Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Post-synthetic diversification of pyrrole-fused benzosultams via *trans*-sulfonylations and reactions on the periphery of pyrrole

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1. GENERAL CONSIDERATIONS

Unless noted otherwise, all reagents and solvents were purchased from commercial sources and used as received. All palladium-catalyzed reactions were performed in a screw-cap sealed tube. The ^{1}H and ^{13}C NMR spectra were obtained in $CDCl_3$ as solvent using a 400 MHz spectrometer with Me_4Si as an internal standard. Coupling constants (*J* values) are reported in Hz. Column chromatography was performed using silica gel (100-200 mesh). High resolution mass spectra (HRMS) were obtained using electron spray ionisation (ESI) technique and as TOF mass analyser. All melting points were taken using a melting point apparatus equipped with a calibrated thermometer and are uncorrected. New compounds were characterized by melting point, IR, ^{1}H NMR, ^{13}C NMR, and HRMS data.

2. EXPERIMENTAL SECTION

2.1 General Procedure for synthesis of pyrrole sultam by intramolecular cyclization

Following a literature procedure,[1] in an oven-dried screw cap vial equipped with a magnetic stir bar, pyrrole substrate (0.5 mmol), $Pd(OAc)_2$ (10 mol%), AgOAc (1.5 mmol), CsOPiv (20 mol%), 3 mL pivalic acid as solvent was heated at 130 ºC for 12 h. The reaction mixture was allowed to cool to room temperature and neutralized by the addition of saturated solution of Na_2CO_3 (10 mL). Then, it was extracted with ethyl acetate (2 x 10 mL). The combined organic layer was dried (Na_2SO_4), concentrated under reduced pressure, and purified by column chromatography on silica using (EtOAc/ hexanes = 2:8) as an eluent to give the desired product.

2.2 General procedure for the synthesis of sulfonylated pyrroles

To a solution of 2-substituted pyrrole (0.5 mmol) in dichloromethane (2.5 mL) was added KOH (1.5 equiv) and tetrabutylammonium hydrogensulfate (10 mol%) and was allowed to stir for 15 mins followed by addition of solution of sulfonyl chloride (1.2 equiv) in dichloromethane (1.0 mL) and the mixture was stirred at room temperature till the starting material was consumed. Water (20 mL) was added and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layer was dried (Na_2SO_4) and concentrated, which upon chromatography [silica, EtOAc - hexanes = 1: 19 to 1: 9] gave the *N*-sulfonylated pyrroles.

2.3 Synthesis of *ortho*-sulfonylated compounds by nucleophilic ring opening

2.3.1 Procedure for N-S bond cleavage by Fluoride source

In an oven-dried screw cap vial equipped with a magnetic stir bar, a solution of substrate (0.25 mmol) in acetonitrile (2 mL) was treated with tetrabutylammonium fluoride trihydrate (0.5 mmol) for 1 h at room temperature. After completion, the mixture was diluted with H_2O (5 mL) and extracted with EtOAc (10 mL X 2). The combined organic layer was dried (Na_2SO_4) and concentrated, which upon chromatography [silica, MeOH - EtOAc = 1:9] gave the corresponding sulfonic acid.

2.3.2. Procedure for N-S bond cleavage by amines

In an oven-dried screw cap vial equipped with a magnetic stir bar, substrate (0.25 mmol) was treated with amine (1 mL) at 40 ºC for 2 h. After completion, the mixture was diluted with H_2O (5 mL) and extracted with EtOAc (10 mL X 2). The combined organic layer was dried (Na_2SO_4) and concentrated, which upon chromatography [silica, EtOAc -hexanes = 2:8/ ~ 1:1] gave the corresponding amide.

2.3.3. Procedure for N-S bond cleavage using NaOEt

In an oven-dried screw cap vial equipped with a magnetic stir bar, a solution of substrate (0.25 mmol) in THF (2 mL) was treated with freshly prepared sodium ethoxide solution in ethanol (0.26 mmol) at room temperature. It was quenched as soon as addition was complete with H_2O (5 mL) and extracted with EtOAc (2 x 10 mL). The combined organic layer was dried (Na_2SO_4) and concentrated, which upon chromatography [silica, EtOAc-hexanes = 1:9] gave the corresponding sulfonate ester.

2.4 General Procedure for regioselective bromination

To an oven dried round bottom flask equipped with magnetic stir bar was charged with N-tosyl pyrrole (**8a**), N-tosyl methyl pyrrole-2-caboxylate (**16a**), **20** or **22** (1 mmol), NaBr (1.1 equiv) and oxone® (1.5 equiv) and then nitromethane (2 mL) was added. Reaction mixture was allowed to stir 5 h depending on substrate to give corresponding C-3 brominated products **35** and **36** in good to moderate yields.

2.5 General Procedure for Suzuki coupling with **42**

In an oven-dried screw cap vail equipped with a magnetic stir bar, substrate (0.1 mmol), $Pd(PPh_3)_4$ (5 mol%), Na_2CO_3 (4 equiv), **42** (2.2 equiv) and THF:water (4:1) was added and heated at 70 ^oC for 12 h. Then, reaction mixture was allowed to come to room temperature, water was added. Then, extratcted with EtOAc (10 mL X 2), layers were separated and organic layer was dried (Na_2SO_4) and concentrated, which upon chromatography [silica, EtOAc-hexanes = 1:9] gave the desired products **38** and **39**.

2.6 Procedure for reduction of *N*-tosyl pyrrole-2-carboxaldehyde by sodium borohydride

To a solution of *N*-tosyl pyrrole-2-carboxaldehyde in ethanol was added $NaBH_4$ (1.5 equiv) and stirred at room temperature for 30 mins. Water (20 mL) was added and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layer was dried (Na_2SO_4) and concentrated, which upon column chromatography [silica, EtOAc -hexanes = 1: 4] gave the desired product.

2.7 Procedure for alkylation of hydroxyl group (10a)

A dried round bottom flask equipped with a magnetic stirrer bar was charged with (1-Tosyl-1*H*-pyrrol-2-yl)methanol and THF (5 mL) under nitrogen atmosphere. The reaction mixture was cool down to 0 $^{\circ}C$ and NaH (1.2 equiv) was added and stirred for 15 mins. After which alkyl halide (1.1 equiv) was added and continued the stirring for 1 h. After completion of the reaction, it was quenched with water (10 mL) and was extracted with ethyl acetate (3 x 20 mL). The combined organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure to give **10a**.

2.8 Procedure for C-2 arylation of pyrrole (9a)[2]

Following a literature procedure, in an oven-dried screw cap vial equipped with a magnetic stir bar, pyrrole substrate (0.5 mmol), $Pd(OAc)_2$ (10 mol%), phenyl boronic acid (1.5 equiv) and acetic acid (5 mL) as solvent under O_2 atmoshpere was stirred at room temperature for 8 h. The reaction mixture was quenched by the addtion of saturated solution of $NaHCO_3$ (10 mL). Then, it was extracted with ethyl acetate (2 x 10 mL). The combined organic layer was dried (Na_2SO_4),

concentrated under reduced pressure, and purified by column chromatography on silica using (dichloromethane/ hexane:1:4) as an eluent to give the desired product.

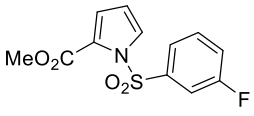
2.9 General Procedure for the synthesis of 2,4-disubstitued pyrrole (15a)[3,4]

Following a literatue protocol[3,4], to an oven-dried round bottom flask was charged with a magnetic stir bar, DMF (1.1 equiv) was added and it was cooled to 0 ^{o}C, then $POCl_3$ (1.1 equiv) was added dropwise to it, the reaction mixture becomes canarary yellow following which it was allowed to run at room temperature for 15 min, followed by addition of solvent DCE (5 mL) was added, followed by addition of ethyl-2-pyrrole carboxylate (5 mmol) dissolved in DCE (5 mL). Reaction mixture was refluxed at 90 ^{o}C for 1 h. Following which, satd solution of sodium bicarbonate was added until CO_2 effervescence ceased, then it was diluted with EtOAc (10 mL), layers were separated, organic layer was collected and concentrated under reduced pressure.

This reaction mixture was further diluted with DMSO (4 mL) and then, $NH_2OH.HCl$ (1.2 equiv) was added. Reaction mixture was heated at 90 ^{o}C for 1 h, following which cold water was added then, EtOAc (5 mL) was added, layers were separated, organic laers was collected and concentrated followed by silica gel chromatography (EtOAc:Hexanes = 2:8) to give desired 2,4-disubsittuted pyrrole in 40% yield.

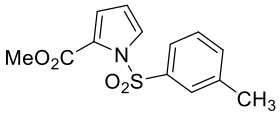
3. CHARACTERIZATION DATA

Methyl 1-((3-fluorophenyl)sulfonyl)-1*H*-pyrrole-2-carboxylate (5)



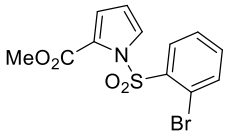
Off-white solid; Yield 77% (217 mg); mp.128-130 $^{\circ}$C; ^{1}H NMR($CDCl_3$): δ 7.82-7.79 (m, 1H), 7.73-7.69 (m, 2H), 7.57-7.51 (m, 1H), 7.37-7.32 (m, 1H), 7.10 (q, J = 1.8 Hz, 1H), 6.37 (t, J = 3.4 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR($CDCl_3$): δ 163.2 (d, J = 251 Hz), 159.0, 140.7 (d, J = 29 Hz), 130.6 (d, J = 31 Hz), 129.1, 125.0, 123.8 (d, J = 13 Hz), 123.6, 121.2 (d, J = 21 Hz), 115.6, 115.3, 110.0, 51.8; HRMS: calcd for $C_{12}H_{11}FNO_4S$ $[M+H]^+$ 284.0393, found 284.0396; IR (KBr): 2926, 2855, 1731, 1447, 756 cm^{-1}.

Methyl 1-(m-tolylsulfonyl)-1*H*-pyrrole-2-carboxylate (6)



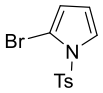
Off-white solid; Yield 86% (184 mg); mp.70-75 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81-7.80 (m, 1H), 7.75-7.74 (m, 2H), 7.44-7.43 (m, 2H), 7.09-7.08 (m, 1H), 6.35 (t, J = 3.4 Hz, 1H), 3.74 (s, 3H), 2.49 (s, 3H); ^{13}C NMR($CDCl_3$): δ 159.0, 139.1, 138.7, 134.6, 129.2, 128.6, 128.0, 125.2, 124.9, 123.3, 110.4, 51.7, 21.3; HRMS: calcd for $C_{13}H_{14}NO_4S$ $[M+H]^+$ 280.0644, found 280.0649; IR (KBr): 2923, 1725, 1448, 1105, 756 cm^{-1}.

Methyl 1-((2-bromophenyl)sulfonyl)-1*H*-pyrrole-2-carboxylate (7)



Whitish solid; Yield 45% (154 mg); mp. 86-87 °C ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.43 (dd, J = 8.0, 1.6 Hz, 1H), 7.92-7.91 (m, 1H), 7.71 (dd, J = 7.9, 1.2 Hz, 1H), 7.60 (dt, J = 7.6, 1.2, 1H), 7.50 (dt, J = 7.7, 1.7 Hz, 1H), 7.14-7.12 (m, 1H), 6.35 (t, J = 3.5 Hz, 1H), 3.69 (s, 3H); ^{13}C NMR($CDCl_3$): δ 158.9, 138.0, 135.1, 134.7, 133.8, 131.7, 127.1, 124.7, 123.9, 120.1, 109.9, 51.7; HRMS: calcd for $C_{12}H_{11}BrNO_4S$ $[M+H]^+$ 343.9592, found 343.9599; IR (KBr): 2919, 1730, 1100, 750 cm^{-1}.

2-bromo-1-tosyl-1*H*-pyrrole (8)

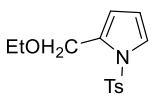


Whitish solid; Yield 55% (165 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, J = 7.9 Hz, 2H), 7.49-7.47 (m, 1H), 7.35 (d, J = 8.2 Hz, 2H), 6.31-6.29 (m, 1H), 6.27-6.25 (m, 1H), 2.44 (s, 3H), ^{13}C NMR($CDCl_3$): δ 145.4, 135.1, 129.9, 127.8, 124.2, 117.9, 112.5, 100.0, 21.7; HRMS: calcd for $C_{11}H_{11}BrNO_2S$ $[M+H]^+$ 301.1780, found 301.1778; IR (KBr): 2999, 1555, 736 cm^{-1}.

2-Phenyl-1-tosyl-1*H*-pyrrole (31)[2]

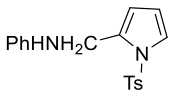
Brown solid; Yield 68% (100 mg); ^{1}H NMR($CDCl_3$): δ 7.46 (dd, J = 3.2, 1.8 Hz, 1H), 7.40-7.36 (m, 1H), 7.35-7.30 (m, 2H), 7.25 (d, J = 8.4 Hz, 4H), 7.12 (d, J = 8.1 Hz, 2H), 6.33 (d, J = 3.3 Hz, 1H), 6.18 (dd, J = 1.8, 3.1 Hz, 1H), 2.37 (s, 3H).

2-(Ethoxymethyl)-1-tosyl-1*H*-pyrrole (10a)[2]



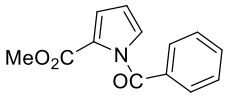
Whitish semi-solid; Yield 44% (123 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, J = 8.3 Hz, 2H), 7.32-7.31 (m, 1H), 7.29-7.27 (m, 2H), 6.27-6.22 (m, 2H), 4.61 (s, 2H), 3.44 (q, J = 7.1 Hz, 2H), 2.41 (s, 3H), 1.10 (t, J = 7.2 Hz, 3H); HRMS: calcd for $C_{14}H_{18}NO_3S$ $[M+H]^+$ 280.1007, found 280.1003; IR (KBr): 2990, 1560, 1441, 1110, 749 cm^{-1}.

N-((1-tosyl-1*H*-pyrrol-2-yl)methyl)aniline (10b)



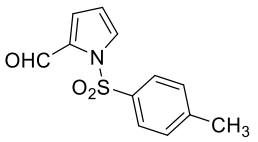
Yellow liquid; Yield 54% (176 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d J = 7.8 Hz, 2H), 7.36-7.28 (m, 3H), 7.14 (t, J = 7.8 Hz, 2H), 6.72 (t, J = 7.2 Hz, 1H), 6.49 (d, J = 8.0 Hz, 2H), 6.23 (s, 2H), 4.41 (s, 2H), 4.08 (s, 1H), 2.47 (s, 3H); ^{13}C NMR($CDCl_3$): δ 147.2, 145.0, 136.3, 132.5, 130.0, 129.1, 126.7, 123.2, 117.7, 114.4, 113.1, 111.4, 40.6, 21.6 ; HRMS: calcd for $C_{18}H_{19}N_2O_2S$ $[M+H]^+$ 327.1167, found 327.1167; IR (KBr): 2921, 1141, 749 cm^{-1}.

Methyl 1-benzoyl-1H-pyrrole-2-carboxylate (11)



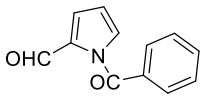
Yellow Liquid; Yield 60% (137 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 7.1 Hz, 2H), 7.65 (t, J = 7.5 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.26-7.25 (m , 1H), 7.10-7.09 (m,1H), 6.33-6.32 (m, 1H), 3.60 (s, 3H); ^{13}C NMR($CDCl_3$): δ 168.3, 160.7, 133.5, 133.4, 129.8, 128.6, 127.7, 126.0, 121.3, 110.6, 51.6; HRMS: calcd for $C_{13}H_{12}NO_3$ $[M+H]^+$ 230.0817, found 230.0810; IR (KBr): 2925, 1730, 1549, 748 cm^{-1}.

1-Tosyl-1*H*-pyrrole-2-carbaldehyde (12)



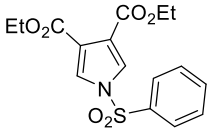
Bluish solid, Yield 85% (105 mg); mp.107-109 $^{\circ}$C; ^{1}H NMR($CDCl_3$): δ 9.98 (s, 1H), 7.82 (d, J = 8.4 Hz, 2H), 7.63 (dd, J = 3.0, 1.8 Hz, 1H), 7.34 (d, J = 8.1 Hz, 2H), 7.17 (dd, J = 3.7, 1.7 Hz, 1H), 6.41 (t, J = 3.3 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR($CDCl_3$): δ 178.9, 145.9, 135.2, 133.5, 130.1, 129.4, 127.4, 124.4, 112.4, 21.6; HRMS: calcd for $C_{12}H_{12}NO_3S$ $[M+H]^+$ 250.0538, found 250.0537; IR (KBr): 2895, 1666, 1538, 1421, 1251, 1153, 670 cm^{-1}.

1-benzoyl-1*H*-pyrrole-2-carbaldehyde (13)



Yellow Liquid; Yield 46% (91 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.05 (s, 1H), 7.82 (d, J = 7.3 Hz, 2H), 7.71 (t, J = 7.4 Hz, 1H), 7.58 (t, J = 7.7 Hz, 2H), 7.34-7.33 (m, 1H), 7.24 (m, 1H), 6.41-6.39 (m, 1H); ^{13}C NMR($CDCl_3$): δ 172.1, 133.8, 130.2, 129.3, 128.5; HRMS: calcd for $C_{12}H_{10}NO_2$ $[M+H]^+$ 200.0712, found 200.0710; IR (KBr): 2921, 1735, 748 cm^{-1}.

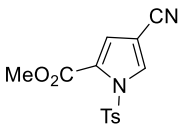
Diethyl 1-(phenylsulfonyl)-1H-pyrrole-3,4-dicarboxylate (14)



Brownish liquid; Yield 87% (304 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (dd, J = 8.3, 1 Hz, 2H), 7.73 (dt, J = 7.5, 1.7 Hz, 1H), 7.67 (s, 2H), 7.62 (dt, J = 8.0, 1.5 Hz, 2H), 4.33 (q, J = 7.2 Hz, 4H), 1.36 (t, J = 7.2 Hz, 6H); ^{13}C

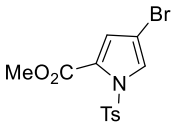
NMR($CDCl_3$): δ 162.0, 135.5, 130.9, 130.1, 129.5, 128.8, 127.7, 127.6, 65.5, 63.0, 19.1; HRMS: calcd for $C_{16}H_{18}NO_6S$ $[M+H]^+$ 352.0855, found 352.0850; IR (KBr): 2962, 1740, 1597, 1365, 1147, 794 cm^{-1}.

Methyl 4-cyano-1-tosyl-1H-pyrrole-2-carboxylate (15)



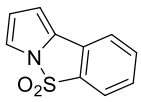
Whitish solid; Yield 40% (142 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, J = 1.9 Hz, 1H), 7.96 (d, J = 8.2 Hz, 2H), 7.40 (d, J = 8.3 Hz, 2H), 7.19 (d, J = 1.9 Hz, 1H), 4.28 (q, J = 7.1 Hz, 2H), 2.47 (s, 3H), 1.32 (t, J = 7.1 Hz, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$):157.5, 146.3, 134.0, 133.9, 129.7, 129.0, 126.3, 122.8, 113.5, 95.8, 61.6, 21.8, 14.1 ; HRMS: calcd for $C_{14}H_{13}N_2O_4S$ $[M+H]^+$ 305.0596, found 305.0599; IR (KBr): 2927, 2233, 1730, 994 cm^{-1}.

Methyl 4-bromo-1-tosyl-1H-pyrrole-2-carboxylate (16)



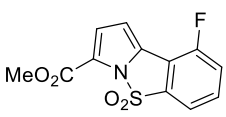
Whitish solid; Yield 40% (142 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, J = 8.4 Hz, 2H), 7.72 (d, J = 2.0 Hz, 1H), 7.37 (d, J = 8.3 Hz, 2H), 7.02 (d, J = 1.9 Hz, 1H), 3.76 (s, 3H), 2.46 (s, 3H)); ^{13}C NMR (100 MHz, $CDCl_3$):158.2, 145.5, 135.1, 129.5, 128.5, 127.7, 125.1, 124.6, 98.9, 52.0, 21.7, 14.1; HRMS: calcd for $C_{13}H_{13}BrNO_4S$ $[M+H]^+$ 357.9749, found 357.9755; IR (KBr): 2883, 1735, 779 cm^{-1}.

Benzo[d]pyrrolo[1,2-b]isothiazole 5,5-dioxide (17)



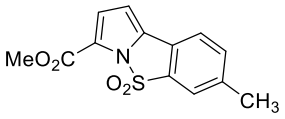
Whitish solid; Yield 77%(79 mg); mp 80-81 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (dd, J = 1.0, 7.8 Hz, 1H), 7.78 (dt, J = 7.8, 1.3 Hz, 1H), 7.64 (t, J = 7.8 Hz, 1H), 7.57 (d, J = 7.7 Hz, 1H), 7.17-7.16 (m, 1H), 6.51-6.50 (m, 1H), 6.45-6.43 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 134.9, 134.2, 133.7, 129.9, 127.9, 127.6, 122.5, 120.8, 119.6, 117.2; HRMS: calcd for $C_{10}H_8NO_2S$ $[M+H]^+$ 206.0276, found 206.277; IR (KBr): 2920, 1490, 742 cm^{-1}.

Methyl 9-fluorobenzo[d]pyrrolo[1,2-b]isothiazole-3-carboxylate 5,5-dioxide (18)



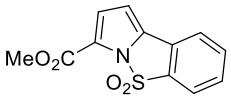
Whitish solid; Yield 44% (30 mg); mp. 280-282 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, J = 7.6 Hz, 1H), 7.53-7.48 (m, 1H), 7.41 (t, J = 8.7 Hz, 1H), 7.09 (d, J = 3.7 Hz, 1H), 6.63 (d, J = 3.5 Hz, 1H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.2, 157.4, 139.3, 131.0, 125.2, 123.2, 121.5, 121.3, 118.8, 108.4, 108.4, 52.5; HRMS: calcd for $C_{12}H_9FNO_4S$ $[M+H]^+$ 282.0236, found 282.0244; IR (KBr): 2920, 2845, 1735, 723 cm^{-1}.

Methyl 7-methylbenzo[d]pyrrolo[1,2-b]isothiazole-3-carboxylate 5,5-dioxide (19)



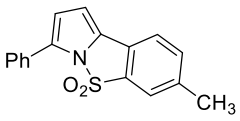
Whitish solid; Yield 44% (30 mg); mp 75-76 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (s, 1H), 7.50-7.44 (m, 2H), 7.05 (d, J = 3.7 Hz, 1H), 6.46 (d, J = 3.7 Hz, 1H), 3.97 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.4, 140.2, 137.6, 134.9, 134.2, 124.4, 123.5, 123.1, 123.0, 121.3, 104.5, 52.3, 21.5; HRMS: calcd for $C_{13}H_{12}NO_4S$ $[M+H]^+$ 278.0487, found 278.0499; IR (KBr): 2925, 1730, 1440, 745 cm^{-1}.

Methyl benzo[d]pyrrolo[1,2-*b*]isothiazole-3-carboxylate 5,5-dioxide (20)



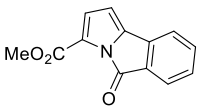
Whitish solid; Yield 34% (45 mg); mp 140-145 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, J = 7.8 Hz, 1H), 7.68-7.60 (m, 2H), 7.52 (t, J = 7.6 Hz, 1H), 7.07 (d, J = 3.7 Hz, 1H), 6.52 (d, J = 3.7 Hz, 1H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.1, 146.5, 134.4, 134.2, 133.9, 129.2, 124.8, 123.0, 122.8, 121.5, 105.1, 52.3; HRMS: calcd for $C_{12}H_{10}NO_4S$ $[M+H]^+$ 264.0331, found 264.0325; IR (KBr): 2955, 2813, 1732, 722 cm^{-1}.

7-methyl-3-phenylbenzo[d]pyrrolo[1,2-b]isothiazole 5,5-dioxide (21)



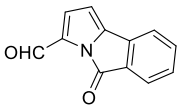
Yellowish semi-solid; Yield 42% (62 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, J = 7.4 Hz, 2H), 7.64 (d, J = 8.0 Hz, 1H), 7.49 (t, J = 7.4 Hz, 2H), 7.40-7.36 (m, 2H), 7.20 (d, J = 7.88 Hz, 1H), 6.54-6.51 (m, 2H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 145.3, 136.3, 134.1, 131.0, 130.0, 128.9, 128.4, 128.3, 127.9, 127.3, 122.2, 120.9, 115.4, 106.0, 21.9; HRMS: calcd for $C_{17}H_{14}NO_2S$ $[M+H]^+$ 296.0745, found 296.0744; IR (KBr): 2925, 1530, 1440, 745 cm^{-1}.

Methyl 5-oxo-5H-pyrrolo[2,1-*a*]isoindole-3-carboxylate (22)



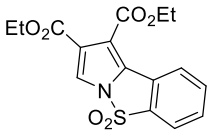
Yellow solid; Yield 78% (44 mg); mp 90-95 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, J = 7.6 Hz, 1H), 7.50 (t, J = 8 Hz, 1H), 7.38 (d, J = 7.5 Hz, 1H), 7.31 (t, J = 7.5 Hz, 1H), 6.99 (d, J = 3.7 Hz, 1H), 6.27 (d, J = 3.7 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.2, 138.2, 134.5, 128.6, 128.5, 126.2, 124.5, 120.1, 118.5, 105.8, 51.9 ; HRMS: calcd for $C_{13}H_{10}NO_3$ $[M+H]^+$ 228.0661, found 228.0659; IR (KBr): 2912, 2830, 1739, 1266, 720 cm^{-1}.

Methyl 5-oxo-5H-pyrrolo[2,1-*a*]isoindole-3-carboxylate (23)



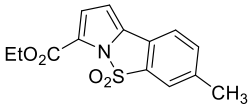
Yellow solid; Yield 60% (30 mg); mp 122-123 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.22 (s, 1H), 7.78 (d, J = 7.5 Hz, 1H), 7.58 (t, J = 7.5 Hz, 1H), 7.45 (d, J = 7.6 Hz, 1H), 7.38 (d, J = 7.4 Hz, 1H), 7.10-7.09 (m, 1H), 6.38-6.37 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 179.4, 165.5, 135.0, 133.4, 129.0, 124.7, 121.0, 108.7, 107.3, 104.6; HRMS: calcd for $C_{12}H_8NO_2$ $[M+H]^+$ 198.0555, found 198.0550; IR (KBr): 2923, 2852, 1739, 1262, 748 cm^{-1}.

