Electronic Supplementary Material (ESI) for Chemical Communications

Support Information

A *Trans* Diacyloxylation of Indoles

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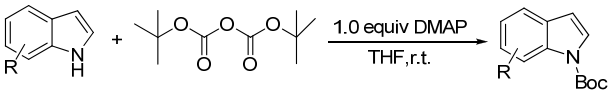
General Considerations

All manipulations were carried out using standard Schlenk techniques. Unless otherwise stated, analytical grade solvents and commercially available reagents were used as received. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum ether (bp. 30-60 ^{o}C). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum ether to the ethyl acetate, which were listed below as volume/volume ratios. All new compounds were characterized by ^{1}H NMR, ^{13}C NMR and HRMS. The known compounds were characterized by ^{1}H NMR. The ^{1}H and ^{13}C NMR spectra were recorded on a Varian Mercury 300 MHz NMR spectrometer. The characterization data of **1q** and **4q** were reported by us previously.[1] The chemical shifts (δ) were given in part per million relative to internal tetramethylsilane (TMS, 0 ppm for ^{1}H) and $CDCl_3$ (77.3 ppm for ^{13}C). High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument and accurate masses were reported for the molecular ion (M^+). X-ray crystallographic analysis was manipulated on a Bruker SMART CCD area-detector diffractometer. All the structures were analyzed at 298 K using graphite monochromated Mo Kα radiation (λ = 0.71073Å) and solved by direct methods using SHELXS-97 program.

Experimental Procedures

General procedure for the synthesis of *tert*-butyl 1*H*-indole-1-carboxylate from substituted indoles with di-*tert*-butyl dicarbonate (5 mmol scale). A 50 mL flask equipped with a stir-bar was charged with substituted indole (5 mmol) and *N*, *N*-dimethylpyridin-4-amine (DMAP) (5.0 mmol). 10 mL of THF was added to the flask and the solution was stirred under room temperature. To the mixture (*tert*-butyl carbonic) 3, 3-dimethylbutanoic anhydride (10 mmol) was added dropwise. The reaction mixture was stirred at room temperature and monitored by TLC. After reaction the mixture was then quenched by water (20 mL) and extracted by ethyl acetate (3 x 20 mL). Combined organic phase were dried over anhydrous Na_2SO_4, and concentrated under vacuum. The residue was then purified by flash chromatography on silica gel with a mixture eluent of petroleum ether, ethyl acetate. After concentrating the fractions containing the product, the residue was dried under reduced pressure.



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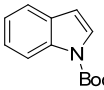
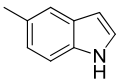
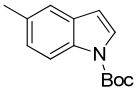
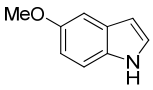
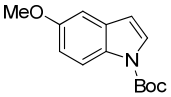
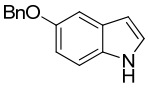
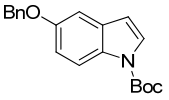
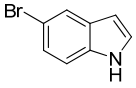
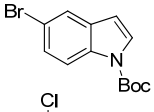
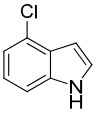
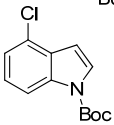
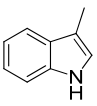
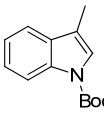
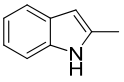
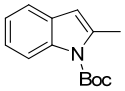
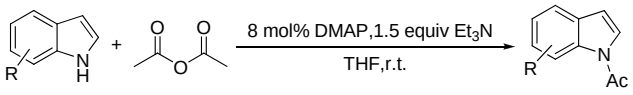
1		 **1c**	92
2		 **1b**	97
3		 **1g**	76
4		 **1e**	87
5		 **1i**	84
6		 **1k**	99
7		 **1p**	86
8		 **1o**	93

General procedure for the synthesis of 1-(1*H*-indol-1-yl)ethanone from substituted indoles with acetic anhydride (5 mmol scale). A 25 mL flask equipped with a stir-bar was charged with substituted indole (5 mmol) and *N*, *N*-dimethylpyridin-4-amine (DMAP) (0.4 mmol). 4 mL of

acetic anhydride was added to the flask and the solution was stirred under room temperature. To the mixture 1.3 mL of triethylamine was added dropwise. The reaction mixture was stirred at room temperature overnight and then quenched by saturated sodium bicarbonate solution (20 mL) and extracted by ethyl acetate (3 x 20 mL). Combined organic phase were dried over anhydrous Na_2SO_4, and concentrated under vacuum. The residue was then purified by flash chromatography on silica gel with a mixture eluent of petroleum ether, ethyl acetate. After concentrating the fractions containing the product, the residue was dried under reduced pressure.



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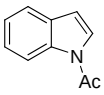
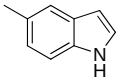
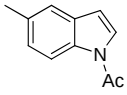
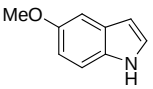
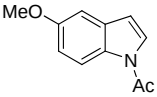
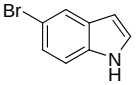
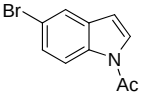
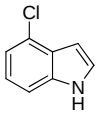
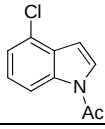
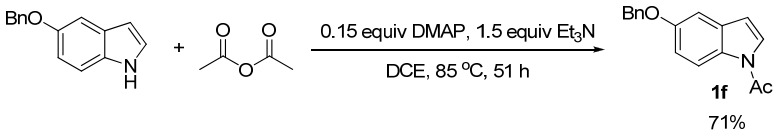
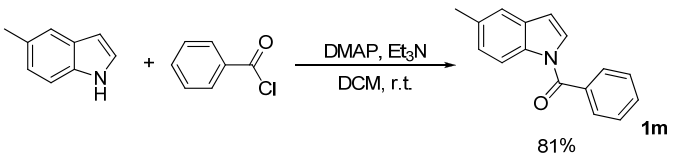
1			**1a**	80
2			**1d**	98
3			**1h**	98
4			**1j**	81
5			**1l**	88

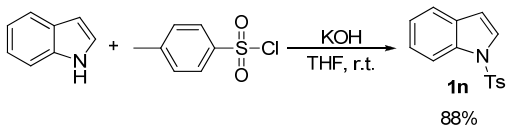
Synthesis of 1-(5-(benzyloxy)-1*H*-indol-1-yl)ethanone 1f from 5-(benzyloxy)-1*H*-indole with acetic anhydride (3 mmol scale) was reference to the literature method.[2]



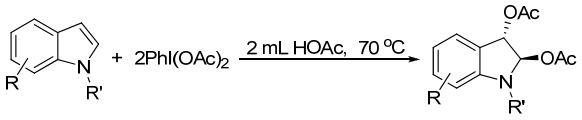
Synthesis of (5-methyl-1*H*-indol-1-yl)(phenyl)methanone 1m from 5-methyl-1*H*-indole with benzoyl chloride (5 mmol scale) was reference to the literature method.[2]



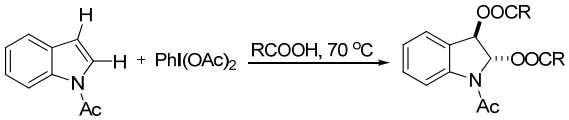
Synthesis of 1-tosyl-1*H*-indole 1n from 1*H*-indole with 4-methylbenzene-1-sulfonyl chloride (5 mmol scale) was reference to the literature method.[3]



General procedure for the diacetoxylation reaction of *N*-protected indole derivatives 1 with (diacetoxyiodo)benzene 2 (0.5 mmol scale). A 10 ml Schlenk tube equipped with a stir-bar was charged with substrate (0.5 mmol), (diacetoxyiodo)benzene (1 mmol). The reaction tube was purged with nitrogen. 2 mL of acetic acid was then added to the reaction tube via a syringe. The Schlenk tube was placed in an oil-bath and heated to 70 ^{o}C and monitored by TLC. After reaction, the reaction mixture was cooled to room temperature and then quenched by sodium bisulphite solution (10 mL) and extracted by ethyl acetate (3 x 10 mL). Combined organic phase were dried over anhydrous Na_2SO_4, and concentrated under vacuum. The residue was then purified by flash chromatography on silica gel with a mixture eluent of petroleum ether, ethyl acetate. After concentrating the fractions containing the product, the residue was dried under reduced pressure.



General procedure for the diacyloxylation reaction of 1-(1*H*-indol-1-yl)ethanone 1a with (diacetoxyiodo)benzene 2 (0.5 mmol scale). A 10 ml Schlenk tube equipped with a stir-bar was charged with substrate (0.5 mmol), (diacetoxyiodo)benzene (1 mmol). The reaction tube was purged with nitrogen. 2 mL of carboxylic acid was then added to the reaction tube via a syringe. The Schlenk tube was placed in an oil-bath and heated to 70 ^{o}C for 48 h. After reaction, the reaction mixture was cooled to room temperature and then quenched by sodium bisulphite solution (10 mL) and extracted by ethyl acetate (3 x 10 mL). Combined organic phase were washed with saturated sodium carbonate solution (3 x 10 mL) and dried over anhydrous Na_2SO_4, and concentrated under vacuum. The residue was then purified by flash chromatography on silica gel with a mixture eluent of petroleum ether, ethyl acetate. After concentrating the fractions containing the product, the residue was dried under reduced pressure.



Procedure for synthesis of *tert*-butyl 3-acetoxy-5-methoxy-1*H*-indole-1-carboxylate 4g from 1-(*tert*-butoxycarbonyl)-5-methoxyindoline-2, 3-diyl diacetate 3g (0.5 mmol scale). A 10 ml Schlenk tube equipped with a stir-bar was charged with substrate (0.5 mmol). The reaction tube was purged with nitrogen. 2 mL of acetic acid was then added to the reaction tube via a syringe. The Schlenk tube was placed in an oil-bath and heated to 70 ^{o}C for 13 h. After reaction, the reaction mixture was cooled to room temperature and extracted by ethyl acetate (3 x 10 mL). Combined organic phase were dried over anhydrous Na_2SO_4, and concentrated under vacuum. The residue was then purified by flash chromatography on silica gel with a mixture eluent of petroleum ether, ethyl acetate (PE/EA=1:70). After concentrating the fractions containing the

product, the residue was dried under reduced pressure.

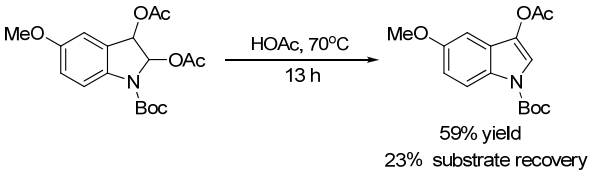
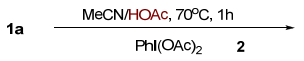


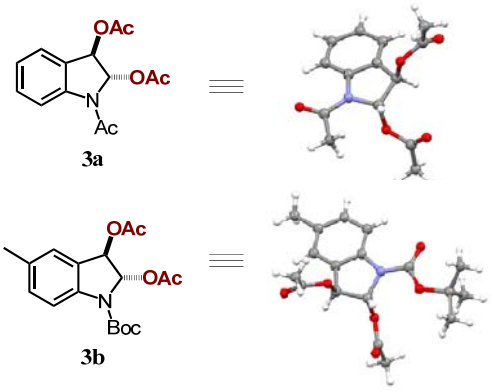
Table S1. The optimization for the diacetoxylation reaction of **1a**[a]



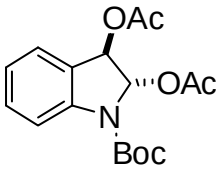
Entry	HOAc/MeCN[b]	Conversion (%)[c]	Yield (%)[c]
1	1 : 156	28	N.D.
2	1 : 78	26	N.D.
3	1 : 39	26	N.D.
4	1 : 5	28	N.D.
5	1 : 3	16	16
6	1 : 1	39	24
7	3 : 1	65	51
8	5 : 1	90	70
9[d]	HOAc	100	78

[a] Reaction conditions: **1** (0.5 mmol), **2** (1 mmol) in 2 mL of MeCN and HOAc mixture at 70 °C. [b] Volume ratio of HOAc to MeCN; [c] Conversion and yield were determined by GC. [d] **1** (0.5 mmol), **2** (1 mmol) in 2 mL of HOAc without MeCN at 70 °C

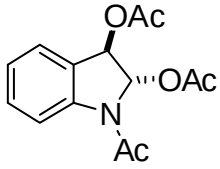
Figure S1. X-Ray crystal structures of **3a** and **3b**



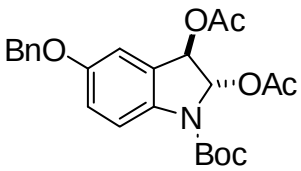
Characterization of Products and Reactants



1-(*tert*-butoxycarbonyl)indoline-2, 3-diyl diacetate (3c): 1c (51 uL, 0.25 mmol), **2** (162.3 mg, 0.50 mmol), HOAc (2 mL), 70 ^{o}C, 1 hour. After column chromatography (PE/EA=1:50) 70.3 mg (84%) of a light yellow liquid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.86 (br, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.77 (s, 1H), 5.90 (s, 1H), 2.09 (s, 6H), 1.56 (s, 9H); ^{13}C NMR (75MHz, $CDCl_3$): δ 170.2, 169.3, 151.1, 143.5, 131.3, 127.3, 126.6, 123.7, 115.4, 86.8, 82.8, 76.1, 28.6, 21.2, 21.1. HRMS (APCI) calculated for $C_{17}H_{21}NO_6Na$ (M^+):358.1267; found: 358.1263.

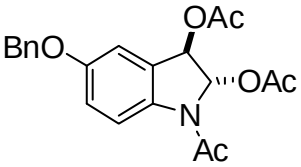


1-acetylindoline-2, 3-diyl diacetate (3a): 1a (80.2 mg, 0.5 mmol) **2** (325.1 mg, 1.0 mmol), HOAc (4 mL), 70 ^{o}C, 1 hour. After column chromatography (PE/EA=1:50) 94.6 mg (68%) of a light yellow solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.21 (br, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.67 (s, 1H), 5.92 (s, 1H), 2.30 (s, 3H), 2.13 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): δ 170.1, 169.9, 169.0, 143.9, 131.4, 130.3, 127.3, 125.0, 117.6, 87.8, 76.3, 23.5, 21.2, 20.8. HRMS (APCI) calculated for $C_{14}H_{15}NO_5Na$ (M^+): 300.0848; found: 300.0846.

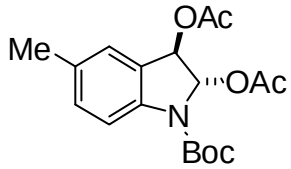


5-(benzyloxy)-1-(*tert*-butoxycarbonyl)indoline-2, 3-diyl diacetate (3e): 1e (161.5 mg, 0.5mmol), **2** (322.3 mg, 1.0 mmol), HOAc (4 mL), 70 ^{o}C, 2 hours. After column chromatography (PE/EA=1:50) 144.1 mg (65%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.70 (br, 1H), 7.33-7.21 (m, 5H), 7.01 (s, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 6.67 (s, 1H), 5.76 (s, 1H), 4.92 (s, 2H), 1.99 (s, 6H), 1.45 (s, 9H);

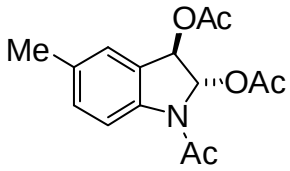
^{13}C NMR (75MHz, $CDCl_3$): δ 170.3, 169.4, 155.4, 151.0, 137.0, 128.8, 128.3, 127.8, 118.0, 116.1, 113.6, 86.9, 82.5, 76.2, 70.8, 28.5, 21.2. HRMS (APCI) calculated for $C_{24}H_{27}NO_7$ (M^+): 441.1788; found: 441.1782.



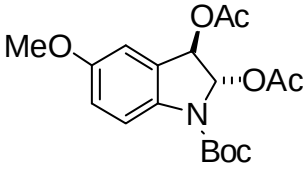
1-acetyl-5-(benzyloxy)indoline-2, 3-diyl diacetate (3f): 1f (54.3 mg, 0.2 mmol), **2** (129.1 mg, 0.4 mmol), HOAc (2 mL), 70 °C, 2.5 hours. After column chromatography (PE/EA=1:20) 58.3 mg (76%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.7 Hz, 1H), 7.36-7.25 (m, 5H), 7.05 (s, 1H), 6.95 (d, *J* = 8.7 Hz, 1H), 6.57 (s, 1H), 5.80 (s, 1H), 4.96 (s, 2H), 2.19 (s, 3H), 2.05 (s, 3H), 2.02 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): δ 170.2, 168.5, 156.2, 137.8, 136.9, 128.9, 128.4, 127.9, 118.5, 117.9, 113.4, 88.1, 76.4, 70.8, 23.3, 21.2. HRMS (APCI) calculated for $C_{21}H_{21}NO_6$ (M^+):383.1369; found: 383.1367.



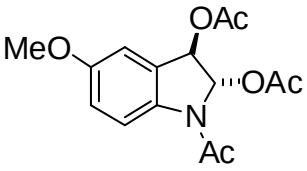
1-(*tert*-butoxycarbonyl)-5-methylindoline-2, 3-diyl diacetate (3b): 1b (55 uL, 0.25 mmol), **2** (162.3 mg, 0.50 mmol), HOAc (2 mL), 70 °C, 1 hour. After column chromatography (PE/EA=1:5) 71.8 mg (82%) of a light yellow solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.66 (br, 1H), 7.19 (br, 1H), 7.12-7.10 (m, 1H), 6.68 (s, 1H), 5.79 (s, 1H), 2.24 (s, 3H), 2.02-2.00 (m, 6H), 1.48 (s, 9H); ^{13}C NMR (75MHz, $CDCl_3$): δ 170.2, 169.3, 151.0, 141.2, 133.3, 131.8, 127.7, 126.5, 115.0, 86.9, 82.5, 76.1, 28.5, 21.2, 21.1. HRMS (APCI) calculated for $C_{18}H_{23}NO_6Na$ (M^+): 372.1423; found: 372.1421.



1-acetyl-5-methylindoline-2, 3-diyl diacetate (3d): 1d (87.5 mg, 0.50 mmol), **2** (326.1 mg, 1.0 mmol), HOAc (4 mL), 70 ^{o}C, 1 hour. After column chromatography (PE/EA=1:5) 125.0 mg (86%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.99 (br, 1H), 7.22 (br, 1H), 7.15-7.12 (m, 1H), 6.58 (s, 1H), 5.81 (s, 1H), 2.26 (s, 3H), 2.20 (s, 3H), 2.04 (s, 3H), 2.02 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): δ 169.8, 169.5, 168.4, 141.3, 134.4, 131.6, 127.3, 126.5, 116.9, 87.6, 76.0, 23.1, 20.9. HRMS (APCI) calculated for $C_{15}H_{17}NO_5$ (M^+): 291.1107; found: 291.1106.

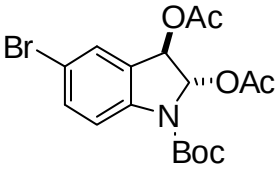


1-(*tert*-butoxycarbonyl)-5-methoxyindoline-2, 3-diyl diacetate (3g): 1g (62.0 mg, 0.25 mmol), **2** (160.7 mg, 0.50mmol), HOAc (2 mL), 70 ^{o}C, 1 hour. After column chromatography (PE/EA=1:5) 87.7 mg (96%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.80 (br, 1H), 7.01 (br, 1H), 6.93 (d, *J* = 9.0 Hz, 1H), 6.75 (s, 1H), 5.85 (s, 1H), 3.78 (s, 3H), 2.10 (s, 3H), 2.09 (s, 3H), 1.54 (s, 9H); ^{13}C NMR (75MHz, $CDCl_3$): δ 170.3, 169.4, 156.4, 151.2, 137.2, 127.4, 117.1, 116.1, 112.5, 87.1, 82.6, 76.2,56.1, 28.6, 21.3, 21.2. HRMS (APCI) calculated for $C_{18}H_{23}NO_7Na$ (M^+): 388.1373; found: 388.1369.

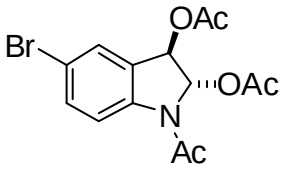


1-acetyl-5-methoxyindoline-2, 3-diyl diacetate (3h): 1h (97.4 mg, 0.50 mmol), **2** (324.7 mg, 1.0 mmol), HOAc (4 mL), 70 ^{o}C, 1 hour. After column chromatography (PE/EA=1:5) 100.8 mg (66%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.12-8.09 (m, 1H), 7.02 (br, 1H), 6.95-6.92 (m, 1H), 6.64 (s, 1H), 5.87 (s, 1H), 3.78 (s, 3H), 2.26 (s, 3H), 2.12 (s, 3H), 2.09 (s, 3H);

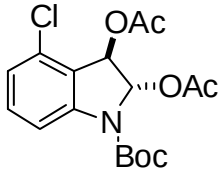
^{13}C NMR (75MHz, $CDCl_3$): δ 170.2, 170.0, 168.6, 157.2, 137.6, 128.1, 118.5, 117.0, 112.3, 88.1, 76.4, 56.0, 23.3, 21.2. HRMS (APCI) calculated for $C_{15}H_{17}NO_6Na$ (M^+): 330.0954; found: 330.0948.



5-bromo-1-(*tert*-butoxycarbonyl)indoline-2, 3-diyl diacetate (3i): 1i (148.5 mg, 0.5 mmol), **2** (322.1 mg, 1.0 mmol), HOAc (4 mL), 70 °C, 29 hours. After column chromatography (PE/EA=1:50) 102.2 mg (50%) of a whilte solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.72 (br, 1H), 7.57 (s, 1H), 7.47 (d, J = 8.4 Hz, 1H), 6.73 (s, 1H), 5.82 (s, 1H), 2.09 (s, 3H), 2.07 (s, 3H), 1.53 (s, 9H); ^{13}C NMR (75MHz, $CDCl_3$): δ 170.2, 169.3, 150.9, 142.7, 134.2, 130.4, 128.7, 116.9, 116.1, 86.7, 83.3, 75.6, 28.6, 21.2, 21.1. HRMS (APCI) calculated for $C_{17}H_{20}BrNO_6$ (M^+): 413.0474; found: 413.0477.

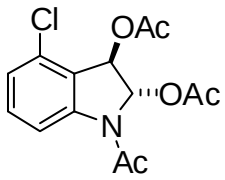


1-Benzyl-5-bromo-1*H*-indol-3-yl acetate (3j): 1j (239.6 mg, 1.0 mmol), **2** (644.6 mg, 2.0 mmol), HOAc (8 mL), 70 °C, 23 hours. After column chromatography (PE/EA=1:5) 263.8 mg (74%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.09 (br, 1H), 7.65-7.63 (m, 1H), 7.61-7.49 (m, 1H), 6.65 (s, 1H), 5.88 (s, 1H), 2.28 (s, 3H), 2.20-2.10 (m, 6H); ^{13}C NMR (75MHz, $CDCl_3$): δ 169.7, 169.5, 168.6, 142.6, 133.9, 130.0, 128.7, 118.7, 117.0, 87.4, 75.4, 23.1, 20.8. HRMS (APCI) calculated for $C_{14}H_{14}BrNO_5$ (M^+): 355.0055; found: 355.0052.

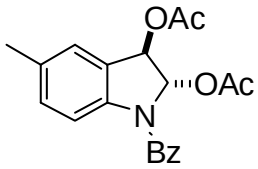


1-(*tert*-butoxycarbonyl)-4-chloroindoline-2, 3-diyl diacetate (3k): 1k (63 uL, 0.25 mmol), **2** (161.5 mg, 0.50 mmol), HOAc (2 mL), 70 °C, 12 hours.

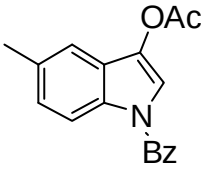
After column chromatography (PE/EA=1:5) 83.2 mg (90%) of a light yellow liquid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.76 (br, 1H), 7.32 (t, *J* = 8.4 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 1H), 6.71 (s, 1H), 6.09 (s, 1H), 2.13 (s, 3H), 2.09 (s, 3H), 1.52 (s, 9H); ^{13}C NMR (75MHz, $CDCl_3$): δ 169.7, 168.6, 150.9, 145.2, 132.7, 132.2, 123.9, 113.8, 86.4, 83.3, 74.4, 28.5, 21.1, 21.0. HRMS (APCI) calculated for $C_{17}H_{20}NO_6ClNa$ (M^+): 392.0877; found: 392.0871.



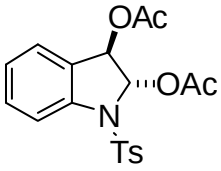
1-acetyl-4-chloroindoline-2, 3-diyl diacetate (3l): 1l (97.0 mg, 0.5 mmol), **2** (323.0mg, 1 mmol), HOAc (4 mL), 70 °C, 53.5 hours. After column chromatography (PE/EA=1:5) 117.0 mg (75%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.10 (br, 1H), 7.36 (t, *J* = 8.1 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 1H), 6.64 (s, 1H), 6.12 (s, 1H), 2.26 (s, 3H), 2.14 (s, 6H); ^{13}C NMR (75MHz, $CDCl_3$): δ 169.6, 169.4, 145.4, 132.9, 131.9, 125.8, 125.1, 115.9, 87.4, 74.7, 23.6, 21.2, 21.0. HRMS (APCI) calculated for $C_{14}H_{14}ClNO_5$ (M^+): 311.0561; found: 311.0556.



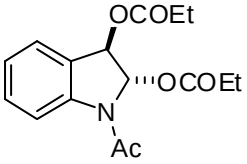
1-benzoyl-5-methylindoline-2, 3-diyl diacetate (3m): 1m (118.5 mg ,0.5 mmol), **2** (322.6 mg, 1 mmol), HOAc (4 mL), 70 °C, 7 hours. After column chromatography (PE/EA=1:5) 125.9 mg (71%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.73 (br, 1H), 7.56-7.42 (m, 5H), 7.33 (s, 1H), 7.19 (d, *J* = 8.1 Hz, 1H), 6.52 (s, 1H), 5.85 (s, 1H), 2.34 (s, 3H), 2.08 (s, 3H), 1.97 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): δ 169.7, 169.0, 168.8, 141.1, 135.1, 134.7, 131.3, 130.8, 128.5, 127.6, 126.7, 116.9, 105.4, 88.2, 75.5, 20.8, 20.5. HRMS (APCI) calculated for $C_{20}H_{19}NO_5$ (M^+): 353.1263; found: 353.1260.



