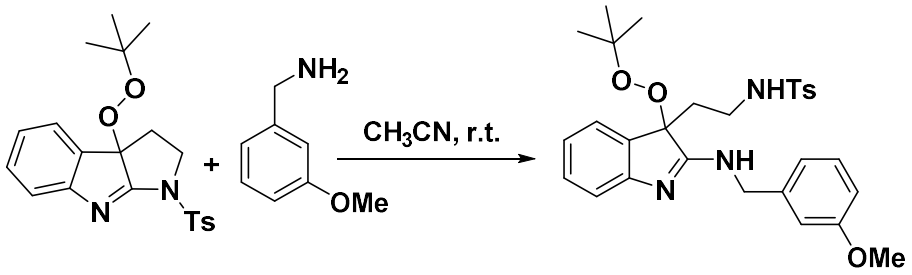
TLC: R_f = 0.40 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 8.21 (d, *J* = 8.8 Hz, 2H), 7.84 (d, *J* = 8.9 Hz, 2H), 7.36 (d, *J* = 7.2 Hz, 2H), 7.35 – 7.31 (m, 2H), 7.31 – 7.27 (m, 1H), 7.23 – 7.20 (m, 1H), 7.07 (d, *J* = 7.3 Hz, 1H), 7.03 (d, *J* = 7.7 Hz, 1H), 6.93 – 6.86 (m, 1H), 4.77 (d, *J* = 14.6 Hz, 1H), 4.53 (d, *J* = 14.6 Hz, 1H), 2.91 – 2.77 (m, 2H), 2.32 – 2.21 (m, 1H), 2.17 – 2.09 (m, 1H), 1.11 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 149.98, 145.66, 137.68, 131.88, 130.72, 128.89, 128.70, 128.28, 127.90, 127.23, 127.03, 124.38, 123.09, 121.88, 117.00, 89.94, 81.06, 47.01, 38.39, 35.26, 26.45.

HRMS (ESI): calcd for $C_{27}H_{31}N_4O_6S$ $[M + H]^+$ m/z: 539.1959, found 539.1956.

Compound 3



N-(2-(3-(tert-butylperoxy)-2-((3-methoxybenzyl) amino)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) in CH_3CN (3 mL) was added *(3-methoxyphenyl)methanamine* (42 μL, 0.44 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 3 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether: EtOAc = 2:1) to give the desired product (153 mg, 95%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 116 - 118 °C.

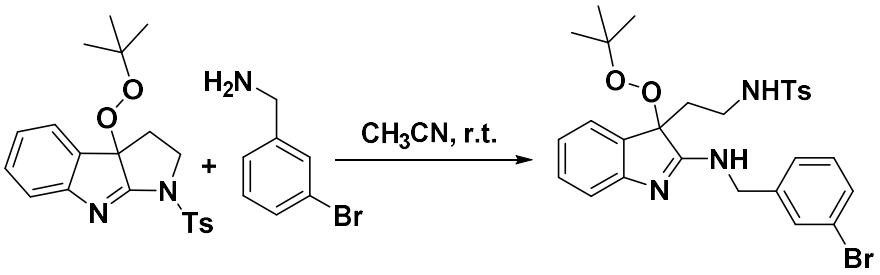
TLC: R_f = 0.32 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.24 (d, *J* = 9.0 Hz, 2H), 7.21 (s, 1H), 7.19 (d, *J* = 1.3 Hz, 1H), 7.08 (d, *J* = 7.7 Hz, 1H), 6.98 – 6.96 (m, 1H), 6.95 (s, 1H), 6.93 (t, *J* = 2.0 Hz, 1H), 6.87 – 6.84 (m, 1H), 6.84 – 6.80 (m, 1H), 5.54 (s, 1H), 5.06 (s, 1H), 4.74 (d, *J* = 14.6 Hz, 1H), 4.50 (d, *J* = 14.6 Hz, 1H), 3.77 (s, 3H), 2.90 – 2.83 (m, 1H), 2.83 – 2.76 (m, 1H), 2.38 (s, 3H), 2.26 – 2.20 (m, 1H), 2.06 – 2.00 (m, 1H), 1.11 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$: CD_3OD = 10:1) δ 172.19, 159.88, 154.74, 143.50, 139.26, 136.52, 131.81, 130.39, 129.71, 126.96, 123.05, 121.62, 120.02, 116.51, 113.59, 90.44, 80.76, 55.24, 46.89, 37.85, 35.03, 26.28, 21.41.

HRMS (ESI): calcd for $C_{29}H_{36}N_3O_5S$ $[M + H]^+$ m/z: 538.2370, found 538.2358.

Compound 4



N-(2-(2-((3-bromobenzyl) amino)-3-(tert-butylperoxy)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (160 mg, 0.4 mmol) *(3-bromophenyl) methanamine* (55 mg, 0.44 mmol) in CH_3CN (4 mL) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (220 mg, 94%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 150 - 152 °C.

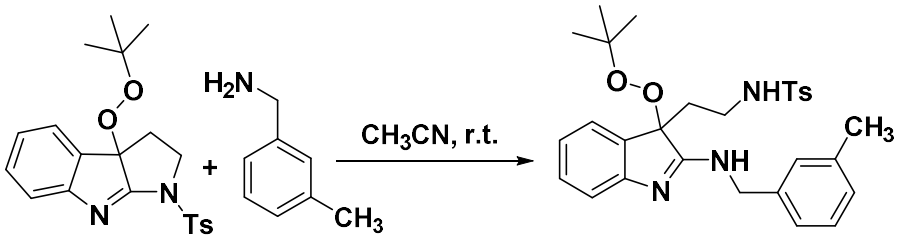
TLC: R_f = 0.30 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.9 Hz, 2H), 7.50 (d, *J* = 2.3 Hz, 1H), 7.40 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.22 (s, 1H), 7.21 – 7.17 (m, 1H), 7.09 (d, *J* = 6.7 Hz, 1H), 6.99 (d, *J* = 7.2 Hz, 1H), 6.87 (t, *J* = 7.4 Hz, 1H), 5.56 (s, 1H), 4.93 (s, 1H), 4.84 (d, *J* = 15.0 Hz, 1H), 4.47 (d, *J* = 15.0 Hz, 1H), 2.90 – 2.76 (m, 2H), 2.39 (s, 3H), 2.27 – 2.20 (m, 1H), 2.09 – 2.03 (m, 1H), 1.13 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.41, 155.40, 143.60, 140.36, 136.61, 132.22, 130.80, 130.61, 130.57, 130.36, 129.81, 127.14, 126.42, 123.09, 122.84, 121.77, 117.36, 90.28, 81.06, 45.91, 38.28, 35.09, 26.51, 21.60.

HRMS (ESI): calcd for $C_{28}H_{33}BrN_3O_4S$ $[M + H]^+$ *m/z* 586.1370, found 586.1365.

Compound 5



N-(2-(3-(tert-butylperoxy)-2-((3-methylbenzyl) amino)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (160 mg, 0.4 mmol) in CH_3CN (4 mL) was added *m-tolylmethanamine* (55 μL, 0.44 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 3 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (203 mg, 97%) as yellow oil.

Physical state: yellow oil.

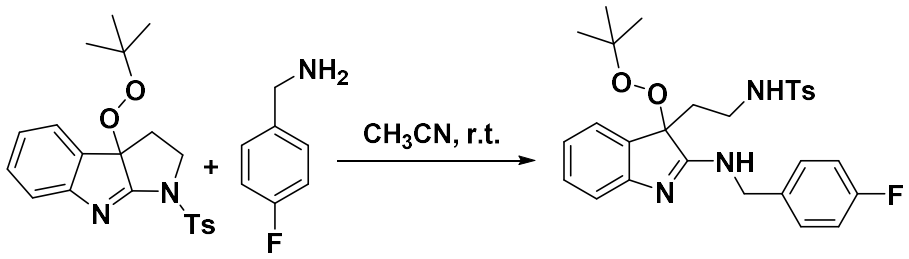
TLC: R_f = 0.35 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 4.8 Hz, 2H), 7.23 (s, 1H), 7.22 – 7.21 (m, 1H), 7.18 (s, 1H), 7.17 (d, *J* = 7.2 Hz, 1H), 7.12 (s, 1H), 7.11 (s, 1H), 6.97 – 6.94 (m, 1H), 6.88 – 6.83 (m, 1H), 5.46 (s, 1H), 4.87 (s, 1H), 4.74 (d, *J* = 14.4 Hz, 1H), 4.51 (s, 1H), 2.92 – 2.86 (m, 1H), 2.86 – 2.79 (m, 1H), 2.40 (s, 3H), 2.35 (s, 3H), 2.28 – 2.21 (m, 1H), 2.07 – 1.99 (m, 1H), 1.12 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.42, 155.61, 143.53, 138.59, 137.67, 136.68, 132.06, 130.60, 129.79, 128.79, 128.72, 128.60, 127.17, 125.03, 123.10, 121.62, 117.29, 90.27, 81.00, 55.34, 37.42, 33.06, 26.45, 21.59, 21.49.

HRMS (ESI): calcd for $C_{29}H_{36}N_3O_4S$ $[M + H]^+$ m/z 522.2421, found 522.2408.

Compound 6



N-(2-(3-(tert-butylperoxy)-2-((4-fluorobenzyl) amino)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (160 mg, 0.4 mmol) in CH_3CN (4 mL) was added *(4-fluorophenyl) methanamine* (50 μL, 0.44 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 4 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (197 mg, 94%) as a cream white solid.

Physical state: cream white solid.

Melting point: 55 - 56 °C.

TLC: R_f = 0.38 (petroleum ether/EtOAc = 1:2).

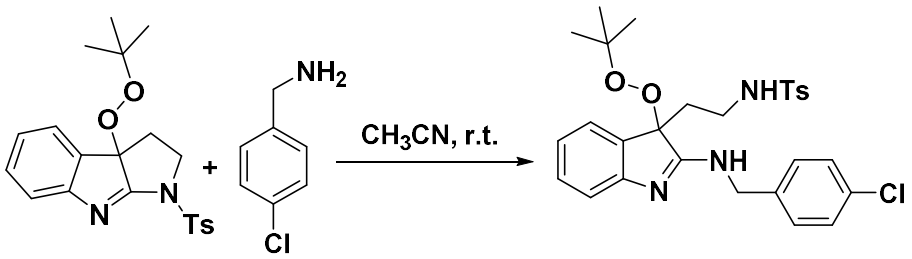
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.38 – 7.33 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.23 – 7.21 (m, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 7.01 (t, *J* = 8.7 Hz, 2H), 6.97 (d, *J* = 8.6 Hz, 1H), 6.89 – 6.85 (m, 1H), 5.49 (s, 1H), 4.80 (s, 1H), 4.76 (s, 1H), 4.50 (d, *J* = 14.6 Hz, 1H), 2.93 – 2.84 (m, 1H), 2.84 – 2.74 (m, 1H), 2.40 (s, 3H), 2.27 – 2.19 (m, 1H), 2.11 – 2.03 (m, 1H), 1.11 (s, 9H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 171.61, 161.65 (d, *J* = 240.0 Hz), 156.67, 143.24, 137.53, 136.15 (d, *J* = 3.1 Hz), 133.46, 130.15, 129.47 (d, *J* = 8.0 Hz), 126.97, 123.32, 120.89, 116.38, 115.27 (d, *J* = 21.2 Hz), 89.59, 80.19, 44.75, 37.90, 34.44, 26.81, 21.46.

^{19}F NMR (471 MHz, DMSO-d_6) δ -116.29.

HRMS (ESI): calcd for $C_{28}H_{33}FN_3O_4S$ $[M + H]^+$ m/z 526.2170, found 526.2175.

Compound 7



N-(2-(3-(tert-butylperoxy)-2-((4-chlorobenzyl) amino)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (160 mg, 0.4 mmol) in CH_3CN (4 mL) was added *(4-chlorophenyl)methanamine* (54 μL, 0.44 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 5 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (206 mg, 95%) as a yellow oil.

Physical state: yellow oil.

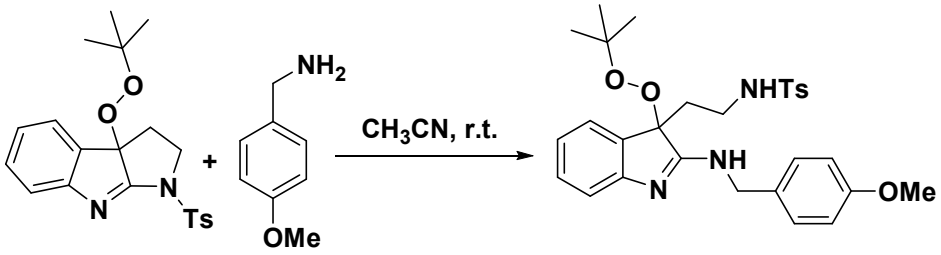
TLC: R_f = 0.33 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 1.7 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.31 – 7.28 (m, 2H), 7.26 – 7.24 (m, 2H), 7.24 – 7.21 (m, 1H), 7.10 (d, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 7.3 Hz, 1H), 6.90 – 6.85 (m, 1H), 5.53 (s, 1H), 4.79 (d, *J* = 26.1 Hz, 2H), 4.51 (d, *J* = 14.9 Hz, 1H), 2.91 – 2.76 (m, 2H), 2.41 (d, *J* = 1.7 Hz, 3H), 2.27 – 2.20 (m, 1H), 2.12 – 2.04 (m, 1H), 1.12 (s, 9H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 171.59, 156.60, 143.23, 139.11, 137.54, 133.47, 131.67, 130.17, 129.37, 128.52, 126.96, 123.33, 120.92, 116.39, 89.58, 80.20, 79.67, 44.78, 37.89, 34.46, 26.82, 21.48.

HRMS (ESI): calcd for $C_{28}H_{33}ClN_3O_4S$ $[M + H]^+$ m/z 542.1875, found 542.1860.

Compound 8



N-(2-(3-(tert-butylperoxy)-2-((4-methoxybenzyl) amino)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) in CH_3CN (3 mL) was added *(4-methoxyphenyl)methanamine* (43 μL, 0.33 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 3 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (150 mg, 93%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 101 - 103 °C.

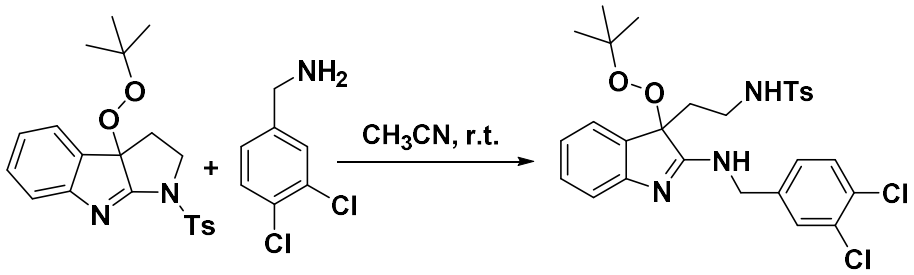
TLC: R_f = 0.33 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 6.9 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.25 – 7.22 (m, 2H), 7.10 (s, 1H), 6.98 – 6.92 (m, 1H), 6.86 (s, 2H), 6.85 (s, 1H), 5.45 (s, 1H), 4.99 (s, 1H), 4.70 (d, *J* = 13.4 Hz, 1H), 4.47 (d, *J* = 12.9 Hz, 1H), 3.79 (s, 3H), 2.82 (d, *J* = 33.1 Hz, 2H), 2.39 (s, 3H), 2.22 (s, 1H), 2.03 (d, *J* = 28.9 Hz, 1H), 1.10 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.02, 143.51, 139.38, 136.67, 132.11, 130.54, 129.89, 129.78, 127.16, 123.09, 121.64, 120.14, 117.19, 113.73, 113.10, 90.19, 80.97, 55.35, 46.78, 38.26, 35.04, 26.44, 21.58.

HRMS (ESI): calcd for $C_{29}H_{36}N_3O_5S$ $[M + H]^+$ m/z: 538.2370, found 538.2370.

Compound 9



N-(2-(3-(tert-butylperoxy)-2-((3,4-dichlorobenzyl) amino)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of 3*a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) in CH_3CN (3 mL) was added *(3,4-dichlorophenyl) methanamine* (44 μL, 0.33 mmol) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (163 mg, 94%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 98 - 100 °C.

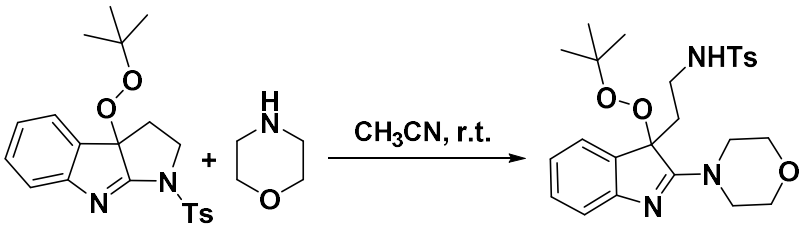
TLC: R_f = 0.33 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.45 (d, *J* = 1.9 Hz, 1H), 7.38 – 7.34 (m, 1H), 7.25 – 7.23 (m, 2H), 7.23 (s, 1H), 7.21 (t, *J* = 3.5 Hz, 1H), 7.07 (d, *J* = 7.9 Hz, 1H), 7.00 (d, *J* = 7.2 Hz, 1H), 6.88 (t, *J* = 7.4 Hz, 1H), 5.56 (s, 1H), 4.95 (s, 1H), 4.84 (d, *J* = 15.0 Hz, 1H), 4.46 (d, *J* = 15.3 Hz, 1H), 2.89 – 2.73 (m, 2H), 2.40 (s, 3H), 2.26 – 2.20 (m, 1H), 2.13 – 2.06 (m, 1H), 1.13 (s, 9H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 171.56, 156.43, 143.23, 141.38, 137.52, 133.44, 131.36, 130.75, 130.20, 130.13, 129.65, 129.34, 127.86, 126.98, 123.81, 121.04, 116.48, 89.55, 80.27, 44.37, 37.88, 34.47, 26.82, 21.48.

HRMS (ESI): calcd for $C_{28}H_{32}Cl_2N_3O_4S$ $[M + H]^+$ *m/z* :576.1485, found 576.1475.

Compound 10



N-(2-(3-(tert-butylperoxy)-2-morpholino-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added *morpholine* (48 μL, 0.55mol) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:1) to give the desired product (236 mg, 97%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 65 - 67 °C.

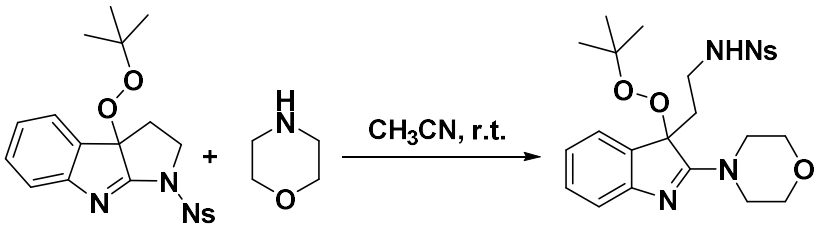
TLC: R_f = 0.21 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.59 (d, *J* = 8.3 Hz, 2H), 7.24 (s, 2H), 7.21 – 7.17 (m, 1H), 7.03 (d, *J* = 7.7 Hz, 1H), 7.01 – 6.98 (m, 1H), 6.89 – 6.83 (m, 1H), 4.53 (s, 1H), 3.97 – 3.82 (m, 4H), 3.81 (s, 4H), 2.73 – 2.63 (m, 2H), 2.41 (s, 3H), 2.25 – 2.17 (m, 2H), 1.09 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.74, 153.96, 143.56, 136.60, 133.30, 130.09, 129.77, 127.09, 122.32, 121.40, 116.50, 91.29, 80.68, 66.87, 46.12, 38.38, 35.36, 26.50, 21.57.

HRMS (ESI): calcd for $C_{25}H_{34}N_3O_5S$ $[M + H]^+$ m/z: 488.2214, found 488.2220.

Compound 11



N-(2-(3-(tert-butylperoxy)-2-morpholino-3H-indol-3-yl) ethyl)-4-nitrobenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-((4-nitrophenyl) sulfonyl)-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (216 mg, 0.5 mmol) in CH_3CN (5 mL) was added *morpholine* (48 μL, 0.55mol) to form a homogeneous solution. The mixture was stirred at r.t. for 2 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:2) to give the desired product (252 mg, 97%) as a yellow solid.

Physical state: yellow solid.

Melting point: 159 - 160 °C.

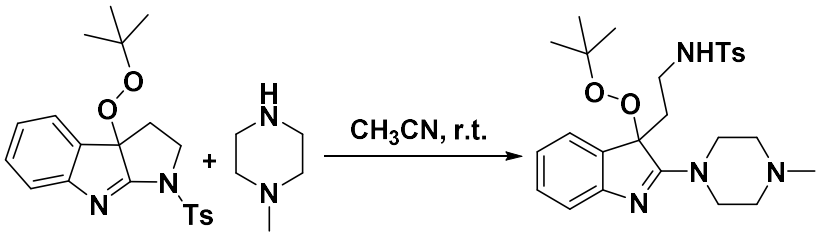
TLC: R_f = 0.22 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 Hz, $CDCl_3$) δ 8.28 (d, *J* = 8.9 Hz, 2H), 7.85 (d, *J* = 8.8 Hz, 2H), 7.23 – 7.18 (m, 1H), 7.04 (d, *J* = 7.3 Hz, 1H), 7.01 (d, *J* = 7.7 Hz, 1H), 6.92 – 6.86 (m, 1H), 4.81 (s, 1H), 3.92 (s, 4H), 3.83 (s, 4H), 2.77 – 2.63 (m, 2H), 2.36 – 2.19 (m, 2H), 1.10 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.76, 145.40, 133.16, 130.29, 128.27, 124.40, 122.31, 121.64, 116.49, 91.14, 80.86, 77.42, 77.17, 76.92, 66.85, 46.19, 38.62, 35.36, 26.49.

HRMS (ESI): calcd for $C_{24}H_{31}N_4O_7S$ $[M + H]^+$ m/z: 519.1908, found 519.1900.

Compound 12



N-(2-(3-(tert-butylperoxy)-2-(4-methylpiperazin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added *1-methylpiperazine* (61 µL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 6 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:2) to give the desired product (225 mg, 90%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 106 - 108 °C.

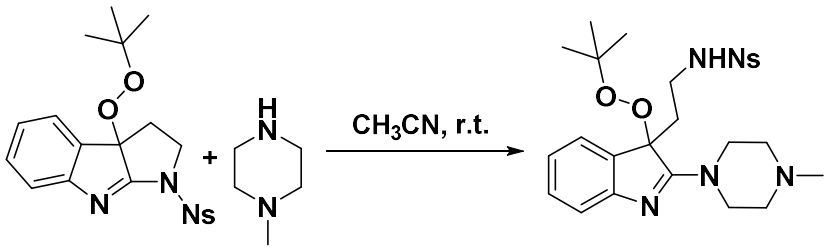
TLC: R_f = 0.21 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 7.6 Hz, 2H), 7.13 (t, *J* = 7.7 Hz, 1H), 6.97 (s, 1H), 6.94 (s, 1H), 6.86 – 6.77 (m, 1H), 5.07 (s, 1H), 3.97 – 3.60 (m, 4H), 2.71 – 2.56 (m, 2H), 2.51 – 2.43 (m, 4H), 2.36 (s, 3H), 2.29 (s, 3H), 2.25 – 2.10 (m, 2H), 1.06 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.73, 154.12, 143.45, 136.59, 133.42, 130.12, 129.89, 127.16, 122.38, 121.16, 116.32, 91.20, 54.93, 45.54, 37.77, 35.42, 26.49.

HRMS (ESI): calcd for $C_{26}H_{37}N_4O_4S$ $[M + H]^+$ m/z: 501.2530, found 501.2535.

Compound 13



N-(2-(3-(tert-butylperoxy)-2-(4-methylpiperazin-1-yl)-3H-indol-3-yl) ethyl)-4-nitrobenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-((4-nitrophenyl) sulfonyl)-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (130 mg, 0.3 mmol) in CH_3CN (3 mL) was added *1-methylpiperazine* (37 μL, 0.33 mmol) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (143 mg, 90%) as a yellow oil.

Physical state: yellow oil.

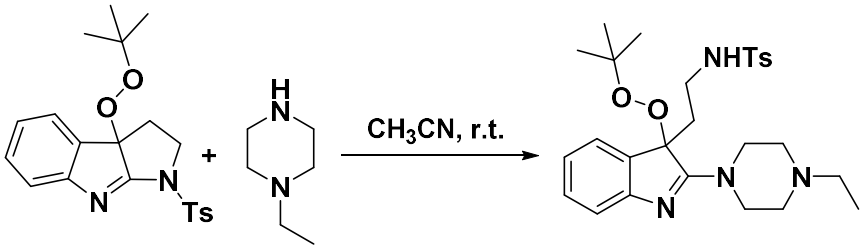
TLC: R_f = 0.23 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 9.3 Hz, 2H), 7.73 (t, *J* = 8.2 Hz, 2H), 7.10 – 7.03 (m, 1H), 6.99 (t, *J* = 5.3 Hz, 1H), 6.83 – 6.76 (m, 2H), 5.27 (s, 1H), 3.79 (s, 4H), 2.53 – 2.44 (m, 2H), 2.42 (s, 3H), 2.21 (d, *J* = 4.3 Hz, 4H), 2.19 – 2.12 (m, 2H), 1.01 (s, 9H).

^{13}C NMR (126 MHz $CDCl_3$) δ 209.82, 170.50, 153.92, 149.87, 145.62, 133.29, 130.06, 128.20, 124.29, 122.22, 121.36, 116.20, 90.92, 80.62, 55.98, 54.84, 46.56, 46.13, 45.52, 38.27, 35.50, 26.43.

HRMS (ESI): calcd for $C_{25}H_{34}N_5O_6S$ $[M + H]^+$ m/z: 532.2224, found 532.2230.

Compound 14



N-(2-(3-(tert-butylperoxy)-2-(4-ethylpiperazin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) in CH_3CN (3 mL) was added *1-ethylpiperazine* (42 μL, 0.33 mmol) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (CH_2CH_2:MeOH = 20:1) to give the desired product (139 mg, 90%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 118 - 119 °C.

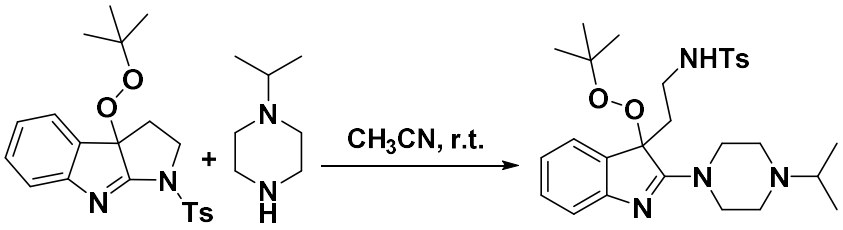
TLC: R_f = 0.22 (CH_2CH_2/MeOH = 20:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.01 (d, *J* = 7.7 Hz, 1H), 6.97 (d, *J* = 7.3 Hz, 1H), 6.84 (t, *J* = 7.4 Hz, 1H), 4.51 (s, 1H), 3.85 (d, *J* = 16.4 Hz, 4H), 2.73 – 2.65 (m, 2H), 2.55 (d, *J* = 24.3 Hz, 4H), 2.48 (d, *J* = 7.1 Hz, 2H), 2.40 (s, 3H), 2.25 – 2.17 (m, 2H), 1.09 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.69, 153.93, 143.48, 136.58, 133.31, 130.02, 129.76, 127.10, 122.28, 121.24, 116.38, 91.27, 80.56, 52.64, 52.41, 45.60, 38.40, 35.48, 26.49, 21.58, 11.96.

HRMS (ESI): calcd for $C_{27}H_{39}N_4O_4S$ $[M + H]^+$ m/z: 515.2687 ,found 515.2689.

Compound 15



N-(2-(3-(tert-butylperoxy)-2-(4-isopropylpiperazin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (160 mg, 0.4 mmol) in CH_3CN (4 mL) was added *1-isopropylpiperazine* (63 µL, 0.44 mmol) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (190 mg, 90%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 125 - 127 °C.

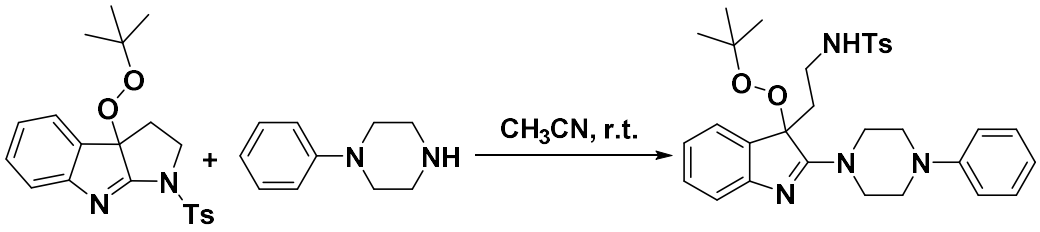
TLC: R_f = 0.26 (CH_2CH_2/MeOH = 20:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.56 (d, *J* = 8.5 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 7.15 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 3.9 Hz, 1H), 6.95 (s, 1H), 6.81 (t, *J* = 7.4 Hz, 1H), 4.96 (s, 1H), 3.95 – 3.70 (m, 4H), 2.78 – 2.66 (m, 2H), 2.64 (s, 1H), 2.62 (t, *J* = 4.9 Hz, 4H), 2.38 (s, 3H), 2.25 – 2.14 (m, 2H), 1.07 (s, 9H), 1.05 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.66, 154.06, 143.46, 136.59, 133.34, 130.00, 129.74, 127.11, 122.28, 121.14, 116.37, 91.25, 81.51, 54.75, 48.62, 45.98, 38.43, 35.45, 26.50, 21.58, 18.50.

HRMS (ESI): calcd for $C_{27}H_{41}N_4O_4S$ $[M + H]^+$ m/z: 529.2843 ,found 529.2843.

Compound 16



N-(2-(3-(tert-butylperoxy)-2-(4-phenylpiperazin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added *1-phenylpiperazine* (84 µL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 4 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:2) to give the desired product (267 mg, 95%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 103 - 105 °C.

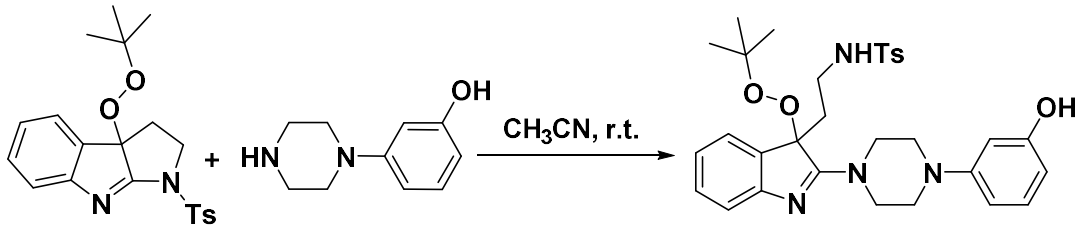
TLC: R_f = 0.50 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.58 (d, *J* = 8.3 Hz, 2H), 7.33 – 7.28 (m, 2H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.21 – 7.18 (m, 1H), 7.04 (d, *J* = 7.7 Hz, 1H), 7.02 – 6.99 (m, 1H), 6.97 (d, *J* = 7.6 Hz, 2H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.89 – 6.85 (m, 1H), 4.52 (s, 1H), 4.03 (d, *J* = 5.8 Hz, 2H), 3.98 (s, 2H), 3.33 – 3.25 (m, 4H), 2.76 – 2.64 (m, 2H), 2.38 (s, 3H), 2.26 (t, *J* = 6.8 Hz, 2H), 1.10 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.64, 153.99, 151.19, 143.55, 136.54, 133.35, 130.11, 129.80, 129.35, 127.14, 122.36, 121.38, 120.50, 116.72, 116.50, 91.32, 83.41, 49.60, 45.58, 38.44, 35.50, 26.55, 21.57.

HRMS (ESI): calcd for $C_{31}H_{39}N_4O_4S$ $[M + H]^+$ m/z: 563.2687 found 563.2689

Compound 17



N-(2-(3-(tert-butylperoxy)-2-(4-(3-hydroxyphenyl) piperazin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) *3-(piperazin-1-yl) phenol* (98 mg, 0.55 mmol) in CH_3CN (5 mL) to form a homogeneous solution. The mixture was stirred at r.t. for 6 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:2) to give the desired product (260 mg, 90%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 114 - 116 °C.

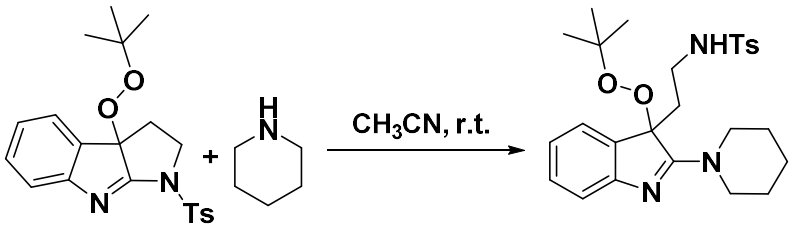
TLC: R_f = 0.56 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.57 (d, *J* = 7.9 Hz, 2H), 7.18 (s, 1H), 7.17 (s, 1H), 7.16 (s, 1H), 7.05 (d, *J* = 6.6 Hz, 2H), 7.03 (s, 1H), 6.88 (t, *J* = 7.3 Hz, 1H), 6.42 (d, *J* = 8.3 Hz, 1H), 6.40 – 6.37 (m, 1H), 6.36 (s, 1H), 5.21 (s, 1H), 4.16 – 3.69 (m, 4H), 3.23 – 3.06 (m, 4H), 2.67 (d, *J* = 6.9 Hz, 2H), 2.34 (s, 3H), 2.25 (d, *J* = 7.0 Hz, 2H), 1.09 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.33, 157.87, 152.75, 152.36, 143.64, 136.36, 132.78, 130.23, 130.15, 129.84, 127.13, 122.50, 121.70, 116.22, 108.35, 107.87, 104.10, 91.27, 80.84, 50.50, 44.24, 38.29, 35.52, 26.53, 21.57, 11.33.

HRMS (ESI): calcd for $C_{31}H_{39}N_4O_5S$ $[M + H]^+$ m/z: 579.2636,found 579.2642.

Compound 18



N-(2-(3-(tert-butylperoxy)-2-(piperidin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added *piperidine* (50 µL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (235 mg, 98%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 137 - 138 °C.

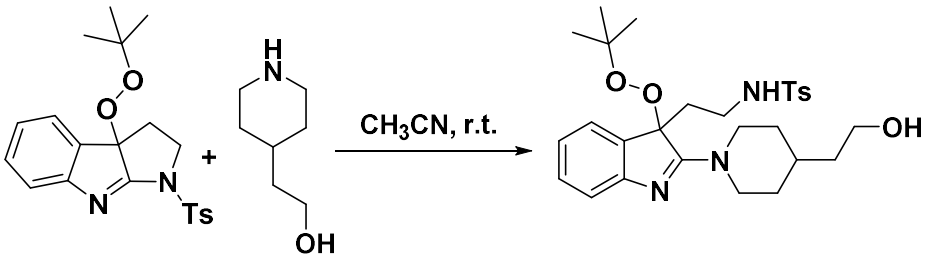
TLC: R_f = 0.62 (CH_2CH_2/MeOH = 50:1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.3 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.14 – 7.10 (m, 1H), 6.97 – 6.95 (m, 1H), 6.94 (d, J = 7.5 Hz, 1H), 6.81 – 6.76 (m, 1H), 5.11 (s, 1H), 3.73 (d, *J* = 20.7 Hz, 4H), 2.67 – 2.58 (m, 2H), 2.36 (s, 3H), 2.19 (t, *J* = 7.0 Hz, 2H), 1.64 (s, 4H), 1.08 (s, 9H).

^{13}C NMR (126 MHz $CDCl_3$) δ 170.51, 154.27, 143.37, 136.65, 133.20, 129.90, 129.71, 122.28, 120.77, 116.03, 91.23, 80.40, 46.81, 38.47, 35.41, 26.50, 26.14, 24.43, 21.55.

HRMS (ESI): calcd for $C_{26}H_{36}N_3O_4S$ $[M + H]^+$ m/z: 486.2421,found 486.2417.

Compound 19



N-(2-(3-(tert-butylperoxy)-2-(4-(2-hydroxyethyl) piperidin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (160 mg, 0.4 mmol) *2-(piperidin-4-yl) ethan-1-ol* (57 mg, 0.44 mmol) in CH_3CN (4 mL) to form a homogeneous solution. The mixture was stirred at r.t. for 5h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (CH_2CH_2/MeOH = 20:1) to give the desired product (192 mg, 91%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 94 - 95 °C.

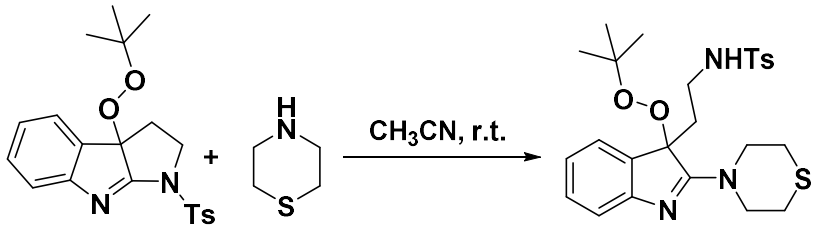
TLC: R_f = 0.32 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 6.6 Hz, 2H), 7.16 – 7.11 (m, 1H), 6.97 (s, 1H), 6.95 (d, *J* = 6.6 Hz, 1H), 6.80 (t, *J* = 7.4 Hz, 1H), 5.16 (s, 1H), 4.53 (t, *J* = 17.1 Hz, 2H), 3.68 (t, *J* = 5.3 Hz, 2H), 3.03 (d, *J* = 19.5 Hz, 2H), 2.61 (s, 2H), 2.37 (s, 3H), 2.26 – 2.14 (m, 2H), 1.77 (d, *J* = 13.3 Hz, 2H), 1.72 (s, 1H), 1.57 – 1.47 (m, 2H), 1.35 (t, *J* = 10.7 Hz, 2H), 1.07 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.51, 154.03, 143.43, 136.63, 133.10, 129.96, 129.78, 127.07, 122.31, 120.94, 115.99, 91.26, 80.48, 59.98, 46.17, 39.15, 38.44, 35.55, 32.44, 26.52, 21.58.

