Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Divergent Synthesis of 4-Amino Indoles with Free Amine Groups via Tandem Reaction of 2-Alkynylanilines

Xiaohua Li, Qiuqin He*, Renhua Fan*

*Corresponding author: Email: rhfan@fudan.edu.cn

Supplementary Information

Content

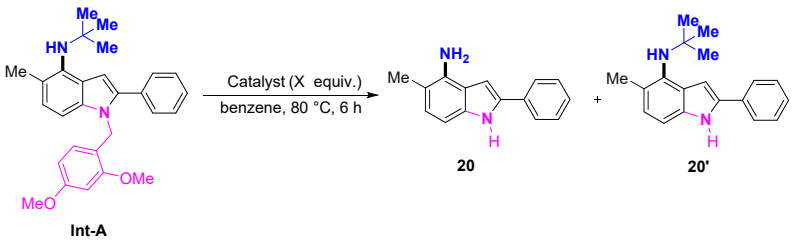
Supplementary Methods

1. General Information

All reactions were performed in a 25 mL of Sealed tubes under air atmosphere. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr (house vacuum) at 35–40 °C. Commercial reagents and solvents were used as received. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. High Resolution Mass spectra was recorded by Bruker MicroTOF II (ESI^{+}).

2. Evaluation of Conditions

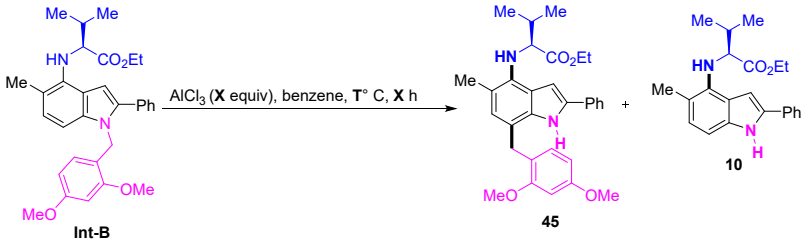
Table S1. Evaluation of Conditions



Entry	Catalyst	Equiv of Catalyst	Yield of 20	Yield of 20'
1	$ZnCl_2$	2.0	0	82
2	$In(OTf)_3$	2.0	0	79
3	$Sc(OTf)_3$	2.0	0	79
4	$Bi(OTf)_3$	2.0	0	50

5	**$AlCl_3$**	**5.0**	**91**	**0**
6	$AlBr_3$	5.0	51	0
7	$BF_3{\cdot}Et_2O$	10.0	90	0
8	$SnCl_4$	5.0	63	0
9	$FeCl_3$	5.0	0	0
10	$Cu(OTf)_2$	2.0	0	0
11	$Yb(OTf)_3$	2.0	0	0
12	$TsOH{\cdot}H_2O$	5.0	49	0
13	CF_3COOH	5.0	0	0

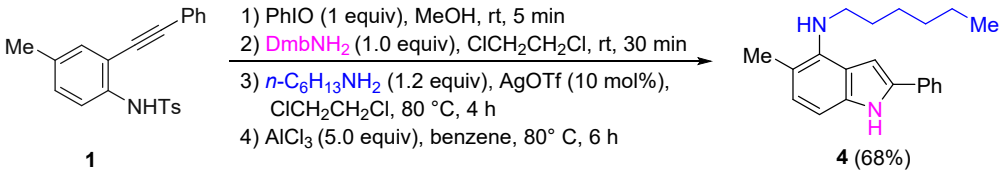
Table S2. Evaluation of Deprotection Conditions



Entry	Equiv. of $AlCl_3$	T/°C	X/h	Yield of 45	Yield of 10
1	**5.0**	**40**	**12**	**0**	**80**
2	2.0	40	12	45	33
3	**2.0**	**40**	**20**	**60**	**20**
4	2.0	60	20	40	33
5	3.0	40	20	52	35
6	4.0	40	12	20	56
7	4.0	80	6	0	70

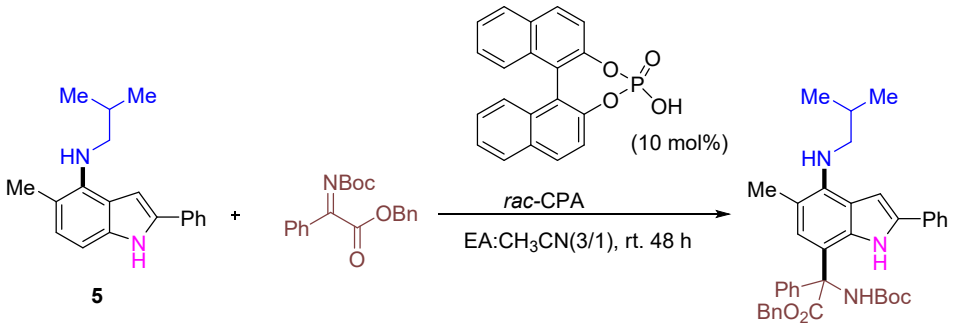
3. Representative Procedure and Characterization of Products

3.1 Representative Procedure



PhIO (0.1 mmol) was added to a solution of compound **1** (0.1 mmol) in MeOH (2.0 mL) at 25 ℃. After 5 min, the reaction mixture was concentrated *in vacuo*. The resulting crude product was dissolved in 1,2-dichloroethane (2.0 mL), (2,4-dimethoxyphenyl)methanamine ($DmbNH_2$) (0.1 mmol) was added and the resulting mixture was stirred at the room temperature for 30 min. Treating with 1.2 equivalents of hexan-1-amine (*n*-$C_6H_{13}NH_2$) in the presence of 10 mol% of AgOTf in 1,2-dichloromethane at 80 °C for 4 hours led to the formation of 4-hexylamino indole. Then the reaction mixture was filtered through a short silica gel column to remove $TsNH_2$ and AgOTf (eluent: petroleum ether/ ethyl acetate 10:1). Next, The resulting crude product that was concentrated *in vacuo* was dissolved in Benzene (2 mL) and added anhydrous $AlCl_3$ (0.5 mmol). The solution was stirred at 80 ℃ for another 6 h. After the intermediate was completely consumed (monitored by TLC analysis), the mixture was cooled to the room temperature, the reaction was quenched by the addition of H_2O (5 mL) and the organic compounds were extracted with ethyl acetate (5 mL ×3) for three times. The organic layers were washed with brine (10 mL ×2), dried over anhydrous Na_2SO_4, and the solvent was removed under reduced pressure. The obtained residue was purified by flash column chromatography on silica gel (eluent: petroleum ether/ ethyl acetate 10:1) to furnish the desired compound **4** (20.8 mg, 68% yield).

3.2 General procedure for the synthesis of the racemic compound 49

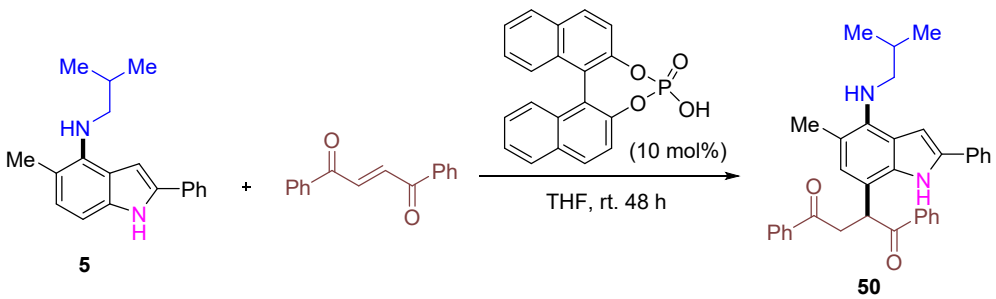


N-isobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine **5** (0.1 mmol, 1.0 equiv.) was added to a mixture of solution catalyst (*rac*)-CPA (0.01 mmol, 0.1 equiv.) and benzyl (*E*)-2-((*tert*-butoxycarbonyl)imino)-2-phenylacetate (0.15 mmol, 1.5 equiv.) in EA/CH_3CN (1.5 mL : 0.5 mL) at room temperature for 48 h. After completion (monitored by TLC), the mixture was directly purified by silica gel column chromatography (eluent: dichloromethane / petroleum ether = 4:1) to afford the compound **49**.

References:

(1) Y. Zhao, L. Cai, T. Huang, S. Meng, A. S. C. Chan and J Zhao. *Adv. Synth. Catal.*, 2020, **362**, 1309.

3.3 General procedure for the synthesis of the racemic compound 50



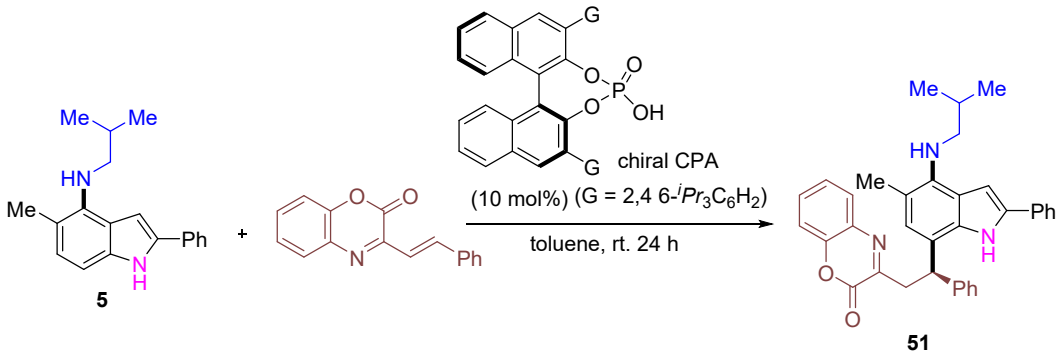
The (*E*)-1,4-diphenylbut-2-ene-1,4-dione (0.12 mmol, 1.2 equiv.) was added to a solution of catalyst (*rac*)-CPA (0.01 mmol, 0.1 equiv.) and *N*-isobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine **5** (0.1 mmol, 1.0 equiv.) in THF (2 mL) at room temperature for 48 h. After completion (monitored by TLC), the mixture was concentrated and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether /

ethyl acetate = 5:1) to afford the compound **50**.

References:

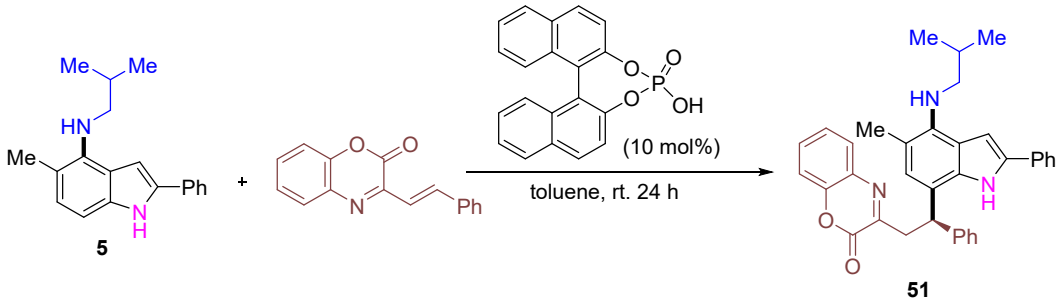
(2) T. Huang, Y. Zhao, S. Meng, A. S. C. Chan and J. Zhao. *Adv. Synth. Catal.*, 2019, **361**, 3632.

3.4 General procedure for the synthesis of the compound 51



The (*E*)-3-styryl-2*H*-benzo[*b*] [1,4] oxazin-2-one (0.12 mmol, 1.2 equiv.) was added to a solution of catalyst (S) or (R)-CPA (0.01 mmol, 0.1 equiv.) and *N*-isobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine **5** (0.1 mmol, 1.0 equiv.) in dry toluene (2 mL) at room temperature for 24 h. After completion (monitored by TLC), the mixture was concentrated and the residue was purified by flash chromatography on silica gel (eluent : petroleum ether / ethyl acetate = 5:1) to afford the title compound **51**.

3.5 General procedure for the synthesis of the racemic compounds 51

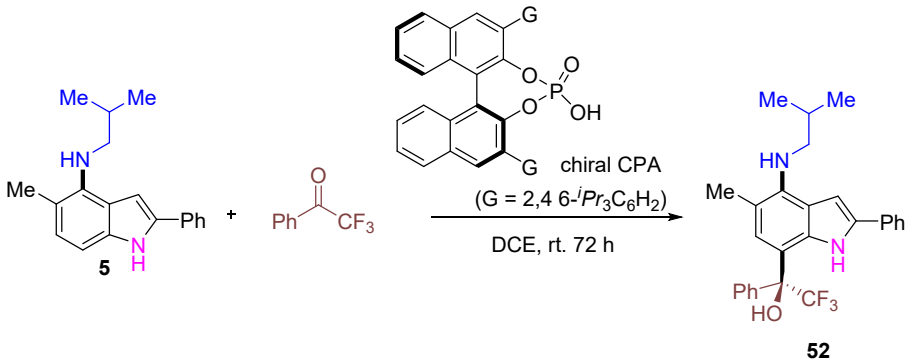


The (*E*)-3-styryl-2*H*-benzo[*b*][1,4]oxazin-2-one (0.12 mmol, 1.2 equiv.) was added to a solution of catalyst (*rac*)-CPA (0.01 mmol, 0.1 equiv.) and *N*-isobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine **5** (0.1 mmol, 1.0 equiv.) in dry toluene (2 mL) at room temperature for 24 h. After completion (monitored by TLC), the mixture was concentrated and the residue was purified by flash chromatography on silica gel (eluent : petroleum ether / ethyl acetate = 5:1) to afford the title compound **51**.

References:

(3) W. Xun, B. Xu, B. Chen, S. Meng, A. S. C. Chan, F. G. Qiu and J. Zhao, *Org. Lett.*, 2018, **20**, 590.

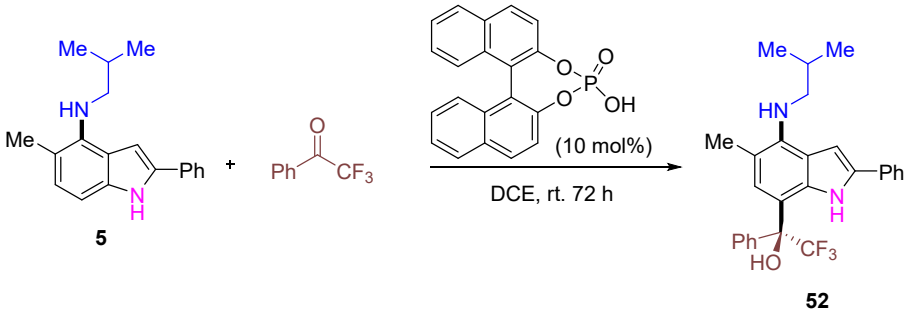
3.6 General procedure for the synthesis of the compound 52



2,2,2-trifluoro-1-phenylethan-1-one (0.15 mmol, 1.5 equiv.) was added to a solution of catalyst (S) or (R)-CPA (0.01 mmol, 0.1 equiv.) and *N*-isobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine **5** (0.1 mmol, 1.0 equiv.) in DCE (2 mL) at room temperature for 72 h. After completion (monitored by TLC), the mixture was concentrated and the residue was purified by flash chromatography on silica gel (eluent : dichloromethane /

petroleum ether = 2:1) to afford the compound **52**.

3.7 General procedure for the synthesis of the racemic compound 52

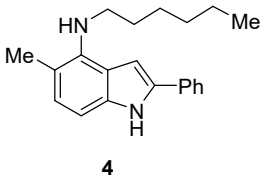


2,2,2-trifluoro-1-phenylethan-1-one (0.15 mmol, 1.5 equiv.) was added to a solution of catalyst (*rac*)-CPA (0.01 mmol, 0.1 equiv.) and *N*-isobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine **5** (0.1 mmol, 1.0 equiv.) in DCE (2 mL) at room temperature for 72 h. After completion (monitored by TLC), the mixture was concentrated and the residue was purified by flash chromatography on silica gel (eluent : dichloromethane / petroleum ether = 2:1) to afford the compound **52**.

References:

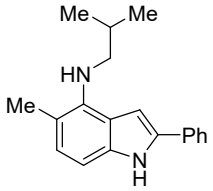
(4) L. Cai, Y. Zhao, T. Huang, S. Meng, X. Jia, A. S. C. Chan and J. Zhao, *Org. Lett.*, 2019, **21**, 3538.

3.8 Characterization of Products



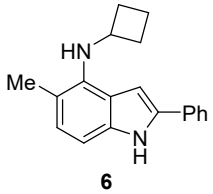
***N*-hexyl-5-methyl-2-phenyl-1*H*-indol-4-amine (4)** (eluent: petroleum ether/ethyl acetate 10:1), 20.8 mg, 68% yield; green solid, m.p. : 81-82 ℃; ^{1}H NMR (400 MHz,

$CDCl_3$) δ 8.22 (br s, 1H), 7.61 (d, *J* = 7.3 Hz, 2H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.26 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.91 (s, 1H), 6.79 (d, *J* = 8.1 Hz, 1H), 3.54 (t, *J* = 7.2 Hz, 2H), 3.02 (br s, 1H), 2.27 (s, 3H), 1.71 – 1.63 (m, 2H), 1.45 – 1.41 (m, 2H), 1.33 – 1.31 (m, 4H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 137.8, 135.9, 132.6, 128.9, 127.2, 125.9, 124.8, 119.8, 113.6, 101.9, 98.8, 48.0, 31.7, 31.1, 26.8, 22.6, 17.6, 14.0. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{21}H_{27}N_2$ 307.2169; Found : 307.2182.



5

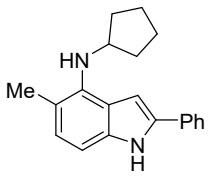
***N*-isobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine (5)** (eluent: petroleum ether/ethyl acetate 10:1), 17.5 mg, 63% yield; green solid, m.p. : 134-135 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.19 (br s, 1H), 7.61 (d, J = 7.3 Hz, 2H), 7.40 (t, J = 7.7 Hz, 2H), 7.27 (t, J = 7.4 Hz, 1H), 6.91 (d, J = 8.2 Hz, 1H), 6.90 (s, 1H), 6.79 (d, J = 8.1 Hz, 1H), 3.37 (d, J = 6.7 Hz, 2H), 2.28 (s, 3H), 2.00 – 1.88 (m, 1H), 1.03 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 137.8, 135.9, 132.6, 128.9, 127.2, 126.0, 124.8, 119.6, 113.3, 101.7, 98.8, 55.6, 29.4, 20.5, 17.6. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{23}N_2$ 279.1856; Found : 279.1876.



6

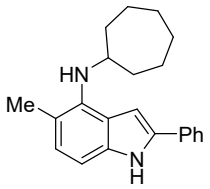
***N*-cyclobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine (6)** (eluent: petroleum ether/ethyl acetate 10:1), 18.2 mg, 66% yield; green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (br s, 1H), 7.63 (d, *J* = 7.4 Hz, 2H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.88 (d, *J* = 1.5 Hz, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 4.39

(p, J = 7.7 Hz, 1H), 3.14 (br s, 1H), 2.49 – 2.42 (m, 2H), 2.28 (s, 3H), 1.99 – 1.89 (m, 2H), 1.81 – 1.65 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 137.6, 136.0, 132.6, 128.9, 127.2, 125.8, 124.8, 119.6, 113.4, 101.9, 98.5, 52.4, 33.4, 17.7, 14.3. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{21}N_2$ 277.1699; Found : 277.1697.



7

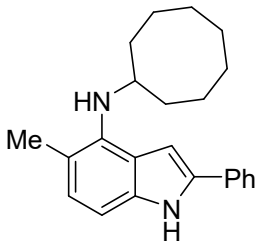
***N*-cyclopentyl-5-methyl-2-phenyl-1*H*-indol-4-amine (7)** (eluent: petroleum ether/ethyl acetate 10:1), 21.5 mg, 74% yield; green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (br s, 1H), 7.63 (d, J = 7.3 Hz, 2H), 7.41 (t, J = 7.7 Hz, 2H), 7.28 (t, J = 7.4 Hz, 1H), 6.92 (d, J = 8.1 Hz, 1H), 6.90 (d, J = 1.5 Hz, 1H), 6.82 (d, J = 8.1 Hz, 1H), 4.35 (p, J = 5.7 Hz, 1H), 2.78 (br s, 1H), 2.27 (s, 3H), 2.04 – 1.96 (m, 2H), 1.77 – 1.58 (m, 2H), 1.68 – 1.55 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.2, 137.6, 135.9, 132.6, 128.9, 127.2, 125.9, 124.8, 120.1, 114.1, 102.0, 98.8, 58.1, 34.5, 23.8, 17.8. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{20}H_{23}N_2$ 291.1856; Found : 291.1866.



8

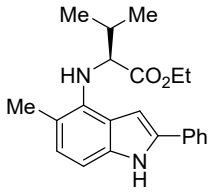
***N*-cycloheptyl-5-methyl-2-phenyl-1*H*-indol-4-amine (8)** (eluent: petroleum ether/ethyl acetate 10:1), 20.0 mg, 63% yield; green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (br s, 1H), 7.64 (d, J = 7.4 Hz, 2H), 7.42 (t, J = 7.7 Hz, 2H), 7.28 (t, J = 7.4 Hz, 1H), 6.93 (d, J = 8.1 Hz, 1H), 6.84 (d, J = 8.3 Hz, 1H), 6.82 (s, 1H), 3.92 – 3.86 (m, 1H), 2.74 (br s, 1H), 2.28 (s, 3H), 2.13 – 2.08 (m, 2H), 1.71 – 1.42 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 137.4, 136.0, 132.6, 128.9, 127.2, 125.9, 124.8, 120.9,

115.0, 102.5, 98.5, 57.3, 36.2, 28.4, 24.0, 17.8. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{27}N_2$ 319.2169; Found : 319.2189.



9

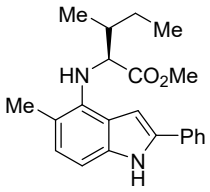
***N*-cyclooctyl-5-methyl-2-phenyl-1*H*-indol-4-amine (9)** (eluent: petroleum ether/ethyl acetate 10:1), 14.9 mg, 45% yield; green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (br s, 1H), 7.64 (d, *J* = 7.9 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.93 (d, *J* = 8.1 Hz, 1H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.82 (s, 1H), 3.97 – 3.87 (m, 1H), 2.28 (s, 3H), 2.03 – 1.97 (m, 2H), 1.72 – 1.55 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 137.4, 136.0, 132.7, 128.9, 127.2, 125.9, 124.9, 121.0, 115.2, 102.5, 98.5, 56.2, 33.2, 27.5, 25.7, 23.8, 17.8. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{29}N_2$ 333.2325; Found : 333.2337.



10

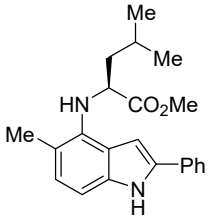
Ethyl (5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-valinate (10) (eluent: petroleum ether/ethyl acetate 5:1), 24.5 mg, 70% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (br s, 1H), 7.63 (d, *J* = 7.9 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.3 Hz, 1H), 6.84 (s, 1H), 4.36 (d, *J* = 5.6 Hz, 1H), 4.20 – 4.04 (m, 3H), 2.37 (s, 3H), 2.26 – 2.18 (m, 1H), 1.19 (t, *J* = 6.7 Hz, 3H), 1.18 (d, *J* = 6.7 Hz, 3H) 1.11 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 138.1, 137.4, 136.2, 132.5, 129.0, 127.3, 126.1, 124.9, 120.4, 115.4, 103.2, 98.1, 64.8, 60.7, 32.5, 18.9, 18.9, 17.5, 14.20. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for

$C_{22}H_{26}N_2O_2$ 350.1994; Found : 350.1991.



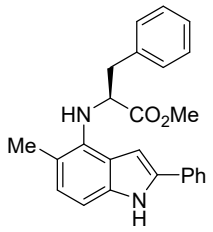
11

Methyl (5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-isoleucinate (11) (eluent: petroleum ether/ethyl acetate 5:1), 28.7 mg, 82% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (br s, 1H), 7.62 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.2 Hz, 1H), 6.82 (s, 1H), 4.45 (d, *J* = 5.8 Hz, 1H), 4.26 (br s, 1H), 3.64 (s, 3H), 2.36 (s, 3H), 2.04 – 1.94 (m, 1H), 1.84 – 1.77 (m, 1H), 1.42 – 1.33 (m, 1H), 1.05 (d, *J* = 7.0 Hz, 3H), 1.01 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 138.0, 137.4, 136.3, 132.5, 129.0, 127.4, 126.1, 124.9, 120.5, 115.6, 103.3, 98.0, 63.7, 51.6, 39.3, 25.9, 17.5, 15.4, 11.9. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{27}N_2O_2$ 351.2067; Found : 351.2077.



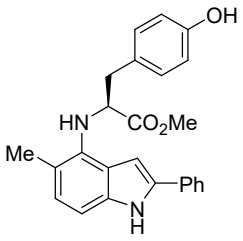
12

Methyl (5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-leucinate (12) (eluent: petroleum ether/ethyl acetate 5:1), 21.0 mg, 60% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (br s, 1H), 7.62 (d, *J* = 7.7 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.2 Hz, 1H), 6.82 (s, 1H), 4.55 (t, *J* = 7.1 Hz, 1H), 3.63 (s, 3H), 2.36 (s, 3H), 1.95 – 1.85 (m, 1H), 1.77 – 1.73 (m, 2H), 1.02 (d, *J* = 6.3 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 137.8, 137.3, 136.3, 132.5, 128.9, 127.3, 126.0, 124.9, 120.7, 115.8, 103.6, 97.8, 58.2, 51.8, 43.9, 25.0, 22.8, 22.7, 17.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{27}N_2O_2$ 351.2067; Found : 351.2085.



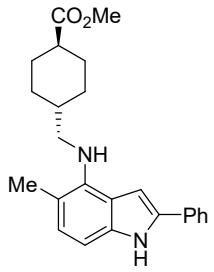
13

Methyl (5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-phenylalaninate (13) (eluent: petroleum ether/ethyl acetate 5:1), 21.9 mg, 57% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (br s, 1H), 7.55 (d, *J* = 7.7 Hz, 2H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.34 – 7.23 (m, 6H), 6.90 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.1 Hz, 1H), 6.49 (s, 1H), 4.73 (t, *J* = 6.2 Hz, 1H), 3.61 (s, 3H), 3.17 (t, *J* = 5.8 Hz, 2H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 137.6, 137.4, 137.2, 136.4, 132.5, 129.7, 129.0, 128.5, 127.4, 126.9, 126.0, 124.9, 120.9, 116.1, 103.7, 97.9, 61.1, 52.0, 40.6, 17.4. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{25}H_{25}N_2O_2$ 385.1911; Found : 385.1929.



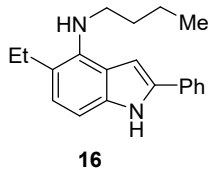
14

Methyl (5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-tyrosinate (14) (eluent: petroleum ether/ethyl acetate 2:1), 22.4 mg, 56% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (br s, 1H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.27 (t, *J* = 7.4 Hz, 1H), 7.09 (d, *J* = 8.2 Hz, 2H), 6.90 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.1 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 2H), 6.50 (s, 1H), 4.68 (t, *J* = 6.2 Hz, 1H), 3.61 (s, 3H), 3.10 (dd, *J* = 5.7 Hz, 3.5 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 154.6, 137.5, 137.3, 136.4, 132.4, 130.7, 129.0, 128.9, 127.4, 125.9, 124.9, 120.9, 116.0, 115.3, 103.6, 97.8, 61.1, 52.0, 39.5, 17.4. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{25}H_{25}N_2O_3$ 401.1860; Found : 401.1866.



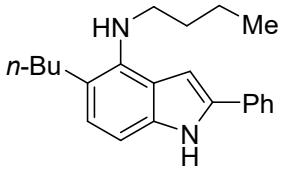
15

Methyl (1r, 4r)-4-(((5-methyl-2-phenyl-1*H*-indol-4-yl)amino)methyl)cyclohexane -1-carboxylate (15) (eluent: petroleum ether/ethyl acetate 5:1), 29.3 mg, 78% y ield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (br s, 1H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.86 (d, *J* = 1.3 Hz, 1H), 6.81 (d, *J* = 8.1 Hz, 1H), 3.66 (s, 3H), 3.39 (d, *J* = 6.5 Hz, 2H), 2.32 – 2.24 (m, 4H), 2.04 – 2.01 (m, 5H), 1.51 – 1.41 (m, 2H), 1.14 – 1.04 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.4, 13 9.6, 137.8, 136.0, 132.6, 128.9, 127.3, 125.9, 124.9, 119.7, 113.6, 102.0, 98.6, 54.1, 51.5, 43.4, 38.4, 30.2, 28.6, 17.6. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{29}N_2O_2$ 377.2224; Found : 377.2228.



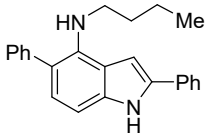
16

***N*-butyl-5-ethyl-2-phenyl-1*H*-indol-4-amine (16)** (eluent: petroleum ether/ethyl acetate 10:1), 22.2 mg, 76% yield; yellow solid. m.p. : 80-81 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (br s, 1H), 7.67 (d, *J* = 7.4 Hz, 2H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 8.2 Hz, 1H), 6.95 (d, *J* = 1.3 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 3.57 (t, *J* = 7.2 Hz, 2H), 3.19 (br s, 1H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.75 – 1.68 (m, 2H), 1.56 – 1.47 (m, 2H), 1.30 (t, *J* = 7.6 Hz, 3H), 1.01 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 137.6, 136.0, 132.7, 129.0, 128.7, 127.3, 124.9, 124.4, 120.4, 102.4, 99.1, 48.1, 33.5, 24.4, 20.4, 14.9, 14.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{20}H_{25}N_2$ 293.2012; Found : 293.2027.



17

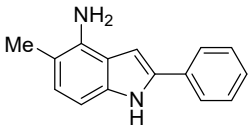
***N*, 5-dibutyl-2-phenyl-1*H*-indol-4-amine (17)** (eluent: petroleum ether/ethyl acetate 10:1), 18.9 mg, 59% yield; green solid. mp: 74-75 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (br s, 1H), 7.63 (d, *J* = 7.4 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 6.93 (d, *J* = 8.1 Hz, 1H), 6.91 (s, 1H), 6.85 (d, *J* = 8.1 Hz, 1H), 3.52 (t, *J* = 7.2 Hz, 2H), 2.94 (br s, 1H), 2.61 (t, *J* = 7.2 Hz, 2H), 1.71 – 1.64 (m, 2H), 1.64 – 1.56 (m, 2H), 1.52 – 1.38 (m, 4H), 0.98 (t, *J* = 7.3Hz, 3H), 0.95 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 137.6, 136.0, 132.7, 129.0, 127.3, 125.3, 124.90, 120.5, 119.2, 102.4, 99.1, 48.2, 33.4, 32.8, 31.3, 22.8, 20.4, 14.1, 14.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{29}N_2$ 321.2325; Found : 321.2328.



19

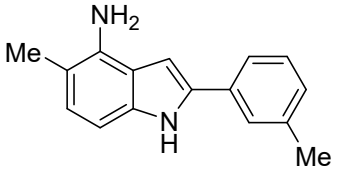
***N*-butyl-2,5-diphenyl-1*H*-indol-4-amine (19)** (eluent: petroleum ether/ethyl acetate 10:1), 15.6 mg, 46% yield; green oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (br s, 1H), 7.62 (d, *J* = 7.6 Hz, 2H), 7.44 - 7.38 (m, 6H), 7.35 – 7.26 (m, 2H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.96 (s, 1H), 6.88 (d, *J* = 8.2 Hz, 1H), 3.95 (br s, 1H), 3.44 (t, *J* = 7.1 Hz, 2H), 1.48 (dt, *J* = 14.7, 7.2 Hz, 2H), 1.28 (dq, *J* = 14.3, 7.3 Hz, 2H), 0.86 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 139.4, 138.3, 136.2, 132.5, 130.0, 128.9, 128.7, 127.3, 126.5, 125.7, 124.9, 120.7, 119.6, 102.1, 99.5, 47.7, 32.9, 20.1, 13.9. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{25}N_2$ 341.4775; Found : 341.4780.



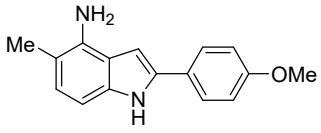
20

5-methyl-2-phenyl-1*H*-indol-4-amine (20): (eluent: petroleum ether/ethyl acetate 5:1), 17.1 mg, 77% yield; green solid; m.p. : 140-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (br s, 1H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 6.71 (d, *J* = 1.9 Hz, 1H), 3.90 (br s, 2H), 2.27 (s, 3H). 13C NMR (100 MHz, $CDCl_3$) δ 136.6, 136.5, 136.4, 132.5, 129.7, 127.0, 125.9, 124.8, 118.8, 111.1, 101.4, 95.9, 16.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{15}N_2$ 223.1230; Found : 223.1231.



21

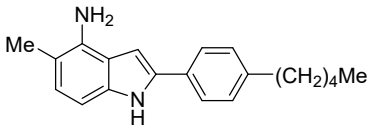
5-methyl-2-(m-tolyl)-1*H*-indol-4-amine (21) (eluent: petroleum ether/ethyl acetate 5:1), 13.0 mg, 55% yield; green solid; m.p. : 152-153 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.47 (s, 1H), 7.44 (d, *J* = 8.2 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 1H), 6.92 (d, *J* = 8.2 Hz, 1H), 6.80 (d, *J* = 8.2 Hz, 1H), 6.70 (dd, *J* = 2.1, 0.8 Hz, 1H), 3.90 (br s, 2H), 2.41 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 136.6, 136.5, 136.5, 132.5, 128.9, 128.1, 125.8, 125.6, 122.0, 118.8, 111.1, 101.4, 95.8, 21.5, 16.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{17}N_2$ 237.1386; Found : 237.1390.



22

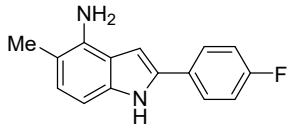
2-(4-methoxyphenyl)-5-methyl-1*H*-indol-4-amine (22) (eluent: petroleum ether/ethyl acetate 5:1), 13.6 mg, 54% yield; green solid; m.p. : 206-207 °C; ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 10.19 (br s, 1H), 7.72 (d, *J* = 8.6 Hz, 2H), 6.98 (d, *J* = 8.6 Hz,

2H), 6.83 (d, *J* = 1.2 Hz, 1H), 6.75 (d, *J* = 8.1 Hz, 1H), 6.65 (d, *J* = 8.1 Hz, 1H), 4.52 (br s, 2H), 3.82 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, $(CD_3)_2CO$) δ 159.0, 137.7, 137.2, 135.7, 126.1, 125.9, 125.1, 119.0, 114.3, 109.2, 100.4, 94.9, 54.8, 16.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{17}N_2O$ 253.1335; Found : 253.1350.



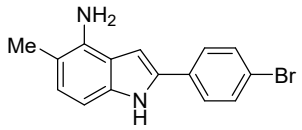
23

5-methyl-2-(4-pentylphenyl)-1*H*-indol-4-amine (23) (eluent: petroleum ether/ethyl acetate 5:1), 19.6 mg, 67% yield; green solid; m.p. : 193-194 °C; ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 10.28 (br s, 1H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 8.1 Hz, 2H), 6.95 (d, *J* = 1.4 Hz, 1H), 6.78 (d, *J* = 8.1 Hz, 1H), 6.66 (d, *J* = 8.2 Hz, 1H), 4.58 (br s, 2H), 2.64 (t, *J* = 7.6 Hz, 2H), 2.21 (s, 3H), 1.65 (dt, *J* = 14.8, 7.4 Hz, 2H) 1.38 – 1.33 (m, 4H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $(CD_3)_2CO$) δ 141.4, 137.8, 137.3, 135.8, 130.8, 128.8, 125.3, 124.5, 118.9, 109.2, 100.4, 95.6, 35.3, 31.4, 31.1, 22.3, 16.2, 13.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{20}H_{25}N_2$ 293.2012; Found : 293.2025.



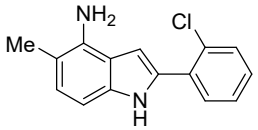
24

2-(4-fluorophenyl)-5-methyl-1*H*-indol-4-amine (24) (eluent: petroleum ether/ethyl acetate 5:1), 11.8 mg, 49% yield; green solid; m.p. : 193-194 °C; ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 10.30 (br s, 1H), 7.81 (dd, *J* = 8.5, 5.4 Hz, 2H), 7.18 (t, *J* = 8.7 Hz, 2H), 6.94 (d, *J* = 1.8 Hz, 1H), 6.79 (d, *J* = 8.1 Hz, 1H), 6.67 (d, *J* = 8.1 Hz, 1H), 4.57 (br s, 2H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $(CD_3)_2CO$) δ 161.8 (d, $^1J_{CF}$ = 244.1 Hz), 138.0, 137.4, 134.7, 129.9 (d, $^4J_{CF}$ = 3.0 Hz), 126.4 (d, $^3J_{CF}$ = 7.9 Hz), 125.7, 118.8, 115.6 (d, $^2J_{CF}$ = 21.8 Hz), 109.3, 100.4, 96.2, 16.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}FN_2$ 241.1136; Found : 241.1140.



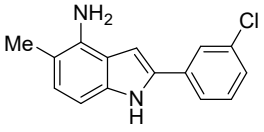
25

2-(4-bromophenyl)-5-methyl-1*H*-indol-4-amine (25) (eluent: petroleum ether/ethyl acetate 5:1), 16.9 mg, 56% yield; green solid; m.p. : 211-212 °C; ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 10.36 (br s, 1H), 7.75 – 7.71 (m, 2H), 7.58 – 7.55 (m, 2H), 7.02 (d, *J* = 1.6 Hz, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 6.67 (d, *J* = 8.1 Hz, 1H), 4.61 (br s, 2H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $(CD_3)_2CO$) δ 138.1, 137.6, 134.3, 132.5, 131.8, 126.3, 126.0, 119.6, 118.8, 109.3, 100.4, 97.0, 16.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}BrN_2$ 301.0335; Found : 301.0326.



26

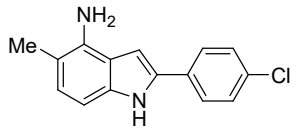
2-(2-chlorophenyl)-5-methyl-1*H*-indol-4-amine (26) (eluent: petroleum ether/ethyl acetate 5:1), 18.2 mg, 71% yield; green solid; m.p. : 190-191 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 br (s, 1H), 7.65 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.46 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.32 (td, *J* = 7.6, 1.4 Hz, 1H), 7.26 – 7.22 (m, 1H), 6.95 (d, *J* = 8.2 Hz, 1H), 6.82 (d, *J* = 8.2 Hz, 1H), 6.76 (dd, *J* = 2.2, 0.8 Hz, 1H), 3.92 (s, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.6, 136.1, 133.5, 131.3, 131.1, 130.8, 130.4, 128.4, 127.2, 126.2, 117.9, 110.9, 101.5, 99.6, 16.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}ClN_2$ 257.0840; Found : 257.0846.



27

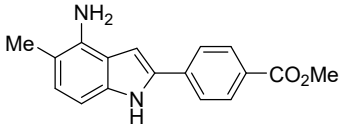
2-(3-chlorophenyl)-5-methyl-1*H*-indol-4-amine (27) (eluent: petroleum ether/ethyl acetate 5:1), 16.6 mg, 65% yield; green solid; m.p. : 184-185 °C; ^{1}H NMR (400 MHz,

$(CD_3)_2CO$) δ 10.40 (br s, 1H), 7.81 (t, *J* = 1.8 Hz, 1H), 7.74 (ddd, *J* = 7.9, 1.7, 1.0 Hz, 1H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.26 (ddd, *J* = 8.0, 2.1, 0.9 Hz, 1H), 7.08 (dd, *J* = 2.3, 0.8 Hz, 1H), 6.81 (d, *J* = 8.1 Hz, 1H), 6.68 (d, *J* = 8.1 Hz, 1H), 4.62 (br s, 2H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $(CD_3)_2CO$) δ 138.2, 137.6, 135.3, 134.4, 133.8, 130.5, 126.2, 124.1, 122.8, 118.7, 109.3, 100.3, 97.5, 16.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}ClN_2$ 257.0840; Found : 257.0848.



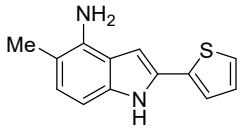
28

2-(4-chlorophenyl)-5-methyl-1*H*-indol-4-amine (28) (eluent: petroleum ether/ethyl acetate 5:1), 20.0 mg, 78% yield; green solid; m.p. : 187-188 ℃; ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 10.37 (br s, 1H), 7.79 (d, *J* = 8.5 Hz, 2H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.01 (d, *J* = 1.7 Hz, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 6.67 (d, *J* = 8.1 Hz, 1H), 4.61 (br s, 2H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $(CD_3)_2CO$) δ 137.7, 137.2, 133.9, 131.8, 131.3, 128.5, 126.0, 125.6, 118.4, 108.9, 100.0, 96.6, 15.8. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}ClN_2$ 257.0840; Found : 257.0849.



