Electronic Supplementary Material (ESI) for Chemical Communications.

Regiocontrolled Direct C4 and C2-Methyl Thiolation of Indoles under Rhodium Catalyzed Mild Conditions

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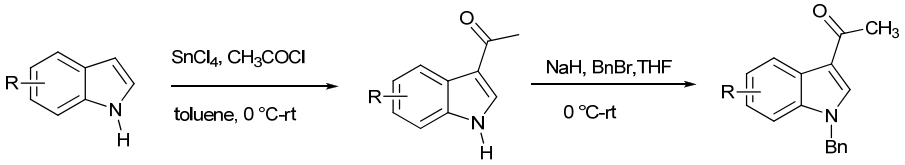
Supporting information

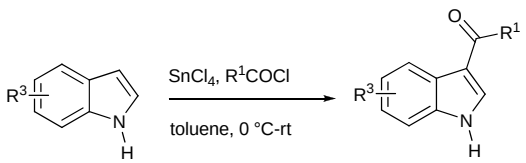
General:

All commercially available compounds were used without further purification. Solvents for elution in column were distilled. Analytical thin layer chromatography (TLC) was performed on pre- coated silica gel 60 F_{254}. Visualization on TLC was achieved by the use of UV light (254 nm). Column chromatography was undertaken on silica gel (230-400 mesh). ^{1}H NMR spectra were recorded on BRUKER ULTRA SHIELD (400 MHz and 600 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, m = multiplet. Coupling constants, *J*, were reported in hertz unit (Hz). ^{13}C NMR spectras were recorded on BRUKER (100 MHz and 150 MHz) and was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the centre of a triplet at 77.16 ppm of chloroform-d. ^{19}F NMR spectra were recorded on BRUKER (376 MHz). Infrared (IR) spectra were recorded using Spectrum BX FT-IR instrument from Perkin Elmer. Frequencies are given in reciprocal centimeters (cm^{-1}), only selected absorbance peaks are reported and KBr is used as the matrix. GC-MS were obtained from Thermo Scientific TRACE 1300. LC-MS were obtained from Agilent Technologies A6120BW (single quadruple mass analyzer). High resolution mass spectra were obtained from waters XEVO-G2QTOF by using TOF MS ES+ method. Materials were obtained from commercial suppliers or prepared according to standard procedures unless otherwise noted.

1. Synthesis of starting material:

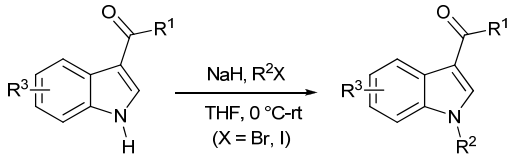


1.1 General procedure for the synthesis of 3-acetyl indole derivatives[1]:



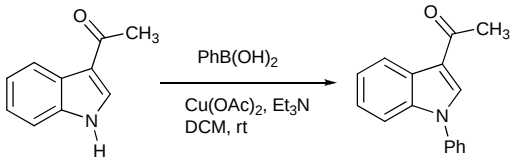
To a stirred solution of indole derivative (1 equiv) in dry toluene, acid chloride (2 equiv) was added. The reaction mixture was cooled to 0 ^{o}C and stirred for 10 min. Next, stannic chloride (2 equiv) was added drop wise to the reaction mixture and stirred for 12 h. After completion of reaction (as monitored by TLC), it was cooled to 0 ^{0}C, quenched by saturated $NaHCO_3$ solution and extracted with ethyl acetate. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to provide desired product.

1.2. General procedure for preparation of *N*-substituted 3-acetyl indole:



To a stirred suspension of NaH (60 wt% in mineral oil, 1.5 equiv) in dry THF, solution of 3-acetyl indole derivative (1 equiv) was added at 0 ^{o}C and stirred for 15 min. Then corresponding alkyl halide (1.1 equiv) was added drop wise to the reaction mixture and stirred overnight at rt. After completion of the reaction (as monitored by TLC), it was cooled to 0 ^{0}C and quenched by addition of water and extracted with ethyl acetate. Combined organic layers were washed with water, brine, and dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to obtain desired *N*-alkylated 3-acetyl indole derivatives.

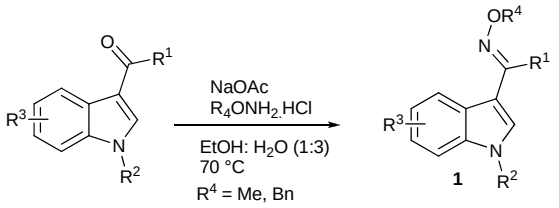
1.3. Procedure for synthesis of *N*-phenyl indole[2]:



In a flame-dried sealed tube, 3-acetyl indole (1 equiv) dissolved in CH_2Cl_2 (6 mL), phenylboronic acid (2 equiv), anhydrous copper(II) acetate (2 equiv), and triethylamine (2 equiv) were added. The mixture was stirred at room temperature for 3 days, concentrated in *vacuo*, diluted with chloroform and water. The organic layer was separated, washed with brine and dried

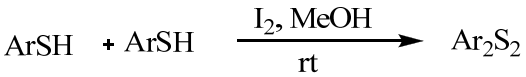
over anhydrous Na_2SO_4, concentrated in *vacuo*, and purified by column chromatography (EtOAc/hexane) to obtain pure product.

1.4. General procedure for preparation of ketoximes[3]:



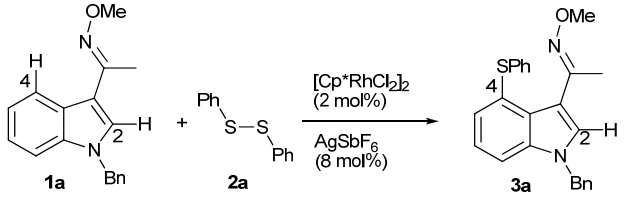
To a 50 mL round bottom flask equipped with a stir bar was charged with ketone (1 equiv), $R^4ONH_2{\cdot}HCl$ (2.7 equiv), NaOAc (4.4 equiv), and EtOH:H_2O (1:3). The reaction mixture was heated at 70 ^{0}C. After completion of reaction (as monitored by TLC), it was cooled to rt and EtOH was removed under vacuum. The mixture was extracted with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to yield the desired analytically pure ketoxime **1** in moderate to good yield.

2. General procedure for preparation of disulfides[4]**:**



To a stirred solution of thiol compounds (1 mmol) in methanol (5 ml) was added iodine (0.5 mmol, 0.5 equiv) at room temperature. After completion of reaction (as monitored by TLC), it was quenched with saturated sodium thiosulfate solution and extracted with ethyl acetate. The combined organic layers were washed with brine and dried over anhydrous Na_2SO_4 and concentrated under vacuum to afford pure disulfide compounds.

Optimization Table S1. Optimization studies for the rhodium-catalyzed C4-thiolation of indole derivatives[a]

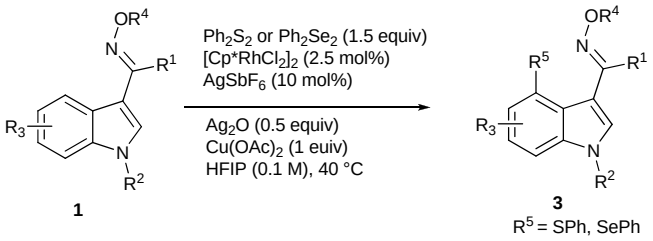


entry	solvent	Ag salt (equiv)	additive (1 equiv)	temp (°C)	yield (%)[b]
1	DCE	-	$Cu(OAc)_2$	80	36
2	DCE	Ag_2CO_3(1)	-	80	65
3	MeCN	Ag_2CO_3(1)	-	80	nd
4	^{t}AmOH	Ag_2CO_3(1)	-	80	43
5	Dioxane	Ag_2CO_3(1)	-	80	30
6	TCE	Ag_2CO_3(1)	-	80	57
7	THF	Ag_2CO_3(1)	-	80	25
8	toluene	Ag_2CO_3(1)	-	80	nd
9	DCE	$AgPF_6$(1)	-	80	nd
10	DCE	Ag_3PO_4(1)	-	80	62
11	DCE	AgOAc(1)	-	80	62
12	DCE	Ag_2O(1)	-	80	72
13	DCE	Ag_2O(1)	LiOAc	80	54
14	DCE	Ag_2O(1)	NaOAc	80	10
15	DCE	Ag_2O(1)	$Cu(OAc)_2$	80	77
16	TFE	Ag_2O(0.5)	$Cu(OAc)_2$	80	75
17[c]	DCE	Ag_2O(0.5)	$Cu(OAc)_2$	40	47
18[c]	**HFIP**	**Ag_2O(0.5)**	**$Cu(OAc)_2$**	**40**	**83**
19[c]	HFIP	Ag_2O(0.5)	-	40	28
20[d]	DCE	Ag_2CO_3(1)	-	80	trace
21[e]	DCE	Ag_2CO_3(1)	-	80	35

[a]Reaction conditions: **1a** (0.1 mmol), **2a** (0.15 mmol), $[Cp^*RhCl_2]_2$ (2 mol%), $AgSbF_6$ (8 mol%), Ag salt, additive (0.1 mmol), solvent (0.1 M), 14-18 h. [b]Isolated yields. [c]$[Cp^*RhCl_2]_2$ (2.5 mol%). [d]$[Cp^*IrCl_2]_2$(2.5

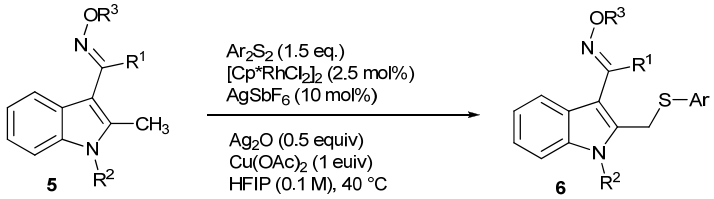
mol%). [e][Ru(*p*-cymene)Cl_2]$_2$ (5 mol%). DCE = 1,2-dichloroethane; TCE = 1,1,2,2-tetracholoroethane; TFE = trifluoroethanol; HFIP = hexafluoroisopropanol. nd = not detected.

3.1. General procedure for the synthesis of C4-chalcogenation using Rh(III) catalyst:



To an oven-dried 10 mL screw cap vial ketoxime **1** (0.1 mmol) was taken in HFIP (0.1 M). Followingly, [Cp*$RhCl_2$]$_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), Ag_2O (0.05 mmol), $Cu(OAc)_2$ (0.1 mmol), Ph_2S_2 or Ph_2Se_2 (0.15 mmol) were added to it and stirred at 40 ^{0}C for 8-16 h. After completion of the reaction (as monitored by TLC), the solvent was evaporated under reduced pressure. The crude reaction mixture was diluted with diethyl ether and passed through a Celite bed, and repeatedly washed with diethyl ether. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography using EtOAc/hexane mixture (1:9-1:5) as eluent to obtain desired pure product **3**.

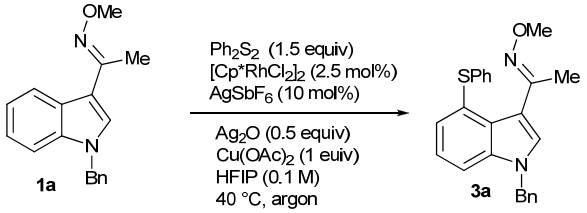
3.2. General procedure for the synthesis of C2-methyl thiolation using Rh(III) catalyst:



Compound **6** was prepared *via* general procedure for the synthesis of compound **3**.

Control experiments:

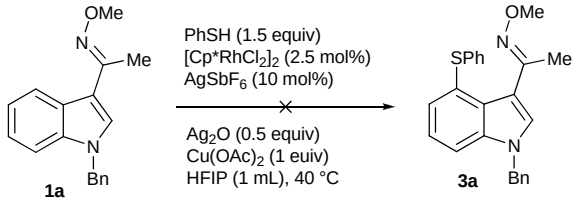
4. Reaction in absence of oxygen atmosphere:



To a pre-dried 10 mL round bottom flask, ketoxime **1a** (27.8 mg, 0.1 mmol) was taken in deoxygenated HFIP (1 mL) under argon atmosphere. Next, [Cp*$RhCl_2$]$_2$ (1.5 mg, 2.5 mol%),

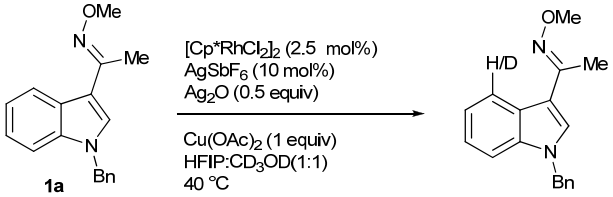
$AgSbF_6$ (3.4 mg, 10 mol%), Ag_2O (11.6 mg, 0.05 mmol), $Cu(OAc)_2$ (18.2mg, 0.1 mmol), Ph_2S_2 (32.7 mg, 0.15 mmol) were added under argon atmosphere. The reaction mixture was stirred at 40 ^{0}C for 14 h. After completion of the reaction (as monitored by TLC), the solvent was evaporated under reduced pressure. The crude reaction mixture was diluted with diethyl ether and passed through a Celite bed, and repeatedly washed with diethyl ether. The combined organic layers were concentrated under reduced pressure and the crude product was purified by silica gel column chromatography (EtOAc/hexane = 1:9) to obtain pure product **3a** (30.1 mg, 78% yield).

5. Reaction with thiophenol under standard condition:



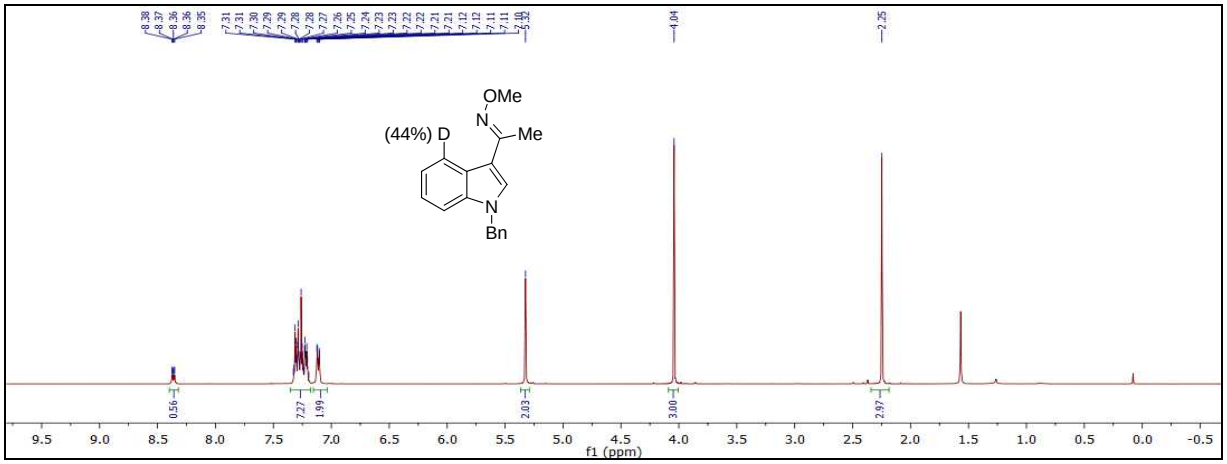
In a pre-dried 10 mL screw cap vial, ketoxime **3a** (27.8 mg, 0.1 mmol) was taken in HFIP (1 mL). Next, $[Cp^*RhCl_2]_2$ (1.5 mg, 2.5 mol%), $AgSbF_6$ (3.4 mg, 10 mol%), Ag_2O (11.6 mg, 0.05 mmol), $Cu(OAc)_2$ (18.2 mg, 0.1 mmol), and PhSH (17 mg, 1.5 mmol) were added and stirred at 40 ^{0}C for 24 h. Major amount of starting material **1a** remained intact without any desired product formation.

6.1. Deuterium incorporation studies in absence of 2a:

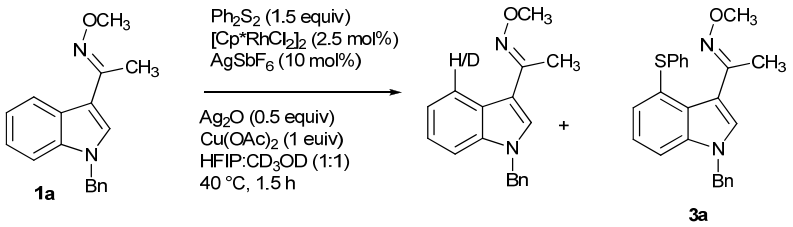


To a oven-dried 10 mL screw cap vial, ketoxime **1a** (27.8 mg, 0.1 mmol) was taken in CD_3OD: HFIP (0.5 mL:0.5 mL). Next, $[Cp^*RhCl_2]_2$ (1.5 mg, 2.5 mol%), $AgSbF_6$ (3.5 mg, 10 mol%), Ag_2O (11.6 mg, 0.05 mmol), $Cu(OAc)_2$ (18.2 mg, 1 equiv) were added and stirred at 40 ^{0}C for 14 h. The solvent was evaporated under reduced pressure. Then, the crude reaction mixture was diluted with diethyl ether and passed through a Celite bed, and repeatedly washed with diethyl ether. The combined organic layers were concentrated under reduced pressure and purified by silica gel column chromatography using EtOAc/hexane mixture as eluent. The

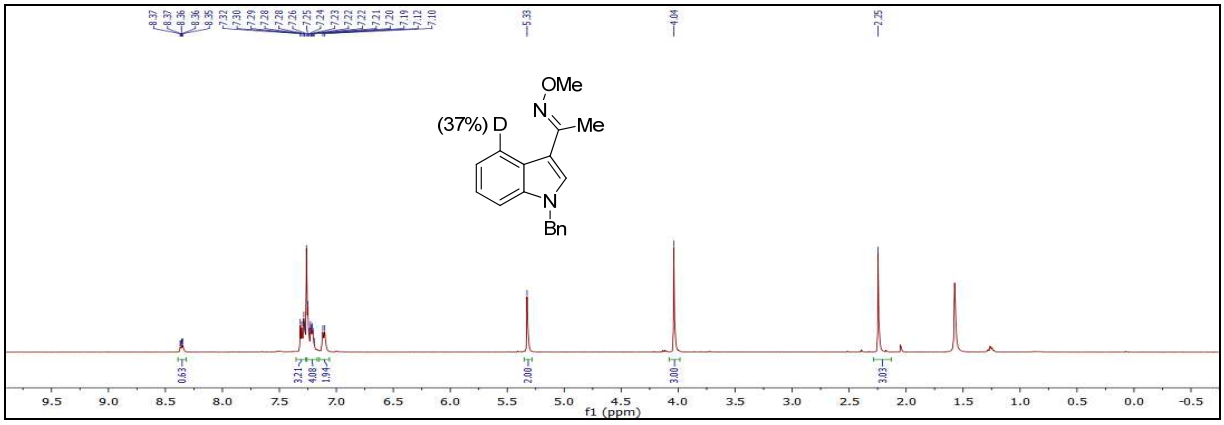
purified product was analyzed by ^{1}H NMR which showed that 44% deuterium incorporation at C-4 position of indole **1a** was happened under standard reaction conditions.



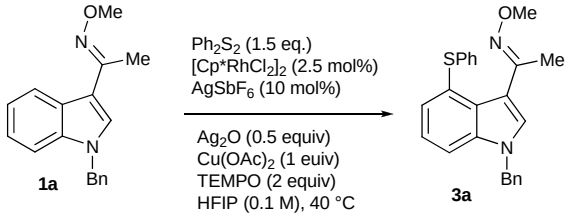
6.2. Study of deuterium incorporation in presence of 2a:



To a stirred solution of ketoxime **1a** (0.1 mmol) in HFIP:CD_3OD (0.5 mL: 0.5 mL), $[Cp^*RhCl_2]_2$ (2.5 mol%), $AgSbF_6$ (10 mol%), Ag_2O (0.05 mmol), $Cu(OAc)_2$ (1 equiv), and Ph_2S_2 (1.5 equiv) were added and stirred at 40 ^{0}C. After 1.5 h, the reaction mixture was filtered through Celite bed and washed with EtOAc. The organic layer was concentrated under vaccum and purified by silica gel column chromatography using EtOAc/hexane as elluent. The isolated starting material and product was characterized by ^{1}H NMR. The ^{1}H NMR analysis of the recovered starting material showed that 37% deuterium incorporation occurred at the C-4 position of **1a**.

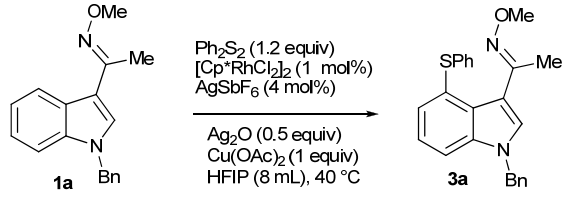


7. Reaction in presence of TEMPO:



To a oven-dried 10 mL screw cap vial, ketoxime **1a** (27.8 mg, 0.1 mmol) was added in HFIP (1 mL). Then, $[Cp^*RhCl_2]_2$ (1.5 mg, 2.5 mol%), $AgSbF_6$ (3.4 mg, 10 mol%), Ag_2O (11.6 mg, 0.05 mmol), $Cu(OAc)_2$ (18.2 mg, 0.1 mmol), Ph_2S_2 (32.7 mg, 0.15 mmol) and TEMPO (31.2 mg, 0.2 mmol) were added to the reaction mixture and stirred at 40 ^{0}C for 6 h. After completion of the reaction (as monitored by TLC), the solvent was evaporated under reduced pressure. The crude reaction mixture was diluted with diethyl ether and passed through a Celite bed, and repeatedly washed with diethyl ether. The combined organic layers were concentrated under reduced pressure and the crude product was purified by silica gel column chromatography using EtOAc/hexane mixture as eluent to obtain pure product **3a** (31 mg, 80%).

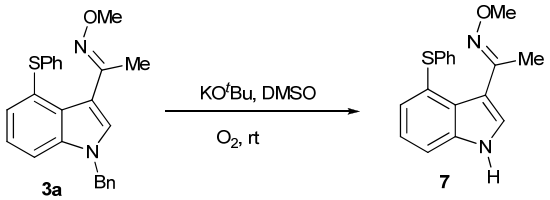
8. Large scale experiment:



To a solution of **1a** (1.0 g, 3.59 mmol) in HFIP (8 mL), $[Cp^*RhCl_2]_2$ (22 mg, 1 mol%), $AgSbF_6$ (50 mg, 4 mol%), Ag_2O (0.42 g, 0.05 mmol), anhydrous $Cu(OAc)_2$ (0.65 g, 1.0 equiv), and phenyldisulfide (0.94 g, 4.31 mmol) were added. After being stirred at 40 ^{0}C (until complete consumption of starting material), the reaction mixture was filtered by short silica gel and washed with ethyl acetate. The combined organic layer was dried over Na_2SO_4 and concentrated under vaccum. The crude product was purified by short silica gel column chromatography using EtOAc/hexane as eluent to afford desired product (0.90 g, 65%) as yellow oil.

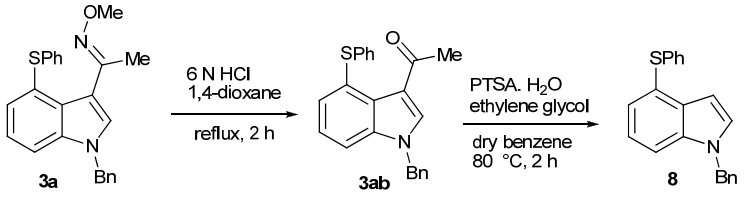
9. Product modification:

9.1. Deprotection of benzyl group:



To a stirred solution of compound **3a** (38.6 mg, 0.1 mmol) dissolved in dry DMSO (1.5 mL), KO^{t}Bu (90 mg, 0.8 mmol) was added. Oxygen was then bubbled into the solution until complete consumption of starting material (as monitored by TLC). After completion, the reaction mixture was quenched by saturated solution of ammonium chloride and extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to obtain pure product **7** (23 mg, 78%) as yellow oil.

9.2. Stepwise removal of oxime directing group:

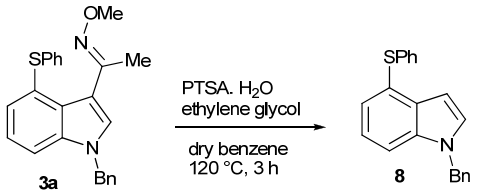


O-Methyl oxime compound **3a** (50 mg, 0.13 mmol) was dissolved in 1,4-dioxane (4 mL) and stirred for 15 min, then 6N HCl (1.5 mL) was added. The reaction was heated at 80 ^{0}C and stirred at the same temperature for 2 h. After completion, the reaction mixture was quenched with saturated sodium bicarbonate and extracted with EtOAc. The combined organic layers were

dried over anhydrous Na_2SO_4 and concentrated under vacuum. The crude product was purified by silica gel column chromatography to obtain pure product **3ab** (35 mg, 75%) as yellow oil.

Next, to a stirred solution of compound **3ab** (30 mg, 0.08 mmol) in dry benzene (2 mL) ethylene glycol (0.1 mL) and *p*-toluenesulfonic acid monohydrate (20 mg, 1.1 equiv) were added and heated under reflux condition for 2 h. After completion (as monitored by TLC), the reaction mixture was cooled, quenched with saturated sodium bicarbonate solution and extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under vaccum. The crude product was purified by silica gel column chromatography to obtain pure product **8** (19 mg, 72%) as yellow oil.

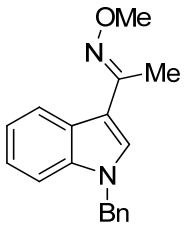
9.3. One step removal of oxime directing group:



O-Methyl oxime compound **3a** (38.6 mg, 0.1 mmol) in dry benzene was taken in a sealed tube. Next, ethylene glycol (0.4 mL) and *p*-toluenesulfonic acid monohydrate (100 mg, 5 equiv) were added consecutively. The reaction mixture was heated at 120 ^{0}C for 3 h. The reaction mixture was cooled, quenched with saturated sodium bicarbonate solution and extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to obtain pure product **8** (17 mg, 55%) as yellowish liquid.

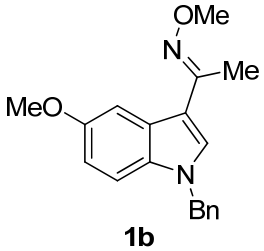
10. Characterization data

10.1. Characterization data for starting materials:



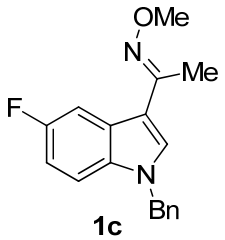
1a

(*E*)-1-(1-Benzyl-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1a): White amorphous solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.37 (dd, J = 6.7, 2.9 Hz, 1H), 7.49–7.18 (m, 7H), 7.11 (d, J = 6.7 Hz, 2H), 5.32 (s, 2H), 4.05 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.7, 137.4, 136.9, 128.8, 128.7, 127.8, 126.7, 125.5, 123.5, 122.9, 120.9, 113.5, 109.6, 61.8, 50.2, 13.01; FT-IR: $\tilde{\nu}$ = 2928, 2366, 1460, 1182, 1052 cm^{-1}; GC-MS: $C_{18}H_{18}N_2O$ $[M]^+$: 278.15.



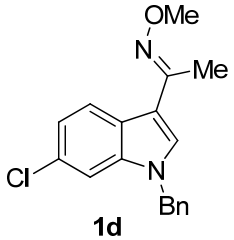
1b

(*E*)-1-(1-Benzyl-5-methoxy-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1b): White amorphous solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.91 (d, J = 2.6 Hz, 1H), 7.33 – 7.25 (m, 4H), 7.13 (d, J = 8.9 Hz, 1H), 7.10 (d, J = 6.9 Hz, 2H), 6.88 (dd, J = 8.9, 2.6 Hz, 1H), 5.28 (s, 2H), 4.05 (s, 3H), 3.89 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.3, 152.1, 137.1, 132.7, 129.4, 129.0, 127.9, 126.8, 126.0, 113.1, 112.9, 110.6, 105.5, 61.9, 55.9, 50.5, 13.1; FT-IR: $\tilde{\nu}$ = 2934, 2818, 1598, 1540, 1484, 1454, 1393, 1358, 1272, 1222, 1184, 1144, 1050 cm^{-1}; GC-MS: $C_{19}H_{20}N_2O_2$ $[M]^+$: 308.08.



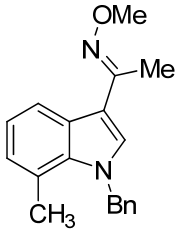
1c

(*E*)-1-(1-Benzyl-5-fluoro-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1c): White amorphous solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.05 (dd, J = 10.1, 2.6 Hz, 1H), 7.40 – 7.27 (m, 4H), 7.14 (dd, J = 8.9, 4.3 Hz, 1H), 7.10 (d, J = 6.9 Hz, 2H), 6.96 (td, J = 9.0, 2.6 Hz, 1H), 5.30 (s, 2H), 4.04 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ: 158.9 (d, J = 235.3 Hz), 151.5, 136.8, 134.1, 130.2, 129.1, 128.1, 126.8, 126.0 (d, J = 13.2 Hz), 113.6 (d, J = 6.6 Hz), 111.4 (d, J = 26.5 Hz), 110.5 (d, J = 9.7 Hz), 108.9 (d, J = 24.6 Hz), 62.0, 50.7, 13.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -123.16; FT-IR: $\tilde{\nu}$ = 2934, 2812, 1620, 1598, 1540, 1478, 1392, 1367, 1258, 1184, 1112, 1054 cm^{-1}; GC-MS: $C_{18}H_{17}FN_2O$ $[M]^+$: 296.09.



1d

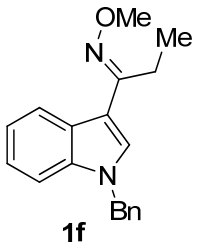
(*E*)-1-(1-Benzyl-6-chloro-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1d): White amorphous solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.29 (d, J = 8.5 Hz, 1H), 7.37 – 7.21 (m, 5H), 7.17 (dd, J = 8.5, 2.0 Hz, 1H), 7.10 (d, J = 6.4 Hz, 2H), 5.25 (s, 2H), 4.04 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.4, 137.9, 136.5, 129.4, 129.1, 129.0, 128.1, 126.8, 124.7, 124.1, 121.8, 113.8, 109.8, 62.0, 50.4, 13.0; FT-IR: $\tilde{\nu}$ = 2942, 2820,1604, 1538, 1494, 1468, 1376, 1332, 1267, 1228, 1176, 1050 cm^{-1}; LCMS (ESI): $C_{18}H_{18}{}^{35}ClN_2O$ $[M+H]^+$: 313.2.



1e

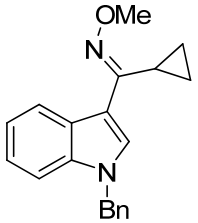
(*E*)-1-(1-Benzyl-7-methyl-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1e): White amorphous solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.29 (d, J= 8.0 Hz, 1H), 7.31 – 7.21 (m, 4H), 7.11 (t, J = 7.6 Hz, 1H), 6.93 (dd, J = 12.4, 7.1 Hz, 3H), 5.58 (s, 2H), 4.05 (s, 3H), 2.51 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ: 151.8, 139.2, 136.3, 131.0, 129.1, 127.6, 126.7, 126.0, 125.5,

121.7, 121.4, 121.0, 113.5, 61.9, 52.7, 19.6, 13.2; FT-IR: $\tilde{\nu}$ = 2956, 2810, 1596, 1546, 1489, 1452, 1419, 1385, 1328, 1260, 1182, 1048 cm^{-1}; GC-MS: $C_{19}H_{20}N_2O$ $[M]^+$: 292.13.



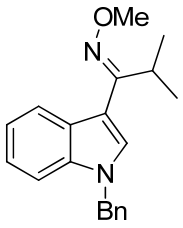
1f

(*E*)-1-(1-Benzyl-1*H*-indol-3-yl)propan-1-one *O*-methyl oxime (1f): Yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ: 8.37 (m, 1H), 7.36–7.18 (m, 7H), 7.11 (dd, J = 7.4, 1.8 Hz, 2H), 5.33 (s, 2H), 4.04 (s, 3H), 2.72 (q, J = 7.6 Hz, 2H), 1.22 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.1, 137.5, 136.9, 128.8, 128.6, 127.8, 126.7, 125.8, 123.6, 122.9, 120.9, 112.2, 109.6, 61.7, 50.2, 20.9, 12.1; FT-IR: $\tilde{\nu}$ = 2936, 2812, 2360, 1540, 1466, 1388, 1180, 1050 cm^{-1}; GC-MS: $C_{19}H_{20}N_2O$ $[M]^+$: 292.09.



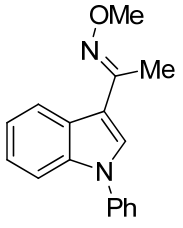
1g

(*E*)-(1-Benzyl-1*H*-indol-3-yl)(cyclopropyl)methanone *O*-methyl oxime (1g): Colorless oil; ^1H NMR (600 MHz,$CDCl_3$) δ: 8.05 (m, 1H), 8.00 (s, 1H), 7.32– 7.27 (m, 4H), 7.22 – 7.16 (m, 2H), 7.15 (d, J = 7.1 Hz, 2H), 5.35 (s, 2H), 3.92 (s, 3H), 2.04 (m, 1H), 1.08 – 1.05 (m, 2H), 0.95 – 0.91 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ: 152.0, 136.9, 136.1, 132.7, 129.0, 127.9, 127.1, 126.9, 122.3, 122.3, 120.6, 110.2, 109.0, 61.8, 50.6, 15.7, 7.0; FT-IR: $\tilde{\nu}$ = 2934, 2856, 1584, 1514, 1468, 1384, 1358, 1247, 1221, 1180, 1044 cm^{-1}; GC-MS: $C_{20}H_{20}N_2O$ $[M]^+$: 304.13.



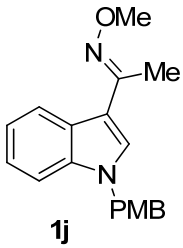
1h

(*E*)-1-(1-Benzyl-1*H*-indol-3-yl)-2-methylpropan-1-one *O*-methyl oxime (1h): Colorless oil; ^{1}H NMR (400 MHz,$CDCl_3$) δ: 7.62 (d, J = 7.9 Hz, 1H), 7.48 (s, 1H), 7.34 – 7.23 (m, 3H), 7.20–7.12 (m, 5H), 5.33 (s, 2H), 3.90 (s, 3H), 3.06 (m, 1H), 1.20 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.0, 137.0, 136.2, 129.6, 129.0, 127.9, 127.0, 126.9, 122.23, 122.17, 120.3, 110.1, 108.8, 61.6, 50.4, 34.5, 21.1; FT-IR: $\tilde{\nu}$ = 2932, 2864, 1614, 1524, 1466, 1368, 1361, 1243, 1223, 1182, 1042 cm^{-1}; GC-MS: $C_{20}H_{22}N_2O$ $[M]^+$: 306.17.



1i

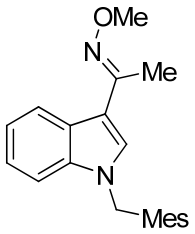
(*E*)-1-(1-Phenyl-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1i): White amorphous solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.39 (m, 1H), 7.56 –7.44 (m, 6H), 7.36 (m, 1H), 7.25 (m, 2H), 4.05 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.6, 139.4, 137.2, 129.8, 128.5, 127.1, 126.1, 124.8, 123.8, 123.5, 121.7, 115.2, 100.1, 62.0, 13.1; FT-IR: $\tilde{\nu}$ = 2928, 2810, 1596, 1546, 1502, 1456, 1411, 1300, 1228, 1179, 1135, 1056 cm^{-1}; GC-MS: $C_{17}H_{16}N_2O$ $[M]^+$: 264.10.



1j

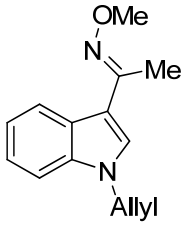
(*E*)-1-(1-(4-Methoxybenzyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1j): Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.41 (dd, J = 6.3, 2.9 Hz, 1H), 7.33–7.20 (m, 4H), 7.08 (d, J = 8.7 Hz, 2H), 6.88–6.81 (m, 2H), 5.23 (s, 2H), 4.07 (s, 3H), 3.79 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (150

MHz, $CDCl_3$) δ: 159.3, 151.8, 137.4, 128.9, 128.7, 128.3, 125.6, 123.6, 122.9, 121.0, 114.3, 113.3, 109.8, 61.8, 55.3, 49.8, 13.1; FT-IR: $\tilde{\nu}$ = 2934, 2836, 1612, 1546, 1514, 1466, 1388, 1338, 1297, 1248, 1176, 1057 cm^{-1}; GC-MS: $C_{19}H_{20}N_2O_2$ $[M]^+$: 308.09.



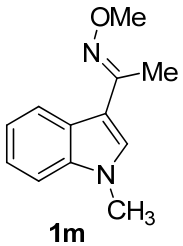
1k

(*E*)-1-(1-(2,4,6-Trimethylbenzyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1k): Amorphous solid; ^1H NMR (400 MHz, $CDCl_3$) δ: 8.36 (d, J = 7.8 Hz, 1H), 7.47 (d, J = 7.8 Hz, 1H), 7.32 (t, J = 7.8 Hz, 1H), 7.25 (m, 1H), 6.96 (s, 2H), 6.76 (s, 1H), 5.19 (s, 2H), 4.01 (s, 3H), 2.34 (s, 3H), 2.22 (s, 6H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.9, 138.3, 138.1, 137.6, 129.5, 128.3, 126.3, 125.6, 123.5, 122.6, 121.0, 112.8, 109.2, 61.7, 43.8, 21.1, 19.7, 13.1; FT-IR: $\tilde{\nu}$ = 2932, 2886, 2366, 1614, 1536, 1460, 1382, 1220, 1052 cm^{-1}; GC-MS: $C_{21}H_{24}N_2O$ $[M]^+$: 320.17.



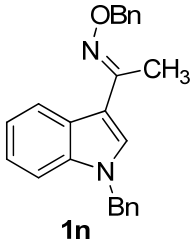
1l

(*E*)-1-(1-Allyl-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1l): Pale yellow oil; ^1H NMR (400 MHz, $CDCl_3$) δ: 8.39 (dd, J = 7.1, 1.6 Hz, 1H), 7.57 – 6.94 (m, 4H), 6.01 (m, 1H), 5.25 (d, J = 10.3 Hz, 1H), 5.12 (d, J = 17.1 Hz, 1H), 4.73 (d, J = 5.2 Hz, 2H), 4.07 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.8, 137.3, 133.0, 128.5, 125.5, 123.6, 122.8, 120.9, 117.8, 113.2, 109.6, 61.8, 49.0, 13.1; FT-IR: $\tilde{\nu}$ = 2934, 2814, 1651, 1598, 1542, 1468, 1388, 1338, 1249, 1186, 1149, 1054 cm^{-1}; GC-MS: $C_{14}H_{16}N_2O$ $[M]^+$: 228.10.



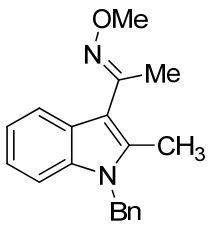
1m

(*E*)-1-(1-Methyl-1*H*-indol-3-yl)ethanone *O*-methyl oxime (1m): Greenish oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.40 (d, J = 7.7 Hz, 1H), 7.34–7.24 (m, 3H), 7.21 (s, 1H), 4.09 (s, 3H), 3.75 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.8, 137.8, 129.5, 125.3, 123.4, 122.7, 120.7, 112.7, 109.2, 61.8, 33.0, 13.0; FT-IR: $\tilde{\nu}$ = 2936, 2814, 1598, 1540, 1472, 1419, 1372, 1328, 1271, 1236, 1152, 1101, 1048 cm^{-1}; GC-MS: $C_{12}H_{14}N_2O$ $[M]^+$: 202.09.



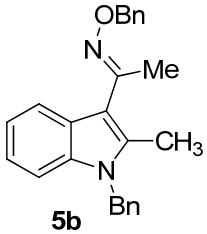
1n

(*E*)-1-(1-Benzyl-1*H*-indol-3-yl)ethanone *O*-benzyl oxime (1n): Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.29 (dd, J = 6.5, 1.7 Hz, 1H), 7.49 (d, J = 7.5 Hz, 2H), 7.37 (t, J = 7.4 Hz, 2H), 7.33 – 7.27 (m, 5H), 7.25 –7.16 (m, 3H), 7.11 (d, J = 6.5 Hz, 2H), 5.32 (s, 2H), 5.29 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.2, 138.8, 137.5, 137.1, 129.0, 128.9, 128.44, 128.35, 127.9, 127.7, 126.9, 125.6, 123.7, 123.0, 121.1, 113.7, 109.7, 76.1, 50.4, 13.5; FT-IR: $\tilde{\nu}$ = 2928, 2887, 1598, 1542, 1498, 1466, 1433, 1388, 1363, 1246, 1186, 1028 cm^{-1}; LCMS [ESI]: $C_{24}H_{23}N_2O$ $[M+H]^+$: 355.4.



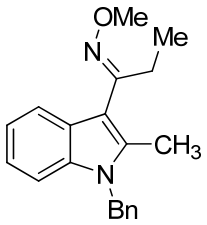
5a

(*E*)-1-(1-Benzyl-2-methyl-1*H*-indol-3-yl)ethanone *O*-methyl oxime (5a): Greenish oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.78 (m, 1H), 7.33 – 7.22 (m, 4H), 7.18 – 7.16 (m, 2H), 7.04 (d, J = 6.8 Hz, 2H), 5.35 (s, 2H), 4.04 (s, 3H), 2.53 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.0, 137.4, 136.7, 135.8, 128.9, 127.5, 126.7, 126.2, 121.7, 120.4, 119.9, 110.7, 109.5, 61.8, 46.7, 16.4, 11.8; FT-IR: $\tilde{\nu}$ = 2934, 2814, 1604, 1548, 1468, 1416, 1360, 1328, 1218, 1154, 1109, 1056 cm^{-1}; GC-MS: $C_{19}H_{20}N_2O$ $[M]^+$: 292.10.



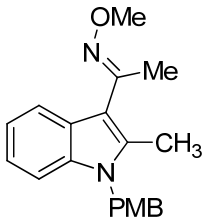
5b

(*E*)-1-(1-Benzyl-2-methyl-1*H*-indol-3-yl)ethanone *O*-benzyl oxime (5b): Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.73 (dd, J = 7.8, 1.9 Hz, 1H), 7.51 (d, J = 7.5 Hz, 2H), 7.42 (t, J = 7.5 Hz, 2H), 7.36 (d, J = 7.3 Hz, 1H), 7.34 – 7.22 (m, 4H), 7.22 – 7.12 (m, 2H), 7.03(d, J = 7.5 Hz, 2H), 5.34 (s, 2H), 5.30 (s, 2H), 2.47 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.3, 138.8, 137.3, 136.6, 135.8, 128.8, 128.3, 128.2, 127.6, 127.4, 126.6, 126.1, 121.5, 120.3, 119.8, 110.6, 109.3, 75.7, 46.6, 16.6, 11.7; FT-IR: $\tilde{\nu}$ = 2940, 2882, 1590, 1542, 1462, 1446, 1420, 1388, 1363, 1246, 1186, 1154, 1050 cm^{-1}; GC-MS: $C_{25}H_{24}N_2O$ $[M]^+$: 368.11.



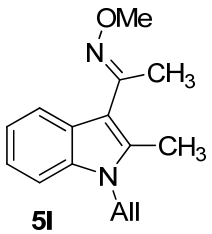
5c

(*E*)-1-(1-Benzyl-2-methyl-1*H*-indol-3-yl)propan-1-one *O*-methyl oxime (5c): Greenish oil; ^{1}H NMR (400 MHz,$CDCl_3$) δ: 7.66 (m, 1H), 7.34 – 7.18 (m, 4H), 7.18 – 7.09 (m, 2H), 7.02 (d, J = 6.8 Hz, 2H), 5.34 (s, 2H), 3.99 (s, 3H), 2.86 (q, J = 7.5 Hz, 2H), 2.47 (s, 3H), 1.13 (t, J = 7.5 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ: 158.3, 137.5, 136.8, 136.1, 128.9, 127.5, 127.1, 126.2, 121.6, 120.3, 119.5, 109.5, 61.7, 46.8, 23.1, 11.6, 10.9; FT-IR: $\tilde{\nu}$ = 2936, 2814, 1606, 1556, 1468, 1454, 1415, 1380, 1352, 1214, 1156, 1114, 1050 cm^{-1}; GC-MS: $C_{20}H_{22}N_2O$ $[M]^+$: 306.09.



5k

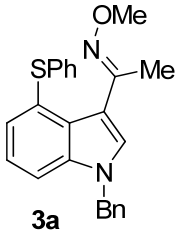
(*E*)-1-(1-(4-Methoxybenzyl)-2-methyl-1*H*-indol-3-yl)ethanone *O*-methyl oxime (5k): Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.76 (m, 1H), 7.27 (m, 1H), 7.19 – 7.12 (m, 2H), 6.97 (d, J = 8.2 Hz, 2H), 6.82 (d, J = 8.2 Hz, 2H), 5.28 (s, 2H), 4.03 (s, 3H), 3.77 (s, 3H), 2.52 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.0, 153.0, 136.7, 135.7, 129.4, 127.5, 126.7, 121.6, 120.3, 119.8, 114.3, 110.6, 109.5, 61.7, 55.4, 46.2, 16.4, 11.9; FT-IR: $\tilde{\nu}$ = 2934, 2836, 1612, 1512, 1466, 1416, 1360, 1293, 1248, 1176, 1110, 1056 cm^{-1}; GC-MS: $C_{20}H_{22}N_2O_2$ $[M]^+$: 322.07.



5l

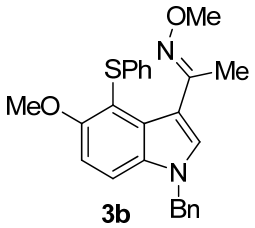
(*E*)-1-(1-Allyl-2-methyl-1*H*-indol-3-yl)ethanone *O*-methyl oxime (5l): Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.72 (d, J = 7.8 Hz, 1H), 7.28 (m, 1H), 7.20-7.10 (m, 2H), 5.93 (m, 1H), 5.15 (dd, J = 10.4, 1.2 Hz, 1H), 4.90 (dd, J = 17.1, 1.2 Hz, 1H), 4.71 (m, 2H), 4.01 (s, 3H), 2.53 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.9, 136.2, 135.4, 132.8, 126.6, 121.3, 120.1, 119.6, 116.6, 110.3, 109.2, 61.6, 45.4, 16.2, 11.4; FT-IR: $\tilde{\nu}$ = 2930, 2810, 1596, 1542, 1472, 1382, 1249, 1179, 1149, 1054 cm^{-1}; GC-MS: $C_{15}H_{18}N_2O$ $[M]^+$: 242.10.

10.2. Characterization data for the final thiolated products:



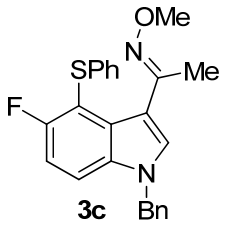
3a

(*E*)-1-(1-Benzyl-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3a): Pale yellow oil, 83%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.40–7.30 (m, 3H), 7.30–7.11 (m, 11H), 5.30 (s, 2H), 3.86 (s, 3H), 2.27 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 152.8, 137.5, 137.3, 136.4, 129.3, 128.93, 128.91, 128.6, 127.9, 127.3, 127.2, 126.4, 125.9, 122.8, 114.5, 110.1, 61.5, 50.5, 19.2; FT-IR: $\tilde{\nu}$ =: 3060, 2932, 2814, 2362, 1724, 1550, 1432, 1358, 1248, 1176, 1050, 769 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{23}N_2OS$ $[M+H]^+$: 387.1526, found 387.1511.



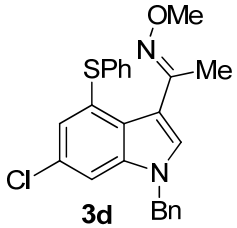
3b

(*E*)-1-(1-Benzyl-5-methoxy-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3b): Yellow oil, 72%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.39–7.30 (m, 4H), 7.22 (d, J = 7.8 Hz, 2H), 7.17 (s, 1H), 7.14 (d, J = 7.8 Hz, 2H), 7.07–7.01 (m, 3H), 6.99 (d, J = 8.9 Hz, 1H), 5.27 (s, 2H), 3.83 (s, 3H), 3.79 (s, 3H), 2.17 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 156.2 , 153.5, 138.9, 136.6, 132.9, 130.6, 130.0, 129.0, 128.6, 128.1, 127.4, 126.4, 124.6, 114.4, 112.2, 110.1, 109.4, 61.5, 57.8, 50.7, 19.6; FT-IR: $\tilde{\nu}$ = 2931, 2835, 1590, 1542, 1463, 1428, 1363, 1328, 1262, 1220, 1179, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2O_2S$ $[M+H]^+$: 417.1631, found 417.1623.



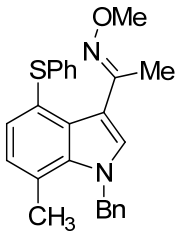
3c

(*E*)-1-(1-Benzyl-5-fluoro-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3c): White crystaline solid, 91%; mp = 105-107 ^{0}C; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.40–7.32 (m, 3H), 7.30 (dd, J = 9.0, 4.0 Hz, 1H), 7.24–7.17 (m, 5H), 7.11 (d, J = 8.3 Hz, 3H), 7.06 (m, 1H), 5.29 (s, 2H), 3.83 (s, 3H), 2.20 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 159.2 (d, J = 238.3 Hz), 152.6, 137.6, 136.1, 133.6, 130.3, 129.43, 129.42, 128.9 (d, J = 29.8 Hz), 128.1, 127.2, 127.0, 125.3, 114.9 (d, J = 5.1 Hz), 112.4 (d, J = 9.8 Hz), 111.2 (d, J = 28.6 Hz), 109.3 (d, J = 21.3 Hz), 61.4, 50.7, 19.3; ^{19}F NMR ($CDCl_3$, 376 MHz) δ: -115.8; FT-IR: $\tilde{\nu}$ = 3064, 2932, 2814, 1582, 1459, 1434, 1226, 1160, 1052, 796 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}FN_2OS$ $[M+H]^+$: 405.1431, found 405.1415.



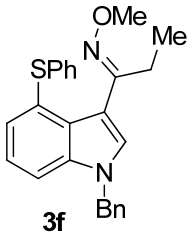
3d

(*E*)-1-(1-Benzyl-6-chloro-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3d): White amorphous solid, 74%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.36–7.20 (m, 8H), 7.19 (d, J = 1.8 Hz, 1H), 7.17–7.14 (m, 2H), 7.13 (s, 1H), 7.01 (d, J = 1.8 Hz, 1H), 5.22 (s, 2H), 3.86 (s, 3H), 2.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.2, 137.4, 135.9, 135.6, 130.7, 129.2, 129.1, 129.0, 128.9, 128.5, 128.2, 127.1, 126.9, 125.1, 124.6, 114.8, 109.3, 61.6, 50.5, 18.9; FT-IR: $\tilde{\nu}$ = 3062, 2932, 2814, 2364, 1546, 1426, 1220, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}{}^{35}ClN_2OS$ $[M+H]^+$: 421.1136, found 421.1120.



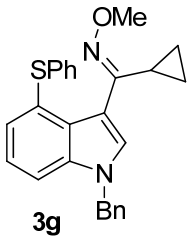
3e

(*E*)-1-(1-Benzyl-7-methyl-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3e): Yellow oil, 83%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.36-7.27 (m, 3H), 7.24-7.19 (m, 2H), 7.16 (d, J = 7.3 Hz, 1H), 7.15-7.12 (m, 3H), 7.11 (s, 1H), 7.01 (d, J = 7.4 Hz, 2H), 6.91 (d, J = 7.4 Hz, 1H), 5.58 (s, 2H), 3.80 (s, 3H), 2.56 (s, 3H), 2.24 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 153.1, 138.8, 138.7, 136.1, 130.7, 129.1, 128.9, 128.8, 128.3, 127.9, 127.7, 126.1, 125.8, 125.6, 122.6, 122.2, 114.7, 61.5, 52.5, 19.7, 19.6; FT-IR: $\tilde{\nu}$ = 2962, 2927, 2814, 1584, 1476, 1446, 1406, 1363, 1258, 1180, 1044, 738 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2OS$ $[M+H]^+$: 401.1682, found 401.1692.



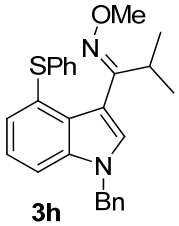
3f

(*E*)-1-(1-Benzyl-4-(phenylthio)-1*H*-indol-3-yl)propan-1-one *O*-methyl oxime (3f): White amorphous solid, 79%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.40-7.29 (m, 3H), 7.27-7.10 (m, 11H), 5.32 (s, 2H), 3.80 (s, 3H), 2.83 (q, J = 7.6 Hz, 2H), 0.99 (t, J = 7.6 Hz, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 158.3, 137.5, 137.3, 136.7, 129.7, 129.03, 129.02, 128.0, 127.9, 127.2, 126.4, 126.2, 122.8, 112.6, 110.0, 61.5, 50.6, 25.3, 10.6; FT-IR: $\tilde{\nu}$ = 3060, 2932, 1552, 1432, 1332, 1220, 1046, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2OS$ $[M+H]^+$: 401.1682, found 401.1665.



