Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Rhodium-Catalyzed Ylide Formation/Smiles Rearrangement Reaction of Chalcogenide Ether and Triazoles

Jiafeng He,[†] Xun-Shen Liu,[†] Mingjia Li,[†] Shaoting Peng,[†] Zhi-Yao Si,[†] and Lu Liu[†‡]*

[†]*School of Chemistry and Molecular Engineering, East China Normal University, 500 Dongchuan Road, Shanghai 200241, P. R. China*

[‡]*Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, East China Normal University, Shanghai 200062, P. R. China*

E-mail : lliu@chem.ecnu.edu.cn

Contents

1. General Information

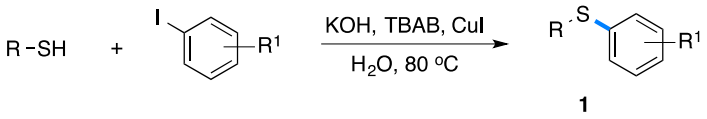
Unless otherwise noted, all reactions were carried out in standard Schlenk techniques with magnetic stirring bar under air. Materials obtained from commercial suppliers were used directly without further purification. ^{1}H NMR spectra were recorded on a BRUKER 500 (500 MHz) or BRUKER 600 (600 MHz) spectrometer in $CDCl_3$. Chemical shifts are reported in ppm with tetramethylsilane (TMS: 0 ppm) with the solvent resonance as the internal standard. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, quint = quintus, sext = sextus, sept = septimum, m = multiplet), coupling constants (Hz), and integration. $^{13}C\{^{1}H\}$ NMR spectra were recorded on a BRUKER 500 (126 MHz) or BRUKER 600 (151 MHz) spectrometer in $CDCl_3$ with complete proton decoupling. Chemical shifts are reported in ppm with the deuterium solvent as the internal standard (e.g. $CDCl_3$: 77.0 ppm). HRMS spectra were recorded on BRUKER maXis impact, Source type is electrospray ionization (ESI-TOF).

Anhydrous toluene and tetrahydrofuran (THF) were distilled from sodium and benzophenone to use; Anhydrous dichloromethane (DCM) and dichloroethane (DCE) were distilled from CaH_2. $Mn(OTf)_2$, $Cu(OTf)_2$, $Bi(OTf)_2$, $Sc(OTf)_3$ and $Rh_2(OAc)_4$ were purchased from Energy Chemical Company and used directly.

Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed on silica gel 60 (particle size 200-400 mesh ASTM, purchased from Yantai, China) and eluted with petroleum ether/ethyl acetate (PE/EA) or petroleum ether/ diethyl ether (PE/Et_2O). Without special instructions, heating reactions are carried out through an oil bath.

2. General procedure for the synthesis of 1 and 4

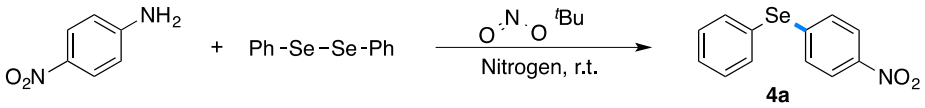
General procedure for synthesis sulfur ether compounds 1



1

Thiophenol (1.0 equiv), aryl iodine compounds (1.1 equiv), tetrabutylammonium bromide (TBAB, 1.0 equiv), and KOH (1.5 equiv) in water (1 mL/mmol), CuI (0.1 equiv) was added to this stirred solution at room temperature. Then the solution was heated at 80 °C by oil bath and keep this temperature for 12 hours. The reaction was monitored by TLC. Upon completion, the reaction was cooled to room temperature and the solution extracted with ethyl ether. The organic layer was washed with water and brine, then dried over Na_2SO_4. The solvent was evaporated under reduced pressure and the crude product was purified with silica column chromatography (PE: EA = 20: 1) to afford the pure product. Compound **1a-1t** were prepared with the above described method.[1]

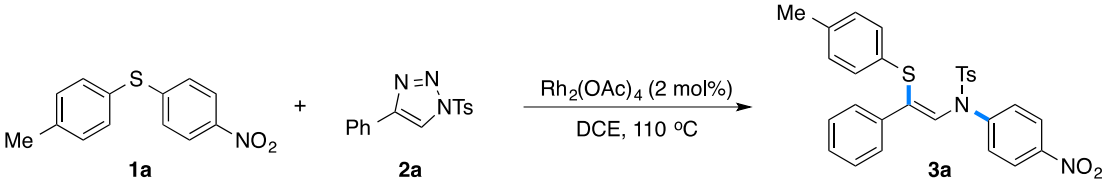
The method for synthesis selenium ether compounds 4a



4a

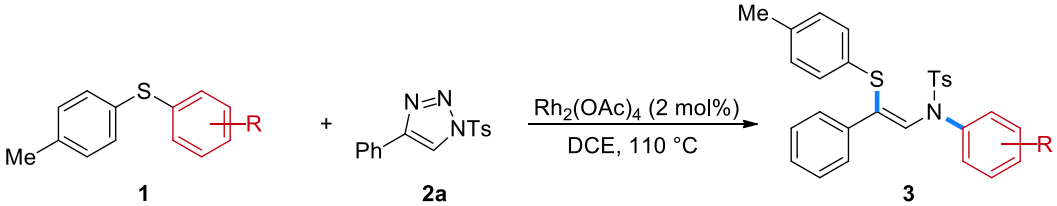
Diphenyl diselenide (1.0 equiv), *p*-nitroaniline (1.0 equiv) and tert-butyl nitrite (2.6 equiv) were introduced into a dried Schlenk tube under nitrogen protection, and the mixture was stirred at room temperature for 1 h. The reaction was monitored by TLC. Upon completion, the mixture was extracted with ethyl acetate and the organic layer washed with water and brine, then dried over Na_2SO_4. The organic layer was quickly filtered through celite. The filtrate was evaporated under reduced pressure and the crude product was purified with silica column chromatography (PE: EA = 20: 1) to afford the pure product **4a**.[2]

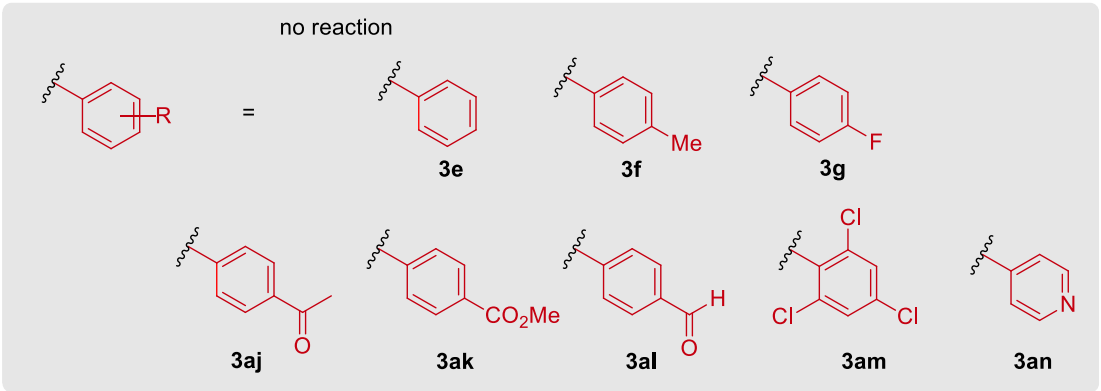
3. General procedure for the synthesis of 3 and 5



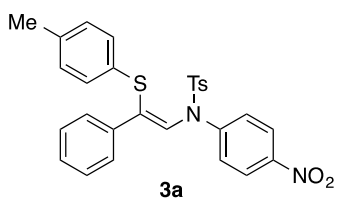
General procedure (Method A): Thioether **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), triazole **2a** (187.2 mg, 0.6 mmol, 1.5 equiv), $Rh_2(OAc)_4$ (3.6 mg, 0.008 mmol, 2.0 mol%) and dry 1,2-dichloroethane (4 ml, 0.1 M) were introduced into a sealed pressure tube under Argon protection, then the solution was heated at 110 °C by oil bath and keep this temperature for 4 hours. The reaction was monitored by TLC. Upon completion, the reaction was cooled to room temperature and open the sealed pressure tube carefully, then the solvent was evaporated under reduced pressure and the mixture was purified by column chromatography on silica gel using PE: EA = 10: 1 as the eluent and concentrated to obtain the product **3a** (190.1 mg, 92%). Unless otherwise specified, the synthesis of other trisubstituted vinyl sulfides/selenides refers to this method.

Table S1 Unsuccessful examples





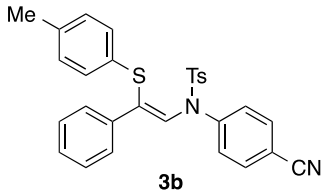
1) (*Z*)-4-methyl-N-(4-nitrophenyl)-N-(2-phenyl-2-(p-tolylthio)vinyl)benzene-sulfonamide. (3a)



3a

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6 PE/EA =5:1). After purification by column chromatography (PE/EA = 10:1), **3a** (190.1 mg, 92%) was obtained as yellow solid; m.p. =131.3 – 132.8 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 9.0 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.45 - 7.43 (m, 2H), 7.35 (d, *J* = 9.0 Hz, 2H), 7.31 (d, *J* = 8.5 Hz, 2H), 7.26 – 7.25 (m, 3H), 7.02 (s, 1H), 6.84 (d, *J* = 8 Hz, 2H), 6.76 (d, *J* = 8 Hz, 2H), 2.45 (s, 3H), 2.19 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.2, 145.6, 144.9, 137.1, 136.6, 134.5, 133.7, 130.0, 129.9, 129.3, 129.2, 128.6, 128.3, 128.2, 127.8, 127.6, 127.0, 124.3, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{24}N_2NaO_4S_2$ 539.1075, found 539.1081.

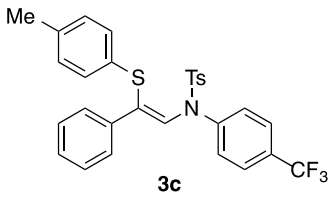
2) (*Z*)-N-(4-cyanophenyl)-4-methyl-N-(2-phenyl-2-(p-tolylthio)vinyl)benzene-sulfonamide. (3b)



3b

The general procedure was followed using **1b** (90.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (179.6 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.7, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3b** (141.5 mg, 71% yield) was obtained as white solid; m.p. =123.5 – 124.8 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.57 – 7.54 (m, 4H), 7.42 – 7.40 (m, 2H), 7.30 – 7.27 (m, 4H), 6.98 (s, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.73 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H), 2.17 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 144.8, 144.5, 137.2, 136.5, 134.5, 133.0, 132.7, 129.90, 129.87, 129.32, 129.30, 128.5, 128.3, 128.1, 128.0, 127.6, 127.5, 118.4, 110.2, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{29}H_{24}N_2NaO_2S_2$ 519.1177, found 519.1171.

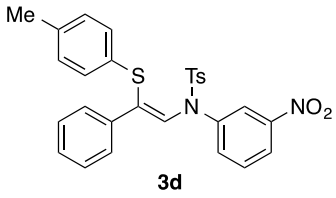
3) (*Z*)-4-methyl-N-(2-phenyl-2-(p-tolylthio)vinyl)-N-(4-(trifluoromethyl)phenyl) benzene-sulfonamide. (3c)



3c

The general procedure was followed using **1c** (107.3 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (179.6 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3c** (119.9 mg, 59% yield) was obtained as white solid; m.p. =141.2 – 142.6 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.46 – 7.44 (m, 2H), 7.31 – 7.29 (m, 4H), 7.26 – 7.24 (m, 3H), 7.05 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.75 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H), 2.19 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 144.6, 143.5, 137.5, 136.3, 134.6, 132.3, 129.9, 129.8, 129.6, 129.2, 128.9 (*J* = 32.5 Hz), 128.8, 128.32, 128.26, 128.1, 127.8, 127.7, 125.8 (*J* = 3.6 Hz), 123.8 (*J* = 270.5 Hz), 21.6, 20.9; **^{19}F NMR** (470 MHz, $CDCl_3$) δ -62.4; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{29}H_{24}F_3NNaO_2S_2$ 562.1098, found 562.1083.

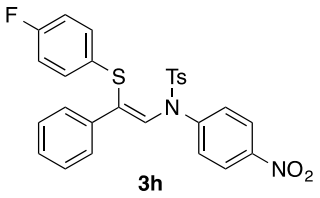
4) (*Z*)-4-methyl-N-(3-nitrophenyl)-N-(2-phenyl-2-(p-tolylthio)vinyl)benzene-sulfonamide. (3d)



3d

The general procedure was followed using **1d** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (179.6 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.5, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3d** (90.9 mg, 44% yield) was obtained as yellow solid; m.p. =128.1 – 129.6 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.0 Hz, 2H), 7.83 – 7.80 (m, 1H), 7.64 – 7.60 (m, 1H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.47 – 7.43 (m, 3H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.25 – 7.24 (m, 3H), 7.10 (s, 1H), 6.80 (d, *J* = 8.0 Hz, 2H), 6.68 (d, *J* = 8.5 Hz, 2H), 2.45 (s, 3H), 2.16 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 148.1, 144.9, 141.1, 137.5, 136.3, 134.4, 134.3, 130.6, 130.0, 129.6, 129.3, 129.1, 128.8, 128.5, 128.3, 128.1, 127.6, 122.3, 122.0, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{24}N_2NaO_4S_2$ 539.1075, found 539.1067.

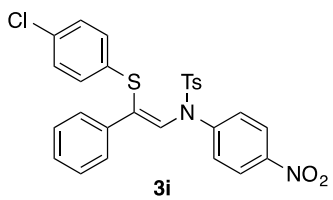
5) (*Z*)-N-(2-((4-fluorophenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3h)



3h

The general procedure was followed using **1h** (99.7 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3h** (175 mg, 84%) was obtained as yellow solid; m.p. =125.6 – 127.2 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 9.0 Hz, 2H), 7.61 – 7.59 (m, 2H), 7.40 – 7.36 (m, 4H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.23 (m, 3H), 6.99 – 6.97 (m, 1H), 6.89 – 6.86 (m, 2H), 6.76 – 6.68 (m, 2H), 2.43 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 161.7 (d, *J* = 247.5 Hz), 146.2, 145.6, 145.0, 136.5, 134.3, 134.2, 132.3 (d, *J* = 8.2 Hz), 129.9, 128.7, 128.4, 128.2, 127.8 (d, *J* = 3.1 Hz), 127.6, 127.5, 126.9, 124.3, 115.7 (d, *J* = 22.1 Hz), 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{21}FN_2NaO_4S_2$ 543.0824, found 543.0828.

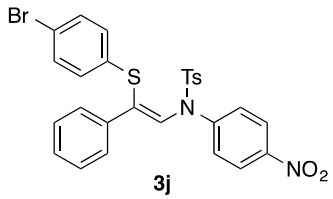
6) (*Z*)-N-(2-((4-chlorophenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3i)



3i

The general procedure was followed using **1i** (106.3 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.5, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3i** (171.4 mg, 80%) was obtained as yellow solid; m.p. =130.2 – 131.9 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 9.0 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.42 - 7.40 (m, 2H), 7.33 – 7.28 (m, 4H), 7.28 - 7.25 (m, 3H), 7.06 (s, 1H), 7.00 (d, *J* = 8.5 Hz, 2H), 6.80 (d, *J* = 8.5 Hz, 2H), 2.44 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.0, 145.8, 145.1, 136.7, 134.3, 132.6, 131.9, 131.6, 130.8, 130.0, 128.9, 128.8, 128.7, 128.5, 128.0, 127.6, 127.2, 124.4, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{21}ClN_2NaO_4S_2$ 559.0529, found 559.0528.

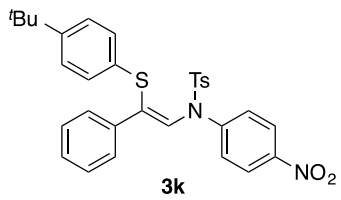
7) (*Z*)-N-(2-((4-bromophenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3j)



3j

The general procedure was followed using **1j** (124 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3j** (211.7 mg, 91%) was obtained as yellow solid; m.p. =133.8 – 135.0 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 9.0 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.43 – 7.41 (m, 2H), 7.31 – 7.28 (m, 4H), 7.27 – 7.26 (m, 3H), 7.14 (d, *J* = 8.5 Hz, 2H), 7.09 (s, 1H), 6.73 (d, *J* = 8.5 Hz, 2H), 2.44 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.0, 145.8, 145.1, 136.7, 134.3, 132.4, 131.7, 131.4, 130.9, 130.0, 129.2, 128.8, 128.6, 128.0, 127.5, 127.2, 124.4, 120.5, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{21}BrN_2NaO_4S_2$ 603.0024, found 603.0020.

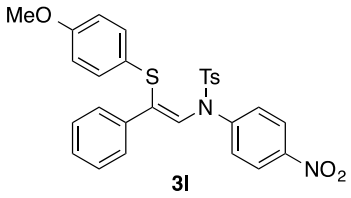
8) (*Z*)-N-(2-((4-(tert-butyl)phenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl)benzenesulfonamide. (3k)



3k

The general procedure was followed using **1k** (115 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.7, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3k** (197 mg, 88%) was obtained as yellow solid; m.p. =126.3 – 128.1 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 (d, *J* = 9.0 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.46 – 7.44 (m, 2H), 7.30 – 7.28 (m, 4H), 7.26 – 7.24 (m, 3H), 7.07 (s, 1H), 7.02 (d, *J* = 8.5 Hz, 2H), 6.73 (d, *J* = 8.5 Hz, 2H), 2.43 (s, 3H), 1.18 (s, 9H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 149.7, 146.0, 145.6, 144.9, 137.4, 134.6, 132.3, 129.9, 129.5, 129.1, 128.53, 128.48, 128.4, 128.0, 127.6, 127.2, 125.6, 124.2, 34.3, 31.1, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{31}H_{30}N_2NaO_4S_2$ 581.1545, found 581.1555.

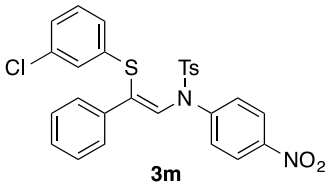
9) (*Z*)-N-(2-((4-methoxyphenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3l)



3l

The general procedure was followed using **1l** (104.5 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3l** (163.1 mg, 77%) was obtained as yellow solid; m.p. =125.4 – 127.1 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 9.5 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.41 – 7.36 (m, 4H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.22 – 7.21 (m, 3H), 3.65 (s, 3H), 2.43 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 158.8, 146.4, 145.4, 144.8, 136.7, 136.2, 134.5, 132.7, 129.9, 128.5, 128.3, 128.2, 127.5, 126.6, 126.2, 124.3, 122.8, 114.2, 55.1, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{24}N_2NaO_5S_2$ 555.1024, found 555.1015.

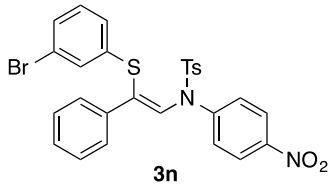
10) (*Z*)-N-(2-((3-chlorophenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3m)



3m

The general procedure was followed using **1m** (106.3 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3m** (162.4 mg, 76%) was obtained as yellow solid; m.p. =128.8 – 130.2 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 9.0 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.41 (m, 2H), 7.32 – 7.25 (m, 7H), 7.14 (s, 1H), 6.99 – 6.93 (m, 2H), 6.79 (s. 1H), 6.74 (d, *J* = 7.5 Hz, 1H), 2.44 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 145.9, 145.8, 145.1, 136.8, 135.2, 134.30, 134.27, 130.7, 130.0, 129.8, 129.6, 128.9, 128.8, 128.6, 127.9, 127.6, 127.4, 127.2, 126.6, 124.3, 21.7; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{21}ClN_2NaO_4S_2$ 559.0529, found 559.0535.

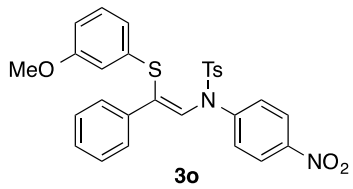
11) (*Z*)-N-(2-((3-bromophenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3n)



3n

The general procedure was followed using **1n** (124 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3n** (186.1 mg, 80%) was obtained as yellow solid; m.p. =132.6 – 133.8 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.5 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.46 – 7.40 (m, 2H), 7.31 – 7.27 (m, 7H), 7.15 – 7.11 (m, 2H), 6.93 (s, 1H), 6.91 – 6.86 (m, 1H), 6.81 – 6.77 (m, 1H), 2.44 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 145.9, 145.8, 145.1, 136.8, 135.2, 134.3, 134.2, 130.6, 130.0, 129.8, 129.6, 128.9, 128.8, 128.6, 127.9, 127.6, 127.4, 127.2, 126.6, 124.3, 21.7; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{21}BrN_2NaO_4S_2$ 603.0024, found 603.0014.

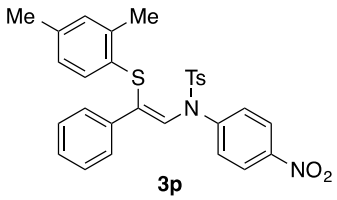
12) (*Z*)-N-(2-((3-methoxyphenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3o)



3o

The general procedure was followed using **1o** (104 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3o** (211.7 mg, 91%) was obtained as yellow solid; m.p. =126.2 – 127.9 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.5 Hz, 2H), 7.57 (d, *J* = 7 Hz, 2H), 7.46 – 7.45 (m, 2H), 7.31 – 7.27 (m, 4H), 7.26 – 7.25 (m, 3H), 7.10 (s, 1H), 6.95 – 6.89 (m, 1H), 6.55 (dd, *J* = 2 Hz, 7 Hz, 1H), 6.43 (d, *J* = 6.5 Hz, 1H), 6.38 (s, 1H), 3.62 (s, 3H), 2.44 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 159.5, 146.0, 145.7, 145.0, 137.3, 134.5, 134.3, 131.6, 130.3, 129.4, 129.1, 128.7, 128.5, 128.0, 127.6, 127.3, 124.2, 121.5,114.5, 112.5, 55.1, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{24}N_2NaO_5S_2$ 555.1024, found 555.1019.

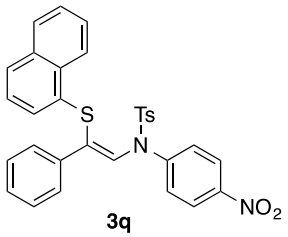
13) (*Z*)-N-(2-((2,4-dimethylphenyl)thio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl)benzenesulfonamide. (3p)



3p

The general procedure was followed using **1p** (103.7 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.7, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3p** (192.1 mg, 90%) was obtained as yellow solid; m.p. =122.6 – 124.4 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 9.0 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.40 – 7.38 (m, 2H), 7.33 – 7.28 (m, 4H), 7.23 – 7.22 (m, 3H), 6.98 (s, 1H), 6.80 – 6.73 (m, 2H), 6.69 – 6.63 (m, 1H), 2.43 (s, 3H), 2.14 (s, 3H), 2.03 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.0, 145.5, 144.8, 138.0, 137.1, 137.0, 134.4, 133.7, 131.1, 130.9, 129.9, 128.5, 128.2, 128.03, 127.98, 127.6, 127.23, 127.17, 126.8, 124.1, 21.6, 20.8, 20.1 HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{29}H_{26}BrN_2NaO_4S_2$ 553.1232, found 553.1236.

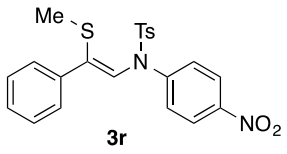
14) (*Z*)-4-methyl-N-(2-(naphthalen-1-ylthio)-2-phenylvinyl)-N-(4-nitrophenyl) benzenesulfonamide. (3q)



3q

The general procedure was followed using **1q** (112 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3q** (211.7 mg, 91%) was obtained as yellow solid; m.p. =130.9 – 131.4 ℃ ; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 9.0 Hz, 2H), 7.91 – 7.87 (m, 1H), 7.72 – 7.70 (m, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.59 – 7.57 (m, 1H), 7.45 – 7.40 (m, 2H), 7.39 – 7.38 (m, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.29 – 7.28 (m, 2H), 7.17 – 7.13 (m, 5H), 7.07 (s, 1H), 2.46 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 145.7, 145.6, 145.0, 137.1, 134.4, 133.6, 133.1, 132.4, 130.0, 129.8, 129.4, 128.5, 128.3, 128.2, 128.0, 127.8, 127.7, 127.6, 127.3, 126.3, 126.1, 125.2, 124.5, 124.1, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{31}H_{24}N_2NaO_4S_2$ 575.1075, found 575.1070.

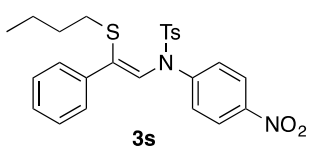
15) (*Z*)-4-methyl-N-(2-(methylthio)-2-phenylvinyl)-N-(4-nitrophenyl)benzene-sulfonamide. (3r)



3r

The general procedure was followed using **1r** (67.6 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3r** (211.7 mg, 91%) was obtained as yellow solid; m.p. =104.3 – 105.6 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 9.0 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.43 – 7.42 (m, 7H), 7.29 (d, *J* = 8.5 Hz, 2H), 6.66 (s, 1H), 2.43 (s, 3H), 1.74 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.6, 145.2, 144.7, 138.5, 136.1, 134.5, 129.8, 128.8, 128.7, 128.4, 127.5, 126.1, 124.5, 124.4, 21.6, 15.2; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{22}H_{20}N_2NaO_4S_2$ 463.0762, found 463.0757.

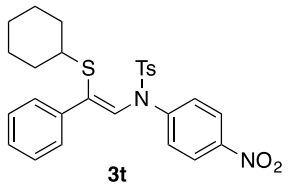
16) (*Z*)-N-(2-(butylthio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl)benzene-sulfonamide. (3s)



3s

The general procedure was followed using **1s** (84.5 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.7, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3s** (44.7 mg, 23%) was obtained as yellow solid; m.p. =108.2 – 109.9 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 9 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.44 – 7.36 (m, 7H), 7.28 (d, *J* = 8.5 Hz, 2H), 6.69 (s, 1H), 2.42 (s, 3H), 2.17 (t, *J* = 7.5 Hz, 2H), 1.08 – 0.98 (m, 4H), 0.64 (t, *J* = 7.0 Hz, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.8, 145.2, 144.7, 138.0, 136.6, 134.8, 129.9, 128.8, 128.6, 128.3, 127.5, 126.3, 125.7, 124.4, 31.9, 31.6, 21.6, 21.4, 13.4; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{25}H_{26}N_2NaO_4S_2$ 505.1232, found 505.1228.

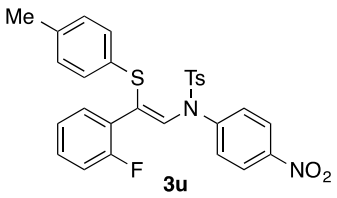
17) (*Z*)-N-(2-(cyclohexylthio)-2-phenylvinyl)-4-methyl-N-(4-nitrophenyl)benzene-sulfonamide. (3t)



3t

The general procedure was followed using **1t** (94.9 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.7, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3t** (76.6 mg, 38%) was obtained as yellow solid; m.p. =115.2 – 116.4 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 9.0 Hz, 2H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.47 – 7.45 (m, 2H), 7.39 – 7.37 (m, 5H), 7.28 (d, *J* = 8.5 Hz, 2H), 6.71 (s, 1H), 2.42 (s, 3H), 1.52 – 1.44 (m, 4H), 1.42 – 1.35 (m, 1H), 1.28 – 1.23 (m, 1H), 0.99 – 0.92 (m, 4H), 0.88 (t, *J* = 7.0 Hz, 1H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.9, 145.2, 144.7, 137.4, 137.3, 134.7, 129.9, 128.7, 128.6, 128.1, 127.5, 126.6, 126.5, 124.3, 44.3, 33.1, 25.5, 25.3, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{28}N_2NaO_4S_2$ 531.1388, found 531.1389.

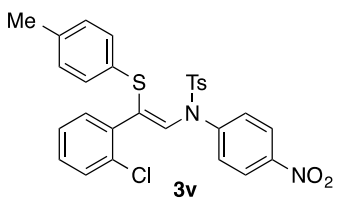
18) (*Z*)-N-(2-(2-fluorophenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3u)



3u

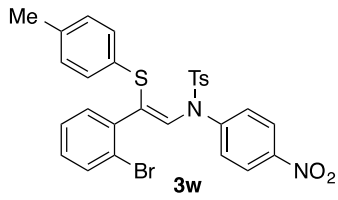
The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2u** (190.4 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3u** (184.5 mg, 95% yield) was obtained as yellow solid; m.p. =126.5 – 128.1 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$); δ 8.15 (d, *J* = 9.0 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 9.0 Hz, 2H), 7.33 – 7.27 (m, 3H), 7.16 – 7.12 (m, 1H), 6.98 – 6.92 (m, 3H), 6.83 – 6.77 (m, 4H), 2.43 (s, 3H), 2.16 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 160.4 (d, *J* = 246.4 Hz), 145.9, 145.5, 144.9, 137.3, 134.4, 131.3 (d, *J* = 2.3 Hz), 131.1, 129.9, 129.8, 129.3, 129.2 (d, *J* = 4.0 Hz), 128.2, 127.6, 127.4, 126.9, 124.6 (d, *J* = 13.0 Hz), 124.3, 123.8 (d, *J* = 3.5 Hz), 115.5 (d, *J* = 22.4 Hz), 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{23}FN_2NaO_4S_2$ 557.0981, found 557.0990.

19) (*Z*)-N-(2-(2-chlorophenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3v)



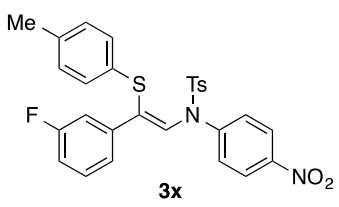
The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2v** (200 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3v** (183 mg, 83%) was obtained as yellow solid; m.p. =124.5 – 126.2 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 9.0 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 9.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.24 – 7.23 (m, 1H), 7.20 – 7.18 (m, 1H), 7.13 – 7.06 (m, 2H), 6.88 (d, *J* = 8.2 Hz, 2H), 6.83 (d, *J* = 8.1 Hz, 2H), 6.74 (s, 1H), 2.45 (s, 3H), 2.18 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 145.8, 145.5, 144.9, 138.0, 135.3, 134.4, 133.6, 132.8, 132.2, 131.8, 129.9, 129.5, 129.3, 129.2, 127.6, 127.14, 127.07, 126.98, 126.3, 124.3, 21.6, 21.0; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{23}ClN_2NaO_4S_2$ 573.0685, found 573.0687.

20) (*Z*)-N-(2-(2-bromophenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3w)



The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2w** (226.9 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3w** (178.7 mg, 75%) was obtained as yellow solid; m.p. =128.6 – 130.2 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 9.5 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 9.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.18 – 7.16 (m, 1H), 7.12 – 7.08 (m, 1H), 7.04 – 7.01 (m, 1H), 6.90 (d, *J* = 8.0 Hz, 2H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.73 (s, 1H), 2.45 (s, 3H), 2.19 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 145.6, 144.9, 138.0, 137.1, 134.4, 133.6, 133.0, 132.8, 131.9, 129.9, 129.5, 129.2, 127.6, 127.2, 126.98, 126.96, 126.8, 124.3, 123.8, 21.6, 21.0; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{23}BrN_2NaO_4S_2$ 617.0180, found 617.0189.

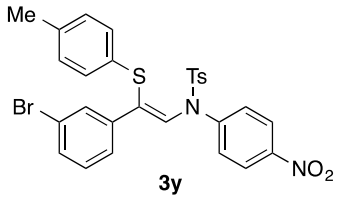
21) (*Z*)-N-(2-(3-fluorophenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3x)



3x

The general procedure was followed using **1a** (98.2mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2x** (190.4 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3x** (150.5 mg, 77% yield) was obtained as yellow solid; m.p. =125.9 – 127.5 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 – 8.10 (m, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.29 (m, 4H), 7.21 – 7.19 (m, 2H), 7.14 – 7.11 (m, 1H), 7.07 (s, 1H), 6.93 – 6.90 (m, 1H), 6.84 (d, *J* = 8.5 Hz, 2H), 6.73 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H), 2.18 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 162.3 (d, *J* = 244.9 Hz), 145.9, 145.8, 145.0, 139.7 (d, *J* = 7.8 Hz), 136.8, 134.4, 131.0 (d, *J* = 2.4 Hz), 130.0, 129.9, 129.8, 129.5, 129.0, 128.9, 127.6, 127.4, 124.3, 123.7 (d, *J* = 12 Hz), 115.4 (d, *J* = 21.3 Hz), 115.0 (d, *J* = 22.6 Hz), 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{23}FN_2NaO_4S_2$ 557.0981, found 557.0979.

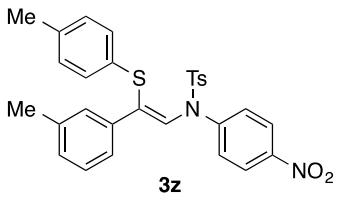
22) (*Z*)-N-(2-(3-bromophenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3y)



3y

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2y** (226.9 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3y** (187.7 mg, 79% yield) was obtained as yellow solid; m.p. =129.6 – 130.8 ℃; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 9.0 Hz, 2H), 7.57 – 7.54 (m, 3H), 7.34 (d, *J* = 7.5 Hz, 2H), 7.31 – 7.29 (m, 4H). 7.13 – 7.07 (m, 1H), 7.04 (s, 1H), 6.85 (d, *J* = 8.0 Hz, 2H), 6.73 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H), 2.18 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 145.8, 145.1, 139.5, 137.0, 134.3, 131.4, 130.9, 130.8, 130.7, 130.0, 129.9, 129.8, 129.5, 129.0, 128.7, 127.5, 127.4, 126.8, 124.3, 122.4, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{23}BrN_2NaO_4S_2$ 617.0180, found 617.0188.

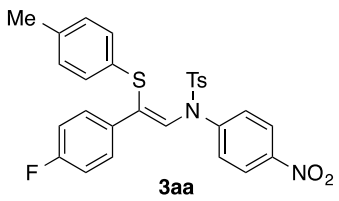
23) (*Z*)-4-methyl-N-(4-nitrophenyl)-N-(2-(m-tolyl)-2-(p-tolylthio)vinyl)benzene-sulfonamide. (3z)



3z

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2z** (188 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3z** (176 mg, 83% yield) was obtained as yellow solid; m.p. =118.7 – 120.3 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 9.0 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.33 – 7.27 (m, 4H), 7.24 – 7.20 (m, 2H), 7.15 – 7.10 (m, 1H), 7.06 – 7.03 (m, 1H), 6.99 (s, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.74 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H), 2.29 (s, 3H), 2.17 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.2, 145.5, 144.9, 138.0, 137.1, 136.6, 134.6, 133.7, 129.92, 129.86, 129.4, 129.34, 129.32, 128.8, 128.2, 127.7, 127.6, 127.0, 125.3, 124.3, 21.6, 21.3, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{29}H_{26}N_2NaO_4S_2$ 553.1232, found 553.1237.

24) (*Z*)-N-(2-(4-fluorophenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3aa)

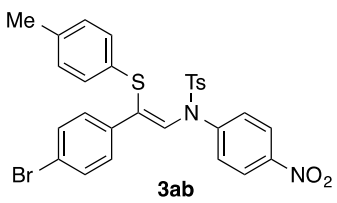


3aa

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (190.4 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3aa** (180.4 mg, 84% yield) was obtained as yellow solid; m.p. =120.1 – 121.5 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 9.0 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.39 – 7.36 (m, 2H), 7.33 (d, *J* = 9.0 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 6.93 – 6.90 (m, 3H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.72 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H), 2.17 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 162.8 (d, *J* = 247.3 Hz), 146.2, 145.6, 144.9, 136.9, 134.5, 133.2, 133.0 (d, *J* = 3.1 Hz), 130.3, 130.0, 129.9 (d, *J* = 8.3 Hz), 129.4, 128.8, 127.5, 127.4, 127.0, 124.4, 115.4 (d, *J* = 22.0 Hz), 21.6, 20.9;

HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{23}FN_2NaO_4S_2$ 557.0981, found 557.0963.

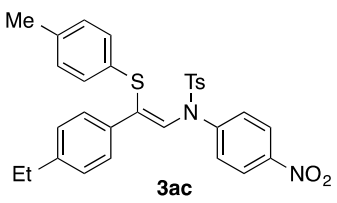
25) (*Z*)-N-(2-(4-bromophenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3ab)



3ab

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2b** (226.9 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3ab** (182.3 mg, 84% yield) was obtained as yellow solid; m.p. =132.2 – 133.9 ℃; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 – 8.11 (m, 2H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.36-7.34 (m, 2H), 7.32 – 7.31 (m, 1H), 7.30 – 7.27 (m, 5H), 7.01 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.71 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H), 2.18 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.0, 145.7, 145.0, 136.9, 136.2, 134.4, 131.9, 131.5, 130.0, 129.9, 129.6, 129.5, 128.8, 128.4, 127.5, 127.3, 124.3, 122.6, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{23}BrN_2NaO_4S_2$ 617.0180, found 617.0189.

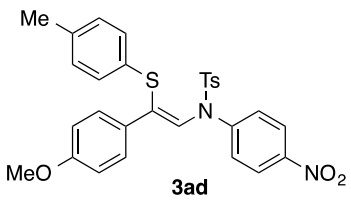
26) (*Z*)-N-(2-(4-ethylphenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3ac)



3ac

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2c** (196.4 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **3ac** (173.3 mg, 87% yield) was obtained as yellow solid; m.p. =121.5 – 123.2 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (d, *J* = 9.0 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.36 – 7.28 (m, 6H), 7.07 (d, *J* = 8 Hz, 2H), 6.98 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.73 (d, *J* = 8.0 Hz, 2H), 2.58 (q, *J* = 7.6 Hz, 2H), 2.43 (s, 3H), 2.17 (s, 3H), 1.18 (t, *J* = 7.6 Hz, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.3, 145.5, 145.0, 144.8, 136.4, 134.6, 134.4, 133.7, 129.9, 129.7, 129.5, 129.3, 128.1, 127.9, 127.6, 127.4, 126.9, 124.2, 28.5, 21.6, 20.9, 15.3; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{30}H_{28}N_2NaO_4S_2$ 567.1388, found 567.1385.

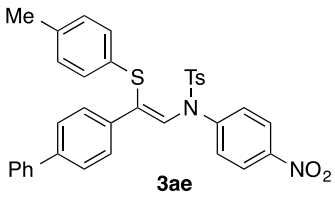
27) (*Z*)-N-(2-(4-methoxyphenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3ad)



3ad

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2d** (197.6 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.4, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3ad** (76.8 mg, 39% yield) was obtained as yellow solid; m.p. =124.6 – 125.8 ℃; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 – 8.10 (m, 2H), 7.6 (d, *J* = 8.0 Hz, 2H), 7.36-7.33 (m, 4H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.88 (s, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.77 – 6.72 (m, 4H), 3.76 (s, 3H), 2.43 (s, 3H), 2.18 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 160.0, 146.5, 145.4, 144.8, 136.5, 134.8, 134.7, 130.0, 129.9, 129.4, 129.34, 129.32, 129.2, 127.5, 126.7, 126.3, 124.3, 113.8, 55.2, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{29}H_{26}N_2NaO_5S_2$ 569.1181, found 569.1169.

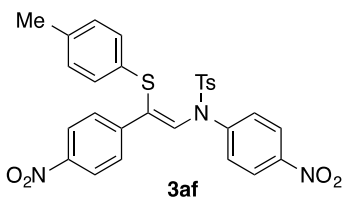
28) (*Z*)-N-(2-([1,1'-biphenyl]-4-yl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl)benzenesulfonamide. (3ae)



3ae

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2e** (225 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.5, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3ae** (208.6 mg, 88%) was obtained as yellow solid; m.p. =129.8 – 131.5 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 9.5 Hz, 2H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.56 – 7.48 (m, 6H), 7.45 – 7.40 (m, 2H), 7.38 – 7.33 (m, 3H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.10 (s, 1H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.5 Hz, 2H), 2.44 (s, 3H), 2.18 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.2, 145.6, 144.9, 141.3, 140.0, 136.6, 136.1, 134.5, 132.8, 129.9, 129.7, 129.4, 129.3, 128.8, 128.5, 128.1, 127.6, 127.09, 126.96, 126.86, 124.3, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{34}H_{28}N_2NaO_4S_2$ 615.1388, found 615.1398.

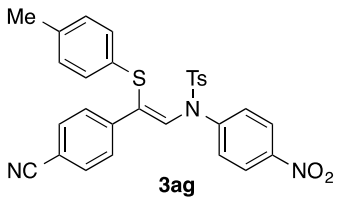
29) (*Z*)-4-methyl-N-(4-nitrophenyl)-N-(2-(4-nitrophenyl)-2-(p-tolylthio)vinyl) benzenesulfonamide. (3af)



3af

The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2f** (207 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.4, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3af** (179.7 mg, 80% yield) was obtained as yellow solid; m.p. =141.2 – 142.6 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.5 Hz, 2H), 8.10 (d, *J* = 8.5 Hz, 2H), 7.60 – 7.57 (m, 4H), 7.34 – 7.31 (m, 4H), 7.28 (s, 1H), 6.86 (d, *J* = 8.0 Hz, 2H), 6.74 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H), 2.19 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 147.3, 146.2, 145.4, 145.2, 144.4, 137.2, 134.0, 131.2, 130.1, 129.7, 129.6, 128.6, 128.5, 128.0, 127.6, 127.5, 124.4, 123.6, 21.7, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{23}N_3NaO_6S_2$ 584.0926, found 584.0910.

