Supporting Information

Transformation of Anionically Activated Trifluoromethyl Groups to Heterocycles under Mild Aqueous Conditions

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1. General Experimental Information

Commercially available regents were used without further purification. Products were obtained either by filtration or further purification by using either recrystalization from solvents such as MeOH, or by using normal phase silica gel chromatography. Normal phase chromatography was carried out using prepacked SiO_2 cartridges eluted with gradients of hexanes and ethyl acetate or methylene chloride and methanol. Low resolution MS chromatograms were obtained on a Shimadzu HPLC system running DISCOVERY VP® software, coupled with a Waters ZQ mass spectrometer running MassLynx version 3.5 software using the following methods:

Method A: A linear gradient using solvent A (10% methanol, 90% water, 0.1% of TFA) and solvent B (90% methanol, 10% water, 0.1% of TFA); 0-100% of solvent B over 4 min and then 100% of solvent B over 1 min. Column: PHENOMENEX® Luna 5 μm C18 (4.5 × 50 mm). Flow rate was 4 ml/min. and UV detection was set to 220 nm.

Method B: A linear gradient using solvent A (10% methanol, 90% water, 0.1% of TFA) and solvent B (90% methanol, 10% water, 0.1% of TFA); 0-100% of solvent B over 2 min and then 100% of solvent B over 1 min. Column: PHENOMENEX® Luna 5 μm C18 (2.0 × 30 mm). Flow rate was 1 ml/min. and UV detection was set to 220 nm.

Method C: A linear gradient using solvent A (98% water, 2% methanol, 0.1% formic acid) and solvent B (methanol, 0.1% formic acid); 0-100% of solvent B over 2 min and then 100% of solvent B over 1 min. Column: PHENOMENEX® Luna 3 μm C18 (2.0 × 30 mm). Flow rate was 1 ml/min. and UV detection was set to 220 nm.

All the compounds were confirmed for molecular weight using accurate mass LCMS. A Thermo Fisher LTQ Orbitrap mass spectrometer in line with a Waters Acquity UPLC allowed collection of molecular ion data with accuracy <5 ppm.

^{1}H NMR and ^{13}C NMR spectra were recorded on either Bruker or JEOL fourier transform spectrometers operating at frequencies as follows: ^{1}H NMR: 400 MHz (Bruker or JEOL) or 500MHz (JEOL). ^{13}C NMR: 100 MHz (Bruker or JEOL). Spectra data are reported in the format: chemical shift (multiplicity, coupling constants, and number of hydrogens). Chemical shifts are specified in ppm downfield of a tetramethylsilane internal standard (δ units, tetramethylsilane = 0 ppm) and/or referenced to solvent peaks, which in ^{1}H NMR spectra appear

at 2.49 ppm for CD_3SOCD_3, 3.30 ppm for CD_3OD, 7.24 ppm for $CDCl_3$, and 11.50 ppm for CF_3COOD and which in ^{13}C NMR spectra appear at 39.7 ppm for CD_3SOCD_3, 49.0 ppm for CD_3OD, 77.0 ppm for $CDCl_3$, and 164.20 and 116.60 for CF_3COOD. All ^{13}C NMR spectra were proton decoupled.

The purity of the compounds was checked by using the following orthogonal HPLC conditions:

Method A: A linear gradient using solvent A (5% acetonitrile, 95% water, 0.05% TFA) and solvent B (95% acetonitrile, 5% water, 0.05% TFA); 10-100% of solvent B over 10 min and then 100% of solvent B over 5 min. Column: Sunfire C18 3.5 μm (4.6 × 150 mm). Flow rate was 2 ml/min, and UV detection was set to 220 nm. The LC column was maintained at room temperature.

Method B: A linear gradient using solvent A (5% acetonitrile, 95% water, 0.05% TFA) and solvent B (95% acetonitrile, 5% water, 0.05% TFA); 10-100% of solvent B over 10 min and then 100% of solvent B over 5 min. Column: Xbridge Phenyl 3.5 μm (4.6 × 150 mm). Flow rate was 2 ml/min, and UV detection was set to 220 nm. The LC column was maintained at room temperature.

2. Representative Procedure and Characterization Data of Compounds

General procedures: To a reaction vessel (such as a 20-ml scintillation vial or a round bottomed flask) equipped with a magnetic stirring bar was added the anionically activated aromatic/heteroaromatics CF_3 substrate (1 mmol) and the amine nucleophile (1–1.4 mmol), followed by the addition of 1 N NaOH solution (3 or 4 mL, 3 or 4 equiv). The resulting reaction mixture was heated using a heating block or an oil bath while stirring at 40–90 ℃ for the time period indicated in the tables in the manuscript. The reaction was cooled to room temperature and the mixture was neutralized by addition of either 1 N HCl or HOAc. The precipitate was collected by filtration, and was rinsed with either 1 N HCl (2 ×) followed by H_2O (2 ×), or with H_2O (4 ×). (Caution: During the work-up to neutralize the mixture with 1N HCl or HOAc, highly toxic HF may be generated, and the corresponding waste should be neutralized with an inorganic base and then properly disposed.) The filter cake was dried under vacuum and the purity was checked by orthogonal HPLC. For compounds with purity less than 95%, the solids were either

recrystallized from methanol or further purified by silica gel column chromatography by using either hexanes/ethyl acetate or methylene chloride/methanol as the eluent.

Representative procedure for transformation of anionically activated aromatic CF_3 group to heterocyclic compound 2-(Benzo[d]oxazol-2-yl)phenol (**3**): 2-(Trifluoromethyl)phenol (163 mg, 1 mmol) and 2-aminophenol (132 mg, 1.2 mmol) were stirred in 1 N NaOH (3 mL, 3 mmol) in a capped 20-ml scintillation vial on a Pie-Block. The mixture was heated at 80 °C for 2 h. After cooling, 1 N HCl (ca. 3 mL) was added with stirring and the resulting slurry was filtered. The filter cake was rinsed with cold 1 N HCl (2 × 5 mL), H_2O (3 × 5 mL), and then dried under vacuum for 16 h to give compound **3**[1] (200 mg, 94 % yield) as a light tan solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.46 (s, 1H), 8.01 (d, *J* = 7.5 Hz, 1H), 7.85 – 7.67 (m, 1H), 7.67 – 7.51 (m, 1H), 7.53 – 7.29 (m, 3H), 7.11 (d, *J* = 8.1 Hz, 1H), 7.00 (t, *J* = 7.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.10, 158.93, 149.33, 140.21, 133.76, 127.32, 125.58, 125.21, 119.77, 119.45, 117.62, 110.86. LCMS (ESI) 212.1 (M+H), retention time = 4.21 min (Method A). HRMS $(M + H)^+$ calcd for $C_{13}H_{10}NO_2$ 212.07060, found 212.07025. Orthogonal HPLC purity: 96.5%, retention time = 12.439 min (Method A); 96.1%, retention time = 10.103 min (Method B).

Representative procedure for transformation of anionically activated NH-containing heteroaromatic CF_3 group to heterocyclic compound 2-(1H-Imidazol-4-yl)-5-nitrobenzo[d]oxazole (**24**): In a 100-mL three-neck round-bottomed flask equipped with a condenser, a thermometer and a magnetic stirring bar, a mixture of 4-(trifluoromethyl)-1H-imidazole (0.272 g, 2 mmol), 2-amino-4-nitrophenol (0.308 g, 2 mmol) and 1 N NaOH (8 mL, 2 mmol) was heated to 90 ^{o}C in an oil bath under nitrogen for 4 h. After cooling to room temperature, the mixture was neutralized with 1 N HCl (8 mL). The resulting suspension was filtered. The filter cake was washed with water (3 × 10 mL) and dried by vacuum suction for 18 h. The filter cake was then crystallized from MeOH (reflux then cooled down to 5 ^{o}C) to afford **24** (0.41 g, 1.781 mmol, 89 % yield) as off-white solids. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.55 (d, *J* = 2.2 Hz, 1H), 8.29 (dd, *J* = 9.2 and 2.2 Hz, 1H), 8.20 (s, 1H), 8.03 (s, 1H), 7.97 (d, *J* = 9.1 Hz, 1H). ^{13}C NMR (75 MHz, DMSO-d_6), δ 161.35, 152.76, 144.19, 141.42, 137.58, 126.50, 122.28, 119.97, 114.11, 110.53. LCMS (ESI) 231.0 (M+H), retention time = 1.27 min (Method B). HRMS $(M + H)^+$ calcd for $C_{10}H_7N_4O_3$ 231.05130, found 231.05128. Orthogonal HPLC

purity: 96.8, retention time = 4.415 min (Method A); 96.6 %, retention time = 4.500 min (Method B).

The following examples were made according to similar procedures as those for compounds **3** and **24**:

2-(Benzo[d]thiazol-2-yl)phenol (**4**):[2] 88% yield. White solids. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.50 (s, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 7.8 Hz, 1H), 7.64 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.46 (dd, *J* = 11.1, 4.0 Hz, 1H), 7.40 – 7.30 (m, 2H), 7.10 (d, *J* = 8.2 Hz, 1H), 6.91 (dd, *J* = 11.2, 4.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.46, 158.07, 151.91, 132.86, 132.69, 128.53, 126.78, 125.62, 122.26, 121.60, 119.63, 117.98, 116.89. LCMS (ESI) 228.0 (M+H), retention time = 2.28 min (Method B). HRMS $(M + H)^+$ calcd for $C_{13}H_{10}NOS$ 228.04780, found 228.04784. Orthogonal HPLC purity: 98.6%, retention time = 14.929 min (Method A); 99.6%, retention time = 12.479 min (Method B).

2-(1-Methyl-1H-benzo[d]imidazol-2-yl)phenol (**5**):[3] 71% yield. White solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.27 (s, 1H), 7.81 – 7.55 (m, 3H), 7.39 (ddd, *J* = 8.3, 7.4, 1.7 Hz, 1H), 7.28 (dtd, *J* = 15.0, 7.3, 1.2 Hz, 2H), 7.05 (dd, *J* = 8.2, 0.9 Hz, 1H), 6.98 (td, *J* = 7.5, 1.1 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 156.61, 151.77, 141.35, 135.70, 131.35, 130.25, 122.37, 121.94, 119.00, 118.43, 116.43, 115.79, 110.31, 31.64. LCMS (ESI) 225.1 (M+H), retention time = 1.90 min (Method A). HRMS $(M + H)^+$ calcd for $C_{14}H_{13}N_2O$ 225.10230, found 225.10187. Orthogonal HPLC purity: 99.6%, retention time = 3.691 min (Method A); 100%, retention time = 4.510 min (Method B).

2-(4,5-Dihydrooxazol-2-yl)phenol (**6**):[4] 55% yield. White solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.22 (s, 1H), 7.61 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.42 (ddd, *J* = 8.6, 7.3, 1.7 Hz, 1H), 6.97 (ddd, *J* = 9.0, 3.7, 1.0 Hz, 1H), 6.94 – 6.87 (m, 1H), 4.46 (t, *J* = 9.5 Hz, 2H), 4.06 (t, *J* = 9.4 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.30, 159.01, 133.49, 127.68, 118.81, 116.34, 110.15, 66.94, 52.86. LCMS (ESI) 164.1 (M+H), retention time = 0.98 min (Method C). HRMS $(M + H)^+$ calcd for $C_9H_{10}NO_2$ 164.07060, found 164.06981. Orthogonal HPLC purity: 100%, retention time = 5.381 min (Method A); 100%, retention time = 4.661 min (Method B).

2-(4,5-Dihydrothiazol-2-yl)phenol (**7**): 74% yield. White solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.63 (s, 1H), 7.93 – 7.14 (m, 2H), 7.17 – 6.60 (m, 2H), 5.23 – 4.15 (m, 2H), 3.52 – 3.37 (m, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 171.51, 158.28, 133.06, 130.42, 119.09, 116.62, 115.78, 63.13, 31.36. LCMS (ESI) 178.0 (M-H), 180.1 (M+H), retention time = 1.85

min (Method C). HRMS $(M + H)^+$ calcd for $C_9H_{10}NOS$ 180.04780, found 180.04723. Orthogonal HPLC purity: 100%, retention time = 3.715 min (Method A); 100%, retention time = 4.553 min (Method B).

2-(Oxazolo[5,4-b]pyridin-2-yl)phenol (**8**): 68% yield. White solids. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.00 (s, 1H), 8.39 (dd, J = 4.9, 1.5 Hz, 1H), 8.27 (dd, J = 7.9, 1.5 Hz, 1H), 8.01 (dd, J = 7.9, 1.6 Hz, 1H), 7.52 (ddd, J = 7.9, 4.8, 1.7 Hz, 2H), 7.17 – 6.94 (m, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.35, 158.09, 158.04, 144.85, 134.43, 131.52, 128.24, 128.09, 121.83, 120.06, 117.33, 110.24. LCMS (ESI) 213.0 (M+H), retention time = 2.00 min (Method C). HRMS $(M + H)^+$ calcd for $C_{12}H_9N_2O_2$ 213.06590, found 213.06534. Orthogonal HPLC purity: 99.8%, retention time = 10.088 min (Method A); 99.4%, retention time = 8.456 min (Method B).

2-(1H-Perimidin-2-yl)phenol (**9**): 82% yield. Dark reddish solids. ^{1}H NMR (400 MHz, DMSO-d_6) δ 14.80 (s, br, 1H), 10.72 (s, br, 1H), 7.97 (dd, J = 8.0, 1.4 Hz, 1H), 7.41 (d, J = 7.0 Hz, 1H), 7.26 – 7.17 (m, 2H), 7.13 (d, J = 8.2 Hz, 2H), 7.01 – 6.87 (m, 2H), 6.70 (dd, J = 7.2, 0.7 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.11, 154.67, 134.77, 133.29, 126.20, 120.98, 117.95, 112.77. LCMS (ESI) 261.1 (M+H), retention time = 1.53 min (Method B). HRMS $(M + H)^+$ calcd for $C_{17}H_{13}N_2O$ 261.10230, found 261.10159. Orthogonal HPLC purity: 93.8%, retention time = 5.623 min (Method A); 93.2%, retention time = 5.946 min (Method B).

5-(5-(Dimethylamino)-1,3,4-thiadiazol-2-yl)pyrimidine-2,4(1H,3H)-dione (**10**): 69% yield. Light yellow solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.62 (s, 2H), 8.14 (s, 1H), 3.06 (s, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 171.73, 162.05, 150.26, 148.13, 139.10, 104.41, 40.88. LCMS (ESI) 240.1 (M+H), retention time = 0.77 min (Method A). HRMS $(M + H)^+$ calcd for $C_8H_{10}N_5O_2S$ 240.05500, found 240.05449. Orthogonal HPLC purity: 94.6%, retention time = 1.74 min (Method A); 100%, retention time = 1.93 min (Method B).

5-(5-Methyl-1,3,4-oxadiazol-2-yl)pyrimidine-2,4(1H,3H)-dione (**11**): 77% yield. Slightly yellowish solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.61 (m, *br*, 2H), 8.10 (s, 1H), 2.50 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 163.34, 160.14, 150.47, 145.06, 98.23, 10.49. LCMS (ESI) 195.0 (M+H), retention time = 0.52 min (Method A). HRMS $(M + H)^+$ calcd for $C_7H_7N_4O_3$ 195.05130, found 195.05078. Orthogonal HPLC purity: 86.5%, retention time = 2.158 min (Method A); 100%, retention time = 2.200 min (Method B).

5-(3-Methyl-1,2,4-oxadiazol-5-yl)pyrimidine-2,4(1H,3H)-dione (**12**): 80% yield. Off-white solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.93 (s, br, 1H), 11.58 (s, 1H), 8.33 (s, 1H), 2.32 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 171.69, 166.43, 159.68, 150.34, 147.57, 98.51, 11.07. LCMS (ESI) 195.0 (M+H), retention time = 0.74 min (Method A). HRMS $(M + H)^+$ calcd for $C_7H_7N_4O_3$ 195.05130, found 195.05090. Orthogonal HPLC purity: 100%, retention time = 3.548 min (Method A); 100%, retention time = 4.148 min (Method B).

2-(2-Hydroxyphenyl)benzo[d]oxazole-6-sulfonamide (**15**): 97% yield. Off-white solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.96 (s, 1H), 8.22 (d, J = 1.5 Hz, 1H), 8.05 – 7.96 (m, 2H), 7.91 (dd, J = 8.6, 1.8 Hz, 1H), 7.57 – 7.45 (m, 3H), 7.11 (dd, J = 8.3, 0.7 Hz, 1H), 7.09 – 7.04 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.29, 157.94, 150.80, 141.59, 139.98, 134.62, 128.43, 123.68, 120.23, 117.48, 117.10, 111.75, 110.49. LSMS (ESI) = 291.0, retention time = 1.84 min (Method B). HRMS $(M + H)^+$ calcd for $C_{13}H_{11}N_2O_4S$ 291.04340, found 291.04300. Orthogonal HPLC purity: 96.7%, retention time = 12.211 min (Method A), 97.2%, retention time =12.423 min (Method B).

2-(5-(Ethylsulfonyl)benzo[d]oxazol-2-yl)phenol (**16**): 94% yield. Slightly tan solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.91 (s, 1H), 8.32 (d, J = 0.8 Hz, 1H), 8.07 (d, J = 8.5 Hz, 1H), 8.00 (d, J = 7.2 Hz, 1H), 7.95 (dd, J = 8.5, 1.2 Hz, 1H), 7.52 (d, J = 7.3 Hz, 1H), 7.11 (d, J = 8.3 Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H), 3.38 (q, J = 7.3 Hz, 2H), 1.12 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.32, 157.86, 151.88, 140.26, 135.58, 134.46, 128.29, 125.40, 119.94, 119.40, 117.29, 111.95, 110.20, 49.44, 7.19. LCMS 304.1 (M+H), retention time = 2.01 min (Method B). HRMS $(M + H)^+$ calcd for $C_{15}H_{14}NO_4S$ 304.06380, found 304.06378. Orthogonal HPLC purity: 97.2%, retention time = 13.976 min (Method A); 97.4%, retention time = 13.782 min (Method B).

2-(2-Hydroxyphenyl)-N,N-dimethylbenzo[d]oxazole-6-sulfonamide (**17**): 91% yield. White solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.97 (s, 1H), 8.22 (d, J = 1.5 Hz, 1H), 8.06 (d, J = 8.5 Hz, 1H), 8.03 (dd, J = 7.9, 1.6 Hz, 1H), 7.81 (dd, J = 8.3, 1.7 Hz, 1H), 7.62 – 7.44 (m, 1H), 7.14 (dd, J = 8.3, 0.7 Hz, 1H), 7.12 – 7.06 (m, 1H), 2.65 (s, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.01, 157.97, 148.67, 143.41, 134.62, 131.77, 128.39, 124.70, 120.03, 119.74, 117.36, 110.94, 110.27, 37.61. LCMS 319.1 (M+H), retention time = 2.10 min (Method B). HRMS $(M + H)^+$ calcd for $C_{15}H_{15}N_2O_4S$ 319.07470, found 319.07352. Orthogonal HPLC purity: 98.9%, retention time = 14.801 min (Method A); 99.0%, retention time = 14.424 min (Method B).

2-(2-Hydroxyphenyl)benzo[d]oxazole-5-sulfonic acid (**18**): 92% yield. Pale yellowish solids. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.13 (s, 1H), 8.47 – 7.85 (m, 2H), 7.75 (q, *J* = 8.3 Hz, 2H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.34 – 6.74 (m, 2H), 3.28 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.92, 157.64, 148.64, 146.20, 138.81, 133.94, 127.63, 123.80, 119.92, 117.14, 116.15, 110.39, 110.05. LCMS 292.0 (M+H), retention time = 2.89 min (Method A). HRMS $(M + H)^+$ calcd for $C_{13}H_{10}NO_5S$ 292.02740, found 292.02747. Orthogonal HPLC purity: 97.4%, retention time = 7.441 min (Method A); 100.0%, retention time = 4.863 min (Method B).