1-benzoyl-5-methyl-1*H*-indol-3-yl acetate (4m): 1m (118.5 mg ,0.5 mmol), **2** (322.6 mg, 1 mmol), HOAc (4 mL), 70 ^{o}C, 7 hours. After column chromatography (PE/EA=1:5) 23.4 mg (16%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.7 Hz, 1H), 7.65 (d, *J* = 6.9 Hz, 2H), 7.51-7.43 (m, 4H), 7.16 (d, *J* = 8.4 Hz, 1H), 7.27 (s, 1H), 2.40 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): δ 168.8, 168.2, 134.6, 134.3, 134.1, 132.2, 132.0, 129.4, 128.9, 127.7, 124.5, 117.7, 116.6, 116.1, 21.8, 21.3. HRMS (APCI) calculated for $C_{18}H_{15}NO_3$ (M^+): 293.1052; found: 293.1055.

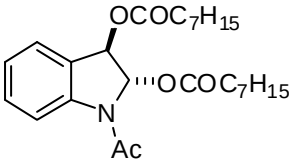


1-tosylindoline-2, 3-diyl diacetate (3n): 1n (271.4 mg, 1.0 mmol), **2** (644.6 mg, 2 mmol), HOAc (6 mL), 70 ^{o}C, 19 hours. After column chromatography (PE/EA=1:5) 287.8 mg (74%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.1 Hz, 2H), 7.57 (d, *J* = 8.7 Hz, 1H), 7.32 (t, *J* = 6.3 Hz, 2H), 7.29-7.19 (m, 2H), 7.05 (t, *J* = 7.8 Hz, 1H), 6.59 (s, 1H), 5.69 (s, 1H), 2.31 (s, 3H), 2.00 (s, 3H), 1.78 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): δ 169.4, 169.0, 144.5, 142.4, 135.2, 131.2, 129.6, 127.5, 127.3, 124.7, 115.2, 88.4, 76.0, 21.5, 20.8, 20.5. HRMS (APCI) calculated for $C_{19}H_{19}NO_6S$ (M^+): 389.0933; found: 389.0938.

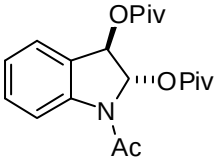


Diethyl 1-acetylindoline-2,3-dicarboxylate (3r) 1a (80.2 mg, 0.5 mmol), **2** (323.0 mg, 1 mmol), EtCOOH (4 mL), 70 ^{o}C, 40 hours. After column chromatography (PE/EA=1:50) 95.6 mg (63%) of a light yellow liquid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.06 (s, 1H), 7.48-7.40 (m, 2H), 7.16 (t, *J* = 7.5

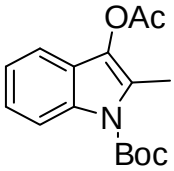
Hz, 1H), 6.73 (s, 1H), 5.97 (s, 1H), 2.41-2.31 (m, 4H), 2.26 (s, 3H), 1.06-1.00 (m, 6H); ^{13}C NMR (75MHz, $CDCl_3$): δ 172.7, 172.5, 168.9, 143.3, 130.8, 126.9, 124.3, 116.1, 86.9, 75.3, 26.5, 23.0, 8.7, 8.5. HRMS (APCI) calculated for $C_{16}H_{19}NO_5$ (M^+): 305.1263; found: 305.1261.



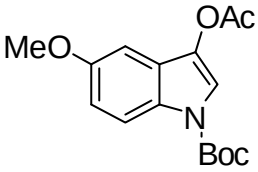
Diheptyl 1-acetylindoline-2,3-dicarboxylate (3s) 1a (80.2 mg, 0.5 mmol), **2** (322.2 mg, 1 mmol), $C_7H_{15}COOH$ (4 mL), 70 °C, 40 hours. After column chromatography (PE/EA=1:50) 110.4 mg (50%) of a light yellow liquid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.06 (s, 1H), 7.44 (t, *J* = 7.2 Hz, 2H), 7.16 (t, *J* = 7.5 Hz, 1H), 6.72 (s, 1H), 5.95 (s, 1H), 2.39-2.30 (m, 4H), 2.25 (s, 3H), 1.54 (br, 4H), 1.22 (br, 16H), 0.85-0.81 (m, 6H); ^{13}C NMR (75MHz, $CDCl_3$): δ 172.0, 168.8, 130.8, 126.8, 124.3, 116.1, 87.0, 75.2, 33.1, 31.0, 28.1, 24.2, 24.0, 21.9, 13.8. HRMS (APCI) calculated for $C_{26}H_{35}NO_5$ (M^+): 445.2828; found: 445.2829.



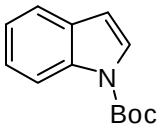
Diheptyl 1-acetylindoline-2,3-dicarboxylate (3t) 1a (80.2 mg, 0.5 mmol), **2** (323.1 mg, 1 mmol), PivOH (4 mL), 70 °C, 40 hours. After column chromatography (PE/EA=1:50) 63.4 mg (35%) of a light yellow liquid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.46-7.41 (m, 2H), 7.16 (t, *J* = 7.5 Hz, 1H), 6.65 (s, 1H), 5.90 (s, 1H), 2.24 (s, 3H), 1.14 (s, 18H); ^{13}C NMR (75MHz, $CDCl_3$): δ 176.5, 176.2, 169.0, 143.2, 130.8, 126.6, 126.4, 124.3, 116.1, 87.9, 75.8, 26.5, 26.4, 22.9. HRMS (APCI) calculated for $C_{20}H_{27}NO_5$ (M^+): 361.1889; found: 361.1892.



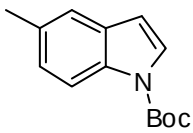
***tert*-butyl 3-acetoxy-2-methyl-1*H*-indole-1-carboxylate (4o): 1o** (115.6 mg, 0.5 mmol), **2a** (324.6 mg, 1.0 mmol), HOAc (4 mL), 70 °C, 1 hour. After column chromatography (PE/EA=1:50) 118.7 mg (82%) of a white solid was obtained. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.07 (d, *J* = 8.7 Hz, 1H), 7.20-7.15 (m, 3H), 2.37 (s, 3H), 2.32 (s, 3H). 1.59 (s, 9H); ^{13}C NMR (75MHz, $CDCl_3$): δ 169.3, 150.8, 134.0, 131.9, 126.9, 124.4, 123.5, 123.1, 116.8, 116.1, 84.3, 28.6, 20.9, 12.9. HRMS (APCI) calculated for $C_{16}H_{19}NO_4$ (M^+): 289.1314; found: 289.1310.



***tert*-butyl 3-acetoxy-5-methoxy-1*H*-indole-1-carboxylate (4g): 3g** (174.8 mg, 0.48 mmol), HOAc (4 mL), 70 °C, 13 hours. After column chromatography (PE/EA=1:70) 90.6 mg (62%) of a white solid was obtained with 27% of substrate recovery. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.04 (br, 1H), 7.65 (s, 1H), 6.97-6.92 (m, 2H), 3.86 (s, 3H), 2.37 (s, 3H), 1.65 (s, 9H); ^{13}C NMR (75MHz, $CDCl_3$): δ 168.3, 156.3, 149.9, 133.4, 127.9, 124.6, 116.6, 115.2, 114.7, 100.1, 84.0, 56.0, 28.5, 21.3. HRMS (APCI) calculated for $C_{16}H_{19}NO_5Na$ (M^+): 328.1161; found: 328.1159.

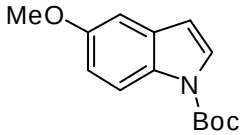


***tert*-butyl 1H-indole-1-carboxylate (1c)** ^{1}H NMR (300MHz, $CDCl_3$): δ 8.15 (d, *J* = 7.5 Hz, 1H), 7.60-7.54 (m, 2H), 7.31 (t, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 3 Hz, 1H), 1.67 (s, 9H).[4]

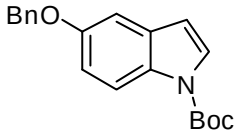


***tert*-butyl 5-methyl-1H-indole-1-carboxylate (1b)** ^{1}H NMR (300MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.1 Hz, 1H), 7.44 (s, 1H), 7.21 (s, 1H), 7.11 (d, *J* = 8.7

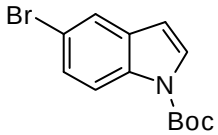
Hz, 1H), 6.37-6.36 (m, 1H), 2.32 (s, 3H), 1.55 (s, 9H).[2]



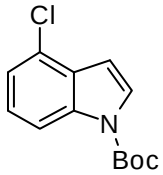
***tert*-butyl 5-methoxy-1H-indole-1-carboxylate (1g)** ^{1}H NMR (300MHz, $CDCl_3$): δ 7.94 (d, *J* = 7.2 Hz, 1H), 7.48 (s, 1H), 6.94 (s, 1H), 6.84 (d, *J* = 9.0 Hz, 1H), 6.41 (s, 1H), 3.76 (s, 3H), 1.58 (s, 9H) .[2]



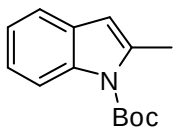
***tert*-butyl 5-(benzyloxy)-1*H*-indole-1-carboxylate (1e)** ^{1}H NMR (300MHz, $CDCl_3$): δ 7.94 (d, *J* = 7.8 Hz, 1H), 7.48-7.47 (m, 1H), 7.37 (d, *J* = 6.9 Hz, 2H), 7.32-7.23 (m, 3H), 7.01-7.00 (m, 1H), 6.92 (dd, *J1* = 9.0 Hz, *J2* = 2.7 Hz, 1H), 6.40 (d, *J* = 3.6 Hz, 1H), 5.02 (s, 2H), 1.58 (s, 9H).[5]



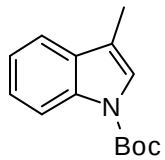
***tert*-butyl 5-bromo-1*H*-indole-1-carboxylate (1i)** ^{1}H NMR (300MHz, $CDCl_3$): δ 7.92 (d, *J* = 8.4 Hz, 1H), 7.56 (s, 1H), 7.48-7.47 (m, 1H), 7.28 (d, *J* = 8.7 Hz, 1H), 6.39-6.38 (m, 1H), 1.56 (s, 9H).[6]



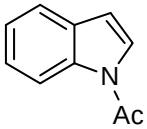
***tert*-butyl 4-chloro-1*H*-indole-1-carboxylate (1k)** ^{1}H NMR (300MHz, $CDCl_3$): δ 7.97 (t, *J* = 4.2 Hz, 1H), 7.53 (d, *J* = 3.3 Hz, 1H), 7.12 (d, *J* = 4.5 Hz, 2H), 6.59 (d, *J* = 3.6 Hz, 1H), 1.58 (s, 9H).[7]



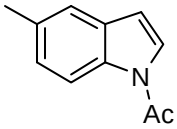
***tert*-butyl 3-methyl-1*H*-indole-1-carboxylate (1o)** ^{1}H NMR (300MHz, $CDCl_3$): 8.17 (d, *J* = 8.1 Hz, 1H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.32-7.25 (m, 2H), 6.38 (s, 1H), 2.66 (s, 3H), 1.75 (s, 9H).[4]



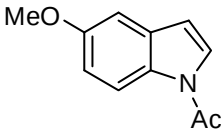
***tert*-butyl 2-methyl-1*H*-indole-1-carboxylate (1p)** ^{1}H NMR (300MHz, $CDCl_3$): δ 8.04 (d, *J* = 5.7 Hz, 1H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.27-7.14 (m, 3H), 2.19 (s, 3H), 1.58 (s, 9H).[8]



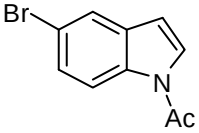
1-(1*H*-indol-1-yl)ethanone (1a) ^{1}H NMR (300MHz, $CDCl_3$): δ 8.54 (d, *J* = 8.1 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.52-7.36 (m, 3H), 6.74 (s, 1H), 2.74 (s, 3H).[9]



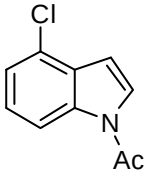
1-(5-methyl-1*H*-indol-1-yl)ethanone (1d) ^{1}H NMR (300MHz, $CDCl_3$): δ 8.20 (d, *J* = 8.1 Hz, 1H), 7.24 (s, 2H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.45-6.44 (m, 1H), 2.48 (s, 3H), 2.38 (s, 3H).[2]



1-(5-methoxy-1*H*-indol-1-yl)ethanone (1h) ^{1}H NMR (300MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.27-7.26 (m, 1H), 6.93-6.92 (m, 1H), 6.87-6.83(m, 1H), 6.46-6.45(m, 1H), 3.75 (s, 3H), 2.49 (s, 3H).[10]

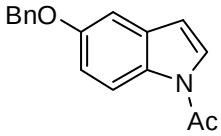


1-(5-bromo-1*H*-indol-1-yl)ethanone (1j) ^{1}H NMR (300MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.59 (s, 1H), 7.34-7.31 (m, 2H), 6.48-6.47(m, 1H), 2.53 (s, 3H).[2]

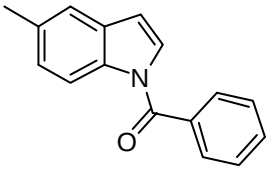


1-(4-chloro-1*H*-indol-1-yl)ethanone (1l) ^{1}H NMR (300MHz, $CDCl_3$): δ 8.26 (t, *J* = 4.5 Hz, 1H), 7.36 (d *J* = 3.9 Hz, 1H), 7.19 (d, *J* = 4.2 Hz, 2H), 6.68 (d, *J* = 4.2

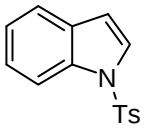
Hz, 1H), 2.56 (s, 3H).[11]



1-(5-(benzyloxy)-1*H*-indol-1-yl)ethanone (1f) ^{1}H NMR (300MHz, $CDCl_3$): δ 8.24 (d, *J* = 8.1 Hz, 1H), 7.37-7.25 (m, 6H), 6.99-6.93 (m, 2H), 6.44 (s, 1H), 5.00 (s, 2H), 2.48 (s, 3H).[12]



(5-methyl-1*H*-indol-1-yl)(phenyl)methanone (1m) ^{1}H NMR (300MHz, $CDCl_3$): δ 8.19 (d, *J* = 8.4 Hz, 1H), 7.31 (d, *J* = 6.9 Hz, 2H), 7.50-7.37 (m, 3H), 7.28 (s, 1H), 7.14-7.08 (m, 2H), 6.42 (d, *J* = 3.6 Hz, 1H), 2.36 (s, 3H).[2]



1-tosyl-1*H*-indole (1n) ^{1}H NMR (300MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 2H), 7.56-7.51 (m, 2H), 7.30-7.20 (m, 5H), 6.65 (s, 1H), 2.33 (s, 3H).[9]

References

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X-Ray Crystallographic data

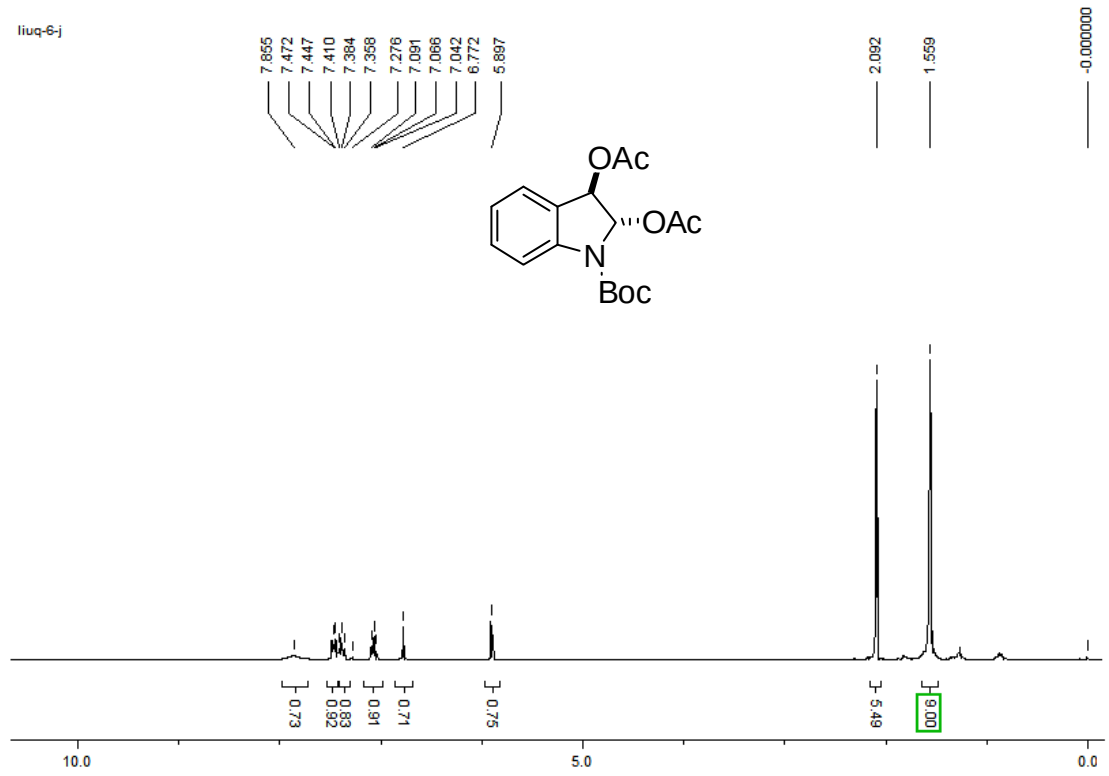
Single crystals of product **3a** suitable for X-ray crystallographic analysis were obtained via slow evaporation of CH_2Cl_2–CH_3OH solution. Crystal data of **3a** (C14 H15 N1 O5): Mw = 277.27, Space group P21/c, Z=4, Bond precision: C-C = 0.0035 A, Wavelength=0.71073; Cell: a=8.8633(10) b=18.912(2) c=8.4229(9); alpha=90, beta=94.108(2), gamma=90, V=1408.2, R(reflections)= 0.0595(2132) wR2(reflections)= 0.1555(2529).

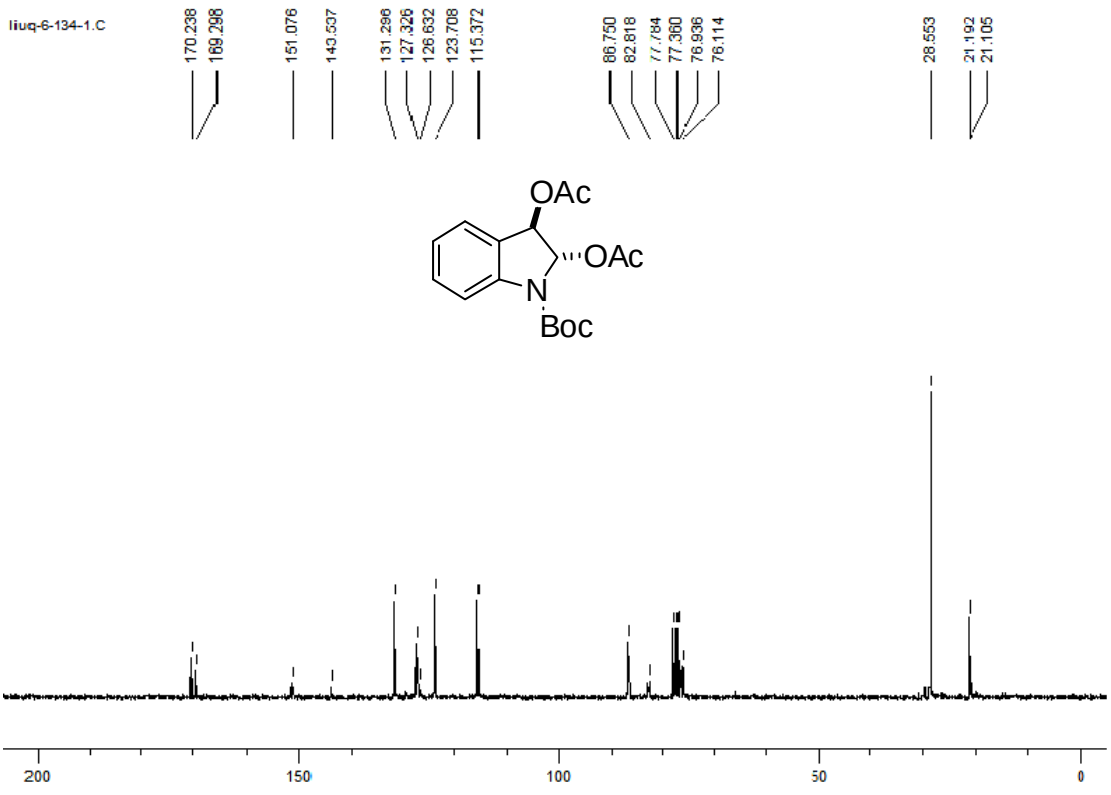
Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Centre with deposition No. CCDC 822882. Copy of the data can be obtained, free of charge, on application to the CCDC, 12 Union Road, Cambridge CB2 1EZ UK (Email: deposit@ccdc.cam.ac.uk).

Single crystals of product **3b** suitable for X-ray crystallographic analysis were obtained via slow evaporation of CH_2Cl_2–CH_3OH solution. Crystal data of **3b** (C18 H23 N1 O6): Mw = 349.37, Space group P-1, Z=4, Bond precision: C-C = 0.0052 A, Wavelength= 0.71073; Cell: a=9.1850(7) b=13.9246(11) c=16.2335(13); alpha=75.704(2) beta=87.418(2) gamma=72.161(2), V=1914.1, R(reflections)= 0.0638(3393) wR2(reflections)= 0.1515(7448).

Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Centre with deposition No. CCDC 822881. Copy of the data can be obtained, free of charge, on application to the CCDC, 12 Union Road, Cambridge CB2 1EZ UK (Email: deposit@ccdc.cam.ac.uk).

NMR Spectra of Products and Reactants





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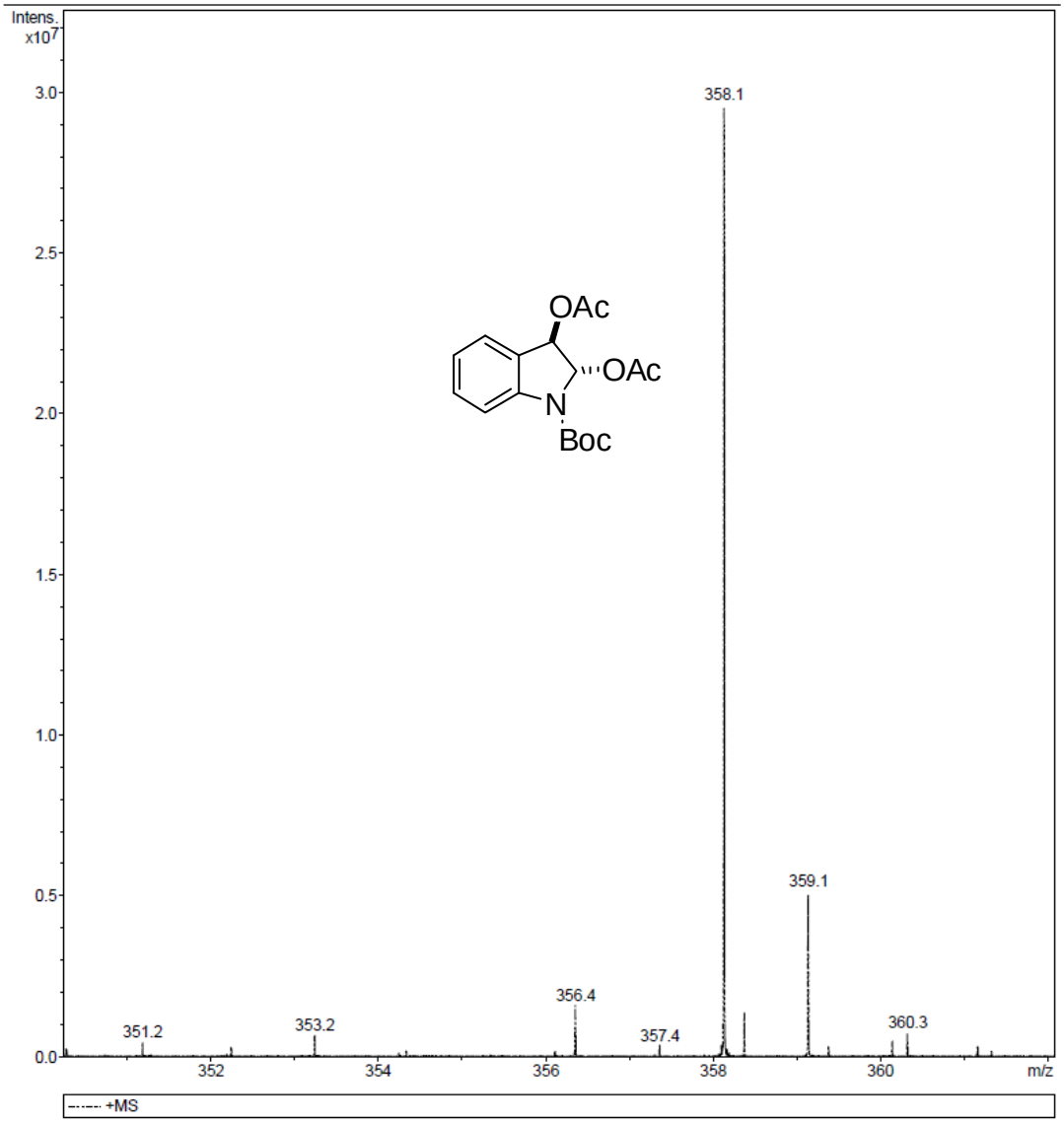