HRMS (ESI): calcd for $C_{28}H_{40}N_3O_5S$ $[M + H]^+$ m/z: 530.2683, found 530.2680.

Compound 20



N-(2-(3-(tert-butylperoxy)-2-thiomorpholino-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) in CH_3CN (3 mL) was added *thiomorpholine* (33 µL, 0.33 mmol) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (143 mg, 95%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 113 - 115 °C.

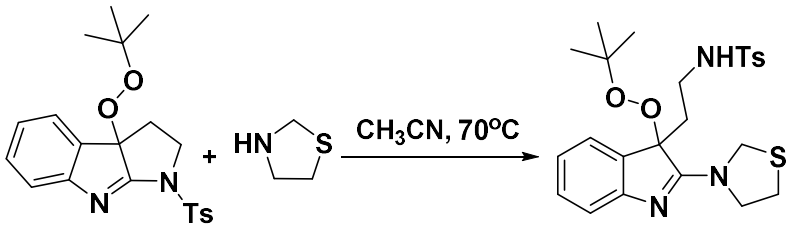
TLC: R_f = 0.38 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.58 (d, *J* = 7.8 Hz, 2H), 7.25 (d, *J* = 7.1 Hz, 2H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.99 (s, 1H), 6.86 (t, *J* = 7.4 Hz, 1H), 4.43 (d, *J* = 5.2 Hz, 1H), 4.04 (d, *J* = 43.1 Hz, 4H), 2.76 (s, 4H), 2.69 – 2.62 (m, 2H), 2.41 (s, 3H), 2.24 – 2.14 (m, 2H), 1.10 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.43, 153.79, 143.59, 136.49, 133.27, 130.06, 129.79, 127.12, 122.39, 121.39, 116.52, 91.29, 81.99, 48.33, 38.38, 35.31, 27.60, 26.53, 21.60.

HRMS (ESI): calcd for $C_{25}H_{34}N_3O_4S_2$ $[M + H]^+$ m/z: 504.1985 found 504.1985.

Compound 21



N-(2-(3-(tert-butylperoxy)-2-(thiazolidin-3-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added *thiazolidine* (43 µL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at 70 °C for 3 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAC = 2:1) to give the desired product (184 mg, 75%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 70 - 72 °C.

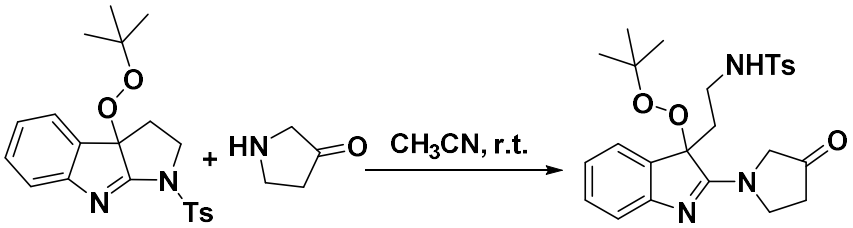
TLC: R_f = 0.56 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.57 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.19 – 7.14 (m, 1H), 7.01 (s, 1H), 6.99 (d, *J* = 9.0 Hz, 1H), 6.86 (t, *J* = 7.2 Hz, 1H), 5.15 (s, 1H), 4.78 (s, 2H), 4.39 – 3.78 (m, 2H), 3.12 – 3.02 (m, 2H), 2.69 – 2.62 (m, 2H), 2.38 (s, 3H), 2.33 – 2.13 (m, 2H), 1.09 (s, 9H).

^{13}C NMR (126 MHz, DMSO-d6) δ 169.04, 154.78, 143.37, 137.42, 133.91, 130.18, 127.10, 122.78, 121.74, 116.66, 90.69, 80.53, 79.71, 49.60, 37.76, 33.86, 30.55, 26.61, 21.49.

HRMS (ESI): calcd for $C_{24}H_{32}N_3O_4S_2$ $[M + H]^+$ m/z: 490.1829 found 490.1832.

Compound 22



N-(2-(3-(tert-butylperoxy)-2-(3-oxopyrrolidin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) *3-pyrrolidinone* (40 mg, 0.33 mmol) in CH_3CN (3 mL) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:1) to give the desired product (117 mg, 80%) as a black oil.

Physical state: black oil.

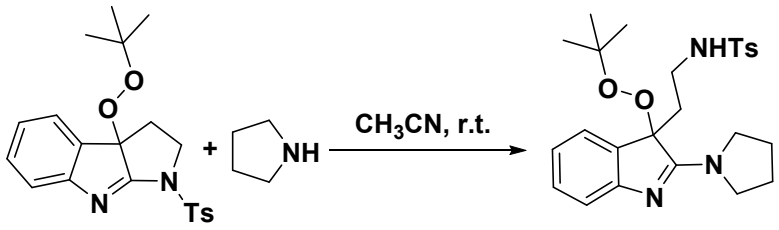
TLC: R_f = 0.32 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 Hz, $CDCl_3$)δ 7.58 (d, *J* = 7.9 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 7.5 Hz, 1H), 7.07 (d, *J* = 7.7 Hz, 1H), 7.03 (d, *J* = 7.2 Hz, 1H), 6.89 (t, *J* = 7.4 Hz, 1H), 4.74 (s, 1H), 4.23 (s, 2H), 4.14 (s, 1H), 2.85 – 2.75 (m, 1H), 2.75 – 2.65 (m, 2H), 2.64 – 2.54 (m, 1H), 2.39 (s, 3H), 2.35 (d, *J* = 4.4 Hz, 1H), 2.16 (s, 1H), 1.10 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 210.74, 170.66, 154.14, 143.53, 136.67, 132.93, 130.19, 129.75, 127.01, 122.50, 121.89, 116.63, 91.32, 80.79, 53.43, 44.66, 38.24, 34.21, 29.76, 26.50, 21.54.

HRMS (ESI): calcd for $C_{25}H_{32}N_3O_5S$ $[M + H]^+$ m/z: 486.2057, found 486.2057.

Compound 23



N-(2-(3-(tert-butylperoxy)-2-(pyrrolidin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added *pyrrolidine* (46 µL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 20 minutes. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (CH_2Cl_2/MeOH = 20:1) to give the desired product (200 mg, 85%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 75 - 76 °C.

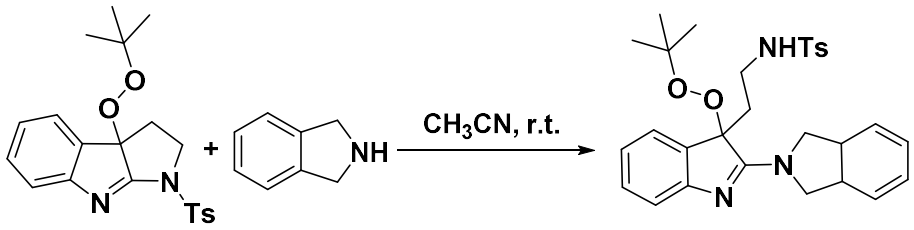
TLC: R_f = 0.32 (CH_2CH_2/MeOH = 20:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.59 (d, *J* = 8.3 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.14 (m, 1H), 7.04 (d, *J* = 7.7 Hz, 1H), 7.00 – 6.96 (m, 1H), 6.85 – 6.79 (m, 1H), 4.98 (s, 1H), 4.16 (s, 1H), 3.78 – 3.71 (m, 2H), 3.70 (d, *J* = 14.1 Hz, 1H), 2.75 (t, *J* = 6.7 Hz, 1H), 2.59 (t, *J* = 6.8 Hz, 1H), 2.48 – 2.42 (m, 1H), 2.39 (s, 3H), 2.20 – 2.14 (m, 1H), 2.11 – 2.03 (m, 1H), 1.98 (s, 2H), 1.11 (s, 9H).

^{13}C NMR (126 MHz, CD_3OD) δ 169.71, 154.35, 143.36, 136.70, 132.47, 130.02, 129.77, 127.06, 122.49, 120.96, 115.74, 91.13, 80.38, 46.27, 38.37, 34.02, 26.53, 24.02, 21.58.

HRMS (ESI): calcd for $C_{25}H_{34}N_3O_4S$ $[M + H]^+$ m/z: 472.2265, found 472.2269.

Compound 24



N-(2-(3-(tert-butylperoxy)-2-(1,3,3a,7a-tetrahydro-2H-isoindol-2-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) and *isoindoline* (66 mg, 0.55 mmol) in CH_3CN (5 mL) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (242 mg, 93%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 172 -174 °C.

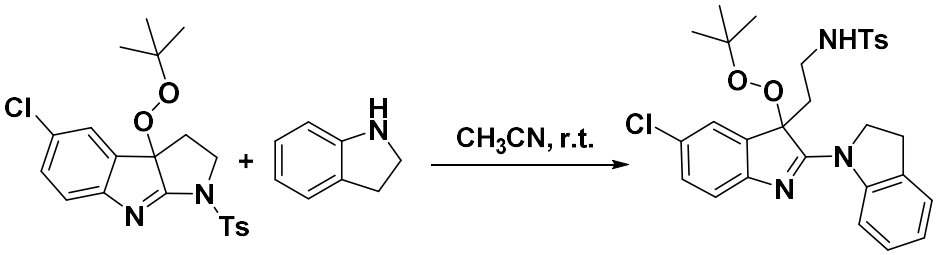
TLC: R_f=0.29 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.52 (d, *J* = 6.5 Hz, 2H), 7.34 (s, 2H), 7.23 – 7.19 (m, 1H), 7.13 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 7.7 Hz, 1H), 7.03 (d, *J* = 7.4 Hz, 1H), 6.87 (t, *J* = 7.4 Hz, 1H), 5.37 (d, *J* = 14.1 Hz, 1H), 5.10 (d, *J* = 14.6 Hz, 2H), 4.89 (d, *J* = 14.8 Hz, 1H), 4.64 (s, 1H), 2.79 – 2.70 (m, 2H), 2.47 – 2.39 (m, 1H), 2.34 (s, 3H), 2.32 – 2.26 (m, 1H), 1.10 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.21, 154.95, 143.44, 136.50, 133.09, 130.13, 129.70, 127.64, 127.61, 127.07, 122.77, 122.55, 121.30, 116.58, 91.37, 80.60, 55.61, 51.95, 38.42, 33.48, 26.54, 21.54.

HRMS (ESI): calcd for $C_{29}H_{34}N_3O_4S$ $[M + H]^+$ m/z: 520.2265, found 520.2272.

Compound 25



N-(2-(3-(tert-butylperoxy)-5-chloro-2-(indolin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-5-chloro-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (217 mg, 0.5 mmol) in CH_3CN (5 mL) was added *indoline* (62 μL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 5 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (266 mg, 96%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 105 - 107 °C.

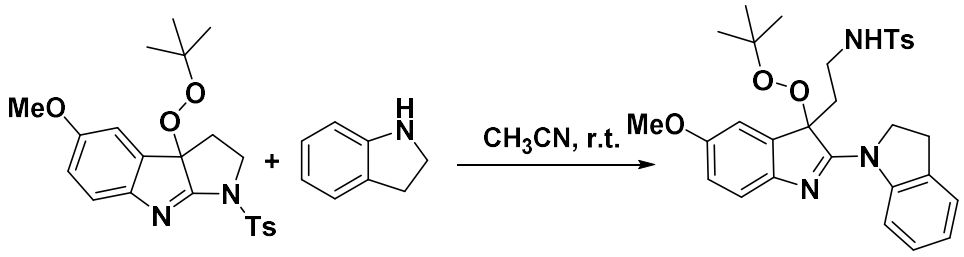
TLC: R_f= 0.80 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 8.45 (d, *J* = 8.2 Hz, 1H), 7.50 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 4.6 Hz, 1H), 7.26 – 7.24 (m, 1H), 7.19 – 7.17 (m, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.08 – 7.05 (m, 1H), 7.05 – 7.03 (m, 1H), 7.00 (d, *J* = 2.1 Hz, 1H), 4.67 – 4.60 (m, 1H), 4.46 (s, 1H), 4.37 – 4.30 (m, 1H), 3.29 – 3.15 (m, 2H), 2.78 – 2.63 (m, 2H), 2.45 – 2.39 (m, 1H), 2.37 (s, 3H), 2.32 – 2.24 (m, 1H), 1.12 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 167.83, 153.34, 144.15, 143.68, 136.03, 134.67, 131.89, 129.93, 129.83, 127.58, 127.16, 127.11, 124.66, 123.54, 122.49, 118.39, 117.49, 92.31, 80.89, 62.72, 47.91, 38.22, 33.79, 28.77, 26.54, 21.64.

HRMS (ESI): calcd for $C_{29}H_{33}ClN_3O_4S$ $[M + H]^+$ m/z: 554.1875, found 554.1876.

Compound 26



N-(2-(3-(tert-butylperoxy)-2-(indolin-1-yl)-5-methoxy-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-5-methoxy-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (215 mg, 0.5 mmol) in CH_3CN (5 mL) was added *indoline* (62 μL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 5 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (264 mg, 96%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 137 - 139 °C.

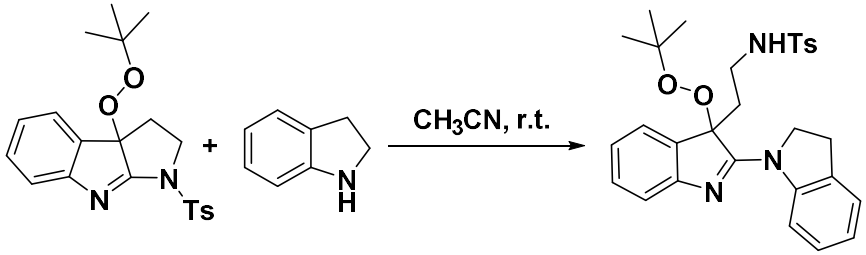
TLC: R_f=0.50 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 8.43 – 8.38 (m, 1H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.11 (d, *J* = 2.9 Hz, 1H), 7.09 (d, *J* = 3.4 Hz, 1H), 7.08 – 7.05 (m, 1H), 7.03 – 6.98 (m, 1H), 6.79 – 6.74 (m, 1H), 6.71 (t, *J* = 3.3 Hz, 1H), 4.63 – 4.54 (m, 1H), 4.44 (s, 1H), 4.33 – 4.25 (m, 1H), 3.78 (s, 3H), 3.19 (d, *J* = 8.1 Hz, 2H), 2.78 – 2.62 (m, 2H), 2.36 (s, 3H), 2.35 – 2.21 (m, 2H), 1.12 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.68, 155.78, 147.91, 144.52, 143.45, 136.26, 134.31, 131.62, 129.74, 127.51, 127.09, 124.51, 122.88, 117.75, 117.04, 114.09, 109.69, 92.51, 80.63, 55.87, 47.92, 38.31, 34.01, 28.75, 26.60, 21.59.

HRMS (ESI): calcd for $C_{30}H_{36}N_3O_5S$ $[M + H]^+$ m/z: 550.2370, found 550.2368.

Compound 27



N-(2-(3-(tert-butylperoxy)-2-(indolin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added *indoline* (62 µL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 1 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (252 mg, 97%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 83 - 85 °C.

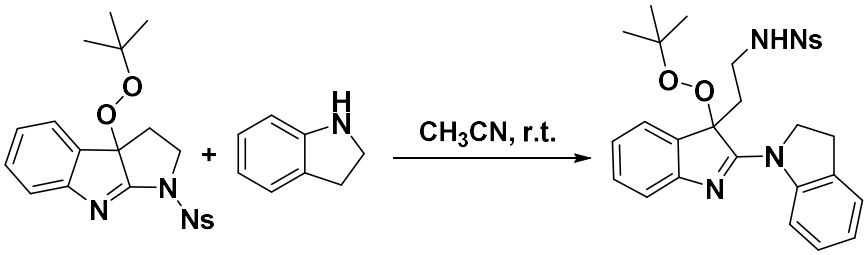
TLC: R_f = 0.58 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 8.46 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 2.0 Hz, 1H), 7.24 (d, *J* = 3.4 Hz, 1H), 7.24 – 7.21 (m, 1H), 7.16 – 7.14 (m, 1H), 7.13 (d, *J* = 7.7 Hz, 2H), 7.08 – 7.05 (m, 1H), 7.05 – 7.01 (m, 1H), 6.94 – 6.91 (m, 1H), 4.68 – 4.61 (m, 1H), 4.36 – 4.29 (m, 2H), 3.26 – 3.14 (m, 2H), 2.82 – 2.66 (m, 2H), 2.38 (s, 3H), 2.37 – 2.28 (m, 2H), 1.11 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 167.77, 154.72, 144.41, 143.45, 136.29, 132.85, 131.79, 130.04, 129.73, 127.53, 127.12, 124.54, 123.20, 122.32, 122.08, 117.63, 117.44, 92.42, 80.61, 47.93, 38.38, 33.82, 28.78, 26.58, 21.59.

HRMS (ESI): calcd for $C_{29}H_{34}N_3O_4S$ $[M + H]^+$ m/z: 520.2265, found 520.2271.

Compound 28



N-(2-(3-(tert-butylperoxy)-2-(indolin-1-yl)-3H-indol-3-yl) ethyl)-4-nitrobenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-((4-nitrophenyl) sulfonyl)-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (216 mg, 0.5 mmol) in CH_3CN (5 mL) was added *indoline* (62 µL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 2 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:2) to give the desired product (252 mg, 97%) as a yellow solid.

Physical state: yellow solid.

Melting point: 80 - 82 °C.

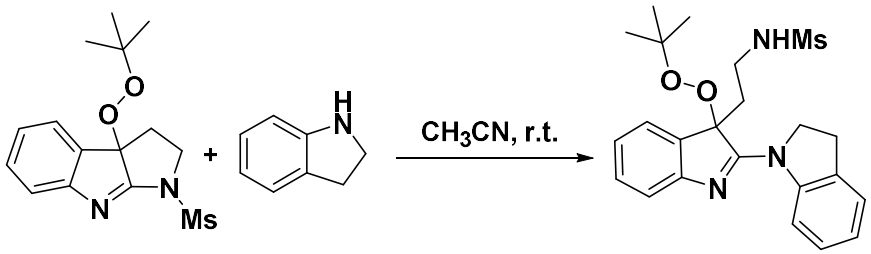
TLC: R_f= 0.68 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 8.38 (d, *J* = 8.1 Hz, 1H), 8.09 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.26 (d, *J* = 1.4 Hz, 1H), 7.25 – 7.23 (m, 1H), 7.20 (d, *J* = 7.3 Hz, 1H), 7.14 – 7.13 (m, 1H), 7.12 (d, *J* = 4.1 Hz, 1H), 7.05 – 7.02 (m, 1H), 6.99 – 6.95 (m, 1H), 5.06 (d, *J* = 6.4 Hz, 1H), 4.66 – 4.59 (m, 1H), 4.38 – 4.32 (m, 1H), 3.25 – 3.18 (m, 2H), 2.73 – 2.64 (m, 2H), 2.52 – 2.46 (m, 1H), 2.33 – 2.27 (m, 1H), 1.10 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 167.73, 154.52, 149.95, 145.00, 144.20, 132.74, 131.82, 130.29, 128.27, 127.59, 124.76, 124.33, 123.55, 122.36, 122.26, 117.67, 117.23, 92.27, 80.77, 48.06, 38.57, 33.85, 28.73, 26.54.

HRMS (ESI): calcd for $C_{28}H_{31}N_4O_6S$ $[M + H]^+$ m/z: 551.1959, found 551.1960.

Compound 29



N-(2-(3-(tert-butylperoxy)-2-(indolin-1-yl)-3H-indol-3-yl) ethyl) methanesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-(methylsulfonyl)-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (162 mg, 0.5 mmol) in CH_3CN (5 mL) was added *indoline* (62 μL, 0.55 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 2 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (215 mg, 97%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 75 - 77 °C.

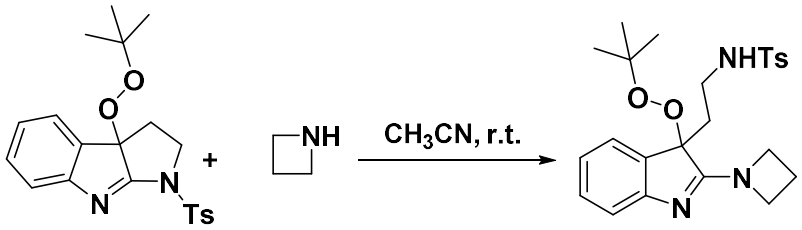
TLC: R_f= 0.38 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.27 (m, 1H), 7.25 (s, 1H), 7.23 (d, *J* = 1.3 Hz, 1H), 7.22 – 7.21 (m, 1H), 7.19 (d, *J* = 1.2 Hz, 1H), 7.04 – 7.01 (m, 1H), 7.01 – 6.97 (m, 1H), 4.76 – 4.67 (m, 1H), 4.46 – 4.37 (m, 1H), 4.20 – 4.09 (m, 1H), 3.24 (t, *J* = 8.3 Hz, 2H), 3.02 – 2.86 (m, 2H), 2.73 (s, 3H), 2.52 – 2.30 (m, 2H), 1.26 (d, *J* = 17.2 Hz, 3H), 1.12 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 167.88, 154.85, 144.39, 133.01, 131.90, 130.24, 127.56, 124.62, 123.31, 122.36, 122.24, 117.61, 117.41, 92.43, 80.66, 48.05, 40.01, 38.55, 34.45, 28.77, 26.58.

HRMS (ESI): calcd for $C_{23}H_{30}N_3O_4S$ $[M + H]^+$ m/z: 444.1952, found 444.1948.

Compound 30



N-(2-(2-(azetidin-1-yl)-3-(tert-butylperoxy)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) and *azetidine* (31 mg, 0.33 mmol) in CH_3CN (3 mL) to form a homogeneous solution. The mixture was stirred at r.t. for 6 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:2) to give the desired product (135 mg, 98%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 139 – 141 °C.

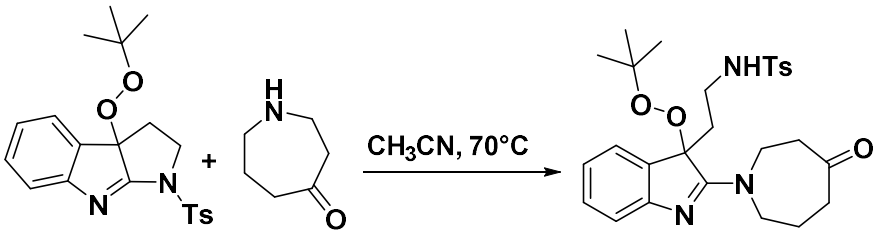
TLC: R_f = 0.22 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.3 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.18 – 7.14 (m, 1H), 7.01 (d, *J* = 7.7 Hz, 1H), 6.96 (d, *J* = 6.0 Hz, 1H), 6.81 (t, *J* = 7.9 Hz, 1H), 4.76 (s, 1H), 4.53 – 4.39 (m, 2H), 4.38 – 4.31 (m, 1H), 2.78 – 2.69 (m, 2H), 2.46 (s, 2H), 2.40 (s, 3H), 2.22 – 2.14 (m, 2H), 1.12 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 171.09, 155.13, 143.37, 136.77, 132.41, 130.13, 129.72, 127.09, 122.79, 121.06, 116.28, 91.00, 80.46, 77.42, 77.17, 76.91, 51.62, 38.37, 33.97, 26.53, 21.56, 17.79.

HRMS (ESI): calcd for $C_{24}H_{32}N_3O_4S$ $[M + H]^+$ m/z: 458.2108, found 458.2110.

Compound 31



N-(2-(3-(tert-butylperoxy)-2-(4-oxoazepan-1-yl)-3H-indol-3-yl)ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) and *azepan-4-one* (49 mg, 0.33 mmol) in CH_3CN (3 mL) to form a homogeneous solution. The mixture was stirred at 70°C for 1 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 1:1) to give the desired product (137 mg, 89%) as a yellow oil.

Physical state: yellow oil.

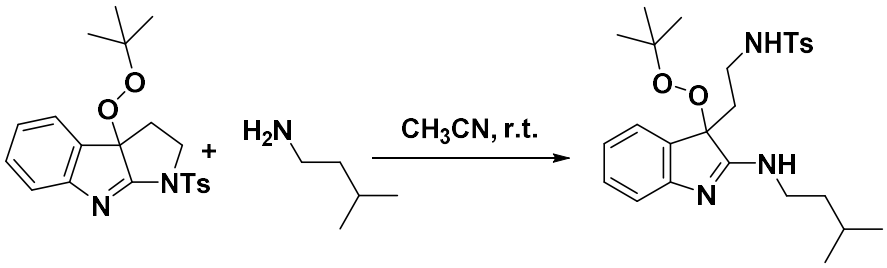
TLC: R_f = 0.26 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.55 (d, *J* = 7.9 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.15 (m, 1H), 7.02 (s, 1H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.85 (t, *J* = 7.4 Hz, 1H), 4.83 (s, 1H), 4.35 – 3.93 (m, 2H), 3.81 (t, *J* = 34.6 Hz, 2H), 2.95 (d, *J* = 34.3 Hz, 1H), 2.71 (d, *J* = 6.2 Hz, 2H), 2.69 (s, 1H), 2.61 – 2.55 (m, 2H), 2.38 (s, 3H), 2.25 (t, *J* = 7.0 Hz, 2H), 1.99 (d, *J* = 22.6 Hz, 2H), 1.08 (s, 9H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 211.81, 170.15, 153.94, 143.54, 136.56, 133.31, 130.10, 129.77, 127.06, 122.09, 121.38, 116.59, 91.51, 80.91, 50.37, 42.73, 38.45, 35.34, 26.54, 21.57.

HRMS (ESI): calcd for $C_{27}H_{36}N_3O_5S$ $[M + H]^+$ m/z: 514.2370, found 514.2375.

Compound 32



N-(2-(3-(tert-butylperoxy)-2-(isopentylamino)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (120 mg, 0.3 mmol) in CH_3CN (3 mL) was added *3-methylbutan-1-amine* (38 μL, 0.33 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 1 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (142 mg, 97%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 79 – 82 °C.

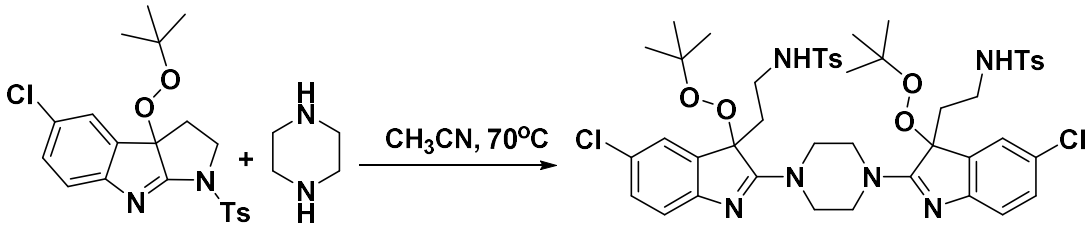
TLC: R_f = 0.37 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 Hz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.23 – 7.19 (m, 1H), 7.10 (d, *J* = 7.7 Hz, 1H), 6.94 – 6.90 (m, 1H), 6.85 – 6.81 (m, 1H), 5.18 (s, 1H), 4.70 (s, 1H), 3.56 – 3.48 (m, 1H), 3.48 – 3.40 (m, 1H),2.91 – 2.84 (m, 1H), 2.84 – 2.74 (m, 1H), 2.42 (s, 3H), 2.29 – 2.20 (m, 1H), 2.07 – 2.00 (m, 1H), 1.74 – 1.67 (m, 1H), 1.58 – 1.49 (m, 2H), 1.17 (s, 9H), 0.96 (d, *J* = 1.5 Hz, 3H), 0.95 (d, *J* = 1.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.46, 155.86, 143.51, 136.64, 131.97, 130.45, 129.74, 127.13, 123.07, 121.30, 117.01, 90.16, 80.88, 41.00, 38.17, 35.07, 26.49, 25.92, 22.53, 21.57.

HRMS (ESI): calcd for $C_{26}H_{38}N_3O_4S$ $[M + H]^+$ m/z: 488.2578, found 488.2586.

Compound 33



N, N'-((piperazine-1,4-diylbis(3-(tert-butylperoxy)-5-chloro-3H-indole-2,3-diyl)) bis(ethane-2,1-diyl)) bis(4-methylbenzenesulfonamide)

To a solution of *3a-(tert-butylperoxy)-5-chloro-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (174 mg, 0.4 mmol) piperazine and (17 mg, 0.2 mmol) in CH_3CN (4 mL) to form a homogeneous solution. The mixture was stirred at 70 ^oC for 4 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether: EtOAc = 4:1) to give the desired product (126 mg, 66%) as a creamy white oil.

Physical state: creamy white oil.

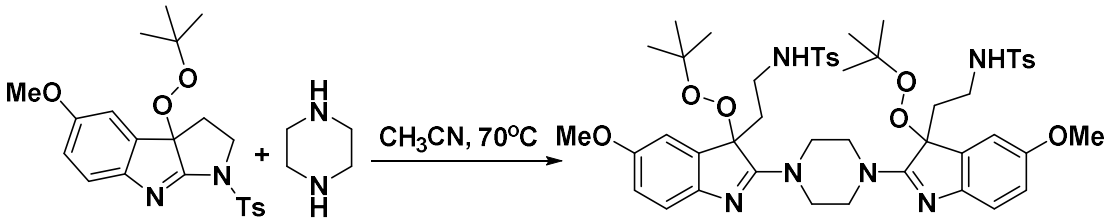
TLC: R_f = 0.56 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 – 7.52 (m, 4H), 7.24 – 7.18 (m, 4H), 7.15 – 7.11 (m, 2H), 6.99 – 6.96 (m, 2H), 6.91 – 6.88 (m, 2H), 5.11 (s, 1H), 4.43 – 3.53 (m, 7H), 2.69 – 2.54 (m, 4H), 2.36 (s, 6H), 2.32 – 2.18 (m, 4H), 1.11 (s, 18H).

^{13}C NMR (126 MHz $CDCl_3$) δ 170.71, 152.63, 143.74, 136.28, 135.20, 129.99, 129.88, 127.05, 126.62, 122.56, 117.29, 91.21, 81.10, 45.36, 38.24, 35.55, 26.49, 21.59.

HRMS (ESI): calcd for $C_{46}H_{57}Cl_2N_6O_8S_2$ $[M + H]^+$ m/z: 955.3051, found 955.3053.

Compound 34



N, N'-((piperazine-1,4-diylbis(3-(tert-butylperoxy)-5-methoxy-3H-indole-2,3-diyl)) bis(ethane-2,1-diyl)) bis(4-methylbenzenesulfonamide)

To a solution of *3a-(tert-butylperoxy)-5-methoxy-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (172 mg, 0.4 mmol) and piperazine (17 mg, 0.2 mmol) in CH_3CN (4 mL) to form a homogeneous solution. The mixture was stirred at 70 °C for 4 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (CH_2CH_2/MeOH = 50:1) to give the desired product (125 mg, 66%) as a creamy white oil.

Physical state: creamy white oil.

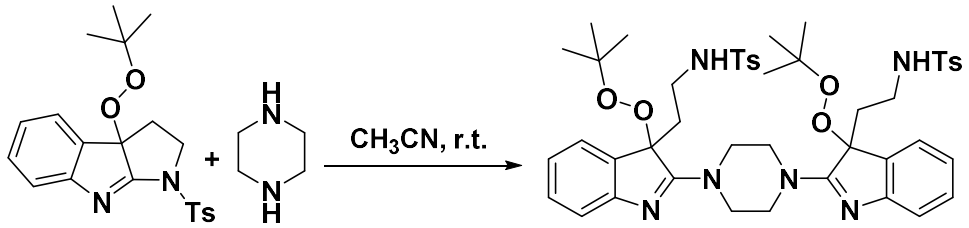
TLC: R_f = 0.39 (CH_2CH_2/MeOH = 20:1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.51 (m, 4H), 7.18 (t, *J* = 8.4 Hz, 4H), 6.92 – 6.87 (m, 2H), 6.73 – 6.69 (m, 2H), 6.68 (d, *J* = 2.6 Hz, 2H), 5.13 (s, 2H), 3.94 (s, 8H), 3.74 (s, 6H), 2.69 – 2.55 (m, 4H), 2.35 (s, 6H), 2.27 – 2.16 (m, 4H), 1.11 (s, 18H).

^{13}C NMR (126 MHz $CDCl_3$) δ 169.67, 155.35, 147.14, 143.51, 136.50, 134.76, 129.85, 129.72, 116.60, 114.31, 109.67, 91.43, 80.81, 55.89, 44.57, 38.30, 35.73, 26.55, 21.54.

HRMS (ESI): calcd for $C_{48}H_{63}N_6O_{10}S_2$ $[M + H]^+$ m/z: 947.4042, found 947.4042.

Compound 35



N, N'-((piperazine-1,4-diylbis(3-(tert-butylperoxy)-3H-indole-2,3-diyl)) bis(ethane-2,1-diyl)) bis(4-methylbenzenesulfonamide)

To a solution of 3*a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) and piperazine (22 mg, 0.25 mmol) in CH_3CN (5 mL) to form a homogeneous solution. The mixture was stirred at r.t overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (170 mg, 70%) as a creamy white solid.

Physical state: creamy white solid.

Melting point: 120 - 122 °C.

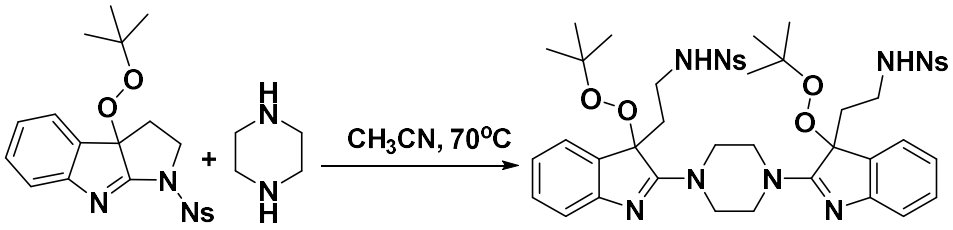
TLC: R_f = 0.16 (petroleum ether/EtOAc = 1:2).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 4H), 7.22 (d, *J* = 7.5 Hz, 4H), 7.20 (s, 2H), 7.05 (s, 2H), 7.03 (d, *J* = 6.7 Hz, 2H), 6.89 (t, *J* = 7.5 Hz, 2H), 4.75 (s, 2H), 4.11 (t, *J* = 36.4 Hz, 8H), 2.71 – 2.59 (m, 4H), 2.38 (s, 6H), 2.35 – 2.22 (m, 4H), 1.12 (s, 18H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.63, 170.51, 153.92, 143.55, 143.51, 136.56, 136.48, 133.32, 133.26, 130.11, 129.80, 129.77, 127.05, 127.03, 122.40, 121.53, 116.53, 116.46, 91.34, 89.36, 84.44, 45.62, 38.39, 35.69, 35.53, 26.53, 21.58.

HRMS (ESI): calcd for $C_{46}H_{59}N_6O_8S_2$ $[M + H]^+$ m/z: 887.3830, found 887.3830.

Compound 36



N, N'-((piperazine-1,4-diylbis(3-(tert-butylperoxy)-3H-indole-2,3-diyl)) bis(ethane-2,1-diyl)) bis(4-nitrobenzenesulfonamide)

To a solution of 3*a-(tert-butylperoxy)-1-((4-nitrophenyl) sulfonyl)-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (173 mg, 0.4 mmol) and piperazine (17 mg, 0.2 mmol) in CH_3CN (4 mL) to form a homogeneous solution. The mixture was stirred at 70 °C for 4h.TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether: EtOAc = 1:2) to give the desired product (133 mg, 70%) as a yellow solid.

Physical state: yellow solid.

Melting point: 122 - 124 °C.

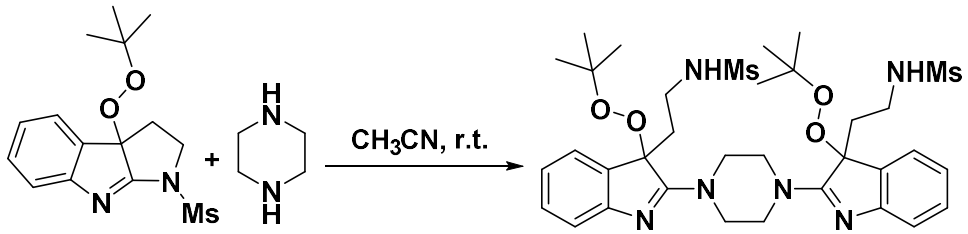
TLC: R_f = 0.26 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (t, *J* = 8.8 Hz, 4H), 7.84 – 7.78 (m, 4H), 7.22 – 7.17 (m, 2H), 7.09 (d, *J* = 8.5 Hz, 2H), 6.97 (d, *J* = 7.7 Hz, 2H), 6.94 – 6.89 (m, 2H), 5.60 (s, 1H), 4.12 (d, *J* = 53.9 Hz, 8H), 2.72 – 2.66 (m, 2H), 2.65 – 2.56 (m, 2H), 2.43 – 2.34 (m, 2H), 2.32 – 2.24 (m, 2H), 1.12 (s, 16H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.57, 153.61, 150.02, 145.28, 133.11, 130.30, 128.28, 124.44, 122.41, 121.85, 116.37, 91.19, 81.02, 45.51, 38.57, 35.69, 26.51.

HRMS (ESI): calcd for $C_{44}H_{53}N_8O_{12}S_2$ $[M + H]^+$ m/z: 949.3219, found 949.3219.