2-Amino-3-(2-(2-hydroxyphenyl)benzo[d]oxazol-5-yl)propanoic acid (**19**): 87% yield. Off-white solids. ^{1}H NMR (500 MHz, CF_3COOD) δ 8.33 (dd, *J* = 8.0, 2.3 Hz, 1H), 8.02 (s, 1H), 7.96 (dd, *J* = 8.6, 3.6 Hz, 1H), 7.81 (ddd, *J* = 17.2, 9.1, 4.4 Hz, 2H), 7.32 (ddd, *J* = 16.2, 8.2, 3.5 Hz, 2H), 4.80 (s, 1H), 3.84 (d, *J* = 14.7 Hz, 1H), 3.70 (dd, *J* = 11.4, 8.3 Hz, 1H). ^{13}C NMR (126 MHz, CF_3COOD) δ 173.76, 165.51, 161.06, 149.90, 142.42, 136.47, 132.39, 131.81, 130.89, 124.69, 119.26, 118.47, 107.19, 57.18, 37.25. LCMS 299.1 (M+H), retention time = 2.99 min (Method A). HRMS $(M + H)^+$ calcd for $C_{16}H_{15}N_2O_4$ 299.10270, found 299.10266. Orthogonal HPLC purity: 96.5%, retention time = 4.626 min (Method A); 96.4%, retention time = 5.228 min (Method B).

1-(2-(2-Hydroxyphenyl)-5-methylbenzo[d]oxazol-7-yl)ethanone (**20**): 96% yield. Off-white solids. ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.26 – 11.25 (m, 1H), 8.00 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.71 (dd, *J* = 27.7, 0.8 Hz, 2H), 7.55 – 7.31 (m, 1H), 7.10 (dd, *J* = 8.4, 0.5 Hz, 1H), 7.05 – 6.88 (m, 1H), 2.87 (s, 3H), 2.50 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.78, 163.54, 158.99, 146.32, 141.70, 135.41, 134.21, 127.32, 126.80, 124.46, 121.35, 119.95, 117.77, 110.27, 30.58, 21.54. LSMS (ESI) = 268.1, retention time = 2.33 min (Method B). HRMS $(M + H)^+$ calcd for $C_{16}H_{14}NO_3$ 268.09680, found 268.09668. Orthogonal HPLC purity: 100%, retention time = 16.312 min (Method A); 100%, retention time = 14.996 min (Method B).

2-(5-Chloro-7-nitrobenzo[d]oxazol-2-yl)phenol (**21**): 98% yield. Light tan solids. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.75 (s, 1H), 8.69 (s, 1H), 8.45 (s, 1H), 8.03 (d, *J* = 7.7 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.33 – 6.58 (m, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.57, 158.36, 149.99, 145.92, 141.85, 135.32, 128.96, 121.55, 120.45, 117.70, 116.01, 114.55, 110.23. LCMS (ESI) 291.0 (M+H), retention time = 2.41 min (Method B). HRMS $(M - H)^+$ calcd for $C_{13}H_6ClN_2O_4$ 289.00210, found 289.00153. Orthogonal HPLC purity: 97.6%, retention time = 16.672 min (Method A); 96.9%, retention time = 15.856 min (Method B).

2-(6-Bromo-5-methoxybenzo[d]oxazol-2-yl)phenol (**22**): 93% yield. Off-white solids. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.15 (s, 1H), 8.05 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.44 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.16 – 7.07 (m, 3H), 7.00 (dd, *J* = 11.5, 4.3 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.91, 158.90, 158.35, 142.44, 141.35, 134.17, 127.56, 119.91, 117.66, 116.92, 110.41, 102.66, 102.09, 56.44. LCMS (ESI) 320.0, 322.0 (M+H), retention time = 2.57 min (Method B). HRMS $(M + H)^+$ calcd for $C_{14}H_{11}BrNO_3$ 319.99170, found 319.99219. Orthogonal HPLC purity: 97.4%, retention time = 13.757 min (Method A); 95.0%, retention time = 11.148 min (Method B).

2-(2-(4-Chlorophenyl)-1H-imidazol-4-yl)benzo[d]oxazole-5-carbonitrile (**23**): 92 % yield. Off-white solids. ^{1}H NMR (300 MHz, DMSO-d_6) δ 13.49 (bs, 1H), 8.30 – 7.32 (m, 2H), 8.07 (d, *J* = 8.4 Hz, 2H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.83 – 7.86 (m, 1H), 7.57 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (75 MHz, DMSO-d_6), δ 151.59, 145.49, 141.39, 132.98, 128.29, 127.70, 126.44, 122.95, 118.15, 111.49, 106.70. LCMS (ESI) 321.0 (M+H), retention time = 1.99 min (Method B). HRMS $(M + H)^+$ calcd for $C_{17}H_{10}ClN_4O$ 321.05380, found 321.05359. Orthogonal HPLC purity: 95.8%, retention time = 8.658 min (Method A); 100%, retention time = 7.691 min (Method B).

4-Hydroxy-phenyl-benzoxazole (**25**):[5] 98% yield. White solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.31 (s, 1H), 8.18–7.92 (m, 2H), 7.72 (ddd, *J* = 5.7, 3.8, 2.4 Hz, 2H), 7.44 – 7.25 (m, 2H), 7.06 – 6.85 (m, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.72, 160.92, 150.00, 141.74, 129.26, 124.67, 124.54, 119.21, 117.13, 116.07, 110.53. LC-MS (ESI) 212.2 (M+H), retention time = 1.94 min (Method B). HRMS $(M + H)^+$ calcd for $C_{13}H_{10}NO_2$ 212.07060, found 212.07074. Orthogonal HPLC purity: 98.6%, retention time = 7.721 min (Method A); 99.6%, retention time = 6.550 min (Method B).

6-(Benzo[d]oxazol-2-yl)pyridin-3-ol (**26**): 95% yield. Light brownish solids. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.84 (s, 1H), 8.30 (d, *J* = 2.7 Hz, 1H), 8.19 (d, *J* = 8.7 Hz, 1H), 7.85 – 7.71 (m, 2H), 7.50 – 7.30 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.67, 156.08, 150.29, 141.43, 138.65, 136.11, 125.44, 125.04, 124.81, 122.87, 119.81, 110.99.LCMS (ESI) 213.1 (M+H), retention time = 1.61 min (Method B). HRMS $(M + H)^+$ calcd for $C_{12}H_9N_2O_2$ 213.06590, found 213.06630. Orthogonal HPLC purity: 95.0%, retention time = 6.335 min (Method A); 95.3%, retention time = 5.623 min (Method B).

2-Amino-phenyl-benzoxazole (**27**):[6] 42% yield. Off-white solids. ^{1}H NMR (400 MHz, MeOD) δ 7.99 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.81 – 7.67 (m, 1H), 7.65 – 7.53 (m, 1H), 7.44 – 7.32 (m, 2H), 7.24 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 6.87 (dd, *J* = 8.3, 0.8 Hz, 1H), 6.72 (ddd, *J* = 8.2, 7.2, 1.1 Hz, 1H), 4.80 (s, 2H). ^{13}C NMR (101 MHz, MeOD) δ 164.77, 150.66, 150.28, 143.27, 133.64, 129.53, 126.04, 125.65, 120.30, 117.52, 117.29, 111.30, 109.13. LCMS (ESI) 211.1 (M+H), retention time = 2.23 min (Method B). HRMS $(M + H)^+$ calcd for $C_{13}H_{11}N_2O$ 211.08860, found 211.08731. Orthogonal HPLC purity: 99.1%, retention time = 11.308 min (Method A); 99.3%, retention time = 9.479 min (Method B)

4-Amino-phenyl-benzoxazole (**28**):[7] 84% yield. White solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.98 – 7.76 (m, 2H), 7.65 (dd, *J* = 6.4, 2.6 Hz, 2H), 7.30 (ddd, *J* = 6.4, 5.4, 3.7 Hz, 2H), 6.88 – 6.57 (m, 2H), 5.97 (s, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 163.55, 152.47, 149.83, 142.06, 128.90, 124.27, 123.96, 118.67, 113.50, 112.70, 110.19. LCMS (ESI) 211.1 (M+H), retention time = 1.71 min (Method B). HRMS $(M + H)^+$ calcd for $C_{13}H_{11}N_2O$ 211.08860, found 211.08731. Orthogonal HPLC purity: 98.8%, retention time = 8.451 min (method A); 99.8%, retention time = 7.155 min (Method B).

5-(Benzo[d]oxazol-2-yl)pyridin-2-amine (**29**): 84% yield. White solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.73 (d, *J* = 2.2 Hz, 1H), 8.06 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.82 – 7.54 (m, 2H), 7.33 (ddd, *J* = 4.6, 2.1, 0.8 Hz, 2H), 6.81 (s, 2H), 6.59 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.05, 161.70, 149.77, 148.37, 141.69, 135.62, 124.48, 124.39, 118.90, 110.53, 110.38, 107.92. LCMS (ESI) 212.1, retention time = 2.14 min (Method A). HRMS $(M + H)^+$ calcd for $C_{12}H_{10}N_3O$ 212.08190, found 212.08192. Orthogonal HPLC purity: 98.3%, retention time = 3.876 min (Method A); 96.6%, retention time = 4.386 min (Method B).

4-(Benzo[d]oxazol-2-yl)thiazol-2-amine (**30**): 45% yield. Brownish solids. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.71 (ddd, *J* = 9.2, 4.9, 1.9 Hz, 1H), 7.60 (s, 1H), 7.46 – 7.27 (m, 5H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 169.03, 158.49, 149.64, 141.35, 138.25, 125.21, 124.69, 119.62, 112.55, 110.69. LC-MS (ESI) 218.0 (M+H), retention time = 1.53 min (Method B). HRMS $(M + H)^+$ calcd for $C_{10}H_8N_3OS$ 218.03830, found 218.03876. Orthogonal HPLC purity: 98.2%, retention time = 9.348 min (Method A); 98.1%, retention time = 9.861 min (Method B).

5-(Benzo[d]oxazol-2-yl)pyrimidine-2,4(1H,3H)-dione (**31**): 98% yield. Light tan solids. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.05 – 11.66 (m, 1H), 11.56 (s, 1H), 8.34 (s, 1H), 7.91 – 7.53 (m, 2H), 7.55 – 7.16 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.15, 158.95, 150.51, 149.68,

146.37, 141.06, 124.86, 124.58, 119.22, 110.58, 100.75. LCMS (ESI) 230.1 (M+H), retention time = 2.08 min (Method A). HRMS $(M + H)^+$ calcd for $C_{11}H_8N_3O_3$ 230.05600, found 230.05580. Orthogonal HPLC purity: 96.5%, retention time = 4.146 min (Method A); 96.4%, retention time = 3.868 min (Method B).

2-(1H-Pyrazol-3-yl)benzo[d]oxazole (**32**):86% yield. Light brownish solids. ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.61 (s, 1H), 7.99 (s, 1H), 7.87 – 7.65 (m, 2H), 7.51 – 7.27 (m, 2H), 6.99 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.57, 149.73, 141.25, 139.60, 130.68, 125.28, 124.74, 119.62, 110.87, 106.02. LC-MS (ESI) 184.1 (M–H), 186.1 (M+H), retention time = 2.92 min (Method A). HRMS $(M + H)^+$ calcd for $C_{10}H_8N_3O$ 186.06620, found 186.06656. Orthogonal HPLC purity: 97.3%, retention time = 6.121 min (Method A); 97.8%, retention time = 5.393 min (Method B).

2-(1H-Imidazol-4-yl)benzo[d]oxazole (**33**): 76 % yield. Off-white solids. . ^{1}H NMR (300 MHz, DMSO-d_6) δ 12.85 (bs, 1H), 8.05 (s, 1H), 7.93 (s, 1H), 7.71 – 7.73 (m, 2H), 7.31-7.39 (m, 2H). ^{13}C NMR (75 MHz, DMSO-d_6), δ 148.82, 140.88, 137.09, 123.84, 123.77, 118.40, 109.79. LCMS (ESI) 186.0 (M+H), retention time = 1.18 (Method B). HRMS $(M + H)^+$ calcd for $C_{10}H_8N_3O$ 186.06620, found 186.06656. Orthogonal HPLC purity: 97.5%, retention time = 3.486 min (Method A); 98.9%, retention time = 3.760 min (Method B).

5-(1H-Indol-2-yl)-N,N-dimethyl-1,3,4-thiadiazol-2-amine (**34**): 58% yield. Light tan solids. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.89 (s, 1H), 7.55 (d, J = 8.0 Hz, 1H), 7.45 – 7.35 (m, 1H), 7.22 – 7.09 (m, 1H), 7.03 (dd, J = 11.4, 4.1 Hz, 1H), 6.81 (d, J = 1.9 Hz, 1H), 3.14 (s, 6H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6) δ 170.74, 149.75, 137.05, 128.53, 127.72, 122.95, 120.53, 119.77, 111.78, 102.76, 41.25 ppm. LCMS (ESI) 245.1 (M+H), retention time = 3.24 (Method A). HRMS $(M – H)^-$ calcd for $C_{12}H_{11}N_4S$ 243.07100, found 243.07037. Orthogonal HPLC purity: 97.7%, retention time = 7.723 min (Method A); 98.9%, retention time = 7.105 min (Method B).

