Kinetic Resolution of Sulfur-Stereogenic Sulfoximines by Pd(II)-MPAA Catalyzed C−H Arylation and Olefination

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SUPPORTING INFORMATION

Table of Contents **Page**

1. General Experimental Information:

All the reactions were performed in oven-dried screw capped tubes. Commercial grade solvents were distilled prior to use. Column chromatography was performed using either 100–200 Mesh or 230–400 Mesh silica gel. Thin layer chromatography (TLC) was performed on silica gel GF254 plates. Visualization of spots on TLC plates was accomplished with UV light (254 nm) and staining over I_2 chamber.

Proton, carbon, and fluorine nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR, and ^{19}F NMR) were recorded based on the resonating frequencies as follows:(^{1}H NMR, 400 MHz; ^{13}C NMR, 101 MHz; ^{19}F NMR, 376 MHz) and (^{1}H NMR, 500 MHz; ^{13}C NMR, 126 MHz; ^{19}F NMR, 470 MHz) having the solvent resonance as internal standard (^{1}H NMR, $CDCl_3$ at 7.26 ppm; ^{13}C NMR, $CDCl_3$ at 77.0 ppm). In few cases, tetramethylsilane (TMS) was used as reference standard at 0.00 ppm. Data for ^{1}H NMR are reported as follows: chemical shift (ppm), multiplicity (s = singlet; bs = broad singlet; d = doublet; bd = broad doublet, t = triplet; bt = broad triplet; q = quartet; m = multiplet), coupling constants, *J*, in (Hz), and integration. Data for ^{13}C NMR, ^{19}F NMR were reported in terms of chemical shift (ppm). IR spectra were reported in cm^{-1}. LC–MS spectra were obtained with ionization voltage of 70 ev; data was reported in the form of *m/z* (intensity relative to base peak = 100). Melting points were determined by electro–thermal heating and are uncorrected. High resolution mass spectra were obtained in ESI mode. X-ray data was collected at 298K using graphite monochromated Mo–Kα radiation (0.71073 Å).

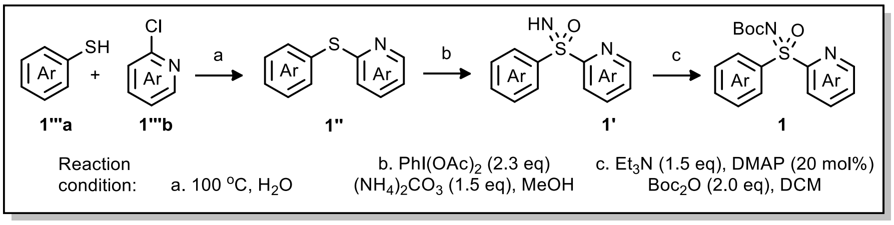
Enantiomeric ratios (er) were determined on a Shimadzu LC-20AD HPLC system using commercially available chiral columns. All racemic products were prepared under the same procedure than the chiral products although with the employment of a racemic monoprotected amino acid ligand.

Materials: Unless otherwise noted, all the reagents and intermediates were obtained commercially and used without purification. Dichloromethane (DCM), 1,2-dichloroethane (DCE), and 1,4-dioxane were distilled over CaH_2. $Pd(OAc)_2$, trifluoro toluene (TFT), quinones, acrylates, boronic acids and amino acid ligands were purchased from Sigma Aldrich Ltd, and used as received. Analytical and spectral data of all the known compounds are exactly matching with reported values.

2. Experimental Procedures:

2.1 Preparation of substrates

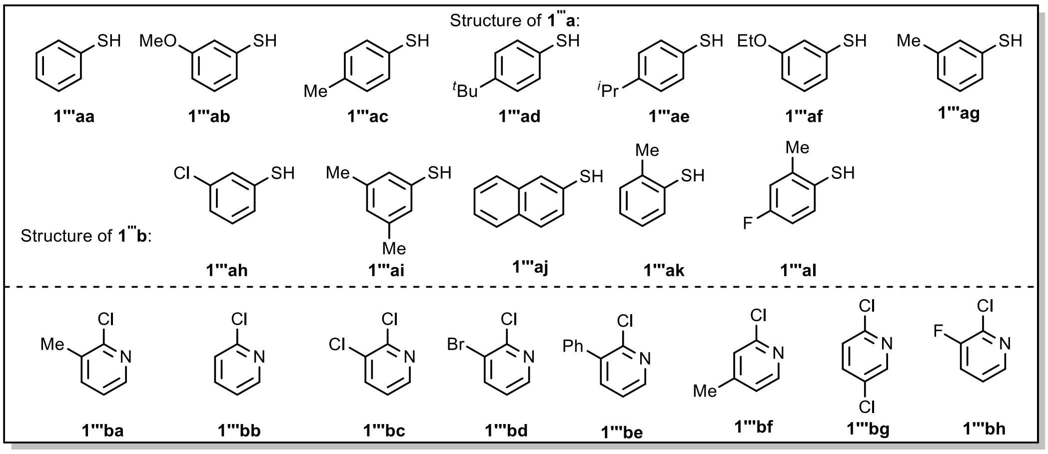
General procedure for the synthesis of racemic (rac) 1a–1l (GP-1):[1]



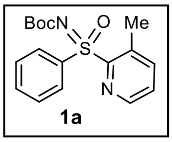
A suspension mixture of thiol **1‴a** (5.5 mmol) and substituted-2-chloro pyridine **1‴b** (5.0 mmol) in H_2O (5.0 mL) was taken in a 50 mL screw capped tube and stirred at 100 °C for 6 h. After reaction completion, the product was extracted with EtOAc (2 × 100 mL). Then the combined organic extracts were washed with $NaHCO_3$ solution (2 × 100 mL). Finally the organic layer was dried over Na_2SO_4. The solvent was removed under reduced pressure to give the crude sulfide product **1″**, which was used for the next step without further purification.

To a stirred solution of sulfide **1″** in MeOH (10 mL) was added $(NH_4)_2CO_3$ (0.72 g, 7.5 mmol). Subsequently, $PhI(OAc)_2$ (3.7 g, 11.5 mmol) was added and the resulting mixture was stirred at rt. Upon disappearance of sulfide (checked by TLC), the solvent was removed under reduced pressure. The phenyl iodide and other non polar impurities were eliminated though a short column filtration eluenting with hexane: ethyl acetate 90:10 mixture at first and then with 100% ethyl acetate. The crude sulfoximine product **1′** was collected; which was used for the next step without further purification.

To a stirred solution of crude sulfoximine **1′** in dry CH_2Cl_2 (100 mL) was added triethylamine (10 mmol) and 4-N,N-dimethylamino pyridine (DMAP; 1.0 mol %). The reaction mixture was stirred for 30 min at 0°C. Next, a solution of Boc_2O (10 mmol) in dry CH_2Cl_2 (50 mL) was added. The solution was warmed to rt and stirred for 5 h. Evaporation of organic solvent and purification by column chromatography eluting with hexane: ethyl acetate 3:2 mixture gave the corresponding N-Boc protected aryl-2-pyridyl sulfoximine products **1a**, **1a-1**, **1a–2**, **1a–3**, and **1b–1l**.

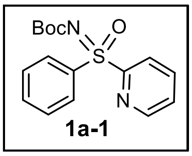


***N*-Boc-protected 3-methyl-2-(phenylsulfonimidoyl)pyridine (1a):**



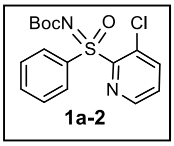
1a (864 mg, 52%) as colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, J = 4.8 Hz, 1H), 8.10–8.04 (m, 2H), 7.63–7.55 (m, 2H), 7.54–7.46 (m, 2H), 7.32–7.24 (m, 1H), 2.74 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 155.1, 146.4, 141.7, 136.9, 135.0, 133.5, 129.2, 128.8, 126.5, 80.3, 27.8, 19.1; IR (KBr) ν_{max} 2918, 2850, 1734, 1464, 1261, 1150, 804 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{20}N_2NaO_3S$ $(M+Na)^+$: calcd. 355.1087, found 355.1096.

***N*-Boc-protected 2-(phenylsulfonimidoyl)pyridine (1a-1):**



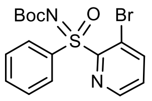
1a-1 (860 mg, 54%) as colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64–8.59 (m, 1H), 8.35–8.29 (m, 1H), 8.15–8.08 (m, 2H), 7.91 (t, J = 7.75 Hz, 1H), 7.61–7.54 (m, 1H), 7.50 (t, J = 7.5 Hz, 2H), 7.45–7.39 (m, 1H), 1.31 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 157.3, 150.2, 138.1, 136.7, 133.6, 129.04, 129.00, 126.6, 123.4, 80.6, 27.8; IR (KBr) ν_{max} 2976, 1677, 1451, 1238, 911 cm^{-1}; **HRMS (ESI)** for $C_{16}H_{18}N_2NaO_3S^+$$(M+H)^+$: calcd. 341.0930, found 341.0944.

***N*-Boc-protected 3-chloro-2-(phenylsulfonimidoyl)pyridine (1a-2):**



1a-2 (864 mg, 49%) as pale-yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61–8.55 (m, 1H), 8.17–8.11 (m, 2H), 7.78 (dt, J = 8.0, 1.2 Hz, 1H), 7.64–7.57 (m, 1H), 7.54–7.47 (m, 2H), 7.42 (dd, J = 8.0, 4.5 Hz, 1H), 1.34 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.9, 153.3, 147.2, 140.7, 135.8, 134.0, 130.8, 129.4, 129.0, 127.7, 80.7, 27.8; IR (KBr) ν_{max} 2977, 2923, 1738, 1700, 1246, 1151, 1084 cm^{-1}; **HRMS (ESI)** for $C_{16}H_{17}ClN_2NaO_3S^+$ $(M+Na)^+$: calcd. 375.0541, found 375.0551.

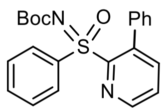
***N*-Boc-protected 3-bromo-2-(phenylsulfonimidoyl)pyridine (1a-3):**



1a-3

1a-3 (1.05 g, 53%) as yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (dd, *J* = 4.5, 1.0 Hz, 1H), 8.21–8.15 (m, 2H), 8.02 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.63 (t, *J* = 7.25 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 2H), 7.32 (dd, *J* = 8.0, 4.5 Hz, 1H), 1.37 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 154.7, 147.7, 144.3, 135.8, 134.0, 129.6, 129.0, 127.5, 118.6, 80.8, 27.9; IR (KBr) ν_{max} 2980, 2926, 1665, 1273, 1247, 1153 cm^{-1}; **HRMS (ESI)** for $C_{16}H_{17}BrN_2NaO_3S^+$ $(M+Na)^+$: calcd. 419.0035, found 419.0043.

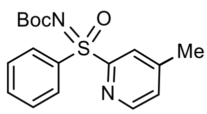
***N*-Boc-protected 3-phenyl-2-(phenylsulfonimidoyl)pyridine (1a-4):**



1a-4

1a-4 (828 mg, 42%) as colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (bd, *J* = 4.5 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 6.5 Hz, 1H), 7.55 (d, *J* = 7.25 Hz, 1H), 7.52–7.46 (m, 1H), 7.45–7.35 (m, 5H), 7.30–7.27 (m, 2H), 1.40 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 154.8, 148.0, 141.7, 138.9, 137.6, 136.2, 133.3, 129.3, 129.2, 128.7, 128.3, 127.7, 126.1, 80.4, 28.0; **HRMS (ESI)** for $C_{22}H_{23}N_2O_3S^+$ $(M+H)^+$: calcd. 395.1424, found 395.1424.

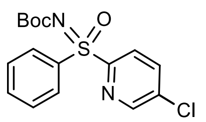
***N*-Boc-protected 4-methyl-2-(phenylsulfonimidoyl)pyridine (1a-5):**



1a-5

1a-5 (914 mg, 55%) as colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 5.0 Hz, 1H), 8.18–8.08 (m, 3H), 7.61–7.54 (m, 1H), 7.54–7.48 (m, 2H), 7.22 (bd, *J* = 4.5 Hz, 1H), 2.45 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 157.4, 150.1, 150.0, 137.0, 133.5, 129.03, 128.96, 127.4, 124.1, 80.6, 27.9, 21.2; **HRMS (ESI)** for $C_{17}H_{21}N_2O_3S^+$ $(M+H)^+$: calcd. 333.1267, found 333.1269.

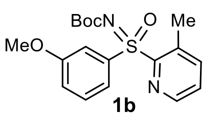
***N*-Boc-protected 5-chloro-2-(phenylsulfonimidoyl)pyridine (1a-6):**



1a-6

1a-6 (864 mg, 49%) as colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (dd, *J* = 2.5, 0.5 Hz, 1H), 8.29 (dd, *J* = 8.25, 1.25 Hz, 1H), 8.15–8.09 (m, 2H), 7.89 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.65–7.58 (m, 1H), 7.57–7.50 (m, 2H), 1.36 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 156.0, 149.2, 137.7, 136.3, 135.6, 133.9, 129.2, 129.1, 124.5, 80.9, 27.9; **HRMS (ESI)** for $C_{16}H_{18}ClN_2O_3S^+$ $(M+H)^+$: calcd. 353.0721, found 353.0720.

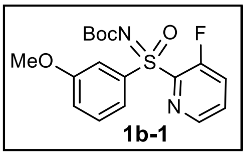
***N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):**



1b

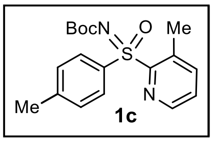
1b (761 mg, 42%) as colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 4.5 Hz, 1H), 7.69–7.57 (m, 3H), 7.42 (t, *J* = 8.25 Hz, 1H), 7.31 (dd, *J* = 7.5, 4.5 Hz, 1H), 7.16–7.10 (m, 1H), 3.84 (s, 3H), 2.77 (s, 3H), 1.34 (s, 9H); ^{13}C NMR (126 MHz, CDCl3) δ 159.8, 157.5, 155.3, 146.4, 141.7, 138.3, 135.0, 129.8, 126.5, 121.5, 120.2, 113.7, 80.4, 55.7, 27.9, 19.2; IR (KBr) ν_{max} 2970, 2926, 1739, 1649, 1367, 1241, 1038 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{22}N_2NaO_4S^+$ $(M+Na)^+$: calcd. 385.1192, found 385.1202.

***N*-Boc-protected 3-fluoro-2-(3-methoxyphenylsulfonimidoyl)pyridine (1b-1):**



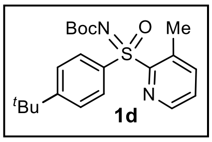
1b-1 (769 mg, 42%) as colorless solid. ^1H NMR (500 MHz, $CDCl_3$) δ 8.52–8.47 (m, 1H), 7.79–7.74 (m, 1H) 7.68–7.64 (m, 1H), 7.57–7.50 (m, 2H), 7.46–7.38 (m, 1H), 7.17–7.11 (m, 1H), 3.84 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.0, 157.9, 156.5 (d, *J* = 193 Hz), 145.3, 145.26, 137.6, 130.2, 129.3, 126.4 (d, *J* = 20 Hz), 121.1 (d, *J* = 36 Hz), 113.1, 80.9, 55.8, 27.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ, ppm: −114 (s); **HRMS (ESI)** for $C_{17}H_{20}FN_2O_4S^+$ $(M+H)^+$: calcd. 367.1122, found 367.1122.

***N*-Boc-protected 3-methyl-2-(4-methylphenylsulfonimidoyl)pyridine (1c):**



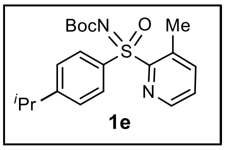
1c (831 mg, 48%) as colorless solid. ^1H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 4.0 Hz, 1H), 7.97–7.91 (m, 2H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.32–7.24 (m, 3H), 2.72 (s, 3H), 2.38 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.5, 155.3, 146.3, 144.5, 141.6, 134.7, 133.7, 129.4, 129.1, 126.4, 80.2, 27.8, 21.5, 19.1; IR (KBr) ν_{max} 2980, 2923, 2847, 1664, 1272, 1152, 1090 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{22}N_2NaO_3S^+$ $(M+Na)^+$: calcd. 369.1243, found 369.1258.

***N*-Boc-protected 2-(4-(*tert*-butyl)phenylsulfonimidoyl)-3-methylpyridine (1d):**



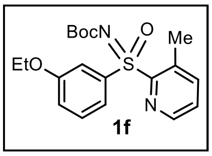
1d (1.01 g, 52%) as colorless solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 4.4 Hz, 1H), 8.04–7.97 (m, 2H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.56–7.50 (m, 2H), 7.31 (dd, *J* = 7.8, 4.6 Hz, 1H), 2.76 (s, 3H), 1.34 (s, 9H), 1.32 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 157.4, 155.5, 146.5, 141.6, 134.9, 133.9, 129.1, 126.4, 125.9, 80.3, 35.2, 31.0, 27.9, 19.3; IR (KBr) ν_{max} 2968, 1699, 1239, 1223, 1148, 1069, 909 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{28}N_2NaO_3S^+$ $(M+Na)^+$: calcd. 411.1713, found 411.1724.

***N*-Boc-protected 2-(4-isopropylphenylsulfonimidoyl)-3-methylpyridine (1e):**



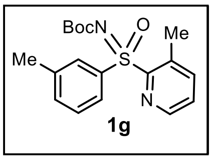
1e (1.05 g, 56%) as light red solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 4.4 Hz, 1H), 8.03–7.96 (m, 2H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 2H), 7.30 (dd, *J* = 7.8, 4.6 Hz, 1H), 3.03–2.89 (m, 1H), 2.75 (s, 3H), 1.34 (s, 9H), 1.24 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 155.5, 155.1, 146.5, 141.6, 134.9, 134.2, 129.4, 127.0, 126.4, 80.3, 34.2, 27.9, 23.5, 19.3; IR (KBr) ν_{max} 2970, 1663, 1269, 1245, 1151, 1093, 896 cm^{-1}; **HRMS (ESI)** for $C_{20}H_{27}N_2O_3S^+$ $(M+H)^+$: calcd. 375.1737, found 375.1747.

N-Boc-protected 2-(3-ethoxyphenylsulfonimidoyl)-3-methylpyridine (1f):



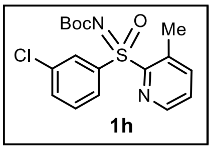
1f (866 mg, 46%) as yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40–8.35 (m, 1H), 7.67–7.55 (m, 3H), 7.44–7.36 (m, 1H), 7.34–7.27 (m, 1H), 7.14–7.07 (m, 1H), 4.05 (q, J = 7.07 Hz, 2H), 2.75 (s, 3H), 1.38 (t, J = 7.0 Hz, 3H), 1.33 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 157.4, 155.2, 146.4, 141.7, 138.1, 134.9, 129.7, 126.5, 121.3, 120.6, 114.3, 80.3, 64.0, 27.9, 19.2, 14.5; IR (KBr) ν_{max} 2980, 2929, 1671, 1598, 1471, 1245, 1154 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{24}N_2NaO_4S^+$ $(M+Na)^+$: calcd. 399.1349, found 399.1358.

N-Boc-protected 3-methyl-2-(3-methylphenylsulfonimidoyl)pyridine (1g):



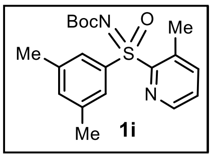
1g (883 mg, 51%) as colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, J = 4.0 Hz, 1H), 7.93–7.84 (m, 2H), 7.61 (d, J = 7.5 Hz, 1H), 7.42–7.37 (m, 2H), 7.33–7.27 (m, 1H), 2.75 (s, 3H), 2.39 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.6, 155.2, 146.5, 141.7, 139.1, 136.8, 135.0, 134.4, 129.4, 128.6, 126.5, 126.3, 80.3, 27.9, 21.3, 19.2; IR (KBr) ν_{max} 2974, 1671, 1264, 1244, 1145, 1095, 894 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{22}N_2NaO_3S^+$ $(M+Na)^+$: calcd. 369.1243, found 369.1259.

N-Boc-protected 2-(3-chlorophenylsulfonimidoyl)-3-methylpyridine (1h):



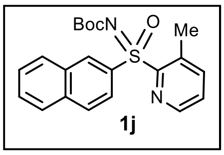
1h (899 mg, 49%) as yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35 (d, J = 5.0 Hz, 1H), 8.12–8.07 (m, 1H), 8.00–7.94 (m, 1H), 7.64 (d, J = 8.0 Hz, 1H),7.60–7.54 (m, 1H), 7.47 (t, J = 8.0 Hz, 1H), 7.32 (dd, J = 7.5 Hz, 1H), 2.79 (s, 3H), 1.34 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.2, 154.9, 146.4, 141.8, 139.0, 135.3, 135.1, 133.6, 129.9, 129.4, 127.6, 126.7, 80.7, 27.9, 19.1; IR (KBr) ν_{max} 2977, 2926, 1699, 1666, 1271, 1235, 1147 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{19}ClN_2NaO_3S^+$ $(M+Na)^+$: calcd. 389.0697, found 389.0709.

N-Boc-protected 2-(3,5-dimethylphenylsulfonimidoyl)-3-methylpyridine (1i):



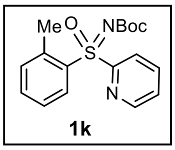
1i (1.03 g, 57%) as colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, J = 4.5 Hz, 1H), 7.69 (bs, 2H), 7.61 (d, J = 7.0 Hz, 1H), 7.30 (dd, J = 7.5, 4.5 Hz, 1H), 7.20 (bs, 1H), 2.75 (s, 3H), 2.35 (s, 6H), 1.34 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 155.3, 146.6, 141.7, 138.9, 136.6, 135.4, 135.0, 126.5, 126.4, 80.3, 27.9, 21.2, 19.3; IR (KBr) ν_{max} 2977, 2929, 2850, 1741, 1700, 1666, 1273, 1157 cm^{-1}; **HRMS (ESI)** for $C_{19}H_{24}N_2NaO_3S^+$ $(M+Na)^+$: calcd. 383.1400, found 383.1409.

***N*-Boc-protected 3-methyl-2-(naphthalene-2-sulfonimidoyl)pyridine (1j):**



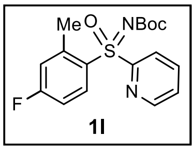
1j (1.16 g, 61%) as colorless solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (s, 1H), 8.37–8.32 (m, 1H), 8.06–8.01 (m, 1H), 8.00–7.91 (m, 2H), 7.90–7.86 (m, 1H), 7.67–7.55 (m, 3H), 7.32–7.26 (m, 1H), 2.82 (s, 3H), 1.35 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.6, 155.5, 146.4, 141.7, 135.2, 135.1, 134.1, 132.1, 131.0, 129.5, 129.2, 128.9, 127.8, 127.4, 126.4, 124.1, 80.4, 27.9, 19.2; IR (KBr) ν_{max} 3012, 2970, 2929, 1744, 1662, 1062, 857 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{22}N_2NaO_3S^+$ $(M+Na)^+$: calcd. 405.1243, found 405.1251.

***N*-Boc-protected 2-(2-methylphenylsulfonimidoyl)pyridine (1k):**



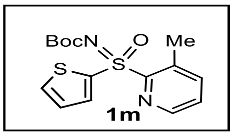
1k (864 mg, 52%) as colorless solid.; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 4.8 Hz, 1H), 8.44 (d, J = 8.0 Hz, 1H), 8.37 (d, J = 8.0 Hz, 1H), 7.94 (td, J = 7.8, 1.9 Hz, 1H), 7.52–7.37 (m, 3H), 7.22 (d, J = 7.6 Hz, 1H), 2.42 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 156.8, 150.1, 138.4, 137.8, 135.0, 133.7, 132.7, 131.4, 126.8, 126.5, 123.8, 80.5, 27.8, 20.5; IR (KBr) ν_{max} 2973, 2929, 1666, 1450, 1232, 1142, 752 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{20}N_2NaO_3S^+$ $(M+Na)^+$: calcd. 355.87, found 355.1087.

***N*-Boc-protected 2-(4-fluoro-2-methylphenylsulfonimidoyl)pyridine (1l):**



1l (823 mg, 47%) as colorless solid.; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (bd, J = 4.8 Hz, 1H), 8.42–8.32 (m, 2H), 7.94 (td, J = 7.8, 1.7 Hz, 1H), 7.49–7.42 (m, 1H), 7.10–7.01 (m, 1H), 6.91 (dd, J = 9.2, 2.4 Hz, 1H), 2.39 (s, 3H), 1.29 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4 (d, J = 258 Hz), 157.2, 156.6, 150.1, 141.8 (d, J = 9.1 Hz), 137.9, 134.3 (d, J = 10 Hz), 130.6, 126.9, 123.6, 119.5 (d, J = 22 Hz), 113.6 (d, J = 22 Hz), 80.5, 27.7, 20.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ, ppm: –104.9 (s). IR (KBr) ν_{max} 2981, 1660, 1576, 1276, 1144, 1118, 856 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{19}FN_2NaO_3S^+$ $(M+Na)^+$: calcd. 373.0993, found 373.1001.

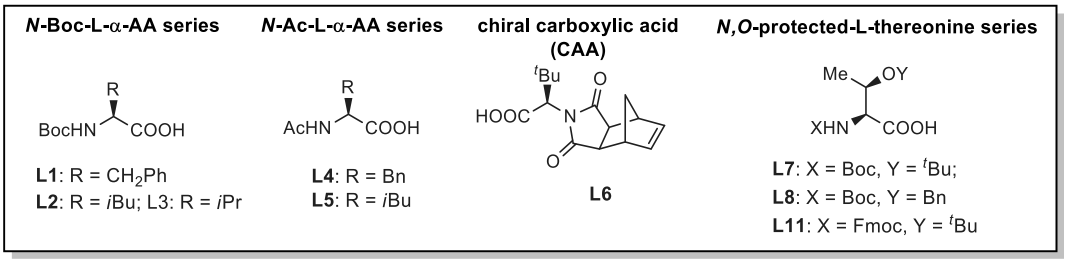
***N*-Boc-protected 3-methyl-2-(thiophene-2-sulfonimidoyl)pyridine (1m):**



1m (880 mg, 52%) as colorless solid.; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (bd, J = 4.5 Hz, 1H), 7.81–7.73 (m, 2H), 7.63 (d, J = 8.0 Hz, 1H), 7.32 (dd, J = 7.5, 4.5 Hz, 1H), 7.11 (bt, J = 4.25 Hz, 1H), 2.77 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 155.4, 146.5, 141.8, 137.3, 135.7, 135.4, 134.7, 127.6, 126.7, 80.6, 27.8, 19.2; **HRMS (ESI)** for $C_{15}H_{19}N_2O_3S_2^+$ $(M+H)^+$: calcd. 339.0832, found 339.0833.

2.2 Synthesis of chiral ligands (GP-2):[2]

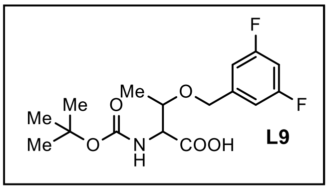
All mono protected amino acids ligands **L1–L8** and **L11** were purchased from commercial sources or synthesized following the known procedures.[2]



Synthesis of L9 and L10 ligands:

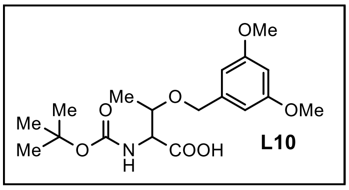
To a solution of L-Boc-Thr-OH (5.0 g, 22 mmol) in DMF (80 mL) was added sodium hydride (55% dispersion in mineral oil, 2.1 g, 48 mmol) at –20 °C. After being stirred for 2 h, benzyl bromide derivatives (24 mmol) was added to the reaction. The resulting mixture was stirred at room temperature for 5 h and then quenched with saturated NH_4Cl solution. The reaction mixture was poured into water (100 mL) and washed with diethyl ether (2 × 25 mL). The aqueous solution was acidified with citric acid and extracted with EtOAc (3 × 50 mL). The combined extracts were washed with brine (3 × 30 mL), and then dried over anhydrous Na_2SO_4. The solution was concentrated in reduced pressure and was purified by flash chromatography using a mixture of hexane and EtOAc (2 : 1 v/v) to give a thick colorless syrupy liquid.

2-((*tert*-Butoxycarbonyl)amino)-3-((3,5-difluorobenzyl)oxy)butanoic acid (L9):



L9: 5.2 g, 68% yield, colorless viscous liquid, **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.64 (s, 1H), 6.82–6.72 (m, 2H), 6.64 (t, *J* = 9.0 Hz, 1H), 5.33 (d, *J* = 9.5 Hz, 1H), 4.51 (d, *J* = 12.5 Hz, 1H), 4.41–4.33 (m, 1H), 4.19–4.13 (m, 1H), 1.43 (s, 9H), 1.25 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 175.6, 162.9 (dd, *J* = 249, 13 Hz), 156.3, 142.0 (t, *J* = 8.6 Hz), 109.8 (dd, *J* = 19, 6.5 Hz), 102.8 (t, *J* = 25 Hz), 80.3, 75.2, 69.7, 57.9, 28.2, 16.1; ^{19}F NMR (471 MHz, $CDCl_3$) δ –109.8 (s). IR (KBr) ν_{max} 2979, 1712, 1627, 1597, 1160, 1115, 847 cm^{-1}; **HRMS (ESI)** for $C_{16}H_{21}F_2NNaO_5^+$ $(M+Na)^+$: calcd. 368.1280, 368.1288.

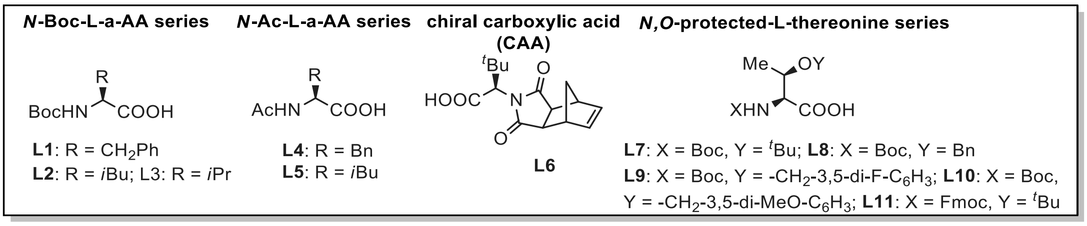
2-((*tert*-Butoxycarbonyl)amino)-3-((3,5-dimethoxybenzyl)oxy)butanoic acid (L10):

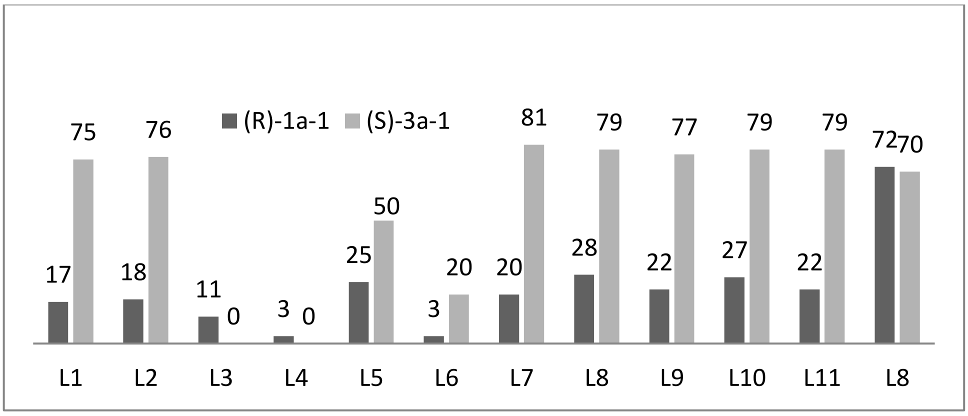


L10: 5.5 g, 68% yield, brown solid, **^{1}H NMR (500 MHz, $CDCl_3$)** δ 6.42 (bd, *J* = 2.0 Hz, 2H), 6.35 (s, 1H), 5.36 (d, *J* = 9.0 Hz, 1H), 4.50 (d, *J* = 12.0 Hz, 1H), 4.38 (d, *J* = 12.0 Hz, 1H), 4.33 (d, *J* = 9.5 Hz, 1H), 4.20–4.15 (m, 1H), 3.74 (s, 6H), 1.44 (s, 9H), 1.24 (d, *J* = 5.2 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 175.2, 160.7, 156.2, 140.1, 105.4, 99.7, 80.1, 74.5, 71.0, 58.0, 55.3, 28.3, 16.2; IR (KBr) ν_{max} 3433, 2936, 1680, 1597, 1519, 1152, 1053 cm^{-1}; **HRMS (ESI)** for $C_{18}H_{27}NNaO_7^+$ $(M+Na)^+$: calcd. 392.1680, found 392.1689.

2.3 Optimization of reaction conditions for C–H alkenylative kinetic resolution:

Table S1. Ligands screening [a]

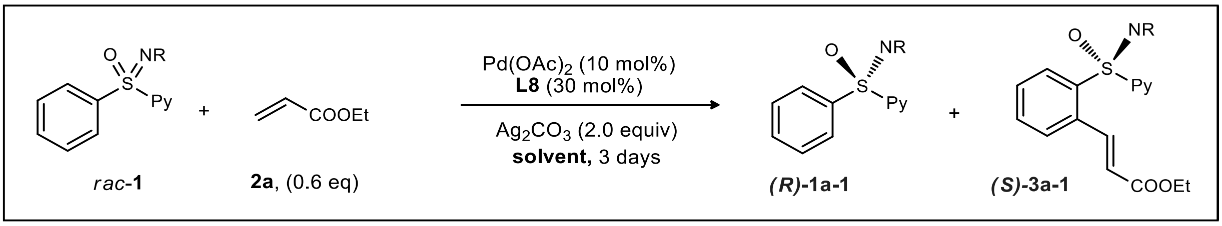




	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L8
s[d]	8	9	–	–	4	–	12	11	10	11	11	12[e]
c[c]	18	19	–	–	33	–	20	26	22	25	22	50[e]

[a]Reaction conditions: ***rac*-1a-1** (0.1 mmol), ethyl acrylate **2a** (0.6 equiv), $Pd(OAc)_2$ (10 mol%), ligand (30 mol%), Ag_2CO_3 (2.0 equiv), 1,2-DCE (1.0 mL), N_2, 75 °C, 3 days. [b]Calculated conversion, C = eeSM/(eeSM + eePR). [c]Determined by chiral HPLC analysis. [d]Selectivity factor (*s*) = ln[(1 − C)(1 − eeSM)]/ln[(1 − C)(1 + eeSM)]. [e]Ethyl acrylate (2.0 equiv) was used.

Table S2. Solvent screening[a]

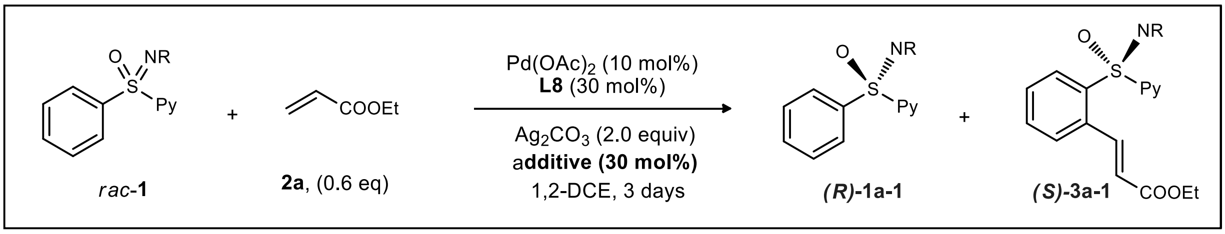


Entry	solvent	Conversion[b]	*ee* [%][c]		s[d]
			***(R)*-1a-1**	***(S)*-3a-1**	
1	THF	trace	–	–	–
2	CH_3CN	trace	–	–	–
3	DIOXANE	trace	–	–	–
4	HFIP	trace	–	–	–
5	Tol	12.76	12	82	11
6	TFT	24.78	28	85	16
7	2-chloro toluene	16.33	16	82	12
8	3-methoxy anisole	27.27	30	80	12
9	1,2-dimethoxy propane	9.9	09	82	11
10	4-Cl-TFT	17	17	83	13
11	TFE	trace	–	–	–
12	2-methoxy propen	trace	–	–	–

13	2-methyl anisole	20.75	22	84	14

[a]Reaction conditions: ***rac*-1a-1** (0.1 mmol), ethyl acrylate **2a** (0.6 equiv), $Pd(OAc)_2$ (10 mol%), **L8** (30 mol%), Ag_2CO_3 (2.0 equiv), solvent (1.0 mL), N_2, 75 °C, 3 days. [b]Calculated conversion, C = eeSM/(eeSM + eePR). [c]Determined by chiral HPLC analysis. [d]Selectivity factor (*s*) = ln[(1 − C)(1 − eeSM)]/ln[(1 − C)(1 + eeSM)]. [e]Ethyl acrylate (2.0 equiv) was used.

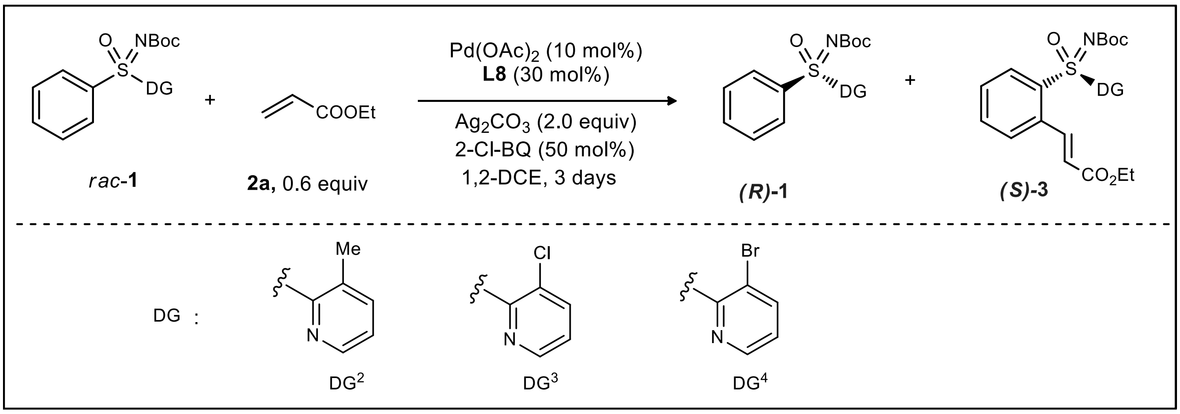
Table S3. Additive screening [a]



Entry	Additive	Conversion[b]	*ee* [%][c]		*s*[d]
			(*R*)-**1a-1**	(*S*)-**3a-1**	
1	BQ	18	17	78	10
2	2-chloro BQ	39	50	77	13
3	2, 5-dichloro BQ	35	40	75	10

[a]Reaction conditions: **rac-1a-1** (0.1 mmol), ethyl acrylate **2a** (0.6 equiv), $Pd(OAc)_2$ (10 mol%), L8 (30 mol%), Ag_2CO_3 (2.0 equiv), additives (0.3 equiv), 1,2-DCE (1.0 mL), N_2, 75 °C, 3 days. [b]Calculated conversion, C = eeSM/(eeSM + eePR). [c]Determined by chiral HPLC analysis. [d]Selectivity factor (*s*) = ln[(1 − C)(1 − eeSM)]/ln[(1 − C)(1 + eeSM)].

Table S4. Directing group screening [a]

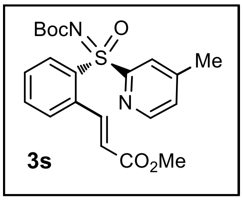


Entry	DG	Conversion[b]	*ee* [%][c]		*s*[d]
			(***R***)- **1a**	(*S*)-**3a**	
1	DG^2	17	20	96	58
2	DG^3	nr	–	–	–
3	DG^4	nr	–	–	–
4[e]	DG^2	22	27	95	48
5[f]	DG^2	27	35	94	44
6[f,g]	DG^2	34	50	96	85

[a]Reaction conditions: **rac-1** (0.1 mmol), ethyl acrylate **2a** (0.6 equiv), $Pd(OAc)_2$ (10 mol%), L8 (30 mol%), Ag_2CO_3 (2.0 equiv), additives (0.3 equiv), 1,2-DCE (1.0 mL), N_2, 75 °C, 3 days. [b]Calculated conversion, C = eeSM/(eeSM + eePR).

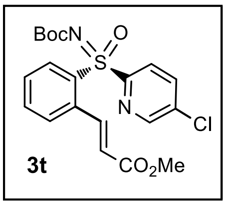
[c]Determined by chiral HPLC analysis. [d]Selectivity factor (s) = ln[(1 − C)(1 − eeSM)]/ln[(1 − C)(1 + eeSM)]. [e]Ethyl acrylate (2.0 equiv) was used. [f]Methyl acrylate instead ethyl acrylate. [g]2-Cl-BQ (50 mol%) was used.

N-Boc-protected (S,E)-methyl 3-(2-(4-methylpyridine-2-sulfonimidoyl)phenyl)acrylate (3s):



3s: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45–8.37 (m, 3H), 8.33 (bs, 1H), 7.64–7.55 (m, 2H), 7.51 (d, J = 7.0 Hz, 1H), 7.23 (bd, J = 4.5 Hz, 1H), 6.03 (d, J = 15.5 Hz, 1H), 3.77 (s, 3H), 2.45 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.1, 157.1, 156.7, 150.0, 149.9, 141.4, 135.9, 135.2, 133.8, 131.3, 129.8, 128.9, 127.7, 124.9, 122.2, 80.6, 51.8, 27.9, 21.2; **HRMS (ESI)** for $C_{21}H_{25}N_2O_5S^+$ $(M+H)^+$: calcd. 417.1479, found 417.1478.

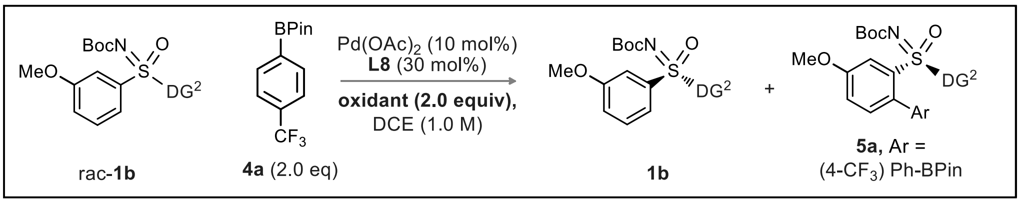
N-Boc-protected (S,E)-methyl 3-(2-(5-chloropyridine-2-sulfonimidoyl)phenyl)acrylate (3t):



3t: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (bd, J = 2.0 Hz, 1H), 8.48–8.37 (m, 3H), 7.91 (dd, J = 8.5, 2.0 Hz, 1H), 7.66–7.57 (m, 2H), 7.57–7.53 (m, 1H), 6.11 (d, J = 16 Hz, 1H), 3.79 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.1, 156.6, 155.3, 149.2, 141.1, 137.5, 136.0, 135.4, 135.3, 134.2, 131.5, 130.0, 129.1, 125.1, 122.5, 81.0, 51.9, 27.9; **HRMS (ESI)** for $C_{20}H_{22}ClN_2O_5S^+$ $(M+H)^+$: calcd. 437.0932, found 437.0933.

2.4 Optimization of reaction conditions (arylation):

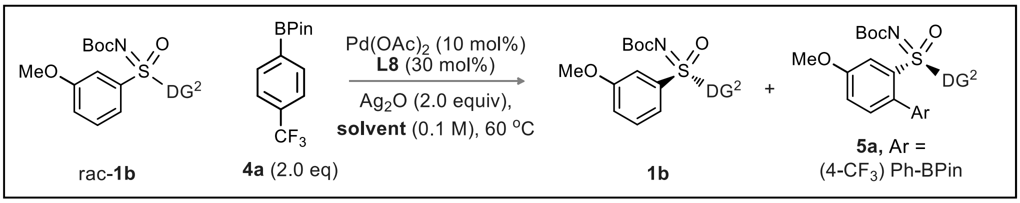
Table S5. Oxidant screening[a]



Entry	Oxidant	Conversion (c)[b]	*ee* [%][c]		
			***(R)*-1b**	***(S)*-5a**	***s***[d]
1	Ag_2CO_3	17.54	20	94	39
2	Ag_2O	47.56	78	86	31
3	AgOAc	11.76	12	90	21
4[e]	Ag_2O	43.21	70	92	50

[a]Reaction conditions: *rac*-**1b** (0.1 mmol), **4a** (2.0 equiv), $Pd(OAc)_2$ (10 mol%), **L8** (30 mol%), oxidant (2.0 equiv), 2-Cl-BQ (0.5 equiv), 1,2-DCE (1.0 mL), N_2, 75 °C, 3 days. [b]Calculated conversion, C = eeSM/(eeSM + eePR). [c]Determined by chiral HPLC analysis. [d]Selectivity factor (s) = ln[(1 − C)(1 − eeSM)]/ln[(1 − C)(1 + eeSM)]. [e]Reaction is performed in 60 °C.

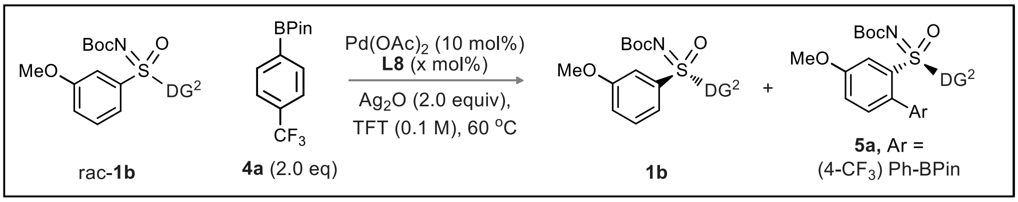
Table S6. Solvent screening:



Entry	Solvent	Conversion (c)[b]	*ee* [%][c]		
			***(R)*-1b**	***(S)*-5a**	s[d]
1	TFT	41.25	66	94	64
2	THF	31.43	44	96	75
3	*t*-Amyl-OH	36.0	54	96	84

[a]Reaction conditions: *rac*-**1b** (0.1 mmol), **4a** (2.0 equiv), $Pd(OAc)_2$ (10 mol%), **L8** (30 mol%), Ag_2O (2.0 equiv), 2-Cl-BQ (0.5 equiv), solvent (1.0 mL), N_2, 60 °C, 3 days. [b]Calculated conversion, C = eeSM/(eeSM + eePR). [c]Determined by chiral HPLC analysis. [d]Selectivity factor (*s*) = ln[(1 − C)(1 − eeSM)]/ln[(1 − C)(1 + eeSM)].

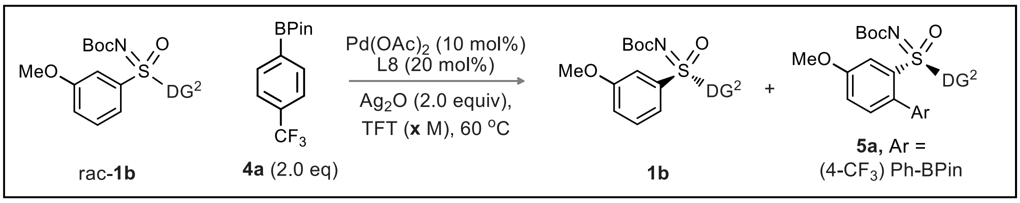
Table S7. Screening of ligand loading[a]



Entry	Ligand loading (x mol%)	Conversion (c)[b]	*ee* [%][c]		
			***(R)*-1b**	***(S)*-5a**	*s*[d]
1	10 mol%	40.51	64	94	62
2	15 mol%	41.97	68	94	66
3	20 mol%	45.98	80	94	79
4	40 mol%	39.74	62	94	61

[a]Reaction conditions: *rac*-**1b** (0.1 mmol), **4a** (2.0 equiv), $Pd(OAc)_2$ (10 mol%), **L8** (x mol%), Ag_2O (2.0 equiv), 2-Cl-BQ (0.5 equiv), TFT (1.0 mL), N_2, 60 °C, 3 days. [b]Calculated conversion, C = eeSM/(eeSM + eePR). [c]Determined by chiral HPLC analysis. [d]Selectivity factor (*s*) = ln[(1 − C)(1 − eeSM)]/ln[(1 − C)(1 + eeSM)].

Table S8. Screening of solvent loading[a]

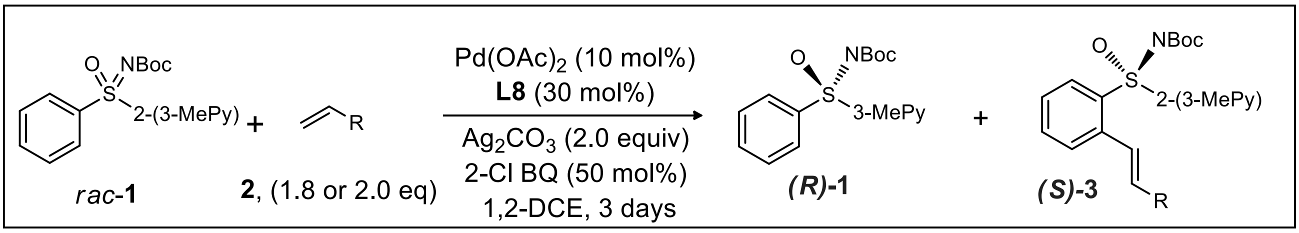


Entry	Molarity	Conversion	*ee* [%][c]	

		(c)[b]	*(R)*-1b	*(S)*-5a	s[d]
1	0.2 M	40.51	64	94	62
2	0.13 M	41.25	66	94	64
3	0.067 M	48.35	88	94	95
4	0.05 M	47.19	84	94	86

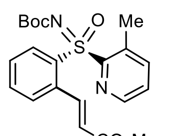
[a]Reaction conditions: *rac*-**1b** (0.1 mmol), **4a** (2.0 equiv), $Pd(OAc)_2$ (10 mol%), **L8** (20 mol%), Ag_2O (2.0 equiv), 2-Cl-BQ (0.5 equiv), TFT (x M), N_2, 60 °C, 3 days. [b]Calculated conversion, C = eeSM/(eeSM + eePR). [c]Determined by chiral HPLC analysis. [d]Selectivity factor (*s*) = ln[(1 − C)(1 − eeSM)]/ln[(1 − C)(1 + eeSM)].

2.5 General procedures for kinetic resolution via Pd-catalyzed C(sp^2)–H olefination (GP-3):



To an oven-dried 10 mL screw-capped vial was added $Pd(OAc)_2$ (0.025 mmol) **L8** (0.075 mmol) and 1,2-DCE (2.5 mL). The mixture was stired for 2 h at 50 °C. The reaction mixture was cooled to rt. The substrate (0.25 mmol), olefin (0.45–0.5 mmol), 2-chlorobenzoquinone (0.075–0.125 mmol), Ag_2CO_3 (0.5 mmol) was then added. The mixture was stirred for 48–72 h at 70 °C. The resulting mixture was then cooled to rt and filtered through a small pad of Celite and concentrated in vacuo. The residue was purified by preparative TLC using hexane/EtOAc as the eluent to afford the chiral product.

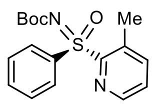
***N*-Boc-protected (*S*,*E*)-methyl 3-(2-(3-methylpyridine-2-sulfonimidoyl)phenyl)acrylate (3b):**



3b

3b: 27 mg, 26% yield, 96% ee, colorless solid, $[\alpha]_D^{25}$ = +37.5 (c = 0.01, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.40 (d, *J* = 8.0 Hz, 1H), 8.31–8.23 (m, 2H), 7.65 (t, *J* = 7.5 Hz, 2H), 7.60 (t, *J* = 8.0 Hz, 2H), 7.31 (dd, *J* = 7.5, 5.0 Hz, 1H), 6.11 (d, *J* = 15.5 Hz, 1H), 3.74 (s, 3H), 2.86 (s, 3H), 1.33 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.2, 157.0, 155.0, 146.0, 141.8, 141.7, 136.3, 136.2, 135.8, 133.7, 131.0, 129.6, 128.8, 126.6, 122.0, 80.5, 51.8, 27.9, 19.0; IR (KBr) ν_{max} 3021, 2926, 2853, 1738, 1367, 1216 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{25}N_2O_5S^+$ $(M+H)^+$: calcd. 417.1479, found 417.1487; **HPLC condition**: Daicel IG-3, *i*-PrOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 18.6 min (major) and tR = 22.8 min (minor).

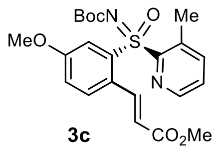
N-Boc-protected (R)-3-methyl-2-(phenylsulfonimidoyl)pyridine (1a):



1a

1a: 42 mg, 51% yield, 52% ee; $[\alpha]_D^{25}$ = −17.5 (c = 0.016, $CHCl_3$); **HPLC condition**: Daicel IG-3, *i*-PrOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 22.0 min (major) and tR = 20.3 min (minor).

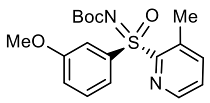
N-Boc-protected (S,E)-methyl 3-(4-methoxy-2-(3-methylpyridine-2-sulfonimidoyl)phenyl) acrylate (3c):



3c

3c: 39 mg, 35% yield, 97% ee, colorless solid, $[\alpha]_D^{25}$ = +55.3 (c = 0.13, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.25 (dd, J = 4.75, 1.25 Hz, 1H), 8.19 (d, J = 16.0, 1H), 7.90 (d, J = 3.0 Hz, 1H), 7.66 (dd, J = 7.75, 0.75 Hz, 1H), 7.55 (d, J = 8.5 Hz, 1H), 7.31 (dd, J = 7.75, 4.75 Hz, 1H), 7.13 (dd, J = 8.5, 2.5 Hz, 1H), 6.05 (d, J = 16.0 Hz, 1H), 3.90 (s, 3H), 3.71 (s, 3H), 2.85 (s, 3H), 1.33 (s, 9H); **^{13}C NMR (126 MHz, CDCl3)** δ 166.4, 160.5, 157.0, 154.9, 146.0, 141.7, 141.2, 137.5, 135.6, 130.0, 128.1, 126.6, 120.0, 119.9, 115.6, 80.5, 55.8, 51.6, 27.9, 18.9; IR (KBr) ν_{max} 2970, 2923, 1720, 1272, 1232, 1155, 1035 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{26}N_2NaO_6S^+$ (M+Na)$^+$: calcd. 469.1404, found 469.1413; **HPLC condition**: Phenomenex Chiralpak cellulose-2, n-hexane/i-PrOH =60/40, Flow rate = 0.4 mL/min, UV = 254 nm, tR = 57.7 min (major) and tR = 50.9 min (minor).

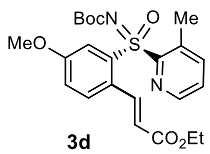
N-Boc-protected (R)-2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



1b

1b: 42 mg, 46% yield, 71% ee $[\alpha]_D^{25}$ = −41.5 (c = 0.378, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 14.5 min (major) and tR = 10.2 min (minor).

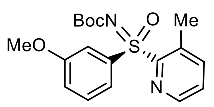
N-Boc-protected (S,E)-ethyl 3-(4-methoxy-2-(3-methylpyridine-2-sulfonimidoyl)phenyl) acrylate (3d):



3d

3d: 38 mg, 33% yield, 90% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +25.2 (c = 0.138, $CHCl_3$); **1H NMR (400 MHz, CDCl3)** δ 8.27 (d, J = 4.8 Hz, 1H), 8.17 (d, J = 15.6 Hz, 1H), 7.94 (d, J = 2.8 Hz, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.54 (d, J = 8.4 Hz, 1H), 7.34–7.28 (m, 1H), 7.17–7.10 (m, 1H), 6.04 (d, J = 15.6 Hz, 1H), 4.19 (q, J = 7.2 Hz, 2H), 3.92 (s, 3H), 2.87 (s, 3H), 1.35 (s, 9H), 1.28 (t, J = 7.0 Hz, 3H); **13C NMR (101 MHz, CDCl3)** δ 166.0, 160.4, 157.0, 155.0, 146.1, 141.6, 140.8, 137.6, 135.8, 130.0, 128.1, 126.6, 120.5, 119.9, 115.5, 80.5, 60.4, 55.9, 27.9, 19.1, 14.3; IR (KBr) ν_{max} 2969, 1738, 1366, 1229, 1216, 1156 cm^{-1}; **HRMS (ESI)** for $C_{23}H_{28}N_2NaO_6S^+$ (M+Na)$^+$: calcd. 483.1560, found 483.1571; **HPLC condition**: Amylose-C Neo, n-hexane/i-PrOH (0.1% DEA) =65/35, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 13.2 min (major) and tR = 18.2 min (minor).

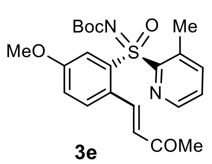
_N_-Boc-protected (_R_)-2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



1b

1b: 40 mg, 45% yield, 74% ee; $[\alpha]_D^{25}$ = –29.8 (c = 0.12, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 14.4 min (major) and tR = 10.0 min (minor).

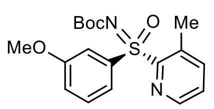
_N_-Boc-protected (_S_,_E_)-4-(4-methoxy-2-(3-methylpyridine-2-sulfonimidoyl)phenyl)but-3-en-2-one (3e):



3e

3e: 37 mg, 35% yield, 91% ee, colorless solid, $[\alpha]_D^{25}$ = +97 (c = 0.06, $CHCl_3$); **1H NMR (500 MHz, $CDCl_3$)** δ 8.46 (d, _J_ = 16.5, 1H), 8.33 (dd, _J_ = 4.5, 1.0 Hz, 1H), 7.87 (d, _J_ = 3.0 Hz, 1H), 7.67 (d, _J_ = 7.0 Hz, 1H), 7.63 (d, _J_ = 8.5 Hz, 1H), 7.36 (dd, _J_ = 8.0, 4.5 Hz, 1H), 7.15 (dd, _J_ = 8.75, 2.75 Hz, 1H), 6.30 (d, _J_ = 16.5 Hz, 1H), 3.91 (s, 3H), 2.75 (s, 3H), 2.35 (s, 3H), 1.34 (s, 9H); **^{13}C NMR (126 MHz, CDCl3)** δ 199.1, 160.8, 157.0, 154.8, 145.9, 142.0, 141.3, 137.5, 135.3, 129.9, 129.4, 128.1, 127.0, 119.8, 115.9, 80.6, 55.9, 27.9, 26.1, 19.0; IR (KBr) ν_{max} 2974, 2923, 2363, 1738, 1668, 1366, 1232, 1152 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{27}N_2O_5S^+$ $(M+H)^+$: calcd. 431.1635, found 431.1641; **HPLC condition**: Daicel OT (+), n-hexane/i-PrOH =70/30, Flow rate = 0.2 mL/min, UV = 254 nm, tR = 45.1 min (major) and tR = 39.9 min (minor).

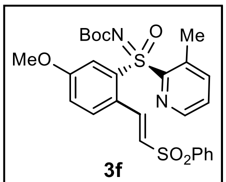
_N_-Boc-protected (R)-2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine(1b):



1b

1b: 39 mg, 43% yield, 67 % ee; $[\alpha]_D^{25}$ = –28.0 (c = 0.114, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 14.6 min (major) and tR = 10.1 min (minor).

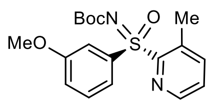
_N_-Boc-protected (_S_,_E_)-2-(5-methoxy-2-(2-(phenylsulfonyl)vinyl)phenylsulfonimidoyl)-3-methyl pyridine (3f):



3f

3f: 35.7 mg, 27% yield, 89% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +12.42 (c = 1.0, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.31–8.22 (m, 2H), 7.91–7.85 (m, 3H), 7.70 (d, _J_ = 7.5 Hz, 1H), 7.60–7.53 (m, 1H), 7.52–7.46 (m, 3H), 7.33 (dd, _J_ = 7.5, 4.5 Hz, 1H), 7.10 (dd, _J_ = 8.5, 2.5 Hz, 1H), 6.57 (d, _J_ = 15.5 Hz, 1H), 3.90 (s, 3H), 2.87 (s, 3H), 1.33 (s, 9H); **^{13}C NMR (126 MHz, CDCl3)** δ 161.1, 156.7, 154.6, 146.1, 142.0, 140.2, 139.3, 138.4, 135.7, 133.2, 130.3, 129.2, 128.6, 127.9, 126.8, 125.6, 119.6, 116.1, 80.7, 55.9, 27.9, 19.1; IR (KBr) ν_{max} 2969, 2927, 1738, 1246, 1145, 1083, 733 cm^{-1}; **HRMS (ESI)** for $C_{26}H_{28}N_2NaO_6S_2^+$ $(M+H)^+$: calcd. 551.1281, found 551.1292; **HPLC condition**: Daicel ODH, n-hexane/i-PrOH =50/50, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 20.7 min (major) and tR = 18.9 min (minor).

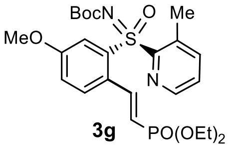
***N*-Boc-protected (*R*)-2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):**



1b

1b: 41 mg, 45% yield, 48% ee; $[\alpha]_D^{25}$ = –18.8 (c = 0.258, $CHCl_3$); HPLC condition: Daicel ODH, *n*-hexane/**i**-PrOH =50/50, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 10.1 min (major) and tR = 8.6 min (minor).

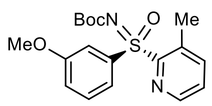
***N*-Boc-protected (*S*,*E*)-diethyl 4-methoxy-2-(3-methylpyridine-2-sulfonimidoyl)styrylphosphonate (3g):**



3g

3g: 43 mg, 33% yield, 95% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +14.1 (c = 0.058, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.29 (dd, *J* = 4.75, 1.25 Hz, 1H), 7.96–7.84 (m, 2H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 1H), 7.32 (dd, *J* = 7.75, 4.75 Hz, 1H), 7.14 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.01–5.90 (m, 1H), 4.10–3.98 (m, 4H), 3.91 (s, 3H), 2.83 (s, 3H), 1.33 (s, 9H), 1.31–1.22 (m, 6H); **^{13}C NMR (126 MHz, CDCl3)** δ 160.4, 156.8, 154.8, 146.0, 143.7 (*J* = 8.8 Hz), 141.8, 137.2, 135.5, 129.9, 128.5 (d, *J* = 25.2 Hz), 126.7, 119.8, 116.6 (d, *J* = 191.5 Hz), 115.5, 80.5, 62.03 (d, *J* = 6.3 Hz), 62.01 (d, *J* = 5.0 Hz), 55.9, 27.9, 19.0, 16.34, 16.3; IR (KBr) ν_{max} 2969, 2920, 2850, 1738, 1366, 1228, 1216 cm^{-1}; **HRMS (ESI)** for $C_{24}H_{33}N_2NaO_7PS^+$ $(M+Na)^+$: calcd. 547.1638, found 546.2053; **HPLC condition**: Daicel IC-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, t_R = 16.7 min (major) and t_R = 15.8 min (minor).

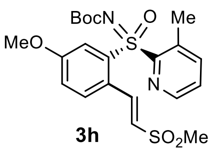
***N*-Boc-protected (*R*)-2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):**



1b

1b: 37 mg, 41% yield, 62% ee; $[\alpha]_D^{25}$ = –21.0 (c = 0.348, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 14.8 min (major) and tR = 10.2 min (minor).

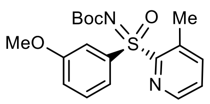
***N*-Boc-protected (*S*,*E*)-2-(5-methoxy-2-(2-(methylsulfonyl)vinyl)phenylsulfonimidoyl)-3-methyl pyridine (3h):**



3h

3h: 38 mg, 33%, 99% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +16.9 (c = 0.16, $CHCl_3$); **^{1}H NMR (400 MHz, CDCl3)** δ 8.35–8.26 (m, 2H), 7.84 (d, *J* = 2.4 Hz, 1H), 7.70 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.36 (dd, *J* = 7.6, 4.4 Hz, 1H), 7.16 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.60 (d, *J* = 15.2 Hz, 1H), 3.91 (s, 3H), 3.03 (s, 3H), 2.83 (s, 3H), 1.31 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 161.2, 156.5, 154.6, 146.2, 142.15, 142.09, 138.3, 135.5, 130.5, 128.3, 127.0, 126.0, 119.6, 116.2, 80.8, 56.0, 43.0, 27.9, 19.0; IR (KBr) ν_{max} 2977, 2932, 2367, 1738, 1242, 1153, 1127 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{26}N_2NaO_6S_2^+$ $(M+H)^+$: calcd. 489.1124, found 489.1134; **HPLC condition**: Daicel IC-3, i-PrOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 52.9 min (major) and tR = 36.8 min (minor).

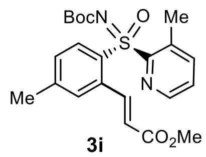
***N*-Boc-protected (*R*)-2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):**



1b

1b: 38 mg, 42% yield, 70% ee; $[\alpha]_D^{25} = -44.56$ (c = 0.364, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 13.9 min (major) and tR = 10.2 min (minor).

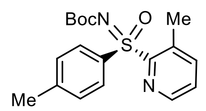
***N*-Boc-protected (*S*,*E*)-methyl 3-(5-methyl-2-(3-methylpyridine-2-sulfonimidoyl)phenyl) acrylate (3i):**



3i

3i: 33 mg, 31% yield, 96% ee, colorless viscous liquid, $[\alpha]_D^{25} = +29.4$ (c = 0.108, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.29–8.20 (m, 3H), 7.64 (dd, *J* = 7.75, 0.75 Hz, 1H), 7.41–7.36 (m, 2H), 7.29 (dd, *J* = 7.75, 4.75 Hz, 1H), 6.09 (d, *J* = 15.5 Hz, 1H), 3.73 (s, 3H), 2.83 (s, 3H), 2.44 (s, 3H), 1.33 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.2, 157.1, 155.1, 145.9, 144.7, 141.9, 141.6, 136.1, 135.6, 133.1, 131.1, 130.3, 129.5, 126.5, 121.7, 80.3, 51.7, 27.9, 21.5, 19.0; IR (KBr) ν_{max} 2969, 2923, 1722, 1366, 1273, 1226, 1154 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{27}N_2O_5S^+$ $(M+H)^+$: calcd. 431.1635, found 431.1646; **HPLC condition**: Daicel ODH, n-hexane/i-PrOH = 70/30, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 22.8 min (major) and tR = 25.5 min (minor).

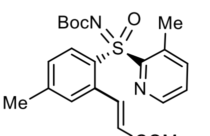
***N*-Boc-protected (*R*)-3-methyl-2-(4-methylphenylsulfonimidoyl)pyridine (1c):**



1c

1c: 40 mg, 46% yield, 52% ee; $[\alpha]_D^{25} = -22.3$ (c = 0.182, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 19.2 min (major) and tR = 10.6 min (minor).

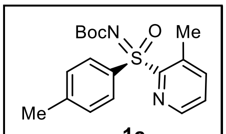
***N*-Boc-protected (*S*,*E*)-4-(5-methyl-2-(3-methylpyridine-2-sulfonimidoyl)phenyl)but-3-en-2-one (3j):**



3j

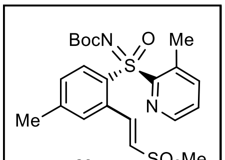
3j: 31 mg, 30% yield, 96% ee, colorless viscous liquid, $[\alpha]_D^{25} = +96.2$ (c = 0.08, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.49 (d, *J* = 16.5 Hz, 1H), 8.32 (d, *J* = 4.5 Hz, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.45 (bs, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.34 (dd, *J* = 8.0, 4.5 Hz, 1H), 6.32 (d, *J* = 16.5 Hz, 1H), 2.72 (s, 3H), 2.44 (s, 3H), 2.37 (s, 3H), 1.34 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 199.1, 157.2, 154.9, 145.8, 145.0, 141.9, 141.8, 136.0, 135.2, 132.9, 131.00, 130.97, 130.5, 129.3, 126.9, 80.5, 27.9, 26.2, 21.5, 19.0; IR (KBr) ν_{max} 2969, 2922, 1738, 1671, 1228, 1154 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{27}N_2O_4S^+$ $(M+H)^+$: calcd. 415.1686, found 415.1694; **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 26.0 min (major) and tR = 29.9 min (minor).

***N*-Boc-protected (*R*)-3-methyl-2-(4-methylphenylsulfonimidoyl)pyridine (1c):**



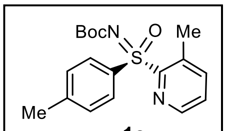
1c: 39 mg, 45% yield, 59% ee; $[\alpha]_D^{25}$ = –35.6 (c = 0.114, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 19.5 min (major) and tR = 10.9 min (minor).

***N*-Boc-protected (*S*,*E*)-3-methyl-2-(4-methyl-2-(2-(methylsulfonyl)vinyl)phenyl sulfonimidoyl) pyridine (3k):**



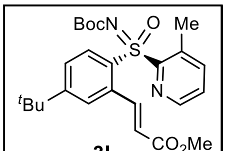
3k: 35 mg, 31% yield, 94% ee, colorless solid, $[\alpha]_D^{25}$ = +67.2 (c = 0.136, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.37 (d, *J* = 15.5 Hz, 1H), 8.31 (d, *J* = 3.5 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 7.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.39–7.30 (m, 2H), 6.65 (d, *J* = 15.0 Hz, 1H), 3.04 (s, 3H), 2.79 (s, 3H), 2.45 (s, 3H), 1.29 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 156.6, 154.8, 146.2, 145.1, 142.9, 142.0, 135.4, 134.2, 133.6, 131.0, 130.9, 130.0, 126.9, 80.6, 42.9, 27.8, 21.4, 19.0 (1 carbon overlap); IR (KBr) ν_{max} 2969, 2932, 1739, 1228 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{26}N_2NaO_5S_2^+$ $(M+H)^+$: calcd. 473.1175, found 473.1181; **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 12.6 min (major) and tR = 18.0 min (minor).

***N*-Boc-protected (*R*)-3-methyl-2-(4-methylphenylsulfonimidoyl)pyridine (1c):**



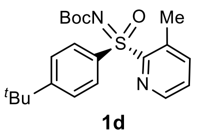
1c: 37 mg, 43% yield, 50% ee; $[\alpha]_D^{25}$ = –17.3 (c = 0.252, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 18.3 min (major) and tR = 10.5 min (minor).

***N*-Boc-protected (*S*,*E*)-methyl 3-(5-(tert-butyl)-2-(3-methylpyridine-2-sulfonimidoyl) phenyl) acrylate (3l):**



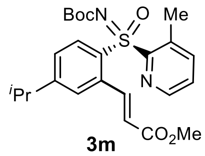
3l: 38 mg, 32% yield, 98% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +41.9 (c = 0.16, $CHCl_3$); **^{1}H NMR (400 MHz, CDCl3)** δ 8.32–8.29 (d, *J* = 2.0 Hz, 1H), 8.28–8.24 (m, 2H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.61–7.53 (m, 2H), 7.29 (dd, *J* = 7.6, 4.4 Hz, 1H), 6.10 (d, *J* = 15.6 Hz, 1H), 3.74 (s, 3H), 2.83 (s, 3H), 1.35 (s, 9H), 1.32 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.2, 157.5, 157.0, 155.2, 146.0, 142.4, 141.6, 135.8, 135.6, 133.2, 130.9, 126.8, 126.5, 126.0, 121.6, 80.3, 51.7, 35.2, 30.9, 27.9, 19.0; IR (KBr) ν_{max} 2968, 2360, 1721, 1366, 1271, 1249, 1154 cm^{-1}; **HRMS (ESI)** for $C_{25}H_{32}N_2NaO_5S^+$ $(M+Na)^+$: calcd. 495.1924, found 495.1937; **HPLC condition**: cellulose-2, n-hexane/i-PrOH = 50/50, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 20.1 min (major) and tR = 32.2 min (minor).

***N*-Boc-protected (*R*)-2-(4-(tert-butyl)phenylsulfonimidoyl)-3-methylpyridine (1d):**



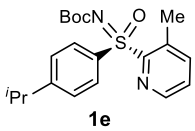
1d: 42 mg, 43% yield, 59% ee; , $[\alpha]_D^{25}$ = +33.3 (c = 0.1, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 31.5 min (major) and tR = 12.2 min (minor).

***N*-Boc-protected (*S*,*E*)-methyl 3-(5-isopropyl-2-(3-methylpyridine-2-sulfonimidoyl)phenyl) acrylate (3m):**



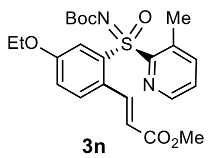
3m: 34 mg, 30% yield, 94% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +27.6 (c = 0.55, $CHCl_3$); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.32–8.23 (m, 3H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.46–7.39 (m, 2H), 7.30 (dd, *J* = 7.6, 4.4 Hz, 1H), 6.11 (d, *J* = 15.6 Hz, 1H), 3.75 (s, 3H), 3.07–2.94 (m, 1H), 2.84 (s, 3H), 1.33 (s, 9H), 1.29 (d, *J* = 6.8 Hz, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.2, 157.1, 155.2, 146.0, 142.2, 141.6, 136.2, 135.6, 133.5, 131.2, 127.8, 127.1, 126.5, 121.7, 80.3, 51.7, 34.1, 27.9, 23.53, 23.46, 19.0 (1 carbon is overlapped); IR (KBr) ν_{max} 2986, 1720, 1666, 1267, 1247, 1151, 1041 cm^{-1}; **HRMS (ESI)** for $C_{24}H_{31}N_2O_5S^+$ $(M+H)^+$: calcd. 459.1948, found 459.1959; **HPLC condition**: Daicel IG-3, *i*-PrOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 30.1 min (major) and tR = 57.6 min (minor).

***N*-Boc-protected (*R*)-2-(4-isopropylphenylsulfonimidoyl)-3-methylpyridine (1e):**



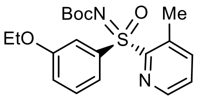
1e: 42 mg, 45% yield, 57% ee; $[\alpha]_D^{25}$ = –28.9 (c = 0.588, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 23.4 min (major) and tR = 12.0 min (minor).

***N*-Boc-protected (*S*,*E*)-methyl 3-(4-ethoxy-2-(3-methylpyridine-2-sulfonimidoyl)phenyl) acrylate (3n):**



3n: 48 mg, 42% yield, 85% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +50.1 (c = 0.11, $CHCl_3$); **1H NMR (500 MHz, $CDCl_3$)** δ 8.26 (dd, *J* = 4.5, 0.75 Hz, 1H), 8.19 (d, *J* = 16.0 Hz, 1H), 7.89 (d, *J* = 3.0 Hz, 1H), 7.68–7.62 (m, 1H), 7.53 (d, *J* = 8.5 Hz, 1H), 7.30 (dd, *J* = 8.0, 4.5 Hz, 1H), 7.11 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.04 (d, *J* = 15.5 Hz, 1H), 4.13 (q, *J* = 6.83 Hz, 2H), 3.71 (s, 3H), 2.84 (s, 3H), 1.42 (t, *J* = 7.0 Hz, 3H), 1.33 (s, 9H); **13C NMR (126 MHz, CDCl3)** δ 166.5, 159.9, 156.9, 155.0, 146.0, 141.6, 141.2, 137.5, 135.6, 129.9, 127.8, 126.6, 120.1, 119.8, 116.3, 80.4, 64.3, 51.6, 27.9, 18.9, 14.5; IR (KBr) ν_{max} 2921, 2850, 1737, 1366, 1230, 1156 cm^{-1}; **HRMS (ESI)** for $C_{23}H_{29}N_2O_6S^+$ $(M+H)^+$: calcd. 461.1741, found 489.1749; **HPLC condition**: Daicel IC-3, *i*-PrOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 37.7 min (major) and tR = 28.6 min (minor).

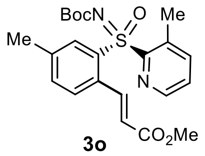
N-Boc-protected (R)-2-(3-ethoxyphenylsulfonimidoyl)-3-methylpyridine (1f):



1f

1f: 32 mg, 34% yield, 88% ee; $[\alpha]_D^{25}$ = −18.8 (c = 0.258, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 34.1 min (major) and tR = 16.8 min (minor).

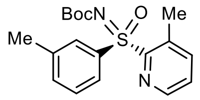
N-Boc-protected (S,E)-methyl 3-(4-methyl-2-(3-methylpyridine-2-sulfonimidoyl)phenyl) acrylate (3o):



3o

3o: 38 mg, 35% yield, 96% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +29.7 (c = 0.03, $CHCl_3$); **1H NMR (500 MHz, CDCl₃)** δ 8.26 (d, *J* = 3.5 Hz, 1H), 8.25–8.18 (m, 2H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 1H), 7.30 (dd, *J* = 8.0, 4.5 Hz, 1H), 6.08 (d, *J* = 16.0 Hz, 1H), 3.73 (s, 3H), 2.87 (s, 3H), 2.47 (s, 3H), 1.34 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.3, 157.1, 155.2, 146.0, 141.62, 141.60, 140.4, 136.1, 135.9, 134.5, 133.3, 131.3, 128.7, 126.5, 121.2, 80.4, 51.7, 27.9, 21.3, 19.0; IR (KBr) ν_{max} 2969, 2853, 1738, 1366, 1228, 1216, 1156 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{26}N_2NaO_5S^+$ $(M+Na)^+$: calcd. 453.1455, found 453.1469; **HPLC condition**: Cellulose-1, n-hexane/i-PrOH = 70/30, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 28.0 min (major) and tR = 24.1 min (minor).

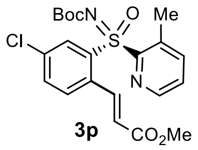
N-Boc-protected (R)-3-methyl-2-(3-methylphenylsulfonimidoyl)pyridine (1g):



1g

1g: 36 mg, 42% yield, 68% ee; $[\alpha]_D^{25}$ = −66.7 (c = 0.006, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 18.2 min (major) and tR = 16.4 min (minor).

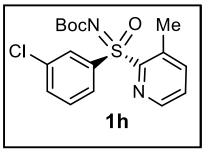
N-Boc-protected (S,E)-methyl 3-(4-chloro-2-(3-methylpyridine-2-sulfonimidoyl)phenyl) acrylate (3p):



3p

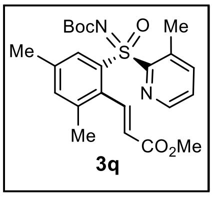
3p: 25 mg, 22% yield, 89% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +32.1 (c = 0.07, $CHCl_3$); **1H NMR (500 MHz, CDCl₃)** δ 8.37 (d, *J* = 2.0 Hz, 1H), 8.24 (dd, *J* = 4.5, 1.0 Hz, 1H), 8.18 (d, *J* = 15.5 Hz, 1H), 7.69 (dd, *J* = 7.75, 0.75 Hz, 1H), 7.61 (dd, *J* = 8.25, 2.25 Hz, 1H), 7.53 (d, *J* = 8.5 Hz, 1H), 7.33 (dd, *J* = 7.75, 4.75 Hz, 1H), 6.11 (d, *J* = 16 Hz, 1H), 3.74 (s, 3H), 2.88 (s, 3H), 1.34 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.0, 156.8, 154.7, 146.0, 141.8, 140.7, 137.8, 136.1, 135.9, 134.7, 133.8, 131.0, 129.9, 126.8, 122.3, 80.8, 51.9, 27.9, 18.9; IR (KBr) ν_{max} 2969, 2851, 1727, 1221, 1208, 1100 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{23}ClN_2NaO_5S^+$ $(M+Na)^+$: calcd. 473.0908, found 473.0919; **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.2 mL/min, UV = 254 nm, tR = 23.1 min (major) and tR = 22.0 min (minor).

N-Boc-protected (R)-2-(3-chlorophenylsulfonimidoyl)-3-methylpyridine (1h):



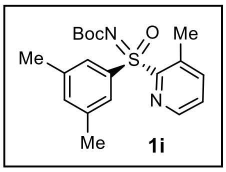
1h: 33 mg, 36% yield, 35% ee; $[\alpha]_D^{25}$ = –46 (c = 0.05, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.2 mL/min, UV = 254 nm, tR = 32.4 min (major) and tR = 24.3 min (minor).

N-Boc-protected (S,E)-methyl 3-(2,4-dimethyl-6-(3-methylpyridine-2-sulfonimidoyl)phenyl) acrylate (3q):



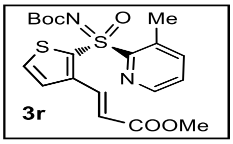
3q: 40 mg, 36% yield, 96% ee, colorless solid, $[\alpha]_D^{25}$ = +8.3 (c = 0.1, $CHCl_3$); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.25 (dd, *J* = 4.6, 1.0 Hz, 1H), 8.18 (bs, 1H), 7.76 (d, *J* = 16.4 Hz, 1H), 7.58 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.33–7.27 (m, 2H), 5.48 (d, *J* = 16.4 Hz, 1H), 3.72 (s, 3H), 2.78 (s, 3H), 2.42 (s, 3H), 2.25 (s, 3H), 1.36 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 165.8, 157.3, 155.3, 146.0, 141.3, 141.2, 138.3, 137.4, 136.7, 136.5, 136.4, 132.5, 128.9, 126.4, 125.1, 80.3, 51.6, 28.0, 21.1, 20.8, 19.1; IR (KBr) ν_{max} 2966, 2920, 2851, 1725, 1258, 1154, 1014 cm^{-1}; **HRMS (ESI)** for $C_{23}H_{29}N_2O_5S^+$ $(M+H)^+$: calcd. 445.1792, found 445.1799; **HPLC condition**: Daicel IC-3, i-PrOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 44.2 min (major) and tR = 57.5 min (minor).

N-Boc-protected (R)-2-(3,5-dimethylphenylsulfonimidoyl)-3-methylpyridine (1i):



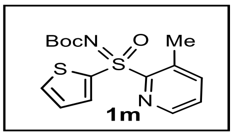
1i: 34 mg, 38% yield, 76% ee; $[\alpha]_D^{25}$ = –29.3 (c = 0.028, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 14.1 min (major) and tR = 10.1 min (minor).

N-Boc-protected (R,E)-methyl 3-(2-(3-methylpyridine-2-sulfonimidoyl)thiophen-3-yl)acrylate (3r):



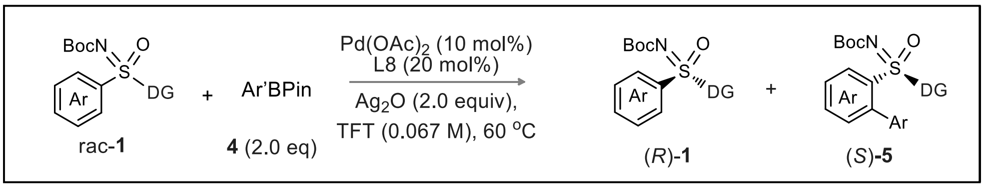
3r: 34 mg, 32% yield, 92% ee, colorless viscous liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (d, *J* = 4.5 Hz, 1H), 8.04 (d, *J* = 16 Hz, 1H), 7.73–7.64 (m, 2H), 7.36 (d, *J* = 5.5 Hz, 1H), 7.35–7.30 (m, 1H), 6.27 (d, *J* = 16 Hz, 1H), 3.74 (s, 3H), 2.83 (s, 3H), 1.32 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.4, 156.6, 155.3, 146.4, 141.9, 136.3, 135.1, 134.6, 133.5, 127.3, 126.8, 122.5, 121.7, 80.8, 51.8, 27.9, 19.1; **HRMS (ESI)** for $C_{19}H_{23}N_2O_5S_2^+$ $(M+H)^+$: calcd. 423.1043, found 423.1043. **HPLC condition**: Daicel IF-3, *n*-hexane/*i*-PrOH = 50/50, Flow rate = 0.6 mL/min, UV = 254 nm, tR = 14.9 min (major) and tR = 20.0 min (minor).

N-Boc-protected 3-methyl-2-(thiophene-2-sulfonimidoyl)pyridine (1m):



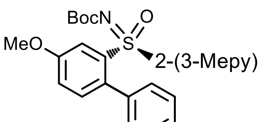
1m: 36 mg, 42% yield, 66% ee; **HPLC condition**: Daicel IF-3, *n*-hexane/*i*-PrOH = 85/15, Flow rate = 0.6 mL/min, UV = 254 nm, tR = 13.8 min (major) and tR = 12.9 min (minor).

2.6 General Procedures for kinetic resolution via Pd-Catalyzed C(sp^2)–H Arylation (GP-4):



To an oven-dried 10 mL screw-capped vial was added substrate (0.2 mmol), ArBPin (0.4 mmol), $Pd(OAc)_2$ (4.6 mg, 0.02 mmol), L8 (0.04 mmol), Ag_2O (56 mg, 0.4 mmol), 2-chloro benzoquinone (0.1 mmol), TFT (3.0 mL). The mixture was stirred for 72 h at 60 °C. The resulting mixture was then cooled to rt and filtered through a small pad of Celite and concentrated in vacuo. The residue was purified by Silica gel column chromatography using hexane/EtOAc as eluent to afford the chiral product and chiral starting material.

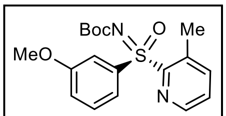
(*S*)-*N*-Boc-protected 2-(4-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-sulfonimidoyl)-3-methyl-pyridine (5a):



5a

5a: 42 mg, 42% yield, 92% ee, colorless solid, $[\alpha]_D^{25}$ = +39.7 (c = 0.216, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.24–8.18 (m, 2H), 7.37–7.30 (m, 3H), 7.18 (dd, *J* = 7.5, 4.5 Hz, 1H), 7.18– 7.12 (m, 1H), 7.12–6.60 (m, 3H), 3.96 (s, 3H), 2.30 (s, 3H), 1.32 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 159.1, 157.0, 154.9, 146.0, 141.8, 140.9, 138.1, 136.6, 133.3, 132.9, 130.2, 129.4 (q, *J* = 33 Hz), 126.3, 124.0 (q, *J* = 274 Hz), 123.98 (q, *J* = 4.0 Hz), 119.5, 114.7, 80.3, 55.9, 27.9, 18.8; **^{19}F NMR (471 MHz, $CDCl_3$)** δ – 62.76, IR (KBr) ν_{max} 2969, 1663, 1600, 1322, 1106, 822, 800 cm^{-1}; **HRMS (ESI)** for $C_{25}H_{26}F_3N_2O_4S^+$ $(M+H)^+$: calcd. 507.1560, found 507.1569; **HPLC condition**: Daicel Chiralpak IG-3, MeOH /*i*-PrOH = 95/5, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 17.2 min (major) and tR = 14.5 min (minor).

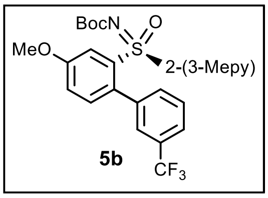
(*R*)-*N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



1b

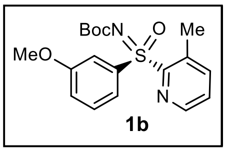
1b: 32 mg, 44% yield, 89% ee; $[\alpha]_D^{25}$ = –35.7 (c = 0.172, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.7 mL/min, UV = 254 nm, tR = 7.3 min (minor) and tR = 10.3 min (major).

(*S*)-*N*-Boc-protected 2-(4-methoxy-3'-(trifluoromethyl)-[1,1'-biphenyl]-2-sulfonimidoyl)-3-methyl-pyridine (5b):



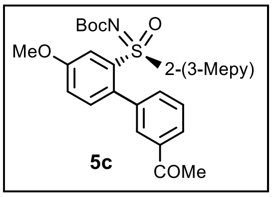
5b: 43 mg, 43% yield, 93% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +46.7 (c = 0.06, $CHCl_3$); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.26–8.19 (m, 2H), 7.45 (d, *J* = 7.2 Hz, 1H), 7.37–7.29 (m, 3H), 7.20 (dd, *J* = 7.6, 4.4 Hz, 1H), 7.19–7.12 (m, 1H), 7.11–7.06 (m, 1H), 6.93–6.82 (m, 1H), 3.98 (s, 3H), 2.28 (s, 3H), 1.34 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 159.0, 157.1, 154.7, 146.0, 141.0, 138.8, 138.0, 136.6, 133.9, 133.6, 132.7, 129.5 (q, *J* = 32 Hz), 127.7, 126.5, 125.8, 124.2 (q, *J* = 4.0 Hz), 123.7 (q, *J* = 274 Hz), 119.5, 114.7, 80.3, 55.9, 27.9, 18.8; **^{19}F NMR (471 MHz, $CDCl_3$)** δ – 62.49; IR (KBr) ν_{max} 2985, 1645, 1276, 1246, 1158, 1119, 901 cm^{-1}; **HRMS (ESI)** for $C_{25}H_{26}F_3N_2O_4S^+$ $(M+H)^+$: calcd. 507.1560, found 507.1566; **HPLC condition**: Daicel Chiralpak AS-H, n-hexane/*i*-PrOH = 90/10, Flow rate = 1.00 mL/min, UV = 254 nm, tR = 13.3 min (major) and tR = 15.5 min (minor).

(*R*)-*N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



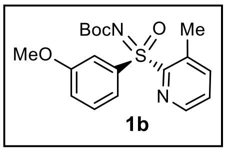
1b: 30 mg, 41% yield, 90% ee; $[\alpha]_D^{25}$ = –34.9 (c = 0.129, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 15.4 min (major).and tR = 10.7 min (minor).

(*S*)-*N*-Boc-protected 1-(4'-methoxy-2'-(3-methylpyridine-2-sulfonimidoyl)-[1,1'-biphenyl]-3-yl)-ethanone (5c):



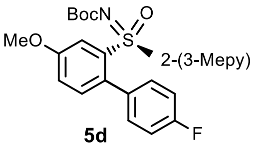
5c: 39 mg, 41% yield, 95% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = + 70.0 (c = 0.01, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.24–8.16 (m, 2H), 7.78 (d, *J* = 7.5 Hz, 1H), 7.45–7.37 (m, 1H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.25–7.07 (m, 5H), 3.95 (s, 3H), 2.46 (s, 3H), 2.25 (s, 3H), 1.32 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 197.5, 159.0, 157.0, 154.9, 146.0, 140.8, 138.5, 138.0, 136.4, 136.0, 134.5, 133.6, 133.3, 129.9, 127.6, 127.0, 126.2, 119.5, 114.8, 80.2, 55.9, 27.9, 26.5, 18.8; IR (KBr) ν_{max} 2969, 2926, 1738, 1365, 1275, 1229, 1156 cm^{-1}; **HRMS (ESI)** for $C_{26}H_{28}N_2NaO_5S^+$ $(M+Na)^+$: calcd. 503.1611, found 503.1619; **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 20.1 min (major) and tR = 25.4 min (minor).

(*R*)-*N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



1b: 30 mg, 42% yield, 82% ee; $[\alpha]_D^{25}$ = –62 (c = 0.01, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 24.7 min (major) and tR = 17.1 min (minor).

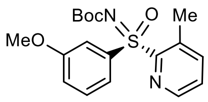
(*S*)-*N*-Boc-protected 2-(4'-fluoro-4-methoxy-[1,1'-biphenyl]-2-sulfonimidoyl)-3-methylpyridine (5d):



5d

5d: 36 mg, 40% yield, 97% ee, light yellow solid, $[\alpha]_D^{25}$ = +61 (c = 0.22, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.25–8.20 (m, 1H), 8.20 (d, *J* = 3.0 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.20 (dd, *J* = 7.5, 4.5 Hz, 1H), 7.15– 7.09 (m, 1H), 7.08–7.03 (m, 1H), 6.78–6.73 (m, 4H), 3.94 (s, 3H), 2.33 (s, 3H), 1.32 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 162.1 (d, *J* = 248 Hz), 158.8, 157.0, 155.0, 145.9, 140.9, 138.1, 136.6, 134.0, 133.9, 133.5, 131.5, 126.2, 119.5, 114.6, 114.0 (d, *J* = 21 Hz), 80.2, 55.8, 27.9, 18.9; IR (KBr) ν_{max} 2969, 1663, 1600, 1322, 1106, 822, 800 cm^{-1}; **^{19}F NMR (376 MHz, $CDCl_3$)** δ – 114.76; **HPLC condition**: Daicel Chiralpak IH-3, *i*-PrOH, Flow rate = 0.4 mL/min, UV = 254 nm, tR = 13.5 min (major) and tR = 15.4 min (minor).

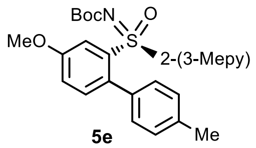
(*R*)-*N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



1b

1b: 30 mg, 42% yield, 85% ee; $[\alpha]_D^{25}$ = –56 (c = 0.025, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 15.7 min (major) and tR = 11.1 min (minor).

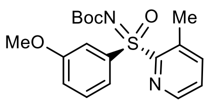
(*S*)-*N*-Boc-protected 2-(4-methoxy-4'-methyl-[1,1'-biphenyl]-2-sulfonimidoyl)-3-methylpyridine (5e):



5e

5e: 37 mg, 41% yield, 94% ee, colorless solid, $[\alpha]_D^{25}$ = +84.3 (c = 0.122, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.20 (d, *J* = 2.5 Hz, 2H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.20–7.14 (m, 1H), 7.13–7.09 (m, 1H), 7.08–7.04 (m, 1H), 6.95–6.70 (m, 4H), 3.95 (s, 3H), 2.28 (s, 6H), 1.32 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 158.5, 157.1 155.1, 145.9, 140.7, 138.0, 136.9, 136.8, 135.1, 134.7, 133.9, 129.6, 127.8, 126.0, 119.6, 114.2, 80.1, 55.9, 27.9, 21.1, 18.9; IR (KBr) ν_{max} 2974, 2924, 1658, 1268, 1245, 1155, 1032 cm^{-1}; **HRMS (ESI)** for $C_{25}H_{29}N_2O_4S^+$ $(M+H)^+$: calcd. 453.1843, found 453.1844; **HPLC condition**: Daicel Chiralpak IG-3, MeOH /i-PrOH =95/5, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 17.9 min (minor).and tR = 19.6 min (major).

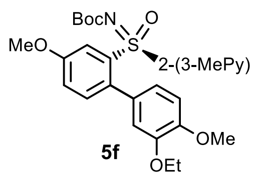
(*R*)-*N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



1b

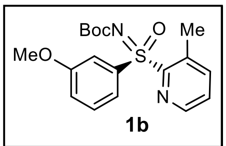
1b: 33 mg, 46% yield, 80% ee; $[\alpha]_D^{25}$ = –34.75 (c = 0.175, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.7 mL/min, UV = 254 nm, tR = 7.3 min (minor) and tR = 10.3 min (major).

(*S*)-*N*-Boc-protected 2-(3'-ethoxy-4,4'-dimethoxy-[1,1'-biphenyl]-2-sulfonimidoyl)-3-methyl-pyridine (5f):



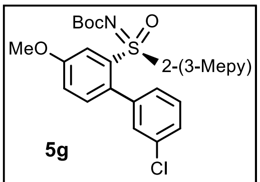
5f: 45 mg, 44% yield, 93% ee, colorless solid, $[\alpha]_D^{25}$ = + 51.4 (c = 0.01, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.21–8.17 (m, 2H), 7.30 (d, *J* = 7.5 Hz, 1H), 7.13 (dd, *J* = 7.5, 4.5 Hz, 1H), 7.10–7.04 (m, 2H), 6.85–6.10 (m, 3H), 3.92 (s, 3H), 3.90–3.80 (m, 2H), 3.79 (s, 3H), 2.30 (s, 3H), 1.36 (t, *J* = 7.0 Hz, 3H), 1.30 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 158.4, 157.1, 154.9, 148.3, 146.7, 145.7, 140.5, 138.3, 136.7, 134.1, 133.9, 130.3, 125.8, 122.0, 119.4, 114.4, 114.0, 110.2, 79.9, 63.8, 55.9, 55.8, 27.8, 18.8, 14.6; IR (KBr) ν_{max} 3028, 2974, 2850, 1738, 1366, 1228, 1216 cm^{-1}; **HRMS (ESI)** for $C_{27}H_{33}N_2O_6S^+$ $(M+H)^+$: calcd. 513.2054, found 513.2062; **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 20.4 min (major) and tR = 18.4 min (minor).

(R)-*N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



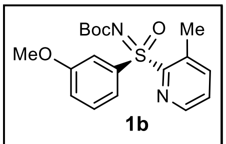
1b: 33 mg, 46% yield, 83% ee; $[\alpha]_D^{25}$ = –68.0 (c = 0.01, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 24.6 min (major) and tR = 17.1 min (minor).

(*S*)-*N*-Boc-protected 2-(3'-chloro-4-methoxy-[1,1'-biphenyl]-2-sulfonimidoyl)-3-methylpyridine (5g):



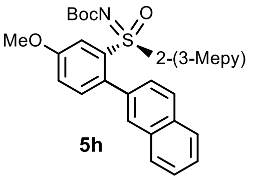
5g: 37 mg, 39% yield, 96% ee, colorless solid, $[\alpha]_D^{25}$ = + 40.0 (c = 0.01, $CHCl_3$); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.25 (d, *J* = 4.8 Hz, 1H), 8.22 (d, *J* = 2.8 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.26–7.20 (m, 2H), 7.19–7.09 (m, 3H), 7.09–7.03 (m, 2H), 3.96 (s, 3H), 2.33 (s, 3H), 1.34 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 158.9, 157.1, 154.9, 146.0, 140.9, 139.8, 138.2, 136.9, 133.5, 132.9, 132.8, 128.5, 127.5, 126.2, 119.5, 114.6, 80.2, 55.9, 28.0, 19.9 (2 carbons missing); **HRMS (ESI)** for $C_{24}H_{26}ClN_2O_4S^+$ $(M+H)^+$: calcd. 473.1296, found 473.1305; **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 18.1 min (major) and tR = 20.0 min (minor).

(*R*)-*N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



1b: 32 mg, 44% yield, 83% ee; $[\alpha]_D^{25}$ = –70.0 (c = 0.01, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 24.2 min (major) and tR = 16.9 min (minor).

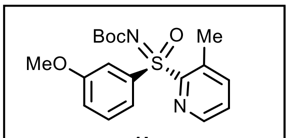
(*S*)-*N*-Boc-protected 2-(5-methoxy-2-(naphthalen-1-yl)phenylsulfonimidoyl)-3-methylpyridine (5h):



5h

5h: 37 mg, 38% yield, 98% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = +44 (c = 0.029, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.30–8.26 (m, 1H), 8.22–8.17 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.65–7.38 (m, 5H), 7.20–7.14 (m, 3H), 7.12–7.06 (m, 1H), 7.06–7.02 (m, 1H), 3.99 (s, 3H), 1.96 (s, 3H), 1.31 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 158.7, 157.1, 155.1, 145.9, 140.6, 138.3, 137.0, 135.5, 134.5, 133.8, 132.3, 132.2, 128.0, 127.4, 126.6, 126.1, 126.0, 125.9, 119.5, 114.4, 80.1, 55.9, 27.9, 18.5; IR (KBr) ν_{max} 2974, 2931, 1662, 1452, 1366, 1247, 1148 cm^{-1}; **HRMS (ESI)** for $C_{28}H_{28}N_2NaO_4S^+$ $(M+Na)^+$: calcd. 511.1662, found 511.1672; **HPLC condition**: Phenomenex Chiralpak Amylose2, n-hexane/i-PrOH =50/50, Flow rate = 0.7 mL/min, UV = 254 nm, tR = 11.7 min (major) and tR = 16.7 min (minor).

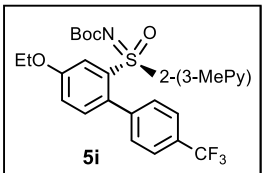
(*R*)-*N*-Boc-protected 2-(3-methoxyphenylsulfonimidoyl)-3-methylpyridine (1b):



1b

1b: 37 mg, 51% yield, 71% ee; $[\alpha]_D^{25}$ = –31.28 (c = 0.186, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 10.7 min (major) and tR = 15.4 min (minor).

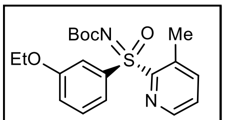
(*S*)-*N*-Boc-protected 2-(4-ethoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-sulfonimidoyl)-3-methylpyridine (5i):



5i

5i: 36 mg, 35% yield, 99% ee, colorless solid, $[\alpha]_D^{25}$ = +46.23 (c = 0.334, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.23–8.18 (m, 2H), 7.39–7.30 (m, 3H), 7.20 (dd, *J* = 7.5, 4.5 Hz, 1H), 7.14 (dd, *J* = 8.25, 2.75 Hz, 1H), 7.10–6.70 (m, 3H), 4.20 (q, *J* = 7.0 Hz, 2H), 2.29 (s, 3H), 1.47 (t, *J* = 7.0 Hz, 3H), 1.32 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 158.5, 157.0, 154.9, 146.0, 141.9, 140.9, 138.0, 136.5, 133.3, 132.7, 130.3, 129.4 (q, *J* = 32 Hz), 126.3, 124.03 (q, *J* = 274 Hz), 123.97 (q, *J* = 6.0 Hz), 119.7, 115.5, 80.3, 64.3, 27.9, 18.8, 14.7; **^{19}F NMR (471 MHz, $CDCl_3$)** δ –62.7; **HRMS (ESI)** for $C_{26}H_{27}F_3N_2NaO_4S^+$ $(M+Na)^+$: calcd. 543.1536, found 543.1544; IR (KBr) ν_{max} 2974, 1662, 1325, 1270, 1246, 1072, 1042 cm^{-1}; **HPLC condition**: Phenomenex Chiralpak Amylose2, n-hexane/i-PrOH =85/15, Flow rate = 0.4 mL/min, UV = 254 nm, tR = 21.4 min (major) and tR = 35.0 min (minor).

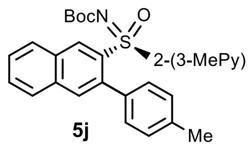
(*R*)-*N*-Boc-protected 2-(3-ethoxyphenylsulfonimidoyl)-3-methylpyridine (1f):



1f

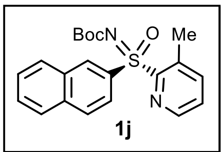
1f: 36 mg, 48% yield, 68% ee; $[\alpha]_D^{25}$ = –20.8 (c = 0.221, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 13.2 min (minor) and tR = 26.5 min (major).

(*S*)-*N*-Boc-protected 3-methyl-2-(3-(*p*-tolyl)naphthalene-2-sulfonimidoyl)pyridine (5j):



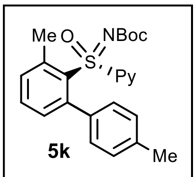
5j: 40 mg, 42% yield, 94% ee, colorless solid, $[\alpha]_D^{25}$ = +220 (c = 0.006, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.33 (s, 1H), 8.18 (dd, *J* = 4.5, 1.0 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 7.5 Hz, 1H), 7.68–7.58 (m, 3H), 7.35–7.30 (m, 1H), 7.17 (dd, *J* = 8.0, 4.5 Hz, 1H), 7.10–6.52 (m, 4H), 2.32 (s, 3H), 2.29 (s, 3H), 1.35 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 157.2, 155.0, 145.9, 140.7, 137.4, 137.3, 137.0, 135.3, 134.7, 134.6, 132.10, 132.07, 131.0, 129.7, 129.4, 127.7, 127.35, 127.28, 126.0, 80.1, 28.0, 21.1, 18.9 (1 carbon overlapped); IR (KBr) ν_{max} 2971, 1662, 1275, 1248, 1151, 1060, 890 cm^{-1}; **HRMS (ESI)** for $C_{28}H_{29}N_2O_3S^+$ $(M+H)^+$: calcd. 473.1893, found 473.1896; **HPLC condition**: YMC Amylose C-neo, n-hexane/i-PrOH = 70/30, Flow rate = 0.4 mL/min, UV = 254 nm, tR = 21.8 min (minor) and tR = 24.3 min (major).

(*R*)-*N*-Boc-protected 3-methyl-2-(naphthalene-2-sulfonimidoyl)pyridine (1j):



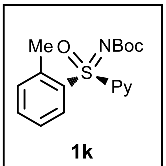
1j: 31 mg, 41% yield, 91% ee; $[\alpha]_D^{25}$ = –35.90 (c = 0.078, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.7 mL/min, UV = 254 nm, tR = 9.6 min (minor). and tR = 29.4 min (major).

(*S*)-*N*-Boc-protected 2-(3,4'-dimethyl-[1,1'-biphenyl]-2-sulfonimidoyl)pyridine (5k):



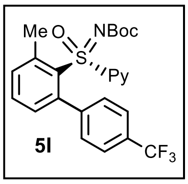
5k: 21 mg, 25% yield, 87% ee, colorless solid, $[\alpha]_D^{25}$ = −17.31 (c = 0.35, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.55–8.49 (m, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.53–7.46 (m, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.37–7.28 (m, 2H), 7.15 (d, *J* = 7.0 Hz, 1H), 7.07 (d, *J* = 7.5 Hz, 1H), 6.99–6.94 (m, 1H), 6.64 (d, *J* = 8.0 Hz, 1H), 6.27 (d, *J* = 8.0 Hz, 1H), 2.93 (s, 3H), 2.29 (m, 3H), 1.41 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 158.3, 156.8, 149.6, 143.0, 142.7, 137.0, 136.9, 136.7, 134.9, 132.8, 131.7, 131.1, 130.0, 128.2, 127.8, 127.5, 126.3, 123.0, 80.2, 28.1, 23.4, 21.1; **HRMS (ESI)** for $C_{24}H_{27}N_2O_3S^+$ $(M+H)^+$: calcd. 423.1737, found 423.1747; **HPLC condition**: Phenomenex Chiralpak Amylose2, n-hexane/*i*-PrOH = 85/15, Flow rate = 0.7 mL/min, UV = 254 nm, tR = 24.8 min (minor) and tR = 29.2 min (major)

(*R*)-*N*-Boc-protected 2-(2-methylphenylsulfonimidoyl) pyridine (1k):



1k: 30 mg, 46% yield, 41% ee; $[\alpha]_D^{25}$ = 8.0 (c = 0.166, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 10.5 min (major) and tR = 14.1 min (minor).

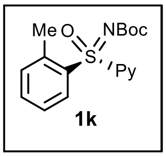
(*S*)-*N*-Boc-protected 2-(3-methyl-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-sulfonimidoyl) pyridine (5l):



5l

5l: 28 mg, 29% yield, 86% ee, colorless solid, $[\alpha]_D^{25}$ = –81.68 (c = 0.214, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.56 (d, *J* = 4.0 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.64–7.57 (m, 1H), 7.56–7.51 (m, 1H), 7.50–7.43 (m, 2H), 7.42–7.35 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.0 (d, *J* = 7.5 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 2.81 (s, 3H), 1.39 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ – 62.49; **^{13}C NMR (101 MHz, $CDCl_3$)** δ 158.0, 156.7, 149.8, 144.0, 142.2, 142.1, 137.5, 134.4, 133.4, 132.0, 130.8, 130.0, 129.0 (q, *J* = 32 Hz), 128.9, 126.8, 124.0 (q, *J* = 272 Hz), 123.8 (q, *J* = 3.8 Hz), 122.8, 80.5, 28.0, 23.1 (one peak missing); IR (KBr) ν_{max} 2979, 2938, 1660, 1279, 1243, 1156, 1120 cm^{-1}; **HRMS (ESI)** for $C_{24}H_{23}F_3N_2NaO_3S^+$ $(M+Na)^+$: calcd. 499.1274, found 499.1283; **HPLC condition**: Phenomenex Chiralpak Amylose2, n-hexane/i-PrOH =90/10, Flow rate = 0.6 mL/min, UV = 254 nm, tR = 23.7 min (minor) and tR = 27.8 min (major).

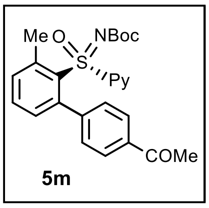
(*R*)-*N*-Boc-protected 2-(2-methylphenylsulfonimidoyl) pyridine (1k):



1k

1k: 33mg, 49% yield, 50% ee; $[\alpha]_D^{25}$ = + 12.63 (c = 0.41, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 10.4 min (major) and tR = 14.0 min (minor).

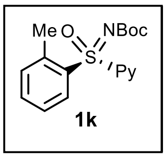
(*S*)-*N*-Boc-protected 1-(3'-methyl-2'-(pyridine-2-sulfonimidoyl)-[1,1'-biphenyl]-4-yl) ethanone (5m):



5m

5m: 30 mg, 33% yield, 84% ee, colorless solid, $[\alpha]_D^{25}$ = –22.91 (c = 0.213, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.60–8.55 (m, 1H), 7.92–7.83 (m, 2H), 7.66–7.57 (m, 2H), 7.50–7.34 (m, 4H), 7.04–6.99 (m, 1H), 6.84–6.79 (m, 1H), 2.79 (s, 3H), 2.59 (s, 3H), 1.39 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 197.7, 158.2, 156.6, 149.8, 145.5, 142.9, 142.0, 137.5, 135.5, 134.4, 133.3, 132.0, 130.7, 129.8, 128.8, 127.05, 126.96, 126.8, 122.9, 80.5, 28.0, 26.6, 23.1; IR (KBr) ν_{max} 2974, 1673, 1646, 1280, 1237, 1111, 890 cm^{-1}; **HRMS (ESI)** for $C_{25}H_{26}N_2NaO_4S^+$ $(M+Na)^+$: calcd. 473.1505, found 473.1515; **HPLC condition**: YMC Amylose C-neo, n-hexane/i-PrOH = 50/50, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 9.7 min (minor) and tR = 11.8 min (major).

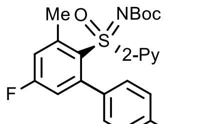
(*R*)-*N*-Boc-protected 2-(2-methylphenylsulfonimidoyl)pyridine(1k):



1k

1k: 32 mg, 48% yield, 51% ee; $[\alpha]_D^{25}$ = + 14.63 (c = 0.45, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 10.9 min (major) and tR = 14.5 min (minor).

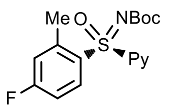
(*S*)-*N*-Boc-protected 2-(5-fluoro-3-methyl-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-sulfonimidoyl)-pyridine (5n):



5n

5n: 22 mg, 22% yield, 89% ee, colorless solid, $[\alpha]_D^{25}$ = –79.78 (c = 0.275, $CHCl_3$); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.56 (dd, *J* = 4.2, 0.6 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.63 (td, *J* = 7.8, 1.7 Hz, 1H), 7.57–7.52 (m, 1H), 7.45–7.43 (m, 1H), 7.43–7.37 (m, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.09 (dd, *J* = 8.8, 2.8 Hz, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 6.74 (dd, *J* = 8.4, 2.8 Hz, 1H), 2.79 (s, 3H), 1.41 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 164.6, 162.1, 157.9, 156.7, 149.8, 145.9, 145.8, 145.3, 145.2, 143.0, 137.6, 134.9, 130.4, 130.37, 130.0, 129.7, 129.67, 129.3, 129.0, 128.7, 128.0, 126.9, 125.3, 124.2, 124.0, 123.97, 123.9, 122.8, 122.6, 120.0, 119.9, 119.8, 118.0, 117.7, 80.6, 28.0, 24.8, 23.4; IR (KBr) ν_{max} 3070, 2931, 1657, 1581, 1322, 1282, 1126 cm^{-1}; **^{19}F NMR (376 MHz, $CDCl_3$)** δ – 62.59, –106.89; **HRMS (ESI)** for $C_{24}H_{22}F_4N_2NaO_3S^+$ $(M+Na)^+$: calcd. 517.1179, found 517.1190; **HPLC condition**: Phenomenex Chiralpak Amylose2, n-hexane/i-PrOH = 90/10, Flow rate = 0.7 mL/min, UV = 254 nm, tR = 16.1 min (minor) and tR = 18.8 min (major).

(*R*)-*N*-Boc-protected 2-(4-fluoro-2-methylphenylsulfonimidoyl)pyridine(1l):



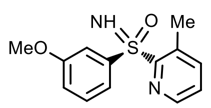
1l

1l: 36 mg, 51% yield, 37% ee; $[\alpha]_D^{25}$ = +10.23 (c = 0.088, $CHCl_3$); **HPLC condition**: Daicel IG-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 10.2 min (major) and tR = 12.9 min (minor).

2.7 Synthesis of chiral sulfoximine 6 (GP-5):

Chiral (*R*)-**1b** (0.2 mmol, 1.0 equiv) was dissolved in CH_2Cl_2 (2.0 mL) and TFA (10.0 equiv) was added. The mixture was stirred at 70 °C for 3 h. After concentration, the resulting residue was purified by flash column using hexane/EtOAc as the eluent to afford the desired product **6**.

(R)-2-(3-Methoxyphenylsulfonimidoyl)pyridine (6):



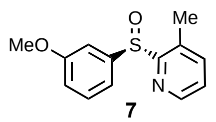
6

6: 46 mg, 88% yield, 95% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = –42.2 (c = 0.14, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.48 (d, *J* = 4.5 Hz, 1H), 7.62–7.56 (m, 2H), 7.52 (t, *J* = 2.25 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.39–7.32 (m, 1H), 7.10 (dd, *J* = 8.25, 2.25 Hz, 1H), 3.83 (s, 3H), 2.53 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 158.7, 156.0, 145.2, 140.9, 140.5, 132.2, 128.7, 125.8, 120.5, 118.6, 112.6, 54.7, 18.2; IR (KBr) ν_{max} 3028, 2969, 1738, 1366, 1229, 1216 cm^{-1}; **HRMS (ESI)** for $C_{13}H_{15}N_2O_2S^+$ $(M+H)^+$: calcd. 263.0849, found 263.0858; **HPLC condition**: IH-3, MeOH/DEA = 99.9/0.1, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 9.4 min (major) and tR = 10.2 min (minor).

2.8 Synthesis of chiral sulfoxide 7 (GP-6):

Chiral (*R*)-6 (0.2 mmol, 1.0 equiv) was dissolved in $CHCl_3$ (2.0 mL) under air and ^{t}BuONO (1.1 equiv) was added. The mixture was stirred at rt for 2 h. After concentration, the resulting residue was purified by preparative TLC using hexane/EtOAc as the eluent to afford the desired product **7**.

(*R*)- 2-((3-Methoxyphenyl)sulfinyl)pyridine (7):

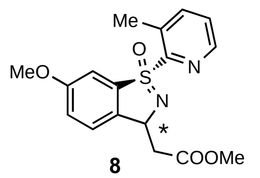


7: 39 mg, 78% yield, 90% ee, colorless viscous liquid, $[\alpha]_D^{25}$ = –63 (c = 0.13, $CHCl_3$); **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.47–8.40 (m, 1H), 7.25–7.18 (m, 2H), 7.18–7.08 (m, 2H), 6.88–7.80 (m, 1H), 3.68 (s, 3H), 2.37 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 160.5, 159.9, 147.5, 144.3, 139.8, 132.9, 129.7, 125.0, 117.04, 116.97, 109.4, 55.2, 16.5; IR (KBr) ν_{max} 3456, 2925, 1592, 1479, 1283, 1245, 1038 cm^{-1}; **HRMS (ESI)** for $C_{13}H_{13}NNaO_2S^+$ $(M+Na)^+$: calcd. 270.0559, found 270.0570; **HPLC condition**: IC-3, MeOH, Flow rate = 0.5 mL/min, UV = 254 nm, tR = 14.0 min (major) and tR = 14.8 min (minor).

2.9 Synthesis of Michael product 8 (GP-7):

Chiral (*R*)-**3c** (0.2 mmol, 1.0 equiv) was dissolved in CH_2Cl_2 (2.0 mL) and TFA (10.0 equiv) was added. The mixture was stirred at 70 ºC for 3 h. After concentration, the resulting residue was purified by flash column using hexane/EtOAc as the eluent to afford the desired product **8**.

Methyl 2-((1S)-6-methoxy-1-(3-methylpyridin-2-yl)-1-oxidobenzo[d]isothiazol-3-yl)acetate (8):

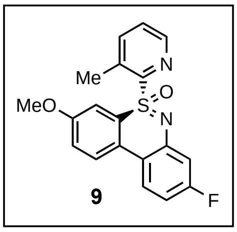


8: 46 mg, 66% yield, 95% ee , colorless viscous liquid. $[\alpha]_D^{25}$ = +47.3 (c = 0.114, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) 8.34–8.29 (m, 1H), 7.63 (dd, *J* = 7.75, 0.75 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.28 (dd, *J* = 7.5, 4.5 Hz, 1H), 7.18–7.12 (m, 2H), 5.29 (t, *J* = 1.5 Hz, 1H), 3.80 (s, 3H), 3.71 (s, 3H), 2.89 (dd, *J* = 6.75, 3.25 Hz, 2H), 2.66 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.7, 160.2, 156.9, 146.2, 141.4, 141.1, 137.9, 133.1, 126.0, 124.1, 121.0, 106.5, 65.3, 55.8, 51.7, 43.1, 18.9; IR (KBr) ν_{max} 2969, 2360, 2340, 1736, 1264, 1231, 1039 cm^{-1}; **HRMS (ESI)** for $C_{17}H_{19}N_2O_4S^+$ $(M+H)^+$: calcd. 347.1060, found 347.1070; **HPLC condition**: IG-3, MeOH, Flow rate = 0.3 mL/min, UV = 254 nm, tR = 22.8 min (major) and tR = 30.4 min (minor).

2.10 Synthesis of thiazine 9 (GP-8):

Chiral (*R*)-**5d** (0.2 mmol, 1.0 equiv) was dissolved in CH_2Cl_2 (2.0 mL) and TFA (10.0 equiv) was added. The mixture was stirred at 70 ºC for 1 h. After basic work-up followed by concentration, the crude was further subjected with $Pd(OAc)_2$ (10 mol%), $PhI(OAc)_2$ (2.0 equiv) in toluene at 75 ºC for 12 h. Next the crude was purified by flash column using hexane/EtOAc as the eluent to afford the desired product **9**.

(S)-8-fluoro-3-methoxy-5-(3-methylpyridin-2-yl)dibenzo[c,e][1,2]thiazine 5-oxide (9):

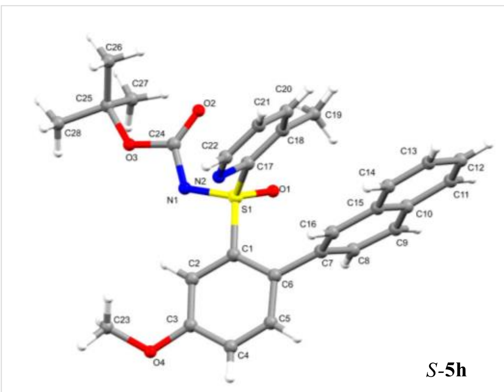


9: 44 mg, 62% yield, 93% ee, colorless viscous liquid. $[\alpha]_D^{25}$ = +63.1 (c = 0.014, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) 8.50 (d, J = 4.5 Hz, 1H), 8.08 (d, J = 9.0 Hz, 1H), 7.93 (dd, J = 9.0, 6.0 Hz, 1H), 7.66 (d, J = 7.5 Hz, 1H), 7.39 (dd, J = 7.5, 4.5 Hz, 1H), 7.30 (dd, J = 9.0, 2.5 Hz, 1H), 6.99 (d, J = 2.5 Hz, 1H), 6.92 (dd, J = 10.5, 2.5 Hz, 1H), 6.83–6.75 (m, 1H), 3.76 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5 (d, J = 247 Hz), 158.7, 155.1, 146.5, 143.7 (d, J = 12 Hz), 141.9, 134.3, 128.4, 127.0, 124.8, 124.4 (d, J = 10 Hz), 123.2, 122.0, 113.5, 110.7 (d, J = 23 Hz), 108.7 (d, J = 22 Hz), 108.3, 55.7, 19.0; IR (KBr) ν_{max} 2940, 2350, 2230, 1213, 1201, 1019 cm^{-1}; **^{19}F NMR (471 MHz, $CDCl_3$)** δ – 111.99; **HPLC condition**: IH-3, MeOH, Flow rate = 0.4 mL/min, UV = 254 nm, tR = 15.1 min (major) and tR = 15.8 min (minor).

X-ray crystallography: Single crystal X-ray data for the compound **5h** was collected using the Bruker D8 Quest CMOS detector system [λ(Mo-Kα) = 0.71073 Å] at 299K, graphite monochromator with a ω scan width of 0.3o , crystal-detector distance 60 mm, collimator 0.5 mm. The SMART software[3] was used for the intensity data acquisition and the SAINTPLUS Software was S23 used for the data extraction. In each case, absorption correction was performed with the help of SADABS program,[3] an empirical absorption correction using equivalent reflections was performed with the program. The structure was solved using SHELXS-97,[4] and full-matrix least-squares refinement against F2 was carried out using SHELXL-97.[4] All non-hydrogen atoms were refined anisotropically. Aromatic and methyl hydrogens were introduced on calculated positions and included in the refinement riding on their respective parent atoms.

Absolute configuration of **5h** and **3l** have been determined from the diffraction measurement Flack 0.02(4) and 0.04(5) respectively.

a



b

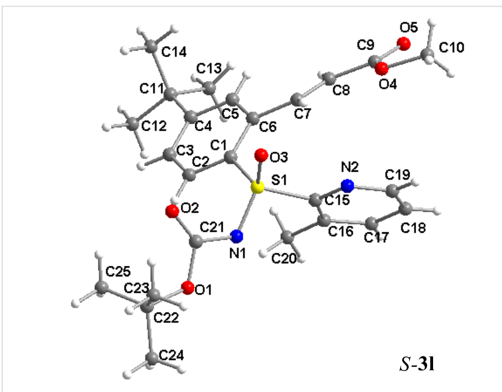


Figure S1. Thermal ellipsoidal plot of compound **5h** and **3l** with atom labeling scheme. Displacement ellipsoids are drawn at 50% probability level except for the H atoms, which are shown as circles of arbitrary radius**.**

Table S10. Crystal data for 5h

Identification code	**5h**
Formula	C28 H28 N2 O4 S
Fw	488.58
T (K)	292
λ (Å)	0.71073
Crystal system	Monoclinic
Space group	P 6_1
a(Å)	22.7073(5)
b (Å)	22.7073(5)
c (Å)	9.0908(2)
α (°)	90
β (°)	90
γ(°)	120
V ($Å^3$)	4059.4(2)
Z	6
ρ_{calcd} (Mg m^{-3})	1.199
μ (mm^{-1})	0.154
F(000)	1548
Reflections collected	5690
Unique reflections	3797
Completeness (%)	99.93
T_{max}, T_{min}	1.000, 0.673
GOF (F^2)	1.015
R1[I>2σ(I)]	0.0519
wR2 (all data)	0.1450(5690)
Flack	0.02(4)
CCDC Number	2088890

Table S11. Crystal data for 3l

Identification code	**3l**
Formula	C25H32N2O5S
Fw	472.58
T (K)	111K
λ (Å)	0.71073
Crystal system	Orthorhombic
Space group	P $2_12_12_1$
a(Å)	9.2225 (2)
b (Å)	15.1104 (3)

c (Å)	18.1484 (4)
α (°)	90
β (°)	90
γ(°)	90
V (Å^3)	2529.08 (9)
Z	4
ρ_{calcd} (Mg m^{-3})	1.241
μ (mm^{-1})	0.165
F(000)	1009.0
Reflections collected	5105
Unique reflections	4889
Completeness (%)	99.43
T_{max}, T_{min}	1.000, 0.651
GOF (F^2)	1.035
R1[I>2σ(I)]	0.0298
wR2 (all data)	0.0749(5105)
Flack	0.04(5)
CCDC Number	2109210

Density Functional Theory (DFT) Calculations:

Density-functional theory (DFT) calculations were performed using the Gaussian16 software[5] to understand the origin of this chiral resolution (Figure S2a). To diminish computational costs, we selected the simplest experimentally tested system, **1a**. We carried out geometry optimizations with the recently developed MN15 functional[6] coupled with the def2-TZVPPD basis set for Pd and the def2-SVP basis set for the other atoms.[7–9] This functional has proved to provide much better energetic values for the reaction barriers in transition metal catalysis than other commonly employed ones.[6] Effects of DCE as solvent on the Gibbs energy profile were considered with single-point calculations using the same functional and the def2-QZVPP basis set. The Gibbs energy were evaluated at 343.15 K.

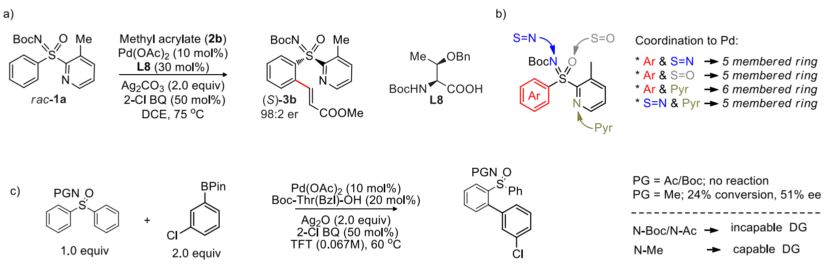


Figure S2. a) Selected model reaction for the computational mechanism elucidation. b) Coordination centres of the starting material **1a**. c) Comparision of directing capability of various N-protected sulfoximine imine

Since this is the study of a kinetic resolution, transition states are the most important species for the reaction path. From literature, mono-*N*-protected aminoacid (MPAA) C-H activations such as the one presented here, follows three steps: concerted metalation-deprotonation (CMD), insertion and a β-hydride elimination (Fig S3). The last one has no effect on the chiral outcome of the reaction. The CMD is a key step, since once the C-Pd bond is formed, the absolute configuration of the sulfur atom of the sulfoximine group in the unreacted substrate and in the reaction product gets defined. This concept has been presented as the relay of chirality from MPAA by Zhang, Yu and Wu.[10] The challenge in this scenario lies in the different coordination centers the sulfoximine substrate **1a** offers to the metal center (Fig S2b). In addition to the aryl group where the C-H activation takes place, there are three other possible coordination sites: S=N (**int-1$_{S=N}$**) or S=O (**int-1$_{S=O}$**) groups from the sulfoximine functionality, which form a five-membered palladacycle, and the pyridyl group (**int-1$_{Pyr}$**), which gives rise to a 6-membered ring. It should be underlined that at ground state, every directing groups can be interconverted by rotation of a dihedral angle.

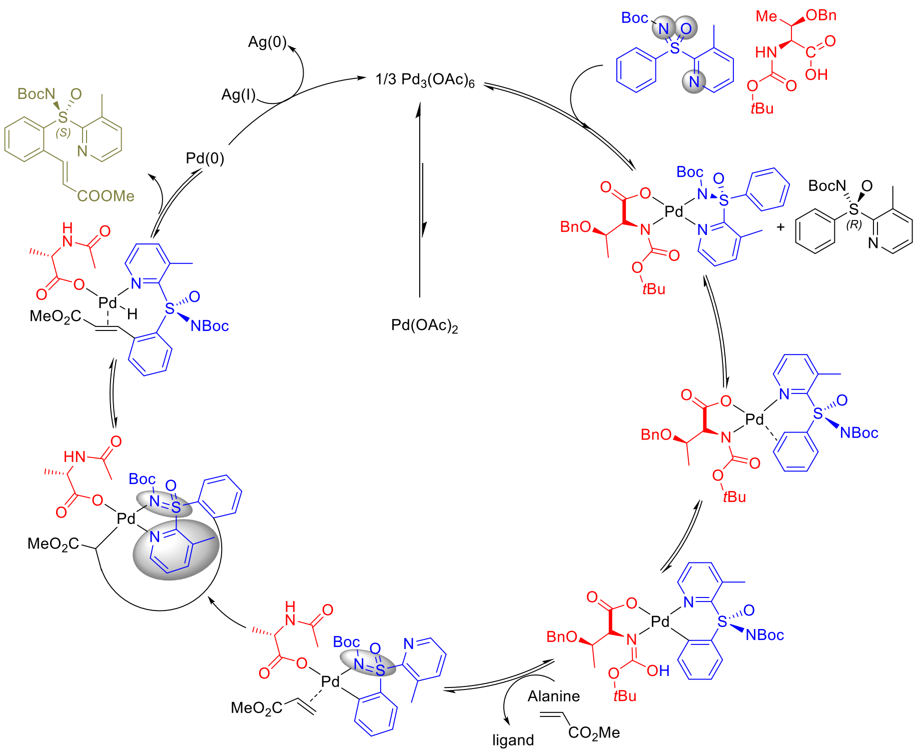


Figure S3. Mechanistic proposal for the kinetic resolution of sulfoximine.

The MPAA is known to lower the energy barrier of the CMD step by coordination to the metal center, forming a semi planar five membered ring (*vide infra*).[11] With the additional coordination of both nitrogen atoms available in the sulfoximine substrate **1a**, **int-0** is formed after displacement of 2 molecules of acetic acid. This intermediate is energetically favored, with the *S* configuration being 1.0 kcal/mol more stable than the *R* isomer. Consecutively, the aryl group should coordinate to Pd prior to the deprotonation, in a *cis* relationship with the MPAA amino group since it serves as a base in this process through its carbamate carbonyl.[11] This coordination gives rise to intermediates **int-1$_{S=N}$**, **int-1$_{S=O}$** and **int-1$_{Pyr}$**

depending on the group of the sulfoximine substrate coordinated to the metal. These intermediates undergo the CMD, defining the absolute configuration of the sulfur atom. As shown in Fig S4, it was found that pyridyl is the directing group which gives the lowest energy barriers, $\Delta\Delta G^{\neq}$ 22.91 kcal/mol for the *S* isomer and $\Delta G^{\neq}$ 25.35 kcal/mol for the *R* isomer. The calculated selectivity of this directing group is in excellent agreement with experimental observations (calc. 98:2, exp. 98:2). Additionally, the thermodynamics of this step (**int-2$_{Pyr}$**) highly favors the experimentally observed isomer by over 6 kcal/mol. From **int-1$_{S=N}$** and **int-1$_{S=O}$**, the CMD transition states lie much higher and the respective $\Delta\Delta G^{\neq}$ do not coincide with the experimental findings.

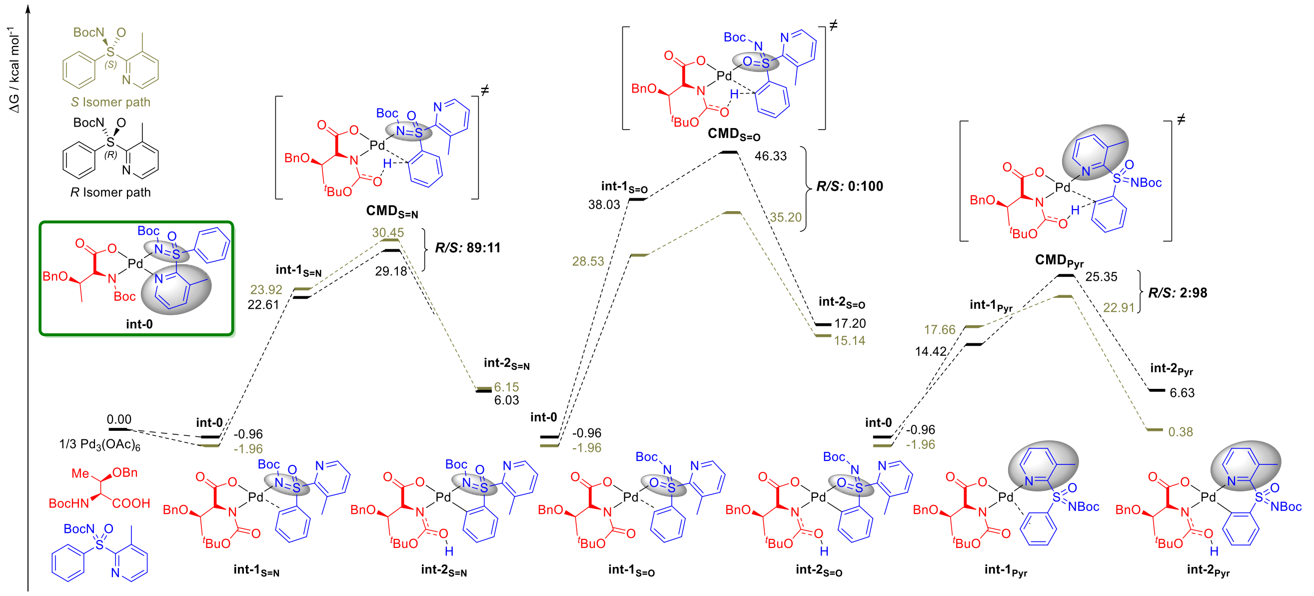


Figure S4. Comparison of the different energy profiles for the CMD of each possible coordination of the sulfoximine to the metal centre. Free energies at 343.15 K in DCE in kcal/mol. *R*/*S* selectivity highlighted at the transition state of each diagram.

The rationalization of the selectivity of the reaction can be done considering the findings of Cheng *et al*, who also focused on the CMD as determining step.[10] Considering the plane defined by the coordination of the MPAA to the Pd, the orientation of the bulky side chain pushes the carbamate to the other side to avoid steric interactions (for simplicity, the side chain will be defined above the plane, Fig S5). To this Pd-MPAA complex, the coordination of the phenyl group of the sulfoximine substrate can point upwards (U) or downwards (D) that plane, with any of both configurations (*R* or *S*). This translates into a total of 4 possible CMD approaches: **CMD$_{Pyr-UR}$, CMD$_{Pyr-US}$, CMD$_{Pyr-DR}$** and **CMD$_{Pyr-DS}$**. In all of them, the 6-membered cycle of the sulfoximine substrate with the Pd adopts a twisted boat conformation. In both scenarios where the phenyl group points upwards (**CMD$_{Pyr-UR}$** and **CMD$_{Pyr-US}$**), the sulfur atom and its substituents get located above the Pd plane. In agreement with Cheng observations, the C1-N2-Pd-O3 dihedral angle for these approaches are *ca.* -170°, which generates a higher steric interaction when compared with the ca. 140° of **CMD**$_{\mathbf{Pyr\text{-}DR}}$ and **CMD**$_{\mathbf{Pyr\text{-}DS}}$. These last transition structures also present the possibility of hydrogen bonds, making the combination of steric and electronic effects account for a difference of nearly 10 kcal/mol for each enantiomer. As can be seen in Figure S5, the geometry of the most stable transition structure for each enantiomer is very similar. The almost 2.5 kcal/mol difference between them lies in the fact that in the *R* configuration, given the size of the NBoc group, there is a steric clash with the methyl group from the pyridine moiety and in consequence with the phenyl group, causing an energetically demanding arrangement. Meanwhile, for the *S* configuration, the oxygen atom does not present such interactions. Additionally, the smaller distance of N···H in comparison with O···H could account with stabilizing electronic effects assisting the deprotonation. Of note, the CMD process through **int-1**$_{\mathbf{pyr}}$ is endergonic, so the calculated *R*/*S* ratio is only relevant if the next steps display lower free energies of activation than the **CMD**$_{\mathbf{pyr}}$ transition states.

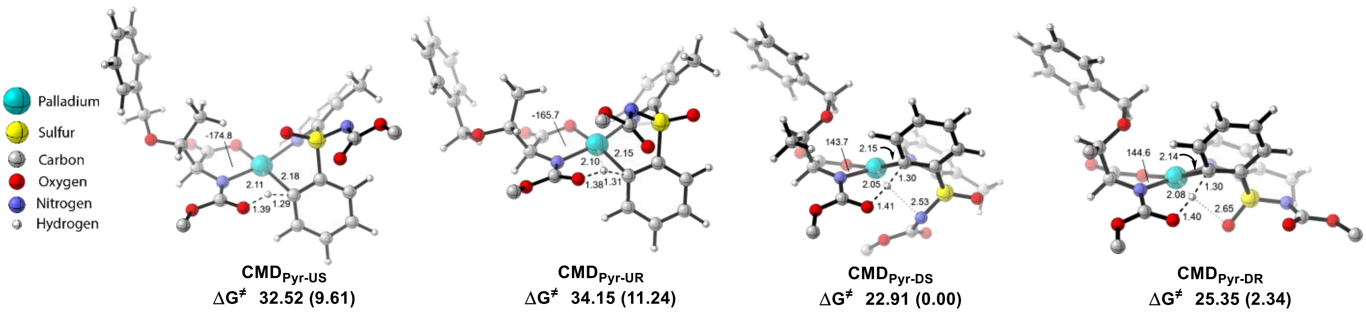


Figure S5. Transition structures for each **CMD**$_{\mathbf{Pyr}}$ approach. *tert*-Butyl group from NBoc removed from all models to simplify visualization. Free energies in kcal/mol, distances in Å. Free energies at 343.15 K in DCE in kcal/mol. Relative free energies in parentheses.

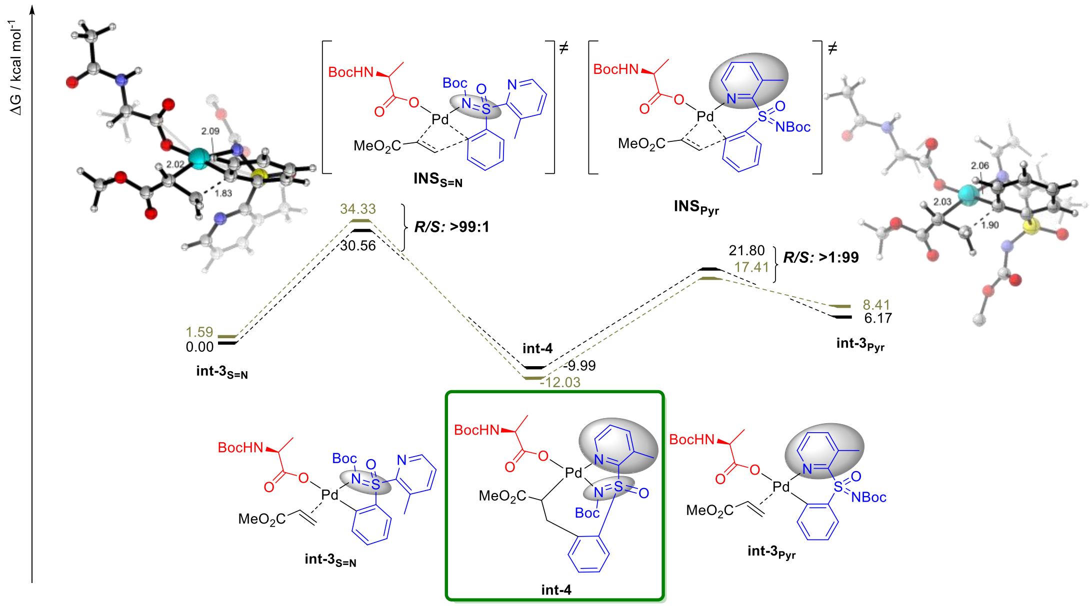


Figure S6. Comparison of the different energy profiles for the insertion step (INS) of the possible nitrogenated coordinations of the sulfoximine to the metal centre. Free energies at 343.15 K in DCE in kcal/mol. *R*/*S* selectivity highlighted at the transition state of each diagram.

To corroborate the outcome of this analysis, we studied the mechanism for the insertions step. At this stage, the MPAA is known to act as a monodentate ligand, so it is has been replaced as an acetate group for modelling purposes.[9,11] However, since we aim to distinguish the chiral center at the sulfur atom, we employed Acetyl-*L*-Alanine as a chiral MPAA. To further simplify the model, we only considered the prochiral center of methyl acrylate as *R*. Towards the product of the insertion, we considered the coordination of pyr and N=S in the metalated sulfoximine (Figure S6).

We found that the most stable of these **int-3** systems, is the one corresponding to N=S with *S* configuration, which is higher in energy than any int-2. However, the analysis of the transition states (**INS**) revealed that, as occurred in the CMD, when pyridine acts as a directing group (**INS$_{Pyr}$**), it provides the lowest energy barriers (36.08 kcal/mol for the *S* isomer and 40.47 for the *R* isomer). This gives a final selectivity >99:1, which is in perfect agreement with experimental observations (98:2). The study of this step confirms the selectivity observed at the CMD and shows the irreversibility of the reaction. Interestingly, **int-4$_{Pyr}$** and **int-4$_{N=S}$** present the same coordination pattern (**int-4**), since in both the two Nitrogenated groups (N=S and Pyr) are coordinated to the metal center.

Based on experimental observations and the computational results, we depicted the mechanism in Figure S7.

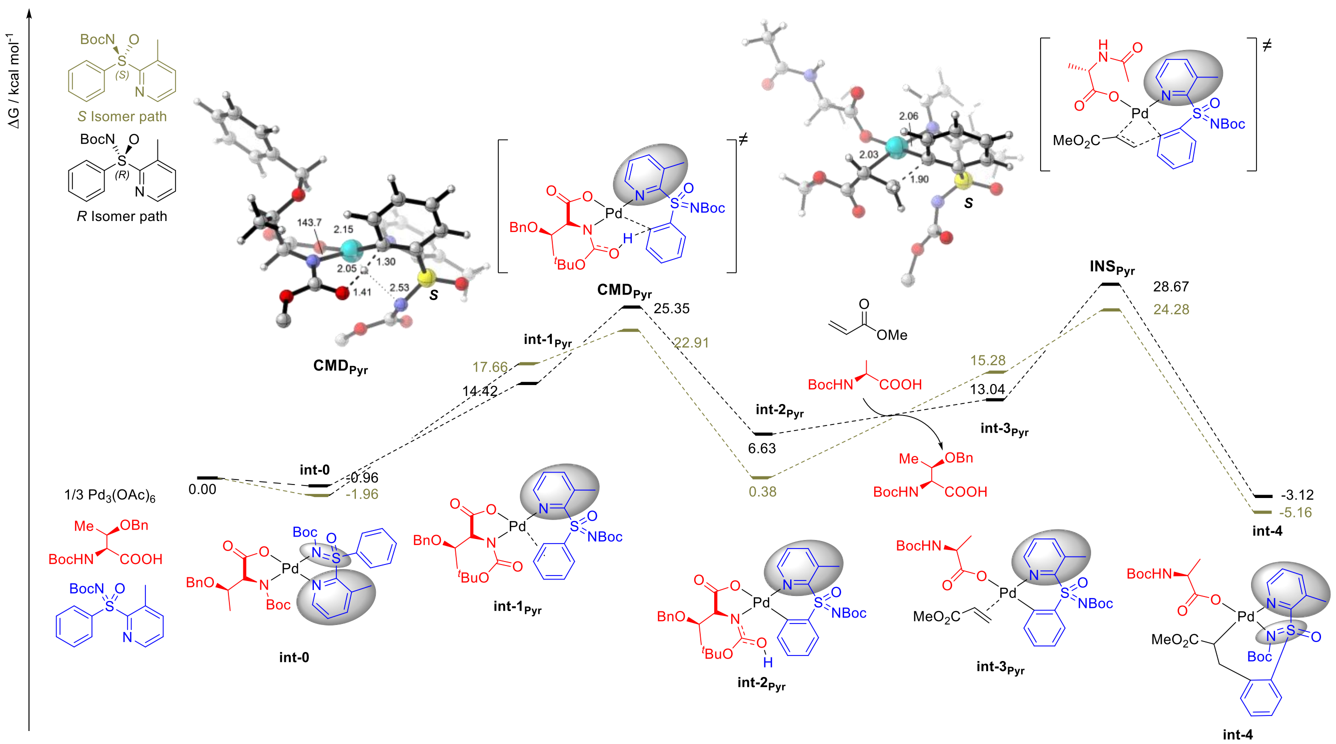


Figure S7. Complete free energy profile of the studied mechanism. Free energies at 343.15 K in DCE in kcal/mol

Catalytic effect of the mono *N*-Protected aminoacid

We studied the effect of the mono *N*-protected aminoacid (MPAA) as ligand for the concerted metalation deprotonation (CMD) of the sulfoximine. To this end, we modelled the uncatalyzed reaction via the new intermediates that contain two acetate groups instead of the bidentate aminoacid (**int-1$_{AcO}$**; **CMD$_{AcO}$** and **int-2$_{AcO}$**) as shown on Figure S8. The comparison on the effect of the MPAA is made with the coordination of the pyridyl from the sulfoximine since it is the most stable among all studied ones. Additionally, it should be mentioned that without a chirality transfer from an auxiliar ligand (MPAA for this reaction), the acetate groups are not able to provide the resolution observed in this work. As described above, the presence of a MPAA gives rise to an intermediate more stable than the starting materials. Furthermore, the intermediate where the phenyl and pyridyl group are coordinated to the metal centre is almost 15 kcal/mol more stable for the catalysed reaction. This energetic difference can also be observed at the transition state, where the difference is almost 10 kcal/mol.