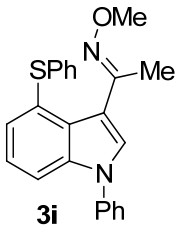
3g

(*E*)-(1-Benzyl-4-(phenylthio)-1*H*-indol-3-yl)(cyclopropyl)methanone *O*-methyl oxime (3g): White amorphous solid, 57%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.37 – 7.29 (m, 3H), 7.28 – 7.23 (m, 4H), 7.22 – 7.12 (m, 4H), 7.12 – 7.07 (m, 2H), 7.01 (s, 1H), 5.28 (s, 2H), 3.80 (s, 3H), 2.57 (m, 1H), 0.86 – 0.79 (m, 2H), 0.52–0.49 (m, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 158.4, 137.6, 136.8, 136.5, 129.9, 129.3, 128.9, 128.8, 127.9, 127.1, 126.9, 126.1, 125.8, 122.8, 109.6 , 108.1, 99.9, 61.6, 50.4, 11.6, 5.9; FT-IR: $\tilde{\nu}$ = 2920, 2850, 1577, 1546, 1481, 1432, 1389, 1328, 1262, 1220, 1170, 1038, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{25}N_2OS$ $[M+H]^+$: 413.1682, found 413.1662.



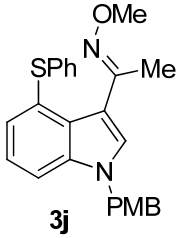
3h

(*E*)-1-(1-Benzyl-4-(phenylthio)-1*H*-indol-3-yl)-2-methylpropan-1-one *O*-methyl oxime (3h): Pale yellow oil, 54%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.35– 7.31 (m, 2H), 7.30 – 7.22 (m, 5H), 7.18 (d, J = 7.8 Hz, 2H), 7.15 (d, J = 7.8 Hz, 2H), 7.09 – 7.04 (m, 2H), 6.98 (d, J = 7.9 Hz, 1H), 5.32 (s, 2H), 3.75 (s, 3H), 3.54 (m, 1H), 1.07 (d, J = 6.9 Hz, 6H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 160.9, 136.9, 136.7, 136.6, 130.7, 128.9, 128.8, 128.4, 128.1, 127.8, 127.4, 126.9, 126.3, 124.7, 122.7, 110.3, 109.1, 61.4, 50.4, 28.9, 19.6; FT-IR: $\tilde{\nu}$ = 2962, 2870, 1554, 1476, 1430, 1393, 1332, 1248, 1214, 1176, 1036, 736 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{27}N_2OS$ $[M+H]^+$: 415.1839, found 415.1823.



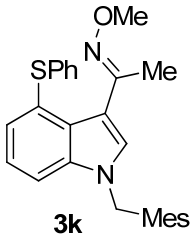
3i

(*E*)-1-(1-Phenyl-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3i): White amorphous solid, 65%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.62–7.46 (m, 5H), 7.46 –7.38 (m, 1H), 7.37(s, 1H), 7.33–7.12 (m, 7H), 3.84 (s, 3H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 152.8, 139.0, 137.8, 137.2, 129.9, 129.14, 129.08, 128.5, 128.1, 127.5, 127.4, 126.0, 125.9, 125.0, 123.5, 116.0, 111.1 , 61.6, 19.3; FT-IR: $\tilde{\nu}$ = 2930, 2812, 1584, 1537, 1498, 1463, 1430, 1324, 1248, 1176, 1135, 1050, 748 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{23}H_{21}N_2OS$ $[M+H]^+$: 373.1369, found 373.1355.



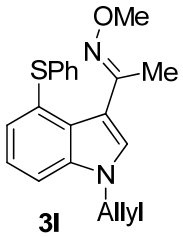
3j

(*E*)-1-(1-(4-Methoxybenzyl)-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3j): Yellow oil, 63%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.31 (dd, J = 8.0, 1.0 Hz, 1H), 7.25-7.21 (m, 2H), 7.20-7.13 (m, 8H), 6.88 (d, J = 8.4 Hz, 2H), 5.23 (s, 2H), 3.84 (s, 3H), 3.81(s, 3H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 159.4, 152.8, 137.6, 137.3, 129.2, 128.9, 128.7, 128.4, 128.3, 127.4, 126.4, 125.9, 125.8, 122.7, 114.3, 110.0, 61.4, 55.3, 49.9, 19.1; FT-IR: $\tilde{\nu}$ = 2922, 2852, 1512, 1434, 1220, 1048, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2O_2S$ $[M+H]^+$: 417.1631, found 417.1616.



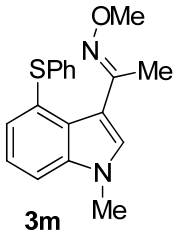
3k

(*E*)-1-(4-(Phenylthio)-1-(2,4,6-trimethylbenzyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3k): Amorphous solid, 62%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.46 (dd, J = 7.7, 1.5 Hz, 1H), 7.30–7.10 (m, 7H), 6.94 (s, 2H), 6.66 (s, 1H), 5.19 (s, 2H), 3.78 (s, 3H), 2.32 (s, 3H), 2.23 (s, 6H), 2.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 152.9, 138.4, 138.1, 137.5, 137.4, 129.5, 129.4, 128.9, 128.1, 127.3, 126.4, 126.2, 126.0, 125.9, 122.5, 113.9, 109.4, 61.3, 43.9, 21.0, 19.8, 19.2; FT-IR: $\tilde{\nu}$ = 3064, 2924, 2845, 1542, 1424, 1228, 1178, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{27}H_{29}N_2OS$ $[M+H]^+$: 429.1995, found 429.1976.



3l

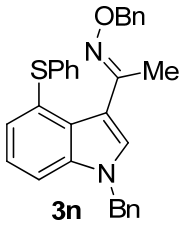
(*E*)-1-(1-Allyl-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3l): Pale yellow oil, 85%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.32 (dd, J = 7.7, 1.6 Hz, 1H), 7.24-7.19 (m, 4H), 7.18-7.12 (m, 4H), 6.03 (m, 1H), 5.29 (dd, J = 10.0, 1.6 Hz, 1H), 5.23 (dd, J = 17.4, 1.6 Hz, 1H), 4.73 (d, J = 5.7 Hz, 2H), 3.84 (s, 3H), 2.25 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.8, 137.7, 137.1, 132.7, 129.0, 128.9, 128.2, 127.4, 126.6, 125.8, 125.6, 122.6, 118.3, 114.2, 110.0, 61.4, 49.2, 19.1; FT-IR: $\tilde{\nu}$ = 2920, 1446, 1220, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{20}H_{21}N_2OS$ $[M+H]^+$: 337.1369, found 337.1355.



3m

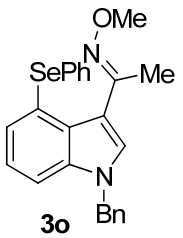
(*E*)-1-(1-Methyl-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3m): Pale yellow oil, 74%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.30 (dd, J = 7.3, 1.8 Hz, 1H), 7.24-7.17 (m, 4H), 7.14-7.09 (m, 4H), 3.81 (s, 3H), 3.78 (s, 3H), 2.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.8, 137.8, 137.7, 129.3, 128.8, 127.3, 126.7, 125.7, 122.6, 113.9, 109.7, 61.4, 32.9, 19.1; FT-IR: $\tilde{\nu}$ =

3056, 2932, 1542, 1456, 1411, 1330, 1244, 1124, 1050, 769 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{18}H_{19}N_2OS$ $[M+H]^+$: 311.1213, found 311.1220.



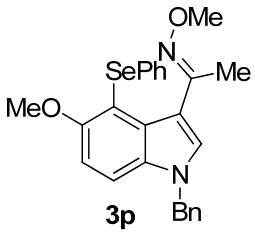
3n

(*E*)-1-(1-Benzyl-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-benzyl oxime (3n): Yellow oil, 71%; ^1H NMR ($CDCl_3$, 600 MHz) δ: 7.42 (d, J = 7.2 Hz, 2H), 7.39-7.30 (m, 6H), 7.27-7.13 (m, 11H), 5.31 (s, 2H), 5.12 (s, 2H), 2.33 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 153.5, 138.3, 137.6, 137.3, 136.5, 129.5, 128.93, 128.90, 128.7, 128.3, 127.9, 127.8, 127.5, 127.3, 127.2, 126.3, 126.1, 126.0, 122.8, 114.5, 109.9, 75.6, 50.5, 19.6; FT-IR: $\tilde{\nu}$ = 3030, 2922, 2858, 2362, 1550, 1432, 1362, 1220, 1024, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{30}H_{27}N_2OS$ $[M+H]^+$: 463.1839, found 463.1848.



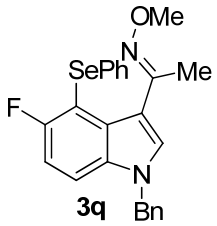
3o

(*E*)-1-(1-Benzyl-4-(phenylselanyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3o): White amorphous solid, 94%; ^1H NMR ($CDCl_3$, 400 MHz) δ: 7.57–7.47 (m, 2H), 7.40–7.25 (m, 6H), 7.23 (s, 1H), 7.20–7.15 (m, 3H), 7.09-6.99 (m, 2H), 5.29 (s, 2H), 4.01 (s, 3H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 152.3, 136.9, 136.5, 133.9, 132.2, 129.2, 128.9, 128.6, 127.9, 127.3, 127.1, 126.9, 125.7, 124.6, 123.0, 115.1, 108.9, 61.6, 50.4, 18.1; FT-IR: $\tilde{\nu}$ = 3058, 2932, 1550, 1432, 1220, 1176, 1048, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{23}N_2OSe$ $[M+H]^+$: 435.0970, found 435.0955.



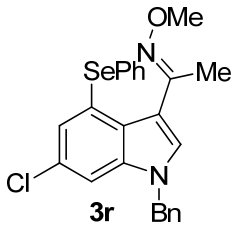
3p

(*E*)-1-(1-Benzyl-5-methoxy-4-(phenylselanyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3p): Yellow oil, 60%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.39-7.27 (m, 4H), 7.24-7.19 (m, 4H), 7.18 (s, 1H), 7.16-7.08 (m, 3H), 6.97 (d, J = 9.4 Hz, 1H), 5.27 (s, 2H), 3.86 (s, 3H), 3.78 (s, 3H), 2.19 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 155.4, 153.2, 136.5, 134.3, 132.6, 130.7, 129.8, 129.3, 128.9, 128.7, 127.9, 127.2, 125.4, 114.9, 111.9, 109.3, 107.9, 61.4, 57.8, 50.5, 19.7; FT-IR: $\tilde{\nu}$ = 2932, 2848, 2362, 1546, 1454, 1430, 1218, 1186, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2O_2Se$ $[M+H]^+$: 465.1076, found 465.1089.



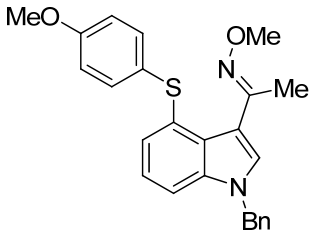
3q

(*E*)-1-(1-Benzyl-5-fluoro-4-(phenylselanyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3q): White amorphous solid, 93%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.39-7.31 (m, 3H), 7.30-7.26 (m, 3H), 7.24 (s, 1H), 7.21 (d, J = 7.8 Hz, 2H), 7.19-7.13 (m, 3H), 7.03 (t, J = 8.5 Hz, 1H), 5.29 (s, 2H), 3.90 (s, 3H), 2.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 158.8 (d, J = 235.3 Hz), 152.7, 136.3, 133.4, 133.0, 130.3, 130.2, 129.8 (d, J = 3.3 Hz), 129.1, 128.2, 127.3, 126.2, 115.6 (d, J = 4.2 Hz), 112.2 (d, J = 9.8 Hz), 111.0 (d, J = 30.0 Hz), 106.0 (d, J = 26.0 Hz), 61.6, 50.8, 19.5; ^{19}F NMR ($CDCl_3$, 376 MHz) δ: -109.6; FT-IR: $\tilde{\nu}$ = 2932, 2366, 1465, 1434, 1220, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}FN_2OSe$ $[M+H]^+$: 453.0876, found 453.0852.



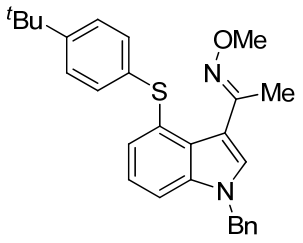
3r

(*E*)-1-(1-Benzyl-6-chloro-4-(phenylselanyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3r): White amorphous solid, 88%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.59-7.54 (m, 2H), 7.39-7.30 (m, 6H), 7.21 (s, 1H), 7.16 (d, J = 7.0 Hz, 2H), 7.14 (d, J = 1.8 Hz, 1H), 6.93 (d, J = 1.8 Hz, 1H), 5.25 (s, 2H), 4.04 (s, 3H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 151.7, 137.1, 135.9, 134.8, 130.9, 129.5, 129.2, 129.1, 128.9, 128.1, 128.0, 127.1, 126.9, 124.9, 124.5, 115.5, 108.4, 61.7, 50.5, 17.7; FT-IR: $\tilde{\nu}$ = 3062, 2932, 2814, 2360, 1540, 1430, 1244, 1176, 1050, 740 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}{}^{35}ClN_2OSe$ $[M+H]^+$: 469.0580, found 469.0559.



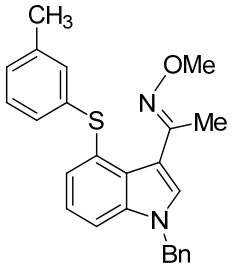
4a

(*E*)-1-(1-Benzyl-4-(4-methoxyphenylthio)-1H-indol-3-yl)ethanone *O*-methyl oxime (4a): Colorless oil, 72%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.40 – 7.28 (m, 5H), 7.23 – 7.11 (m, 4H), 7.06 (t, J = 7.8 Hz, 1H), 6.86 (t, J = 8.1 Hz, 3H), 5.28 (s, 2H), 3.95 (s, 3H), 3.80 (s, 3H), 2.33 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 159.2, 152.9, 137.1, 136.5, 133.9, 129.7, 128.9, 128.3, 127.9, 127.1, 126.0, 125.5, 122.7, 114.8, 114.4, 108.5, 61.6, 55.3, 50.4, 19.2; FT-IR: $\tilde{\nu}$ = 3045, 2928, 2886, 1590, 1487, 1440, 1248, 1166, 1138, 1050, 1025, 740 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2O_2S$ $[M+H]^+$: 417.1631, found 417.1615.



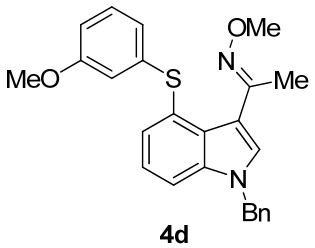
4b

(*E*)-1-(1-Benzyl-4-(4-*tert*-butylphenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4b): Colorless oil, 47%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.37-7.30 (m, 3H), 7.29-7.25 (m, 2H), 7.24-7.14 (m, 6H), 7.13-7.08 (m, 2H), 5.30 (s, 2H), 3.86 (s, 3H), 2.27 (s, 3H), 1.29 (s, 9H)); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.9, 149.4, 137.2, 136.5, 133.4, 129.9, 128.9, 128.5, 127.9, 127.2, 127.1, 126.1, 125.9, 125.3, 122.8, 114.5, 109.5, 61.4, 50.4, 34.5, 31.3, 19.2; FT-IR: $\tilde{\nu}$ = 3072, 2962, 2818, 1548, 1459, 1432, 1360, 1176, 1052, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{28}H_{31}N_2OS$ $[M+H]^+$: 443.2152, found 443.2160.



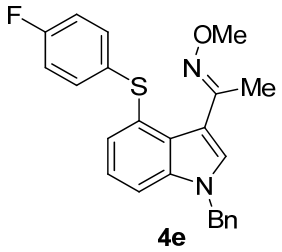
4c

(*E*)-1-(1-Benzyl-4-(*m*-tolylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4c): Yellow oil, 61%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.37-7.28 (m, 3H), 7.25-7.05 (m, 8H), 6.98 (d, J = 8.3 Hz, 2H), 5.23 (s, 2H), 3.86 (s, 3H), 2.27 (s, 3H), 2.25 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 152.9, 138.6, 137.3, 136.9, 136.5, 130.4, 128.9, 128.8, 128.5, 127.9, 127.2, 127.1, 127.0, 126.9, 126.6, 125.8, 122.7, 114.5, 109.7, 61.4, 50.4, 21.3, 19.2; FT-IR: $\tilde{\nu}$ = 3060, 2926, 2358, 1550, 1430, 1220, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2OS$ $[M+H]^+$: 401.1682, found 401.1693.



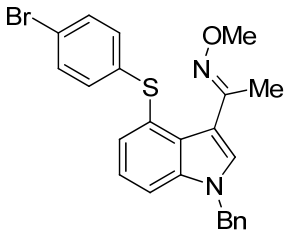
4d

(*E*)-1-(1-Benzyl-4-(3-methoxyphenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4d): Pale yellow oil, 58%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.38-7.29 (m, 3H), 7.27 (d, J = 7.8 Hz, 1H), 7.23-7.18 (m, 4H), 7.17-7.12 (m, 2H), 6.80-6.69 (m, 3H), 5.31 (s, 2H), 3.88 (s, 3H), 3.74 (s, 3H), 2.25 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 159.9, 152.8, 138.9, 137.3, 136.4, 129.7, 128.9, 128.6, 127.9, 127.3, 127.2, 126.6, 125.7, 122.8, 121.7, 114.5, 111.9, 110.1, 61.4, 55.2, 50.4, 19.1; FT-IR: $\tilde{\nu}$ = 3064, 2928, 1592, 1494, 1450, 1248, 1176, 1138, 1050, 1030, 740 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2O_2S$ $[M+H]^+$: 417.1631, found 417.1642.



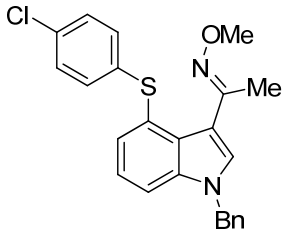
4e

(*E*)-1-(1-Benzyl-4-(4-fluorophenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4e): Colorless oil, 68%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.37-7.30 (m, 3H), 7.26 (dd, J = 8.0, 1.2 Hz, 1H), 7.23-7.19 (m, 5H), 7.16-7.09 (m, 2H), 6.96 (t, J = 8.6 Hz, 2H), 5.27 (s, 2H), 3.85 (s, 3H), 2.26 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 161.8 (d, J = 246.2 Hz), 152.7, 137.3, 136.4 , 132.1 (d, J = 2.6 Hz), 131.9 (d, J = 8.3 Hz), 128.9, 128.6, 127.9, 127.2, 126.8 (d, J = 17.8 Hz), 125.5, 122.8, 116.1 (d, J = 21.9 Hz), 114.4, 109.8, 99.9, 61.5, 50.5, 19.1; ^{19}F NMR ($CDCl_3$, 376 MHz) δ: -115.9; FT-IR: $\tilde{\nu}$ = 3062, 2932, 2814, 1588, 1488, 1430, 1222, 1050, 774 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}FN_2OS$ $[M+H]^+$: 405.1431, found 405.1445.



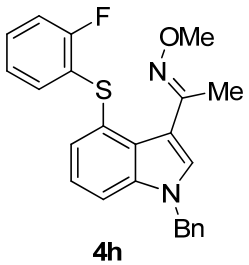
4f

(*E*)-1-(1-Benzyl-4-(4-bromophenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4f): White amorphous solid, 76%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.38-7.27 (m, 6H), 7.24-7.14 (m, 5H), 6.98 (d, J = 8.0 Hz, 2H), 5.30 (s, 2H), 3.82 (s, 3H), 2.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.5, 137.4, 137.3, 136.3, 131.9, 130.1, 128.9, 128.8, 128.0, 127.5, 127.2, 126.7, 124.6, 122.8, 119.4, 114.4, 110.7, 61.4, 50.5, 19.1; FT-IR: $\tilde{\nu}$ = 2932, 2814, 2372, 1600, 1548, 1470, 1428, 1174, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}{}^{79}BrN_2OS$ $[M+H]^+$: 465.0631, found 465.0615.



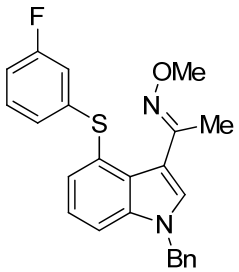
4g

(*E*)-1-(1-Benzyl-4-(4-chlorophenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4g): Amorphous solid, 85%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.39-7.30 (m, 4H), 7.25 (d, J = 7.1 Hz, 1H), 7.23-7.16 (m, 6H), 7.08 (d, J = 8.3 Hz, 2H), 5.31 (s, 2H), 3.85 (s, 3H), 2.26 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.6, 137.4, 136.5, 136.3, 131.7, 130.0, 129.0, 128.9, 128.8, 128.0, 127.4, 127.2, 127.0, 124.9, 122.8, 114.5, 110.6, 61.4, 50.5, 19.1; FT-IR: $\tilde{\nu}$ = 2932, 2818, 1552, 1472, 1220, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}{}^{35}ClN_2OS$ $[M+H]^+$: 421.1136, found 421.1119.



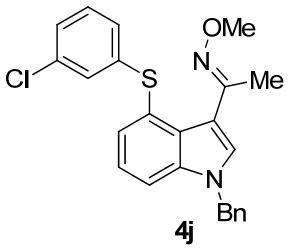
4h

(*E*)-1-(1-Benzyl-4-(2-fluorophenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4h): Yellow oil, 94%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.39-7.27 (m, 4H), 7.23-7.12 (m, 6H), 7.06 (m, 1H), 6.98-6.88 (m, 2H), 5.30 (s, 2H), 3.83 (s, 3H), 2.26 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 160.1 (d, J = 245.6 Hz), 152.7, 137.5 , 136.5, 131.4, 129.0, 128.9, 128.1, 127.7 (d, J = 7.3 Hz), 127.4, 127.3, 126.7, 124.9 (d, J = 17.0 Hz), 124.7 (d, J = 3.4 Hz), 124.1, 122.9, 115.5 (d, J = 21.5 Hz), 114.6, 110.5, 61.5, 50.6, 19.1; ^{19}F NMR ($CDCl_3$, 376 MHz) δ: -110.8; FT-IR: $\tilde{\nu}$ = 3064, 2934, 2814, 1550, 1472, 1439, 1220, 1171, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}FN_2OS$ $[M+H]^+$: 405.1431, found 405.1442.



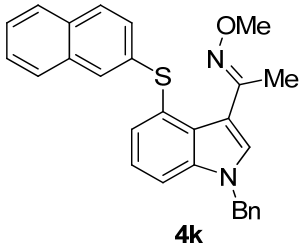
4i

(*E*)-1-(1-Benzyl-4-(3-fluorophenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4i): Pale yellow oil, 64%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.38-7.29 (m, 5H), 7.21 (d, J = 7.7 Hz, 3H), 7.19 (s, 1H), 7.16 (m, 1H), 6.89 (d, J = 8.0 Hz, 1H), 6.83-6.78 (m, 2H), 5.32 (s, 2H), 3.83 (s, 3H), 2.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 163.1 (d, J = 247.4 Hz), 152.7, 140.9 (d, J = 7.8 Hz), 137.6, 136.5, 130.1 (d, J = 8.2 Hz), 129.1, 128.9, 128.2, 128.1, 128.0, 127.3, 124.0, 123.8 (d, J = 2.4 Hz), 122.9, 115.1 (d, J = 23.6 Hz), 114.6, 112.6 (d, J = 21.7 Hz), 111.1, 61.5, 50.6, 19.2; ^{19}F NMR ($CDCl_3$, 376 MHz) δ: -112.7; FT-IR: $\tilde{\nu}$ = 3064, 2934, 2814, 2358, 1598, 1472,1430, 1176, 1050, 774 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}FN_2OS$ $[M+H]^+$: 405.1431, found 405.1445.



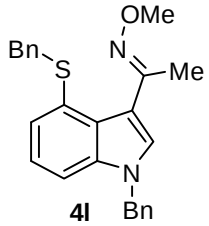
4j

(*E*)-1-(1-Benzyl-4-(3-chlorophenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4j): Yellow oil, 90%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.39-7.27 (m, 5H), 7.23-7.18 (m, 4H), 7.17-7.07 (m, 3H), 6.97 (dt, J = 7.8, 1.8 Hz, 1H), 5.32 (s, 2H), 3.85 (s, 3H), 2.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.5, 140.4, 137.4, 136.3, 134.6, 132.9, 129.8, 128.9, 128.0, 127.9, 127.7, 127.2, 126.4, 125.7, 124.0, 122.8, 114.4, 110.9, 61.4, 50.5, 19.1; FT-IR: $\tilde{\nu}$ = 3060, 2932, 2814, 1574, 1456, 1433, 1176, 1050, 774 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{24}H_{22}{}^{35}ClN_2OS$ $[M+H]^+$: 421.1136, found 421.1136.



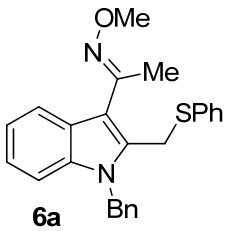
4k

(*E*)-1-(1-Benzyl-4-(naphthalen-2-ylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4k): Amorphous solid, 62%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.78 (d, J = 8.4 Hz, 1H), 7.75 (s, 1H), 7.72-7.68 (m, 2H), 7.47-7.40 (m, 2H), 7.39-7.25 (m, 5H), 7.23 (t, J = 7.8 Hz, 3H), 7.19 (s, 1H), 7.16 (m, 1H), 5.32 (s, 2H), 3.71 (s, 3H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.9 , 137.5, 136.6 , 134.9, 133.9, 132.0, 129.0, 128.8, 128.6, 128.1, 128.0, 127.8, 127.7, 127.4, 127.3, 126.42, 126.40, 126.3, 125.7, 122.9, 114.7, 110.1, 61.4, 50.6, 19.3; FT-IR: $\tilde{\nu}$ = 3054, 2932, 2362, 1550, 1430, 1356, 1174, 1050, 742 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{28}H_{25}N_2OS$ $[M+H]^+$: 437.1682, found 437.1692.



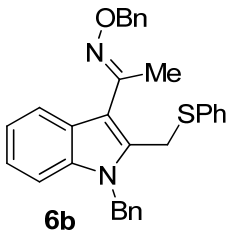
4l

(*E*)-1-(1-Benzyl-4-(benzylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (4l): Colorless oil, 26%; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.34-7.28 (m, 3H), 7.25-7.19 (m, 5H), 7.19-7.14 (m, 4H), 7.13-7.05 (m, 2H), 5.28 (s, 2H), 4.09 (s, 2H), 3.99 (s, 3H), 2.34 (s, 3H); ^{13}C NMR ($CDCl_3$,150 MHz) δ: 154.0, 137.9, 137.1, 136.7, 129.2, 129.0, 128.5, 128.27, 128.25, 128.0, 127.2, 127.12, 127.09, 124.1, 122.7, 114.5, 109.4, 61.7, 50.5, 40.7, 19.8; FT-IR: $\tilde{\nu}$ = 2930, 2852, 1650, 1540, 1454, 1428, 1359, 1339, 1248, 1176, 1050, 769 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2OS$ $[M+H]^+$: 401.1682, found 401.1699.



6a

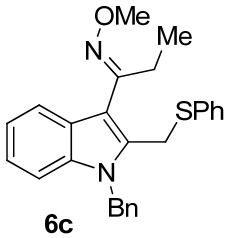
(*E*)-1-(1-Benzyl-2-(phenylthiomethyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6a): Yellow oil, 65%; ^{1}H NMR ($CDCl_3$, 600 MHz) *δ*: 7.69 (d, *J* = 7.8 Hz, 1H), 7.34-7.31 (m, 2H), 7.30-7.22 (m, 7H), 7.21-7.13 (m, 2H), 7.01 (d, *J* = 7.8 Hz, 2H), 5.52 (s, 2H), 4.48 (s, 2H), 3.98 (s, 3H), 2.19 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) *δ*: 152.5, 137.2, 137.1, 134.9, 133.5, 131.4, 128.9, 128.8, 127.5, 127.1, 126.2, 126.1, 122.5, 120.5, 120.2, 112.7, 109.8, 61.7, 46.9, 29.5, 15.9; FT-IR: $\tilde{\nu}$ = 2932, 2814, 1585, 1546, 1466, 1433, 1360, 1234, 1197, 1160, 1052, 742 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{25}N_2OS$ $[M+H]^+$: 401.1682, found 401.1688.



6b

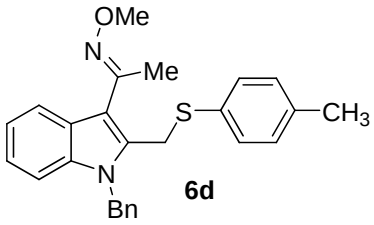
(*E*)-1-(1-Benzyl-2-(phenylthiomethyl)-1*H*-indol-3-yl)ethanone *O*-benzyl oxime (6b): Yellow oil, 63%; ^{1}H NMR ($CDCl_3$, 600 MHz) *δ*: 7.62 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.36

(t, J = 7.3 Hz, 2H), 7.31 (d, J = 7.8 Hz, 1H), 7.25-7.16 (m, 8H), 7.15-7.10 (m, 3H), 6.98 (d, J = 7.3 Hz, 2H), 5.49 (s, 2H), 5.20 (s, 2H), 4.32 (s, 2H), 2.20 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.9, 138.6, 137.2, 135.9, 134.9, 133.5, 131.4, 128.9, 128.8, 128.4, 128.2, 127.7, 127.6, 127.5, 126.9, 126.2, 122.5, 120.4, 120.2, 112.8, 109.8, 75.8, 46.9, 29.3, 16.2; FT-IR: $\tilde{\nu}$ = 3028, 2922, 1548, 1464, 1360, 1220, 1160, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{31}H_{29}N_2OS$ $[M+H]^+$: 477.1995, found 477.2005.



6c

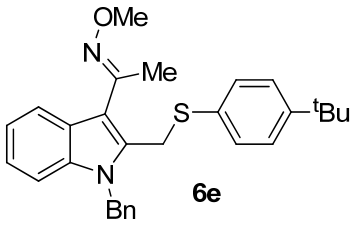
(*E*)-1-(1-Benzyl-2-(phenylthiomethyl)-1*H*-indol-3-yl)propan-1-one *O*-methyl oxime (6c): Yellow oil, 67%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.70 (d, J = 7.5 Hz, 1H), 7.35 (d, J = 9.0 Hz, 2H), 7.32-7.23 (m, 7H), 7.22-7.14 (m, 2H), 6.99 (d, J = 8.2 Hz, 2H), 5.40 (s, 2H), 4.47 (s, 2H), 3.97 (s, 3H), 2.81 (q, J = 7.5 Hz, 2H), 1.13 (t, J = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 157.7, 137.2, 137.1, 135.9, 133.9, 130.6, 128.9, 128.8, 127.4, 126.8, 126.6, 126.1, 122.5, 120.5, 120.1, 111.5, 109.9, 61.6, 46.9, 29.6, 23.0, 10.8; FT-IR: $\tilde{\nu}$ = 2932, 2848, 1581, 1537, 1464, 1411, 1352, 1284, 1220, 1192, 1158, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{27}N_2OS$ $[M+H]^+$: 415.1839, found 415.1838.



6d

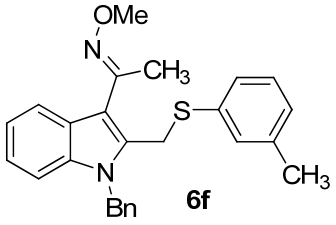
(*E*)-1-(1-Benzyl-2-(*p*-tolylthiomethyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6d): Pale yellow oil, 49%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.70 (d, J = 7.8 Hz, 1H), 7.30-7.24 (m, 4H), 7.23-7.14 (m, 4H), 7.08 (d, J = 7.8 Hz, 2H), 7.02 (d, J = 7.8 Hz, 2H), 5.53 (s, 2H), 4.43 (s, 2H), 3.99 (s, 3H), 2.34 (s, 3H), 2.18 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.5, 137.4, 137.2, 137.1, 133.8, 132.2, 131.1, 129.7, 128.8, 127.4, 126.2, 122.5, 120.4, 120.2, 112.7, 109.8, 99.9,

61.7, 46.9, 30.1, 21.1, 15.9; FT-IR: $\tilde{\nu}$ = 3028, 2932, 2814, 2362, 1548, 1464, 1356, 1220, 1052, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{27}N_2OS$ $[M+H]^+$: 415.1839, found 415.1840.



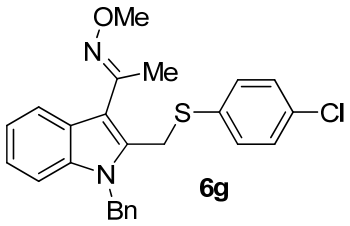
6e

(*E*)-1-(1-Benzyl-2-((4-*tert*-butylphenylthio)methyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6e): Yellow oil, 55%; ^1H NMR ($CDCl_3$, 400 MHz) δ: 7.66 (d, J = 7.8 Hz, 1H), 7.31-7.22 (m, 8H), 7.21-7.10 (m, 2H), 7.00 (dd, J = 7.8, 1.8 Hz, 2H), 5.51 (s, 2H), 4.42 (s, 2H), 3.97 (s, 3H), 2.12 (s, 3H), 1.30 (s, 9H).; ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.5, 150.5, 137.2, 137.1, 133.8, 131.9, 131.2, 128.8, 127.4, 126.2, 126.1, 125.9, 122.4, 120.4, 120.2, 112.7, 109.8, 61.6, 46.9, 34.5, 31.2, 29.9, 15.9; FT-IR: $\tilde{\nu}$ = 2960, 2904, 2859, 1462, 1416, 1360, 1220, 1160, 1052, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{29}H_{33}N_2OS$ $[M+H]^+$: 457.2308, found 457.2317.



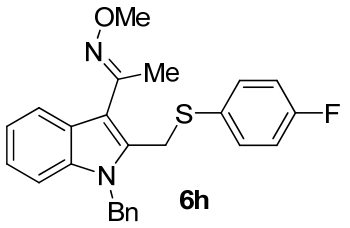
6f

(*E*)-1-(1-Benzyl-2-(*m*-tolylthiomethyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6f): Yellowish liquid, 62%; ^1H NMR ($CDCl_3$, 600 MHz) δ: 7.70 (d, J = 8.0 Hz, 1H), 7.29-7.23 (m, 4H), 7.20 (dt, J = 8.0, 1.1 Hz, 1H), 7.18-7.11 (m, 4H), 7.04 (d, J = 8.0 Hz, 1H), 7.02 (d, J = 8.0 Hz, 2H), 5.32 (s, 2H), 4.48 (s, 2H), 4.00 (s, 3H), 2.30 (s, 3H), 2.20 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.5, 138.7, 137.2, 137.1, 134.7, 133.7, 131.9, 128.8, 128.7, 128.3, 127.9, 127.5, 126.2, 122.5, 120.4, 120.2, 112.7, 109.8, 61.7, 46.9, 29.4, 21.2, 15.9; FT-IR: $\tilde{\nu}$ = 3030, 2930, 1540, 1460, 1413, 1220, 1160, 1052, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{27}N_2OS$ $[M+H]^+$: 415.1839, found 415.1838.



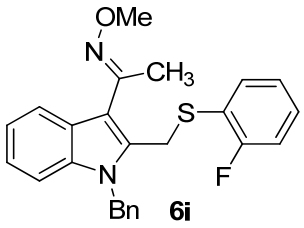
6g

(*E*)-1-(1-Benzyl-2-((4-chlorophenylthio)methyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6g): Yellow oil, 51%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.68 (d, J = 7.8 Hz, 1H), 7.27-7.24 (m, 4H), 7.23-7.19 (m, 5H), 7.16 (m, 1H), 7.01 (d, J = 7.8 Hz, 2H), 5.52 (s, 2H), 4.46 (s, 2H), 3.97 (s, 3H), 2.20 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.3, 137.2, 137.1, 133.3, 133.1, 132.9, 129.0, 128.8, 127.5, 126.1, 126.0, 122.6, 120.6, 120.3, 112.9, 109.9, 61.7, 46.9, 29.7, 15.9; FT-IR: $\tilde{\nu}$ = 3060, 2932, 2841, 1604, 1470, 1420, 1356, 1160, 1089, 1052, 742 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{24}{}^{35}ClN_2OS$ $[M+H]^+$: 435.1292, found 435.1299.



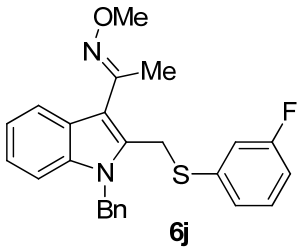
6h

(*E*)-1-(1-Benzyl-2-((4-fluorophenylthio)methyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6h): Yellow oil, 46%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.68 (d, J = 8.0 Hz, 1H), 7.32-7.23 (m, 6H), 7.21 (t, J = 8.0 Hz, 1H), 7.16 (t, J = 8.0 Hz, 1H), 7.02 (d, J = 7.6 Hz, 2H), 6.95 (t, J = 8.6 Hz, 2H), 5.52 (s, 2H), 4.43 (s, 2H), 3.97 (s, 3H), 2.16 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 162.6 (d, J = 247.9 Hz), 152.5, 137.3 (d, J = 4.3 Hz), 134.8 (d, J = 7.9 Hz), 133.6 , 129.7, 128.9 , 127.7 , 126.3 , 126.2, 122.7, 120.7, 120.4, 116.1 (d, J = 21.9 Hz), 113.1, 109.9, 61.8, 47.0, 30.6, 16.1; ^{19}F NMR ($CDCl_3$, 376 MHz) δ: -113.9; FT-IR: $\tilde{\nu}$ = 3021, 2948, 2856, 1605, 1542, 1427, 1218, 1160, 1052, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{24}FN_2OS$ $[M+H]^+$: 419.1588, found 419.1590.



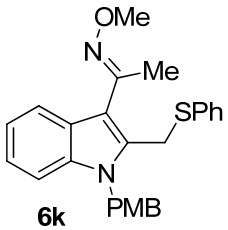
6i

(*E*)-1-(1-Benzyl-2-((2-fluorophenylthio)methyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6i): Yellow oil, 74%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.69 (d, J = 8.0 Hz, 1H), 7.34-7.24 (m, 6H), 7.21 (dt, J = 8.0, 1.1 Hz, 1H), 7.16 (dt, J = 8.0, 1.1 Hz, 1H), 7.09 (m, 1H), 7.06-7.00 (m, 3H), 5.62 (s, 2H), 4.48 (s, 2H), 3.99 (s, 3H), 2.16 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 162.5 (d, J = 246.4 Hz), 152.3, 137.3 (d, J = 2.2 Hz), 135.0, 133.4, 130.1 (d, J = 8.0 Hz), 128.9, 127.6, 126.30, 126.28, 124.5 (d, J = 3.8 Hz), 122.7, 121.4, 120.5 (d, J = 29.9 Hz), 115.9 (d, J = 23.0 Hz), 113.1, 110.0, 61.8, 47.0, 28.9, 15.9; ^{19}F NMR ($CDCl_3$, 376 MHz) δ: -107.6; FT-IR: $\tilde{\nu}$ = 3062, 2930, 2856, 1542, 1470, 1358, 1220, 1160, 1052, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{24}FN_2OS$ $[M+H]^+$: 419.1588, found 419.1596.



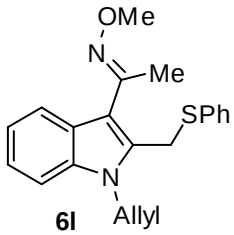
6j

(*E*)-1-(1-Benzyl-2-((3-fluorophenylthio)methyl)-1H-indol-3-yl)ethanone *O*-methyl oxime (6j): Yellow oil, 59%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.69 (d, J = 7.6 Hz, 1H), 7.32 – 7.11 (m, 7H), 7.11 – 6.96 (m, 4H), 6.91 (m, 1H), 5.32 (s, 2H), 4.51 (s, 2H), 3.98 (s, 3H), 2.26 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 162.8 (d, J = 249.0 Hz), 152.6, 137.7, 137.3 (d, J = 20.8 Hz), 133.0, 130.3 (d, J = 8.7 Hz), 129.0, 127.7, 126.33, 126.30 (d, J = 2.9 Hz), 126.25, 122.8, 120.7, 120.4, 117.5 (d, J = 22.5 Hz), 113.9 (d, J = 21.5 Hz), 113.1, 110.1, 61.9, 47.1, 29.2, 16.1; ^{19}F NMR ($CDCl_3$, 376 MHz) δ: -112.07; FT-IR: $\tilde{\nu}$ = 2974, 2908, 1700, 1540, 1472, 1218, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{25}H_{24}FN_2OS$ $[M+H]^+$: 419.1588, found 419.1598.



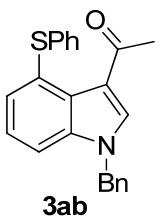
6k

(*E*)-1-(1-(4-Methoxybenzyl)-2-(phenylthiomethyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6k): Pale yellow oil, 56%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.68 (d, J = 8.0 Hz, 1H), 7.35-7.30 (m, 2H), 7.27-7.22 (m, 4H), 7.21-7.11 (m, 2H), 6.95 (d, J = 8.0 Hz, 2H), 6.81 (d, J = 8.0 Hz, 2H), 5.45 (s, 2H), 4.48 (s, 2H), 3.98 (s, 3H), 3.78 (s, 3H), 2.19 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 158.9, 152.5, 137.1, 133.5, 131.4, 129.2, 128.9, 127.4, 127.1, 126.2, 122.5, 120.4, 120.2, 114.2, 112.7, 109.9, 99.9, 61.7, 55.3, 46.4, 29.5, 15.9; FT-IR: $\tilde{\nu}$ = 2941, 2893, 1612, 1512, 1462, 1253, 1220, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{26}H_{27}N_2O_2S$ $[M+H]^+$: 431.1788, found 431.1786.



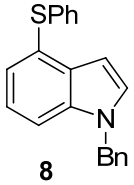
6l

(*E*)-1-(1-Allyl-2-(phenylthiomethyl)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (6l): Yellow oil, 57%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.65 (d, J = 8.0 Hz, 1H), 7.37-7.33 (m, 2H), 7.31-7.21 (m, 5H), 7.14 (t, J = 8.0 Hz, 1H), 5.98 (m, 1H), 5.17 (dd, J = 10.2, 1.1 Hz, 1H), 4.97 (dd, J = 17.2, 1.1 Hz, 1H), 4.92-4.87 (m, 2H), 4.55 (s, 2H), 3.98 (s, 3H), 2.16 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 152.5, 136.7, 135.0, 133.3, 133.1, 131.4, 128.9, 127.1, 126.2, 122.3, 120.3, 120.1, 116.8, 112.5, 109.8, 61.6, 45.8, 29.3, 15.9; FT-IR: $\tilde{\nu}$ = 3067, 2930, 2362, 1464, 1362, 1220, 1160, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{21}H_{23}N_2OS$ $[M+H]^+$: 351.1526, found 351.1527.



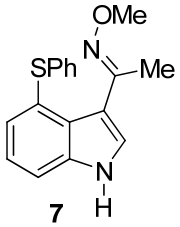
3ab

1-(1-Benzyl-4-(phenylthio)-1*H*-indol-3-yl)ethanone (3ab): Yellow oil, 75%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.73 (s, 1H), 7.51 (dd, J = 8.0, 1.2 Hz, 2H), 7.40-7.30 (m, 6H), 7.16 (d, J= 8.0 Hz, 2H), 7.10-7.03 (m, 2H), 6.81 (d, J = 7.8 Hz, 1H), 5.36 (s, 2H), 2.55 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 192.6, 138.0, 135.6, 135.0, 134.0, 133.1, 129.3, 129.1, 128.3, 127.8, 126.9, 123.9, 123.6, 122.8, 119.7, 110.7, 107.6, 50.8, 28.7; FT-IR: $\tilde{\nu}$ = 3058, 2926, 2360, 1656, 1524, 1436, 1388 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{23}H_{20}NOS$ $[M+H]^+$: 358.1260, found 358.1265.



8

1-Benzyl-4-(phenylthio)-1*H*-indole (8): White amorphous solid, 72%; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 7.38-7.22 (m, 9H), 7.22-7.13 (m, 5H), 6.61 (d, J = 3.3 Hz, 1H), 5.35 (s, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 137.2, 136.8, 136.5, 130.4, 129.4, 128.9, 128.84, 128.82, 127.8, 126.9, 126.0, 125.5, 124.4, 122.2, 109.9, 101.4, 50.4; FT-IR: $\tilde{\nu}$ = 3058, 2922, 1548, 1464, 1360, 1220, 1174, 1026, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{21}H_{18}NS$ $[M+H]^+$: 316.1154, found 316.1147.



7

(*E*)-1-(4-(Phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (7): Yellow oil, 78%; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 8.53 (br s, 1H), 7.35 – 7.25 (m, 1H), 7.23 – 7.06 (m, 8H), 3.83 (s, 3H), 2.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 153.2, 137.8, 136.9, 129.1, 129.0, 127.0, 126.8, 125.9, 125.5, 124.8, 123.2, 115.4, 111.7, 61.5, 19.2; FT-IR: $\tilde{\nu}$ = 3056, 2928,2370, 1584, 1438, 1220, 1158, 1050, 772 cm^{-1}; HRMS (ESI): *m/z* calcd for $C_{17}H_{17}N_2OS$ $[M+H]^+$: 297.1056, found 297.1053.

Reference:

1. J. A. MacKay, R. L. Bishop and V. H. Rawal, *Org*. *Lett*. 2005, **7**, 3421-3424.
2. H. Sano, T. Noguchi, A. Tanatani, Y. Hashimoto and H. Miyachi, *Bioorg*. *Med*. *Chem*. 2005, **13**, 3079-3091.
3. A. S. Tsai, M. Brasse, R. G. Bergman and J. A. Ellman, *Org*. *Lett*. 2011, **13**, 540-542.
4. (a) R. S. Sengar, V. N. Nemykin and P. Basu, *New J*. *Chem*., 2003, **27**, 1115-1123. (b) E. Aoyama, H. Fuchida, Y. Oshikawa, S. Uchinomiya and A. Ojida, *Chem*. *Commun*., 2016, **52**, 7715-7718.

Table 1: Crystal data and structure refinement for (*E*)-1-(1-Benzyl-5-fluoro-4-(phenylthio)-1*H*-indol-3-yl)ethanone *O*-methyl oxime (3c, CCDC: 1570067):

Bond precision: C-C = 0.0046 A Wavelength=0.71069

Cell: a=11.035(5) b=5.298(5) c=35.455(5)
alpha=90 beta=95.937(5) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2062(2)	2062(2)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	C24 H21 F N2 O S	C24 H21 F N2 O S
Sum formula	C24 H21 F N2 O S	C24 H21 F N2 O S
Mr	404.49	404.49
Dx,g cm-3	1.303	1.303
Z	4	4
Mu (mm-1)	0.183	0.183
F000	848.0	848.0
F000'	848.84	
h,k,lmax	14,7,47	14,7,47
Nref	5191	5136
Tmin,Tmax	0.978,0.982	0.978,0.982
Tmin'	0.964	

Correction method= # Reported T Limits: Tmin=0.978 Tmax=0.982
AbsCorr = EMPIRICAL

Data completeness= 0.989 Theta(max)= 28.430

R(reflections)= 0.0597(2396) wR2(reflections)= 0.1580(5136)

S = 0.932 Npar= 268

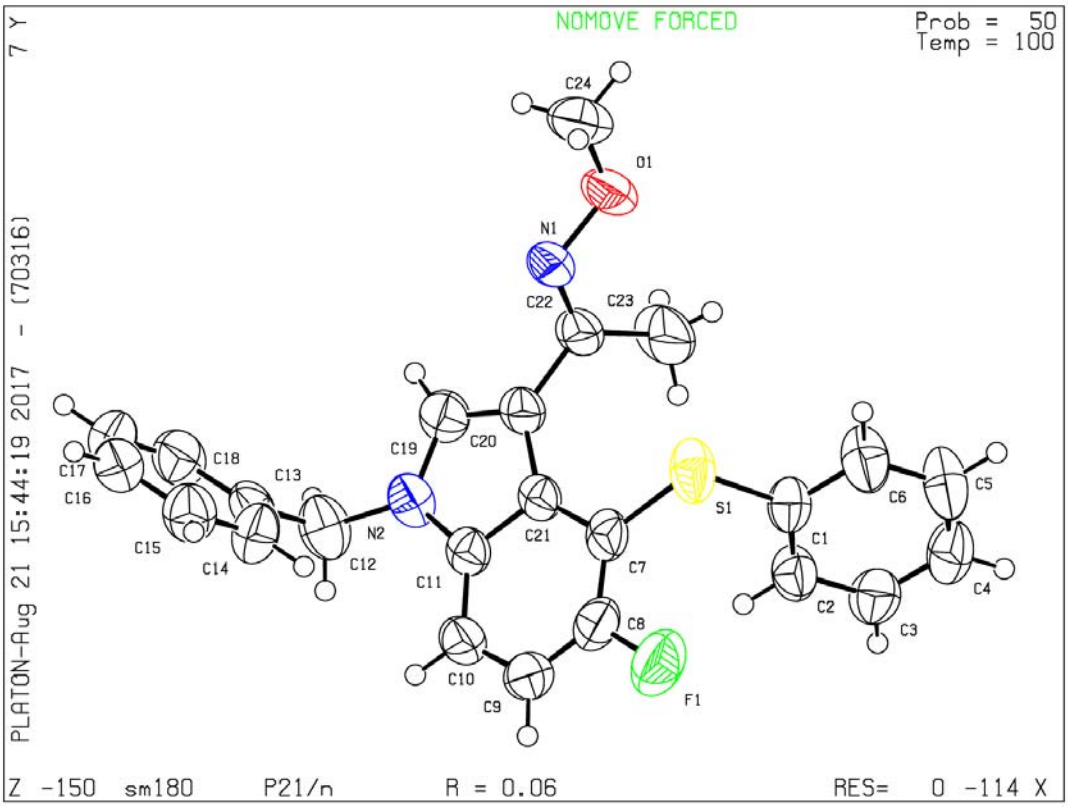
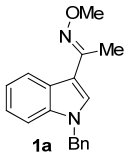
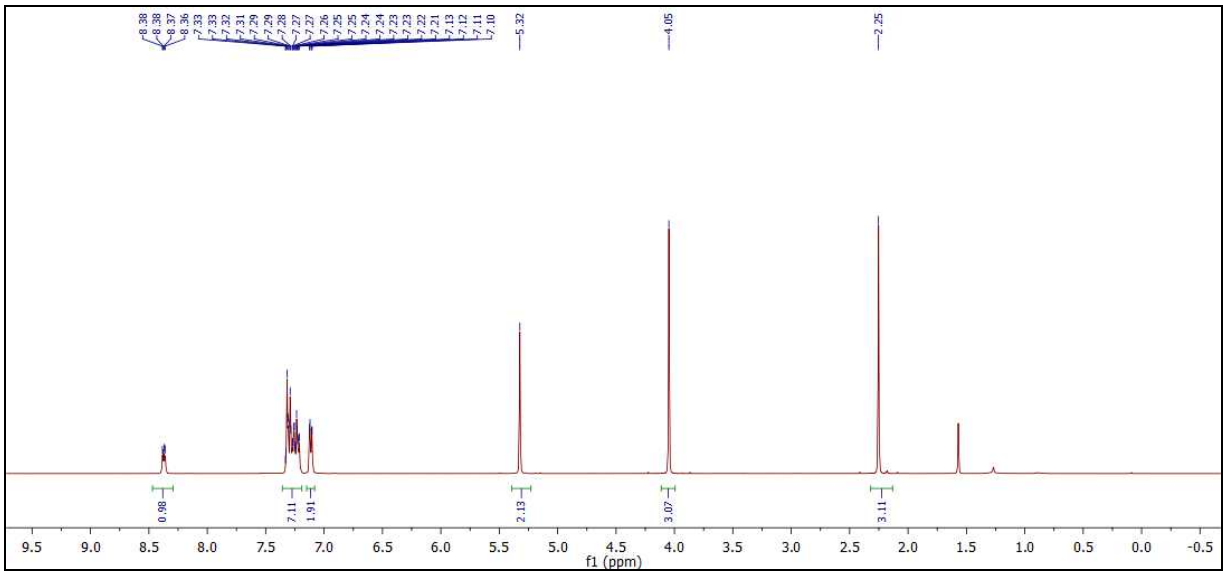


Fig 1. ORTEP diagram of compound **3c**.