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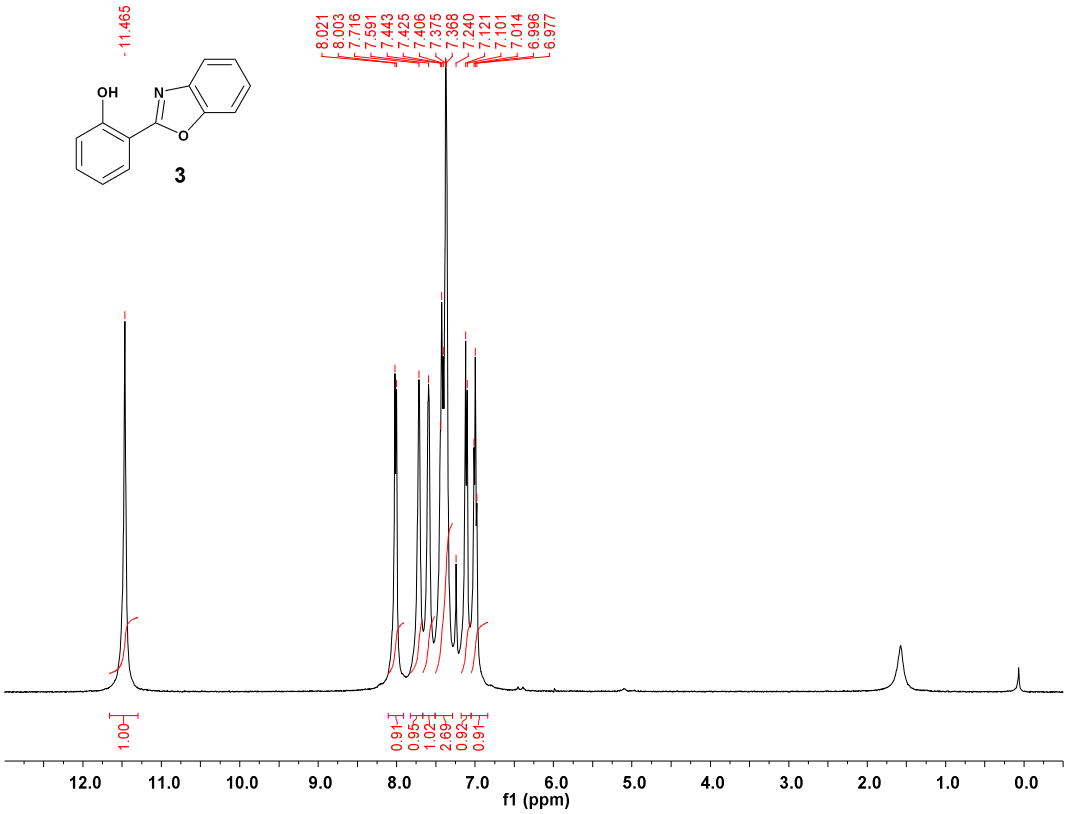
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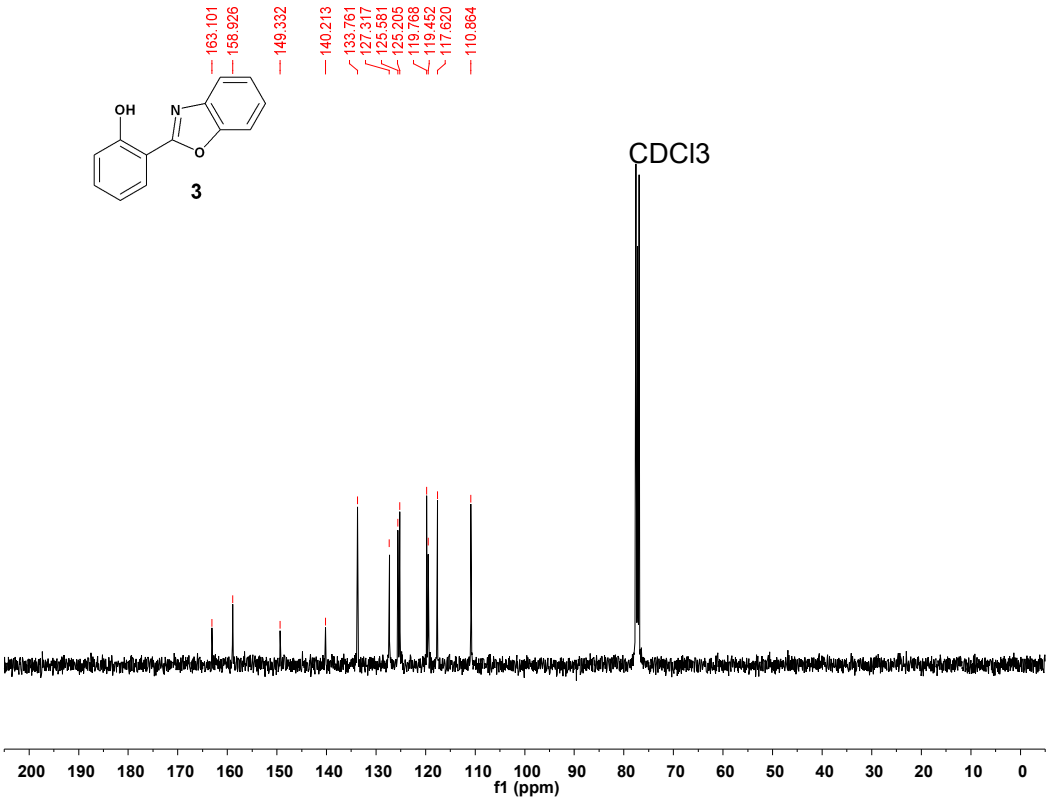
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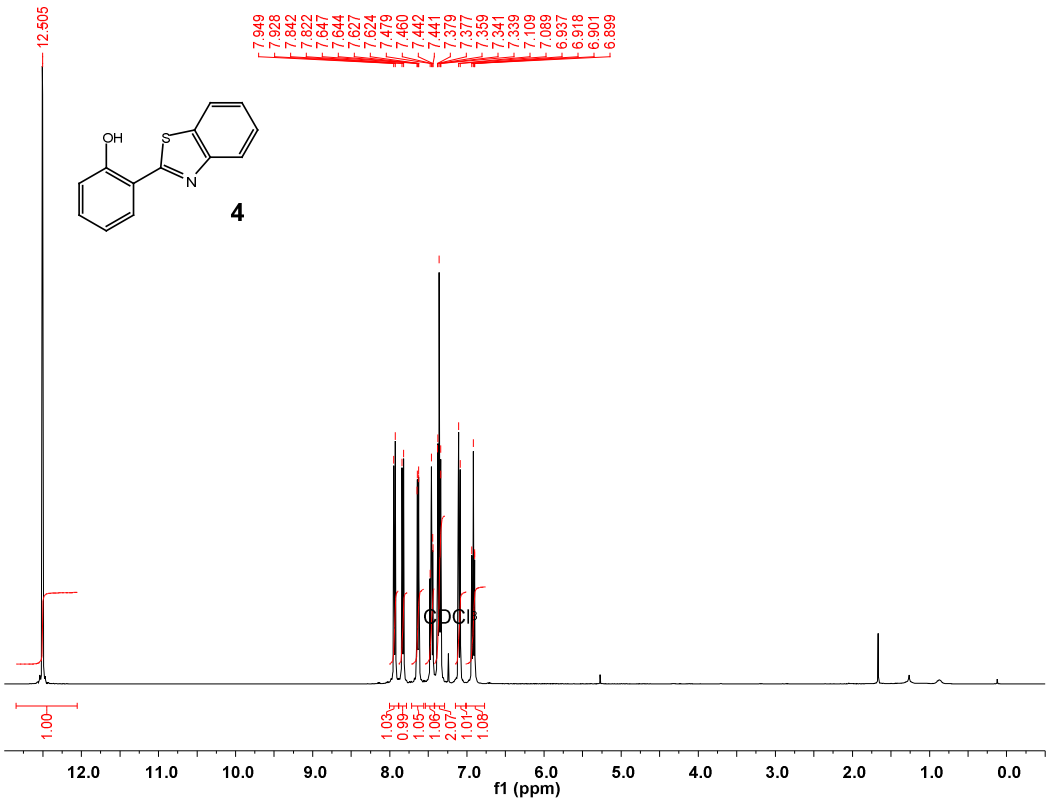
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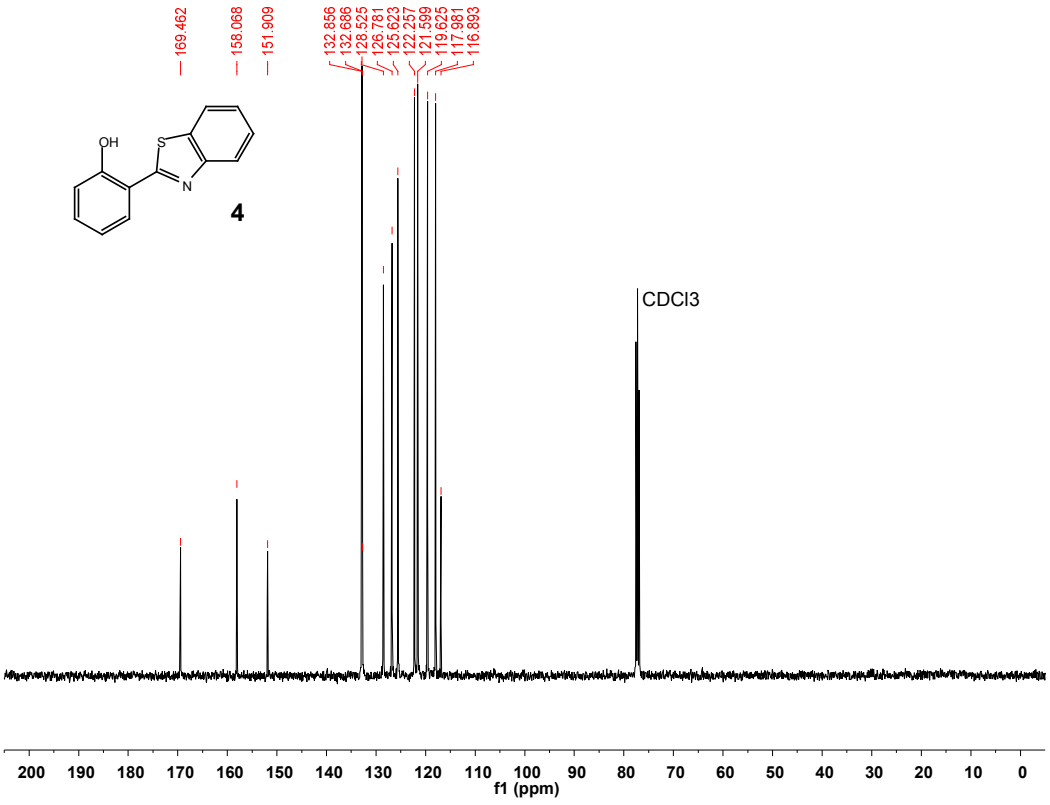
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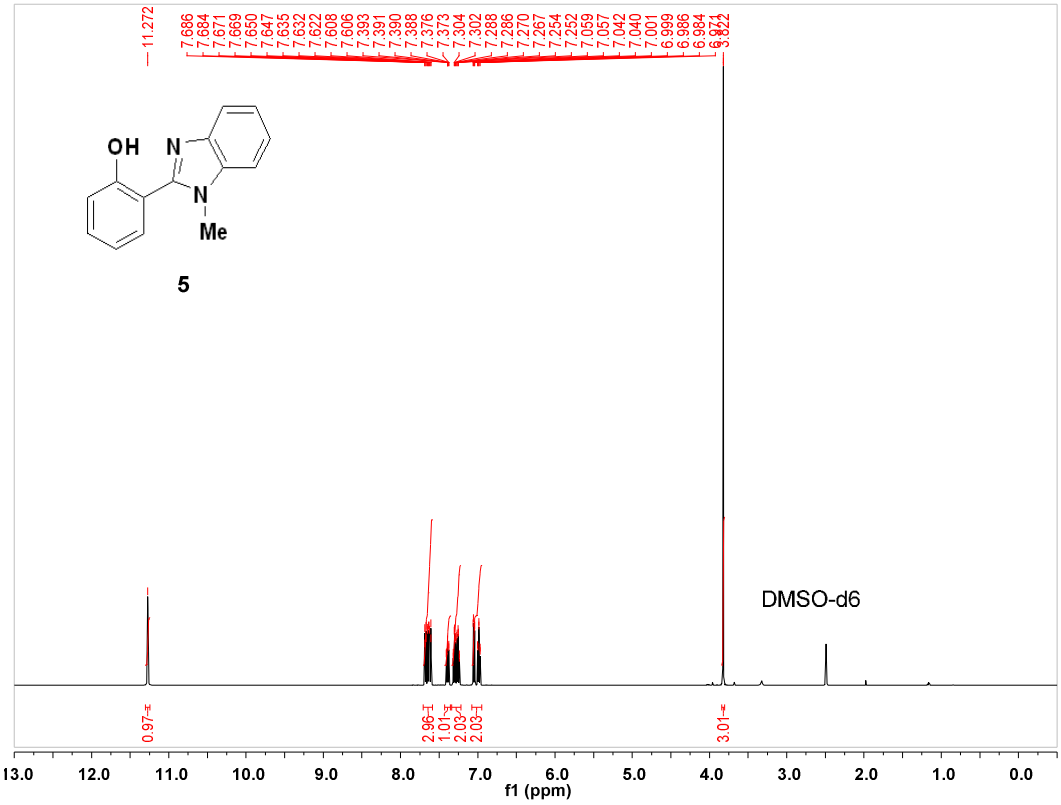
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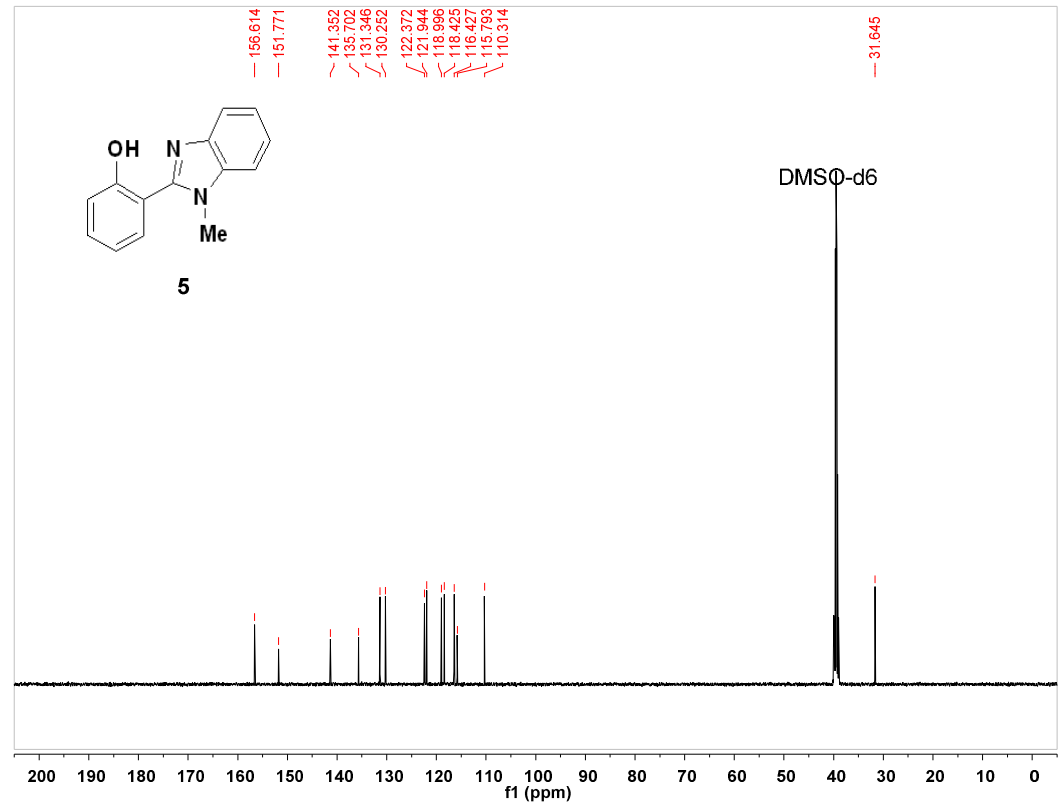
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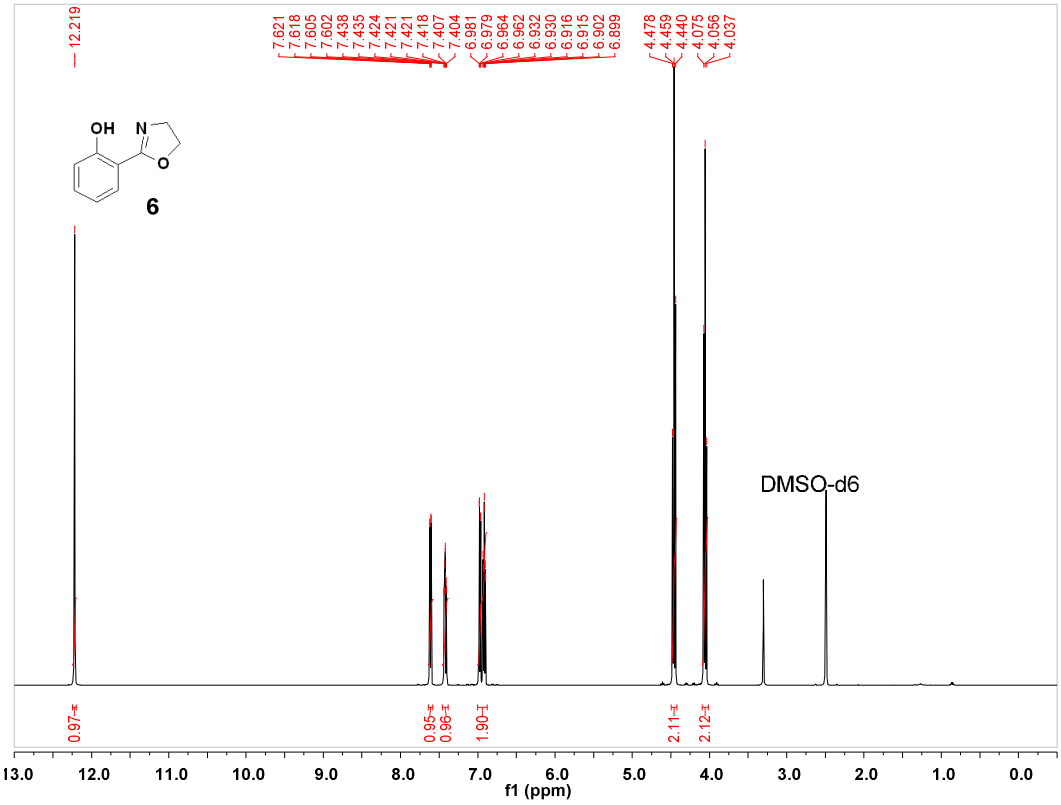
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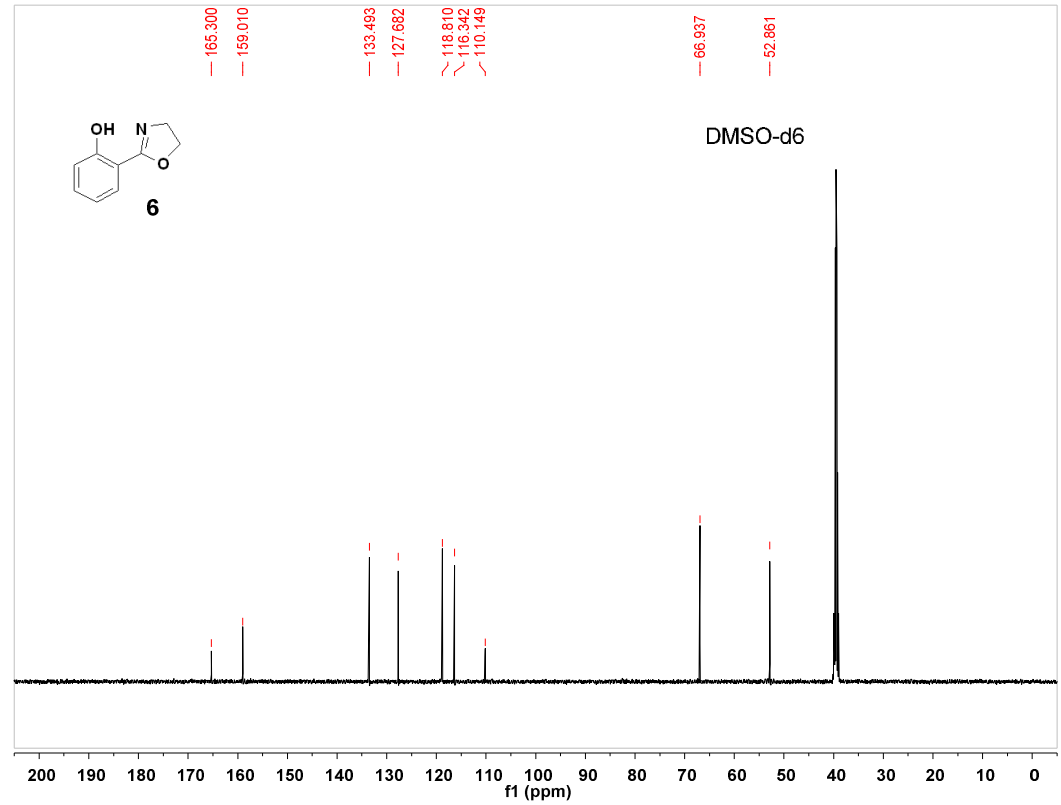
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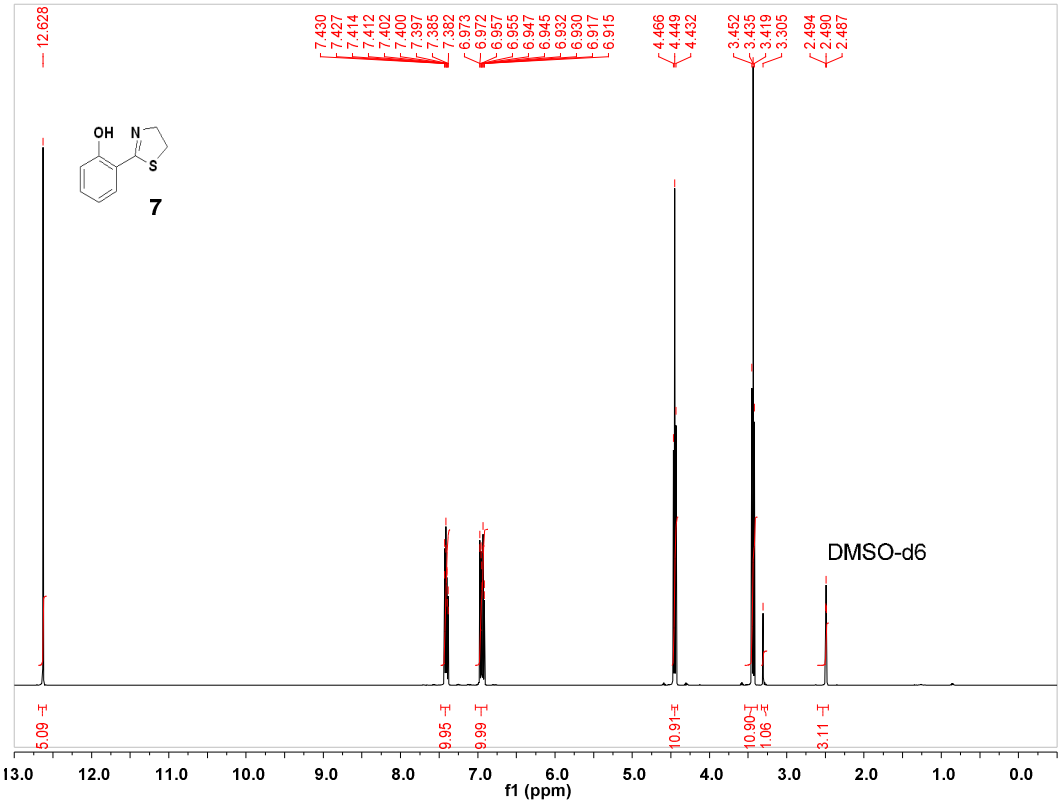
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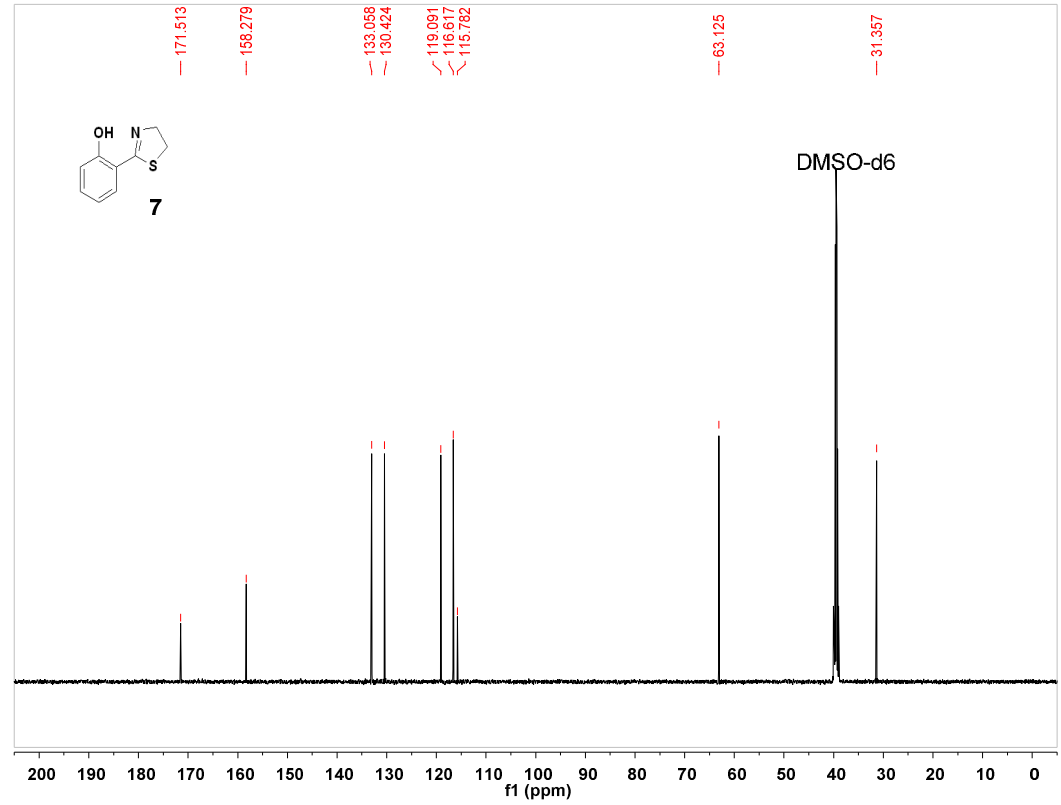
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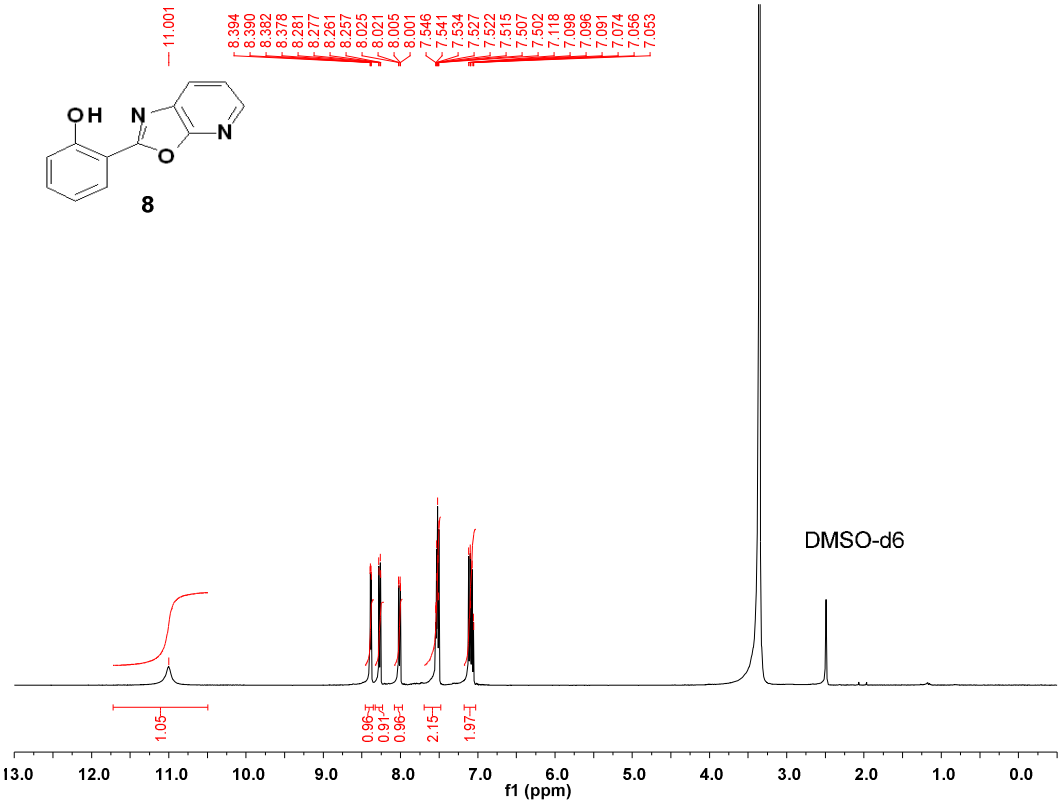
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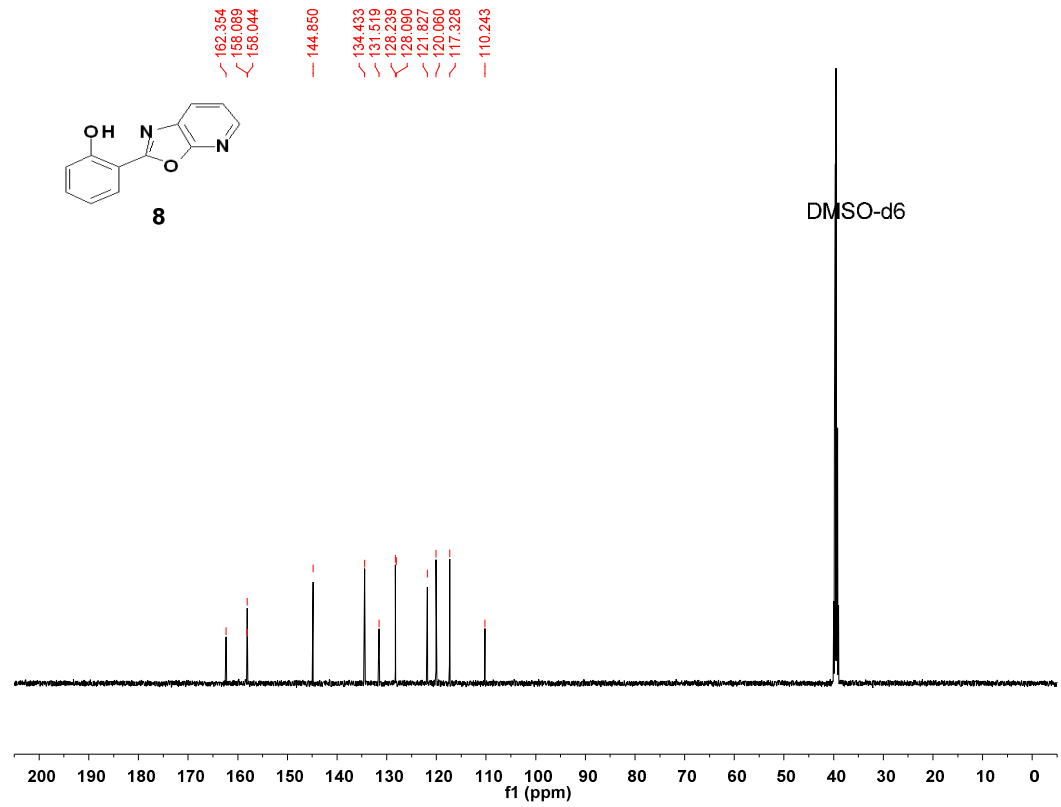
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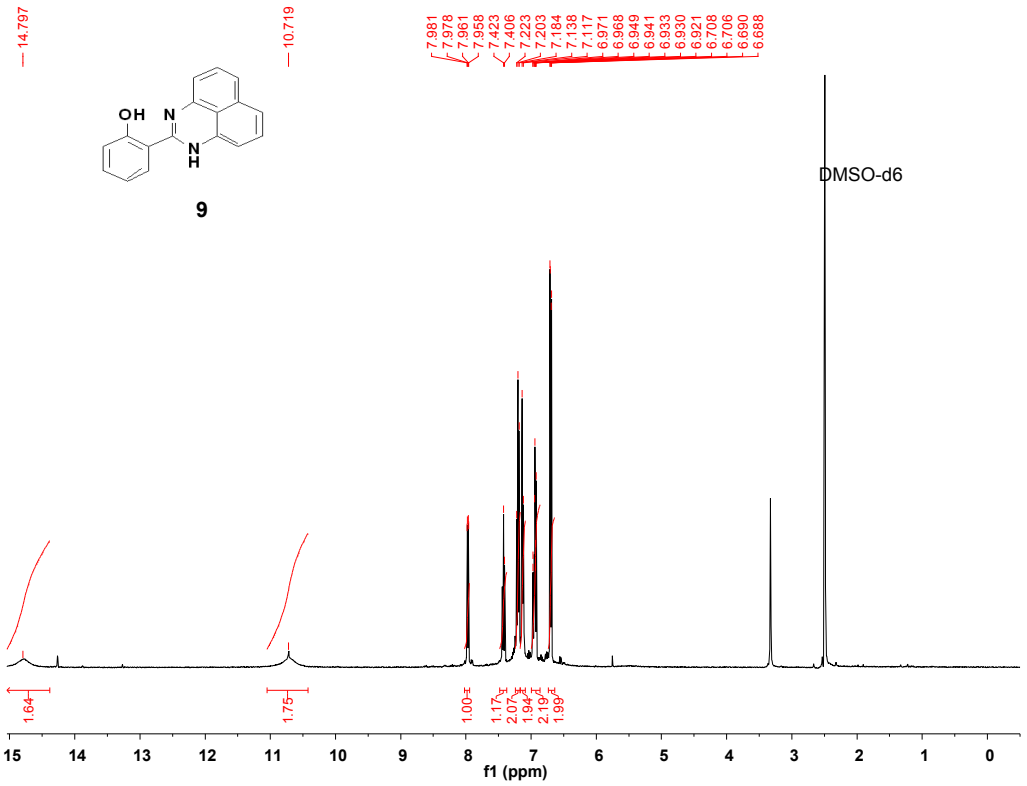
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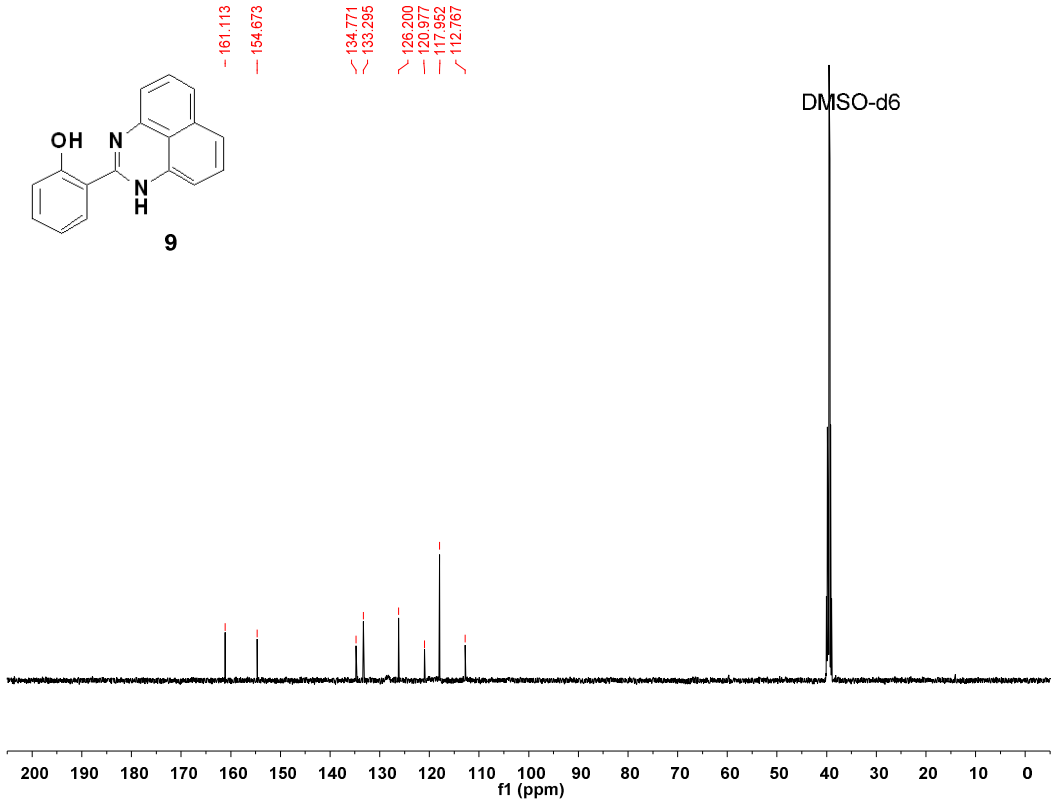
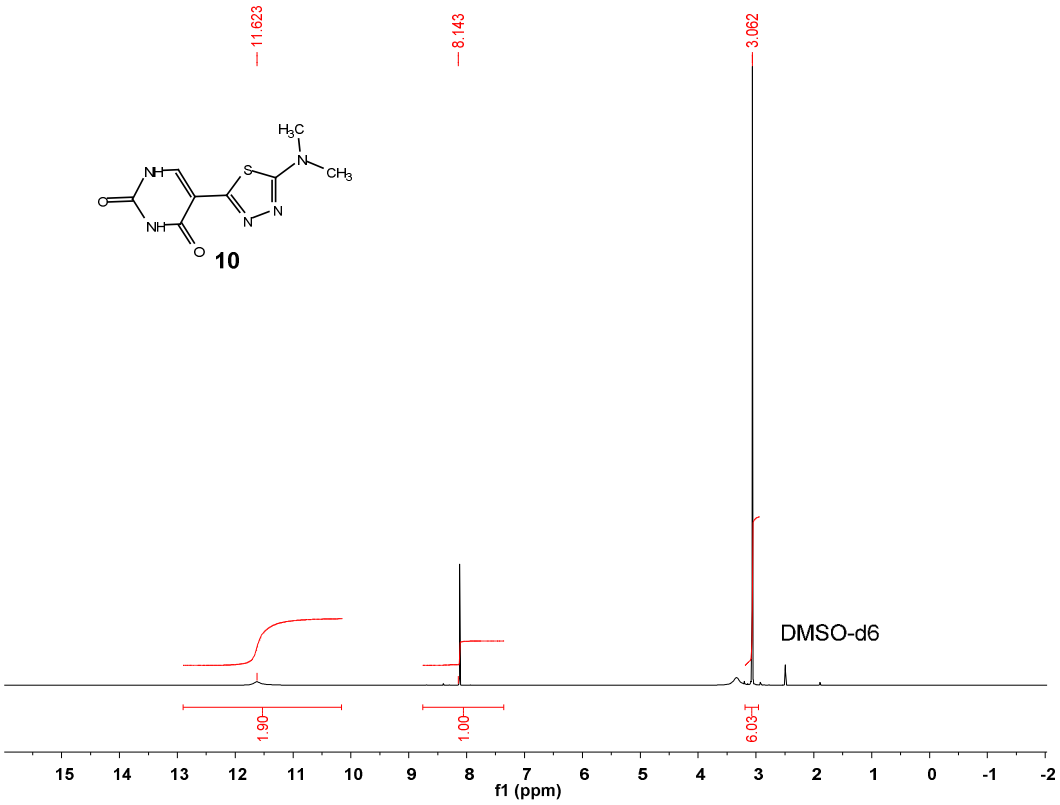
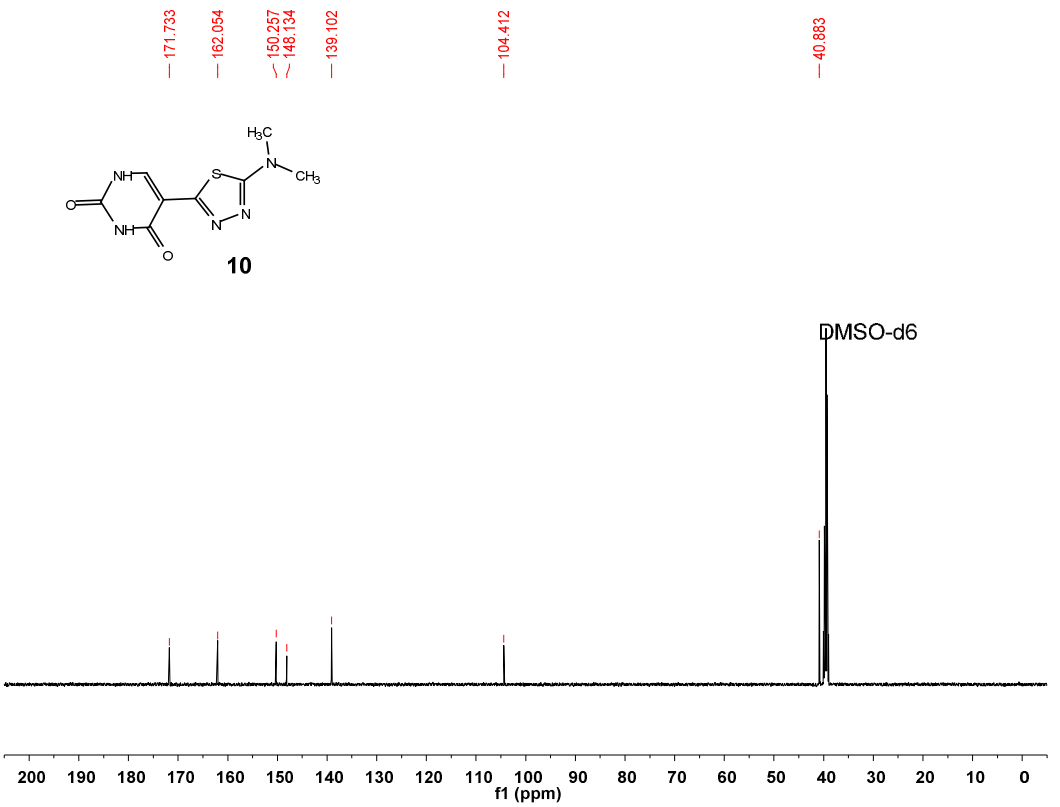
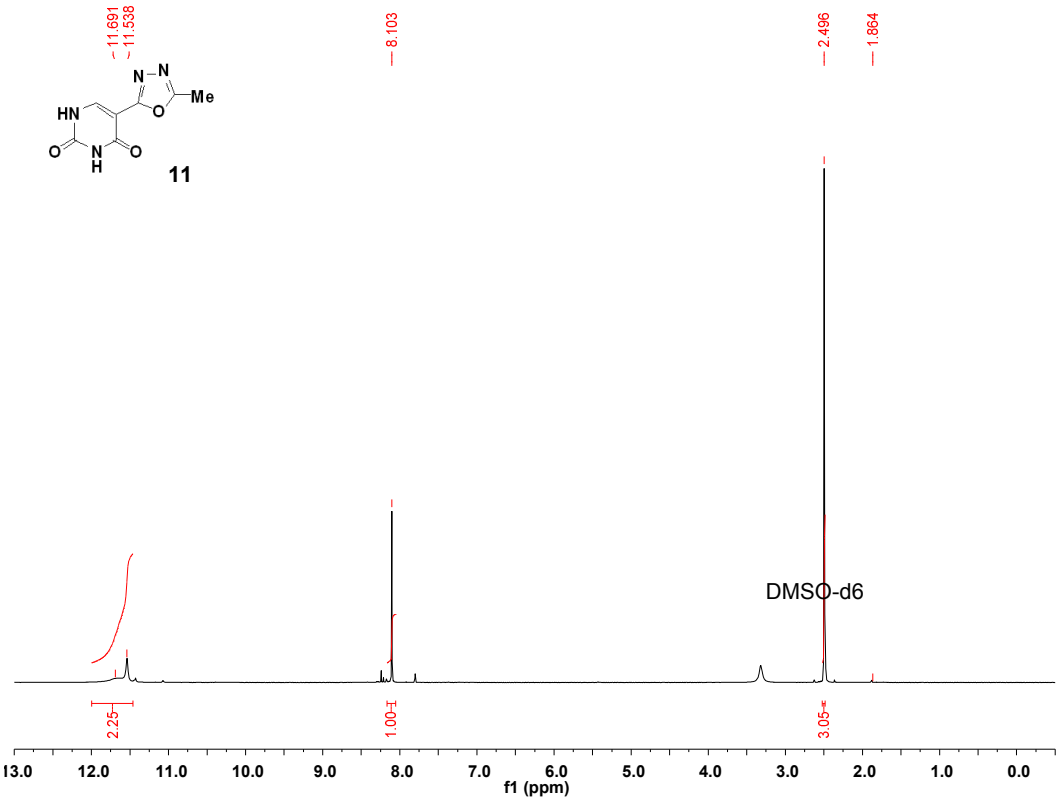
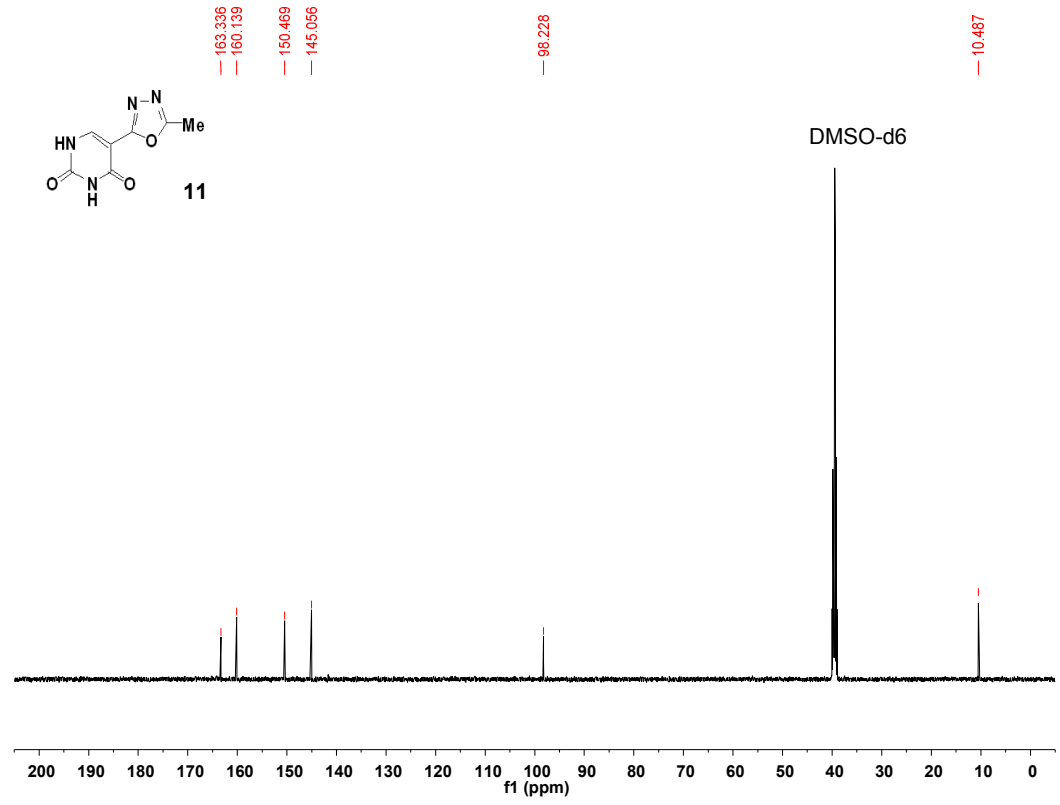
f1 (ppm)

