Supporting Information for

Preparation of 2-Amino-3-arylindoles via Pd-Catalyzed Coupling between 3-Diazoindolin-2-imines and Arylboronic Acids as well as Their Extension to 3-Aryl-3-fluoroindolin-2-imines

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Contents

General Information

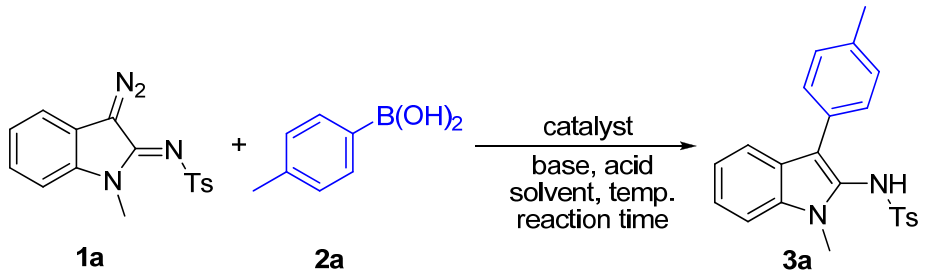
Unless otherwise mentioned, solvents and reagents were purchased from commercial sources and used as received. ^{1}HNMR spectra were obtained on 500 or 400 MHz spectrometer at room temperature. The chemical shifts were reported relative to internal TMS (0 ppm) in $CDCl_3$ or $(CD_3)_2SO$. The following abbreviations were used to describe peak patterns when appropriate: b = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants (*J* values) were reported in Hertz unit (Hz). ^{13}C NMR spectra were recorded on 100 or 125 MHz spectrometer and the chemical shifts were referenced to the central line of the triplet of $CDCl_3$ (77.00 ppm) or the center line of the heptet of $(CD_3)_2SO$ (40.0 ppm). Infrared spectra were obtained on FTIR spectrometer. All high-resolution mass spectra (HRMS) data were obtained by using EI ionization on time-of-flight (TOF) mass spectrometer or ESI ionization on LCMS-IT-TOF mass spectrometer. Melting points were measured with a micro melting point apparatus. Flash column chromatography was performed employing 300-400 mesh silica gel. Thin layer chromatography (TLC) was performed on silica gel HSGF254.

Substrates **1** were prepared according to the published methods.[1]

References

1. (a) Y. P. Xing, G. R. Sheng, J. Wang, P. Lu, Y.G. Wang, *Org. Lett.***2014**, *16*, 1244−1247. (b) G. R. Sheng, K. Huang, Z. H. Chi, H. L. Ding, Y. P. Xing, P. Lu, Y. G. Wang, *Org. Lett.***2014**, *16*,5096–5099.

Table S1. Screening of the reaction conditions[a]



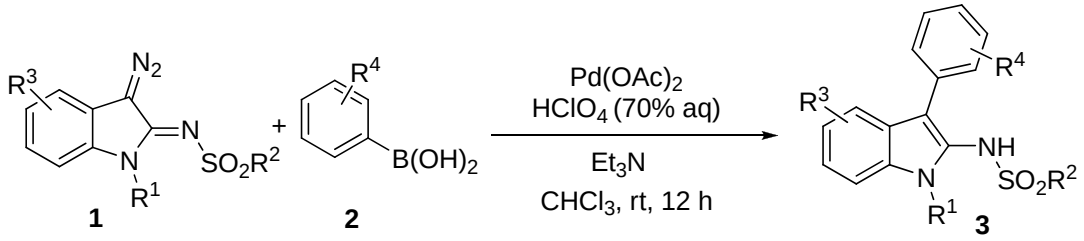
1a **2a** **3a**

entry	catalyst	base	acid	solvent	temp (°C)	time(h)	yield(%)[b]
1	$Pd(OAc)_2$	KF	CH_3COOH	DCE	50	2	27
2	$Pd(PPh_3)_4$	KF	CH_3COOH	DCE	50	2	trace
3	$PdCl_2$	KF	CH_3COOH	DCE	50	2	ND
4	$Pd(OH)_2$	KF	CH_3COOH	DCE	50	2	ND
5	$Pd(OAc)_2$	K_2HPO_4	NONE	DCE	50	2	43
6	$Pd(OAc)_2$	K_2HPO_4	NONE	$CHCl_3$	50	2	44
7	$Pd(OAc)_2$	K_2HPO_4	NONE	DCM	50	2	34
8	$Pd(OAc)_2$	K_2HPO_4	NONE	THF	50	2	20
9	$Pd(OAc)_2$	K_2HPO_4	NONE	PhMe	50	2	29
10	$Pd(OAc)_2$	K_2HPO_4	NONE	MeCN	50	2	trace
11	$Pd(OAc)_2$	K_2HPO_4	NONE	1,4-dioxane	50	2	18
12	$Pd(OAc)_2$	K_2HPO_4	NONE	DMF	50	2	ND
13	$Pd(OAc)_2$	K_2CO_3	CH_3COOH	$CHCl_3$	50	2	49
14	$Pd(OAc)_2$	NaOAc	CH_3COOH	$CHCl_3$	50	2	12
15	$Pd(OAc)_2$	Na_2CO_3	CH_3COOH	$CHCl_3$	50	2	16
16	$Pd(OAc)_2$	Cs_2CO_3	CH_3COOH	$CHCl_3$	50	2	10
17	$Pd(OAc)_2$	$NaHCO_3$	NONE	$CHCl_3$	50	2	42
18	$Pd(OAc)_2$	KH_2PO_4	NONE	$CHCl_3$	50	2	44
19	$Pd(OAc)_2$	K_2CO_3	NONE	$CHCl_3$	50	2	trace
20	$Pd(OAc)_2$	K_2HPO_4	CH_3COOH	$CHCl_3$	50	2	47
21	$Pd(OAc)_2$	K_2CO_3	CF_3COOH	$CHCl_3$	50	2	56
22	$Pd(OAc)_2$	K_2CO_3	CF_3COOH	$CHCl_3$	reflux	1	14
23	$Pd(OAc)_2$	K_2CO_3	CF_3COOH	$CHCl_3$	rt	12	58
24	$Pd(OAc)_2$	K_2CO_3	CF_3COOH	$CHCl_3$	0	12	56
25	$Pd(OAc)_2$	K_2CO_3	$HClO_4$[c]	$CHCl_3$	rt	12	65
26	$Pd(OAc)_2$	Et_3N	$HClO_4$[c]	$CHCl_3$	rt	12	67

27	$Pd(OAc)_2$	Pyridine	$HClO_4$[c]	$CHCl_3$	rt	12	NR
28	$Pd(OAc)_2$	DIEA	$HClO_4$[c]	$CHCl_3$	rt	12	34
29	$Pd(OAc)_2$	DBU	$HClO_4$[c]	$CHCl_3$	rt	12	NR
30	$Pd(OAc)_2$	$(Me_2NCH_2)_2$	$HClO_4$[c]	$CHCl_3$	rt	12	18
31	$Pd(OAc)_2$	Et_3N(5equiv)	$HClO_4$[c](5equiv)	$CHCl_3$	rt	12	78
32	$Pd(OAc)_2$	Et_3N(6equiv)	$HClO_4$[c](6equiv)	$CHCl_3$	rt	12	81
33	$Pd(OAc)_2$	Et_3N(7equiv)	$HClO_4$[c](7equiv)	$CHCl_3$	rt	12	80
34	NONE	Et_3N(6equiv)	$HClO_4$[c](6equiv)	$CHCl_3$	rt	12	ND
35	$Pd(OAc)_2$	Et_3N(6equiv)	NONE	$CHCl_3$	rt	12	25
36	$Pd(OAc)_2$	NONE	$HClO_4$[c](6equiv)	$CHCl_3$	rt	12	21

[a] Reaction condition: **1a** (0.2 mmol), **2a** (0.6 mmol), Pd catalyst (10 mol %), base (3.0 equiv), acid (3.0equiv), solvent (2 mL). [b]Isolated yield. [c] 70% aqueous $HClO_4$ was used.

General Procedure for the Synthesis of 3

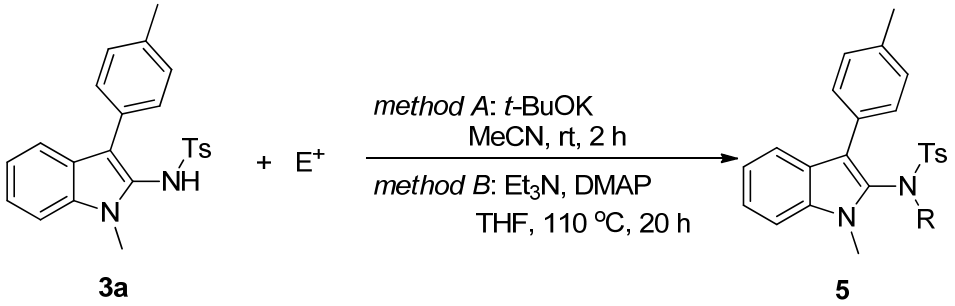


To a solution of **1** (0.2 mmol) and **2** (3.0 equiv) in $CHCl_3$ (2 mL) was added triethylamine (165 μL, 6.0 equiv), $HClO_4$ (70% aq, 68 μL, 6.0 equiv), and $Pd(OAc)_2$ (4.4 mg, 0.1 equiv). Then, the reaction mixture was stirred at room temperature for 12 h (24 h for **3e** and **3f;** 36 h for **3h**, **3q, 3r**, **3v** and **3A;** 3 d for **3t**). After the reaction completed, the solvent was removed in vacuum and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, v/v) to give pure product.

Preparation of 3a in 1 mmol Scale

To a solution of **1a** (1.0 mmol, 326 mg) and **2a** (3.0 equiv) in $CHCl_3$ (10 mL) was added triethylamine (832 μl, 6.0 equiv), $HClO_4$ (70% aq, 342 μl, 6.0 equiv), and $Pd(OAc)_2$ (22.4 mg, 0.1 equiv). Then the reaction mixture was stirred for 12 h at room temperature. After the reaction completed, the solvent was removed in vacuum and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, v/v) to give product **3a** (305 mg, 78% yield).

General Procedure for the Synthesis of 5

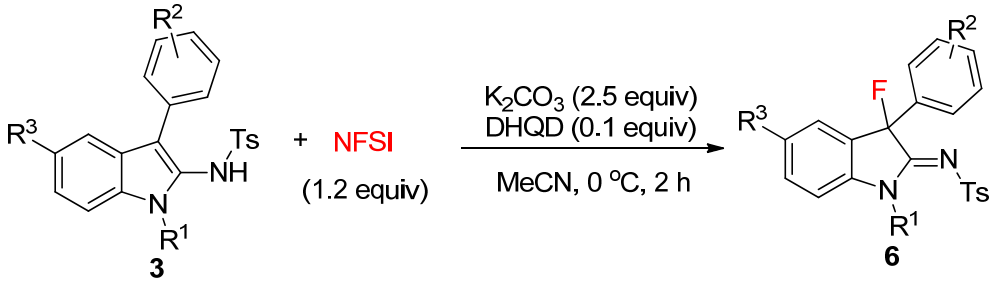


Method A: To a stirring solution of **3a** (78 mg, 0.2 mmol), *t*-BuOK (34 mg, 1.5 equiv) in MeCN (2 mL) was added electrophile (E^+ = benzyl bromide, methyl iodide or allyl bromide) (1.5 equiv) at room temperature. The mixture was stirred at room temperature for 2 h. After the reaction

completed (checked by TLC), the mixture was concentrated under vacuum and filtered through a plug of silica gel (DCM). The solvent was removed in vacuum and the residue was purified by columnchromatography on silica gel (petroleum ether/ethyl acetate = 6:1, v/v) to give pure products **5a-c**.

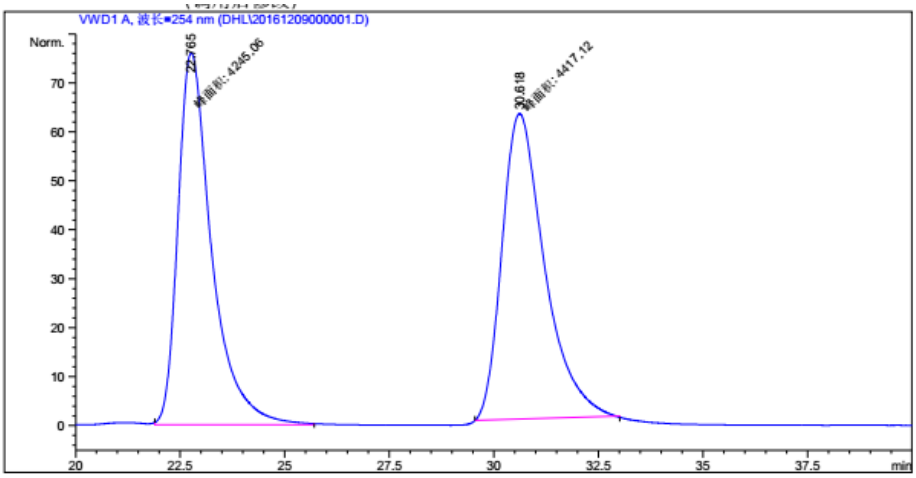
Method B: To a solution of **3a** (78 mg, 0.2 mmol), di-*tert*-butyl dicarbonate (69 μL, 1.5 equiv) in THF (2 mL) was added Et_3N (83 μL, 3.0 equiv) and DMAP (3 mg, 0.1 equiv) at a sealed tube. The mixture was stirred at 110 °C for 20 h. After the reaction completed, the solvent was removed in vacuum and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =6:1, v/v) to give pure **5d.**

General Procedure for the Synthesis of 6



To a stirring solution of **3** (0.2 mmol), K_2CO_3 (69 mg, 2.5 equiv) and hydroquinidine (DHQD) (6 mg, 0.1 equiv) in MeCN (2 mL) was added NFSI (76 mg, 1.2 equiv) at 0 °C. The reaction mixture was stirred for 2 h. After the reaction completed, the solvent was removed in vacuum and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 4:1, v/v) to give pure **6**.

Optimizing the enantiomer excess of **6a**: To a stirring solution of **3a** (39 mg, 0.1mmol), K_2CO_3 (20 mg, 1.0 equiv) and $(DHQD)_2PHAL$ (7 mg, 0.1 equiv) in MeCN (1 mL) was added NFSI (38 mg, 1.2 equiv) at -40 °C. After the reaction mixture was stirred for 24 h, the solvent was quenched with water and the aqueous was extracted with DCM (3 × 10 mL). The combined extracts were washed with water and dried over anhydrous Na_2SO_4. Evaporation of solvents and the residue was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 4:1, v/v) to give **6a** as a white solid (39 mg, 97% yield, 60% ee). HPLC: Chiralcel AD-H column (250 mm); Hexane/*i*-PrOH = 75/25; flow = 0.8 ml/min; detected at 254 nm; Retention time: 23.1 min, 31.1 min (major).



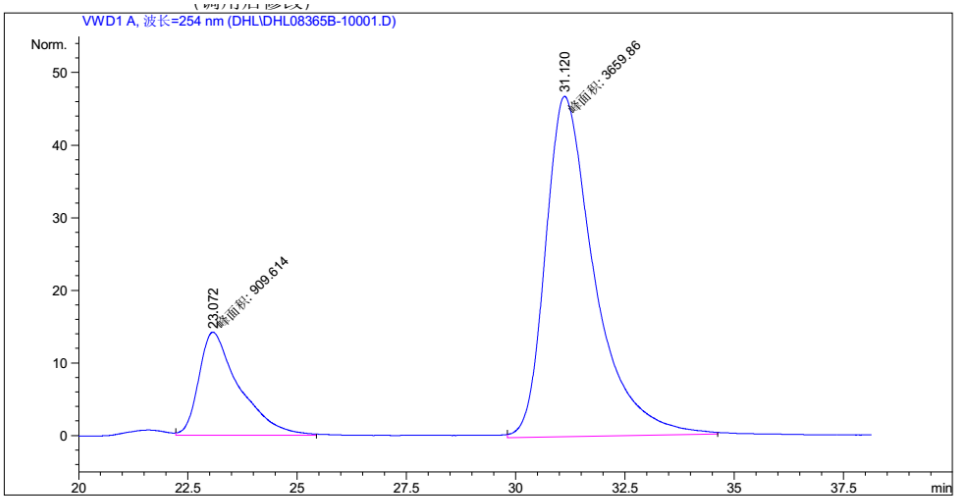
面积百分比报告

排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	22.765	MM	0.9323	4245.05859	75.88873	49.0068
2	30.618	MM	1.1806	4417.12109	62.35790	50.9932

总量 : 8662.17969 138.24662



面积百分比报告

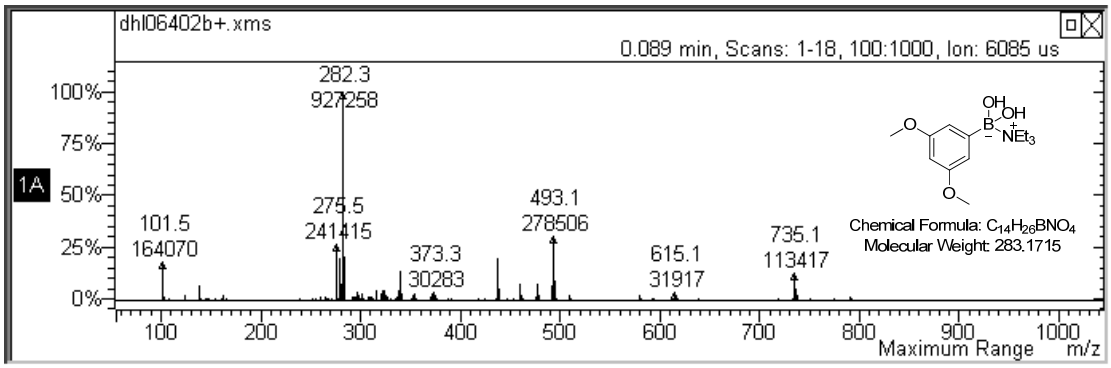
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

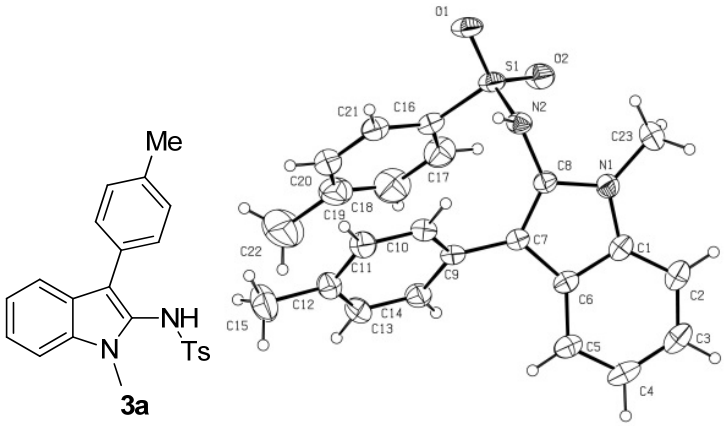
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	23.072	MM	1.0680	909.61407	14.19493	19.9063
2	31.120	MM	1.3007	3659.85571	46.89703	80.0937

总量 : 4569.46979 61.09196

MS of the Combined Speciesfrom Triethylamine and (3,5-Dimethoxyphenyl)-boronic Acid



ORTEP diagram and Crystal Parameters of 3a, 4 and 6a



Datablock: I

```
Bond precision:  C-C = 0.0034 A          Wavelength=0.71073

Cell:            a=28.1291(17)     b=11.3338(5)       c=14.8299(8)
                 alpha=90          beta=91.255(5)     gamma=90
Temperature:     293 K

                 Calculated                Reported
Volume           4726.8(4)                 4726.8(4)
Space group      C 2/c                     C 1 2/c 1
Hall group       -C 2yc                    -C 2yc
Moiety formula   C23 H22 N2 O2 S           C23 H22 N2 O2 S
Sum formula      C23 H22 N2 O2 S           C23 H22 N2 O2 S
Mr               390.49                    390.49
Dx,g cm-3        1.097                     1.097
Z                8                         8
Mu (mm-1)        0.155                     0.155
F000             1648.0                    1648.0
F000'            1649.62
h,k,lmax         33,13,17                  33,13,17
Nref             4333                      4254
Tmin,Tmax        0.927,0.940               0.963,1.000
Tmin'            0.927

Correction method= # Reported T Limits: Tmin=0.963 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.982          Theta(max)= 25.350

R(reflections)= 0.0464( 3144)     wR2(reflections)= 0.1369( 4254)

S = 1.081                 Npar= 260
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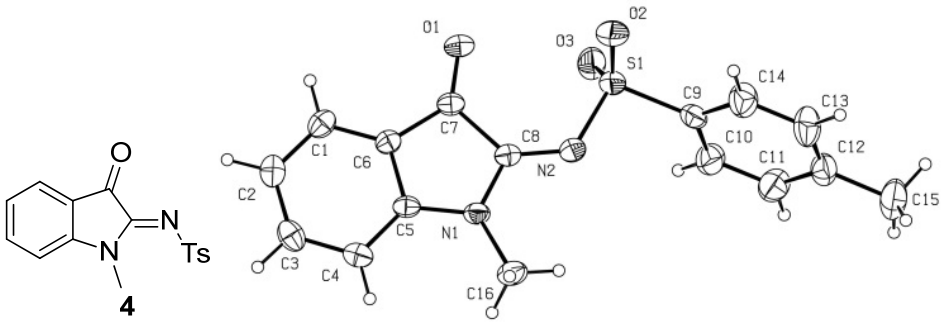


Datablock: 170319_dhl08378a_2

Bond precision: C-C = 0.0065 A Wavelength=0.71073

Cell: a=6.8692(7) b=7.4511(9) c=15.6394(18)
alpha=85.058(9) beta=80.243(9) gamma=68.404(10)
Temperature: 293 K

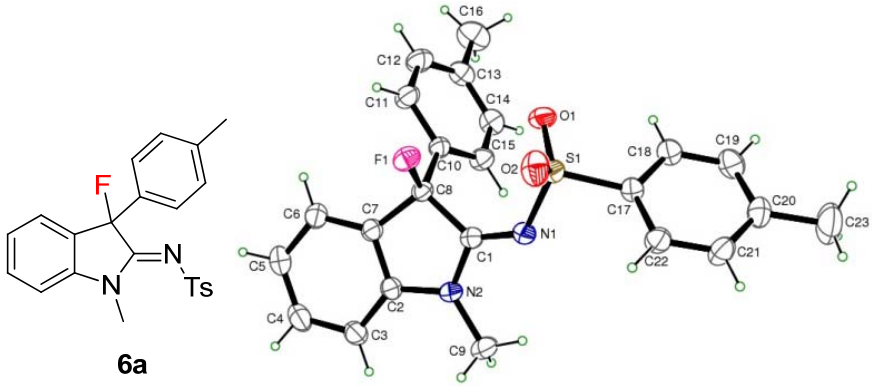
	Calculated	Reported
Volume	733.27(15)	733.26(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H14 N2 O3 S	C16 H14 N2 O3 S
Sum formula	C16 H14 N2 O3 S	C16 H14 N2 O3 S
Mr	314.35	314.35
Dx,g cm-3	1.424	1.424
Z	2	2
Mu (mm-1)	0.235	0.235
F000	328.0	328.0
F000'	328.39	
h,k,lmax	8,8,18	8,8,18
Nref	2683	2667
Tmin,Tmax	0.937,0.977	0.793,1.000
Tmin'	0.932	

Correction method= # Reported T Limits: Tmin=0.793 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.346

R(reflections)= 0.0688(1740) wR2(reflections)= 0.1969(2667)

S = 1.059 Npar= 201



6a

Datablock: dhl330b

```
Bond precision:  C-C = 0.0045 A          Wavelength=0.71073

Cell:            a=8.5856(5)     b=26.6604(15)       c=9.0241(6)
                 alpha=90        beta=98.396(2)      gamma=90
Temperature:     296 K
```

	Calculated	Reported
Volume	2043.4(2)	2043.4(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H21 F N2 O2 S	C23 H21 F N2 O2 S
Sum formula	C23 H21 F N2 O2 S	C23 H21 F N2 O2 S
Mr	408.48	408.48
Dx,g cm-3	1.328	1.328
Z	4	4
Mu (mm-1)	0.189	0.189
F000	856.0	856.0
F000'	856.88	
h,k,lmax	11,34,11	11,34,11
Nref	4689	4662
Tmin,Tmax	0.900,0.952	0.902,0.952
Tmin'	0.900	

```
Correction method= # Reported T Limits: Tmin=0.902 Tmax=0.952
AbsCorr = MULTI-SCAN

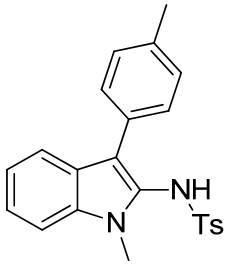
Data completeness= 0.994          Theta(max)= 27.470

R(reflections)= 0.0659( 2797)     wR2(reflections)= 0.1314( 4662)