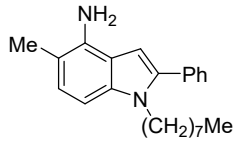
29

Methyl 4-(4-amino-5-methyl-1*H*-indol-2-yl)benzoate (29) (eluent: petroleum ether/ethyl acetate 2:1), 17.6 mg, 63% yield; yellow solid; m.p. : 217-218 ℃; ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 10.49 (br s, 1H), 8.03 (d, *J* = 8.4 Hz, 2H), 7.90 (d, *J* = 8.3 Hz, 2H), 7.18 (d, *J* = 1.2 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 6.69 (d, *J* = 8.1 Hz, 1H), 4.70 (br s, 2H), 3.89 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 166.1, 138.3, 137.9, 137.5, 134.2, 130.0, 127.8, 126.6, 124.1, 118.8, 109.3, 1493900.4, 98.5, 51.4, 16.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{17}N_2O_2$ 281.1285; Found: 281.1299.



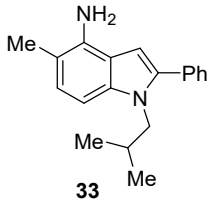
30

5-methyl-2-(thiophen-2-yl)-1*H*-indol-4-amine (28) (eluent: petroleum ether/ethyl acetate 5:1), 12.1 mg, 53% yield; green solid; m.p.: 180-181 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (br s, 1H), 7.24 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.20 (dd, *J* = 3.6, 1.0 Hz, 1H), 7.06 (dd, *J* = 5.0, 3.6 Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 6.76 (d, *J* = 8.1 Hz, 1H), 6.60 (d, *J* = 2.0 Hz, 1H), 3.91 (br s, 1H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5 , 136.2, 135.9, 130.8, 127.8, 126.0, 124.0, 122.3, 118.6, 111.3, 101.3, 96.5, 16.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{13}N_2S$ 229.0794; Found : 229.0798.



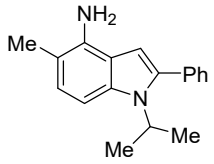
32

5-methyl-1-octyl-2-phenyl-1*H*-indol-4-amine (32) (eluent: petroleum ether/ethyl acetate 10:1), 21.0 mg, 63% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.40 (m, 5H), 6.99 (d, *J* = 8.2 Hz, 1H), 6.81 (d, *J* = 8.2 Hz, 1H), 6.41 (s, 1H), 4.11 (t, *J* = 7.6 Hz, 2H), 2.32 (s, 3H), 1.72 – 1.64 (m, 2H), 1.29 – 1.18 (m, 10H), 0.88 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.9, 137.2, 136.5, 133.6, 129.4, 128.4, 127.7, 125.0, 117.6, 110.8, 100.8, 97.9, 44.1, 31.8, 29.9, 29.1, 29.0, 26.8, 22.6, 16.7, 14.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{31}N_2$ 335.2482; Found : 335.2499.



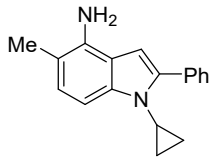
33

1-isobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine (33) (eluent: petroleum ether/ethyl acetate 10:1), 16.1 mg, 58% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.34 (m, 5H), 6.94 (d, *J* = 8.3 Hz, 1H), 6.77 (d, *J* = 8.2 Hz, 1H), 6.36 (s, 1H), 3.95 (d, *J* = 7.5 Hz, 2H), 3.77 (br s, 2H), 2.27 (s, 3H), 2.08 – 1.93 (m, 1H), 0.63 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 137.4, 136.4, 133.8, 129.5, 128.3, 127.5, 124.8, 117.5, 110.7, 101.2, 98.1, 51.3, 28.8, 20.0, 16.6. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{23}N_2$ 279.1856; Found : 279.1869.



34

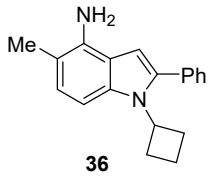
1-isopropyl-5-methyl-2-phenyl-1*H*-indol-4-amine (34) (eluent:petroleum ether/ethyl acetate 10:1), 18.7 mg, 71% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.36 (m, 5H), 7.00 (d, *J* = 8.3 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 6.31 (s, 1H), 4.62 (hept, *J* = 7.0 Hz, 1H), 3.77 (br s, 2H), 2.27 (s, 3H), 1.58 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.9, 136.7, 135.1, 133.9, 129.5, 128.3, 127.7, 124.4, 118.4, 110.5, 103.2, 97.9, 47.8, 21.4, 16.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{21}N_2$ 265.1699; Found : 265.1704.



35

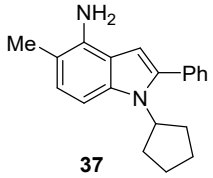
1-cyclopropyl-5-methyl-2-phenyl-1*H*-indol-4-amine (35) (eluent: petroleum ether/ethyl acetate 10:1), 15.7 mg, 60% yield, green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.1 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 1H), 6.98 (d, *J* = 8.3 Hz, 1H), 6.95 (d, *J* = 8.3 Hz, 1H), 6.38 (s, 1H), 3.79 (br s, 2H), 3.41 – 3.36 (m, 1H), 2.27 (s, 3H), 0.93 – 0.89 (m, 2H), 0.66 – 0.62 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 138.7, 136.5, 133.7, 128.6, 128.1, 127.1, 125.0, 117.0, 111.0, 101.7, 97.7, 26.2,

16.6, 9.0. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}N_2$ 263.1543; Found : 263.1557.



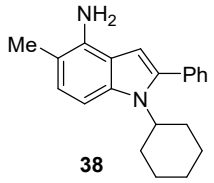
36

1-cyclobutyl-5-methyl-2-phenyl-1*H*-indol-4-amine (36) (eluent: petroleum ether/ethyl acetate 10:1), 17.9 mg, 65% yield, green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.35 (m, 5H), 7.13 (d, *J* = 8.3 Hz, 1H), 6.94 (d, *J* = 8.3 Hz, 1H), 6.31 (s, 1H), 4.94 (p, *J* = 8.9 Hz, 1H), 3.83 (br s, 2H), 3.00 – 2.90 (m, 2H), 2.33 – 2.27 (m, 5H), 1.94 – 1.86 (m, 1H), 1.79 – 1.67 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 136.8, 136.3, 133.8, 129.3, 128.3, 127.6, 124.6, 118.2, 110.7, 102.9, 98.0, 50.9, 29.5, 16.5, 14.4. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{21}N_2$ 277.1699; Found : 277.1698.



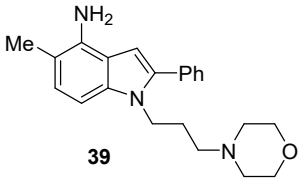
37

1-cyclopentyl-5-methyl-2-phenyl-1*H*-indol-4-amine (37) (eluent: petroleum ether/ethyl acetate 10:1), 16.8 mg, 58% yield, green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.36 (m, 5H), 6.91 (d, *J* = 8.4 Hz, 1H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.32 (s, 1H), 4.74 (p, *J* = 9.0 Hz, 1H), 3.84 (br s, 2H), 2.43 – 2.33 (m, 2H), 2.27 (s, 3H), 1.97 – 1.91 (m, 4H), 1.67 – 1.64 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 136.9, 134.6, 133.9, 129.4, 128.4, 127.6, 124.4, 118.4, 110.5, 102.8, 97.7, 57.1, 29.9, 25.2, 16.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{20}H_{23}N_2$ 291.1856; Found : 291.1879.



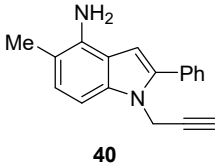
38

1-cyclohexyl-5-methyl-2-phenyl-1*H*-indol-4-amine (38) (eluent: petroleum ether/ethyl acetate 10:1), 18.5 mg, 61% yield, green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.36 (m, 5H), 7.04 (d, *J* = 8.4 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.32 (s, 1H), 4.19 – 4.11 (m, 1H), 3.80 (br s, 2H), 2.38 – 2.32 (m, 2H), 2.26 (s, 3H), 1.89 – 1.86 (m, 4H), 1.27 – 1.20 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 136.6, 135.5, 134.0, 129.5, 128.3, 127.6, 124.3, 118.4, 110.4, 103.5, 98.0, 56.3, 31.3, 26.2, 25.5, 16.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{21}H_{25}N_2$ 305.2012; Found : 305.2036.



39

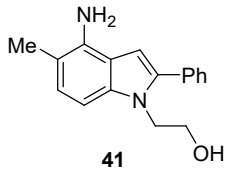
5-methyl-1-(3-morpholinopropyl)-2-phenyl-1*H*-indol-4-amine (39) (eluent: petroleum ether/ethyl acetate 5:1), 20.9 mg, 60% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.37 (m, 5H), 6.95 (d, *J* = 8.3 Hz, 1H), 6.79 (d, *J* = 8.2 Hz, 1H), 6.39 (s, 1H), 4.20 (t, *J* = 7.2 Hz 2H), 3.60 – 3.58 (m, 4H), 2.28 (s, 3H), 2.23 – 2.20 (m, 4H), 2.16 (t, *J* = 6.9 Hz, 2H), 1.80 – 1.73 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 137.3, 136.5, 133.4, 129.3, 128.4, 127.7, 125.0, 117.6, 110.8, 100.6, 98.2, 66.8, 55.5, 53.3, 41.8, 26.5, 16.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{28}N_3O$ 350.2227; Found : 350.2238.



40

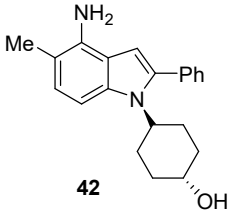
5-methyl-2-phenyl-1-(prop-2-yn-1-yl)-1*H*-indol-4-amine (40) (eluent: petroleum

ether/ethyl acetate 10:1), 17.9 mg, 69% yield, white-off solid, mp: 121-122 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.1 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.02 (d, *J* = 8.2 Hz, 1H), 6.89 (d, *J* = 8.2 Hz, 1H), 6.45 (s, 1H), 4.76 (d, *J* = 2.4 Hz, 2H), 3.87 (br s, 2H), 2.34 (t, *J* = 2.4 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 137.4, 136.6, 132.4, 129.1, 128.7, 127.9, 125.6, 117.5, 111.7, 100.5, 98.5, 79.1, 72.5, 34.2, 16.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{17}N_2$ 261.1386; Found : 260.1390.



41

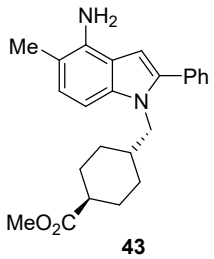
2-(4-amino-5-methyl-2-phenyl-1*H*-indol-1-yl)ethan-1-ol (41) (eluent: petroleum ether/ethyl acetate 2:1), 18.1 mg, 68% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.48 (m, 2H), 7.43 – 7.34 (m, 3H), 6.93 (d, *J* = 8.3 Hz, 1H), 6.77 (d, *J* = 8.2 Hz, 1H), 6.35 (s, 1H), 4.20 (t, *J* = 5.9 Hz, 2H), 3.73 (t, *J* = 5.9 Hz, 2H), 2.23 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 137.4, 136.4, 133.0, 129.6, 128.5, 127.8, 125.3, 117.6, 111.2, 100.7, 98.5, 61.4, 46.0, 16.6. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{19}N_2O$ 267.1492; Found : 267.1501.



42

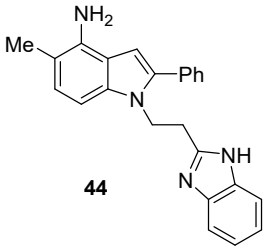
(1s,4s)-4-(4-amino-5-methyl-2-phenyl-1*H*-indol-1-yl)cyclohexan-1-ol (42) (eluent: petroleum ether/ethyl acetate 2:1), 19.2 mg, 60% yield, white-off solid, mp: 95-96 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.38 (m, 5H), 6.94 (d, *J* = 8.4 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.33 (s, 1H), 4.23 – 4.14 (m, 1H), 3.79 – 3.71 (m, 1H), 2.52 – 2.41 (m, 2H), 2.26 (s, 3H), 2.07 – 2.04 (m, 2H), 1.89 – 1.86 (m, 2H), 1.37 – 1.25 (m, 2H). ^{13}C

NMR (100 MHz, $CDCl_3$) δ 140.1, 136.7, 135.3, 133.7, 129.4, 128.4, 127.8, 124.5, 118.3, 110.6, 103.2, 98.3, 69.8, 55.2, 34.9, 28.8, 16.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{21}H_{25}N_2O$ 321.1961; Found : 321.1977.



43

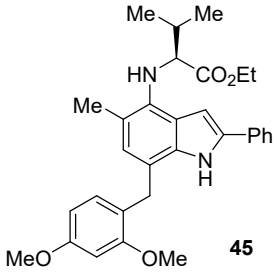
Methyl (1r,4r)-4-((4-amino-5-methyl-2-phenyl-1*H*-indol-1yl)methyl)cyclohexane-1-carboxylate (43) (eluent: petroleum ether/ethyl acetate 5:1), 26.3 mg, 70% yield, yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.41 (m, 5H), 6.99 (d, *J* = 8.2 Hz, 1H), 6.79 (d, *J* = 8.2 Hz, 1H), 6.41 (s, 1H), 4.03 (d, *J* = 7.3 Hz, 2H), 3.90 (br s, 2H), 3.62 (s, 3H), 2.32 (s, 3H), 2.16 – 2.06 (m, 2H), 1.86 – 1.83 (m, 2H), 1.49 – 1.46 (m, 2H), 1.27 – 1.17 (m, 2H), 0.79 – 0.69 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 140.1, 137.5, 136.4, 133.6, 129.5, 128.4, 127.6, 124.9, 117.5, 110.8, 101.0, 98.2, 51.4, 49.8, 42.9, 37.4, 29.7, 28.2, 16.6. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{29}N_2O_2$ 377.2224; Found : 377.2225.



44

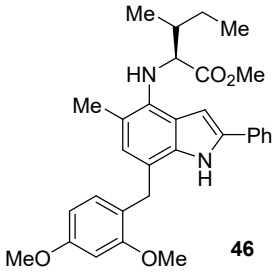
1-(2-(1*H*-benzo[d]imidazol-2-yl)ethyl)-5-methyl-2-phenyl-1*H*-indol-4-amine (44) (eluent: dichloromethane/methanol 10:1), 20.1 mg, 55% yield, yellow solid, m.p. : 200-201°C; ^1H NMR (400 MHz, CD_3OD) δ 7.38 – 7.33 (m, 2H), 7.26 – 7.13 (m, 8H), 6.89 (d, *J* = 8.2 Hz, 1H), 6.85 (d, *J* = 8.2 Hz, 1H), 6.43 (s, 1H), 4.59 (t, *J* = 6.9 Hz, 2H), 3.11 (t, *J* = 6.9 Hz, 2H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, CD_3OD) δ 153.5, 141.1, 139.7,

138.8, 138.4, 134.5, 130.4, 129.7, 128.8, 126.7, 123.6, 120.1, 115.7, 113.2, 102.1, 100.6, 44.1, 30.5, 17.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{24}H_{23}N_4$ 367.1917; Found : 367.1938.



45

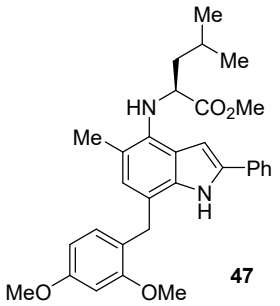
Ethyl (7-(2,4-dimethoxybenzyl)-5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-valinate (45) (eluent: petroleum ether/ethyl acetate 5:1), 30.0 mg, 60% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (br s, 1H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.13 (d, *J* = 8.3 Hz, 1H), 6.84 (s, 1H), 6.78 (s, 1H), 6.51 (s, 1H), 6.42 (d, *J* = 8.4 Hz, 1H), 4.27 (d, *J* = 5.7 Hz, 1H), 4.14 – 4.03 (m, 3H), 4.00 (s, 5H), 3.74 (s, 3H), 2.37 (s, 3H), 2.21 – 2.16 (m, 1H), 1.17 (t, *J* = 6.4 Hz, 3H), 1.16 (d, *J* = 6.5 Hz, 3H), 1.09 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 159.2, 156.6, 136.5, 136.2, 135.8, 133.1, 131.3, 128.9, 127.0, 126.0, 124.7, 121.5, 120.7, 117.0, 115.4, 105.6, 99.0, 98.0, 64.9, 60.5, 56.2, 55.4, 32.4, 30.4, 18.9, 17.5, 14.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{31}H_{37}N_2O_4$ 501.2748; Found : 501.2748.



46

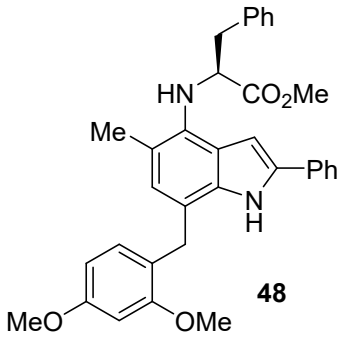
Methyl (7-(2,4-dimethoxybenzyl)-5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-isoleucinate (46) (eluent: petroleum ether/ethyl acetate 5:1), 33.0 mg, 66% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (br s, 1H), 7.65 (d, *J* = 7.5 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 6.89 (s, 1H), 6.82

(s, 1H), 6.56 (d, *J* = 1.7 Hz, 1H), 6.47 (d, *J* = 8.4, 1H), 4.42 (d, *J* = 5.8 Hz, 1H), 4.19 (s, 2H), 4.05 (s, 2H), 4.04 (s, 3H), 3.78 (s, 3H), 3.67 (s, 3H), 2.41 (s, 3H), 2.02 – 1.95 (m, 1H), 1.88 – 1.79 (m, 1H), 1.45 – 1.36 (m, 1H), 1.09 (d, *J* = 7.0 Hz, 3H), 1.05 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 159.2, 156.7, 136.3, 136.1, 135.9, 133.1, 131.3, 128.9, 127.0, 126.0, 124.8, 121.5, 120.9, 117.1, 115.6, 105.6, 99.1, 97.9, 63.8, 56.2, 55.3, 51.5, 39.3, 30.4, 25.9, 17.4, 15.4. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{31}H_{37}N_2O_4$ 501.2748; Found : 501.2765.



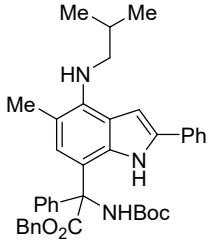
47

Methyl (7-(2,4-dimethoxybenzyl)-5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-leucinate (47) (eluent: petroleum ether/ethyl acetate 5:1), 31.0 mg, 62% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (br s, 1H), 7.59 (d, *J* = 7.7 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 6.84 (s, 1H), 6.76 (s, 1H), 6.51 (s, 1H), 6.43 (d, *J* = 8.3 Hz, 1H), 4.45 (t, *J* = 7.1 Hz, 1H), 4.00 (s, 5H), 3.73 (s, 3H), 3.61 (s, 3H), 2.35 (s, 3H), 1.93 – 1.83 (m, 1H), 1.74 – 1.68 (m, 2H), 1.01 (d, *J* = 6.5 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 159.3, 156.7, 136.2, 136.1, 136.0, 133.1, 131.3, 128.9, 127.1, 126.0, 124.8, 121.5, 121.1, 117.4, 115.9, 105.6, 99.1, 97.8, 58.4, 56.2, 55.4, 51.7, 43.9, 30.4, 25.1, 22.9, 22.7, 17.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{31}H_{37}N_2O_4$ 501.2748; Found : 501.2750.



48

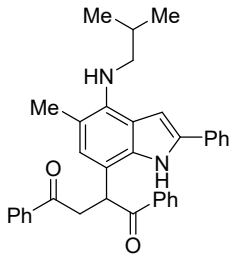
Methyl (7-(2,4-dimethoxybenzyl)-5-methyl-2-phenyl-1*H*-indol-4-yl)-*L*-phenylalaninate (48) (eluent: petroleum ether/ethyl acetate 5:1), 27.2 mg, 51% yield, yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (br s, 1H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.32 – 7.23 (m, 6H), 7.12 (d, *J* = 8.3 Hz, 1H), 6.82 (s, 1H), 6.50 (d, *J* = 1.6 Hz, 1H), 6.43-4.60 (m, 2H), 4.62 (t, *J* = 6.4 Hz, 1H), 3.98 (s, 5H), 3.72 (s, 3H), 3.59 (s, 3H), 3.18 – 3.09 (m, 2H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 159.3, 156.7, 137.3, 136.1, 136.0, 135.9, 133.0, 131.3, 129.6, 128.8, 128.3, 127.0, 126.8, 125.9, 124.7, 121.5, 121.2, 117.6, 116.1, 105.6, 99.1, 97.8, 61.4, 56.2, 55.3, 51.8, 40.6, 30.4, 17.3. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{34}H_{35}N_2O_4$ 535.2591; Found : 535.2597.



49

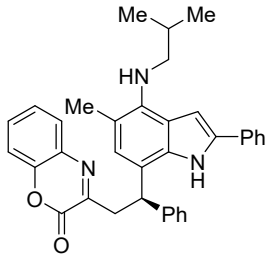
benzyl 2-((*tert*-butoxycarbonyl)amino)-2-(4-(isobutylamino)-5-methyl-2-phenyl-1*H*-indol-7-yl)-2-phenylacetate (49) (eluent: dichloromethane / petroleum ether 4:1), 40.1 mg, 65% yield, green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (br s, 1H), 7.57 - 7.45 (m, 2H), 7.34 – 7.27 (m, 7H), 7.23 – 7.18 (m, 4H), 7.16 – 7.12 (m, 2H), 6.82 (d, *J* = 1.7 Hz, 1H), 6.66 (s, 1H), 6.15 (s, 1H), 5.26 (s, 1H), 5.20 (q, *J* = 12.3 Hz, 2H), 3.39 (d, *J* = 6.7 Hz, 2H), 2.14 (s, 3H), 1.98 – 1.88 (m, 1H), 1.32 (s, 9H), 1.04 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 154.8, 140.5, 135.78, 135.0, 134.8, 132.3, 128.8, 128.4, 128.2, 128.2, 127.8, 127.7, 127.0, 125.2, 124.6, 112.6, 111.9, 97.8, 80.2,

68.7, 67.9, 55.2, 29.5, 28.2, 20.4, 17.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{39}H_{44}N_3O_4$ 618.3326; Found : 618.2248.



50

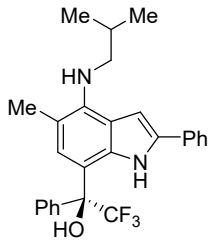
2-(4-(isobutylamino)-5-methyl-2-phenyl-1*H*-indol-7-yl)-1,4-diphenylbutane-1,4-dione (50) (eluent: petroleum ether/ethyl acetate 5:1), 45.7 mg, 89% yield, green oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.57 (s, 1H), 8.13 (d, *J* = 7.4 Hz, 2H), 7.94 (d, *J* = 7.9 Hz, 2H), 7.74 (d, *J* = 7.4 Hz, 2H), 7.53 – 7.37 (m, 9H), 7.29 (t, *J* = 7.4 Hz, 1H), 6.90 (d, *J* = 2.0 Hz, 1H), 6.88 (s, 1H), 5.49 (dd, *J* = 9.7, 3.9 Hz, 1H), 4.48 (dd, *J* = 18.4, 9.8 Hz, 1H), 3.44 (dd, *J* = 18.5, 3.9 Hz, 1H), 3.35 (d, *J* = 6.7 Hz, 2H), 2.23 (s, 3H), 1.96 – 1.85 (m, 1H), 1.02 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.4, 199.0, 139.8, 136.8, 136.5, 136.3, 136.2, 133.3, 133.0, 132.5, 129.0, 129.0, 128.6, 128.5, 128.2, 127.3, 126.8, 124.9, 120.4, 113.6, 110.0, 98.5, 55.3, 46.4, 41.9, 29.5, 20.4, 17.6. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{35}H_{35}N_2O_2$ 515.2693; Found : 515.2689.



51

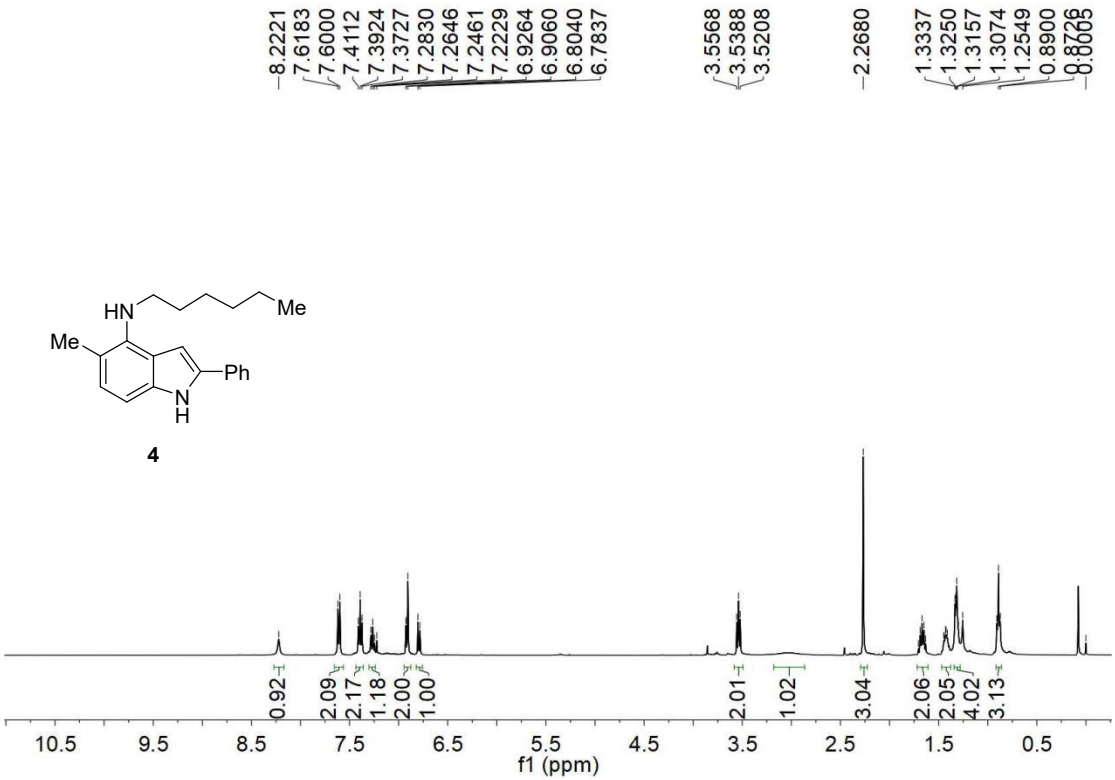
(*R*)-3-(2-(4-(isobutylamino)-5-methyl-2-phenyl-1*H*-indol-7-yl)-2-phenylethyl)-2*H*-benzo[b][1,4]oxazin-2-one (51) (eluent: petroleum ether/ethyl acetate 5:1), 41.1 mg, 78% yield, 99% *ee*, green oil; The enantiomeric excess was determined by HPLC (Daicel Chiralpak AD, hexane/*i*-PrOH = 80:20 (v/v), λ = 254 nm, flow rate = 1.0 mL/min, 25 °C): t_{major} = 37.4 min, t_{minor} = 39.8 min, 60.0 min. ^{1}H NMR (400 MHz,

$CDCl_3$) δ 9.44 (br s, 1H), 7.76 (d, *J* = 7.5 Hz, 2H), 7.65 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.51 – 7.39 (m, 5H), 7.37 – 7.19 (m, 7H), 6.92 (d, *J* = 2.0 Hz, 1H), 6.50 (s, 1H), 5.08 (dd, *J* = 10.0, 4.3 Hz, 1H), 3.82 (dd, *J* = 14.5, 4.3 Hz, 1H), 3.64 (dd, *J* = 14.5, 10.1 Hz, 1H), 3.34 (d, *J* = 6.7 Hz, 2H), 2.18 (s, 3H), 1.97 – 1.86 (m, 1H), 1.03 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.0, 153.9, 146.2, 141.1, 138.8, 136.1, 132.7, 131.2, 130.8, 129.0, 128.9, 128.8, 128.5, 127.1, 126.8, 125.6, 124.7, 124.3, 119.8, 117.9, 116.3, 112.9, 98.7, 55.6, 43.5, 39.9, 29.5, 20.5, 17.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{35}H_{34}N_3O_2$ 528.2646; Found : 528.2650.



52

(*S*)-2,2,2-trifluoro-1-(4-(isobutylamino)-5-methyl-2-phenyl-1*H*-indol-7-yl)-1-phenylethan-1-ol (52) (eluent: dichloromethane / petroleum ether 2:1), 42.9 mg, 95% yield, 77% *ee*, green oil; The enantiomeric excess was determined by HPLC (Daicel Chiralpak AD, hexane/*i*-PrOH = 80:20 (v/v), λ = 254 nm, flow rate = 1.0 mL/min, 25 ^{o}C): t_{major} = 7.4 min, t_{minor} = 10.5 min, 30.0 min. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.63 -7.58 (m, 2H), 7.41 – 7.24 (m, 8H), 7.19-7.16 (m, 1H), 6.92 (s, 1H), 6.64 (d, *J* = 2.0 Hz, 1H), 4.41 (s, 1H), 3.73 (s, 1H), 3.73 – 3.24 (m, 2H), 2.20 (s, 3H), 1.97 – 1.87 (m, 1H), 1.03 (d, *J* = 6.5 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 138.7, 135.6, 135.3, 132.1, 128.8, 128.7, 128.2, 127.5, 127.1, 124.5 (q, *J* = 286.3 Hz), 124.6, 124.2, 120.2, 112.4, 111.9, 97.6, 79.8 (q, *J* = 28.9 Hz), 55.5, 29.3, 20.5, 17.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{27}H_{28}F_3N_2O$ 453.2148; Found : 453.2153.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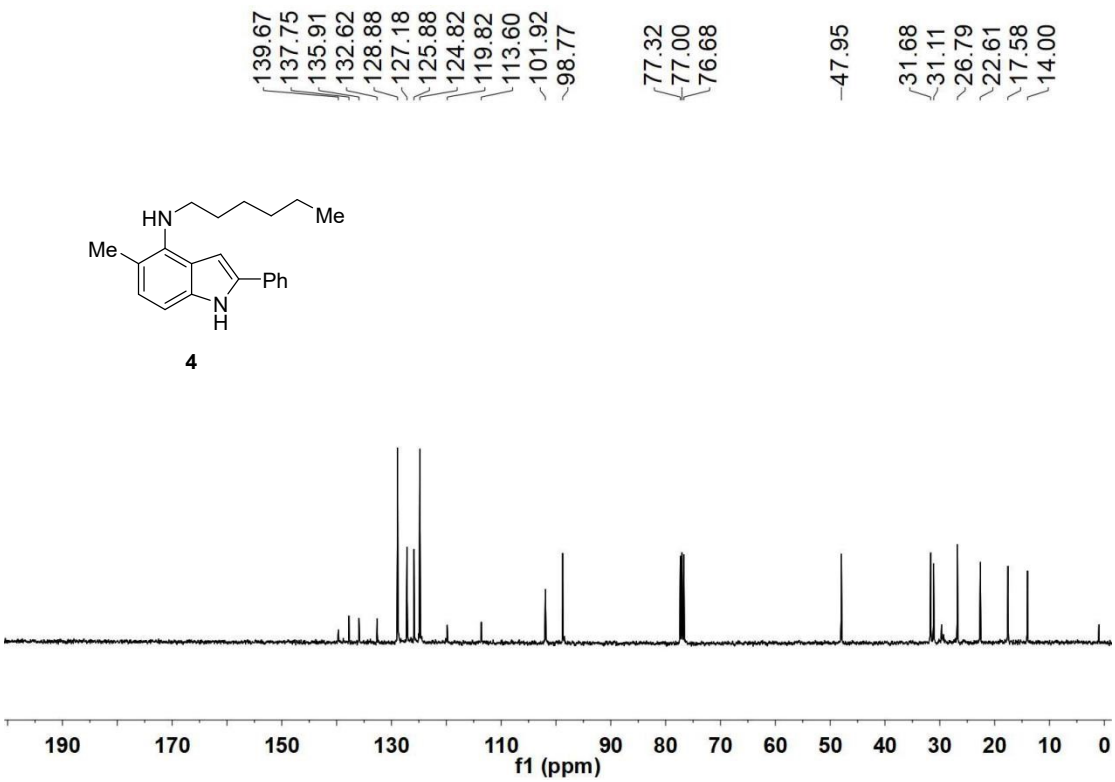
4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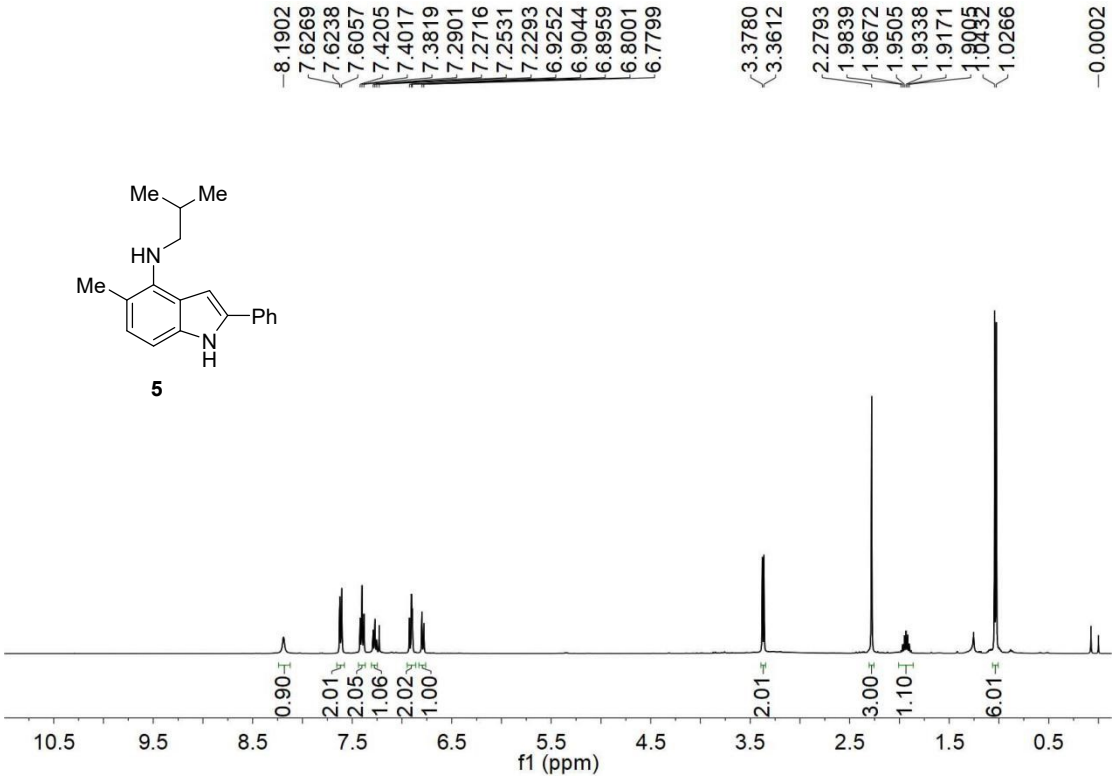
f1 (ppm)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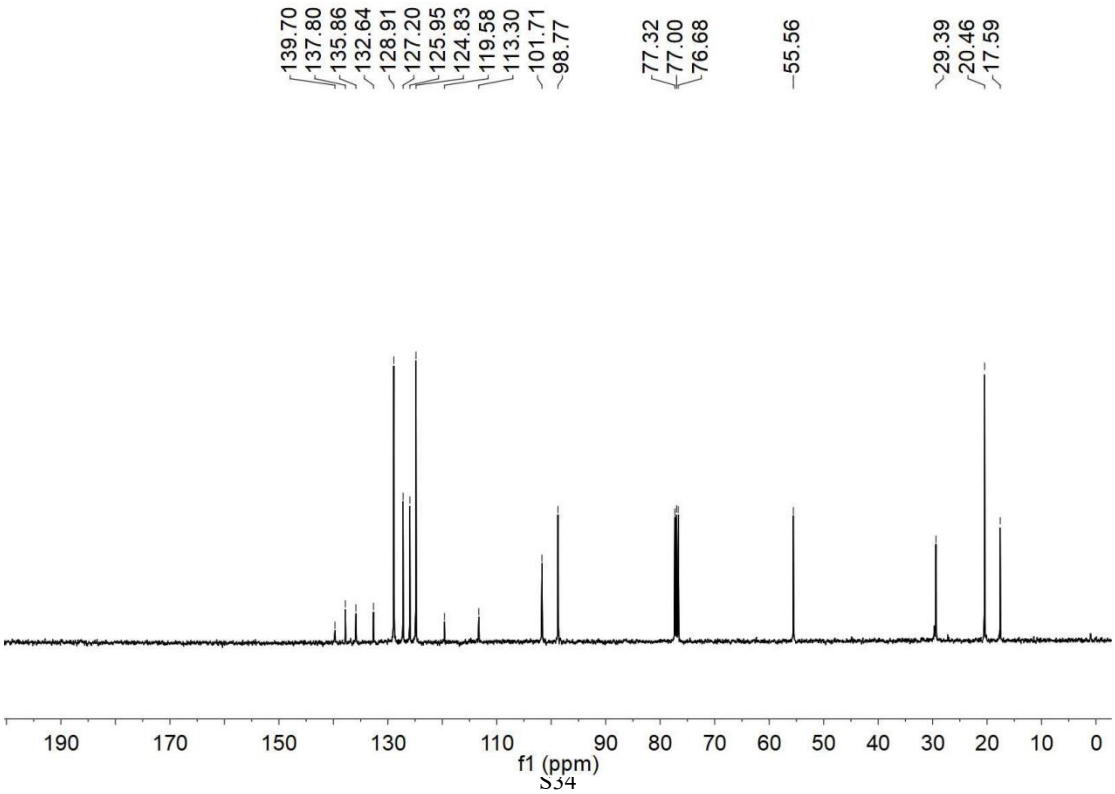
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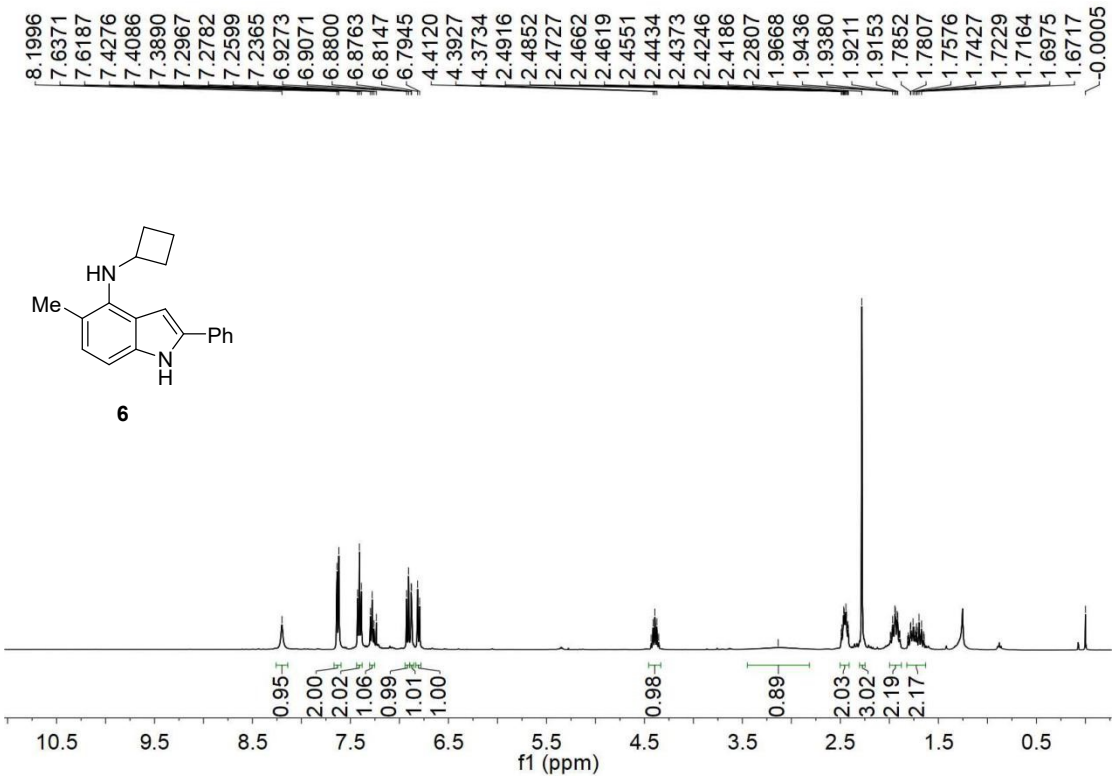
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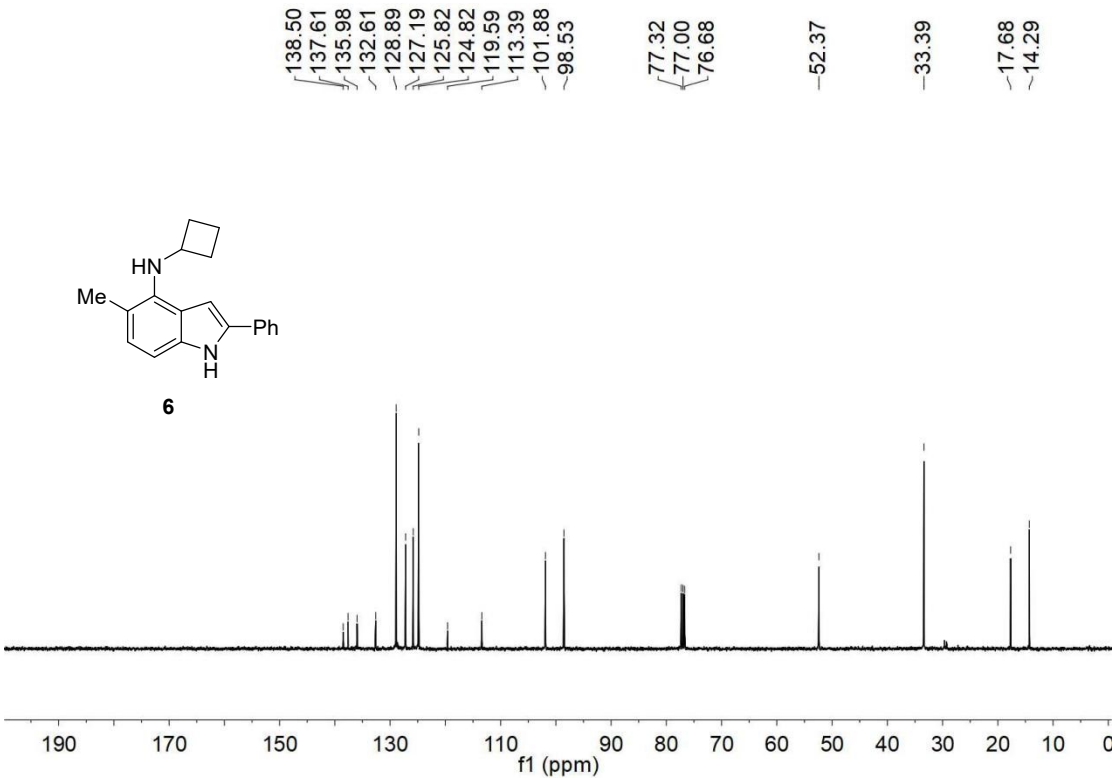
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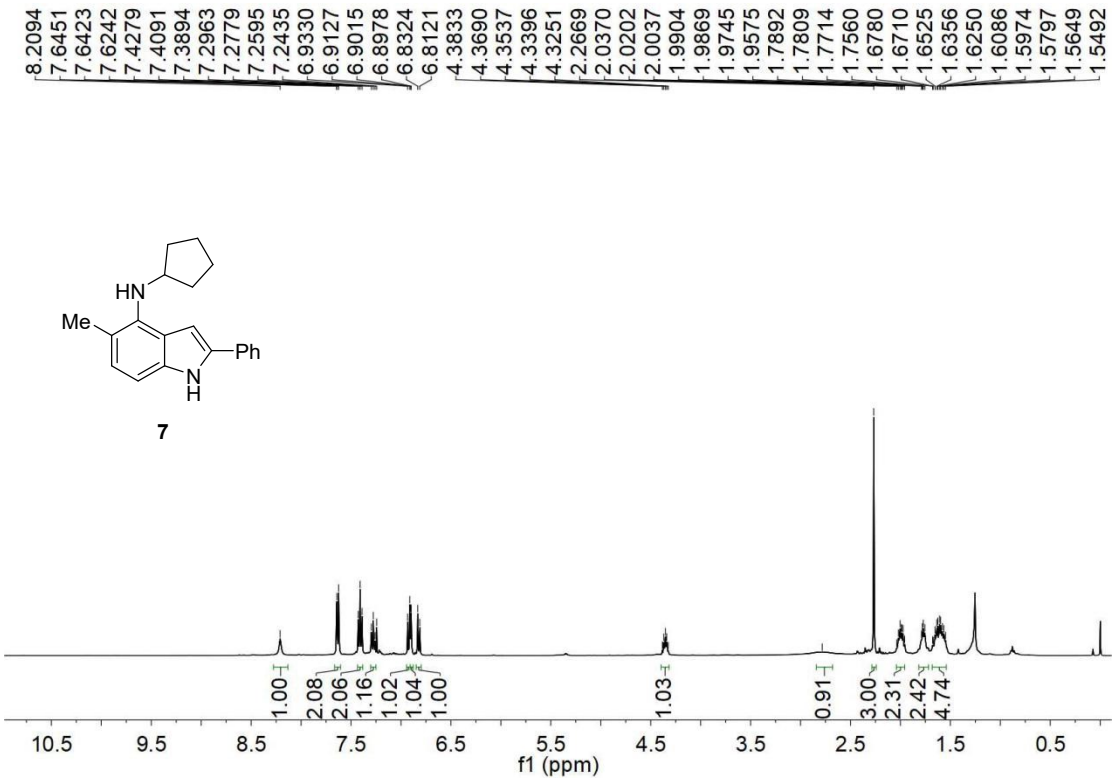
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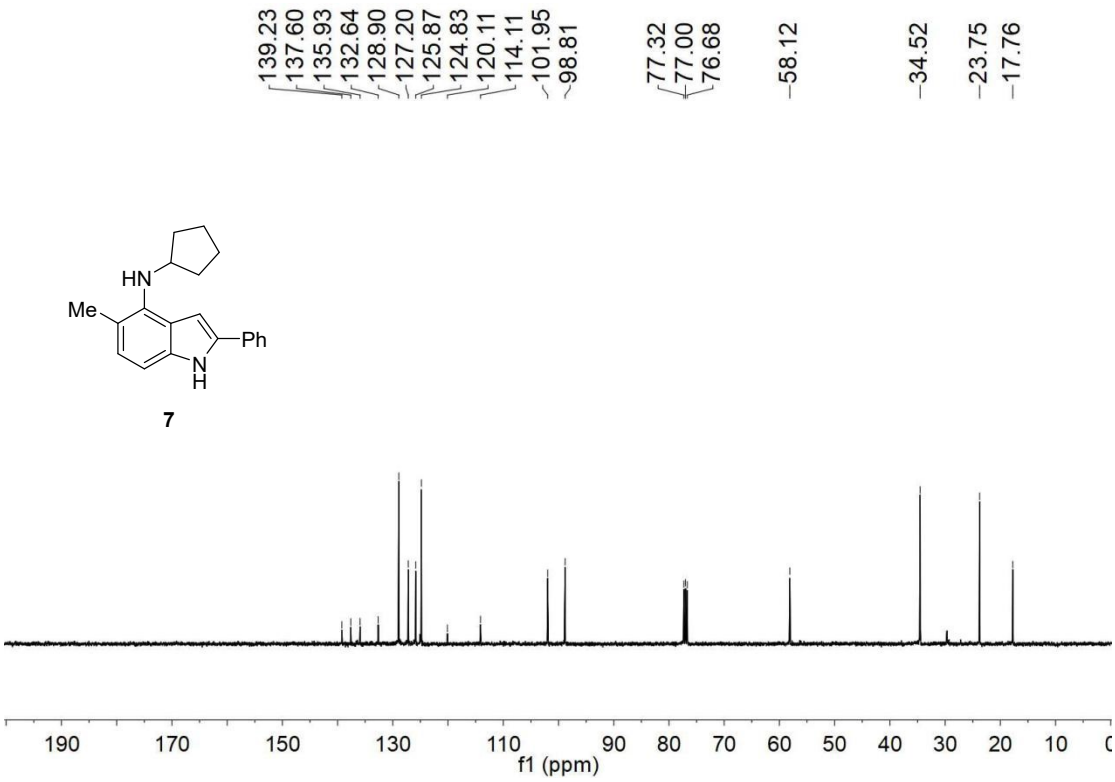
f1 (ppm)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23.75
17.76
HN
Me
Ph
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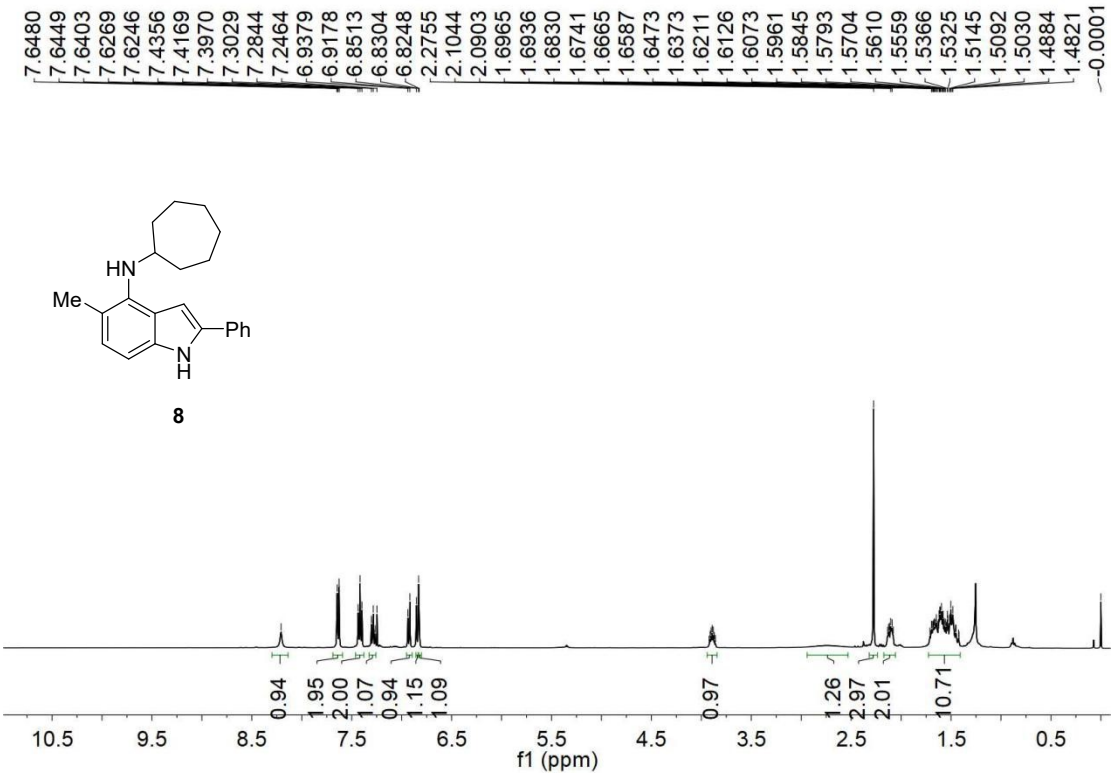
f1 (ppm)