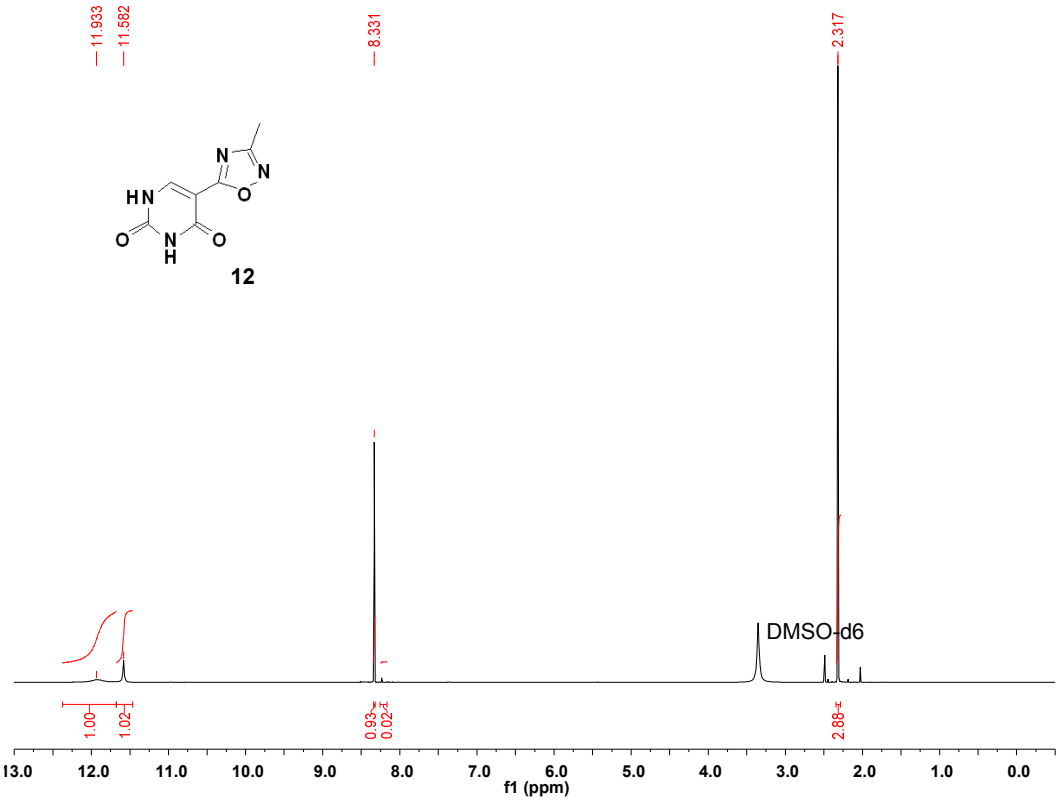

161.113
154.673
134.771
133.295
126.200
120.977
117.952
112.767
OH
N
N
H
9
DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