Diethyl benzo[d]pyrrolo[1,2-b]isothiazole-1,2-dicarboxylate 5,5-dioxide (24)



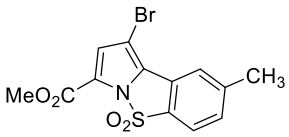
Brownish semi-solid; Yield 78% (68 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (d, J = 7.9 Hz, 1H), 7.82 (d, J = 7.7 Hz, 1H), 7.75 (dt, J = 7.8, 1.0 Hz, 1H), 7.65 (s, 1H), 7.59 (dt, J = 7.8, 1.0 Hz, 1H), 4.47 (q, J = 7.2 Hz, 2H), 4.37 (q, J = 7.2 Hz, 2H), 1.44-1.36 (m 6H); ^{13}C NMR($CDCl_3$): δ 167.7, 167.6, 132.3, 130.9, 130.8, 130.7, 128.8, 128.7, 123.8, 122.4, 119.8, 113.1, 72.3, 71.7, 19.1, 19.,1; HRMS: calcd for $C_{16}H_{16}NO_6S$ $[M+H]^+$ 350.0698, found 350.0699; IR (KBr): 3077, 2962, 1762, 1597, 1365, 1147, 794 cm^{-1}.

Ethyl 7-methylbenzo[d]pyrrolo[1,2-b]isothiazole-3-carboxylate 5,5-dioxide (25)



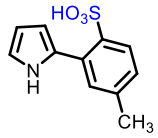
White semi-solid; Yield 45% (32 mg);^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, J = 8.0 Hz, 1H), 7.40 (s, 1H), 7.30-7.28 (m, 1H), 7.06 (d, J = 3.7 Hz, 1H), 6.48 (d, J = 3.7 Hz, 1H), 4.47 (q, J = 7.1 Hz, 2H), 2.48 (s, 3H), 1.46 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.9, 145.3, 135.0, 129.8, 126.3, 125.1, 122.8, 122.5, 121.8, 106.5, 104.7, 61.5, 21.8, 14.1; HRMS: calcd for $C_{14}H_{14}NO_4S$ $[M+H]^+$ 292.0644, found 292.0647; IR (KBr): 2925, 1735, 1529, 745 cm^{-1}.

Methyl 1-bromo-8-methylbenzo[d]pyrrolo[1,2-b]isothiazole-3-carboxylate 5,5-dio xide (26)



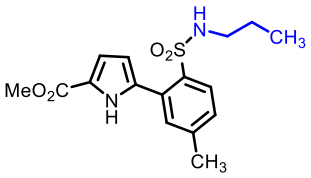
Whitish Solid; Yield 25% (22 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (s, 1H), 7.71 (d, J = 8 Hz, 1H), 7.36 (d, J = 8.1 Hz, 1H), 7.04 (s, 1H), 3.98 (s, 3H), 2.53 (s, 3H); ^{13}C NMR ($CDCl_3$): δ 158.6, 145.7, 134.4, 130.4, 130.2, 125.2, 124.6, 124.4, 122.7, 122.2, 95.0, 52.6, 22.0; HRMS (ESI) m/z calcd for $C_{13}H_{11}BrNO_4S$ $[M+H]^+$ 355.9592, found 355.9599; IR (KBr): 2922, 1739, 1155 cm^{-1}.

2-(5-(Methoxycarbonyl)-1*H*-pyrrol-2-yl)-5-methylbenzenesulfonic acid (31)



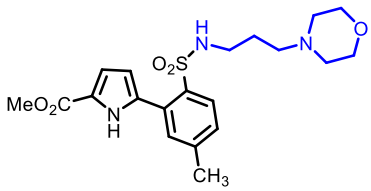
Pale yellow solid; Yield 92% (54 mg); mp.>200 °C; ^{1}H NMR (MeOD): δ 7.95 (d, J = 8.0 Hz, 1H), 7.50 (s, 1H), 7.07 (d, J = 8.0 Hz, 1H), 6.88-6.87 (m, 1H), 6.49-6.48 (m, 1H), 6.16-6.15 (m, 1H), 2.38 (s, 3H); ^{13}C NMR (MeOD): δ 144.3, 140.6, 135.0, 134.2, 134.1, 132.1, 129.3, 122.4, 112.0, 111.7, 23.7; HRMS: calcd for $C_{11}H_{12}NO_3S$ $[M+H]^+$ 238.0538, found 238.0531; IR (KBr): 3369, 2912, 1601, 1481, 1384, 1207, 1094 cm^{-1}.

Methyl 5-(4-methyl-2-(N-propylsulfamoyl)phenyl)-1*H*-pyrrole-2-carboxylate (32)



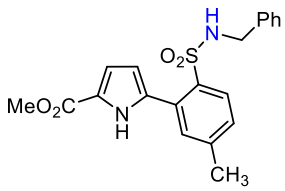
White solid; Yield 87% (139 mg); mp.108-110 °C; ^{1}H NMR($CDCl_3$): δ 10.4 (bs., 1H), 8.03 (d, J = 8.1 Hz, 1H), 7.40 (s, 1H), 7.30 (dd, J = 8.0, 0.6 Hz, 1H), 7.01-6.99 (m, 1H), 6.48-6.46 (m, 1H), 3.92 (bs, 1H), 3.88 (s, 3H), 2.62 (q, J = 7.3 Hz, 2H), 2.45 (s, 3H), 1.29-1.20 (m, 2H), 0.68 (t, J = 6.4 Hz, 3H); ^{13}C NMR($CDCl_3$): δ 160.9, 143.6, 133.8, 132.8, 132.8, 130.4, 129.8, 128.9, 124.0, 116.1, 111.9, 51.7, 44.8, 22.5, 21.3, 10.9; HRMS: calcd for $C_{16}H_{21}N_2O_4S$ $[M+H]^+$ 337.1222, found 337.1229; IR (KBr): 3319, 2924, 2853, 1705, 1459, 1326, 1155, 763 cm^{-1}.

Methyl 5-(4-methyl-2-(N-(3-morpholinopropyl)sulfamoyl)phenyl)-1*H*-pyrrole-2 carboxylate (33)



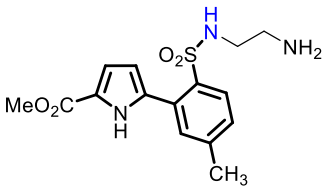
Colorless semi-solid; Yield 85% (89 mg); ^{1}H NMR($CDCl_3$): δ 10.76 (s, 1H), 8.04 (d, J = 8.1 Hz, 1H), 7.42 (d, J = 1.1 Hz, 1H), 7.27 (d, J = 7.0 Hz, 1H), 6.97 (d, J = 3.4 Hz, 1H), 6.48 (d, J = 2.9 Hz, 1H), 3.88 (s, 3H), 3.57 (t, J = 4.4 Hz, 4H), 2.80 (t, J = 5.9 Hz, 2H), 2.44 (s, 3H), 2.28 (t, J = 5.8 Hz, 6H), 1.49 (t, J = 5.9 Hz, 2H); ^{13}C NMR($CDCl_3$): δ 160.0, 143.7, 133.4, 133.3, 132.9, 130.9, 130.3, 128.6, 123.9, 115.9, 111.5, 66.7, 57.7, 53.4, 51.6, 43.0, 29.6, 24.3, 21.3, 14.1; HRMS: calcd for $C_{20}H_{28}N_3O_5S$ $[M+H]^+$ 422.1750, found 422.1752; IR (ATR): 3434, 1634, 1534, 749 cm^{-1}.

Methyl 5-(2-(N-benzylsulfamoyl)-5-methylphenyl)-1H-pyrrole-2-carboxylate (34)



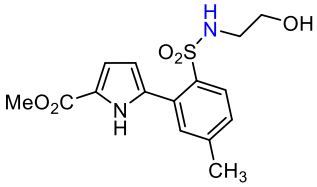
Yellowish liquid; Yield 15% (6 mg); ^{1}H NMR ($CDCl_3$): δ 10.30 (s, 1H), 8.09 (d, J = 8.0 Hz, 1H), 7.36 (s, 1H), 7.33 (d, J = 8.2 Hz, 1H), 7.23-7.18 (m, 3H), 6.96-6.94 (m, 3H), 4.19 (s, 1H), 3.88 (s, 5H), 2.47 (s, 3H); ^{13}C NMR($CDCl_3$): δ 160.8, 143.8, 135.5, 133.9, 132.7, 132.6, 130.5, 130.0, 128.9, 128.5, 127.9, 124.1, 121.9, 116.0, 112.1, 104.8, 51.6, 47.3, 21.3; HRMS: calcd for $C_{20}H_{21}N_2O_4S$ $[M+H]^+$ 385.1222, found 385.1220; IR (ATR): 3490, 1633, 1550, 810 cm^{-1}.

Methyl 5-(2-(N-(3-aminoethyl)sulfamoyl)-5-methylphenyl)-1*H*-pyrrole-2-carboxylate (35)



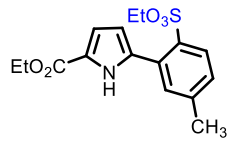
Colorless semi-solid; Yield 70% (24 mg); ^{1}H NMR($CDCl_3$): δ 8.03 (d, J = 8.1 Hz, 1H), 7.39 (s, 1H), 7.29-7.27 (m, 1H), 6.97 (d, J = 3.8 Hz, 1H), 6.45 (d, J = 3.8 Hz, 1H), 3.84 (s, 3H), 2.83-2.80 (m, 2H), 2.66-2.63 (m, 2H), 2.44 (s, 3H); ^{13}C NMR($CDCl_3$): δ 157.7, 153.7, 142.2, 133.1, 132.9, 130.5, 129.0, 120.1, 116.1, 114.3, 111.8, 53.4, 45.0, 29.6, 14.1; HRMS (ESI) m/z calcd for $C_{15}H_{20}N_3O_4S$ $[M+H]^+$ 338.1175, found 338.1177; IR (ATR): 3534, 2830, 1365, 1105 cm^{-1}.

Methyl 5-(2-(N-(3-aminoethyl)sulfamoyl)-5-methylphenyl)-1*H*-pyrrole-2-carboxylate (36)



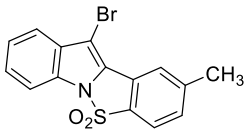
Colorless semi-solid; 55% (19 mg); mp.137-138 $^{\circ}$C ^{1}H NMR($CDCl_3$): δ 10.56 (s, 1H), 8.07 (d, J = 8.1 Hz, 1H), 7.43 (s, 1H), 7.33 (d, J = 7.2 Hz, 1H), 7.03-7.01 (m, 1H), 6.51 (m, 1H), 4.5 (s, 1H), 3.90 (s, 3H), 3.50-3.49 (m 2H), 2.90-2.89 (m, 2H), 2.47 (s, 3H); ^{13}C NMR ($CDCl_3$): δ 161.2, 143.9, 133.7, 133.0, 132.9, 130.5, 130.1, 129.0, 124.1, 116.1, 114.0, 111.8, 60.8, 51.7, 45.0, 22.6; HRMS (ESI) m/z calcd for $C_{15}H_{19}N_2O_5S$ $[M+H]^+$ 339.1015, found 339.1000; IR (ATR, cm^{-1}): 3443, 2923, 1725, 1255 cm^{-1};

Methyl 5-(2-(ethoxysulfonyl)-4-methylphenyl)-1*H*-pyrrole-2-carboxylate (37)



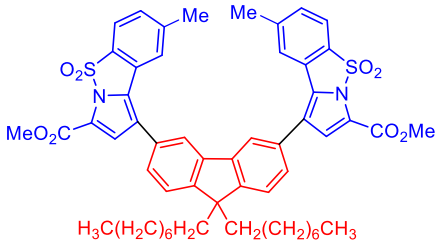
Colorless liquid; Yield 82% (67 mg); ^{1}H NMR ($CDCl_3$): δ 8.04 (d, J = 8.1 Hz, 1H), 7.51 (s, 1H), 7.30–7.28 (m, 1H), 6.99 - 6.97 (m, 1H), 6.50–6.49 (m, 1H), 4.37 (q, J = 7.1 Hz, 2H), 4.02 (q, J = 7.1 Hz, 2H), 2.48 (s, 3H), 1.41 (t, J = 7.0 Hz, 3H), 1.13 (t, J = 7.0 Hz, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.7, 144.9, 132.7, 132.5, 131.1, 130.8, 129.8, 128.4, 124.5, 115.4, 111.8, 67.2, 60.4, 21.4, 14.4; HRMS (ESI) m/z calcd for $C_{15}H_{18}NO_5S$ $[M+H]^+$ 338.1062, found 338.1066; IR (ATR): 3363, 2983, 2926, 1704, 1599, 1249, 1176, 916 cm^{-1}.

11-Bromo-2-methylbenzo[4,5]isothiazolo[2,3-a]indole 5,5-dioxide (41)



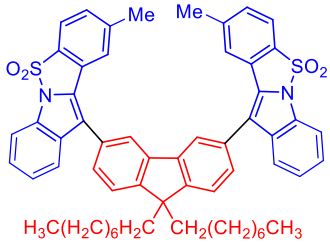
Whitish Solid; Yield 65% (90 mg); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (s, 1H), 7.77-7.72 (m, 2H), 7.62 (d, J = 8 Hz, 1H), 7.46 (t, J = 7.1 Hz, 1H), 7.40-7.36 (m, 2H), 2.57 (s, 3H); ^{13}C NMR ($CDCl_3$): δ 145.4, 130.4, 129.8, 126.9, 123.8, 123.3, 123.1, 122.4, 120.8, 111.9, 22.6; HRMS (ESI) m/z calcd for $C_{15}H_{11}BrNO_2S$ $[M+H]^+$ 347.9694, found 347.9685; IR (KBr): 2855, 1430, 1143, 740 cm^{-1}.

11,11'-(9,9-dioctyl-9H-fluorene-3,6-diyl)bis(Methyl8-methylbenzo[d]pyrrolo[1,2-b] isothiazole-3-carboxylate 5,5-dioxide (43)



Yellowish solid; Yield 70% (66 mg); mp. 257-258 ℃; ^{1}H NMR ($CDCl_3$): δ 7.89 (d, J = 7.7 Hz, 2H), 7.74 (d, J = 8.0 Hz, 2H), 7.57-7.53 (m, 6H), 7.30 (m, 2H), 7.16 (s, 2H), 4.02 (s, 6H), 2.37 (s, 6H), 2.08-2.04 (m, 4H), 1.18-1.09 (m, 12H), 0.8 (m, 6H); ^{13}C NMR ($CDCl_3$): δ 159.3, 151.7, 145.1, 140.6, 134.8, 131.8, 129.8, 129.1, 127.6, 126.7, 124.3, 124.3, 123.0, 122.8, 121.8, 120.3, 55.5, 52.5, 40.2, 31.7, 30.1, 29.3, 29.2, 24.1, 22.5, 21.9, 14.0; HRMS: calcd for $C_{55}H_{61}N_2O_8S_2$ $[M+H]^+$ 941.3869, found 941.3866; IR (KBr): 2926, 2854, 1725, 1186, 758 cm^{-1}.

11,11'-(9,9-dioctyl-9H-fluorene-3,6-diyl)bis(2-methylbenzo[4,5]isothiazolo[2,3-a]indole 5,5-dioxide) (44)



Yellowish solid; Yield 85% (78 mg); mp. 275-276 ℃; ^{1}H NMR($CDCl_3$): δ 8.03 (d, J = 7.8 Hz, 2H), 7.84 (d, J = 8.2 Hz, 2H), 7.79 (d, J = 8.0 Hz, 2H), 7.72-7.70 (m 4H)), 7.65 (d, J = 7.9 Hz, 2H), 7.59 (s, 2H), 7.50 (t, J = 7.4 Hz, 2H), 7.33-7.30 (m, 4H), 2.39 (s, 6H), 2.14-2.10 (4H), 1.13 (m, 12H), 0.80 (t, J = 6.5 Hz, 6H); ^{13}C NMR($CDCl_3$): δ 151.9, 144.9, 140.7, 135.6, 133.2, 132.5, 130.8, 130.0, 128.6, 128.6, 128.2, 126.3, 124.3, 123.5, 122.5, 121.3, 120.5, 118.8 111.9, 55.5, 40.1, 31.7, 30.1, 29.4, 29.2, 24.3, 22.5, 22.0, 14.0; HRMS: calcd for $C_{59}H_{61}N_2O_4S_2$ $[M+H]^+$ 925.4073, found 925.4077; IR (KBr): 2925, 2854, 1339, 1027 cm^{-1}.

4. REFERENCES

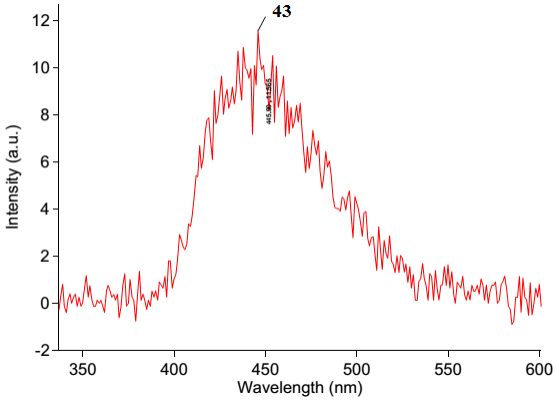
1. J. K. Laha, N. Dayal, K. Jethava, D. V. Prajapati, *Org. Lett.* **2015**, *17*, 1296-1299;

2. J. K. Laha, S. Sharma, R. A. Bhimpuria, N. Dayal, *New J. Chem.* **2017**, DOI: 10.1039/c7nj01709j;

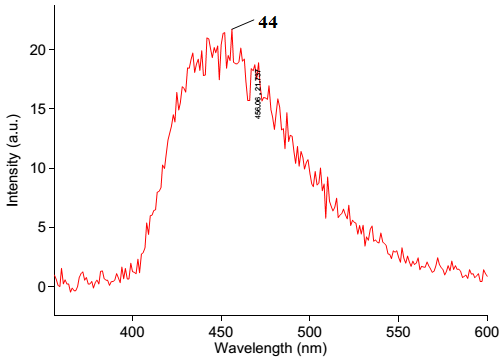
3. C. Schmmuck, *Tetrahedron* **2001**, *57*, 3063-3067;