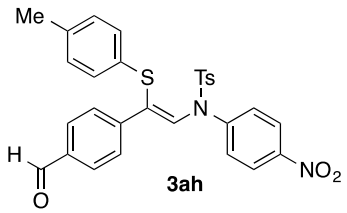
30) (*Z*)-N-(2-(4-cyanophenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3ag)



3ag

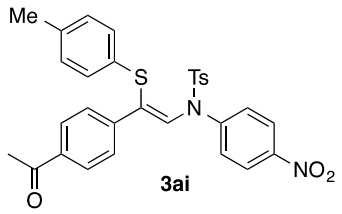
The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2g** (194.6 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3ag** (182.3 mg, 84% yield) was obtained as yellow solid; m.p. =132.9 – 134.4 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 9.0 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.51 (s, 4H), 7.29 (t, *J* = 8.5 Hz, 4H), 7.19 (s, 1H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.70 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H), 2.18 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.1, 145.3, 145.2, 142.3, 137.2, 134.1, 132.1, 130.7, 130.1, 129.7, 129.6, 128.5, 128.4, 127.9, 127.6, 124.3, 118.4, 111.7, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{29}H_{23}N_3NaO_4S_2$ 564.1028, found 564.1024.

31) (*Z*)-N-(2-(4-formylphenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3ah)



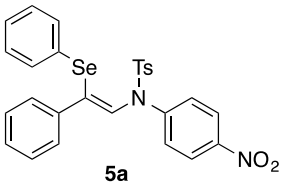
The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2h** (196.4 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.2, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3ah** (91.4 mg, 42% yield) was obtained as yellow solid; m.p. =130.2 – 131.6 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.93 (s, 1H), 8.12 (d, *J* = 9 Hz, 2H), 7.74 (d, *J* = 8 Hz, 2H), 7.59 – 7.55 (m, 4H), 7.30 (d, *J* = 8.5 Hz, 4H), 7.21 (s, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.72 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H), 2.16 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 191.5, 146.0, 145.5, 145.2, 143.7, 137.0, 135.9, 134.2, 130.4, 130.0, 129.7, 129.6, 129.5, 129.4, 128.8, 128.6, 127.8, 127.6, 124.3, 21.7, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{29}H_{24}N_2NaO_5S_2$ 567.1024, found 567.1031.

32) (*Z*)-N-(2-(4-acetylphenyl)-2-(p-tolylthio)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (3ai)



The general procedure was followed using **1a** (98.2 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2i** (204.8 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.2, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **3ai** (207.5 mg, 93% yield) was obtained as yellow solid; m.p. =133.5 – 134.8 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 9.0 Hz, 2H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.33 – 7.28 (m, 4H), 7.16 (s, 1H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.71 (d, *J* = 8.5 Hz, 2H), 2.55 (s, 3H), 2.44 (s, 3H), 2.16 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 197.3, 145.9, 145.7, 145.1, 142.2, 136.9, 136.7, 134.3, 130.1, 130.02, 129.99, 129.6, 129.5, 128.9, 128.4, 128.1, 127.61, 127.56, 124.3, 26.6, 21.6, 20.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{30}H_{26}N_2NaO_5S_2$ 581.1181, found 581.1187.

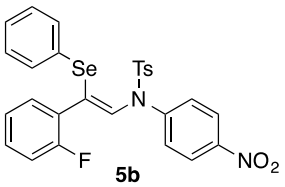
33) (*Z*)-4-methyl-N-(4-nitrophenyl)-N-(2-phenyl-2-(phenylselanyl)vinyl) benzenesulfonamide. (5a)



5a

The general procedure was followed using **4a** (111.3 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (179.6 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **5a** (164.9 mg, 75%) was obtained as yellow solid; m.p. =129.5 – 130.9 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 9.0 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 9.0 Hz, 2H), 7.34 – 7.32 (m, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.21 – 7.16 (m, 3H), 7.05 – 7.04 (m, 1H), 7.00 – 6.99 (m, 4H), 6.94 – 6.93 (m, 1H), 2.43 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.2, 145.5, 144.9, 137.7, 135.1, 134.3, 133.0, 129.9, 128.8, 128.71, 128.68, 128.5, 128.2, 127.6, 127.4, 127.3, 126.8, 124.4, 21.6 ; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{22}N_2NaO_4SSe$ 573.0363, found 573.0368.

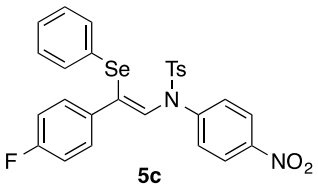
34) (*Z*)-N-(2-(2-fluorophenyl)-2-(phenylselanyl)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (5b)



5b

The general procedure was followed using **4a** (111.3 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2u** (190.4 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.5, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **5b** (163.4 mg, 72%) was obtained as yellow solid; m.p. =127.1 – 128.6 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 9.0 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.47 (d, *J* = 9.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.16 (m, 1H), 7.12 – 7.08 (m, 1H), 7.08 – 7.04 (m, 3H), 7.00 – 6.97 (m, 2H), 6.93 – 6.91 (m, 1H), 6.90 (s, 1H), 6.88 – 6.84 (m, 1H), 2.43 (s, 3H) ; **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 159.6 (d, *J* = 246.5 Hz), 145.8, 145.5, 144.9, 134.3, 134.2, 131.7 (d, *J* = 2.1 Hz), 129.9, 129.8, 128.6, 128.5 (d, *J* = 2.6 Hz), 128.2, 127.9, 127.60, 127.57, 126.7, 125.2 (d, *J* = 13.9 Hz), 124.5, 123.6 (d, *J* = 3.5 Hz), 115.3 (d, *J* = 22.1 Hz), 21.6 ; **^{19}F NMR** (470 MHz, $CDCl_3$) δ 115.2; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{21}FN_2NaO_4SSe$ 591.0269, found 591.0271.

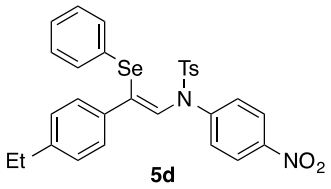
35) (*Z*)-N-(2-(4-fluorophenyl)-2-(phenylselanyl)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (5c)



5c

The general procedure was followed using **4a** (111.3 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2a** (190.4 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **5c** (181.6 mg, 80%) was obtained as yellow solid; m.p. =128.3 – 129.6 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.19 (d *J* = 9.5 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.40 (d, *J* = 9 Hz, 2H), 7.32 – 7.30 (m, 4H), 7.10 – 7.08 (m, 1H), 7.04 – 7.00 (m, 4H), 6.91 – 6.87 (m, 3H), 2.45 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 162.6 (*J* = 247.3 Hz), 146.2, 145.6, 145.0, 134.5, 134.3, 133.7 (*J* = 3.3 Hz), 133.2, 130.5 (*J* = 8.3 Hz), 129.9, 128.8, 128.4, 127.6, 127.5, 127.2, 126.8, 124.5, 115.2 (*J* = 21.6 Hz), 21.6; **^{19}F NMR** (470 MHz, $CDCl_3$) δ -112.7; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{27}H_{21}FN_2NaO_4SSe$ 591.0269, found 591.0272.

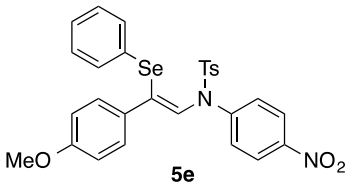
36) (*Z*)-N-(2-(4-ethylphenyl)-2-(phenylselanyl)vinyl)-4-methyl-N-(4-nitrophenyl) benzenesulfonamide. (5d)



5d

The general procedure was followed using **4a** (111.3 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2c** (187.2 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.6, PE/EA = 5:1). After purification by column chromatography (PE/EA = 10:1), **5d** (145.5 mg, 63%) was obtained as yellow solid; m.p. =115.6 – 116.9 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 9.0 Hz, 2H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.36 (d, *J* = 9.0 Hz, 2H), 7.29 – 7.27 (m, 4H), 7.07 – 7.02 (m, 3H), 7.00 – 6.98 (m, 4H), 6.92 (s, 1H), 2.57 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 1.17 (t, *J* = 7.5 Hz, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 146.4, 145.4, 145.0, 144.8, 135.2, 135.0, 134.4, 132.7, 129.9, 129.0, 128.7, 127.7, 127.6, 127.13, 127.09, 126.8, 124.4, 28.5, 21.6, 15.4 ; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{29}H_{26}N_2NaO_4SSe$ 601.0676, found 601.0674.

37) (*Z*)-N-(2-(4-methoxyphenyl)-2-(phenylselanyl)vinyl)-4-methyl-N-(4-nitrophenyl)benzenesulfonamide. (5e)

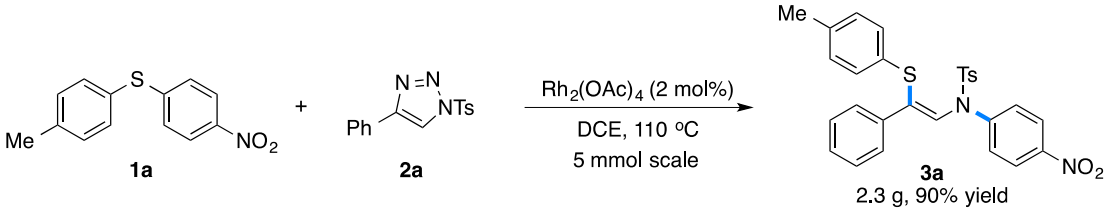


5e

The general procedure was followed using **4a** (111.3 mg, 0.4 mmol, 1.0 equiv), $Rh_2(OAc)_4$ (2 mol%, 3.6 mg) and **2d** (197.6 mg, 0.6 mmol, 1.5 equiv) by method A (R_f = 0.3, PE/EA = 10:1). After purification by column chromatography (PE/EA = 10:1), **5e** (106.6 mg, 46%) was obtained as yellow solid; m.p. =130.2 – 131.6 ℃ ; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.18 (d *J* = 9.0 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 9.0 Hz, 2H), 7.31 – 7.29 (m, 4H), 7.08 – 7.06 (m, 1H), 7.02 – 6.99 (m, 4H), 6.86 (s, 1H), 6.74 (d, *J* = 8.5 Hz, 2H), 3.76 (s, 3H), 2.44 (s, 3H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ 159.9, 146.5, 145.4, 144.8, 136.0, 134.5, 132.8, 130.0, 129.9, 128.9, 128.7, 127.6, 127.2, 126.5, 126.2, 124.4, 113.6, 55.2, 21.6 ; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{24}N_2NaO_5SSe$ 603.0469, found 603.0475.

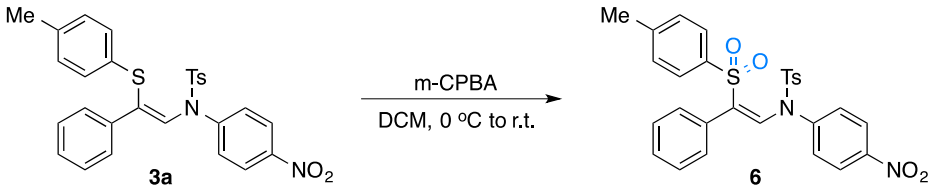
4. Gram scale preparation of 3a and Synthetic Application

4.1 Gram scale preparation of 3a

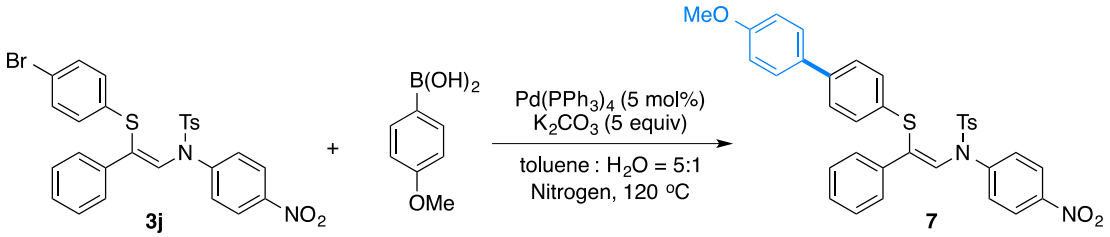


Thioether **1a** (1.23 g, 5.0 mmol, 1.0 equiv), triazole **2a** (2.25 g, 7.5 mmol, 1.5 equiv), $Rh_2(OAc)_4$ (45.0 mg, 0.1 mmol, 2.0 mol%) and dry 1,2-dichloroethane (50 mL, 0.1 M) were introduced into a sealed pressure tube under Argon protection, then the solution was heated at 110 °C by oil bath and keep this temperature for 4 hours. The reaction was monitored by TLC. Upon completion, the reaction was cooled to room temperature and open the sealed pressure tube carefully, then the solvent was evaporated under reduced pressure and the mixture was purified by column chromatography on silica gel using PE: EA = 10: 1 as the eluent and concentrated to obtain the product **3a** (2.3 g, 90%).

4.2 Synthetic Application



3a (258.3 mg, 0.5 mmol, 1.0 equiv) was introduced into a flask, and DCM (10 mL) as a solvent. The solvent stir at 0°C with ice-bath to add m-CPBA (85%, 203.0 mg, 1.0 mmol, 2.0 equiv), then allowed the mixture to stir for 2 hours at room temperature. Consumed completely determined by TLC analysis. Add 10 mL of H_2O, extract three times with DCM, wash the combined organic layer twice with $NaHCO_3$ solution, dry with Na_2SO_4 and filter, then concentrate the solvent and the residue was purified by column chromatography on silica gel using PE: EA = 5: 1 as the eluent and concentrated to obtain the product **6** (222.5 mg, 81%) as white solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.16 (d, *J* = 9.0 Hz, 2H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.41 (d, *J* = 9.0 Hz, 2H), 7.36 – 7.32 (m, 1H), 7.29 – 7.24 (m, 6H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 7.00 (s, 1H), 2.40 (s, 3H), 2.31 (s, 3H); **^{13}C{^{1}H} NMR** (151 MHz, $CDCl_3$) δ 146.9, 146.0, 145.5, 144.5, 136.2, 135.3, 134.7, 132.9, 132.8, 130.3, 130.0, 129.3, 129.1, 128.3, 127.88, 127.85, 127.7, 124.1, 21.6, 21.5; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{24}N_2NaO_6S_2$ 571.0973, found 571.0983.



3j (290.7 mg, 0.5 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (50.1 mg, 0.025 mmol, 5 mol%), K_2CO_3 (345.0 mg, 2.5 mmol, 5.0 equiv) and 4-methoxyphenylboronic acid (91.2 mg, 0.6 mmol, 1.2 equiv) were introduced into a 25mL dried Schlenk tube under N_2 protection. Then add 5 mL solvent (toluene: H_2O = 5:1) and react at 120 °C in oil bath. Consumed completely determined by TLC analysis (R_f = 0.3, PE/EA = 10:1). Concentrate the solvent and then the mixture was purified by column chromatography on silica gel using PE/EA (5:1) as the eluent and concentrated to obtain the product **7** (280.0 mg, 90%) as yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz,

2H), 7.50 – 7.46 (m, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 9.0 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.27 – 7.25 (m, 3H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.11 (s, 1H), 6.92 – 6.89 (m, 4H), 3.82 (s, 3H), 2.43 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 159.2, 146.0, 145.7, 144.9, 139.0, 137.1, 134.5, 132.4, 132.3, 131.2, 130.0, 129.9, 128.7, 128.6, 128.4, 128.1, 127.8, 127.5, 127.2, 126.7, 124.3, 114.2, 55.3, 21.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{34}H_{28}N_2NaO_5S_2$ 631.1337, found 631.1341.

5. X-ray crystal data for 3a

0.5 mL of DCM was added to a 10mL oven-dried glass sample bottle with 25 mg pure **3a** to dissolve the sample, then 8mL *n*-hexane was slowly added to the solution, sealed with rubber stopper and and insert two needles. And then the solvent was slowly dried at room temperature to obtain crystals. Single crystal X-ray diffraction data were collected on Bruker Smart Apex II CCD diffractometer. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC)：2207653

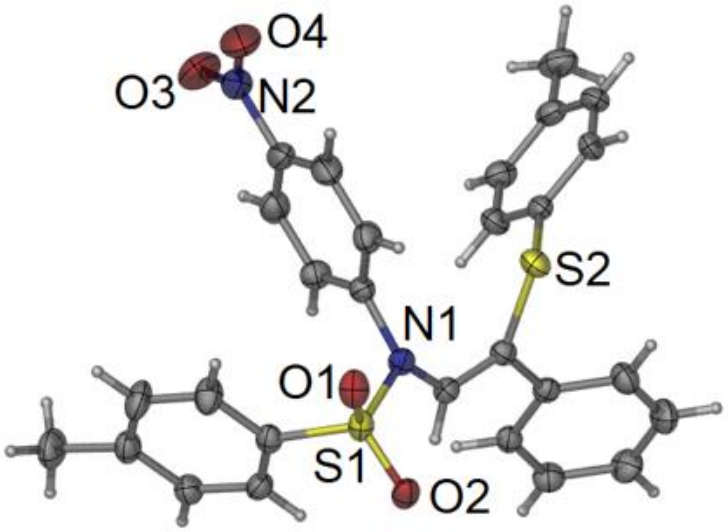


Figure 1. The structure of the **3a**

Table 1. Crystal data for compound **3a**

Compound	**3a**
Empirical formula	$C_{11}H_{18}O_2S$
Formula weight	516.61
Temperature/K	173.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	6.3065(3)

b/Å	12.6515(5)
c/Å	16.4803(5)
α/°	102.313(3)
β/°	93.649(3)
γ/°	98.836(3)
Volume/Å^3	1263.07(9)
Z	2
ρcalcg/cm^3	1.358
μ/mm^{-1}	2.222
F(000)	540.0
Crystal size/mm^3	0.36 × 0.09 × 0.07
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.26 to 134.142
Index ranges	-7 ≤ h ≤ 7, -15 ≤ k ≤ 15, -19 ≤ l ≤ 19
Reflections collected	27050
Independent reflections	4470 [R_{int} = 0.0814, R_{sigma} = 0.0604]
Data/restraints/parameters	4470/0/328
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.1118
Final R indexes [all data]	R_1 = 0.0556, wR_2 = 0.1181
Largest diff. peak/hole / e Å^{-3}	0.30/-0.57

6. References

[1] Rout, L.; Saha, P.; Jammi, S.; Punniyamurthy, T. Efficient Copper(I)-Catalyzed C–S Cross Coupling of Thiols with Aryl Halides in Water. *Eur. J. Org. Chem.* **2008**, 640–643.

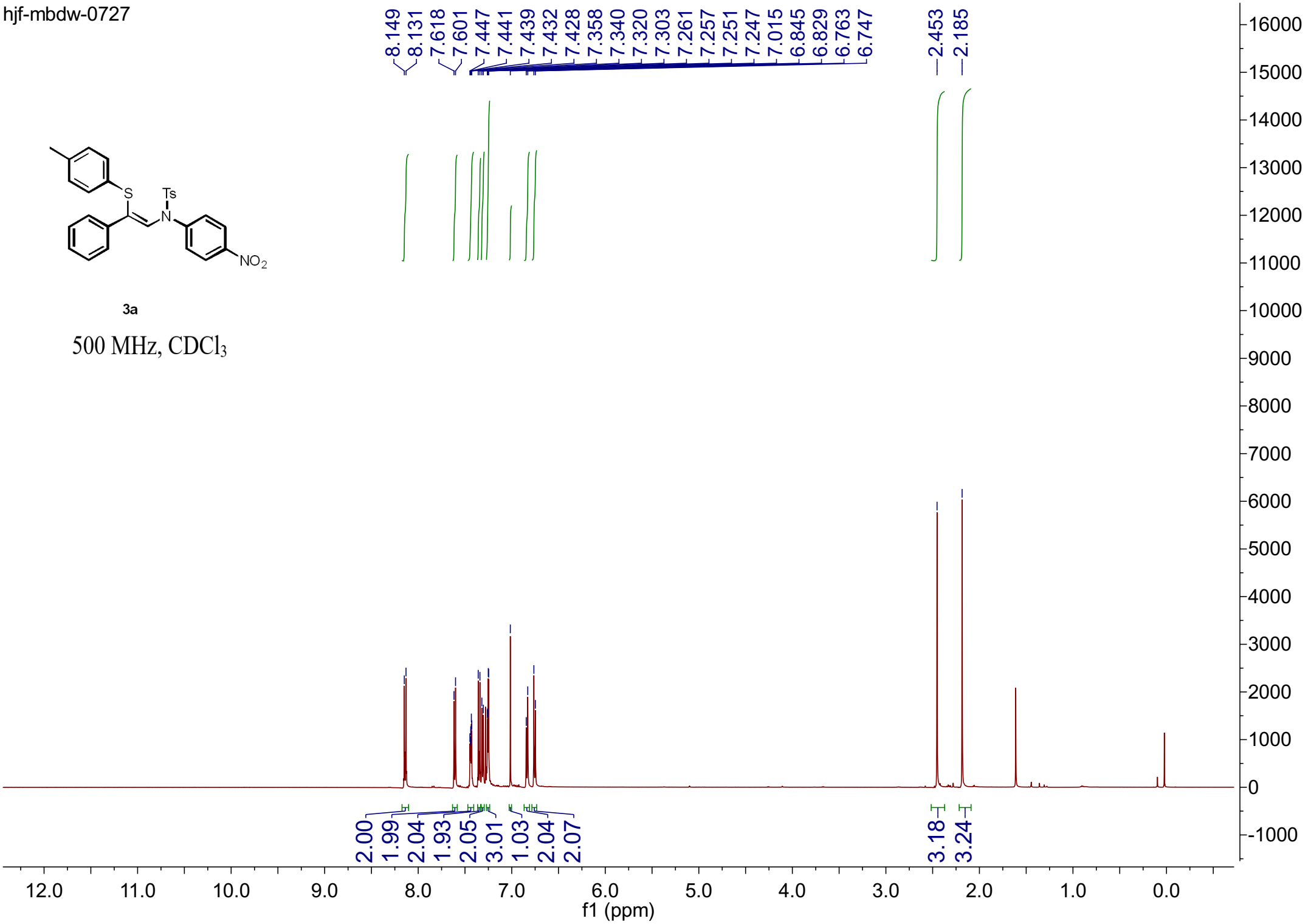
[2] Shieh, Y.-C.; Du, K.; Basha, R. S.; Xue, Y.-J.; Shih, B.-H.; Li, L.; Lee, C.-F. Syntheses of Thioethers and Selenide Ethers from Anilines. *J. Org. Chem.* **2019**, *84*, 6223–6231.

7. NMR and HRMS spectra of new compounds

hjf-mbdw-0727

3a

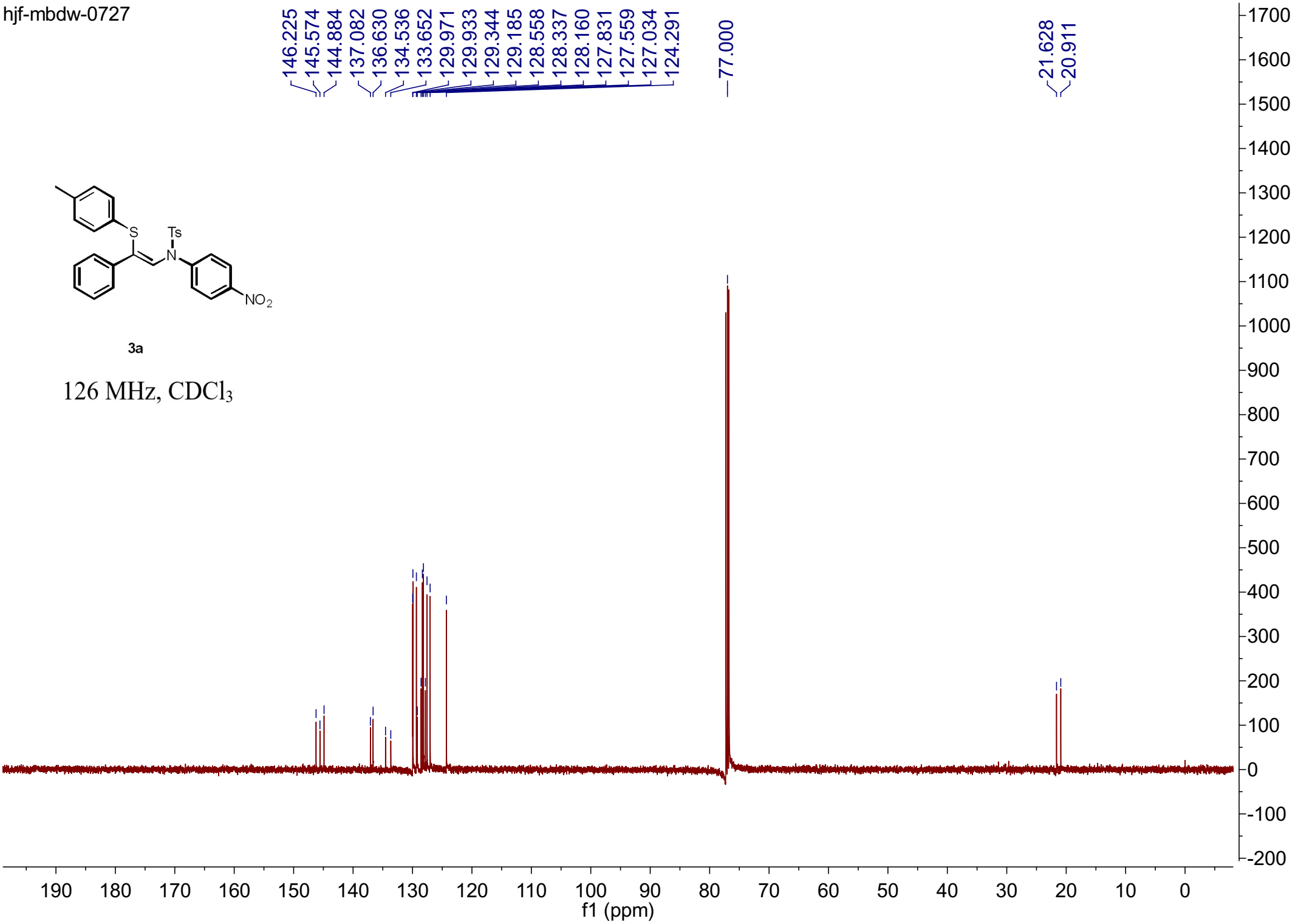
500 MHz, $CDCl_3$



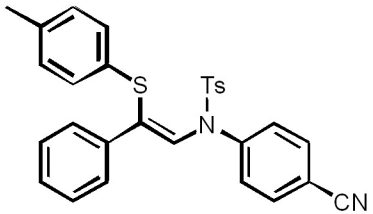
hjf-mbdw-0727

3a

126 MHz, $CDCl_3$

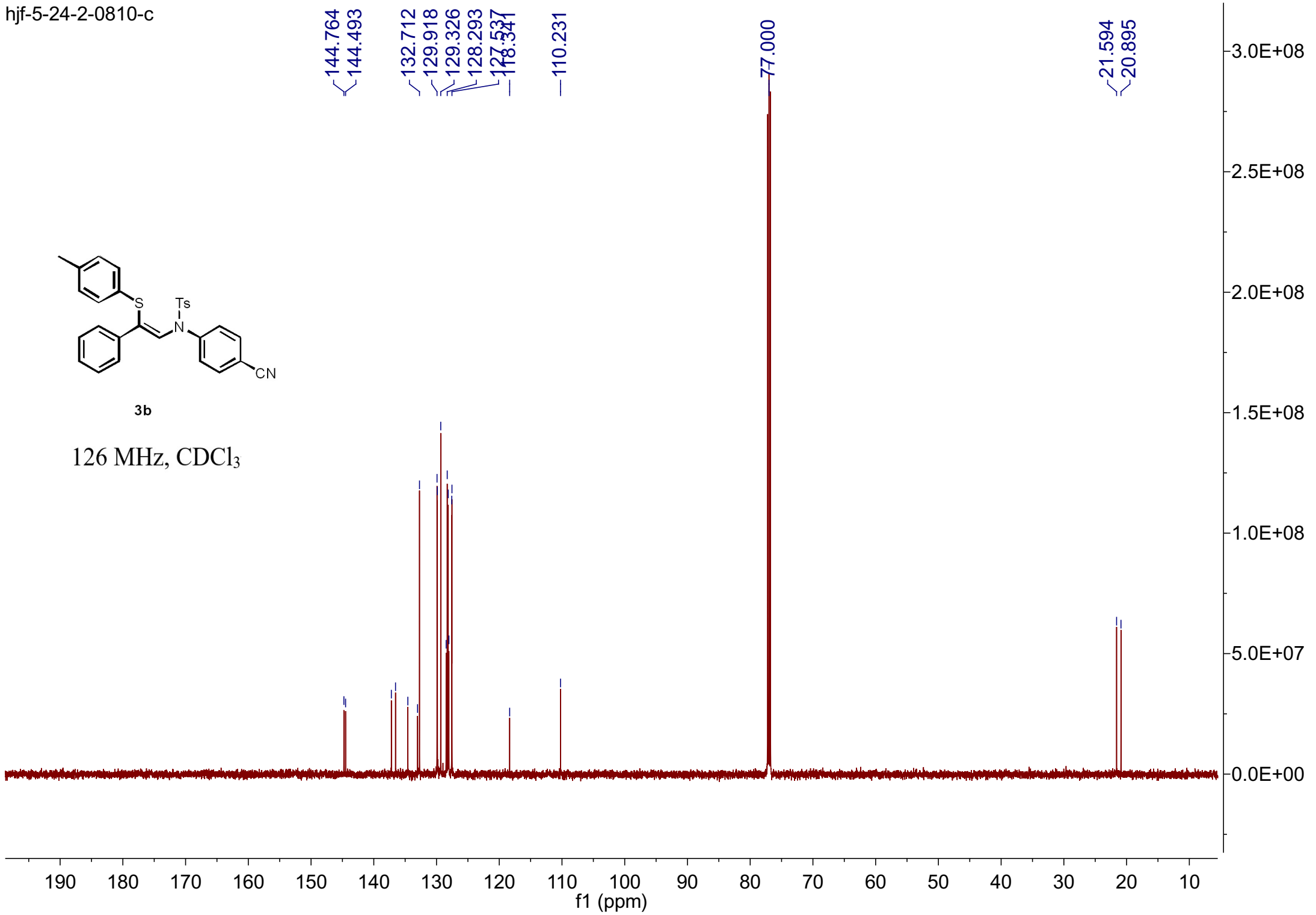


hjf-5-24-2-0810-h

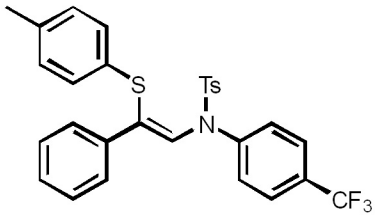


3b

500 MHz, $CDCl_3$


hjf-5-24-2-0810-c
144.764
144.493
132.712
129.918
129.326
128.293
127.537
118.341
110.231
77.000
21.594
20.895
S
Ts
N
CN
3b
126 MHz, CDCl3
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

hjf-5-29-0710-h



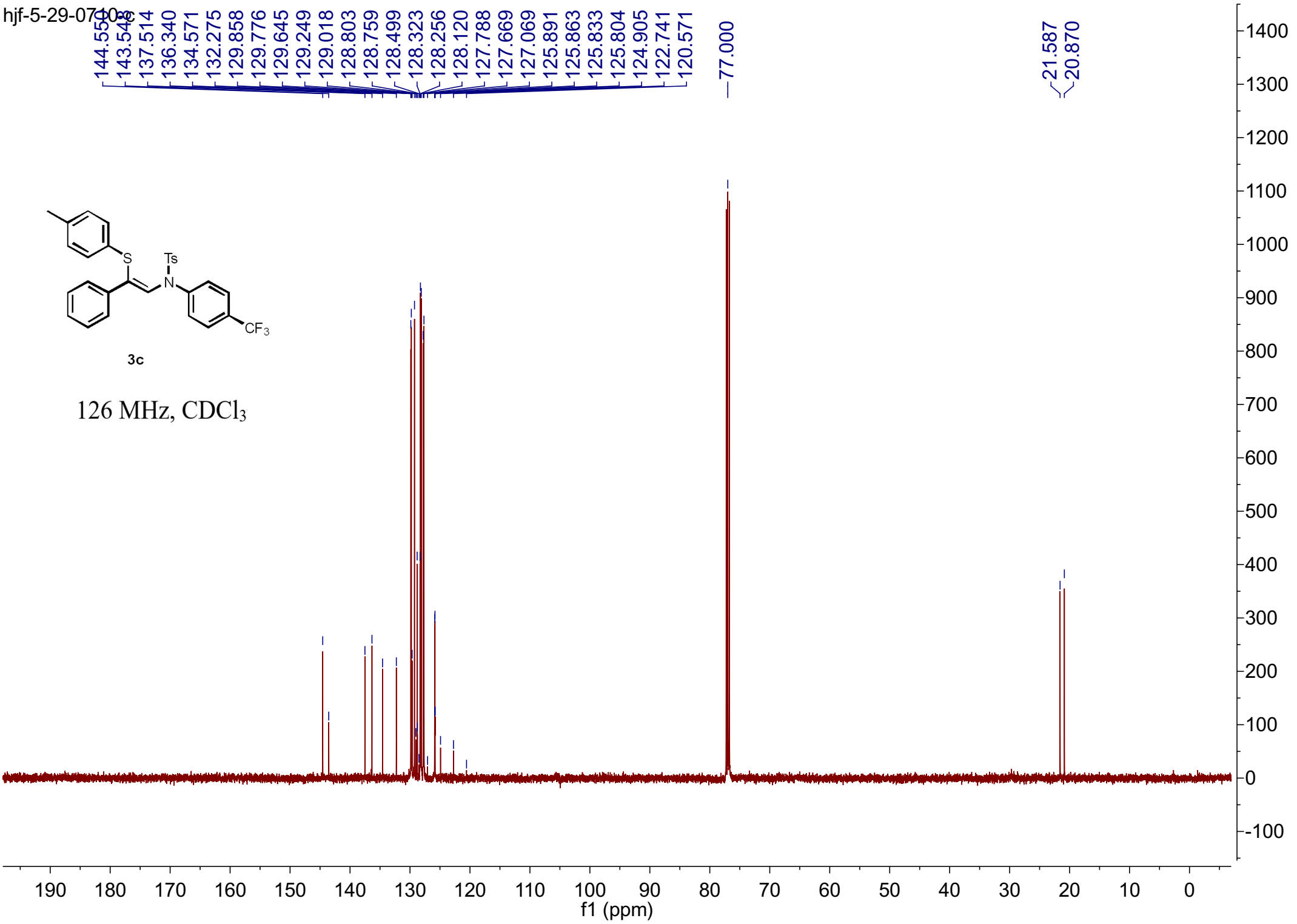
3c

500 MHz, $CDCl_3$

hjf-5-29-0710-c

3c

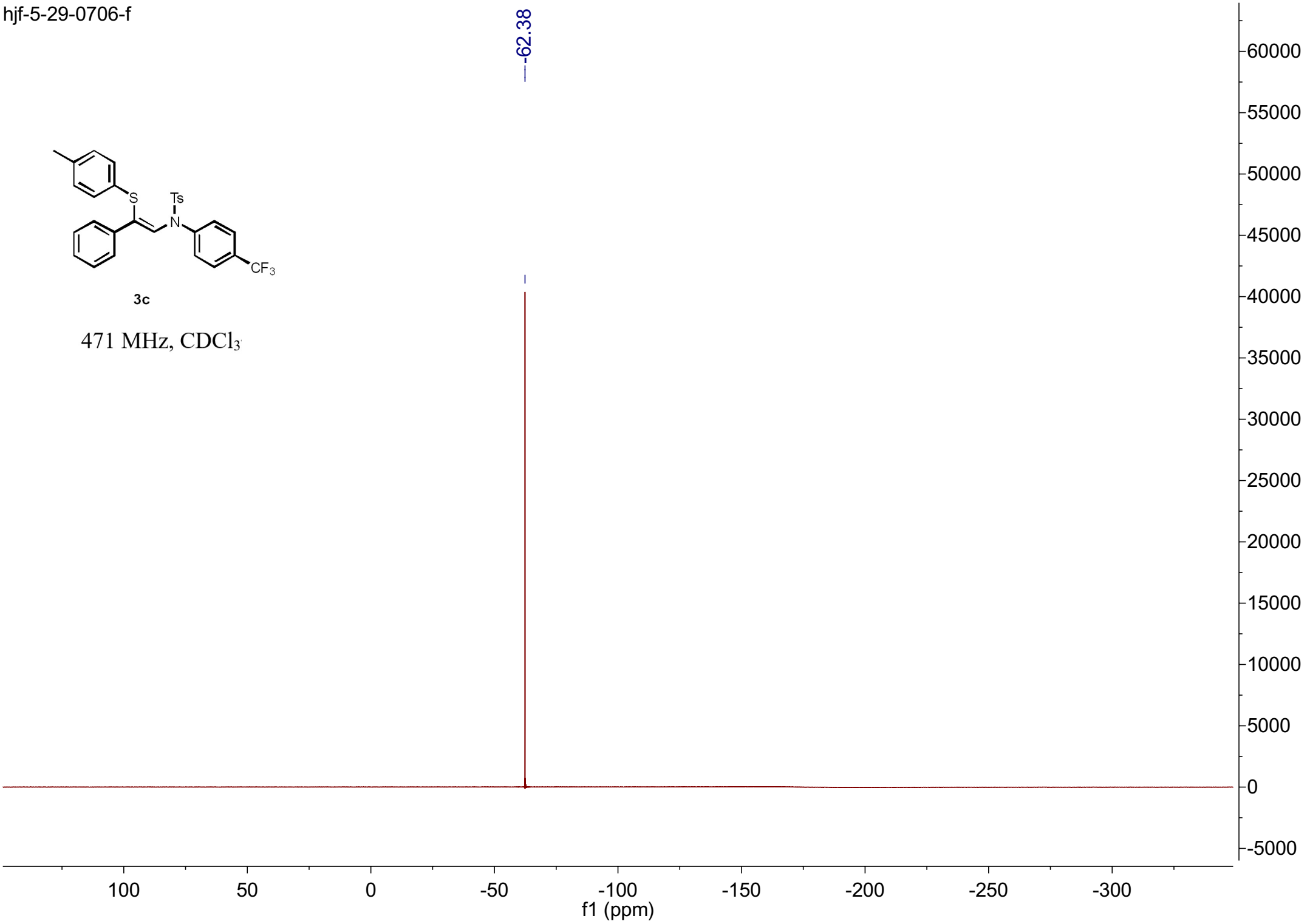
126 MHz, $CDCl_3$



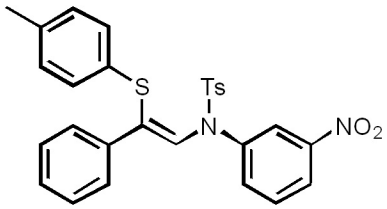
hjf-5-29-0706-f

3c

471 MHz, $CDCl_3$

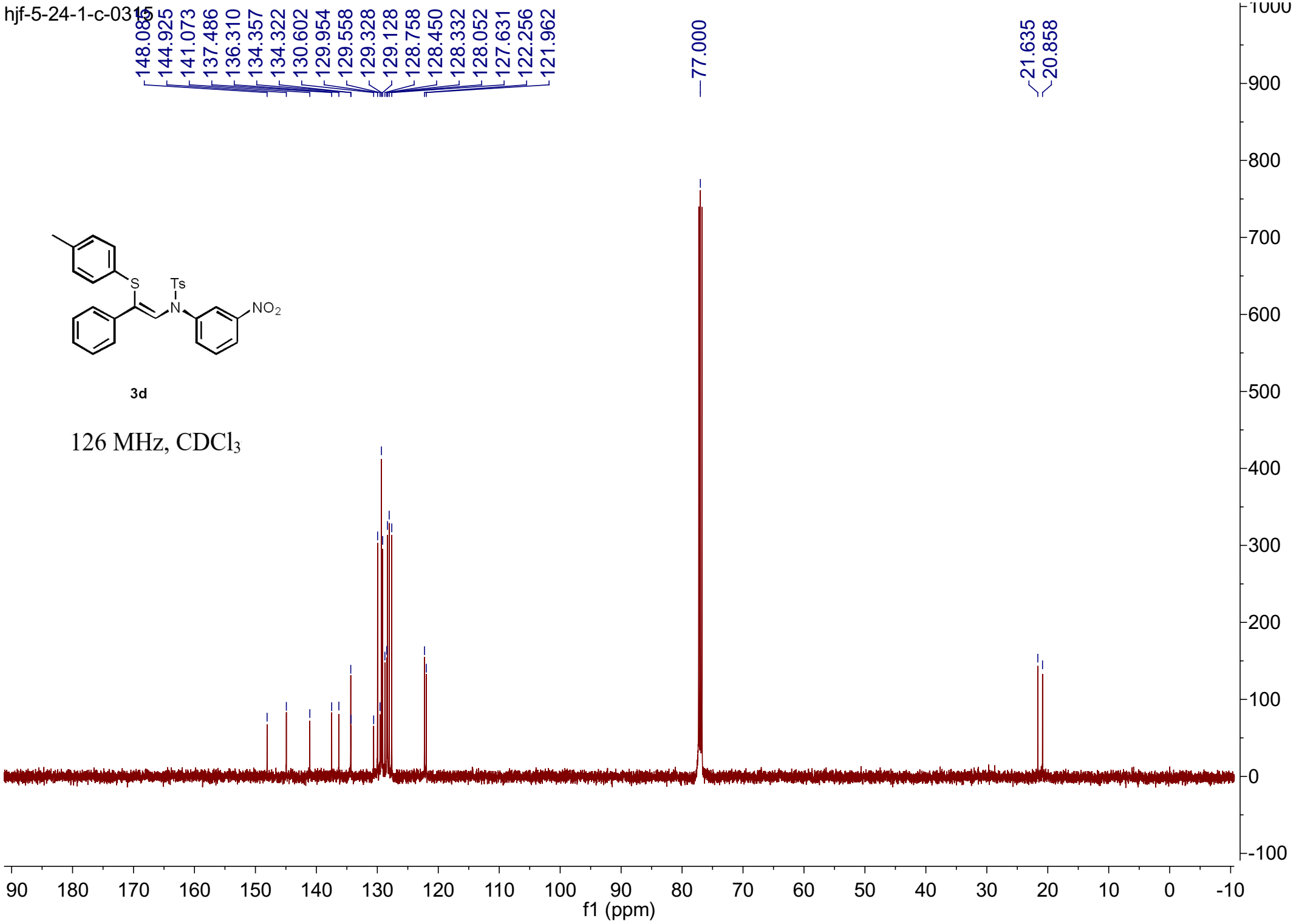


hjf-5-24-1-h-0315

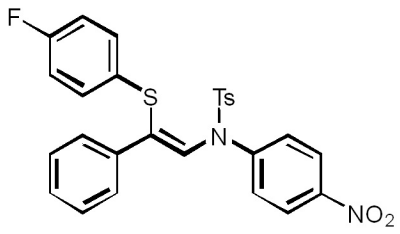


3d

500 MHz, $CDCl_3$


hjf-5-24-1-c-0315
148.085
144.925
141.073
137.486
136.310
134.357
134.322
130.602
129.954
129.558
129.328
129.128
128.758
128.450
128.332
128.052
127.631
122.256
121.962
77.000
21.635
20.858
S
Ts
N
NO2
3d
126 MHz, CDCl3
f1 (ppm)