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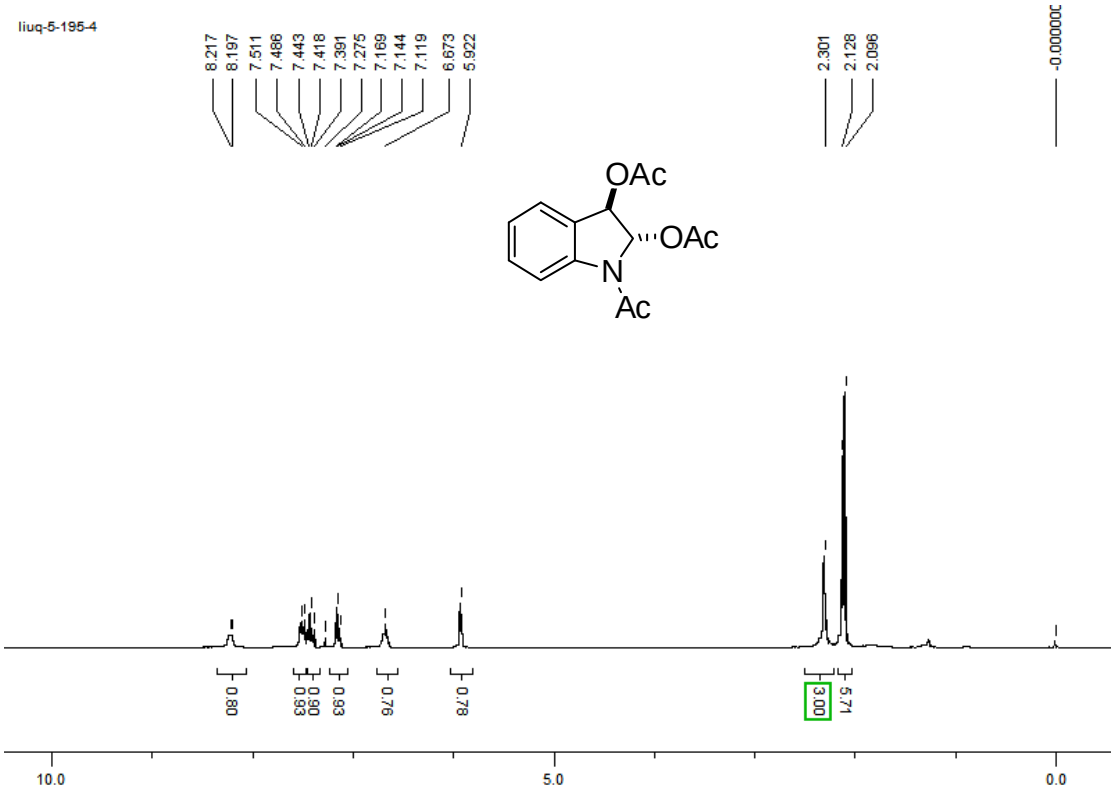
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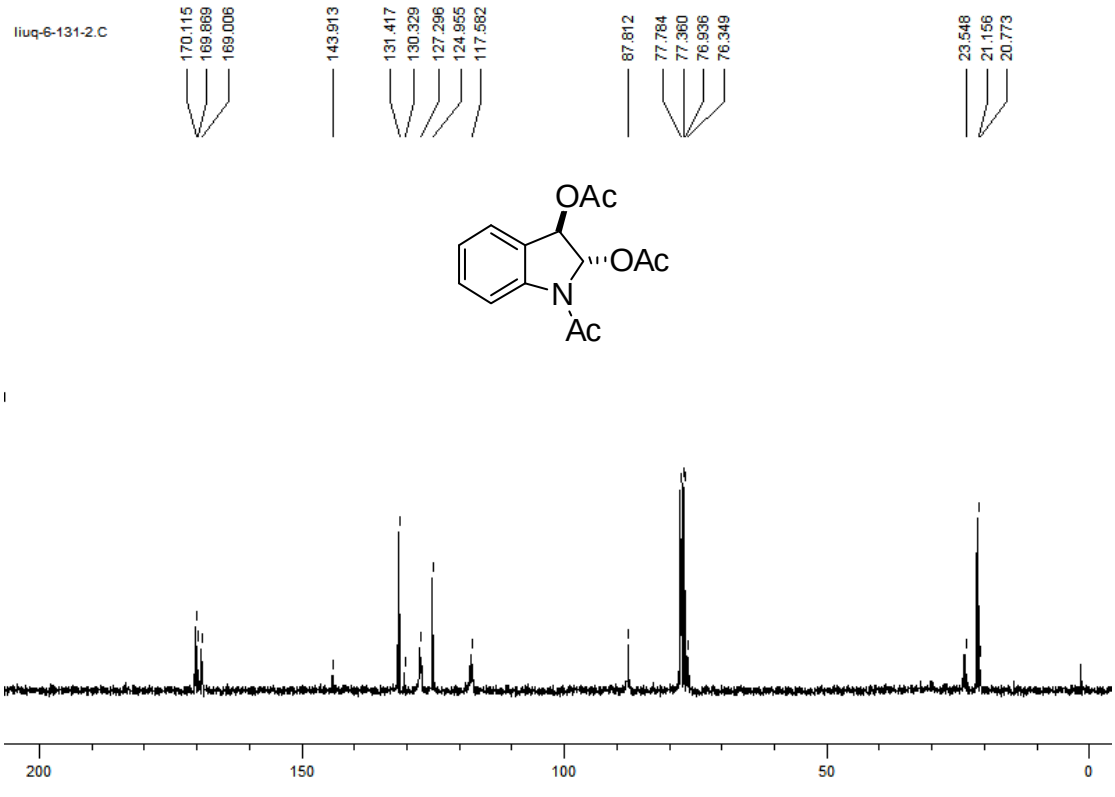
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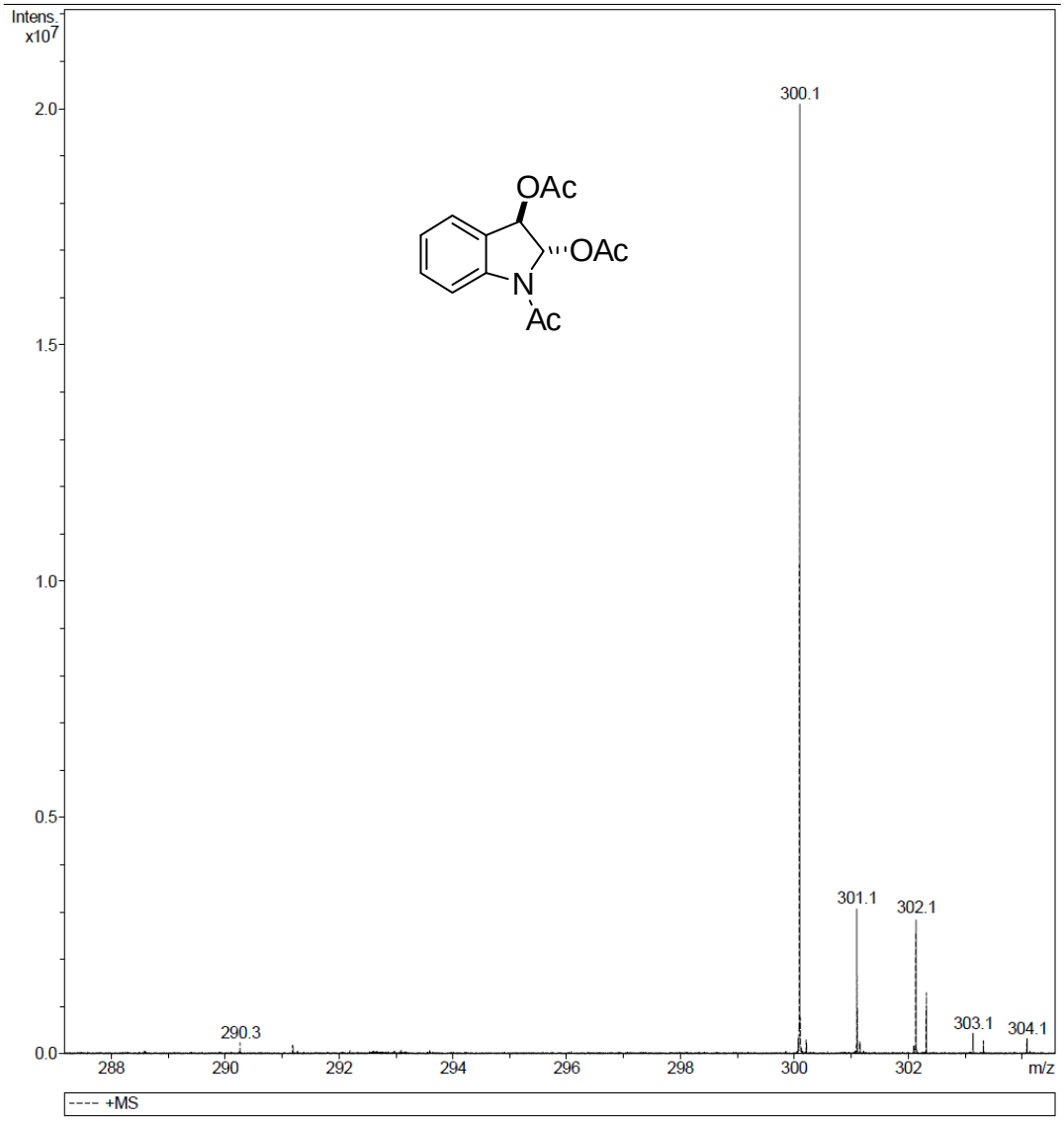

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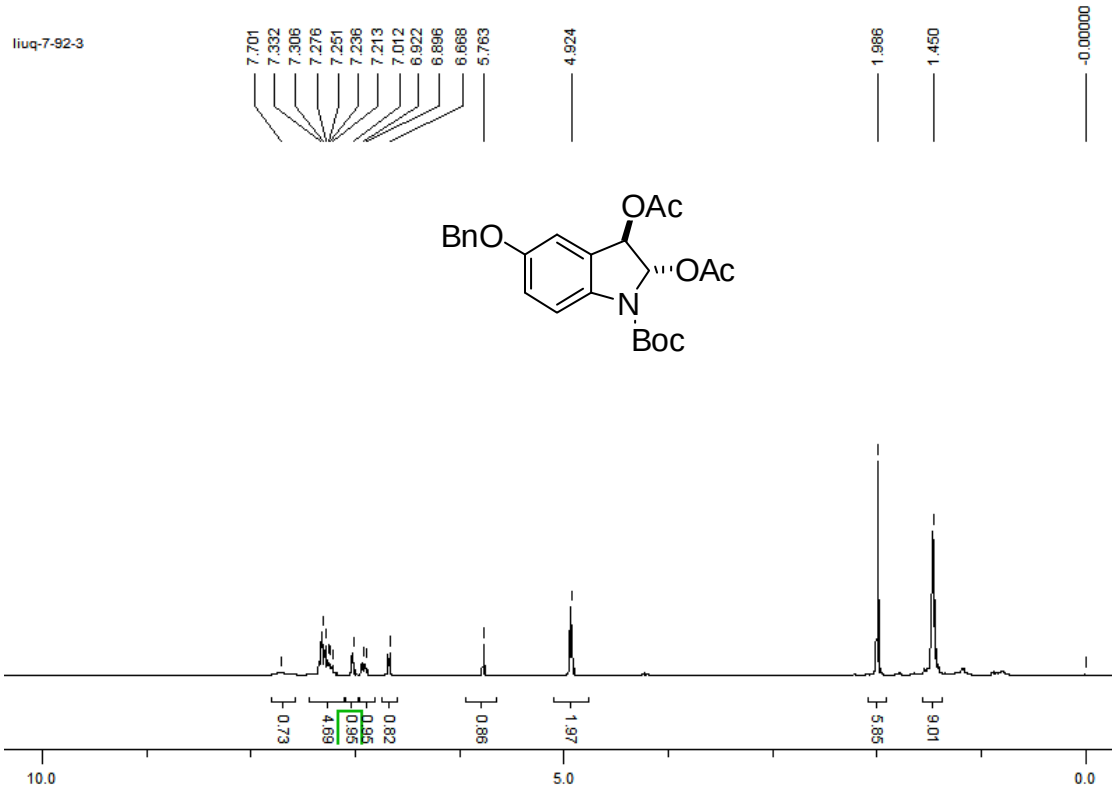
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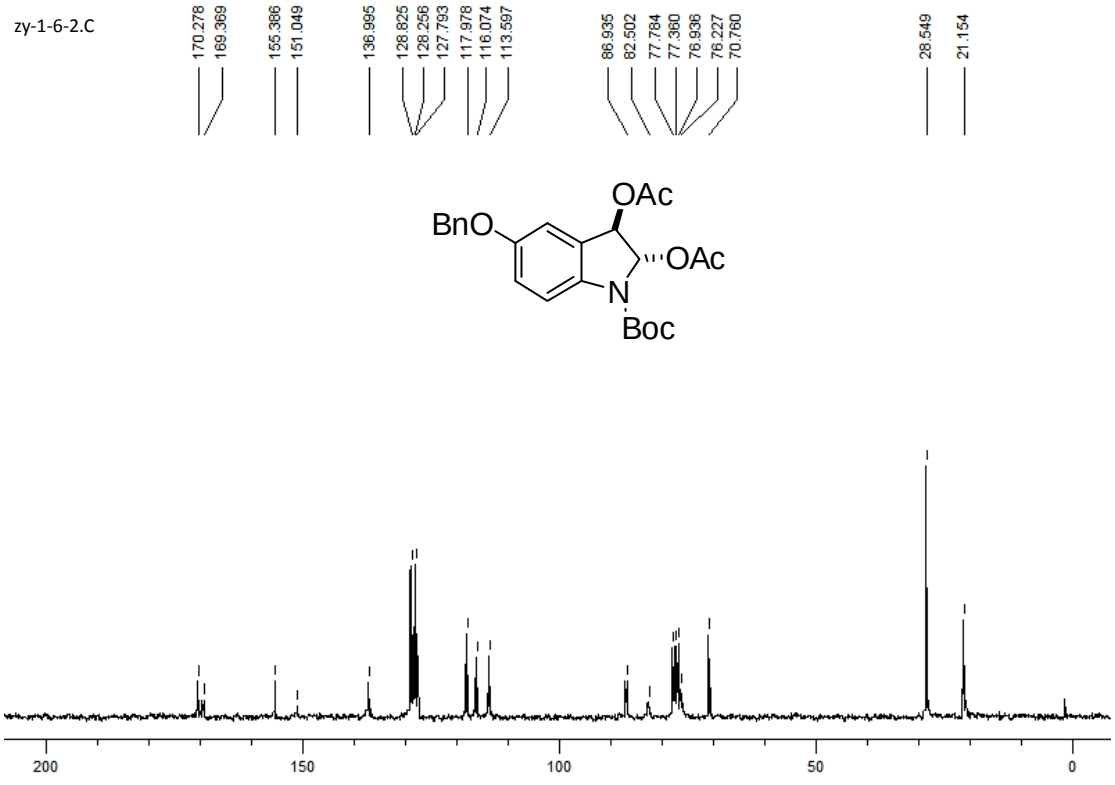
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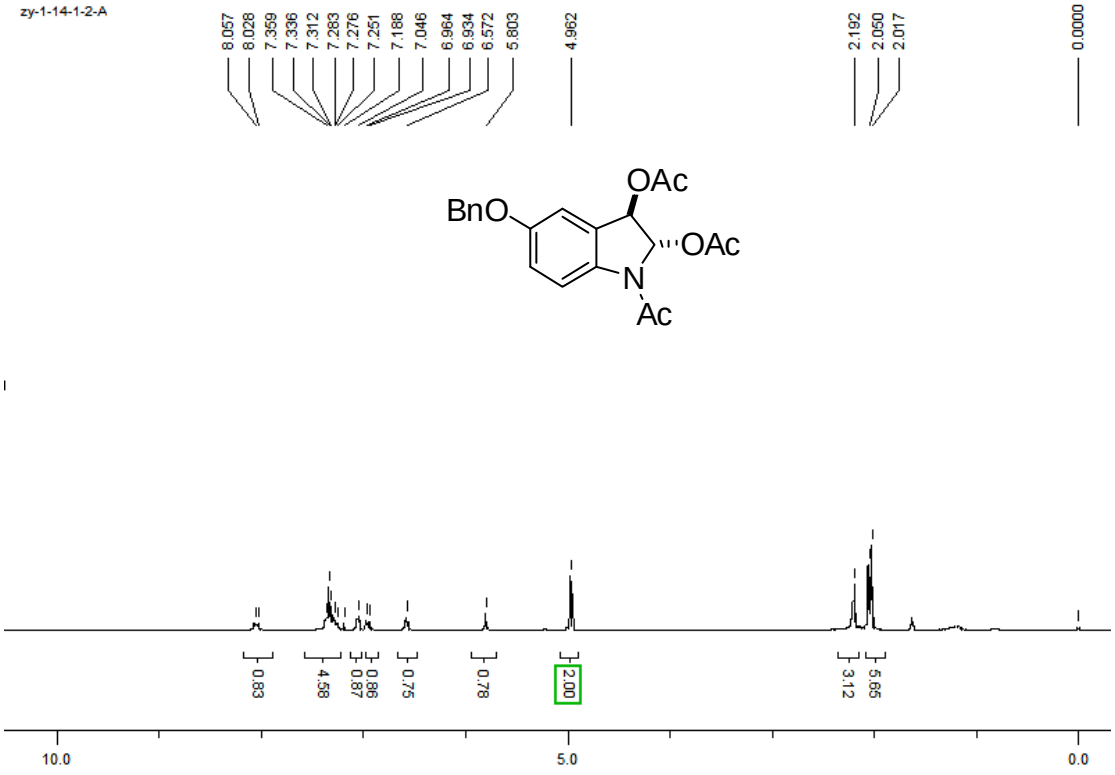
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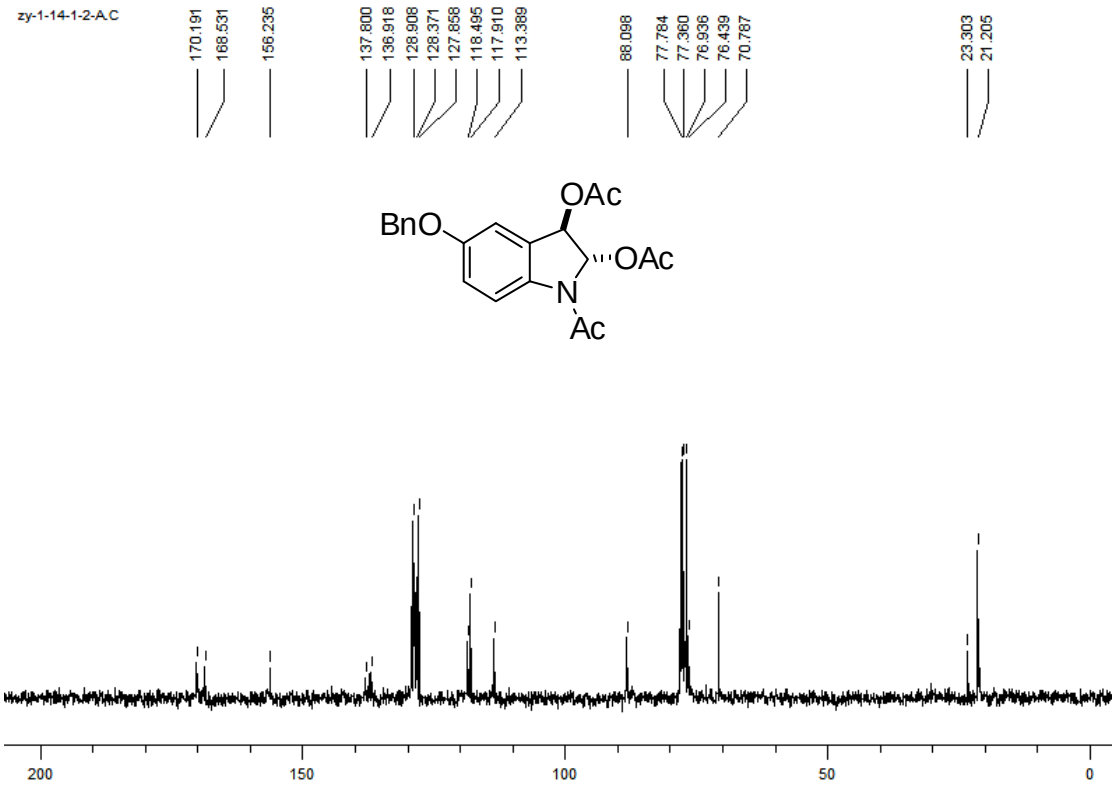
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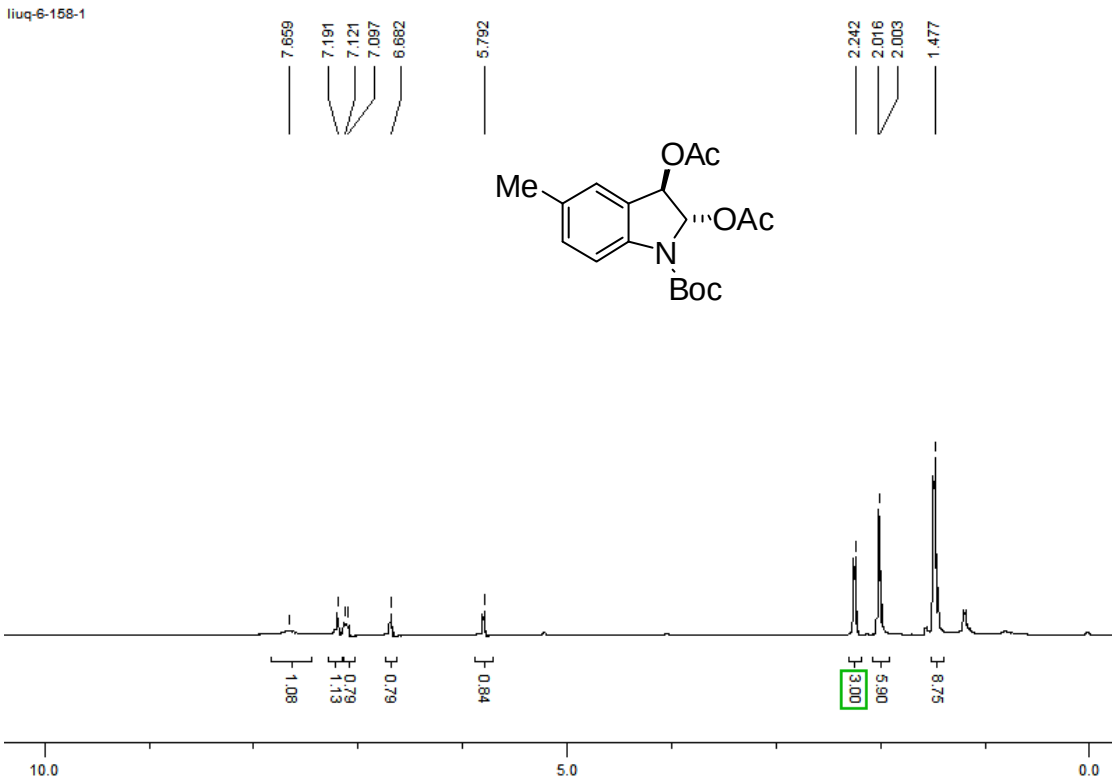
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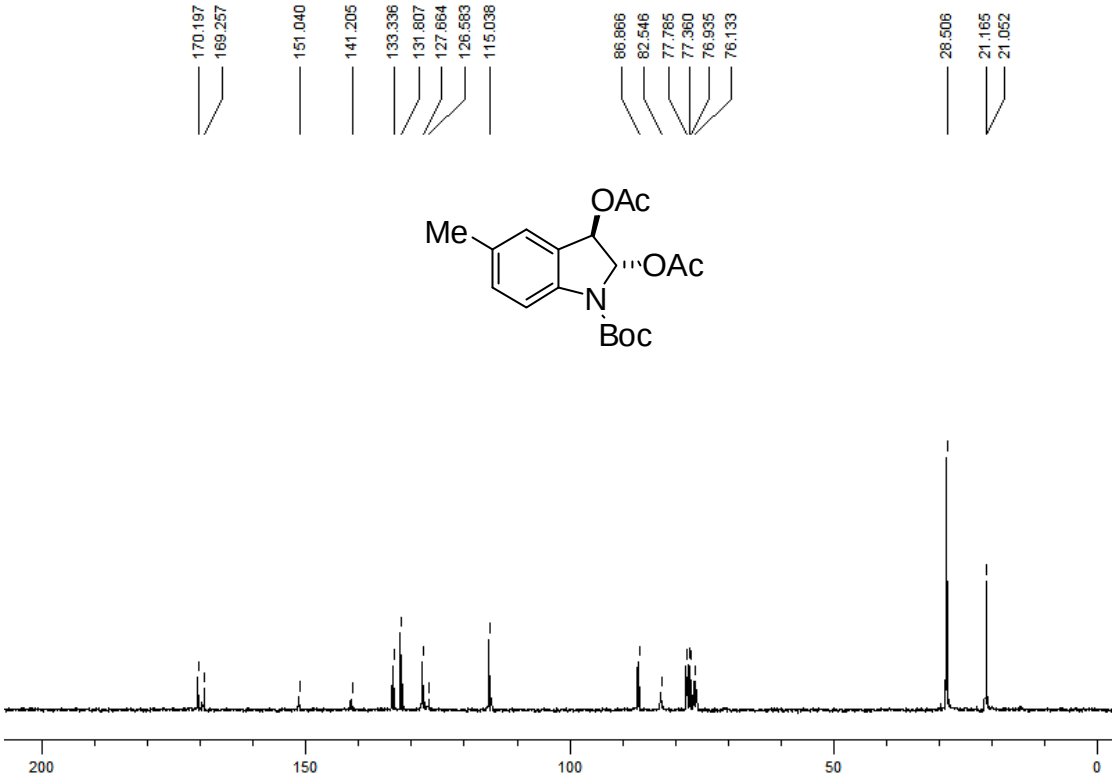
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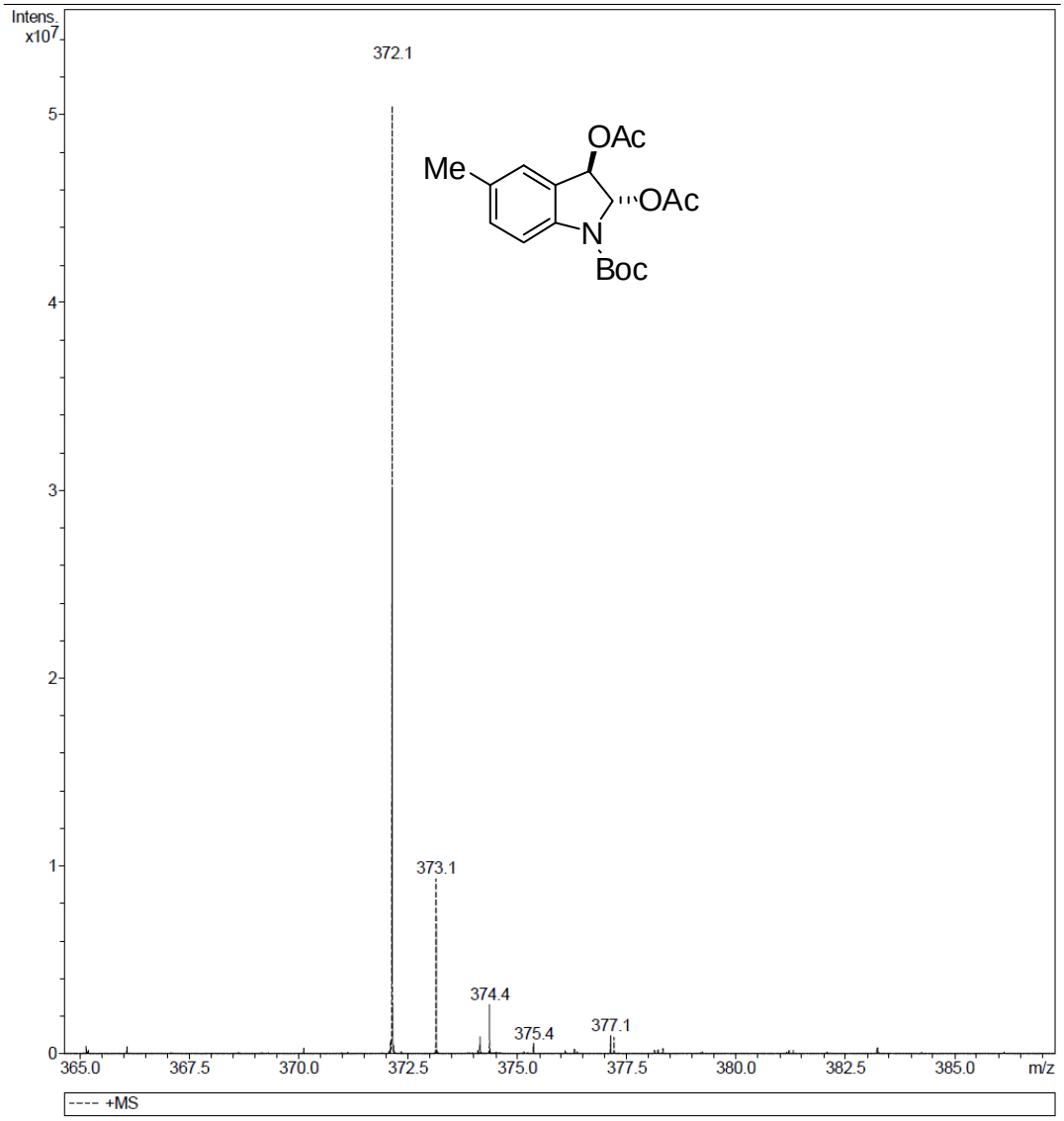