7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6.9178
6.8513
6.8304
6.8248
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2.1044
2.0903
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1.6936
1.6830
1.6741
1.6665
1.6587
1.6473
1.6373
1.6211
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1.6073
1.5961
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1.5030
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1.4821
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Me
Ph
N
H
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0.94
1.15
1.09
0.97
1.26
2.97
2.01
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5.5
4.5
3.5
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1.5
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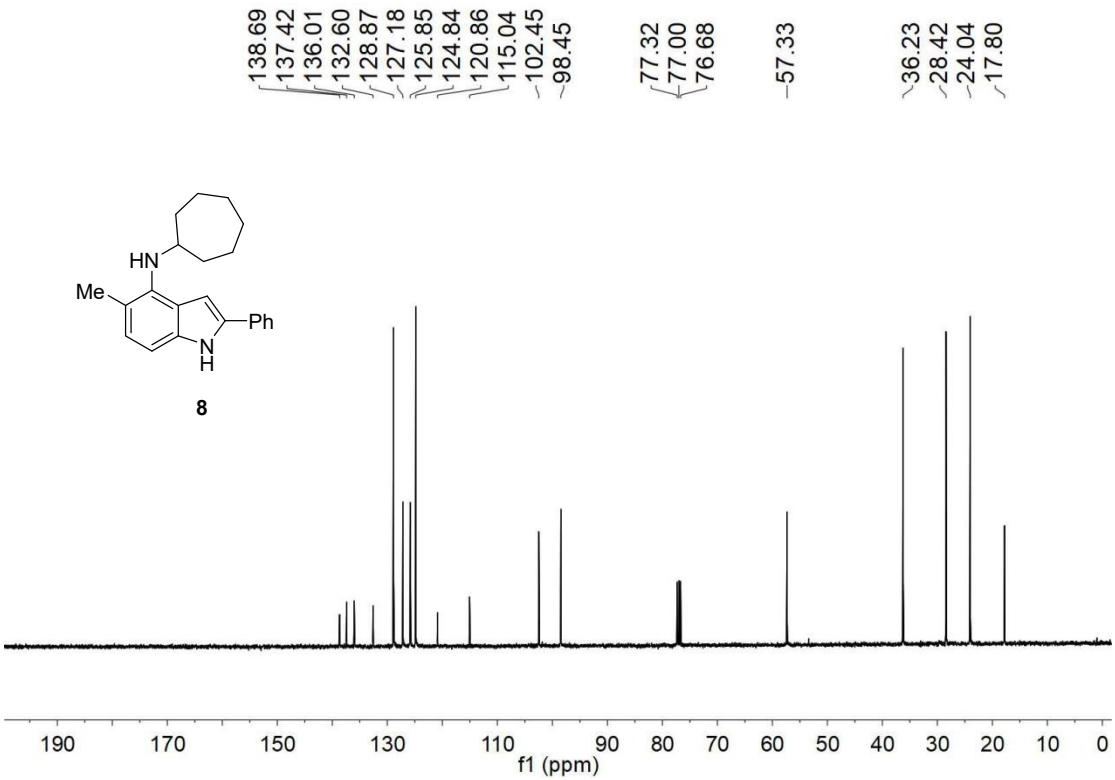
f1 (ppm)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124.84
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115.04
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98.45
77.32
77.00
76.68
57.33
36.23
28.42
24.04
17.80
HN
Me
Ph
N
H
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150
130
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90
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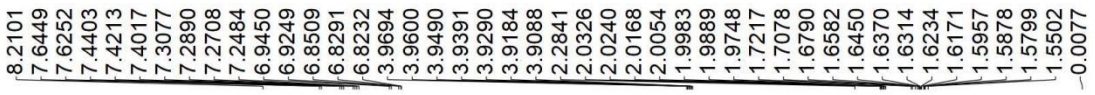
f1 (ppm)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6.9249
6.8509
6.8291
6.8232
3.9694
3.9600
3.9490
3.9391
3.9290
3.9184
3.9088
2.2841
2.0326
2.0240
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2.0054
1.9983
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1.7217
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1.6790
1.6582
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1.5878
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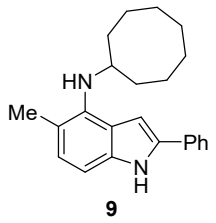
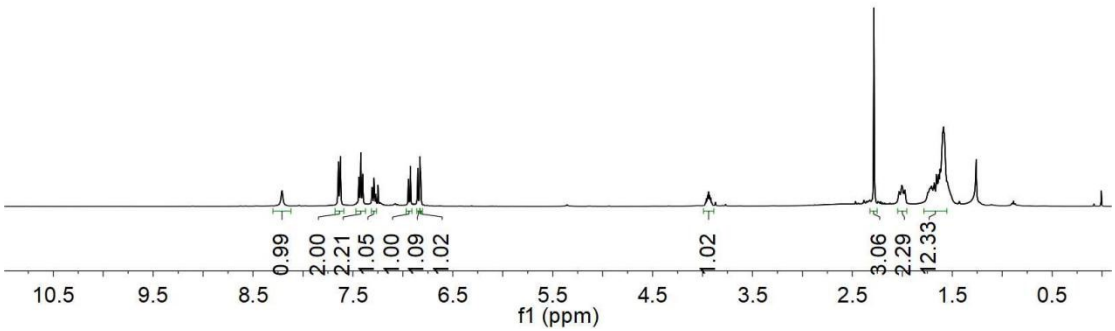
1.5502
0.0077


HN
Me
Ph
N
H

9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1.02
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12.33
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7.5
6.5
5.5
4.5
3.5
2.5
1.5
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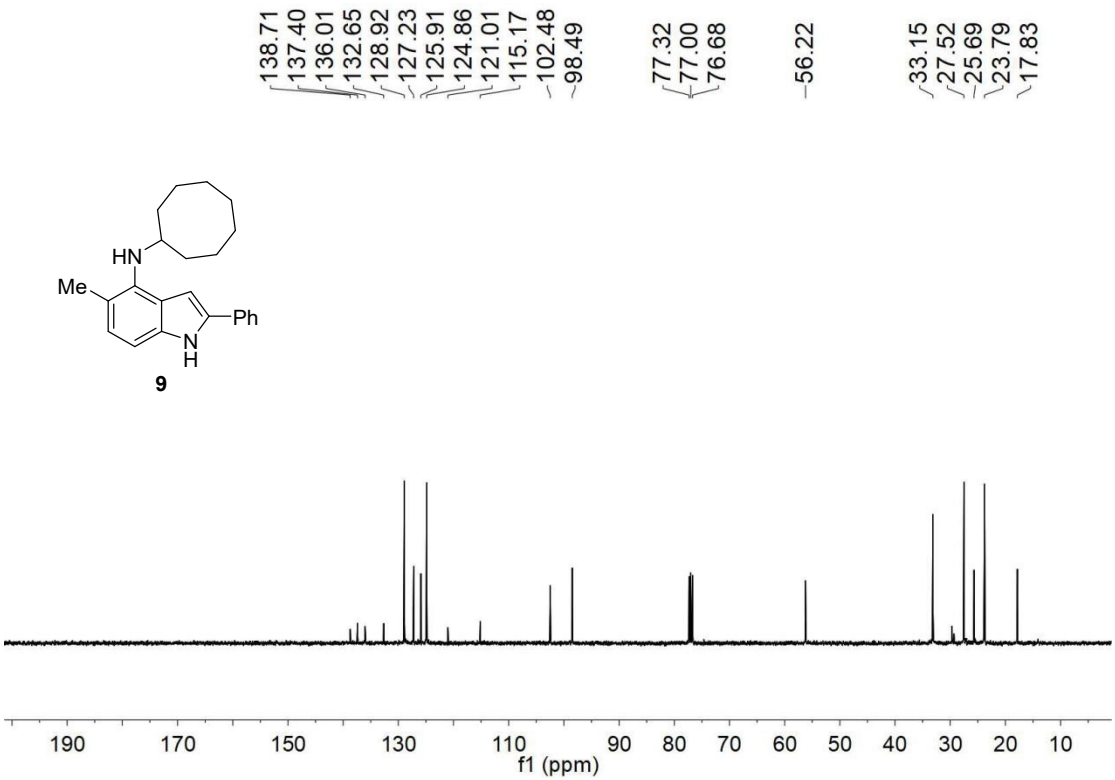
f1 (ppm)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125.91
124.86
121.01
115.17
102.48
98.49
77.32
77.00
76.68
56.22
33.15
27.52
25.69
23.79
17.83
HN
Me
Ph
N
H
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190
170
150
130
110
90
80
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60
50
40
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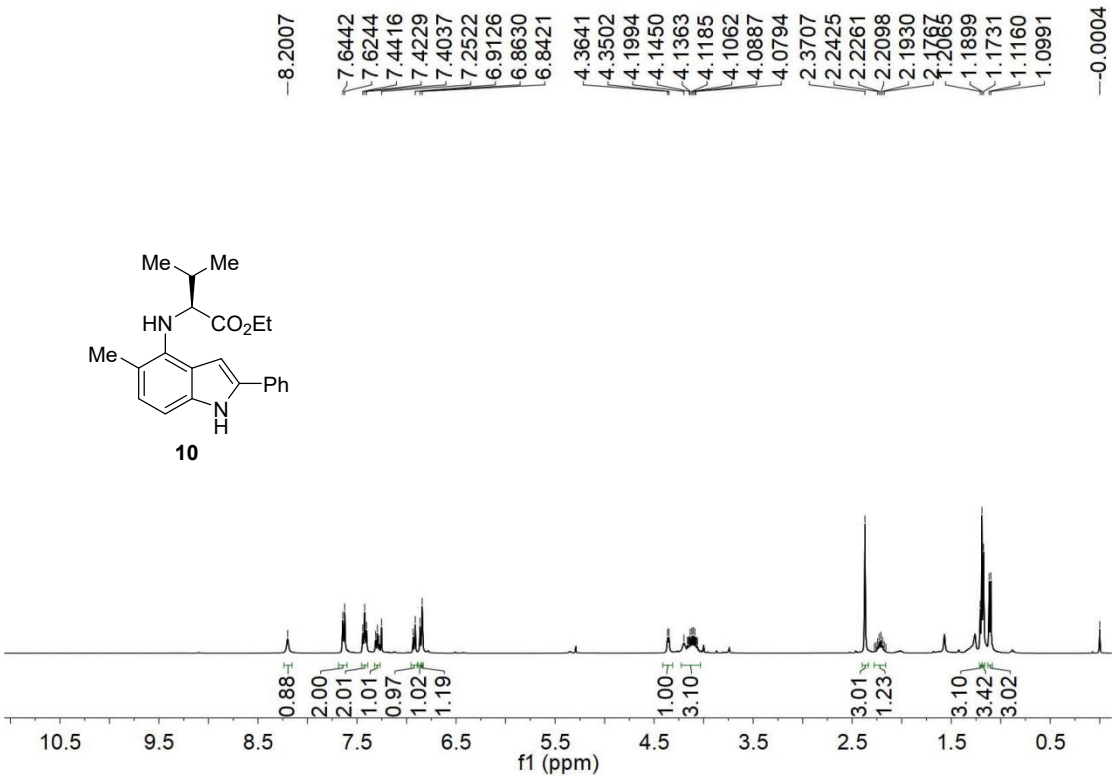
20
10
f1 (ppm)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7.4037
7.2522
6.9126
6.8630
6.8421
4.3641
4.3502
4.1994
4.1450
4.1363
4.1185
4.1062
4.0887
4.0794
2.3707
2.2425
2.2261
2.2098
2.1930
1.1899
1.1731
1.1160
1.0991
0.0004
Me
Me
HN
CO2Et
Me
Ph
N
H
10
0.88
2.00
2.01
1.01
0.97
1.02
1.19
1.00
3.10
3.01
1.23
3.10
3.42
3.02
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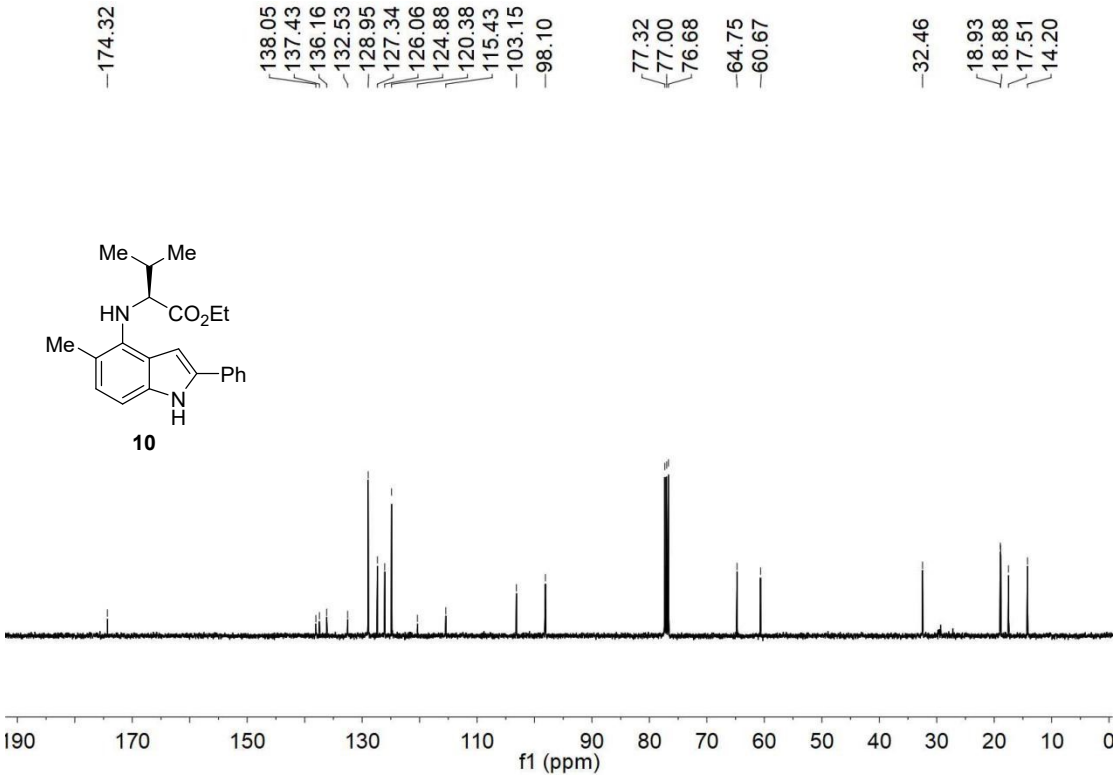
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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127.34
126.06
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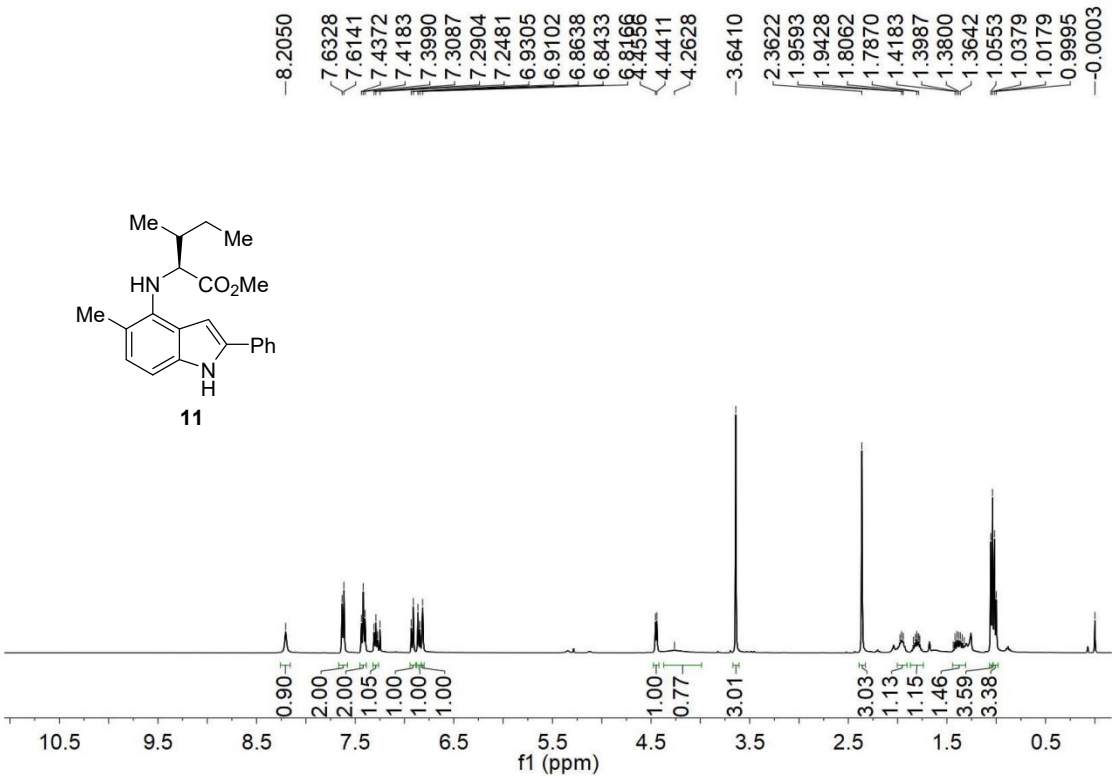
120.38
115.43
103.15
98.10
77.32
77.00
76.68
64.75
60.67
32.46
18.93
18.88
17.51
14.20
Me
Me
HN
CO2Et
Me
Ph
N
H
10
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4183
7.3990
7.3087
7.2904
7.2481
6.9305
6.9102
6.8638
6.8433
4.4411
4.2628
3.6410
2.3622
1.9593
1.9428
1.8062
1.7870
1.4183
1.3987
1.3800
1.3642
1.0553
1.0379
1.0179
0.9995
0.0003
Me
Me
HN
CO2Me
Me
Ph
N
H
11
0.90
2.00
2.00
1.05
1.00
1.00
1.00
1.00
0.77
3.01
3.03
1.13
1.15
1.46
3.59
3.38
10.5
9.5
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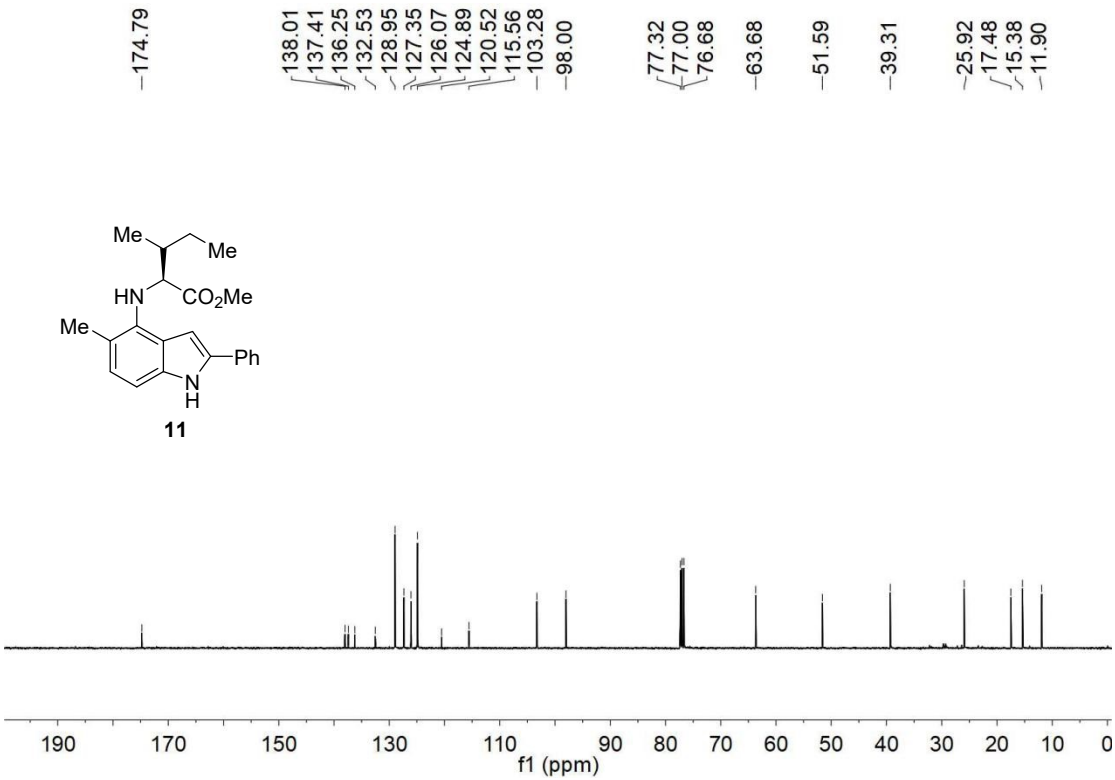
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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115.56
103.28
98.00
77.32
77.00
76.68
63.68
51.59
39.31
25.92
17.48
15.38
11.90
Me
Me
HN
CO2Me
Me
Ph
N
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11
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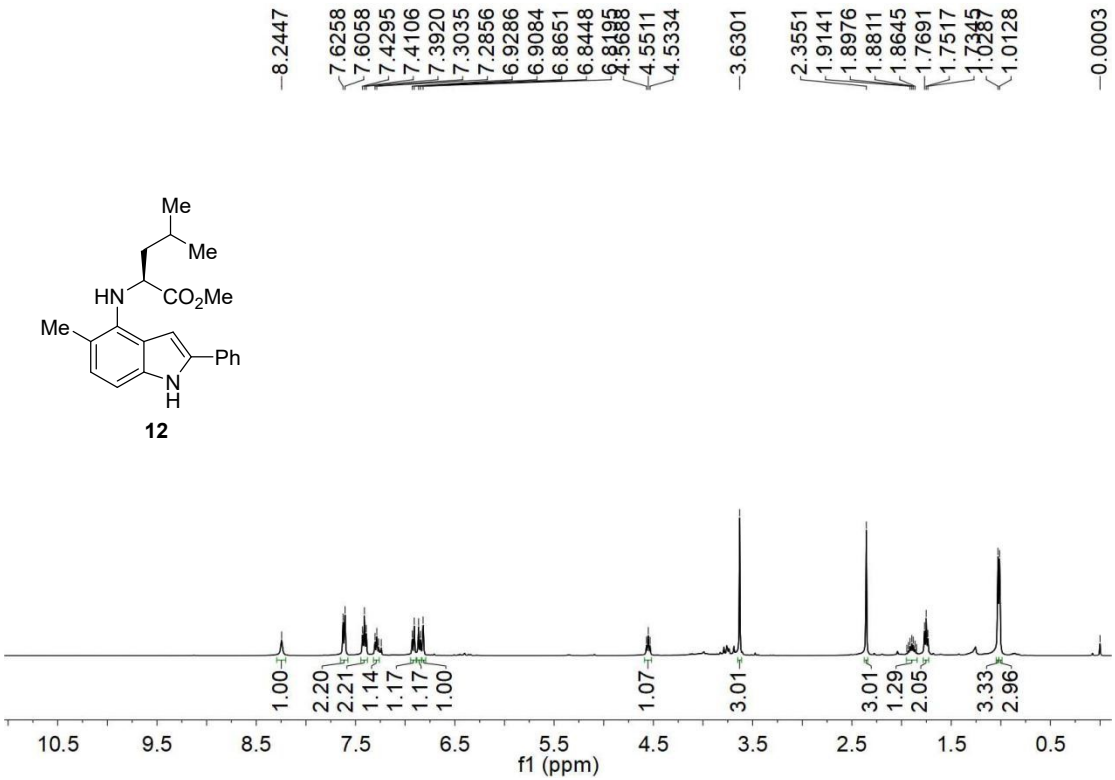
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.8448
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2.3551
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1.8811
1.8645
1.7691
1.7517
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Me
Me
HN
CO2Me
Me
Ph
N
H
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1.00
2.20
2.21
1.14
1.17
1.17
1.00
1.07
3.01
3.01
1.29
2.05
3.33
2.96
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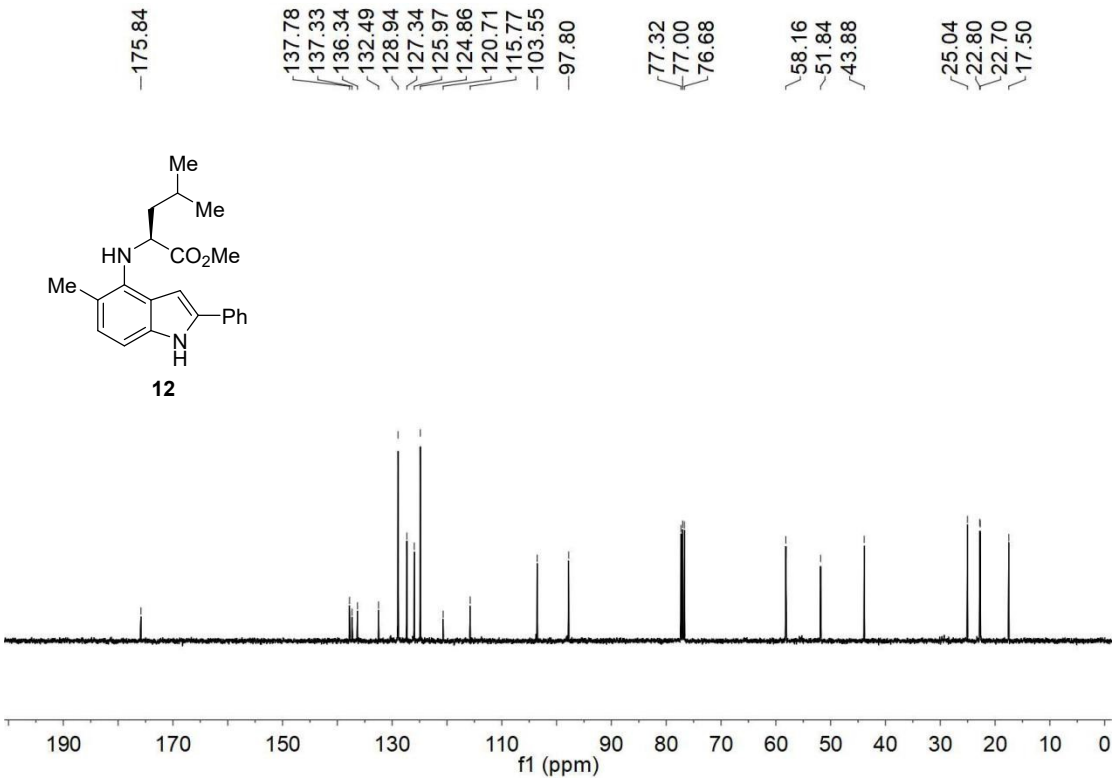
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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136.34
132.49
128.94
127.34
125.97
124.86
120.71
115.77
103.55
97.80
77.32
77.00
76.68
58.16
51.84
43.88
25.04
22.80
22.70
17.50
Me
Me
HN
CO2Me
Me
Ph
N
H
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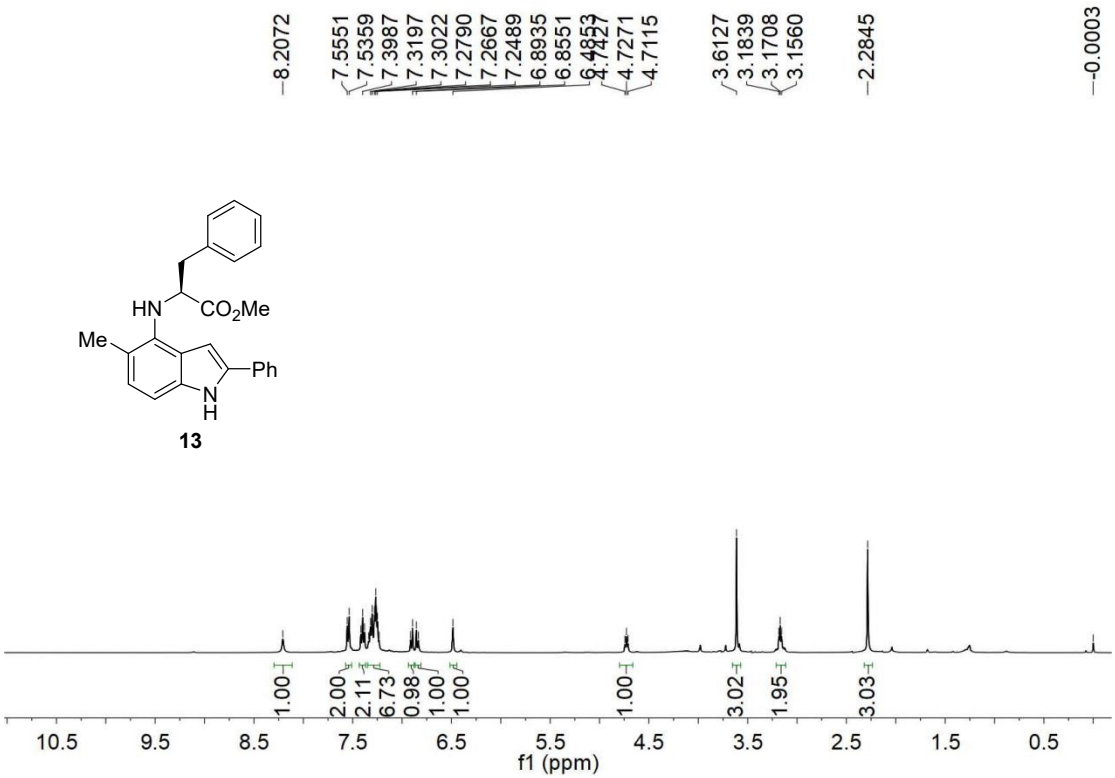
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.2790
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7.2489
6.8935
6.8551
6.4853
4.7271
4.7115
3.6127
3.1839
3.1708
3.1560
2.2845
0.0003
HN
CO2Me
Me
Ph
N
H
13
1.00
2.00
2.11
6.73
0.98
1.00
1.00
1.00
3.02
1.95
3.03
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9.5
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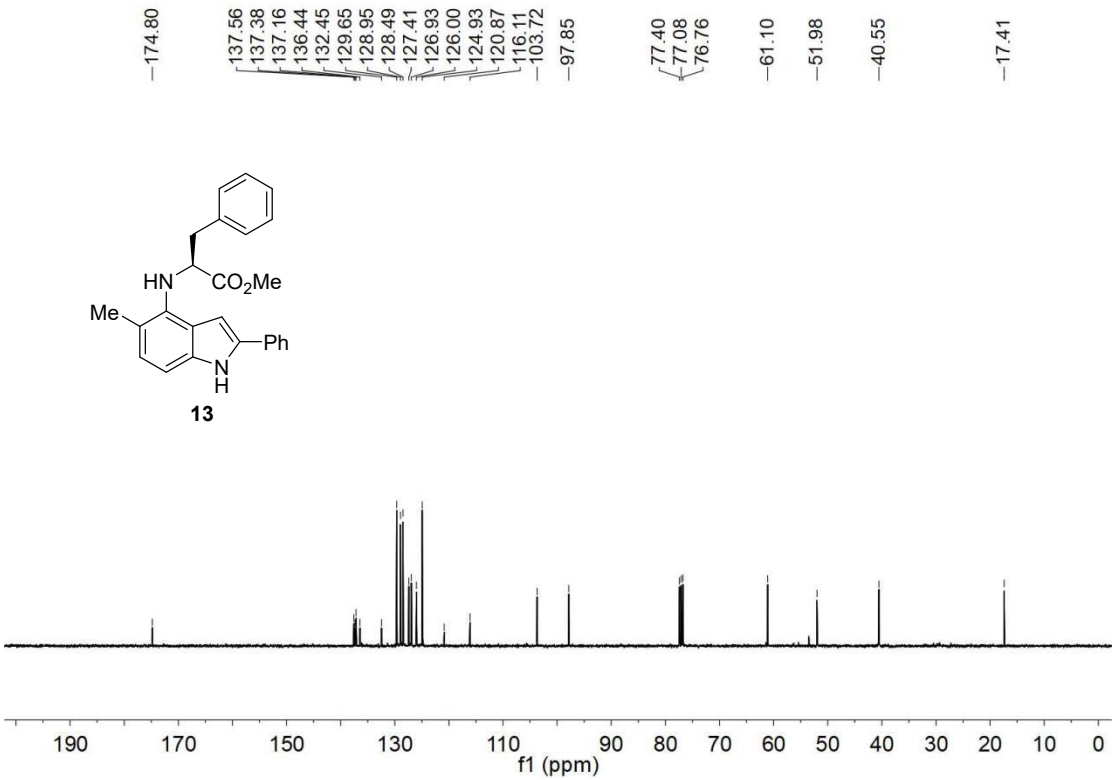
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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128.95
128.49
127.41
126.93
126.00
124.93
120.87
116.11
103.72
97.85
77.40
77.08
76.76
61.10
51.98
40.55
17.41
HN
CO2Me
Me
Ph
N
H
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170
150
130
110
90
80
70
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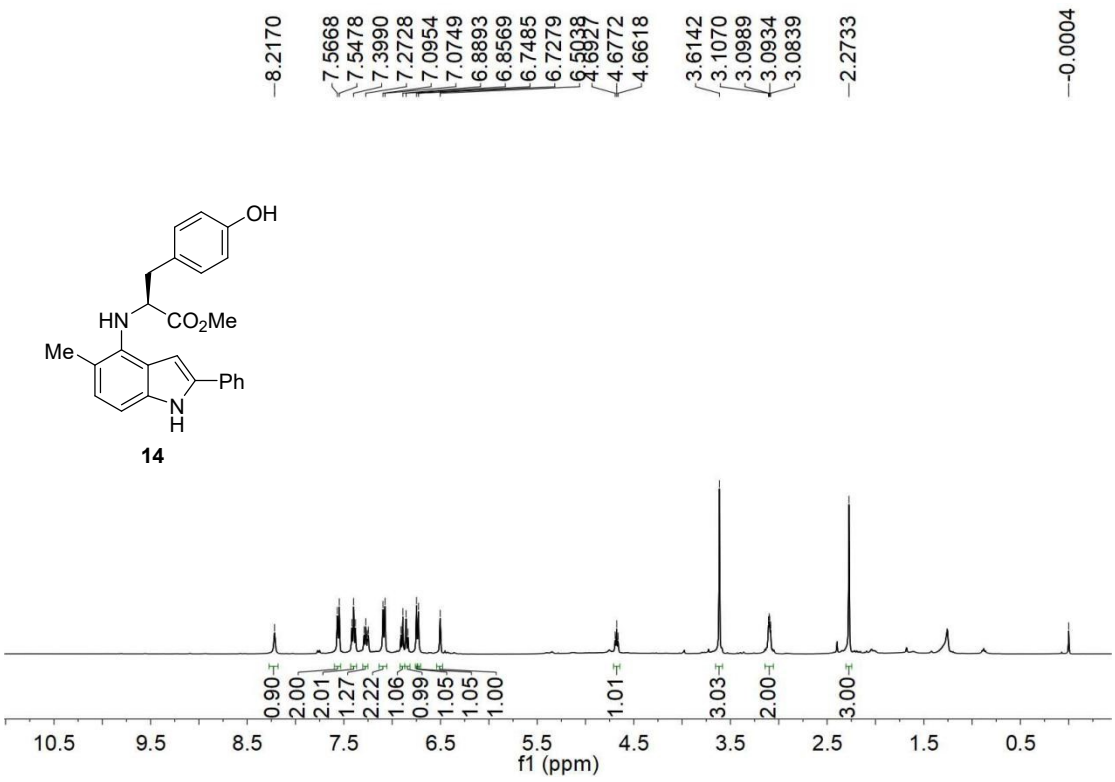
50
40
30
20
10
0
f1 (ppm)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7.0749
6.8893
6.8569
6.7485
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4.6772
4.6618
3.6142
3.1070
3.0989
3.0934
3.0839
2.2733
0.0004
OH
HN
CO2Me
Me
Ph
N
H
14
0.90
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2.01
1.27
2.22
1.06
0.99
1.05
1.05
1.00
1.01
3.03
2.00
3.00
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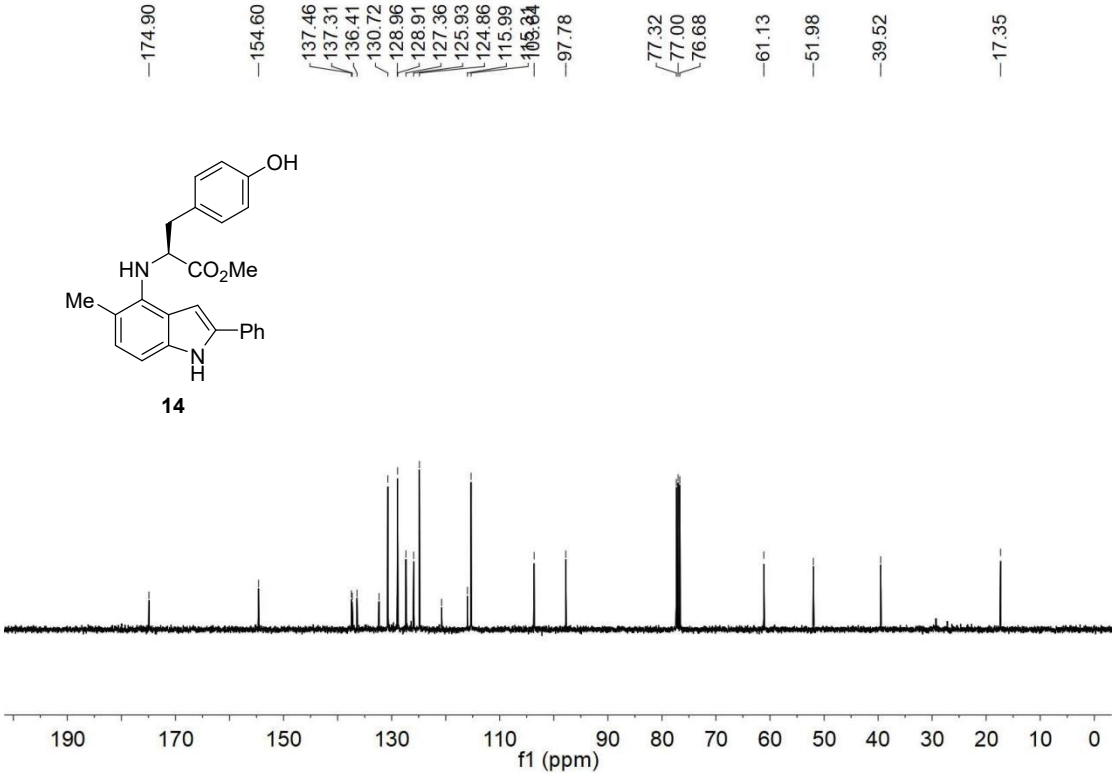
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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128.91
127.36
125.93
124.86
115.99
97.78
77.32
77.00
76.68
61.13
51.98
39.52
17.35
OH
HN
CO2Me
Me
Ph
N
H
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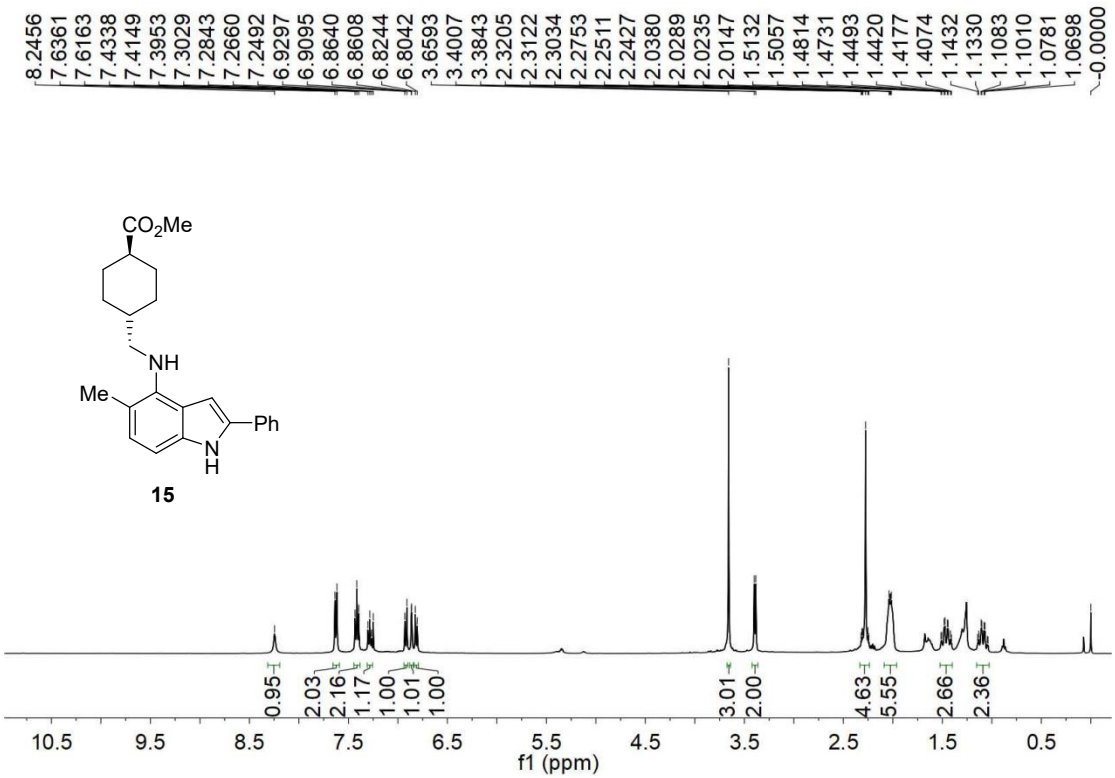
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.2492
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6.8640
6.8608
6.8244
6.8042
3.6593
3.4007
3.3843
2.3205
2.3122
2.3034
2.2753
2.2511
2.2427
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2.0289
2.0235
2.0147
1.5132
1.5057
1.4814
1.4731
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1.4177
1.4074
1.1432
1.1330
1.1083
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1.0781
1.0698
0.0000
CO2Me
NH
Me
Ph
N
H
15
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1.17
1.00
1.01
1.00
3.01
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2.66
2.36
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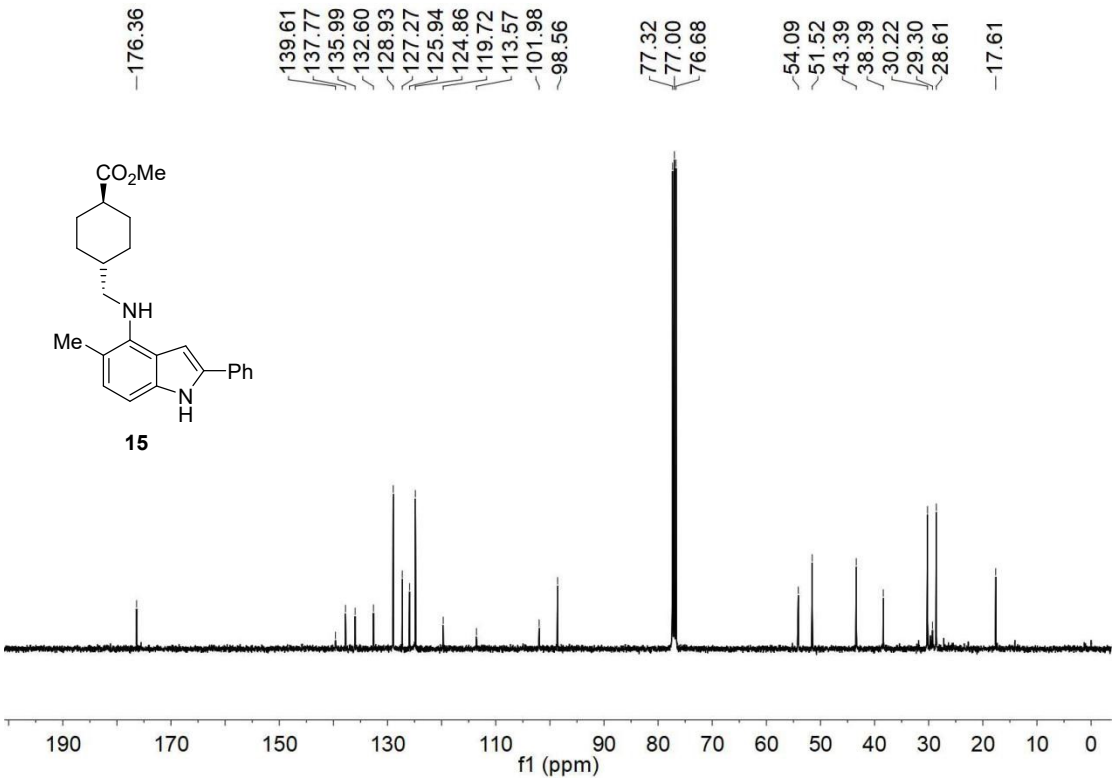
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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125.94
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119.72
113.57
101.98
98.56
77.32
77.00
76.68
54.09
51.52
43.39
38.39
30.22
29.30
28.61
17.61
CO2Me
NH
Me
Ph
N
H
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170
150
130
110
90
80
70
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50
40
30
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10
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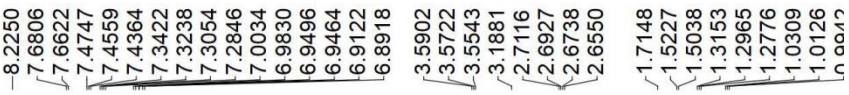
f1 (ppm)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7.2846
7.0034
6.9830
6.9496
6.9464
6.9122
6.8918
3.5902
3.5722
3.5543
3.1881
2.7116
2.6927
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1.5038
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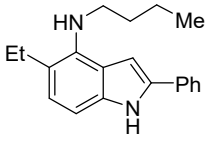
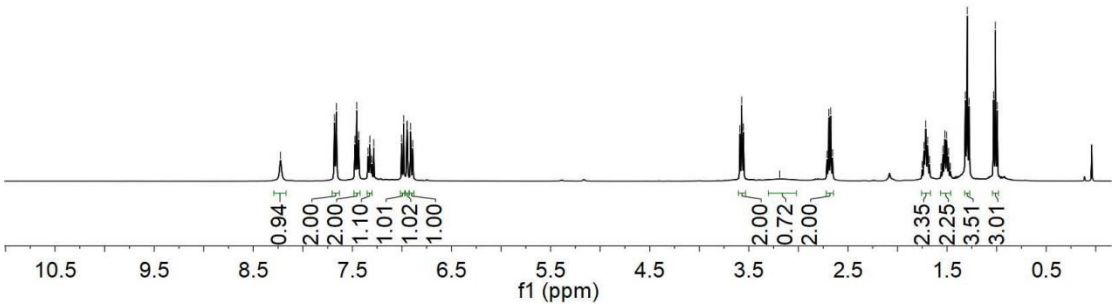
1.2965
1.2776
1.0309
1.0126