4. J. K. Augustine, A. Bombrun, R. N. Atta, *Synlett* **2011**, *15*, 2223-2227.

EMISSION SPECTRA OF 43,44

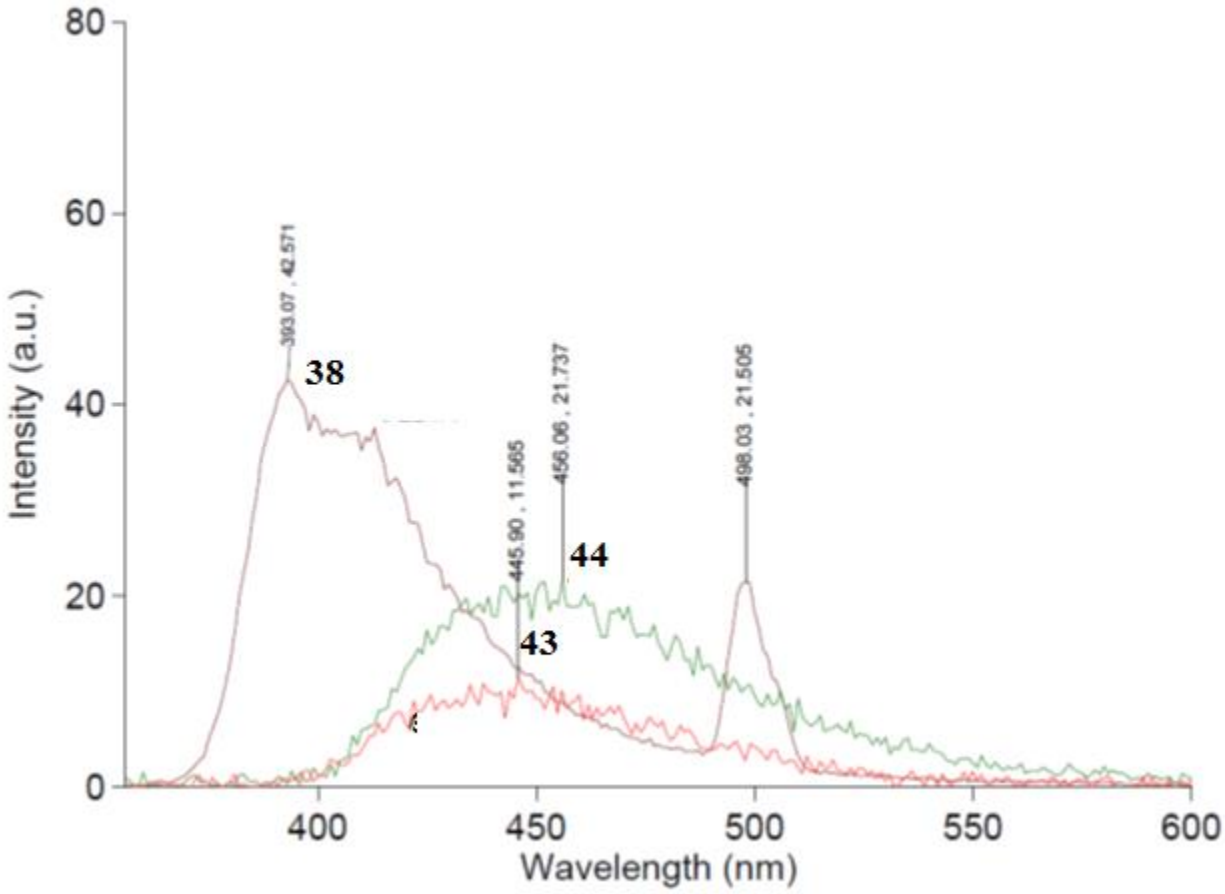


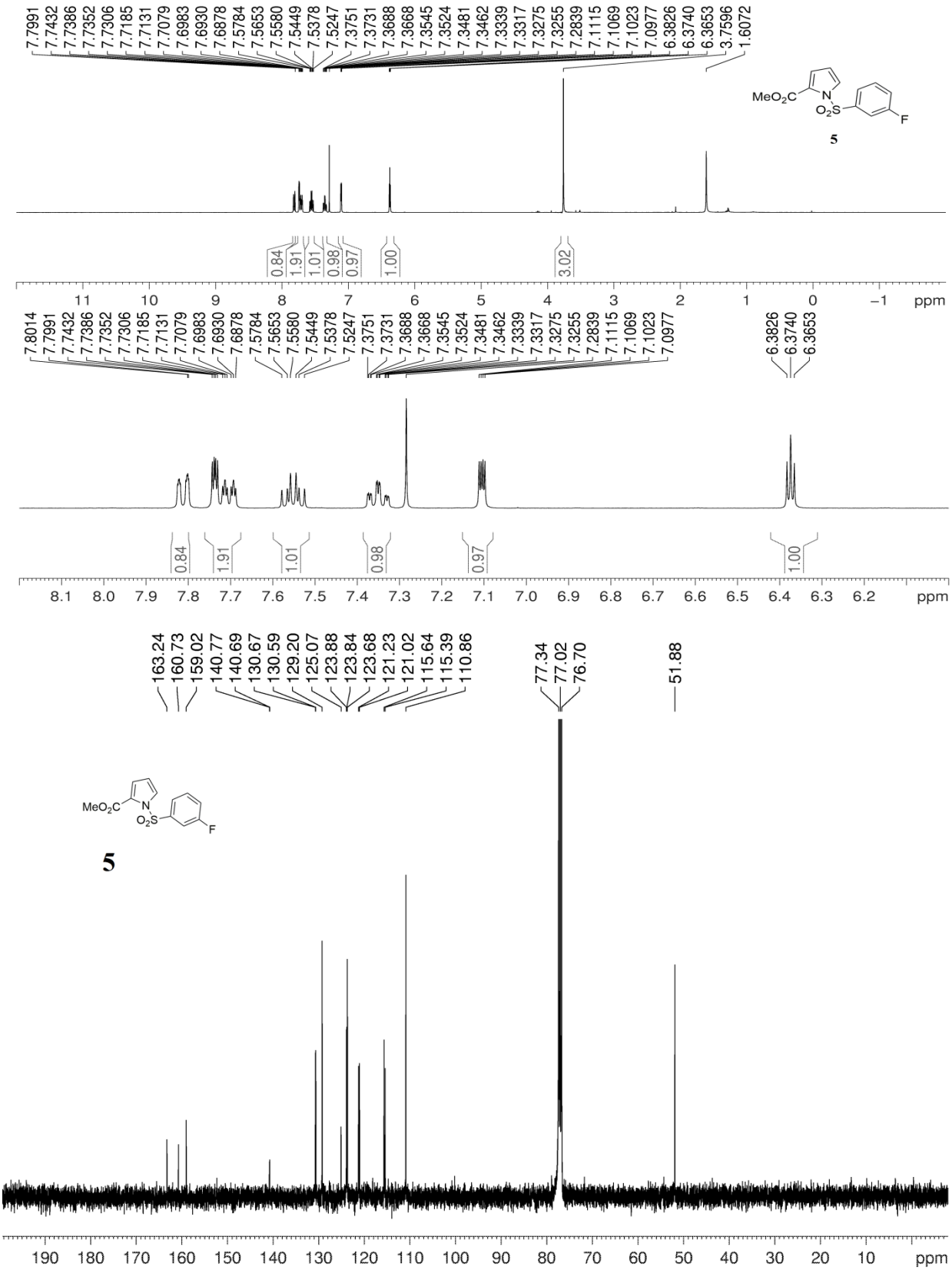
43



44

OVERLAY EMISSION SPECTRA OF 38, 43 and 44

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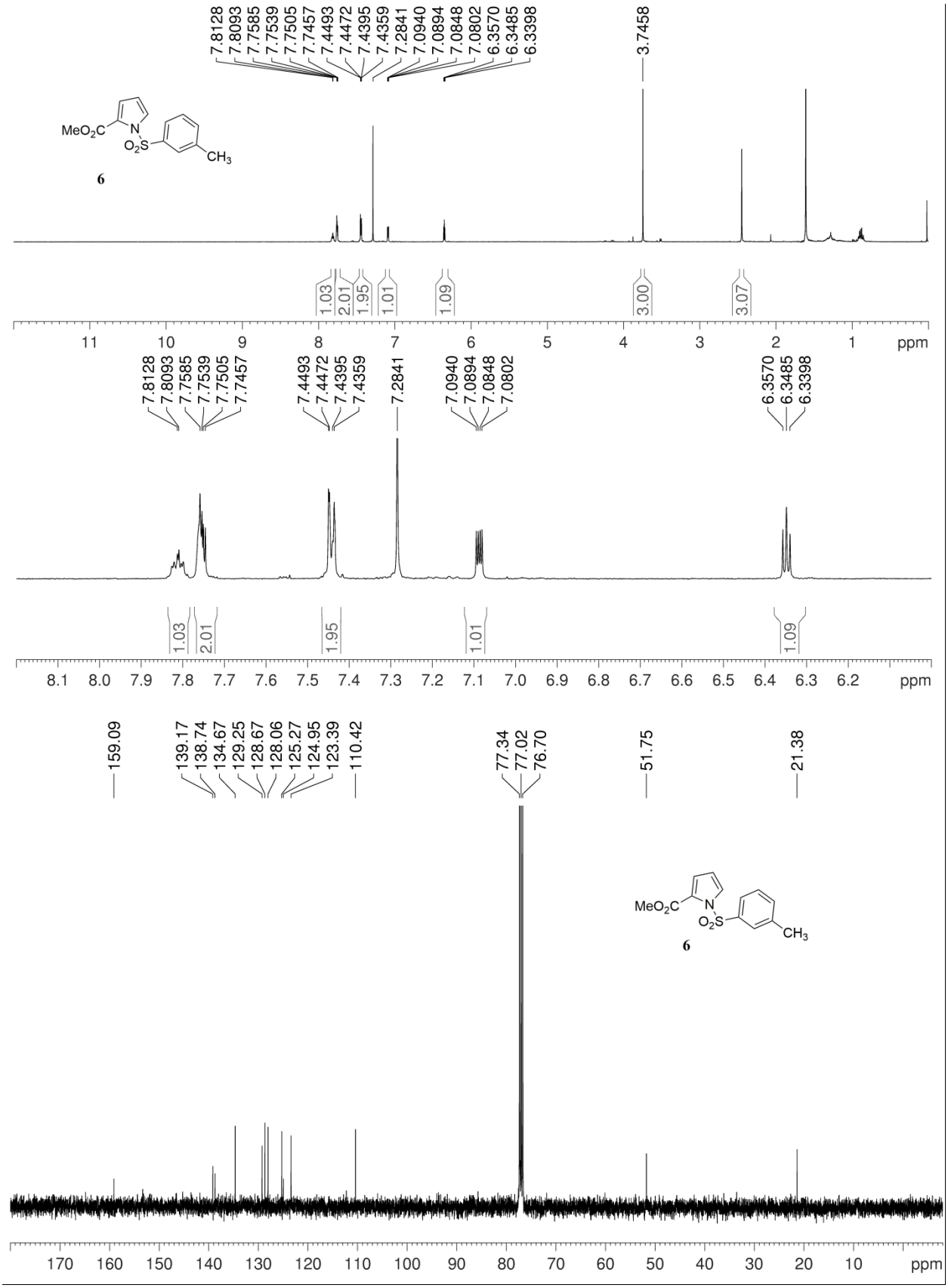
7.7432
7.7386
7.7352
7.7306
7.7185
7.7131
7.7079
7.6983
7.6930
7.6878
7.5784
7.5653
7.5580
7.5449
7.5378
7.5247
7.3751
7.3731
7.3688
7.3668
7.3545
7.3524
7.3481
7.3462
7.3339
7.3317
7.3275
7.3255
7.2839
7.1115
7.1069
7.1023
7.0977
6.3826
6.3740
6.3653
3.7596
1.6072
MeO2C
N
O2S
F
5
0.84
1.91
1.01
0.98
0.97
1.00
3.02
ppm
7.8014
6.3826
6.3740
6.3653
0.84
1.91
1.01
0.98
0.97
1.00
ppm
163.24
160.73
159.02
140.77
140.69
130.67
130.59
129.20
125.07
123.88
123.84
123.68
121.23
121.02
115.64
115.39
110.86
77.34
77.02
76.70
51.88
MeO2C
N
O2S
F
5
ppm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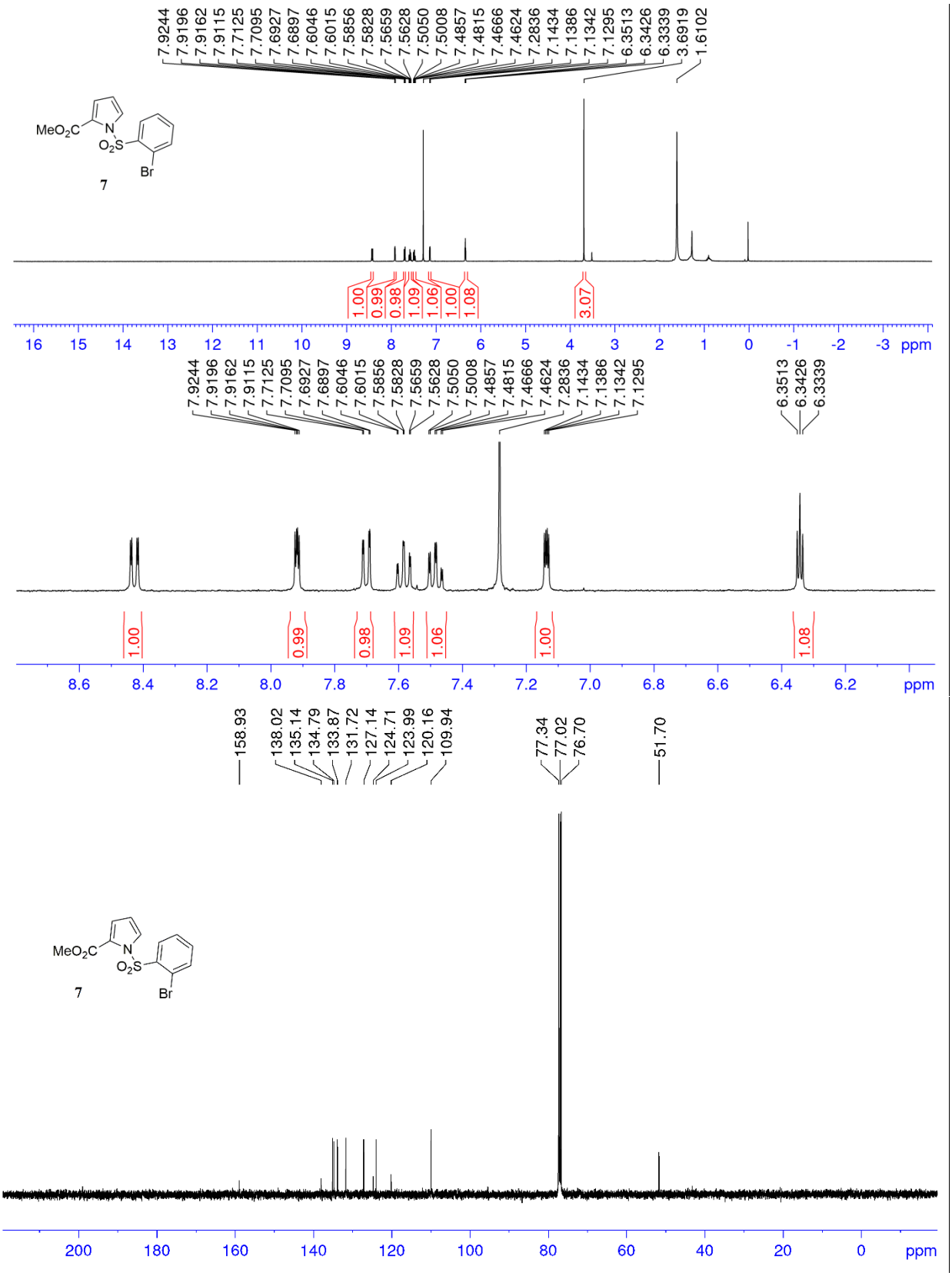
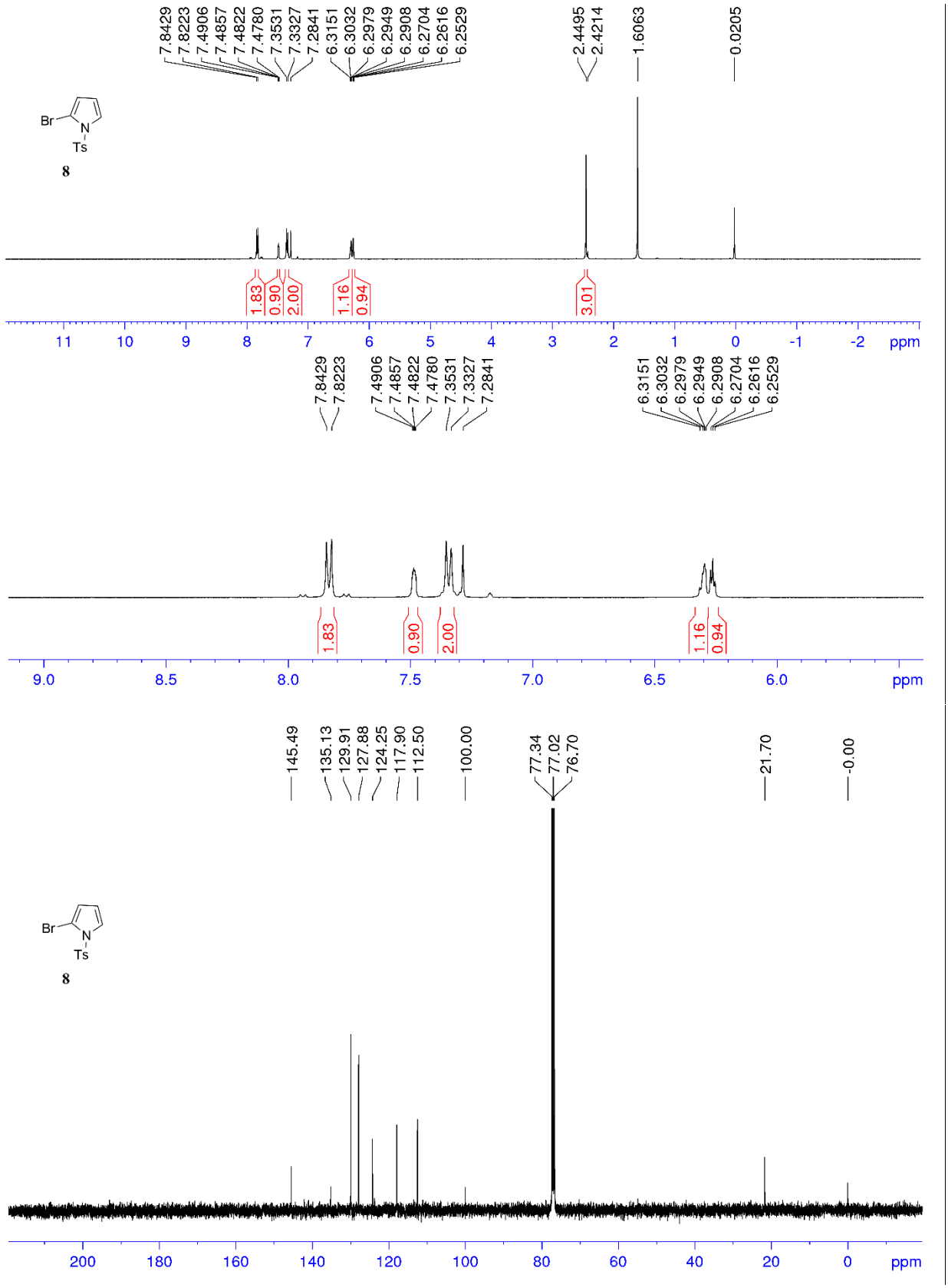
7.8093
7.7585
7.7539
7.7505
7.7457
7.4493
7.4472
7.4395
7.4359
7.2841
7.0940
7.0894
7.0848
7.0802
6.3570
6.3485
6.3398
3.7458
MeO2C
N
O2S
CH3
6
1.03
2.01
1.95
1.01
1.09
3.00
3.07
ppm
159.09
139.17
138.74
134.67
129.25
128.67
128.06
125.27
124.95
123.39
110.42
77.34
77.02
76.70
51.75
21.38