OMe
N
Me
N
Bn

1a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7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.13
7.12
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4.05
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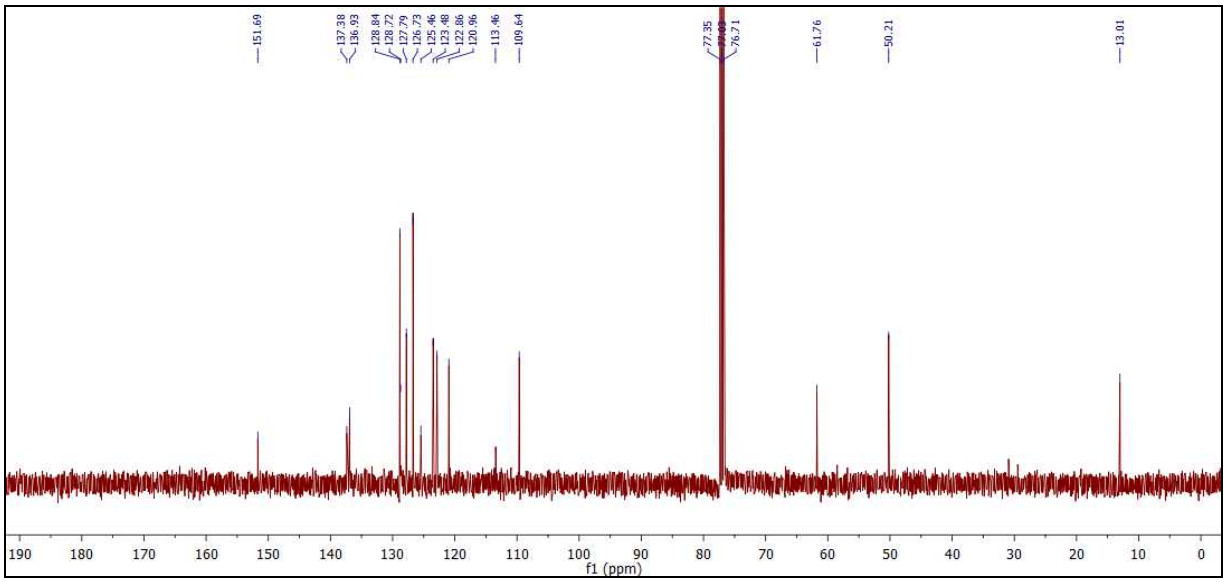
2.13
3.07
3.11
f1 (ppm)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126.73
125.46
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113.46
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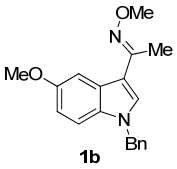
76.71
61.76
50.21
13.01
f1 (ppm)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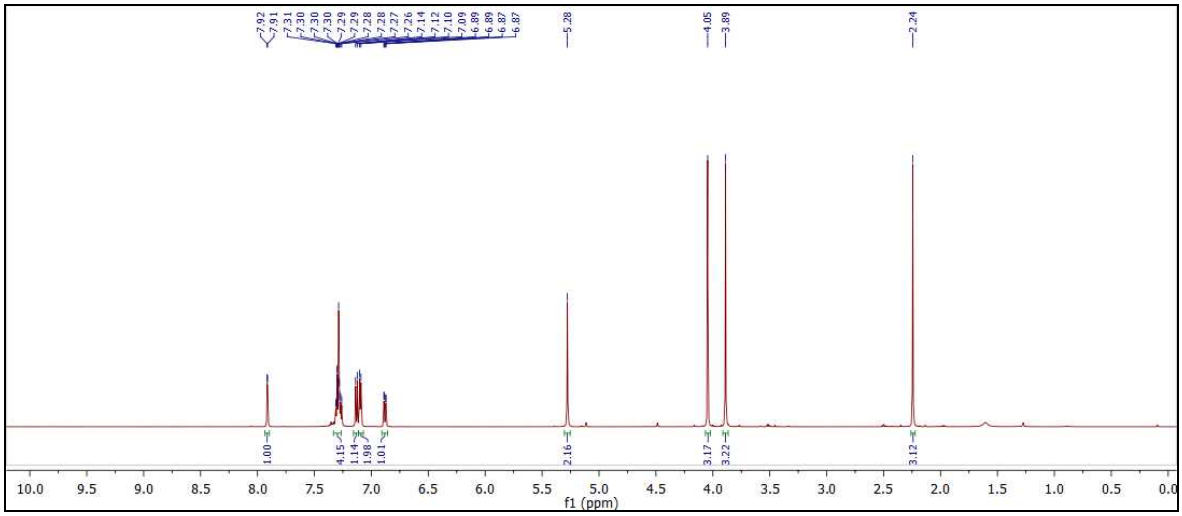
Me
MeO
N
Bn

1b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7.10
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6.87
6.87
5.28
4.05
3.89
2.24
1.00
4.15
1.14
1.98
1.01
2.16
3.17
3.22
3.12
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9.0
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8.0
7.5
7.0
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6.0
5.5
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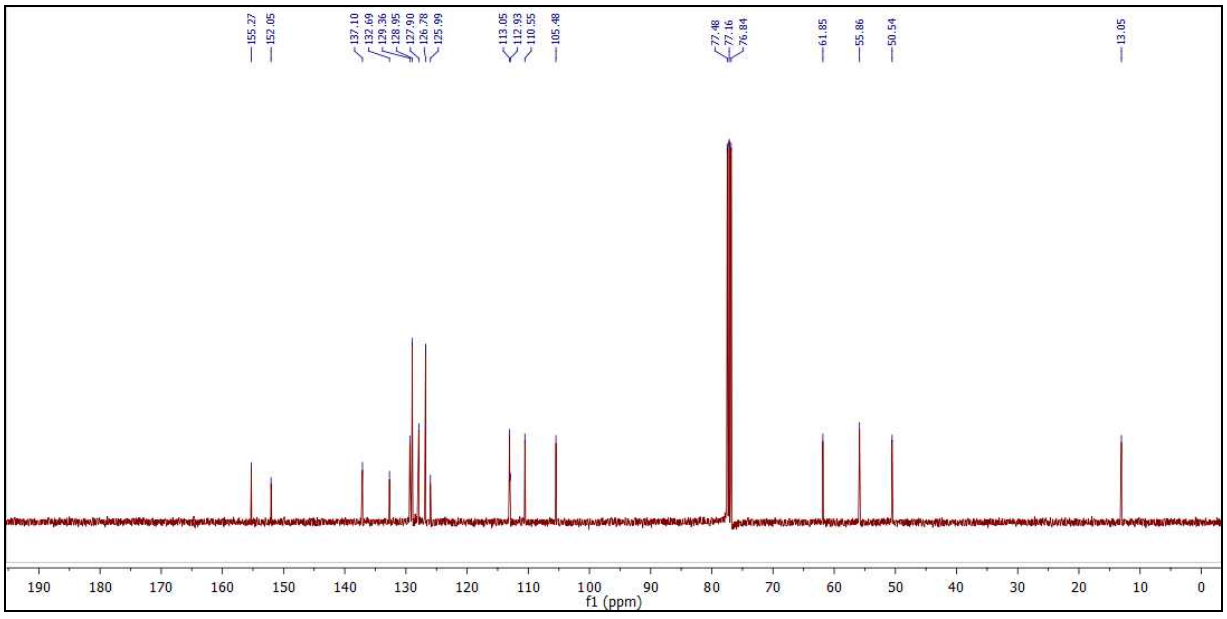
f1 (ppm)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113.05
112.93
110.55
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77.48
77.16
76.84
61.85
55.86
50.54
13.05
190
180
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50
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10
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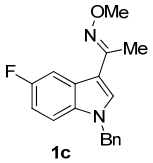
f1 (ppm)


OMe
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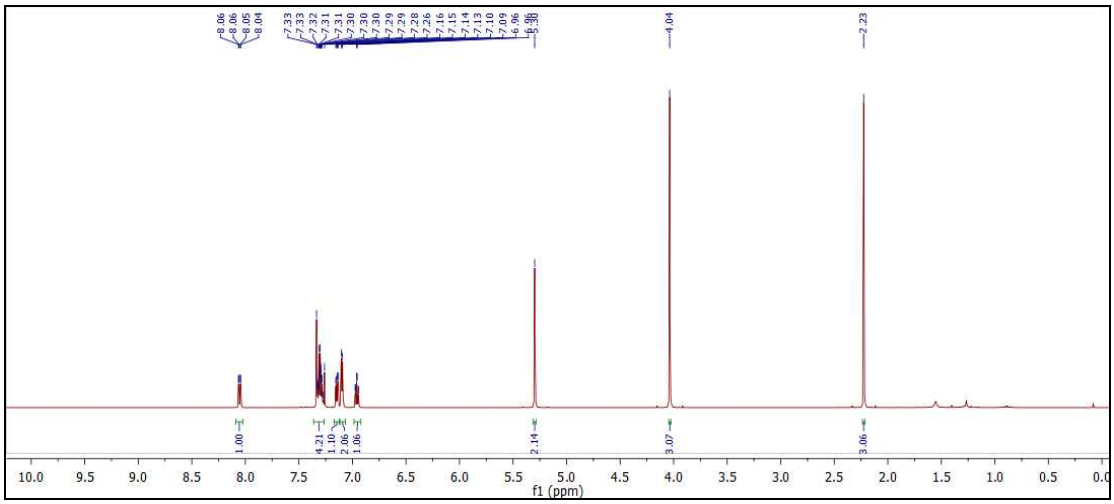
Me
F
N
Bn

1c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7.30
7.29
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7.15
7.14
7.13
7.10
7.09
6.96
6.96
5.30
4.04
2.23
1.00
4.21
1.10
2.06
1.06
2.14
3.07
3.06
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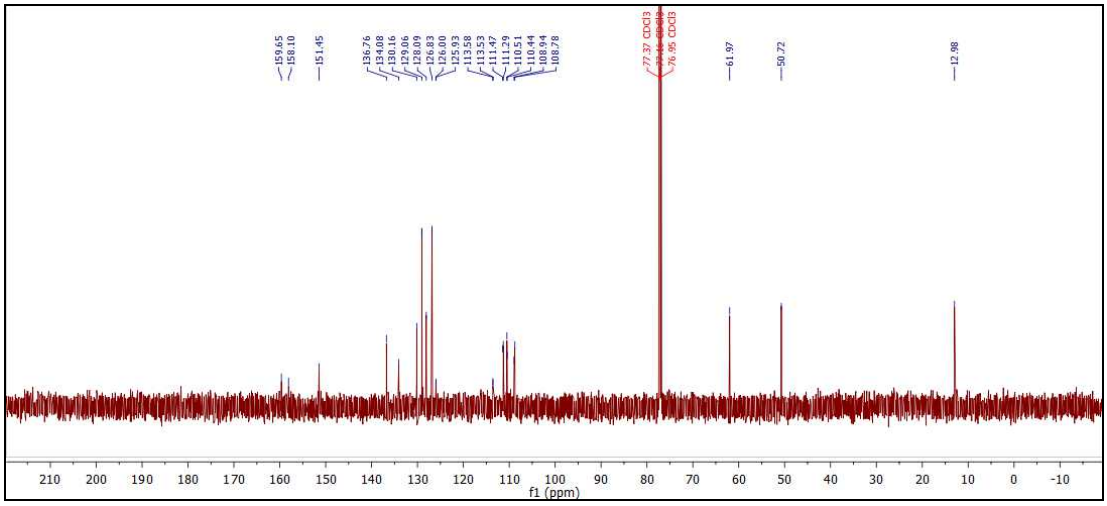
f1 (ppm)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128.09
126.83
126.00
125.93
113.58
113.53
111.47
111.29
110.51
110.44
108.94
108.78
77.37 CDCl3
76.95 CDCl3
61.97
50.72
12.98
210
200
190
180
170
160
150
140
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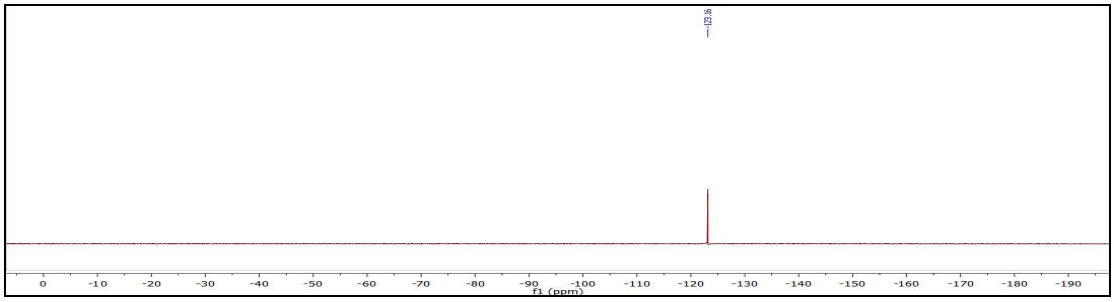
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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-50
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-100
-110
-120
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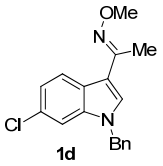
-150
-160
-170
-180
-190
f1 (ppm)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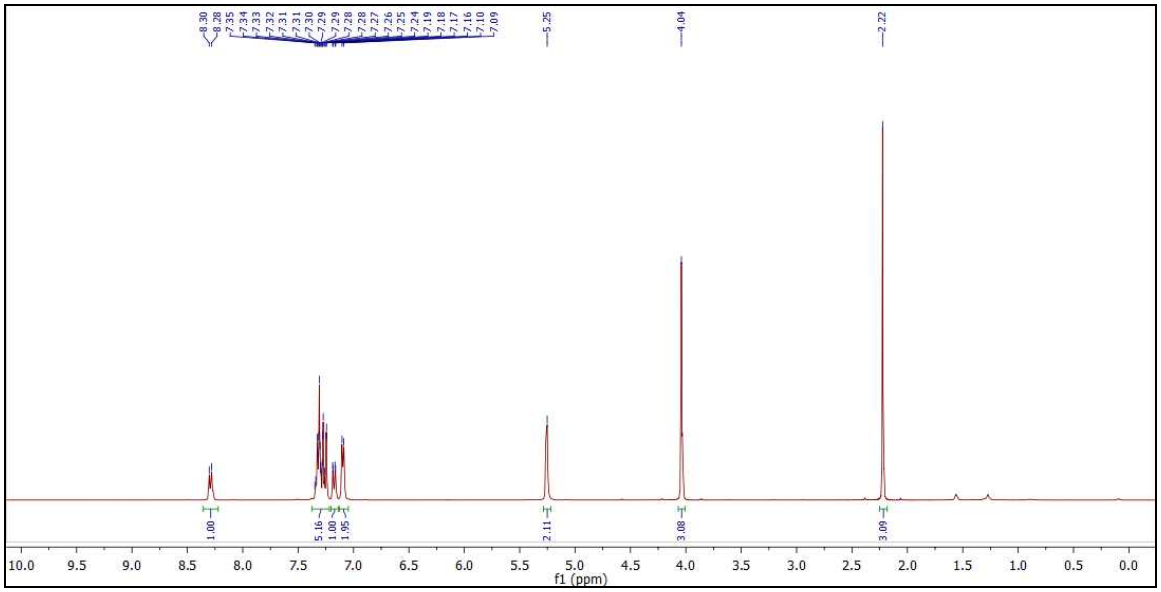
N
Me
Cl
N
Bn

1d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7.18
7.17
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7.10
7.09
5.25
4.04
2.22
1.00
5.16
1.00
1.05
2.11
3.08
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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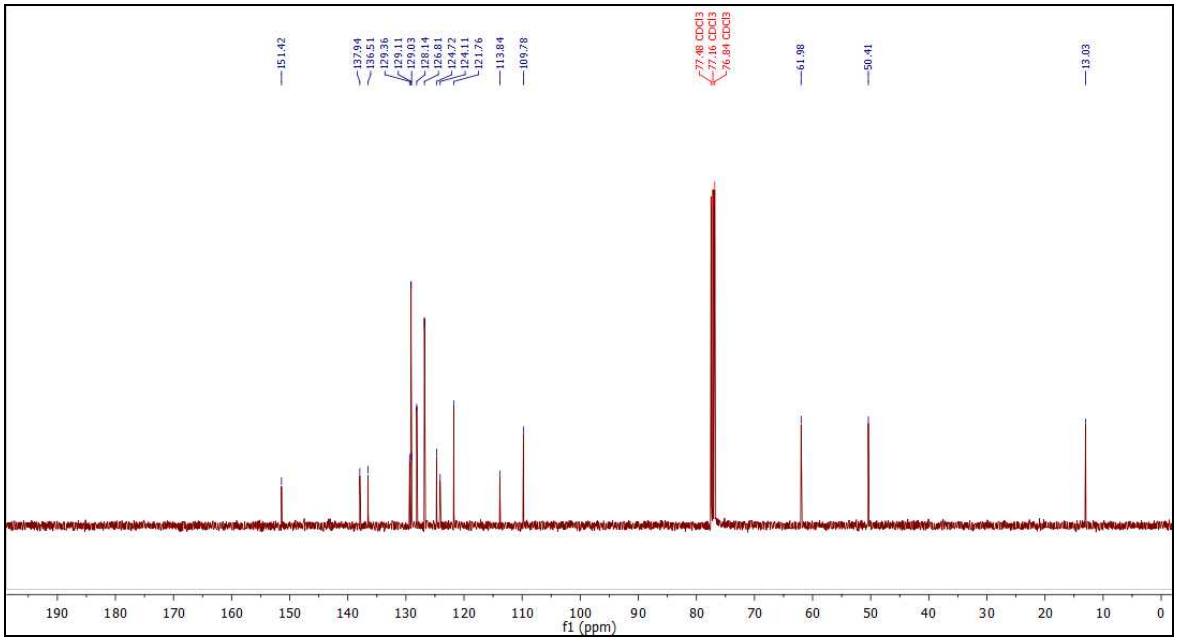
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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124.11
121.76
113.84
109.78
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
61.98
50.41
13.03
190
180
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130
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90
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70
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50
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30
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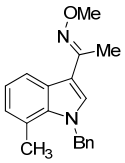
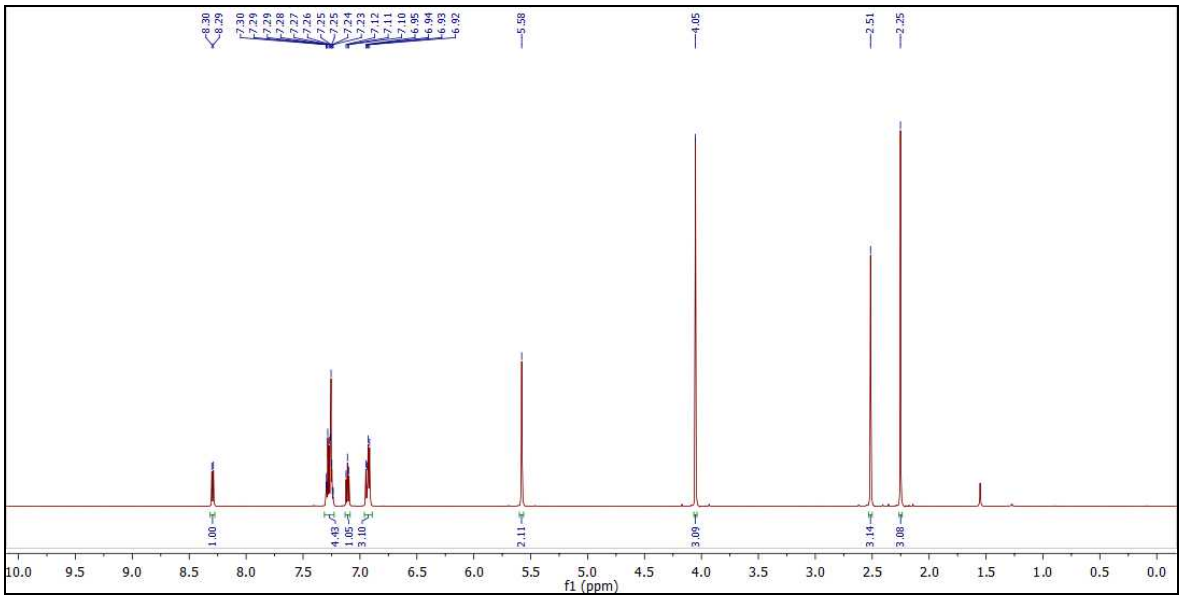
10
0
f1 (ppm)


OMe
N
Me
N
Bn
CH3

1e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7.23
7.12
7.11
7.10
6.95
6.94
6.93
6.92
5.58
4.05
2.51
2.25
1.00
4.48
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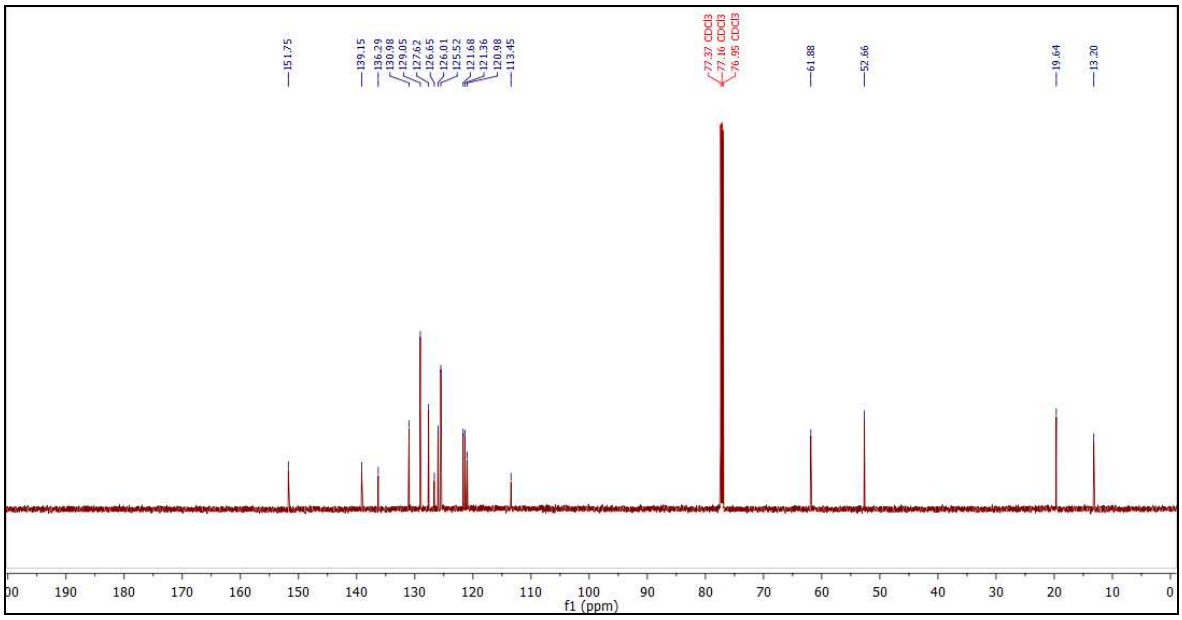
2.11
3.09
3.14
3.08
f1 (ppm)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125.52
121.68
121.36
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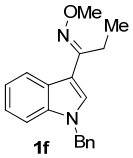
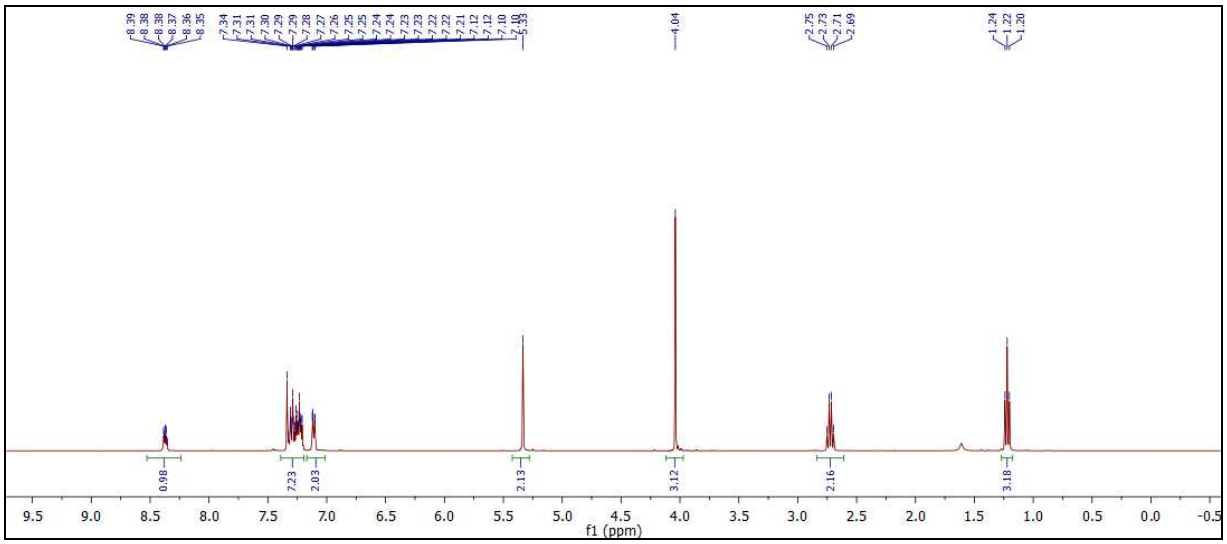
113.45
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
61.88
52.66
19.64
13.20
f1 (ppm)


OMe
N
Me
N
Bn

1f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7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.21
7.12
7.12
7.10
7.10
5.33
4.04
2.75
2.73
2.71
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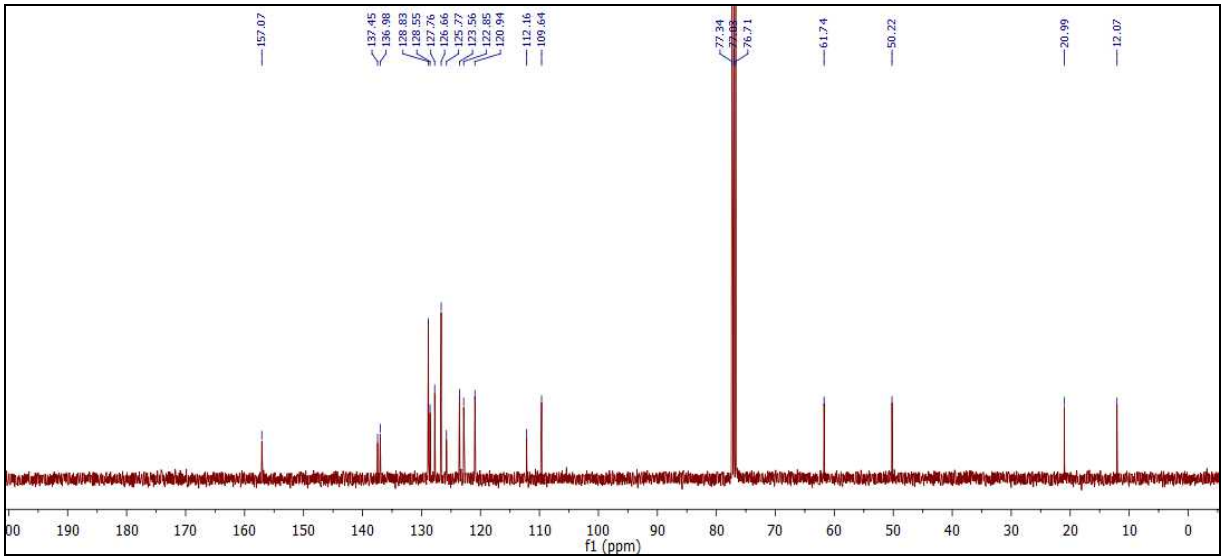
1.20
0.98
7.23
2.03
2.13
3.12
2.16
3.18
f1 (ppm)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109.64
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77.03
76.71
61.74
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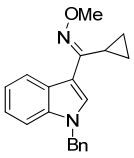
20.99
12.07
f1 (ppm)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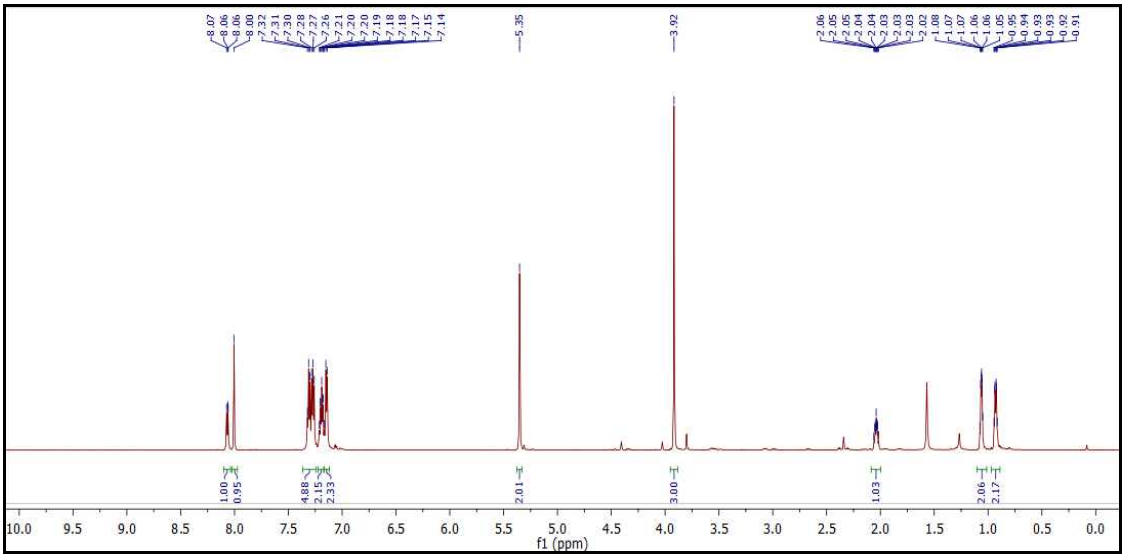
Bn

1g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7.20
7.19
7.18
7.18
7.17
7.15
7.14
5.35
3.92
2.06
2.05
2.05
2.04
2.04
2.03
2.03
2.03
2.02
1.08
1.07
1.07
1.06
1.06
1.05
0.95
0.94
0.93
0.93
0.92
0.91
1.00
0.95
4.88
2.15
2.33
2.01
3.00
1.03
2.06
2.17
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
2.0
1.5
1.0
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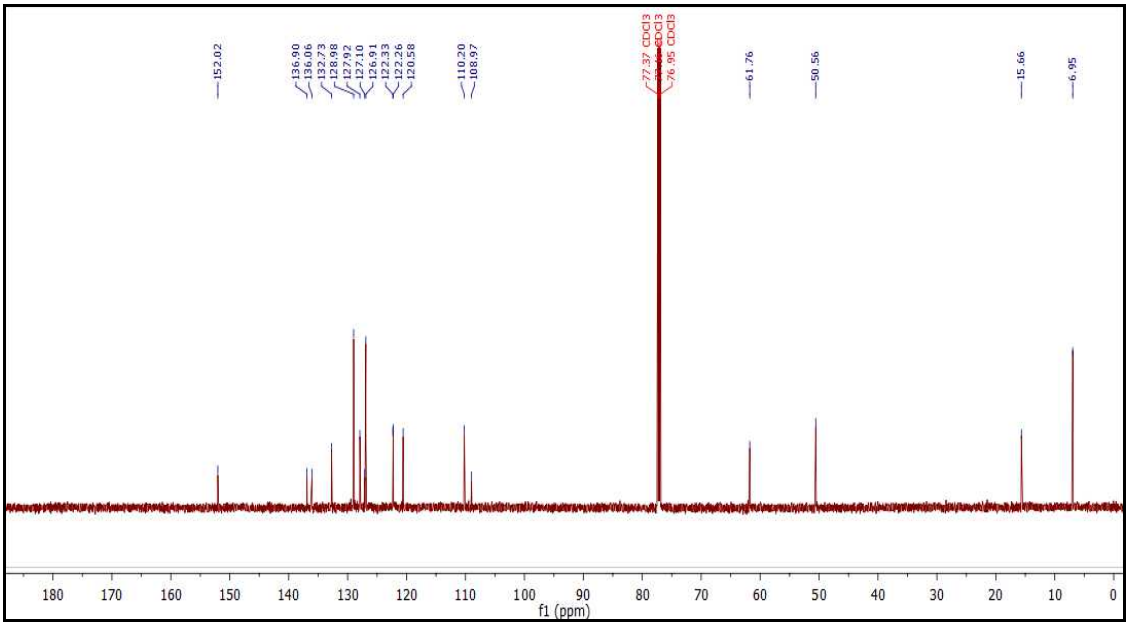
0.0
f1 (ppm)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127.10
126.91
122.33
122.26
120.58
110.20
100.97
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
61.76
50.56
15.66
6.95
180
170
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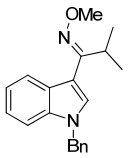
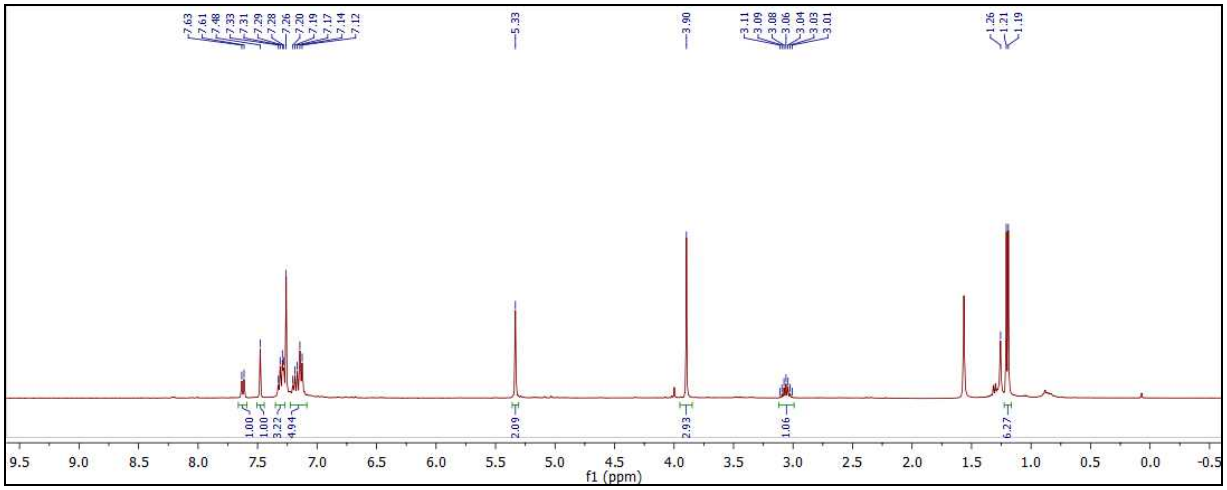
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
N
N
Bn

1h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7.19
7.17
7.14
7.12
5.33
3.90
3.11
3.09
3.08
3.06
3.04
3.03
3.01
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1.21
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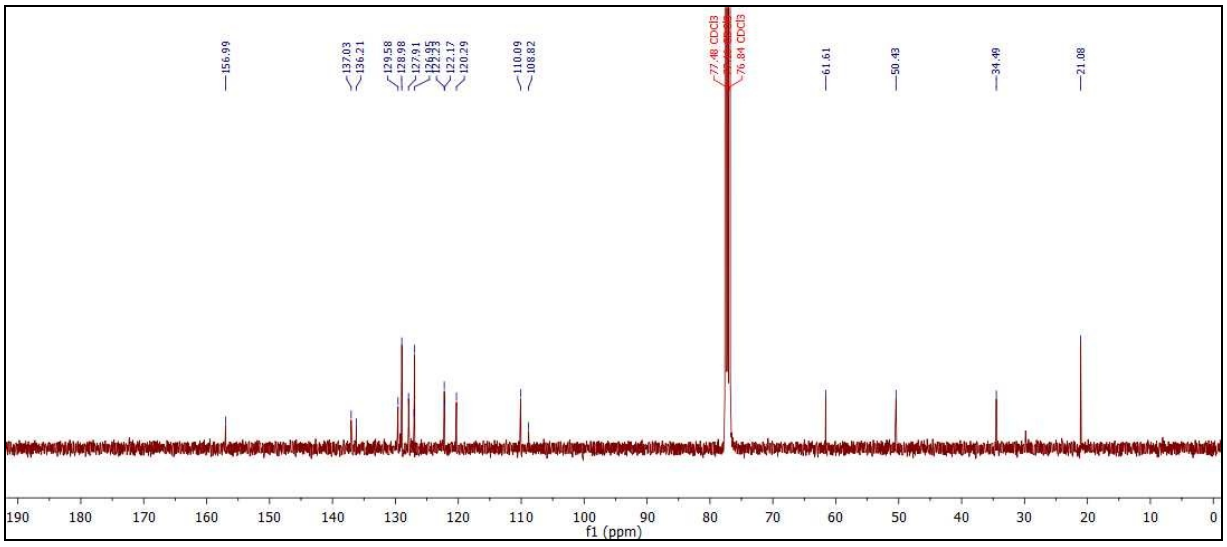
1.00
1.00
3.22
4.94
2.09
2.93
1.06
6.27
f1 (ppm)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127.91
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126.23
122.17
120.29
110.09
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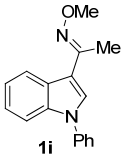
61.61
50.43
34.49
21.08
f1 (ppm)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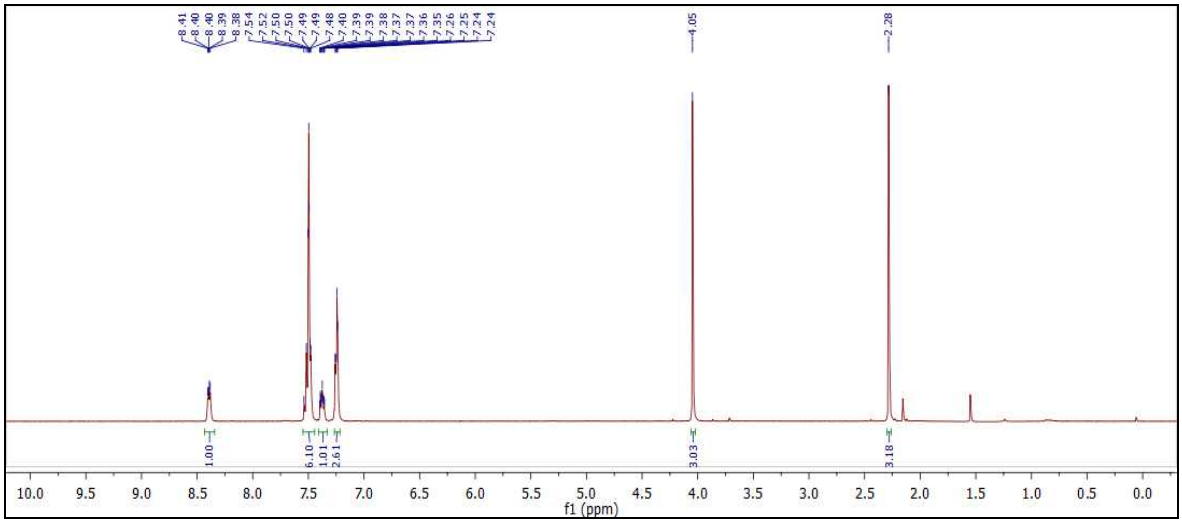
Me
N
Ph

1i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7.39
7.38
7.37
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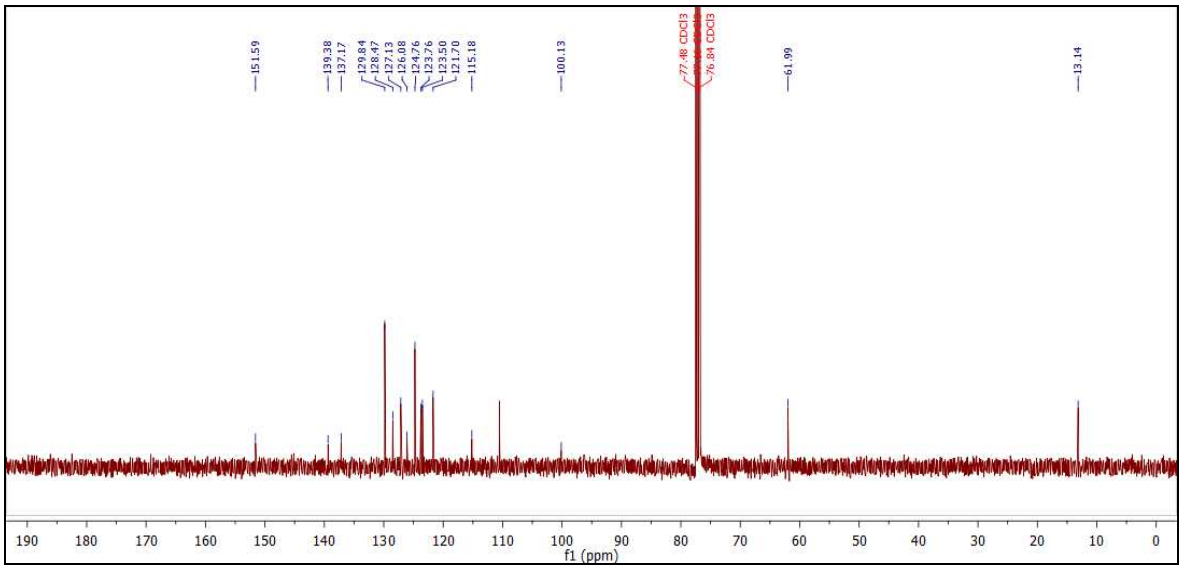
7.36
7.35
7.26
7.25
7.24
7.24
4.05
2.28
1.00
6.10
1.01
2.61
3.03
3.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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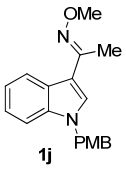
124.76
123.76
123.50
121.70
115.18
100.13
77.48 CDCl3
76.84 CDCl3
61.99
13.14
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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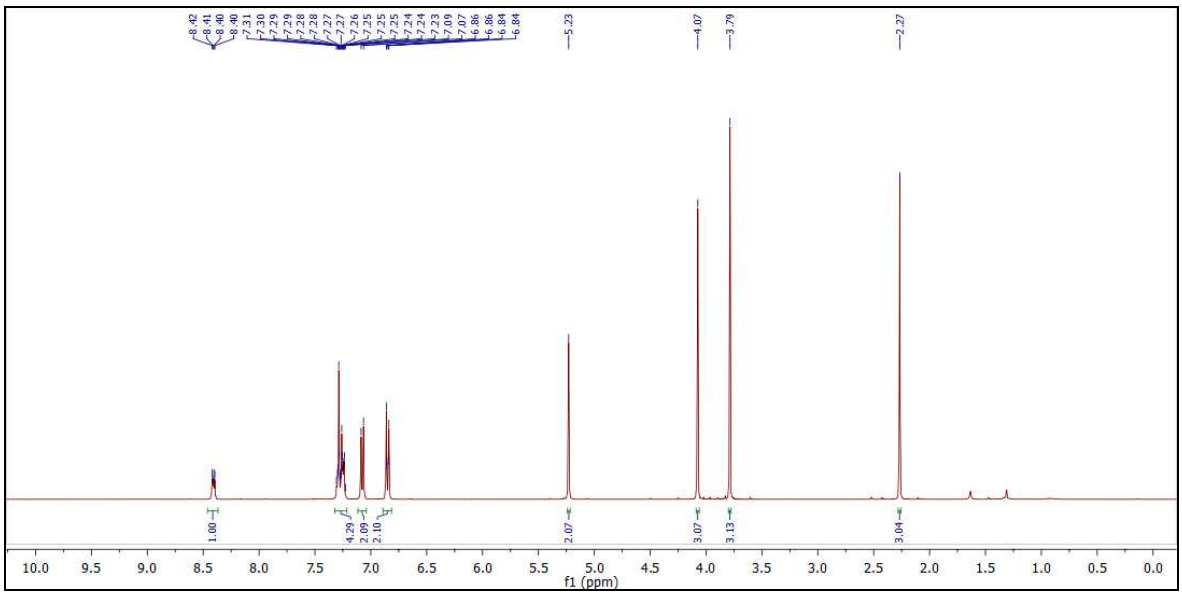
Me
N
PMB

1j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7.26
7.25
7.25
7.25
7.24
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7.23
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7.07
6.86
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6.84
5.23
4.07
3.79
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2.09
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2.07
3.07
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6.0
5.5
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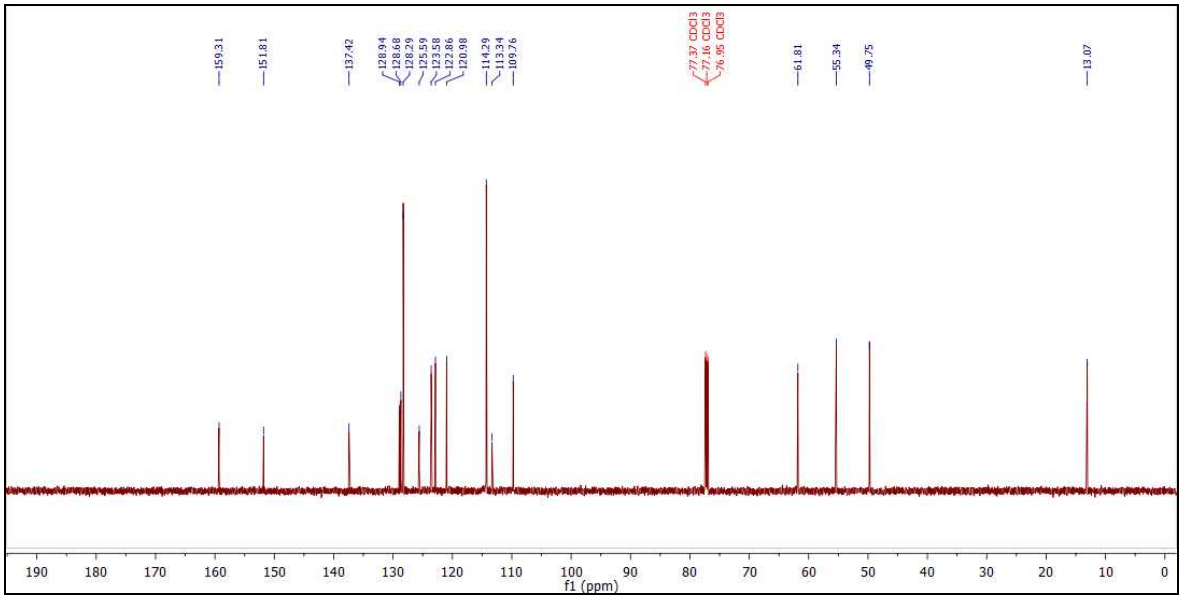
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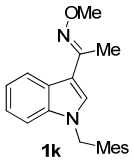
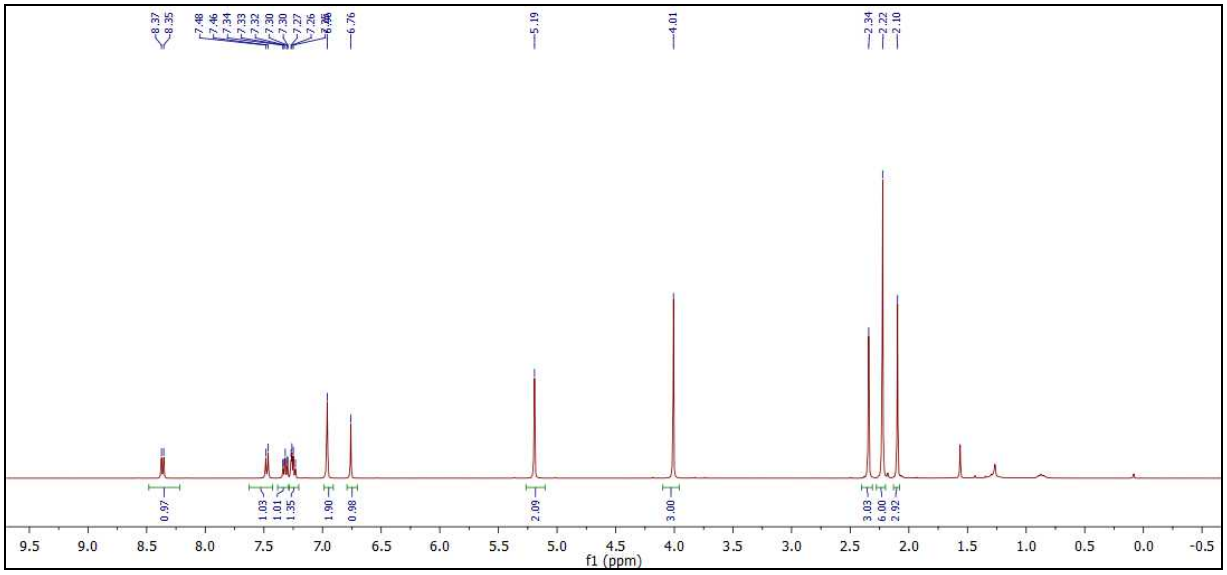
128.94
128.68
128.29
125.59
123.58
122.86
120.98
114.29
113.34
109.76
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
61.81
55.34
49.75
13.07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
N
Me
N
Mes

1k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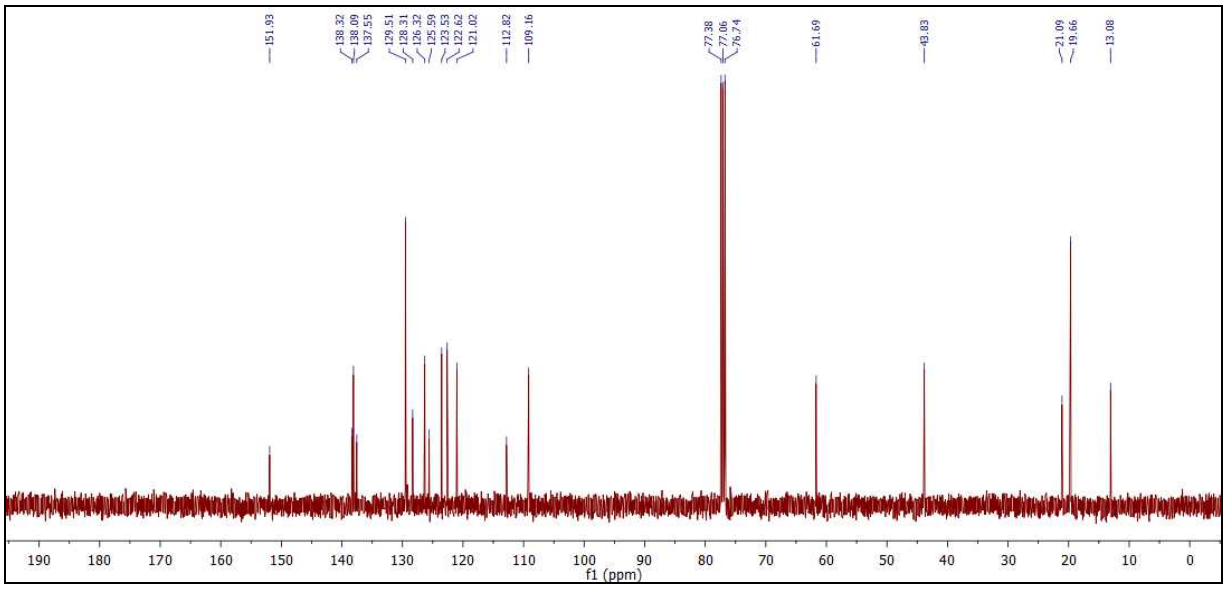
7.33
7.32
7.30
7.30
7.27
7.26
6.76
5.19
4.01
2.34
2.22
2.10
0.97
1.03
1.01
1.35
1.90
0.98
2.09
3.00
3.03
6.00
2.92
f1 (ppm)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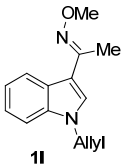
138.09
137.55
129.51
128.31
126.32
125.59
123.53
122.62
121.02
112.82
109.16
77.38
77.06
76.74
61.69
43.83
21.09
19.66
13.08
f1 (ppm)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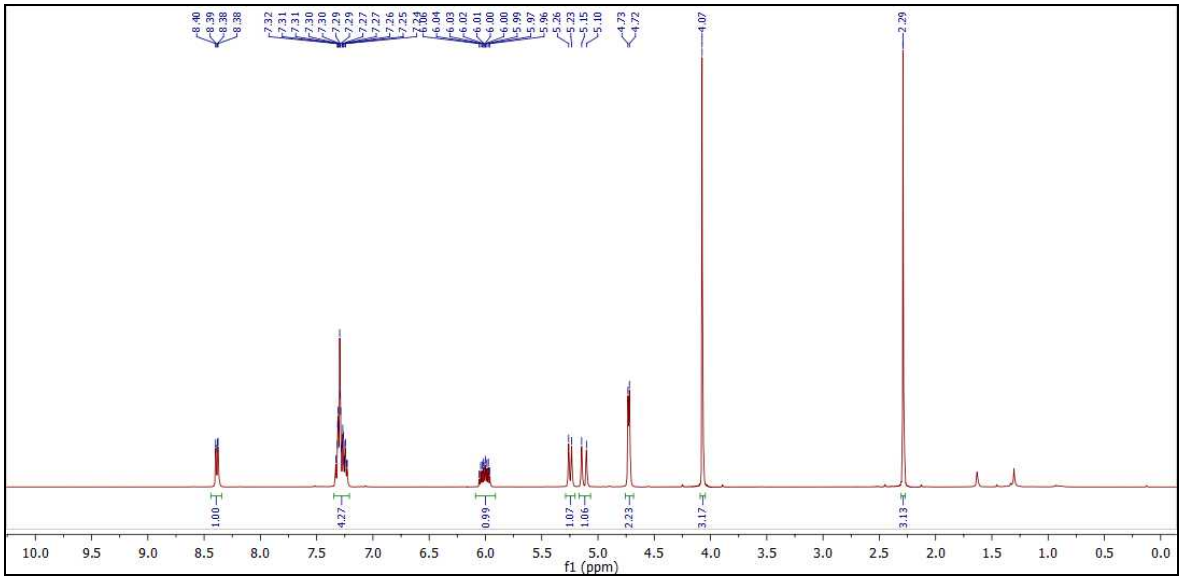
Me
N
Allyl