Compound 37



N, N'-((piperazine-1,4-diylbis(3-(tert-butylperoxy)-3H-indole-2,3-diyl)) bis(ethane-2,1-diyl)) dimethanesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-(methylsulfonyl)-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (130 mg, 0.4 mmol) and piperazine (17 mg, 0.2 mmol) in CH_3CN (4 mL) to form a homogeneous solution. The mixture was stirred at r.t. overnight. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete. Then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether: EtOAc = 2:1) to give the desired product (103 mg, 70%) as a yellow oil.

Physical state: yellow oil.

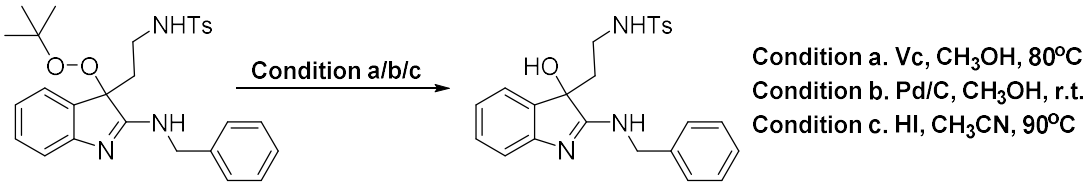
TLC: R_f = 0.23 (PE/EtOAc = 1:1).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 – 7.20 (m, 2H), 7.14 (d, *J* = 7.2 Hz, 2H), 7.09 – 7.04 (m, 2H), 6.93 (t, *J* = 6.8 Hz, 2H), 4.97 (s, 1H), 4.43 – 3.64 (m, 8H), 2.77 (s, 4H), 2.76 (s, 6H), 2.29 (t, *J* = 7.0 Hz, 4H), 1.11 (s, 18H).

^{13}C NMR (126 MHz $CDCl_3$) δ 170.57, 153.71, 133.18, 130.27, 122.37, 121.81, 116.44, 91.27, 80.85, 45.57, 39.97, 38.57, 35.93, 26.52.

HRMS (ESI): calcd for $C_{34}H_{51}N_6O_8S_2$ $[M + H]^+$ m/z: 735.3204, found 735.3210.

Compound 38



N-(2-(2-(benzylamino)-3-hydroxy-3H-indol-3-yl)ethyl)-4-methylbenzenesulfonamide

Condition a: To a solution of compound **1** (0.5 mmol, 254 mg) and Vc (2 mmol, 352mg) in CH_3OH (15 mL). The reaction mixture was stirred for 18 h at 80 °C. The reaction mixture was basified to pH 8−9 using saturated $NaHCO_3$ and extracted with EtOAc (50 mL). Then, the combined organic layers were washed with saturated brine (50 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by chromatography on silica gel (petroleum ether:EtOAc = 1:1) to give the desired product as a white solid (193mg, 89%).

Condition b: To a solution of compound **1** (0.5 mmol, 254 mg) in CH_3CN (3 mL) was added 10% Pd/C (76 mg). The reaction mixture was stirred at r.t. for 15 h. The mixture is filtered through diatomaceous earth. Then, the reaction mixture was basified to pH 8–9 using saturated $NaHCO_3$ and extracted with EtOAc (50 mL). Then, the combined organic layers were washed with saturated brine (50 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by chromatography on silica gel (petroleum ether:EtOAc = 1:1) to give the desired product as a white solid (152mg, 70%).

Condition c: To a solution of compound **1** (0.25 mmol, 127 mg) in CH_3CN (3 mL) was added HI (1 mmol, 9 μL). The reaction mixture was stirred for 5 h at 90 °C. The reaction mixture was basified to pH 8–9 using saturated $NaHCO_3$ and extracted with EtOAc (15 mL). Then, the combined organic layers were washed with saturated brine (15 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by chromatography on silica gel (petroleum ether:EtOAc = 1:1) to give the desired product as a white solid (90mg, 83%).

Physical state: white solid.

Melting point: 113 - 115 °C.

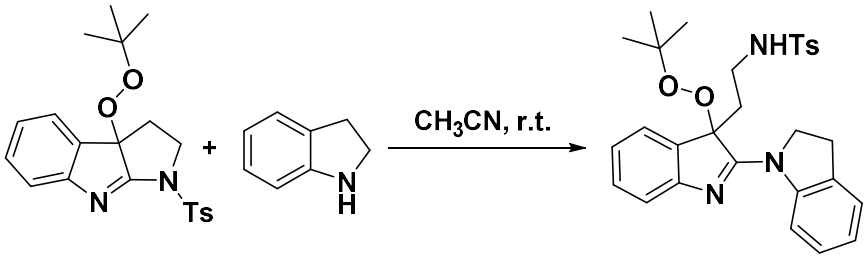
TLC: R_f = 0.35 (petroleum ether/EtOAc = 1:1).

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.31 (s, 1H), 7.99 (s, 1H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.48 (t, *J* = 5.6 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.30 (s, 2H), 7.29 (s, 1H), 7.25 – 7.21 (m, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 7.03 (d, *J* = 7.7 Hz, 1H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.80 (t, *J* = 7.3 Hz, 1H), 5.96 (s, 1H), 4.48 (s, 2H), 2.63 – 2.52 (m, 1H), 2.36 (s, 3H), 2.33 (d, *J* = 7.8 Hz, 1H), 2.12 – 2.03 (m, 1H), 1.92 – 1.85 (m, 1H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 176.13, 156.31, 143.09, 140.07, 137.81, 130.13, 129.57, 128.69, 127.55, 127.14, 126.96, 122.48, 120.81, 115.55, 80.69, 79.71, 45.39, 38.72, 38.34, 21.99.

HRMS (ESI): calcd for $C_{24}H_{26}N_3O_3S$ $[M + H]^+$ m/z: 436.1689, found 436.1689.

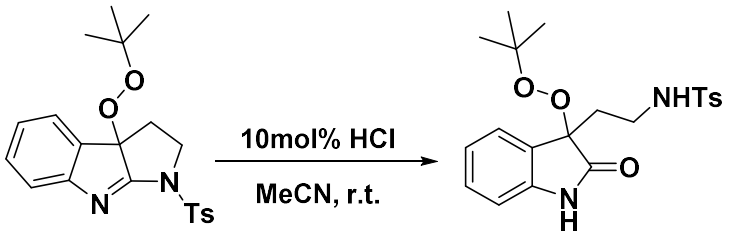
Gram-Scale Synthesis of 27



N-(2-(3-(tert-butylperoxy)-2-(indolin-1-yl)-3H-indol-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (1.2 g, 3 mmol) in CH_3CN (30 mL) was added *indoline* (370 µL, 3.3 mmol) to form a homogeneous solution. The mixture was stirred at r.t. for 1 h. TLC (petroleum ether:EtOAc = 4:1) indicated that the reaction was complete, then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product (1.56 g, 95%) as a creamy white solid.

The synthesis of peroxyoxindole



N-(2-(3-(tert-butylperoxy)-2-oxoindolin-3-yl) ethyl)-4-methylbenzenesulfonamide

To a solution of *3a-(tert-butylperoxy)-1-tosyl-1,2,3,3a-tetrahydropyrrolo[2,3-b] indole* (200 mg, 0.5 mmol) in CH_3CN (5 mL) was added 1N HCl (50 μL, 0.05 mmol). The mixture was stirred at r.t. for 10 min. Then the resulting mixture was diluted with ethyl acetate (20 mL), washed with saturated $NaHCO_3$ (10 mL), water (10 mL) and saturated brine (10 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and then concentrated to dryness under vacuum. The residue was purified by silica gel column chromatography (petroleum ether:EtOAc = 2:1) to give the desired product as a yellow solid (85 mg, 41%).

Physical state: yellow solid.

Melting point: 151 - 152 °C.

TLC: R_f = 0.37 (petroleum ether/EtOAc = 1:1).

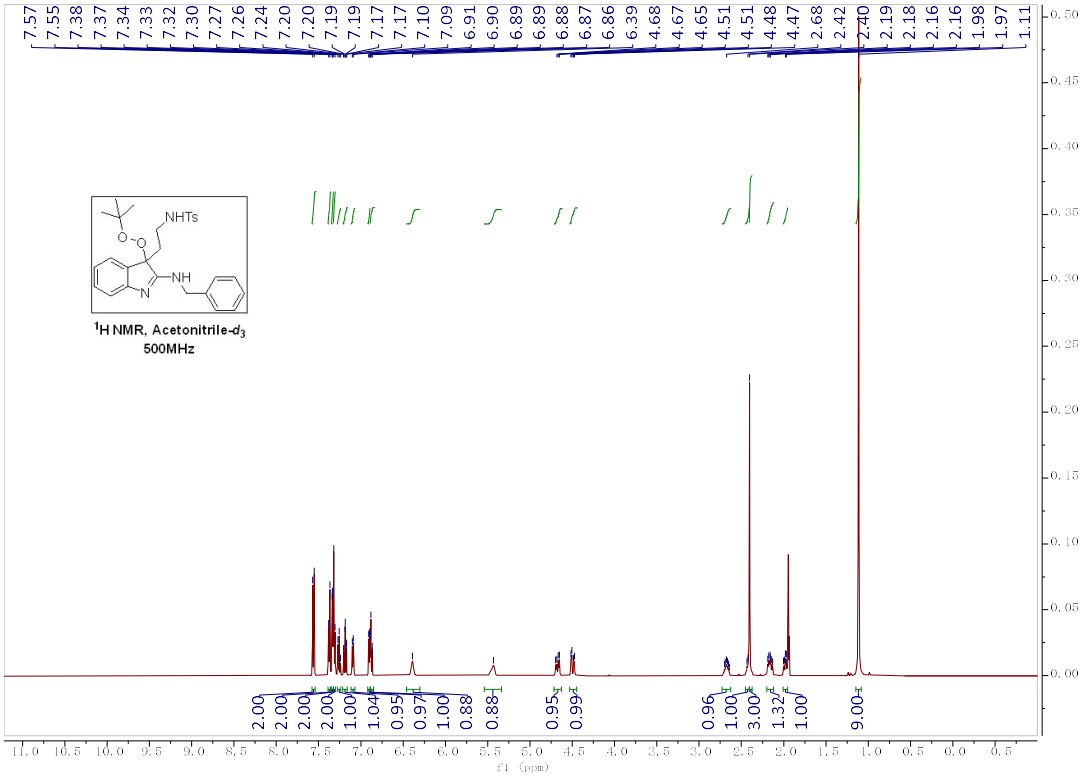
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.95 (s, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 5.9 Hz, 2H), 7.23 (d, *J* = 5.6 Hz, 1H), 7.19 (d, *J* = 7.4 Hz, 1H), 7.04 – 6.99 (m, 1H), 6.87 (d, *J* = 7.7 Hz, 1H), 5.96 – 5.88 (m, 1H), 3.11 – 3.01 (m, 2H), 2.38 (s, 3H), 2.28 – 2.20 (m, 1H), 2.04 – 1.97 (m, 1H), 1.06 (s, 9H).

^{13}C NMR (126 MHz $CDCl_3$) δ 177.04, 143.29, 141.29, 136.85, 130.03, 129.75, 127.91, 127.20, 124.67, 122.66, 110.76, 83.70, 80.87, 38.29, 32.50, 26.93, 21.57.

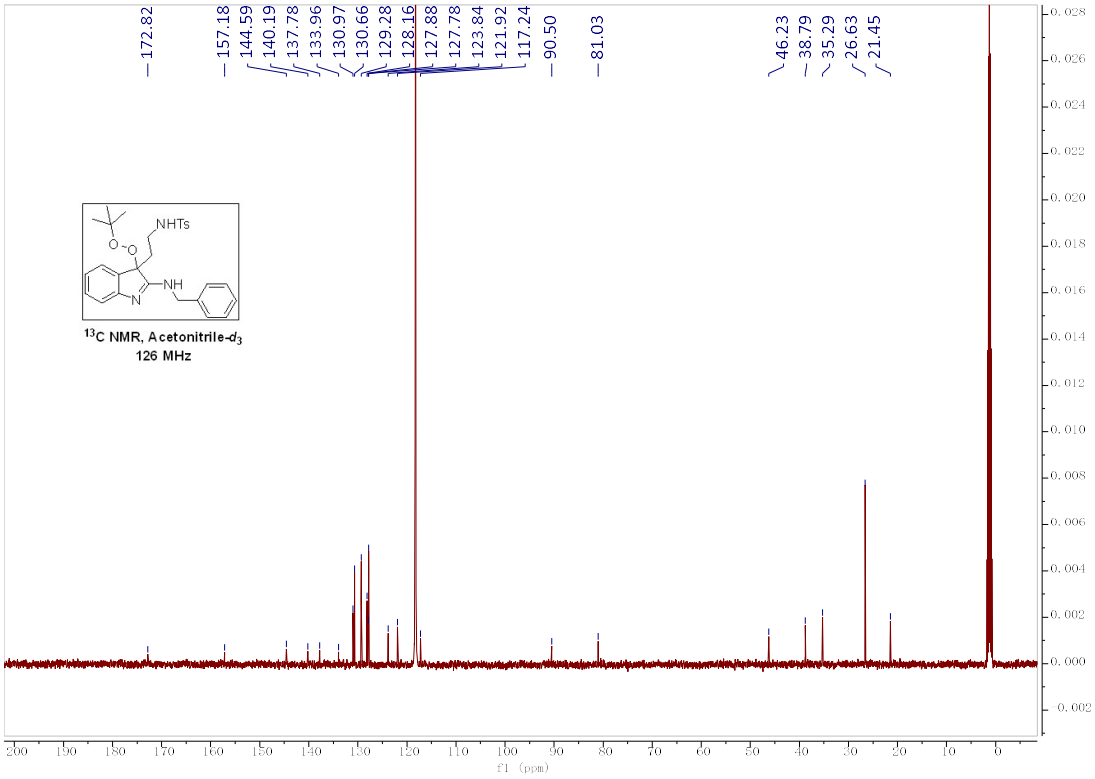
HRMS (ESI): calcd for $C_{21}H_{27}N_2O_5S$ [M + H]+ m/z: 419.1635, found 419.1630.