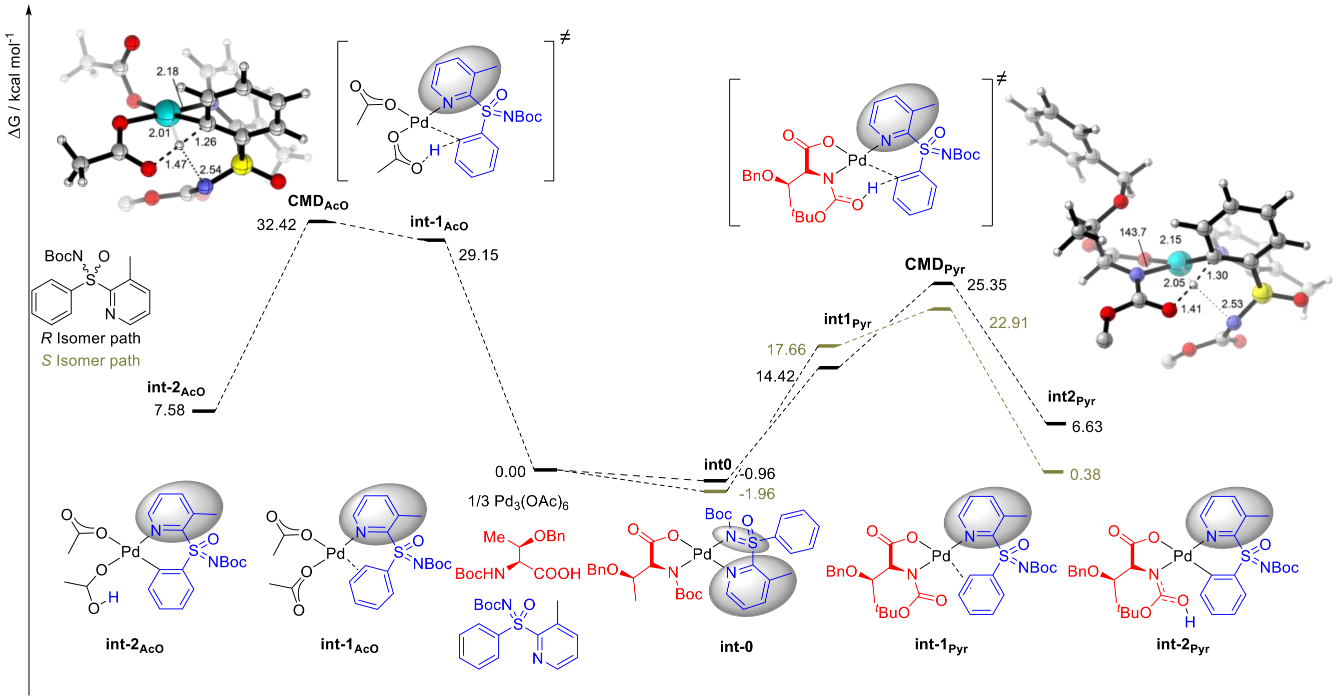


Figure S8. Comparison of the uncatalysed (left) versus MPAA catalysed (right) CMD step. Free energies at 343.15 K in DCE in kcal/mol

Rationalization of the inverse selectivity of NBoc systems

The selectivity outcome of the system in which the NBoc is coordinated to the metal centre for the CMD reaction is inverse to the one observed experimentally. These results can be explained considering, once again, the Relay of chirality previously presented based on the work of Cheng *et al*.[10] Considering the plane defined by the coordination of the MPAA to the Pd, the orientation of the bulky side chain pushes the carbamate to the other side to avoid steric interactions. To this Pd-MPAA complex, the coordination of the phenyl group of the sulfoximine substrate should be able to point upwards (U) or downwards (D) that plane, with any of both configurations (*R* or *S*) generating a total of 4 approaches. However, given the nature of the sulfoximine and the rigidity of the 5-membered palladacycle formed with NBoc compared to the 6-membered one formed with the pyridyl group, the system is not able to adapt the Upwards conformations. Regardless, based on our findings, those conformations are expected to be the higher in energy for each configuration. Hence, for this scenario there is only one approach for the *R* configuration and one for the *S* configuration (**CMD$_{S=N-DR}$** and **CMD$_{S=N-DS}$**). As similarly observed for **CMD$_{Pyr-DR}$** and **CMD$_{Pyr-DS}$**, the C1-N2-Pd-O3 angle values for the S=N analogues are 138.45 and 139.22, respectively (Figure S9). The key difference between both approaches seems to rise from an electronic stabilization via a N···H hydrogen bond in a similar fashion as in the pyridine group CMD (**CMD$_{Pyr-DS}$**). It is worth recall that the difference in selectivity is lower than that for the **CMD$_{Pyr}$** system (*R/S*: 2:98 vs 89:11)

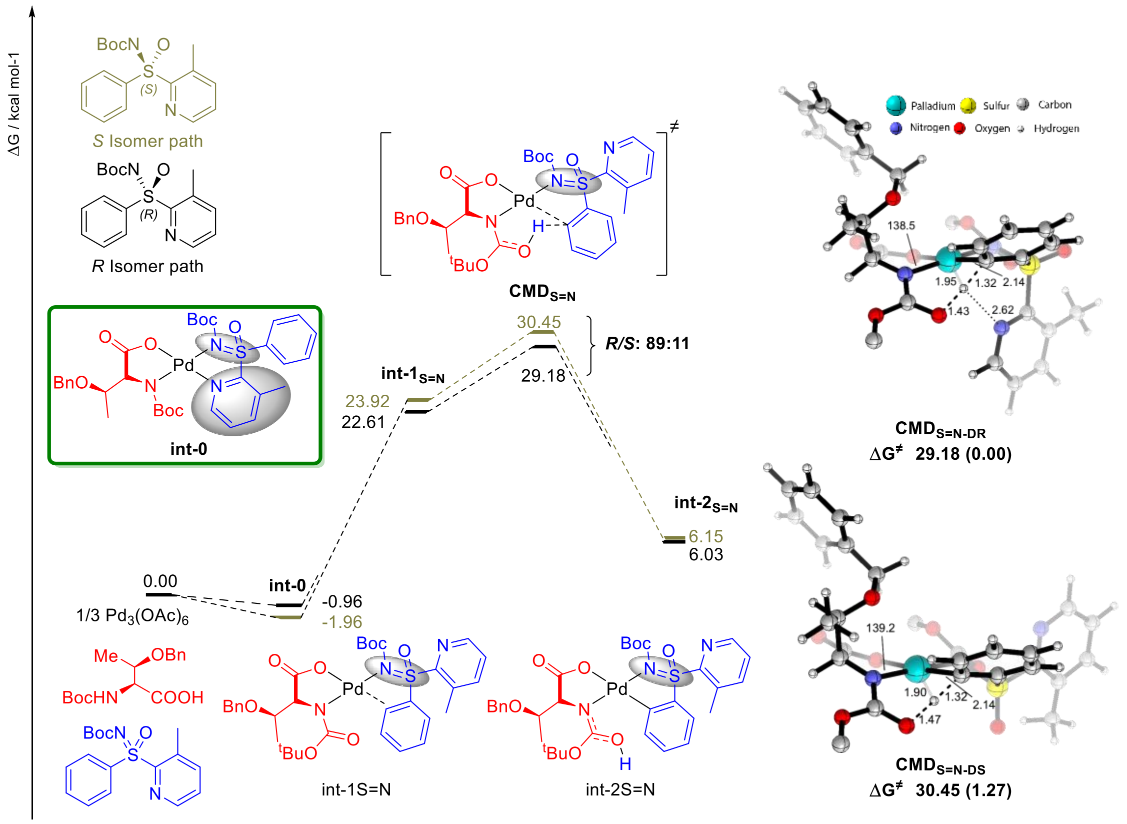


Figure S9. Energy profile for the CMD reaction step with NBoc group coordinated to Pd. Free energies at 343.15 K in DCE in kcal/mol, distances in A. Relative energies between parentheses.

Cartesian Coordinates

Alanine

Imaginary frequencies = 0
E(MN15,DCE) = -476.2579078
$E_{Thermal\ correction}$ = 0.102573

N	0.619667	0.398987	0.169432
H	0.424600	1.335604	0.516050
C	-0.518879	-0.429272	-0.142598
H	-0.406020	-0.824800	-1.167938
C	-0.670996	-1.622188	0.804655
C	-1.748799	0.449888	-0.118568
H	-0.804532	-1.276500	1.840309
H	-1.533268	-2.237973	0.516422
H	0.242308	-2.227641	0.740579
O	-1.752394	1.616790	0.194737
C	1.879771	-0.011381	-0.150720
O	2.089922	-1.098309	-0.664721
C	2.991682	0.956777	0.185443
H	3.609185	1.103809	-0.710409
H	2.629995	1.927479	0.549188
H	3.633997	0.499882	0.951223
O	-2.853768	-0.213922	-0.465226
H	-3.600674	0.407809	-0.409043

CH_3COOH

Imaginary frequencies = 0
E(MN15,DCE) = -229.0394117
$E_{Thermal\ correction}$ = 0.030141

C	-0.091087	0.121523	0.000011
O	-0.637655	1.195512	-0.000002
O	-0.779719	-1.033438	0.000002
H	-1.724070	-0.798117	-0.000029
C	1.391686	-0.112337	0.000004
H	1.672077	-0.701520	0.884210
H	1.672145	-0.700822	-0.884649
H	1.915249	0.848752	0.000375

Methyl-Acrylate

Imaginary frequencies = 0
E(MN15,DCE) = 306.36218632
$E_{Thermal\ correction}$ = 0.059947

C	0.039704	0.103470	0.000004
C	1.318082	-0.654420	-0.000018
O	-0.061421	1.308138	0.000046
O	-1.018880	-0.718082	-0.000029
C	-2.284832	-0.082743	-0.000011
C	2.480276	0.002894	0.000009
H	1.247360	-1.744364	-0.000057
H	-3.039388	-0.876886	-0.000031
H	-2.400918	0.553763	0.889227
H	-2.400920	0.553809	-0.889217
H	3.439466	-0.518765	-0.000006
H	2.477428	1.096789	0.000048

MPAA

Imaginary frequencies = 0
E(MN15,DCE) = -1053.984061
$E_{Thermal\ correction}$ = 0.31034

C	-1.698106	2.685154	-0.111160
O	-2.099343	3.655969	0.478672
C	0.727354	2.168072	-0.034938
C	-0.662085	1.720713	0.447880
N	-0.891738	0.370686	0.016378
O	-2.030489	2.402631	-1.375632
C	1.155106	3.477747	0.605920
O	1.608057	1.109905	0.267088
C	2.869827	1.181437	-0.338185
O	-2.111446	-1.481721	-0.160131
C	-3.315871	-2.285600	-0.107046
C	-2.842104	-3.656208	-0.570922
C	-3.838204	-2.356365	1.324104
C	-4.360492	-1.727306	-1.067782
C	-2.123841	-0.186426	0.174903
O	-3.089385	0.444029	0.565370
C	3.615681	-0.115777	-0.156643
C	3.250713	-1.023450	0.842313

C	3.973652	-2.206137	1.016084
C	5.067497	-2.490375	0.197651
C	5.434949	-1.586487	-0.802459
C	4.710459	-0.408332	-0.979252
H	0.670911	2.277384	-1.138620
H	-0.717869	1.829500	1.545659
H	2.079766	3.863142	0.153988
H	0.372704	4.240526	0.493880
H	1.328117	3.316599	1.680497
H	2.764008	1.404943	-1.419285
H	3.465247	2.008055	0.097046
H	-3.682074	-4.365696	-0.573885
H	-2.428201	-3.592560	-1.587621
H	-2.059501	-4.036790	0.101265
H	-4.679307	-3.063923	1.372456
H	-4.179273	-1.371126	1.664821
H	-3.045662	-2.716750	1.997294
H	-4.701844	-0.737777	-0.739999
H	-3.935804	-1.645496	-2.079688
H	-5.222802	-2.409308	-1.108616
H	2.393660	-0.794221	1.477896
H	3.678867	-2.909803	1.798005
H	5.631172	-3.415706	0.334971
H	6.285829	-1.803893	-1.452007
H	4.995132	0.293119	-1.769426
H	-0.079138	-0.212993	-0.164660
H	-2.698136	3.057512	-1.644345

$PdOAc_2$_trimer

Imaginary frequencies = 0
E(MN15,DCE) = -1753.814649
$E_{Thermal\ correction}$ = 0.22939

Pd	1.573522	0.907091	0.000426
O	2.245203	0.027904	-1.651095
O	2.595465	-0.362384	1.153915
C	2.187389	-1.350109	1.822095
O	1.092580	-1.955737	1.652438
Pd	-0.000951	-1.814734	-0.001731
C	2.268254	-1.223590	-1.817393
O	1.610659	-2.068364	-1.152505
O	1.146620	1.927098	1.652860
O	0.986842	2.427699	-1.153074
C	-0.072139	2.570135	-1.821360
O	-1.144448	1.924622	-1.654011
Pd	-1.573002	0.908284	-0.000253
C	0.074206	2.571992	1.820043
O	-0.984364	2.429399	1.150963
O	-2.239955	0.029097	1.653753
O	-2.598480	-0.359792	-1.152080
C	-2.264499	-1.222458	1.819226
C	-2.192054	-1.347310	-1.821368
O	-1.612643	-2.068001	1.149459
O	-1.095484	-1.951178	-1.656136
C	3.195218	-1.753706	-2.877075
C	-0.073931	3.631858	-2.887205
C	0.071697	3.633608	2.886006
C	-3.185034	-1.753375	2.884068
C	-3.111780	-1.882006	-2.885000
C	3.104054	-1.879776	2.890965
H	0.276350	4.600488	2.402617
H	0.859793	3.437463	3.621144
H	-0.914515	3.690633	3.360779
H	0.927881	3.741055	-3.317421
H	-0.356540	4.585262	-2.416499
H	-0.816836	3.394341	-3.656835
H	-3.716668	-1.072384	-3.308301
H	-2.534166	-2.398309	-3.659913
H	-3.786836	-2.612106	-2.414114
H	3.347494	-0.999579	-3.657428
H	2.803515	-2.688159	-3.293972
H	4.167011	-1.961625	-2.405031
H	3.821656	-2.564325	2.414747
H	3.665342	-1.058079	3.350150
H	2.532273	-2.440989	3.638209
H	-3.369485	-0.985467	3.643498
H	-2.767133	-2.663915	3.328082
H	-4.143585	-2.008281	2.408054

Sulfoximine

Imaginary frequencies = 0
E(MN15,DCE) = -1392.68078
$E_{Thermal\ correction}$ = 0.28523

C	-2.483961	-0.503637	0.229950
S	-0.775257	-0.492155	0.690386

C	-0.149922	1.030096	-0.088748
O	-0.689085	-0.355609	2.146073
C	-3.394436	-0.025599	1.171276
C	-4.748980	-0.006729	0.835926
C	-5.162044	-0.460051	-0.419026
C	-4.230783	-0.940346	-1.345543
C	-2.874144	-0.968619	-1.026124
N	-0.376672	1.030780	-1.391052
C	0.066093	2.050040	-2.122533
C	0.767865	3.110597	-1.546371
C	0.996179	3.086686	-0.172690
C	0.535489	2.026423	0.624070
N	-0.200199	-1.708844	-0.078491
O	1.895742	-0.911741	0.353124
C	3.299258	-0.725741	0.039340
C	3.753745	0.380665	0.982452
C	4.092486	-1.998259	0.321953
C	3.428638	-0.263966	-1.408732
C	1.148701	-1.821411	-0.333384
O	1.618639	-2.634774	-1.091870
C	0.817618	2.001464	2.098579
H	-3.034872	0.302960	2.148249
H	-5.483190	0.355057	1.558407
H	-6.223376	-0.445963	-0.676820
H	-4.565300	-1.301579	-2.320008
H	-2.115826	-1.348742	-1.711743
H	-0.138983	2.019738	-3.196616
H	1.130266	3.935609	-2.161841
H	1.550457	3.898782	0.306340
H	4.830338	0.561355	0.849864
H	3.216913	1.317208	0.771173
H	3.572380	0.092732	2.028551
H	5.166679	-1.788157	0.207212
H	3.805375	-2.804057	-0.362266
H	3.914201	-2.326388	1.357092
H	2.796632	0.626213	-1.568038
H	4.472816	0.008318	-1.623437
H	3.116118	-1.055444	-2.101381
H	1.474399	2.841178	2.365718
H	-0.108521	2.065553	2.685763
H	1.292516	1.053870	2.383407

Int-0-R

Imaginary frequencies = 0
E(MN15,DCE) = -2573.192436
$E_{Thermal\ correction}$ = 0.6076

Pd	-0.360041	0.145477	-0.495033
O	0.080973	-1.684315	-0.997762
C	1.256877	-2.124836	-0.598281
N	1.606993	0.266736	-0.313743
N	-0.886088	1.941569	0.354229
C	2.330469	1.052556	-1.156003
O	1.584498	-3.290386	-0.689017
C	0.021999	2.839994	0.753697
C	-0.366061	4.006942	1.409722
C	-1.713649	4.224513	1.668943
C	-2.681515	3.277892	1.294636
C	-2.180113	2.151156	0.632696
C	-3.617150	-0.020658	1.686255
O	1.568088	2.072384	-1.638631
O	3.510071	0.913956	-1.438559
C	-4.938887	-0.195898	2.090168
C	-5.173871	-0.902054	3.269985
C	-4.102425	-1.417733	4.004997
C	-2.530448	-0.535169	2.394377
C	-2.785444	-1.238517	3.570461
H	-2.038154	5.130760	2.186122
H	0.392422	4.727074	1.719215
H	1.060760	2.589655	0.539836
H	-6.198654	-1.060950	3.610616
H	-4.296334	-1.974367	4.924151
H	-1.509120	-0.405363	2.024560
H	-1.951507	-1.654818	4.139032
H	-5.748762	0.200501	1.474506
C	-3.046345	-1.198297	-1.261995
C	2.133348	3.130100	-2.438933
C	3.198295	3.877456	-1.641034
C	2.684863	2.578922	-3.749997
C	0.939412	4.038231	-2.710159
H	2.771267	4.241513	-0.691471
H	4.049272	3.220573	-1.422508
H	3.551020	4.749531	-2.211761
H	1.905444	2.000604	-4.268350
H	2.990949	3.411625	-4.401323
H	3.546819	1.927814	-3.563465
H	1.242195	4.895108	-3.329420
H	0.150458	3.480292	-3.235259

H	0.525142	4.419686	-1.763185
C	-4.133391	3.500208	1.612413
H	-4.717505	3.660675	0.696457
H	-4.577166	2.631273	2.120413
H	-4.238777	4.375516	2.265981
N	-2.408712	-0.014794	-0.816351
O	-4.571238	1.392686	-0.334063
O	-4.077489	-1.600375	-0.758206
S	-3.320457	0.839515	0.163001
C	-2.505757	-3.126967	-2.635681
C	-2.298292	-4.010649	-1.412018
C	-3.865406	-3.336727	-3.289036
C	-1.365641	-3.323766	-3.621817
H	-1.312422	-3.799076	-0.971633
H	-3.089661	-3.854455	-0.666231
H	-2.323433	-5.063878	-1.728263
H	-3.990453	-2.648834	-4.138709
H	-3.931932	-4.367722	-3.666796
H	-4.675794	-3.168411	-2.567749
H	-1.378381	-4.355864	-4.001174
H	-1.468273	-2.631975	-4.470635
H	-0.409839	-3.135803	-3.112440
O	-2.373619	-1.721743	-2.250897
C	2.173176	-1.042679	-0.027024
C	2.432208	-1.214000	1.484662
H	3.140823	-1.125666	-0.544245
C	1.171121	-1.076708	2.317818
O	2.988825	-2.459379	1.814104
H	3.134616	-0.396517	1.750673
H	0.756198	-0.061496	2.223489
H	1.410379	-1.272891	3.372740
H	0.418615	-1.813032	1.987993
C	4.161995	-2.829531	1.125650
C	5.273429	-1.817740	1.295001
H	4.462844	-3.793000	1.564361
H	3.949367	-3.012584	0.058295
C	5.811681	-1.127140	0.205418
C	5.740092	-1.520335	2.584137
C	6.812215	-0.169321	0.394353
H	5.435035	-1.326458	-0.801713
C	6.736651	-0.565711	2.776922
H	5.304233	-2.047392	3.437999
C	7.277841	0.111147	1.678486
H	7.218014	0.365462	-0.467122
H	7.096582	-0.346938	3.785313
H	8.059063	0.860377	1.827586

Int-0-S

Imaginary frequencies = 0
E(MN15,DCE) = -2573.194026
$E_{Thermal\ correction}$ = 0.60408

Pd	0.028645	0.238672	0.109849
O	-1.248960	-0.768053	1.180059
C	-2.397594	-0.181350	1.446881
N	-1.131944	1.735185	0.660838
N	1.213642	1.257386	-1.219433
C	-0.613155	2.750385	1.400258
O	-3.319038	-0.771246	1.972654
C	0.914360	2.515804	-1.566188
C	1.715885	3.222608	-2.459339
C	2.837359	2.603804	-3.000926
C	3.144471	1.270625	-2.687576
C	2.271279	0.658682	-1.778794
C	4.040862	-1.303646	-0.758887
O	0.747481	2.784560	1.276209
O	-1.236377	3.558118	2.067249
C	4.870418	-2.282697	-1.296863
C	6.143772	-2.432932	-0.747707
C	6.551434	-1.613828	0.309143
C	4.412129	-0.485903	0.309592
C	5.692288	-0.644780	0.838720
H	3.480788	3.141192	-3.701830
H	1.453014	4.247556	-2.724478
H	0.011143	2.926579	-1.110958
H	6.817966	-3.195562	-1.141536
H	7.550726	-1.735902	0.732068
H	3.713509	0.254182	0.713679
H	6.017120	-0.017592	1.670749
H	4.506563	-2.905411	-2.116803
C	1.476746	-2.544904	0.355072
C	1.538201	3.855025	1.819062
C	1.149187	5.176717	1.162543
C	1.408058	3.917665	3.337997
C	2.960426	3.460250	1.430722
H	1.255520	5.100692	0.067589
H	0.109500	5.429418	1.406982
H	1.808280	5.983986	1.515394

H	1.629992	2.931145	3.772191
H	2.127456	4.646365	3.741917
H	0.391469	4.209454	3.625964
H	3.680004	4.222567	1.763456
H	3.220871	2.499950	1.902525
H	3.044343	3.349393	0.336599
C	4.336091	0.590100	-3.300850
H	5.155905	0.501958	-2.570108
H	4.086768	-0.421856	-3.646614
H	4.702826	1.174956	-4.154111
N	1.371593	-1.293845	-0.288614
O	2.334496	-1.825843	-2.718565
O	2.096511	-3.467938	-0.137974
S	2.427566	-1.104334	-1.456753
C	0.288035	-3.699010	2.134143
C	-0.659487	-4.332325	1.124444
C	1.397328	-4.642760	2.580044
C	-0.487082	-3.147517	3.320391
H	-1.388551	-3.574389	0.799924
H	-0.112273	-4.722879	0.254233
H	-1.200276	-5.164594	1.597506
H	2.086370	-4.122308	3.262314
H	0.952890	-5.490205	3.122723
H	1.963044	-5.023510	1.720358
H	-0.936851	-3.980657	3.880376
H	0.187680	-2.596715	3.992093
H	-1.279919	-2.470099	2.972607
O	0.868295	-2.508984	1.512913
C	-2.471546	1.287964	1.008349
C	-3.454037	1.463664	-0.159501
H	-2.871332	1.888303	1.839516
C	-3.181082	0.493021	-1.301299
O	-4.738492	1.350450	0.402593
H	-3.308021	2.500983	-0.530580
H	-2.154325	0.647297	-1.671051
H	-3.873026	0.644794	-2.143016
H	-3.279815	-0.549883	-0.962168
C	-5.829764	1.425727	-0.464376
C	-6.320627	0.070687	-0.931278
H	-6.643437	1.924858	0.089892
H	-5.608048	2.071250	-1.338847
C	-7.138755	-0.038731	-2.061524
C	-5.989169	-1.080718	-0.207024
C	-7.628709	-1.281860	-2.464882
H	-7.392558	0.859527	-2.633958
C	-6.476824	-2.324196	-0.615925
H	-5.331170	-0.989180	0.662479
C	-7.298104	-2.429767	-1.740738
H	-8.265086	-1.355872	-3.350186
H	-6.209796	-3.218903	-0.048372
H	-7.676718	-3.404901	-2.056265

CMD_NBoc_R

Imaginary frequencies = 1 (-1190.6103)
E(MN15,DCE) = -2573.144397
$E_{Thermal\ correction}$ = 0.59945

Pd	-0.263986	0.081872	0.077839
C	1.859826	-0.345225	-1.692661
O	2.731880	-0.914813	-2.322153
C	3.194808	1.072331	-0.112700
C	2.076105	1.085463	-1.171629
N	0.827407	1.538094	-0.607800
N	-3.298703	0.778941	-0.585542
C	-3.853517	-0.321615	-0.110560
C	-5.017991	-0.937426	-0.589826
C	-5.591483	-0.266937	-1.684303
C	-3.858721	1.394938	-1.619880
C	-5.024010	0.892266	-2.206218
S	-2.871259	-0.991460	1.248160
O	-3.670112	-1.889430	2.072323
O	0.724297	-0.895784	-1.349127
C	3.544514	2.472065	0.354053
O	2.792095	0.348524	1.031924
C	3.032550	-1.047251	1.058085
O	0.955483	3.646191	-1.387878
C	0.623410	5.056914	-1.334727
C	1.791518	5.710880	-2.059602
C	-0.685156	5.322365	-2.069709
C	0.573042	5.515886	0.119060
C	0.251484	2.715696	-0.746298
O	-0.905188	2.933709	-0.282886
N	-1.463386	-1.515243	0.682023
O	-0.339417	-3.202749	-0.221993
C	-0.017775	-4.201649	-1.234197
C	-0.542955	-3.760705	-2.595297
C	1.504383	-4.210504	-1.241485
C	-0.595802	-5.540011	-0.793812

C	-1.538623	-2.691009	-0.082661
O	-2.587386	-3.137003	-0.513130
C	4.492807	-1.390615	0.884813
C	4.917973	-2.221975	-0.155948
C	6.274065	-2.526435	-0.306100
C	7.214186	-1.989904	0.573925
C	6.797338	-1.142406	1.605868
C	5.444212	-0.844895	1.758597
C	-5.626027	-2.192392	-0.039758
C	-2.740597	0.469845	3.494762
C	-2.124858	1.387015	4.352503
C	-1.045387	2.147892	3.900152
C	-0.590719	2.024811	2.583477
C	-1.201382	1.141032	1.682241
C	-2.269859	0.382665	2.190605
H	4.071143	0.591129	-0.586052
H	2.396969	1.718979	-2.013735
H	-6.500656	-0.680490	-2.128671
H	-3.362475	2.300828	-1.979682
H	-5.477244	1.400530	-3.058813
H	3.824031	3.117580	-0.491526
H	4.375203	2.430300	1.072501
H	2.670464	2.914534	0.859789
H	2.683048	-1.373706	2.049667
H	2.423609	-1.590208	0.313936
H	1.659284	6.801934	-2.087098
H	2.734677	5.479896	-1.542543
H	1.858028	5.335326	-3.090742
H	-0.855917	6.407395	-2.134177
H	-1.528350	4.857403	-1.544137
H	-0.629713	4.919988	-3.092206
H	1.510185	5.242378	0.629363
H	0.466199	6.609887	0.158617
H	-0.274106	5.058549	0.646793
H	-0.130397	-4.427574	-3.366713
H	-1.638692	-3.803216	-2.640239
H	-0.199765	-2.734986	-2.794213
H	1.869024	-4.999760	-1.915431
H	1.890020	-4.404753	-0.229029
H	1.877752	-3.235972	-1.593363
H	-0.199467	-5.822473	0.192860
H	-1.691690	-5.485437	-0.740163
H	-0.314216	-6.319325	-1.517369
H	4.178779	-2.607427	-0.862929
H	6.596663	-3.176100	-1.122873
H	8.274356	-2.225198	0.454089
H	7.531958	-0.716643	2.293675
H	5.108569	-0.179732	2.559876
H	-6.484621	-2.491758	-0.655282
H	-4.879179	-2.997563	-0.030398
H	-5.957353	-2.051276	0.998008
H	-3.543377	-0.189772	3.831378
H	-2.475887	1.486473	5.381396
H	-0.550756	2.844373	4.580448
H	0.242414	2.637533	2.225151
H	-1.139598	1.767214	0.516638

CMD_NBoc_S

Imaginary frequencies = 1 (-1116.6246)
E(MN15,DCE) = -2573.142368
$E_{Thermal\ correction}$ = 0.59905

Pd	-0.069168	-0.532055	-0.444771
C	-2.049515	1.050396	-1.624985
O	-2.626137	2.034372	-2.050125
C	-3.430553	0.486554	0.388905
C	-2.829242	-0.069652	-0.915829
N	-1.904394	-1.142353	-0.647026
N	4.099345	0.208712	1.774598
C	4.374545	-0.403621	0.636573
C	5.626439	-0.468149	0.006382
C	6.649833	0.170446	0.726963
C	5.086023	0.812442	2.429085
C	6.393732	0.808723	1.936200
S	2.896241	-1.116634	-0.119548
O	3.232331	-2.015332	-1.215061
O	-0.751651	0.888844	-1.660620
C	-4.322767	-0.527291	1.078127
O	-2.406961	0.819434	1.305669
C	-1.856789	2.122763	1.245935
O	-3.333207	-2.822444	-1.094315
C	-3.778077	-4.199682	-0.993882
C	-5.267236	-4.100370	-1.293882
C	-3.071756	-5.061132	-2.033388
C	-3.553155	-4.706203	0.427519
C	-2.096459	-2.442177	-0.781952
O	-1.150982	-3.258692	-0.607226
N	1.891139	0.104838	-0.370030

O	1.590046	2.229850	-0.930042
C	1.627143	3.365186	-1.843581
C	1.621250	2.851156	-3.277718
C	0.330624	4.102635	-1.542162
C	2.847837	4.221268	-1.531591
C	2.423597	1.218710	-1.023673
O	3.523869	1.217784	-1.549614
C	-2.893908	3.204711	1.432903
C	-3.099082	4.181255	0.453256
C	-4.065888	5.173889	0.638457
C	-4.843572	5.187143	1.796525
C	-4.657211	4.201217	2.771219
C	-3.688161	3.215974	2.588592
C	5.899644	-1.074974	-1.336686
C	2.624304	-2.397999	2.318268
C	1.838058	-2.911777	3.351994
C	0.446930	-2.915871	3.236593
C	-0.163135	-2.458859	2.067351
C	0.592812	-1.966827	0.991628
C	1.988291	-1.918679	1.177736
H	-4.009196	1.387390	0.111316
H	-3.651242	-0.393826	-1.573758
H	7.658684	0.173068	0.306361
H	4.829453	1.313796	3.366434
H	7.192929	1.308688	2.485812
H	-5.122421	-0.876938	0.408924
H	-4.767801	-0.082197	1.979192
H	-3.716803	-1.396301	1.383120
H	-1.124695	2.156476	2.067666
H	-1.292329	2.295015	0.312810
H	-5.730520	-5.096460	-1.250776
H	-5.759694	-3.446927	-0.558326
H	-5.425664	-3.678801	-2.296800
H	-3.500576	-6.074388	-2.021913
H	-1.996933	-5.122997	-1.824051
H	-3.217844	-4.635113	-3.037036
H	-4.010000	-4.009328	1.148464
H	-4.030452	-5.689634	0.549810
H	-2.481613	-4.802784	0.645221
H	1.482367	3.697535	-3.966087
H	2.563693	2.345517	-3.527387
H	0.780422	2.152266	-3.399182
H	0.278960	5.023136	-2.142316
H	0.285673	4.375678	-0.476442
H	-0.530397	3.462045	-1.788851
H	2.825628	4.547215	-0.480764
H	3.772665	3.659179	-1.715884
H	2.839755	5.116501	-2.170922
H	-2.513729	4.138954	-0.468738
H	-4.219636	5.931551	-0.133284
H	-5.601751	5.960781	1.939216
H	-5.269186	4.205239	3.676493
H	-3.538114	2.437778	3.342957
H	6.951744	-0.916603	-1.607683
H	5.674901	-2.149032	-1.355974
H	5.251394	-0.600535	-2.087190
H	3.709375	-2.348234	2.420694
H	2.317315	-3.291498	4.256277
H	-0.166699	-3.291485	4.057817
H	-1.250227	-2.505234	1.954650
H	-0.094013	-2.394978	-0.055020

CMD_Pyr_R_cis

Imaginary frequencies = 1 (-1167.3321)
E(MN15,DCE) = -2573.136478
$E_{Thermal\ correction}$ = 0.60122

Pd	-0.491360	-1.081434	-0.923593
C	2.237993	-1.664920	-1.263980
O	3.225141	-2.312458	-1.549462
C	2.921126	0.452078	-0.039900
C	2.217321	-0.135528	-1.313696
N	0.823623	0.285014	-1.389944
N	-1.596462	-2.665424	-0.137577
C	-2.581748	-2.483497	0.753218
C	-3.041758	-3.476379	1.627086
C	-2.455193	-4.741393	1.454499
C	-1.056351	-3.883028	-0.288332
C	-1.487290	-4.958709	0.483483
S	-3.368749	-0.861688	0.745432
O	-4.738113	-1.027776	1.228752
O	1.131106	-2.203382	-0.800939
C	2.937356	-0.505301	1.144809
O	4.172622	1.018963	-0.353228
C	5.178381	0.148611	-0.827116
O	1.462593	2.406833	-1.686856
C	1.490696	3.799437	-1.269947
C	2.869480	4.256743	-1.723390

C	1.385388	3.854374	0.251759
C	0.389207	4.589038	-1.966071
C	0.481449	1.567483	-1.381835
O	-0.693846	1.951376	-1.131108
N	-2.331801	0.026348	1.504227
O	-1.862811	2.118425	2.176389
C	-2.198847	3.498405	2.484997
C	-2.302072	4.347899	1.221331
C	-1.030803	3.956820	3.347863
C	-3.495261	3.530729	3.288527
C	-2.686760	1.371712	1.450029
O	-3.645532	1.796349	0.824866
C	5.937478	-0.562984	0.270445
C	6.182714	-1.937724	0.189718
C	6.901818	-2.586048	1.197375
C	7.369663	-1.866571	2.298237
C	7.113500	-0.495022	2.390871
C	6.401151	0.152186	1.381703
C	-4.050954	-3.262913	2.721233
C	-4.654267	-0.692715	-1.644220
C	-4.698595	-0.476772	-3.023897
C	-3.548085	-0.078300	-3.711395
C	-2.349507	0.118173	-3.023415
C	-2.265408	-0.094029	-1.635216
C	-3.441161	-0.495653	-0.994047
H	2.309483	1.314485	0.255257
H	2.784436	0.217503	-2.189553
H	-2.773016	-5.557626	2.108327
H	-0.234841	-3.960891	-1.001613
H	-1.036381	-5.941084	0.340584
H	3.413600	-0.020108	2.008420
H	1.900831	-0.769233	1.405806
H	3.484009	-1.432792	0.924228
H	5.876447	0.784055	-1.396051
H	4.763362	-0.600949	-1.522395
H	3.065455	5.278682	-1.367690
H	2.937820	4.244084	-2.820977
H	3.626556	3.571607	-1.313846
H	1.233238	4.892978	0.582285
H	0.536374	3.251846	0.607394
H	2.310150	3.476852	0.713832
H	0.446836	4.430175	-3.053309
H	0.532224	5.661784	-1.767057
H	-0.605846	4.285884	-1.618303
H	-2.345162	5.409852	1.507968
H	-3.196718	4.091230	0.643145
H	-1.420840	4.194026	0.583330
H	-1.198356	4.988061	3.690729
H	-0.926845	3.302039	4.224725
H	-0.092399	3.923849	2.776328
H	-3.401028	2.902638	4.187122
H	-4.338766	3.174309	2.683215
H	-3.702781	4.563031	3.606915
H	5.774193	-2.499809	-0.655037
H	7.086191	-3.660723	1.127759
H	7.927978	-2.374022	3.088454
H	7.472136	0.070194	3.254646
H	6.183659	1.221613	1.450008
H	-3.990942	-4.094889	3.435653
H	-5.070945	-3.205698	2.318464
H	-3.874234	-2.318323	3.250803
H	-5.533783	-0.992656	-1.072095
H	-5.638073	-0.614628	-3.563177
H	-3.591050	0.090517	-4.789443
H	-1.457978	0.463588	-3.554870
H	-1.433212	0.786099	-1.140248

CMD_Pyr_R_trans

Imaginary frequencies = 1 (-1113.3083)
E(MN15,DCE) = -2573.1505
$E_{\text{Thermal correction}}$ = 0.59622

Pd	0.528469	-0.317972	-0.713186
C	3.085687	-0.390133	-1.847099
O	4.133229	-0.826334	-2.280089
C	3.930912	0.777424	0.197645
C	3.059130	0.932392	-1.063640
N	1.690041	1.240004	-0.723906
N	-0.577663	-2.098084	-0.913870
C	-1.918503	-2.220322	-0.885446
C	-2.595473	-3.419835	-1.161141
C	-1.761431	-4.521325	-1.430442
C	0.187687	-3.162924	-1.183483
C	-0.379824	-4.408144	-1.436724
S	-2.694301	-0.630203	-0.520279
O	-2.272848	0.318440	-1.544693
O	1.934517	-1.015485	-1.937988
C	4.111175	2.079682	0.952418

O	3.334087	-0.136499	1.099541
C	3.686257	-1.499211	0.979076
O	1.953215	3.463134	-0.943598
C	1.563442	4.853442	-0.776438
C	2.833100	5.608298	-1.144700
C	0.430538	5.200635	-1.734330
C	1.191430	5.112261	0.679280
C	1.143670	2.446278	-0.666420
O	-0.066898	2.604790	-0.360346
N	-4.188312	-0.996626	-0.300305
O	-6.242028	-0.376607	0.283717
C	-7.281908	0.498603	0.787051
C	-7.429897	1.718280	-0.116501
C	-8.530076	-0.370949	0.716767
C	-6.986303	0.890434	2.231484
C	-4.977392	0.033464	0.187066
O	-4.574259	1.138678	0.502974
C	5.166885	-1.740899	1.154819
C	5.939335	-2.260542	0.110939
C	7.311794	-2.462034	0.284246
C	7.920695	-2.132841	1.495677
C	7.156664	-1.594108	2.536152
C	5.787334	-1.398002	2.364332
C	-4.083560	-3.633440	-1.213019
C	-2.481675	-0.643800	2.226864
C	-1.767101	-0.410167	3.403574
C	-0.502347	0.188576	3.358644
C	0.053025	0.574956	2.138495
C	-0.652331	0.373708	0.936876
C	-1.906209	-0.234590	1.026977
H	4.910145	0.395429	-0.145419
H	3.504077	1.714365	-1.700135
H	-2.232680	-5.483212	-1.647222
H	1.263189	-2.980396	-1.231069
H	0.260888	-5.263721	-1.651712
H	4.522298	2.865820	0.303009
H	4.784991	1.919840	1.806138
H	3.137729	2.422665	1.339520
H	3.122290	-2.010766	1.775055
H	3.354303	-1.926774	0.016297
H	2.667367	6.691601	-1.057722
H	3.655305	5.320948	-0.472367
H	3.128432	5.376961	-2.178147
H	0.230192	6.281304	-1.684209
H	-0.484853	4.654338	-1.476354
H	0.719297	4.950372	-2.765978
H	2.013650	4.794058	1.339386
H	1.027442	6.189509	0.829589
H	0.276385	4.572823	0.953776
H	-8.303367	2.305532	0.203882
H	-6.536507	2.352851	-0.070798
H	-7.591833	1.398568	-1.156834
H	-9.403869	0.190273	1.077936
H	-8.404073	-1.269640	1.337844
H	-8.715073	-0.687041	-0.319890
H	-6.833058	-0.012665	2.842341
H	-6.092911	1.523943	2.291654
H	-7.844169	1.441942	2.644064
H	5.459990	-2.473787	-0.848544
H	7.908472	-2.866552	-0.536464
H	8.993760	-2.288302	1.629643
H	7.632566	-1.329746	3.483486
H	5.182715	-0.972537	3.170860
H	-4.284702	-4.662405	-1.540445
H	-4.551635	-3.459743	-0.236242
H	-4.570268	-2.929252	-1.897848
H	-3.459912	-1.129355	2.238733
H	-2.197077	-0.705177	4.363100
H	0.053092	0.348816	4.285139
H	1.050125	1.023327	2.089636
H	-0.442448	1.336760	0.083762

CMD_Pyr_S_cis

Imaginary frequencies = 1 (-1113.8592)
E(MN15,DCE) = -2573.139072
$E_{\text{Thermal correction}}$ = 0.59549

Pd	0.192806	-0.127188	1.557018
C	2.897405	0.457819	2.096570
O	3.870788	0.947654	2.627511
C	3.535546	-0.309365	-0.212415
C	2.987228	-0.754791	1.176162
N	1.655715	-1.329083	1.049633
N	-1.064099	1.489919	2.022942
C	-2.038021	1.943017	1.212983
C	-2.663376	3.189105	1.369873
C	-2.238134	3.923274	2.493407
C	-0.673532	2.213451	3.077880

C	-1.263304	3.443818	3.355313
S	-2.379972	0.740133	-0.091284
O	-1.172647	0.560763	-0.892954
O	1.688933	0.978916	2.190906
C	2.809977	0.905150	-0.773624
O	4.941616	-0.213497	-0.162642
C	5.567208	1.030416	0.031121
O	2.487589	-3.176428	0.081665
C	2.470894	-4.277893	-0.867214
C	3.942106	-4.655902	-0.967668
C	1.947661	-3.794302	-2.214748
C	1.648198	-5.432781	-0.309744
C	1.418268	-2.444345	0.370485
O	0.255369	-2.797124	0.042520
N	-3.706509	1.251765	-0.717882
O	-5.394913	0.929536	-2.129422
C	-6.224446	0.218177	-3.082632
C	-5.424309	-0.106705	-4.339563
C	-7.327216	1.220107	-3.396916
C	-6.809883	-1.034376	-2.438253
C	-4.303159	0.371883	-1.609008
O	-3.901973	-0.750958	-1.858647
C	5.850590	1.763992	-1.261960
C	6.006028	3.154846	-1.267395
C	6.306930	3.833082	-2.449963
C	6.447542	3.126427	-3.646245
C	6.286225	1.738779	-3.649778
C	5.991336	1.062582	-2.464940
C	-3.696482	3.800800	0.464672
C	-3.957139	-0.927649	1.401662
C	-4.144906	-1.964378	2.316688
C	-3.054039	-2.724813	2.750869
C	-1.775366	-2.461182	2.260098
C	-1.548208	-1.424724	1.335489
C	-2.667793	-0.694598	0.927478
H	3.336808	-1.163771	-0.880063
H	3.711055	-1.476788	1.582445
H	-2.693727	4.900413	2.672592
H	0.148967	1.805917	3.666983
H	-0.938686	4.019093	4.222713
H	3.140462	1.112876	-1.800656
H	1.725779	0.708003	-0.788620
H	2.977620	1.807872	-0.166267
H	6.524044	0.809478	0.533099
H	5.010646	1.675569	0.727600
H	4.071854	-5.487772	-1.674685
H	4.324870	-4.962700	0.016230
H	4.531669	-3.794709	-1.315177
H	2.066432	-4.594704	-2.959763
H	0.886963	-3.520150	-2.155831
H	2.526612	-2.921289	-2.554545
H	2.023636	-5.717865	0.684436
H	1.741643	-6.303134	-0.976203
H	0.589833	-5.155522	-0.230516
H	-6.096764	-0.530245	-5.100346
H	-4.628723	-0.830255	-4.124055
H	-4.975819	0.811188	-4.748250
H	-8.033163	0.791042	-4.122455
H	-7.875948	1.483069	-2.480962
H	-6.896869	2.138575	-3.821154
H	-7.334463	-0.768739	-1.507476
H	-6.023455	-1.765496	-2.214480
H	-7.538539	-1.491795	-3.123868
H	5.883860	3.711344	-0.333028
H	6.423403	4.919497	-2.439214
H	6.677138	3.655980	-4.573724
H	6.391447	1.179727	-4.582877
H	5.855999	-0.021564	-2.454898
H	-3.882631	4.835754	0.781869
H	-4.636315	3.234749	0.485199
H	-3.373010	3.791973	-0.582754
H	-4.791470	-0.309652	1.062888
H	-5.147227	-2.179003	2.692962
H	-3.207109	-3.533382	3.468747
H	-0.927197	-3.080508	2.564360
H	-0.575994	-1.827174	0.580985

CMD_Pyr_S_trans

Imaginary frequencies = 1 (-1073.9581)
E(MN15,DCE) = -2573.154389
$E_{\text{Thermal correction}}$ = 0.59956

Pd	-0.256735	-0.359862	0.040000
C	1.792743	-0.094431	-1.858183
O	2.606077	-0.378409	-2.713977
C	3.336033	0.564547	0.004808
C	2.102510	0.990955	-0.815824
N	0.947388	1.165247	0.030520

N	-1.541713	-1.987223	-0.249080
C	-2.831604	-2.025469	0.118468
C	-3.747027	-2.986274	-0.329610
C	-3.205289	-3.990954	-1.146332
C	-1.051319	-2.952680	-1.042201
C	-1.859517	-3.991188	-1.492176
S	-3.330036	-0.672554	1.235003
O	-4.593081	-1.028881	1.874728
O	0.640154	-0.708387	-1.707033
C	3.821876	1.657445	0.936371
O	3.026576	-0.553595	0.816082
C	3.228138	-1.837402	0.261600
O	1.221041	3.389269	0.217770
C	0.955733	4.704878	0.773145
C	2.057584	5.559913	0.162746
C	-0.417334	5.190556	0.325579
C	1.092478	4.664993	2.291145
C	0.511374	2.311384	0.539597
O	-0.499385	2.356338	1.283233
N	-3.086259	0.661732	0.497859
O	-2.541961	1.575388	-1.442883
C	-2.406409	1.676787	-2.884368
C	-3.662930	2.319409	-3.455958
C	-1.186566	2.577441	-3.028642
C	-2.122724	0.313892	-3.510805
C	-3.335980	0.683265	-0.863386
O	-4.128715	-0.040695	-1.445646
C	4.663265	-2.082050	-0.140835
C	5.004409	-2.332447	-1.473841
C	6.339834	-2.540157	-1.831348
C	7.341326	-2.484988	-0.861535
C	7.008083	-2.215141	0.469896
C	5.675803	-2.013213	0.826454
C	-5.223566	-2.946968	-0.062739
C	-2.283467	-1.396206	3.638596
C	-1.224086	-1.515633	4.543351
C	0.033766	-0.987374	4.233088
C	0.244187	-0.313747	3.026926
C	-0.805602	-0.161011	2.104280
C	-2.040197	-0.724086	2.445780
H	4.124407	0.303202	-0.725188
H	2.350367	1.918424	-1.358384
H	-3.871368	-4.769581	-1.526728
H	-0.006767	-2.844967	-1.339864
H	-1.437304	-4.766835	-2.131603
H	4.031367	2.587465	0.388632
H	4.732806	1.323489	1.453042
H	3.050757	1.866574	1.695822
H	2.931762	-2.540718	1.055779
H	2.564238	-2.021672	-0.601562
H	1.961570	6.600699	0.503536
H	3.045338	5.178938	0.462587
H	1.992498	5.538925	-0.934597
H	-0.570714	6.223885	0.670781
H	-1.212070	4.553684	0.733507
H	-0.478735	5.180971	-0.773224
H	2.067465	4.233566	2.567433
H	1.044125	5.688952	2.690122
H	0.291829	4.068062	2.744365
H	-3.546506	2.466716	-4.539935
H	-4.532689	1.671625	-3.279504
H	-3.840508	3.298456	-2.986730
H	-0.961825	2.759606	-4.089160
H	-0.319887	2.088473	-2.555086
H	-1.363163	3.540116	-2.526231
H	-1.296580	-0.182003	-2.976649
H	-3.010806	-0.328896	-3.498697
H	-1.806087	0.465094	-4.553713
H	4.217285	-2.331047	-2.232866
H	6.598164	-2.733515	-2.874940
H	8.385053	-2.644835	-1.141952
H	7.791372	-2.165266	1.230003
H	5.406316	-1.796400	1.864415
H	-5.723663	-3.719717	-0.661453
H	-5.455526	-3.100092	0.998656
H	-5.618421	-1.959437	-0.338898
H	-3.275442	-1.803482	3.843791
H	-1.380875	-2.029259	5.494207
H	0.856601	-1.101009	4.942178
H	1.226167	0.098150	2.772887
H	-0.784869	0.987363	1.497648

CMD_SO-R

Imaginary frequencies = 1 (-1224.1168)
E(MN15,DCE) = -2573.117063
$E_{Thermal\ correction}$ = 0.59648

Pd	-0.060894	-0.070061	-0.200720

C	2.158640	-0.092140	-1.899685
O	2.952092	-0.431060	-2.753989
C	3.633990	-0.204509	0.135642
C	2.647103	0.672278	-0.654552
N	1.495822	1.018655	0.145646
N	-3.496125	-3.112539	0.533602
C	-4.107983	-1.970348	0.255274
C	-5.470837	-1.812657	-0.047413
C	-6.184943	-3.026707	-0.052291
C	-4.196940	-4.238320	0.523315
C	-5.563667	-4.238387	0.223506
S	-2.916595	-0.619127	0.233778
O	-1.838567	-1.092741	-0.706240
O	0.877349	-0.373130	-1.920763
C	4.269136	0.547319	1.289391
O	2.972008	-1.323507	0.687396
C	2.904075	-2.494096	-0.105322
O	2.249378	3.061418	0.707983
C	2.255887	4.270537	1.512879
C	3.634598	4.854688	1.238599
C	1.162044	5.221027	1.041756
C	2.114854	3.904457	2.986486
C	1.259172	2.177093	0.740145
O	0.152019	2.412037	1.299872
N	-3.578191	0.721066	-0.027912
O	-2.171119	1.955494	-1.286936
C	-1.690342	2.637947	-2.485181
C	-2.543916	3.867704	-2.775016
C	-0.273642	3.057086	-2.116570
C	-1.671135	1.639332	-3.635037
C	-3.399945	1.451760	-1.211684
O	-4.282733	1.620225	-2.020759
C	4.268607	-3.018811	-0.484968
C	4.649433	-3.128601	-1.826236
C	5.921517	-3.602957	-2.159832
C	6.823620	-3.956164	-1.155759
C	6.455225	-3.829593	0.187729
C	5.184681	-3.361921	0.519531
C	-6.192299	-0.527106	-0.340218
C	-2.642444	-1.270770	2.941786
C	-1.855098	-1.313725	4.095515
C	-0.577241	-0.750075	4.093453
C	-0.089078	-0.107960	2.953455
C	-0.863159	-0.010703	1.786566
C	-2.128123	-0.627002	1.823074

H	4.407854	-0.528610	-0.584977
H	3.178428	1.574784	-0.998380
H	-7.252901	-2.997874	-0.283311
H	-3.662409	-5.163376	0.756907
H	-6.127799	-5.172439	0.211320
H	4.772194	1.461703	0.942511
H	4.997332	-0.100323	1.797617
H	3.490553	0.830251	2.017096
H	2.375901	-3.230504	0.519518
H	2.294323	-2.343872	-1.012393
H	3.766333	5.792930	1.796166
H	4.416089	4.144878	1.548051
H	3.754320	5.060446	0.165284
H	1.249495	6.176006	1.581079
H	0.167052	4.796355	1.225228
H	1.276282	5.420944	-0.034424
H	2.875503	3.155563	3.258827
H	2.276051	4.799138	3.605607
H	1.116844	3.500972	3.199353
H	-2.079501	4.436968	-3.593814
H	-3.563696	3.591198	-3.066114
H	-2.585078	4.516556	-1.886872
H	0.165218	3.637350	-2.941085
H	0.350068	2.168520	-1.943133
H	-0.281743	3.674705	-1.205461
H	-1.073582	0.759085	-3.348824
H	-2.689787	1.327926	-3.902389
H	-1.203942	2.102952	-4.516388
H	3.950455	-2.808915	-2.603839
H	6.211457	-3.684642	-3.209886
H	7.818549	-4.324154	-1.417396
H	7.161983	-4.099948	0.976055
H	4.888661	-3.254618	1.567403
H	-7.255922	-0.740951	-0.511764
H	-6.099076	0.181933	0.493610
H	-5.783032	-0.004449	-1.216523
H	-3.623573	-1.748329	2.916047
H	-2.236466	-1.806976	4.991669
H	0.043652	-0.810360	4.989574
H	0.906356	0.346187	2.955261
H	-0.510522	1.159600	1.253583

CMD_SO-S

Imaginary frequencies = 1 (-1165.5633)
E(MN15,DCE) = -2573.134812
$E_{Thermal\ correction}$ = 0.59443

Pd	0.327921	-0.267917	-0.122055
C	2.401667	-0.753665	-1.930718
O	3.140009	-1.312994	-2.714474
C	4.002635	-0.206357	-0.078276
C	2.941334	0.371276	-1.029468
N	1.832130	0.932212	-0.293331
N	-2.824905	2.052500	0.379442
C	-2.540948	1.042201	-0.421908
C	-2.250482	1.112518	-1.794142
C	-2.226552	2.428871	-2.285326
C	-2.805278	3.284602	-0.119640
C	-2.491081	3.518090	-1.460173
S	-2.483915	-0.506799	0.524135
O	-1.482155	-1.401489	-0.170119
O	1.144306	-1.076851	-1.734029
C	4.659166	0.870316	0.764082
O	3.412978	-1.131880	0.811417
C	3.394088	-2.493495	0.418712
O	2.518093	3.065513	-0.479005
C	2.484210	4.483687	-0.165221
C	3.790837	4.993575	-0.756770
C	1.290208	5.145075	-0.844358
C	2.472480	4.671410	1.347587
C	1.579352	2.213747	-0.086033
O	0.503593	2.591126	0.462853
N	-3.844828	-1.092101	0.952326
O	-5.914797	-1.744627	0.487585
C	-7.089478	-2.012137	-0.322598
C	-6.763444	-3.046383	-1.394400
C	-8.079574	-2.580456	0.684704
C	-7.620624	-0.714057	-0.920990
C	-4.806242	-1.240763	-0.034870
O	-4.655523	-0.936812	-1.207267
C	4.774051	-3.037590	0.136686
C	5.110487	-3.512939	-1.135043
C	6.397015	-3.998187	-1.387295
C	7.357020	-3.997871	-0.374753
C	7.031899	-3.505837	0.893648
C	5.747158	-3.027326	1.146031
C	-1.989394	-0.051536	-2.702409
C	-2.178158	-0.337814	3.260248
C	-1.341814	-0.135473	4.363955
C	-0.033130	0.322317	4.186887
C	0.455736	0.605780	2.907823
C	-0.359656	0.436579	1.780272
C	-1.660233	-0.040051	2.009806
H	4.754129	-0.707323	-0.716017
H	3.417647	1.128853	-1.671880
H	-2.000005	2.582608	-3.343684
H	-3.037779	4.104958	0.564955
H	-2.462013	4.536462	-1.851594
H	5.103511	1.655120	0.134489
H	5.439829	0.423331	1.395564
H	3.905289	1.334026	1.421615
H	2.942023	-3.027280	1.268362
H	2.740788	-2.661015	-0.454279
H	3.891013	6.073778	-0.579141
H	4.643930	4.477057	-0.292593
H	3.817726	4.808239	-1.840101
H	1.350806	6.234926	-0.706767
H	0.345047	4.781426	-0.421618
H	1.307087	4.932131	-1.923907
H	3.310288	4.116483	1.798133
H	2.596606	5.737523	1.587916
H	1.529349	4.316830	1.781974
H	-7.689522	-3.337681	-1.911761
H	-6.057083	-2.644075	-2.130774
H	-6.329446	-3.945399	-0.931902
H	-9.027484	-2.826617	0.185040
H	-8.276880	-1.847281	1.479866
H	-7.673009	-3.492435	1.144644
H	-7.795266	0.025035	-0.124644
H	-6.914505	-0.298786	-1.650381
H	-8.578787	-0.911043	-1.424261
H	4.362567	-3.470625	-1.931630
H	6.651768	-4.367523	-2.383274
H	8.362935	-4.375331	-0.573118
H	7.783461	-3.500226	1.686795
H	5.484398	-2.637334	2.133985
H	-2.099274	0.270740	-3.746835
H	-0.969273	-0.447168	-2.570089
H	-2.695787	-0.865036	-2.499528
H	-3.192880	-0.729926	3.348651
H	-1.712960	-0.351342	5.367837
H	0.613366	0.458883	5.056290
H	1.476454	0.974695	2.767723

H	-0.048118	1.390491	0.923290

INS_R-NBoc

Imaginary frequencies = 1 (-284.5669)
E(MN15,DCE) = -2301.76728
$E_{Thermal\ correction}$ = 0.479434

Pd	-0.152818	-0.984550	-0.411201
C	2.460993	-0.181812	-0.245223
O	2.393025	-0.493916	-1.435389
N	-2.483478	-0.498189	1.718775
C	-1.748634	-2.029846	-1.275418
C	-1.596324	-2.911864	-2.361964
C	-2.534741	-3.001985	-3.388061
C	-3.679763	-2.203659	-3.364972
C	-3.811537	-1.234096	-2.370613
C	-2.852420	-1.145817	-1.361940
C	-3.120932	0.489512	1.117838
C	-3.894557	1.478602	1.745070
C	-3.956939	1.333224	3.141848
C	-2.543528	-0.604850	3.043427
C	-3.288130	0.305001	3.798167
S	-2.796091	0.499329	-0.655061
O	-3.787307	1.340963	-1.317180
O	1.445044	-0.077200	0.538830
N	-1.245993	0.792744	-0.933551
O	0.348192	2.330517	-1.100082
C	1.098014	3.526331	-0.752743
C	2.433260	3.307556	-1.450965
C	1.260518	3.594808	0.762089
C	0.397507	4.757972	-1.314519
C	-0.843381	2.087696	-0.596285
O	-1.528244	2.856934	0.056373
C	-4.585831	2.623829	1.067186
C	-1.122508	-2.916075	0.201479
C	0.321430	-2.785425	0.367359
H	-0.735603	-3.588186	-2.358328
H	-2.376780	-3.712600	-4.201867
H	-4.435300	-2.289171	-4.147692
H	-4.609086	-0.489184	-2.410258
H	-4.535919	2.063634	3.713164
H	-1.963863	-1.414358	3.493038
H	-3.332178	0.213076	4.884517
H	3.112345	4.145877	-1.237598
H	2.282236	3.238864	-2.537926
H	2.903544	2.371903	-1.117441
H	2.050518	4.316447	1.018591
H	0.324909	3.900659	1.247016
H	1.548042	2.602651	1.138664
H	0.259918	4.656025	-2.401304
H	1.020536	5.645223	-1.127029
H	-0.580078	4.903725	-0.838028
H	-5.358098	2.272495	0.370380
H	-3.861075	3.200235	0.476737
H	-5.048035	3.273960	1.821925
H	0.995320	-3.386647	-0.252661
H	-1.478879	-3.873333	-0.183502
C	0.827964	-2.482948	1.730675
O	0.141357	-2.145020	2.672699
O	2.151341	-2.632275	1.808545
C	2.742165	-2.208743	3.027035
H	3.819022	-2.391771	2.938817
H	2.324363	-2.766103	3.877410
H	2.550405	-1.136372	3.180527
H	-1.695704	-2.569625	1.065463
C	3.831777	0.014158	0.408855
H	4.022244	-0.942658	0.932421
C	3.906753	1.128172	1.445163
N	4.810232	0.159195	-0.647468
H	3.094645	1.020492	2.178068
H	4.877423	1.072330	1.955325
H	3.819918	2.115041	0.968263
H	4.421324	0.092963	-1.588617
C	6.128179	-0.088565	-0.415876
O	6.566286	-0.317502	0.702132
C	7.025099	-0.049412	-1.635473
H	6.484054	0.164680	-2.566450
H	7.795450	0.717862	-1.477707
H	7.541993	-1.014950	-1.722211

INS_R-Pyr

Imaginary frequencies = 1 (-312.4032)
E(MN15,DCE) = -2301.78124
$E_{Thermal\ correction}$ = 0.475181

Pd	-0.913681	-0.517698	0.380593

C	-3.575080	0.276495	0.127297
O	-3.466962	0.409574	1.349070
C	0.673921	-1.080296	1.545819
C	0.404796	-1.372379	2.896268
C	1.288700	-0.987668	3.900076
C	2.471301	-0.308597	3.580587
C	2.743142	0.024312	2.255987
C	1.845594	-0.369769	1.259998
S	2.052563	0.324521	-0.372681
O	1.468136	-0.543562	-1.389931
O	-2.598748	0.035634	-0.671824
C	0.070561	-2.549151	0.436786
C	-1.357183	-2.503865	0.254233
H	-0.507419	-1.922693	3.146139
H	1.058934	-1.222320	4.941525
H	3.171748	-0.023330	4.367513
H	3.630236	0.602602	1.989593
H	-2.025429	-2.850340	1.049500
H	0.468295	-3.218342	1.200472
C	-1.898772	-2.602052	-1.130651
O	-1.238814	-2.528125	-2.139689
O	-3.227263	-2.768150	-1.124268
C	-3.842092	-2.679530	-2.398300
H	-4.912815	-2.860536	-2.247763
H	-3.422458	-3.423127	-3.090472
H	-3.676095	-1.676601	-2.821315
H	0.667102	-2.504498	-0.480839
C	1.026118	1.810666	-0.216581
C	1.409983	3.105614	-0.600314
N	-0.183055	1.510001	0.274573
C	0.438450	4.095935	-0.362149
C	-1.086061	2.468123	0.500371
C	-0.794807	3.797137	0.201213
H	0.677656	5.126744	-0.635902
H	-2.037334	2.141236	0.930581
H	-1.532950	4.575992	0.395281
N	3.491997	0.891544	-0.529714
C	4.488510	-0.072297	-0.503035
O	4.309369	-1.257223	-0.276864
O	5.671648	0.492973	-0.731511
C	6.894396	-0.286961	-0.739461
C	7.966048	0.753243	-1.036300
C	6.844669	-1.334093	-1.846869
C	7.126083	-0.914859	0.631264
H	7.971256	1.528653	-0.256641
H	7.770541	1.234583	-2.005214
H	8.956649	0.277417	-1.070026
H	6.076265	-2.089107	-1.640796
H	7.823289	-1.830905	-1.923054
H	6.626468	-0.852145	-2.811610
H	8.117957	-1.390167	0.652760
H	6.363467	-1.671987	0.850879
H	7.101341	-0.137503	1.410493
C	2.708162	3.508213	-1.242077
H	2.950601	2.869264	-2.099595
H	3.550142	3.398439	-0.546713
H	2.637143	4.553155	-1.572962
C	-4.933573	0.429553	-0.563105
H	-5.141557	-0.568020	-0.993424
C	-4.822017	1.443094	-1.702235
N	-5.913785	0.771161	0.439543
H	-4.045156	1.126297	-2.411185
H	-5.776205	1.541223	-2.238219
H	-4.551624	2.431908	-1.300742
H	-5.524852	0.950480	1.367200
C	-7.275104	0.675811	0.376446
O	-7.979002	0.918578	1.341508
C	-7.881521	0.278456	-0.956126
H	-8.005871	1.172715	-1.585711
H	-7.273525	-0.447328	-1.514691
H	-8.875838	-0.137302	-0.757025

INS_S-NBoc

Imaginary frequencies = 1 (-299.8047)
E(MN15,DCE) = -2301.761265
$E_{\text{Thermal correction}}$ = 0.478895

Pd	0.275862	-0.991151	-0.168560
C	2.793547	-0.164914	-1.040784
O	2.795414	-1.263191	-1.589506
N	-4.387075	0.370107	-1.141960
C	-1.151810	-2.485539	-0.251695
C	-0.926853	-3.570060	-1.118288
C	-1.965929	-4.136561	-1.852681
C	-3.268823	-3.645200	-1.729531
C	-3.516877	-2.524218	-0.936773
C	-2.458283	-1.948229	-0.237938
C	-4.128869	0.406717	0.154269

C	-4.907539	1.034565	1.139650
C	-6.075648	1.630826	0.635471
C	-5.497354	0.948428	-1.589533
C	-6.381933	1.592614	-0.721027
S	-2.542607	-0.360695	0.547155
O	-2.354316	-0.483532	1.989697
O	1.830925	0.333818	-0.342904
N	-1.424178	0.382766	-0.334554
O	-0.403870	2.305133	-0.801289
C	0.237664	3.550135	-0.407987
C	1.366277	3.682501	-1.418885
C	0.800167	3.382835	0.999217
C	-0.741042	4.712432	-0.518820
C	-1.341403	1.747298	-0.062946
O	-2.063721	2.316076	0.741897
C	-4.553580	1.160408	2.590695
C	-0.058438	-2.672432	1.237824
C	1.324158	-2.378164	0.883387
H	0.081720	-3.990255	-1.176501
H	-1.761233	-4.981578	-2.513120
H	-4.088970	-4.111486	-2.277954
H	-4.512603	-2.083824	-0.902203
H	-6.738255	2.148052	1.334139
H	-5.684370	0.902795	-2.666052
H	-7.287264	2.065923	-1.104539
H	1.968960	4.576173	-1.201729
H	0.962441	3.763604	-2.438728
H	1.998030	2.785690	-1.360046
H	1.416451	4.256883	1.256643
H	-0.005496	3.294025	1.740511
H	1.423431	2.475372	1.031137
H	-1.168697	4.752289	-1.531984
H	-0.205779	5.655805	-0.333544
H	-1.554181	4.611297	0.210314
H	-3.579603	1.661506	2.684108
H	-4.450829	0.181169	3.075287
H	-5.323227	1.746578	3.109863
H	1.915468	-3.083716	0.292800
H	-0.346228	-3.724078	1.305060
C	2.095743	-1.519684	1.825283
O	1.602581	-0.858214	2.712955
O	3.403959	-1.554285	1.566477
C	4.209460	-0.678693	2.342153
H	5.253486	-0.906132	2.099987
H	4.010826	-0.820189	3.413558
H	3.976044	0.366981	2.082049
H	-0.441490	-2.081625	2.078890
C	4.041528	0.717604	-1.173315
H	3.904107	1.601651	-0.532455
C	4.223712	1.123352	-2.634285
N	5.156134	-0.071295	-0.681372
H	3.368966	1.715164	-2.994941
H	5.143308	1.713492	-2.764498
H	4.297116	0.211147	-3.243587
H	5.072109	-1.080562	-0.810644
C	6.259462	0.365931	-0.012867
O	7.099876	-0.406800	0.422383
C	6.367090	1.861959	0.203871
H	7.368612	2.073725	0.593689
H	6.192285	2.432288	-0.719796
H	5.619418	2.189344	0.944276

INS_S-Pyr

Imaginary frequencies = 1 (-302.9509)
E(MN15,DCE) = -2301.788241
$E_{Thermal\ correction}$ = 0.475399

Pd	0.345787	-0.377223	0.715493
C	3.036618	-0.115610	0.032828
O	3.169212	-0.909676	0.970723
C	-1.189168	-1.013067	1.940801
C	-0.840591	-1.614751	3.165647
C	-1.545812	-2.705203	3.667417
C	-2.641781	-3.216143	2.964821
C	-2.979732	-2.676147	1.725052
C	-2.245799	-1.598443	1.223731
S	-2.504405	-1.283122	-0.526710
O	-3.735890	-1.980632	-0.895724
O	1.907924	0.244802	-0.463597
C	-0.952190	0.860845	2.116963
C	0.400208	1.296847	1.863944
H	-0.014958	-1.185244	3.741592
H	-1.250194	-3.148105	4.620752
H	-3.219620	-4.048312	3.371183
H	-3.793552	-3.084487	1.123846
H	1.154766	1.232747	2.654470
H	-1.263735	0.792700	3.159807
C	0.624980	2.355132	0.842313

O	-0.214260	2.751005	0.062130
O	1.879265	2.808201	0.873573
C	2.248818	3.649086	-0.208612
H	3.288898	3.948110	-0.036922
H	1.597857	4.533220	-0.258065
H	2.161856	3.092262	-1.153848
H	-1.723479	1.304877	1.482279
C	-1.098310	-2.164394	-1.249720
C	-1.262938	-2.931378	-2.411030
N	0.064704	-2.008567	-0.618004
C	-0.104350	-3.597545	-2.843657
C	1.157710	-2.653767	-1.040690
C	1.100041	-3.483246	-2.157394
H	-0.163869	-4.209736	-3.747342
H	2.071106	-2.477844	-0.464845
H	1.994042	-4.009732	-2.493166
N	-2.240921	0.158228	-1.041708
C	-3.091447	1.120395	-0.512287
O	-3.813322	0.934753	0.459359
O	-3.000697	2.245300	-1.194045
C	-3.677365	3.457542	-0.773651
C	-3.078309	4.508173	-1.697920
C	-3.357572	3.800497	0.679416
C	-5.174963	3.293200	-1.001204
H	-3.260874	4.239599	-2.748340
H	-1.992212	4.556665	-1.532485
H	-3.524079	5.493271	-1.497503
H	-3.855360	3.112989	1.374100
H	-3.702076	4.825294	0.884809
H	-2.269713	3.758262	0.833402
H	-5.692664	4.233548	-0.759713
H	-5.573022	2.495150	-0.360007
H	-5.376026	3.045590	-2.054152
C	-2.535853	-3.031381	-3.203761
H	-2.987045	-2.041836	-3.353844
H	-3.287923	-3.636856	-2.680608
H	-2.323359	-3.483854	-4.181473
C	4.254089	0.483413	-0.661968
H	4.209720	1.577702	-0.517033
C	4.219306	0.205040	-2.163406
N	5.443882	-0.024172	-0.020125
H	3.315073	0.643470	-2.606886
H	5.109759	0.647406	-2.629588
H	4.215293	-0.880375	-2.352213
H	5.282161	-0.741823	0.684965
C	6.636883	0.613126	-0.151545
O	6.780375	1.586299	-0.877330
C	7.783294	0.033276	0.650134
H	7.487974	-0.813944	1.283088
H	8.569813	-0.289256	-0.046084
H	8.210610	0.828934	1.275281

Int-1_NBoc_R

Imaginary frequencies = 0
E(MN15,DCE) = -2573.154866
$E_{\text{Thermal correction}}$ = 0.602481

Pd	-0.248231	0.320511	-0.161893
C	1.802778	-0.536541	-1.811637
O	2.535624	-1.290179	-2.423666
C	3.179187	0.325390	0.072487
C	2.319155	0.735787	-1.140627
N	1.172086	1.514886	-0.735357
N	-3.439552	1.370056	-0.403594
C	-4.027299	0.316020	0.134712
C	-5.318554	-0.151141	-0.146256
C	-5.999750	0.632472	-1.093605
C	-4.104054	2.092885	-1.299131
C	-5.406526	1.750240	-1.673154
S	-2.899763	-0.532693	1.257292
O	-3.626890	-1.430698	2.145157
O	0.530034	-0.782417	-1.598223
C	3.779849	1.527130	0.773762
O	2.389175	-0.356403	1.031264
C	2.300291	-1.769594	0.946038
O	2.156616	3.438513	-1.314337
C	2.338666	4.868434	-1.264172
C	3.765172	5.056573	-1.764736
C	1.349451	5.565473	-2.192229
C	2.216319	5.362432	0.175590
C	1.043273	2.845197	-0.829707
O	0.033824	3.470299	-0.496432
N	-1.660976	-1.121800	0.437071
O	-0.910603	-2.937087	-0.608192
C	-0.842952	-3.924559	-1.681007
C	-1.327920	-3.294919	-2.980846
C	0.642655	-4.240840	-1.768684
C	-1.659081	-5.146800	-1.281855

C	-1.989286	-2.240575	-0.351520
O	-3.131960	-2.491923	-0.691417
C	3.649869	-2.442920	1.005865
C	4.114214	-3.214189	-0.064821
C	5.372489	-3.820564	-0.004038
C	6.179101	-3.647978	1.121085
C	5.728492	-2.862322	2.187175
C	4.471432	-2.262961	2.127713
C	-5.949706	-1.373670	0.448868
C	-2.203761	0.630177	3.574325
C	-1.395416	1.444663	4.375740
C	-0.440687	2.282375	3.797511
C	-0.293337	2.338683	2.407525
C	-1.100907	1.545918	1.592073
C	-2.043965	0.703283	2.196423
H	3.975525	-0.340984	-0.308062
H	2.954247	1.281482	-1.854257
H	-7.013701	0.339530	-1.378302
H	-3.584075	2.954905	-1.725112
H	-5.943102	2.347847	-2.411686
H	4.367923	2.143209	0.078196
H	4.419489	1.194578	1.603645
H	2.965414	2.145484	1.185393
H	1.688406	-2.064616	1.812645
H	1.751385	-2.097992	0.047090
H	4.024311	6.125043	-1.789049
H	4.472687	4.535371	-1.102274
H	3.868715	4.643197	-2.778357
H	1.568642	6.643555	-2.225746
H	0.322112	5.414250	-1.839499
H	1.443043	5.160960	-3.211226
H	2.871065	4.763456	0.829248
H	2.536263	6.413392	0.237455
H	1.180001	5.282584	0.528072
H	-1.113226	-3.980316	-3.813749
H	-2.408196	-3.099954	-2.954763
H	-0.783335	-2.353627	-3.145211
H	0.811005	-5.028771	-2.517569
H	1.015058	-4.596114	-0.795321
H	1.201870	-3.338772	-2.063304
H	-1.294070	-5.554706	-0.327465
H	-2.721622	-4.889010	-1.181253
H	-1.552739	-5.923981	-2.053076
H	3.489993	-3.311537	-0.957315
H	5.726956	-4.420280	-0.845449
H	7.163488	-4.119667	1.167438
H	6.360747	-2.721242	3.067126
H	4.112499	-1.643343	2.954932
H	-6.935512	-1.541762	-0.004324
H	-5.308464	-2.247785	0.270409
H	-6.063807	-1.276752	1.536804
H	-2.924640	-0.069936	4.001237
H	-1.505106	1.407377	5.461282
H	0.193796	2.901571	4.434503
H	0.424250	3.007637	1.927683
H	-1.145057	1.831136	0.496362

Int-1_NBoc_S

Imaginary frequencies = 0
E(MN15,DCE) = -2573.152779
$E_{\text{Thermal correction}}$ = 0.601732

Pd	-0.278994	-0.705414	-0.604806
C	-1.826366	1.320177	-1.684205
O	-2.129000	2.418223	-2.112387
C	-2.912849	1.181481	0.551532
C	-2.779014	0.492721	-0.822100
N	-2.216033	-0.830012	-0.690139
N	3.889286	-0.225695	1.681863
C	4.122591	-1.093800	0.712922
C	5.377817	-1.468044	0.211001
C	6.451681	-0.851007	0.874881
C	4.925423	0.349077	2.284898
C	6.239028	0.052812	1.910801
S	2.592170	-1.710823	-0.018420
O	2.824294	-2.831118	-0.918091
O	-0.638304	0.784356	-1.846328
C	-3.891499	0.457521	1.454262
O	-1.664038	1.188825	1.222577
C	-0.810495	2.305432	1.034001
O	-4.220096	-1.804601	-0.888893
C	-5.157337	-2.891251	-0.741044
C	-6.510911	-2.199612	-0.843663
C	-4.984410	-3.901961	-1.869626
C	-4.999340	-3.536895	0.633727
C	-2.889317	-1.987805	-0.744779
O	-2.363128	-3.098025	-0.650285
N	1.790558	-0.427535	-0.528305

O	1.949051	1.651866	-1.303514
C	2.235993	2.657784	-2.320963
C	2.064291	2.020886	-3.693711
C	1.167830	3.714315	-2.082977
C	3.634537	3.221702	-2.103596
C	2.547209	0.484971	-1.274684
O	3.628537	0.198908	-1.760755
C	-1.457010	3.608635	1.436797
C	-1.697926	4.610117	0.489836
C	-2.314232	5.806243	0.869353
C	-2.705230	6.002612	2.194180
C	-2.484974	4.997445	3.141758
C	-1.865797	3.807281	2.763117
C	5.616795	-2.366473	-0.964623
C	1.943923	-2.368193	2.623258
C	0.989786	-2.685365	3.595914
C	-0.359398	-2.803762	3.261167
C	-0.771843	-2.642566	1.936558
C	0.168260	-2.338536	0.949937
C	1.515956	-2.181663	1.314342
H	-3.249912	2.217714	0.363046
H	-3.767450	0.472432	-1.304817
H	7.468161	-1.080625	0.545297
H	4.704785	1.065465	3.080955
H	7.078562	0.534376	2.414712
H	-4.877748	0.360413	0.977775
H	-3.992925	0.997817	2.406225
H	-3.504306	-0.552854	1.664544
H	0.065097	2.100086	1.669532
H	-0.438808	2.372579	-0.002089
H	-7.323868	-2.935620	-0.761386
H	-6.621318	-1.457939	-0.038048
H	-6.598784	-1.680485	-1.808957
H	-5.770507	-4.669497	-1.803466
H	-4.000838	-4.383031	-1.806478
H	-5.074703	-3.396276	-2.842639
H	-5.015907	-2.757274	1.412752
H	-5.835945	-4.227122	0.819292
H	-4.055958	-4.093837	0.696780
H	2.131630	2.797877	-4.468952
H	2.841566	1.267903	-3.883914
H	1.071472	1.549906	-3.744607
H	1.306026	4.545825	-2.789752
H	1.245034	4.110399	-1.058277
H	0.165744	3.281053	-2.227497
H	3.727072	3.623351	-1.083144
H	4.398364	2.449121	-2.258085
H	3.807363	4.044231	-2.813375
H	-1.423683	4.428924	-0.553292
H	-2.499602	6.581846	0.122790
H	-3.189108	6.936366	2.490232
H	-2.796362	5.146560	4.178494
H	-1.694167	3.013568	3.496321
H	6.693290	-2.429537	-1.170314
H	5.216377	-3.375028	-0.800428
H	5.097913	-1.958058	-1.843745
H	2.991587	-2.249071	2.897180
H	1.311419	-2.830867	4.629012
H	-1.093527	-3.038370	4.033972
H	-1.810713	-2.778191	1.630388
H	-0.170585	-2.512391	-0.122408

Int-1_Pyr_R_cis

Imaginary frequencies = 0
E(MN15,DCE) = -2573.148946
$E_{Thermal\ correction}$ = 0.604898

Pd	-0.850818	-0.339006	-1.046024
C	1.668673	-1.379033	-1.744543
O	2.487827	-2.186107	-2.129778
C	2.838958	0.174940	-0.059785
C	1.998145	0.058809	-1.371303
N	0.745796	0.792312	-1.216216
N	-2.257107	-1.927755	-0.987976
C	-3.124197	-2.164845	0.006892
C	-3.807106	-3.372322	0.191843
C	-3.569835	-4.343806	-0.797095
C	-2.059299	-2.866247	-1.921932
C	-2.721002	-4.091121	-1.864177
S	-3.409261	-0.753863	1.083758
O	-4.639666	-0.973744	1.835416
O	0.398835	-1.709845	-1.595428
C	2.456091	-0.883535	0.965318
O	4.218956	0.332289	-0.289822
C	4.939109	-0.708792	-0.910773
O	1.975746	2.618614	-1.535163
C	2.404357	3.978363	-1.308326
C	3.853166	3.952638	-1.779228

C	2.341287	4.297428	0.180983
C	1.572329	4.950590	-2.136480
C	0.768130	2.140576	-1.184773
O	-0.186098	2.861311	-0.887438
N	-2.009629	-0.560921	1.727722
O	-0.580118	0.907742	2.602714
C	-0.152001	2.127296	3.271116
C	-0.662711	3.366432	2.539448
C	1.363428	2.039892	3.175239
C	-0.621773	2.085527	4.719595
C	-1.859903	0.673884	2.357021
O	-2.781965	1.431248	2.603466
C	5.302606	-1.840869	0.024494
C	5.104662	-3.173511	-0.350674
C	5.460275	-4.210652	0.516322
C	6.005635	-3.922579	1.768263
C	6.193932	-2.591302	2.153157
C	5.844191	-1.557794	1.285222
C	-4.716068	-3.698172	1.345729
C	-5.026245	0.697815	-0.556931
C	-5.264611	1.587283	-1.609991
C	-4.204431	2.261760	-2.218789
C	-2.893409	2.077727	-1.768153
C	-2.640680	1.184703	-0.724052
C	-3.714792	0.505659	-0.140542
H	2.546899	1.155015	0.344775
H	2.611065	0.491499	-2.178027
H	-4.069999	-5.311511	-0.707929
H	-1.327244	-2.635693	-2.695702
H	-2.543022	-4.838169	-2.638082
H	3.017856	-0.731812	1.898554
H	1.378414	-0.789764	1.185967
H	2.658864	-1.903387	0.605935
H	5.865121	-0.239051	-1.280703
H	4.395534	-1.111625	-1.780274
H	4.339578	4.919082	-1.582129
H	3.899713	3.745302	-2.858447
H	4.392363	3.153047	-1.249318
H	2.721128	5.314784	0.357644
H	1.309910	4.238754	0.553156
H	2.973316	3.592592	0.743861
H	1.571472	4.637877	-3.191569
H	2.013880	5.956813	-2.075126
H	0.538276	4.984982	-1.772603
H	-0.068395	4.236689	2.858522
H	-1.720239	3.556367	2.755168
H	-0.540887	3.243938	1.451525
H	1.830165	2.899202	3.677973
H	1.724915	1.109861	3.637624
H	1.663828	2.041963	2.117300
H	-0.234340	1.187829	5.223916
H	-1.719307	2.085172	4.766764
H	-0.249181	2.972814	5.252511
H	4.638940	-3.388051	-1.316041
H	5.299068	-5.248822	0.216021
H	6.279185	-4.733271	2.447768
H	6.615780	-2.361144	3.134671
H	5.973872	-0.512839	1.580493
H	-4.928666	-4.775440	1.343473
H	-5.662935	-3.145935	1.280441
H	-4.266990	-3.421822	2.307390
H	-5.835984	0.165066	-0.054763
H	-6.287983	1.756008	-1.951396
H	-4.401625	2.955630	-3.038250
H	-2.050783	2.637169	-2.176298
H	-1.628762	1.249022	-0.232850

Int-1_Pyr_R_trans

Imaginary frequencies = 0
E(MN15,DCE) = -2573.167924
$E_{\text{Thermal correction}}$ = 0.599995

Pd	0.435158	0.079871	-1.116286
C	3.086938	-0.553514	-1.560272
O	4.028186	-1.283527	-1.788210
C	3.362446	-0.103090	0.886927
C	3.126115	0.533883	-0.491747
N	1.886584	1.282316	-0.548172
N	-0.801390	-1.408124	-1.976233
C	-2.138740	-1.318900	-1.991361
C	-2.985197	-2.142349	-2.742656
C	-2.338645	-3.176619	-3.436485
C	-0.206235	-2.404858	-2.648099
C	-0.957943	-3.324478	-3.375258
S	-2.740606	0.067945	-1.046328
O	-2.801218	1.248606	-1.899172
O	1.920147	-0.661985	-2.168798
C	3.596380	0.945543	1.955301

O	2.233122	-0.865573	1.278799
C	2.195866	-2.223155	0.895330
O	3.062718	3.180032	-0.375425
C	3.223606	4.602938	-0.197402
C	4.684644	4.737956	0.213242
C	2.965119	5.341928	-1.506085
C	2.313944	5.093037	0.926758
C	1.856735	2.629706	-0.654467
O	0.868800	3.298197	-0.932180
N	-4.007452	-0.528220	-0.365230
O	-5.627494	-0.342289	1.147385
C	-6.357481	0.230055	2.262271
C	-6.896136	1.607304	1.889772
C	-7.502376	-0.752694	2.466815
C	-5.468488	0.279159	3.500844
C	-4.531936	0.237568	0.664661
O	-4.048468	1.277850	1.078857
C	3.340636	-3.026784	1.464474
C	4.290536	-3.619498	0.626263
C	5.355421	-4.342913	1.171208
C	5.482680	-4.466379	2.555108
C	4.546265	-3.859390	3.398532
C	3.482646	-3.141848	2.854195
C	-4.470417	-1.954124	-2.849914
C	-1.318962	-0.711884	1.189381
C	-0.621039	-0.384651	2.329440
C	-0.082297	0.913866	2.487179
C	-0.224898	1.869393	1.502502
C	-0.940271	1.568011	0.319313
C	-1.450089	0.274680	0.172926
H	4.246920	-0.760508	0.791588
H	3.989459	1.178759	-0.713335
H	-2.941179	-3.862278	-4.037684
H	0.885680	-2.412448	-2.619350
H	-0.450986	-4.127976	-3.910464
H	4.483228	1.551353	1.720471
H	3.733447	0.460714	2.932565
H	2.725438	1.617703	2.005378
H	1.234787	-2.602005	1.282399
H	2.170011	-2.342835	-0.203210
H	4.940771	5.795320	0.373502
H	4.870453	4.183155	1.145423
H	5.338663	4.330736	-0.571486
H	3.200280	6.409681	-1.379906
H	1.916881	5.234799	-1.809711
H	3.611653	4.936743	-2.298939
H	2.461358	4.464965	1.821089
H	2.569903	6.130342	1.189360
H	1.260555	5.050914	0.622213
H	-7.553062	1.971284	2.693721
H	-6.078861	2.324126	1.744693
H	-7.487626	1.542748	0.964155
H	-8.139194	-0.423848	3.300593
H	-7.109062	-1.754077	2.693887
H	-8.115410	-0.817196	1.556389
H	-5.057448	-0.720507	3.708829
H	-4.642077	0.987318	3.363847
H	-6.067743	0.592431	4.368597
H	4.204288	-3.482064	-0.455307
H	6.094467	-4.801297	0.510286
H	6.316290	-5.029971	2.980435
H	4.647803	-3.949517	4.482613
H	2.748709	-2.658516	3.506141
H	-4.851689	-2.509167	-3.717475
H	-4.975089	-2.300341	-1.937533
H	-4.728158	-0.891912	-2.956731
H	-1.779021	-1.694282	1.053755
H	-0.481338	-1.128277	3.116492
H	0.462773	1.154561	3.402166
H	0.191767	2.871882	1.617513
H	-1.158704	2.338601	-0.421382

Int-1_Pyr_S_cis

Imaginary frequencies = 0
E(MN15,DCE) = -2573.147976
$E_{Thermal\ correction}$ = 0.59943

Pd	0.272048	0.184045	-1.299306
C	2.951451	-0.630974	-1.505670
O	3.913436	-1.289906	-1.838998
C	3.289540	0.301736	0.859022
C	3.027189	0.624373	-0.648827
N	1.769165	1.346326	-0.802646
N	-0.995964	-1.443314	-1.838417
C	-2.015355	-1.913433	-1.096366
C	-2.598549	-3.175962	-1.271745
C	-2.088291	-3.911735	-2.358439
C	-0.534700	-2.165835	-2.865009

C	-1.081443	-3.410741	-3.168689
S	-2.501548	-0.693740	0.136080
O	-1.385191	-0.459053	1.047499
O	1.722310	-0.989173	-1.834161
C	2.678062	-1.026118	1.287841
O	4.635855	0.483668	1.232480
C	5.622917	-0.312706	0.617566
O	2.889646	3.121657	-0.063781
C	3.064966	4.308239	0.741928
C	4.563018	4.304248	1.018666
C	2.284363	4.172864	2.045382
C	2.648537	5.545670	-0.044089
C	1.680724	2.630358	-0.390689
O	0.643149	3.285779	-0.320380
N	-3.884513	-1.197020	0.625506
O	-5.737197	-0.817966	1.798652
C	-6.680860	-0.069382	2.609405
C	-6.032073	0.339426	3.927308
C	-7.799173	-1.073346	2.853007
C	-7.202774	1.133923	1.831238
C	-4.599676	-0.273754	1.379270
O	-4.240614	0.869395	1.598316
C	5.750092	-1.697448	1.213745
C	5.847756	-2.824403	0.391143
C	5.982947	-4.097478	0.951980
C	6.009688	-4.253878	2.338621
C	5.899186	-3.131363	3.165424
C	5.770492	-1.861208	2.604930
C	-3.666982	-3.801417	-0.418589
C	-3.824199	0.823203	-1.731034
C	-3.876572	1.858696	-2.667708
C	-2.804386	2.745486	-2.808424
C	-1.672553	2.622872	-1.999234
C	-1.609716	1.593011	-1.052899
C	-2.686531	0.715253	-0.938633
H	2.765474	1.105224	1.398619
H	3.873192	1.238017	-0.994171
H	-2.505795	-4.902962	-2.552280
H	0.309860	-1.748705	-3.413653
H	-0.695024	-3.981124	-4.013676
H	2.842043	-1.190787	2.362074
H	1.591457	-0.999989	1.098837
H	3.109886	-1.877122	0.740250
H	6.570691	0.230012	0.766880
H	5.454409	-0.397881	-0.468704
H	4.832414	5.128412	1.695261
H	5.123427	4.419103	0.079084
H	4.846797	3.343234	1.473531
H	2.499778	5.034661	2.694340
H	1.204608	4.133029	1.853428
H	2.592812	3.258539	2.576399
H	3.185766	5.578938	-1.003838
H	2.903697	6.451099	0.527232
H	1.568779	5.531580	-0.237773
H	-6.791753	0.791847	4.581794
H	-5.226669	1.065583	3.762668
H	-5.621574	-0.545536	4.436185
H	-8.588754	-0.617848	3.467651
H	-8.236343	-1.397030	1.897350
H	-7.409024	-1.958310	3.375787
H	-7.615292	0.807726	0.864193
H	-6.404789	1.865824	1.656311
H	-8.009541	1.615802	2.403073
H	5.783844	-2.696122	-0.692622
H	6.055829	-4.972464	0.301514
H	6.110667	-5.249534	2.777148
H	5.913914	-3.249743	4.251733
H	5.668999	-0.977561	3.241034
H	-3.777181	-4.857235	-0.700338
H	-4.629557	-3.287634	-0.537697
H	-3.426536	-3.731553	0.648613
H	-4.645643	0.112128	-1.615569
H	-4.762741	1.971451	-3.295816
H	-2.858459	3.546757	-3.547936
H	-0.832577	3.317050	-2.047762
H	-0.795051	1.620682	-0.289065

Int-1_Pyr_S_trans

Imaginary frequencies = 0
E(MN15,DCE) = -2573.162753
$E_{\text{Thermal correction}}$ = 0.601621

Pd	-0.294236	-0.196865	-0.039593
C	1.725545	0.169180	-1.915086
O	2.505885	-0.108779	-2.800477
C	3.291698	0.522858	0.013083
C	2.099061	1.107780	-0.768474
N	0.946876	1.294689	0.083182

N	-1.540438	-1.861458	-0.471056
C	-2.779169	-2.058893	0.007233
C	-3.686110	-2.995388	-0.502228
C	-3.181543	-3.817186	-1.522354
C	-1.086327	-2.658645	-1.450977
C	-1.880159	-3.669516	-1.984442
S	-3.215995	-0.955202	1.384662
O	-4.373409	-1.500035	2.085545
O	0.512539	-0.348224	-1.832941
C	3.840789	1.504102	1.029133
O	2.896969	-0.631946	0.732657
C	2.969463	-1.873129	0.065704
O	1.405608	3.480754	0.278328
C	1.290453	4.796349	0.866385
C	2.504861	5.531623	0.314301
C	0.002095	5.468898	0.405100
C	1.376699	4.701684	2.386707
C	0.554793	2.482864	0.592468
O	-0.450269	2.634971	1.280454
N	-3.105384	0.492647	0.869939
O	-2.736191	1.698635	-0.946765
C	-2.713309	2.032154	-2.358949
C	-4.011583	2.741170	-2.718914
C	-1.507256	2.958286	-2.448867
C	-2.480834	0.788746	-3.213241
C	-3.478189	0.722427	-0.448204
O	-4.318813	0.082253	-1.058918
C	4.373328	-2.226968	-0.365242
C	4.691113	-2.399819	-1.716065
C	5.999555	-2.711474	-2.097114
C	6.998641	-2.838599	-1.131700
C	6.690694	-2.647296	0.219286
C	5.384931	-2.341261	0.598610
C	-5.126423	-3.096982	-0.091461
C	-1.745447	-2.213471	3.304480
C	-0.556485	-2.427995	4.009077
C	0.548342	-1.591529	3.815628
C	0.474435	-0.508098	2.936108
C	-0.714496	-0.269481	2.236372
C	-1.790874	-1.139894	2.422022
H	4.067902	0.262625	-0.730934
H	2.424294	2.058620	-1.219774
H	-3.841158	-4.569729	-1.961892
H	-0.086421	-2.435457	-1.827262
H	-1.483098	-4.304773	-2.776663
H	4.149170	2.443199	0.548008
H	4.700270	1.059118	1.550063
H	3.061607	1.739586	1.772422
H	2.597547	-2.611649	0.794815
H	2.293837	-1.913170	-0.808037
H	2.523681	6.567159	0.683791
H	3.430939	5.027319	0.629262
H	2.472572	5.548365	-0.784785
H	-0.033754	6.500324	0.787161
H	-0.873643	4.917394	0.769674
H	-0.026307	5.507329	-0.694682
H	2.284891	4.148358	2.674383
H	1.439518	5.712512	2.816561
H	0.497691	4.190472	2.797528
H	-3.983463	3.059398	-3.771556
H	-4.865251	2.063701	-2.578028
H	-4.148647	3.631415	-2.087612
H	-1.387865	3.338887	-3.473469
H	-0.599991	2.401228	-2.163114
H	-1.627959	3.804220	-1.756336
H	-1.599988	0.238515	-2.845191
H	-3.357674	0.130016	-3.217220
H	-2.269130	1.106020	-4.245327
H	3.910934	-2.256940	-2.468786
H	6.239856	-2.842697	-3.154553
H	8.021566	-3.079416	-1.430211
H	7.472907	-2.739548	0.976498
H	5.136280	-2.183461	1.652252
H	-5.648525	-3.793952	-0.760207
H	-5.239077	-3.433820	0.946710
H	-5.596164	-2.105870	-0.160760
H	-2.618277	-2.857560	3.429158
H	-0.489401	-3.263117	4.709484
H	1.474771	-1.784992	4.359825
H	1.329362	0.148845	2.764665
H	-0.878706	0.713398	1.713039

int-1_SO-R

Imaginary frequencies = 0
E(MN15,DCE) = -2573.130298
$E_{Thermal\ correction}$ = 0.598023

Pd	-0.143251	0.566133	-0.865557

C	2.326996	0.488974	-2.130523
O	3.318828	-0.031578	-2.612630
C	3.297285	0.833833	0.221751
C	2.529371	1.475805	-0.950938
N	1.222855	1.962599	-0.528337
N	-0.861221	-3.289771	1.303763
C	-0.859224	-2.916399	0.036433
C	-0.024249	-3.409034	-0.978808
C	0.904567	-4.362484	-0.526520
C	0.023105	-4.201183	1.698714
C	0.944110	-4.757752	0.806761
S	-2.070379	-1.628848	-0.282582
O	-1.553801	-0.800121	-1.439946
O	1.097000	0.284410	-2.482014
C	3.812875	1.878191	1.193865
O	2.477130	-0.030966	0.973048
C	2.243611	-1.318250	0.447045
O	1.912157	4.113167	-0.348002
C	1.827329	5.443514	0.257503
C	3.271194	5.920434	0.208604
C	0.927864	6.338576	-0.583402
C	1.352894	5.320239	1.700907
C	0.963747	3.208533	-0.326813
O	-0.274435	3.629040	-0.122563
N	-3.403220	-2.387625	-0.452157
O	-4.341858	-0.327240	-0.424046
C	-5.369487	0.668585	-0.212120
C	-6.173666	0.336017	1.040268
C	-4.562701	1.944415	-0.001369
C	-6.250868	0.759852	-1.450961
C	-4.588874	-1.651430	-0.491530
O	-5.683163	-2.146988	-0.568715
C	3.447369	-2.228410	0.498864
C	4.105067	-2.611505	-0.676028
C	5.200026	-3.479540	-0.616769
C	5.646551	-3.962091	0.614239
C	5.001738	-3.570267	1.792471
C	3.908543	-2.706834	1.733016
C	-0.047798	-2.992627	-2.420696
C	-2.649314	-0.799149	2.266224
C	-2.500418	0.088150	3.328464
C	-1.623034	1.172467	3.196783
C	-0.915047	1.397154	2.012929
C	-1.082487	0.560735	0.893124
C	-1.942412	-0.528282	1.096436
H	4.138286	0.279856	-0.237794
H	3.146791	2.302428	-1.336967
H	1.613216	-4.782945	-1.244838
H	0.003717	-4.491035	2.753010
H	1.684407	-5.481056	1.152584
H	4.458358	2.610978	0.688334
H	4.376994	1.391241	2.000459
H	2.958216	2.407275	1.647153
H	1.430726	-1.734765	1.064408
H	1.871156	-1.272243	-0.592737
H	3.347330	6.932521	0.630108
H	3.913695	5.243056	0.789937
H	3.630714	5.940978	-0.829811
H	0.977518	7.366367	-0.195057
H	-0.116236	6.003555	-0.553013
H	1.272303	6.347649	-1.627578
H	1.968242	4.583305	2.240270
H	1.467058	6.291984	2.202402
H	0.297290	5.024611	1.760196
H	-6.862240	1.164684	1.262507
H	-6.755134	-0.584326	0.904221
H	-5.494179	0.212758	1.898546
H	-5.235173	2.803156	0.139243
H	-3.919509	2.131840	-0.875135
H	-3.922429	1.840627	0.890147
H	-5.637177	0.979182	-2.337108
H	-6.783817	-0.186843	-1.609017
H	-6.986514	1.568422	-1.326244
H	3.763982	-2.205807	-1.634008
H	5.709706	-3.772763	-1.537412
H	6.501667	-4.640624	0.659266
H	5.353130	-3.943227	2.757558
H	3.394560	-2.399588	2.648754
H	0.504580	-3.726965	-3.021995
H	-1.073670	-2.913447	-2.803432
H	0.420882	-2.002239	-2.560128
H	-3.290797	-1.682286	2.327425
H	-3.042336	-0.073803	4.262081
H	-1.479224	1.851295	4.041038
H	-0.212635	2.234330	1.975350
H	-0.869574	2.845661	-0.167289

int-1_SO-S

Imaginary frequencies = 0
E(MN15,DCE) = -2573.145439
$E_{Thermal\ correction}$ = 0.598038

Pd	0.371397	0.018444	-0.205769
C	2.349366	-0.839458	-2.011726
O	3.035469	-1.540223	-2.734884
C	3.797935	-0.733519	0.031344
C	3.070679	0.108967	-1.027880
N	2.087410	0.993457	-0.413352
N	-3.226860	2.307529	-0.054395
C	-2.785110	1.236511	-0.690394
C	-2.603962	1.099489	-2.077016
C	-2.916398	2.267008	-2.793745
C	-3.521407	3.393572	-0.764005
C	-3.370312	3.416014	-2.151889
S	-2.458778	-0.092976	0.498070
O	-1.436874	-1.011315	-0.136778
O	1.057915	-0.850362	-1.921939
C	4.605057	0.113140	0.996880
O	2.875017	-1.475185	0.798685
C	2.565800	-2.791308	0.361760
O	3.435760	2.803158	-0.603790
C	3.941005	4.079942	-0.098593
C	5.382403	4.083353	-0.586117
C	3.162305	5.235135	-0.713819
C	3.888980	4.076568	1.424311
C	2.288641	2.258869	-0.269260
O	1.346980	3.068011	0.181784
N	-3.746160	-0.694853	1.103793
O	-5.793842	-1.522745	0.876164
C	-6.975538	-2.010625	0.191244
C	-6.625835	-3.224013	-0.663449
C	-7.895352	-2.412542	1.336277
C	-7.605452	-0.892298	-0.632385
C	-4.733461	-1.080855	0.212545
O	-4.646472	-1.013710	-1.003604
C	3.790187	-3.667480	0.257307
C	4.216265	-4.153184	-0.983903
C	5.365384	-4.944362	-1.072452
C	6.100576	-5.243382	0.075297
C	5.689464	-4.745578	1.316130
C	4.540731	-3.960542	1.404692
C	-2.152465	-0.138575	-2.789993
C	-2.209150	1.026899	3.010510
C	-1.392871	1.541203	4.016484
C	-0.013781	1.657639	3.800411
C	0.568021	1.280015	2.585970
C	-0.220923	0.772910	1.539317
C	-1.590934	0.663253	1.818329
H	4.464183	-1.409674	-0.534730
H	3.819604	0.684183	-1.592031
H	-2.805841	2.252223	-3.881191
H	-3.885734	4.266245	-0.214449
H	-3.612039	4.315973	-2.719922
H	5.306597	0.772285	0.463590
H	5.165930	-0.537767	1.681997
H	3.921395	0.732857	1.600754
H	1.875943	-3.184628	1.123071
H	2.024718	-2.783513	-0.598823
H	5.883791	5.008429	-0.268754
H	5.927841	3.223766	-0.170160
H	5.414159	4.021313	-1.683013
H	3.655529	6.181724	-0.448447
H	2.127680	5.265764	-0.351982
H	3.157718	5.145472	-1.809852
H	4.417164	3.194118	1.816748
H	4.391558	4.976445	1.807152
H	2.855217	4.075175	1.795203
H	-7.550235	-3.662774	-1.067493
H	-5.970997	-2.944789	-1.497704
H	-6.122273	-3.985318	-0.049184
H	-8.843435	-2.804145	0.940384
H	-8.108628	-1.543980	1.975768
H	-7.418960	-3.189012	1.951631
H	-7.797698	-0.016544	0.005692
H	-6.950296	-0.598033	-1.461327
H	-8.566294	-1.238187	-1.041599
H	3.653513	-3.878252	-1.880624
H	5.691452	-5.320164	-2.044963
H	6.998860	-5.861389	0.005102
H	6.265454	-4.976085	2.215617
H	4.211942	-3.566306	2.370934
H	-2.310788	-0.015011	-3.869883
H	-1.084556	-0.348795	-2.617586
H	-2.722218	-1.007489	-2.437617
H	-3.284991	0.886144	3.130267
H	-1.825596	1.839065	4.973298
H	0.622480	2.041860	4.601597
H	1.651773	1.364928	2.453818

H	0.560812	2.522514	0.414460

Int-2_NBoc_R

Imaginary frequencies = 0
E(MN15,DCE) = -2573.181292
$E_{Thermal\ correction}$ = 0.60518

Pd	-0.229916	-0.013062	0.138375
C	1.801907	-0.203500	-1.790517
O	2.748015	-0.667904	-2.408841
C	3.060964	1.203202	-0.099535
C	1.959460	1.209717	-1.172201
N	0.676145	1.597910	-0.607596
N	-3.254676	0.654887	-0.540124
C	-3.720507	-0.490283	-0.055762
C	-4.838655	-1.185598	-0.544537
C	-5.448386	-0.577620	-1.656505
C	-3.852855	1.205616	-1.592354
C	-4.964398	0.610214	-2.191536
S	-2.735671	-1.126800	1.334636
O	-3.552205	-2.024932	2.140038
O	0.680793	-0.796384	-1.546974
C	3.381139	2.603304	0.388467
O	2.669892	0.453555	1.029139
C	2.923013	-0.942786	1.007149
O	0.714476	3.694328	-1.470649
C	0.397585	5.110704	-1.310742
C	1.592933	5.796730	-1.955674
C	-0.886137	5.453858	-2.056039
C	0.321241	5.446442	0.174146
C	0.089129	2.717229	-0.846174
O	-1.175817	2.926745	-0.519378
N	-1.317581	-1.642129	0.767950
O	-0.118573	-3.208858	-0.235402
C	0.222307	-4.179418	-1.268222
C	-0.422118	-3.791677	-2.593955
C	1.736126	-4.057244	-1.371424
C	-0.209642	-5.560330	-0.793057
C	-1.348576	-2.802504	-0.016741
O	-2.377339	-3.324421	-0.407026
C	4.395948	-1.257831	0.902103
C	4.907352	-1.947785	-0.202197
C	6.276085	-2.218518	-0.291338
C	7.142300	-1.790332	0.714920
C	6.639544	-1.083854	1.812658
C	5.274064	-0.818920	1.903407
C	-5.391168	-2.463779	0.013944
C	-2.886628	0.695552	3.350775
C	-2.360307	1.774903	4.056640
C	-1.167956	2.373234	3.622379
C	-0.488652	1.916590	2.489103
C	-0.991171	0.834702	1.748123
C	-2.181813	0.277074	2.222735
H	3.948186	0.750028	-0.579748
H	2.267281	1.895961	-1.976275
H	-6.319880	-1.065293	-2.100902
H	-3.432127	2.144569	-1.964664
H	-5.439771	1.072459	-3.057916
H	3.672590	3.259115	-0.445396
H	4.196710	2.566233	1.123744
H	2.493050	3.032054	0.881906
H	2.516461	-1.317413	1.958701
H	2.366095	-1.452287	0.200855
H	1.478867	6.888319	-1.896527
H	2.519556	5.506907	-1.439262
H	1.675017	5.505339	-3.012383
H	-1.015795	6.546092	-2.067655
H	-1.763582	5.001983	-1.577866
H	-0.821684	5.103922	-3.096685
H	1.253797	5.146644	0.676634
H	0.198003	6.532065	0.297587
H	-0.526826	4.944546	0.660020
H	0.008987	-4.414837	-3.391502
H	-1.509076	-3.941212	-2.575839
H	-0.190893	-2.737127	-2.803375
H	2.124765	-4.816355	-2.066346
H	2.200533	-4.211335	-0.385239
H	2.002253	-3.056398	-1.747061
H	0.273047	-5.804694	0.164939
H	-1.300461	-5.598464	-0.667656
H	0.088346	-6.315833	-1.535104
H	4.226454	-2.243464	-1.004703
H	6.666556	-2.756993	-1.157863
H	8.212083	-2.000781	0.643728
H	7.316377	-0.743668	2.600185
H	4.872082	-0.265116	2.756978
H	-6.212365	-2.818990	-0.622759
H	-4.604809	-3.227842	0.065062

H	-5.763520	-2.318789	1.036988
H	-3.795978	0.177050	3.664325
H	-2.865027	2.142936	4.951754
H	-0.755587	3.209956	4.192127
H	0.448692	2.388995	2.178246
H	-1.575444	2.087097	-0.177594

Int-2_NBoc_S

Imaginary frequencies = 0
E(MN15,DCE) = -2573.181108
$E_{\text{Thermal correction}}$ = 0.604568

Pd	-0.184117	-0.589017	-0.535453
C	-1.921432	1.272723	-1.714959
O	-2.362184	2.351736	-2.086890
C	-3.062073	1.092452	0.541607
C	-2.819704	0.397397	-0.810442
N	-2.168200	-0.890960	-0.621865
N	3.841503	-0.467508	1.830146
C	4.158865	-1.018088	0.671895
C	5.451450	-1.159712	0.143667
C	6.459949	-0.665871	0.987909
C	4.816359	-0.002803	2.604612
C	6.156128	-0.089562	2.217360
S	2.691234	-1.574504	-0.222533
O	3.056018	-2.490990	-1.296595
O	-0.745838	0.800601	-1.955490
C	-4.091683	0.358870	1.380552
O	-1.879383	1.146810	1.306537
C	-1.011188	2.250423	1.093429
O	-4.086880	-2.057066	-0.944890
C	-4.941371	-3.208729	-0.664122
C	-6.340349	-2.629611	-0.816510
C	-4.699083	-4.308024	-1.690129
C	-4.708359	-3.676569	0.767684
C	-2.789041	-2.011129	-0.740330
O	-2.146104	-3.166945	-0.695224
N	1.821083	-0.261354	-0.550387
O	1.782589	1.875809	-1.160114
C	2.002351	2.966872	-2.102535
C	1.948397	2.402847	-3.516526
C	0.822492	3.894337	-1.854968
C	3.323904	3.658862	-1.791846
C	2.505313	0.776197	-1.178276
O	3.633538	0.648989	-1.624856
C	-1.639362	3.561397	1.500573
C	-2.065489	4.481732	0.534621
C	-2.678068	5.677221	0.922074
C	-2.875780	5.957175	2.274718
C	-2.465269	5.036219	3.243966
C	-1.852732	3.845161	2.856767
C	5.787410	-1.724104	-1.203860
C	2.121802	-3.210802	1.907993
C	1.232311	-3.729990	2.844691
C	-0.105587	-3.314864	2.828259
C	-0.571296	-2.411310	1.870300
C	0.288561	-1.880896	0.890843
C	1.627367	-2.290387	0.983046
H	-3.419011	2.110585	0.298092
H	-3.790683	0.284580	-1.316302
H	7.498194	-0.730637	0.652142
H	4.524437	0.450742	3.555917
H	6.944895	0.295786	2.865609
H	-5.038894	0.233777	0.835138
H	-4.276792	0.911019	2.311946
H	-3.701096	-0.637201	1.647953
H	-0.125564	2.036703	1.710634
H	-0.664822	2.301993	0.047809
H	-7.092589	-3.408476	-0.628123
H	-6.491715	-1.808451	-0.100765
H	-6.481847	-2.238555	-1.833921
H	-5.455849	-5.095415	-1.559021
H	-3.704351	-4.755587	-1.578048
H	-4.797239	-3.902255	-2.707463
H	-4.842008	-2.835335	1.465157
H	-5.444769	-4.452840	1.020989
H	-3.702962	-4.098832	0.897834
H	1.962727	3.229427	-4.241871
H	2.806322	1.746030	-3.716327
H	1.011413	1.838072	-3.633421
H	0.906707	4.779871	-2.502309
H	0.813083	4.229756	-0.806027
H	-0.123122	3.375738	-2.078122
H	3.334311	4.004035	-0.746884
H	4.171011	2.981140	-1.955637
H	3.434385	4.537414	-2.444883
H	-1.934850	4.236210	-0.523708
H	-3.007796	6.388580	0.161394

H	-3.353471	6.892247	2.576909
H	-2.621307	5.252036	4.303739
H	-1.530173	3.119598	3.609270
H	6.865118	-1.624033	-1.389410
H	5.500156	-2.780670	-1.284073
H	5.226607	-1.182544	-1.977968
H	3.177426	-3.495375	1.909270
H	1.579827	-4.443778	3.593717
H	-0.796529	-3.703200	3.580614
H	-1.620119	-2.097364	1.884446
H	-1.192963	-2.975335	-0.550378

Int-2_Pyr_R_cis

Imaginary frequencies = 0
E(MN15,DCE) = -2573.173279
$E_{Thermal\ correction}$ = 0.607921

Pd	-1.017651	-0.546091	-0.874483
C	1.556632	-1.538322	-1.376797
O	2.403850	-2.245814	-1.900857
C	2.890609	0.227242	-0.099484
C	1.826551	-0.028553	-1.219829
N	0.576949	0.681816	-0.890863
N	-2.454774	-2.009299	-0.827809
C	-3.585705	-1.929651	-0.114197
C	-4.528579	-2.960874	-0.027138
C	-4.215860	-4.114767	-0.766936
C	-2.167680	-3.124119	-1.512426
C	-3.044374	-4.205738	-1.506662
S	-3.755710	-0.382070	0.806625
O	-5.097106	-0.289781	1.377677
O	0.442465	-1.962072	-0.872330
C	2.875643	-0.856421	0.971221
O	4.161224	0.552146	-0.610189
C	4.860633	-0.423637	-1.357061
O	1.667413	2.589256	-1.337561
C	2.135932	3.943136	-1.055505
C	3.525528	3.933065	-1.677050
C	2.226245	4.178651	0.446581
C	1.216241	4.943603	-1.740949
C	0.625818	1.981713	-0.816615
O	-0.296007	2.731393	-0.277695
N	-2.571697	-0.516856	1.810030
O	-0.878686	0.122952	3.067305
C	-0.016800	1.052454	3.771644
C	0.850616	1.867295	2.816539
C	0.856513	0.133611	4.614994
C	-0.884628	1.950609	4.644435
C	-1.736135	0.508508	2.132319
O	-1.738243	1.643782	1.644833
C	5.589669	-1.433336	-0.499531
C	5.480770	-2.802823	-0.763109
C	6.169570	-3.728547	0.025318
C	6.961303	-3.292892	1.089189
C	7.061156	-1.925794	1.365801
C	6.378513	-1.002288	0.574751
C	-5.790202	-2.921742	0.790767
C	-4.673069	1.691275	-0.681677
C	-4.572881	2.602762	-1.728764
C	-3.420840	2.614011	-2.525768
C	-2.362681	1.735954	-2.280851
C	-2.421285	0.808023	-1.226691
C	-3.594301	0.828047	-0.472210
H	2.578009	1.164317	0.384615
H	2.250496	0.356431	-2.160914
H	-4.913607	-4.955589	-0.738086
H	-1.205079	-3.135517	-2.027117
H	-2.796263	-5.106881	-2.068047
H	3.548822	-0.587725	1.798767
H	1.845719	-0.963232	1.352236
H	3.183131	-1.832541	0.572124
H	5.594788	0.140605	-1.954843
H	4.185562	-0.953021	-2.048389
H	4.028574	4.894380	-1.500236
H	3.454243	3.763844	-2.761156
H	4.115100	3.114575	-1.237941
H	2.753258	5.127197	0.624816
H	1.234389	4.242175	0.910514
H	2.804311	3.374092	0.927708
H	1.144523	4.717662	-2.814951
H	1.630132	5.956523	-1.628411
H	0.210558	4.922144	-1.301064
H	1.722957	2.258928	3.362034
H	0.297043	2.706233	2.380706
H	1.214927	1.220387	2.004490
H	1.510018	0.728425	5.269211
H	0.229284	-0.522479	5.234489
H	1.483022	-0.494074	3.963767

H	-1.478443	1.346524	5.345935
H	-1.561264	2.550065	4.019112
H	-0.247210	2.634814	5.223739
H	4.819462	-3.134789	-1.567966
H	6.075764	-4.796661	-0.184670
H	7.495612	-4.017378	1.708359
H	7.674995	-1.581202	2.201744
H	6.439472	0.068292	0.789551
H	-6.301212	-3.890801	0.717665
H	-6.466915	-2.128665	0.447332
H	-5.578586	-2.703611	1.845222
H	-5.550159	1.635779	-0.034238
H	-5.388930	3.299831	-1.928413
H	-3.348063	3.323895	-3.353599
H	-1.472753	1.775373	-2.916447
H	-0.922549	2.227746	0.327733

Int-2_Pyr_R_trans

Imaginary frequencies = 0
E(MN15,DCE) = -2573.180328
$E_{\text{Thermal correction}}$ = 0.601486

Pd	0.608865	-0.484375	-0.489126
C	3.025035	-0.088202	-1.862190
O	4.121572	-0.312653	-2.348754
C	3.818913	0.940539	0.305310
C	2.898870	1.130837	-0.910198
N	1.508878	1.282391	-0.509430
N	-0.400805	-2.237031	-0.818314
C	-1.741446	-2.333171	-0.790202
C	-2.435134	-3.493431	-1.176077
C	-1.613953	-4.566977	-1.570368
C	0.355552	-3.264786	-1.220133
C	-0.230161	-4.468177	-1.598231
S	-2.506390	-0.766818	-0.281329
O	-2.079135	0.274128	-1.236966
O	1.956480	-0.804559	-2.016001
C	3.860430	2.169538	1.192301
O	3.374649	-0.133610	1.111978
C	3.857250	-1.427431	0.804429
O	1.538756	3.532042	-0.675356
C	0.960940	4.849613	-0.931030
C	2.197970	5.721937	-1.093065
C	0.147411	4.825555	-2.218651
C	0.142427	5.300114	0.272326
C	0.870314	2.406053	-0.548602
O	-0.436279	2.492767	-0.456116
N	-4.010750	-1.122448	-0.146866
O	-6.118284	-0.505371	0.177330
C	-7.212176	0.366763	0.552071
C	-7.310600	1.540832	-0.416495
C	-8.433387	-0.533897	0.422348
C	-7.044350	0.830108	1.996060
C	-4.854522	-0.076280	0.186662
O	-4.505772	1.057161	0.463596
C	5.358754	-1.533752	0.926115
C	6.155130	-1.771170	-0.199516
C	7.545310	-1.847334	-0.072608
C	8.146168	-1.674540	1.174804
C	7.355835	-1.417891	2.299964
C	5.969429	-1.346239	2.173979
C	-3.924946	-3.695934	-1.222366
C	-2.494315	-0.408039	2.457793
C	-1.823349	-0.072519	3.628883
C	-0.448970	0.207494	3.591256
C	0.273548	0.147332	2.398061
C	-0.376519	-0.190851	1.198181
C	-1.746886	-0.437790	1.275666
H	4.821955	0.722522	-0.104457
H	3.249635	2.018641	-1.460147
H	-2.099042	-5.497520	-1.875279
H	1.431373	-3.079962	-1.262778
H	0.393341	-5.302533	-1.920342
H	4.166209	3.059915	0.624271
H	4.563386	2.006123	2.021143
H	2.859723	2.353617	1.615675
H	3.368067	-2.092214	1.533848
H	3.541642	-1.751872	-0.202698
H	1.901723	6.763881	-1.279077
H	2.810340	5.684841	-0.180396
H	2.806466	5.370003	-1.938351
H	-0.150309	5.853143	-2.473483
H	-0.759535	4.217291	-2.114818
H	0.755868	4.429989	-3.045474
H	0.749195	5.233077	1.187514
H	-0.154047	6.350023	0.132378
H	-0.762679	4.693505	0.396083
H	-8.217952	2.122358	-0.194831

H	-6.435112	2.195525	-0.329118
H	-7.382036	1.170663	-1.450278
H	-9.345017	0.022980	0.682770
H	-8.341673	-1.399319	1.094489
H	-8.525467	-0.902541	-0.609409
H	-6.918024	-0.041040	2.657521
H	-6.174981	1.491157	2.098434
H	-7.946201	1.374134	2.313923
H	5.675364	-1.861459	-1.178231
H	8.160868	-2.031690	-0.956022
H	9.232805	-1.733084	1.272413
H	7.824583	-1.277062	3.276848
H	5.343788	-1.142807	3.048145
H	-4.135719	-4.701376	-1.611011
H	-4.379341	-3.580249	-0.230943
H	-4.415973	-2.948725	-1.856866
H	-3.563046	-0.629410	2.454051
H	-2.368052	-0.025132	4.573743
H	0.067591	0.468050	4.518684
H	1.351573	0.333481	2.381640
H	-0.895471	1.623971	-0.602812

Int-2_Pyr_S_cis

Imaginary frequencies = 0
E(MN15,DCE) = -2573.163713
$E_{Thermal\ correction}$ = 0.602274

Pd	0.176787	-0.104581	-1.566213
C	2.914454	-0.889279	-1.482156
O	3.968338	-1.454175	-1.726662
C	3.144569	0.328715	0.754883
C	2.919109	0.480082	-0.789317
N	1.642424	1.178903	-1.022327
N	-1.073629	-1.695783	-1.932737
C	-2.181262	-1.961586	-1.218420
C	-2.925153	-3.144124	-1.364569
C	-2.441661	-4.027864	-2.347625
C	-0.622622	-2.562964	-2.846601
C	-1.302739	-3.751728	-3.089916
S	-2.493968	-0.650672	-0.007456
O	-1.325230	-0.564543	0.865550
O	1.736959	-1.384261	-1.695851
C	2.658865	-1.007478	1.299860
O	4.450276	0.693585	1.139306
C	5.528487	-0.077143	0.646151
O	2.710943	3.049840	-0.370622
C	2.853271	4.206016	0.516975
C	4.361119	4.281422	0.705228
C	2.164331	3.917397	1.843865
C	2.311399	5.453475	-0.166596
C	1.598637	2.423594	-0.665459
O	0.485529	3.122102	-0.595889
N	-3.888647	-1.017362	0.574400
O	-5.492842	-0.660376	2.069604
C	-6.243849	0.062331	3.074966
C	-5.396677	0.263586	4.327178
C	-7.413982	-0.867333	3.368189
C	-6.746516	1.386252	2.507002
C	-4.377440	-0.154517	1.539006
O	-3.884627	0.916962	1.846494
C	5.769842	-1.353867	1.419435
C	5.928120	-2.571365	0.748996
C	6.166260	-3.745436	1.468655
C	6.235197	-3.712245	2.862349
C	6.062614	-2.499821	3.537552
C	5.831681	-1.327618	2.818524
C	-4.144562	-3.552662	-0.584733
C	-3.820531	1.396287	-1.288787
C	-3.866481	2.459461	-2.188008
C	-2.706644	2.839221	-2.871201
C	-1.497904	2.169446	-2.659285
C	-1.406946	1.101718	-1.744950
C	-2.593095	0.762348	-1.083885
H	2.516952	1.107307	1.215144
H	3.754820	1.077703	-1.182041
H	-2.984170	-4.962647	-2.509534
H	0.311060	-2.297098	-3.344284
H	-0.929458	-4.449508	-3.839830
H	2.826318	-1.048871	2.385421
H	1.579811	-1.104826	1.098037
H	3.179364	-1.857242	0.836106
H	6.414257	0.572767	0.734407
H	5.387833	-0.320387	-0.420062
H	4.612406	5.076105	1.422060
H	4.855924	4.498100	-0.252546
H	4.724395	3.313362	1.080145
H	2.306413	4.776242	2.515650
H	1.084870	3.758389	1.716795

H	2.613712	3.033548	2.320893
H	2.762816	5.563813	-1.163418
H	2.580446	6.336206	0.431954
H	1.219643	5.417947	-0.268840
H	-6.018953	0.699188	5.123186
H	-4.551763	0.933111	4.125828
H	-5.012063	-0.704834	4.680702
H	-8.068825	-0.424050	4.132193
H	-8.000942	-1.040995	2.454654
H	-7.046076	-1.836290	3.735069
H	-7.303529	1.207353	1.574201
H	-5.912045	2.068986	2.305263
H	-7.429023	1.859370	3.228615
H	5.824117	-2.592517	-0.339364
H	6.285091	-4.692936	0.937693
H	6.416300	-4.631163	3.424989
H	6.109000	-2.471100	4.629002
H	5.682515	-0.376339	3.337015
H	-4.453252	-4.556914	-0.905135
H	-4.971865	-2.847511	-0.730766
H	-3.952133	-3.555977	0.494620
H	-4.714353	1.066709	-0.757171
H	-4.806183	2.987336	-2.360617
H	-2.746877	3.664008	-3.586845
H	-0.607883	2.482072	-3.213934
H	-0.282512	2.533724	-0.774746

Int-2_Pyr_S_trans

Imaginary frequencies = 0
E(MN15,DCE) = -2573.154389
$E_{Thermal\ correction}$ = 0.599563

Pd	-0.123873	-0.540648	0.130092
C	1.801042	0.186498	-1.789190
O	2.682307	0.099443	-2.628611
C	3.249174	0.684989	0.218559
C	2.030687	1.148337	-0.596104
N	0.828509	1.196152	0.219226
N	-1.301145	-2.172346	-0.242644
C	-2.588837	-2.212703	0.124344
C	-3.494356	-3.185743	-0.319776
C	-2.942492	-4.172589	-1.152279
C	-0.801312	-3.108805	-1.061620
C	-1.602835	-4.146355	-1.524170
S	-3.102862	-0.840964	1.221992
O	-4.420525	-1.128014	1.777192
O	0.697075	-0.495268	-1.766186
C	3.619474	1.671571	1.308377
O	2.991938	-0.552992	0.854000
C	3.290253	-1.732655	0.132502
O	0.978429	3.419139	0.562773
C	0.415735	4.763457	0.632846
C	1.631017	5.643635	0.374929
C	-0.618686	4.936300	-0.471141
C	-0.150655	5.038238	2.020902
C	0.281785	2.299577	0.621227
O	-0.922062	2.371028	1.121558
N	-2.829698	0.505653	0.443908
O	-2.527443	1.434414	-1.547597
C	-2.509383	1.474683	-3.004945
C	-3.873126	1.925518	-3.511165
C	-1.434526	2.511788	-3.295022
C	-2.095850	0.121609	-3.577467
C	-3.196525	0.492344	-0.891605
O	-3.980880	-0.299415	-1.389093
C	4.750904	-1.838494	-0.236694
C	5.153404	-1.825748	-1.576406
C	6.510203	-1.905957	-1.903340
C	7.470680	-1.986031	-0.894426
C	7.074908	-1.979685	0.447122
C	5.721507	-1.904420	0.772743
C	-4.967325	-3.184465	-0.033601
C	-2.285686	-0.986654	3.804949
C	-1.296629	-0.919849	4.782175
C	0.037441	-0.704077	4.406361
C	0.406642	-0.557363	3.066252
C	-0.566985	-0.619156	2.054923
C	-1.880194	-0.822466	2.477820
H	4.076767	0.577650	-0.506117
H	2.265096	2.141268	-1.012668
H	-3.600505	-4.958694	-1.531121
H	0.241767	-2.978817	-1.358249
H	-1.183014	-4.904658	-2.185588
H	3.805106	2.672339	0.892865
H	4.518261	1.322052	1.835578
H	2.794450	1.745472	2.035048
H	3.006908	-2.556144	0.806888
H	2.670866	-1.821933	-0.777349

H	1.336945	6.702770	0.379192
H	2.389216	5.483683	1.155318
H	2.076223	5.403033	-0.601130
H	-1.008706	5.964397	-0.449769
H	-1.459604	4.239909	-0.348194
H	-0.152586	4.763239	-1.452655
H	0.593240	4.777601	2.788227
H	-0.373338	6.111888	2.109415
H	-1.068919	4.469764	2.206401
H	-3.838507	2.044985	-4.604229
H	-4.640895	1.181529	-3.260988
H	-4.147498	2.892969	-3.064412
H	-1.285111	2.613059	-4.379244
H	-0.485777	2.192536	-2.834090
H	-1.724666	3.489529	-2.884133
H	-1.168984	-0.224849	-3.093145
H	-2.887270	-0.627080	-3.450155
H	-1.895644	0.242239	-4.652682
H	4.394663	-1.718230	-2.356603
H	6.816948	-1.894027	-2.951694
H	8.530999	-2.046959	-1.150767
H	7.825688	-2.036848	1.238902
H	5.403085	-1.895175	1.819393
H	-5.450805	-3.992457	-0.598273
H	-5.178111	-3.309665	1.035852
H	-5.396991	-2.218604	-0.332668
H	-3.340081	-1.144035	4.041993
H	-1.560516	-1.030972	5.835605
H	0.807038	-0.654125	5.181047
H	1.453311	-0.409063	2.783940
H	-1.526209	1.590779	0.895931

int-2_SO-R

Imaginary frequencies = 0
E(MN15,DCE) = -2573.163493
$E_{Thermal\ correction}$ = 0.603373

Pd	-0.066576	0.255464	-0.275784
C	2.039145	-0.132637	-2.033087
O	2.711661	-0.619783	-2.917145
C	3.385725	-0.609711	0.017542
C	2.675529	0.492532	-0.789883
N	1.634486	1.124864	-0.013794
N	-3.337907	-3.001901	0.374754
C	-4.016455	-1.863165	0.354531
C	-5.410457	-1.728530	0.236898
C	-6.079732	-2.962280	0.120300
C	-3.999174	-4.146985	0.266519
C	-5.391131	-4.169006	0.127512
S	-2.887775	-0.464169	0.387313
O	-1.904145	-0.740953	-0.713480
O	0.721143	-0.153764	-2.022777
C	4.115136	-0.051599	1.223580
O	2.447477	-1.552214	0.504094
C	2.165921	-2.676172	-0.309416
O	2.938859	2.876157	0.468673
C	3.307701	4.078928	1.176533
C	4.763246	4.283842	0.776385
C	2.453966	5.253835	0.709818
C	3.199603	3.851724	2.681714
C	1.720221	2.314936	0.600750
O	0.795526	2.833712	1.229950
N	-3.618677	0.866486	0.387022
O	-2.346980	2.233368	-0.881750
C	-1.981593	3.001191	-2.075129
C	-2.830604	4.263848	-2.169039
C	-0.521238	3.367004	-1.849038
C	-2.125445	2.089754	-3.286838
C	-3.570497	1.735690	-0.716664
O	-4.541972	2.000153	-1.384216
C	3.397796	-3.488677	-0.630242
C	3.826323	-3.647772	-1.952233
C	4.978158	-4.387961	-2.234587
C	5.714664	-4.961033	-1.197246
C	5.301949	-4.788709	0.128126
C	4.150407	-4.054762	0.408348
C	-6.203413	-0.451654	0.231014
C	-2.026567	-1.584105	2.836359
C	-1.074573	-1.606830	3.862643
C	-0.037126	-0.673803	3.897858
C	0.052496	0.322303	2.921486
C	-0.903425	0.379325	1.905569
C	-1.920142	-0.590416	1.873092
H	4.097544	-1.100476	-0.672069
H	3.430046	1.222505	-1.120753
H	-7.167858	-2.952638	0.017903
H	-3.411123	-5.068723	0.286633
H	-5.922340	-5.117112	0.029238

H	4.832726	0.728687	0.931492
H	4.644033	-0.861462	1.746009
H	3.381498	0.391294	1.917118
H	1.455631	-3.279656	0.276911
H	1.653089	-2.392061	-1.243755
H	5.168726	5.185498	1.257799
H	5.366852	3.416352	1.083138
H	4.845269	4.396638	-0.314324
H	2.845000	6.189112	1.138269
H	1.410081	5.122375	1.019779
H	2.494750	5.331534	-0.387483
H	3.758942	2.944289	2.960821
H	3.636995	4.705976	3.219842
H	2.150698	3.739007	2.983707
H	-2.454643	4.882071	-2.997517
H	-3.886019	4.029695	-2.348745
H	-2.741723	4.846999	-1.240039
H	-0.185605	4.031240	-2.658940
H	0.113254	2.467677	-1.854165
H	-0.396189	3.879426	-0.884118
H	-1.527348	1.176605	-3.134385
H	-3.176460	1.820977	-3.459284
H	-1.745213	2.605817	-4.180567
H	3.264474	-3.159626	-2.753468
H	5.306682	-4.506315	-3.269669
H	6.616296	-5.537114	-1.418391
H	5.880820	-5.231052	0.942551
H	3.822793	-3.909363	1.442152
H	-7.272813	-0.691871	0.161127
H	-6.025778	0.134207	1.142826
H	-5.927238	0.210296	-0.602396
H	-2.813105	-2.336781	2.787723
H	-1.140775	-2.376603	4.634106
H	0.707063	-0.720933	4.694842
H	0.841195	1.076989	2.929167
H	-0.919671	1.287713	1.244258

int-2_SO-S

Imaginary frequencies = 0
E(MN15,DCE) = -2573.166767
$E_{\text{Thermal correction}}$ = 0.600628

Pd	0.358568	0.185830	-0.367552
C	2.305312	-0.765542	-2.090994
O	2.890842	-1.489654	-2.866763
C	3.730099	-0.773135	-0.065645
C	3.050530	0.136357	-1.106191
N	2.090635	1.024953	-0.491782
N	-3.186899	2.375579	0.525232
C	-2.805667	1.468543	-0.357151
C	-2.658103	1.647369	-1.741905
C	-2.936949	2.960651	-2.159097
C	-3.447444	3.606409	0.096323
C	-3.324953	3.943627	-1.254276
S	-2.481664	-0.103988	0.472833
O	-1.499857	-0.859799	-0.381721
O	0.992338	-0.753987	-1.956274
C	4.513925	0.011557	0.966907
O	2.752318	-1.524561	0.632299
C	2.465672	-2.832074	0.163259
O	3.540564	2.726617	-0.475802
C	4.049492	3.999151	-0.019179
C	5.512584	3.960899	-0.441348
C	3.321632	5.144781	-0.714050
C	3.940067	4.088576	1.500656
C	2.286258	2.320372	-0.196740
O	1.424874	3.055931	0.289543
N	-3.732331	-0.832576	1.003829
O	-5.760196	-1.672461	0.660770
C	-6.960252	-2.032528	-0.075209
C	-6.613172	-2.997322	-1.203411
C	-7.813868	-2.725448	0.977682
C	-7.656157	-0.776399	-0.587619
C	-4.747881	-1.046589	0.082167
O	-4.708522	-0.692991	-1.085583
C	3.693933	-3.705487	0.079770
C	4.138449	-4.193721	-1.153639
C	5.289765	-4.983292	-1.225182
C	6.009734	-5.277687	-0.066673
C	5.580717	-4.776879	1.166863
C	4.429523	-3.993716	1.237789
C	-2.273945	0.592540	-2.736214
C	-1.885047	-0.153582	3.159640
C	-0.975126	0.057935	4.202240
C	0.228140	0.730484	3.976244
C	0.538434	1.224243	2.705470
C	-0.360557	1.029491	1.656465
C	-1.556368	0.342298	1.906917

H	4.400905	-1.449101	-0.626680
H	3.825806	0.695895	-1.650618
H	-2.847305	3.196927	-3.222429
H	-3.756634	4.342077	0.843763
H	-3.534556	4.960462	-1.590005
H	5.260754	0.663940	0.491758
H	5.015776	-0.682030	1.656679
H	3.818815	0.639916	1.547555
H	1.754572	-3.245207	0.894712
H	1.954697	-2.813820	-0.813614
H	6.015951	4.896642	-0.158148
H	6.028377	3.120125	0.046486
H	5.590107	3.832315	-1.530588
H	3.793013	6.101143	-0.441326
H	2.265210	5.164081	-0.420431
H	3.389543	5.024552	-1.805688
H	4.395749	3.195775	1.958463
H	4.482368	4.975409	1.861075
H	2.890266	4.161250	1.812268
H	-7.541651	-3.364748	-1.664857
H	-6.005614	-2.505655	-1.972856
H	-6.060860	-3.861486	-0.805186
H	-8.767295	-3.049736	0.536675
H	-8.022985	-2.039096	1.810695
H	-7.288513	-3.605806	1.374498
H	-7.843899	-0.082010	0.245126
H	-7.048477	-0.271945	-1.348768
H	-8.624435	-1.052658	-1.030502
H	3.586744	-3.923776	-2.058783
H	5.630115	-5.360609	-2.192184
H	6.910524	-5.893366	-0.122950
H	6.145842	-5.002433	2.074436
H	4.088377	-3.594719	2.197807
H	-2.447164	0.969711	-3.752837
H	-1.212690	0.309342	-2.647677
H	-2.870082	-0.315281	-2.578539
H	-2.821234	-0.697946	3.293574
H	-1.208856	-0.317971	5.200279
H	0.929302	0.877046	4.799928
H	1.457722	1.779046	2.506092
H	-0.187172	1.659610	0.728963

int-3-R-NBoc

Imaginary frequencies = 0
E(MN15,DCE) = -2301.795904
$E_{Thermal\ correction}$ = 0.481799

Pd	-0.686136	1.095086	-0.359637
C	2.135979	0.484218	-1.016048
O	1.952558	0.927055	-2.155550
N	-1.082932	-0.707207	-1.648442
C	-2.611725	1.575076	-0.488871
C	-3.247734	2.775374	-0.829383
C	-4.644131	2.860343	-0.867789
C	-5.452354	1.760809	-0.563599
C	-4.854454	0.555211	-0.203464
C	-3.461219	0.508773	-0.175842
C	-1.922475	-1.617806	-1.166129
C	-2.129853	-2.889532	-1.704634
C	-1.402755	-3.139472	-2.879900
C	-0.385996	-0.963897	-2.759796
C	-0.542285	-2.185466	-3.415526
S	-2.710708	-0.995163	0.338862
O	-3.699969	-1.932808	0.852896
O	1.250725	0.412385	-0.086731
N	-1.516098	-0.450171	1.231965
O	0.187934	-1.056533	2.549426
C	1.162829	-1.956709	3.147677
C	1.973880	-1.039149	4.050465
C	2.049769	-2.565547	2.068239
C	0.439928	-3.015742	3.972312
C	-0.676852	-1.486992	1.654004
O	-0.772291	-2.634085	1.241249
C	-2.979733	-3.946487	-1.065139
C	-0.070591	2.966686	-1.128487
C	-0.225318	3.051424	0.261137
H	-2.668330	3.671959	-1.063282
H	-5.110096	3.810955	-1.138286
H	-6.539708	1.848720	-0.592788
H	-5.433194	-0.328440	0.074829
H	-1.508113	-4.115162	-3.361648
H	0.318623	-0.191368	-3.078402
H	0.026849	-2.389428	-4.323225
H	2.719575	-1.623254	4.608277
H	1.313049	-0.526900	4.765063
H	2.497505	-0.282761	3.449560
H	2.937461	-3.018556	2.533445
H	1.514485	-3.330609	1.493592

H	2.377755	-1.771482	1.382554
H	-0.199796	-2.538863	4.729993
H	1.182624	-3.640722	4.489832
H	-0.175751	-3.658924	3.331007
H	-4.030821	-3.638610	-0.989204
H	-2.627342	-4.121700	-0.038547
H	-2.916016	-4.878589	-1.641716
H	-1.121704	3.459802	0.735819
H	-0.836437	3.321183	-1.819342
C	0.998683	3.016371	1.119772
O	2.122943	3.200869	0.717112
O	0.693695	2.781274	2.395678
C	1.791329	2.714296	3.289513
H	1.400174	2.351895	4.246325
H	2.247997	3.707397	3.415343
H	2.558742	2.029948	2.902916
H	0.932749	2.824287	-1.537031
C	3.514019	-0.058001	-0.629185
H	3.398983	-1.144858	-0.459281
C	4.040148	0.565945	0.660195
N	4.407443	0.131873	-1.748576
H	3.328249	0.377439	1.476408
H	5.009322	0.110610	0.905119
H	4.149445	1.653111	0.546410
H	4.034821	0.698680	-2.508355
C	5.552002	-0.588033	-1.869495
O	5.916398	-1.389028	-1.020478
C	6.365431	-0.318254	-3.118792
H	5.842864	0.312439	-3.850362
H	7.303540	0.174554	-2.826389
H	6.632105	-1.279227	-3.577981

Int-3-R-Pyr

Imaginary frequencies = 0
E(MN15,DCE) = -2301.806145
$E_{\text{Thermal correction}}$ = 0.477554

Pd	-0.878932	-0.897568	0.100660
C	1.995722	-1.140587	0.340999
O	2.116311	-1.125996	-0.883198
N	-1.132881	0.118584	1.924738
C	-2.611654	-0.115127	-0.496784
C	-3.741465	-0.786117	-0.980580
C	-4.888525	-0.074677	-1.348533
C	-4.940407	1.318808	-1.253400
C	-3.836866	2.012327	-0.764076
C	-2.706950	1.277049	-0.398048
C	-1.278039	1.442919	1.973956
C	-1.267776	2.189858	3.157044
C	-1.098021	1.432005	4.328148
C	-0.958041	-0.586748	3.046047
C	-0.943492	0.050631	4.283841
S	-1.366891	2.190191	0.334300
O	-1.767774	3.592410	0.427093
O	0.919354	-1.420338	0.993719
N	0.066594	1.823313	-0.136174
O	1.696303	1.898960	-1.622724
C	2.364181	1.898372	-2.910954
C	3.834656	1.882167	-2.518719
C	2.006314	3.172103	-3.667604
C	2.015153	0.644417	-3.705177
C	0.377735	1.855085	-1.492482
O	-0.427452	1.831922	-2.405753
C	-1.393331	3.685647	3.228967
C	-0.696874	-1.471064	-2.032890
C	-0.504461	-2.587233	-1.253256
H	-3.728608	-1.871362	-1.095885
H	-5.755276	-0.623876	-1.724080
H	-5.837308	1.861837	-1.557144
H	-3.827107	3.099135	-0.664709
H	-1.075488	1.954434	5.287997
H	-0.805080	-1.660752	2.930461
H	-0.801437	-0.531390	5.194827
H	4.472667	1.837678	-3.412783
H	4.033160	1.002722	-1.889067
H	4.088120	2.784565	-1.943492
H	2.599654	3.228120	-4.592329
H	0.940011	3.182731	-3.928609
H	2.237201	4.055976	-3.054216
H	2.223244	-0.244714	-3.092895
H	2.641538	0.607331	-4.608908
H	0.960491	0.652936	-4.010333
H	-2.357633	4.026036	2.829552
H	-0.623141	4.179166	2.621986
H	-1.296723	4.013520	4.272249
H	0.499410	-2.852769	-0.918038
H	0.166956	-0.859714	-2.303789

C	-1.567373	-3.616153	-1.063088
O	-2.620180	-3.660116	-1.658969
O	-1.207703	-4.520452	-0.149762
C	-2.142814	-5.559901	0.089867
H	-2.354610	-6.109940	-0.837970
H	-3.089607	-5.148718	0.468624
H	-1.691723	-6.224991	0.833577
H	-1.646499	-1.311332	-2.548079
C	3.166449	-0.720697	1.230268
H	3.175304	-1.389385	2.105943
C	2.873430	0.717701	1.679109
N	4.390092	-0.851173	0.476086
H	1.932472	0.754623	2.251336
H	3.689316	1.110017	2.304049
H	2.757062	1.360700	0.793484
H	4.270570	-0.877068	-0.537591
C	5.657804	-1.037057	0.948781
O	6.615944	-1.150215	0.204543
C	5.802791	-1.129376	2.456108
H	5.322575	-0.285756	2.972225
H	5.335150	-2.055153	2.826222
H	6.872517	-1.150123	2.690811

Int-3-S-NBoc

Imaginary frequencies = 0
E(MN15,DCE) = -2301.813447
$E_{Thermal\ correction}$ = 0.479417