7.9244
7.9196
7.9162
7.9115
7.7125
7.7095
7.6927
7.6897
7.6046
7.6015
7.5856
7.5828
7.5659
7.5628
7.5050
7.5008
7.4857
7.4815
7.4666
7.4624
7.2836
7.1434
7.1386
7.1342
7.1295
6.3513
6.3426
6.3339
3.6919
1.6102
MeO2C
N
O2S
Br
7
1.00
0.99
0.98
1.09
1.06
1.00
1.08
3.07
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 ppm
158.93
138.02
135.14
134.79
133.87
131.72
127.14
124.71
123.99
120.16
109.94
77.34
77.02
76.70
51.70
200 180 160 140 120 100 80 60 40 20 0 ppm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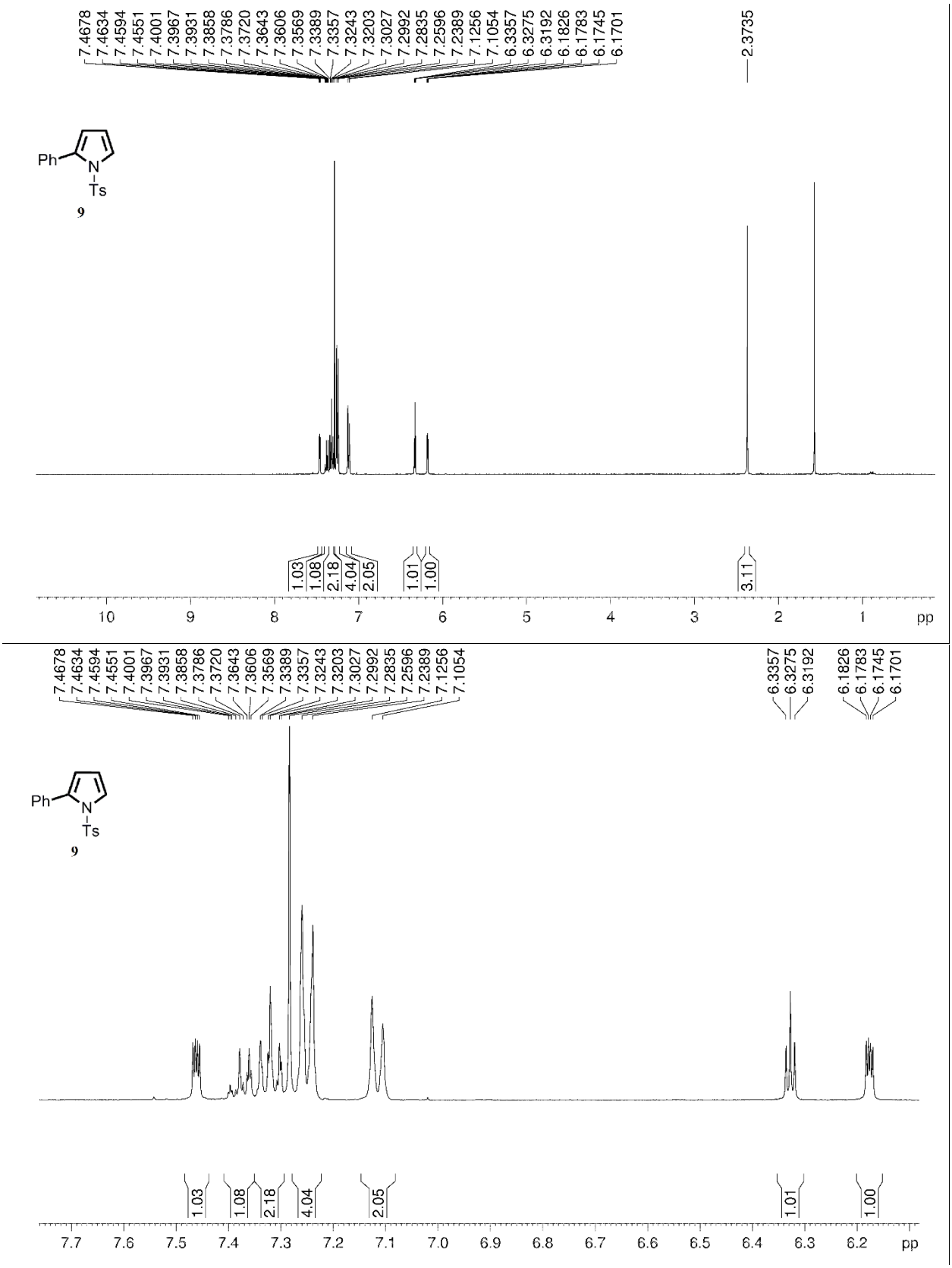
7.4906
7.4857
7.4822
7.4780
7.3531
7.3327
7.2841
6.3151
6.3032
6.2979
6.2949
6.2908
6.2704
6.2616
6.2529
2.4495
2.4214
1.6063
0.0205
Br
N
Ts
8
1.83
0.90
2.00
1.16
0.94
3.01
ppm
145.49
135.13
129.91
127.88
124.25
117.90
112.50
100.00
77.34
77.02
76.70
21.70
-0.00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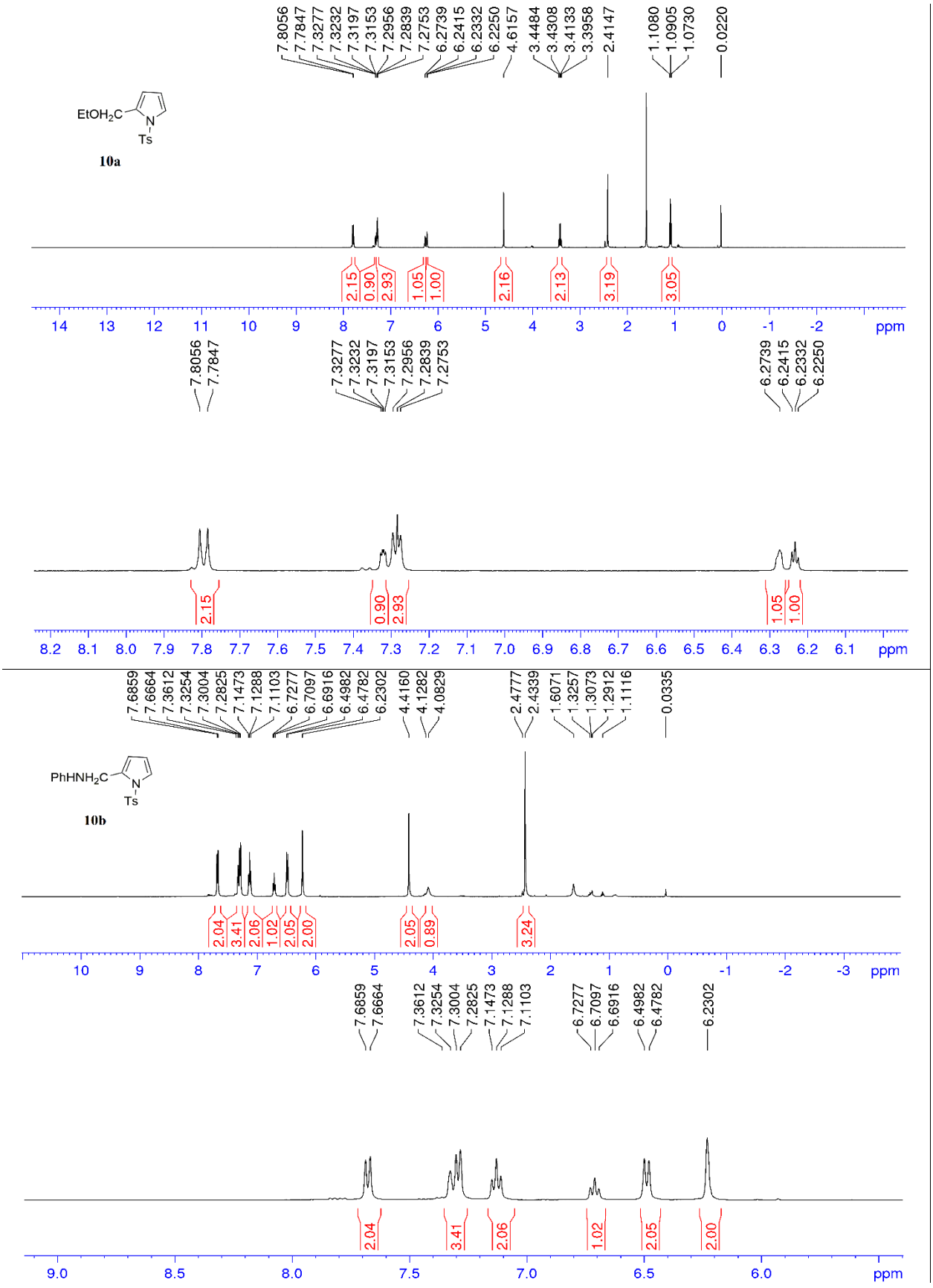
7.4634
7.4594
7.4551
7.4001
7.3967
7.3931
7.3858
7.3786
7.3720
7.3643
7.3606
7.3569
7.3389
7.3357
7.3243
7.3203
7.3027
7.2992
7.2835
7.2596
7.2389
7.1256
7.1054
6.3357
6.3275
6.3192
6.1826
6.1783
6.1745
6.1701
2.3735
Ph
N
Ts
9
1.03
1.08
2.18
4.04
2.05
1.01
1.00
3.11
10
9
8
7
6
5
4
3
2
1
pp
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2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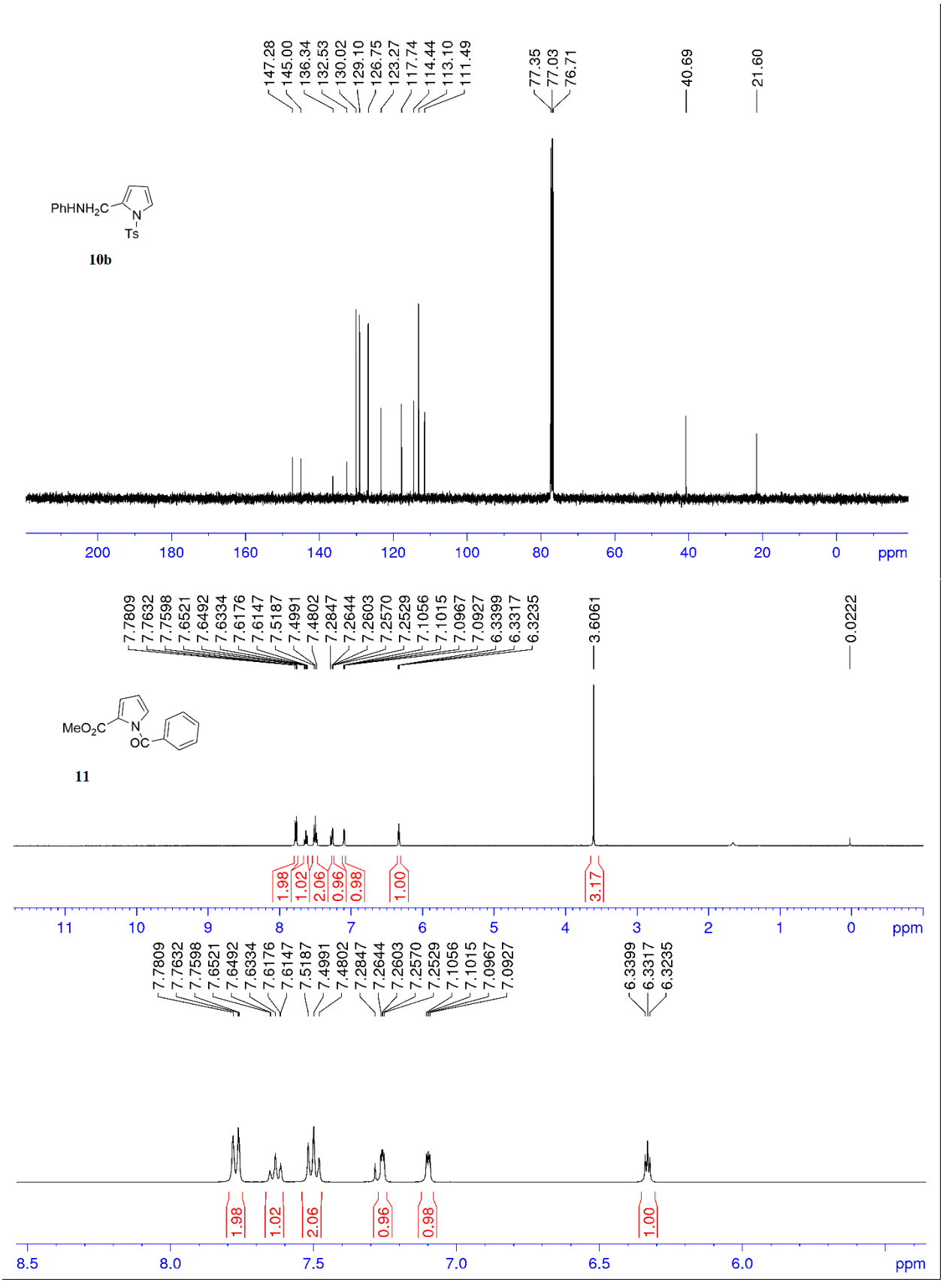
7.7847
7.3277
7.3232
7.3197
7.3153
7.2956
7.2839
7.2753
6.2739
6.2415
6.2332
6.2250
4.6157
3.4484
3.4308
3.4133
3.3958
2.4147
1.1080
1.0905
1.0730
0.0220
EtOH2C
N
Ts
10a
2.15
0.90
2.93
1.05
1.00
2.16
2.13
3.19
3.05
ppm
7.6859
7.6664
7.3612
7.3254
7.3004
7.2825
7.1473
7.1288
7.1103
6.7277
6.7097
6.6916
6.4982
6.4782
6.2302
4.4160
4.1282
4.0829
2.4777
2.4339
1.6071
1.3257
1.3073
1.2912
1.1116
0.0335
PhHNH2C
N
Ts
10b
2.04
3.41
2.06
1.02
2.05
2.00
2.05
0.89
3.24
ppm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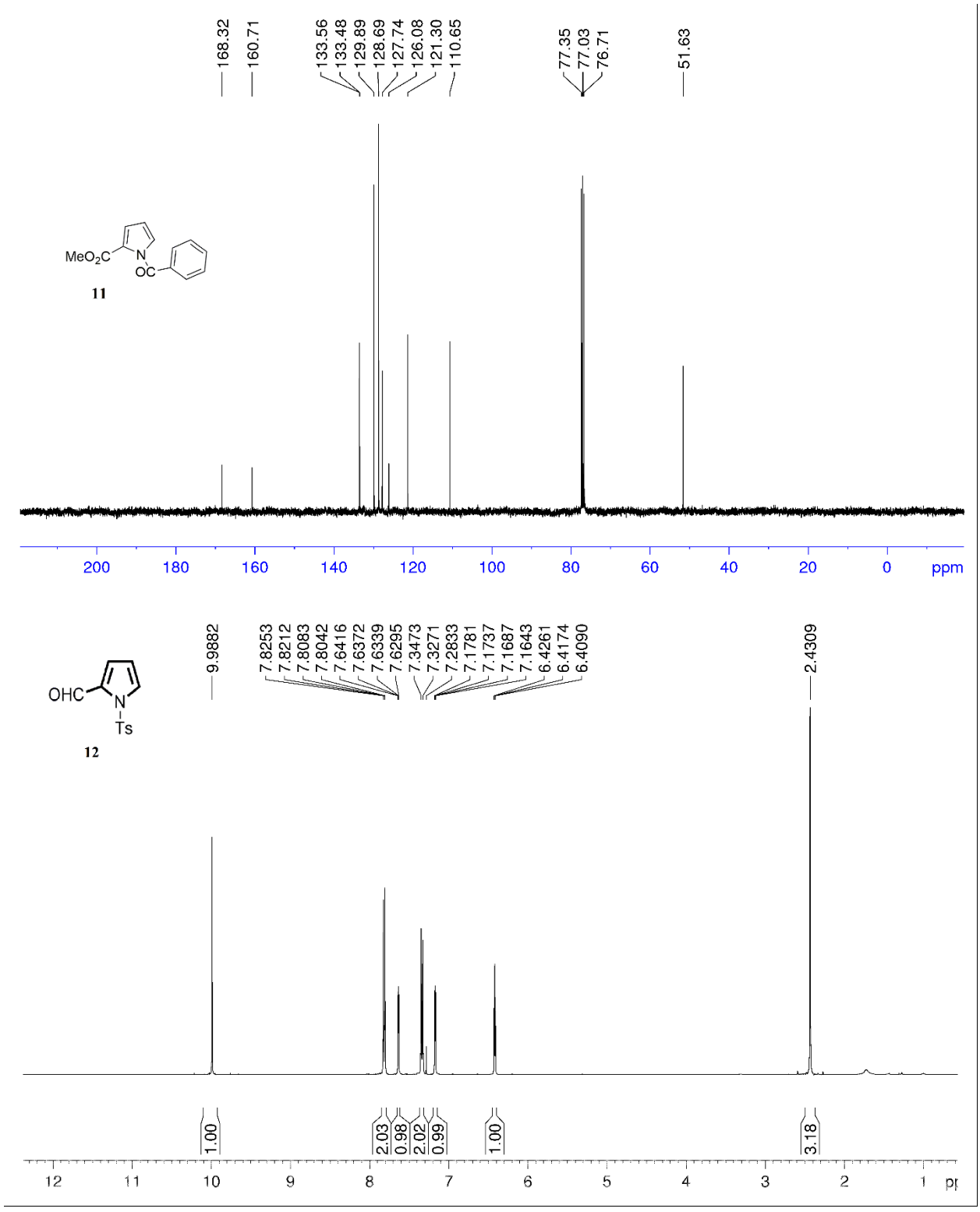
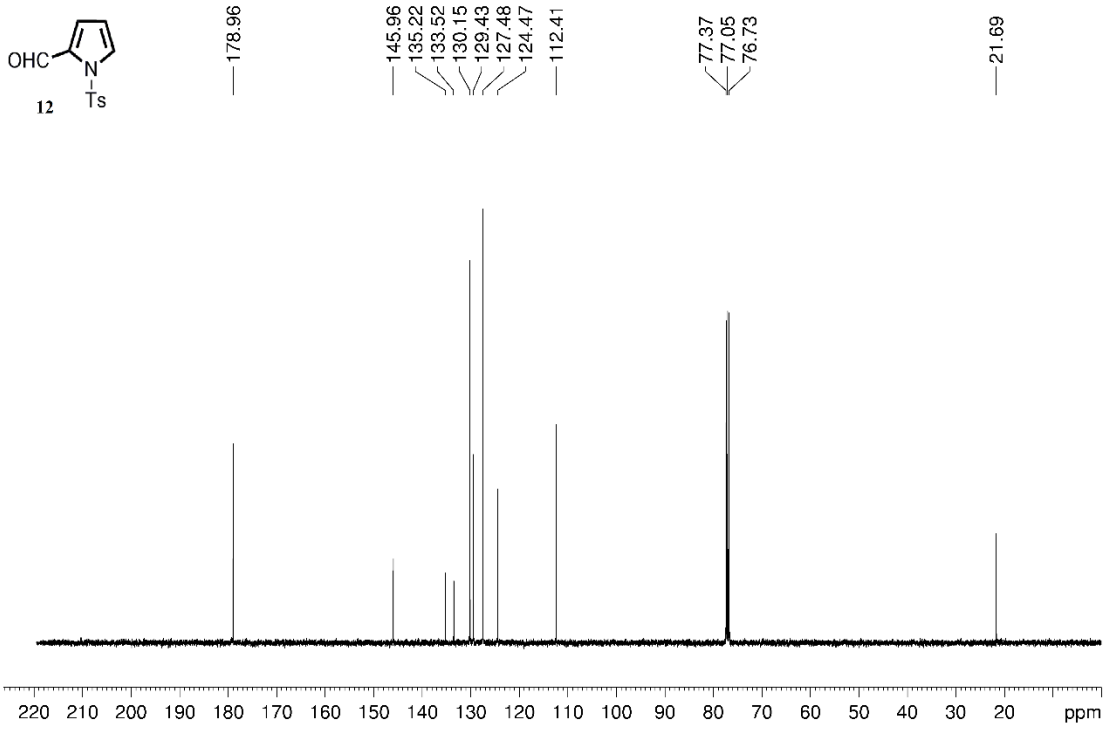
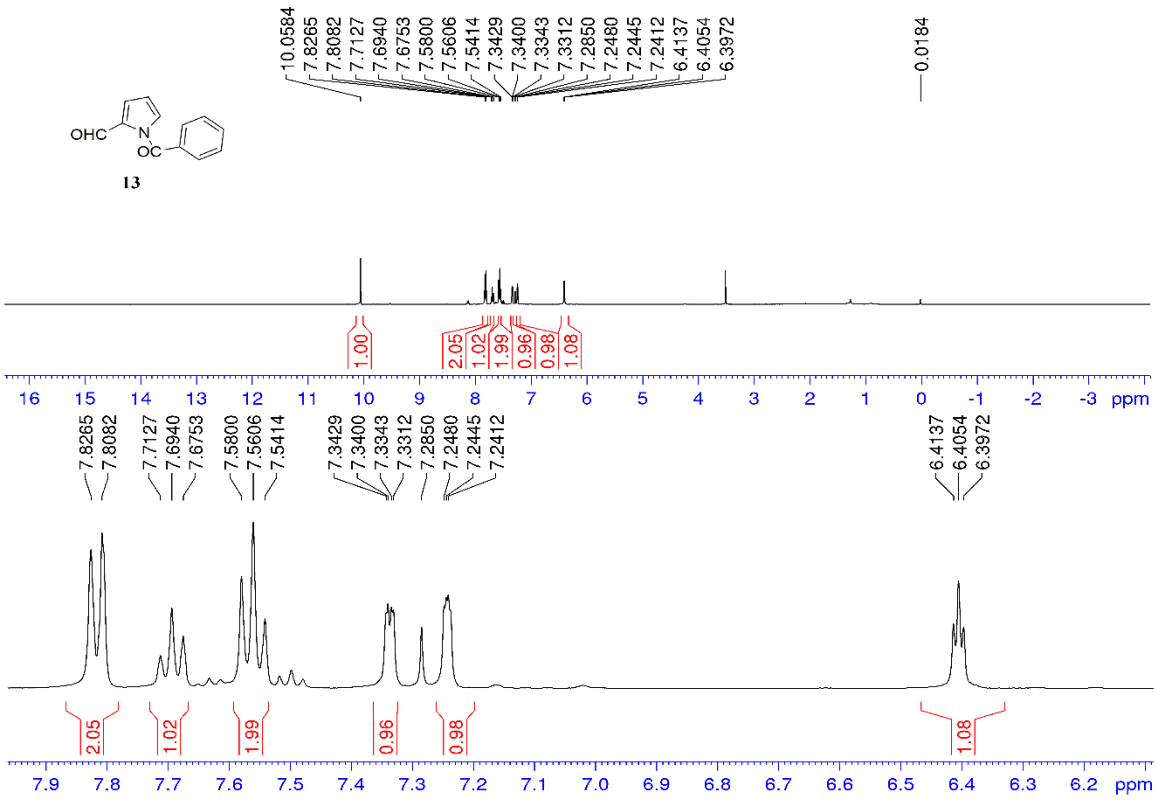
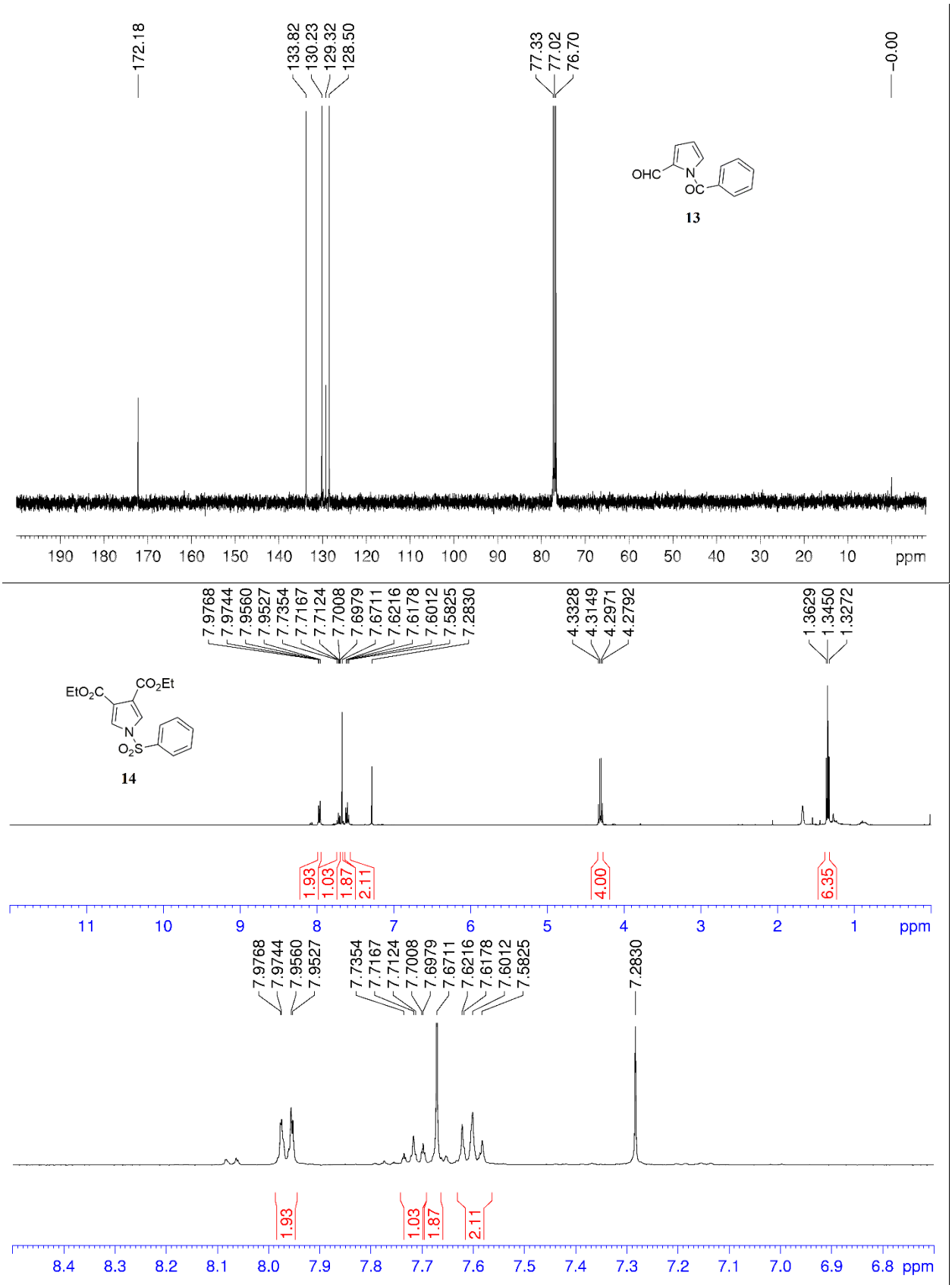
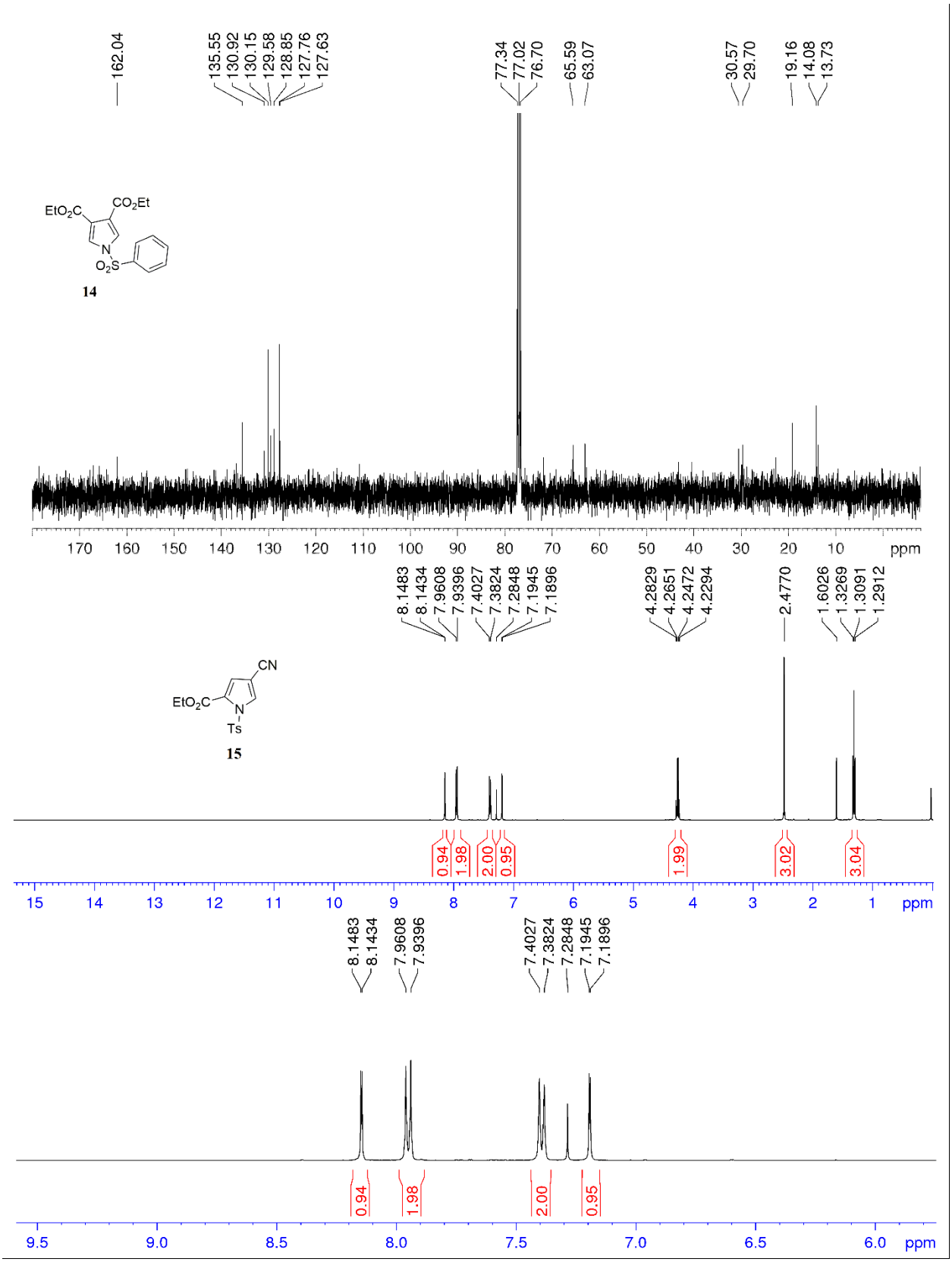
145.00
136.34
132.53
130.02
129.10
126.75
123.27
117.74
114.44
113.10
111.49
77.35
77.03
76.71
40.69
21.60
PhHNH2C
N
Ts
10b
200
180
160
140
120
100
80
60
40
20
0
ppm
7.7809
7.7632
7.7598
7.6521
7.6492
7.6334
7.6176
7.6147
7.5187
7.4991
7.4802
7.2847
7.2644
7.2603
7.2570
7.2529
7.1056
7.1015
7.0967
7.0927
6.3399
6.3317
6.3235
3.6061
0.0222
MeO2C
N
OC
11
1.98
1.02
2.06
0.96
0.98
1.00
3.17
11
10
9
8
7
6
5
4
3
2
1
0
ppm
8.5
8.0
7.5
7.0
6.5
6.0
ppm


168.32
160.71
133.56
133.48
129.89
128.69
127.74
126.08
121.30
110.65
77.35
77.03
76.71
51.63
MeO2C
N
OC
11
200
180
160
140
120
100
80
60
40
20
0
ppm
9.9882
7.8253
7.8212
7.8083
7.8042
7.6416
7.6372
7.6339
7.6295
7.3473
7.3271
7.2833
7.1781
7.1737
7.1687
7.1643
6.4261
6.4174
6.4090
2.4309
OHC
N
Ts
12
1.00
2.03
0.98
2.02
0.99
1.00
3.18
12
11
10
9
8
7
6
5
4
3
2
1
ppm


OHC
N
Ts
12
178.96
145.96
135.22
133.52
130.15
129.43
127.48
124.47
112.41
77.37
77.05
76.73
21.69
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


OHC
N
OC
13
10.0584
7.8265
7.8082
7.7127
7.6940
7.6753
7.5800
7.5606
7.5414
7.3429
7.3400
7.3343
7.3312
7.2850
7.2480
7.2445
7.2412
6.4137
6.4054
6.3972
0.0184
1.00
2.05
1.02
1.99
0.96
0.98
1.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 ppm