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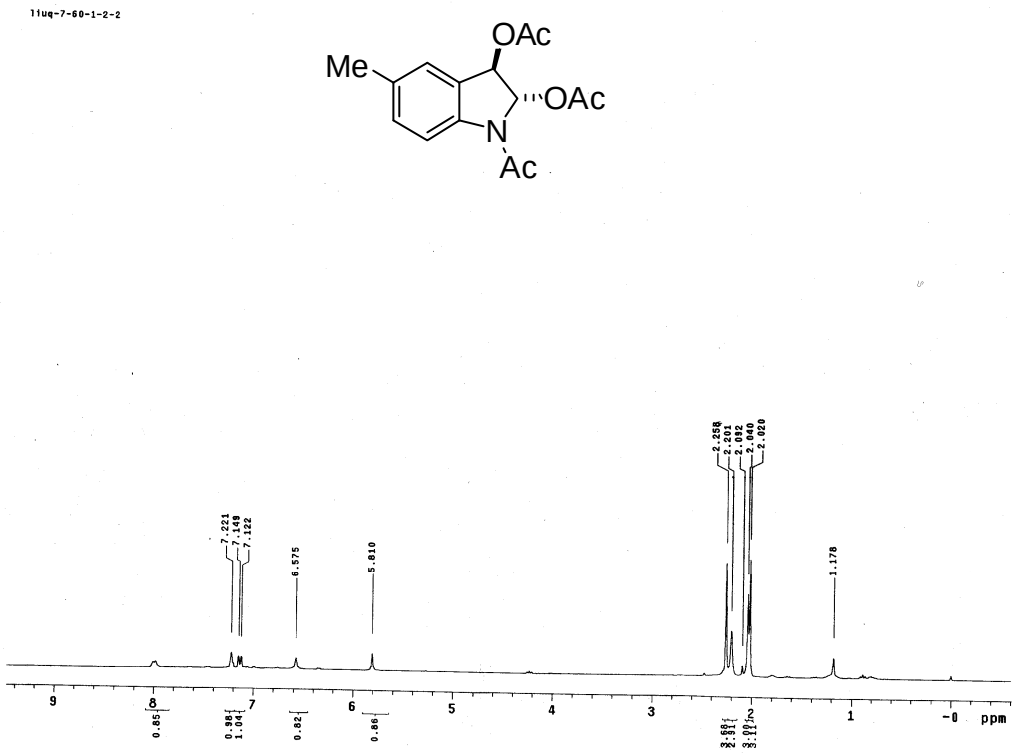
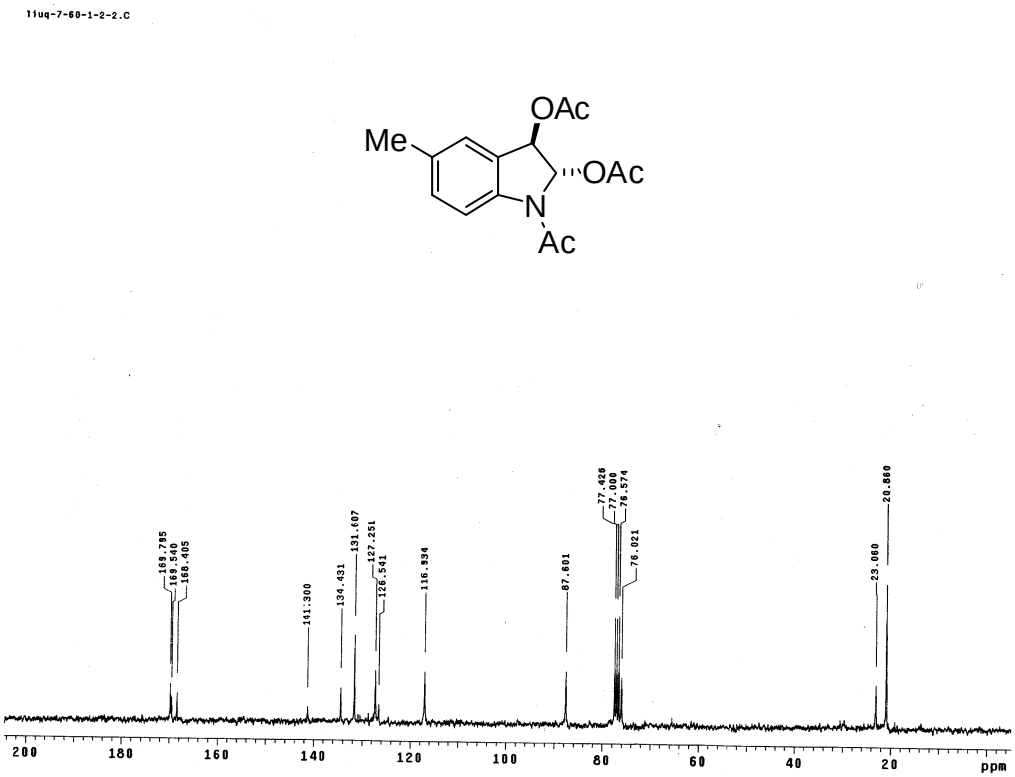
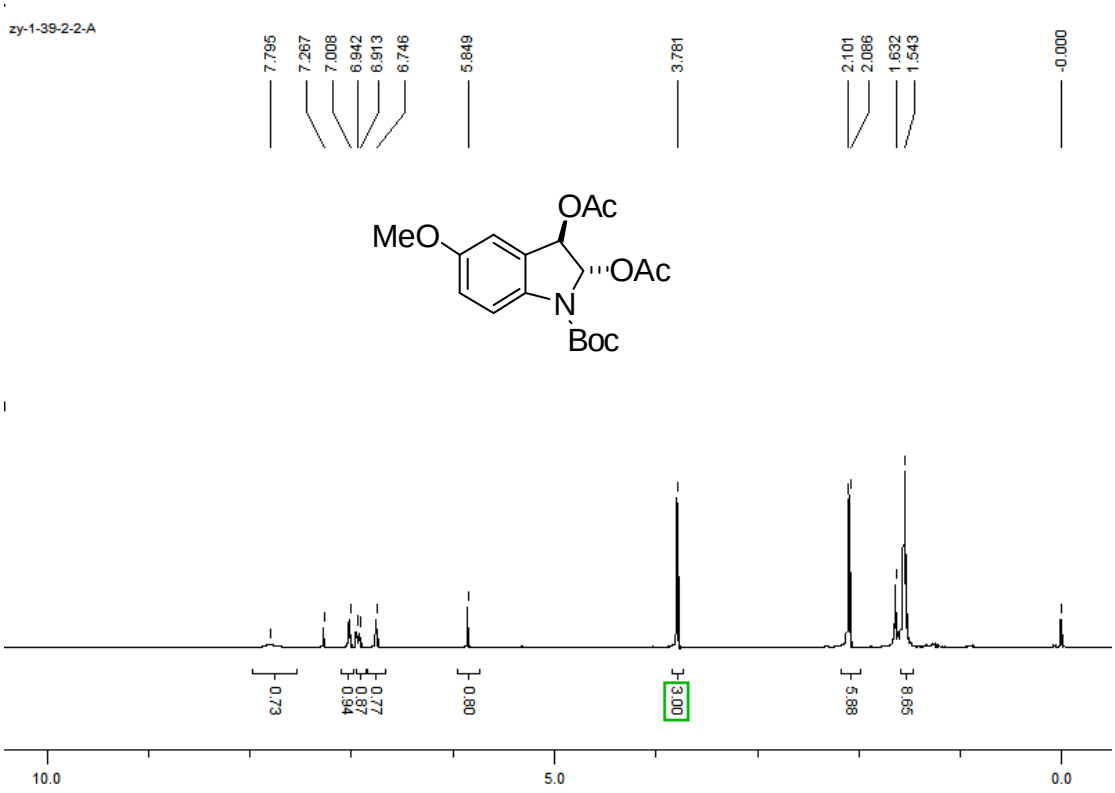
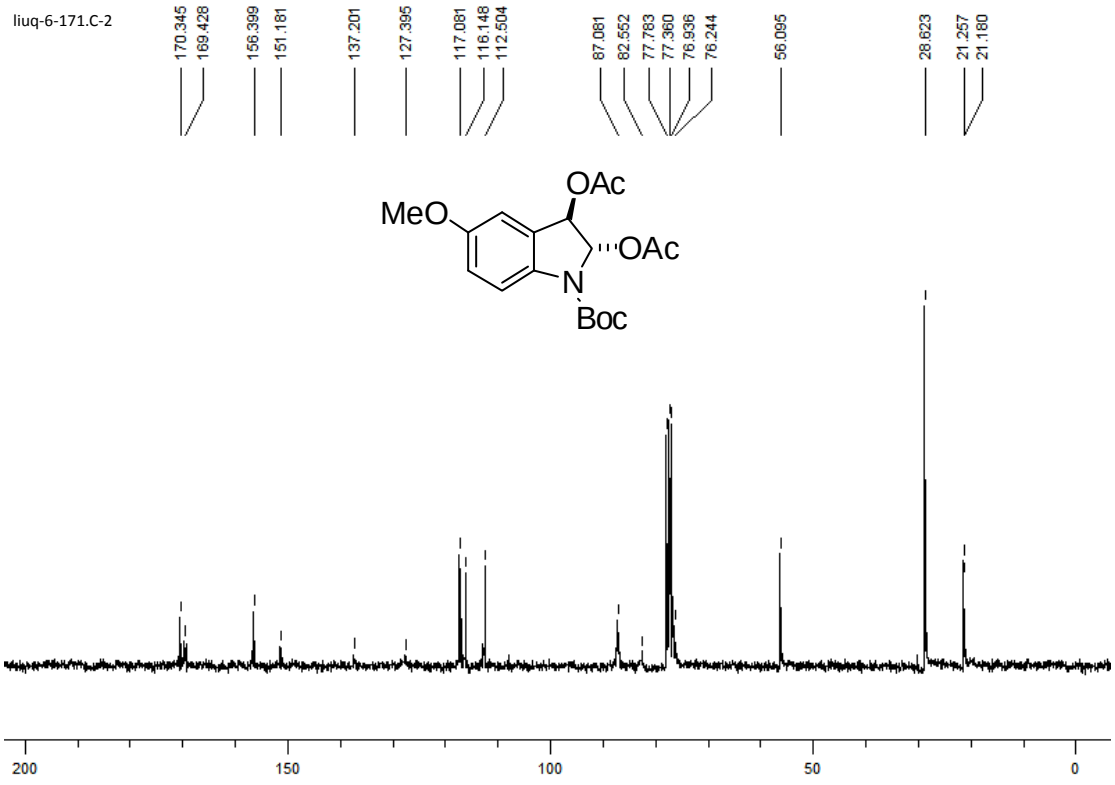

liuq-7-60-1-2-2
OAc
Me
OAc
N
Ac
7.221
7.148
7.122
6.575
5.810
2.258
2.201
2.087
2.040
2.020
1.178
ppm


liuq-7-60-1-2-2.c
OAc
Me
OAc
N
Ac
169.795
169.540
168.405
141.300
134.431
131.607
127.251
126.541
116.934
87.601
77.458
77.000
76.574
76.021
23.060
20.860
ppm


zy-1-39-2-2-A
7.795
7.267
7.008
6.942
6.913
6.746
5.849
3.781
2.101
2.086
1.632
1.543
-0.000
OAc
MeO
OAc
N
Boc
0.73
0.94
0.87
0.77
0.80
3.00
5.88
8.66
10.0
5.0
0.0

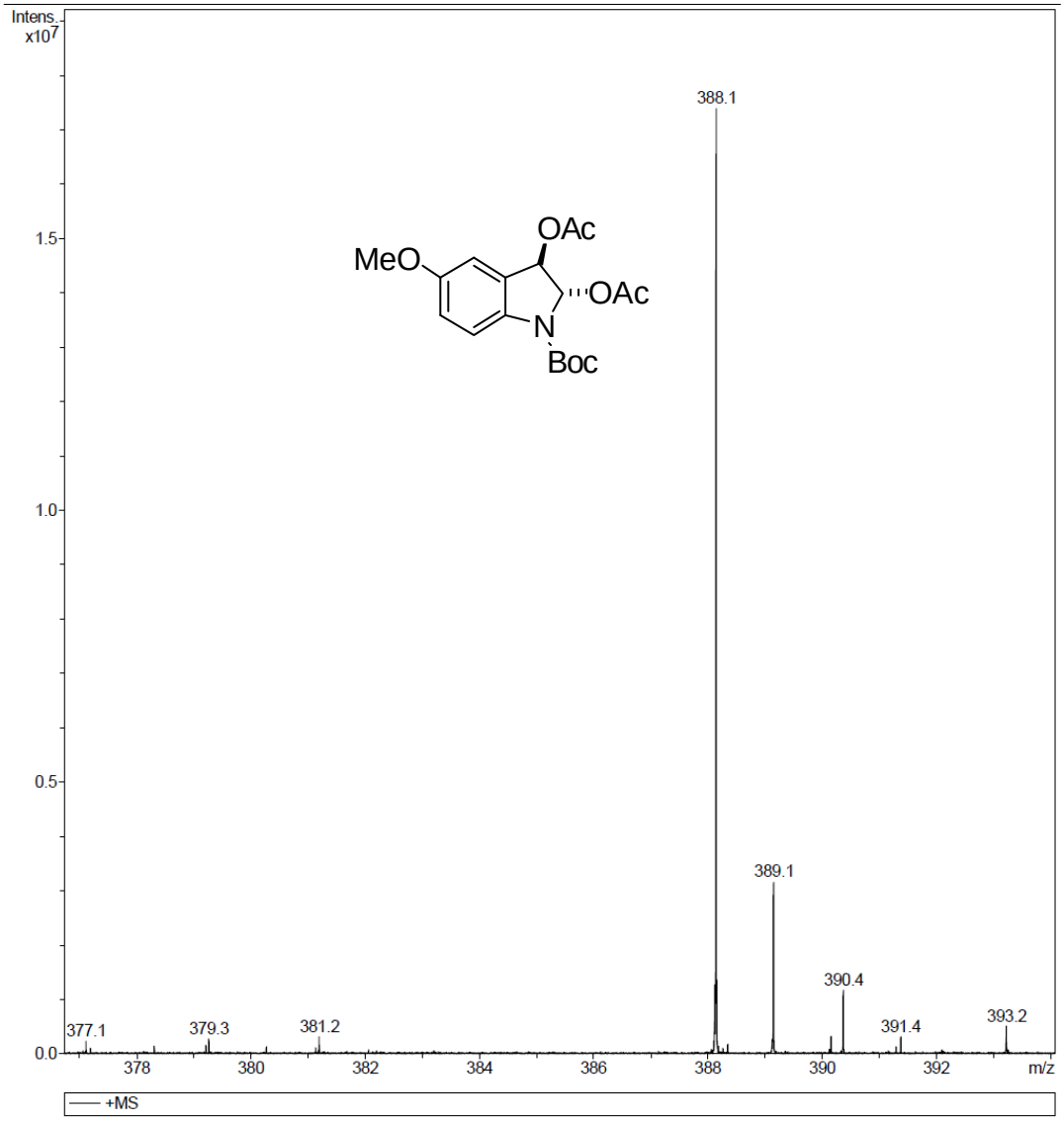

liuq-6-171.C-2
170.345
169.428
156.399
151.181
137.201
127.395
117.081
116.148
112.504
87.081
82.552
77.783
77.360
76.936
76.244
56.095
28.623
21.257
21.180
OAc
MeO
OAc
N
Boc
200
150
100
50
0

Display Report

Analysis Info

Analysis Name	D:\Data\zfj\2010915_000020.d	Acquisition Date	9/15/2010 4:05:09 PM
Method	XMASS_Method	Operator	FTMS_USER
Sample Name	184-9	Instrument	apex-III
Comment			

Acquisition Parameter



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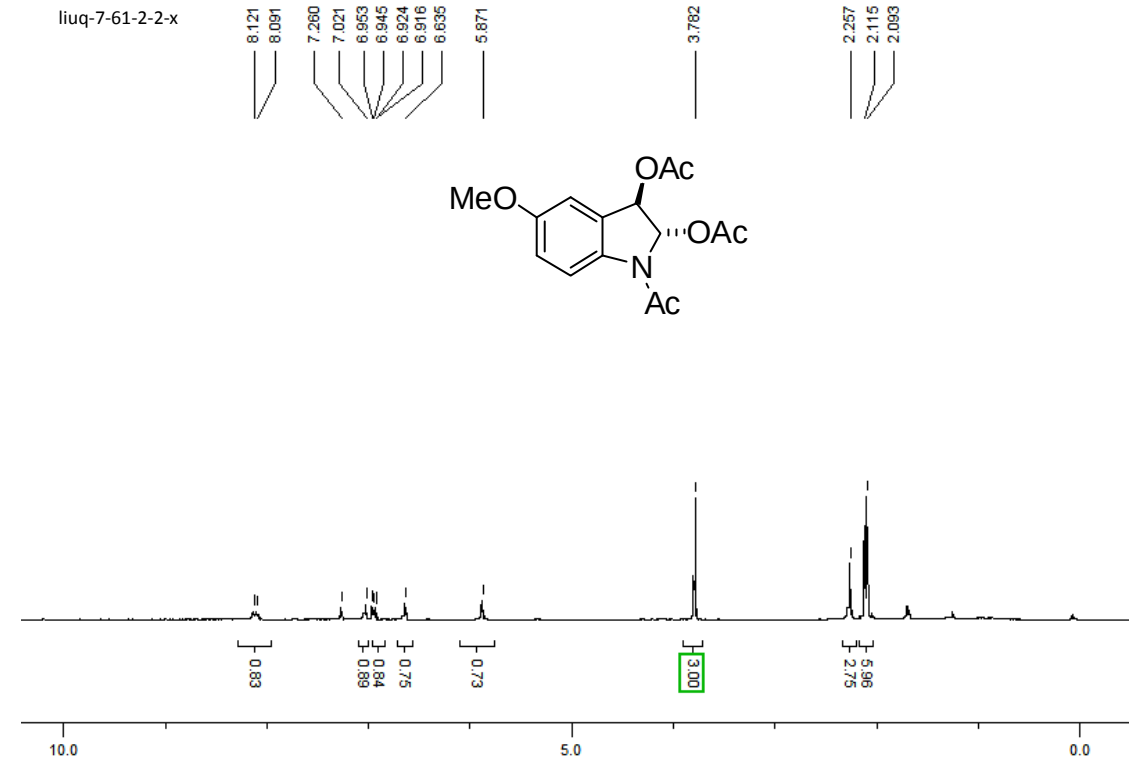
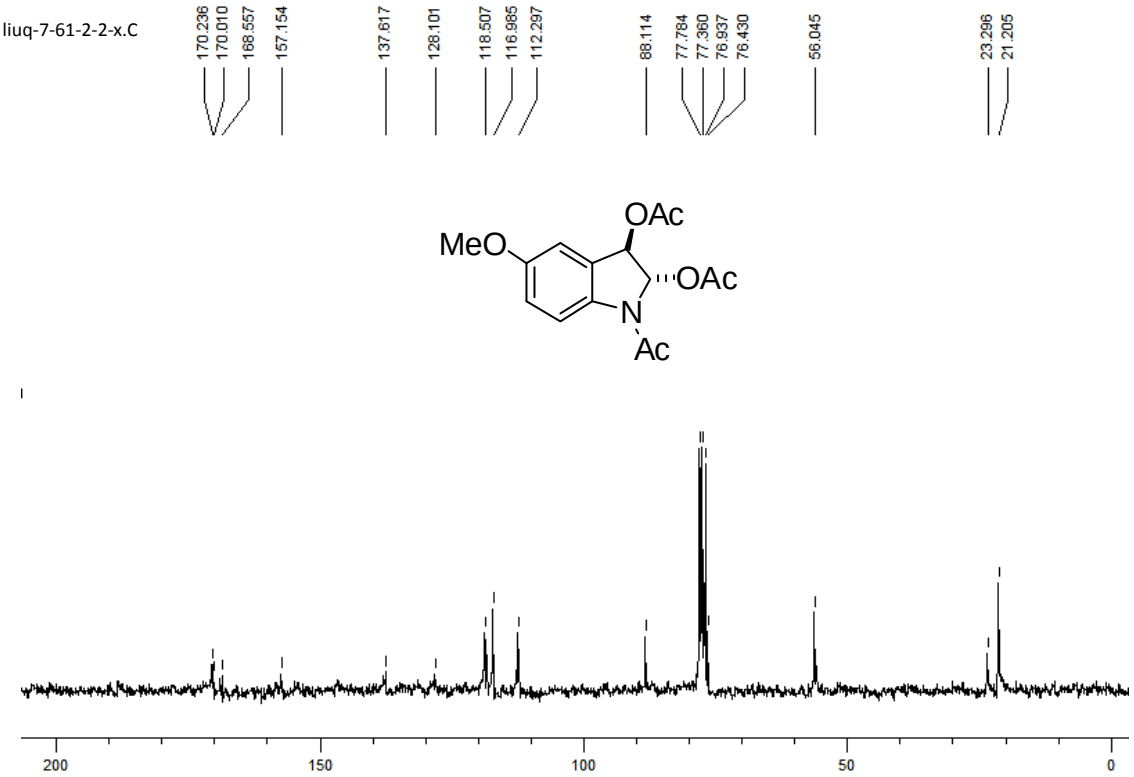

liuq-7-61-2-2-x
8.121
8.091
7.260
7.021
6.953
6.945
6.924
6.916
6.635
5.871
3.782
2.257
2.115
2.093
MeO
OAc
OAc
N
Ac
0.83
0.89
0.84
0.75
0.73
3.00
2.75
5.96
10.0
5.0
0.0

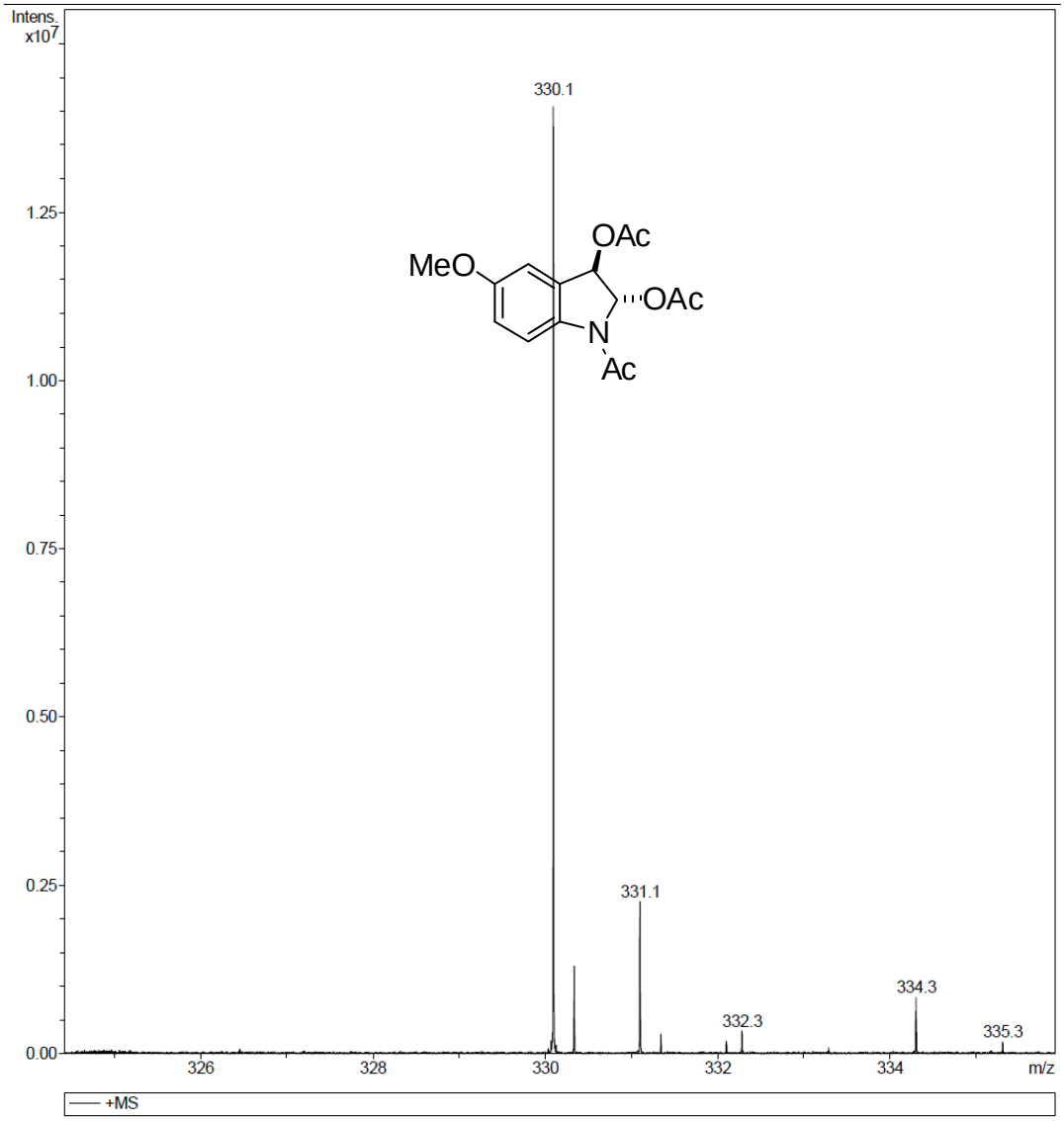

liuq-7-61-2-2-x.C
170.236
170.010
168.557
157.154
137.617
128.101
118.507
116.985
112.297
88.114
77.784
77.360
76.937
76.430
56.045
23.296
21.205
MeO
OAc
OAc
N
Ac
200
150
100
50
0