Pd	-0.914943	0.893110	-0.611984
C	2.057478	0.927389	-0.371362
O	2.208479	0.980864	-1.586894
N	-1.508901	0.155724	1.520736
C	-2.806359	0.716797	-1.187959
C	-3.670663	1.608216	-1.835839
C	-5.004833	1.262372	-2.076272
C	-5.521211	0.022413	-1.684995
C	-4.688000	-0.893678	-1.047390
C	-3.364819	-0.513165	-0.824419
C	-1.977988	-1.081014	1.589061
C	-2.096850	-1.838488	2.756729
C	-1.703069	-1.153142	3.918451
C	-1.119456	0.787113	2.626181
C	-1.219288	0.152269	3.864980
S	-2.291841	-1.692723	-0.085580
O	-2.888563	-3.020743	-0.079816
O	0.935748	0.950559	0.269828
N	-0.930120	-1.361656	-0.856132
O	1.204798	-1.983332	-1.134678
C	2.329373	-2.914111	-1.116529
C	3.265858	-2.337976	-2.167759
C	1.822653	-4.292538	-1.526257
C	3.012290	-2.949146	0.244416
C	0.125612	-2.170229	-0.406090
O	0.008261	-2.948802	0.527952
C	-2.521294	-3.275744	2.788326
C	-0.520277	2.295976	-2.141475
C	-0.886361	2.959967	-0.961384
H	-3.317895	2.588335	-2.168544
H	-5.655608	1.977758	-2.584948
H	-6.562815	-0.231240	-1.889098
H	-5.028536	-1.887213	-0.747025
H	-1.759026	-1.676148	4.876795
H	-0.716059	1.794494	2.494343
H	-0.901847	0.667952	4.772154
H	4.175185	-2.954107	-2.234016
H	3.536390	-1.309401	-1.891059
H	2.774828	-2.313586	-3.150890
H	2.677966	-4.973018	-1.648031
H	1.150242	-4.708767	-0.764313
H	1.289035	-4.230641	-2.486471
H	3.435806	-1.969492	0.505877
H	3.849258	-3.661960	0.198567
H	2.318259	-3.271729	1.029685
H	-1.838785	-3.866520	2.160207
H	-3.529035	-3.413892	2.374770
H	-2.496724	-3.654499	3.818443
H	-1.899736	3.331462	-0.787687
H	-1.240007	2.146709	-2.948870
C	0.151502	3.608855	-0.103803
O	1.276665	3.879325	-0.442043
O	-0.348140	3.916896	1.105602
C	0.530165	4.628620	1.963693
H	-0.031620	4.852492	2.877519
H	0.864339	5.560740	1.485729
H	1.419209	4.026225	2.195437
H	0.543126	2.180252	-2.374152
C	3.270628	0.827246	0.555008
H	3.142780	-0.074648	1.175597

C	3.365542	2.020836	1.502104
N	4.446895	0.656774	-0.263925
H	2.478064	2.042748	2.151602
H	4.262259	1.909800	2.128086
H	3.416849	2.964280	0.939055
H	4.317103	0.894218	-1.247719
C	5.518181	-0.056224	0.174634
O	5.599613	-0.471884	1.322028
C	6.575434	-0.343247	-0.869872
H	6.615975	0.427483	-1.651638
H	7.549923	-0.434280	-0.375910
H	6.342426	-1.308443	-1.346604

Int-3-S-Pyr

Imaginary frequencies = 0
E(MN15,DCE) = -2301.802581
$E_{\text{Thermal correction}}$ = 0.477689

Pd	-1.347972	1.531763	0.149641
C	-2.852709	-0.873168	0.576236
O	-1.999063	-1.393047	-0.128405
N	-0.163145	0.715000	1.688333
C	0.127886	2.825716	-0.272697
C	-0.041583	4.213193	-0.402174
C	1.045295	5.057605	-0.651944
C	2.339876	4.548493	-0.785013
C	2.552149	3.178573	-0.651064
C	1.445791	2.365245	-0.396535
C	1.136302	0.424803	1.533009
C	1.960146	0.034860	2.598995
C	1.309045	-0.108783	3.837645
C	-0.768105	0.561504	2.870718
C	-0.050171	0.130349	3.982281
S	1.637041	0.621874	-0.221079
O	0.619024	-0.071816	-1.002206
O	-2.905753	0.389112	0.868278
N	3.148776	0.356950	-0.452478
O	4.794921	-1.093048	-0.811021
C	5.458724	-2.381351	-0.837387
C	6.852915	-2.039974	-1.346051
C	4.747736	-3.318611	-1.807219
C	5.536309	-2.968022	0.569474
C	3.534962	-0.970407	-0.399971
O	2.839216	-1.887028	0.003408
C	3.438419	-0.227355	2.537637
C	-2.196883	1.944508	-1.799980
C	-2.923339	2.639802	-0.856552
H	-1.030235	4.665107	-0.295182
H	0.875120	6.133128	-0.743685
H	3.178788	5.215687	-0.991077
H	3.538746	2.722326	-0.747965
H	1.903936	-0.417358	4.701227
H	-1.837555	0.781686	2.896649
H	-0.551023	0.006404	4.942901
H	7.461204	-2.952287	-1.426937
H	7.350050	-1.341015	-0.657814
H	6.789027	-1.566479	-2.336078
H	5.322118	-4.252253	-1.901003
H	3.736720	-3.556145	-1.453787
H	4.681676	-2.852207	-2.801452
H	5.955732	-2.222719	1.263741
H	6.202297	-3.843659	0.564251
H	4.545328	-3.279942	0.922678
H	3.954708	0.458445	1.855777
H	3.627201	-1.251307	2.183749
H	3.867533	-0.127303	3.543397
H	-3.827873	2.174306	-0.455030
H	-1.401036	2.407013	-2.389365
C	-2.677373	0.595804	-2.259211
O	-3.780878	0.164306	-2.011000
O	-1.754759	-0.020133	-2.974061
C	-2.006443	-1.381550	-3.307529
H	-1.189078	-1.696841	-3.963683
H	-2.974480	-1.477937	-3.820569
H	-2.011201	-1.979465	-2.385508
H	-2.757022	3.701953	-0.676238
C	-3.987858	-1.705011	1.197458
H	-4.909053	-1.371615	0.691814
C	-4.120983	-1.413088	2.688150
N	-3.807354	-3.118315	0.970850
H	-4.311516	-0.344397	2.849047
H	-4.940949	-2.000148	3.124519
H	-3.189017	-1.680633	3.215233
H	-3.108348	-3.578262	1.552809
C	-3.947168	-3.750134	-0.246101
O	-3.454519	-4.844855	-0.446062
C	-4.788017	-3.036124	-1.278944
H	-5.798825	-2.838537	-0.889464

H	-4.344639	-2.068148	-1.556254
H	-4.857241	-3.683104	-2.160699

Int-4-R

Imaginary frequencies = 0
E(MN15,DCE) = -2301.831898
$E_{Thermal\ correction}$ = 0.480025

Pd	0.149722	0.254788	-0.378175
C	-2.469200	-0.041742	0.572401
O	-2.241662	-1.256630	0.506623
N	0.937029	-0.806973	1.387001
C	2.267407	-0.726673	1.446842
C	3.062607	-1.295086	2.444100
C	2.337465	-1.959622	3.449333
C	0.266953	-1.461506	2.336966
C	0.950661	-2.047208	3.404065
S	2.947159	0.106855	-0.026855
O	4.378910	-0.117510	-0.129888
O	-1.610486	0.888592	0.366064
N	1.952520	-0.383373	-1.178536
O	0.950485	-2.104604	-2.171838
C	0.306075	-3.413932	-2.113936
C	-0.948504	-3.205568	-2.948375
C	-0.073091	-3.727122	-0.669945
C	1.229288	-4.459744	-2.722189
C	1.927028	-1.782460	-1.345581
O	2.675970	-2.543145	-0.766314
C	4.564337	-1.283724	2.463389
C	1.333847	2.212572	-2.082426
C	-0.003620	1.467517	-1.986834
H	2.890327	-2.427245	4.268235
H	-0.815851	-1.522876	2.202773
H	0.396357	-2.578034	4.178937
H	-1.528619	-4.138248	-2.996690
H	-0.682886	-2.899001	-3.970332
H	-1.568729	-2.420547	-2.489443
H	-0.694553	-4.634673	-0.654609
H	0.815793	-3.905890	-0.049233
H	-0.665690	-2.896134	-0.252275
H	1.498903	-4.178760	-3.751010
H	0.714268	-5.431370	-2.751895
H	2.145288	-4.560102	-2.125282
H	4.981690	-0.273992	2.350162
H	4.952704	-1.869445	1.618223
H	4.927855	-1.717753	3.403870
H	-0.168082	0.794360	-2.840924
H	2.055469	1.574546	-2.607442
C	-1.147997	2.403218	-1.820124
O	-1.050660	3.545111	-1.415992
O	-2.323289	1.872618	-2.184110
C	-3.449483	2.695115	-1.940691
H	-3.491482	2.981745	-0.878976
H	-4.337092	2.112972	-2.214188
H	-3.399856	3.616611	-2.539467
H	1.196955	3.127051	-2.681861
C	2.587905	1.833656	0.179723
C	3.138942	2.325745	1.369696
C	1.920624	2.655944	-0.753817
C	2.997603	3.670449	1.692700
C	1.802500	4.004913	-0.387622
C	2.319465	4.507236	0.805375
H	3.411216	4.056962	2.625415
H	1.252525	4.659585	-1.065305
H	2.187319	5.564450	1.043995
H	3.669212	1.648866	2.045950
C	-3.862100	0.459241	0.946743
H	-4.276853	0.953215	0.049867
C	-3.809361	1.494591	2.066708
N	-4.688089	-0.683041	1.265588
H	-3.184595	2.344857	1.760824
H	-4.828972	1.841956	2.279778
H	-3.380909	1.053151	2.979761
H	-4.205951	-1.580379	1.245325
C	-6.044466	-0.595420	1.237915
O	-6.628424	0.460991	1.046707
C	-6.790355	-1.892352	1.474471
H	-6.128760	-2.760512	1.594354
H	-7.410225	-1.780517	2.374798
H	-7.472652	-2.062631	0.630662

Int-4-S

Imaginary frequencies = 0
E(MN15,DCE) = -2301.835162
$E_{Thermal\ correction}$ = 0.479081

Pd	0.144275	-0.411404	-0.214435
C	-2.471755	-0.566221	0.722943
O	-2.403063	0.668670	0.784087
N	0.859808	0.557013	1.620625
C	2.192460	0.619623	1.638733
C	2.953022	1.135247	2.690897
C	2.192278	1.568860	3.792150
C	0.152015	0.992857	2.663137
C	0.803245	1.502925	3.787890
S	2.906865	0.090582	0.041599
O	4.285777	0.536896	-0.061087
O	-1.492785	-1.354759	0.467349
N	1.795254	0.563587	-0.999609
O	0.474166	2.216364	-1.677956
C	-0.320675	3.416540	-1.447451
C	-1.600620	3.104189	-2.206680
C	-0.617673	3.550268	0.042427
C	0.408172	4.624316	-2.017635
C	1.559167	1.955182	-0.980133
O	2.242603	2.744915	-0.360560
C	4.446330	1.297559	2.684028
C	1.470524	-1.966349	-2.226874
C	0.044273	-1.588825	-1.837550
H	2.717984	1.980298	4.657779
H	-0.935207	0.940037	2.558513
H	0.222359	1.855937	4.640777
H	-2.306941	3.943063	-2.126763
H	-1.373267	2.921972	-3.267468
H	-2.059897	2.200045	-1.775655
H	-1.338347	4.368320	0.189536
H	0.290636	3.780415	0.615999
H	-1.074689	2.616155	0.407986
H	0.627477	4.468307	-3.084094
H	-0.227473	5.516865	-1.919960
H	1.349136	4.796784	-1.478537
H	4.973501	0.375753	2.403835
H	4.736306	2.050553	1.937674
H	4.790433	1.618782	3.675733
H	-0.558899	-2.440949	-1.491995
H	1.942927	-1.101543	-2.709510
C	-0.679285	-0.833843	-2.895038
O	-0.177161	-0.308200	-3.864818
O	-2.007896	-0.800417	-2.664725
C	-2.790030	-0.184212	-3.668576
H	-2.654543	-0.692147	-4.635187
H	-3.835637	-0.260479	-3.346862
H	-2.511241	0.870317	-3.798515
H	1.451962	-2.778290	-2.973488
C	2.835360	-1.686399	-0.006557
C	3.540633	-2.248545	1.063808
C	2.273908	-2.465694	-1.044046
C	3.673158	-3.629459	1.165589
C	2.446562	-3.851159	-0.907057
C	3.119888	-4.431067	0.167958
H	4.207212	-4.069082	2.009199
H	2.022601	-4.491979	-1.684144
H	3.212345	-5.517588	0.223077
H	3.979957	-1.597732	1.825194
C	-3.804516	-1.276253	0.940906
H	-3.666416	-2.034528	1.730368
C	-4.240116	-1.993228	-0.337205
N	-4.770836	-0.300190	1.389136
H	-3.469790	-2.709613	-0.652736
H	-5.183945	-2.521193	-0.145143
H	-4.386777	-1.262765	-1.146776
H	-4.481869	0.671631	1.291710
C	-5.929413	-0.667373	1.994055
O	-6.233574	-1.837357	2.174356
C	-6.832864	0.471029	2.422948
H	-6.381141	1.462431	2.284594
H	-7.765450	0.415134	1.844015
H	-7.098184	0.328783	3.479022

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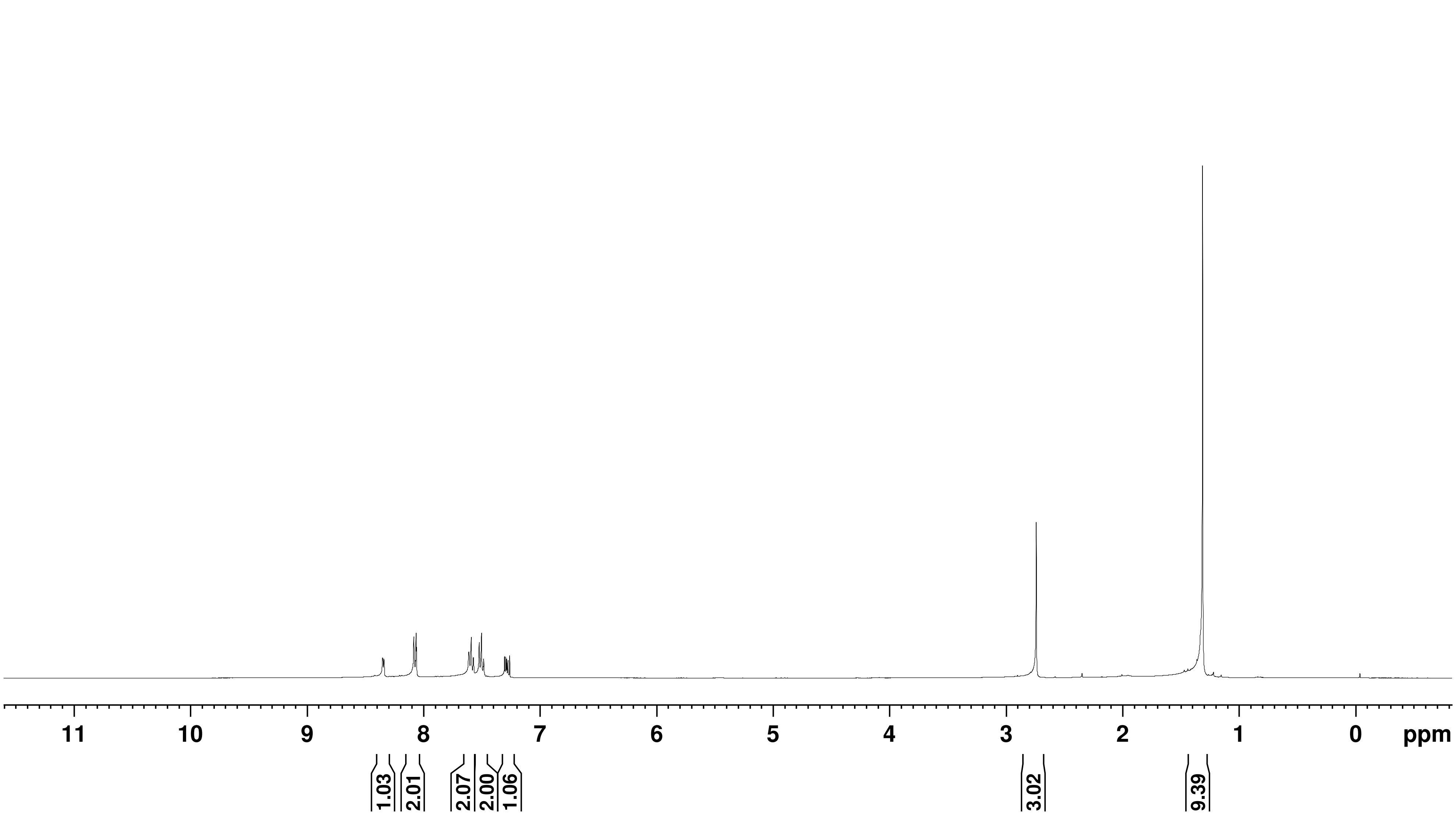
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2.740
1.312
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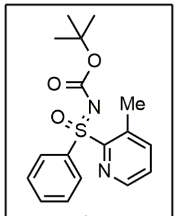
1.03 2.01 2.07 2.00 1.06 3.02 9.39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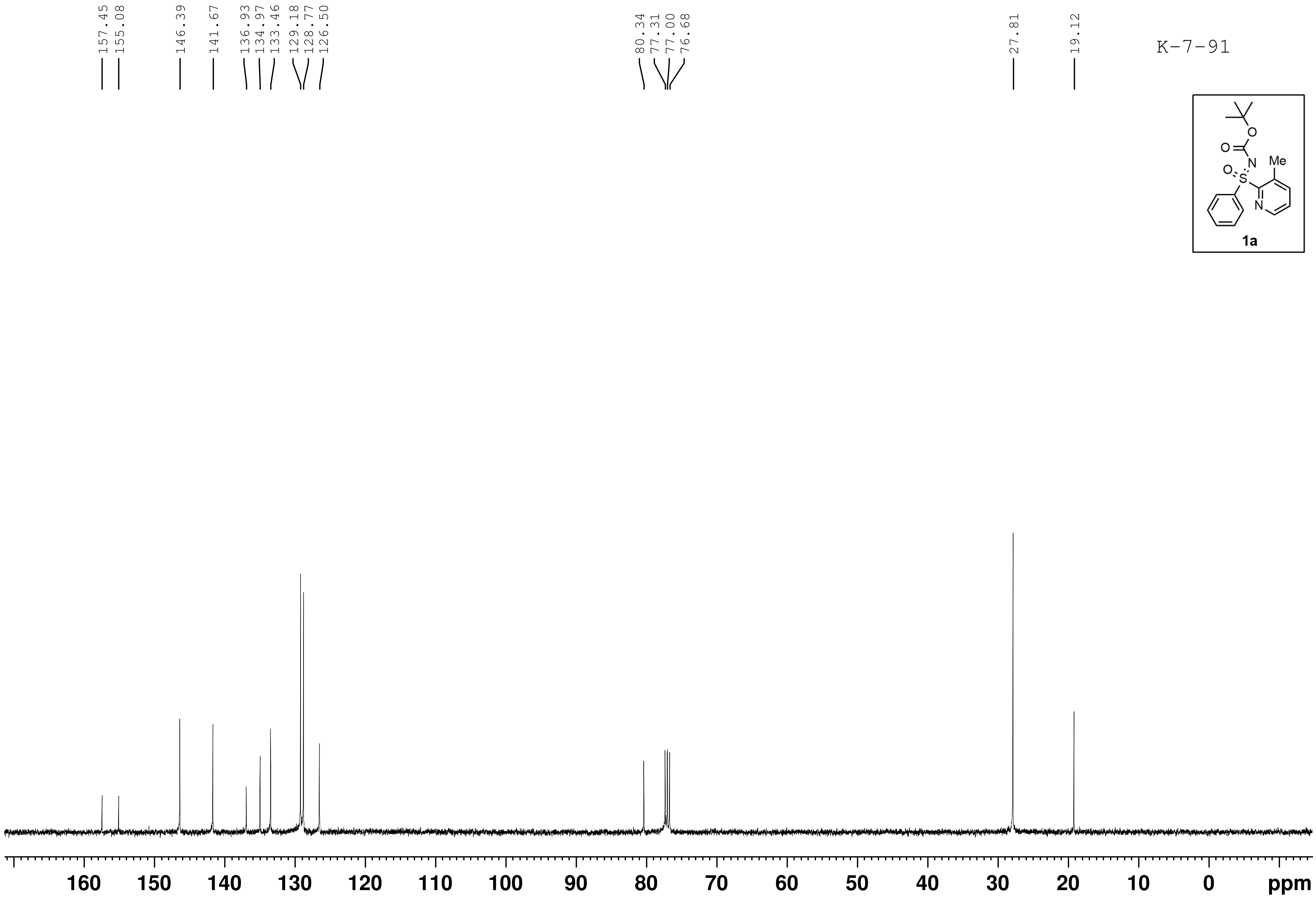
O
N
Me
O
S
N

1a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155.08
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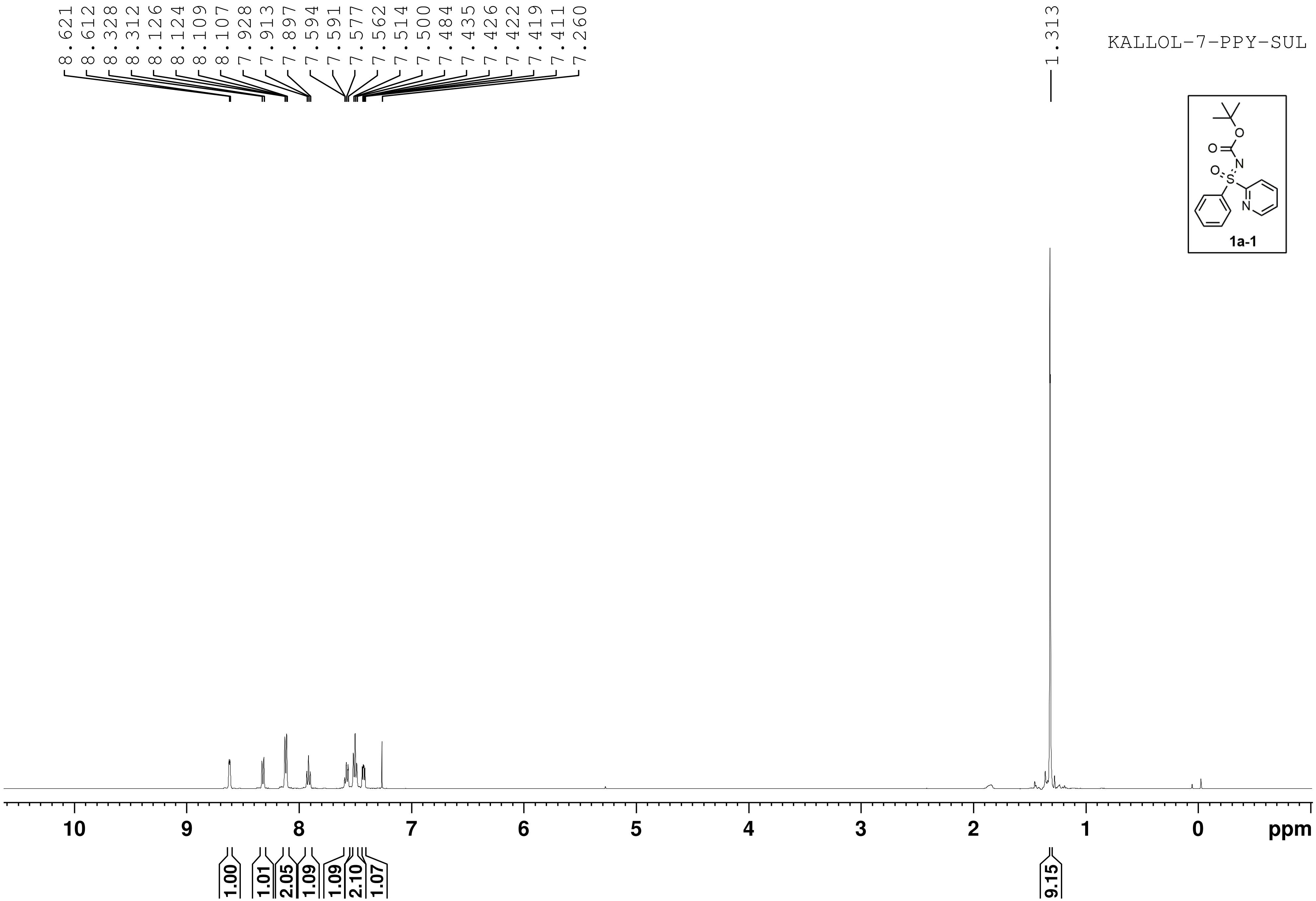
141.67
136.93
134.97
133.46
129.18
128.77
126.50
80.34
77.31
77.00
76.68
27.81
19.12
K-7-91
O
O
N
Me
O
S
N
1a
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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1.313
KALLOL-7-PPY-SUL
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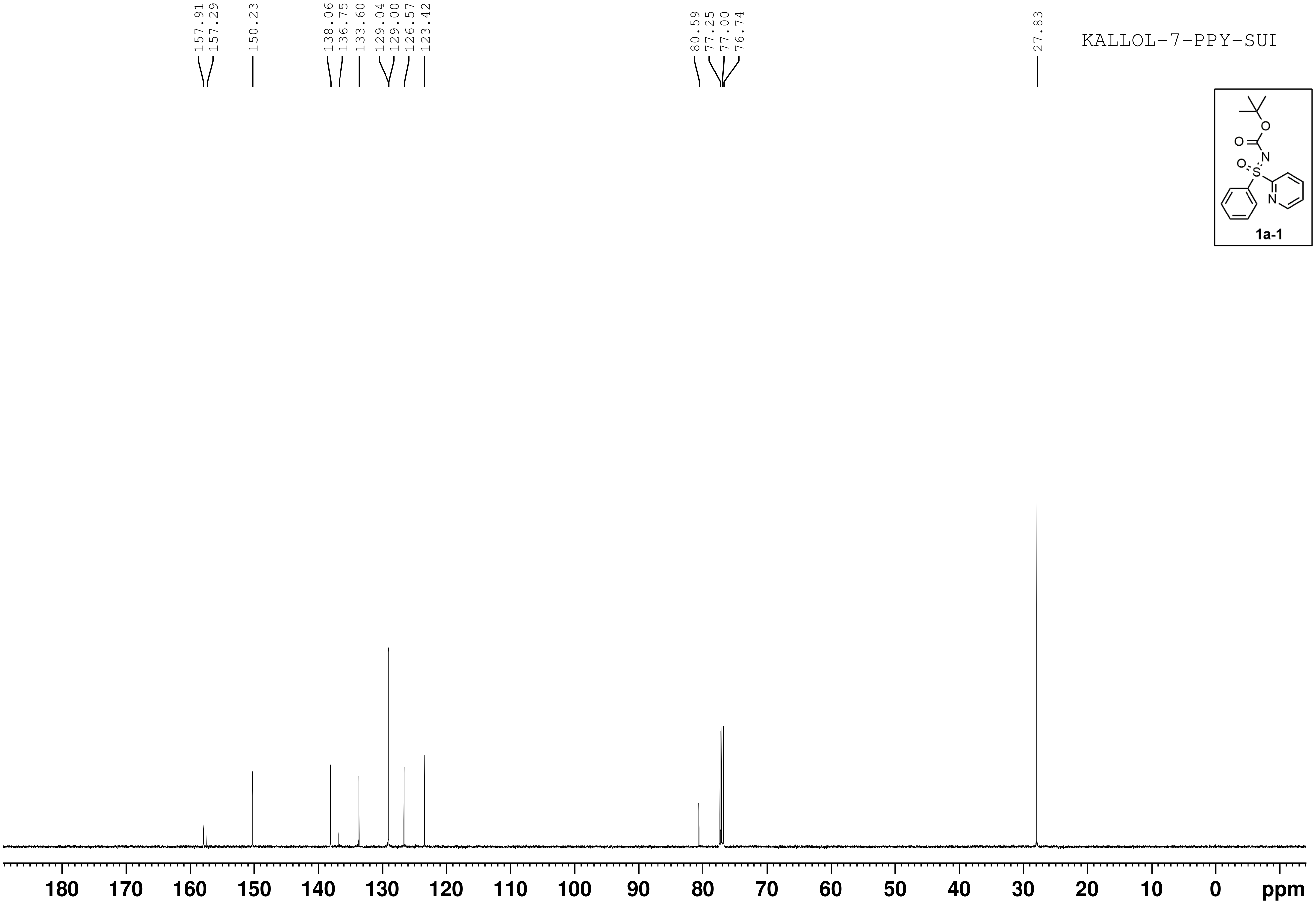
1.00 1.01 2.05 1.09 1.09 2.10 1.07
9.15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136.75
133.60
129.04
129.00
126.57
123.42
80.59
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77.00
76.74
27.83
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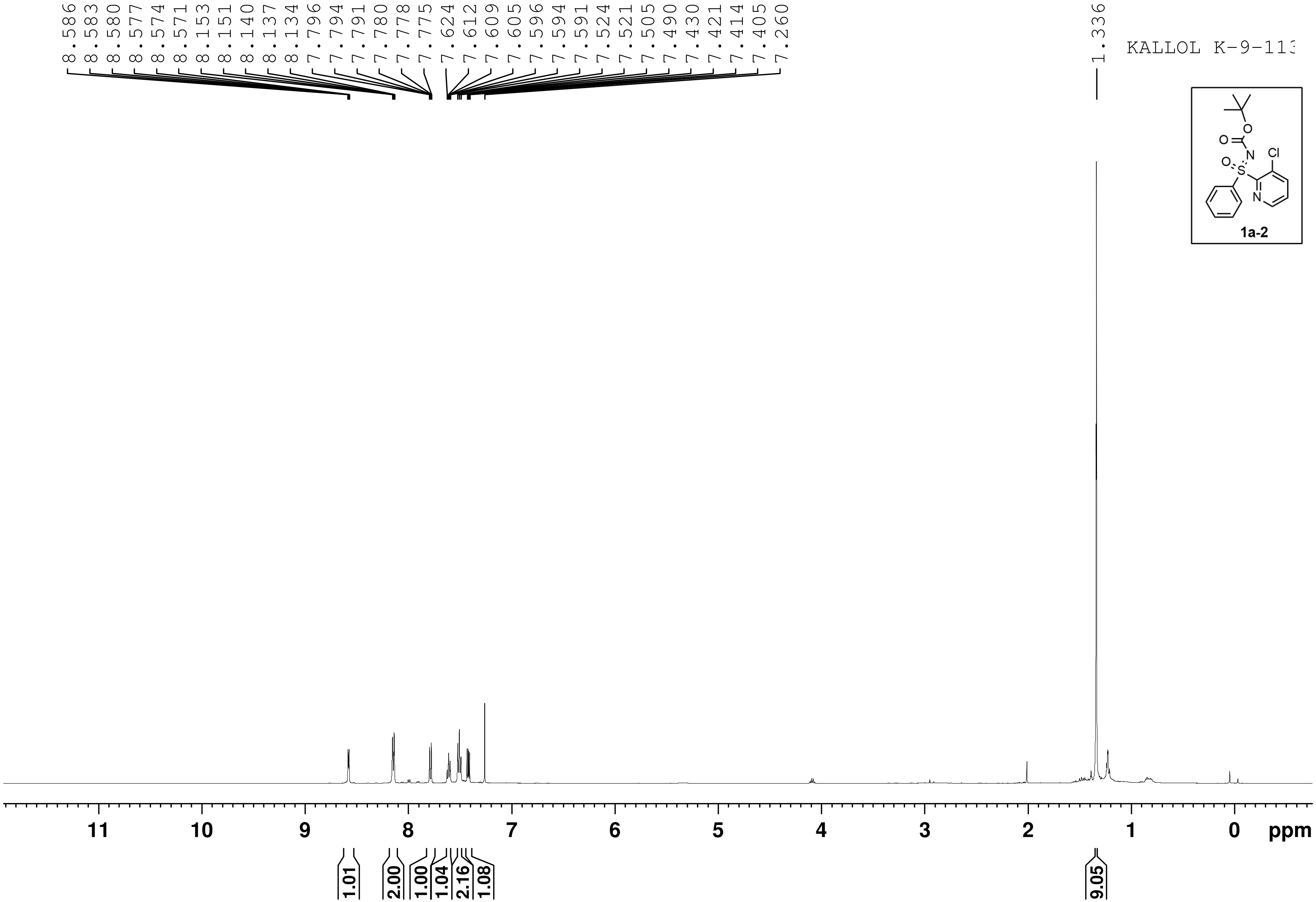
1a-1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8.583
8.580
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8.151
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8.134
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7.794
7.791
7.780
7.778
7.775
7.624
7.612
7.609
7.605
7.596
7.594
7.591
7.524
7.521
7.505
7.490
7.430
7.421
7.414
7.405
7.260
1.336
KALLOL K-9-113
O
O
N
Cl
O
S
N
1a-2
11
10
9
8
7
6
5
4
3
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1
0
ppm
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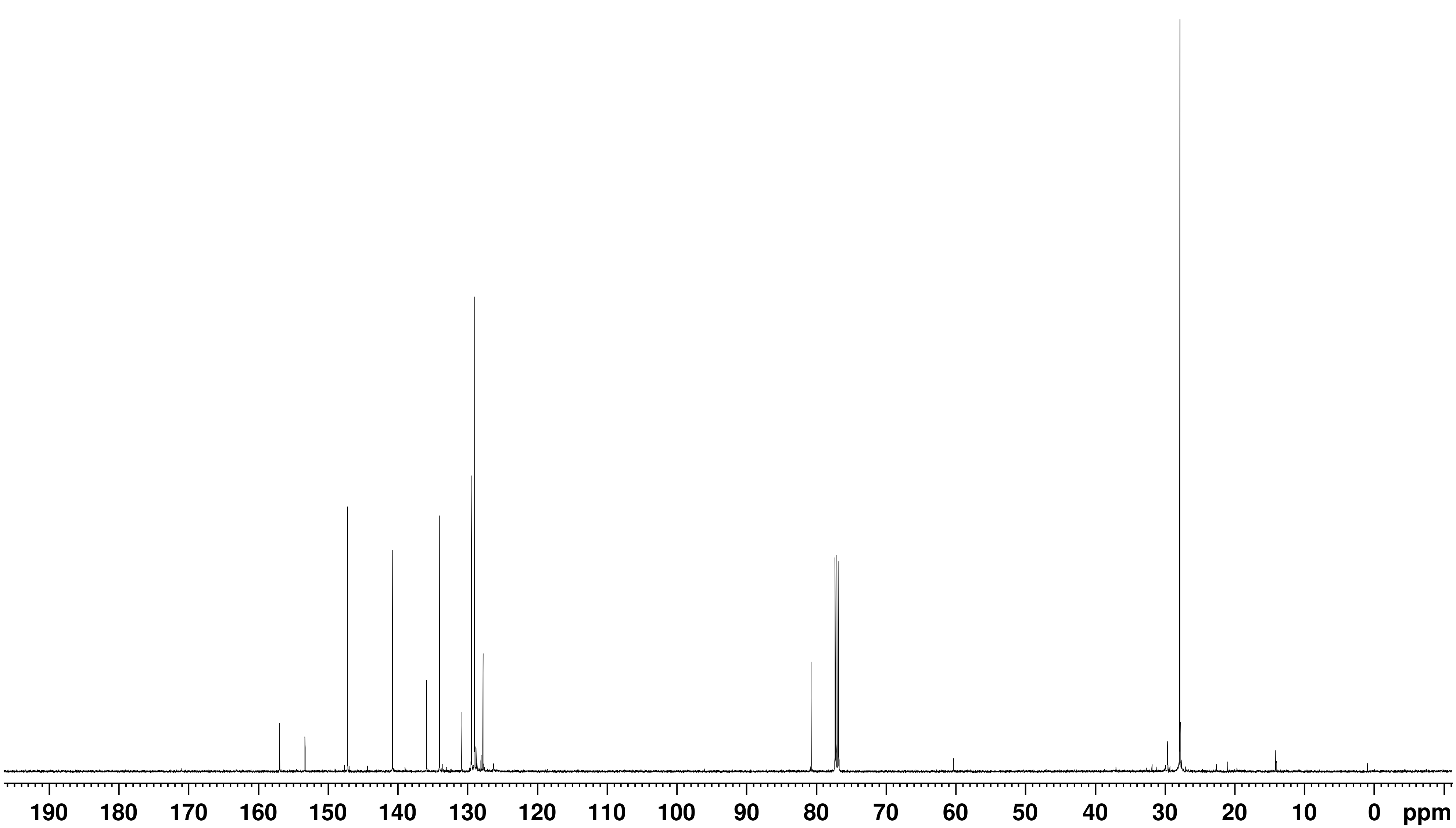
2.00
1.00
1.04
2.16
1.08
9.05

K 9-113



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153.30
147.19
140.73
135.85
134.00
130.80
129.39
128.96
127.75
80.72
77.25
77.00
76.74
27.82
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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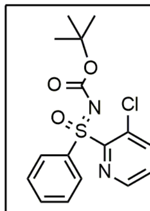
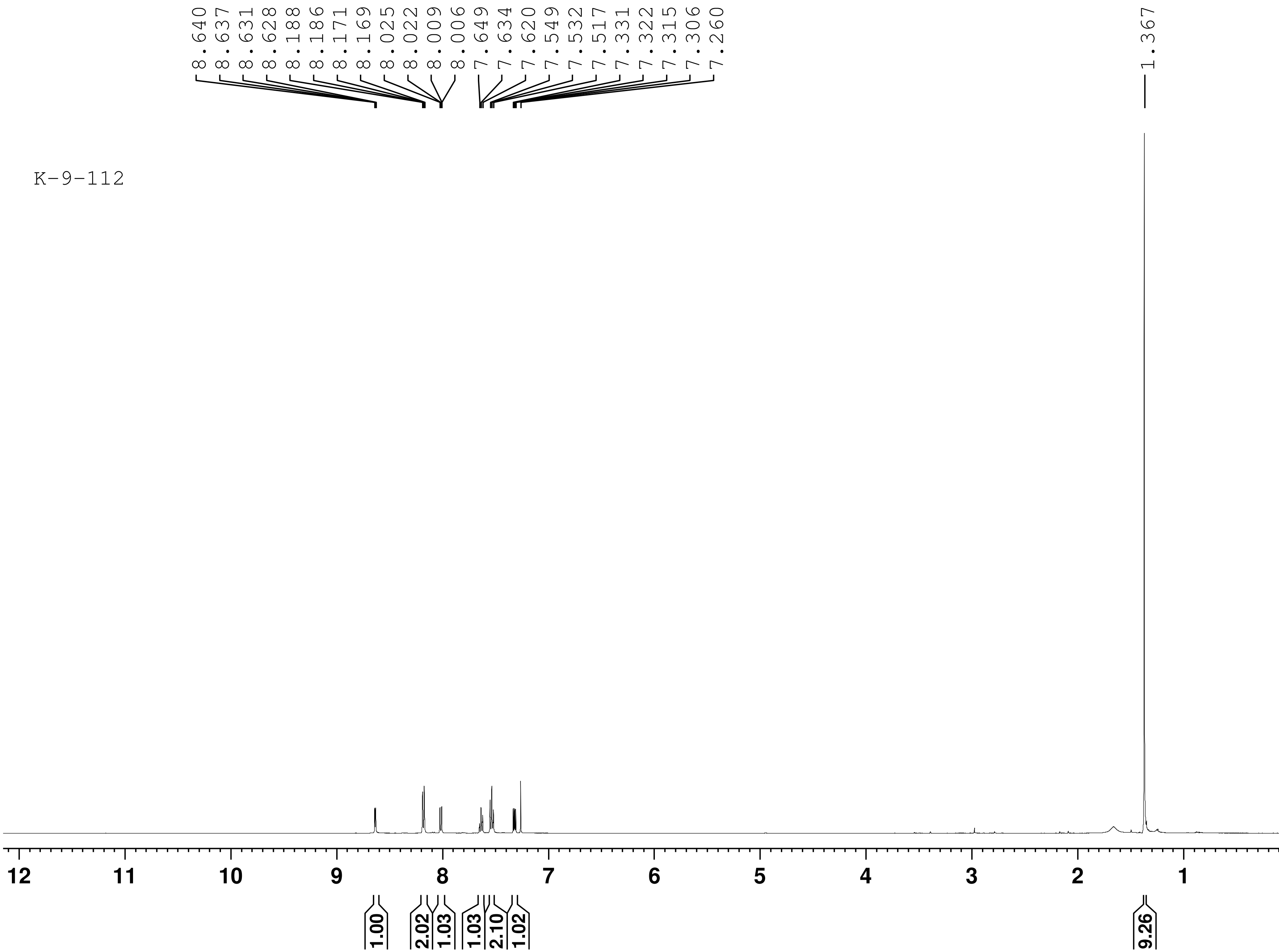
30
20
10
0
ppm



O
O
N
Cl
O
S
O
N

1a-2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8.637
8.631
8.628
8.188
8.186
8.171
8.169
8.025
8.022
8.009
8.006
7.649
7.634
7.620
7.549
7.532
7.517
7.331
7.322
7.315
7.306
7.260
1.367
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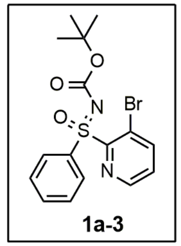
1.00
2.02
1.03
1.03
2.10
1.02
9.26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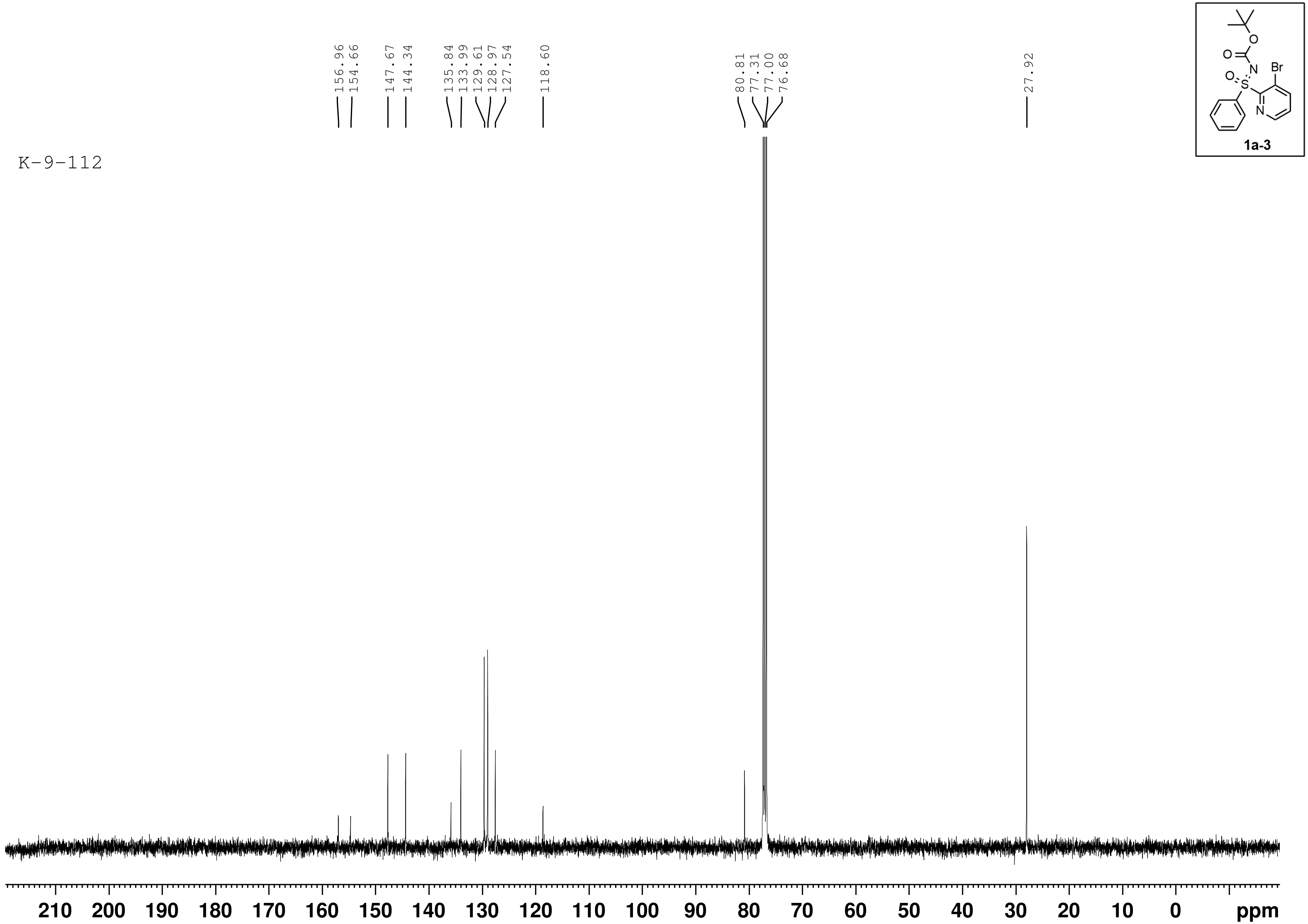
Br
O
S
N
1a-3


K-9-112
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154.66
147.67
144.34
135.84
133.99
129.61
128.97
127.54
118.60
80.81
77.31
77.00
76.68
27.92
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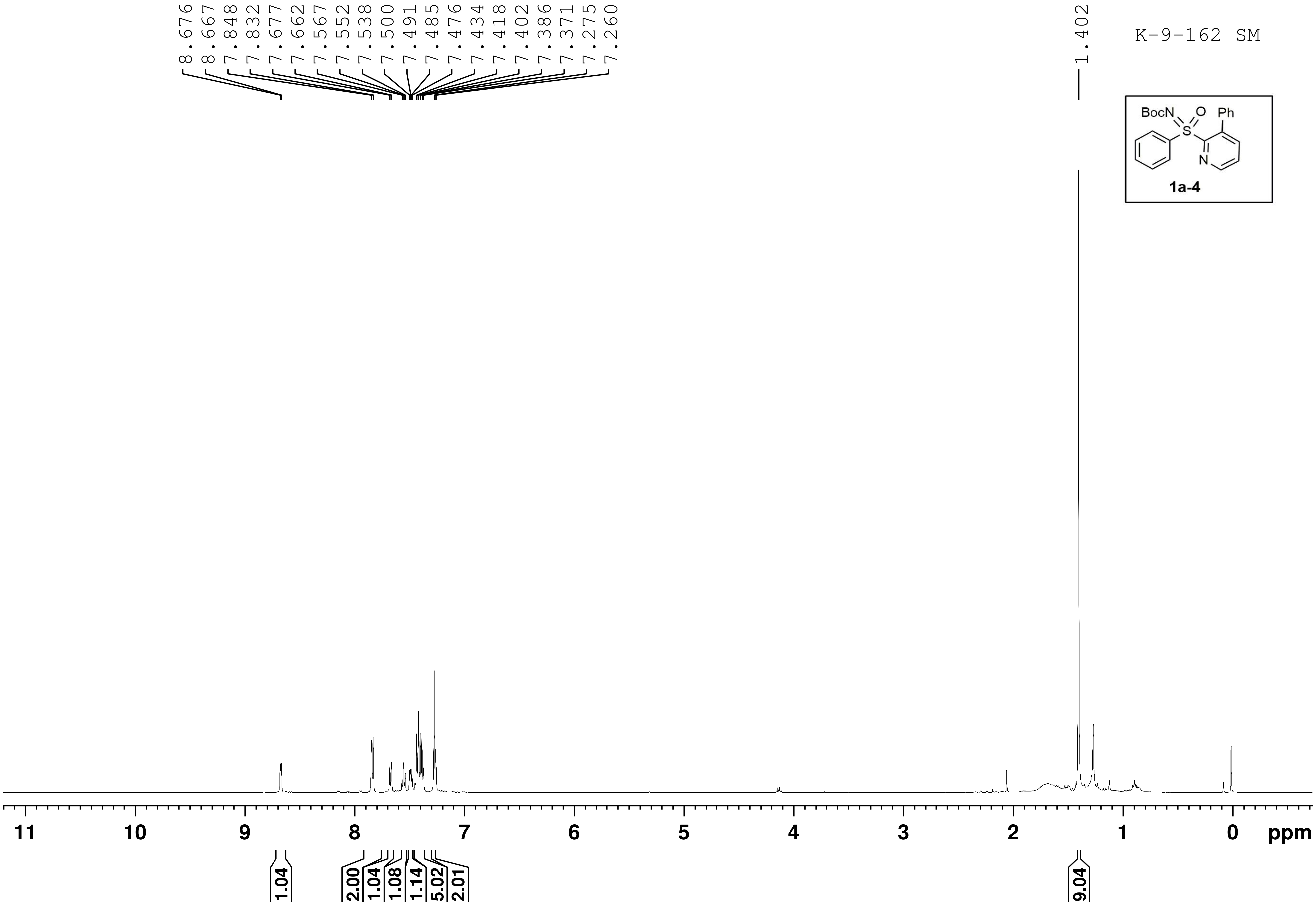
O
O
N
Br
O
S
N
1a-3



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8.667
7.848
7.832
7.677
7.662
7.567
7.552
7.538
7.500
7.491
7.485
7.476
7.434
7.418
7.402
7.386
7.371
7.275
7.260
1.402
K-9-162 SM
BocN
O
S
Ph
N
1a-4
11
10
9
8
7
6
5
4
3
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1
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ppm
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2.00
1.04
1.08
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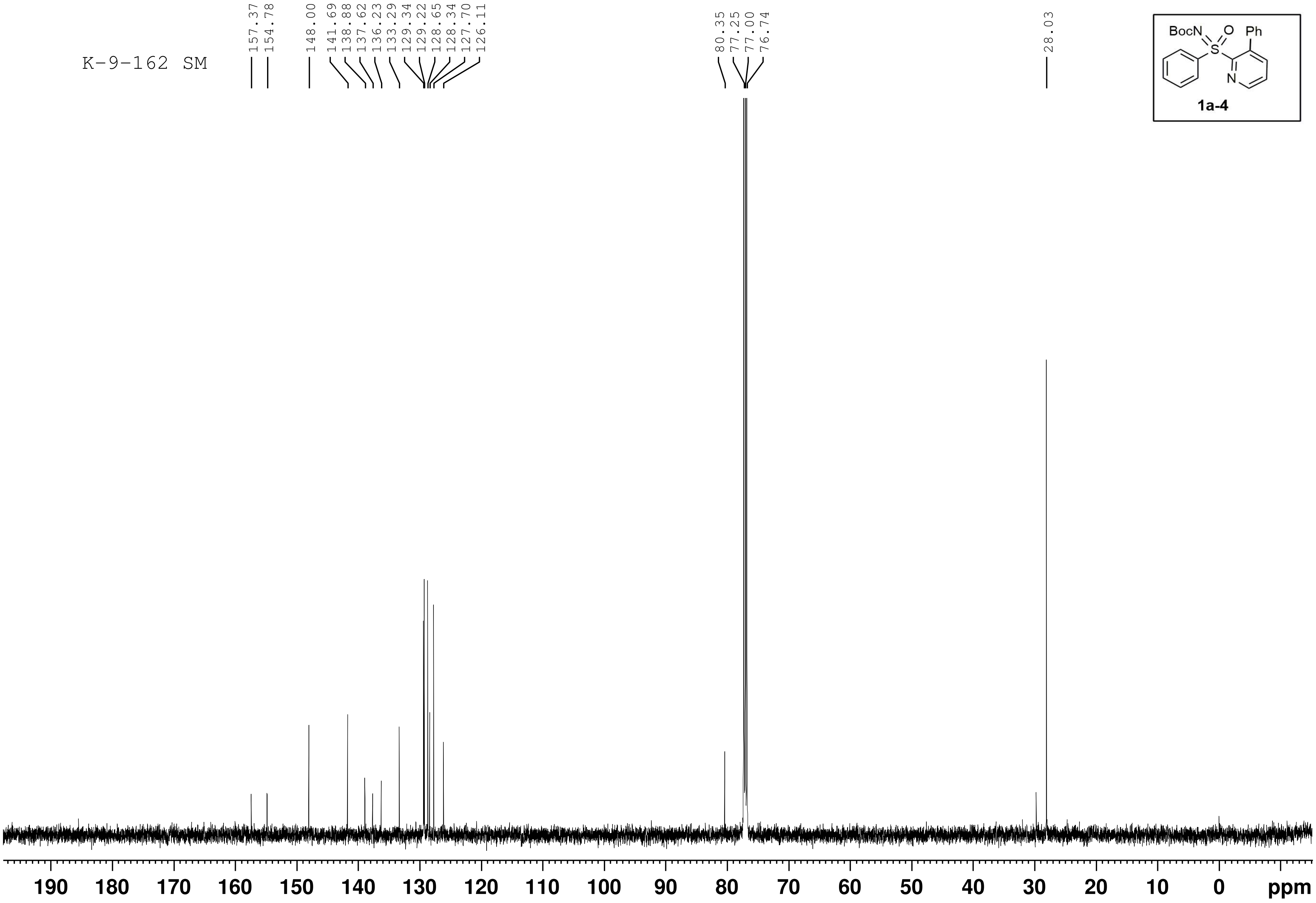
5.02
2.01
9.04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136.23
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129.34
129.22
128.65
128.34
127.70
126.11
80.35
77.25
77.00
76.74
28.03
BocN
O
Ph
S
N
1a-4
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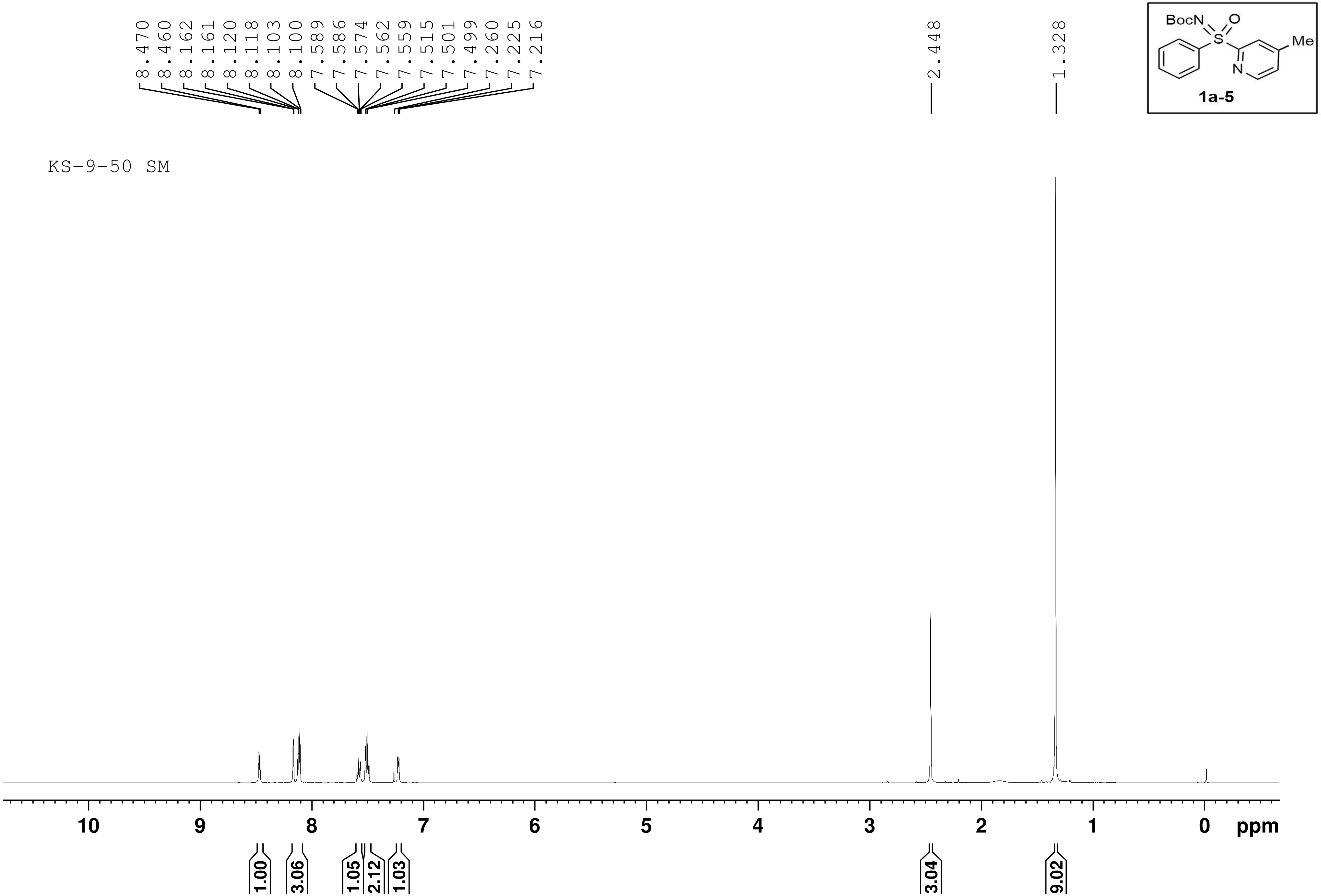
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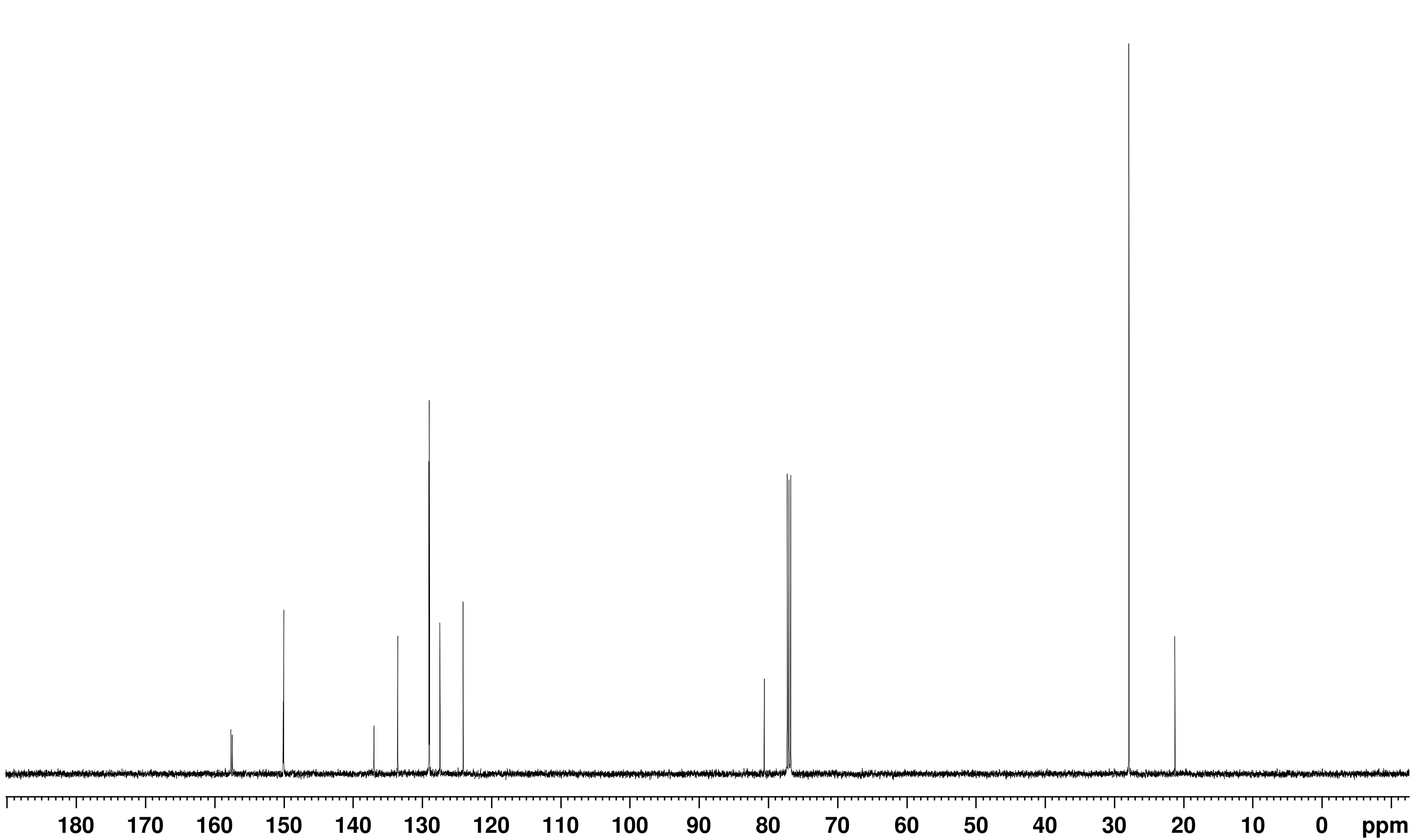
8.460
8.162
8.161
8.120
8.118
8.103
8.100
7.589
7.586
7.574
7.562
7.559
7.515
7.501
7.499
7.260
7.225
7.216
2.448
1.328
KS-9-50 SM
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
3.06
1.05
2.12
1.03
3.04
9.02
BocN
S
O
N
Me

1a-5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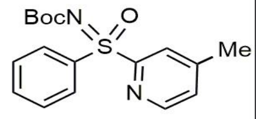
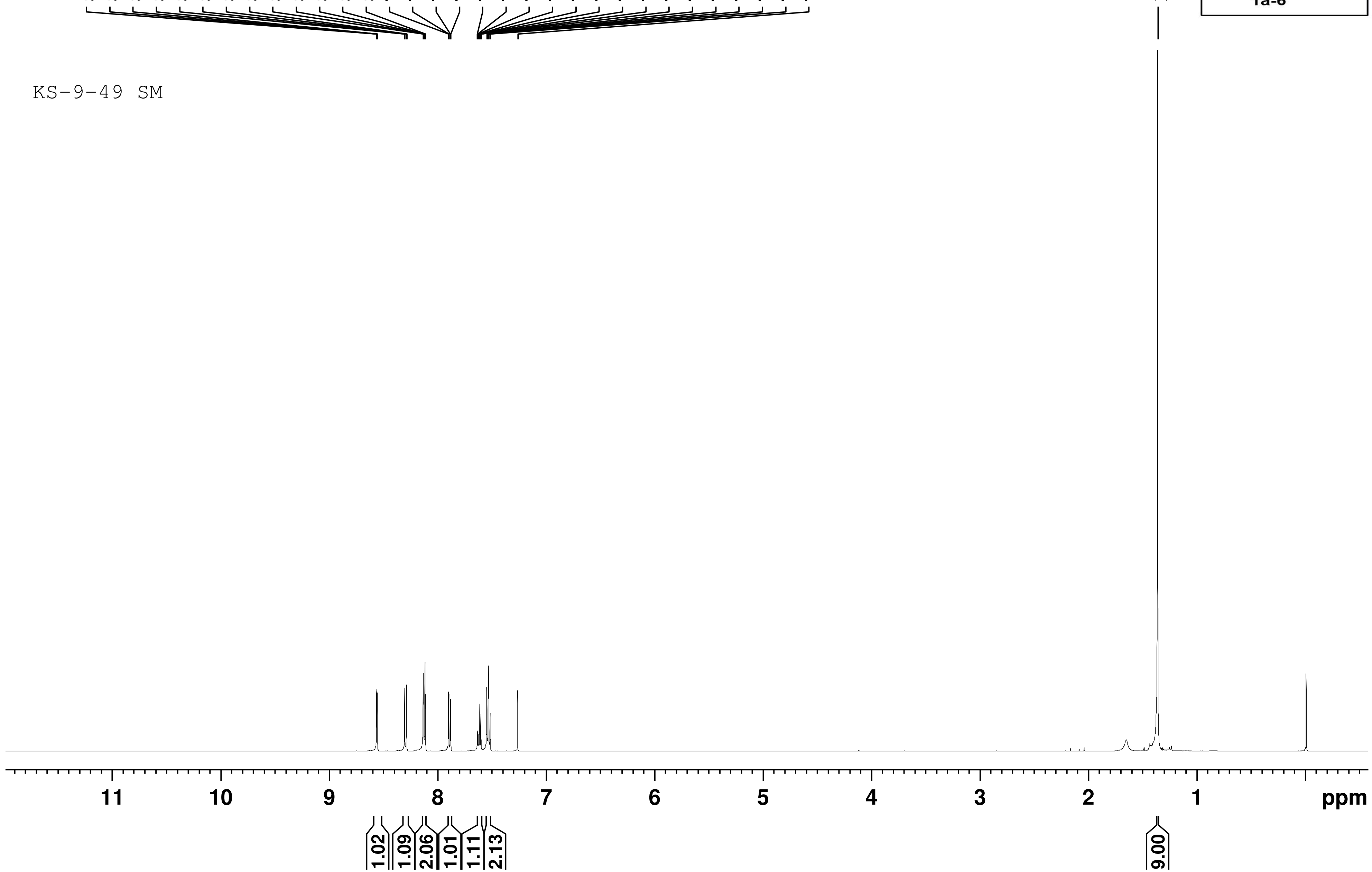
129.03
128.96
127.44
124.10
80.56
77.25
77.00
76.75
27.87
21.22
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


BocN
O
S
N
Me

1a-5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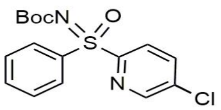
1.361
KS-9-49 SM
11 10 9 8 7 6 5 4 3 2 1 ppm
1.02 1.09 2.06 1.01 1.11 2.13
9.00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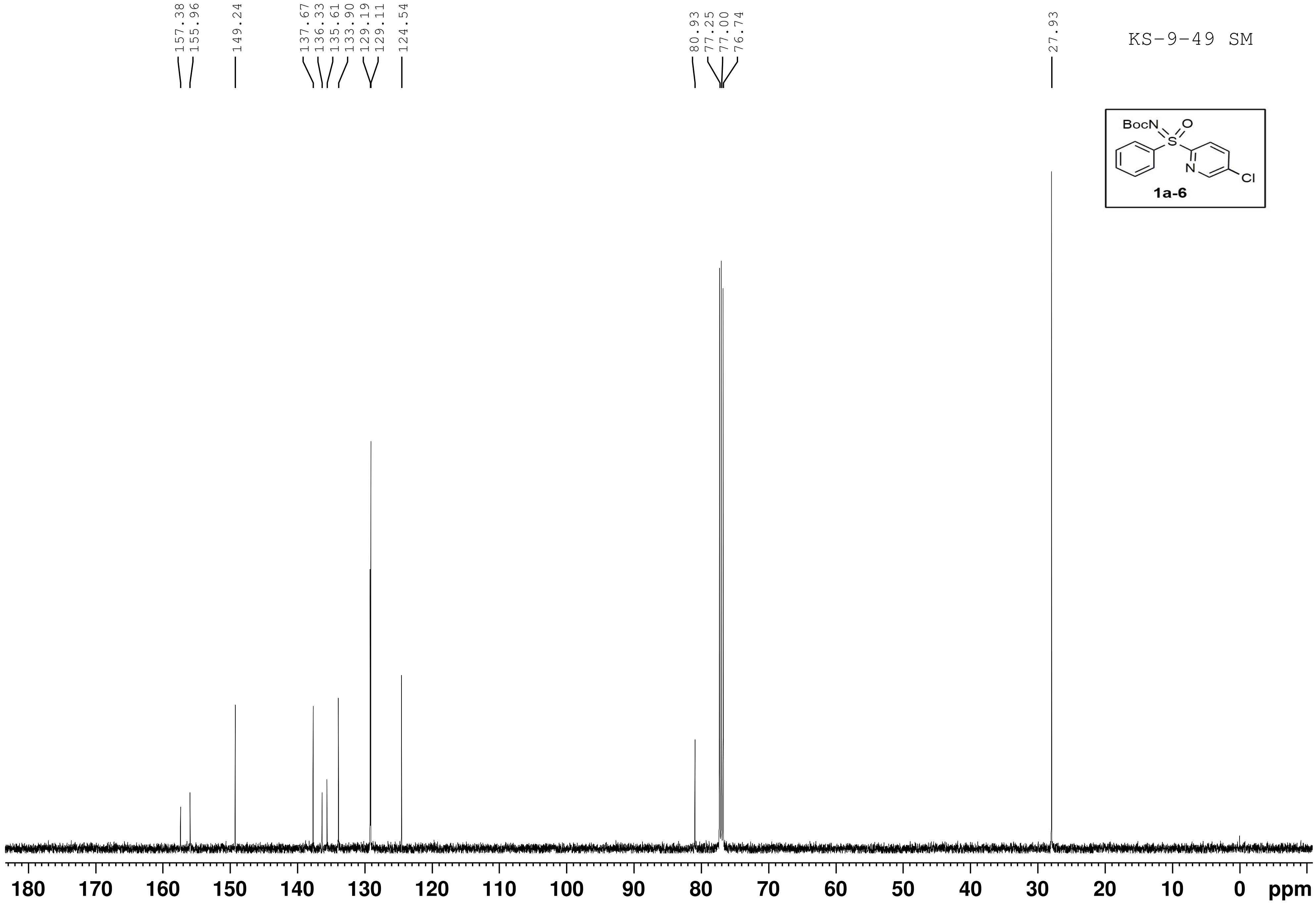
O
S
N
Cl
1a-6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149.24
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136.33
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129.19
129.11
124.54
80.93
77.25
77.00
76.74
27.93
KS-9-49 SM
BocN
O
S
N
Cl
1a-6
180
170
160
150
140
130
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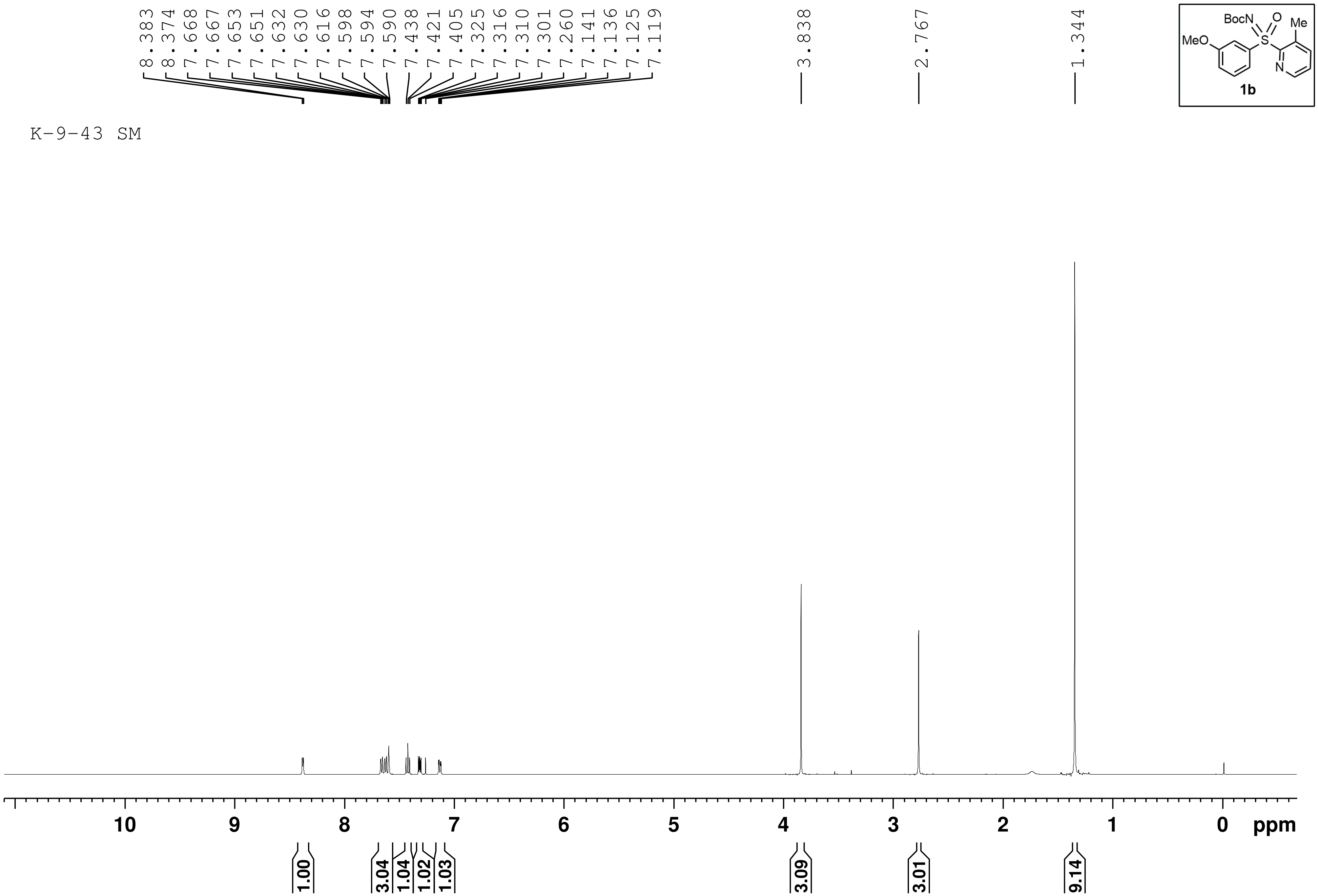
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.667
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7.630
7.616
7.598
7.594
7.590
7.438
7.421
7.405
7.325
7.316
7.310
7.301
7.260
7.141
7.136
7.125
7.119
3.838
2.767
1.344
BocN
O
S
Me
MeO
N
1b
10
9
8
7
6
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4
3
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0
ppm
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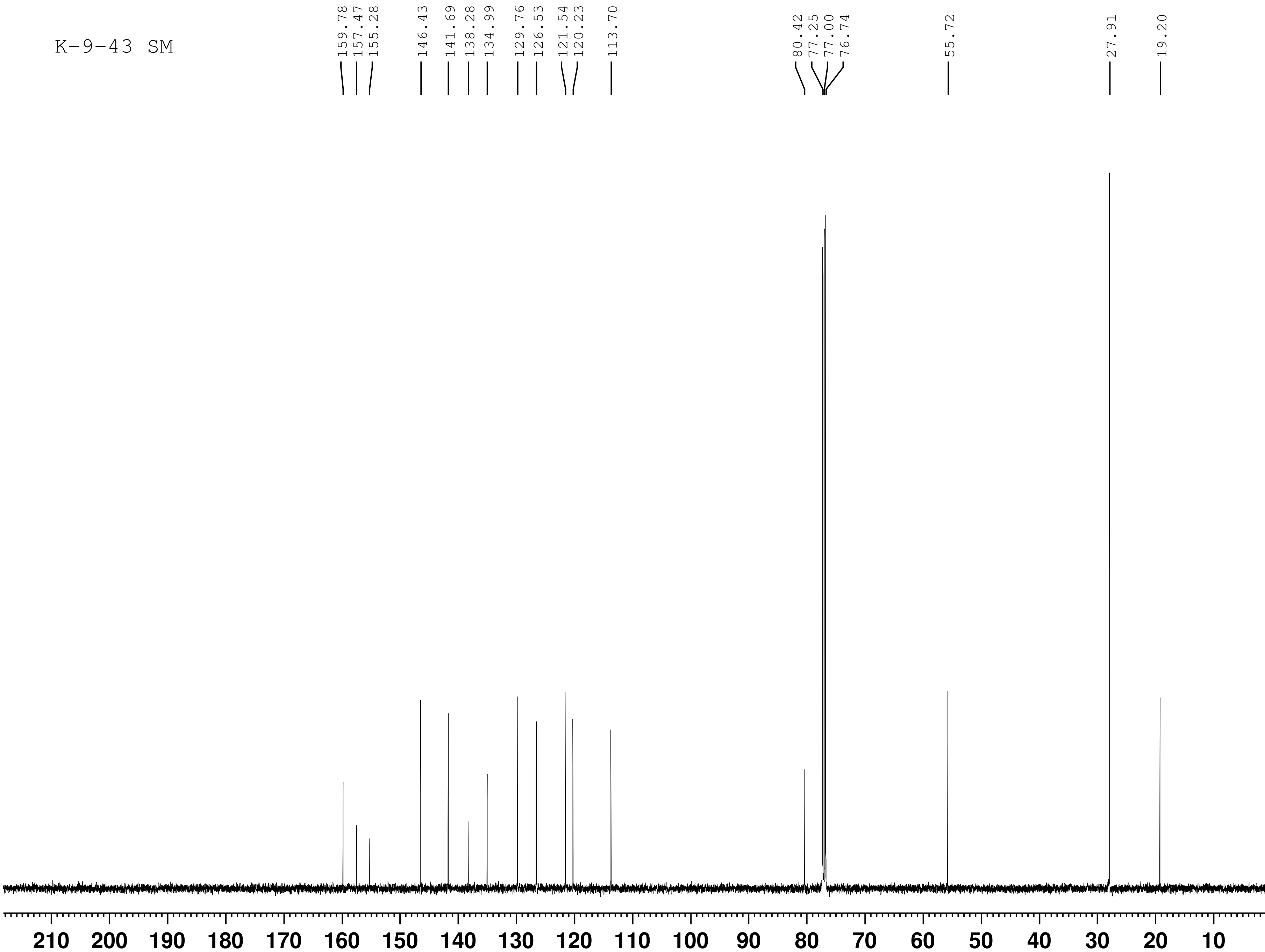
1.04
1.02
1.03
3.09
3.01
9.14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120.23
113.70
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77.00
76.74
55.72
27.91
19.20
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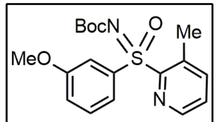
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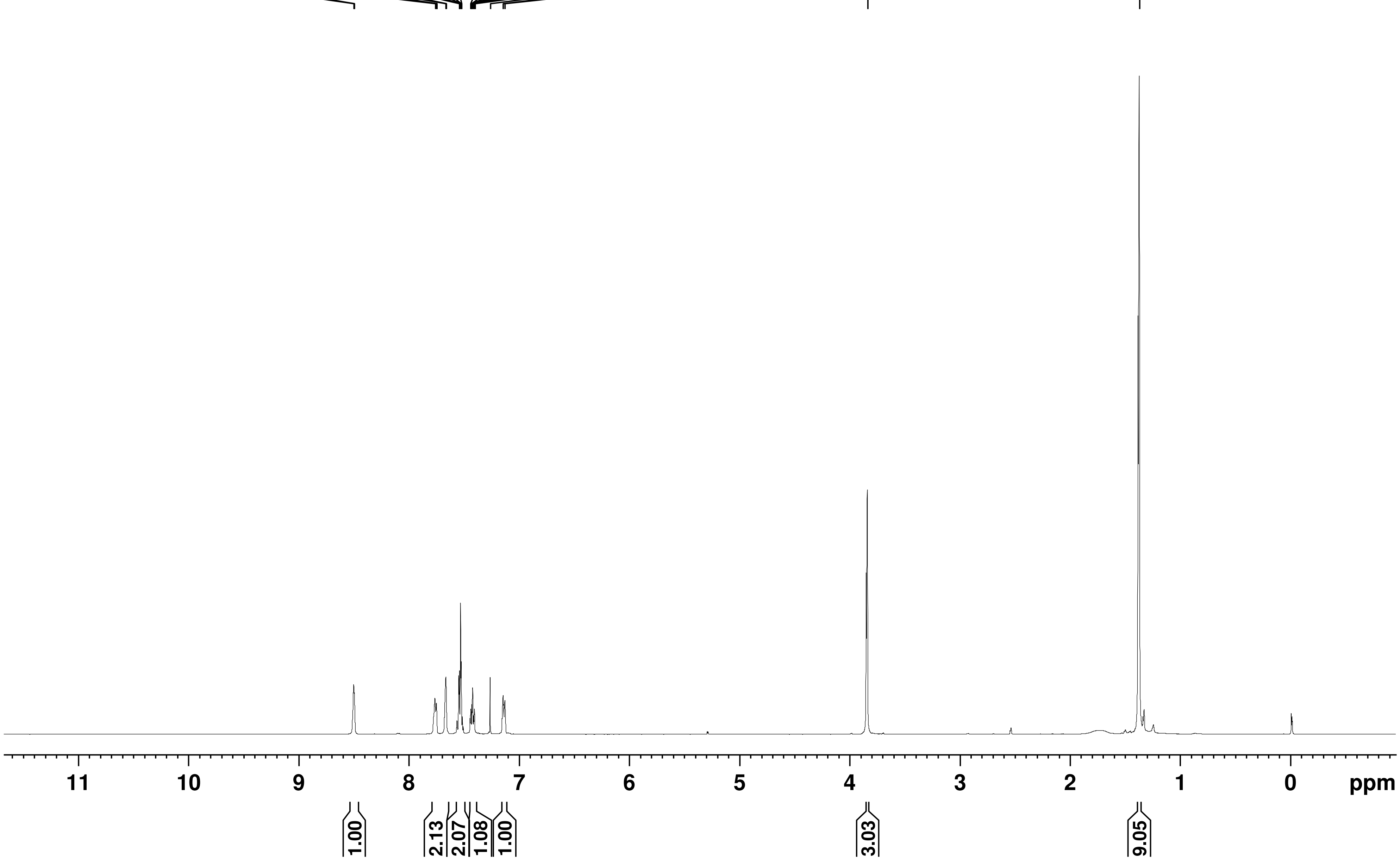
S
N

1b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7.434
7.432
7.426
7.418
7.410
7.402
7.400
7.260
7.145
7.129
3.836
1.368
11
10
9
8
7
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2
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ppm
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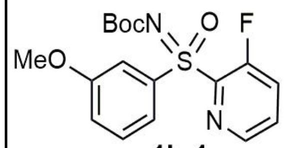
3.03
9.05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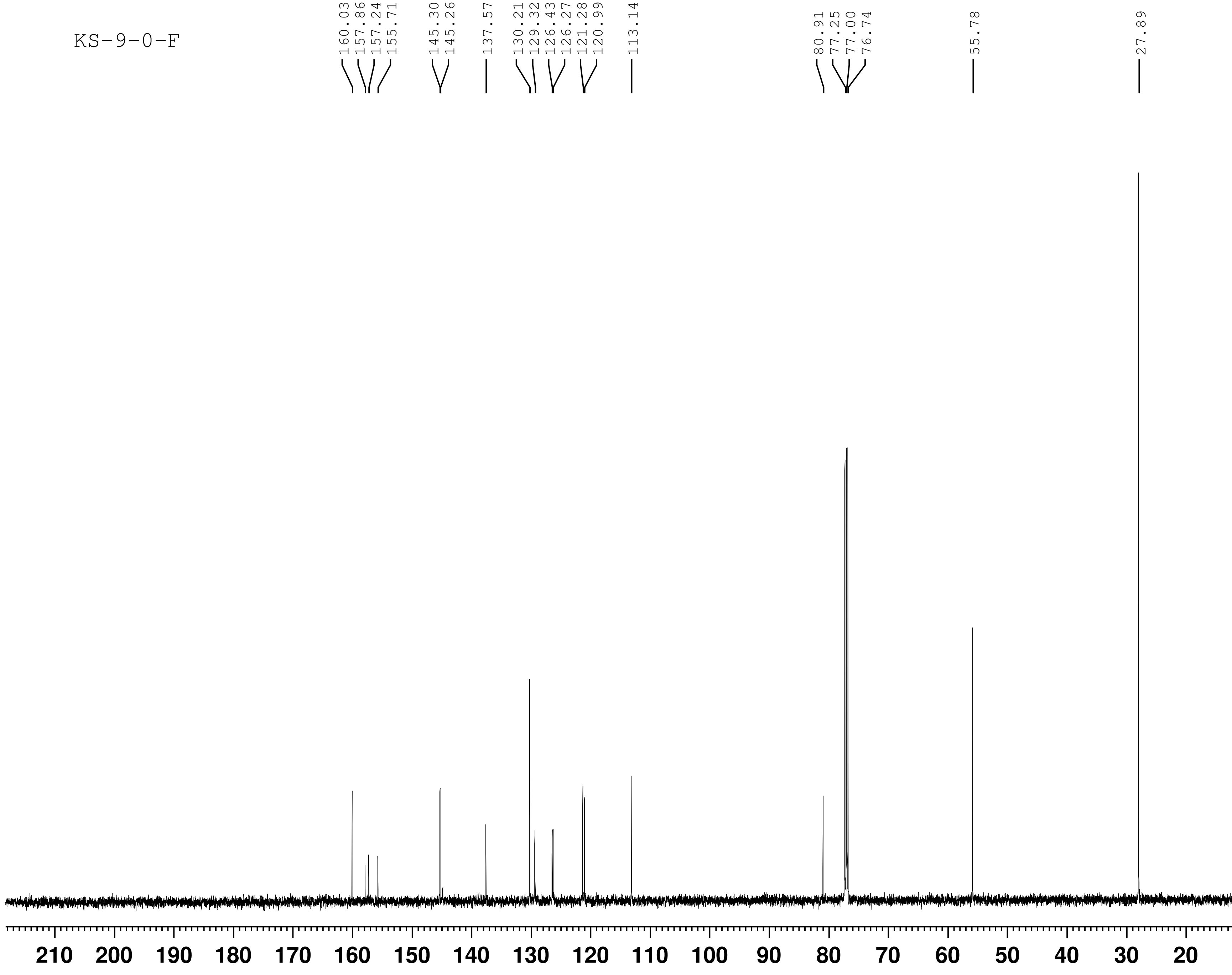
MeO
S
N

1b-1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130.21
129.32
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126.27
121.28
120.99
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77.00
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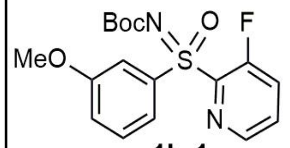
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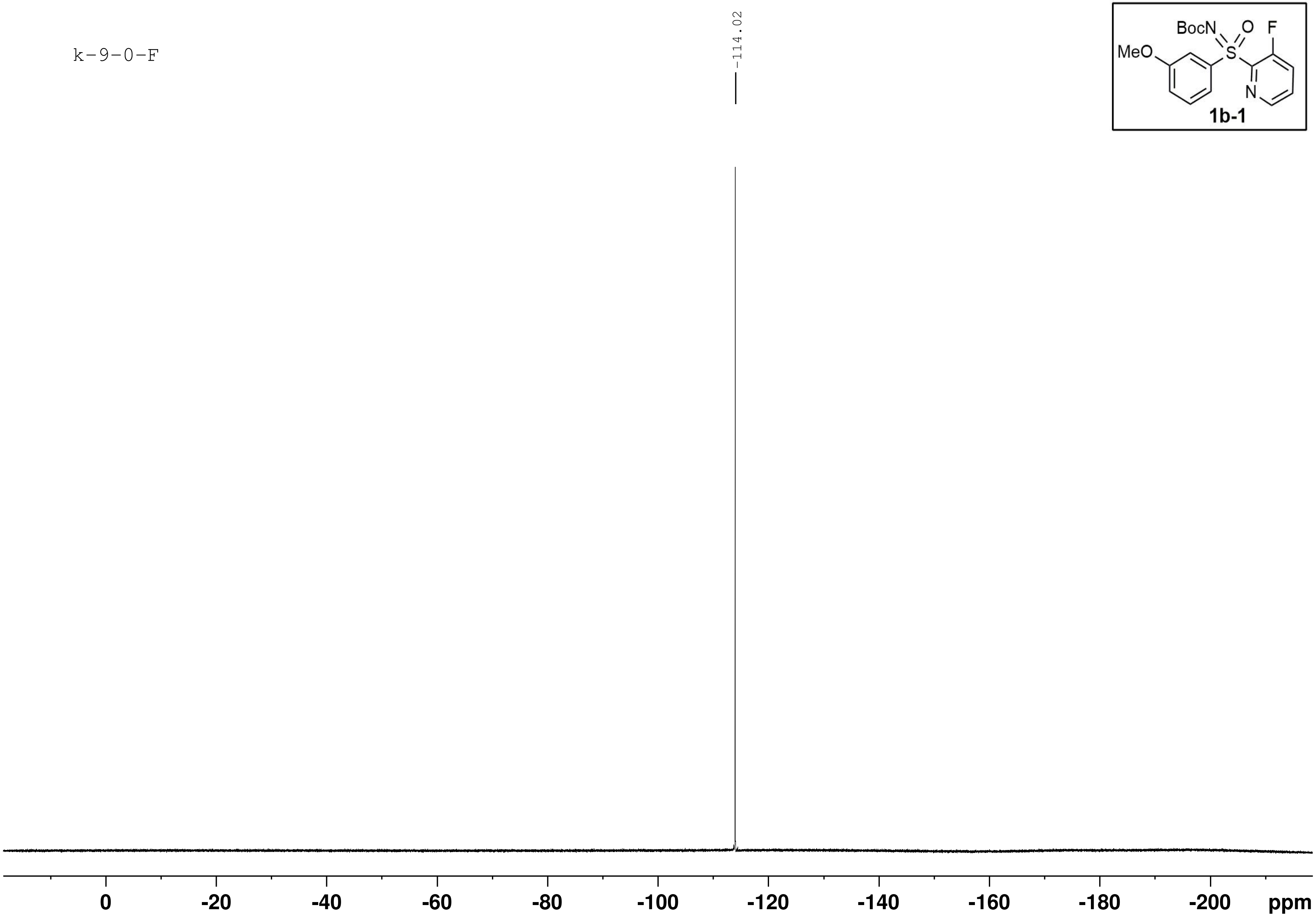
MeO
S
N

1b-1



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F
MeO
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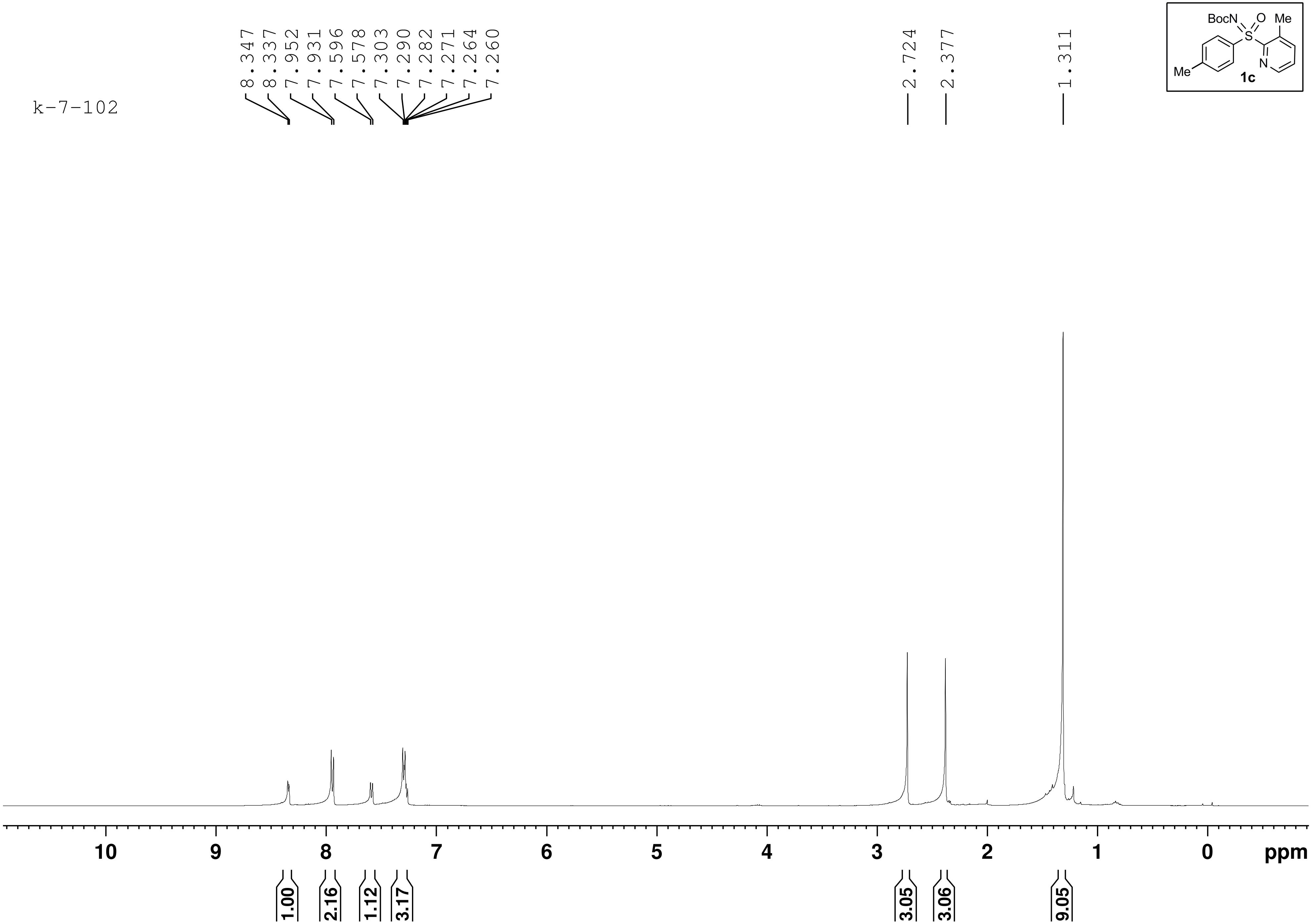
-80
-100
-120
-140
-160
-180
-200
ppm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7.282
7.271
7.264
7.260
2.724
2.377
1.311
BocN
O
Me
S
Me
N
1c
10
9
8
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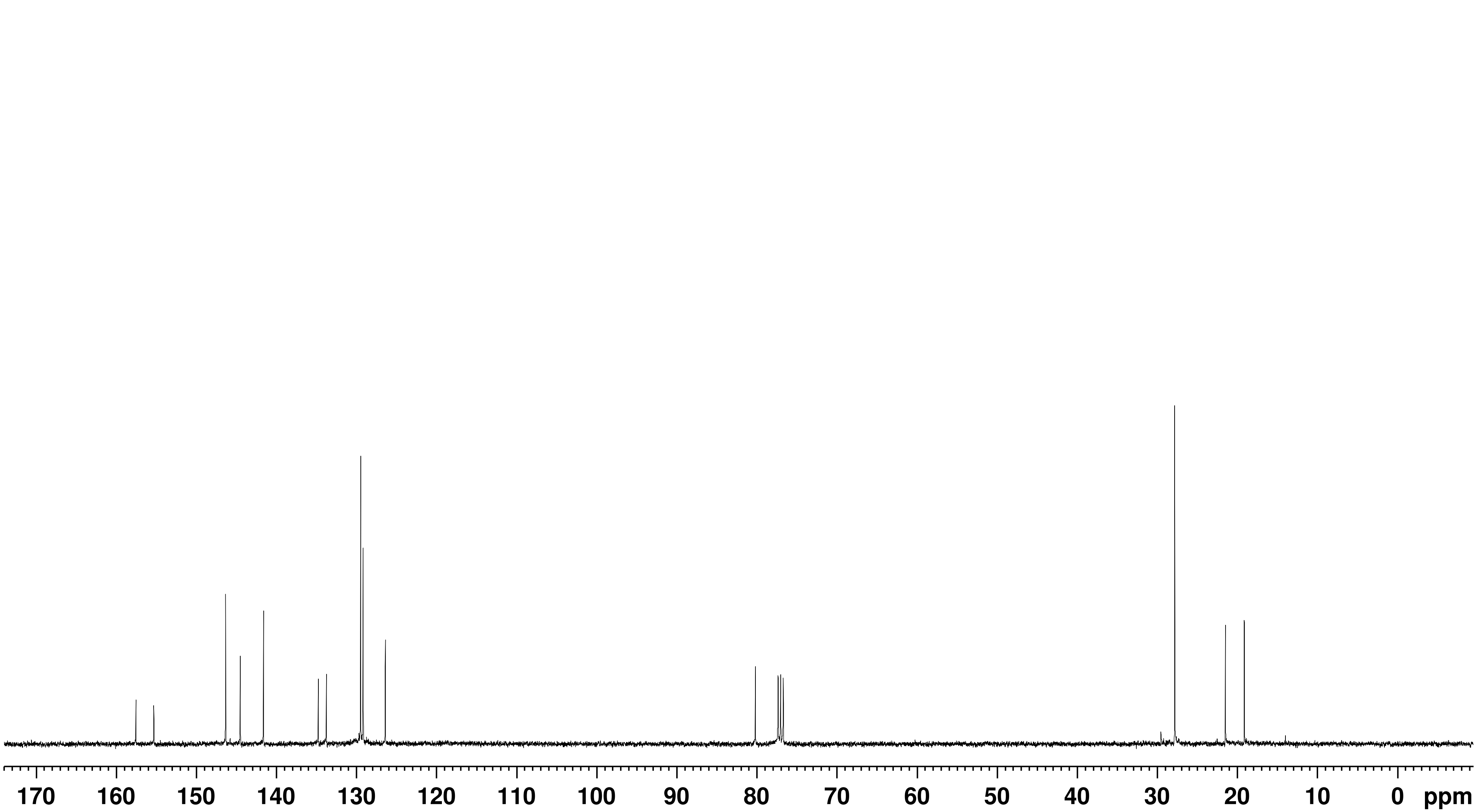
3.06
9.05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126.37
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76.68
27.79
21.46
19.10
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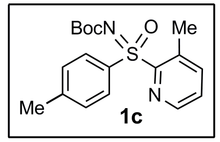
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S
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N
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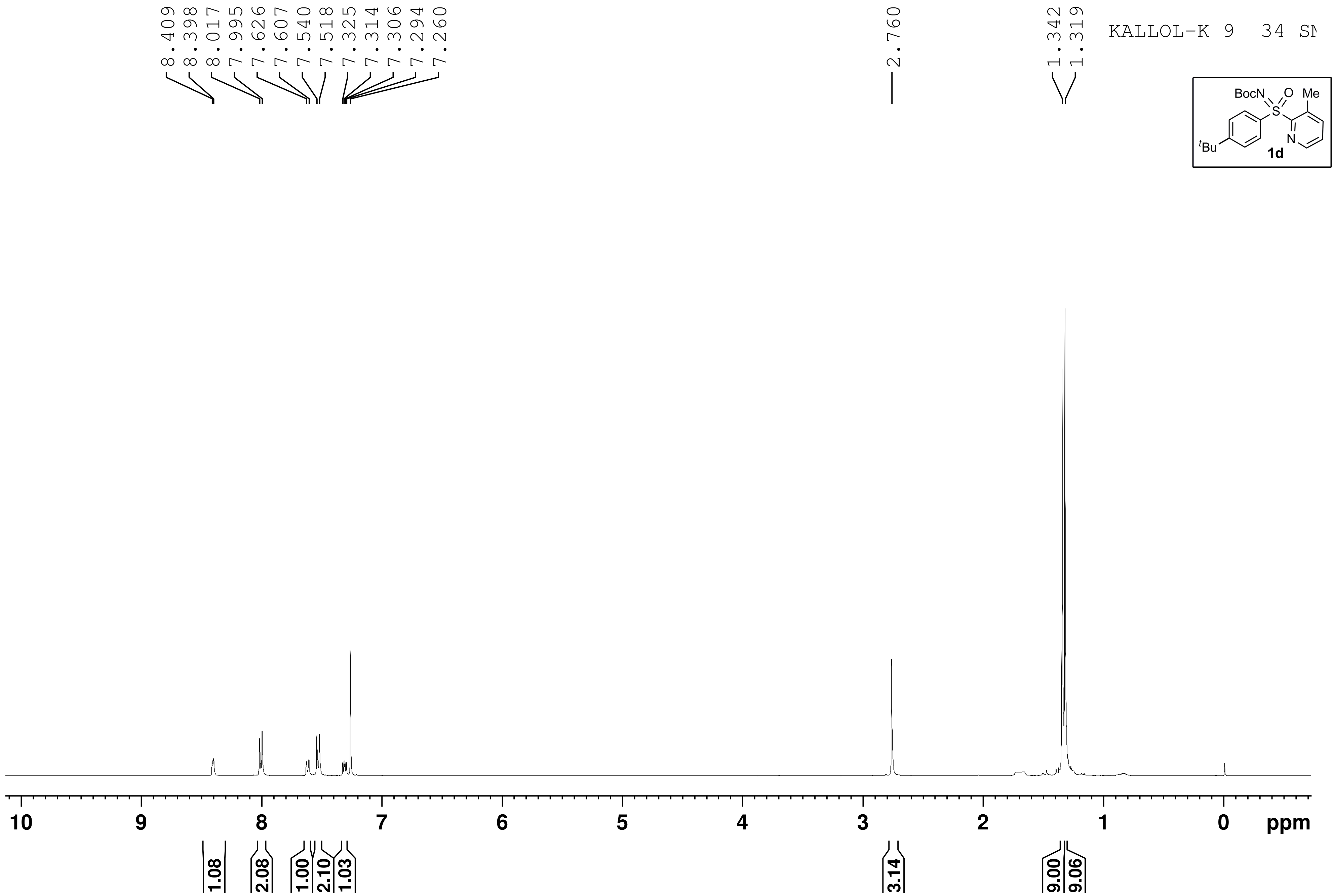
1c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7.626
7.607
7.540
7.518
7.325
7.314
7.306
7.294
7.260
2.760
1.342
1.319
KALLOL-K 9 34 SN
BocN
O
Me
S
N
tBu
1d
10
9
8
7
6
5
4
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2
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ppm
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2.08
1.00
2.10
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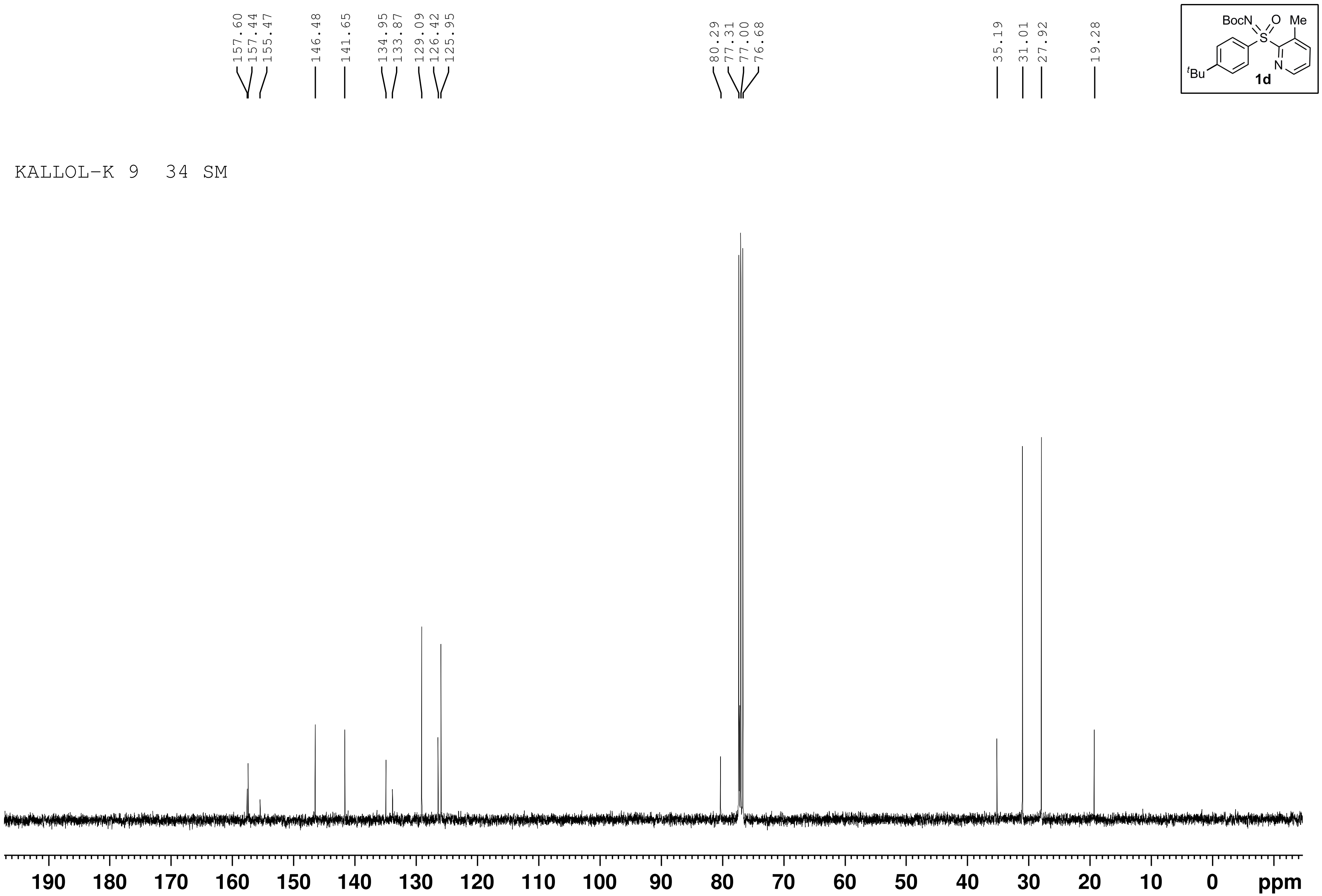
3.14
9.00
9.06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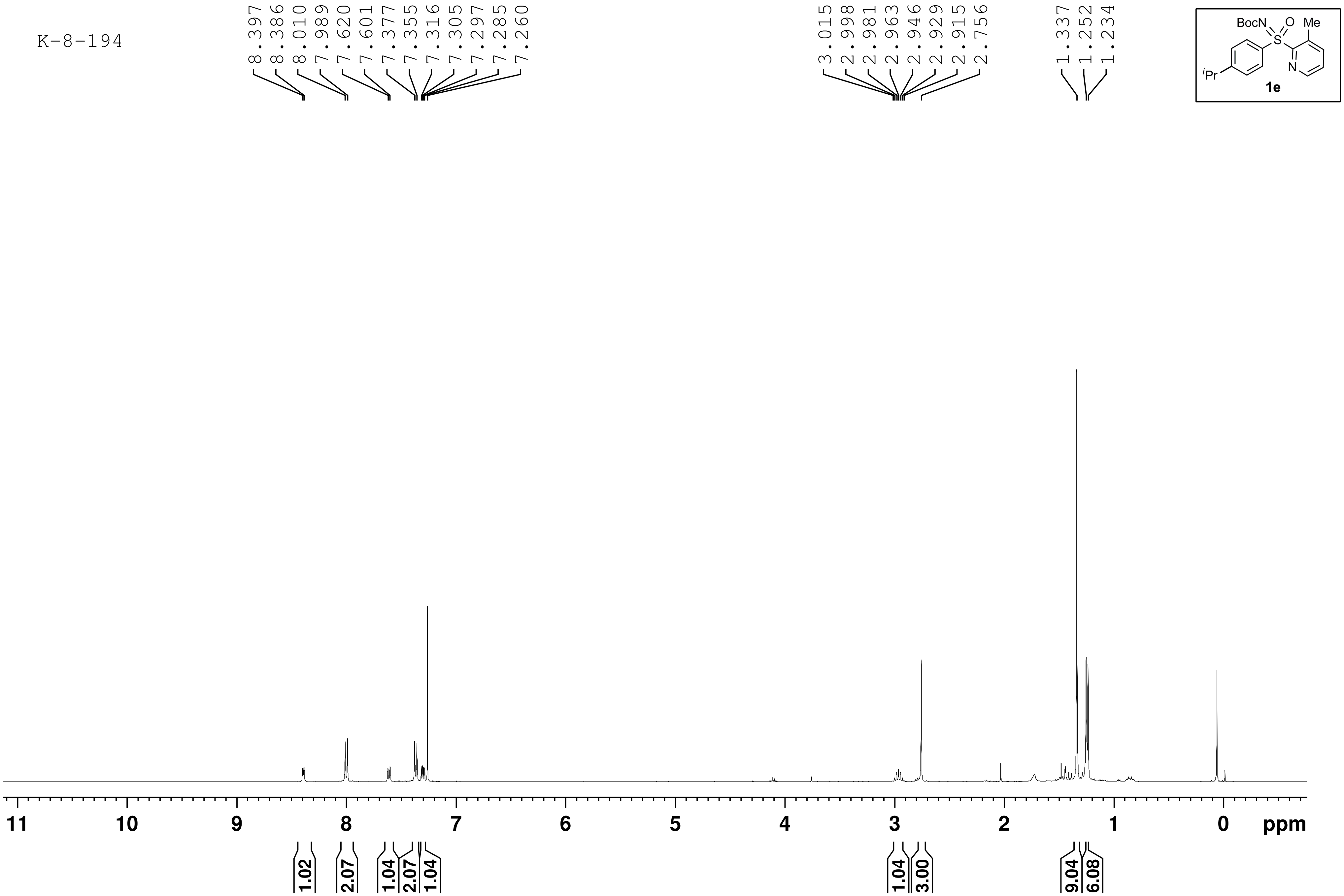
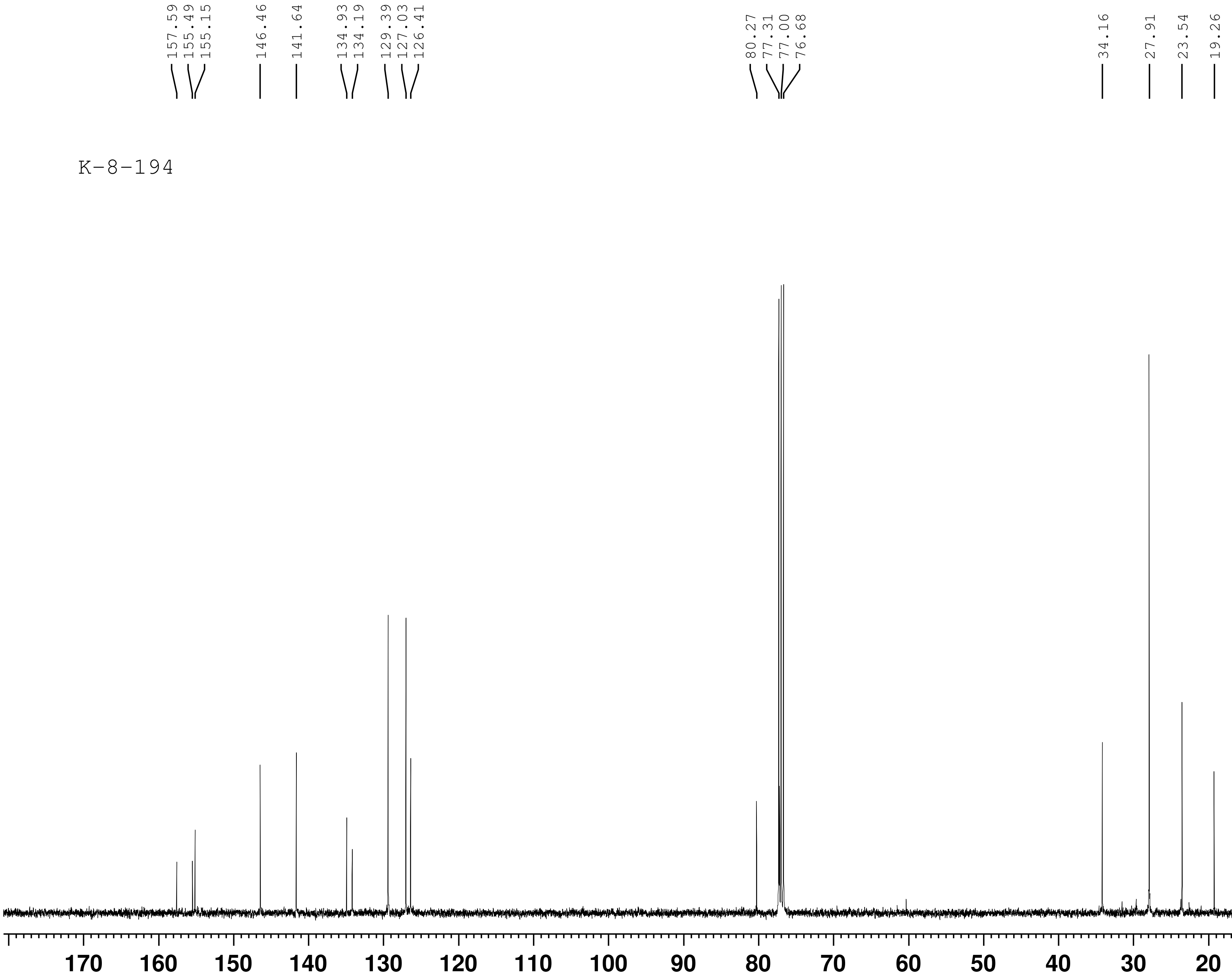
77.00
76.68
35.19
31.01
27.92
19.28
KALLOL-K 9 34 SM
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
BocN
O
S
Me
N
tBu
1d


K-8-194
8.397
8.386
8.010
7.989
7.620
7.601
7.377
7.355
7.316
7.305
7.297
7.285
7.260
3.015
2.998
2.981
2.963
2.946
2.929
2.915
2.756
1.337
1.252
1.234
BocN
O
S
Me
N
iPr
1e
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
2.07
1.04
2.07
1.04
1.04
3.00
9.04
6.08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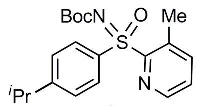
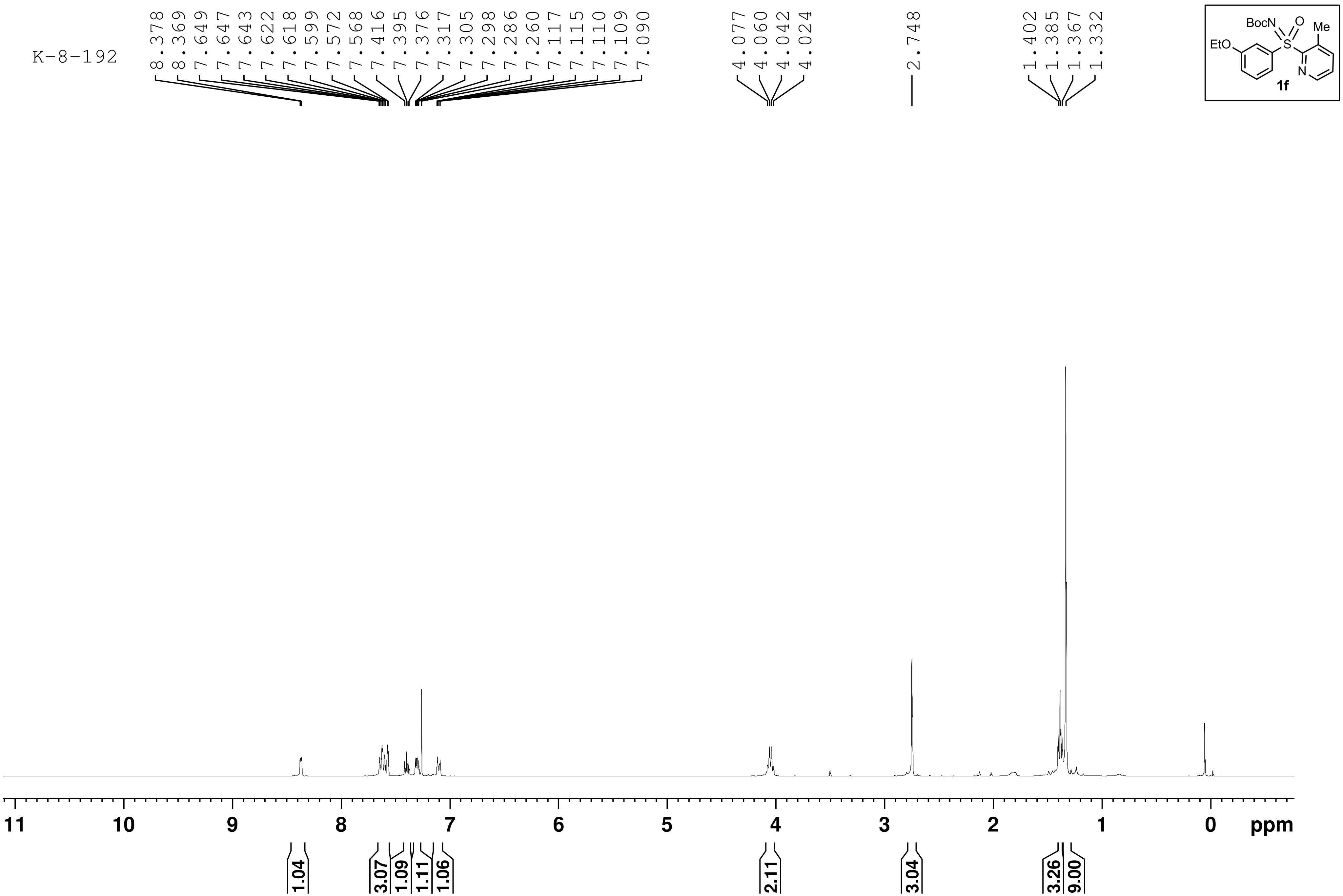
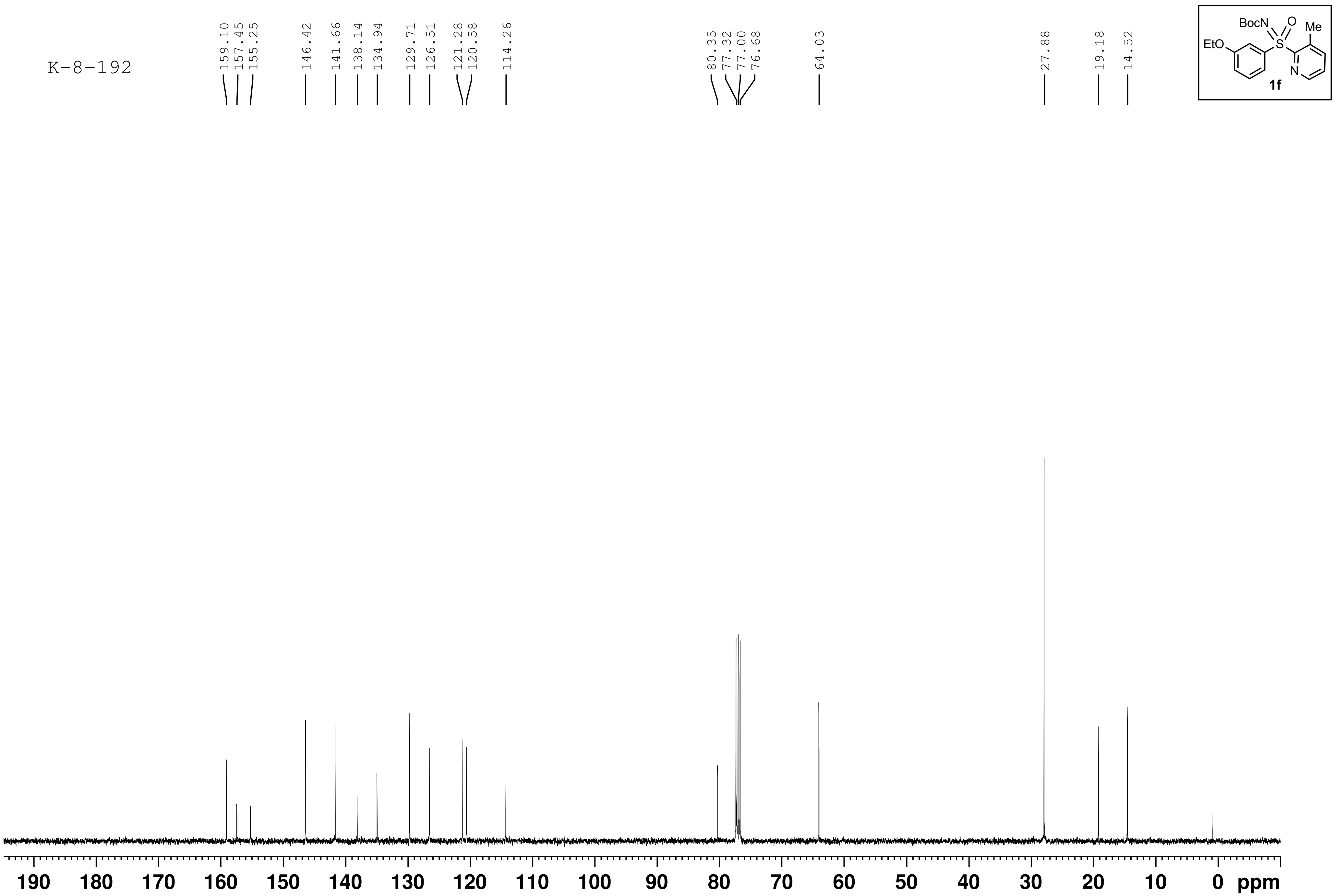
155.49
155.15
146.46
141.64
134.93
134.19
129.39
127.03
126.41
80.27
77.31
77.00
76.68
34.16
27.91
23.54
19.26
K-8-194
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

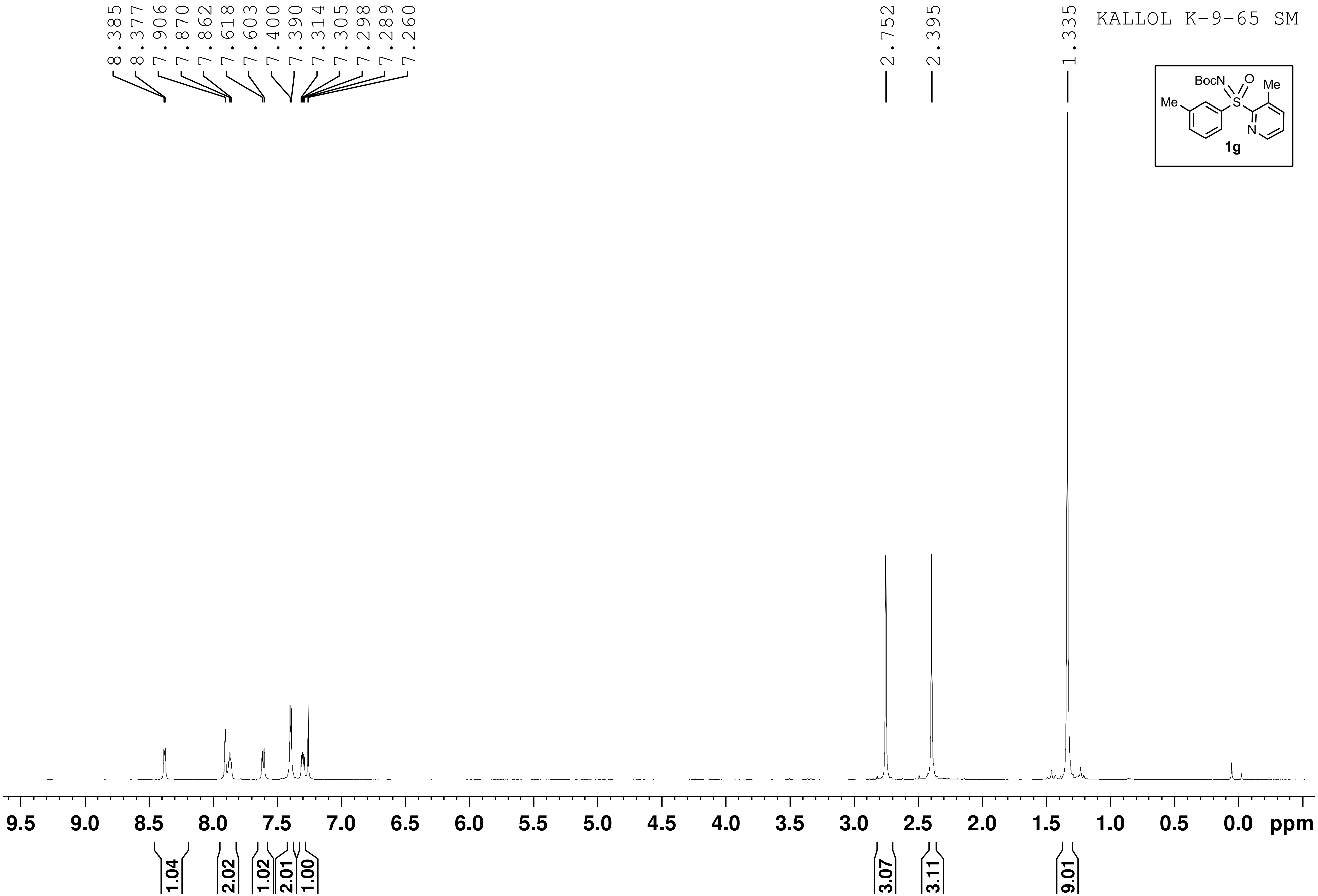

BocN
O
S
Me
N
iPr

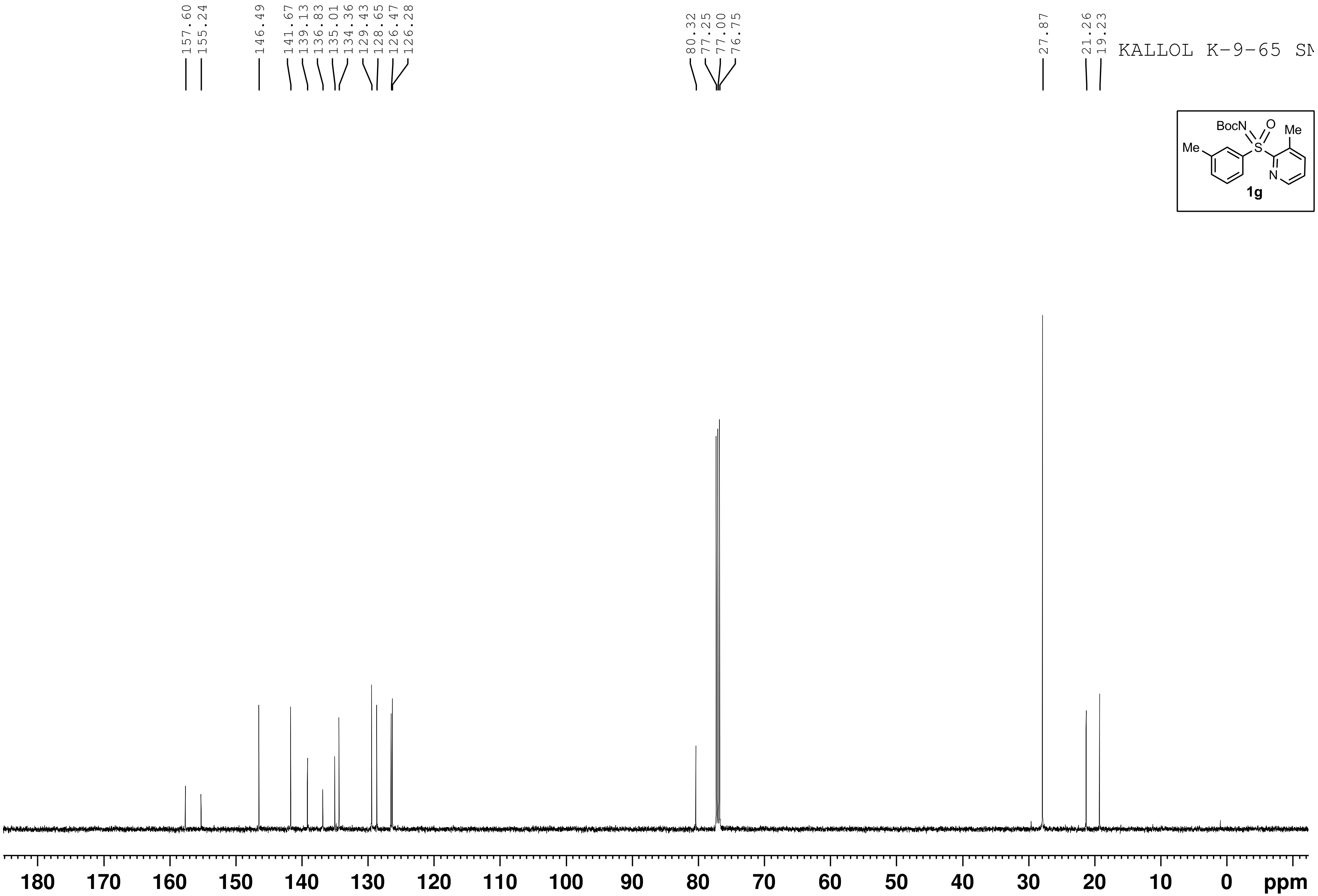
1e

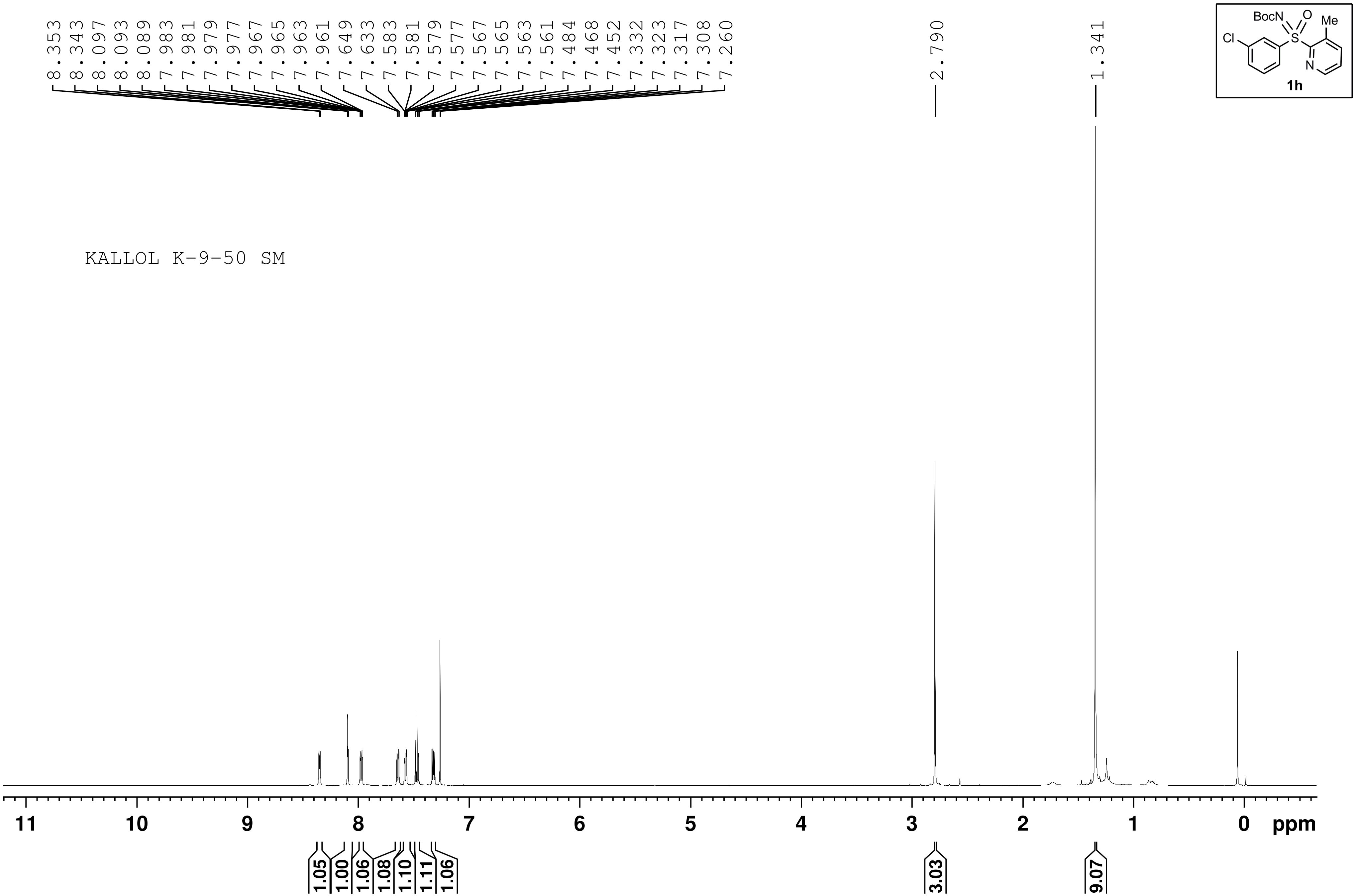

K-8-192
8.378 8.369 7.649 7.647 7.643 7.622 7.618 7.599 7.572 7.568 7.416 7.395 7.376 7.317 7.305 7.298 7.286 7.260 7.117 7.115 7.110 7.109 7.090
4.077 4.060 4.042 4.024
2.748
1.402 1.385 1.367 1.332
BocN
O
Me
EtO
S
N
1f
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.04 3.07 1.09 1.11 1.06 2.11 3.04 3.26 9.00



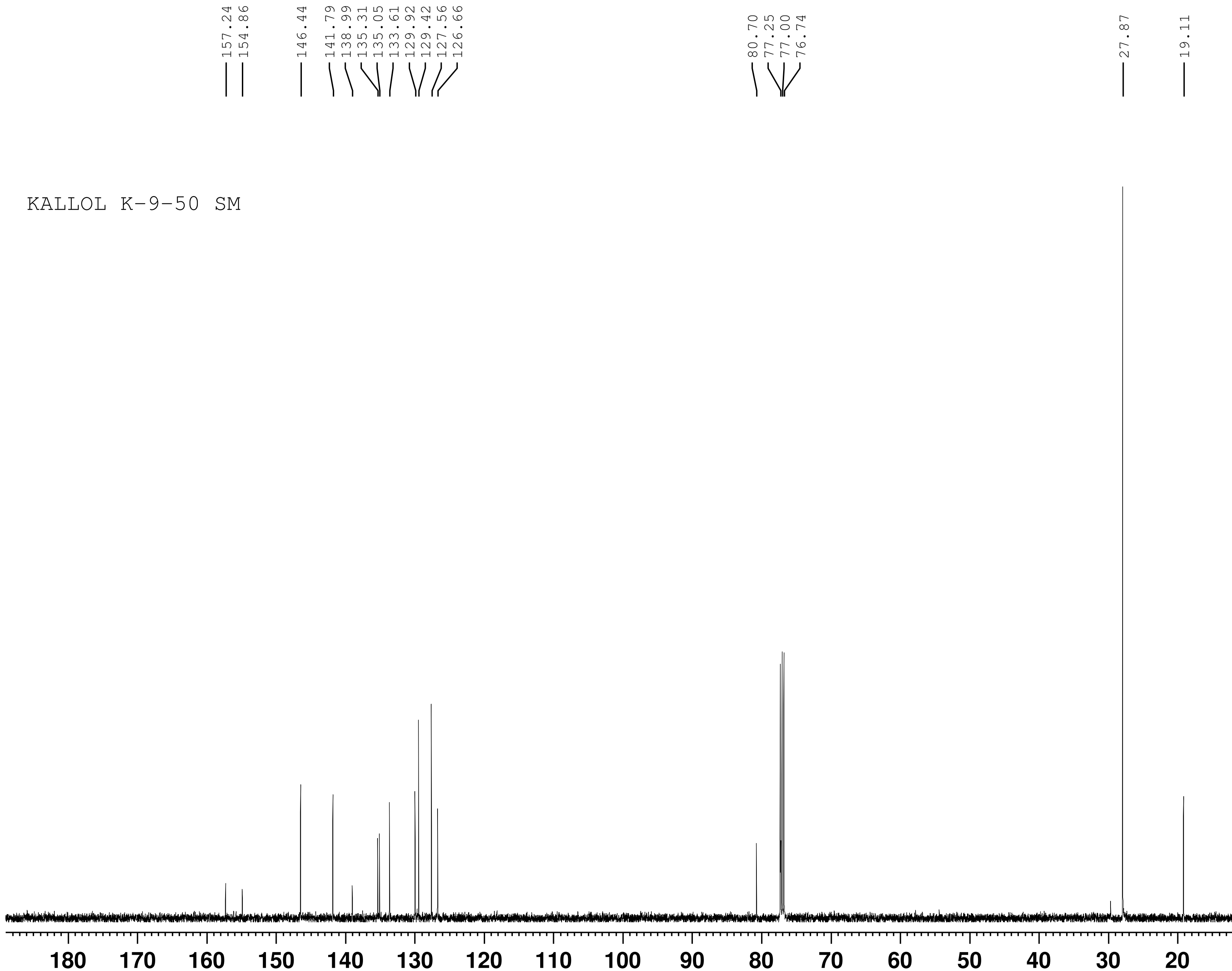
K-8-192
159.10
157.45
155.25
146.42
141.66
138.14
134.94
129.71
126.51
121.28
120.58
114.26
80.35
77.32
77.00
76.68
64.03
27.88
19.18
14.52
BocN
O
Me
EtO
S
N
1f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

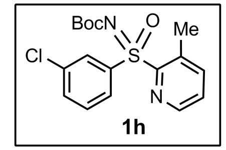

8.385
8.377
7.906
7.870
7.862
7.618
7.603
7.400
7.390
7.314
7.305
7.298
7.289
7.260
2.752
2.395
1.335
KALLOL K-9-65 SM
BocN
O
Me
Me
S
N
1g
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.04
2.02
1.02
2.01
1.00
3.07
3.11
9.01

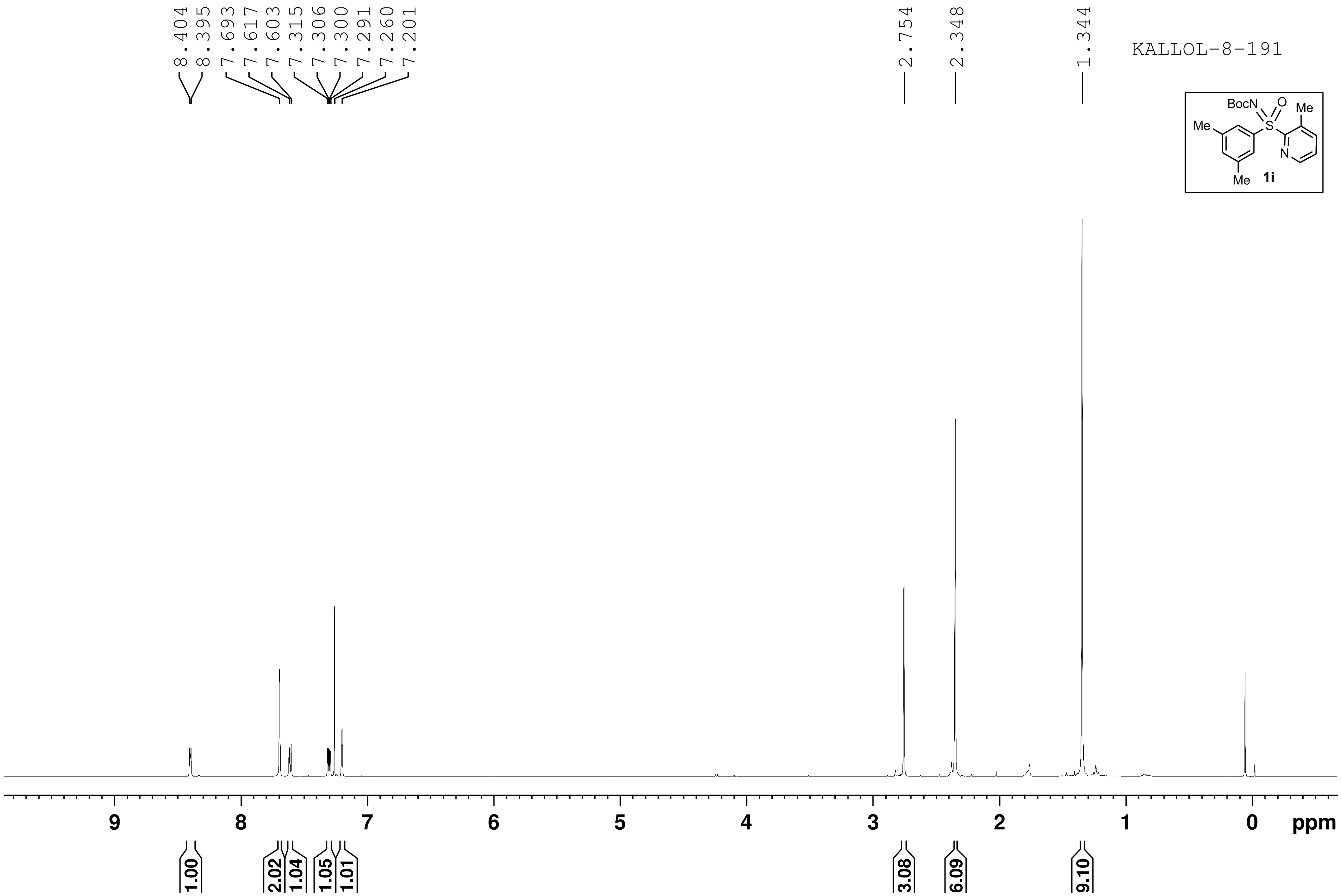

157.60
155.24
146.49
141.67
139.13
136.83
135.01
134.36
129.43
128.65
126.47
126.28
80.32
77.25
77.00
76.75
27.87
21.26
19.23
KALLOL K-9-65 SM
BocN
O
Me
Me
S
N
1g
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.353
8.343
8.097
8.093
8.089
7.983
7.981
7.979
7.977
7.967
7.965
7.963
7.961
7.649
7.633
7.583
7.581
7.579
7.577
7.567
7.565
7.563
7.561
7.484
7.468
7.452
7.332
7.323
7.317
7.308
7.260
2.790
1.341
KALLOL K-9-50 SM
BocN
O
Me
Cl
S
N
1h
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.05
1.00
1.06
1.08
1.10
1.11
1.06
3.03
9.07