172.18
133.82
130.23
129.32
128.50
77.33
77.02
76.70
0.00
OHC
N
OC
13
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
7.9768
7.9744
7.9560
7.9527
7.7354
7.7167
7.7124
7.7008
7.6979
7.6711
7.6216
7.6178
7.6012
7.5825
7.2830
4.3328
4.3149
4.2971
4.2792
1.3629
1.3450
1.3272
EtO2C
CO2Et
N
O2S
14
1.93
1.03
1.87
2.11
4.00
6.35
11 10 9 8 7 6 5 4 3 2 1 ppm
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm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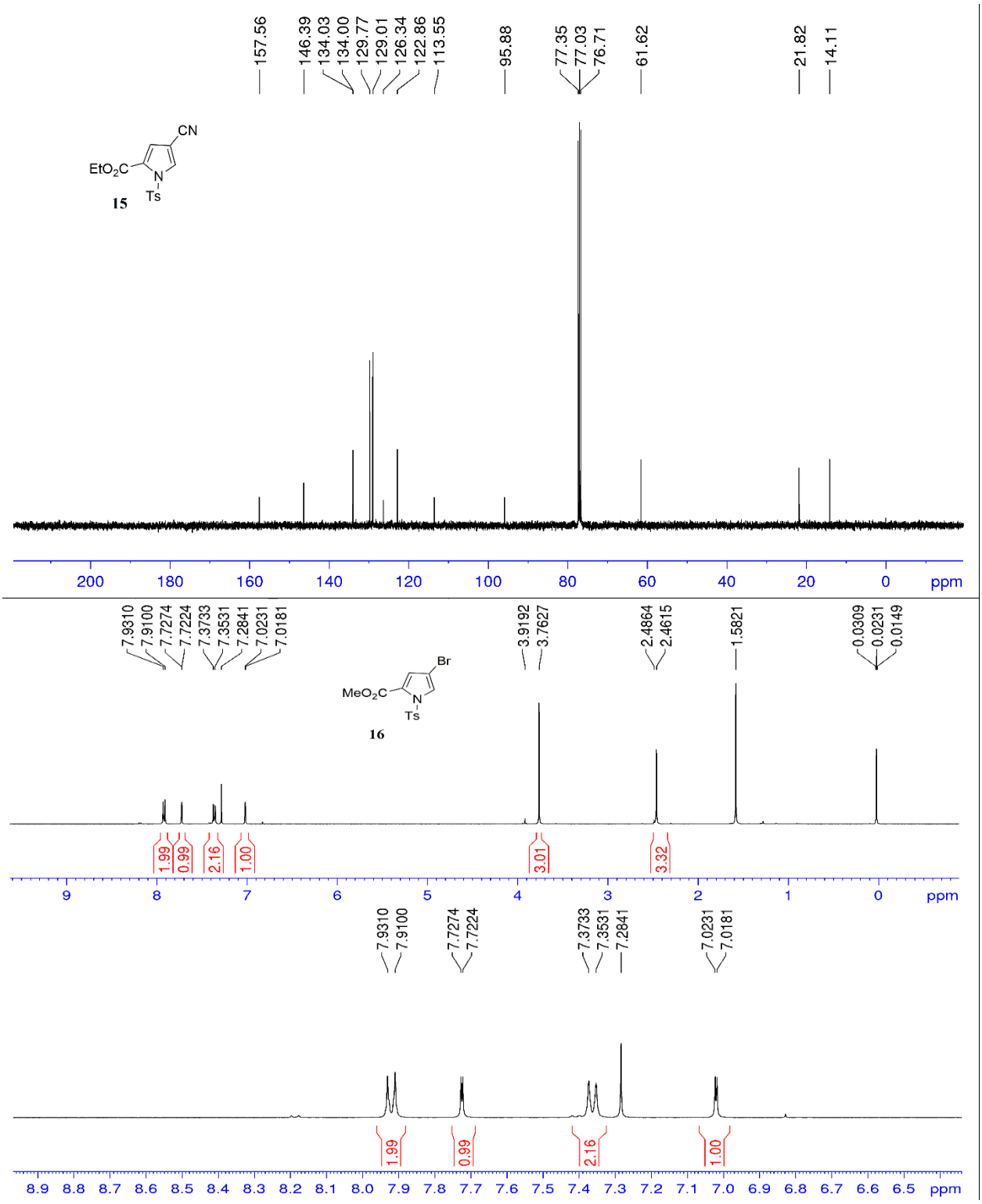
130.92
130.15
129.58
128.85
127.76
127.63
77.34
77.02
76.70
65.59
63.07
30.57
29.70
19.16
14.08
13.73
EtO2C
CO2Et
N
O2S
14
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
8.1483
8.1434
7.9608
7.9396
7.4027
7.3824
7.2848
7.1945
7.1896
4.2829
4.2651
4.2472
4.2294
2.4770
1.6026
1.3269
1.3091
1.2912
CN
EtO2C
N
Ts
15
0.94
1.98
2.00
0.95
1.99
3.02
3.04
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
8.1483
8.1434
7.9608
7.9396
7.4027
7.3824
7.2848
7.1945
7.1896
0.94
1.98
2.00
0.95
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 ppm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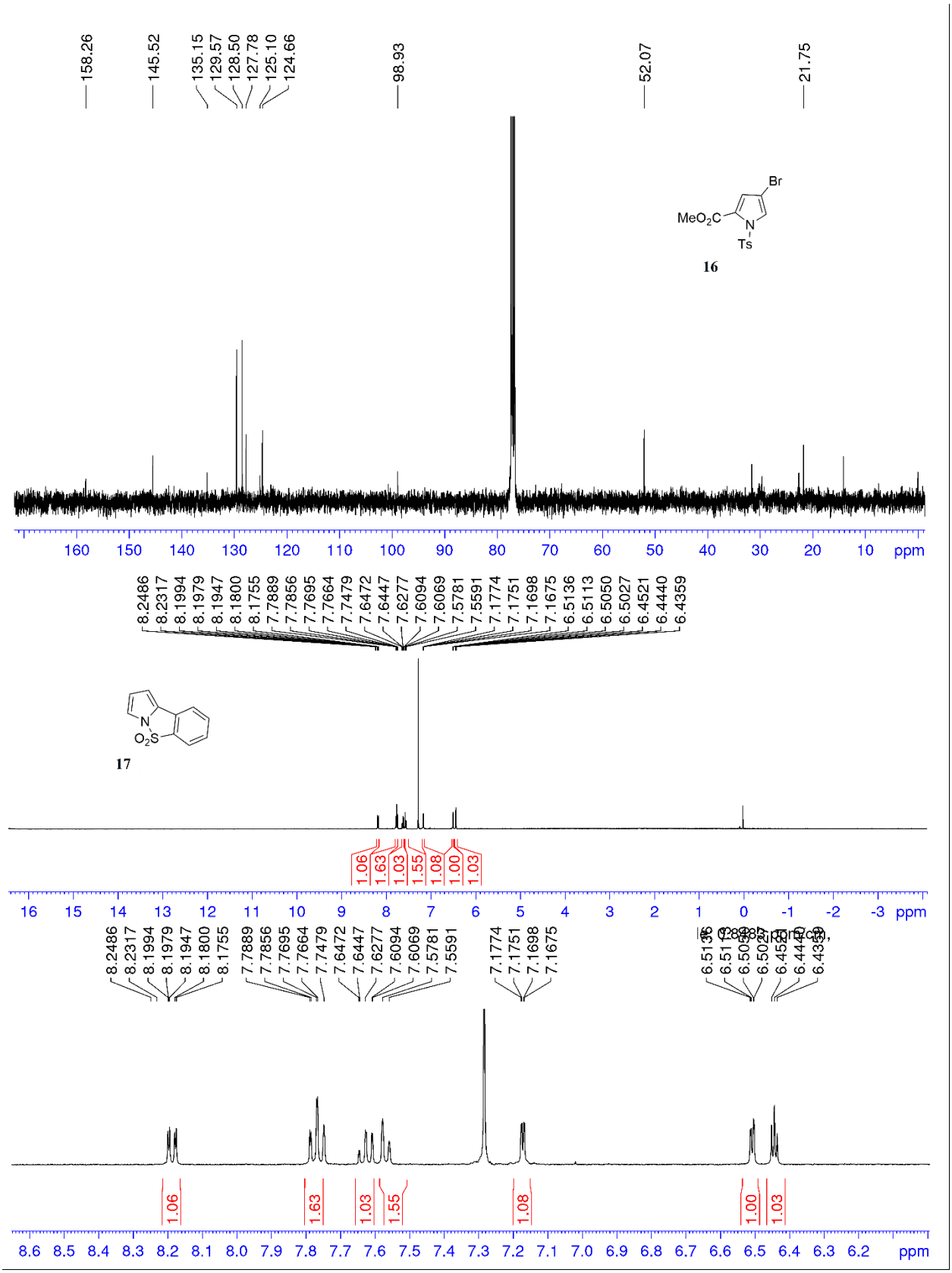
134.00
129.77
129.01
126.34
122.86
113.55
95.88
77.35
77.03
76.71
61.62
21.82
14.11
CN
EtO2C
N
Ts
15
200
180
160
140
120
100
80
60
40
20
0
ppm
7.9310
7.9100
7.7274
7.7224
7.3733
7.3531
7.2841
7.0231
7.0181
3.9192
3.7627
2.4864
2.4615
1.5821
0.0309
0.0231
0.0149
Br
MeO2C
N
Ts
16
1.99
0.99
2.16
1.00
3.01
3.32
9
8
7
6
5
4
3
2
1
0
ppm
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
ppm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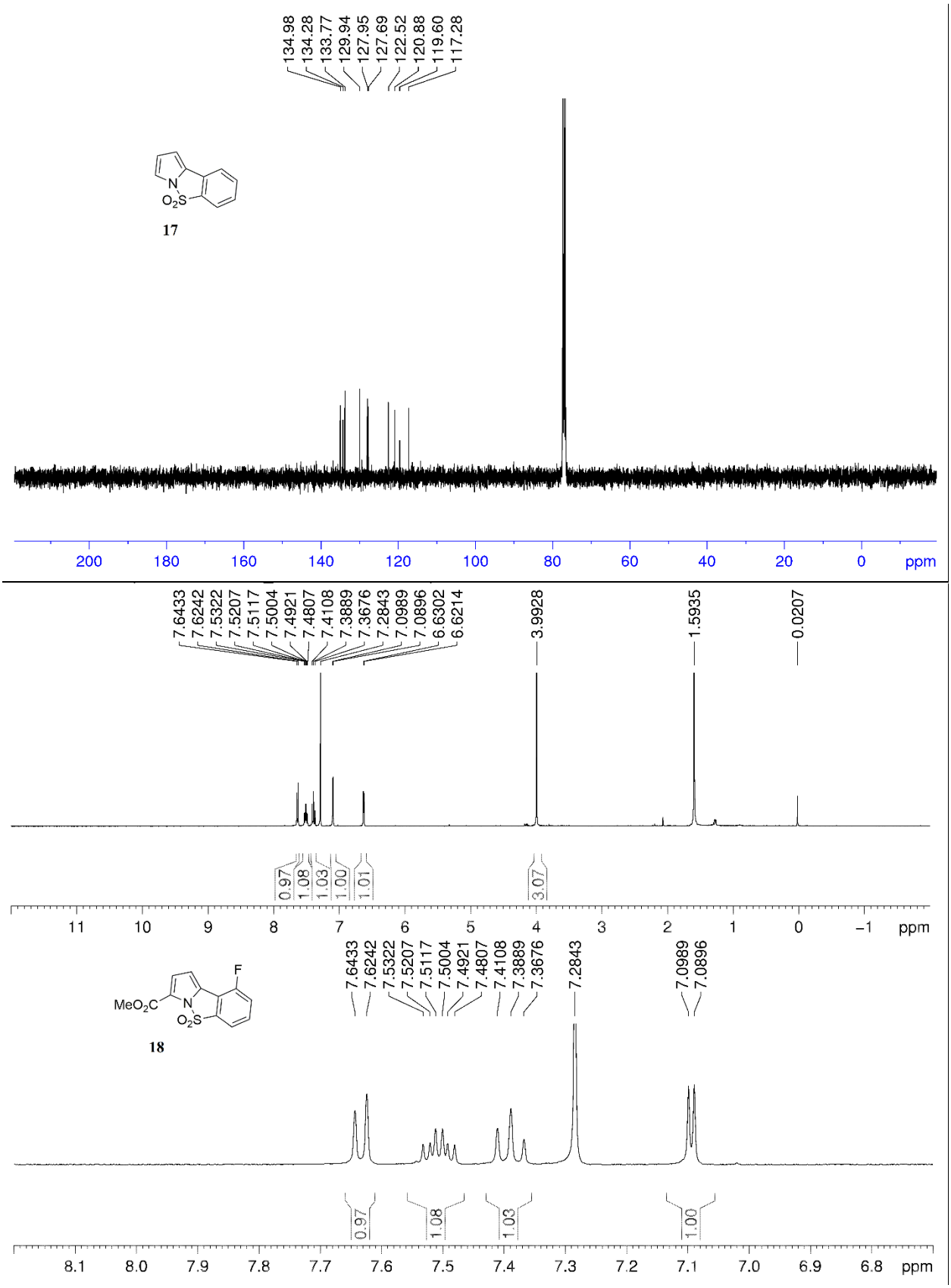
145.52
135.15
129.57
128.50
127.78
125.10
124.66
98.93
52.07
21.75
Br
MeO2C
N
Ts
16
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
8.2486
8.2317
8.1994
8.1979
8.1947
8.1800
8.1755
7.7889
7.7856
7.7695
7.7664
7.7479
7.6472
7.6447
7.6277
7.6094
7.6069
7.5781
7.5591
7.1774
7.1751
7.1698
7.1675
6.5136
6.5113
6.5050
6.5027
6.4521
6.4440
6.4359
N
O2S
17
1.06
1.63
1.03
1.55
1.08
1.00
1.03
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 ppm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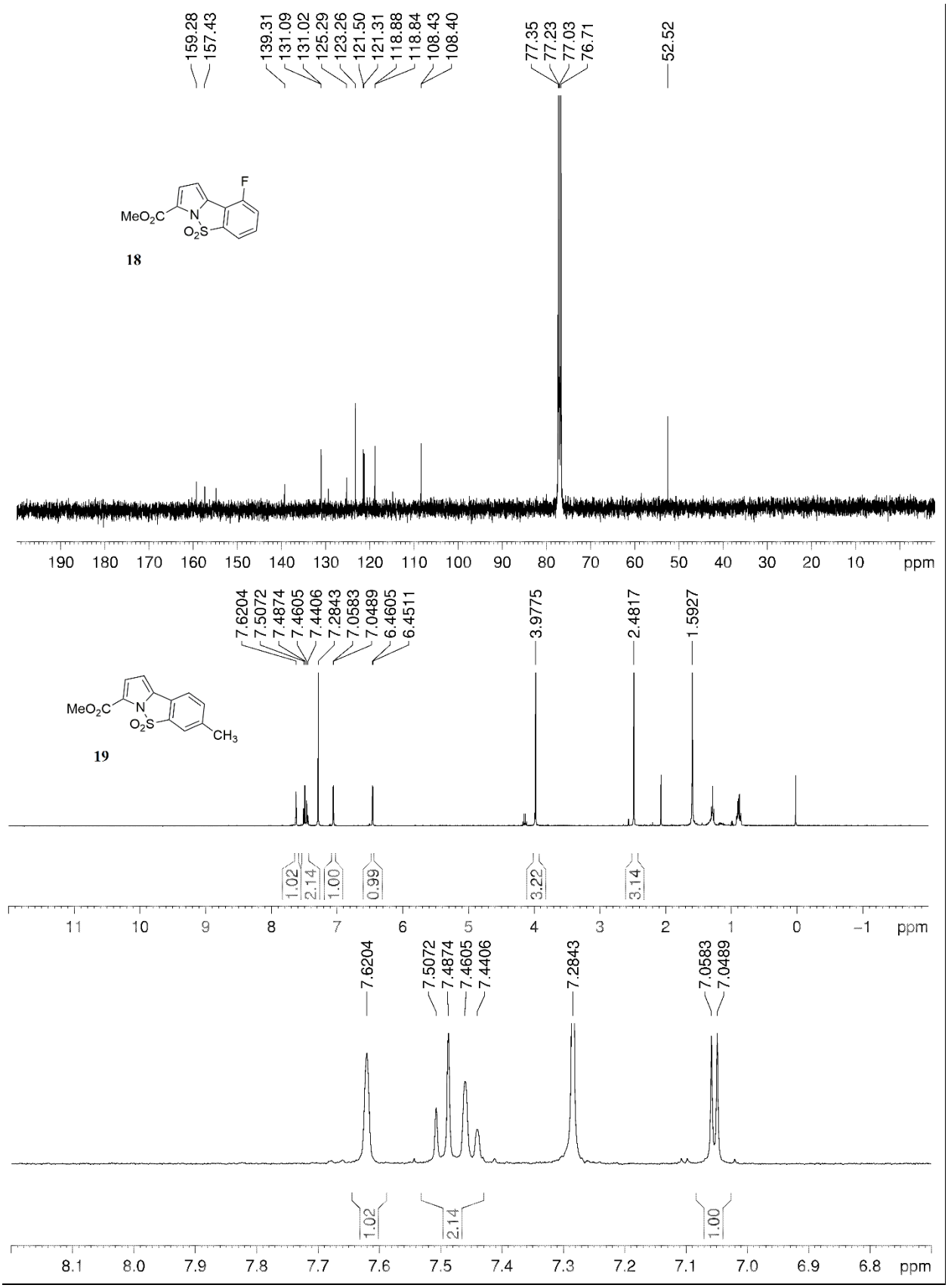
134.28
133.77
129.94
127.95
127.69
122.52
120.88
119.60
117.28
17
200
180
160
140
120
100
80
60
40
20
0
ppm
7.6433
7.6242
7.5322
7.5207
7.5117
7.5004
7.4921
7.4807
7.4108
7.3889
7.3676
7.2843
7.0989
7.0896
6.6302
6.6214
3.9928
1.5935
0.0207
0.97
1.08
1.03
1.00
1.01
3.07
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm
MeO2C
F
18
7.6433
7.6242
7.5322
7.5207
7.5117
7.5004
7.4921
7.4807
7.4108
7.3889
7.3676
7.2843
7.0989
7.0896
0.97
1.08
1.03
1.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm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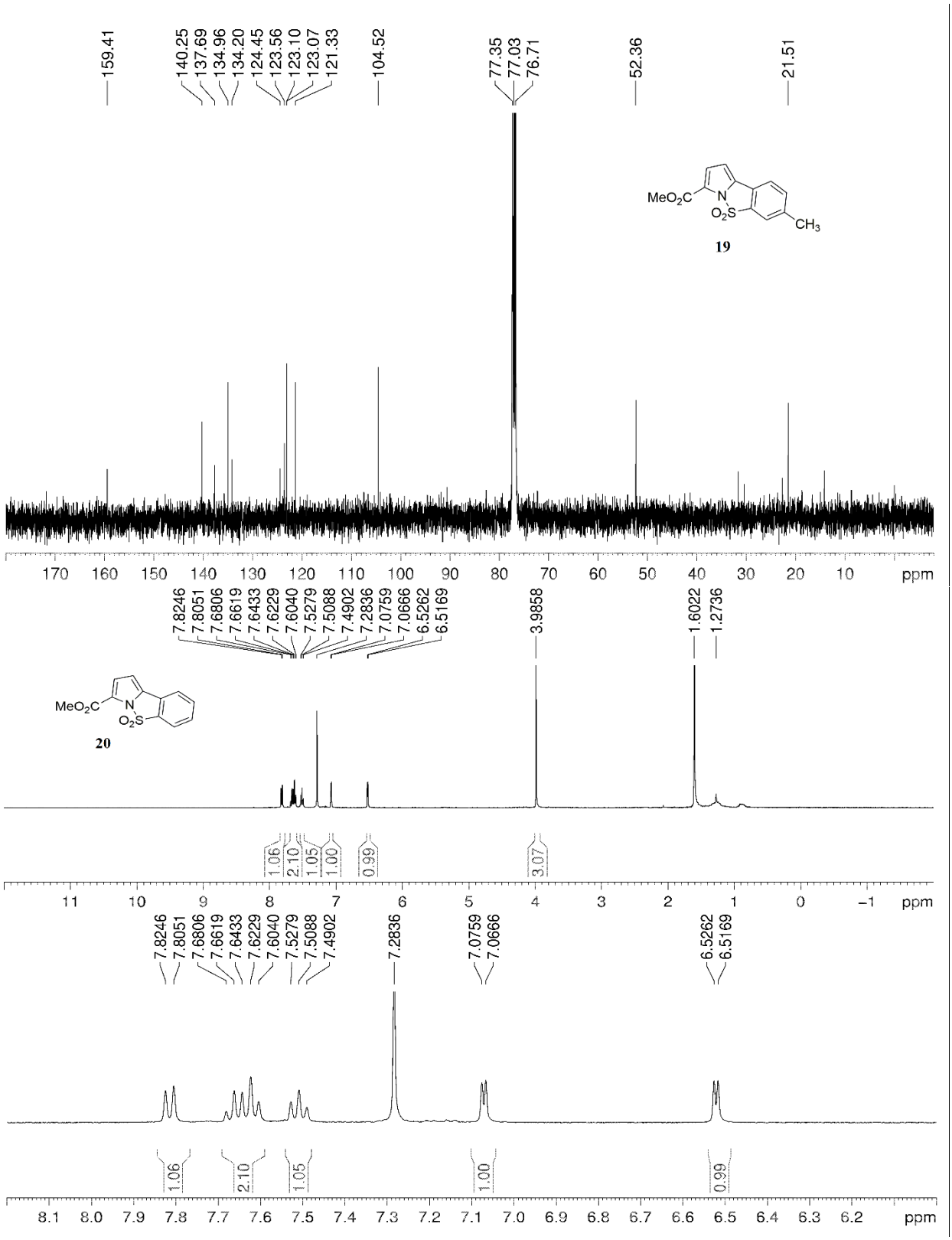
157.43
139.31
131.09
131.02
125.29
123.26
121.50
121.31
118.88
118.84
108.43
108.40
77.35
77.23
77.03
76.71
52.52
F
MeO2C
N
O2S
18
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
7.6204
7.5072
7.4874
7.4605
7.4406
7.2843
7.0583
7.0489
6.4605
6.4511
3.9775
2.4817
1.5927
MeO2C
N
O2S
CH3
19
1.02
2.14
1.00
0.99
3.22
3.14
11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm
7.6204
7.5072
7.4874
7.4605
7.4406
7.2843
7.0583
7.0489
1.02
2.14
1.00
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm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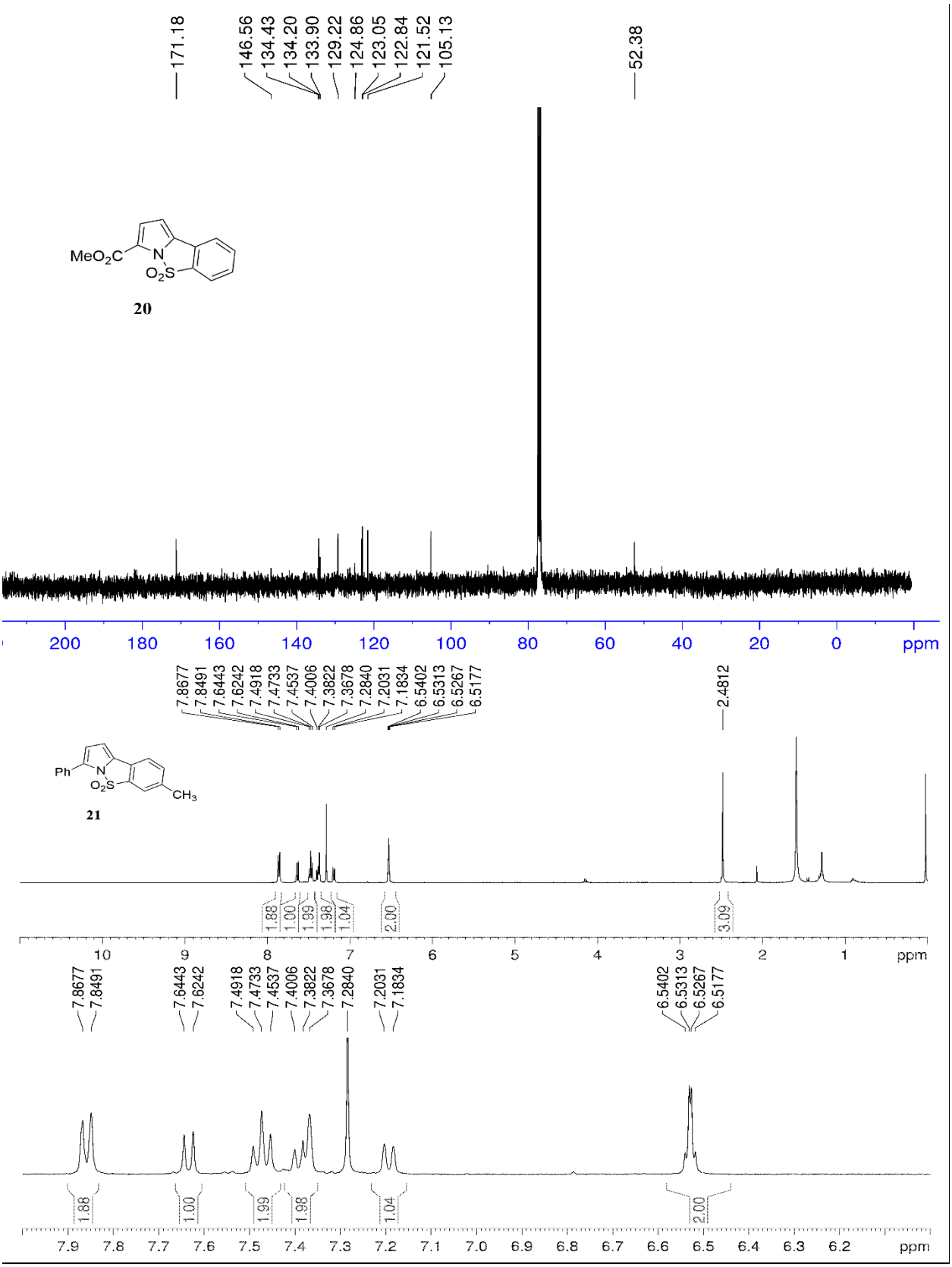
140.25
137.69
134.96
134.20
124.45
123.56
123.10
123.07
121.33
104.52
77.35
77.03
76.71
52.36
21.51
MeO2C
N
O2S
CH3
19
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
7.8246
7.8051
7.6806
7.6619
7.6433
7.6229
7.6040
7.5279
7.5088
7.4902
7.2836
7.0759
7.0666
6.5262
6.5169
3.9858
1.6022
1.2736
MeO2C
N
O2S
20
1.06
2.10
1.05
1.00
0.99
3.07
11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm
7.8246
7.8051
7.6806
7.6619
7.6433
7.6229
7.6040
7.5279
7.5088
7.4902
7.2836
7.0759
7.0666
6.5262
6.5169
1.06
2.10
1.05
1.00
0.99
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 ppm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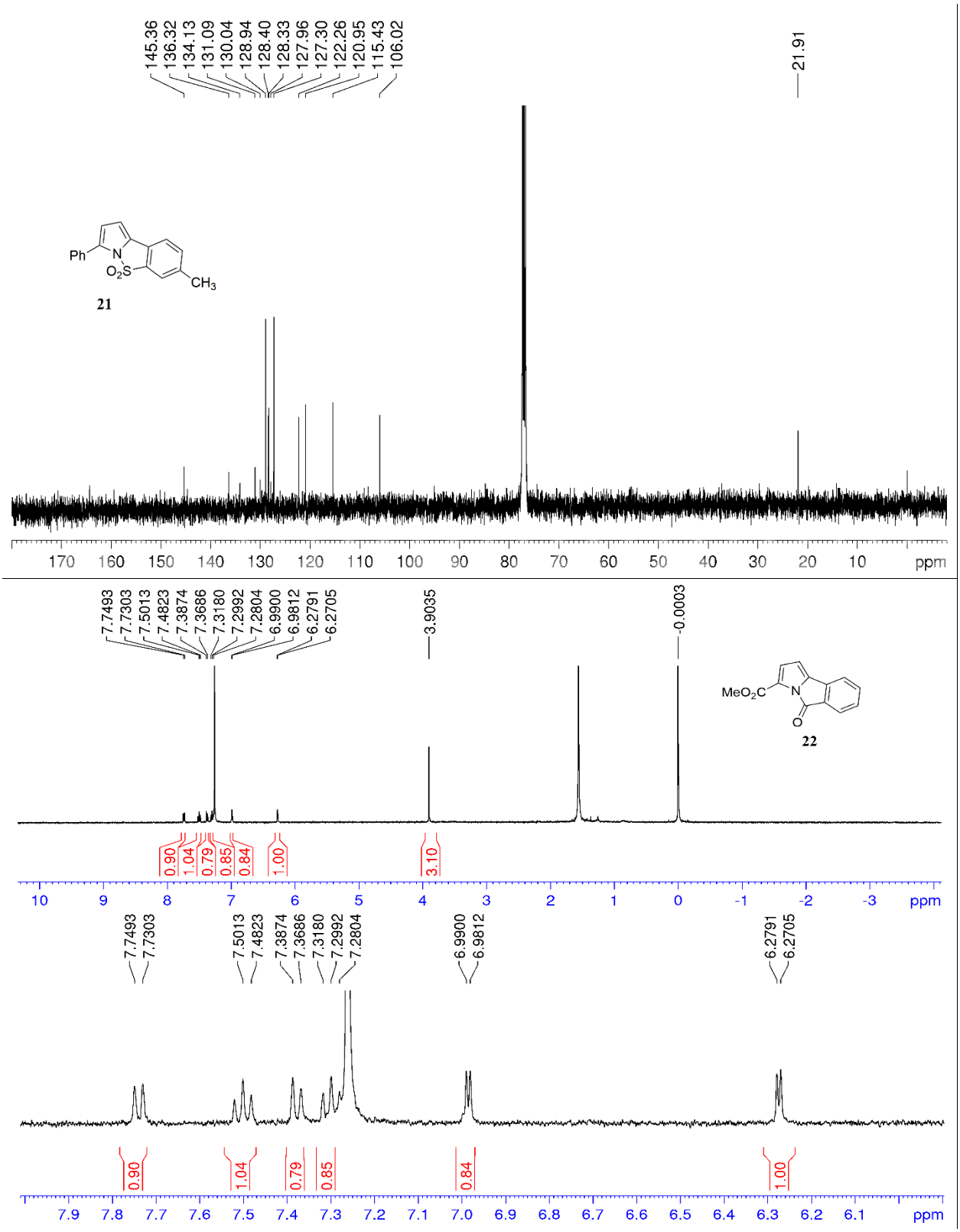
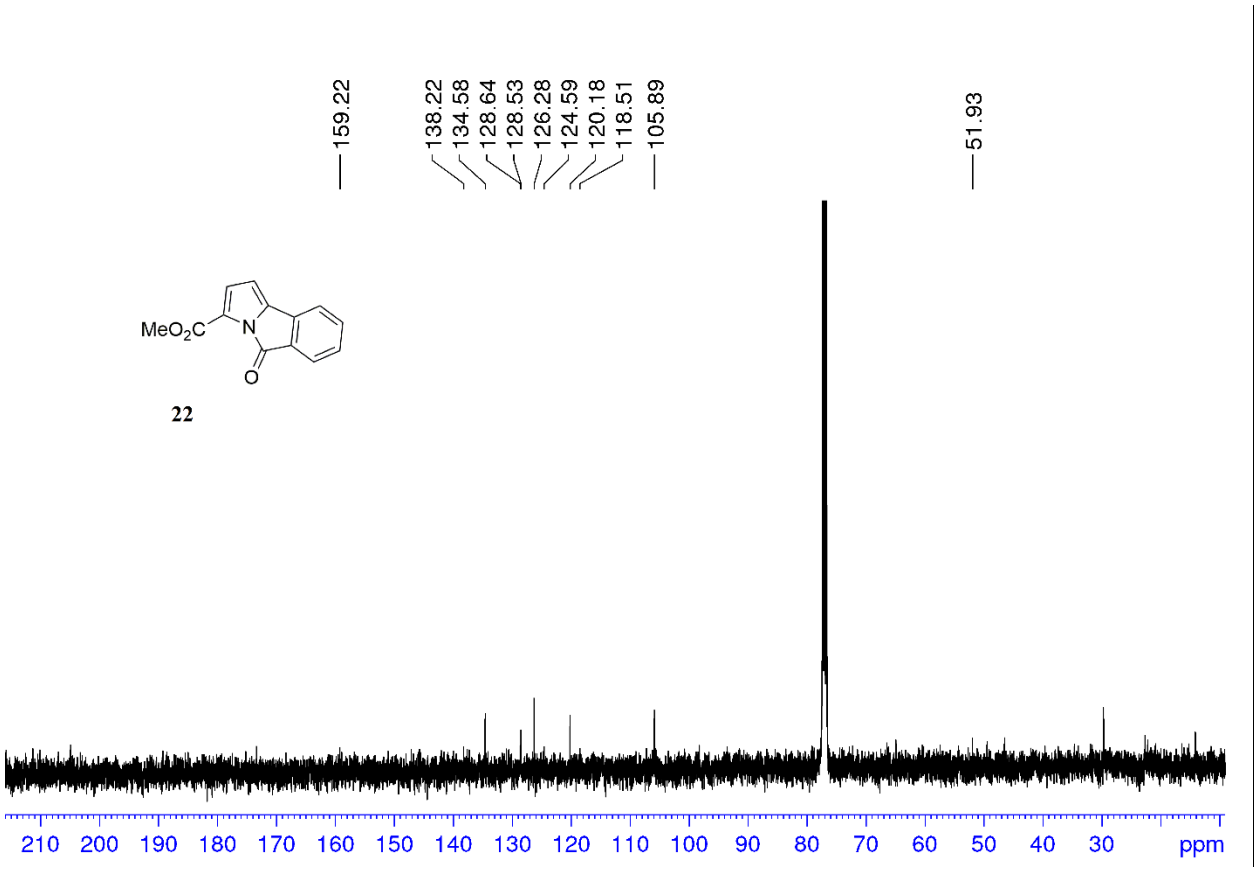
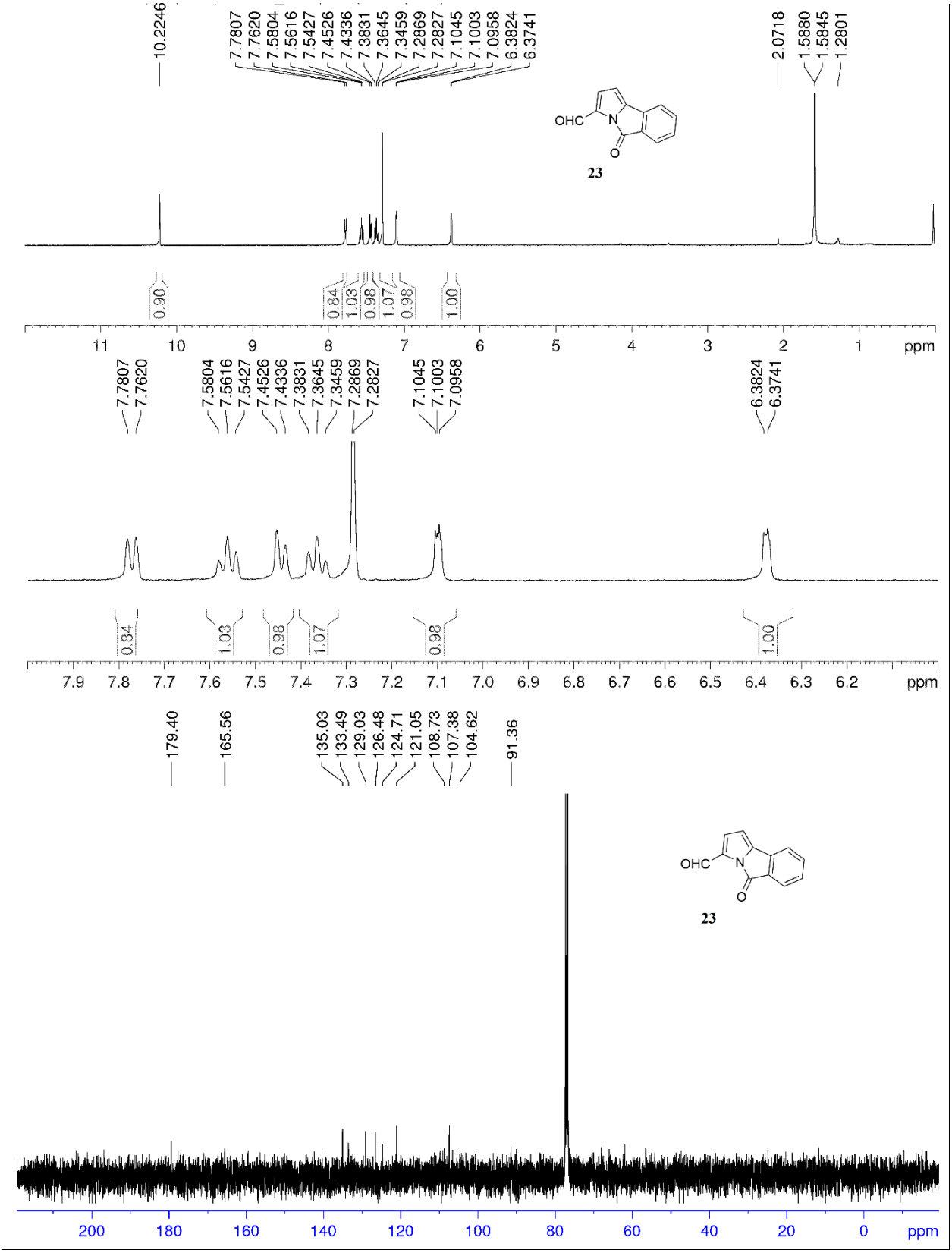
146.56
134.43
134.20
133.90
129.22
124.86
123.05
122.84
121.52
105.13
52.38
MeO2C
N
O2S
20
200
180
160
140
120
100
80
60
40
20
0
ppm
7.8677
7.8491
7.6443
7.6242
7.4918
7.4733
7.4537
7.4006
7.3822
7.3678
7.2840
7.2031
7.1834
6.5402
6.5313
6.5267
6.5177
2.4812
Ph
N
O2S
CH3
21
1.88
1.00
1.99
1.98
1.04
2.00
3.09
10
9
8
7
6
5
4
3
2
1
ppm
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
ppm