S = 1.002                 Npar= 266
```

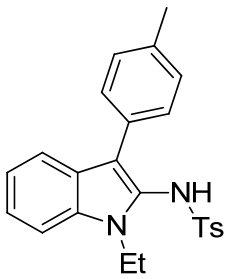
Characterization Data for All Products

4-Methyl-N-(1-methyl-3-(p-tolyl)-1H-indol-2-yl)benzenesulfonamide (3a)



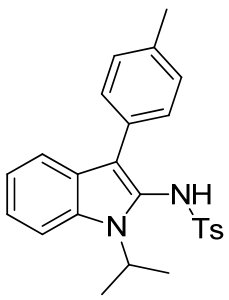
White solid (63 mg, 81%); m.p. 157.3 – 158.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.13 – 7.09 (m, 1H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.92 (s, 1H), 6.83 – 6.79 (m, 4H), 3.91 (s, 3H), 2.35 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 135.5, 135.0, 134.8, 129.9, 128.9, 128.9, 128.5, 127.2, 126.3, 125.1, 122.9, 120.1, 119.7, 112.8, 109.9, 30.0, 21.5, 21.2; IR (neat) *ν* 3269, 3050, 2922, 1598, 1567, 1471, 1373, 1330, 1259, 1162, 1091 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{22}N_2O_2S$]: 390.1402; found: 390.1398.

N-(1-Ethyl-3-(p-tolyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (3b)



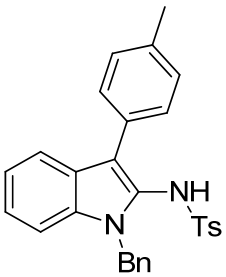
White solid (64 mg, 79%); m.p. 151.4 – 152.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.11 – 7.03 (m, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.79 (d, *J* = 8.0 Hz, 2H), 4.49 (q, *J* = 7.2 Hz, 2H), 2.34 (s, 3H), 2.29 (s, 3H), 1.48 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 135.4, 134.9, 134.0, 130.0, 128.9, 128.8, 128.6, 127.2, 125.5, 125.4, 122.9, 119.9, 119.0, 113.3, 110.2, 38.0, 21.5, 21.2, 14.8; IR (neat) *ν* 3258, 3054, 2979, 1581, 1557, 1510, 1488, 1470, 1403, 1331, 1284, 1162, 1087 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{24}N_2O_2S$]: 404.1558; found: 404.1558.

N-(1-Isopropyl-3-(p-tolyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (3c)



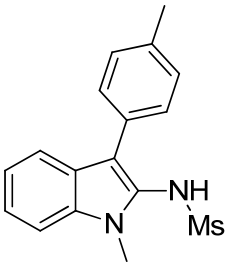
White solid (69 mg, 83%); m.p. 154.7 – 155.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.08 – 7.05 (m, 1H), 6.98 – 6.93 (m, 3H), 6.79 (d, *J* = 8.4 Hz, 4H), 5.35 – 5.24 (m, 1H), 2.34 (s, 3H), 2.30 (s, 3H), 1.73 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 135.4, 134.8, 132.7, 130.0, 128.9, 128.8, 128.6, 127.2, 126.1, 125.4, 122.3, 120.0, 119.5, 112.8, 112.4, 46.9, 21.5, 21.2, 21.1; IR (neat) *ν* 3262, 3051, 2978, 1574, 1510, 1470, 1404, 1336, 1284, 1162, 1086, 1008 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{25}H_{26}N_2O_2S$]: 418.1715; found: 418.1714.

N-(1-Benzyl-3-(p-tolyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (3d)



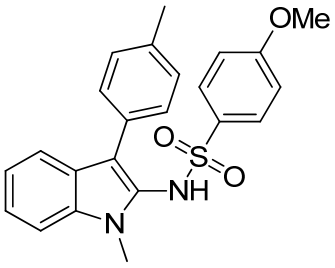
White solid (69 mg, 74%); m.p. 116.3 – 117.5 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 1H), 7.30 – 7.20 (m, 7H), 7.11 – 7.07 (m, 3H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.87 (d, *J* = 8.0 Hz, 2H), 6.81 – 6.77 (m, 3H), 5.66 (s, 3H), 2.34 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 137.7, 135.6, 135.0, 134.8, 129.8, 128.9, 128.8, 128.7, 128.6, 127.3, 127.3, 126.6, 125.9, 125.4, 123.3, 120.3, 119.9, 114.2, 110.6, 46.6, 21.5, 21.2; IR (neat) *v* 3258, 3030, 2921, 1573, 1510, 1496, 1463, 1400, 1333, 1304, 1209, 1162, 1091, 1008 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{29}H_{26}N_2O_2S$]: 466.1715; found: 466.1707.

N-(1-Methyl-3-(p-tolyl)-1H-indol-2-yl)methanesulfonamide (3e)



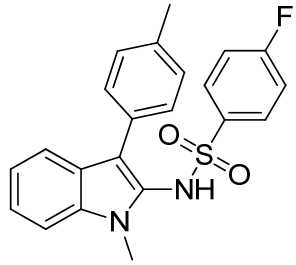
White solid (19 mg, 30%); m.p. 154.0 – 154.9 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.38 – 7.28 (m, 4H), 7.19 – 7.15 (m, 1H), 6.96 – 6.95 (m, 1H), 3.82 (s, 3H), 2.41 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 135.0, 130.4, 129.9, 129.0, 125.8, 124.9, 123.3, 120.4, 119.8, 113.4, 110.0, 39.9, 29.6, 21.2; IR (neat) *v* 3254, 3027, 2927, 1567, 1510, 1471, 1434, 1373,1328, 1158, 1090, 976 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{17}H_{18}N_2O_2S$]: 314.1089; found: 314.1094.

4-Methoxy-N-(1-methyl-3-(p-tolyl)-1H-indol-2-yl)benzenesulfonamide (3f)



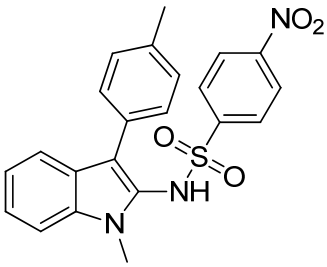
White solid (40 mg, 49%); m.p. 197.7 – 198.5 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.22 (d, *J* = 8.8 Hz, 2H), 7.13 – 7.09 (m, 1H), 6.98 – 6.94 (m, 3H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.47 (d, *J* = 9.2 Hz, 2H), 3.91 (s, 3H), 3.79 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 135.5, 135.1, 130.0, 129.3, 129.2, 129.0, 128.5, 126.4, 125.1, 122.9, 120.1, 119.7, 113.5, 112.7, 109.9, 55.3, 30.0, 21.1; IR (neat) *v* 3280, 3060, 2917, 1596, 1575, 1497, 1459, 1373, 1329, 1261, 1179, 1158, 1092, 1029 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{22}N_2O_3S$]: 406.1351; found: 406.1349.

4-Fluoro-N-(1-methyl-3-(p-tolyl)-1H-indol-2-yl)benzenesulfonamide (3g)



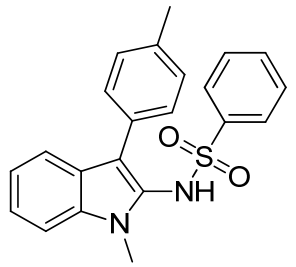
White solid (56 mg, 71%); m.p. 134.4 – 135.4 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.0 Hz, 1H), 7.39 (d, J = 8.4 Hz, 1H), 7.34 – 7.28 (m, 3H), 7.14 – 7.10 (m, 1H), 7.04 – 6.99 (m, 3H), 6.85 (d, J = 7.6 Hz, 2H), 6.66 (dd, $J_1 = J_2$ = 8.4 Hz, 2H), 3.91 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3 (d, J = 253.3 Hz), 164.0, 135.9, 135.1, 133.7, 130.0, 129.9 (d, J = 9.6 Hz), 129.2, 128.4, 125.8, 124.9, 123.2, 120.3, 119.8, 115.5 (d, J = 22.6 Hz), 113.1, 109.9, 29.9, 21.0; IR (neat) ν 3273, 3062, 2922, 1591,1566, 1493, 1470, 1373,1331, 1236, 1169, 1154, 1090, 1014 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{22}H_{19}FN_2O_2S$]: 394.1151; found: 394.1149.

N-(1-Methyl-3-(p-tolyl)-1H-indol-2-yl)-4-nitrobenzenesulfonamide (3h)



Yellow solid (14 mg, 16%); m.p. 179.2 – 180.3^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.8 Hz, 2H), 7.53 (d, J = 8.0 Hz, 1H), 7.48 (d, J = 8.8 Hz, 2H), 7.40 (d, J = 8.4 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.15 – 7.11 (m, 2H), 6.92 (d, J = 7.6 Hz, 2H), 6.82 (d, J = 8.0 Hz, 2H), 3.93 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.0, 143.4, 136.5, 135.1, 129.7, 129.2, 128.5, 128.4, 124.7, 124.6, 123.6, 123.3, 120.5, 119.9, 113.5, 110.0, 29.9, 21.0; IR (neat) v 3287, 3101, 2917, 1557,1531, 1471, 1432, 1348, 1307, 1167, 1140, 1089, 1014 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{22}H_{19}N_3O_4S$]: 421.1096; found: 421.1099.

N-(1-Methyl-3-(p-tolyl)-1H-indol-2-yl)benzenesulfonamide(3i)

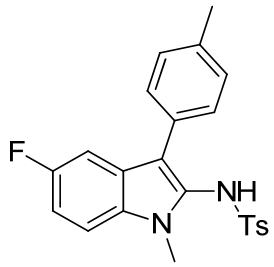


White solid (60 mg, 80%); m.p. 85.2 – 86.4 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 8.0 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.34 – 7.29 (m, 4H), 7.13 – 7.05 (m, 3H), 6.99 – 6.93 (m, 3H),6.80 (d, J = 7.6 Hz, 2H), 3.91 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 135.6, 135.1, 132.7, 129.8, 129.2, 128.5, 128.4, 127.3, 126.1, 125.1, 123.0, 120.1, 119.7, 113.0, 109.9, 30.0, 21.1; IR (neat) ν 3268, 3059, 2921, 1567, 1510, 1470, 1447, 1373, 1329, 1222, 1164, 1090 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{22}H_{20}N_2O_2S$]: 376.1245; found: 376.1248.

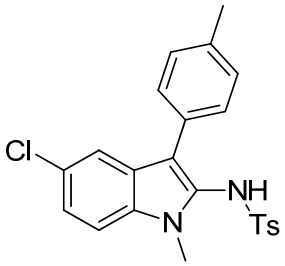
N-(5-Fluoro-1-methyl-3-(p-tolyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (3j)

Light yellow solid (69 mg, 85%); m.p. 208.7 – 209.8 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (dd, J_1 = 8.8 Hz, J_2 =

4.4 Hz, 1H), 7.20 – 7.15 (m, 3H), 7.07 – 7.01 (m, 2H), 6.96 (d, *J* = 7.6 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.77 (d, *J* = 8.0 Hz, 2H), 3.89 (s, 3H), 2.34 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3 (d, *J* = 234.0 Hz), 143.8, 135.8, 134.7, 131.6, 129.5, 129.0, 128.3, 127.6, 127.2, 125.3 (d, *J* = 9.9 Hz), 112.9(d, *J* = 4.9 Hz), 111.5 (d, *J* = 26.1 Hz), 110.7 (d, *J* = 9.3 Hz), 104.5 (d, *J* = 23.8 Hz), 30.2, 21.5, 21.1; IR (neat) *ν* 3278, 3048, 2916, 1624, 1597, 1557, 1488, 1436, 1375, 1324, 1258, 1162, 1089 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{21}FN_2O_2S$]: 408.1308; found: 408.1308.

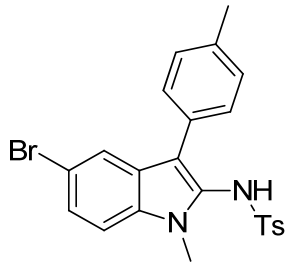


N-(5-Chloro-1-methyl-3-(p-tolyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (3k)



Light yellow solid (71 mg, 84%); m.p. 187.2 – 188.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 1.6 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 7.23 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.10 (b, 1H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.77 (d, *J* = 8.0 Hz, 2H), 3.88 (s, 3H), 2.34 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 135.9, 134.7, 133.4, 129.2, 129.0, 129.0, 128.4, 127.4, 127.2, 126.0, 126.0, 123.3, 119.1, 112.6, 111.0, 30.2, 21.5, 21.1; IR (neat) *ν* 3263, 3028, 2921, 1598, 1563, 1472, 1433, 1372, 1327, 1287, 1162, 1091 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{21}ClN_2O_2S$]: 424.1012; found: 424.1012.