Display Report

Analysis Info

Analysis Name	D:\Data\zfj\2010915_000003.d	Acquisition Date	9/15/2010 9:46:28 AM
Method	XMASS_Method	Operator	FTMS_USER
Sample Name	184-1	Instrument	apex-III
Comment			

Acquisition Parameter



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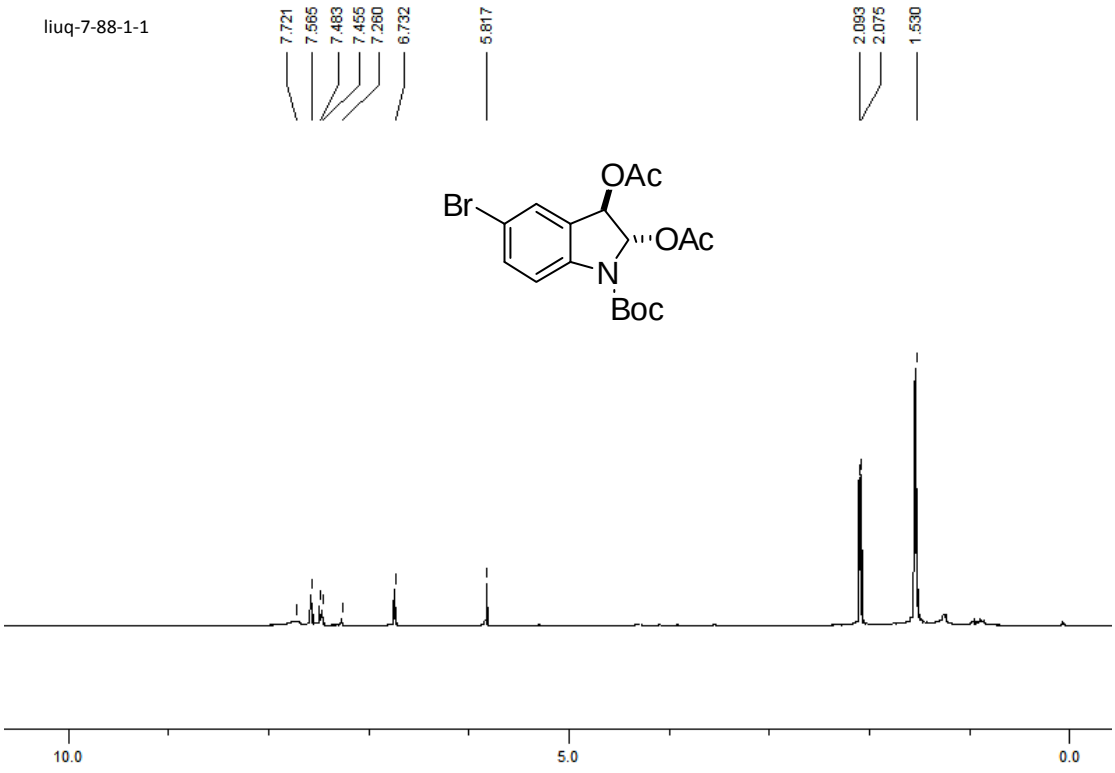
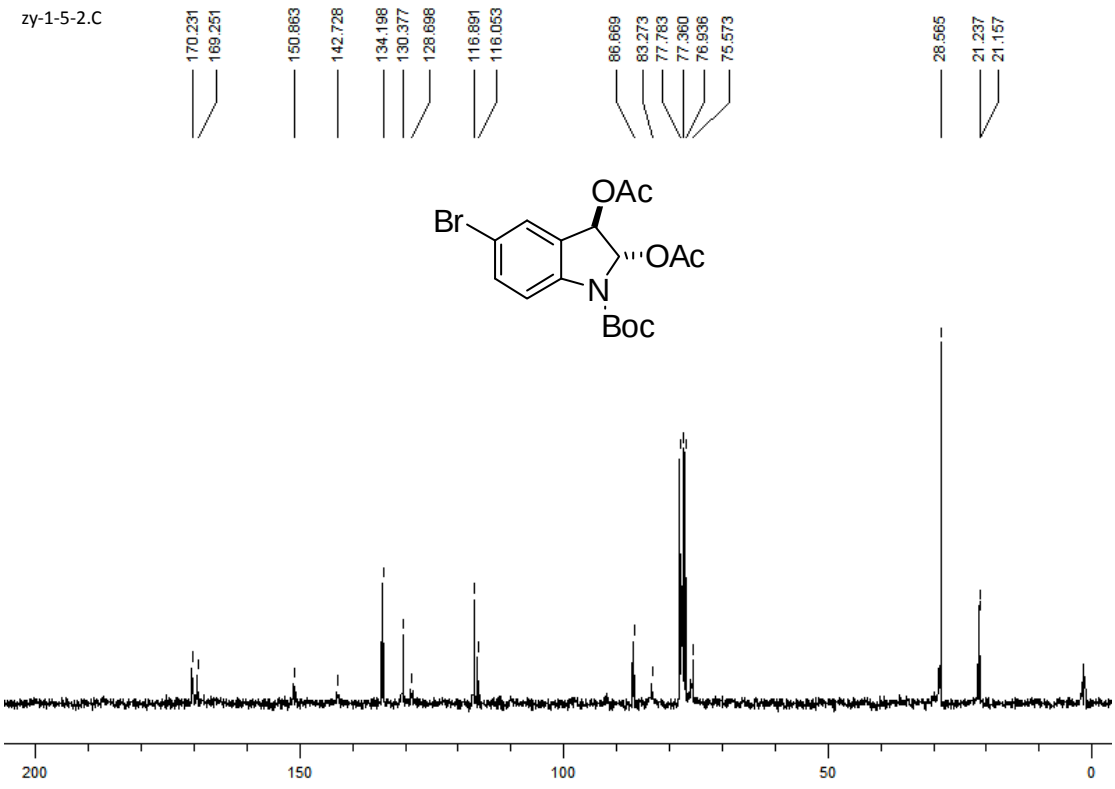
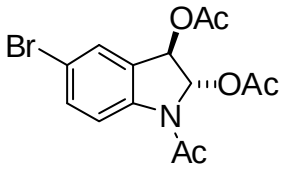
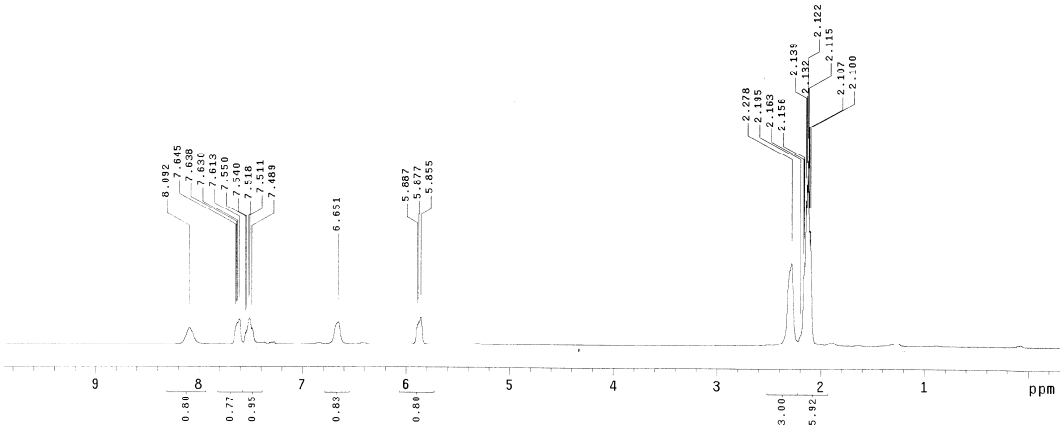

liuq-7-88-1-1
7.721
7.565
7.483
7.455
7.260
6.732
5.817
2.093
2.075
1.530
OAc
Br
OAc
N
Boc
10.0
5.0
0.0


zy-1-5-2.C
170.231
169.251
150.863
142.728
134.198
130.377
128.698
116.891
116.053
86.669
83.273
77.783
77.360
76.936
75.573
28.565
21.237
21.157
OAc
Br
OAc
N
Boc
200
150
100
50
0

zy-1-25-2-2-B

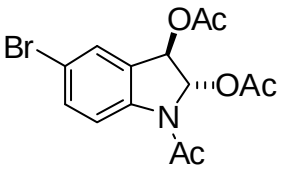


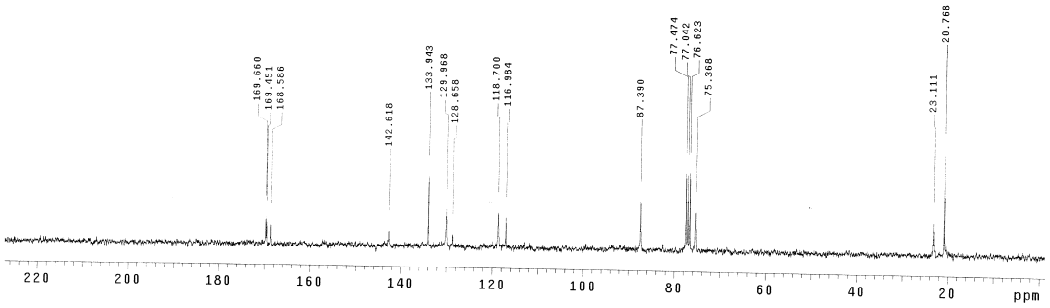


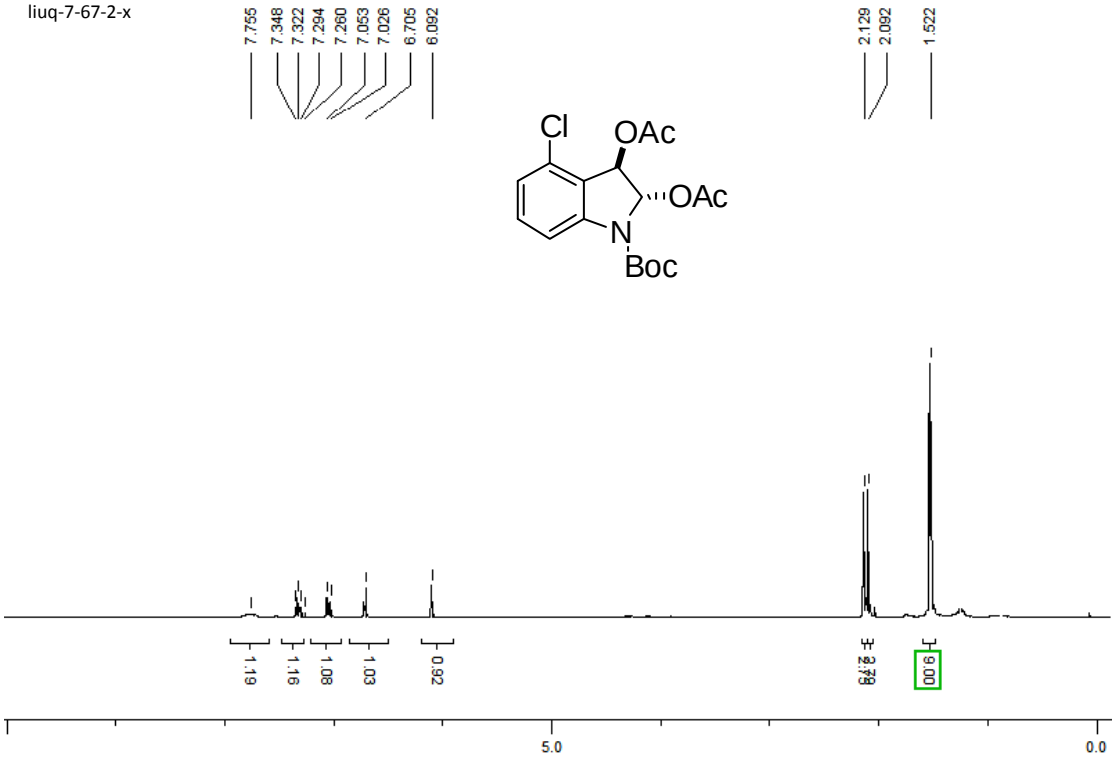
zy-1-25-2-2-B.C

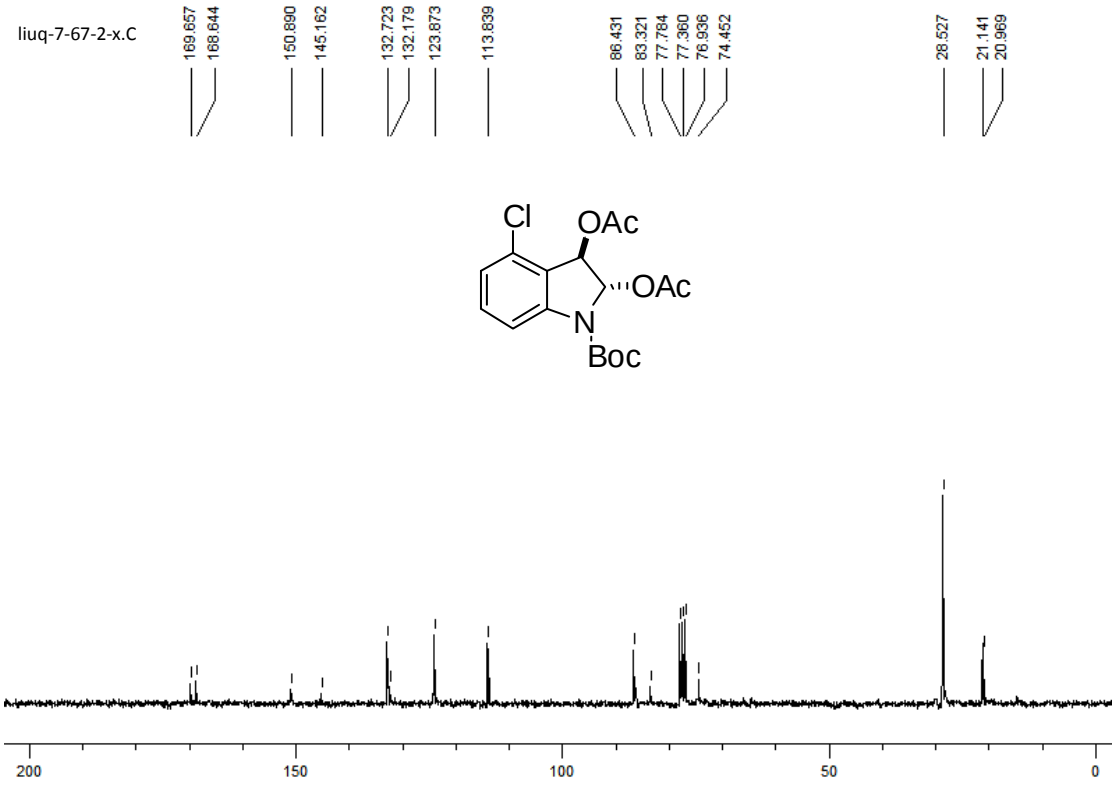
Solvent: DMSO
Ambient temperature
Mercury-300BB "mercury300"

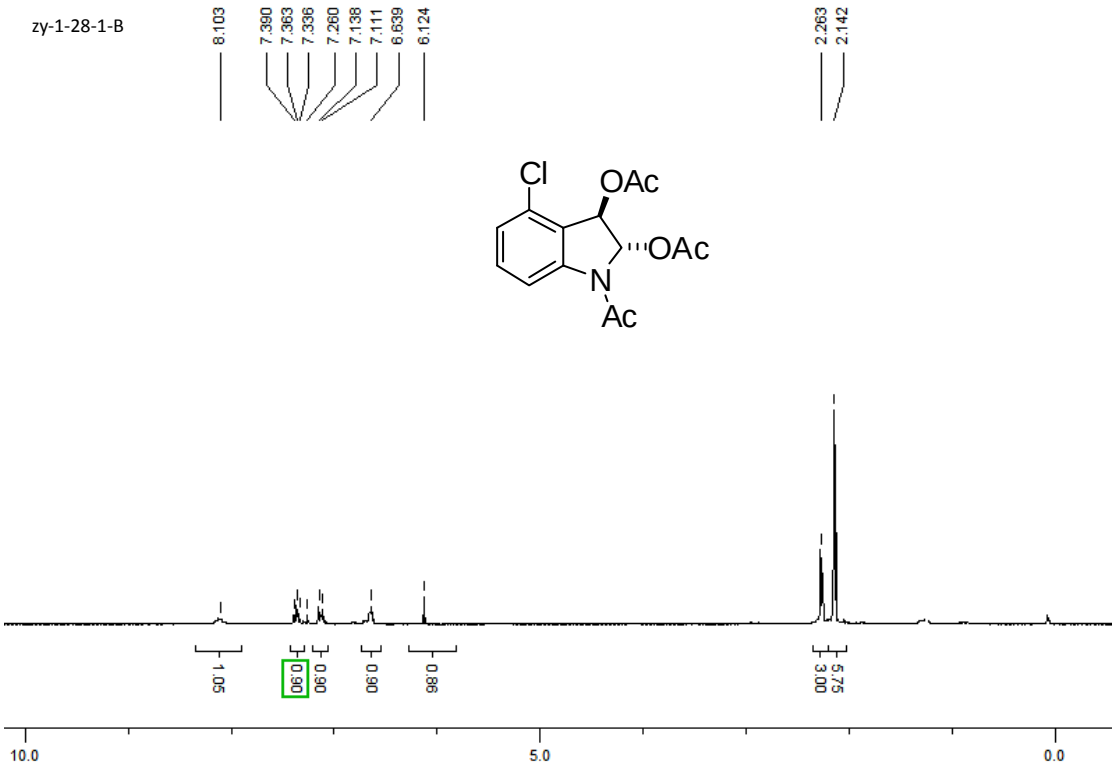
Relax. delay 1.000 sec
Pulse 28.0 degrees
Acq. time 0.501 sec
Width 17241.4 Hz
10240 repetitions
OBSERVE C13, 75.4552408 MHz
DECOUPLE H1, 300.0836216 MHz
Power 40 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 4.0 Hz
FT size 32768
Total time 4 hr, 48 min, 17 sec

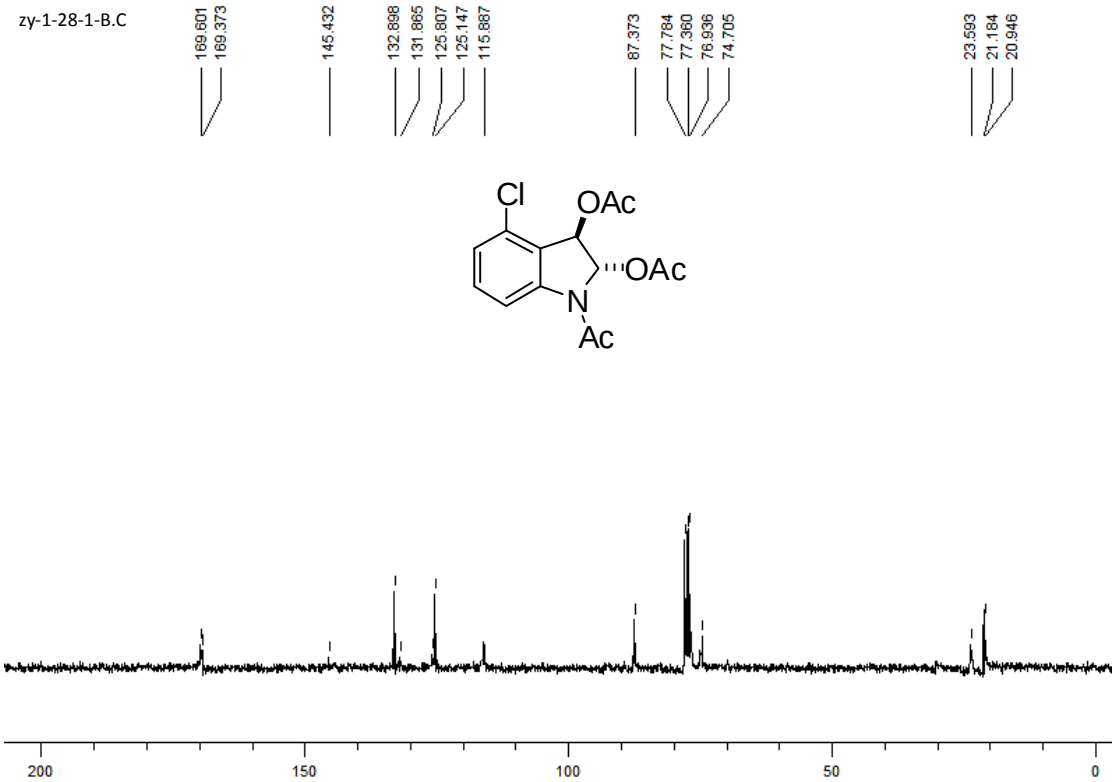




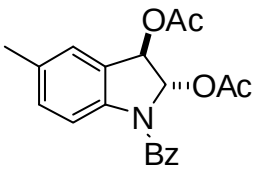

liuq-7-67-2-x
7.755
7.348
7.322
7.294
7.260
7.053
7.026
6.705
6.092
2.129
2.092
1.522
Cl
OAc
OAc
N
Boc
1.19
1.16
1.08
1.03
0.92
2.79
9.00
5.0
0.0

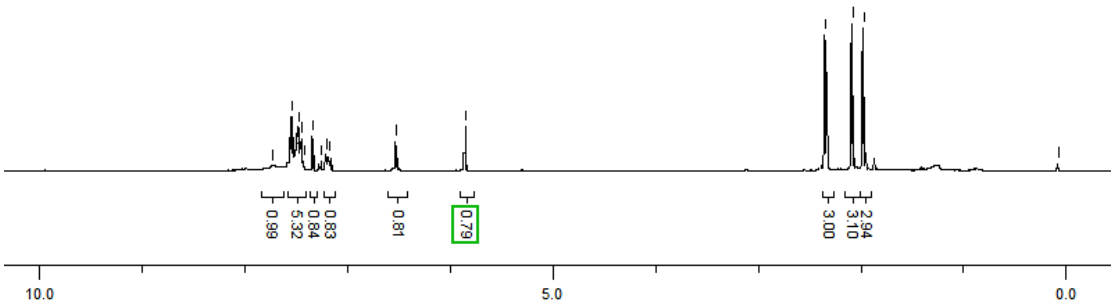

liuq-7-67-2-x.C
169.657
168.644
150.890
145.162
132.723
132.179
123.873
113.839
86.431
83.321
77.784
77.360
76.936
74.452
28.527
21.141
20.969
Cl
OAc
OAc
N
Boc
200
150
100
50
0


zy-1-28-1-B
8.103
7.390
7.363
7.336
7.260
7.138
7.111
6.639
6.124
2.263
2.142
Cl
OAc
OAc
N
Ac
1.05
0.90
0.90
0.90
0.98
3.00
5.75
10.0
5.0
0.0

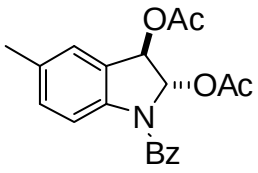

zy-1-28-1-B.C
169.601
169.373
145.432
132.898
131.865
125.807
125.147
115.887
87.373
77.784
77.360
76.936
74.705
23.593
21.184
20.946
Cl
OAc
OAc
N
Ac
200
150
100
50
0