6. NMR Spectra

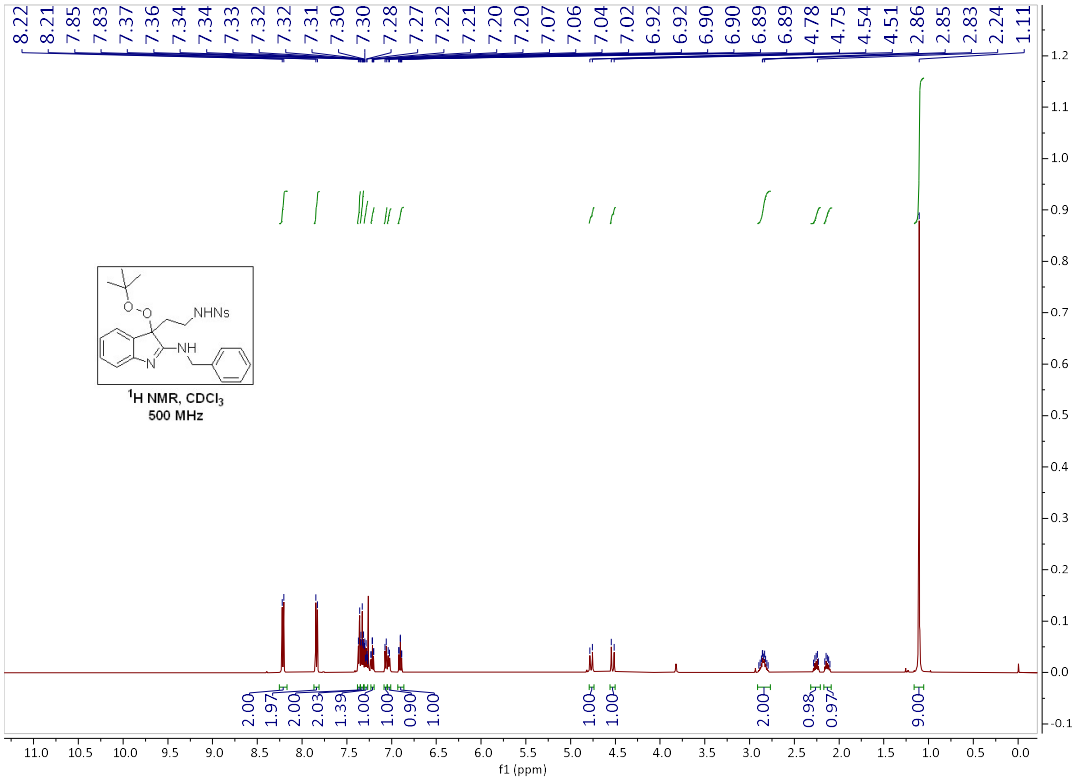
^{1}H NMR Spectrum of 1



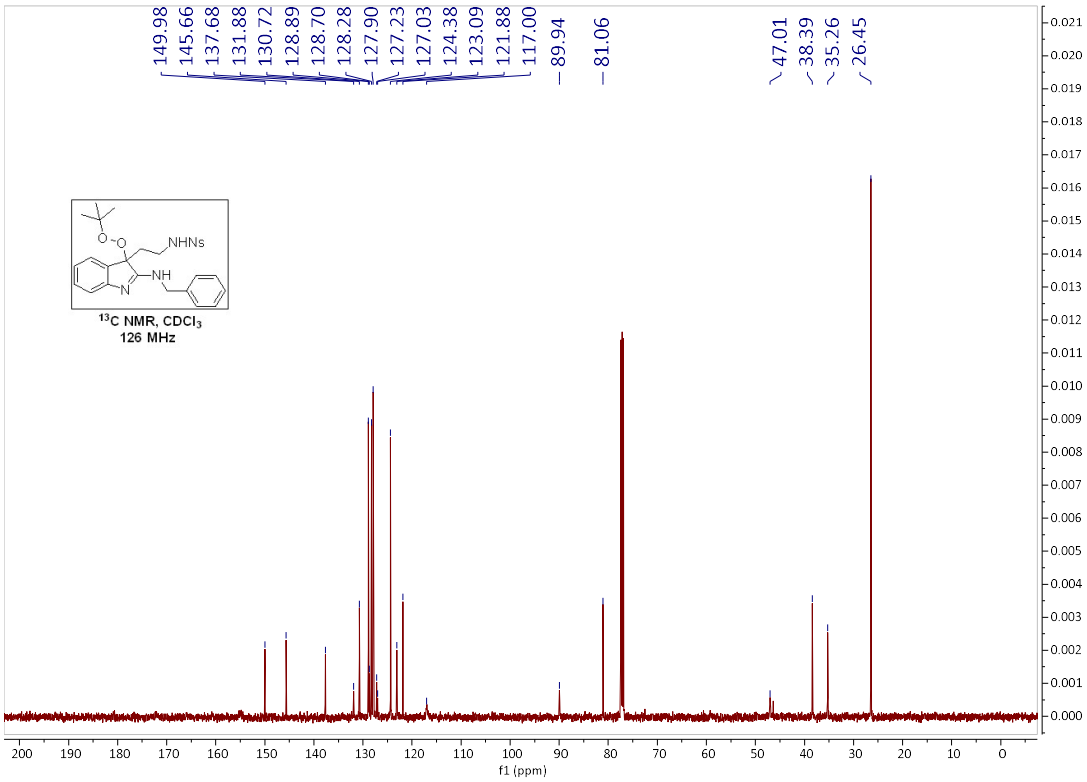
^{13}C NMR Spectrum of 1



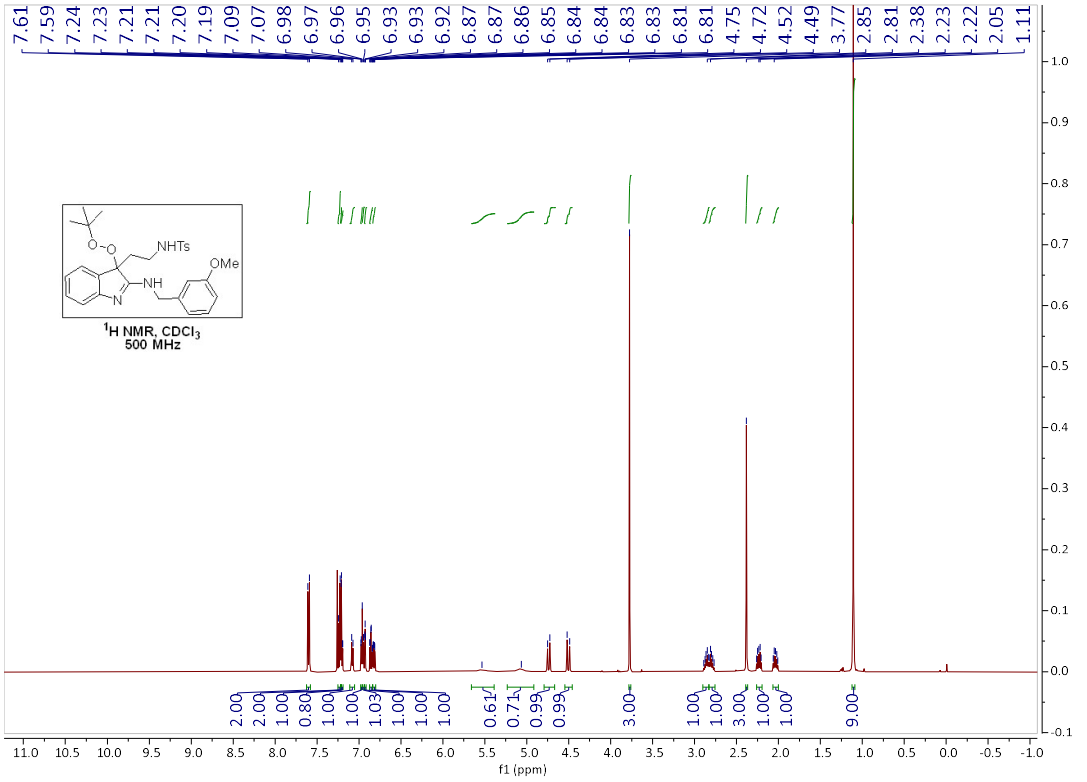
^{1}H NMR Spectrum of 2



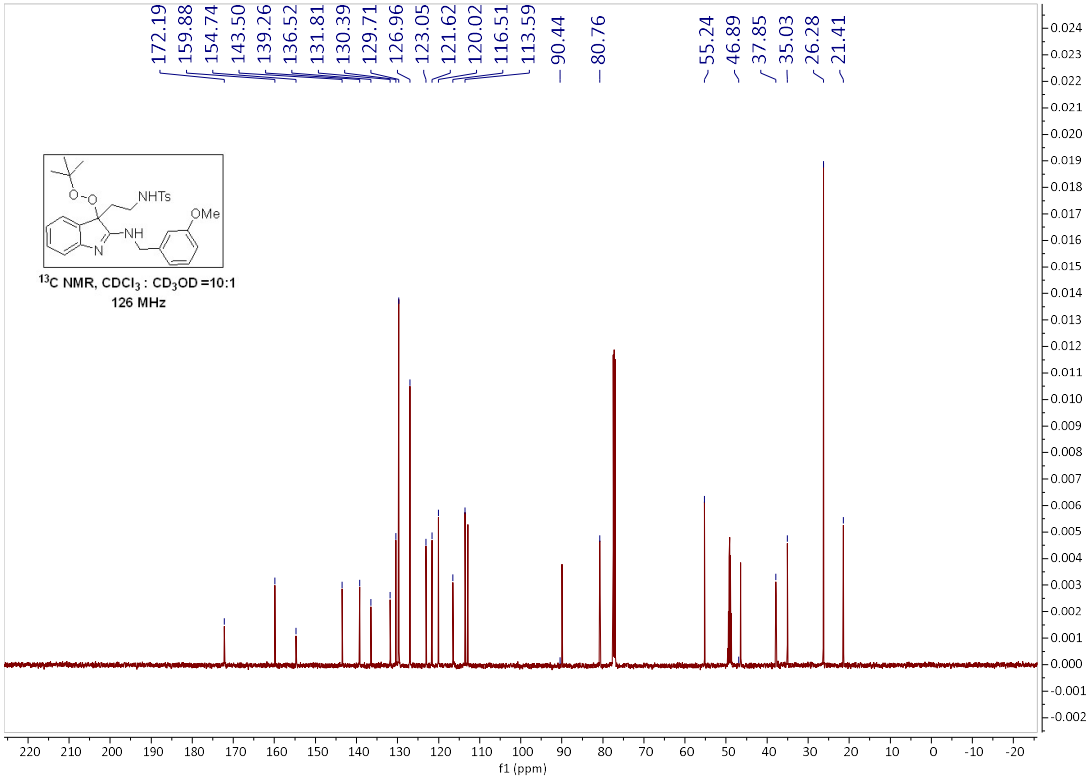
^{13}C NMR Spectrum of 2



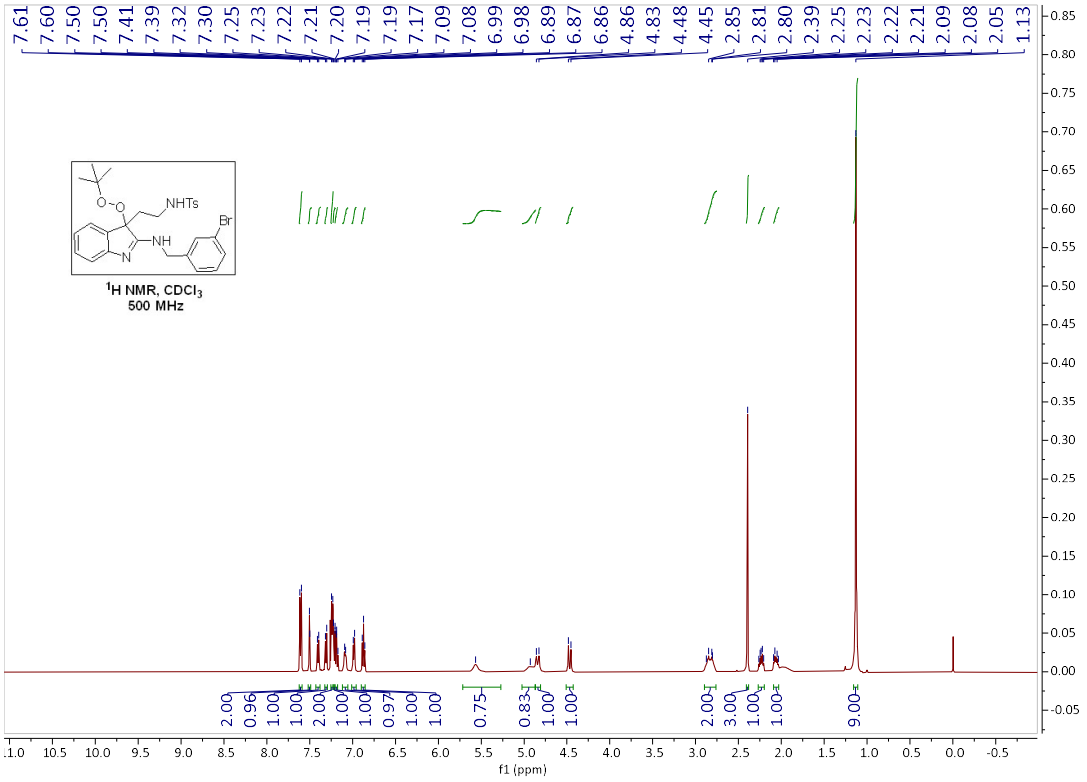
^{1}H NMR Spectrum of 3



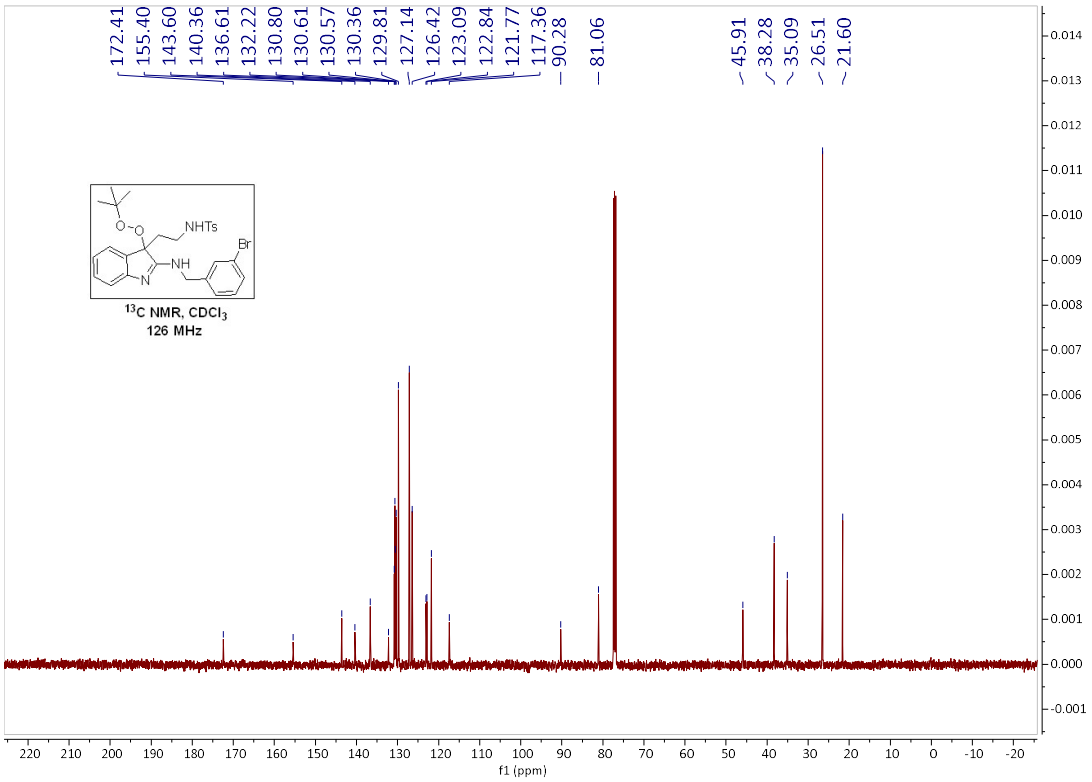
^{13}C NMR Spectrum of 3



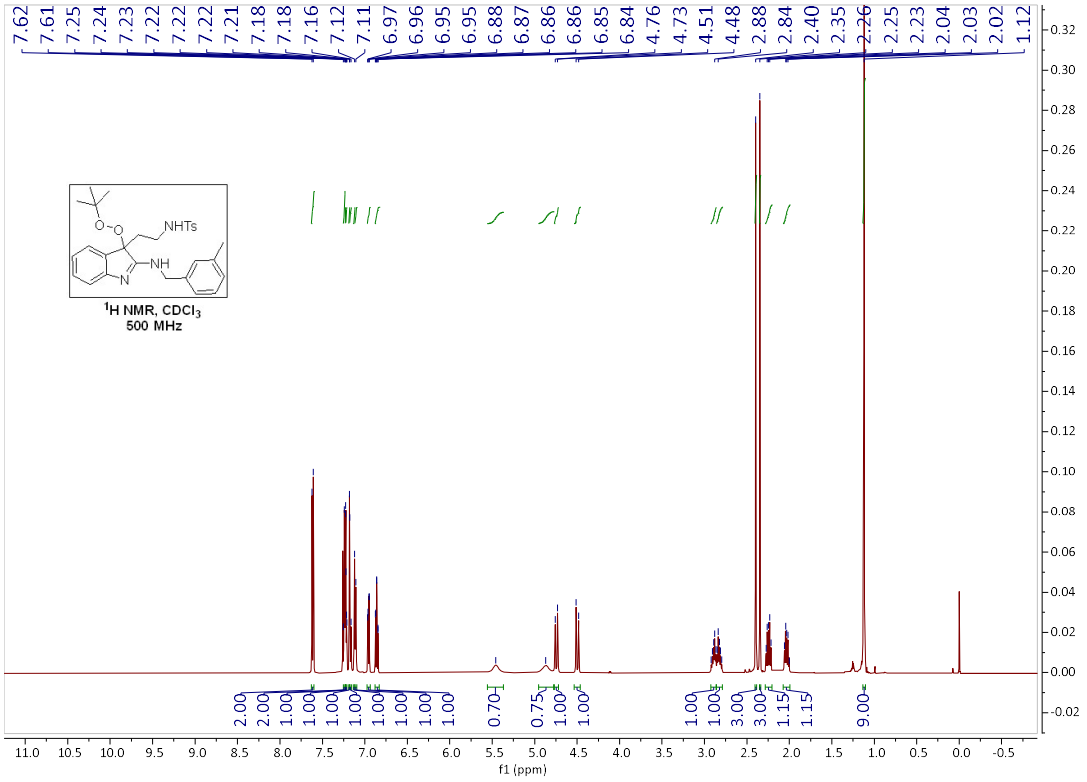
^{1}H NMR Spectrum of 4



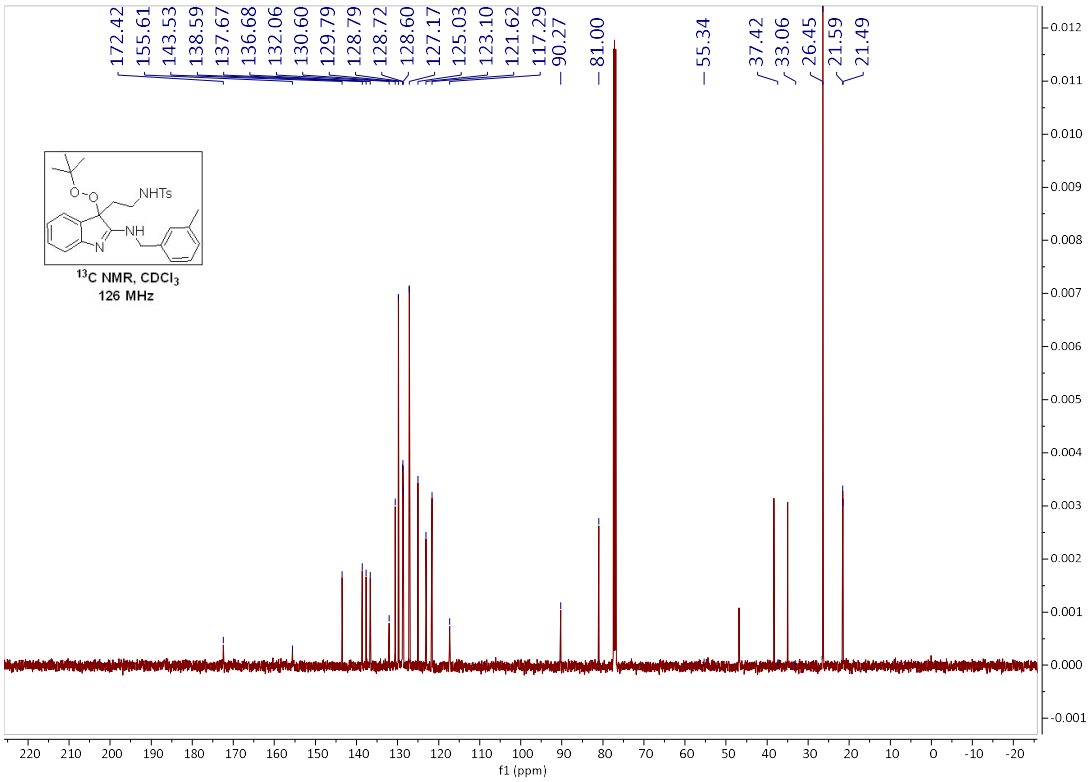
^{13}C NMR Spectrum of 4



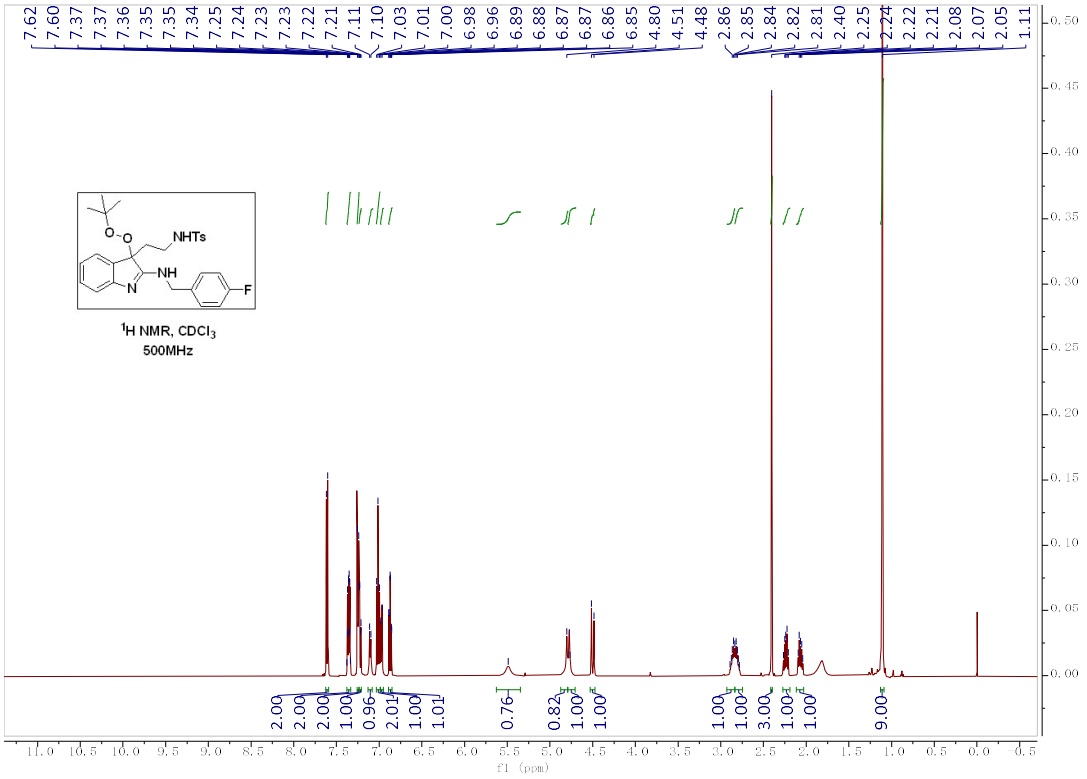
^{1}H NMR Spectrum of 5



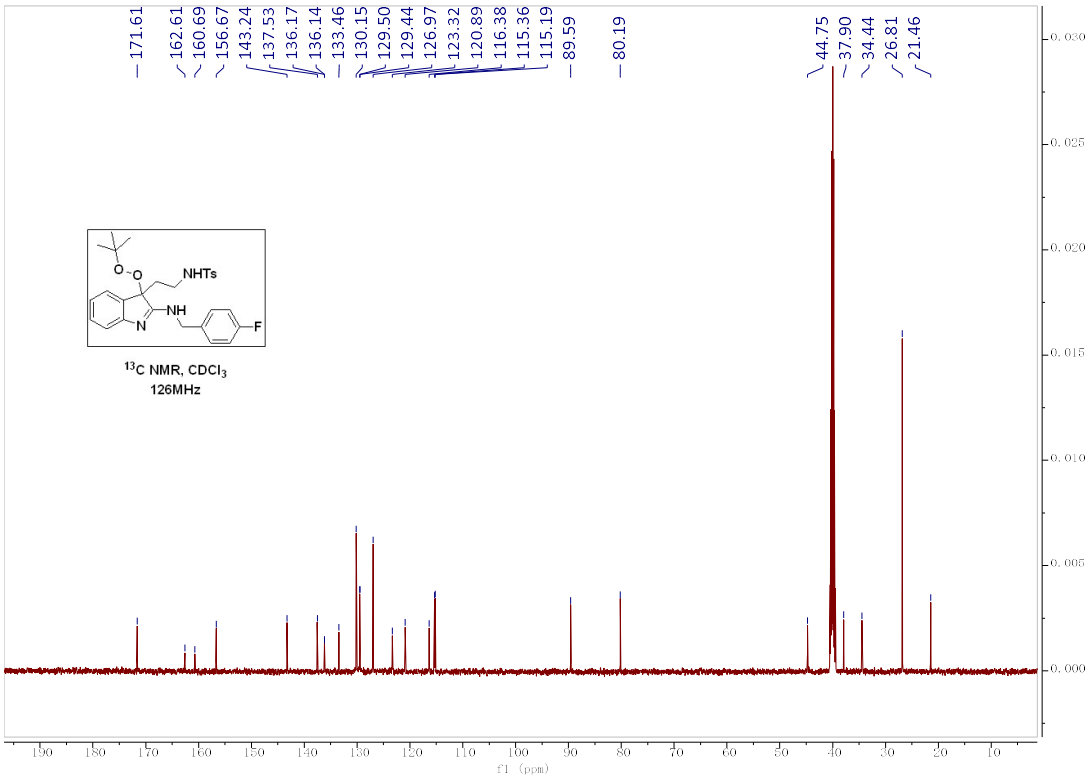
^{13}C NMR Spectrum of 5



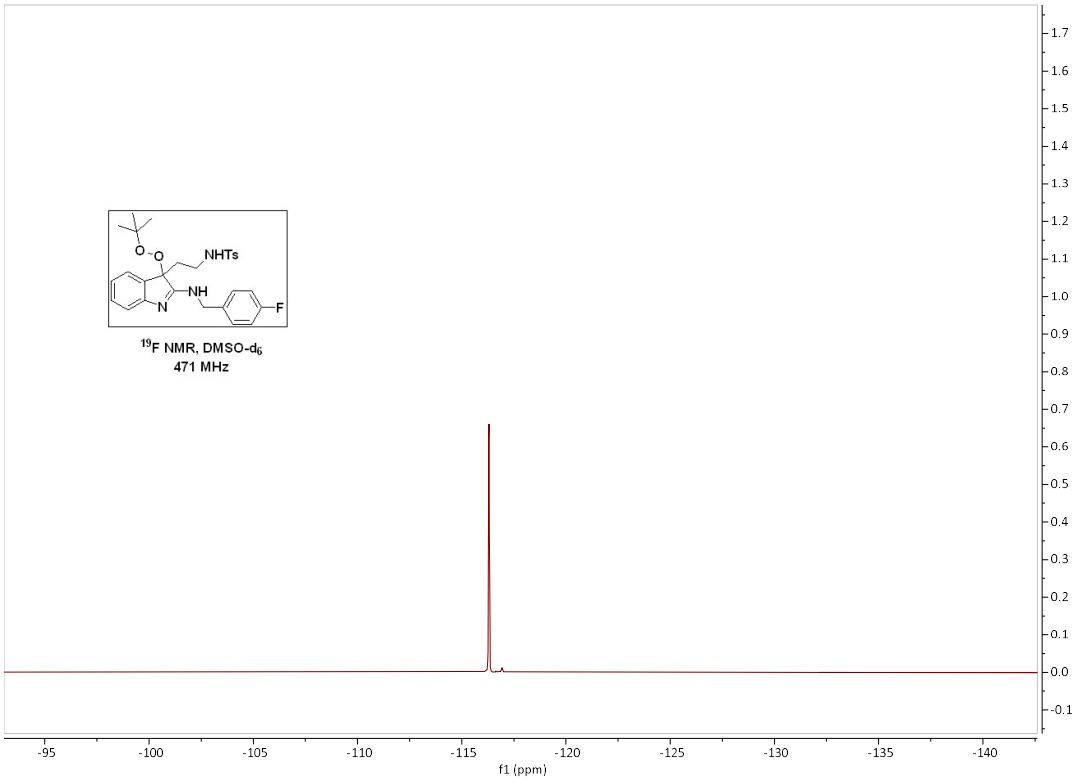
^{1}H NMR Spectrum of 6



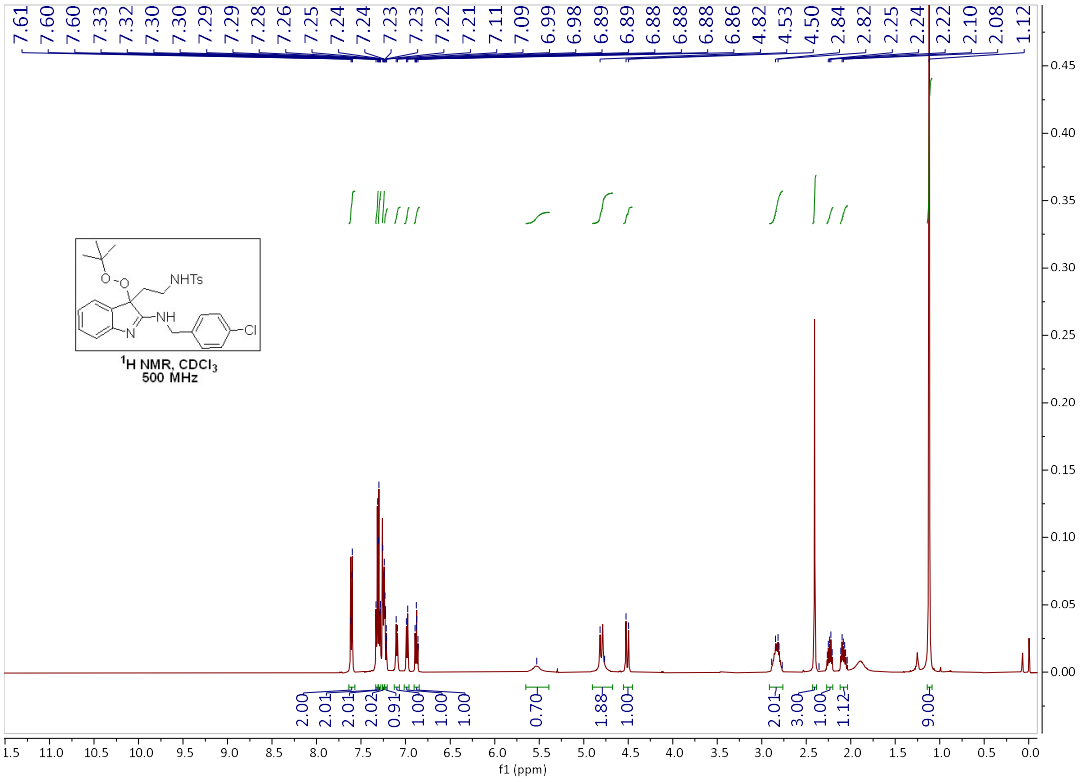
^{13}C NMR Spectrum of 6



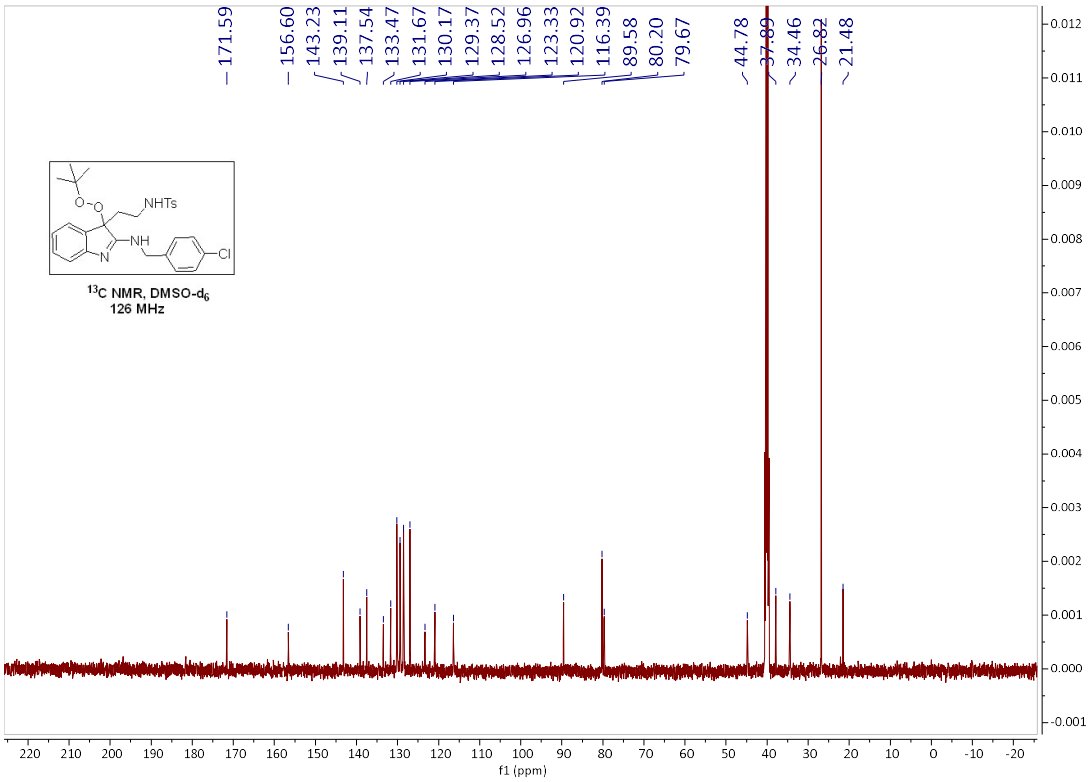
^{19}F NMR Spectrum of 6



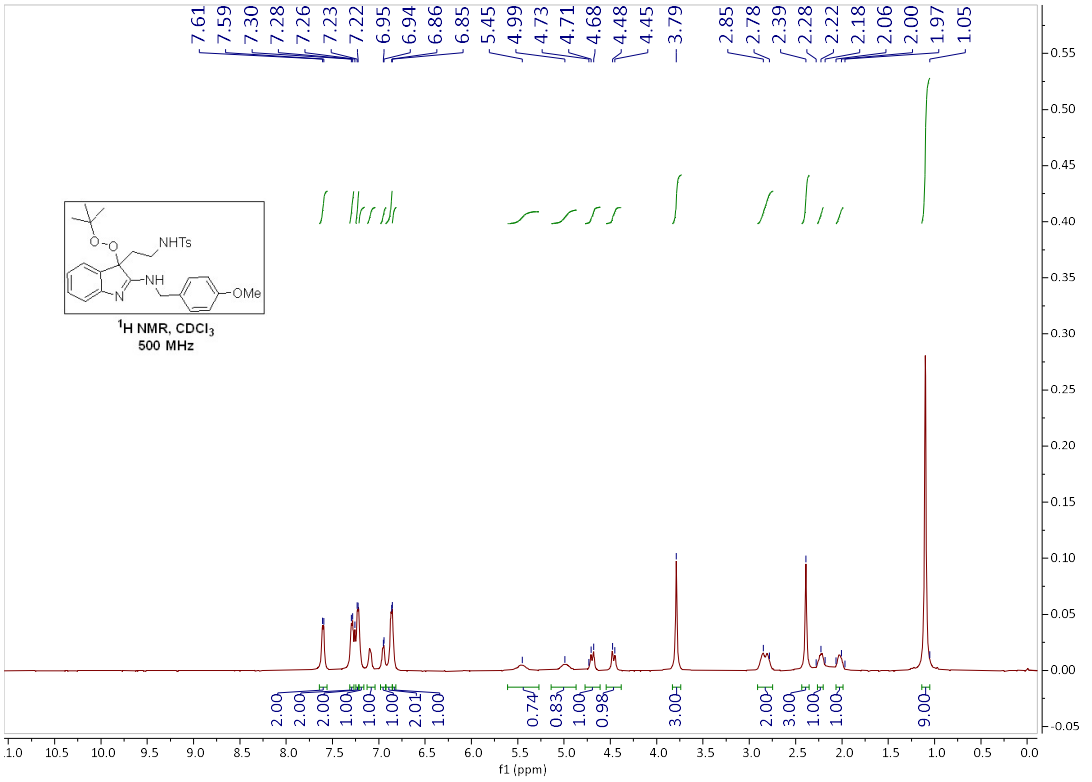
^{1}H NMR Spectrum of 7



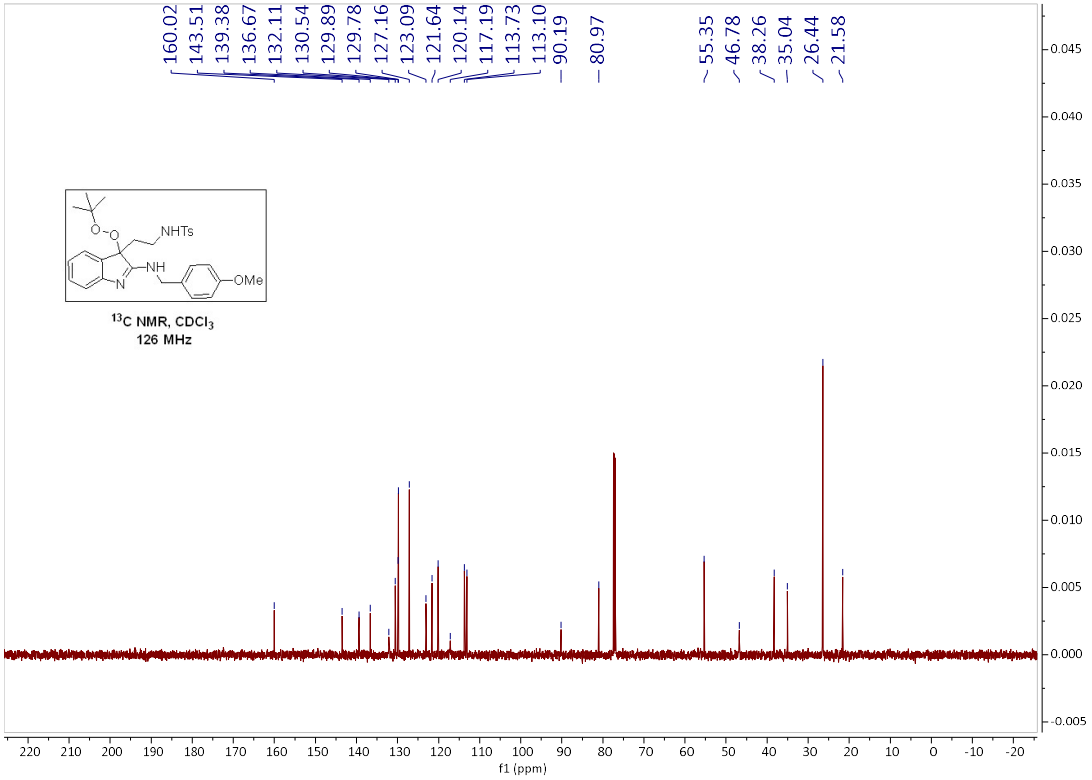
^{13}C NMR Spectrum of 7



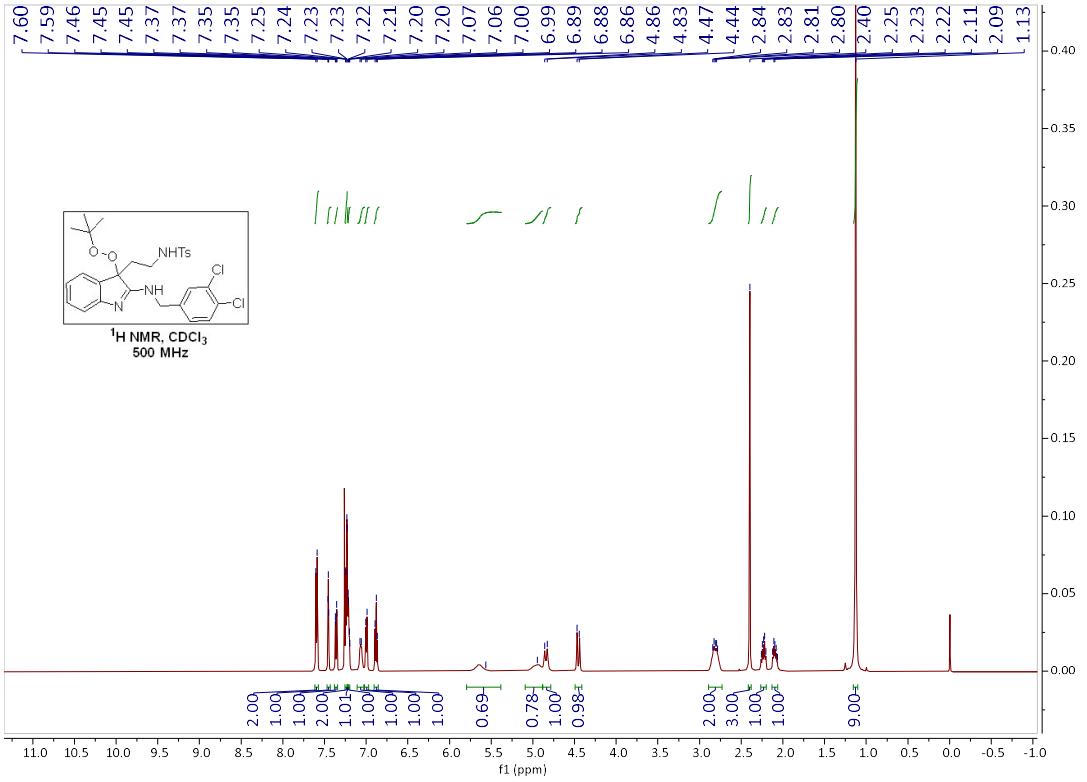
^{1}H NMR Spectrum of 8



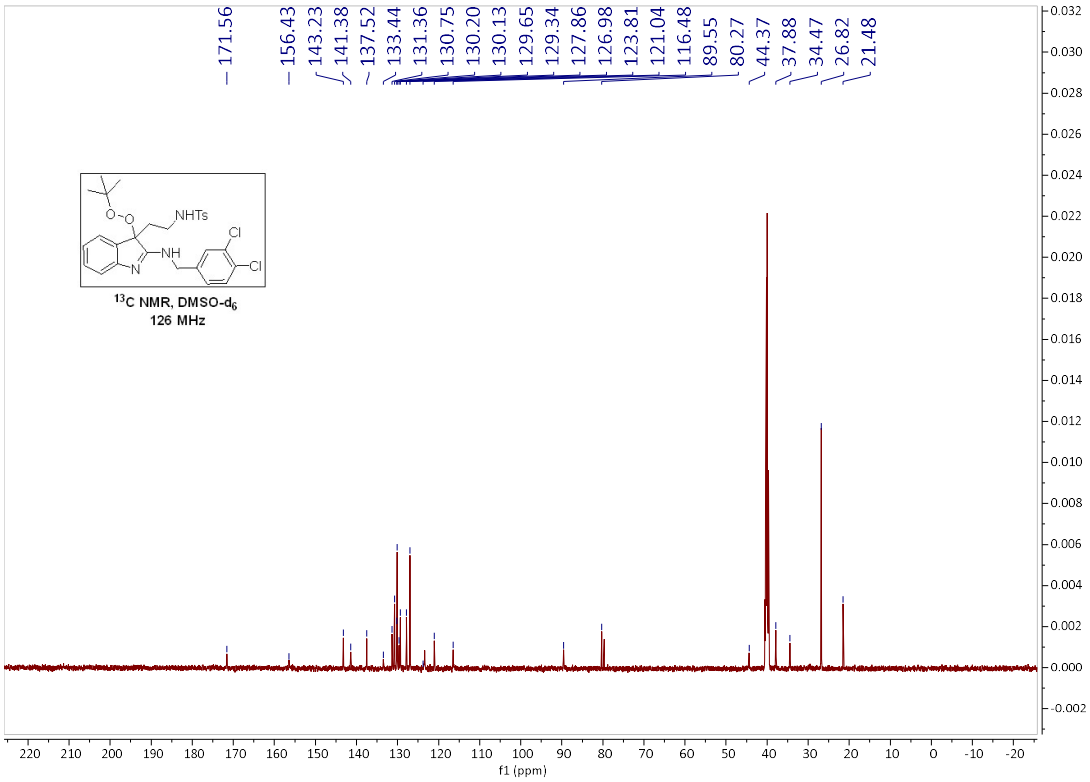
^{13}C NMR Spectrum of 8



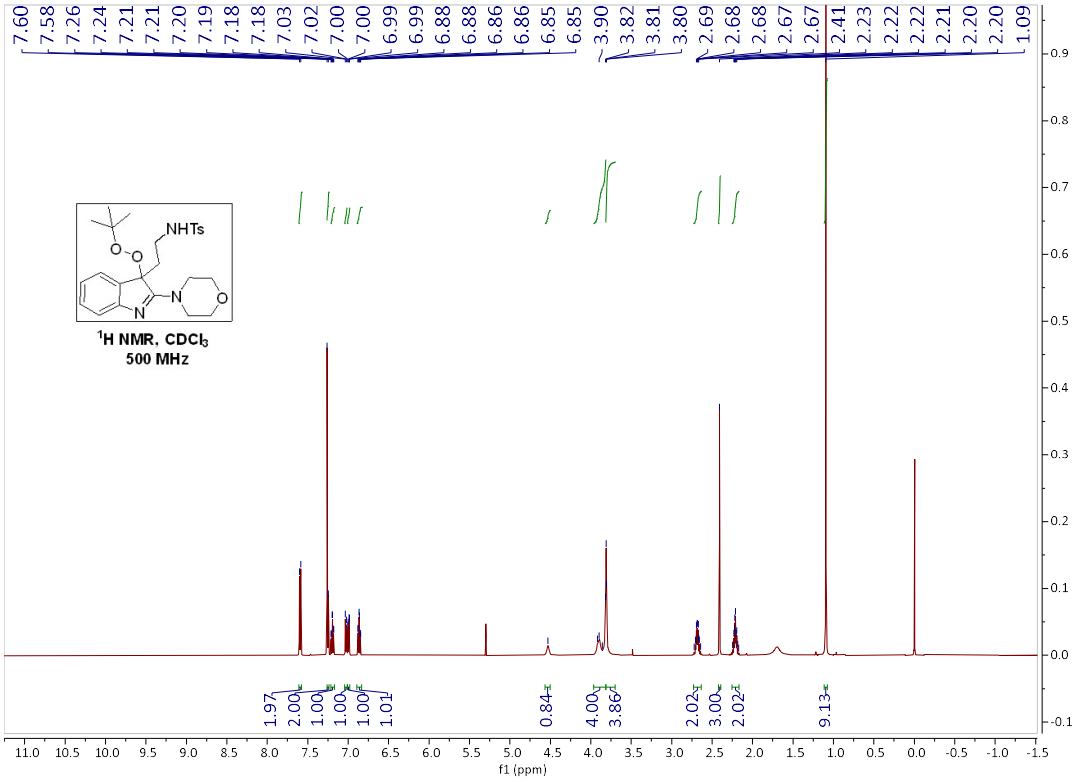
^{1}H NMR Spectrum of 9



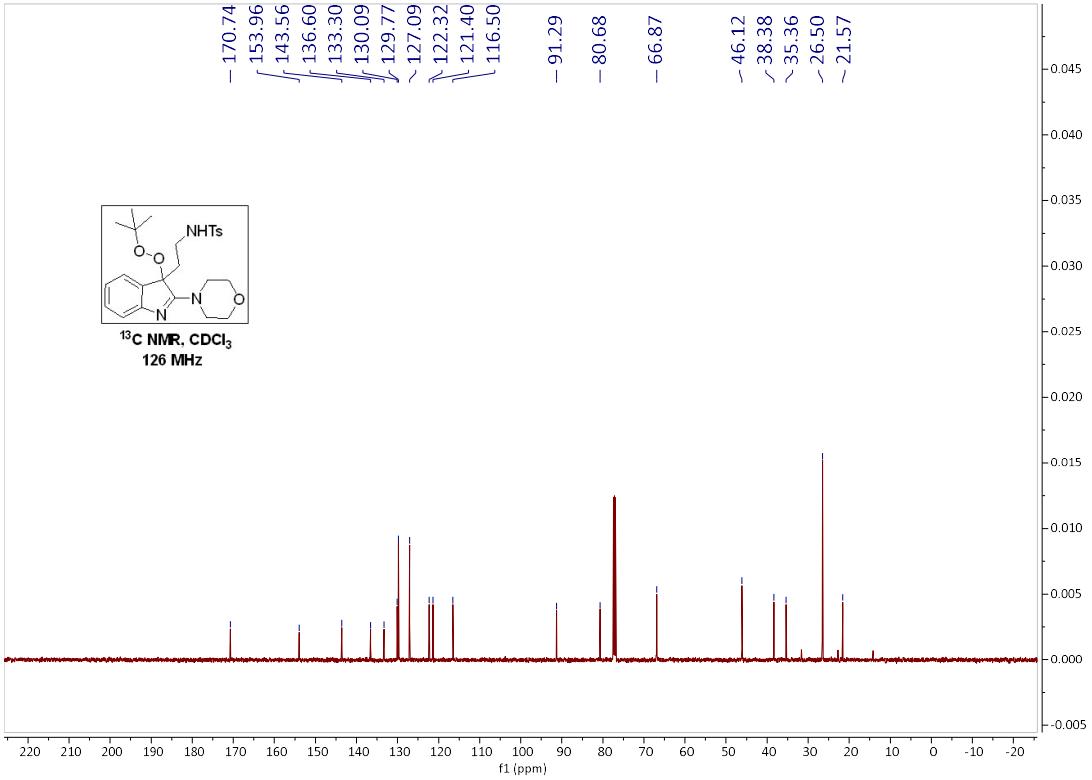