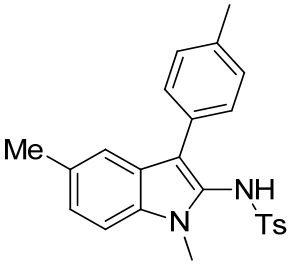
N-(5-Bromo-1-methyl-3-(p-tolyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (3l)



Light yellow solid (72 mg, 77%); m.p. 178.0 – 179.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 2.0 Hz, 1H), 7.37 (dd, J_1 = 8.8 Hz,J_2 = 1.6 Hz, 1H), 7.25 (d, *J* = 2.0 Hz, 1H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.03 (b, 1H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.76 (d, *J* = 8.0 Hz, 2H), 3.88 (s, 3H), 2.34 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 135.9, 134.6, 133.6, 129.2, 129.0, 129.0, 128.4, 127.2, 127.2, 126.7, 125.8, 122.1, 113.5, 112.5, 111.4, 30.2, 21.5, 21.2; IR (neat) *ν* 3265, 3021, 2921, 1598, 1563, 1471, 1431, 1376, 1326, 1287, 1162, 1090 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{21}BrN_2O_2S$]: 468.0507; found: 468.0499.

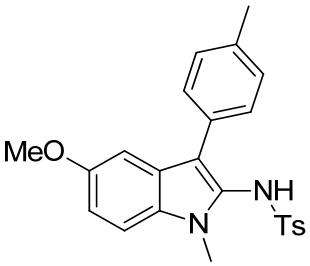
N-(1,5-Dimethyl-3-(p-tolyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (3m)

Light yellow liquid (65 mg, 80 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 2H), 7.18 (d, *J* = 8.4 Hz, 2H),



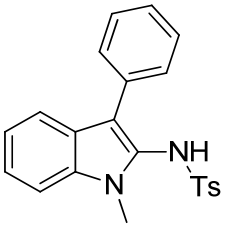
7.13 – 7.11 (m, 1H), 6.96 (d, *J* = 7.6 Hz, 3H), 6.80 (t, *J* = 7.6 Hz, 4H), 3.87 (s, 3H), 2.39 (s, 3H), 2.34 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 135.4, 134.8, 133.4, 130.1, 129.4, 128.9, 128.8, 128.5, 127.2, 126.2, 125.2, 124.6, 119.2, 112.3, 109.6, 30.0, 21.5, 21.4, 21.2; IR (neat) *v* 3264, 3027, 2920, 1567, 1493, 1435, 1392, 1377, 1327, 1296, 1161, 1090 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{24}N_2O_2S$]: 404.1558; found: 404.1559.

N-(5-Methoxy-1-methyl-3-(p-tolyl)-1H-indol-2-yl)-4-methylbenzenesulfonamide (3n)



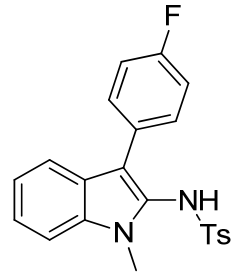
Colorless oil (70 mg, 83%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.26 (m, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.98 – 6.95 (m, 5H), 6.83 – 6.79 (m, 4H), 3.87 (s, 3H), 3.76 (s, 3H), 2.34 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 143.5, 135.4, 134.9, 130.3, 130.1, 128.9, 128.4, 127.2, 126.5, 125.3, 113.4, 112.6, 110.7, 101.1, 55.8, 30.0, 21.5, 21.1; IR (neat) *v* 3271, 3024, 2922, 1622, 1593,1487, 1455, 1397, 1327, 1262, 1197, 1162, 1090, 1033 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{22}N_2O_3S$]: 420.1508; found: 420.1508.

4-Methyl-N-(1-methyl-3-phenyl-1H-indol-2-yl)benzenesulfonamide (3o)



White solid (50 mg, 67%); m.p. 171.4 – 172.3 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.29 (m, 1H), 7.19 – 7.09 (m, 7H), 6.94 – 6.92 (m, 2H), 6.80 (d, *J* = 8.4 Hz, 2H), 3.91 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 135.0, 134.5, 132.9, 129.1, 128.7, 128.2, 127.2, 126.4, 125.8, 125.0, 123.0, 120.2, 119.6, 112.9, 109.9, 30.0, 21.5; IR (neat) *v* 3262, 3057, 2923, 1567, 1488, 1392, 1369, 1331, 1259, 1163, 1090 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{22}H_{20}N_2O_2S$]: 376.1245; found: 376.1241.

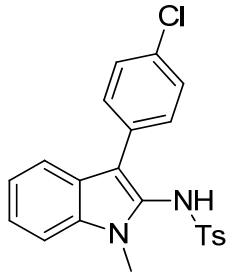
N-(3-(4-Fluorophenyl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3p)



White solid (17 mg, 21%); m.p. 171.4 – 172.3 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.34 – 7.30 (m, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.14 – 7.10 (m, 1H), 7.05 (b, 1H), 6.94 – 6.82 (m, 6H), 3.90 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3 (d, *J* = 243.9 Hz), 143.9, 135.0, 135.0, 130.2(d, *J* = 7.9

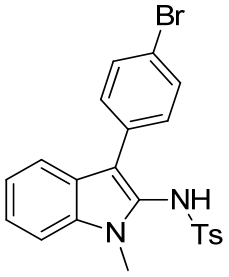
Hz), 129.1, 129.0(d, J = 3.1 Hz), 127.2, 126.2, 125.0, 123.2, 120.3, 119.5, 115.1 (d, J = 21.3 Hz), 112.2, 110.0, 29.9, 21.5; IR (neat) ν 3269, 3061, 2926, 1598, 1564, 1506, 1471, 1373, 1330, 1220, 1185, 1091, 1017 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{22}H_{19}FN_2O_2S$]: 394.1151; found: 394.1156.

N-(3-(4-Chlorophenyl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3q)



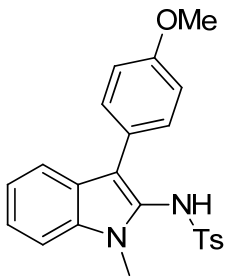
White solid (20 mg, 25%); m.p. 143.9 – 145.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 8.0 Hz, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.23 (d, J = 8.4 Hz, 2H), 7.15 – 7.07 (m, 4H), 6.92 – 6.87 (m, 4H), 3.91 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.1, 135.0, 135.0, 131.8, 131.5, 129.9, 129.1, 128.3, 127.2, 126.3, 124.7, 123.3, 120.5, 119.4, 112.1, 110.1, 29.9, 21.5; IR (neat) ν 3265, 3060, 2947, 1598, 1557, 1492, 1471, 1393, 1331, 1256, 1163, 1092, 1014 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{22}H_{19}ClN_2O_2S$]: 410.0856; found: 410.0850.

N-(3-(4-Bromophenyl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3r)



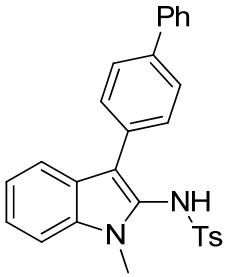
White solid (17 mg, 19%); m.p. 167.6 – 168.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 8.0 Hz, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.27 – 7.22 (m, 4H), 7.15 – 7.11 (m, 1H), 7.07 (b, 1H), 6.89 – 6.84 (m, 4H), 3.91 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 135.0, 135.0, 132.0, 131.3, 130.2, 129.1, 127.2, 126.3, 124.7, 123.3, 120.5, 119.9, 119.4, 112.1, 110.1, 29.9, 21.6; IR (neat) ν 3270, 3060, 2925, 1597, 1558, 1471, 1434, 1392, 1330, 1258, 1162, 1090, 1010 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{22}H_{19}BrN_2O_2S$]: 454.0351; found: 454.0344.

N-(3-(4-Methoxyphenyl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3s)



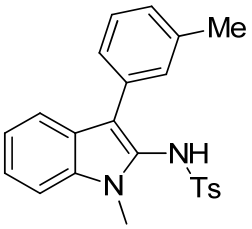
White solid (64 mg, 79%); m.p. 195.8 – 197.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 8.0 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.22 (d, J = 8.4 Hz, 2H), 7.13 – 7.09 (m, 1H), 6.97 (s, 1H), 6.86 – 6.83 (m, 4H), 6.69 (d, J = 8.8 Hz, 2H), 3.90 (s, 3H), 3.82 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 143.6, 135.0, 135.0, 129.7, 129.0, 127.2, 126.1, 125.3, 125.2, 123.0, 120.1, 119.7, 113.7, 112.6, 109.9, 55.2, 30.0, 21.5; IR (neat) ν 3269, 3057, 2935,1730, 1619, 1557, 1506, 1468, 1391, 1280, 1253, 1161, 1084, 1032 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{22}N_2O_3S$]: 406.1351; found: 406.1348.

N-(3-([1,1'-Biphenyl]-4-yl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3t)



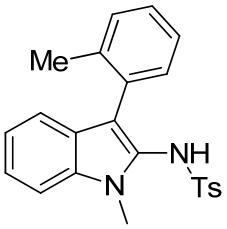
Light yellow solid (30 mg, 33%); m.p. 186.7 – 187.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.59 (m, 3H), 7.51 – 7.47 (m, 2H), 7.42 – 7.31 (m, 5H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.13 (m, 1H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.99 (b, 1H), 6.80 (d, *J* = 8.0 Hz, 2H), 3.94 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 140.7, 138.7, 135.1, 134.8, 132.0, 129.0, 128.9, 128.9, 127.3, 127.2, 126.8, 126.7, 126.5, 125.0, 123.1, 120.3, 119.7, 112.5, 110.0, 30.0, 21.5; IR (neat) *v* 3262, 3057, 2923,1596, 1567, 1487, 1393, 1331, 1257, 1163, 1090 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{28}H_{24}N_2O_2S$]: 452.1558; found: 452.1558.

4-Methyl-N-(1-methyl-3-(*m*-tolyl)-1H-indol-2-yl)benzenesulfonamide (3u)



White solid (63 mg, 81%); m.p. 125.7 – 126.9°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.20 (d, *J* = 8.4 Hz, 2H), 7.13 – 7.03 (m, 3H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.76 – 6.73 (m, 2H), 3.92 (s, 3H), 2.29 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 137.8, 135.1, 134.8, 132.8, 129.3, 129.0, 128.2, 127.2, 126.6, 126.4, 125.7, 125.1, 123.0, 120.2, 119.7, 112.8, 109.9, 30.1, 21.5, 21.4; IR (neat) *v* 3261, 3057, 2922, 1574, 1470, 1385, 1331, 1284, 1163, 1089 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{22}N_2O_2S$]: 390.1402; found: 390.1412.

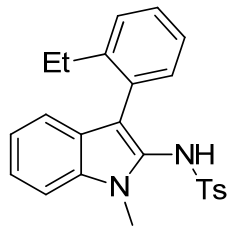
4-Methyl-N-(1-methyl-3-(o-tolyl)-1H-indol-2-yl)benzenesulfonamide (3v)



White solid (50 mg, 64%); m.p. 171.9 – 173.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.4 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.23 – 7.17 (m, 3H), 7.15 – 7.05 (m, 2H), 7.01 – 6.98 (m, 2H), 6.89 (d, *J* = 8.0 Hz, 2H), 6.74 (d, *J* = 7.2 Hz, 2H), 3.92 (s, 3H), 2.34 (s, 3H), 1.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 137.0, 135.3, 135.0, 131.9, 130.5, 130.0, 129.3, 126.9, 126.5, 125.5, 125.5, 122.8, 120.4, 119.9, 112.4, 109.9, 30.1, 21.5, 20.2; IR (neat) *v* 3258, 3058, 2924, 1599, 1567, 1470, 1371, 1330, 1254, 1163, 1092 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{22}N_2O_2S$]: 390.1402; found: 390.1398.