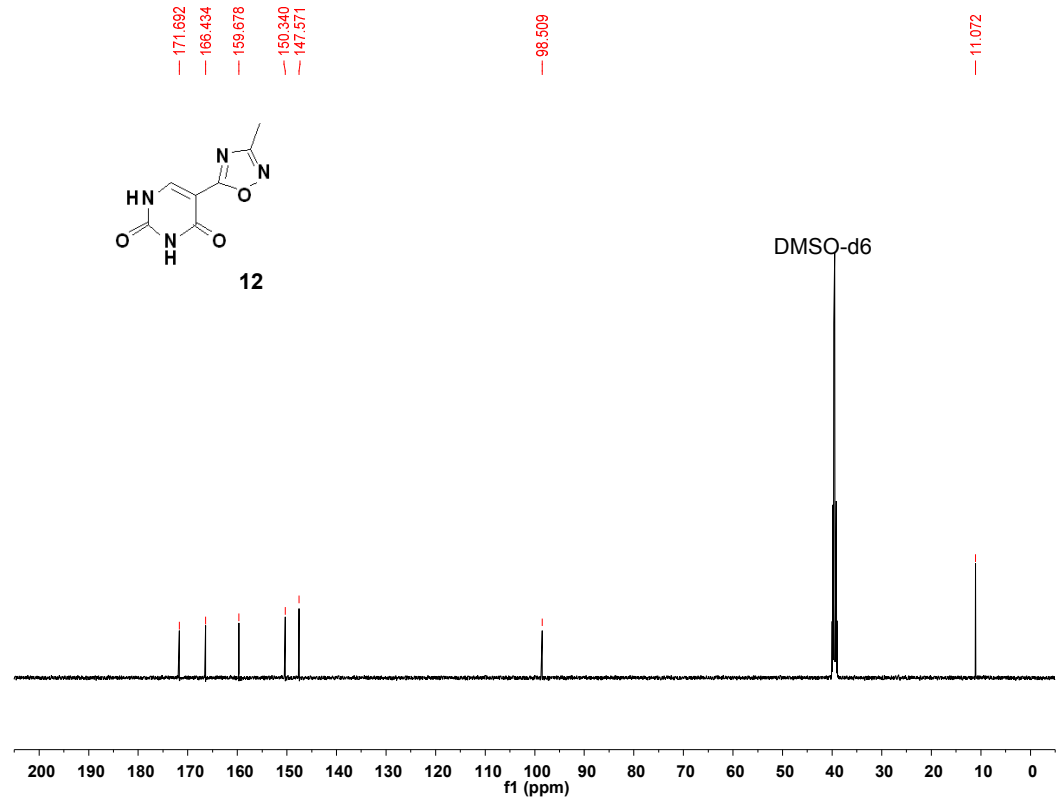

11.623
8.143
3.062
H3C
N
CH3
S
NH
O
N
N
NH
O
10
DMSO-d6
1.90
1.00
6.03
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

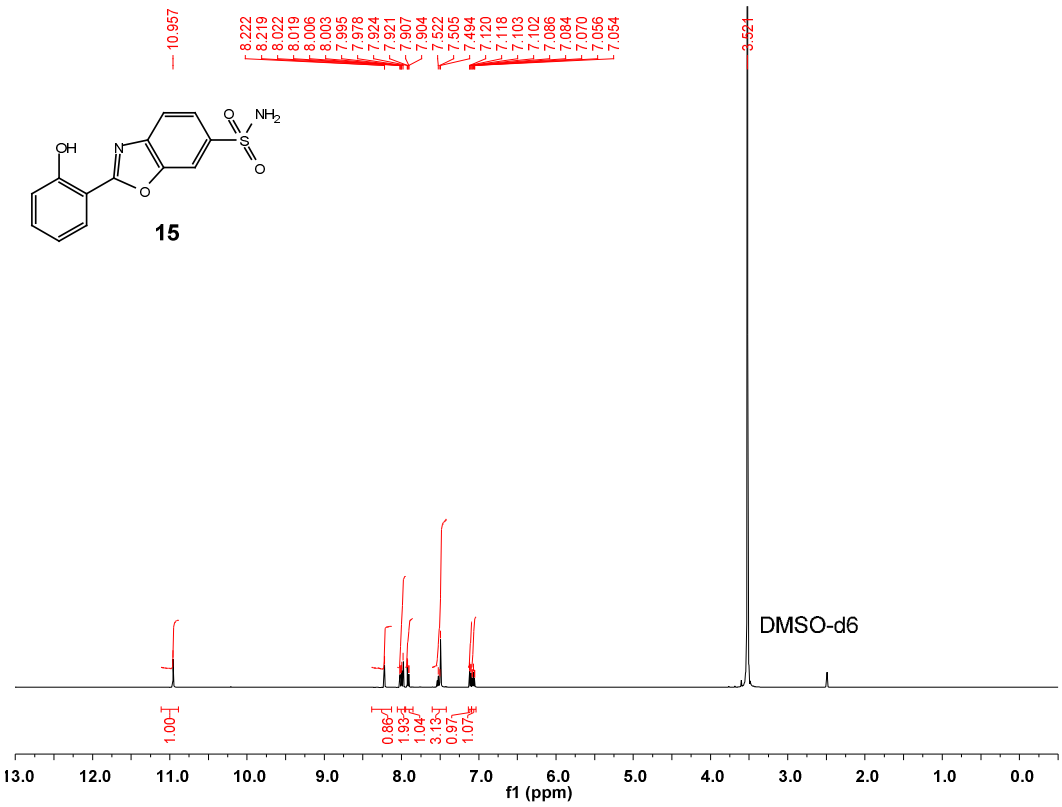

171.733
162.054
150.257
148.134
139.102
104.412
40.883
H3C
N
CH3
S
NH
O
N
N
NH
O
10
DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

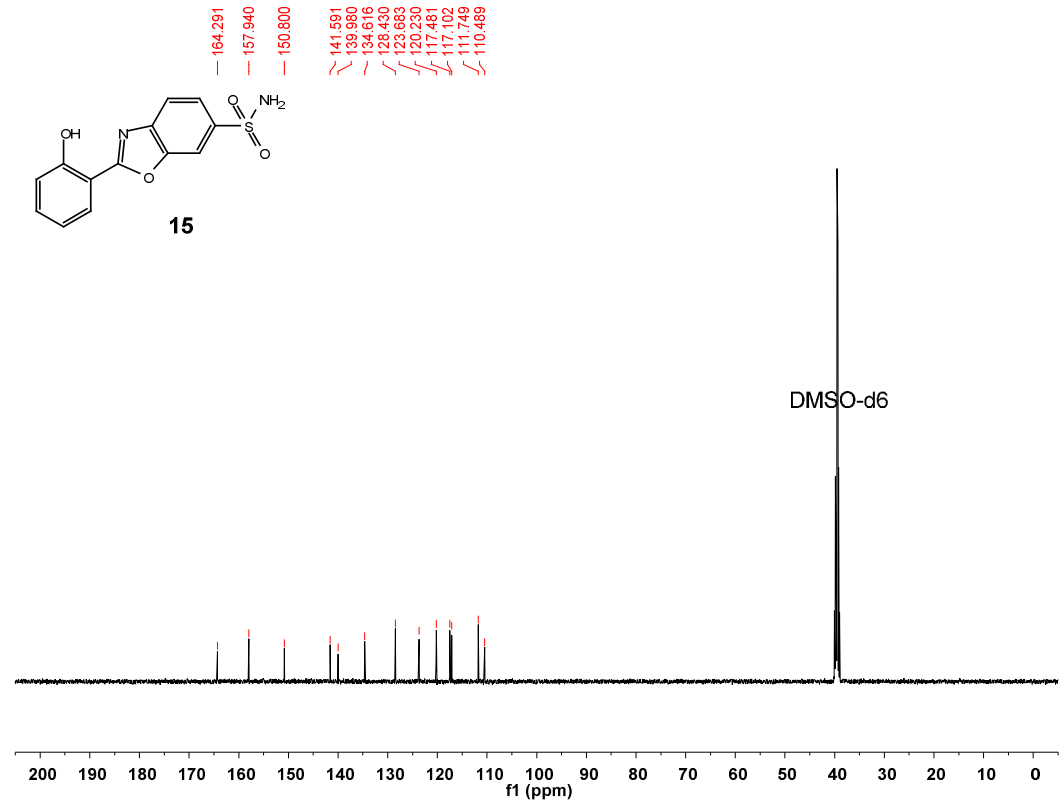

11.691
11.538
8.103
2.496
1.864
HN
N
N
Me
O
O
N
H
O
11
DMSO-d6
2.25
1.00
3.05
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

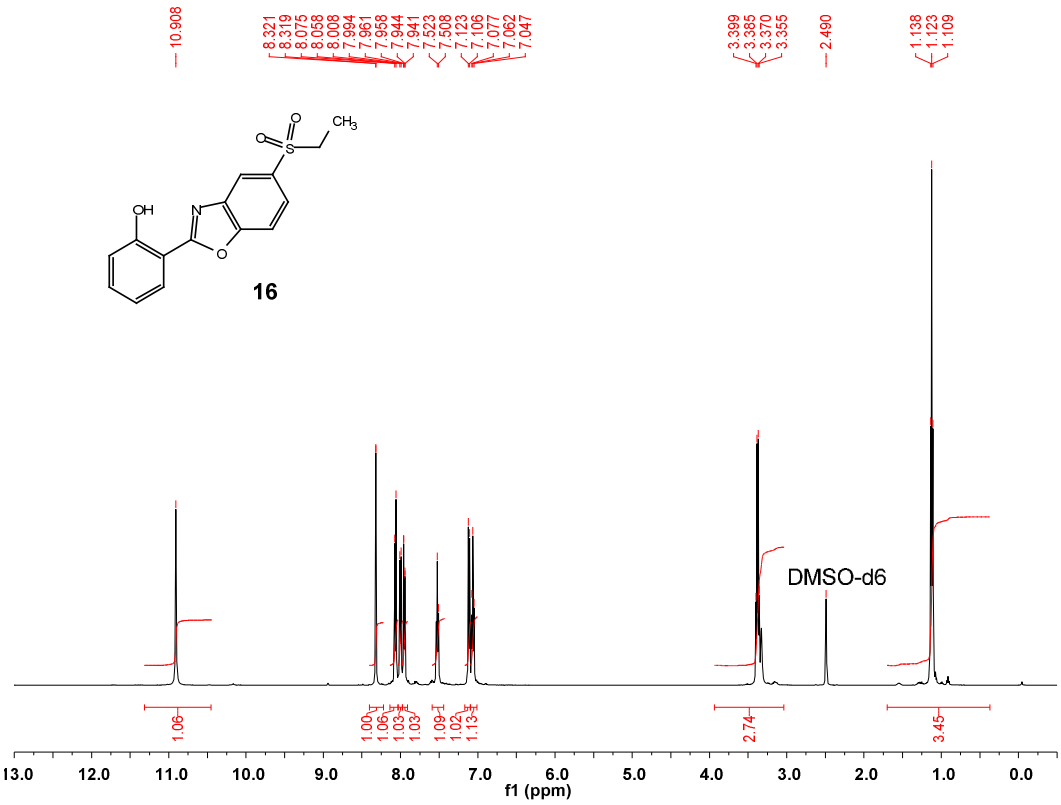

163.336
160.139
150.469
145.056
98.228
10.487
HN
N
N
Me
O
O
N
H
O
11
DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

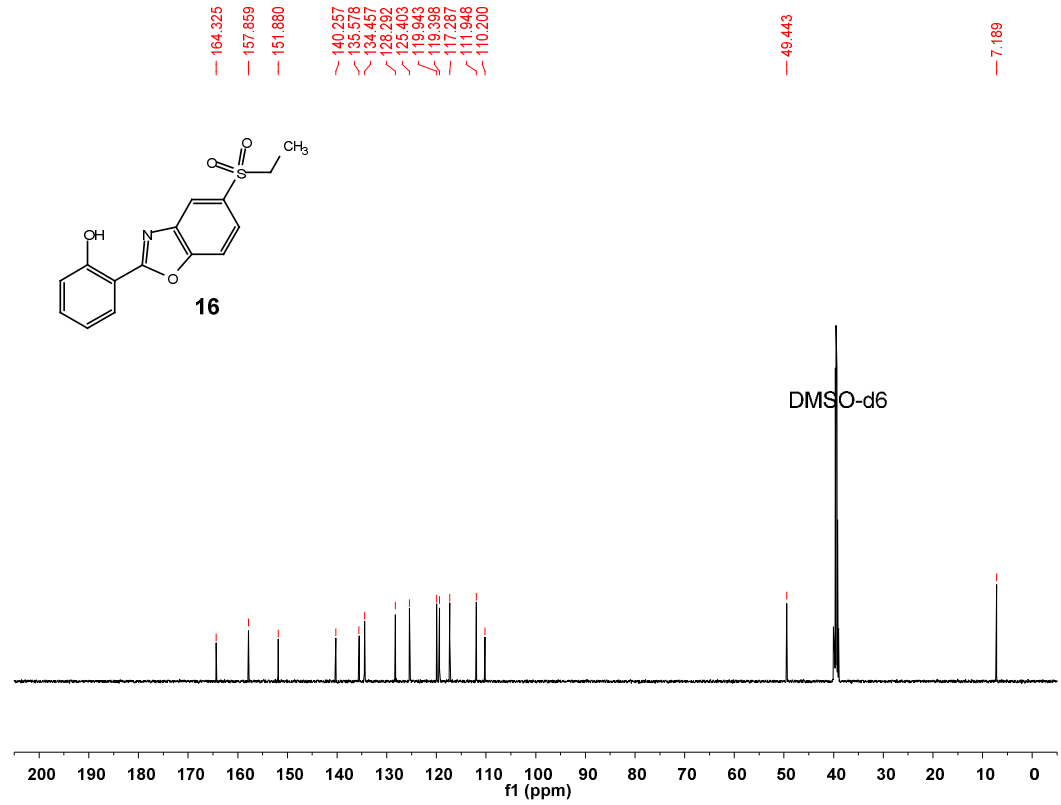

11.933
11.582
8.331
2.317
12
DMSO-d6
1.00
1.02
0.93
0.02
2.88
f1 (ppm)

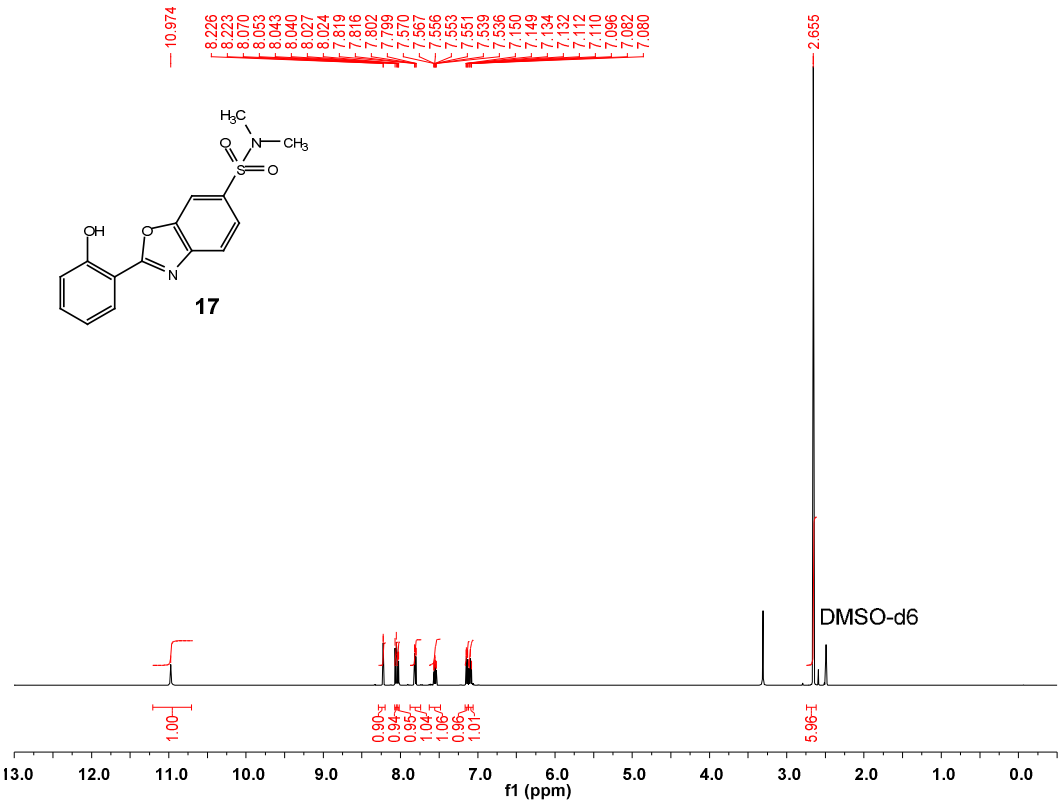

171.692
166.434
159.678
150.340
147.571
98.509
11.072
12
DMSO-d6
f1 (ppm)