HN
Me
Et
Ph
N
H

16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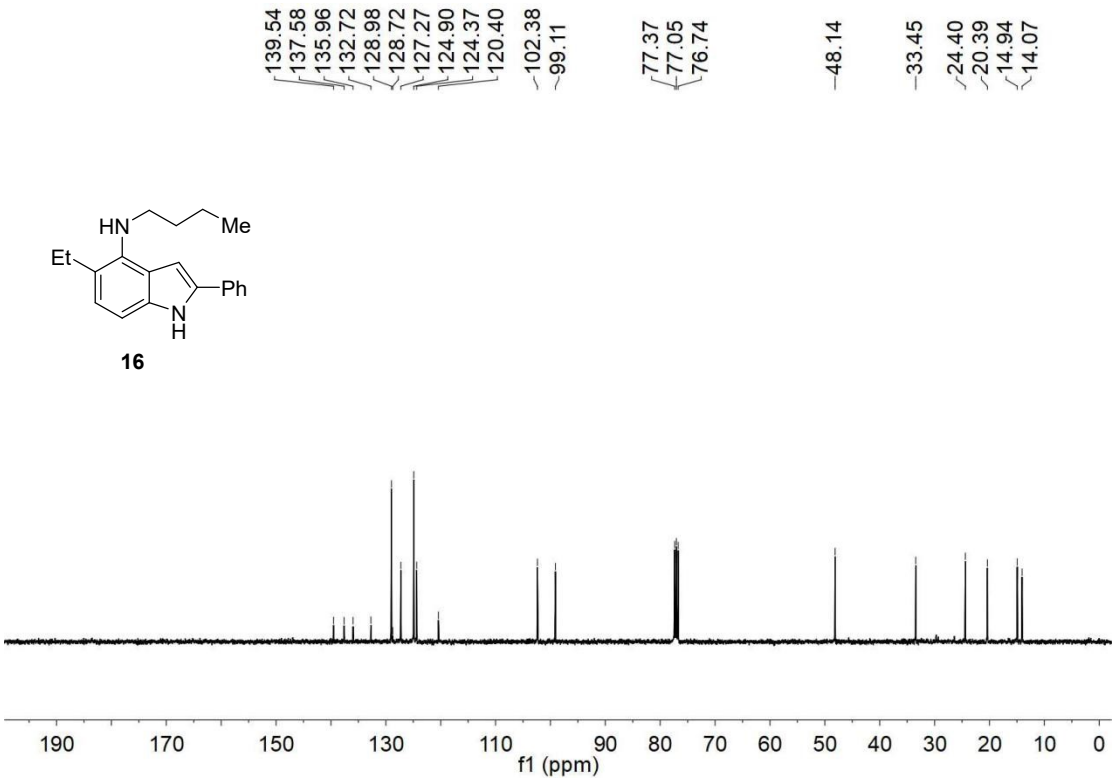
1.02
1.00
2.00
0.72
2.00
2.35
2.25
3.51
3.01
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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128.98
128.72
127.27
124.90
124.37
120.40
102.38
99.11
77.37
77.05
76.74
48.14
33.45
24.40
20.39
14.94
14.07
HN
Me
Et
Ph
N
H
16
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.1905
7.6409
7.6225
7.4342
7.4154
7.3959
7.3015
7.2832
7.2646
7.2473
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6.9163
6.9070
6.8616
6.8412
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2.6145
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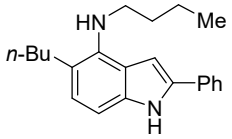
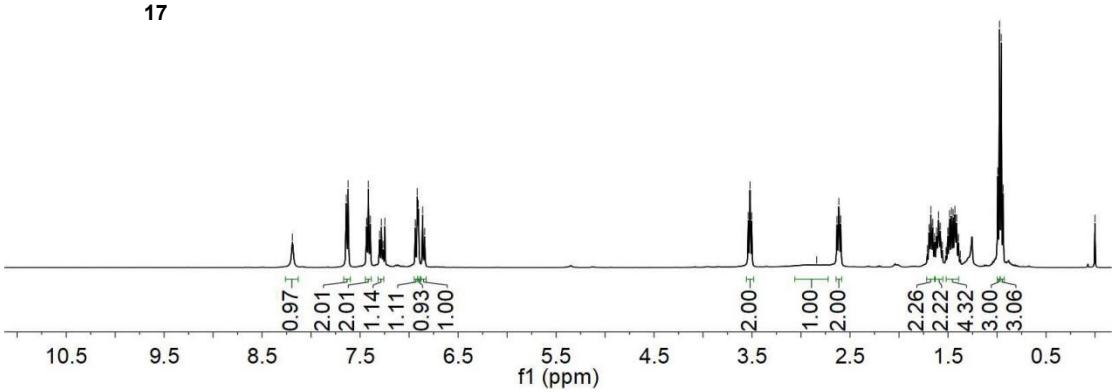
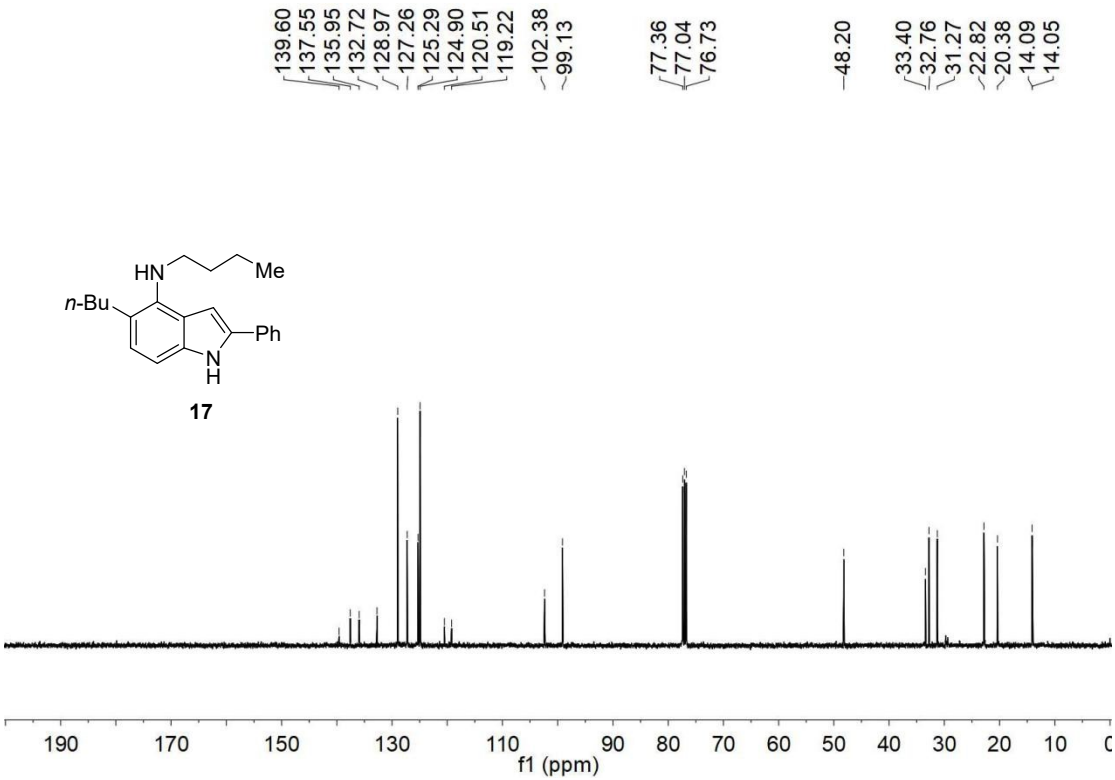
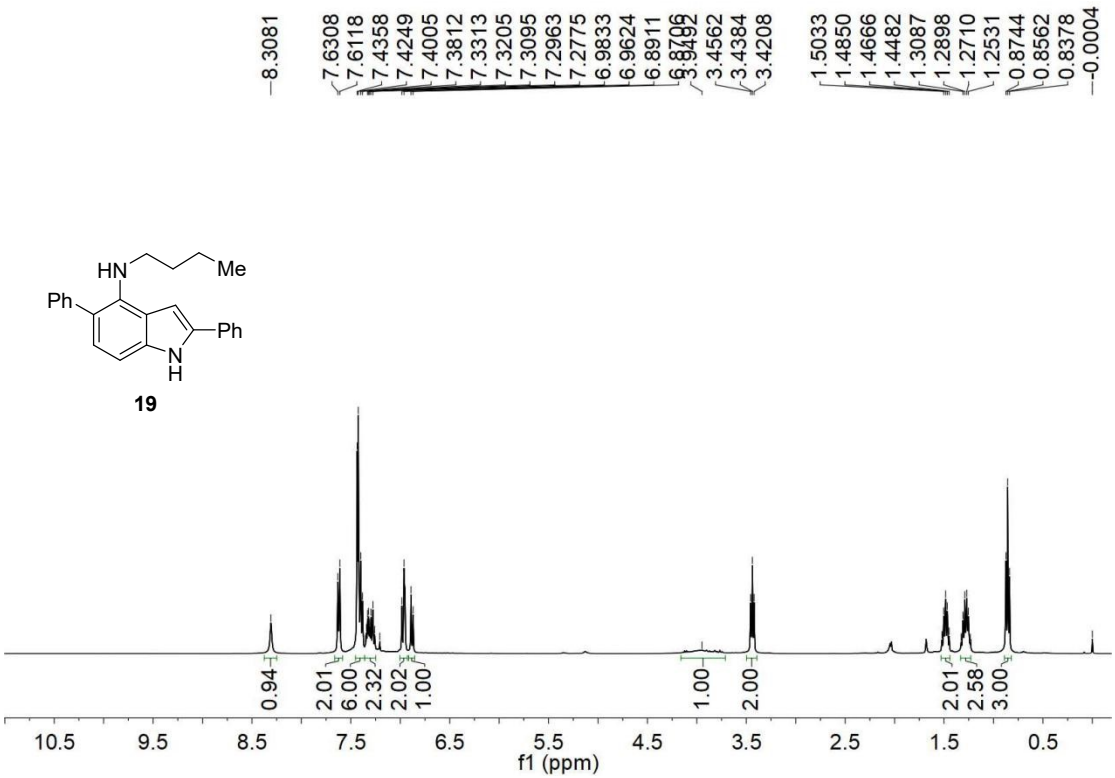
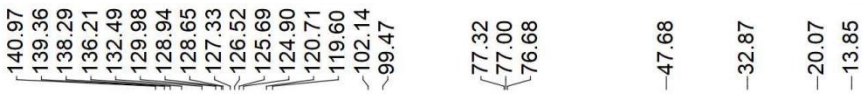

HN
Me
n-Bu
Ph
N
H

17


0.97
2.01
2.01
1.14
1.11
0.93
1.00
2.00
1.00
2.00
2.26
2.22
4.32
3.00
3.06
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


139.60
137.55
135.95
132.72
128.97
127.26
125.29
124.90
120.51
119.22
102.38
99.13
77.36
77.04
76.73
48.20
33.40
32.76
31.27
22.82
20.38
14.09
14.05
HN
Me
n-Bu
Ph
N
H
17
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.3081
7.6308
7.6118
7.4358
7.4249
7.4005
7.3812
7.3313
7.3205
7.3095
7.2963
7.2775
6.9833
6.9624
6.8911
3.4562
3.4384
3.4208
1.5033
1.4850
1.4666
1.4482
1.3087
1.2898
1.2710
1.2531
0.8744
0.8562
0.8378
0.0004
HN
Me
Ph
Ph
N
H
19
0.94
2.01
6.00
2.32
2.02
1.00
1.00
2.00
2.01
2.58
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


140.97
139.36
138.29
136.21
132.49
129.98
128.94
128.65
127.33
126.52
125.69
124.90
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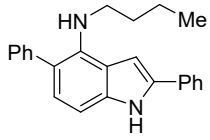
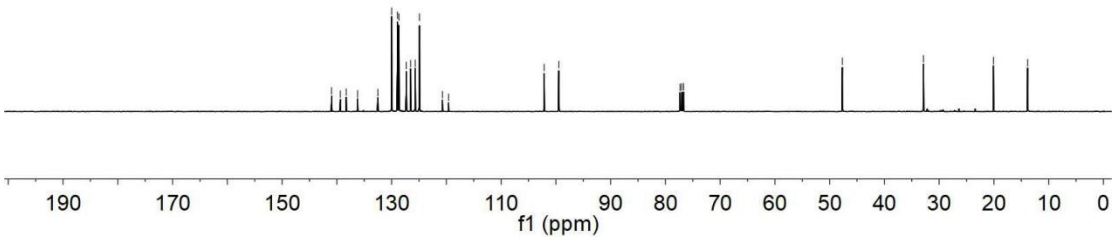
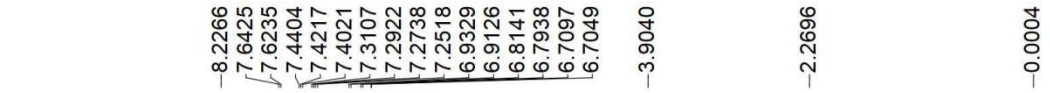
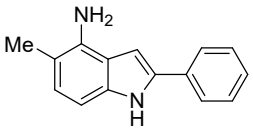
102.14
99.47
77.32
77.00
76.68
47.68
32.87
20.07
13.85


HN
Me
Ph
Ph
N
H

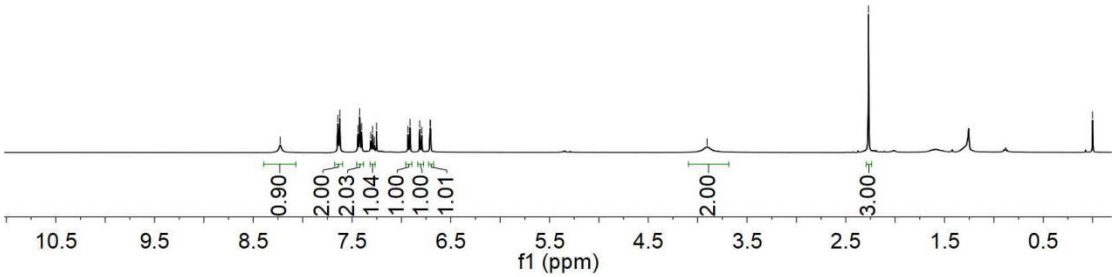
19

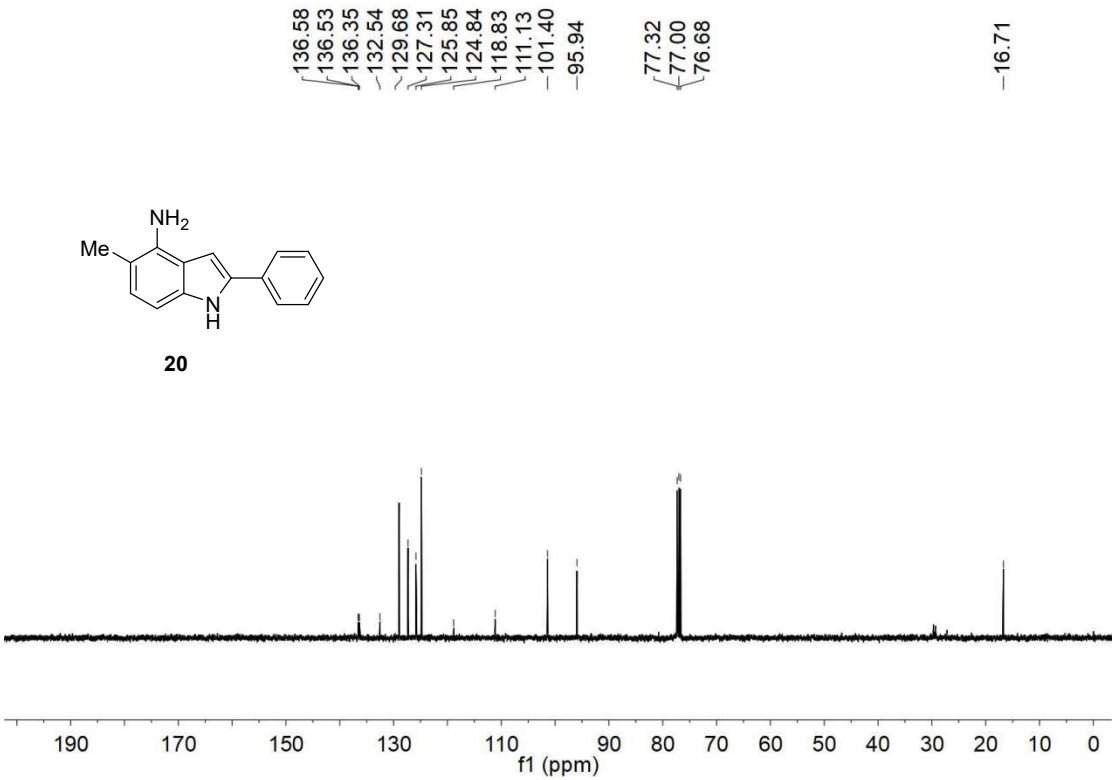

190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.2266
7.6425
7.6235
7.4404
7.4217
7.4021
7.3107
7.2922
7.2738
7.2518
6.9329
6.9126
6.8141
6.7938
6.7097
6.7049
3.9040
2.2696
0.0004

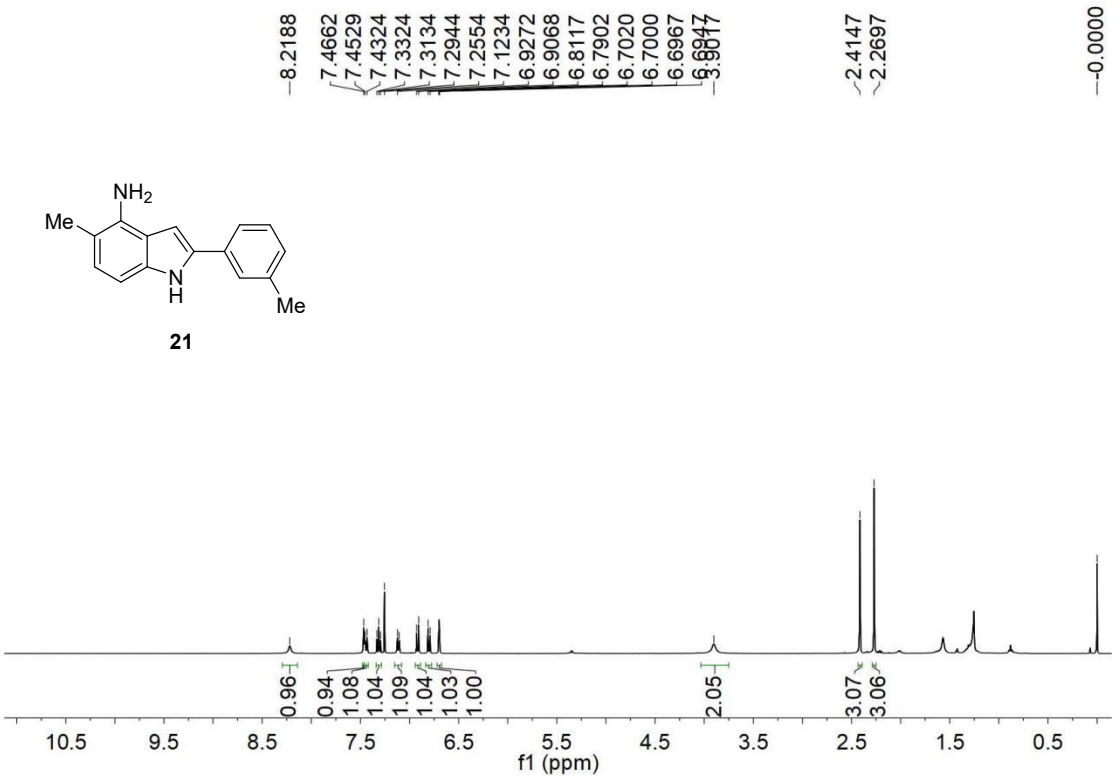

NH2
Me
N
H

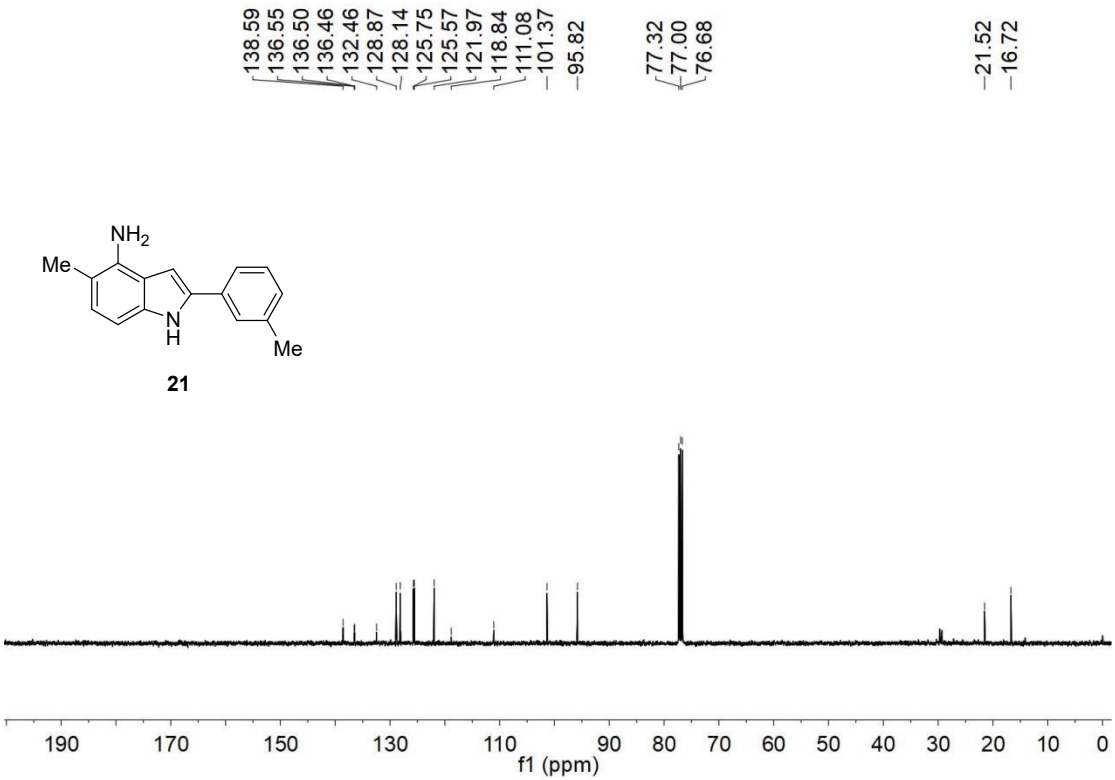
20


0.90
2.00
2.03
1.04
1.00
1.00
1.01
2.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

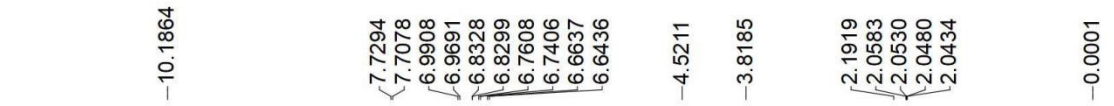

136.58
136.53
136.35
132.54
129.68
127.31
125.85
124.84
118.83
111.13
101.40
95.94
77.32
77.00
76.68
16.71
NH2
Me
N
H
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

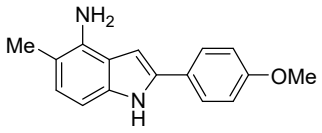
20


8.2188
7.4662
7.4529
7.4324
7.3324
7.3134
7.2944
7.2554
7.1234
6.9272
6.9068
6.8117
6.7902
6.7020
6.7000
6.6967
6.6847
3.9017
2.4147
2.2697
0.0000
NH2
Me
N
H
Me
21
0.96
0.94
1.08
1.04
1.09
1.04
1.03
1.00
2.05
3.07
3.06
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


138.59
136.55
136.50
136.46
132.46
128.87
128.14
125.75
125.57
121.97
118.84
111.08
101.37
95.82
77.32
77.00
76.68
21.52
16.72
NH2
Me
N
H
Me
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

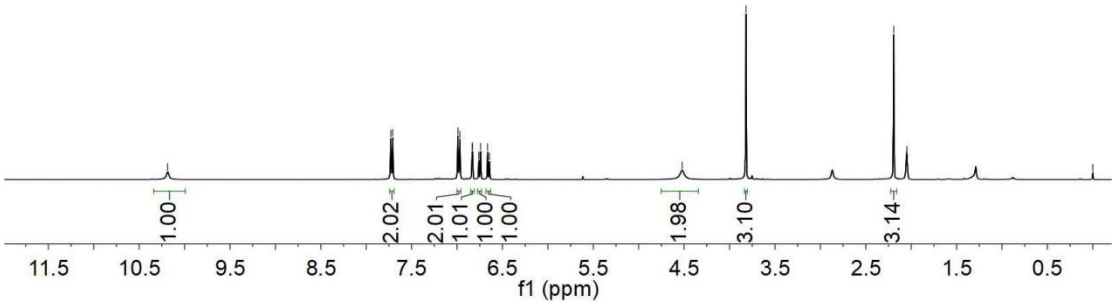
21

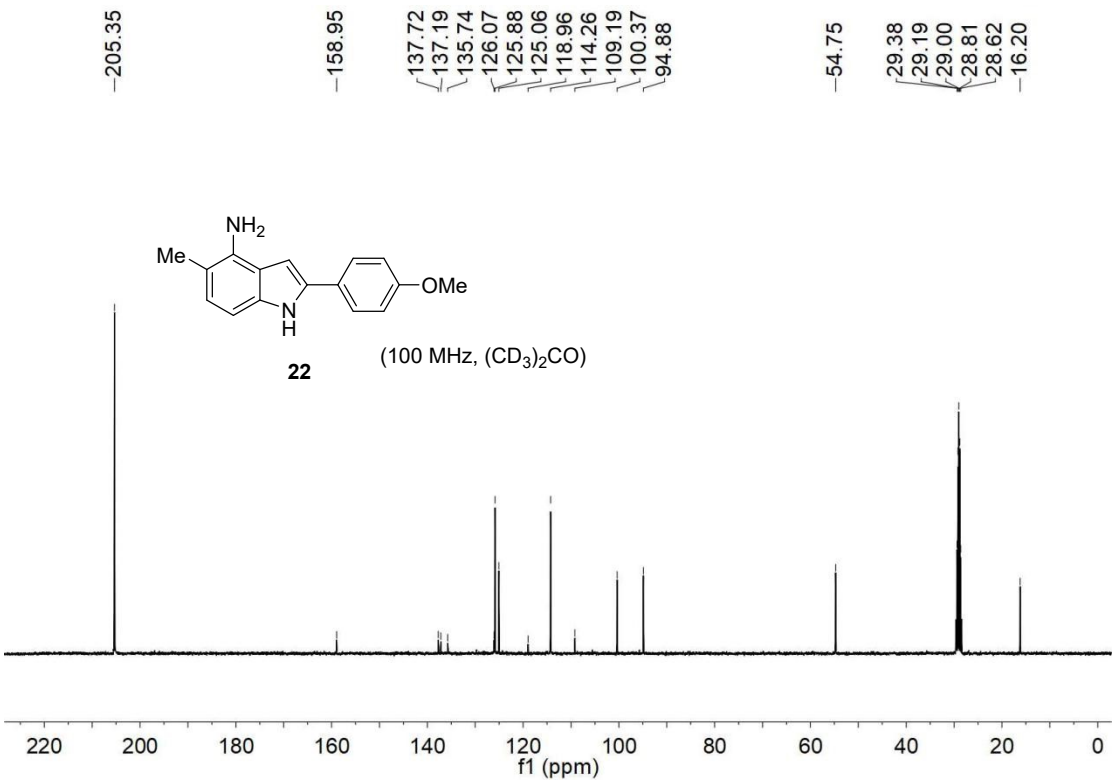


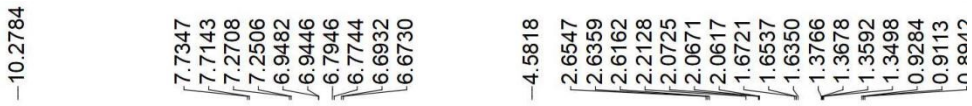


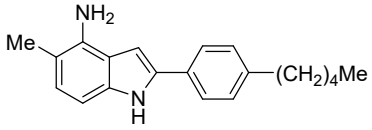
22

(400 MHz, $(CD_3)_2CO$)