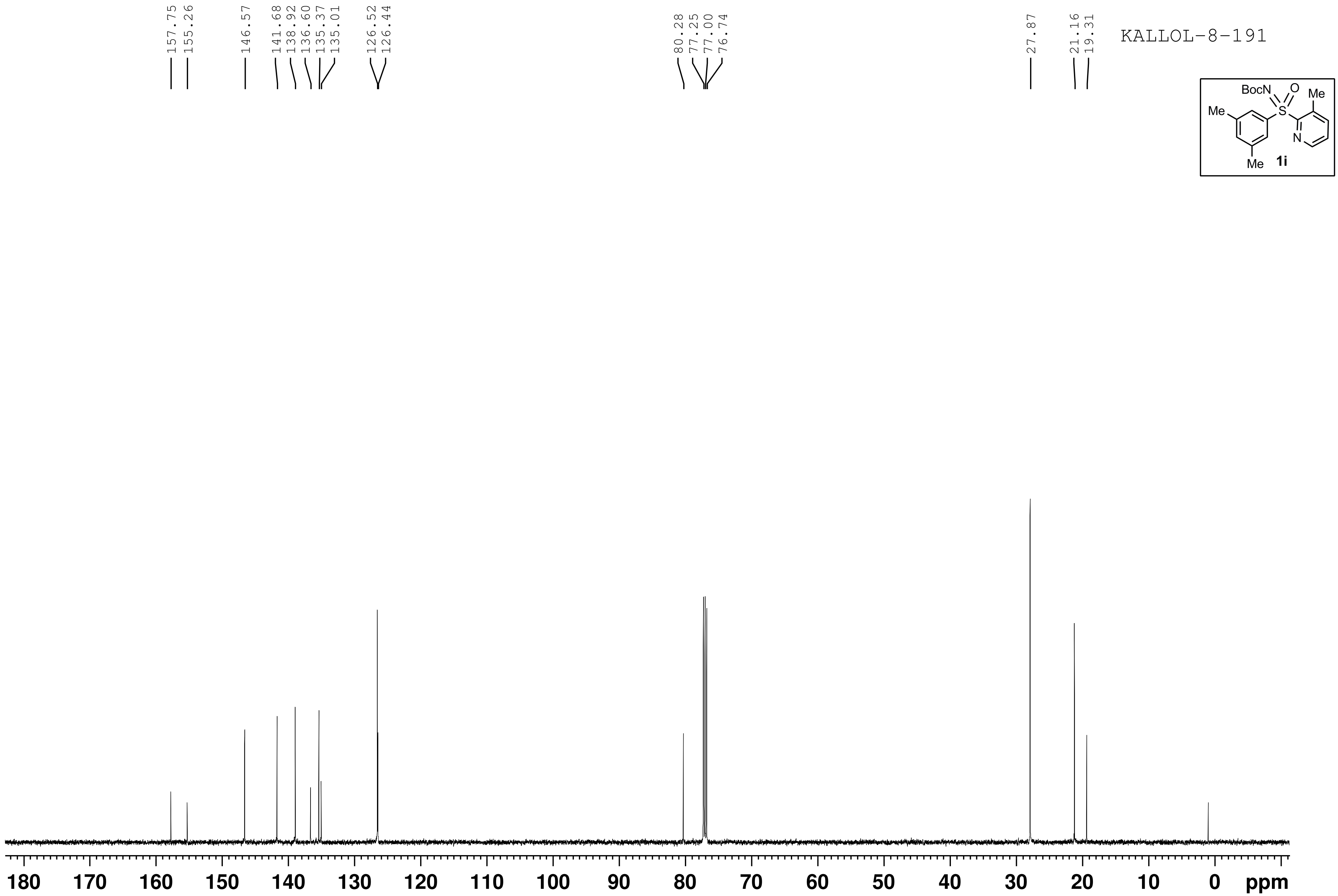
KALLOL K-9-50 SM

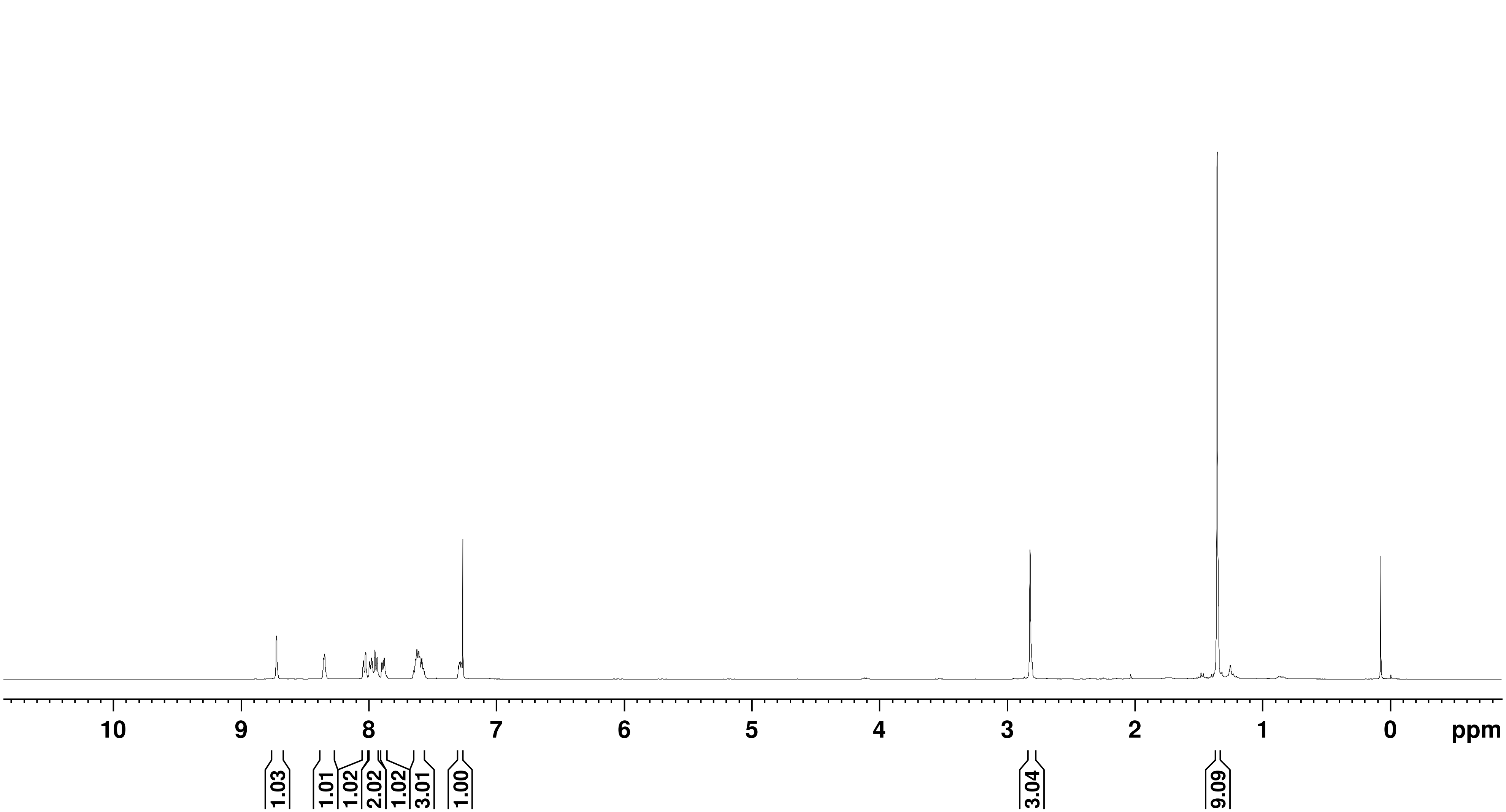


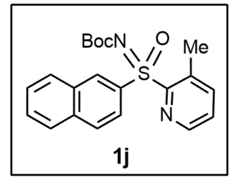


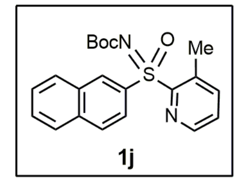


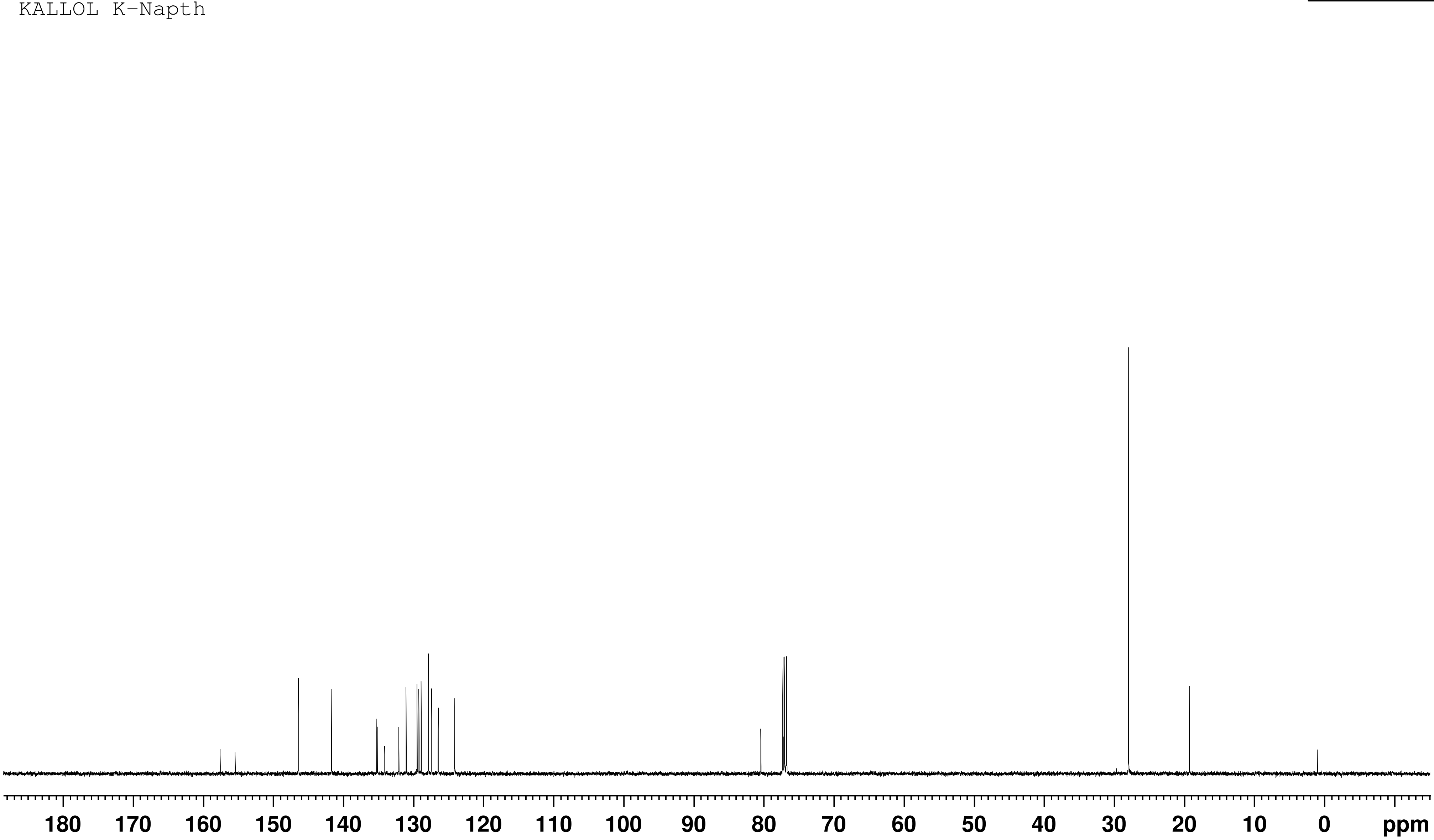
8.404
8.395
7.693
7.617
7.603
7.315
7.306
7.300
7.291
7.260
7.201
2.754
2.348
1.344
KALLOL-8-191
BocN
O
S
Me
Me
N
Me
1i
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.02
1.04
1.05
1.01
3.08
6.09
9.10

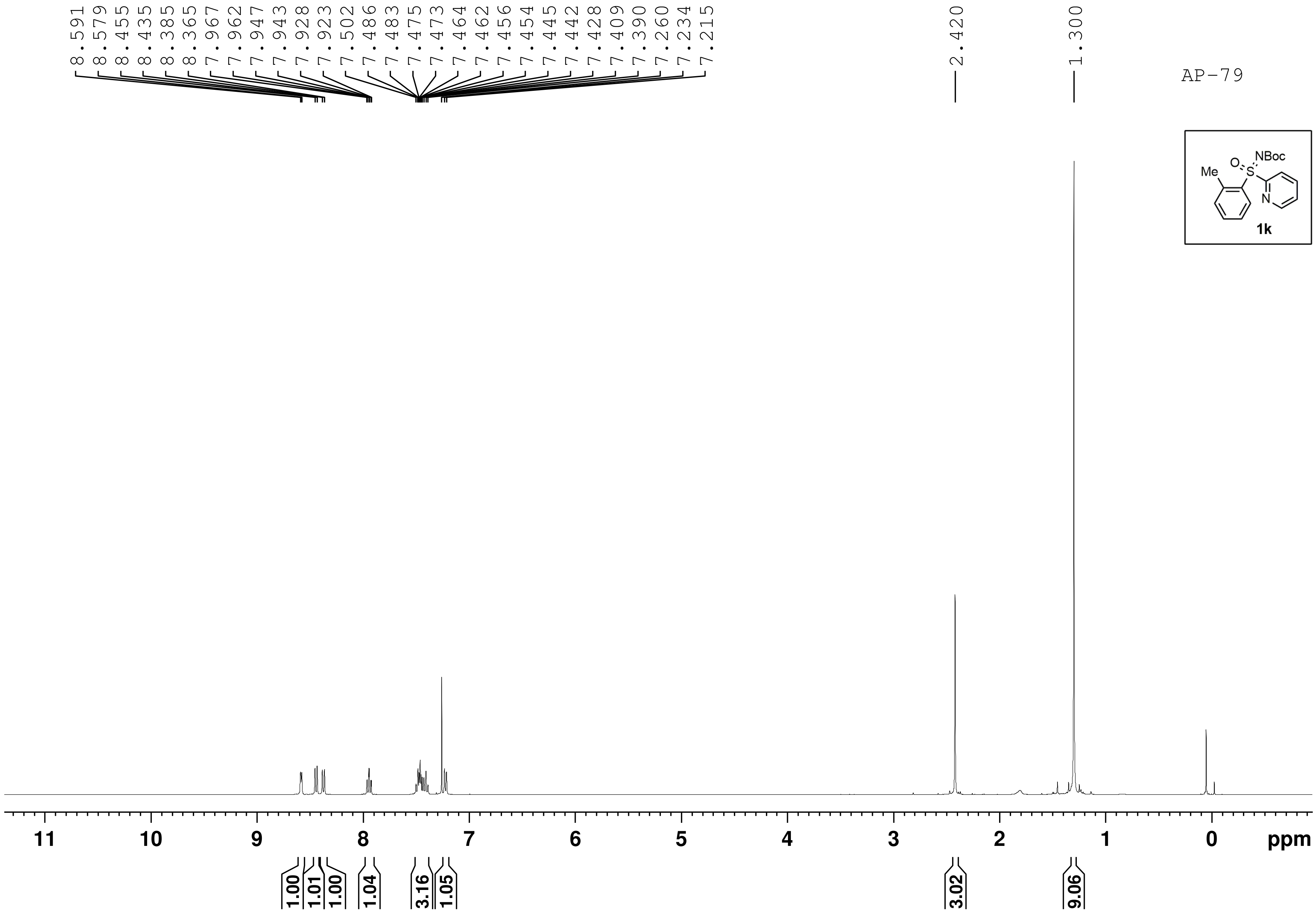

157.75
155.26
146.57
141.68
138.92
136.60
135.37
135.01
126.52
126.44
80.28
77.25
77.00
76.74
27.87
21.16
19.31
KALLOL-8-191
BocN
O
S
Me
N
1i
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

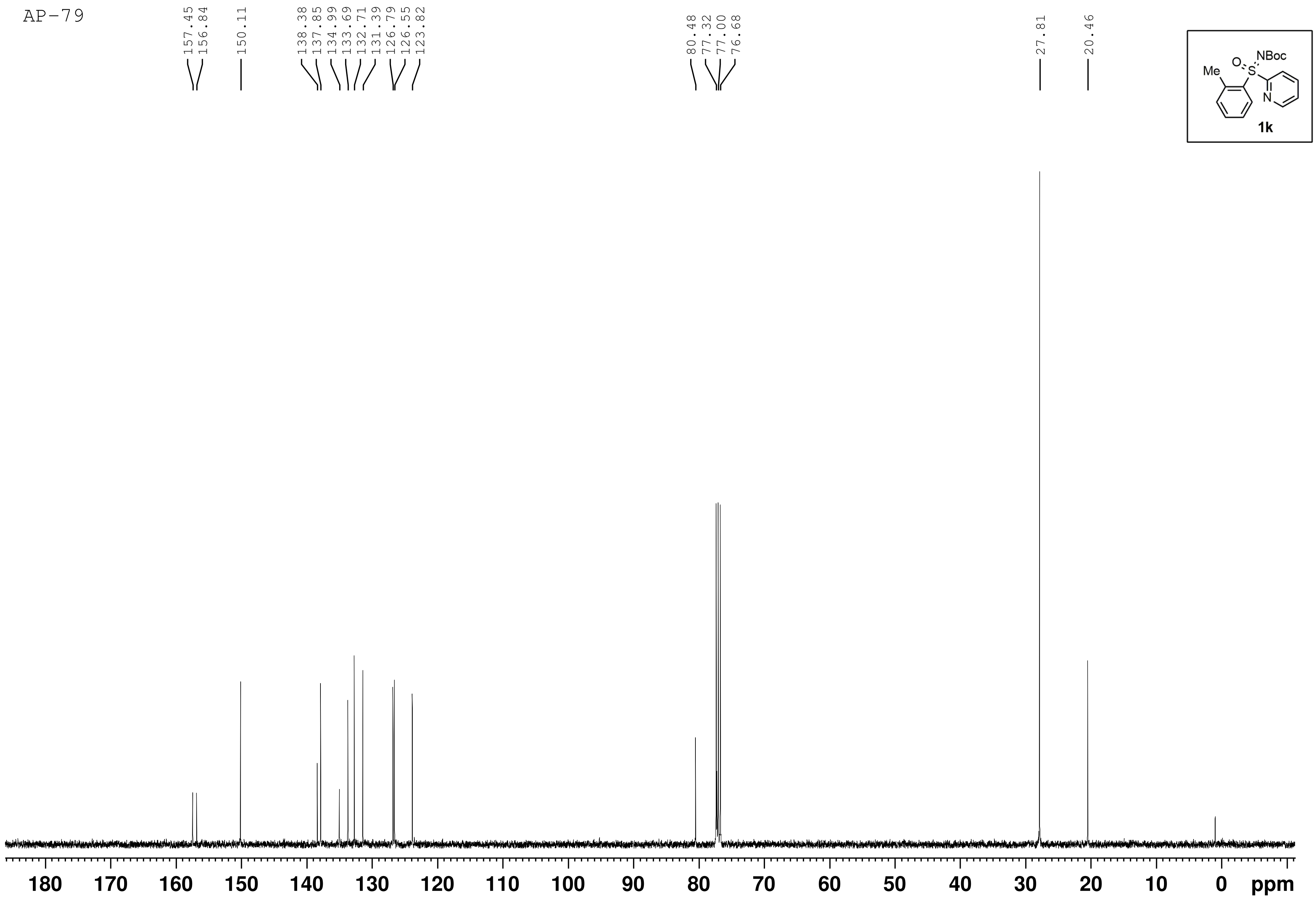

8.719
8.351
8.343
8.039
8.023
7.989
7.974
7.949
7.931
7.893
7.877
7.647
7.644
7.631
7.620
7.618
7.606
7.598
7.581
7.568
7.295
7.286
7.282
7.280
7.270
7.260
2.817
1.352
KALLOL K-Napth
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.01
1.02
2.02
1.02
3.01
1.00
3.04
9.09

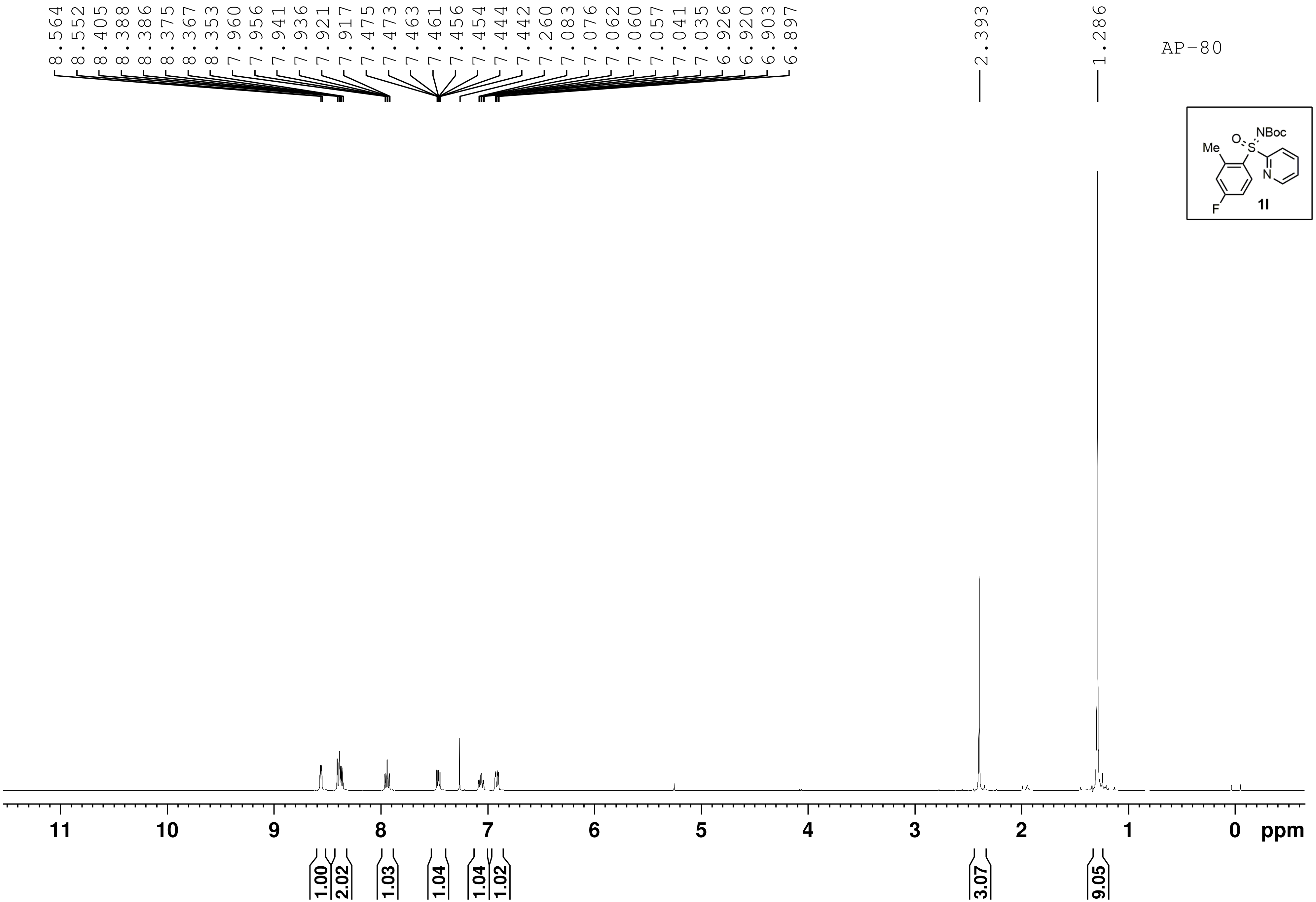

BocN
O
S
Me
N
1j


BocN
O
S
Me
N
1j

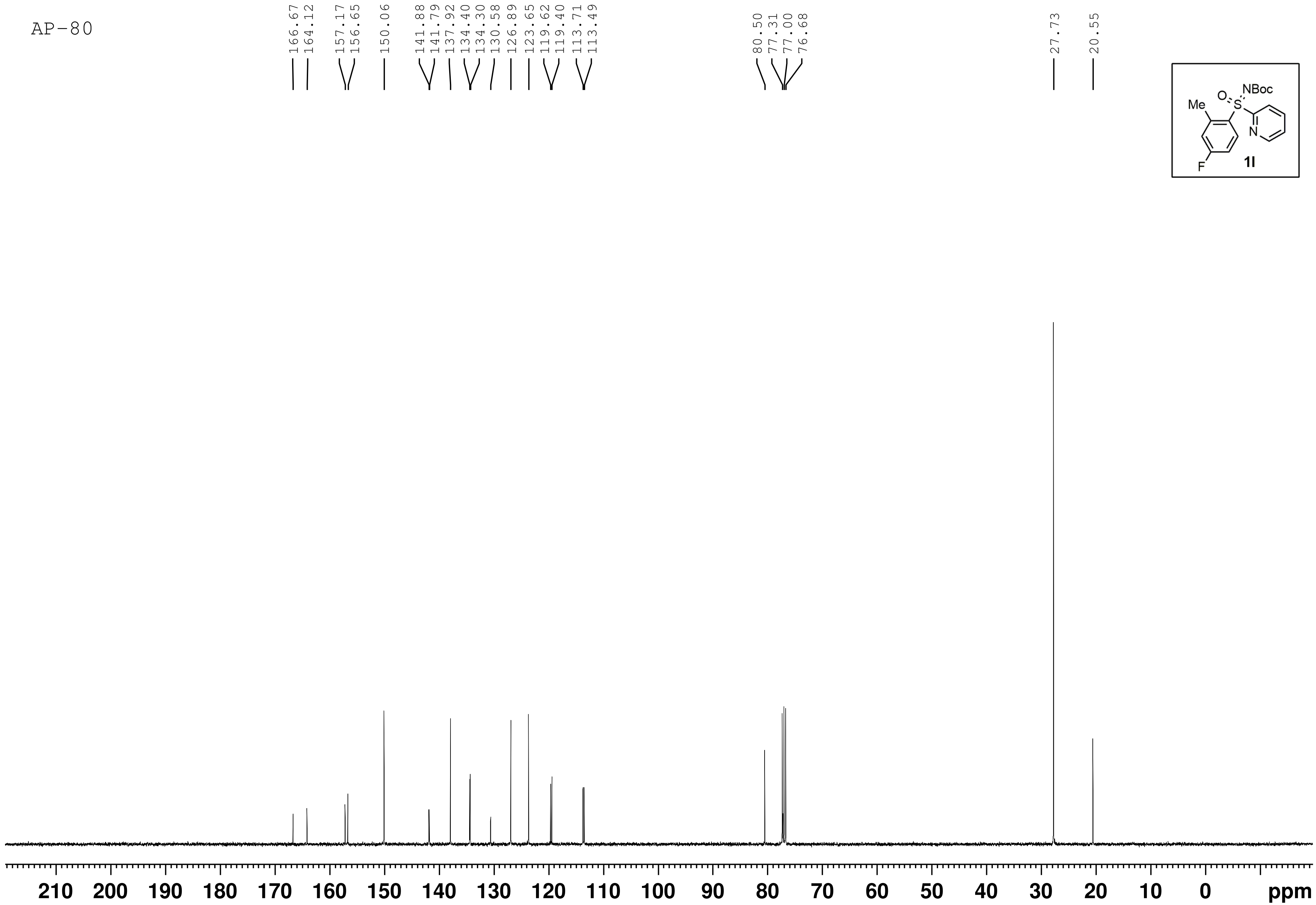

157.57
155.45
146.42
141.66
135.22
135.09
134.10
132.09
131.03
129.47
129.19
128.87
127.83
127.38
126.44
124.10
80.41
77.25
77.00
76.74
27.92
19.22
KALLOL K-Napth
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

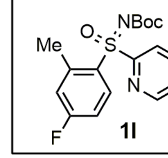

8.591
8.579
8.455
8.435
8.385
8.365
7.967
7.962
7.947
7.943
7.928
7.923
7.502
7.486
7.483
7.475
7.473
7.464
7.462
7.456
7.454
7.445
7.442
7.428
7.409
7.390
7.260
7.234
7.215
2.420
1.300
AP-79
NBoc
O
S
Me
N
1k
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.00
1.04
3.16
1.05
3.02
9.06


AP-79
157.45
156.84
150.11
138.38
137.85
134.99
133.69
132.71
131.39
126.79
126.55
123.82
80.48
77.32
77.00
76.68
27.81
20.46
NBoc
O
S
Me
N
1k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



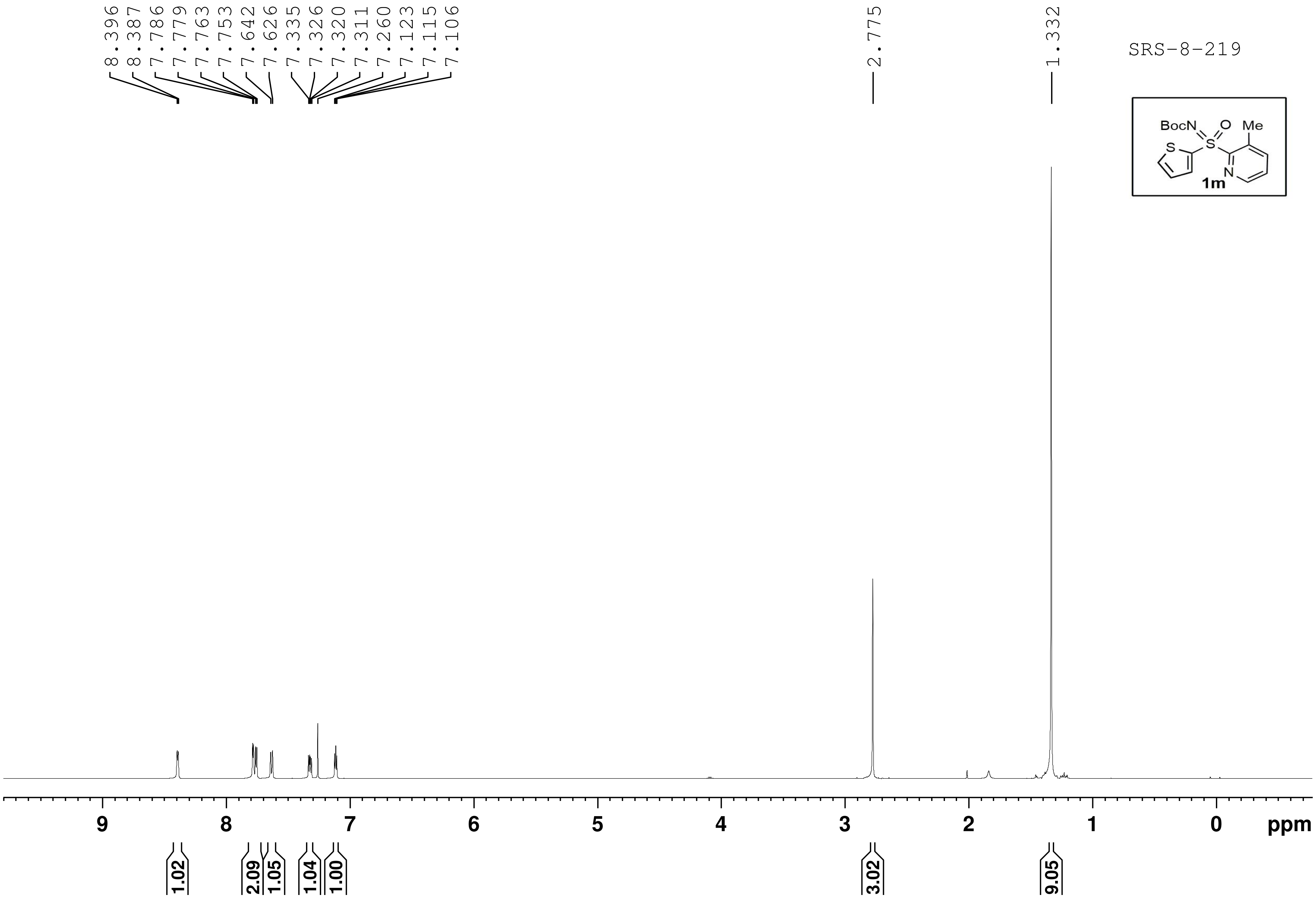
8.564
8.552
8.405
8.388
8.386
8.375
8.367
8.353
7.960
7.956
7.941
7.936
7.921
7.917
7.475
7.473
7.463
7.461
7.456
7.454
7.444
7.442
7.260
7.083
7.076
7.062
7.060
7.057
7.041
7.035
6.926
6.920
6.903
6.897
2.393
1.286
AP-80
Me
O
S
NBoc
N
F
1l
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.02
1.03
1.04
1.04
1.02
3.07
9.05


AP-80
166.67
164.12
157.17
156.65
150.06
141.88
141.79
137.92
134.40
134.30
130.58
126.89
123.65
119.62
119.40
113.71
113.49
80.50
77.31
77.00
76.68
27.73
20.55
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
NBoc
O
S
Me
N
F
1l



1l

AP-80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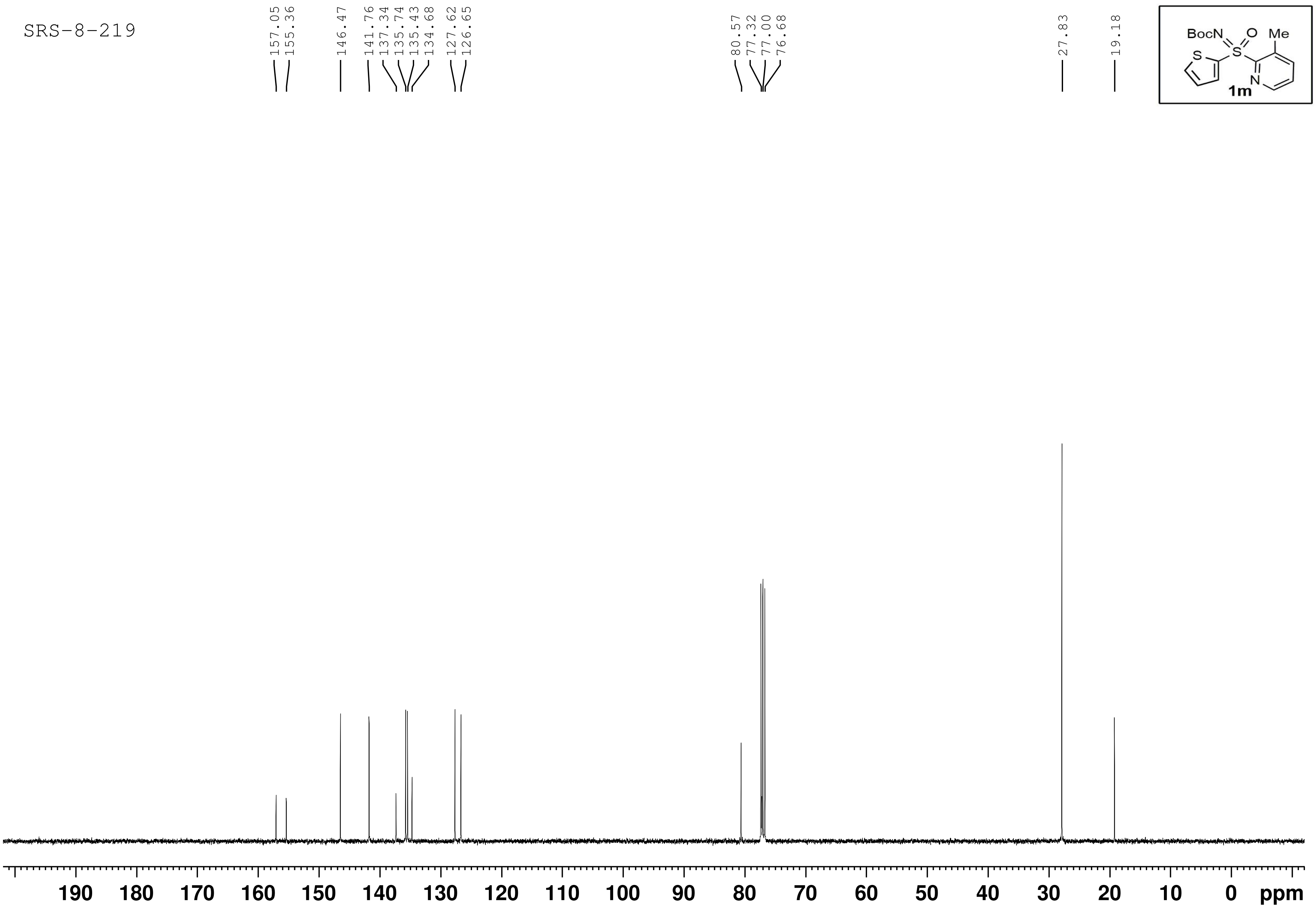
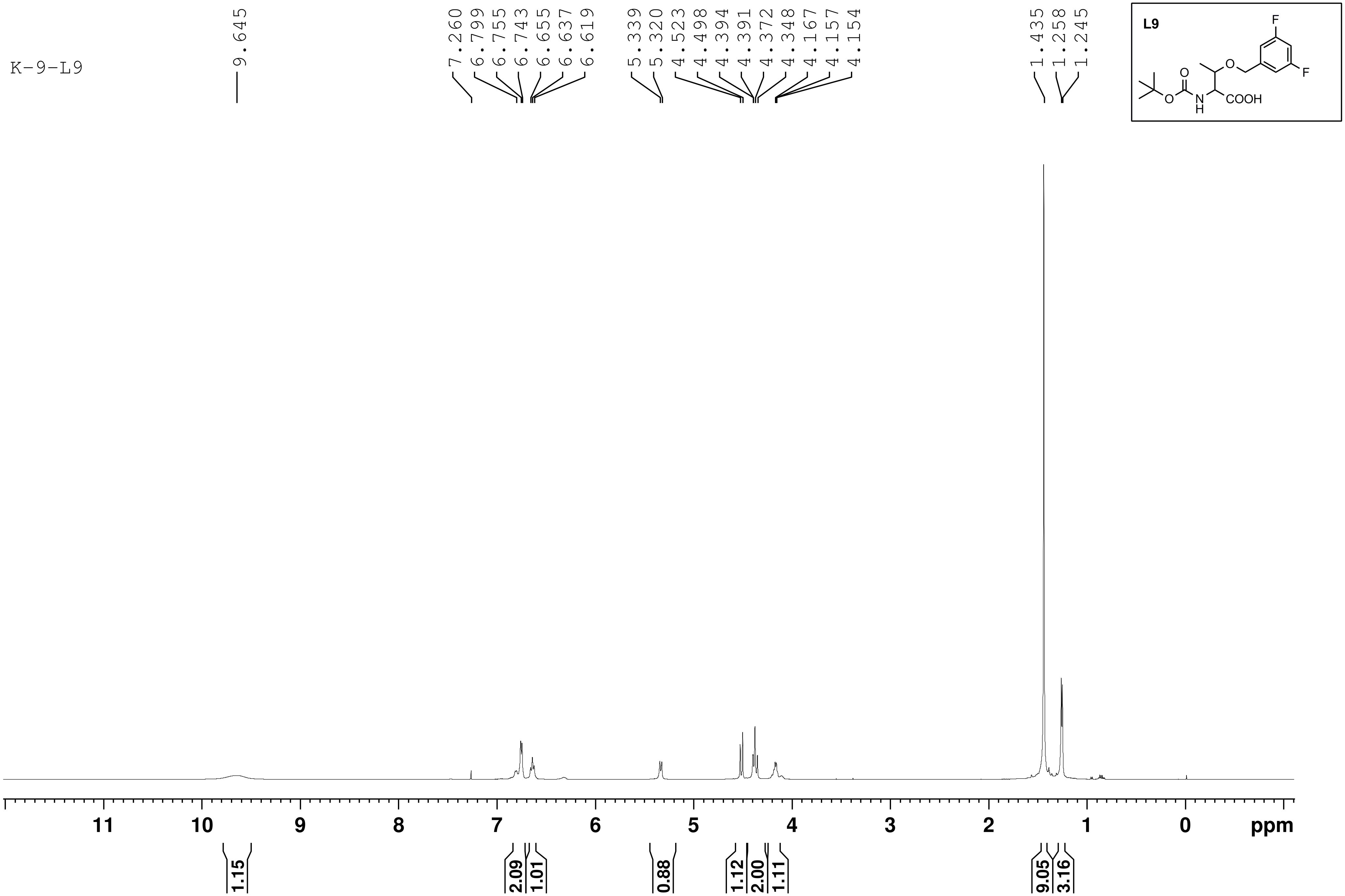
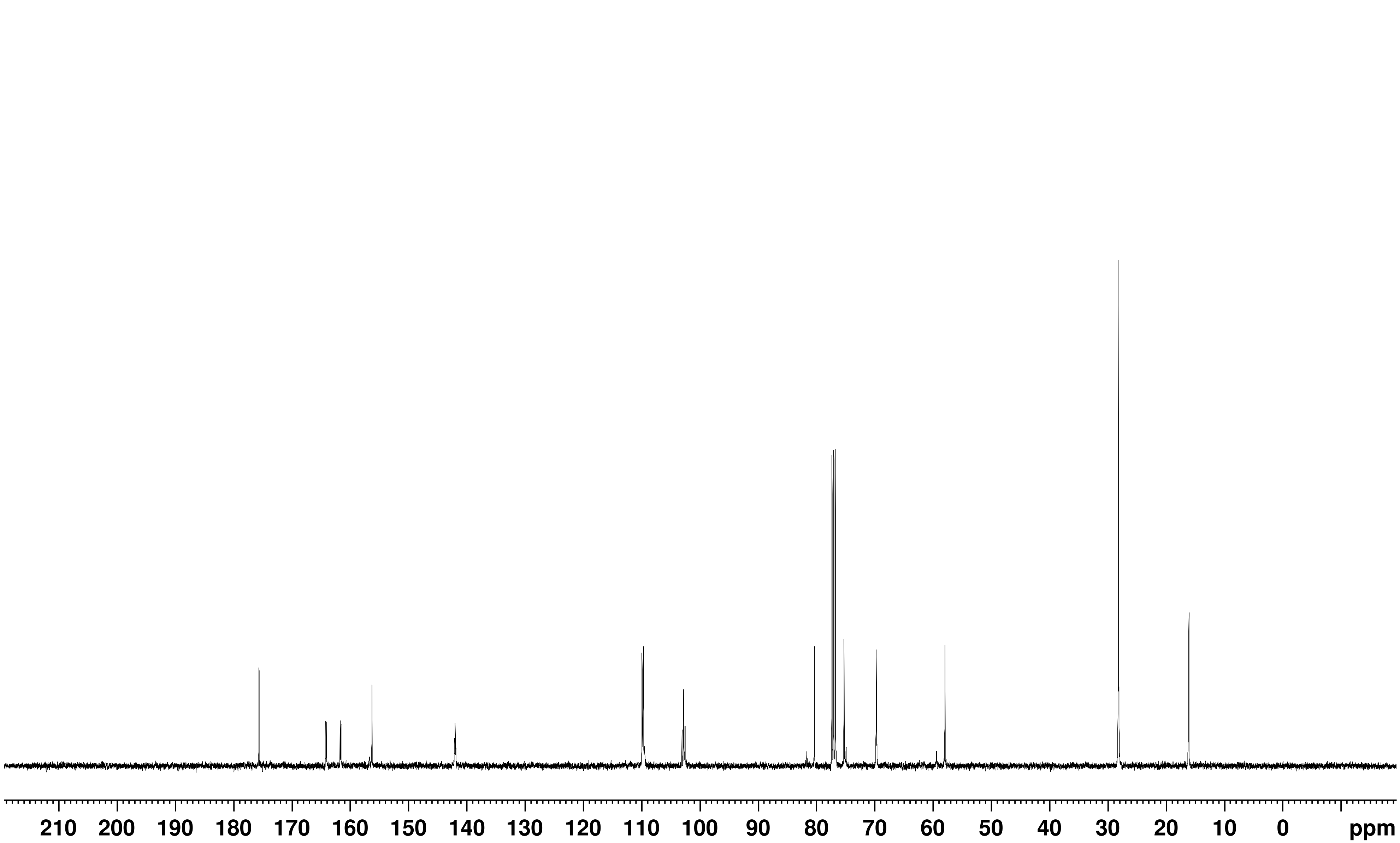
8.387
7.786
7.779
7.763
7.753
7.642
7.626
7.335
7.326
7.320
7.311
7.260
7.123
7.115
7.106
2.775
1.332
SRS-8-219
BocN
O
Me
S
S
N
1m
9
8
7
6
5
4
3
2
1
0
ppm
1.02
2.09
1.05
1.04
1.00
3.02
9.05


SRS-8-219
157.05
155.36
146.47
141.76
137.34
135.74
135.43
134.68
127.62
126.65
80.57
77.32
77.00
76.68
27.83
19.18
BocN
O
Me
S
S
N
1m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

K-9-L9

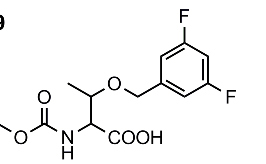

9.645
7.260
6.799
6.755
6.743
6.655
6.637
6.619
5.339
5.320
4.523
4.498
4.394
4.391
4.372
4.348
4.167
4.157
4.154
1.435
1.258
1.245
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.15
2.09
1.01
0.88
1.12
2.00
1.11
9.05
3.16
L9
F
F
O
O
O
N
H
COOH

K-9-L9



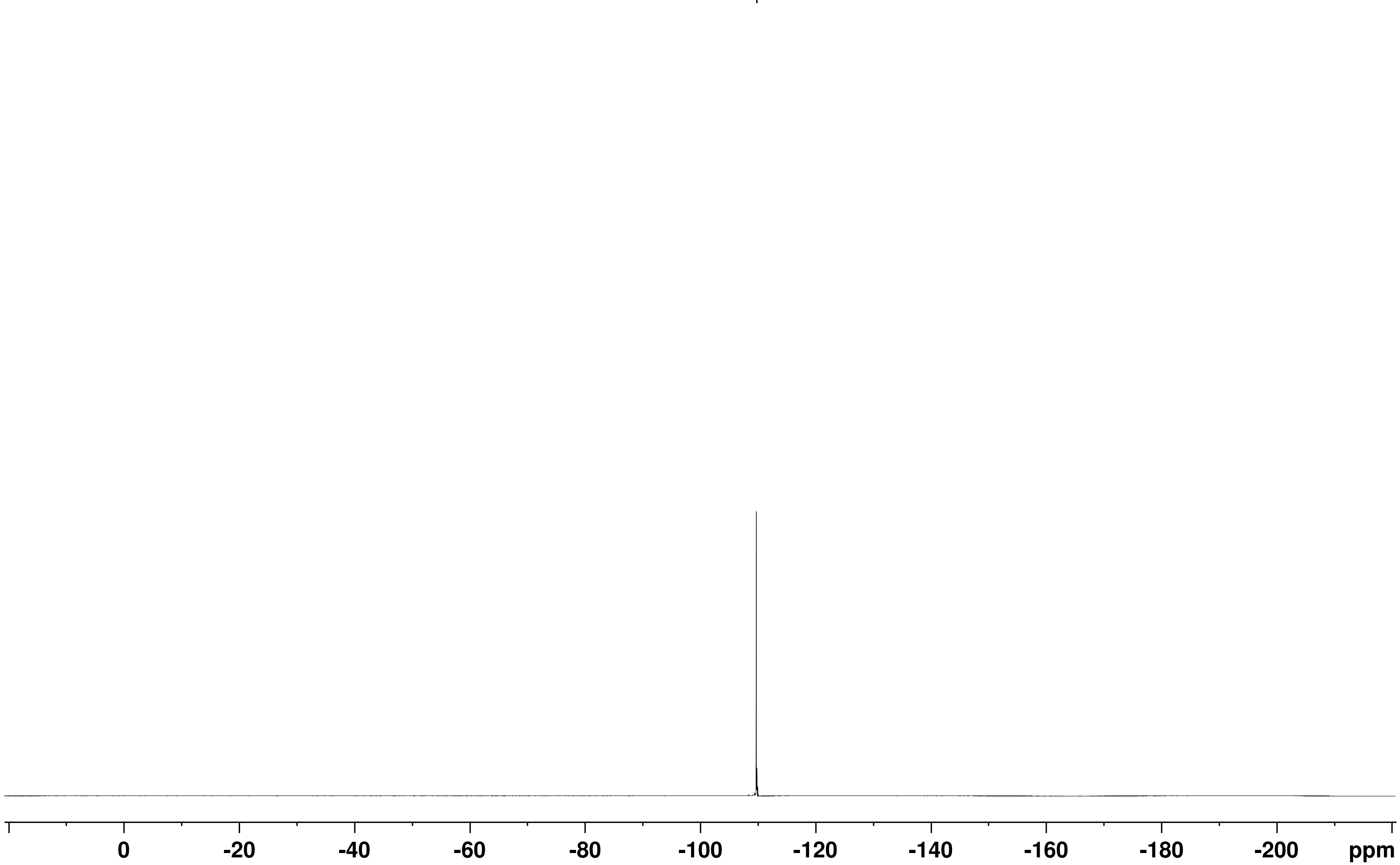
175.63
164.17
164.04
161.70
161.57
156.26
142.05
141.97
141.88
109.91
109.85
109.73
109.66
103.03
102.78
102.53
80.33
77.31
77.00
76.68
75.24
69.72
57.94
28.19
16.07
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

L9

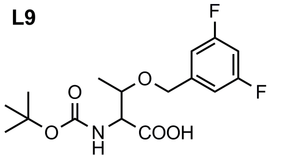


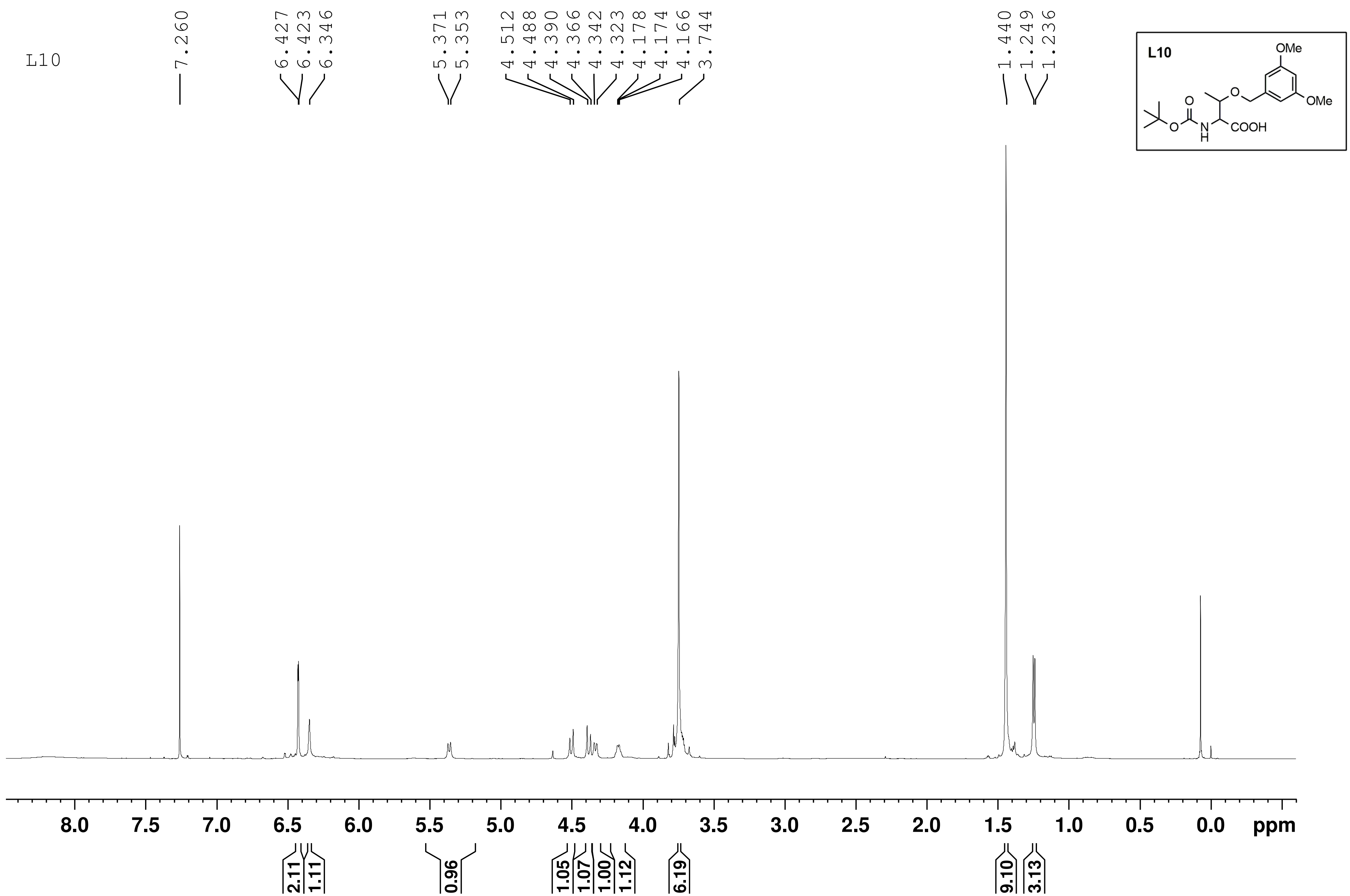
F
O
O
F
O
N
H
COOH

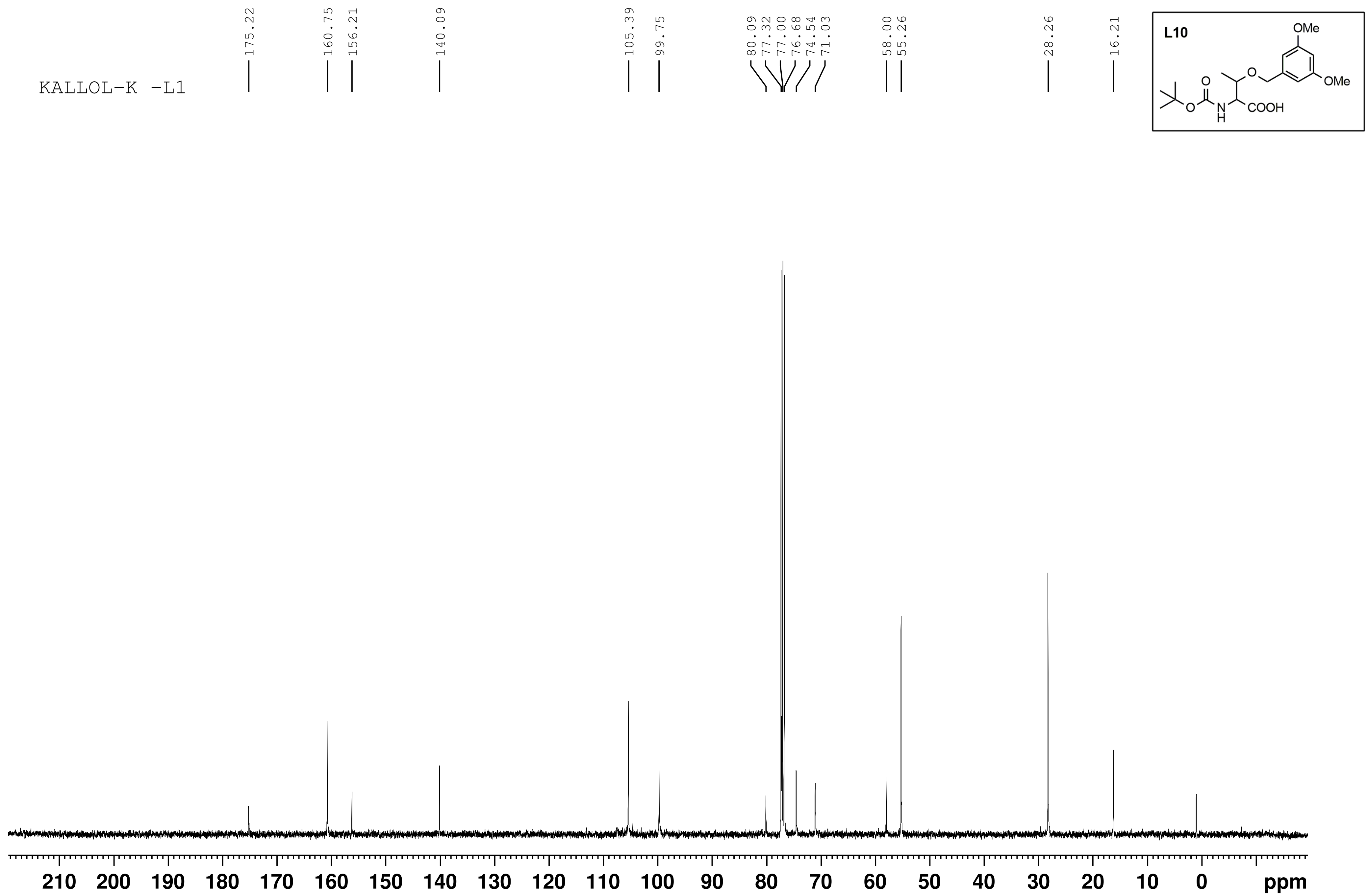
K-L9



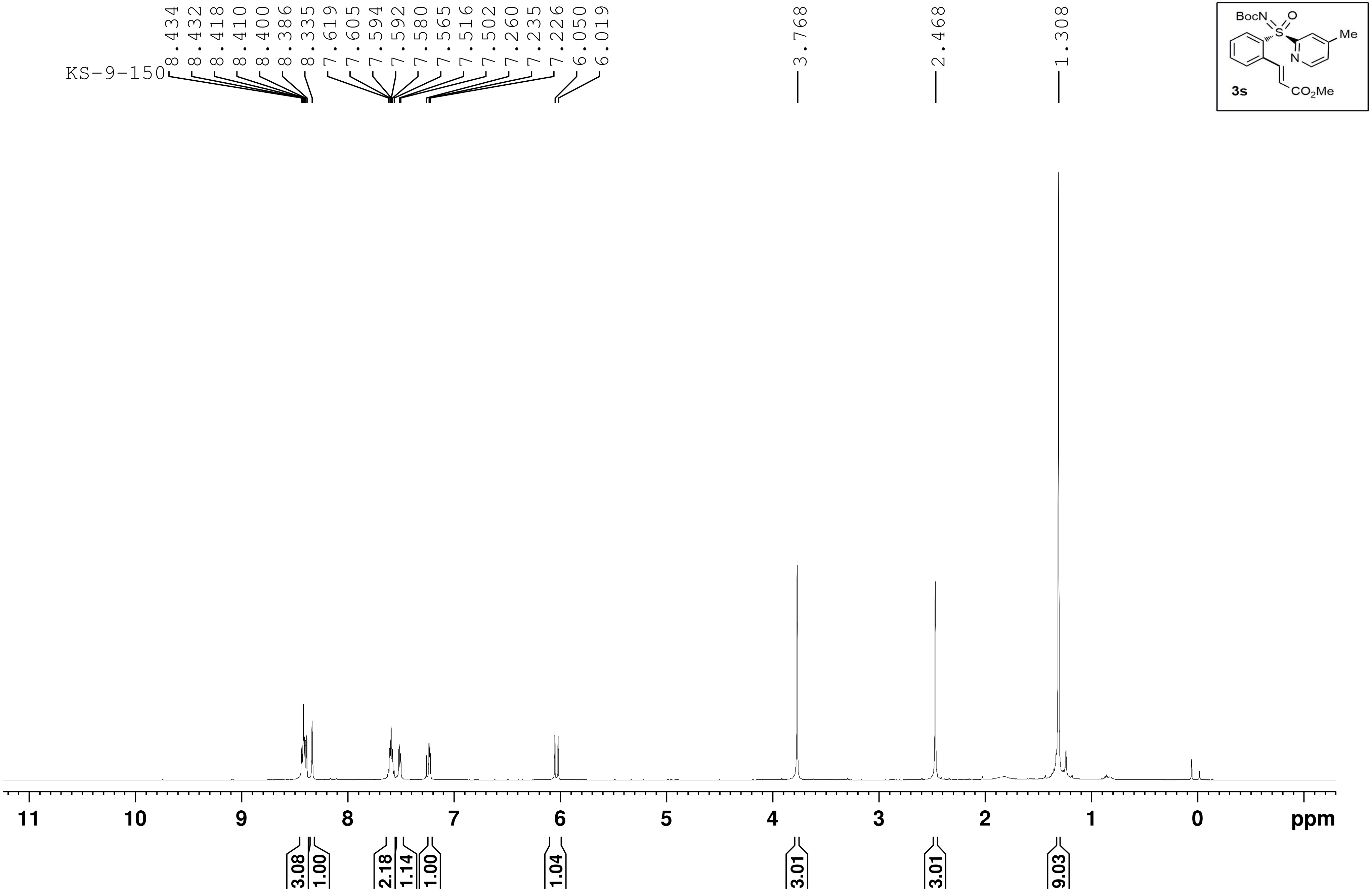
L9

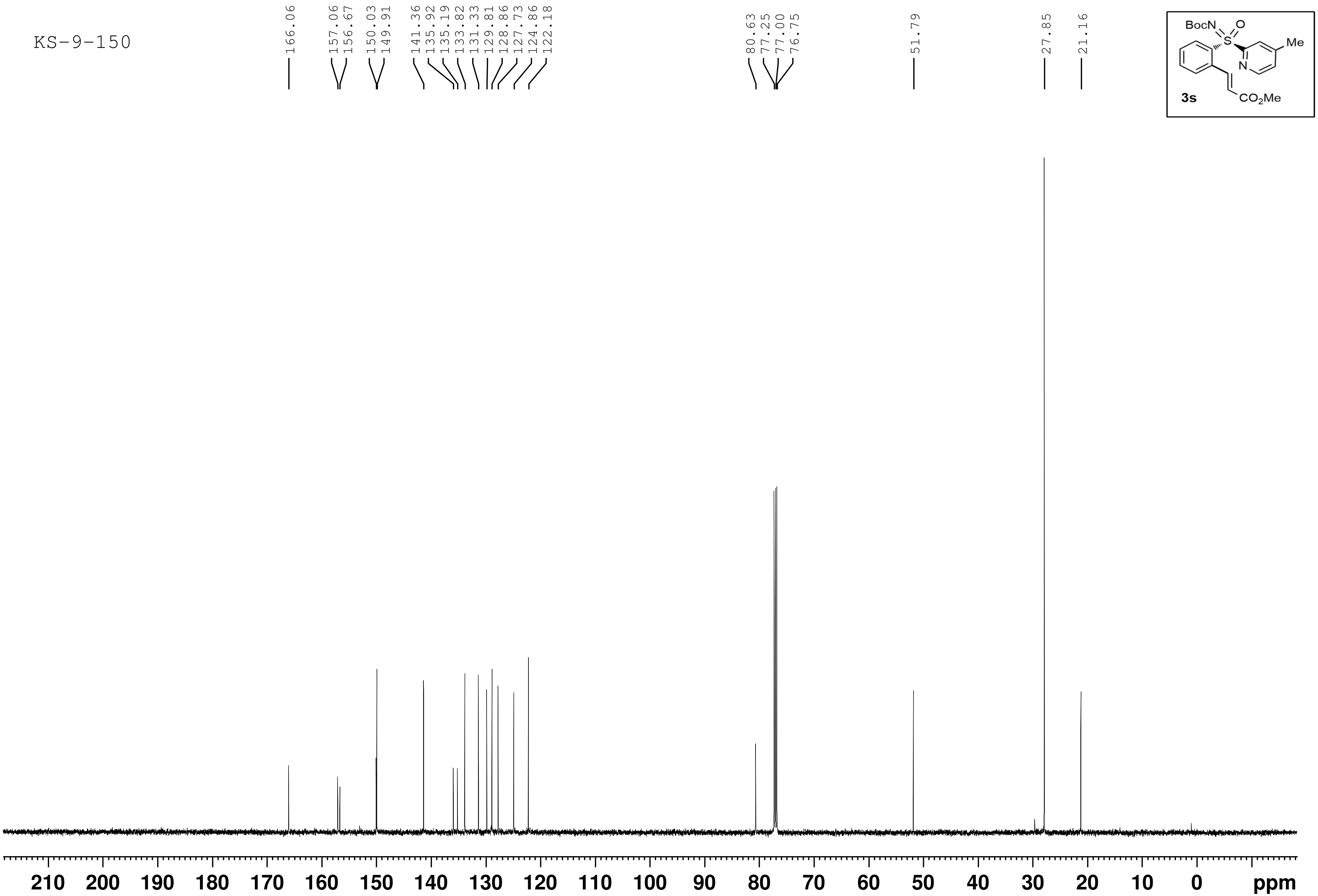


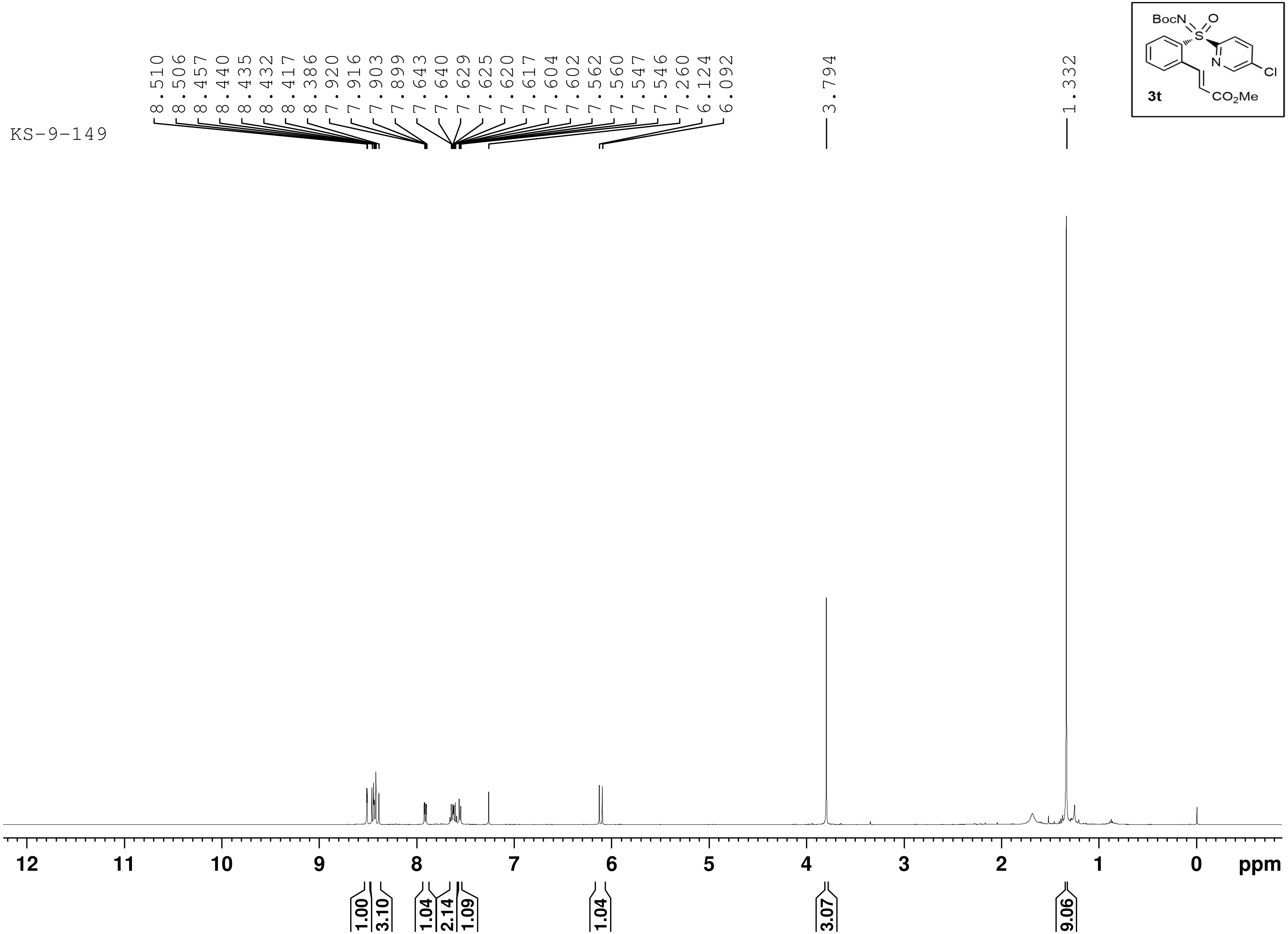

L10
7.260
6.427
6.423
6.346
5.371
5.353
4.512
4.488
4.390
4.366
4.342
4.323
4.178
4.174
4.166
3.744
1.440
1.249
1.236
OMe
O
O
N
H
O
COOH
OMe
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.11
1.11
0.96
1.05
1.07
1.00
1.12
6.19
9.10
3.13



KALLOL-K -L1
175.22
160.75
156.21
140.09
105.39
99.75
80.09
77.32
77.00
76.68
74.54
71.03
58.00
55.26
28.26
16.21
L10
OMe
OMe
O
O
N
H
COOH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


KS-9-150
8.434
8.432
8.418
8.410
8.400
8.386
8.335
7.619
7.605
7.594
7.592
7.580
7.565
7.516
7.502
7.260
7.235
7.226
6.050
6.019
3.768
2.468
1.308
BocN
O
S
N
Me
3s
CO2Me
11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.08
1.00
2.18
1.14
1.00
1.04
3.01
3.01
9.03


KS-9-150
166.06
157.06
156.67
150.03
149.91
141.36
135.92
135.19
133.82
131.33
129.81
128.86
127.73
124.86
122.18
80.63
77.25
77.00
76.75
51.79
27.85
21.16
BocN
O
S
Me
N
3s
CO2Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


KS-9-149
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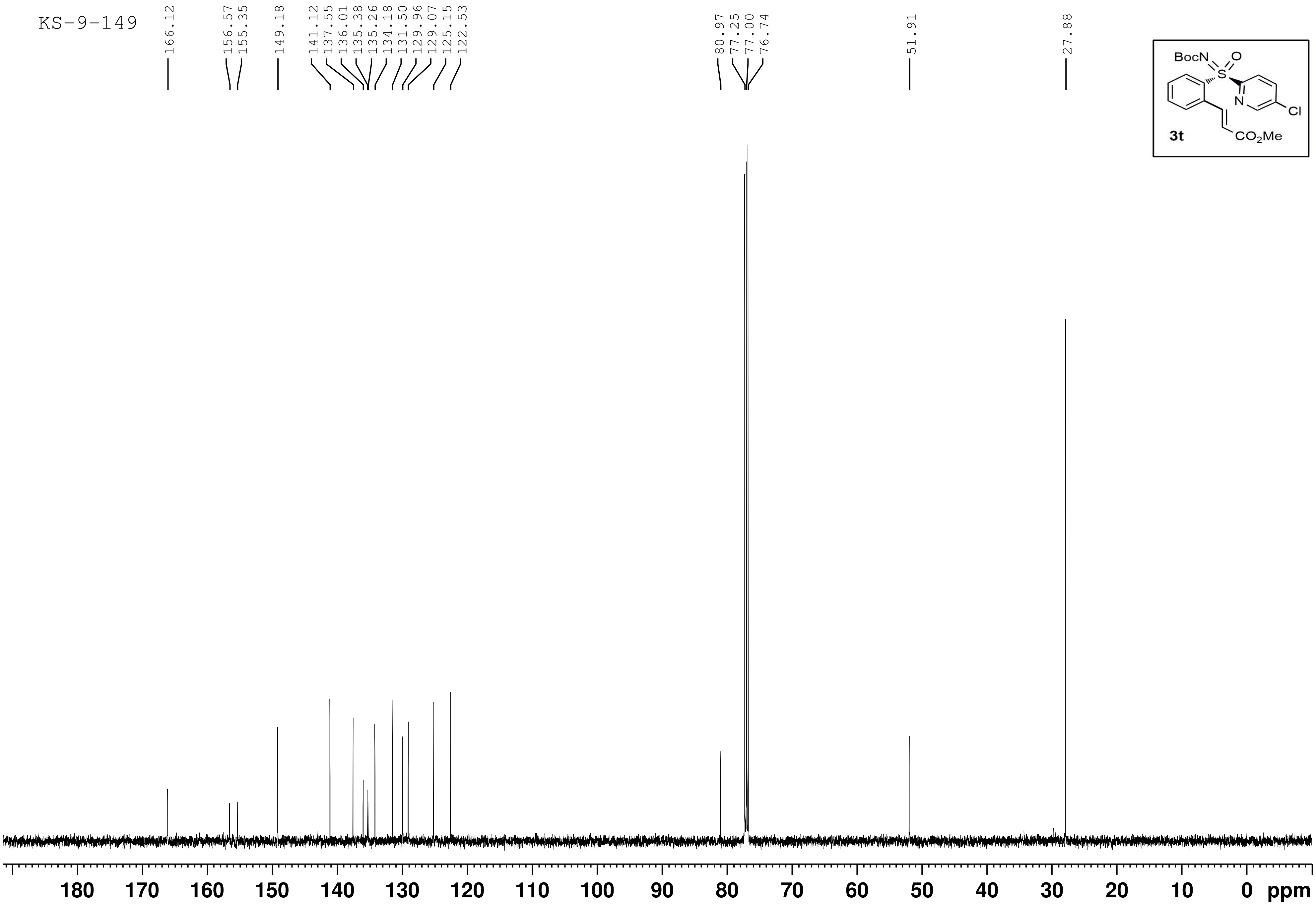
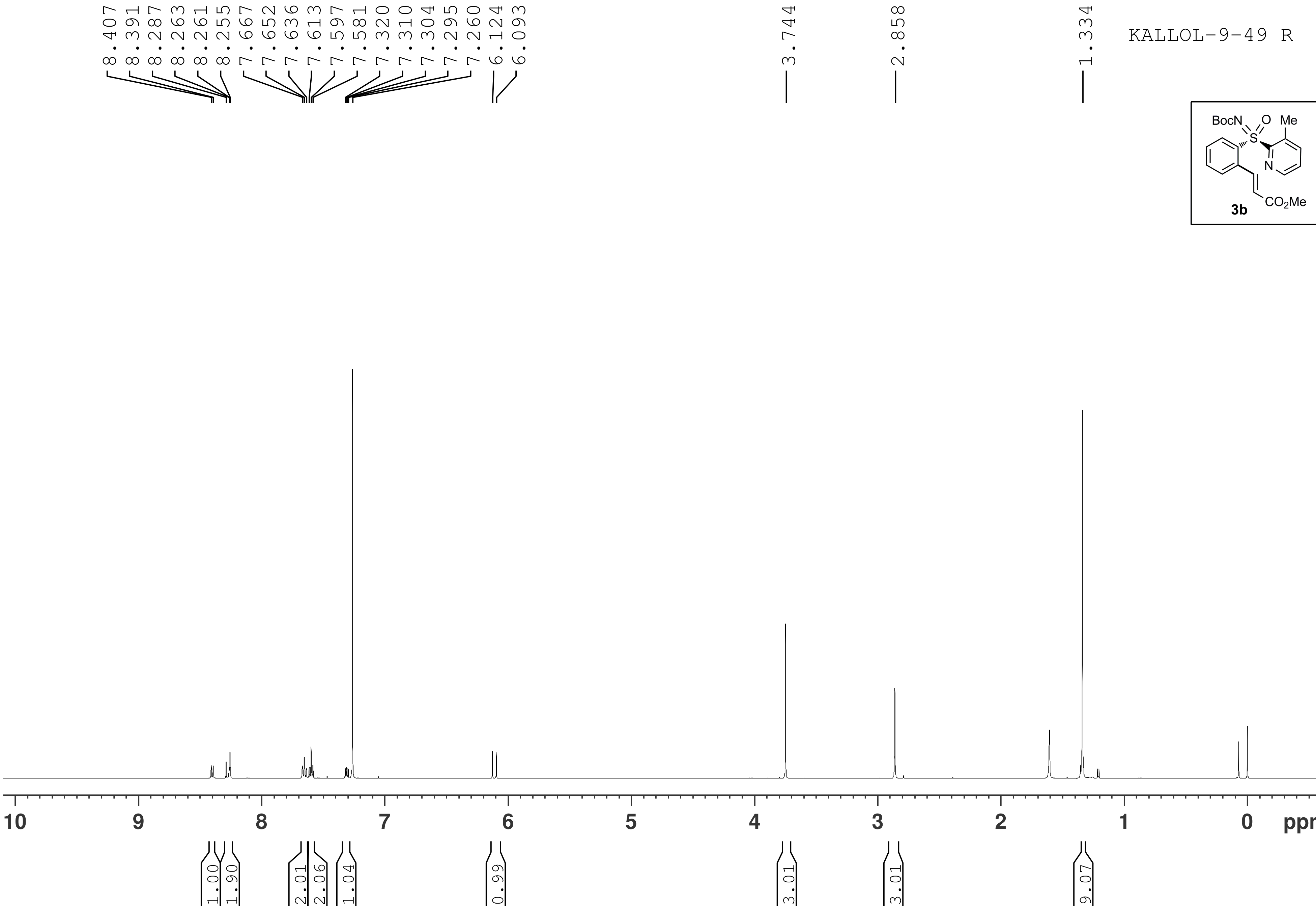
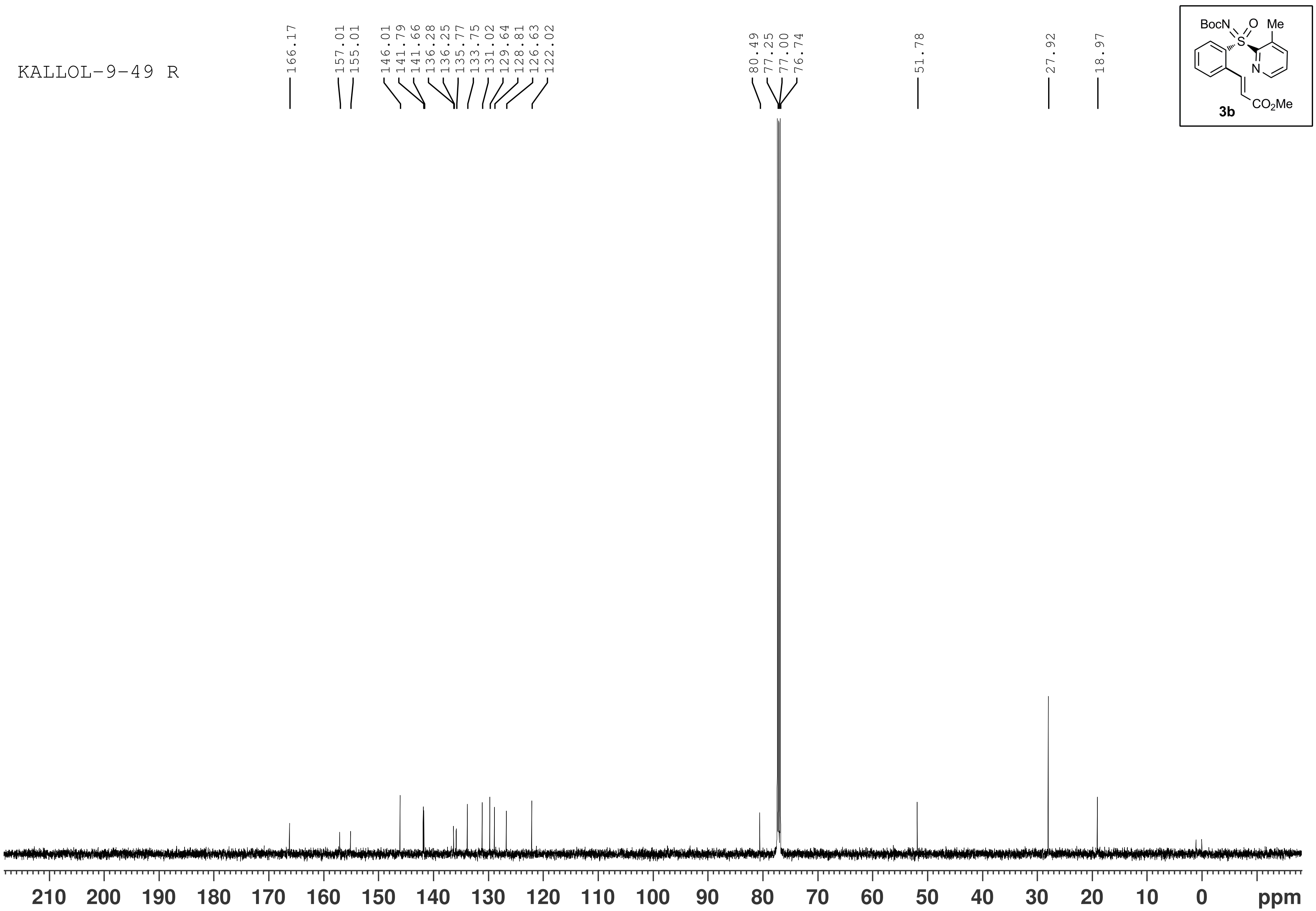
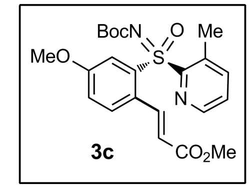
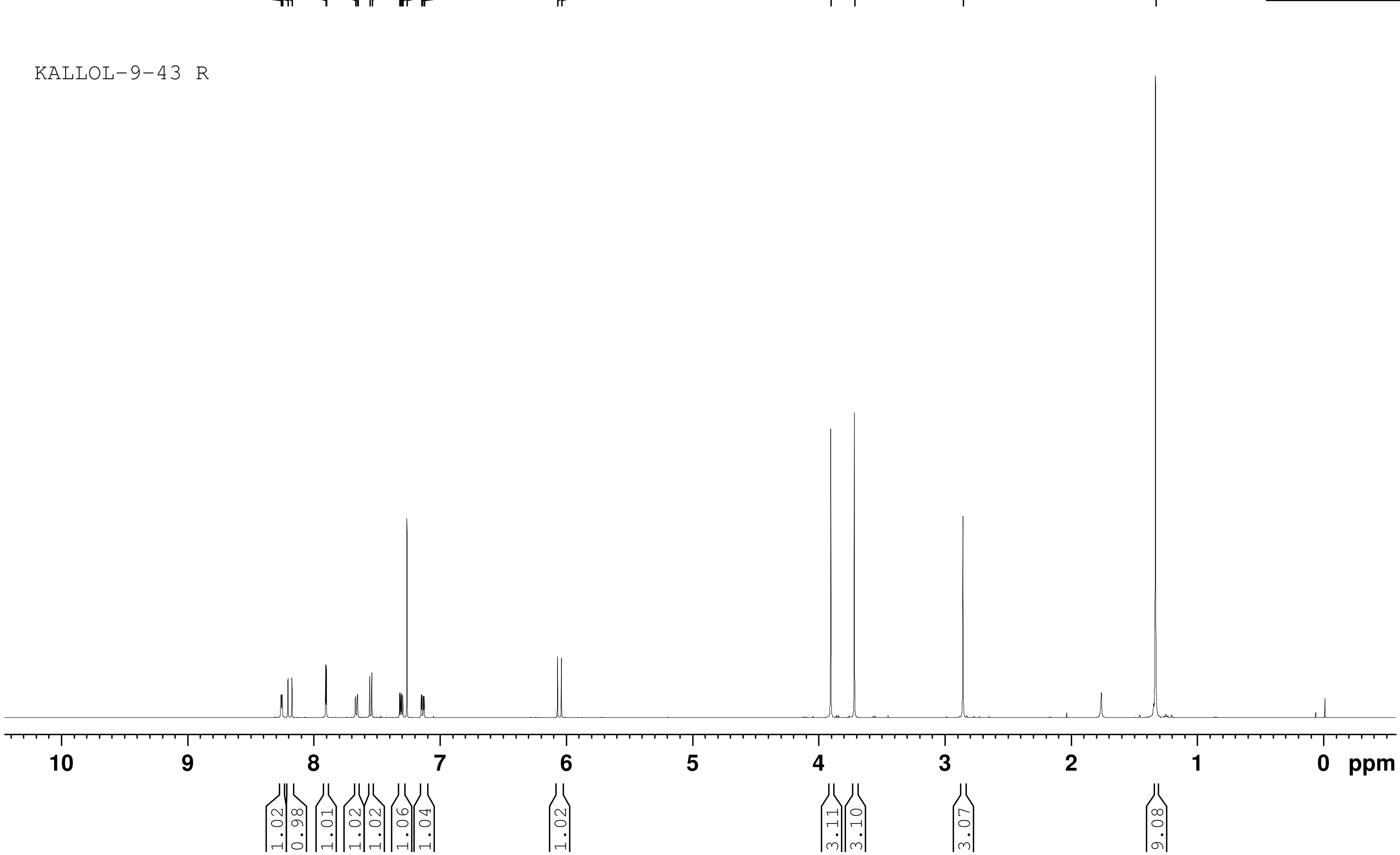
8.506
8.457
8.440
8.435
8.432
8.417
8.386
7.920
7.916
7.903
7.899
7.643
7.640
7.629
7.625
7.620
7.617
7.604
7.602
7.562
7.560
7.547
7.546
7.260
6.124
6.092
3.794
1.332
BocN
S
O
N
Cl
3t
CO2Me
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
3.10
1.04
2.14
1.09
1.04
3.07
9.06


KS-9-149
166.12
156.57
155.35
149.18
141.12
137.55
136.01
135.38
135.26
134.18
131.50
129.96
129.07
125.15
122.53
80.97
77.25
77.00
76.74
51.91
27.88
BocN
O
S
N
Cl
3t
CO_2Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

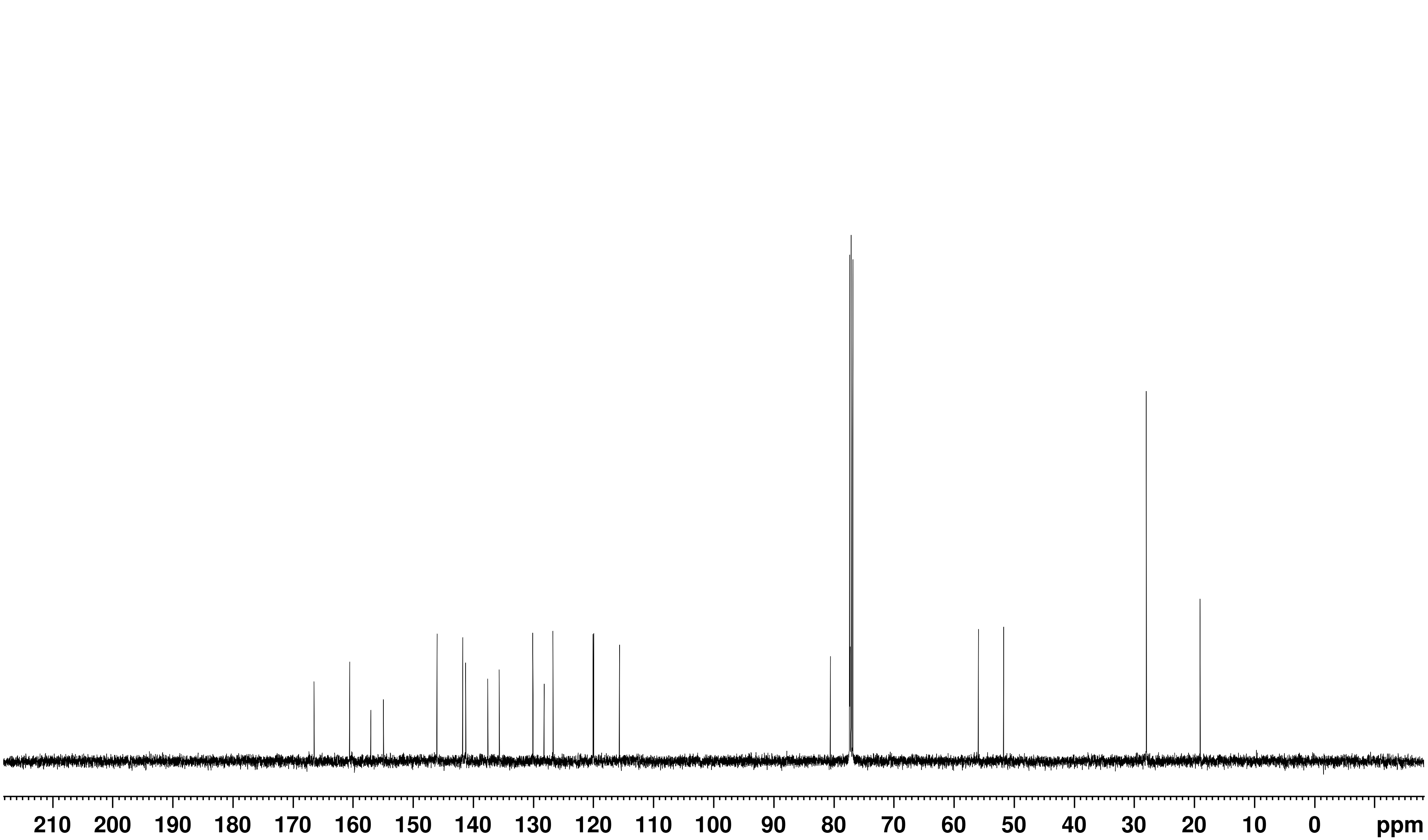

8.407
8.391
8.287
8.263
8.261
8.255
7.667
7.652
7.636
7.613
7.597
7.581
7.320
7.310
7.304
7.295
7.260
6.124
6.093
3.744
2.858
1.334
KALLOL-9-49 R
BocN
O
S
Me
N
CO_2Me
3b
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.90
2.01
2.06
1.04
0.99
3.01
3.01
9.07

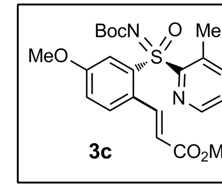

KALLOL-9-49 R
166.17
157.01
155.01
146.01
141.79
141.66
136.28
136.25
135.77
133.75
131.02
129.64
128.81
126.63
122.02
80.49
77.25
77.00
76.74
51.78
27.92
18.97
BocN
O
Me
S
N
CO2Me
3b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

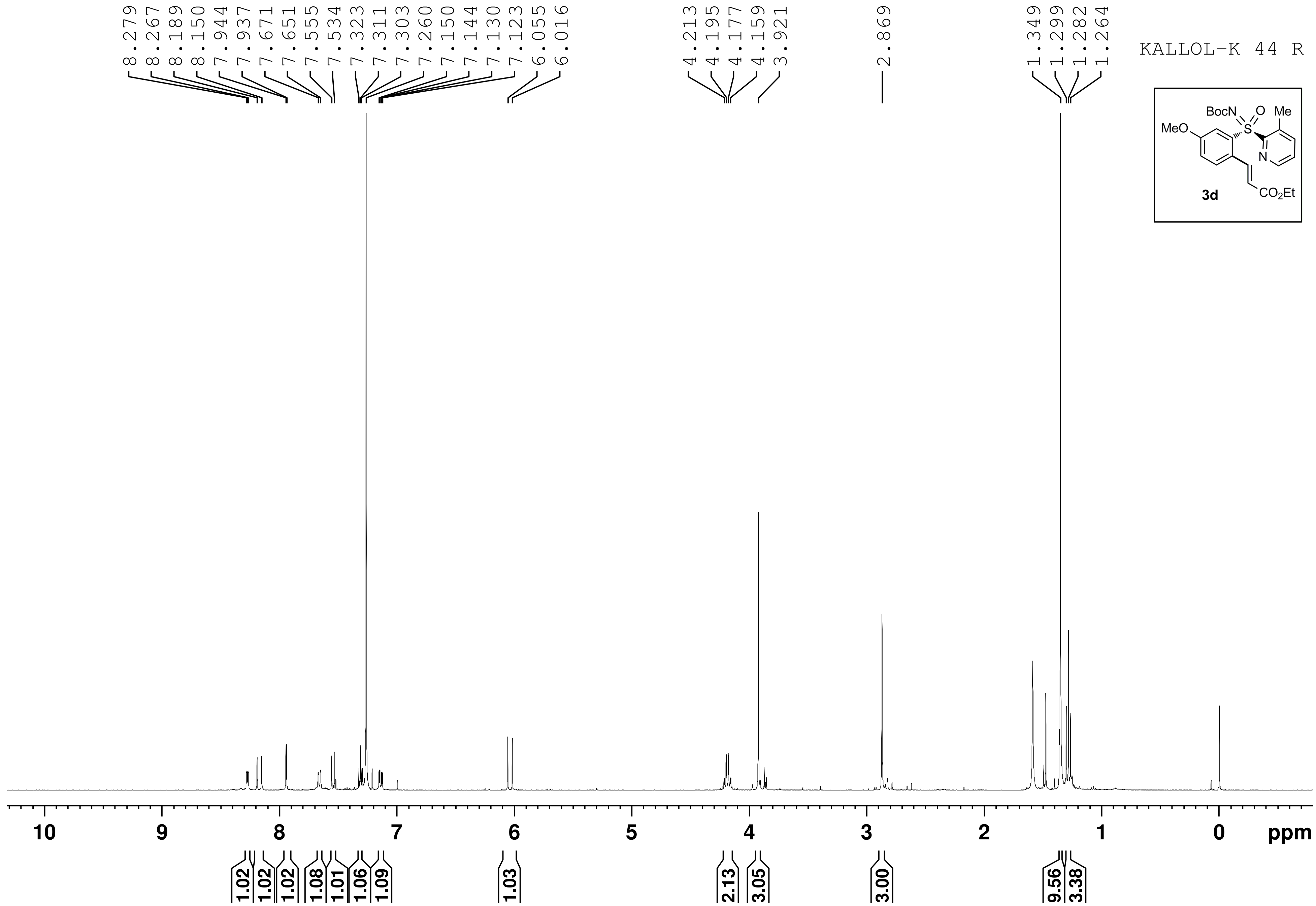

BocN
O
Me
MeO
S
N
CO2Me
3c

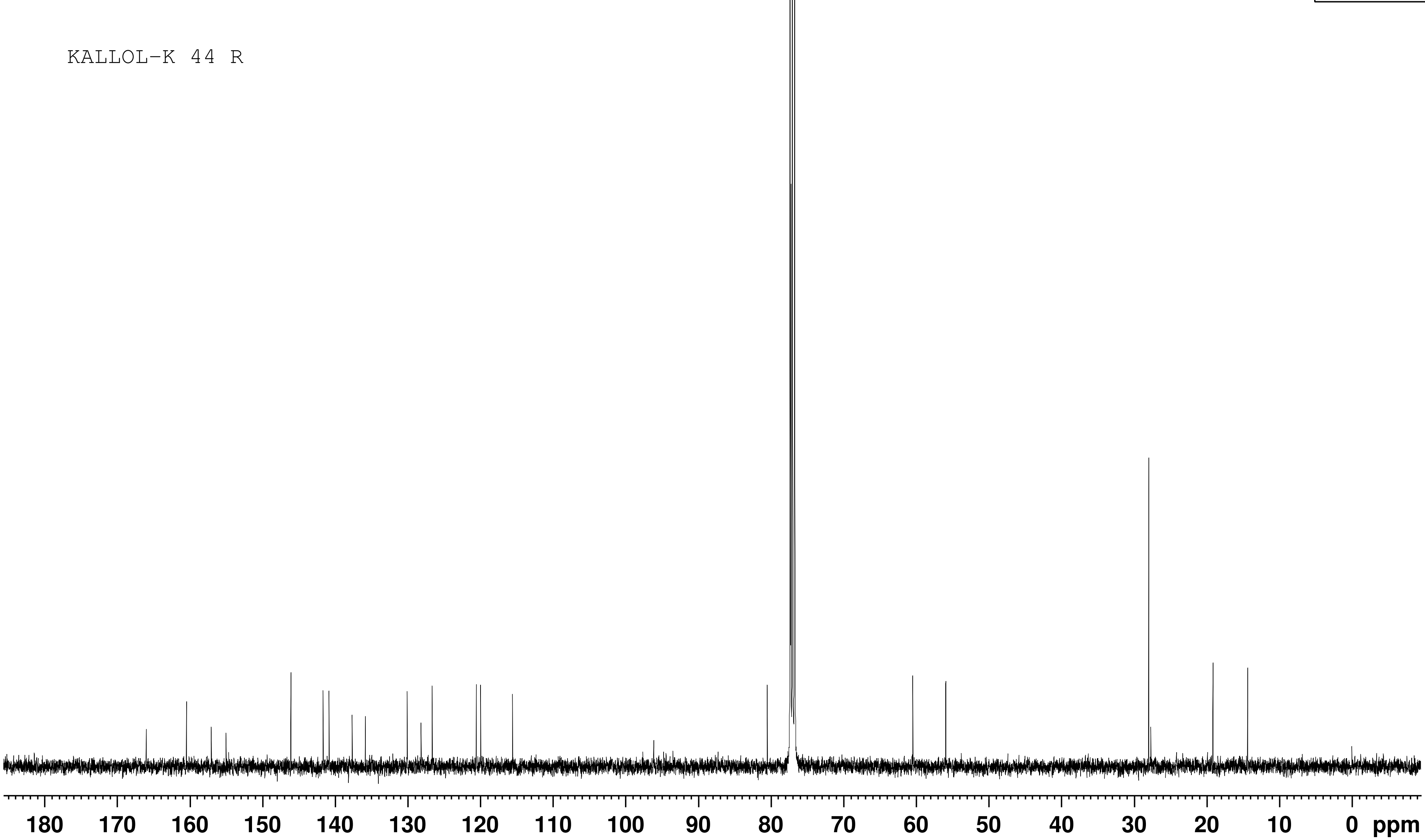

8.259
8.256
8.249
8.247
8.203
8.171
7.904
7.898
7.668
7.667
7.653
7.651
7.555
7.538
7.318
7.309
7.303
7.293
7.260
7.146
7.141
7.129
7.124
6.067
6.035
3.901
3.714
2.854
1.328
KALLOL-9-43 R
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
0.98
1.01
1.02
1.02
1.06
1.04
1.02
3.11
3.10
3.07
9.08

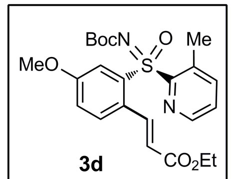
KALLOL-9-43 R


166.43
160.50
156.96
154.91
145.97
141.67
141.17
137.50
135.60
130.00
128.11
126.65
119.98
119.88
115.60
80.47
77.25
77.00
76.74
55.84
51.63
27.88
18.92
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

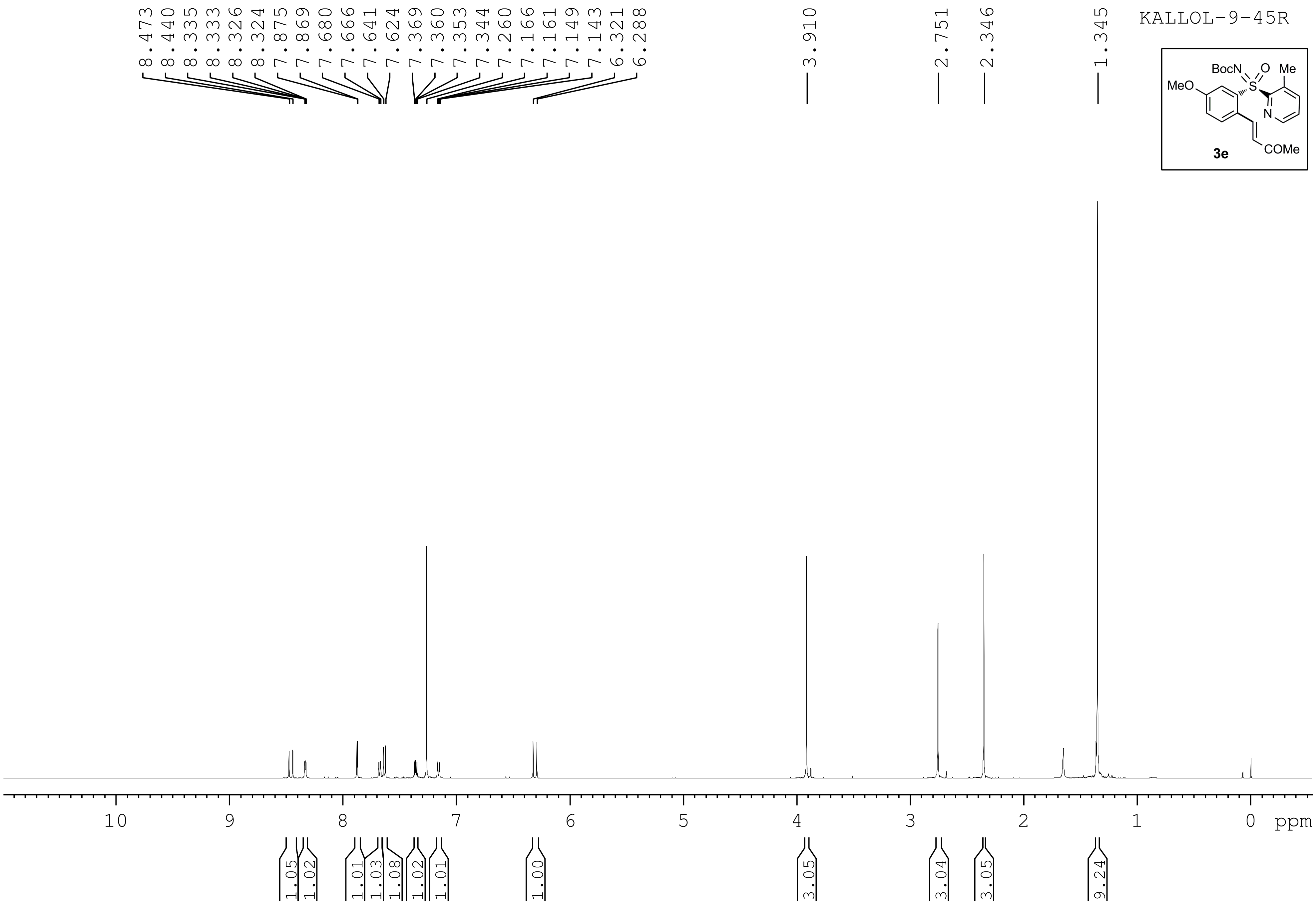

BocN
O
Me
MeO
S
N
3c
CO_2Me

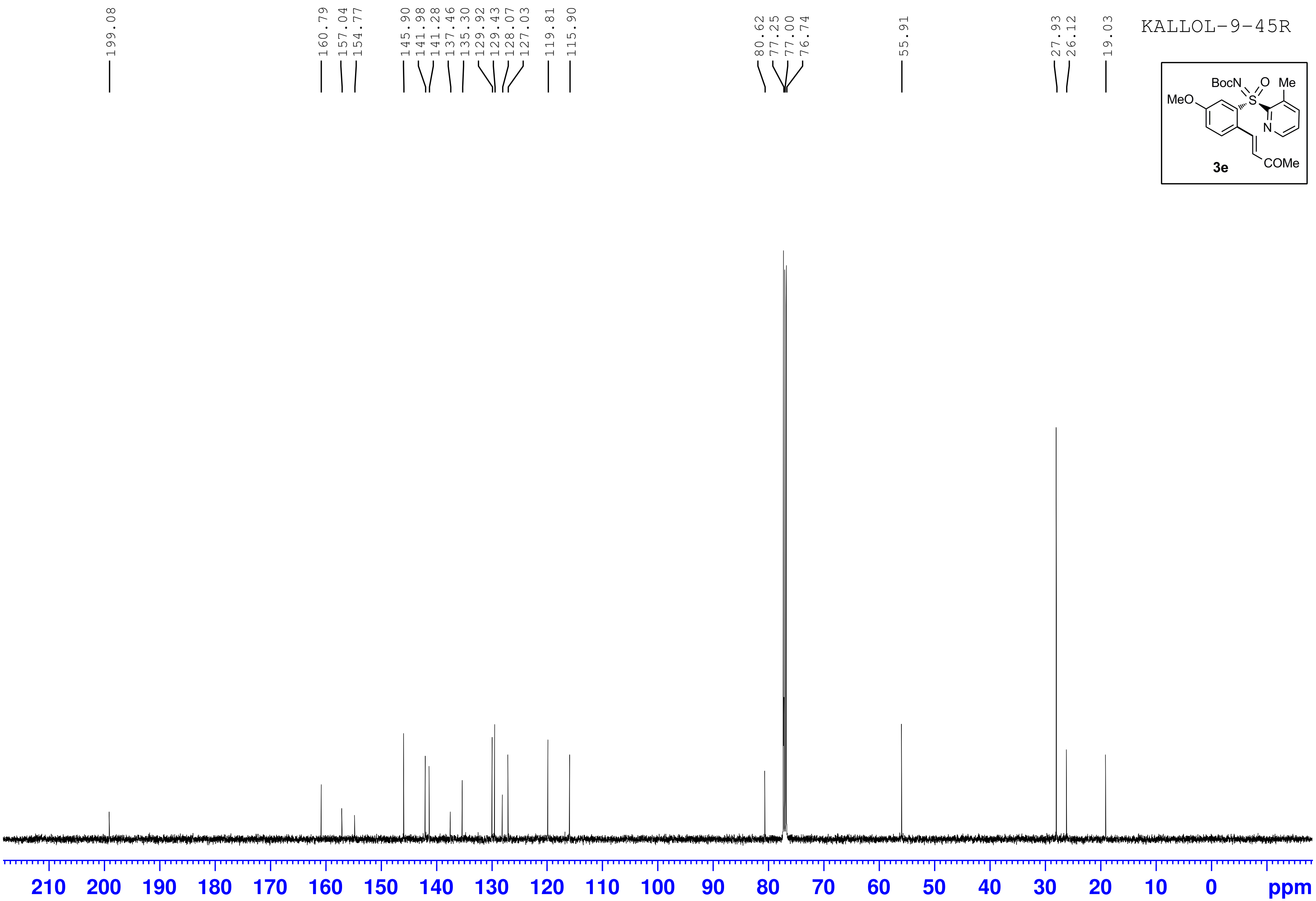

8.279
8.267
8.189
8.150
7.944
7.937
7.671
7.651
7.555
7.534
7.323
7.311
7.303
7.260
7.150
7.144
7.130
7.123
6.055
6.016
4.213
4.195
4.177
4.159
3.921
2.869
1.349
1.299
1.282
1.264
KALLOL-K 44 R
BocN
O
S
Me
MeO
N
CO2Et
3d
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
1.02
1.02
1.08
1.01
1.06
1.09
1.03
2.13
3.05
3.00
9.56
3.38

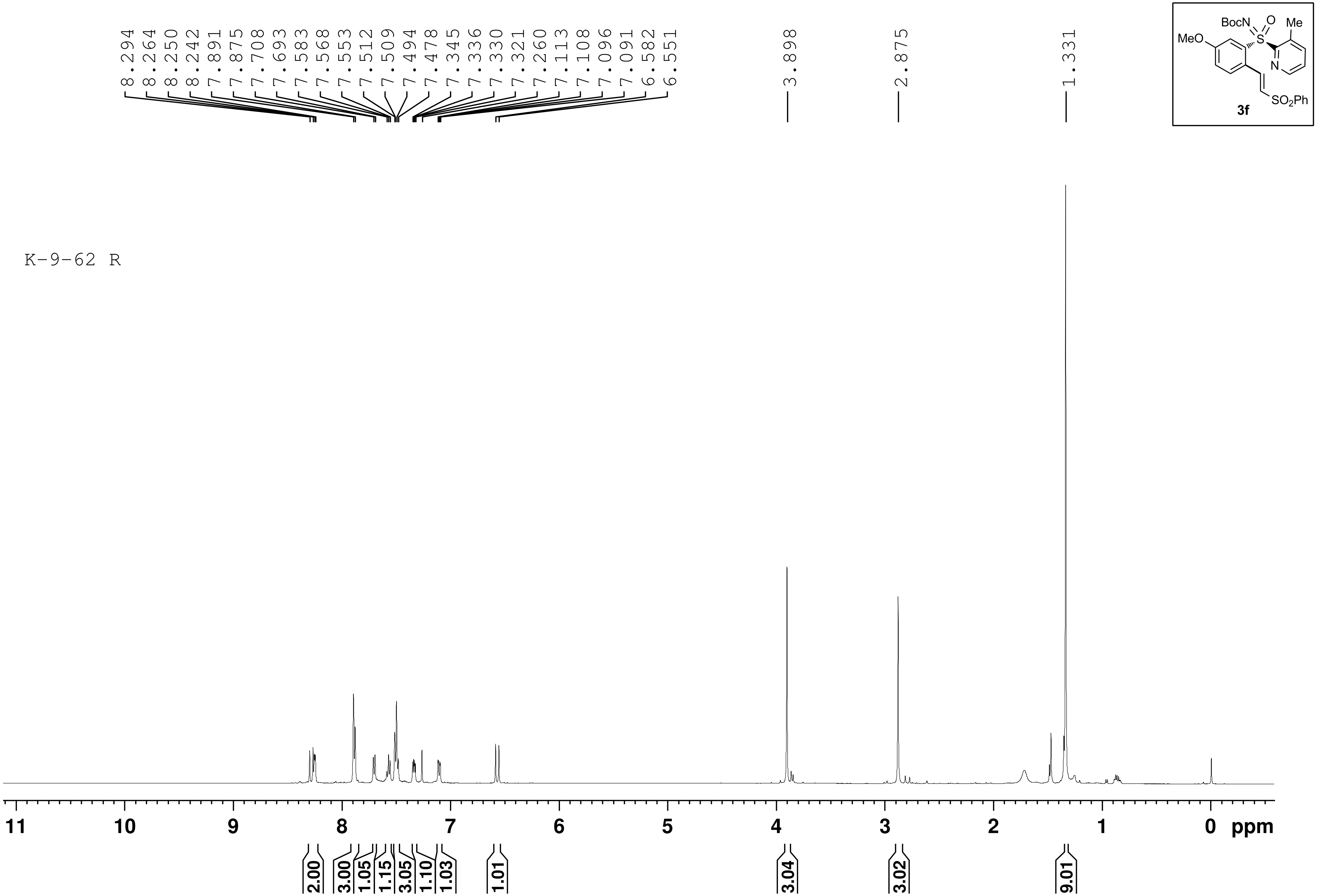

165.99
160.45
157.03
155.01
146.07
141.64
140.82
137.62
135.82
130.05
128.14
126.61
120.53
119.94
115.55
80.47
77.31
77.00
76.68
60.43
55.89
27.94
19.10
14.30
KALLOL-K 44 R
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


BocN
O
Me
MeO
S
N
CO2Et

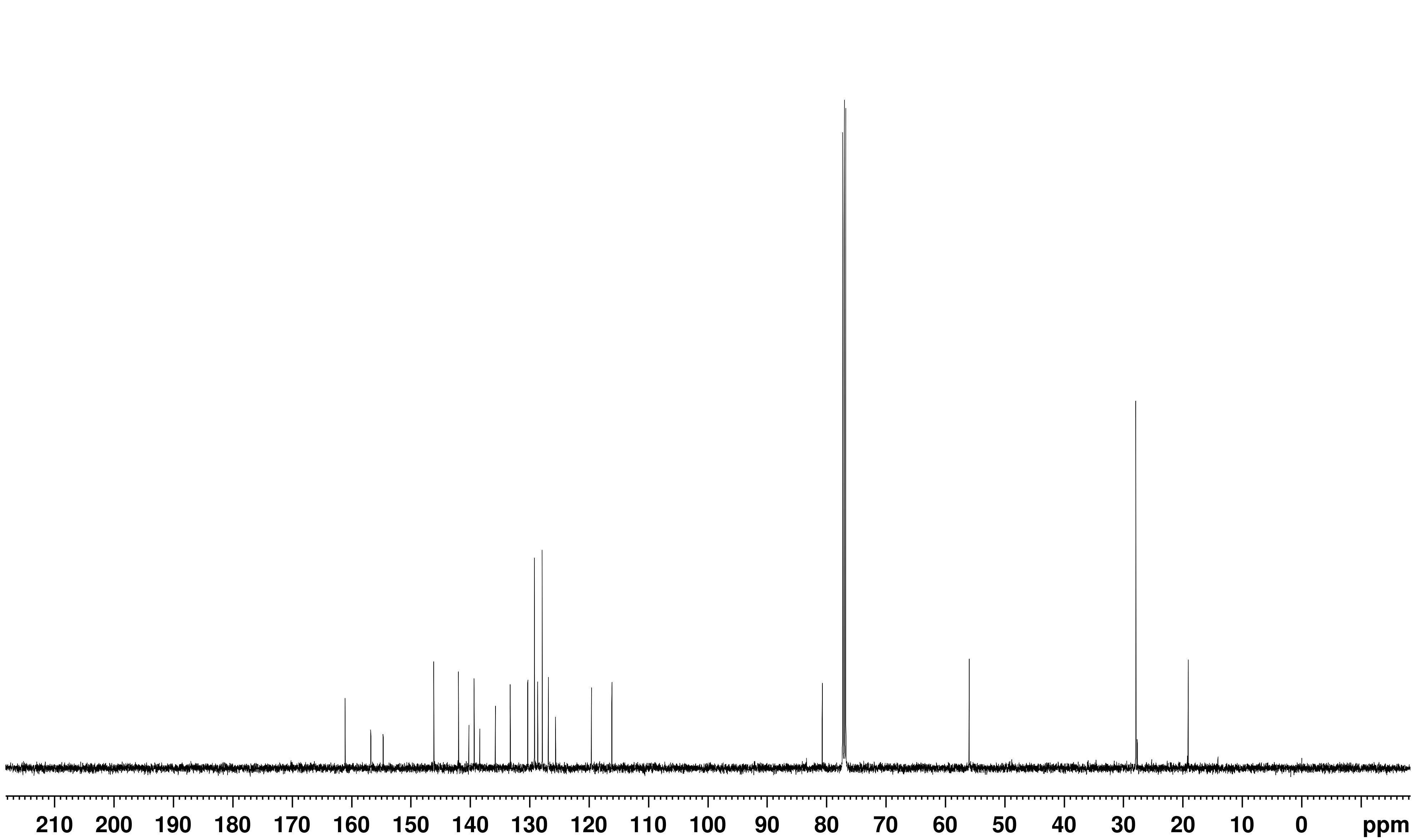
3d

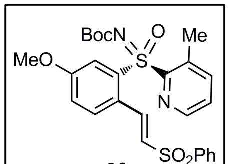

KALLOL-9-45R
8.473
8.440
8.335
8.333
8.326
8.324
7.875
7.869
7.680
7.666
7.641
7.624
7.369
7.360
7.353
7.344
7.260
7.166
7.161
7.149
7.143
6.321
6.288
3.910
2.751
2.346
1.345
BocN
O
Me
MeO
S
N
COMe
3e
10
9
8
7
6
5
4
3
2
1
0
ppm
1.05
1.02
1.01
1.03
1.08
1.02
1.01
1.00
3.05
3.04
3.05
9.24


199.08
160.79
157.04
154.77
145.90
141.98
141.28
137.46
135.30
129.92
129.43
128.07
127.03
119.81
115.90
80.62
77.25
77.00
76.74
55.91
27.93
26.12
19.03
KALLOL-9-45R
BocN
O
Me
MeO
S
N
COMe
3e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

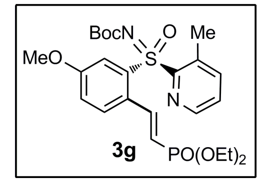

8.294
8.264
8.250
8.242
7.891
7.875
7.708
7.693
7.583
7.568
7.553
7.512
7.509
7.494
7.478
7.345
7.336
7.330
7.321
7.260
7.113
7.108
7.096
7.091
6.582
6.551
3.898
2.875
1.331
BocN
O
S
Me
MeO
N
SO2Ph
3f
K-9-62 R
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.00
1.05
1.15
3.05
1.10
1.03
1.01
3.04
3.02
9.01

K-9-62 R


161.07
156.73
154.65
146.13
141.97
140.22
139.33
138.37
135.75
133.24
130.31
129.19
128.63
127.87
126.82
125.62
119.56
116.13
80.69
77.25
77.00
76.74
55.94
27.87
19.06
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

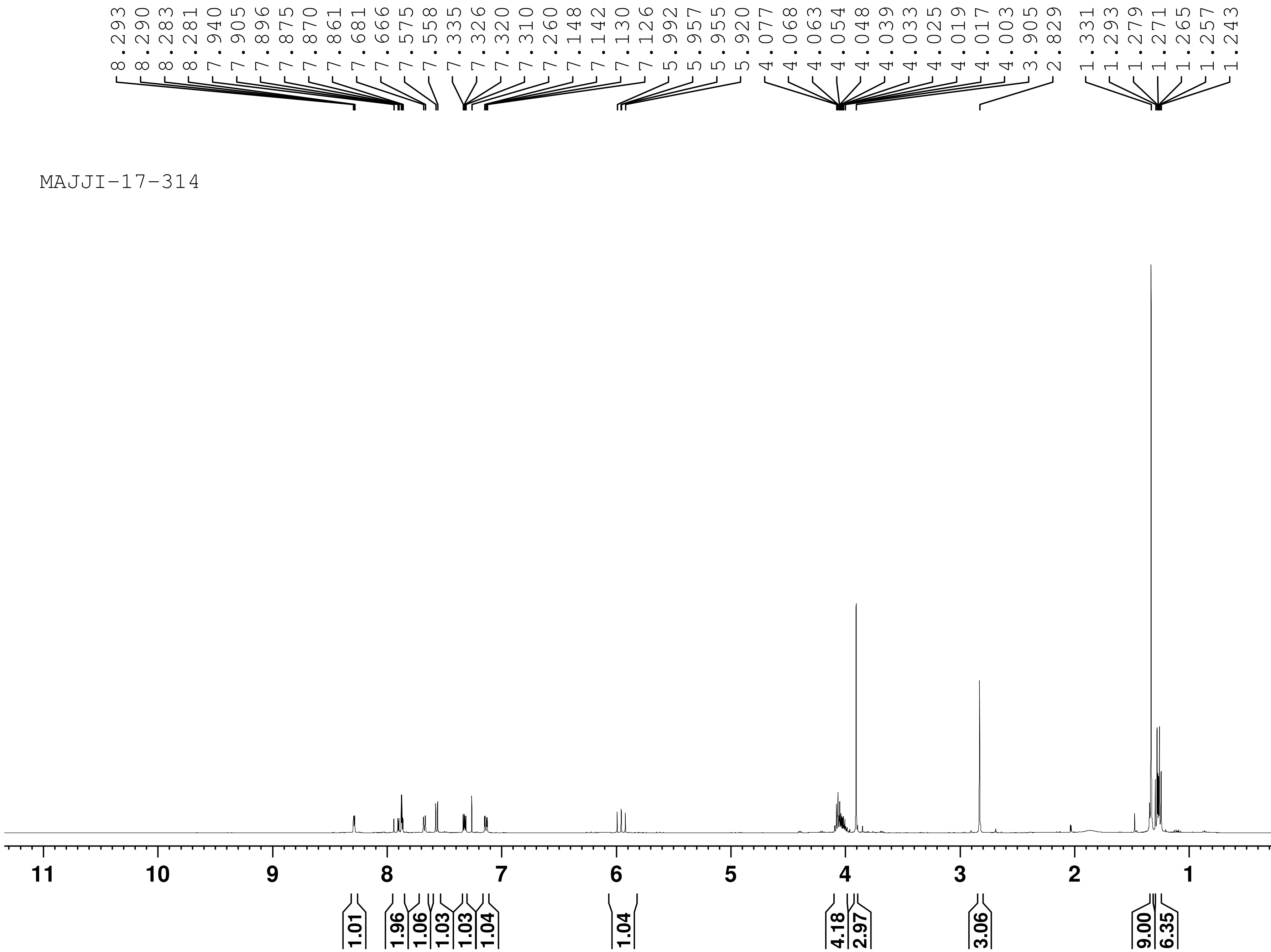

BocN
O
Me
MeO
S
N
SO2Ph

3f

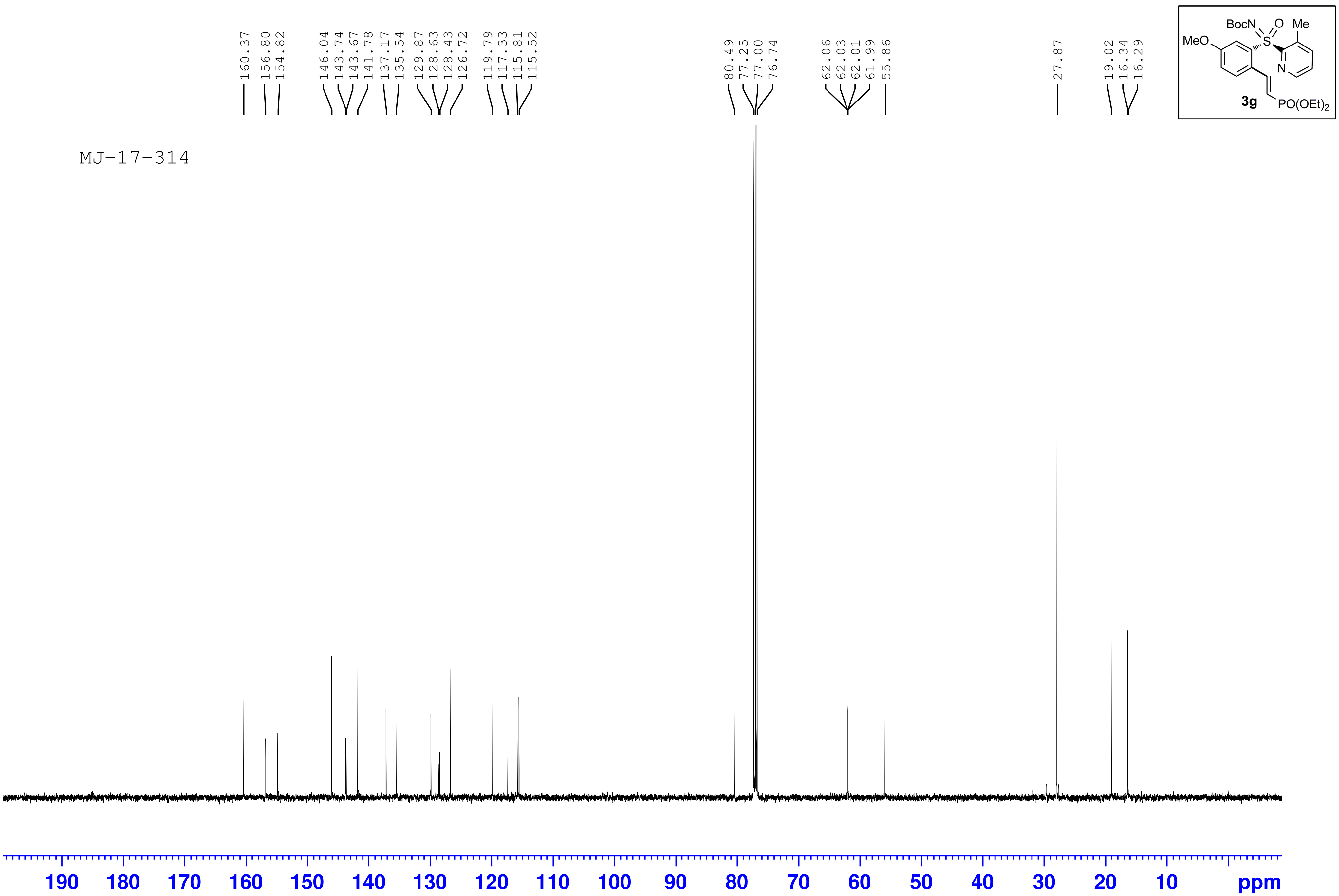


3g

MAJJI-17-314



MJ-17-314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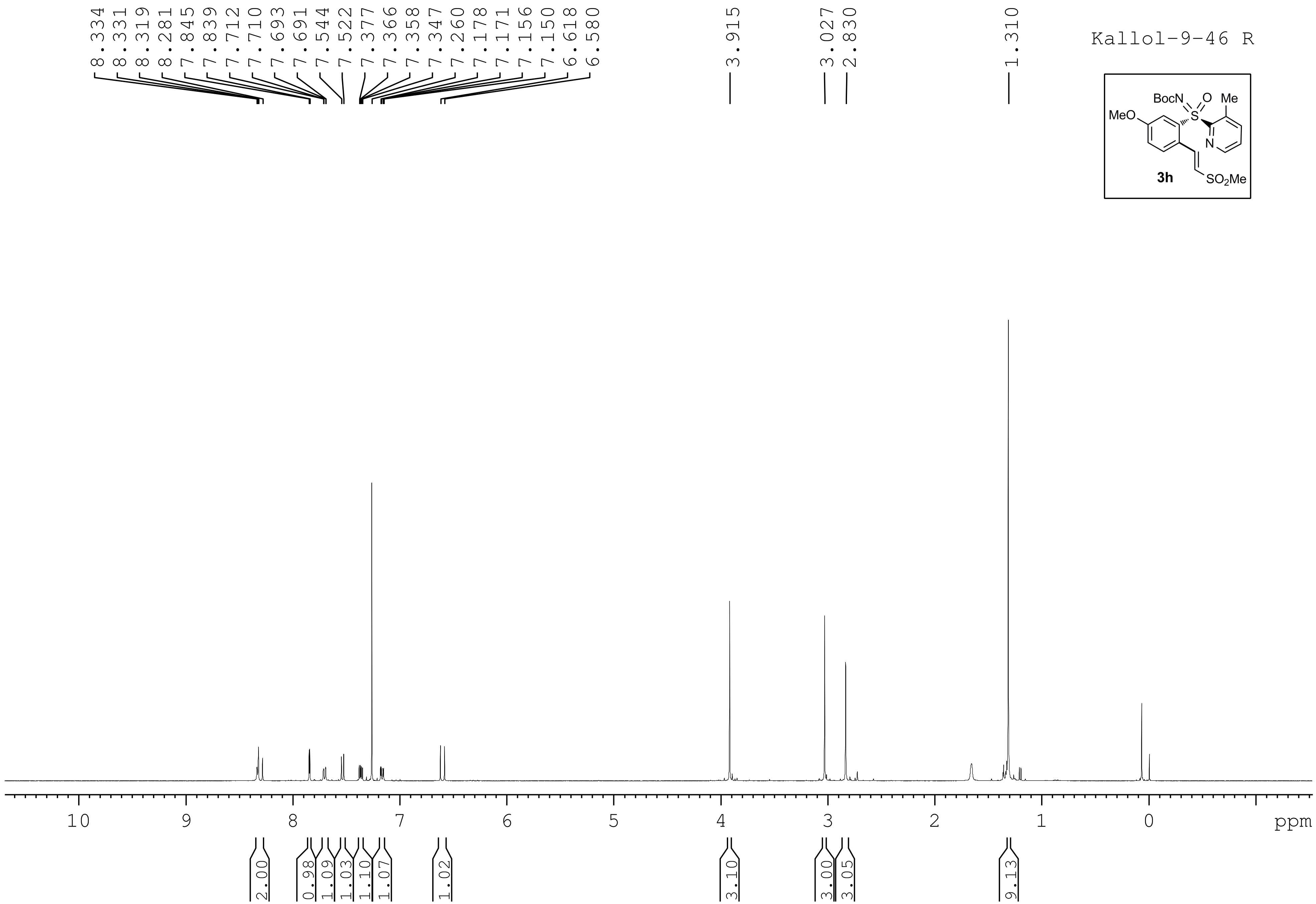
156.80
154.82
146.04
143.74
143.67
141.78
137.17
135.54
129.87
128.63
128.43
126.72
119.79
117.33
115.81
115.52
80.49
77.25
77.00
76.74
62.06
62.03
62.01
61.99
55.86
27.87
19.02
16.34
16.29
BocN
O
Me
MeO
S
N
3g
PO(OEt)2
ppm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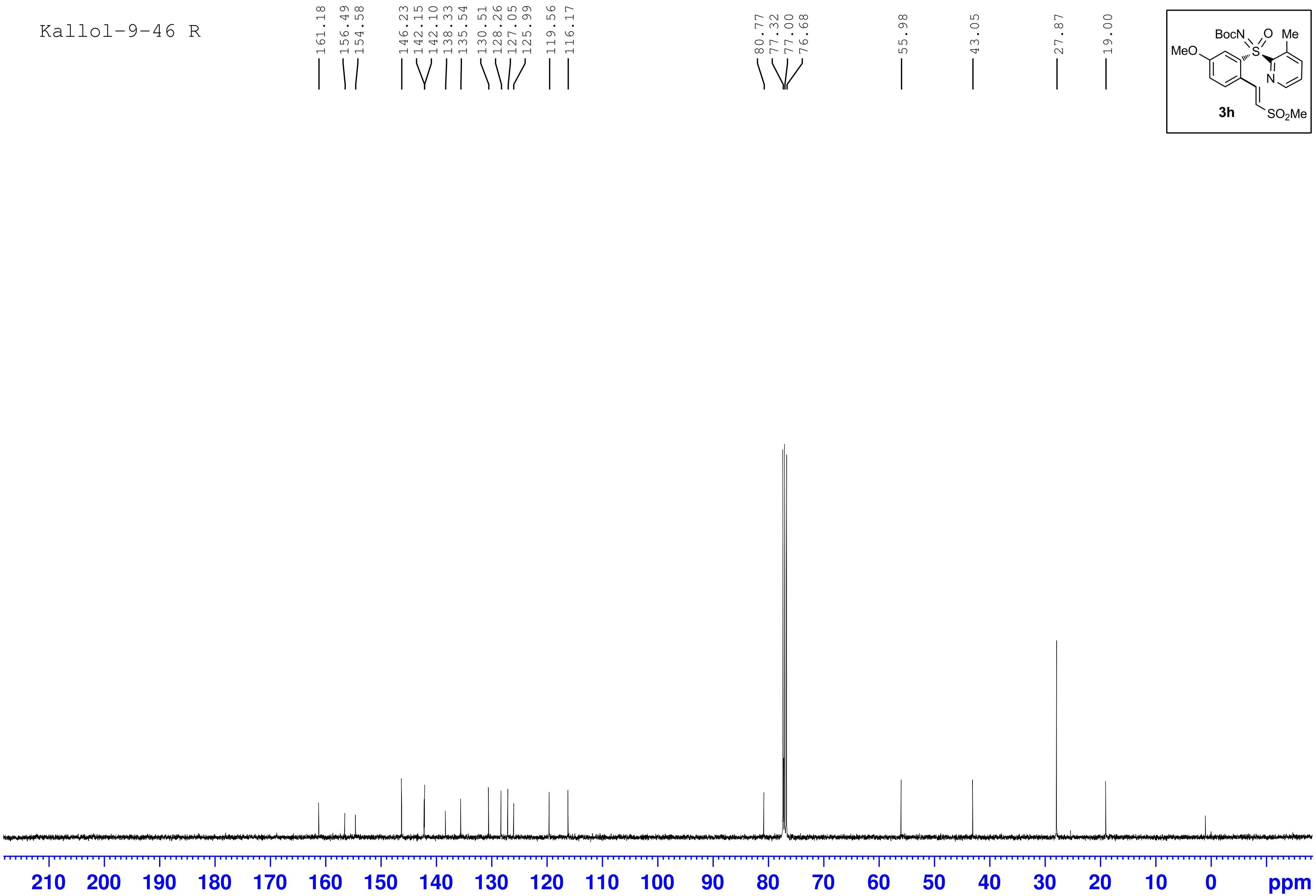
8.331
8.319
8.281
7.845
7.839
7.712
7.710
7.693
7.691
7.544
7.522
7.377
7.366
7.358
7.347
7.260
7.178
7.171
7.156
7.150
6.618
6.580
3.915
3.027
2.830
1.310
Kallol-9-46 R
BocN
O
Me
MeO
S
N
3h
SO2Me
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
0.98
1.09
1.03
1.10
1.07
1.02
3.10
3.00
3.05
9.13



Kallol-9-46 R
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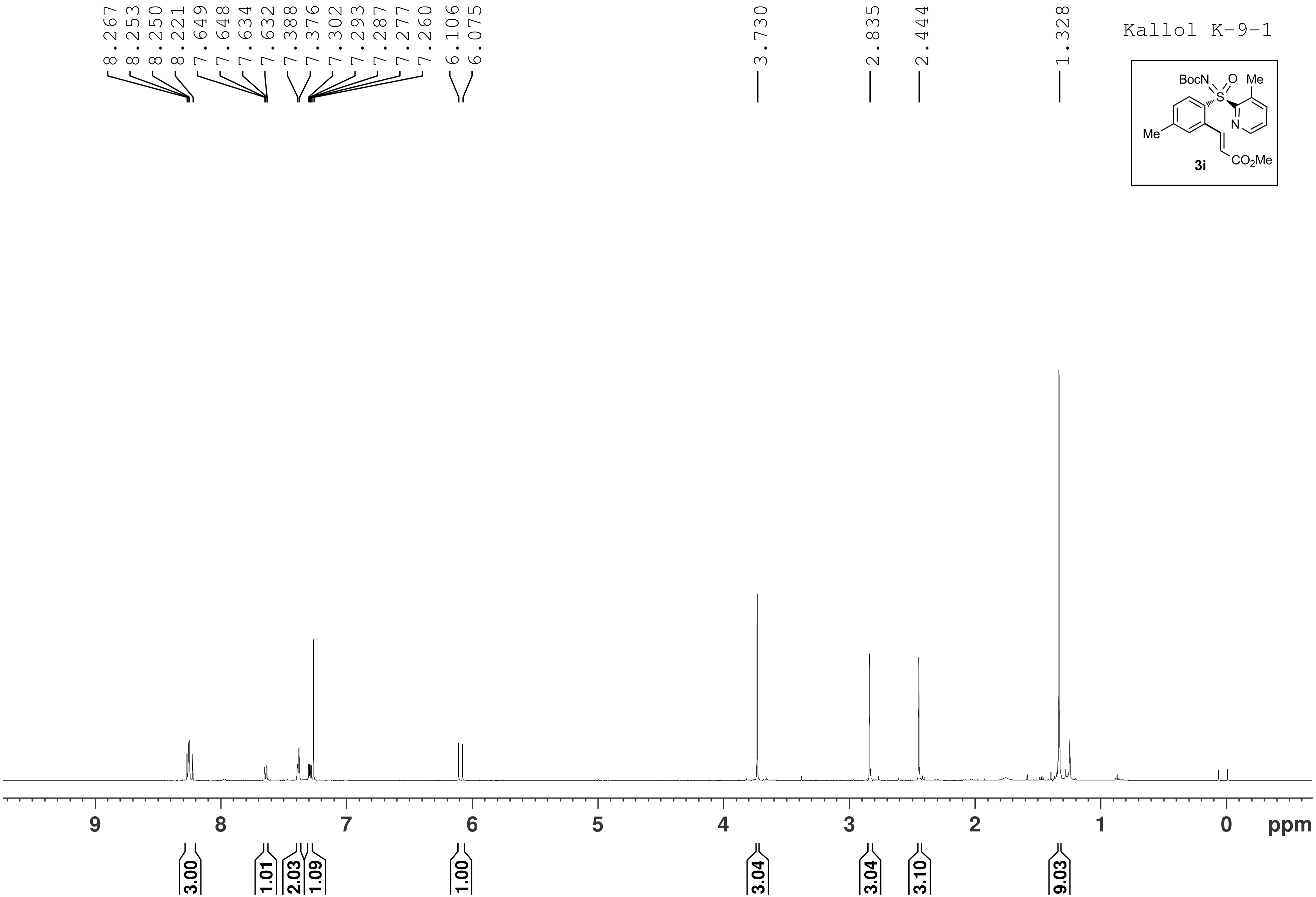
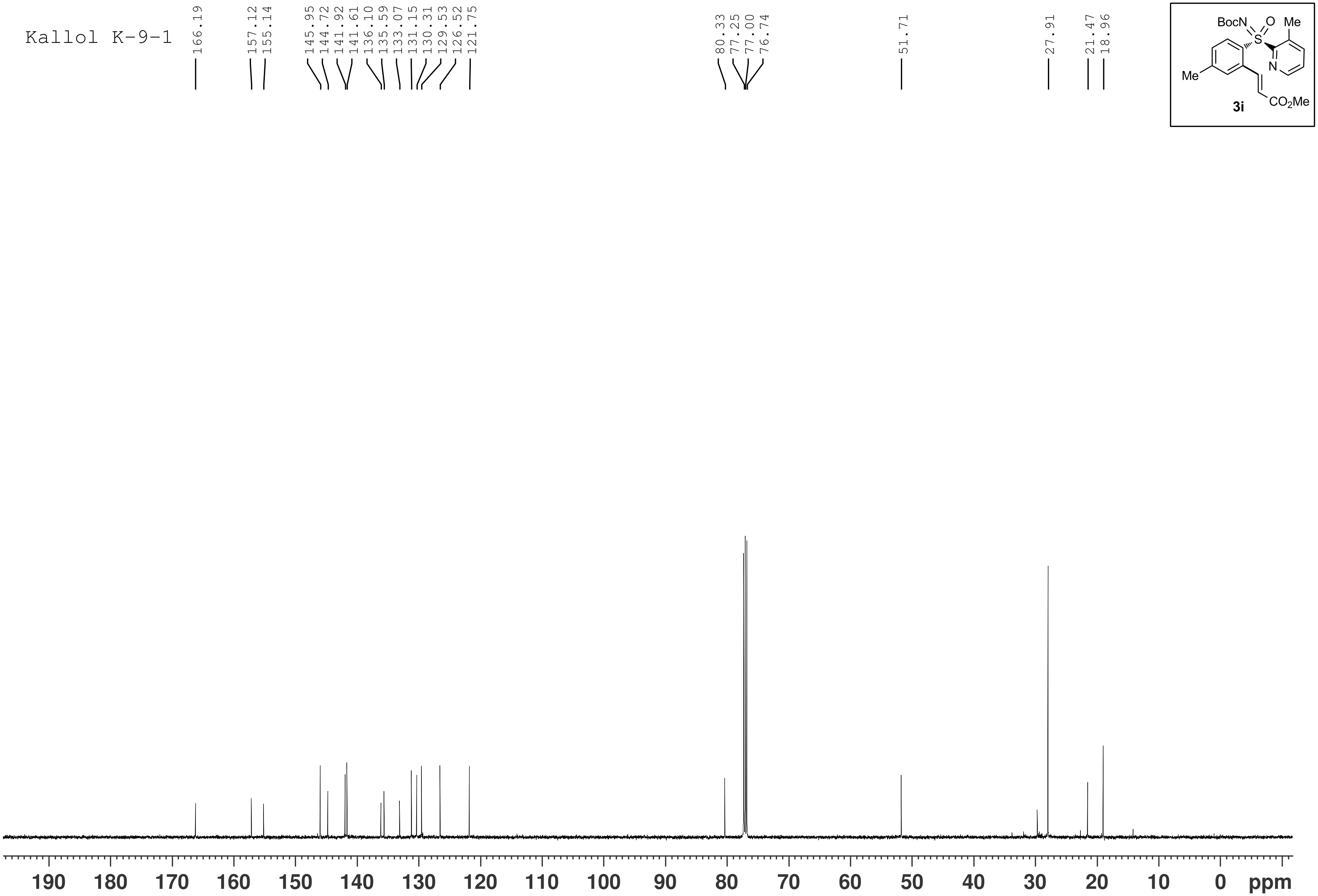
154.58
146.23
142.15
142.10
138.33
135.54
130.51
128.26
127.05
125.99
119.56
116.17
80.77
77.32
77.00
76.68
55.98
43.05
27.87
19.00
BocN
O
Me
MeO
S
N
3h
SO2Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.267
8.253
8.250
8.221
7.649
7.648
7.634
7.632
7.388
7.376
7.302
7.293
7.287
7.277
7.260
6.106
6.075
3.730
2.835
2.444
1.328
Kallol K-9-1
BocN
O
S
Me
N
Me
CO_2Me
3i
9
8
7
6
5
4
3
2
1
0
ppm
3.00
1.01
2.03
1.09
1.00
3.04
3.04
3.10
9.03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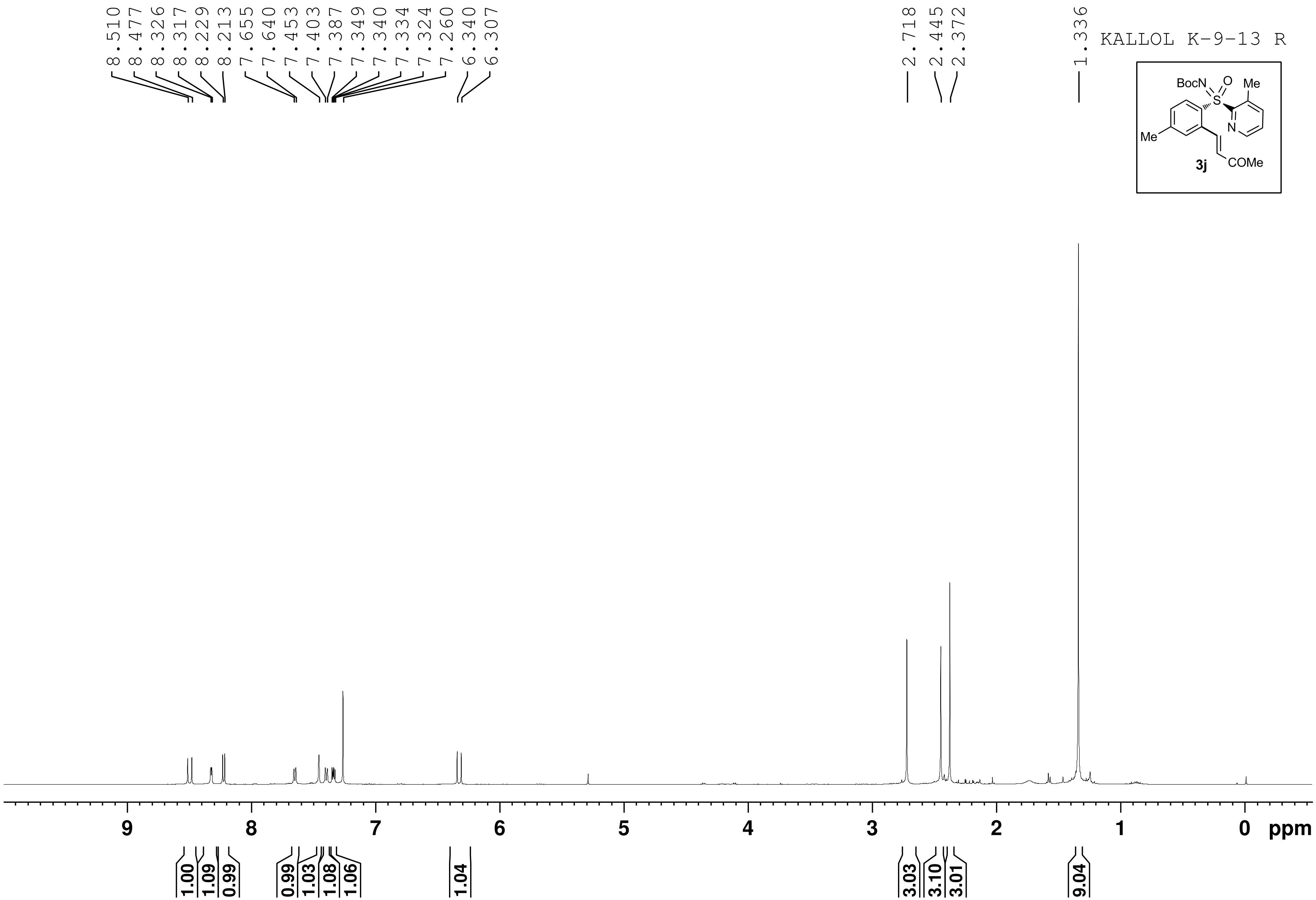
155.14
145.95
144.72
141.92
141.61
136.10
135.59
133.07
131.15
130.31
129.53
126.52
121.75
80.33
77.25
77.00
76.74
51.71
27.91
21.47
18.96
BocN
O
S
Me
N
Me
CO_2Me
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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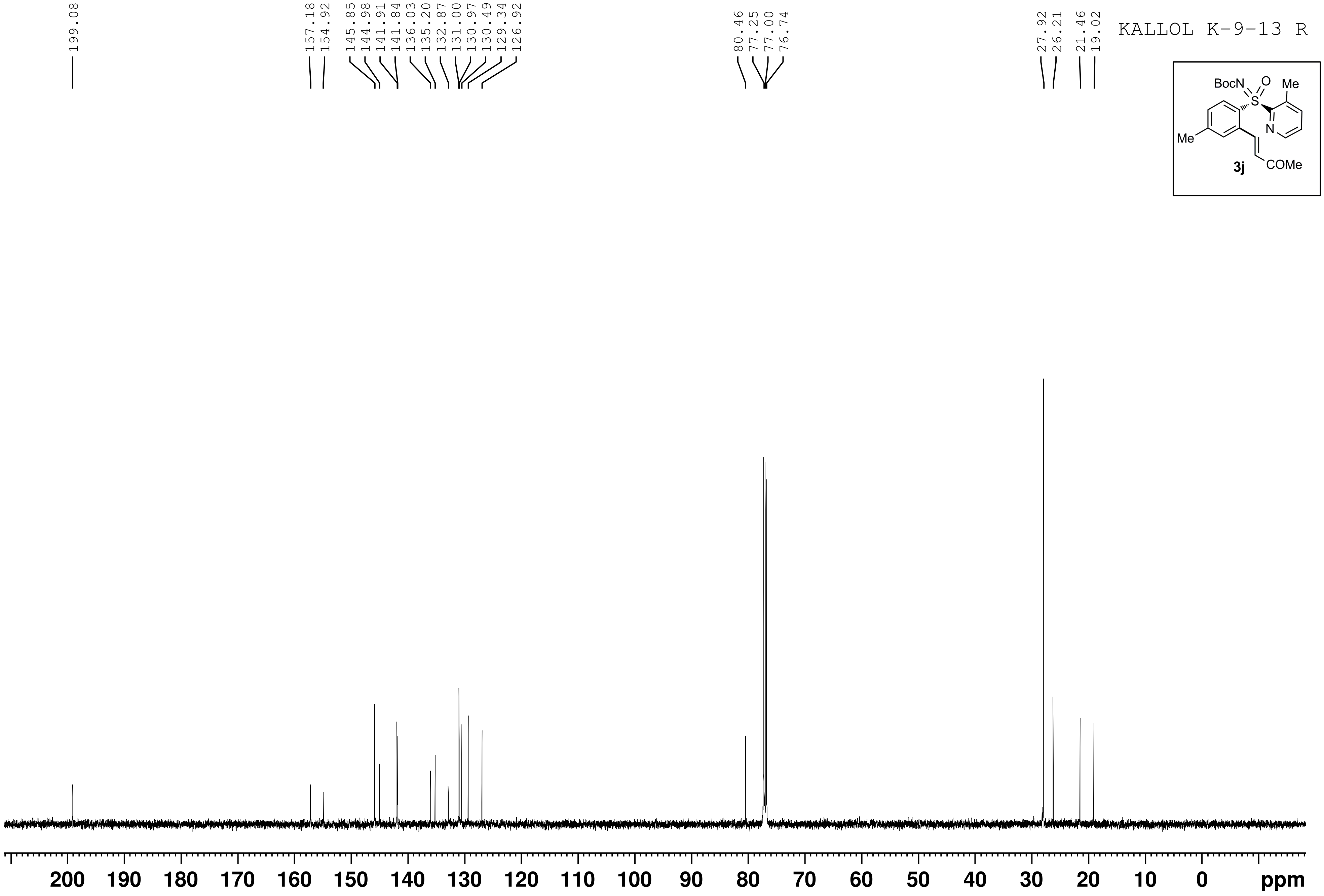
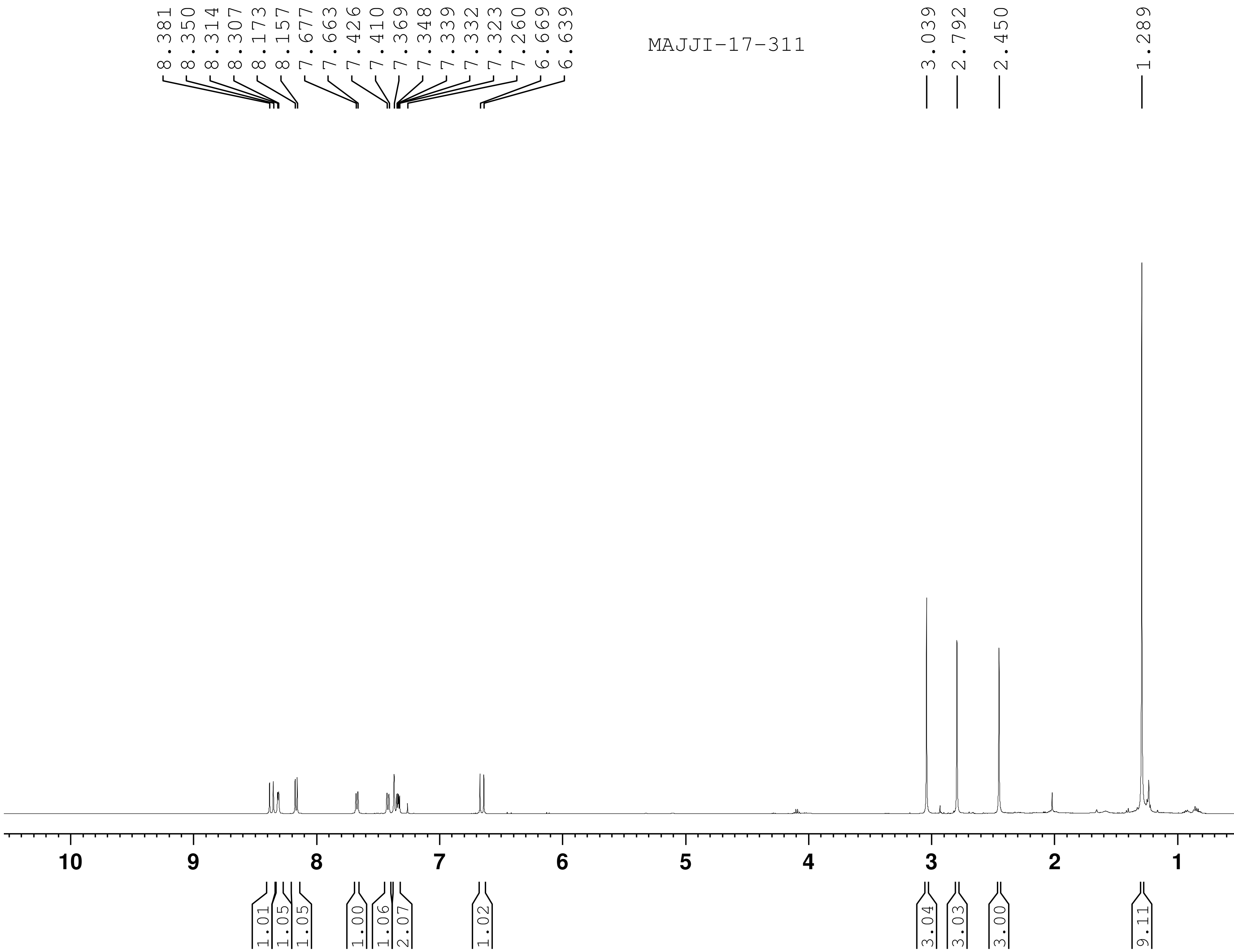
8.326
8.317
8.229
8.213
7.655
7.640
7.453
7.403
7.387
7.349
7.340
7.334
7.324
7.260
6.340
6.307
2.718
2.445
2.372
1.336
KALLOL K-9-13 R
BocN
O
S
Me
N
Me
COMe
3j
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.09
0.99
0.99
1.03
1.08
1.06
1.04
3.03
3.10
3.01
9.04