^{13}C NMR Spectrum of 9



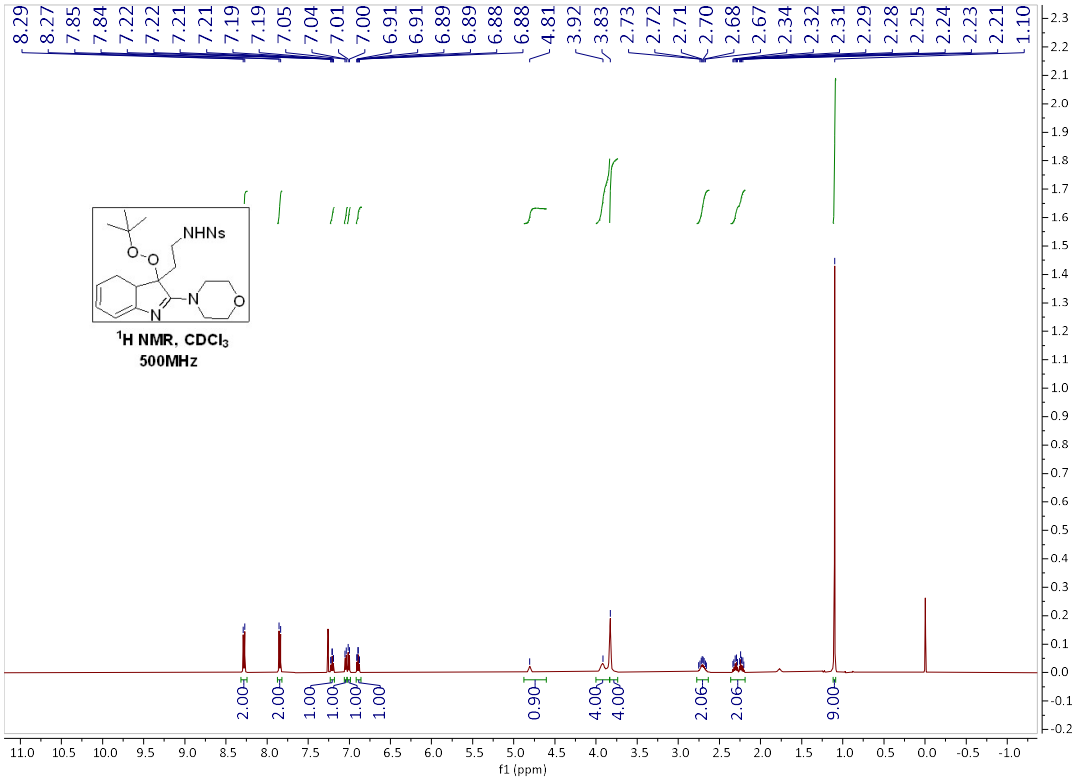
^{1}H NMR Spectrum of 10



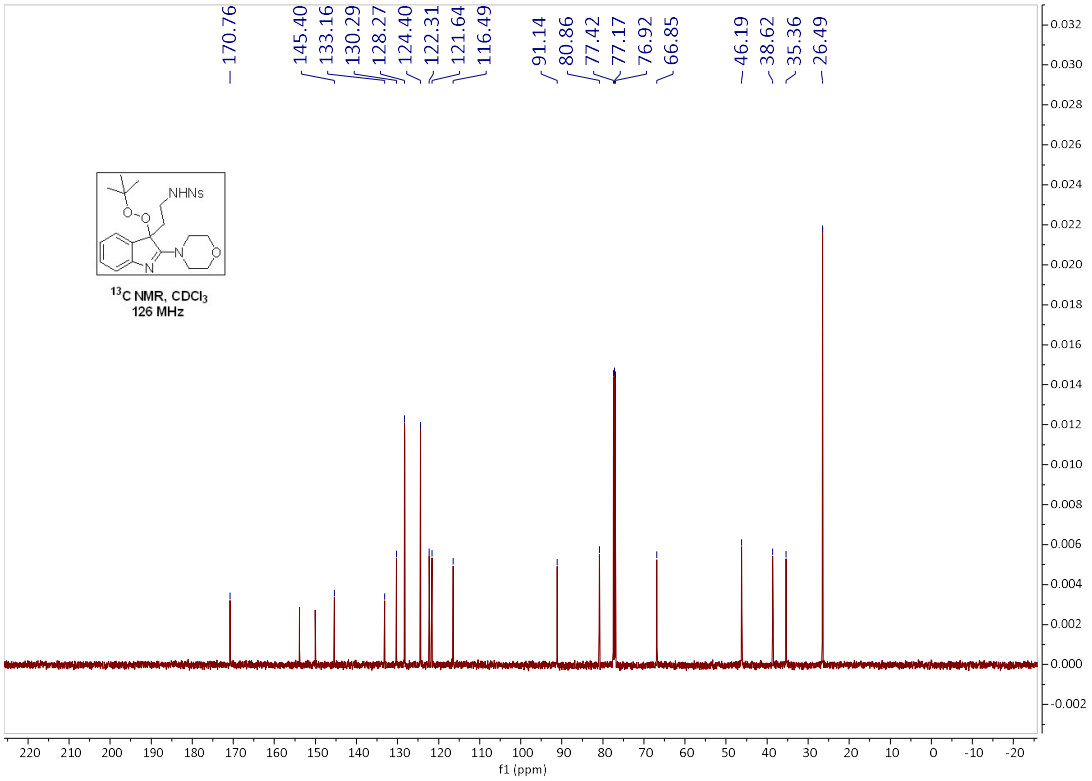
^{13}C NMR Spectrum of 10



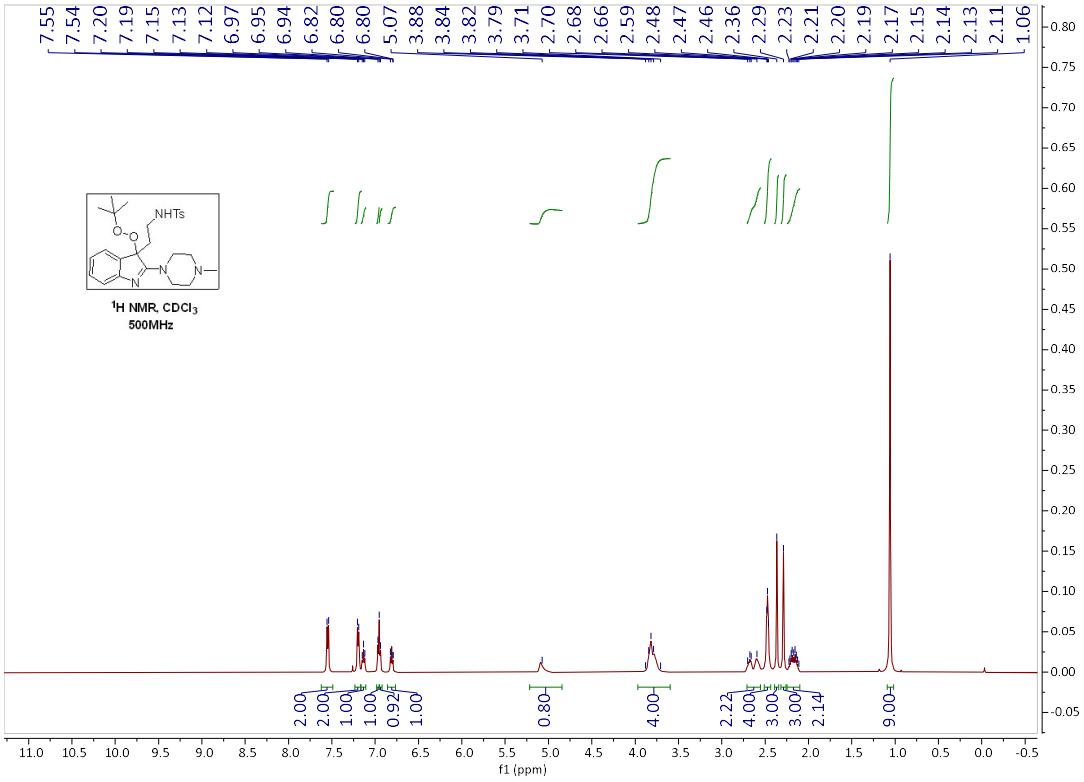
^{1}H NMR Spectrum of 11



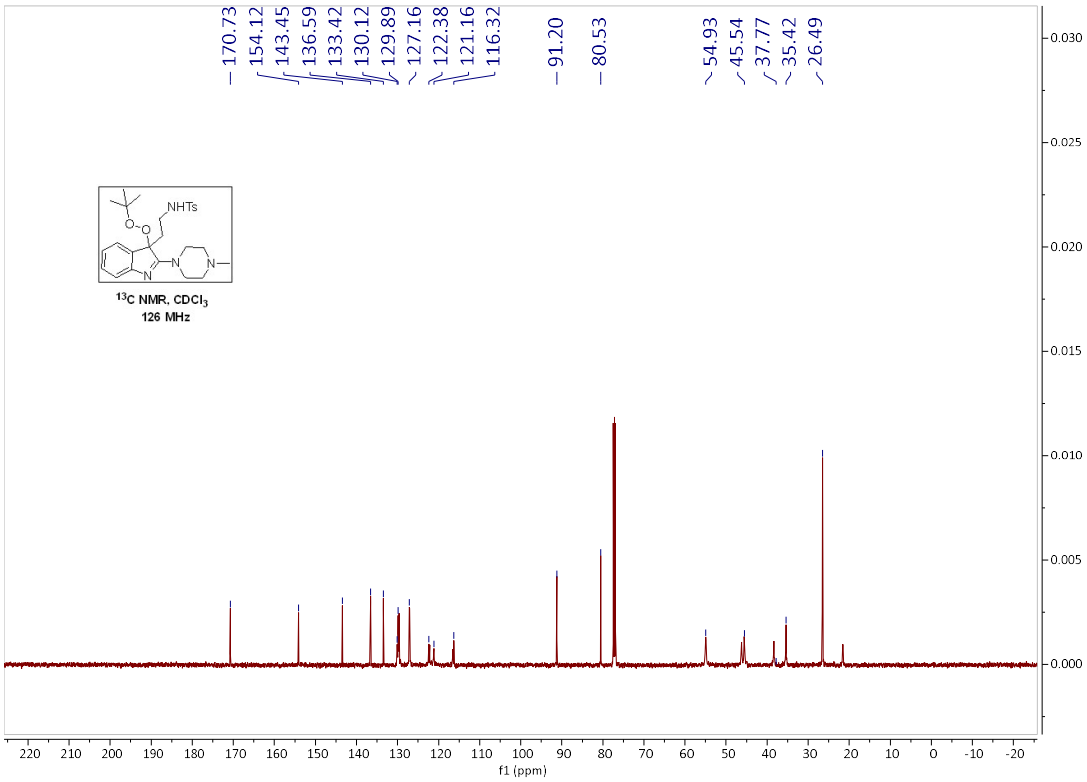
^{13}C NMR Spectrum of 11



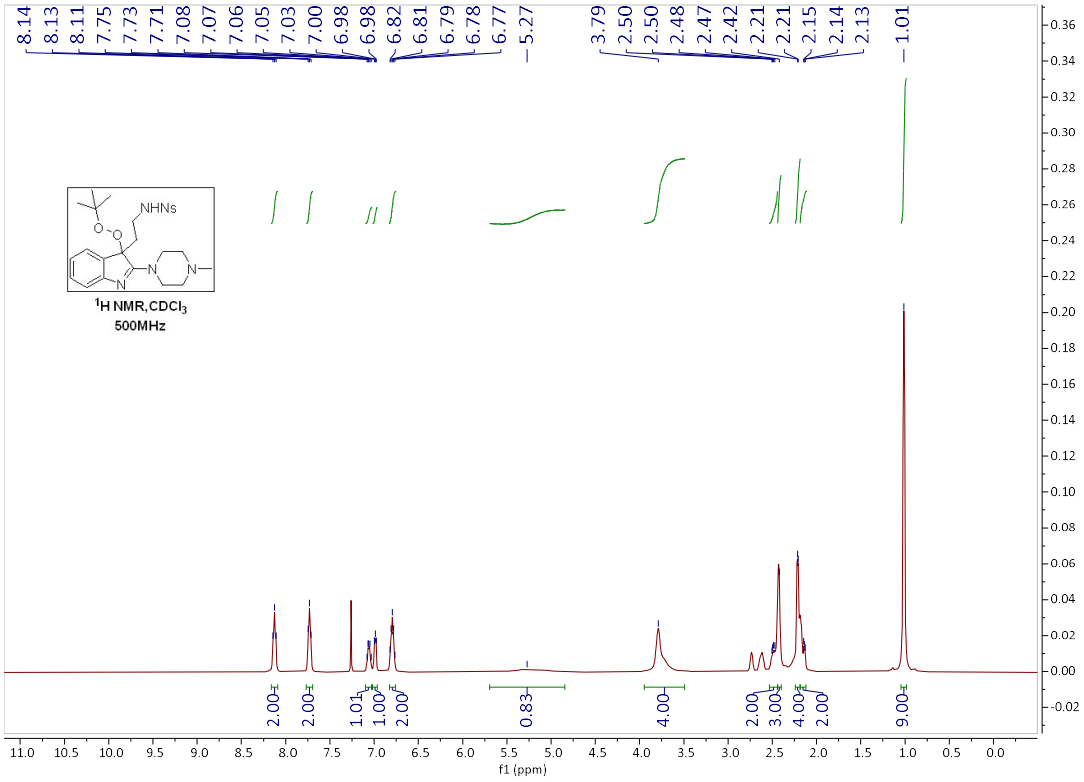
^{1}H NMR Spectrum of 12



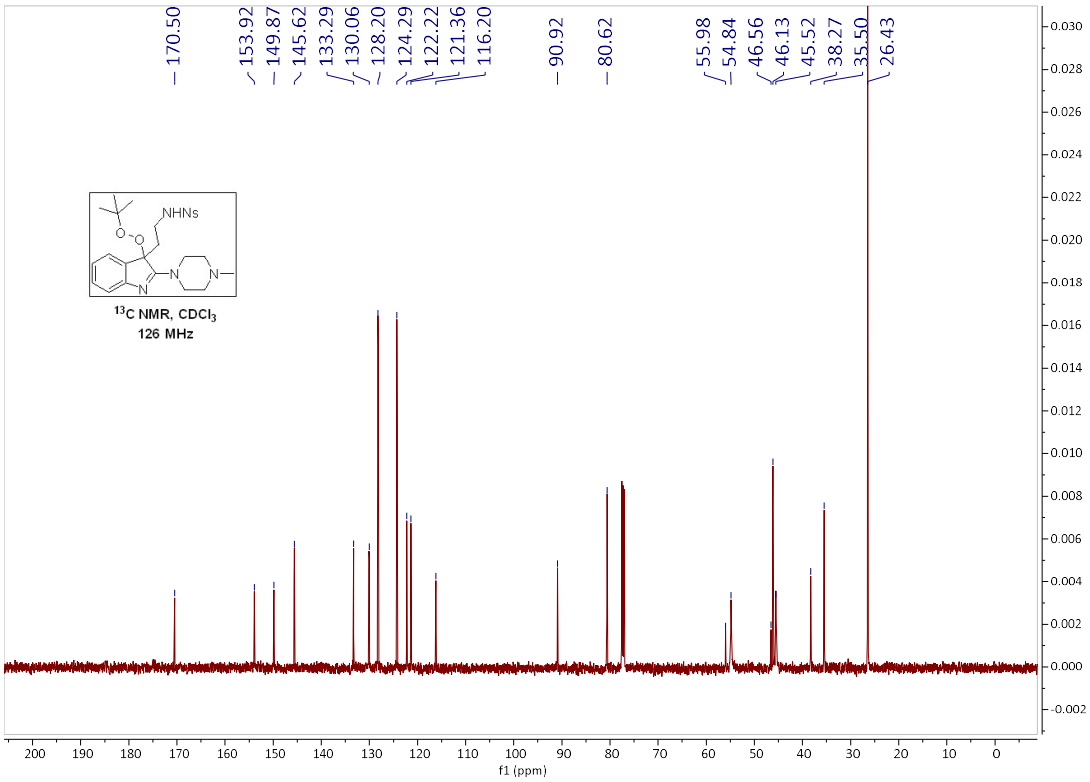
^{13}C NMR Spectrum of 12



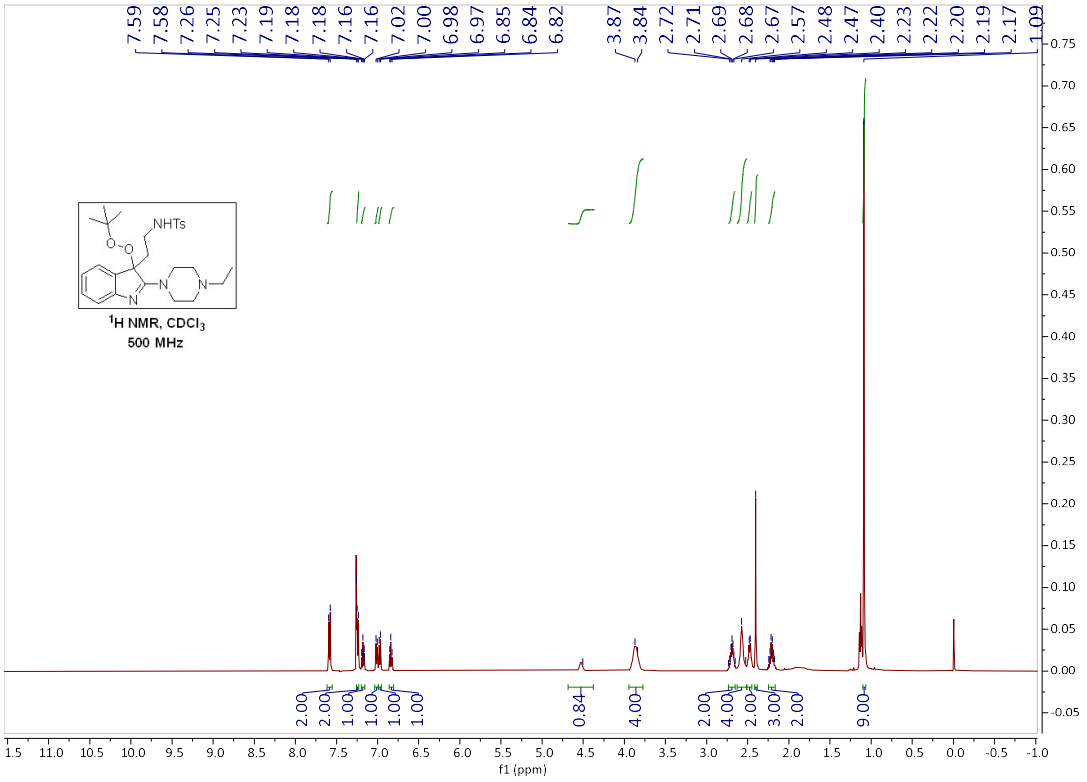
^{1}H NMR Spectrum of 13



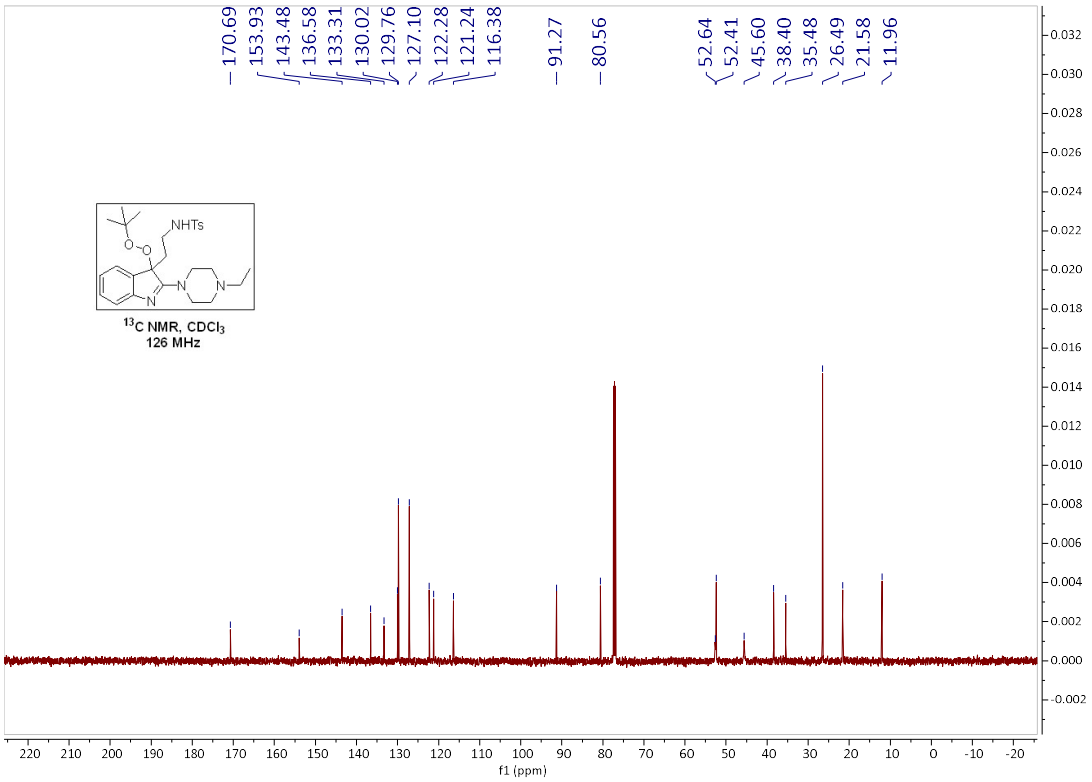
^{13}C NMR Spectrum of 13



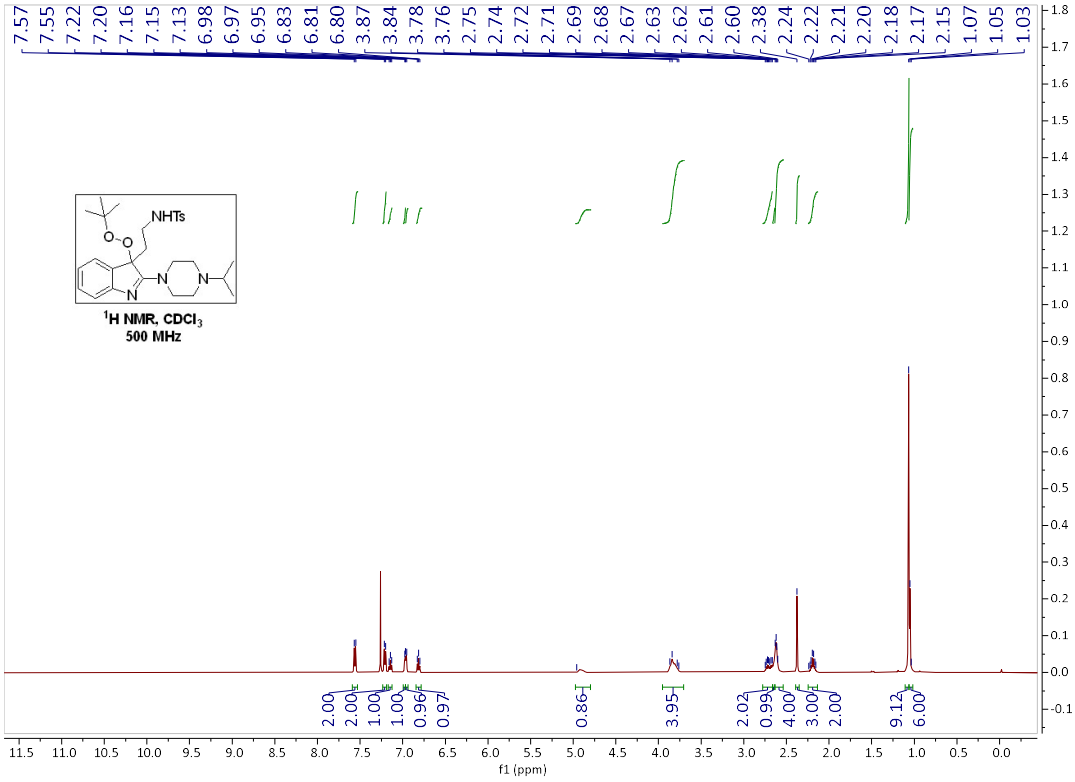
^{1}H NMR Spectrum of 14



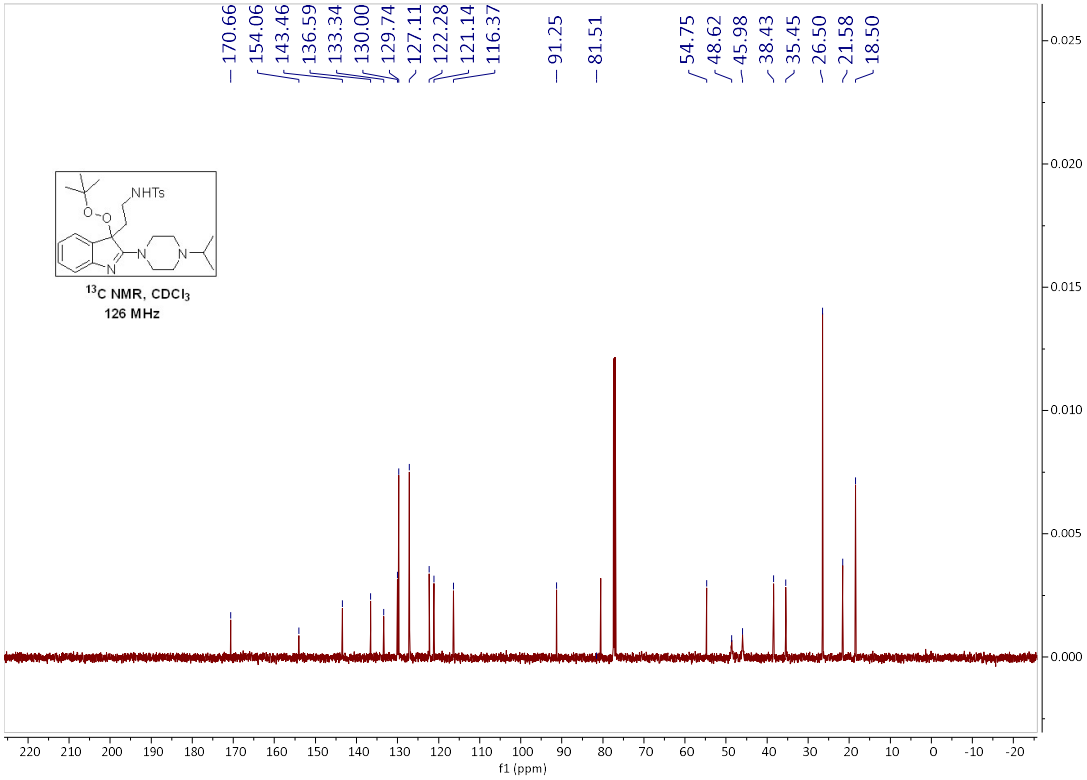
^{13}C NMR Spectrum of 14



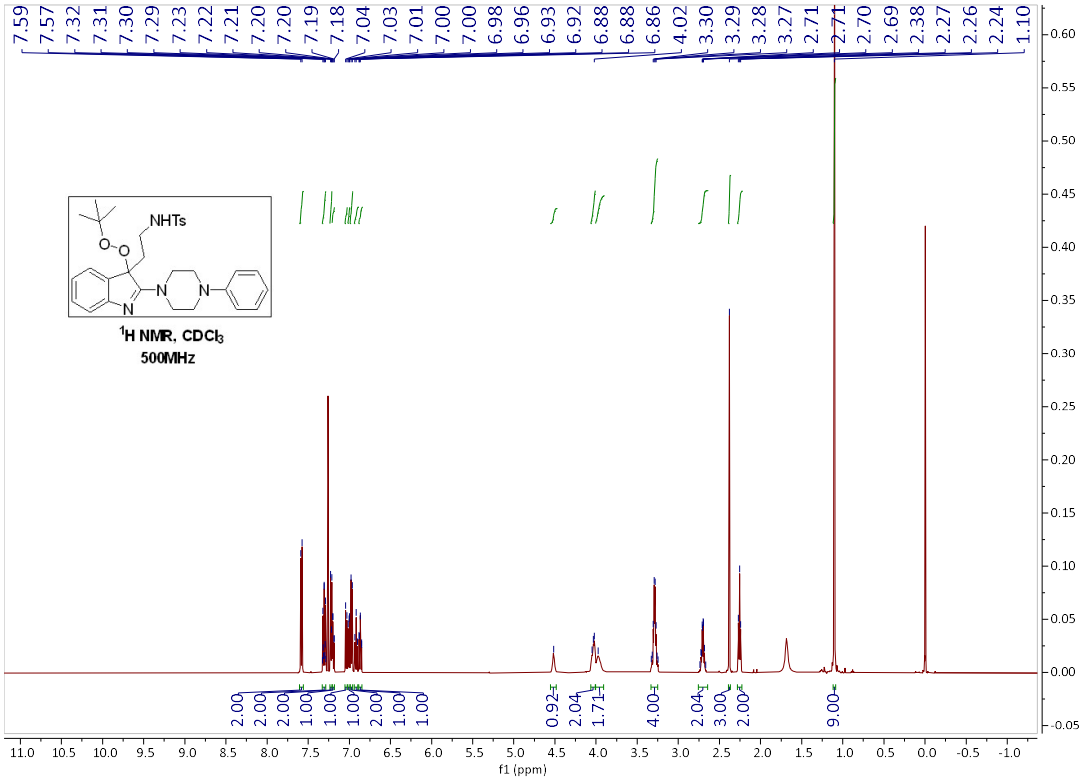
^{1}H NMR Spectrum of 15



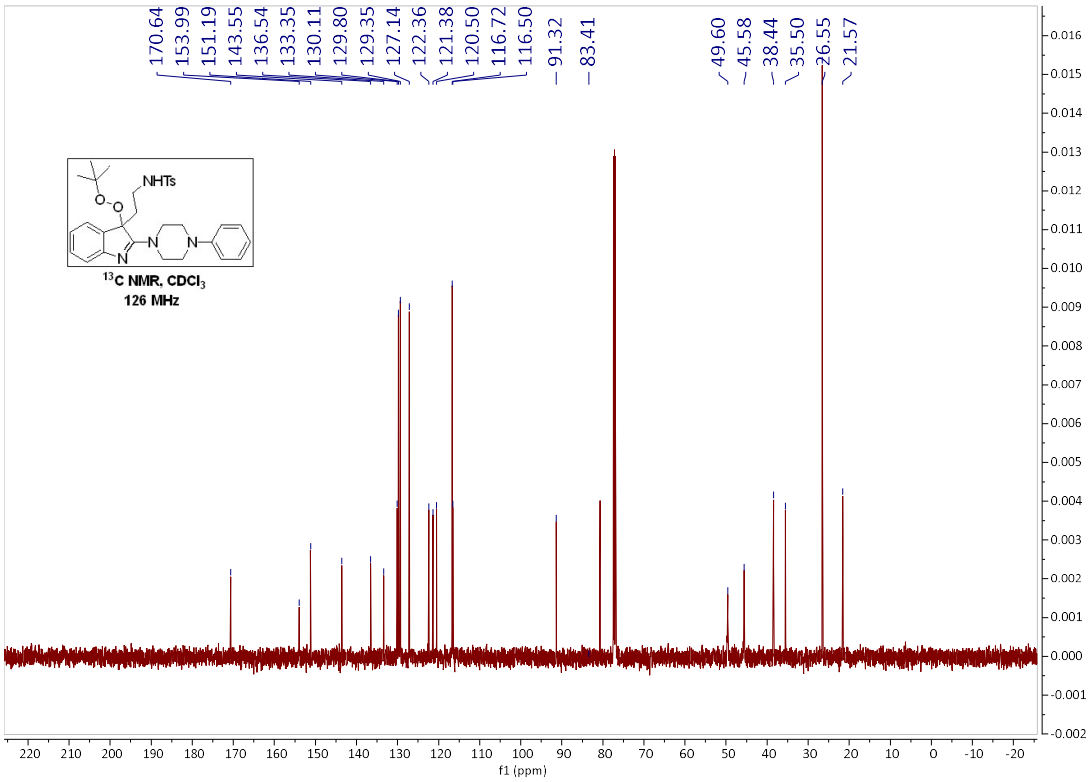
^{13}C NMR Spectrum of 15



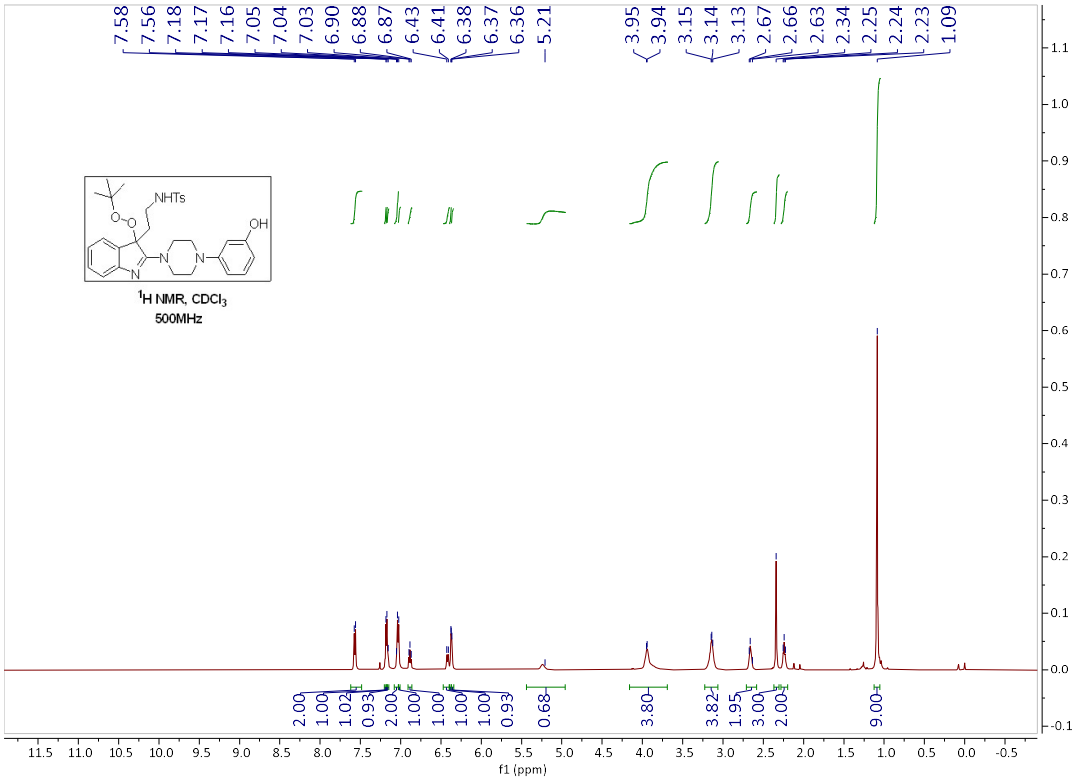
^{1}H NMR Spectrum of 16



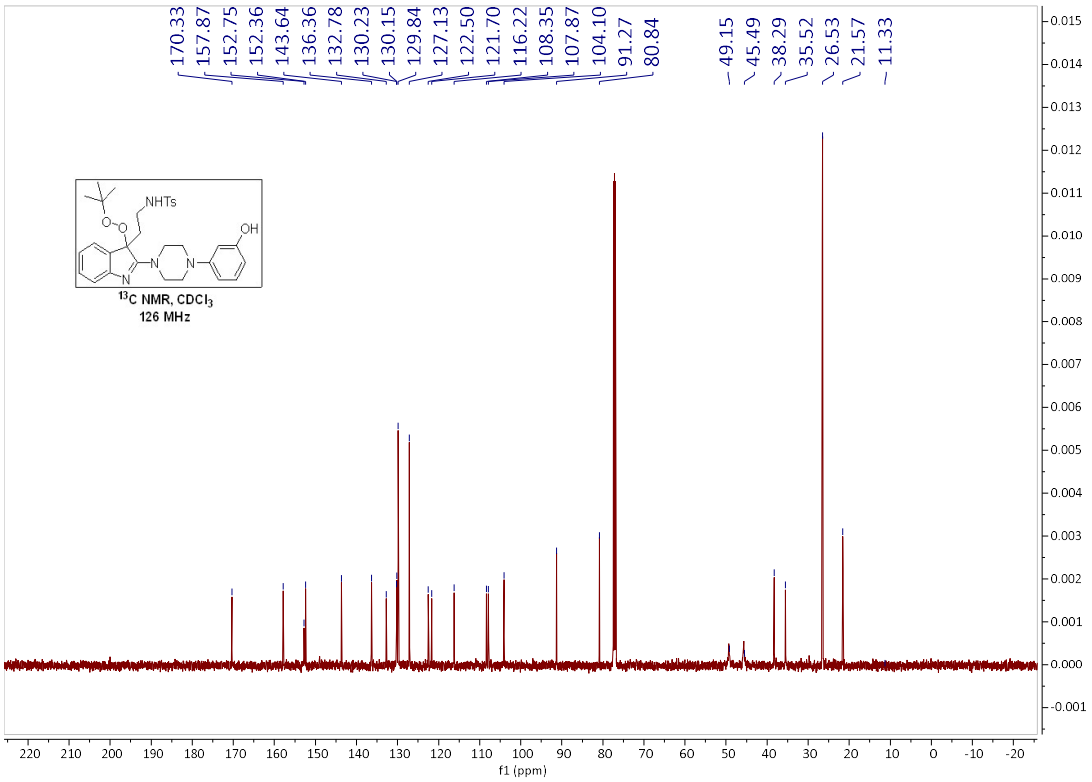
^{13}C NMR Spectrum of 16



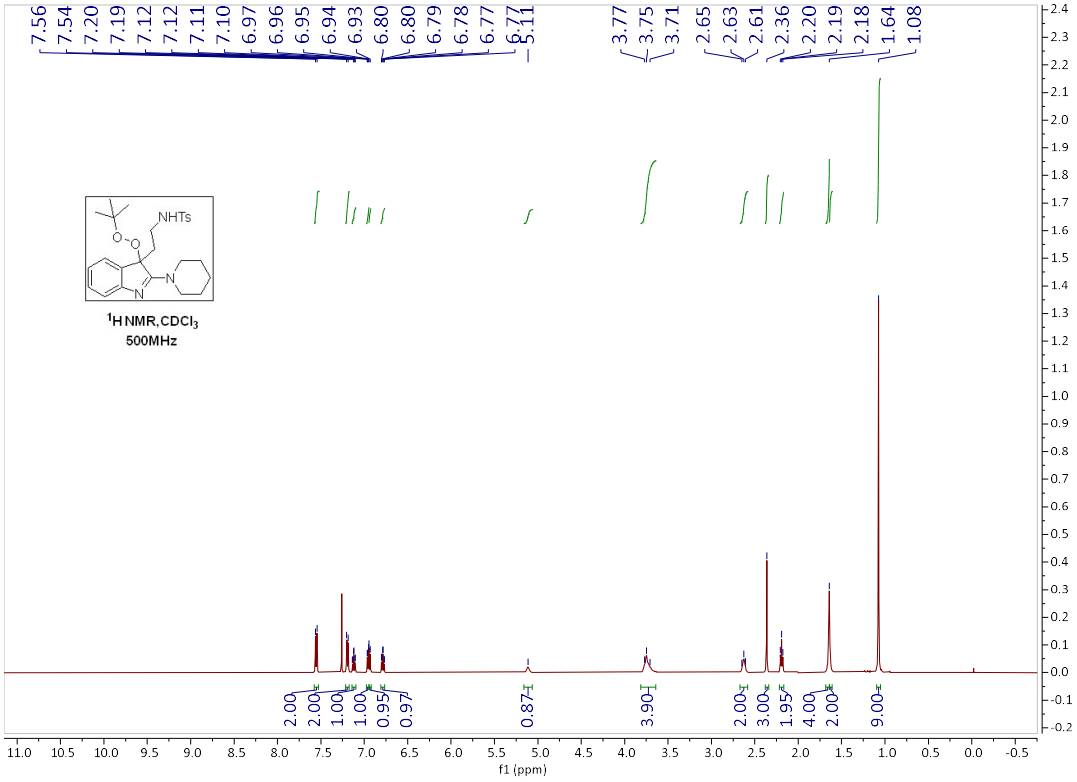
^{1}H NMR Spectrum of 17



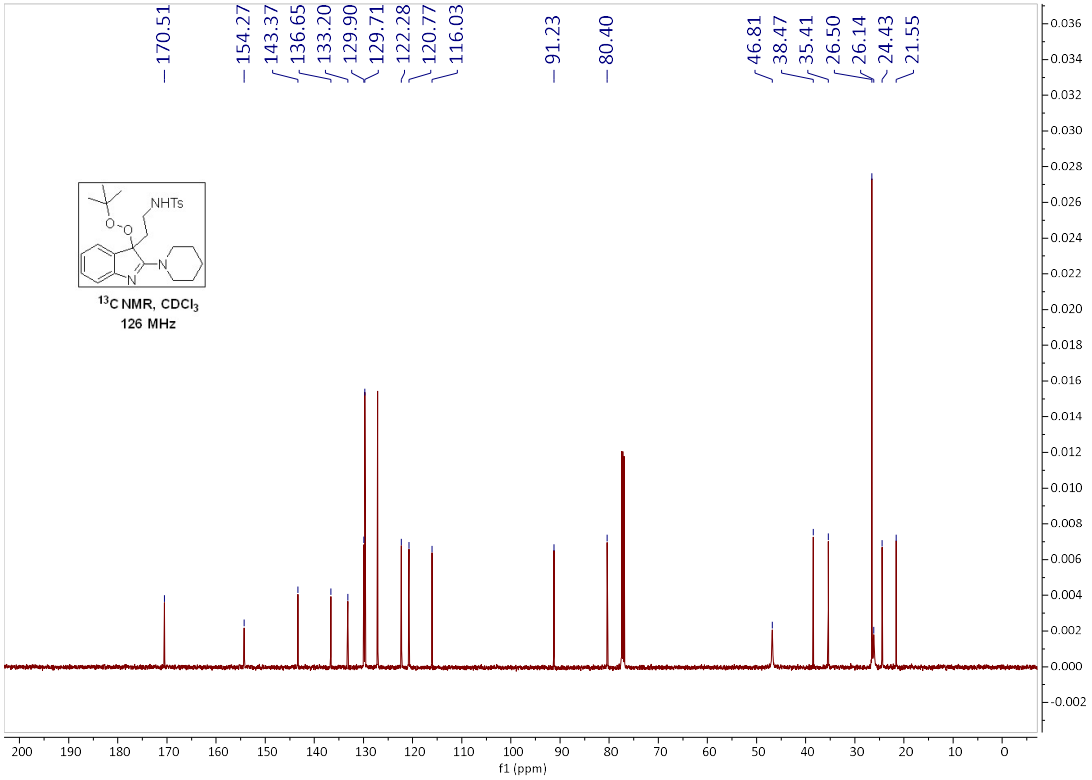
^{13}C NMR Spectrum of 17



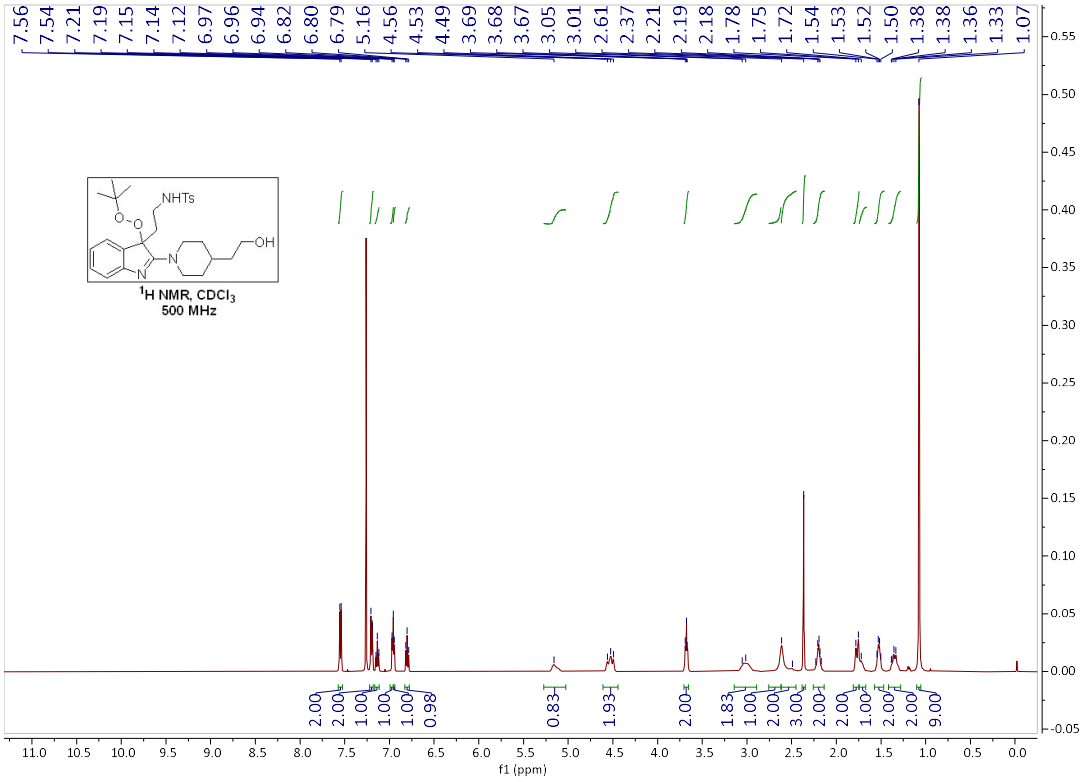
^{1}H NMR Spectrum of 18



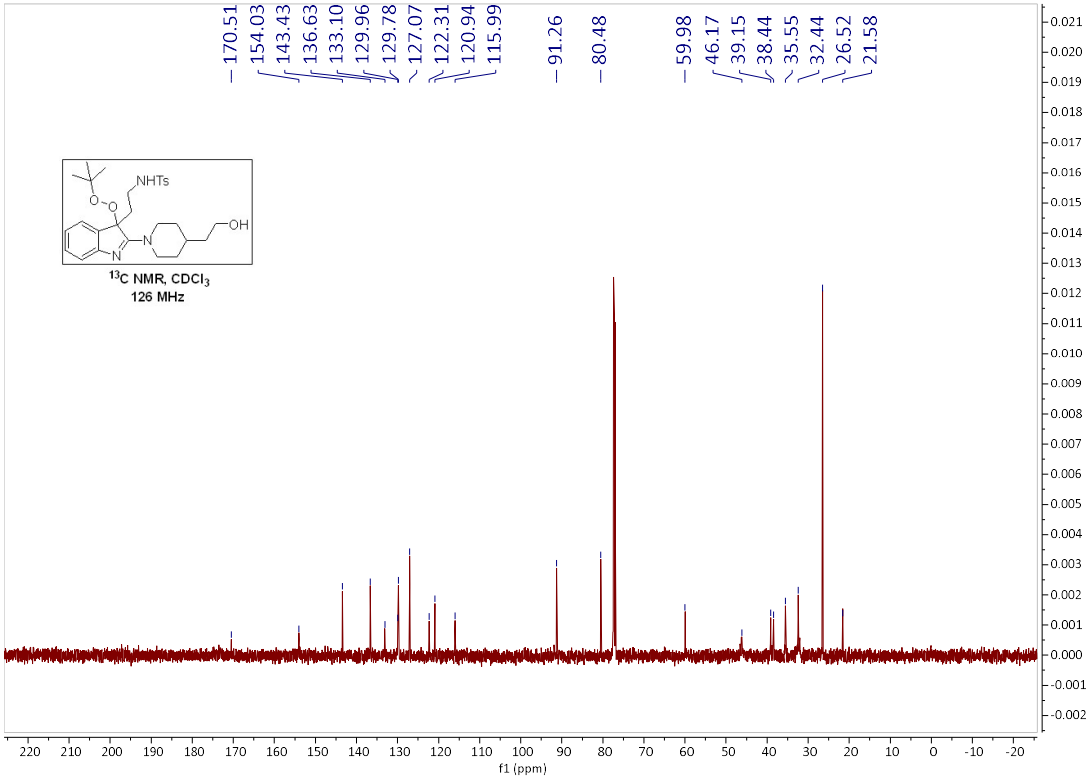