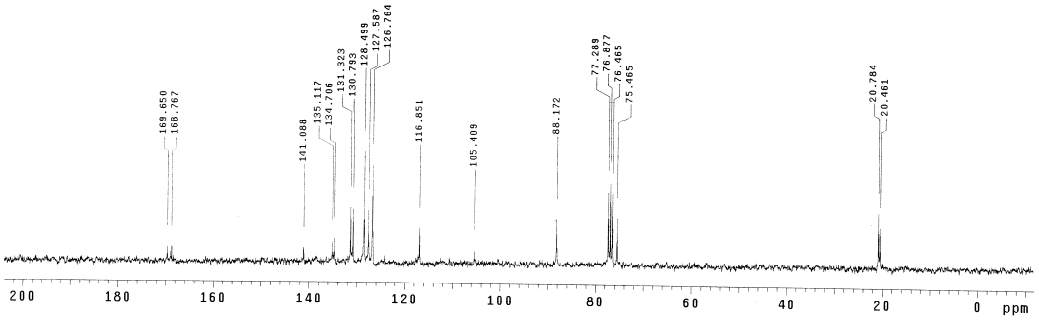
zy-1-29-2-a

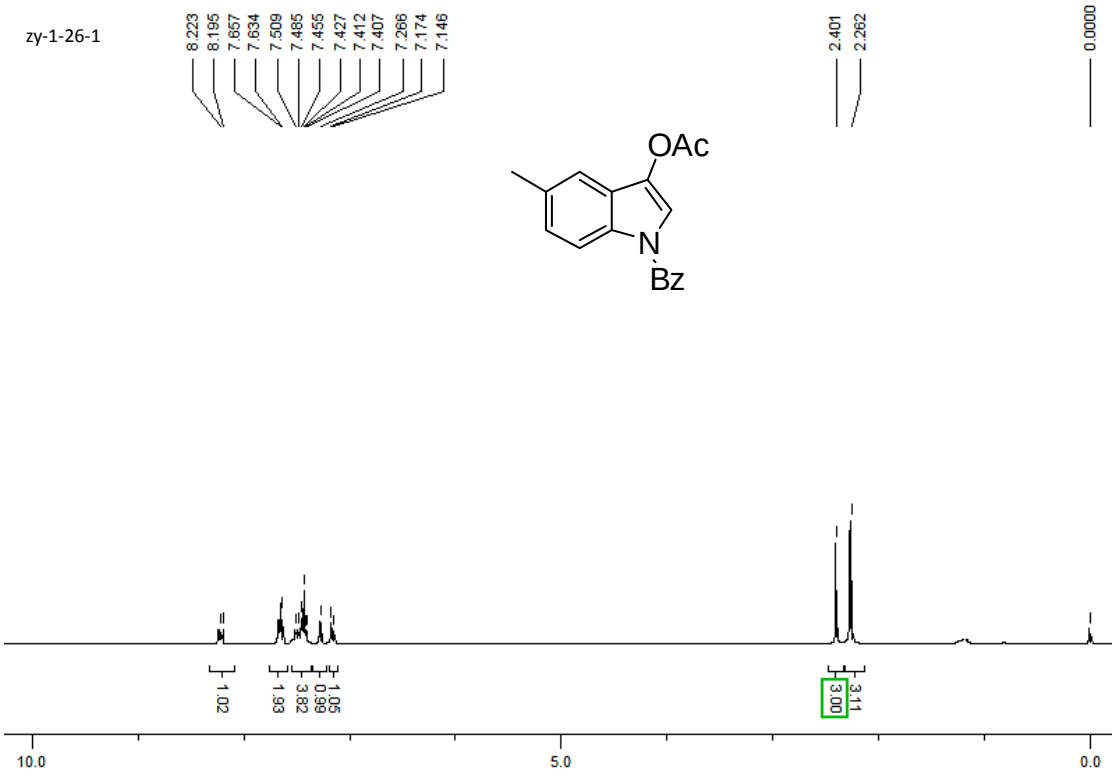


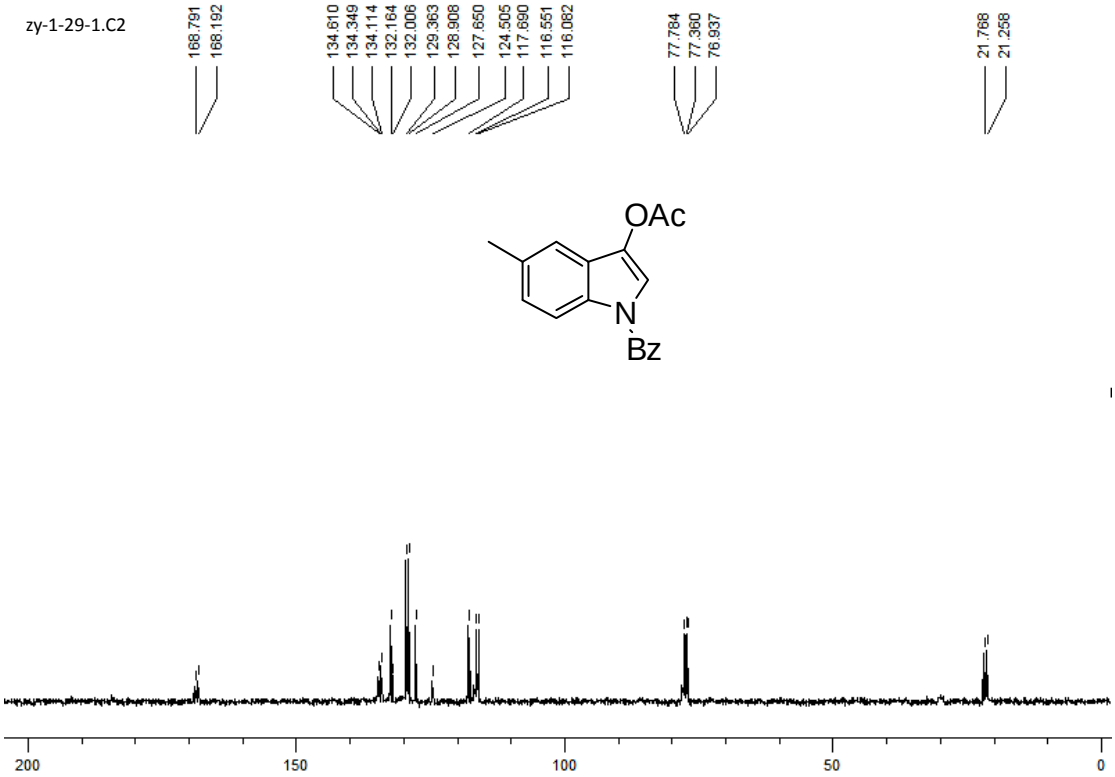


zy-1-29-2-A.C

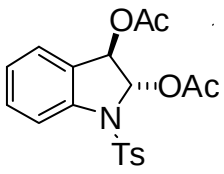


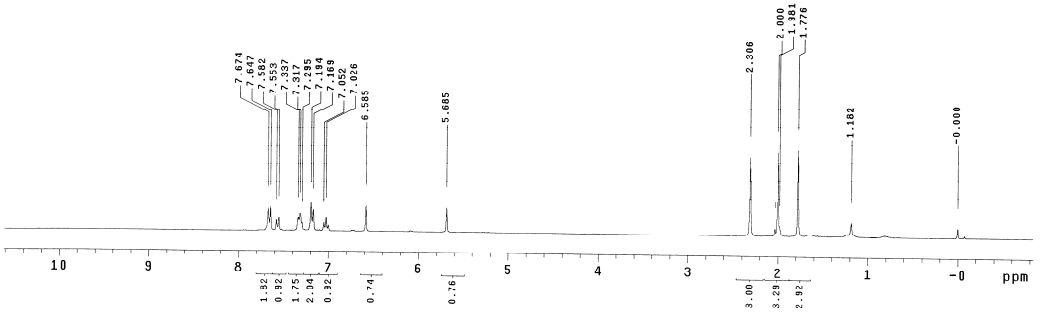



zy-1-26-1
8.223
8.195
7.657
7.634
7.509
7.485
7.455
7.427
7.412
7.407
7.266
7.174
7.146
2.401
2.262
0.0000
OAc
N
Bz
1.02
1.93
3.82
0.99
1.05
3.00
3.11
10.0
5.0
0.0


zy-1-29-1.C2
168.791
168.192
134.610
134.349
134.114
132.164
132.006
129.363
128.908
127.650
124.505
117.690
116.551
116.082
77.784
77.360
76.937
21.768
21.258
OAc
N
Bz
200
150
100
50
0

zy-1-65-B

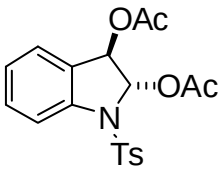


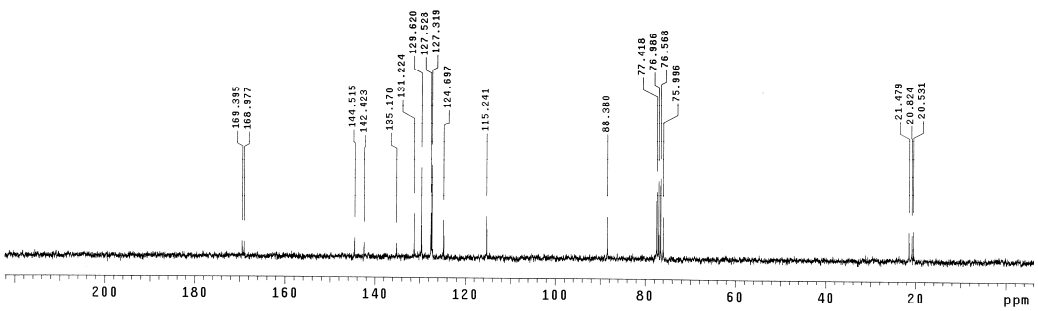


zy-1-65-B.C

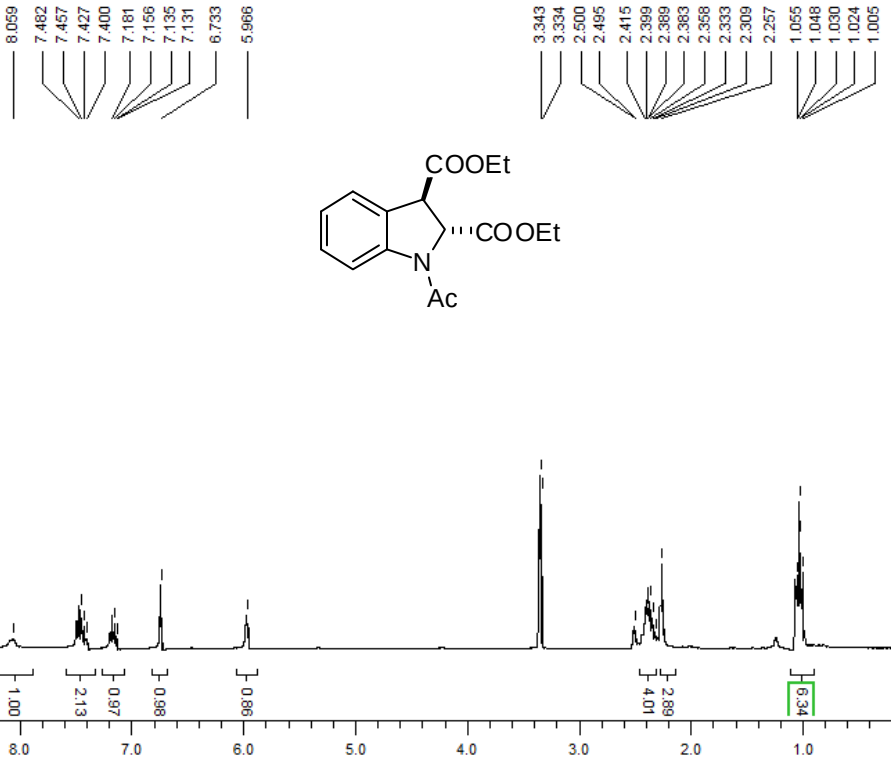
Solvent: CDCl3
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 28.0 degrees
Acq. time 0.501 sec
Width 17241.4 Hz
96 repetitions
OBSERVE C13, 75.4552538 MHz
DECOUPLE H1, 300.0821962 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 32768
Total time 1 hr, 55 min, 18 sec