1l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7.30
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7.29
7.29
7.27
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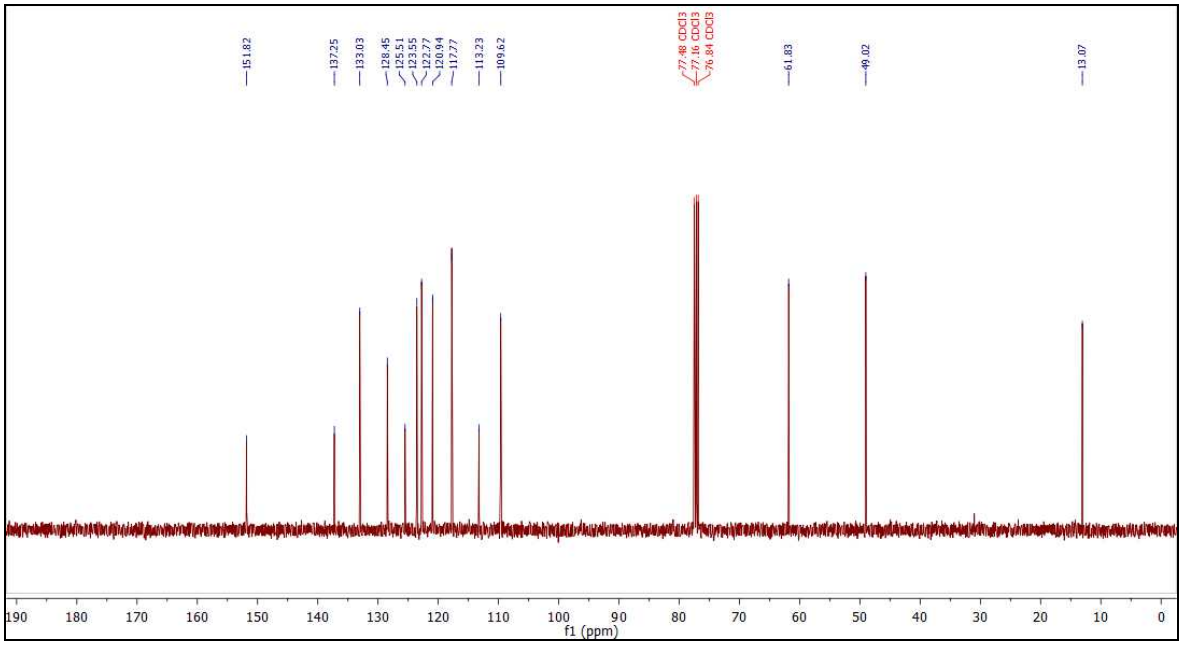
7.26
7.25
7.24
6.06
6.04
6.03
6.02
6.01
6.00
6.00
5.99
5.97
5.96
5.26
5.23
5.15
5.10
4.73
4.72
4.07
2.29
1.00
4.27
0.99
1.07
1.06
2.23
3.17
3.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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137.25
133.03
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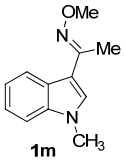
123.55
122.77
120.94
117.77
113.23
109.62
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
61.83
49.02
13.07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
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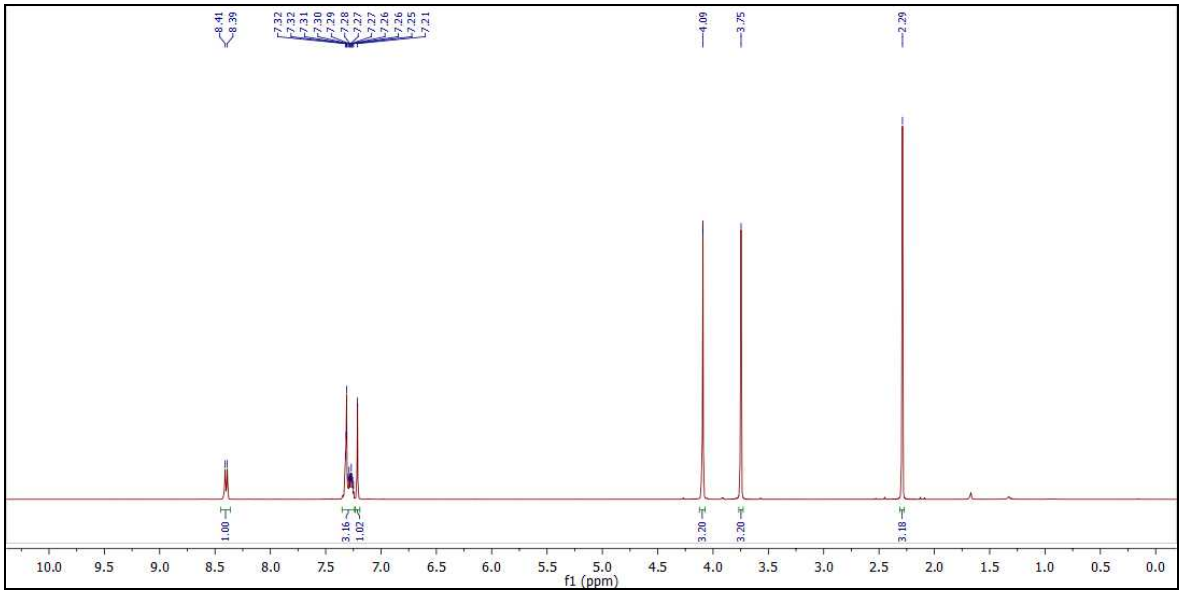
Me
N
CH3

1m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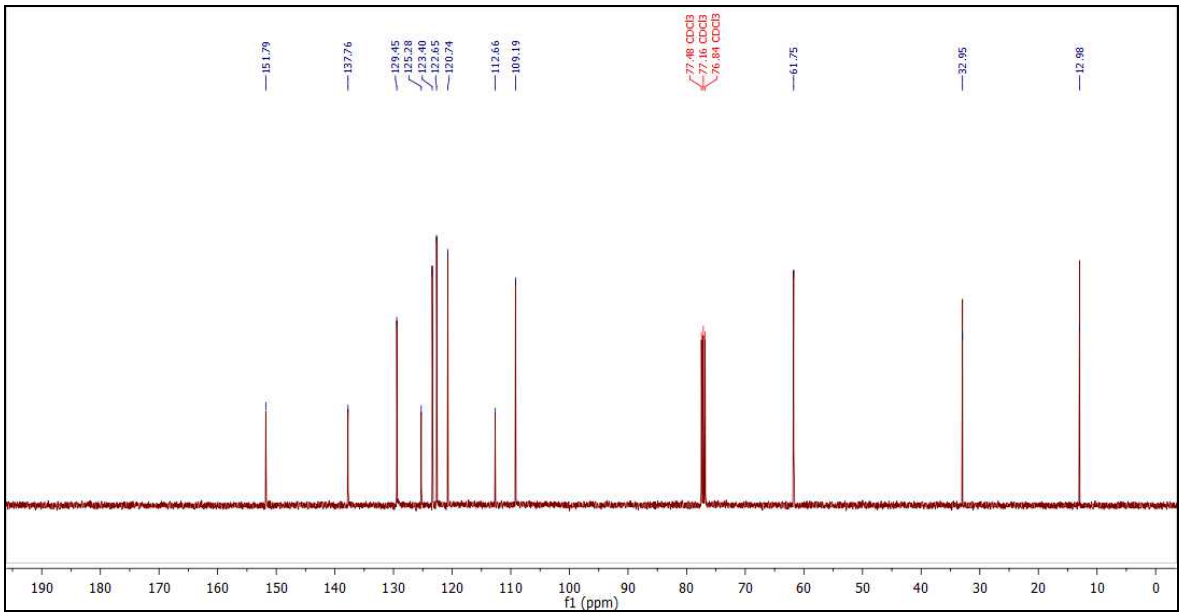
7.30
7.29
7.28
7.27
7.27
7.26
7.26
7.25
7.21
4.09
3.75
2.29
1.00
3.16
1.02
3.20
3.20
3.18
f1 (ppm)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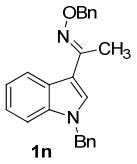
137.76
129.45
125.28
123.40
122.65
120.74
112.66
109.19
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
61.75
32.95
12.98
f1 (ppm)


OBn
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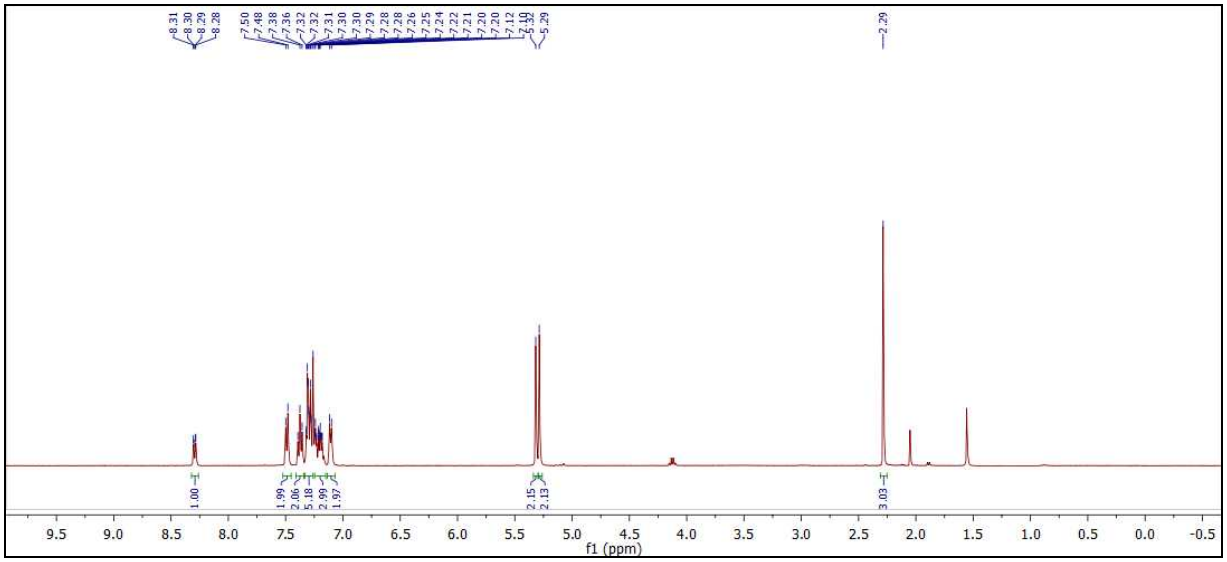
CH3
N
Bn

1n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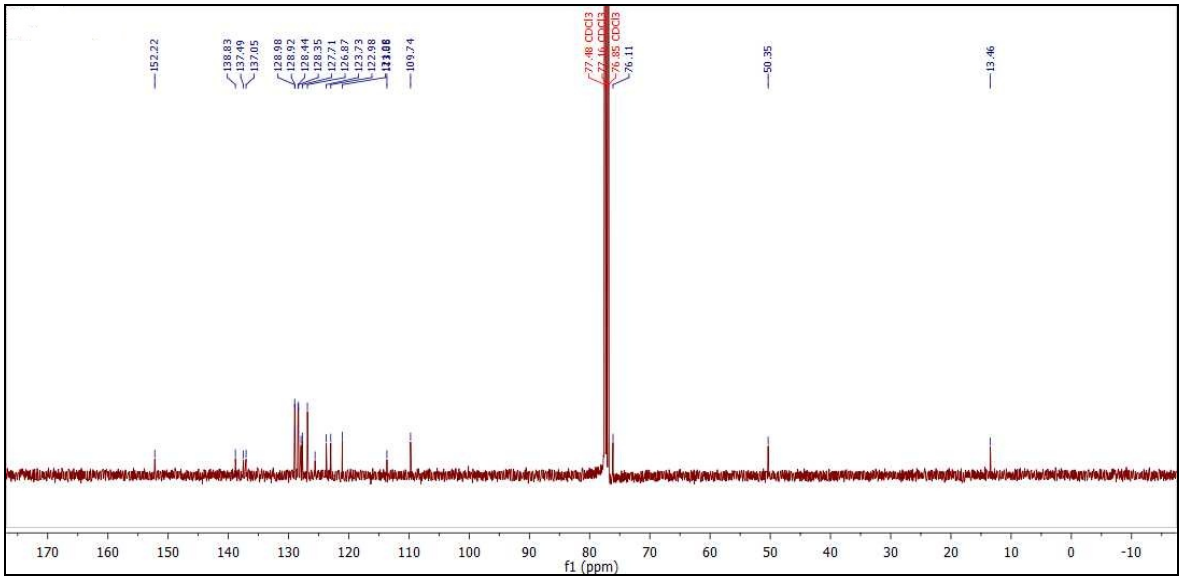
7.38
7.36
7.32
7.32
7.31
7.30
7.30
7.29
7.28
7.28
7.26
7.25
7.24
7.22
7.21
7.20
7.20
7.12
5.30
5.29
2.29
1.00
1.99
2.06
5.18
2.99
1.97
2.15
2.13
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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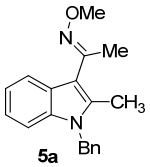
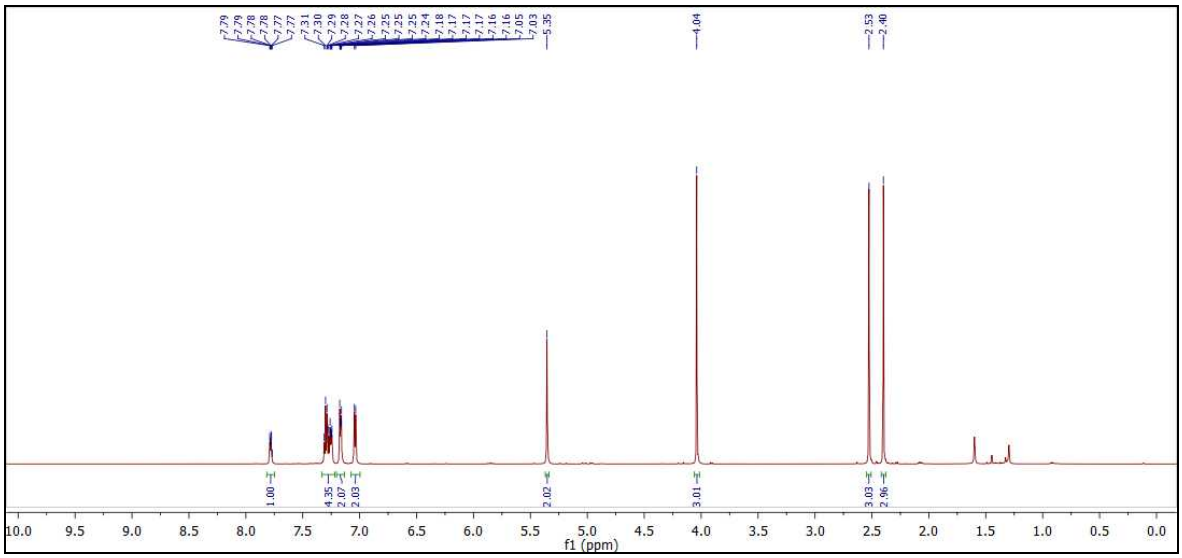
128.98
128.92
128.44
128.35
127.71
126.87
123.73
122.98
121.08
109.74
77.48 CDCl3
77.16 CDCl3
76.85 CDCl3
76.11
50.35
13.46
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OMe
N
Me
CH3
N
Bn

5a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7.79
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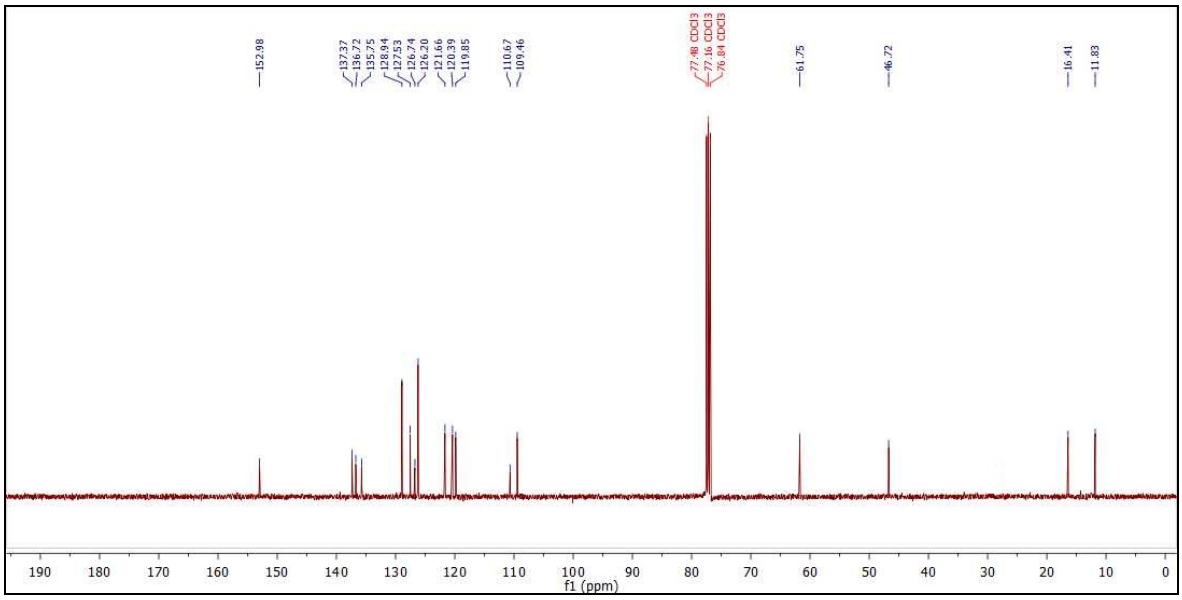
7.78
7.77
7.77
7.31
7.30
7.29
7.28
7.27
7.26
7.25
7.25
7.25
7.24
7.18
7.17
7.17
7.16
7.16
7.05
7.03
5.35
4.04
2.53
2.40
1.00
4.35
2.07
2.03
2.02
3.01
3.03
2.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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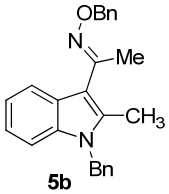
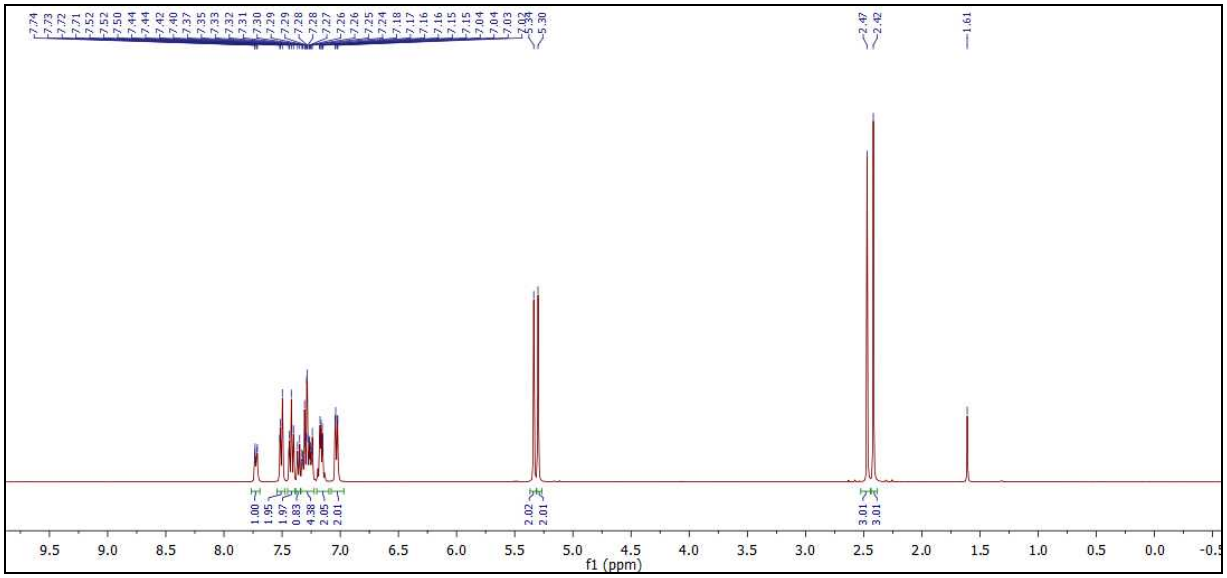
137.37
136.72
135.75
128.94
127.53
126.74
126.20
121.66
120.39
119.85
110.67
109.46
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
61.75
46.72
16.41
11.83
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OBn
N
Me
CH3
N
Bn

5b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7.71
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7.44
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7.40
7.37
7.35
7.33
7.32
7.31
7.30
7.29
7.29
7.28
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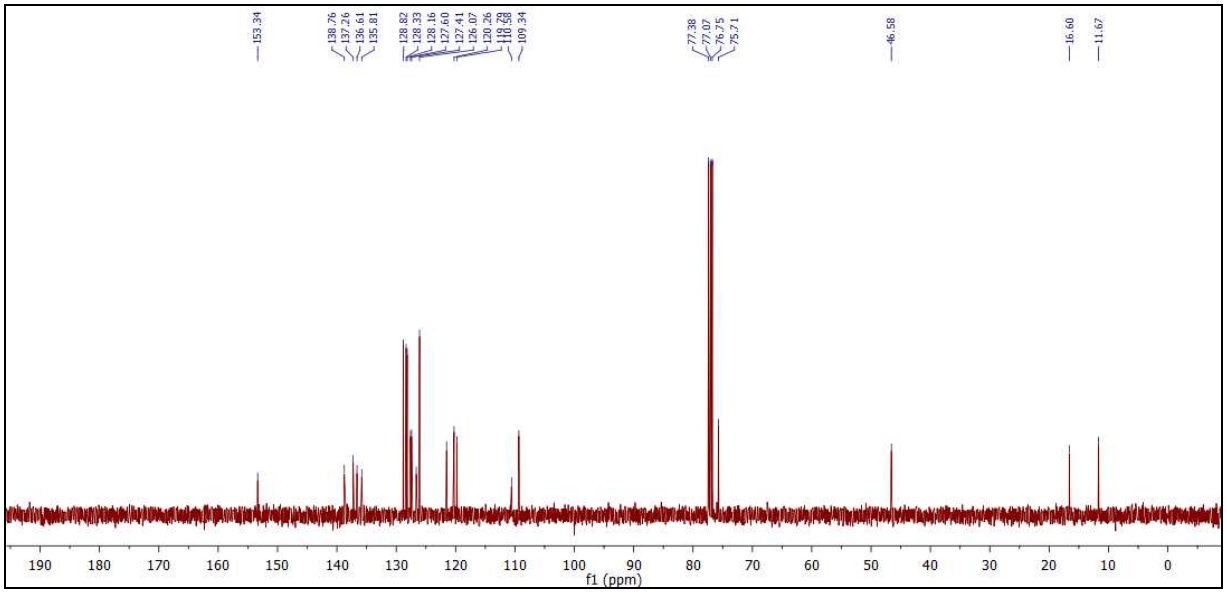
7.27
7.26
7.26
7.25
7.24
7.18
7.17
7.16
7.16
7.15
7.15
7.04
7.03
5.34
5.30
2.47
2.42
1.61
1.00
1.95
1.97
0.83
4.38
2.05
2.01
2.02
2.01
3.01
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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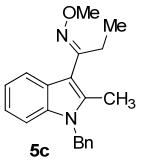
137.26
136.61
135.81
128.82
128.33
128.16
127.60
127.41
126.07
120.26
110.58
109.34
77.38
77.07
76.75
75.71
46.58
16.60
11.67
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
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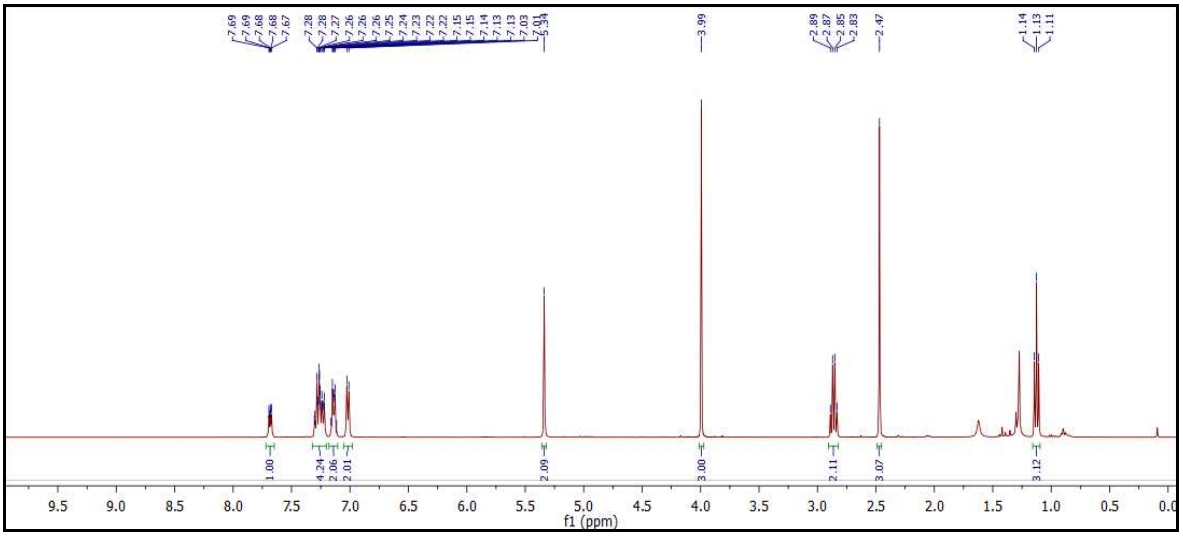
Me
CH3
N
Bn

5c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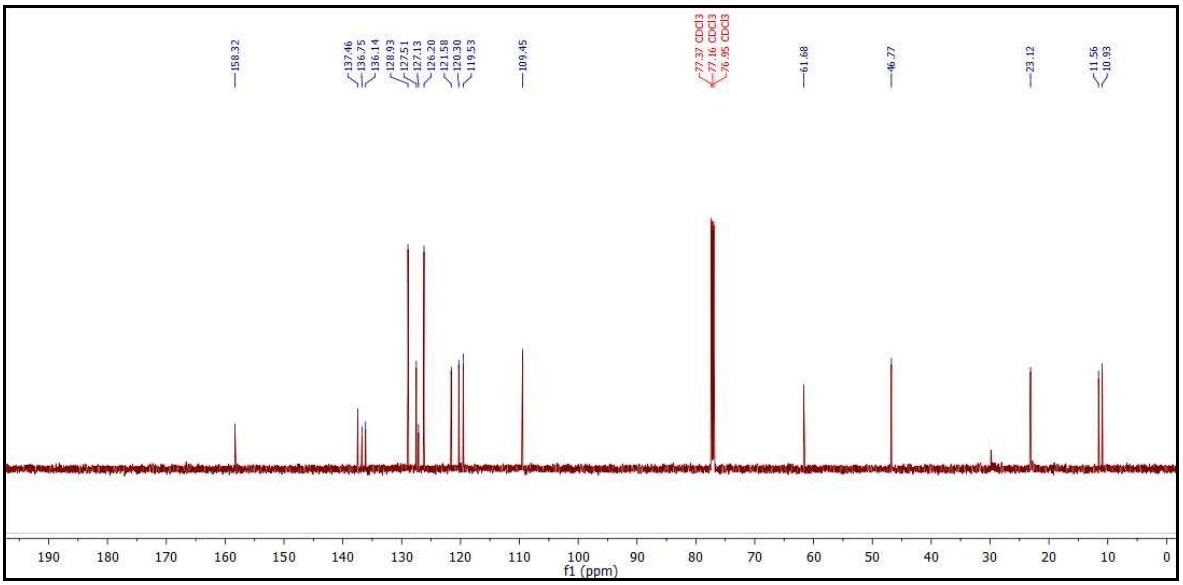
7.23
7.22
7.15
7.14
7.13
7.03
5.34
3.99
2.89
2.87
2.85
2.83
2.47
1.14
1.13
1.11
1.00
4.24
2.06
2.01
2.09
3.00
2.11
3.07
3.12
f1 (ppm)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136.14
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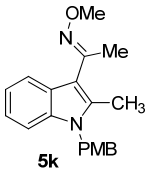
127.51
127.13
126.20
121.58
120.30
119.53
109.45
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
61.68
46.77
23.12
11.56
10.93
f1 (ppm)


OMe
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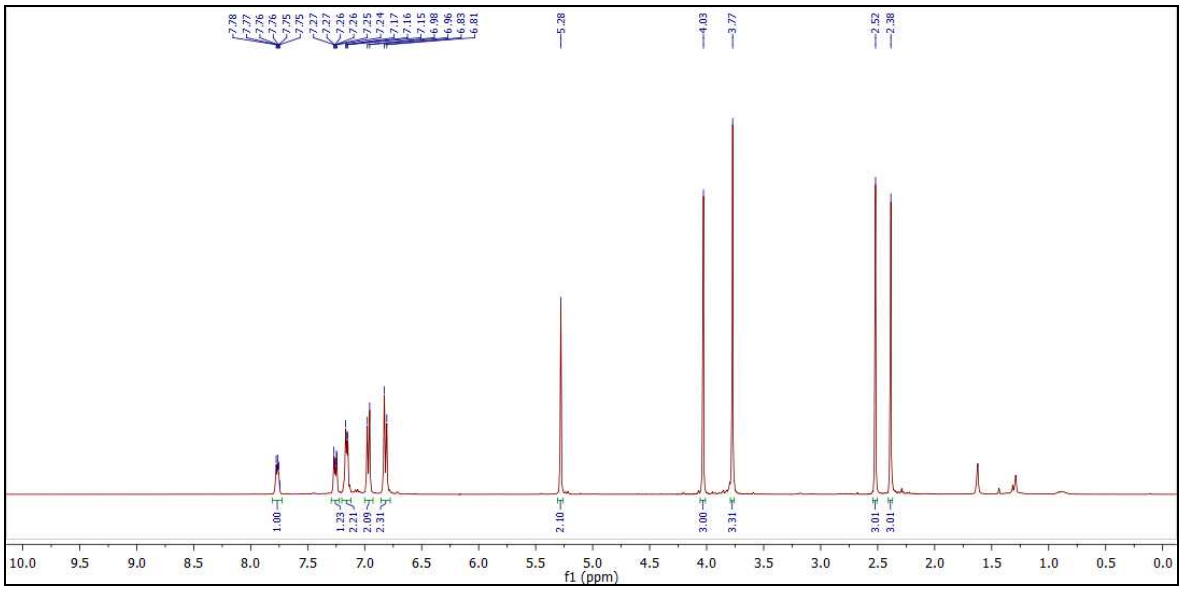
Me
CH3
N
PMB

5k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7.75
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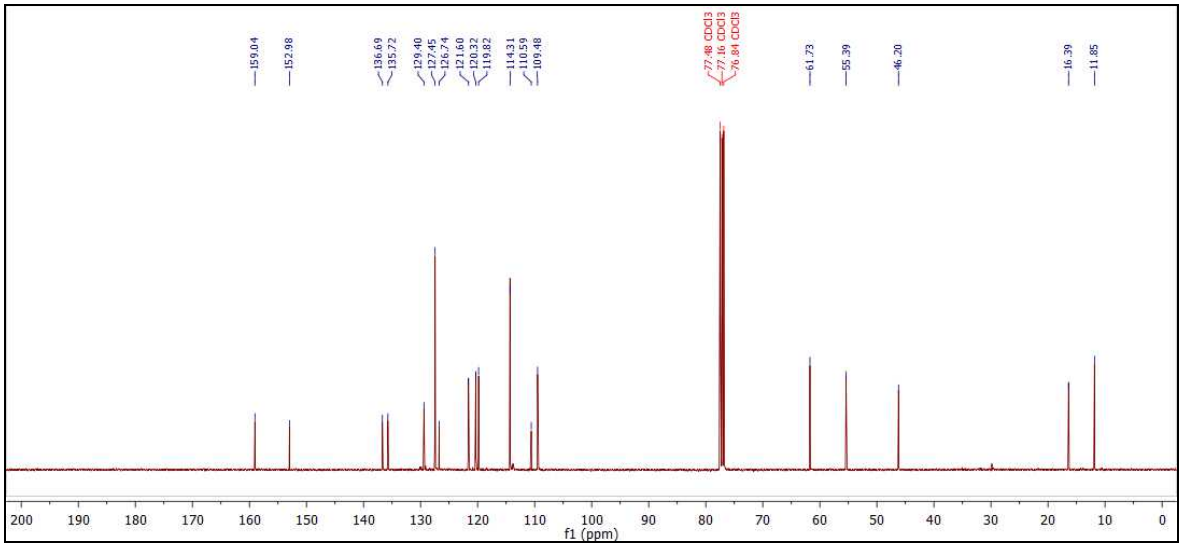
7.26
7.25
7.24
7.17
7.16
7.15
6.98
6.96
6.83
6.81
5.28
4.03
3.77
2.52
2.38
1.00
1.23
2.21
2.09
2.31
2.10
3.00
3.31
3.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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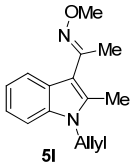
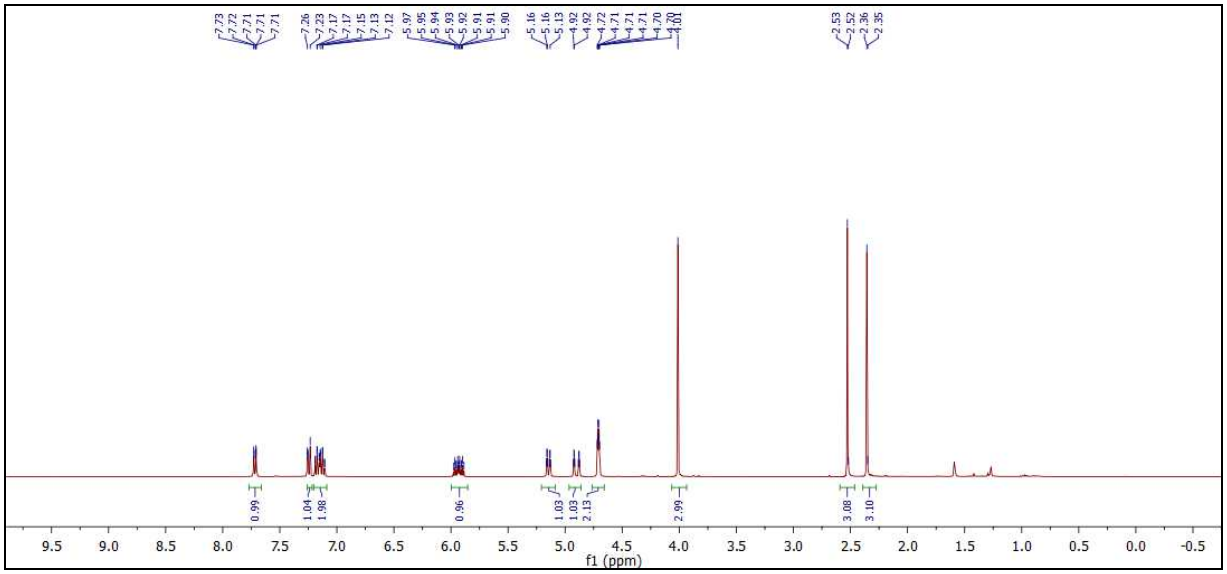
127.45
126.74
121.60
120.32
119.82
114.31
110.59
109.48
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
61.73
55.39
46.20
16.39
11.85
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OMe
N
Me
Me
N
Allyl

5l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7.12
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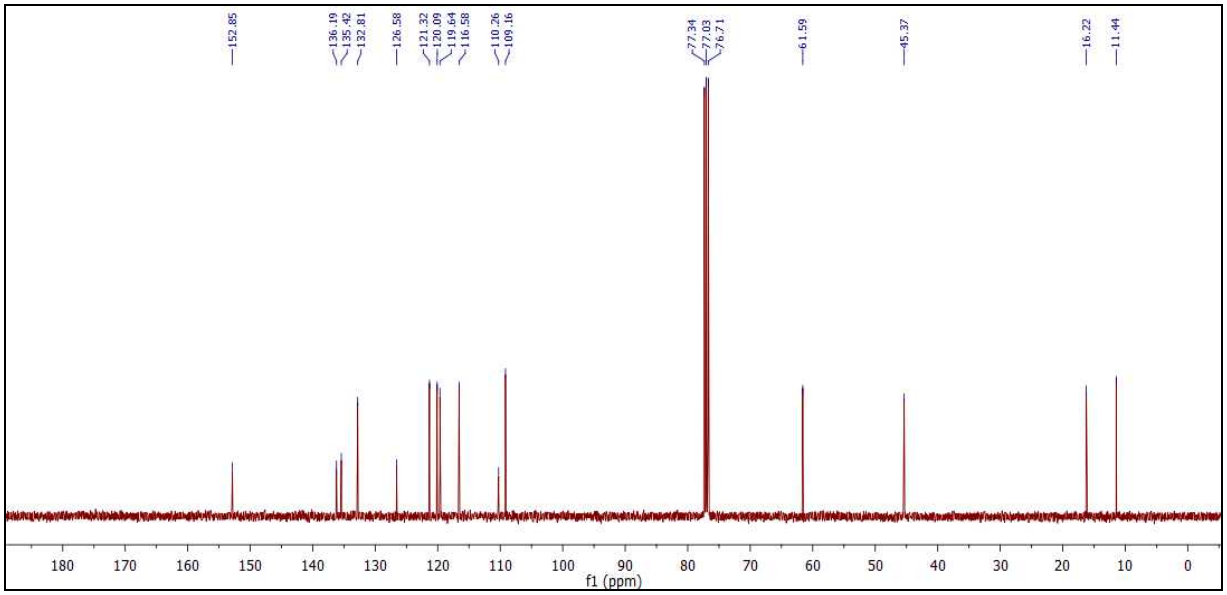
5.92
5.91
5.91
5.90
5.16
5.16
5.15
4.92
4.92
4.72
4.71
4.71
4.71
4.70
4.70
4.01
2.53
2.52
2.36
2.35
0.99
1.04
1.98
0.96
1.03
1.03
2.13
2.99
3.08
3.10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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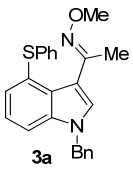
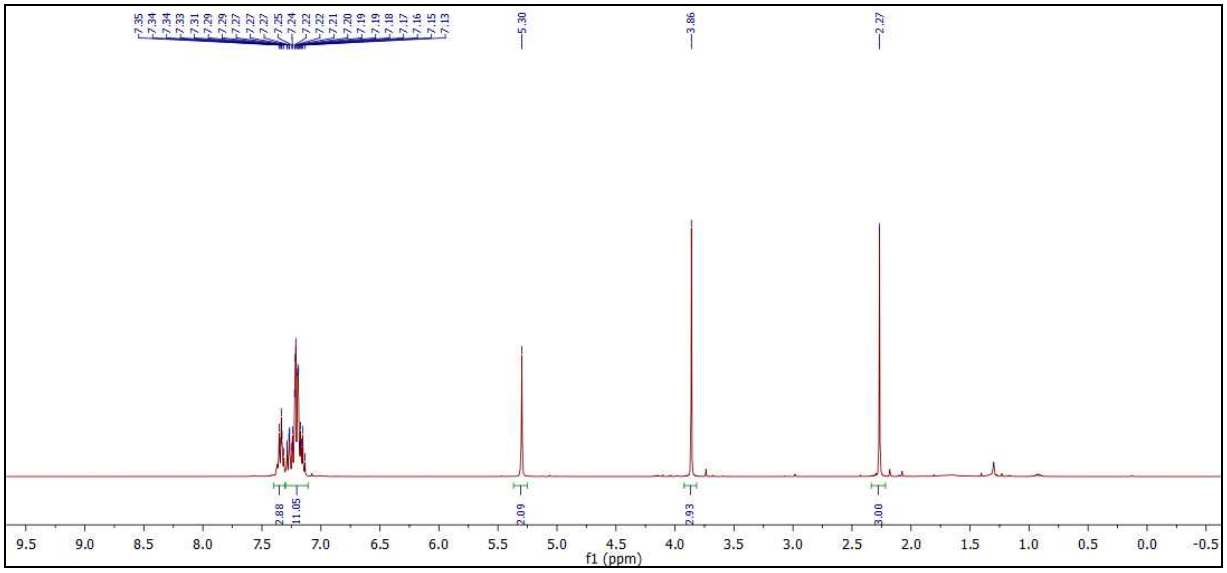
132.81
126.58
121.32
120.09
119.64
116.58
110.26
109.16
77.34
77.03
76.71
61.59
45.37
16.22
11.44
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OMe
N
SPh
Me
N
Bn

3a


7.35
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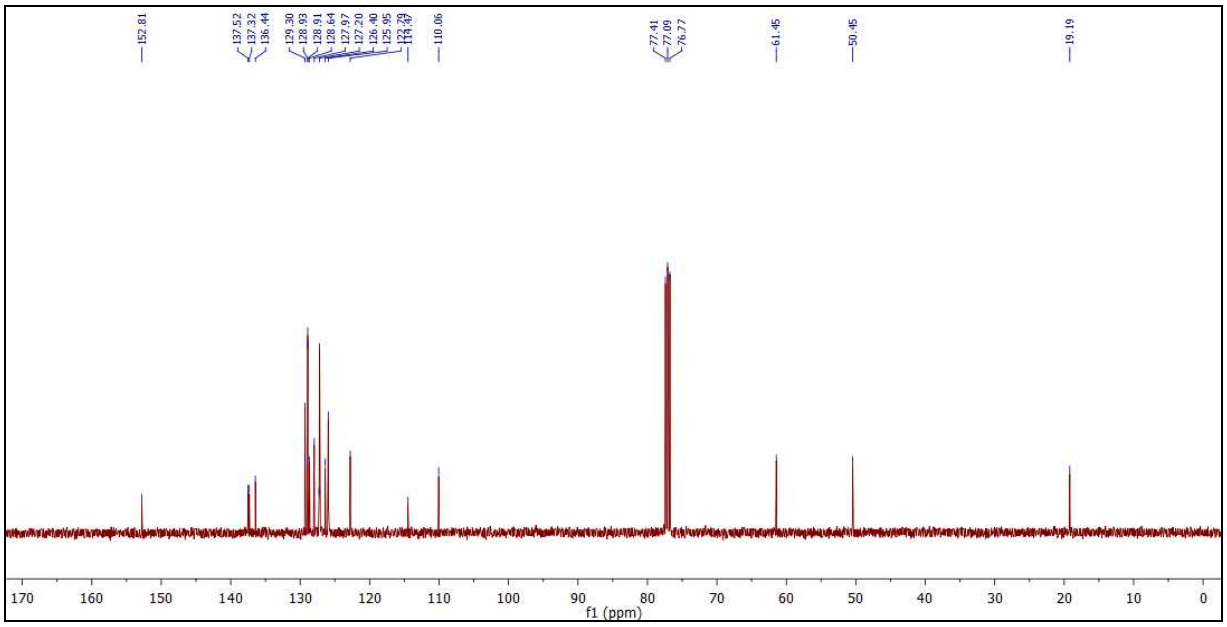
7.29
7.27
7.27
7.27
7.25
7.24
7.22
7.22
7.21
7.20
7.19
7.19
7.18
7.17
7.16
7.15
7.13
5.30
3.86
2.27
2.88
11.05
2.09
2.93
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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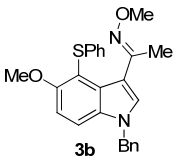
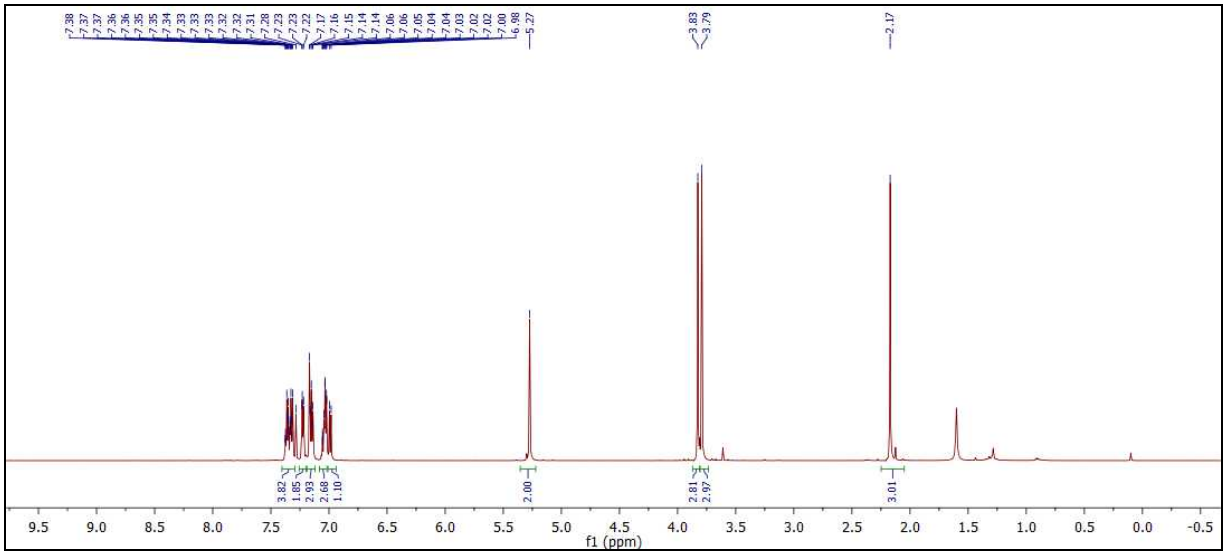
137.32
136.44
129.30
128.93
128.91
128.64
127.97
127.20
126.40
125.95
123.79
114.47
110.06
77.41
77.09
76.77
61.45
50.45
19.19
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
N
SPh
Me
MeO
N
Bn

3b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7.15
7.14
7.14
7.06
7.06
7.05
7.04
7.04
7.03
7.02
7.02
7.00
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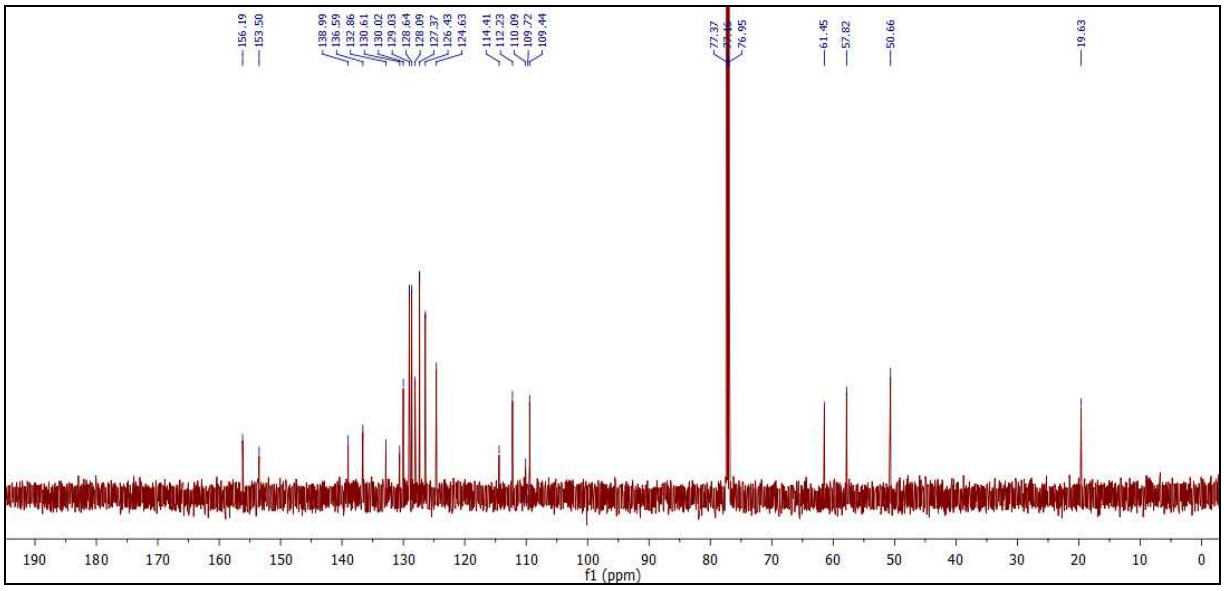
2.81
2.97
3.01
f1 (ppm)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124.63
114.41
112.23
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76.95
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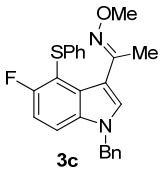
57.82
50.66
19.63
f1 (ppm)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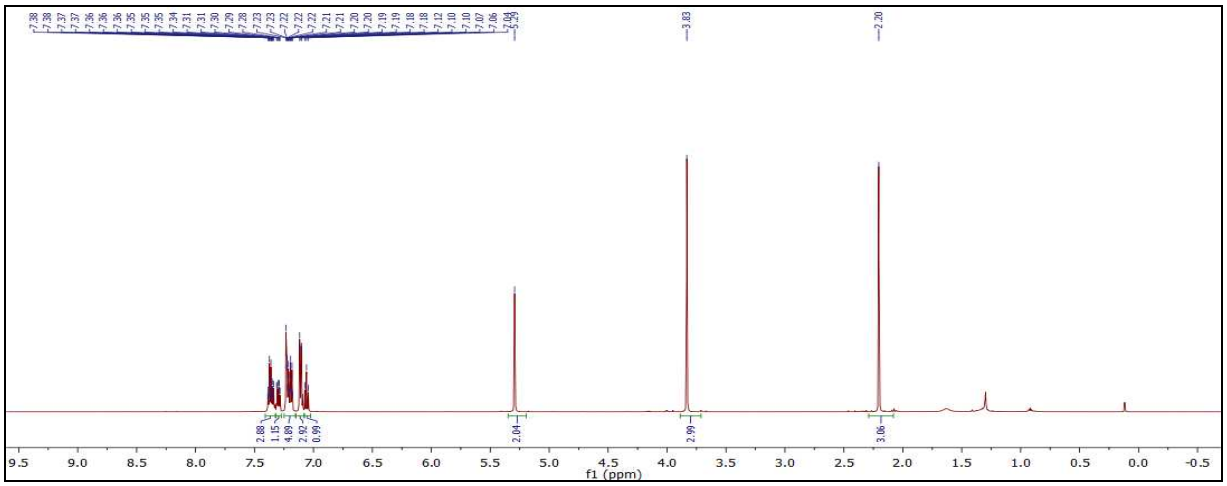
N
SPh
Me
F
N
Bn

3c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4.89
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2.04
2.99
3.06
9.5
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6.0
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5.0
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1.5
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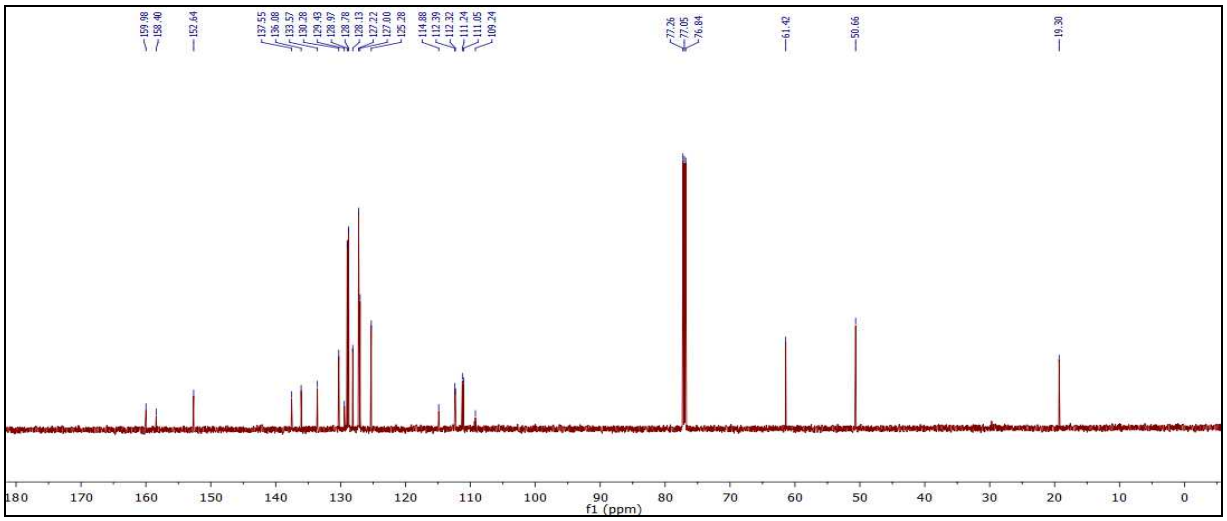
0.5
0.0
-0.5
f1 (ppm)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127.22
127.00
125.28
114.88
112.39
112.32
111.24
111.05
109.24
77.26
77.05
76.84
61.42
50.66
19.30
180
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150
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120
110
100
90
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40
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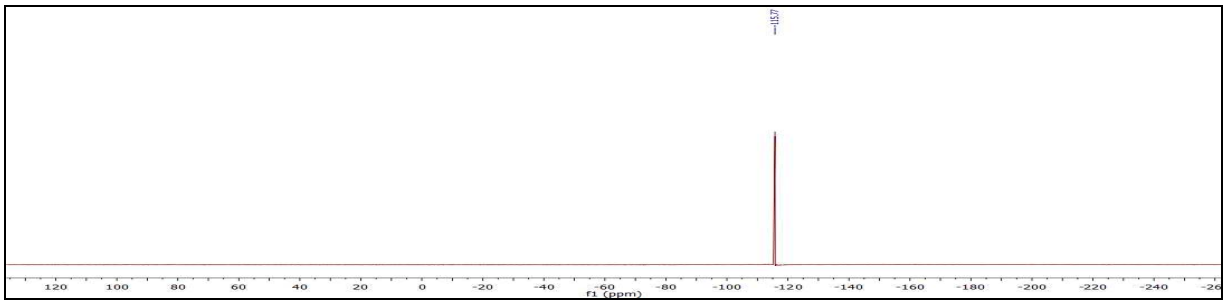
20
10
0
f1 (ppm)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40
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-60
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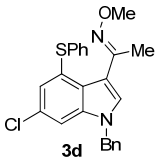
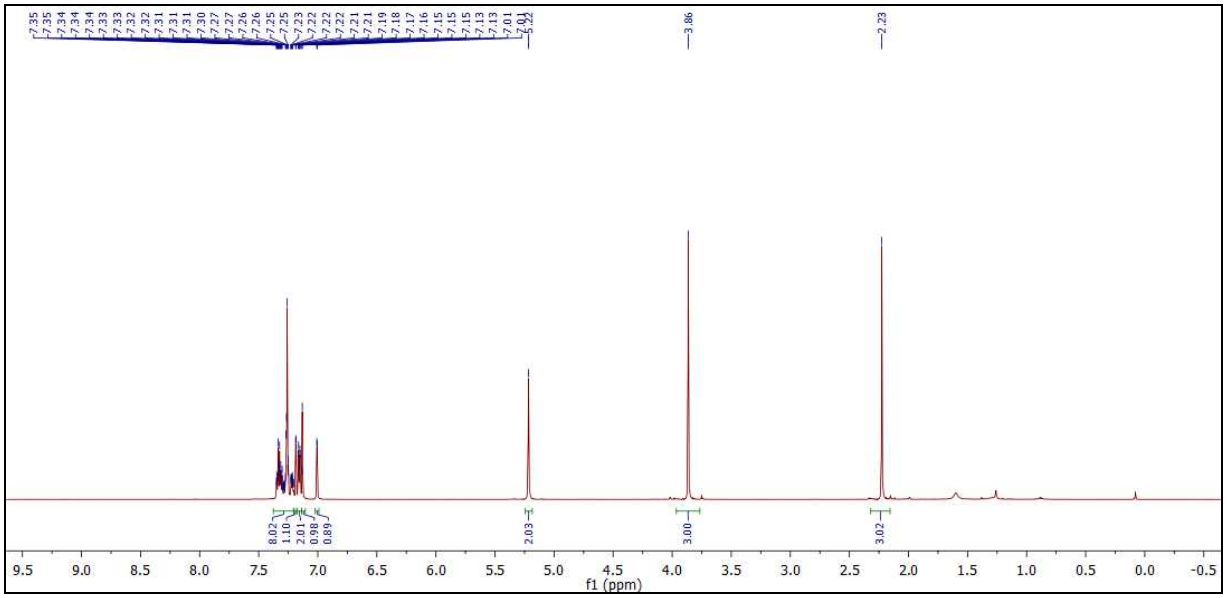
-100
-120
-140
-160
-180
-200
-220
-240
f1 (ppm)