199.08
157.18
154.92
145.85
144.98
141.91
141.84
136.03
135.20
132.87
131.00
130.97
130.49
129.34
126.92
80.46
77.25
77.00
76.74
27.92
26.21
21.46
19.02
KALLOL K-9-13 R
BocN
O
S
Me
N
Me
3j
COMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


MAJJI-17-311
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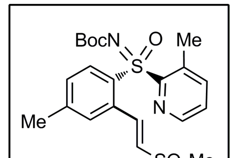
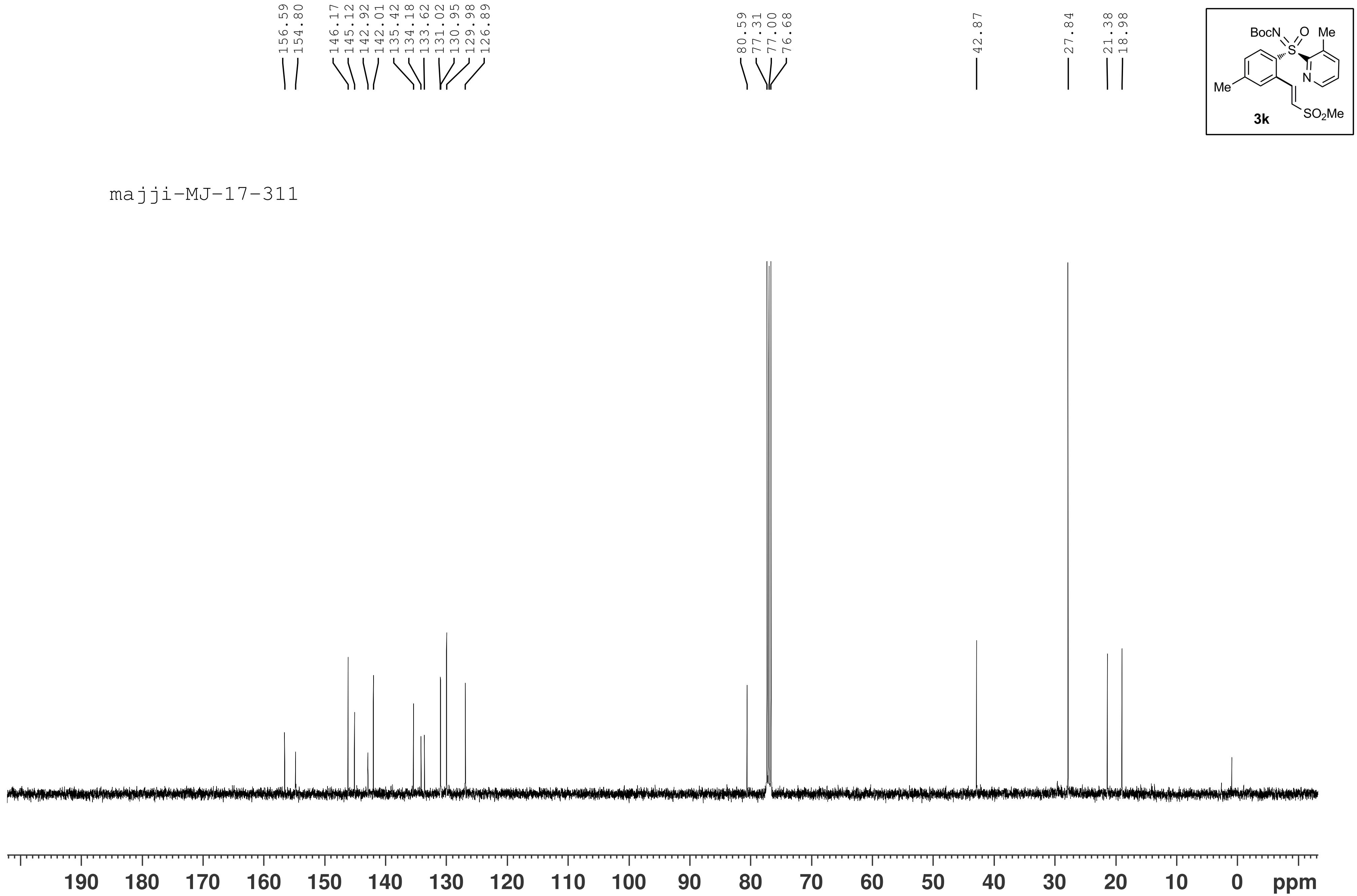
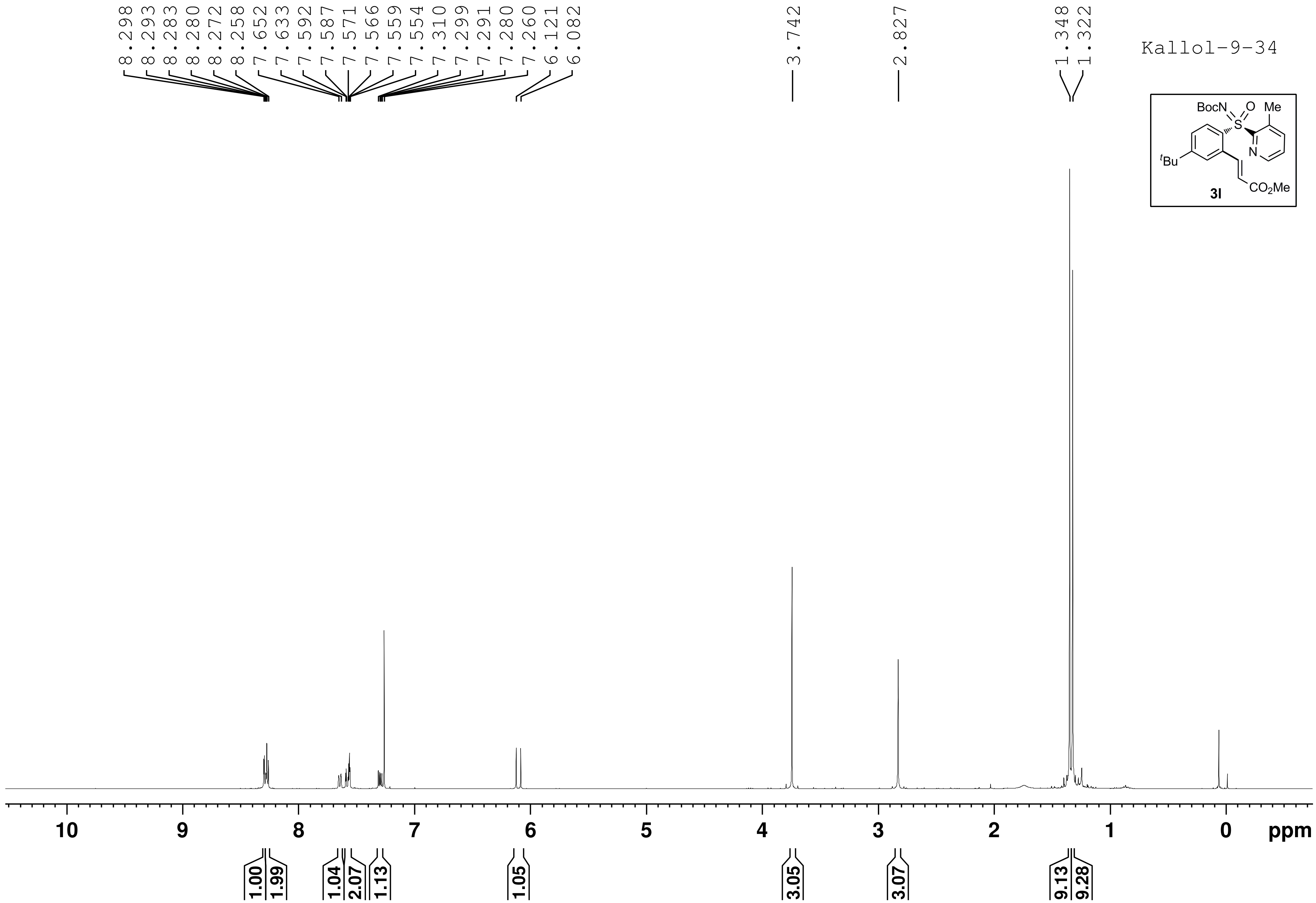
8.314
8.307
8.173
8.157
7.677
7.663
7.426
7.410
7.369
7.348
7.339
7.332
7.323
7.260
6.669
6.639
3.039
2.792
2.450
1.289
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.05
1.05
1.00
1.06
2.07
1.02
3.04
3.03
3.00
9.11

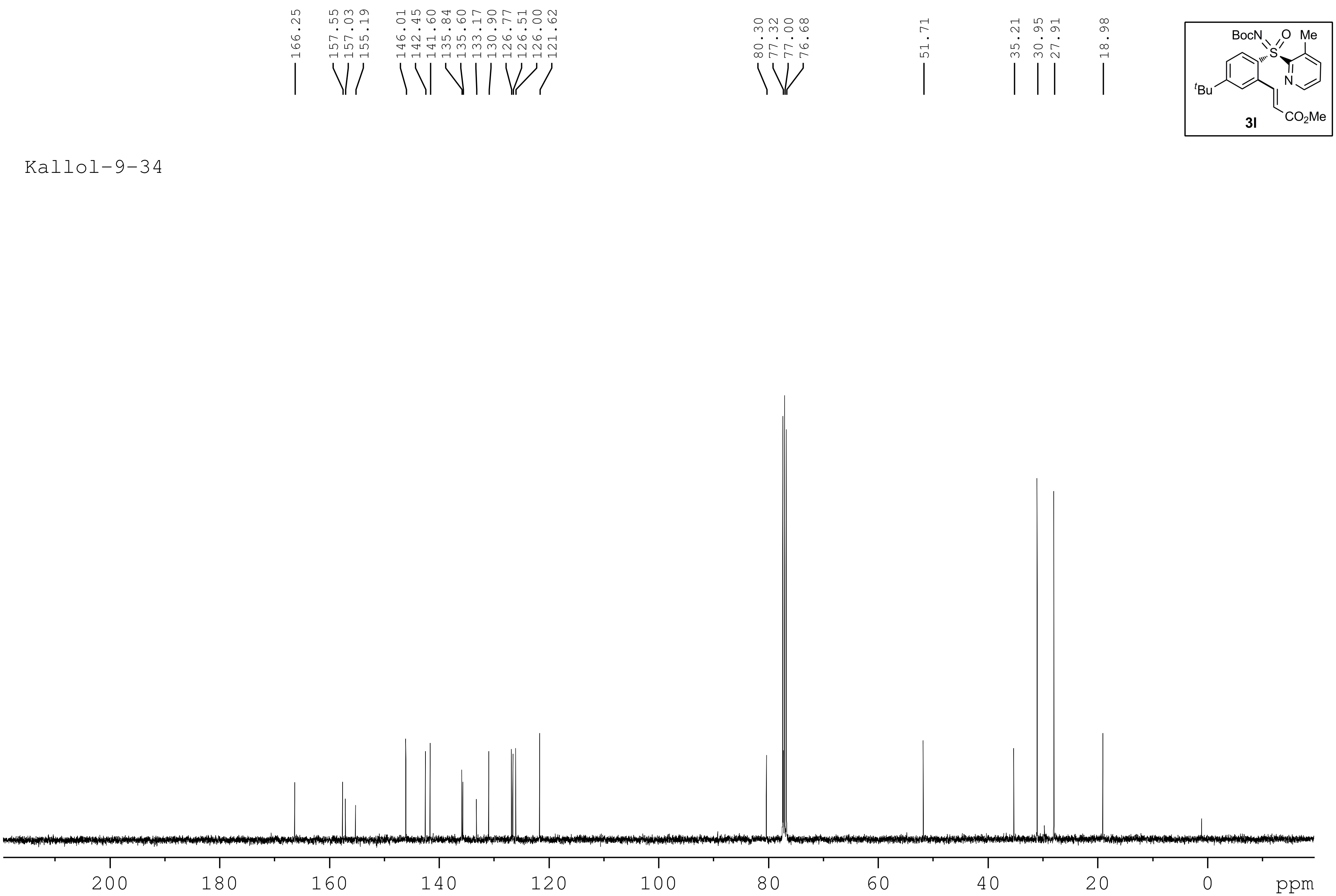

BocN
O
Me
S
N
Me
SO2Me

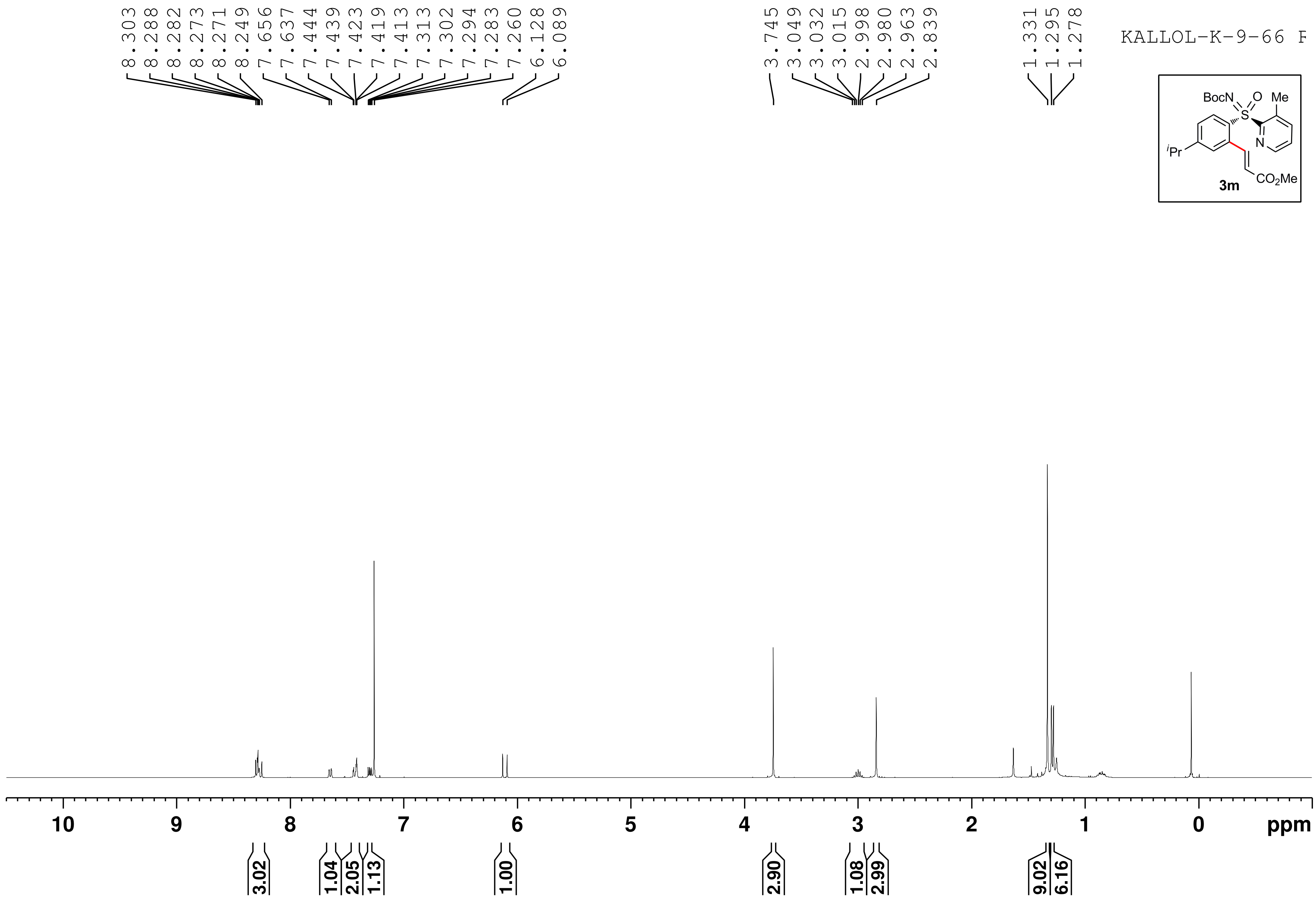
3k

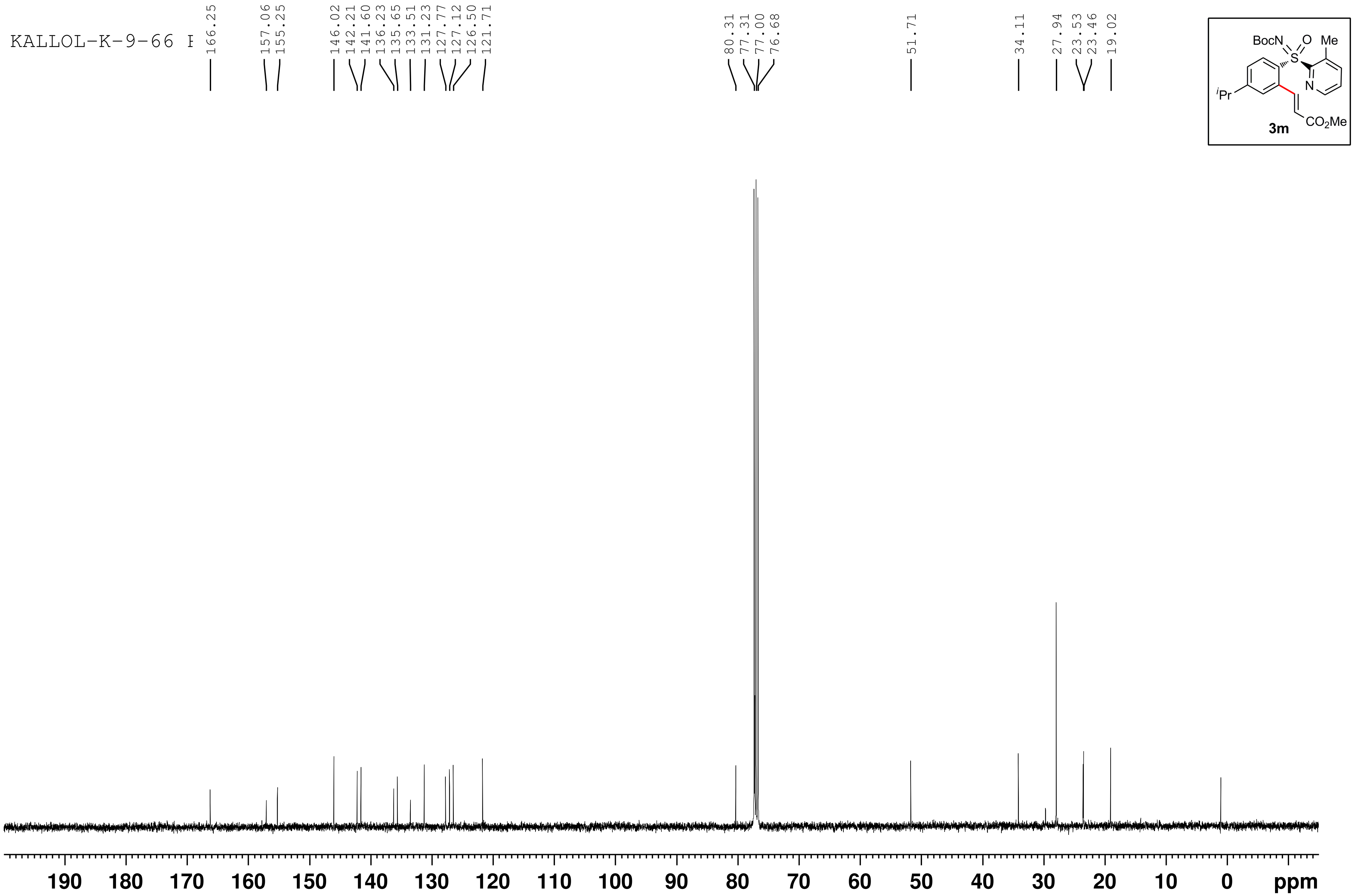

156.59
154.80
146.17
145.12
142.92
142.01
135.42
134.18
133.62
131.02
130.95
129.98
126.89
80.59
77.31
77.00
76.68
42.87
27.84
21.38
18.98
BocN
O
S
Me
N
Me
SO2Me
3k
majji-MJ-17-311
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.298
8.293
8.283
8.280
8.272
8.258
7.652
7.633
7.592
7.587
7.571
7.566
7.559
7.554
7.310
7.299
7.291
7.280
7.260
6.121
6.082
3.742
2.827
1.348
1.322
Kallol-9-34
BocN
O
Me
S
N
tBu
CO2Me
3l
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.99
1.04
2.07
1.13
1.05
3.05
3.07
9.13
9.28

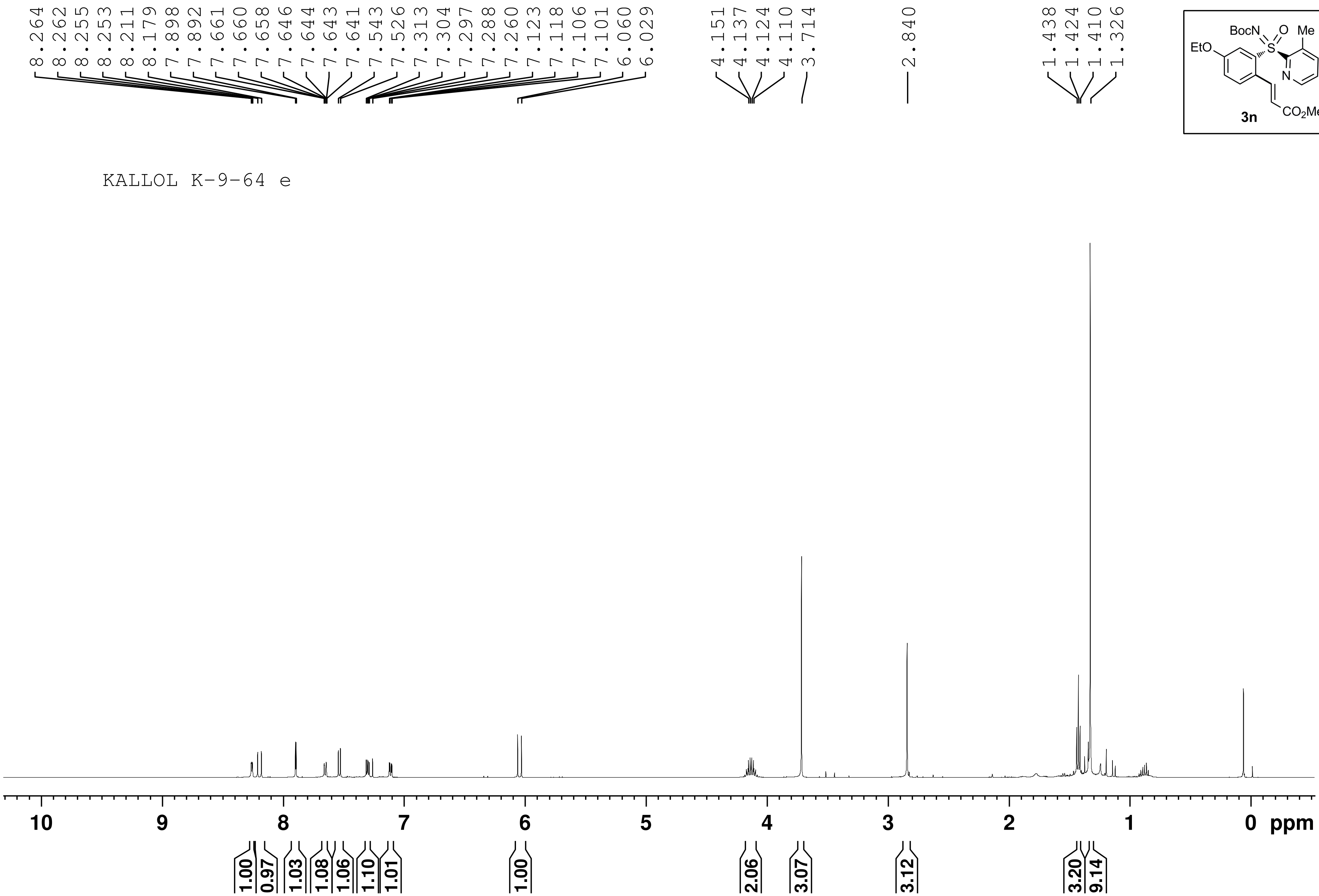
Kallol-9-34

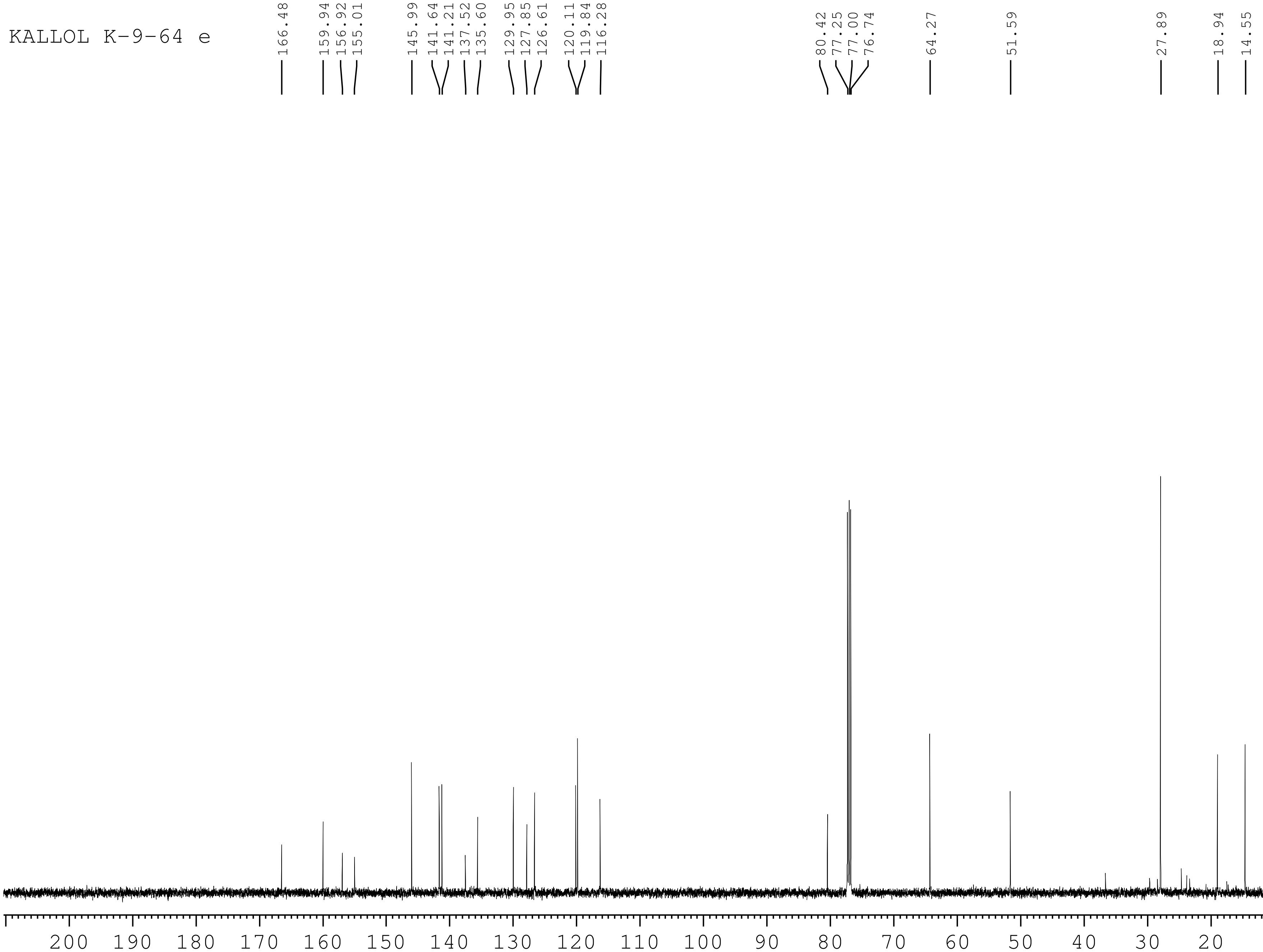

166.25
157.55
157.03
155.19
146.01
142.45
141.60
135.84
135.60
133.17
130.90
126.77
126.51
126.00
121.62
80.30
77.32
77.00
76.68
51.71
35.21
30.95
27.91
18.98
BocN
O
S
Me
N
tBu
CO2Me
3l
200
180
160
140
120
100
80
60
40
20
0
ppm

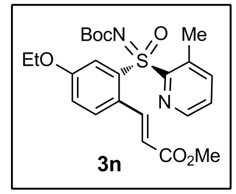

8.303 8.288 8.282 8.273 8.271 8.249 7.656 7.637 7.444 7.439 7.423 7.419 7.413 7.313 7.302 7.294 7.283 7.260 6.128 6.089
3.745 3.049 3.032 3.015 2.998 2.980 2.963 2.839
1.331 1.295 1.278
KALLOL-K-9-66 F
BocN
O
S
Me
N
iPr
CO2Me
3m
10 9 8 7 6 5 4 3 2 1 0 ppm
3.02 1.04 2.05 1.13 1.00 2.90 1.08 2.99 9.02 6.16

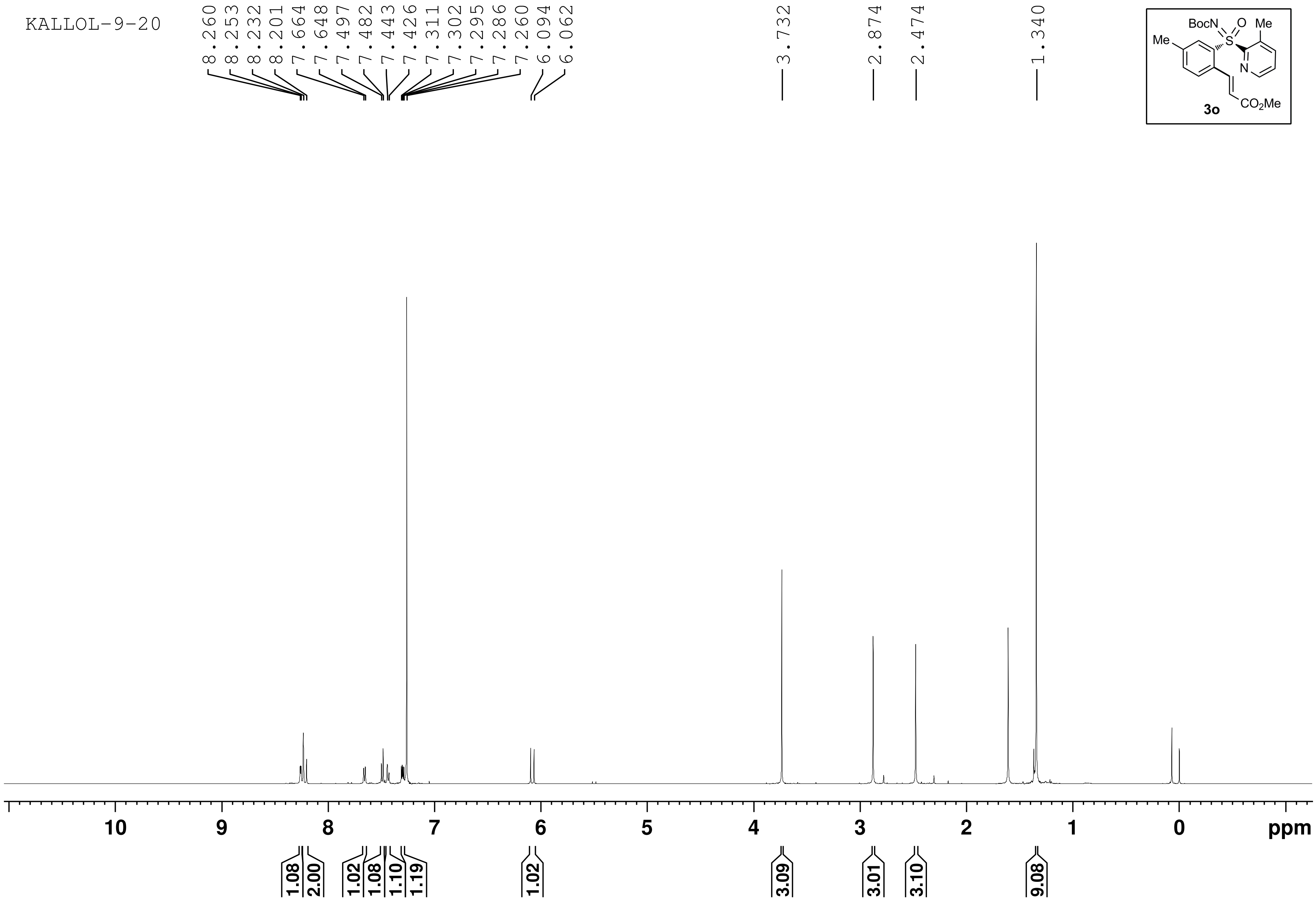


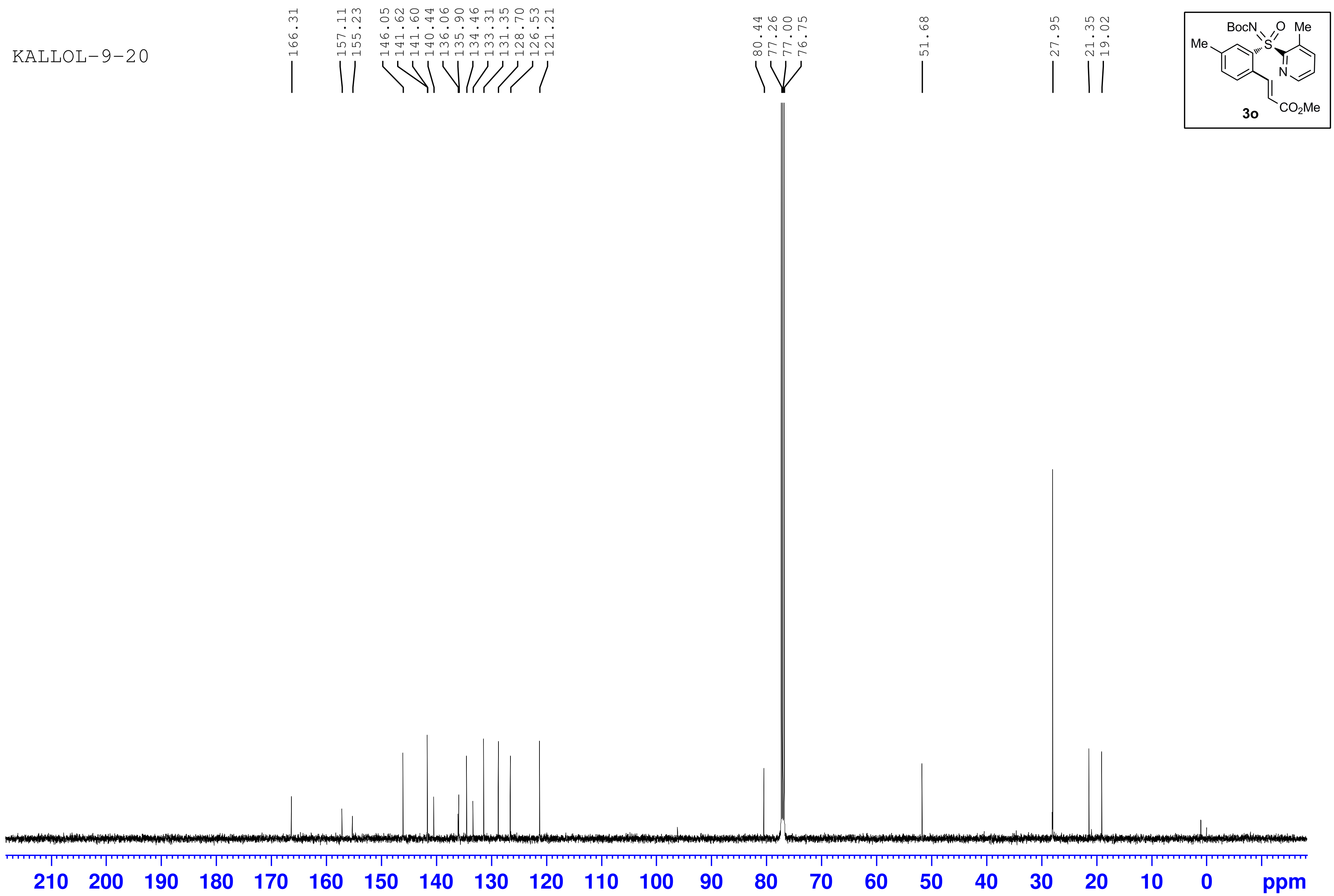
KALLOL-K-9-66 F
166.25
157.06
155.25
146.02
142.21
141.60
136.23
135.65
133.51
131.23
127.77
127.12
126.50
121.71
80.31
77.31
77.00
76.68
51.71
34.11
27.94
23.53
23.46
19.02
BocN
O
S
Me
N
iPr
CO2Me
3m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

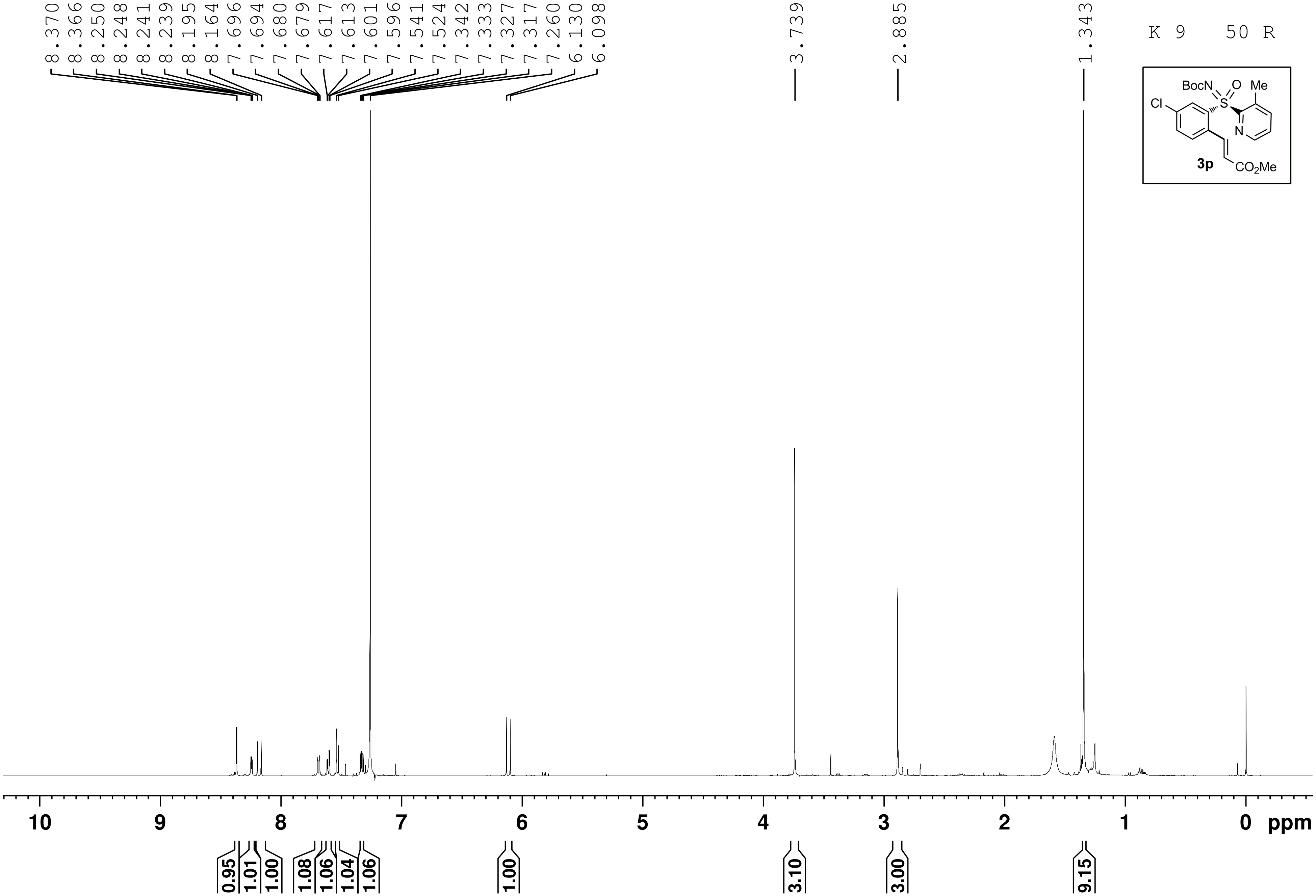

8.264
8.262
8.255
8.253
8.211
8.179
7.898
7.892
7.661
7.660
7.658
7.646
7.644
7.643
7.641
7.543
7.526
7.313
7.304
7.297
7.288
7.260
7.123
7.118
7.106
7.101
6.060
6.029
4.151
4.137
4.124
4.110
3.714
2.840
1.438
1.424
1.410
1.326
BocN
O
Me
EtO
S
N
CO_2Me
3n
KALLOL K-9-64 e
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.97
1.03
1.08
1.06
1.10
1.01
1.00
2.06
3.07
3.12
3.20
9.14

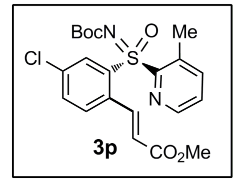

KALLOL K-9-64 e
166.48
159.94
156.92
155.01
145.99
141.64
141.21
137.52
135.60
129.95
127.85
126.61
120.11
119.84
116.28
80.42
77.25
77.00
76.74
64.27
51.59
27.89
18.94
14.55
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


BocN
O
Me
EtO
S
N
CO_2Me
3n

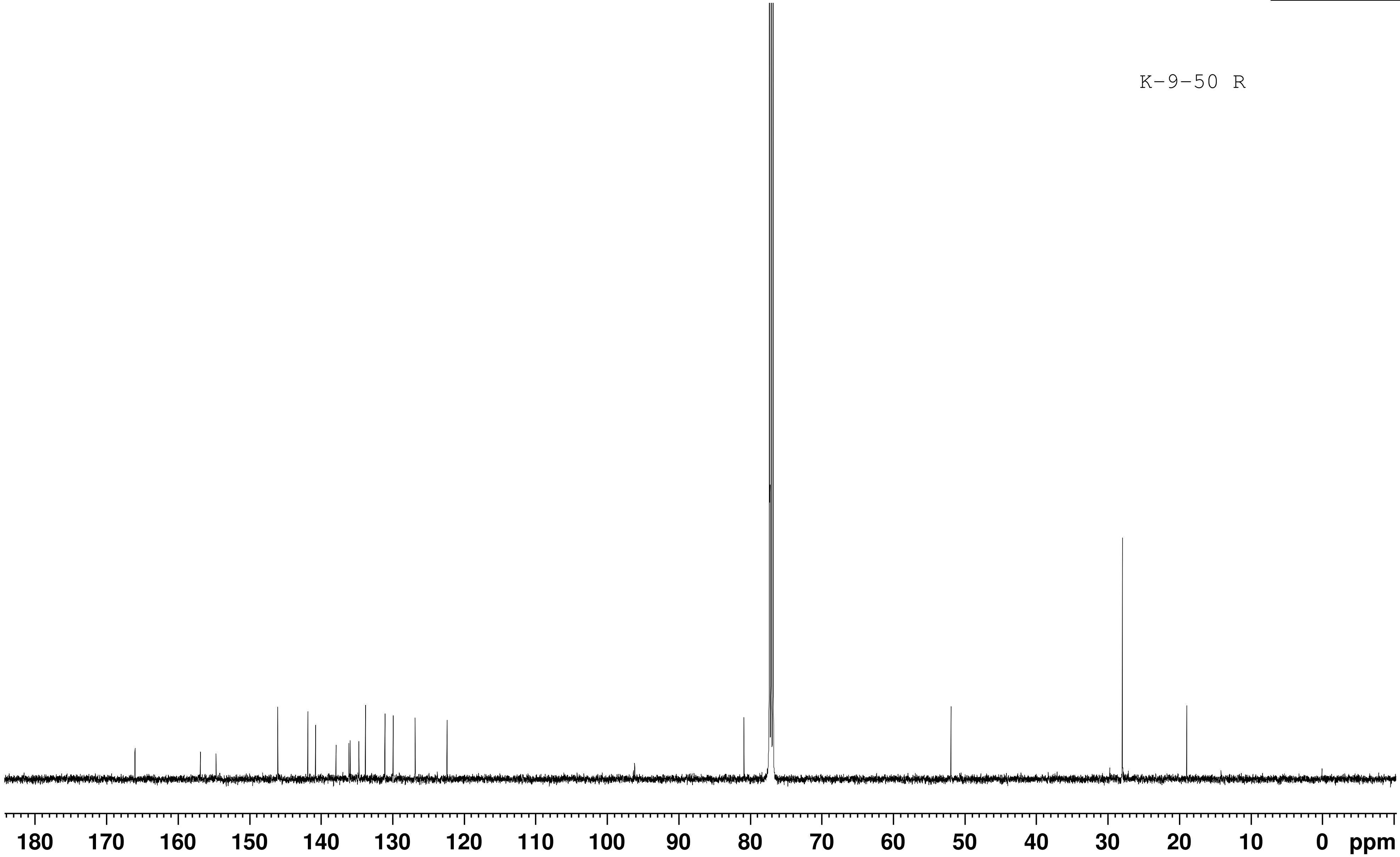

KALLOL-9-20
8.260
8.253
8.232
8.201
7.664
7.648
7.497
7.482
7.443
7.426
7.311
7.302
7.295
7.286
7.260
6.094
6.062
3.732
2.874
2.474
1.340
BocN
O
Me
Me
S
N
CO2Me
3o
10
9
8
7
6
5
4
3
2
1
0
ppm
1.08
2.00
1.02
1.08
1.10
1.19
1.02
3.09
3.01
3.10
9.08


KALLOL-9-20
166.31
157.11
155.23
146.05
141.62
141.60
140.44
136.06
135.90
134.46
133.31
131.35
128.70
126.53
121.21
80.44
77.26
77.00
76.75
51.68
27.95
21.35
19.02
BocN
O
S
Me
Me
N
CO2Me
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

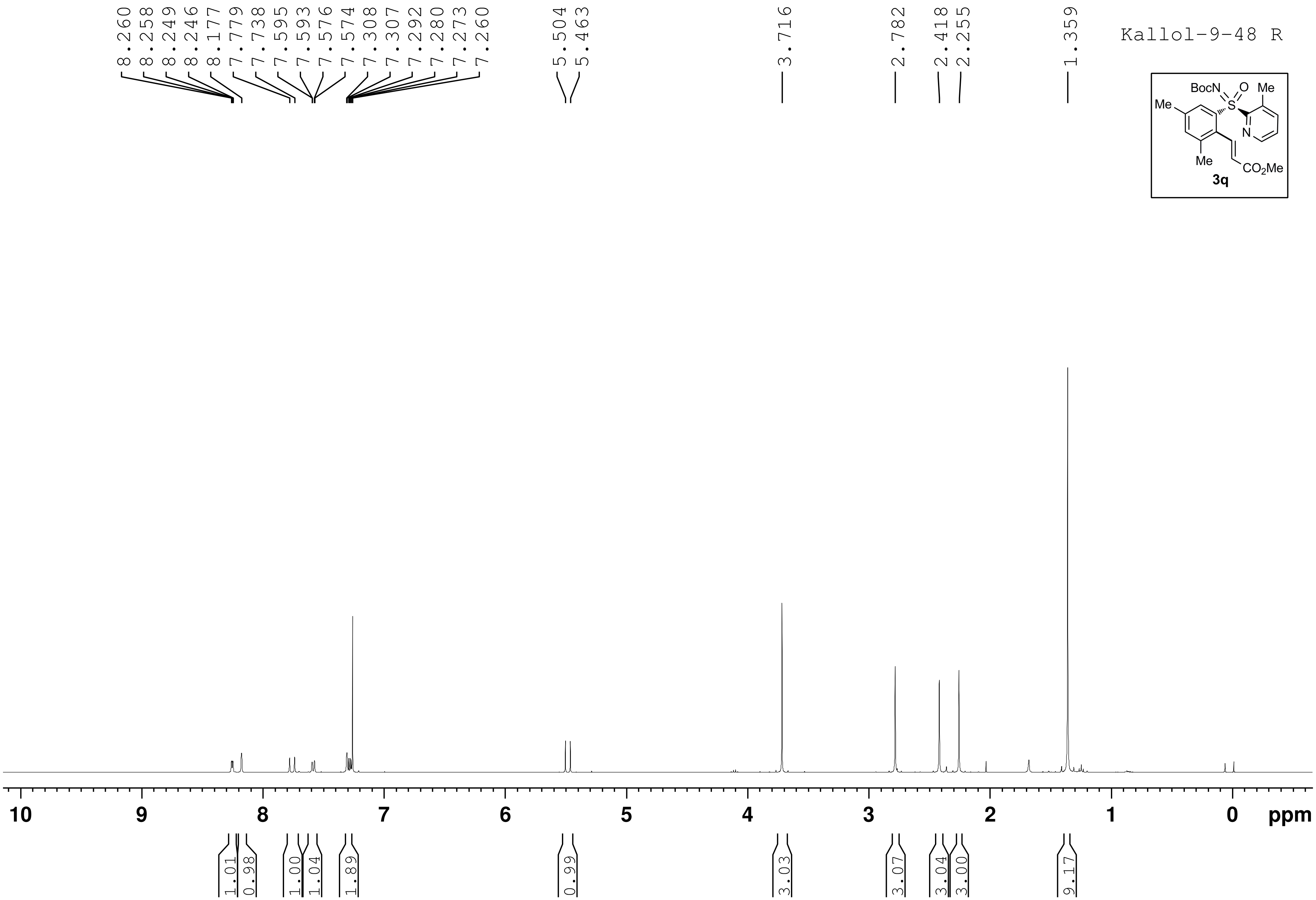

8.370
8.366
8.250
8.248
8.241
8.239
8.195
8.164
7.696
7.694
7.680
7.679
7.617
7.613
7.601
7.596
7.541
7.524
7.342
7.333
7.327
7.317
7.260
6.130
6.098
3.739
2.885
1.343
K 9 50 R
BocN
O
S
Me
Cl
N
3p
CO_2Me
10
9
8
7
6
5
4
3
2
1
0
ppm
0.95
1.01
1.00
1.08
1.06
1.04
1.06
1.00
3.10
3.00
9.15

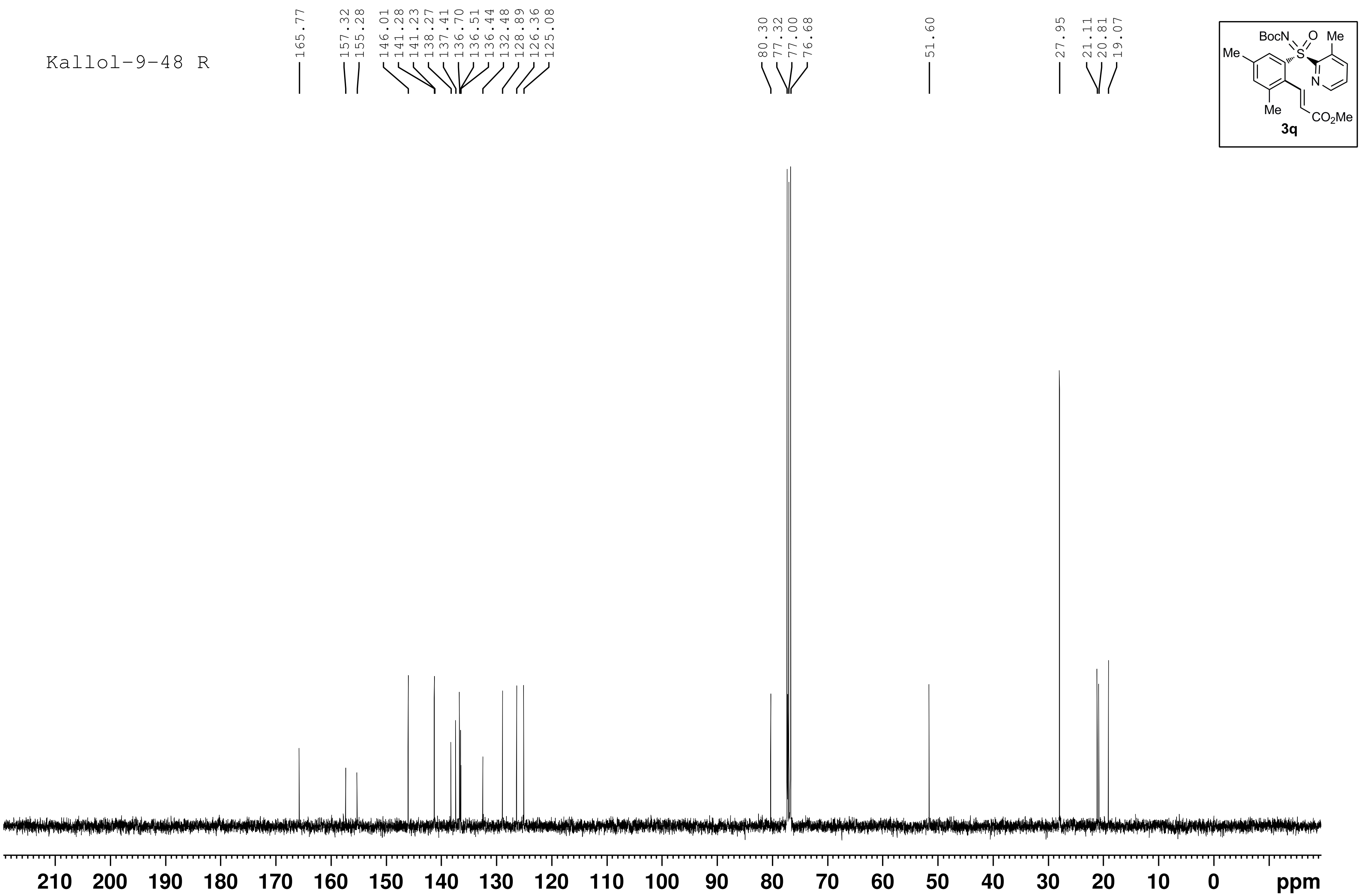


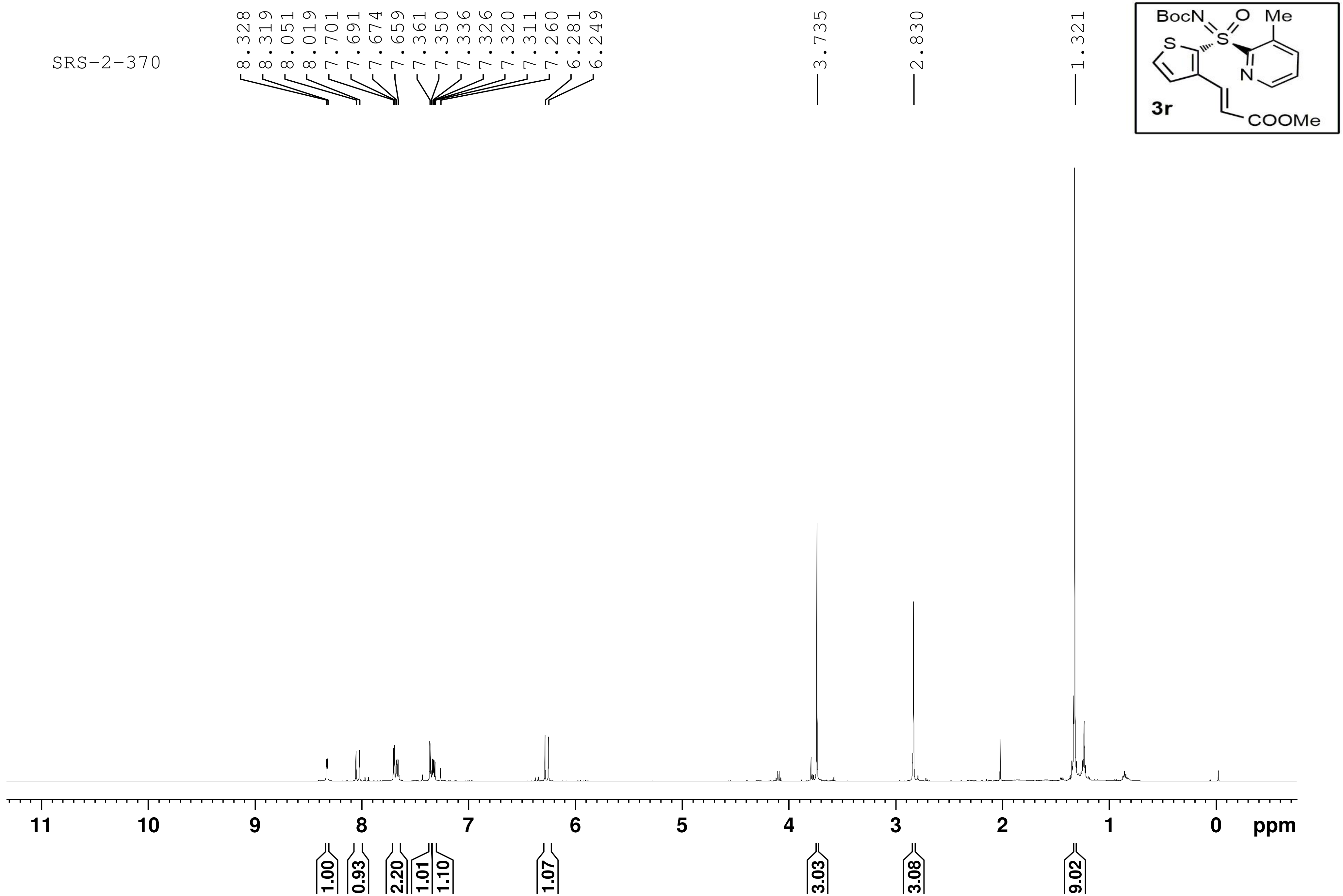
3p
BocN
O
Me
Cl
S
N
CO2Me



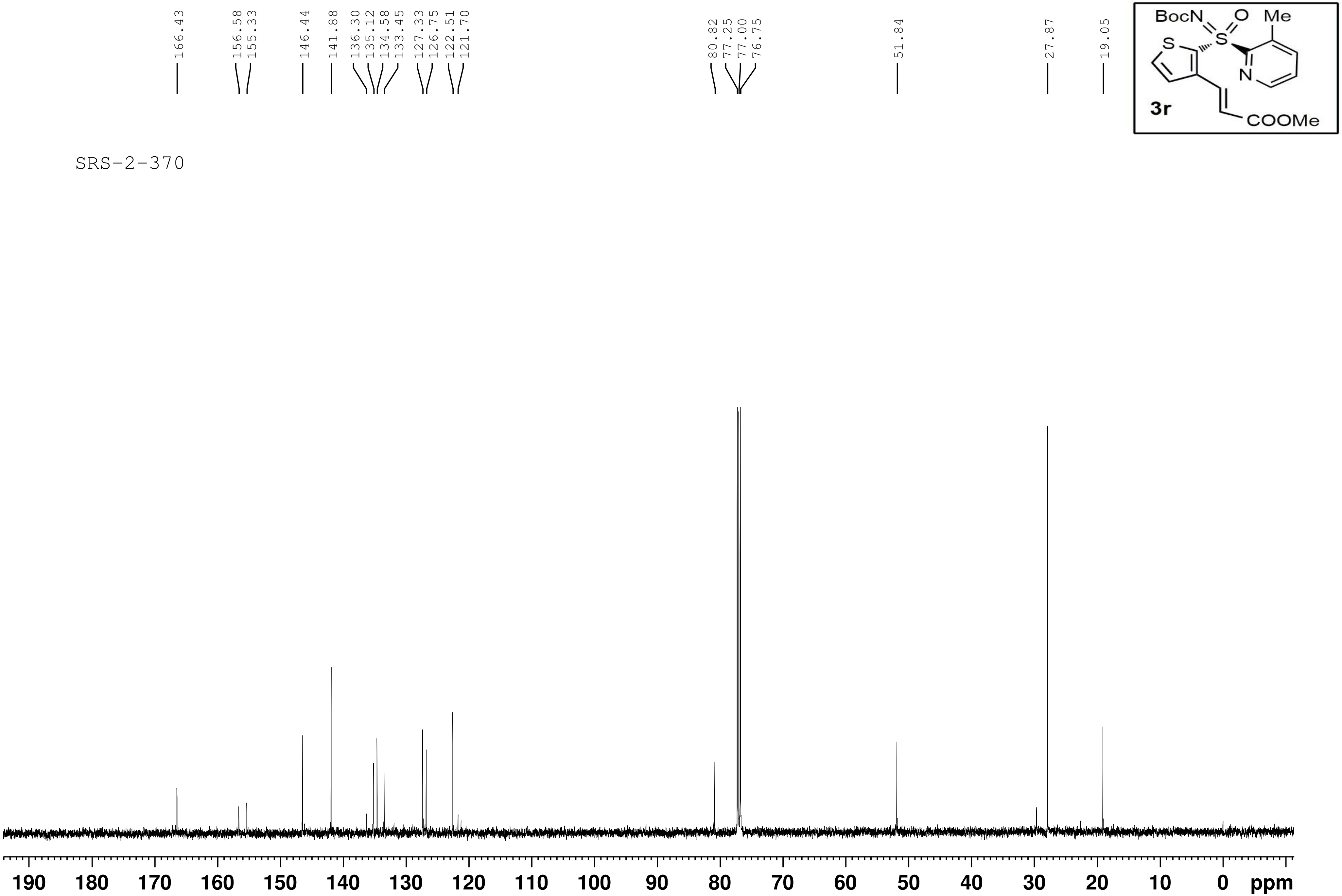
165.98
156.82
154.65
146.02
141.80
140.72
137.84
136.06
135.89
134.68
133.75
131.03
129.87
126.82
122.34
80.83
77.25
77.00
76.74
51.86
27.90
18.88
K-9-50 R
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

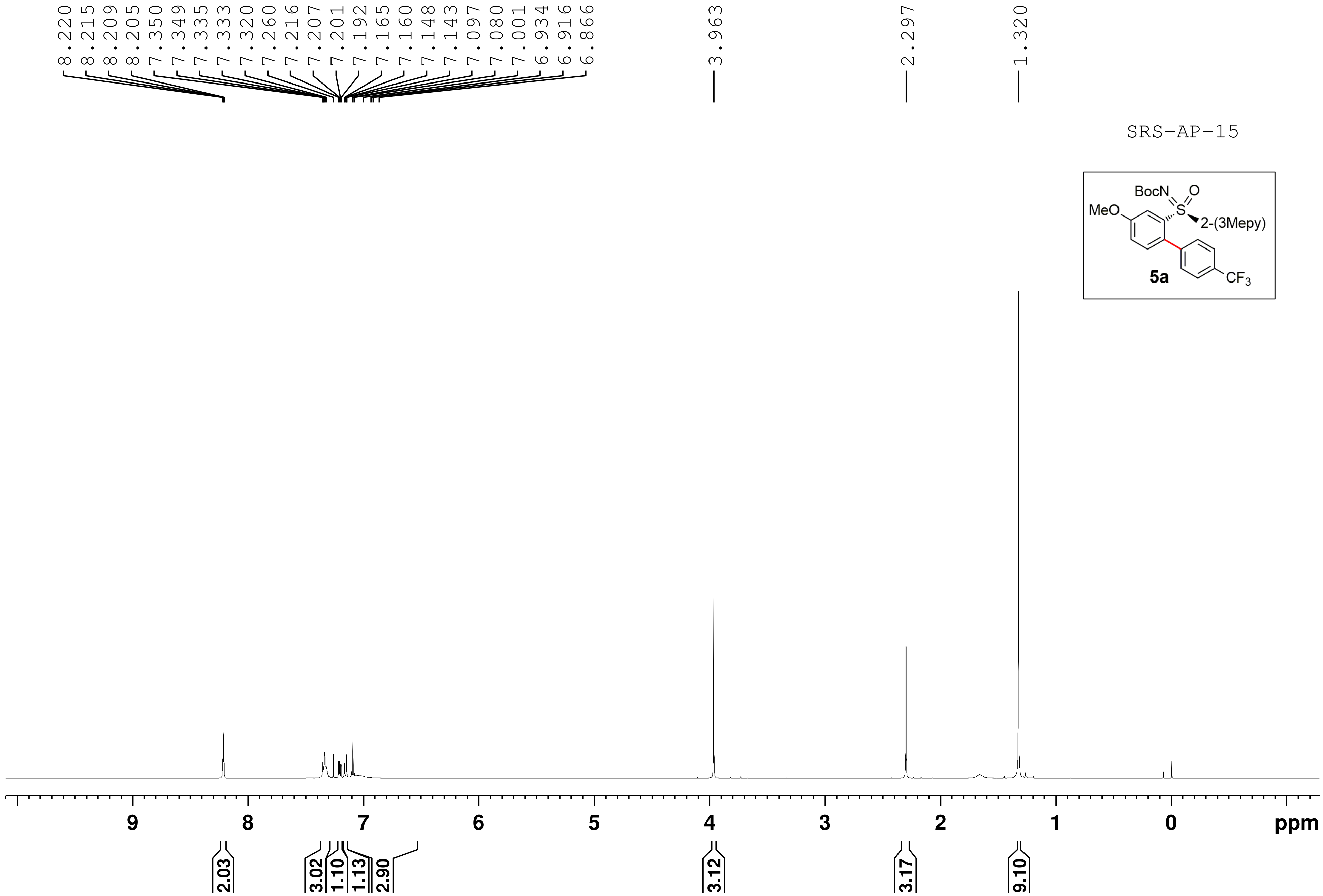

8.260
8.258
8.249
8.246
8.177
7.779
7.738
7.595
7.593
7.576
7.574
7.308
7.307
7.292
7.280
7.273
7.260
5.504
5.463
3.716
2.782
2.418
2.255
1.359
Kallol-9-48 R
BocN
O
S
Me
Me
N
Me
CO2Me
3q
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
0.98
1.00
1.04
1.89
0.99
3.03
3.07
3.04
3.00
9.17


Kallol-9-48 R
165.77
157.32
155.28
146.01
141.28
141.23
138.27
137.41
136.70
136.51
136.44
132.48
128.89
126.36
125.08
80.30
77.32
77.00
76.68
51.60
27.95
21.11
20.81
19.07
BocN
O
S
Me
Me
N
Me
CO_2Me
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

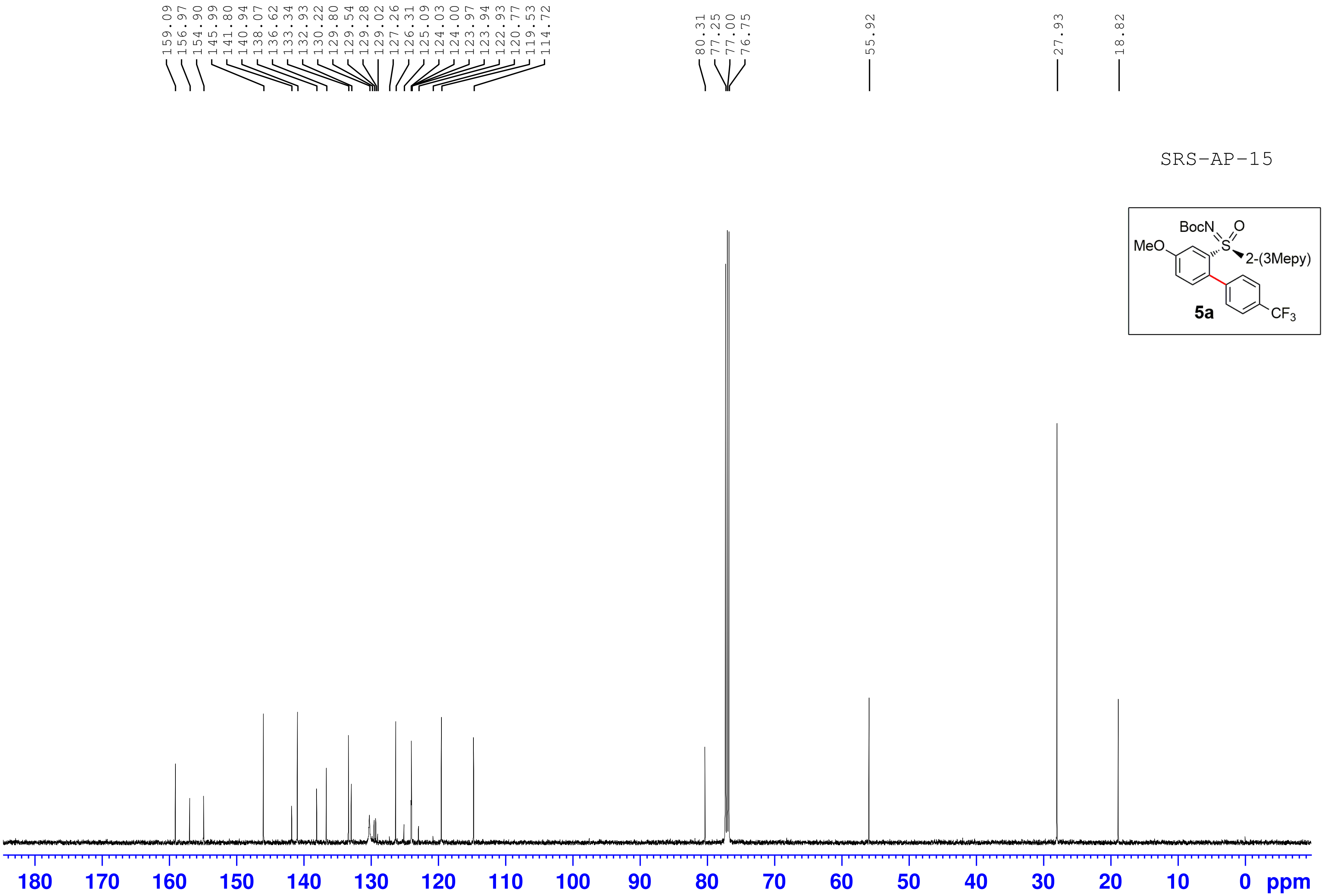

SRS-2-370
8.328
8.319
8.051
8.019
7.701
7.691
7.674
7.659
7.361
7.350
7.336
7.326
7.320
7.311
7.260
6.281
6.249
3.735
2.830
1.321
BocN
O
Me
S
S
N
3r
COOMe
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.93
2.20
1.01
1.10
1.07
3.03
3.08
9.02

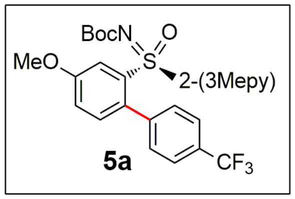
SRS-2-370

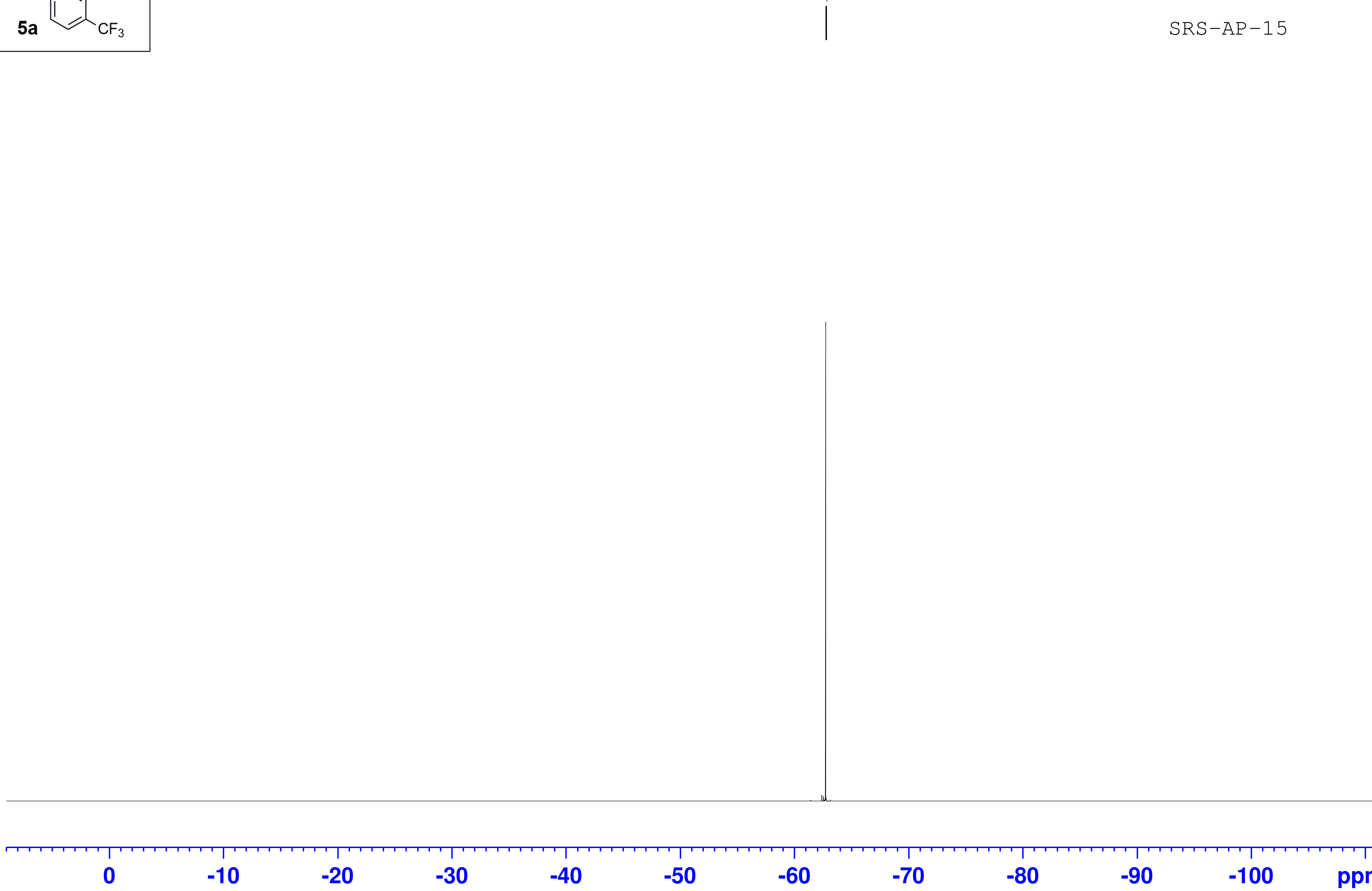

166.43
156.58
155.33
146.44
141.88
136.30
135.12
134.58
133.45
127.33
126.75
122.51
121.70
80.82
77.25
77.00
76.75
51.84
27.87
19.05
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
BocN
O
Me
S
S
N
3r
COOMe

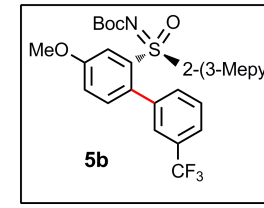

8.220
8.215
8.209
8.205
7.350
7.349
7.335
7.333
7.320
7.260
7.216
7.207
7.201
7.192
7.165
7.160
7.148
7.143
7.097
7.080
7.001
6.934
6.916
6.866
3.963
2.297
1.320
SRS-AP-15
BocN
O
S
MeO
2-(3Mepy)
5a
CF3
9
8
7
6
5
4
3
2
1
0
ppm
2.03
3.02
1.10
1.13
2.90
3.12
3.17
9.10

SRS-AP-15

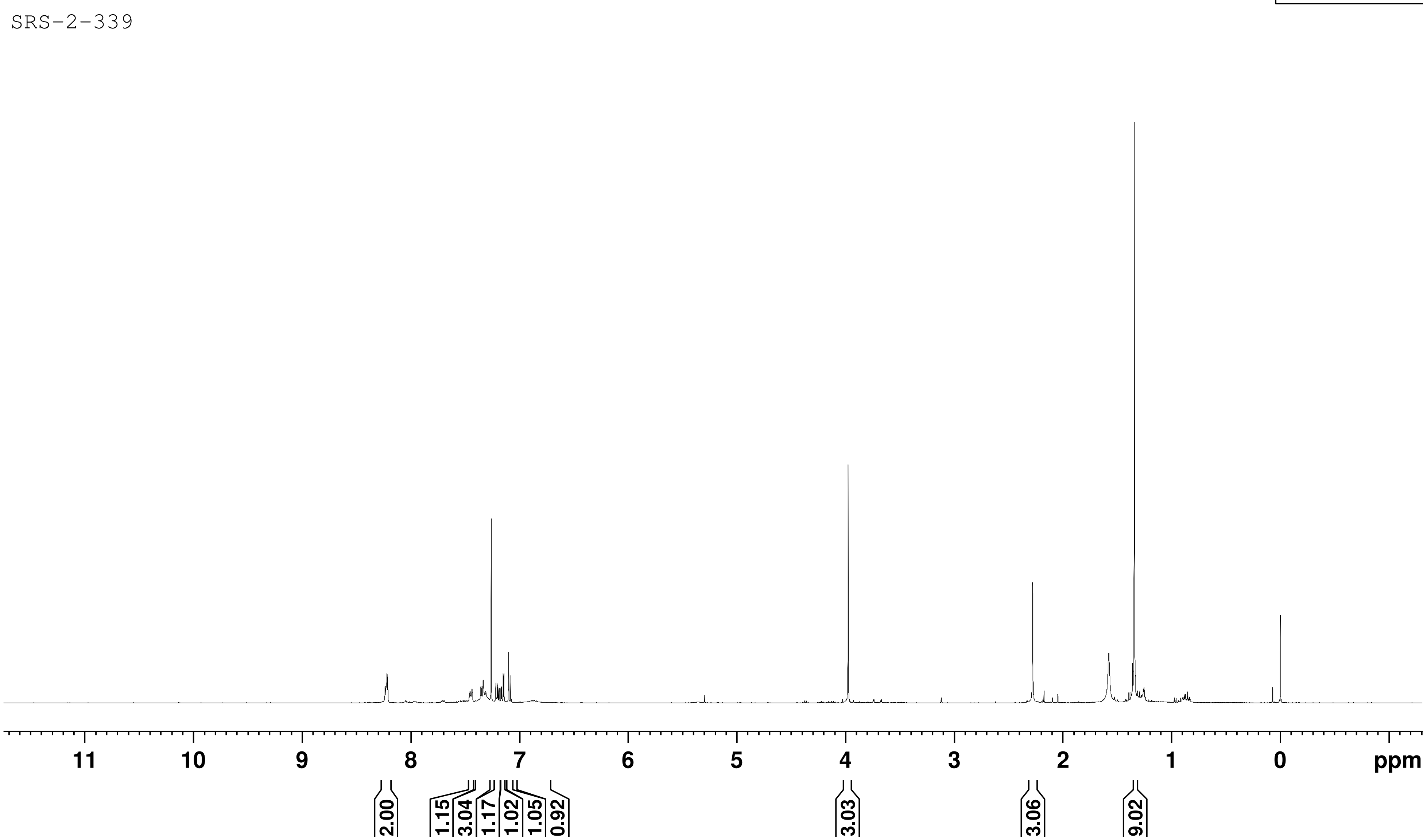

159.09
156.97
154.90
145.99
141.80
140.94
138.07
136.62
133.34
132.93
130.22
129.80
129.54
129.28
129.02
127.26
126.31
125.09
124.03
124.00
123.97
123.94
122.93
120.77
119.53
114.72
80.31
77.25
77.00
76.75
55.92
27.93
18.82
BocN
O
S
MeO
2-(3Mepy)
CF_3
5a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


BocN
O
MeO
S
2-(3Mepy)
5a
CF3

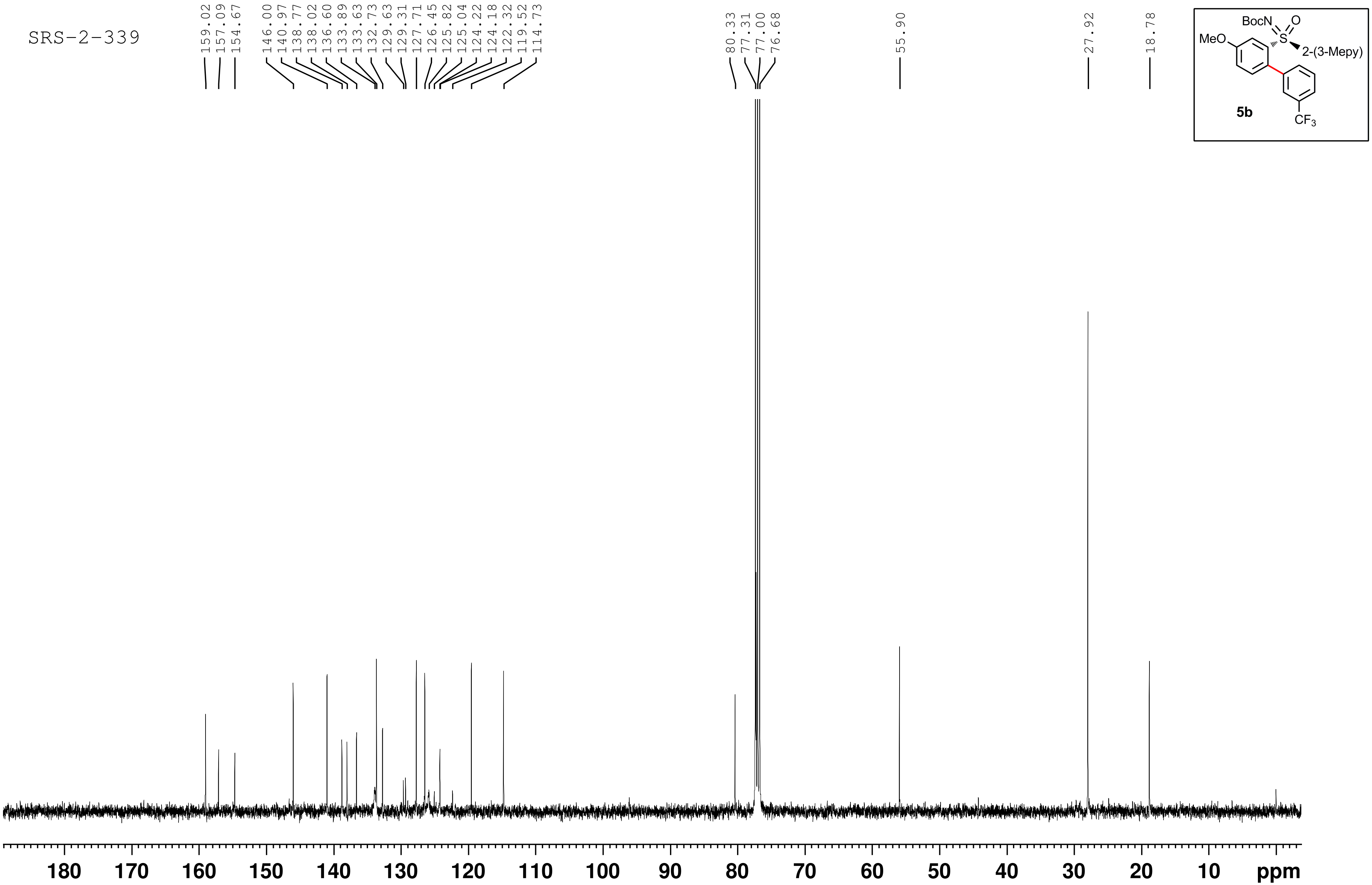

-62.76
SRS-AP-15
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
ppm

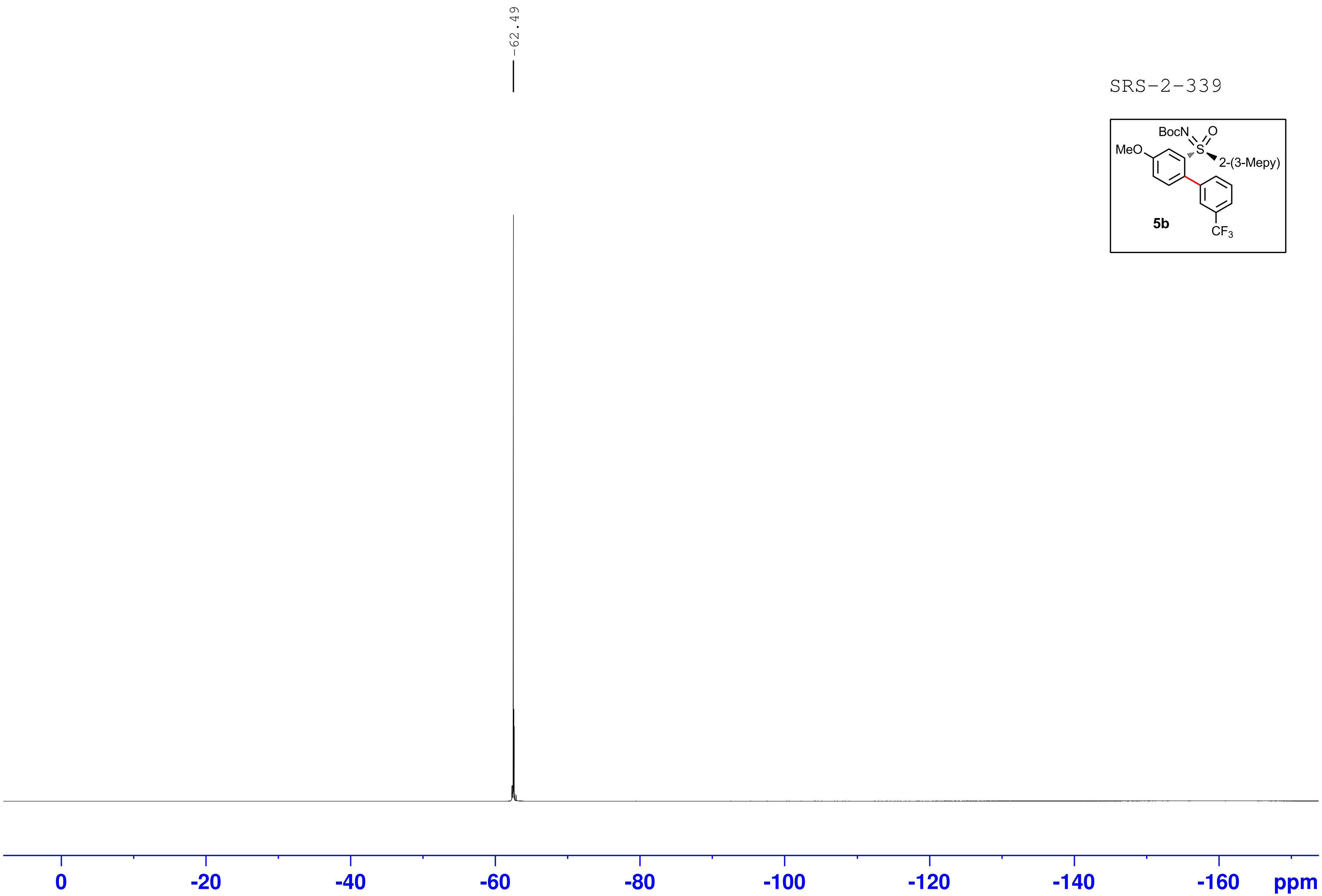


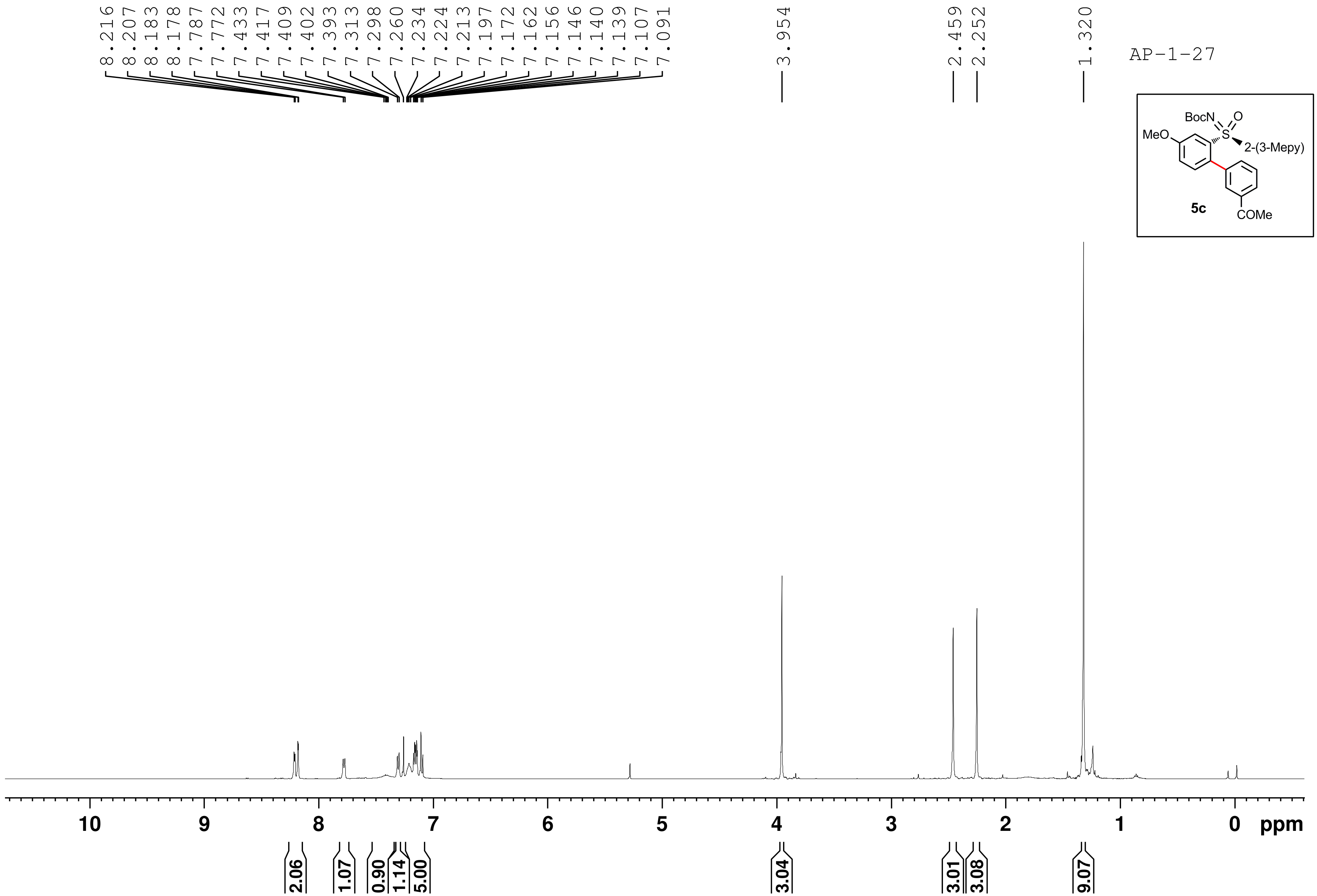
BocN
O
S
MeO
2-(3-Mepy)
5b
CF3



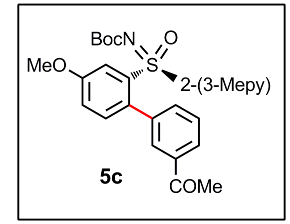
8.237
8.234
8.225
8.219
8.212
7.455
7.437
7.353
7.335
7.333
7.310
7.260
7.216
7.205
7.197
7.186
7.170
7.163
7.149
7.142
7.099
7.078
6.914
6.895
6.884
6.874
6.863
6.845
6.837
3.975
2.276
1.340
SRS-2-339
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.15
3.04
1.17
1.02
1.05
0.92
3.03
3.06
9.02

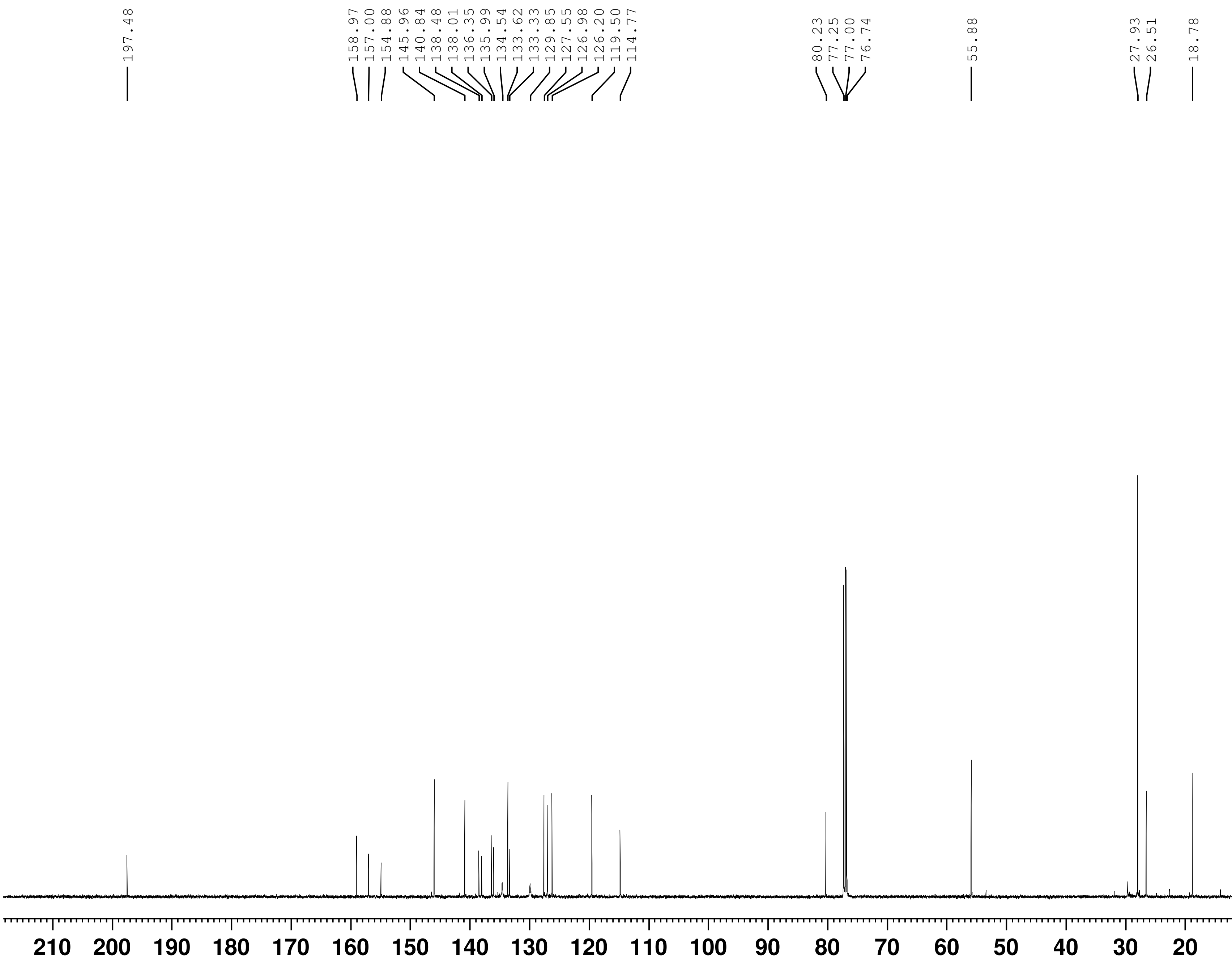

SRS-2-339
159.02
157.09
154.67
146.00
140.97
138.77
138.02
136.60
133.89
133.63
132.73
129.63
129.31
127.71
126.45
125.82
125.04
124.22
124.18
122.32
119.52
114.73
80.33
77.31
77.00
76.68
55.90
27.92
18.78
BocN
O
S
MeO
2-(3-Mepy)
5b
CF3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

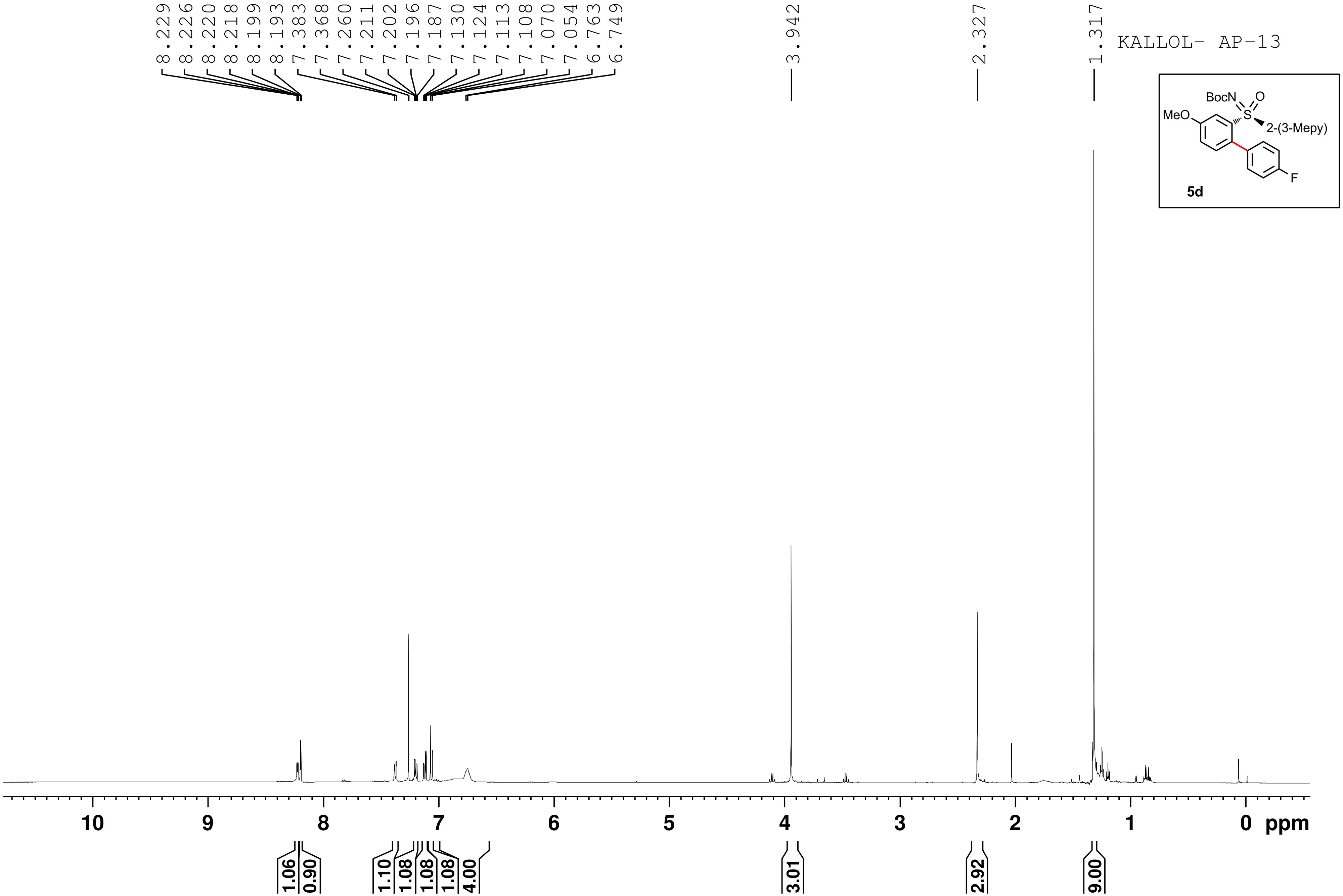

-62.49
SRS-2-339
BocN
O
MeO
S
2-(3-Mepy)
5b
CF3
0
-20
-40
-60
-80
-100
-120
-140
-160
ppm


8.216
8.207
8.183
8.178
7.787
7.772
7.433
7.417
7.409
7.402
7.393
7.313
7.298
7.260
7.234
7.224
7.213
7.197
7.172
7.162
7.156
7.146
7.140
7.139
7.107
7.091
3.954
2.459
2.252
1.320
AP-1-27
BocN
O
S
MeO
2-(3-Mepy)
5c
COMe
10
9
8
7
6
5
4
3
2
1
0
ppm
2.06
1.07
0.90
1.14
5.00
3.04
3.01
3.08
9.07

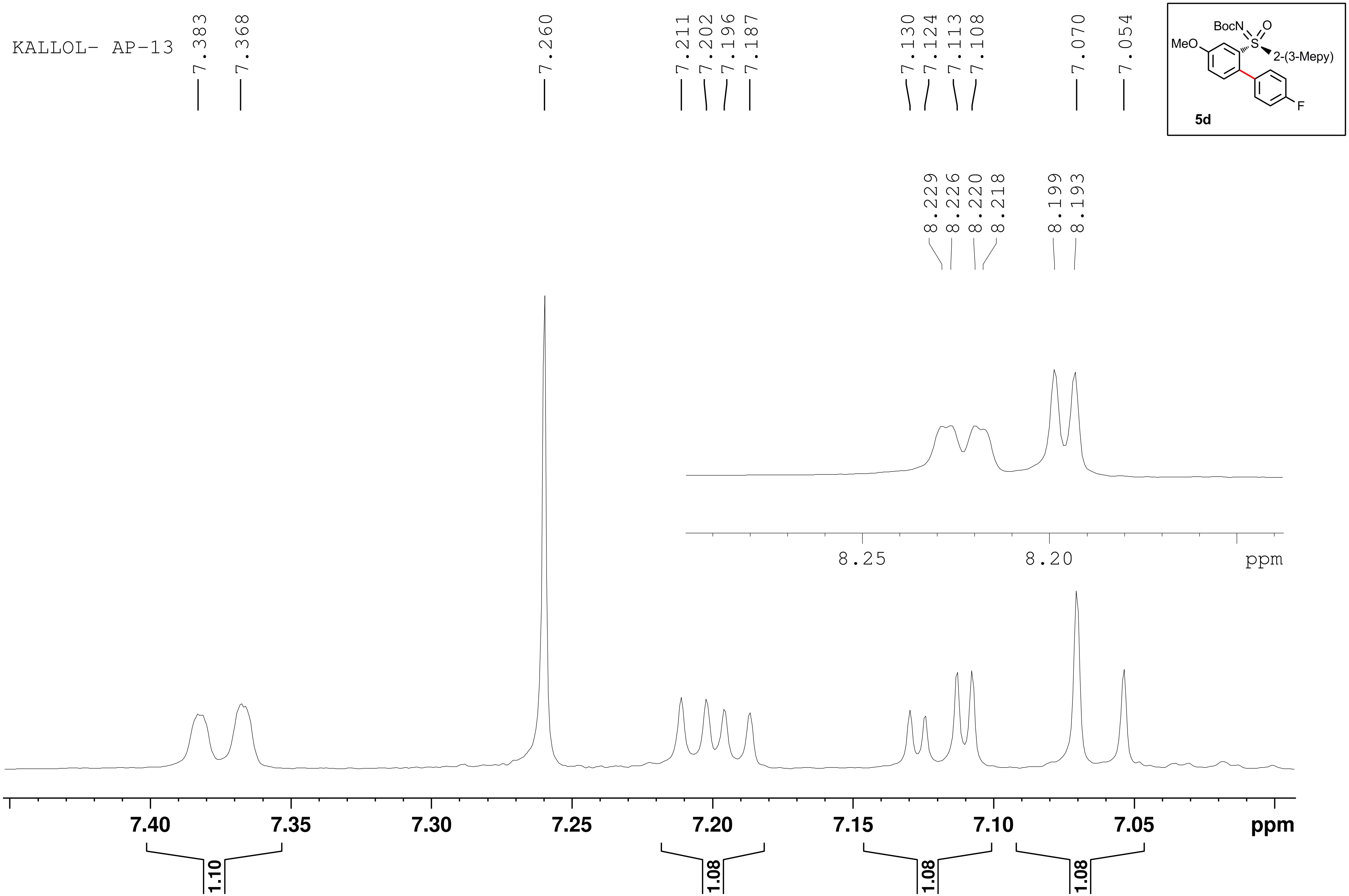
AP-1-27


BocN
O
S
MeO
2-(3-Mepy)
5c
COMe

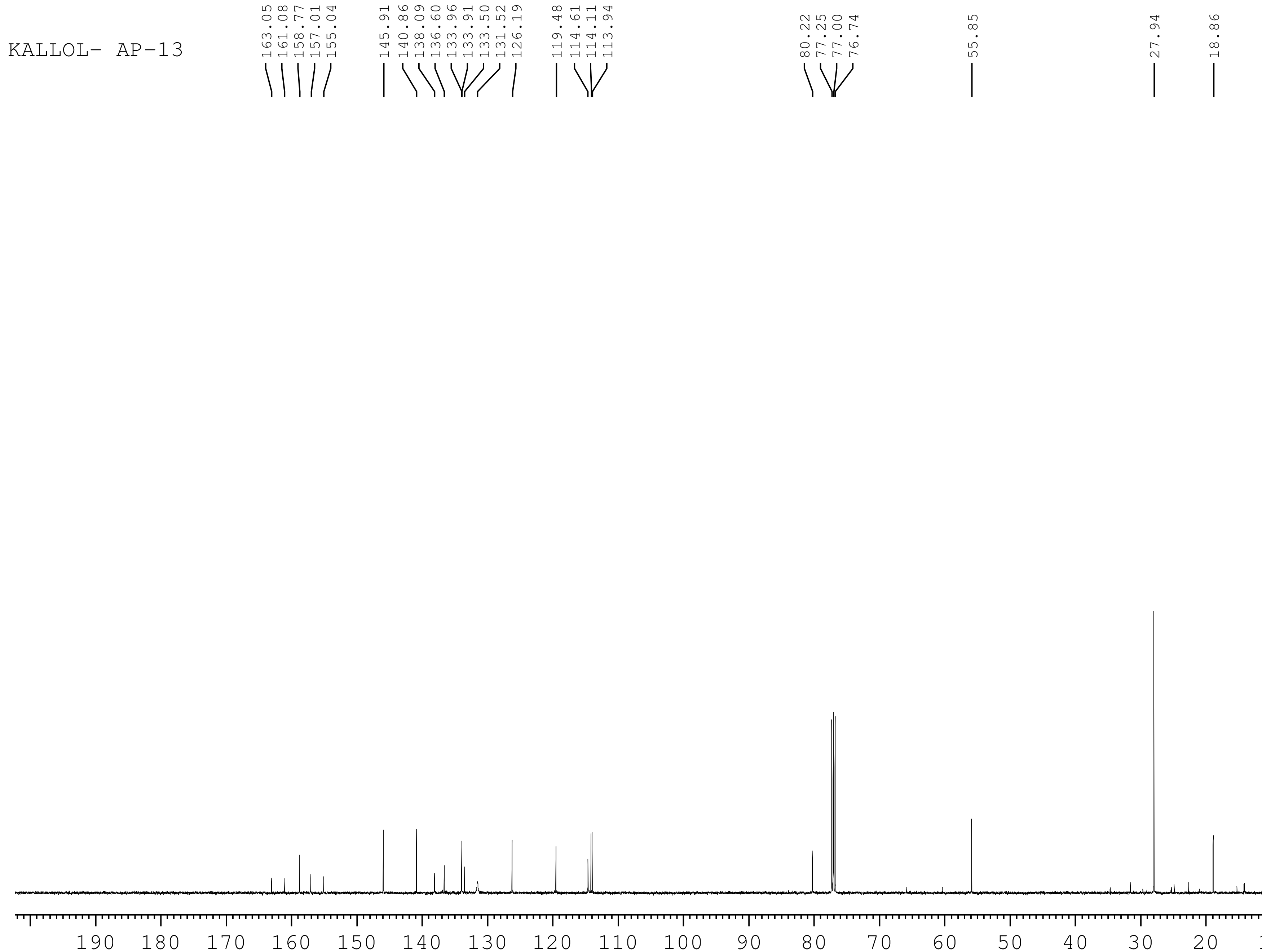

197.48
158.97
157.00
154.88
145.96
140.84
138.48
138.01
136.35
135.99
134.54
133.62
133.33
129.85
127.55
126.98
126.20
119.50
114.77
80.23
77.25
77.00
76.74
55.88
27.93
26.51
18.78
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

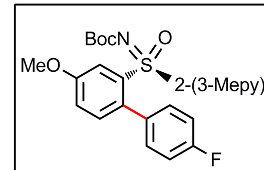


8.229
8.226
8.220
8.218
8.199
8.193
7.383
7.368
7.260
7.211
7.202
7.196
7.187
7.130
7.124
7.113
7.108
7.070
7.054
6.763
6.749
3.942
2.327
1.317
KALLOL- AP-13
BocN
O
S
MeO
2-(3-Mepy)
F
5d
10
9
8
7
6
5
4
3
2
1
0
ppm
1.06
0.90
1.10
1.08
1.08
1.08
4.00
3.01
2.92
9.00



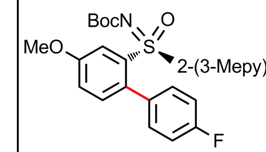
KALLOL- AP-13
7.383
7.368
7.260
7.211
7.202
7.196
7.187
7.130
7.124
7.113
7.108
7.070
7.054
8.229
8.226
8.220
8.218
8.199
8.193
8.25
8.20
ppm
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
ppm
1.10
1.08
1.08
1.08
BocN
O
S
MeO
2-(3-Mepy)
F
5d


KALLOL- AP-13
163.05
161.08
158.77
157.01
155.04
145.91
140.86
138.09
136.60
133.96
133.91
133.50
131.52
126.19
119.48
114.61
114.11
113.94
80.22
77.25
77.00
76.74
55.85
27.94
18.86
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

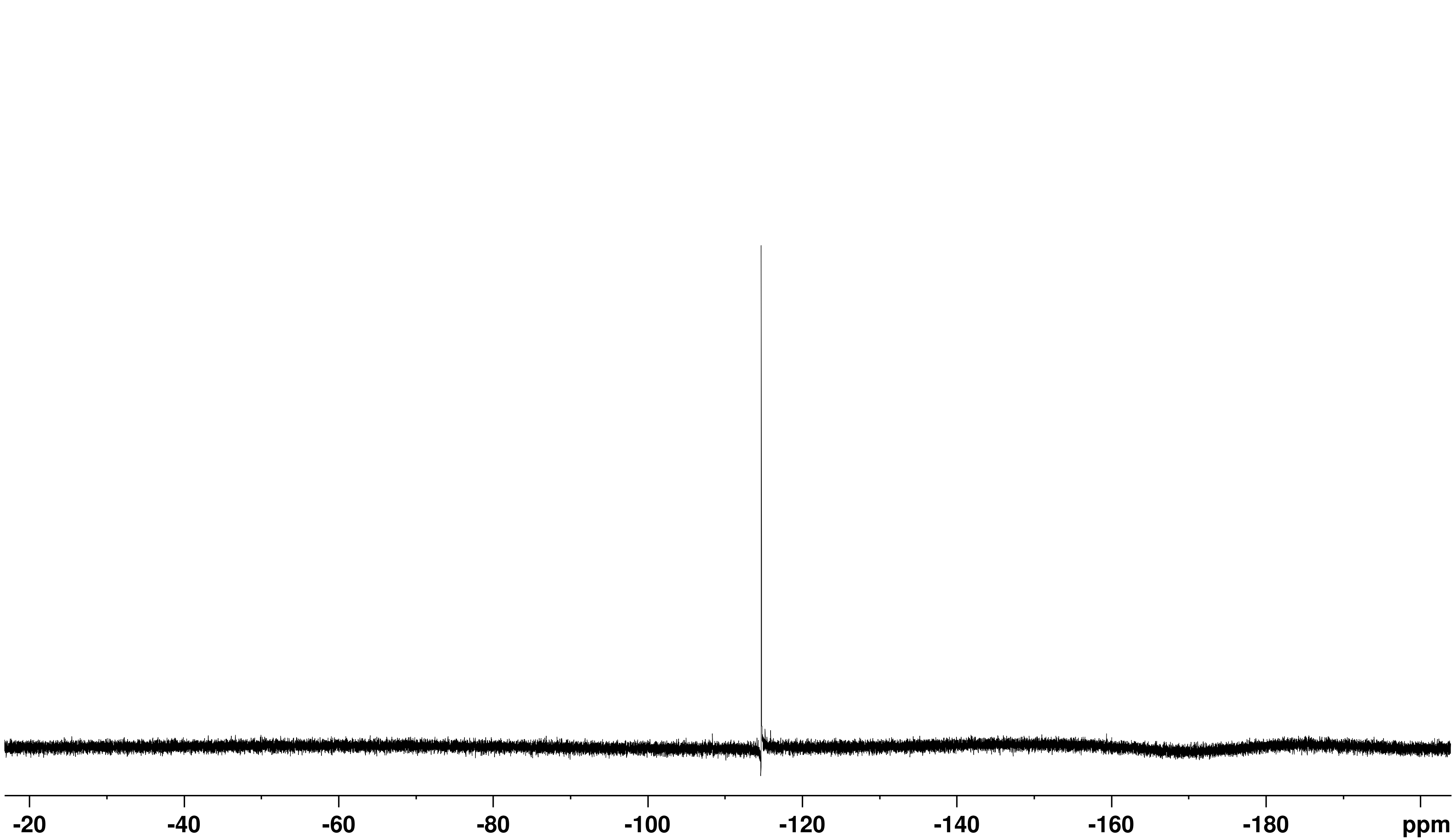

BocN
O
S
MeO
2-(3-Mepy)
F

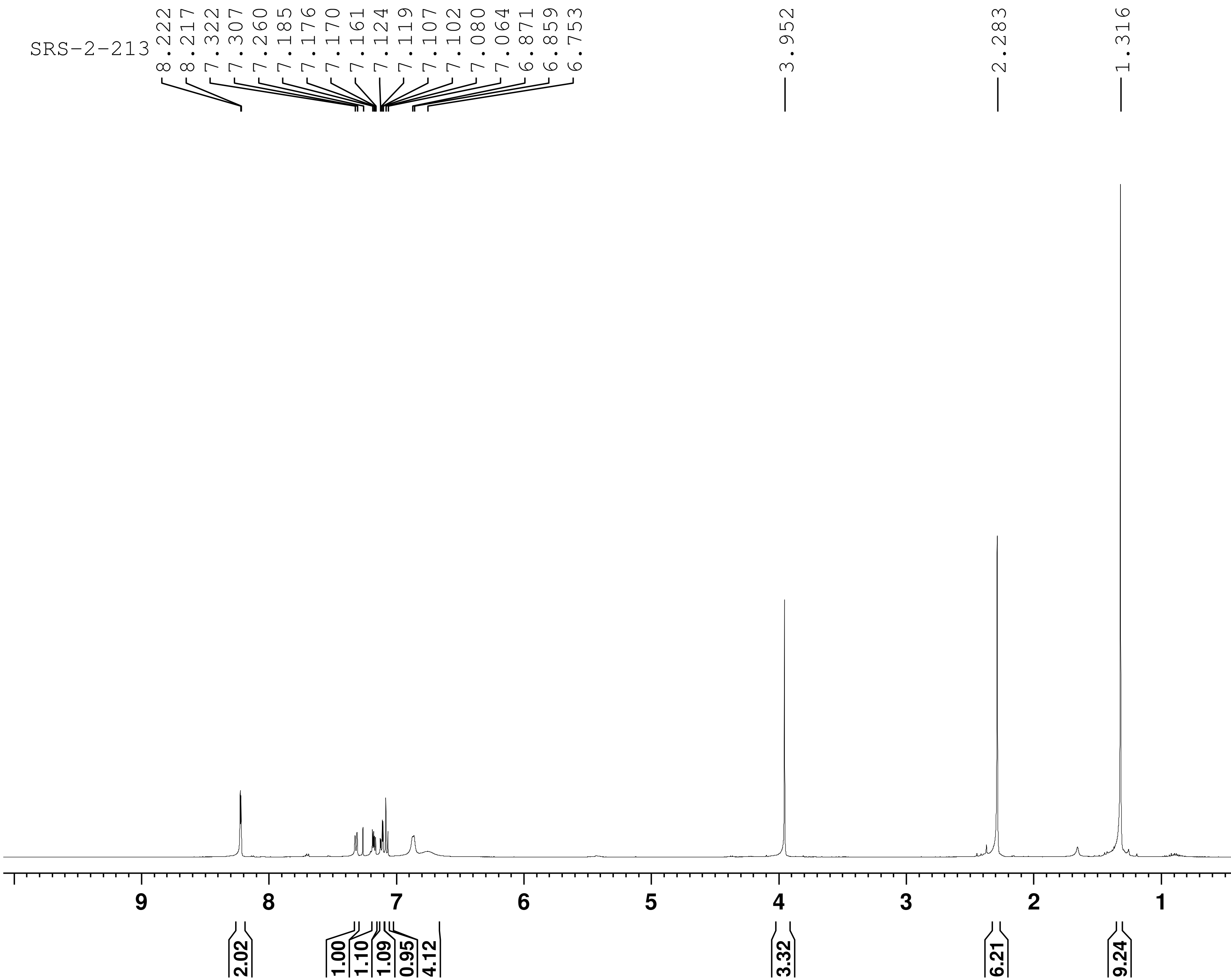
5d

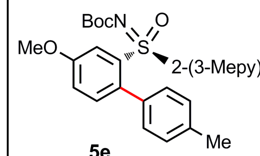
K-S-2-364



5d

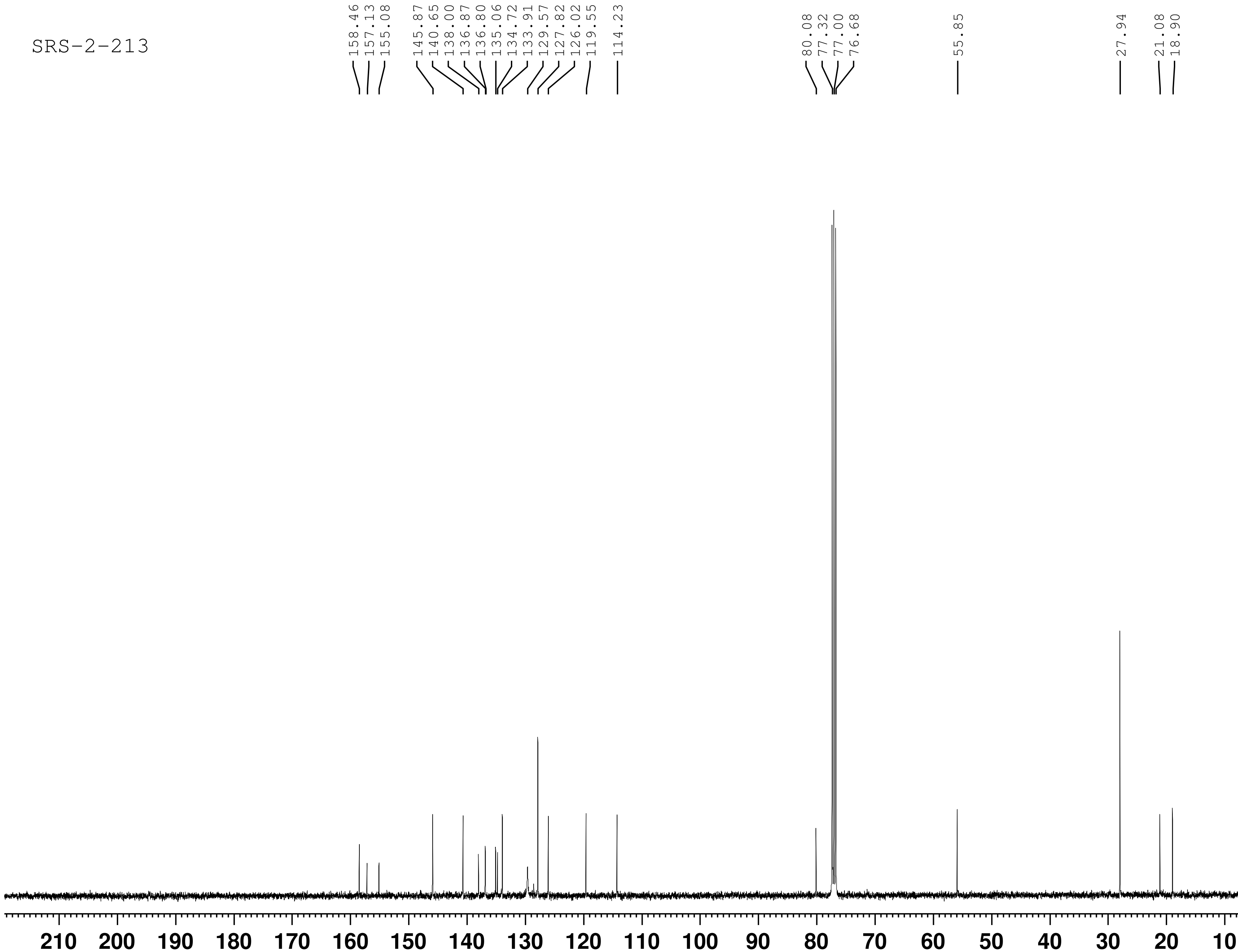


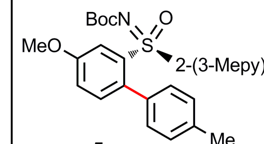

SRS-2-213
8.222
8.217
7.322
7.307
7.260
7.185
7.176
7.170
7.161
7.124
7.119
7.107
7.102
7.080
7.064
6.871
6.859
6.753
3.952
2.283
1.316
9
8
7
6
5
4
3
2
1
0
ppm
2.02
1.00
1.10
1.09
0.95
4.12
3.32
6.21
9.24


BocN
O
S
MeO
2-(3-Mepy)
Me

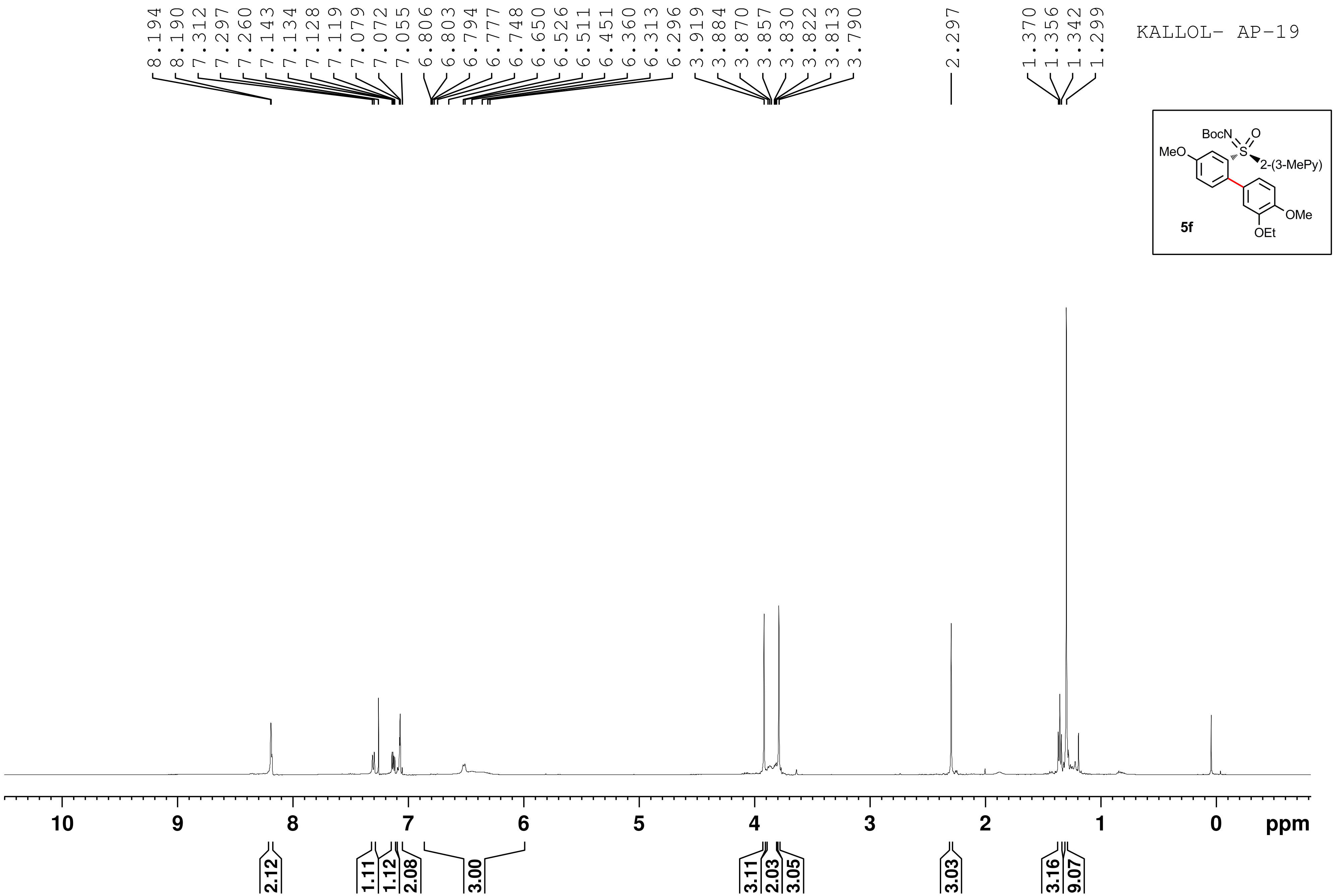
5e

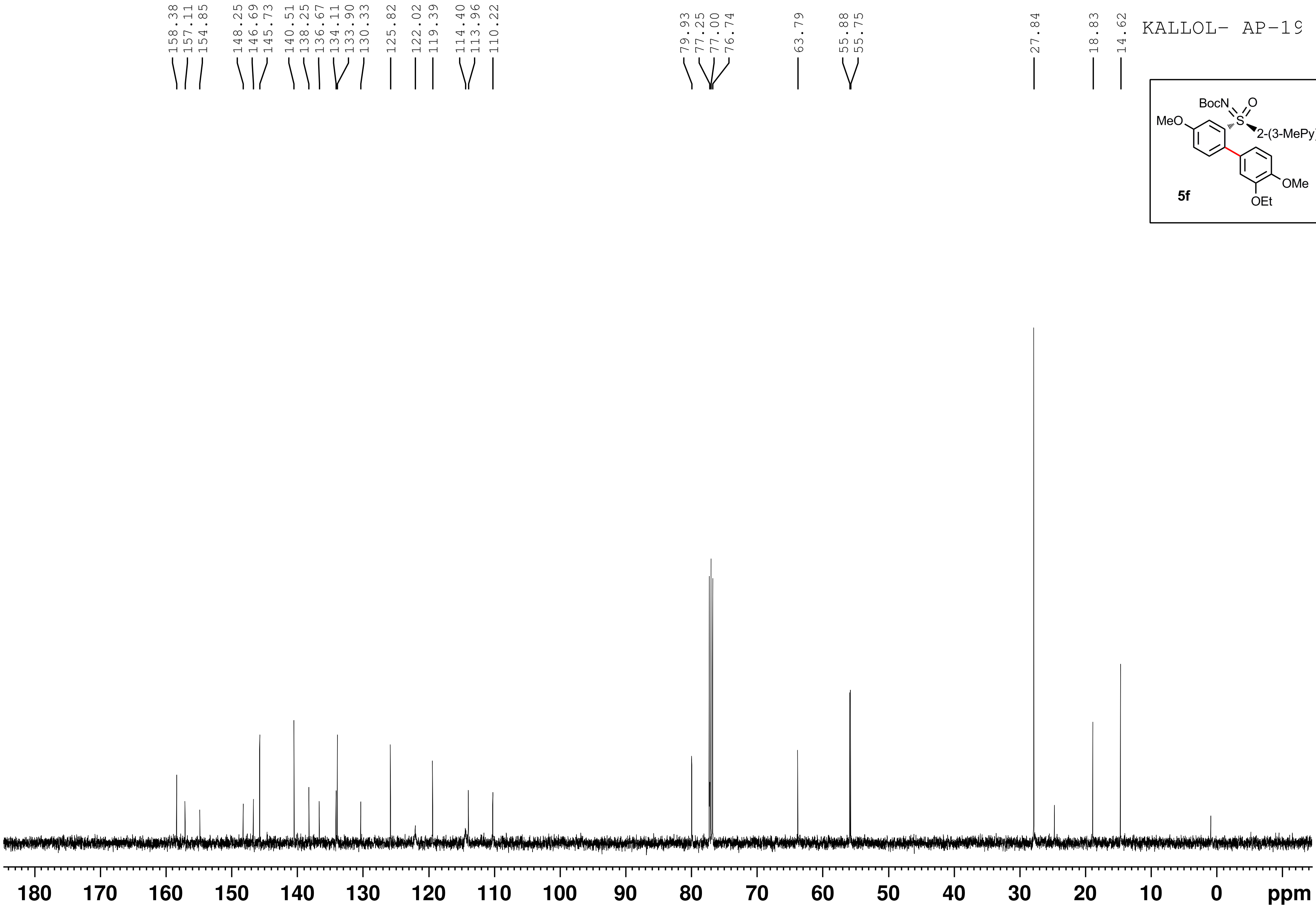
SRS-2-213

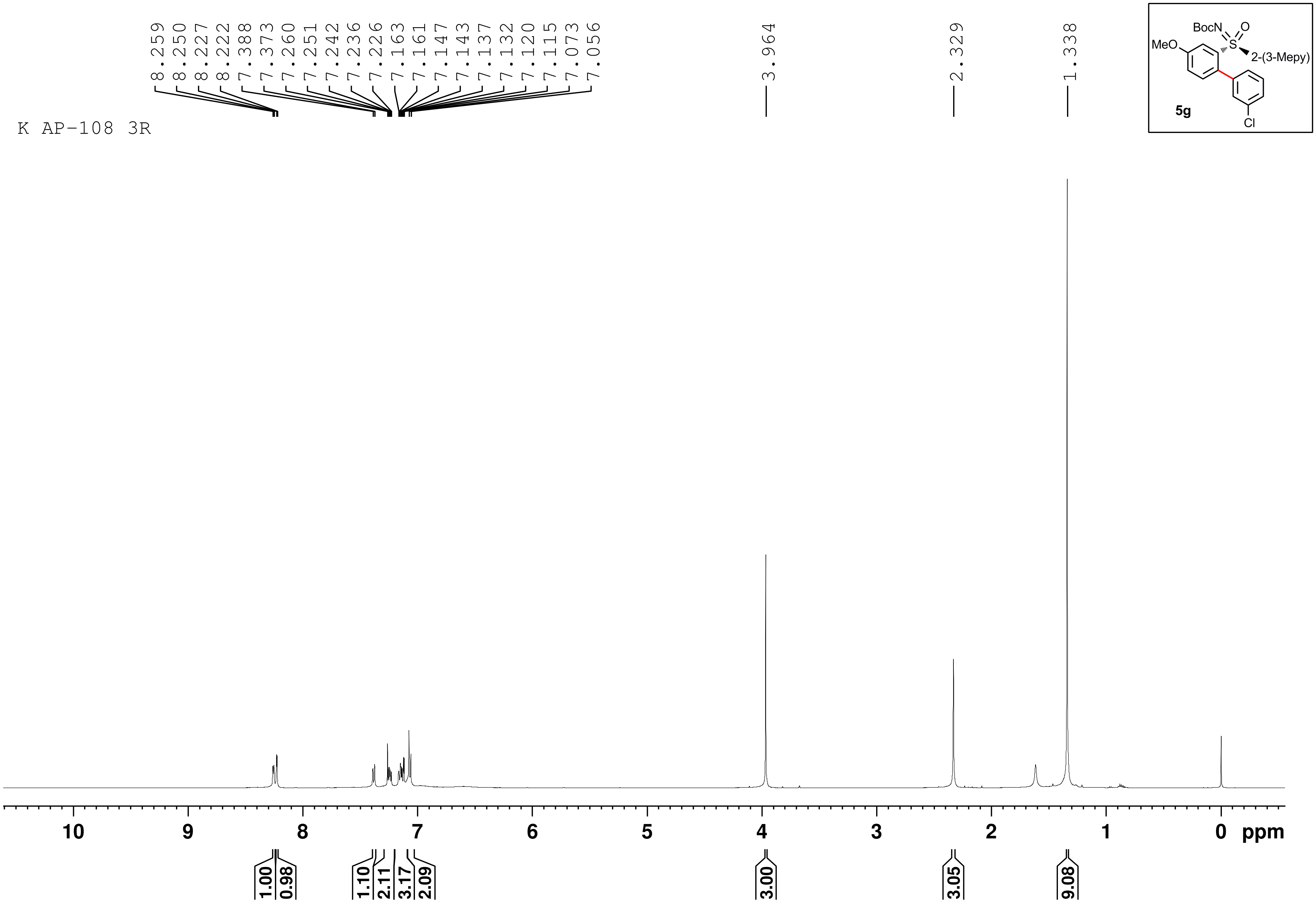

158.46
157.13
155.08
145.87
140.65
138.00
136.87
136.80
135.06
134.72
133.91
129.57
127.82
126.02
119.55
114.23
80.08
77.32
77.00
76.68
55.85
27.94
21.08
18.90
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

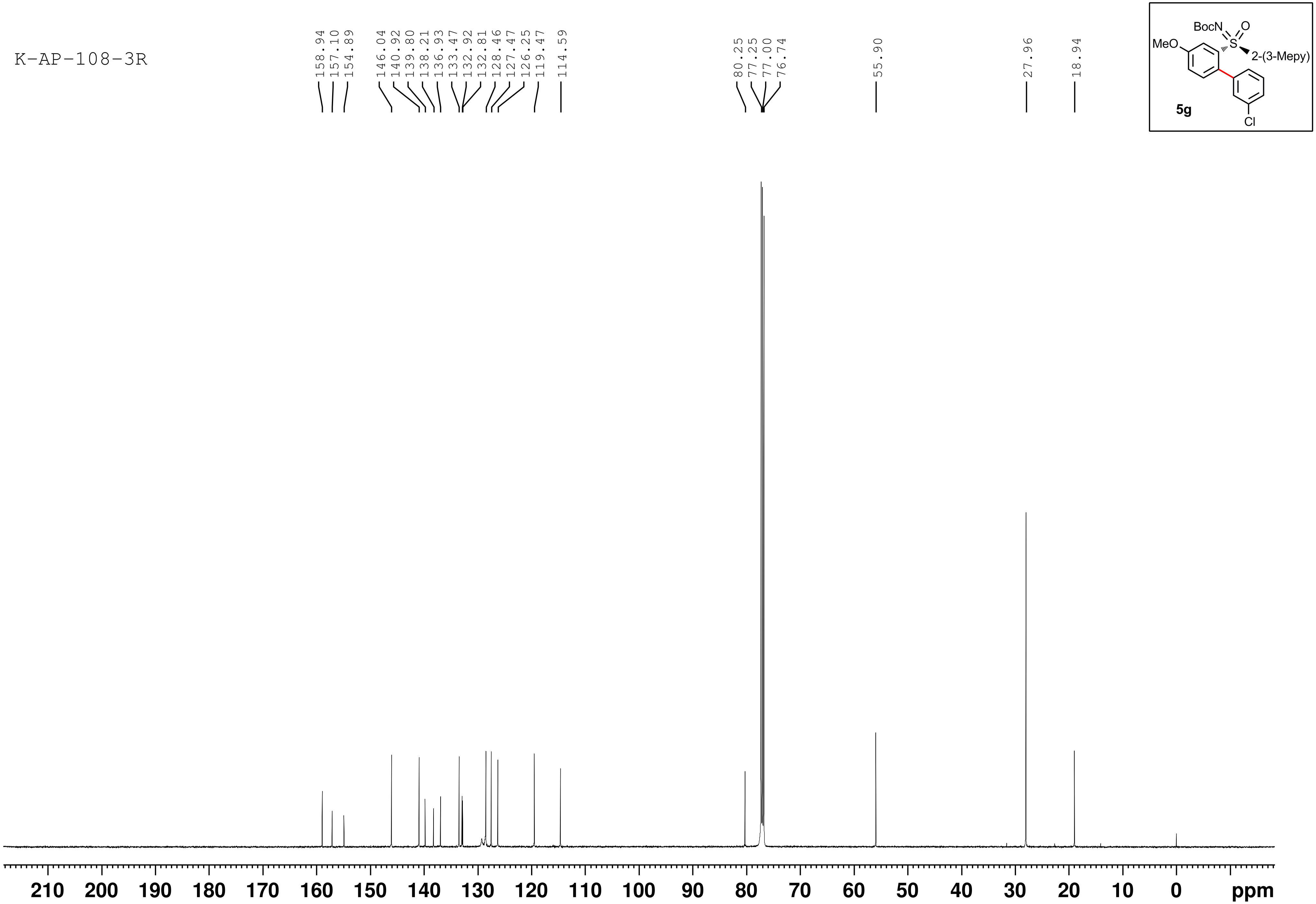

BocN
O
S
MeO
2-(3-Mepy)
Me

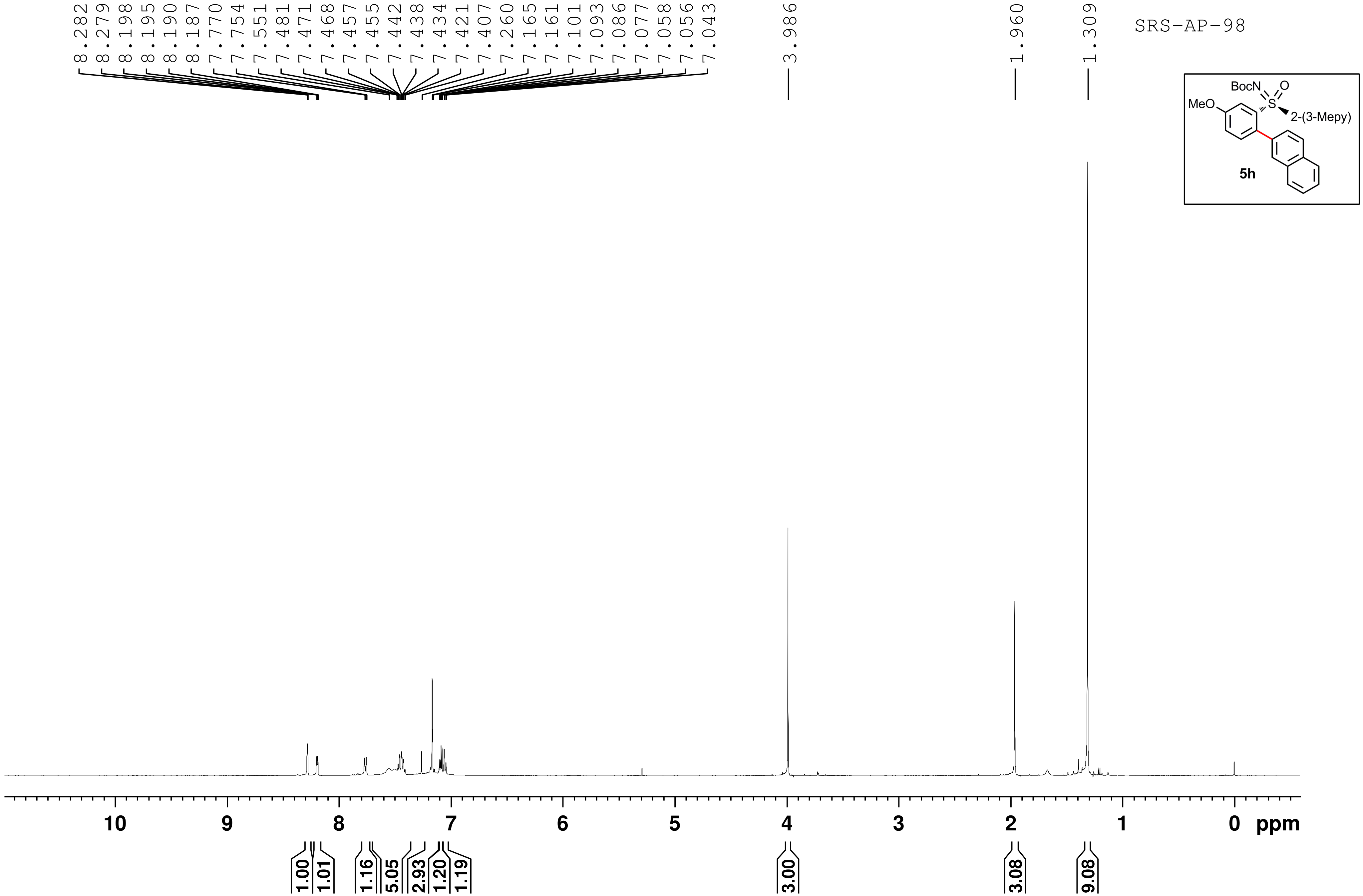
5e


8.194
8.190
7.312
7.297
7.260
7.143
7.134
7.128
7.119
7.079
7.072
7.055
6.806
6.803
6.794
6.777
6.748
6.650
6.526
6.511
6.451
6.360
6.313
6.296
3.919
3.884
3.870
3.857
3.830
3.822
3.813
3.790
2.297
1.370
1.356
1.342
1.299
KALLOL- AP-19
BocN
O
S
MeO
2-(3-MePy)
OMe
OEt
5f
10
9
8
7
6
5
4
3
2
1
0
ppm
2.12
1.11
1.12
2.08
3.00
3.11
2.03
3.05
3.03
3.16
9.07