^{13}C NMR Spectrum of 18



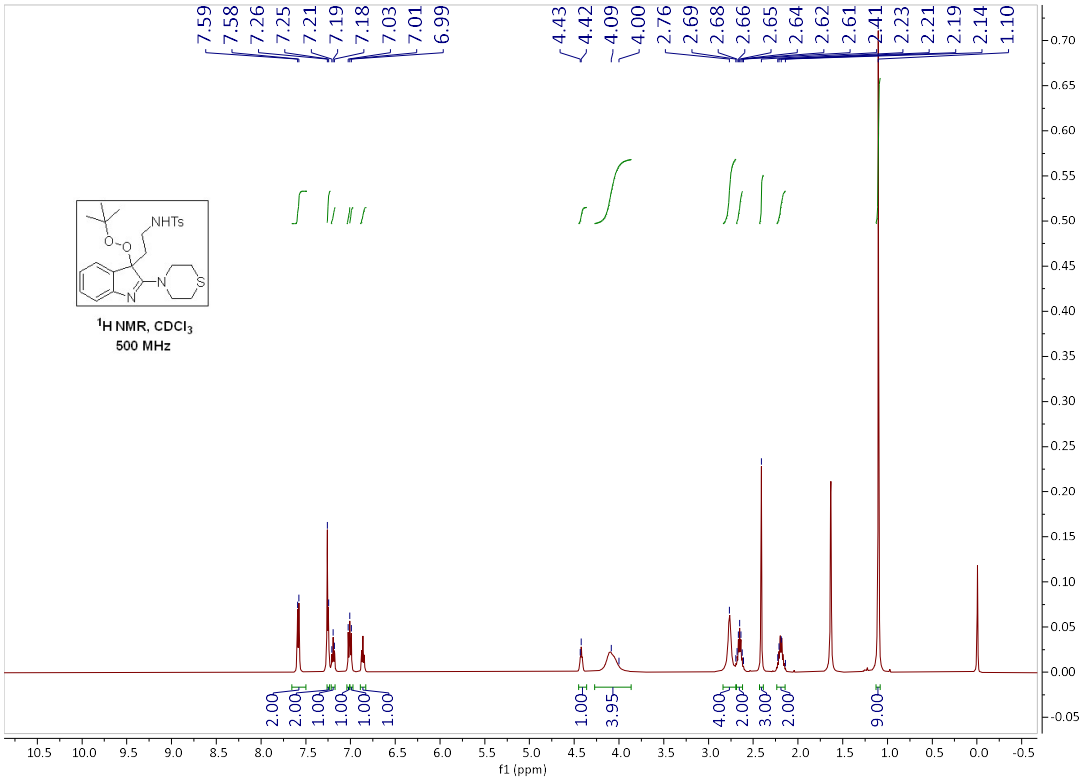
^{1}H NMR Spectrum of 19



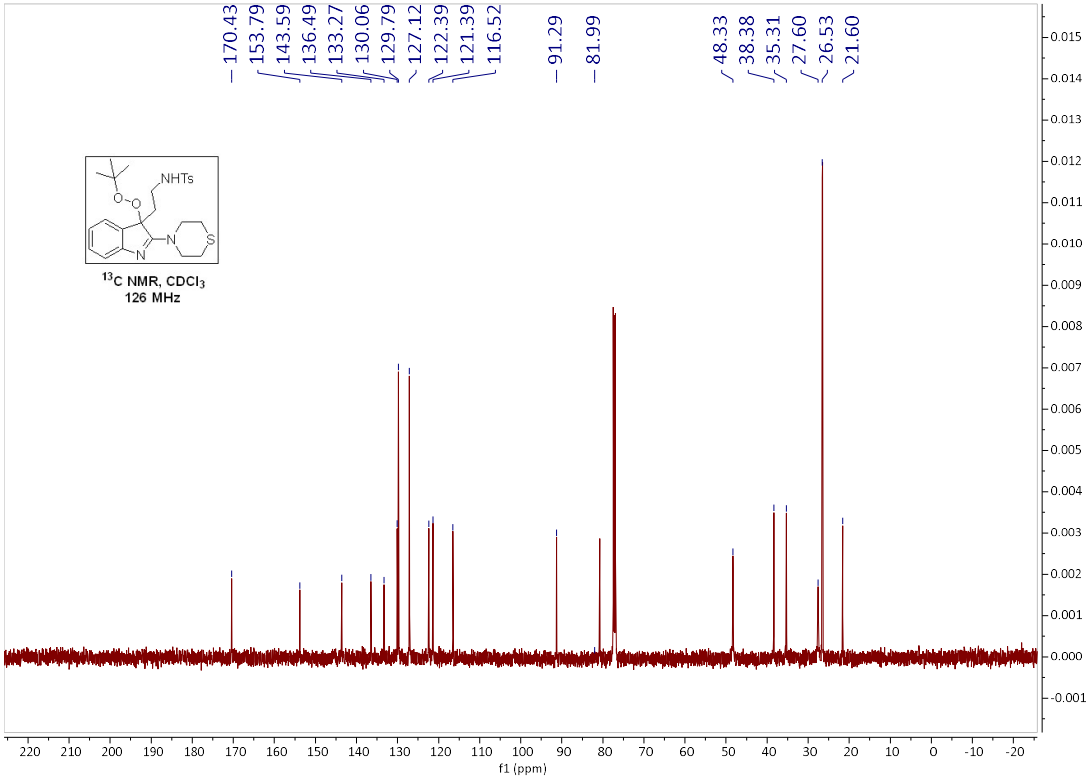
^{13}C NMR Spectrum of 19



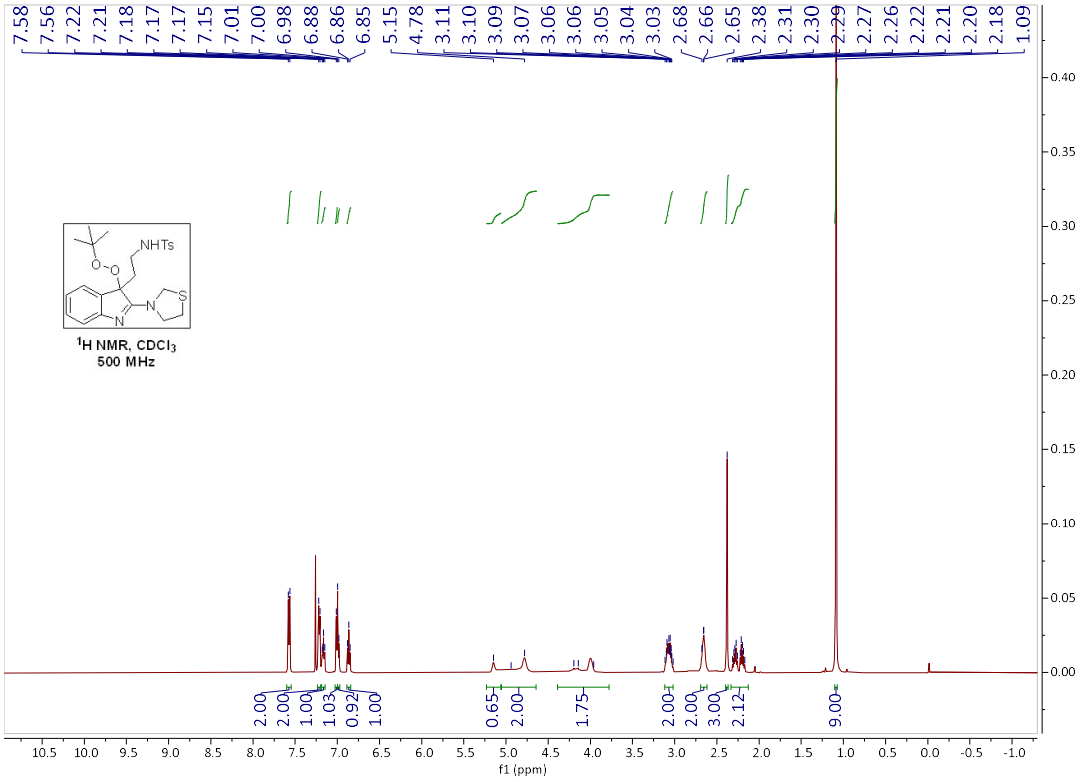
^{1}H NMR Spectrumof 20



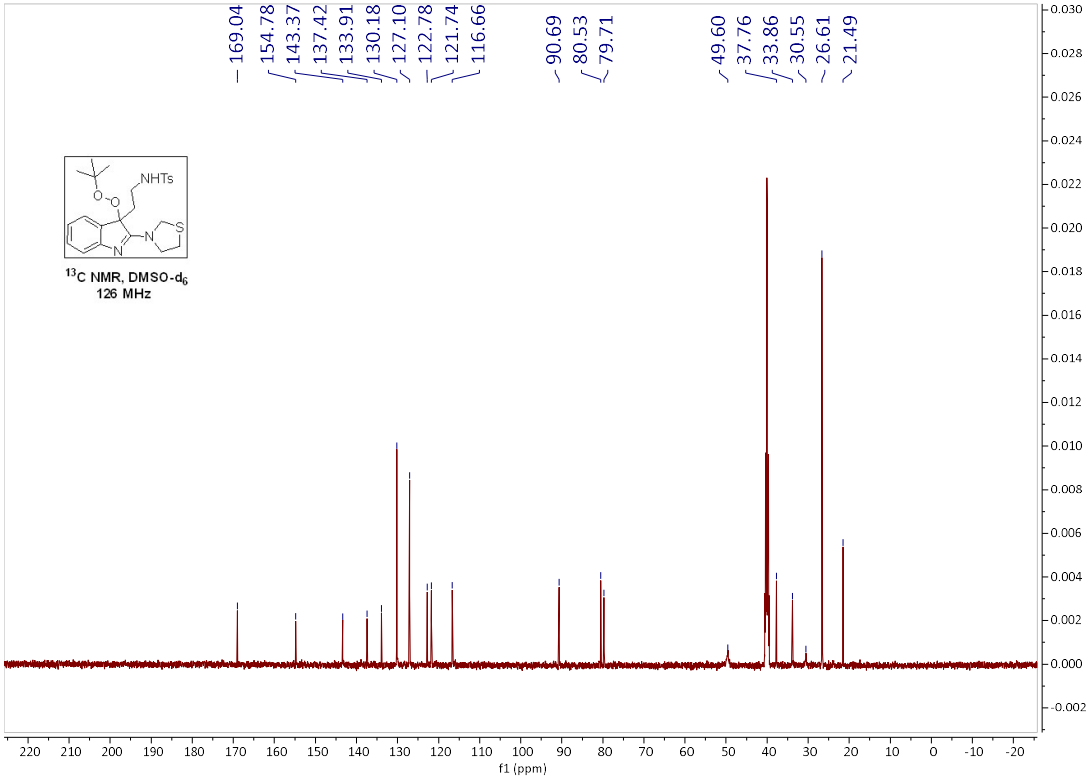
^{13}C NMR Spectrum of 20



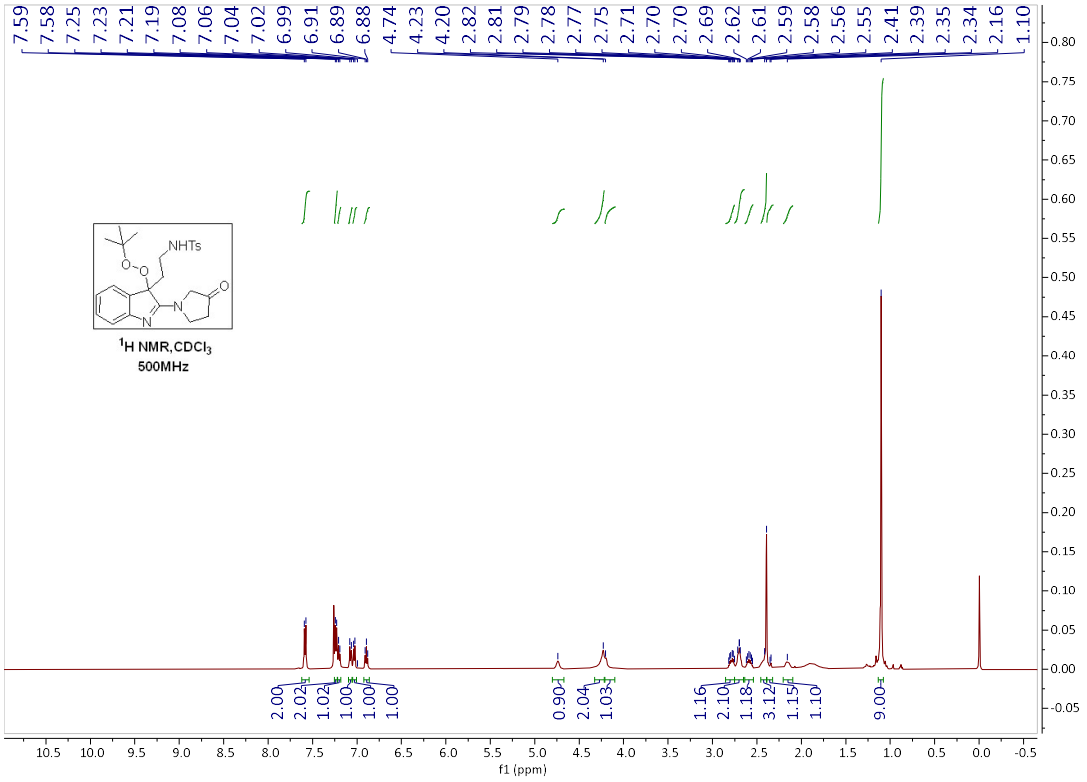
^{1}H NMR Spectrum of 21



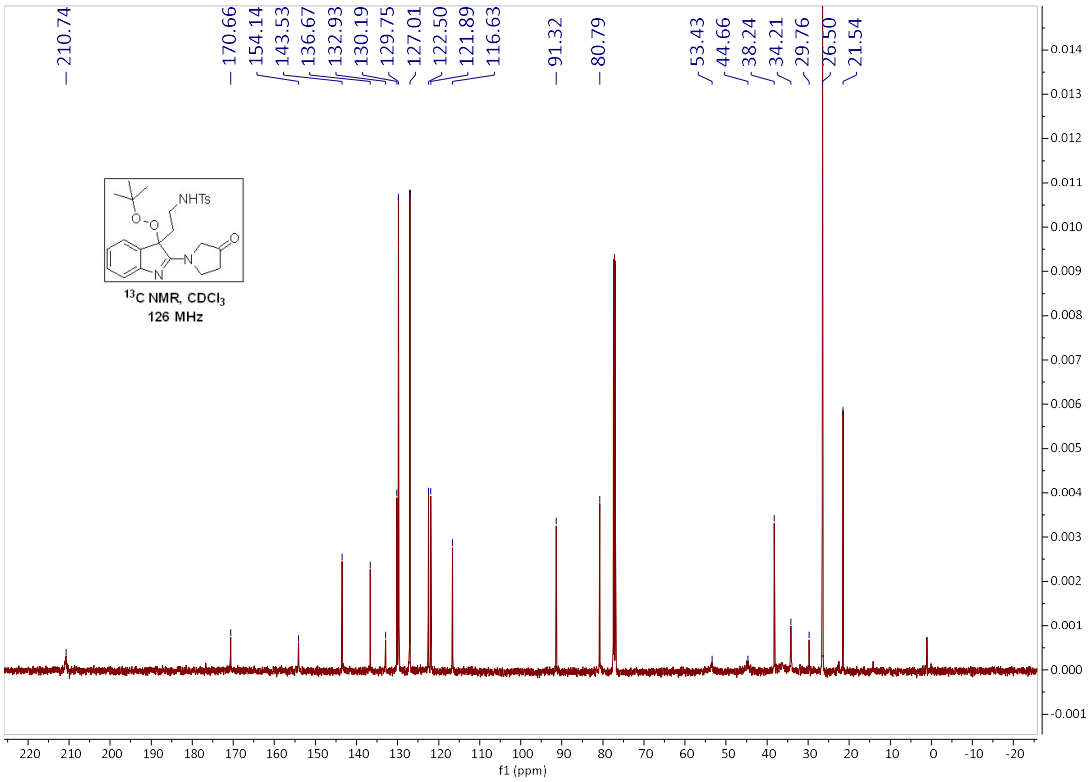
^{13}C NMR Spectrum of 21



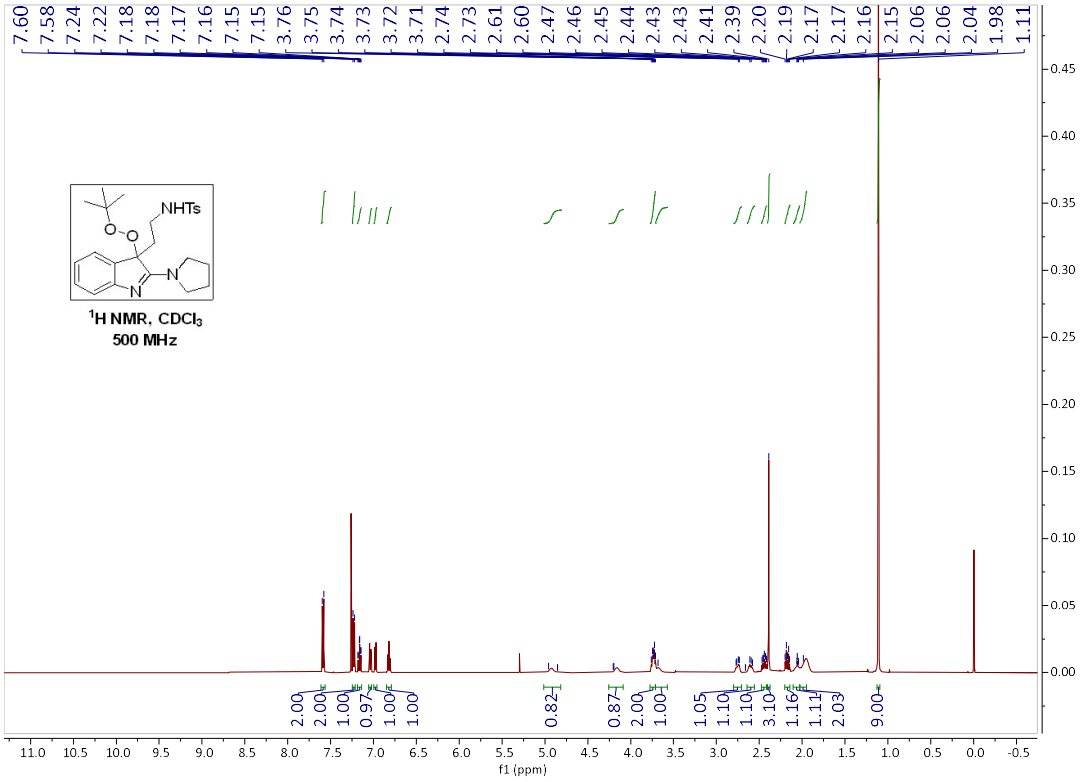
^{1}H NMR Spectrum of 22



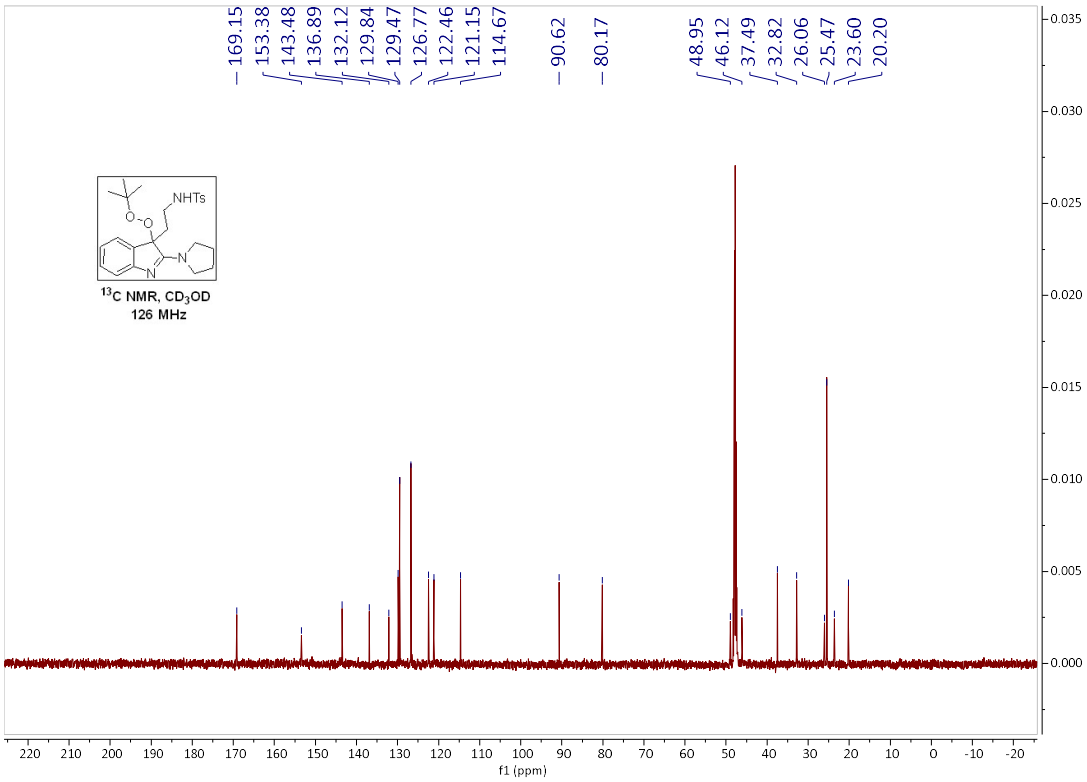
^{13}C NMR Spectrum of 22



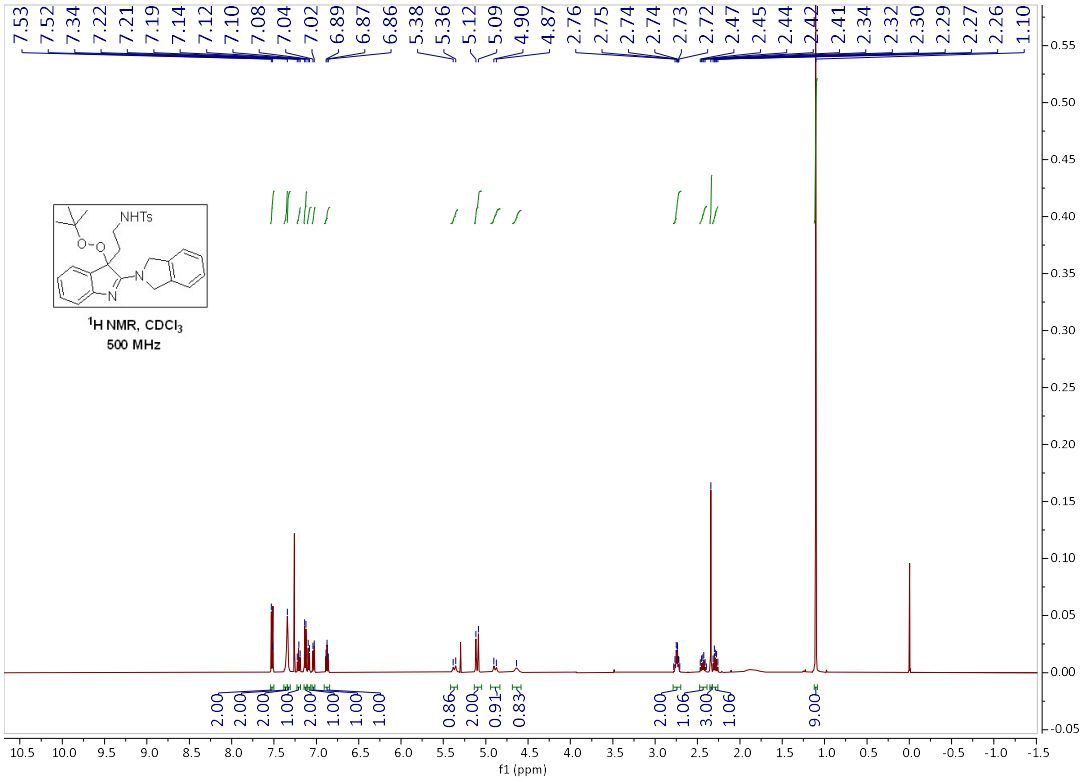
^{1}H NMR Spectrum of 23



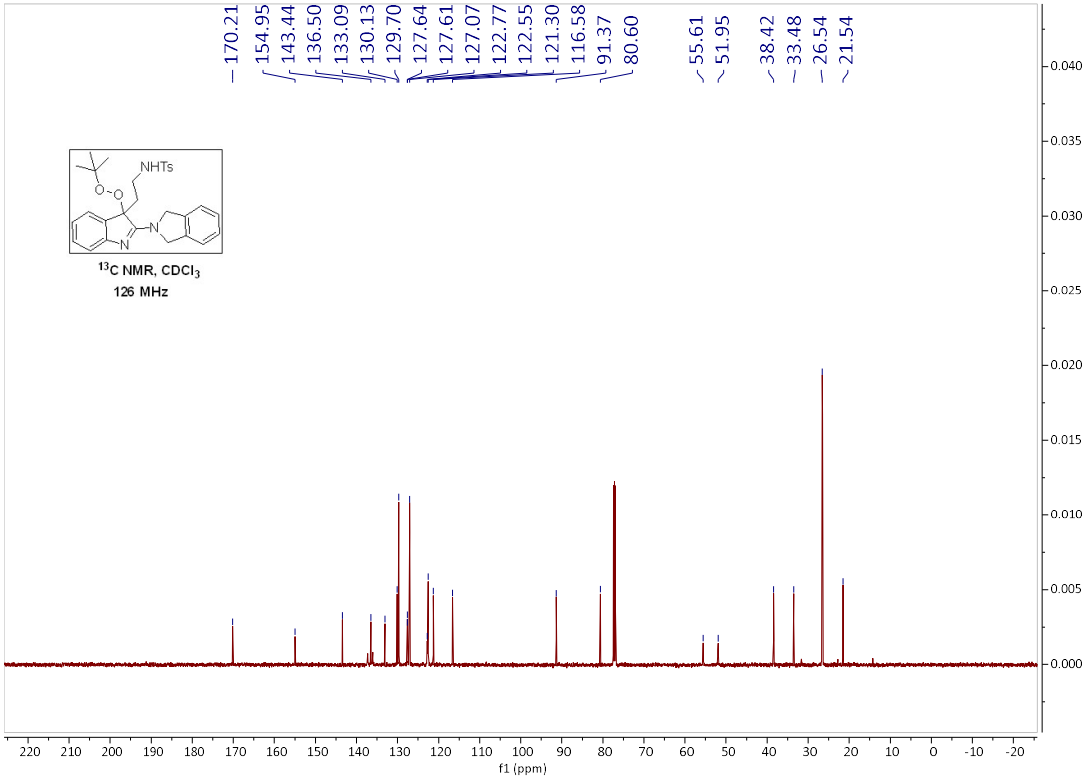
^{13}C NMR Spectrum of 23



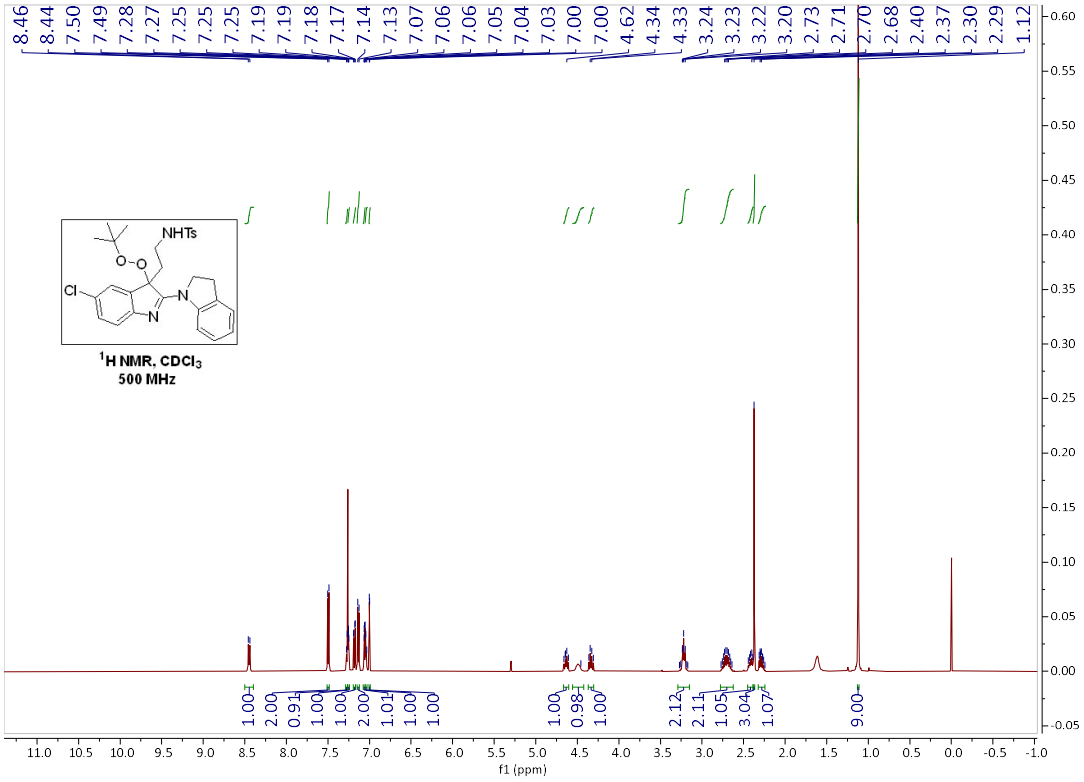
^{1}H NMR Spectrum of 24



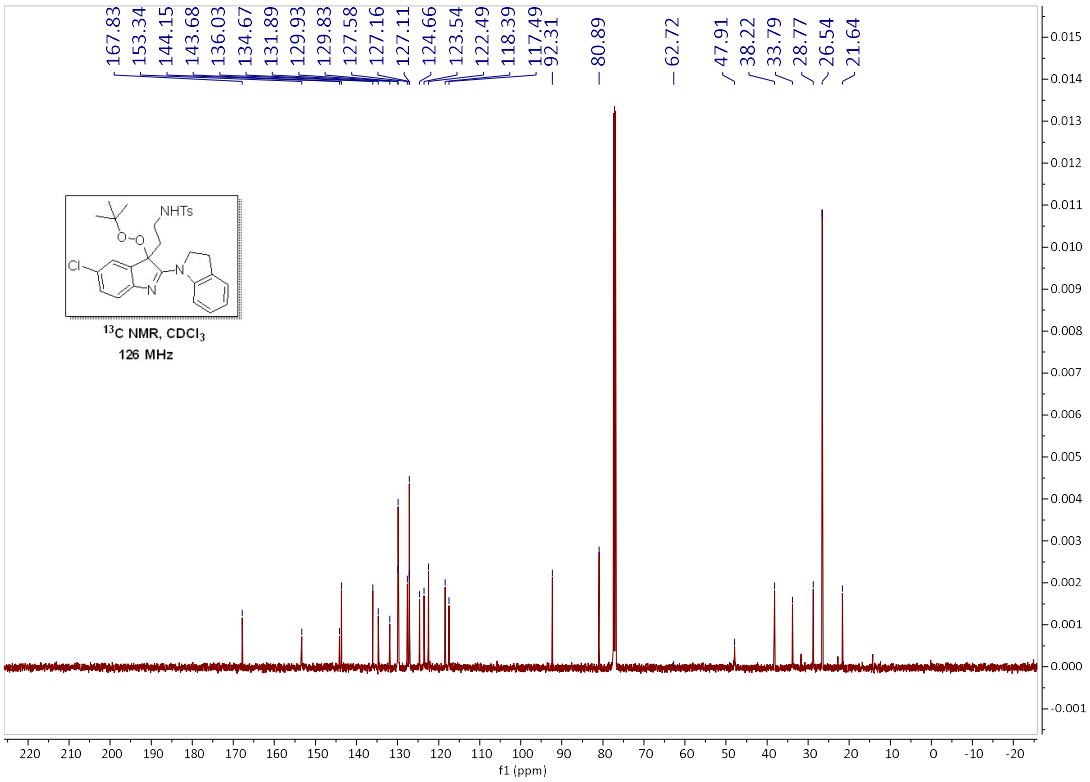
^{13}C NMR Spectrum of 24



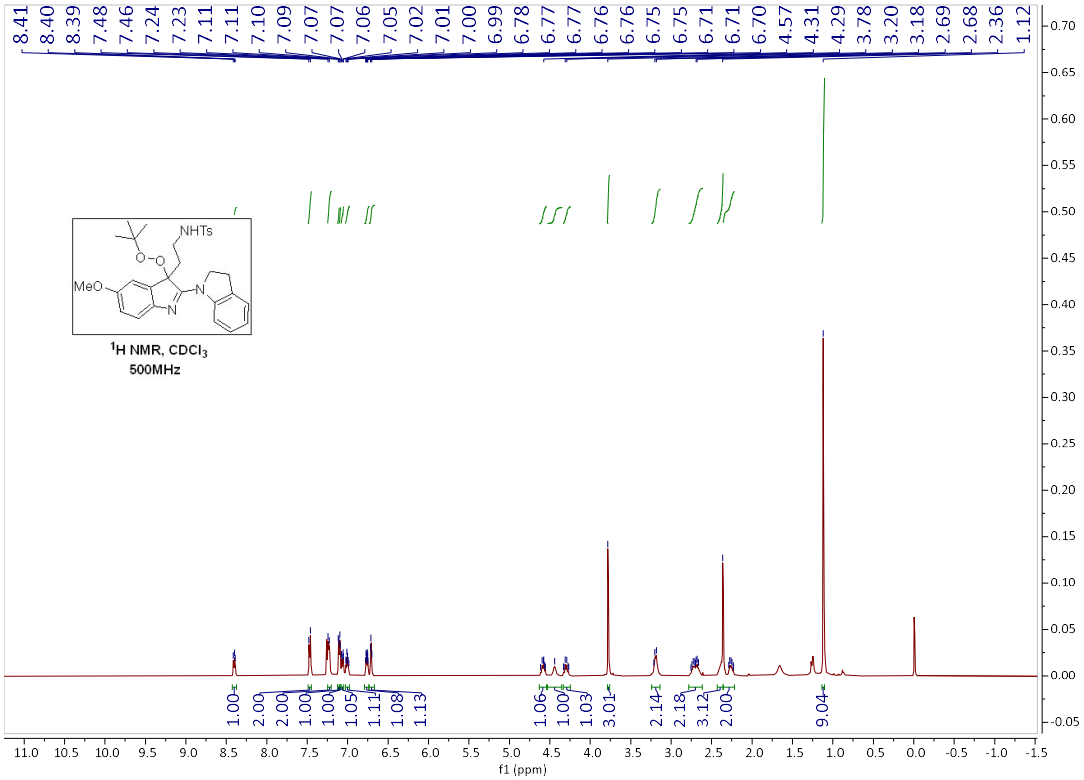
^{1}H NMR Spectrum of 25



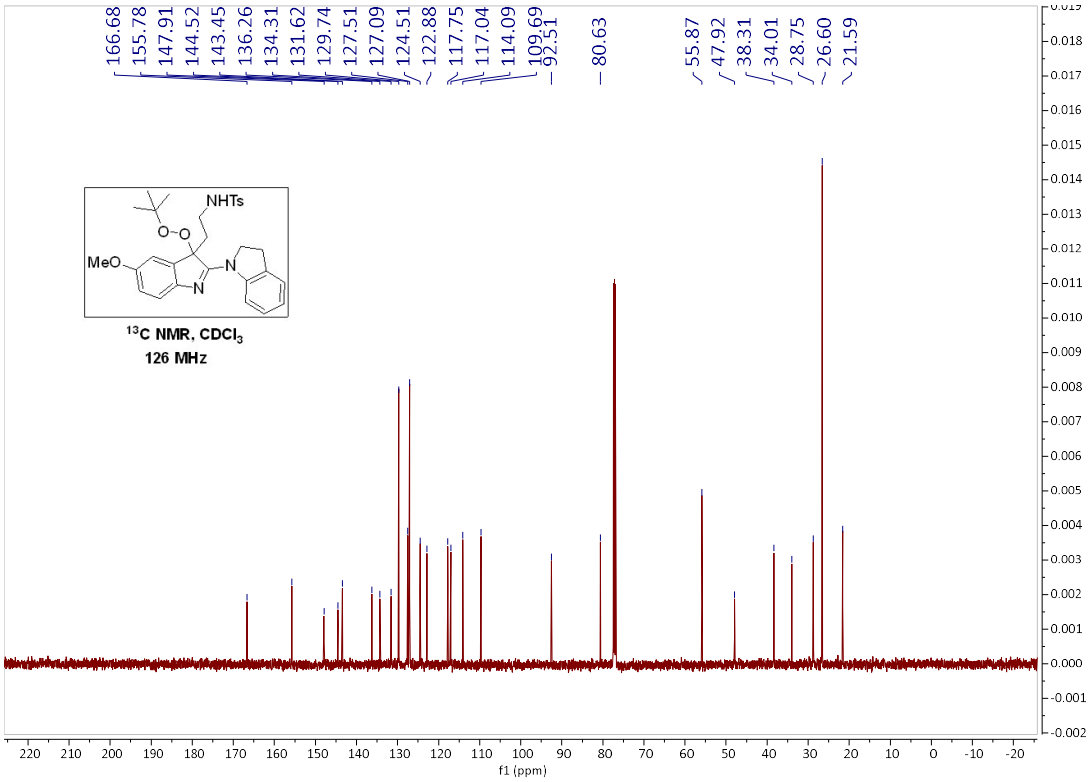
^{13}C NMR Spectrum of 25



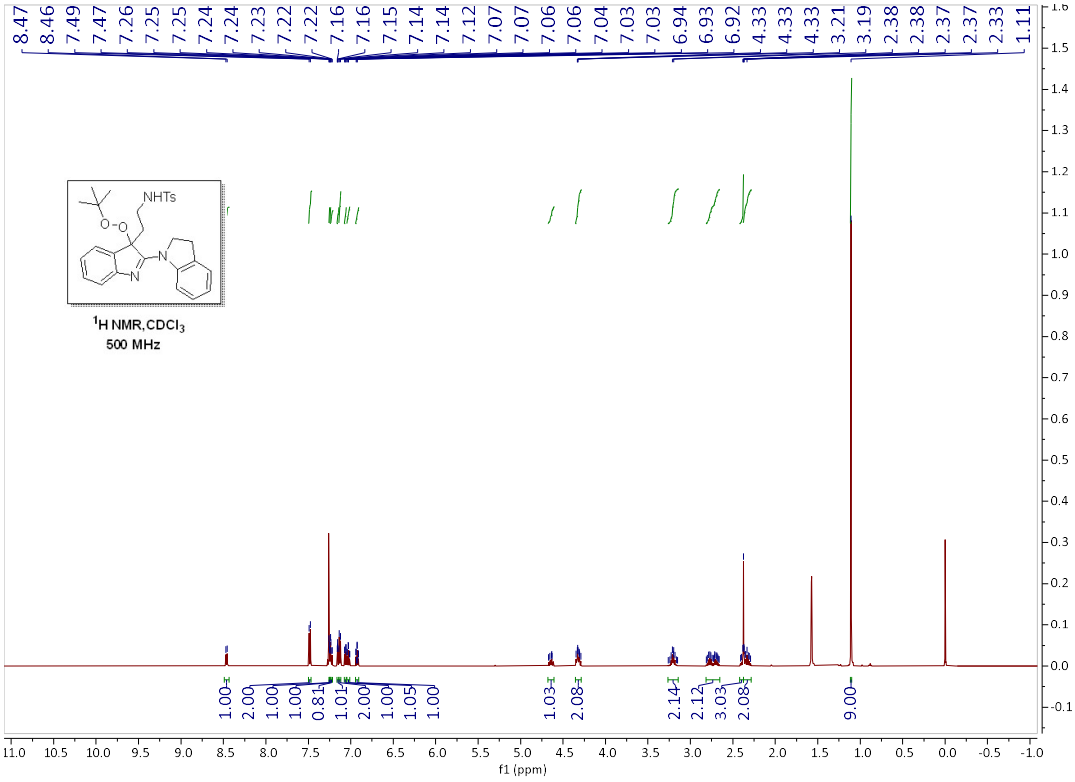
^{1}H NMR Spectrum of 26



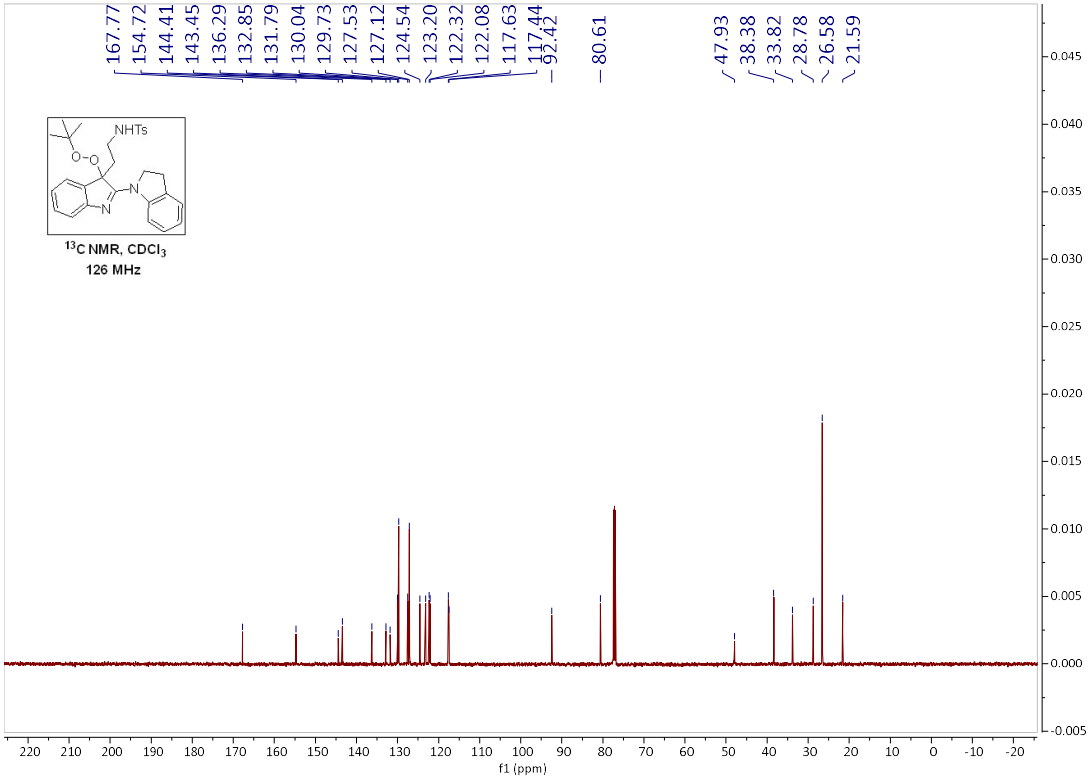
^{13}C NMR Spectrum of 26



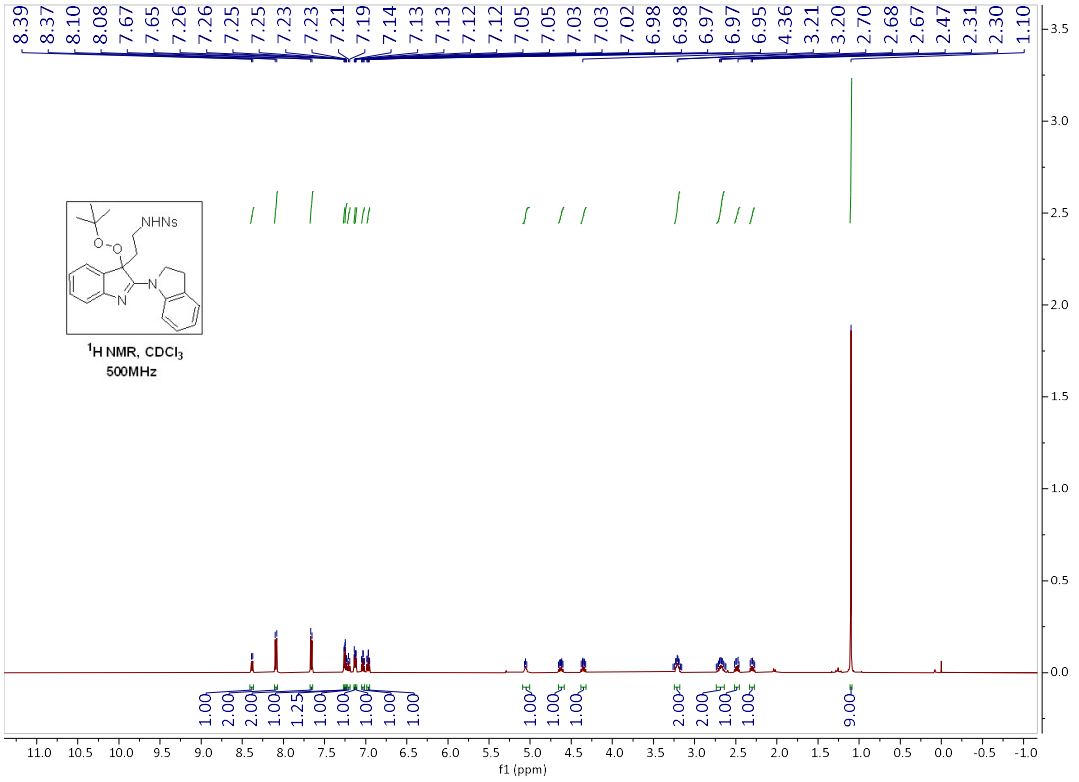
^{1}H NMR Spectrum of 27



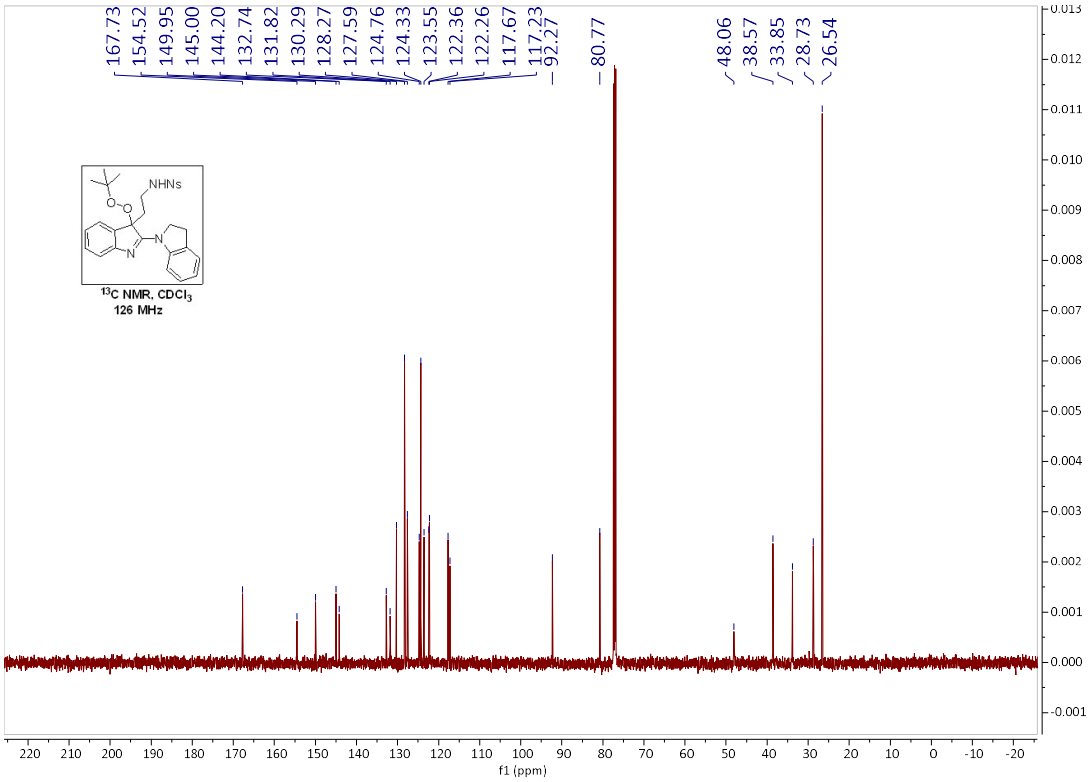
^{13}C NMR Spectrum of 27