OMe
N
SPh
Me
Cl
N
Bn

3d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7.27
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7.17
7.16
7.15
7.15
7.15
7.13
7.13
7.01
6.91
6.90
3.86
2.23
8.02
1.10
2.01
0.98
0.89
2.03
3.00
3.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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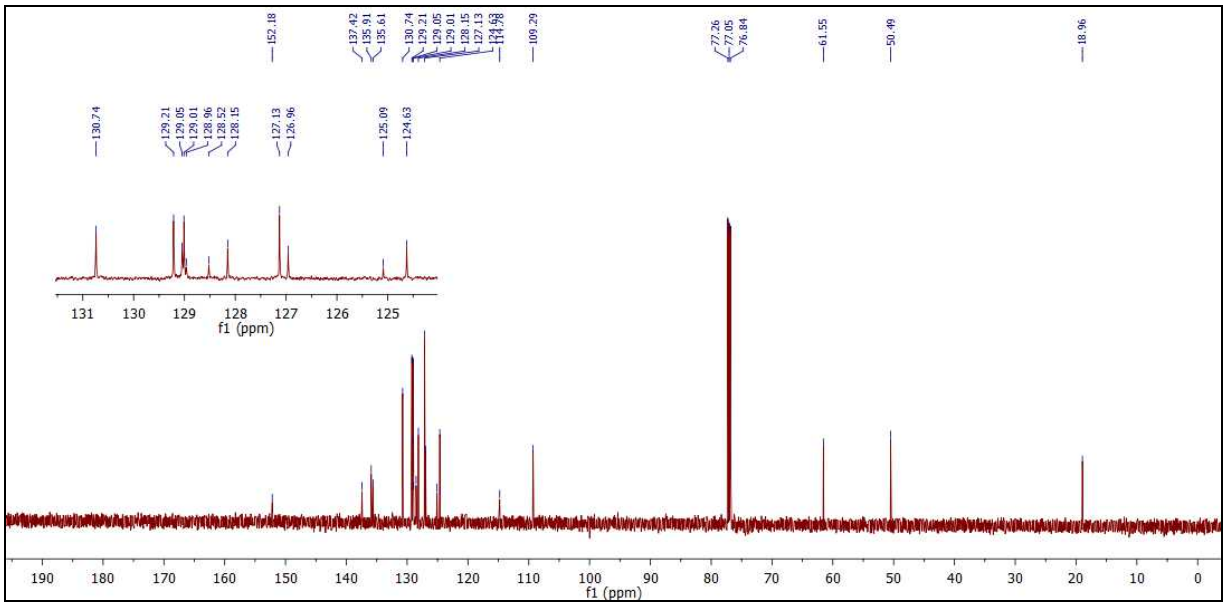
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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129.21
129.05
129.01
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127.13
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124.63
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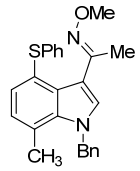
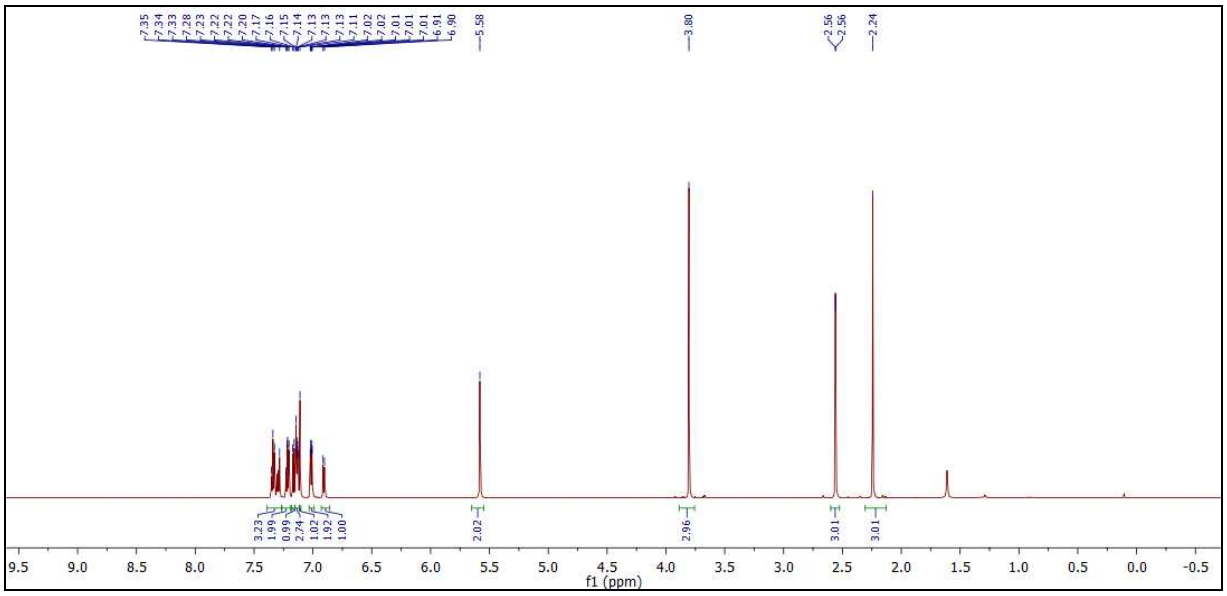
77.26
77.05
76.84
61.55
50.49
18.96
130.74
129.21
129.05
129.01
128.96
128.52
128.15
127.13
126.96
125.09
124.63
131
130
129
128
127
126
125
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
N
SPh
Me
N
Bn
CH3

3e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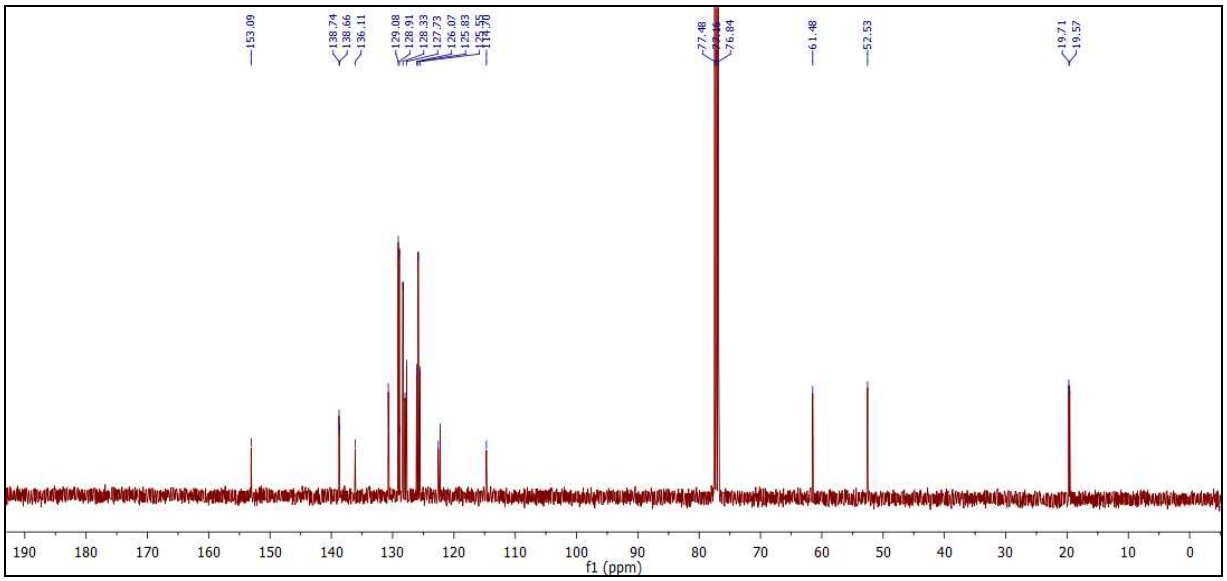
7.13
7.13
7.13
7.11
7.02
7.02
7.01
7.01
7.01
6.91
6.90
5.58
3.80
2.56
2.56
2.24
3.23
1.99
0.99
2.74
1.02
1.92
1.00
2.02
2.96
3.01
3.01
f1 (ppm)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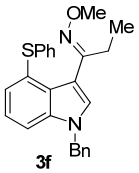
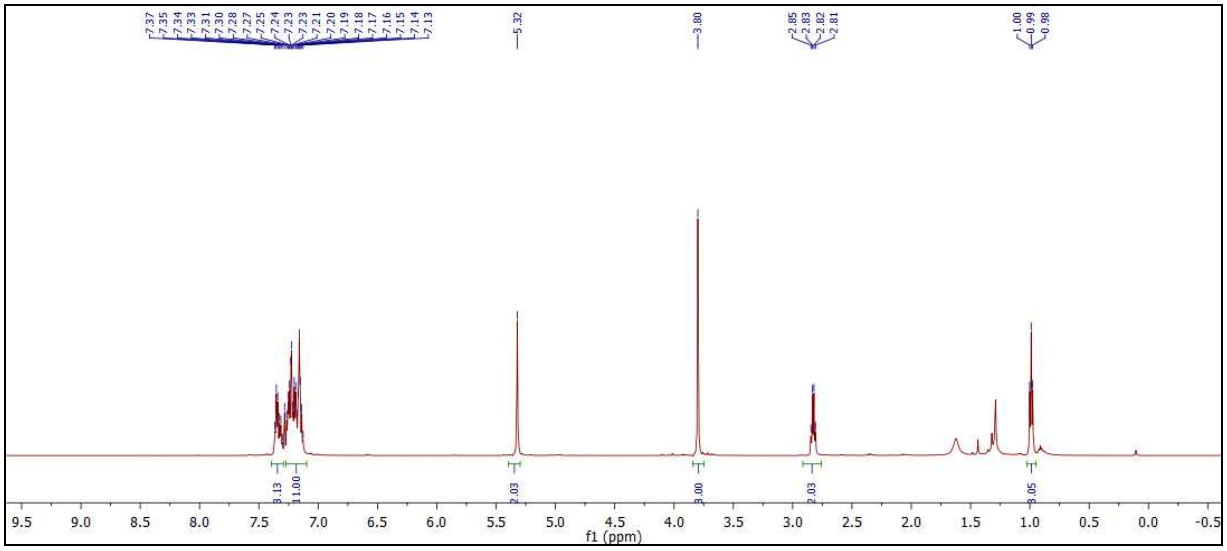
77.48
76.84
61.48
52.53
19.71
19.57
f1 (ppm)


OMe
N
Me
SPh
N
Bn

3f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7.20
7.19
7.18
7.17
7.16
7.15
7.14
7.13
5.32
3.80
2.85
2.83
2.82
2.81
1.00
0.99
0.98
3.13
11.00
2.03
3.00
2.03
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
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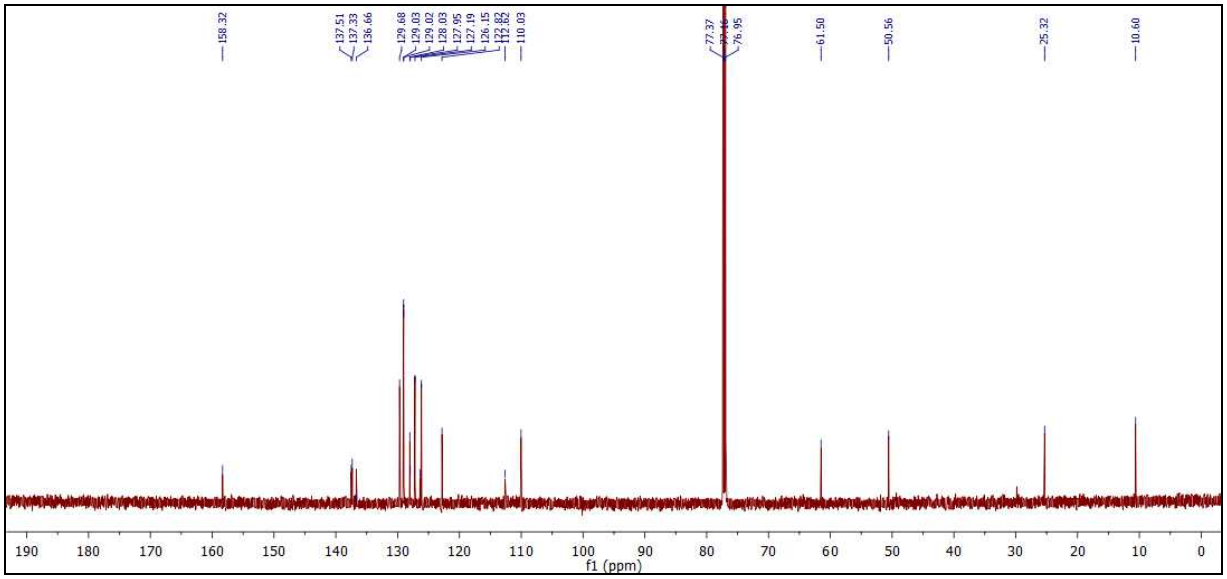
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.19
126.15
122.82
110.03
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77.16
76.95
61.50
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25.32
10.60
190
180
170
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150
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130
120
110
100
90
80
70
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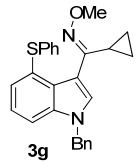
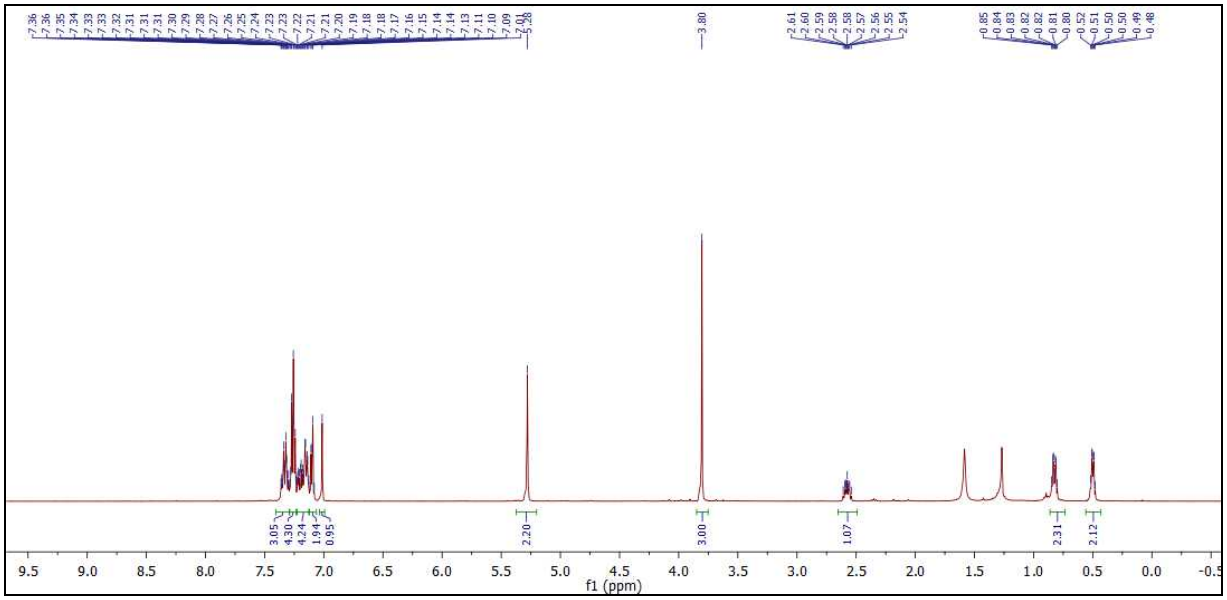
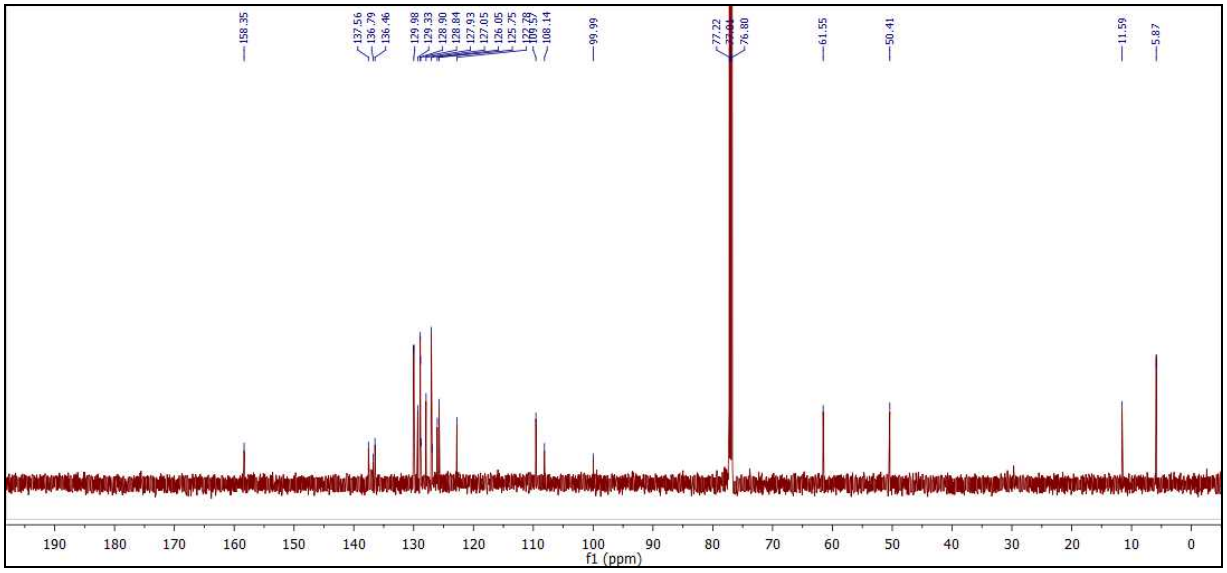
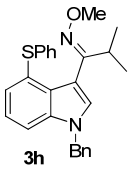
50
40
30
20
10
0
f1 (ppm)



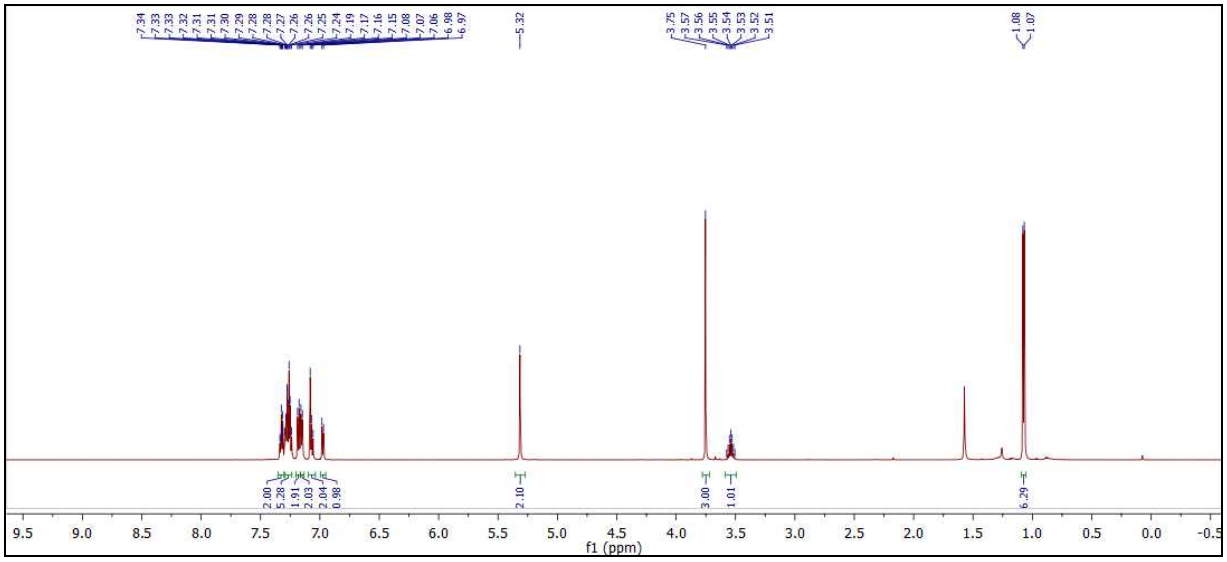
3g






OMe
N
SPh
N
Bn

3h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7.24
7.19
7.17
7.16
7.15
7.08
7.07
7.06
6.98
6.97
5.32
3.75
3.57
3.56
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3.52
3.51
1.08
1.07
2.00
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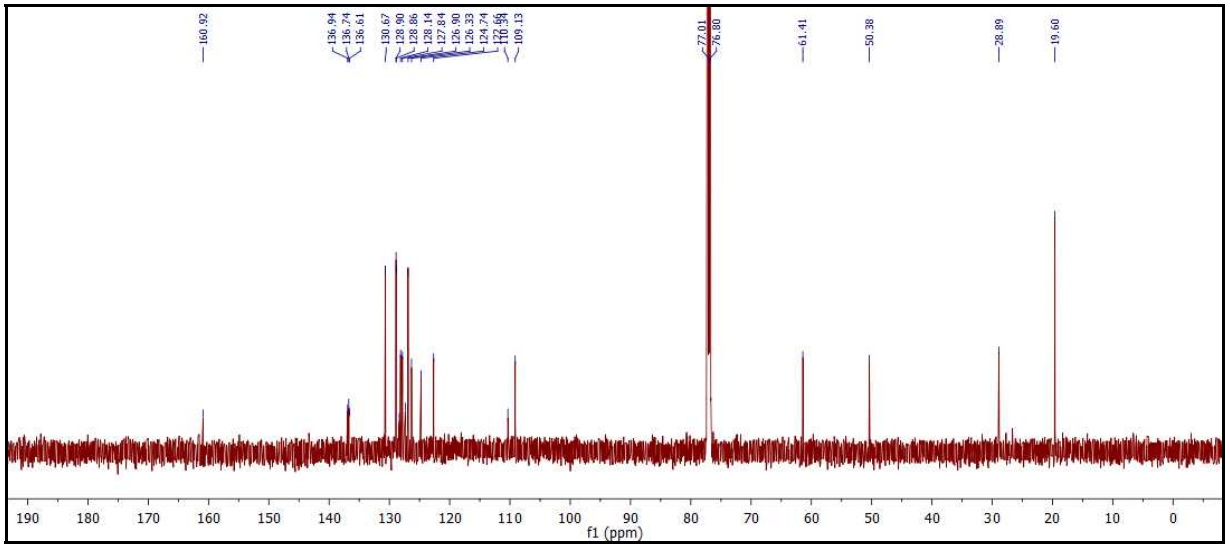
2.03
2.04
0.98
2.10
3.00
1.01
6.29
f1 (ppm)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126.90
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124.74
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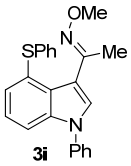
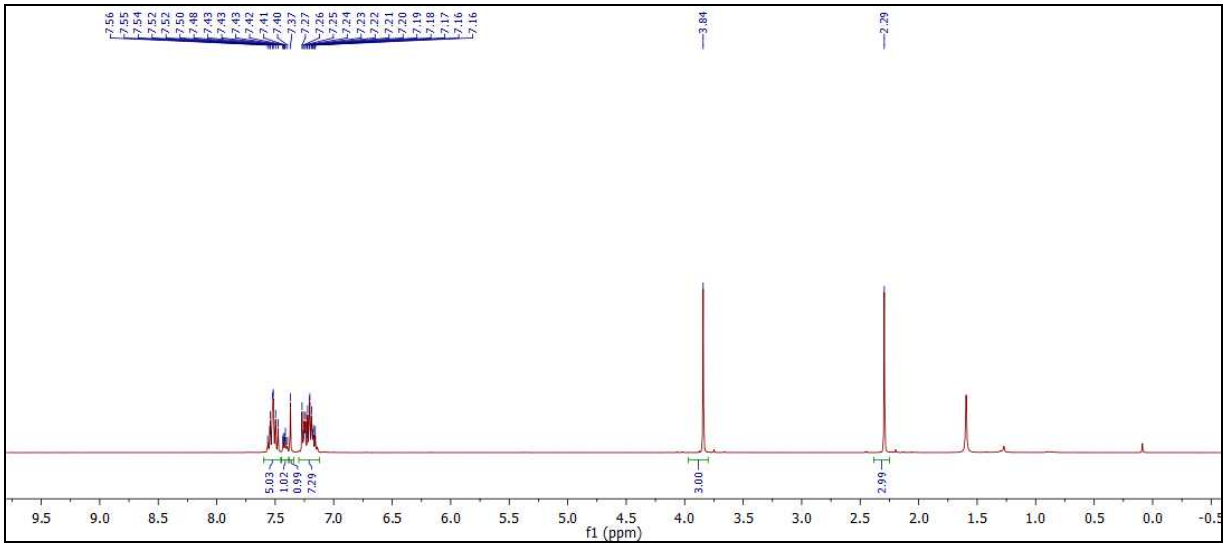
110.94
109.13
77.01
76.80
61.41
50.38
28.89
19.60
f1 (ppm)


OMe
N
SPh
Me
N
Ph

3i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7.24
7.23
7.22
7.21
7.20
7.19
7.18
7.17
7.16
7.16
3.84
2.29
5.03
1.02
0.99
7.29
3.00
2.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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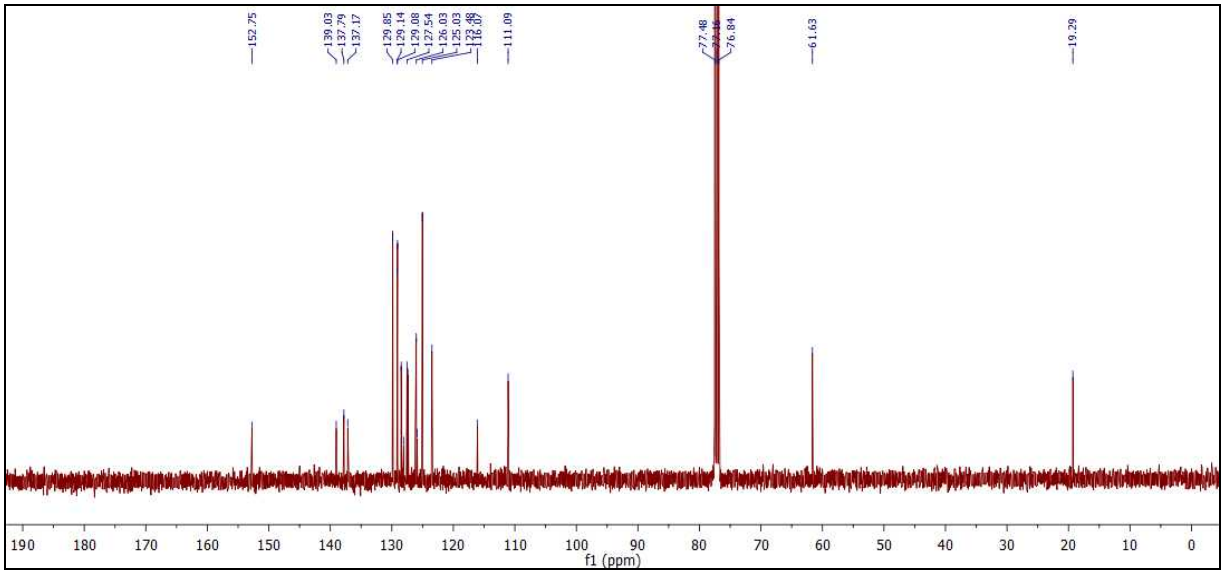
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.54
126.03
125.03
123.48
116.87
111.09
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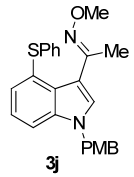
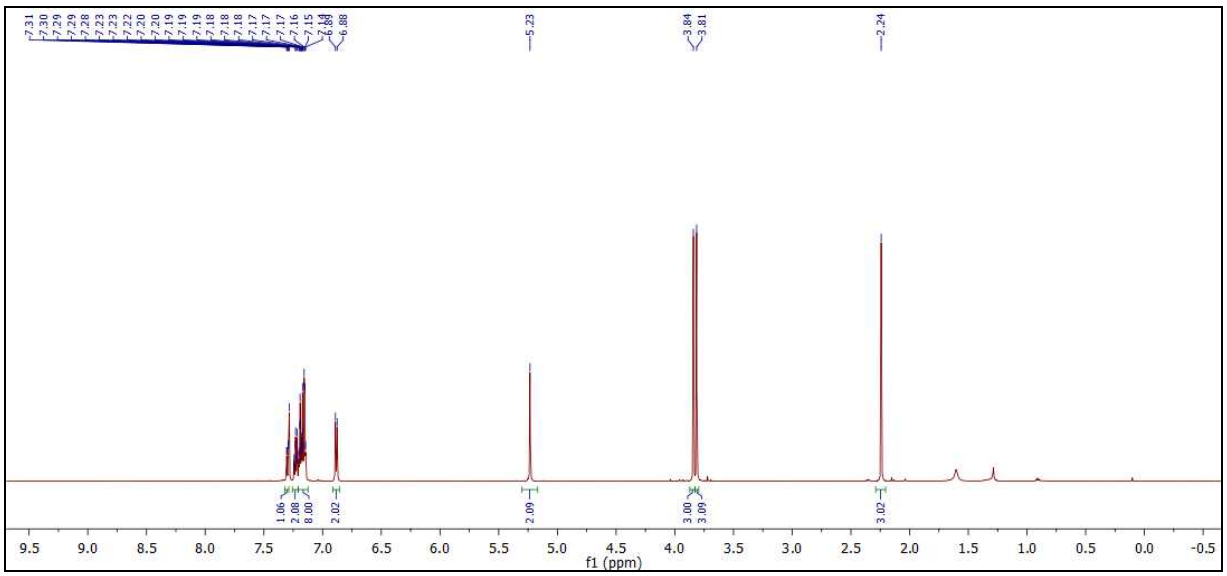
77.16
76.84
61.63
19.29
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
N
SPh
Me
N
PMB

3j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7.18
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7.17
7.17
7.16
7.15
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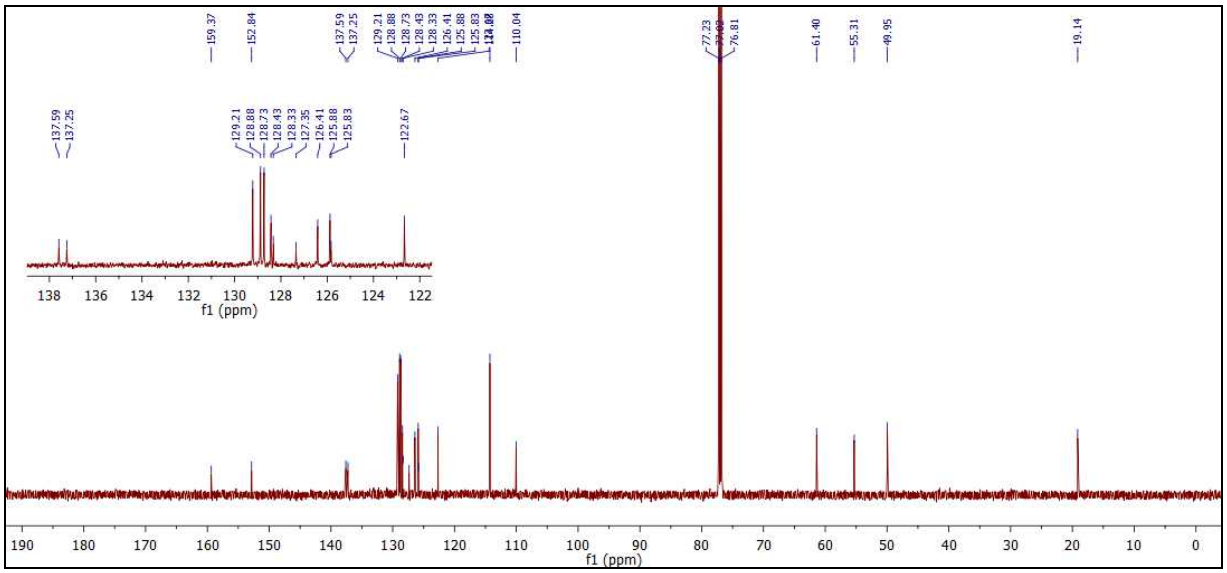
6.88
5.23
3.84
3.81
2.24
1.06
2.08
8.00
2.02
2.09
3.00
3.09
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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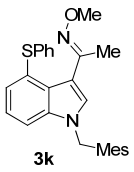
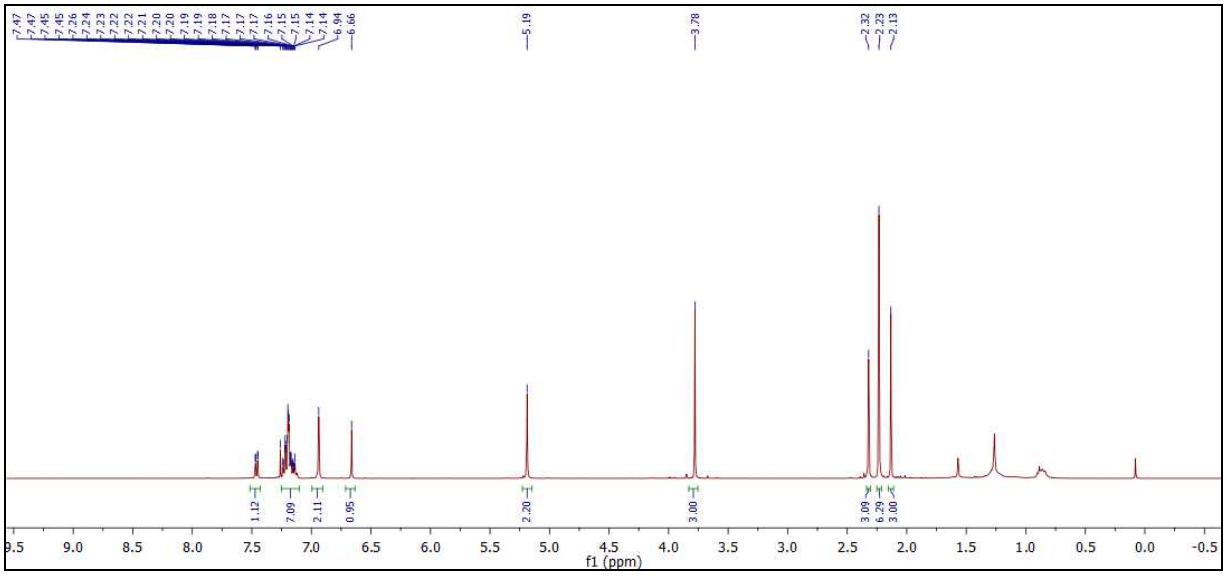
128.33
127.35
126.41
125.88
125.83
110.04
77.23
76.81
61.40
55.31
49.95
19.14
122.67
138 136 134 132 130 128 126 124 122
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OMe
N
SPh
Me
N
Mes

3k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7.18
7.17
7.17
7.17
7.16
7.15
7.15
7.14
7.14
6.94
6.66
5.19
3.78
2.32
2.23
2.13
1.12
7.09
2.11
0.95
2.20
3.00
3.09
6.29
3.00
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9.0
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
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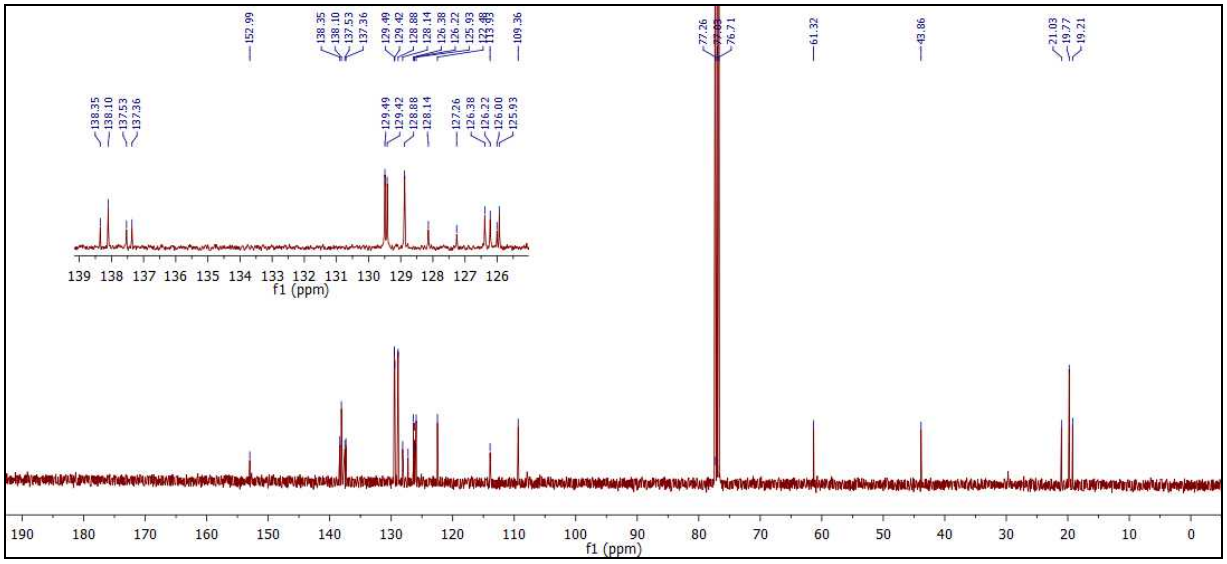
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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126.38
126.22
125.93
113.88
109.36
77.26
77.03
76.71
61.32
43.86
21.03
19.77
19.21
139 138 137 136 135 134 133 132 131 130 129 128 127 126
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
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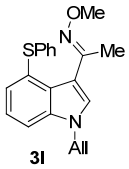
f1 (ppm)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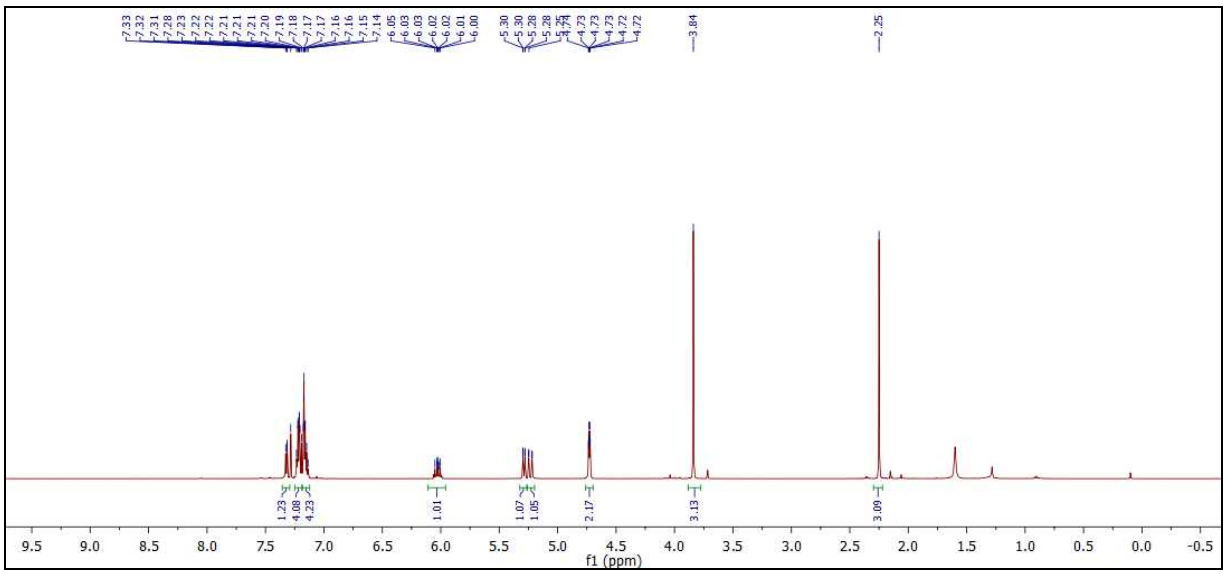
N
SPh
Me
N
All

3l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7.17
7.16
7.16
7.15
7.14
6.05
6.03
6.02
6.02
6.01
6.00
5.30
5.30
5.28
5.28
4.74
4.73
4.73
4.73
4.72
4.72
3.84
2.25
1.23
4.08
4.23
1.01
1.07
1.05
2.17
3.13
3.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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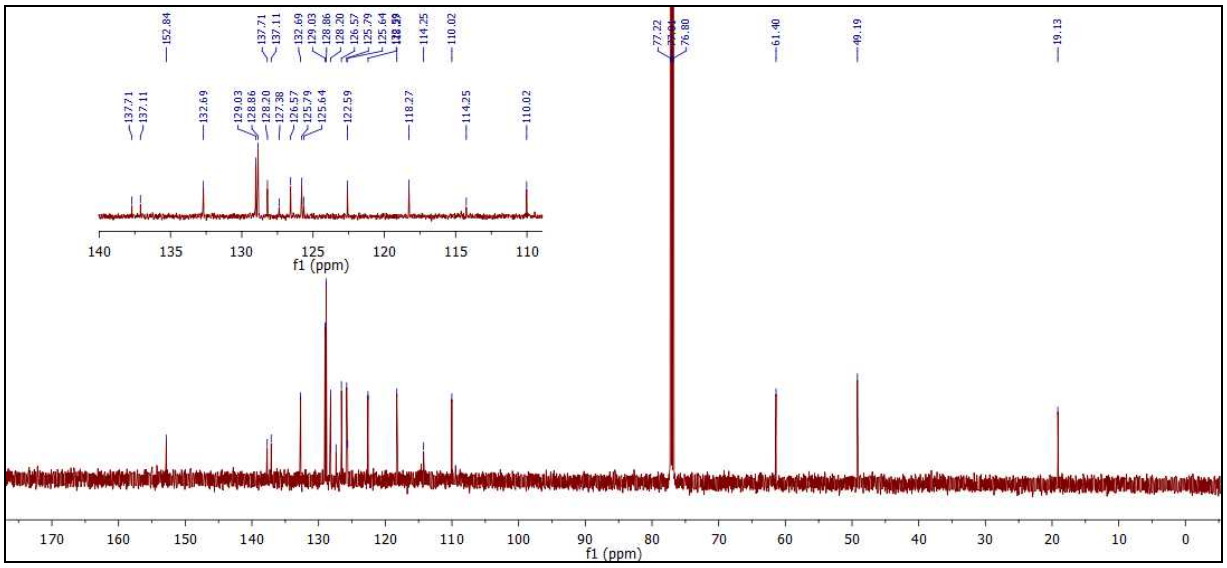
0.5
0.0
-0.5
f1 (ppm)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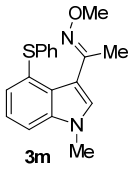
128.86
128.20
126.57
125.79
125.64
114.25
110.02
77.22
76.80
61.40
49.19
19.13
137.71
137.11
132.69
129.03
128.86
128.20
127.98
126.57
125.79
125.64
122.59
118.27
114.25
110.02
140
135
130
125
120
115
110
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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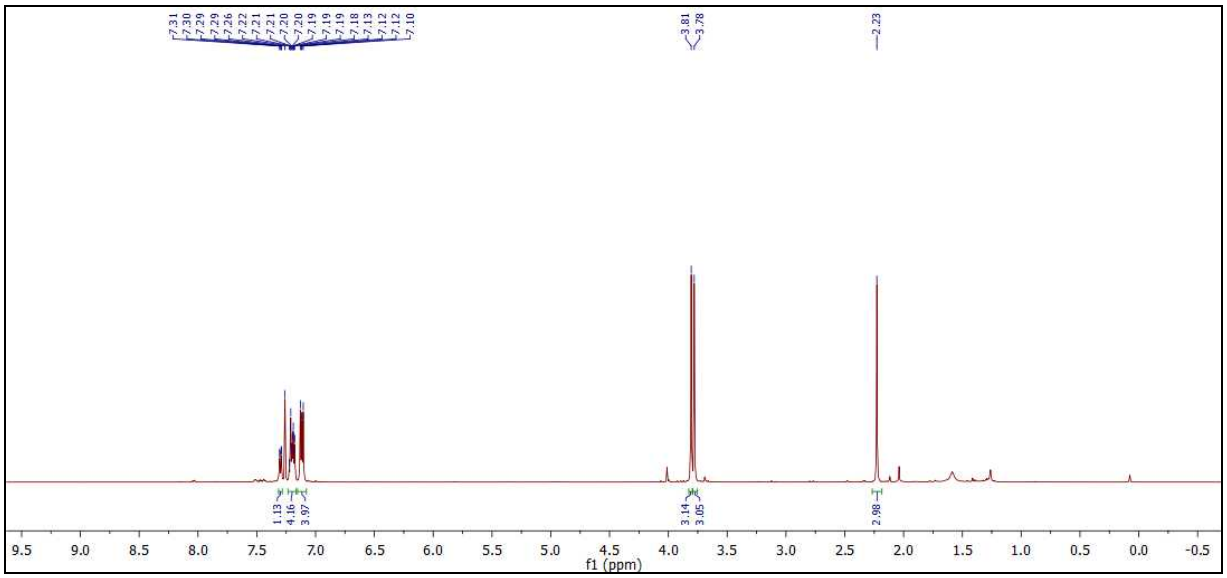
SPh
Me
N
Me

3m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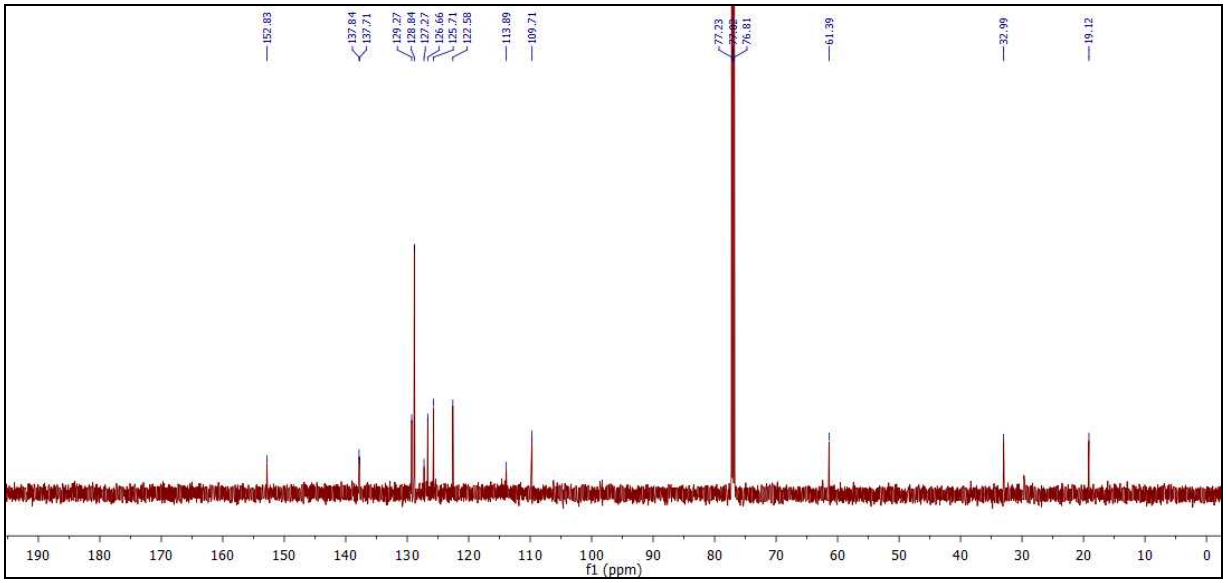
7.19
7.18
7.13
7.12
7.12
7.10
3.81
3.78
2.23
1.13
4.16
3.97
3.14
3.05
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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137.71
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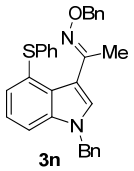
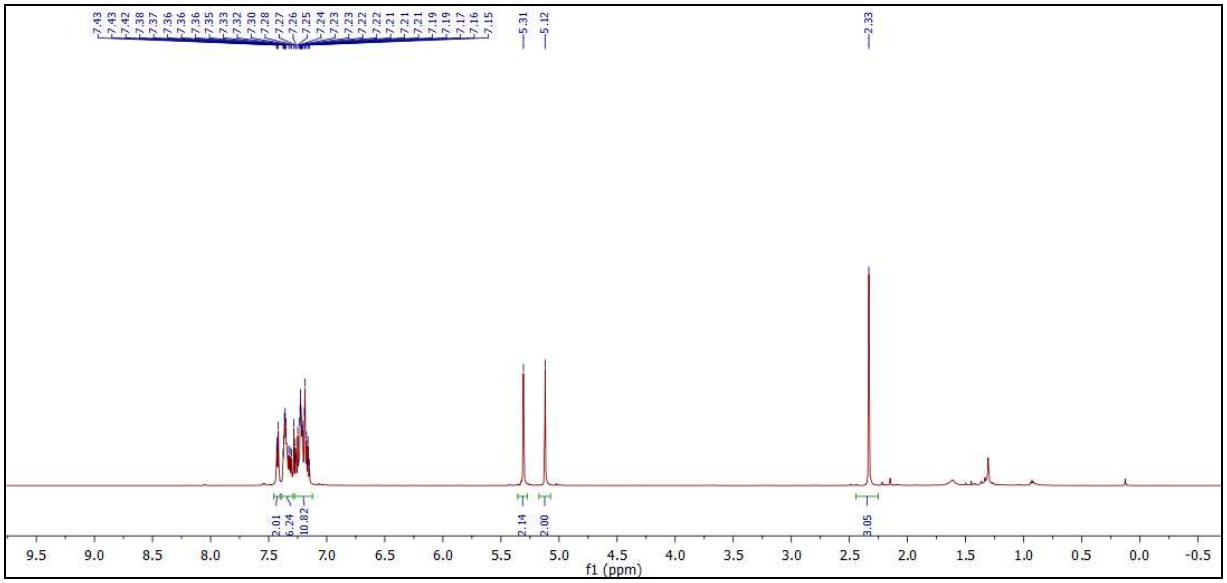
127.27
126.66
125.71
122.58
113.89
109.71
77.23
77.02
76.81
61.39
32.99
19.12
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OBn
N
SPh
Me
N
Bn