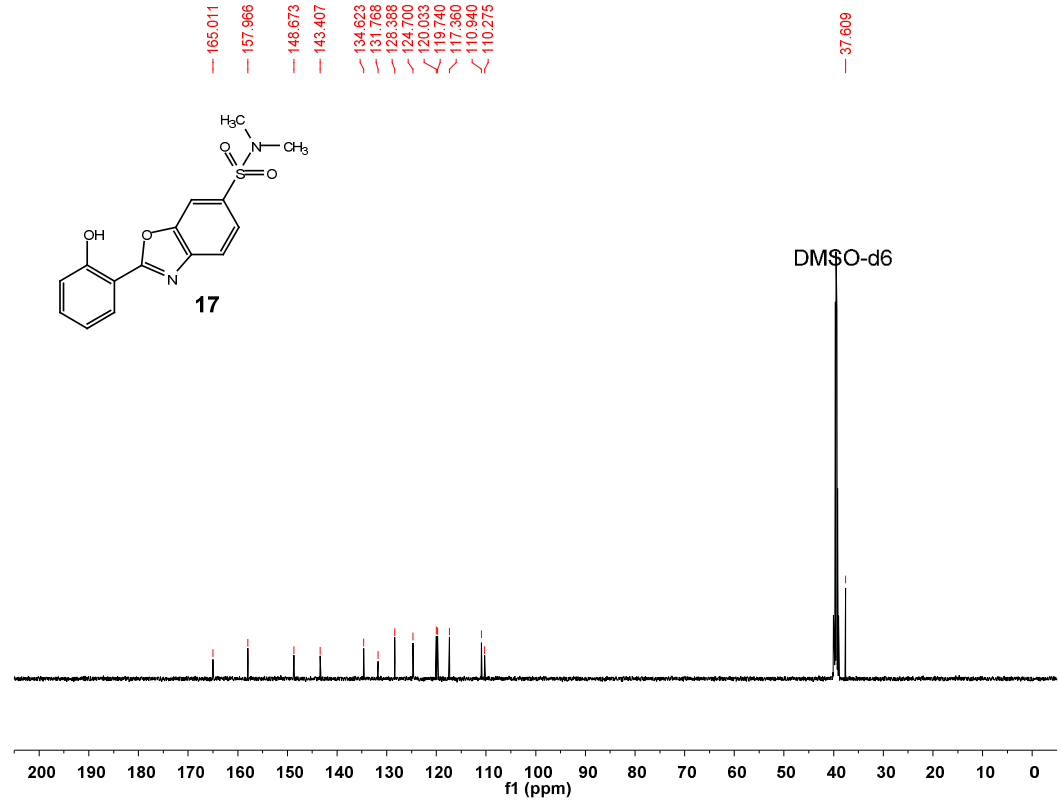

10.957
8.222
8.219
8.022
8.019
8.006
8.003
7.995
7.978
7.924
7.921
7.907
7.904
7.522
7.505
7.494
7.120
7.118
7.103
7.102
7.086
7.084
7.070
7.056
7.054
3.521
OH
N
O
S
O
NH2
15
DMSO-d6
1.00
0.86
1.93
1.04
3.13
0.97
1.07
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


164.291
157.940
150.800
141.591
139.980
134.616
128.430
123.683
120.230
117.481
117.102
111.749
110.489
OH
N
O
S
O
NH2
15
DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

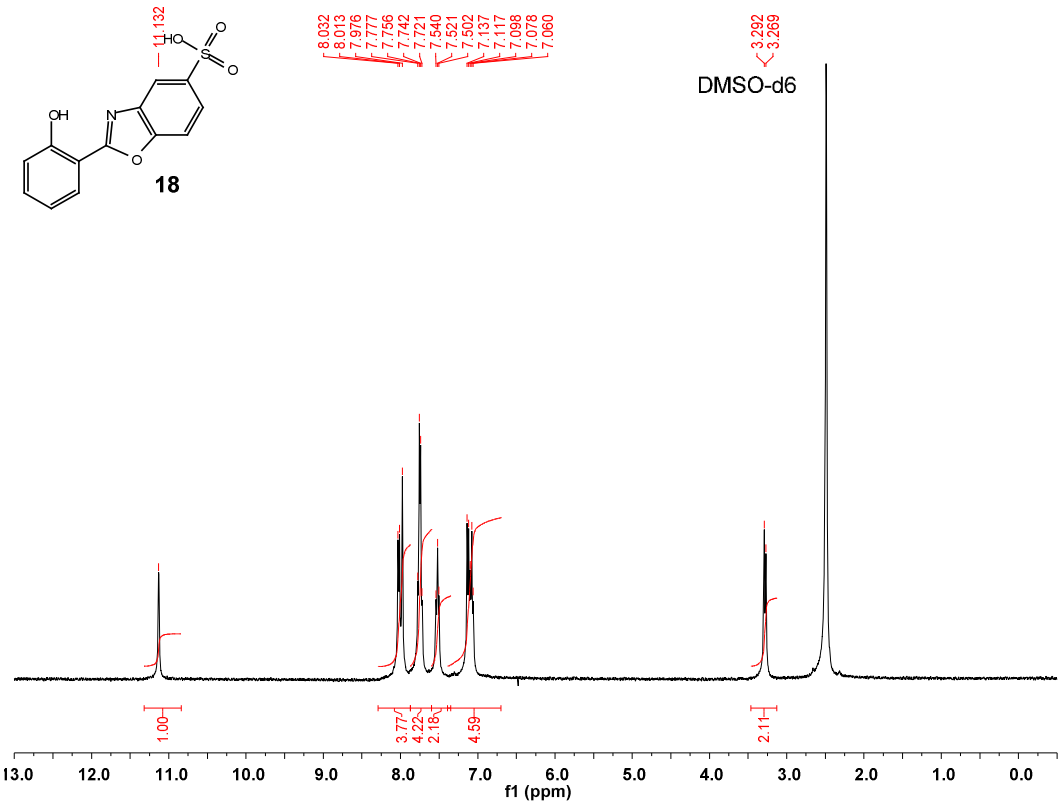

10.908
8.321
8.319
8.075
8.058
8.008
7.994
7.961
7.958
7.944
7.941
7.523
7.508
7.123
7.106
7.077
7.062
7.047
3.399
3.385
3.370
3.355
2.490
1.138
1.123
1.109
OH
N
O
S
O
O
CH3
16
DMSO-d6
1.06
1.00
1.06
1.03
1.03
1.09
1.02
1.13
2.74
3.45
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

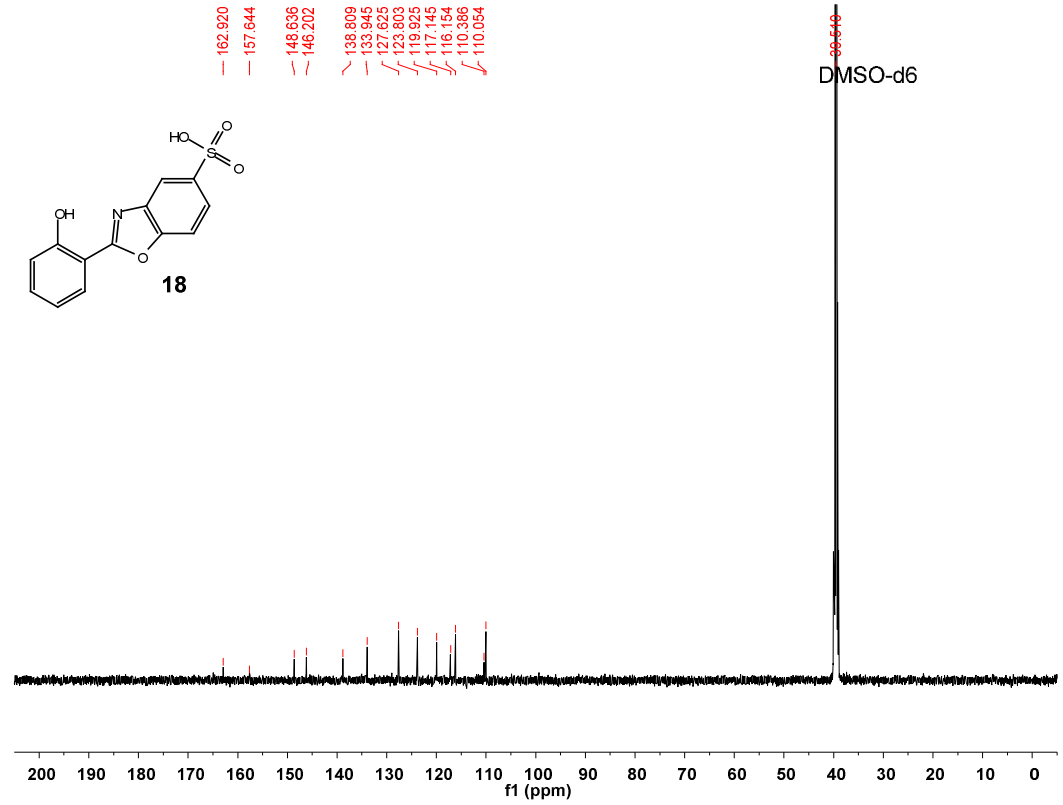

164.325
157.859
151.880
140.257
135.578
134.457
128.292
125.403
119.943
119.398
117.267
111.948
110.200
49.443
7.189
OH
N
O
S
O
O
CH3
16
DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

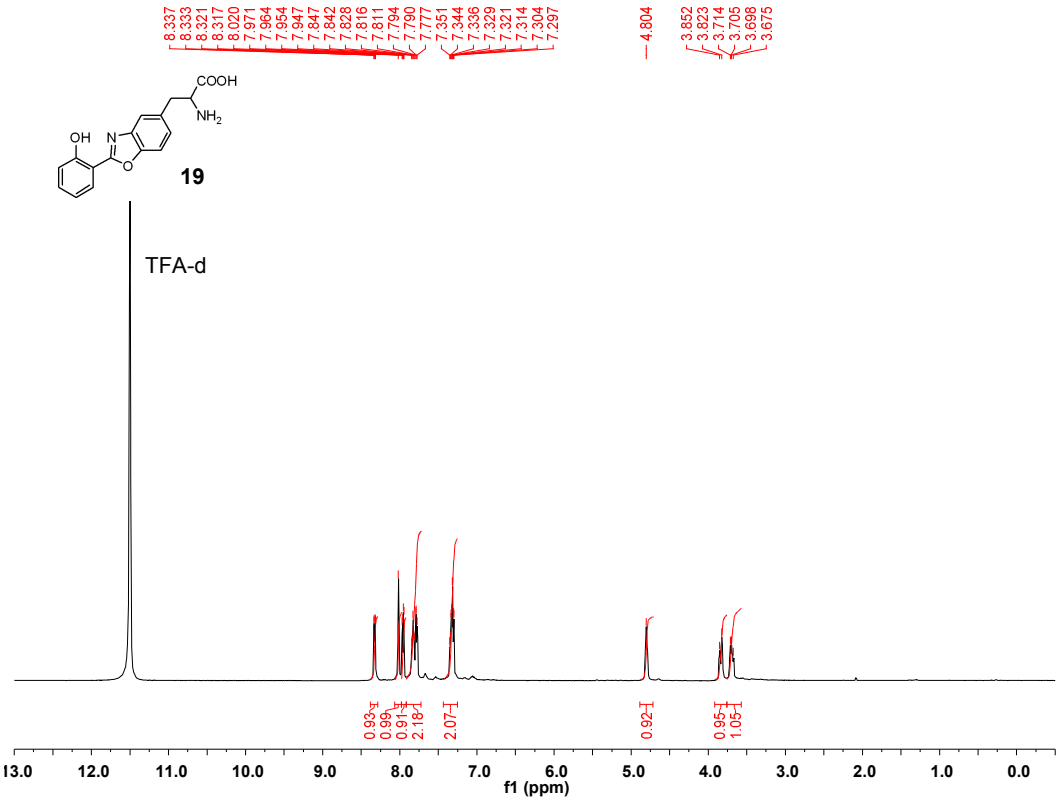

10.974
8.226
8.223
8.070
8.053
8.043
8.040
8.027
8.024
7.819
7.816
7.802
7.799
7.570
7.567
7.556
7.553
7.551
7.539
7.536
7.150
7.149
7.134
7.132
7.112
7.110
7.096
7.082
7.080
2.655
DMSO-d6
1.00
0.90
0.94
0.95
1.04
1.06
0.96
1.01
5.96
f1 (ppm)

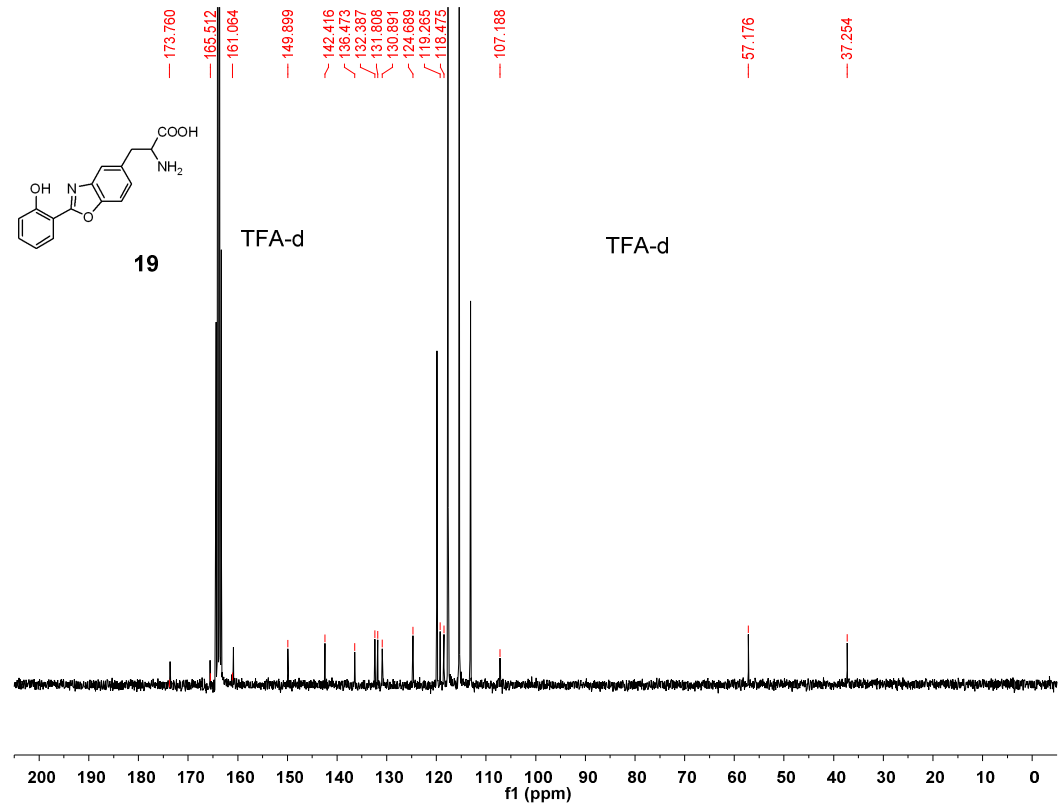

165.011
157.966
148.673
143.407
134.623
131.768
128.388
124.700
120.033
119.740
117.360
110.940
110.275
37.609
DMSO-d6
f1 (ppm)

17


11.132
8.032
8.013
7.976
7.777
7.756
7.742
7.721
7.540
7.521
7.502
7.137
7.117
7.098
7.078
7.060
3.292
3.269
DMSO-d6
OH
N
O
HO
S
O
O
18
1.00
3.77
4.22
2.18
4.59
2.11
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