hjf-5-73-1-h-0901



3h

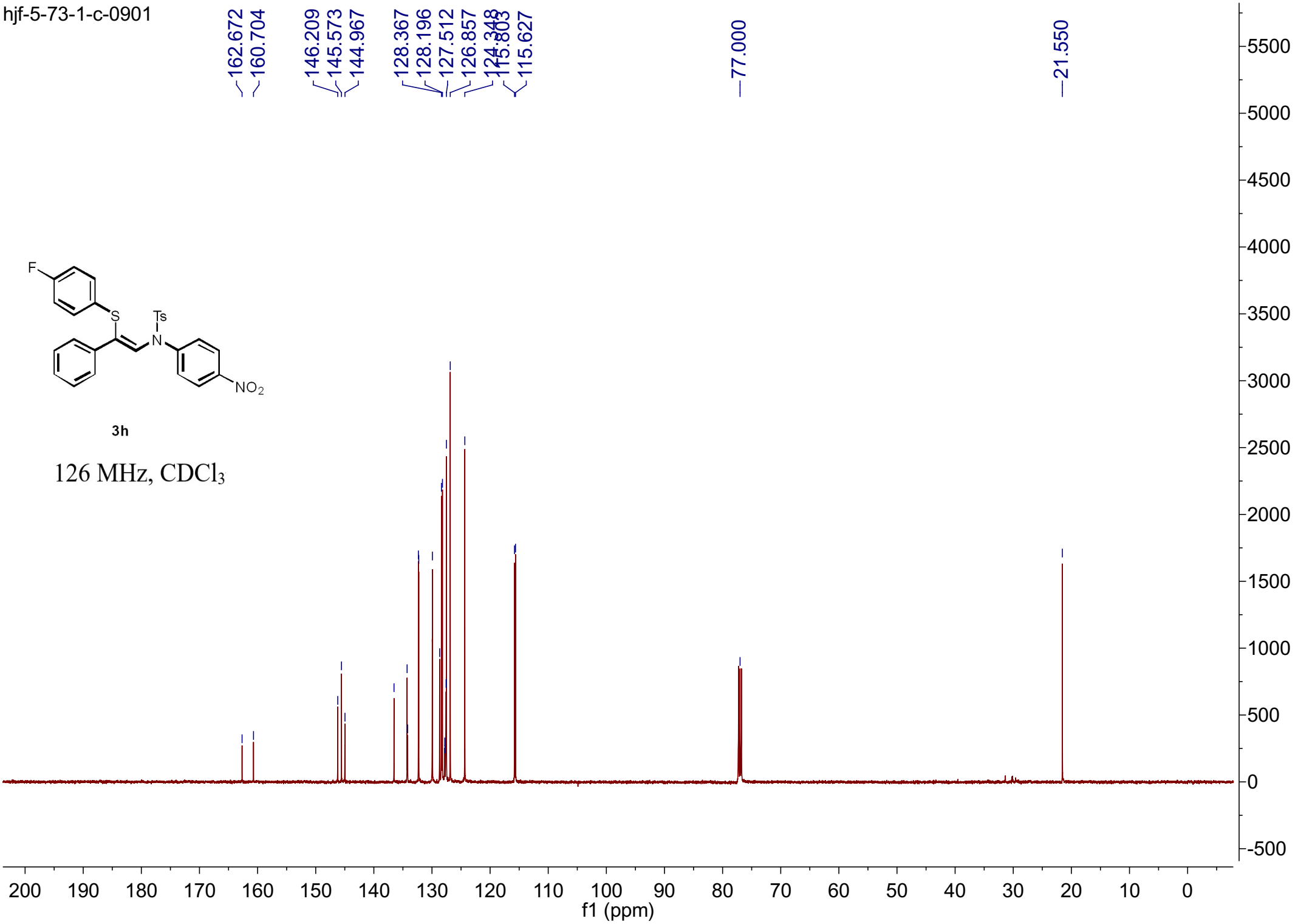
500 MHz, $CDCl_3$

f1 (ppm)

hjf-5-73-1-c-0901

3h

126 MHz, $CDCl_3$



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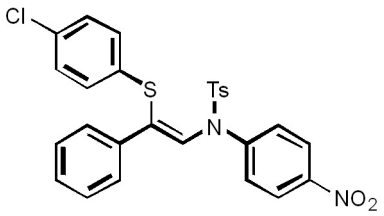
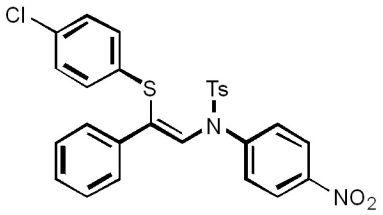


3i

500 MHz, $CDCl_3$

f1 (ppm)

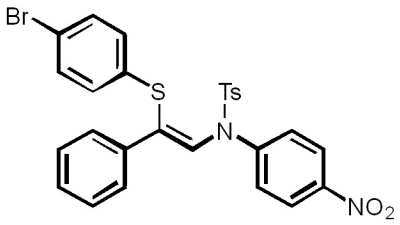
hjf-5-73-2-c-0314



3i

126 MHz, $CDCl_3$

hjf-5-68-5-h



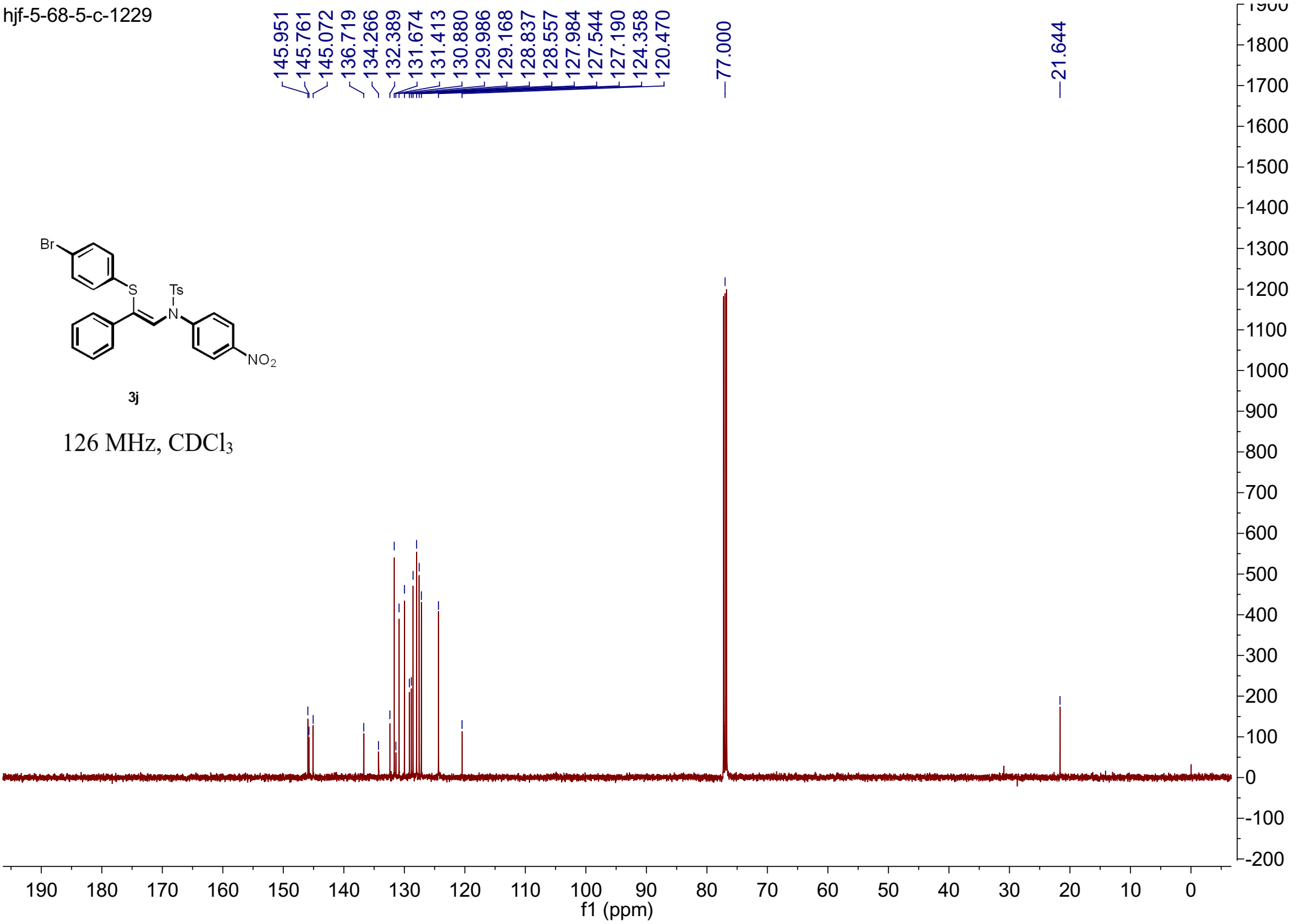
3j

500 MHz, $CDCl_3$

hjf-5-68-5-c-1229

3j

126 MHz, $CDCl_3$



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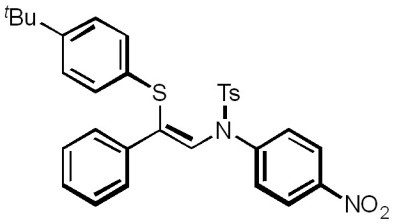
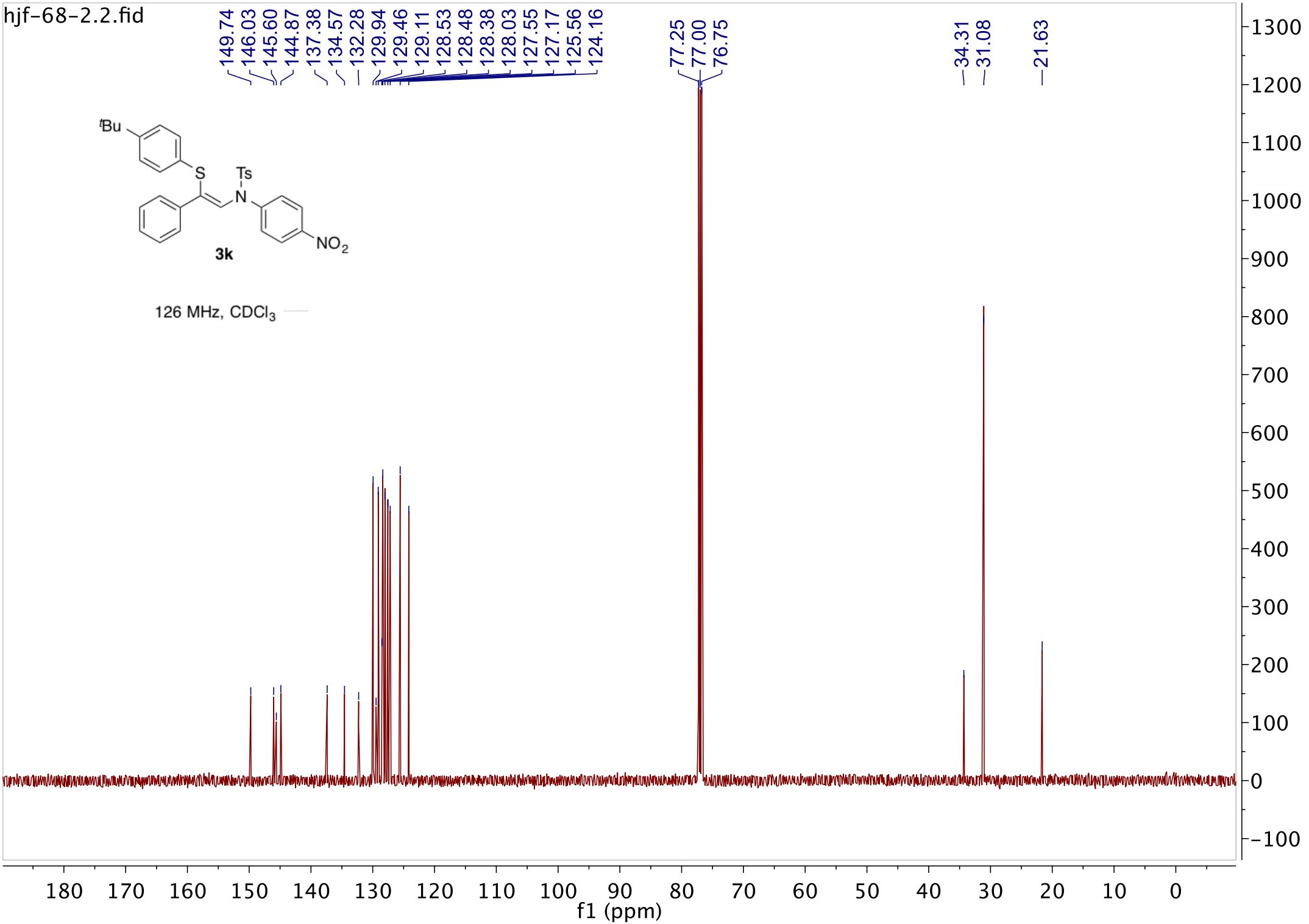
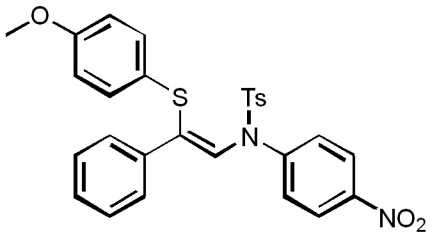


3k

500 MHz, $CDCl_3$


hjf-68-2.2.fid
149.74
146.03
145.60
144.87
137.38
134.57
132.28
129.94
129.46
129.11
128.53
128.48
128.38
128.03
127.55
127.17
125.56
124.16
77.25
77.00
76.75
34.31
31.08
21.63
tBu
S
Ts
N
NO2
3k
126 MHz, CDCl3
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

hjf-5-68-1-h-0902



3l

500 MHz, $CDCl_3$

8.169
8.150
7.620
7.603
7.402
7.384
7.380
7.364
7.361
7.304
7.288
7.221
7.210
7.207
6.862
6.817
6.800
6.558
6.540
3.649
2.429

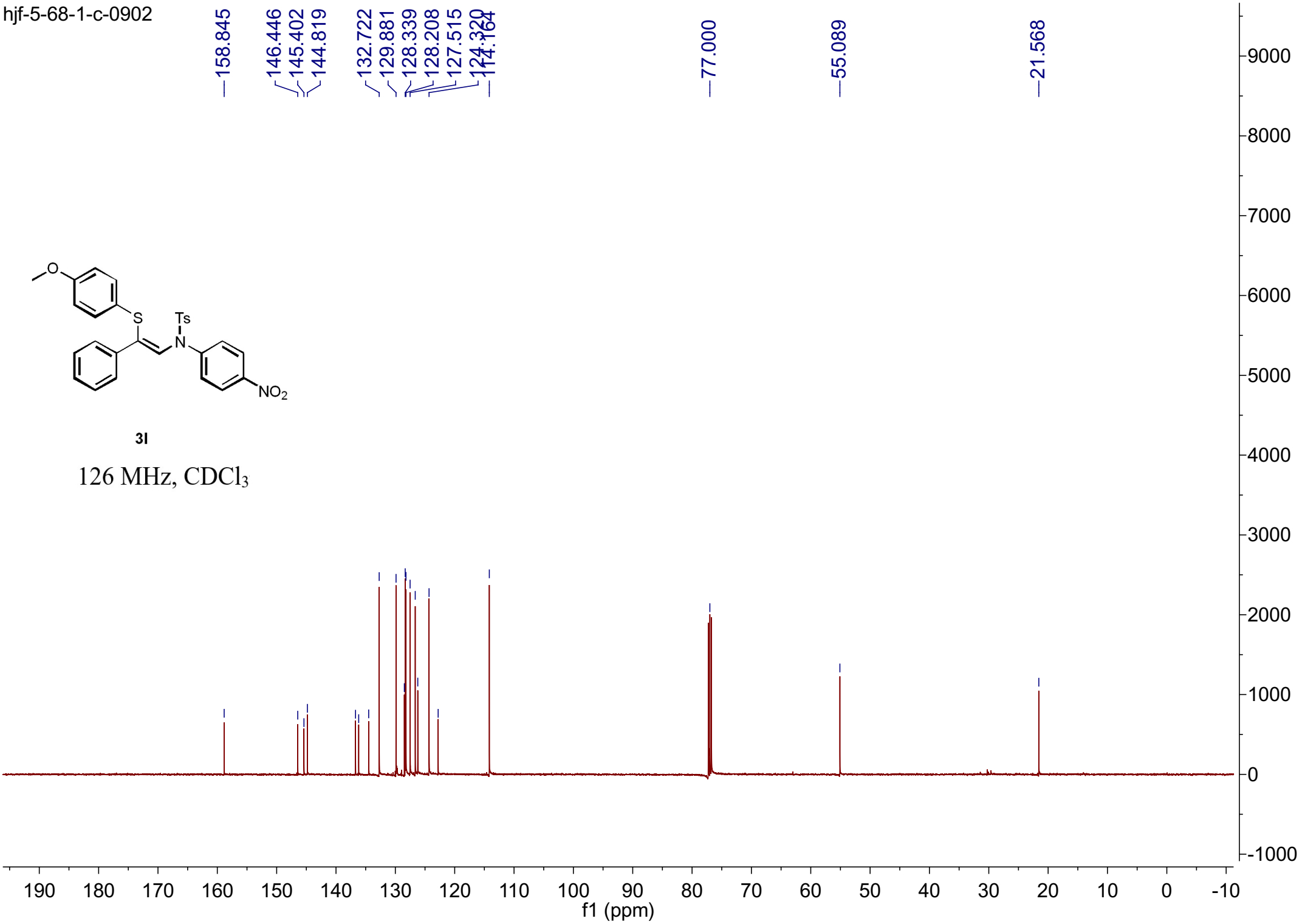
2.00
2.03
4.03
2.16
3.23
0.98
2.09
2.10
3.18
3.23

f1 (ppm)

hjf-5-68-1-c-0902

3l

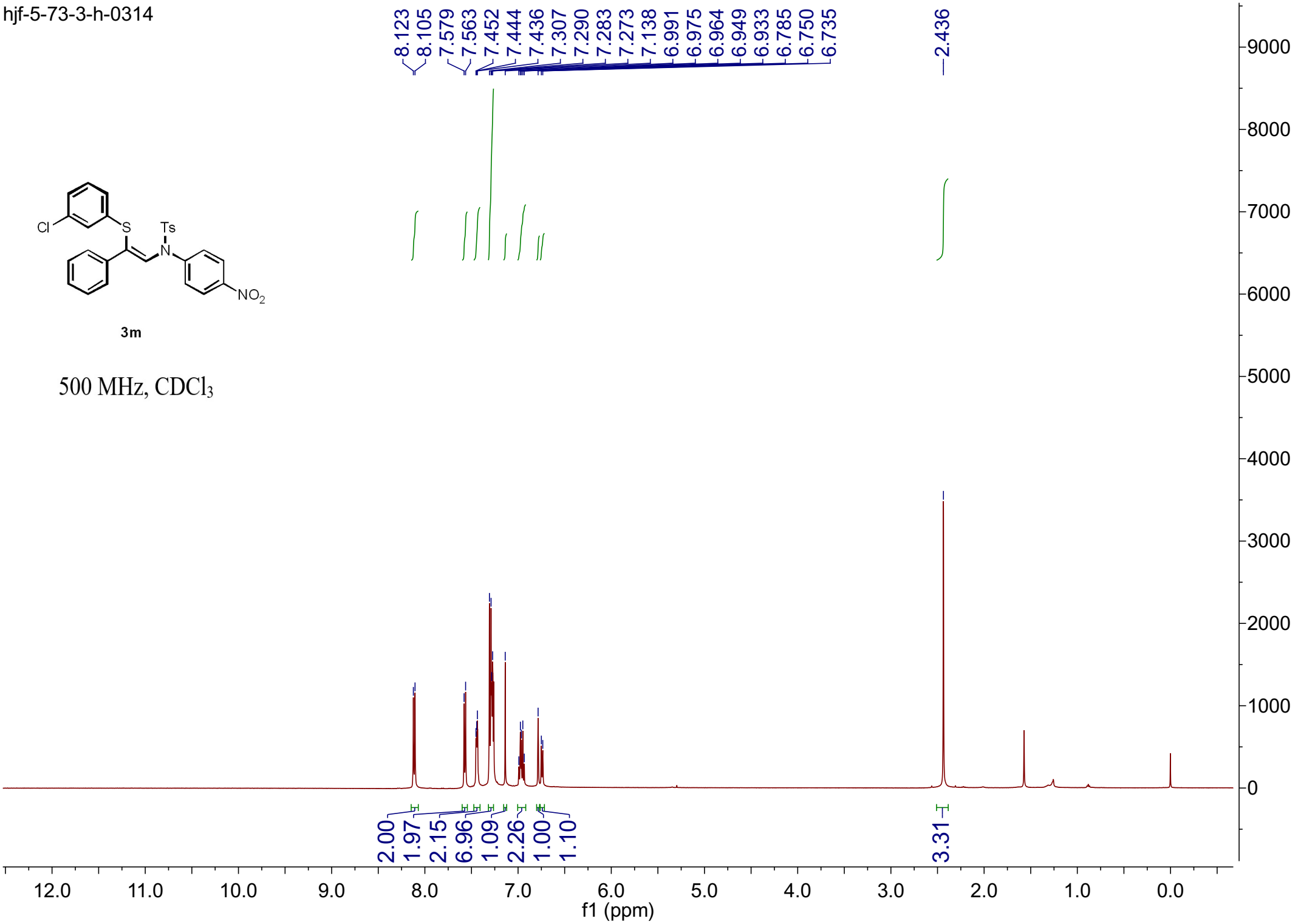
126 MHz, $CDCl_3$



hjf-5-73-3-h-0314

3m

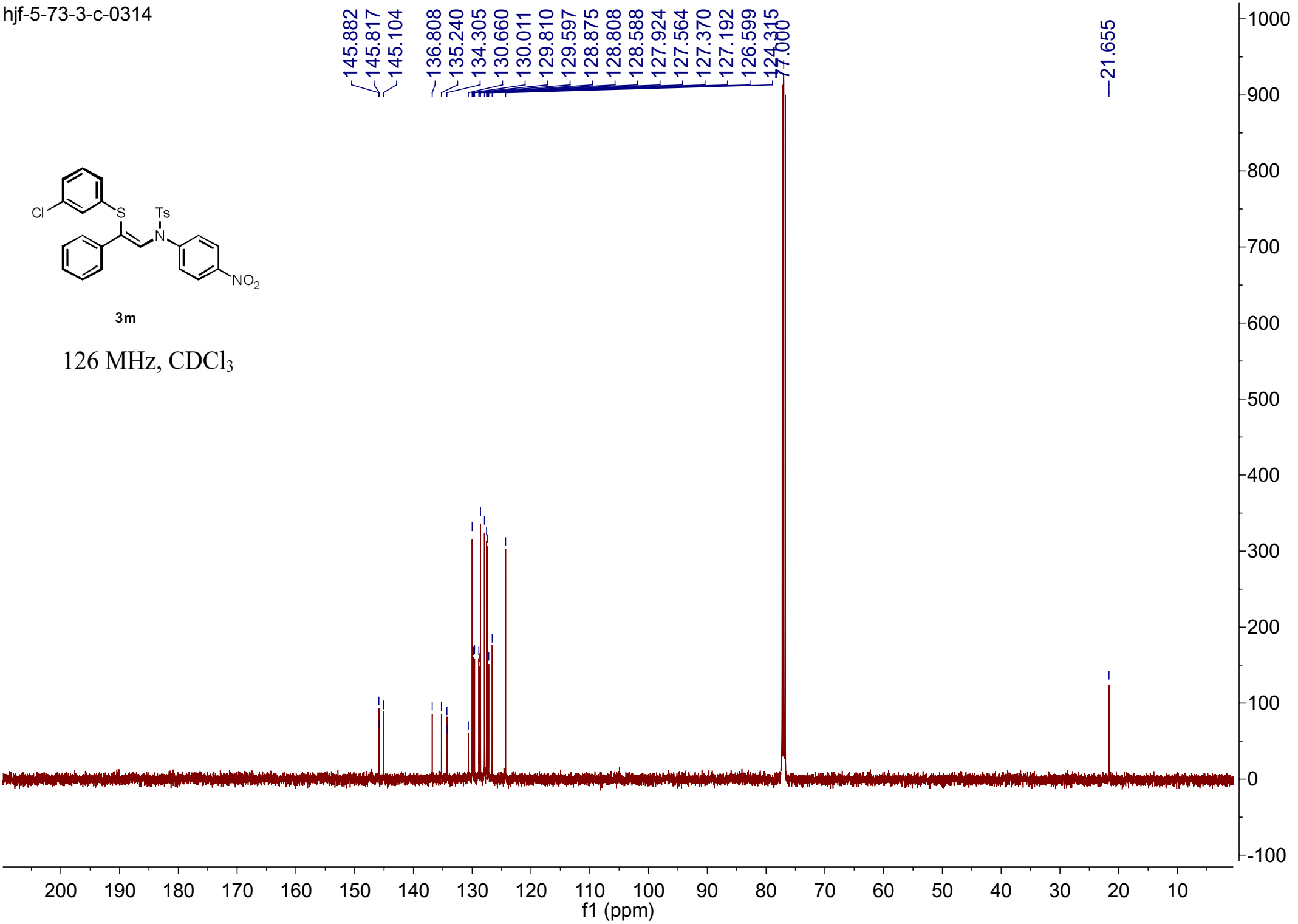
500 MHz, $CDCl_3$



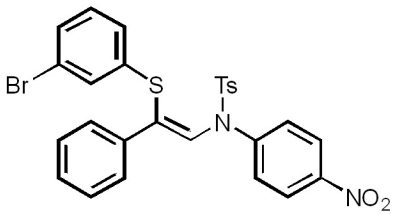
hjf-5-73-3-c-0314

3m

126 MHz, $CDCl_3$



hjf-5-68-4-h-0314



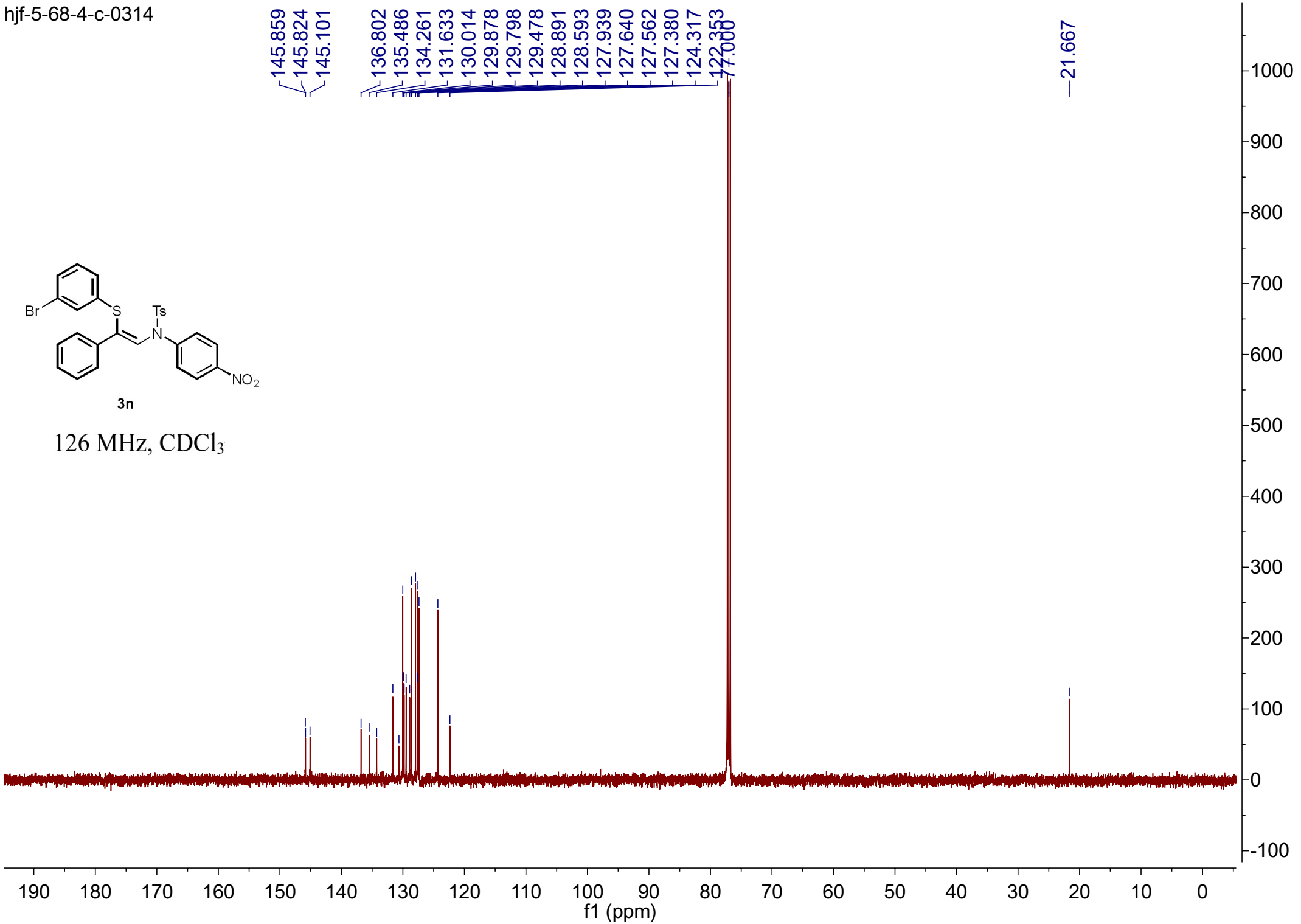
3n

500 MHz, $CDCl_3$

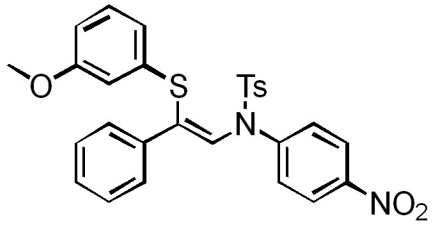
hjf-5-68-4-c-0314

3n

126 MHz, $CDCl_3$

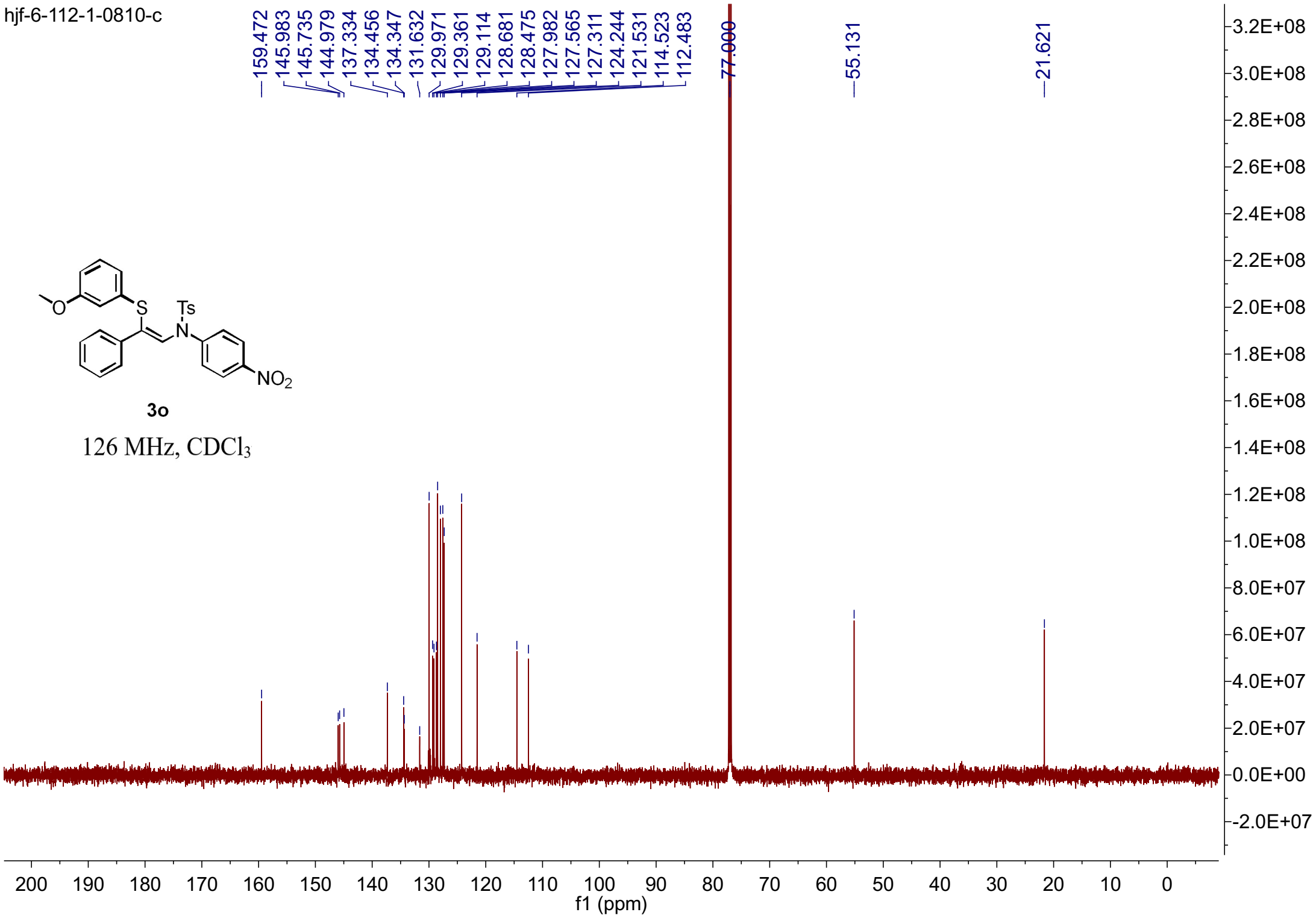


hjf-6-112-1-0810-h

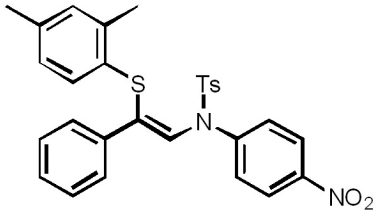


3o

500 MHz, $CDCl_3$


hjf-6-112-1-0810-c
159.472
145.983
145.735
144.979
137.334
134.456
134.347
131.632
129.971
129.361
129.114
128.681
128.475
127.982
127.565
127.311
124.244
121.531
114.523
112.483
77.000
55.131
21.621
O
S
Ts
N
NO2
3o
126 MHz, CDCl3
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