3n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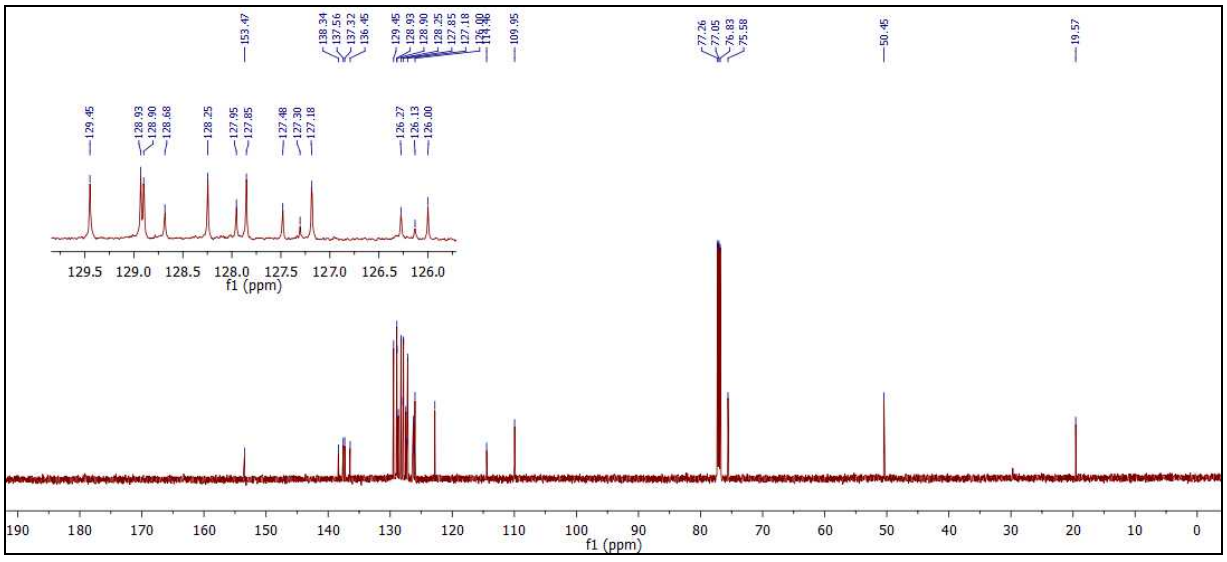
7.22
7.22
7.21
7.21
7.19
7.19
7.17
7.16
7.15
5.31
5.12
2.33
2.01
6.24
10.82
2.14
2.00
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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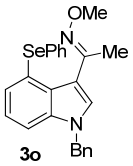
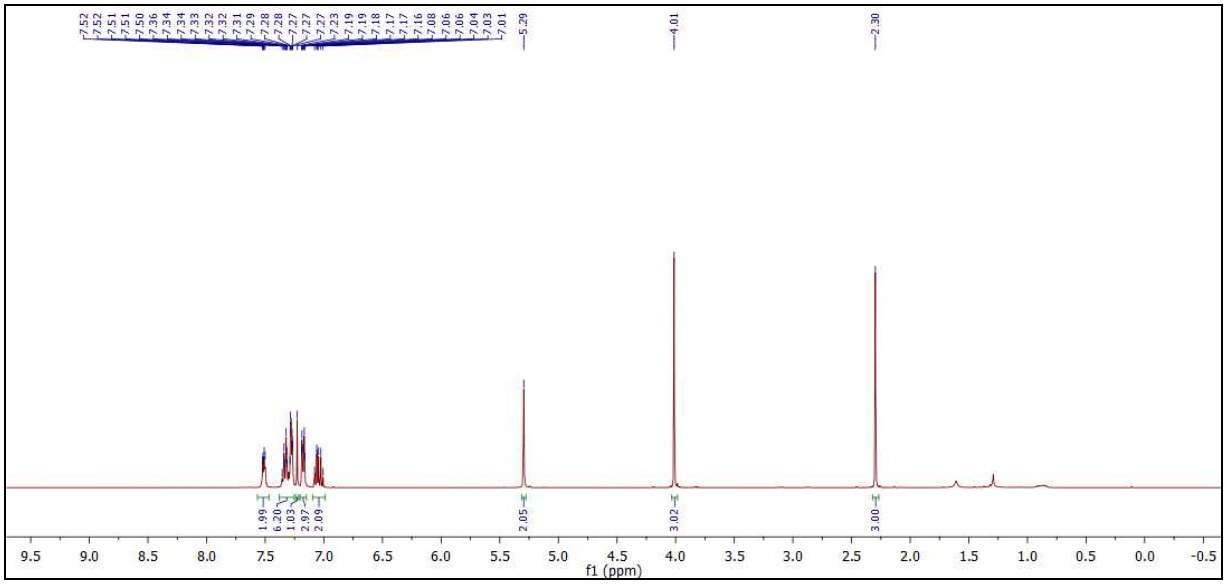
127.85
127.18
109.95
77.26
77.05
76.83
75.58
50.45
19.57
129.45
128.93
128.90
128.68
128.25
127.95
127.85
127.48
127.30
127.18
126.27
126.13
126.00
129.5 129.0 128.5 128.0 127.5 127.0 126.5 126.0
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OMe
N
SePh
Me
N
Bn

3o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7.27
7.27
7.23
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7.19
7.18
7.17
7.17
7.16
7.08
7.06
7.06
7.04
7.03
7.01
5.29
4.01
2.30
1.99
6.20
1.03
2.97
2.09
2.05
3.02
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
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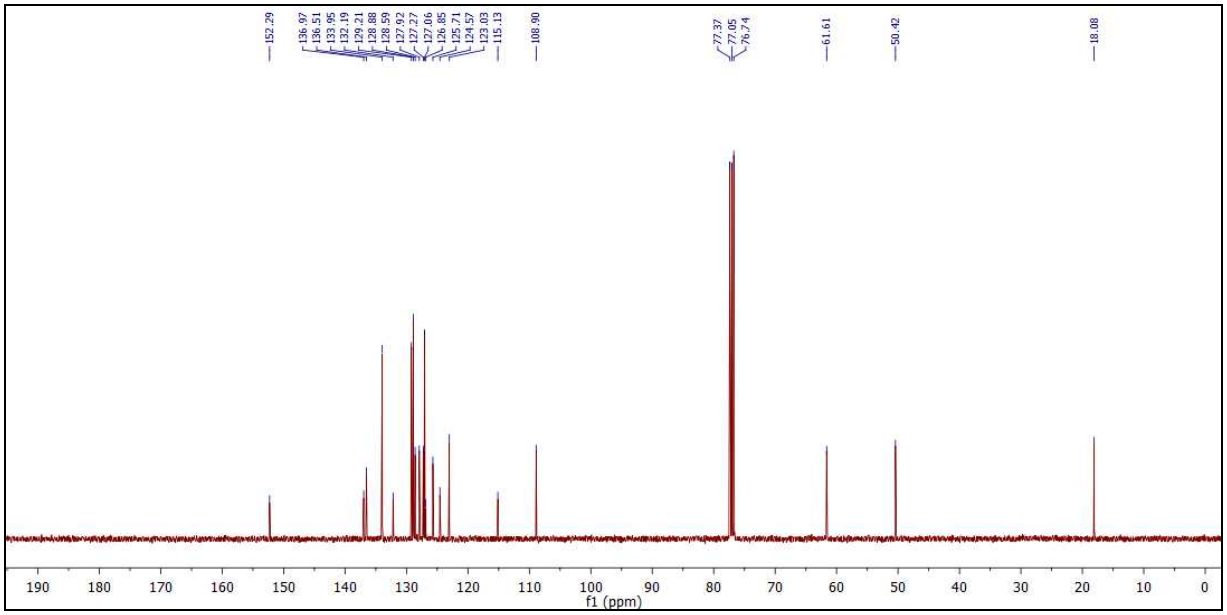
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.06
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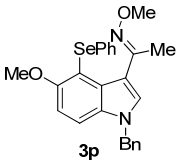
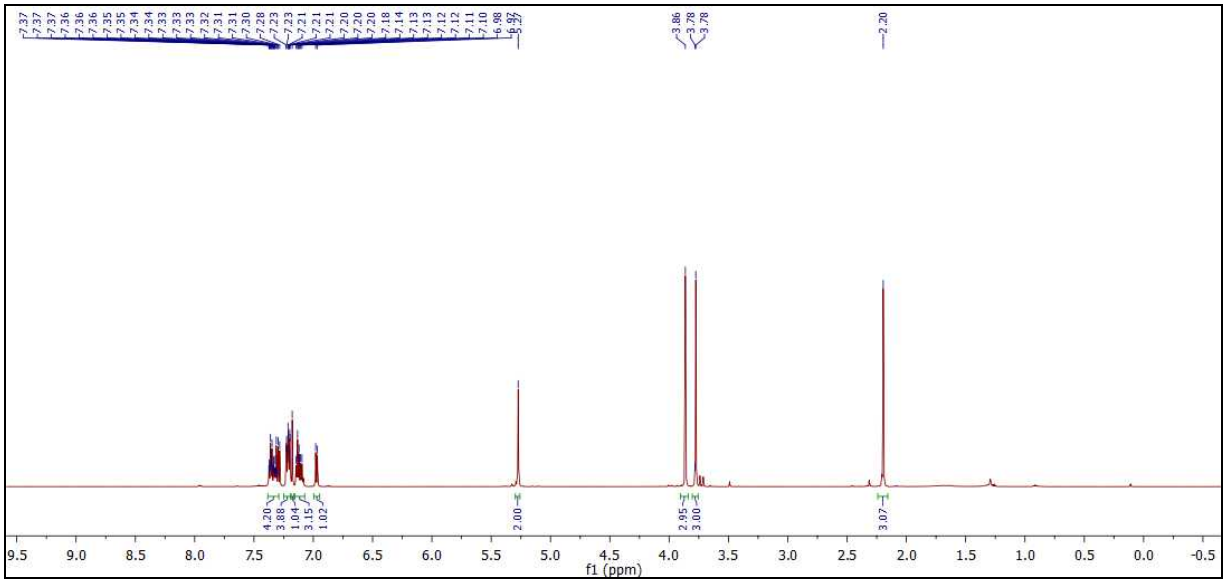
125.71
124.57
123.03
115.13
108.90
77.37
77.05
76.74
61.61
50.42
18.08
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
N
SePh
Me
MeO
N
Bn

3p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7.20
7.18
7.14
7.13
7.13
7.12
7.12
7.11
7.10
6.98
6.97
5.27
3.86
3.78
3.78
2.20
4.20
3.88
1.04
3.15
1.02
2.00
2.95
3.00
3.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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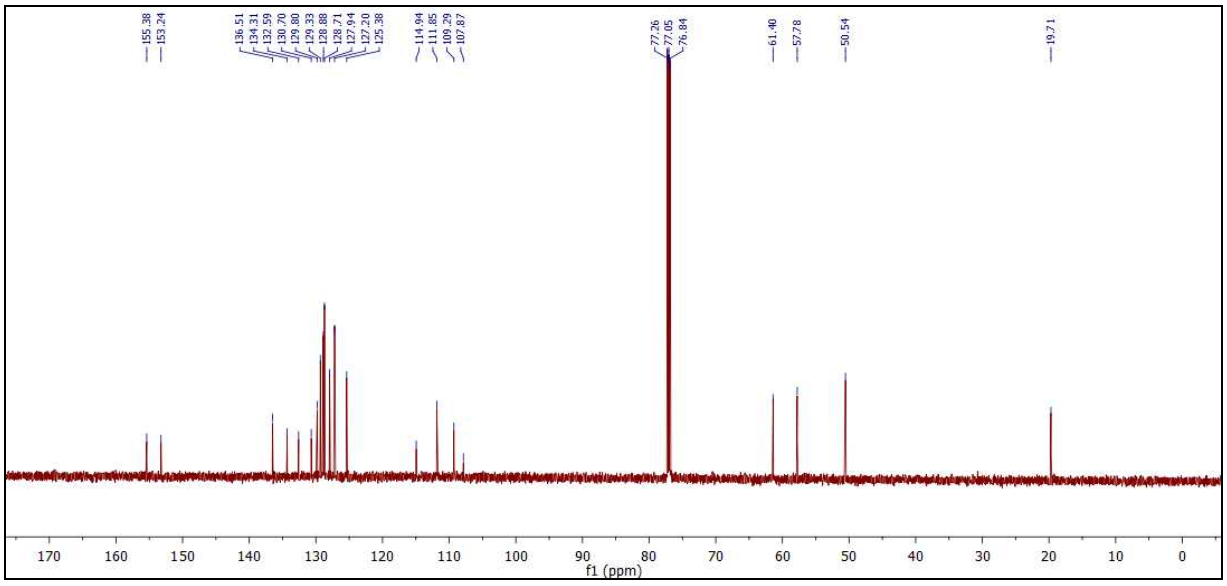
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.94
127.20
125.38
114.94
111.85
109.29
107.87
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77.05
76.84
61.40
57.78
50.54
19.71
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150
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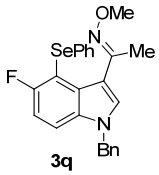
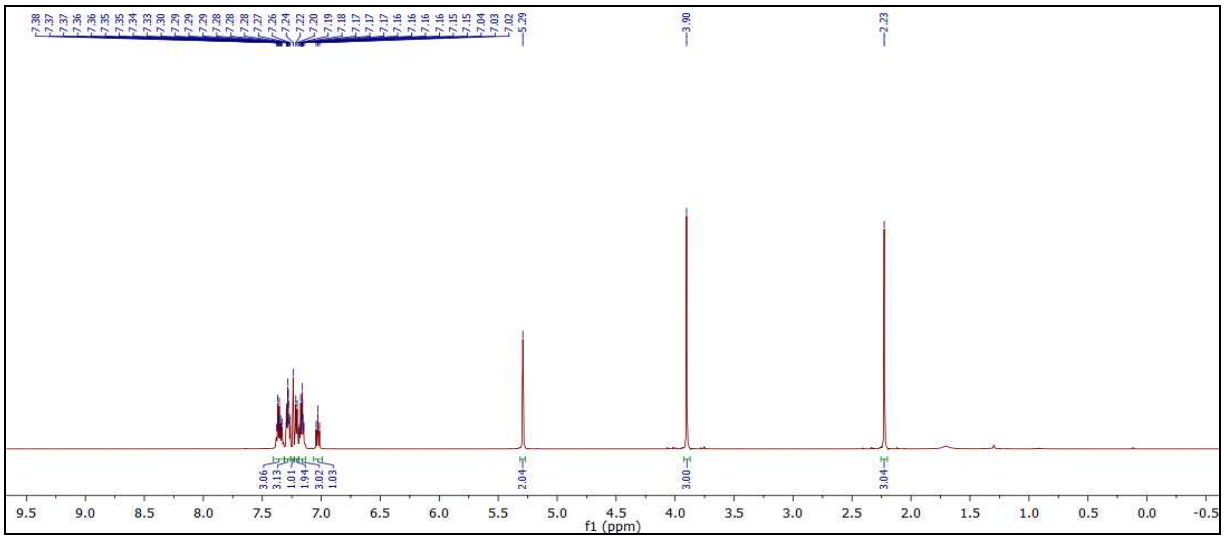
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
N
SePh
Me
F
N
Bn

3q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7.28
7.28
7.27
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7.22
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7.19
7.18
7.17
7.17
7.17
7.16
7.16
7.16
7.16
7.15
7.15
7.04
7.03
7.02
5.29
3.90
2.23
3.06
3.13
1.01
1.94
3.02
1.03
2.04
3.00
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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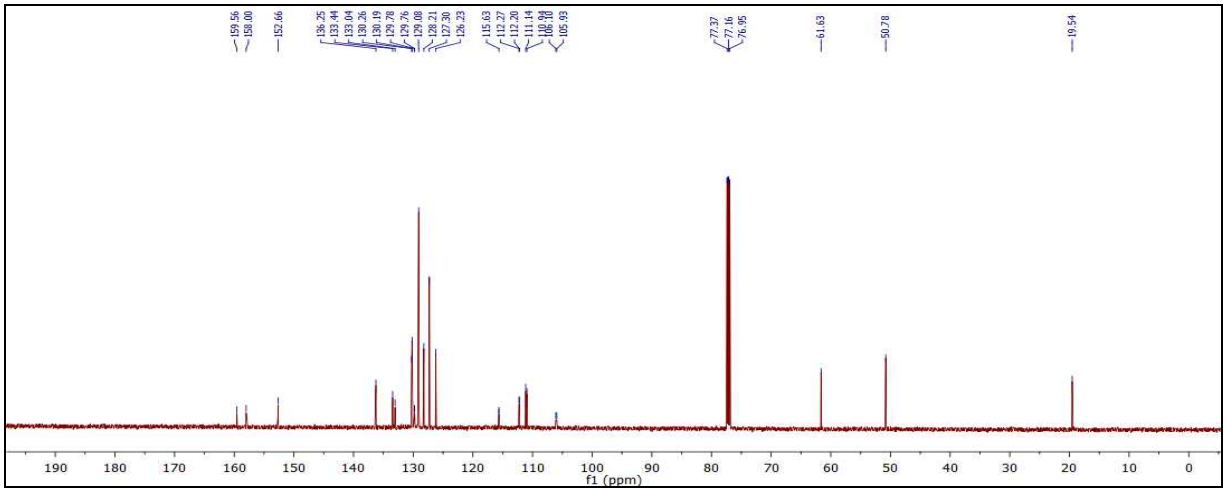
0.5
0.0
-0.5
f1 (ppm)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129.76
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126.23
115.63
112.27
112.20
111.14
110.94
108.10
105.93
77.37
77.16
76.95
61.63
50.78
19.54
190
180
170
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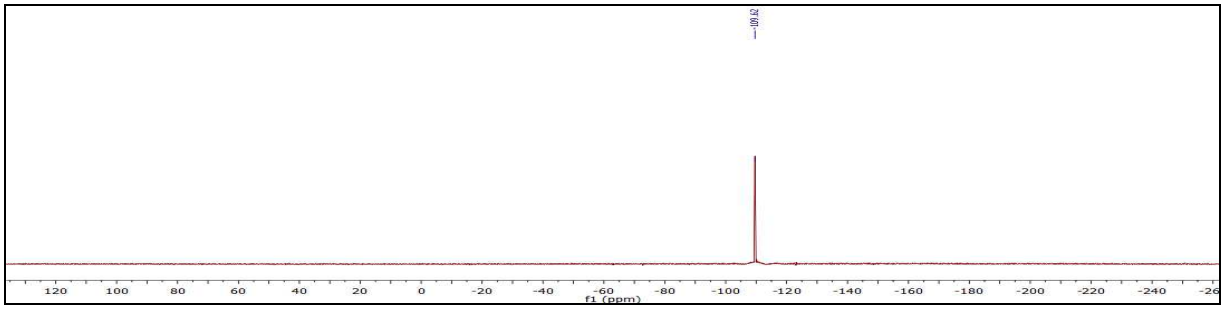
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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120
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60
40
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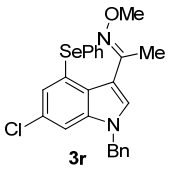
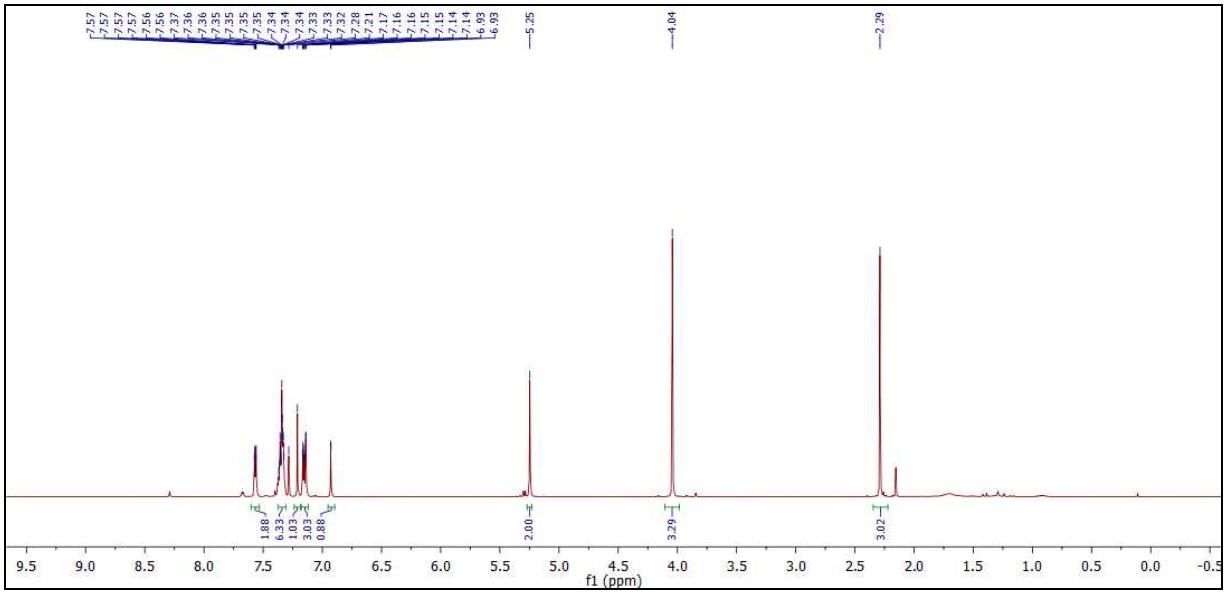
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
f1 (ppm)


OMe
N
SePh
Me
Cl
N
Bn

3r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7.15
7.14
7.14
6.93
6.93
5.25
4.04
2.29
1.88
6.33
1.03
3.03
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2.00
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3.02
9.5
9.0
8.5
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6.0
5.5
5.0
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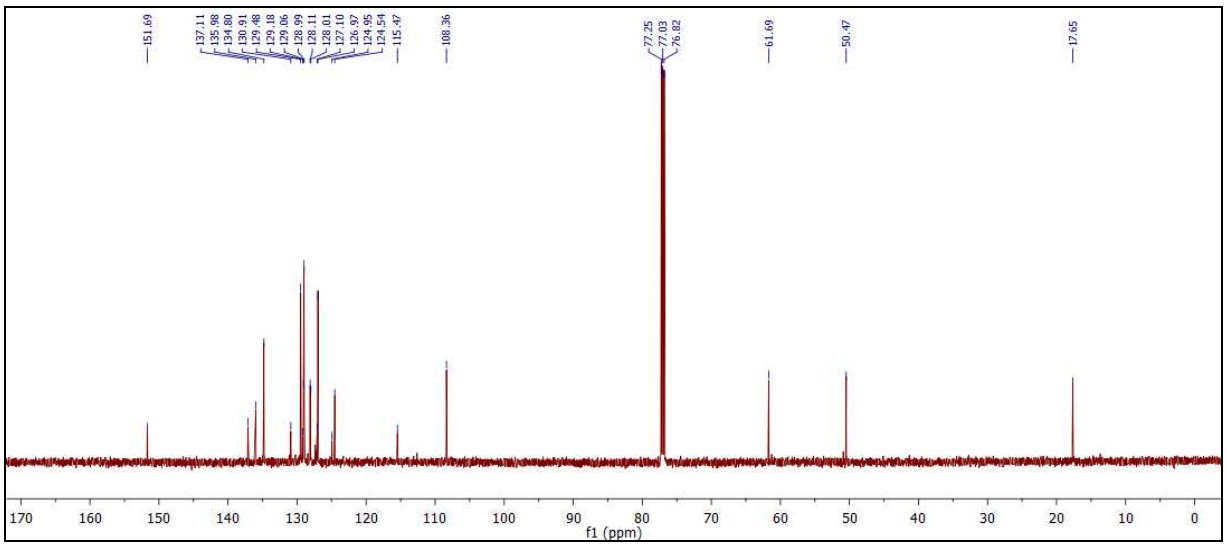
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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128.11
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126.97
124.95
124.54
115.47
108.36
77.25
77.03
76.82
61.69
50.47
17.65
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100
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80
70
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50
40
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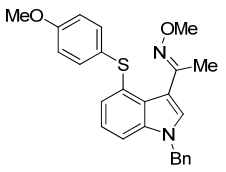
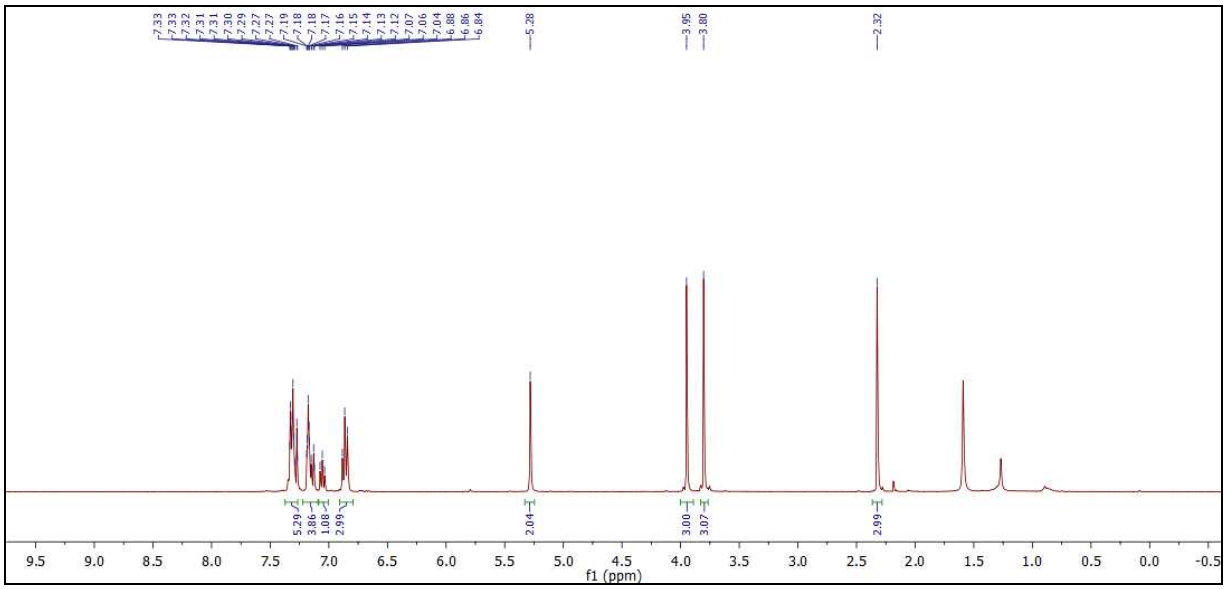
20
10
0
f1 (ppm)


MeO
OMe
N
S
Me
N
Bn

4a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7.18
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7.14
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7.04
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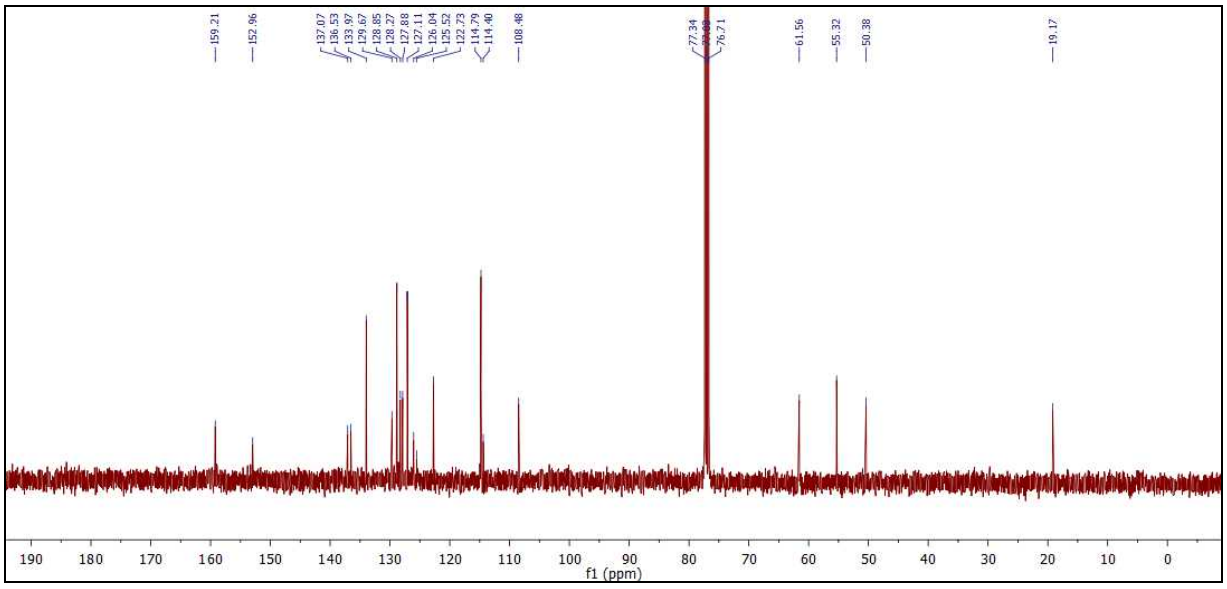
3.95
3.80
2.32
5.29
3.86
1.08
2.99
2.04
3.00
3.07
2.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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152.96
137.07
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128.85
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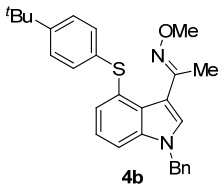
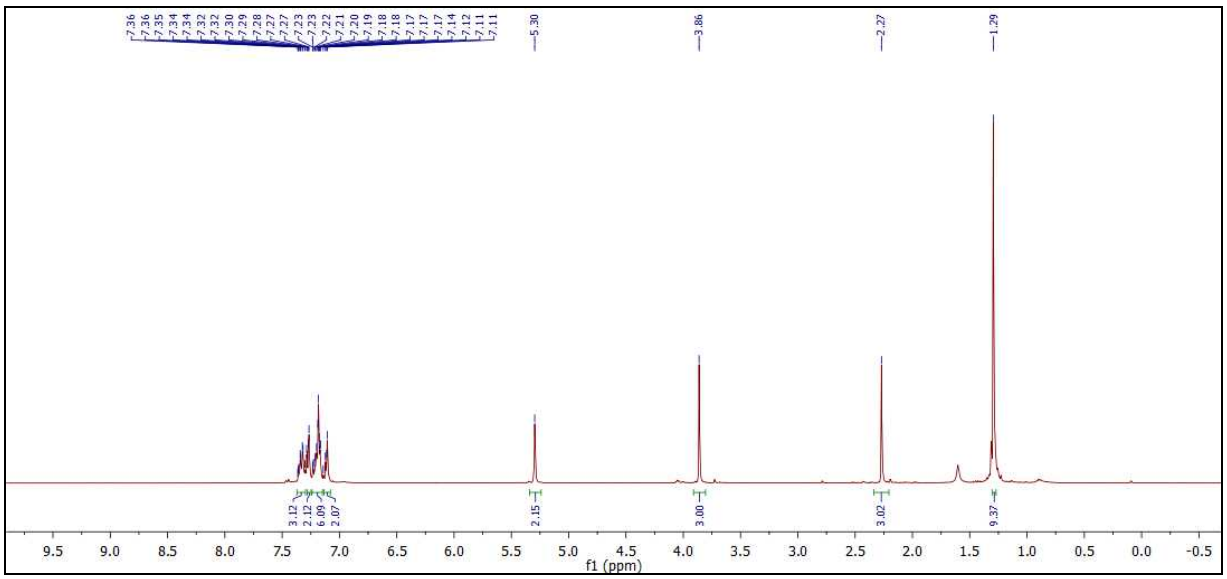
127.88
127.11
126.04
125.52
122.73
114.79
114.40
108.48
77.34
77.03
76.71
61.56
55.32
50.38
19.17
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


tBu
OMe
N
Me
S
N
Bn

4b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7.11
7.11
5.30
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1.29
3.12
2.13
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2.07
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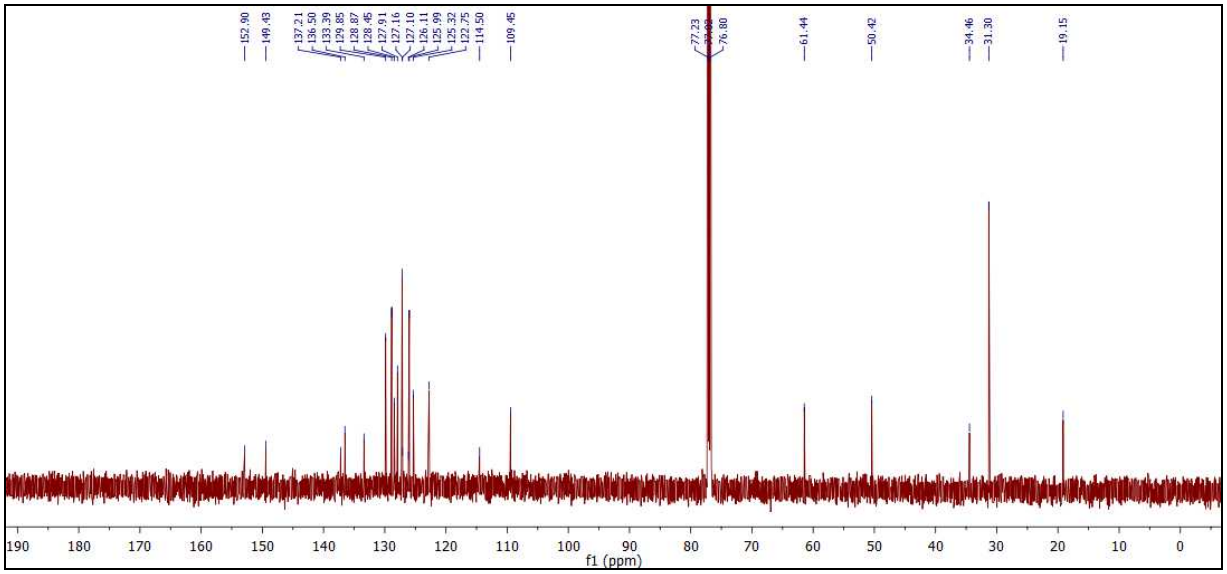
3.00
3.02
9.37
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.45
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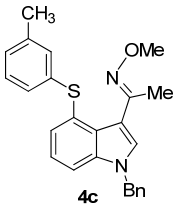
127.16
127.10
126.11
125.99
125.32
122.75
114.50
109.45
77.23
77.03
76.80
61.44
50.42
34.46
31.30
19.15
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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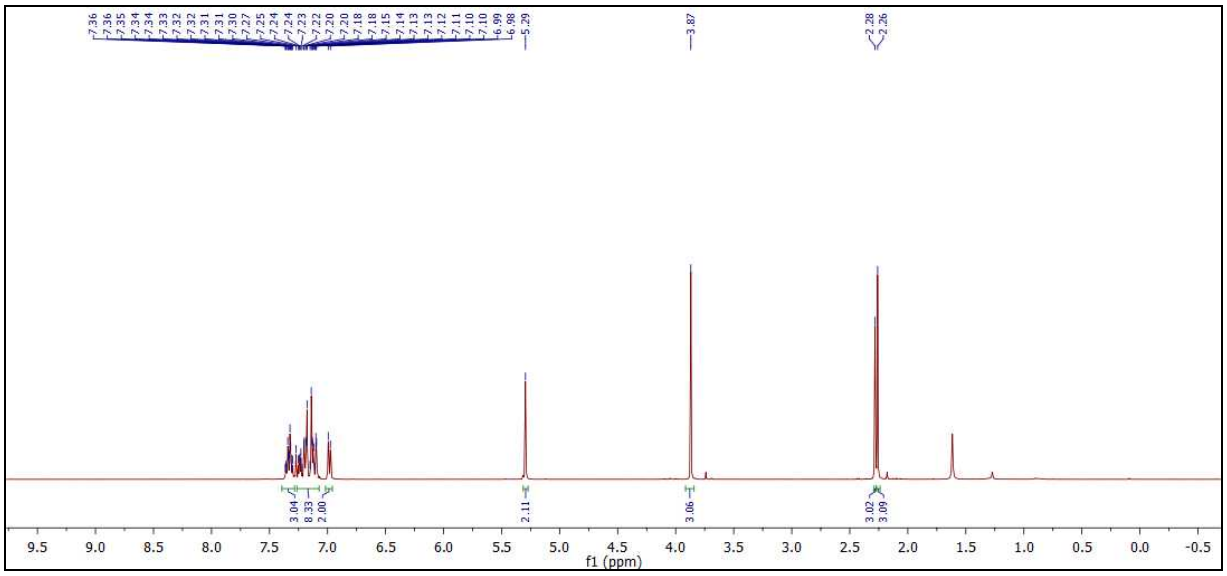
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7.13
7.13
7.12
7.11
7.10
7.10
6.99
6.98
5.29
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2.28
2.26
3.04
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2.00
2.11
3.06
3.02
3.09
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8.5
8.0
7.5
7.0
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6.0
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5.0
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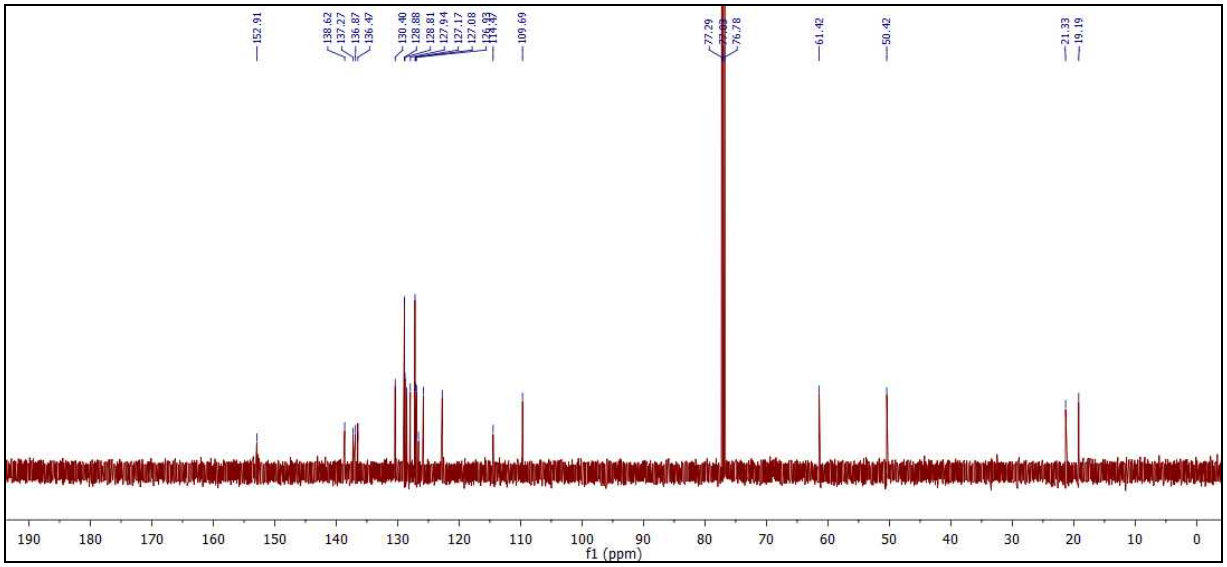
f1 (ppm)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76.78
61.42
50.42
21.33
19.19
190
180
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150
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130
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110
100
90
80
70
60
50
40
30
20
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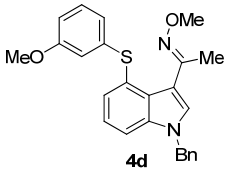
f1 (ppm)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Bn

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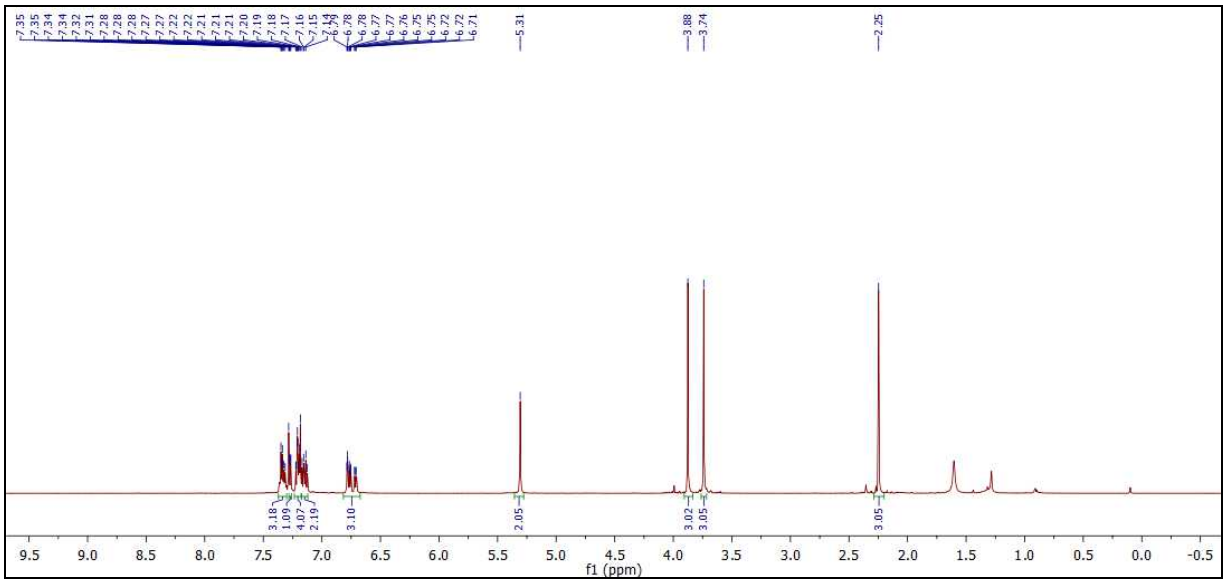
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7.17
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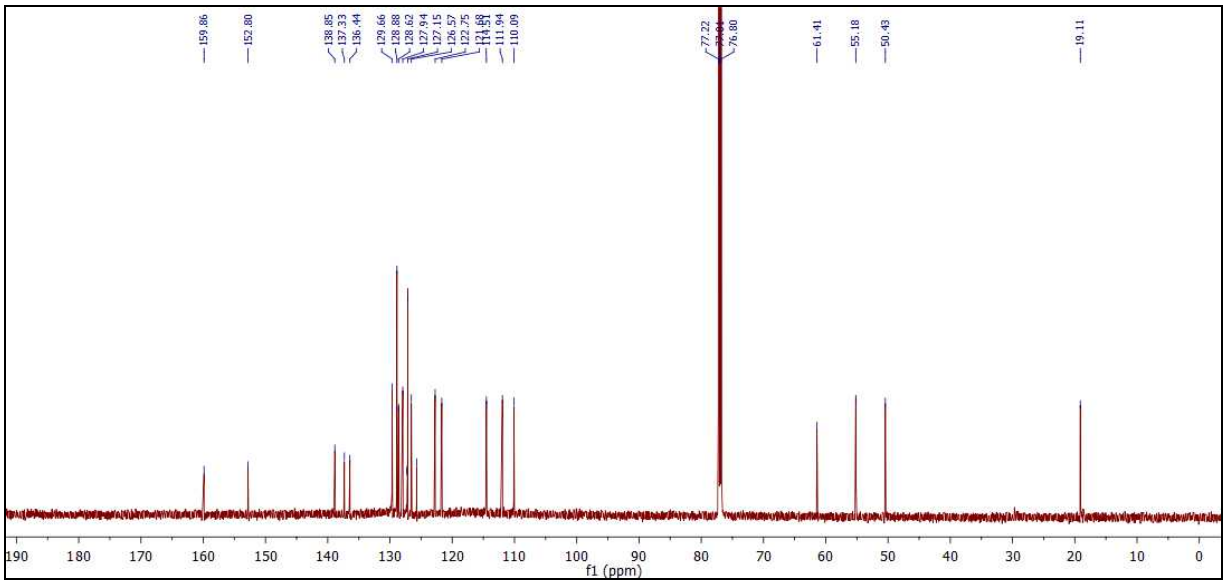
7.15
6.78
6.77
6.76
6.75
6.72
6.71
5.31
3.88
3.74
2.25
3.18
1.09
4.07
2.19
3.10
2.05
3.02
3.05
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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111.94
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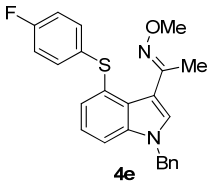
50.43
19.11
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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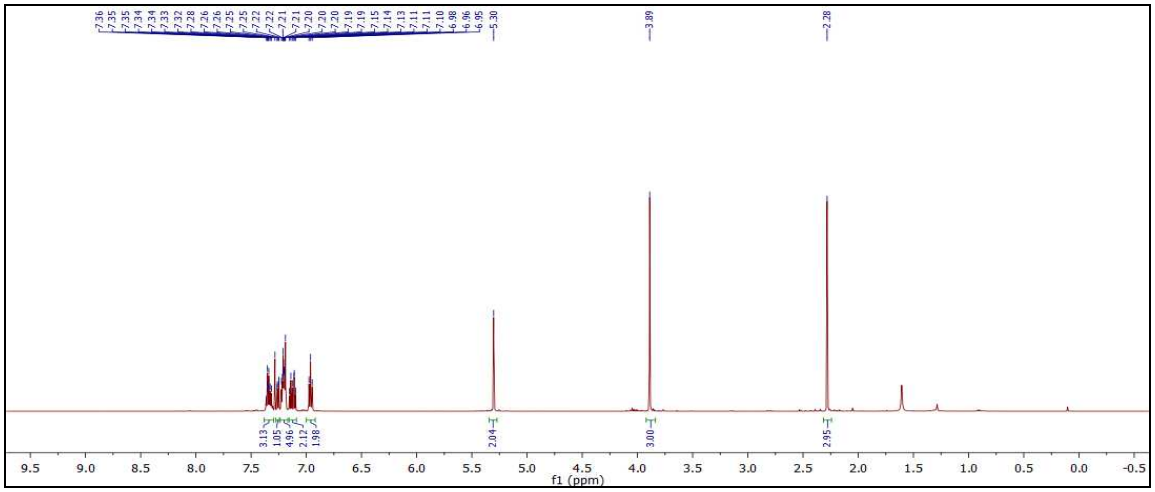
N
Me
N
Bn

4e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7.15
7.14
7.13
7.11
7.11
7.10
6.98
6.96
6.95
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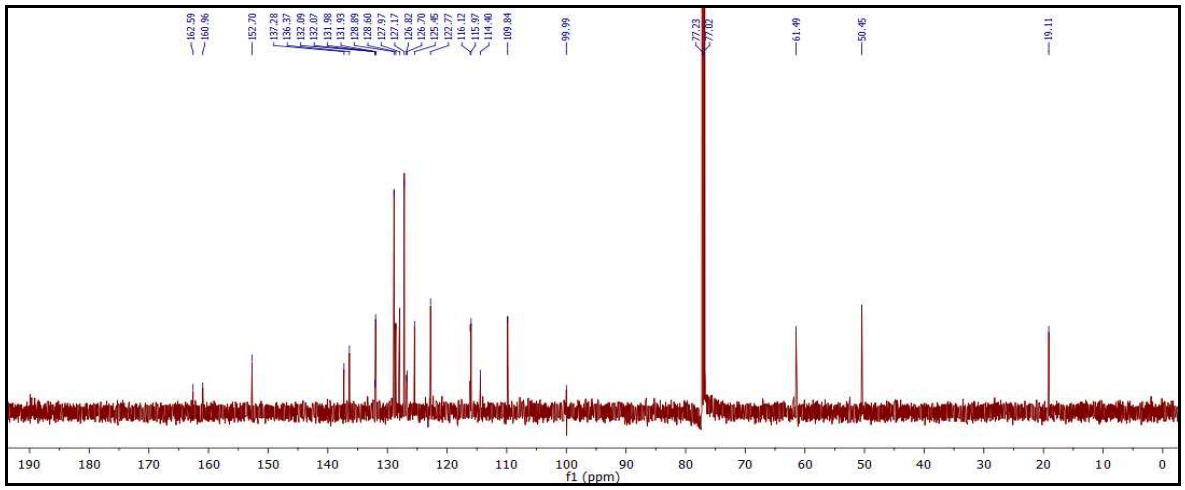
2.04
3.00
2.95
f1 (ppm)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127.97
127.17
126.82
126.70
125.46
122.77
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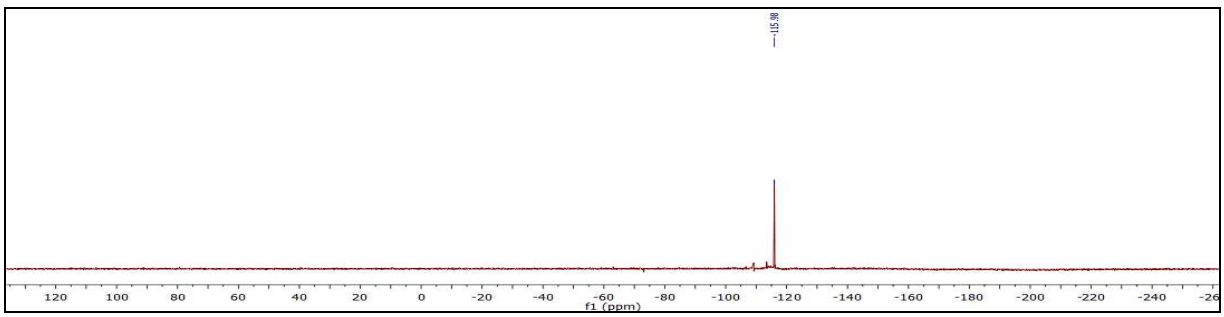
114.40
109.84
99.99
77.23
77.02
61.49
50.45
19.11
f1 (ppm)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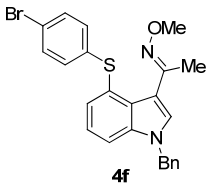
f1 (ppm)


Br
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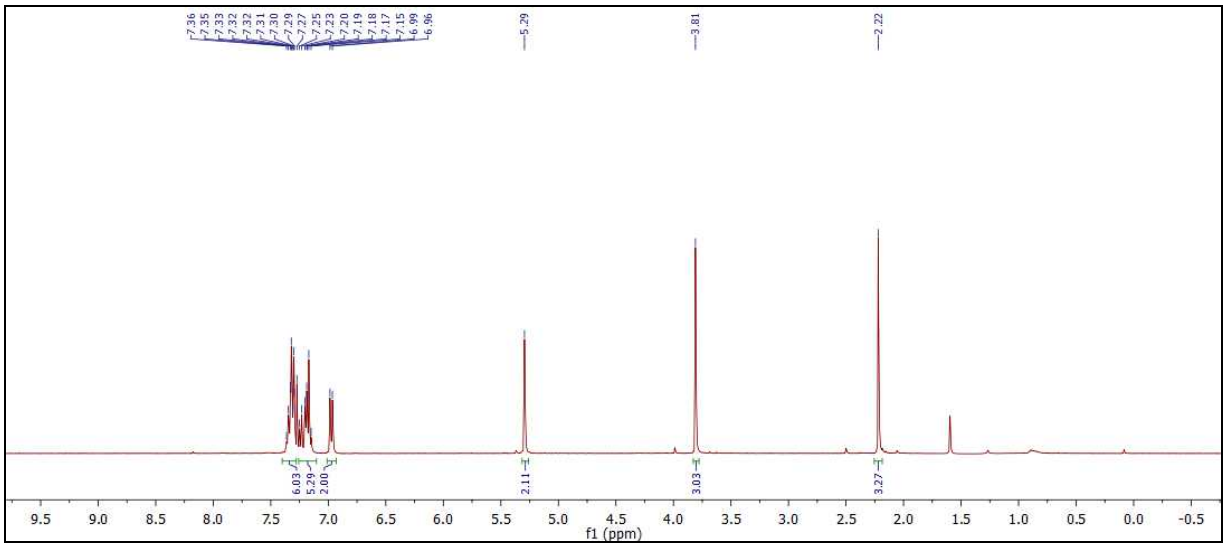
Me
N
Bn

4f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7.19
7.18
7.17
7.15
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6.03
5.29
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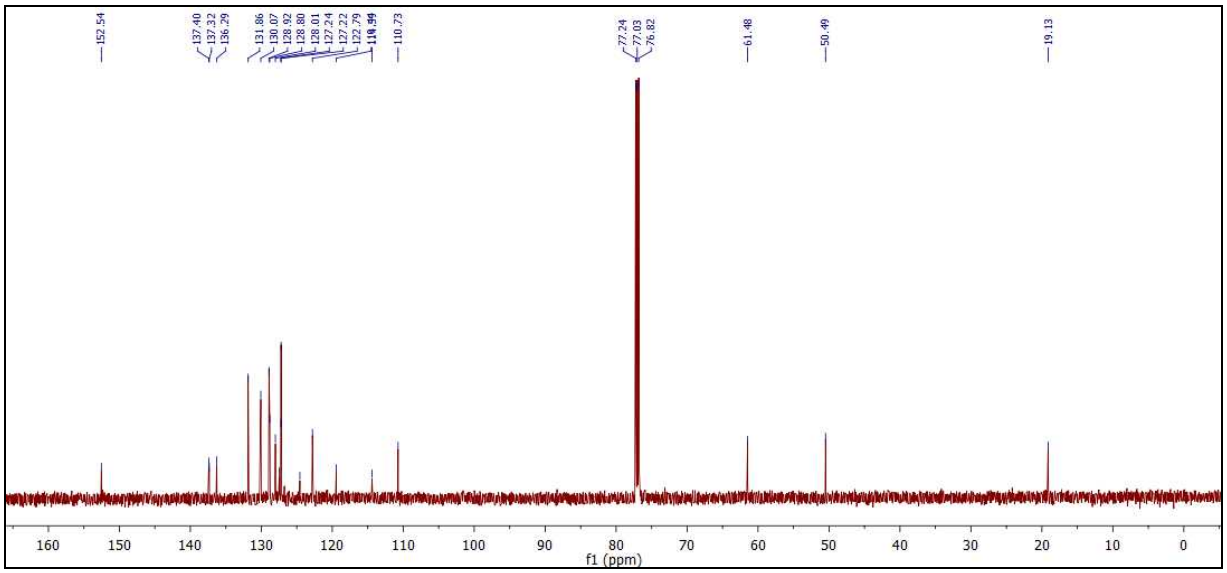
f1 (ppm)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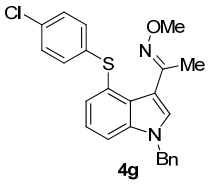
76.82
61.48
50.49
19.13
f1 (ppm)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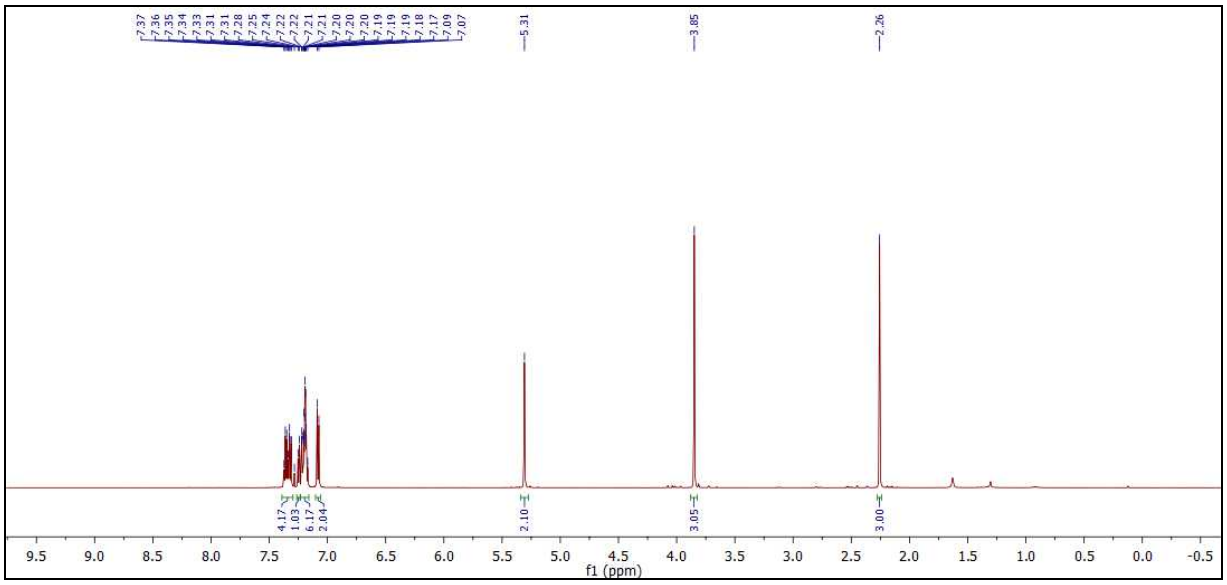
Me
N
Bn