162.920
157.644
148.636
146.202
138.809
133.945
127.625
123.803
119.925
117.145
116.154
110.386
110.054
39.518
DMSO-d6
OH
N
O
HO
S
O
O
18
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.337
8.333
8.321
8.317
8.020
7.971
7.964
7.954
7.947
7.847
7.842
7.828
7.816
7.811
7.794
7.790
7.777
7.351
7.344
7.336
7.329
7.321
7.314
7.304
7.297
4.804
3.852
3.823
3.714
3.705
3.698
3.675
COOH
NH2
OH
N
O
19
TFA-d
0.93
0.99
0.91
2.18
2.07
0.92
0.95
1.05
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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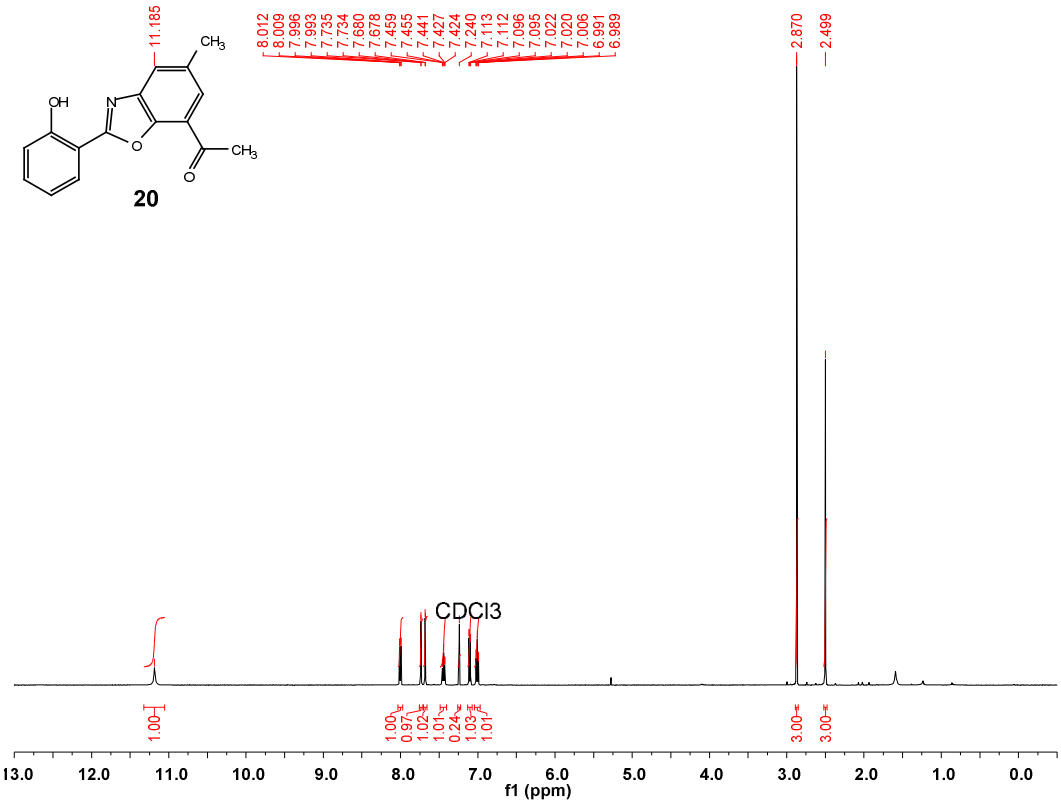
161.064
149.899
142.416
136.473
132.387
131.808
130.891
124.689
119.265
118.475
107.188
57.176
37.254
COOH
NH2
OH
N
O
19
TFA-d
TFA-d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.009
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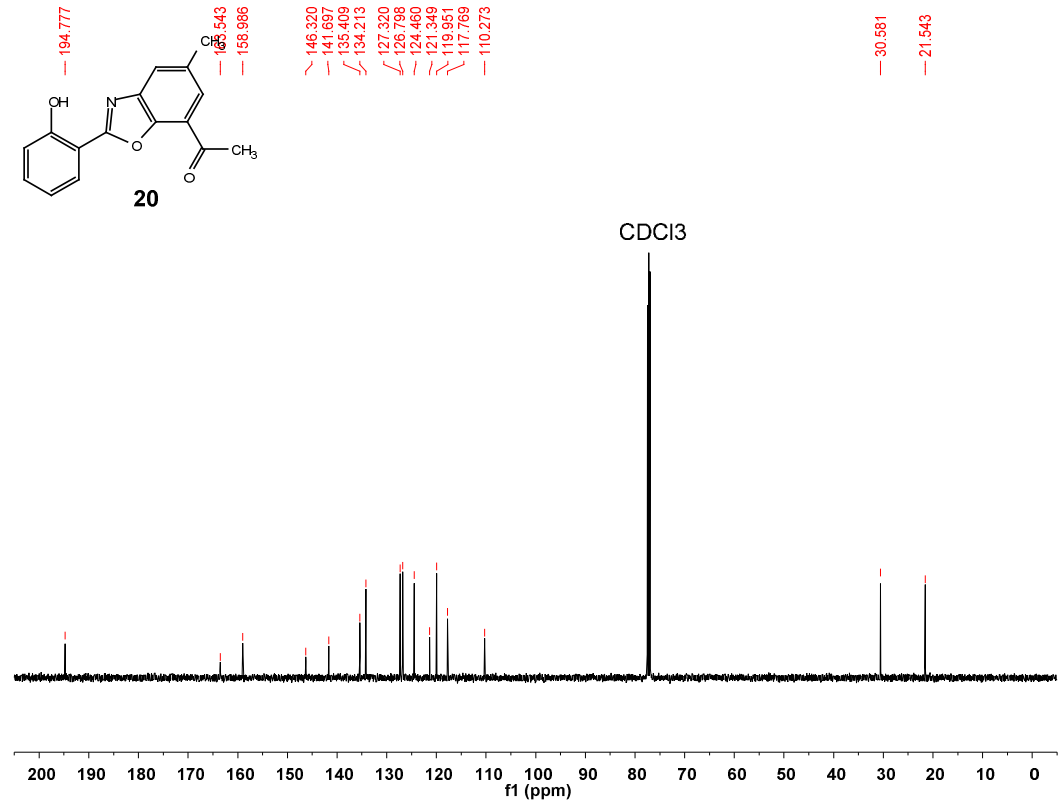
7.993
7.735
7.734
7.680
7.678
7.459
7.455
7.441
7.427
7.424
7.240
7.113
7.112
7.096
7.095
7.022
7.020
7.006
6.991
6.989
2.870
2.499
CH3
OH
N
O
CH3
O
20
CDCl3
1.00
0.97
1.02
1.01
0.24
1.03
1.01
3.00
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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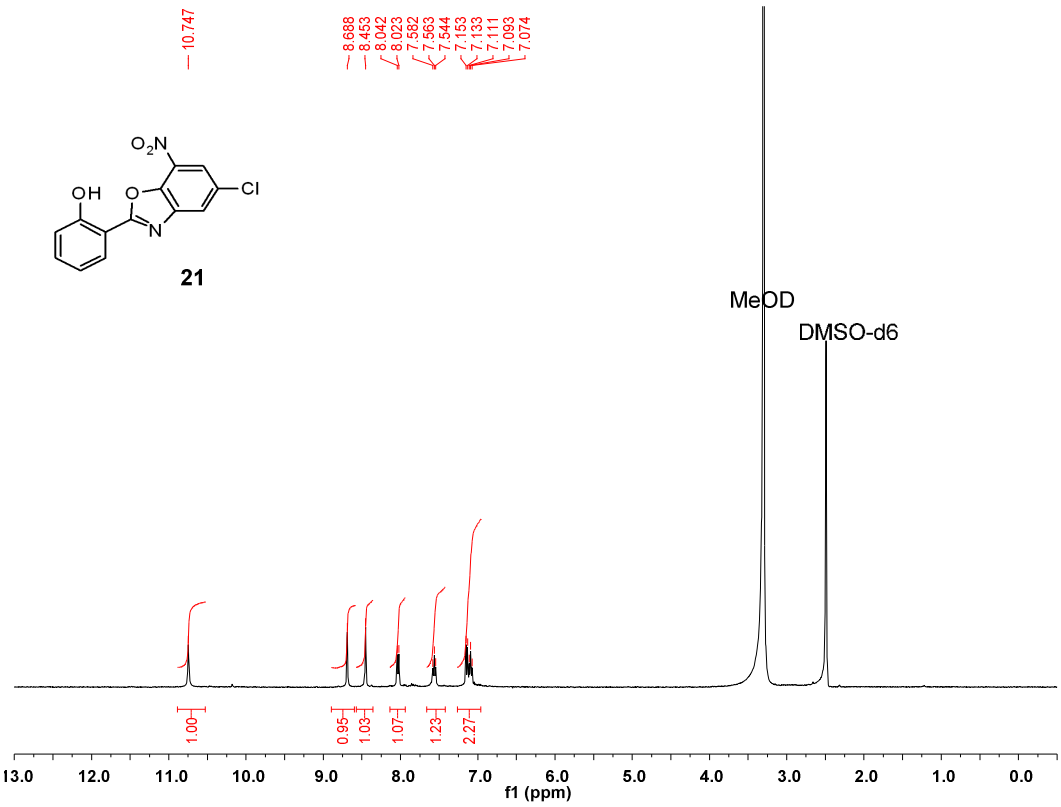
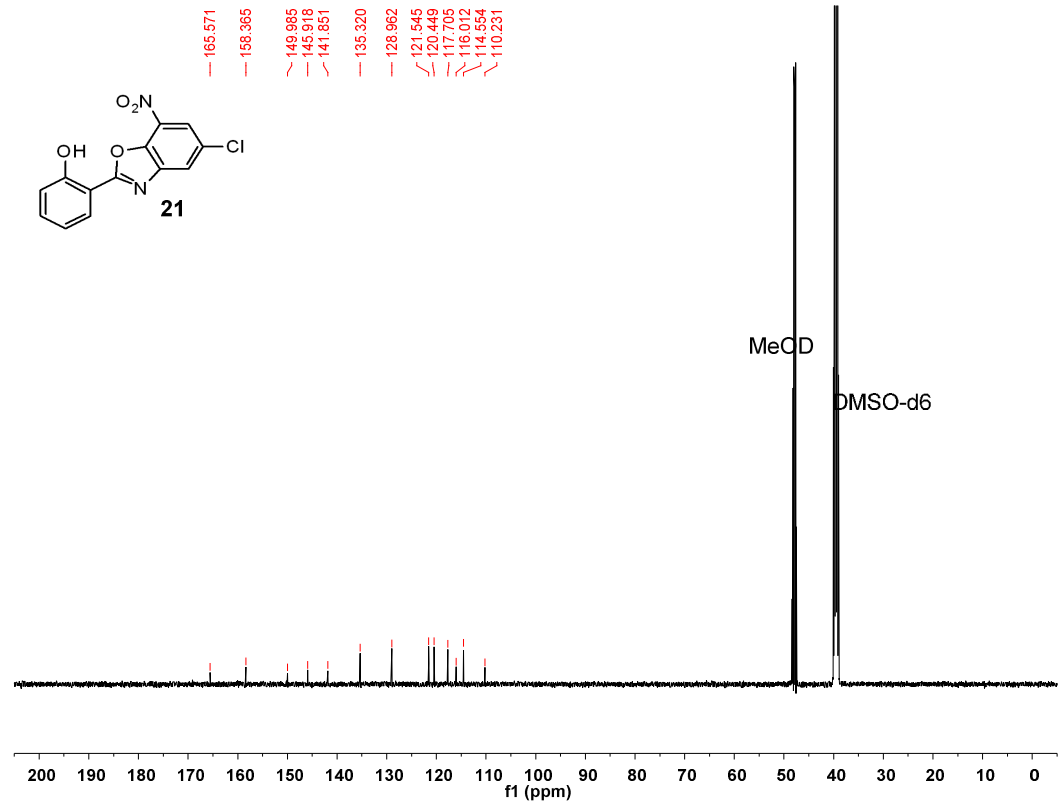
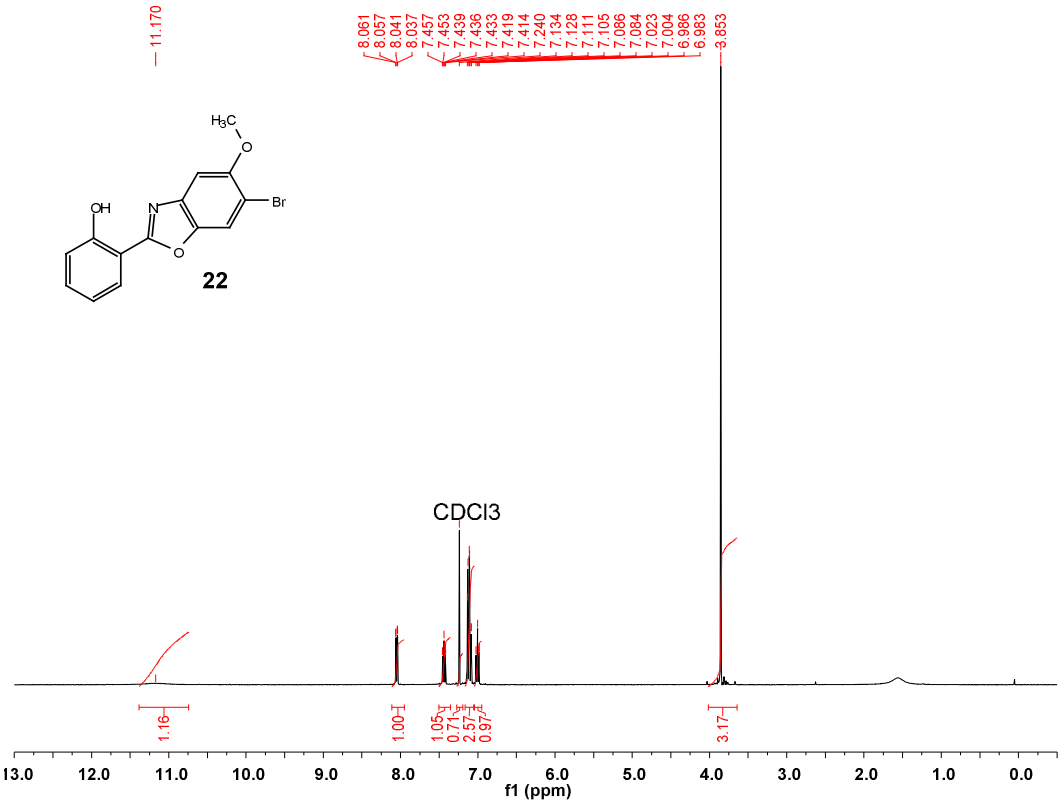
158.986
146.320
141.697
135.409
134.213
127.320
126.798
124.460
121.349
119.951
117.769
110.273
30.581
21.543
CH3
OH
N
O
CH3
O
20
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.747
8.688
8.453
8.042
8.023
7.582
7.563
7.544
7.153
7.133
7.111
7.093
7.074
O2N
OH
O
N
Cl
21
MeOD
DMSO-d6
1.00
0.95
1.03
1.07
1.23
2.27
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


165.571
158.365
149.985
145.918
141.851
135.320
128.962
121.545
120.449
117.705
116.012
114.554
110.231
O2N
OH
O
N
Cl
21
MeOD
DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.170
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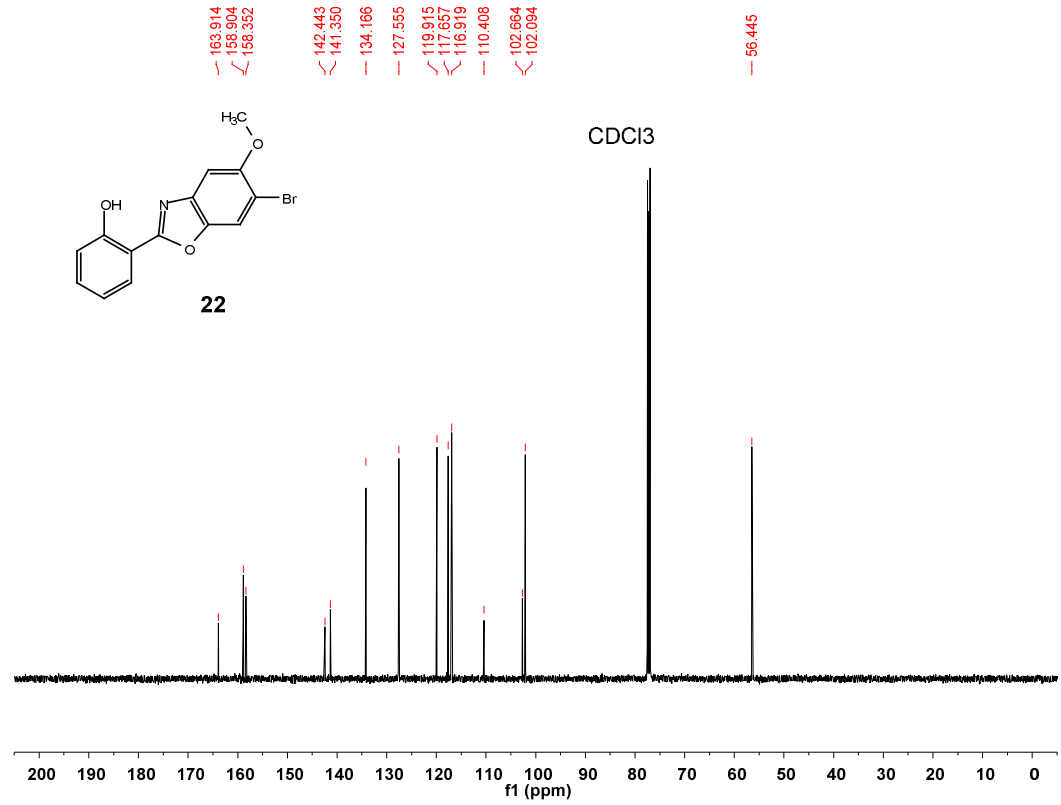
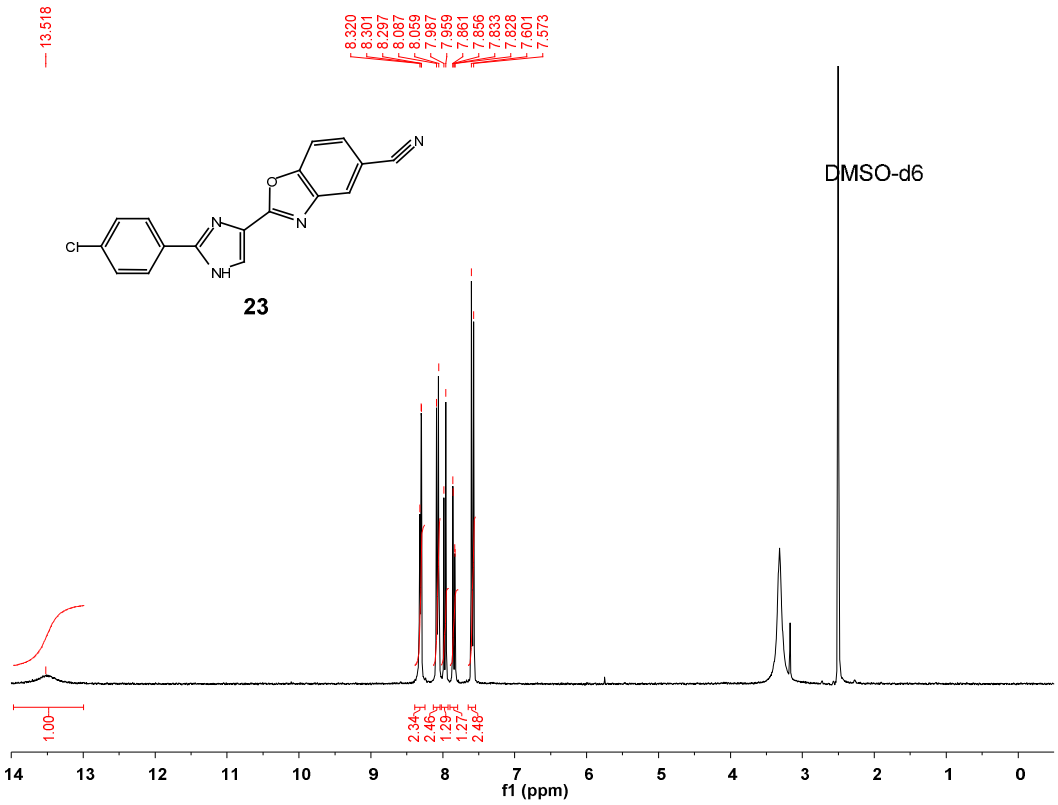
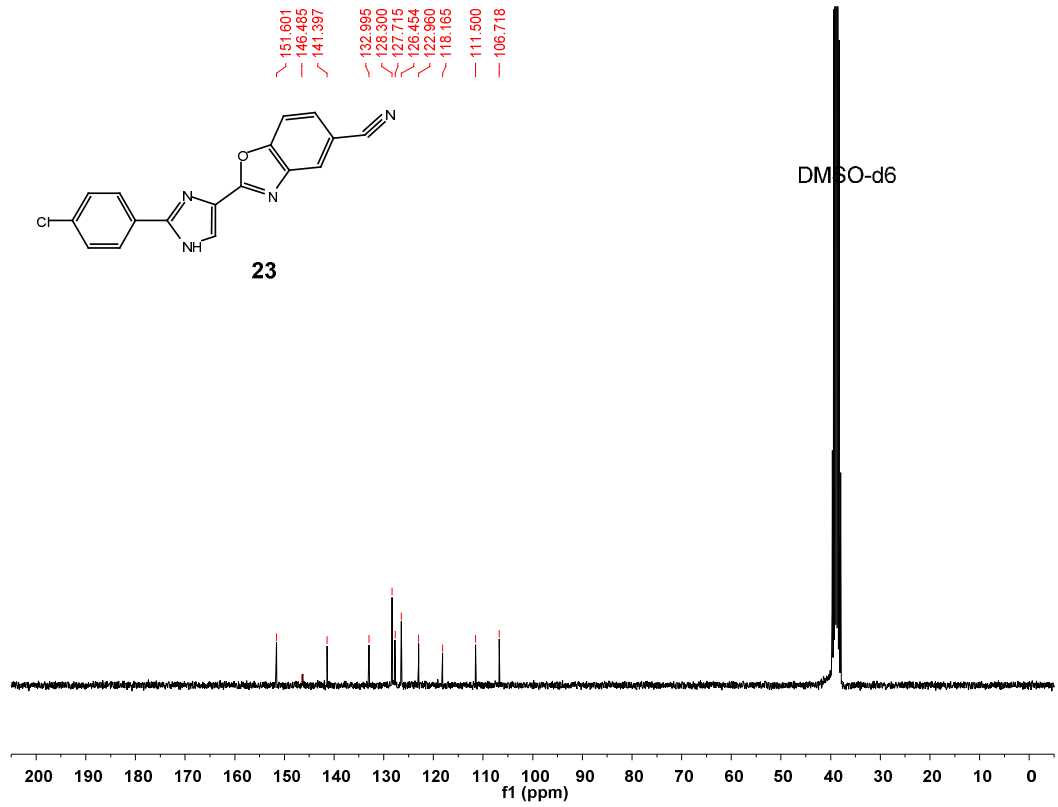
8.057
8.041
8.037
7.457
7.453
7.439
7.436
7.433
7.419
7.414
7.240
7.134
7.128
7.111
7.105
7.086
7.084
7.023
7.004
6.986
6.983
3.853
H3C
O
OH
N
Br
O
22
CDCl3
1.16
1.00
1.05
0.71
2.57
0.97
3.17
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


163.914
158.904
158.352
142.443
141.350
134.166
127.555
119.915
117.657
116.919
110.408
102.664
102.094
56.445
H3C
O
OH
N
Br
O
22
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


13.518
8.320
8.301
8.297
8.087
8.059
7.987
7.959
7.861
7.856
7.833
7.828
7.601
7.573
DMSO-d6
23
1.00
2.34
2.46
1.29
1.27
2.48
f1 (ppm)