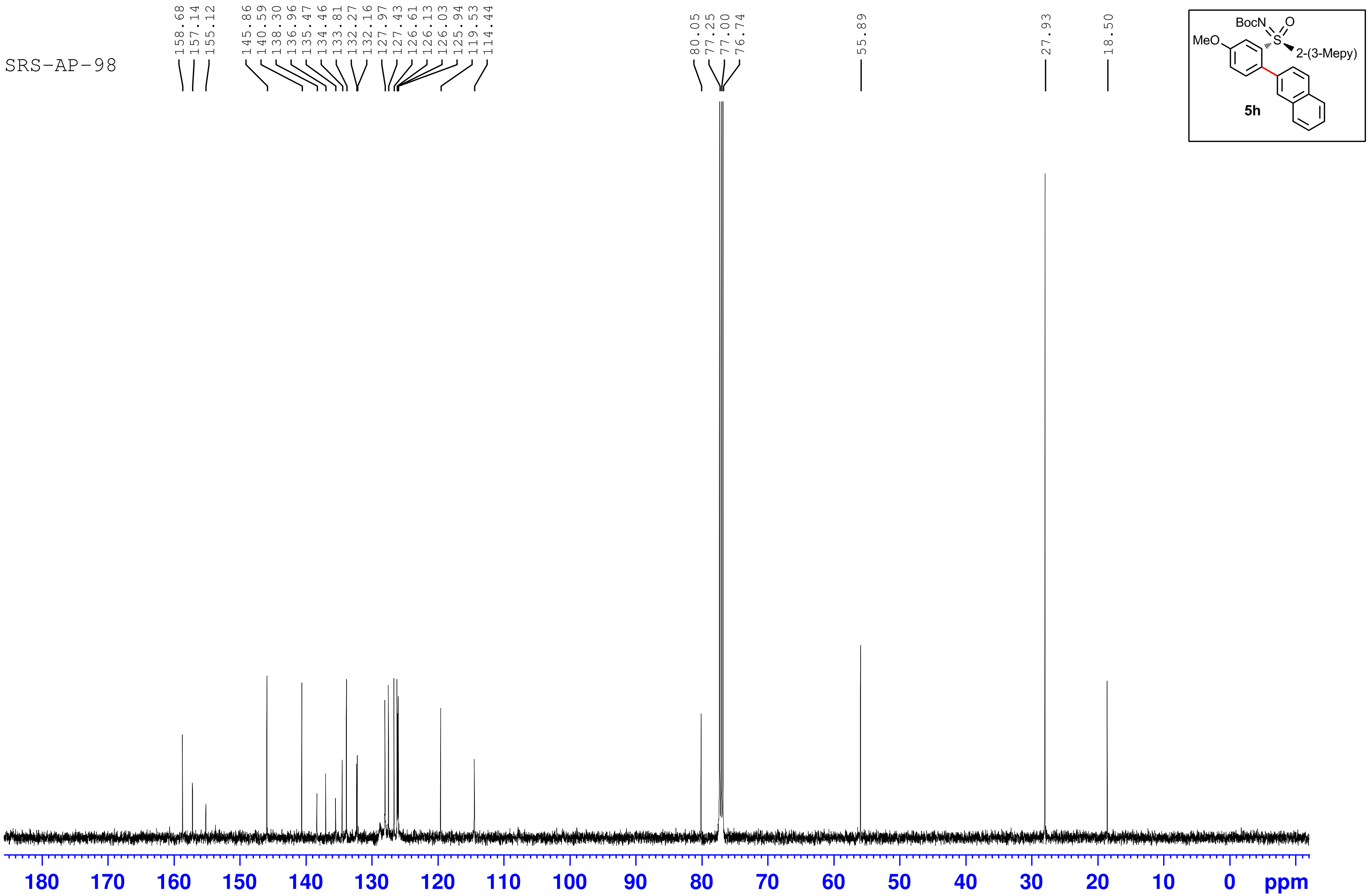

158.38
157.11
154.85
148.25
146.69
145.73
140.51
138.25
136.67
134.11
133.90
130.33
125.82
122.02
119.39
114.40
113.96
110.22
79.93
77.25
77.00
76.74
63.79
55.88
55.75
27.84
18.83
14.62
KALLOL- AP-19
BocN
O
S
MeO
2-(3-MePy)
OMe
OEt
5f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


K AP-108 3R
8.259
8.250
8.227
8.222
7.388
7.373
7.260
7.251
7.242
7.236
7.226
7.163
7.161
7.147
7.143
7.137
7.132
7.120
7.115
7.073
7.056
3.964
2.329
1.338
BocN
O
S
MeO
2-(3-Mepy)
5g
Cl
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.98
1.10
2.11
3.17
2.09
3.00
3.05
9.08

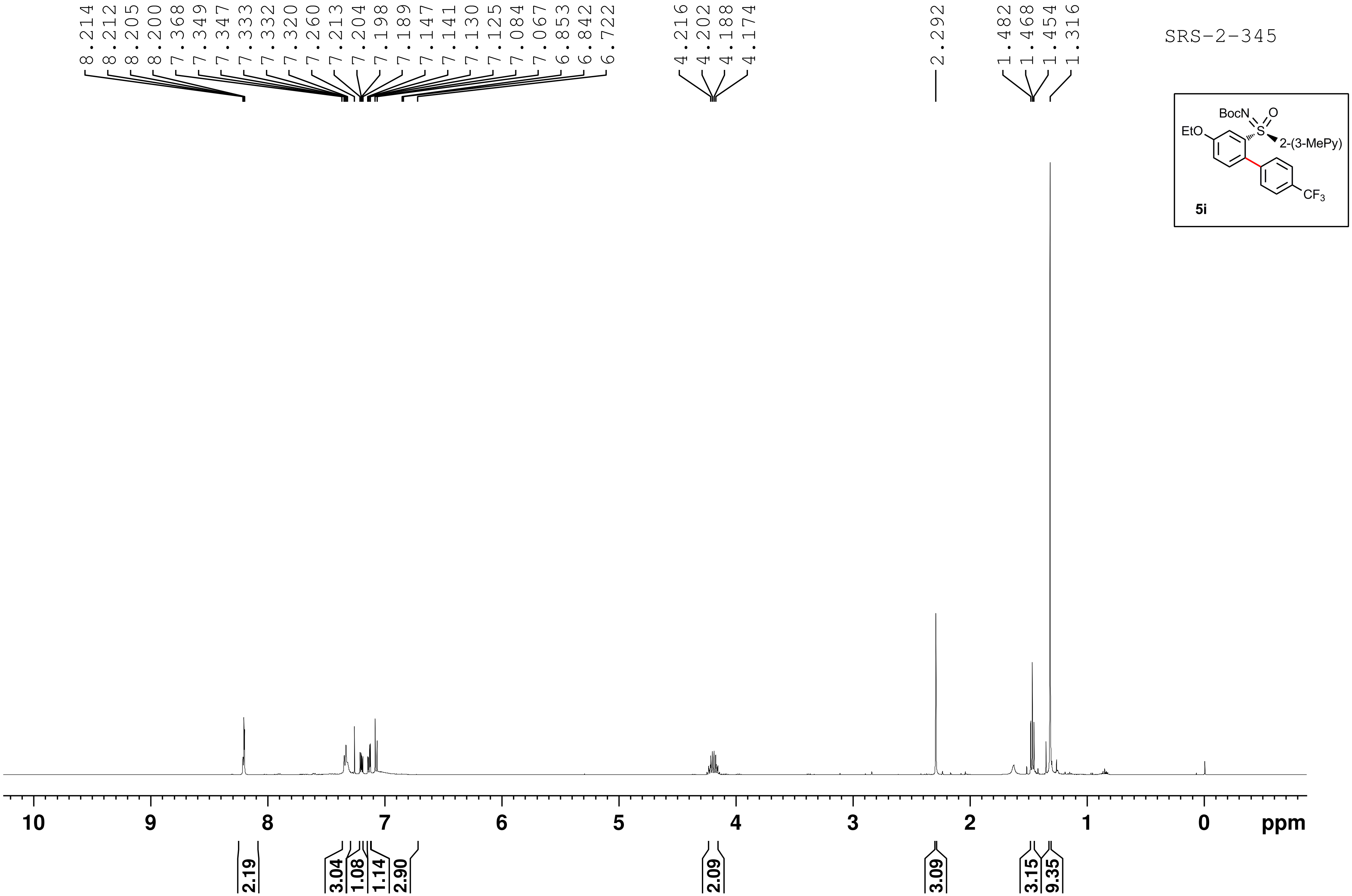

K-AP-108-3R
158.94
157.10
154.89
146.04
140.92
139.80
138.21
136.93
133.47
132.92
132.81
128.46
127.47
126.25
119.47
114.59
80.25
77.25
77.00
76.74
55.90
27.96
18.94
BocN
O
MeO
S
2-(3-Mepy)
5g
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.282
8.279
8.198
8.195
8.190
8.187
7.770
7.754
7.551
7.481
7.471
7.468
7.457
7.455
7.442
7.438
7.434
7.421
7.407
7.260
7.165
7.161
7.101
7.093
7.086
7.077
7.058
7.056
7.043
3.986
1.960
1.309
SRS-AP-98
BocN
O
S
MeO
2-(3-Mepy)
5h
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.16
5.05
2.93
1.20
1.19
3.00
3.08
9.08

SRS-AP-98


158.68
157.14
155.12
145.86
140.59
138.30
136.96
135.47
134.46
133.81
132.27
132.16
127.97
127.43
126.61
126.13
126.03
125.94
119.53
114.44
80.05
77.25
77.00
76.74
55.89
27.93
18.50
BocN
O
MeO
S
2-(3-Mepy)
5h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

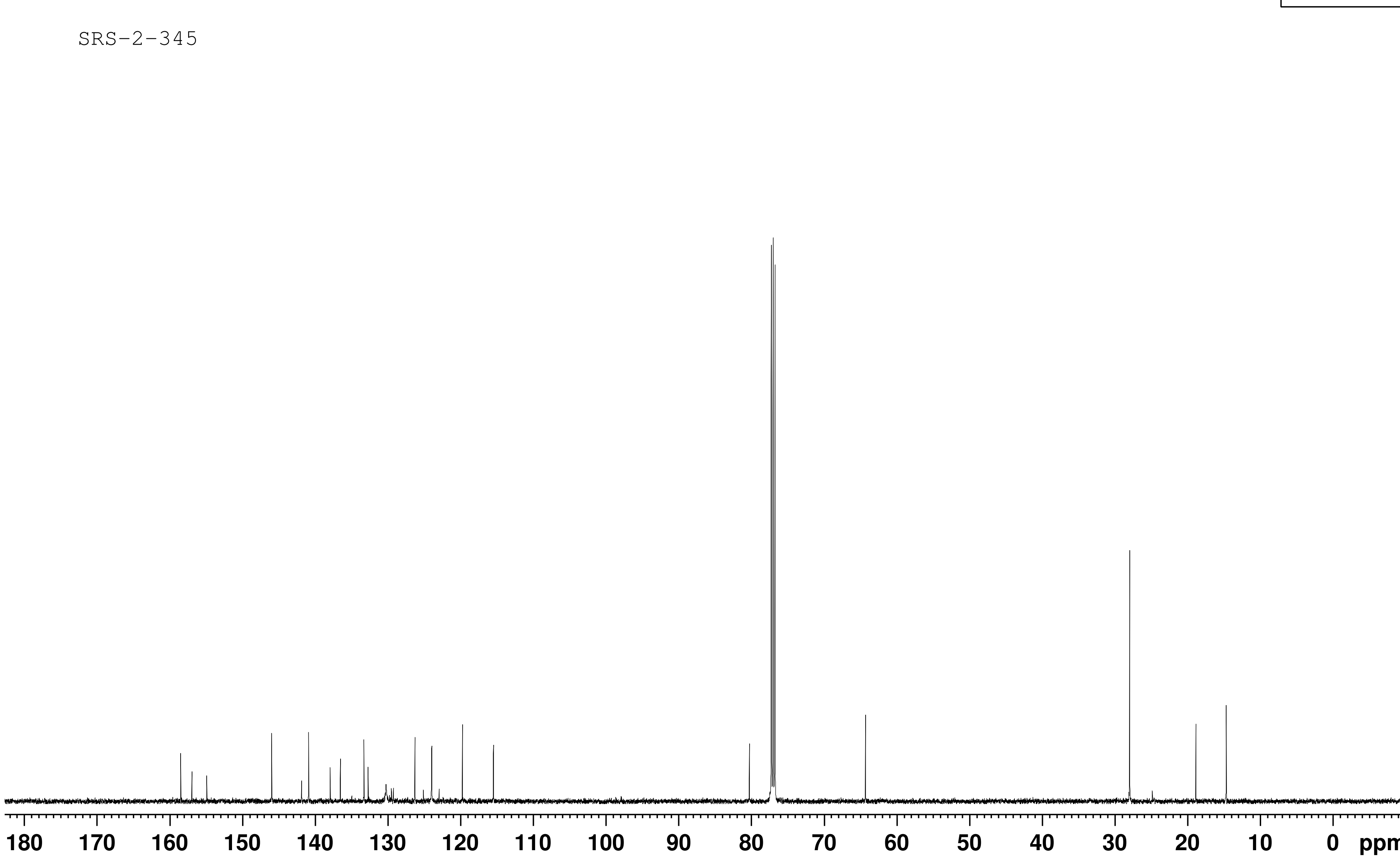
SRS-2-345



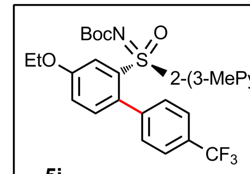
BocN
O
EtO
S
2-(3-MePy)
CF3

5i

8.214
8.212
8.205
8.200
7.368
7.349
7.347
7.333
7.332
7.320
7.260
7.213
7.204
7.198
7.189
7.147
7.141
7.130
7.125
7.084
7.067
6.853
6.842
6.722
4.216
4.202
4.188
4.174
2.292
1.482
1.468
1.454
1.316
10
9
8
7
6
5
4
3
2
1
0
ppm
2.19
3.04
1.08
1.14
2.90
2.09
3.09
3.15
9.35



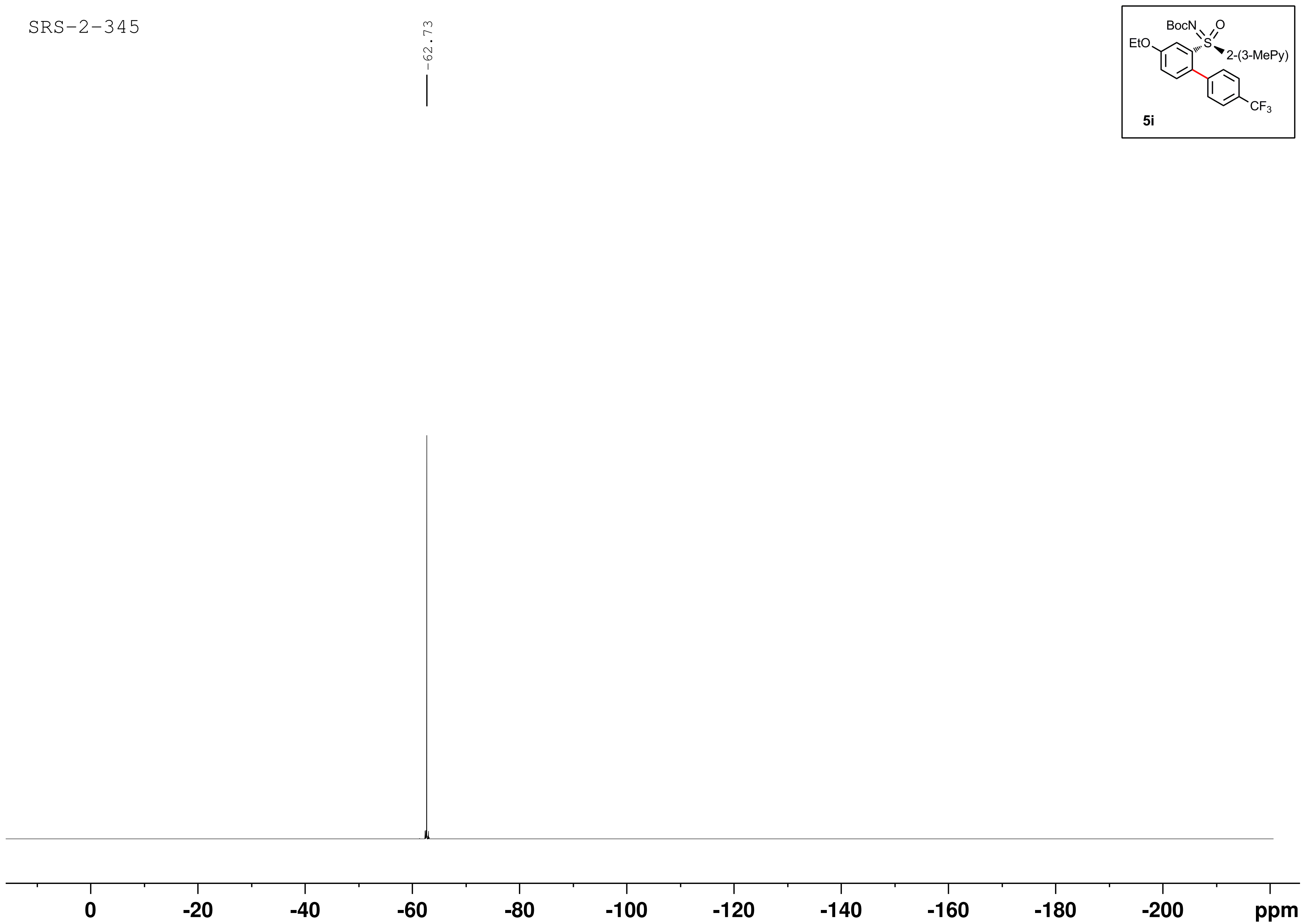
158.49
156.96
154.92
145.98
141.85
140.91
137.95
136.54
133.29
132.71
130.25
129.50
129.24
126.28
125.11
124.02
123.98
123.95
123.93
122.94
119.74
115.47
80.27
77.25
77.00
76.74
64.29
27.93
18.82
14.66
SRS-2-345
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



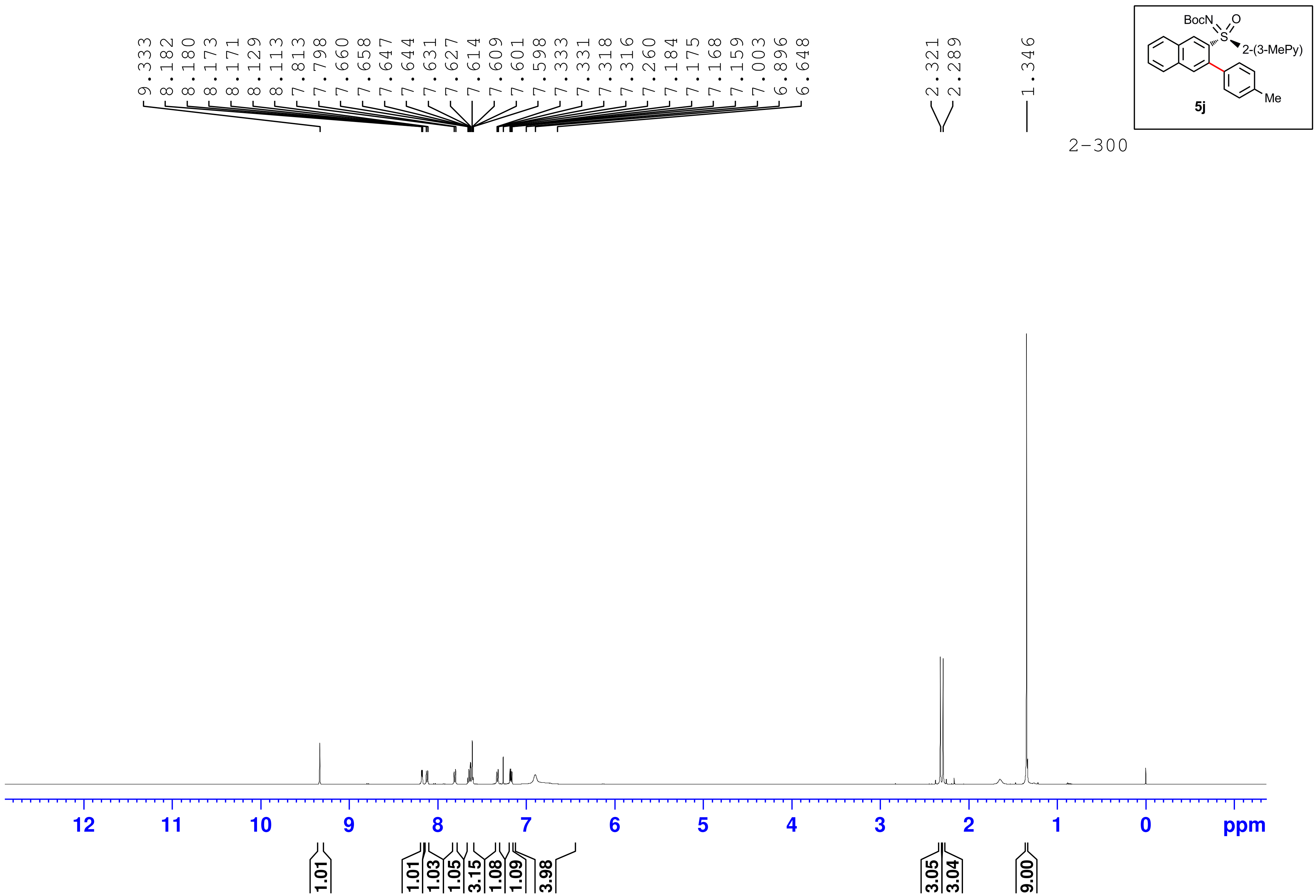
BocN
O
S
EtO
2-(3-MePy)
CF3

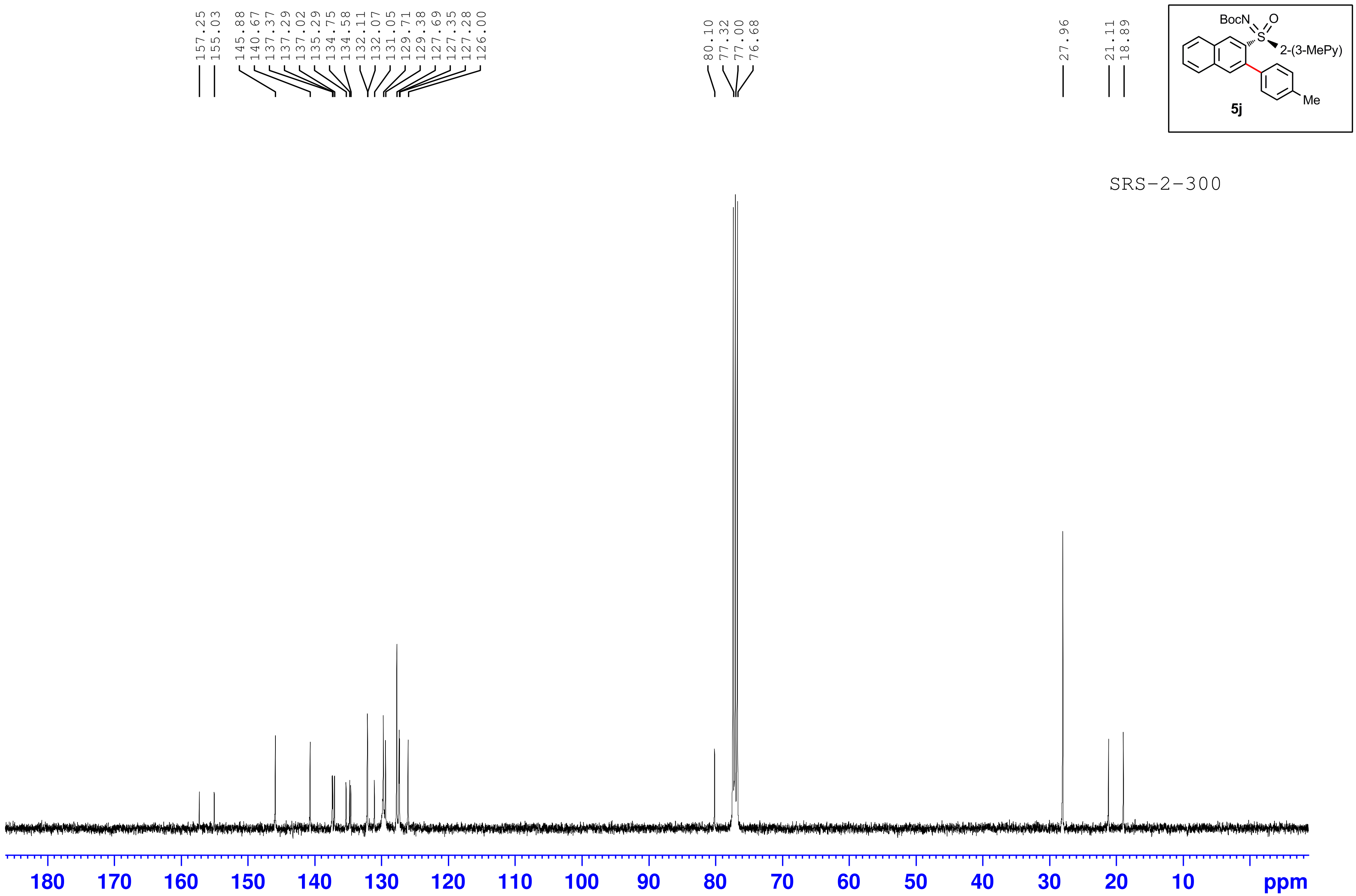
5i

SRS-2-345

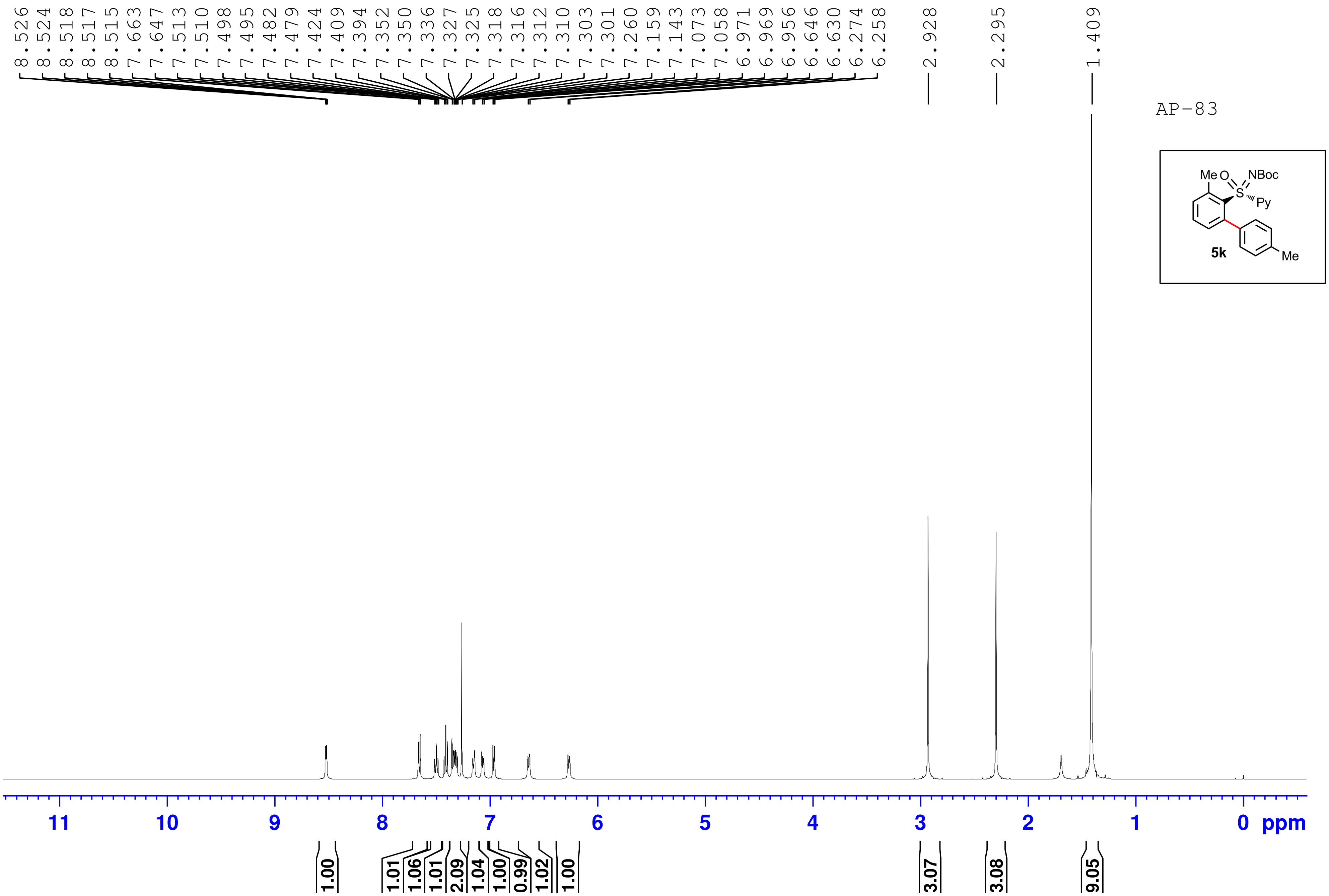

-62.73
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
BocN
O
S
EtO
2-(3-MePy)
CF_3

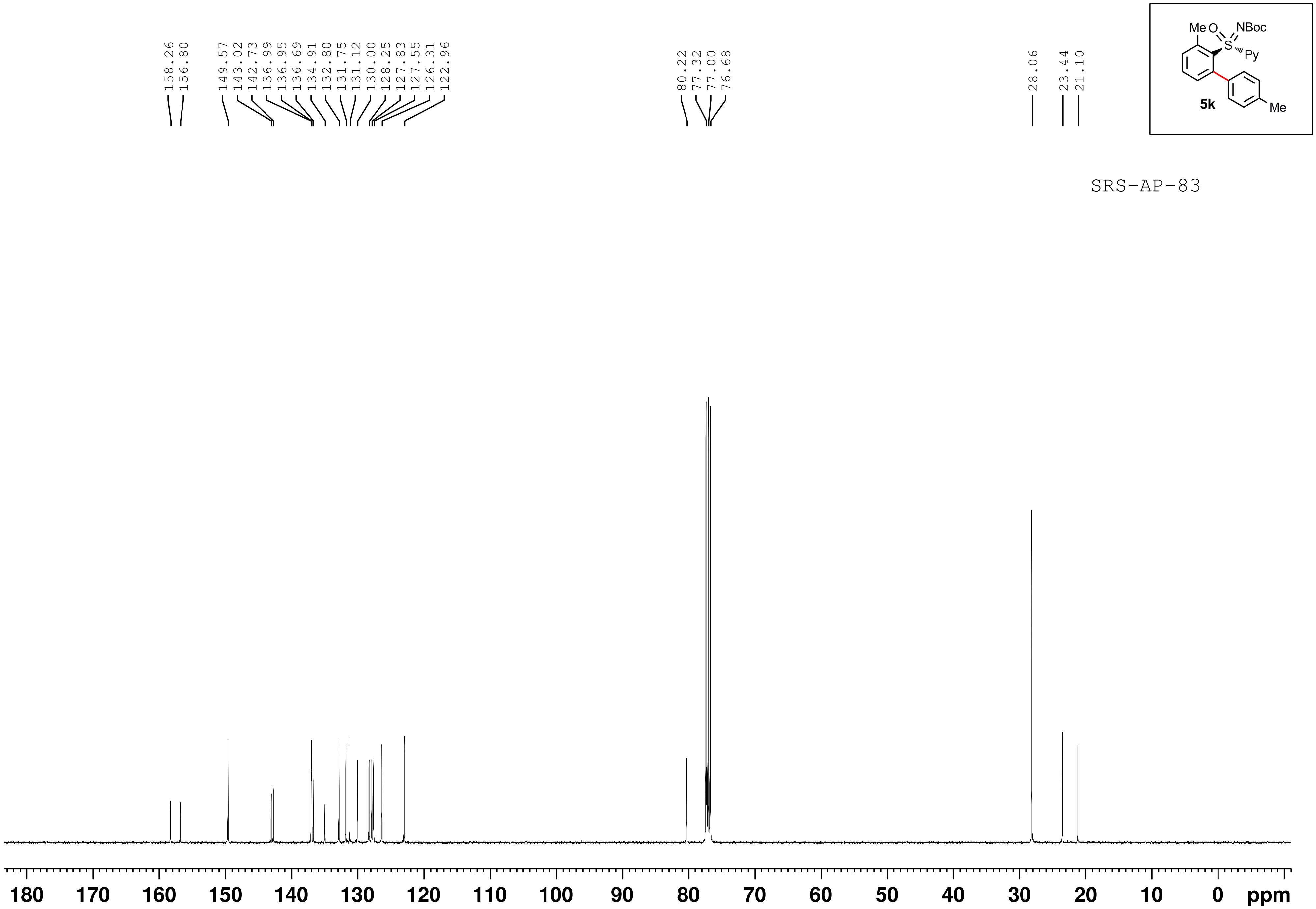
5i

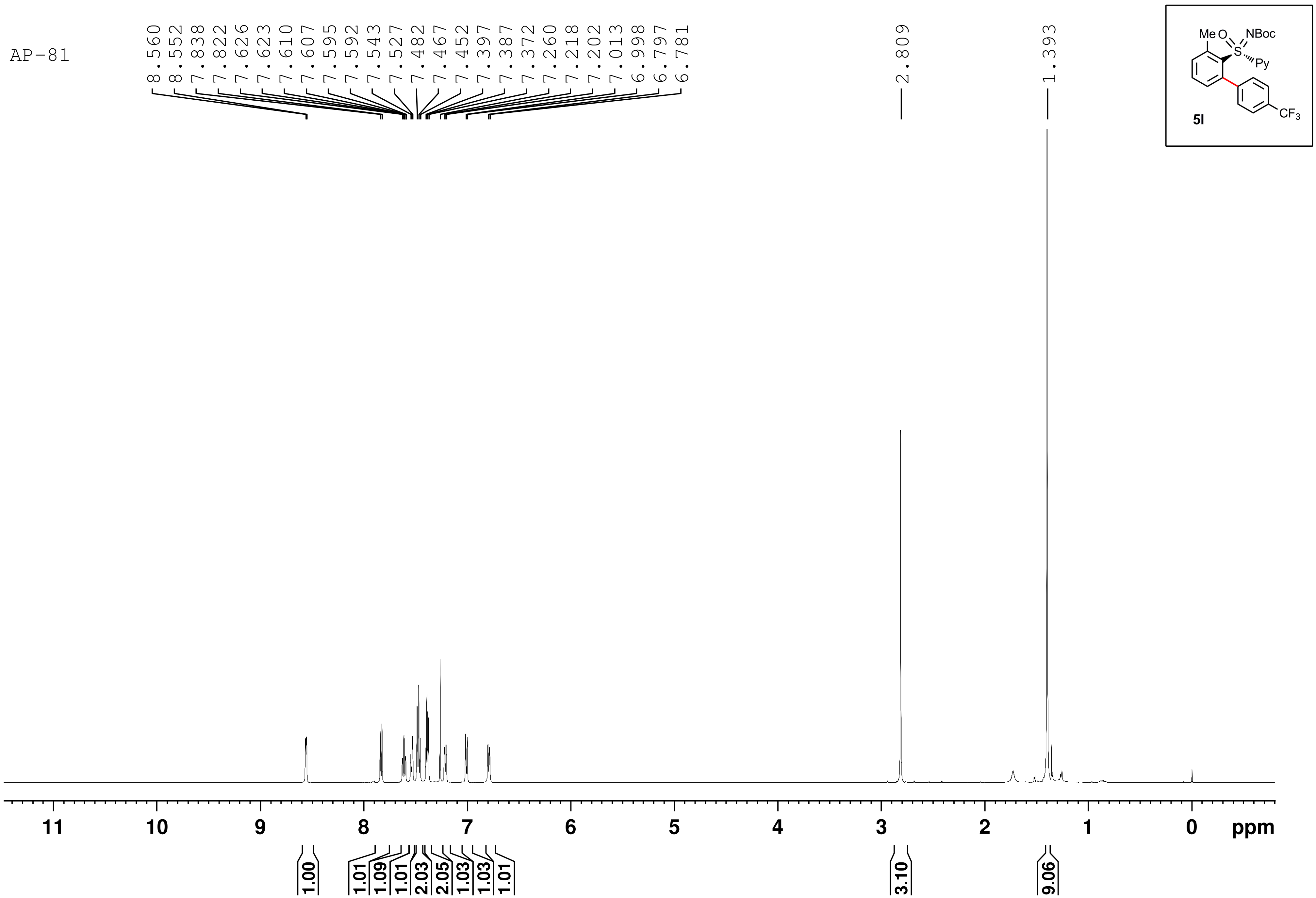

9.333 8.182 8.180 8.173 8.171 8.129 8.113 7.813 7.798 7.660 7.658 7.647 7.644 7.631 7.627 7.614 7.609 7.601 7.598 7.333 7.331 7.318 7.316 7.260 7.184 7.175 7.168 7.159 7.003 6.896 6.648
2.321 2.289
1.346
2-300
BocN
O
S
2-(3-MePy)
Me
5j
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.01 1.01 1.03 1.05 3.15 1.08 1.09 3.98 3.05 3.04 9.00



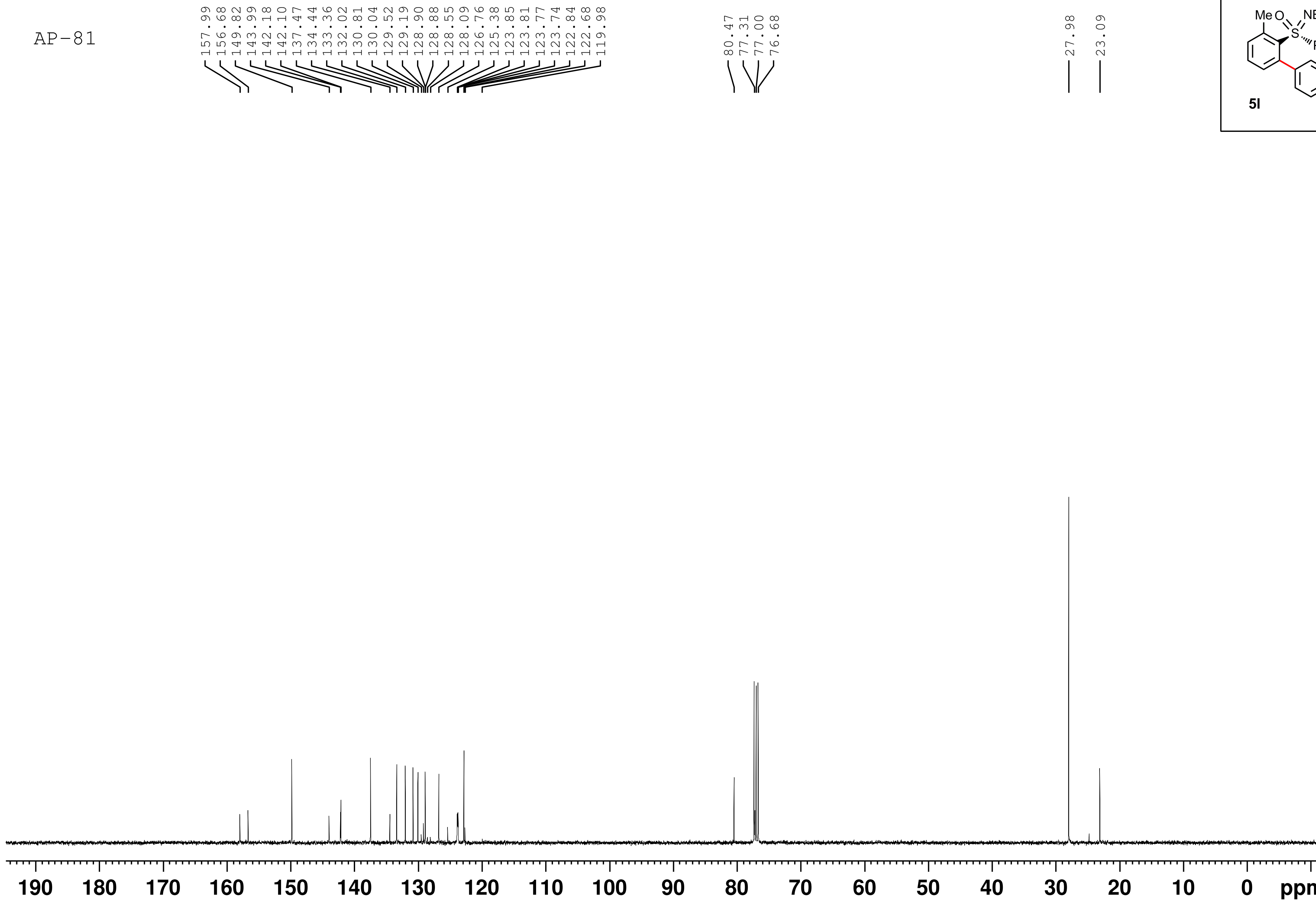
157.25
155.03
145.88
140.67
137.37
137.29
137.02
135.29
134.75
134.58
132.11
132.07
131.05
129.71
129.38
127.69
127.35
127.28
126.00
80.10
77.32
77.00
76.68
27.96
21.11
18.89
BocN
O
S
2-(3-MePy)
Me
5j
SRS-2-300
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

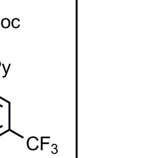

8.526 8.524 8.518 8.517 8.515 7.663 7.647 7.513 7.510 7.498 7.495 7.482 7.479 7.424 7.409 7.394 7.352 7.350 7.336 7.327 7.325 7.318 7.316 7.312 7.310 7.303 7.301 7.260 7.159 7.143 7.073 7.058 6.971 6.969 6.956 6.646 6.630 6.274 6.258
2.928
2.295
1.409
AP-83
Me
O
NBoc
S
Py
5k
Me
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.01 1.06 1.01 2.09 1.04 1.00 0.99 1.02 1.00 3.07 3.08 9.05


158.26
156.80
149.57
143.02
142.73
136.99
136.95
136.69
134.91
132.80
131.75
131.12
130.00
128.25
127.83
127.55
126.31
122.96
80.22
77.32
77.00
76.68
28.06
23.44
21.10
Me O
NBoc
S
Py
5k
Me
SRS-AP-83
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


AP-81
8.560
8.552
7.838
7.822
7.626
7.623
7.610
7.607
7.595
7.592
7.543
7.527
7.482
7.467
7.452
7.397
7.387
7.372
7.260
7.218
7.202
7.013
6.998
6.797
6.781
2.809
1.393
Me O
NBoc
S
Py
CF3
5l
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.09
1.01
2.03
2.05
1.03
1.03
1.01
3.10
9.06

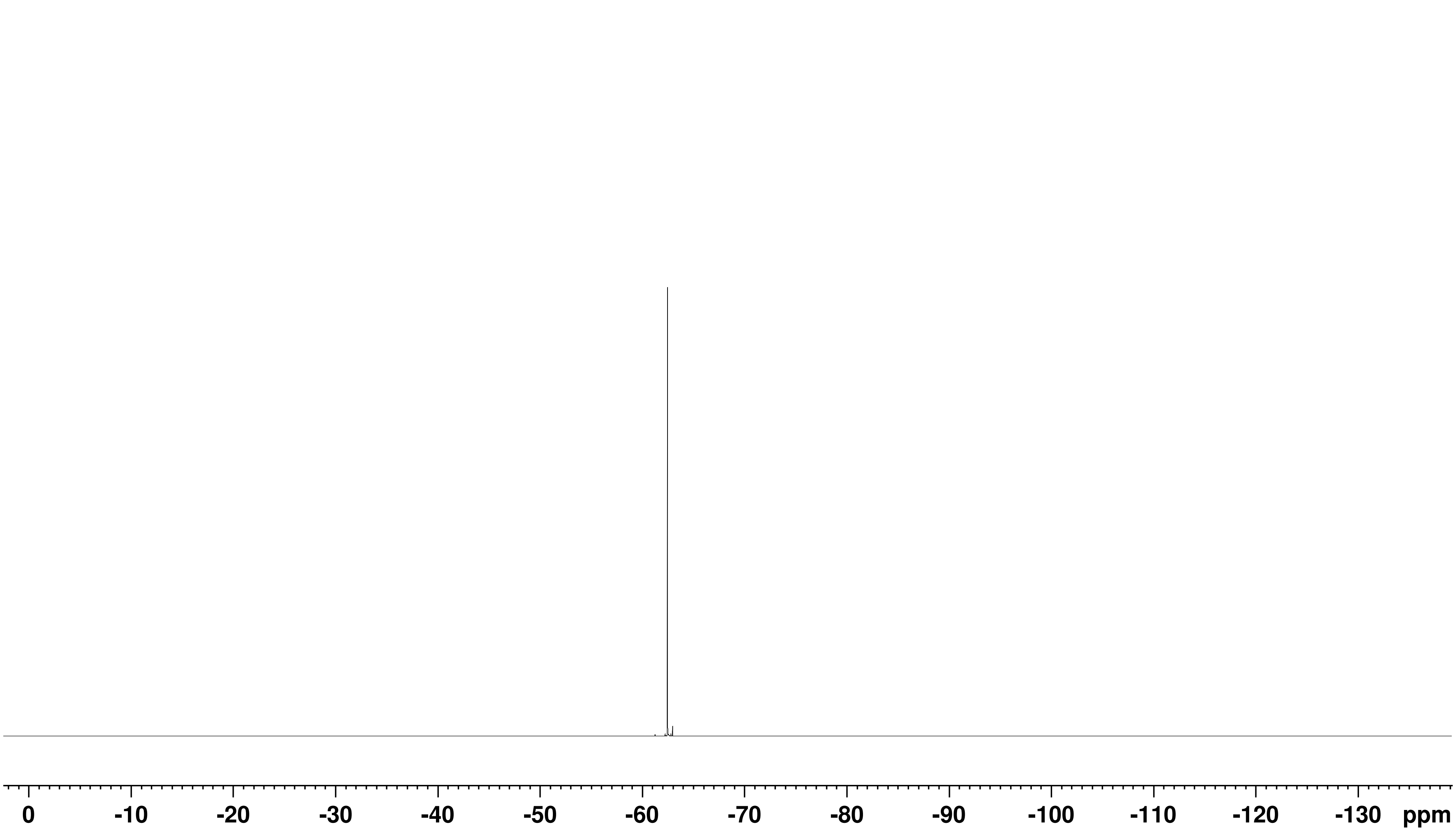
AP-81

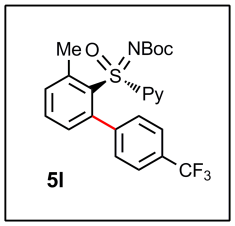

157.99
156.68
149.82
143.99
142.18
142.10
137.47
134.44
133.36
132.02
130.81
130.04
129.52
129.19
128.90
128.88
128.55
128.09
126.76
125.38
123.85
123.81
123.77
123.74
122.84
122.68
119.98
80.47
77.31
77.00
76.68
27.98
23.09
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

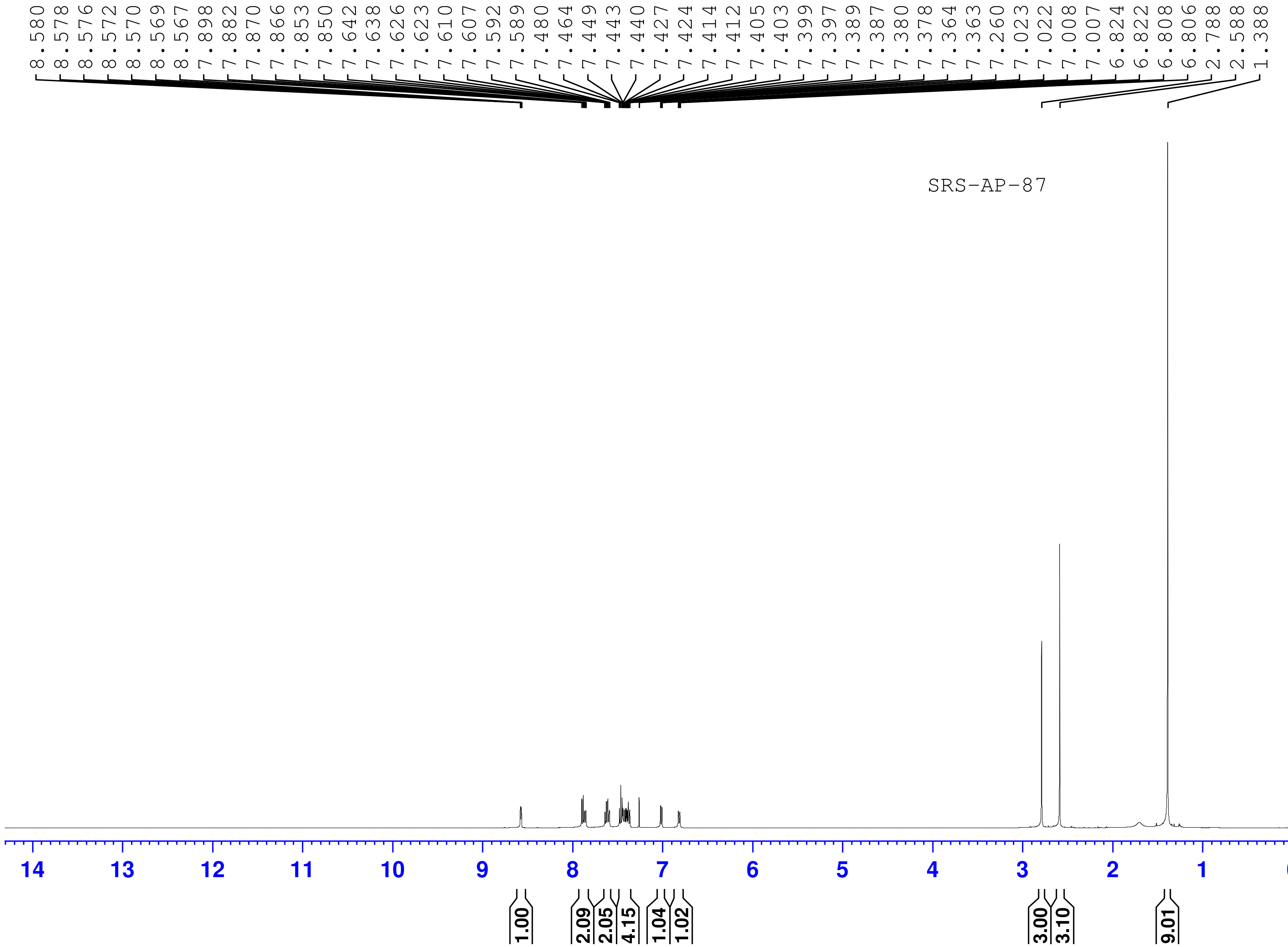

Me
O
NBoc
S
Py
CF3

5l

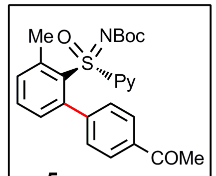
AP-81


-62.49
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
ppm


Me
O
NBoc
S
Py
CF3
5l

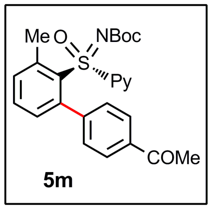


8.580
8.578
8.576
8.572
8.570
8.569
8.567
7.898
7.882
7.870
7.866
7.853
7.850
7.642
7.638
7.626
7.623
7.610
7.607
7.592
7.589
7.480
7.464
7.449
7.443
7.440
7.427
7.424
7.414
7.412
7.405
7.403
7.399
7.397
7.389
7.387
7.380
7.378
7.364
7.363
7.260
7.023
7.022
7.008
7.007
6.824
6.822
6.808
6.806
2.788
2.588
1.388
SRS-AP-87
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
2.09
2.05
4.15
1.04
1.02
3.00
3.10
9.01

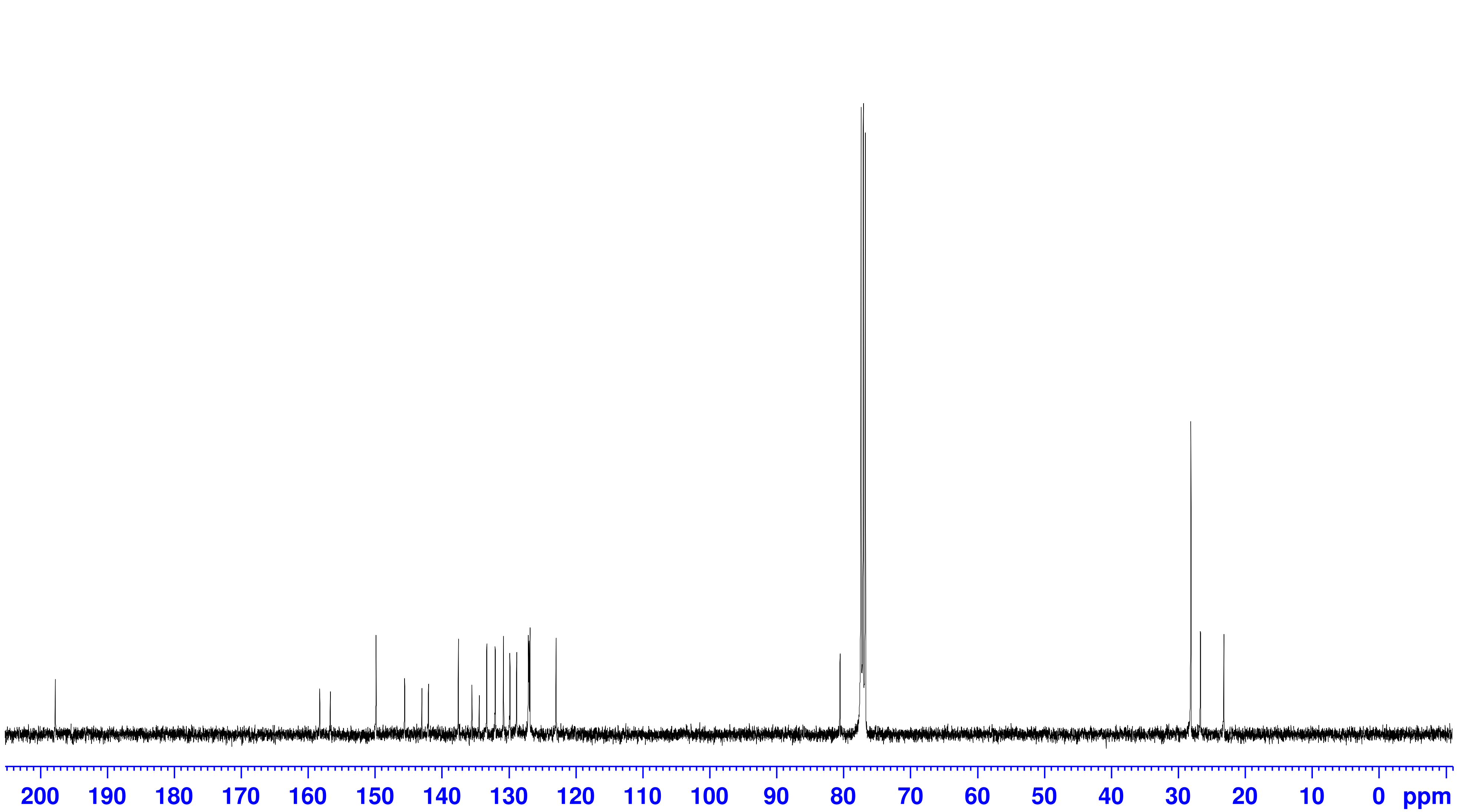


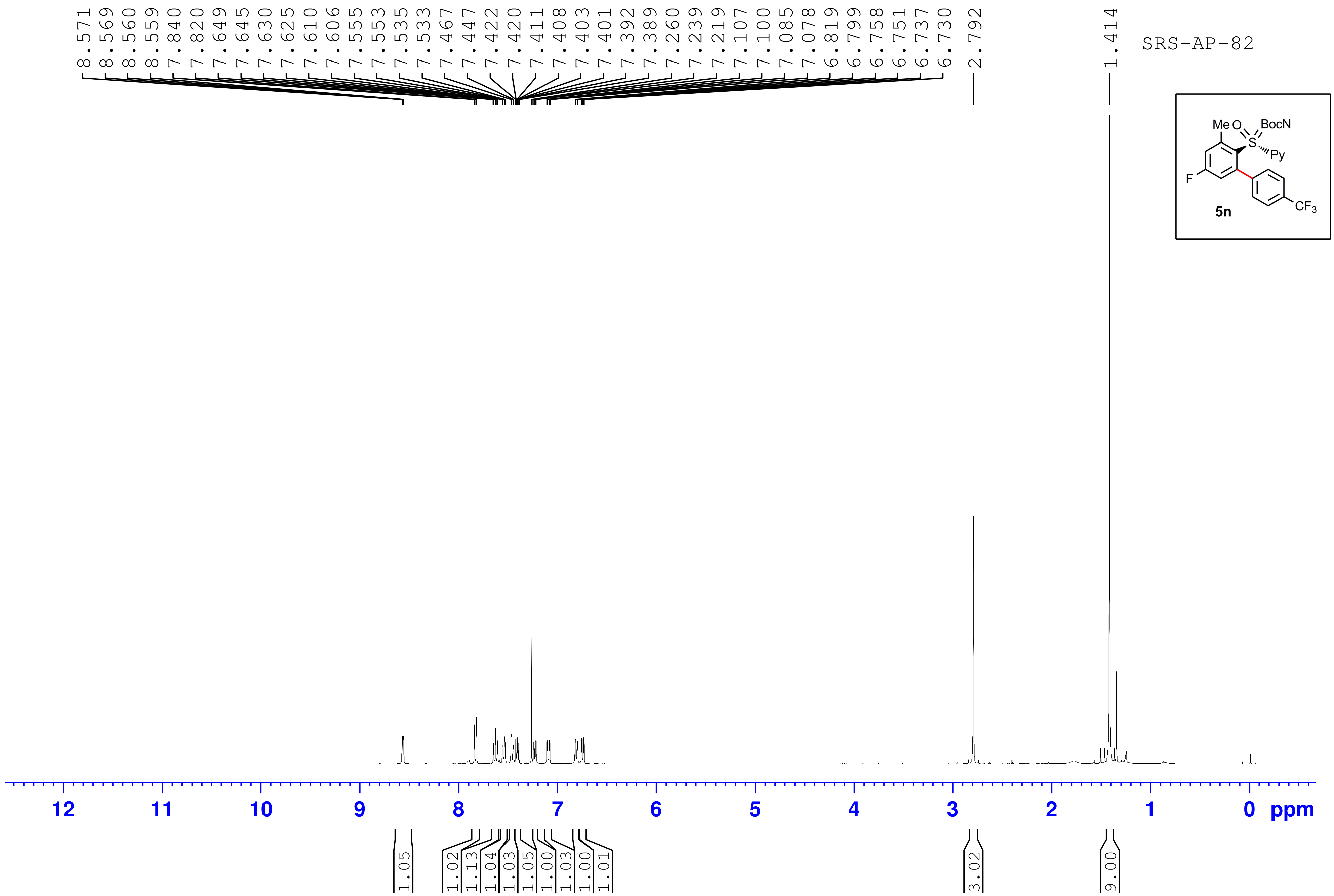
Me O
NBoc
S
Py
COMe

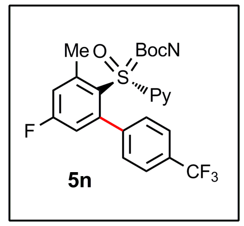
5m


Me O
NBoc
S
Py
COMe
5m

SRS-AP-87

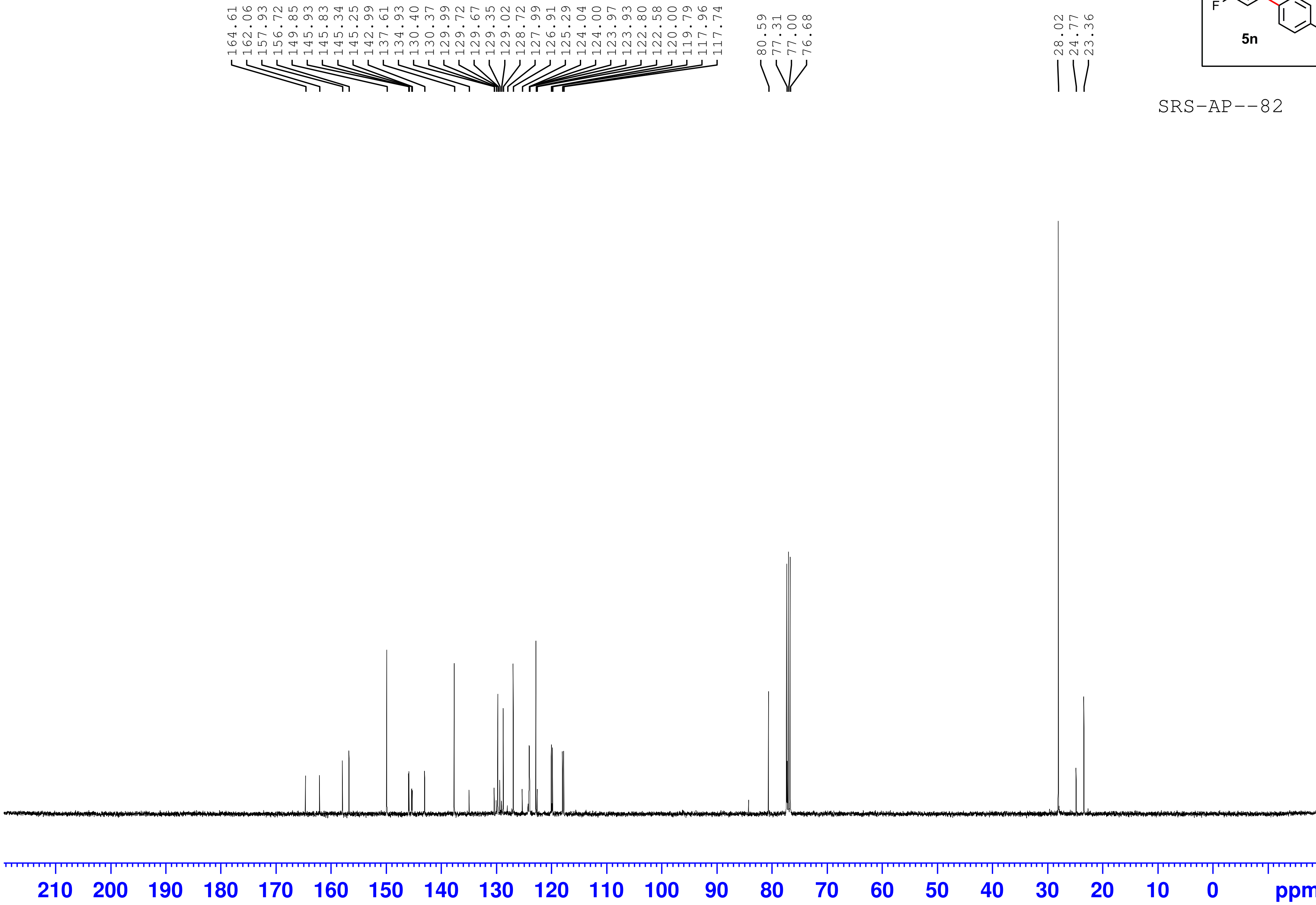

197.73
158.23
156.65
149.82
145.55
142.95
141.99
137.51
135.50
134.38
133.27
132.00
130.75
129.81
128.80
127.05
126.96
126.82
122.90
80.47
77.32
77.00
76.68
28.04
26.62
23.10
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.571
8.569
8.560
8.559
7.840
7.820
7.649
7.645
7.630
7.625
7.610
7.606
7.555
7.553
7.535
7.533
7.467
7.447
7.422
7.420
7.411
7.408
7.403
7.401
7.392
7.389
7.260
7.239
7.219
7.107
7.100
7.085
7.078
6.819
6.799
6.758
6.751
6.737
6.730
2.792
1.414
SRS-AP-82
Me
O
BocN
S
Py
F
CF3
5n
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.05
1.02
1.13
1.04
1.03
1.05
1.00
1.03
1.00
1.01
3.02
9.00

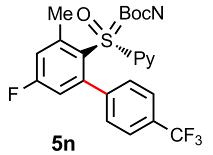


Me
O
BocN
S
Py
F
CF3
5n

SRS-AP--82

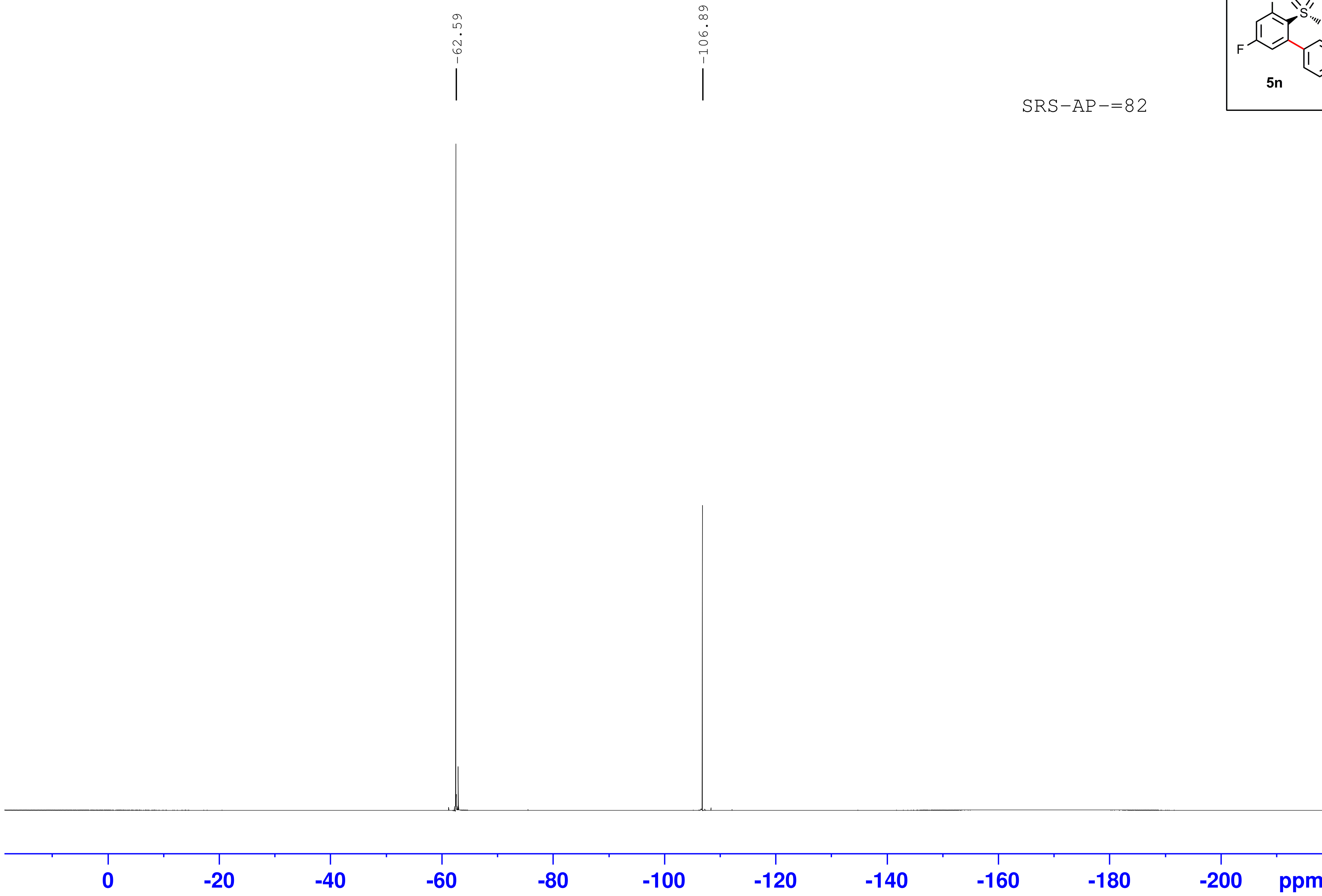


164.61
162.06
157.93
156.72
149.85
145.93
145.83
145.34
145.25
142.99
137.61
134.93
130.40
130.37
129.99
129.72
129.67
129.35
129.02
128.72
127.99
126.91
125.29
124.04
124.00
123.97
123.93
122.80
122.58
120.00
119.79
117.96
117.74
80.59
77.31
77.00
76.68
28.02
24.77
23.36
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

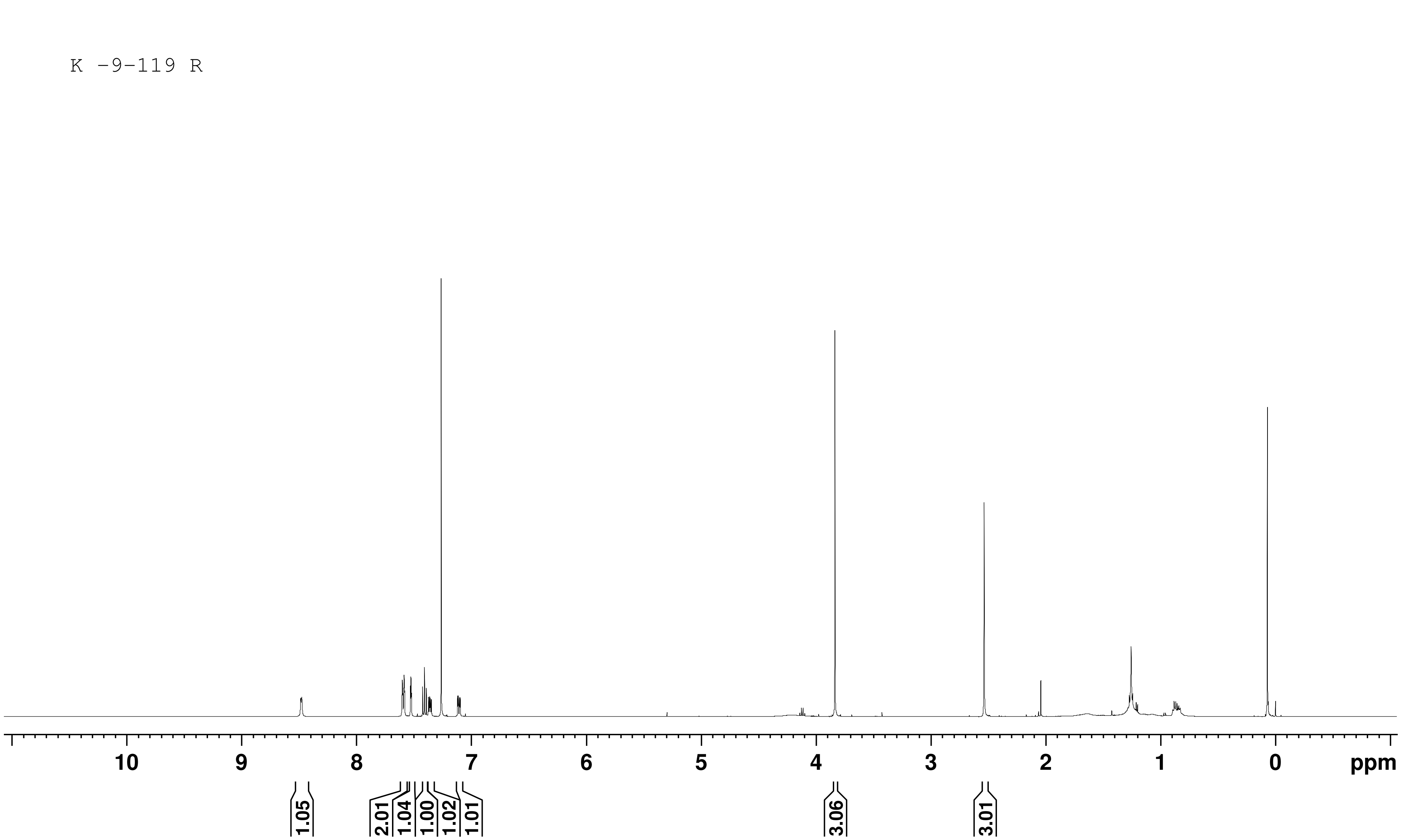


Me
O
BocN
S
Py
F
CF3

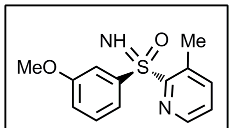
5n



-62.59
-106.89
SRS-AP-=82
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

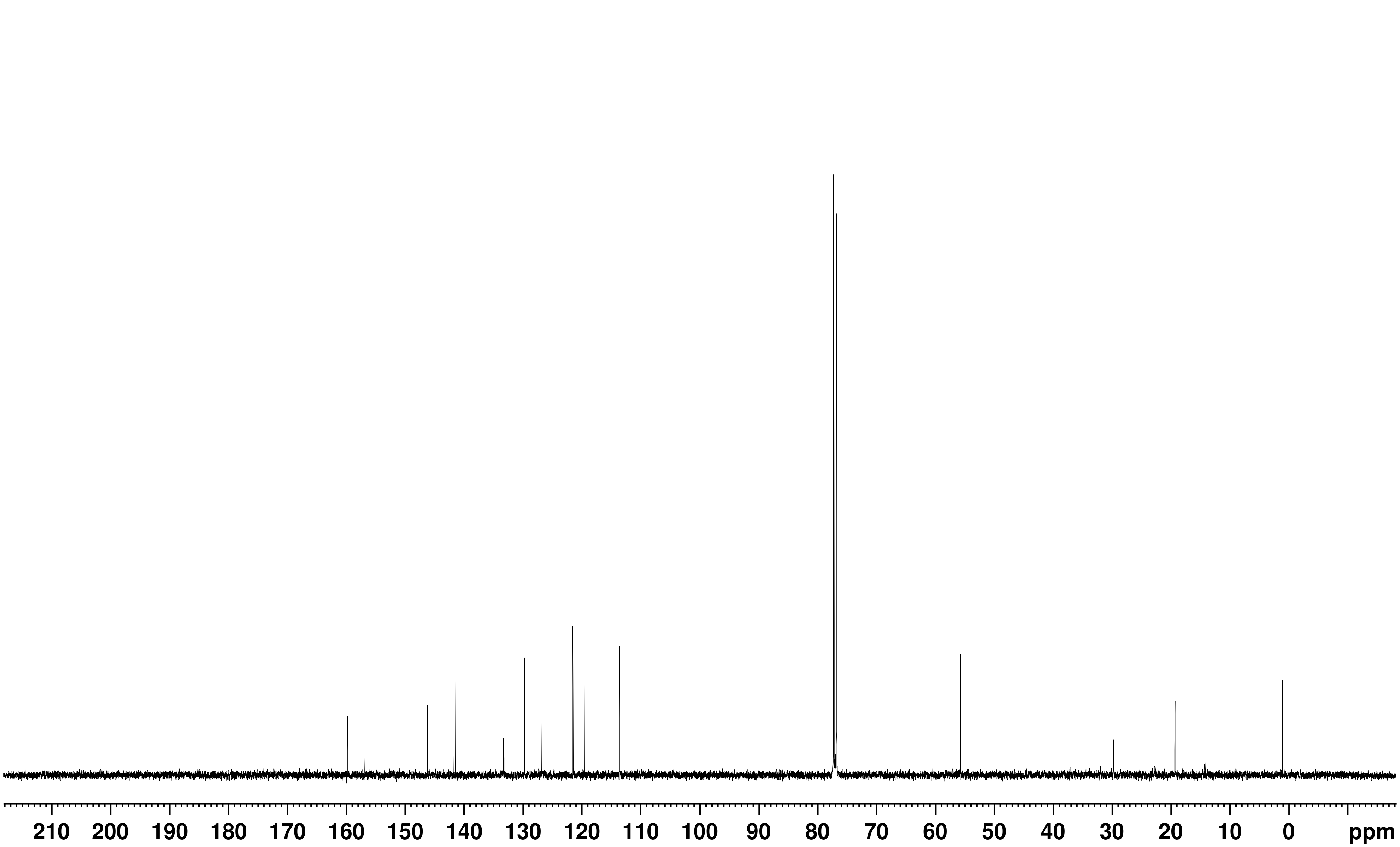


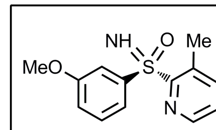
8.482
8.473
7.599
7.597
7.595
7.593
7.585
7.583
7.581
7.580
7.578
7.528
7.523
7.519
7.421
7.405
7.389
7.370
7.361
7.355
7.345
7.260
7.116
7.111
7.099
7.095
3.831
2.532
K -9-119 R
10
9
8
7
6
5
4
3
2
1
0
ppm
1.05
2.01
1.04
1.00
1.02
1.01
3.06
3.01

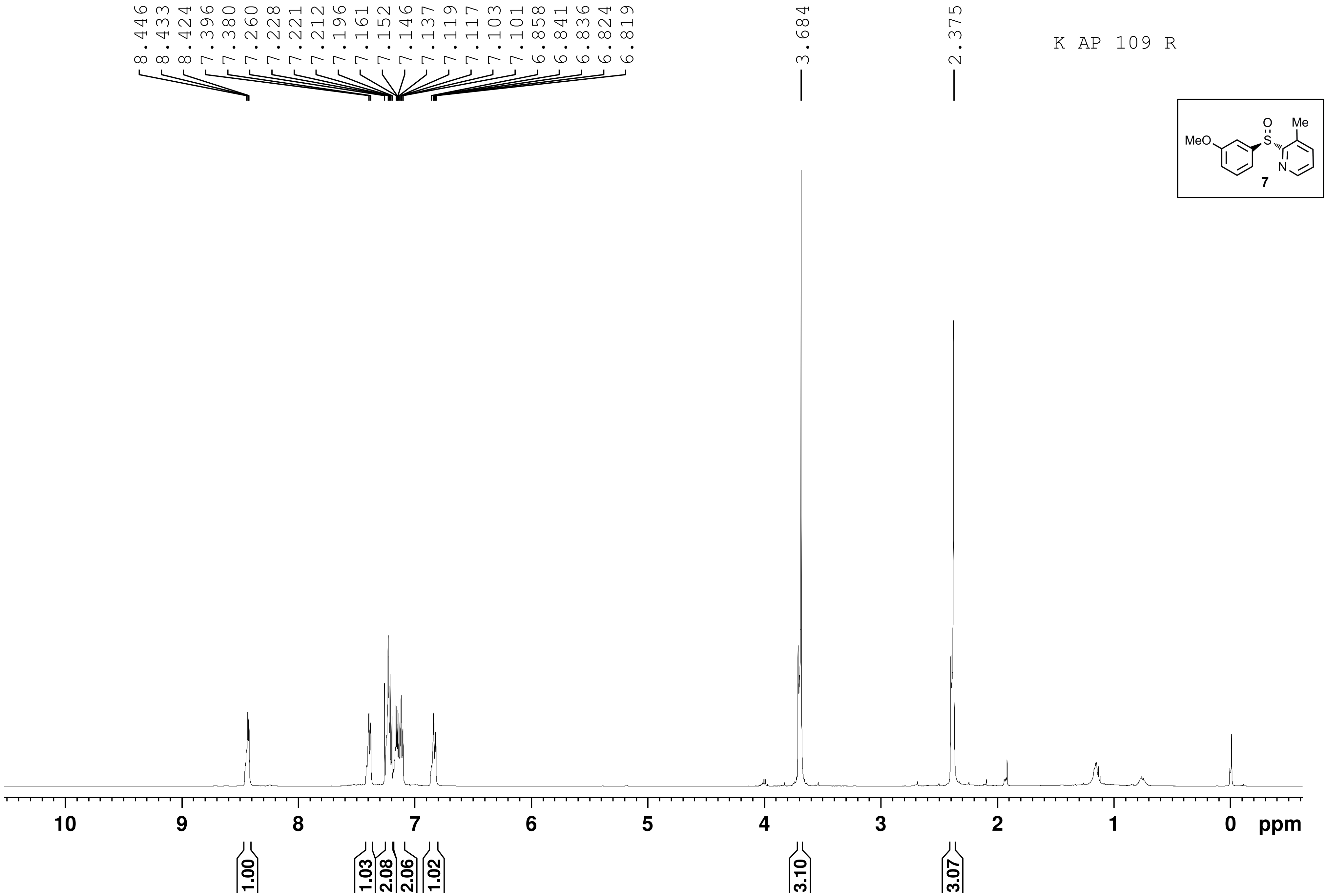


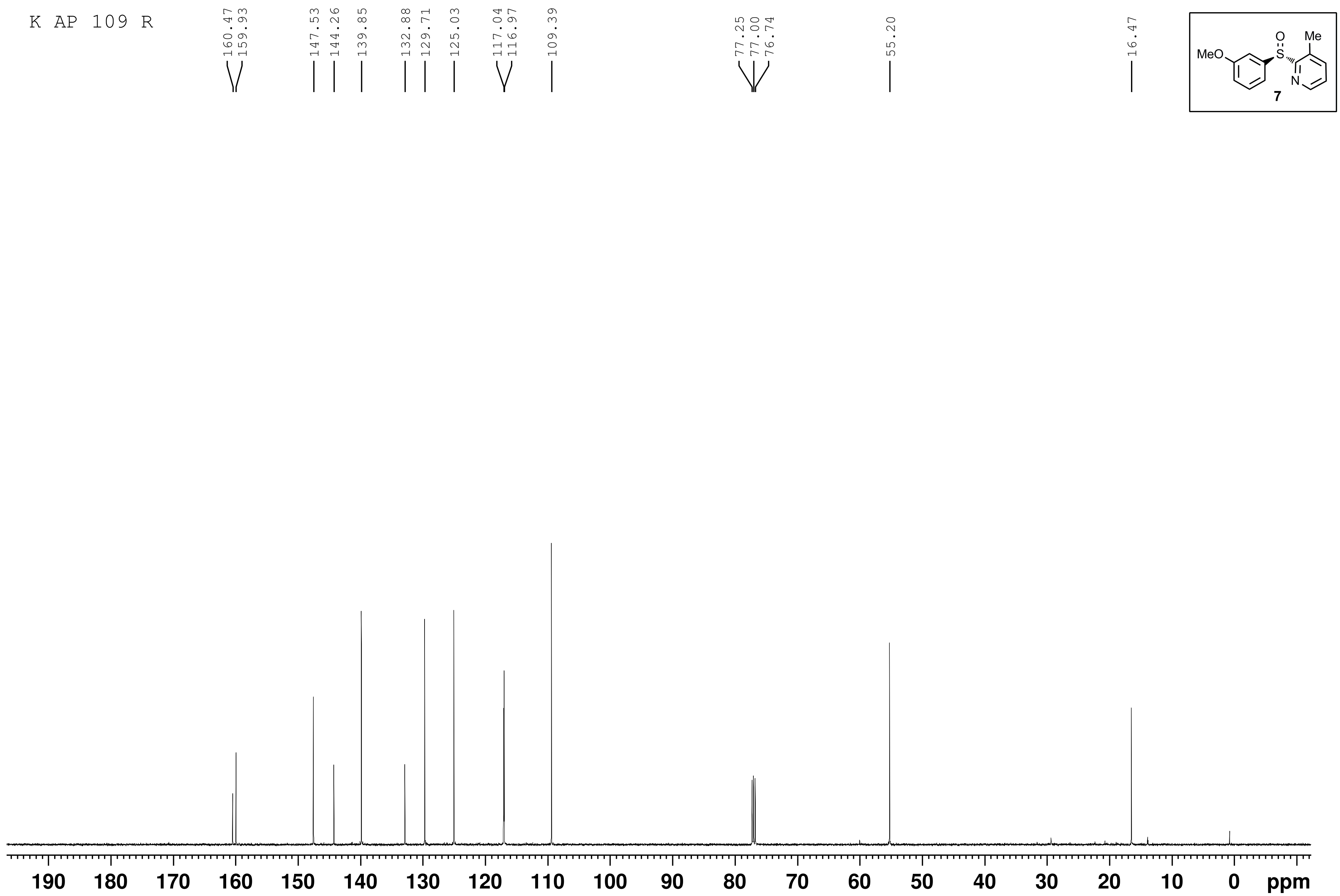
NH
O
Me
MeO
S
N

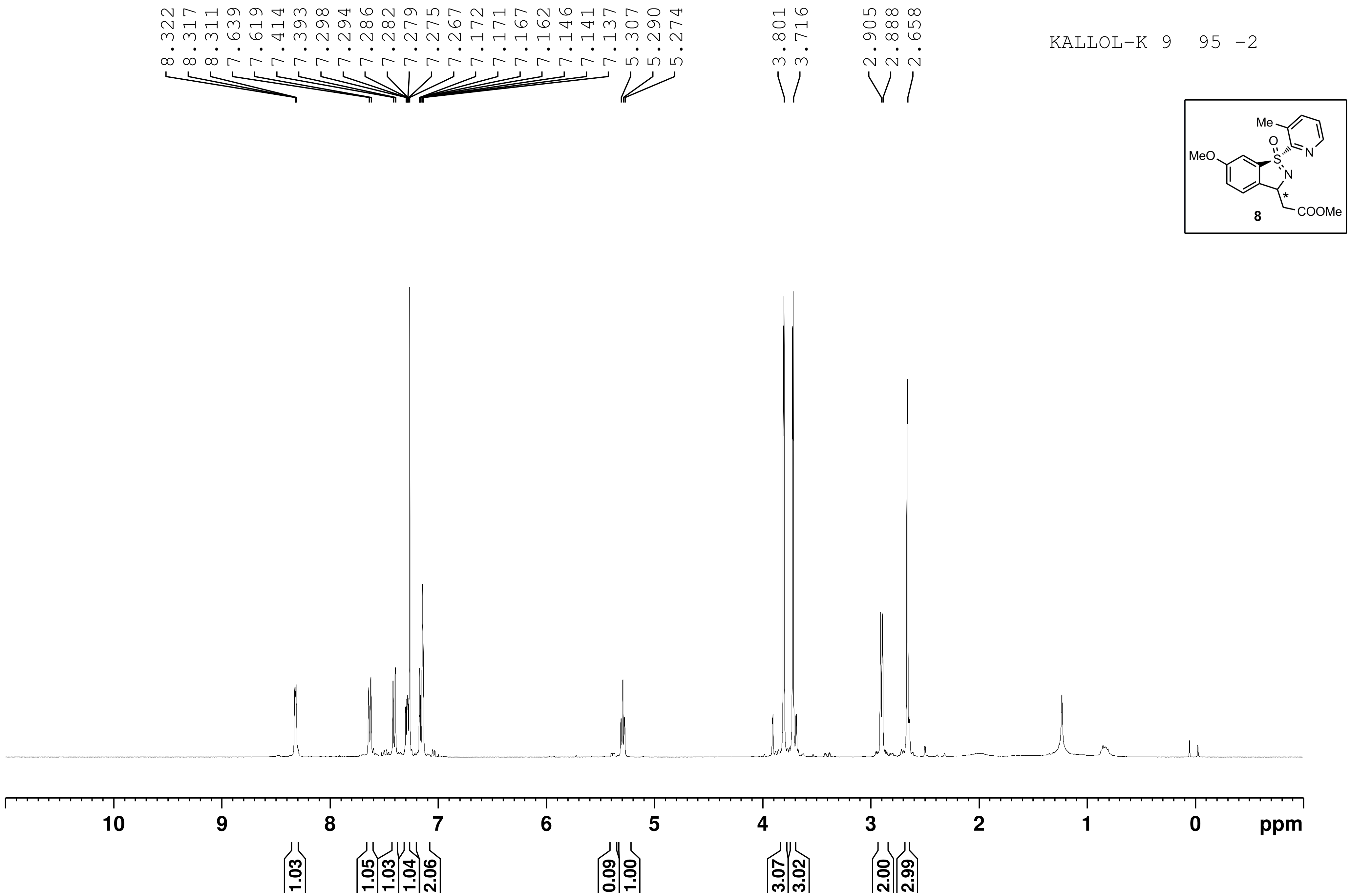
6

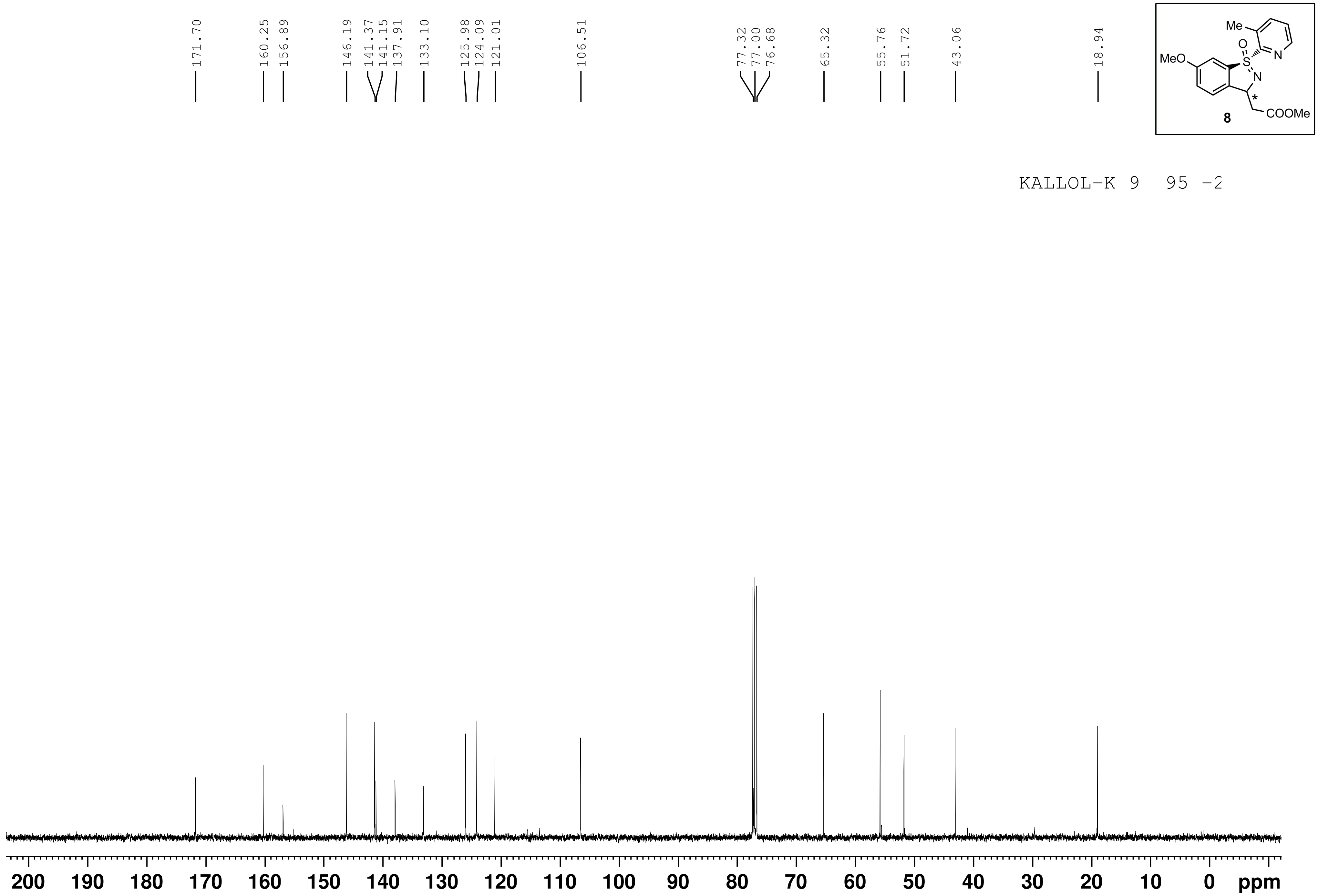

K -9-119 R
159.73
156.97
146.18
141.89
141.52
133.25
129.72
126.76
121.48
119.59
113.59
77.25
77.00
76.74
55.67
19.23
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


NH
O
Me
MeO
S
N
6

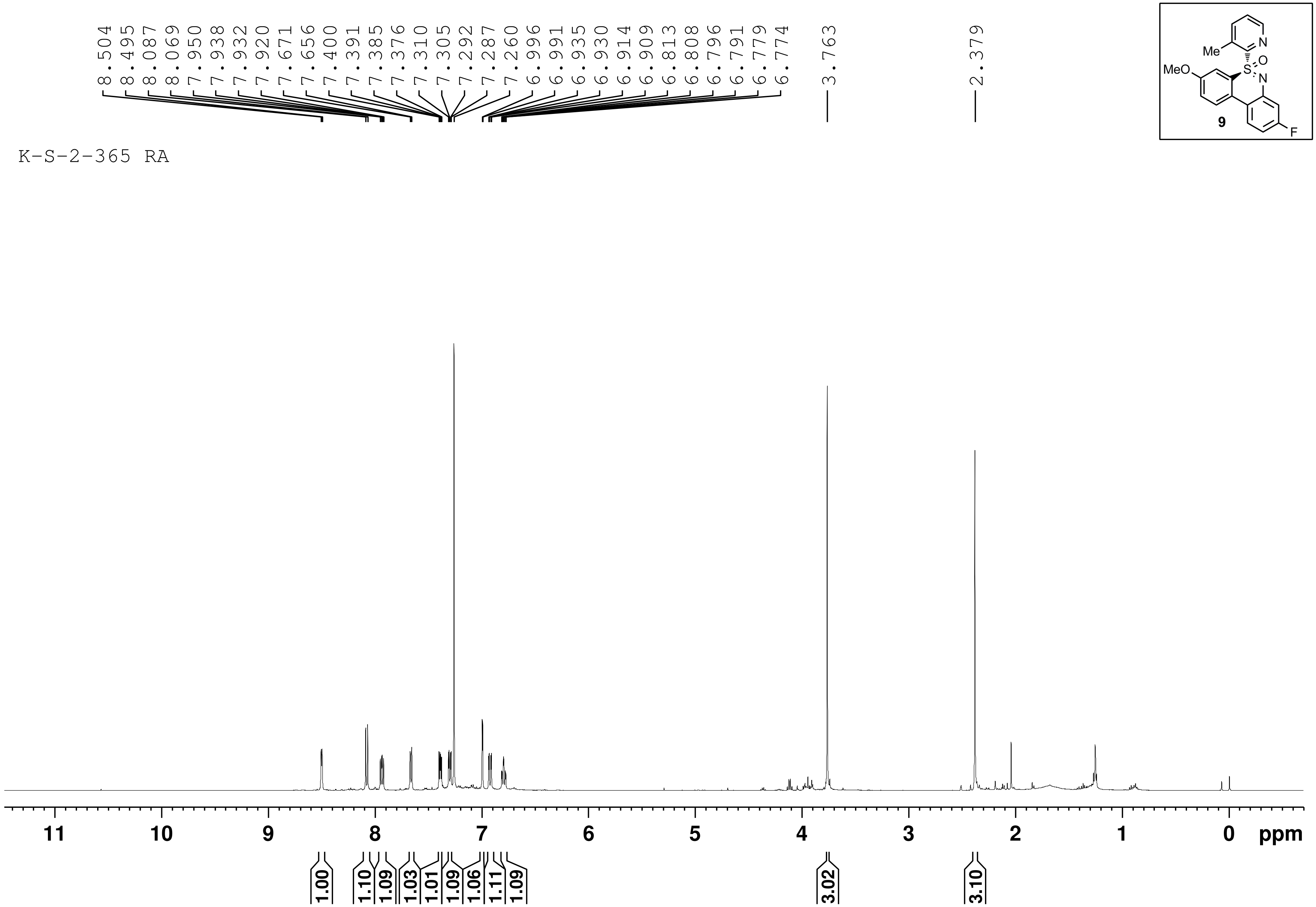

8.446
8.433
8.424
7.396
7.380
7.260
7.228
7.221
7.212
7.196
7.161
7.152
7.146
7.137
7.119
7.117
7.103
7.101
6.858
6.841
6.836
6.824
6.819
3.684
2.375
K AP 109 R
MeO
O
S
Me
N
7
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
2.08
2.06
1.02
3.10
3.07

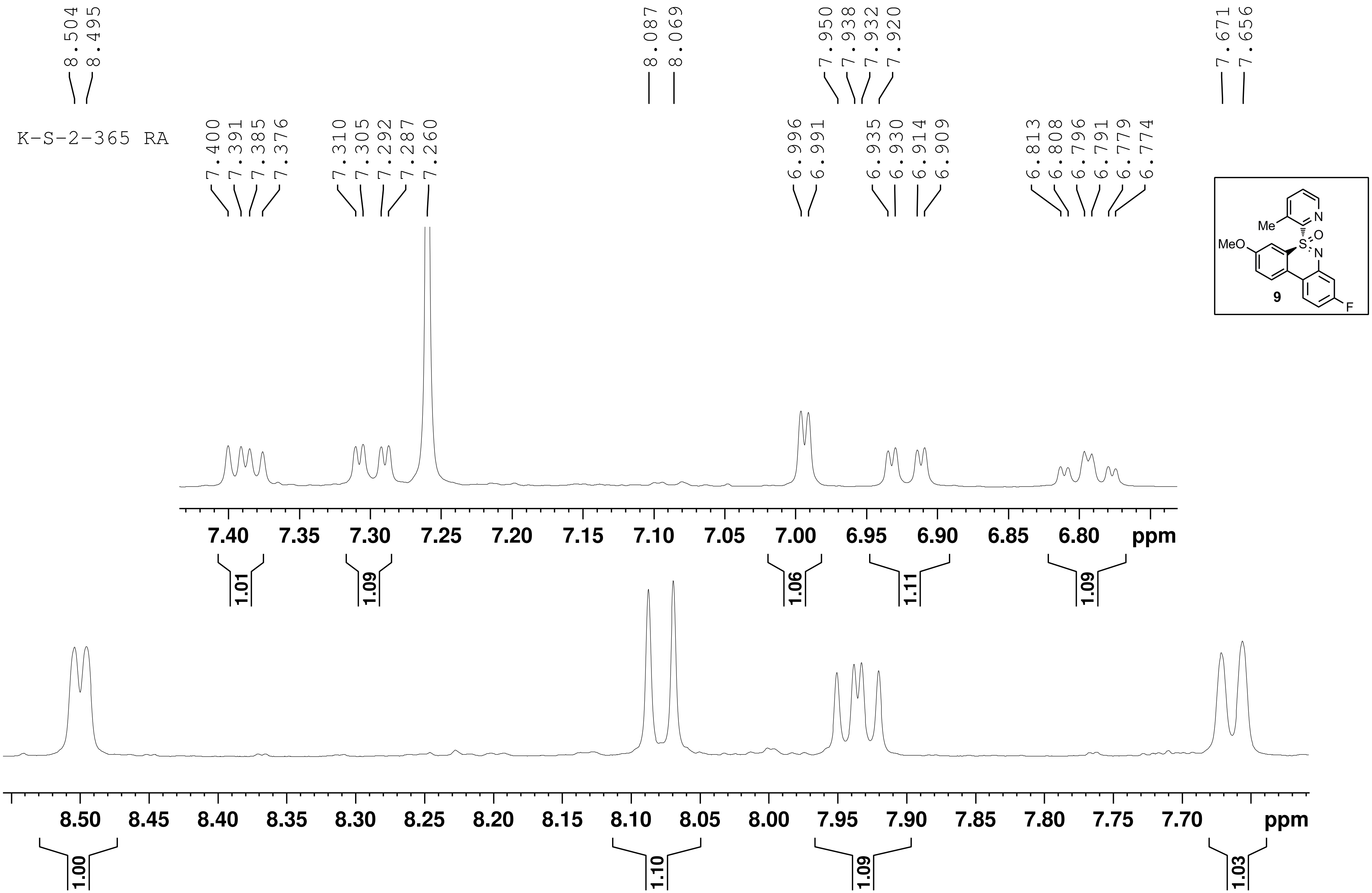

K AP 109 R
160.47
159.93
147.53
144.26
139.85
132.88
129.71
125.03
117.04
116.97
109.39
77.25
77.00
76.74
55.20
16.47
MeO
O
S
Me
N
7
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

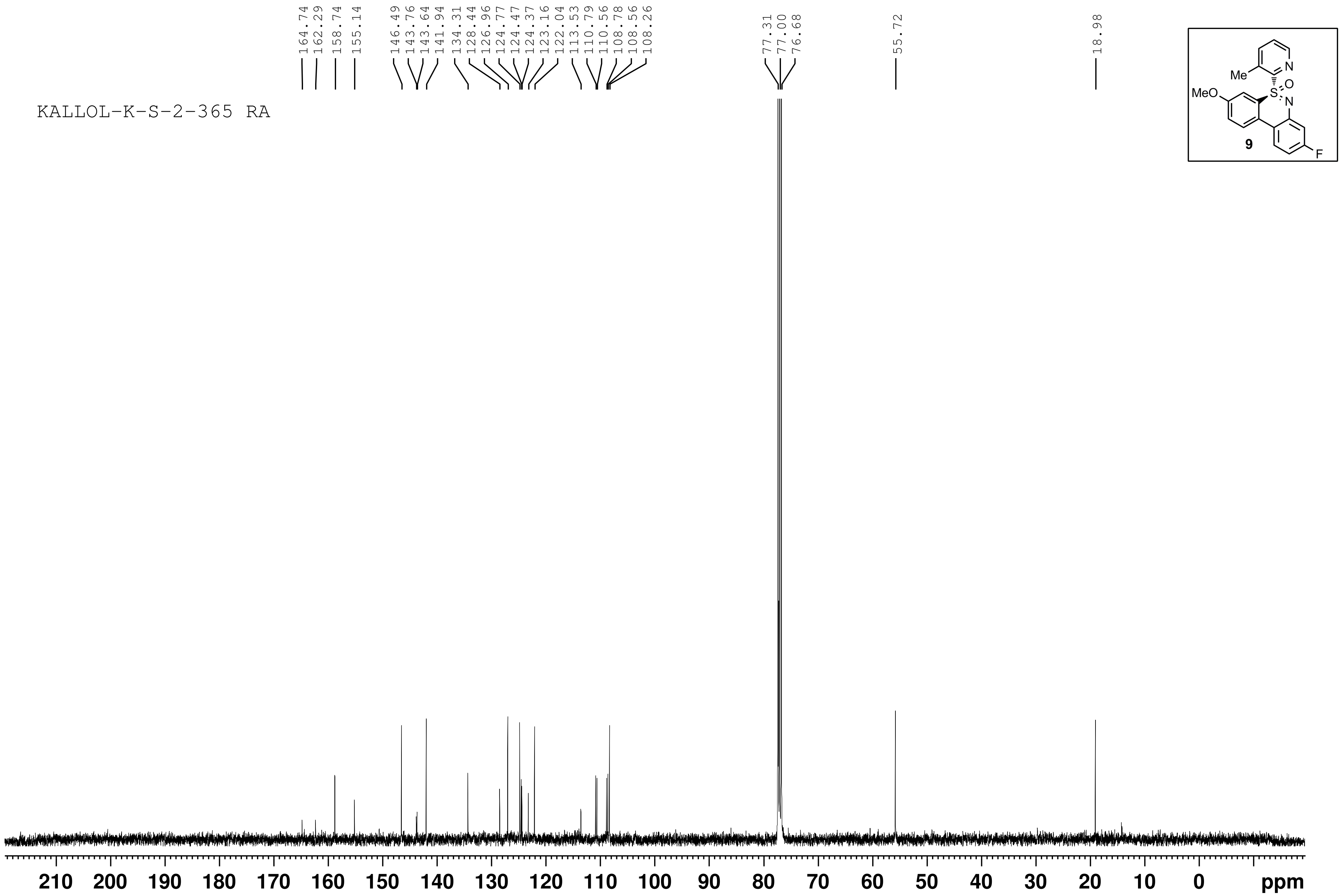

8.322
8.317
8.311
7.639
7.619
7.414
7.393
7.298
7.294
7.286
7.282
7.279
7.275
7.267
7.172
7.171
7.167
7.162
7.146
7.141
7.137
5.307
5.290
5.274
3.801
3.716
2.905
2.888
2.658
KALLOL-K 9 95 -2
Me
O
S
N
MeO
N
*
COOMe
8
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.05
1.03
1.04
2.06
0.09
1.00
3.07
3.02
2.00
2.99


8

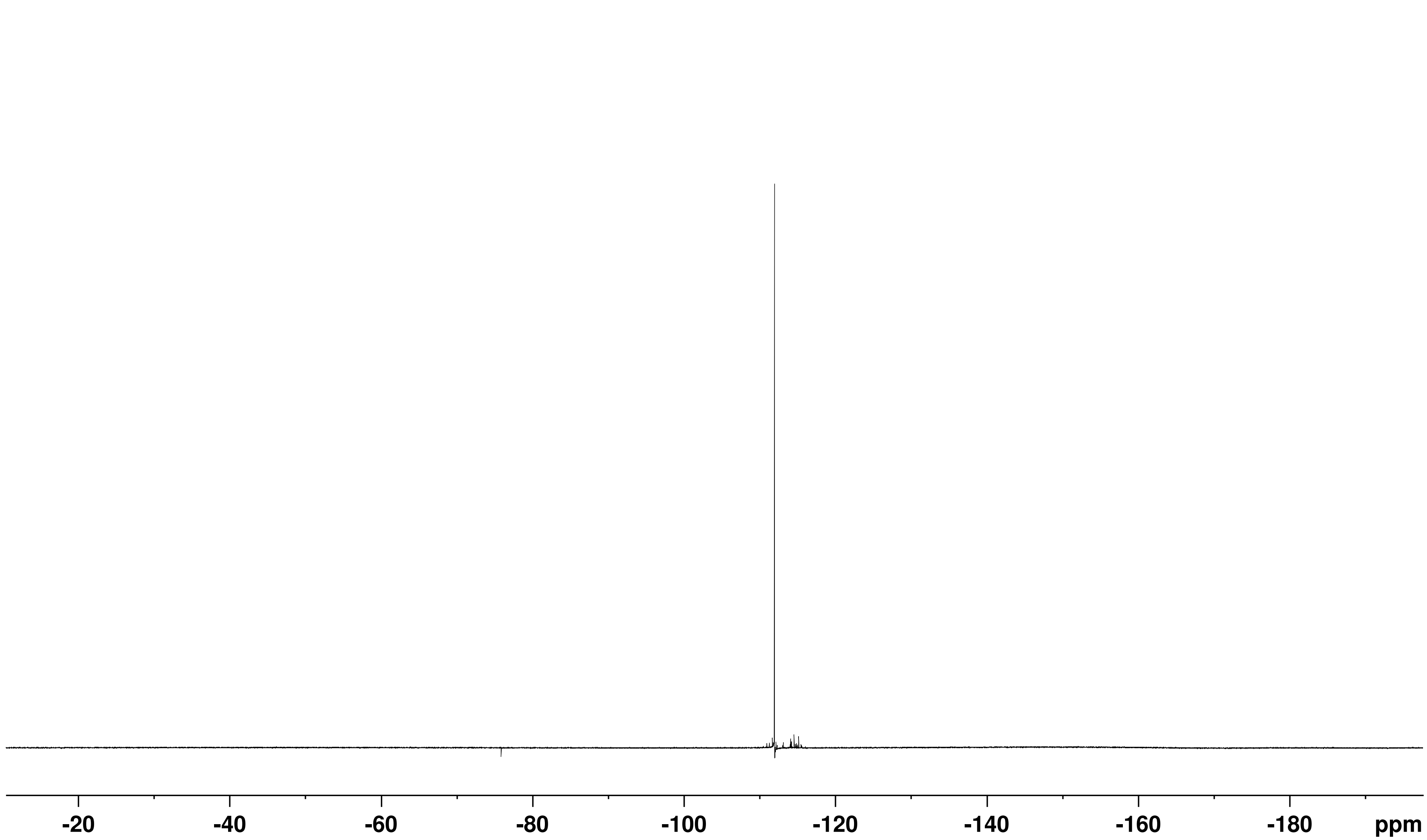
171.70
160.25
156.89
146.19
141.37
141.15
137.91
133.10
125.98
124.09
121.01
106.51
77.32
77.00
76.68
65.32
55.76
51.72
43.06
18.94
KALLOL-K 9 95 -2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

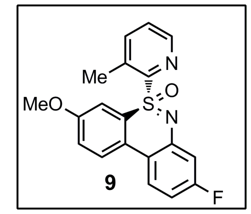

8.504
8.495
8.087
8.069
7.950
7.938
7.932
7.920
7.671
7.656
7.400
7.391
7.385
7.376
7.310
7.305
7.292
7.287
7.260
6.996
6.991
6.935
6.930
6.914
6.909
6.813
6.808
6.796
6.791
6.779
6.774
3.763
2.379
K-S-2-365 RA
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.10
1.09
1.03
1.01
1.09
1.06
1.11
1.09
3.02
3.10
N
Me
S
O
MeO
N
9
F


K-S-2-365 RA
8.504
8.495
8.087
8.069
7.950
7.938
7.932
7.920
7.671
7.656
7.400
7.391
7.385
7.376
7.310
7.305
7.292
7.287
7.260
6.996
6.991
6.935
6.930
6.914
6.909
6.813
6.808
6.796
6.791
6.779
6.774
Me
N
MeO
S
O
N
9
F
7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 ppm
1.01
1.09
1.06
1.11
1.09
8.50 8.45 8.40 8.35 8.30 8.25 8.20 8.15 8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 ppm
1.00
1.10
1.09
1.03


KALLOL-K-S-2-365 RA
164.74
162.29
158.74
155.14
146.49
143.76
143.64
141.94
134.31
128.44
126.96
124.77
124.47
124.37
123.16
122.04
113.53
110.79
110.56
108.78
108.56
108.26
77.31
77.00
76.68
55.72
18.98
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Me
N
S
O
MeO
N
9
F

srs-2-365ra





3b

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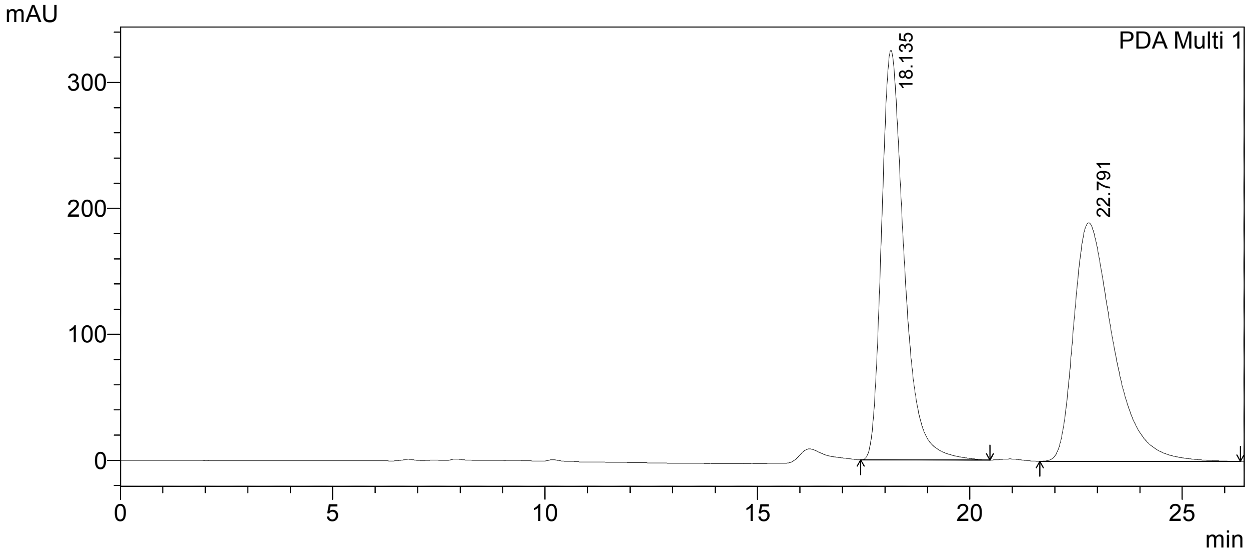


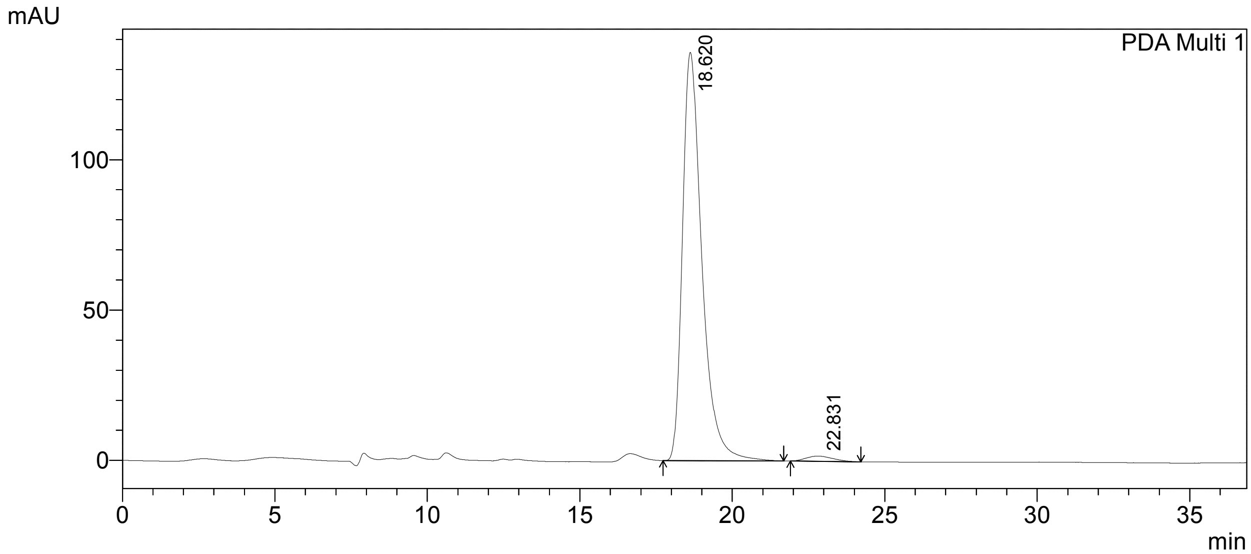
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.135	12140347	325359	49.728	63.208
2	22.791	12273309	189387	50.272	36.792
Total		24413656	514746	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

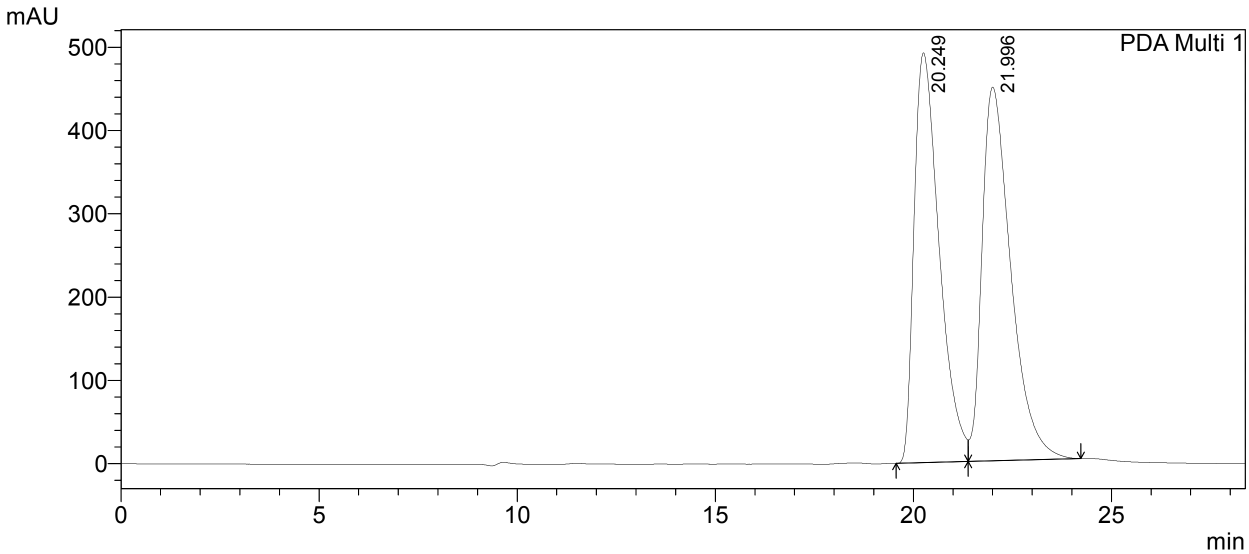
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.620	6030335	135858	98.226	98.712
2	22.831	108928	1773	1.774	1.288
Total		6139263	137631	100.000	100.000

1a

<Chromatogram>



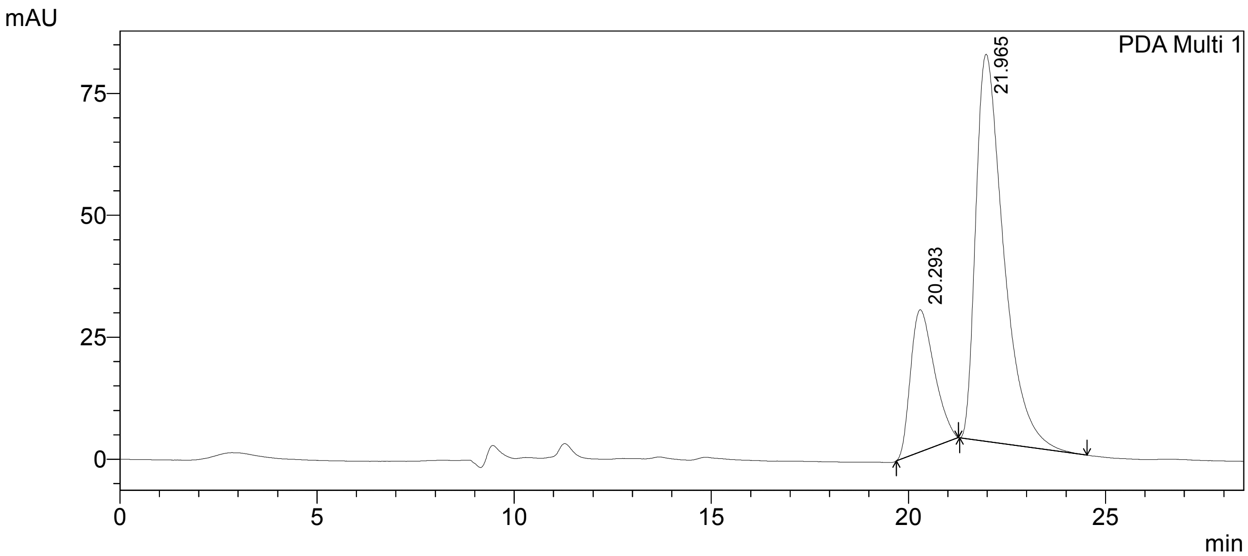
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.249	21759605	492183	48.883	52.303
2	21.996	22753619	448841	51.117	47.697
Total		44513224	941024	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

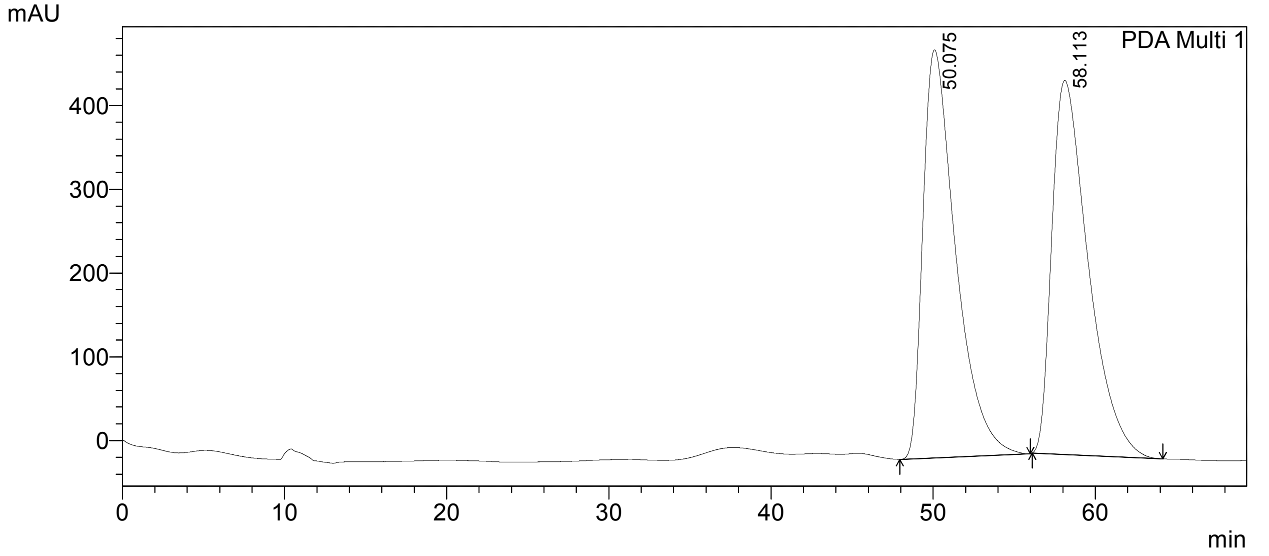
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.293	1222975	29183	23.816	26.872
2	21.965	3912044	79417	76.184	73.128
Total		5135019	108600	100.000	100.000

3c

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	50.075	68565966	487104	49.593	52.170
2	58.113	69690288	446578	50.407	47.830
Total		138256255	933682	100.000	100.000

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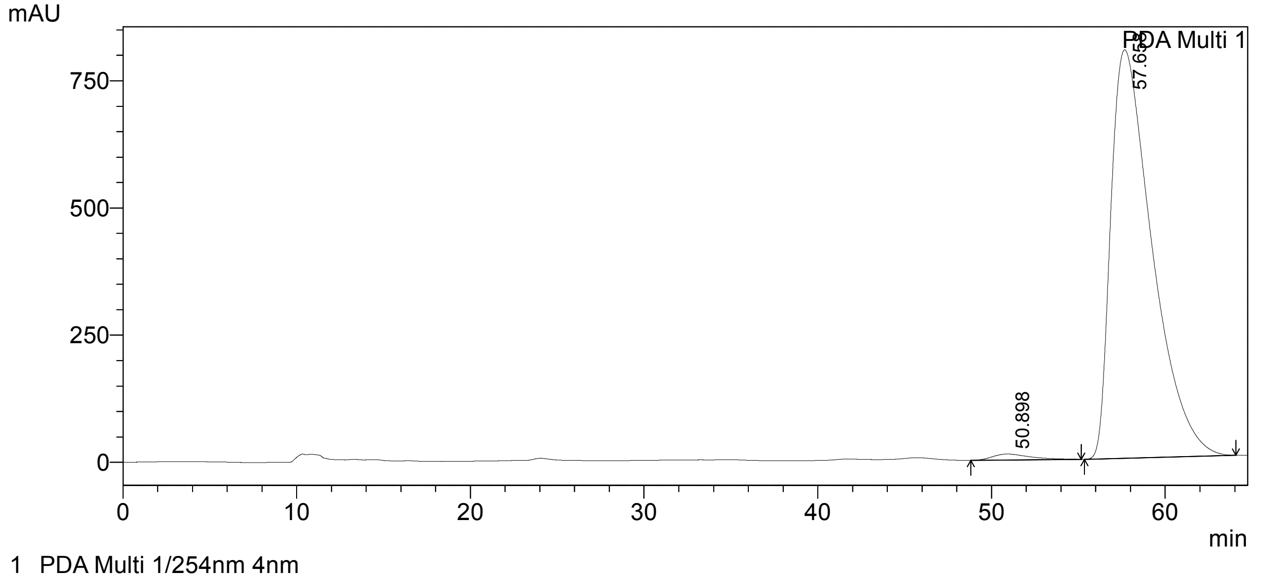

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	50.898	1758161	11717	1.308	1.439
2	57.658	132678713	802741	98.692	98.561
Total		134436874	814458	100.000	100.000

1b

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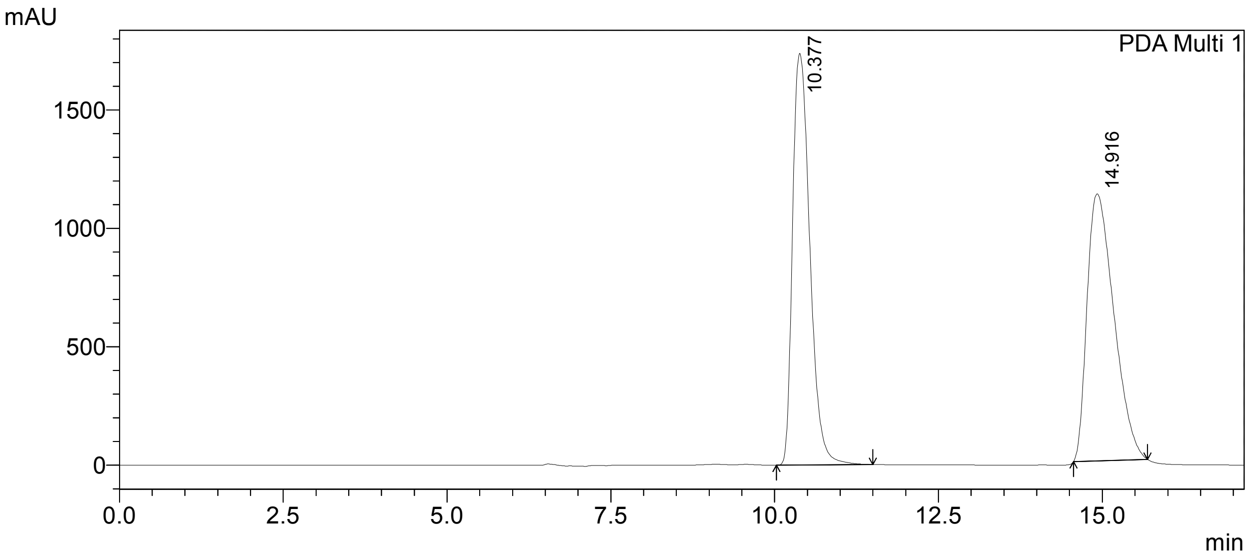


1 PDA Multi 1/254nm 4nm

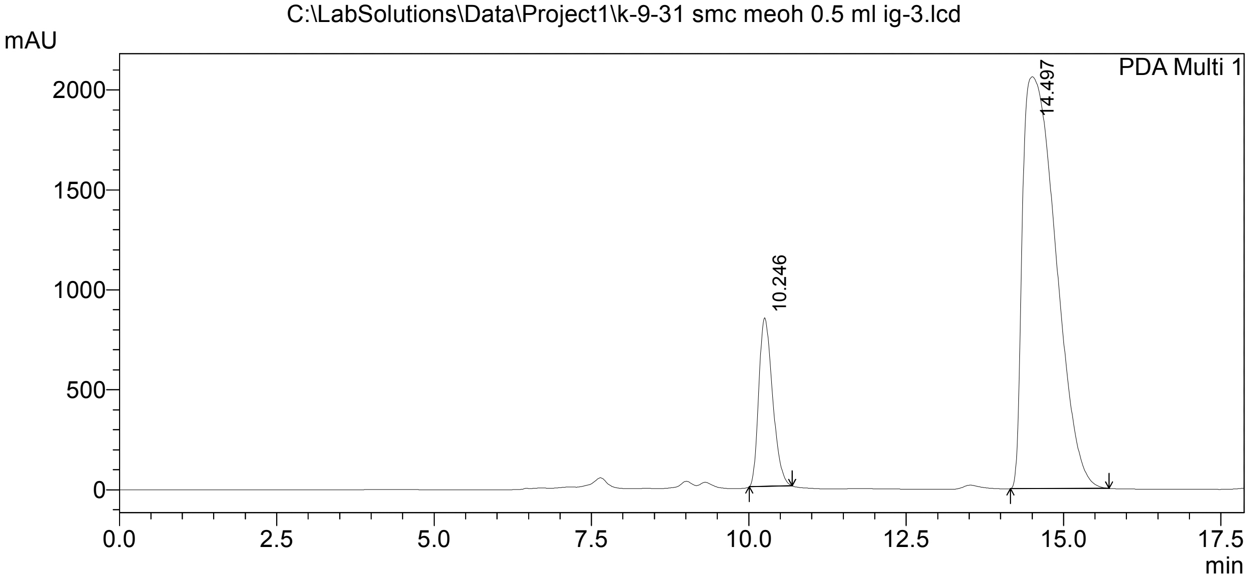
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.377	31942172	1738140	49.810	60.630
2	14.916	32186004	1128662	50.190	39.370
Total		64128176	2866802	100.000	100.000

<Chromatogram>

C:\LabSolutions\Data\Project1\k-9-31 smc meoh 0.5 ml ig-3.lcd



1 PDA Multi 1/254nm 4nm

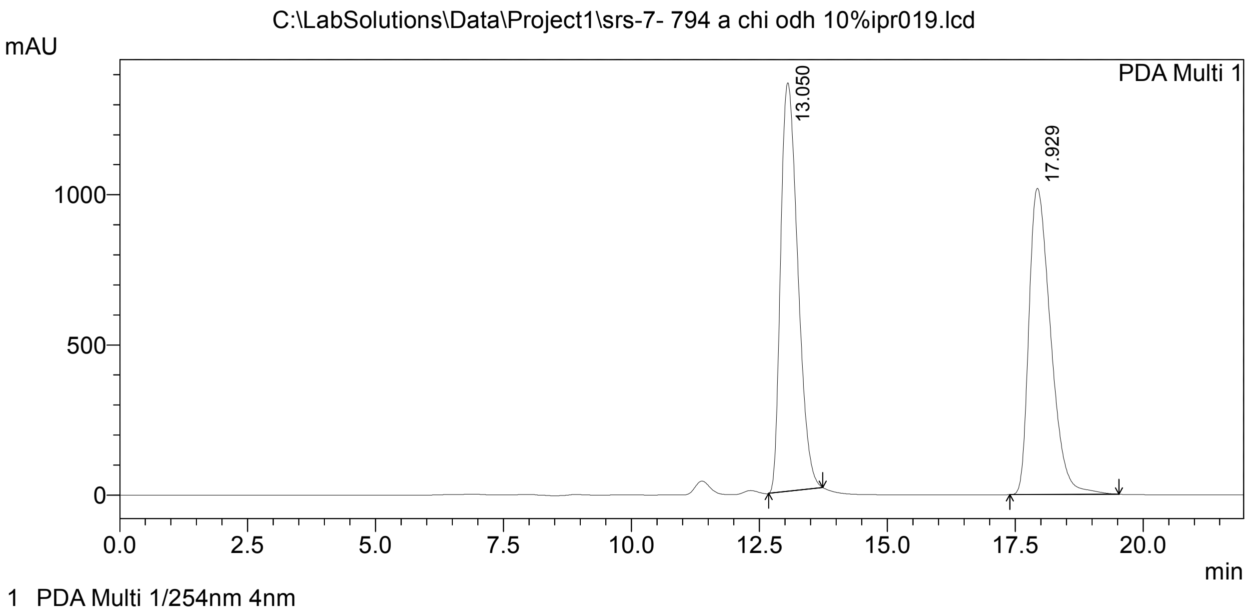
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.246	12888462	843097	14.534	29.044
2	14.497	75787225	2059744	85.466	70.956
Total		88675687	2902841	100.000	100.000

3d

<Chromatogram>



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.050	31775587	1360545	51.362	57.143
2	17.929	30090737	1020410	48.638	42.857
Total		61866323	2380955	100.000	100.000

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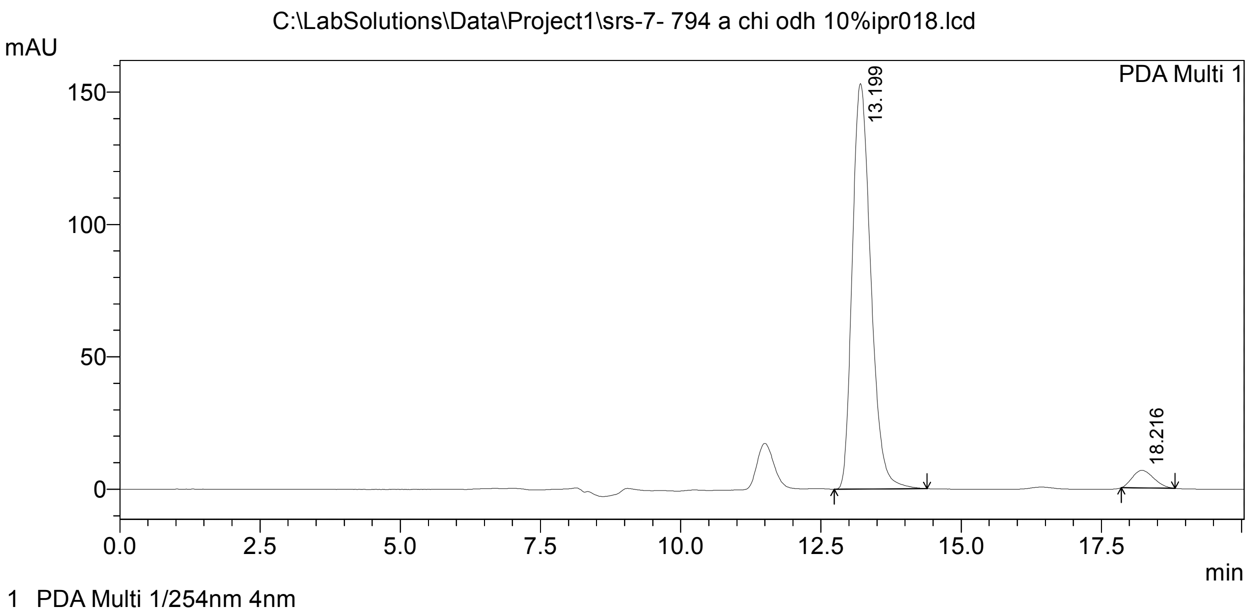

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.199	3523329	153194	95.249	95.851
2	18.216	175761	6632	4.751	4.149
Total		3699090	159826	100.000	100.000

1b

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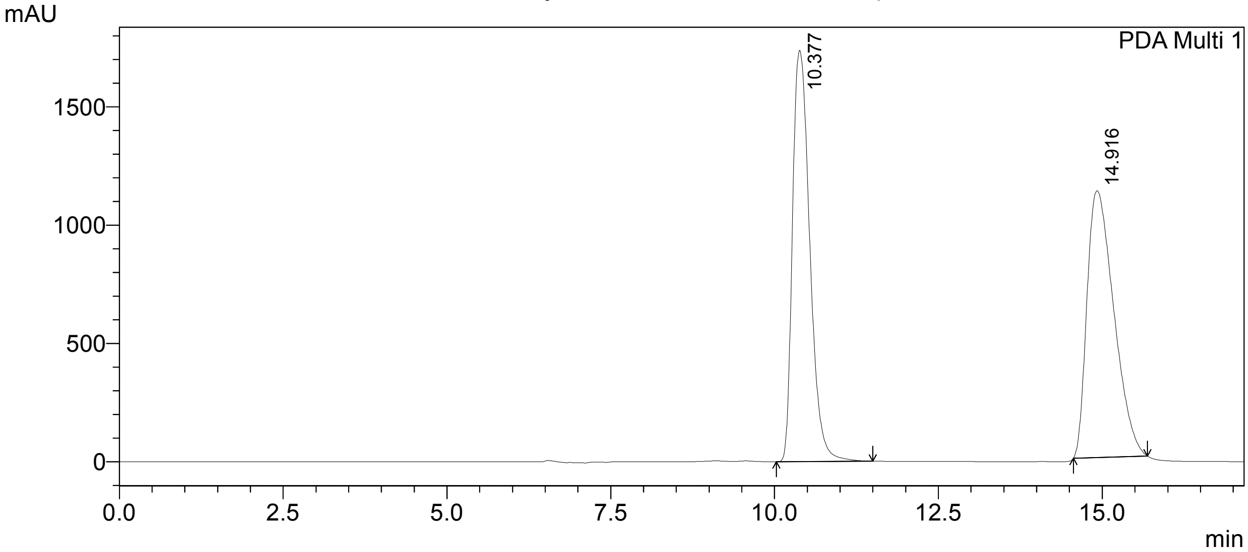

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.377	31942172	1738140	49.810	60.630
2	14.916	32186004	1128662	50.190	39.370
Total		64128176	2866802	100.000	100.000

<Chromatogram>

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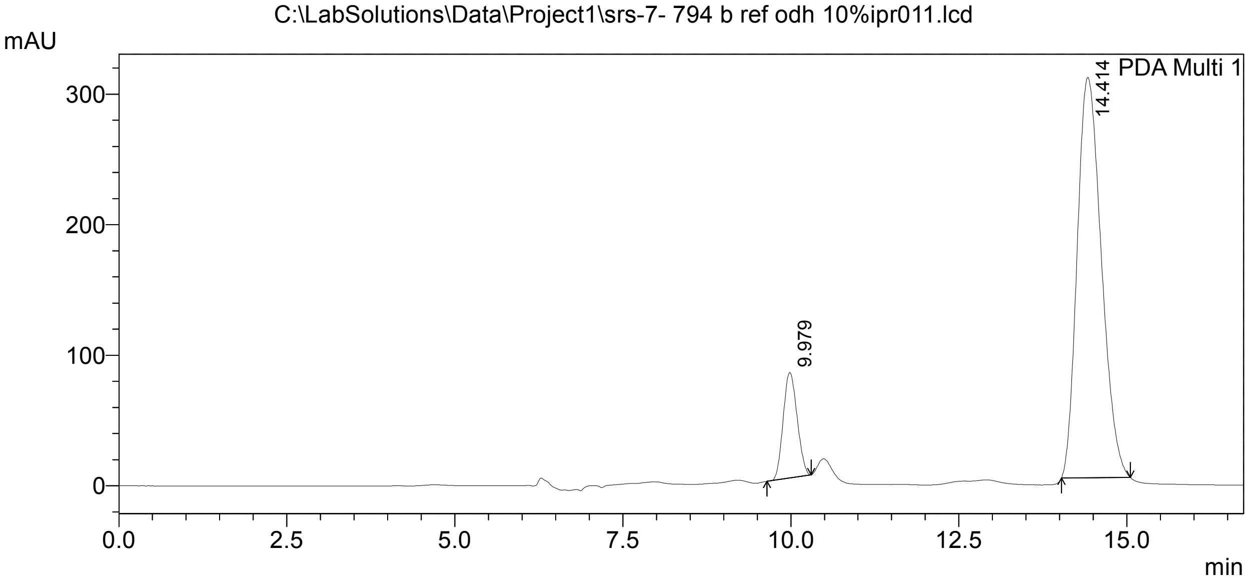

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.979	1168220	80921	13.208	20.881
2	14.414	7676274	306614	86.792	79.119
Total		8844495	387534	100.000	100.000

3e

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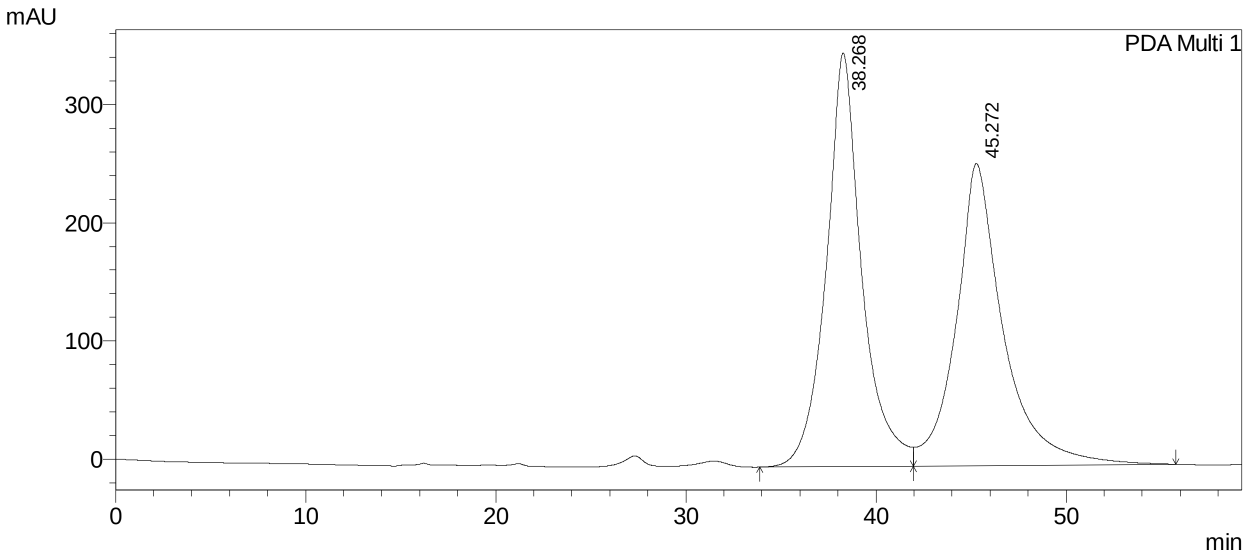

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.268	45546152	350035	50.773	57.781
2	45.272	44158452	255761	49.227	42.219
Total		89704604	605796	100.000	100.000

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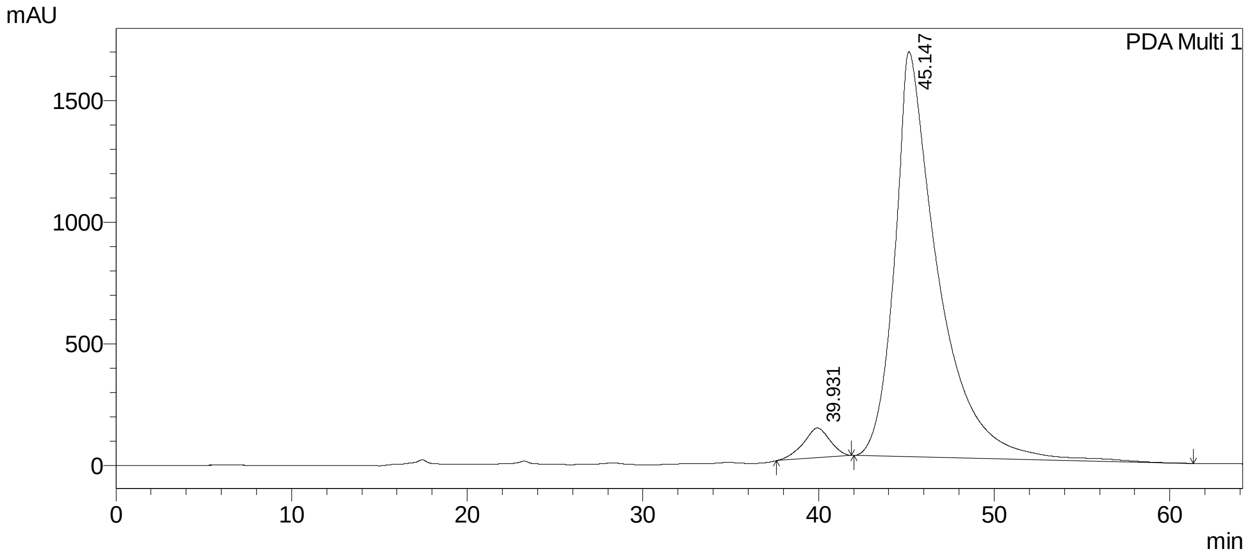