145.36
136.32
134.13
131.09
130.04
128.94
128.40
128.33
127.96
127.30
122.26
120.95
115.43
106.02
21.91
Ph
N
O2S
CH3
21
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
7.7493
7.7303
7.5013
7.4823
7.3874
7.3686
7.3180
7.2992
7.2804
6.9900
6.9812
6.2791
6.2705
3.9035
-0.0003
MeO2C
N
O
22
0.90
1.04
0.79
0.85
0.84
1.00
3.10
10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 ppm


159.22
138.22
134.58
128.64
128.53
126.28
124.59
120.18
118.51
105.89
51.93
MeO2C
N
O
22
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm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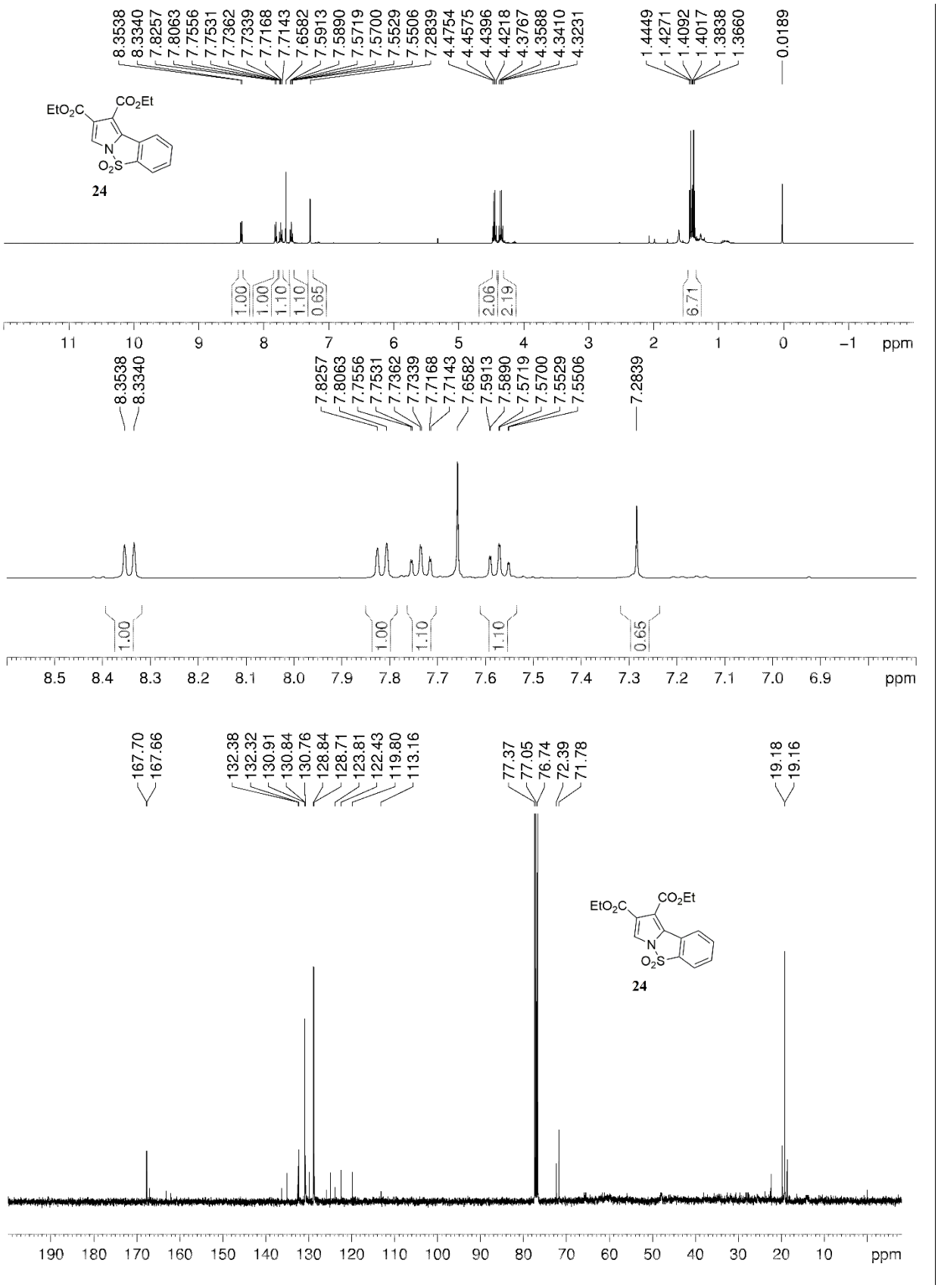
7.7807
7.7620
7.5804
7.5616
7.5427
7.4526
7.4336
7.3831
7.3645
7.3459
7.2869
7.2827
7.1045
7.1003
7.0958
6.3824
6.3741
2.0718
1.5880
1.5845
1.2801
OHC
N
O
23
0.90
0.84
1.03
0.98
1.07
0.98
1.00
ppm
0.84
1.03
0.98
1.07
0.98
1.00
179.40
165.56
135.03
133.49
129.03
126.48
124.71
121.05
108.73
107.38
104.62
91.36
200
180
160
140
120
100
80
60
40
20
0
ppm


8.3538
8.3340
7.8257
7.8063
7.7556
7.7531
7.7362
7.7339
7.7168
7.7143
7.6582
7.5913
7.5890
7.5719
7.5700
7.5529
7.5506
7.2839
4.4754
4.4575
4.4396
4.4218
4.3767
4.3588
4.3410
4.3231
1.4449
1.4271
1.4092
1.4017
1.3838
1.3660
0.0189
EtO2C
CO2Et
N
O2S
24
1.00
1.00
1.10
1.10
0.65
2.06
2.19
6.71
ppm
1.00
1.00
1.10
1.10
0.65
167.70
167.66
132.38
132.32
130.91
130.84
130.76
128.84
128.71
123.81
122.43
119.80
113.16
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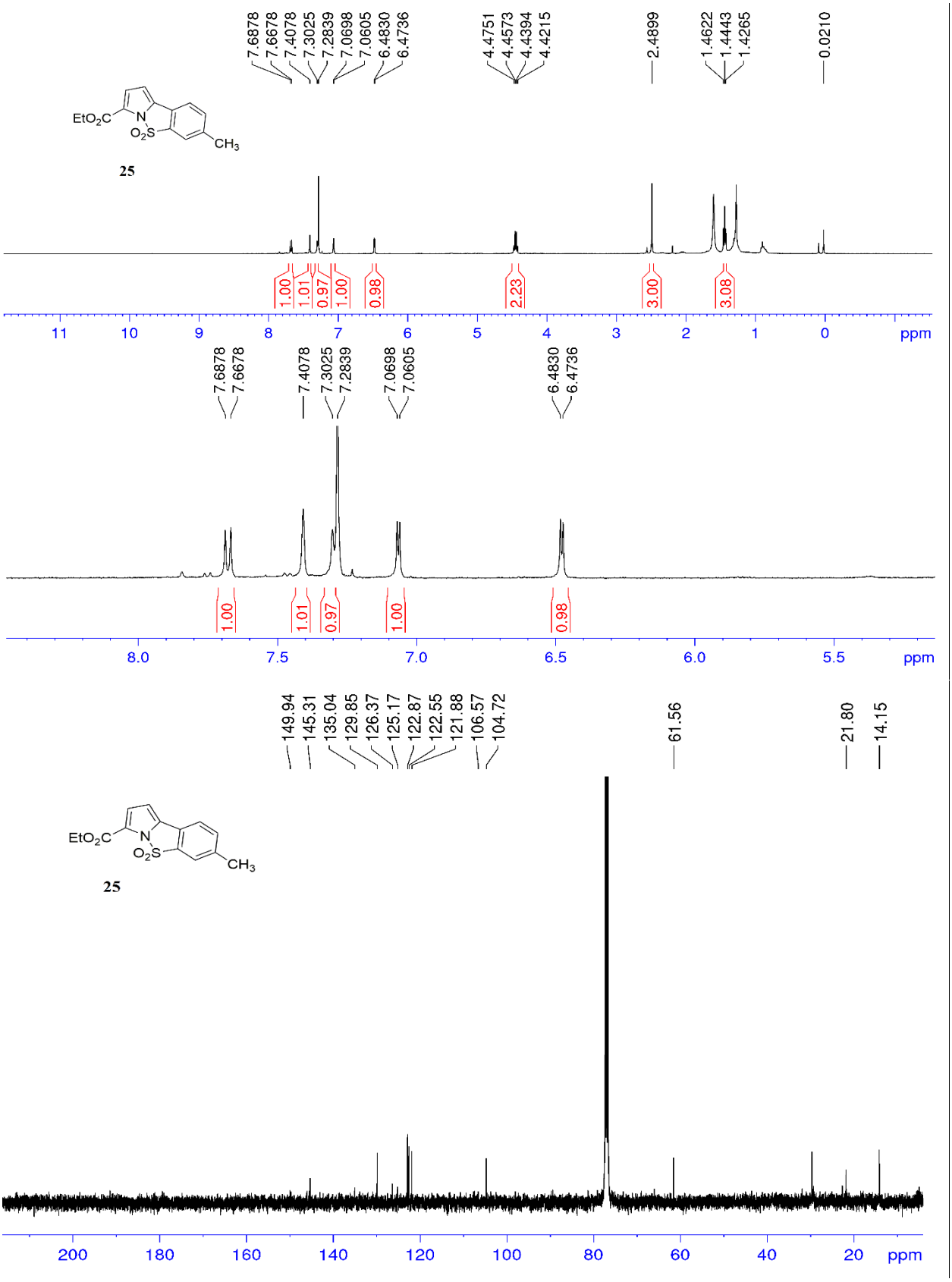
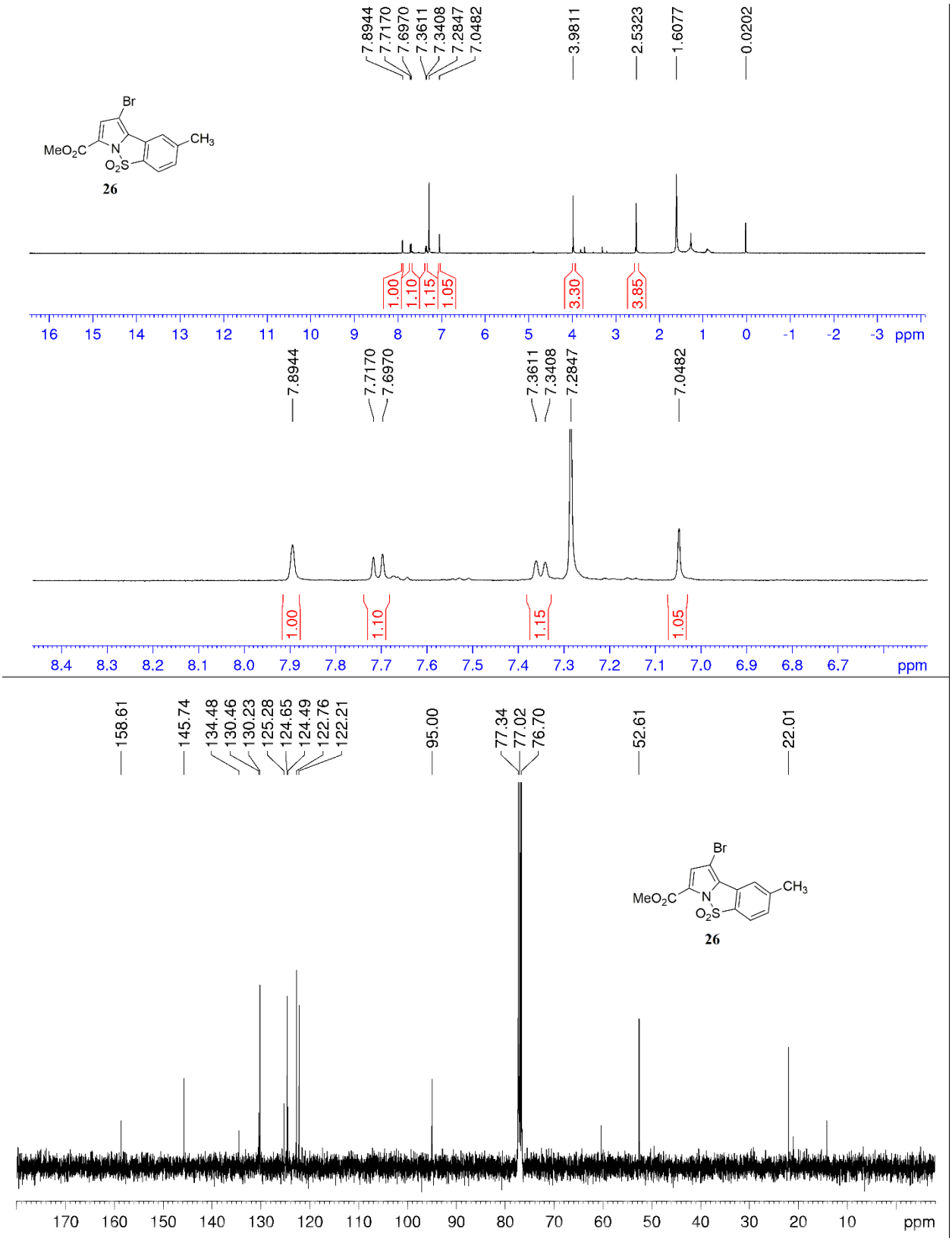
77.05
76.74
72.39
71.78
19.18
19.16