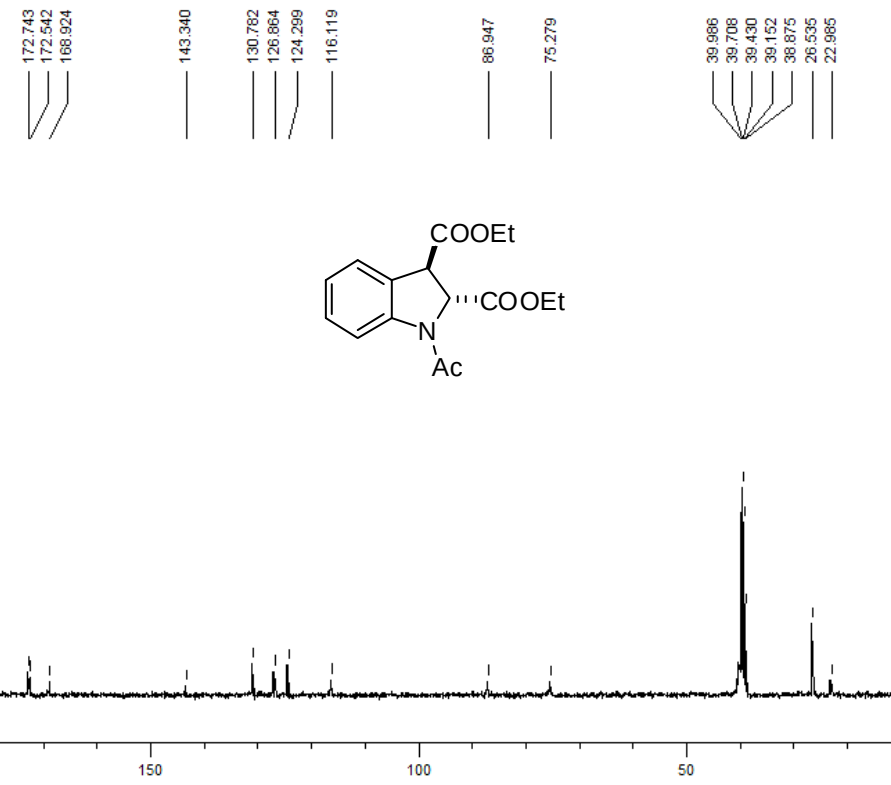




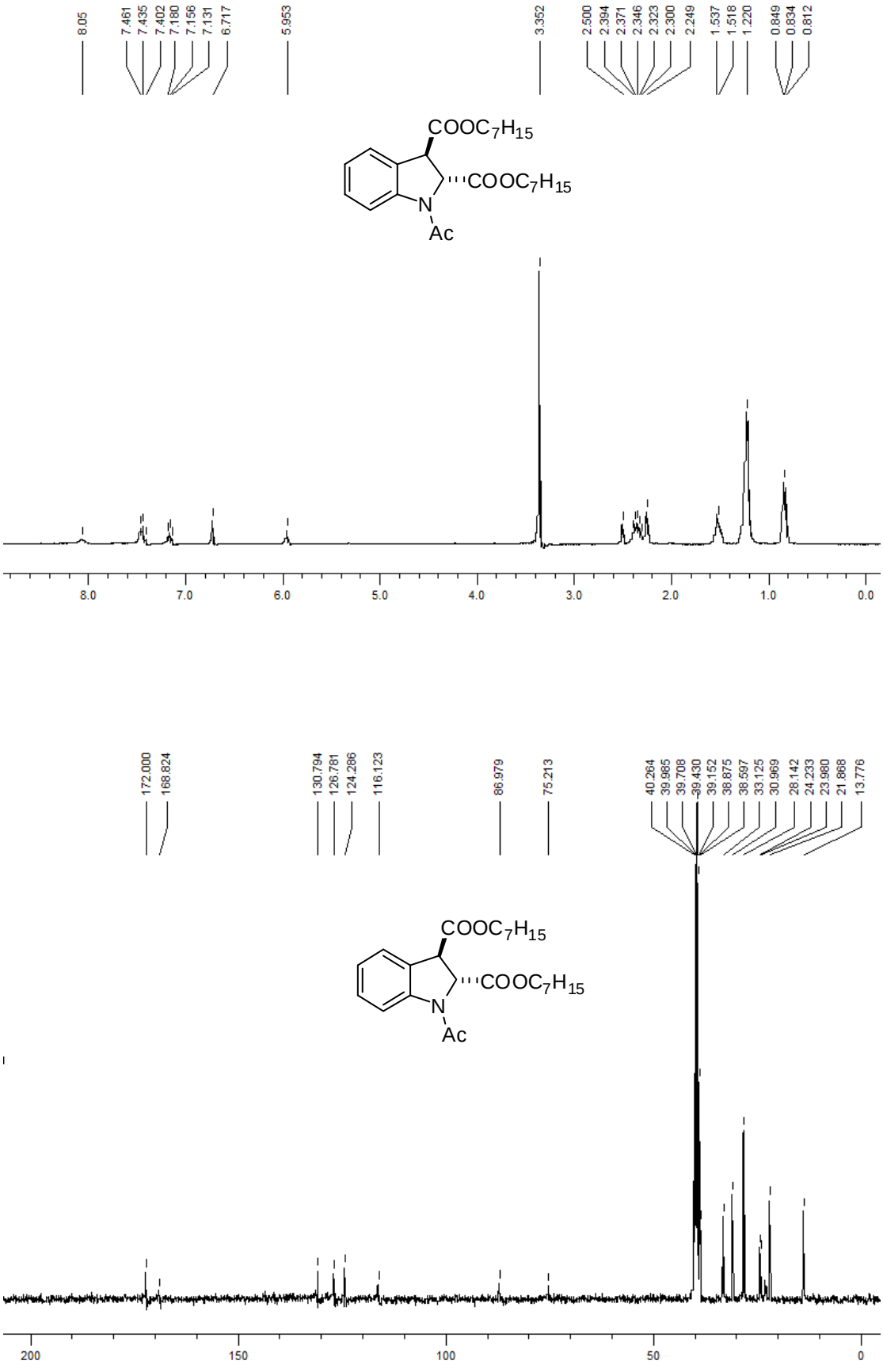
zy-1-124-2-2-a



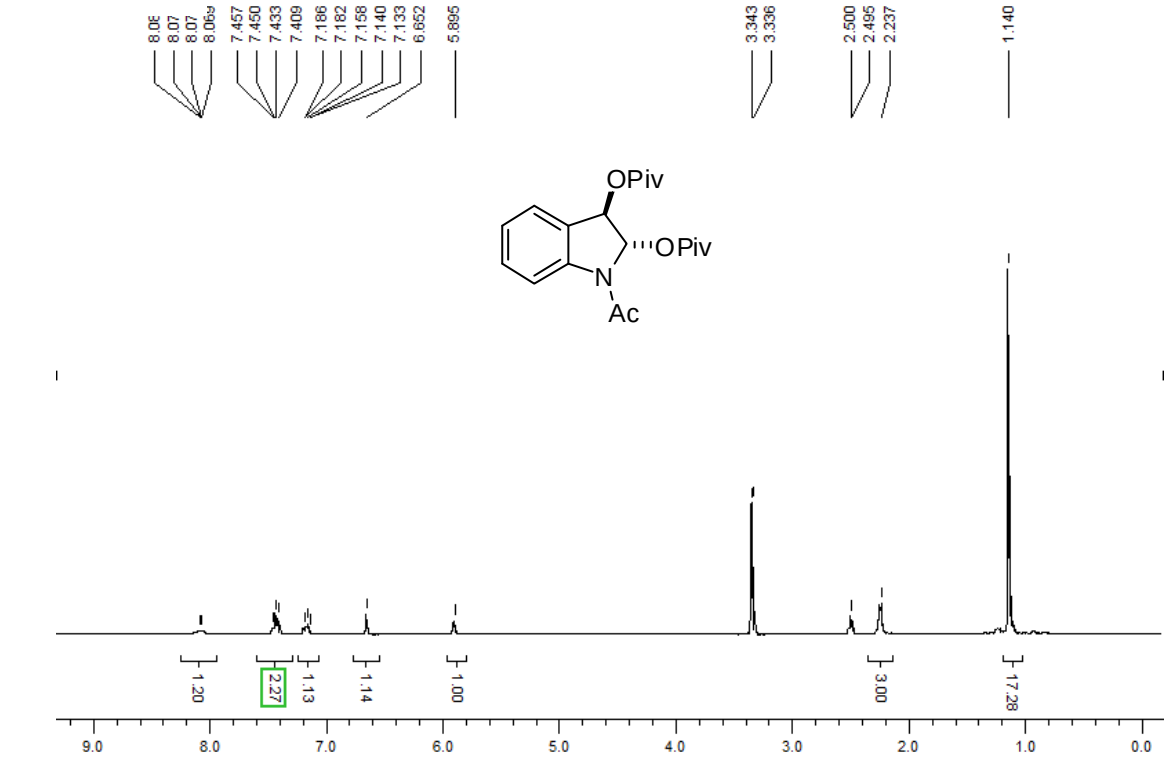
zy-1-124-2-2-a. C



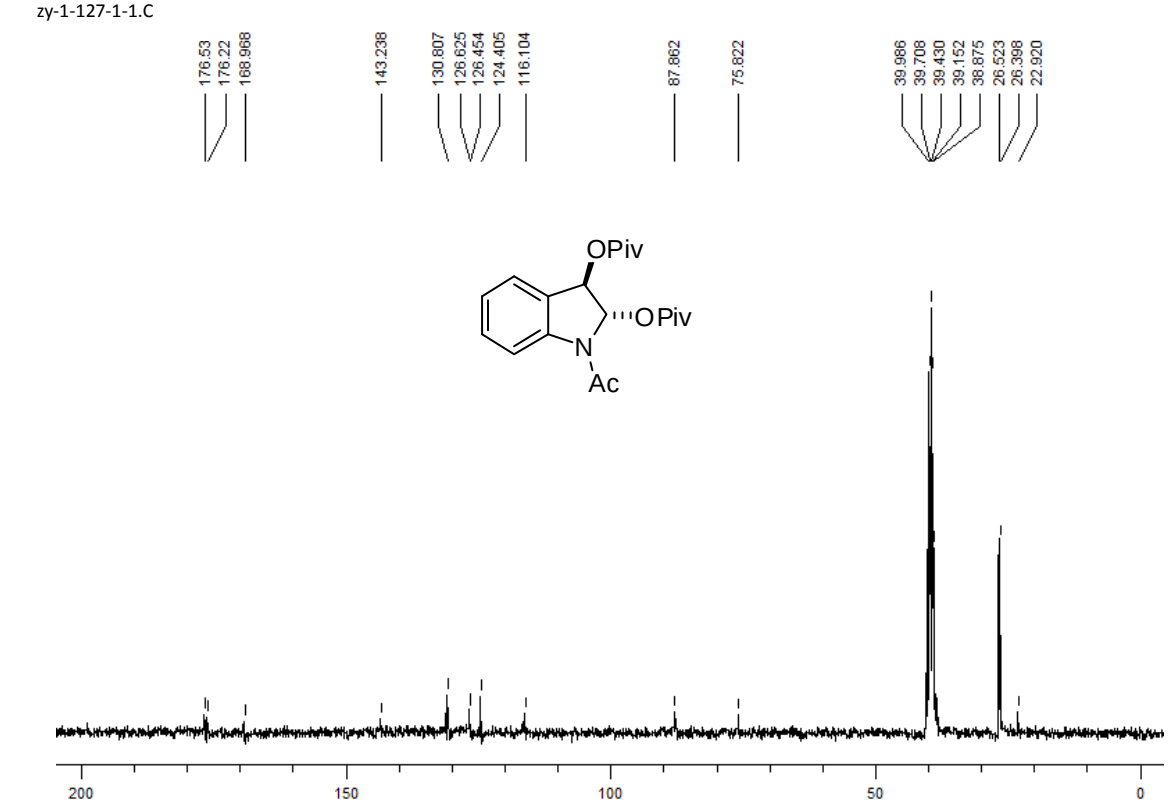
zy-1-129-1-1-DMSO

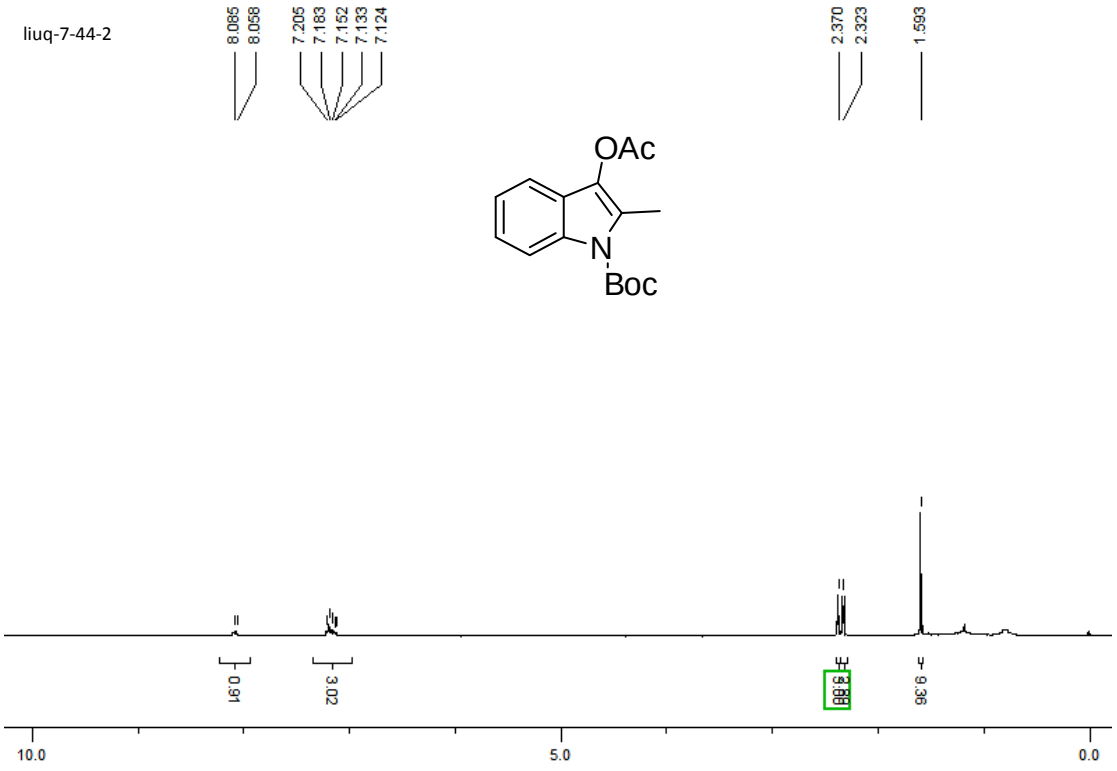


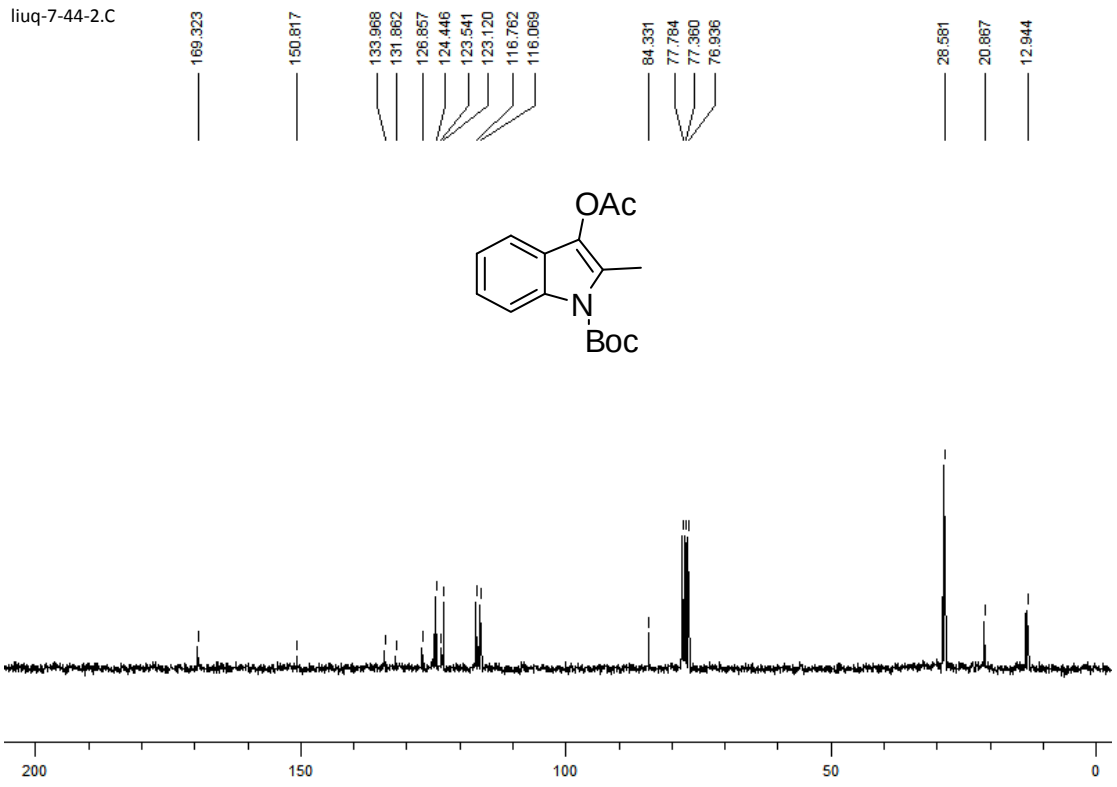
zy-1-127-1-1

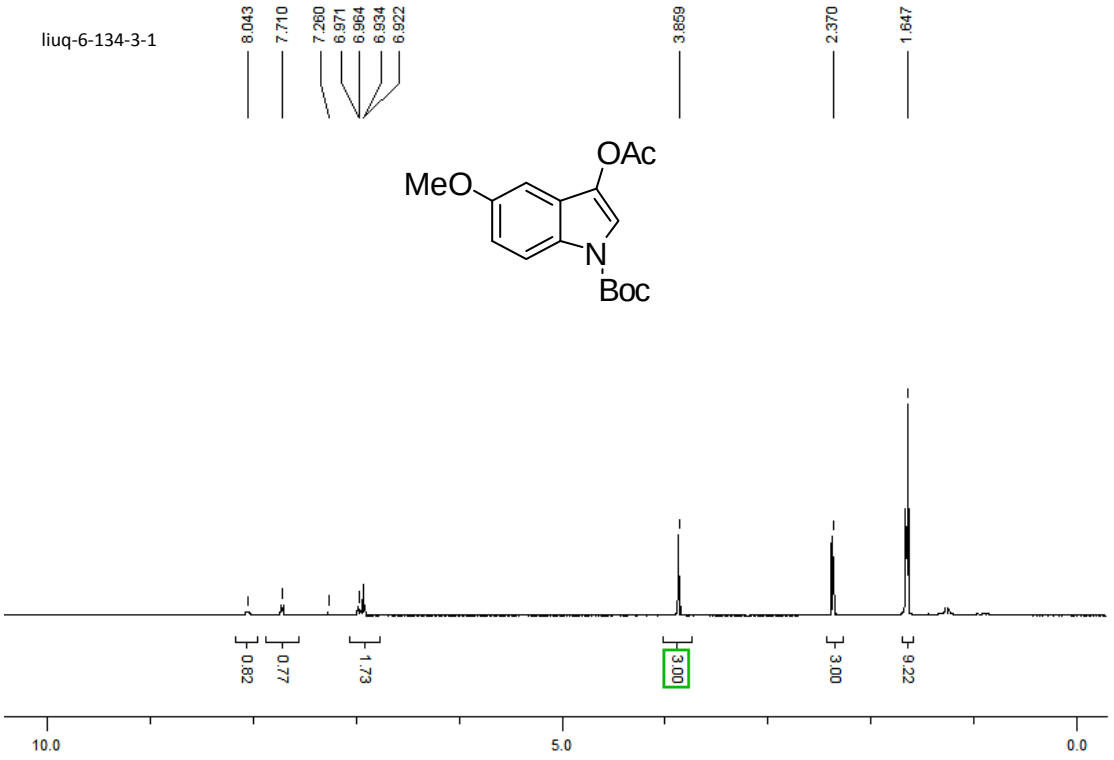


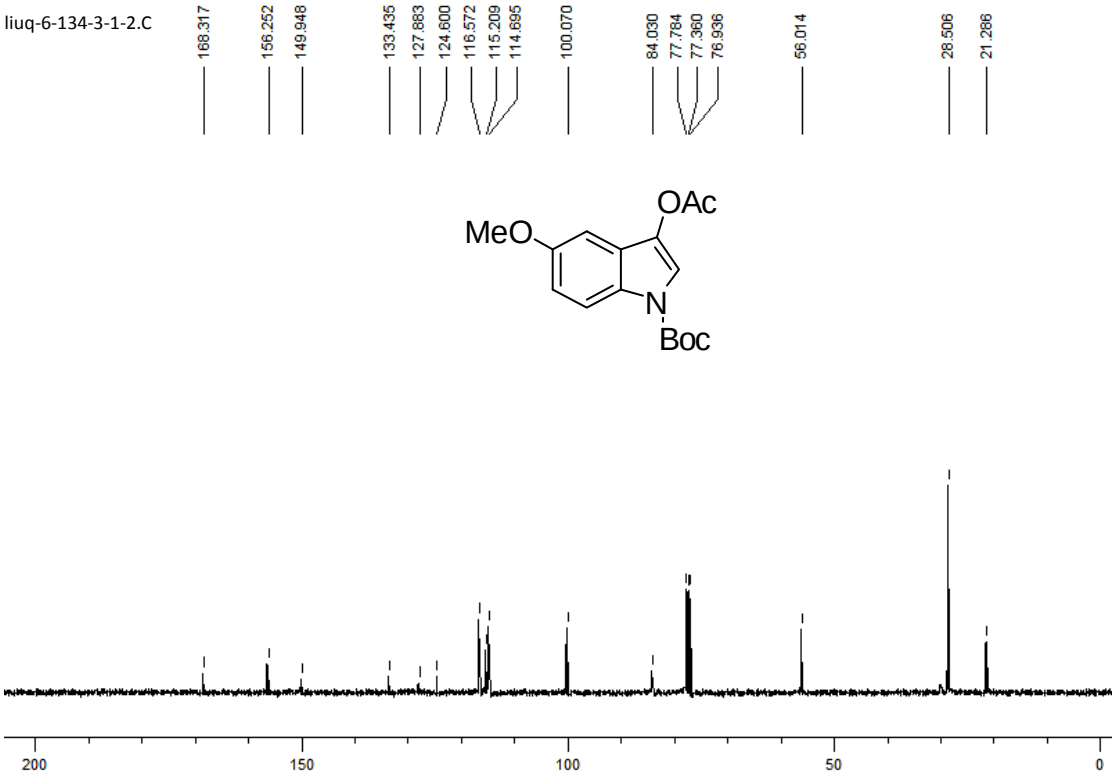
zy-1-127-1-1.C




liuq-7-44-2
8.085
8.058
7.205
7.183
7.152
7.133
7.124
2.370
2.323
1.593
OAc
N
Boc
0.91
3.02
9.36
10.0
5.0
0.0


liuq-7-44-2.C
169.323
150.817
133.968
131.862
126.857
124.446
123.541
123.120
116.762
116.069
84.331
77.784
77.360
76.936
28.581
20.867
12.944
OAc
N
Boc
200
150
100
50
0


liuq-6-134-3-1
8.043
7.710
7.260
6.971
6.964
6.934
6.922
3.859
2.370
1.647
OAc
MeO
N
Boc
0.82
0.77
1.73
3.00
3.00
9.22
10.0
5.0
0.0

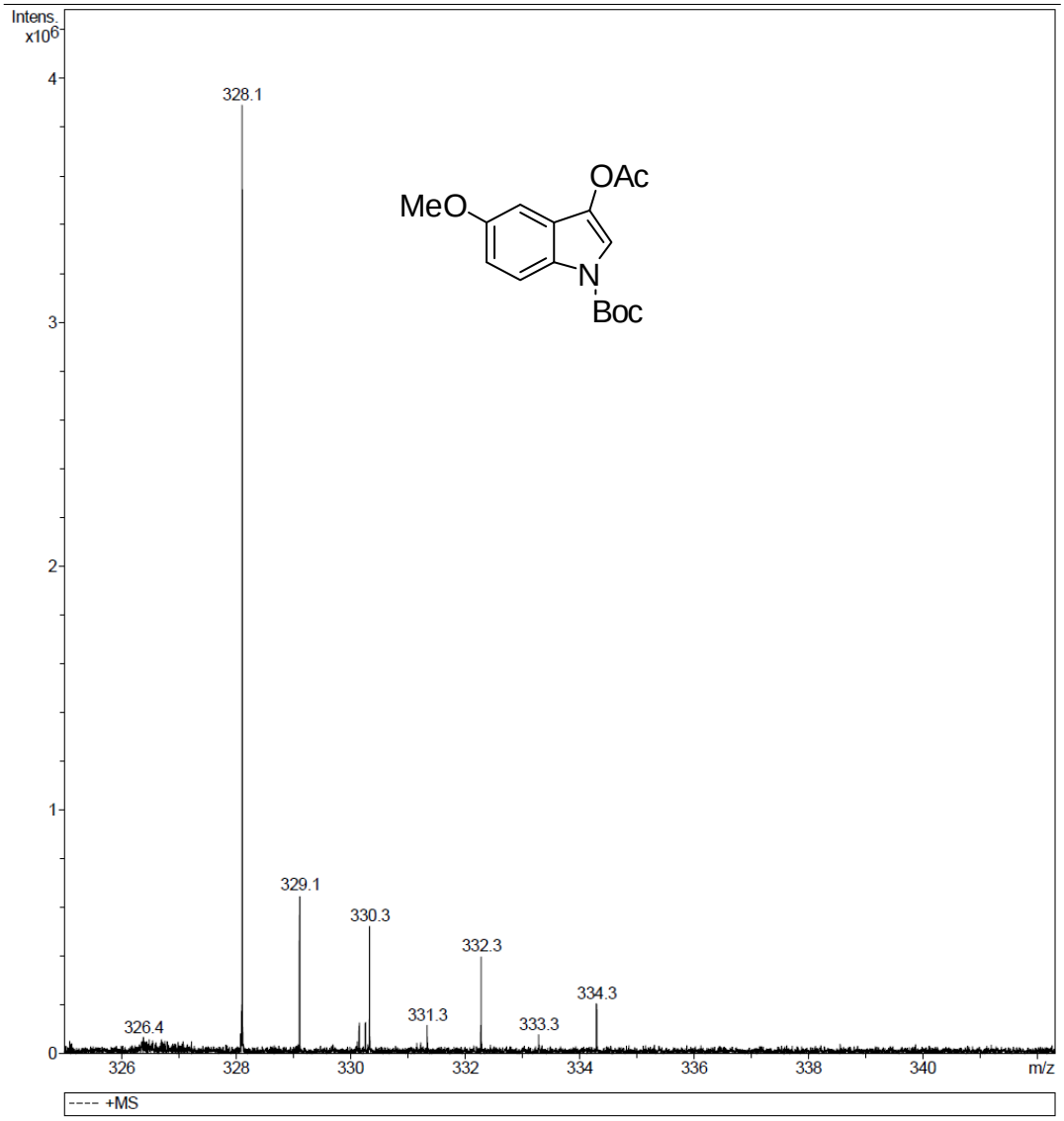

liuq-6-134-3-1-2.C
168.317
156.252
149.948
133.435
127.883
124.600
116.572
115.209
114.695
100.070
84.030
77.784
77.360
76.936
56.014
28.506
21.286
OAc
MeO
N
Boc
200
150
100
50
0

Display Report

Analysis Info

Analysis Name	D:\Data\zfj\2010915_000011.d	Acquisition Date	9/15/2010 1:18:44 PM
Method	XMASS_Method	Operator	FTMS_USER
Sample Name	184-4	Instrument	apex-III
Comment			

Acquisition Parameter



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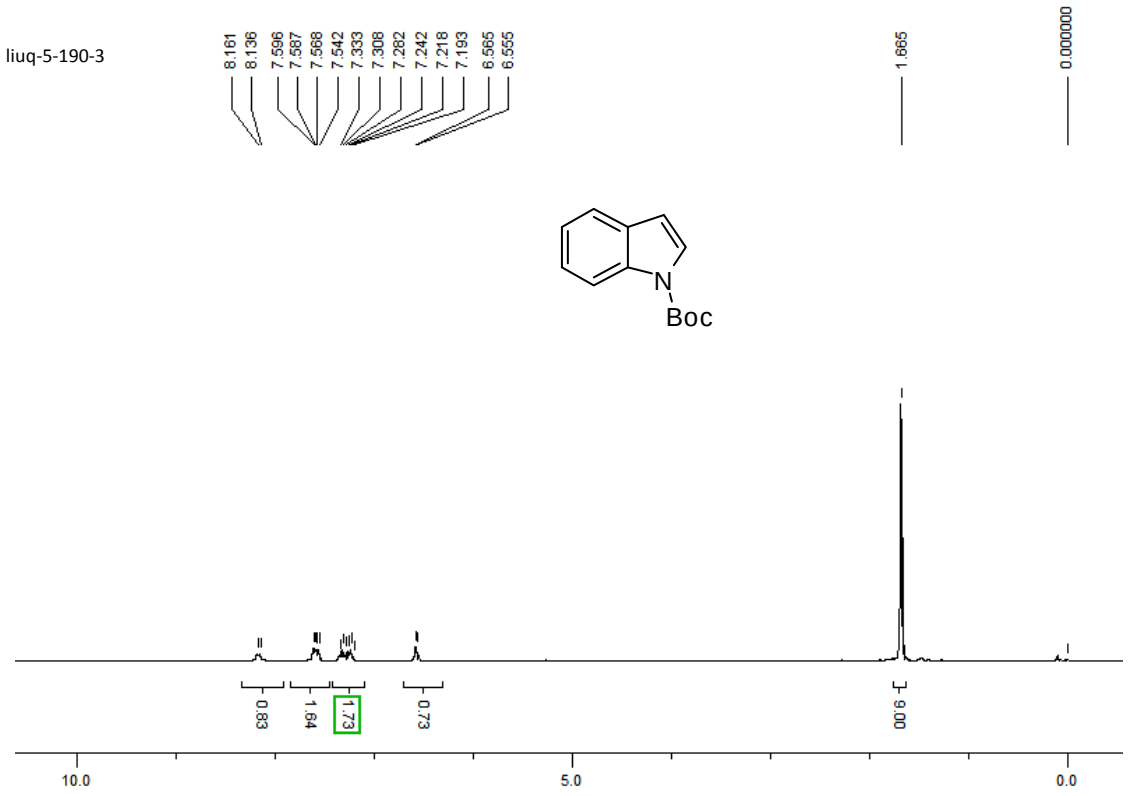
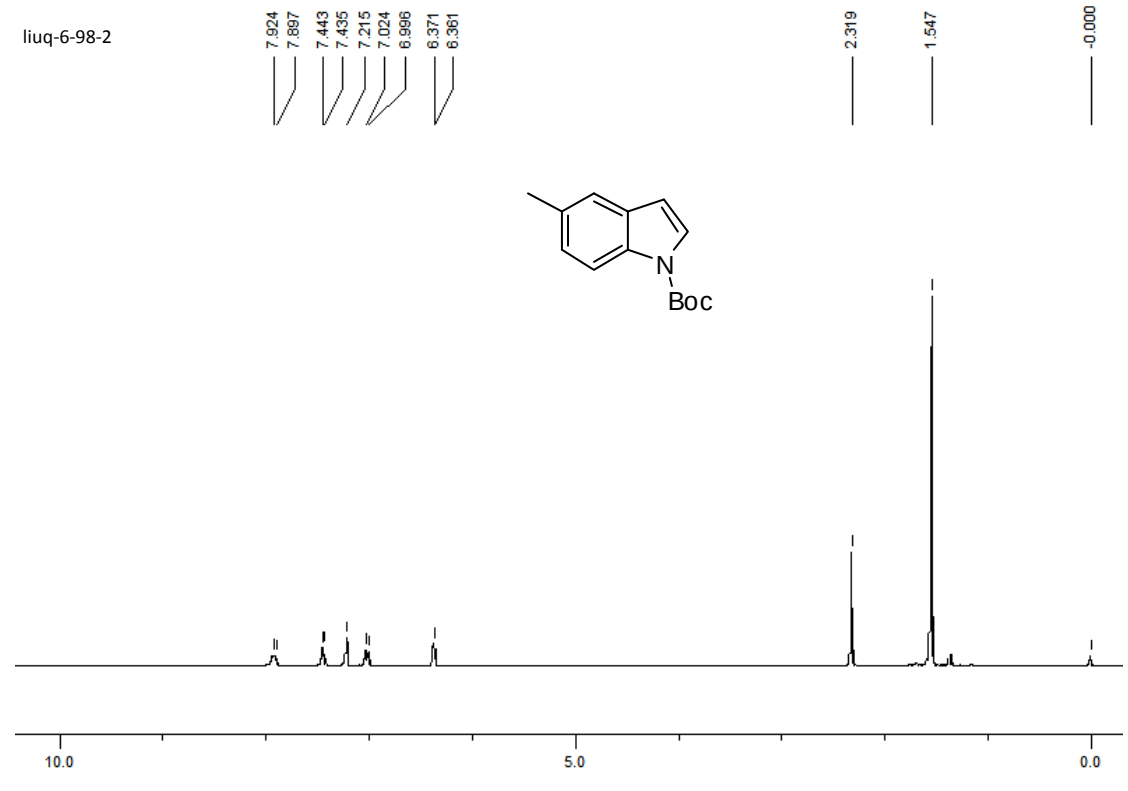
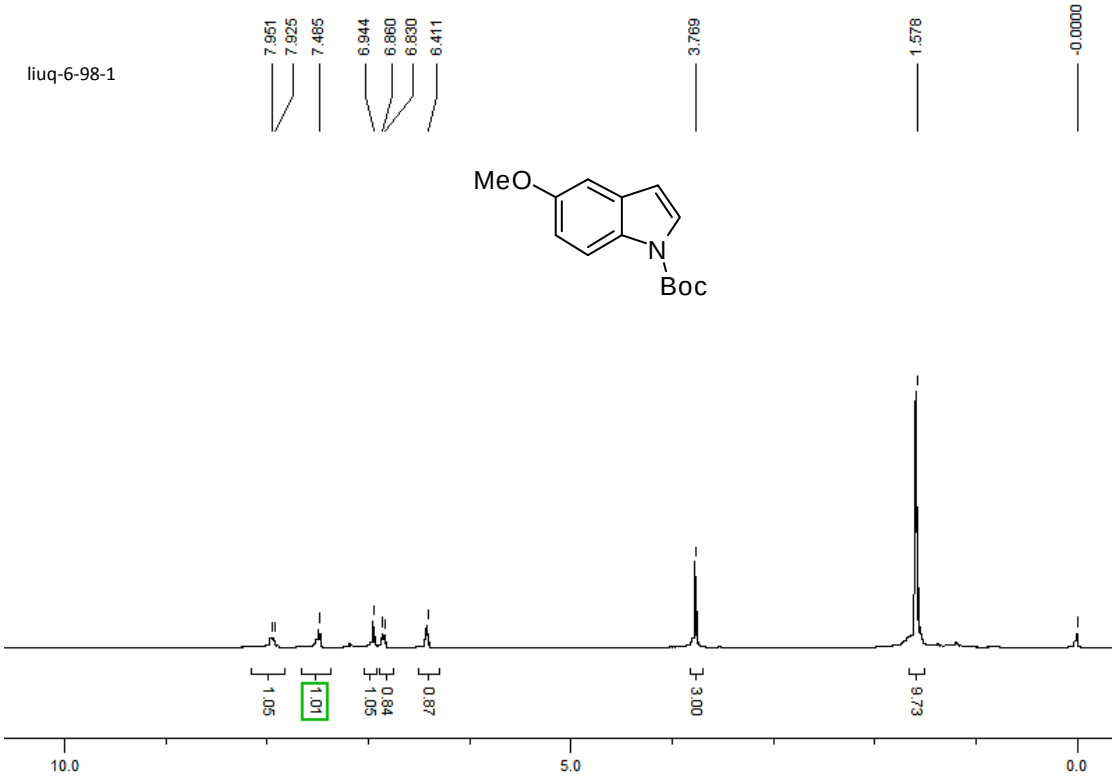
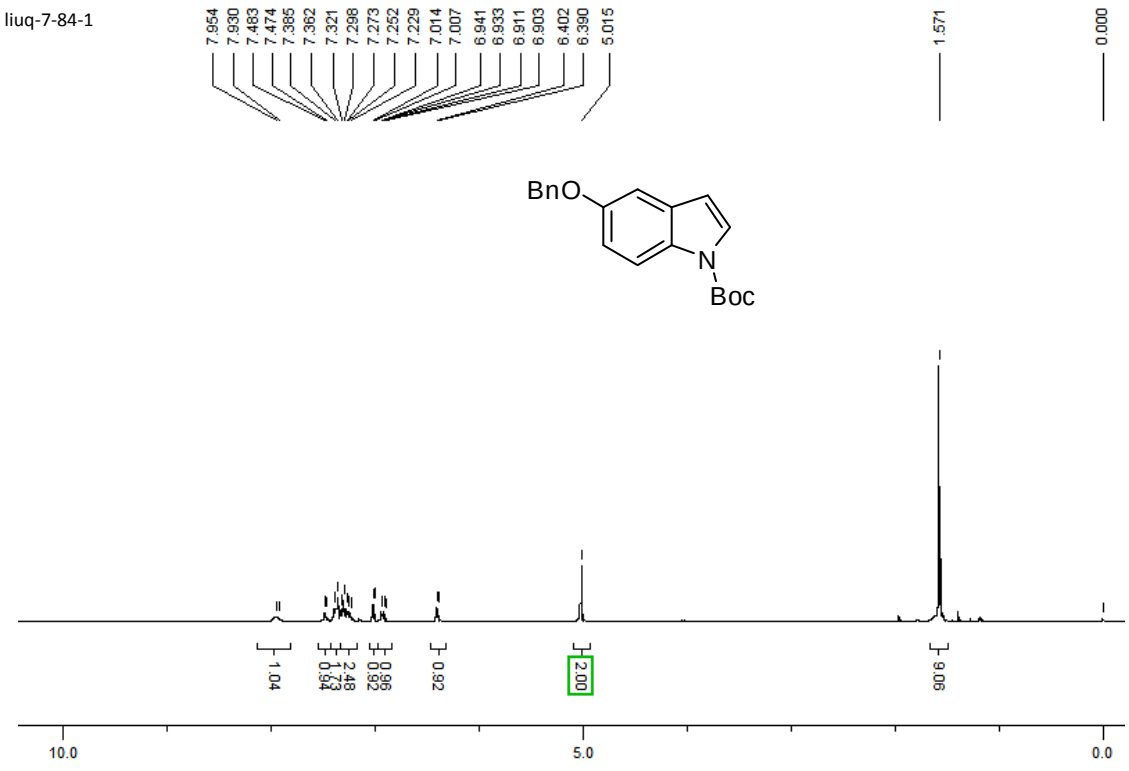

liuq-5-190-3
8.161
8.136
7.596
7.587
7.568
7.542
7.333
7.308
7.282
7.242
7.218
7.193
6.565
6.555
1.665
0.000000
N
Boc
0.83
1.64
1.73
0.73
9.00
10.0
5.0
0.0

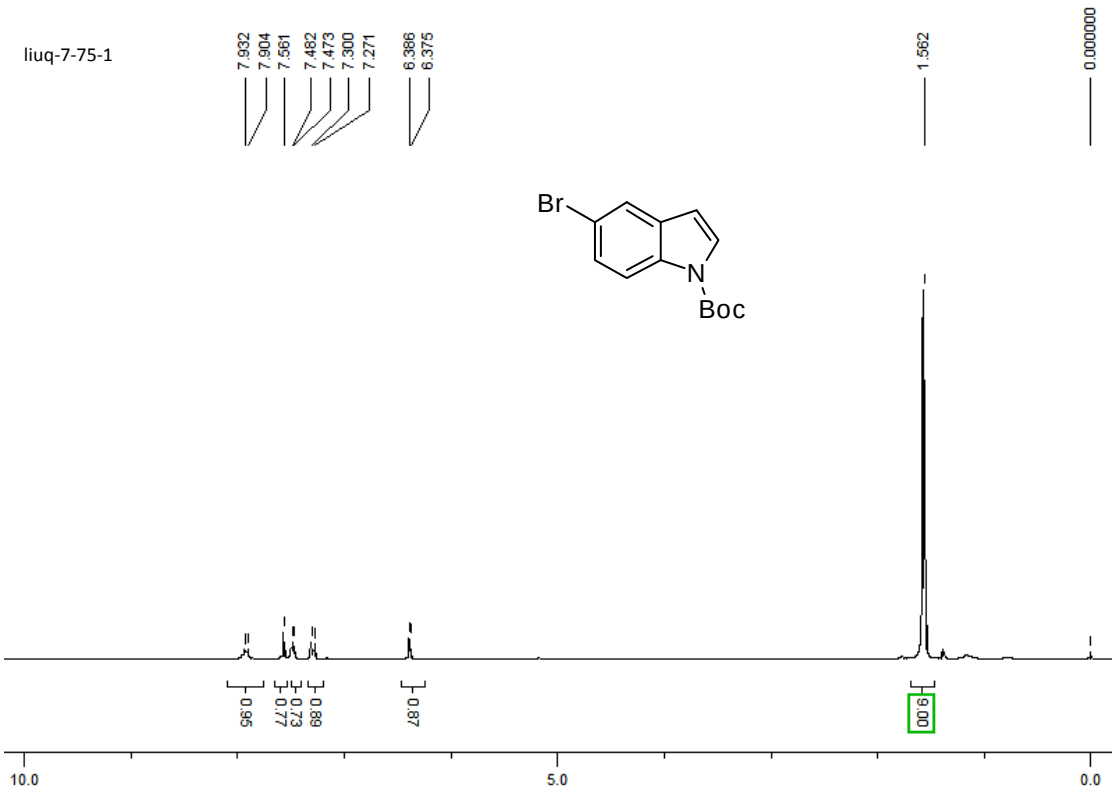

liuq-6-98-2
7.924
7.897
7.443
7.435
7.215
7.024
6.996
6.371
6.361
2.319
1.547
-0.000
N
Boc
10.0
5.0
0.0