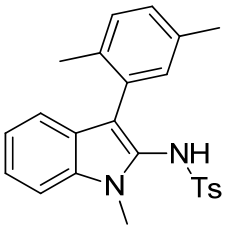
N-(3-(2-Ethylphenyl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3w)

White solid (68 mg, 85%); m.p. 139.4 – 140.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.4 Hz, 1H), 7.31 – 7.17 (m, 4H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.94 – 6,89 (m, 3H),6.55 – 6.53 (m, 2H), 3.91 (s,



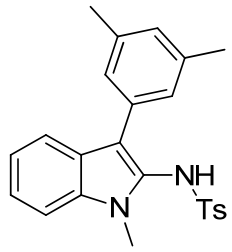
3H), 2.35 – 2.27 (m, 4H), 2.13– 2.04 (m, 1H), 0.95 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ143.6, 142.7, 135.5, 135.1, 131.1, 130.9, 129.3, 127.5, 127.2, 127.0, 126.6, 126.1, 125.3, 122.7, 120.1, 119.9, 112.0, 109.8, 30.2, 25.6, 21.5, 14.6; IR (neat) ν 3254, 3059, 2967, 1599, 1557,1470, 1432, 1390, 1328, 1253, 1162, 1092, 1013 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{24}N_2O_2S$]: 404.1558; found: 404.1554.

N-(3-(2,5-Dimethylphenyl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3x)



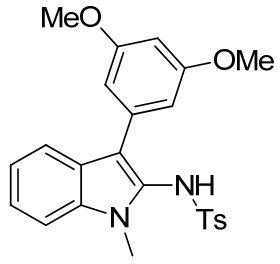
Colorless oil (72 mg, 89%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.29 (s, 1H), 7.45 (d, J = 8.0 Hz, 1H),7.24 – 7.19 (m, 3H), 7.00 – 6.96 (m, 4H), 6.93 – 6,83 (m, 3H),3.68 (s, 3H), 2.29 (s, 3H), 2.21 (s, 3H), 1.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 137.8, 134.7, 134.3, 133.9, 132.3, 132.1, 130.0, 129.4, 127.7, 127.6, 126.4, 125.5, 122.6, 120.1, 120.0, 113.1, 110.7, 29.6, 21.5, 21.0, 20.2; IR (neat) ν 3250, 3048, 2922, 1557, 1494,1470, 1433, 1385, 1328, 1257, 1162, 1091, 1019 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{24}N_2O_2S$]: 404.1558; found: 404.1556.

N-(3-(3,5-Dimethylphenyl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3y)



White solid (67 mg, 83%); m.p. 156.8 – 158.0 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.0 Hz, 1H), 7.38 (d, J = 8.4 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.22 (d, J = 8.0 Hz, 2H), 7.13 – 7.04 (m, 2H), 6.86 (d, J = 8.0 Hz, 2H), 6.76 (s, 1H), 6.56 (s, 2H), 3.91 (s, 3H), 2.29 (s, 3H), 2.22 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 137.7, 135.1, 132.7, 128.9, 127.6, 127.2, 126.4, 126.4, 125.1, 122.9, 120.1, 119.8, 112.8, 109.9, 30.0, 21.5, 21.3; IR (neat) ν 3264, 3030, 2919, 1602, 1557, 1471, 1430, 1379, 1332,1237, 1163, 1091 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{24}N_2O_2S$]: 404.1558; found: 404.1556.

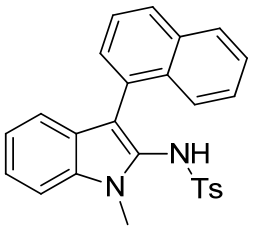
N-(3-(3,5-Dimethoxyphenyl)-1-methyl-1H-indol-2-yl)-4-methylbenzenesulfonamide (3z)



White solid (80 mg, 92%); m.p. 196.4 – 197.2 ^{o}C;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 8.0 Hz, 1H),7.38 (d, J = 8.4 Hz, 1H), 7.33 – 7.29 (m, 1H), 7.26 – 7.24 (m, 2H), 7.14 – 7.10 (m, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.26 (t, J = 2.4 Hz, 1H), 6.10 (d, J = 2.4 Hz, 2H),3.91 (s, 3H), 3.74 (s, 6H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 143.7, 135.0, 134.9, 134.9, 129.0, 127.3, 126.4, 124.9, 123.0, 120.3, 119.7, 112.8, 109.9, 106.8, 98.0, 55.2, 30.0, 21.3; IR (neat) ν 3272, 3006, 2938, 1594, 1471, 1454, 1424, 1394, 1374, 1337,

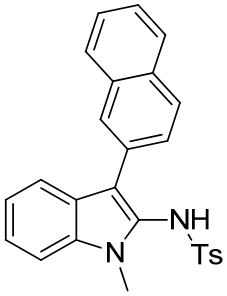
1285, 1204, 1158, 1091, 1064 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{24}N_2O_4S$]: 436.1457; found: 436.1462.

4-Methyl-N-(1-methyl-3-(naphthalen-1-yl)-1H-indol-2-yl)benzenesulfonamide (3A)



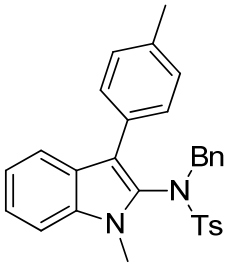
White solid (49 mg, 57%); m.p. 173.5 – 174.6 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.46 – 7.38 (m, 3H), 7.34 – 7.25 (m, 3H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.08 – 7.04 (m, 1H), 6.97 – 6.95 (m, 1H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.83 (b, 1H), 6.47 (d, *J* = 8.4 Hz, 2H), 4.01 (s, 3H), 2.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 135.1, 134.7, 133.7, 131.6, 130.4, 128.8, 128.3, 127.5, 127.5, 127.1, 126.5, 126.1, 126.0, 125.7, 125.7, 125.3, 122.9, 120.4, 120.1, 110.7, 109.9, 30.2, 21.4; IR (neat) v 3259, 3047, 2944,1615, 1595, 1557, 1470, 1411, 1366, 1327, 1247, 1162, 1092 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{26}H_{22}N_2O_2S$]: 426.1402; found: 426.1405.

4-Methyl-N-(1-methyl-3-(naphthalen-2-yl)-1H-indol-2-yl)benzenesulfonamide (3B)



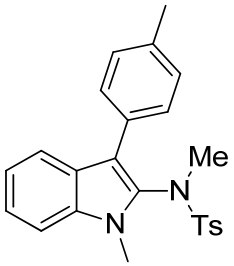
White solid (77 mg, 90%); m.p. 201.7 – 202.9 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.78 (m, 1H), 7.68 – 7.60 (m, 3H), 7.48 – 7.40 (m, 4H), 7.36 – 7.32 (m, 1H), 7.20 – 7.11 (m, 5H), 6.43 (d, *J* = 8.0 Hz, 2H), 3.95 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 135.1, 134.8, 133.5, 131.8, 130.5, 128.7, 127.8, 127.6, 127.4, 127.2, 127.1, 127.0, 126.6, 126.0, 125.5, 125.1, 123.2, 120.4, 119.7, 113.0, 110.0, 30.0, 21.2; IR (neat) *v* 3281, 3051, 2941, 1626, 1599, 1557, 1471, 1397, 1374, 1327, 1162, 1089 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{26}H_{22}N_2O_2S$]: 426.1402; found: 426.1399.

N-Benzyl-4-methyl-N-(1-methyl-3-(p-tolyl)-1H-indol-2-yl)benzenesulfonamide (5a)



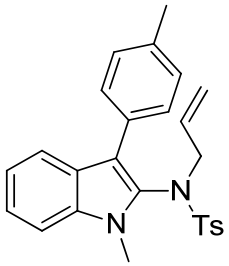
Colorless oil (93 mg, 97%); ^1H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.26 – 7.15 (m, 7H), 7.10 – 7.05 (m, 3H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.84 (d, *J* = 8.0 Hz, 2H), 5.06 (d, *J* = 13.6 Hz, 1H), 4.21 (d, *J* = 14.0 Hz, 1H), 3.24 (s, 3H), 2.45 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 136.9, 136.0, 135.6, 135.0, 130.4, 129.6, 129.5, 129.3, 128.9, 128.5, 128.2, 127.8, 126.1, 122.8, 120.0, 119.8, 114.1, 109.8, 55.7, 29.8, 21.6, 21.2; IR (neat) *v* 3030, 2943, 1598, 1556, 1470, 1353, 1250, 1162, 1091, 1047 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{30}H_{28}N_2O_2S$]: 480.1872; found: 480.1877.

N,4-Dimethyl-N-(1-methyl-3-(p-tolyl)-1H-indol-2-yl)benzenesulfonamide (5b)



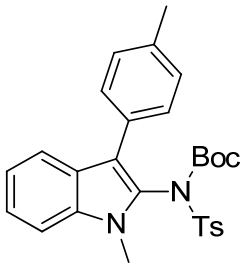
White solid (76 mg, 94%); m.p. 180.5 – 181.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 1H), 7.36 –7.29 (m, 4H), 7.14 – 7.10 (m, 1H), 7.01 – 6.94 (m, 6H), 3.80 (s, 3H), 3.38 (s, 3H), 2.35 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 136.0, 135.7, 134.9, 131.6, 130.6, 129.1, 129.0, 128.8, 127.3, 125.6, 123.1, 120.1, 120.0, 113.9, 109.7, 40.0, 29.6, 21.5, 21.2; IR (neat) *v* 3054, 2922, 1598, 1564, 1510, 1470, 1434, 1385, 1346, 1265, 1162, 1089, 1070 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{24}N_2O_2S$]: 404.1558; found: 404.1555.

N-Allyl-4-methyl-N-(1-methyl-3-(p-tolyl)-1H-indol-2-yl)benzenesulfonamide (5c)



White solid (85 mg, 99%); m.p. 160.8 – 161.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.35 – 7.28 (m, 2H), 7.12 – 7.06 (m, 3H), 6.95 – 6.91 (m, 4H), 5.89–5.79 (m, 1H), 5.06–5.01 (m, 2H), 4.49 (dd, J_1 = 14.4 Hz, J_2 = 6.0 Hz, 1H), 3.88 (dd, J_1 = 14.0 Hz, J_2 = 8.0 Hz, 1H), 3.77 (s, 3H), 2.39 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 136.5, 135.9, 135.0, 132.5, 130.4, 129.8, 129.3, 129.2, 128.8, 128.3, 127.6, 126.4, 125.9, 125.7, 123.0, 120.1, 119.9, 114.4, 109.8, 55.4, 30.3, 21.5, 21.2; IR (neat) *v* 3026, 2922, 1598, 1597, 1563, 1508, 1470, 1429, 1386, 1350, 1255, 1163, 1090, 1058 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{26}H_{26}N_2O_2S$]: 430.1715; found: 430.1719.

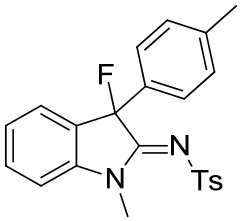
***tert*-Butyl (1-methyl-3-(p-tolyl)-1H-indol-2-yl)(tosyl)carbamate (5d)**



White solid (89 mg, 91%); m.p. 171.6 – 172.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H),7.34– 7.32 (m, 1H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.18– 7.14 (m, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 2H), 3.81 (s, 3H), 3.38 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 144.0, 136.1, 135.7, 135.4, 130.8, 129.3, 128.8, 128.8, 128.6, 126.6, 125.3, 123.2, 120.3, 120.1, 114.5, 109.8, 85.1, 29.1, 27.9, 21.6, 21.2; IR (neat) *v* 2980, 2919, 1738, 1615, 1597, 1567, 1509, 1471, 1433, 1371, 1331, 1287, 1255, 1174, 1148, 1088 cm^{-1}; HRMS (ESI): $[M+H]^+$calcd for $[C_{28}H_{31}N_2O_4S]^+$: 491.1999; found: 491.1996.

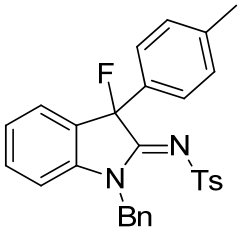
N-(3-Fluoro-1-methyl-3-(p-tolyl)indolin-2-ylidene)-4-methylbenzenesulfonamide (6a)

White solid (40 mg, 97 %); m.p. 198.6 – 199.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 2H), 7.38–7.33 (m, 1H), 7.24 – 7.15 (m, 7H), 7.64 (t, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H),3.44 (s, 3H), 2.38 (s, 3H),



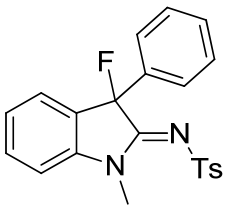