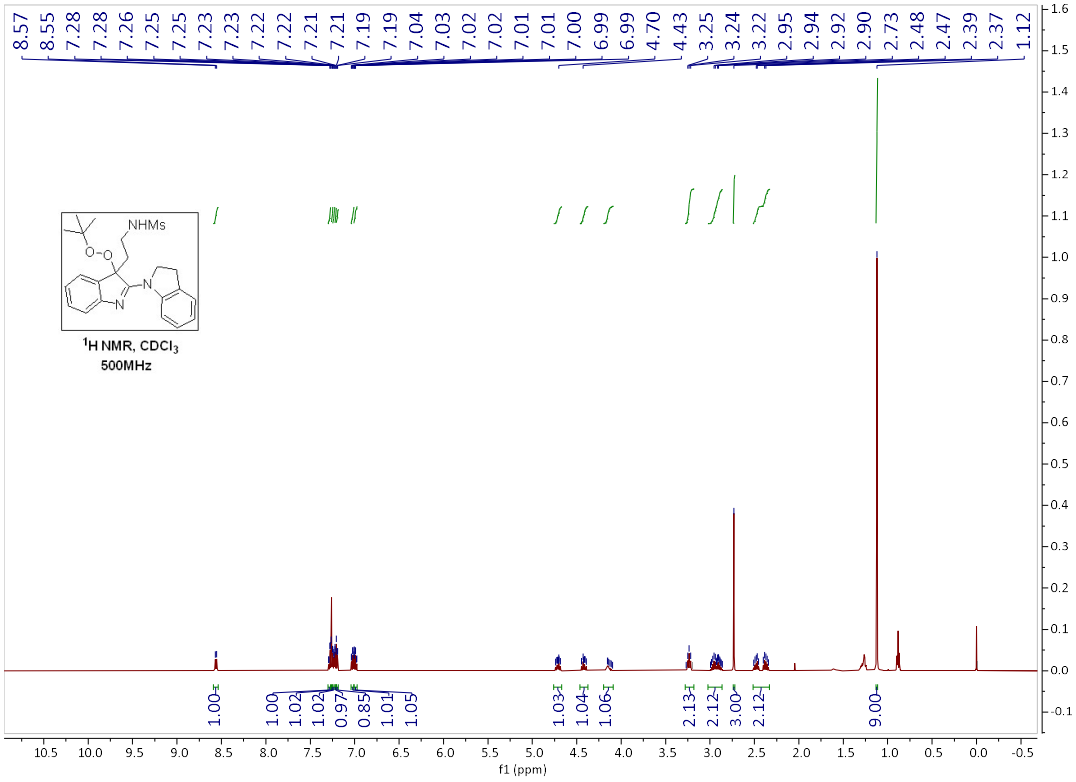
^{1}H NMR Spectrum of 28



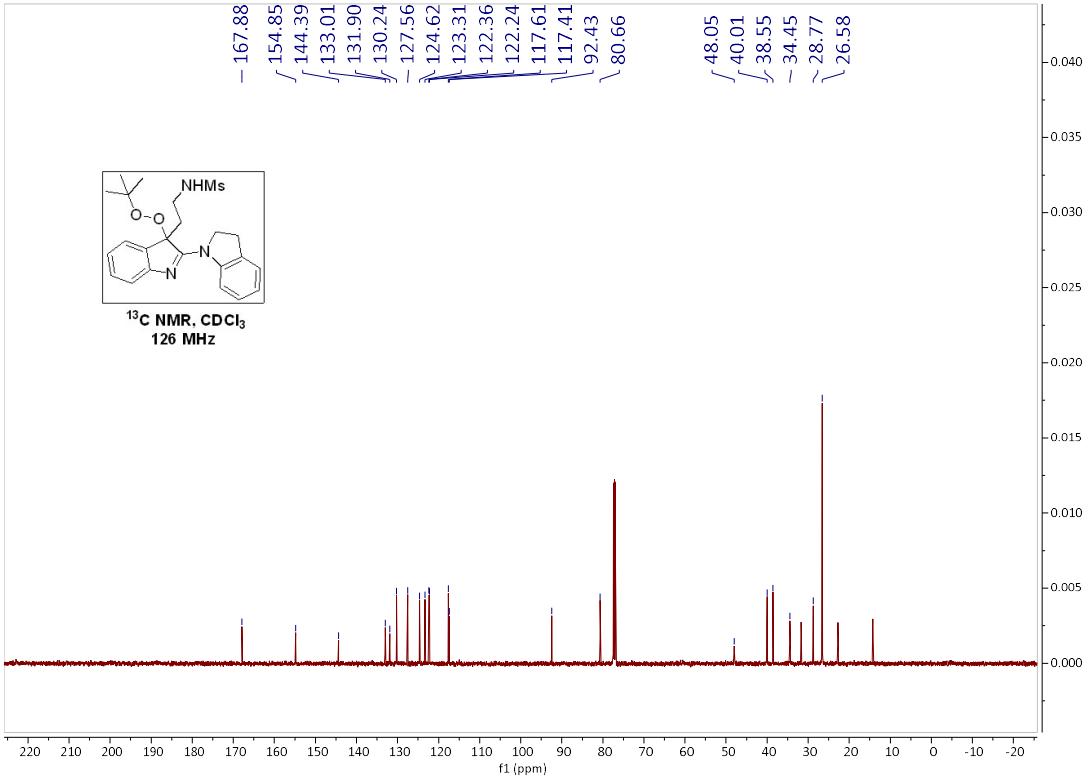
^{13}C NMR Spectrum of 28



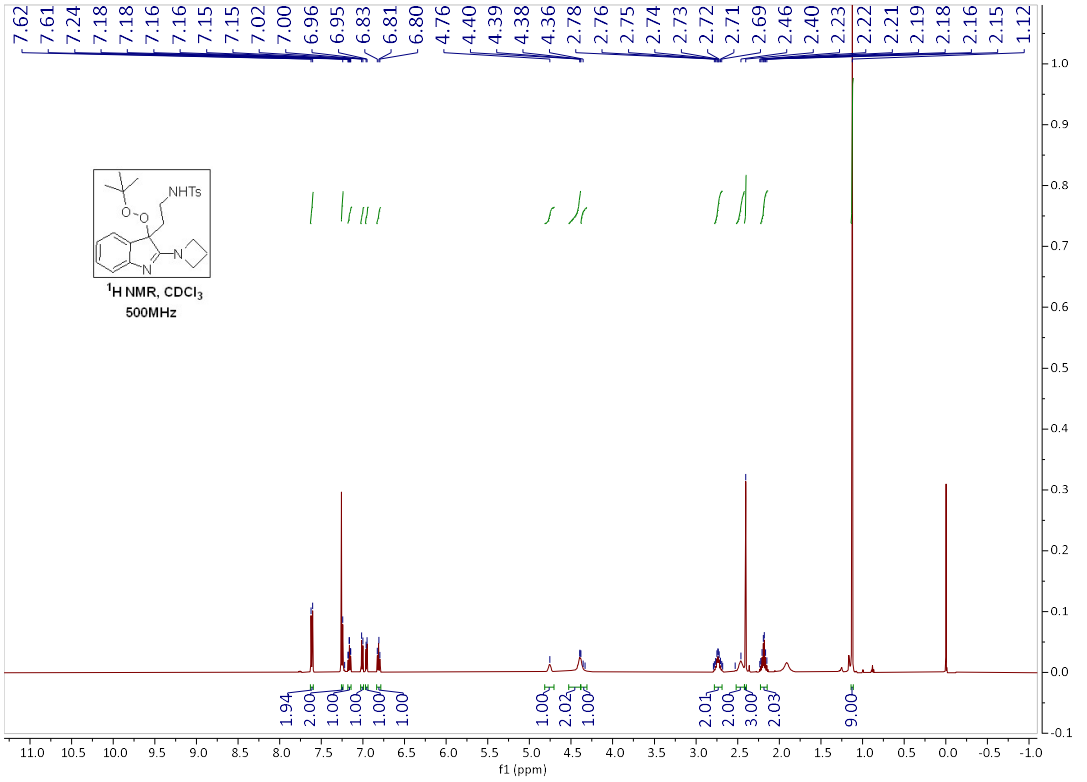
^{1}H NMR Spectrum of 29



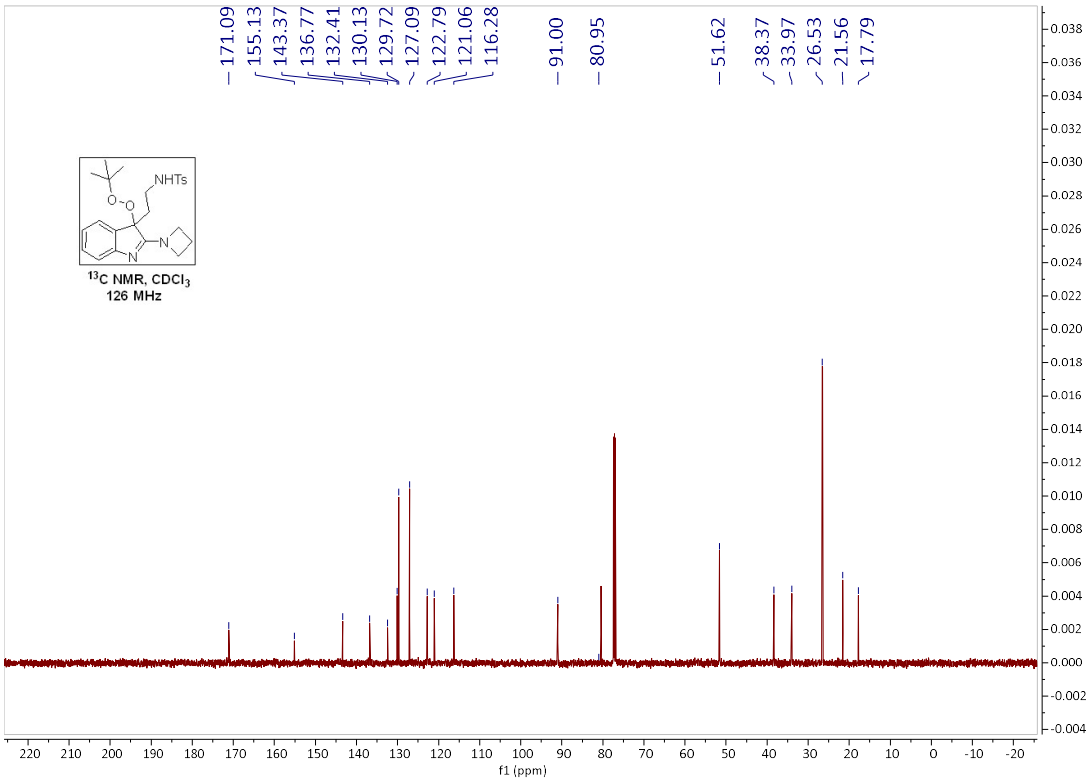
^{13}C NMR Spectrum of 29



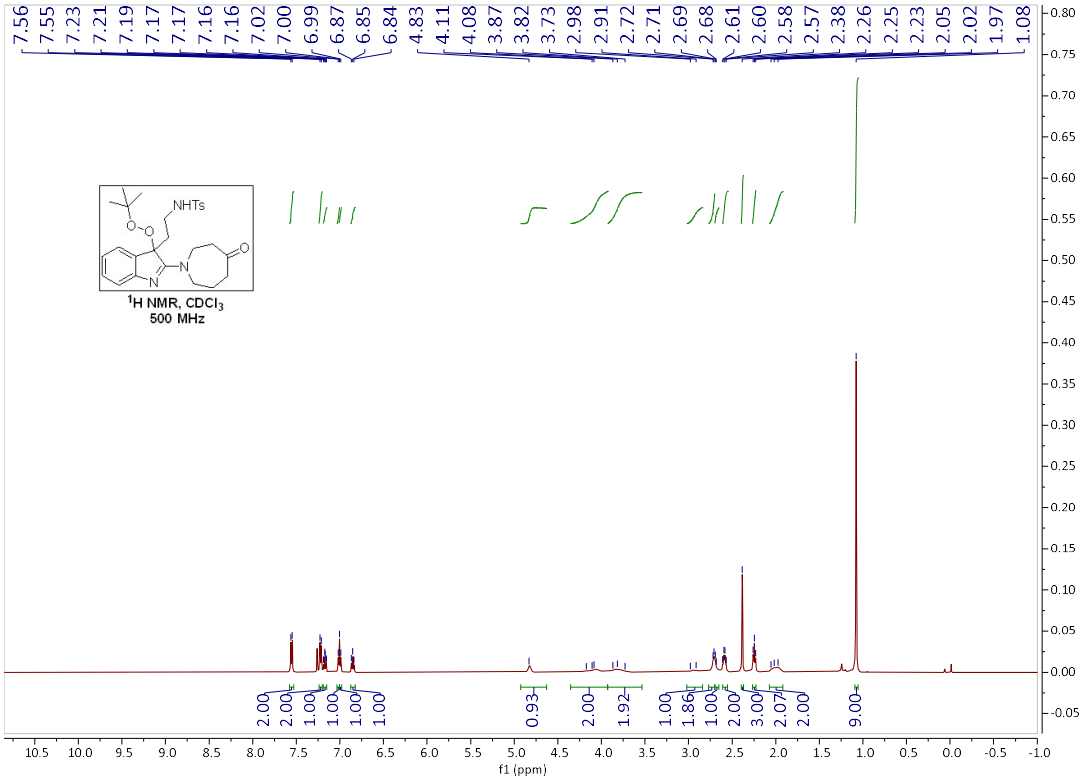
^{1}H NMR Spectrum of 30



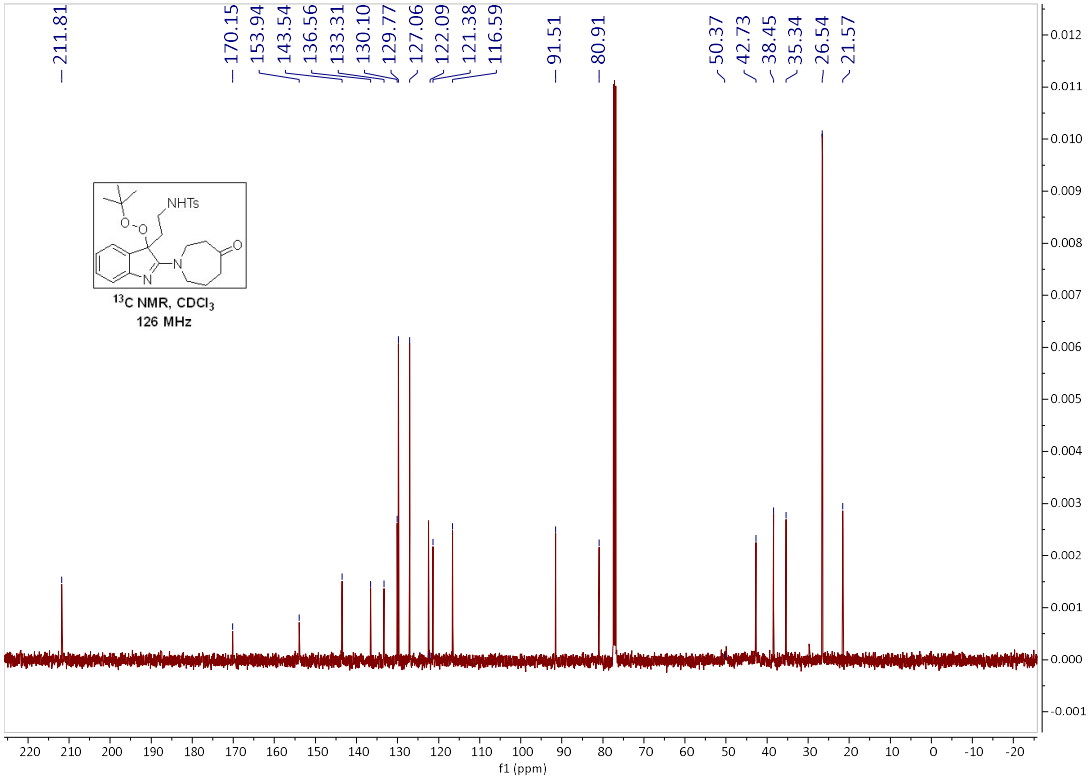
^{13}C NMR Spectrum of 30



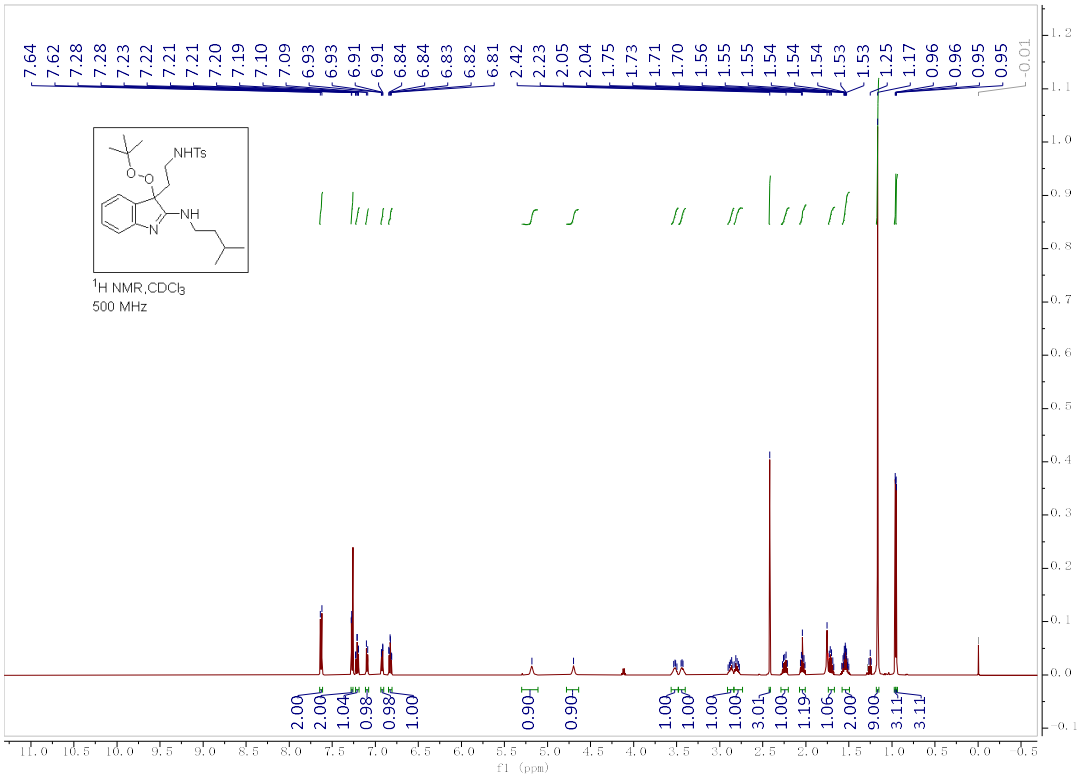
^{1}H NMR Spectrum of 31



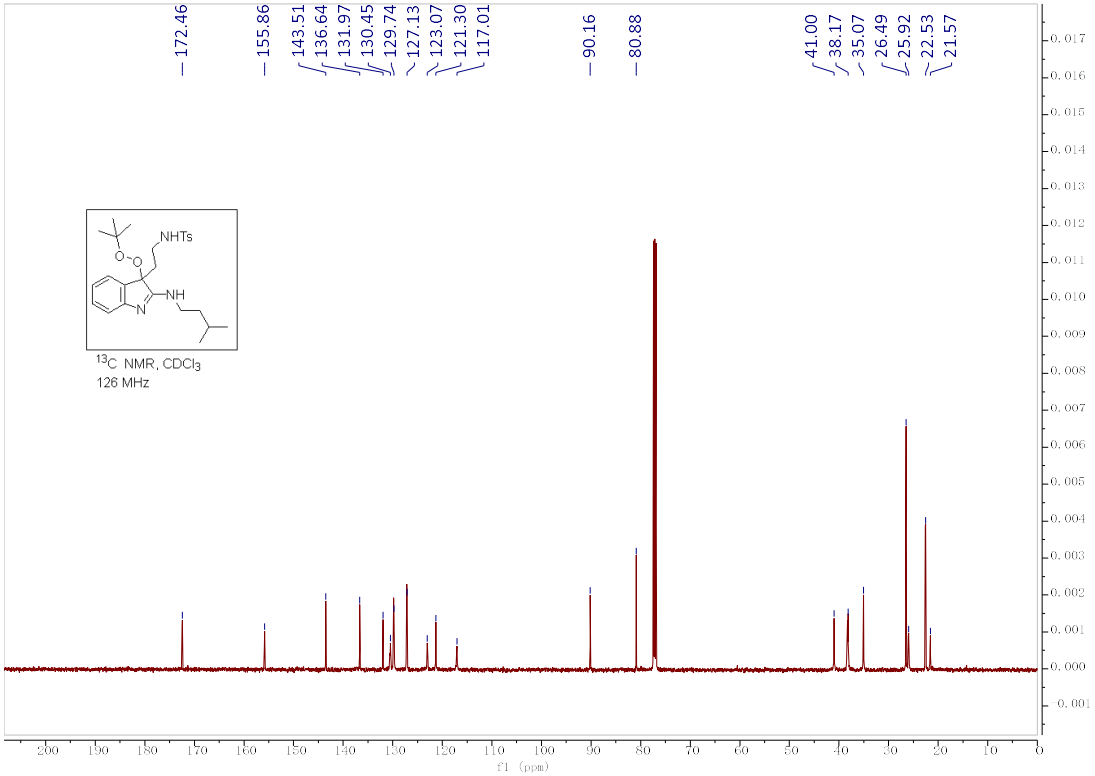
^{13}C NMR Spectrum of 31



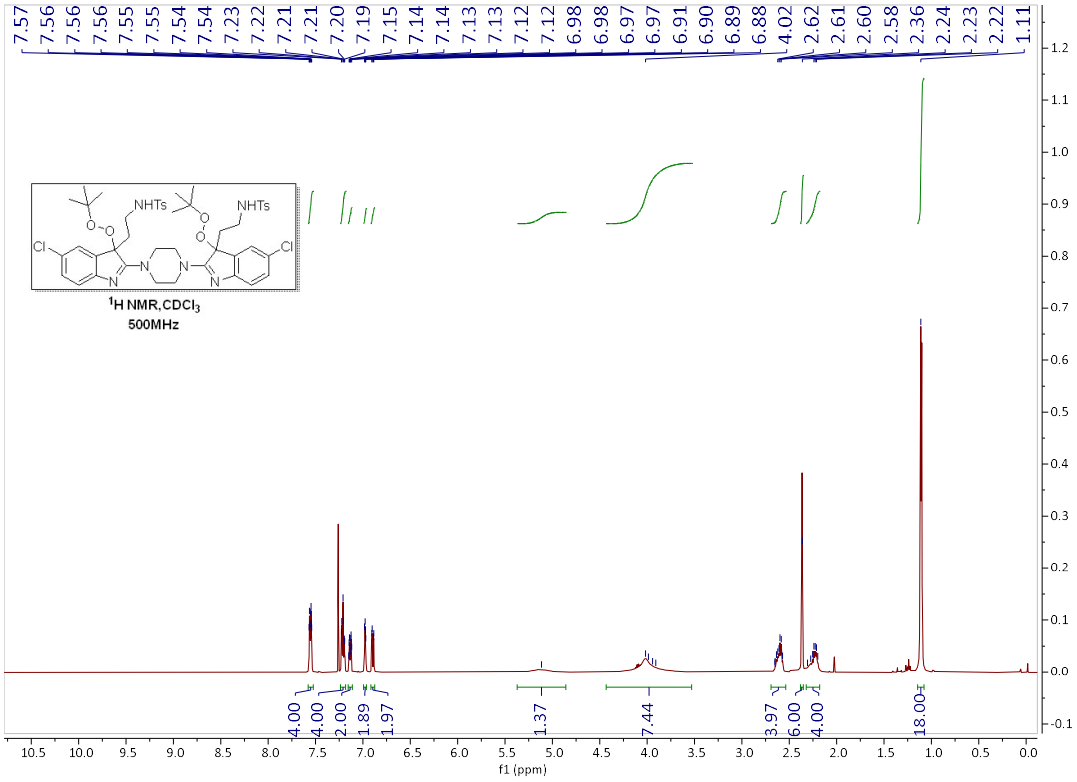
^{1}H NMR Spectrum of 32



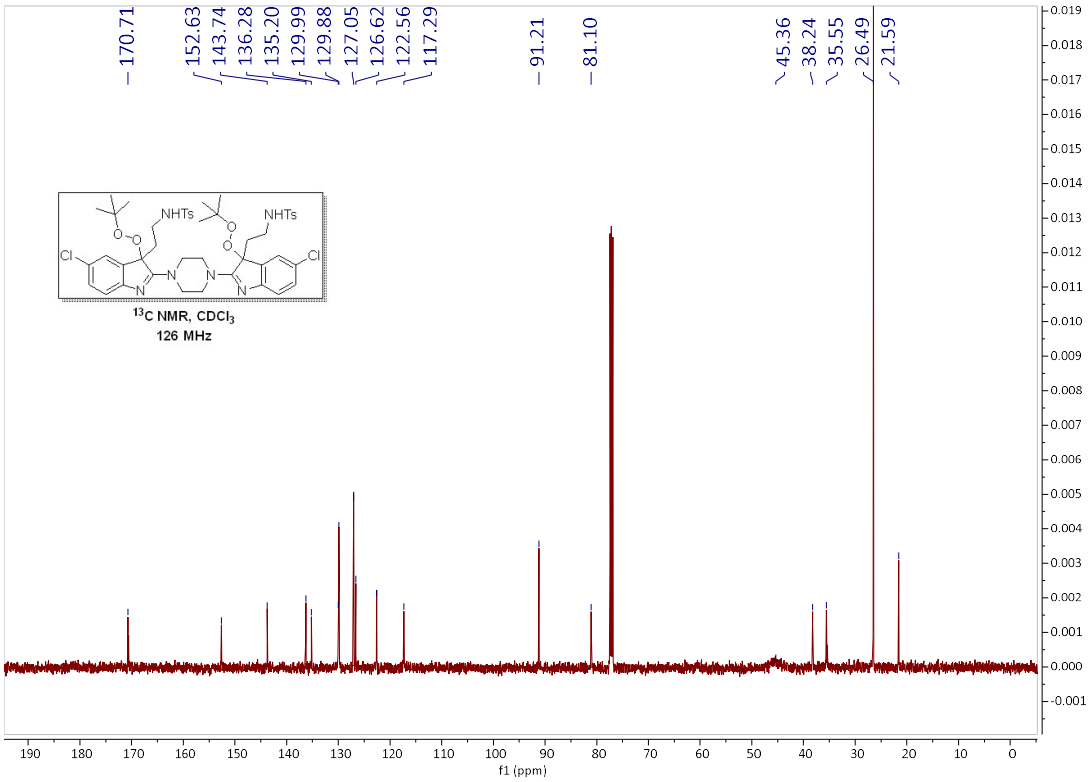
^{13}C NMR Spectrum of 32



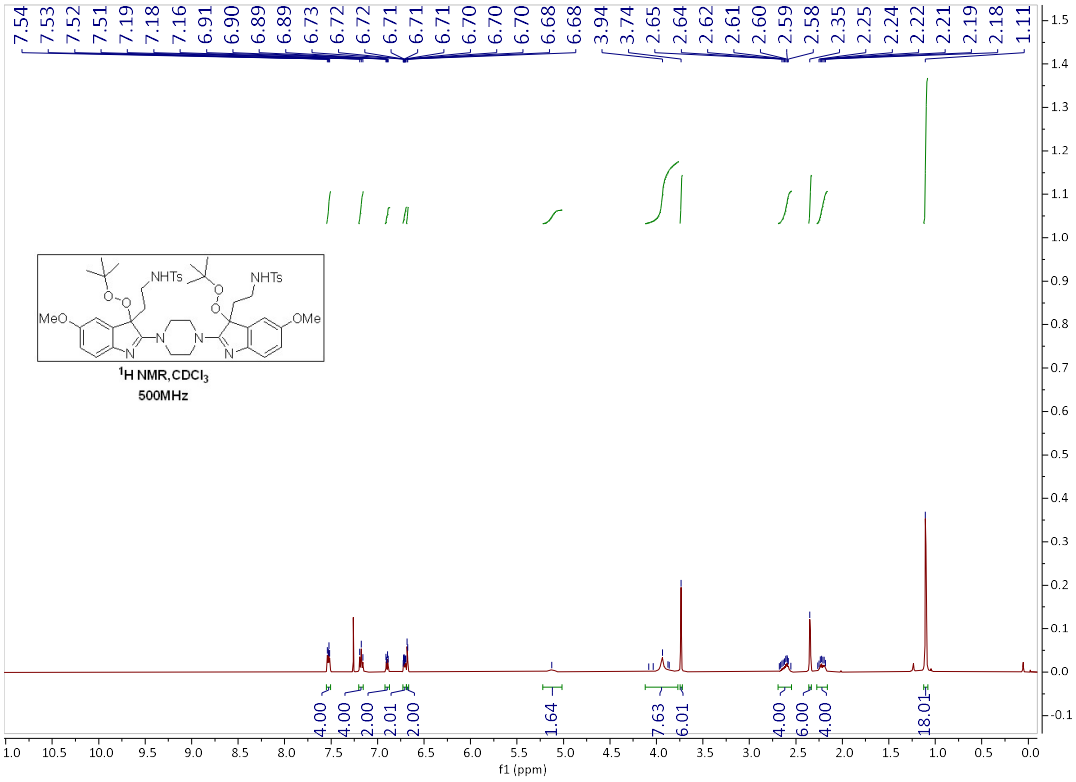
^{1}H NMR Spectrum of 33



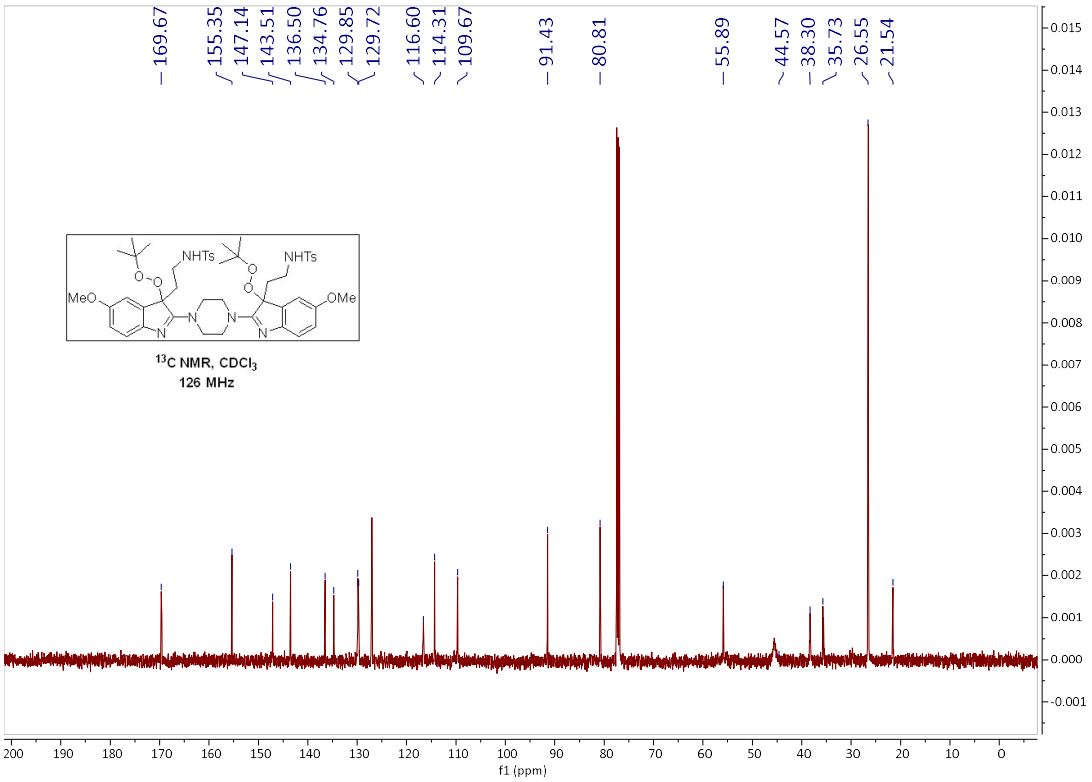
^{13}C NMR Spectrum of 33



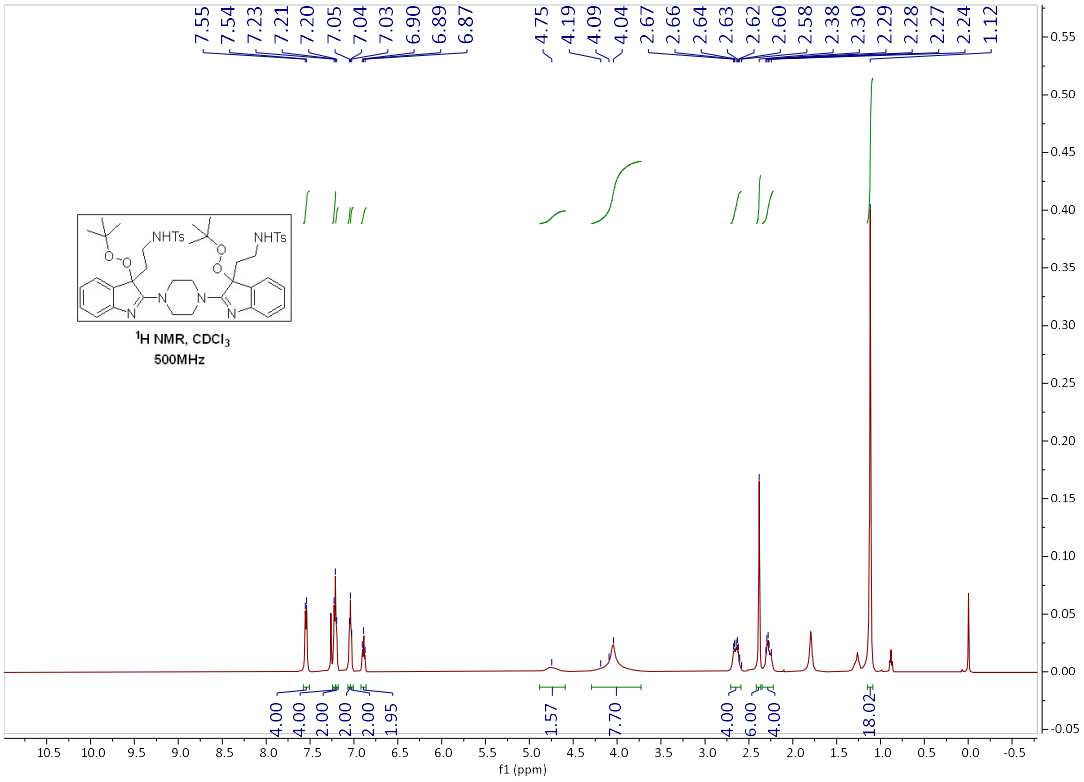
^{1}H NMR Spectrum of 34



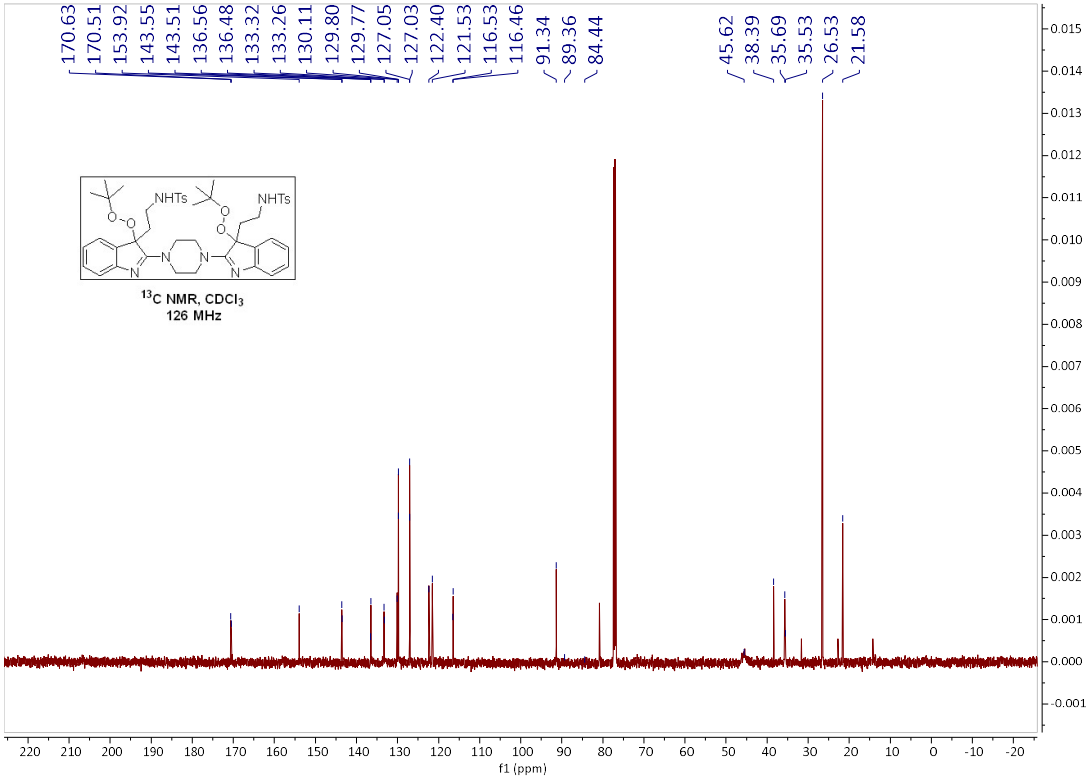
^{13}C NMR Spectrum of 34



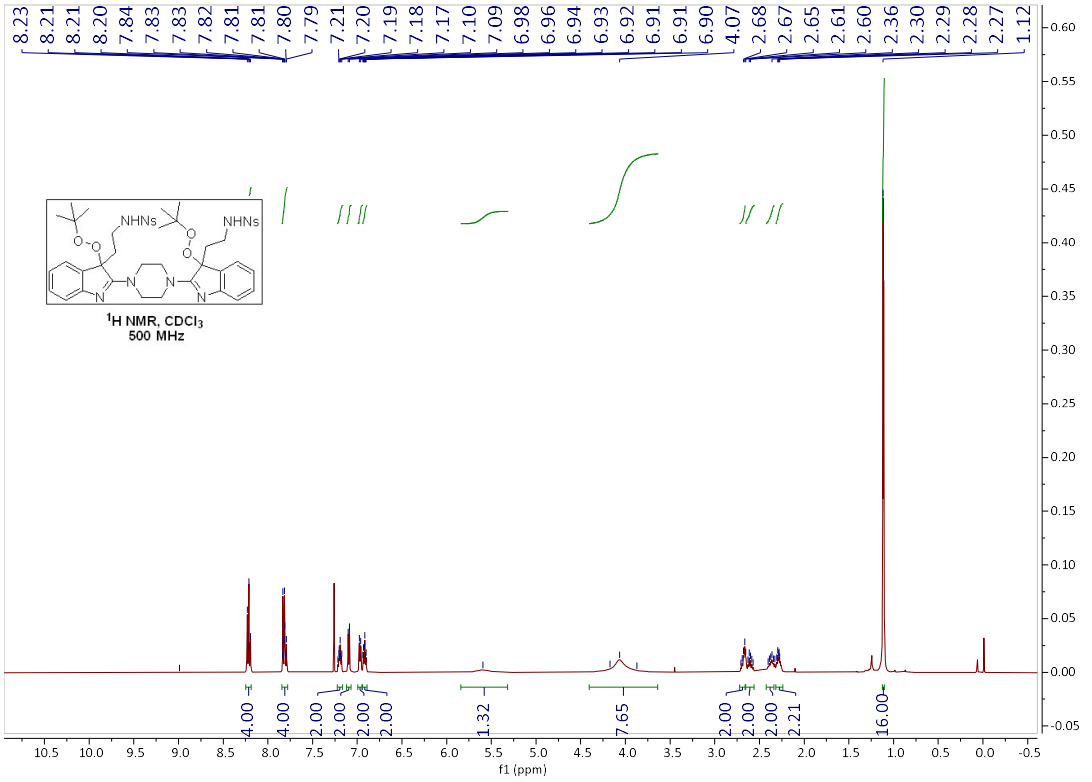
^{1}H NMR Spectrum of 35



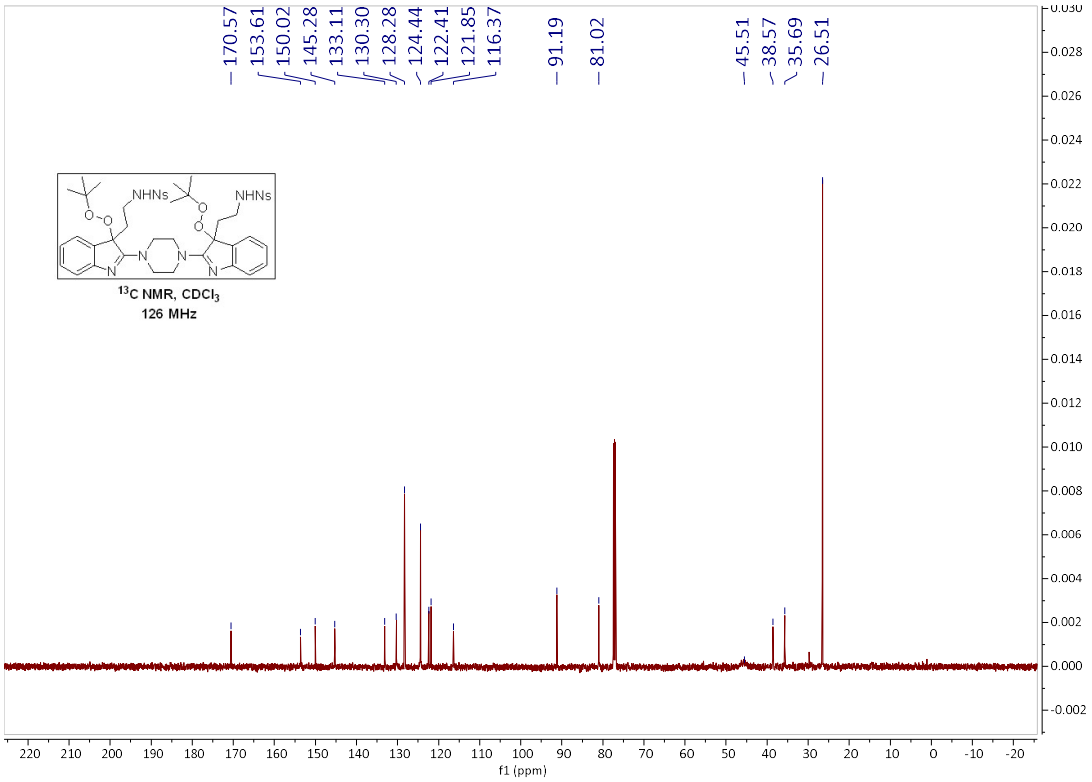
^{13}C NMR Spectrum of 35



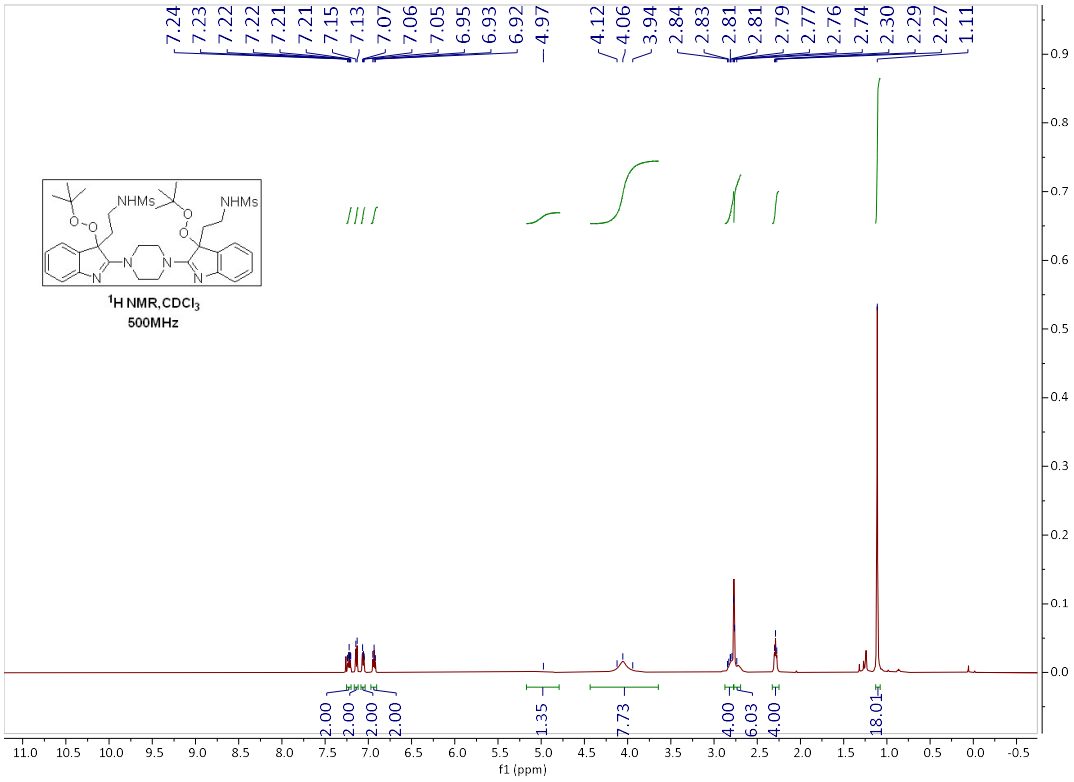
^{1}H NMR Spectrum of 36



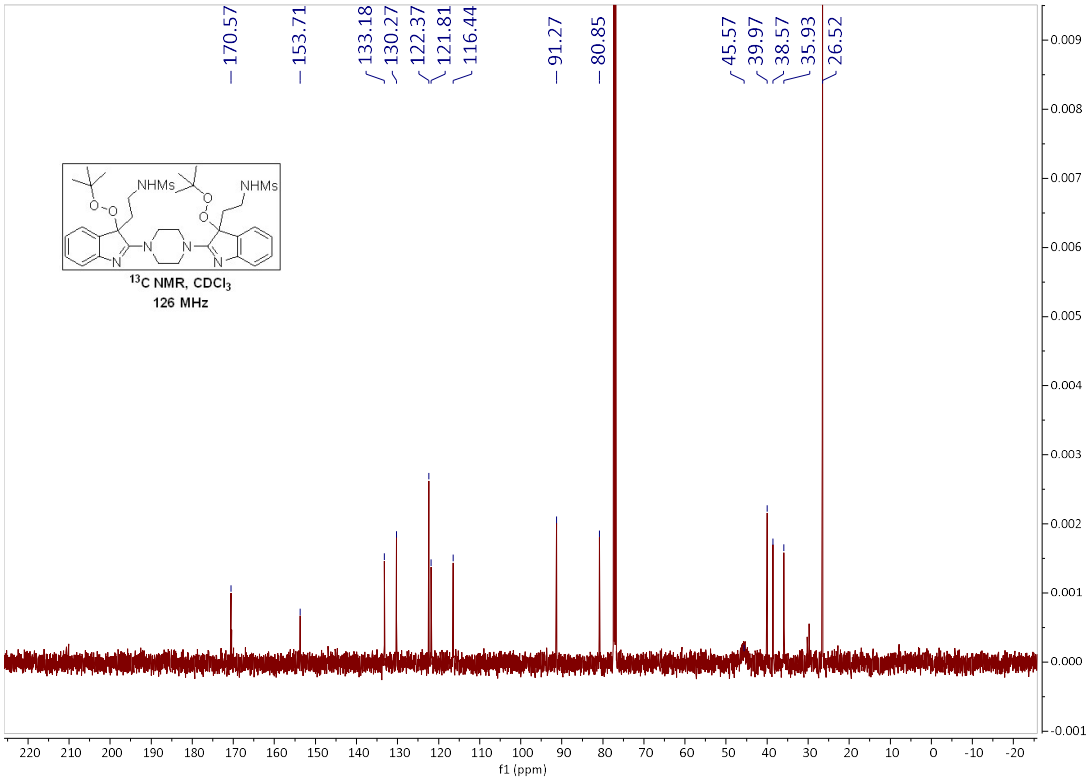
^{13}C NMR Spectrum of 36



^{1}H NMR Spectrum of 37