1 PDA Multi 1/254nm 4nm

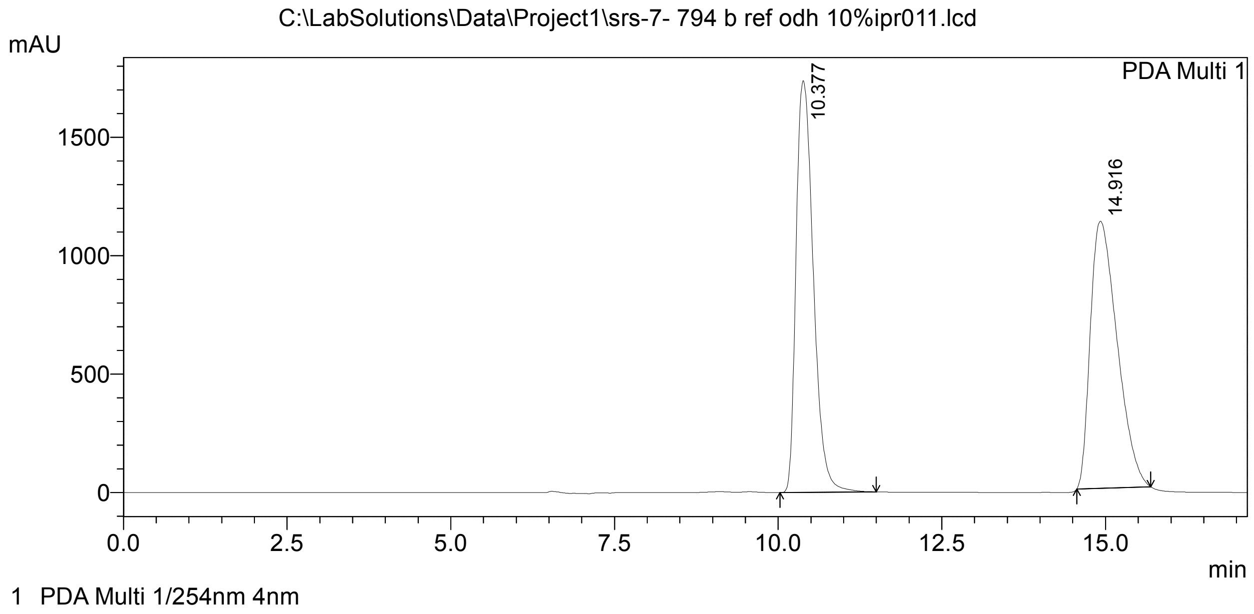
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	39.931	13106862	123021	4.367	6.873
2	45.147	287054445	1667001	95.633	93.127
Total		300161307	1790022	100.000	100.000

1b

<Chromatogram>

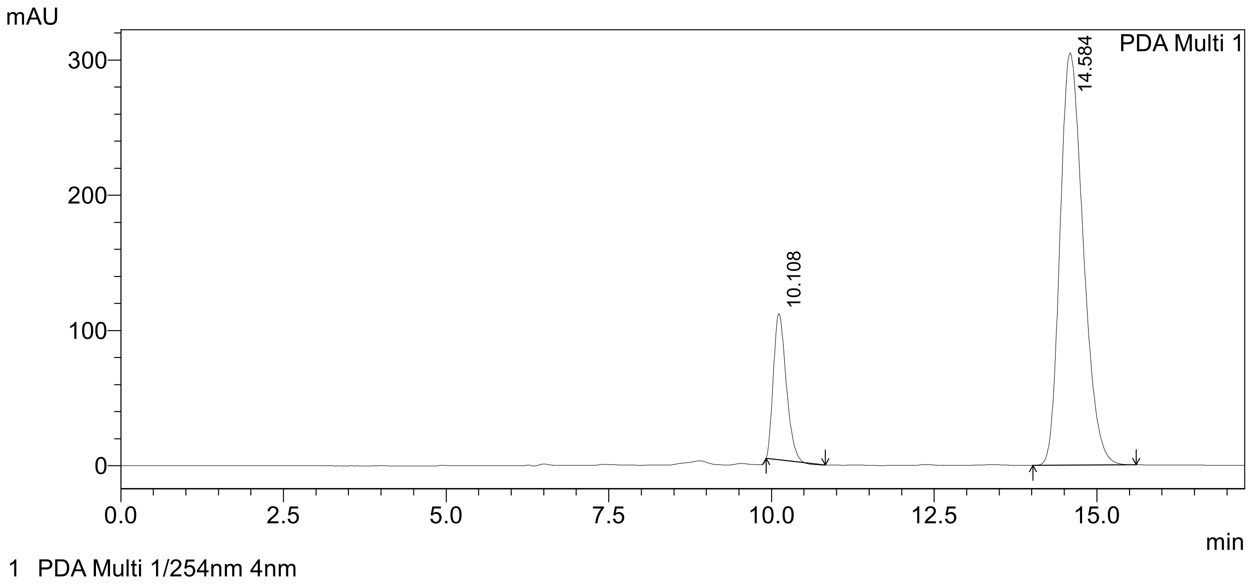


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.377	31942172	1738140	49.810	60.630
2	14.916	32186004	1128662	50.190	39.370
Total		64128176	2866802	100.000	100.000

<Chromatogram>



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.108	1471807	107846	16.268	26.129
2	14.584	7575264	304904	83.732	73.871
Total		9047071	412751	100.000	100.000

3f

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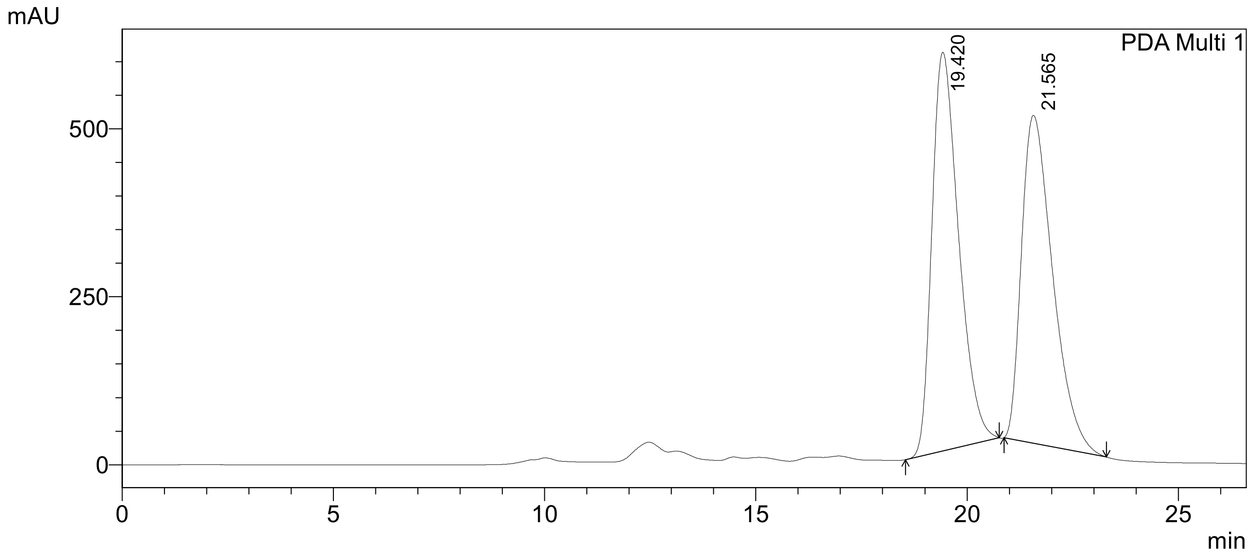


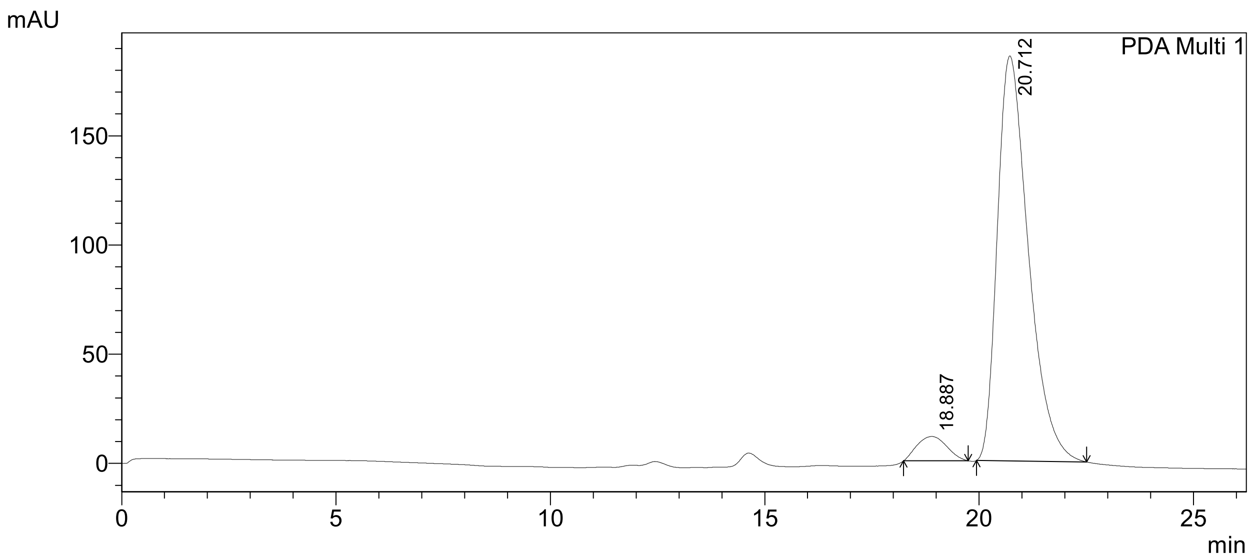
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.420	26150298	593631	51.042	54.881
2	21.565	25082351	488036	48.958	45.119
Total		51232649	1081667	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.887	537356	11121	5.429	5.658
2	20.712	9360507	185421	94.571	94.342
Total		9897863	196542	100.000	100.000

1b

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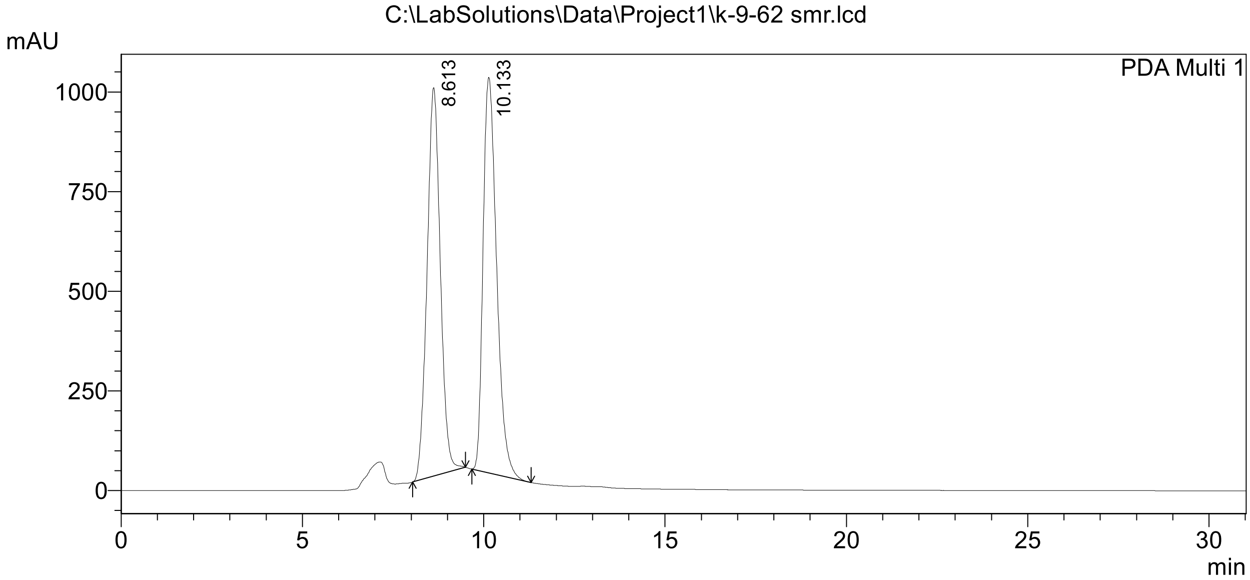


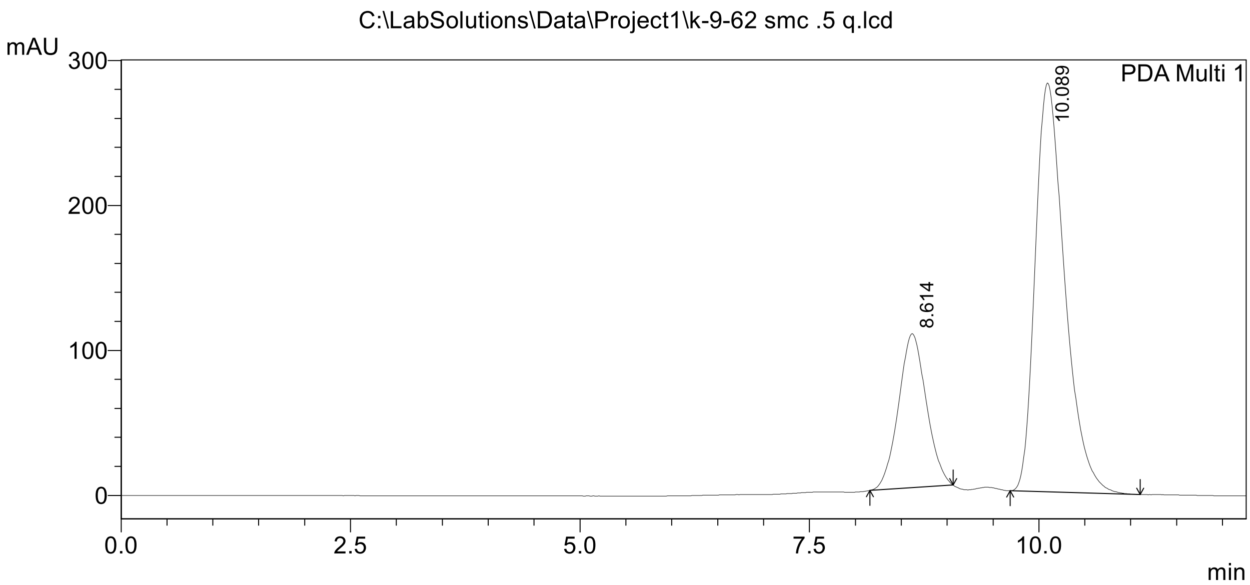
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.613	24842836	974882	49.118	49.567
2	10.133	25735150	991920	50.882	50.433
Total		50577986	1966802	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.614	2249015	106259	26.186	27.366
2	10.089	6339520	282035	73.814	72.634
Total		8588536	388294	100.000	100.000

3g

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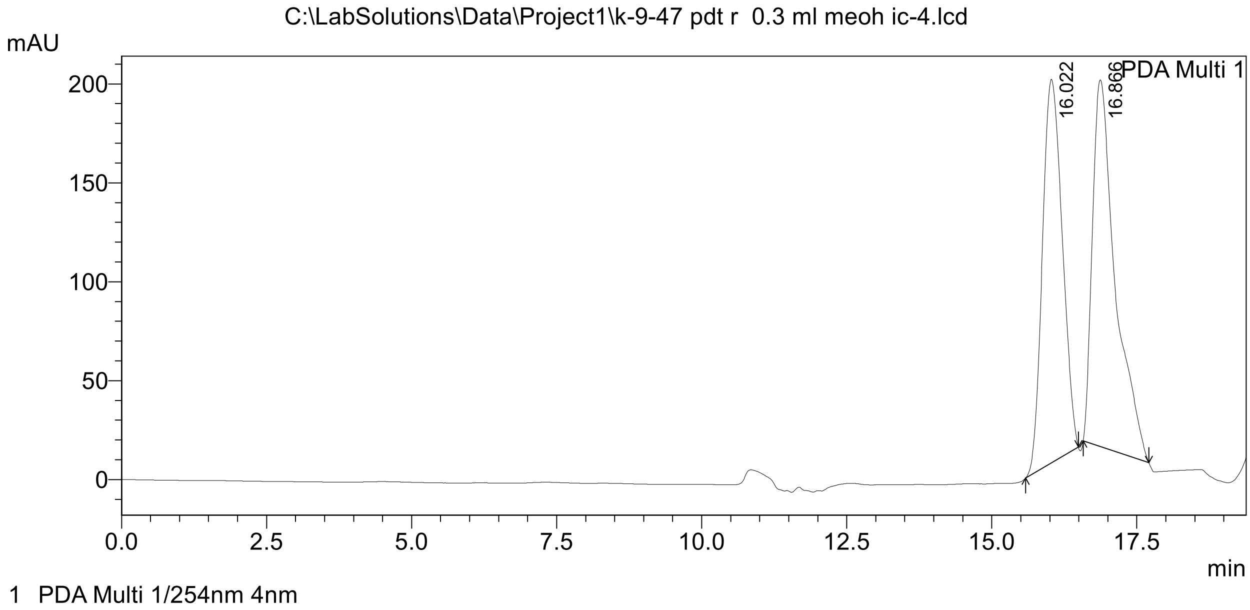
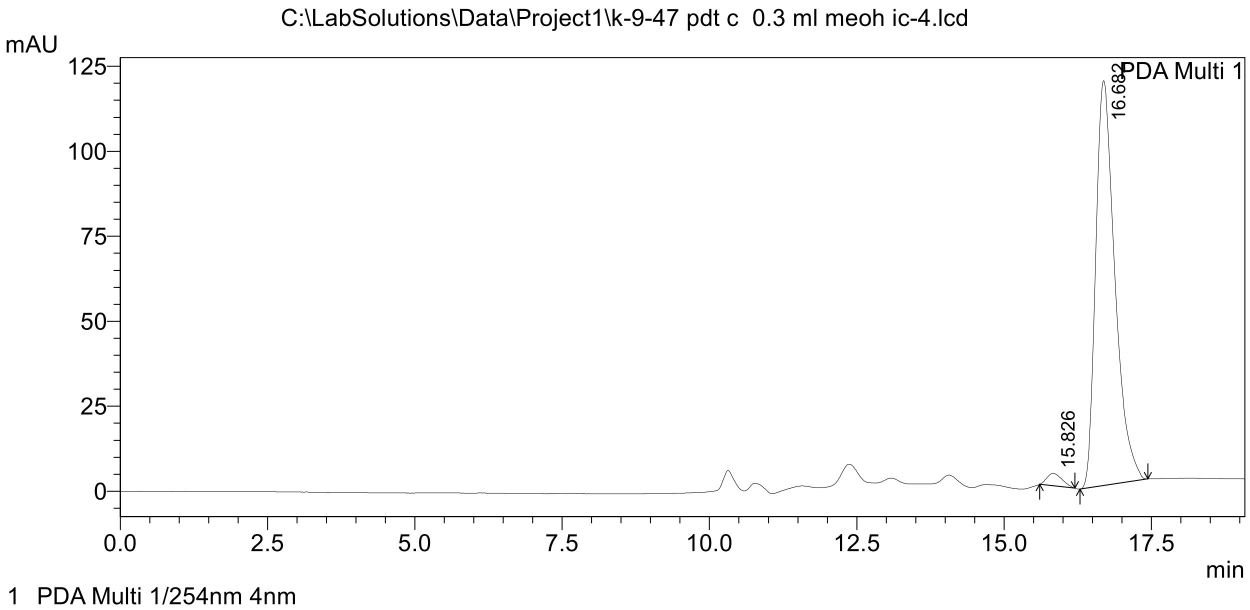


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.022	4618687	194015	47.677	51.124
2	16.866	5068703	185482	52.323	48.876
Total		9687390	379497	100.000	100.000

<Chromatogram>



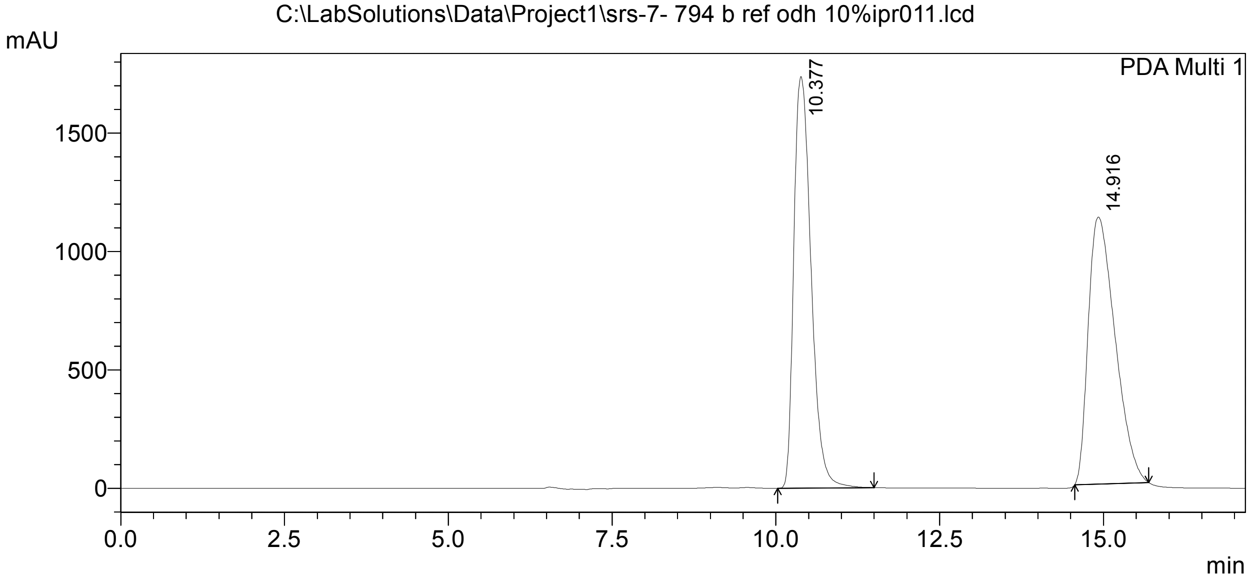
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.826	66458	3673	2.404	2.992
2	16.682	2698595	119086	97.596	97.008
Total		2765053	122759	100.000	100.000

1b

<Chromatogram>



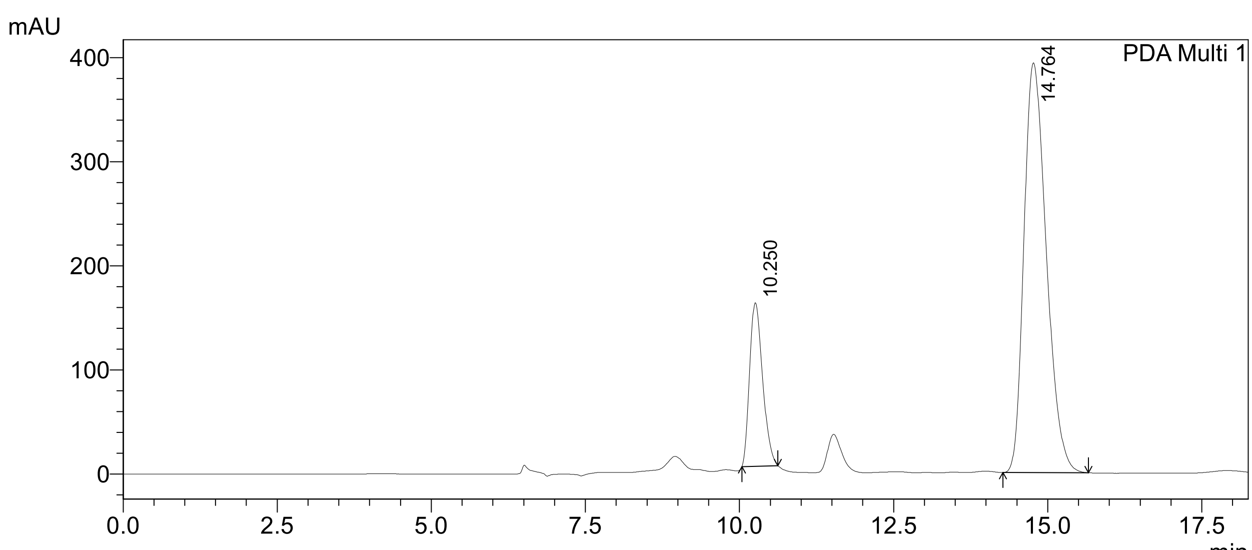
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.377	31942172	1738140	49.810	60.630
2	14.916	32186004	1128662	50.190	39.370
Total		64128176	2866802	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

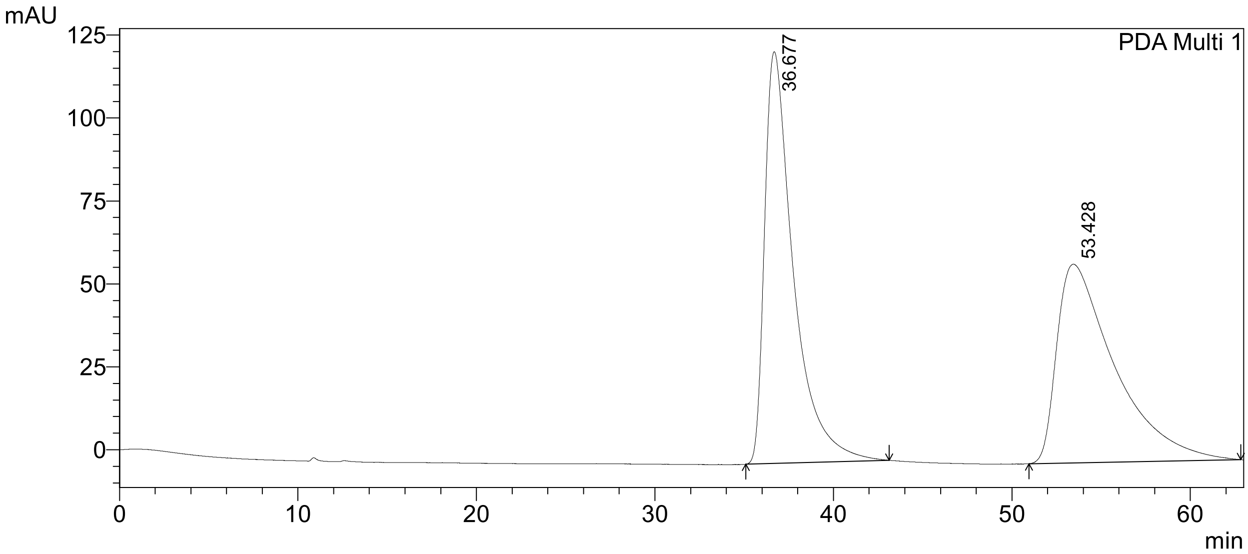
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.250	2314939	157128	18.838	28.522
2	14.764	9973493	393781	81.162	71.478
Total		12288432	550909	100.000	100.000

3h

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	36.677	13955896	124115	50.822	67.463
2	53.428	13504214	59859	49.178	32.537
Total		27460110	183974	100.000	100.000

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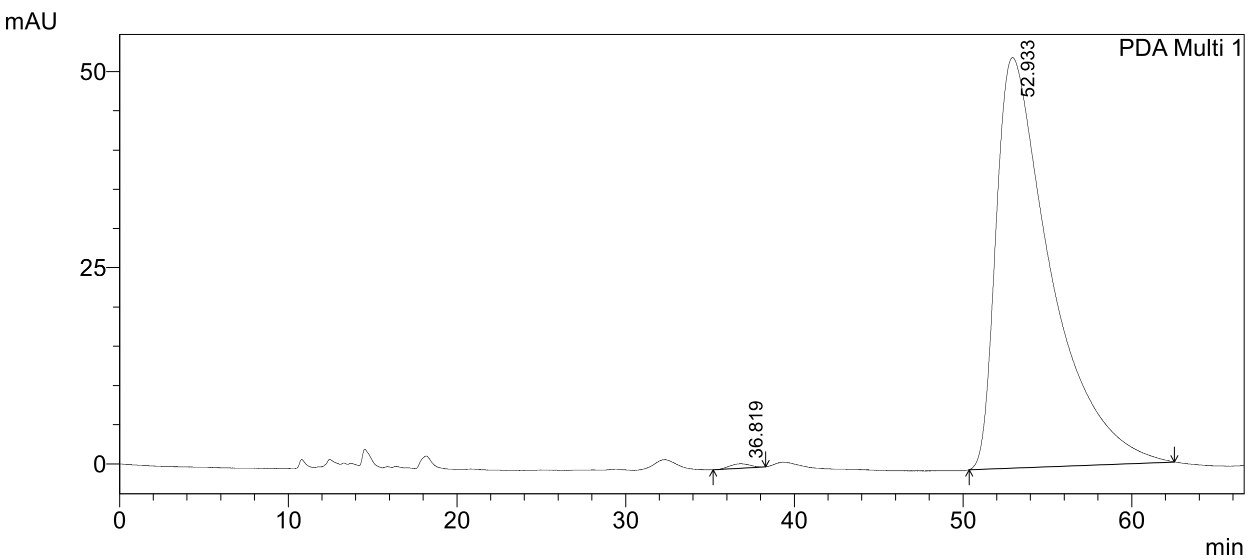

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	36.819	46161	571	0.389	1.081
2	52.933	11817784	52305	99.611	98.919
Total		11863945	52876	100.000	100.000

1b

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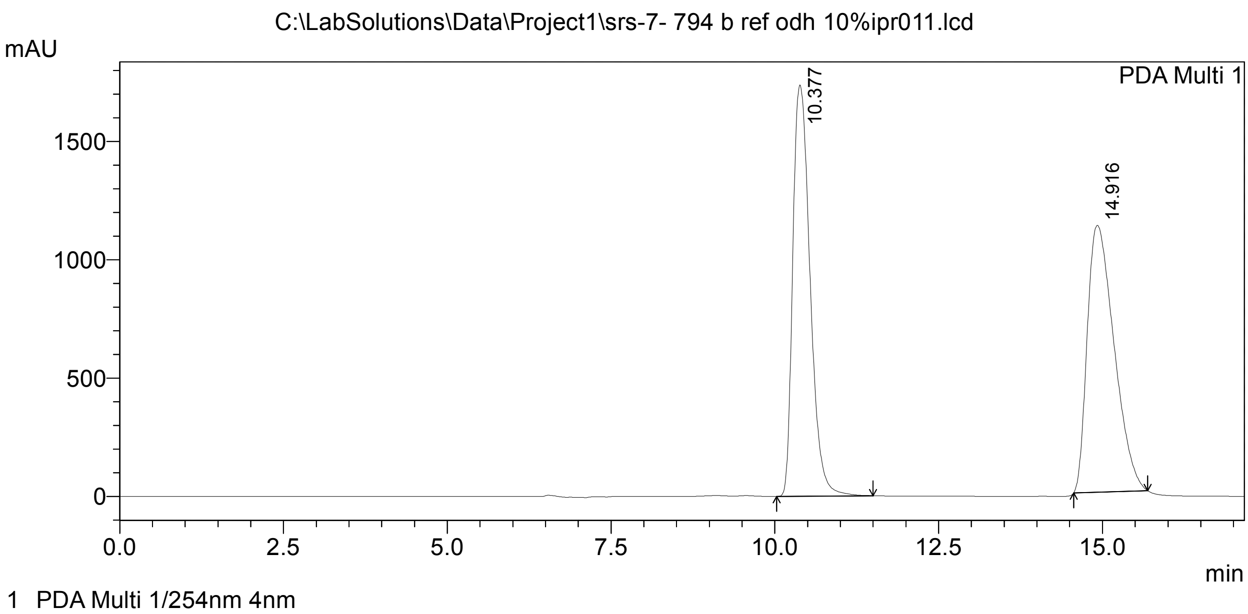
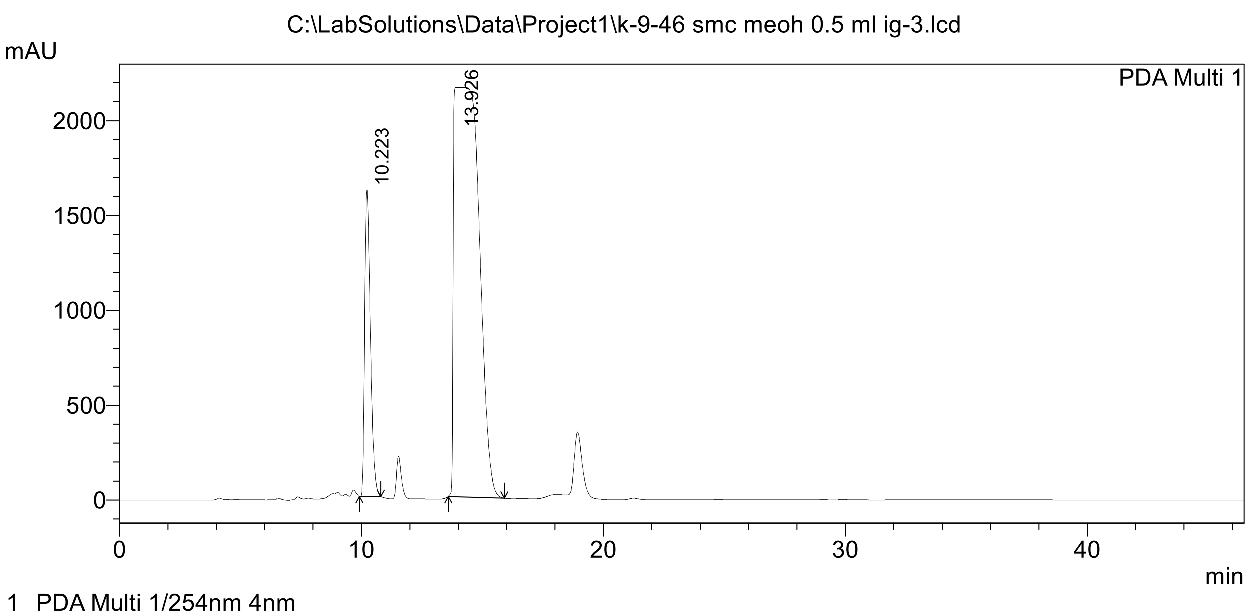


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.377	31942172	1738140	49.810	60.630
2	14.916	32186004	1128662	50.190	39.370
Total		64128176	2866802	100.000	100.000

<Chromatogram>



PeakTable

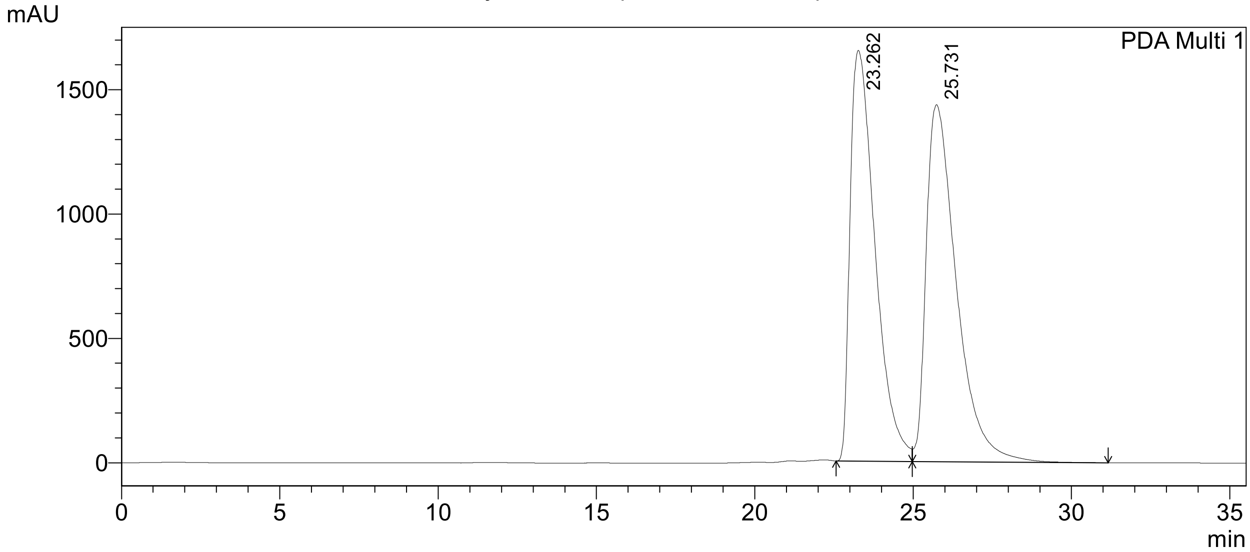
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.223	27274631	1619262	14.961	42.860
2	13.926	155033052	2158732	85.039	57.140
Total		182307683	3777995	100.000	100.000

3i

<Chromatogram>

C:\LabSolutions\Data\Project1\k-9-30 pdt r 0.3 ml 30% ipa in hex odh001.lcd



1 PDA Multi 1/254nm 4nm

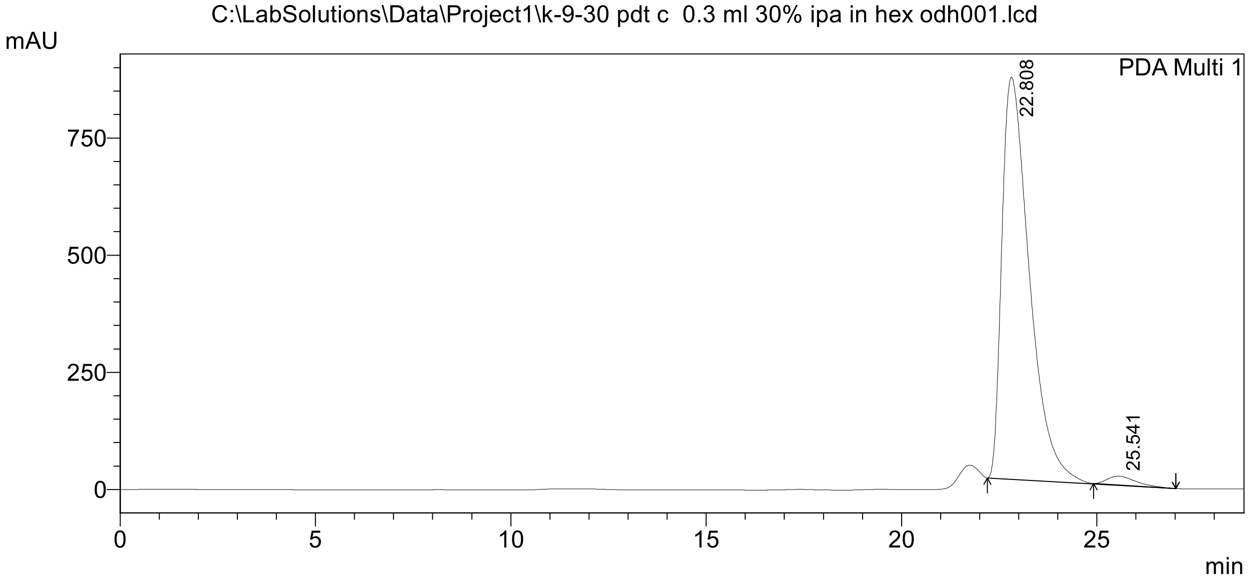
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.262	90779424	1652170	48.757	53.506
2	25.731	95408895	1435667	51.243	46.494
Total		186188319	3087838	100.000	100.000

<Chromatogram>

C:\LabSolutions\Data\Project1\k-9-30 pdt c 0.3 ml 30% ipa in hex odh001.lcd



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.808	42186510	858262	97.801	97.871
2	25.541	948738	18669	2.199	2.129
Total		43135247	876931	100.000	100.000

1c

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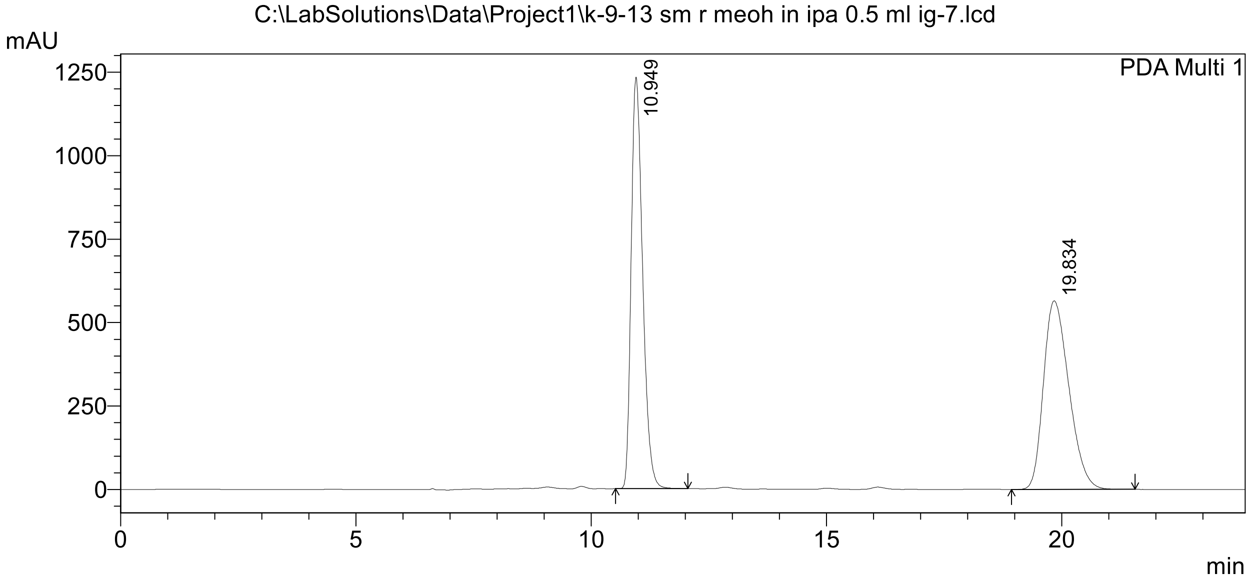

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.949	20823095	1232674	49.514	68.574
2	19.834	21232026	564899	50.486	31.426
Total		42055121	1797574	100.000	100.000

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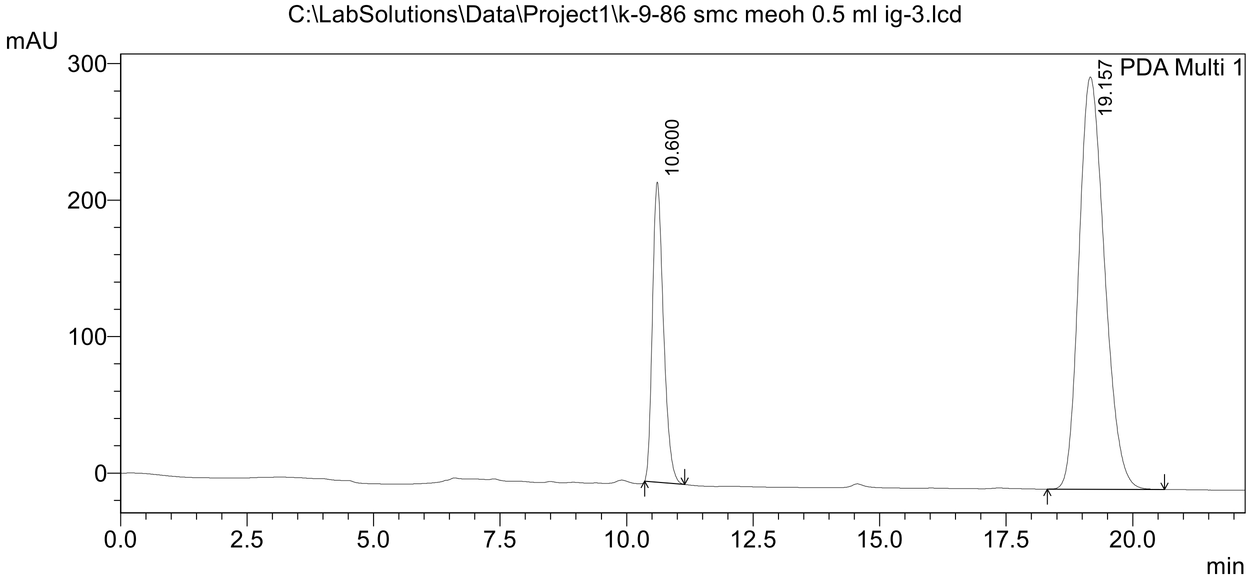

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.600	3343908	220019	23.896	42.148
2	19.157	10649641	301993	76.104	57.852
Total		13993549	522011	100.000	100.000

3j

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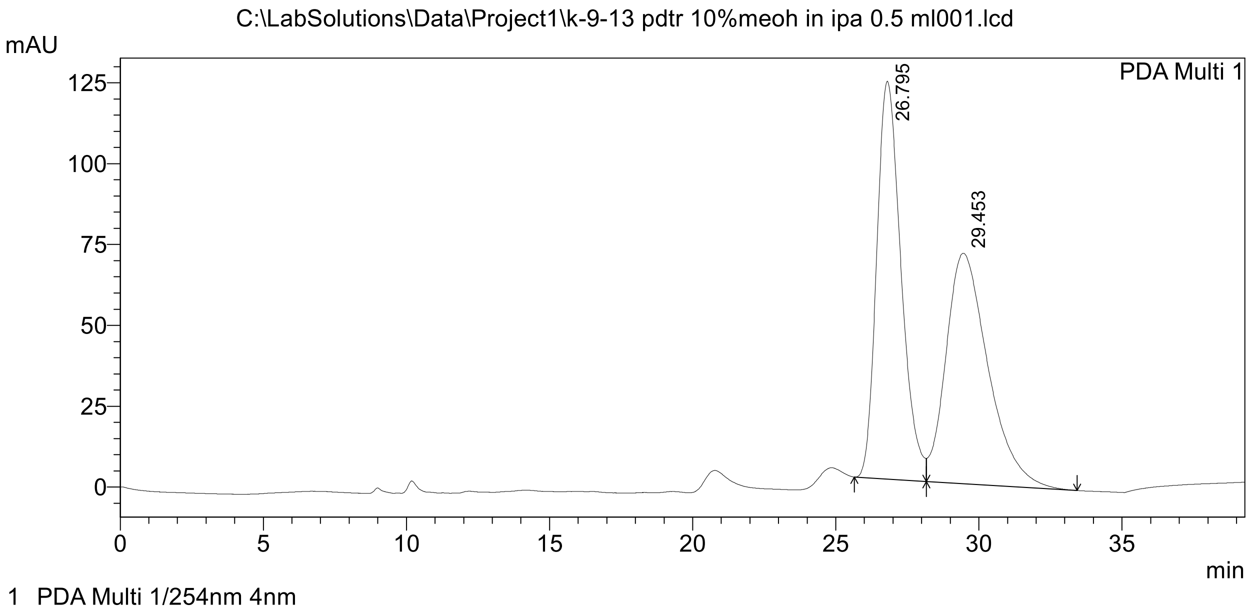

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.795	7304027	123076	50.039	63.329
2	29.453	7292628	71268	49.961	36.671
Total		14596655	194344	100.000	100.000

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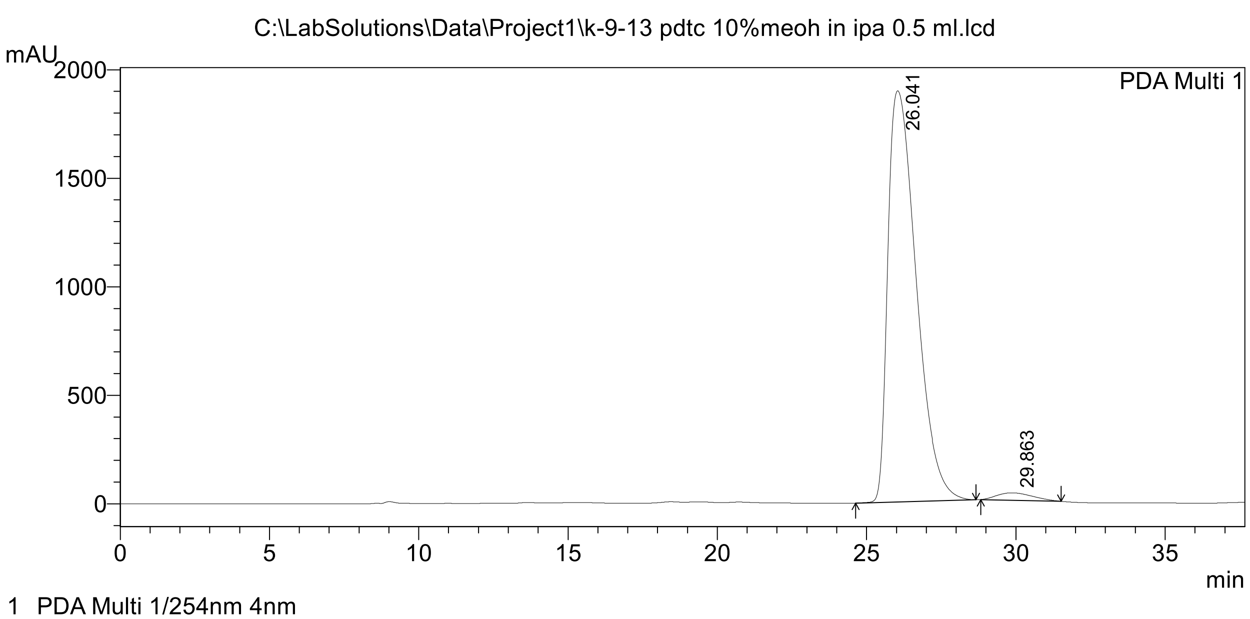


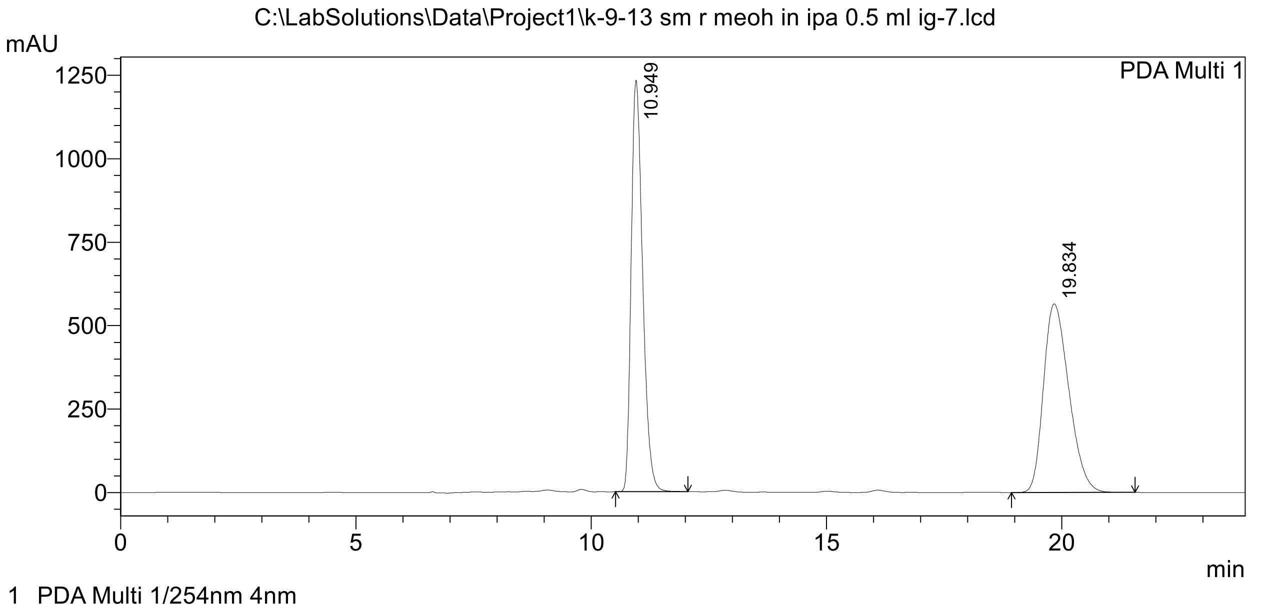
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.041	124890607	1894775	97.759	98.221
2	29.863	2862803	34323	2.241	1.779
Total		127753409	1929098	100.000	100.000

1c

<Chromatogram>

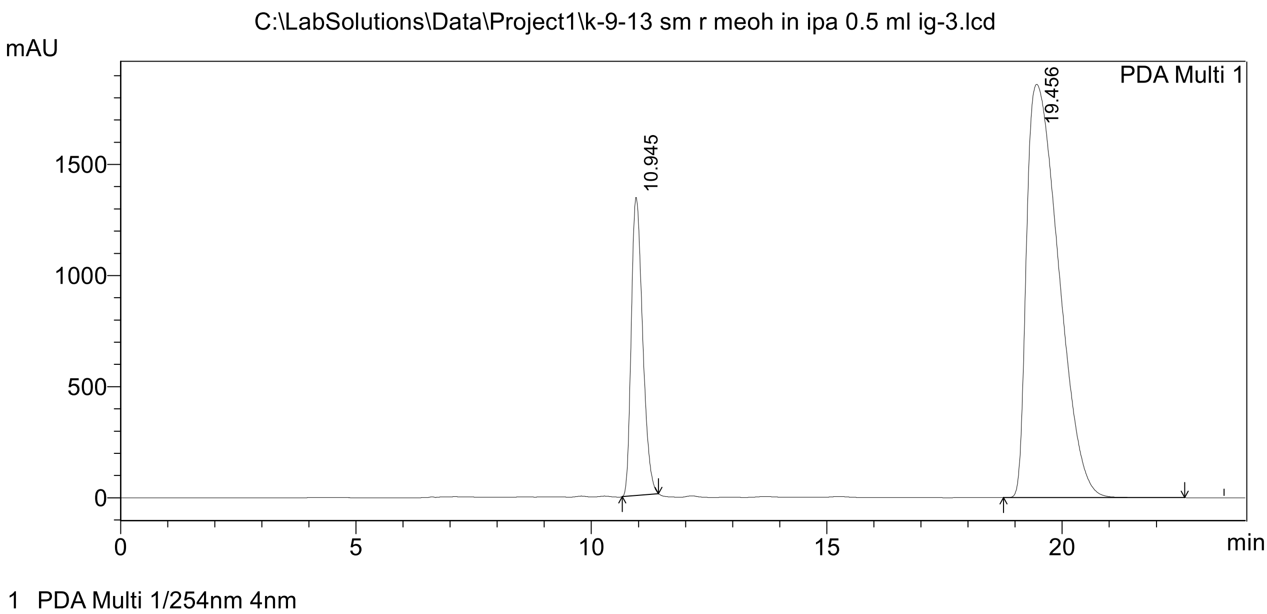


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.949	20823095	1232674	49.514	68.574
2	19.834	21232026	564899	50.486	31.426
Total		42055121	1797574	100.000	100.000

<Chromatogram>



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.945	22495714	1341695	20.344	41.911
2	19.456	88078916	1859586	79.656	58.089
Total		110574630	3201281	100.000	100.000

3k

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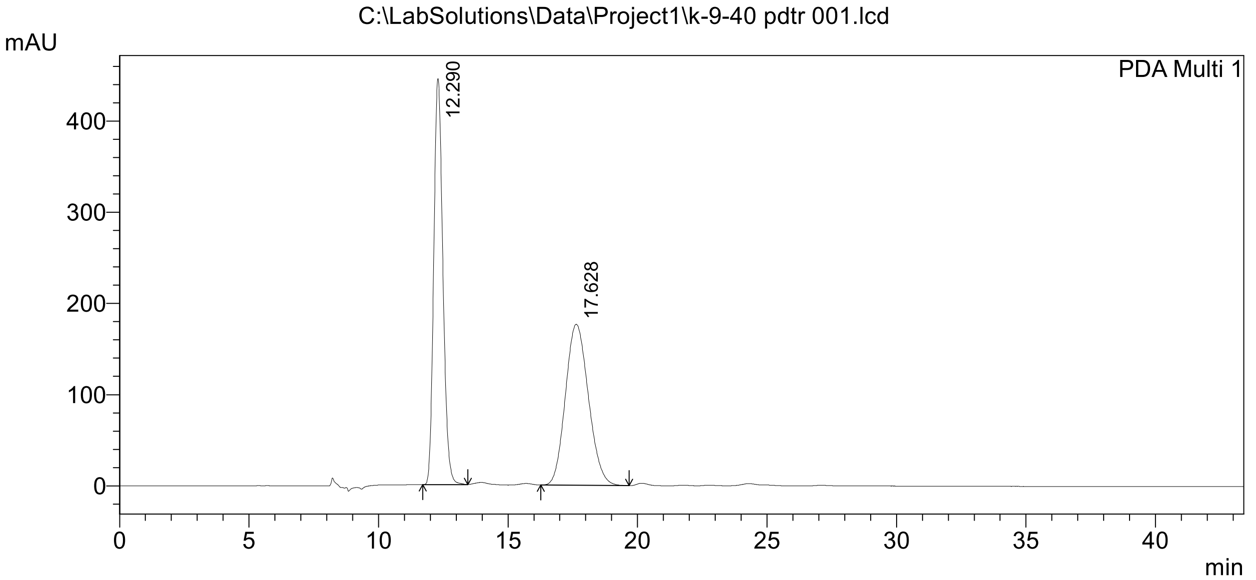

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.290	10915918	445212	49.998	71.606
2	17.628	10916743	176543	50.002	28.394
Total		21832661	621755	100.000	100.000

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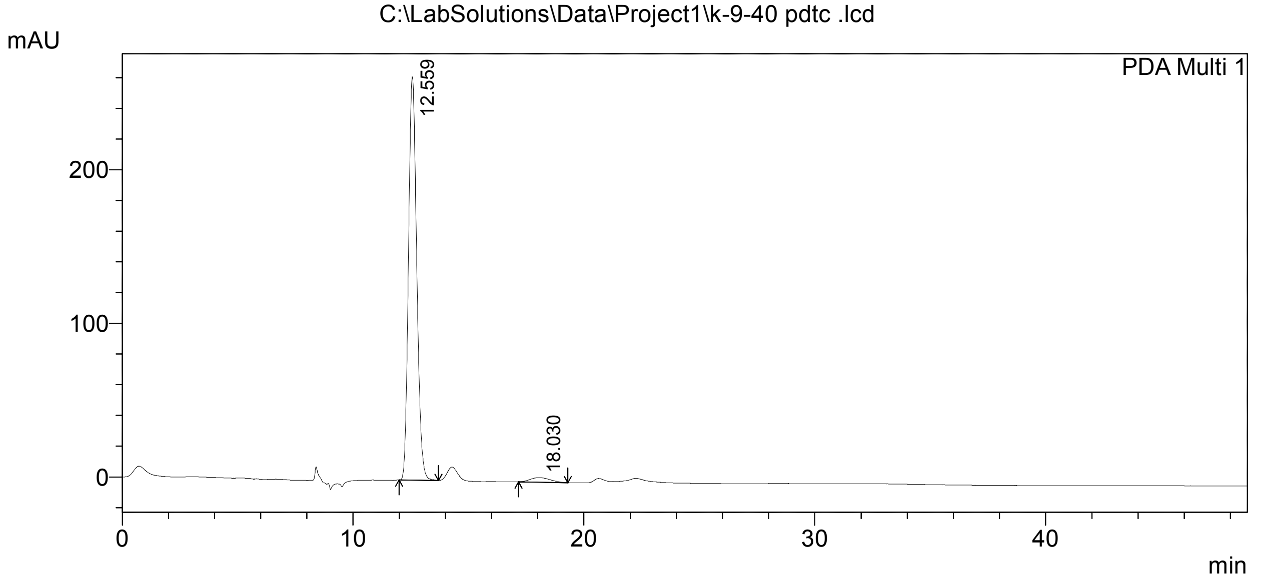

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.559	6506348	262635	97.267	98.853
2	18.030	182849	3047	2.733	1.147
Total		6689198	265683	100.000	100.000

1c

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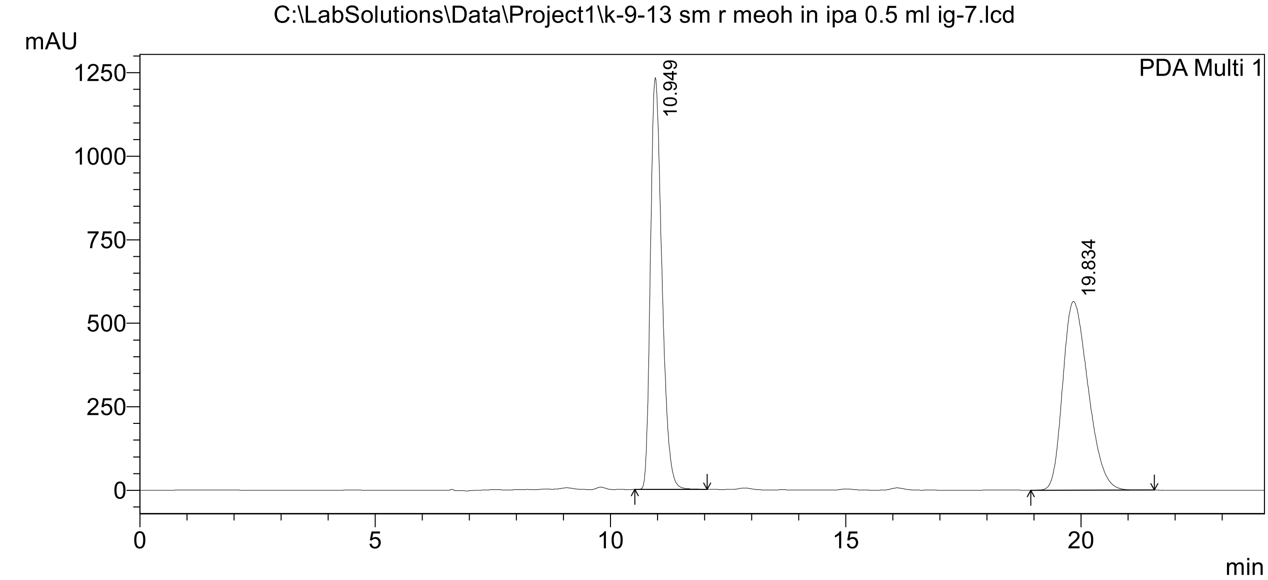

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.949	20823095	1232674	49.514	68.574
2	19.834	21232026	564899	50.486	31.426
Total		42055121	1797574	100.000	100.000

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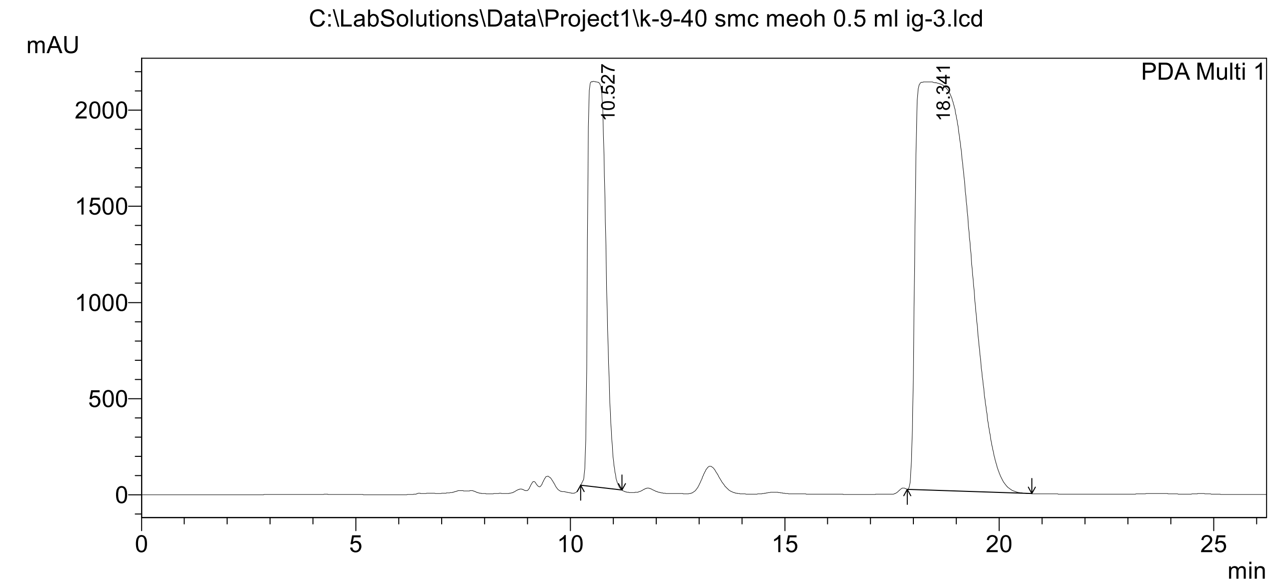

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.527	59522228	2108454	24.931	49.832
2	18.341	179223549	2122649	75.069	50.168
Total		238745776	4231103	100.000	100.000

3l

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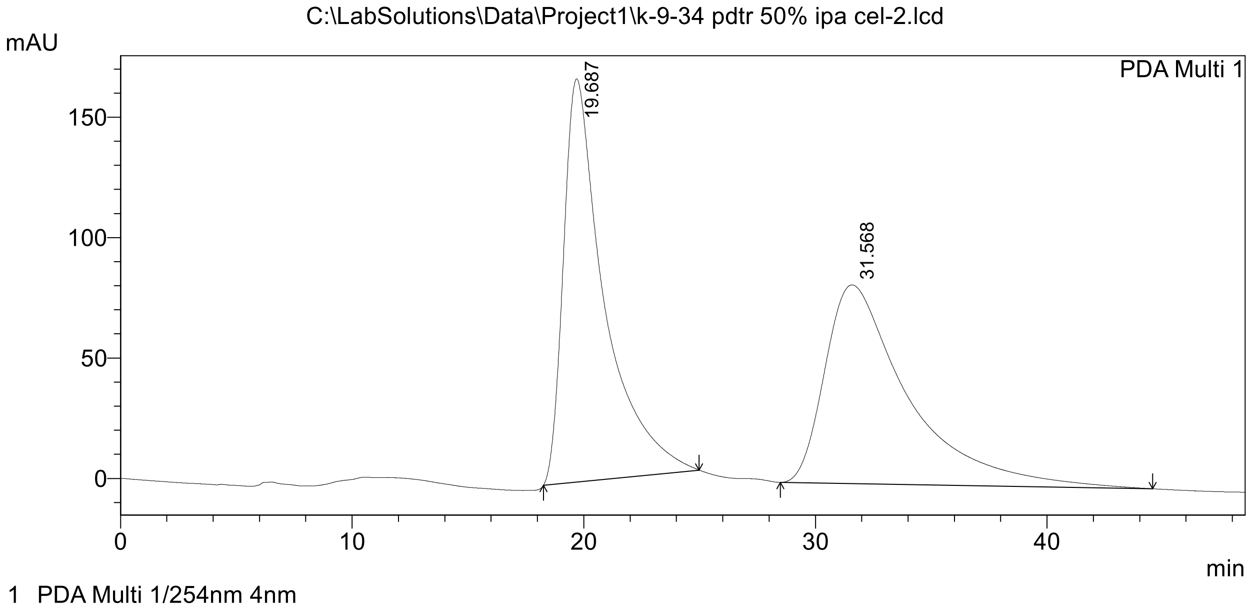
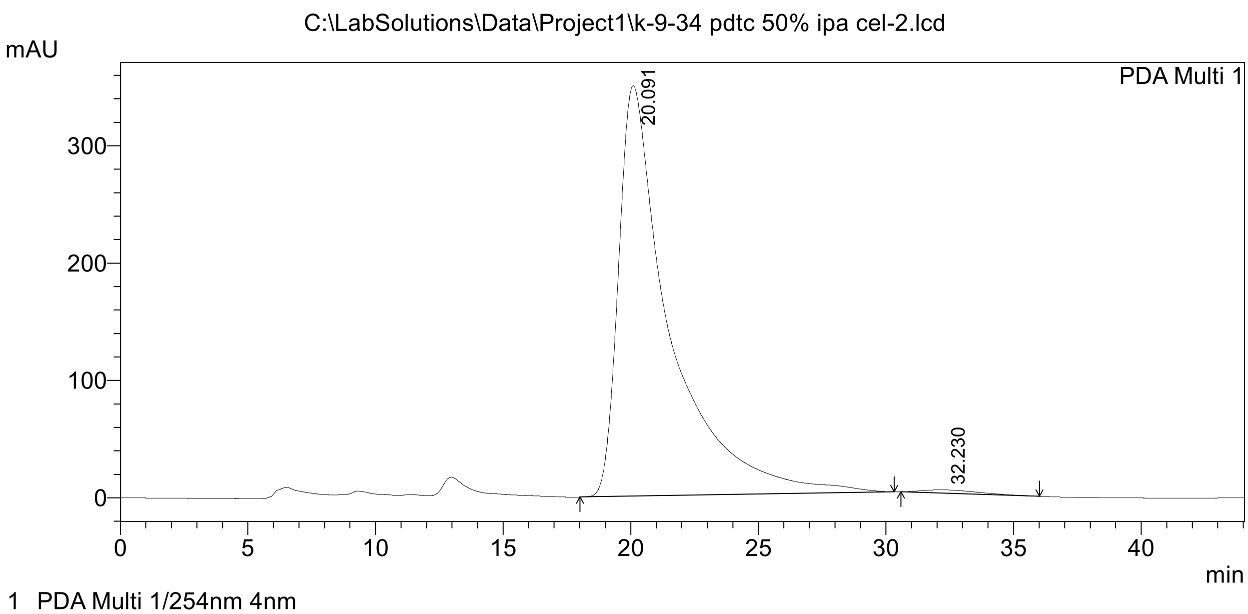


PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.687	20535896	167438	49.966	66.985
2	31.568	20563652	82527	50.034	33.015
Total		41099548	249965	100.000	100.000

<Chromatogram>



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.091	49270866	349792	99.090	99.178
2	32.230	452604	2898	0.910	0.822
Total		49723471	352691	100.000	100.000

1d

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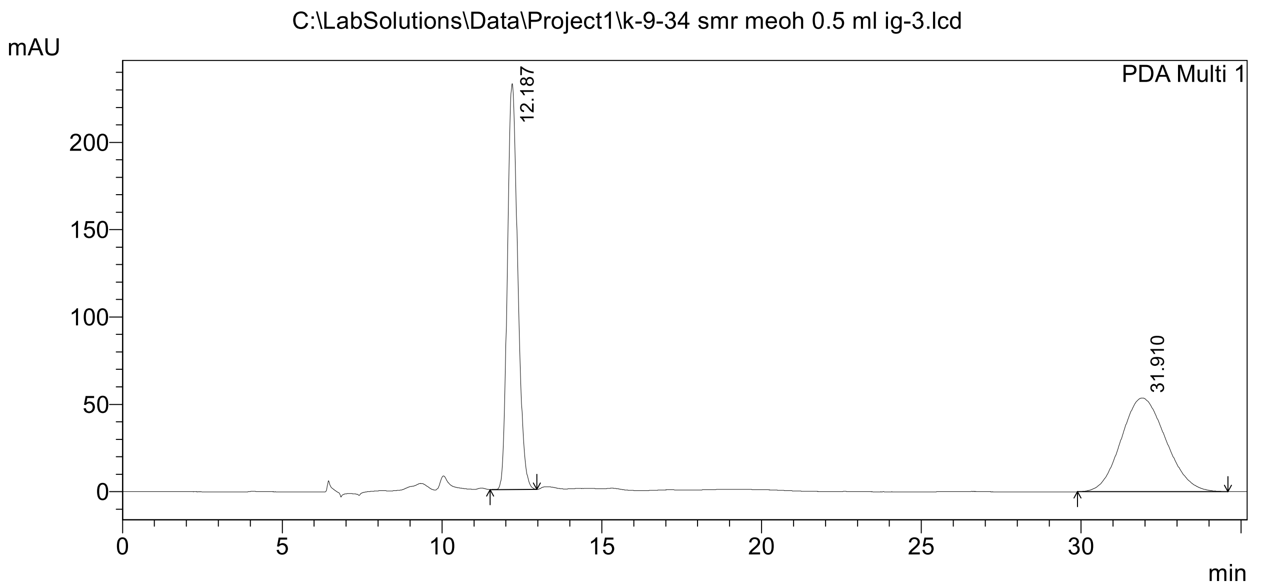

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.187	5258040	232387	50.172	81.240
2	31.910	5222016	53663	49.828	18.760
Total		10480056	286050	100.000	100.000

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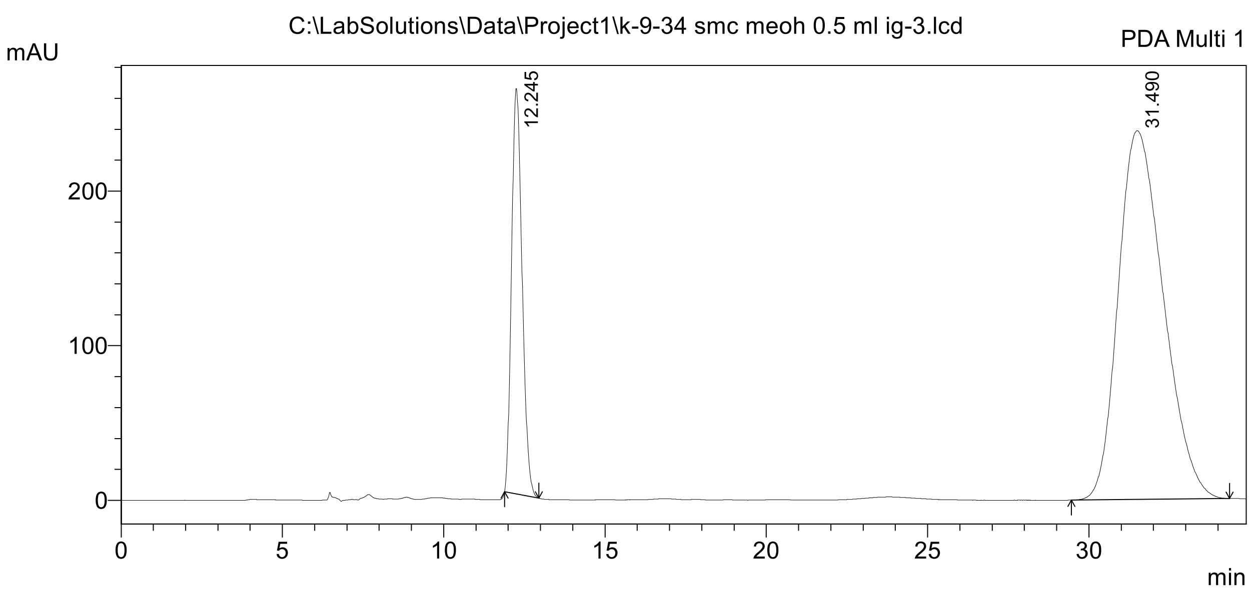

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.245	5957283	262219	20.443	52.364
2	31.490	23183972	238538	79.557	47.636
Total		29141255	500757	100.000	100.000

3m

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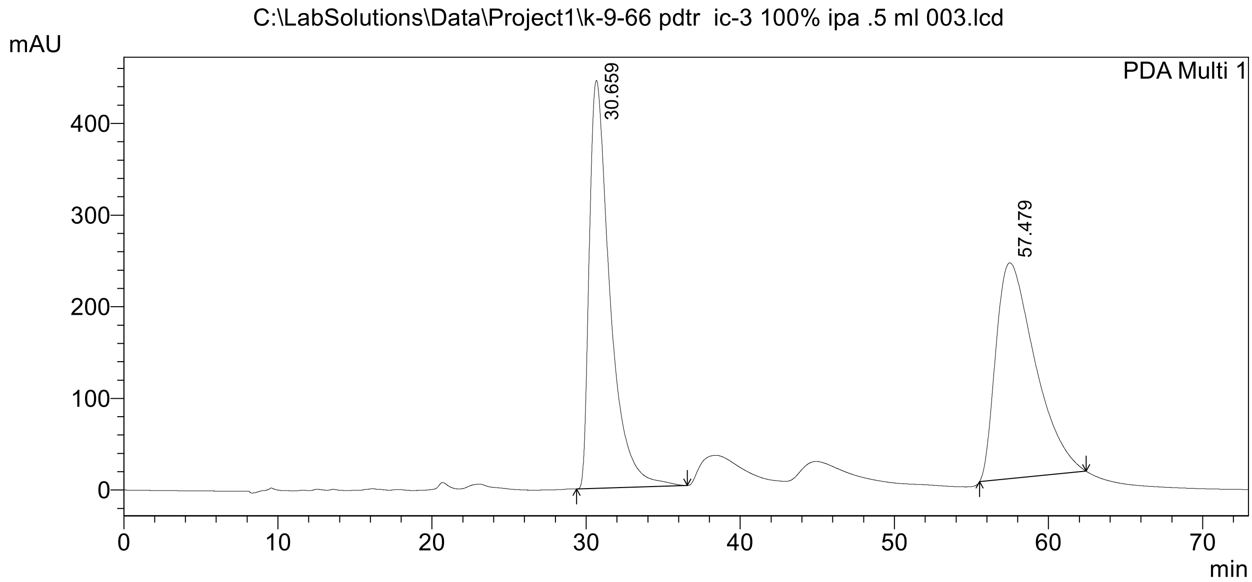

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.659	41675561	445245	49.880	65.387
2	57.479	41875415	235696	50.120	34.613
Total		83550976	680941	100.000	100.000

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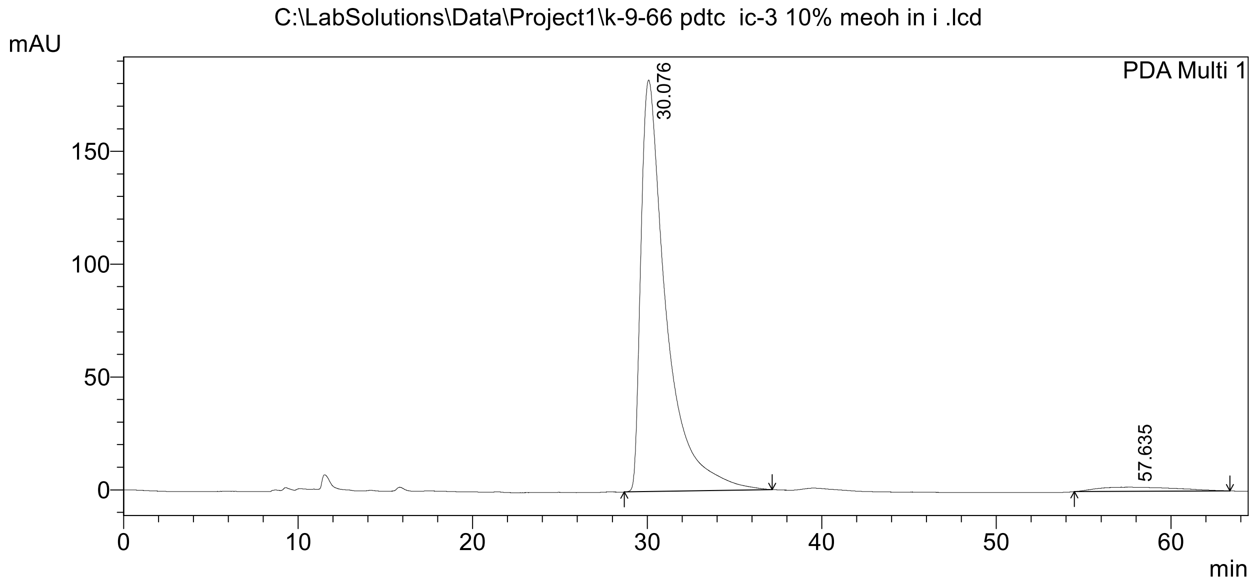

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.076	18403395	182384	96.853	98.991
2	57.635	598034	1860	3.147	1.009
Total		19001429	184244	100.000	100.000

1e

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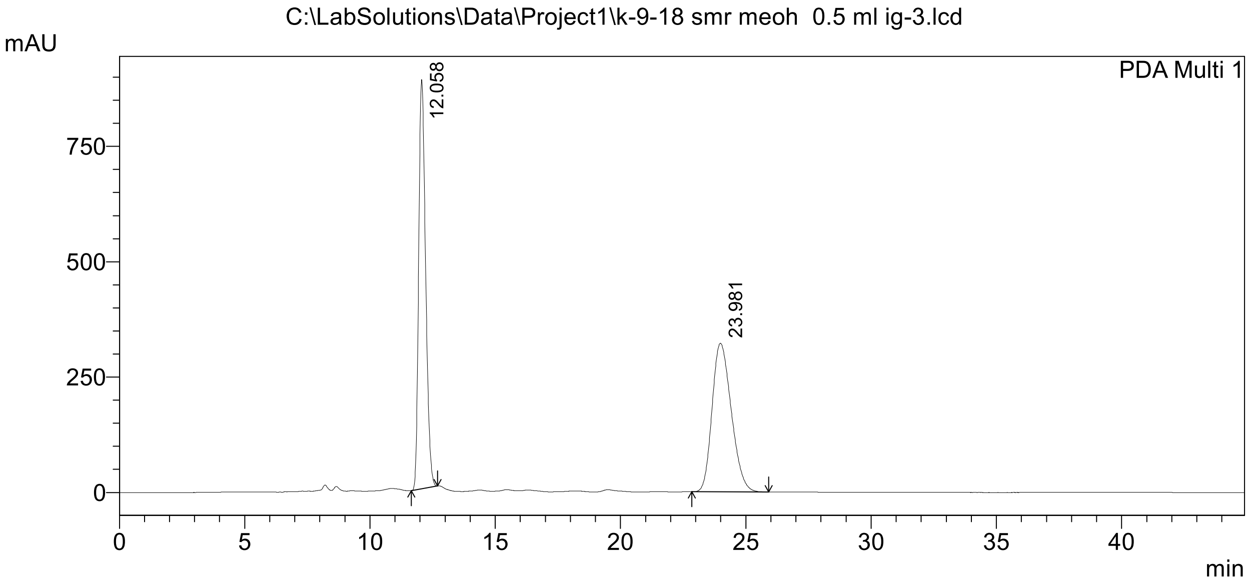

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.058	17027354	887124	49.775	73.369
2	23.981	17181586	322003	50.225	26.631
Total		34208940	1209126	100.000	100.000

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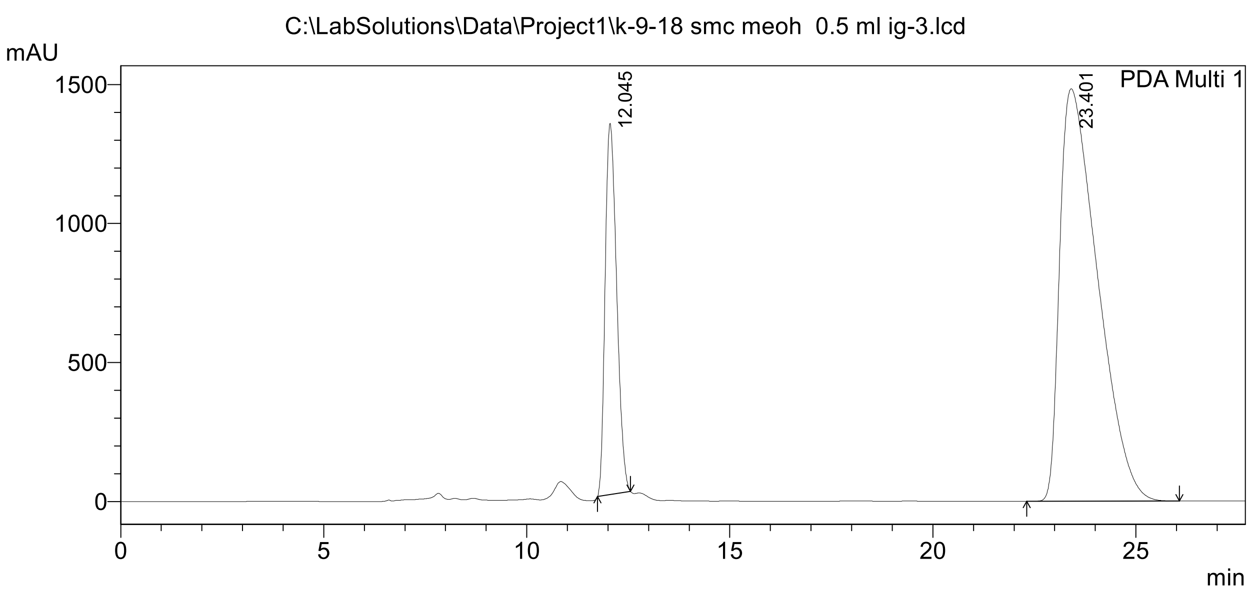

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.045	26400130	1336119	21.534	47.381
2	23.401	96198799	1483842	78.466	52.619
Total		122598929	2819961	100.000	100.000

3n

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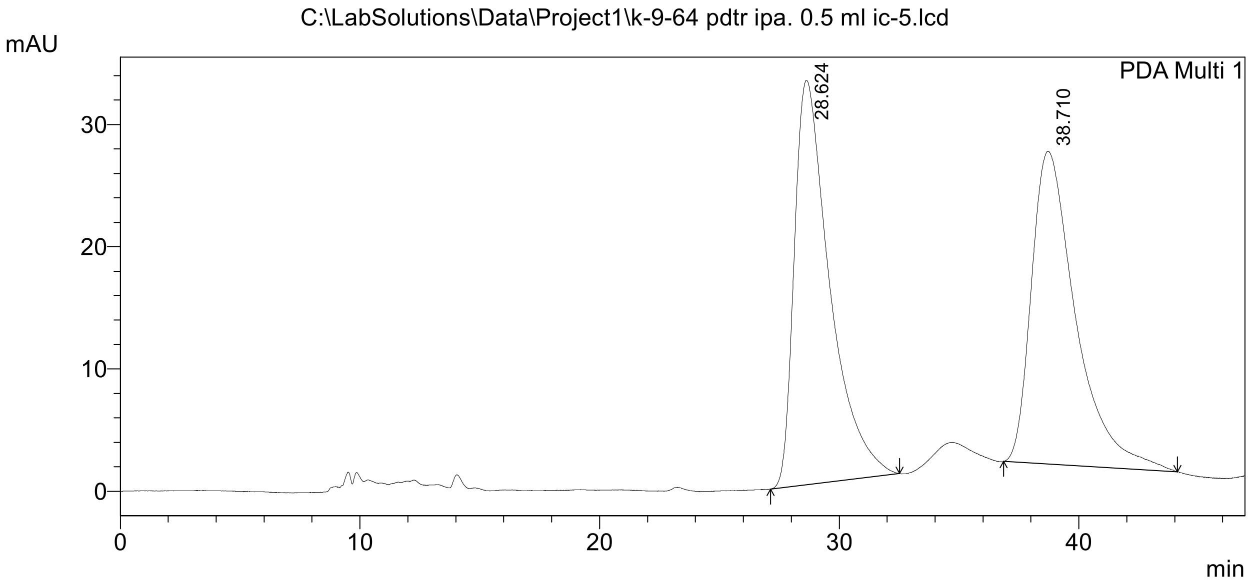


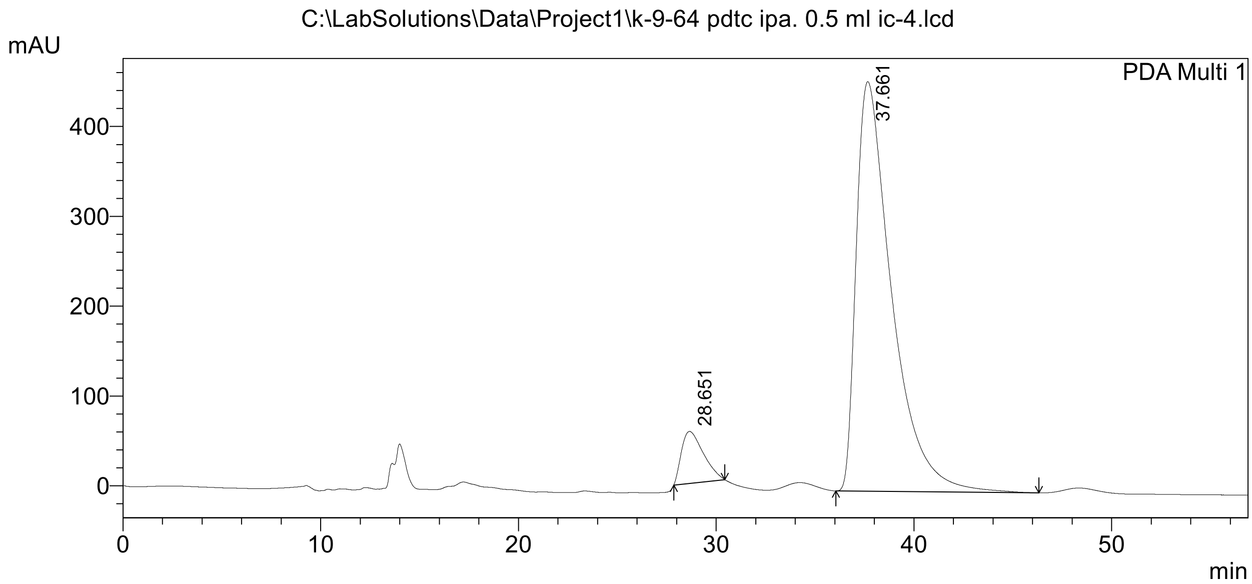
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.624	3412946	33092	50.934	56.394
2	38.710	3287803	25588	49.066	43.606
Total		6700749	58681	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.651	4464027	57867	7.273	11.259
2	37.661	56912944	456077	92.727	88.741
Total		61376971	513944	100.000	100.000

1f

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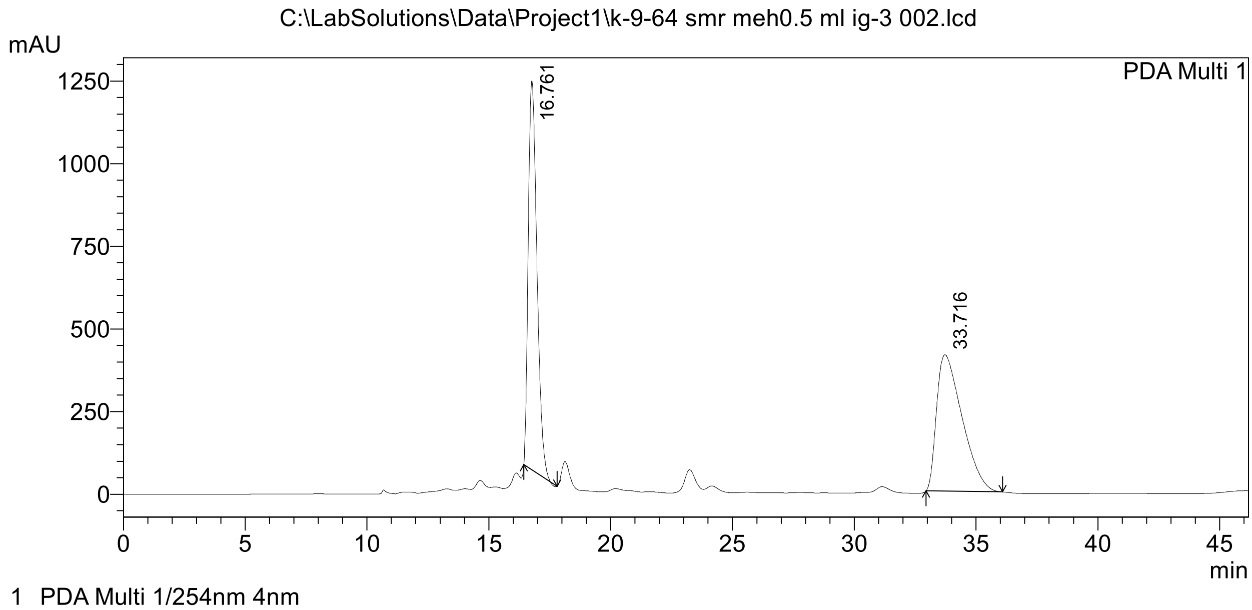

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.761	29212575	1175965	49.290	74.038
2	33.716	30053593	412369	50.710	25.962
Total		59266167	1588335	100.000	100.000

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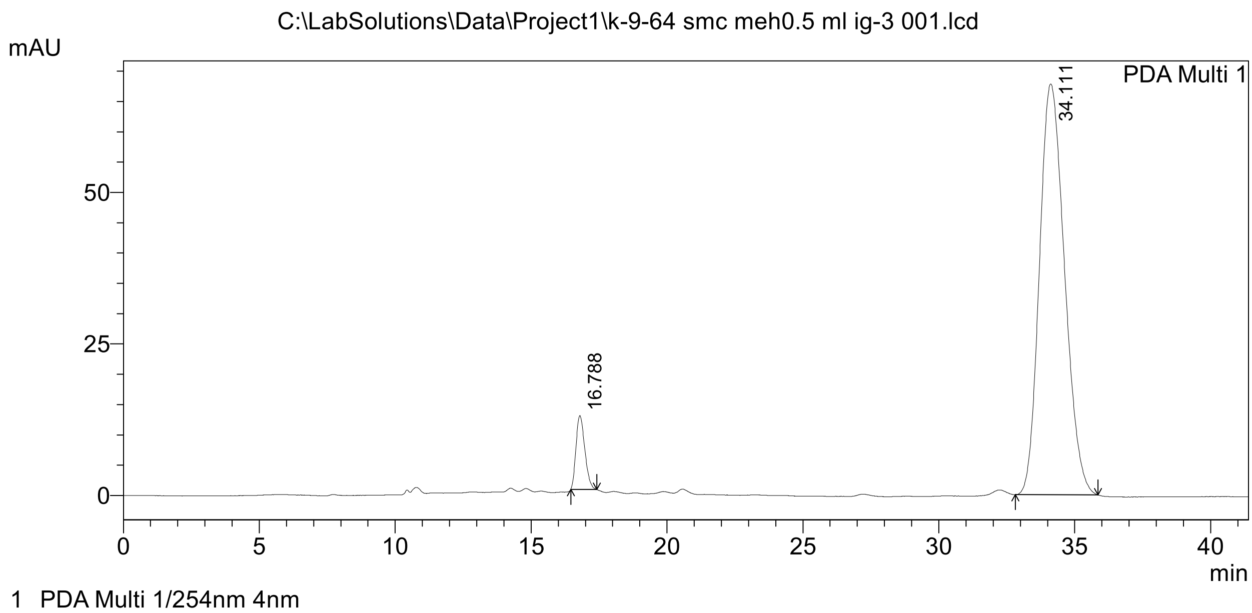

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.788	276605	12214	5.975	15.269
2	34.111	4352747	67782	94.025	84.731
Total		4629352	79996	100.000	100.000

3o

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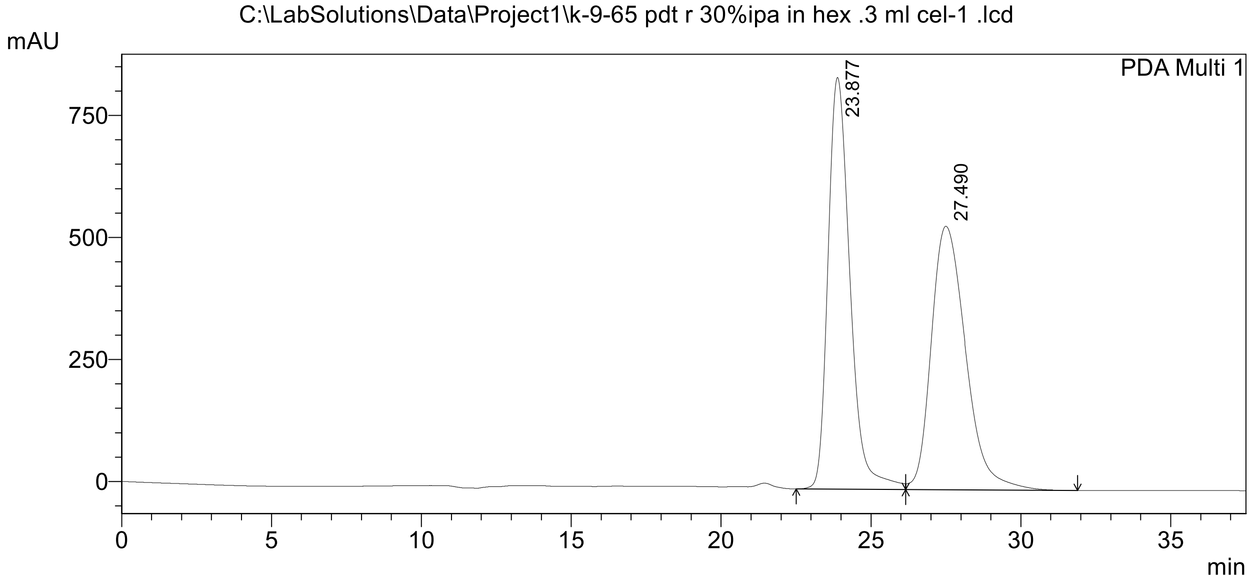

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.877	43176033	843741	49.886	60.974
2	27.490	43373983	540036	50.114	39.026
Total		86550016	1383777	100.000	100.000

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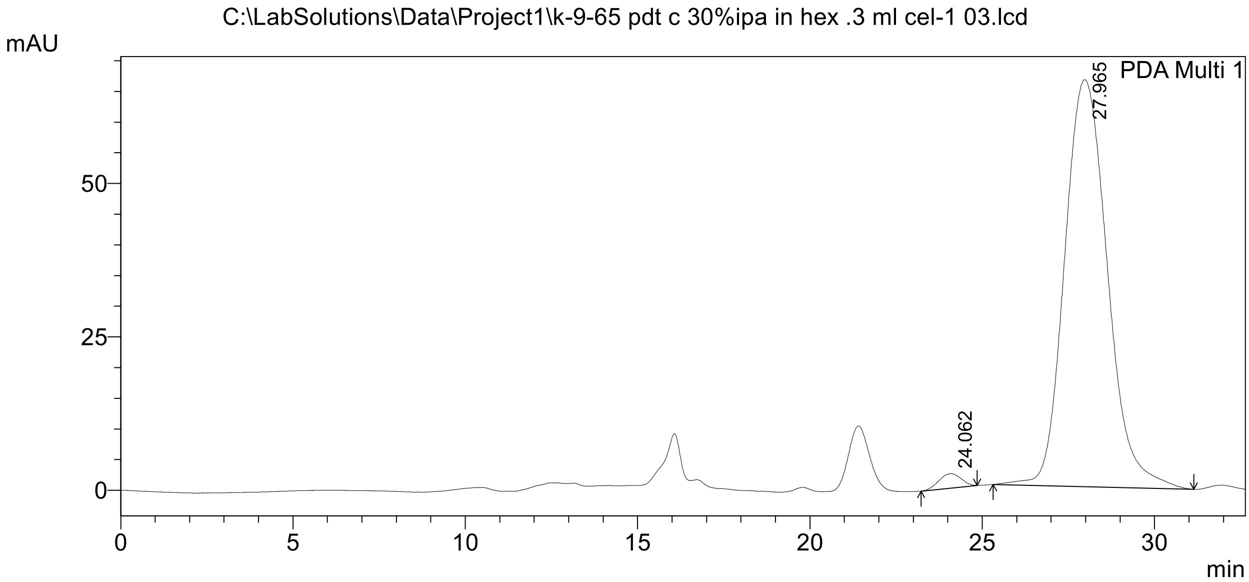

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.062	106164	2369	1.812	3.449
2	27.965	5751505	66325	98.188	96.551
Total		5857669	68695	100.000	100.000

1g

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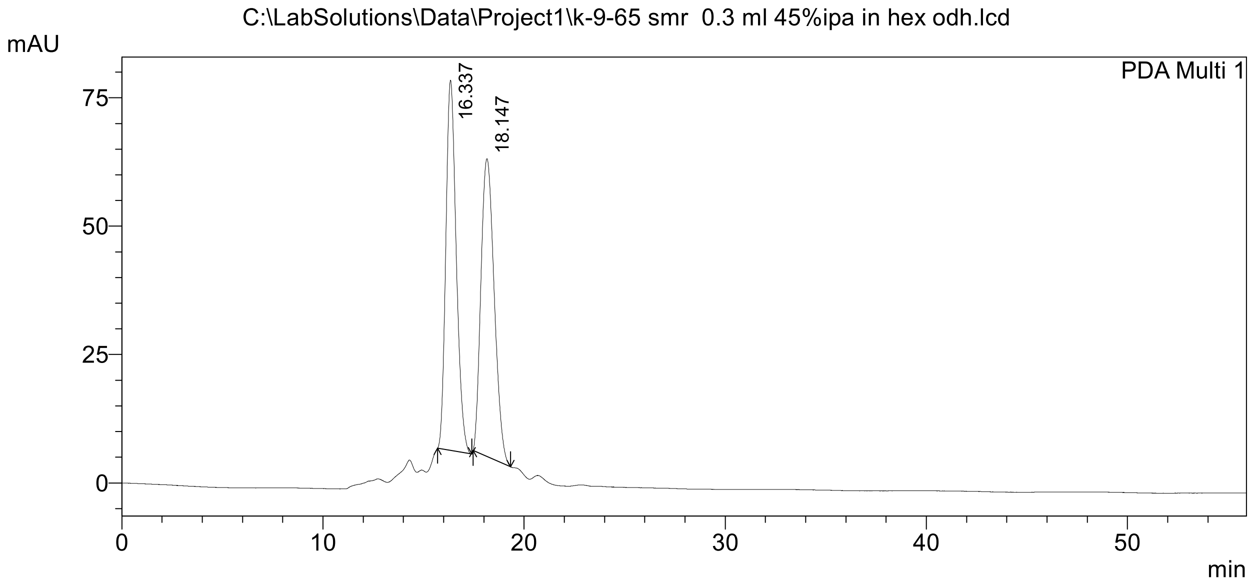

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.337	2601539	72116	49.340	55.421
2	18.147	2671126	58008	50.660	44.579
Total		5272666	130124	100.000	100.000

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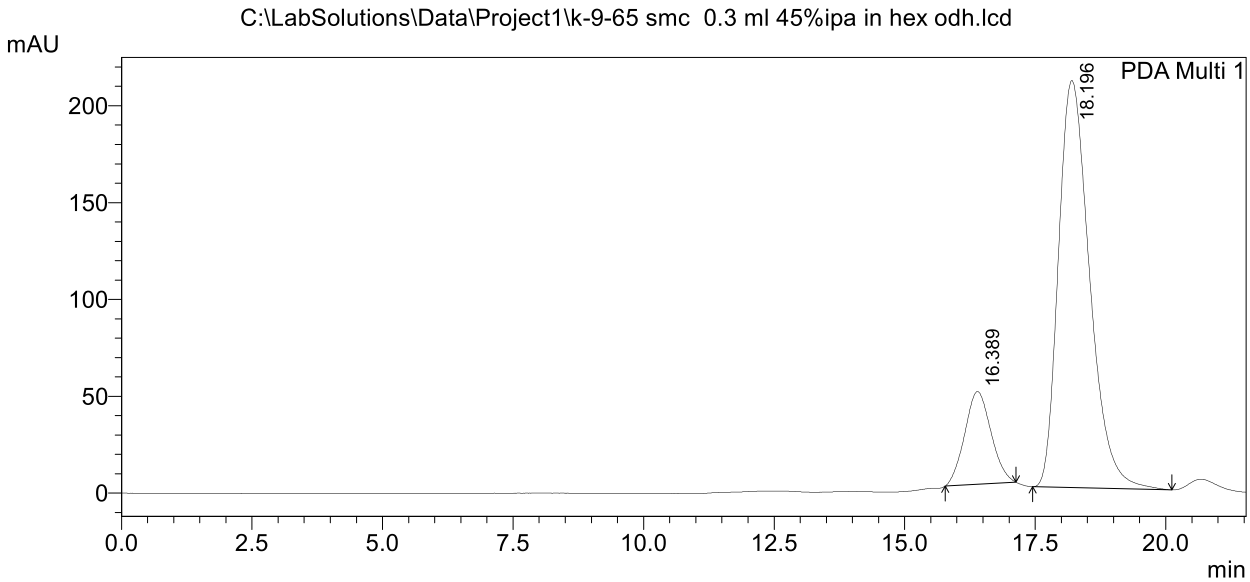

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.389	1680814	47850	16.119	18.548
2	18.196	8747000	210132	83.881	81.452
Total		10427814	257981	100.000	100.000

3p

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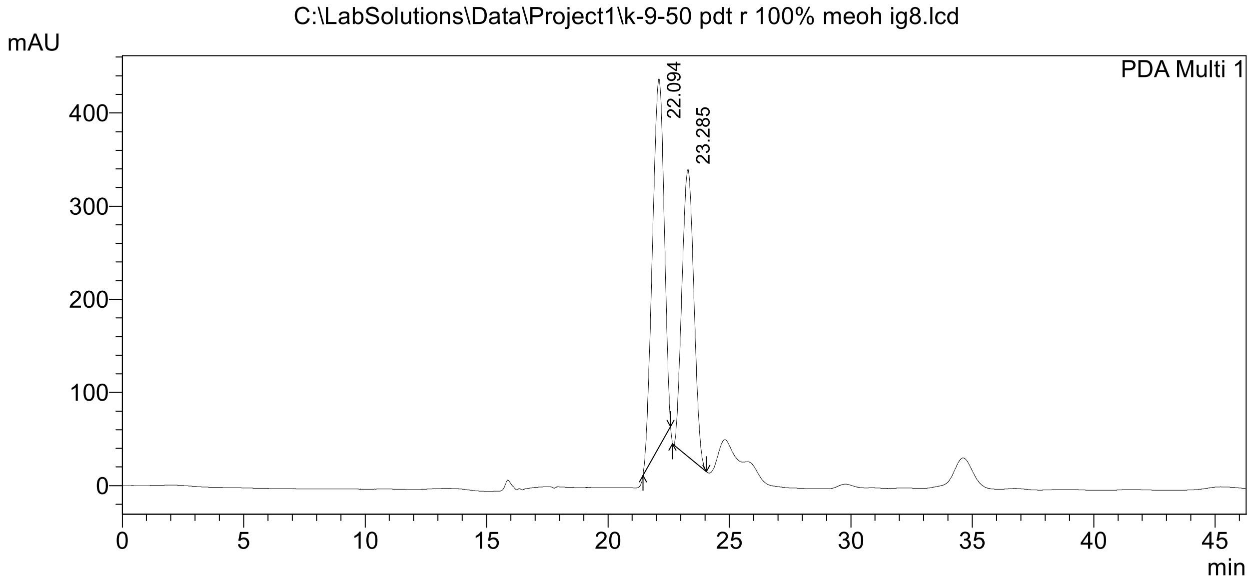

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.094	13299126	395743	55.823	56.244
2	23.285	10524523	307871	44.177	43.756
Total		23823649	703614	100.000	100.000

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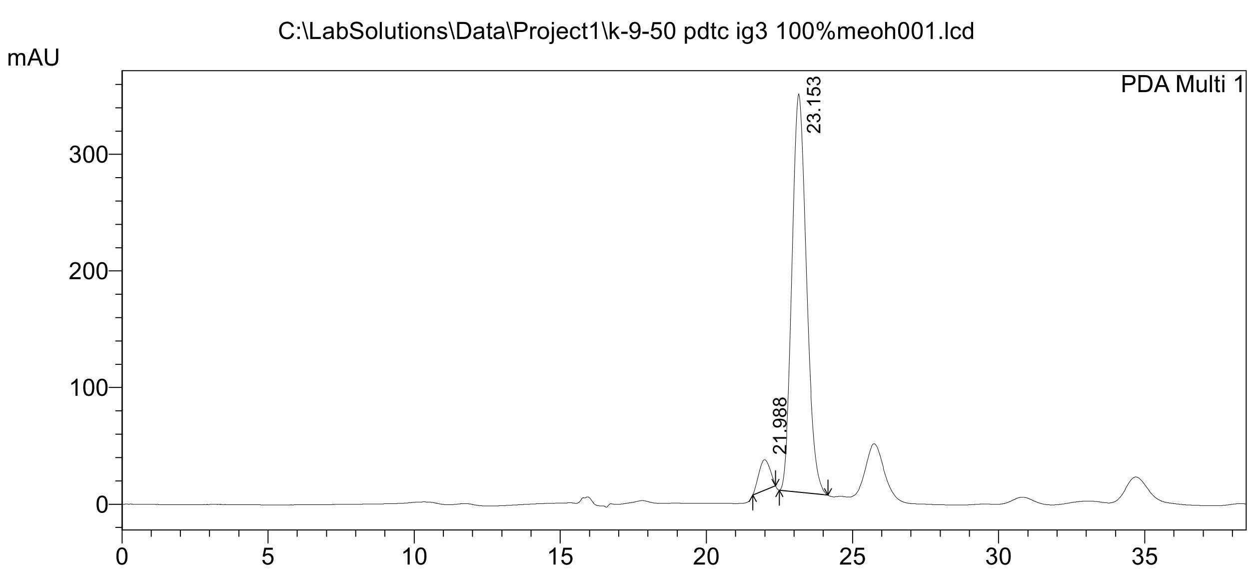

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.988	699413	26146	5.553	7.109
2	23.153	11896041	341651	94.447	92.891
Total		12595454	367797	100.000	100.000

1h

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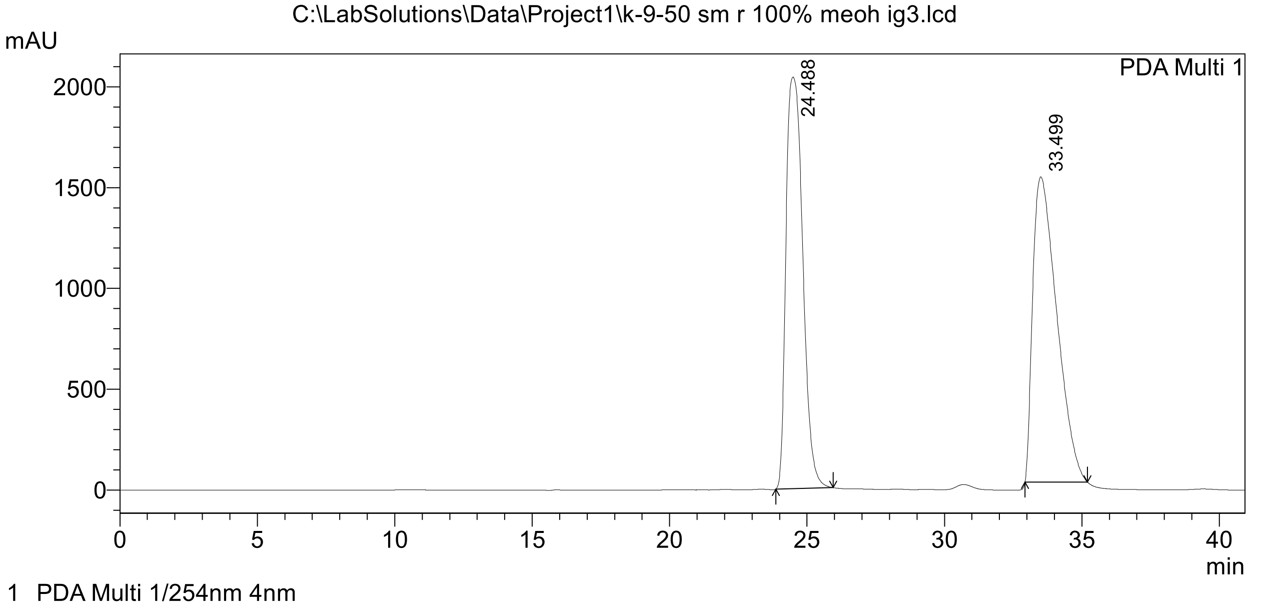

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.488	86660501	2041877	48.480	57.416
2	33.499	92093321	1514387	51.520	42.584
Total		178753821	3556264	100.000	100.000

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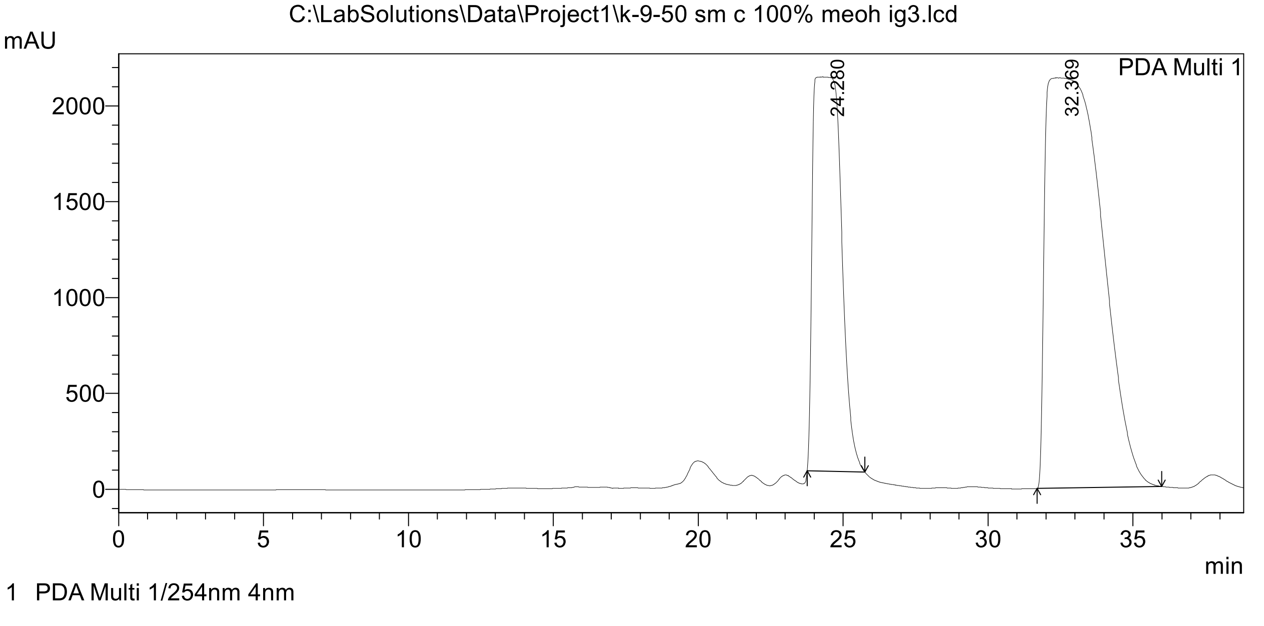

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.280	139464780	2055180	32.601	48.980
2	32.369	288330639	2140754	67.399	51.020
Total		427795418	4195934	100.000	100.000

3q

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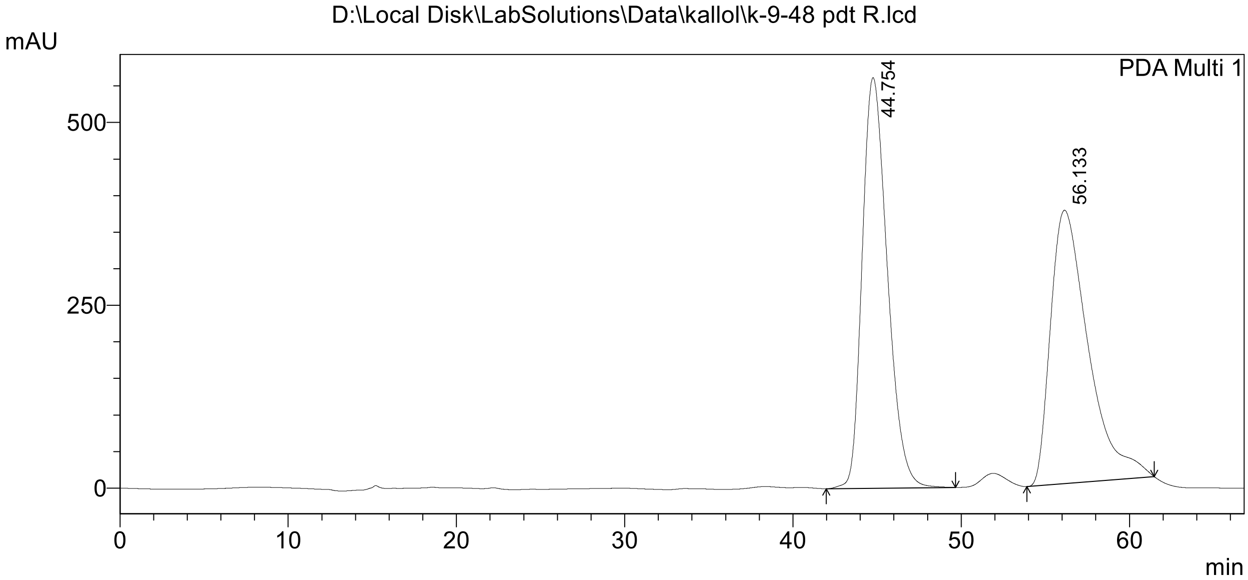

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	44.754	58479508	561698	50.036	60.021
2	56.133	58395815	374143	49.964	39.979
Total		116875323	935842	100.000	100.000

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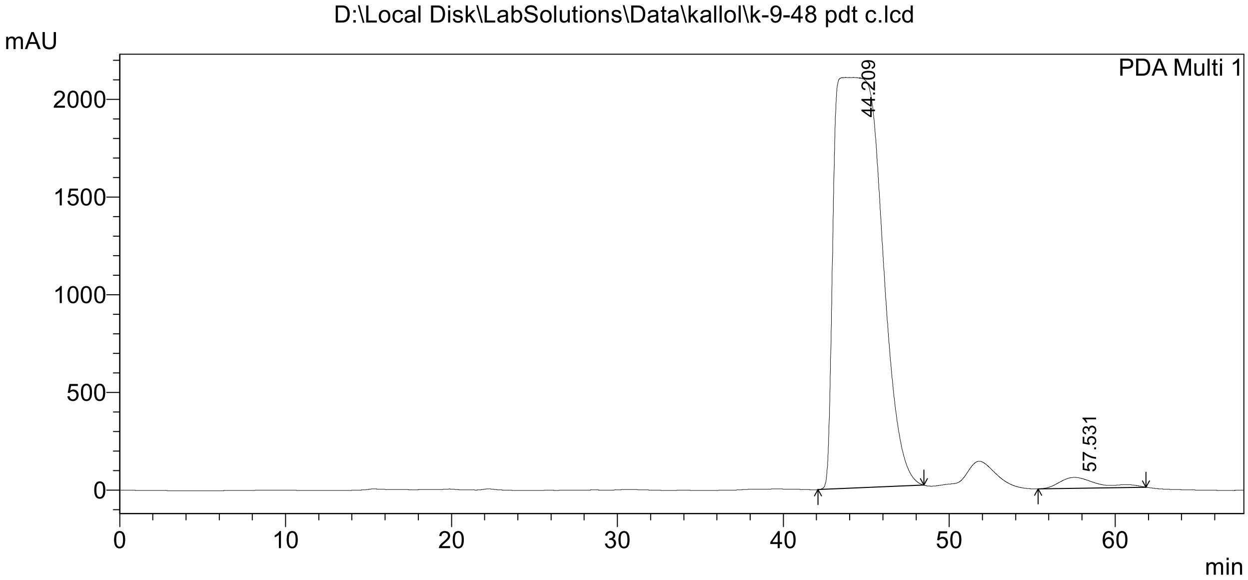

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	44.209	413011528	2102714	97.890	97.424
2	57.531	8904257	55596	2.110	2.576
Total		421915785	2158311	100.000	100.000

1i

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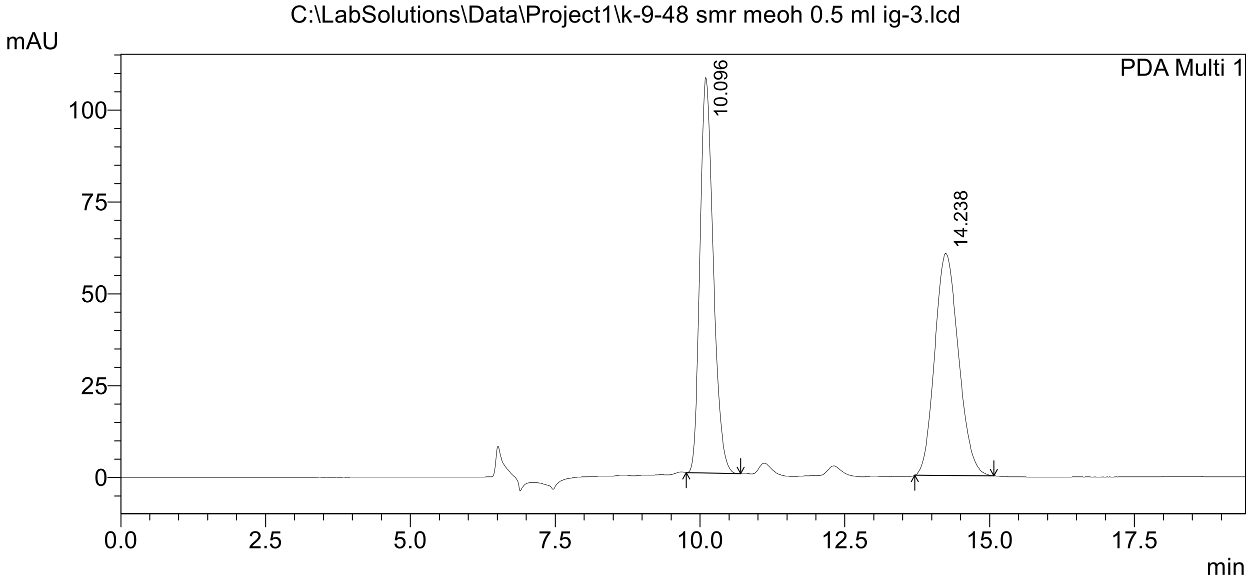

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.096	1724157	107620	50.002	64.029
2	14.238	1723998	60460	49.998	35.971
Total		3448155	168080	100.000	100.000

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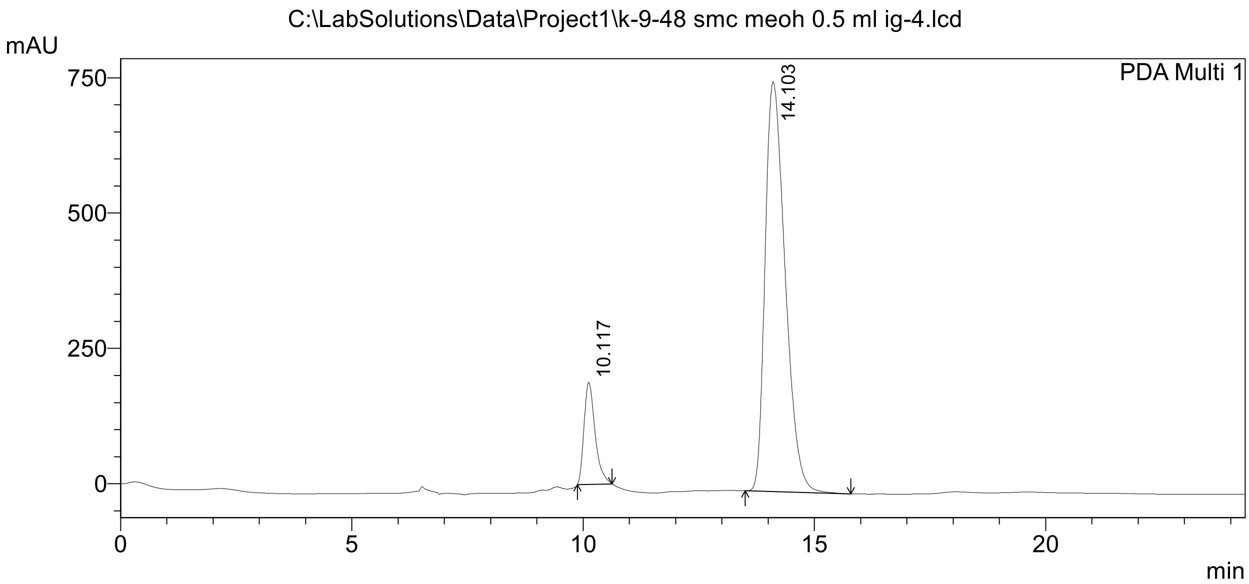

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.117	3138475	188434	12.089	19.932
2	14.103	22823996	756968	87.911	80.068
Total		25962471	945403	100.000	100.000

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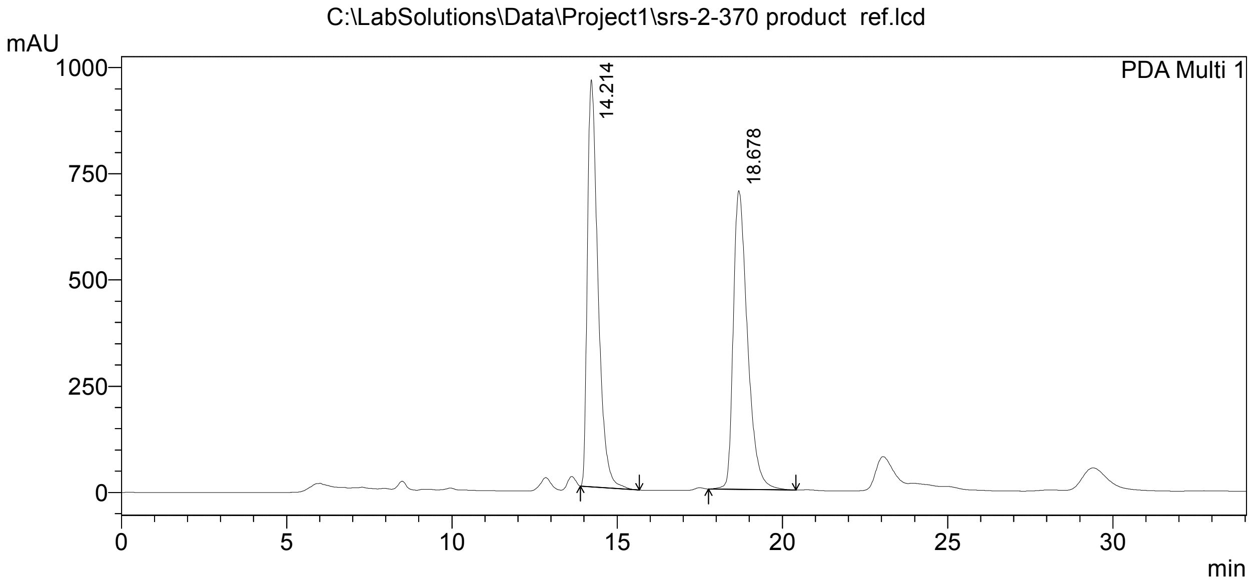
3r-achiral



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.214	21415569	958757	50.409	57.678
2	18.678	21068472	703488	49.591	42.322
Total		42484042	1662245	100.000	100.000

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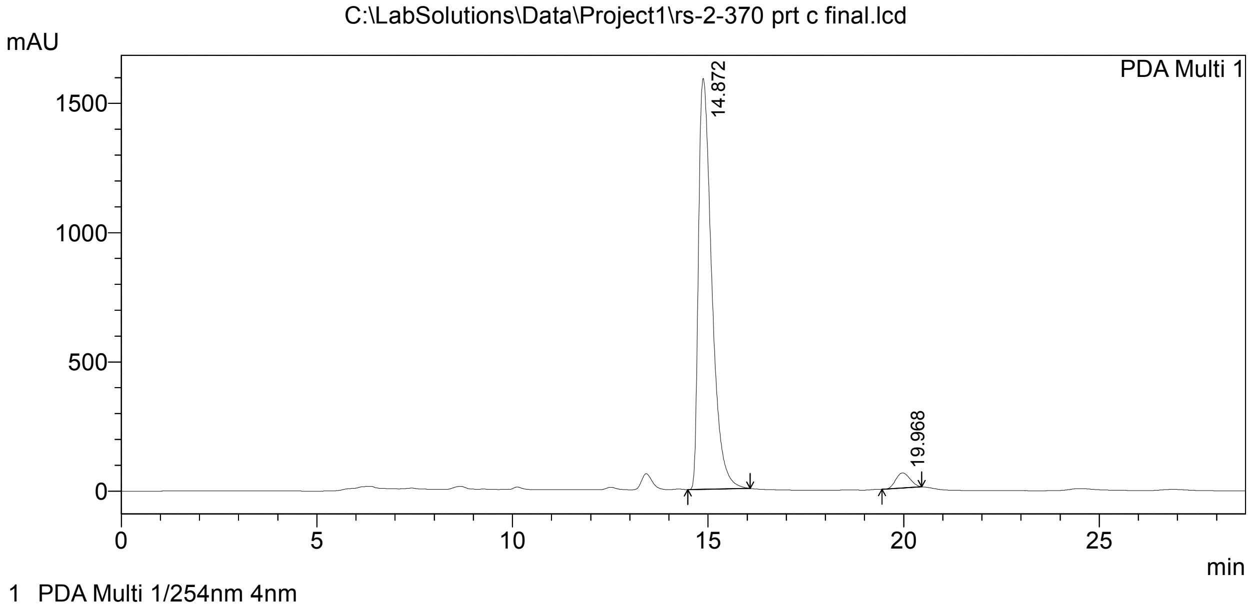

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.872	37609708	1590075	96.236	96.449
2	19.968	1471174	58537	3.764	3.551
Total		39080882	1648612	100.000	100.000

<Chromatogram>

1m-achiral

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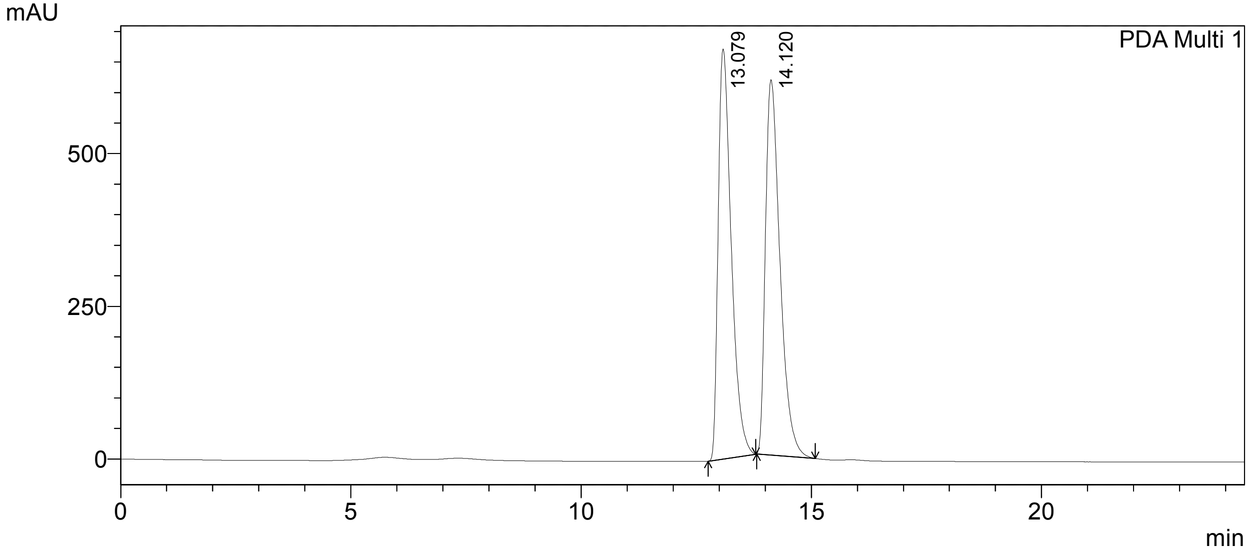

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.079	13274657	671602	49.570	52.217
2	14.120	13505224	614563	50.430	47.783
Total		26779881	1286165	100.000	100.000

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Sample Name : srs-2-370 sm chi

1m-chiral

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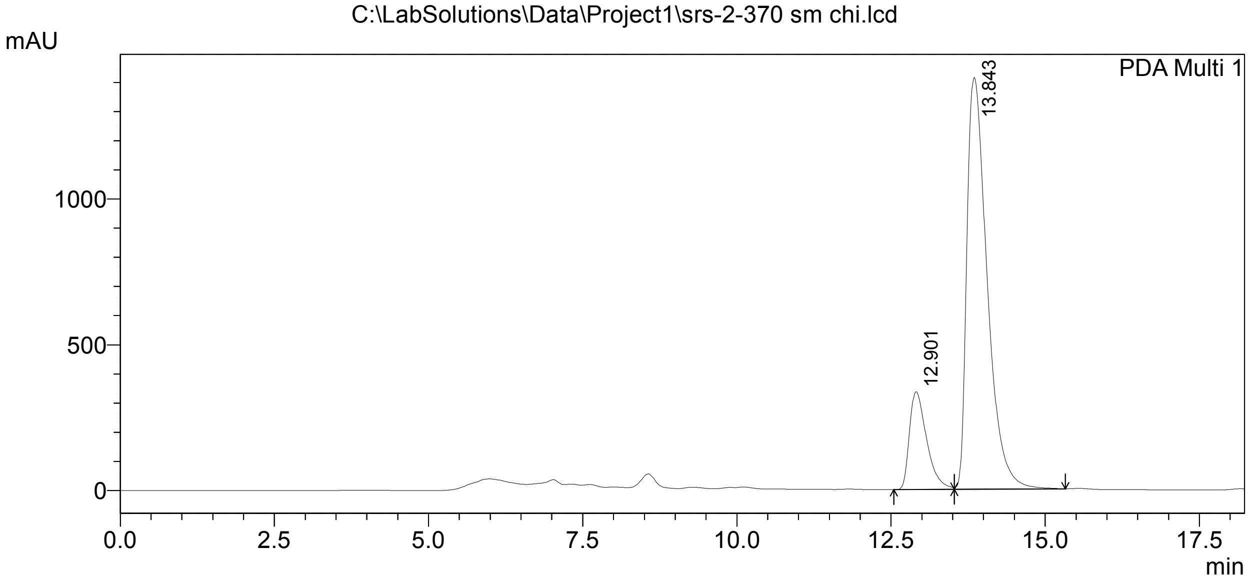

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.901	6569885	336161	16.846	19.214
2	13.843	32429390	1413424	83.154	80.786
Total		38999276	1749585	100.000	100.000

5a

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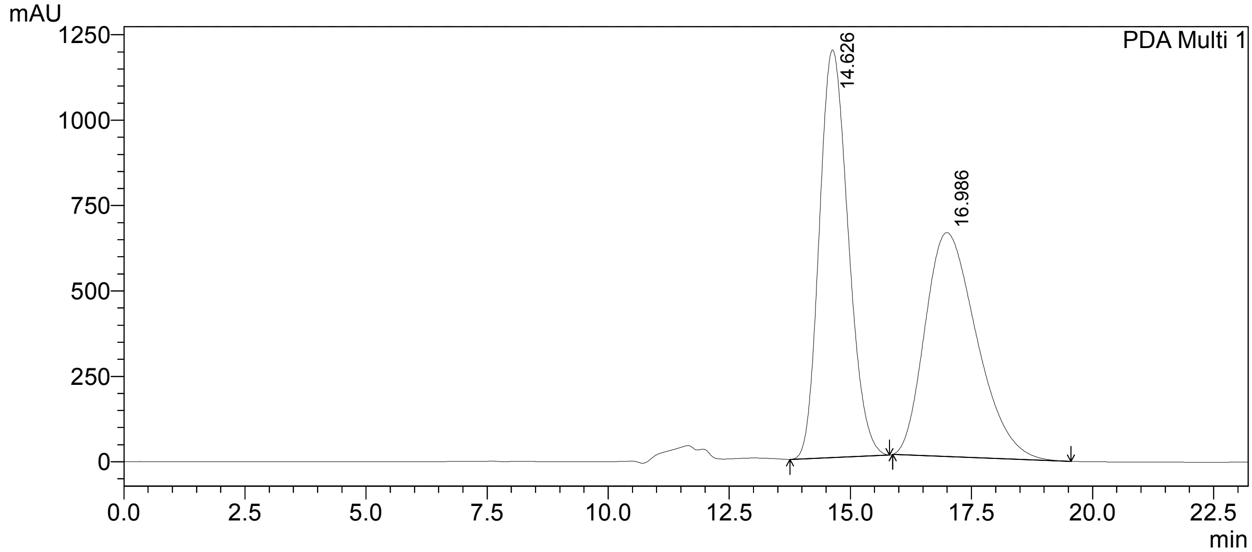

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.626	49645651	1193604	50.530	64.535
2	16.986	48603974	655930	49.470	35.465
Total		98249625	1849534	100.000	100.000

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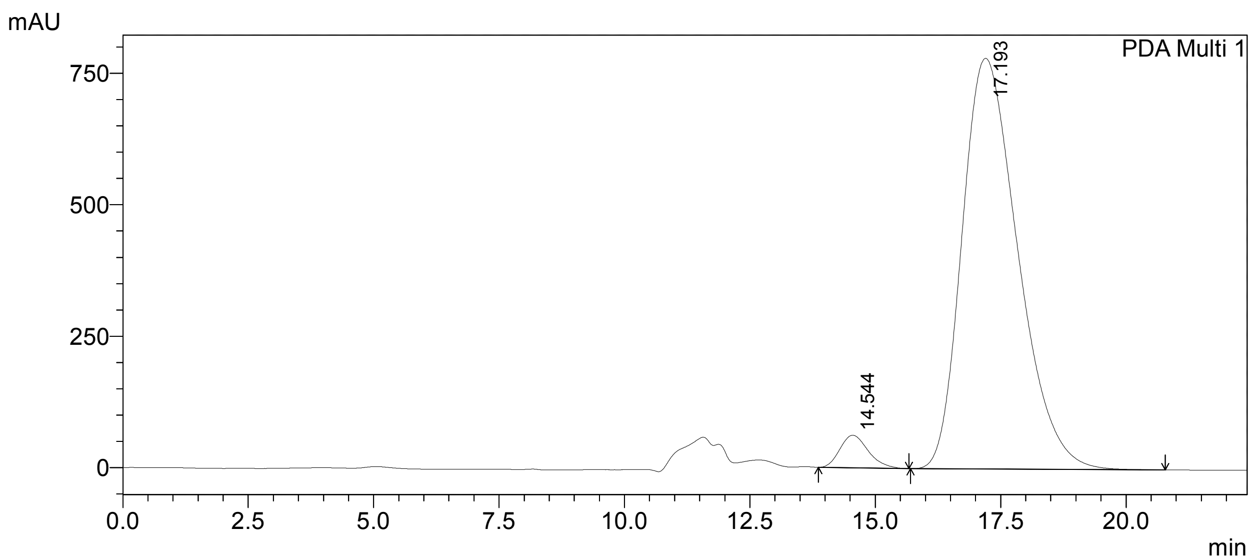

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.544	2433157	61887	3.872	7.340
2	17.193	60402967	781272	96.128	92.660
Total		62836124	843158	100.000	100.000

1b

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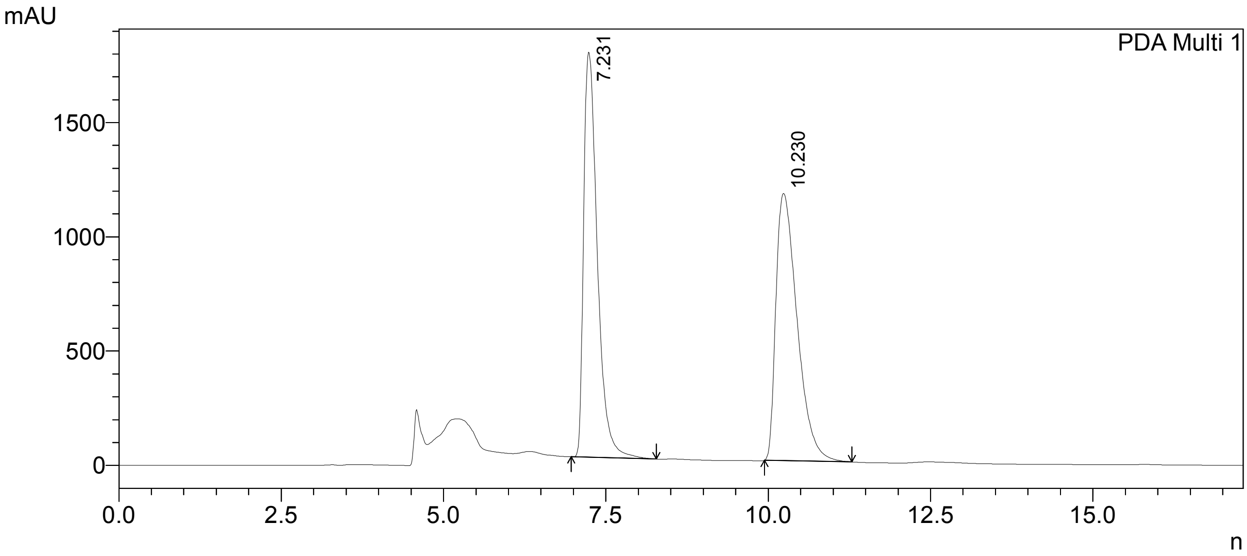

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.231	26089270	1772445	49.517	60.253
2	10.230	26598037	1169216	50.483	39.747
Total		52687308	2941662	100.000	100.000

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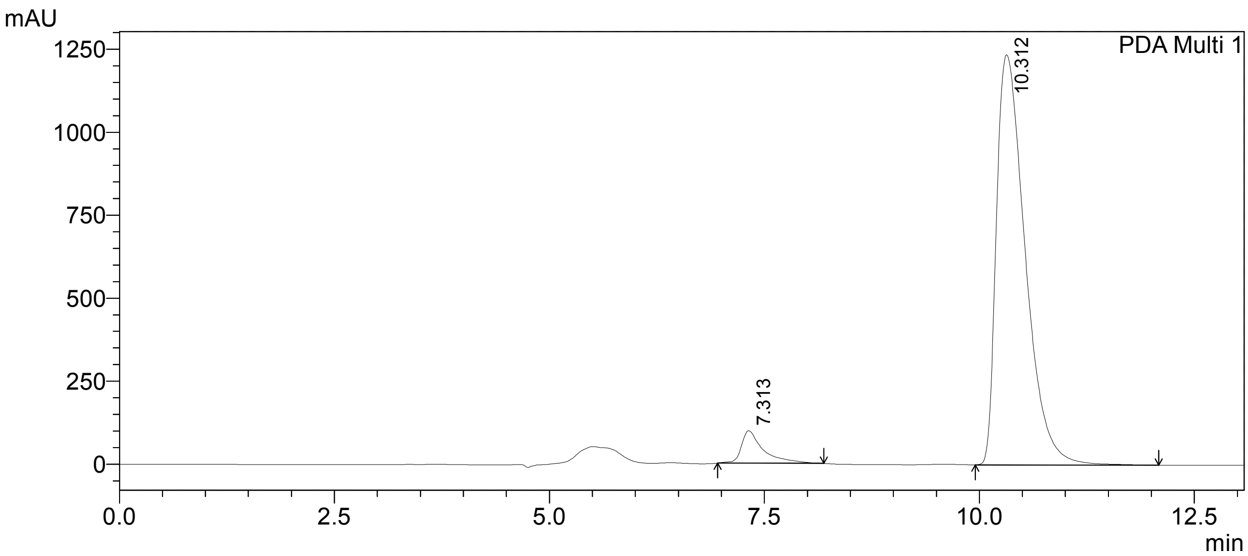

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.313	1742706	97838	5.713	7.337
2	10.312	28763911	1235626	94.287	92.663
Total		30506617	1333464	100.000	100.000