2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4 (d, *J* = 22.6 Hz), 142.5, 142.4, 139.8, 138.4, 134.1 (d, *J* = 26.2 Hz), 131.0 (d, *J* = 2.7 Hz), 130.3 (d, *J* = 20.8 Hz), 129.2 (d, *J* = 0.7 Hz), 129.0, 126.8, 125.1, 124.5 (d, *J* = 2.5 Hz), 123.8 (d, *J* = 6.3 Hz), 109.6, 96.9 (d, *J* = 197.3 Hz), 29.5, 21.5, 21.3; IR (neat) *v* 3058, 3029, 2923, 1633, 1593, 1493, 1471, 1382, 1363, 1316, 1184, 1157, 1088, 1019 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{21}FN_2O_2S$]: 408.1308; found: 408.1309.

N-(1-Benzyl-3-fluoro-3-(*p*-tolyl)indolin-2-ylidene)-4-methylbenzenesulfonamide (6b)



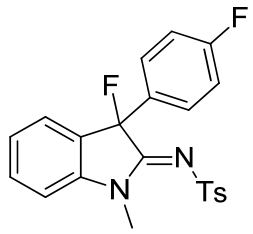
Colorless liquid (47 mg, 98 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.27 – 7.21 (m, 8H), 7.17 – 7.14 (m, 5H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 5.16 (d, *J* = 15.6 Hz, 1H), 4.97 (d, *J* = 15.2 Hz, 1H), 2.37 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4 (d, *J* = 22.6 Hz), 142.4, 141.3(d, *J* = 5.1 Hz), 139.5, 138.3, 134.5, 134.1 (d, *J* = 26.1 Hz), 130.8 (d, *J* = 2.7 Hz), 130.6 (d, *J* = 21.0 Hz), 129.2, 129.2, 128.9, 128.9, 128.0, 127.6, 126.8, 125.1, 124.5(d, *J* = 2.5 Hz), 123.6 (d, *J* = 6.3 Hz), 110.3, 96.7 (d, *J* = 198.3 Hz), 46.1, 21.5, 21.3; IR (neat) *v* 3062, 3031, 2923, 1627, 1592, 1513, 1487, 1470, 1455, 1392, 1351, 1318, 1300, 1209, 1182, 1155, 1050, 1009 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{29}H_{25}FN_2O_2S$]: 484.1621; found: 484.1624.

N-(3-Fluoro-1-methyl-3-phenylindolin-2-ylidene)-4-methylbenzenesulfonamide (6c)



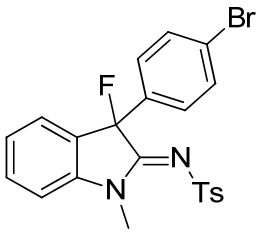
White solid (38 mg, 95%); m.p. 175.8 – 177.0 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.32 (m, 6H), 7.20 – 7.17 (m, 3H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 3.44 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2 (d, *J* = 22.4 Hz), 142.5, 142.4 (d, *J* = 5.2 Hz), 139.6, 137.0 (d, *J* = 26.0 Hz), 131.1 (d, *J* = 2.7 Hz), 130.1 (d, *J* = 20.5 Hz), 129.0, 128.5, 128.5, 128.5, 126.8, 125.1, 124.5(d, *J* = 2.5 Hz), 123.8 (d, *J* = 6.5 Hz), 109.6, 96.8 (d, *J* = 197.9 Hz), 29.5, 21.5; IR (neat) *v* 3063, 3024, 2920, 1633, 1592, 1493, 1471, 1450, 1382, 1364, 1317, 1303, 1197, 1156, 1088, 1019, 994 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{22}H_{19}FN_2O_2S$]: 394.1151; found: 394.1150

N-(3-Fluoro-3-(4-fluorophenyl)-1-methylindolin-2-ylidene)-4-methylbenzenesulfonamide (6d)



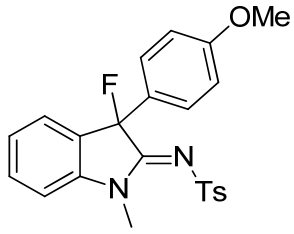
White solid (39 mg, 94 %); m.p. 163.5 – 164.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 2H),7.39 (t, *J* = 8.0 Hz, 1H), 7.34 – 7.30 (m, 2H), 7.22 – 7.17 (m, 3H), 7.12 – 7.02 (m, 3H), 6.96 (d, *J* = 7.6 Hz, 1H), 3.44 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9 (d, *J* = 22.7 Hz), 162.7 (d, *J* = 246.6 Hz), 163.8, 161.5, 161.5, 142.7, 142.5 (d, *J* = 5.3 Hz), 139.6, 132.9 (dd, J_1= 26.7 Hz, J_2 = 3.3 Hz), 131.3 (d, *J* = 2.8 Hz), 129.8 (d, *J* = 20.1 Hz), 129.1, 126.7, 126.1 (d, *J* = 6.7 Hz), 126.0 (d, *J* = 6.6 Hz), 125.1, 124.7 (d, *J* = 2.6Hz), 115.5 (d, *J* = 22.0 Hz), 109.7, 96.4 (d, *J* = 197.8 Hz), 29.6, 21.5; IR (neat) *v* 3066, 3028, 2916, 1633, 1592, 1511, 1493, 1471, 1384, 1360, 1317, 1304, 1223, 1197, 1158,1088, 1019, 996 cm^{-1}; HRMS (ESI): $[M+Na]^+$calcd for $[C_{22}H_{18}F_2N_2NaO_2S]^+$: 435.0949; found: 435.0947.

N-(3-(4-Bromophenyl)-3-fluoro-1-methylindolin-2-ylidene)-4-methylbenzenesulfonamide (6e)



White solid (45 mg, 96 %); m.p. 186.5 – 187.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.41 – 7.37 (m, 1H), 7.21 (d, *J* = 8.4 Hz, 4H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.11– 7.07 (m, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 3.44 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7 (d, *J* = 22.5 Hz), 142.7, 142.5 (d, *J* = 5.0 Hz), 139.5, 136.1 (d, *J* = 26.4 Hz), 132.0, 131.7, 131.4 (d, *J* = 2.7 Hz), 129.6 (d, *J* = 20.4 Hz), 129.1, 127.7 (d, *J* = 43.5 Hz), 126.7, 125.7 (d, *J* = 6.5 Hz), 125.1, 124.7 (d, *J* = 2.4 Hz), 122.7, 109.7, 96.4 (d, *J* = 198.9 Hz), 29.6, 21.5; IR (neat) *v* 3064, 2924, 1731, 1632, 1589, 1488, 1471, 1383, 1316, 1183, 1156, 1087, 1010 cm^{-1}; HRMS (ESI): $[M+H]^+$calcd for $[C_{22}H_{19}BrFN_2O_2S]^+$: 473.0329; found: 473.0319.

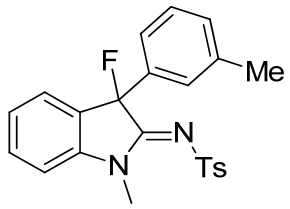
N-(3-Fluoro-3-(4-methoxyphenyl)-1-methylindolin-2-ylidene)-4-methylbenzenesulfonamide (6f)



White solid (38 mg, 90 %); m.p. 189.1 – 190.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.28 – 7.26 (m, 2H), 7.21 – 7.19 (m, 3H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H), 3.45 (s, 3H),2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3 (d, *J* = 22.7 Hz), 159.7, 142.5 (d, *J* = 5.2 Hz), 142.4, 139.8, 131.0 (d, *J* = 2.6 Hz), 130.2 (d, *J* = 20.7 Hz), 129.0, 128.9 (d, *J* = 26.7 Hz), 126.7, 125.5 (d, *J* = 6.3 Hz), 125.1, 124.5 (d, *J* = 2.5 Hz), 113.8, 109.6, 96.8 (d, *J* = 196.7 Hz), 55.2, 29.7, 21.5; IR (neat) *v* 3058, 2935, 2839, 1631, 1593, 1514, 1490, 1471, 1385, 1360, 1316, 1302, 1254, 1179, 1157, 1088, 1031, 994 cm^{-1}; HRMS (ESI): $[M+H]^+$calcd for $[C_{23}H_{22}FN_2O_3S]^+$: 425.1330;

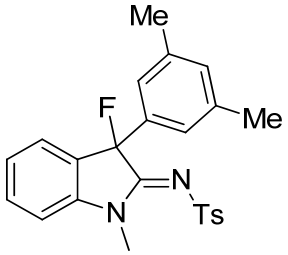
found: 425.1314.

N-(3-Fluoro-1-methyl-3-(m-tolyl)indolin-2-ylidene)-4-methylbenzenesulfonamide (6g)



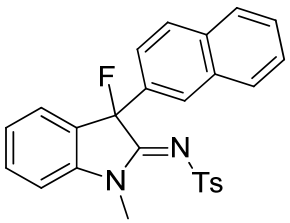
Colorless liquid (40 mg, 98 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.28 – 7.24 (m, 1H), 7.21 – 7.14 (m, 5H), 7.08 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 1H), 3.45 (s, 3H), 2.38 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3 (d, *J* = 22.2 Hz), 142.5, 142.4 (d, *J* = 5.1 Hz), 139.6, 138.2 (d, *J* = 1.0 Hz), 136.9 (d, *J* = 25.9 Hz), 131.0 (d, *J* = 2.7 Hz), 130.2 (d, *J* = 20.8 Hz), 129.4, 129.0, 128.5 (d, *J* = 0.7 Hz), 126.8, 125.1 (d, *J* = 0.6 Hz), 124.5 (d, *J* = 2.5 Hz), 124.2 (d, *J* = 6.1 Hz), 120.9 (d, *J* = 6.6 Hz), 109.6, 96.8 (d, *J* = 197.7 Hz), 29.6, 21.5, 21.5; IR (neat) *ν* 3062, 2924, 2856, 1633, 1594, 1489, 1471, 1382, 1360, 1317, 1300, 1212, 1157, 1087, 1016, 990 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{23}H_{21}FN_2O_2S$]: 408.1308; found: 408.1307.

N-(3-(3,5-Dimethylphenyl)-3-fluoro-1-methylindolin-2-ylidene)-4-methylbenzenesulfonamide (6h)



White solid (38 mg, 91 %); m.p. 184.0 – 185.1 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.95 – 6.91 (m, 4H), 3.45 (s, 3H), 2.37 (s, 3H), 2.27 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3 (d, *J* = 22.1 Hz), 142.4, 142.3 (d, *J* = 5.1 Hz), 139.6, 138.1 (d, *J* = 1.0 Hz), 136.8 (d, *J* = 25.6 Hz), 130.9 (d, *J* = 21.3 Hz), 130.3, 130.1, 128.9, 126.8, 125.1, 124.5(d, *J* = 2.5 Hz), 121.4 (d, *J* = 6.2 Hz), 109.6, 96.8 (d, *J* = 197.5 Hz), 29.6, 21.4, 21.4; IR (neat) *ν* 3067, 3028, 2920, 1633, 1591, 1493, 1471, 1382, 1360, 1317, 1300, 1222, 1157, 1132, 1088, 1016 cm^{-1}; HRMS (EI): M^+ calcd for [$C_{24}H_{23}FN_2O_2S$]: 422.1464; found: 422.1458.

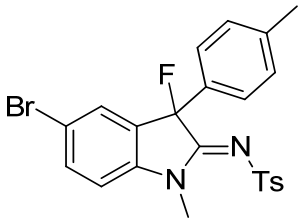
N-(3-Fluoro-1-methyl-3-(naphthalen-2-yl)indolin-2-ylidene)-4-methylbenzenesulfonamide (6i)



White solid (42 mg, 95 %); m.p. 164.2 – 165.1 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.45 (m, 4H), 7.51– 7.47 (m, 4H), 7.39– 7.35 (m, 2H), 7.06 (d, *J* = 7.6 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 1H), 3.50 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2 (d, *J* = 22.4 Hz), 142.5 (d, *J* = 5.2 Hz), 142.4, 139.5, 134.2 (d, *J* = 25.9 Hz), 133.0 (d, *J* = 27.9 Hz), 131.2 (d, *J* = 2.7 Hz), 130.0 (d, *J* = 20.7 Hz), 129.0, 128.9,

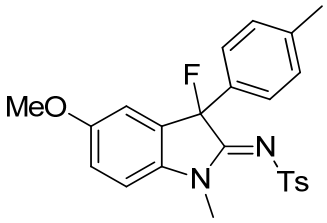
128.5 (d, J = 1.2 Hz), 128.3, 127.7, 127.5 (d, J = 8.2 Hz), 126.7, 126.5 (d, J = 6.3 Hz), 125.2, 124.6 (d, J = 2.5 Hz), 123.1 (d, J = 6.7 Hz), 121.4 (d, J = 6.2 Hz), 109.7, 96.9 (d, J = 198.4 Hz), 29.6, 21.4; IR (neat) ν 3061, 2920, 1730, 1633, 1593, 1489, 1471, 1427, 1385, 1356, 1315, 1230, 1156, 1087, 1020 cm^{-1}; HRMS (ESI): $[M+H]^+$calcd for $[C_{26}H_{22}FN_2O_2S]^+$: 445.1381; found: 445.1373.

N-(5-Bromo-3-fluoro-1-methyl-3-(p-tolyl)indolin-2-ylidene)-4-methylbenzenesulfonamide (6j)



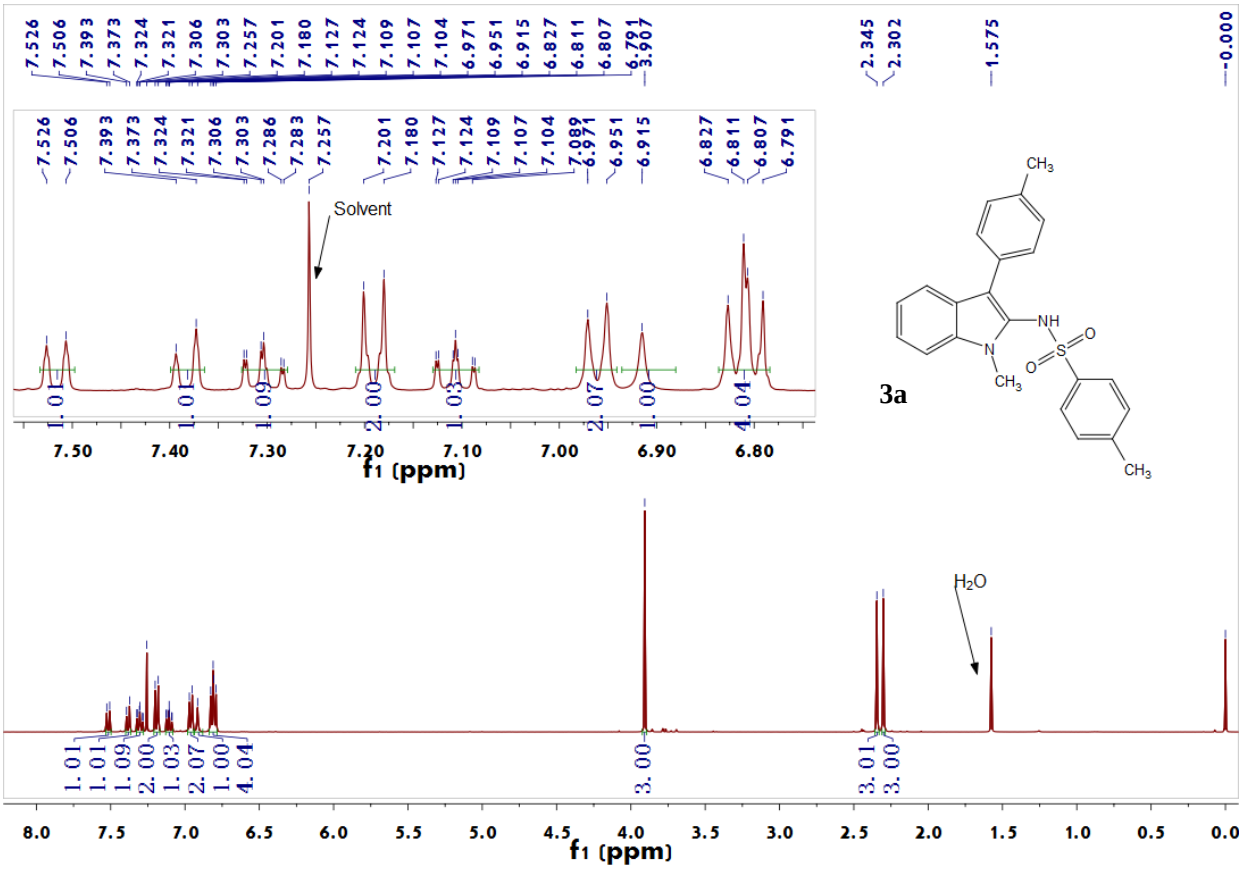