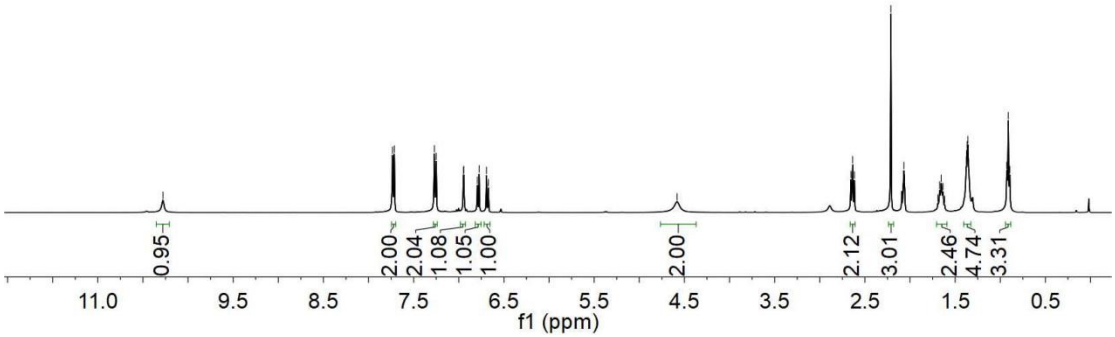


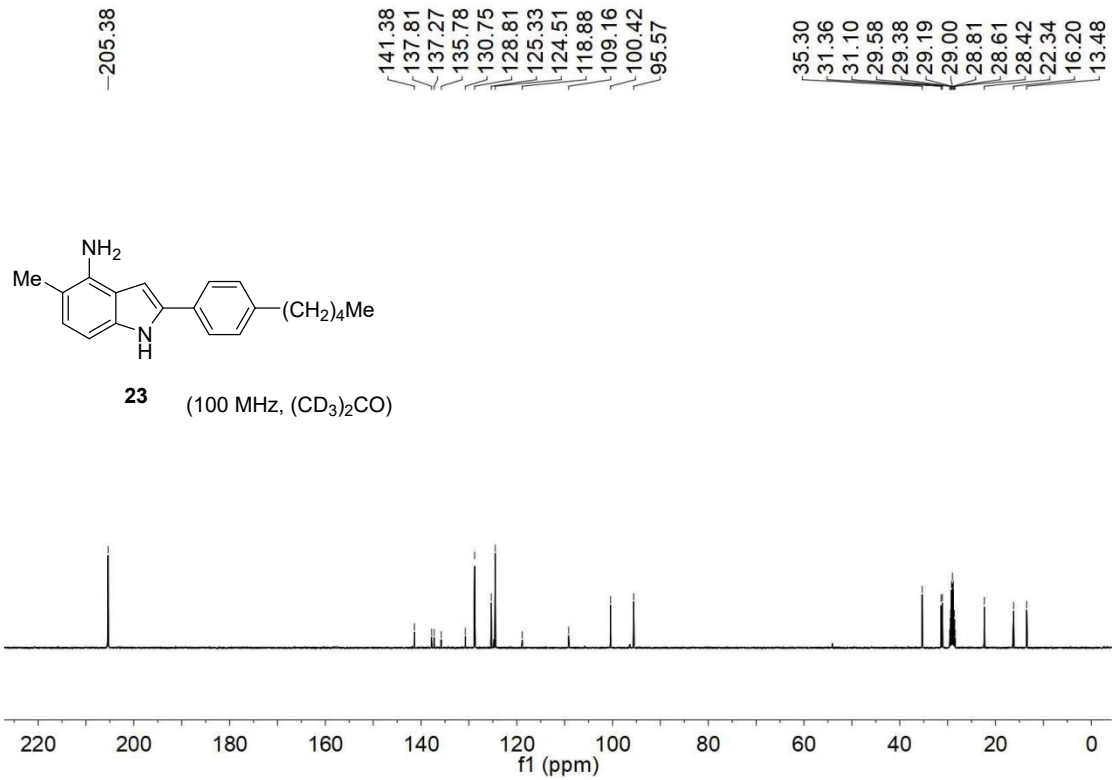

205.35
158.95
137.72
137.19
135.74
126.07
125.88
125.06
118.96
114.26
109.19
100.37
94.88
54.75
29.38
29.19
29.00
28.81
28.62
16.20
NH2
Me
OMe
N
H
22
(100 MHz, (CD3)2CO)
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)



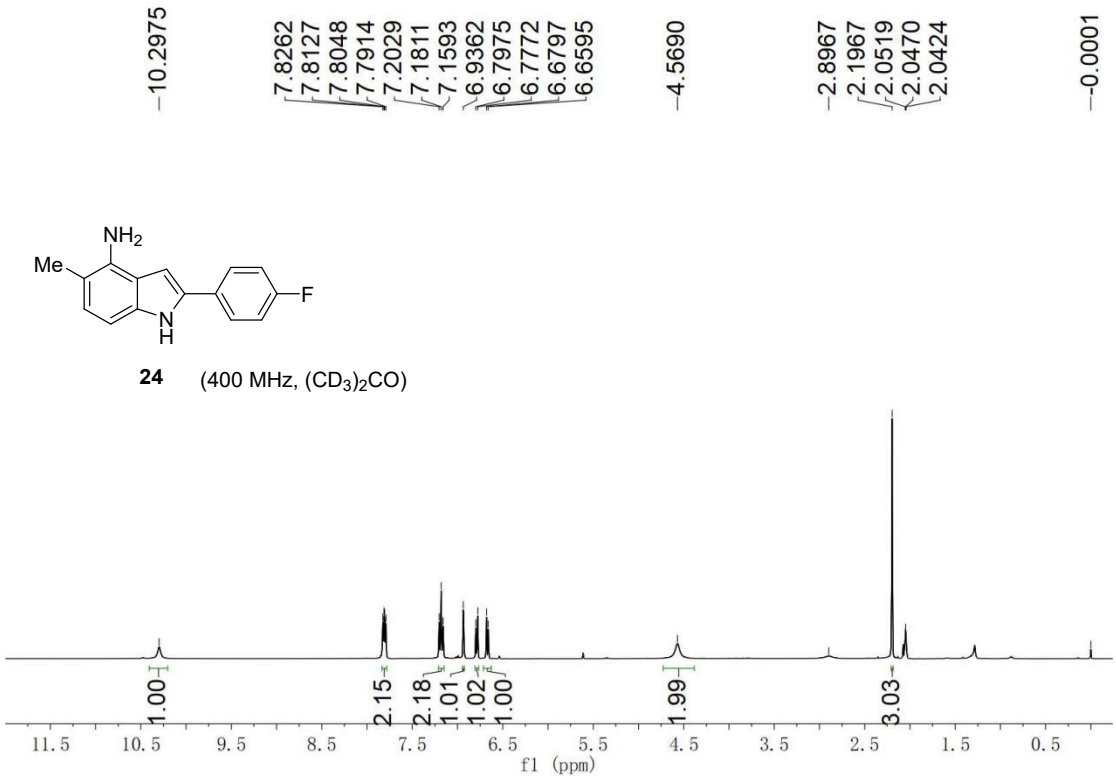


23 (400 MHz, $(CD_3)_2CO$)

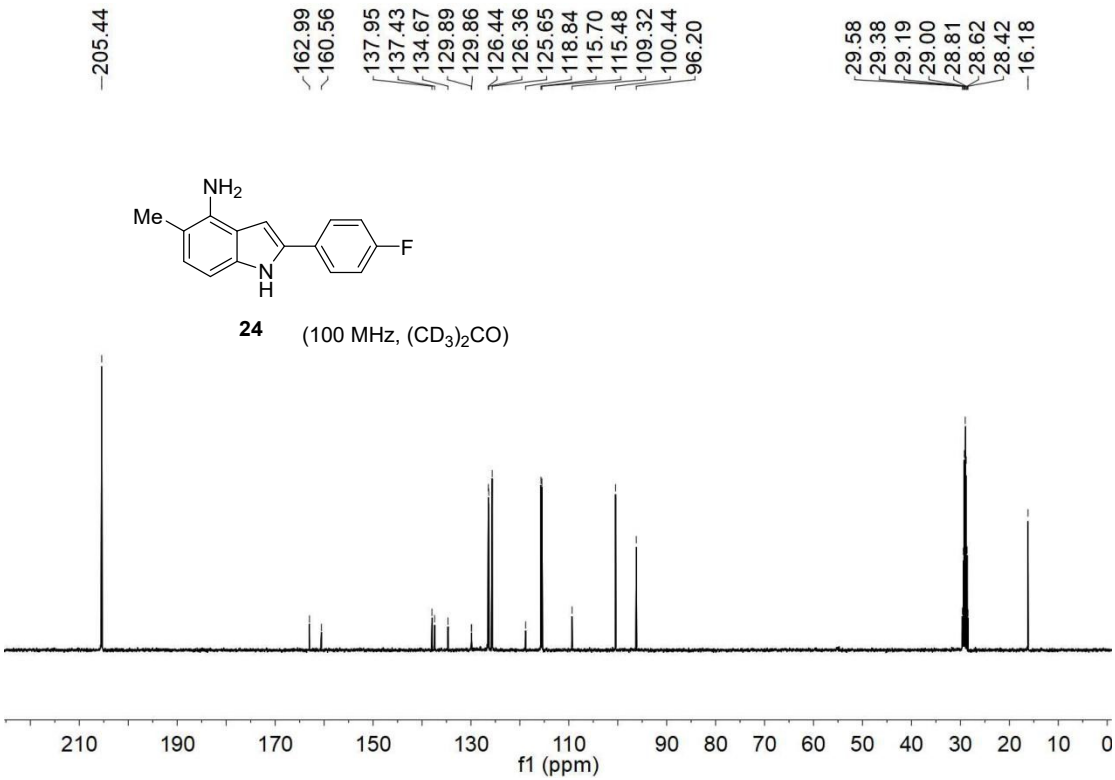




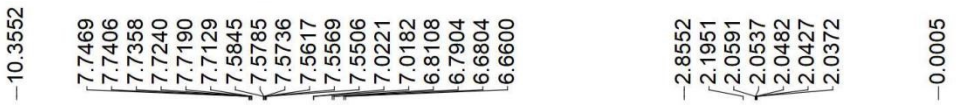
23 (100 MHz, $(CD_3)_2CO$)

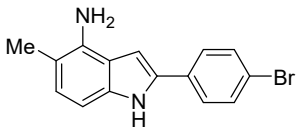


24 (400 MHz, $(CD_3)_2CO$)



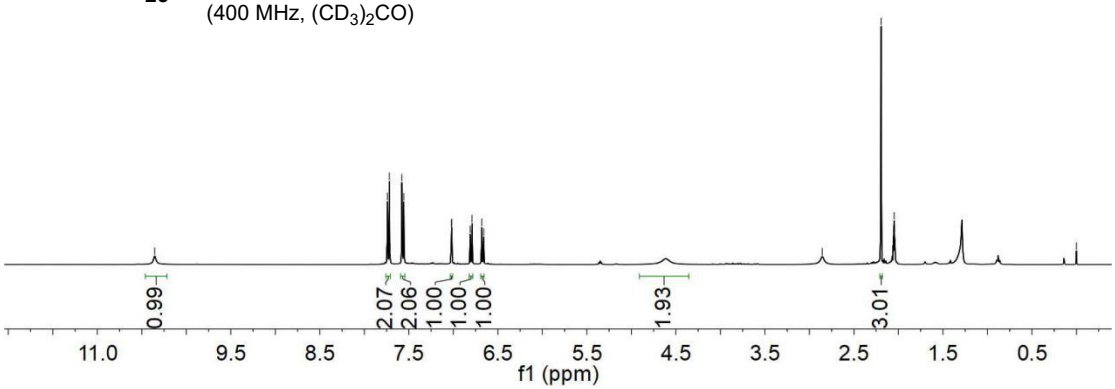
24 (100 MHz, $(CD_3)_2CO$)

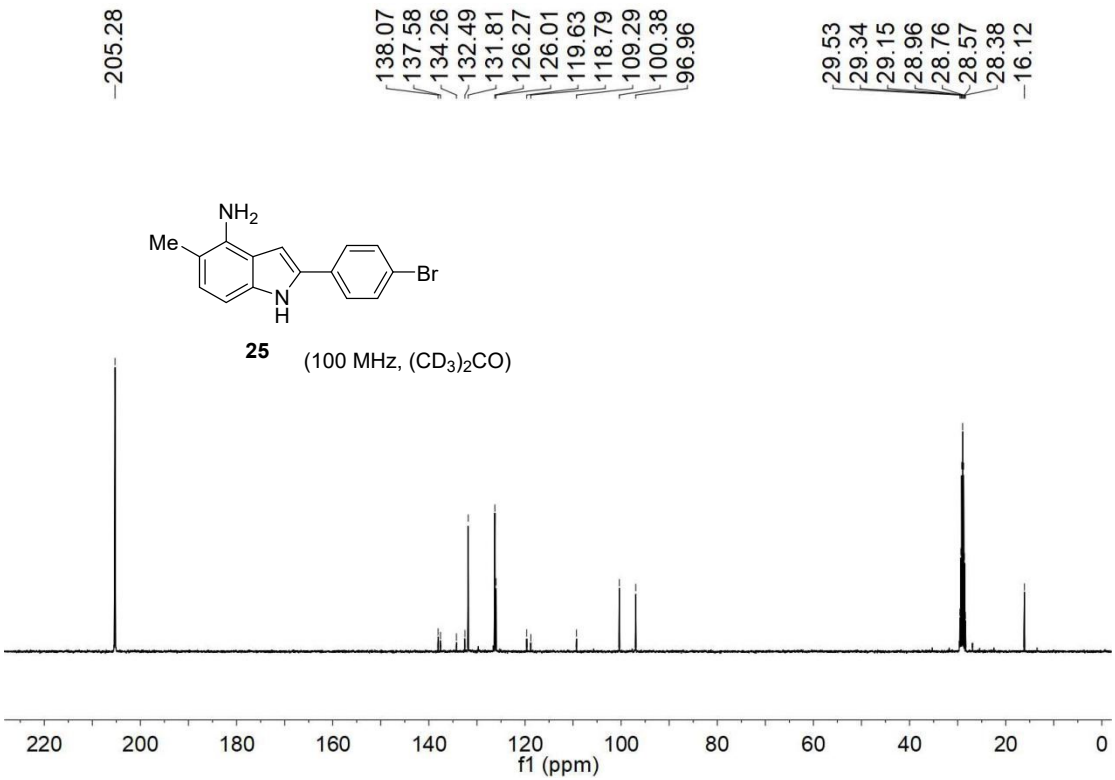




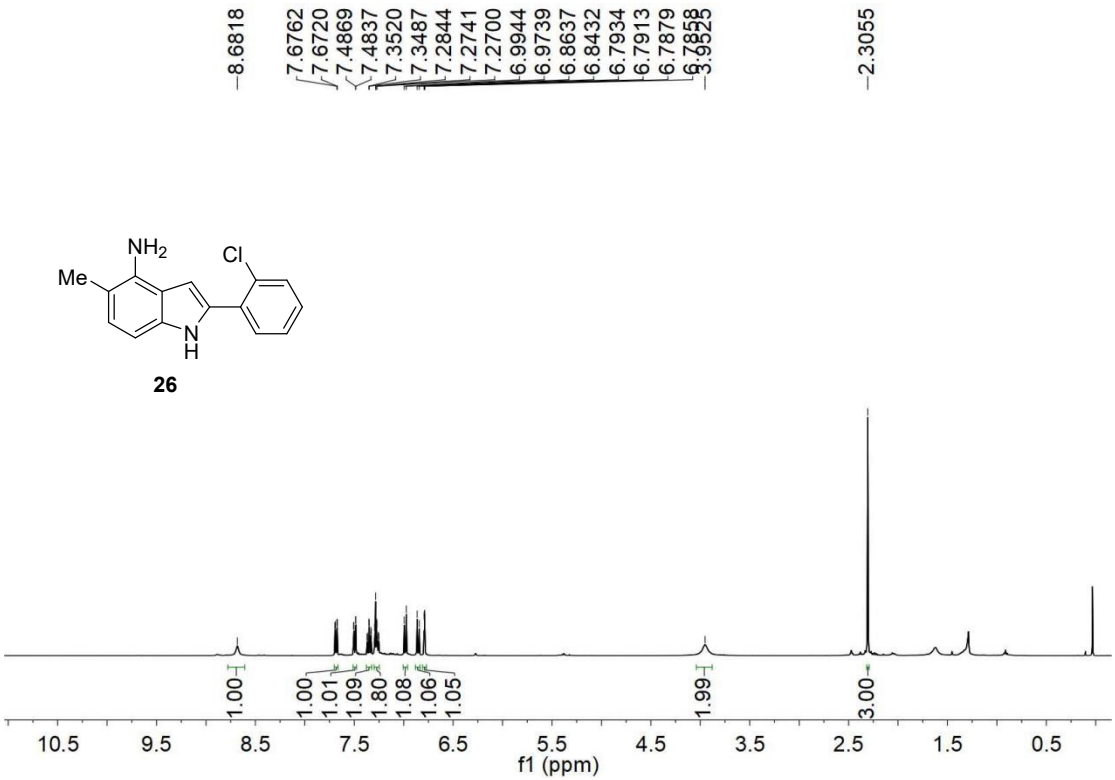
25

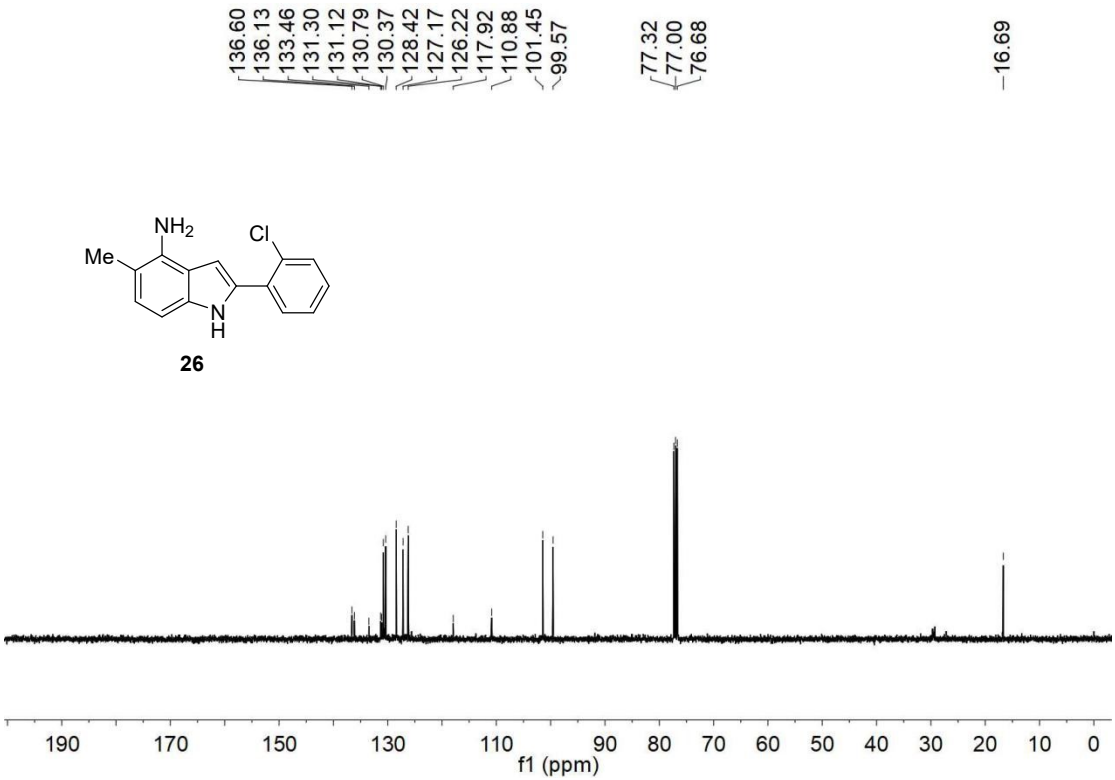
(400 MHz, $(CD_3)_2CO$)

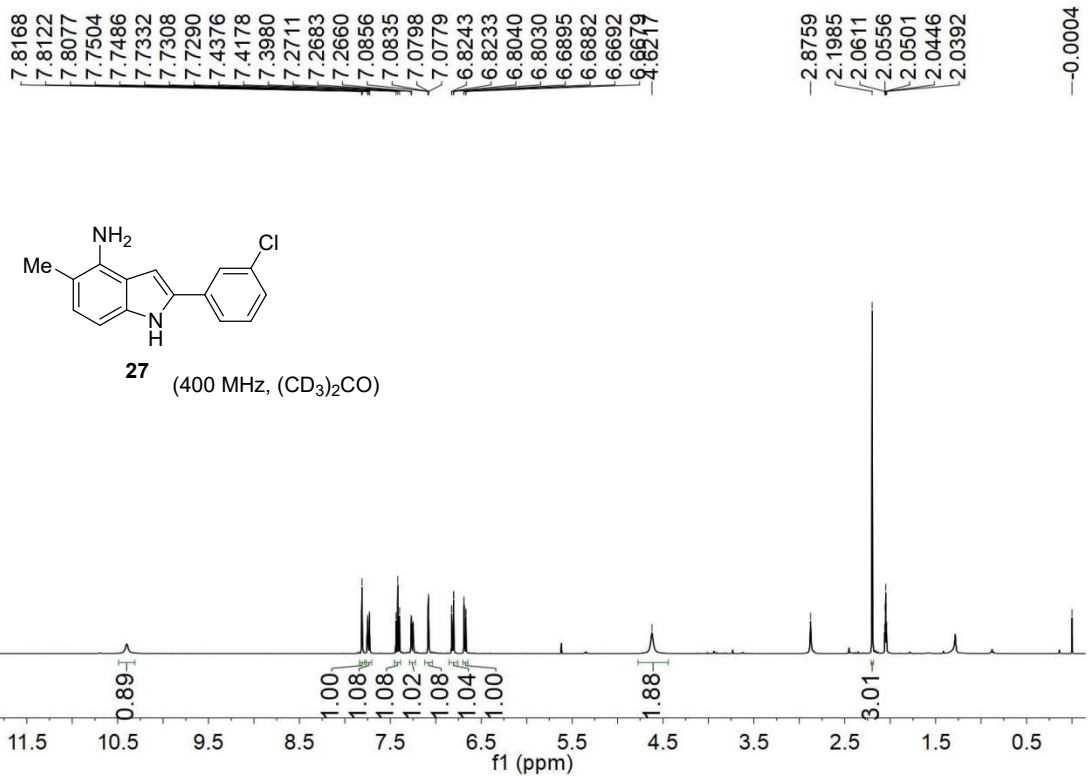




25 (100 MHz, $(CD_3)_2CO$)

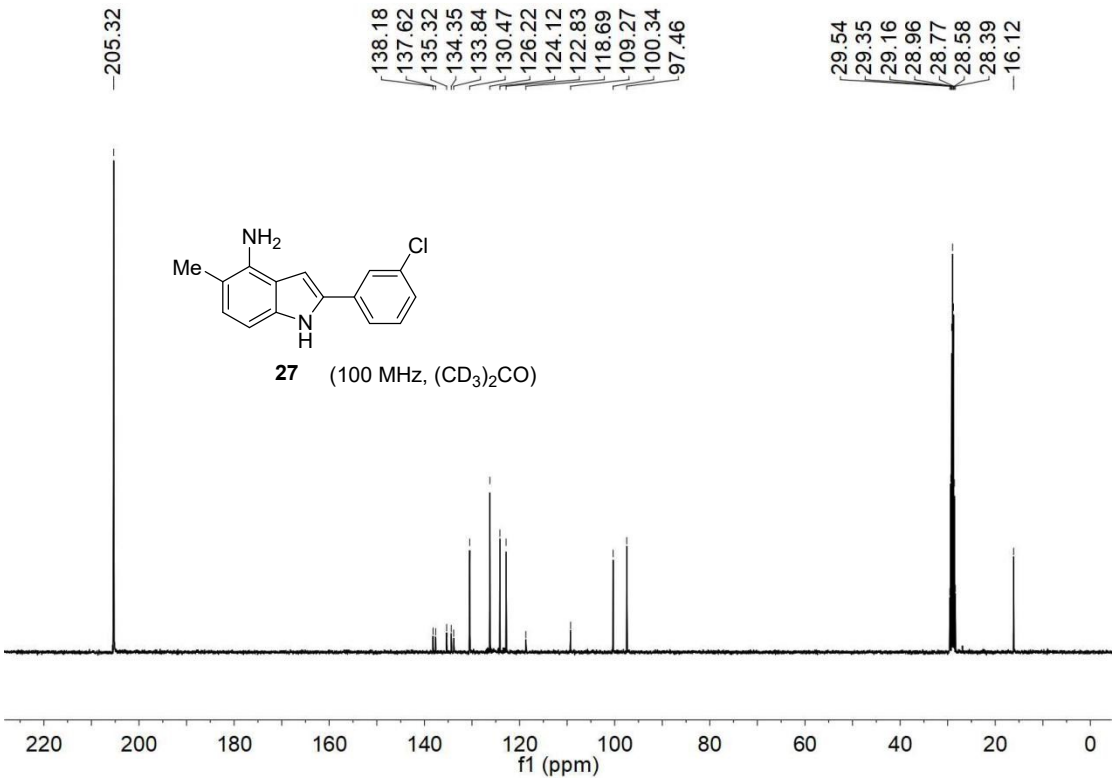

8.6818
7.6762
7.6720
7.4869
7.4837
7.3520
7.3487
7.2844
7.2741
7.2700
6.9944
6.9739
6.8637
6.8432
6.7934
6.7913
6.7879
3.9525
2.3055
NH2
Cl
Me
N
H
26
1.00
1.00
1.01
1.09
1.80
1.08
1.06
1.05
1.99
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


136.60
136.13
133.46
131.30
131.12
130.79
130.37
128.42
127.17
126.22
117.92
110.88
101.45
99.57
77.32
77.00
76.68
16.69
NH2
Cl
Me
N
H
26
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

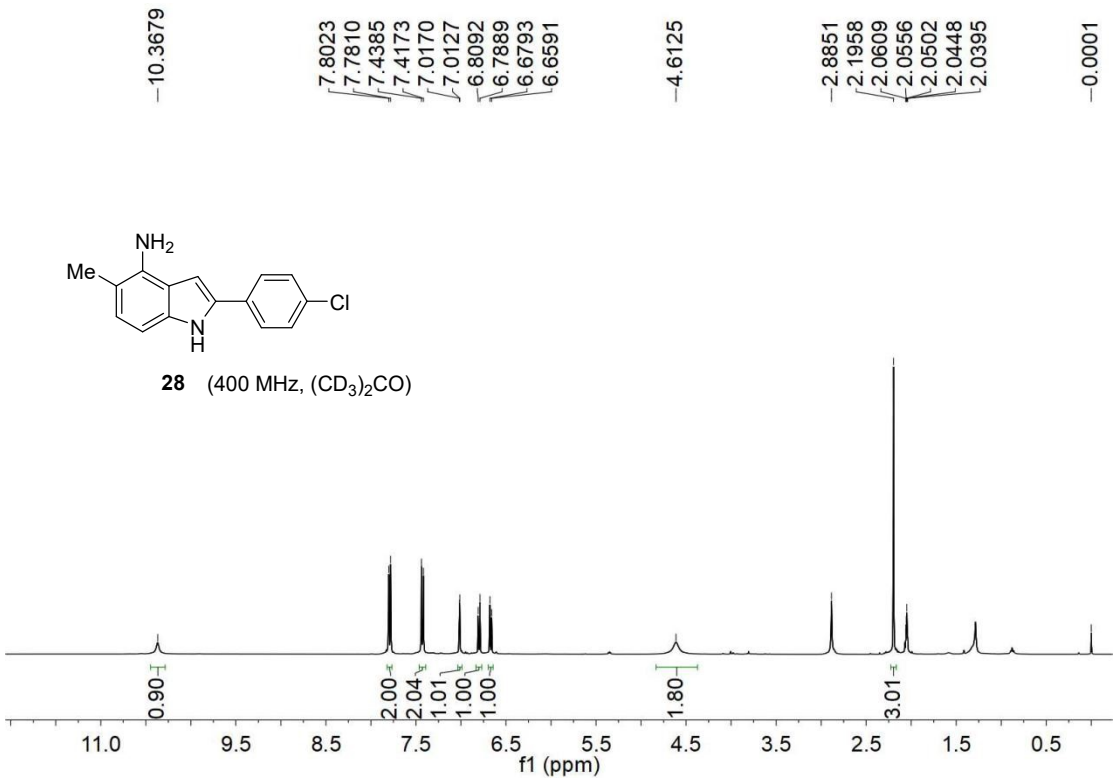


27

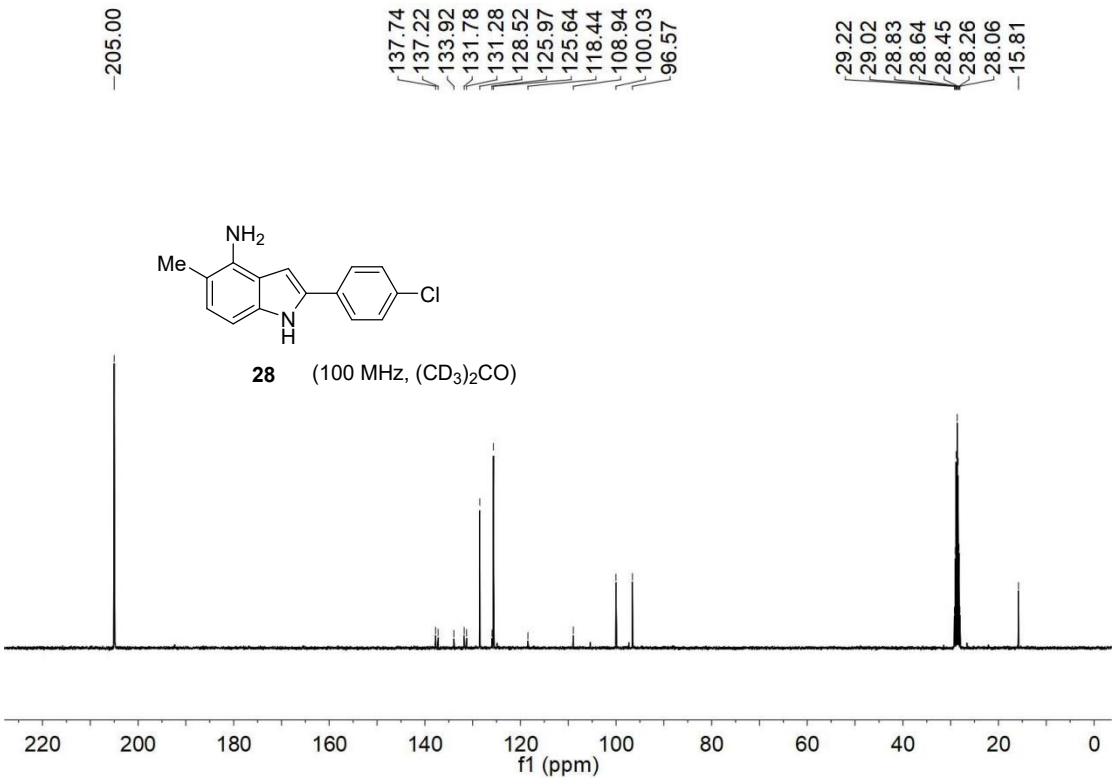
(400 MHz, $(CD_3)_2CO$)



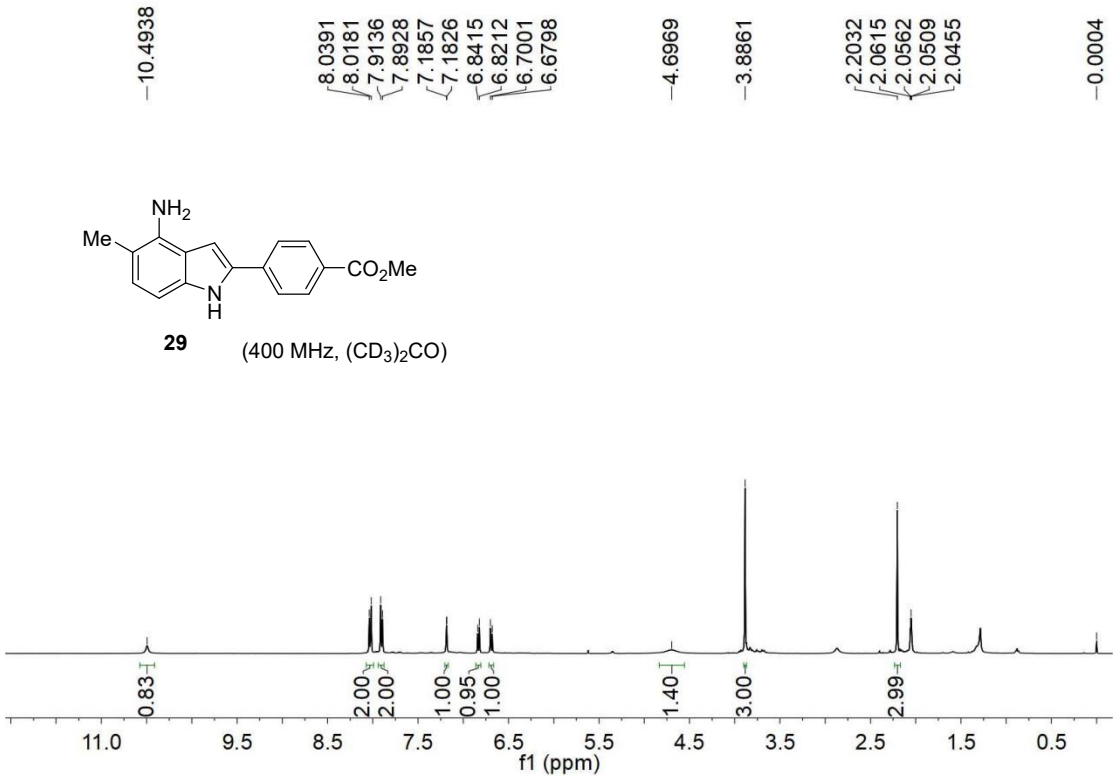
27 (100 MHz, $(CD_3)_2CO$)



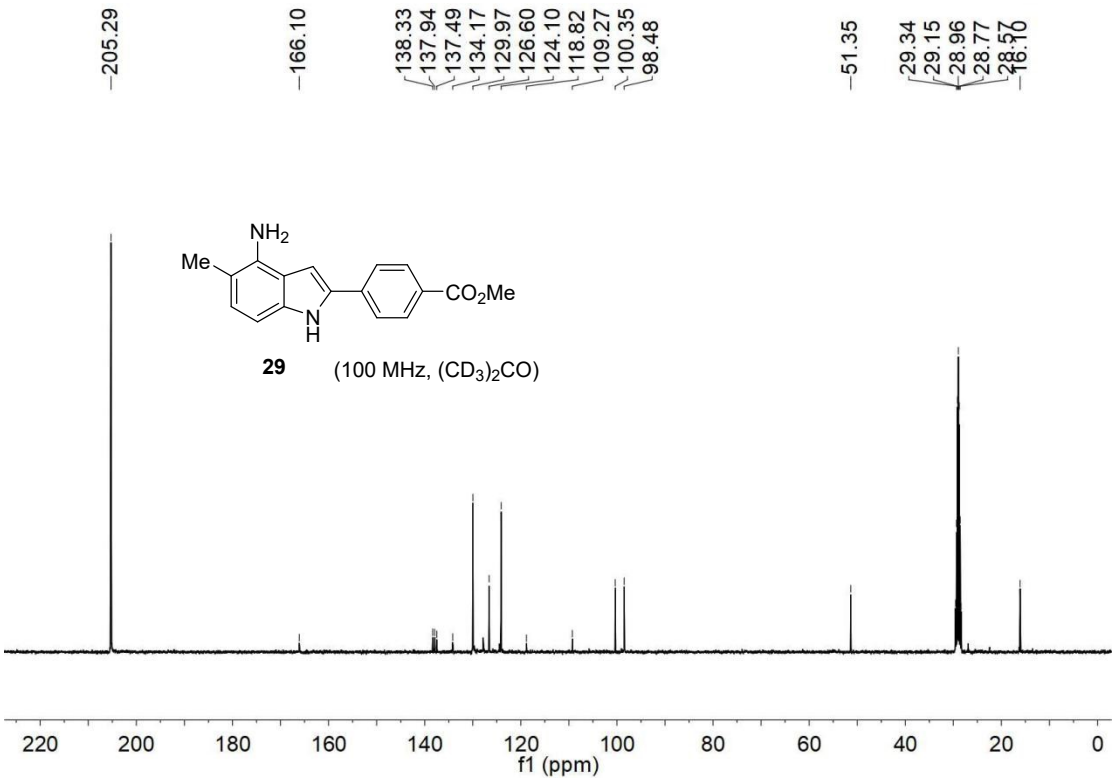
28 (400 MHz, $(CD_3)_2CO$)



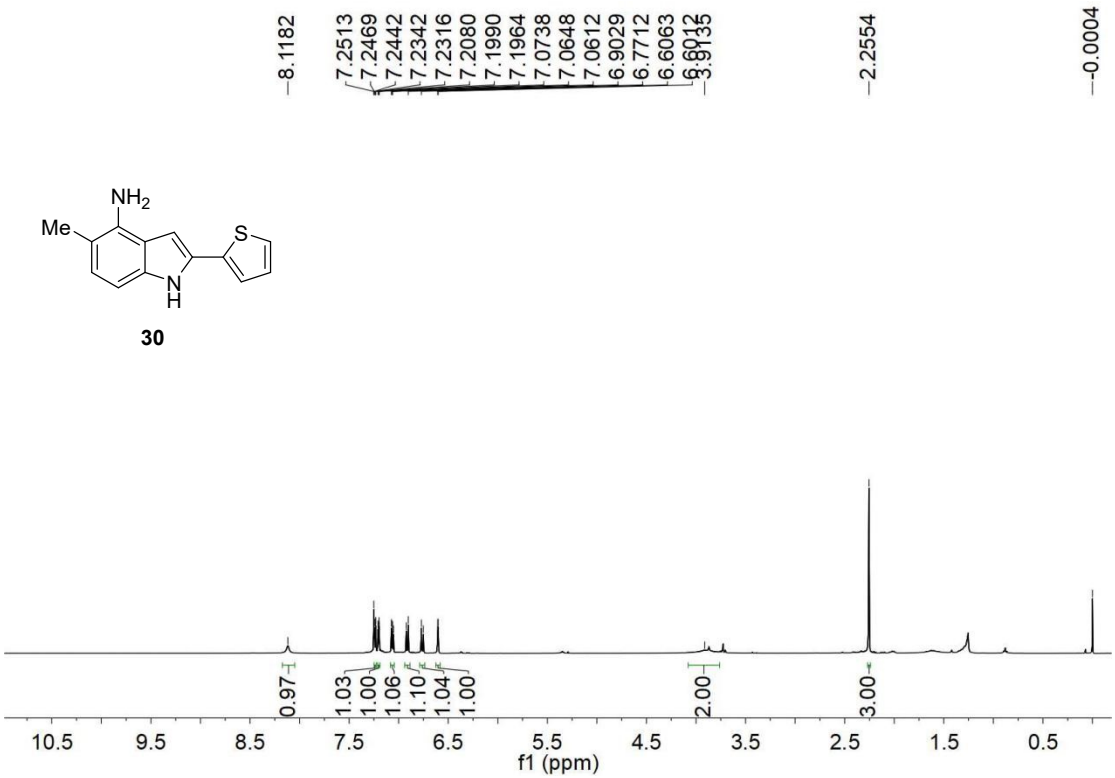
28 (100 MHz, $(CD_3)_2CO$)