7.6878
7.6678
7.4078
7.3025
7.2839
7.0698
7.0605
6.4830
6.4736
4.4751
4.4573
4.4394
4.4215
2.4899
1.4622
1.4443
1.4265
0.0210
EtO2C
N
O2S
CH3
25
1.00
1.01
0.97
1.00
0.98
2.23
3.00
3.08
11
10
9
8
7
6
5
4
3
2
1
0
ppm
7.6878
7.6678
7.4078
7.3025
7.2839
7.0698
7.0605
6.4830
6.4736
1.00
1.01
0.97
1.00
0.98
8.0
7.5
7.0
6.5
6.0
5.5
ppm
149.94
145.31
135.04
129.85
126.37
125.17
122.87
122.55
121.88
106.57
104.72
61.56
21.80
14.15
EtO2C
N
O2S
CH3
25
200
180
160
140
120
100
80
60
40
20
ppm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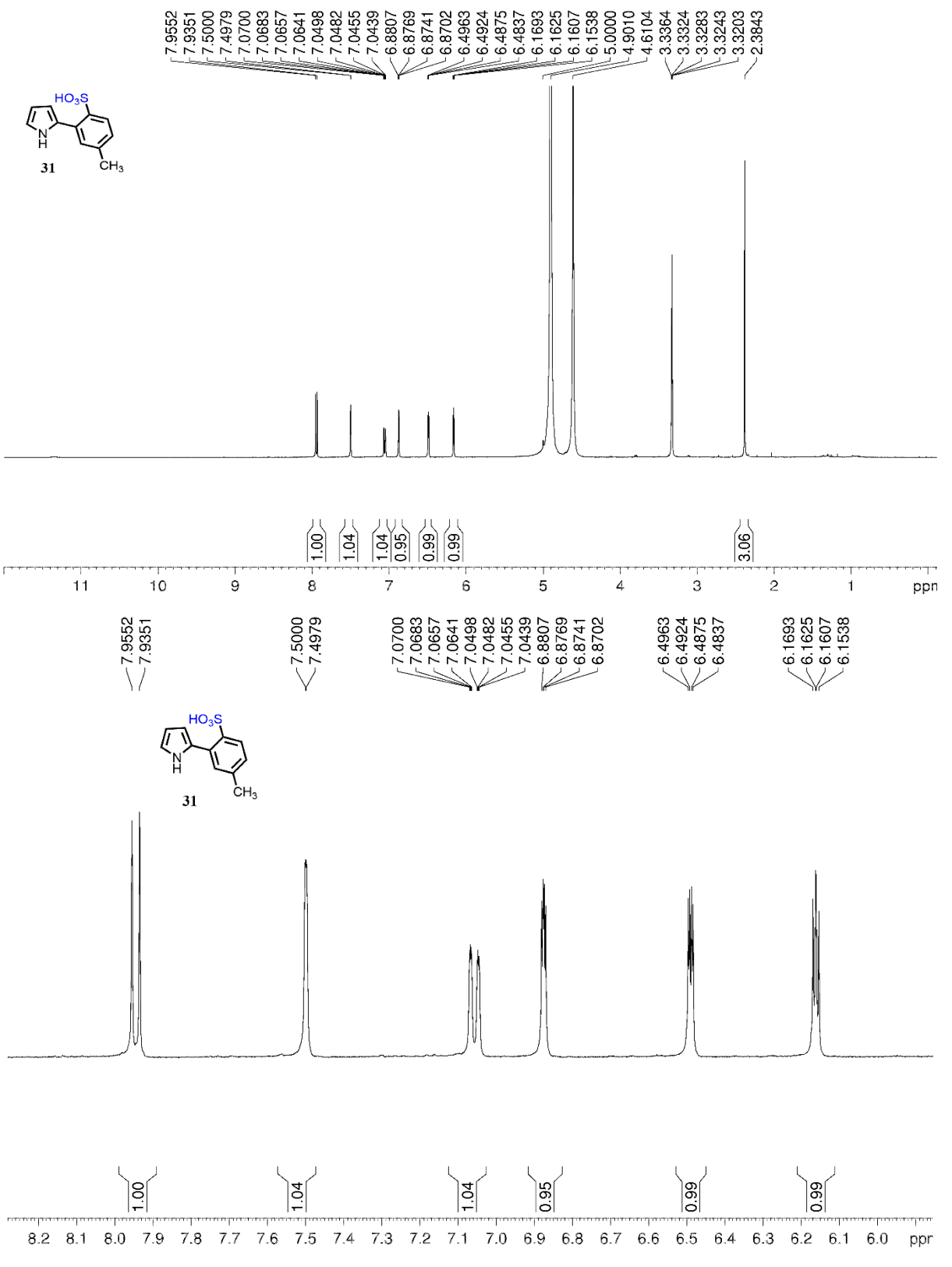
7.7170
7.6970
7.3611
7.3408
7.2847
7.0482
3.9811
2.5323
1.6077
0.0202
Br
MeO2C
N
O2S
CH3
26
1.00
1.10
1.15
1.05
3.30
3.85
ppm
158.61
145.74
134.48
130.46
130.23
125.28
124.65
124.49
122.76
122.21
95.00
77.34
77.02
76.70
52.61
22.01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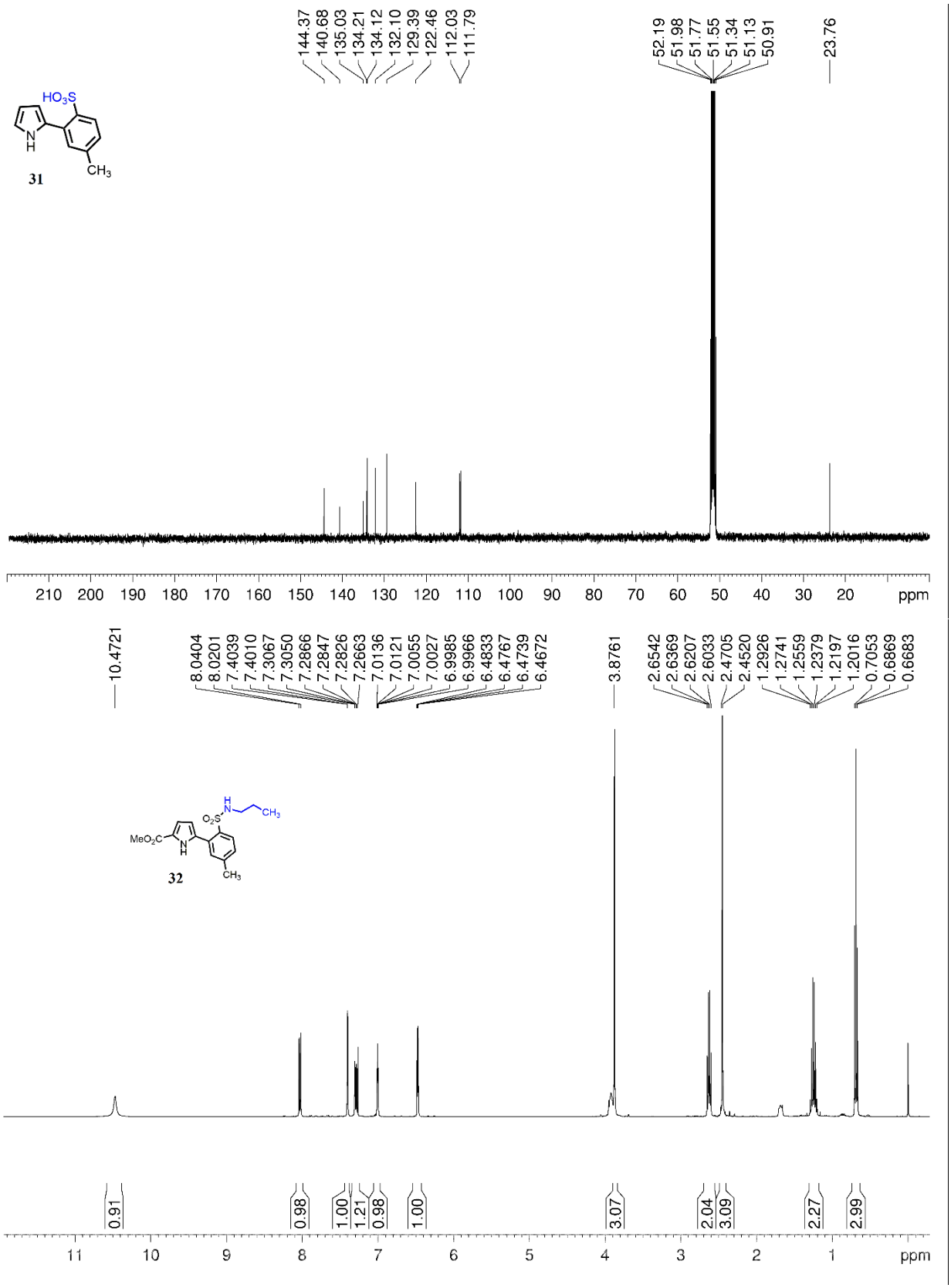
7.9351
7.5000
7.4979
7.0700
7.0683
7.0657
7.0641
7.0498
7.0482
7.0455
7.0439
6.8807
6.8769
6.8741
6.8702
6.4963
6.4924
6.4875
6.4837
6.1693
6.1625
6.1607
6.1538
5.0000
4.9010
4.6104
3.3364
3.3324
3.3283
3.3243
3.3203
2.3843
HO3S
N
H
CH3
31
1.00
1.04
1.04
0.95
0.99
0.99
3.06
11
10
9
8
7
6
5
4
3
2
1
ppm
7.9552
7.9351
7.5000
7.4979
7.0700
7.0683
7.0657
7.0641
7.0498
7.0482
7.0455
7.0439
6.8807
6.8769
6.8741
6.8702
6.4963
6.4924
6.4875
6.4837
6.1693
6.1625
6.1607
6.1538
HO3S
N
H
CH3
31
1.00
1.04
1.04
0.95
0.99
0.99
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
6.0
ppm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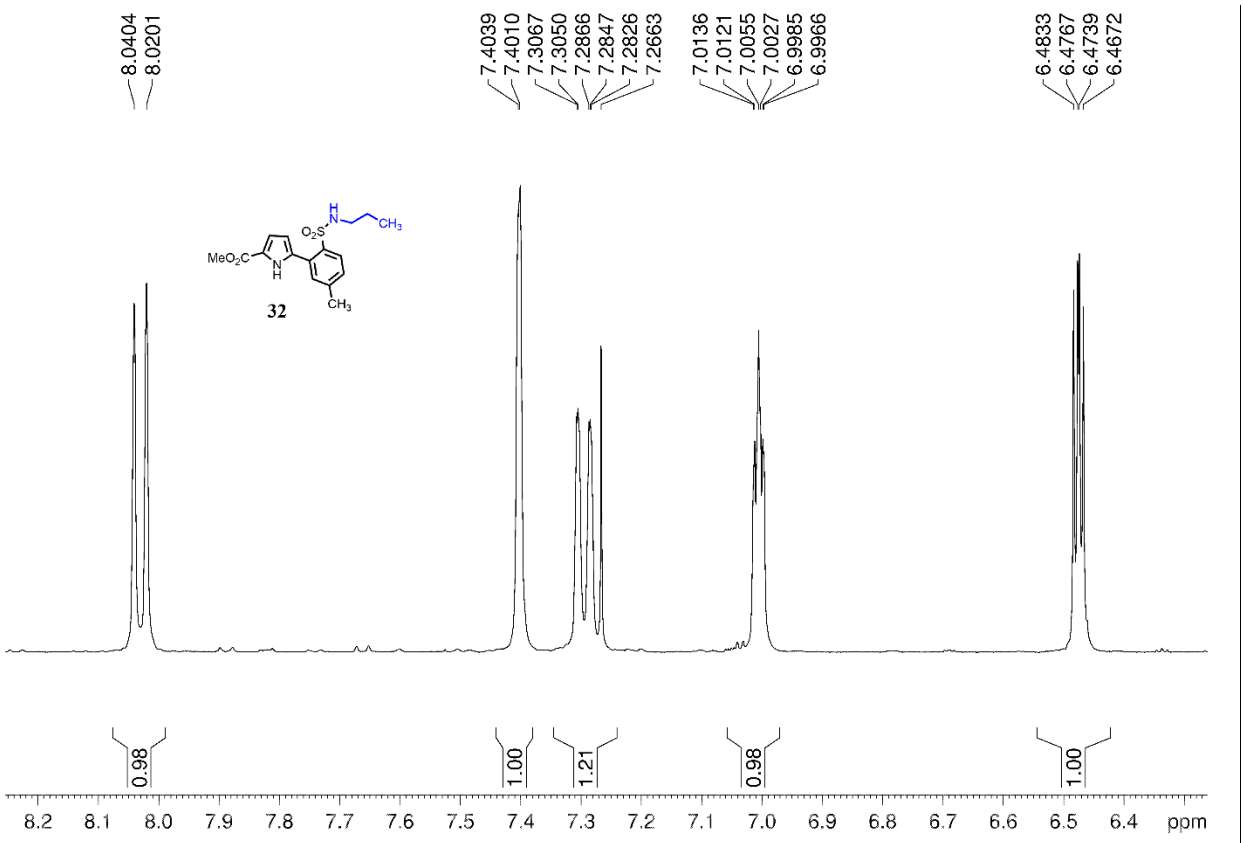
140.68
135.03
134.21
134.12
132.10
129.39
122.46
112.03
111.79
52.19
51.98
51.77
51.55
51.34
51.13
50.91
23.76
HO3S
CH3
31
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
10.4721
8.0404
8.0201
7.4039
7.4010
7.3067
7.3050
7.2866
7.2847
7.2826
7.2663
7.0136
7.0121
7.0055
7.0027
6.9985
6.9966
6.4833
6.4767
6.4739
6.4672
3.8761
2.6542
2.6369
2.6207
2.6033
2.4705
2.4520
1.2926
1.2741
1.2559
1.2379
1.2197
1.2016
0.7053
0.6869
0.6683
MeO2C
O2S
N
H
CH3
CH3
32
0.91
0.98
1.00
1.21
0.98
1.00
3.07
2.04
3.09
2.27
2.99
11 10 9 8 7 6 5 4 3 2 1 ppm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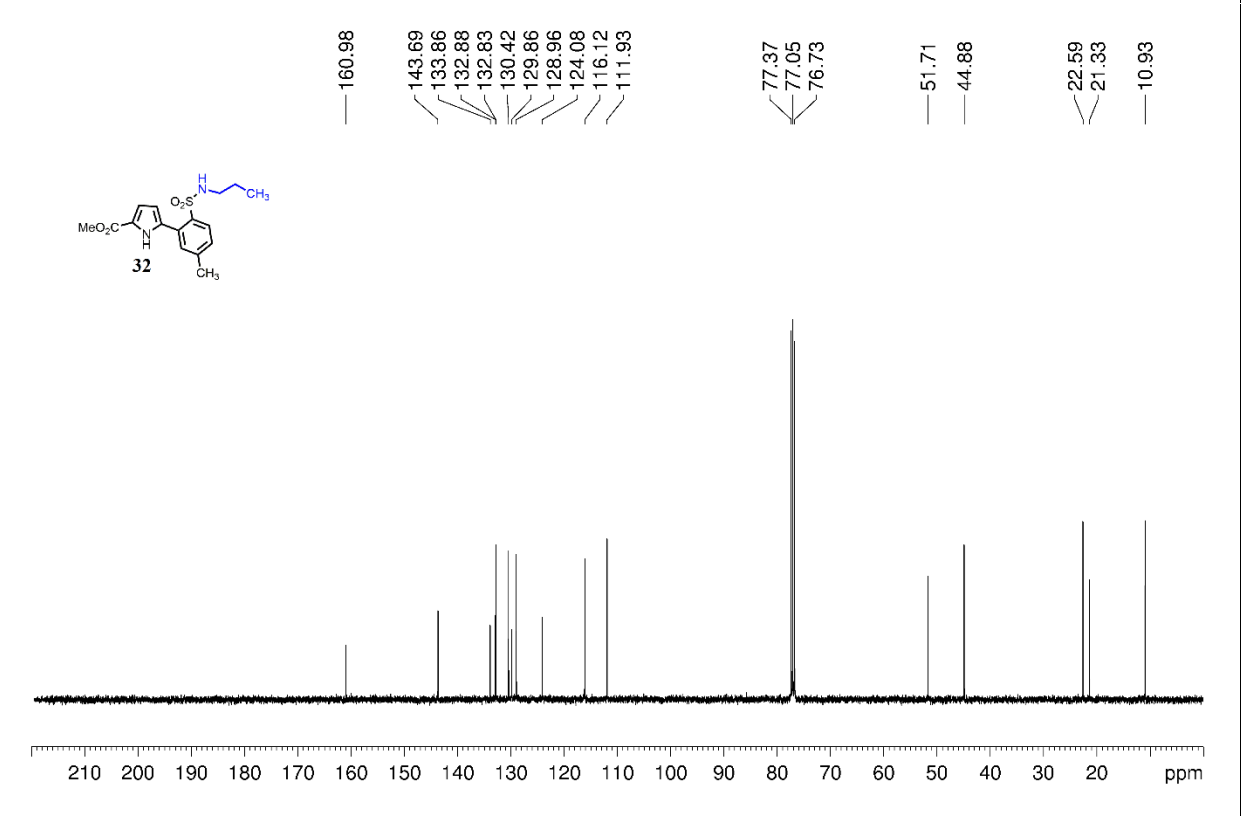
8.0201
7.4039
7.4010
7.3067
7.3050
7.2866
7.2847
7.2826
7.2663
7.0136
7.0121
7.0055
7.0027
6.9985
6.9966
6.4833
6.4767
6.4739
6.4672
32
0.98
1.00
1.21
0.98
1.00
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 ppm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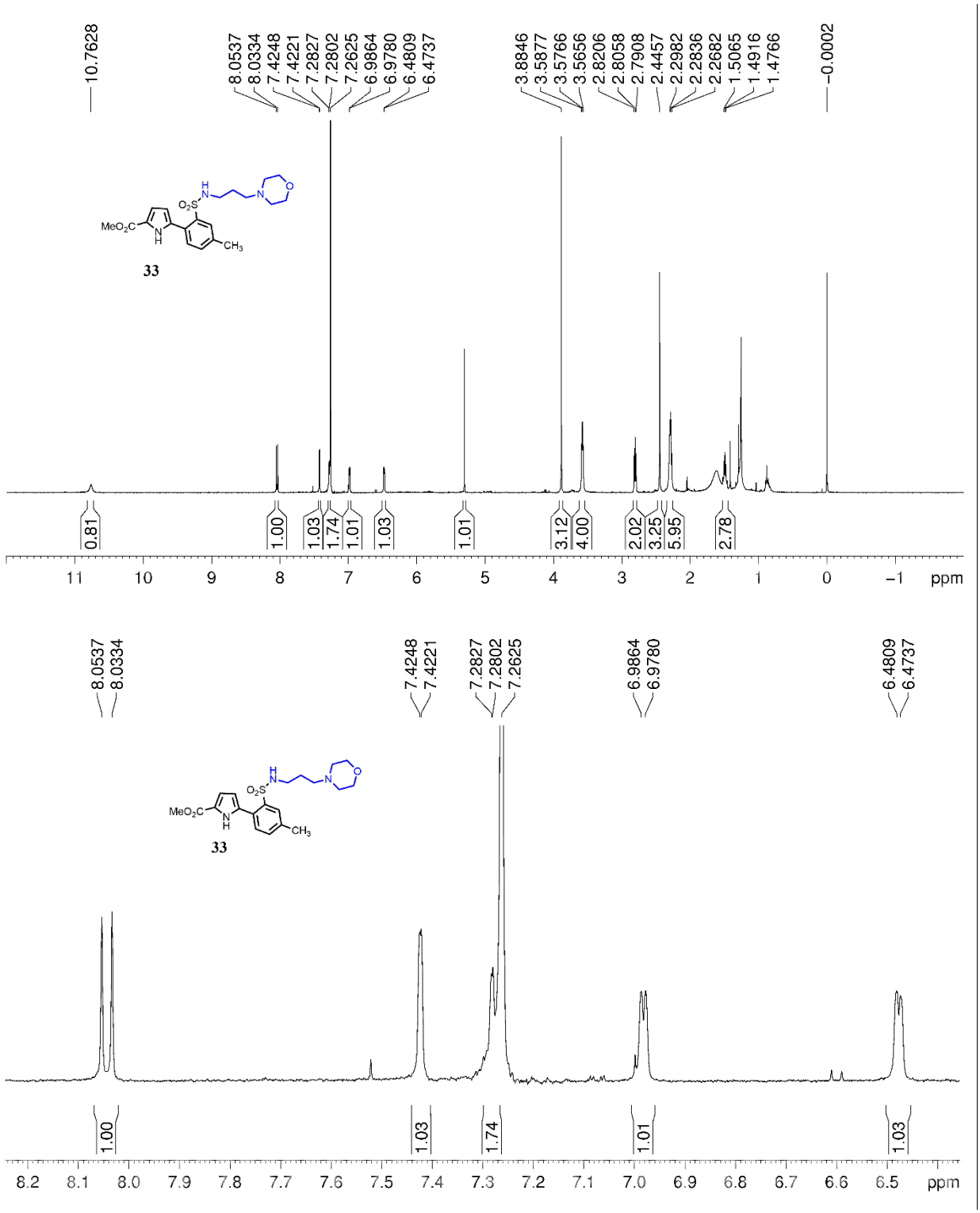
143.69
133.86
132.88
132.83
130.42
129.86
128.96
124.08
116.12
111.93
77.37
77.05
76.73
51.71
44.88
22.59
21.33
10.93
32
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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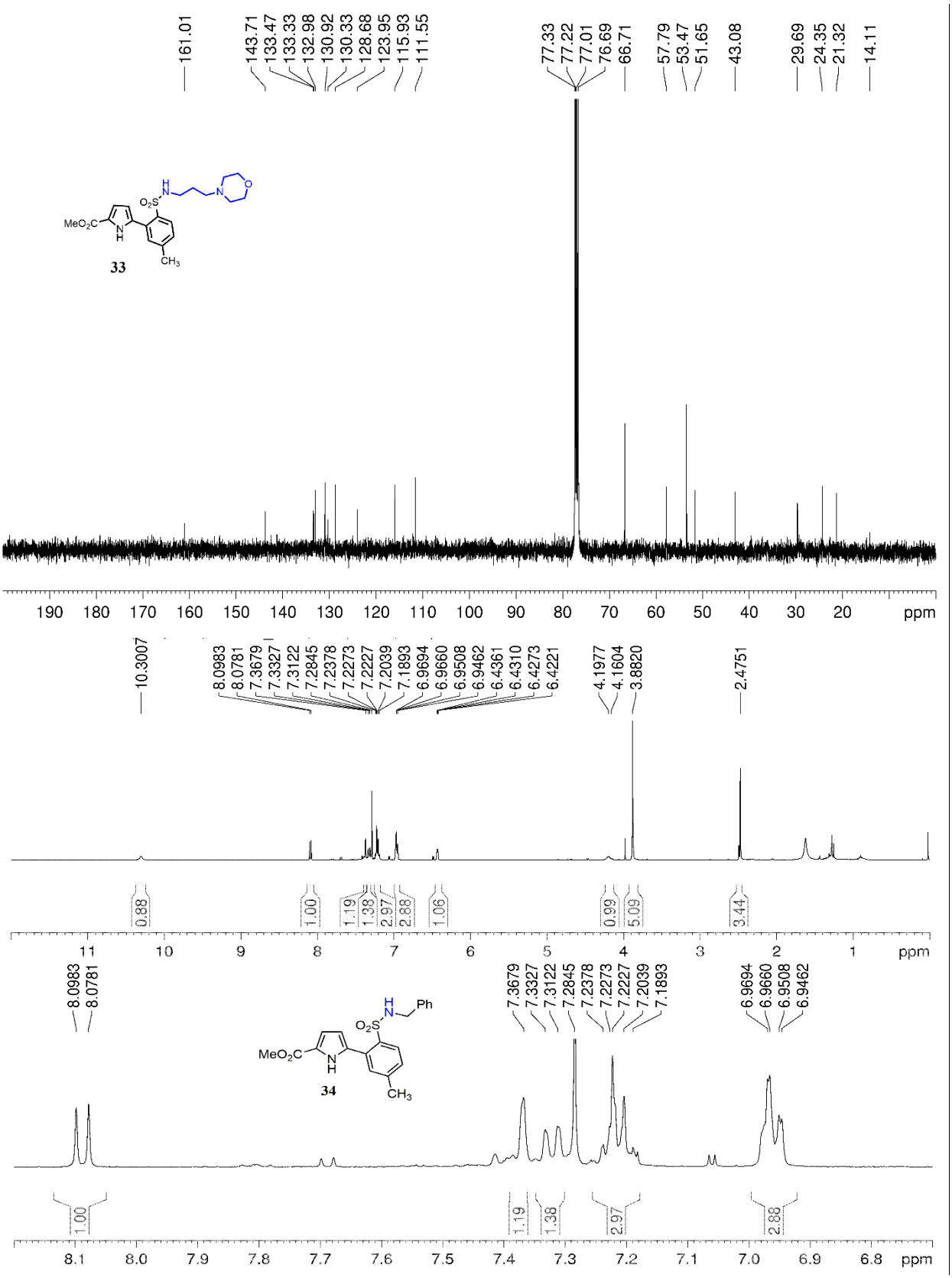
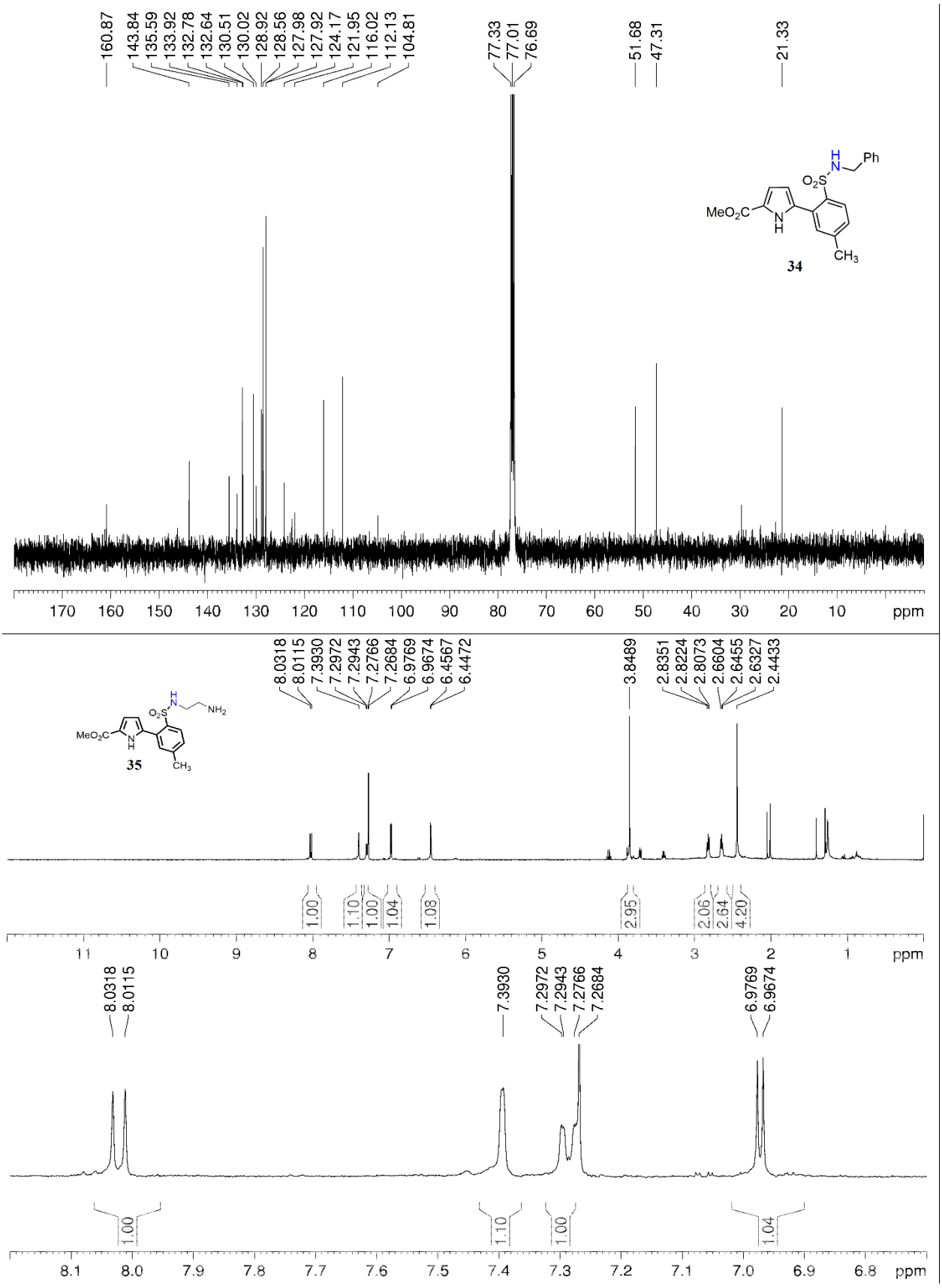
8.0334
7.4248
7.4221
7.2827
7.2802
7.2625
6.9864
6.9780
6.4809
6.4737
3.8846
3.5877
3.5766
3.5656
2.8206
2.8058
2.7908
2.4457
2.2982
2.2836
2.2682
1.5065
1.4916
1.4766
0.0002
33
0.81
1.00
1.03
1.74
1.01
1.03
1.01
3.12
4.00
2.02
3.25
5.95
2.78
ppm
1.00
1.03
1.74
1.01
1.03