White solid (48 mg, 99 %); m.p. 191.2 – 192.3 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 8.4 Hz, 2H), 7.49– 7.46 (m, 1H), 7.29– 7.28 (m, 1H), 7.22 – 7.17 (m, 6H), 6.81 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 3.41 (s, 3H), 2.38 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8 (d, J = 22.5 Hz), 142.7, 141.4 (d, J = 4.9 Hz), 139.4, 138.8, 133.8 (d, J = 2.5 Hz), 133.5 (d, J = 26.0 Hz), 132.0 (d, J = 21.0 Hz), 129.4 (d, J = 0.7 Hz), 129.0, 128.3, 126.9, 123.7 (d, J = 6.3 Hz), 117.2 (d, J = 2.9 Hz), 111.0, 96.4 (d, J = 198.9 Hz), 29.6, 21.5, 21.3; IR (neat) ν 3024, 2923, 1731, 1622, 1594, 1510, 1488, 1417, 1356, 1317, 1282, 1258, 1184, 1158, 1088, 1020 cm^{-1}; HRMS (ESI): $[M+H]^+$calcd for $[C_{23}H_{21}FBrN_2O_2S]^+$: 487.0486; found: 487.0462.

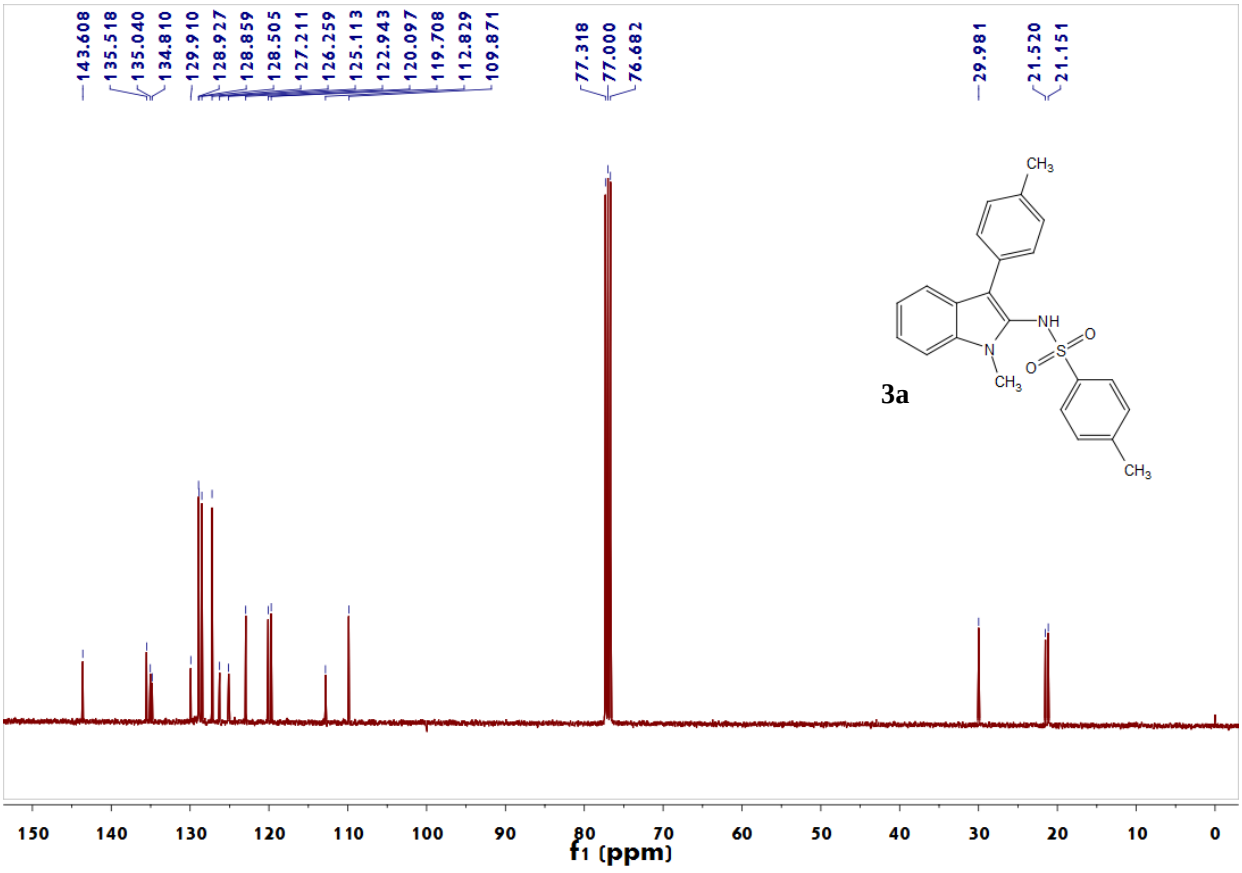
N-(3-Fluoro-5-methoxy-1-methyl-3-(p-tolyl)indolin-2-ylidene)-4-methylbenzenesulfonamide (6k)

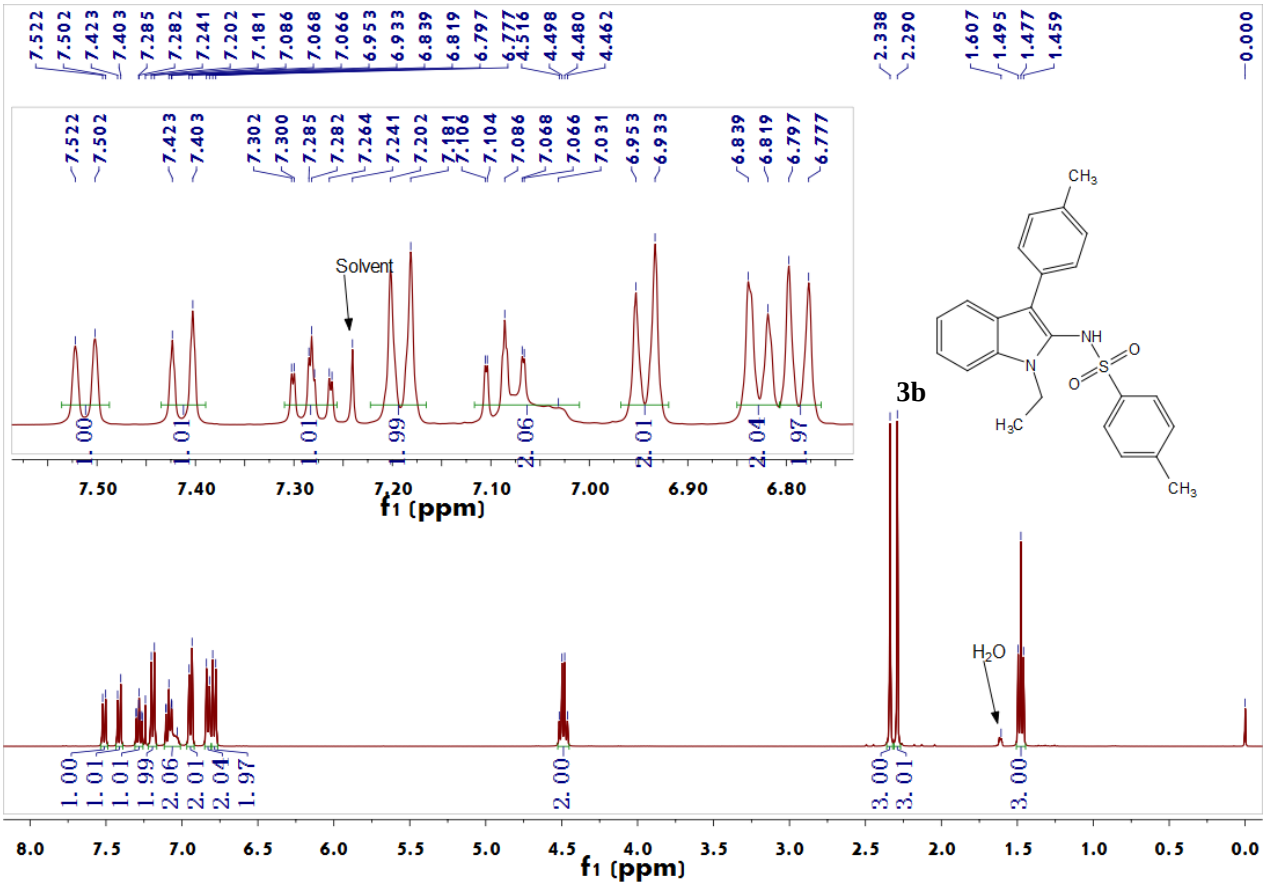


White solid (36 mg, 81 %); m.p. 196.5 – 197.7 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.4 Hz, 2H),7.22 (d, J = 8.4 Hz, 2H), 7.18 – 7.14 (m, 4H), 6.88– 6.83 (m, 2H), 6.77 (s, 1H), 3.72 (s, 3H), 3.43 (s, 3H), 2.37 (s, 3H),2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2 (d, J = 22.5 Hz), 157.3 (d, J = 2.6 Hz), 142.3, 140.0, 138.4, 135.7 (d, J = 5.3 Hz), 134.0 (d, J = 26.2 Hz), 131.4 (d, J = 20.3 Hz), 129.2, 128.9, 126.7, 123.9 (d, J = 6.4 Hz), 115.7 (d, J = 2.6 Hz), 111.7, 110.3, 97.1 (d, J = 197.9 Hz), 55.8, 29.8, 21.4, 21.2; IR (neat) ν 2924, 2834, 1622, 1594, 1496, 1431, 1358, 1315, 1288, 1224, 1155, 1089, 1036, 1002 cm^{-1}; HRMS (ESI): $[M+H]^+$calcd for $[C_{24}H_{24}FN_2O_3S]^+$: 439.1486; found: 439.1474.

The ^{1}H and ^{13}C NMR Spectra of Products



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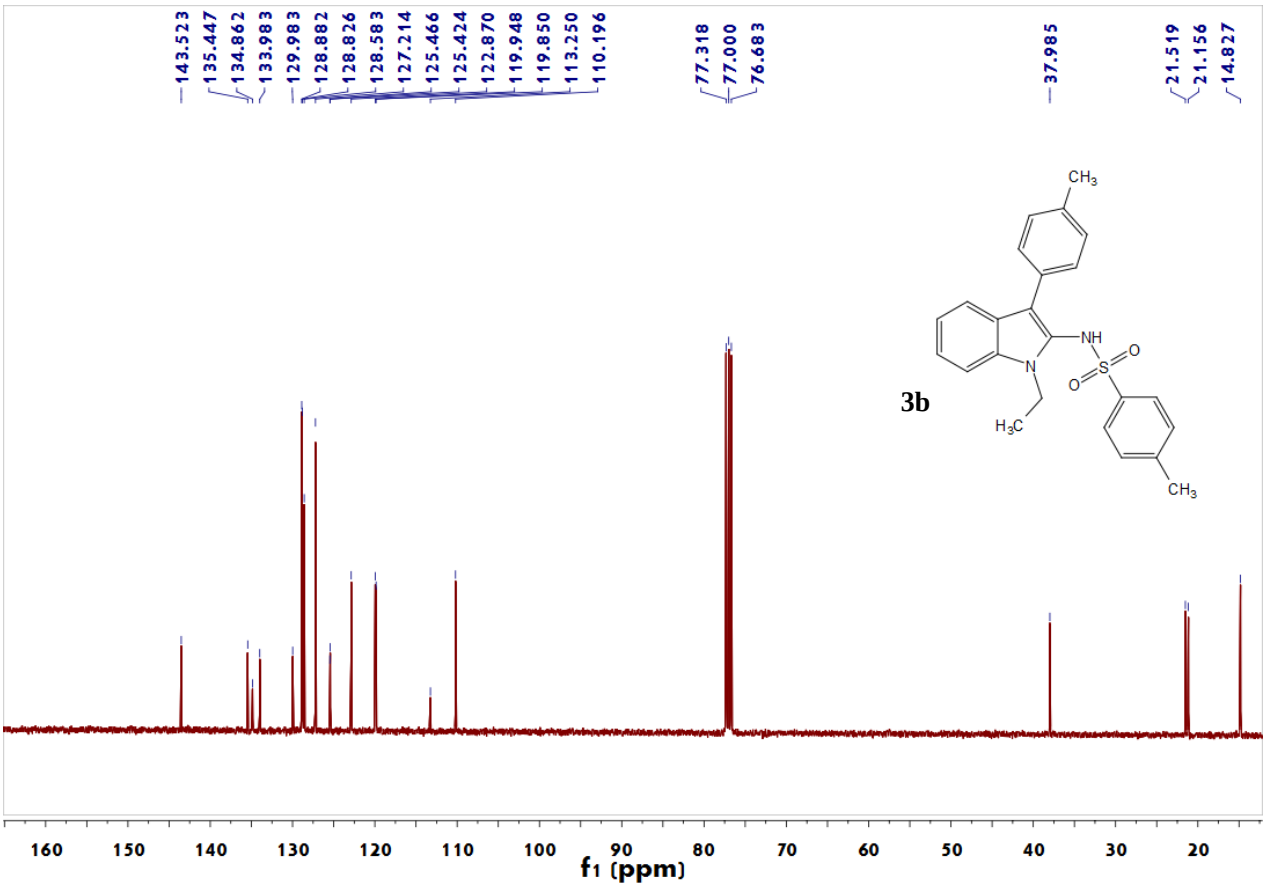
7.502
7.423
7.403
7.285
7.282
7.241
7.202
7.181
7.086
7.068
7.066
6.953
6.933
6.839
6.819
6.797
6.777
4.516
4.498
4.480
4.462
2.338
2.290
1.607
1.495
1.477
1.459
0.000
Solvent
3b
H2O
f1 (ppm)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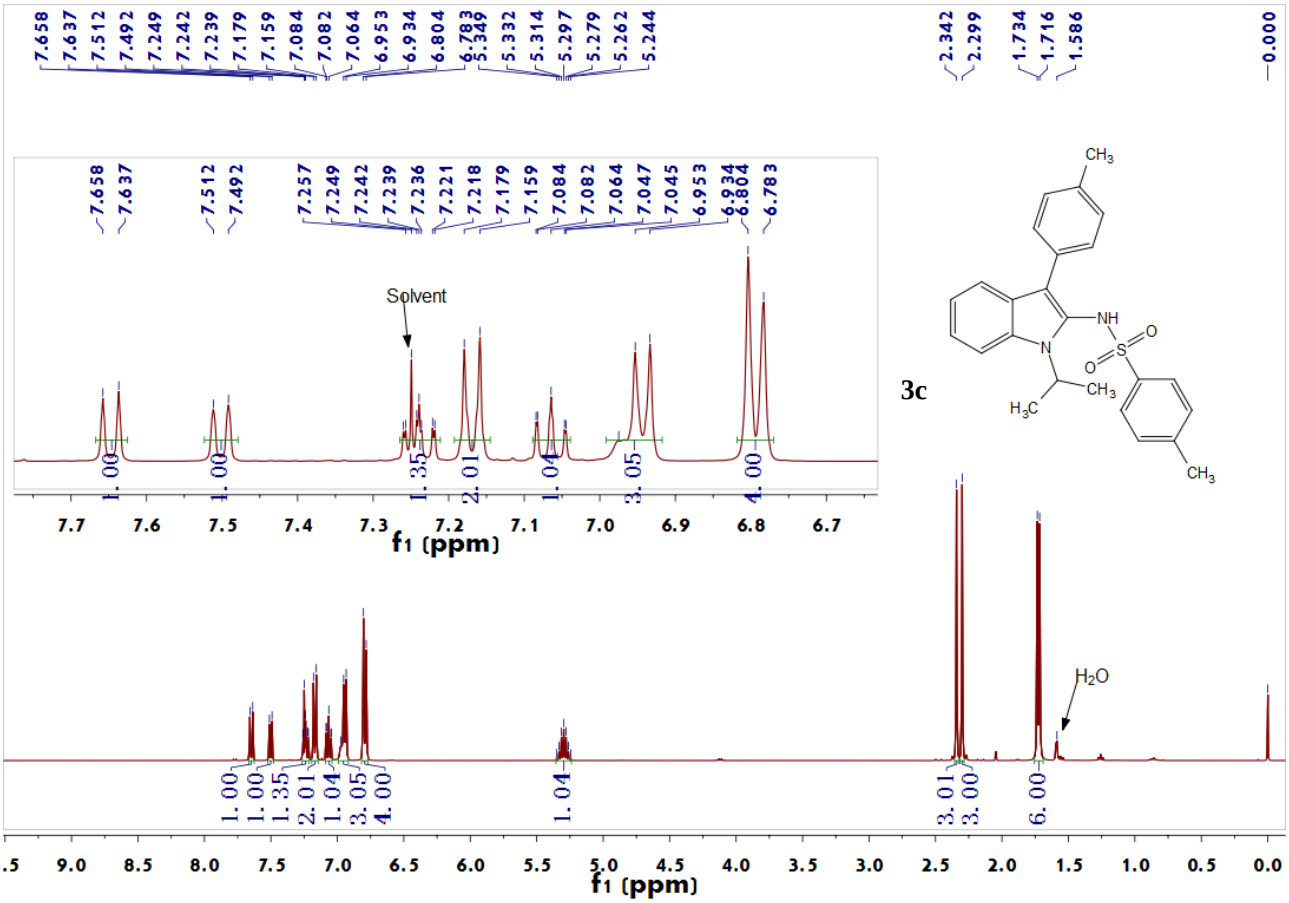
134.862
133.983
129.983
128.882
128.826
128.583
127.214
125.466
125.424
122.870
119.948
119.850
113.250
110.196
77.318
77.000
76.683
37.985
21.519
21.156
14.827
3b
f1 (ppm)


7.658
7.637
7.512
7.492
7.249
7.242
7.239
7.179
7.159
7.084
7.082
7.064
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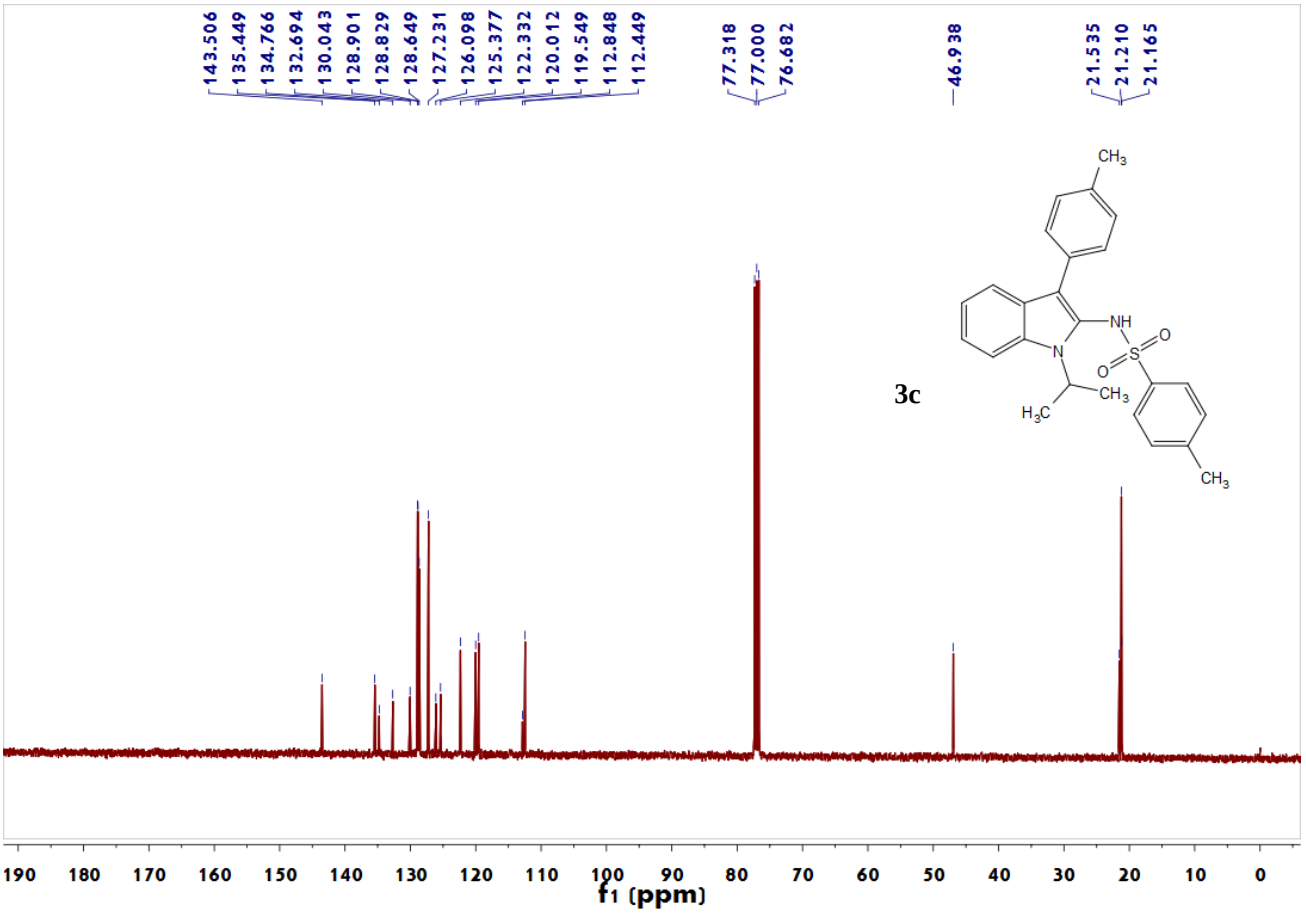
6.934
6.804
6.783
5.349
5.332
5.314
5.297
5.279
5.262
5.244
2.342
2.299
1.734
1.716
1.586
0.000
Solvent
3c
NH
N
S
O
CH3
H3C
H2O
1.00
1.00
1.35
2.01
1.04
3.05
4.00
1.04
3.01
3.00
6.00
f1 (ppm)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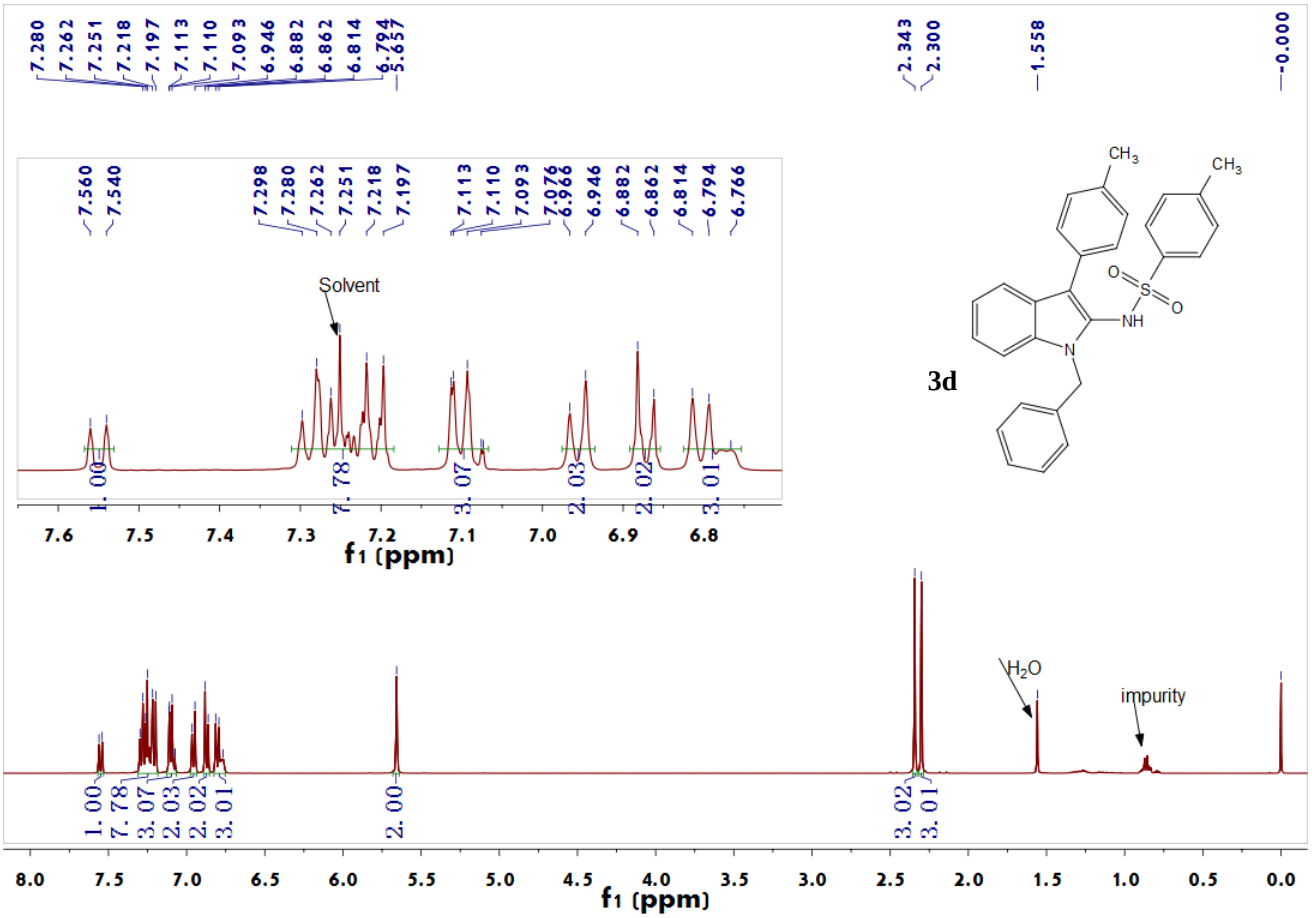
132.694
130.043
128.901
128.829
128.649
127.231
126.098
125.377
122.332
120.012
119.549
112.848
112.449
77.318
77.000
76.682
46.938
21.535
21.210
21.165
3c
NH
N
S
O
CH3
H3C
f1 (ppm)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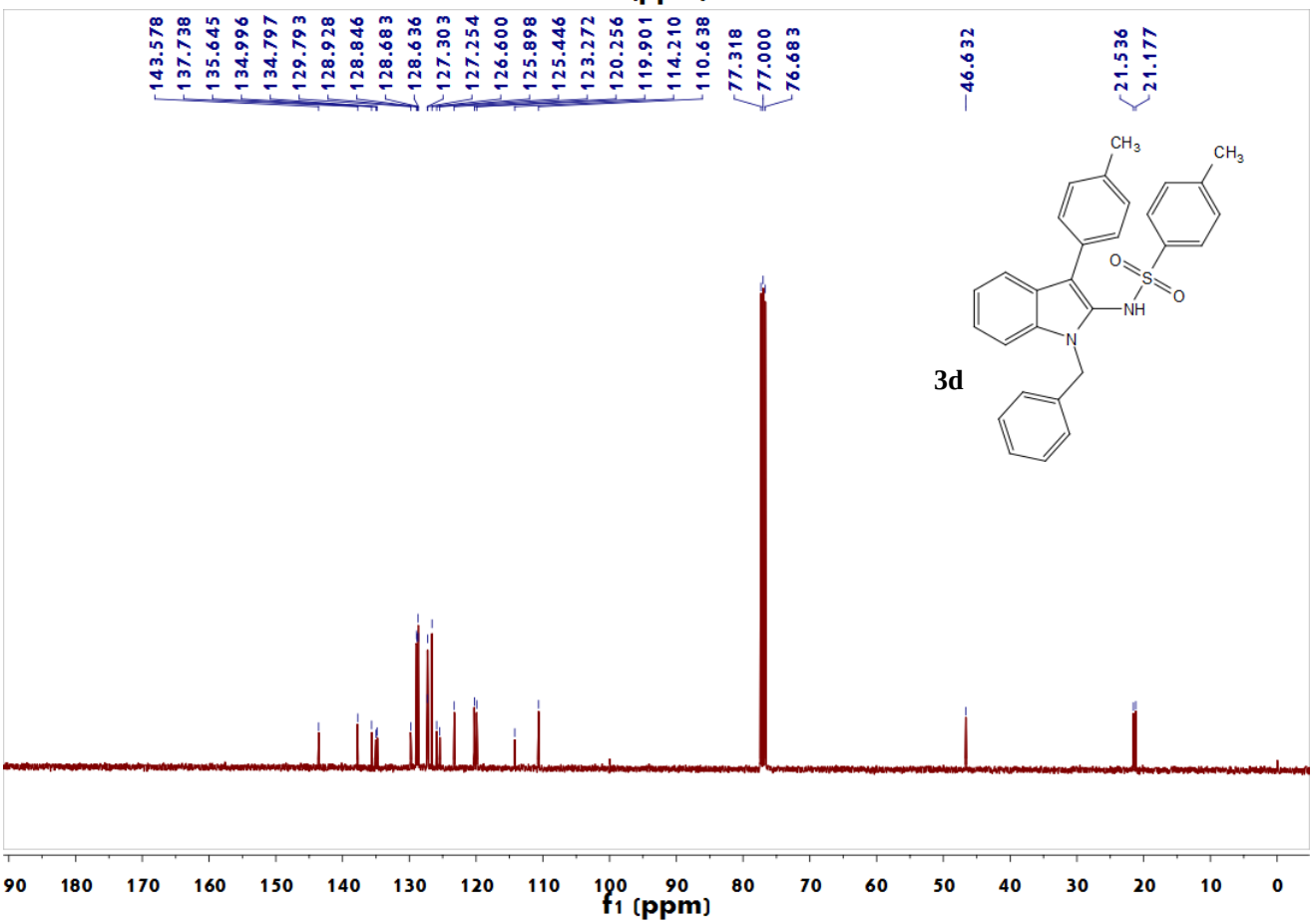
7.262
7.251
7.218
7.197
7.113
7.110
7.093
6.946
6.882
6.862
6.814
6.794
5.657
2.343
2.300
1.558
0.000
7.560
7.540
7.298
7.280
7.262
7.251
7.218
7.197
7.113
7.110
7.093
7.076
6.966
6.946
6.882
6.862
6.814
6.794
6.766
Solvent
1.00
7.78
3.07
2.03
2.02
3.01
f1 (ppm)
CH3
CH3
O
S
O
NH
N
3d
H2O
impurity
1.00
7.78
3.07
2.03
2.02
3.01
2.00
3.02
3.01
f1 (ppm)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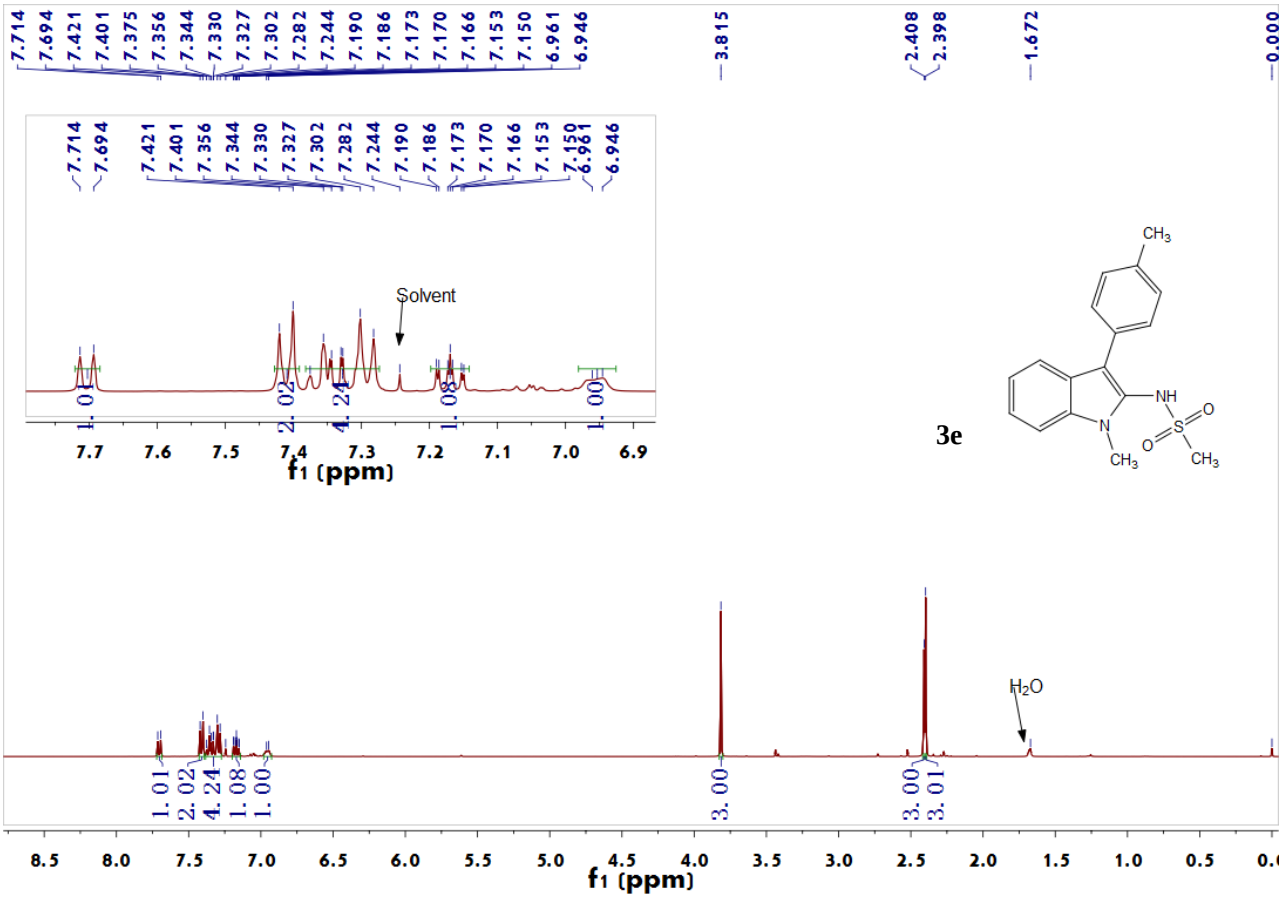
128.683
128.636
127.303
127.254
126.600
125.898
125.446
123.272
120.256
119.901
114.210
110.638
77.318
77.000
76.683
46.632
21.536
21.177
CH3
CH3
O
S
O
NH
N
3d
f1 (ppm)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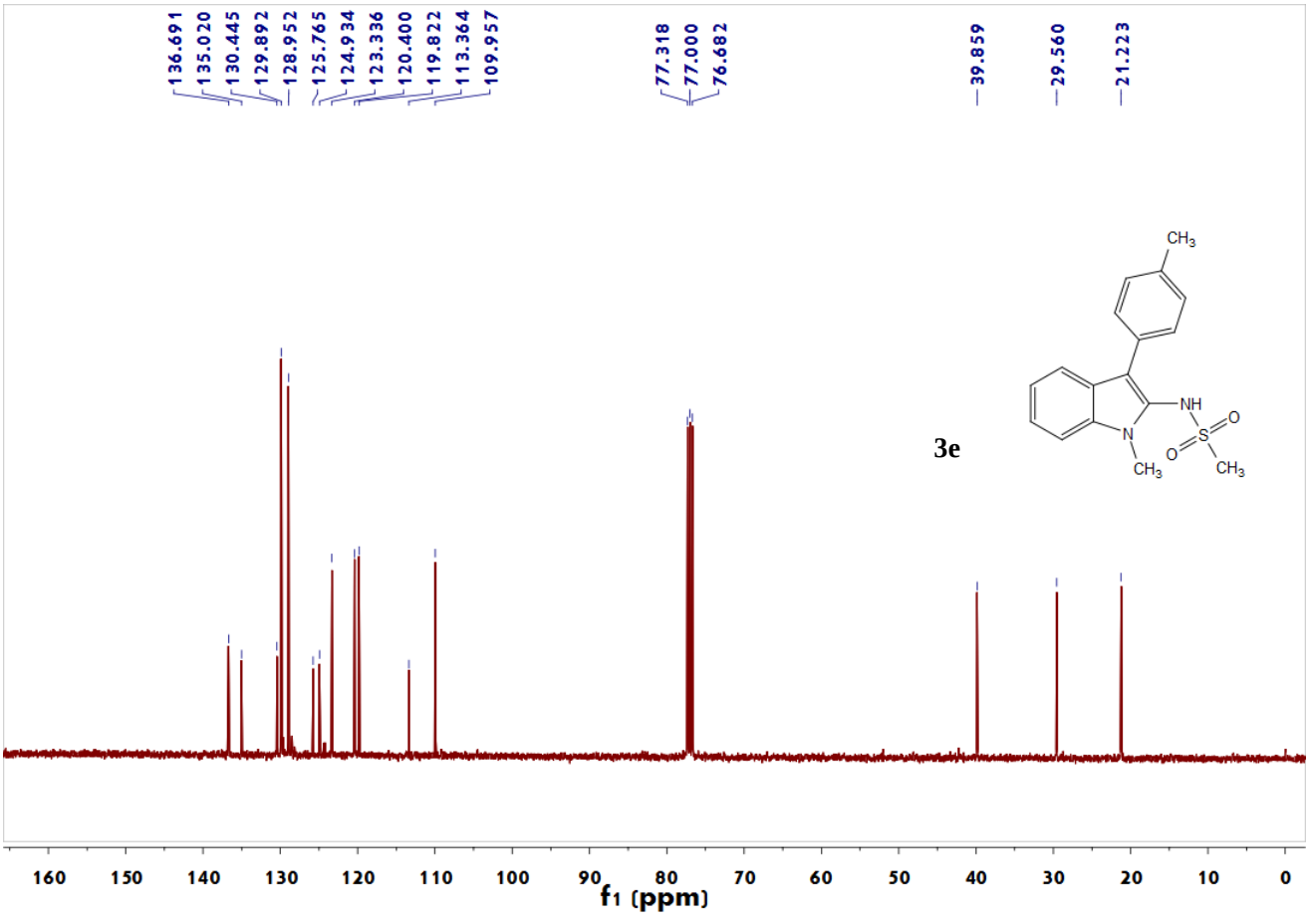
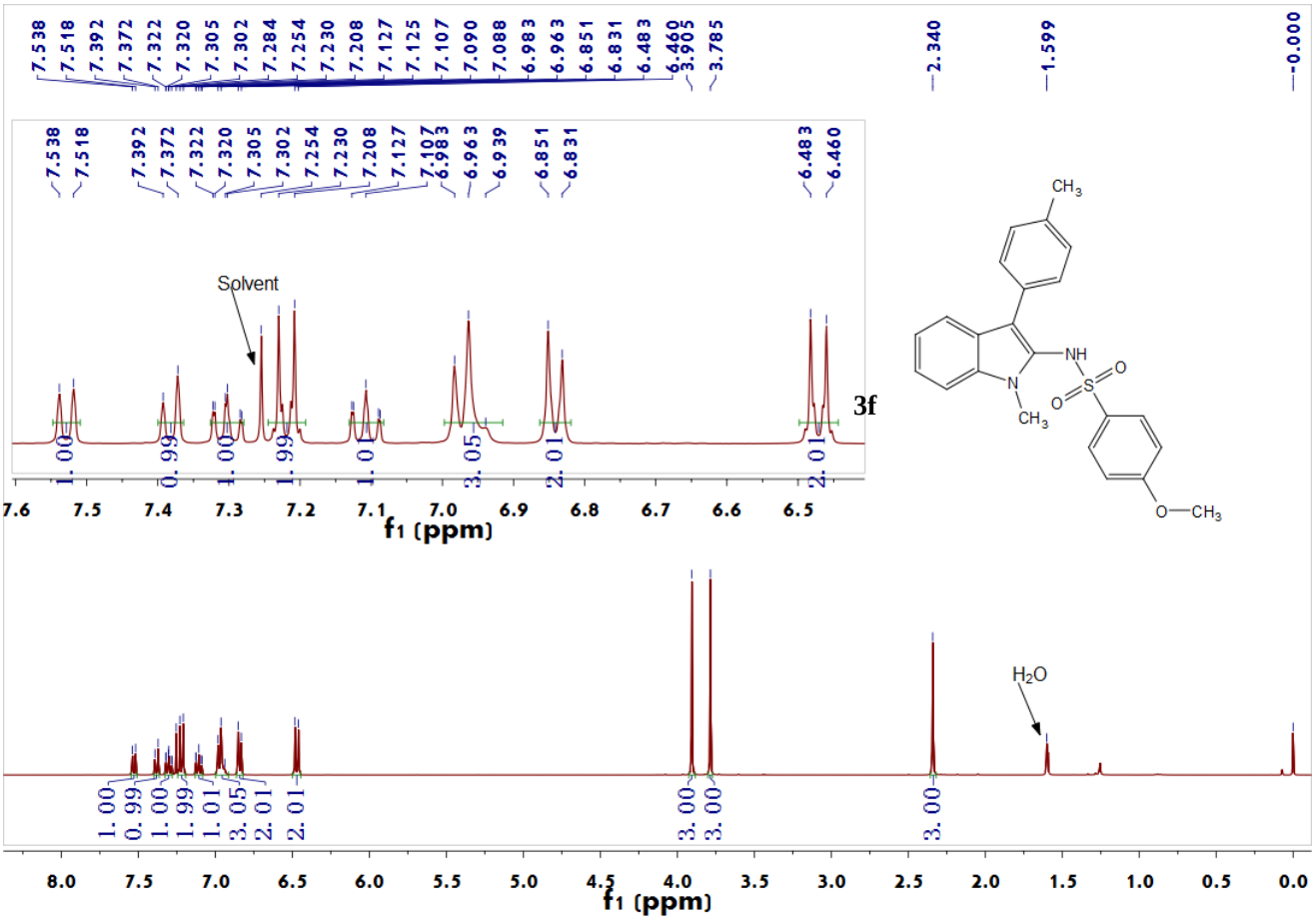
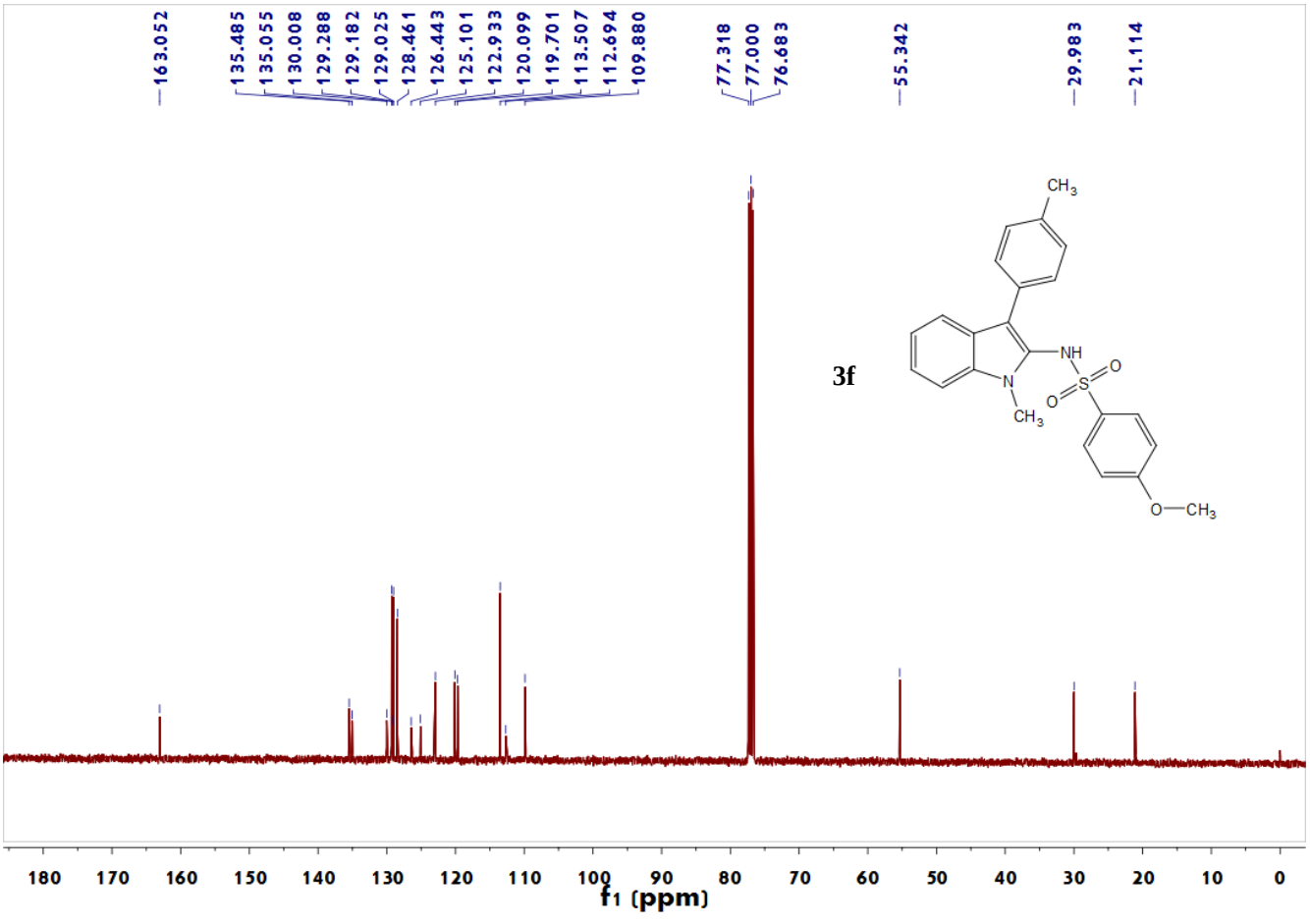
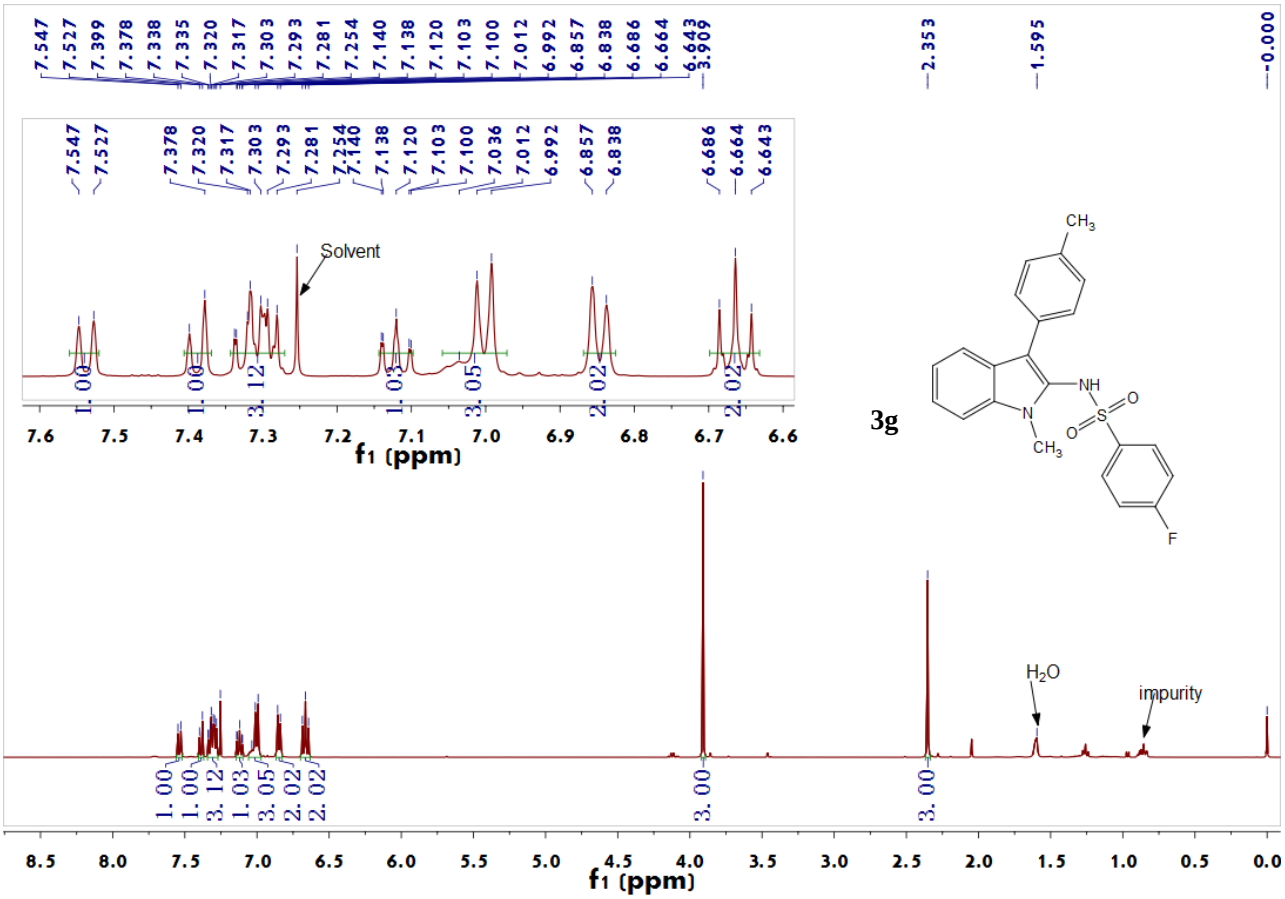
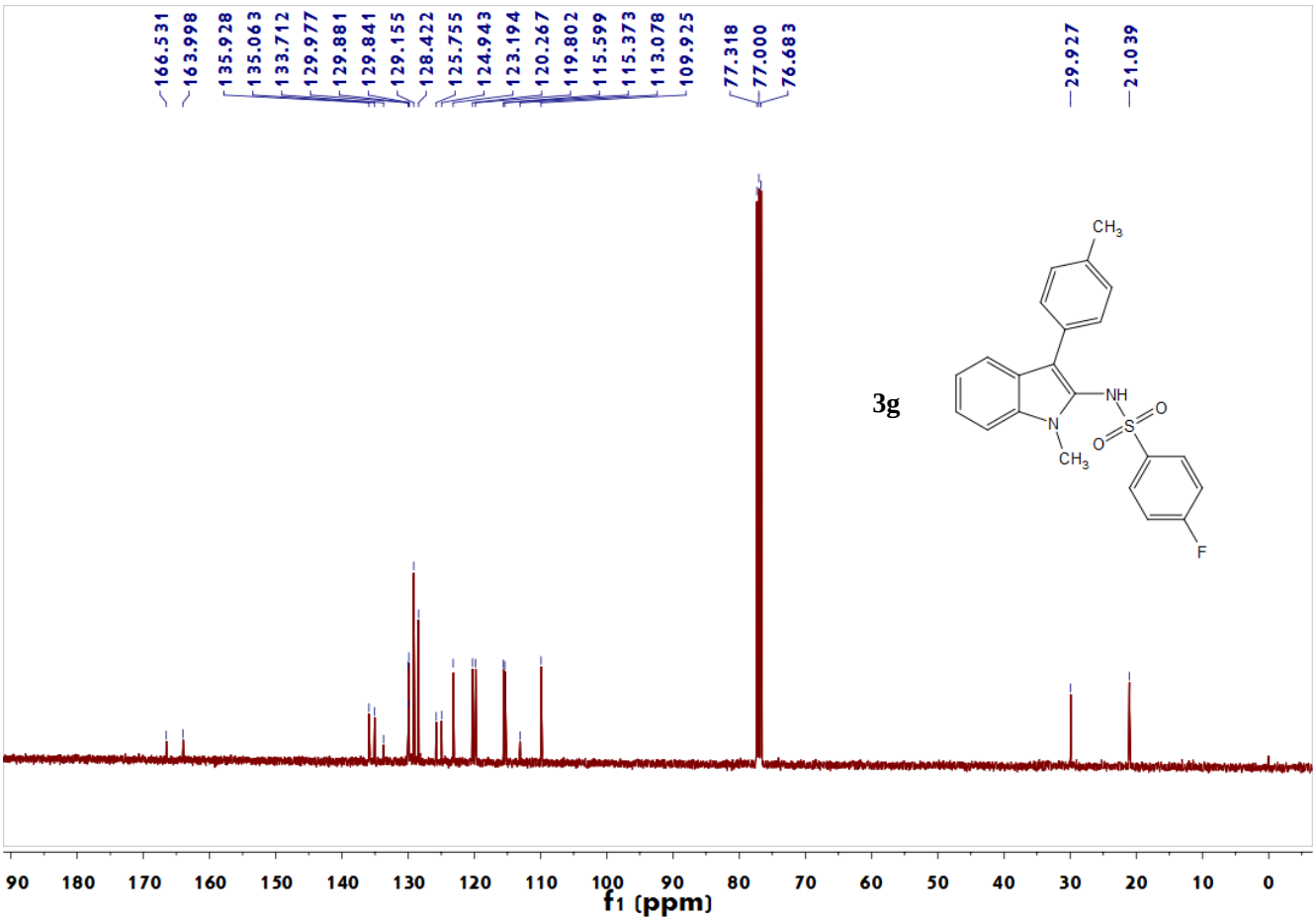
7.694
7.421
7.401
7.375
7.356
7.344
7.330
7.327
7.302
7.282
7.244
7.190
7.186
7.173
7.170
7.166
7.153
7.150
6.961
6.946
3.815
2.408
2.398
1.672
0.000
Solvent
H2O
3e
f1 (ppm)

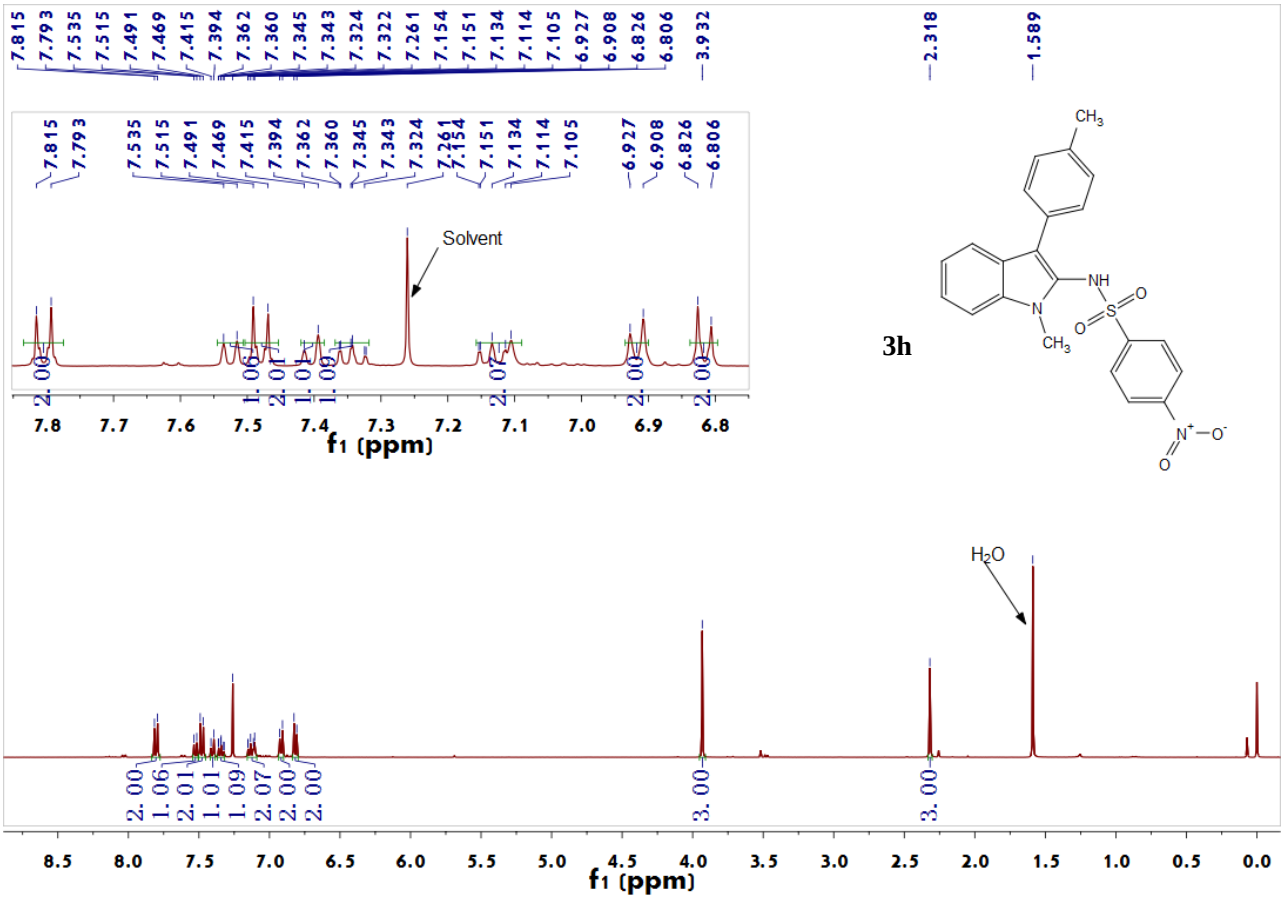

136.691
135.020
130.445
129.892
128.952
125.765
124.934
123.336
120.400
119.822
113.364
109.957
77.318
77.000
76.682
39.859
29.560
21.223
3e
f1 (ppm)


Solvent
3f
H2O
f1 (ppm)


3f
f1 (ppm)


Solvent
3g
H2O
impurity
f1 (ppm)


3g
f1 (ppm)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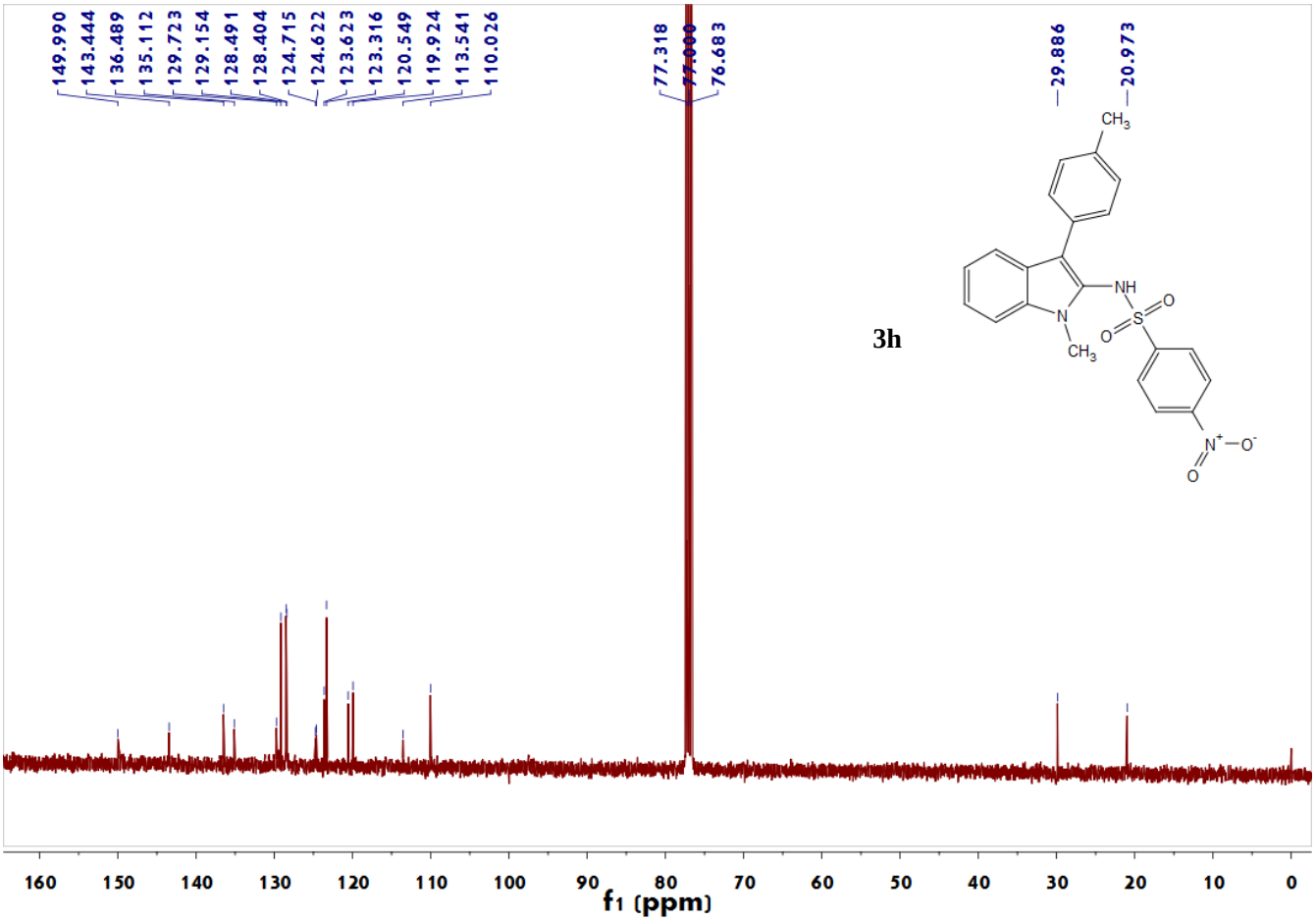
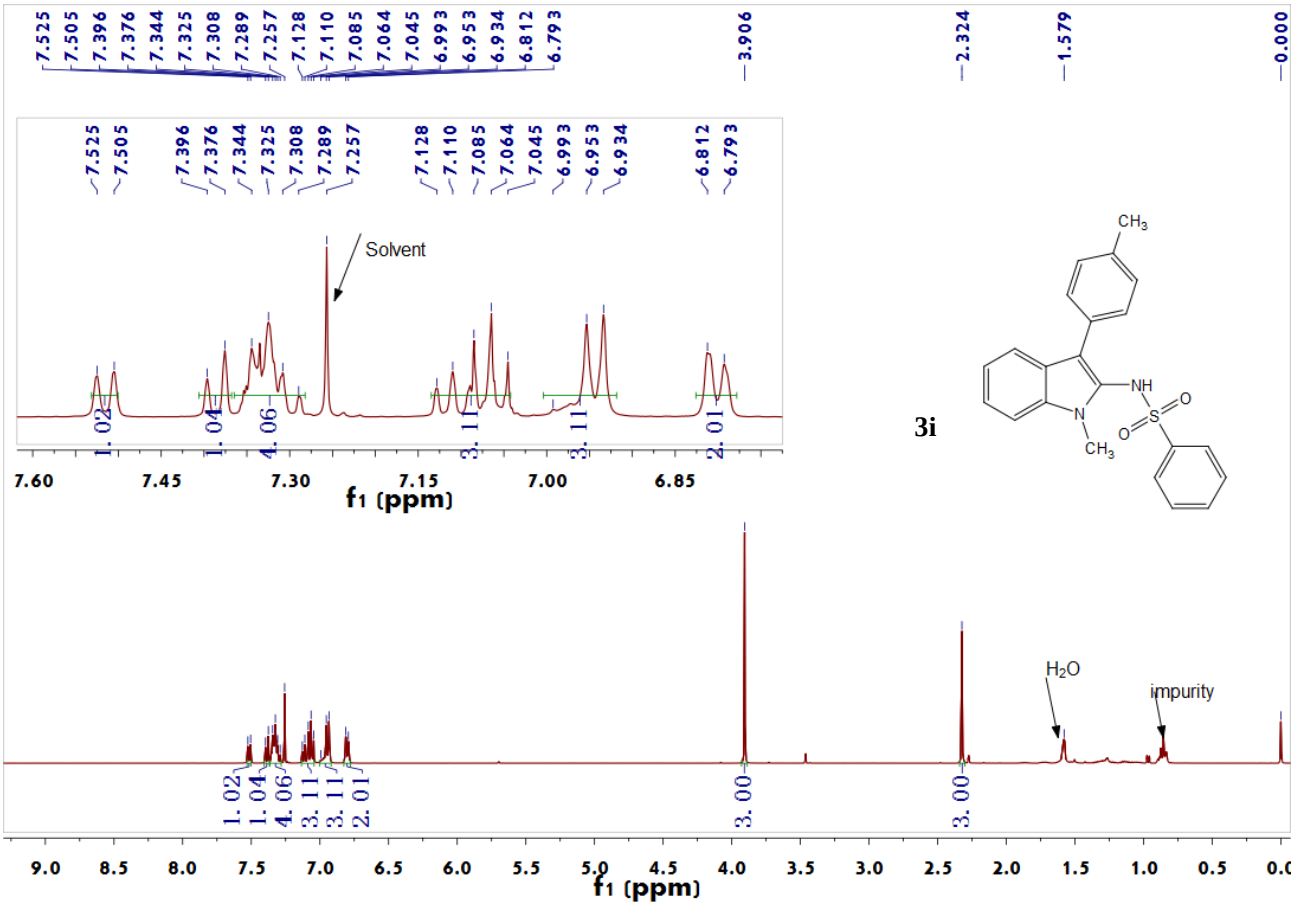
7.793
7.535
7.515
7.491
7.469
7.415
7.394
7.362
7.360
7.345
7.343
7.324
7.322
7.261
7.154
7.151
7.134
7.114
7.105
6.927
6.908
6.826
6.806
3.932
2.318
1.589
Solvent
H2O
f1 (ppm)
3h


149.990
143.444
136.489
135.112
129.723
129.154
128.491
128.404
124.715
124.622
123.623
123.316
120.549
119.924
113.541
110.026
77.318
76.683
29.886
20.973
f1 (ppm)
3h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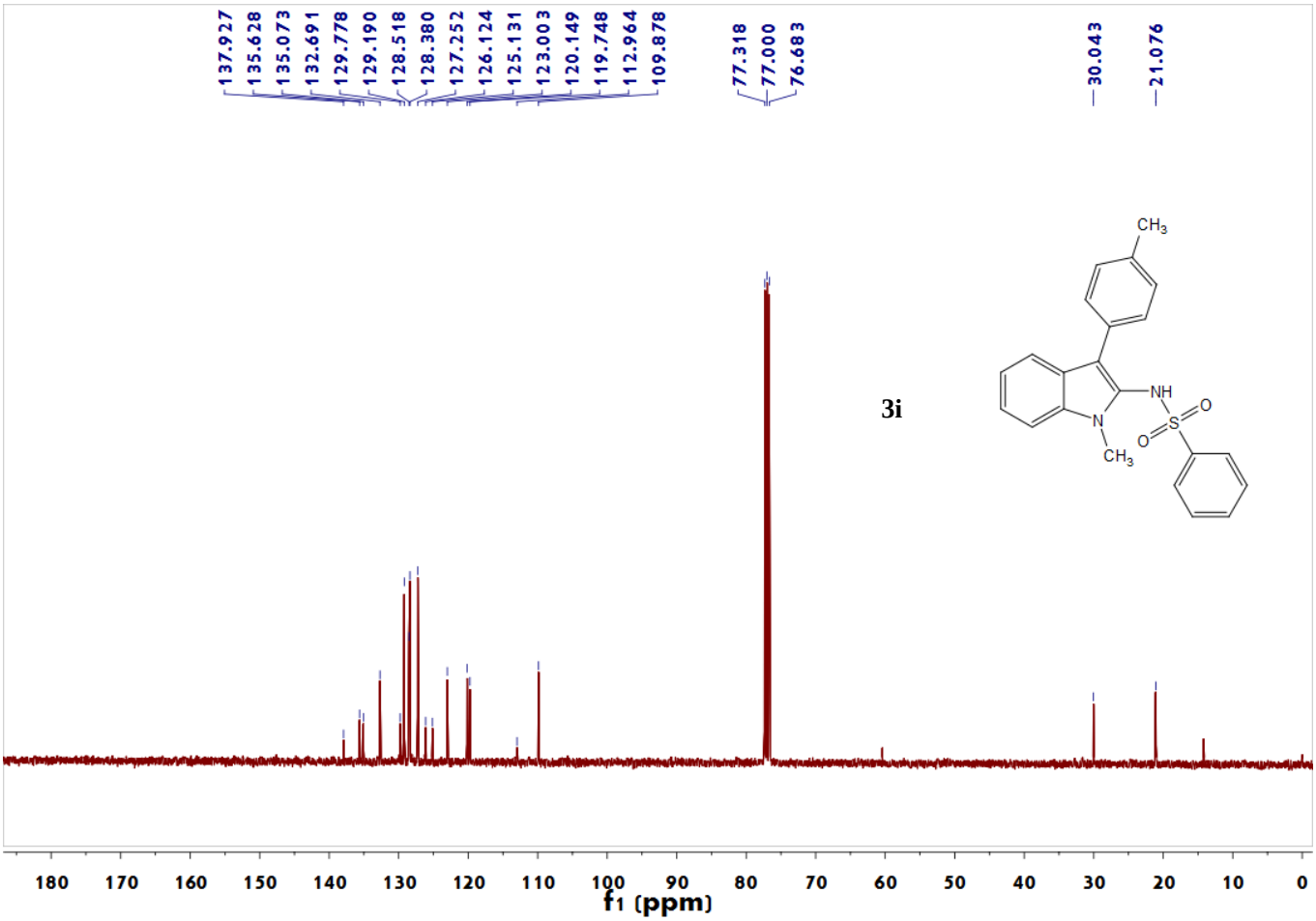
7.505
7.396
7.376
7.344
7.325
7.308
7.289
7.257
7.128
7.110
7.085
7.064
7.045
6.993
6.953
6.934
6.812
6.793
3.906
2.324
1.579
0.000
Solvent
1.02
1.04
4.06
3.11
3.11
2.01
7.60
7.45
7.30
7.15
7.00
6.85
f1 (ppm)
3i
CH3
NH
N
S
O
O
CH3
H2O
impurity
1.02
1.04
4.06
3.11
3.11
2.01
3.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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132.691
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129.190
128.518
128.380
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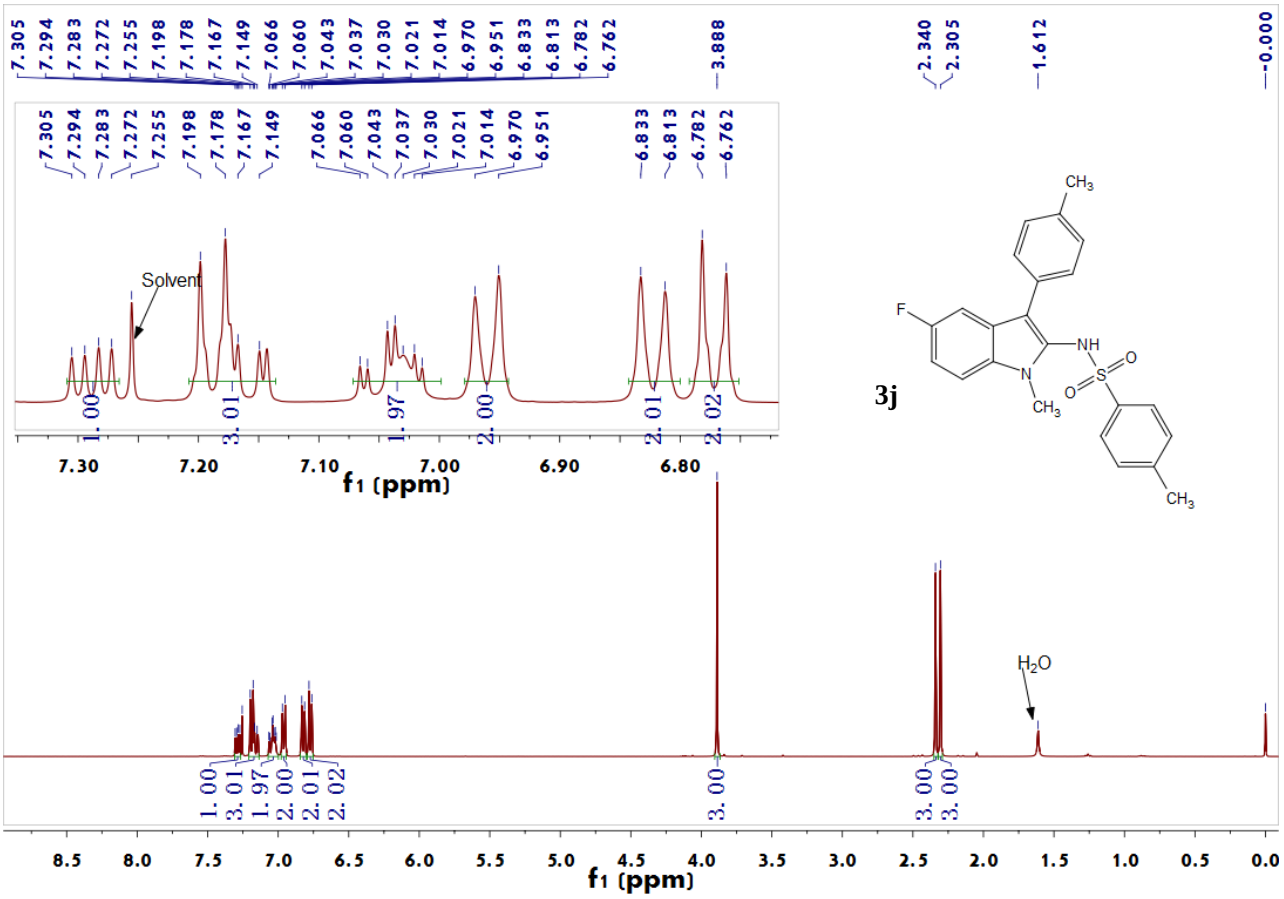
126.124
125.131
123.003
120.149
119.748
112.964
109.878
77.318
77.000
76.683
30.043
21.076
3i
CH3
NH
N
S
O
O
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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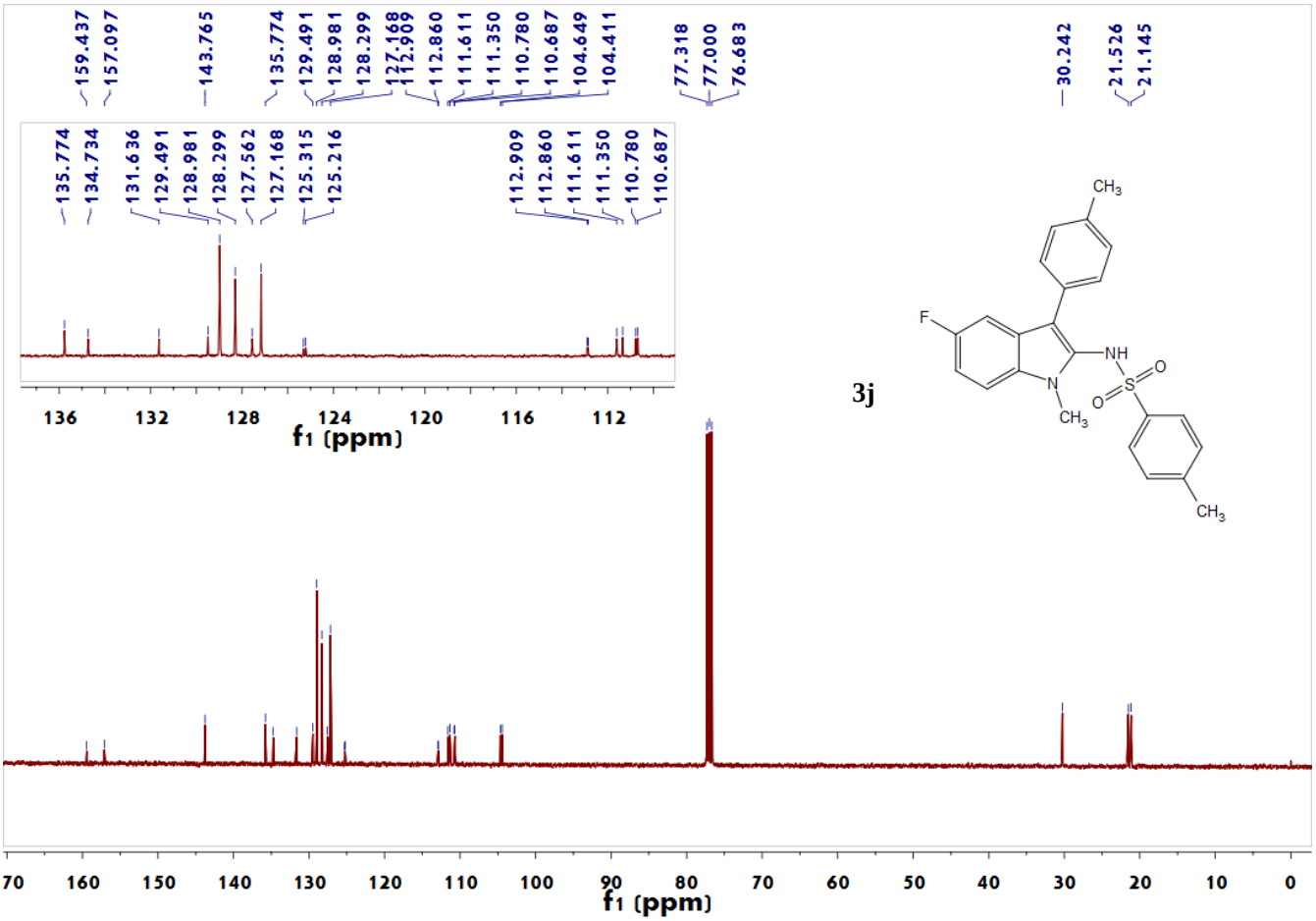
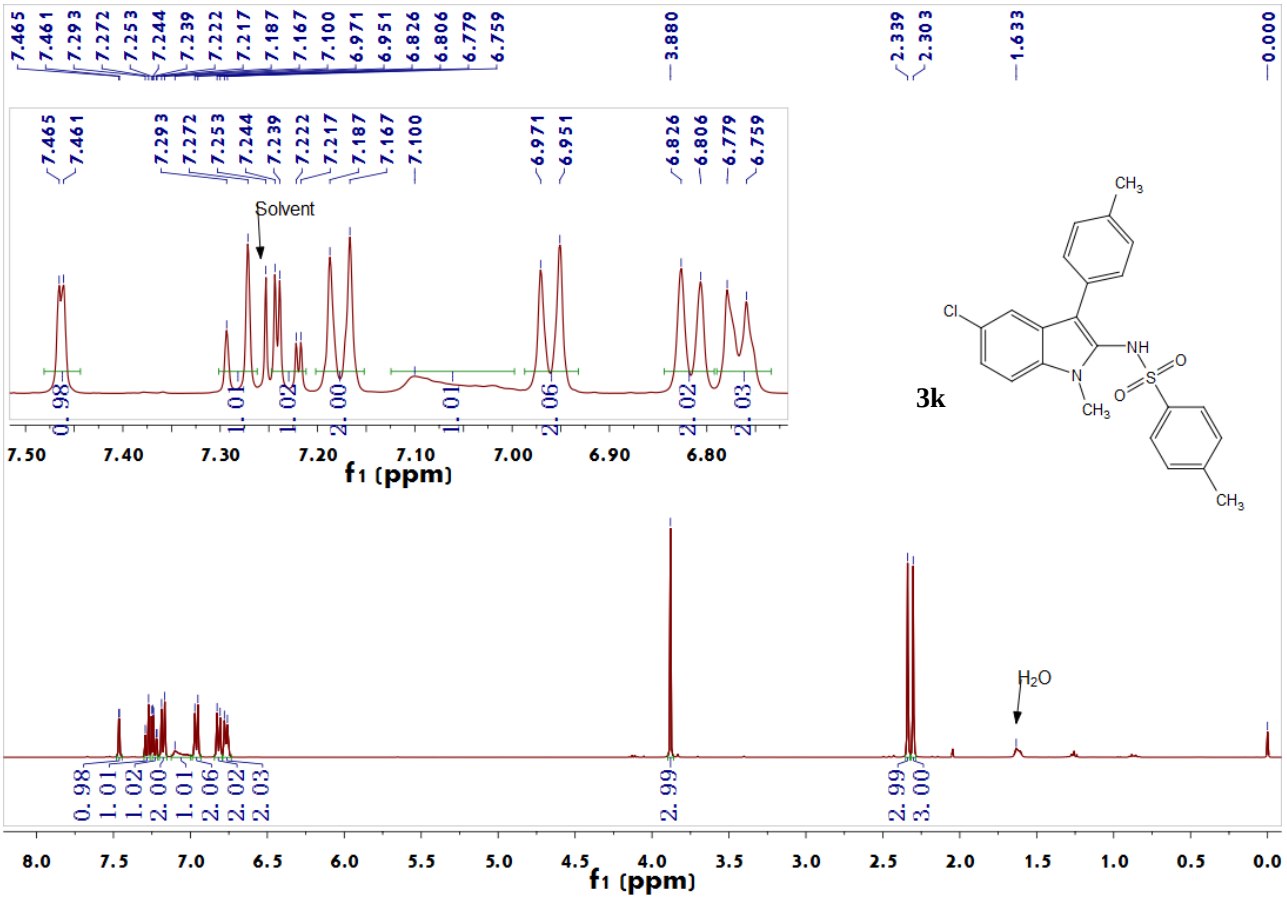
7.294
7.283
7.272
7.255
7.198
7.178
7.167
7.149
7.066
7.060
7.043
7.037
7.030
7.021
7.014
6.970
6.951
6.833
6.813
6.782
6.762
3.888
2.340
2.305
1.612
0.000
Solvent
1.00
3.01
1.97
2.00
2.01
2.02
3.00
3.00
3.00
H2O
f1 (ppm)
3j


159.437
157.097
143.765
135.774
129.491
128.981
128.299
127.562
127.168
125.315
125.216
112.909
112.860
111.611
111.350
110.780
110.687
104.649
104.411
77.318
77.000
76.683
30.242
21.526
21.145
f1 (ppm)
3j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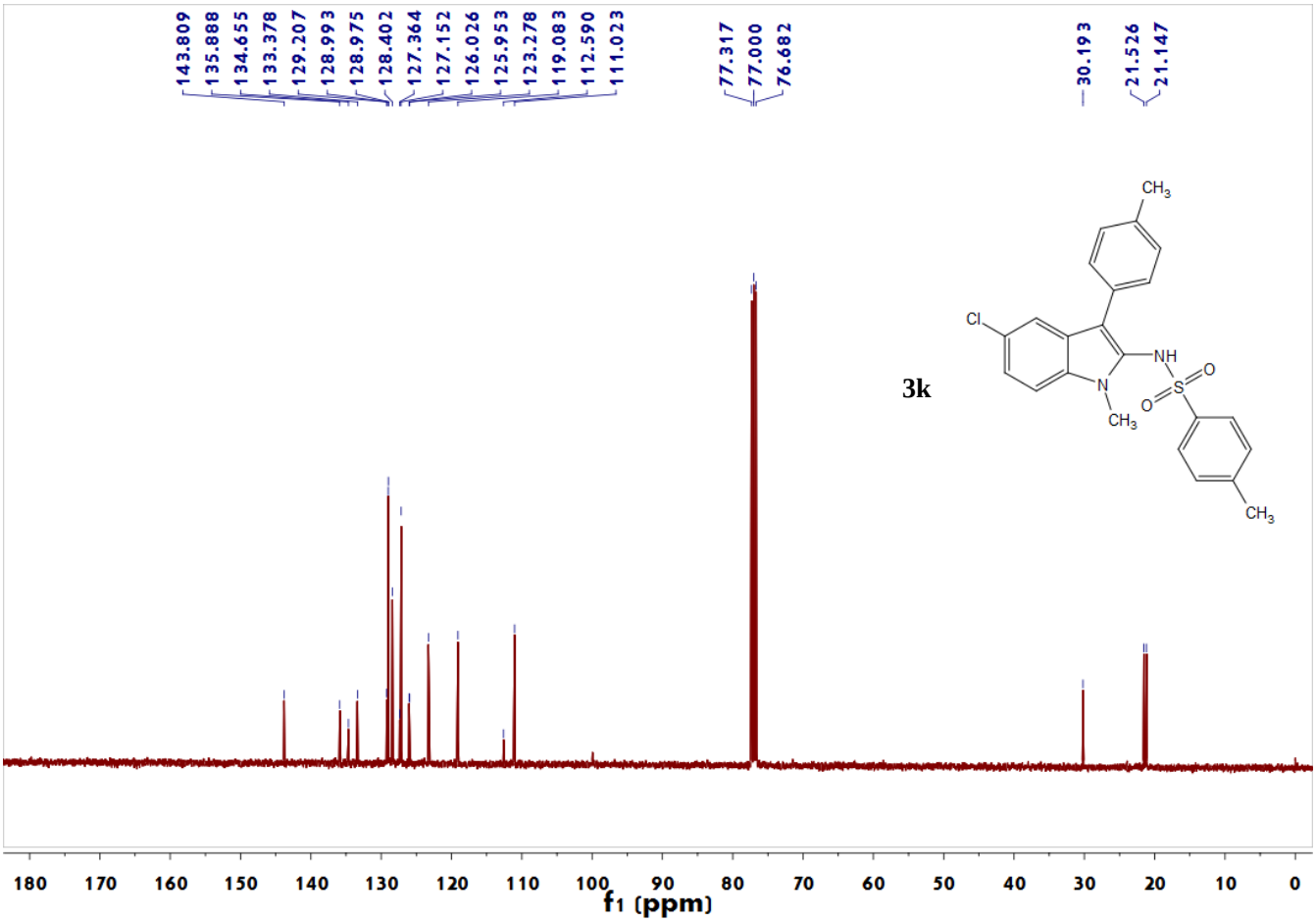
7.293
7.272
7.253
7.244
7.239
7.222
7.217
7.187
7.167
7.100
6.971
6.951
6.826
6.806
6.779
6.759
3.880
2.339
2.303
1.633
0.000
Solvent
0.98
1.01
1.02
2.00
1.01
2.06
2.02
2.03
2.99
2.99
3.00
H2O
3k
f1 (ppm)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128.993
128.975
128.402
127.364
127.152
126.026
125.953
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111.023
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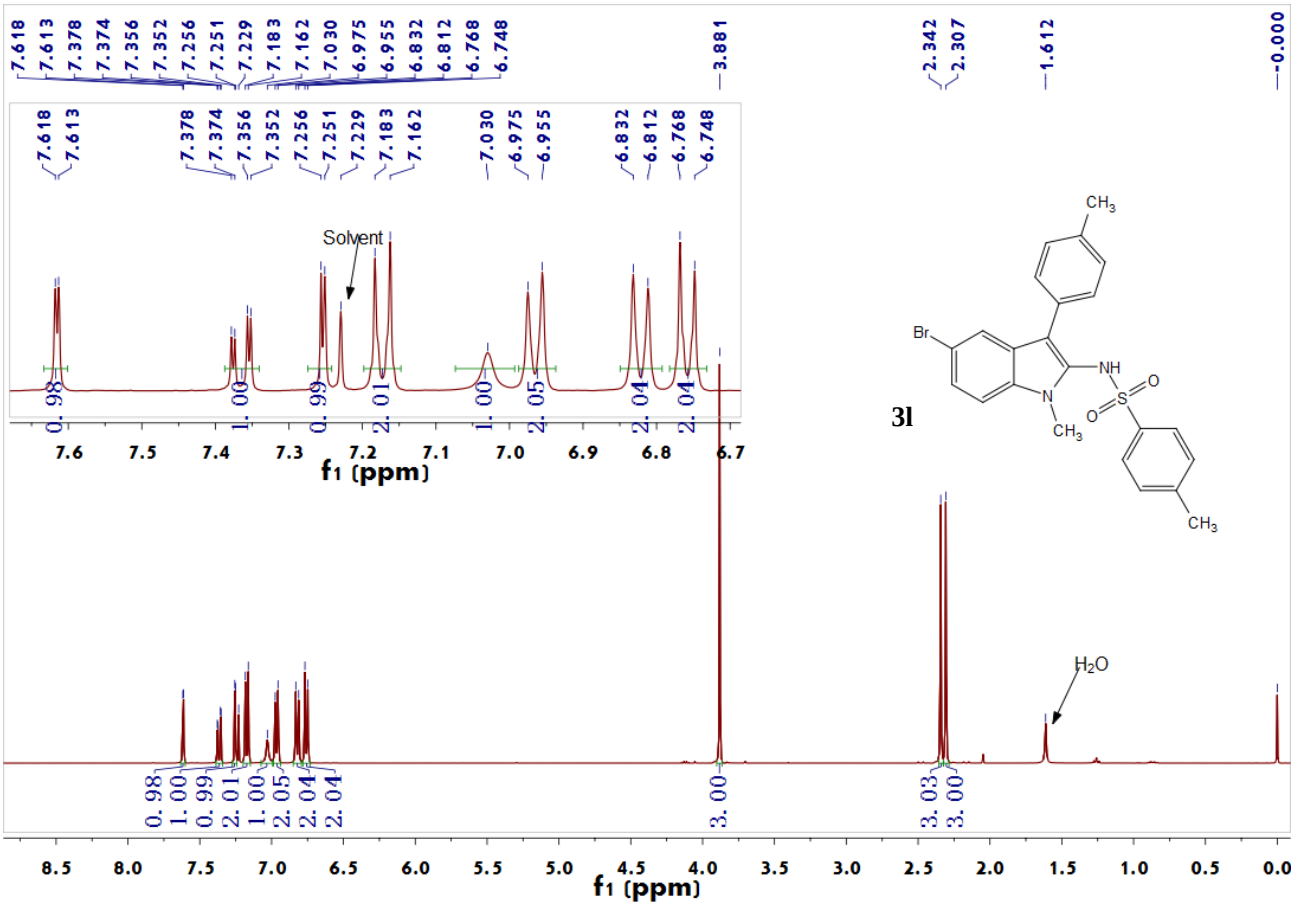
77.000
76.682
30.193
21.526
21.147
3k
f1 (ppm)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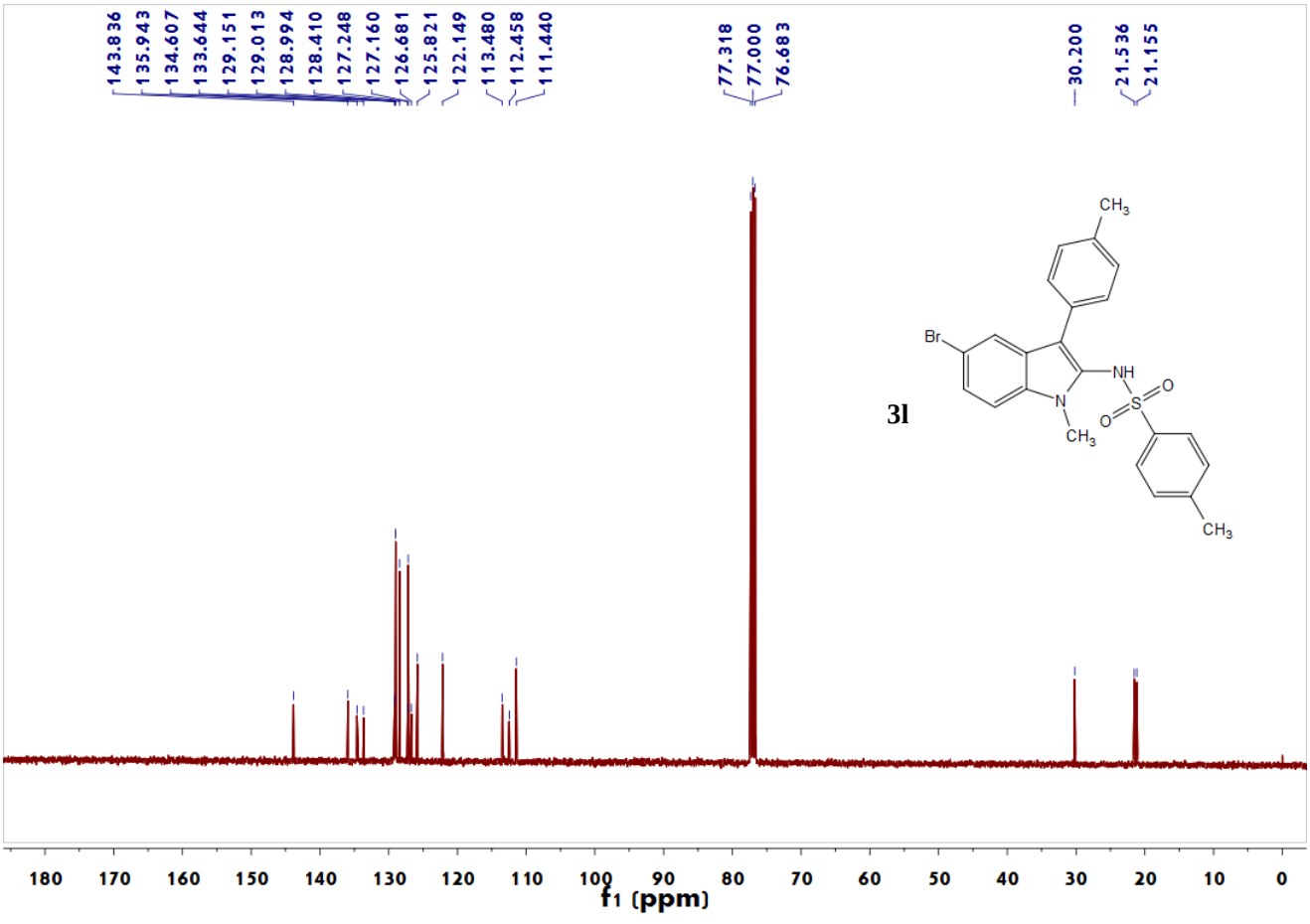
7.256
7.251
7.229
7.183
7.162
7.030
6.975
6.955
6.832
6.812
6.768
6.748
3.881
2.342
2.307
1.612
0.000
Solvent
H2O
3l
f1 (ppm)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125.821
122.149
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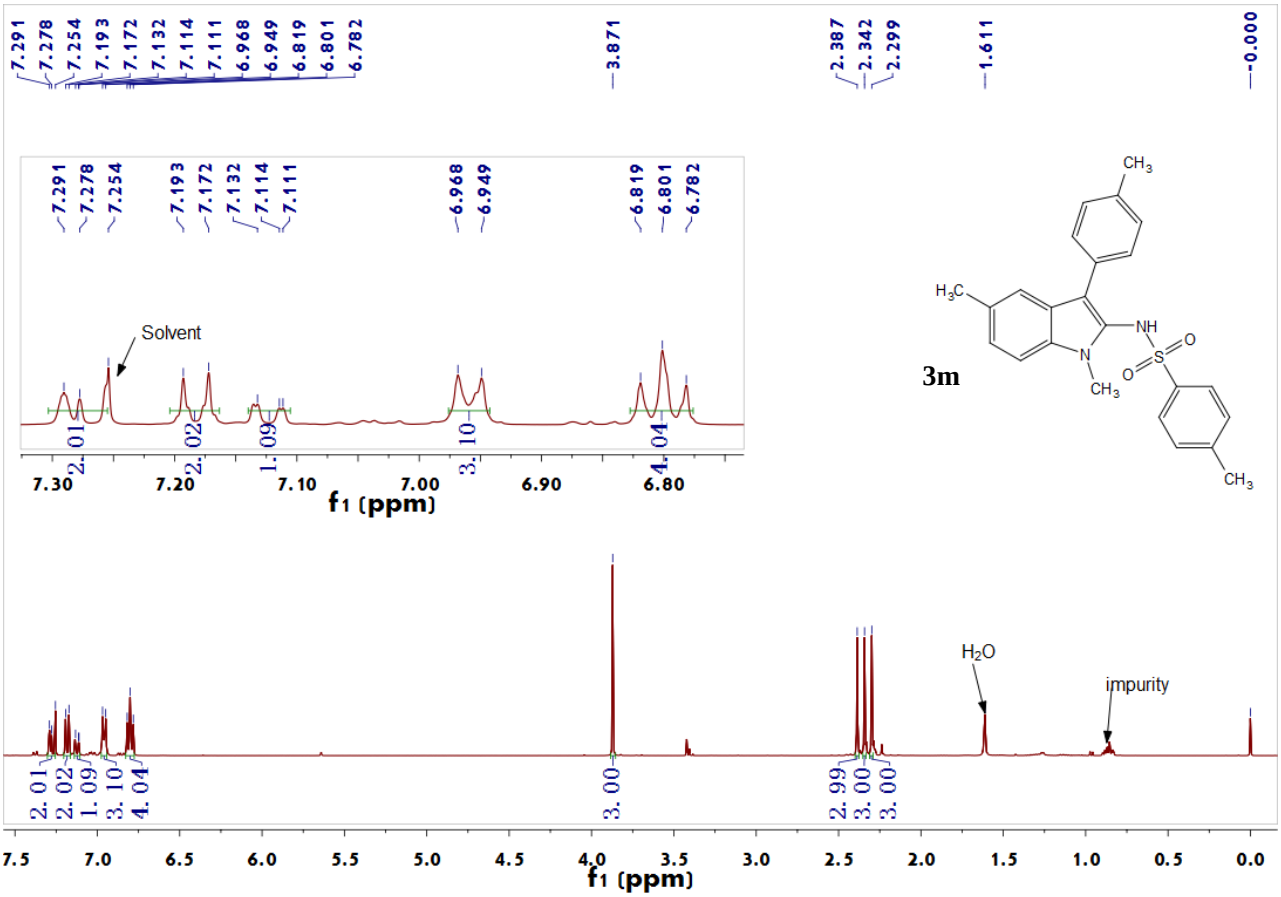
77.000
76.683
30.200
21.536
21.155
3l
f1 (ppm)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6.801
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2.342
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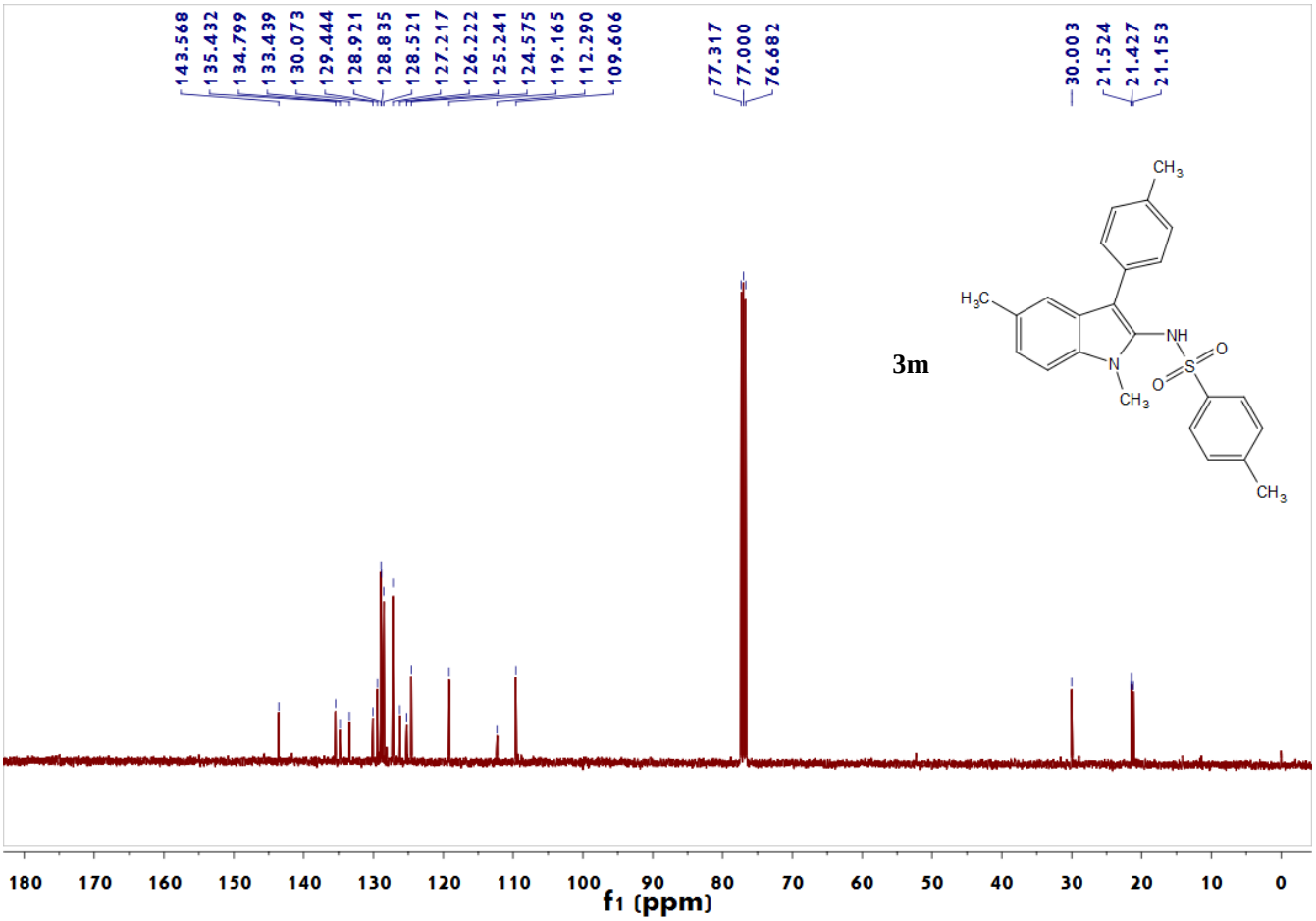
Solvent
3m
H2O
impurity
f1 (ppm)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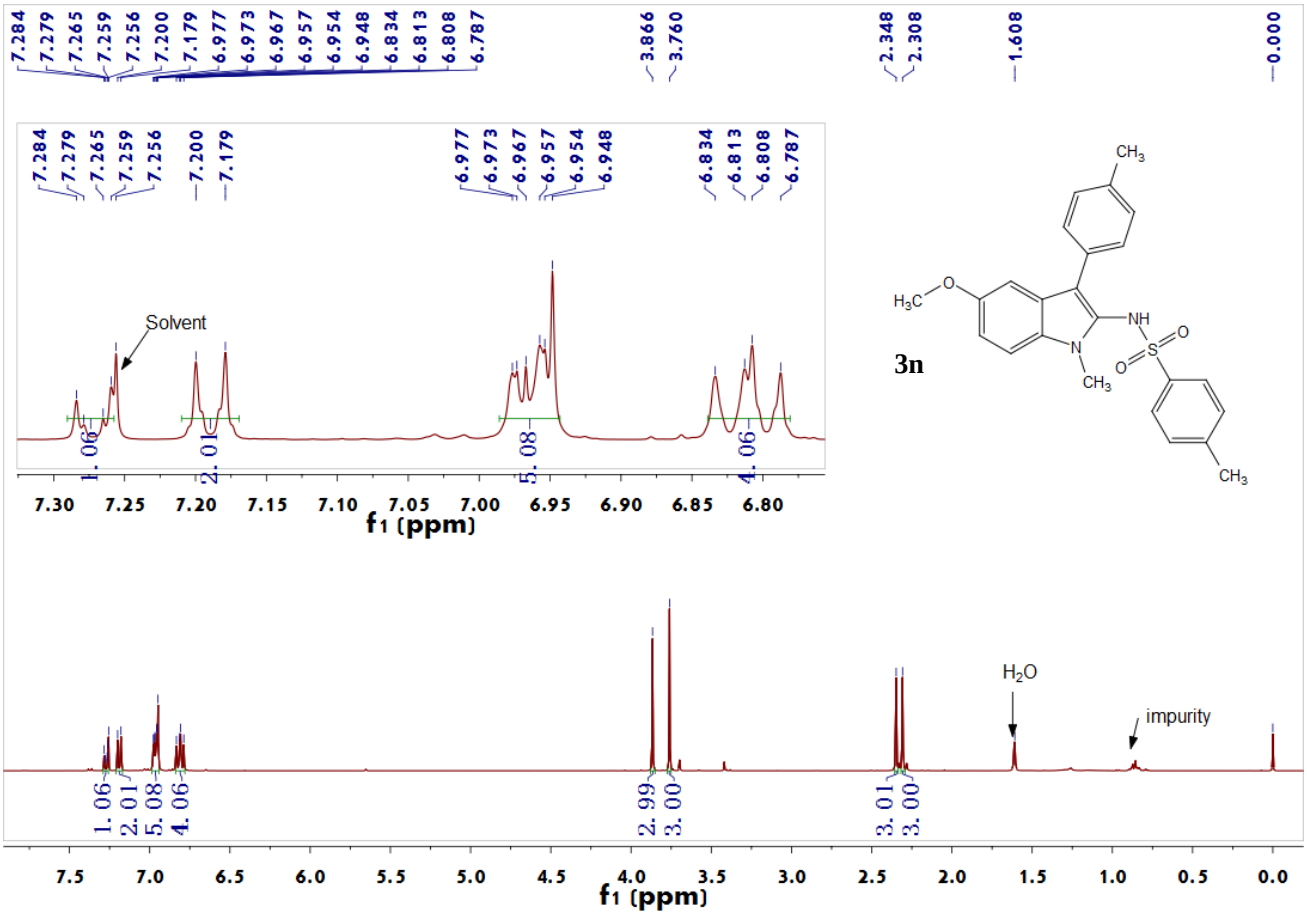
128.921
128.835
128.521
127.217
126.222
125.241
124.575
119.165
112.290
109.606
77.317
77.000
76.682
30.003
21.524
21.427
21.153
3m
f1 (ppm)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7.279
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7.200
7.179
6.977
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6.967
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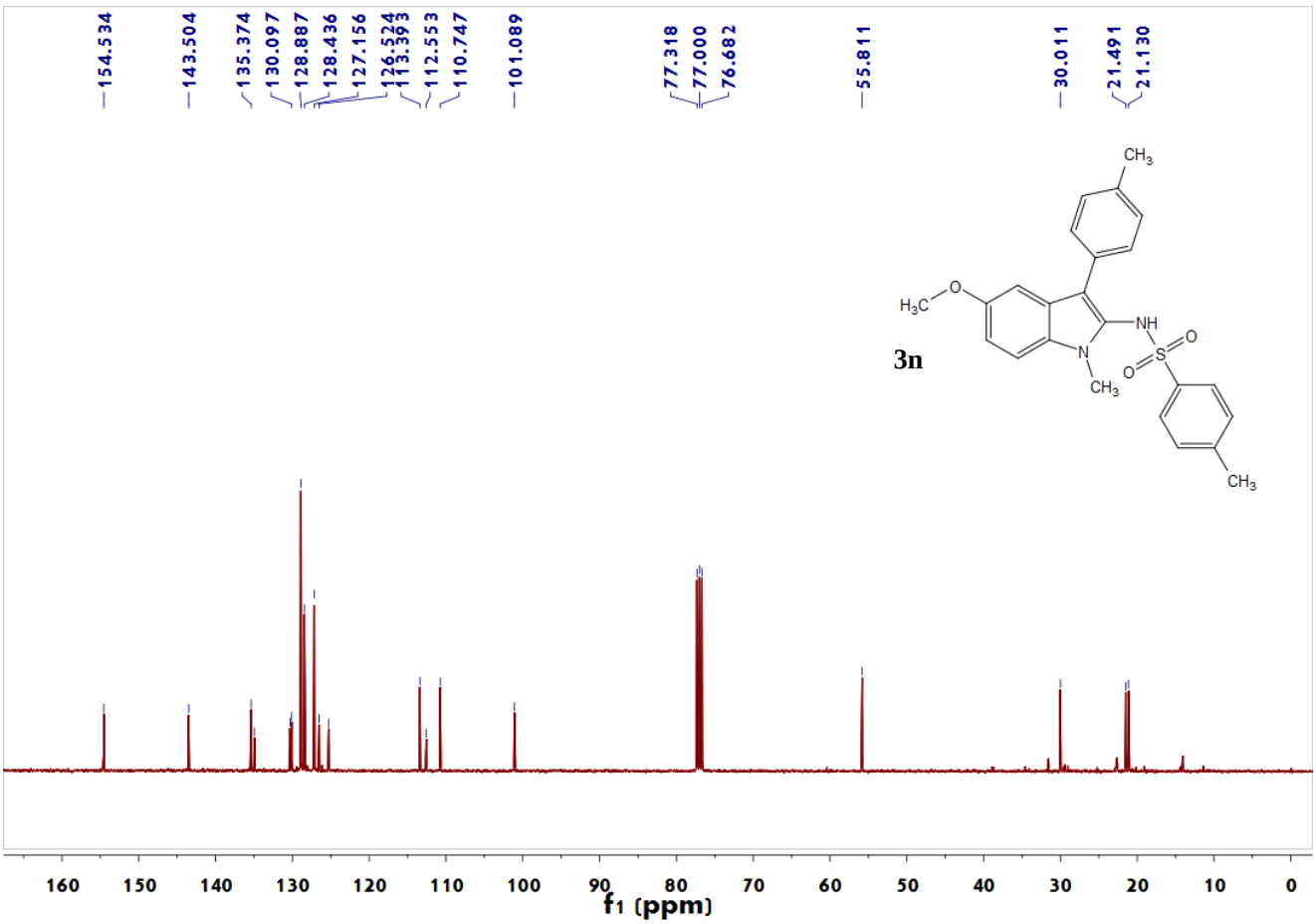
6.954
6.948
6.834
6.813
6.808
6.787
3.866
3.760
2.348
2.308
1.608
0.000
Solvent
1.06
2.01
5.08
4.06
f1 (ppm)
3n
H2O
impurity
2.99
3.00
3.01
3.00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113.393
112.553
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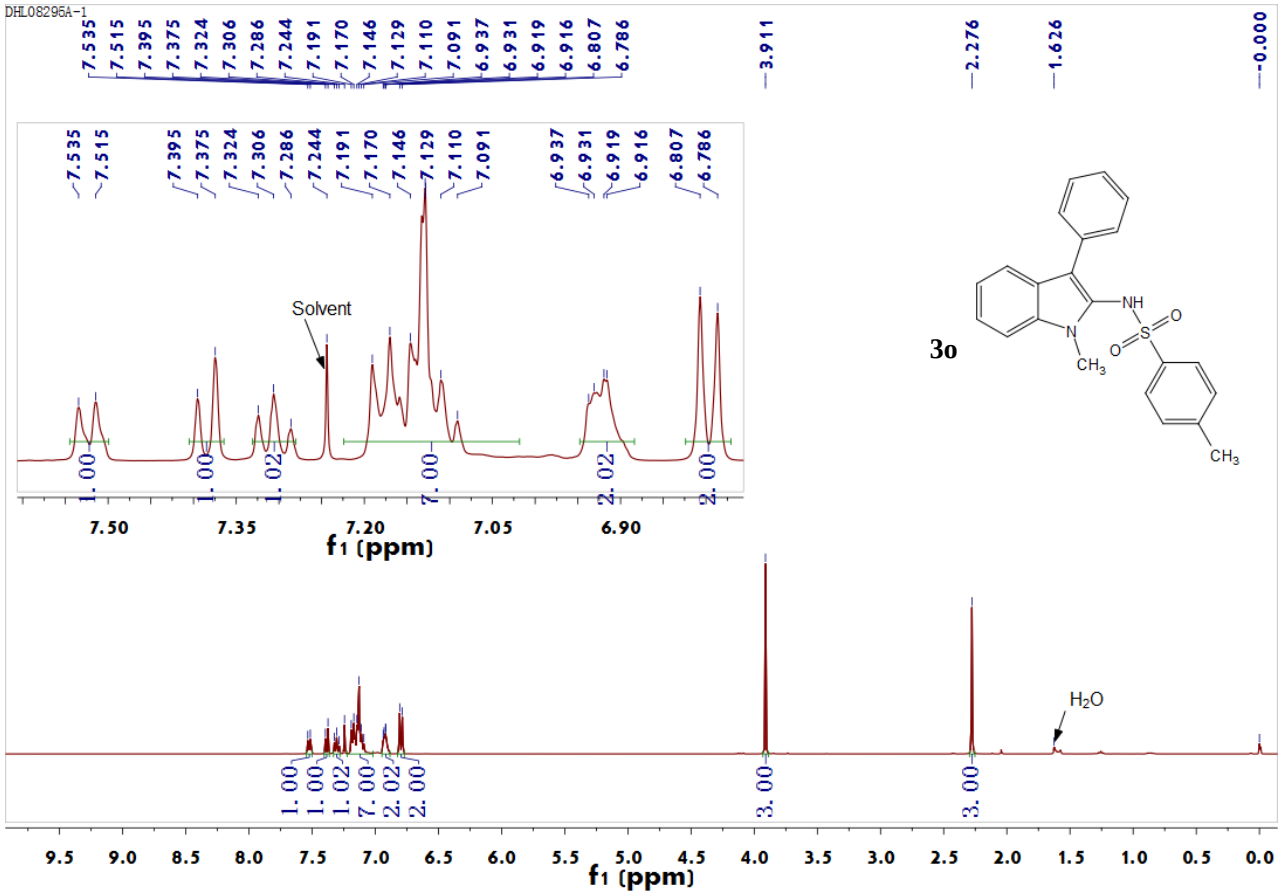
77.318
77.000
76.682
55.811
30.011
21.491
21.130
3n
f1 (ppm)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7.395
7.375
7.324
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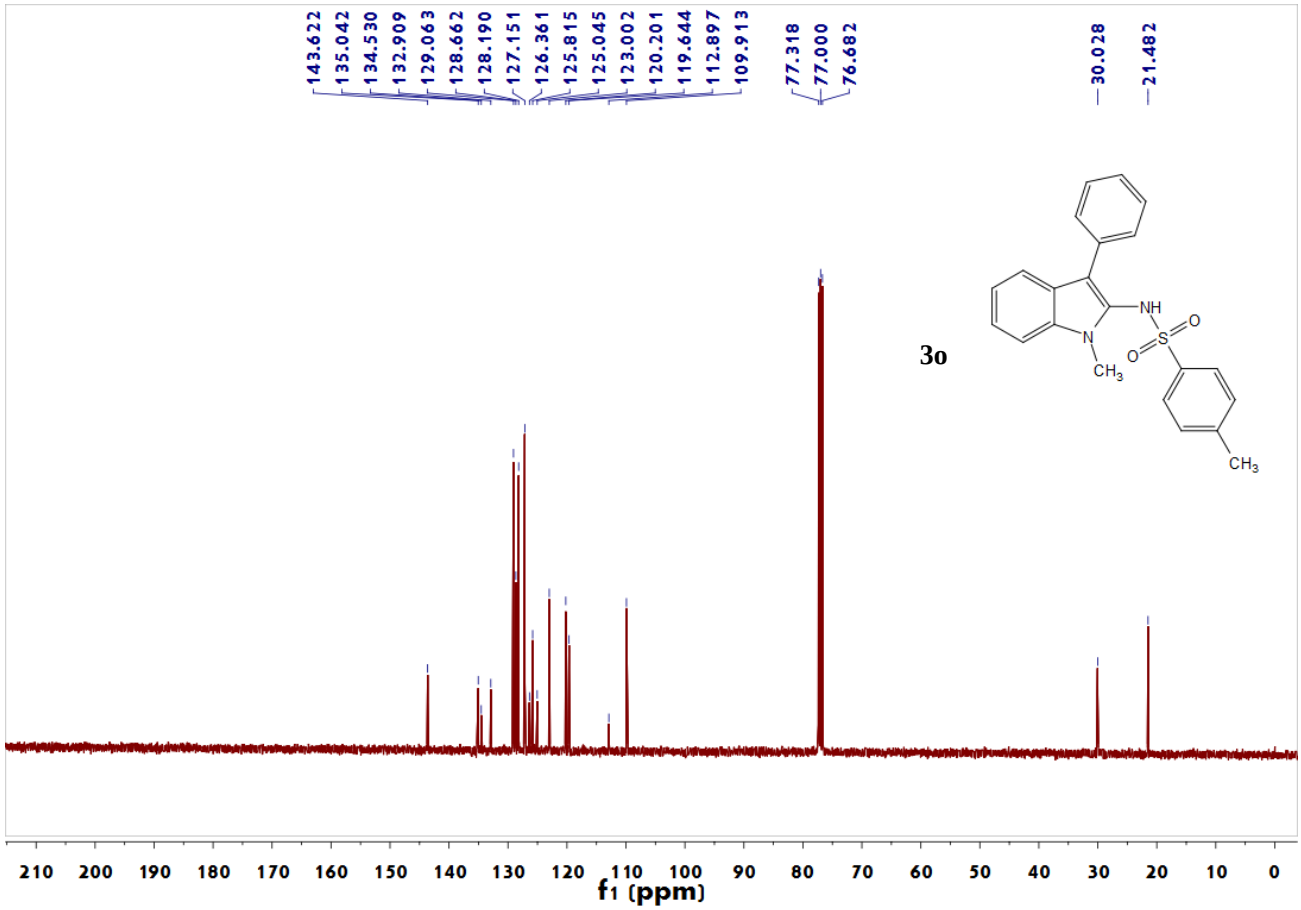
7.129
7.110
7.091
6.937
6.931
6.919
6.916
6.807