hjf-5-79-1-h



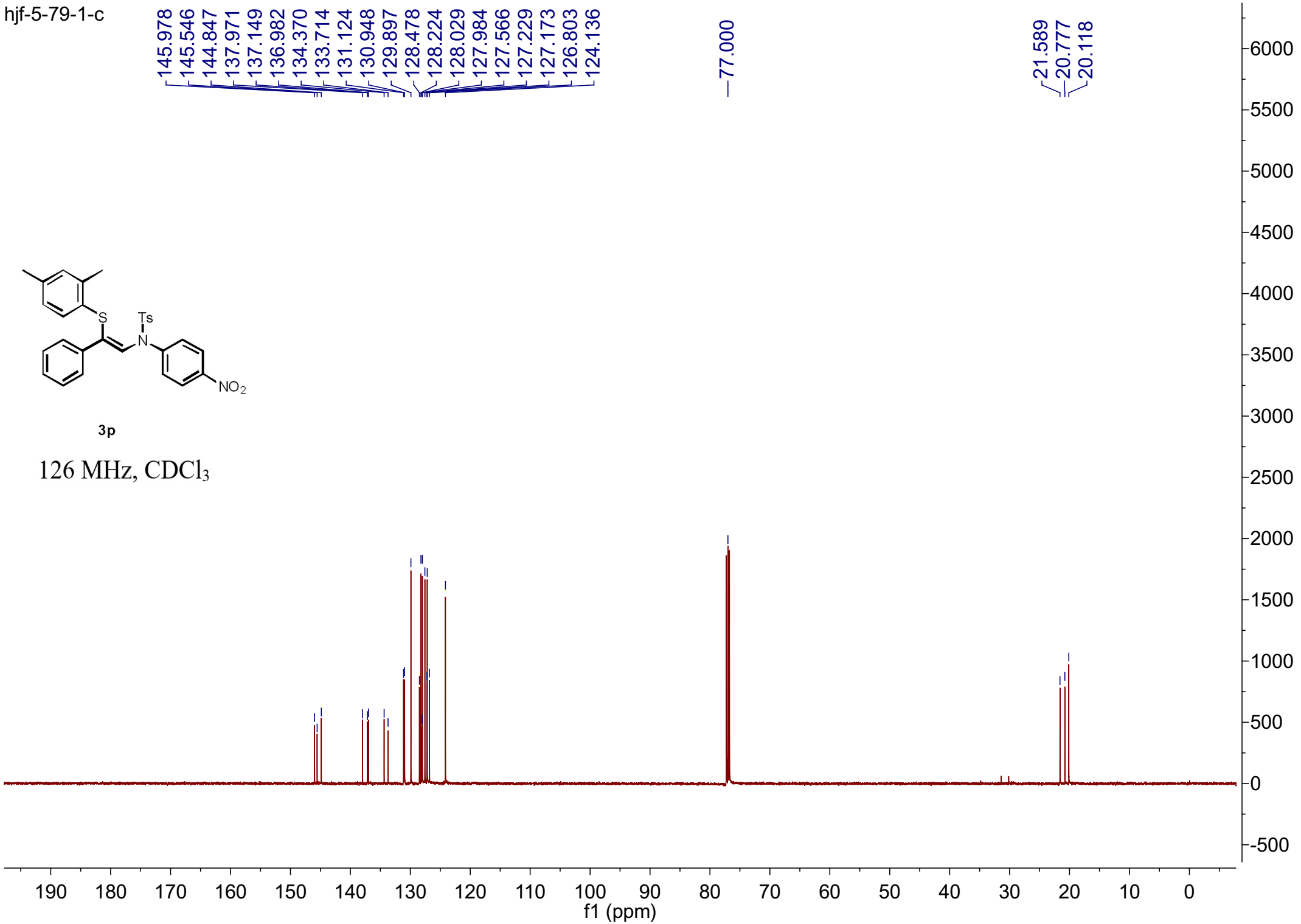
3p

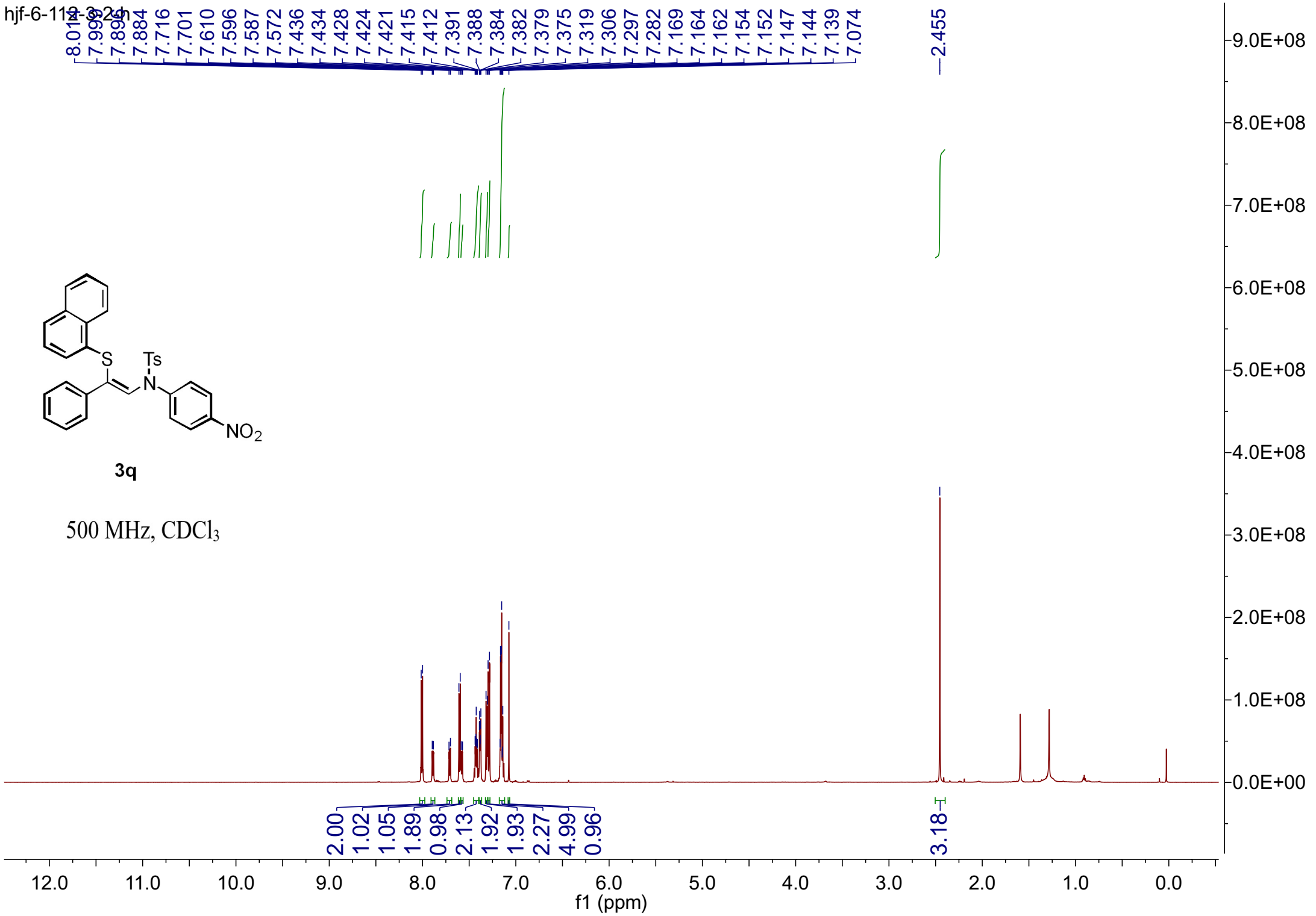
500 MHz, $CDCl_3$

hjf-5-79-1-c

3p

126 MHz, $CDCl_3$

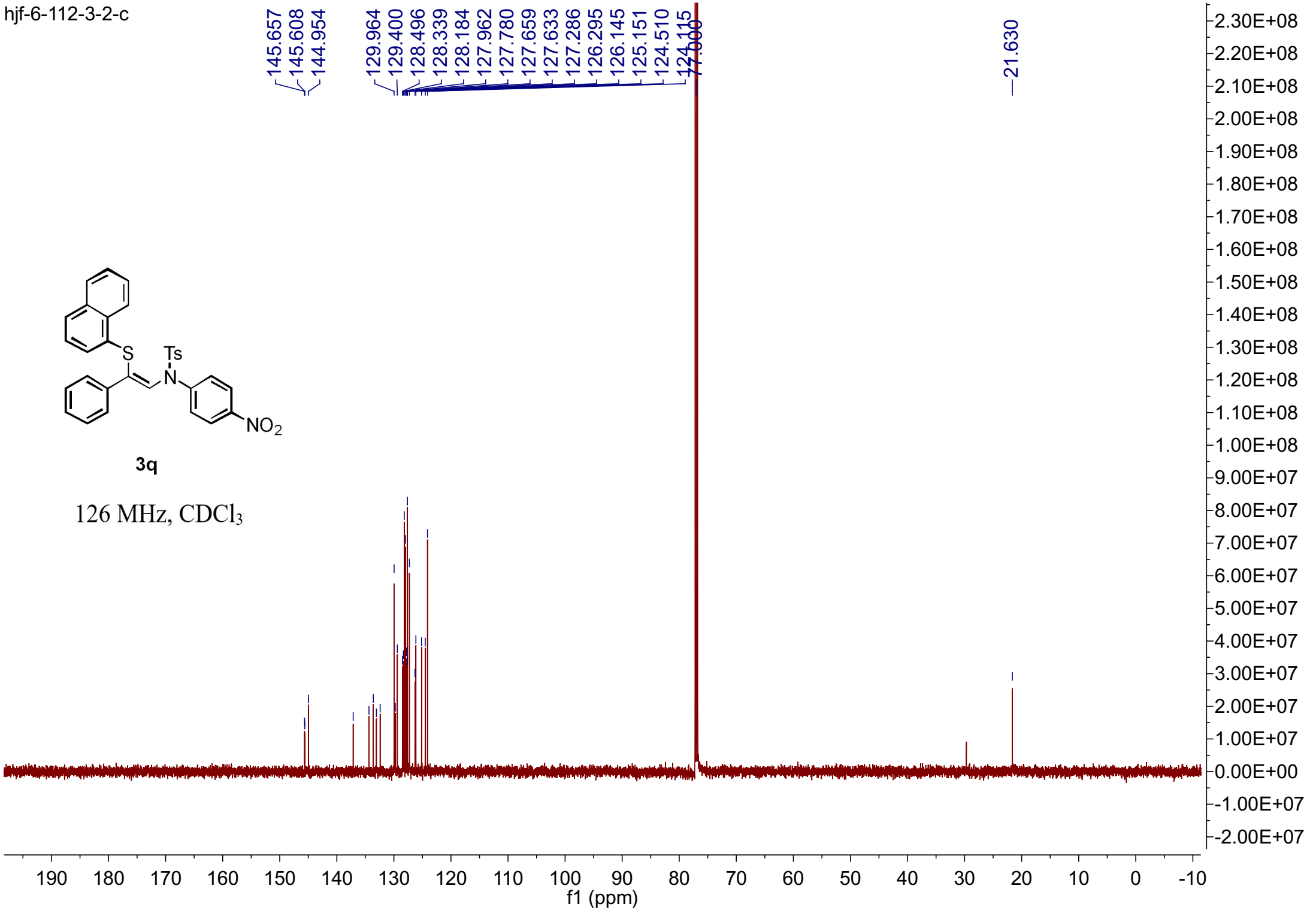



hjf-6-112-3-2-h
8.015
7.999
7.894
7.884
7.716
7.701
7.610
7.596
7.587
7.572
7.436
7.434
7.428
7.424
7.421
7.415
7.412
7.391
7.388
7.384
7.382
7.379
7.375
7.319
7.306
7.297
7.282
7.169
7.164
7.162
7.154
7.152
7.147
7.144
7.139
7.074
2.455
S
Ts
N
NO2
3q
500 MHz, CDCl3
9.0E+08
8.0E+08
7.0E+08
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
2.00
1.02
1.05
1.89
0.98
2.13
1.92
1.93
2.27
4.99
0.96
3.18
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

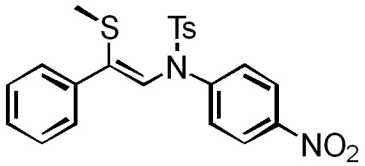
hjf-6-112-3-2-c

3q

126 MHz, $CDCl_3$



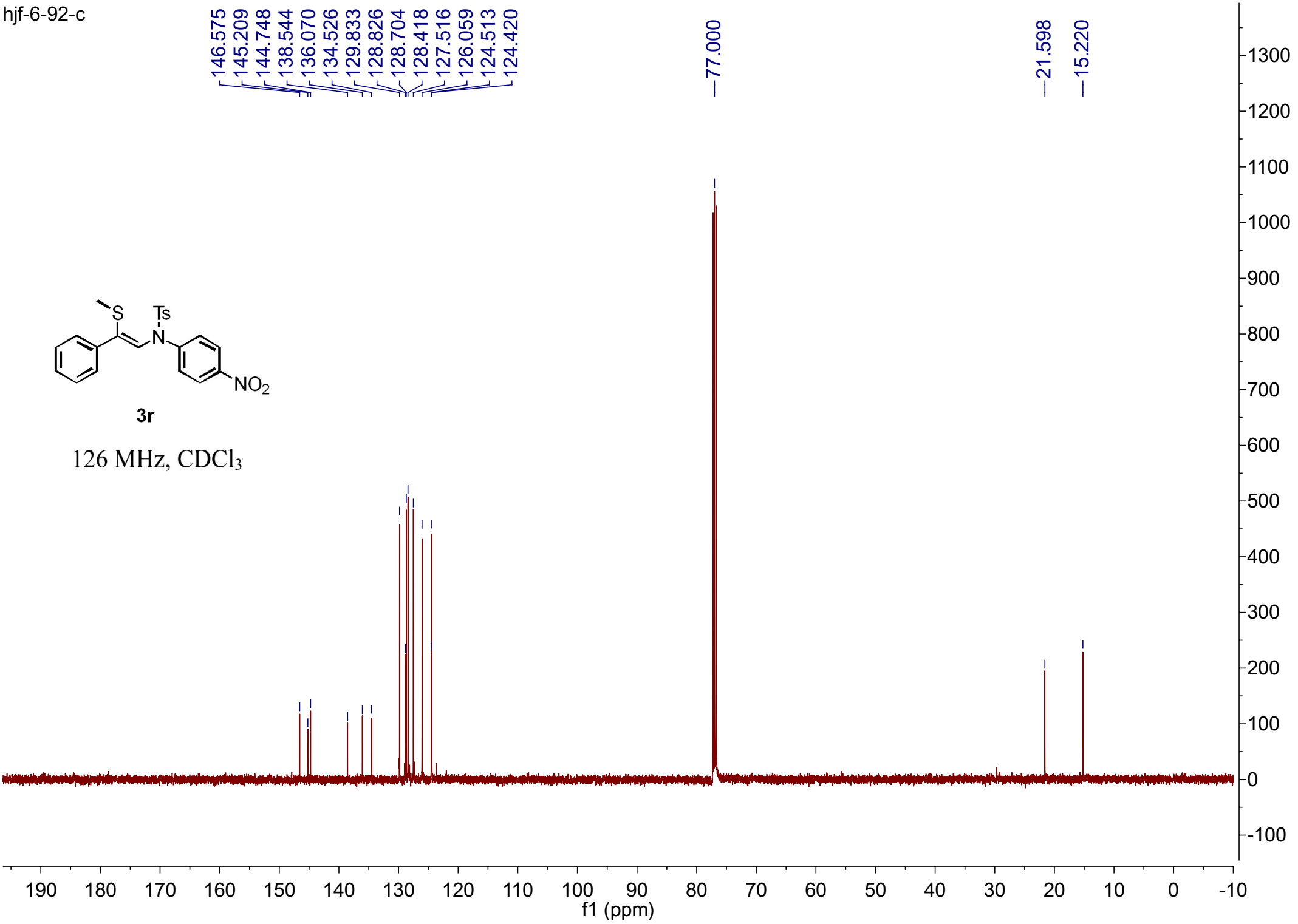
hjf-6-92-h



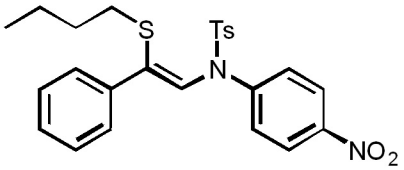
3r

500 MHz, $CDCl_3$

hjf-6-92-c

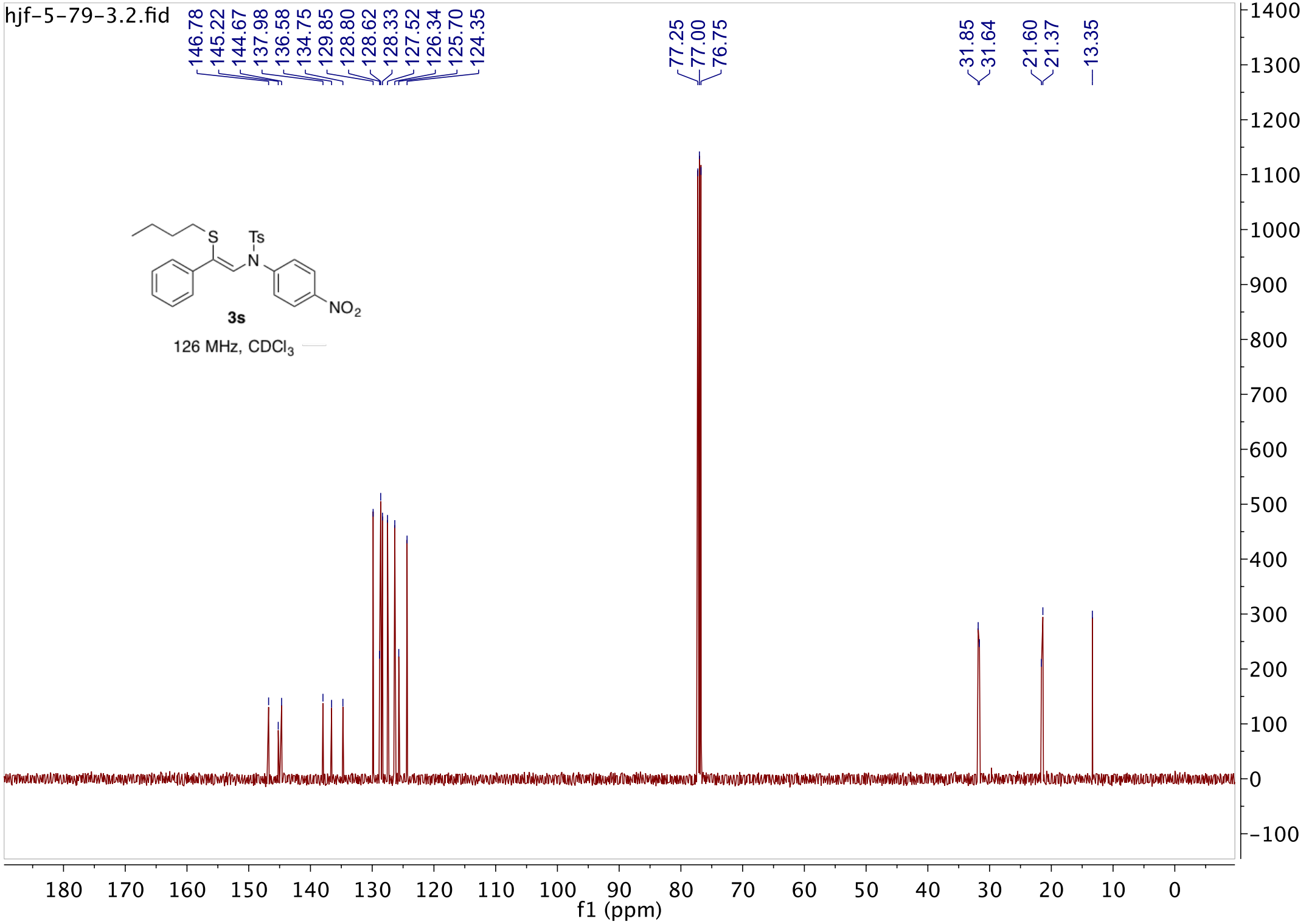

146.575
145.209
144.748
138.544
136.070
134.526
129.833
128.826
128.704
128.418
127.516
126.059
124.513
124.420
77.000
21.598
15.220
S
Ts
N
NO2
3r
126 MHz, CDCl3
f1 (ppm)

hjf-5-79-3-h-1229

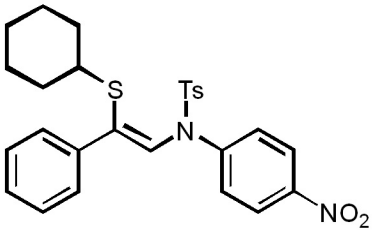


3s

500 MHz, $CDCl_3$


hjf-5-79-3.2.fid
146.78
145.22
144.67
137.98
136.58
134.75
129.85
128.80
128.62
128.33
127.52
126.34
125.70
124.35
77.25
77.00
76.75
31.85
31.64
21.60
21.37
13.35
S
Ts
N
NO2
3s
126 MHz, CDCl3
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

hjf-5-79-2-h-1228



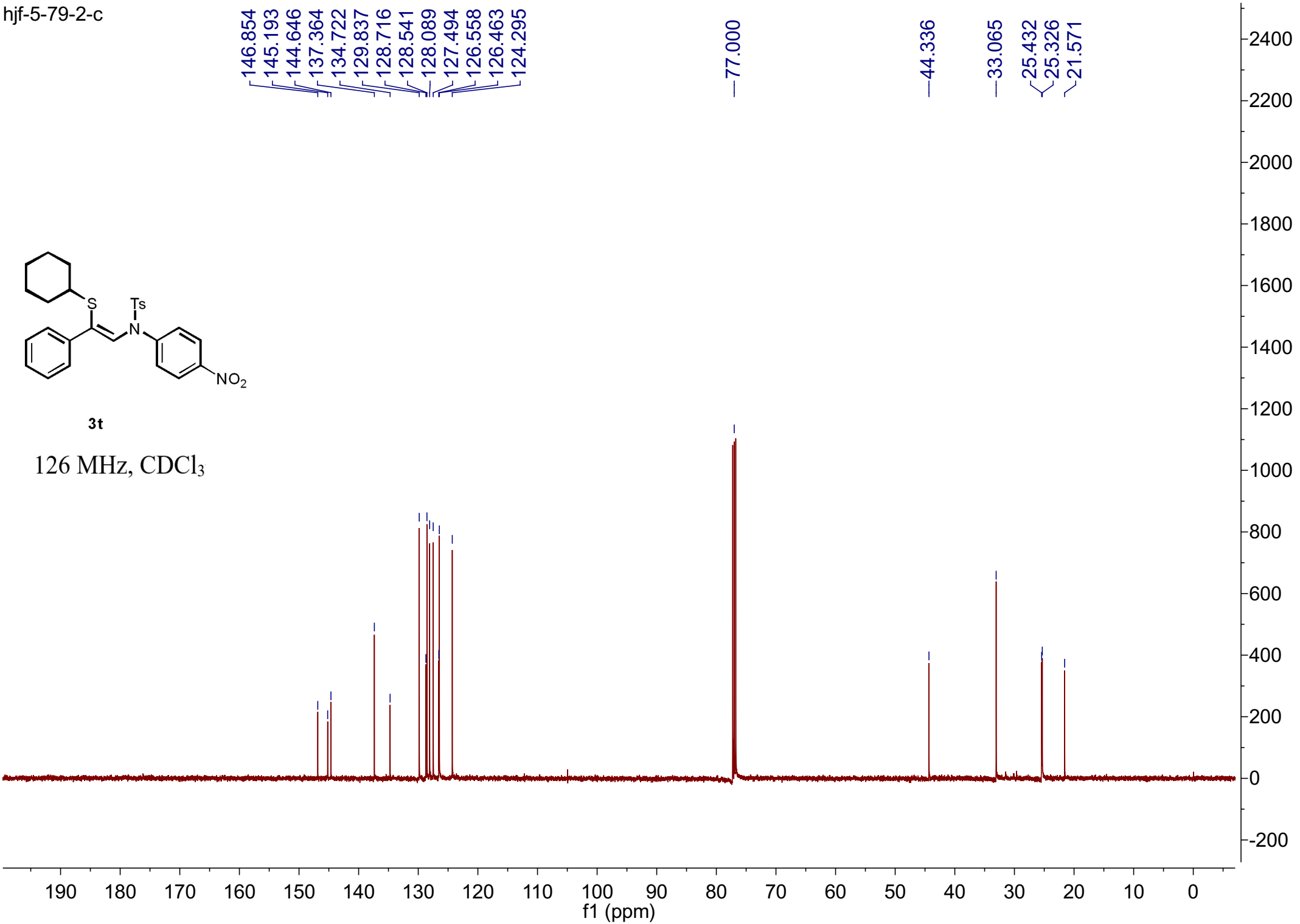
3t

500 MHz, $CDCl_3$

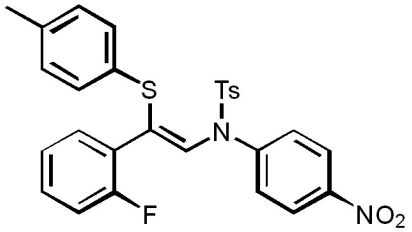
hjf-5-79-2-c

3t

126 MHz, $CDCl_3$



hjf-5-40-1-h-0915



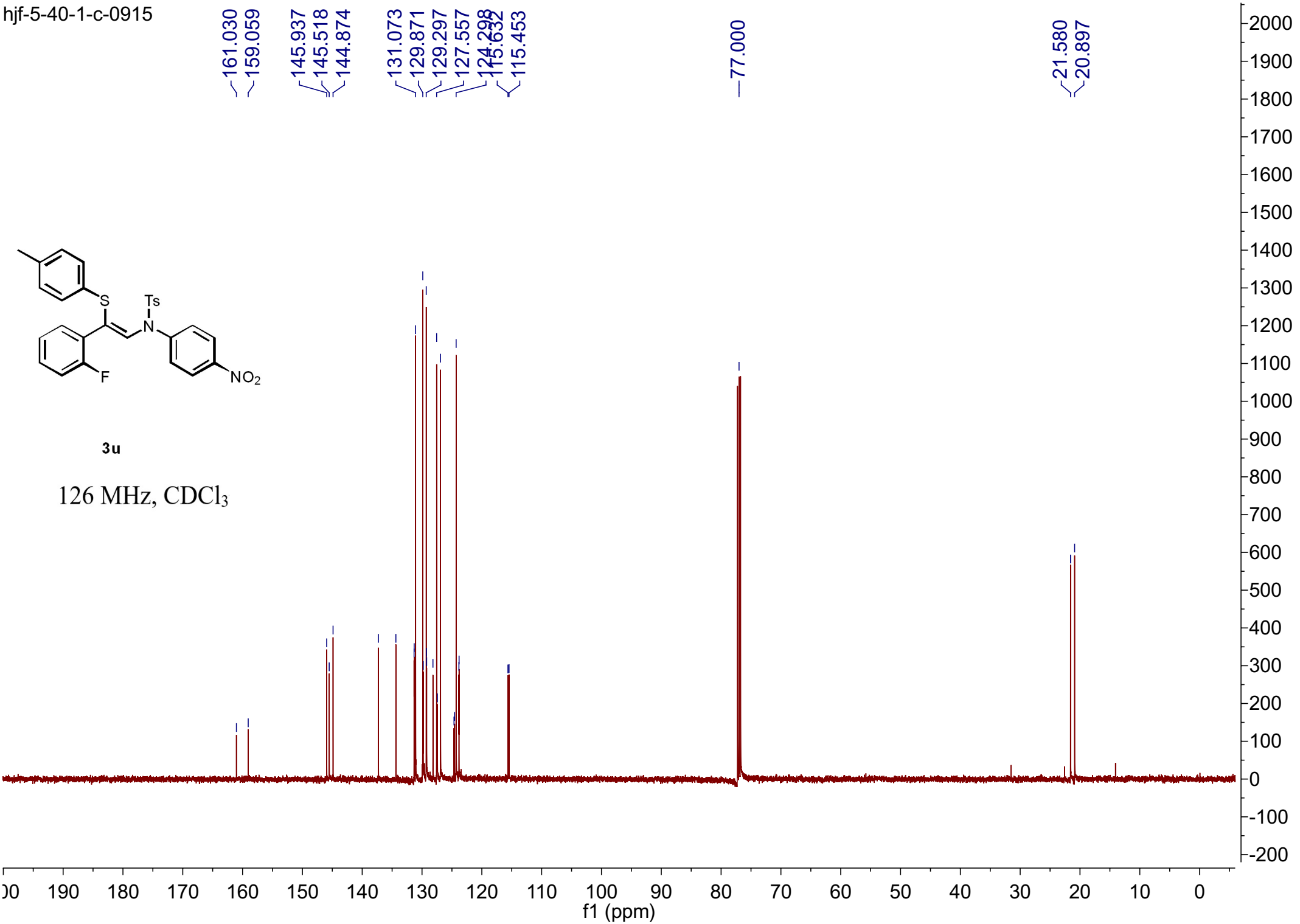
3u

500 MHz, $CDCl_3$

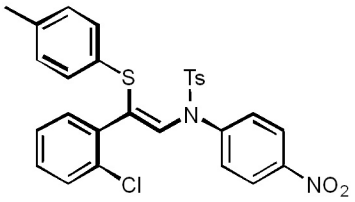
hjf-5-40-1-c-0915

3u

126 MHz, $CDCl_3$



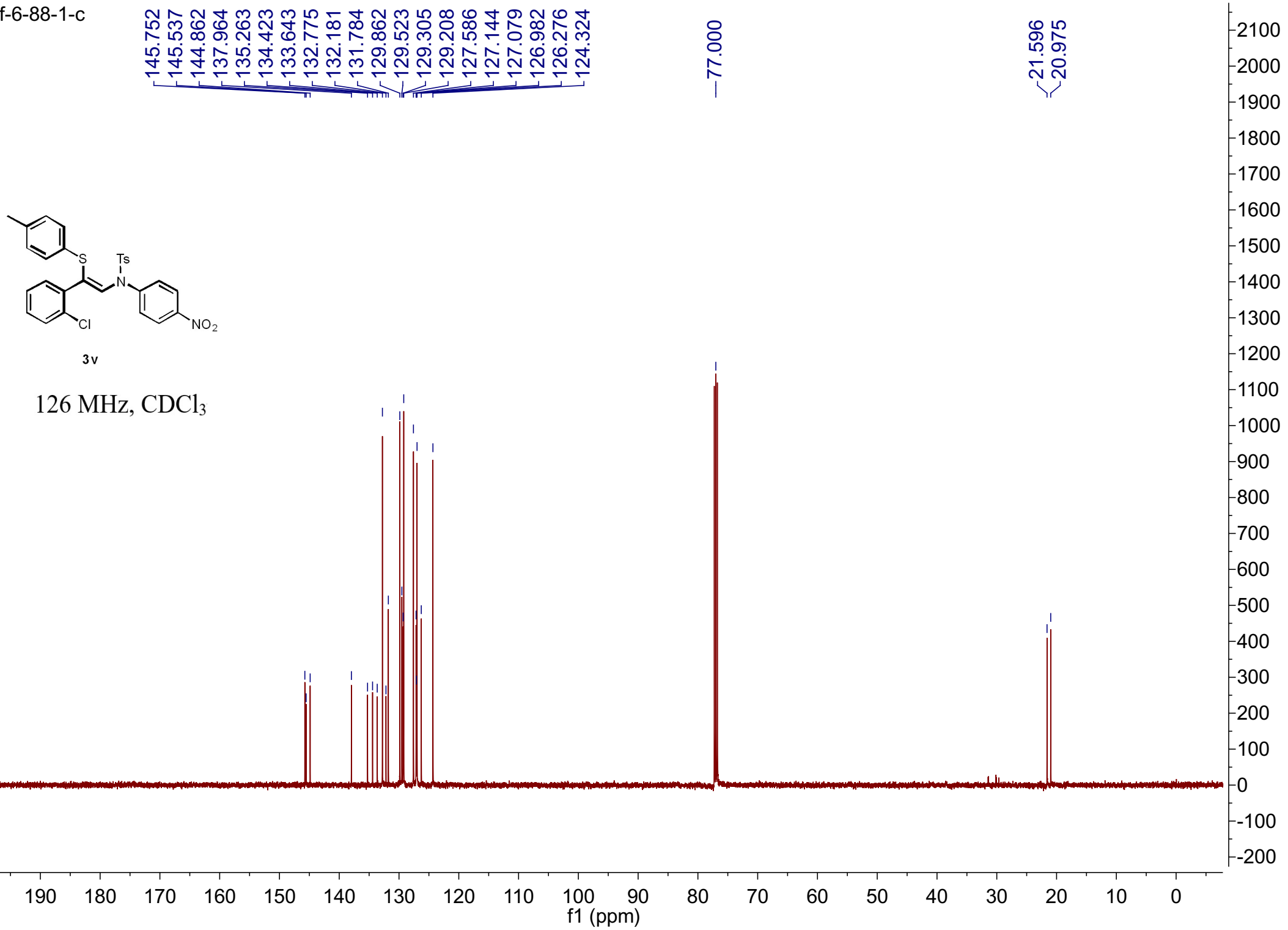
hjf-6-88-1-h



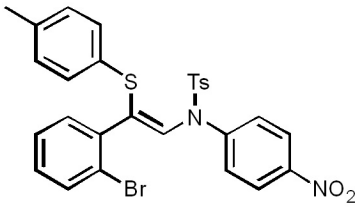
3v

500 MHz, $CDCl_3$

hjf-6-88-1-c


145.752
145.537
144.862
137.964
135.263
134.423
133.643
132.775
132.181
131.784
129.862
129.523
129.305
129.208
127.586
127.144
127.079
126.982
126.276
124.324
77.000
21.596
20.975
S
Ts
N
Cl
NO2
3v
126 MHz, CDCl3
f1 (ppm)

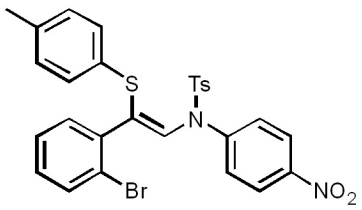
hjf-6-88-2-h



3w

500 MHz, $CDCl_3$

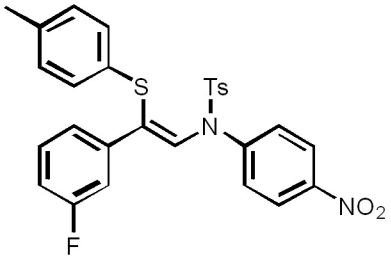
hjf-6-88-2-c



3w

126 MHz, $CDCl_3$

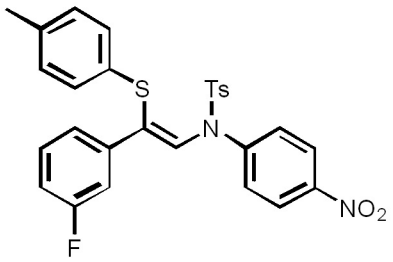
hjf-5-42-1-h-0915



3x

500 MHz, $CDCl_3$

hjf-5-42-1-c-0915



3x

126 MHz, $CDCl_3$

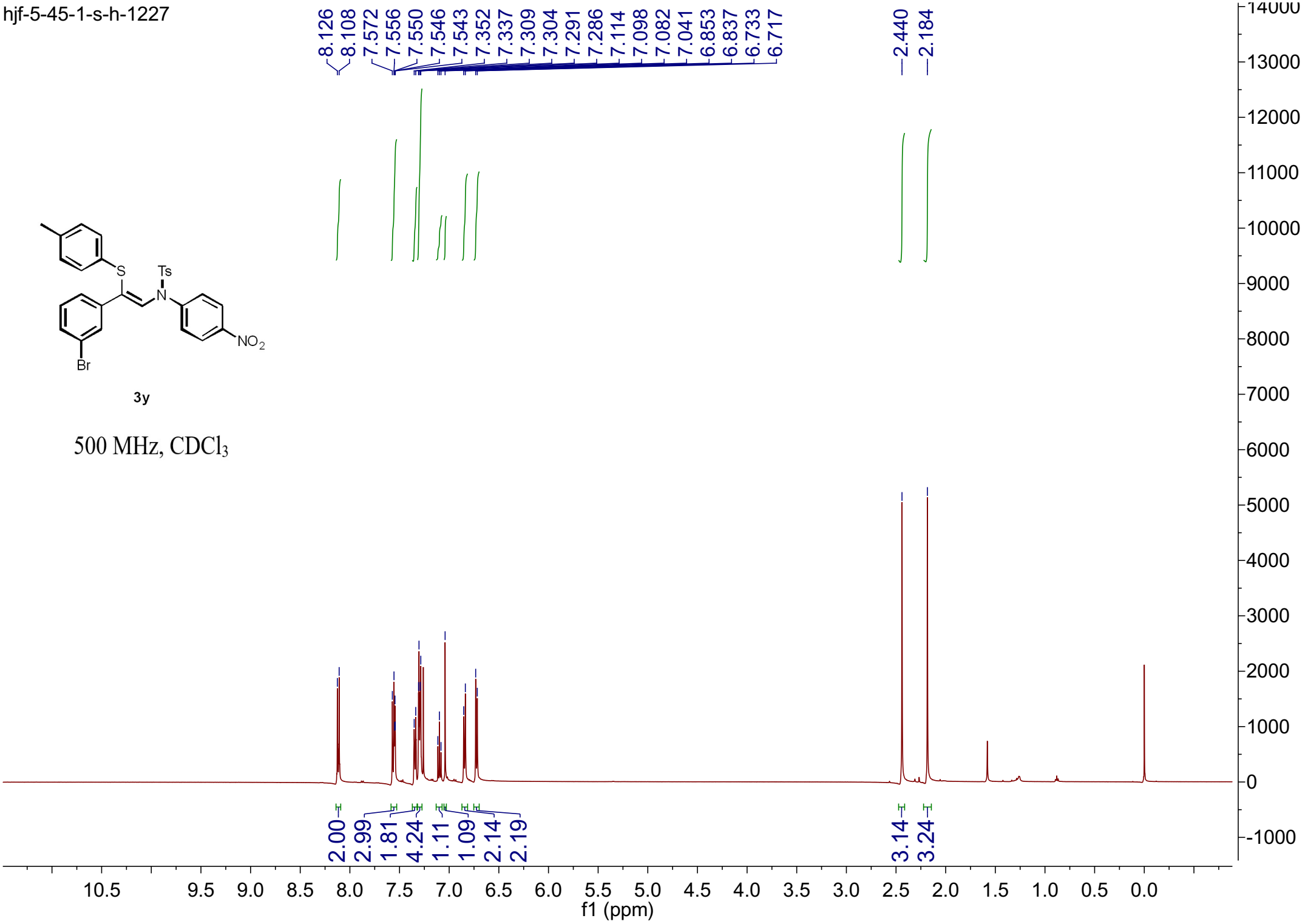
163.558
161.599
145.046
136.843
134.366
129.997
129.775
129.480
129.034
127.551
127.392
124.301
115.469
115.299
115.115
114.934
77.000
21.637
20.911

f1 (ppm)