4g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7.19
7.19
7.18
7.17
7.09
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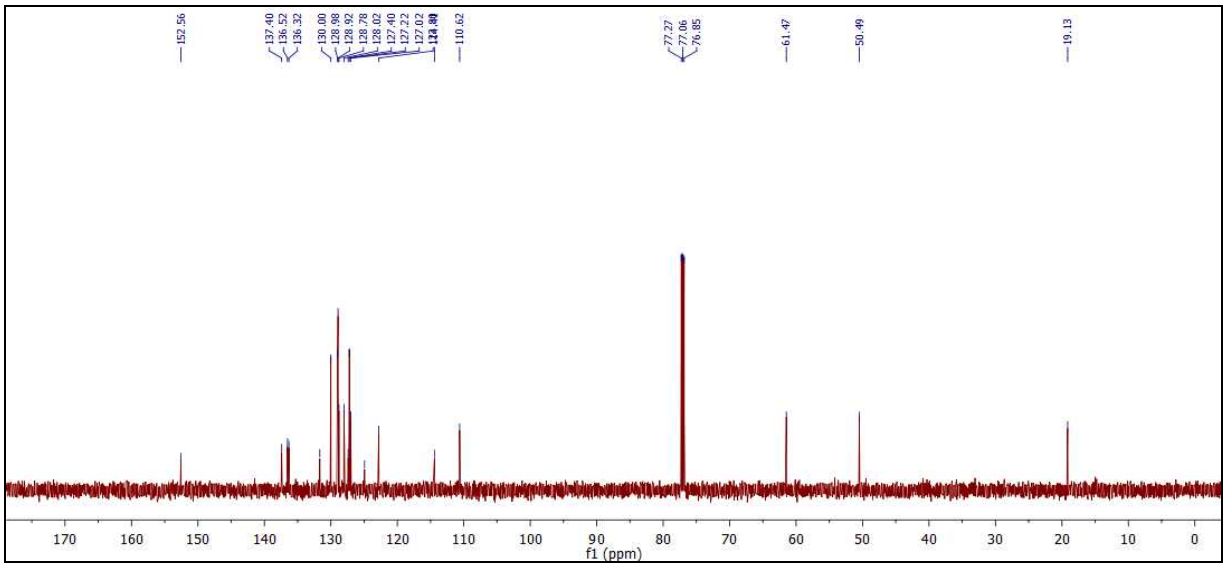
1.03
6.17
2.04
2.10
3.05
3.00
f1 (ppm)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61.47
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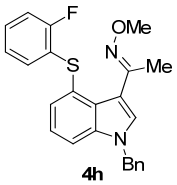
19.13
f1 (ppm)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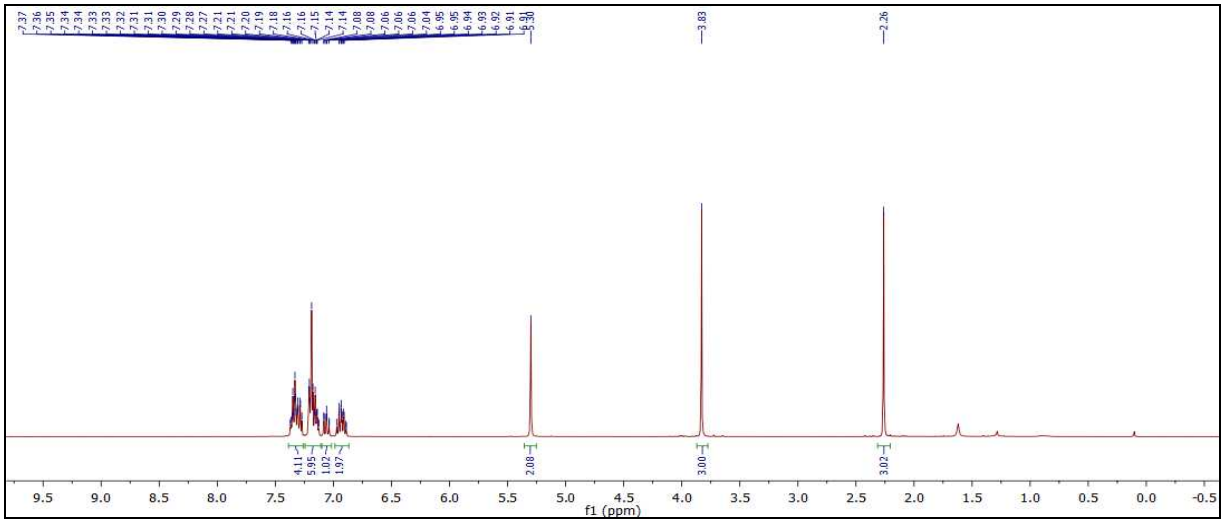
S
N
Bn

4h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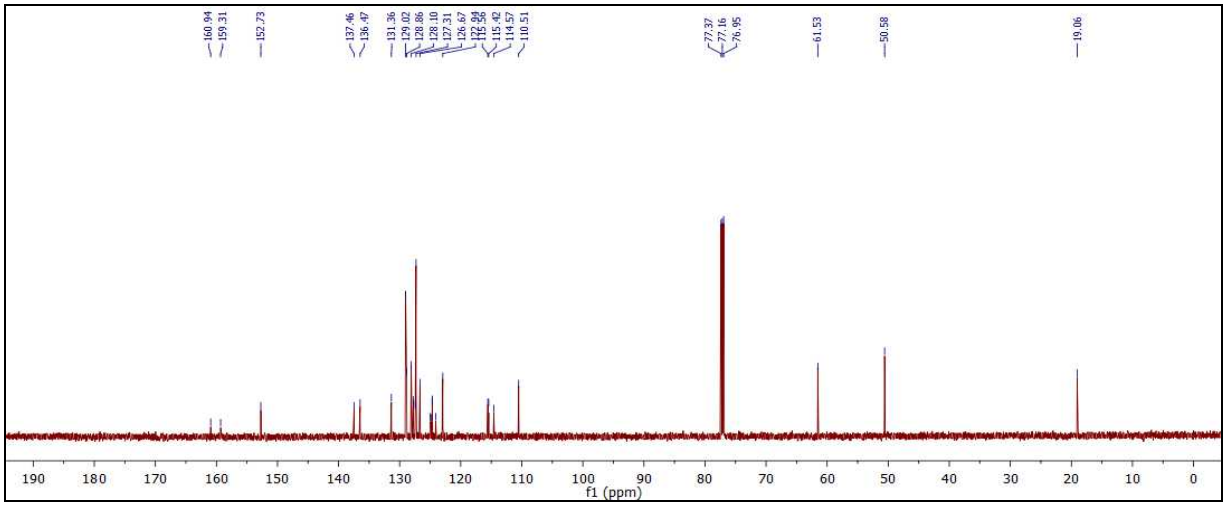
f1 (ppm)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114.57
110.51
77.37
77.16
76.95
61.53
50.58
19.06
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180
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110
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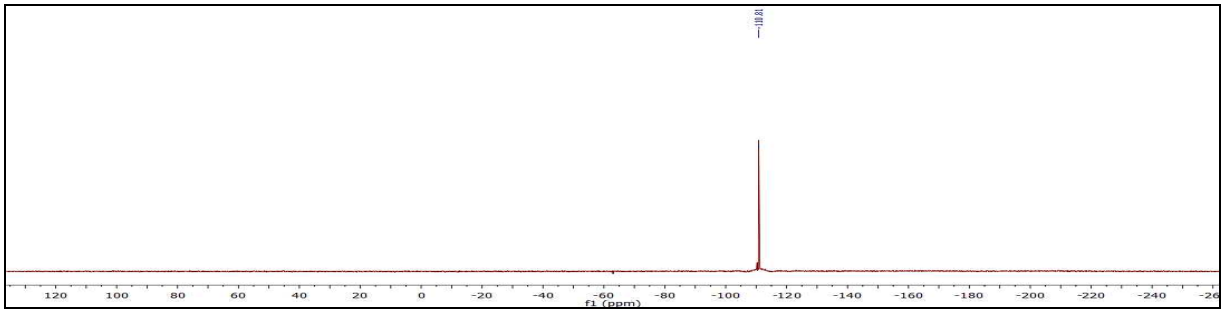
f1 (ppm)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-60
-80
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-120
-140
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-180
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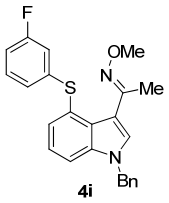
-240
f1 (ppm)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Me
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N
Bn

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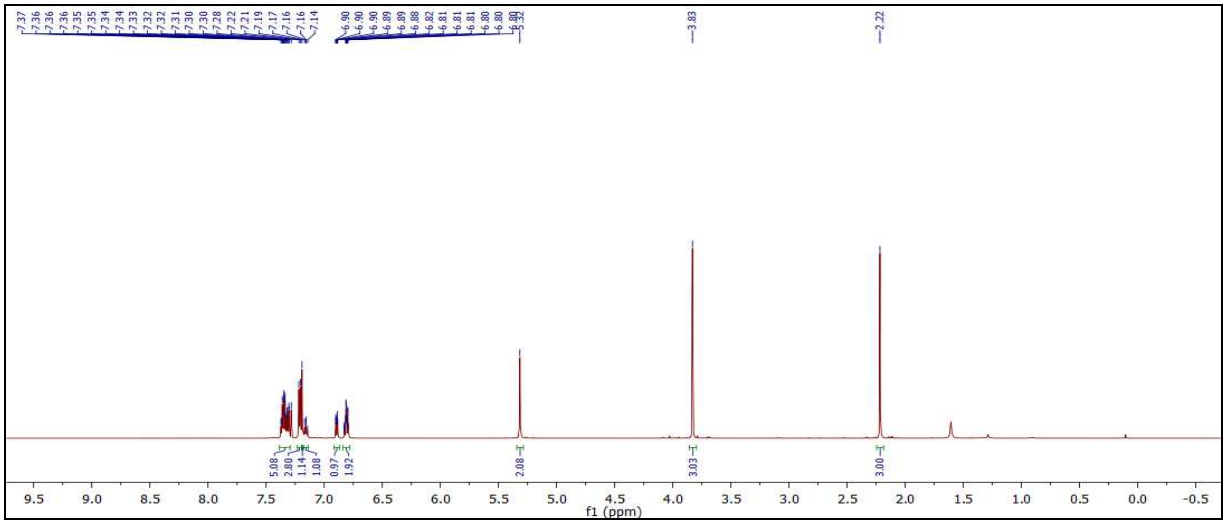
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6.81
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6.80
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5.08
2.80
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1.08
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0.5
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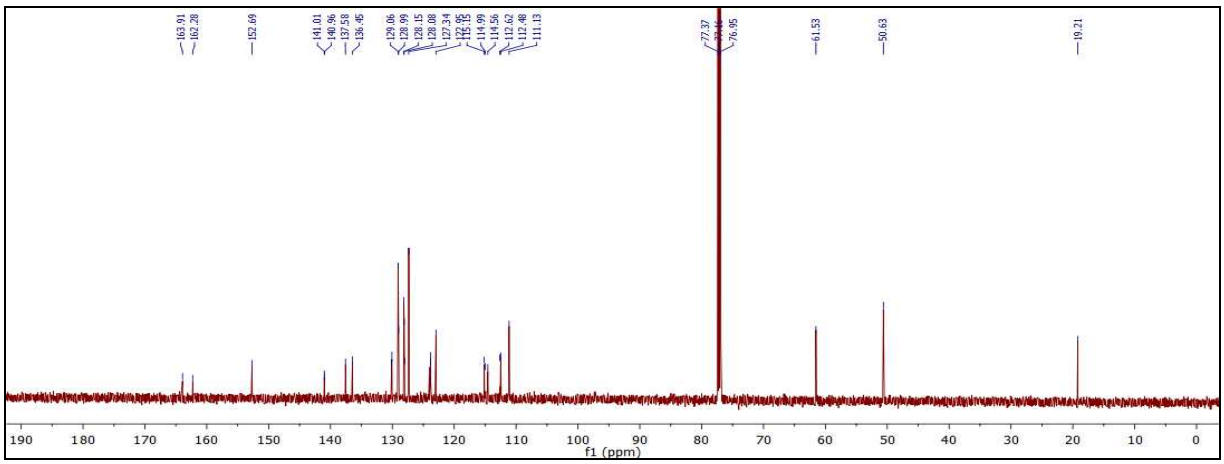
f1 (ppm)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114.99
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112.48
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70
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50
40
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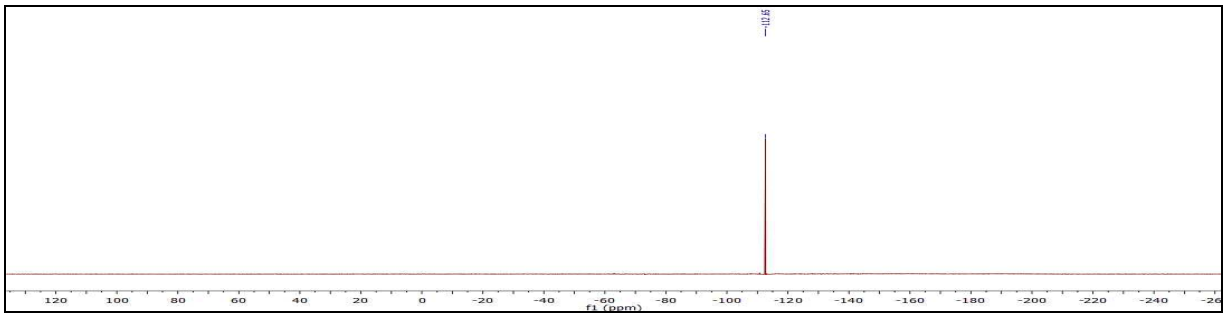
10
0
f1 (ppm)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-20
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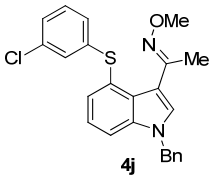
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
f1 (ppm)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Me
N
Bn

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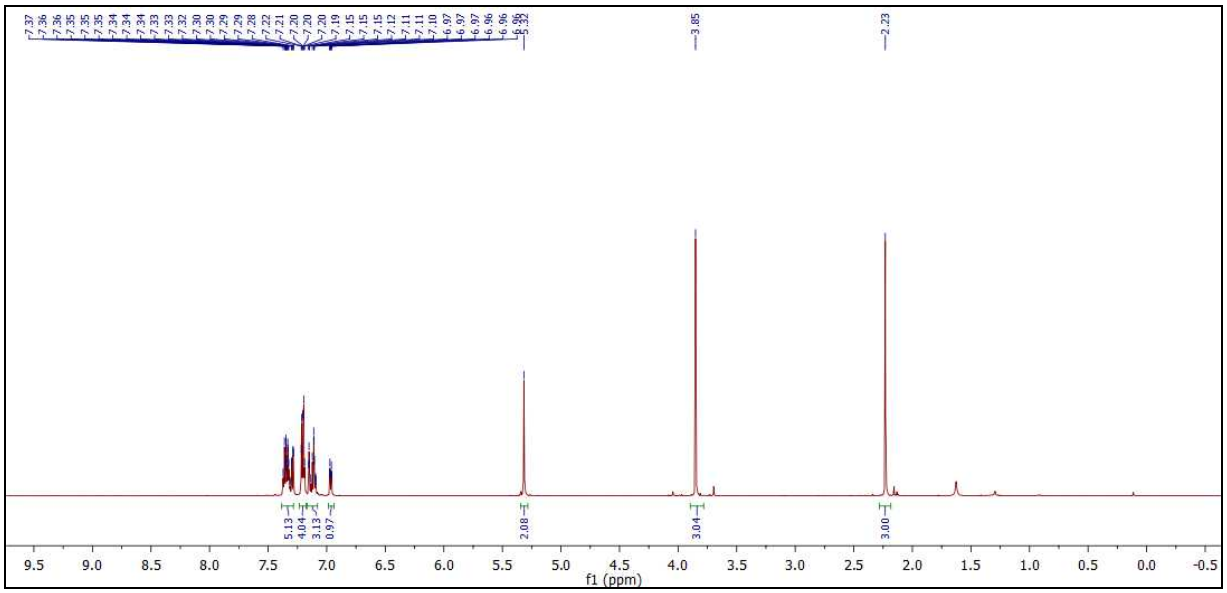
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6.96
5.32
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5.13
4.04
3.13
0.97
2.08
3.04
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
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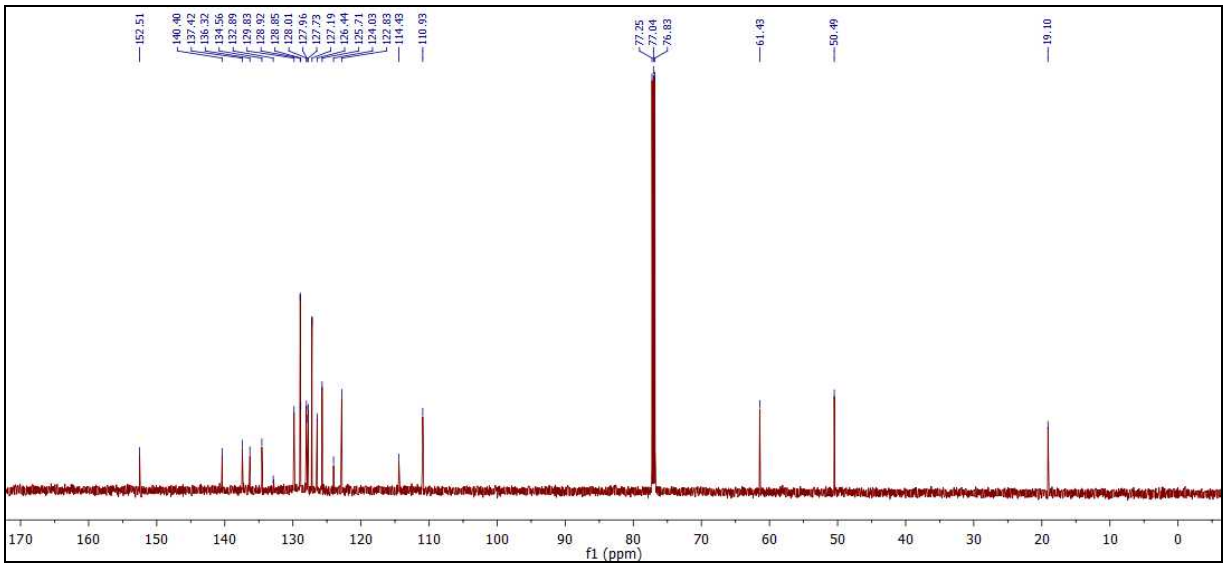
0.5
0.0
-0.5
f1 (ppm)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127.73
127.19
126.44
125.71
124.03
122.83
114.48
110.93
77.25
77.04
76.83
61.43
50.49
19.10
170
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150
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130
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110
100
90
80
70
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50
40
30
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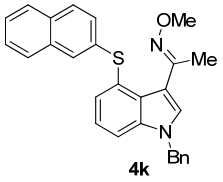
10
0
f1 (ppm)


OMe
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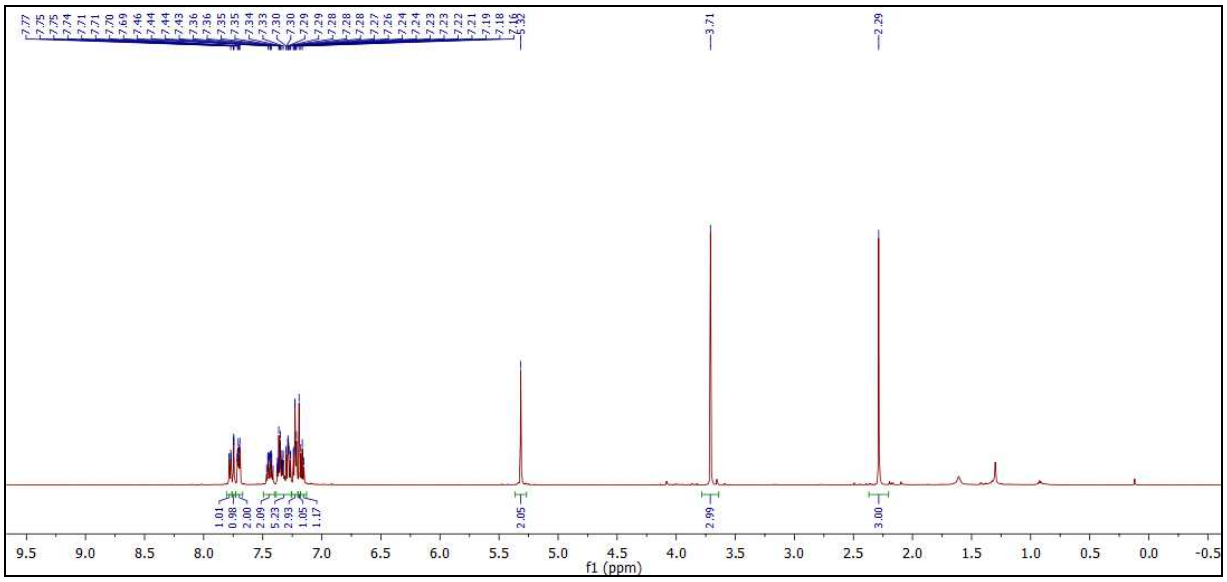
Me
S
N
Bn

4k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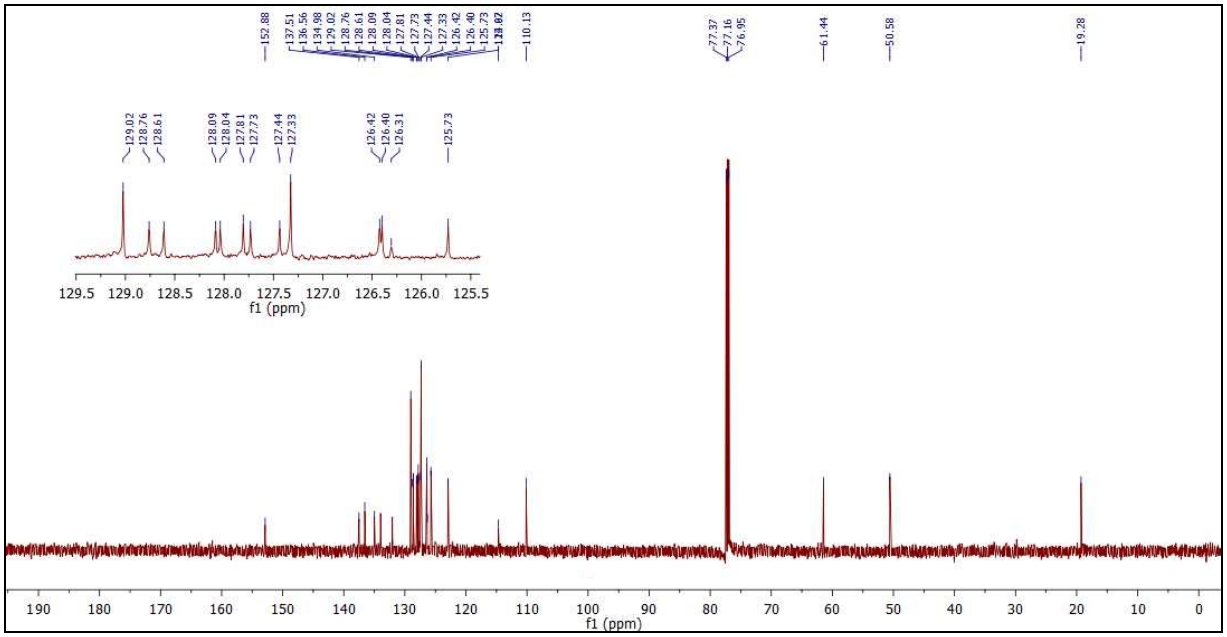
1.05
1.17
2.05
2.99
3.00
f1 (ppm)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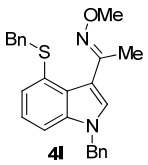
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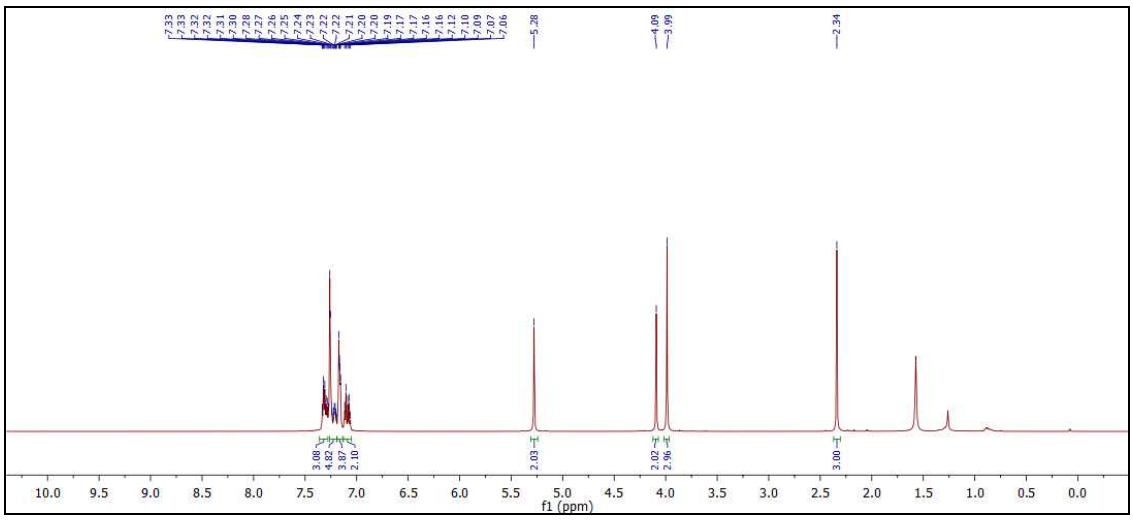
Bn
S
Me
N
Bn

4l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7.19
7.17
7.17
7.16
7.16
7.12
7.10
7.09
7.07
7.06
5.28
4.09
3.99
2.34
3.08
4.82
3.87
2.10
2.03
2.02
2.96
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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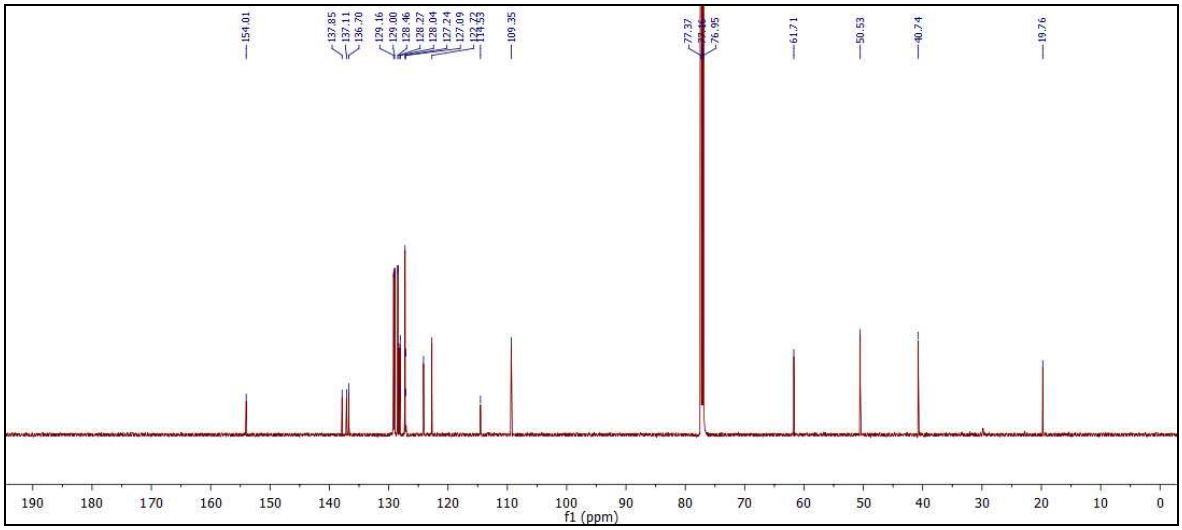
f1 (ppm)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127.24
127.09
123.22
114.53
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77.37
77.16
76.95
61.71
50.53
40.74
19.76
190
180
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90
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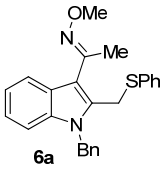
f1 (ppm)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SPh
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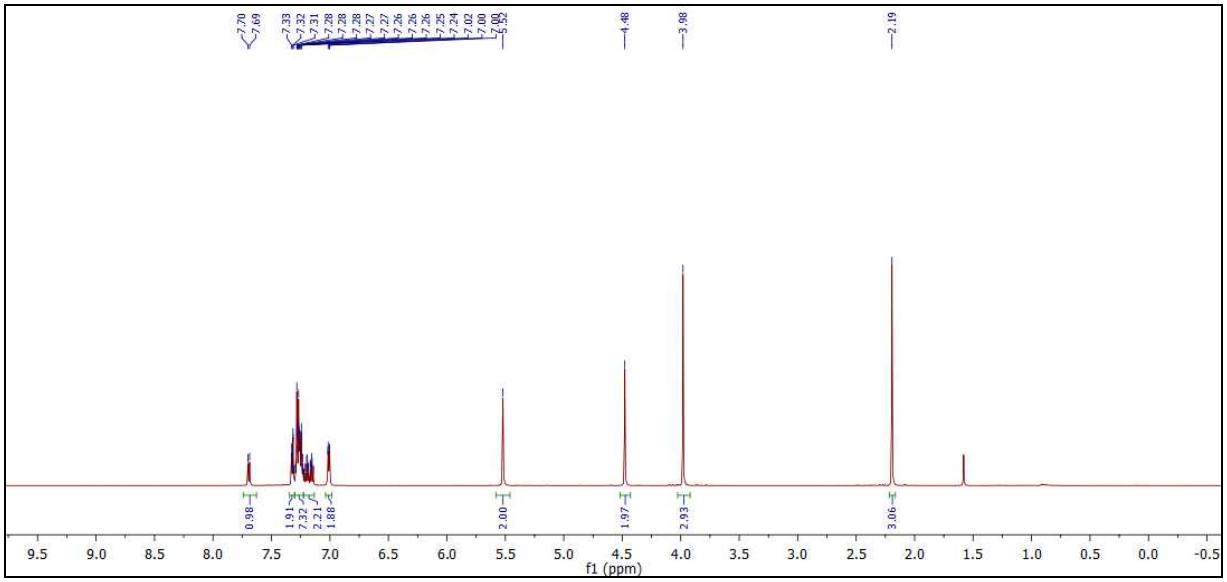
Bn

6a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7.26
7.26
7.26
7.25
7.24
7.02
7.00
5.52
4.48
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2.19
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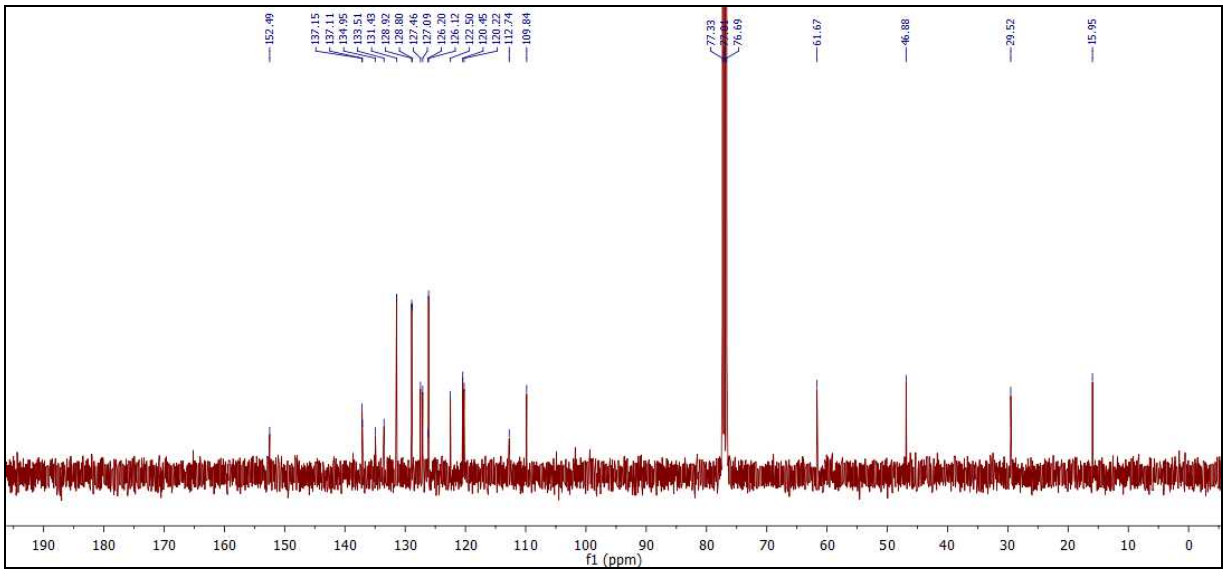
1.91
7.32
2.21
1.88
2.00
1.97
2.93
3.06
f1 (ppm)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131.43
128.92
128.80
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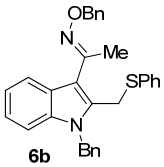
127.09
126.20
126.12
122.50
120.45
120.22
112.74
109.84
77.33
76.69
61.67
46.88
29.52
15.95
f1 (ppm)


OBn
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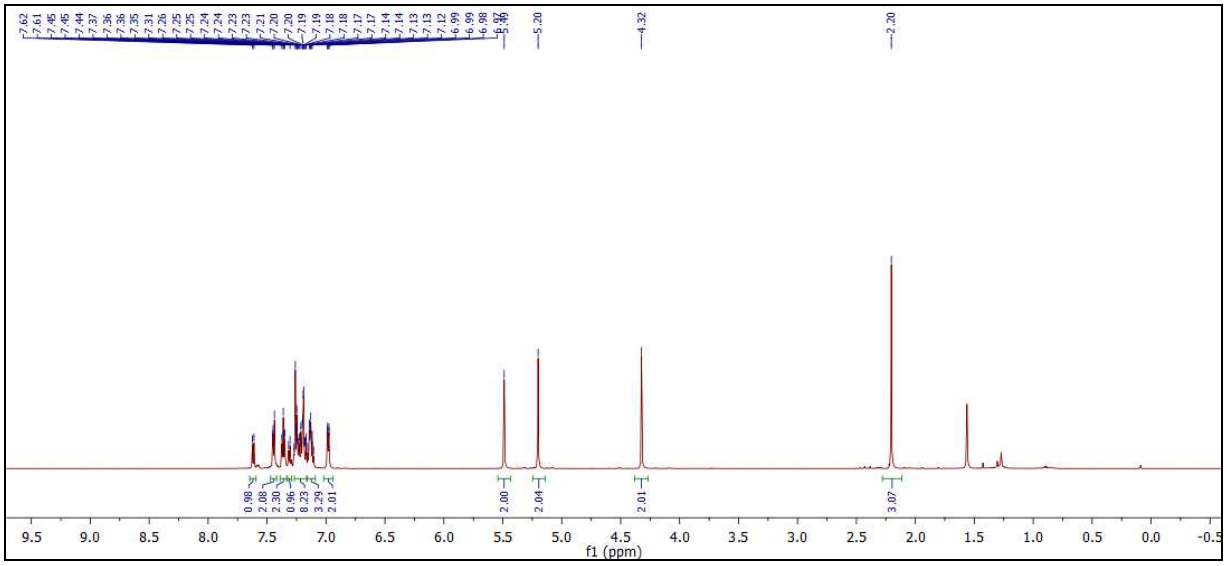
Me
SPh
N
Bn

6b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7.24
7.23
7.23
7.21
7.20
7.20
7.19
7.19
7.18
7.18
7.17
7.17
7.14
7.14
7.13
7.13
7.12
6.99
6.99
6.98
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5.20
4.32
2.20
0.98
2.08
2.30
0.96
8.23
3.29
2.01
2.00
2.04
2.01
3.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
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2.0
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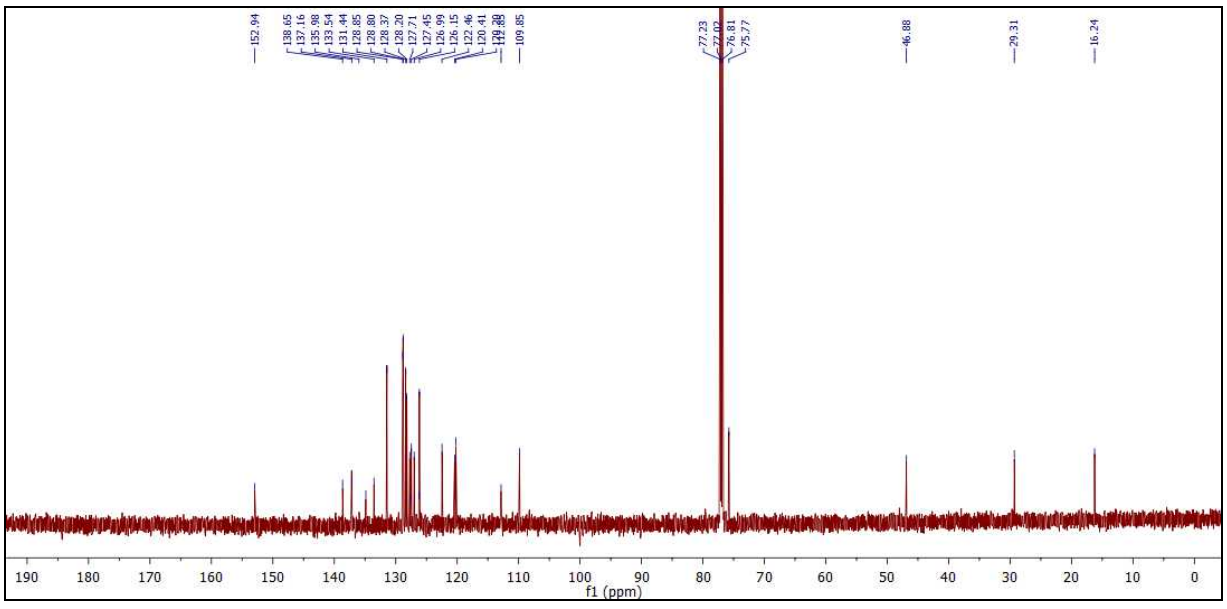
1.0
0.5
0.0
-0.5
f1 (ppm)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126.15
122.46
120.41
109.85
77.23
77.02
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75.77
46.88
29.31
16.24
190
180
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110
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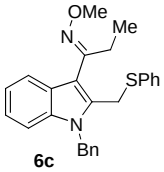
f1 (ppm)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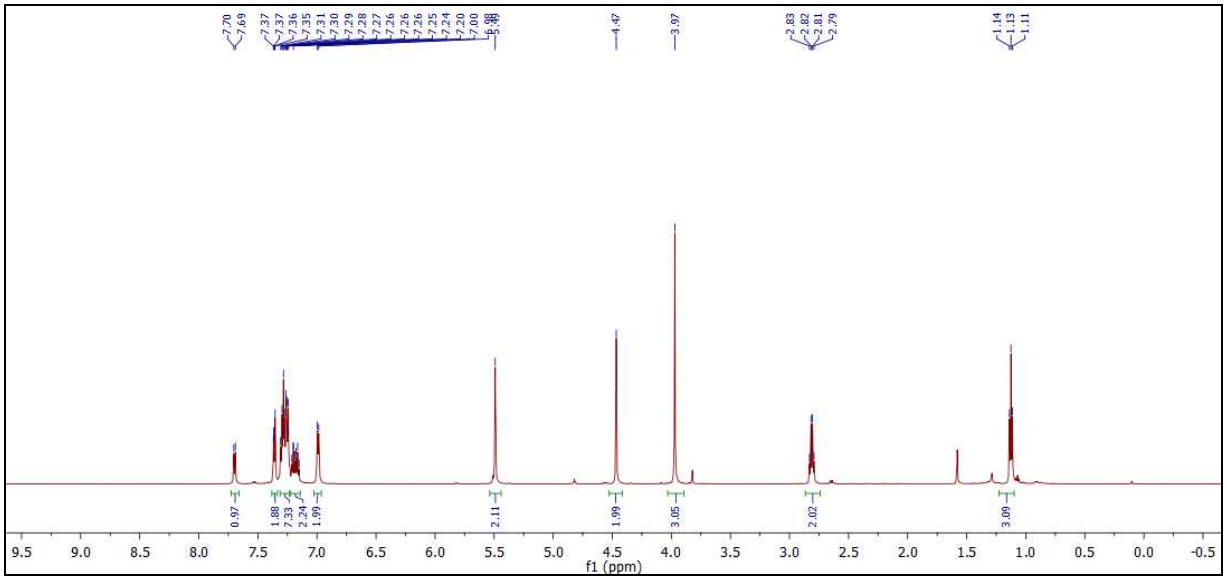
Me
SPh
N
Bn

6c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7.26
7.26
7.25
7.24
7.20
7.00
6.98
6.98
4.47
3.97
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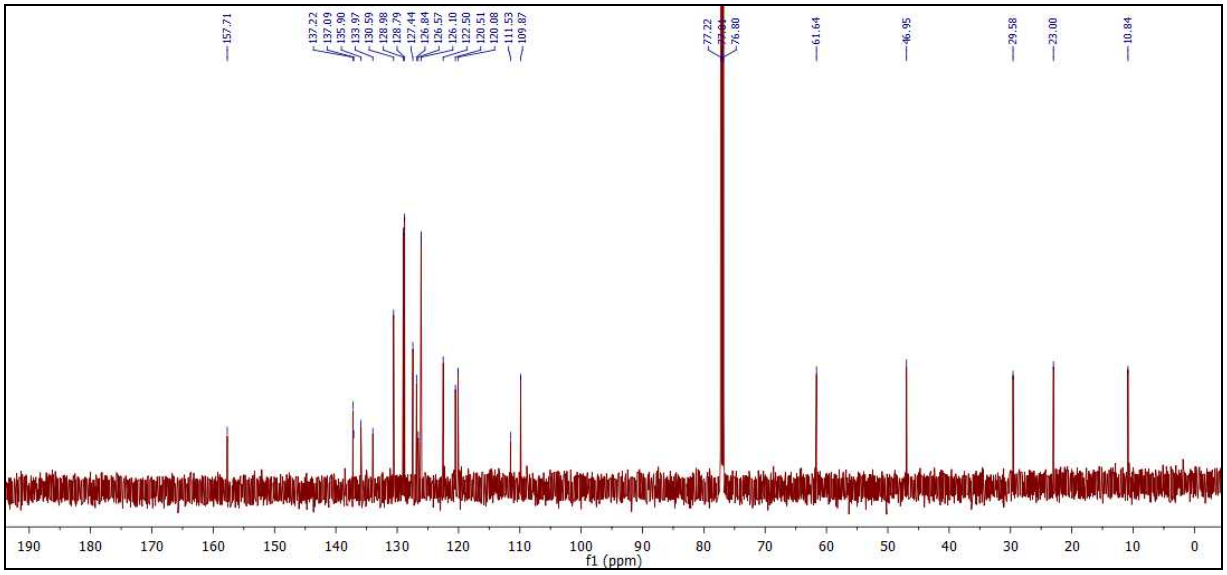
2.82
2.81
2.79
1.14
1.13
1.11
0.97
1.88
7.33
2.24
1.99
2.11
1.99
3.05
2.02
3.09
f1 (ppm)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122.50
120.51
120.08
111.53
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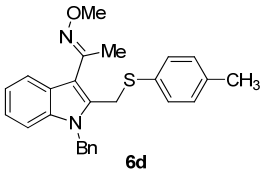
77.01
76.80
61.64
46.95
29.58
23.00
10.84
f1 (ppm)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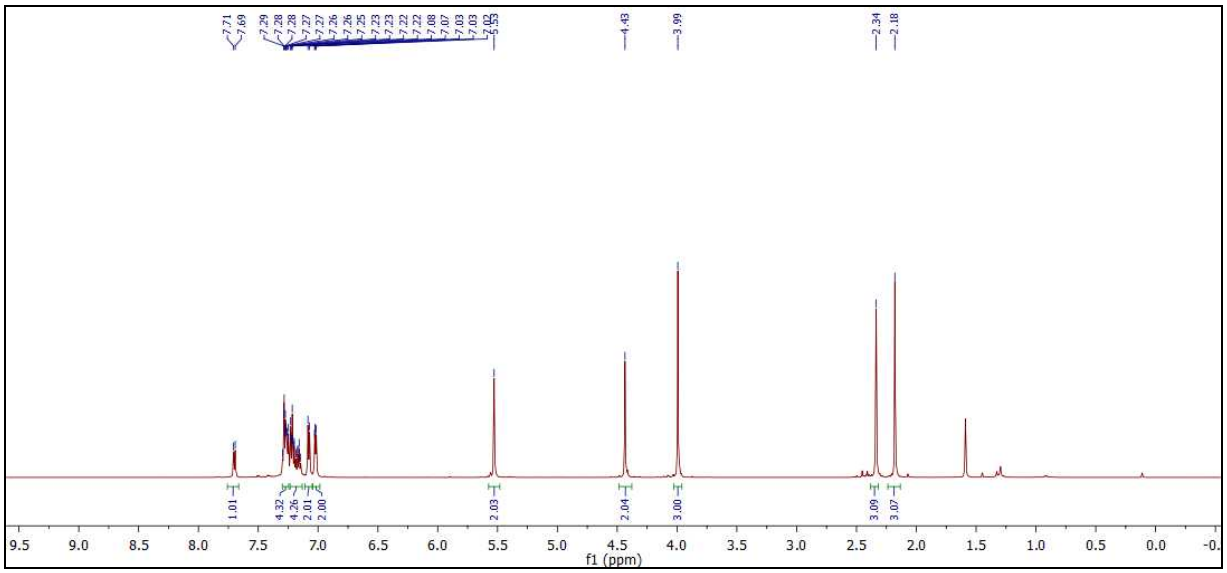
Me
S
CH3
N
Bn

6d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7.08
7.07
7.03
7.03
7.02
5.55
4.43
3.99
2.34
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1.01
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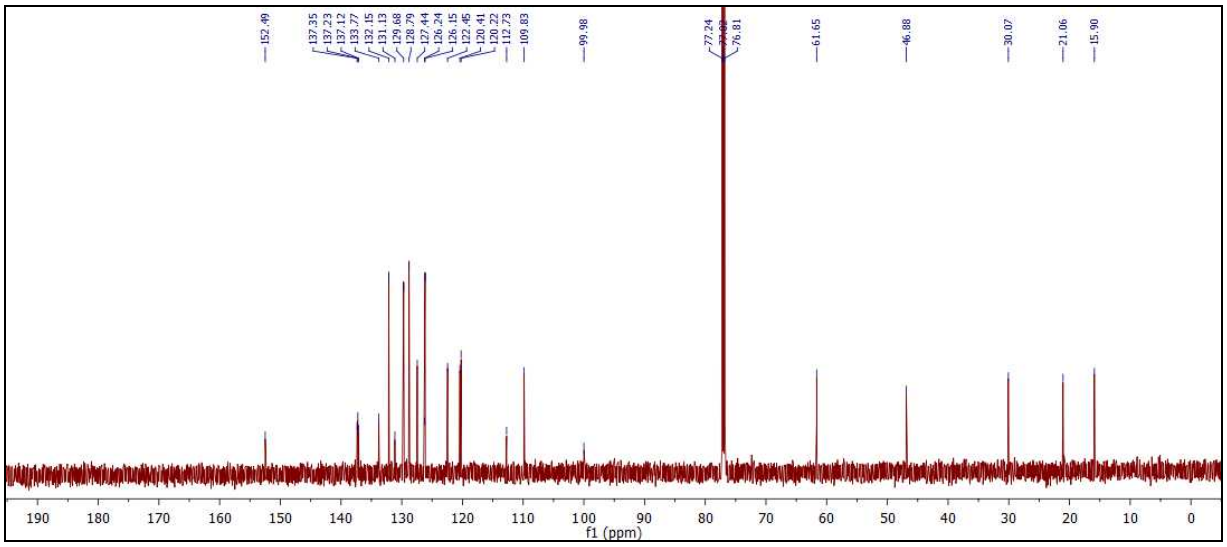
4.26
2.01
2.00
2.03
2.04
3.00
3.09
3.07
f1 (ppm)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122.45
120.41
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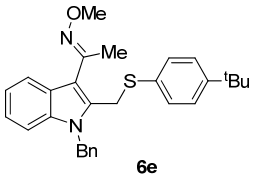
77.24
76.81
61.65
46.88
30.07
21.06
15.90
f1 (ppm)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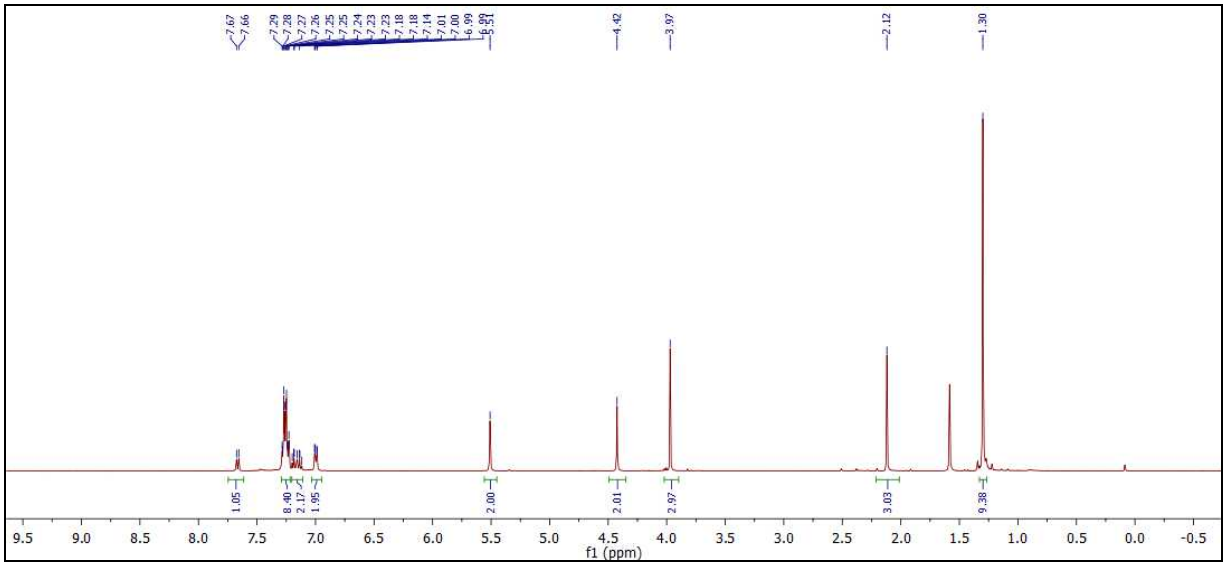
N
Me
S
tBu
N
Bn