6.786
3.911
2.276
1.626
0.000
Solvent
3o
NH
N
CH3
S
O
O
CH3
H2O
1.00
1.00
1.02
7.00
2.02
2.00
3.00
3.00
f1 (ppm)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125.815
125.045
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120.201
119.644
112.897
109.913
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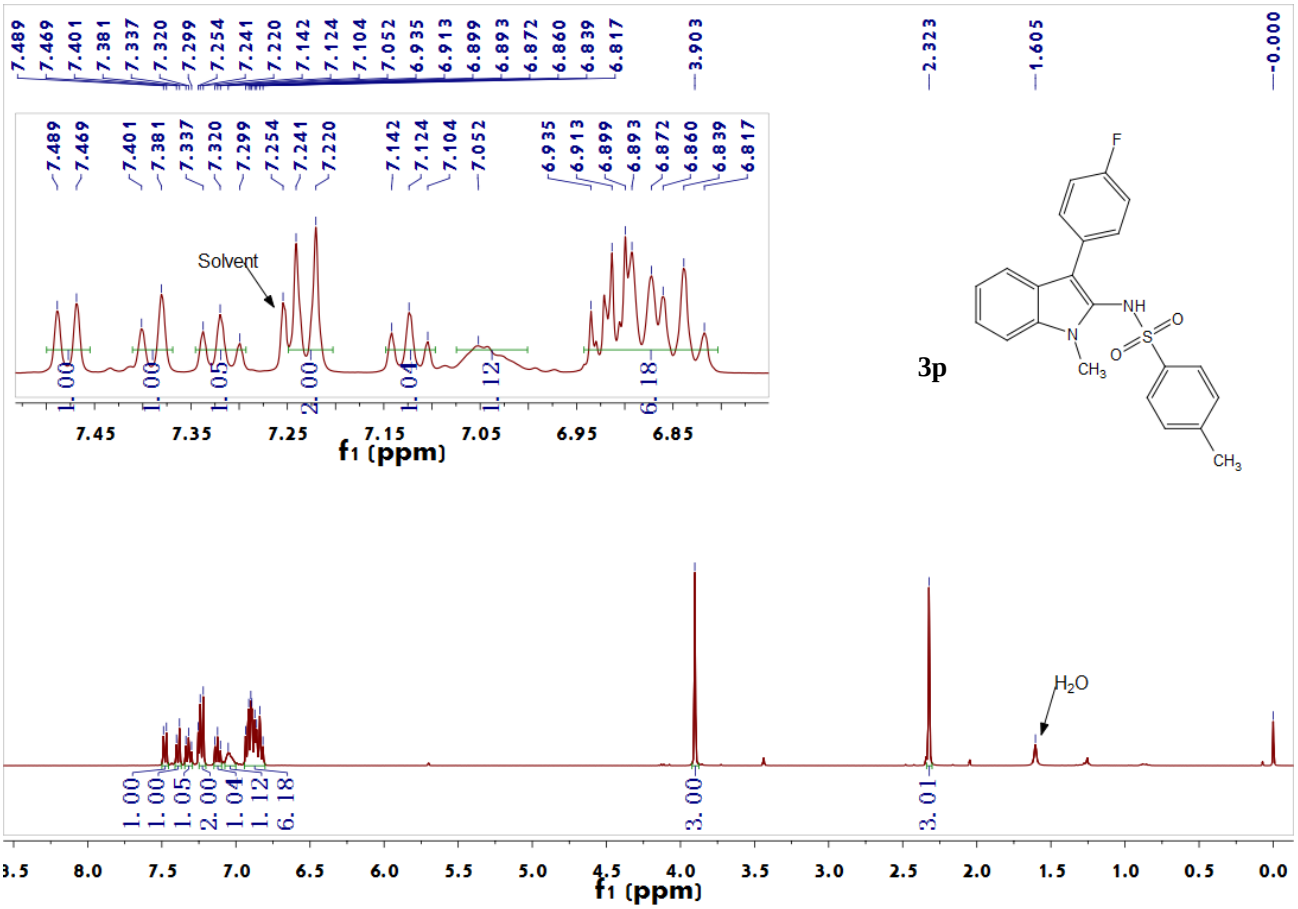
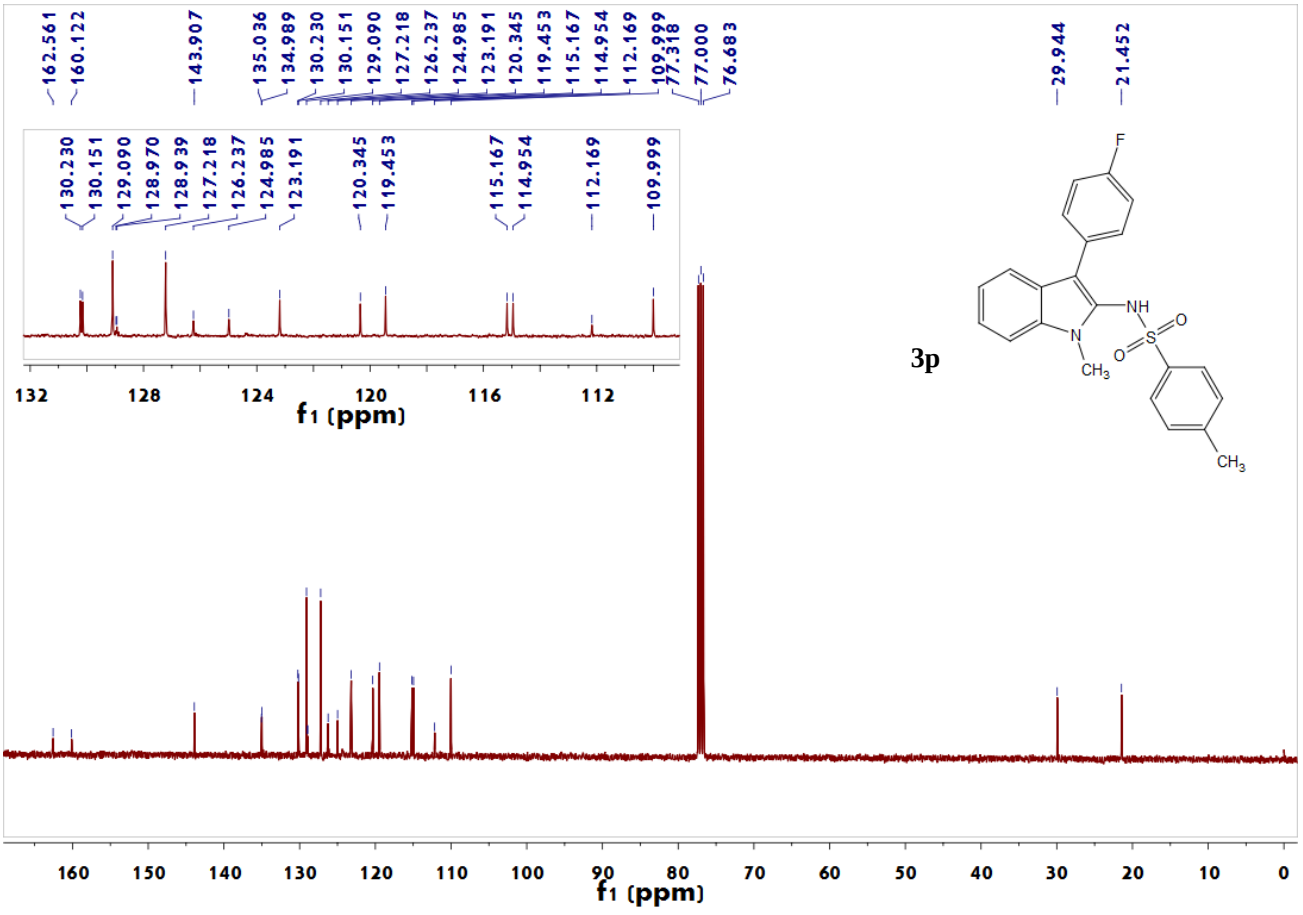
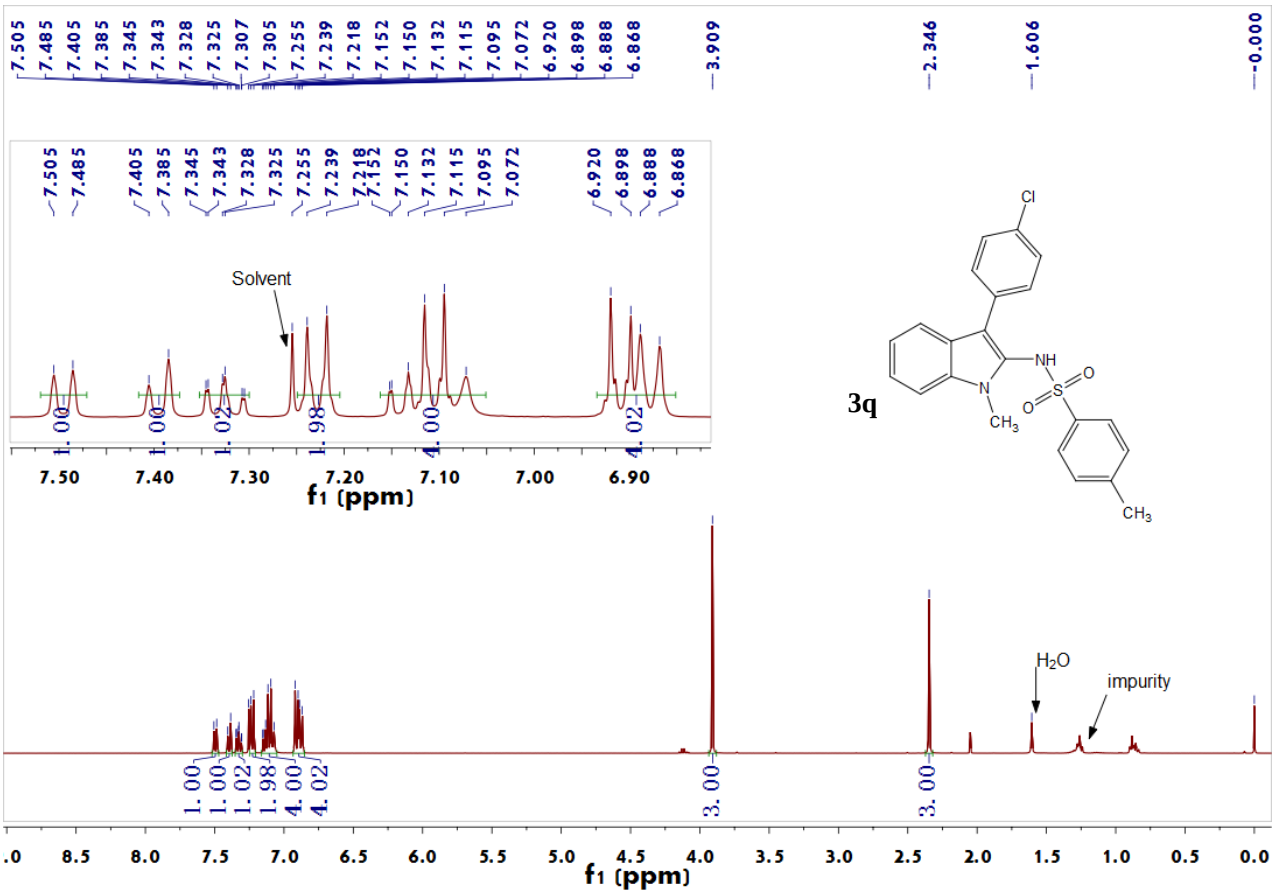
77.000
76.682
30.028
21.482
3o
NH
N
CH3
S
O
O
CH3
f1 (ppm)


Solvent
3p
f1 (ppm)

H2O
f1 (ppm)


3p
f1 (ppm)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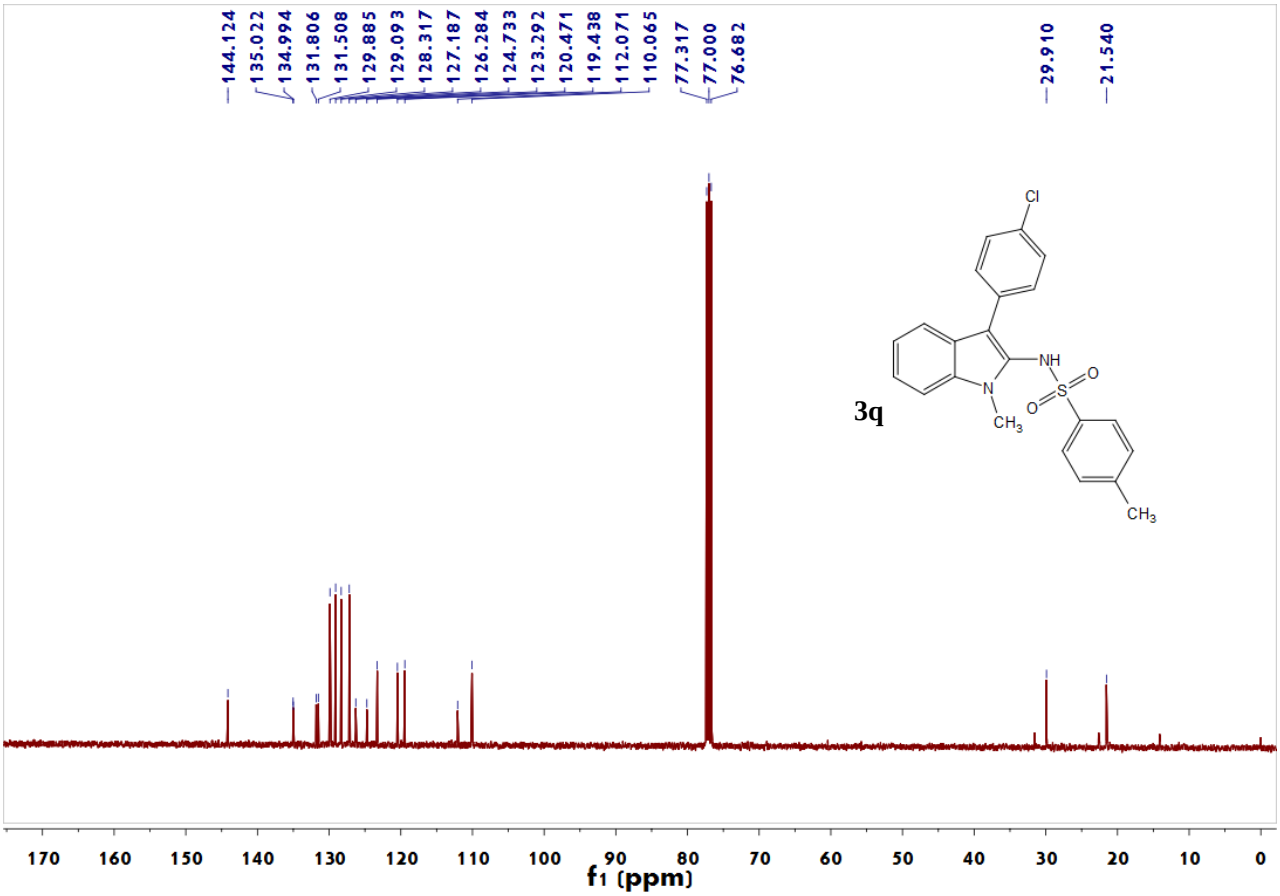
7.385
7.345
7.343
7.328
7.325
7.307
7.305
7.255
7.239
7.218
7.152
7.150
7.132
7.115
7.095
7.072
6.920
6.898
6.888
6.868
3.909
2.346
1.606
0.000
Solvent
1.00
1.00
1.02
1.98
4.00
4.02
3q
Cl
NH
N
CH3
O
S
O
CH3
H2O
impurity
3.00
3.00
f1 (ppm)


144.124
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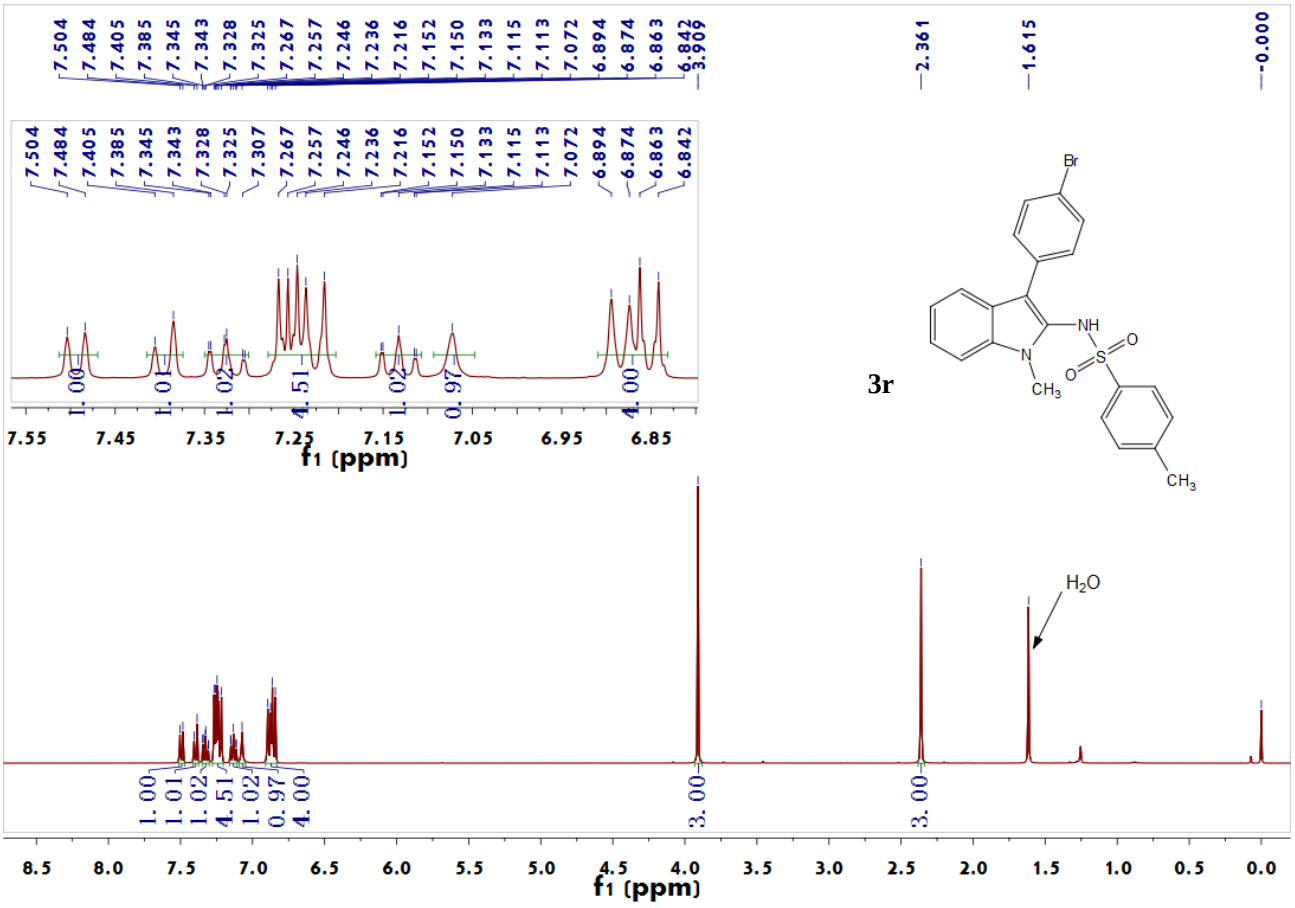
134.994
131.806
131.508
129.885
129.093
128.317
127.187
126.284
124.733
123.292
120.471
119.438
112.071
110.065
77.317
77.000
76.682
29.910
21.540
3q
Cl
NH
N
CH3
O
S
O
CH3
f1 (ppm)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7.484
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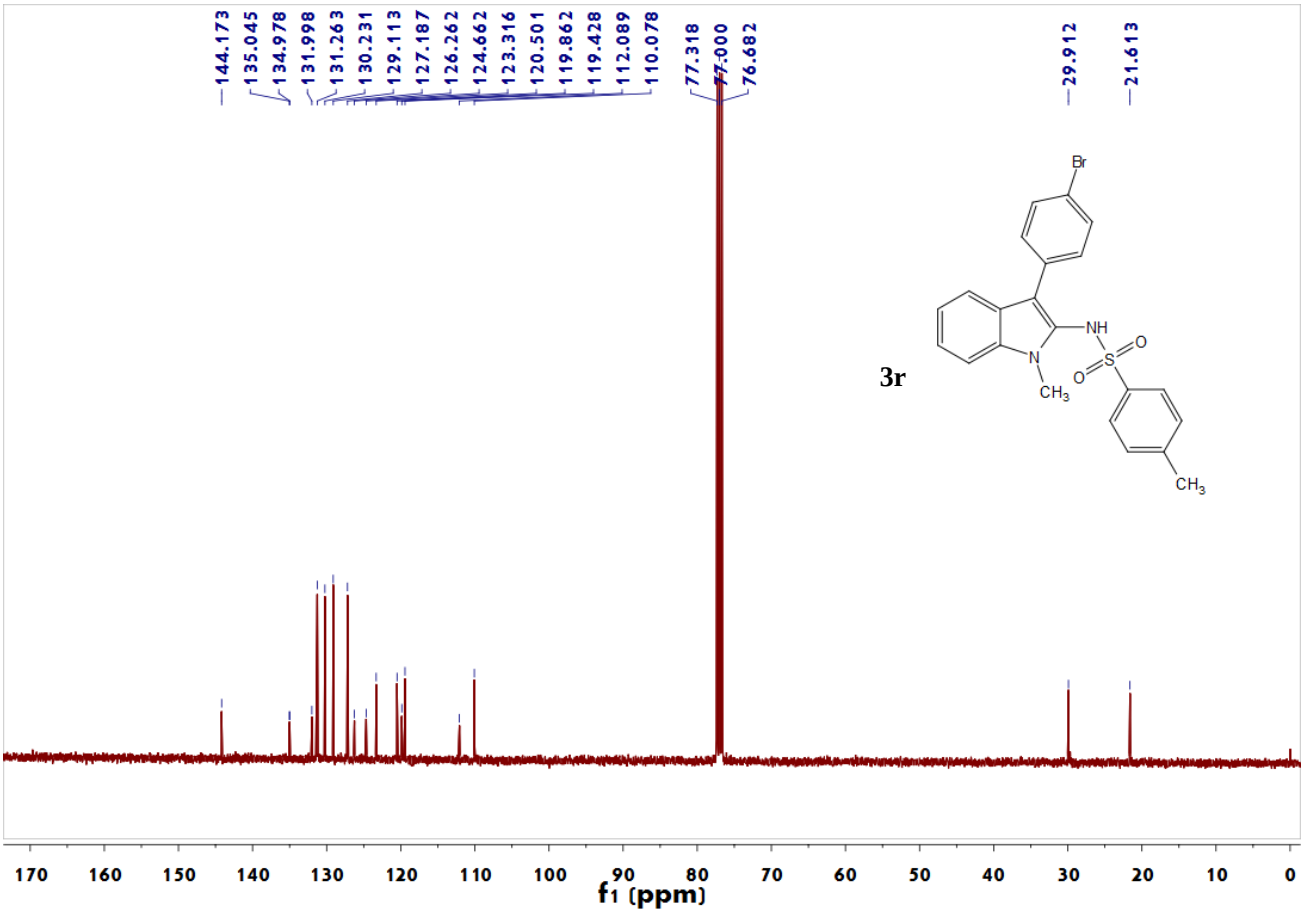
7.385
7.345
7.343
7.328
7.325
7.307
7.267
7.257
7.246
7.236
7.216
7.152
7.150
7.133
7.115
7.113
7.072
6.894
6.874
6.863
6.842
3.909
2.361
1.615
0.000
1.00
1.01
1.02
4.51
1.02
0.97
4.00
3.00
3.00
H2O
f1 (ppm)
3r
Br
NH
N
CH3
S
O
CH3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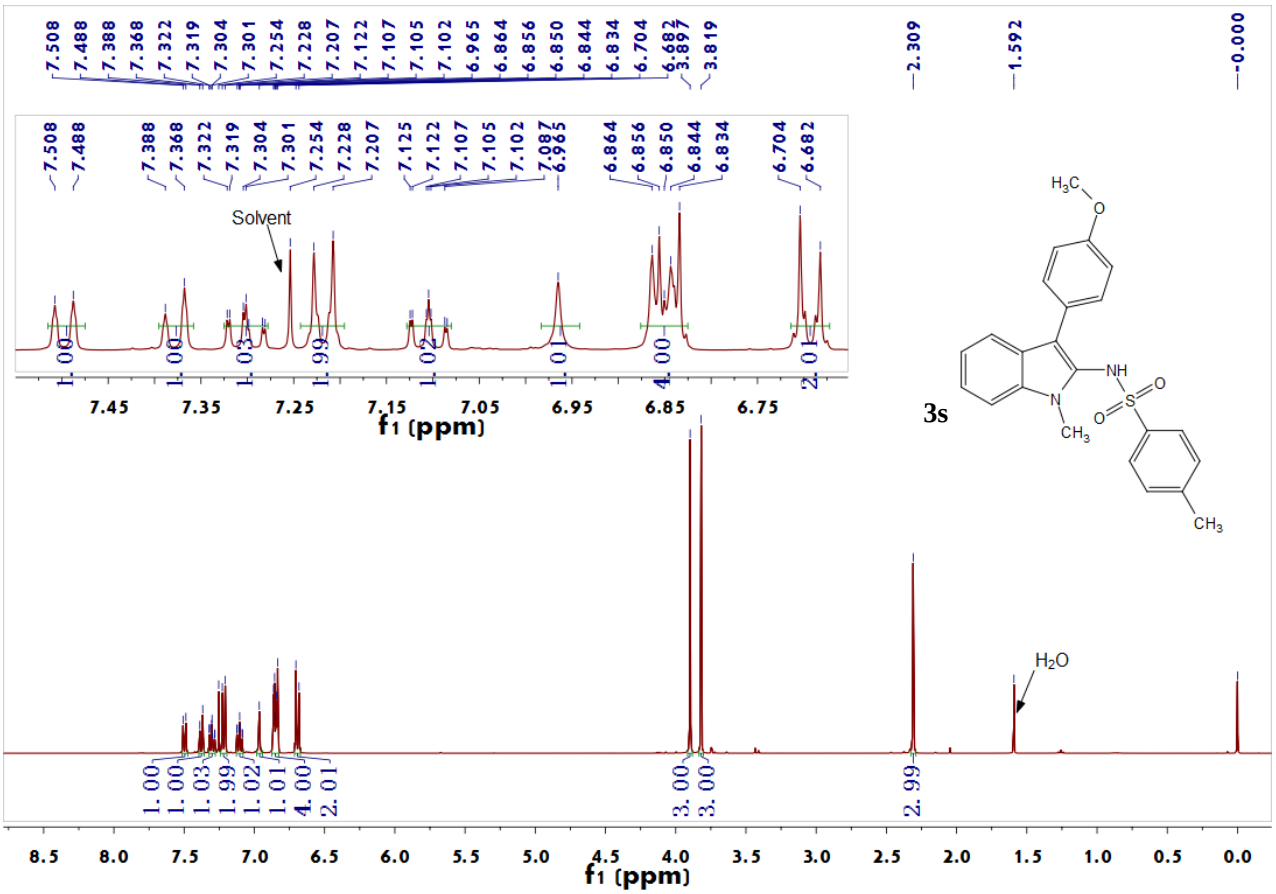
131.263
130.231
129.113
127.187
126.262
124.662
123.316
120.501
119.862
119.428
112.089
110.078
77.318
77.000
76.682
29.912
21.613
f1 (ppm)
3r
Br
NH
N
CH3
S
O
CH3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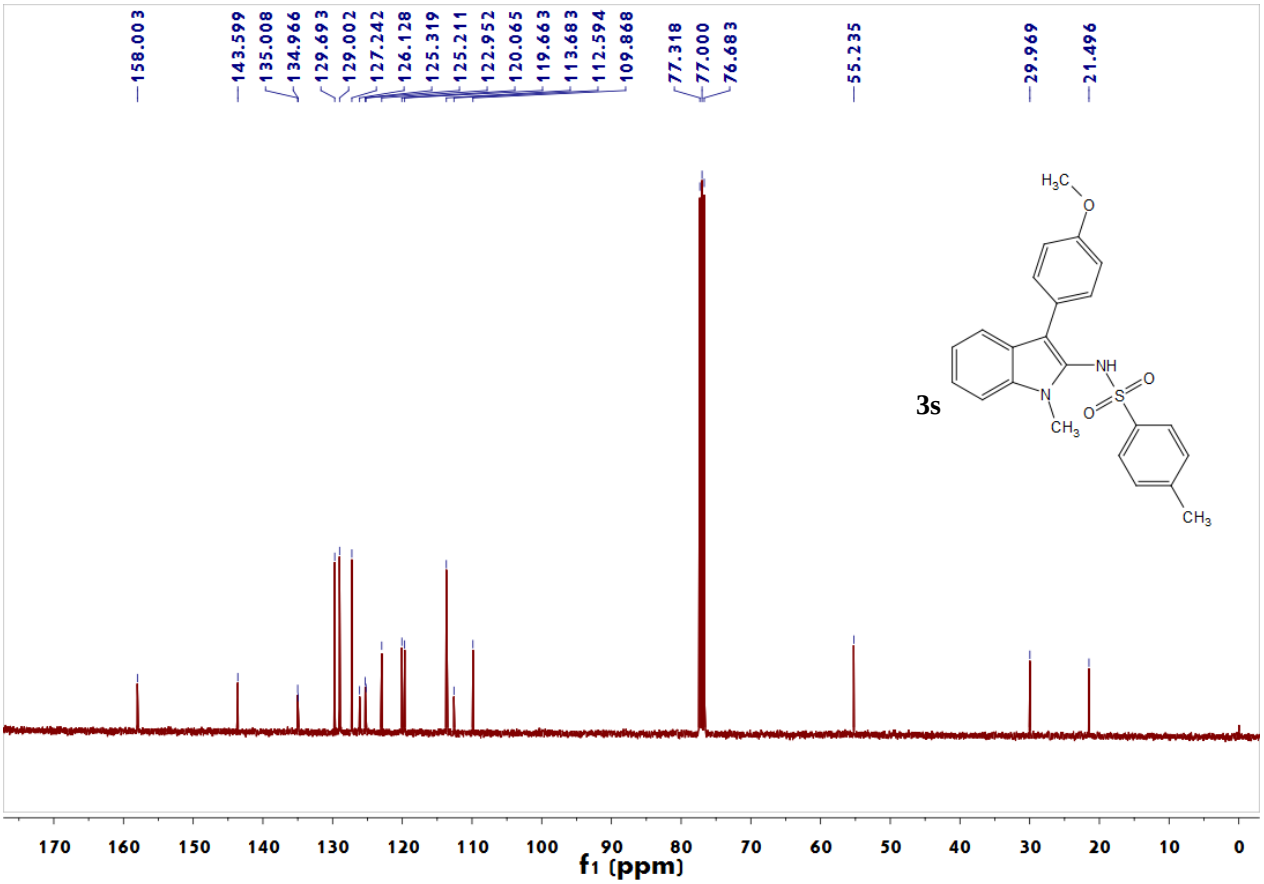
7.488
7.388
7.368
7.322
7.319
7.304
7.301
7.254
7.228
7.207
7.122
7.107
7.105
7.102
6.965
6.864
6.856
6.850
6.844
6.834
6.704
6.682
3.897
3.819
2.309
1.592
0.000
Solvent
1.00
1.00
1.03
1.99
1.02
1.01
4.00
2.01
f1 (ppm)
3s
H2O
3.00
3.00
2.99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134.966
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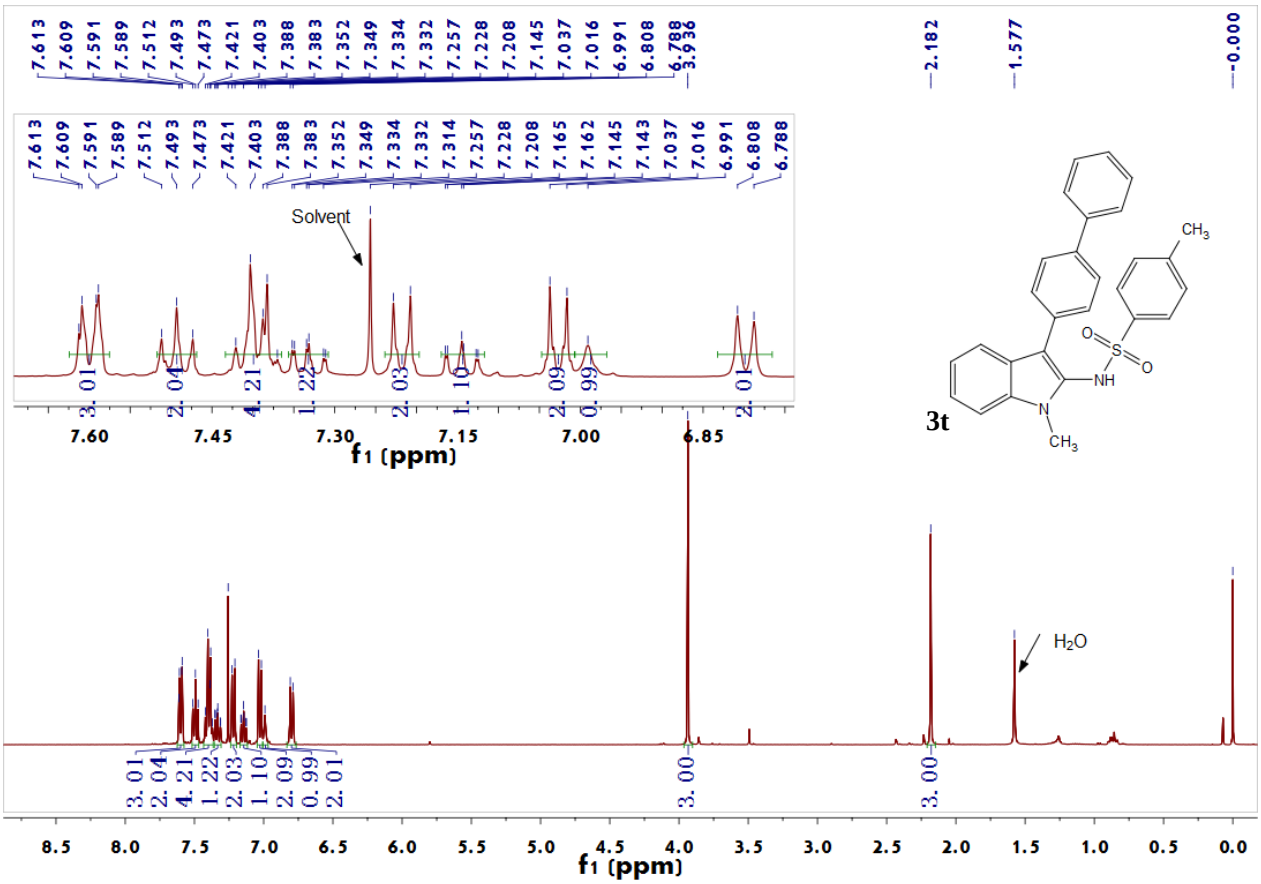
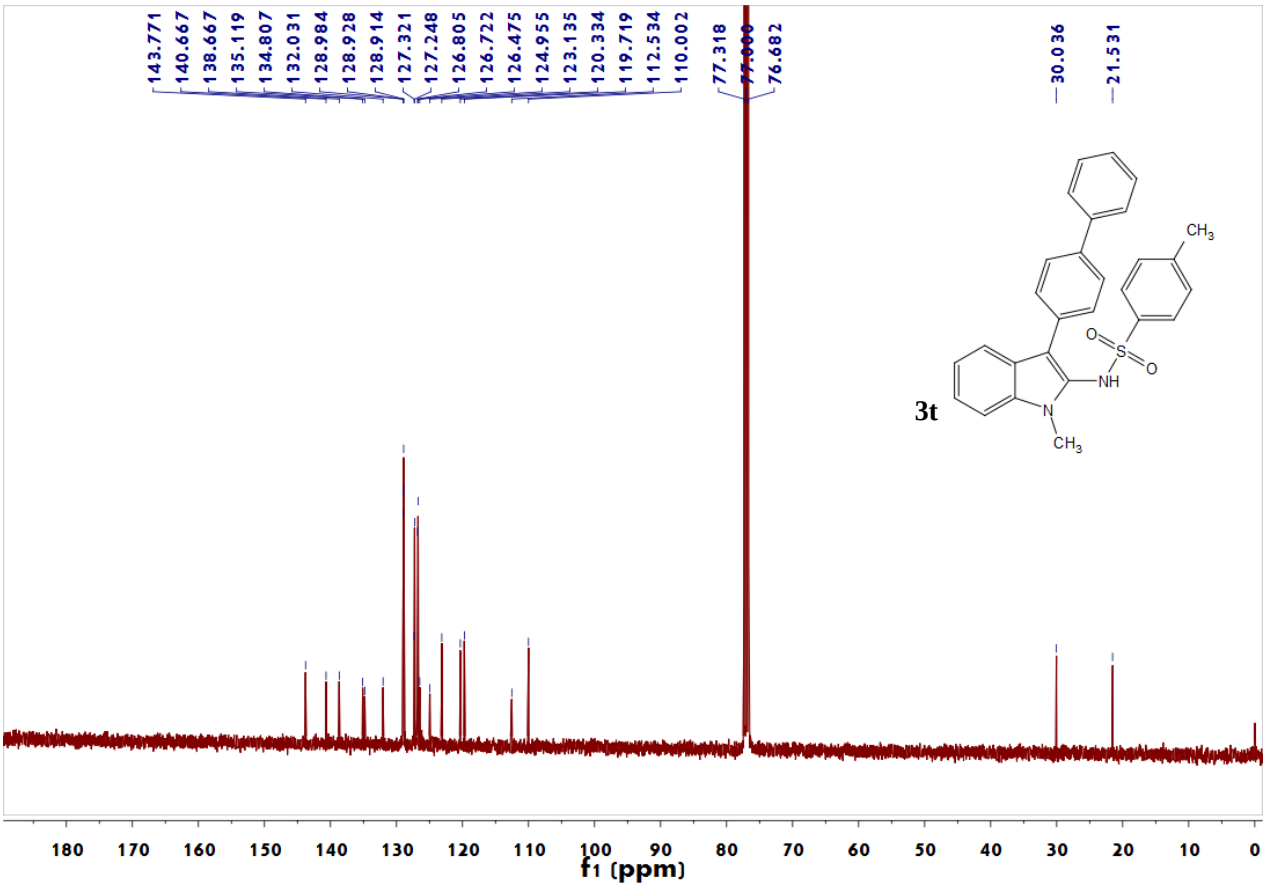
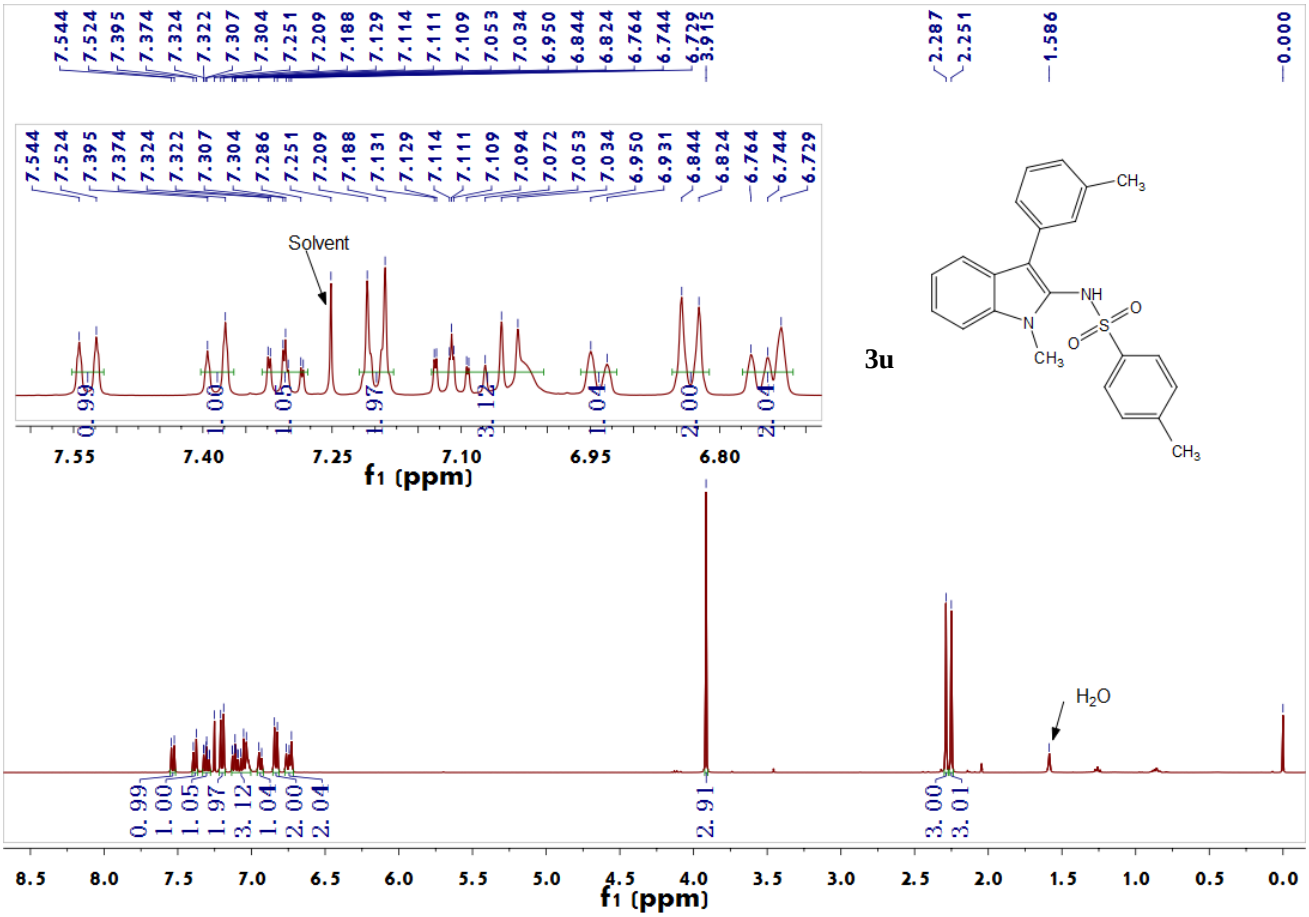
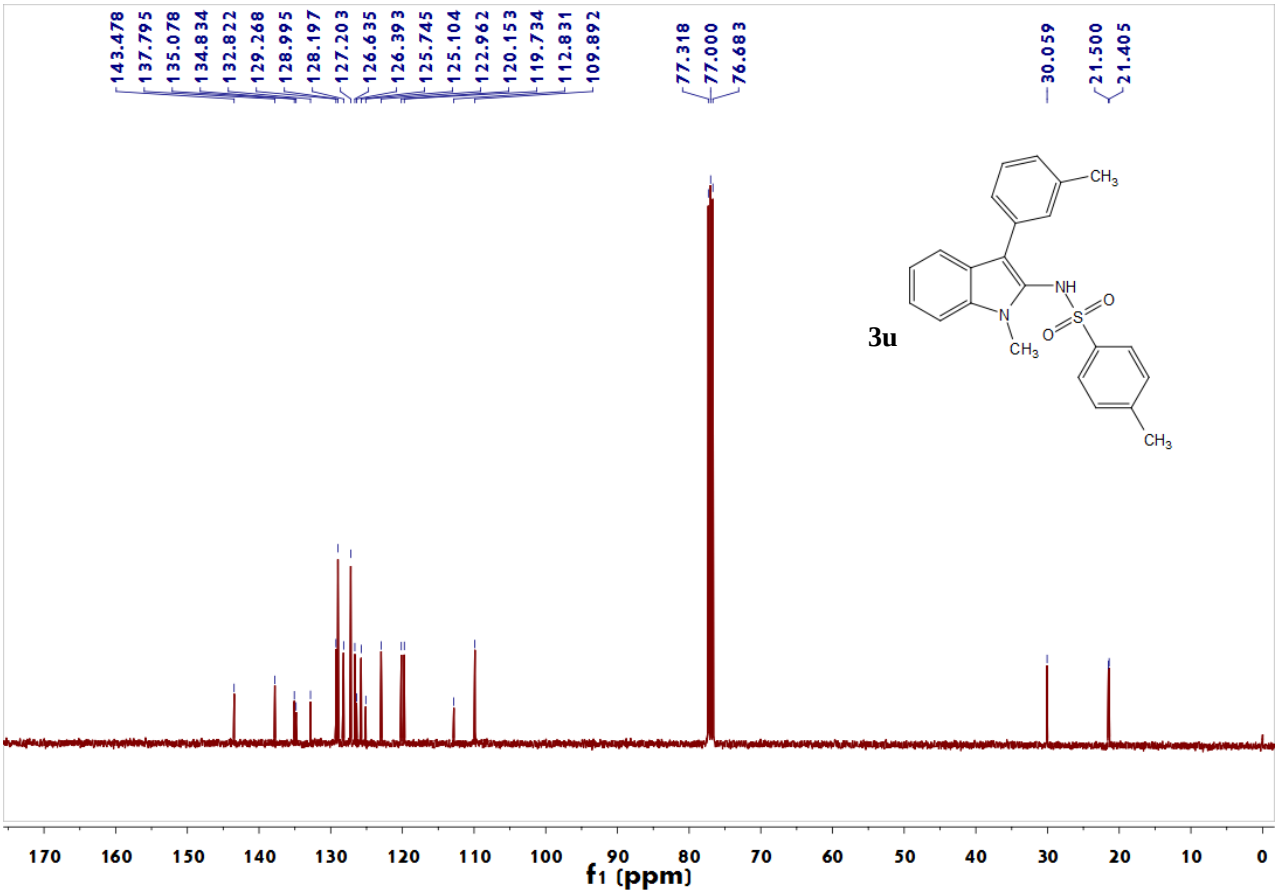
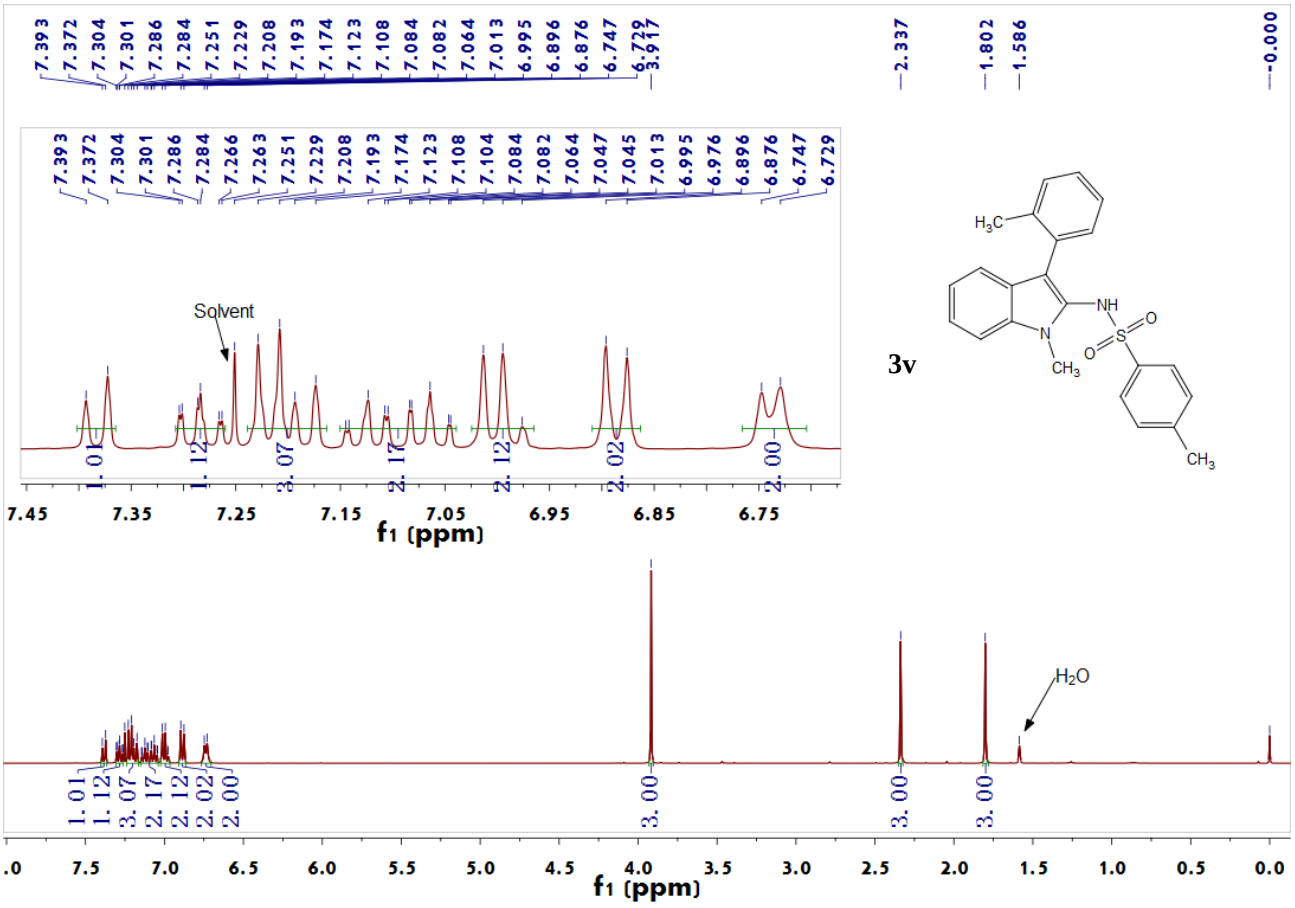
127.242
126.128
125.319
125.211
122.952
120.065
119.663
113.683
112.594
109.868
77.318
77.000
76.683
55.235
29.969
21.496
3s
f1 (ppm)

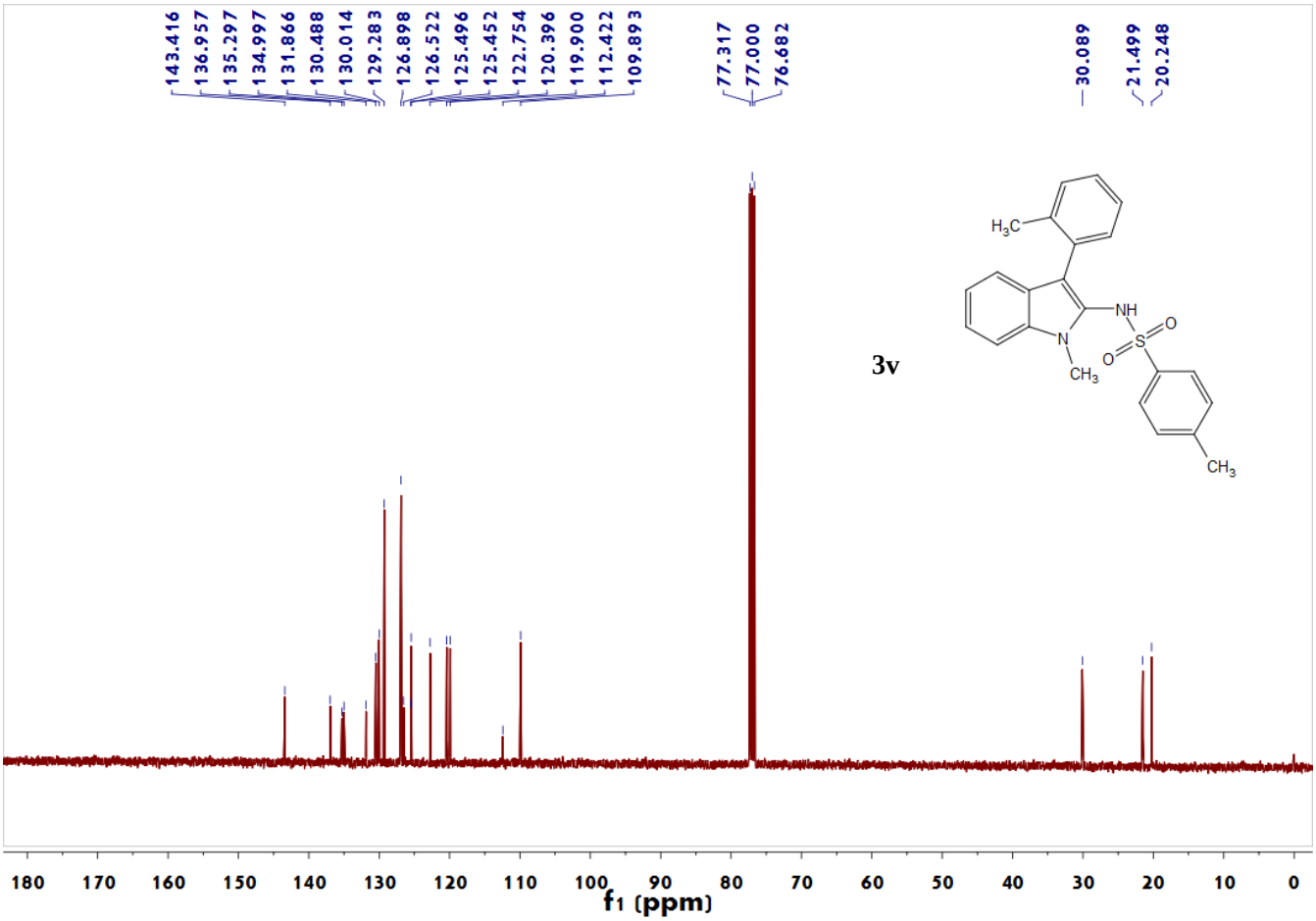

Solvent
3t
H2O
f1 (ppm)


3t
f1 (ppm)


Solvent
3u
H2O
f1 (ppm)


3u
f1 (ppm)


7.393
7.372
7.304
7.301
7.286
7.284
7.251
7.229
7.208
7.193
7.174
7.123
7.108
7.084
7.082
7.064
7.013
6.995
6.896
6.876
6.747
6.729
3.917
2.337
1.802
1.586
0.000
Solvent
1.01
1.12
3.07
2.17
2.12
2.02
2.00
3.00
3.00
3.00
H2O
f1 (ppm)
3v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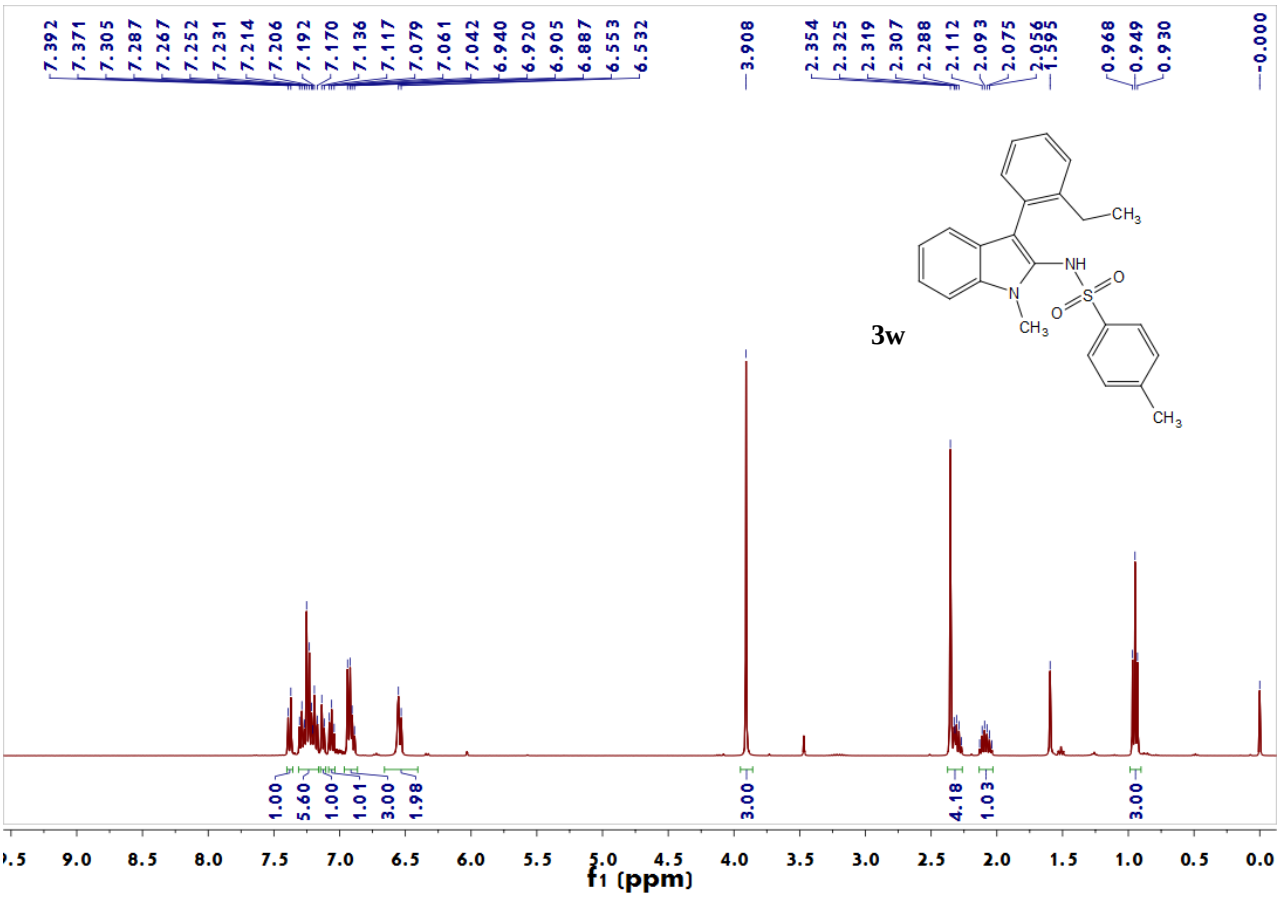
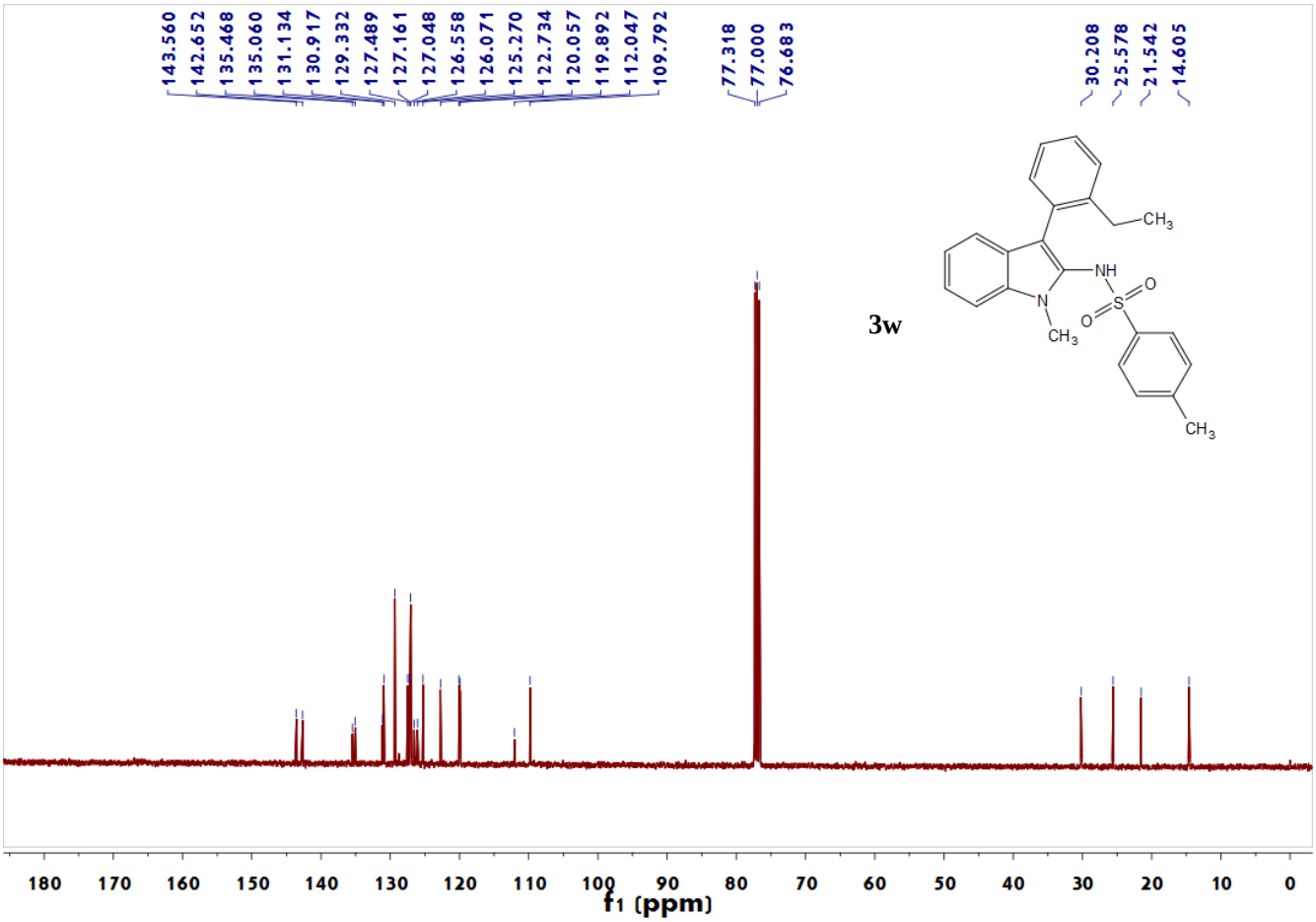
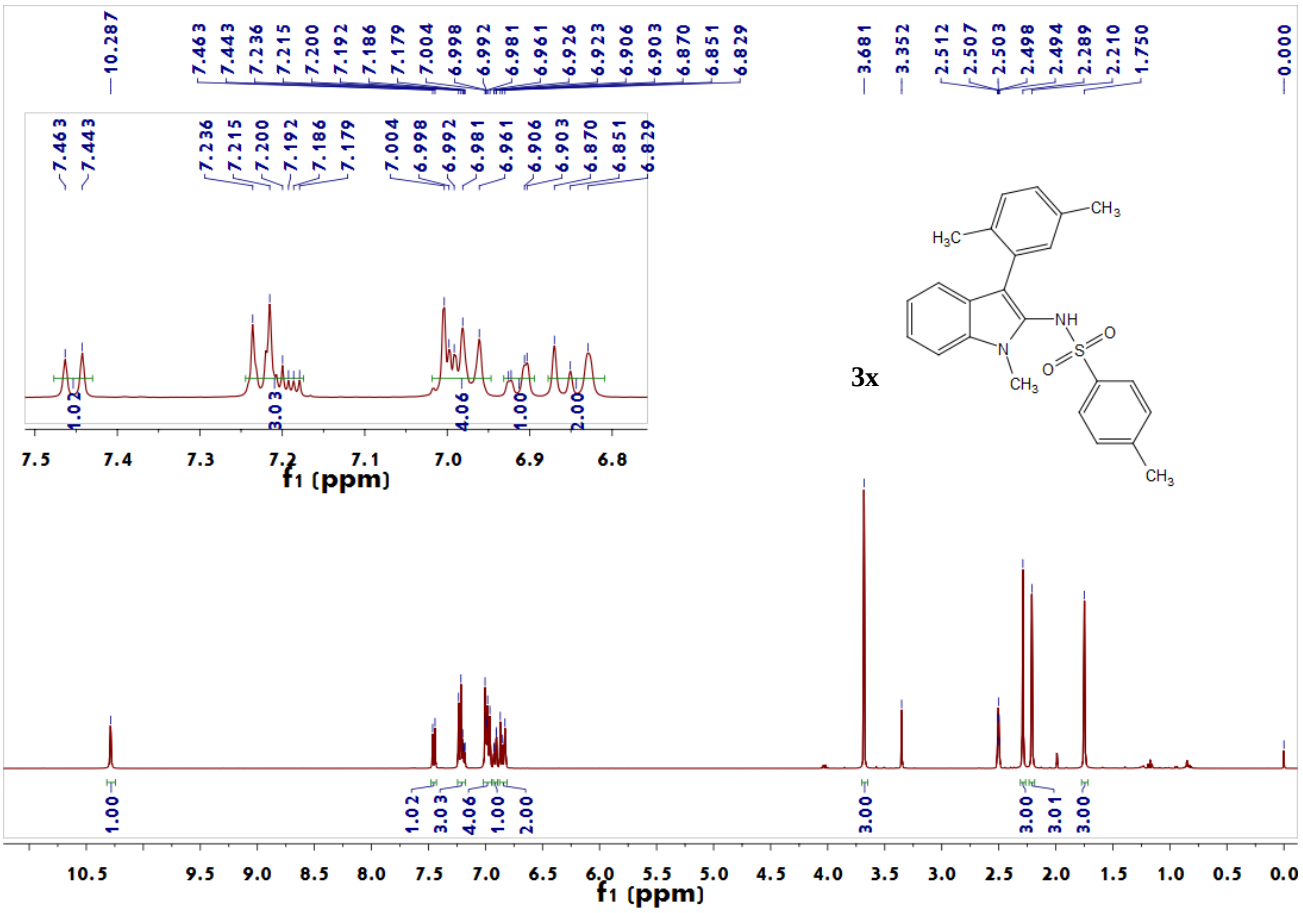
135.297
134.997
131.866
130.488
130.014
129.283
126.898
126.522
125.496
125.452
122.754
120.396
119.900
112.422
109.893
77.317
77.000
76.682
30.089
21.499
20.248
f1 (ppm)
3v


7.392
7.371
7.305
7.287
7.267
7.252
7.231
7.214
7.206
7.192
7.170
7.136
7.117
7.079
7.061
7.042
6.940
6.920
6.905
6.887
6.553
6.532
3.908
2.354
2.325
2.319
2.307
2.288
2.112
2.093
2.075
2.056
1.595
0.968
0.949
0.930
0.000
1.00
5.60
1.00
1.01
3.00
1.98
3.00
4.18
1.03
3.00
f1 (ppm)

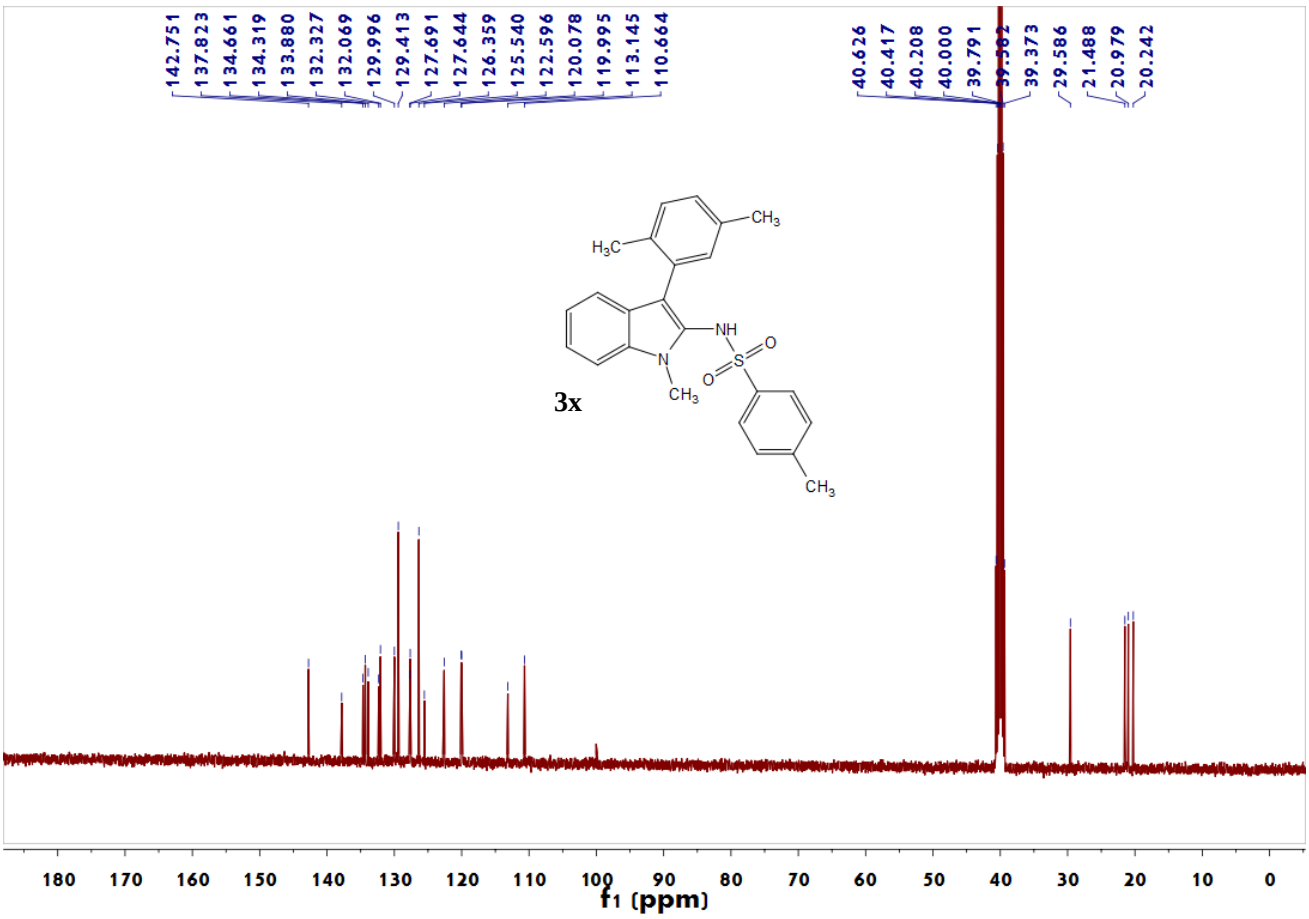
3w


143.560
142.652
135.468
135.060
131.134
130.917
129.332
127.489
127.161
127.048
126.558
126.071
125.270
122.734
120.057
119.892
112.047
109.792
77.318
77.000
76.683
30.208
25.578
21.542
14.605
f1 (ppm)

3w


10.287
7.463
7.443
7.236
7.215
7.200
7.192
7.186
7.179
7.004
6.998
6.992
6.981
6.961
6.926
6.923
6.906
6.903
6.870
6.851
6.829
3.681
3.352
2.512
2.507
2.503
2.498
2.494
2.289
2.210
1.750
0.000
1.02
3.03
4.06
1.00
2.00
3.00
3.01
3.00
f1 (ppm)

3x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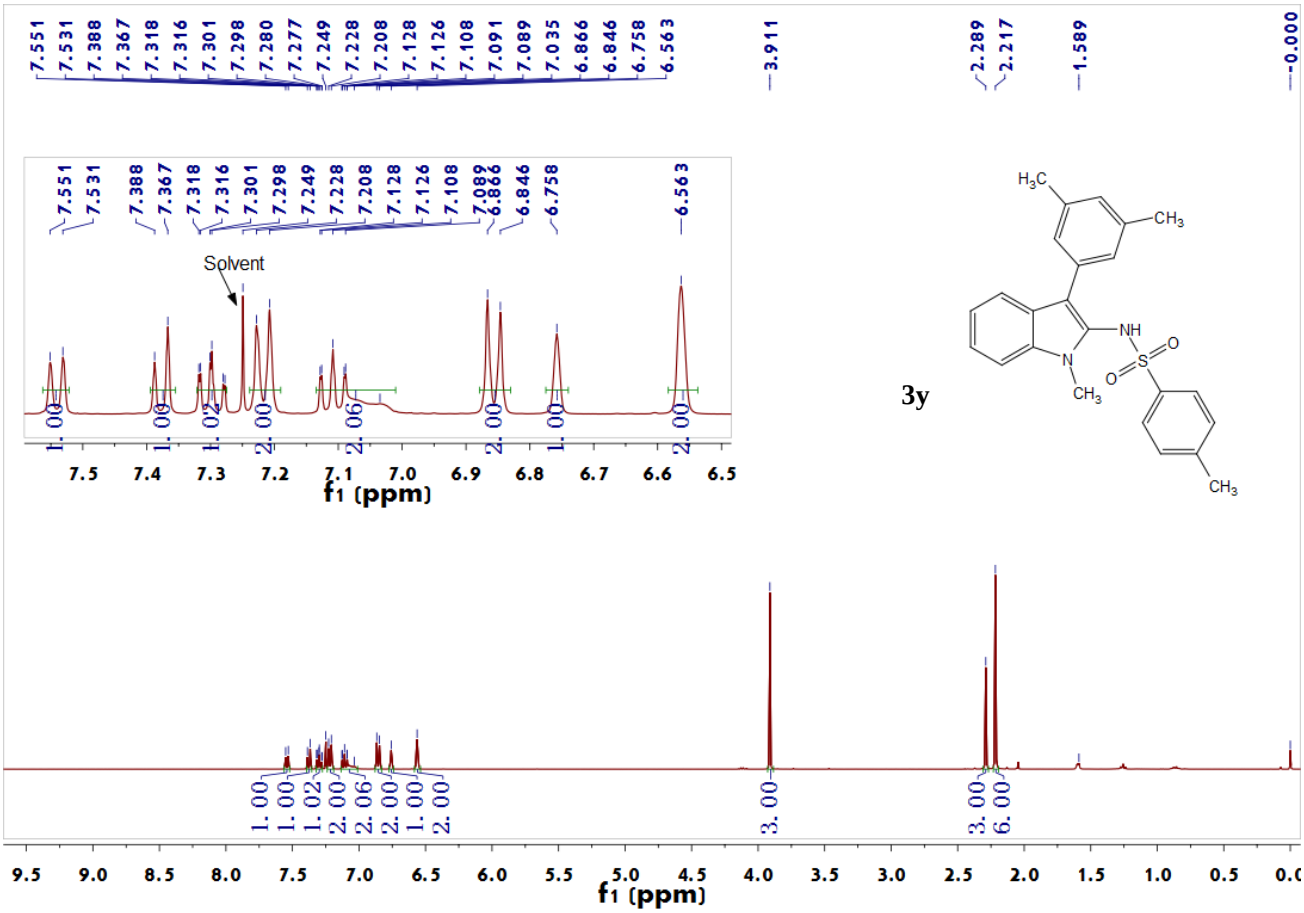
137.823
134.661
134.319
133.880
132.327
132.069
129.996
129.413
127.691
127.644
126.359
125.540
122.596
120.078
119.995
113.145
110.664
40.626
40.417
40.208
40.000
39.791
39.582
39.373
29.586
21.488
20.979
20.242
f1 (ppm)

3x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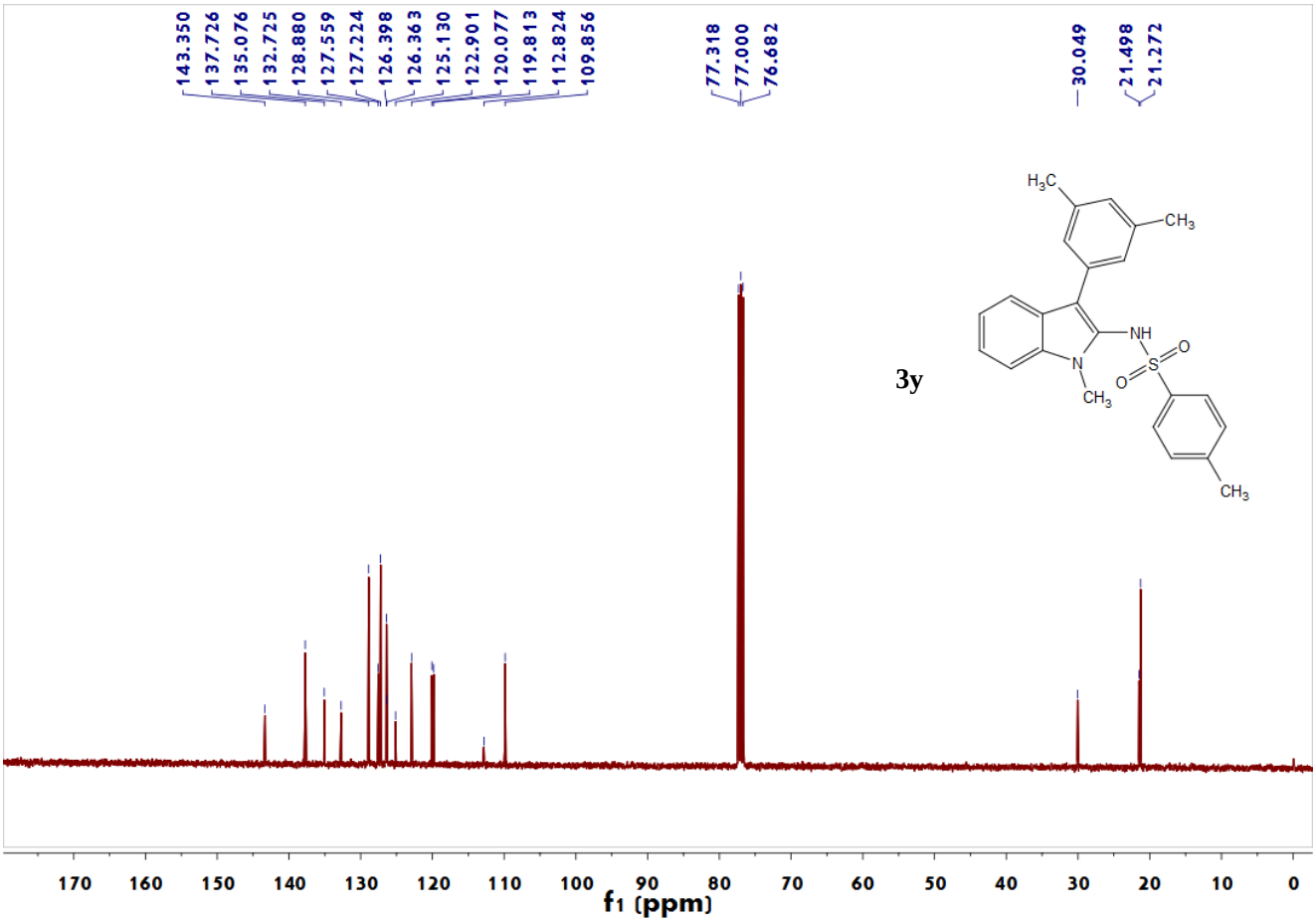
7.388
7.367
7.318
7.316
7.301
7.298
7.280
7.277
7.249
7.228
7.208
7.128
7.126
7.108
7.091
7.089
7.035
6.866
6.846
6.758
6.563
3.911
2.289
2.217
1.589
0.000
Solvent
3y
f1 (ppm)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137.726
135.076
132.725
128.880
127.559
127.224
126.398
126.363
125.130
122.901
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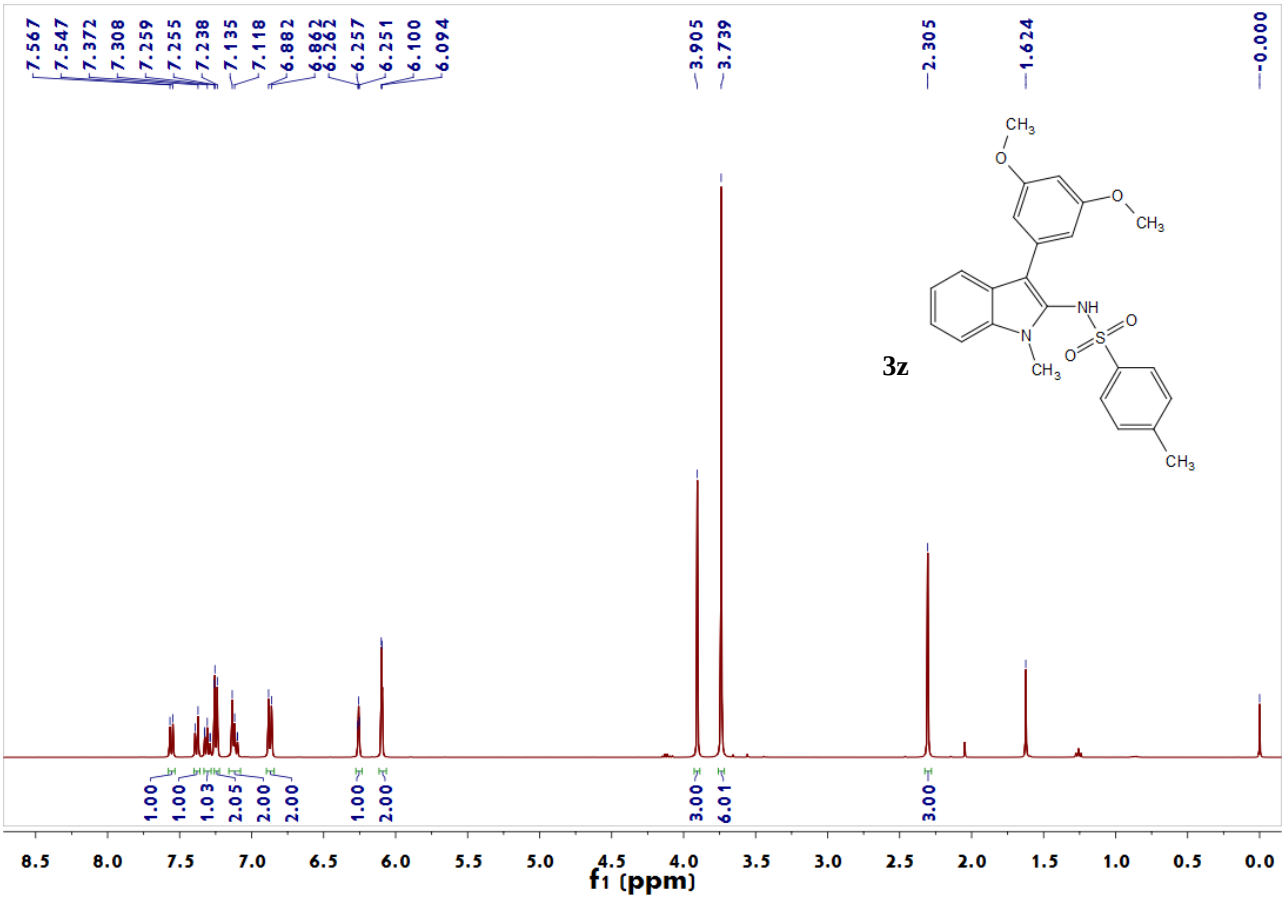
119.813
112.824
109.856
77.318
77.000
76.682
30.049
21.498
21.272
3y
f1 (ppm)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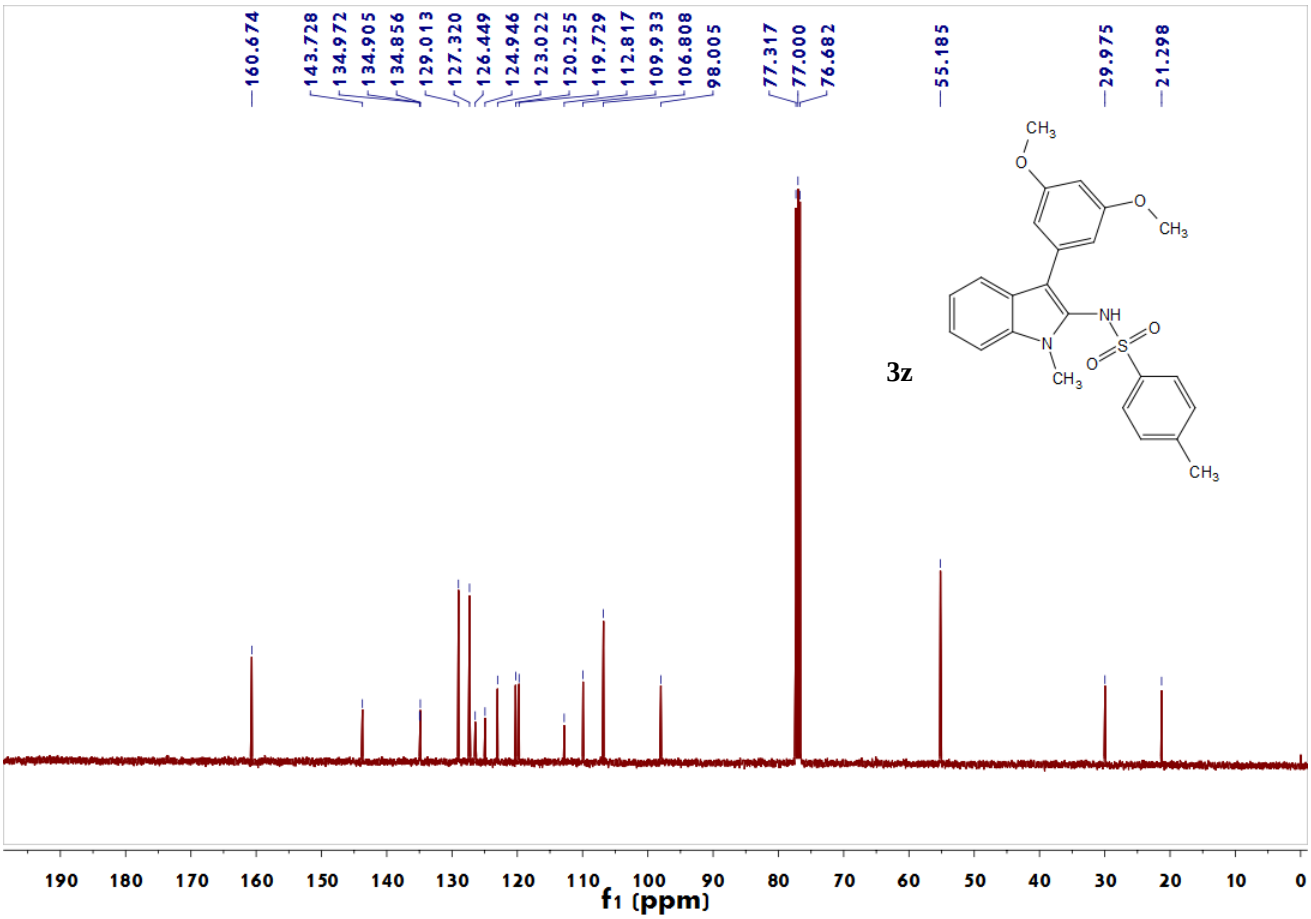
7.372
7.308
7.259
7.255
7.238
7.135
7.118
6.882
6.862
6.282
6.257
6.251
6.100
6.094
3.905
3.739
2.305
1.624
0.000
1.00
1.00
1.03
2.05
2.00
2.00
1.00
2.00
3.00
6.01
3.00
3z
f1 (ppm)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127.320
126.449
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123.022
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119.729
112.817
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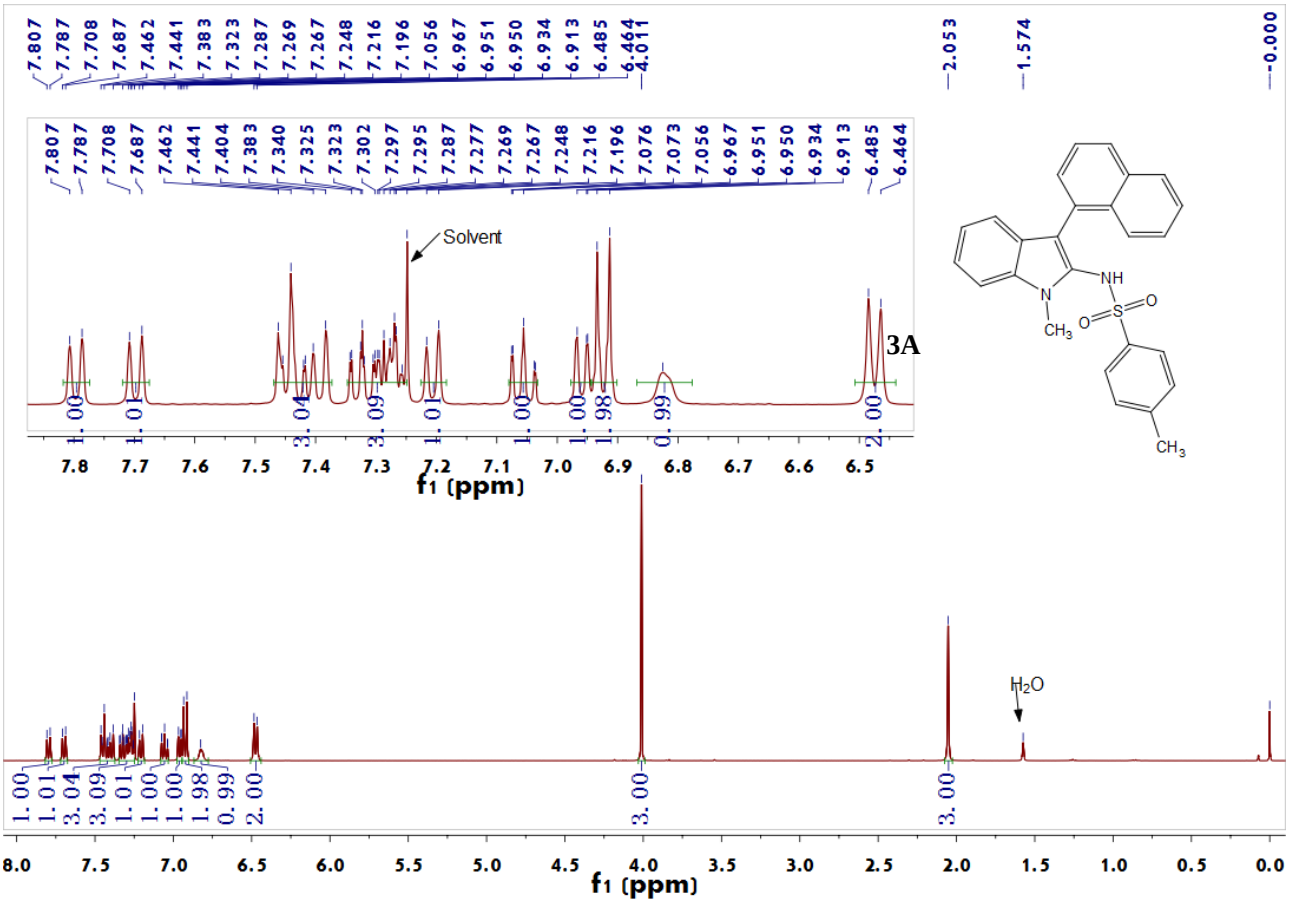
106.808
98.005
77.317
77.000
76.682
55.185
29.975
21.298
3z
f1 (ppm)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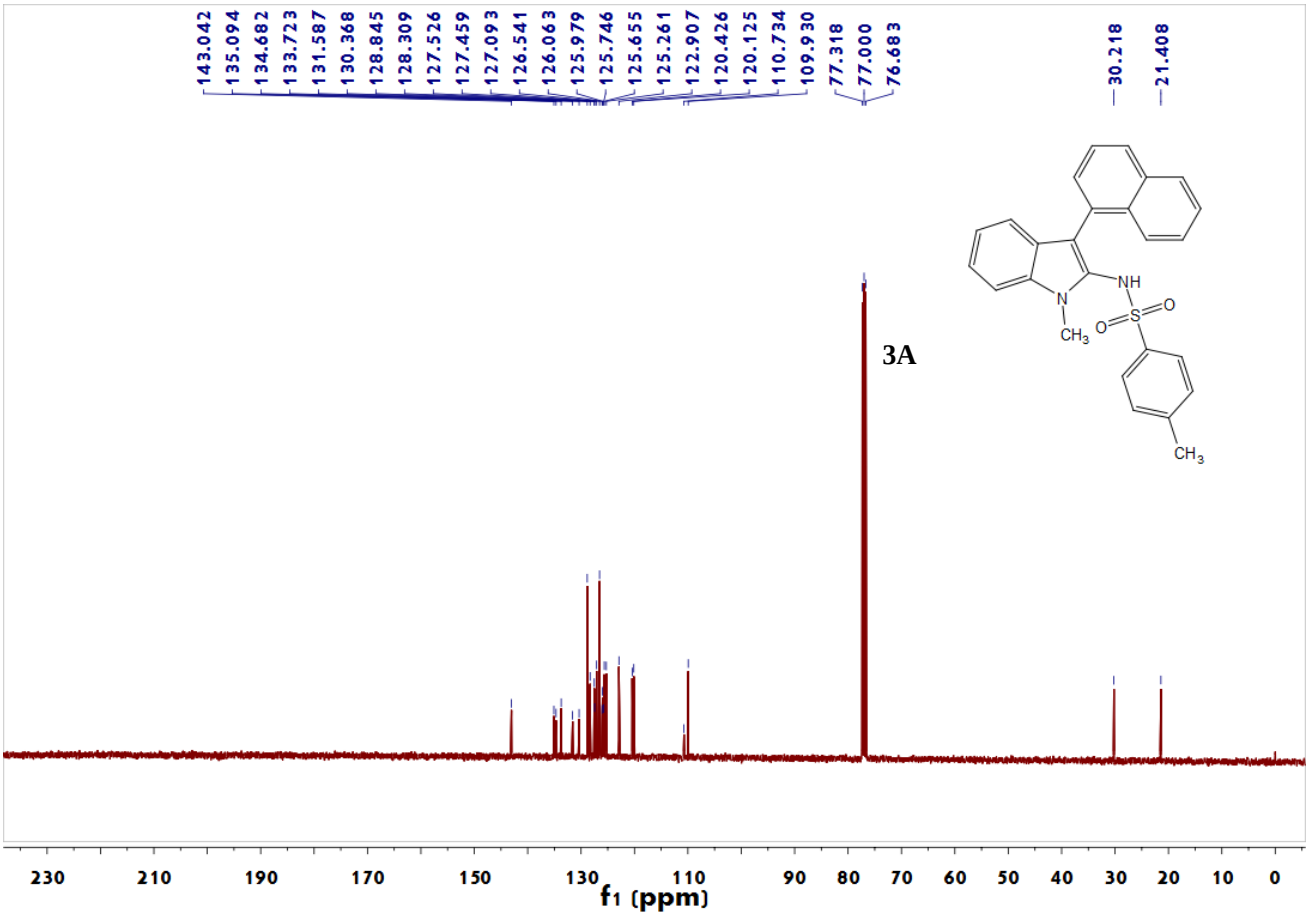
7.687
7.462
7.441
7.383
7.323
7.287
7.269
7.267
7.248
7.216
7.196
7.056
6.967
6.951
6.950
6.934
6.913
6.485
6.464
4.011
2.053
1.574
0.000
Solvent
3A
NH
N
CH3
O
S
O
CH3
H2O
1.00
1.01
3.04
3.09
1.01
1.00
1.00
1.98
0.99
2.00
3.00
3.00
f1 (ppm)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128.309
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127.093
126.541
126.063
125.979
125.746
125.655
125.261
122.907
120.426
120.125
110.734
109.930
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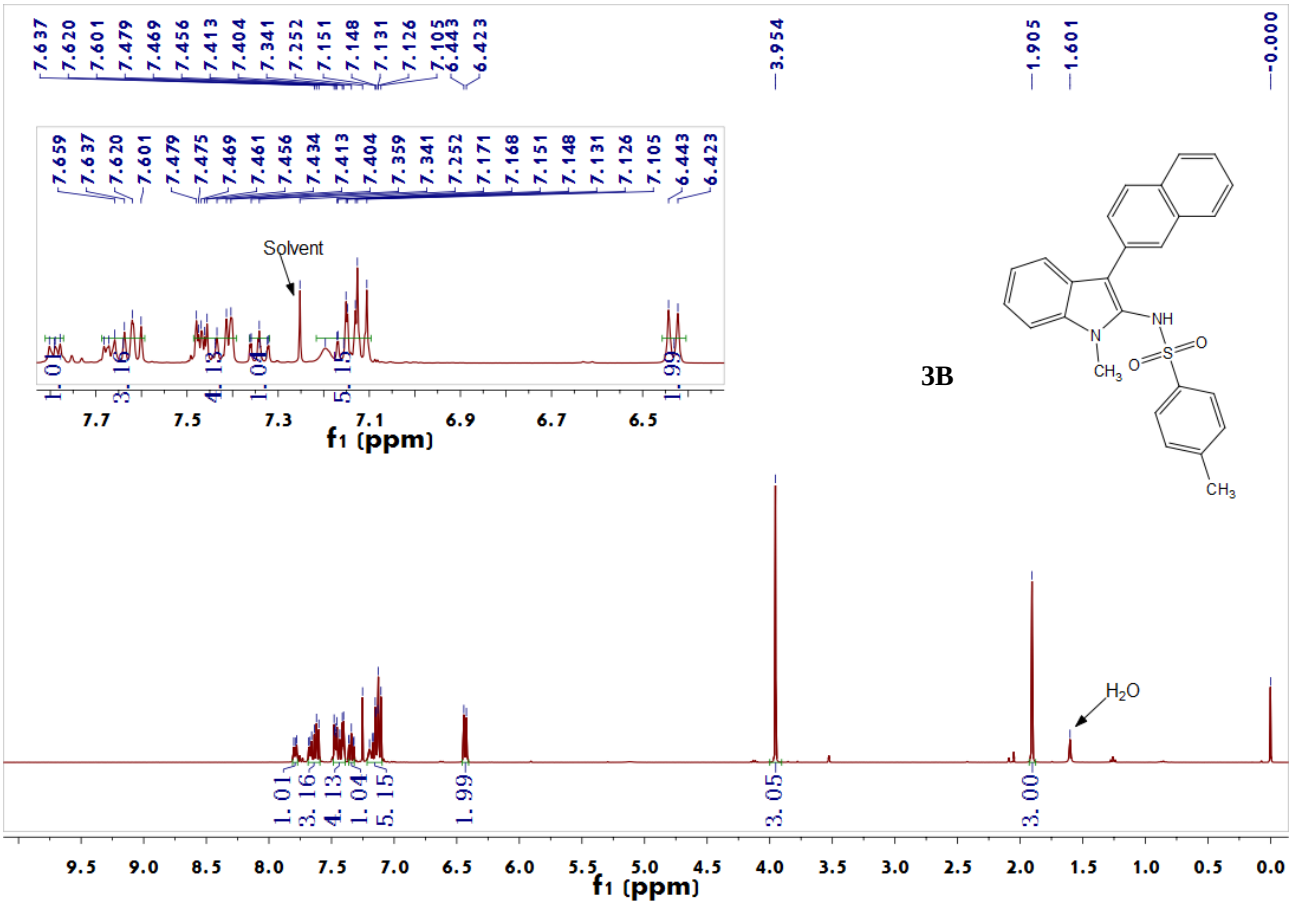
77.000
76.683
30.218
21.408
3A
NH
N
CH3
O
S
O
CH3
f1 (ppm)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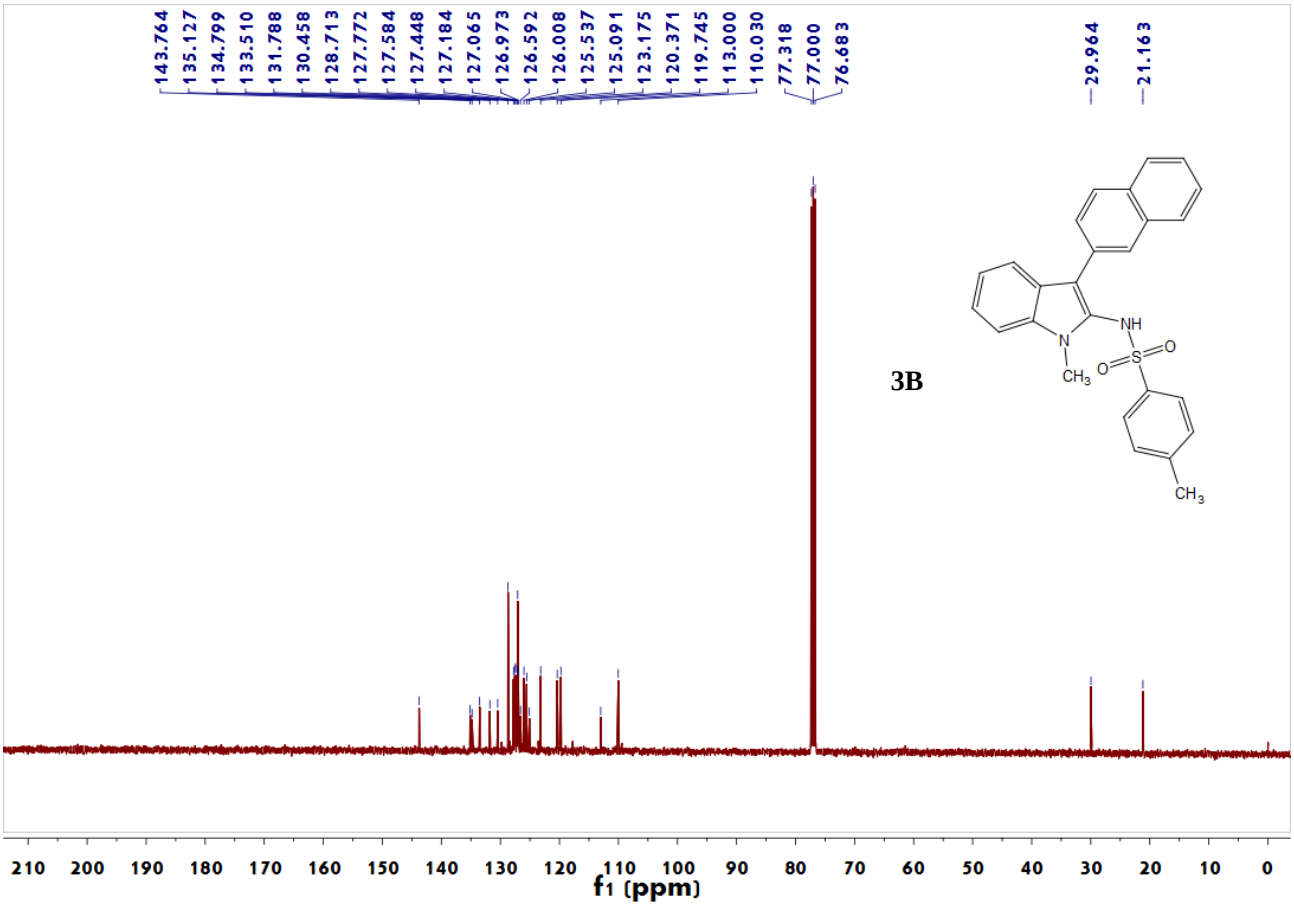
7.404
7.341
7.252
7.151
7.148
7.131
7.126
7.105
6.443
6.423
3.954
1.905
1.601
0.000
Solvent
3B
NH
N
CH3
O
S
O
CH3
H2O
1.01
3.16
4.13
1.04
5.15
1.99
3.05
3.00
f1 (ppm)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133.510
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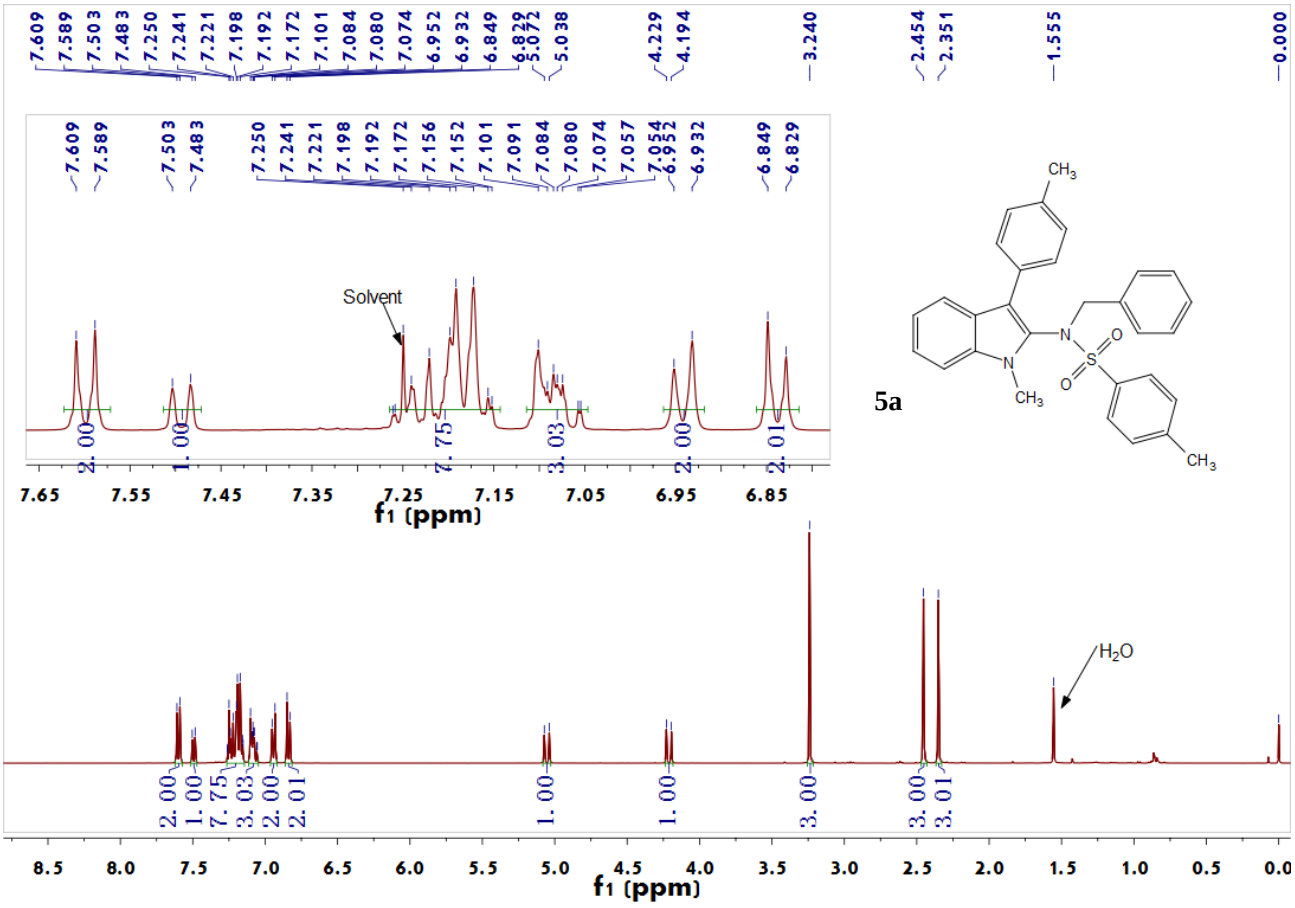
128.713
127.772
127.584
127.448
127.184
127.065
126.973
126.592
126.008
125.537
125.091
123.175
120.371
119.745
113.000
110.030
77.318
77.000
76.683
29.964
21.163
3B
NH
N
CH3
O
S
O
CH3
f1 (ppm)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7.250
7.241
7.221
7.198
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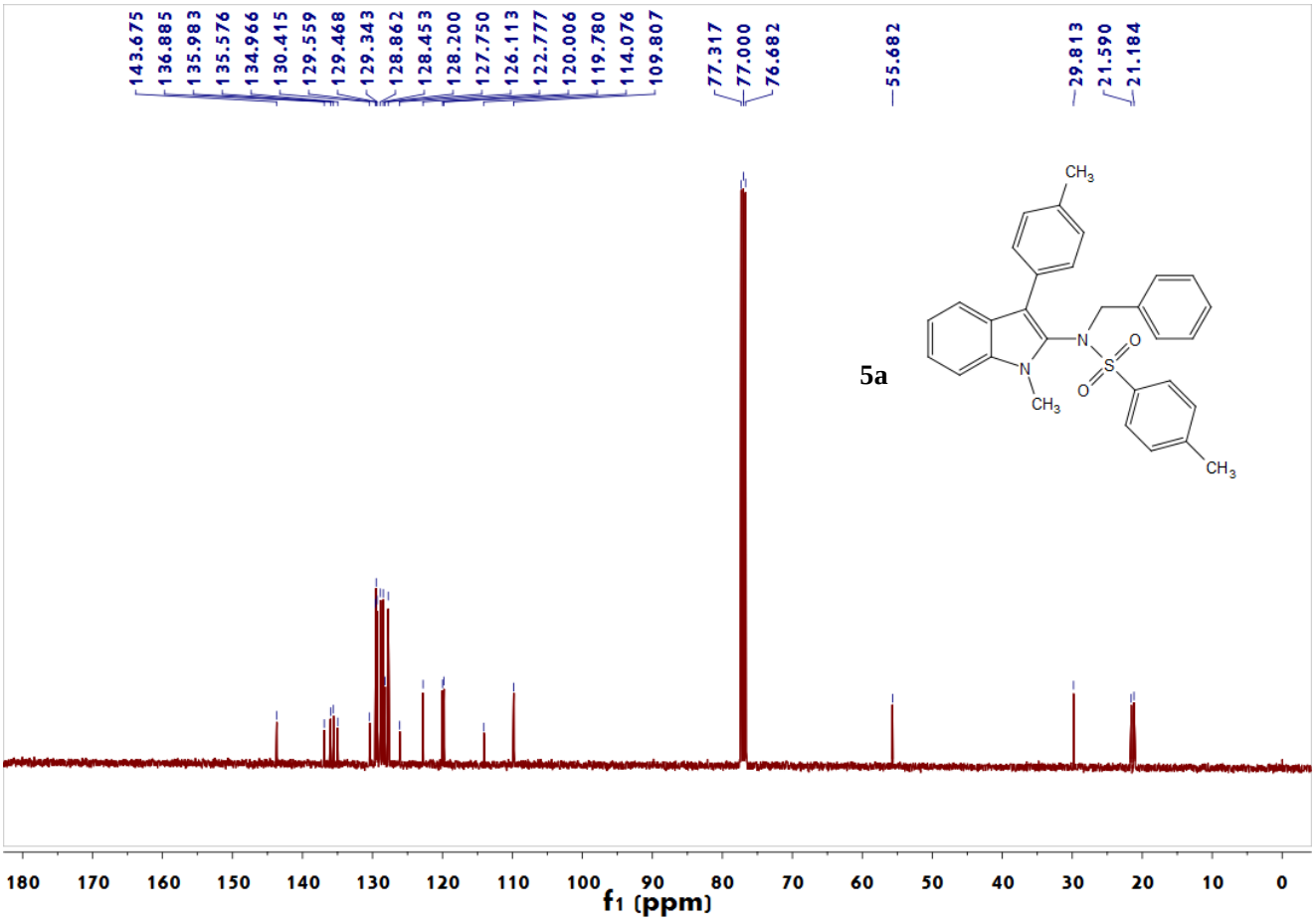
7.172
7.101
7.084
7.080
7.074
6.952
6.932
6.849
6.829
5.072
5.038
4.229
4.194
3.240
2.454
2.351
1.555
0.000
Solvent
2.00
1.00
7.75
3.03
2.00
2.01
f1 (ppm)
5a
H2O
1.00
1.00
3.00
3.00
3.01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129.468
129.343
128.862
128.453
128.200
127.750
126.113
122.777
120.006
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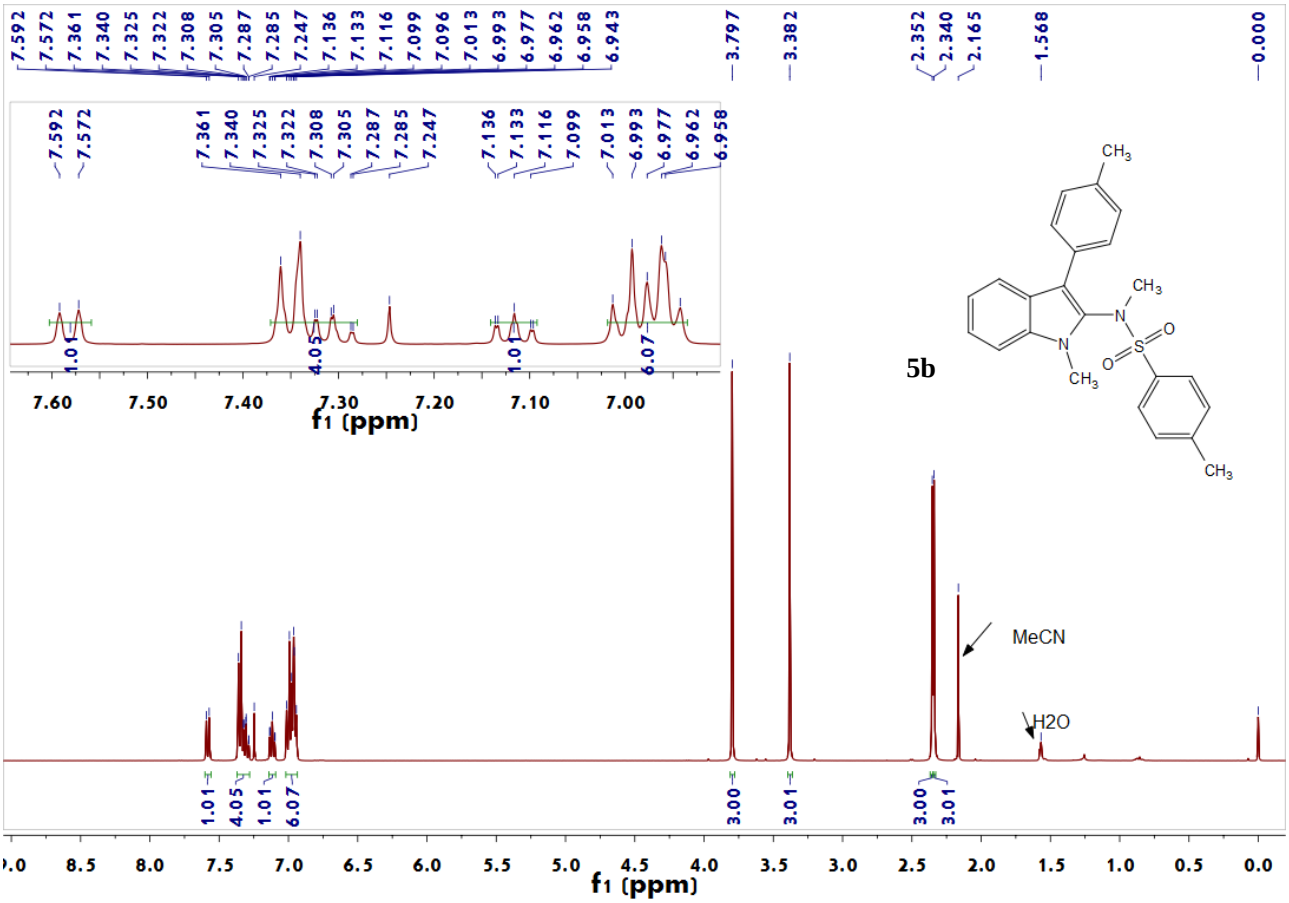
77.000
76.682
55.682
29.813
21.590
21.184
5a
f1 (ppm)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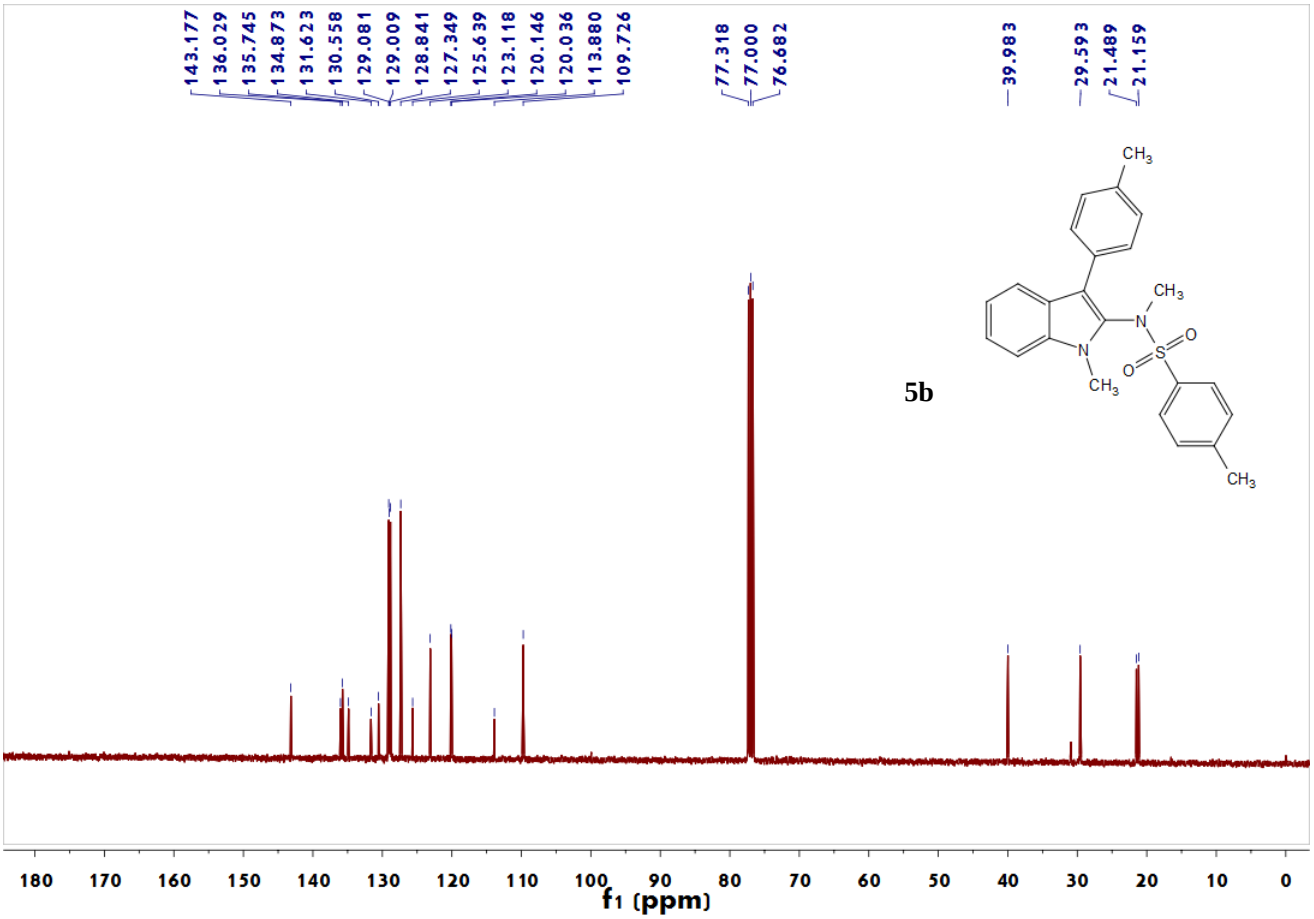
7.322
7.308
7.305
7.287
7.285
7.247
7.136
7.133
7.116
7.099
7.096
7.013
6.993
6.977
6.962
6.958
6.943
3.797
3.382
2.352
2.340
2.165
1.568
0.000
1.01
4.05
1.01
6.07
3.00
3.01
3.00
3.01
MeCN
H2O
5b
f1 (ppm)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131.623
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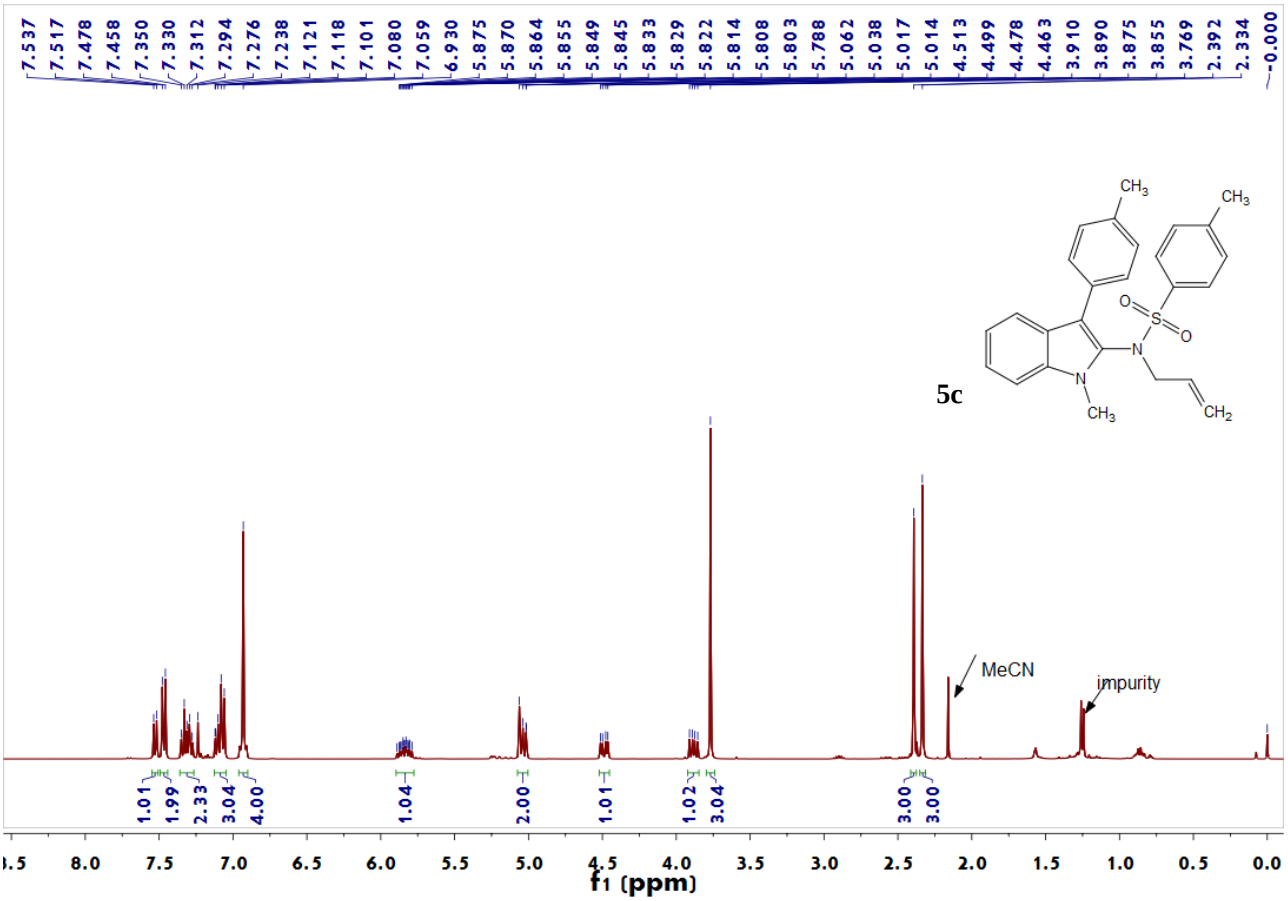
129.081
129.009
128.841
127.349
125.639
123.118
120.146
120.036
113.880
109.726
77.318
77.000
76.682
39.983
29.593
21.489
21.159
5b
f1 (ppm)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7.330
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7.294
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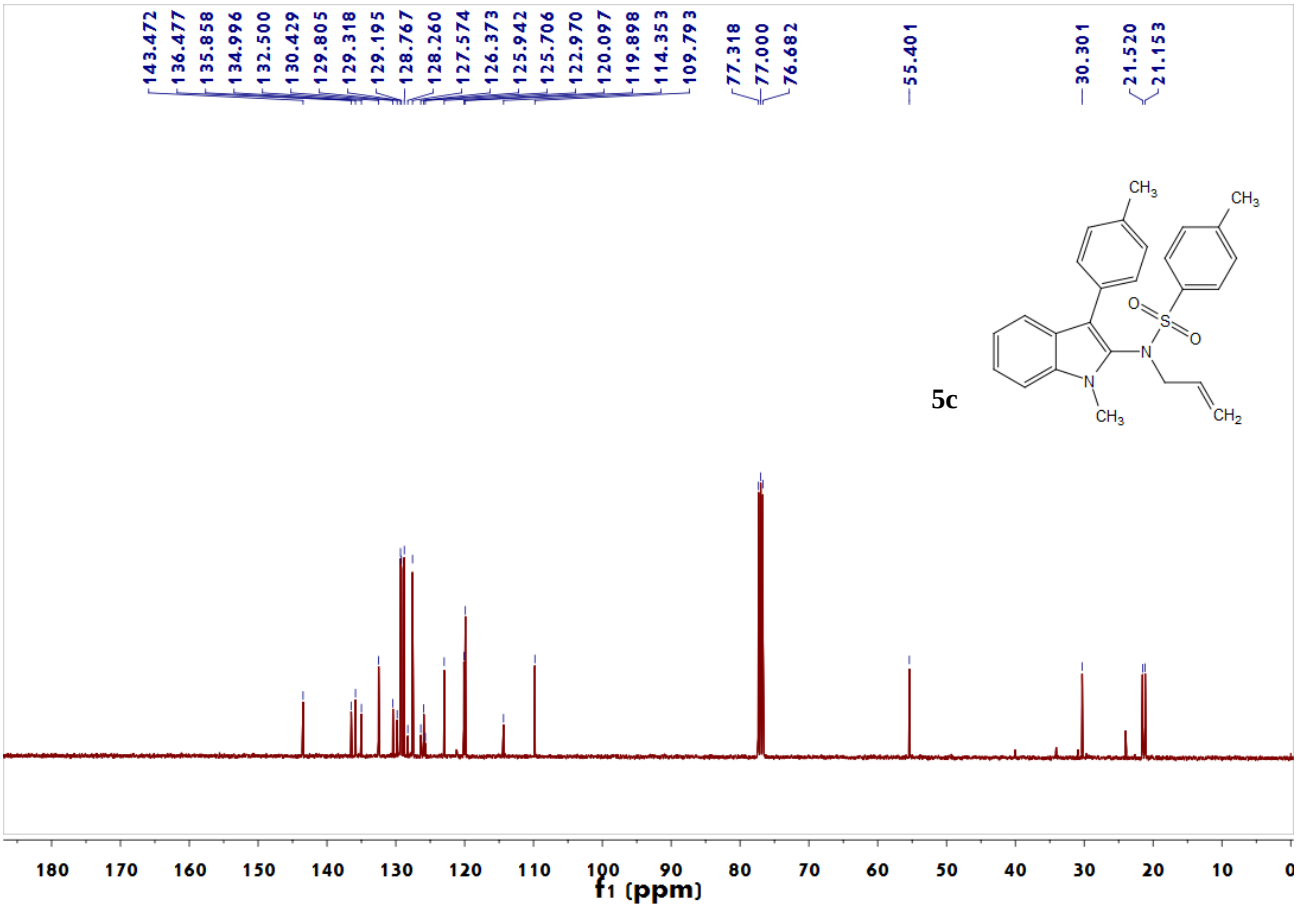