hjf-5-45-1-s-h-1227

3y

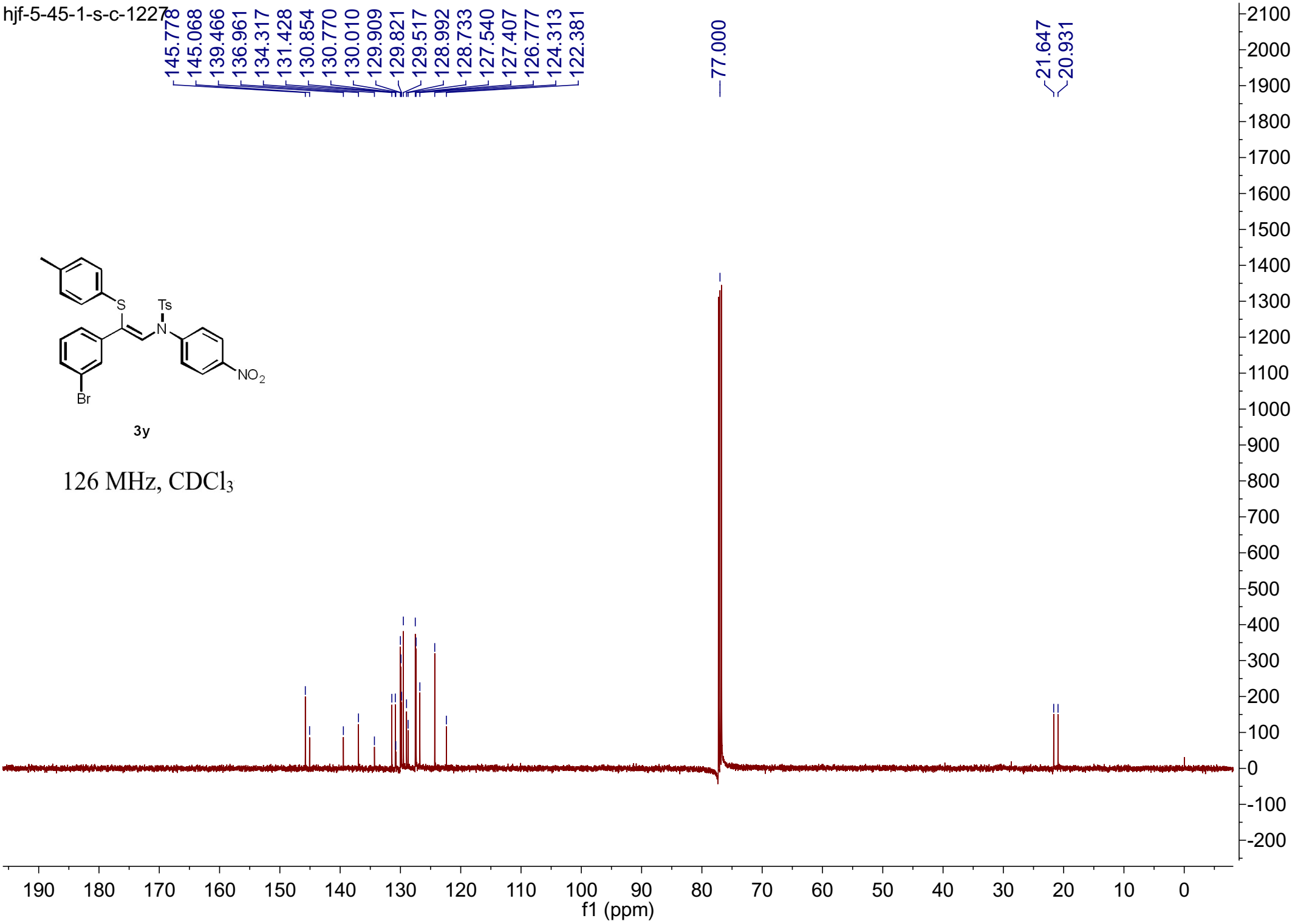
500 MHz, $CDCl_3$



hjf-5-45-1-s-c-1227

3y

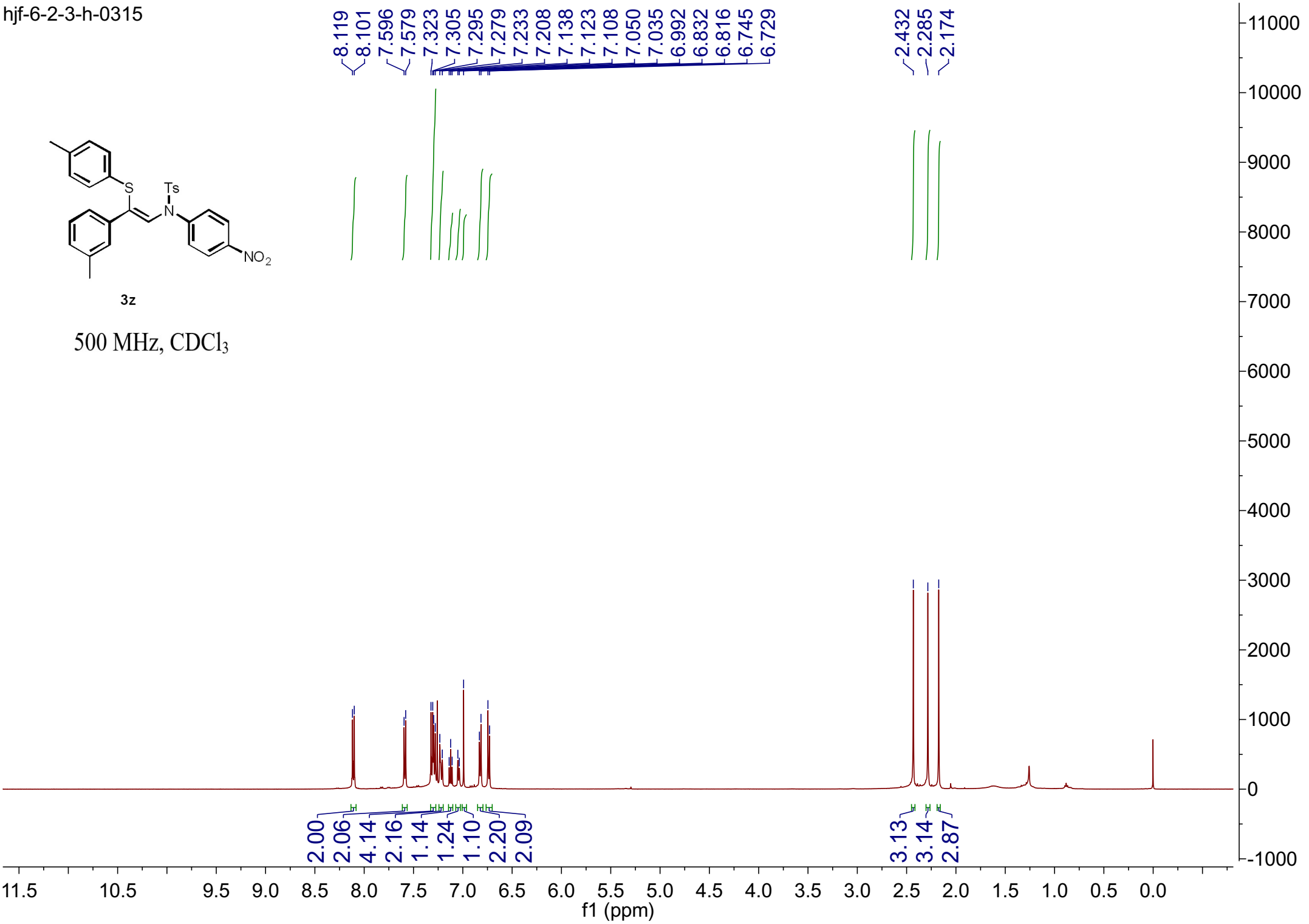
126 MHz, $CDCl_3$

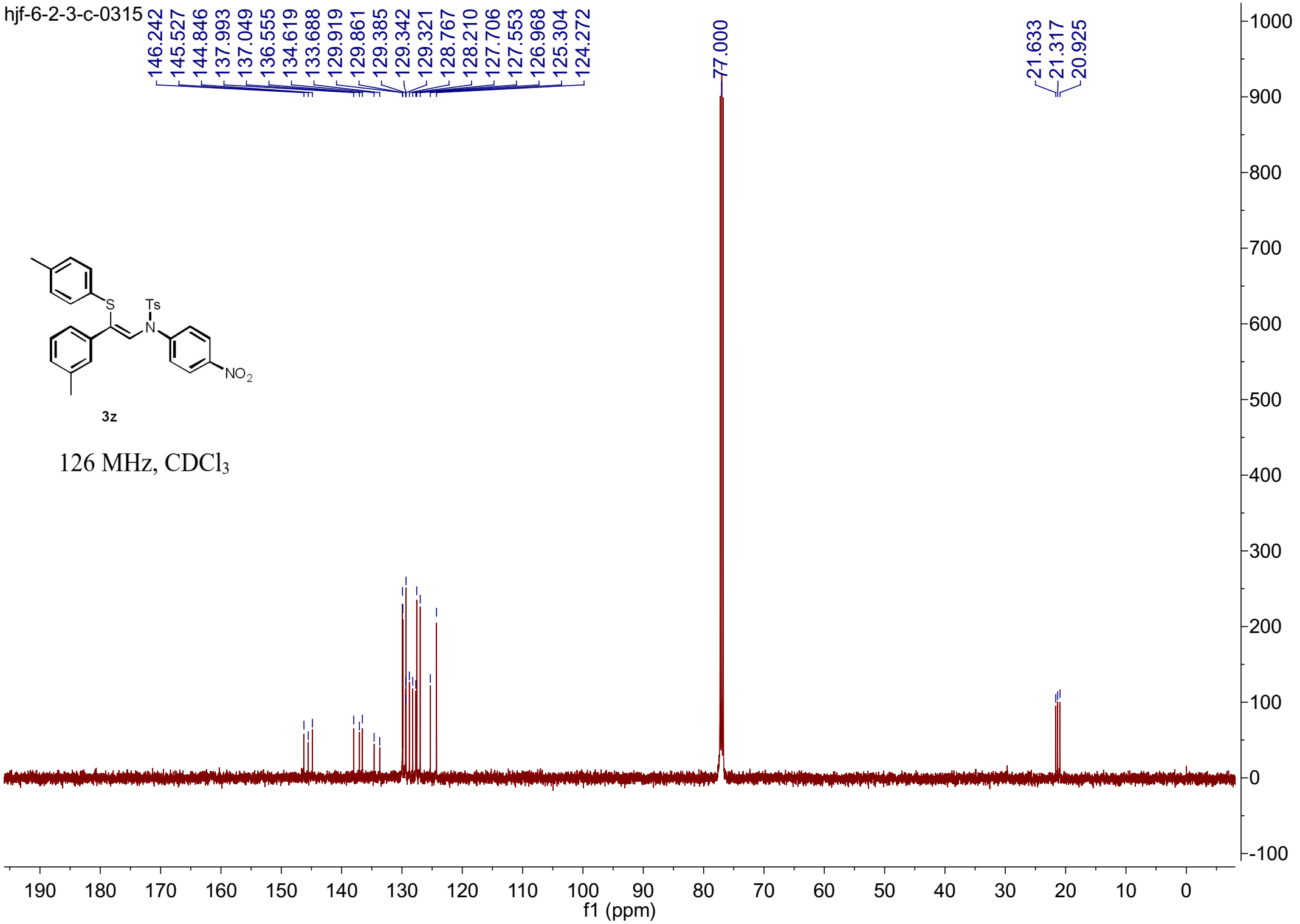


hjf-6-2-3-h-0315

3z

500 MHz, $CDCl_3$

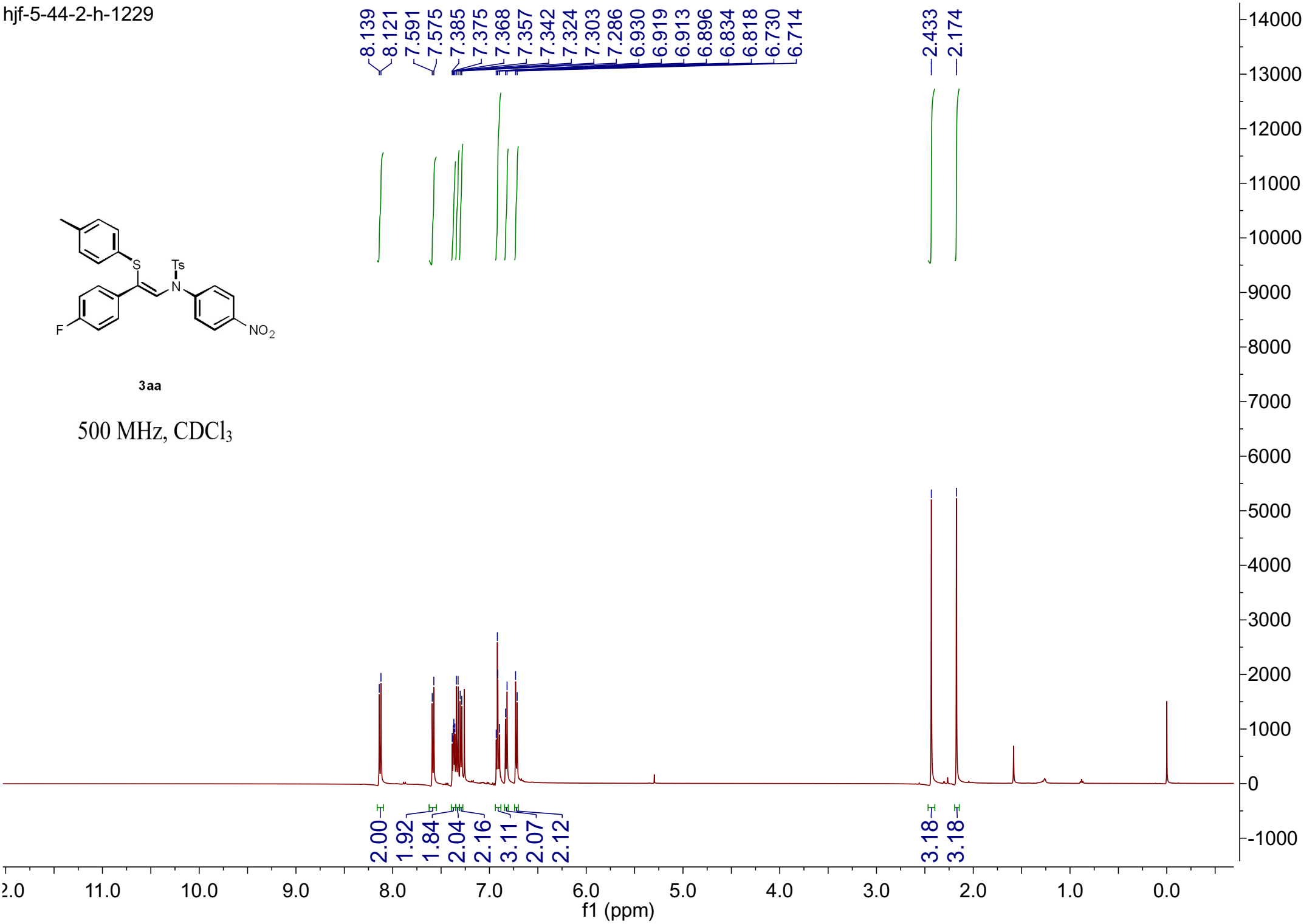



hjf-6-2-3-c-0315
146.242
145.527
144.846
137.993
137.049
136.555
134.619
133.688
129.919
129.861
129.385
129.342
129.321
128.767
128.210
127.706
127.553
126.968
125.304
124.272
77.000
21.633
21.317
20.925
S
Ts
N
NO2
3z
126 MHz, CDCl3
f1 (ppm)

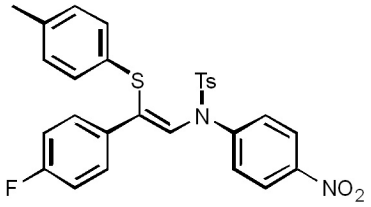
hjf-5-44-2-h-1229

3aa

500 MHz, $CDCl_3$



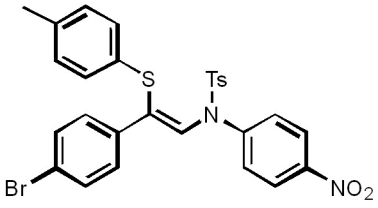
hjf-5-44-2-c-1229



3aa

126 MHz, $CDCl_3$

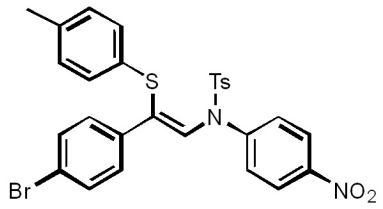
hjf-5-38-2-h-0915



3ab

500 MHz, $CDCl_3$

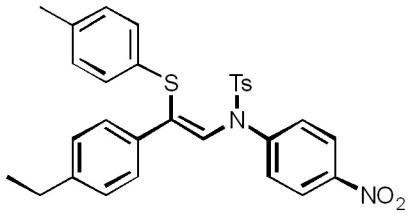
hjf-5-38-2-c-0915



3ab

126 MHz, $CDCl_3$

hjf-5-40-2-h-0817

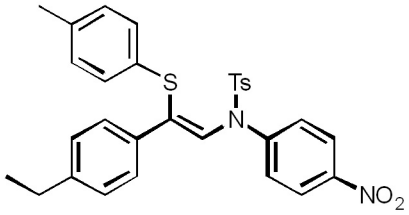


3ac

500 MHz, $CDCl_3$

f1 (ppm)

hjf-5-40-2-c-0817



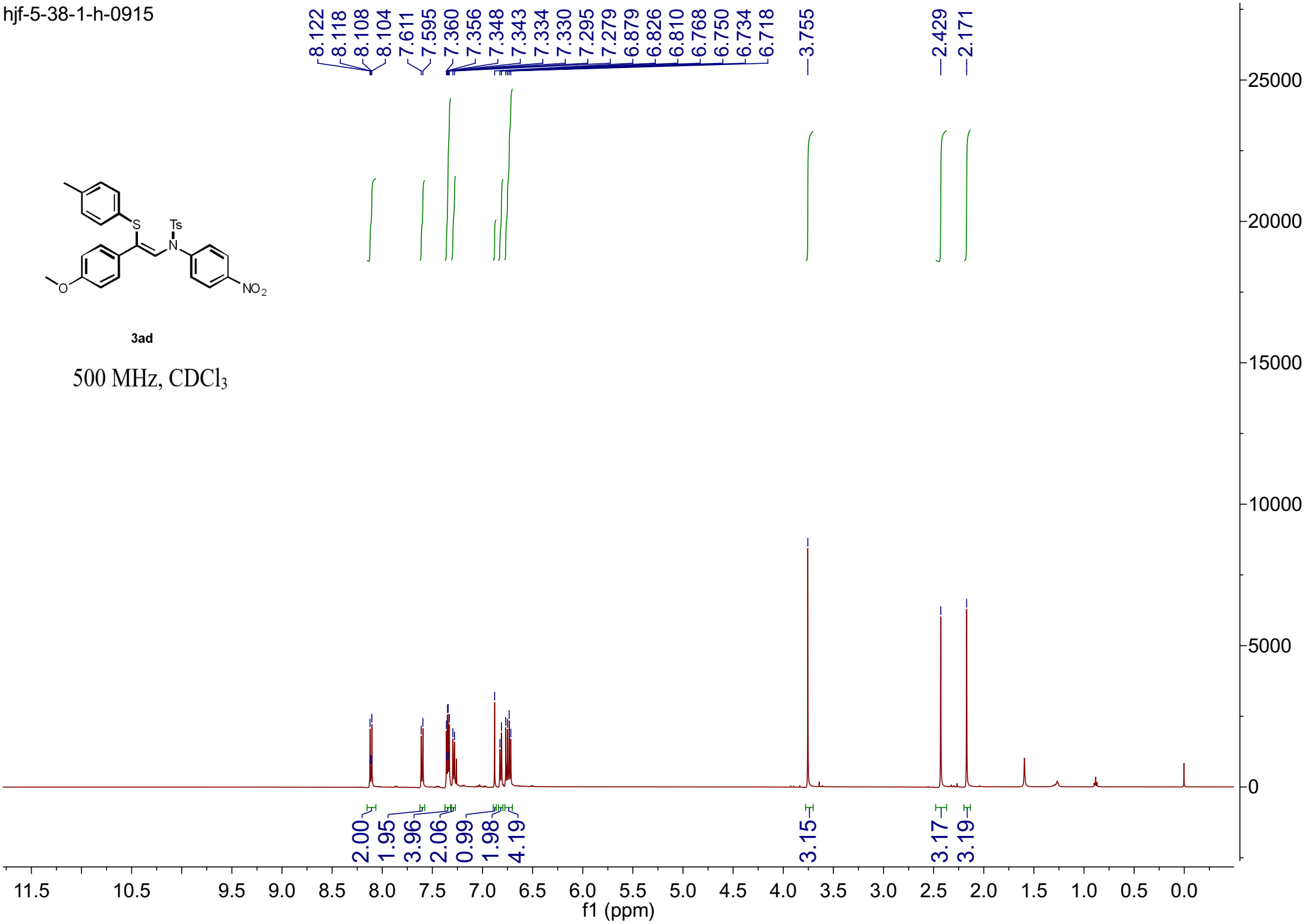
3ac

126 MHz, $CDCl_3$

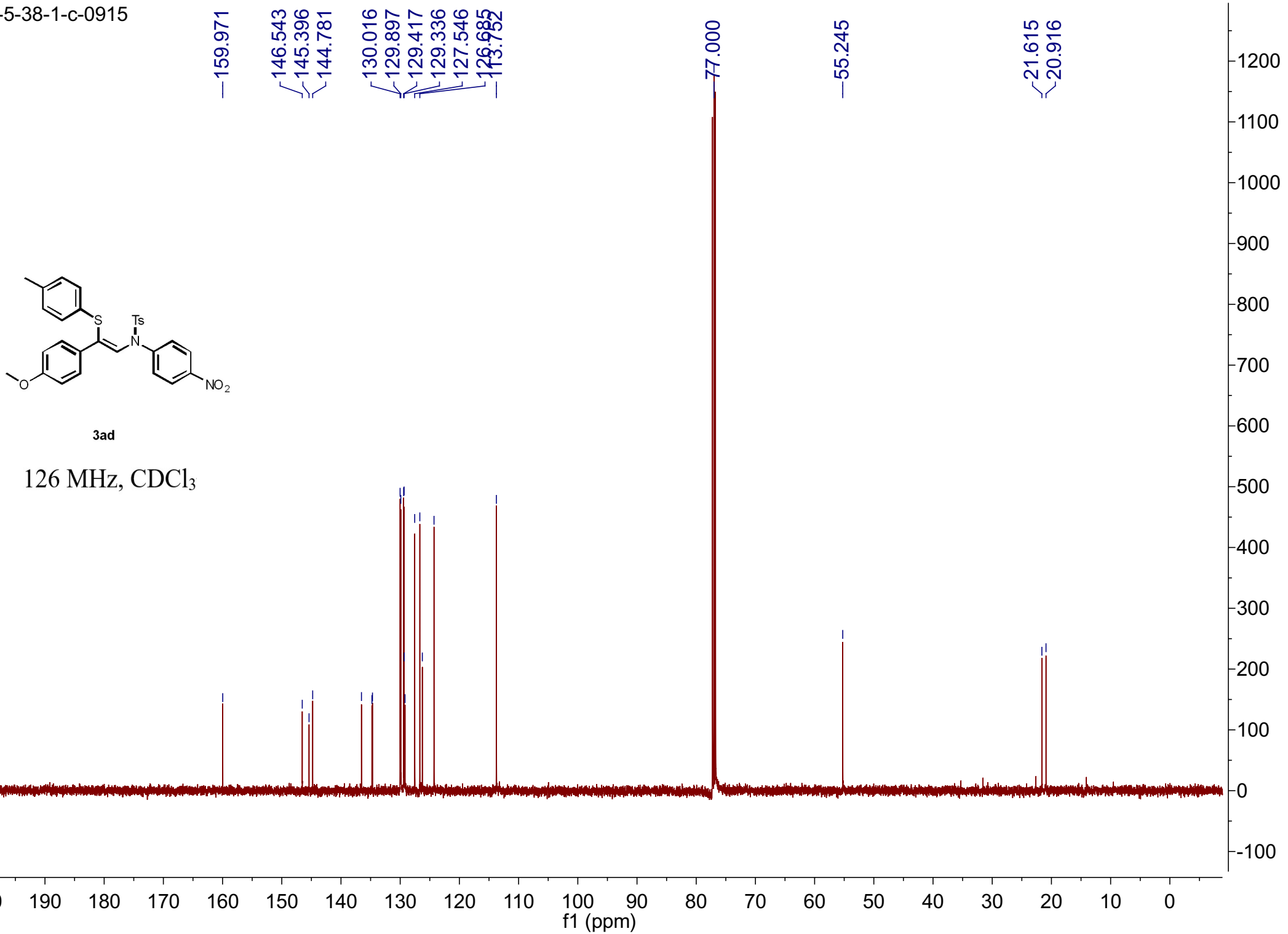
hjf-5-38-1-h-0915

3ad

500 MHz, $CDCl_3$



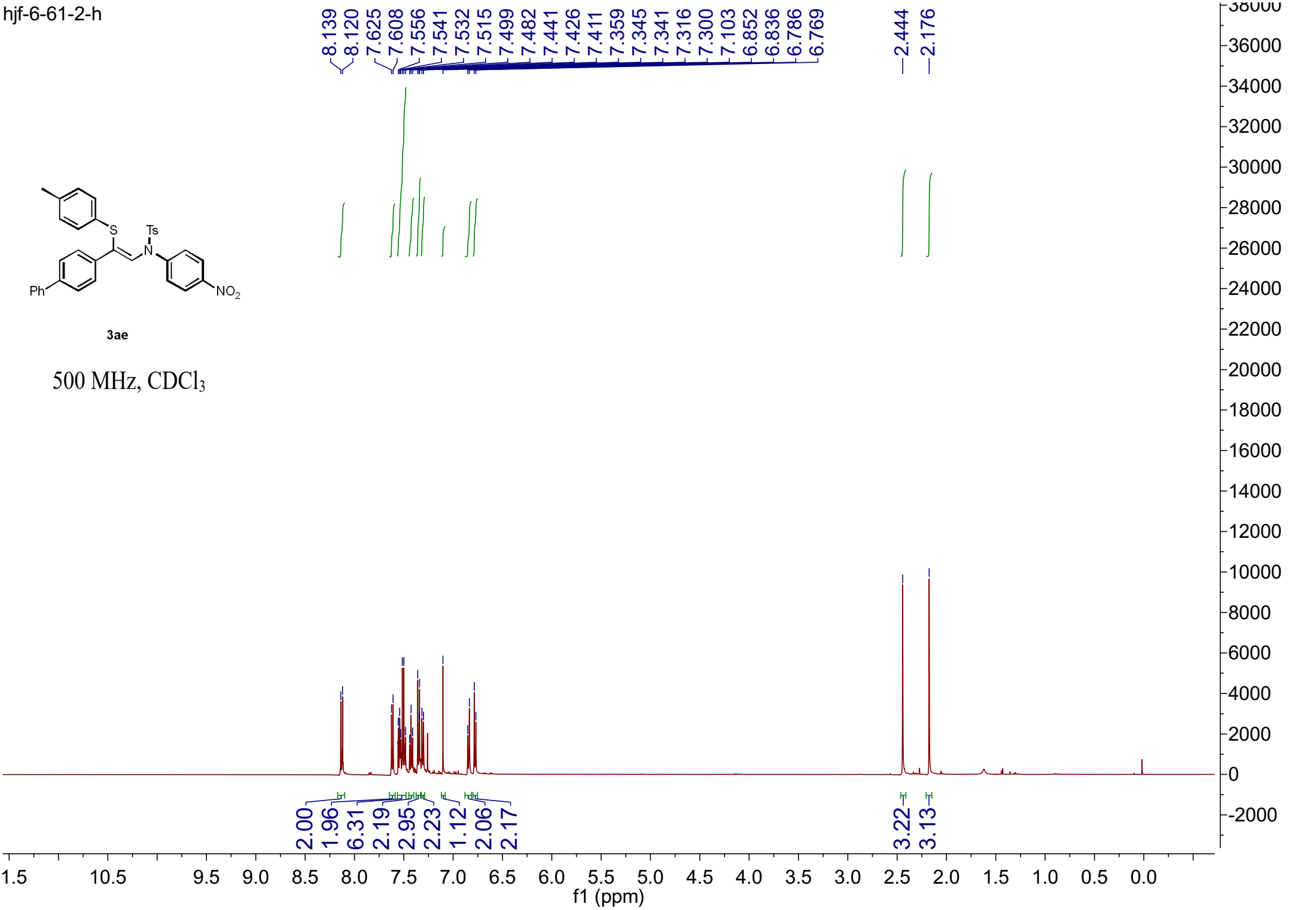
hjf-5-38-1-c-0915



hjf-6-61-2-h

3ae

500 MHz, $CDCl_3$

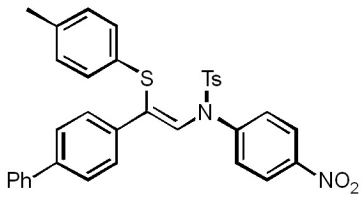


hjf-6-61-2-c

146.193
145.584
144.906
141.254
140.047
136.587
136.078
134.517
132.820
129.946
129.730
129.412
129.295
128.779
128.470
128.066
127.550
127.094
126.960
126.859
124.277

77.000

21.608
20.887

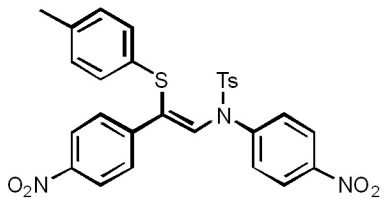


3ae

126 MHz, $CDCl_3$

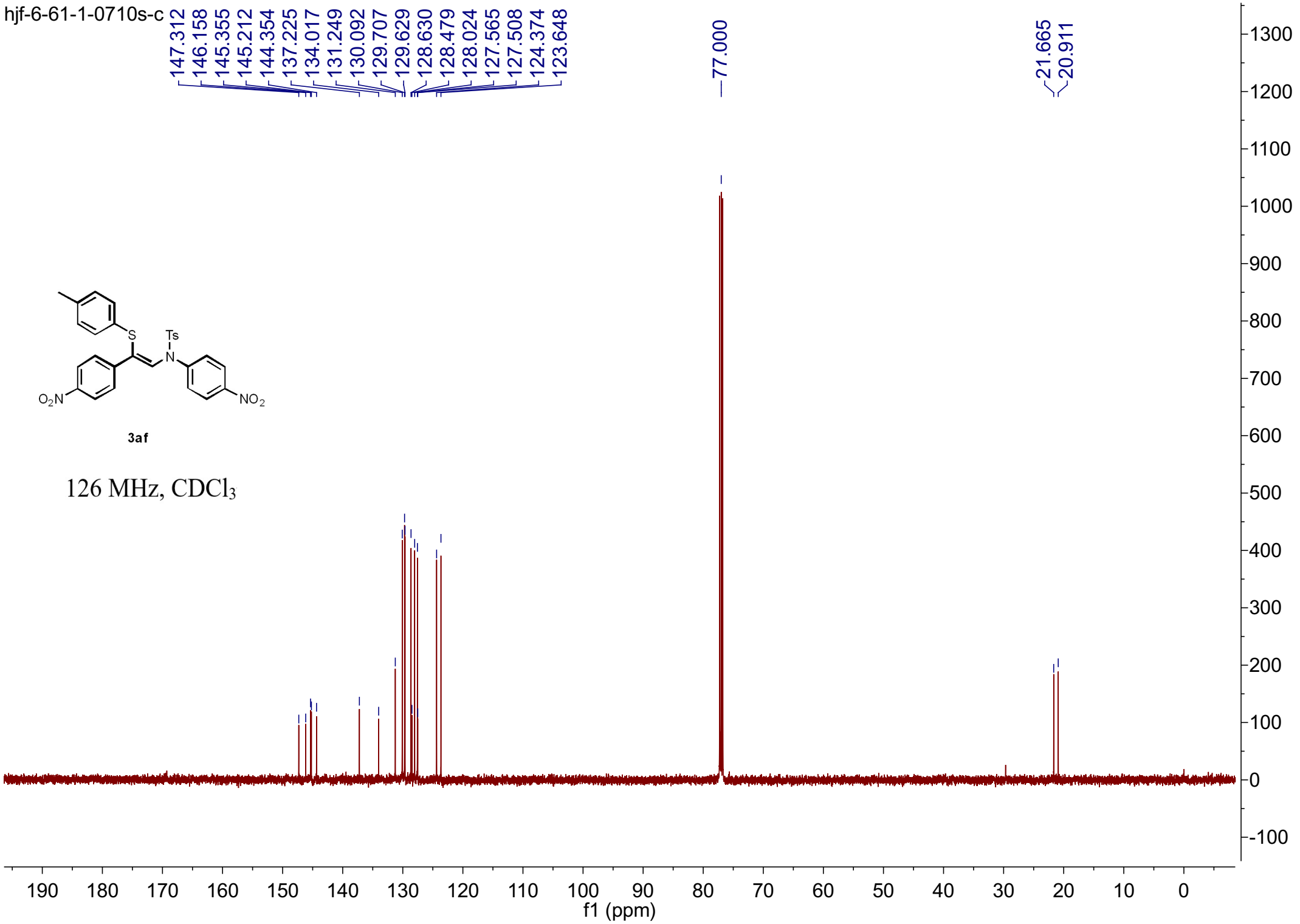
f1 (ppm)

hjf-6-61-1-0710s-h

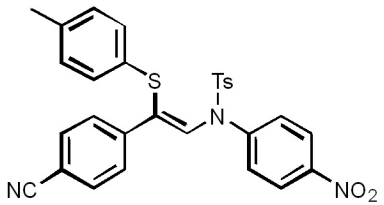


3af

500 MHz, $CDCl_3$

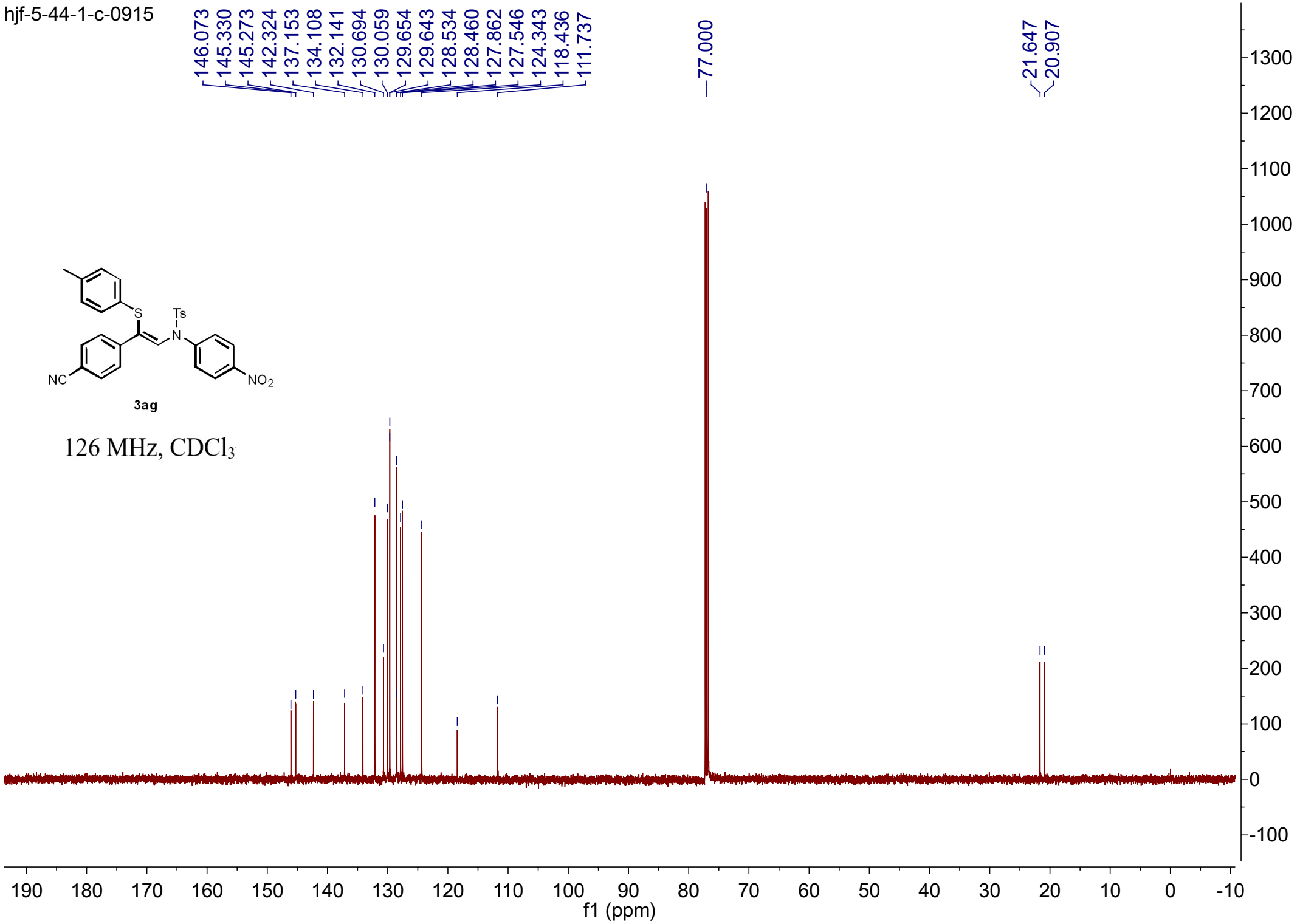

hjf-6-61-1-0710s-c
147.312
146.158
145.355
145.212
144.354
137.225
134.017
131.249
130.092
129.707
129.629
128.630
128.479
128.024
127.565
127.508
124.374
123.648
77.000
21.665
20.911
S
Ts
N
O2N
NO2
3af
126 MHz, CDCl3
f1 (ppm)

hjf-5-44-1-h-0915

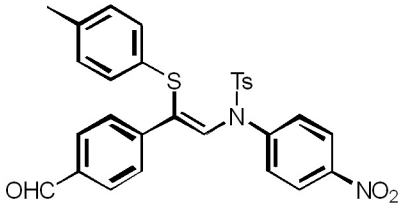


3ag

500 MHz, $CDCl_3$

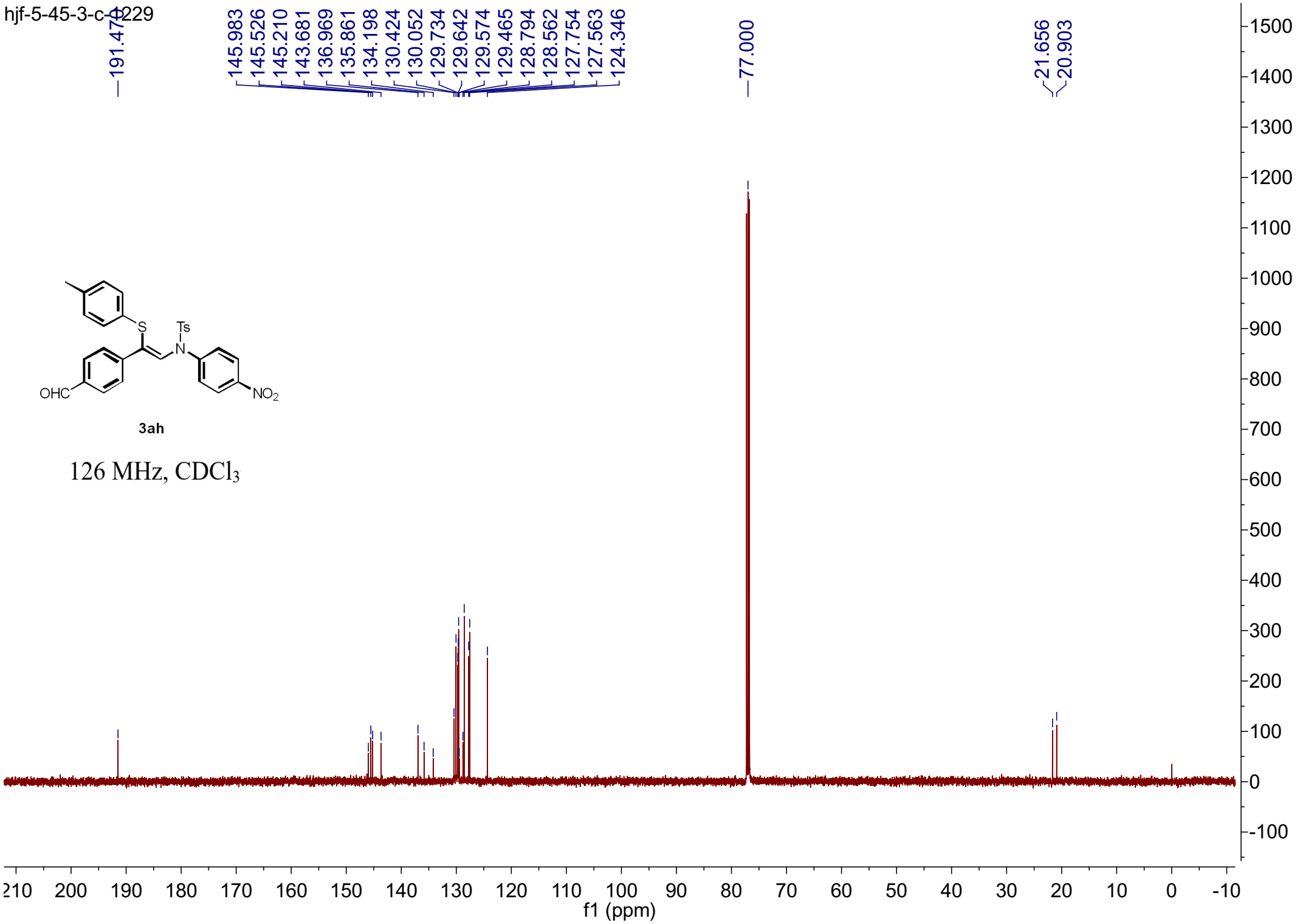

hjf-5-44-1-c-0915
146.073
145.330
145.273
142.324
137.153
134.108
132.141
130.694
130.059
129.654
129.643
128.534
128.460
127.862
127.546
124.343
118.436
111.737
77.000
21.647
20.907
S
Ts
N
NC
NO2
3ag
126 MHz, CDCl3
f1 (ppm)

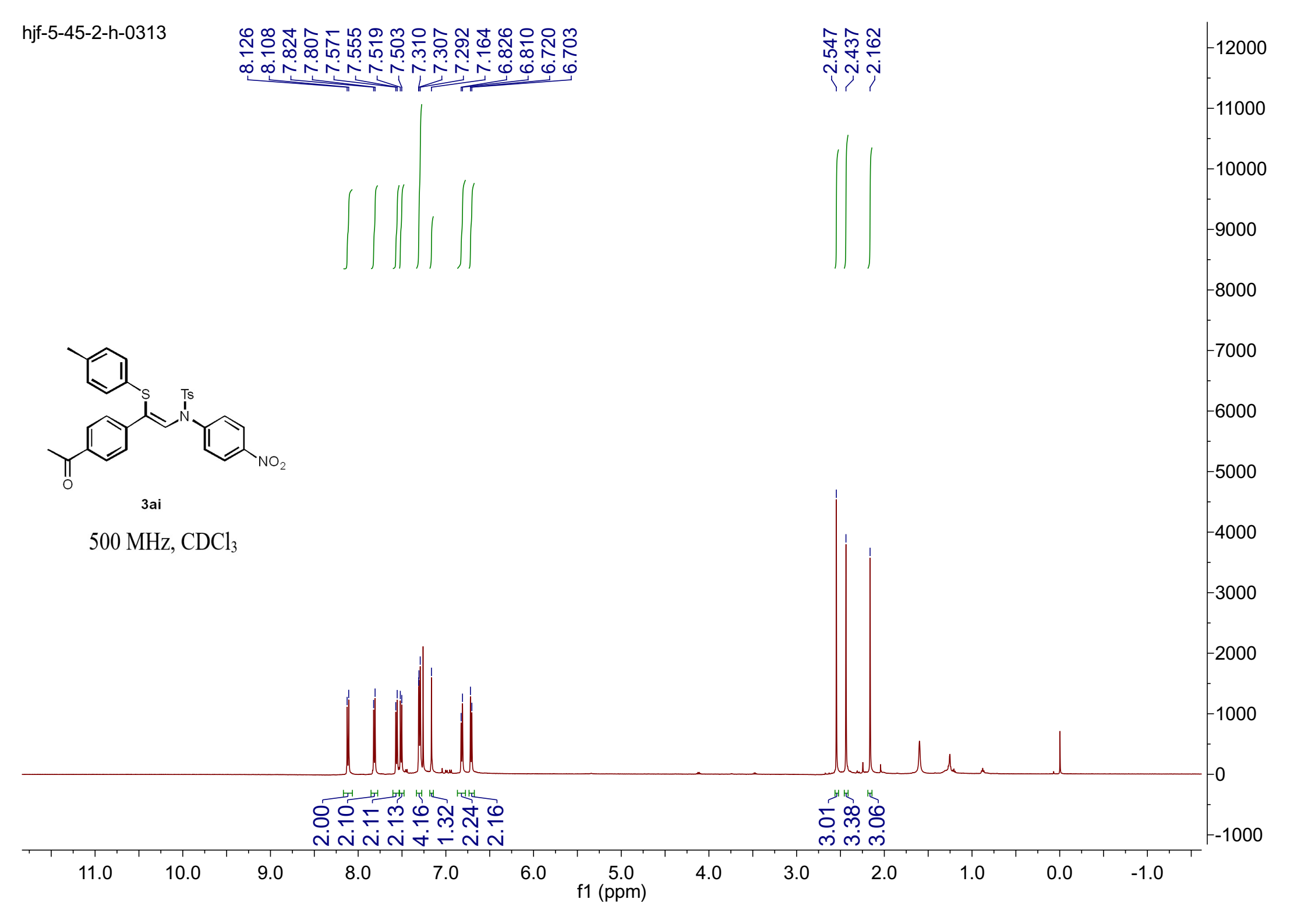
hjf-5-45-3-h-1229

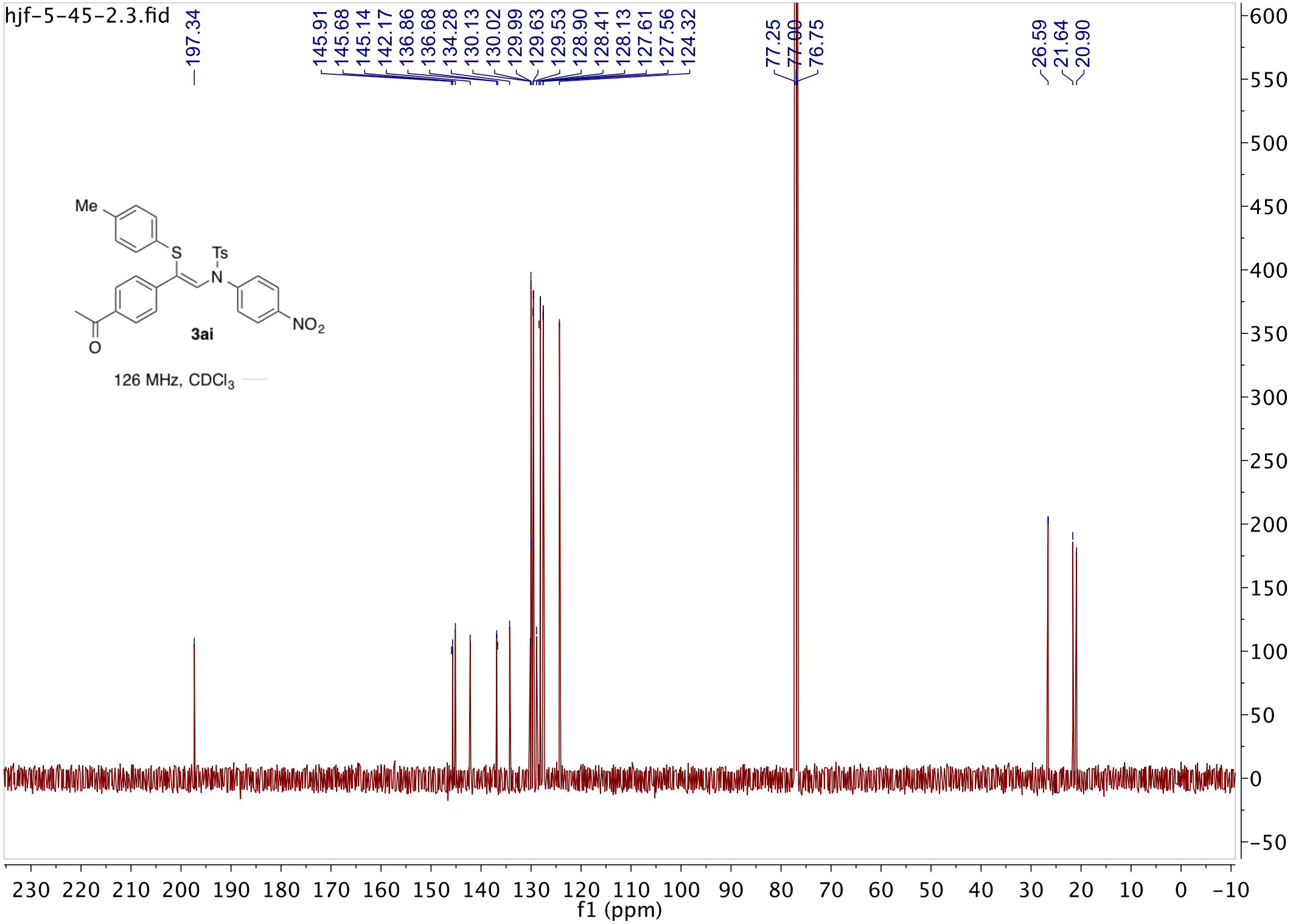


3ah

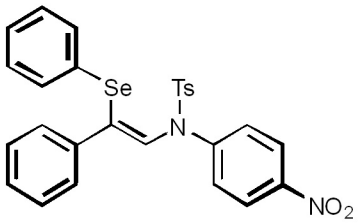
500 MHz, $CDCl_3$


hjf-5-45-3-c-1229
191.470
145.983
145.526
145.210
143.681
136.969
135.861
134.198
130.424
130.052
129.734
129.642
129.574
129.465
128.794
128.562
127.754
127.563
124.346
77.000
21.656
20.903
S
Ts
N
OHC
NO2
3ah
126 MHz, CDCl3
f1 (ppm)


hjf-5-45-2-h-0313
8.126
8.108
7.824
7.807
7.571
7.555
7.519
7.503
7.310
7.307
7.292
7.164
6.826
6.810
6.720
6.703
2.547
2.437
2.162
S
Ts
N
NO2
O
3ai
500 MHz, CDCl3
2.00
2.10
2.11
2.13
4.16
1.32
2.24
2.16
3.01
3.38
3.06
f1 (ppm)


hjf-5-45-2.3.fid
197.34
145.91
145.68
145.14
142.17
136.86
136.68
134.28
130.13
130.02
129.99
129.63
129.53
128.90
128.41
128.13
127.61
127.56
124.32
77.25
77.00
76.75
26.59
21.64
20.90
Me
S
Ts
N
O
NO2
3ai
126 MHz, CDCl3
f1 (ppm)