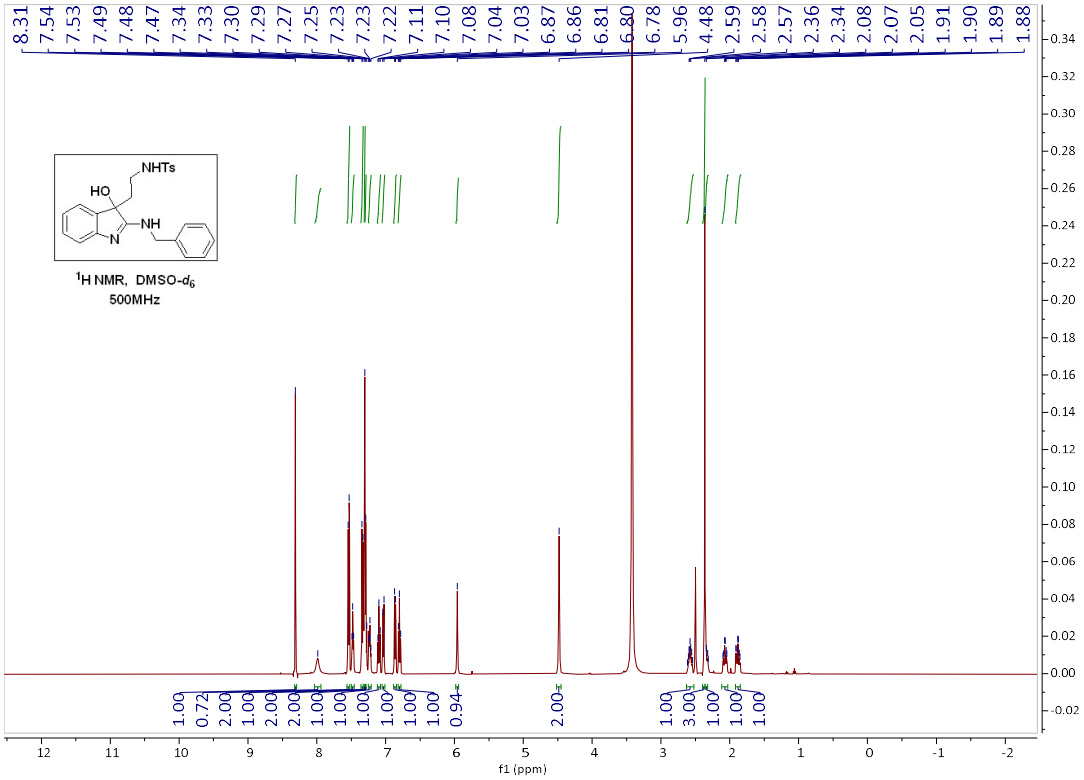


^{13}C NMR Spectrum of 37

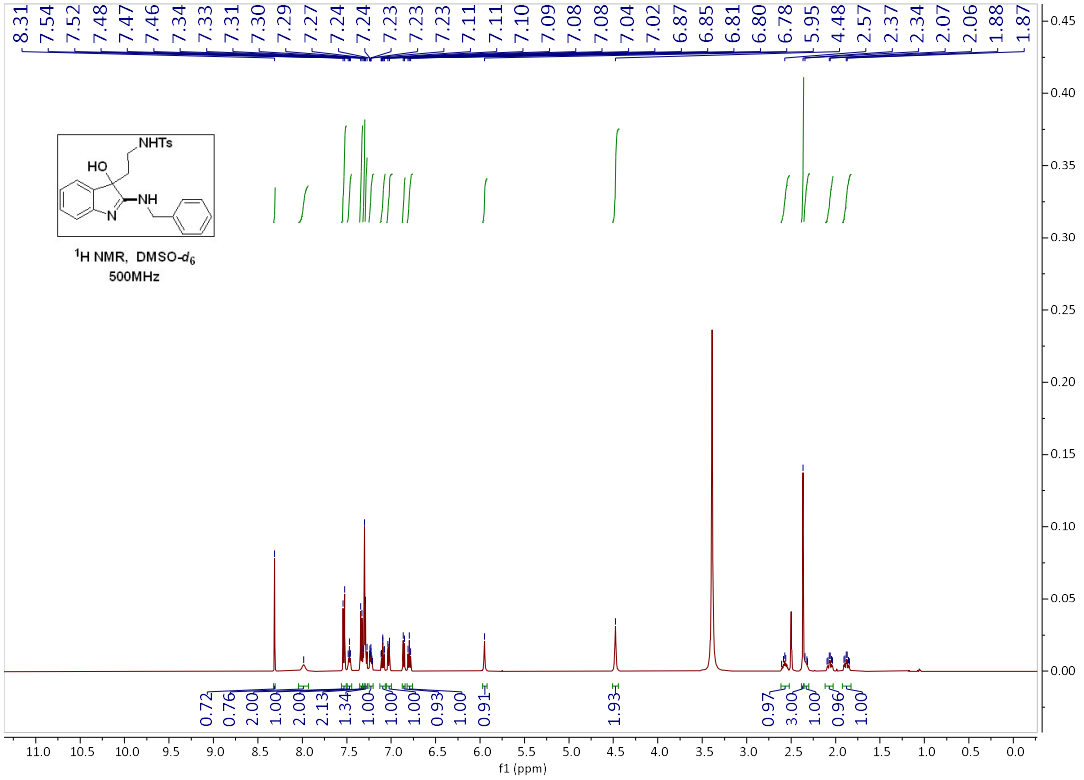


^{1}H NMR Spectrum of 38

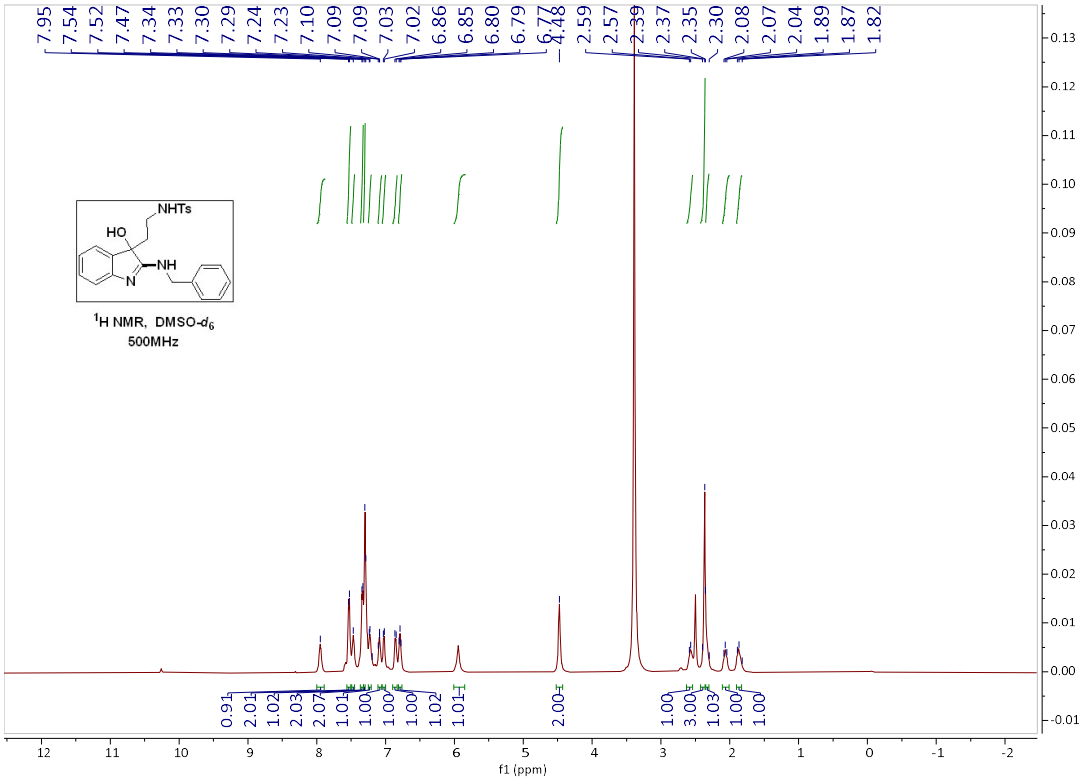
Conditon a:



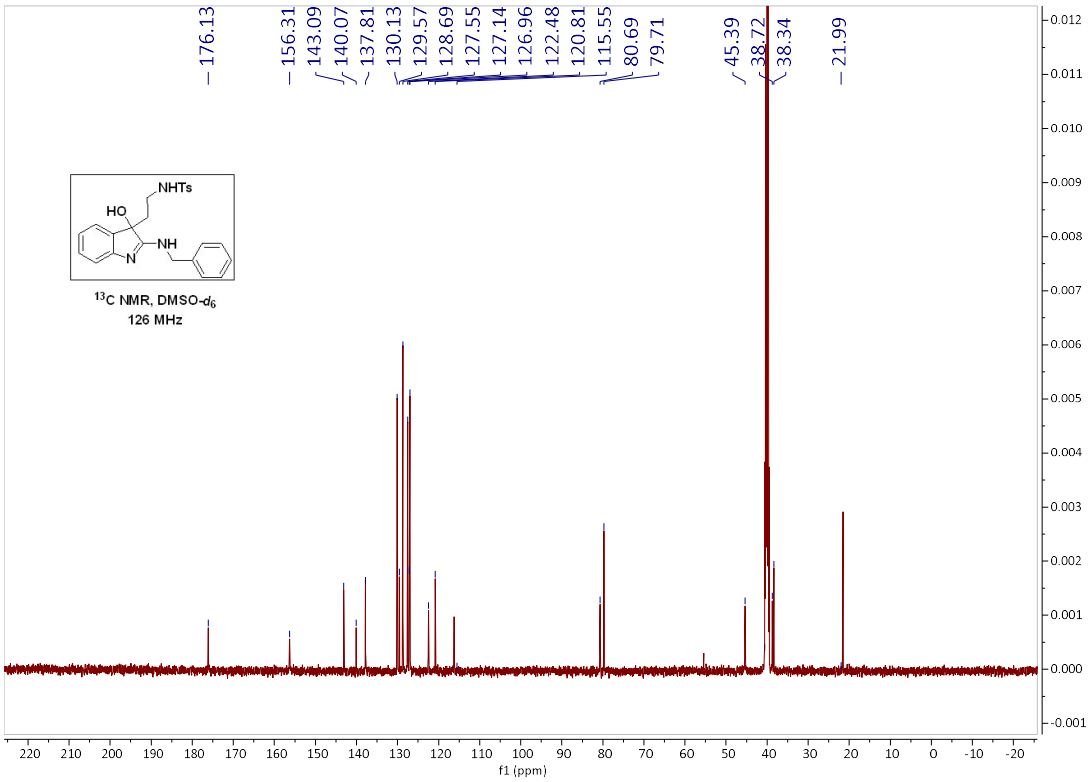
Condition b:



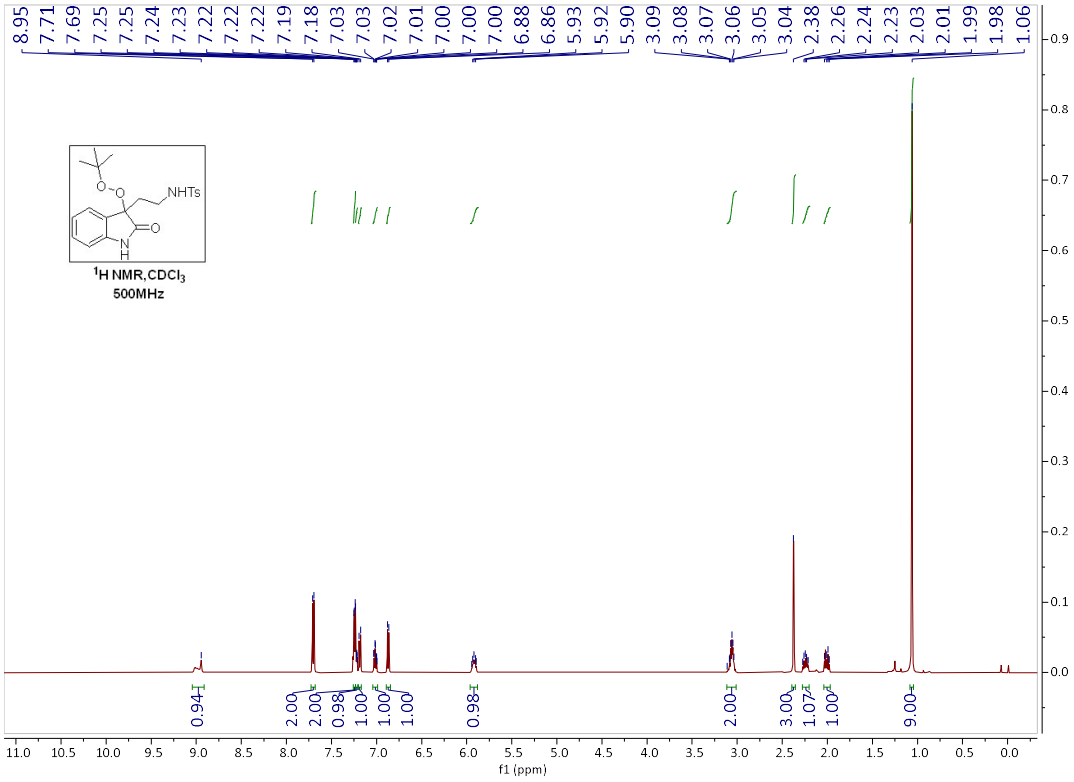
Condition c:



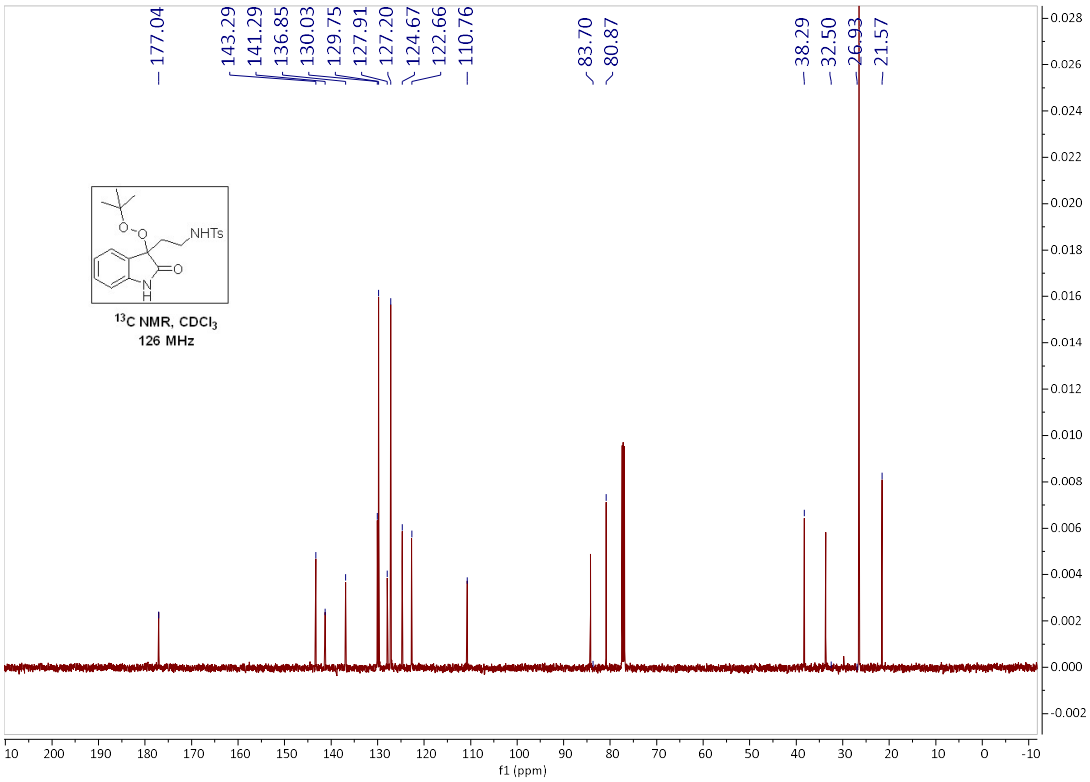
^{13}C NMR Spectrum of 38



^{1}H NMR Spectrum of peroxyoxindole

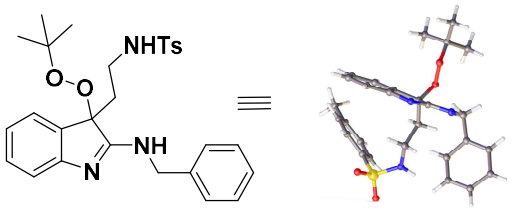


^{13}C NMR Spectrum of peroxyoxindole



7. X-ray Crystal Structure Data

X-ray Crystal Structure Data for compound 1



1

CCDC: 2295779

Identification code	1	
Bond precision	C-C = 0.0055 A; Wavelength=1.54184	
Cell	a=12.9075(2) b=9.8706(2) c=21.4050(4) alpha=90 beta=94.326(2) gamma=90	
Temperature	293 K	
	Calculated	Reported
Volume	2719.33(9)	2719.33(9)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H33 N3 O4 S	C28 H33 N3 O4 S
Sum formula	C28 H33 N3 O4 S	C28 H33 N3 O4 S
Mr	507.63	507.63
Dx, g cm^{-3}	1.240	1.240
Z	4	2
Mu (mm^{-1})	1.360	1.360
F000	1080.0	1080.0
F000’	1084.36	/
h, k, lmax	15,11,25	15,11,25
Nref	4808	4786
Tmin, Tmax	0.878,0.922	0.496,1.000
Tmin’	0.815	/
Data Completeness	0.995	
Theta(max)	66.575	
R(reflections)	0.0693 (3919)	
wR2(reflections)	0.2169 (4786)	
S	1.086	
Npar	331	