7.238
7.121
7.118
7.101
7.080
7.059
6.930
5.875
5.870
5.864
5.855
5.849
5.845
5.833
5.829
5.822
5.814
5.808
5.803
5.788
5.062
5.038
5.017
5.014
4.513
4.499
4.478
4.463
3.910
3.890
3.875
3.855
3.769
2.392
2.334
-0.000
5c
MeCN
impurity
1.01
1.99
2.33
3.04
4.00
1.04
2.00
1.01
1.02
3.04
3.00
3.00
f1 (ppm)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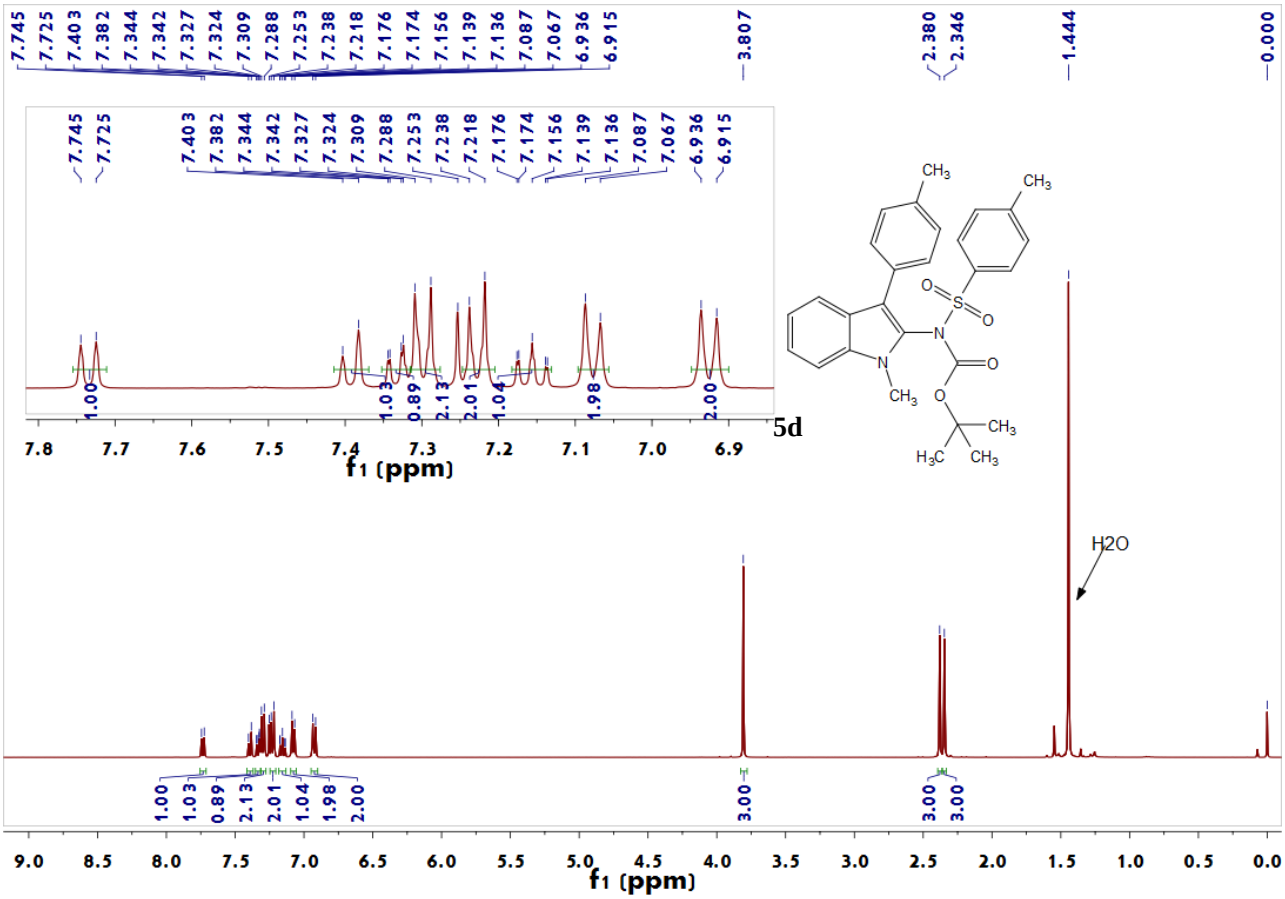
129.805
129.318
129.195
128.767
128.260
127.574
126.373
125.942
125.706
122.970
120.097
119.898
114.353
109.793
77.318
77.000
76.682
55.401
30.301
21.520
21.153
5c
f1 (ppm)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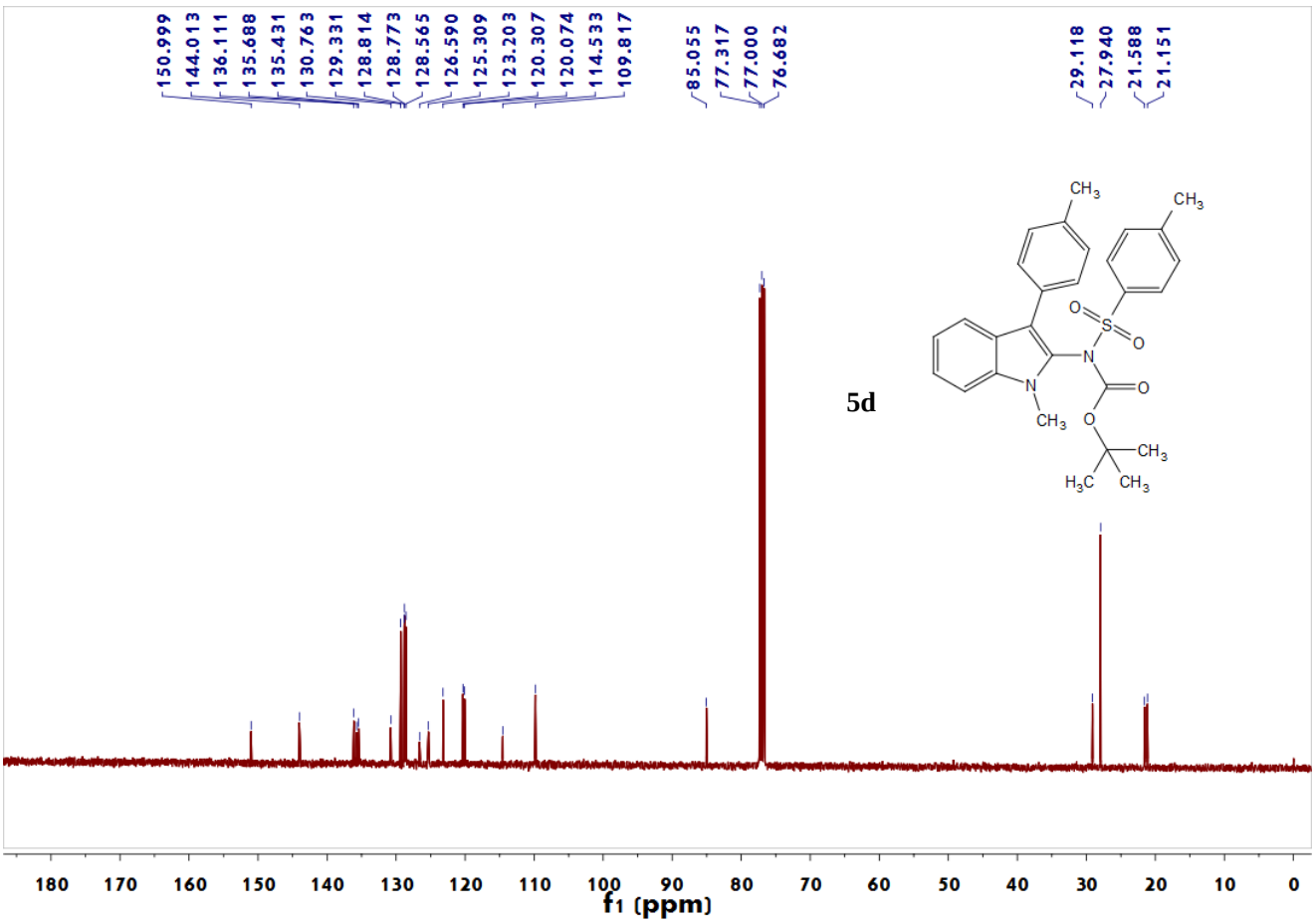
7.382
7.344
7.342
7.327
7.324
7.309
7.288
7.253
7.238
7.218
7.176
7.174
7.156
7.139
7.136
7.087
7.067
6.936
6.915
3.807
2.380
2.346
1.444
0.000
1.00
1.03
0.89
2.13
2.01
1.04
1.98
2.00
3.00
3.00
3.00
H2O
f1 (ppm)

5d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136.111
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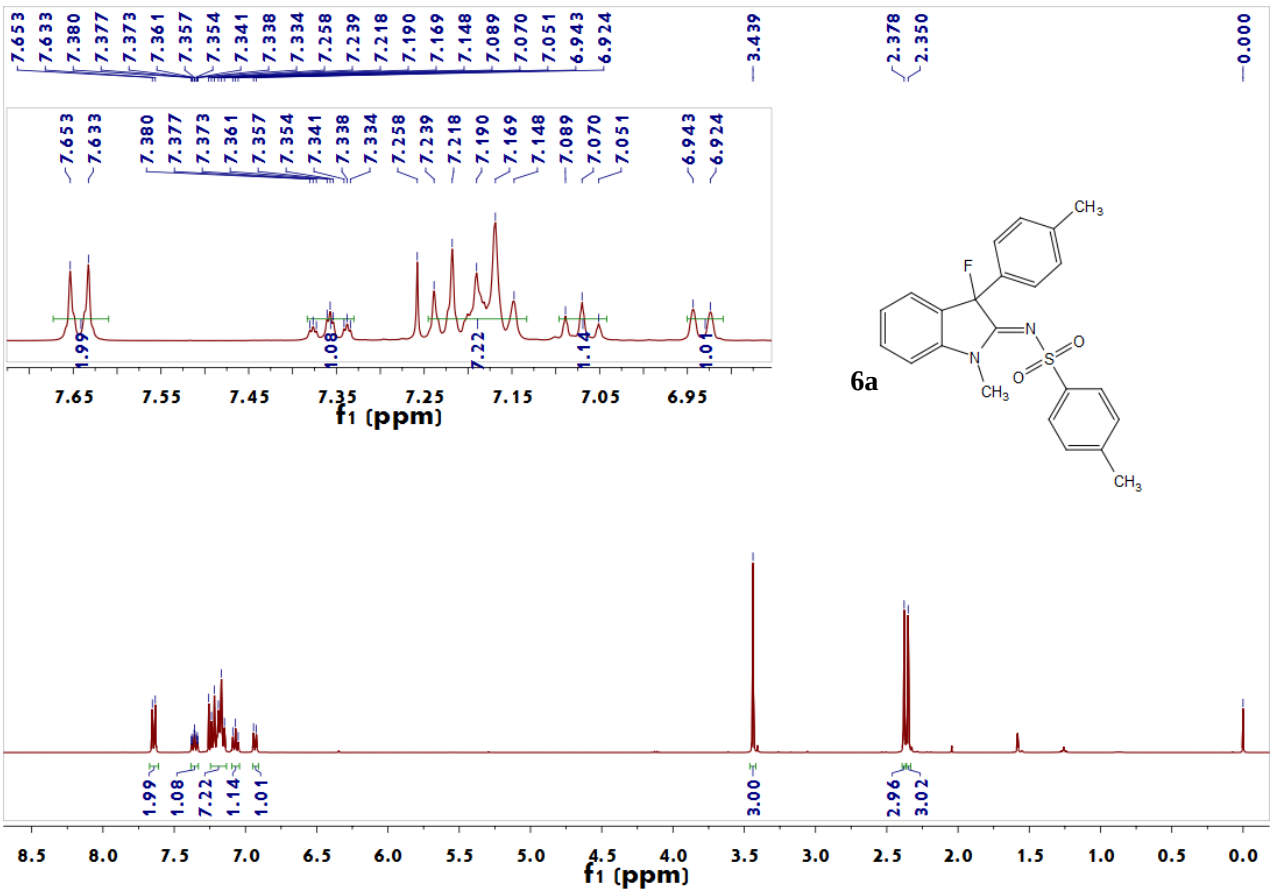
135.431
130.763
129.331
128.814
128.773
128.565
126.590
125.309
123.203
120.307
120.074
114.533
109.817
85.055
77.317
77.000
76.682
29.118
27.940
21.588
21.151
f1 (ppm)

5d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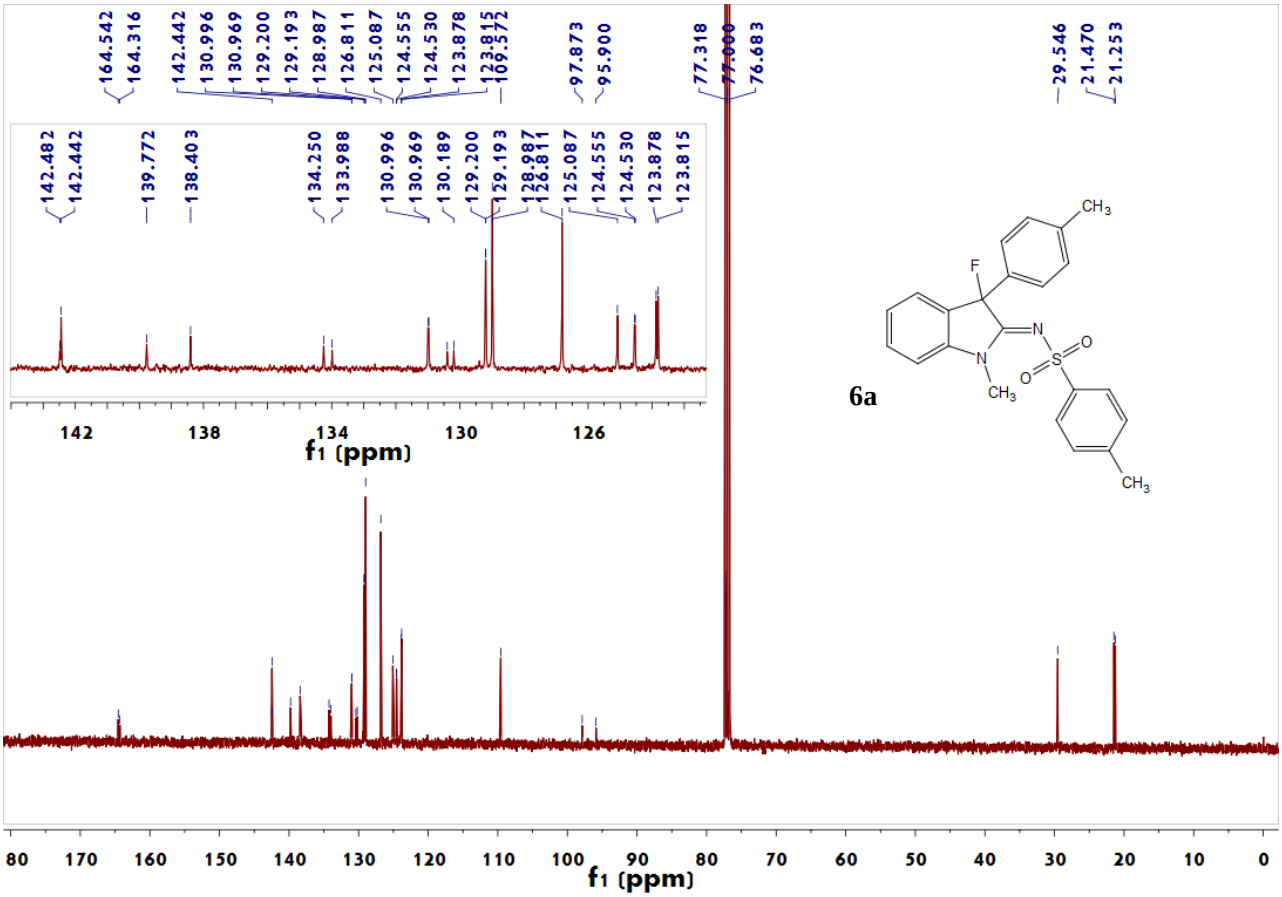
7.633
7.380
7.377
7.373
7.361
7.357
7.354
7.341
7.338
7.334
7.258
7.239
7.218
7.190
7.169
7.148
7.089
7.070
7.051
6.943
6.924
3.439
2.378
2.350
0.000
1.99
1.08
7.22
1.14
1.01
3.00
2.96
3.02
f1 (ppm)
6a
CH3
F
N
O
S
CH3
CH3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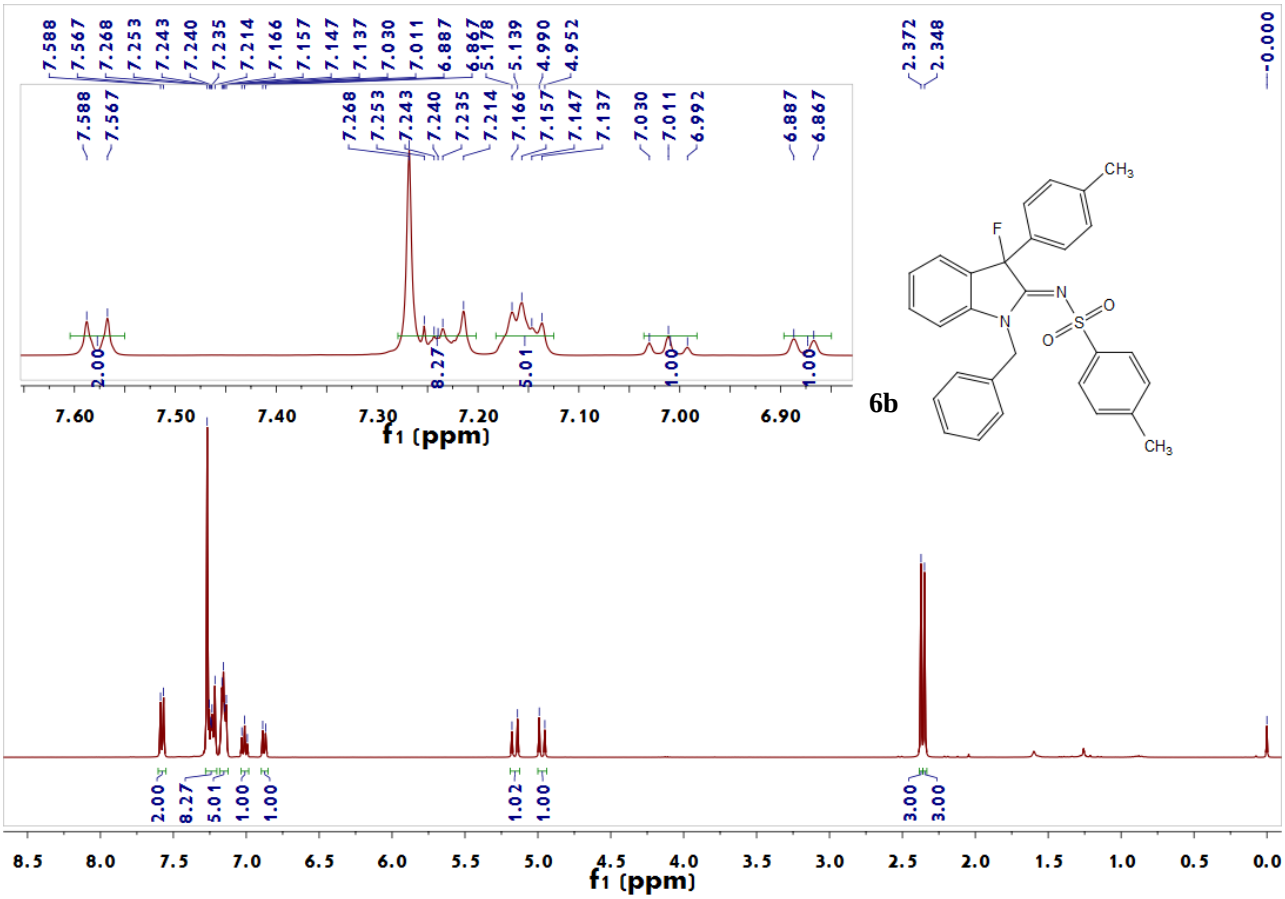
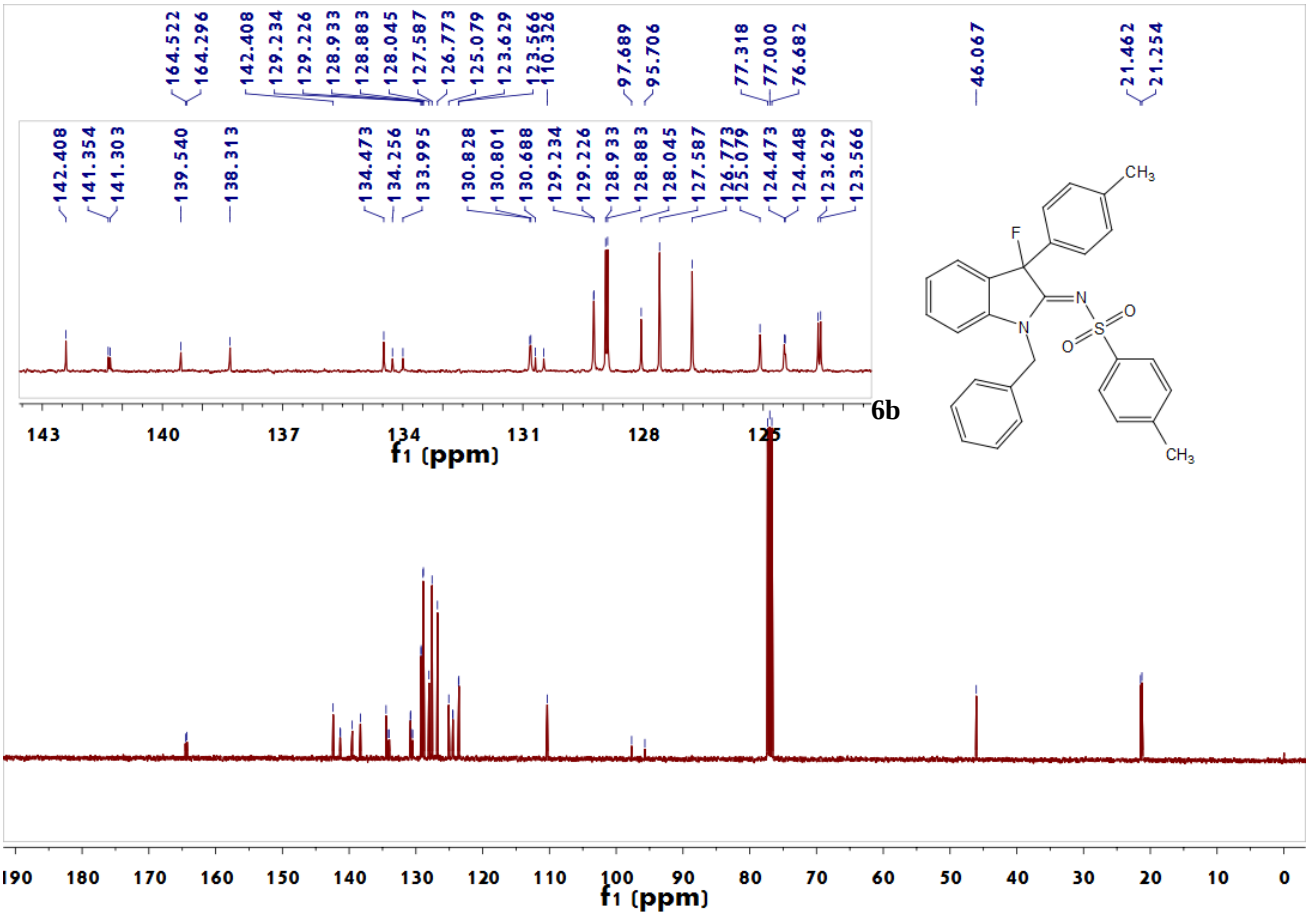
164.316
142.442
130.996
130.969
129.200
129.193
128.987
126.811
125.087
124.555
124.530
123.878
123.815
109.572
97.873
95.900
77.318
77.000
76.683
29.546
21.470
21.253
142.482
142.442
139.772
138.403
134.250
133.988
130.996
130.969
130.189
129.200
129.193
128.987
126.811
125.087
124.555
124.530
123.878
123.815
f1 (ppm)
6a
CH3
F
N
O
S
CH3
CH3


7.588
7.567
7.268
7.253
7.243
7.240
7.235
7.214
7.166
7.157
7.147
7.137
7.030
7.011
6.887
6.867
5.178
5.139
4.990
4.952
2.372
2.348
-0.000
2.00
8.27
5.01
1.00
1.00
1.02
1.00
3.00
3.00
f1 (ppm)
6b
F
N
O
S
CH3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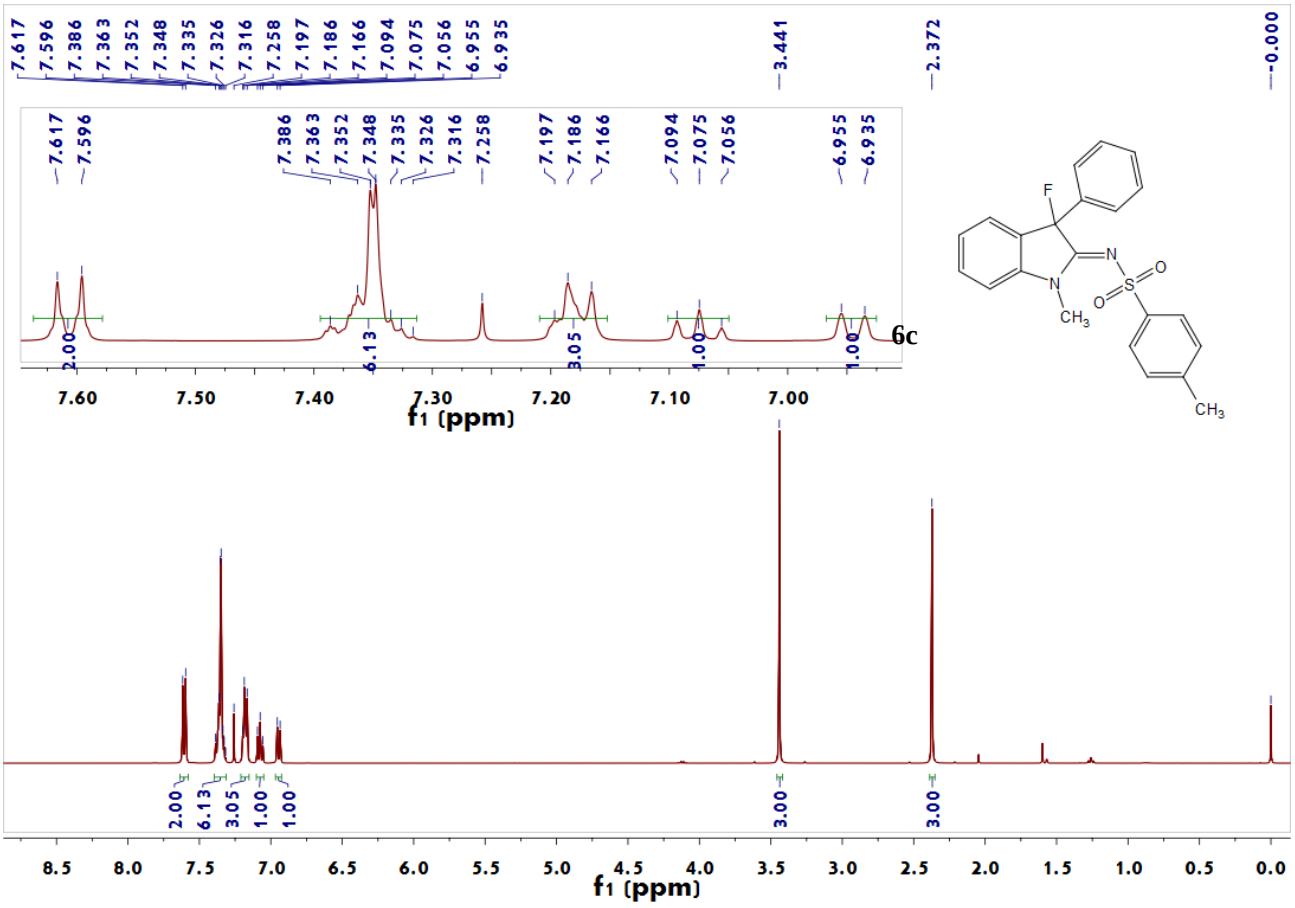
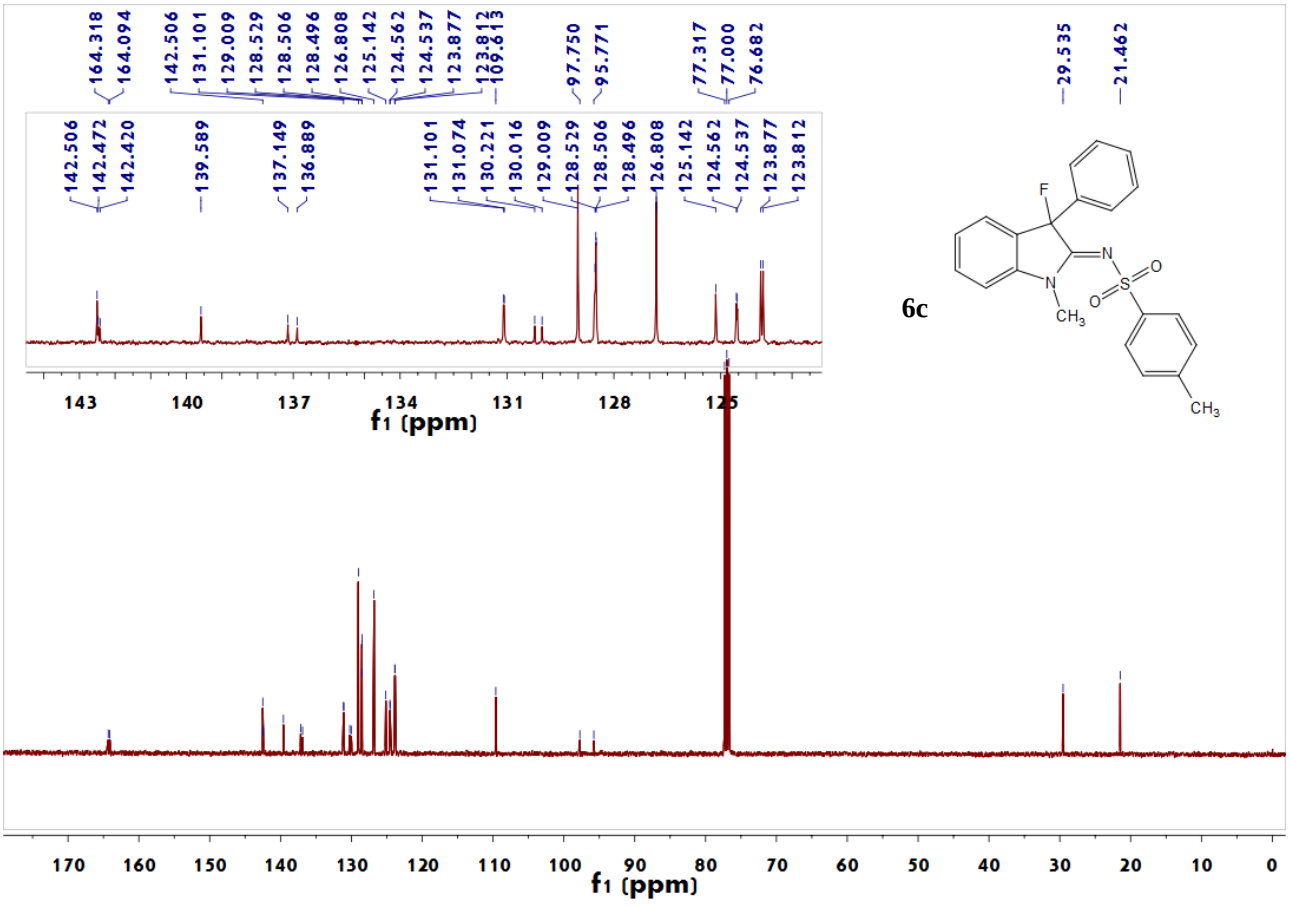
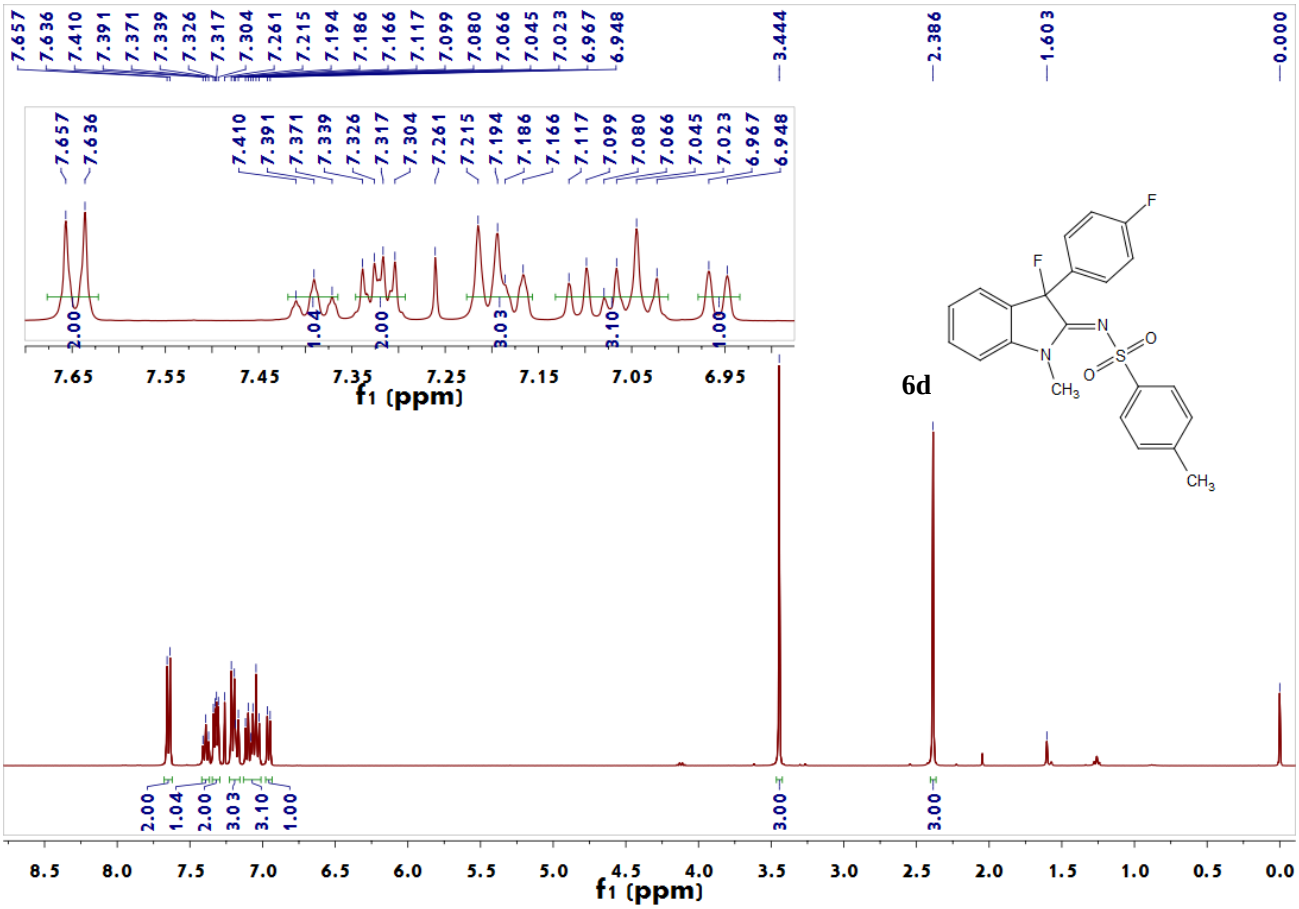
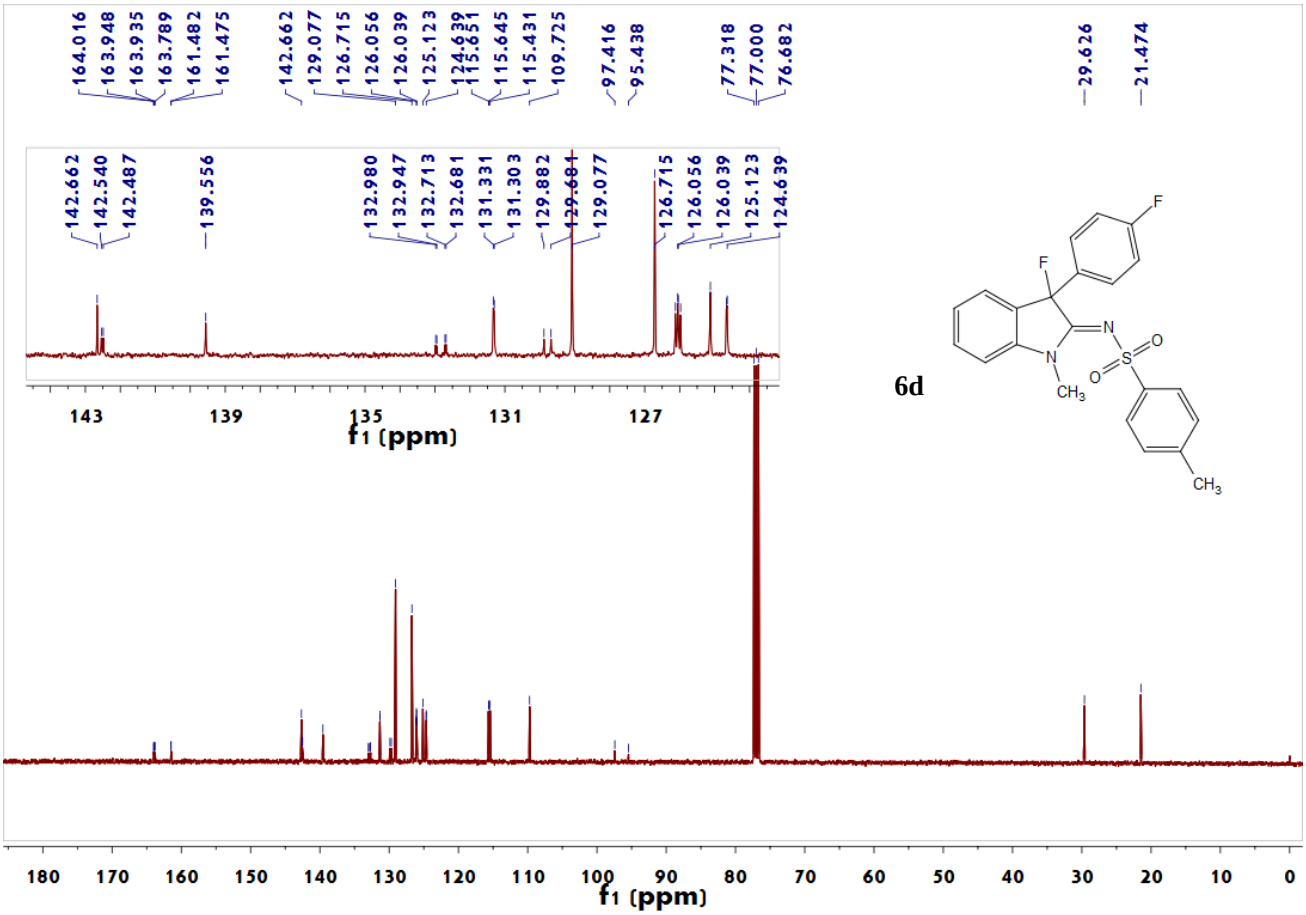
164.296
142.408
129.234
129.226
128.933
128.883
128.045
127.587
126.773
125.079
123.629
123.566
110.326
97.689
95.706
77.318
77.000
76.682
46.067
21.462
21.254
142.408
141.354
141.303
139.540
138.313
134.473
134.256
133.995
130.828
130.801
130.688
129.234
129.226
128.933
128.883
128.045
127.587
126.773
125.079
124.473
124.448
123.629
123.566
f1 (ppm)
6b
F
N
O
S
CH3


7.617
7.596
7.386
7.363
7.352
7.348
7.335
7.326
7.316
7.258
7.197
7.186
7.166
7.094
7.075
7.056
6.955
6.935
3.441
2.372
-0.000
2.00
6.13
3.05
1.00
1.00
3.00
3.00
f1 (ppm)
6c
F
N
O
S
O
N
CH3
CH3


164.318
164.094
142.506
131.101
129.009
128.529
128.506
128.496
126.808
125.142
124.562
124.537
123.877
123.812
109.613
97.750
95.771
77.317
77.000
76.682
29.535
21.462
142.506
142.472
142.420
139.589
137.149
136.889
131.101
131.074
130.221
130.016
129.009
128.529
128.506
128.496
126.808
125.142
124.562
124.537
123.877
123.812
f1 (ppm)
6c
F
N
O
S
O
N
CH3
CH3


7.657
7.636
7.410
7.391
7.371
7.339
7.326
7.317
7.304
7.261
7.215
7.194
7.186
7.166
7.117
7.099
7.080
7.066
7.045
7.023
6.967
6.948
3.444
2.386
1.603
0.000
2.00
1.04
2.00
3.03
3.10
1.00
3.00
3.00
f1 (ppm)
6d
F
F
N
O
S
O
N
CH3
CH3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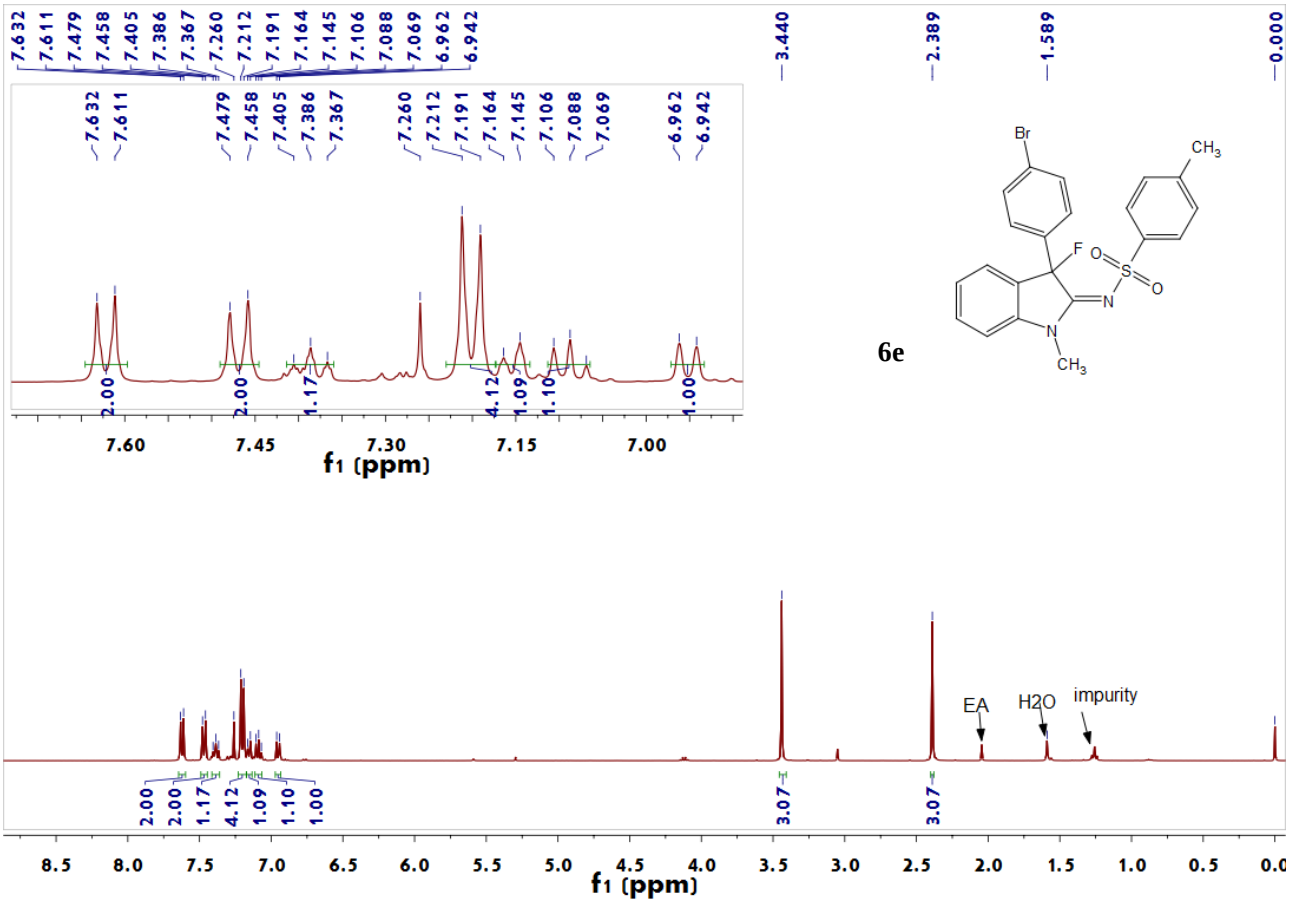
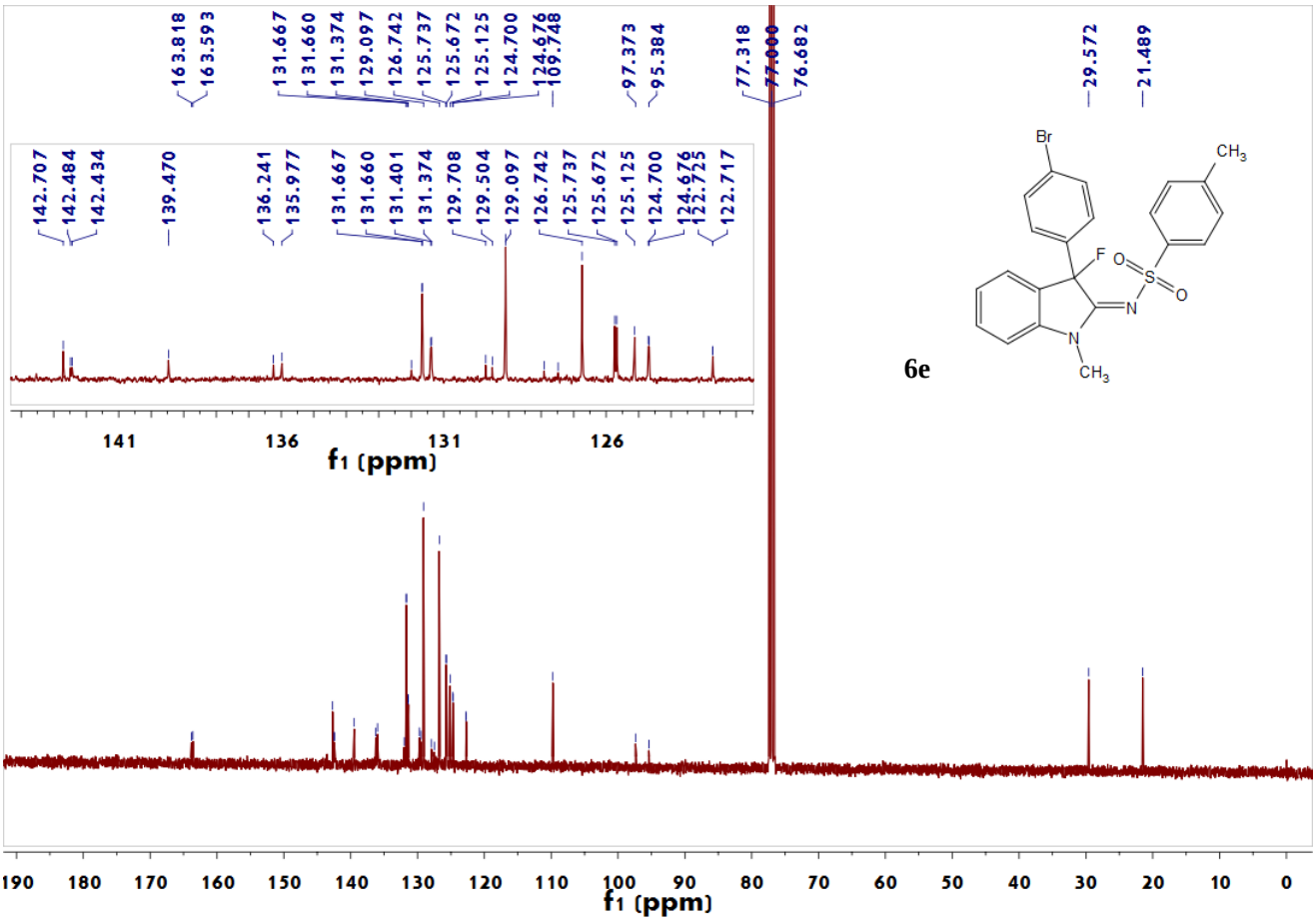
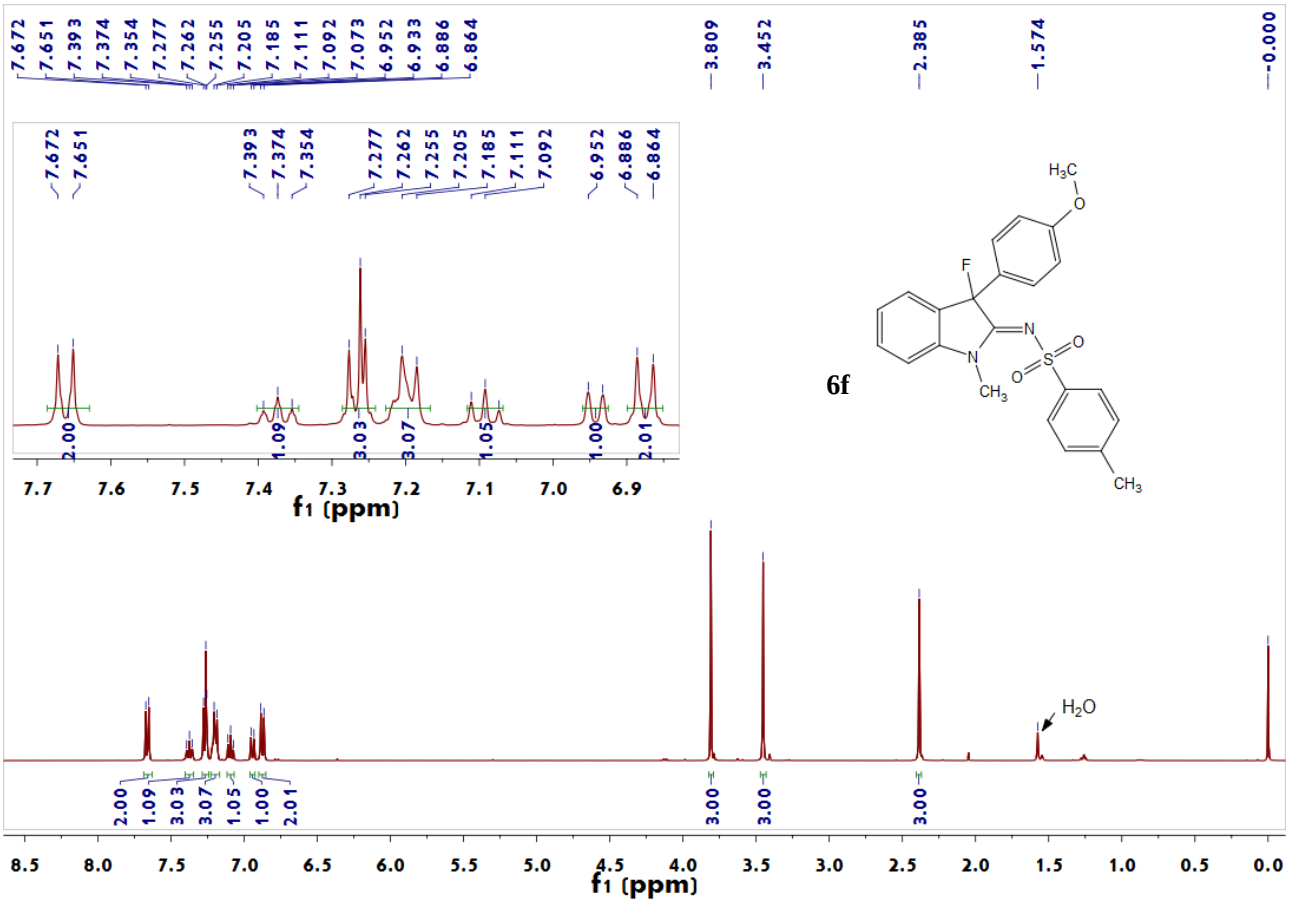
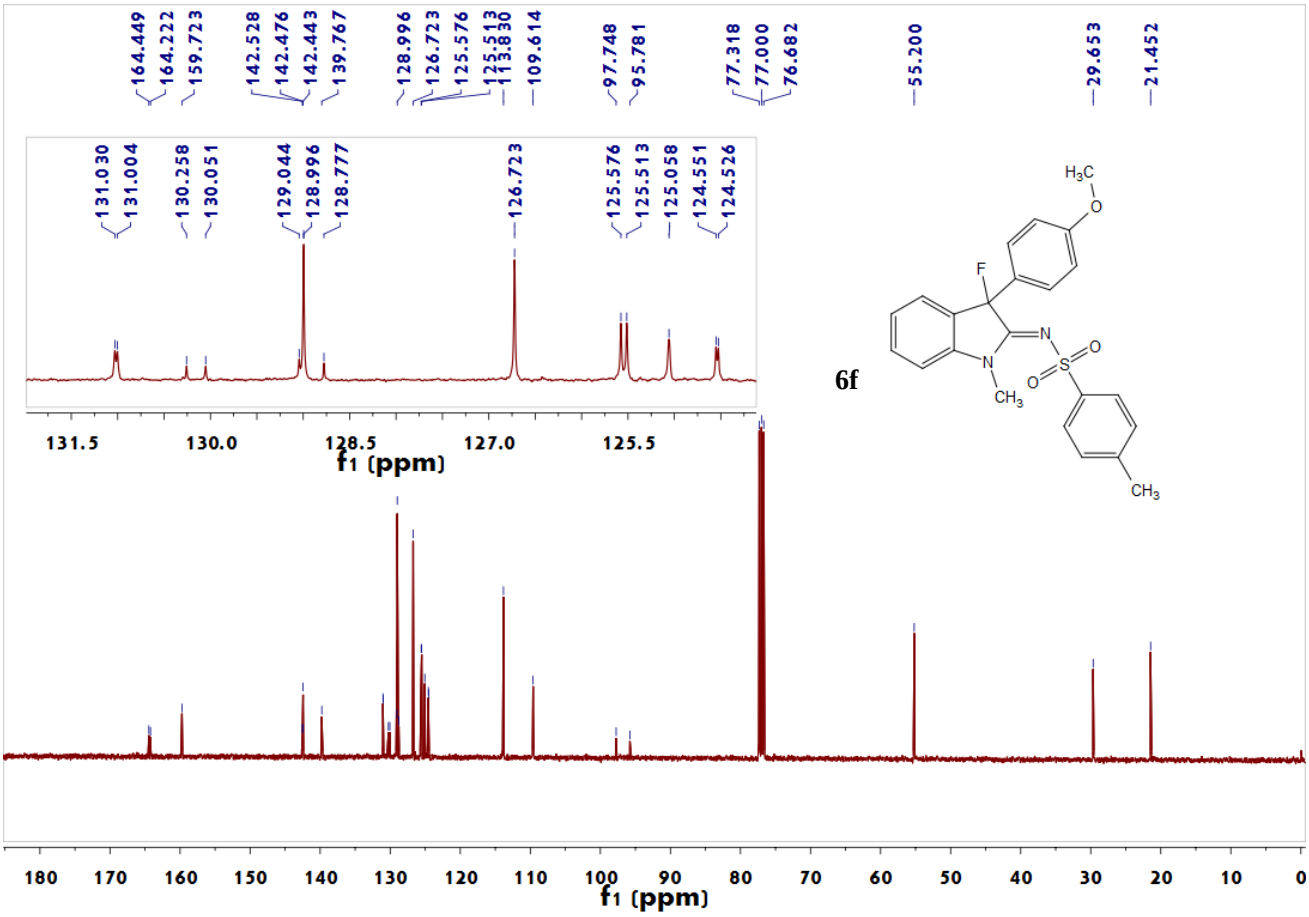
163.948
163.935
163.789
161.482
161.475
142.662
129.077
126.715
126.056
126.039
125.123
124.639
115.651
115.645
115.431
109.725
97.416
95.438
77.318
77.000
76.682
29.626
21.474
142.662
142.540
142.487
139.556
132.980
132.947
132.713
132.681
131.331
131.303
129.882
129.681
129.077
126.715
126.056
126.039
125.123
124.639
f1 (ppm)
6d
F
F
N
O
S
O
N
CH3
CH3


7.632
7.611
7.479
7.458
7.405
7.386
7.367
7.260
7.212
7.191
7.164
7.145
7.106
7.088
7.069
6.962
6.942
3.440
2.389
1.589
0.000
2.00
2.00
1.17
4.12
1.09
1.10
1.00
3.07
3.07
EA
H2O
impurity
f1 (ppm)
Br
CH3
F
O
S
N
6e


163.818
163.593
131.667
131.660
131.374
129.097
126.742
125.737
125.672
125.125
124.700
124.676
109.748
97.373
95.384
77.318
77.000
76.682
29.572
21.489
142.707
142.484
142.434
139.470
136.241
135.977
131.667
131.660
131.401
131.374
129.708
129.504
129.097
126.742
125.737
125.672
125.125
124.700
124.676
122.725
122.717
f1 (ppm)
Br
CH3
F
O
S
N
6e


7.672
7.651
7.393
7.374
7.354
7.277
7.262
7.255
7.205
7.185
7.111
7.092
7.073
6.952
6.933
6.886
6.864
3.809
3.452
2.385
1.574
0.000
2.00
1.09
3.03
3.07
1.05
1.00
2.01
3.00
3.00
3.00
H2O
f1 (ppm)
6f


164.449
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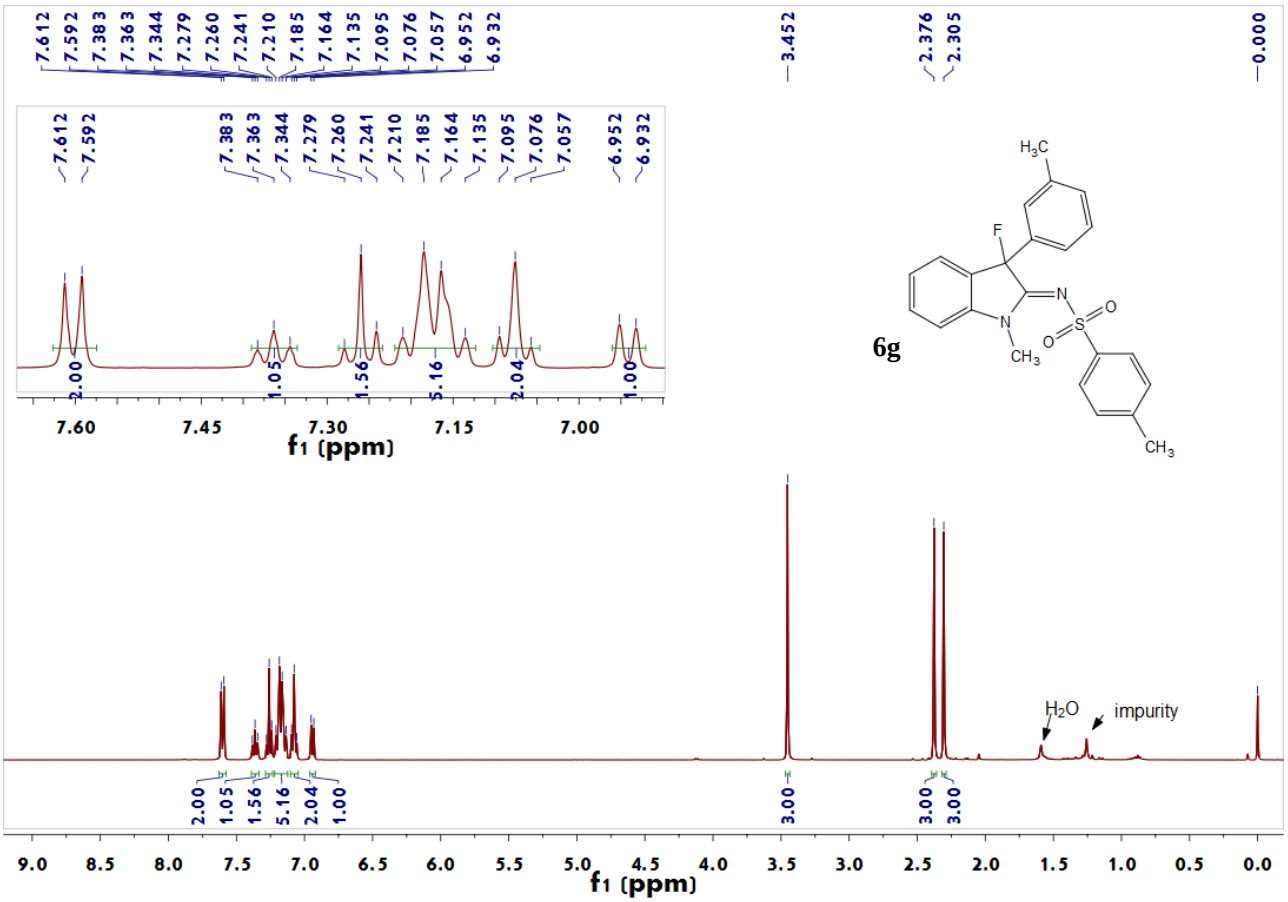
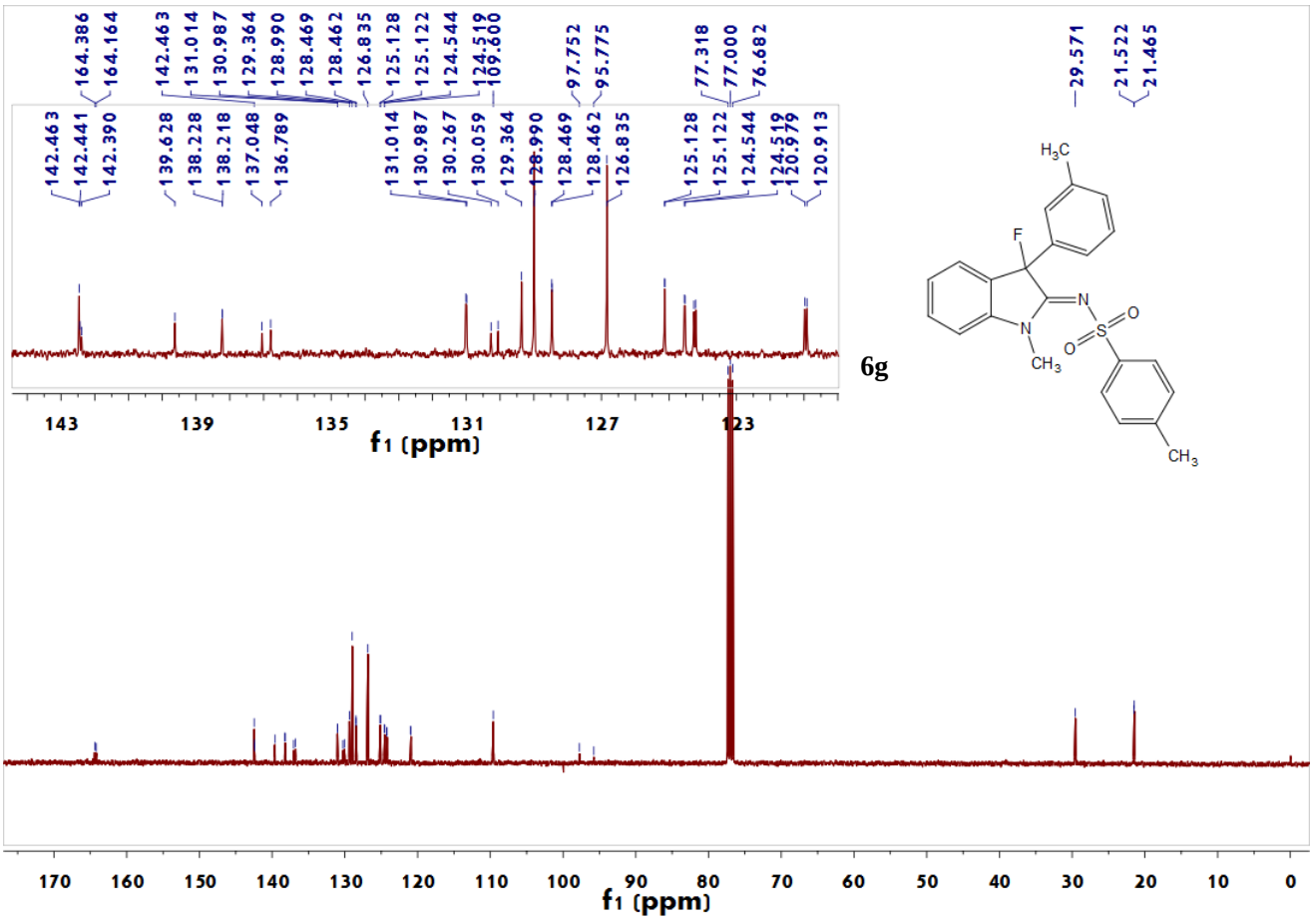
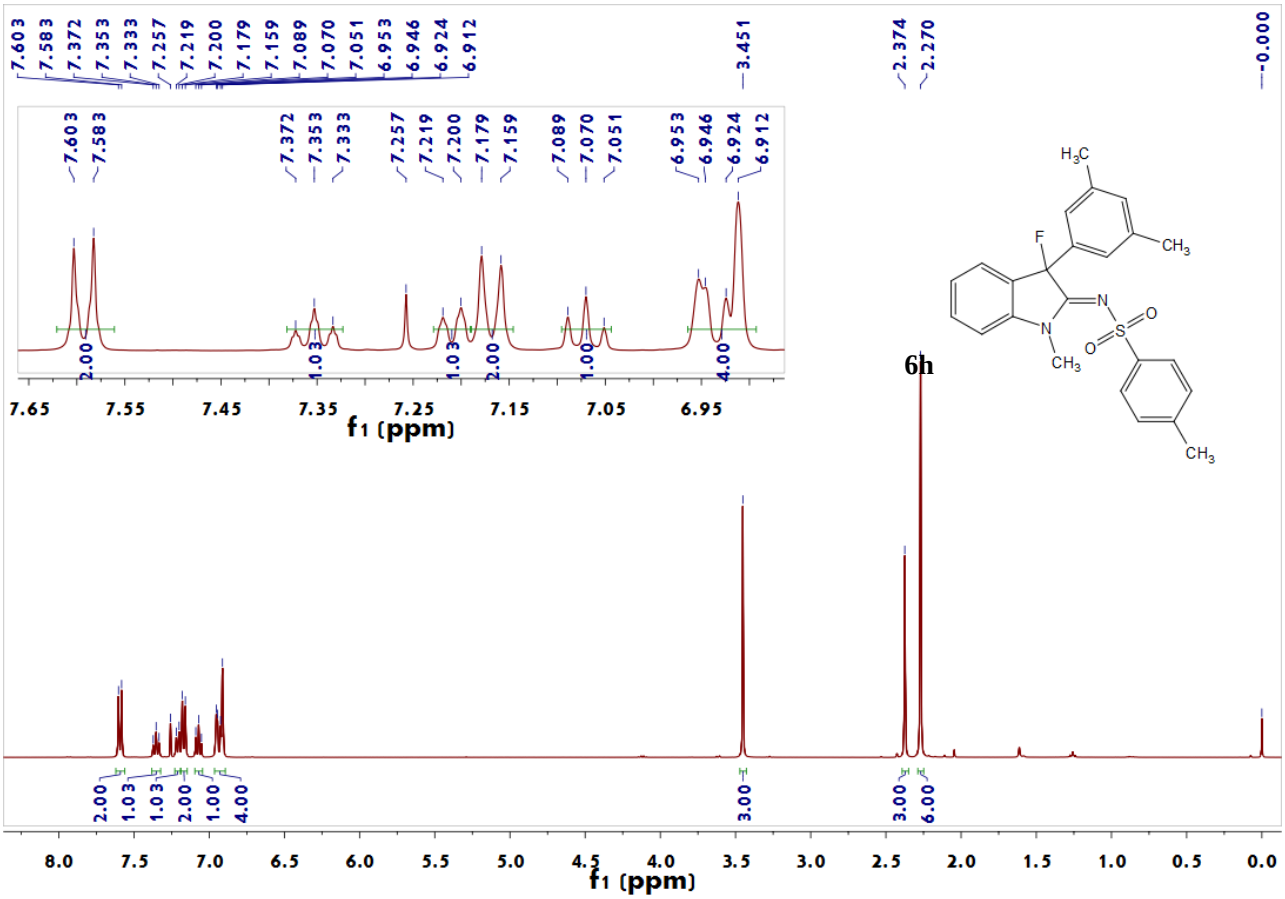
159.723
142.528
142.476
142.443
139.767
128.996
126.723
125.576
125.513
113.830
109.614
97.748
95.781
77.318
77.000
76.682
55.200
29.653
21.452
131.030
131.004
130.258
130.051
129.044
128.996
128.777
126.723
125.576
125.513
125.058
124.551
124.526
f1 (ppm)
6f


7.612
7.592
7.383
7.363
7.344
7.279
7.260
7.241
7.210
7.185
7.164
7.135
7.095
7.076
7.057
6.952
6.932
3.452
2.376
2.305
0.000
2.00
1.05
1.56
5.16
2.04
1.00
3.00
3.00
3.00
H2O
impurity
f1 (ppm)

6g


164.386
164.164
142.463
131.014
130.987
129.364
128.990
128.469
128.462
126.835
125.128
125.122
124.544
124.519
109.600
97.752
95.775
77.318
77.000
76.682
29.571
21.522
21.465
f1 (ppm)

6g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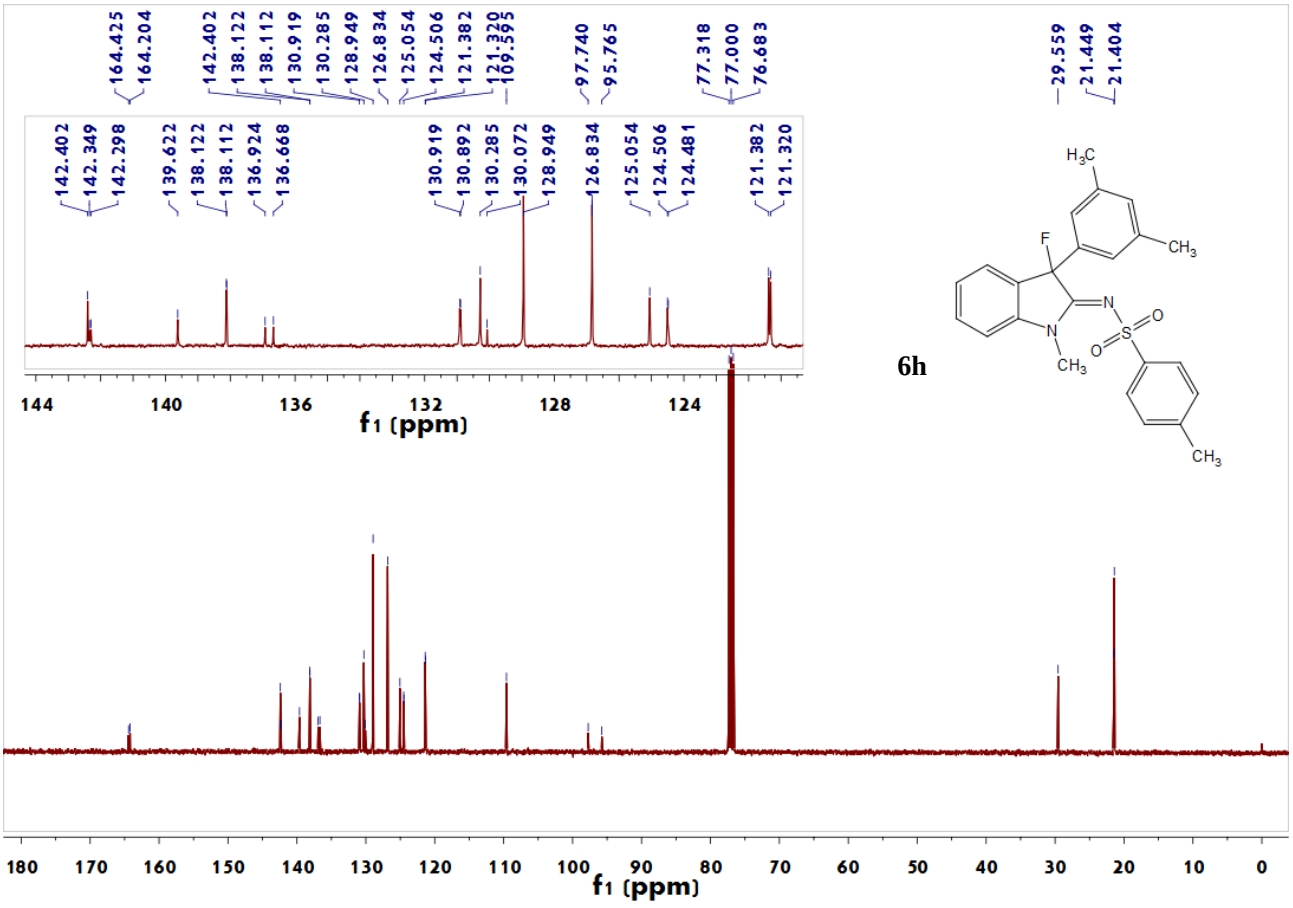
7.333
7.257
7.219
7.200
7.179
7.159
7.089
7.070
7.051
6.953
6.946
6.924
6.912
3.451
2.374
2.270
0.000
2.00
1.03
1.03
2.00
1.00
4.00
3.00
3.00
6.00
f1 (ppm)
6h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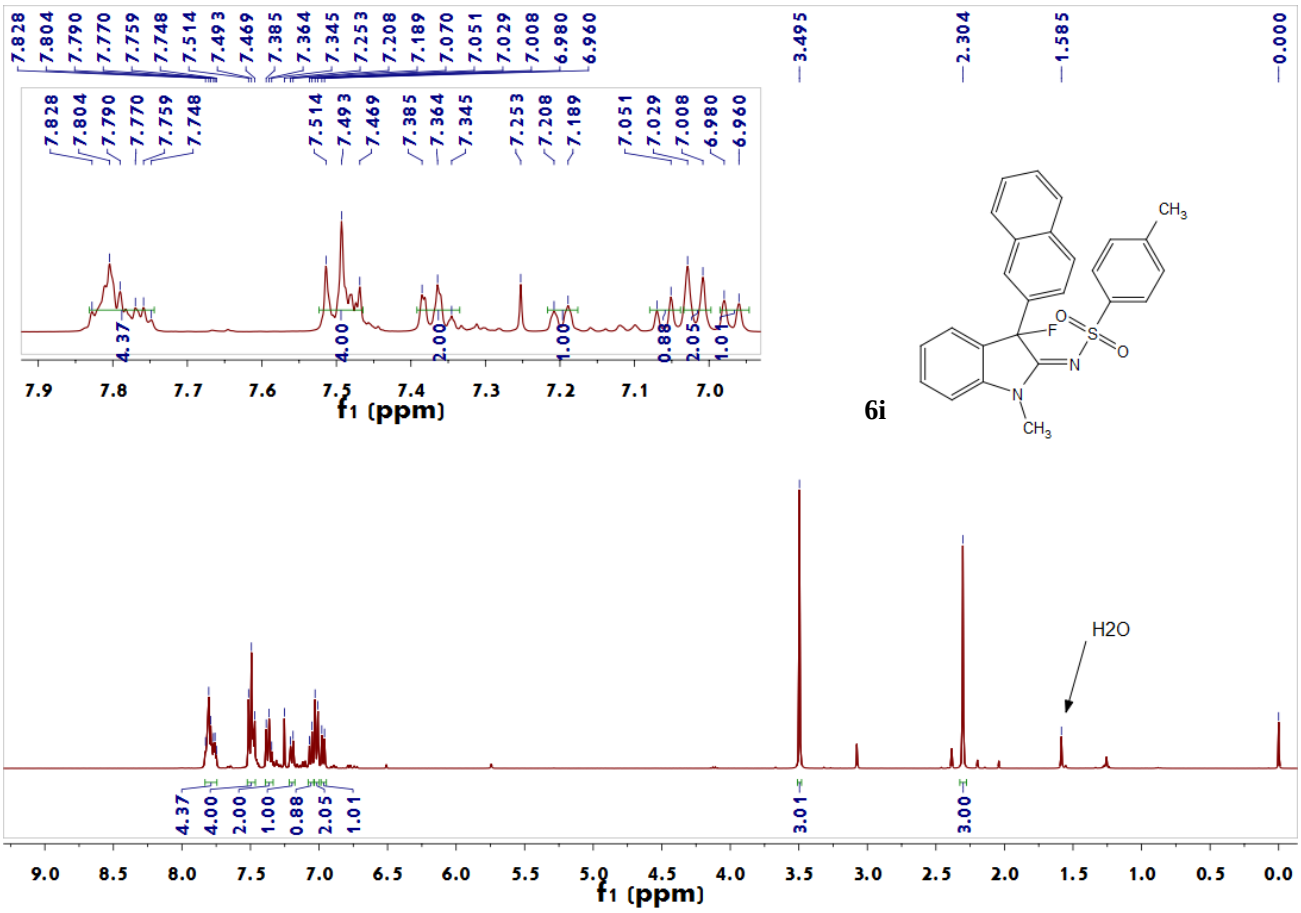
164.204
142.402
138.122
138.112
130.919
130.285
128.949
126.834
125.054
124.506
121.382
121.320
109.595
97.740
95.765
77.318
77.000
76.683
29.559
21.449
21.404
f1 (ppm)
6h


7.828
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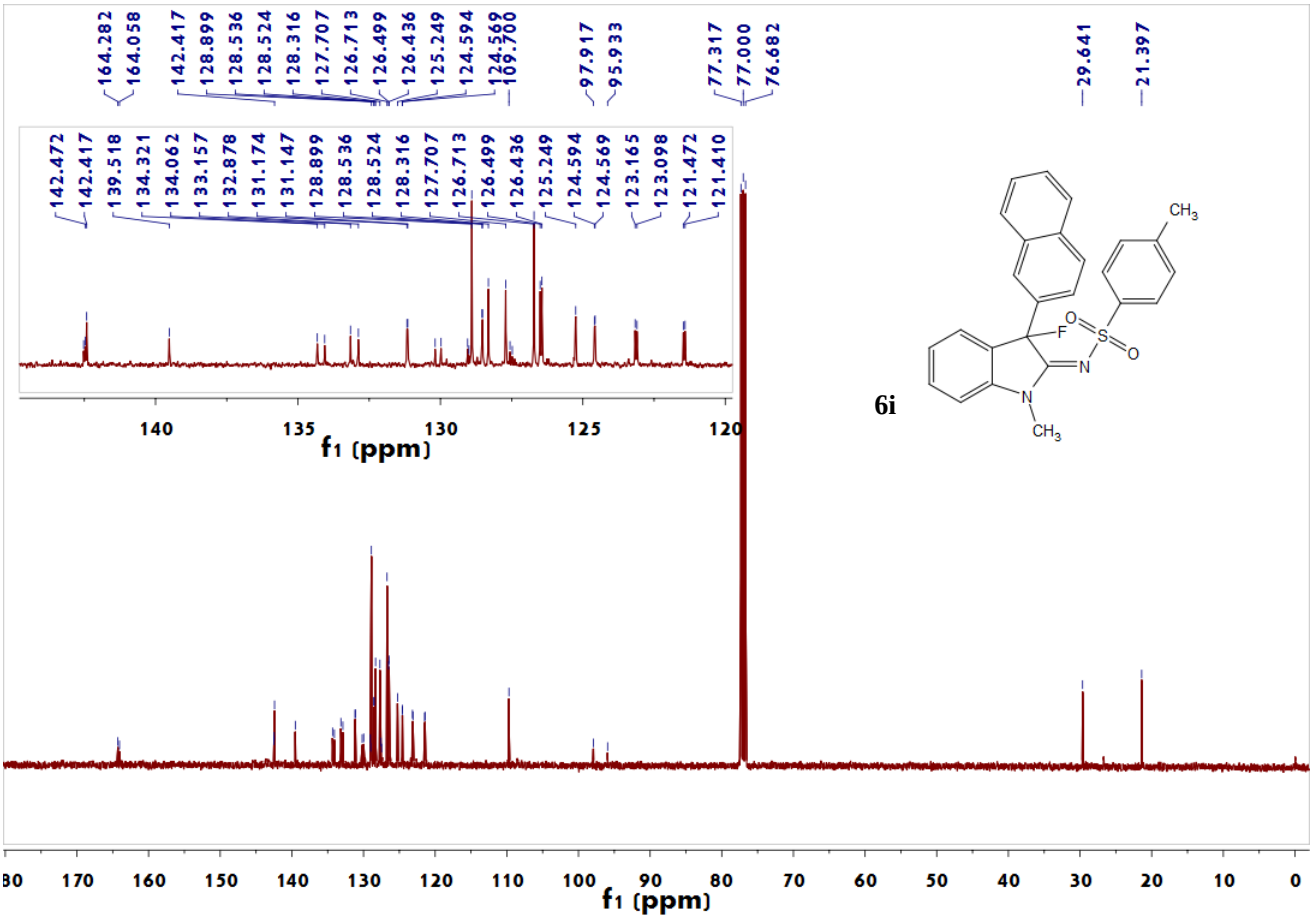
7.790
7.770
7.759
7.748
7.514
7.493
7.469
7.385
7.364
7.345
7.253
7.208
7.189
7.070
7.051
7.029
7.008
6.980
6.960
3.495
2.304
1.585
0.000
4.37
4.00
2.00
1.00
0.88
2.05
1.01
3.01
3.00
H2O
f1 (ppm)
6i
CH3
F
O
S
N
CH3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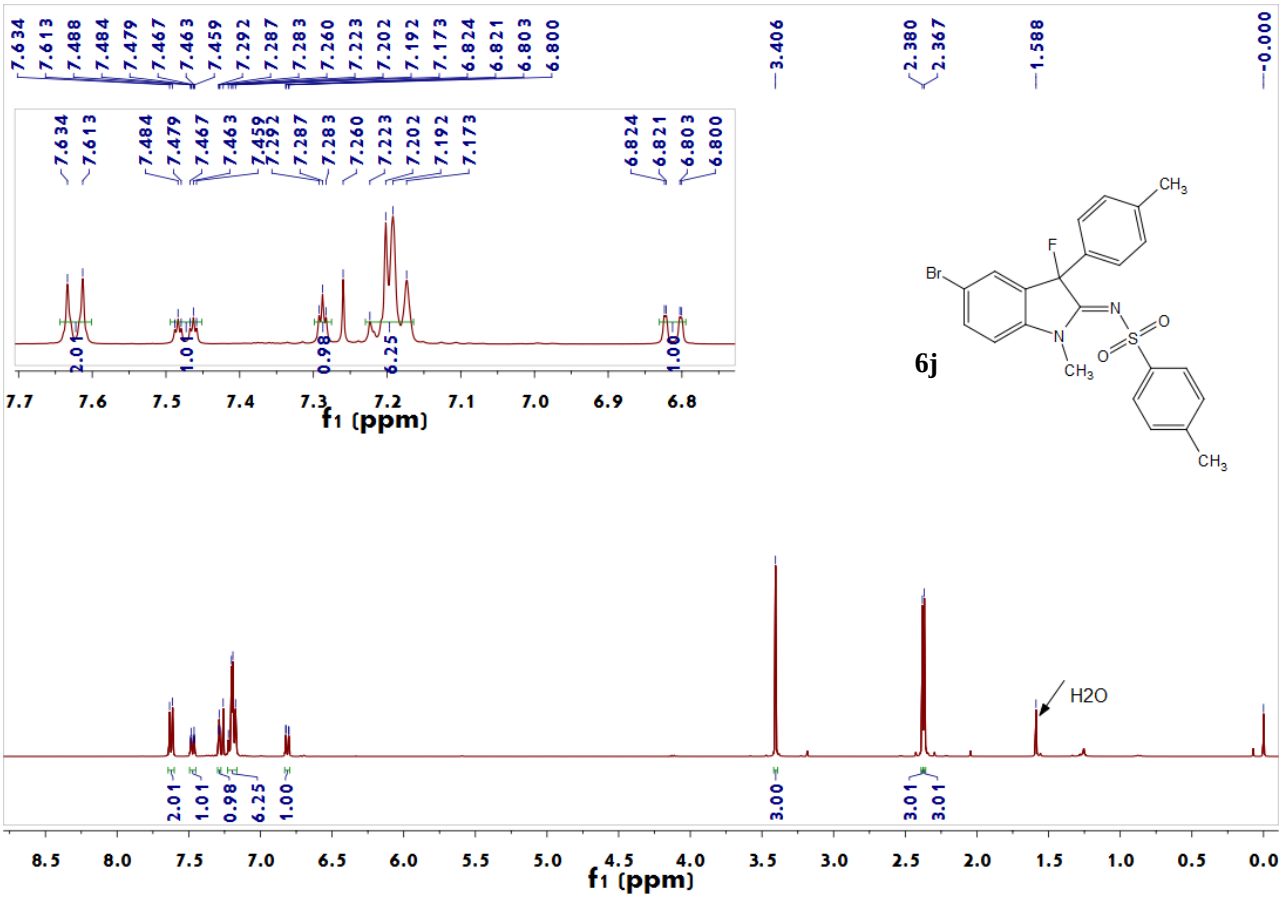
164.058
142.417
128.899
128.536
128.524
128.316
127.707
126.713
126.499
126.436
125.249
124.594
124.569
109.700
97.917
95.933
77.317
77.000
76.682
29.641
21.397
142.472
142.417
139.518
134.321
134.062
133.157
132.878
131.174
131.147
128.899
128.536
128.524
128.316
127.707
126.713
126.499
126.436
125.249
124.594
124.569
123.165
123.098
121.472
121.410
f1 (ppm)
6i
CH3
F
O
S
N
CH3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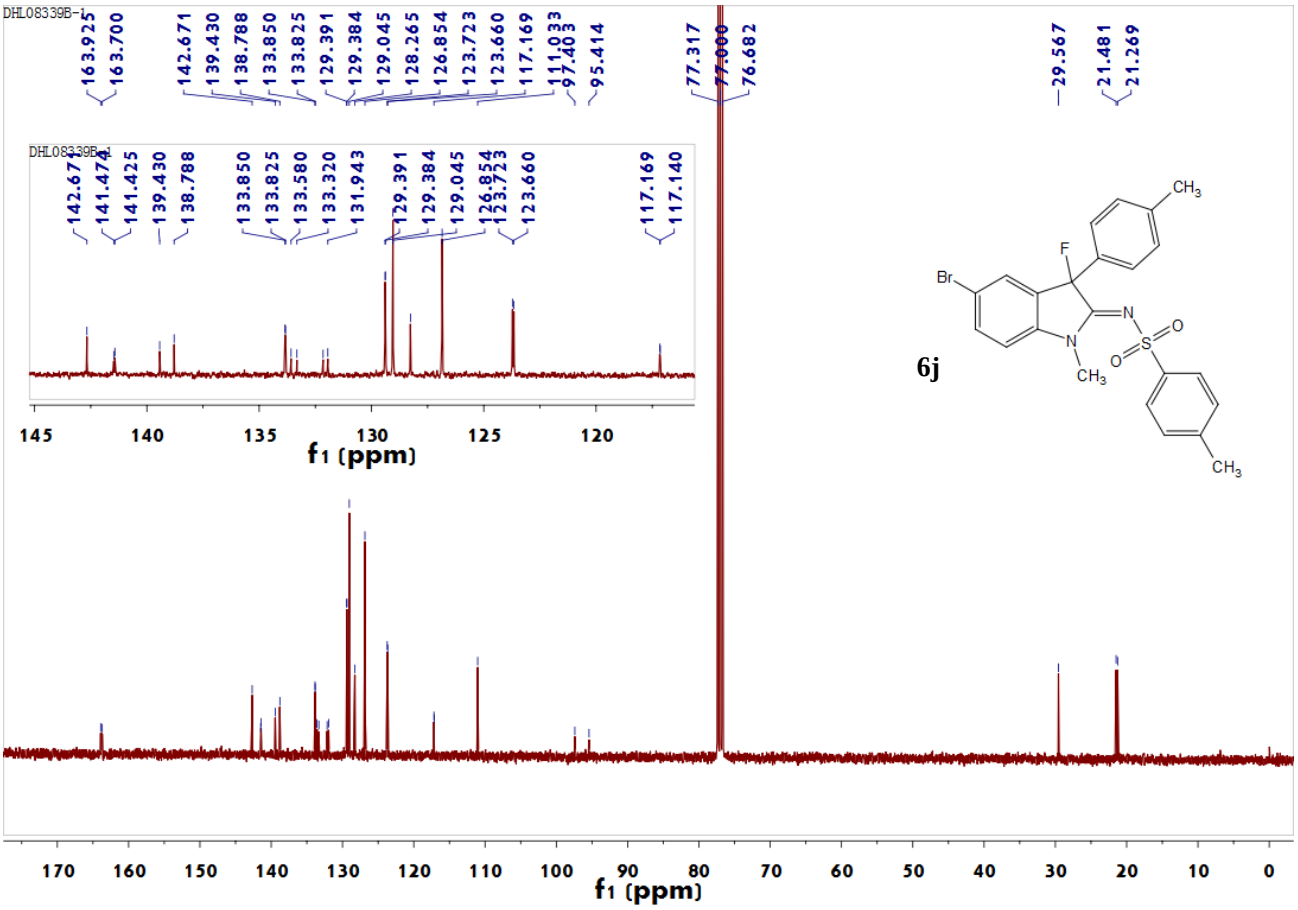
7.488
7.484
7.479
7.467
7.463
7.459
7.292
7.287
7.283
7.260
7.223
7.202
7.192
7.173
6.824
6.821
6.803
6.800
3.406
2.380
2.367
1.588
0.000
2.01
1.01
0.98
6.25
1.00
3.00
3.01
3.01
H2O
6j
f1 (ppm)


DHL08339B-1
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139.430
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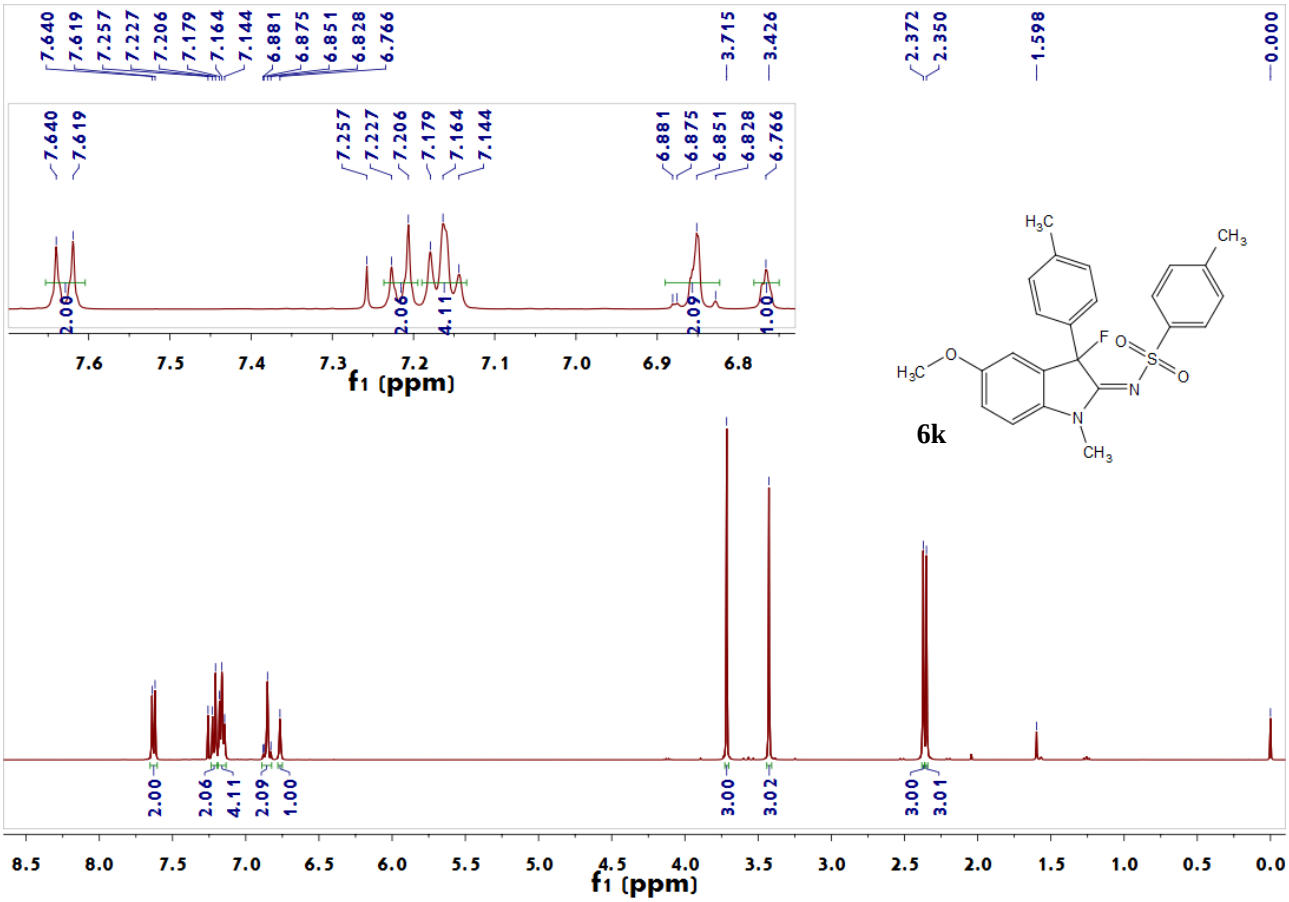
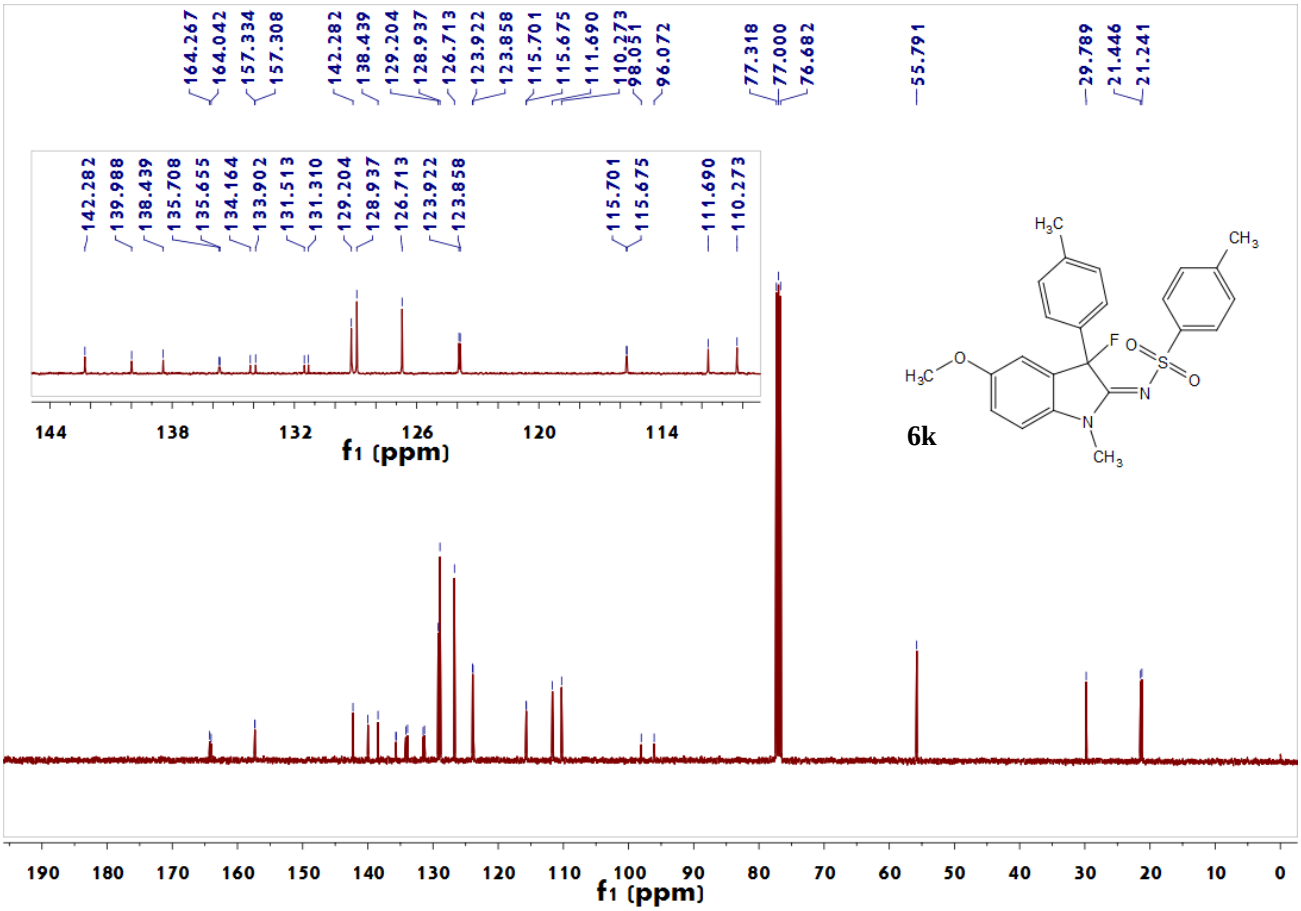
133.850
133.825
129.391
129.384
129.045
128.265
126.854
123.723
123.660
117.169
111.033
97.403
95.414
77.317
77.000
76.682
29.567
21.481
21.269
142.671
141.474
141.425
139.430
138.788
133.850
133.825
133.580
133.320
131.943
129.391
129.384
129.045
126.854
123.723
123.660
117.169
117.140
6j
f1 (ppm)


7.640
7.619
7.257
7.227
7.206
7.179
7.164
7.144
6.881
6.875
6.851
6.828
6.766
3.715
3.426
2.372
2.350
1.598
0.000
2.00
2.06
4.11
2.09
1.00
3.00
3.02
3.00
3.01
f1 (ppm)
6k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157.334
157.308
142.282
138.439
129.204
128.937
126.713
123.922
123.858
115.701
115.675
111.690
110.273
98.051
96.072
77.318
77.000
76.682
55.791
29.789
21.446
21.241
f1 (ppm)
6k