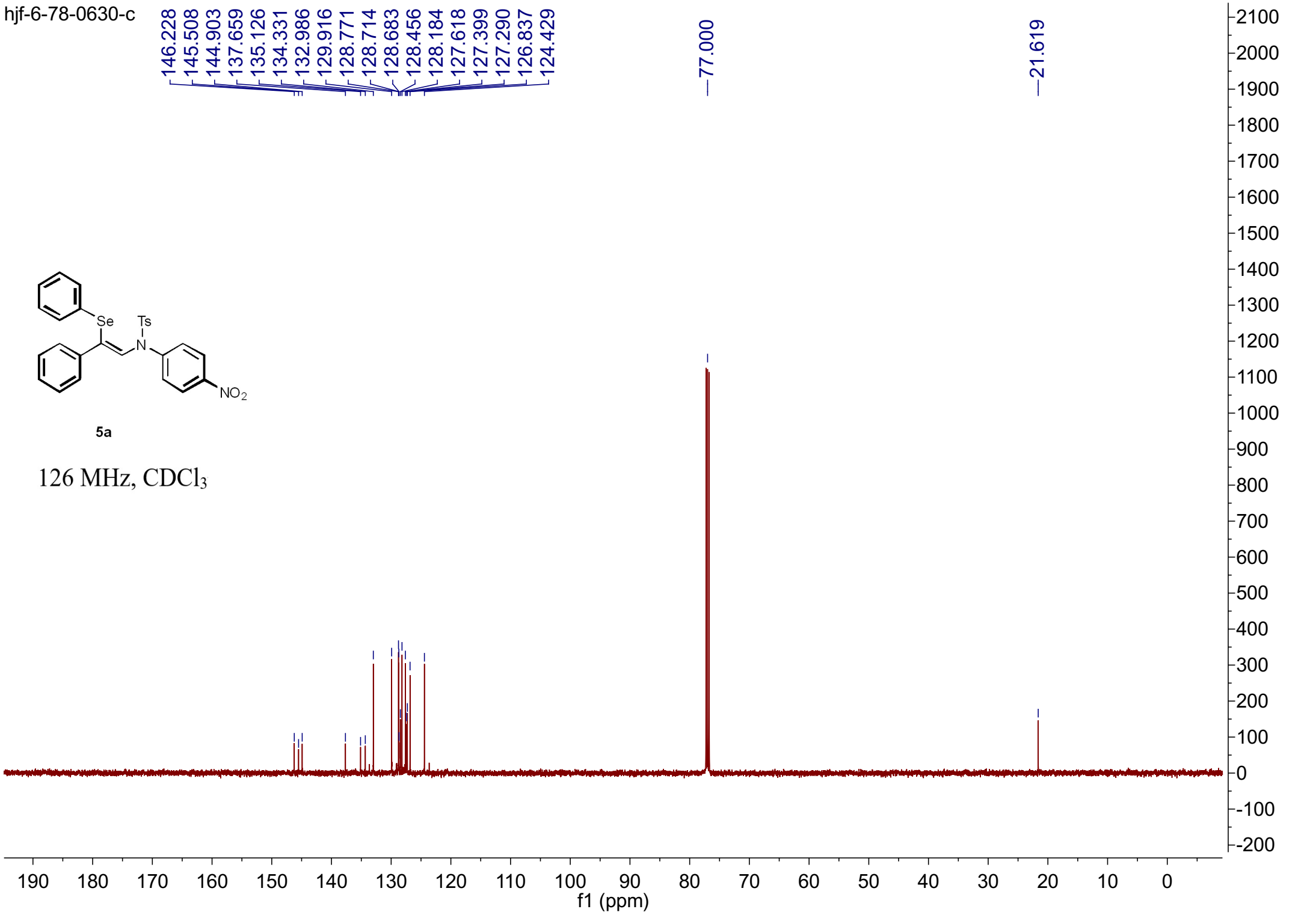
hjf-6-78-0630-h



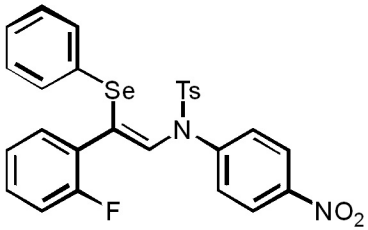
5a

500 MHz, $CDCl_3$

hjf-6-78-0630-c



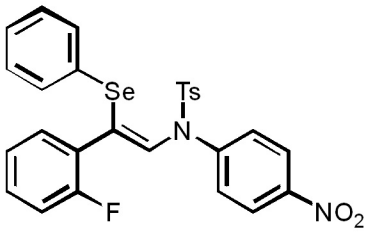
hjf-6-82-2-h



5b

500 MHz, $CDCl_3$

hjf-6-82-2-c



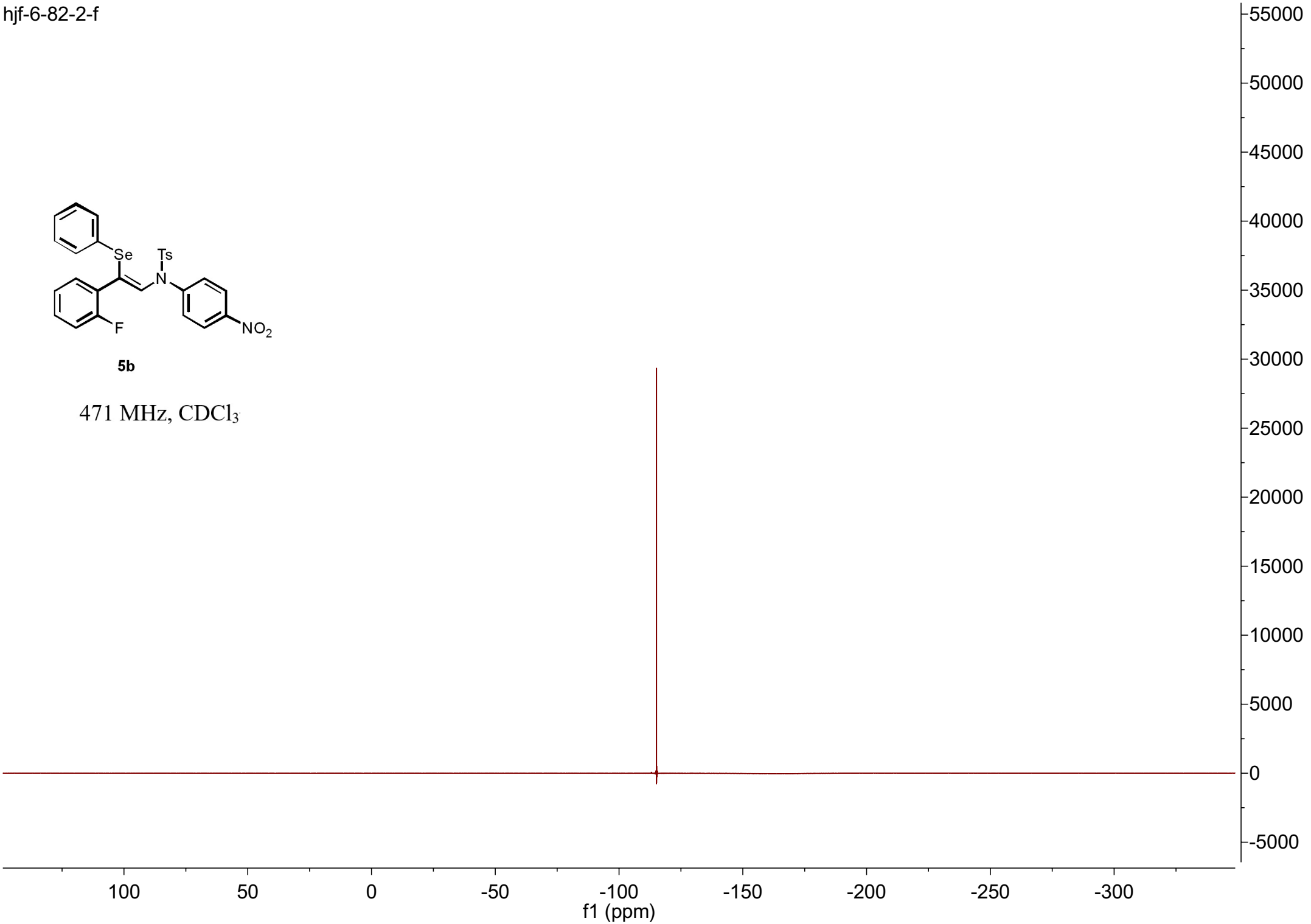
5b

126 MHz, $CDCl_3$

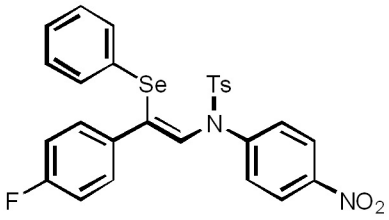
hjf-6-82-2-f

5b

471 MHz, $CDCl_3$



hjf-6-79-4-0710-h

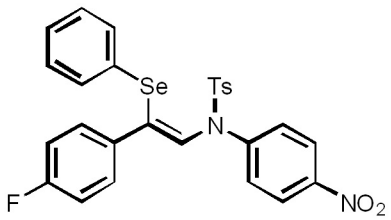


5c

500 MHz, $CDCl_3$

f1 (ppm)

hjf-6-79-4-0710-c



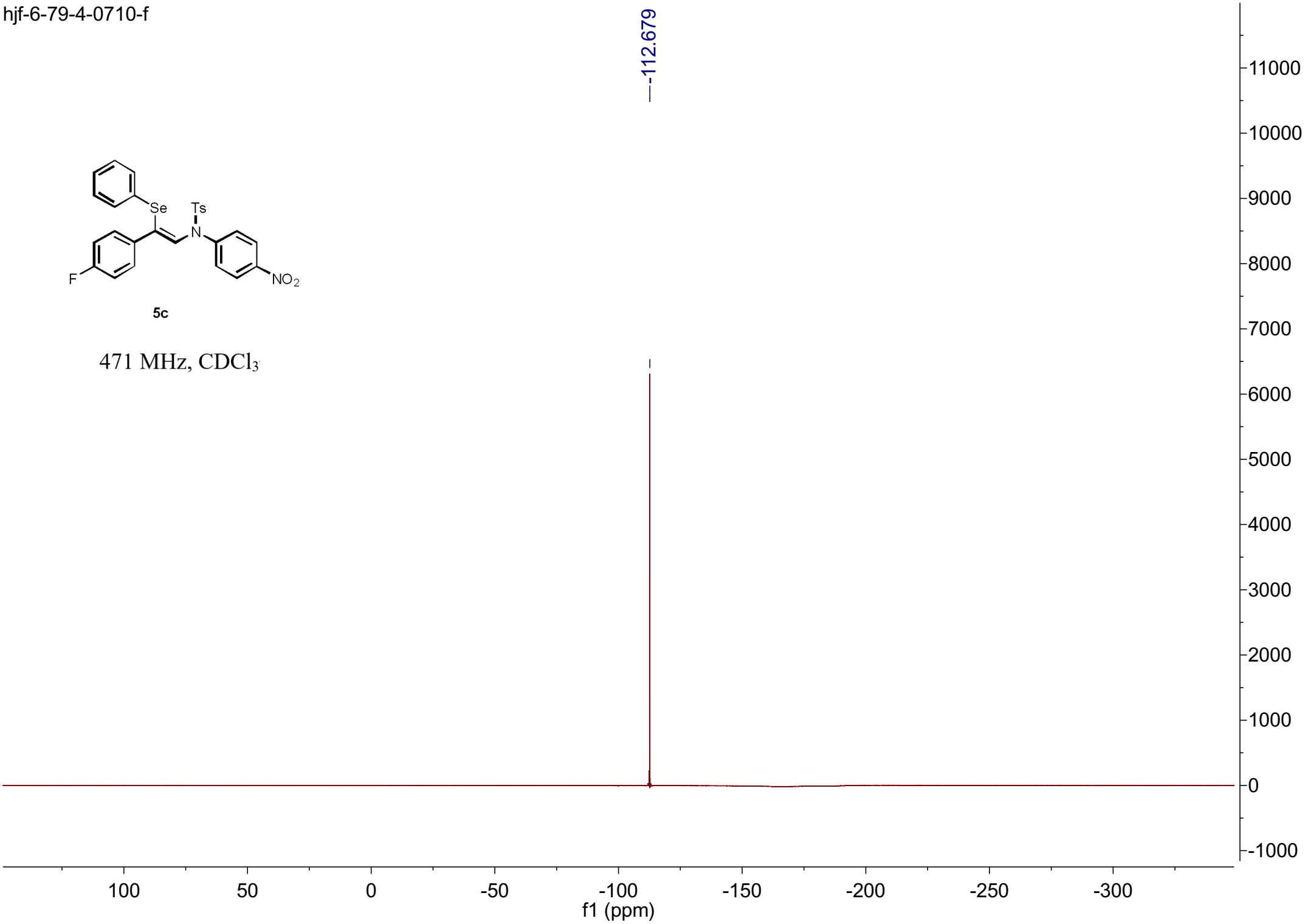
5c

126 MHz, $CDCl_3$

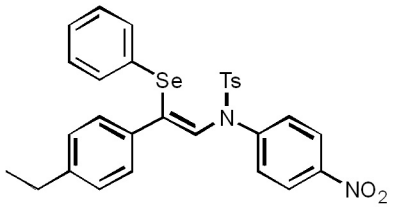
hjf-6-79-4-0710-f

5c

471 MHz, $CDCl_3$

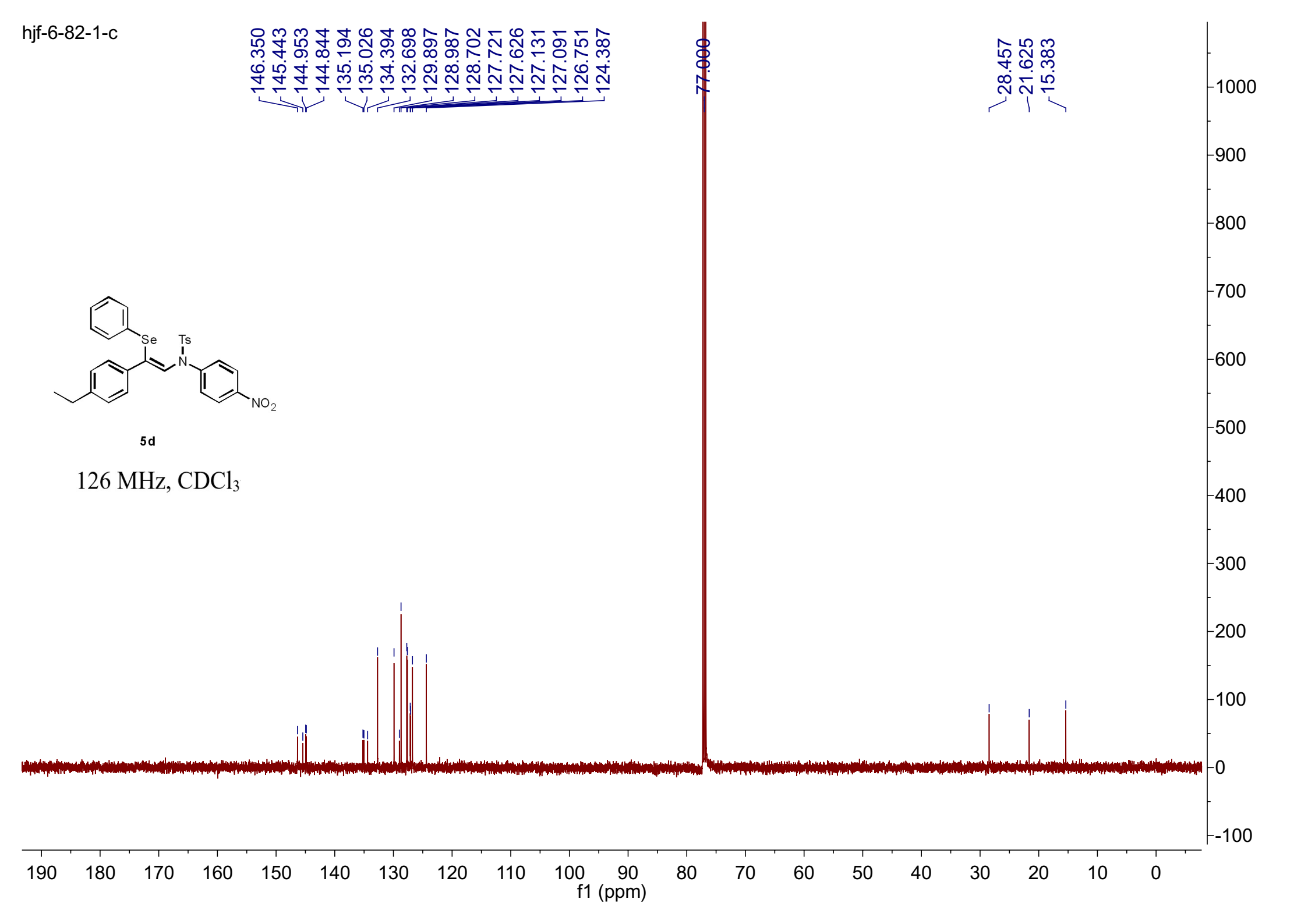


hjf-6-82-1-h

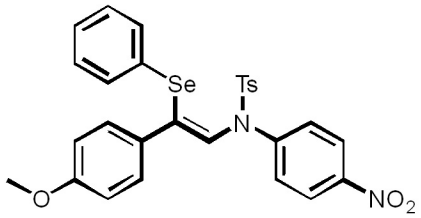


5d

500 MHz, $CDCl_3$

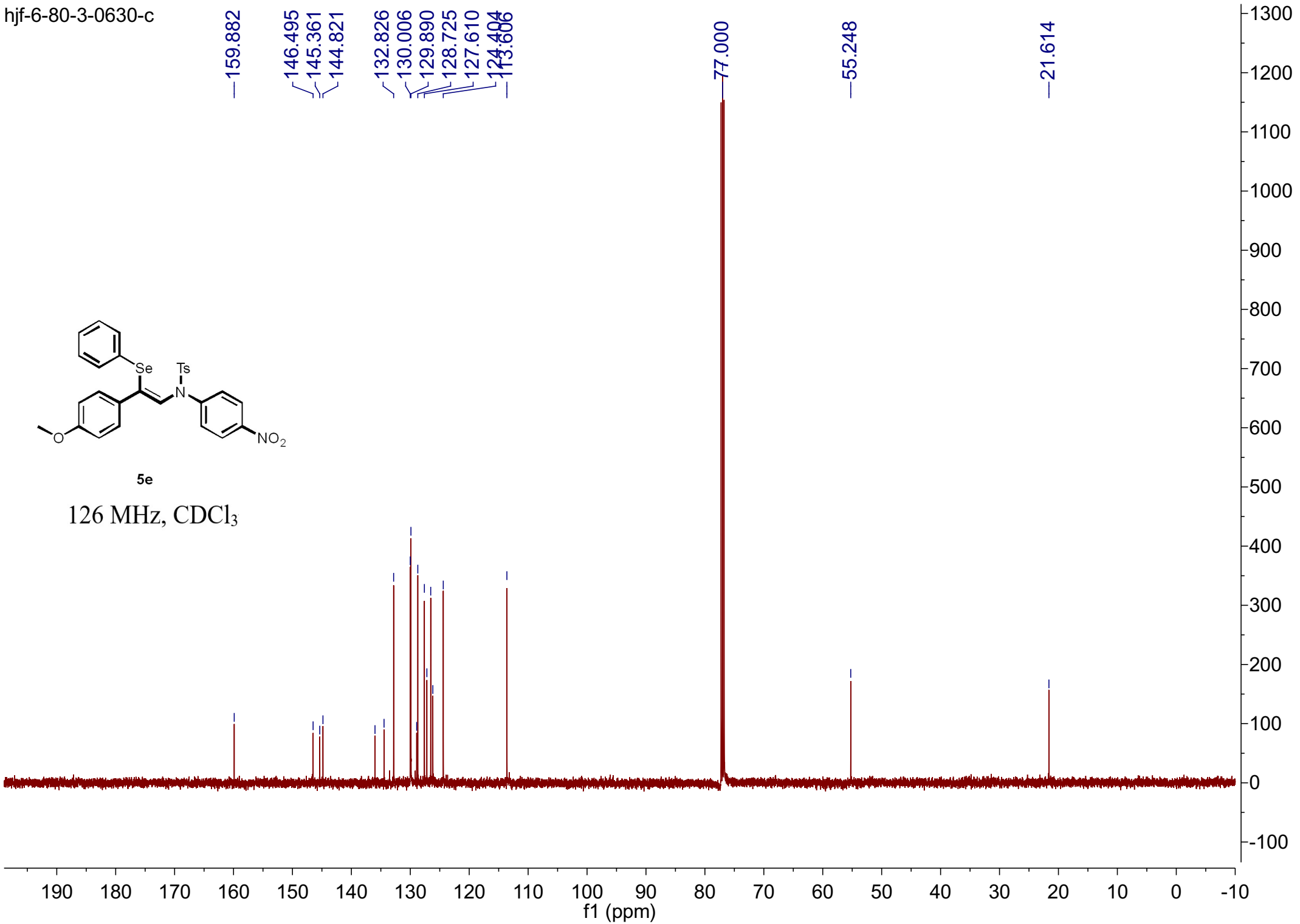

hjf-6-82-1-c
146.350
145.443
144.953
144.844
135.194
135.026
134.394
132.698
129.897
128.987
128.702
127.721
127.626
127.131
127.091
126.751
124.387
77.000
28.457
21.625
15.383
Se
Ts
N
NO2
5d
126 MHz, CDCl3
f1 (ppm)

hjf-6-80-3-0630-h



5e

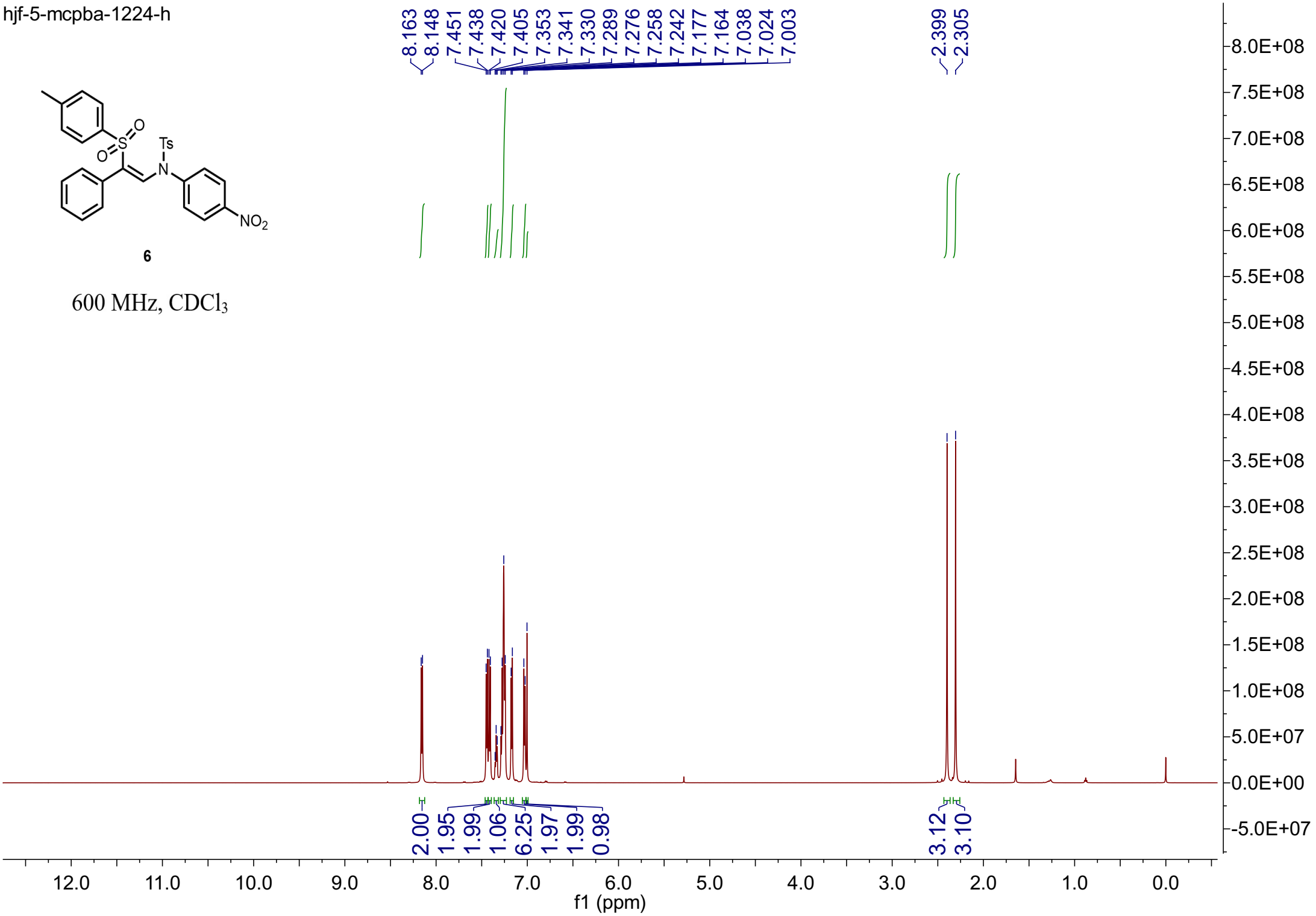
500 MHz, $CDCl_3$


hjf-6-80-3-0630-c
159.882
146.495
145.361
144.821
132.826
130.006
129.890
128.725
127.610
124.404
113.606
77.000
55.248
21.614
Se
Ts
N
O
NO2
5e
126 MHz, CDCl3
f1 (ppm)

hjf-5-mcpba-1224-h

6

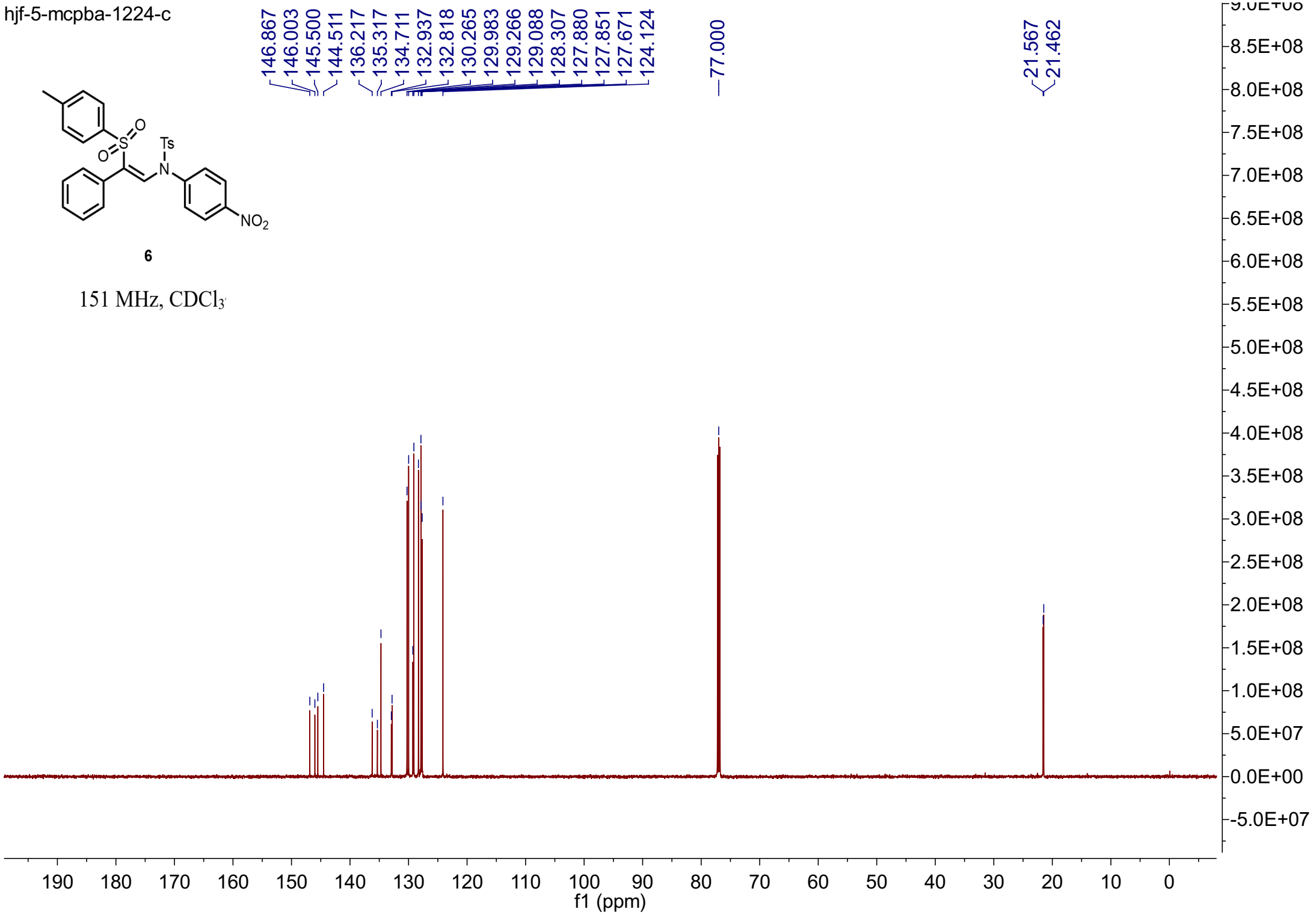
600 MHz, $CDCl_3$



hjf-5-mcpba-1224-c

6

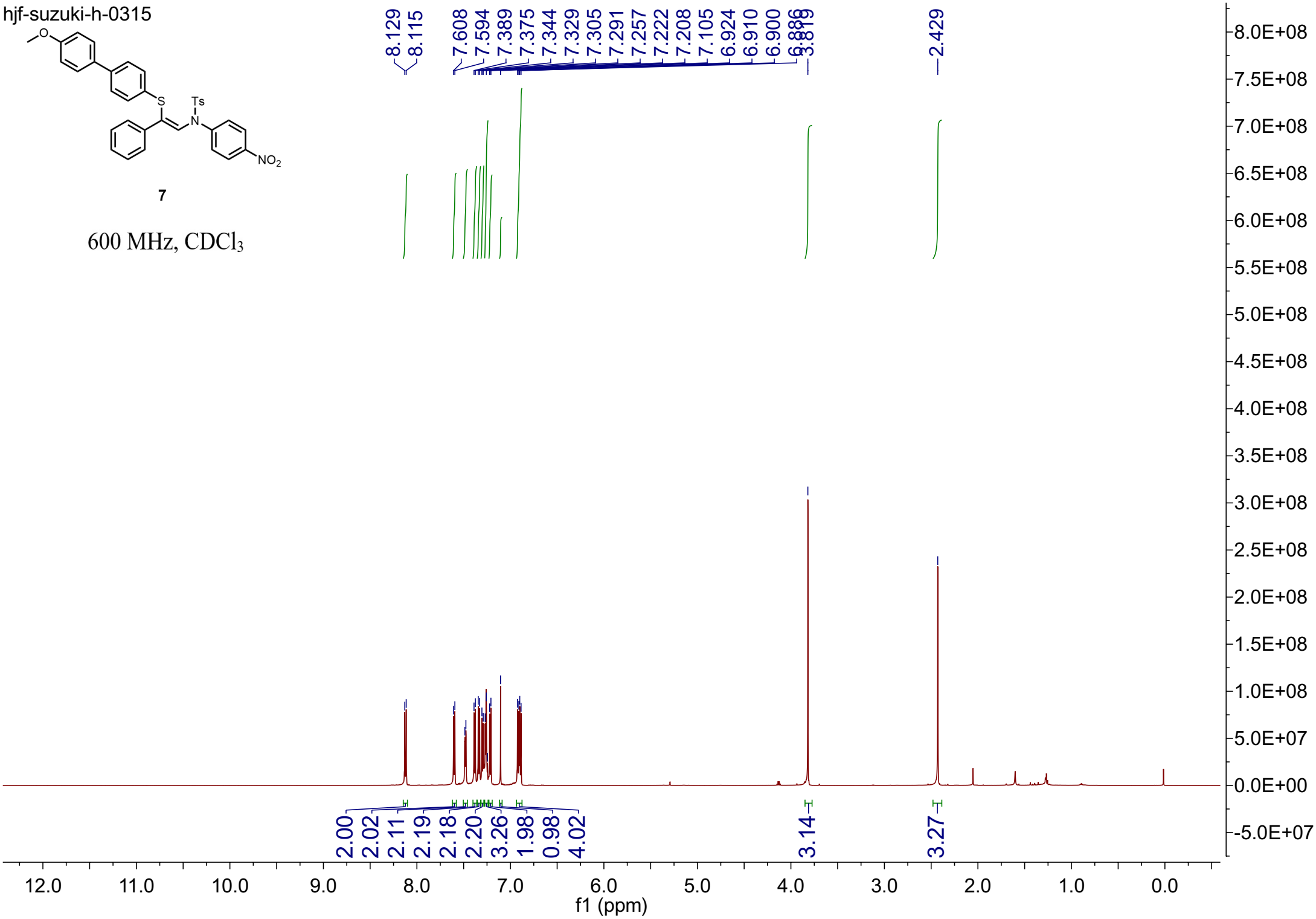
151 MHz, $CDCl_3$



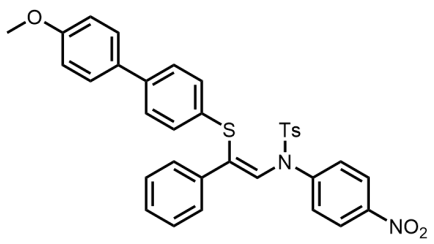
hjf-suzuki-h-0315

7

600 MHz, $CDCl_3$



hjf-suzuki-c-0315



7

151 MHz, $CDCl_3$

159.210
129.950
129.859
128.584
128.446
128.068
127.764
127.548
127.155
126.700
124.279
114.156
77.000
55.280
21.606

4.0E+08
3.8E+08
3.6E+08
3.4E+08
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
-4.0E+07

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

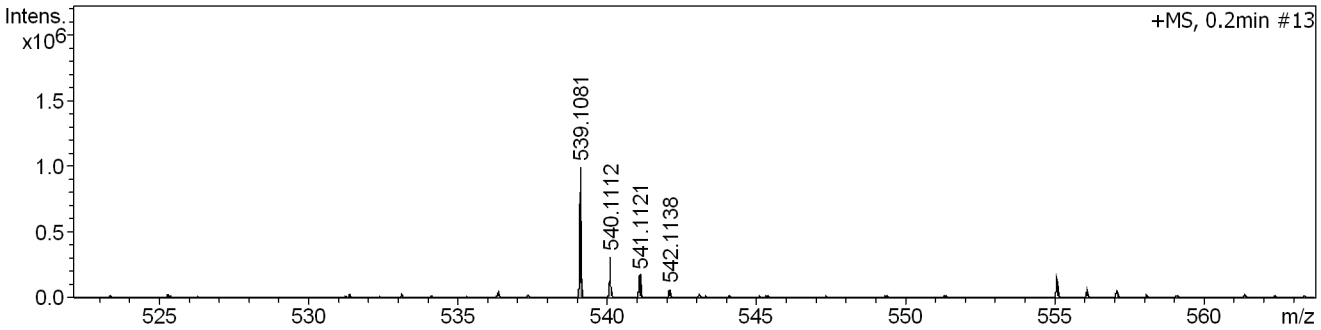
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-MBDW_P1-B-5_01_32731.d	Acquisition Date	7/6/2022 2:06:48 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-MBDW	Instrument	maXis impact 282001.00122
Comment			

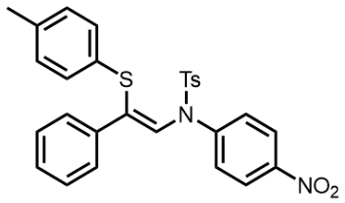
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	539.1081	21843	1081.0	988572	100.0	0.0247
2	540.1112	16365	339.4	310740	31.4	0.0330
3	541.1121	12847	186.0	170500	17.2	0.0421
4	542.1138	11876	68.2	62640	6.3	0.0456

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
539.1081	1	C28H24N2NaO4S2	539.1070	-2.0	19.8	3	73.71	17.5	even	ok



3a

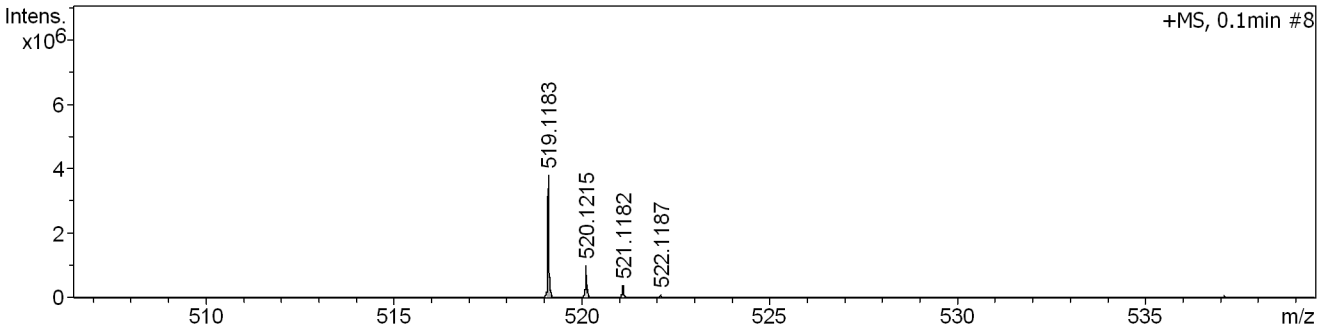
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-24-2_P1-E-3_01_33480.d	Acquisition Date	8/10/2022 12:02:17 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-24-2	Instrument	maXis impact 282001.00122
Comment			

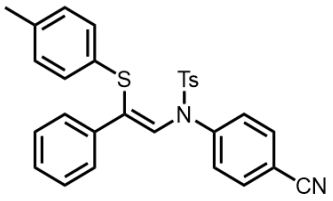
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	519.1183	15371	2498.2	3813760	100.0	0.0338
2	520.1215	22874	657.5	1002872	26.3	0.0227
3	521.1182	16070	245.9	374364	9.8	0.0324
4	522.1187	13857	61.3	93220	2.4	0.0377

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
519.1183	1	C29H24N2NaO2S2	519.1171	-2.3	41.9	7	37.46	18.5	even	ok