6e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7.14
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7.00
6.99
5.51
4.42
3.97
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8.40
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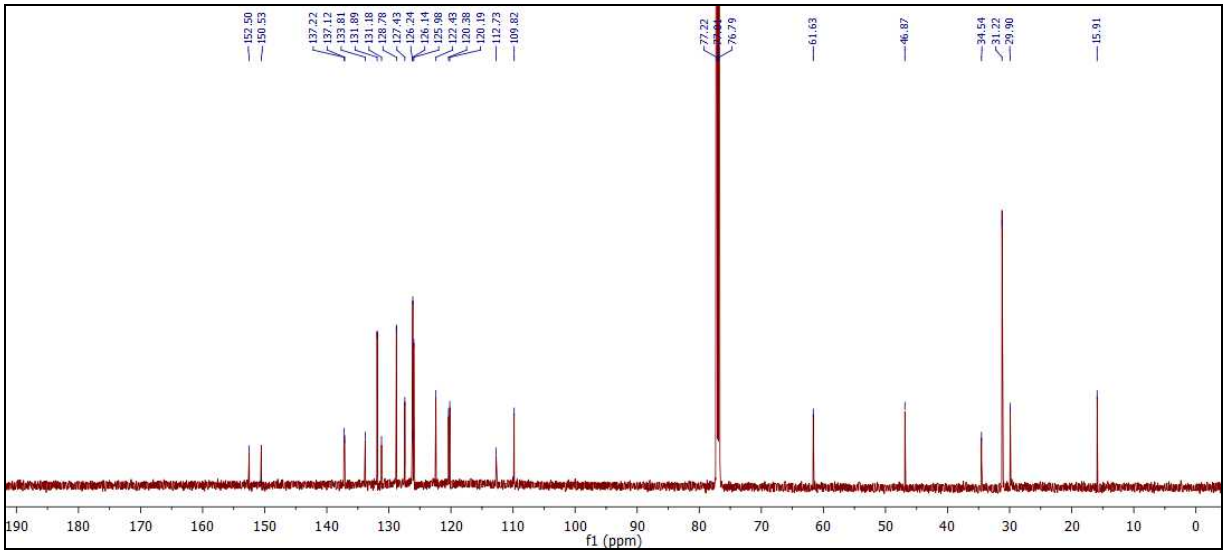
2.00
2.01
2.97
3.03
9.38
f1 (ppm)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126.14
125.98
122.43
120.38
120.19
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76.79
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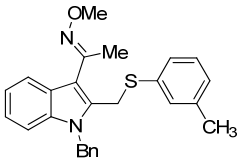
31.22
29.90
15.91
f1 (ppm)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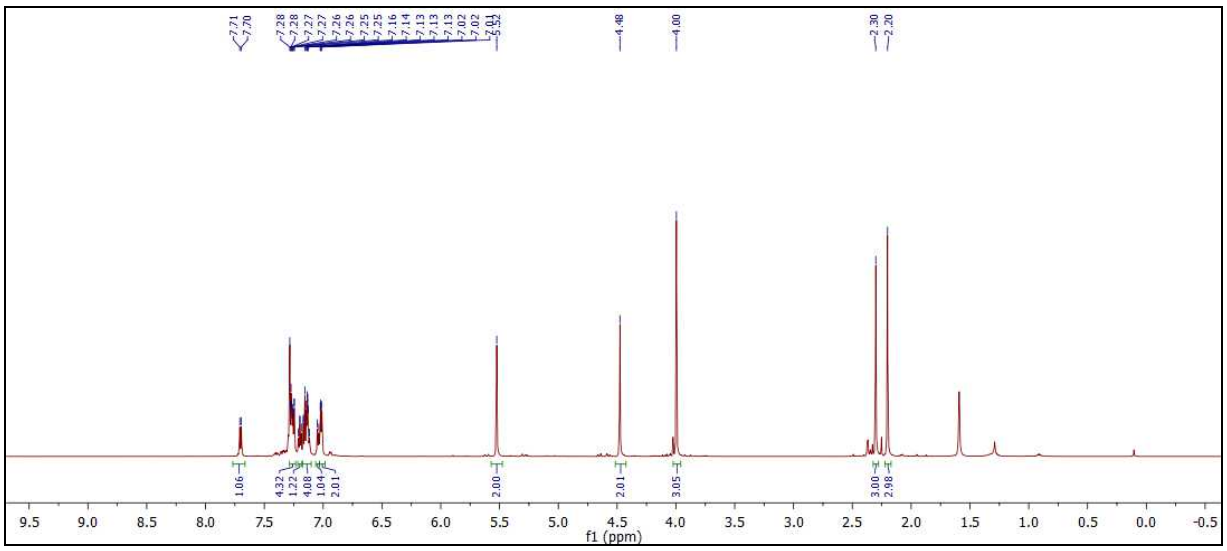
S
N
Bn
CH3

6f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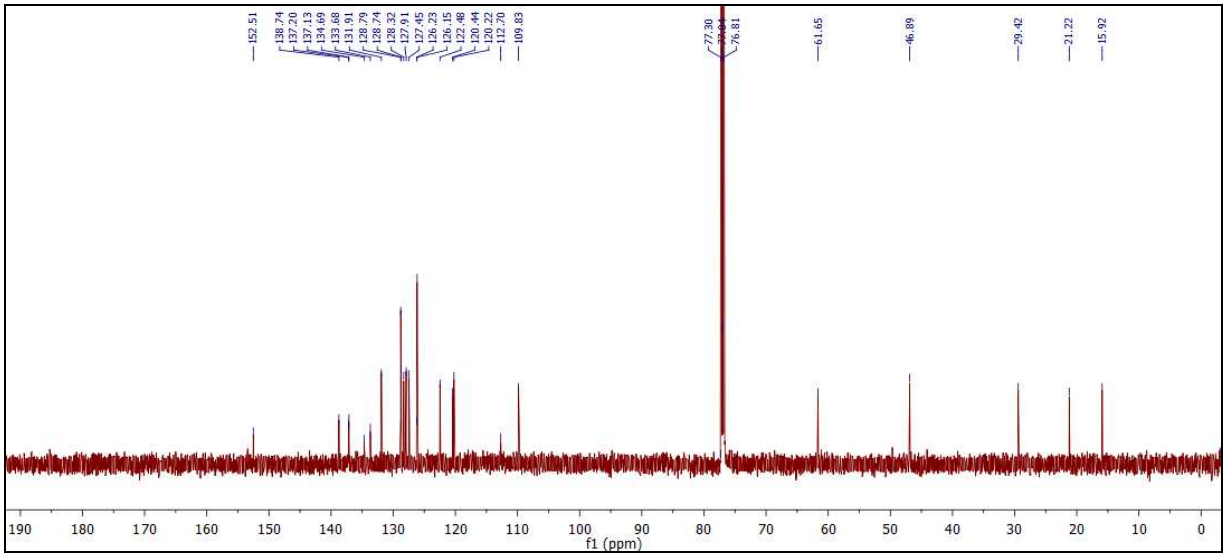
7.14
7.13
7.13
7.02
7.01
5.51
4.48
4.00
2.30
2.20
1.06
4.32
1.22
4.08
1.04
2.01
2.00
2.01
3.05
3.00
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.32
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126.15
122.48
120.44
120.22
112.70
109.83
77.30
77.04
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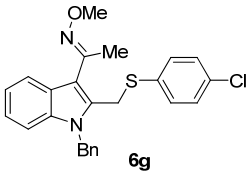
46.89
29.42
21.22
15.92
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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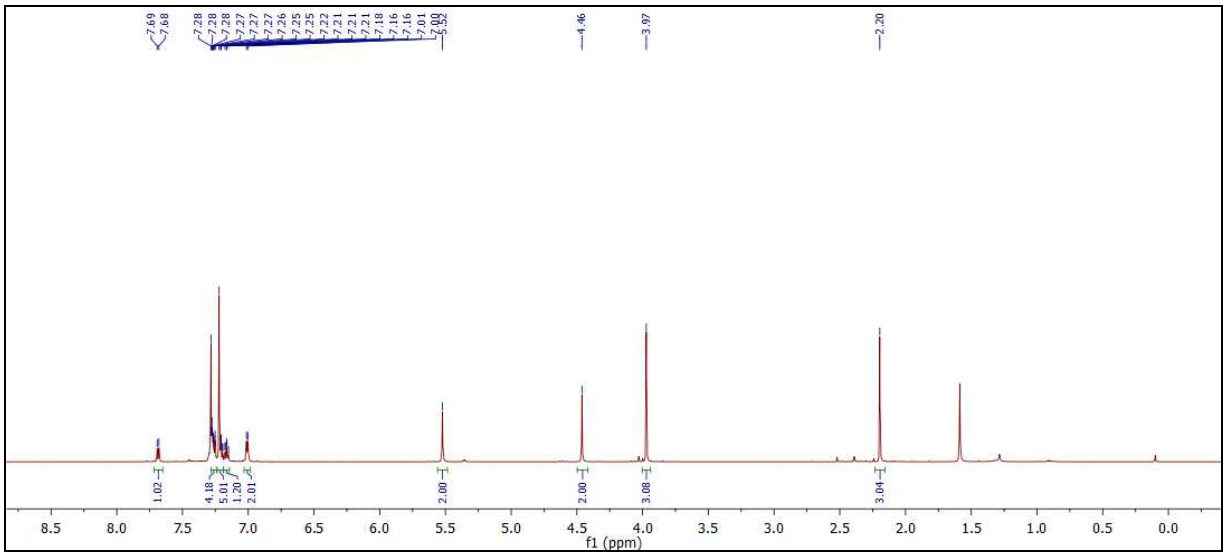
Me
S
Cl
N
Bn

6g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7.25
7.25
7.22
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7.21
7.21
7.18
7.16
7.16
7.01
5.02
4.46
3.97
2.20
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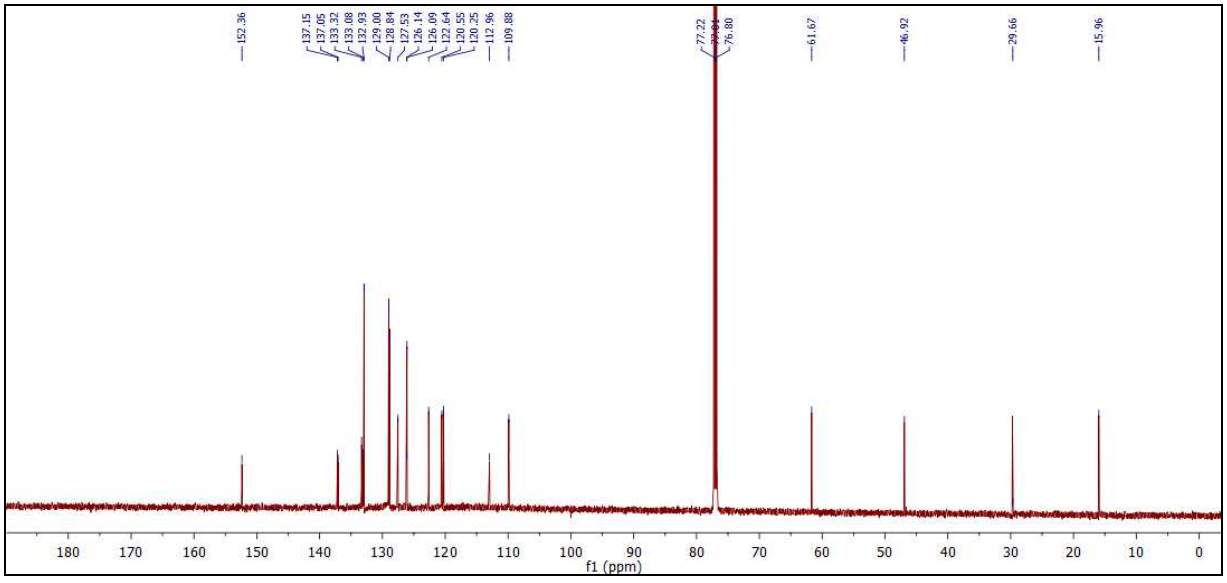
4.18
5.01
1.20
2.01
2.00
2.00
3.08
3.04
f1 (ppm)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126.14
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122.64
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109.88
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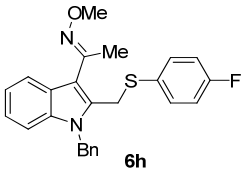
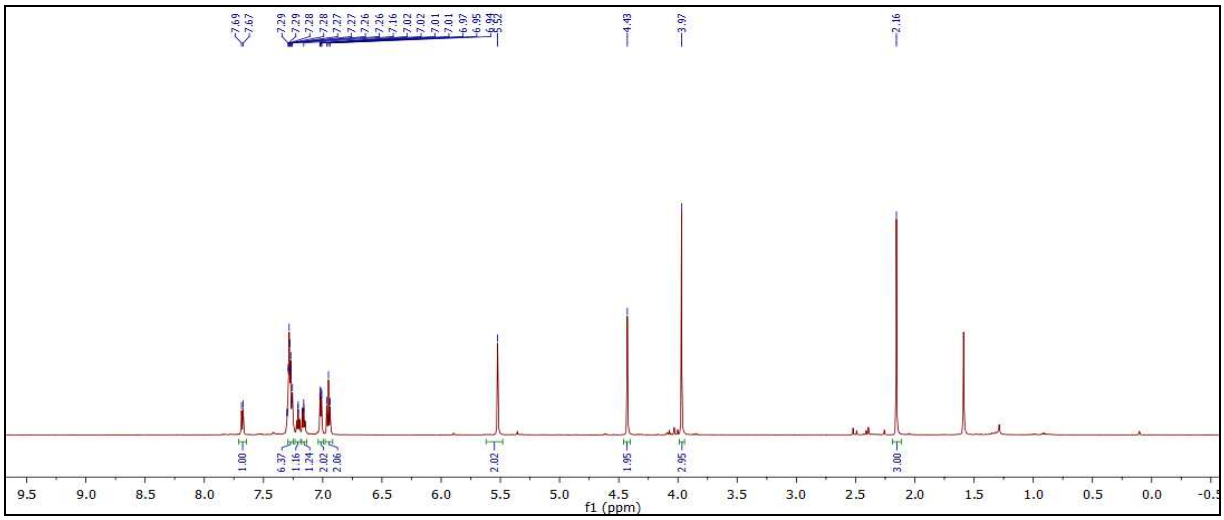
77.01
76.80
61.67
46.92
29.66
15.96
f1 (ppm)


OMe
N
Me
S
F
N
Bn

6h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7.02
7.02
7.01
7.01
6.97
6.95
5.52
5.52
4.43
3.97
2.16
1.00
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1.16
1.24
2.02
2.06
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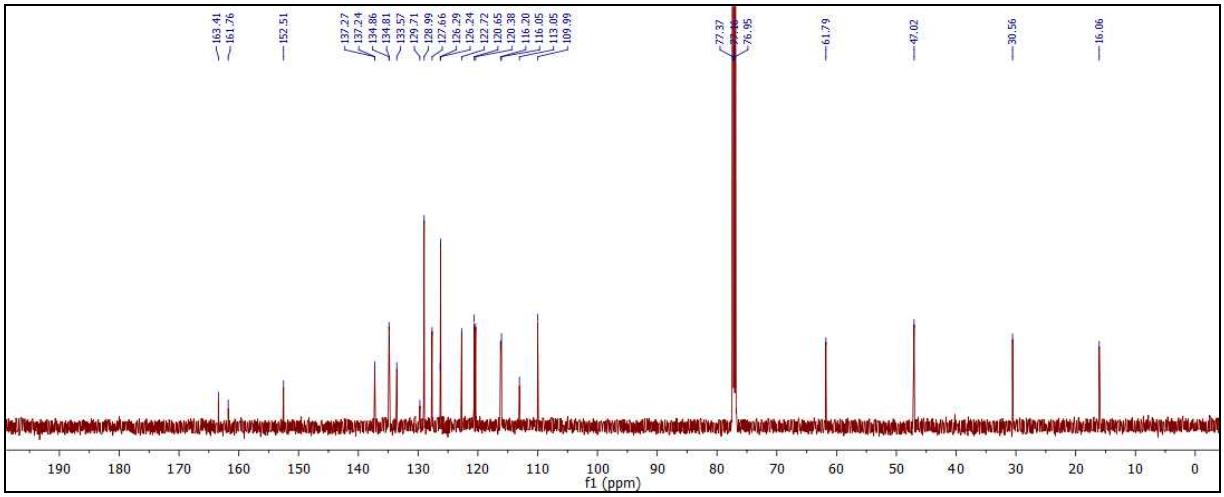
1.95
2.95
3.00
f1 (ppm)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126.24
122.72
120.65
120.38
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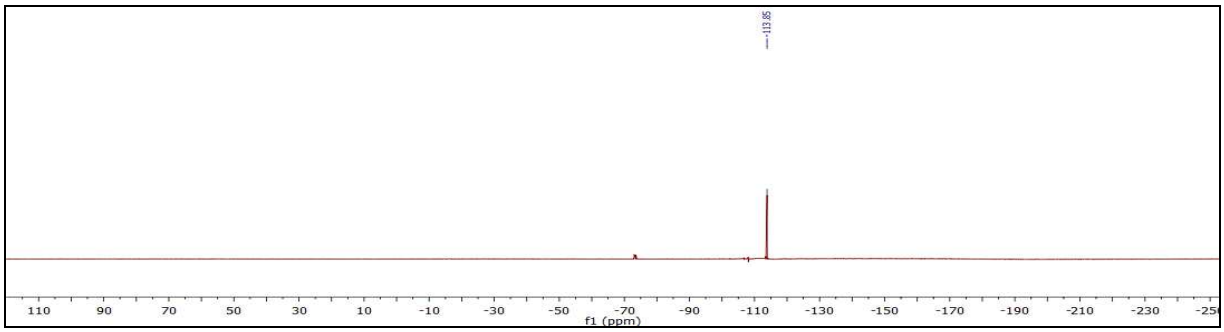
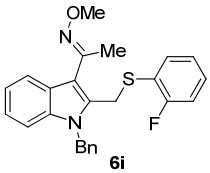
109.99
77.37
77.16
76.95
61.79
47.02
30.56
16.06
f1 (ppm)


-113.85
f1 (ppm)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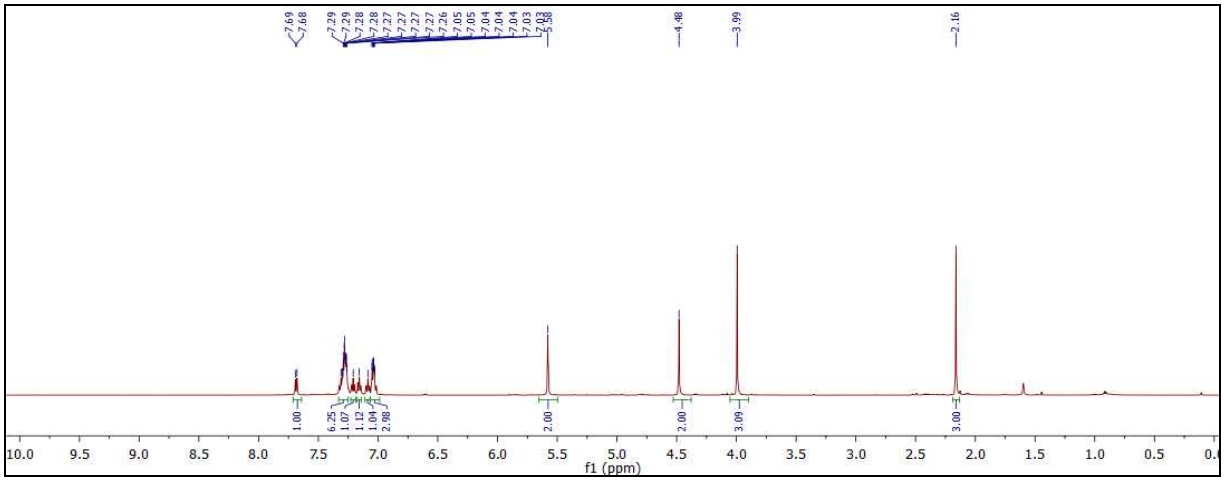
N
Me
S
F
N
Bn

6i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7.04
7.04
7.03
7.03
5.58
4.48
3.99
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1.00
6.25
1.07
1.12
1.04
2.98
2.00
2.00
3.09
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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4.0
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3.0
2.5
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1.5
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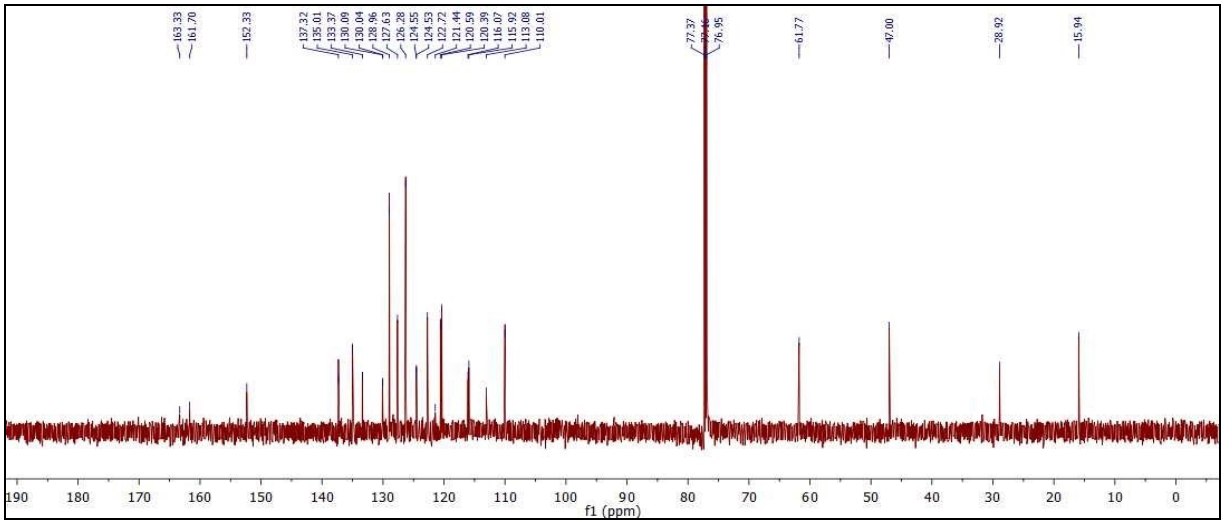
0.5
f1 (ppm)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124.53
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120.59
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116.07
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113.08
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76.95
61.77
47.00
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15.94
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160
150
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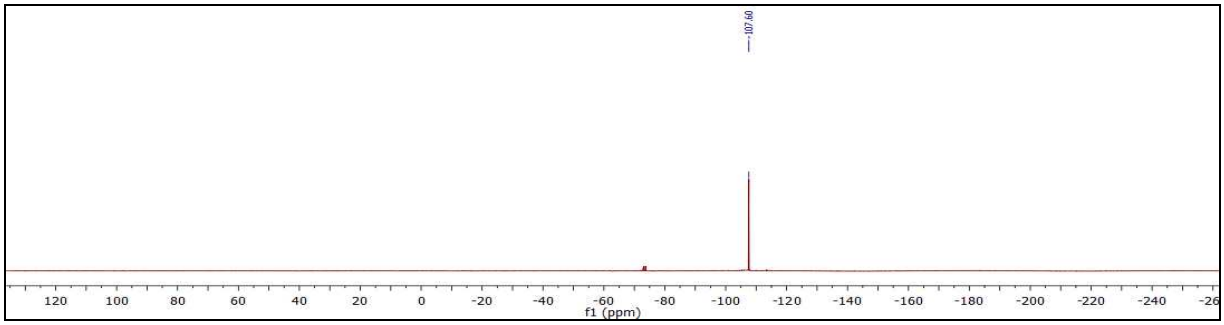
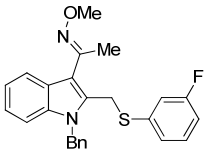
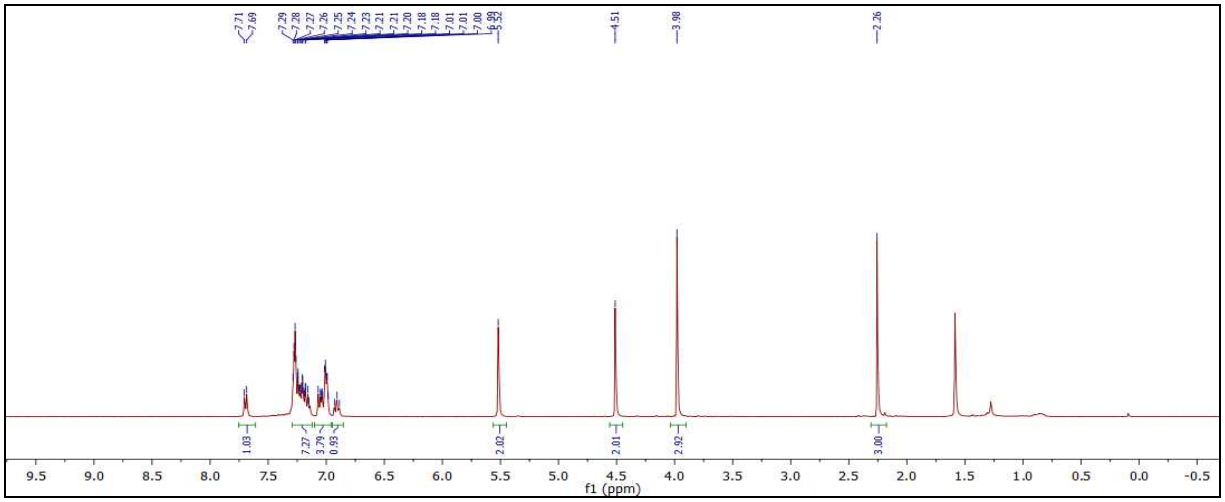
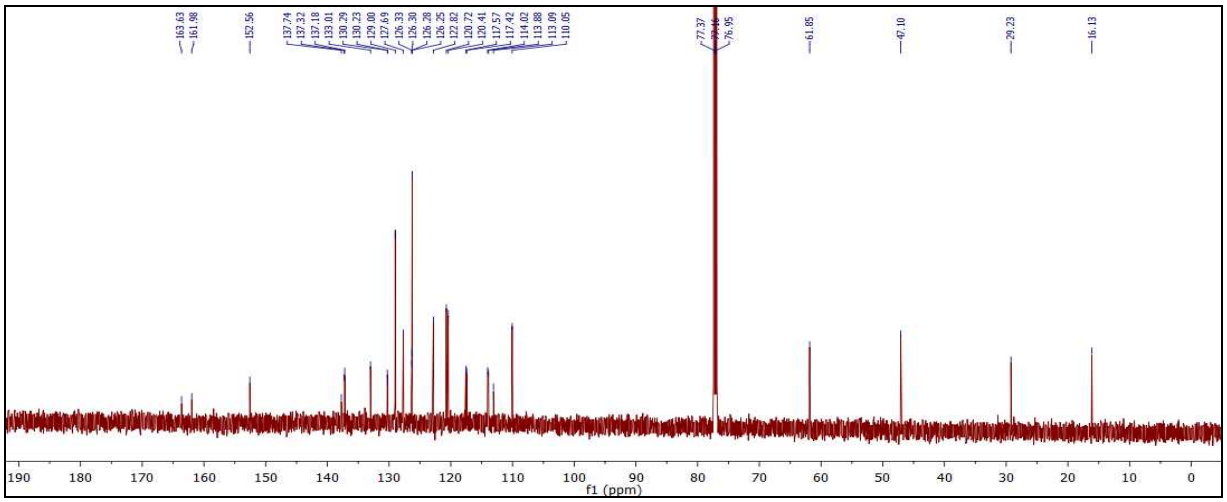
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

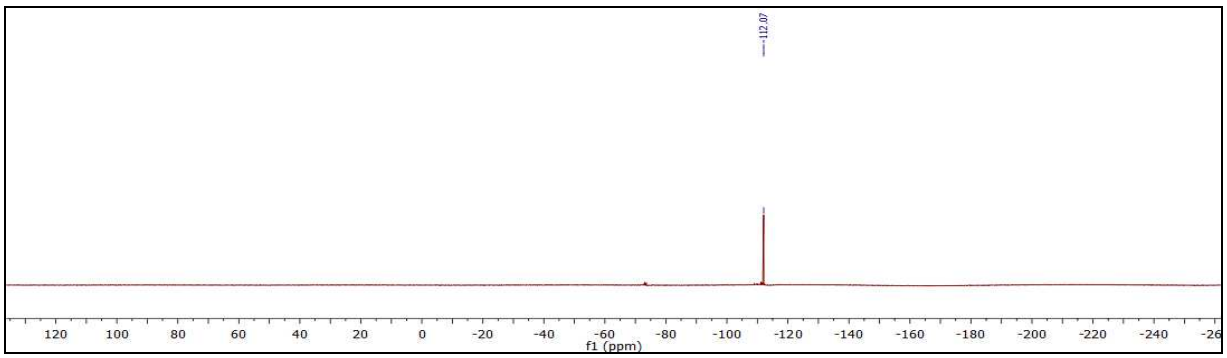

107.60
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
f1 (ppm)

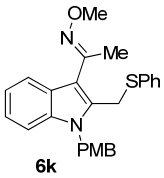

OMe
N
Me
F
S
N
Bn

6j

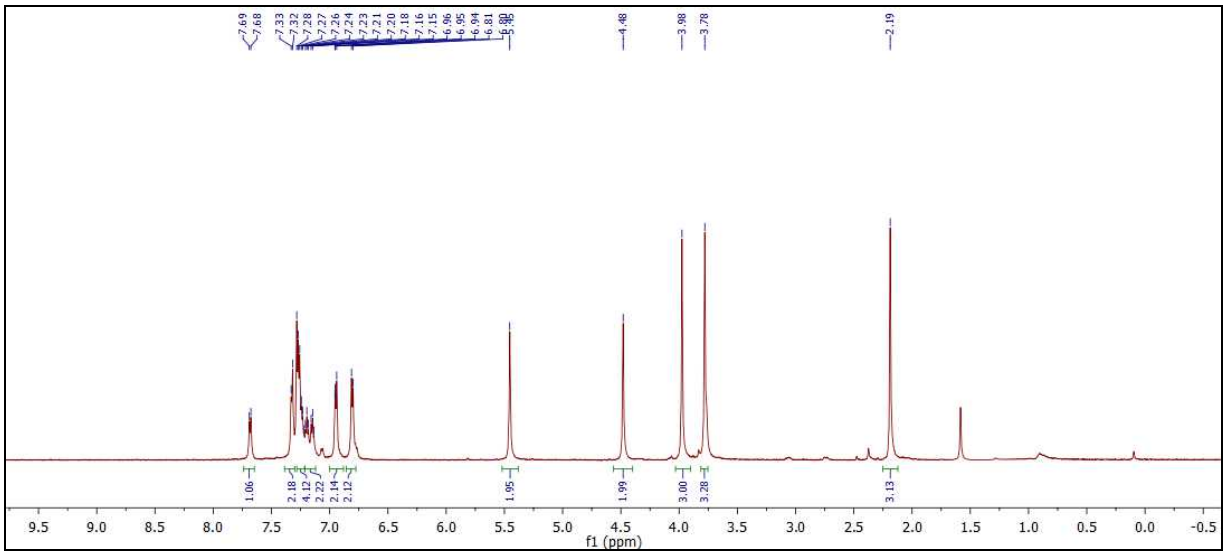

7.71
7.69
7.29
7.28
7.27
7.26
7.25
7.24
7.23
7.21
7.21
7.20
7.18
7.18
7.01
7.01
7.00
6.99
6.98
4.51
3.98
2.26
1.03
7.27
3.79
0.93
2.02
2.01
2.92
3.00
f1 (ppm)


163.63
161.98
152.56
137.74
137.32
137.18
133.01
130.29
130.23
129.00
127.69
126.33
126.30
126.28
126.25
122.82
120.72
120.41
117.57
117.42
114.02
113.88
113.09
110.05
77.37
77.16
76.95
61.85
47.10
29.23
16.13
f1 (ppm)


112.07
f1 (ppm)


OMe
N
Me
SPh
N
PMB

6k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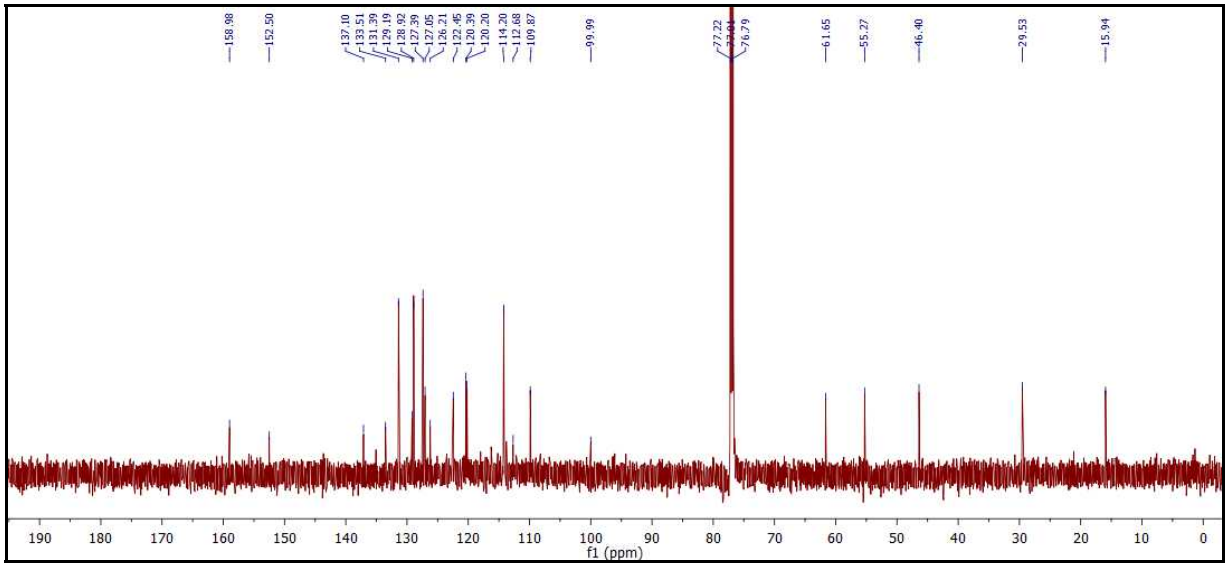
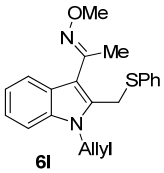
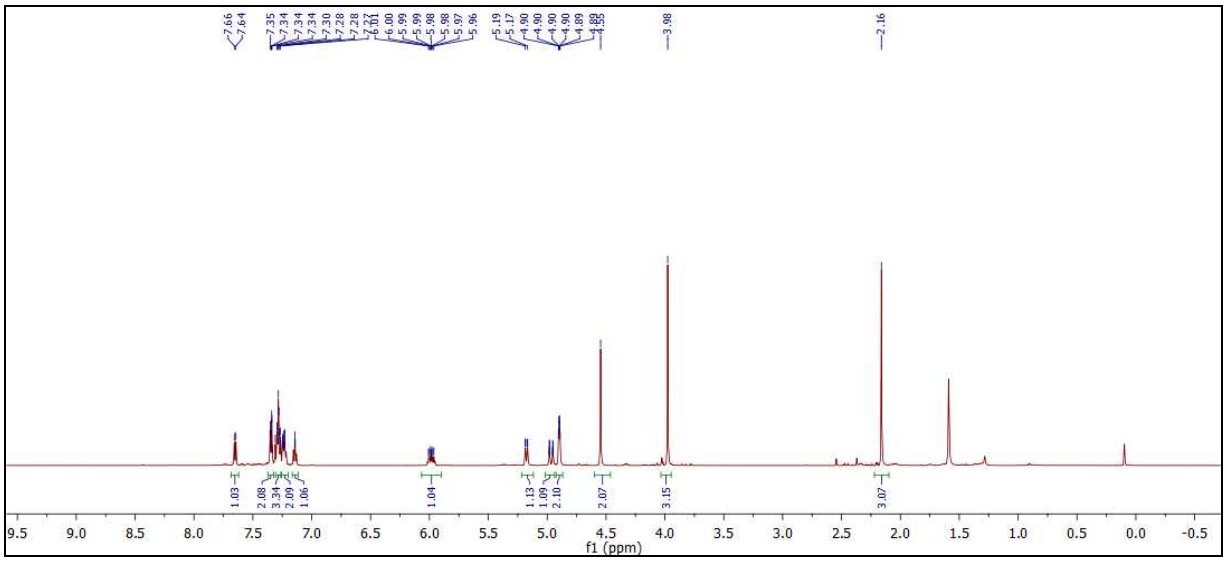
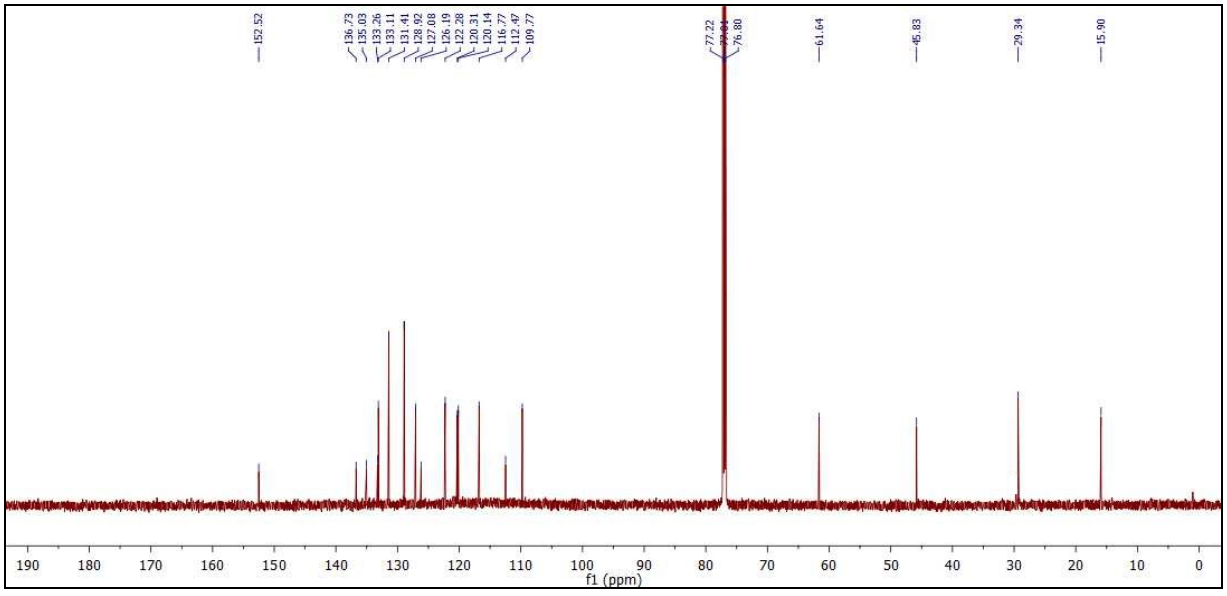
7.68
7.33
7.32
7.28
7.27
7.26
7.24
7.23
7.21
7.20
7.18
7.16
7.15
6.96
6.95
6.94
6.81
6.80
5.48
4.48
3.98
3.78
2.19
1.06
2.18
4.12
2.22
2.14
2.12
1.95
1.99
3.00
3.28
3.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

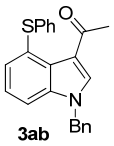

158.98
152.50
137.10
133.51
131.39
129.19
128.92
127.39
127.05
126.21
122.45
120.39
120.20
114.20
112.68
109.87
99.99
77.22
77.01
76.79
61.65
55.27
46.40
29.53
15.94
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OMe
N
Me
SPh
N
Allyl

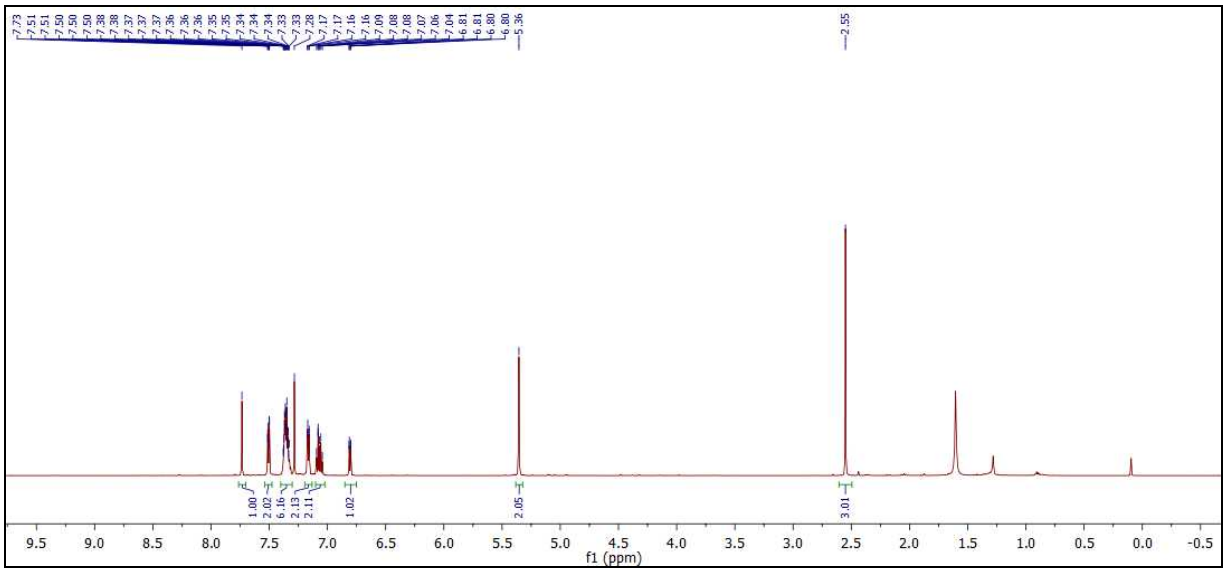
6l

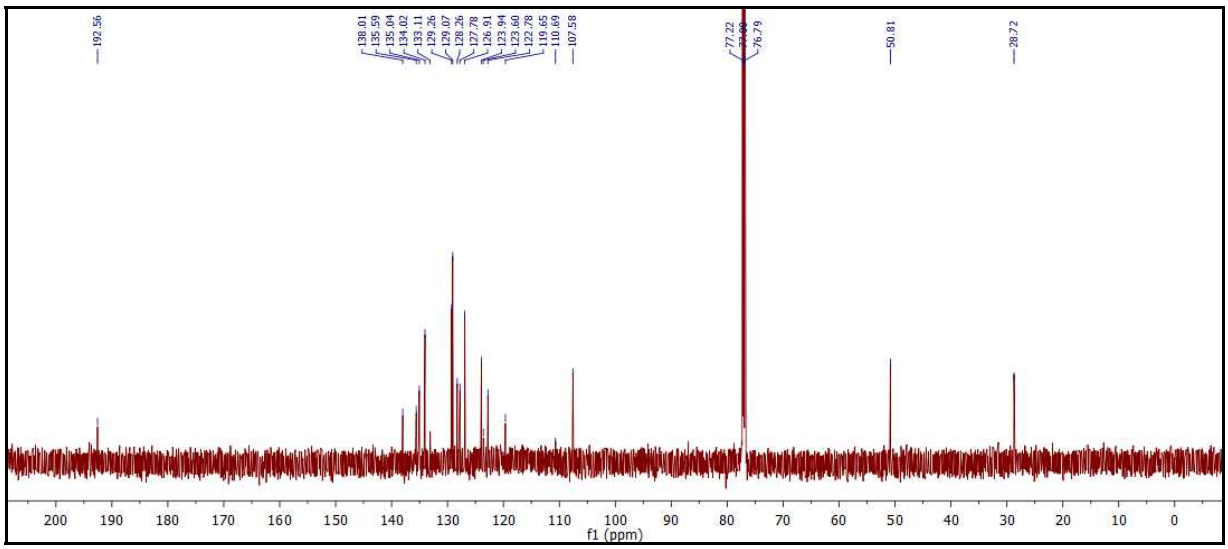

7.66
7.64
7.35
7.34
7.34
7.34
7.30
7.28
7.28
6.00
5.99
5.99
5.98
5.98
5.97
5.96
5.19
5.17
4.90
4.90
4.90
4.90
4.89
3.98
2.16
1.03
2.08
3.34
2.09
1.06
1.04
1.13
1.09
2.10
2.07
3.15
3.07
f1 (ppm)

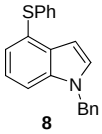

152.52
136.73
135.03
133.26
133.11
131.41
128.92
127.08
126.19
122.28
120.31
120.14
116.77
112.47
109.77
77.22
76.80
61.64
46.83
29.34
15.90
f1 (ppm)


SPh
O
N
Bn

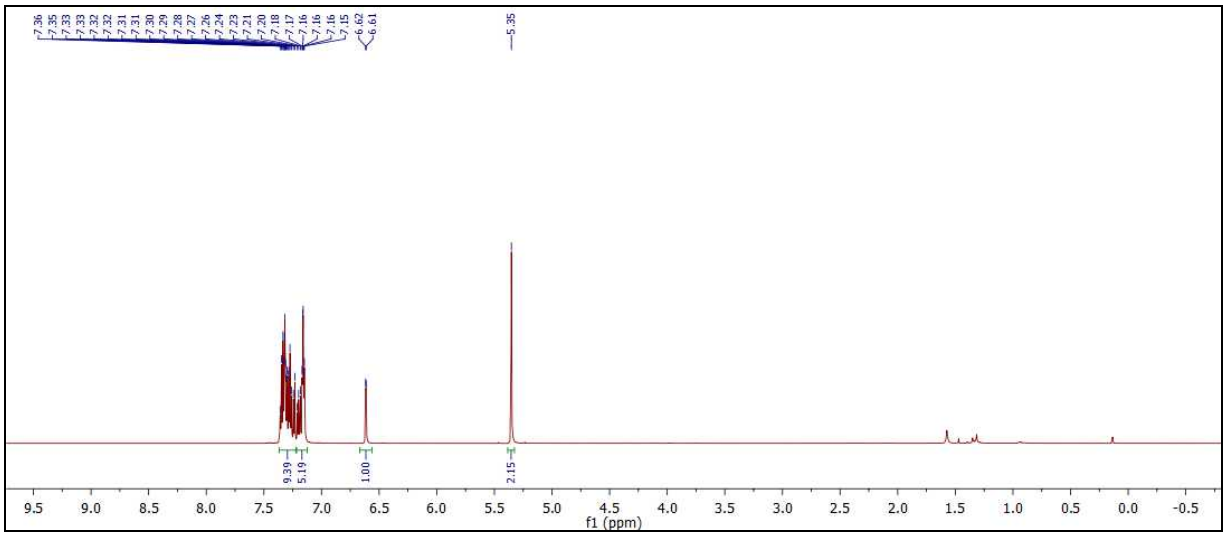
3ab

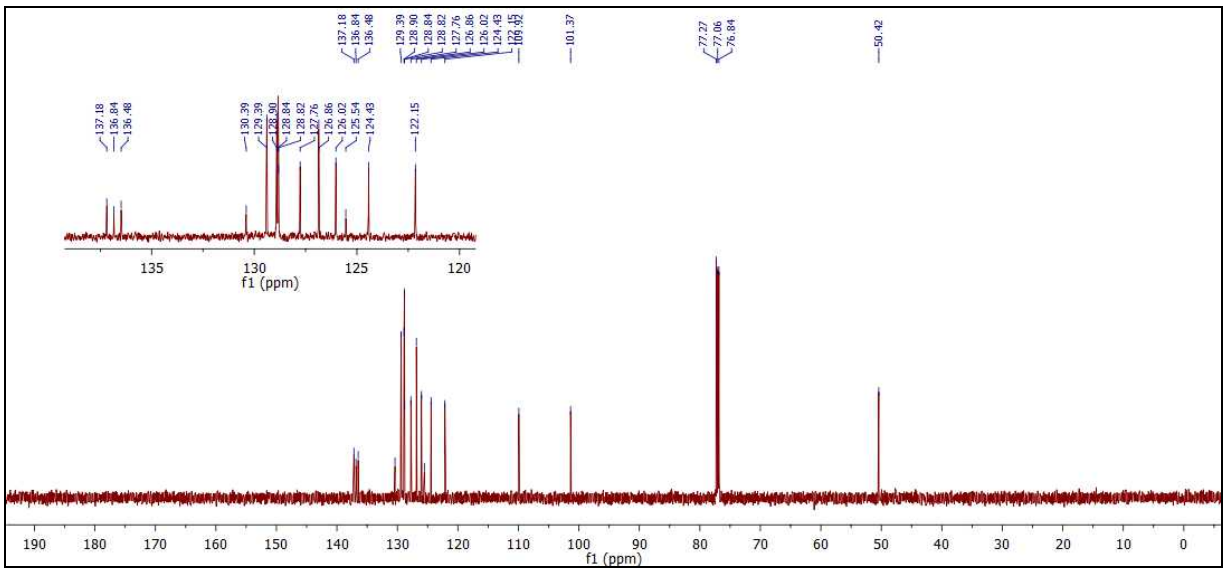

7.73
7.51
7.50
7.38
7.37
7.36
7.35
7.34
7.33
7.28
7.17
7.16
7.09
7.08
7.07
7.06
7.04
6.81
6.80
5.36
2.55
1.00
2.02
6.16
2.13
2.11
1.02
2.05
3.01
f1 (ppm)

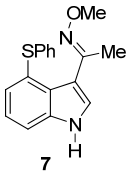

192.56
138.01
135.59
135.04
134.02
133.11
129.26
129.07
128.26
127.78
126.91
123.94
123.60
122.78
119.65
110.69
107.58
77.22
77.00
76.79
50.81
28.72
f1 (ppm)


SPh
N
Bn

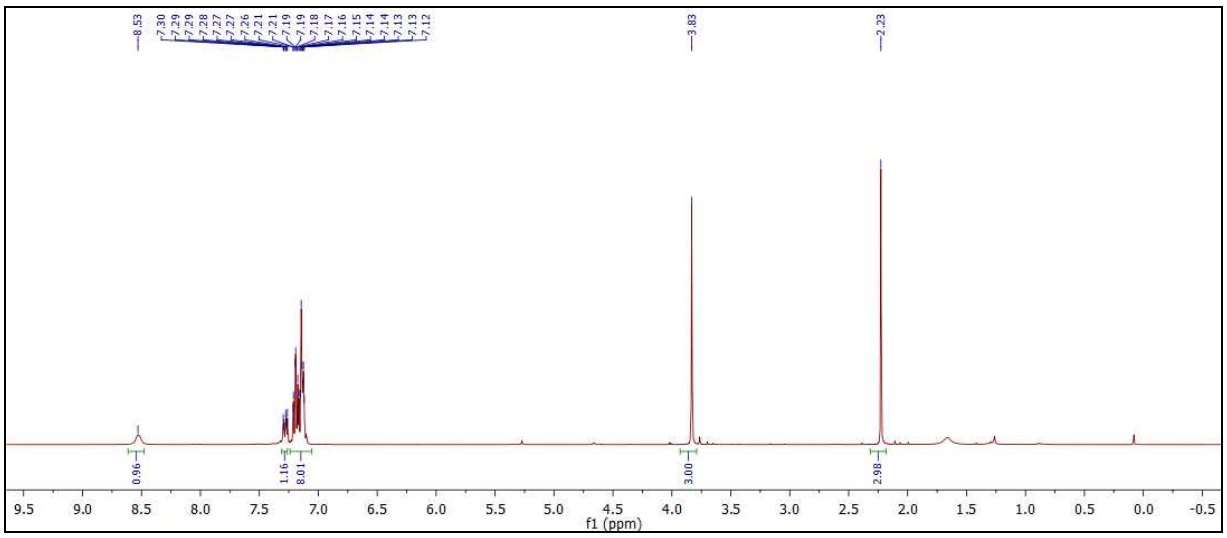
8

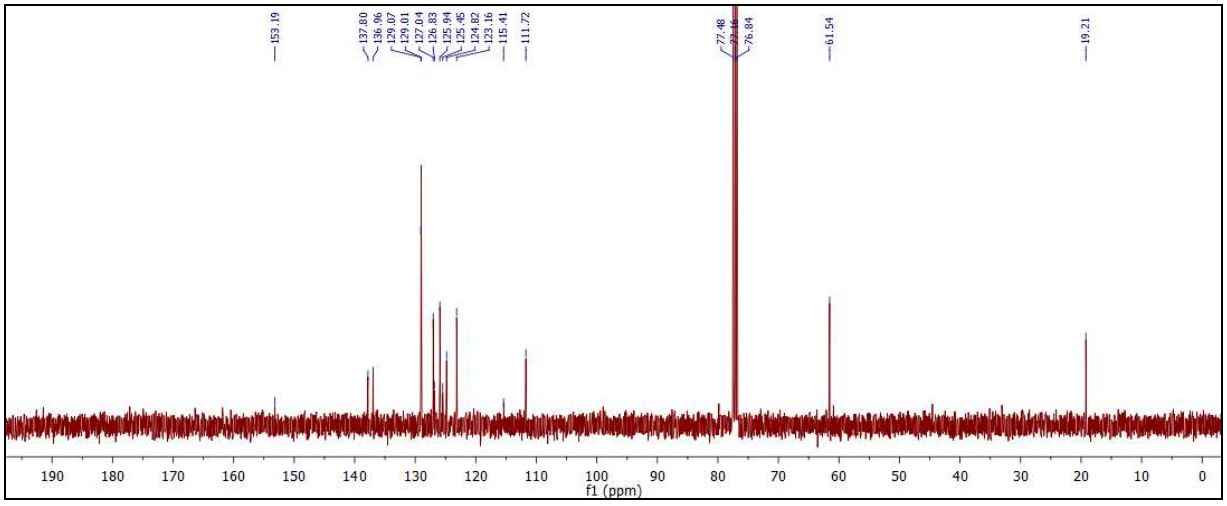

7.36
7.35
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.29
7.28
7.27
7.26
7.24
7.23
7.21
7.20
7.18
7.17
7.16
7.16
7.16
7.15
6.62
6.61
5.35
9.39
5.19
1.00
2.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


137.18
136.84
136.48
129.39
128.90
128.84
128.82
127.76
126.86
126.02
124.43
122.15
109.92
101.37
77.27
77.06
76.84
50.42
135 130 125 120
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


OMe
N
SPh
Me
N
H

7


8.53
7.30
7.29
7.29
7.28
7.27
7.27
7.26
7.21
7.21
7.19
7.19
7.18
7.17
7.16
7.15
7.14
7.14
7.13
7.13
7.12
3.83
2.33
0.96
1.16
8.01
3.00
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


153.19
137.80
136.96
129.07
129.01
127.04
126.83
125.94
125.45
124.82
123.16
115.41
111.72
77.48
77.16
76.84
61.54
19.21
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)