161.01
143.71
133.47
133.33
132.98
130.92
130.33
128.68
123.95
115.93
111.55
77.33
77.22
77.01
76.69
66.71
57.79
53.47
51.65
43.08
29.69
24.35
21.32
14.11
MeO2C
O2S
N
H
CH3
33
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
10.3007
8.0983
8.0781
7.3679
7.3327
7.3122
7.2845
7.2378
7.2273
7.2227
7.2039
7.1893
6.9694
6.9660
6.9508
6.9462
6.4361
6.4310
6.4273
6.4221
4.1977
4.1604
3.8820
2.4751
0.88
1.00
1.19
1.38
2.97
2.88
1.06
0.99
5.09
3.44
11 10 9 8 7 6 5 4 3 2 1 ppm
Ph
34
1.00
1.19
1.38
2.97
2.88
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm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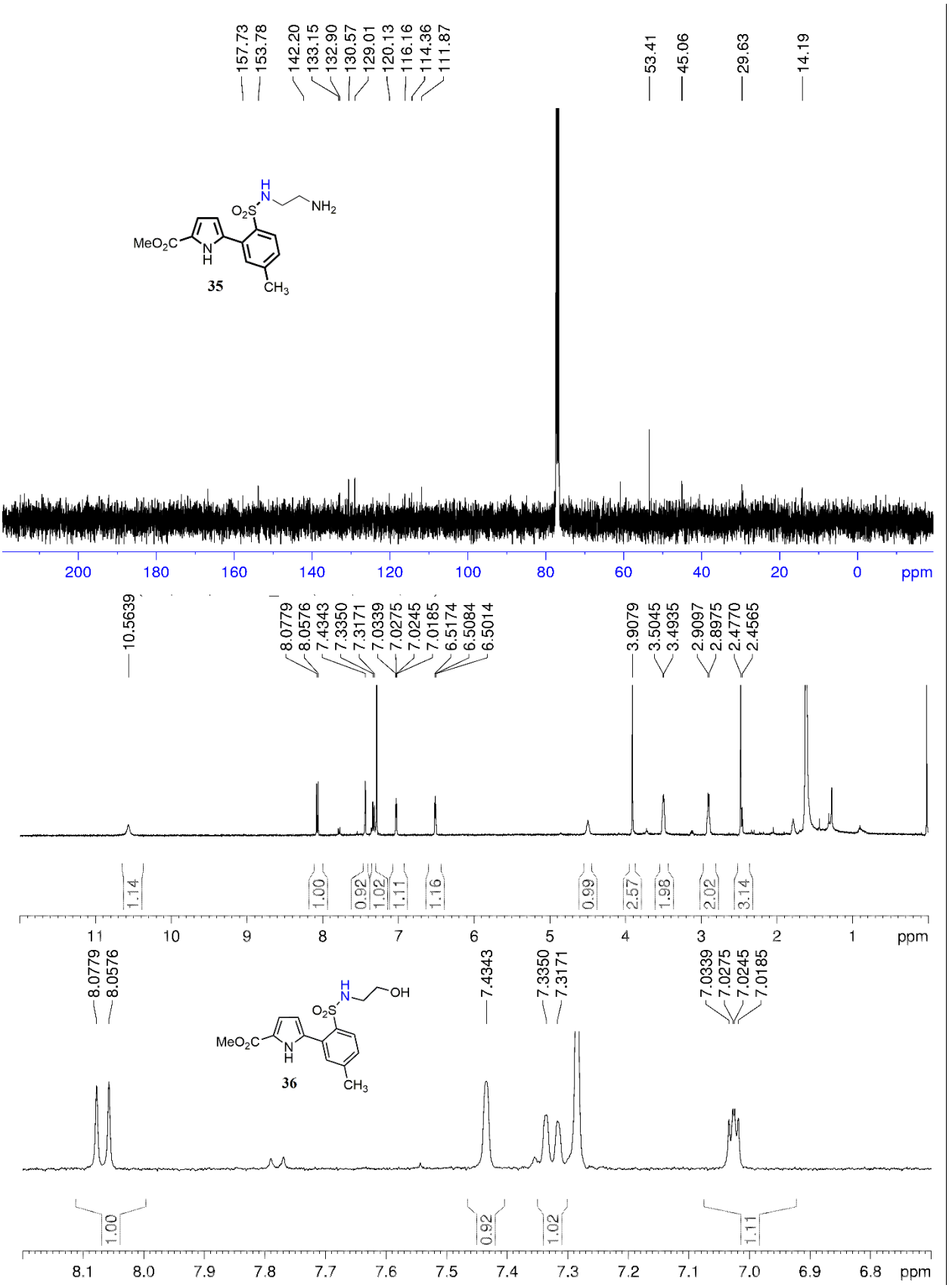
143.84
135.59
133.92
132.78
132.64
130.51
130.02
128.92
128.56
127.98
127.92
124.17
121.95
116.02
112.13
104.81
77.33
77.01
76.69
51.68
47.31
21.33
Ph
MeO2C
O2S
CH3
34
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
8.0318
8.0115
7.3930
7.2972
7.2943
7.2766
7.2684
6.9769
6.9674
6.4567
6.4472
3.8489
2.8351
2.8224
2.8073
2.6604
2.6455
2.6327
2.4433
NH2
MeO2C
O2S
CH3
35
1.00
1.10
1.00
1.04
1.08
2.95
2.06
2.64
4.20
11 10 9 8 7 6 5 4 3 2 1 ppm
8.0318
8.0115
7.3930
7.2972
7.2943
7.2766
7.2684
6.9769
6.9674
1.00
1.10
1.00
1.04
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm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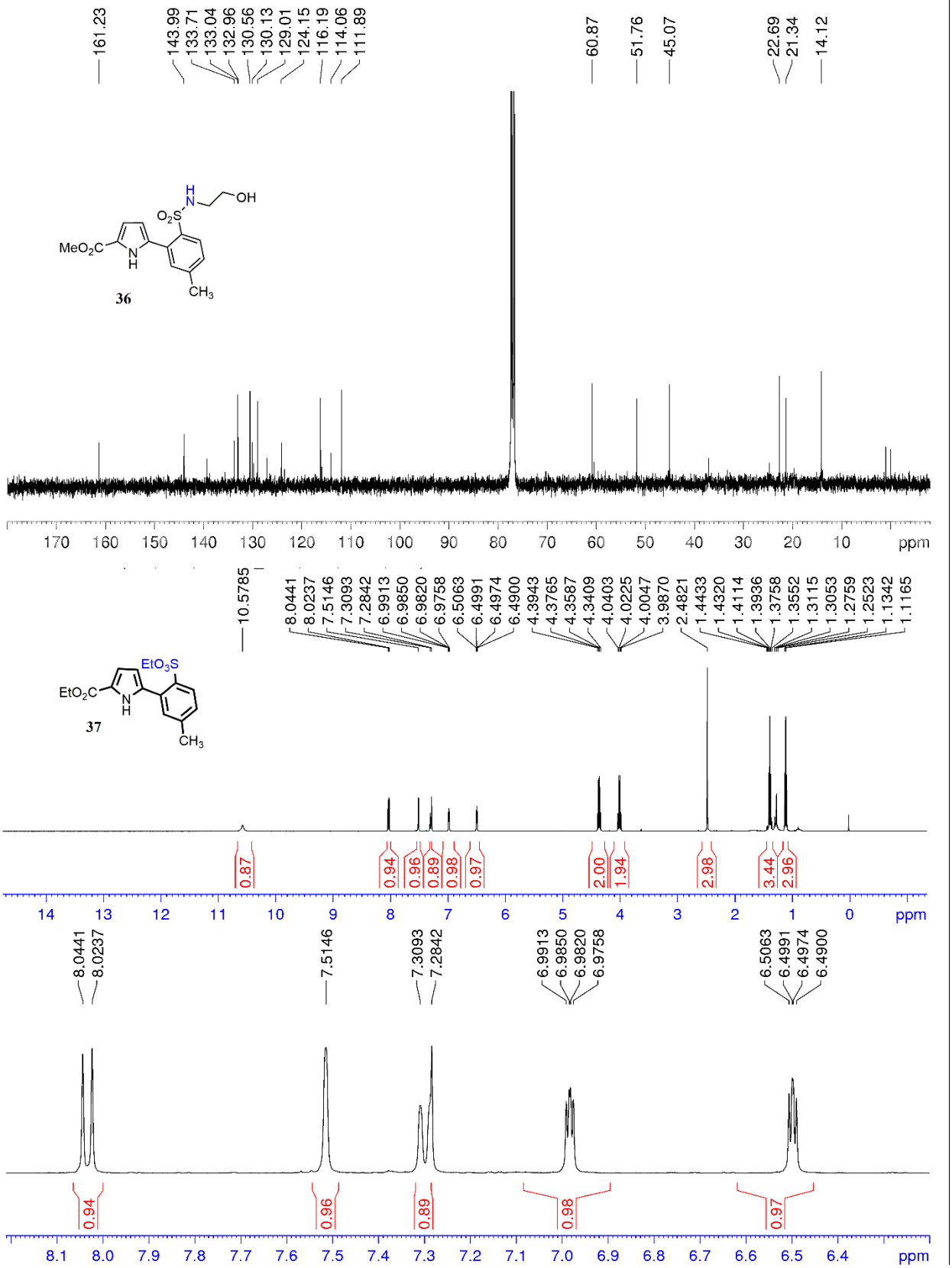
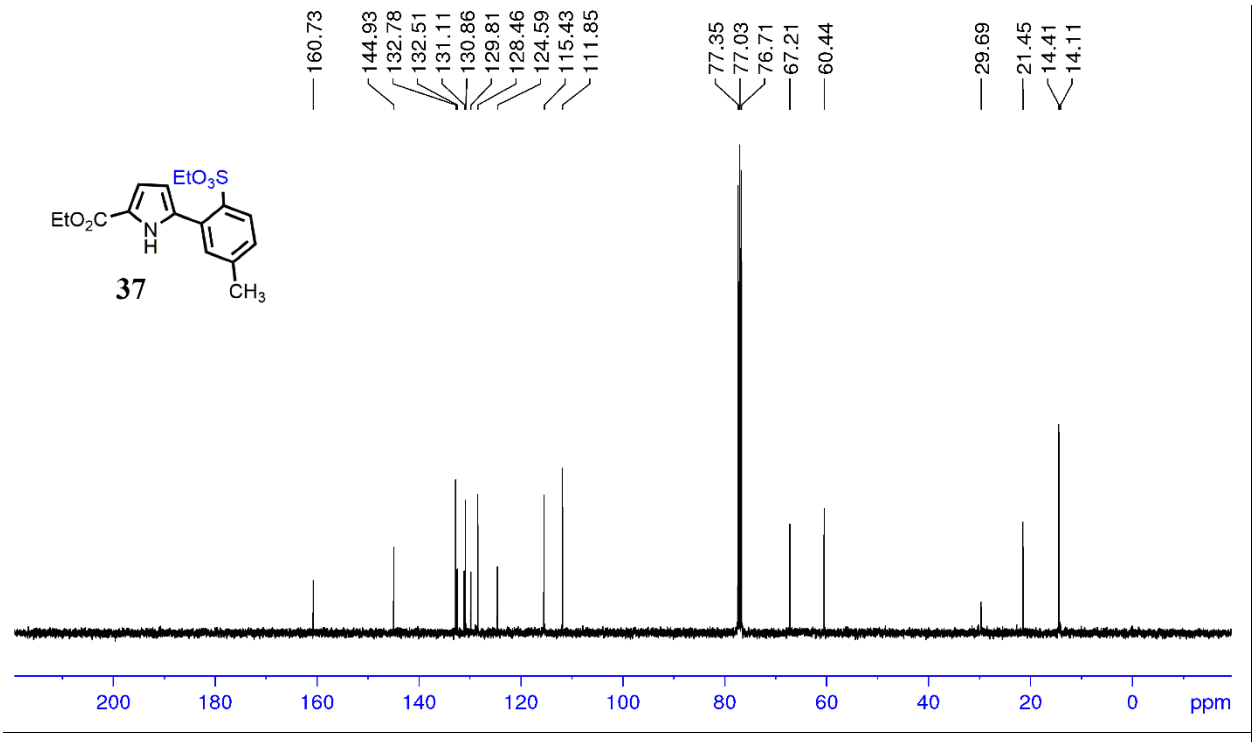
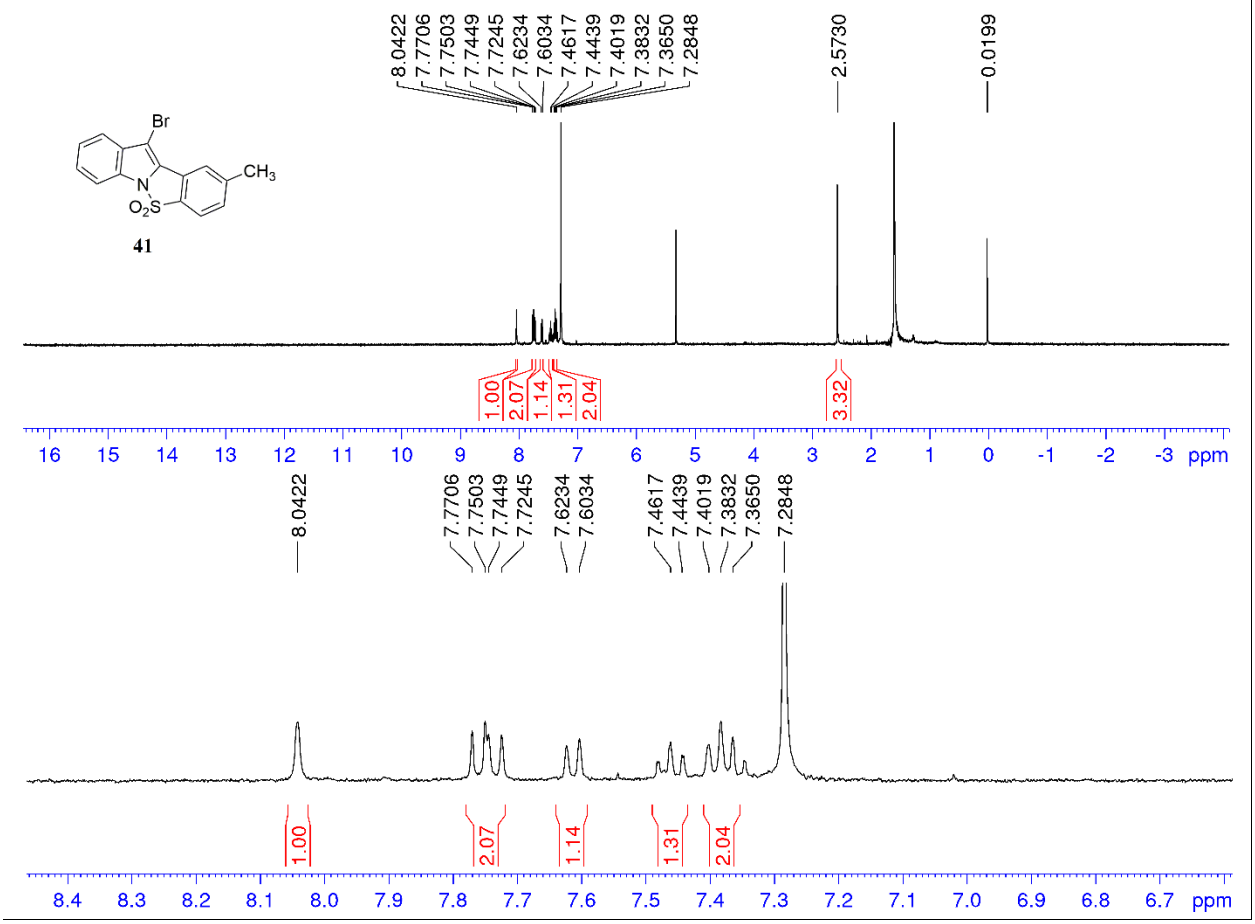
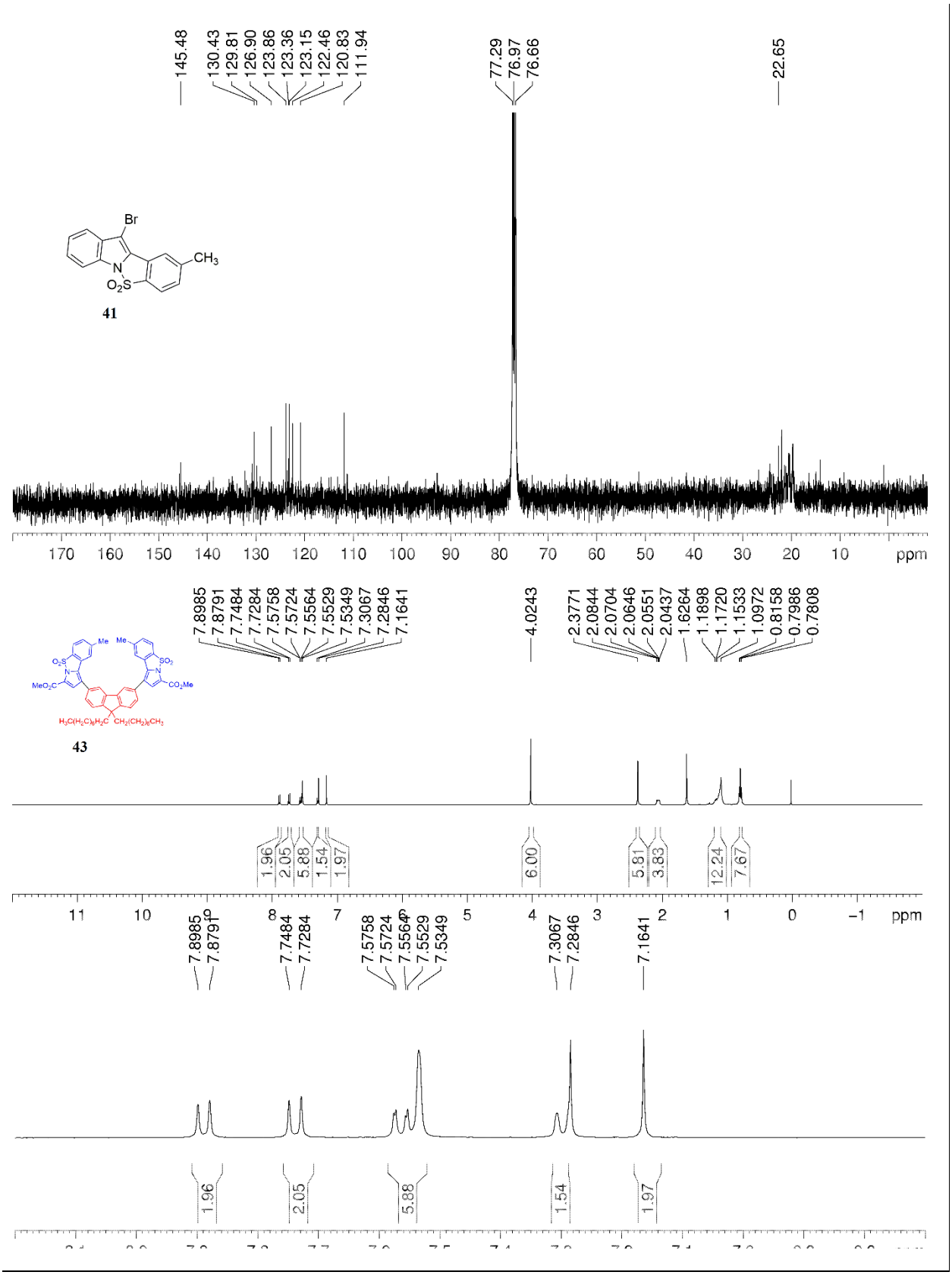
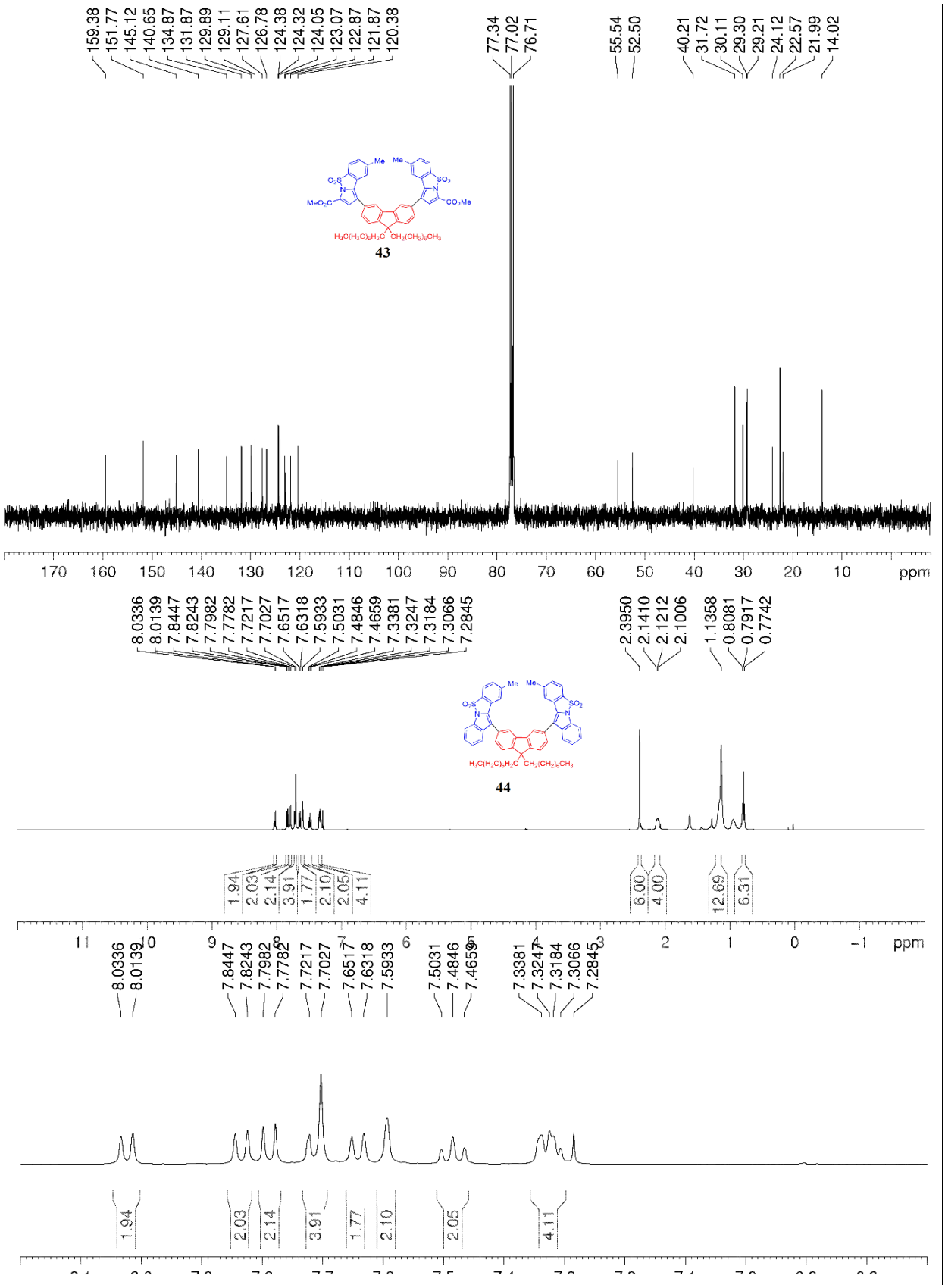
153.78
142.20
133.15
132.90
130.57
129.01
120.13
116.16
114.36
111.87
53.41
45.06
29.63
14.19
35
200
180
160
140
120
100
80
60
40
20
0
ppm
10.5639
8.0779
8.0576
7.4343
7.3350
7.3171
7.0339
7.0275
7.0245
7.0185
6.5174
6.5084
6.5014
3.9079
3.5045
3.4935
2.9097
2.8975
2.4770
2.4565
1.14
1.00
0.92
1.02
1.11
1.16
0.99
2.57
1.98
2.02
3.14
11
10
9
8
7
6
5
4
3
2
1
ppm
8.0779
8.0576
7.4343
7.3350
7.3171
7.0339
7.0275
7.0245
7.0185
36
1.00
0.92
1.02
1.11
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm


161.23
143.99
133.71
133.04
132.96
130.56
130.13
129.01
124.15
116.19
114.06
111.89
60.87
51.76
45.07
22.69
21.34
14.12
MeO2C
O2S
H
N
OH
N
H
CH3
36
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
10.5785
8.0441
8.0237
7.5146
7.3093
7.2842
6.9913
6.9850
6.9820
6.9758
6.5063
6.4991
6.4974
6.4900
4.3943
4.3765
4.3587
4.3409
4.0403
4.0225
4.0047
3.9870
2.4821
1.4433
1.4320
1.4114
1.3936
1.3758
1.3552
1.3115
1.3053
1.2759
1.2523
1.1342
1.1165
EtO3S
EtO2C
N
H
CH3
37
0.87
0.94
0.96
0.89
0.98
0.97
2.00
1.94
2.98
3.44
2.96
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
8.0441
8.0237
7.5146
7.3093
7.2842
6.9913
6.9850
6.9820
6.9758
6.5063
6.4991
6.4974
6.4900
0.94
0.96
0.89
0.98
0.97
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 ppm


160.73
144.93
132.78
132.51
131.11
130.86
129.81
128.46
124.59
115.43
111.85
77.35
77.03
76.71
67.21
60.44
29.69
21.45
14.41
14.11
EtO3S
EtO2C
N
H
37
CH3
200
180
160
140
120
100
80
60
40
20
0
ppm


8.0422
7.7706
7.7503
7.7449
7.7245
7.6234
7.6034
7.4617
7.4439
7.4019
7.3832
7.3650
7.2848
2.5730
0.0199
Br
CH3
N
O2S
41
1.00
2.07
1.14
1.31
2.04
3.32
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
ppm
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
ppm


145.48
130.43
129.81
126.90
123.86
123.36
123.15
122.46
120.83
111.94
77.29
76.97
76.66
22.65
Br
CH3
N
O2S
41
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
7.8985
7.8791
7.7484
7.7284
7.5758
7.5724
7.5564
7.5529
7.5349
7.3067
7.2846
7.1641
4.0243
2.3771
2.0844
2.0704
2.0646
2.0551
2.0437
1.6264
1.1898
1.1720
1.1533
1.0972
0.8158
0.7986
0.7808
Me
Me
O2S
SO2
MeO2C
CO2Me
H3C(H2C)8H2C
CH2(CH2)8CH3
43
1.96
2.05
5.88
1.54
1.97
6.00
5.81
3.83
12.24
7.67
11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm
7.8985
7.8791
7.7484
7.7284
7.5758
7.5724
7.5564
7.5529
7.5349
7.3067
7.2846
7.1641
1.96
2.05
5.88
1.54
1.97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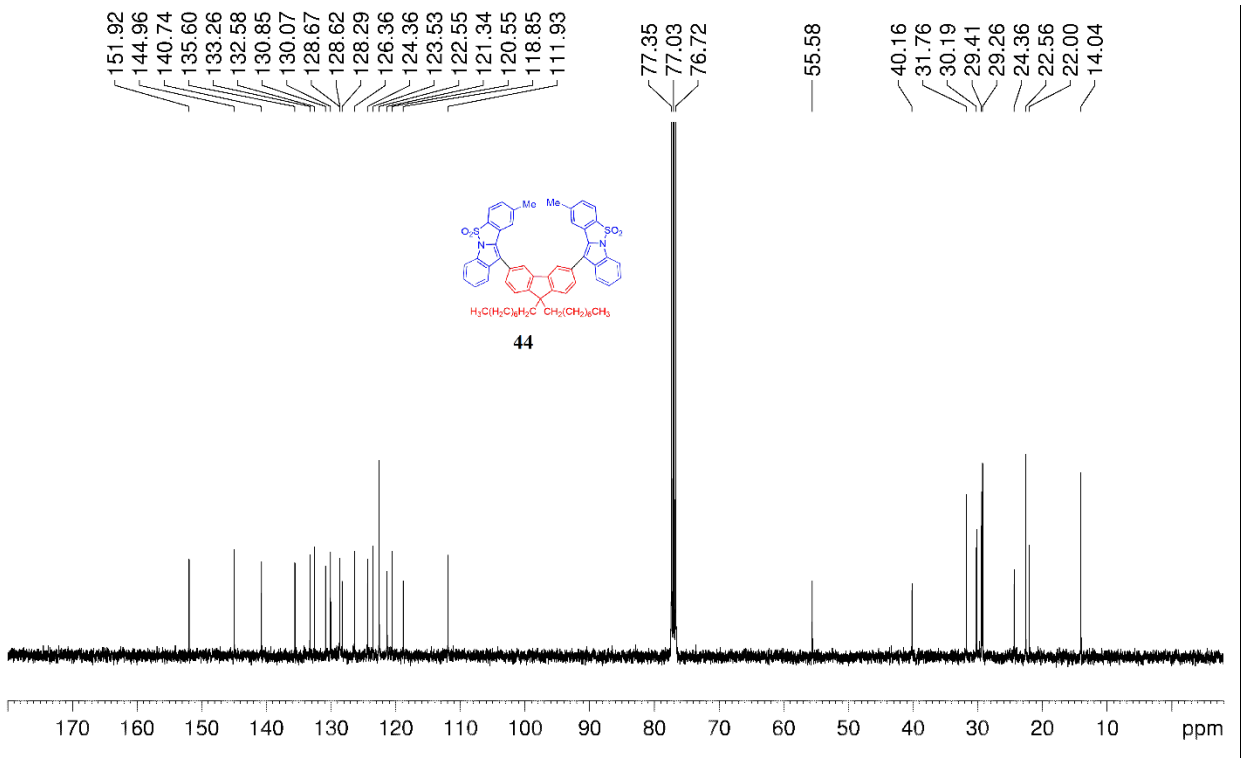
151.77
145.12
140.65
134.87
131.87
129.89
129.11
127.61
126.78
124.38
124.32
124.05
123.07
122.87
121.87
120.38
77.34
77.02
76.71
55.54
52.50
40.21
31.72
30.11
29.30
29.21
24.12
22.57
21.99
14.02
43
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
8.0336
8.0139
7.8447
7.8243
7.7982
7.7782
7.7217
7.7027
7.6517
7.6318
7.5933
7.5031
7.4846
7.4659
7.3381
7.3247
7.3184
7.3066
7.2845
2.3950
2.1410
2.1212
2.1006
1.1358
0.8081
0.7917
0.7742
44
1.94
2.03
2.14
3.91
1.77
2.10
2.05
4.11
6.00
4.00
12.69
6.31
11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm


151.92
144.96
140.74
135.60
133.26
132.58
130.85
130.07
128.67
128.62
128.29
126.36
124.36
123.53
122.55
121.34
120.55
118.85
111.93
77.35
77.03
76.72
55.58
40.16
31.76
30.19
29.41
29.26
24.36
22.56
22.00
14.04
Me
Me
SO2
SO2
N
N
H3C(H2C)8H2C
CH2(CH2)8CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

44