3b

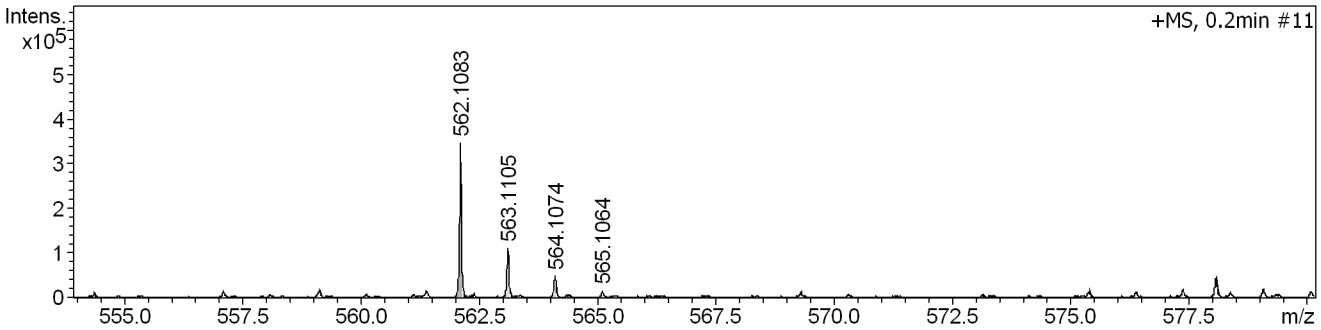
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-29_P1-D-6_01_32944.d	Acquisition Date	7/15/2022 10:58:25 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-29	Instrument	maXis impact 282001.00122
Comment			

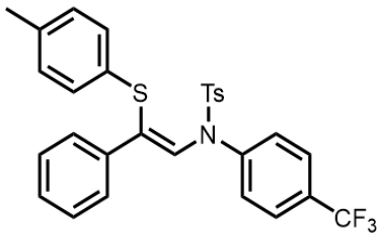
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	562.1083	16215	332.9	346716	100.0	0.0347
2	563.1105	13502	106.7	111112	32.0	0.0417
3	564.1074	11953	46.2	48188	13.9	0.0472
4	565.1064	15732	14.9	15520	4.5	0.0359

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
562.1083	1	C29H24F3NNaO2S2	562.1093	1.7	9.3	4	87.07	16.5	even	ok



3c

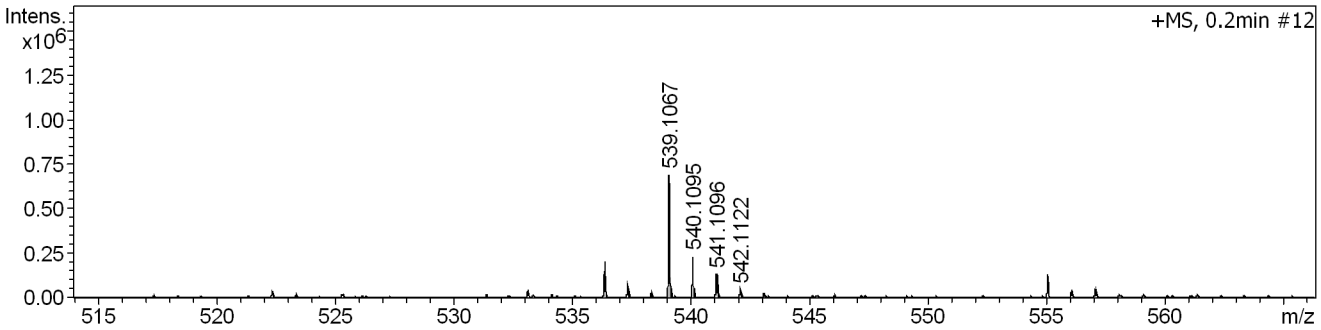
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-24-1_P1-D-5_01_32943.d	Acquisition Date	7/15/2022 10:55:17 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-24-1	Instrument	maXis impact 282001.00122
Comment			

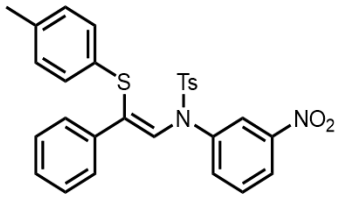
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	539.1067	19562	595.4	690132	100.0	0.0276
2	540.1095	14136	200.0	231904	33.6	0.0382
3	541.1096	11633	113.0	131044	19.0	0.0465
4	542.1122	10732	36.7	42620	6.2	0.0505

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
539.1067	1	C28H24N2NaO4S2	539.1070	0.4	23.4	1	100.00	17.5	even	ok



3d

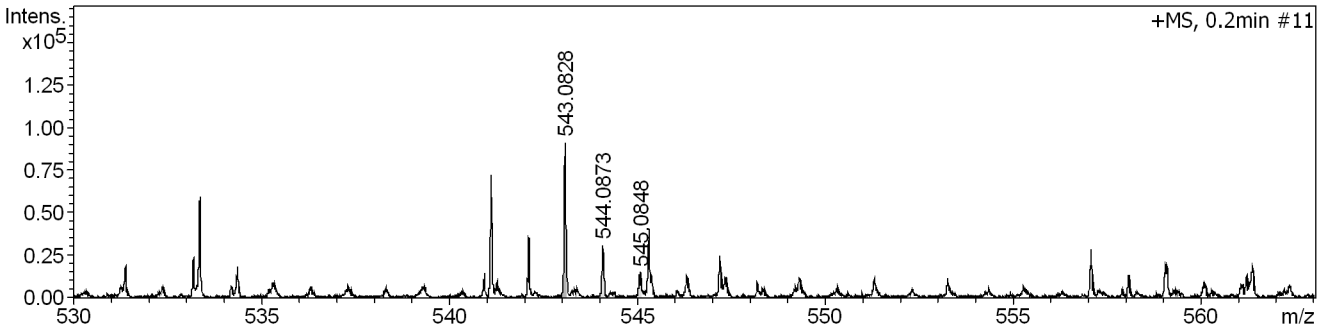
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-73-1_P1-F-6_01_32793.d	Acquisition Date	7/6/2022 5:23:01 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-73-1	Instrument	maXis impact 282001.00122
Comment			

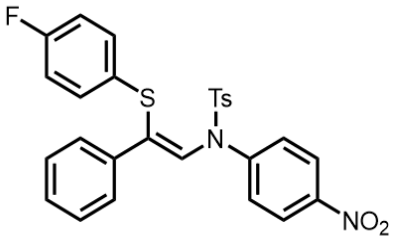
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	543.0828	12517	89.0	90804	100.0	0.0434
2	544.0873	10700	30.2	30832	34.0	0.0508
3	545.0848	9206	14.3	14648	16.1	0.0592

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
543.0828	1	C27H21FN2NaO4S2	543.0819	-1.6	12.8	3	75.04	17.5	even	ok



3h

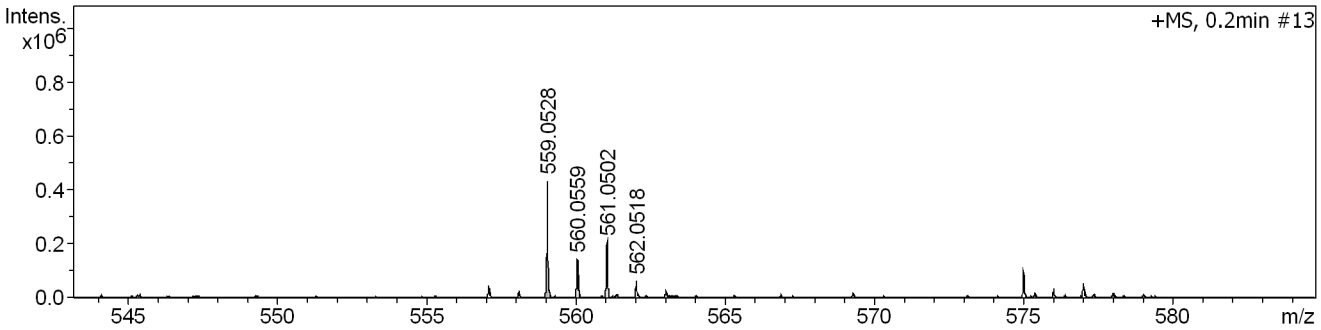
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-73-2_P1-F-7_01_32794.d	Acquisition Date	7/6/2022 5:26:08 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-73-2	Instrument	maXis impact 282001.00122
Comment			

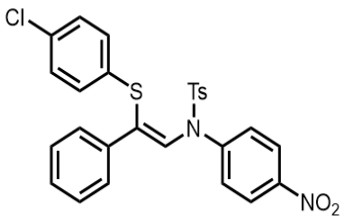
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	559.0528	16423	350.1	432808	100.0	0.0340
2	560.0559	13950	116.9	144324	33.3	0.0401
3	561.0502	14852	166.5	205480	47.5	0.0378
4	562.0518	13594	50.5	62276	14.4	0.0413

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
559.0528	1	C27H21ClN2NaO4S2	559.0523	-0.8	7.7	2	100.00	17.5	even	ok



3i

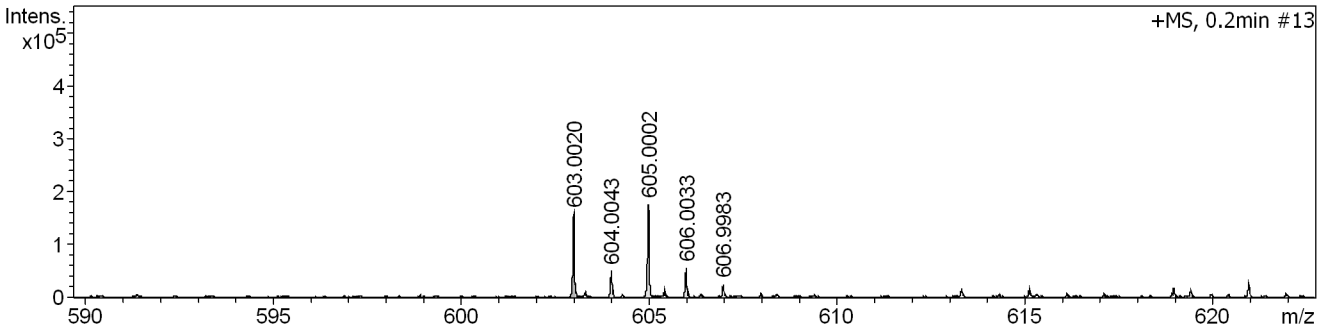
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-68-5_P1-F-5_01_32792.d	Acquisition Date	7/6/2022 5:19:53 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-68-5	Instrument	maXis impact 282001.00122
Comment			

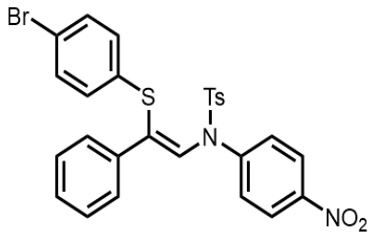
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	603.0020	14753	132.8	158544	90.3	0.0409
2	604.0043	14517	42.6	50872	29.0	0.0416
3	605.0002	14636	147.5	175644	100.0	0.0413
4	606.0033	13535	47.6	56576	32.2	0.0448
5	606.9983	11675	21.4	25448	14.5	0.0520

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
603.0020	1	C27H21BrN2NaO4S2	603.0018	-0.3	8.5	1	100.00	17.5	even	ok



3j

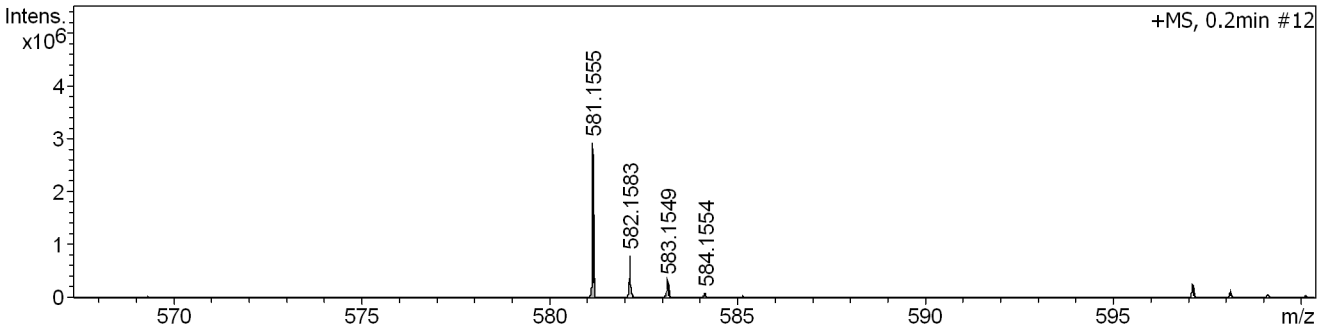
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/6/2022 5:13:38 PM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-5-68-2_P1-F-3_01_32790.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-68-2	Instrument	maXis impact 282001.00122
Comment			

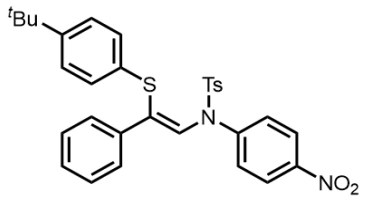
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	581.1555	21699	2734.0	2919224	100.0	0.0268
2	582.1583	21492	751.8	802016	27.5	0.0271
3	583.1549	16582	294.5	313968	10.8	0.0352
4	584.1554	13251	79.1	84324	2.9	0.0441

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
581.1555	1	C31H30N2NaO4S2	581.1539	-2.8	46.9	8	23.75	17.5	even	ok



3k

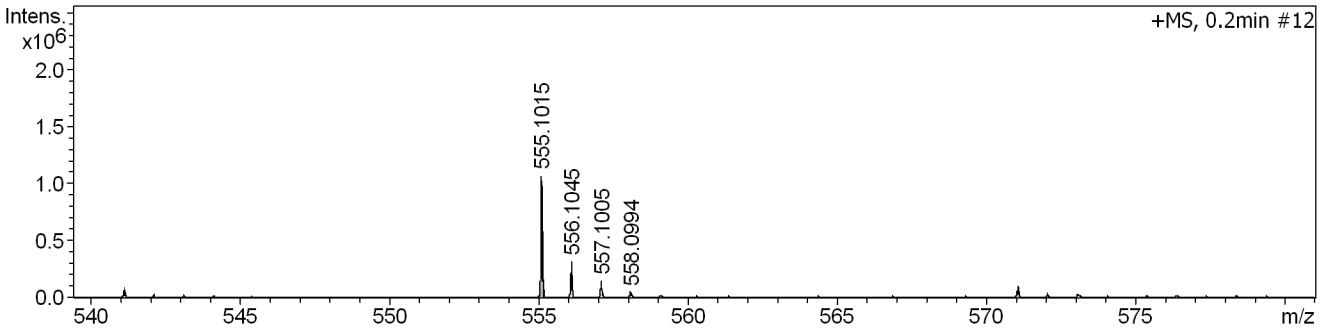
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-68-1_P1-D-8_01_32946.d	Acquisition Date	7/15/2022 11:04:42 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-68-1	Instrument	maXis impact 282001.00122
Comment			

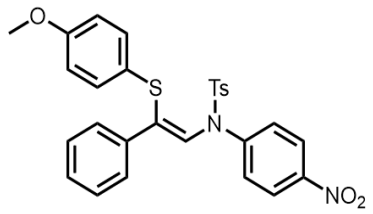
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	555.1015	22473	938.2	1071724	100.0	0.0247
2	556.1045	14946	277.7	317128	29.6	0.0372
3	557.1005	11726	127.4	145404	13.6	0.0475
4	558.0994	10137	38.4	43820	4.1	0.0551

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
555.1015	1	C28H24N2NaO5S2	555.1019	0.7	17.7	1	100.00	17.5	even	ok



3l

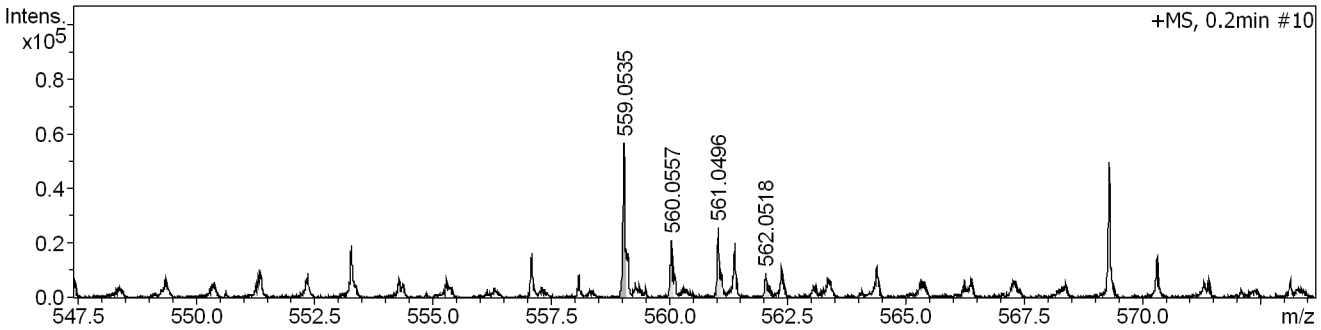
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-73-3_P1-A-6_01_32723.d	Acquisition Date	7/6/2022 1:41:40 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-73-3	Instrument	maXis impact 282001.00122
Comment			

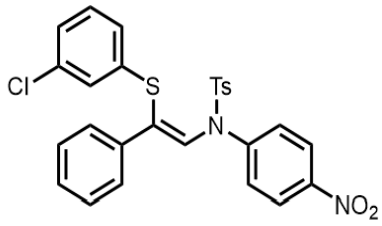
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	559.0535	14052	61.4	56596	100.0	0.0398
2	560.0557	14844	23.2	21348	37.7	0.0377
3	561.0496	11272	28.0	25816	45.6	0.0498
4	562.0518	14500	10.0	9216	16.3	0.0388

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
559.0535	1	C27H21ClN2NaO4S2	559.0523	-2.1	28.6	2	49.97	17.5	even	ok



3m

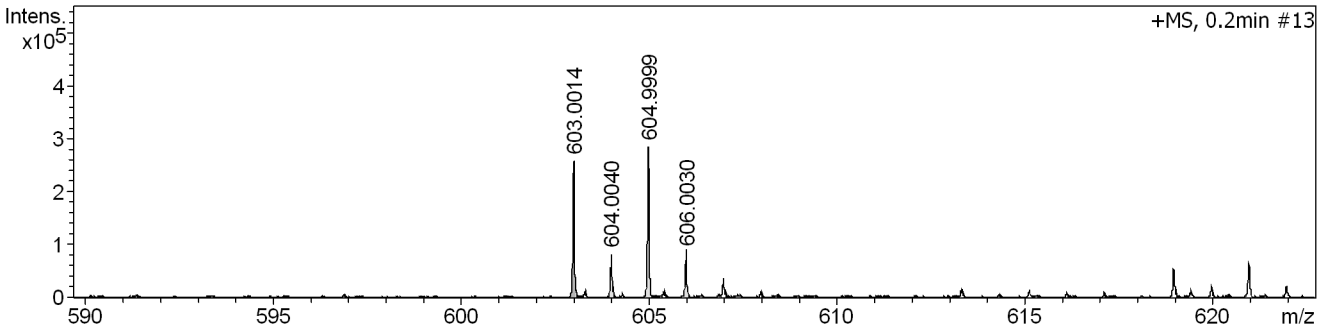
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-68-4_P1-F-4_01_32791.d	Acquisition Date	7/6/2022 5:16:45 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-68-4	Instrument	maXis impact 282001.00122
Comment			

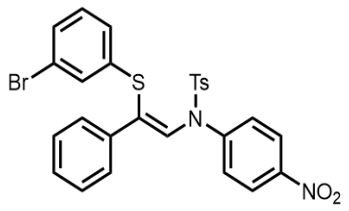
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	603.0014	16015	207.9	257552	90.4	0.0377
2	604.0040	14701	67.7	83752	29.4	0.0411
3	604.9999	17773	230.6	284996	100.0	0.0340
4	606.0030	14211	69.7	86084	30.2	0.0426

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
603.0014	1	C27H21BrN2NaO4S2	603.0018	0.7	8.8	1	100.00	17.5	even	ok



3n

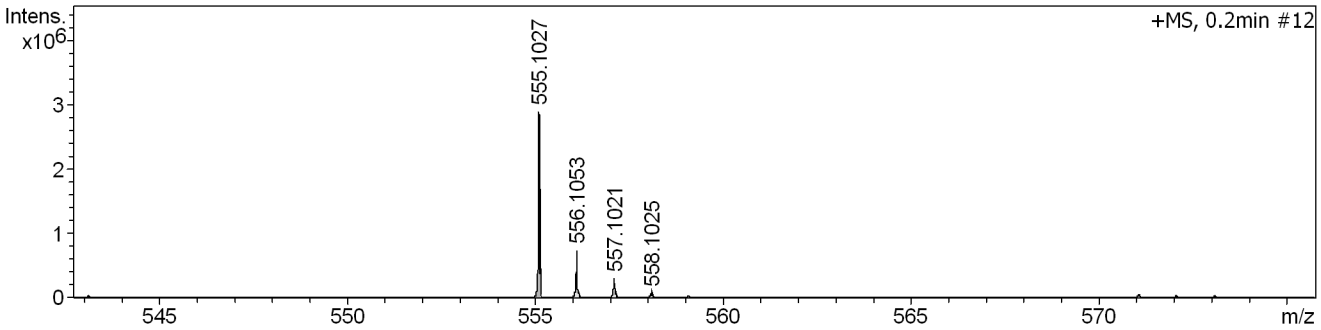
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-112-1_P1-E-5_01_33482.d	Acquisition Date	8/10/2022 12:08:33 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-112-1	Instrument	maXis impact 282001.00122
Comment			

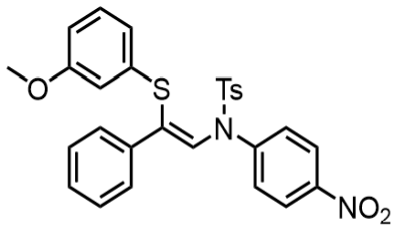
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	555.1027	18337	1757.4	2889568	100.0	0.0303
2	556.1053	20868	456.5	748372	25.9	0.0266
3	557.1021	15797	185.8	303804	10.5	0.0353
4	558.1025	12139	45.4	74044	2.6	0.0460

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
555.1027	1	C28H24N2NaO5S2	555.1019	-1.5	38.8	7	54.91	17.5	even	ok



3o

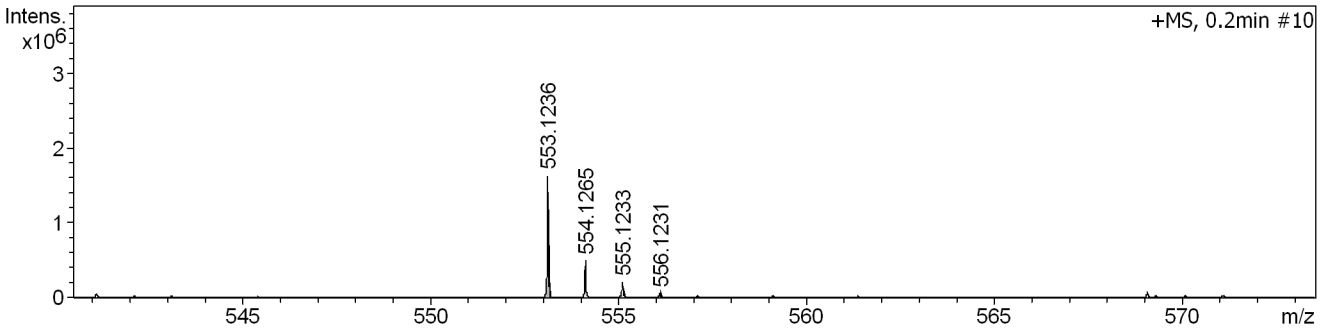
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-79-1_P1-A-8_01_32725.d	Acquisition Date	7/6/2022 1:47:59 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-79-1	Instrument	maXis impact 282001.00122
Comment			

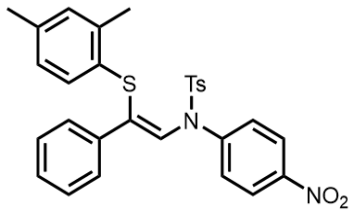
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	553.1236	25065	1872.8	1633748	100.0	0.0221
2	554.1265	19915	569.5	496724	30.4	0.0278
3	555.1233	15960	239.2	208792	12.8	0.0348
4	556.1231	13343	60.0	52372	3.2	0.0417

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
553.1236	1	C29H26N2NaO4S2	553.1226	-1.8	20.7	3	76.76	17.5	even	ok



3p

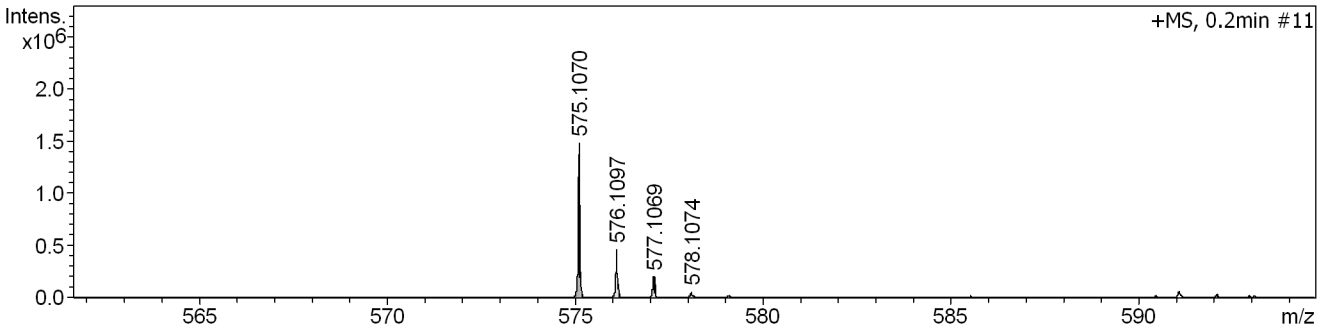
Mass Spectrum List Report

Analysis Info

Acquisition Date	8/24/2022 2:04:25 PM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-6-112-3-2_P1-A-5_01_33715.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-112-3-2	Instrument	maXis impact 282001.00122
Comment			

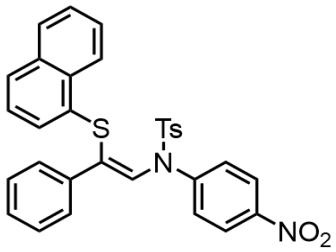
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	575.1070	24939	1025.8	1479032	100.0	0.0231
2	576.1097	17562	322.1	463672	31.3	0.0328
3	577.1069	14267	139.5	200508	13.6	0.0405
4	578.1074	11863	36.3	52168	3.5	0.0487

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
575.1070	1	C31H24N2NaO4S2	575.1070	-0.0	25.1	4	100.00	20.5	even	ok



3q

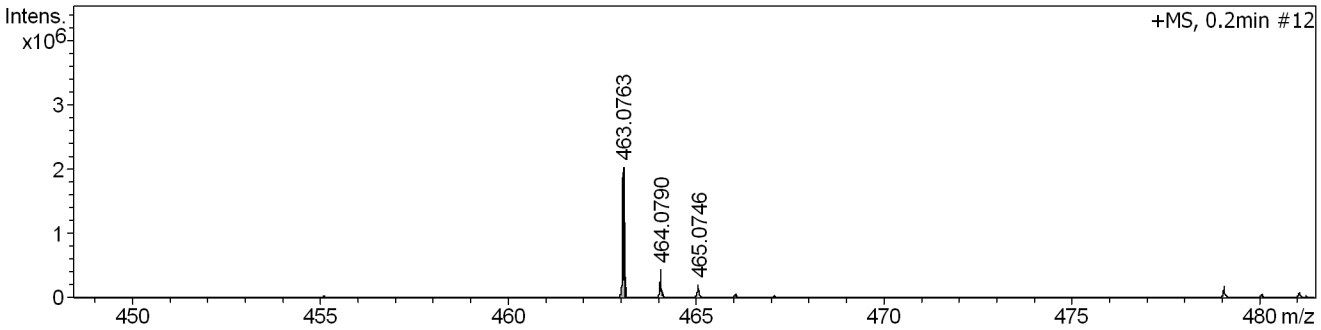
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-92_P1-E-4_01_33481.d	Acquisition Date	8/10/2022 12:05:25 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-92	Instrument	maXis impact 282001.00122
Comment			

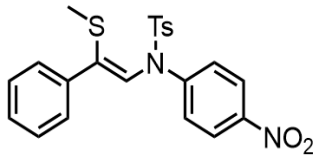
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	463.0763	21398	1509.2	2030596	100.0	0.0216
2	464.0790	16364	322.4	434788	21.4	0.0284
3	465.0746	13159	147.8	199688	9.8	0.0353
4	466.0755	10881	32.6	44224	2.2	0.0428

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
463.0763	1	C22H20N2NaO4S2	463.0757	-1.3	27.3	4	82.33	13.5	even	ok



3r

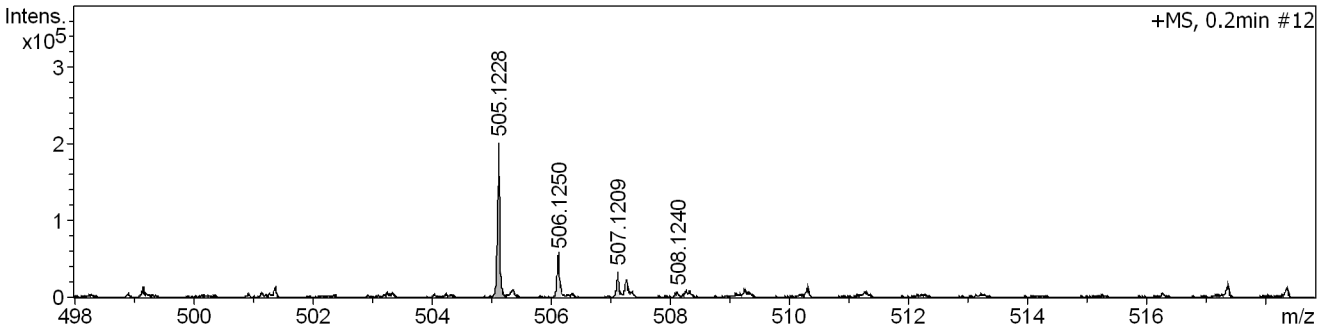
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-79-3_P1-A-9_01_32726.d	Acquisition Date	7/6/2022 1:51:06 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-79-3	Instrument	maXis impact 282001.00122
Comment			

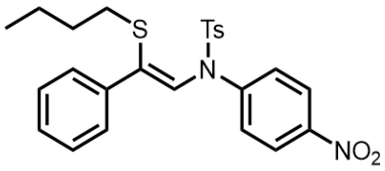
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	505.1228	14679	174.8	201216	100.0	0.0344
2	506.1250	11508	48.3	55716	27.7	0.0440
3	507.1209	14530	29.5	34116	17.0	0.0349
4	508.1240	12464	6.7	7752	3.9	0.0408

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
505.1228	1	C25H26N2NaO4S2	505.1226	-0.3	18.2	1	100.00	13.5	even	ok



3s

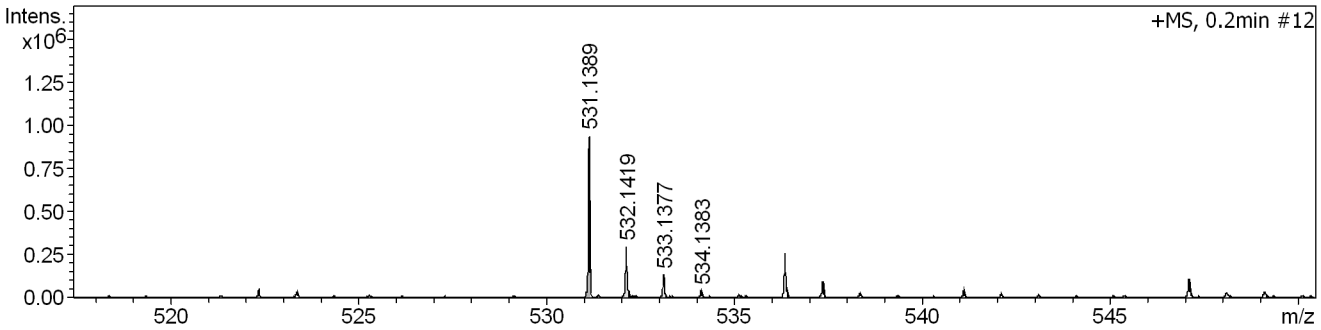
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/15/2022 10:39:31 AM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-5-79-2_P1-C-9_01_32938.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-79-2	Instrument	maXis impact 282001.00122
Comment			

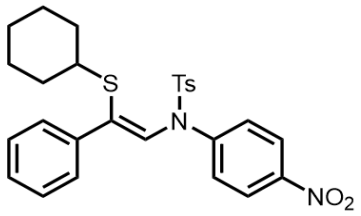
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	531.1389	20427	747.8	937656	100.0	0.0260
2	532.1419	16086	235.4	295120	31.5	0.0331
3	533.1377	12823	106.2	133056	14.2	0.0416
4	534.1383	13939	28.3	35416	3.8	0.0383

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
531.1389	1	C27H28N2NaO4S2	531.1383	-1.2	4.8	1	100.00	14.5	even	ok



3t

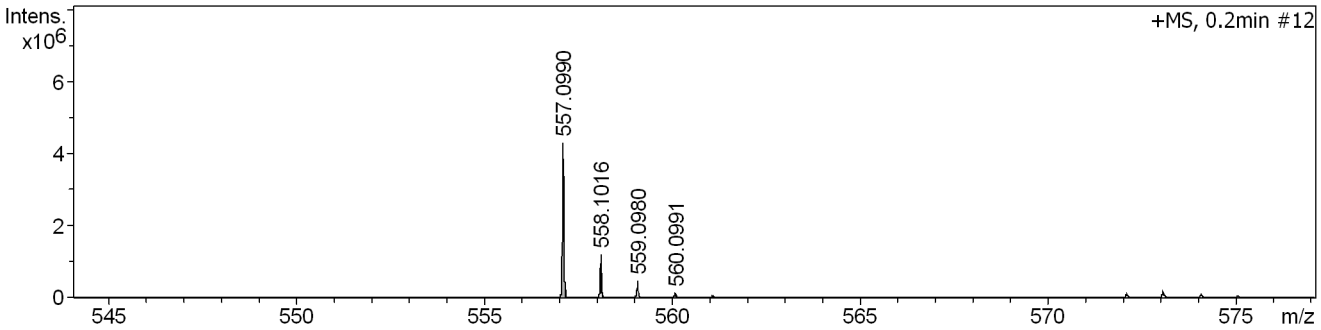
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-40-1_P1-B-6_01_32732.d	Acquisition Date	7/6/2022 2:09:57 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-40-1	Instrument	maXis impact 282001.00122
Comment			

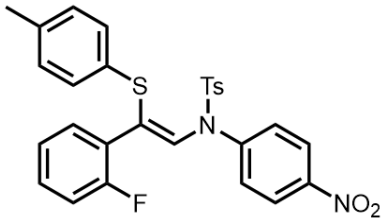
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	557.0990	14316	3718.7	4293832	100.0	0.0389
2	558.1016	23219	1038.9	1198728	27.9	0.0240
3	559.0980	17958	396.2	456708	10.6	0.0311
4	560.0991	16589	110.1	126696	3.0	0.0338

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
557.0990	1	C28H23FN2NaO4S2	557.0975	-2.5	30.3	121	30.96	17.5	even	ok



3u

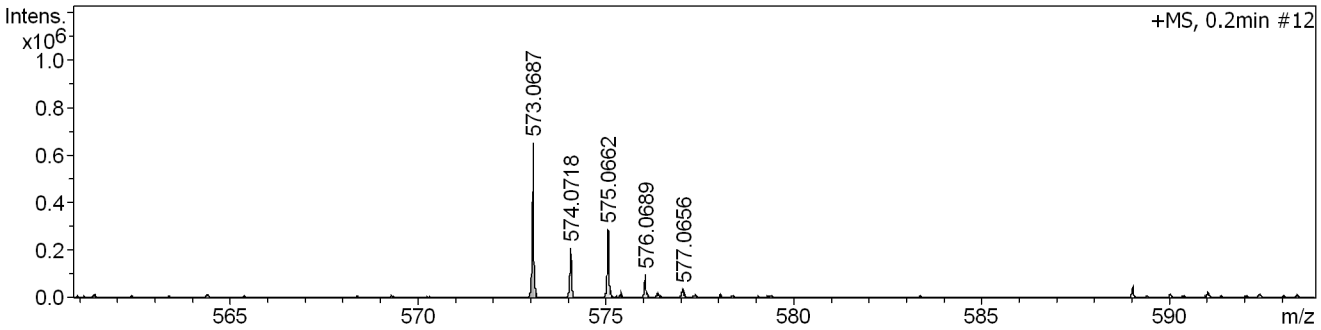
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-88-1_P1-C-2_01_32931.d	Acquisition Date	7/15/2022 10:17:32 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-88-1	Instrument	maXis impact 282001.00122
Comment			

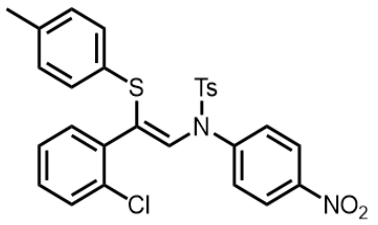
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	573.0687	20016	524.6	650724	100.0	0.0286
2	574.0718	14764	169.2	209484	32.2	0.0389
3	575.0662	15950	233.2	288432	44.3	0.0361
4	576.0689	15367	78.6	97124	14.9	0.0375
5	577.0656	11821	29.4	36236	5.6	0.0488

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
573.0687	1	C28H23ClN2NaO4S2	573.0680	-1.2	12.0	1	100.00	17.5	even	ok



3v

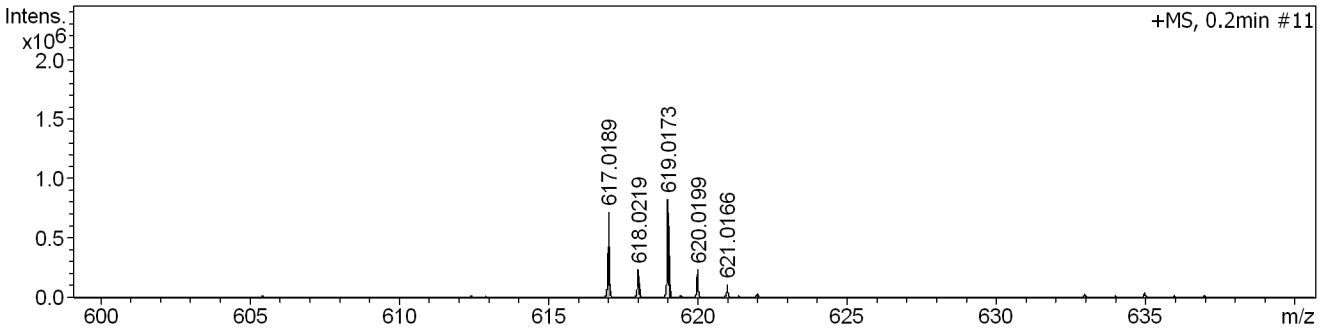
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-88-2_P1-C-3_01_32932.d	Acquisition Date	7/15/2022 10:20:41 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-88-2	Instrument	maXis impact 282001.00122
Comment			

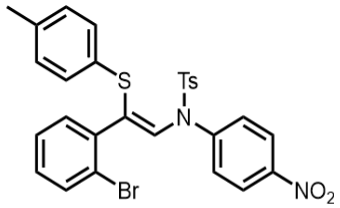
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	617.0189	22258	727.6	719960	87.2	0.0277
2	618.0219	17137	239.5	236640	28.7	0.0361
3	619.0173	24795	836.6	825388	100.0	0.0250
4	620.0199	16204	238.0	234488	28.4	0.0383
5	621.0166	15109	106.6	104892	12.7	0.0411

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
617.0189	1	C28H23BrN2NaO4S2	617.0175	-2.3	15.6	1	60.61	17.5	even	ok



3w

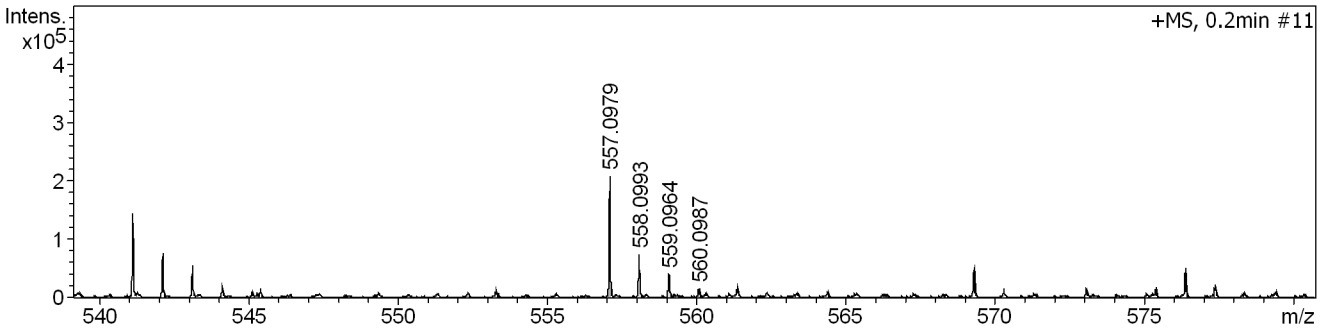
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/6/2022 2:19:20 PM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-5-42-1_P1-B-9_01_32735.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-42-1	Instrument	maXis impact 282001.00122
Comment			

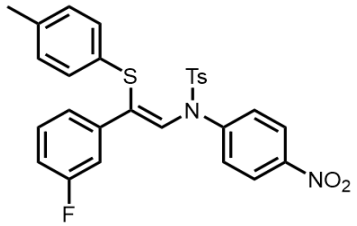
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	557.0979	15396	195.0	208276	100.0	0.0362
2	558.0993	13364	69.6	74316	35.7	0.0418
3	559.0964	11612	37.8	40392	19.4	0.0481
4	560.0987	13466	14.3	15272	7.3	0.0416