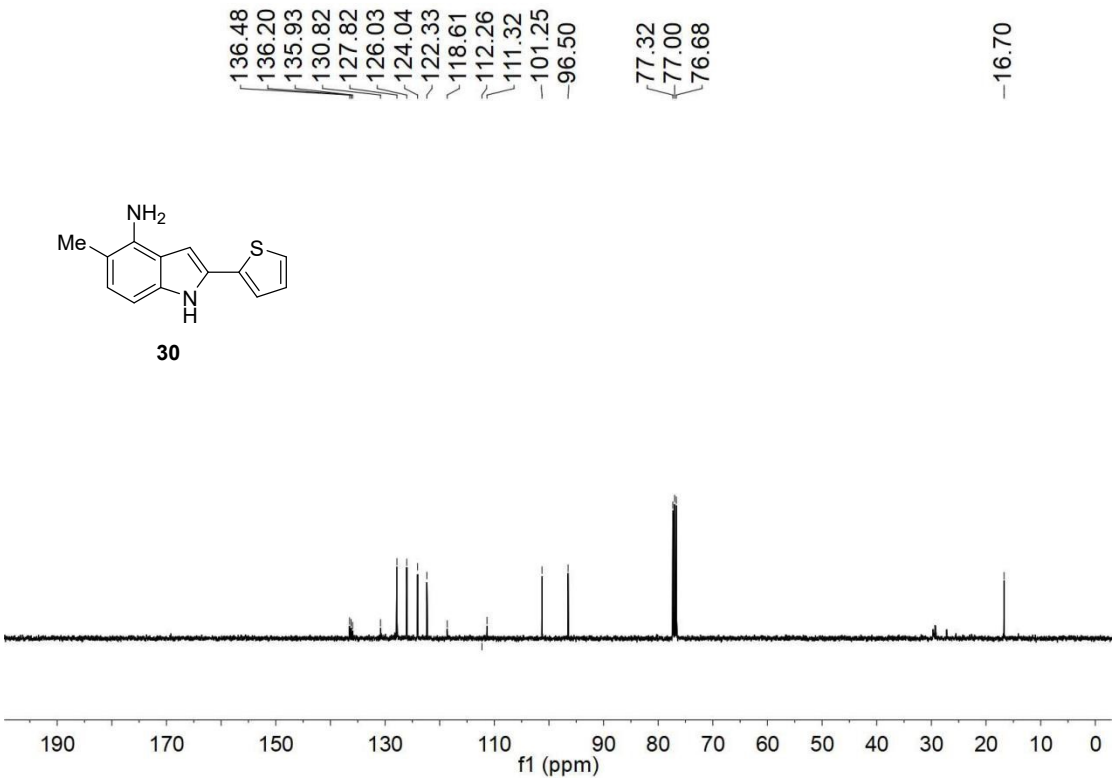


29 (400 MHz, $(CD_3)_2CO$)

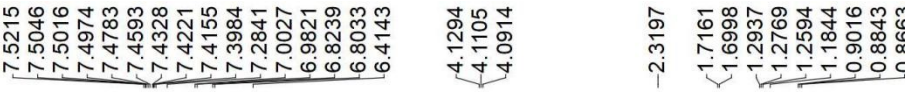


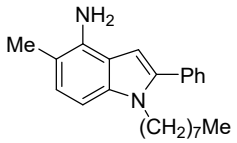
29 (100 MHz, $(CD_3)_2CO$)


8.1182
7.2513
7.2469
7.2442
7.2342
7.2316
7.2080
7.1990
7.1964
7.0738
7.0648
7.0612
6.9029
6.7712
6.6063
3.9135
2.2554
0.0004
NH2
Me
S
N
H
30
0.97
1.03
1.00
1.06
1.10
1.04
1.00
2.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

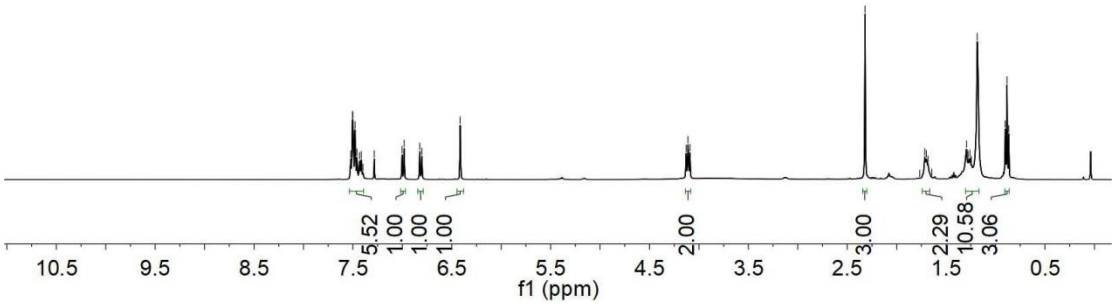

136.48
136.20
135.93
130.82
127.82
126.03
124.04
122.33
118.61
112.26
111.32
101.25
96.50
77.32
77.00
76.68
16.70
NH2
Me
S
N
H
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

30


7.5215
7.5046
7.5016
7.4974
7.4783
7.4593
7.4328
7.4221
7.4155
7.3984
7.2841
7.0027
6.9821
6.8239
6.8033
6.4143
4.1294
4.1105
4.0914
2.3197
1.7161
1.6998
1.2937
1.2769
1.2594
1.1844
0.9016
0.8843


NH2
Me
Ph
N
(CH2)7Me

32


5.52
1.00
1.00
1.00
2.00
3.00
2.29
10.58
3.06
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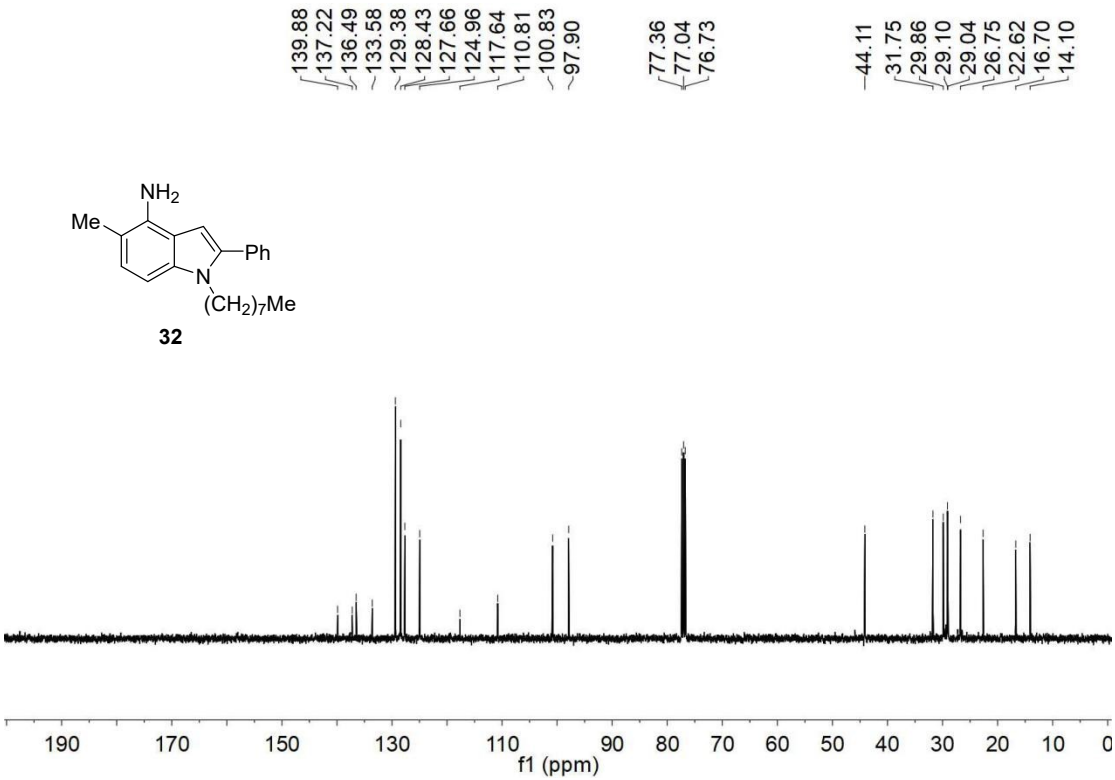
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97.90
77.36
77.04
76.73
44.11
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29.04
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16.70
14.10
NH2
Me
Ph
N
(CH2)7Me
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50
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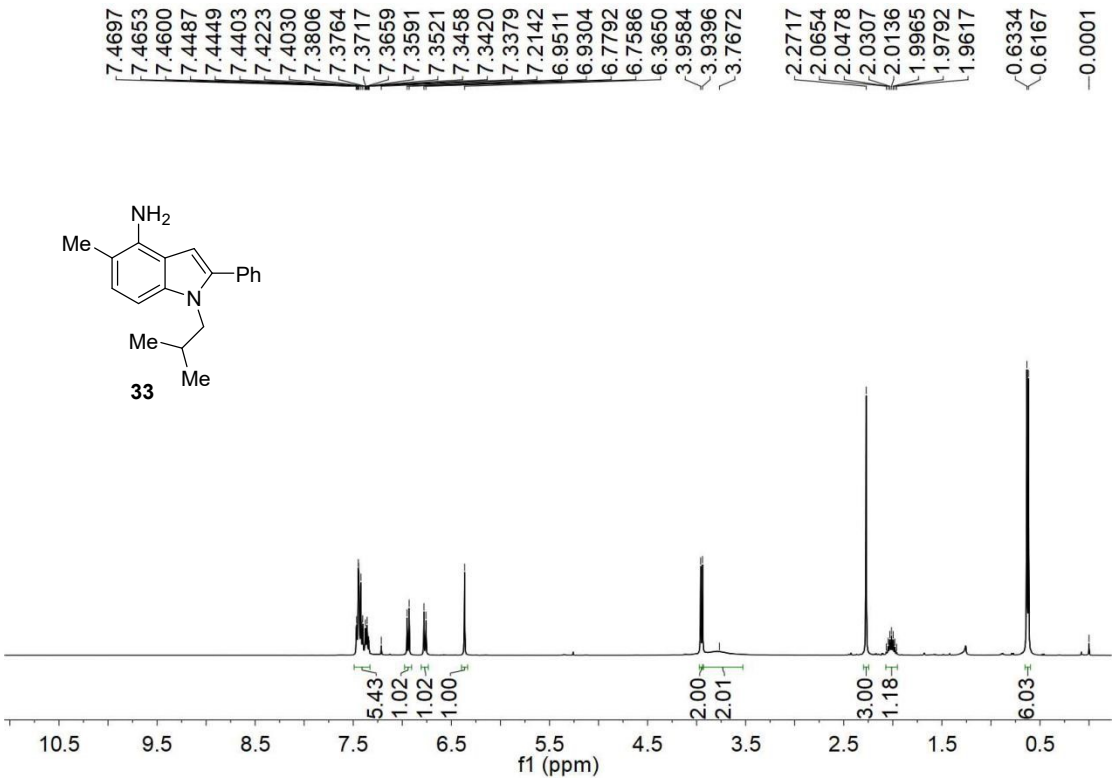
f1 (ppm)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7.4223
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7.3659
7.3591
7.3521
7.3458
7.3420
7.3379
7.2142
6.9511
6.9304
6.7792
6.7586
6.3650
3.9584
3.9396
3.7672
2.2717
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2.0307
2.0136
1.9965
1.9792
1.9617
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NH2
Me
Ph
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Me
Me
33
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1.00
2.00
2.01
3.00
1.18
6.03
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2.5
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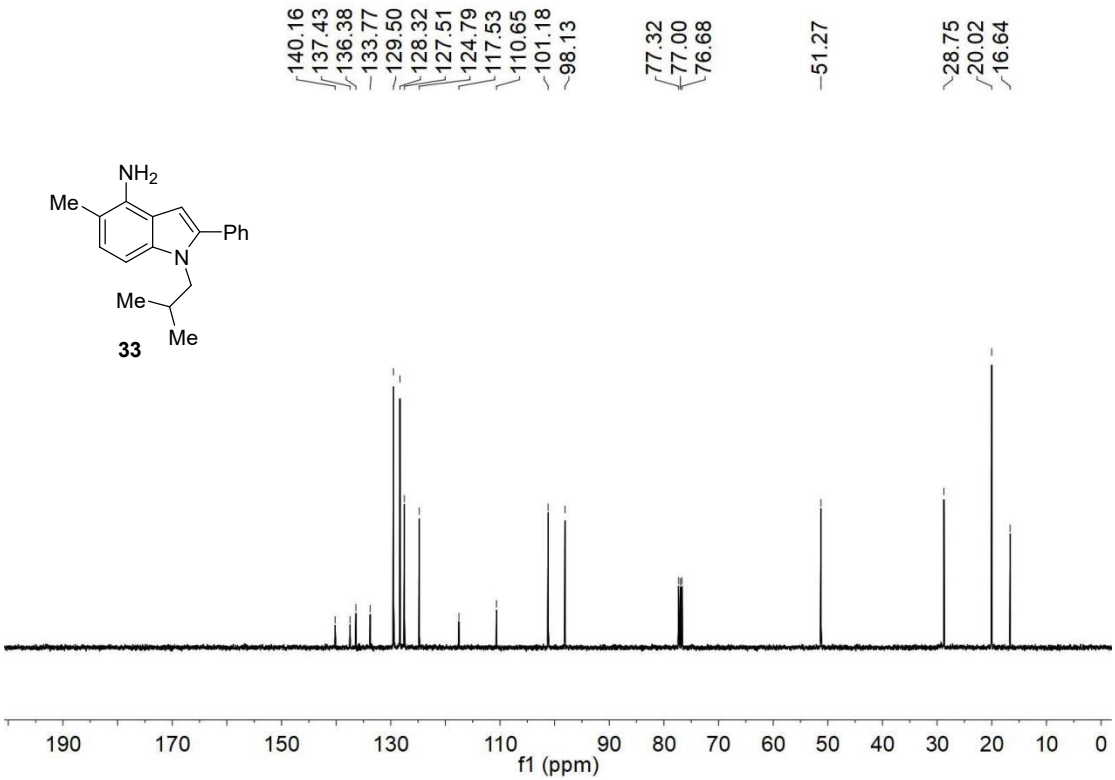
f1 (ppm)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77.00
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51.27
28.75
20.02
16.64
NH2
Me
Ph
N
Me
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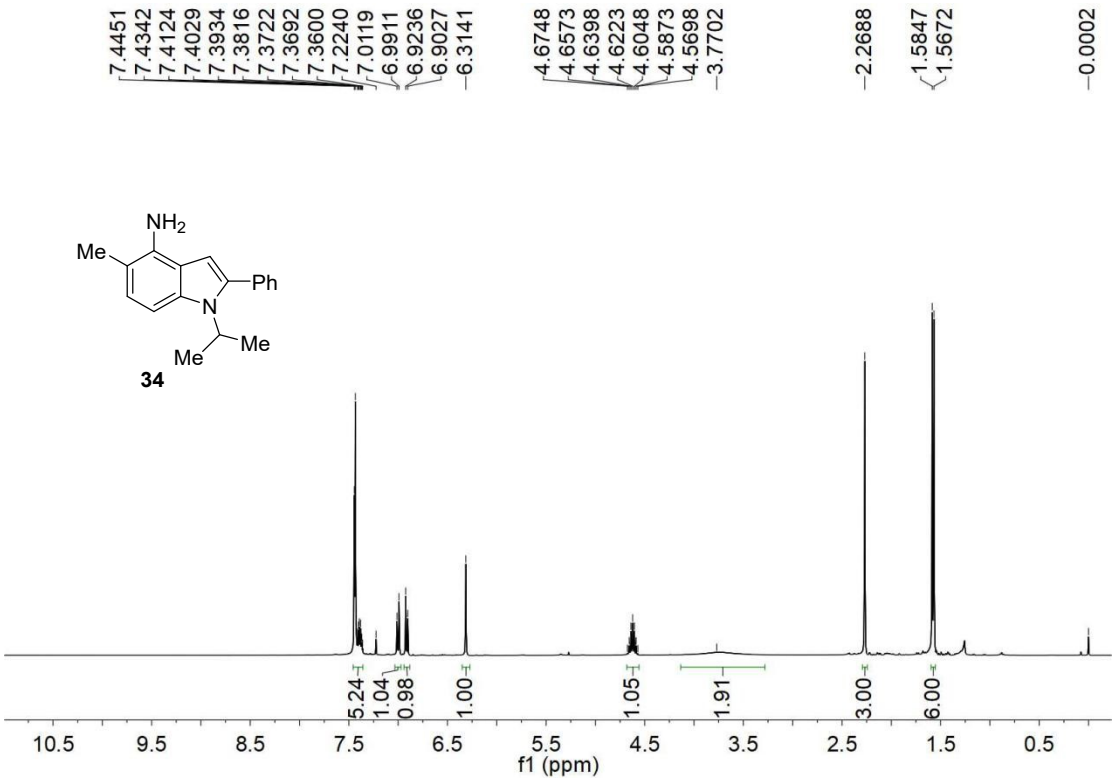
f1 (ppm)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6.9027
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4.5873
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2.2688
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0.0002
NH2
Me
Ph
N
Me
Me
34
5.24
1.04
0.98
1.00
1.05
1.91
3.00
6.00
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6.5
5.5
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3.5
2.5
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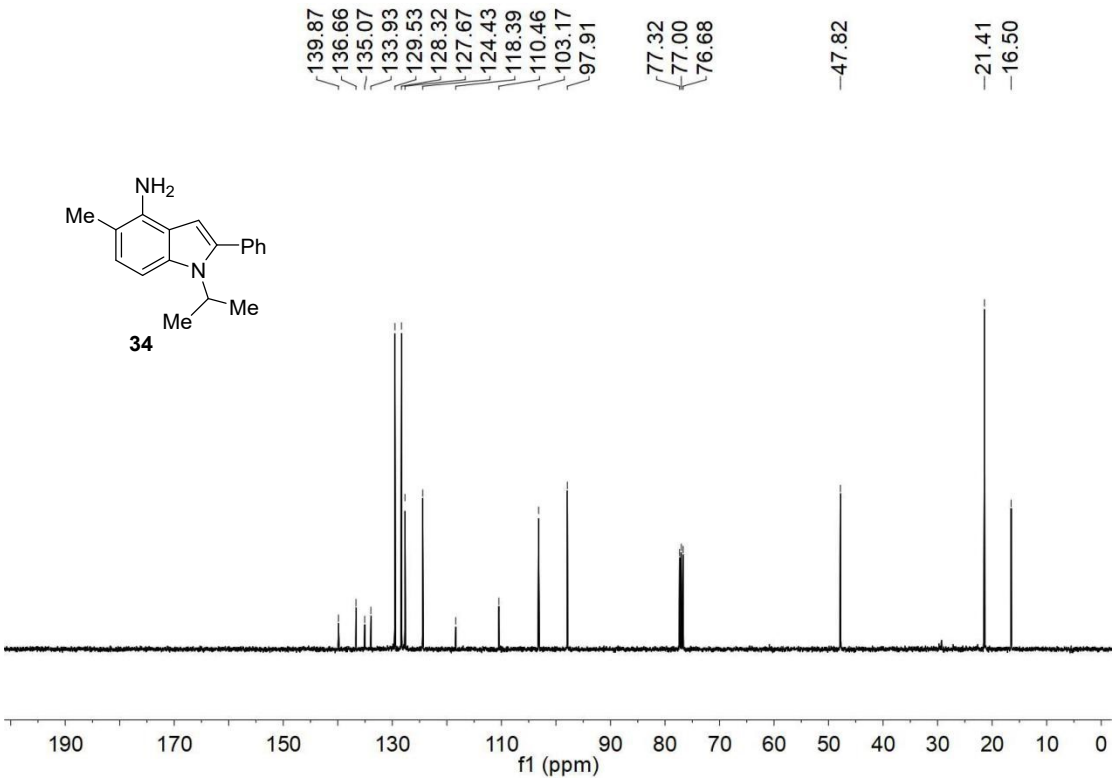
f1 (ppm)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97.91
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47.82
21.41
16.50
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Me
Ph
N
Me
Me
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130
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90
80
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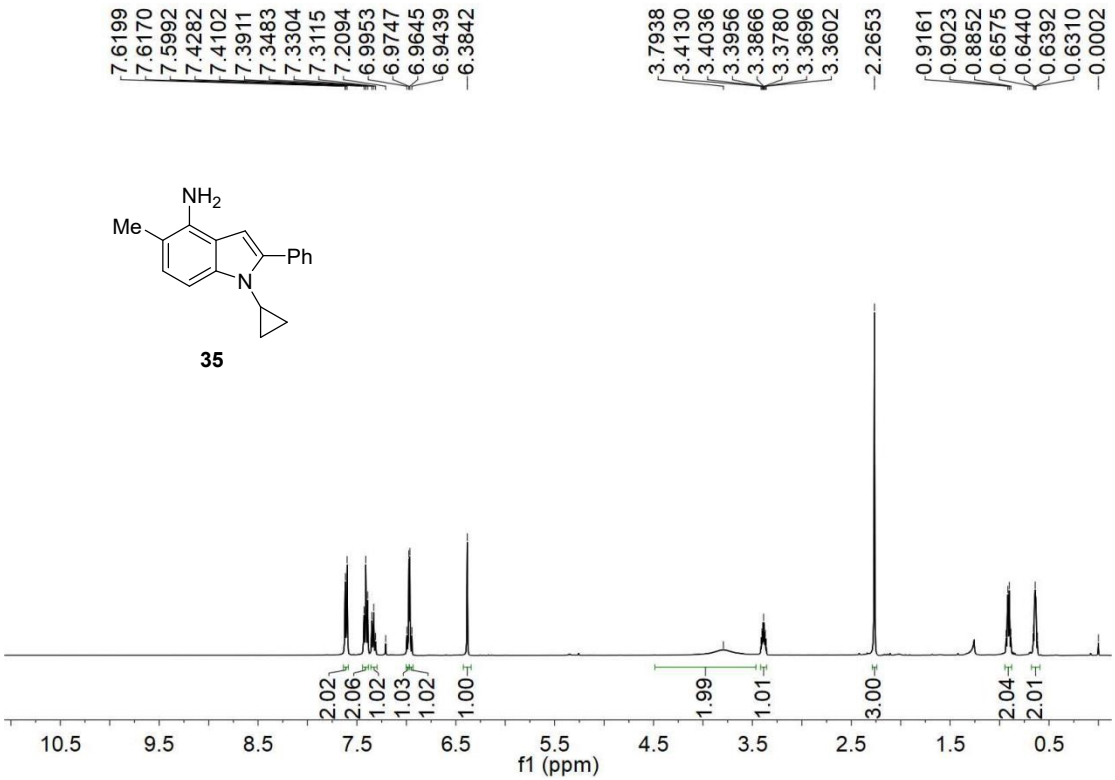
f1 (ppm)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7.3115
7.2094
6.9953
6.9747
6.9645
6.9439
6.3842
3.7938
3.4130
3.4036
3.3956
3.3866
3.3780
3.3696
3.3602
2.2653
0.9161
0.9023
0.8852
0.6575
0.6440
0.6392
0.6310
0.0002
NH2
Me
Ph
N
35
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1.02
1.03
1.02
1.00
1.99
1.01
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2.04
2.01
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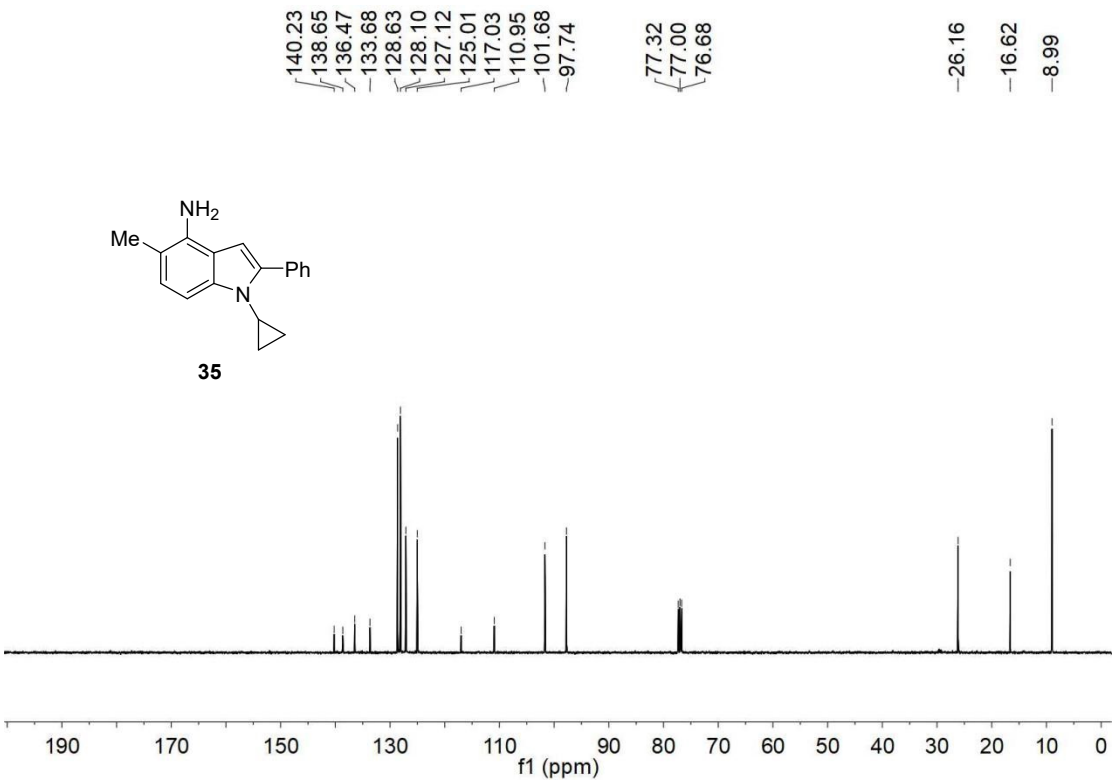
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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97.74
77.32
77.00
76.68
26.16
16.62
8.99
NH2
Me
Ph
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170
150
130
110
90
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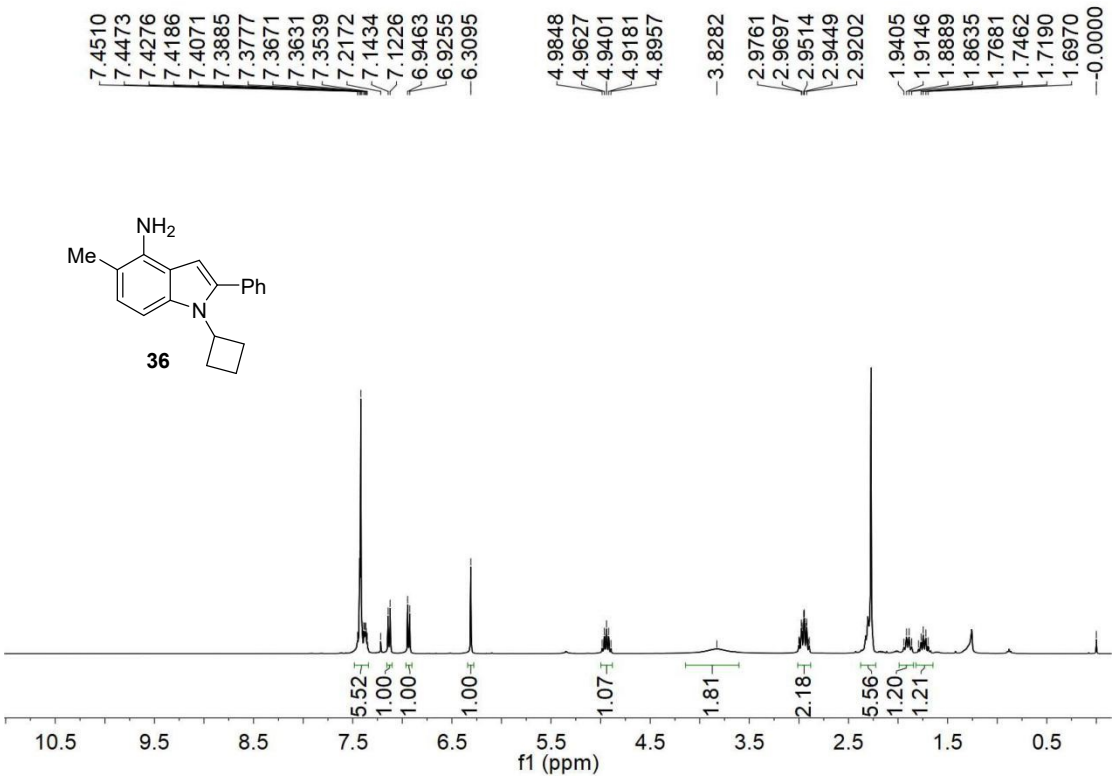
50
40
30
20
10
0
f1 (ppm)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7.3631
7.3539
7.2172
7.1434
7.1226
6.9463
6.9255
6.3095
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4.9627
4.9401
4.9181
4.8957
3.8282
2.9761
2.9697
2.9514
2.9449
2.9202
1.9405
1.9146
1.8889
1.8635
1.7681
1.7462
1.7190
1.6970
0.0000
NH2
Me
Ph
N
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1.00
1.00
1.07
1.81
2.18
5.56
1.20
1.21
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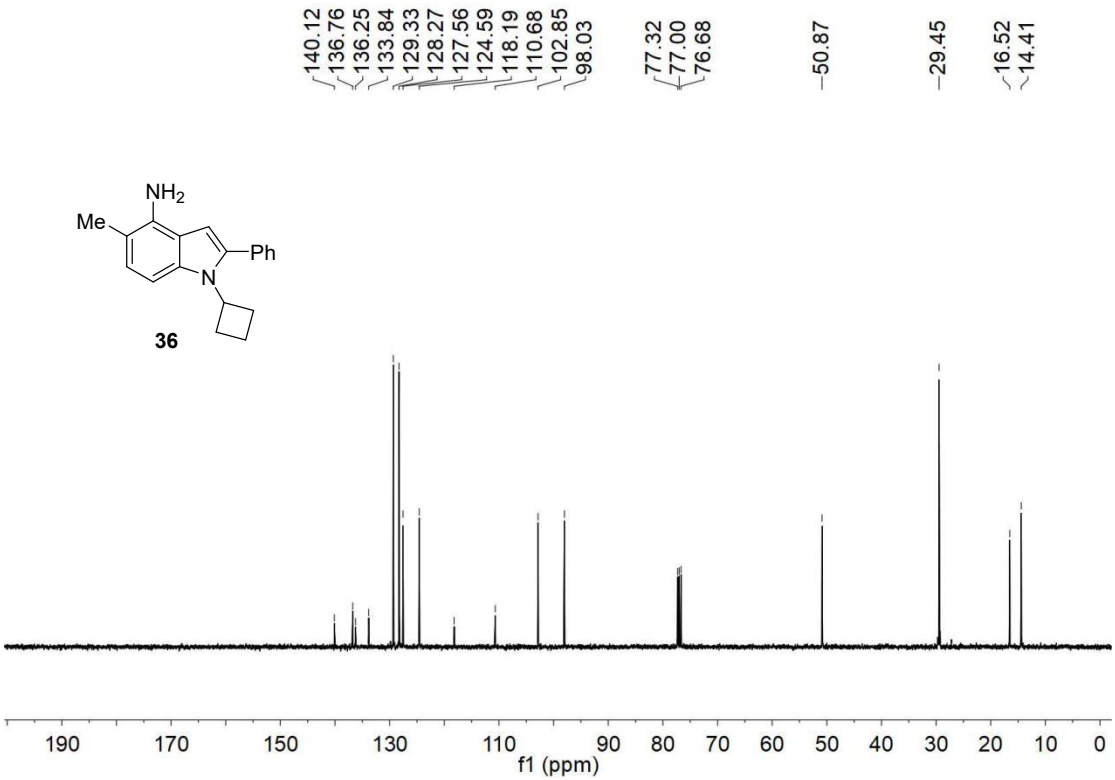
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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102.85
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77.32
77.00
76.68
50.87
29.45
16.52
14.41
NH2
Me
Ph
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170
150
130
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90
80
70
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50
40
30
20
10
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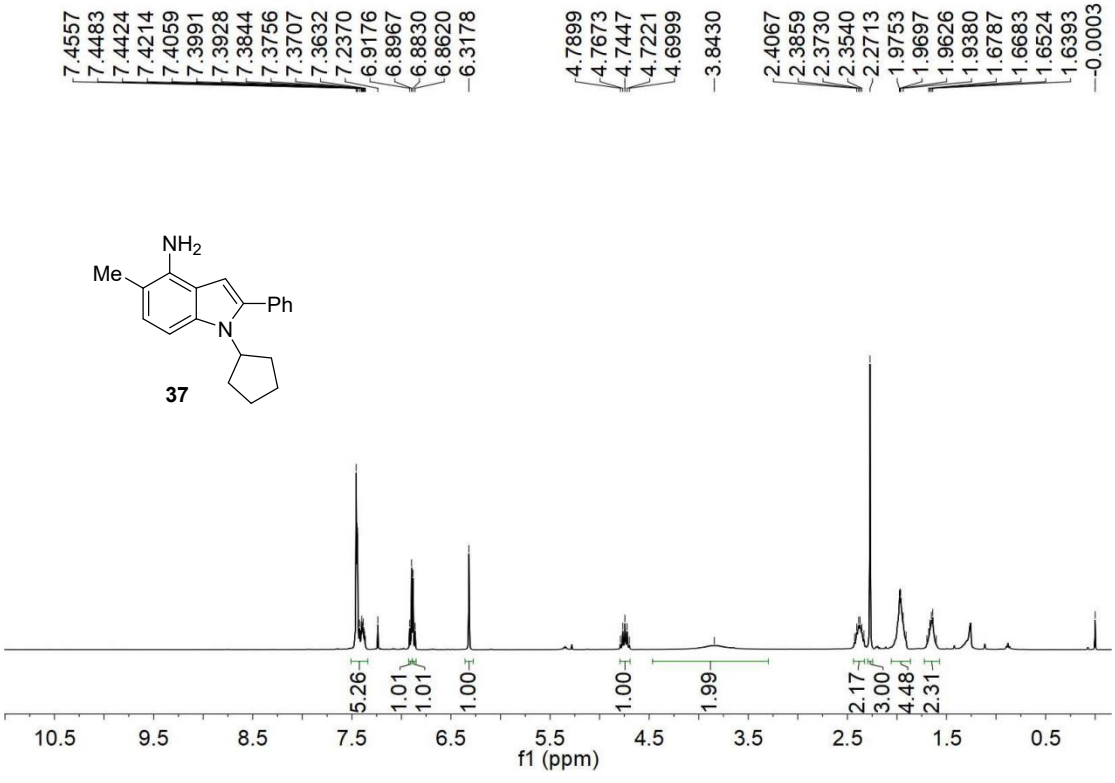
f1 (ppm)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6.8620
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4.7673
4.7447
4.7221
4.6999
3.8430
2.4067
2.3859
2.3730
2.3540
2.2713
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1.9697
1.9626
1.9380
1.6787
1.6683
1.6524
1.6393
0.0003
NH2
Me
Ph
N
37
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1.01
1.00
1.00
1.99
2.17
3.00
4.48
2.31
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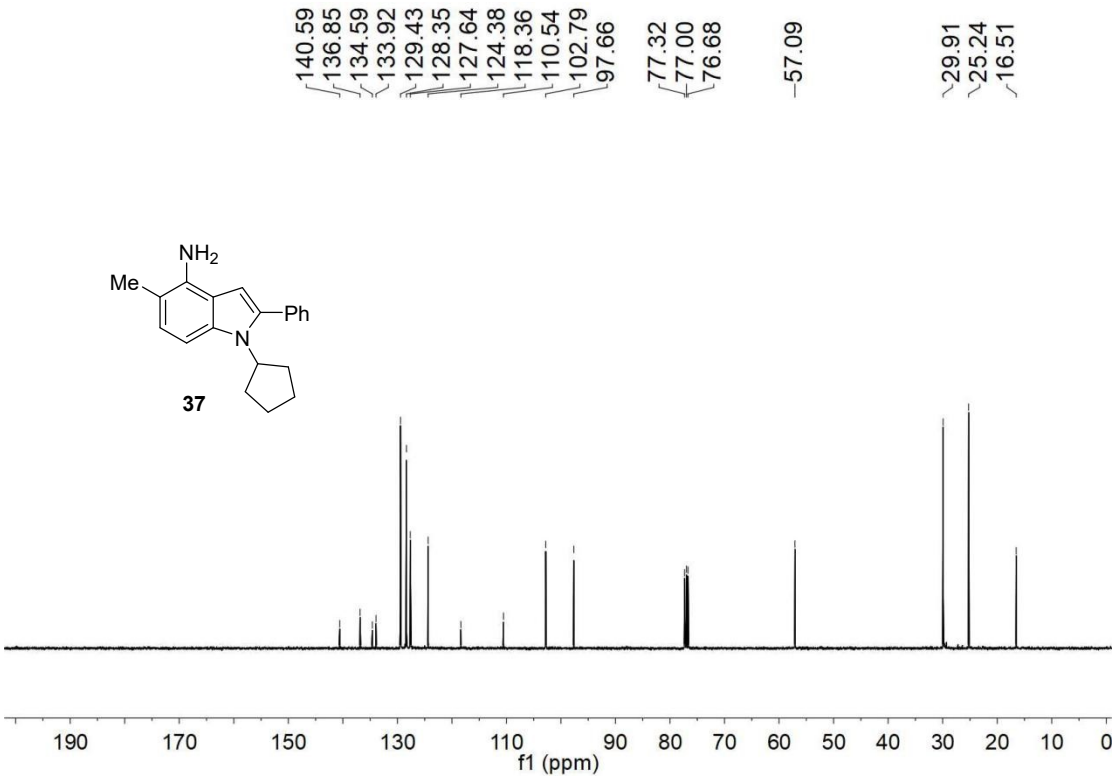
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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124.38
118.36
110.54
102.79
97.66
77.32
77.00
76.68
57.09
29.91
25.24
16.51
NH2
Me
Ph
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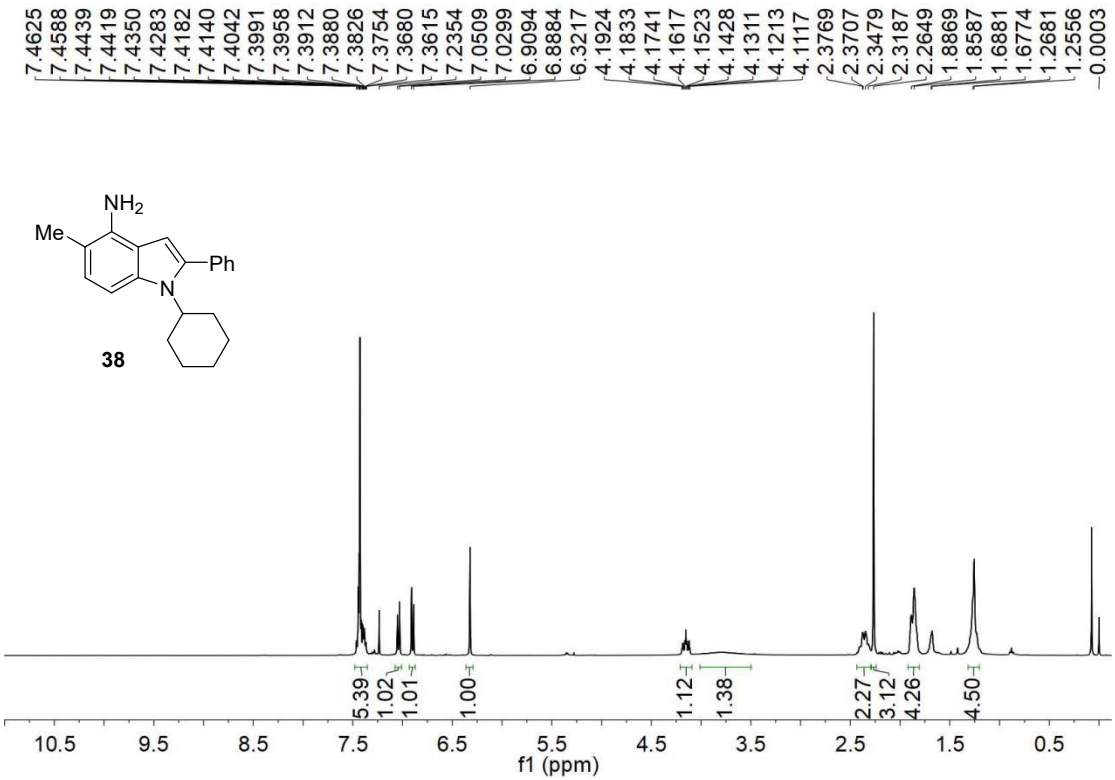
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.3912
7.3880
7.3826
7.3754
7.3680
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7.2354
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4.1833
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4.1617
4.1523
4.1428
4.1311
4.1213
4.1117
2.3769
2.3707
2.3479
2.3187
2.2649
1.8869
1.8587
1.6881
1.6774
1.2681
1.2556
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Me
Ph
N
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5.39
1.02
1.01
1.00
1.12
1.38
2.27
3.12
4.26
4.50
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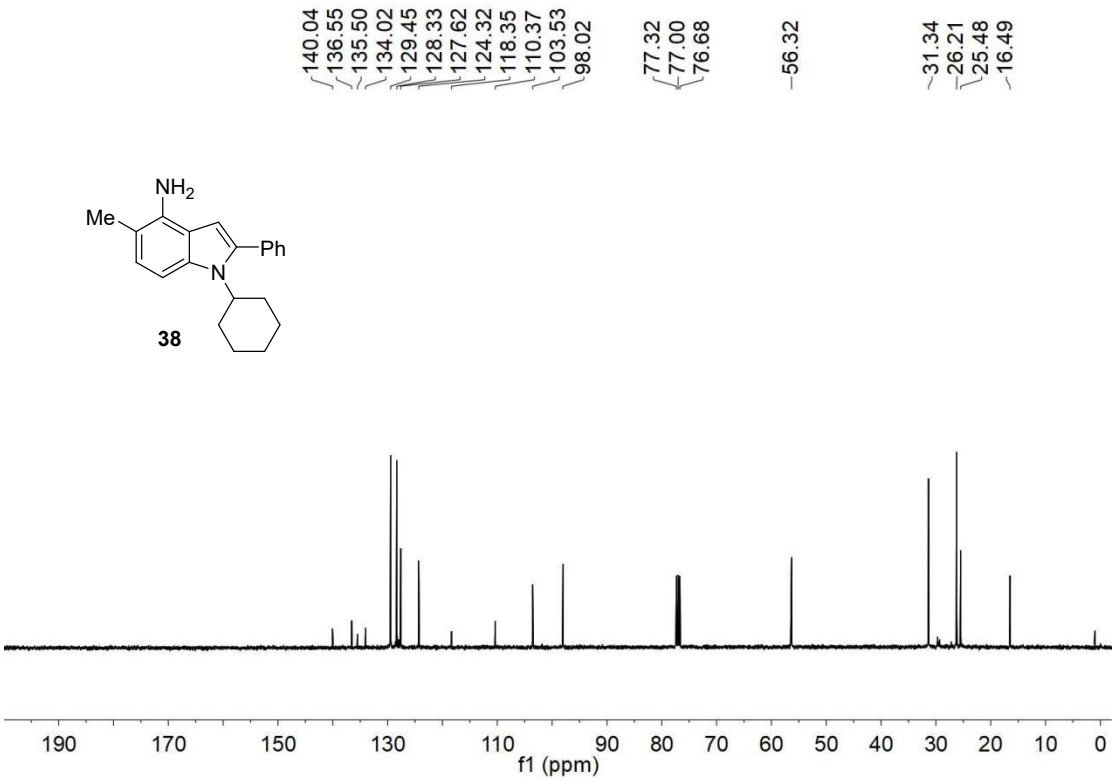
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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124.32
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103.53
98.02
77.32
77.00
76.68
56.32
31.34
26.21
25.48
16.49
NH2
Me
Ph
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170
150
130
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90
80
70
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50
40
30
20
10
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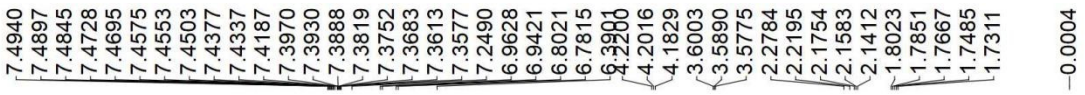
f1 (ppm)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7.4187
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7.3930
7.3888
7.3819
7.3752
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7.3613
7.3577
7.2490
6.9628
6.9421
6.8021
6.7815
4.2200
4.2016
4.1829
3.6003
3.5890
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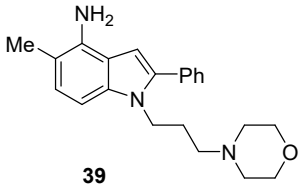
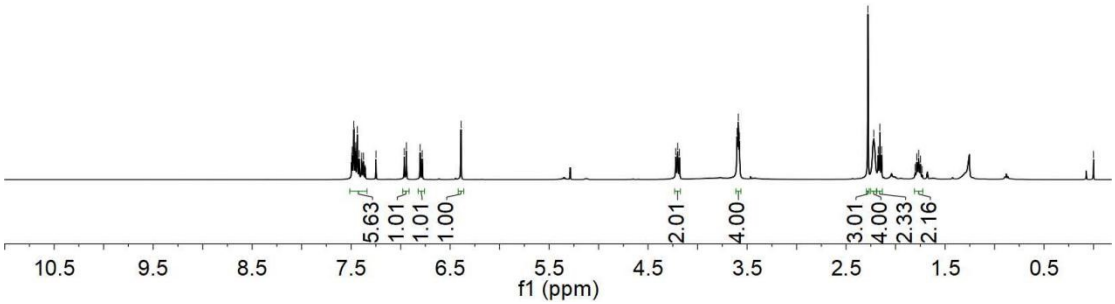