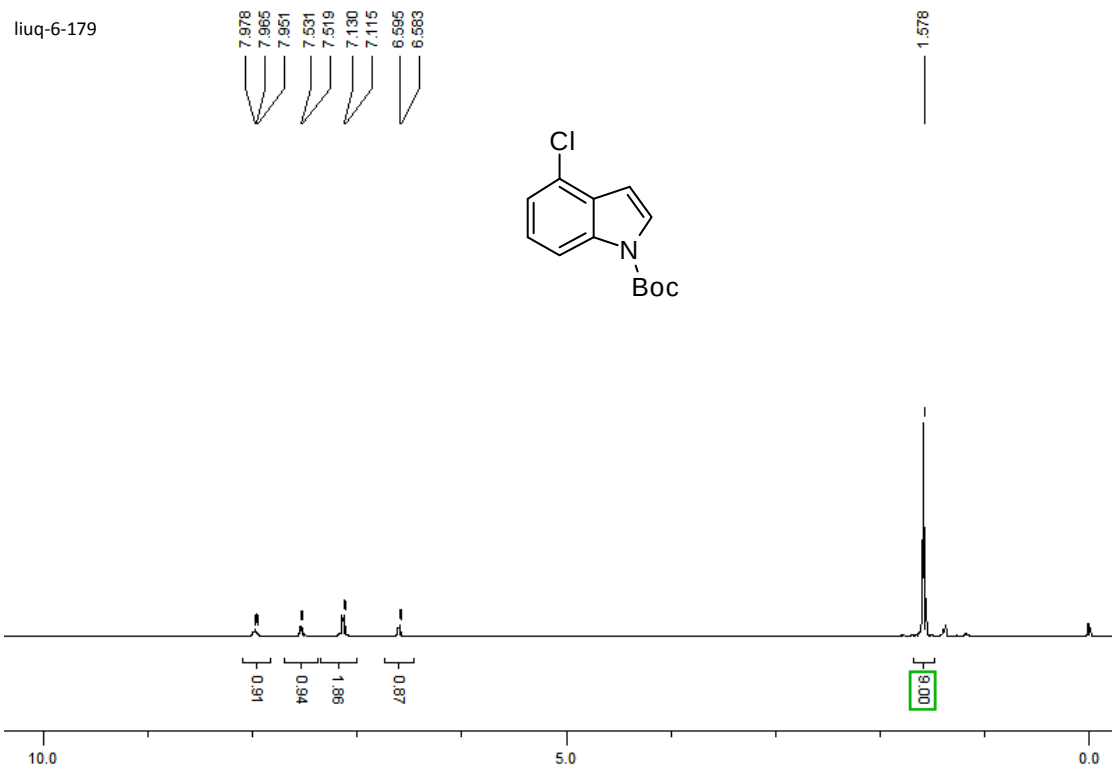
liuq-6-98-1

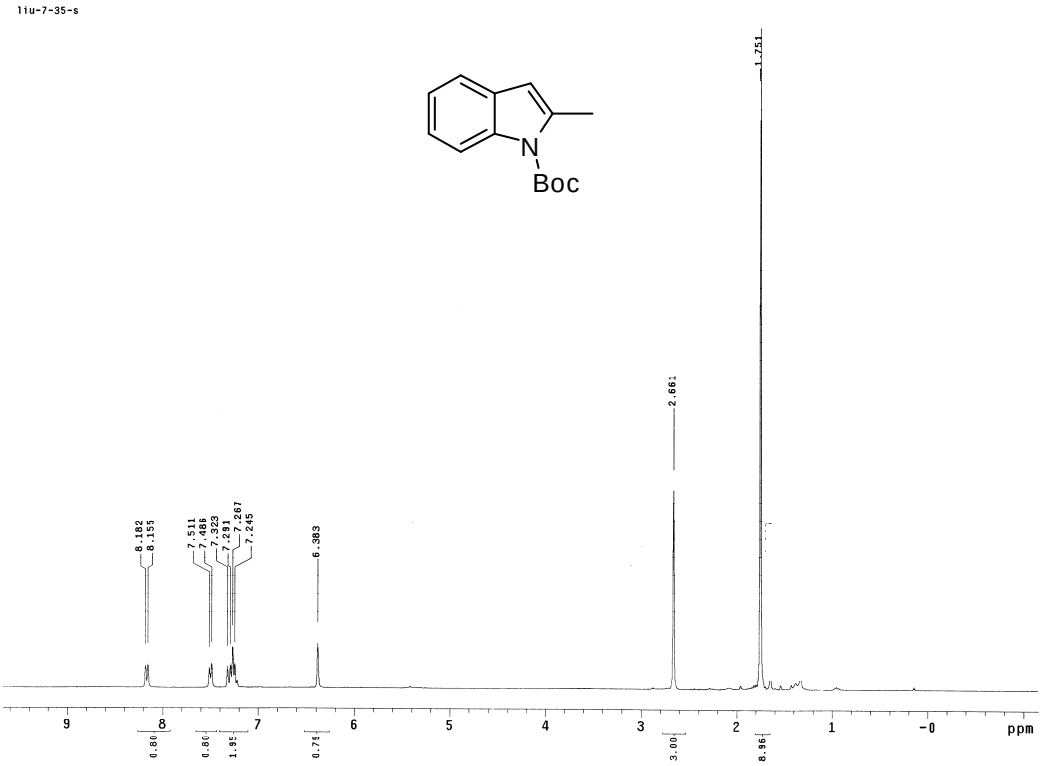


liuq-7-84-1

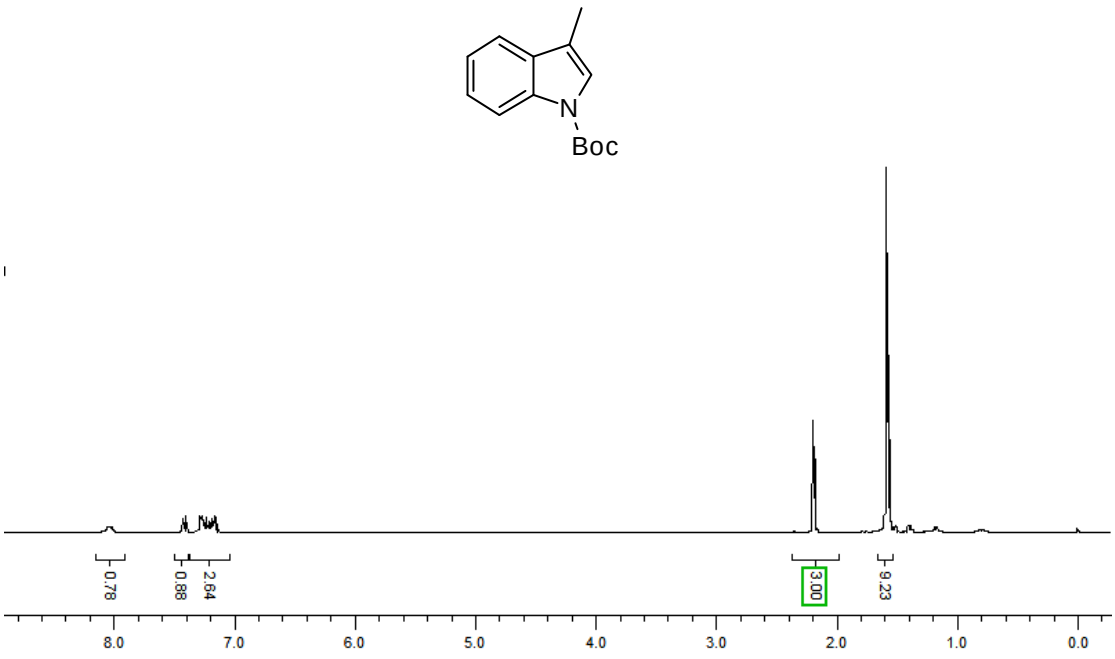



liuq-7-75-1
7.932
7.904
7.561
7.482
7.473
7.300
7.271
6.386
6.375
1.562
0.000000
Br
N
Boc
0.96
0.77
0.73
0.89
0.87
9.00
10.0
5.0
0.0

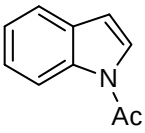

liuq-6-179
7.978
7.965
7.951
7.531
7.519
7.130
7.115
6.595
6.583
1.578
Cl
N
Boc
0.91
0.94
1.86
0.87
9.00
10.0
5.0
0.0

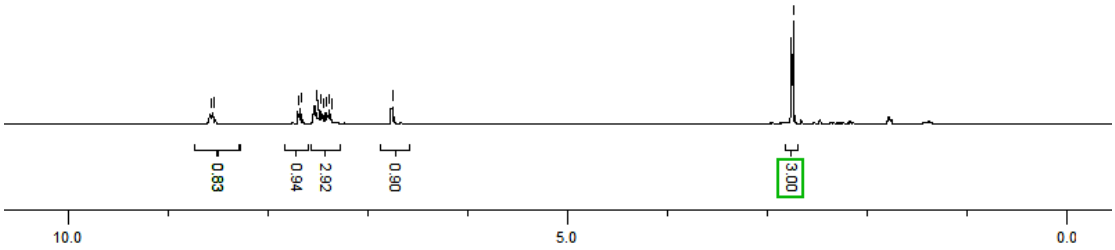

liu-7-35-s
N
Boc
8.182
8.155
7.511
7.486
7.323
7.291
7.287
7.245
6.383
2.661
1.751
ppm

liuq-7-35

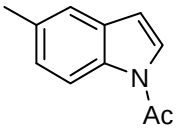

N
Boc
0.78
0.88
2.64
3.00
9.23

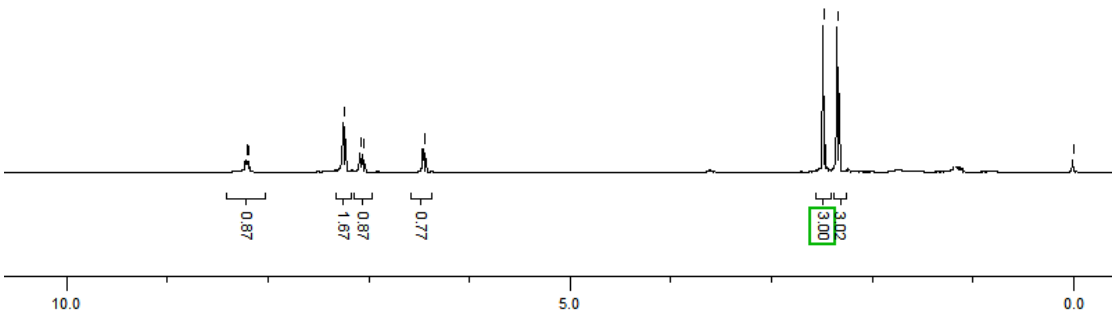
liuq-6-81-3

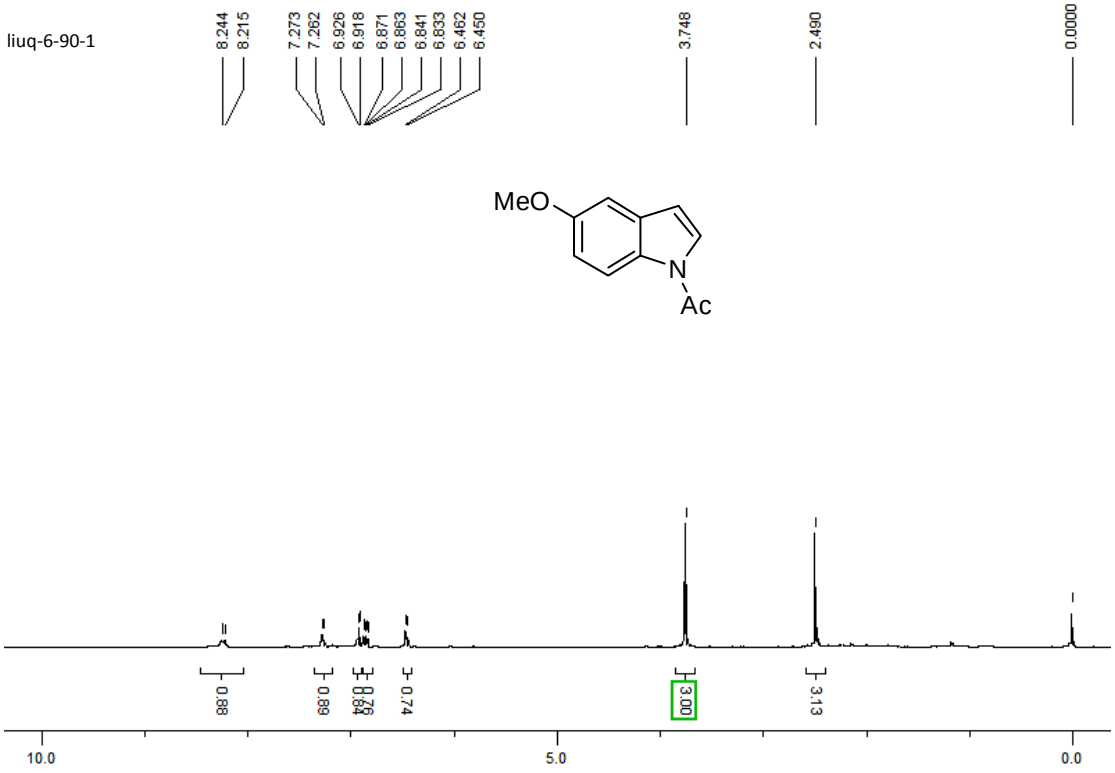


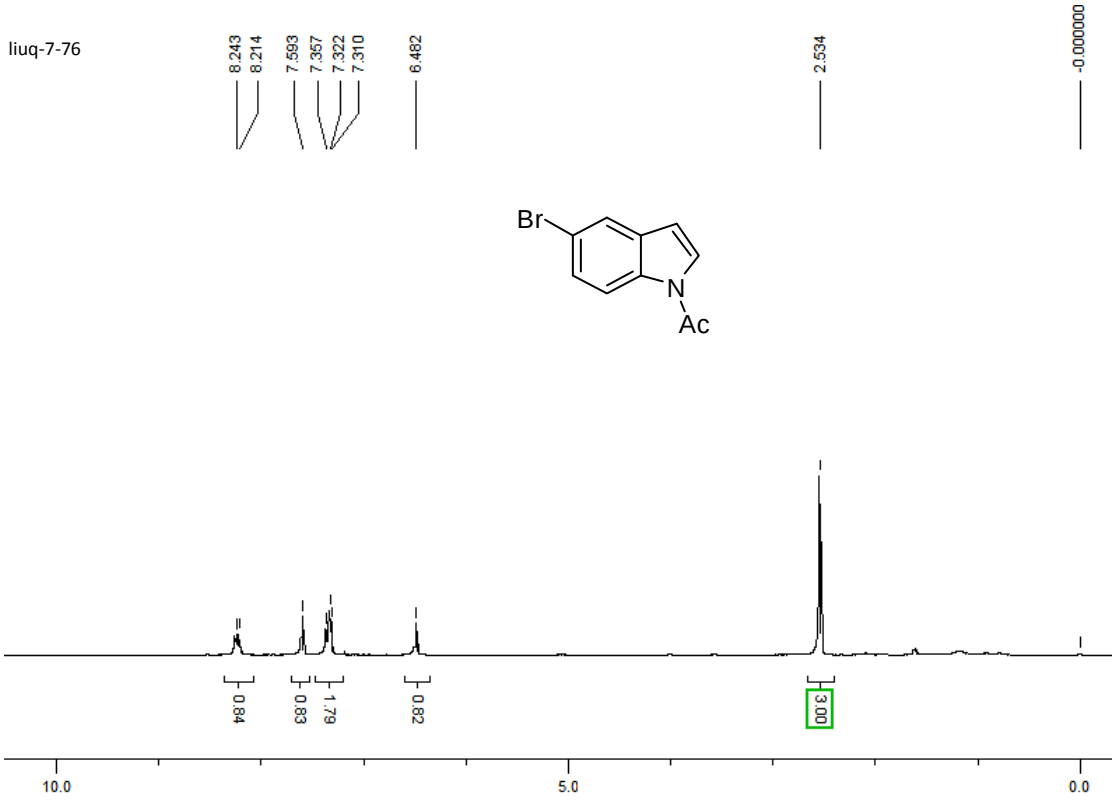


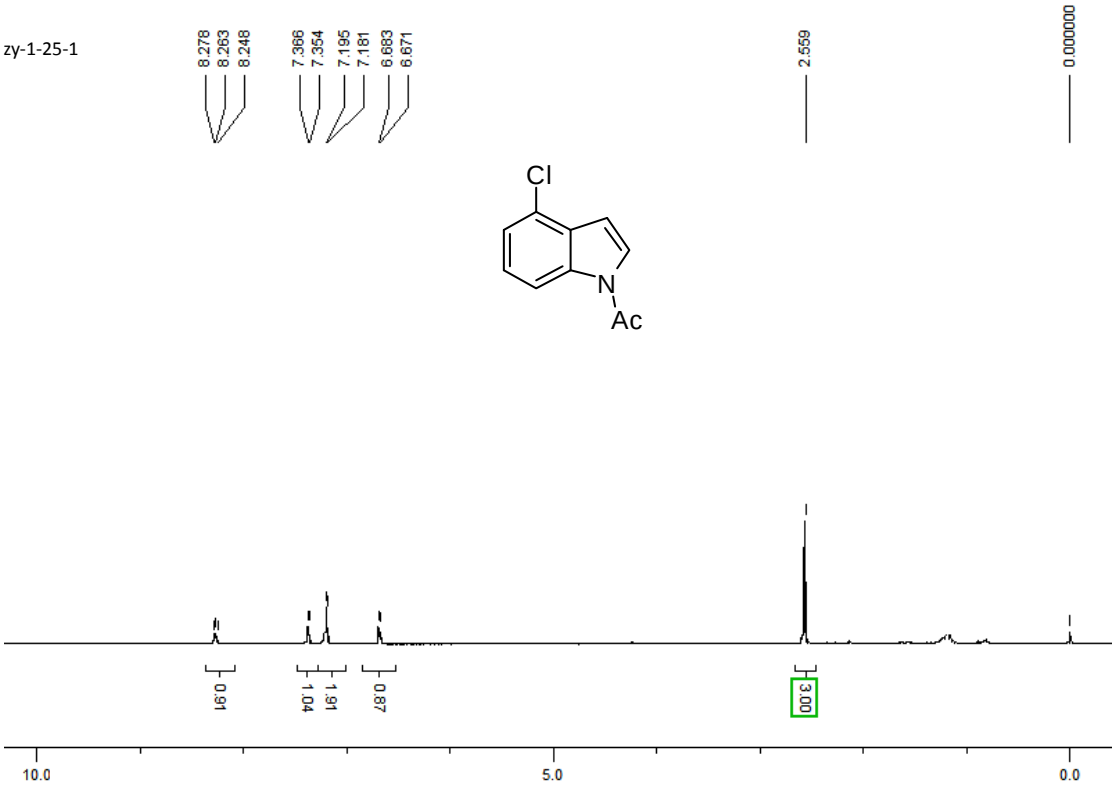
liuq-6-90-2

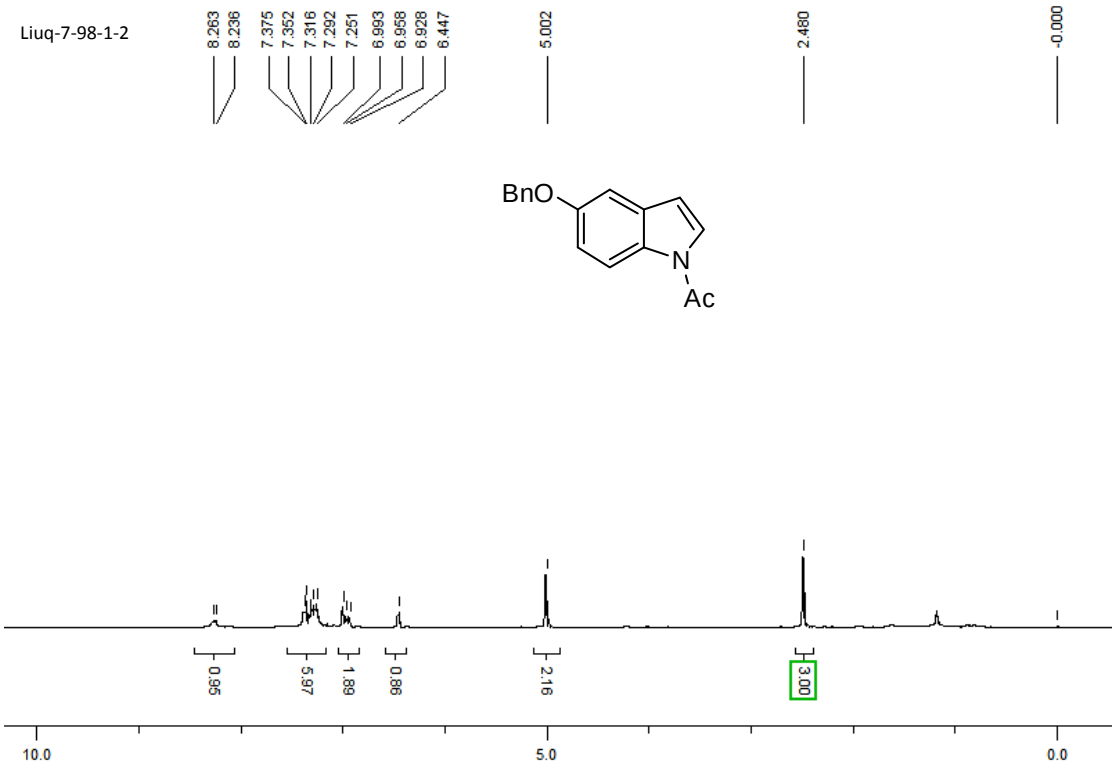


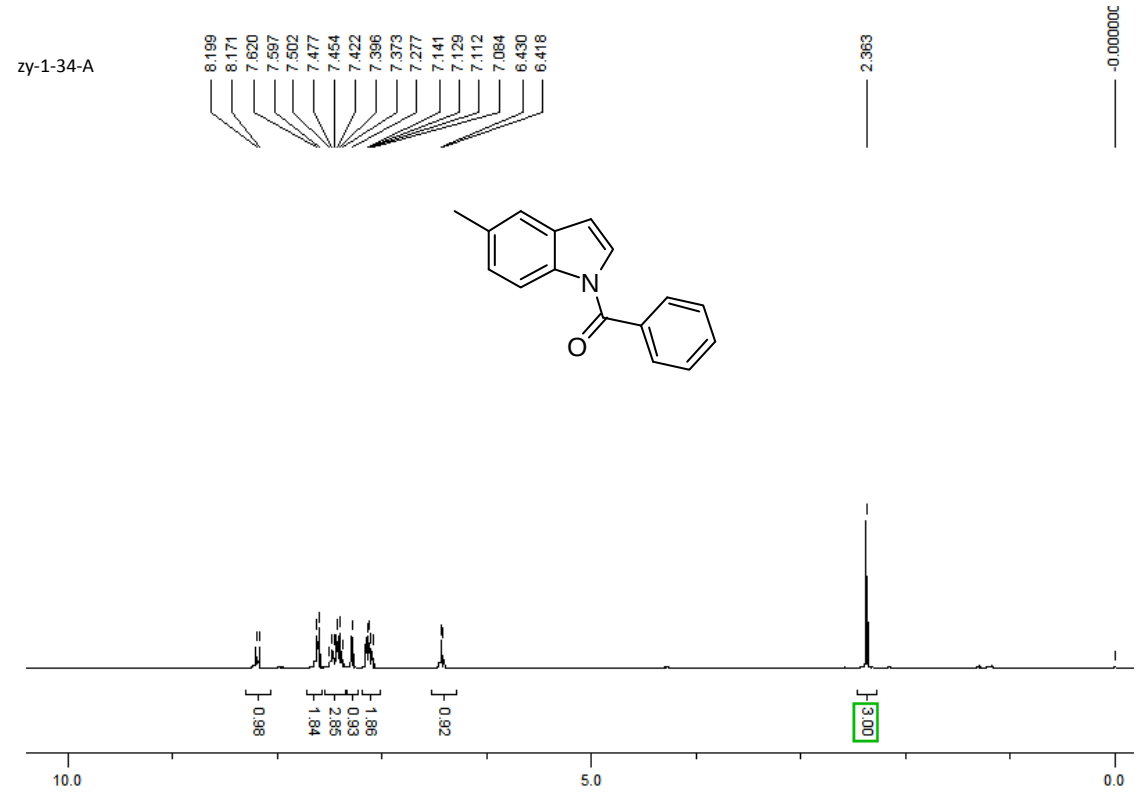


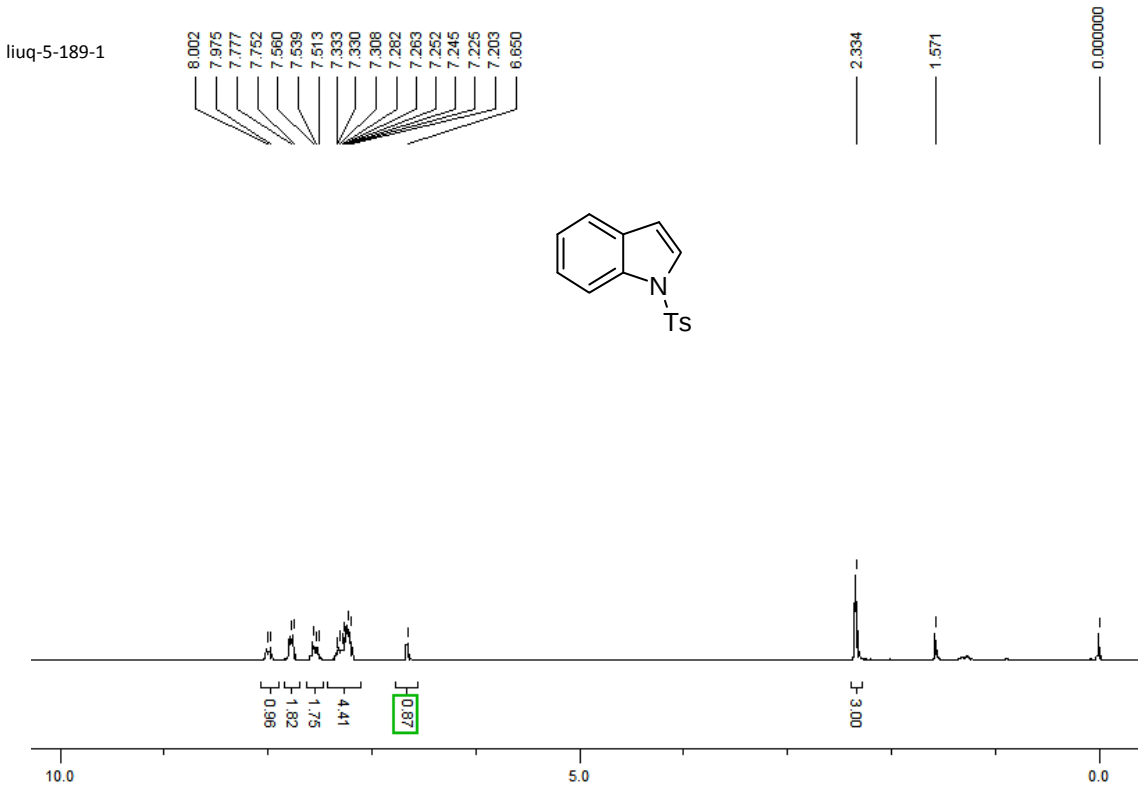

liuq-6-90-1
8.244
8.215
7.273
7.262
6.926
6.918
6.871
6.863
6.841
6.833
6.462
6.450
3.748
2.490
0.0000
MeO
N
Ac
0.88
0.89
0.84
0.76
0.74
3.00
3.13
10.0
5.0
0.0


liuq-7-76
8.243
8.214
7.593
7.357
7.322
7.310
6.482
2.534
-0.000000
Br
N
Ac
0.84
0.83
1.79
0.82
3.00
10.0
5.0
0.0


zy-1-25-1
8.278
8.263
8.248
7.366
7.354
7.195
7.181
6.683
6.671
2.559
0.000000
Cl
N
Ac
0.91
1.04
1.91
0.87
3.00
10.0
5.0
0.0


Liuq-7-98-1-2
8.263
8.236
7.375
7.352
7.316
7.292
7.251
6.993
6.958
6.928
6.447
5.002
2.480
-0.000
BnO
N
Ac
0.95
5.97
1.89
0.86
2.16
9.13
10.0
5.0
0.0


zy-1-34-A
8.199
8.171
7.620
7.597
7.502
7.477
7.454
7.422
7.396
7.373
7.277
7.141
7.129
7.112
7.084
6.430
6.418
2.363
-0.000000
N
O
0.98
1.84
2.86
0.93
1.86
0.92
3.00
10.0
5.0
0.0


liuq-5-189-1
8.002
7.975
7.777
7.752
7.560
7.539
7.513
7.333
7.330
7.308
7.282
7.263
7.252
7.245
7.225
7.203
6.650
2.334
1.571
0.000000
N
Ts
0.96
1.82
1.75
4.41
0.87
3.00
10.0
5.0
0.0