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
557.0979	1	C28H23FN2NaO4S2	557.0975	-0.6	29.6	6	96.34	17.5	even	ok



3x

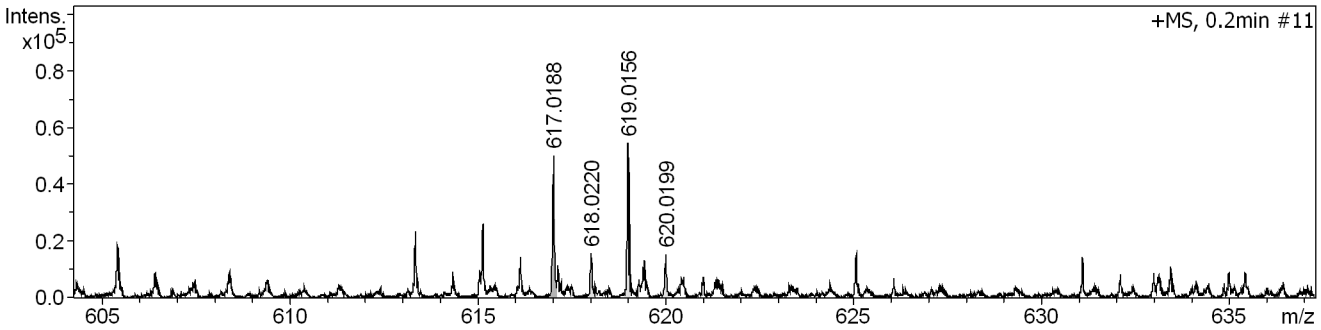
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-45-1_P1-B-2_01_32728.d	Acquisition Date	7/6/2022 1:57:23 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-45-1	Instrument	maXis impact 282001.00122
Comment			

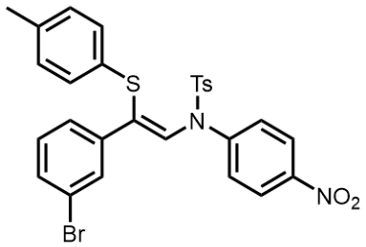
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	617.0188	15114	51.5	50144	91.9	0.0408
2	618.0220	14290	16.3	15876	29.1	0.0432
3	619.0156	15585	56.1	54540	100.0	0.0397
4	620.0199	14156	16.1	15632	28.7	0.0438

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
617.0188	1	C28H23BrN2NaO4S2	617.0175	-2.1	16.8	1	61.82	17.5	even	ok



3y

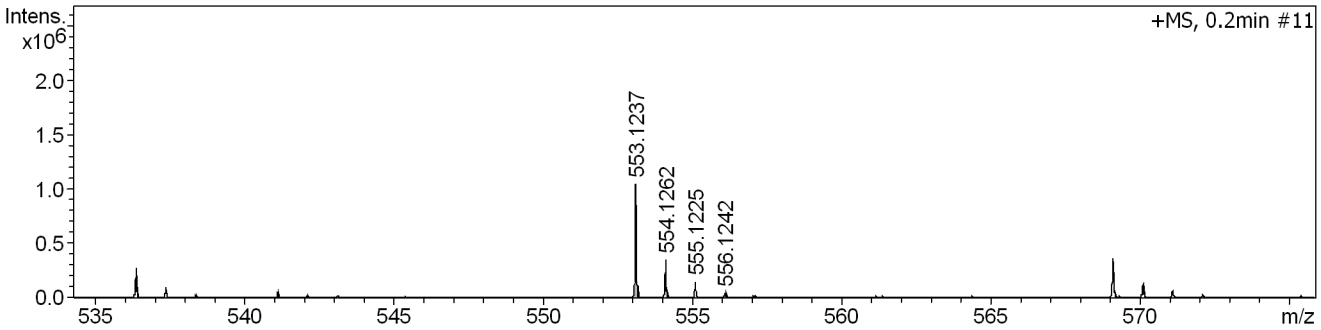
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-2-3_P1-D-2_01_32940.d	Acquisition Date	7/15/2022 10:45:47 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-2-3	Instrument	maXis impact 282001.00122
Comment			

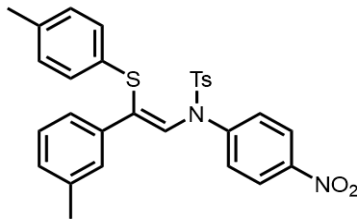
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	553.1237	23962	859.3	1048268	100.0	0.0231
2	554.1262	17799	286.9	350016	33.4	0.0311
3	555.1225	13961	120.6	147084	14.0	0.0398
4	556.1242	14133	31.5	38396	3.7	0.0393

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
553.1237	1	C29H26N2NaO4S2	553.1226	-1.9	7.7	1	78.01	17.5	even	ok



3z

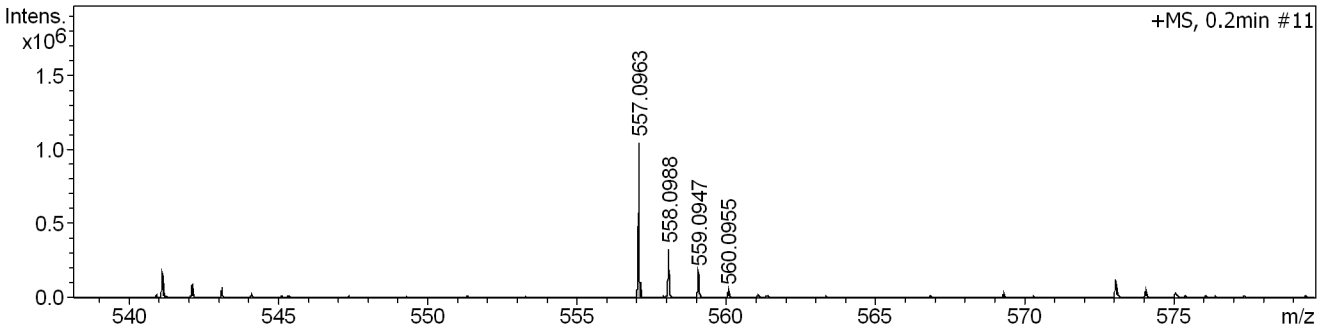
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/6/2022 2:25:36 PM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-5-44-2_P1-C-2_01_32737.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-44-2	Instrument	maXis impact 282001.00122
Comment			

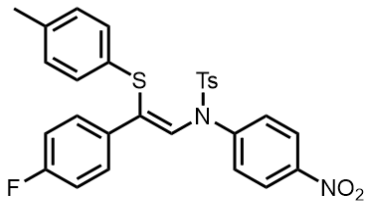
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	557.0963	22546	991.2	1043656	100.0	0.0247
2	558.0988	15519	311.2	327884	31.4	0.0360
3	559.0947	14960	165.2	174132	16.7	0.0374
4	560.0955	11201	42.9	45236	4.3	0.0500

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
557.0963	1	C28H23FN2NaO4S2	557.0975	2.2	11.4	2	65.38	17.5	even	ok



3aa

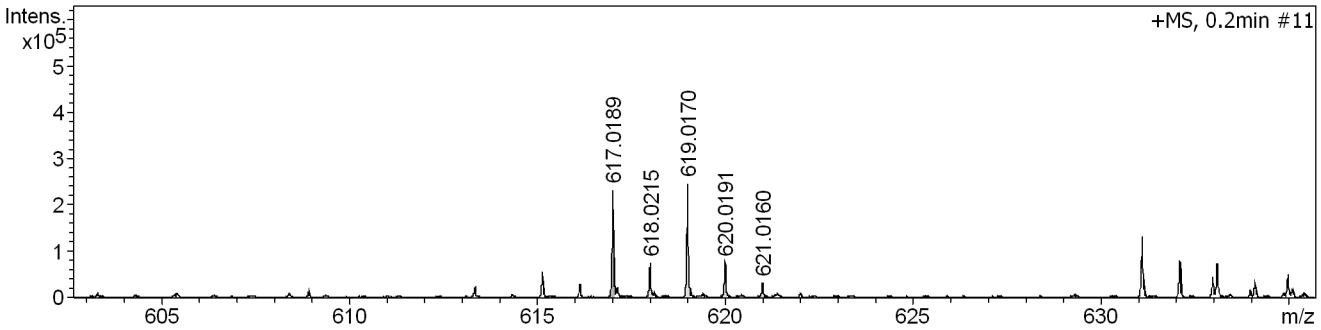
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-38-2_P1-B-8_01_32734.d	Acquisition Date	7/6/2022 2:16:13 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-38-2	Instrument	maXis impact 282001.00122
Comment			

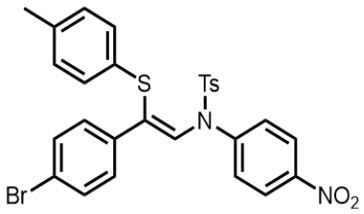
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	617.0189	16992	213.5	232148	94.4	0.0363
2	618.0215	15139	69.8	75828	30.8	0.0408
3	619.0170	17110	226.8	245996	100.0	0.0362
4	620.0191	13916	69.3	75112	30.5	0.0446
5	621.0160	14123	29.4	31884	13.0	0.0440

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
617.0189	1	C28H23BrN2NaO4S2	617.0175	-2.3	21.8	1	52.34	17.5	even	ok



3ab

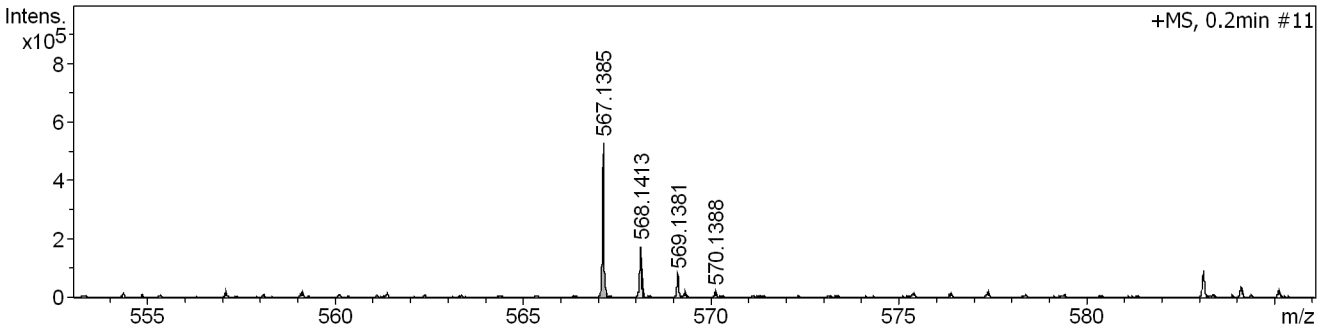
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-40-2_P1-D-7_01_32945.d	Acquisition Date	7/15/2022 11:01:32 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-40-2	Instrument	maXis impact 282001.00122
Comment			

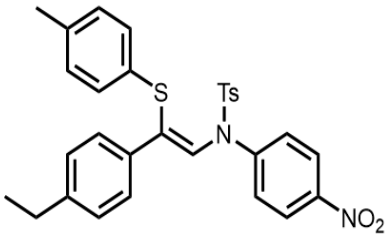
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	567.1385	19223	467.6	527236	100.0	0.0295
2	568.1413	14826	156.7	176848	33.5	0.0383
3	569.1381	12630	69.9	78824	15.0	0.0451
4	570.1388	11993	17.7	19924	3.8	0.0475

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
567.1385	1	C30H28N2NaO4S2	567.1383	-0.4	8.6	1	100.00	17.5	even	ok



3ac

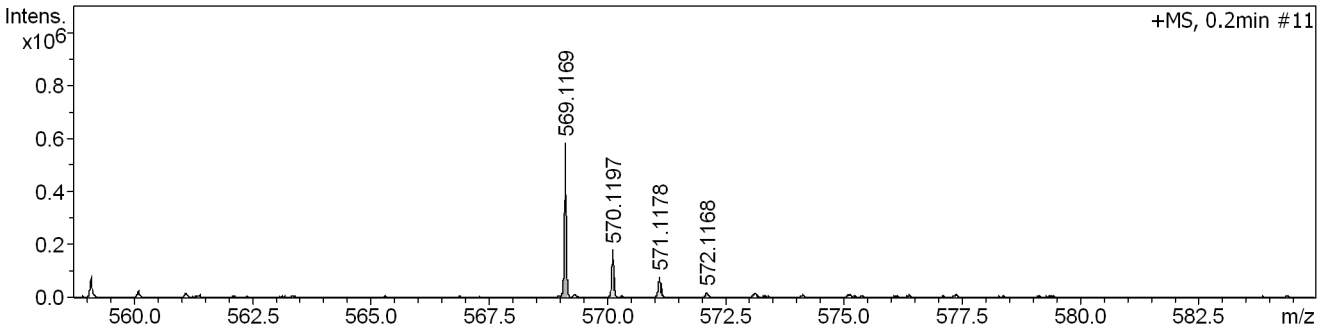
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-38-1_P1-B-7_01_32733.d	Acquisition Date	7/6/2022 2:13:04 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-38-1	Instrument	maXis impact 282001.00122
Comment			

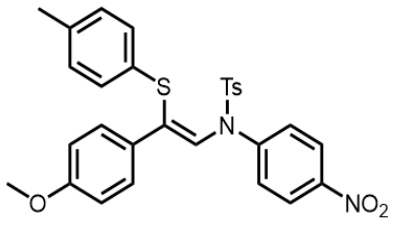
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	569.1169	20341	467.8	583068	100.0	0.0280
2	570.1197	14238	144.6	180392	30.9	0.0400
3	571.1178	12515	64.4	80240	13.8	0.0456
4	572.1168	11658	15.0	18668	3.2	0.0491

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
569.1169	1	C29H26N2NaO5S2	569.1175	1.2	19.3	1	90.72	17.5	even	ok



3ad

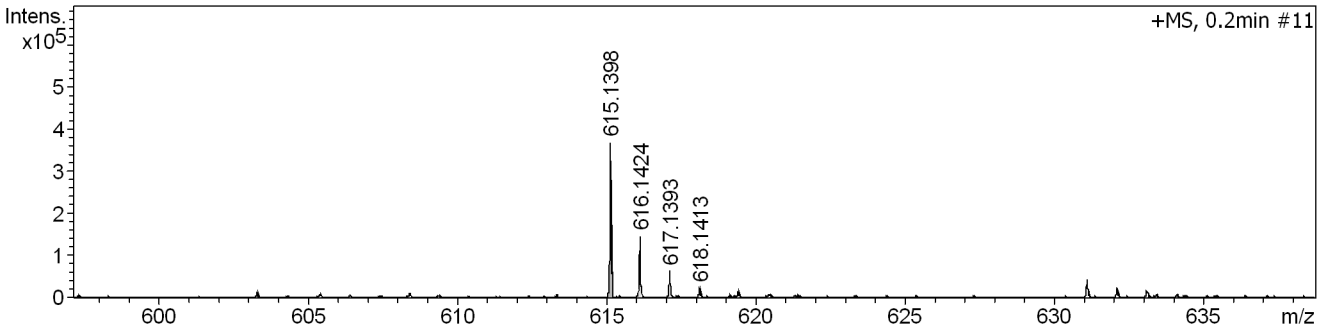
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-61-2_P1-D-4_01_32942.d	Acquisition Date	7/15/2022 10:52:10 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-61-2	Instrument	maXis impact 282001.00122
Comment			

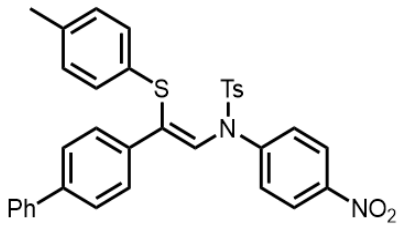
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	615.1398	19942	385.4	366920	100.0	0.0308
2	616.1424	16519	152.4	144804	39.5	0.0373
3	617.1393	13504	65.3	61952	16.9	0.0457
4	618.1413	14290	22.2	21068	5.7	0.0433

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
615.1398	1	C34H28N2NaO4S2	615.1383	-2.5	6.0	1	53.98	21.5	even	ok



3ae

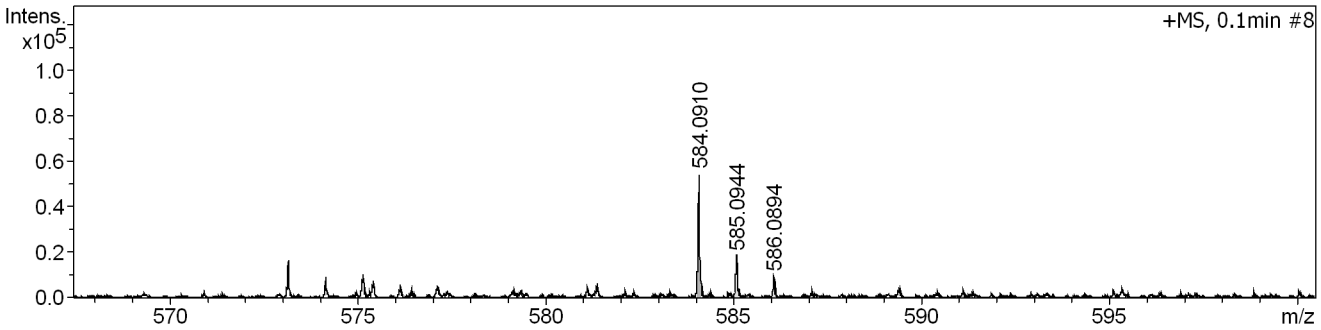
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-61-1_P1-D-3_01_32941.d	Acquisition Date	7/15/2022 10:48:54 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-61-1	Instrument	maXis impact 282001.00122
Comment			

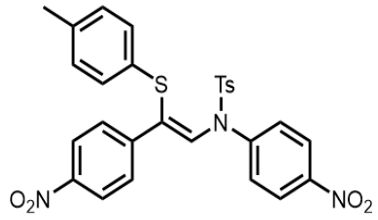
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	584.0910	13424	62.0	53920	100.0	0.0435
2	585.0944	14711	20.6	17876	33.2	0.0398
3	586.0894	15388	10.2	8852	16.4	0.0381

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
584.0910	1	C28H23N3NaO6S2	584.0920	1.7	18.3	1	70.69	18.5	even	ok



3af

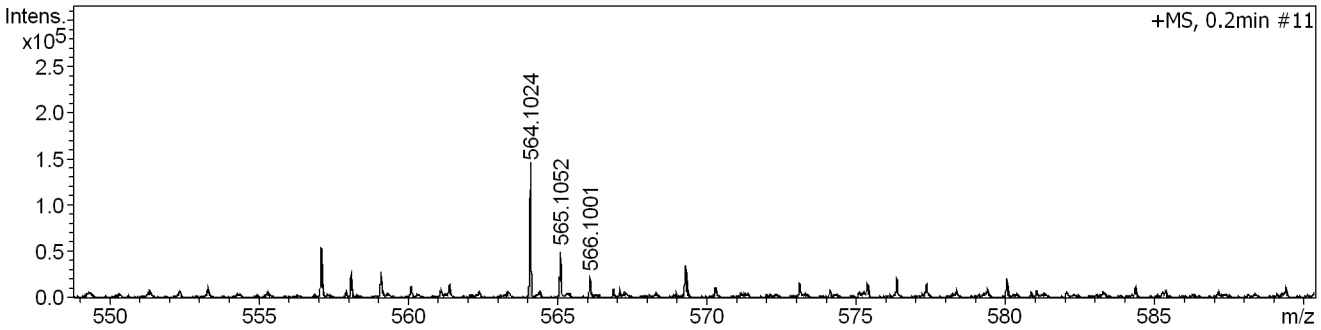
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-5-44-1_P1-C-1_01_32736.d	Acquisition Date	7/6/2022 2:22:29 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-44-1	Instrument	maXis impact 282001.00122
Comment			

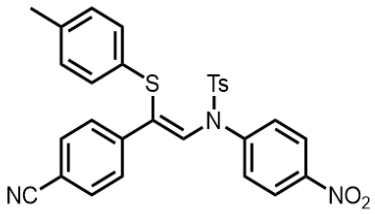
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	564.1024	14161	130.4	141400	100.0	0.0398
2	565.1052	12553	45.5	49400	34.9	0.0450
3	566.1001	13313	20.5	22188	15.7	0.0425

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
564.1024	1	C29H23N3NaO4S2	564.1022	-0.2	5.2	1	100.00	19.5	even	ok



3ag

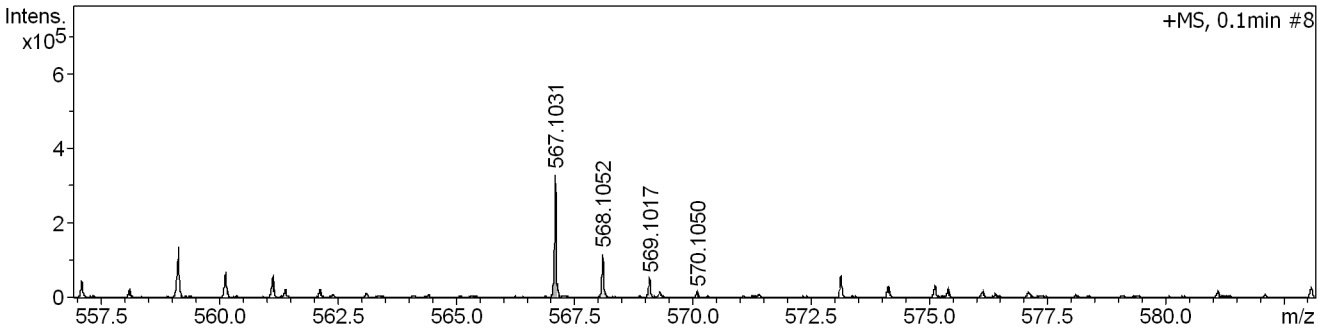
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/6/2022 2:03:39 PM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-5-45-3_P1-B-4_01_32730.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-45-3	Instrument	maXis impact 282001.00122
Comment			

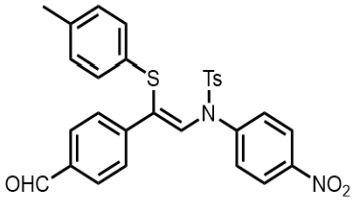
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	567.1031	16662	290.2	328948	100.0	0.0340
2	568.1052	14877	104.1	118016	35.9	0.0382
3	569.1017	13347	44.8	50700	15.4	0.0426
4	570.1050	12768	10.9	12376	3.8	0.0446

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
567.1031	1	C29H24N2NaO5S2	567.1019	-2.2	8.0	2	50.56	18.5	even	ok



3ah

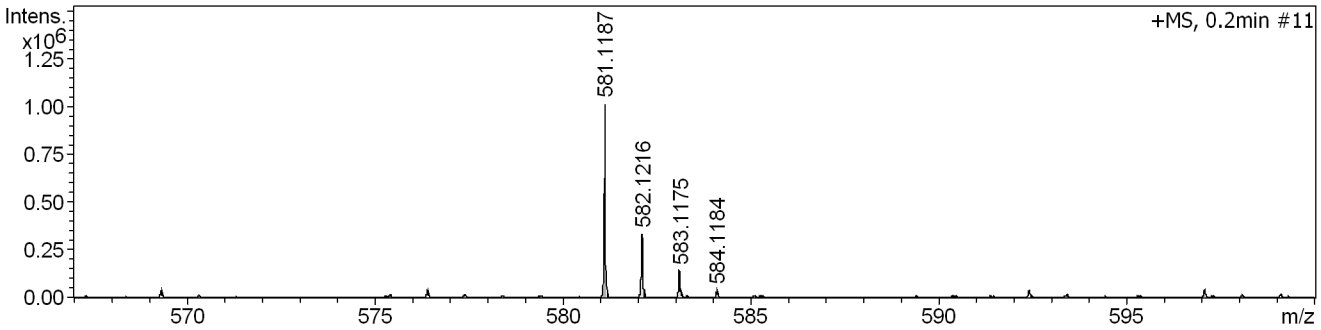
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/6/2022 2:00:31 PM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-5-45-2_P1-B-3_01_32729.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-5-45-2	Instrument	maXis impact 282001.00122
Comment			

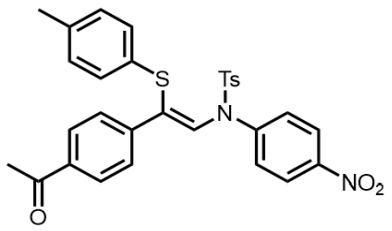
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	581.1187	23819	1015.4	1012768	100.0	0.0244
2	582.1216	18708	334.3	333568	32.9	0.0311
3	583.1175	14867	140.6	140308	13.9	0.0392
4	584.1184	13511	35.4	35328	3.5	0.0432

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
581.1187	1	C30H26N2NaO5S2	581.1175	-2.1	14.4	1	69.88	18.5	even	ok



3ai

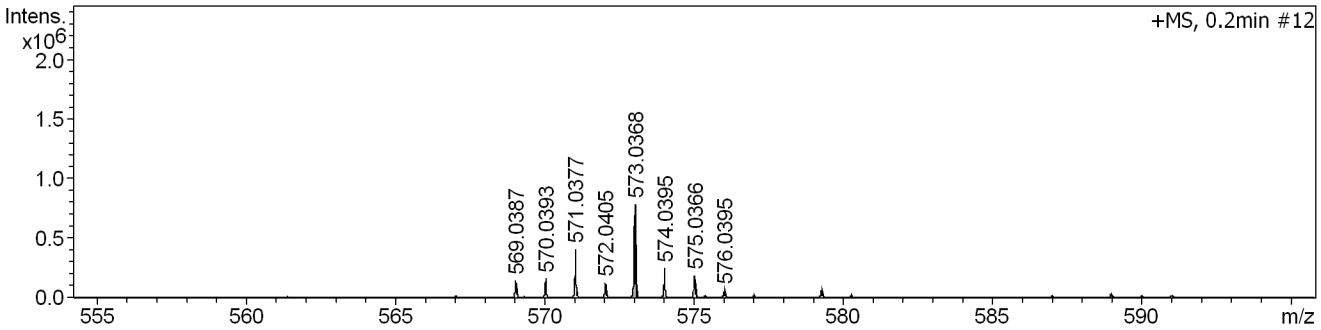
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/15/2022 10:23:49 AM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-6-78_P1-C-4_01_32933.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-78	Instrument	maXis impact 282001.00122
Comment			

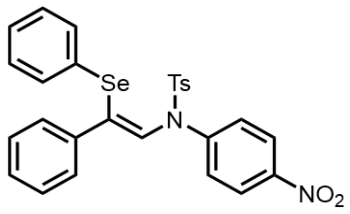
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	569.0387	14932	121.5	139664	17.9	0.0381
2	570.0393	15005	140.8	161616	20.7	0.0380
3	571.0377	17951	353.4	404860	51.8	0.0318
4	572.0405	15797	109.4	125104	16.0	0.0362
5	573.0368	21569	685.4	781996	100.0	0.0266
6	574.0395	17393	214.5	244184	31.2	0.0330
7	575.0366	15019	167.2	190104	24.3	0.0383
8	576.0395	13892	50.0	56756	7.3	0.0415

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
573.0368	1	C27H22N2NaO4SSe	573.0359	-1.6	6.7	1	80.38	17.5	even	ok



5a

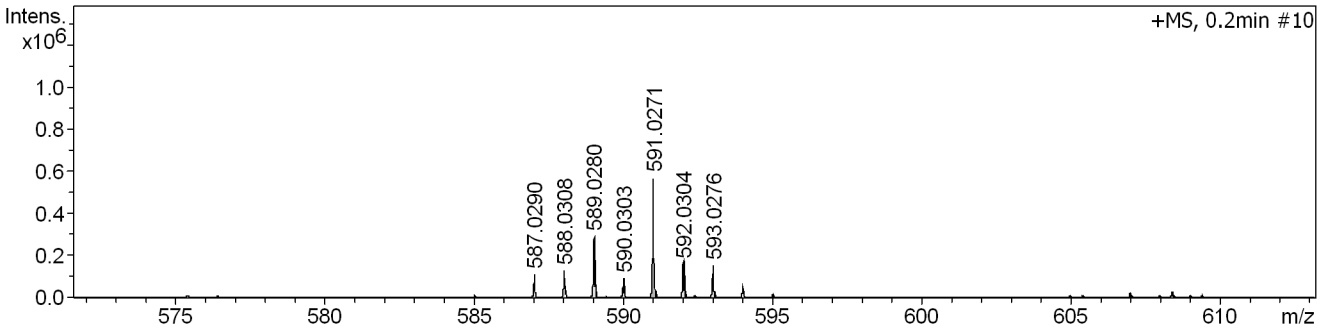
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/15/2022 10:36:23 AM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-6-82-2_P1-C-8_01_32937.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-82-2	Instrument	maXis impact 282001.00122
Comment			

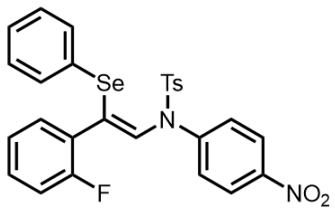
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	587.0290	16054	134.2	110068	19.4	0.0366
2	588.0308	16945	155.4	127280	22.4	0.0347
3	589.0280	16881	353.8	289252	51.0	0.0349
4	590.0303	16110	110.4	90112	15.9	0.0366
5	591.0271	21669	696.3	567128	100.0	0.0273
6	592.0304	15268	192.5	156688	27.6	0.0388
7	593.0276	18294	186.9	151964	26.8	0.0324

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
591.0271	1	C27H21FN2NaO4SSe	591.0265	-1.0	11.7	6	81.51	17.5	even	ok



5b

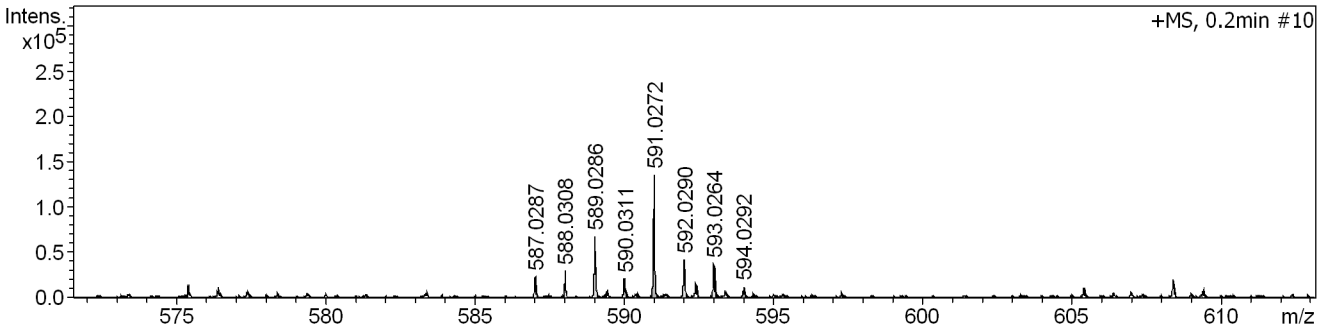
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-79-4_P1-C-5_01_32934.d	Acquisition Date	7/15/2022 10:26:57 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-79-4	Instrument	maXis impact 282001.00122
Comment			

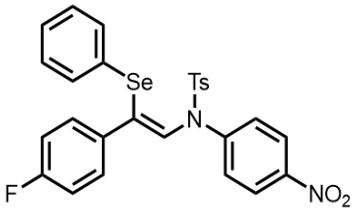
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	587.0287	12151	27.1	23420	17.3	0.0483
2	588.0308	16091	34.0	29368	21.7	0.0365
3	589.0286	15080	78.4	67696	50.1	0.0391
4	590.0311	14744	24.3	20960	15.5	0.0400
5	591.0272	17056	157.1	135208	100.0	0.0347
6	592.0290	15379	48.9	42040	31.1	0.0385
7	593.0264	15076	43.5	37356	27.6	0.0393
8	594.0292	17981	14.2	12216	9.0	0.0330

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
591.0272	1	C27H21FN2NaO4SSe	591.0265	-1.2	10.2	1	78.88	17.5	even	ok



5c

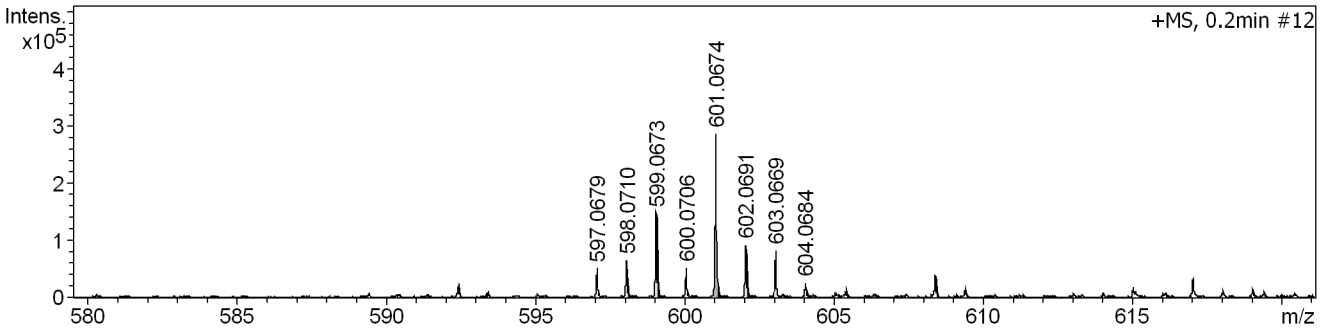
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-82-1_P1-C-7_01_32936.d	Acquisition Date	7/15/2022 10:33:14 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-82-1	Instrument	maXis impact 282001.00122
Comment			

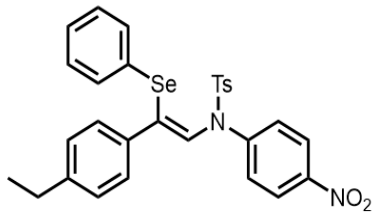
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	597.0679	12789	42.1	51724	18.1	0.0467
2	598.0710	15170	53.7	65896	23.1	0.0394
3	599.0673	14267	120.0	147080	51.5	0.0420
4	600.0706	14835	42.7	52244	18.3	0.0404
5	601.0674	17041	233.5	285504	100.0	0.0353
6	602.0691	13956	75.7	92396	32.4	0.0431
7	603.0669	15152	67.9	82840	29.0	0.0398
8	604.0684	14034	20.9	25404	8.9	0.0430

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e^- Conf	N-Rule
601.0674	1	C29H26N2NaO4SSe	601.0672	-0.3	11.5	1	100.00	17.5	even	ok



5d

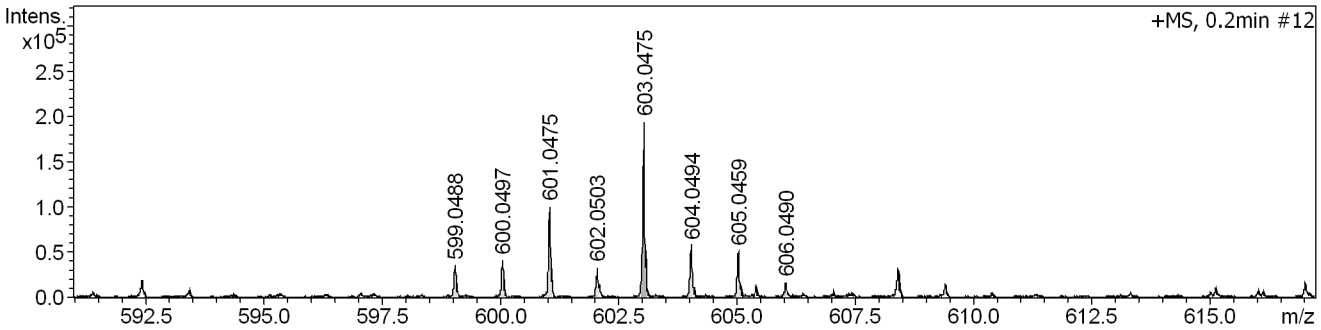
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\HJF-6-80-3_P1-C-6_01_32935.d	Acquisition Date	7/15/2022 10:30:06 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-6-80-3	Instrument	maXis impact 282001.00122
Comment			

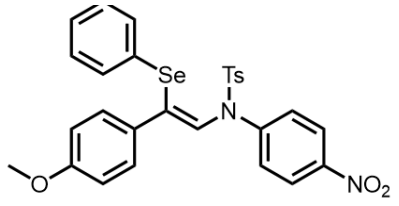
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	599.0488	13486	29.8	35272	18.3	0.0444
2	600.0497	15164	34.8	41152	21.3	0.0396
3	601.0475	14186	84.8	100000	51.7	0.0424
4	602.0503	13436	28.0	32920	17.0	0.0448
5	603.0475	17186	164.2	193264	100.0	0.0351
6	604.0494	13147	48.4	56860	29.4	0.0459
7	605.0459	13162	43.3	50824	26.3	0.0460
8	606.0490	12246	13.5	15856	8.2	0.0495

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
603.0475	1	C28H24N2NaO5SSe	603.0465	-1.8	7.9	1	73.55	17.5	even	ok



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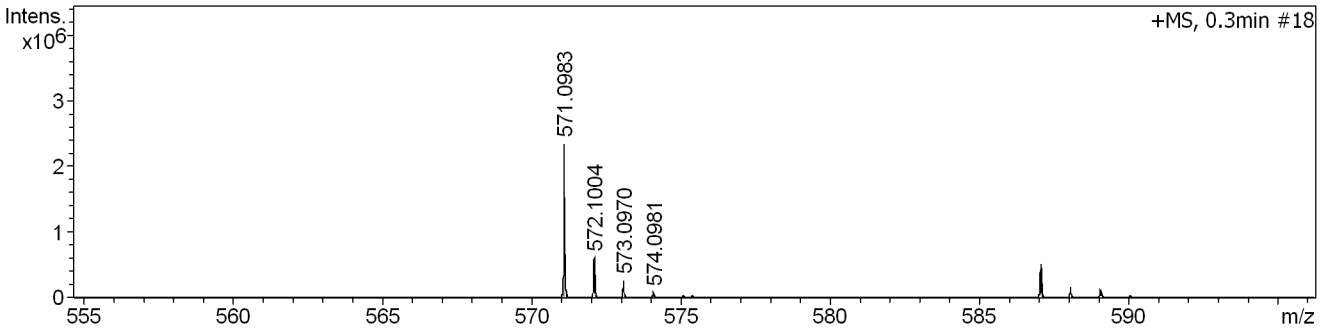
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/6/2022 3:03:12 PM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-OXYGEN_P1-D-5_01_32749.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-OXYGEN	Instrument	maXis impact 282001.00122
Comment			

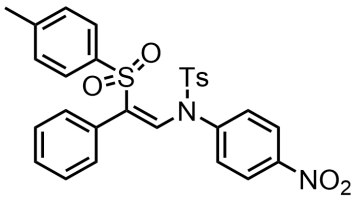
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	571.0983	22900	2144.0	2350040	100.0	0.0249
2	572.1004	19432	564.9	617948	26.3	0.0294
3	573.0970	15500	237.3	259068	11.0	0.0370
4	574.0981	14900	68.8	74952	3.2	0.0385

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
571.0983	1	C28H24N2NaO6S2	571.0968	-2.6	36.5	7	39.60	17.5	even	ok



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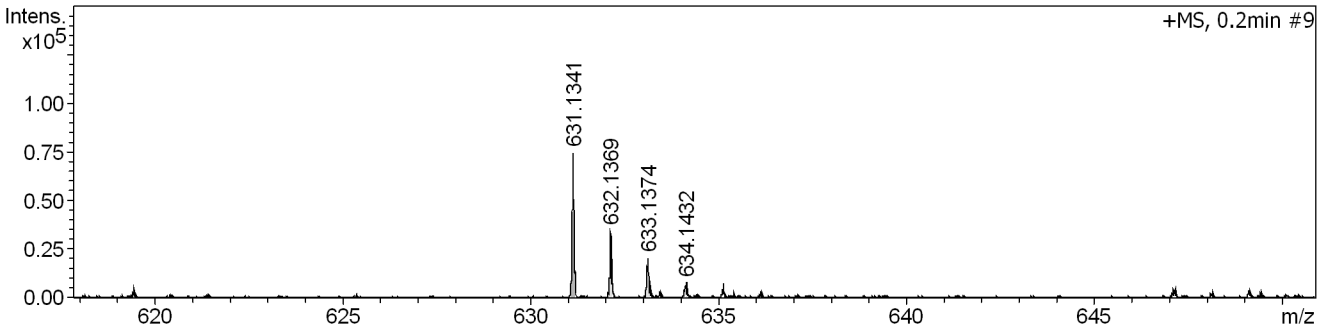
Mass Spectrum List Report

Analysis Info

Acquisition Date	7/15/2022 11:07:50 AM		
Analysis Name	D:\Data\chem. dep\liulu\HJF-SUZUKI-0712_P1-D-9_01_32947.d		
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	HJF-SUZUKI-0712	Instrument	maXis impact 282001.00122
Comment			

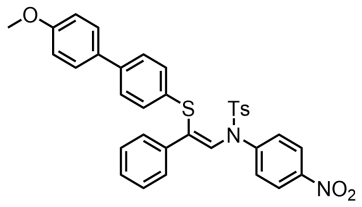
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	631.1341	13857	102.8	74152	100.0	0.0455
2	632.1369	16771	47.5	34224	46.2	0.0377
3	633.1374	12596	28.4	20424	27.5	0.0503
4	634.1432	21868	10.0	7180	9.7	0.0290

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
631.1341	1	C34H28N2NaO5S2	631.1332	-1.4	57.7	3	20.74	21.5	even	ok



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