NH2
Me
Ph
N
N
O

39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4.00
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2.16
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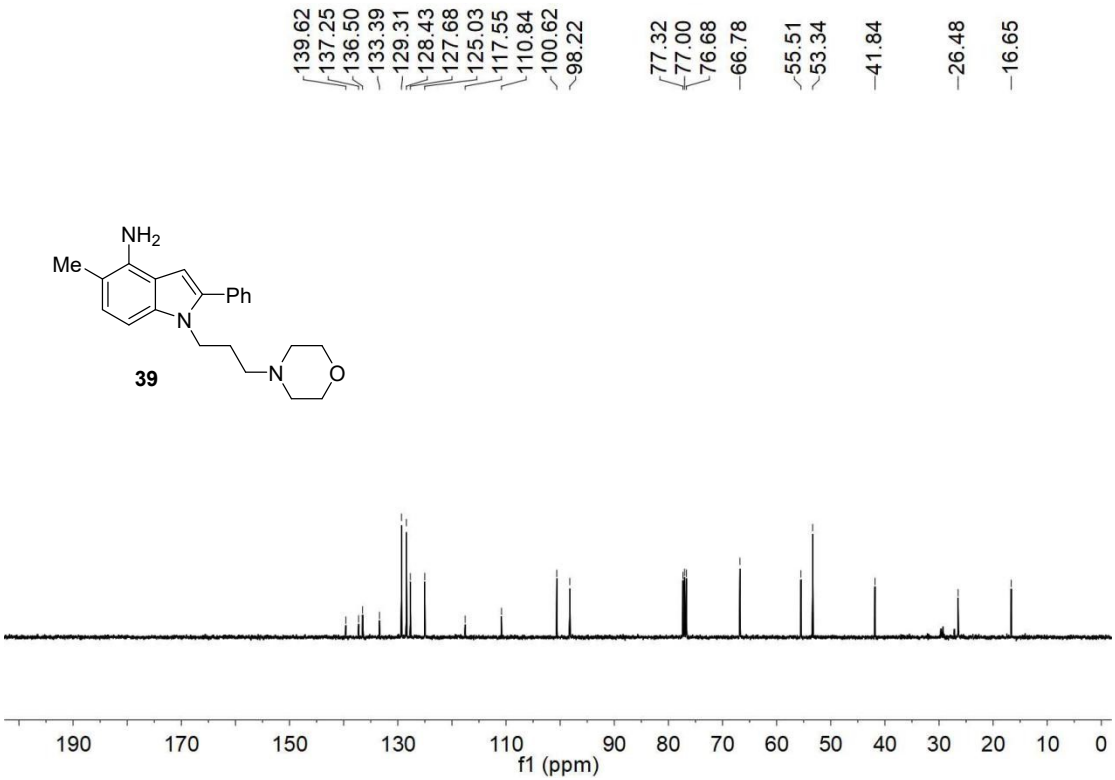
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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125.03
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100.62
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77.32
77.00
76.68
66.78
55.51
53.34
41.84
26.48
16.65
NH2
Me
Ph
N
N
O
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170
150
130
110
90
80
70
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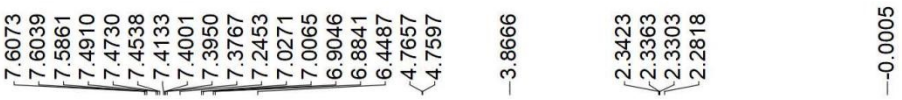
50
40
30
20
10
0
f1 (ppm)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7.4730
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7.4001
7.3950
7.3767
7.2453
7.0271
7.0065
6.9046
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2.2818
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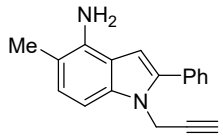
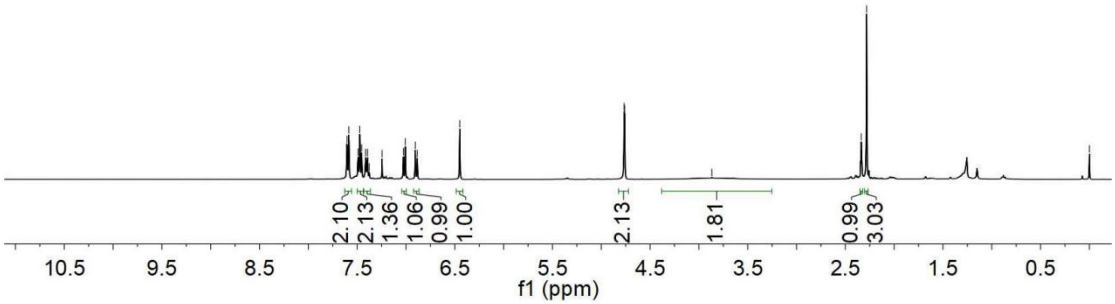

NH2
Me
Ph
N

40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1.00
2.13
1.81
0.99
3.03
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7.5
6.5
5.5
4.5
3.5
2.5
1.5
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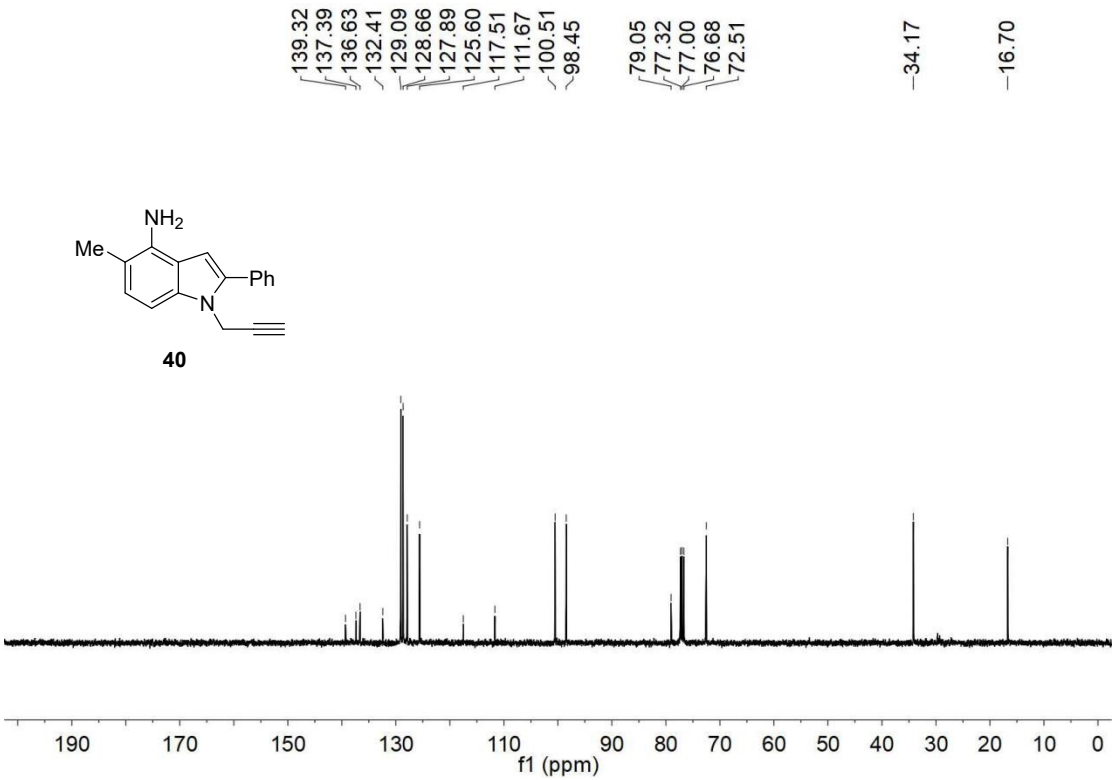
f1 (ppm)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125.60
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111.67
100.51
98.45
79.05
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77.00
76.68
72.51
34.17
16.70
NH2
Me
Ph
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130
110
90
80
70
60
50
40
30
20
10
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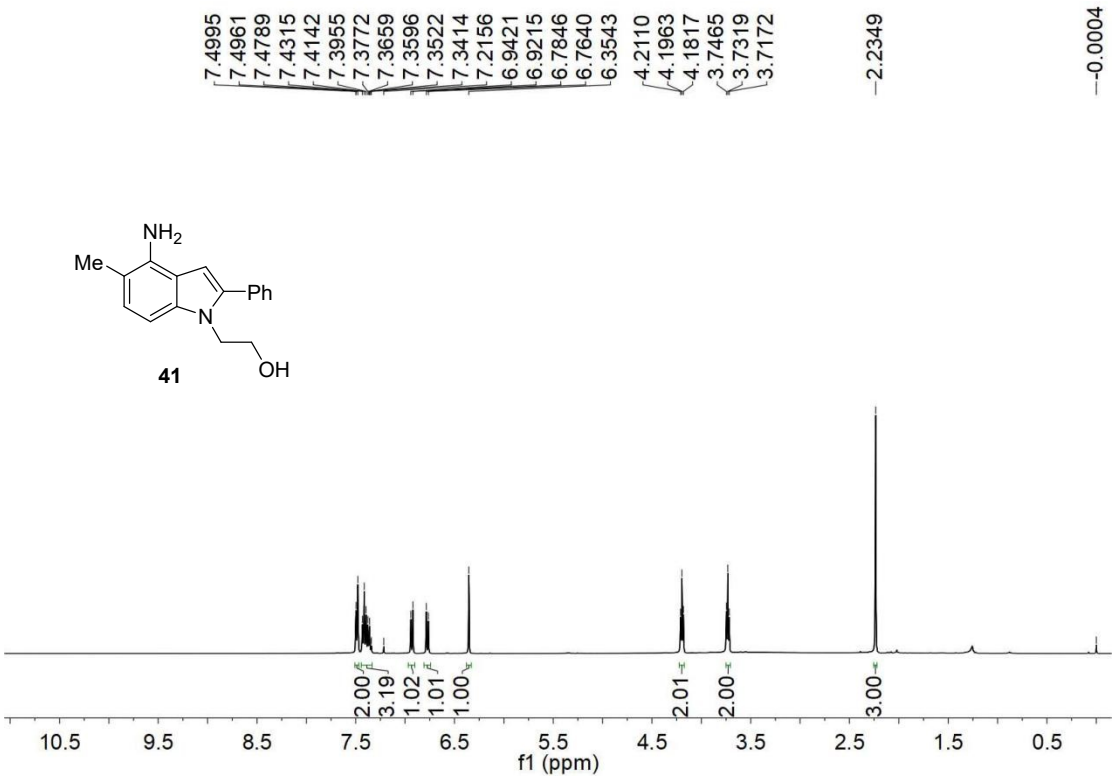
f1 (ppm)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7.2156
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6.9215
6.7846
6.7640
6.3543
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4.1963
4.1817
3.7465
3.7319
3.7172
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Me
Ph
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OH
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1.01
1.00
2.01
2.00
3.00
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7.5
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5.5
4.5
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2.5
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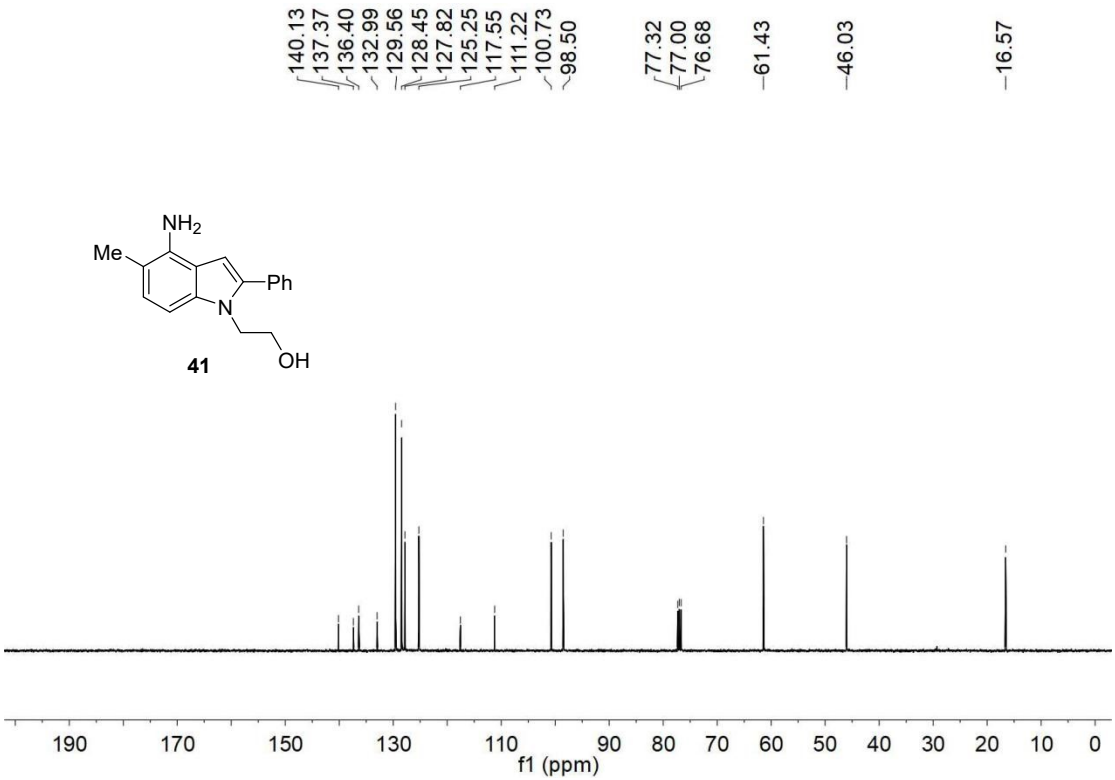
f1 (ppm)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117.55
111.22
100.73
98.50
77.32
77.00
76.68
61.43
46.03
16.57
NH2
Me
Ph
N
OH
41
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


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7.4204
7.4037
7.3990
7.3892
7.3819
7.2437
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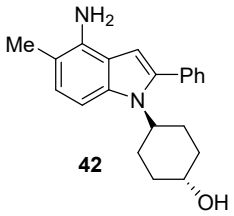
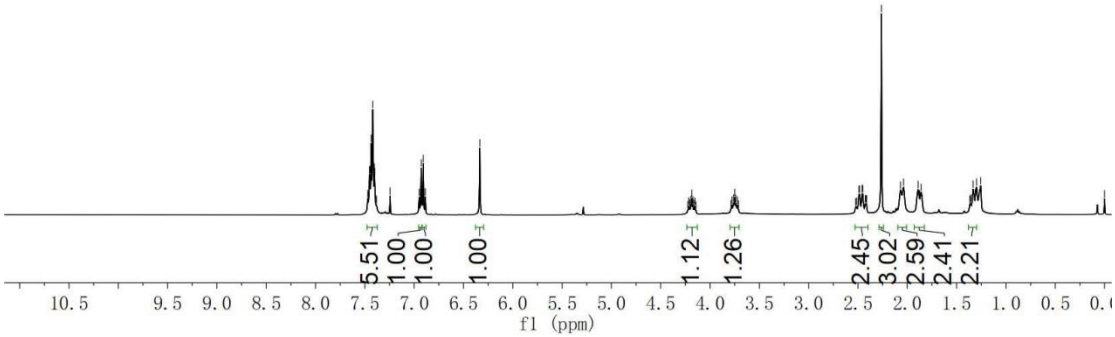

NH2
Me
Ph
N
OH

42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1.00
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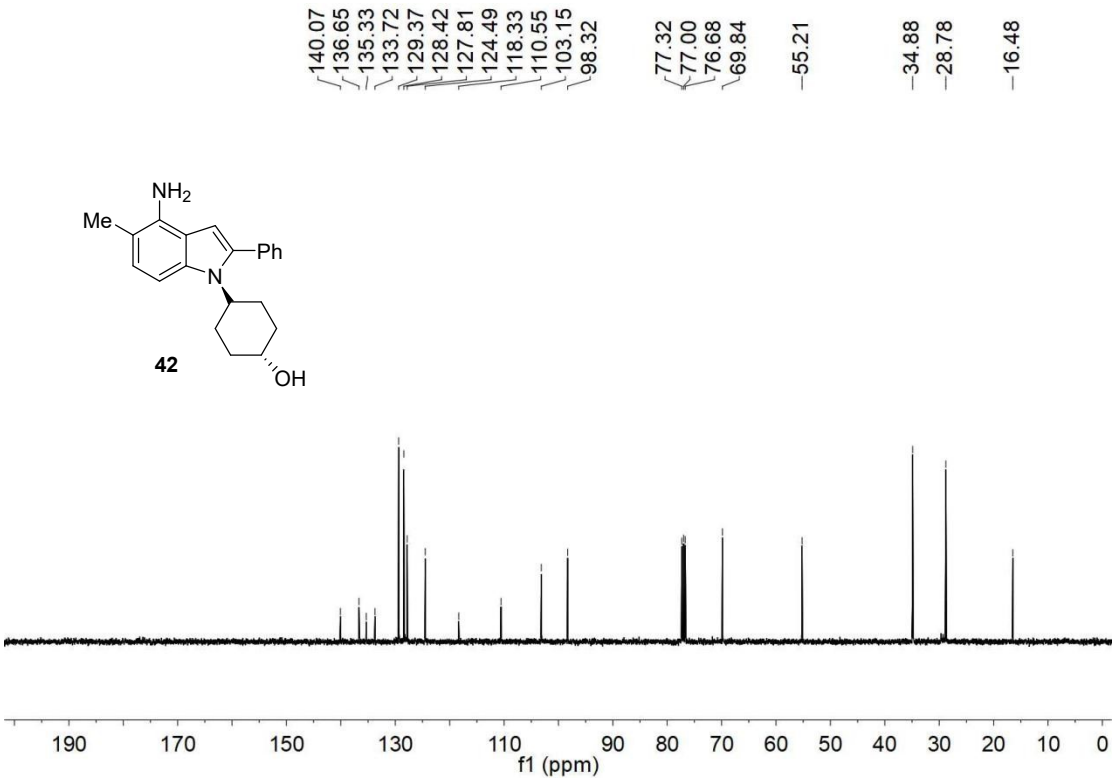
3.02
2.59
2.41
2.21
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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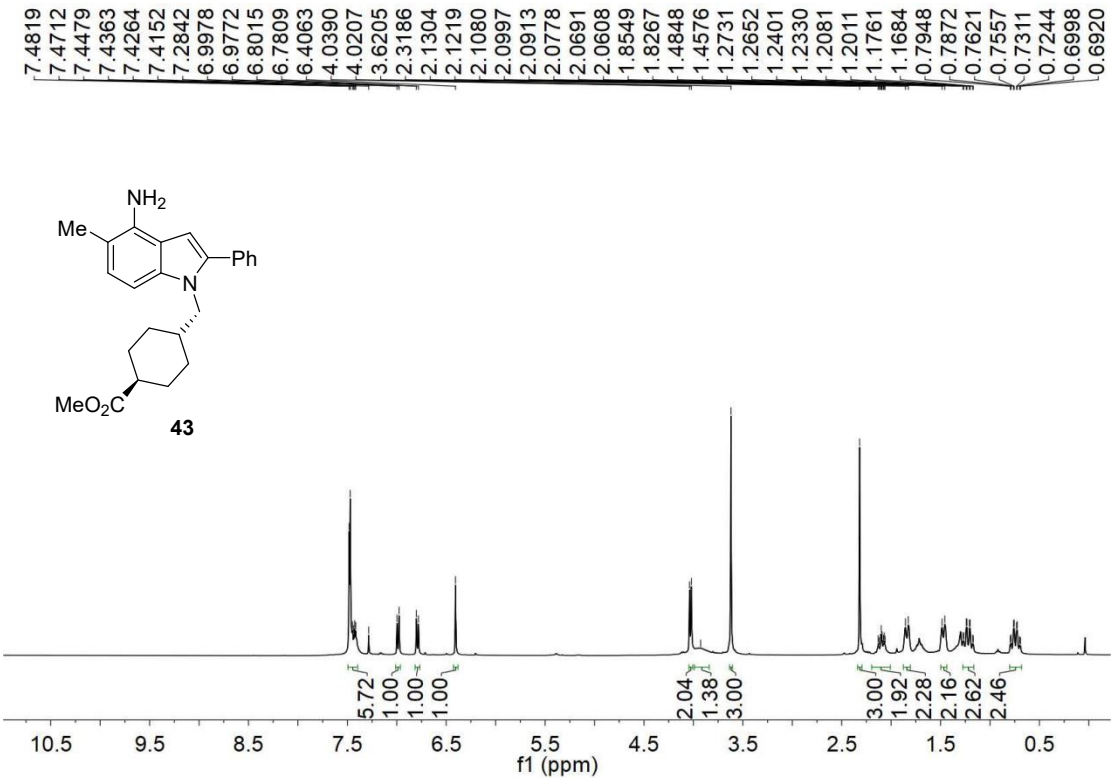
136.65
135.33
133.72
129.37
128.42
127.81
124.49
118.33
110.55
103.15
98.32
77.32
77.00
76.68
69.84
55.21
34.88
28.78
16.48
NH2
Me
Ph
N
OH
42
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4363
7.4264
7.4152
7.2842
6.9978
6.9772
6.8015
6.7809
6.4063
4.0390
4.0207
3.6205
2.3186
2.1304
2.1219
2.1080
2.0997
2.0913
2.0778
2.0691
2.0608
1.8549
1.8267
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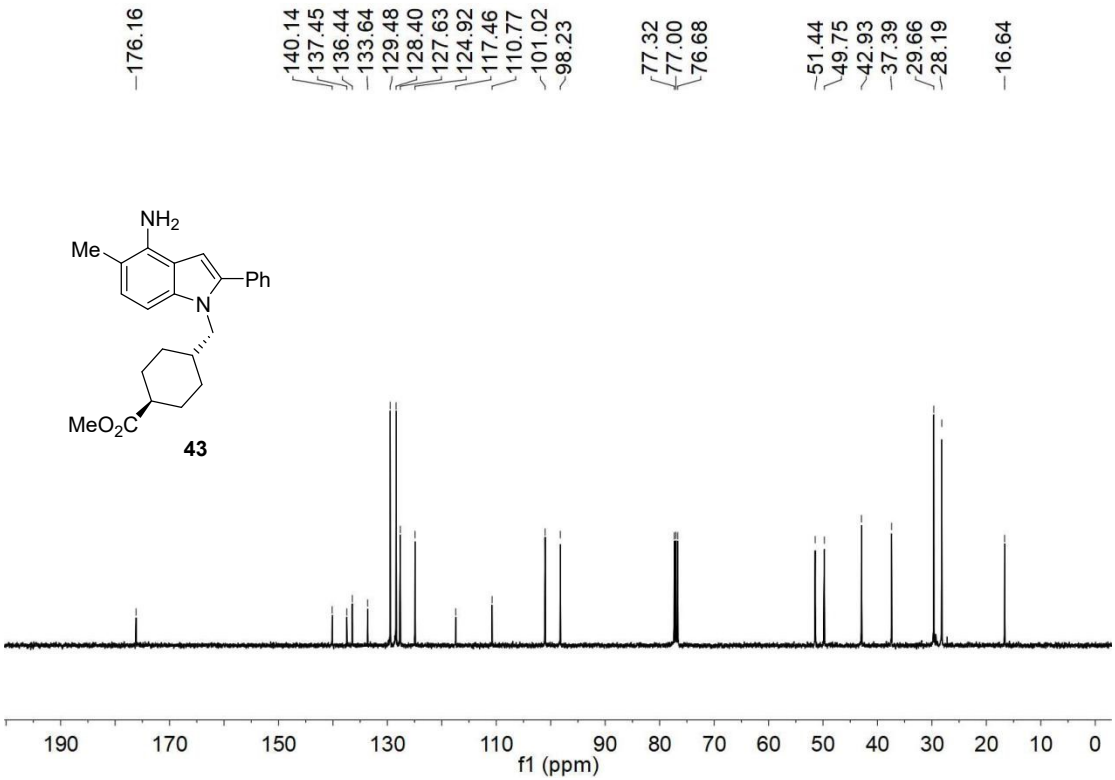
1.4576
1.2731
1.2652
1.2401
1.2330
1.2081
1.2011
1.1761
1.1684
0.7948
0.7872
0.7621
0.7557
0.7311
0.7244
0.6998
0.6920
NH2
Me
Ph
N
MeO2C
43
5.72
1.00
1.00
1.00
2.04
1.38
3.00
3.00
1.92
2.28
2.16
2.62
2.46
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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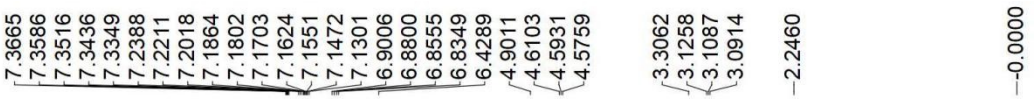
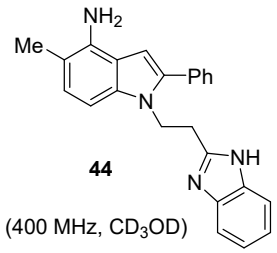
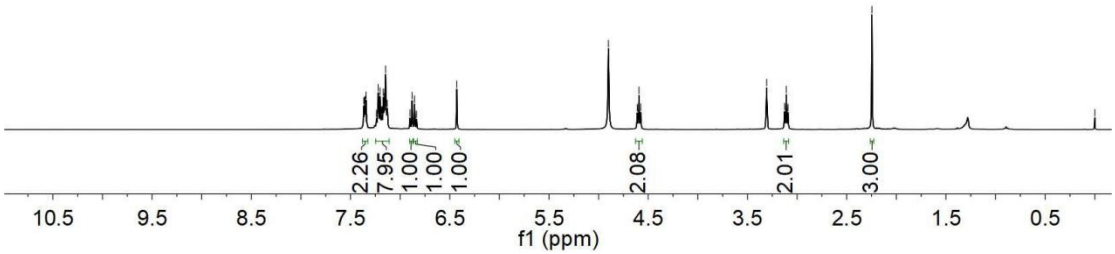
136.44
133.64
129.48
128.40
127.63
124.92
117.46
110.77
101.02
98.23
77.32
77.00
76.68
51.44
49.75
42.93
37.39
29.66
28.19
16.64
NH2
Me
Ph
N
MeO2C
43
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

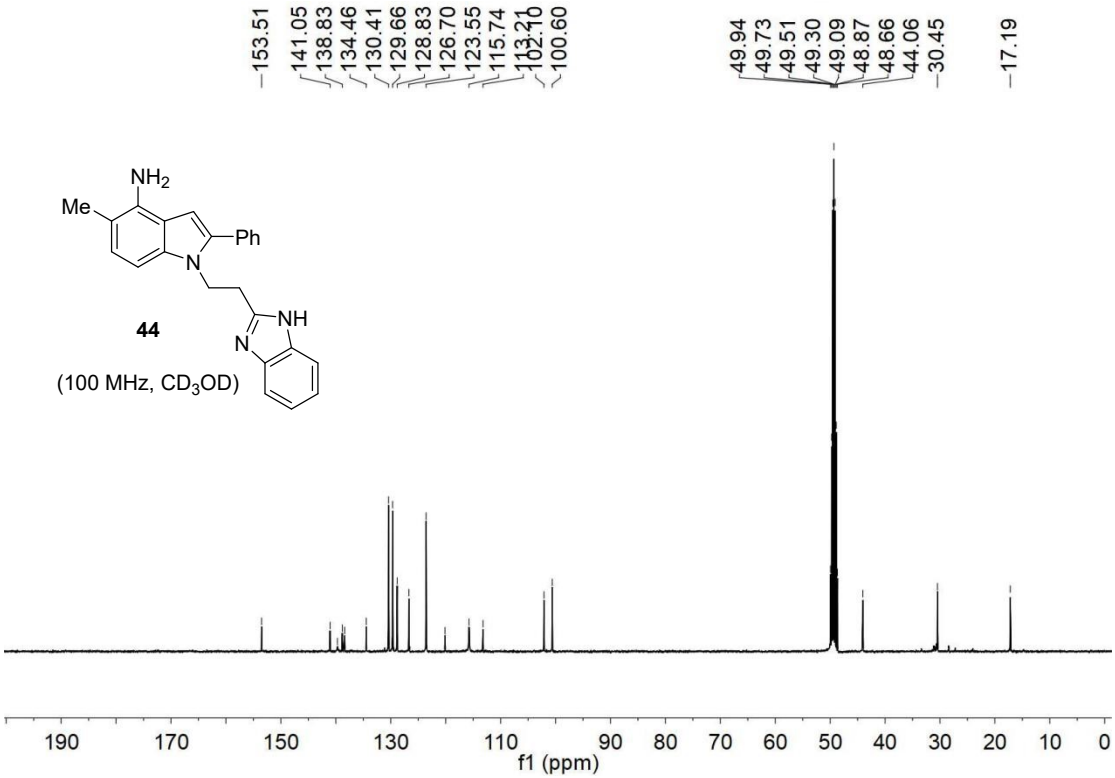




44

(400 MHz, CD_3OD)