5b

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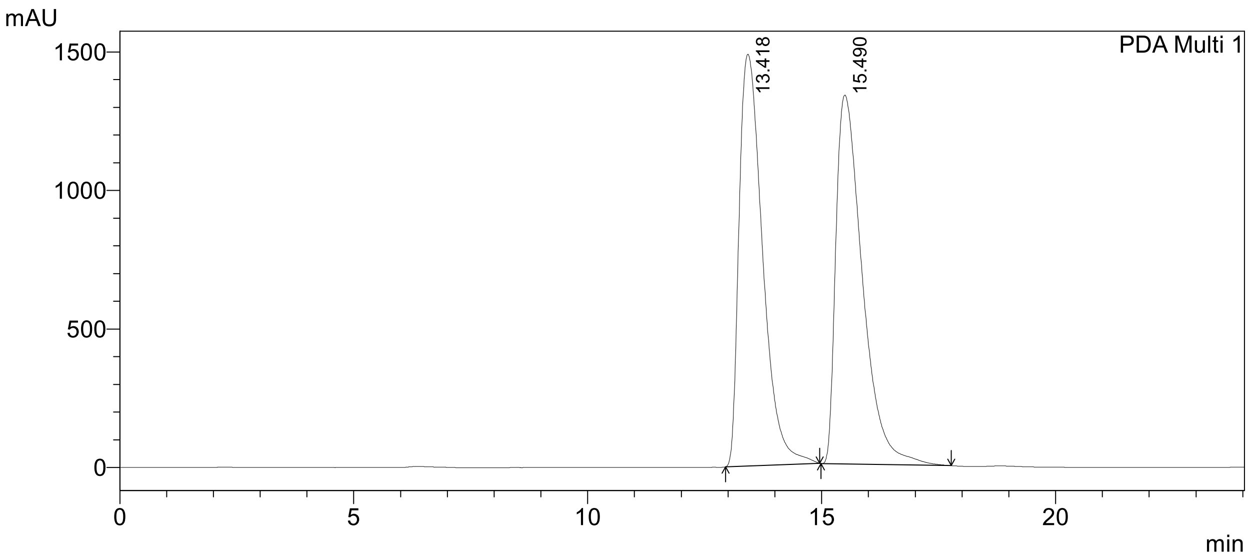

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.418	52008345	1486007	49.746	52.734
2	15.490	52540227	1331918	50.254	47.266
Total		104548572	2817925	100.000	100.000

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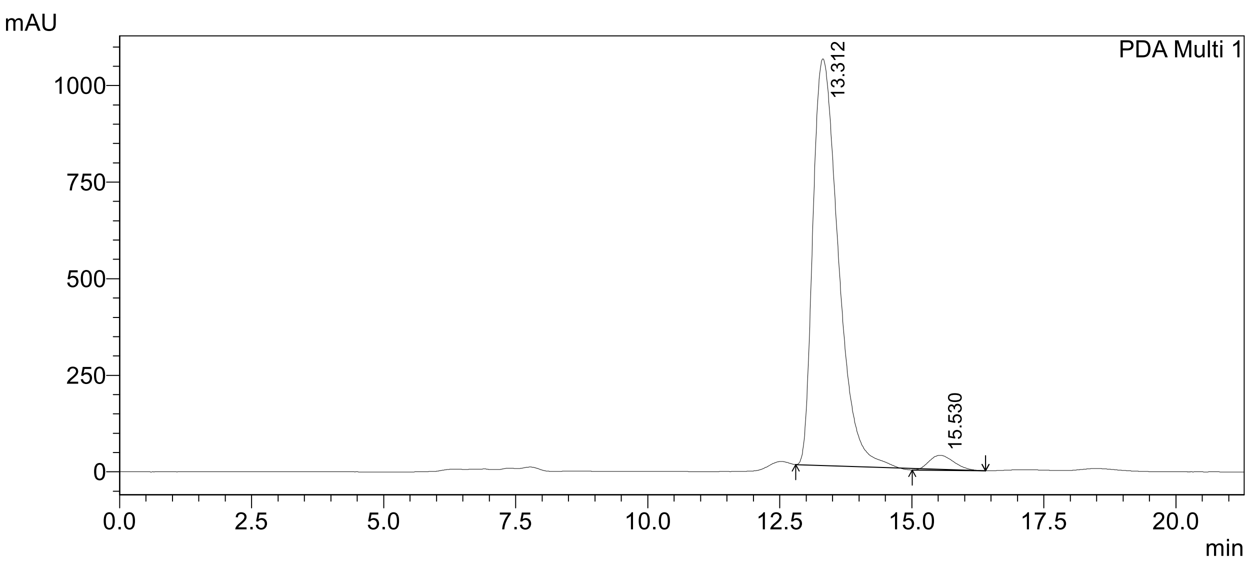

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.312	35106062	1052275	96.449	96.431
2	15.530	1292648	38940	3.551	3.569
Total		36398710	1091216	100.000	100.000

1b

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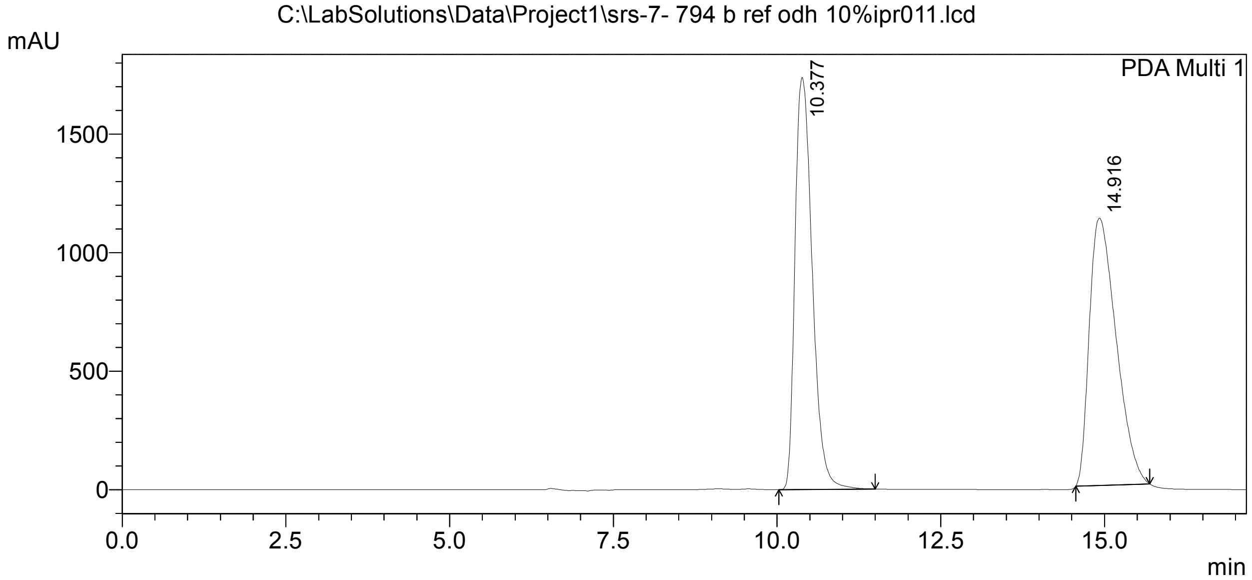

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.377	31942172	1738140	49.810	60.630
2	14.916	32186004	1128662	50.190	39.370
Total		64128176	2866802	100.000	100.000

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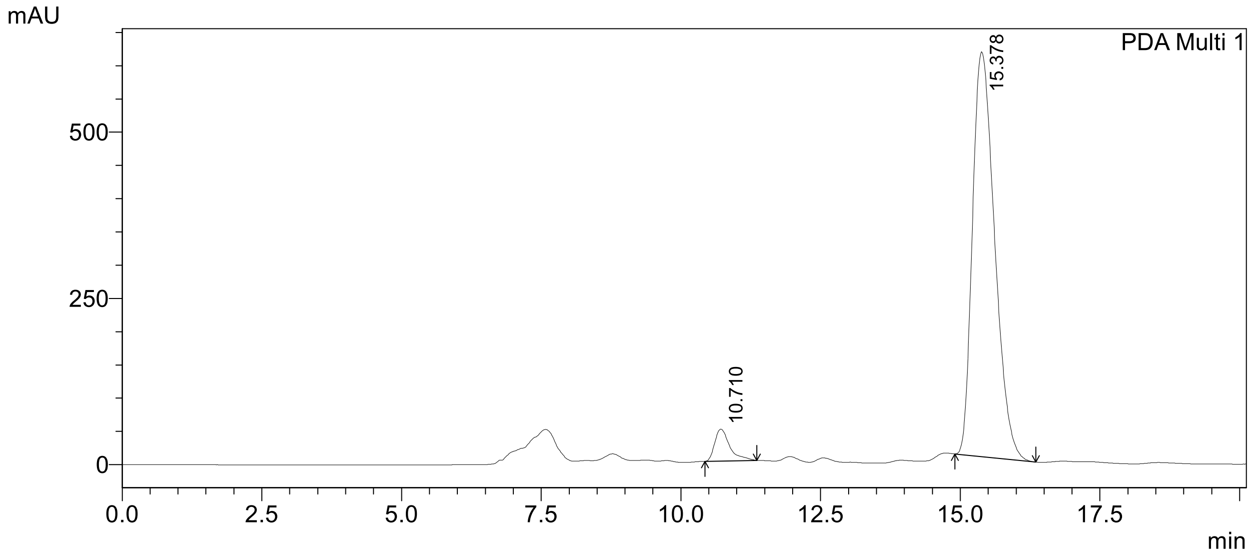

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.710	902526	48196	5.099	7.336
2	15.378	16798035	608796	94.901	92.664
Total		17700561	656993	100.000	100.000

5c

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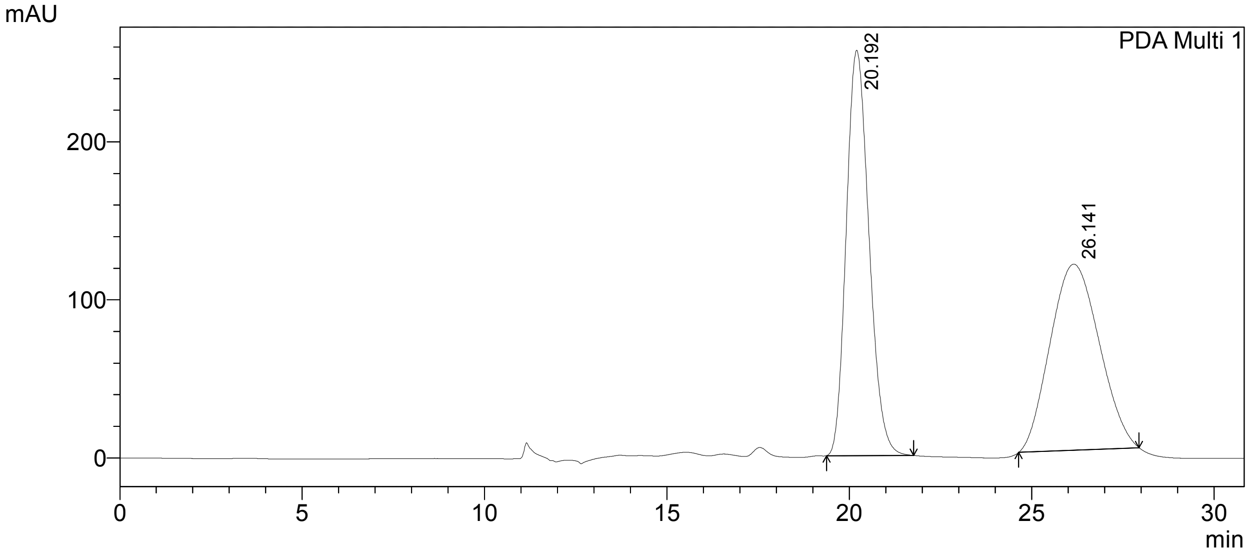

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.192	11131465	256491	50.235	68.529
2	26.141	11027220	117787	49.765	31.471
Total		22158685	374279	100.000	100.000

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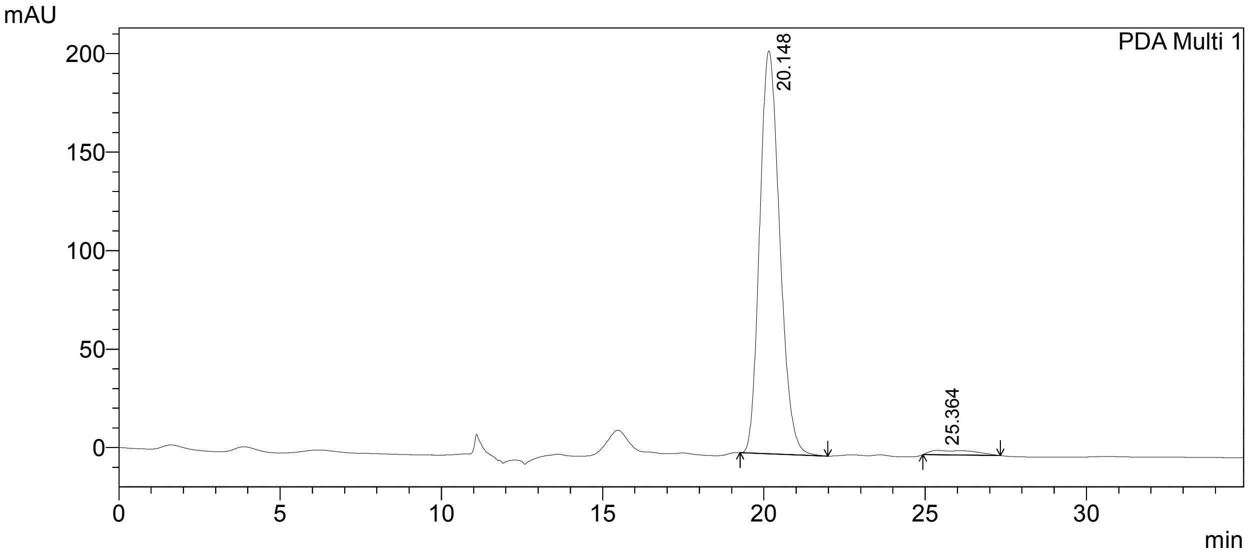

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.148	8855069	204455	97.517	98.914
2	25.364	225464	2245	2.483	1.086
Total		9080533	206699	100.000	100.000

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Sample Name : rs-2-370 prt c final

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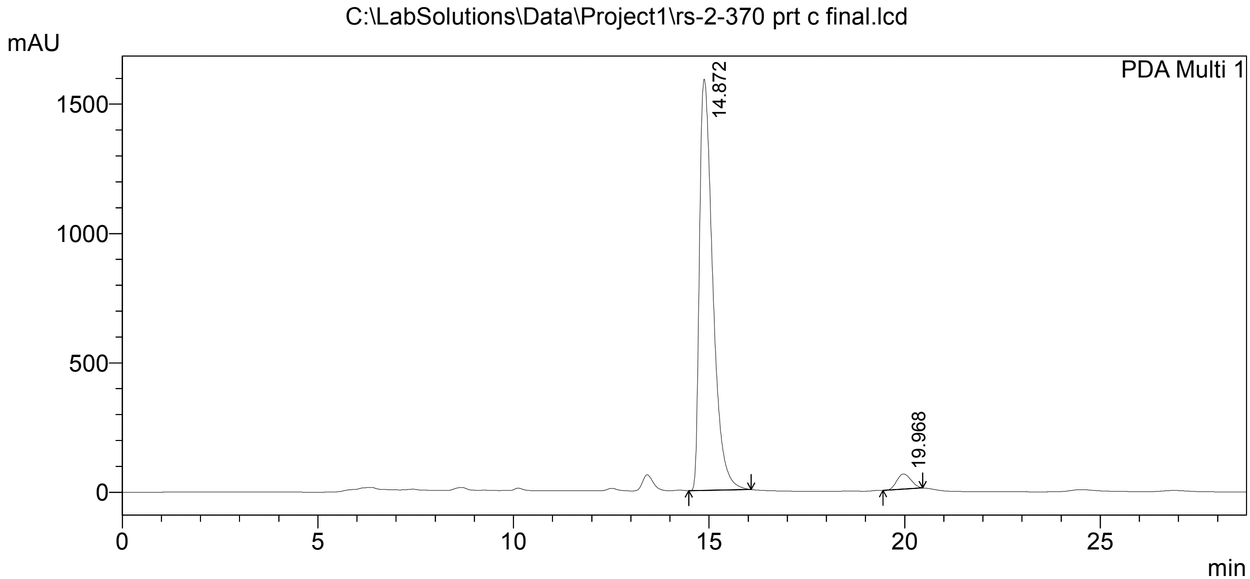

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.872	37609708	1590075	96.236	96.449
2	19.968	1471174	58537	3.764	3.551
Total		39080882	1648612	100.000	100.000

1b

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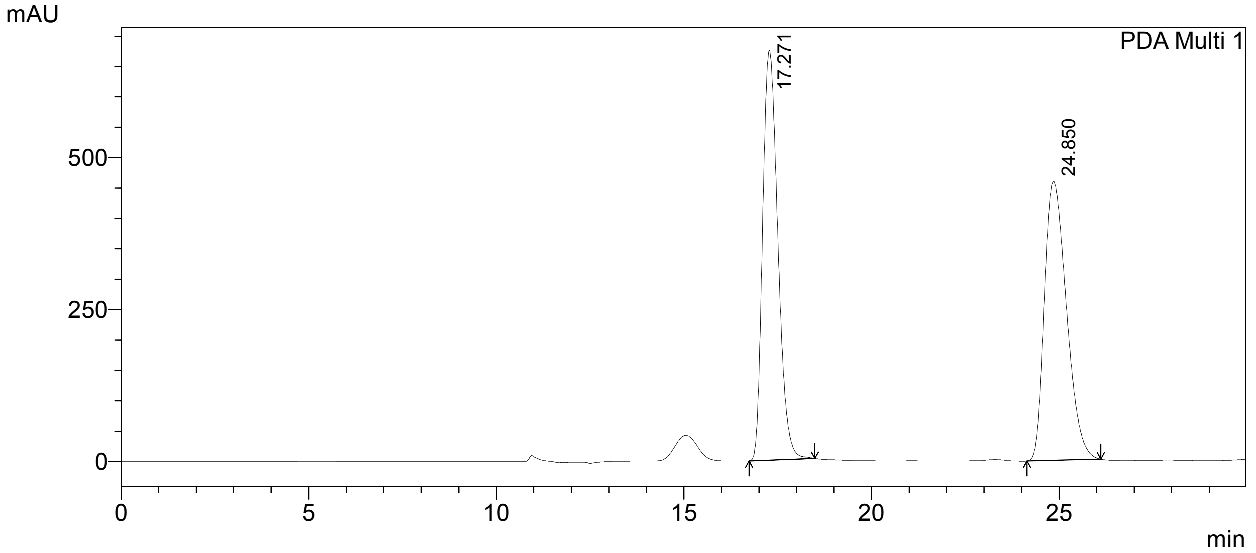

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.271	18958640	674279	50.127	59.478
2	24.850	18862778	459374	49.873	40.522
Total		37821418	1133653	100.000	100.000

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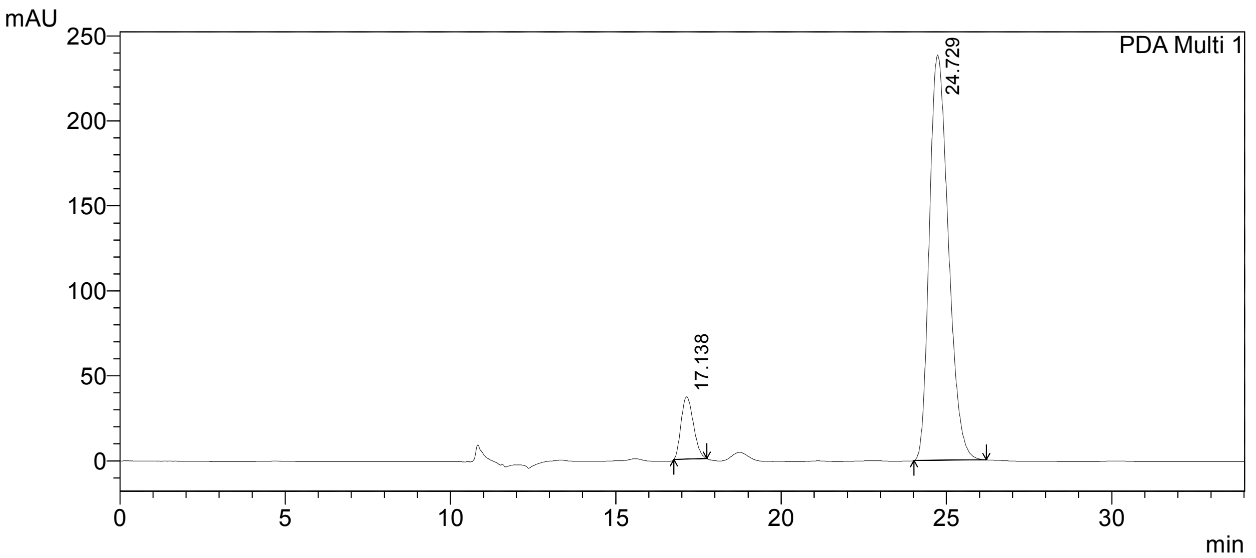

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.138	954272	36682	9.086	13.334
2	24.729	9548608	238425	90.914	86.666
Total		10502880	275107	100.000	100.000

5d

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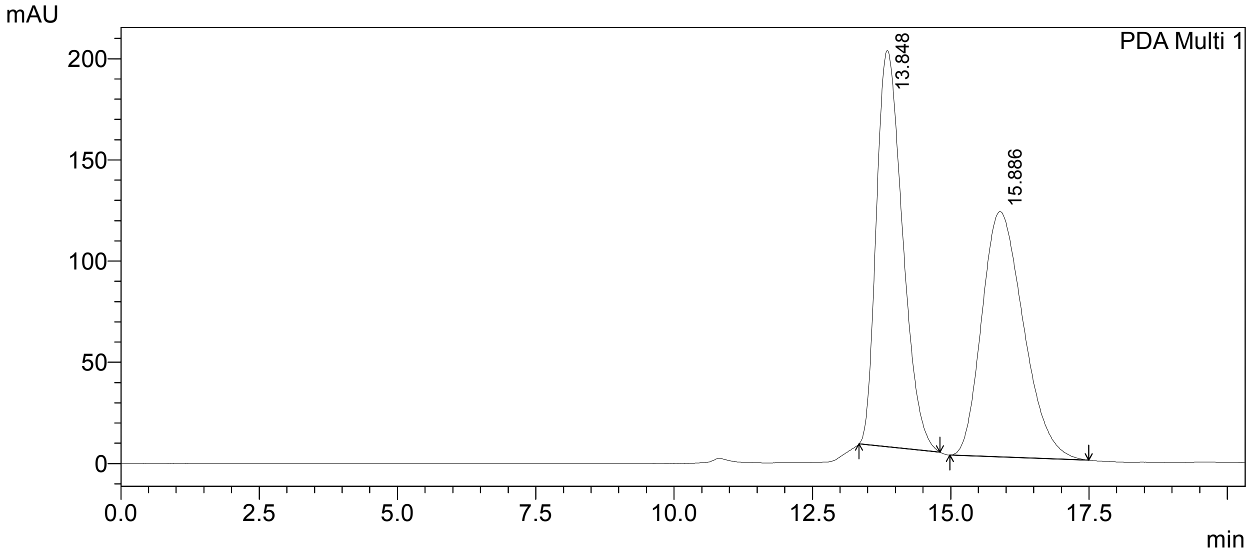

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.848	6459542	195687	50.444	61.750
2	15.886	6345730	121216	49.556	38.250
Total		12805273	316903	100.000	100.000

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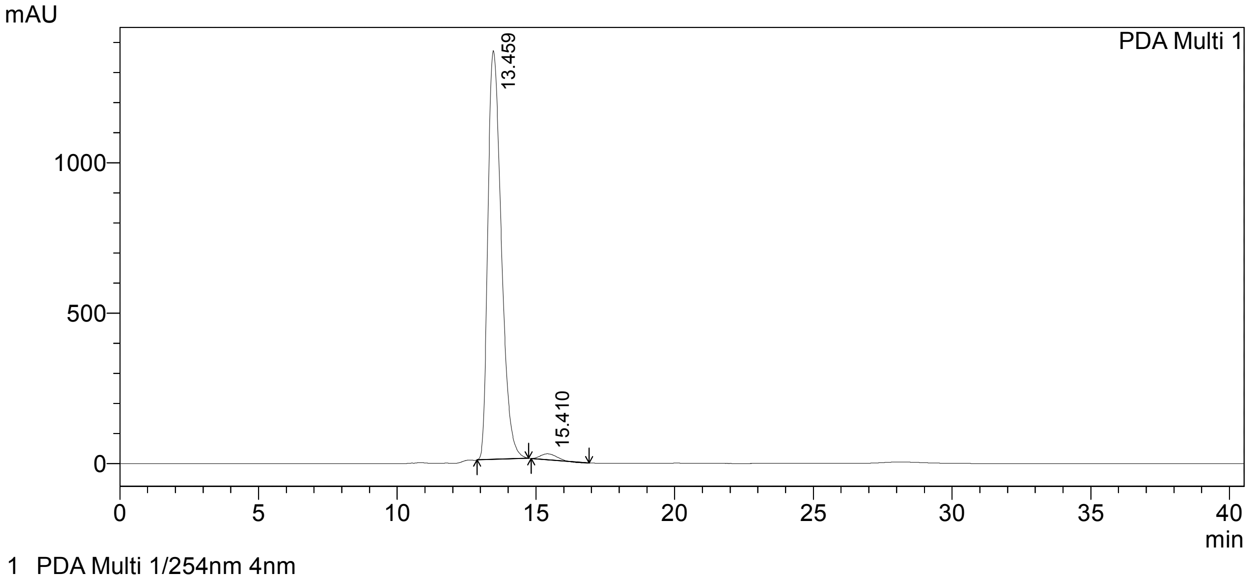

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.459	45762050	1358767	98.394	98.580
2	15.410	746867	19568	1.606	1.420
Total		46508917	1378335	100.000	100.000

1b

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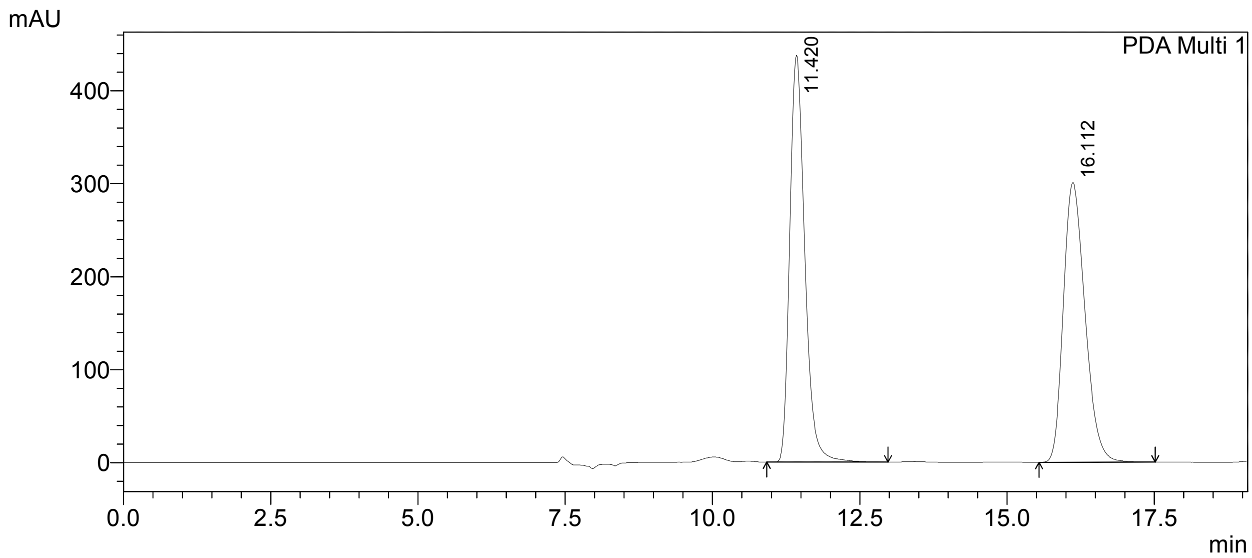

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.420	7798366	437529	50.358	59.253
2	16.112	7687439	300879	49.642	40.747
Total		15485805	738408	100.000	100.000

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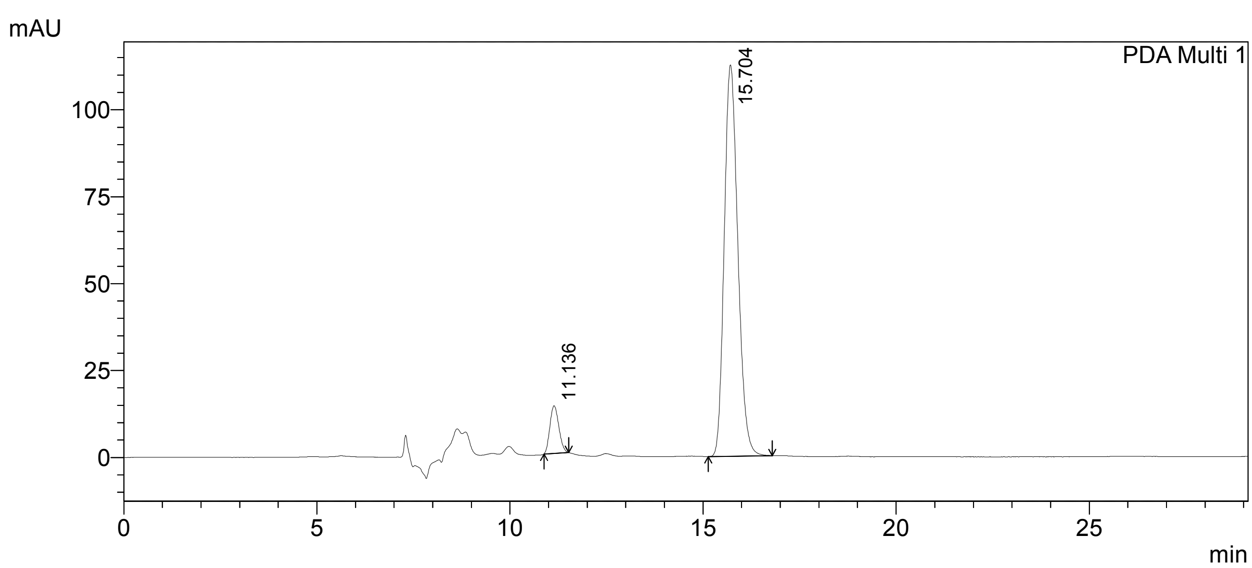

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.136	220820	13672	7.406	10.831
2	15.704	2760768	112555	92.594	89.169
Total		2981588	126227	100.000	100.000

5e

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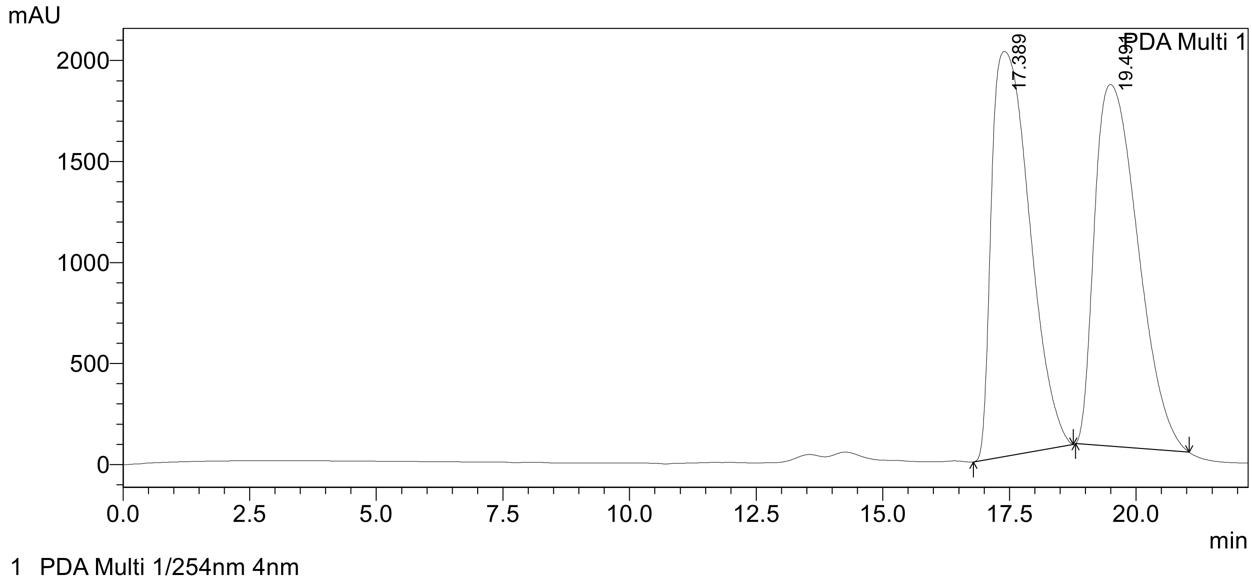

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.389	105162585	2005464	49.608	52.825
2	19.491	106823489	1790977	50.392	47.175
Total		211986074	3796441	100.000	100.000

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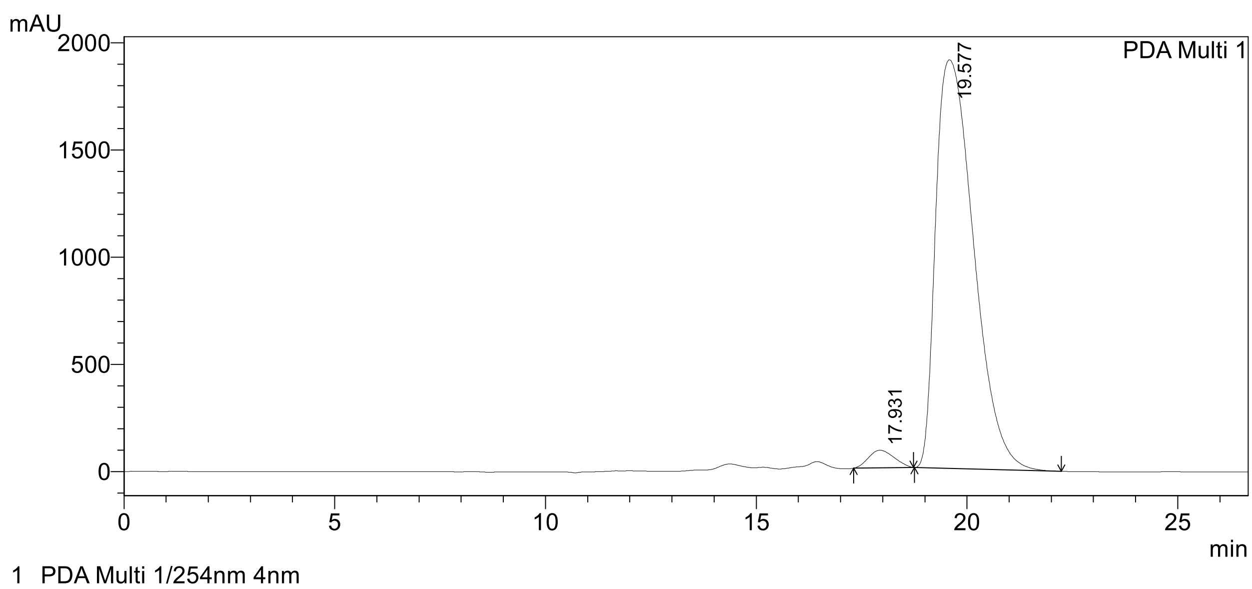

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.931	3446148	82357	2.797	4.140
2	19.577	119741785	1906799	97.203	95.860
Total		123187933	1989156	100.000	100.000

1b

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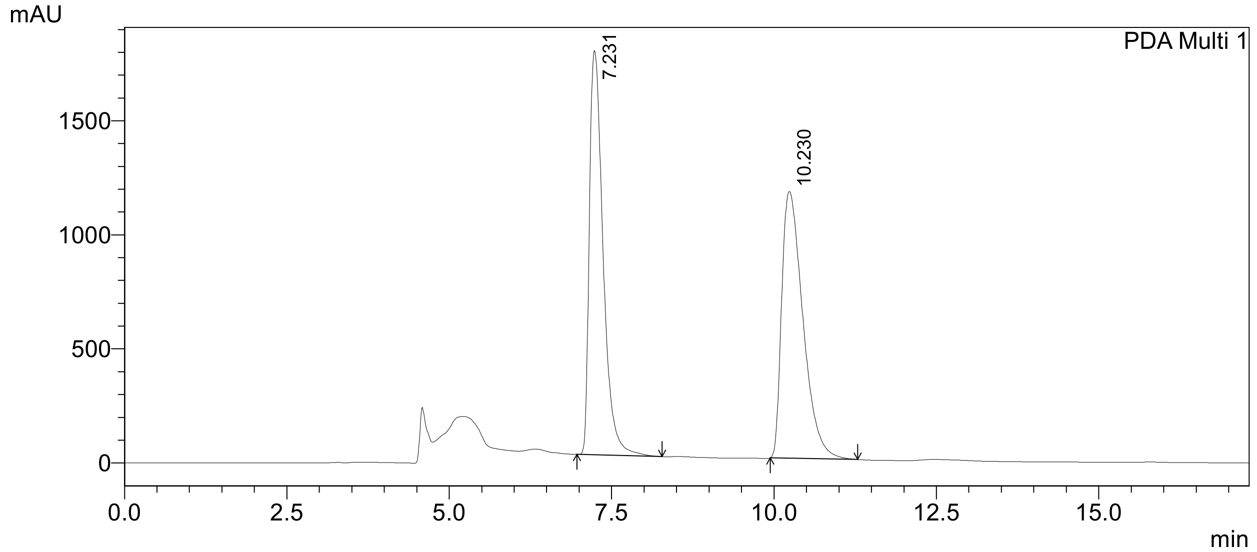

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.231	26089270	1772445	49.517	60.253
2	10.230	26598037	1169216	50.483	39.747
Total		52687308	2941662	100.000	100.000

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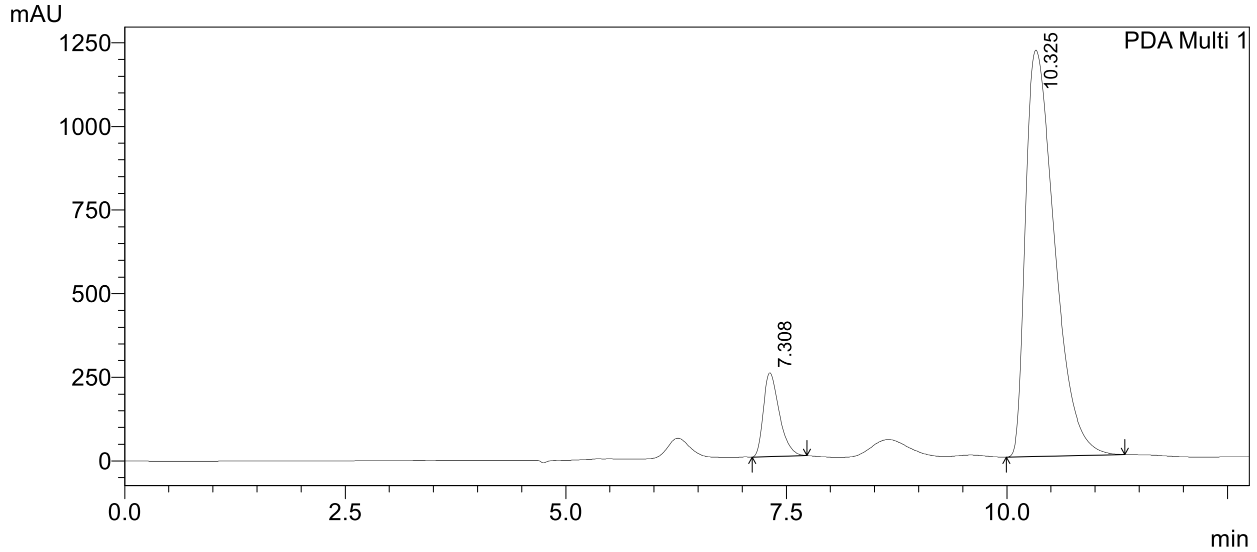

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.308	3145344	250549	10.112	17.103
2	10.325	27958366	1214421	89.888	82.897
Total		31103710	1464970	100.000	100.000

5f

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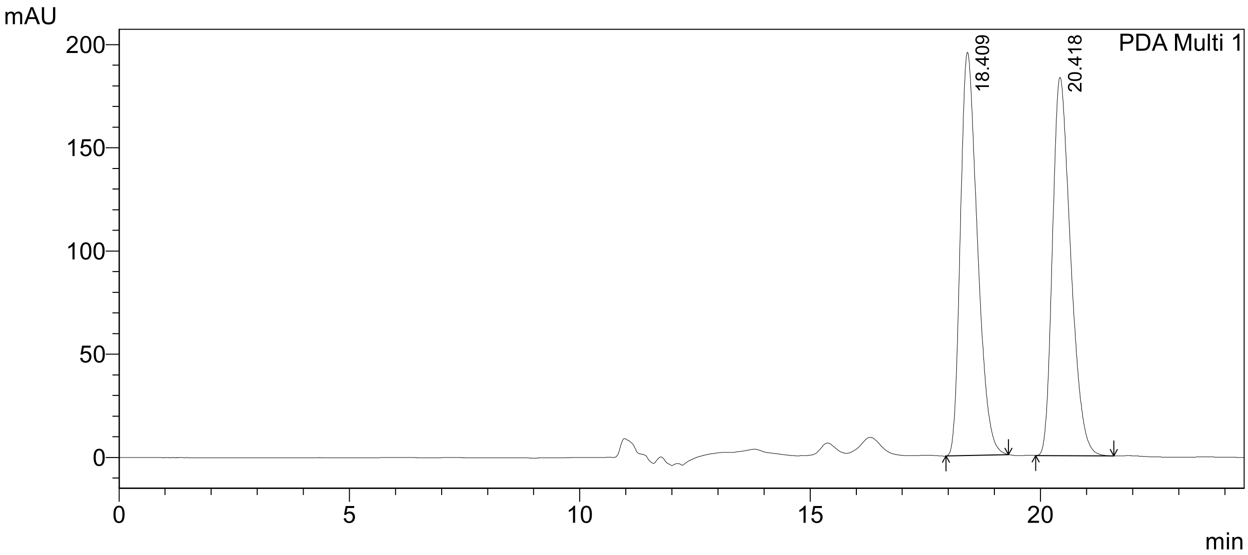


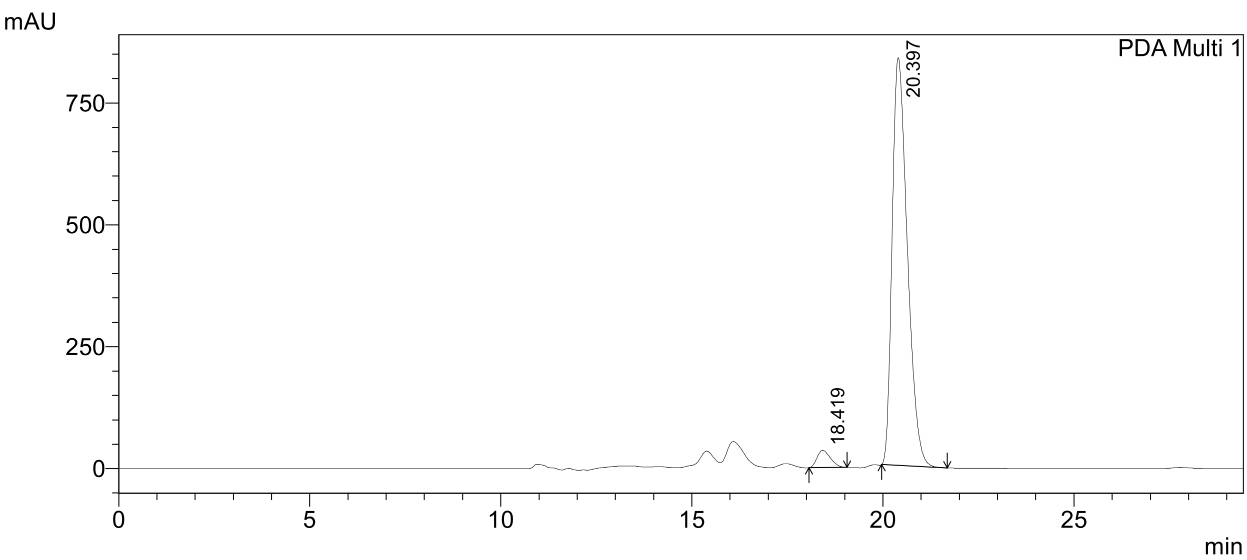
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.409	5013677	195249	49.904	51.579
2	20.418	5033050	183297	50.096	48.421
Total		10046727	378546	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

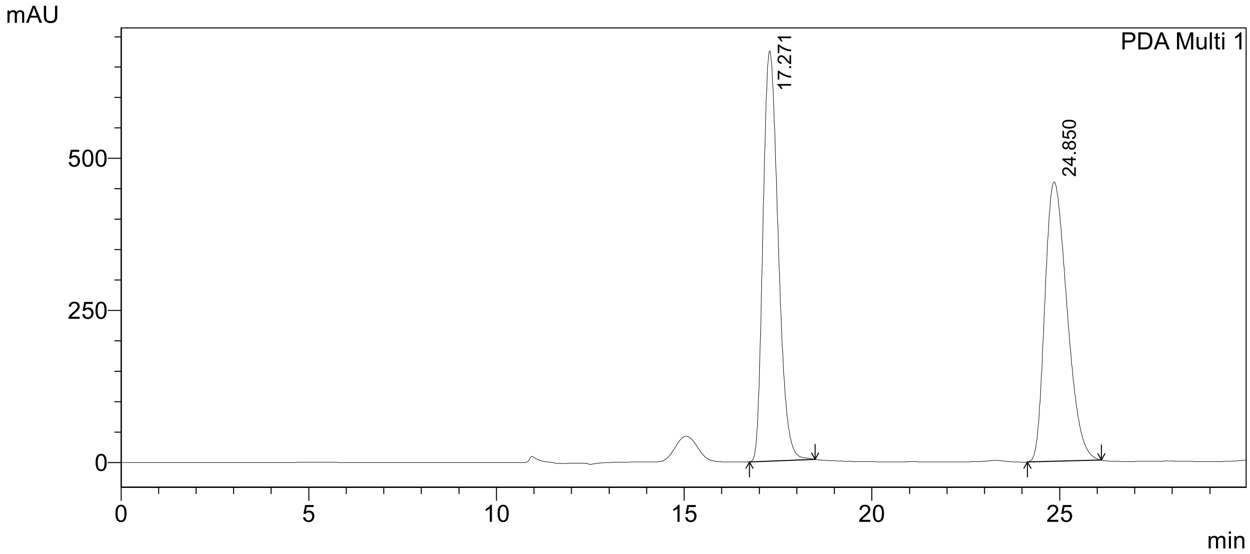
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.419	870514	35639	3.627	4.088
2	20.397	23129703	836137	96.373	95.912
Total		24000218	871776	100.000	100.000

1b

<Chromatogram>



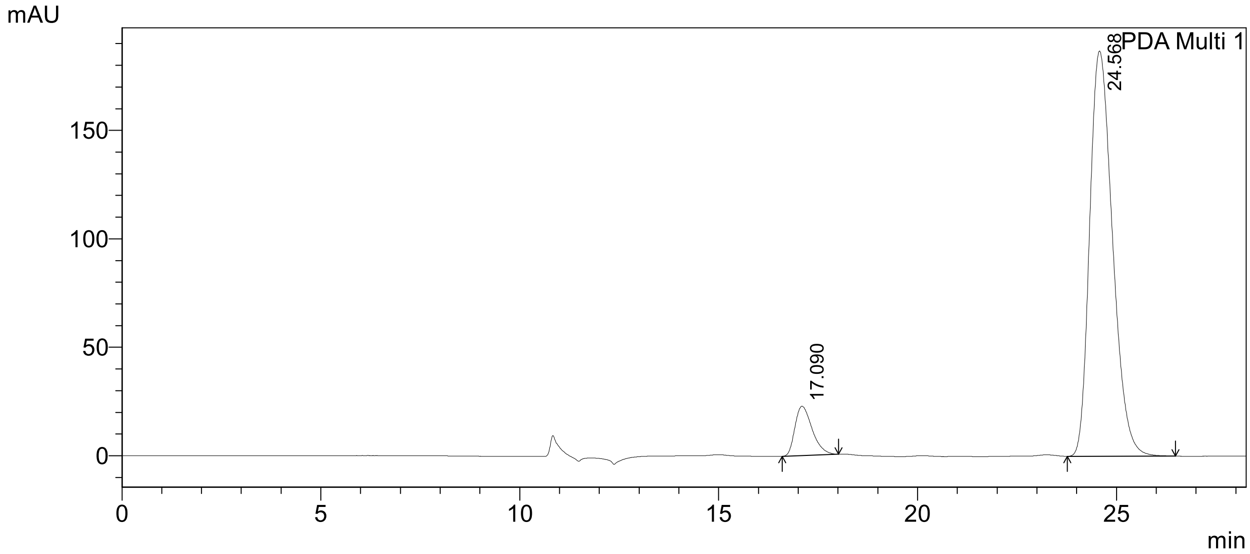
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.271	18958640	674279	50.127	59.478
2	24.850	18862778	459374	49.873	40.522
Total		37821418	1133653	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

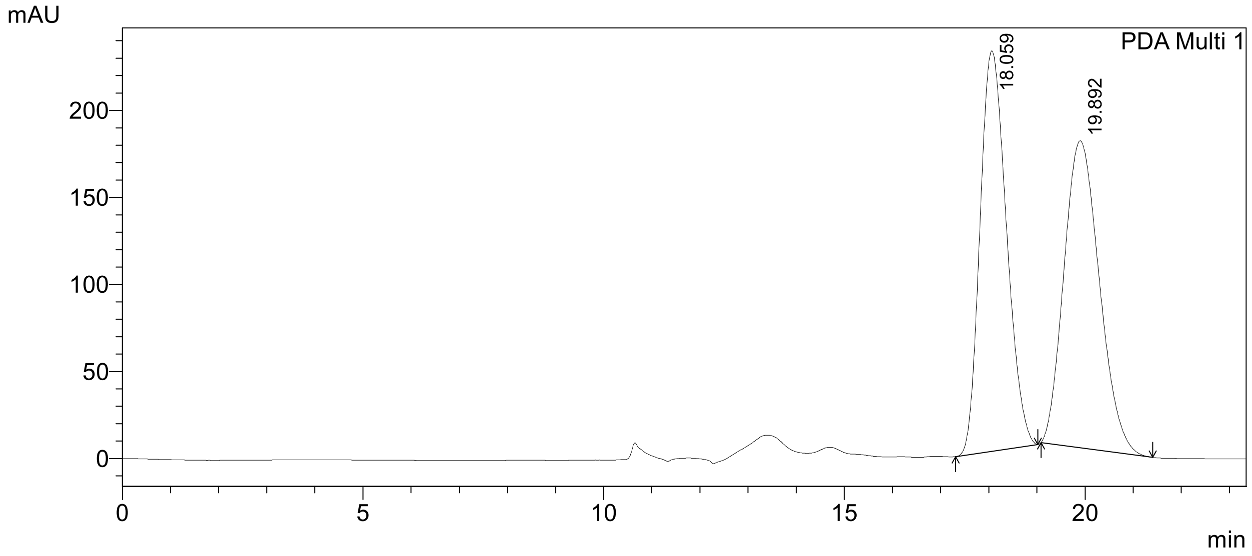
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.090	686679	22760	8.408	10.858
2	24.568	7479913	186858	91.592	89.142
Total		8166592	209618	100.000	100.000

5g

<Chromatogram>



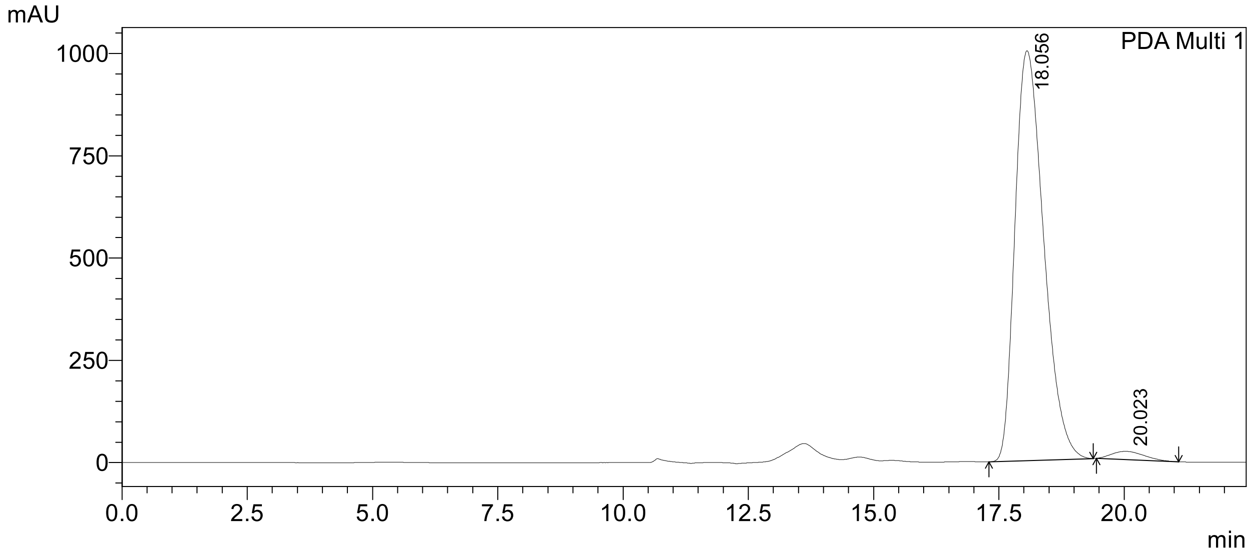
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.059	8814243	230016	49.417	56.600
2	19.892	9022313	176371	50.583	43.400
Total		17836556	406387	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.056	39949816	1002137	97.776	98.037
2	20.023	908766	20066	2.224	1.963
Total		40858582	1022204	100.000	100.000

1b

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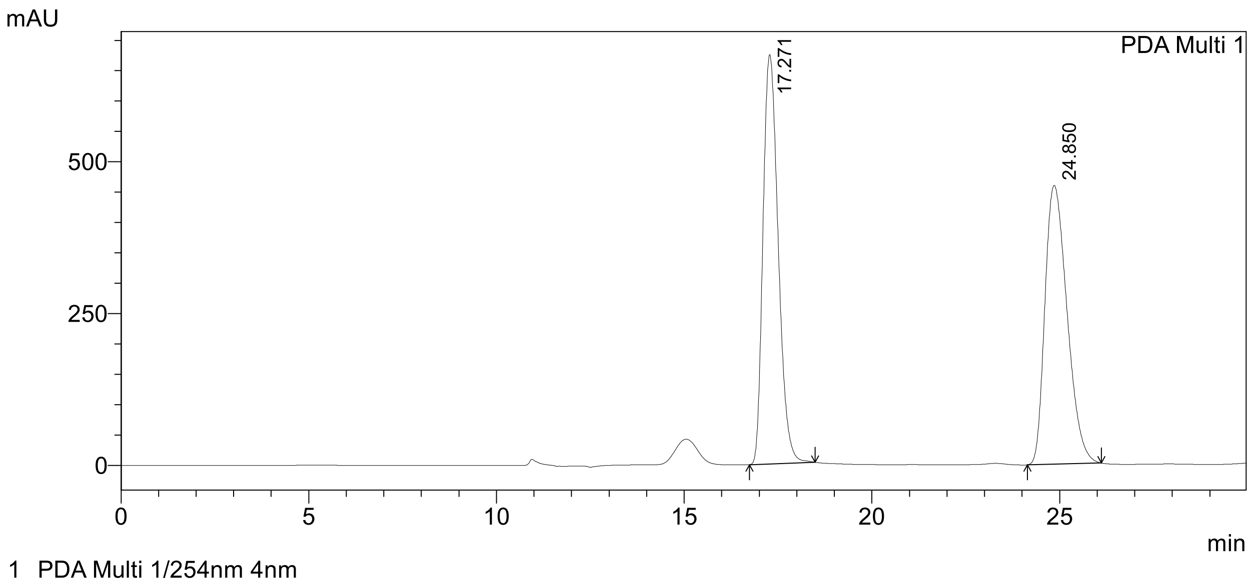

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.271	18958640	674279	50.127	59.478
2	24.850	18862778	459374	49.873	40.522
Total		37821418	1133653	100.000	100.000

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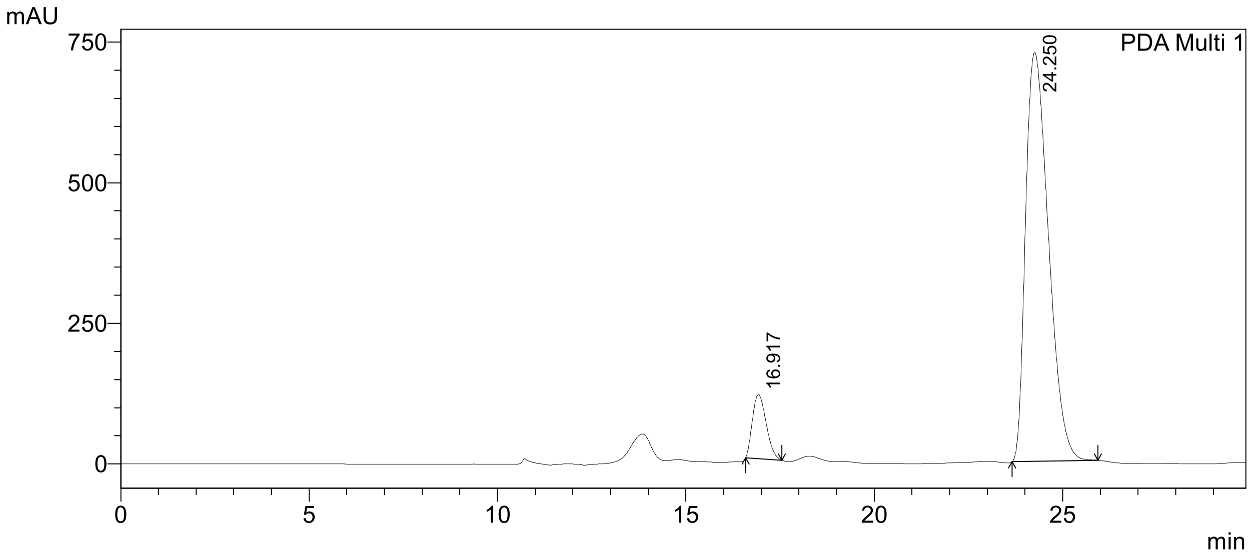

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.917	2901997	113836	8.631	13.540
2	24.250	30721397	726925	91.369	86.460
Total		33623394	840761	100.000	100.000

5h

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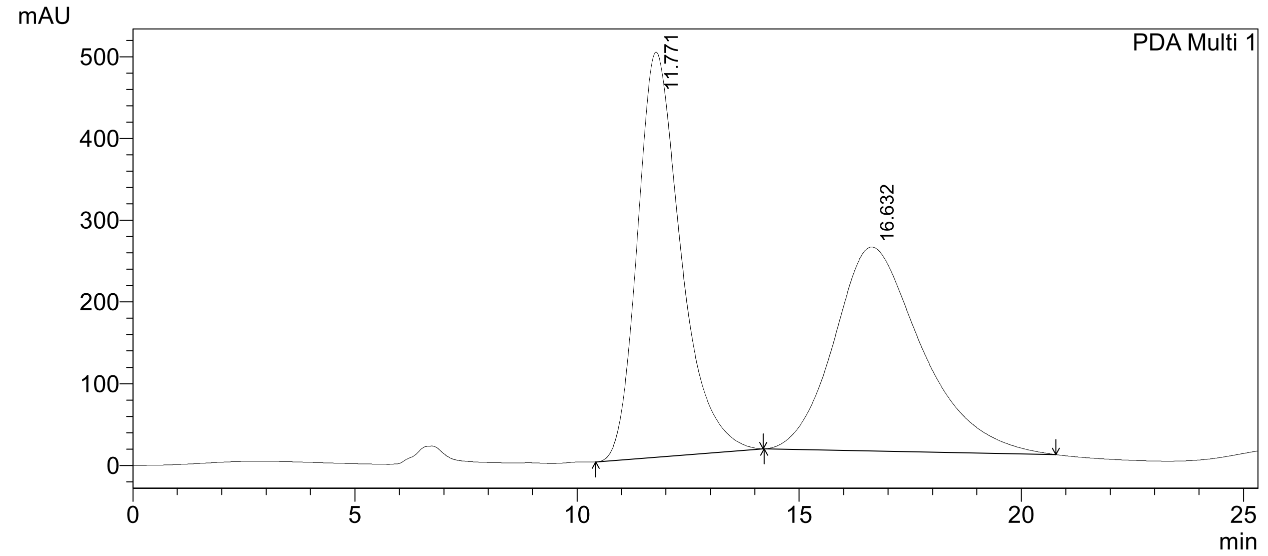


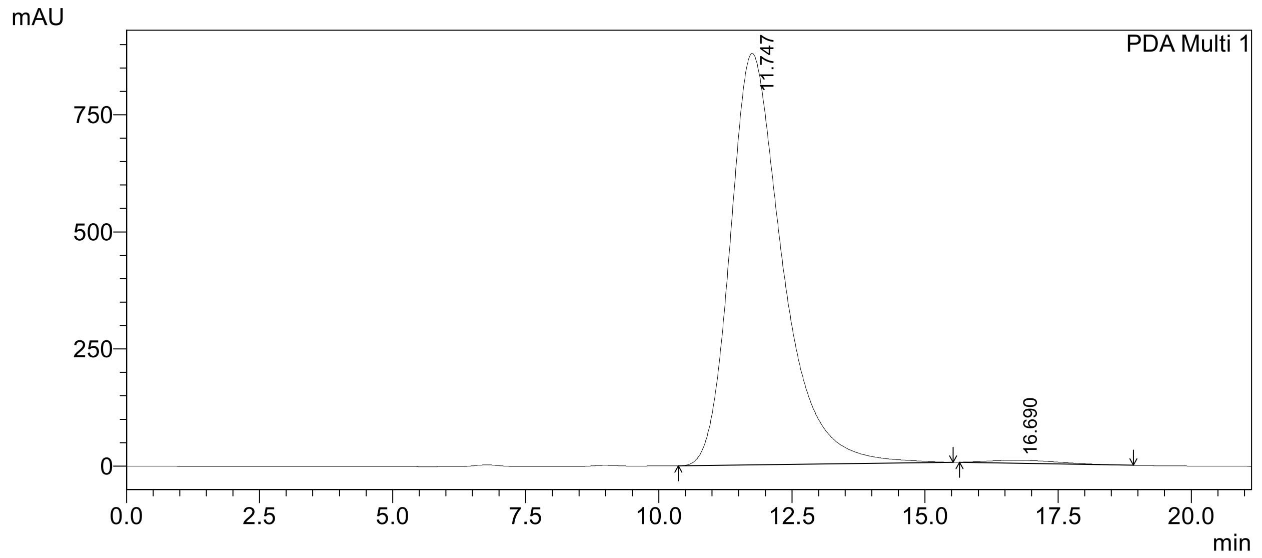
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.771	33787977	495700	49.659	66.527
2	16.632	34251614	249415	50.341	33.473
Total		68039591	745115	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.747	60303928	878479	99.033	99.283
2	16.690	589082	6340	0.967	0.717
Total		60893009	884820	100.000	100.000

1b

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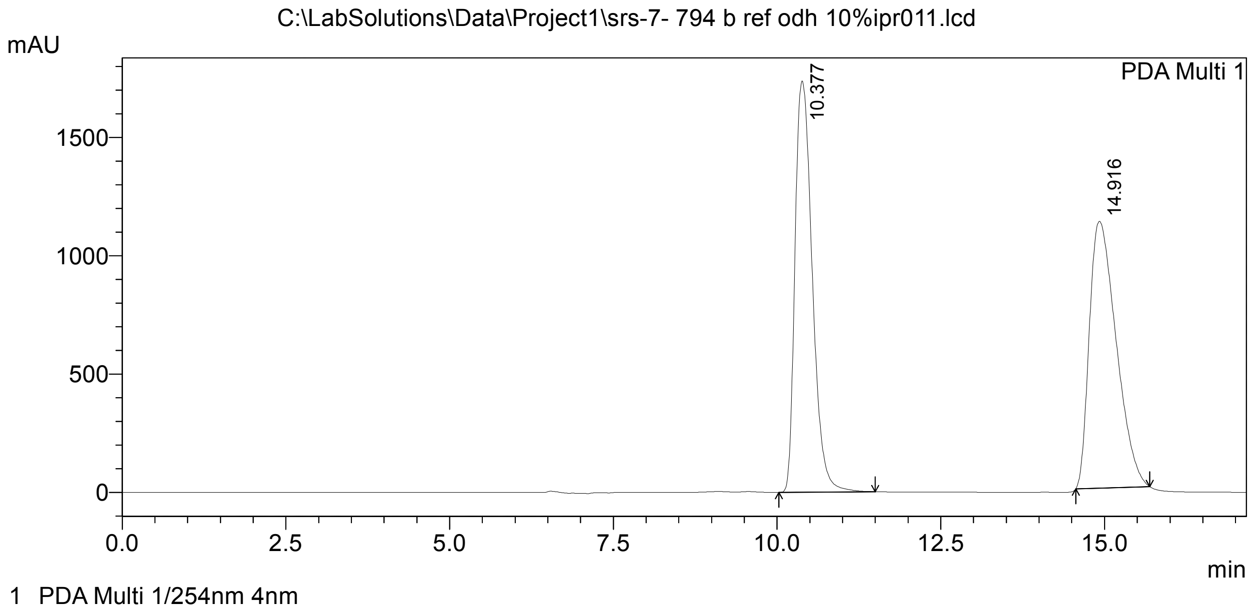

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.377	31942172	1738140	49.810	60.630
2	14.916	32186004	1128662	50.190	39.370
Total		64128176	2866802	100.000	100.000

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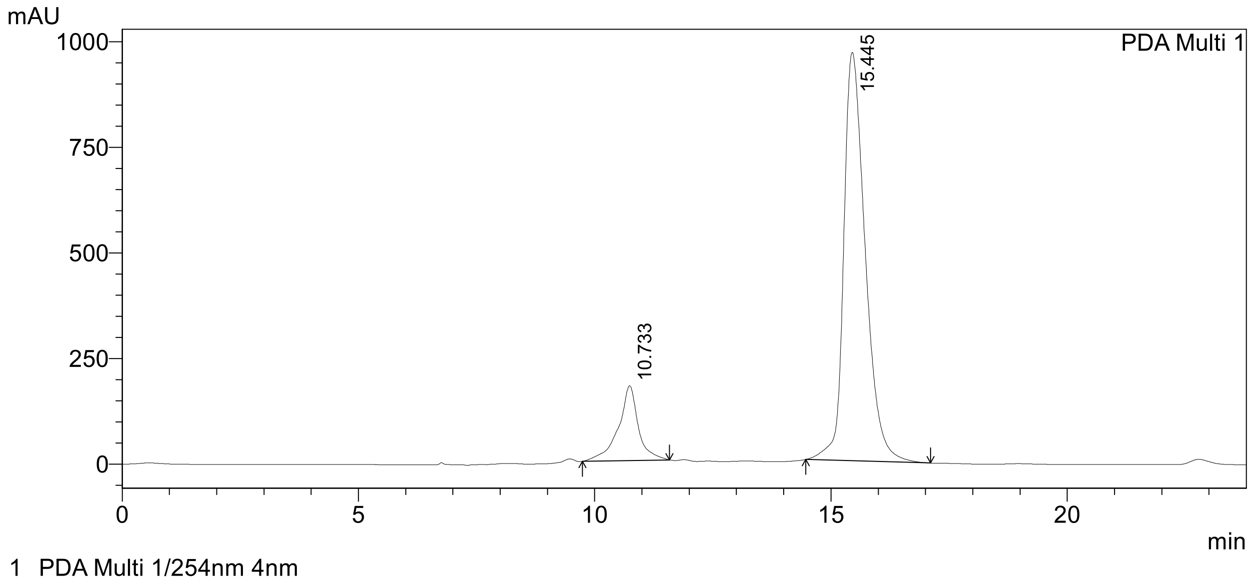

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.733	5222002	177377	14.533	15.493
2	15.445	30708885	967512	85.467	84.507
Total		35930888	1144889	100.000	100.000

5i

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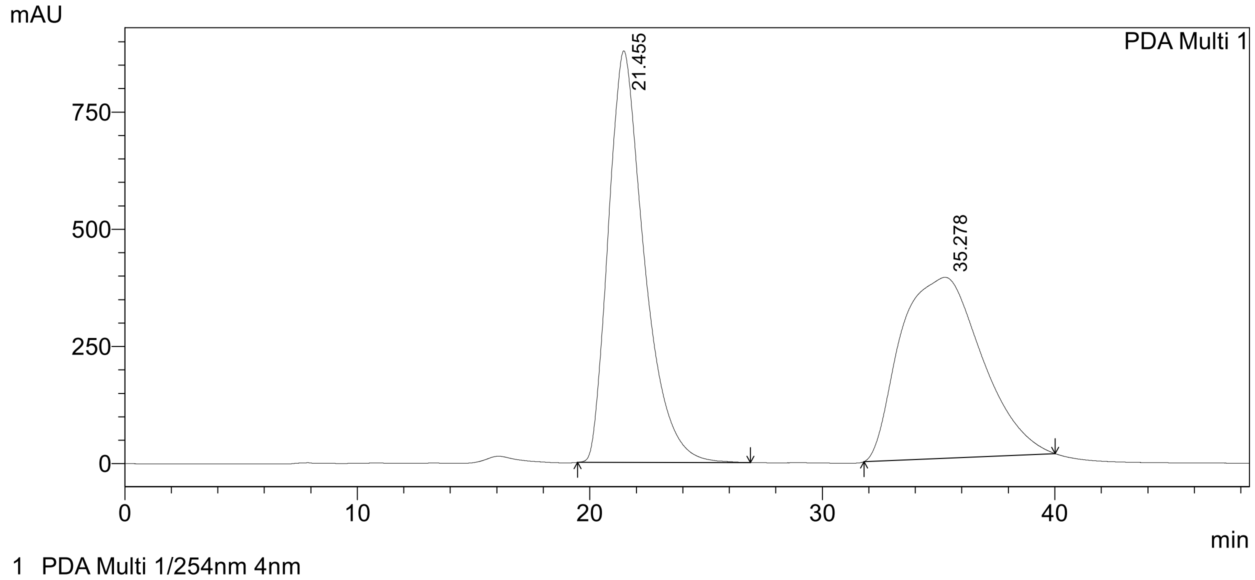

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.455	94365214	877835	49.988	69.465
2	35.278	94410770	385869	50.012	30.535
Total		188775984	1263704	100.000	100.000

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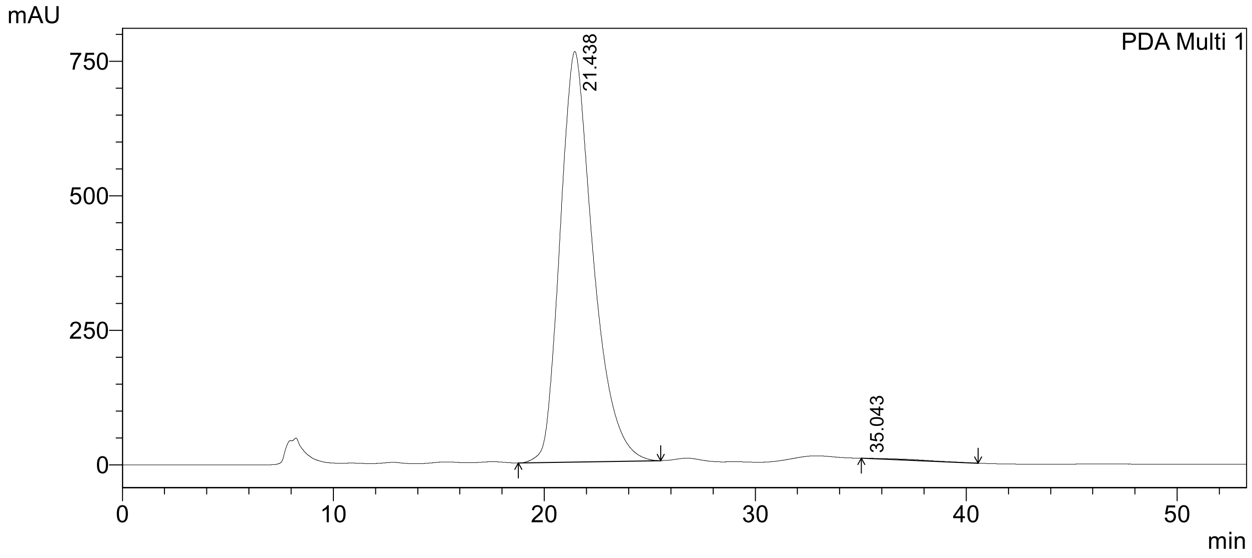

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.438	83256759	763282	99.716	99.998
2	35.043	237325	13	0.284	0.002
Total		83494084	763295	100.000	100.000

1f

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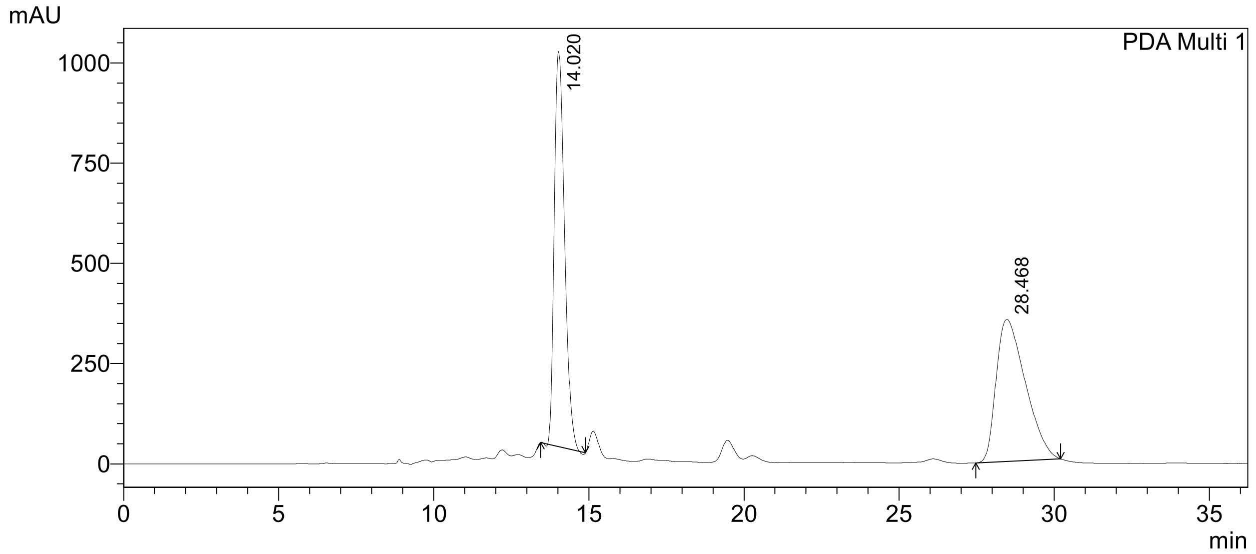

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.020	22748450	985525	49.482	73.558
2	28.468	23224648	354266	50.518	26.442
Total		45973098	1339792	100.000	100.000

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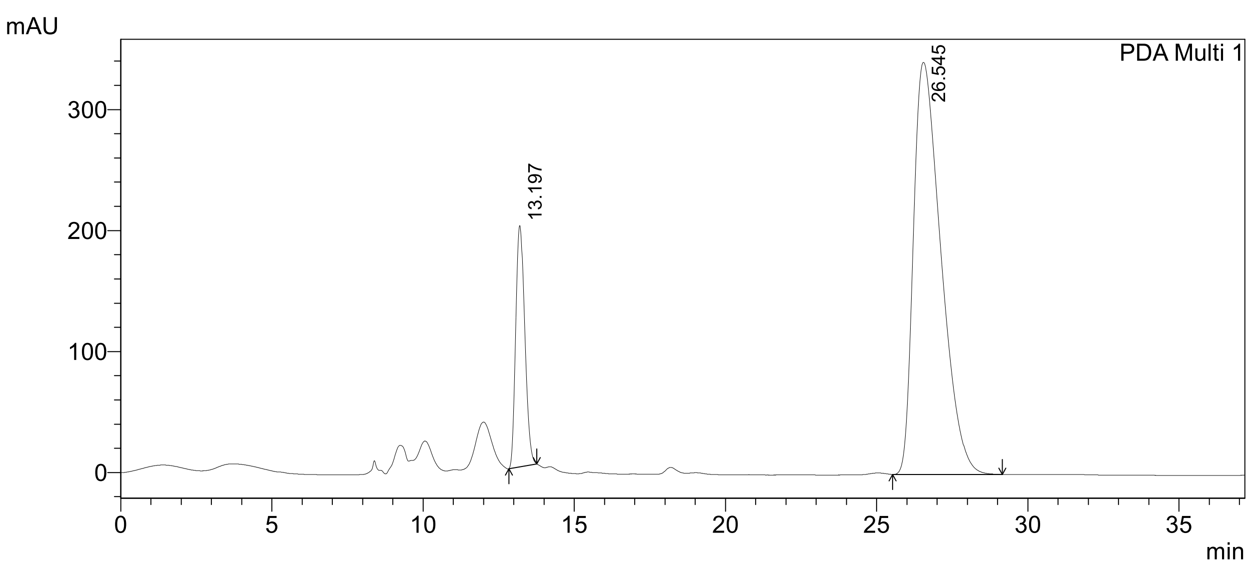

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.197	4111421	199464	16.067	36.937
2	26.545	21478532	340553	83.933	63.063
Total		25589953	540017	100.000	100.000

5j

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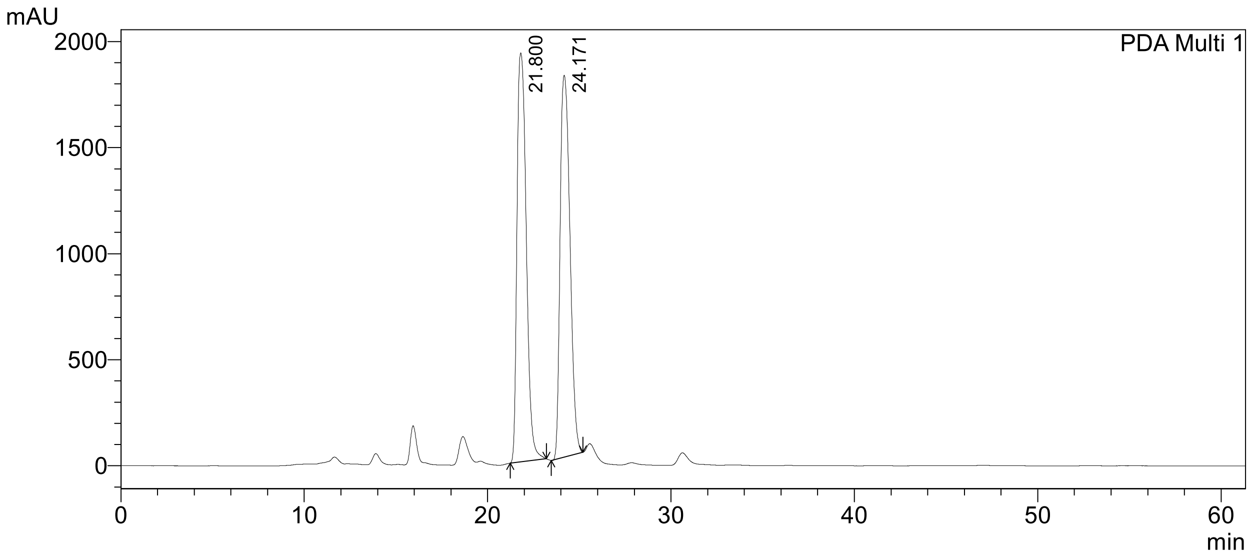

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.800	67872722	1928393	50.217	51.700
2	24.171	67285562	1801594	49.783	48.300
Total		135158285	3729987	100.000	100.000

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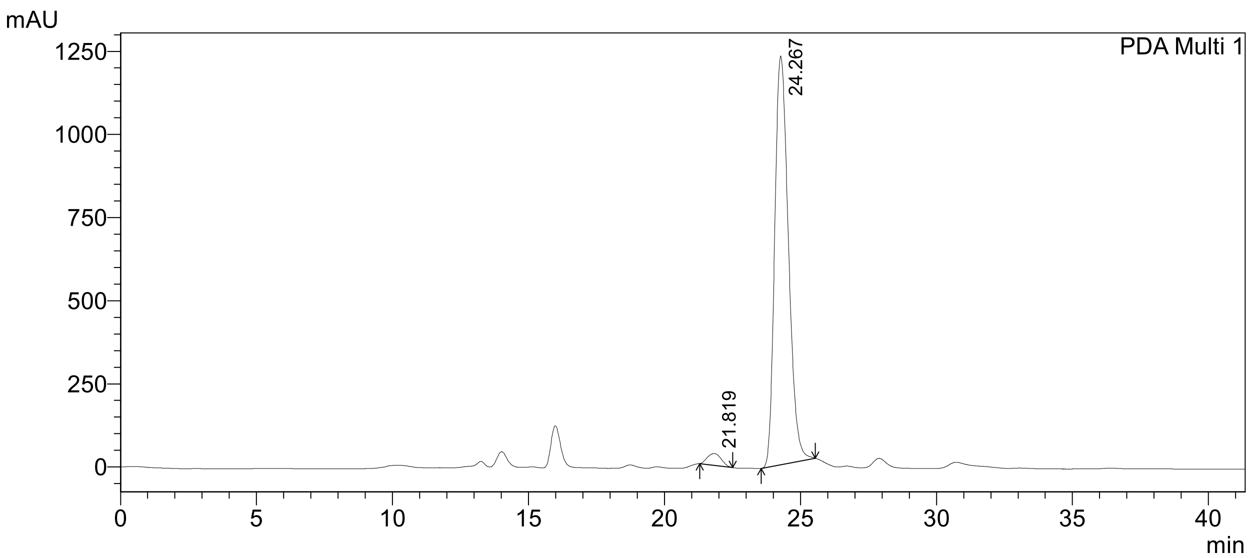

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.819	1251192	35317	2.823	2.793
2	24.267	43063472	1229095	97.177	97.207
Total		44314664	1264412	100.000	100.000

1j

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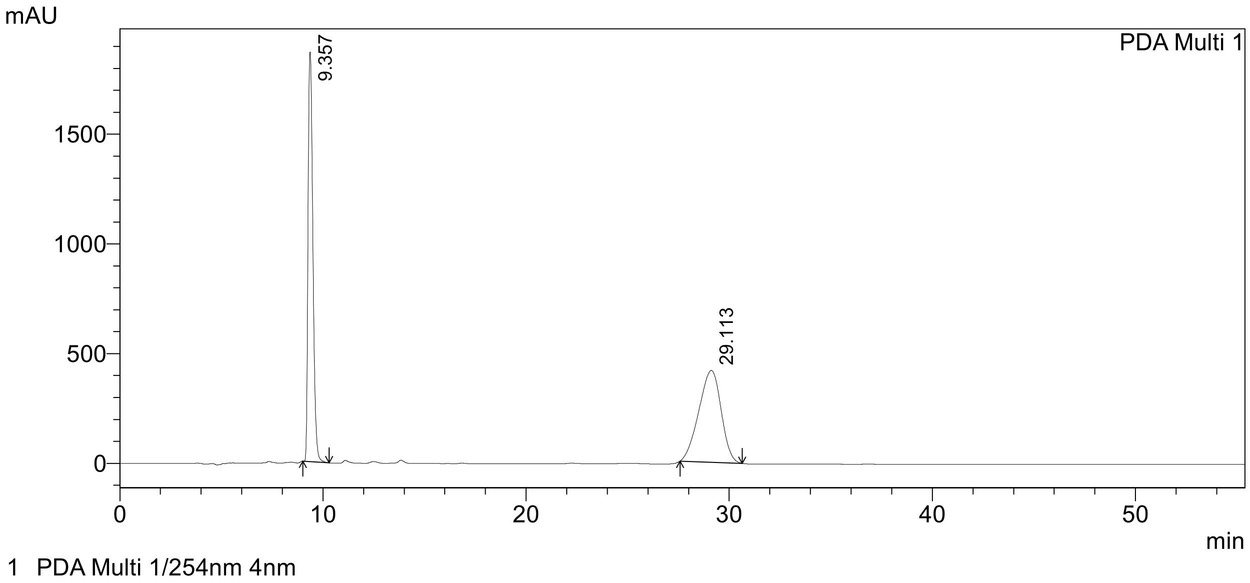

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.357	30828699	1867298	49.075	81.677
2	29.113	31990796	418893	50.925	18.323
Total		62819494	2286191	100.000	100.000

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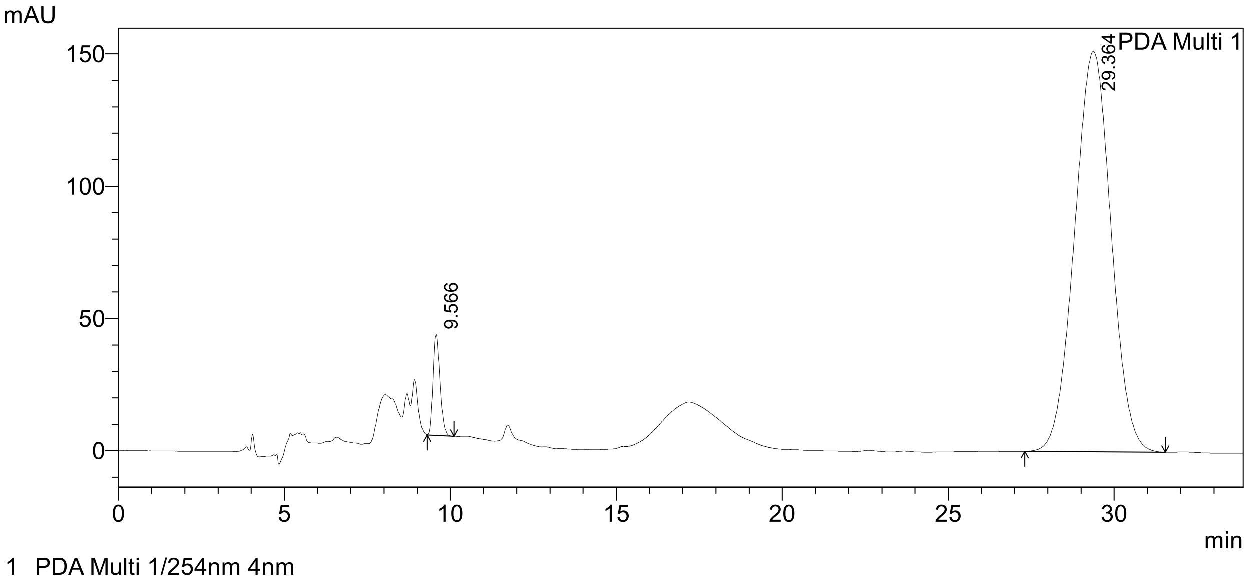

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.566	560389	38144	4.606	20.124
2	29.364	11605033	151397	95.394	79.876
Total		12165422	189541	100.000	100.000

5k

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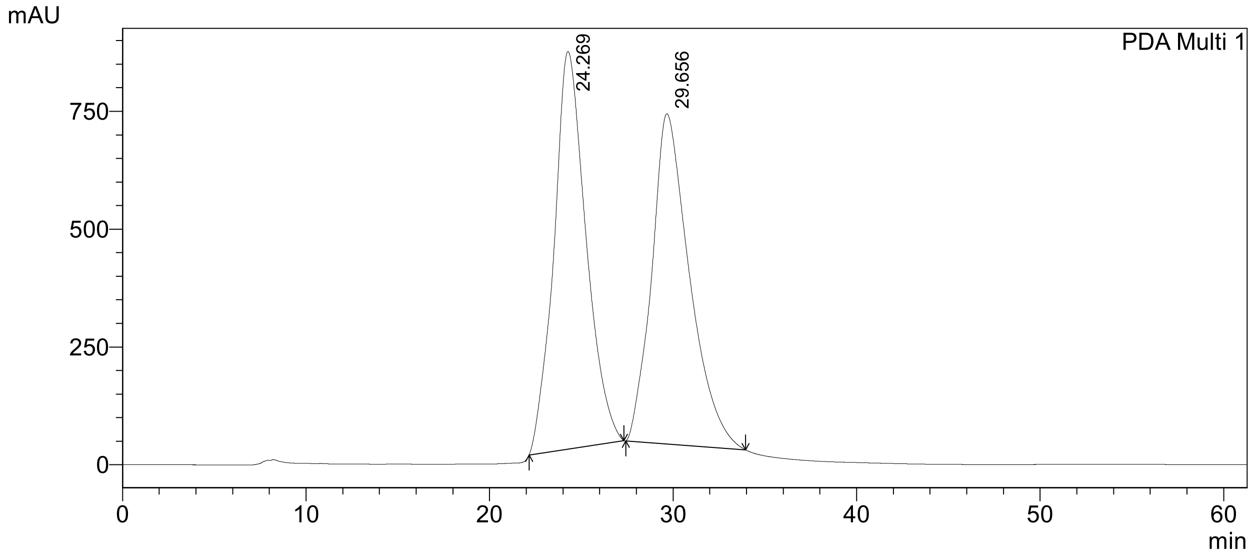

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.269	102763034	843938	50.617	54.640
2	29.656	100257551	700599	49.383	45.360
Total		203020586	1544537	100.000	100.000

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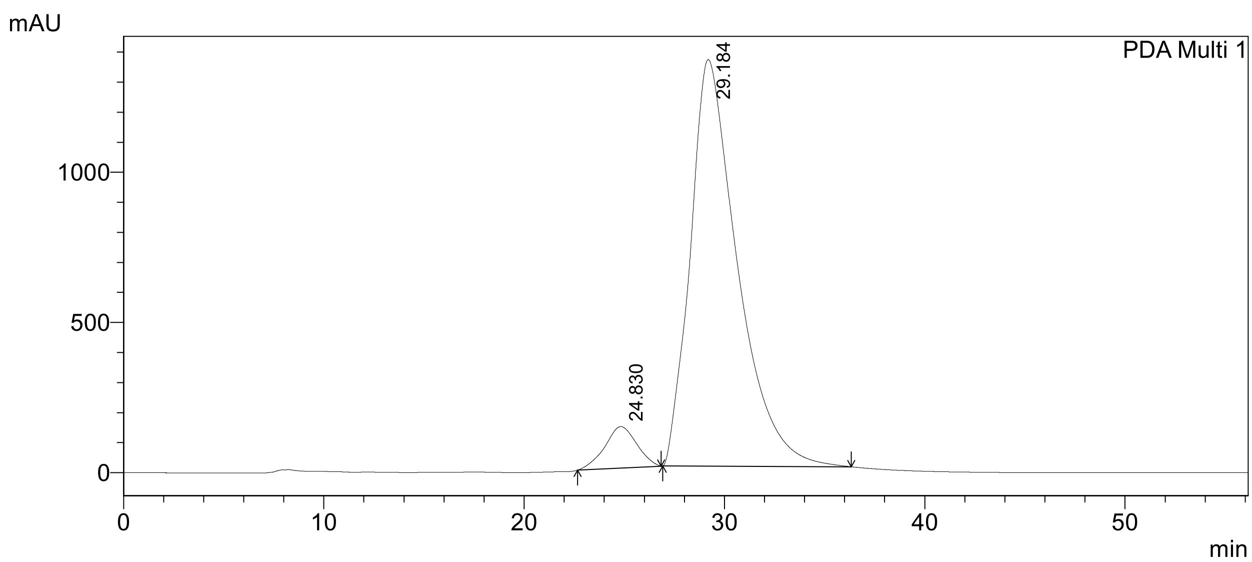

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.830	15403629	138170	6.514	9.260
2	29.184	221073709	1353881	93.486	90.740
Total		236477338	1492051	100.000	100.000

1k

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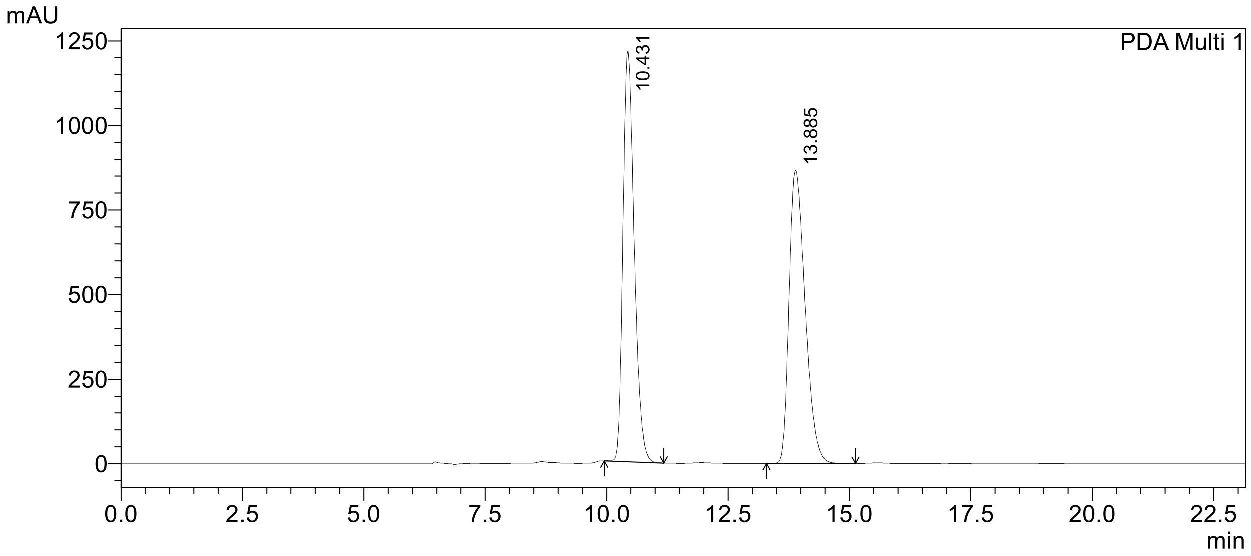

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.431	19640864	1212073	49.566	58.307
2	13.885	19985158	866715	50.434	41.693
Total		39626022	2078788	100.000	100.000

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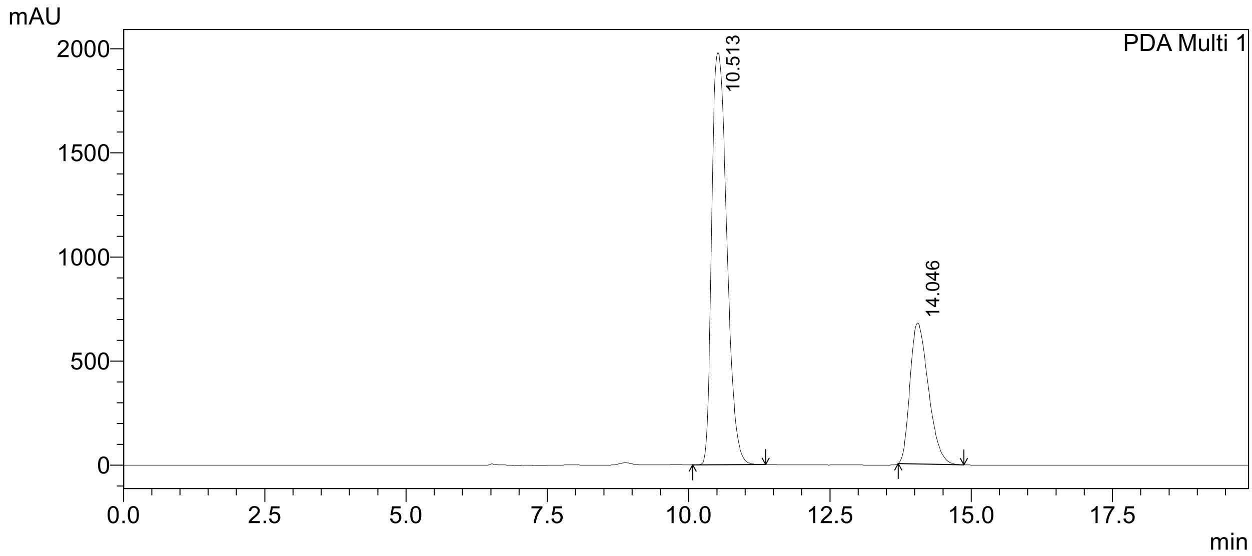

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.513	36849841	1979617	70.583	74.522
2	14.046	15357711	676808	29.417	25.478
Total		52207552	2656426	100.000	100.000

5l

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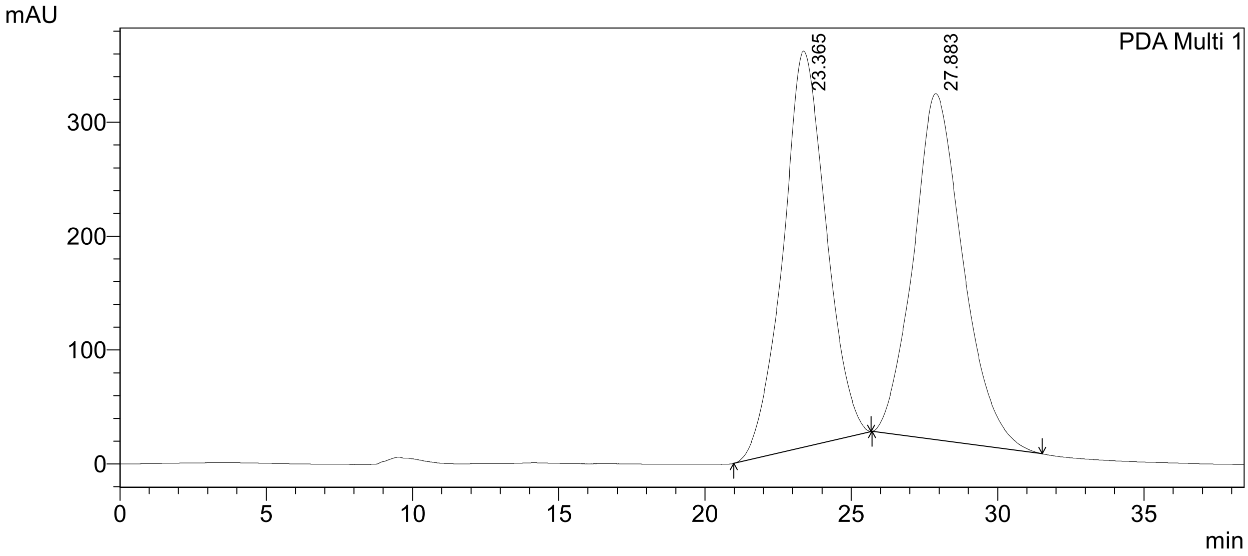

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.365	35747840	347773	49.828	53.362
2	27.883	35995019	303945	50.172	46.638
Total		71742859	651718	100.000	100.000

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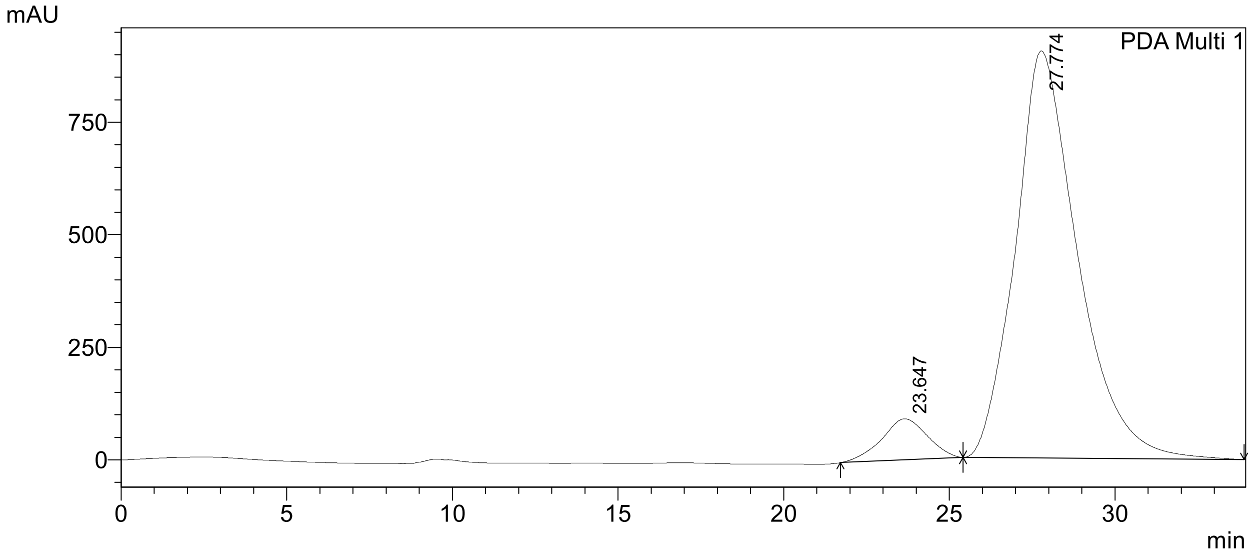

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.647	8757720	91343	6.894	9.173
2	27.774	118280555	904399	93.106	90.827
Total		127038275	995742	100.000	100.000

1k

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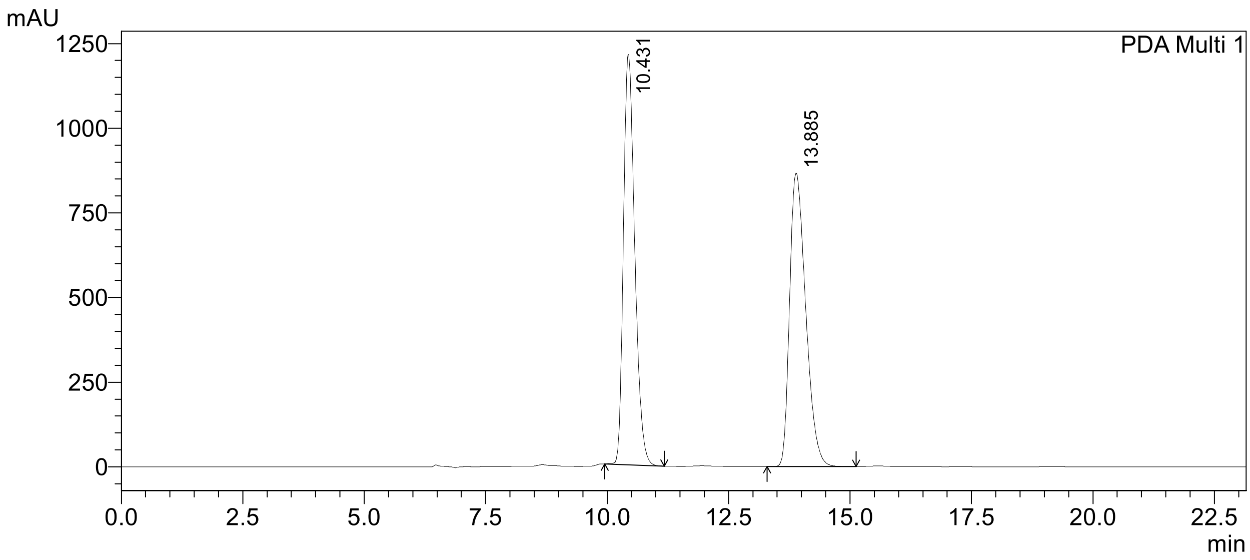

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.431	19640864	1212073	49.566	58.307
2	13.885	19985158	866715	50.434	41.693
Total		39626022	2078788	100.000	100.000

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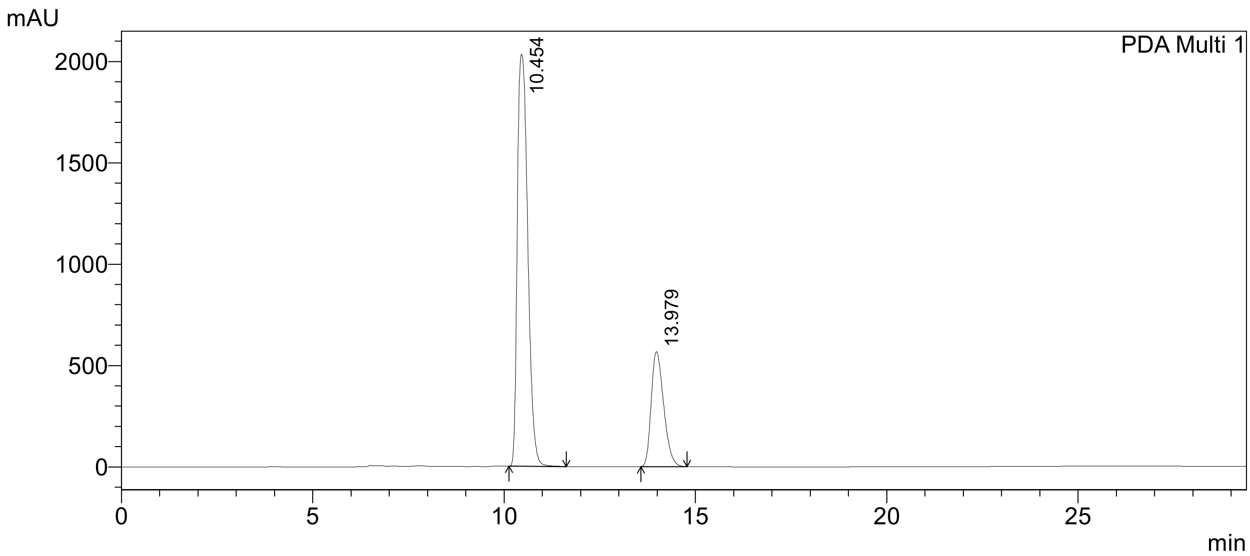

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.454	38519376	2032138	74.999	78.168
2	13.979	12840536	567565	25.001	21.832
Total		51359912	2599704	100.000	100.000

5m

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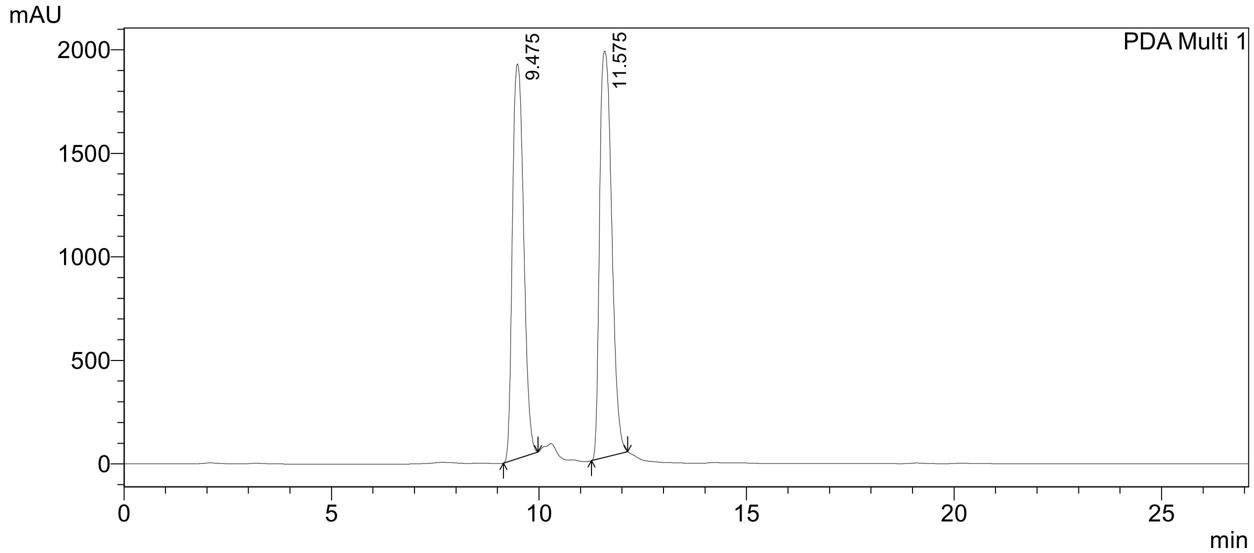

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.475	35926556	1906995	47.389	49.275
2	11.575	39884760	1963087	52.611	50.725
Total		75811317	3870082	100.000	100.000

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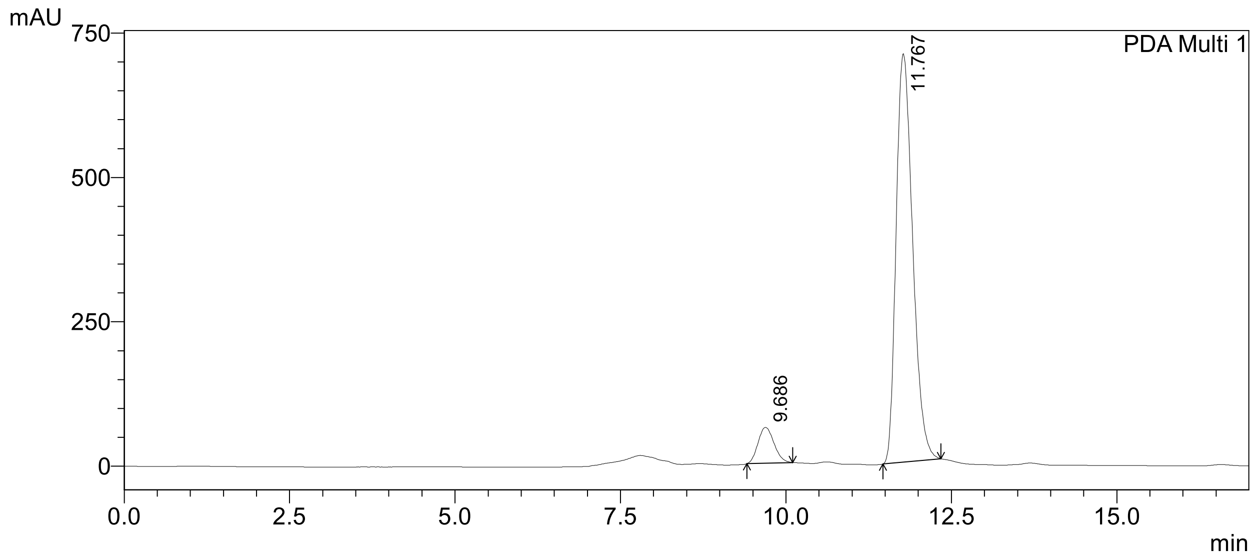

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.686	1046527	62130	7.845	8.075
2	11.767	12292855	707275	92.155	91.925
Total		13339382	769405	100.000	100.000

1k

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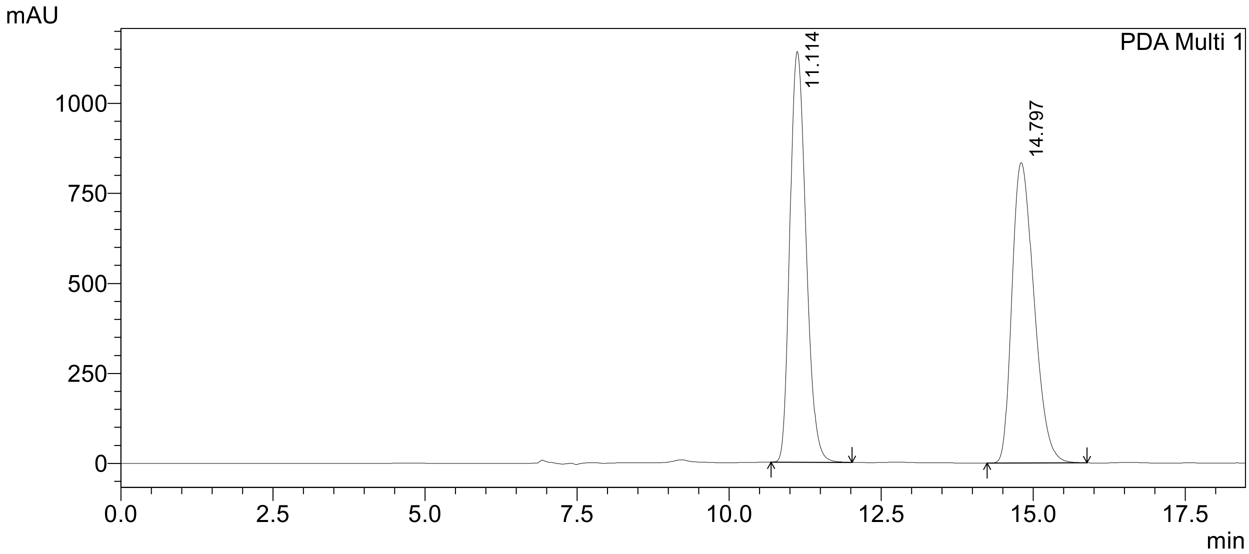

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.114	21078625	1140511	49.926	57.739
2	14.797	21141260	834759	50.074	42.261
Total		42219884	1975271	100.000	100.000

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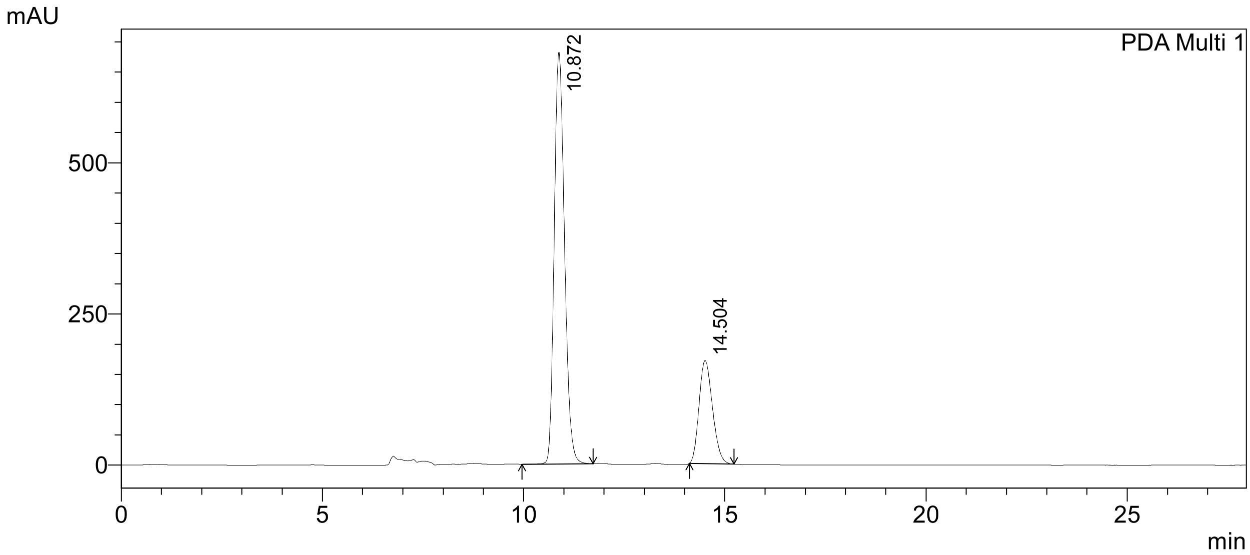

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.872	12162751	680972	75.373	79.972
2	14.504	3973901	170536	24.627	20.028
Total		16136652	851508	100.000	100.000

5n

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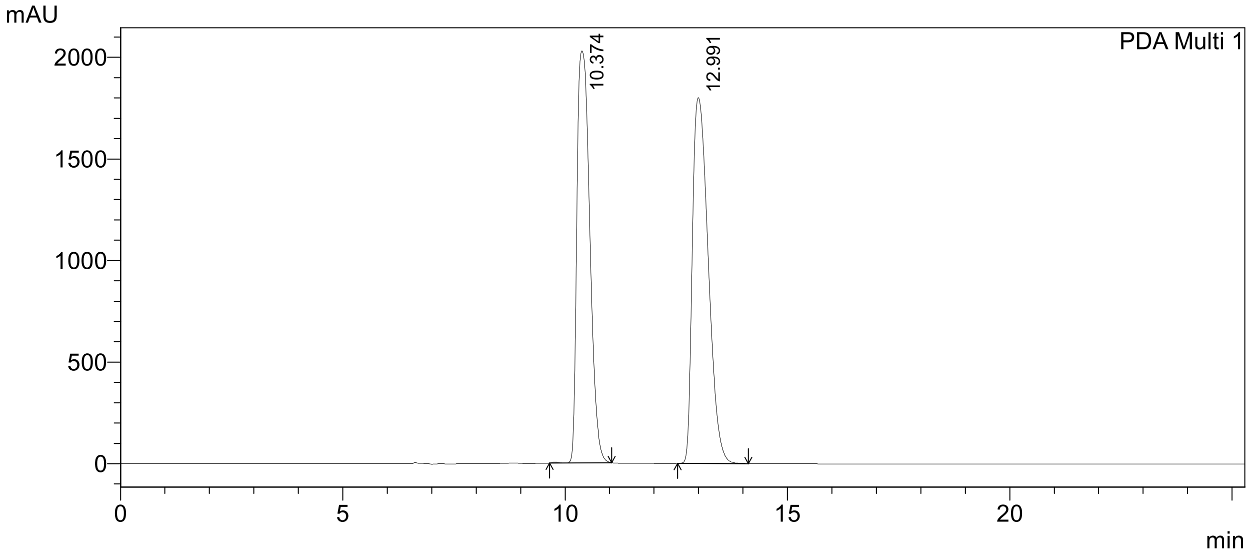

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.374	40875133	2027593	47.712	52.972
2	12.991	44794891	1800071	52.288	47.028
Total		85670024	3827665	100.000	100.000

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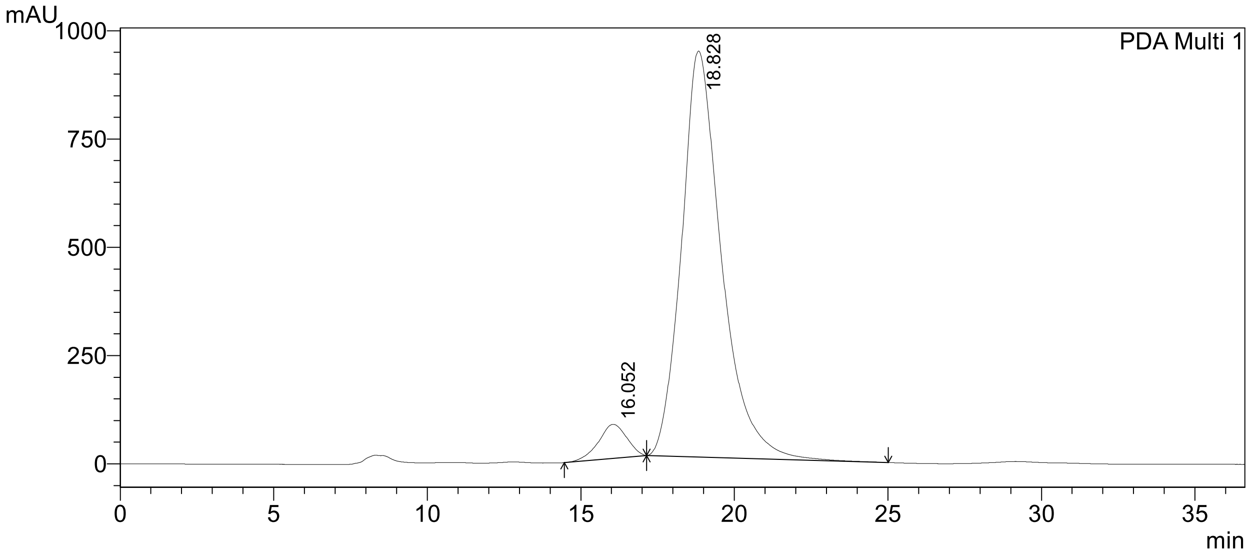

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.052	5031965	78539	5.595	7.733
2	18.828	84911612	937119	94.405	92.267
Total		89943577	1015658	100.000	100.000

1l

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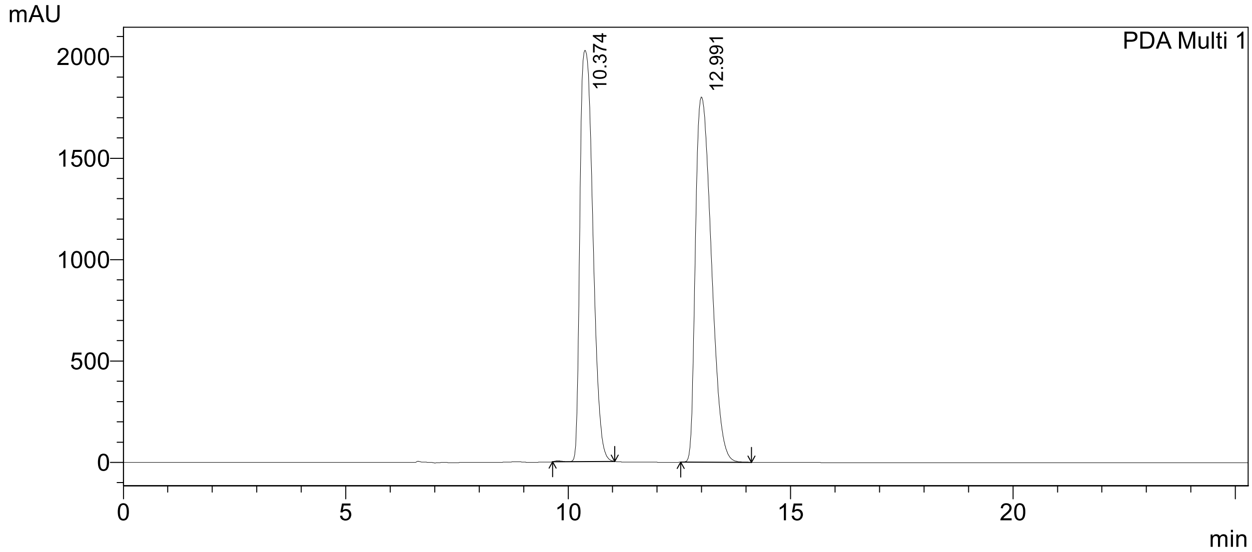

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.374	40875133	2027593	47.712	52.972
2	12.991	44794891	1800071	52.288	47.028
Total		85670024	3827665	100.000	100.000

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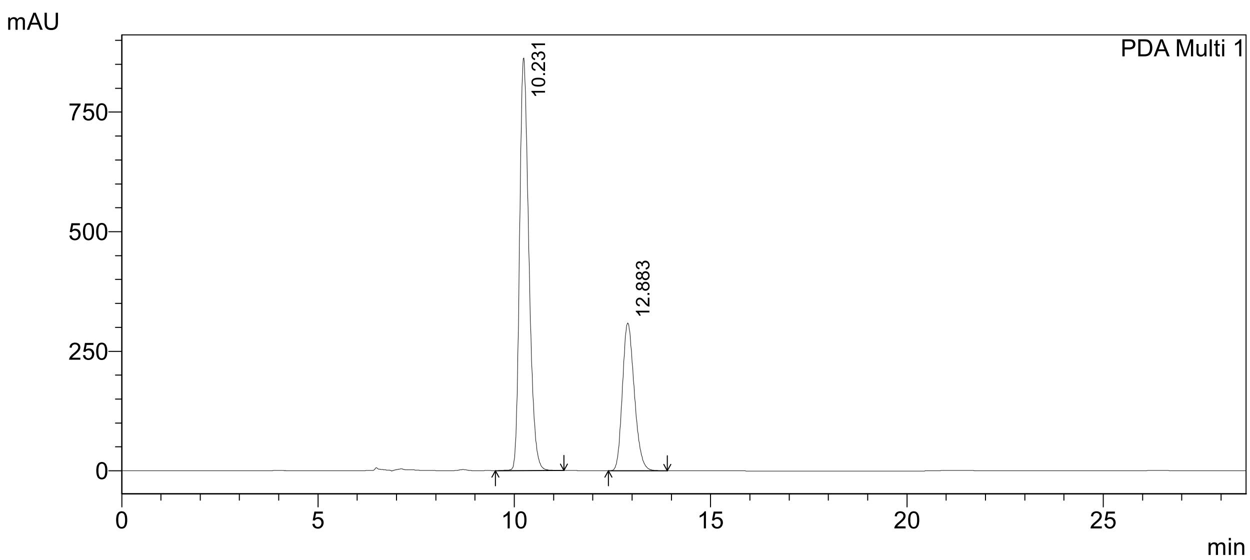

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.231	14252814	862872	68.621	73.634
2	12.883	6517599	308969	31.379	26.366
Total		20770413	1171841	100.000	100.000

6

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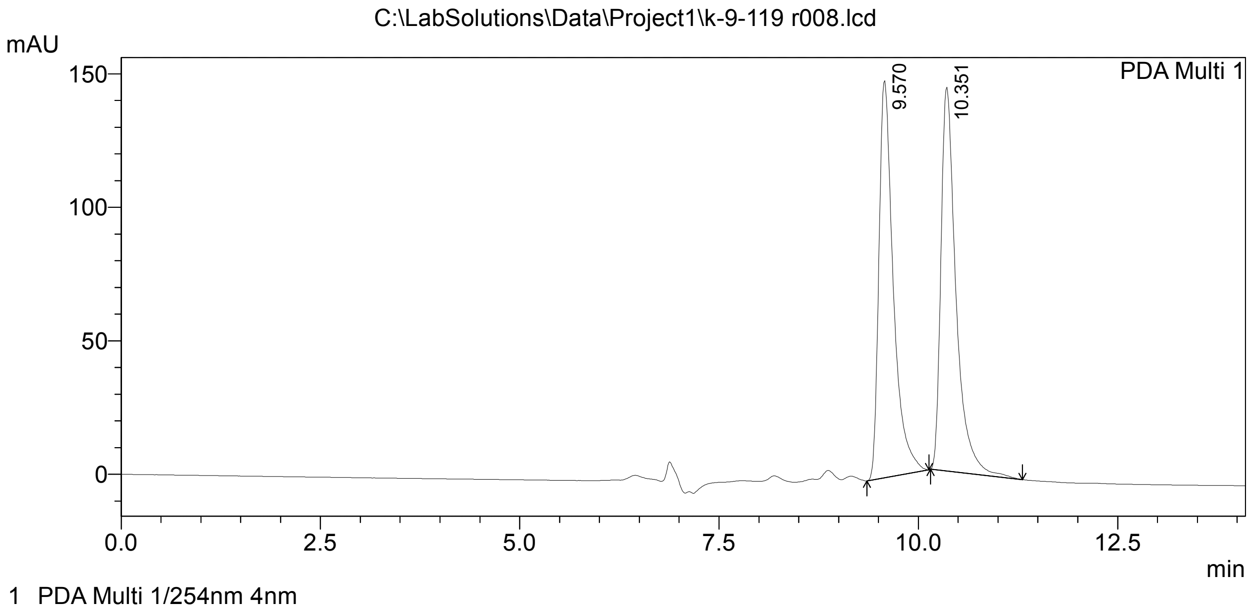

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.570	1878728	148766	49.833	50.831
2	10.351	1891344	143901	50.167	49.169
Total		3770072	292667	100.000	100.000

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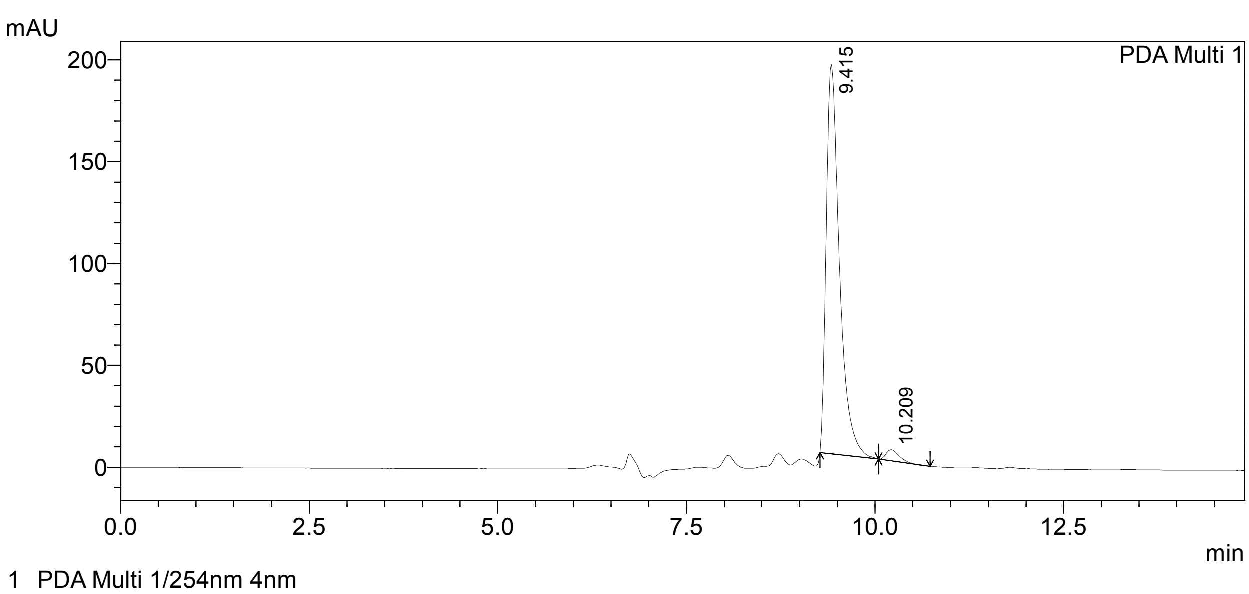

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.415	2321911	191176	97.395	97.268
2	10.209	62099	5369	2.605	2.732
Total		2384009	196546	100.000	100.000

7

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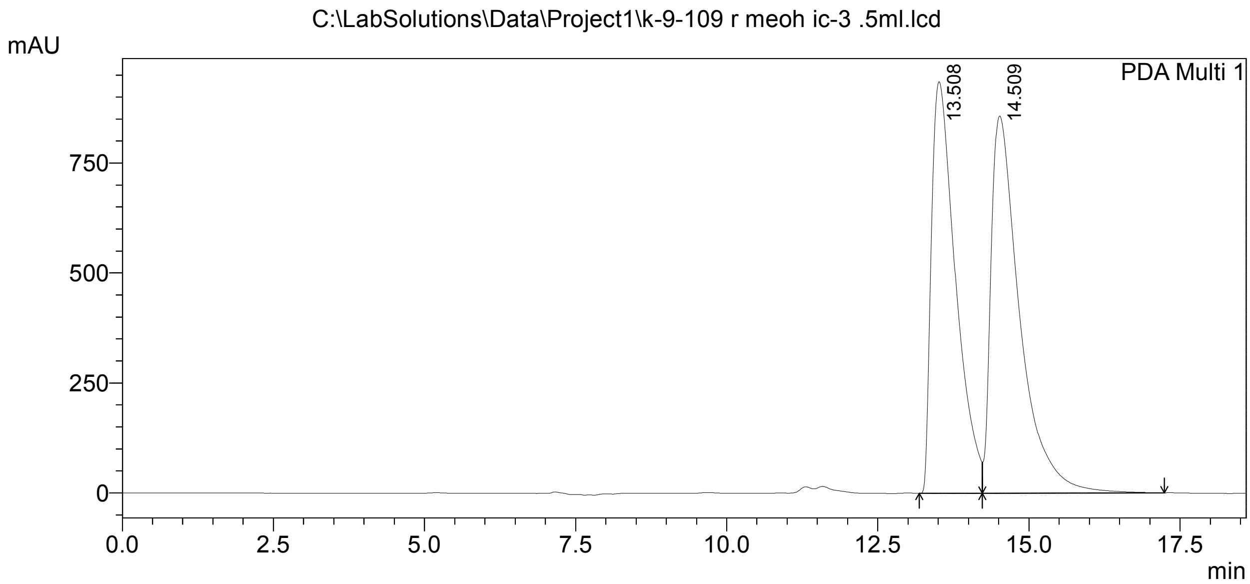

1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.508	26248588	935689	47.985	52.173
2	14.509	28452965	857757	52.015	47.827
Total		54701554	1793446	100.000	100.000

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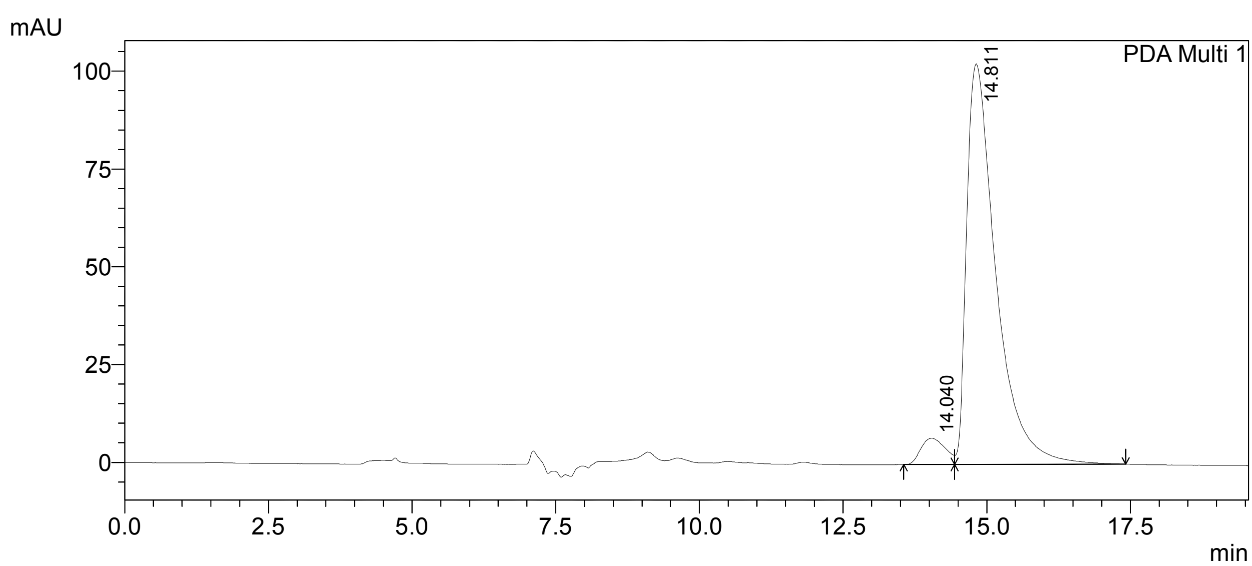


1 PDA Multi 1/254nm 4nm

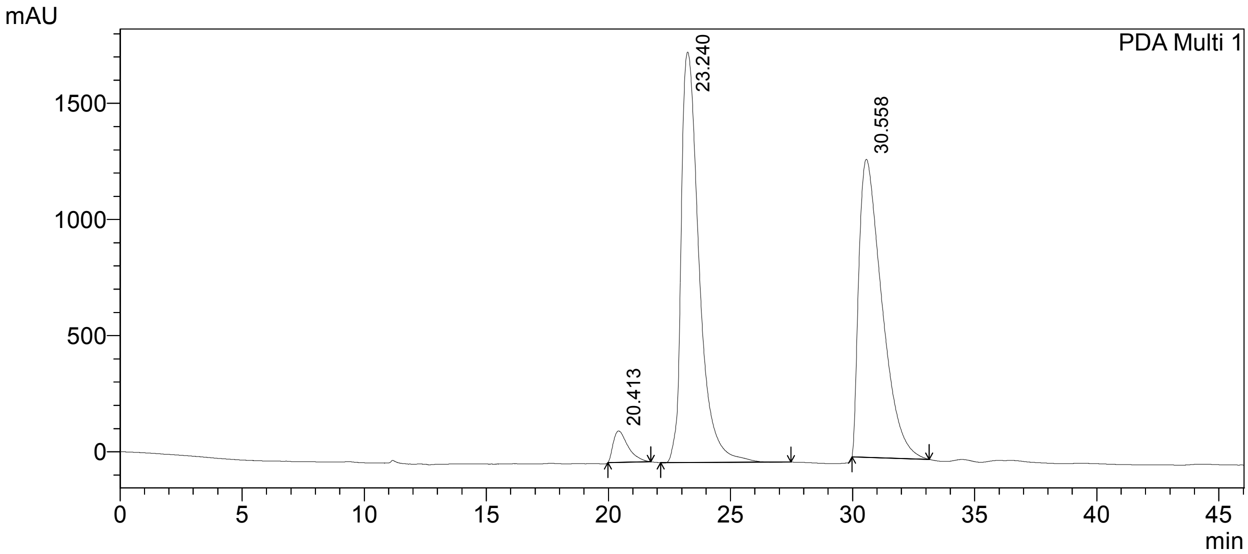
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.040	198773	6698	5.192	6.139
2	14.811	3629324	102416	94.808	93.861
Total		3828097	109114	100.000	100.000

8

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.413	5714931	134883	3.172	4.234
2	23.240	90191223	1767086	50.066	55.467
3	30.558	84238011	1283869	46.761	40.299
Total		180144165	3185837	100.000	100.000

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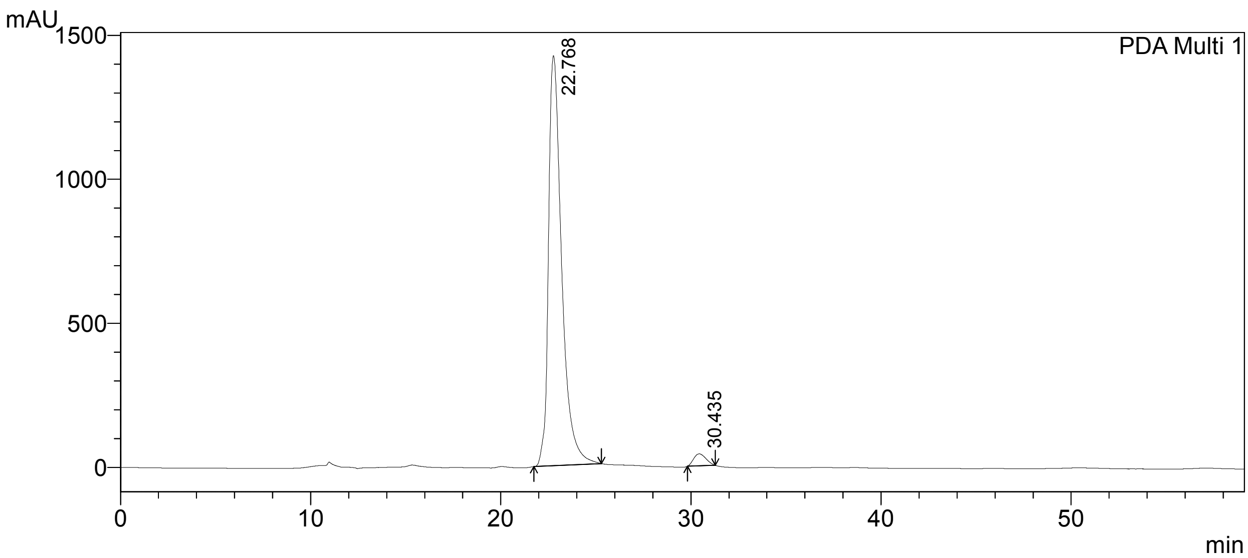


1 PDA Multi 1/254nm 4nm

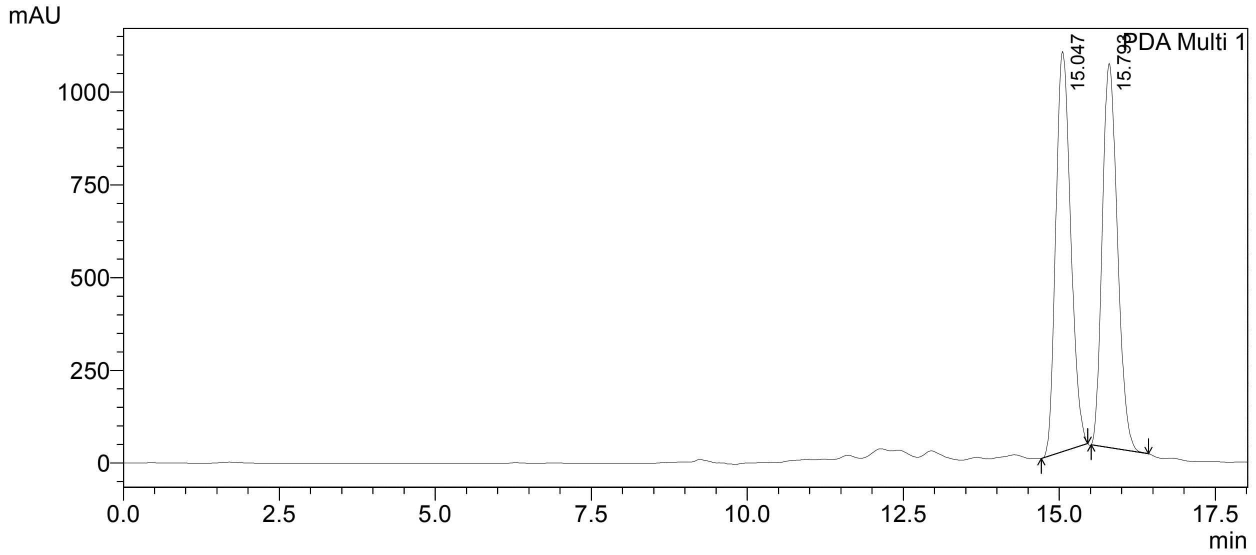
PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.768	68670177	1424000	97.307	97.136
2	30.435	1900279	41990	2.693	2.864
Total		70570456	1465990	100.000	100.000

9

<Chromatogram>



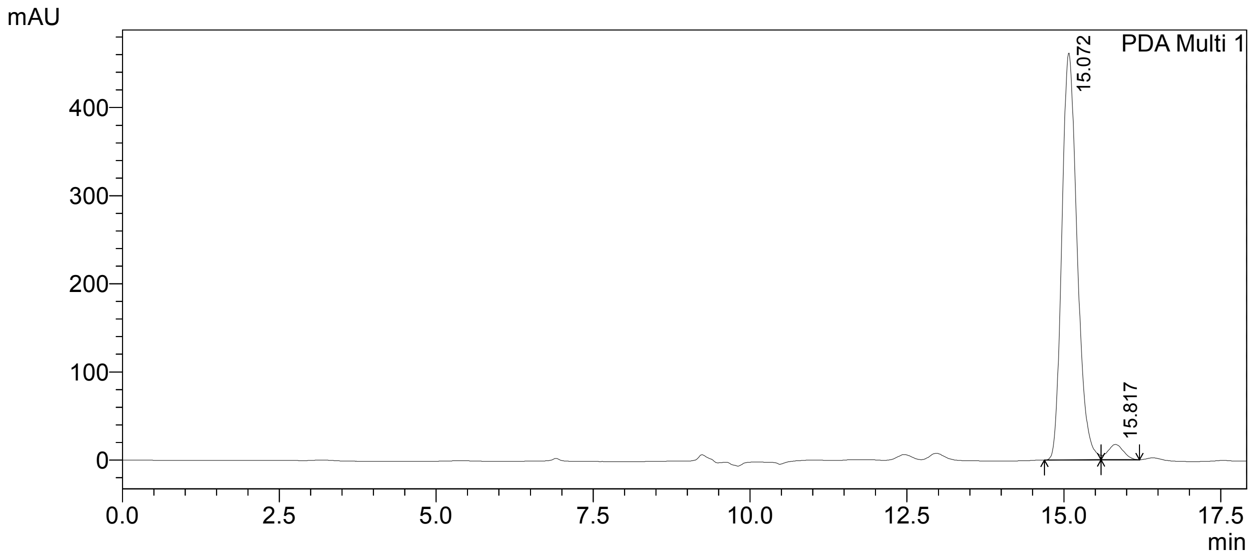
1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.047	18019031	1079131	50.627	51.021
2	15.793	17572866	1035948	49.373	48.979
Total		35591897	2115078	100.000	100.000

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.072	7834091	461689	96.284	96.368
2	15.817	302331	17402	3.716	3.632
Total		8136422	479091	100.000	100.000