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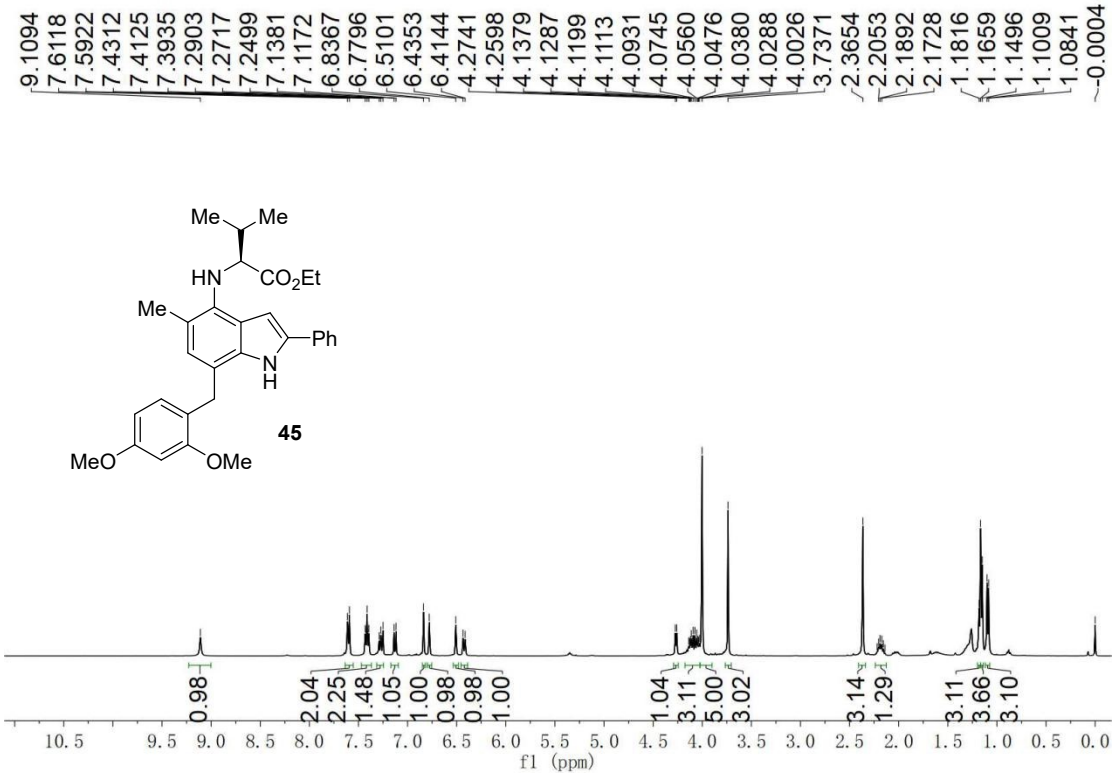
141.05
138.83
134.46
130.41
129.66
128.83
126.70
123.55
115.74
113.21
102.10
100.60
49.94
49.73
49.51
49.30
49.09
48.87
48.66
44.06
30.45
17.19
NH2
Me
Ph
N
NH
N
44
(100 MHz, CD3OD)
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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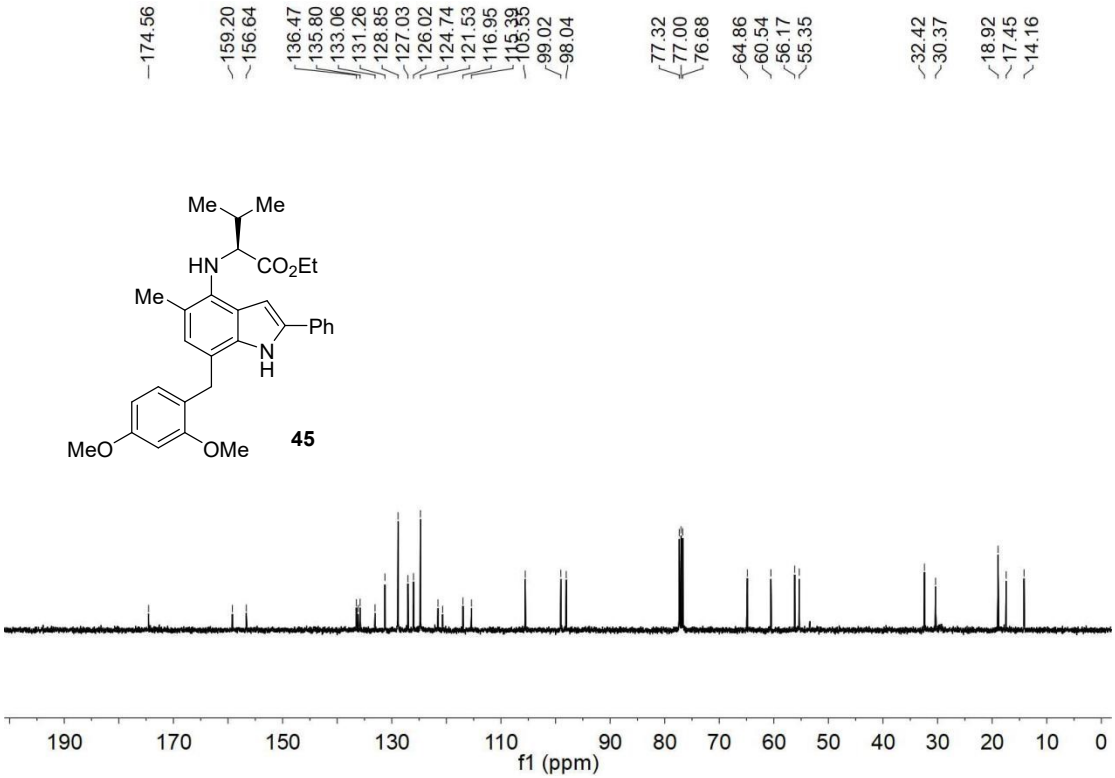
7.5922
7.4312
7.4125
7.3935
7.2903
7.2717
7.2499
7.1381
7.1172
6.8367
6.7796
6.5101
6.4353
6.4144
4.2741
4.2598
4.1379
4.1287
4.1199
4.1113
4.0931
4.0745
4.0560
4.0476
4.0380
4.0288
4.0026
3.7371
2.3654
2.2053
2.1892
2.1728
1.1816
1.1659
1.1496
1.1009
1.0841
-0.0004
Me
Me
HN
CO2Et
Me
Ph
N
H
45
MeO
OMe
0.98
2.04
2.25
1.48
1.05
1.00
0.98
0.98
1.00
1.04
3.11
5.00
3.02
3.14
1.29
3.11
3.66
3.10
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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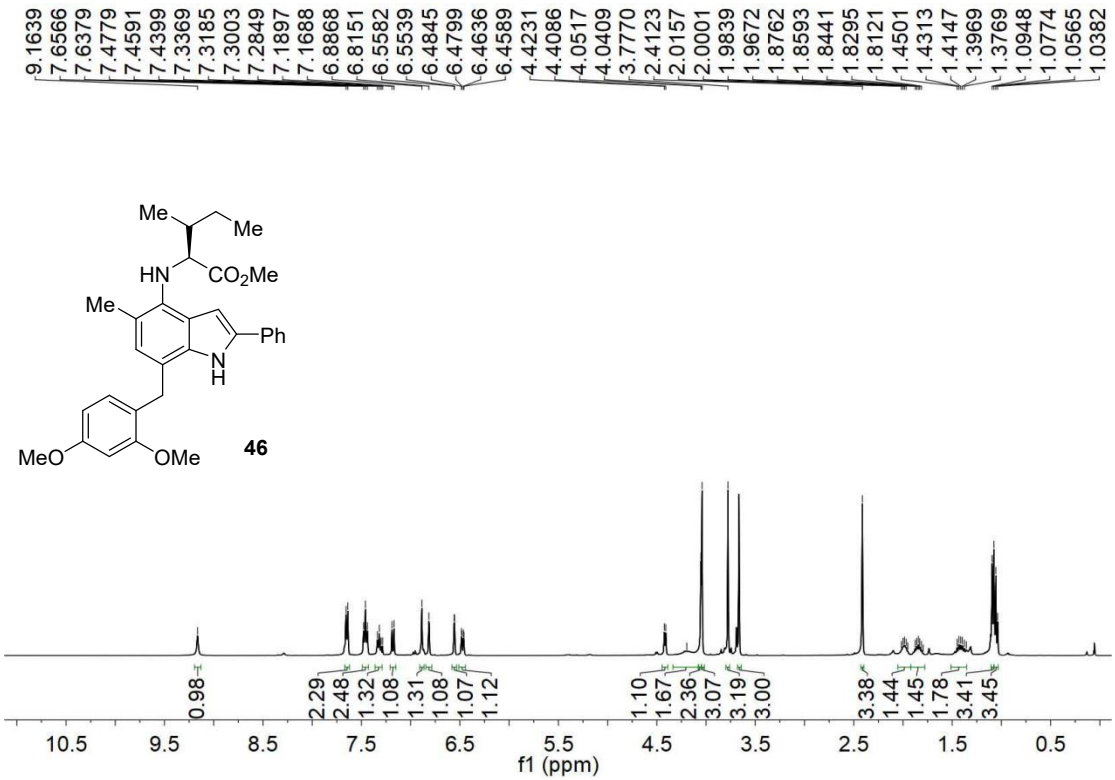
159.20
156.64
136.47
135.80
133.06
131.26
128.85
127.03
126.02
124.74
121.53
116.95
115.39
105.55
99.02
98.04
77.32
77.00
76.68
64.86
60.54
56.17
55.35
32.42
30.37
18.92
17.45
14.16
Me
Me
HN
CO2Et
Me
Ph
N
H
MeO
OMe
45
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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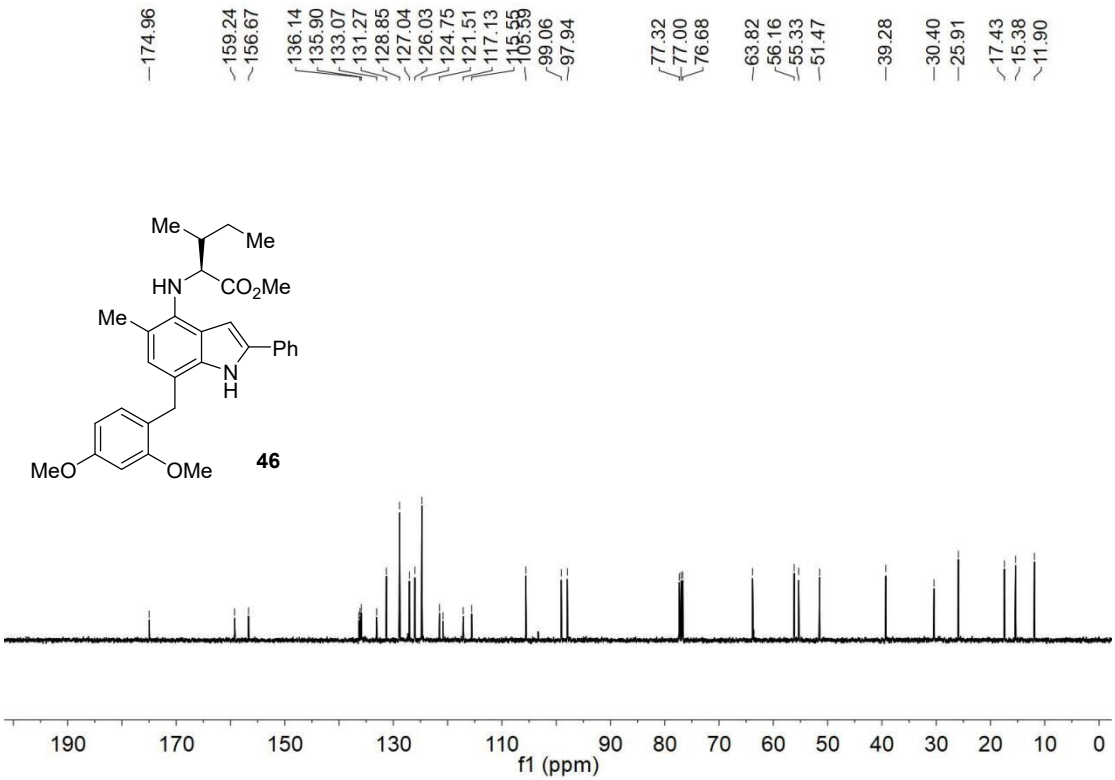
7.4591
7.4399
7.3369
7.3185
7.3003
7.2849
7.1897
7.1688
6.8868
6.8151
6.5582
6.5539
6.4845
6.4799
6.4636
6.4589
4.4231
4.4086
4.0517
4.0409
3.7770
2.4123
2.0157
2.0001
1.9839
1.9672
1.8762
1.8593
1.8441
1.8295
1.8121
1.4501
1.4313
1.4147
1.3969
1.3769
1.0948
1.0774
1.0565
1.0382
Me
Me
HN
CO2Me
Me
Ph
N
H
MeO
OMe
46
0.98
2.29
2.48
1.32
1.08
1.31
1.08
1.07
1.12
1.10
1.67
2.36
3.07
3.19
3.00
3.38
1.44
1.45
1.78
3.41
3.45
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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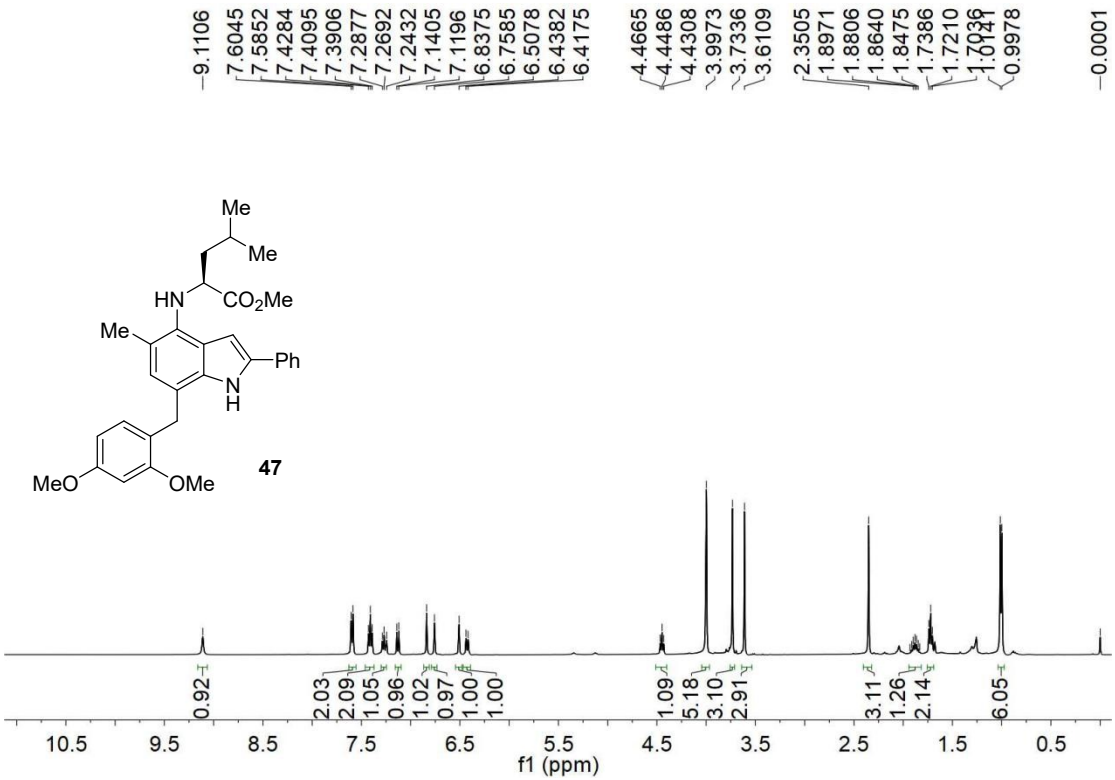
135.90
133.07
131.27
128.85
127.04
126.03
124.75
121.51
117.13
115.55
105.59
99.06
97.94
77.32
77.00
76.68
63.82
56.16
55.33
51.47
39.28
30.40
25.91
17.43
15.38
11.90
Me
Me
HN
CO2Me
Me
Ph
N
H
MeO
OMe
46
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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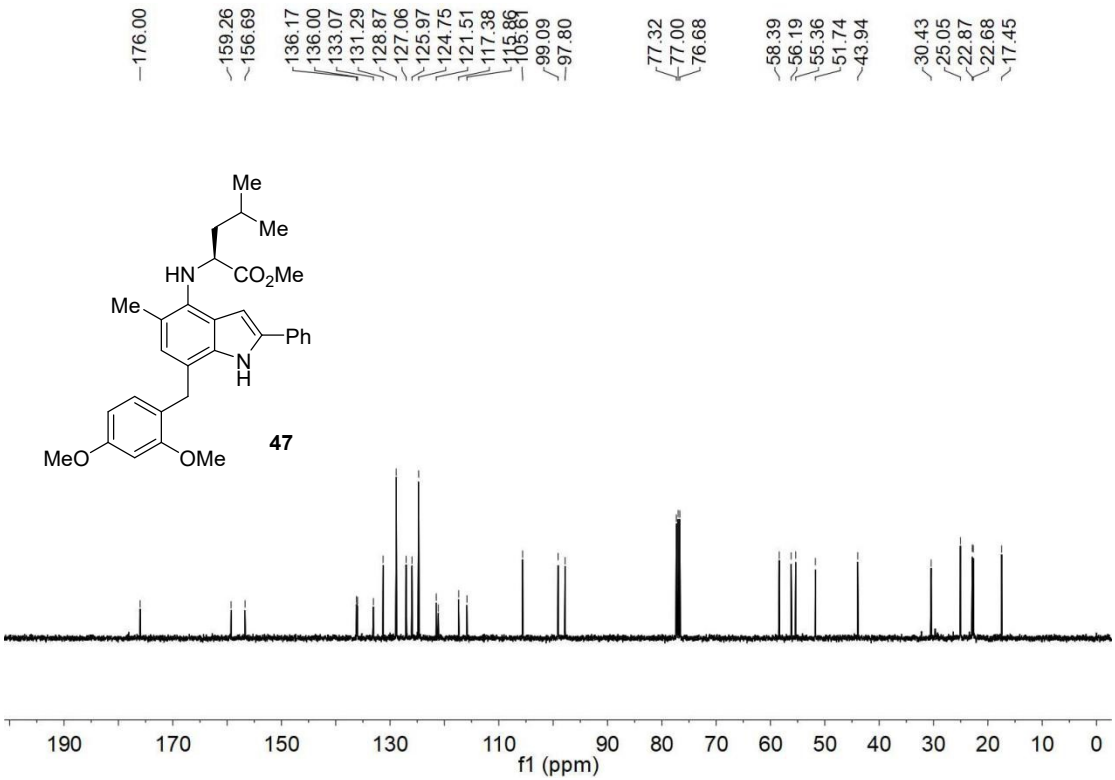
7.5852
7.4284
7.4095
7.3906
7.2877
7.2692
7.2432
7.1405
7.1196
6.8375
6.7585
6.5078
6.4382
6.4175
4.4665
4.4486
4.4308
3.9973
3.7336
3.6109
2.3505
1.8971
1.8806
1.8640
1.8475
1.7386
1.7210
1.7036
1.0141
0.9978
0.0001
Me
Me
HN
CO2Me
Me
Ph
N
H
MeO
OMe
47
0.92
2.03
2.09
1.05
0.96
1.02
0.97
1.00
1.00
1.09
5.18
3.10
2.91
3.11
1.26
2.14
6.05
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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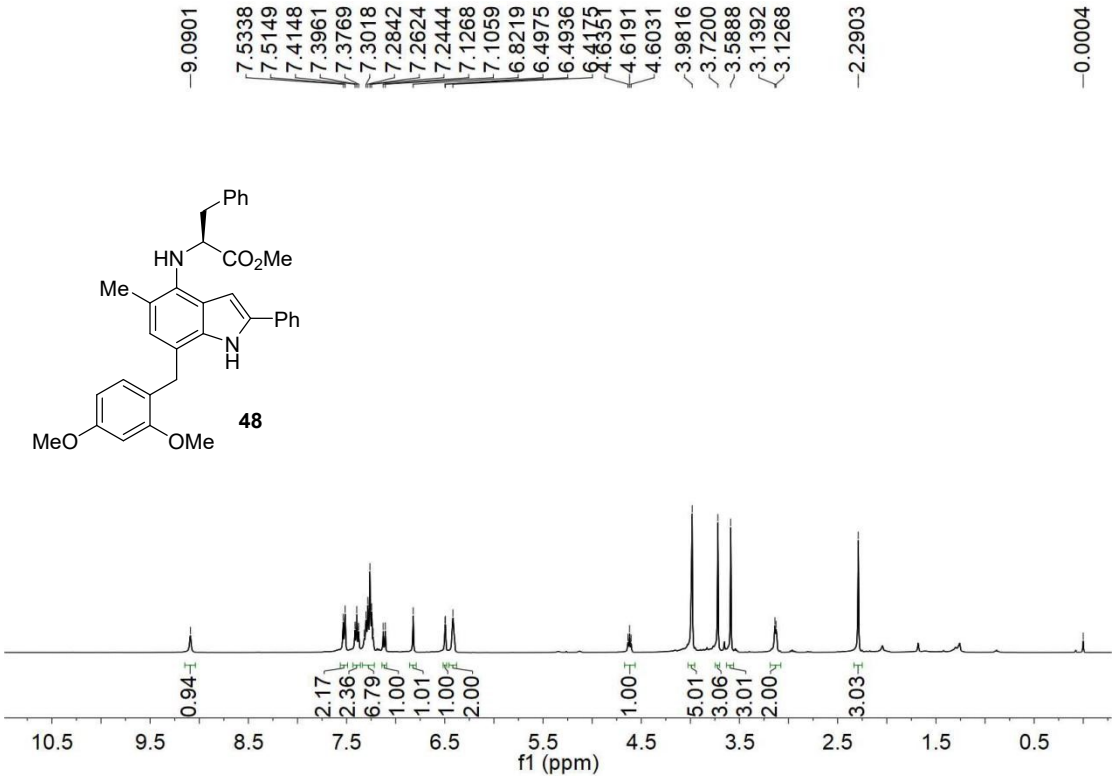
159.26
156.69
136.17
136.00
133.07
131.29
128.87
127.06
125.97
124.75
121.51
117.38
115.86
105.81
99.09
97.80
77.32
77.00
76.68
58.39
56.19
55.36
51.74
43.94
30.43
25.05
22.87
22.68
17.45
Me
Me
HN
CO2Me
Me
Ph
N
H
MeO
OMe
47
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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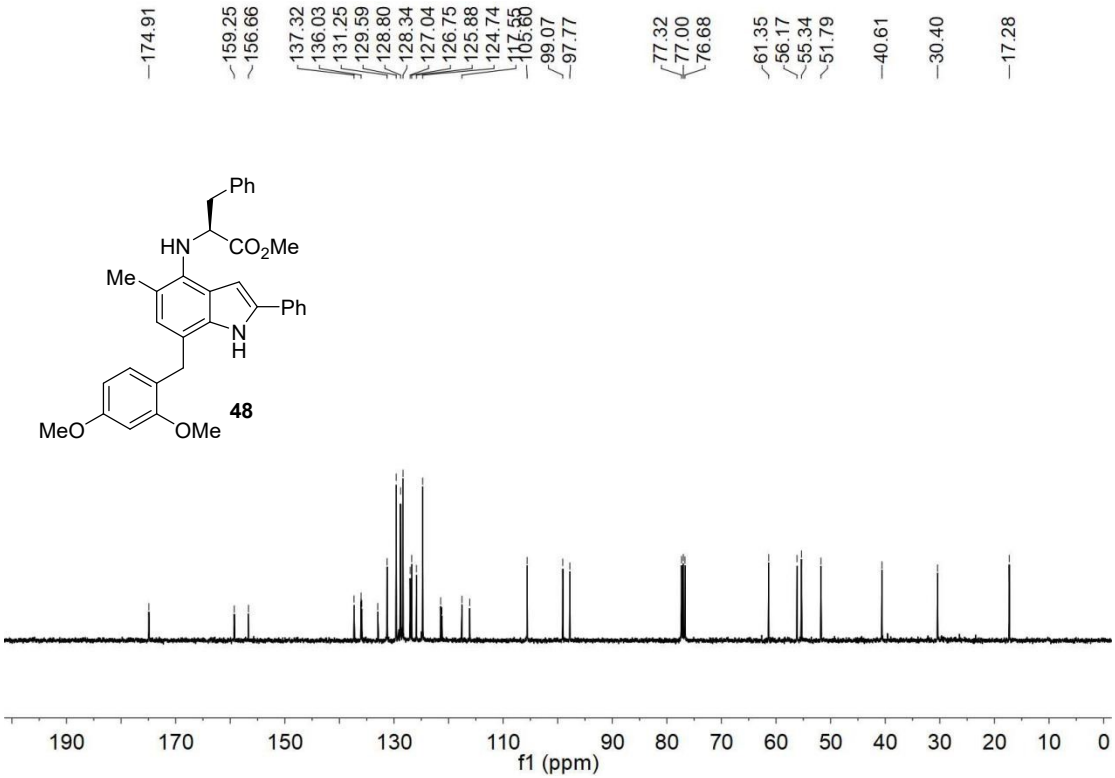
7.3018
7.2842
7.2624
7.2444
7.1268
7.1059
6.8219
6.4975
6.4936
6.4175
6.4151
4.6191
4.6031
3.9816
3.7200
3.5888
3.1392
3.1268
2.2903
0.0004
Ph
HN
CO2Me
Me
Ph
N
H
MeO
OMe
48
0.94
2.17
2.36
6.79
1.00
1.01
1.00
2.00
1.00
5.01
3.06
3.01
2.00
3.03
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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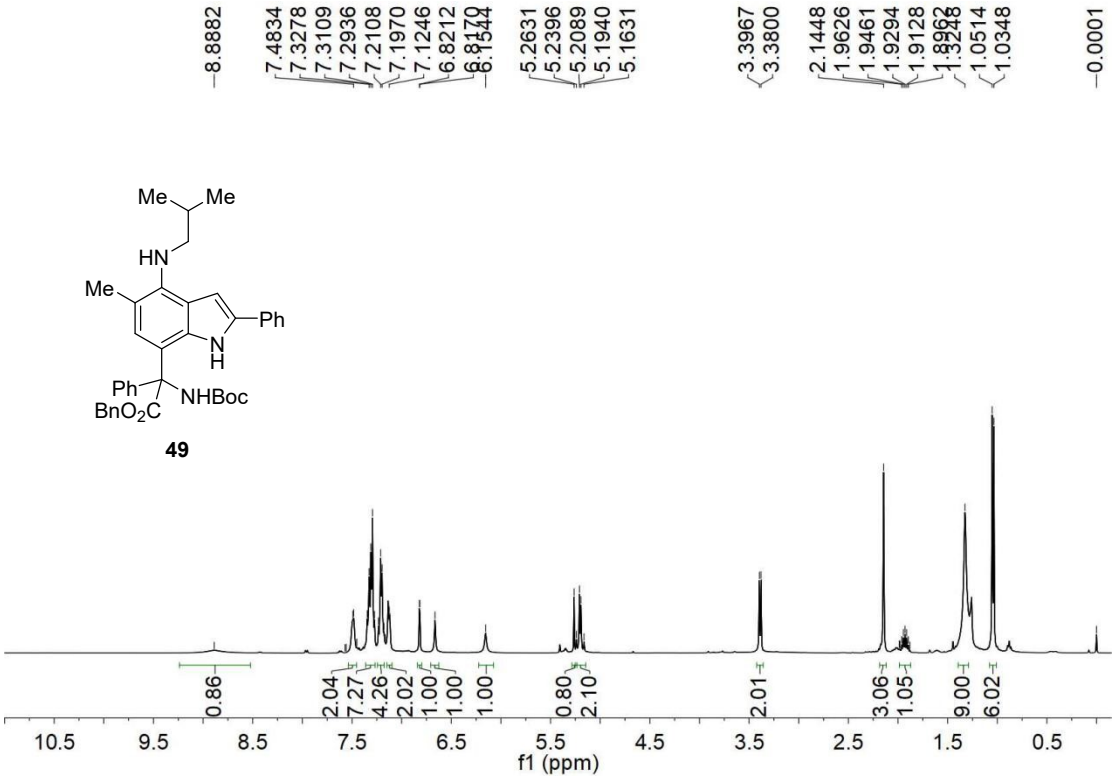
137.32
136.03
131.25
129.59
128.80
128.34
127.04
126.75
125.88
124.74
105.60
99.07
97.77
77.32
77.00
76.68
61.35
56.17
55.34
51.79
40.61
30.40
17.28
Ph
HN
CO2Me
Me
Ph
N
H
MeO
OMe
48
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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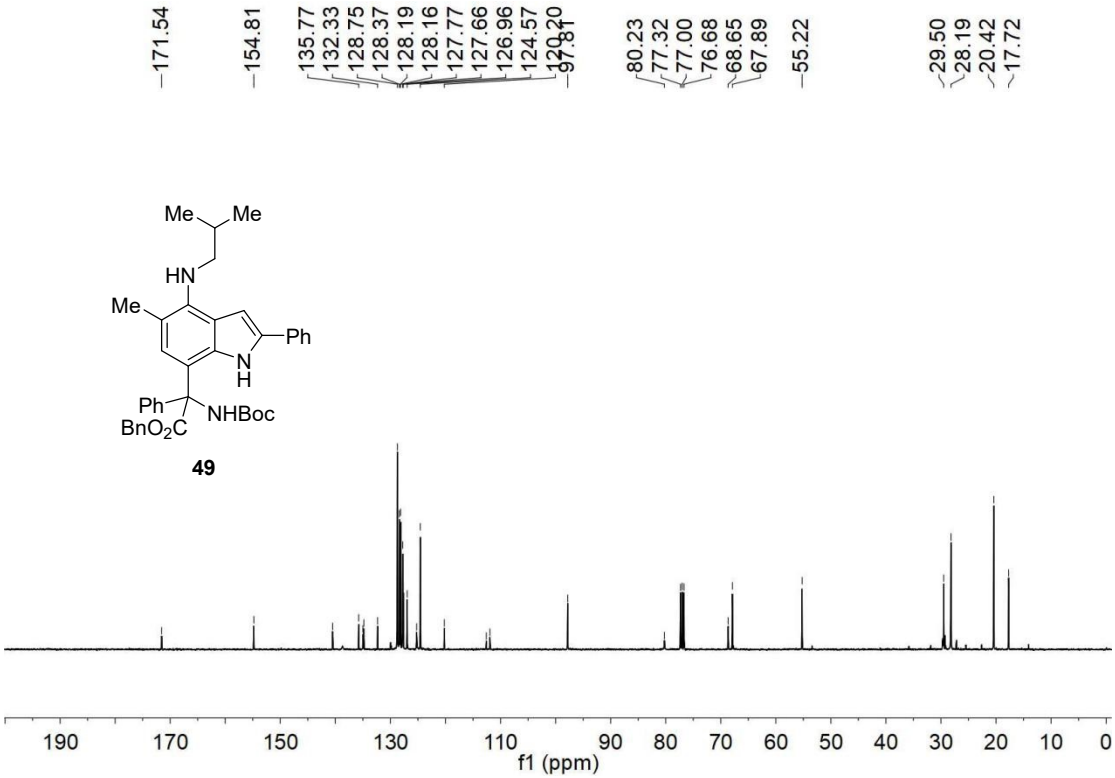
7.2936
7.2108
7.1970
7.1246
6.8212
5.2631
5.2396
5.2089
5.1940
5.1631
3.3967
3.3800
2.1448
1.9626
1.9461
1.9294
1.9128
1.3248
1.0514
1.0348
0.0001
Me
Me
HN
Me
Ph
N
H
Ph
NHBoc
BnO2C
49
0.86
2.04
7.27
4.26
2.02
1.00
1.00
1.00
0.80
2.10
2.01
3.06
1.05
9.00
6.02
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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128.37
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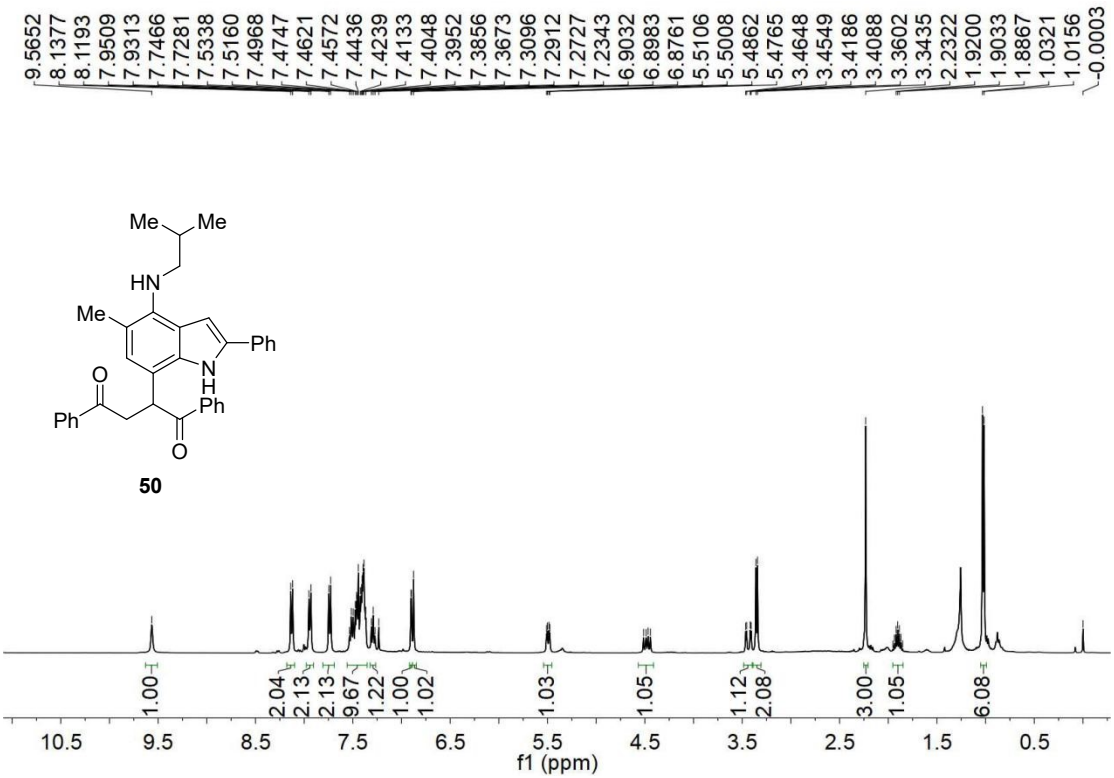
127.66
126.96
124.57
120.20
97.81
80.23
77.32
77.00
76.68
68.65
67.89
55.22
29.50
28.19
20.42
17.72
Me
Me
HN
Me
Ph
N
H
Ph
BnO2C
NHBoc
49
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4747
7.4621
7.4572
7.4436
7.4239
7.4133
7.4048
7.3952
7.3856
7.3673
7.3096
7.2912
7.2727
7.2343
6.9032
6.8983
6.8761
5.5106
5.5008
5.4862
5.4765
3.4648
3.4549
3.4186
3.4088
3.3602
3.3435
2.2322
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1.9033
1.8867
1.0321
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HN
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Ph
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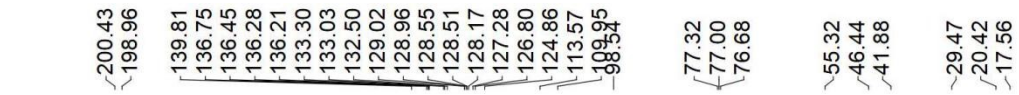
1.02
1.03
1.05
1.12
2.08
3.00
1.05
6.08
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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136.45
136.28
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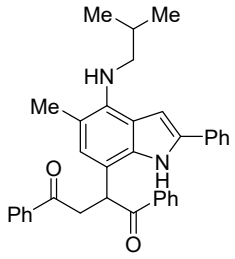
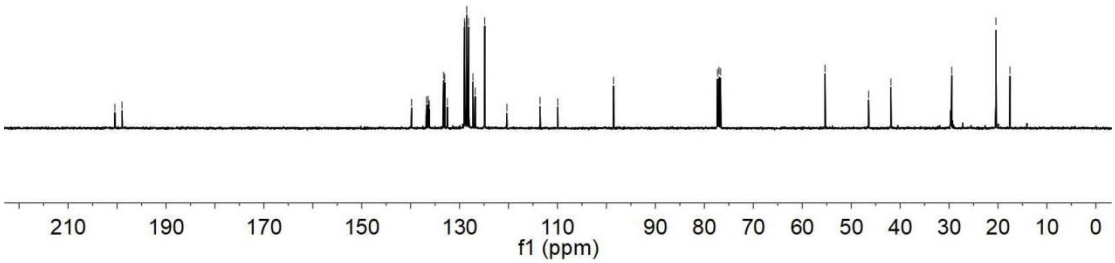
133.30
133.03
132.50
129.02
128.96
128.55
128.51
128.17
127.28
126.80
124.86
113.57
109.95
98.54
77.32
77.00
76.68
55.32
46.44
41.88
29.47
20.42
17.56


Me
Me
HN
Me
Ph
N
H
O
Ph
Ph
O

50


210
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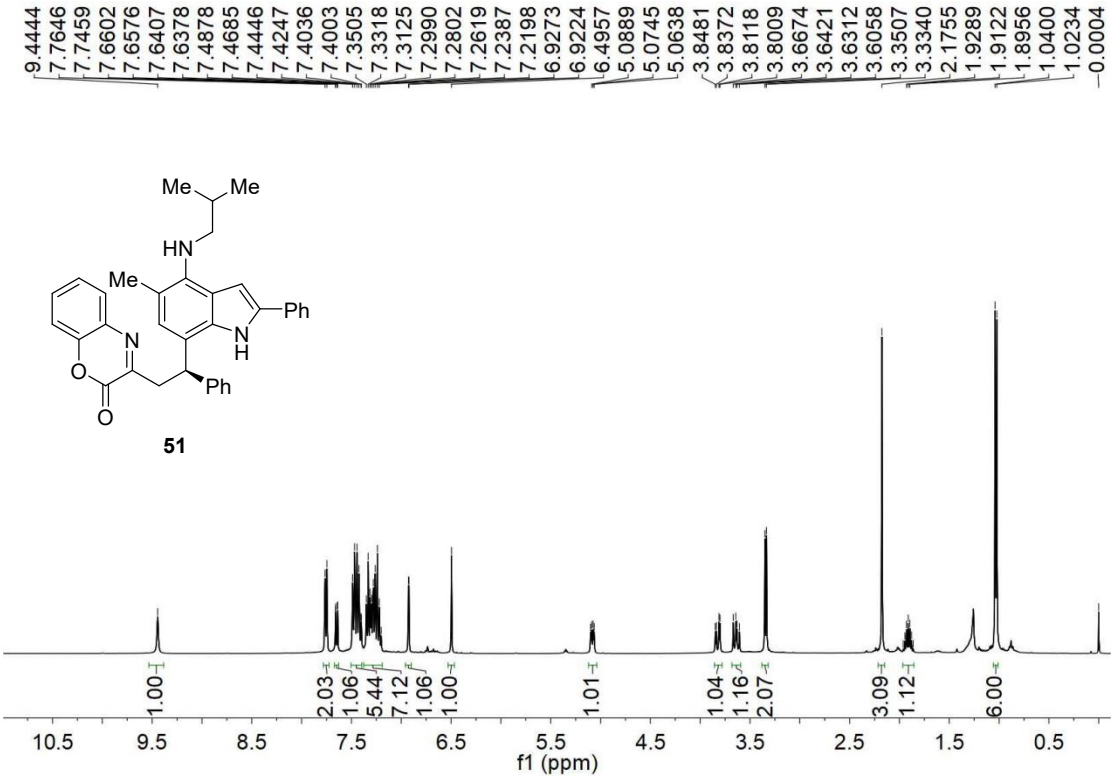
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.6378
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7.4685
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7.4247
7.4036
7.4003
7.3505
7.3318
7.3125
7.2990
7.2802
7.2619
7.2387
7.2198
6.9273
6.9224
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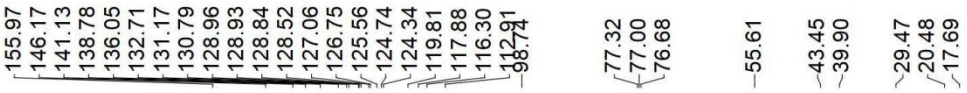
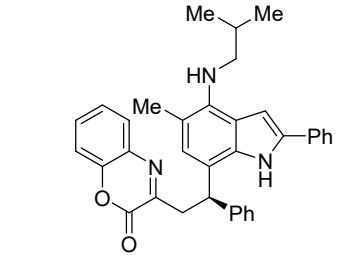
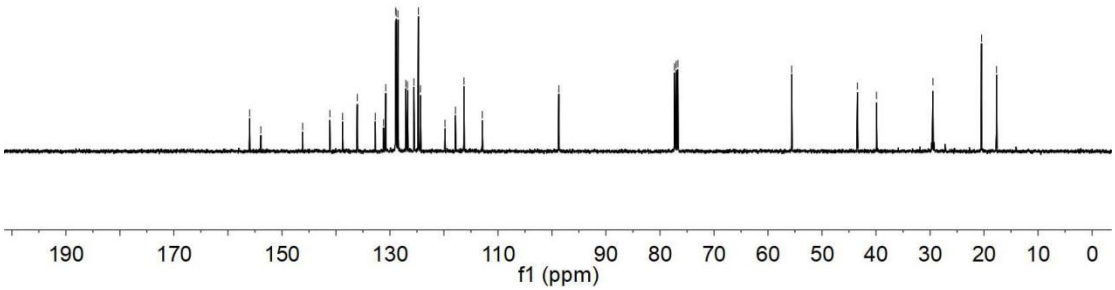
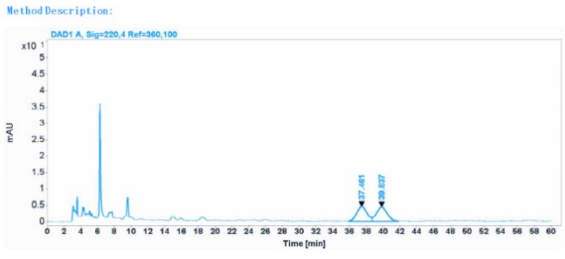
3.6312
3.6058
3.3507
3.3340
2.1755
1.9289
1.9122
1.8956
1.0400
1.0234
0.0004
Me
Me
HN
Me
Ph
N
H
N
O
O
Ph
O
51
1.00
2.03
1.06
5.44
7.12
1.06
1.00
1.01
1.04
1.16
2.07
3.09
1.12
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

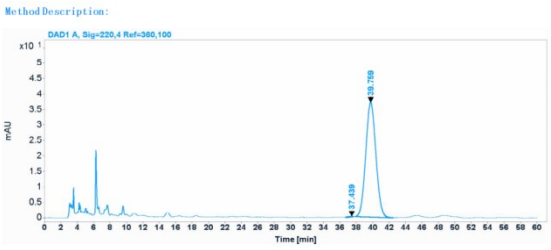

155.97
146.17
141.13
138.78
136.05
132.71
131.17
130.79
128.96
128.93
128.84
128.52
127.06
126.75
125.56
124.74
124.34
119.81
117.88
116.30
112.91
98.74
77.32
77.00
76.68
55.61
43.45
39.90
29.47
20.48
17.69


Me
Me
HN
Me
Ph
N
H
N
O
Ph
O

51


190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Method Description:
DAD1 A, Sig=220,4 Ref=360,100
mAU
Time [min]

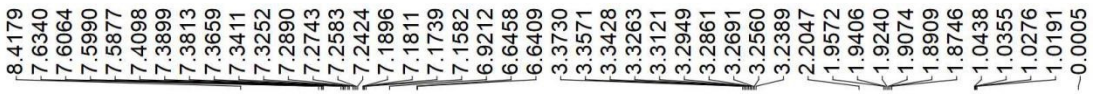

Method Description:
DAD1 A, Sig=220,4 Ref=360,100
mAU
Time [min]

Signal: DAD1 A, Sig=220,4 Ref=360,100

RT [min]	Width [min]	Area [mAU*S]	Height [mAU]	Area%
37.461	1.417	376.167	4.425	49.6489
39.837	1.475	381.487	4.311	50.3511
	Sum	757.6540		

Signal: DAD1 A, Sig=220,4 Ref=360,100

RT [min]	Width [min]	Area [mAU*S]	Height [mAU]	Area%
37.439	0.837	8.395	0.167	0.2630
39.759	1.432	3184.358	37.066	99.7370
	Sum	3192.7535		


8.4179
7.6340
7.6064
7.5990
7.5877
7.4098
7.3899
7.3813
7.3659
7.3411
7.3252
7.2890
7.2743
7.2583
7.2424
7.1896
7.1811
7.1739
7.1582
6.9212
6.6458
6.6409
3.3730
3.3571
3.3428
3.3263
3.3121
3.2949
3.2861
3.2691
3.2560
3.2389
2.2047
1.9572
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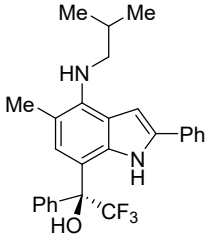
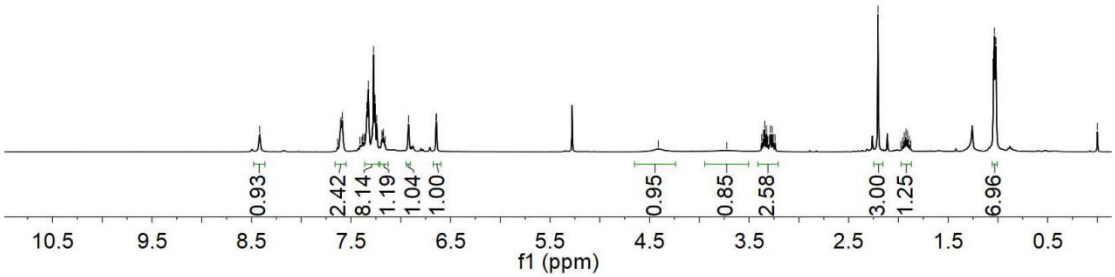
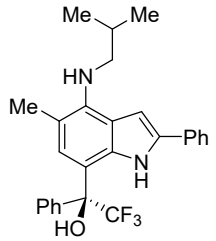
1.0438
1.0355
1.0276
1.0191
0.0005


Me
Me
HN
Me
Ph
N
H
Ph
HO
CF3

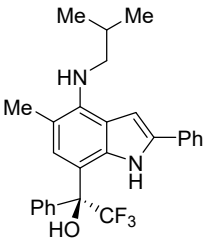
52


0.93
2.42
8.14
1.19
1.04
1.00
0.95
0.85
2.58
3.00
1.25
6.96
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

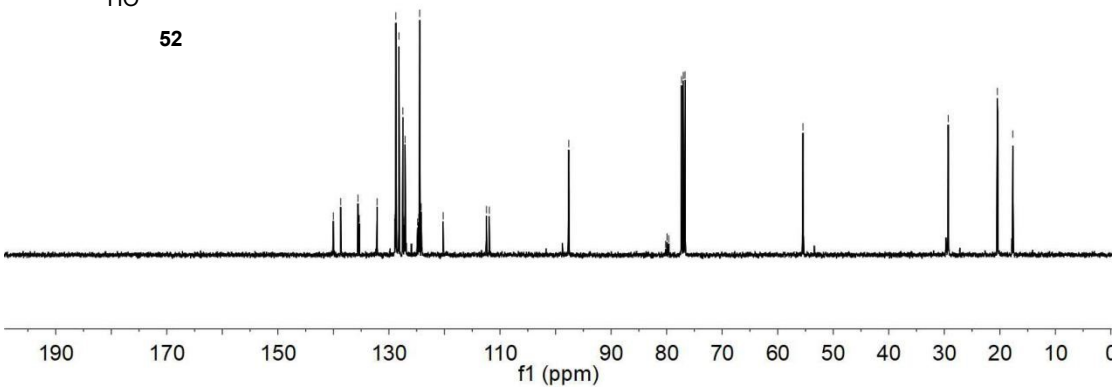

Me
Me
HN
Me
Ph
N
H
Ph
HO
CF3

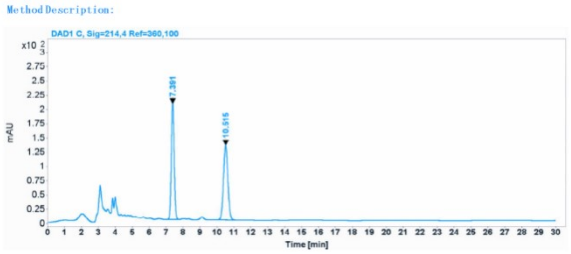
52

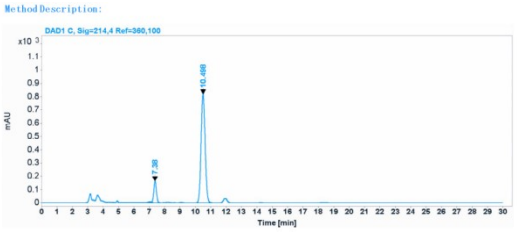
-74.48
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
f1 (ppm)



52







Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Area [mAU*S]	Height [mAU]	Area%
7.391	0.180	2361.089	203.157	50.1865
10.515	0.279	2343.540	130.931	49.8135
	Sum	4704.6292		

Signal: DAD1 C, Sig=214,4 Ref=360,100

RT [min]	Width [min]	Area [mAU*S]	Height [mAU]	Area%
7.380	0.183	1993.488	162.397	11.8143
10.498	0.285	14879.990	816.560	88.1857
	Sum	16873.4778		