151.601
146.485
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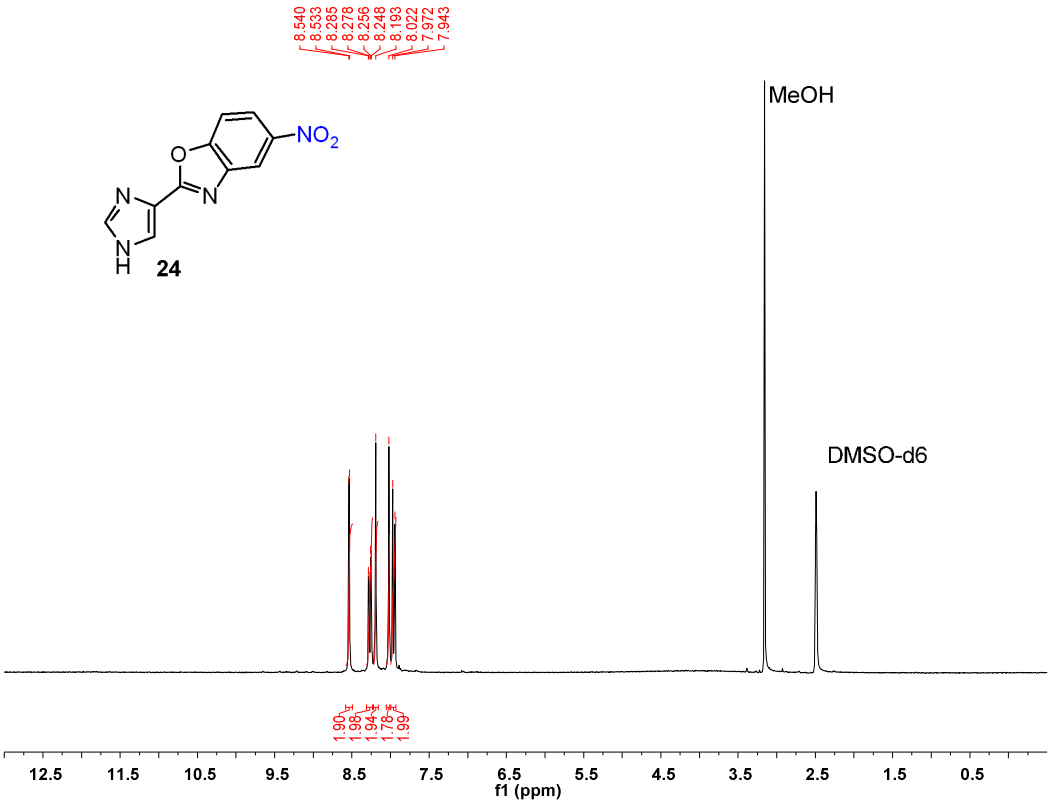
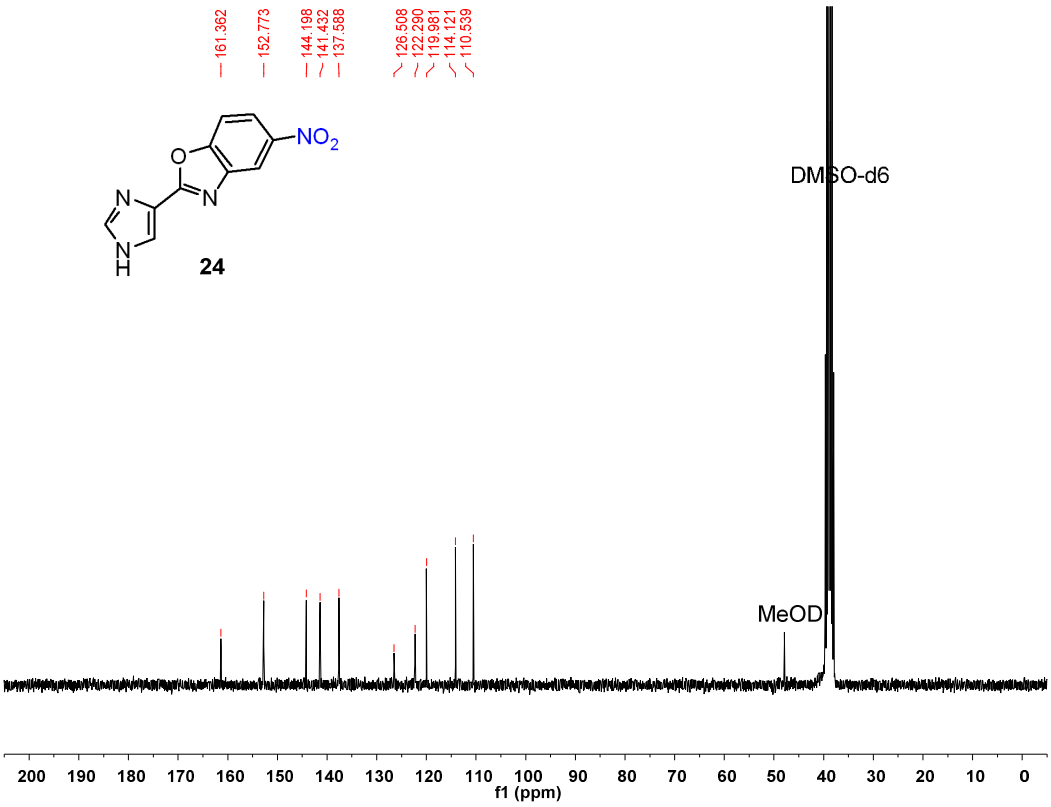
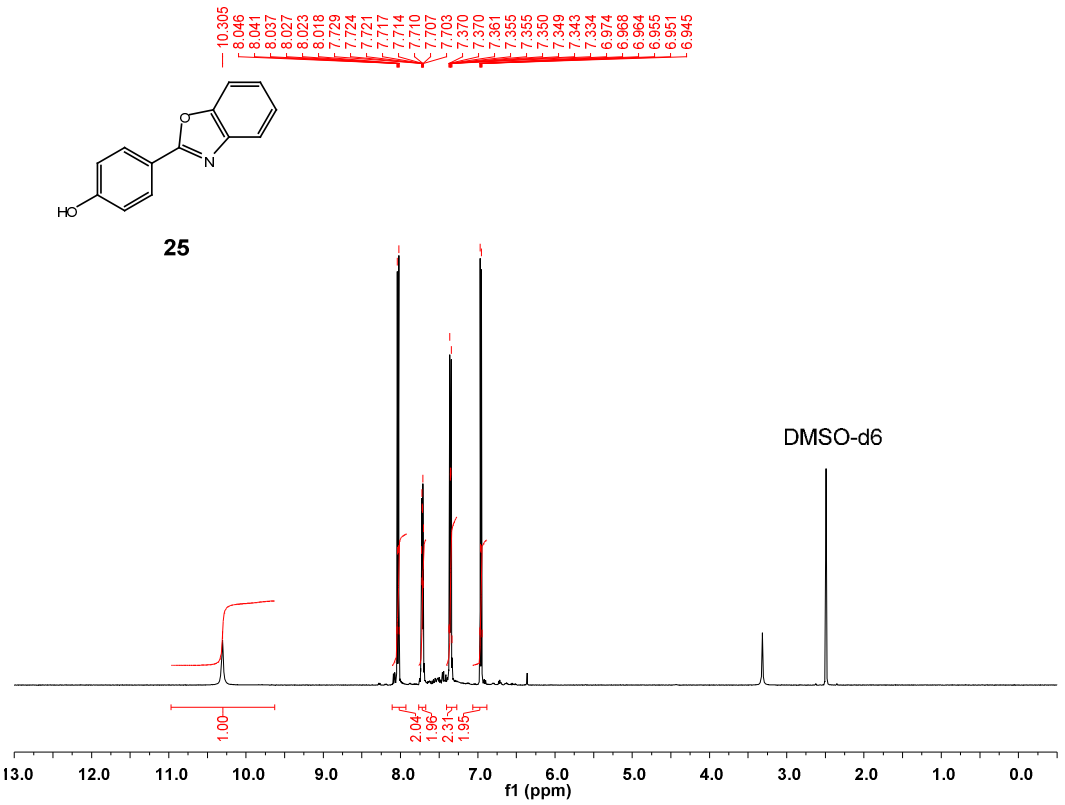
127.715
126.454
122.960
118.165
111.500
106.718
DMSO-d6
23
f1 (ppm)


8.540
8.533
8.285
8.278
8.256
8.248
8.193
8.022
7.972
7.943
NO2
O
N
N
N
H
24
MeOH
DMSO-d6
1.90
1.98
1.94
1.78
1.99
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


161.362
152.773
144.198
141.432
137.588
126.508
122.290
119.981
114.121
110.539
NO2
O
N
N
N
H
24
DMSO-d6
MeOD
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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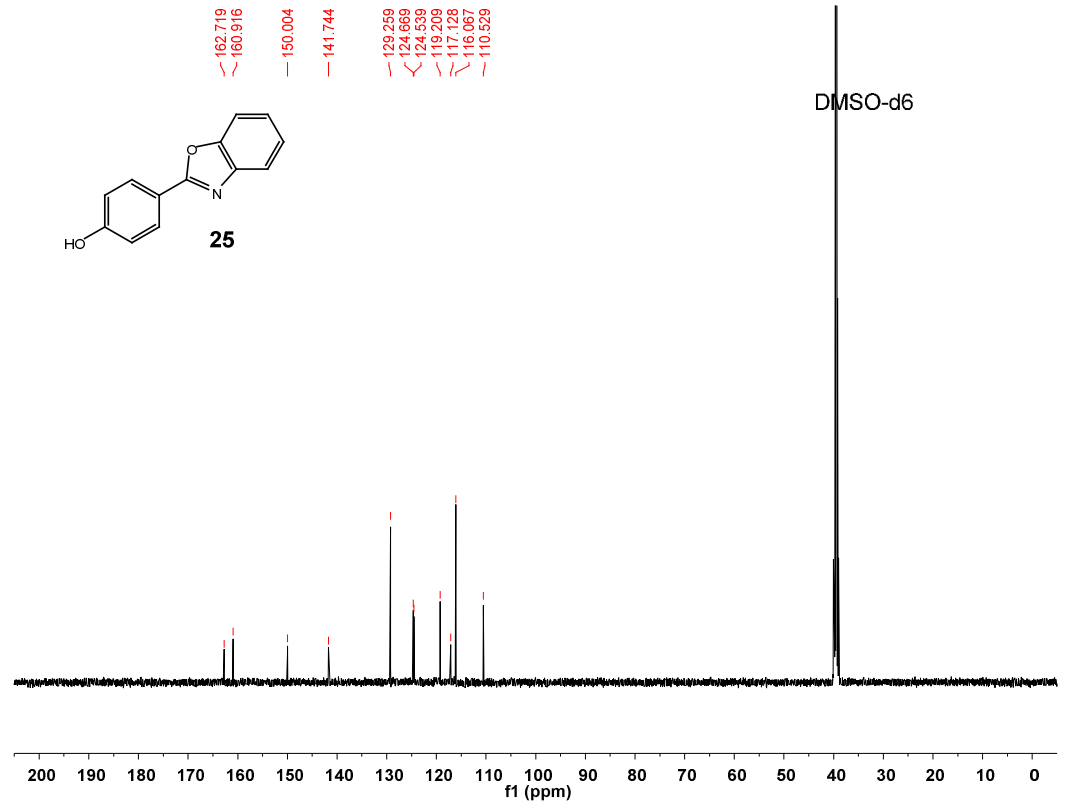
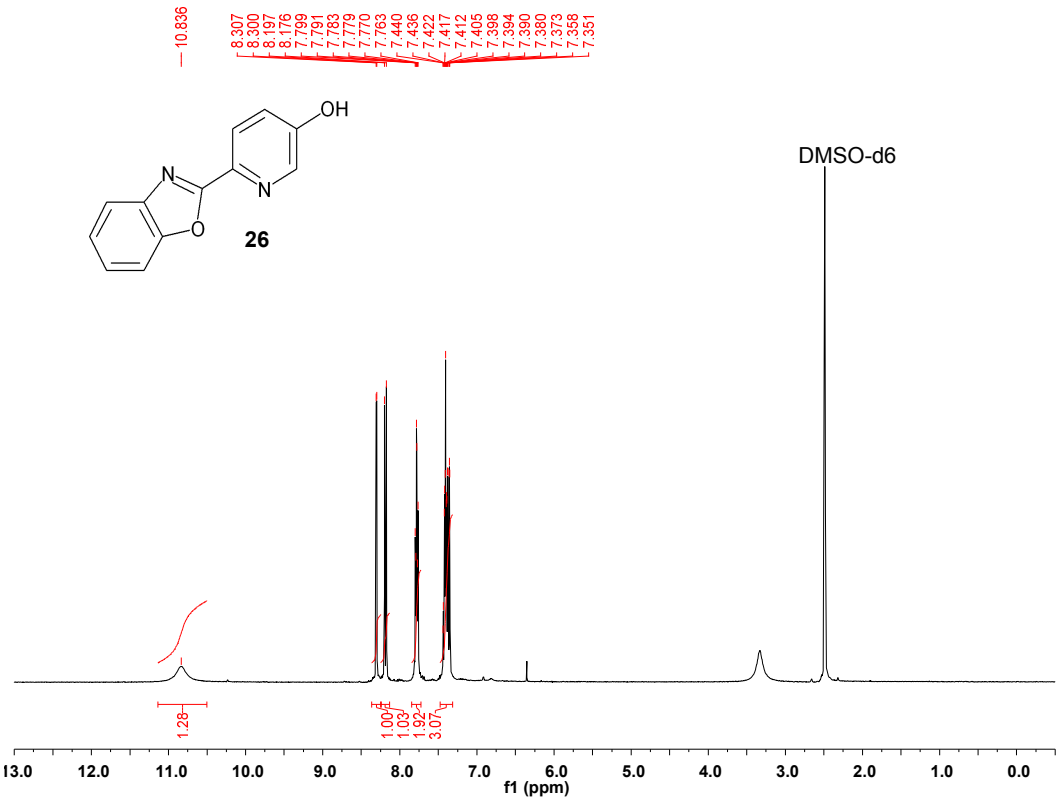
8.046
8.041
8.037
8.027
8.023
8.018
7.729
7.724
7.721
7.717
7.714
7.710
7.707
7.703
7.370
7.370
7.361
7.355
7.355
7.350
7.349
7.343
7.334
6.974
6.968
6.964
6.955
6.951
6.945
O
N
HO
25
DMSO-d6
1.00
2.04
1.96
2.31
1.95
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


162.719
160.916
150.004
141.744
129.259
124.669
124.539
119.209
117.128
116.067
110.529
O
N
HO
25
DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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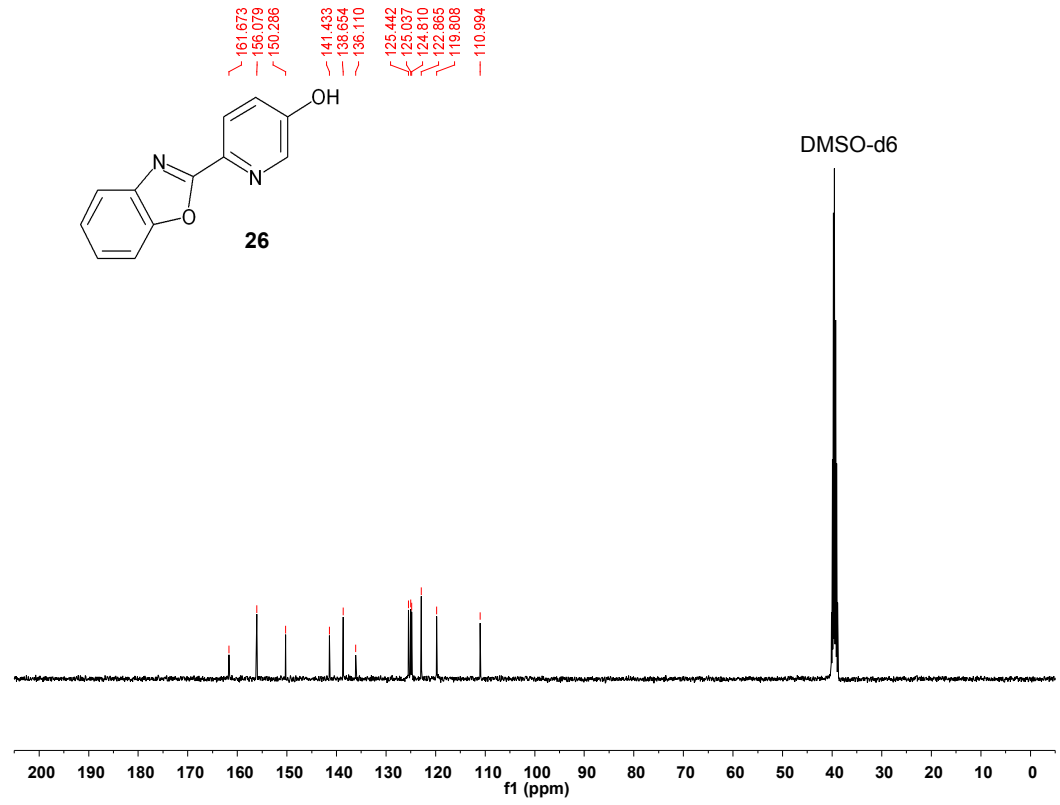
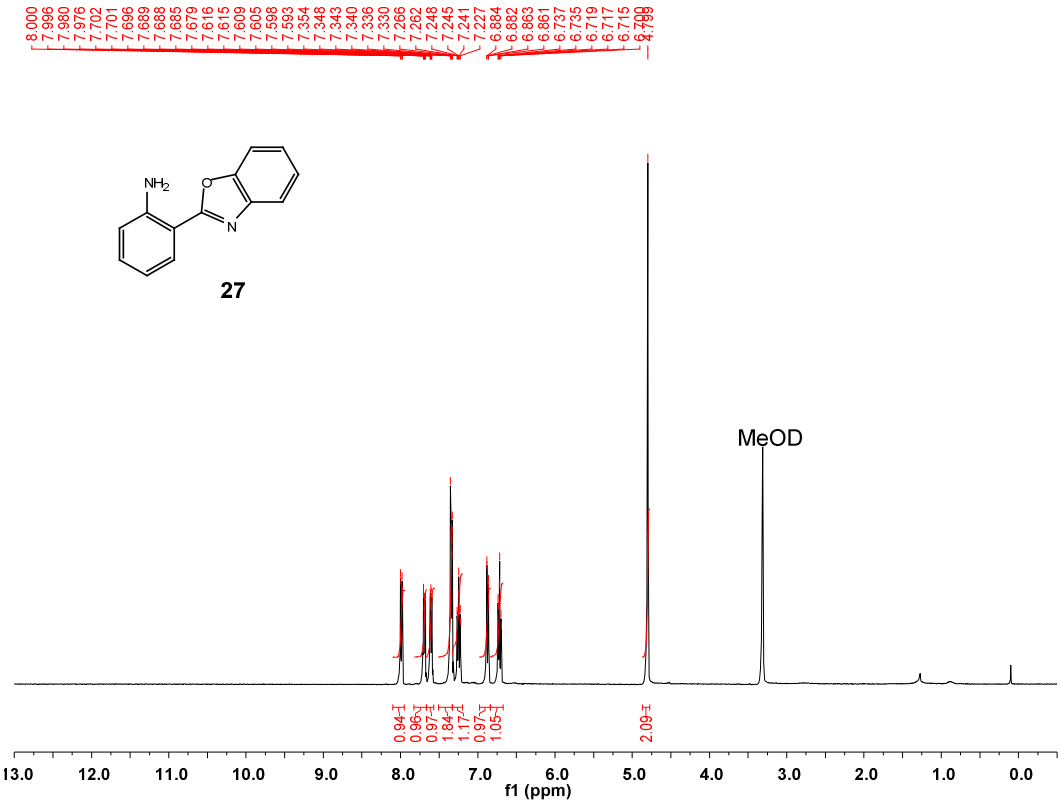
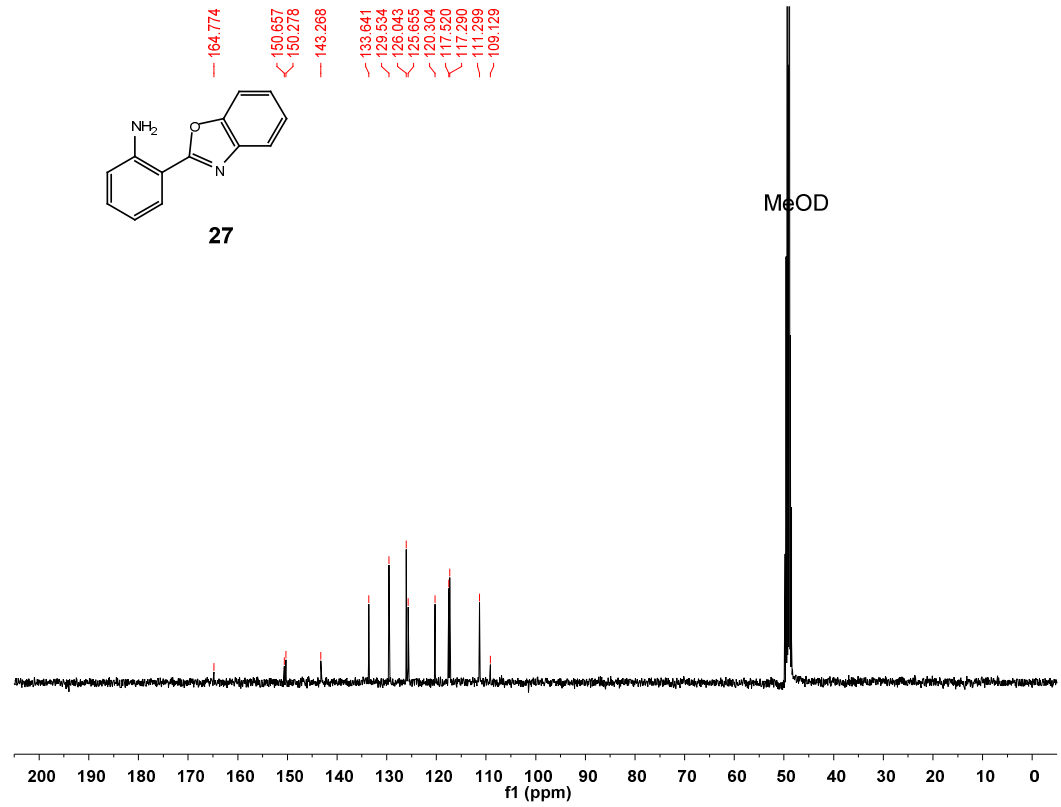
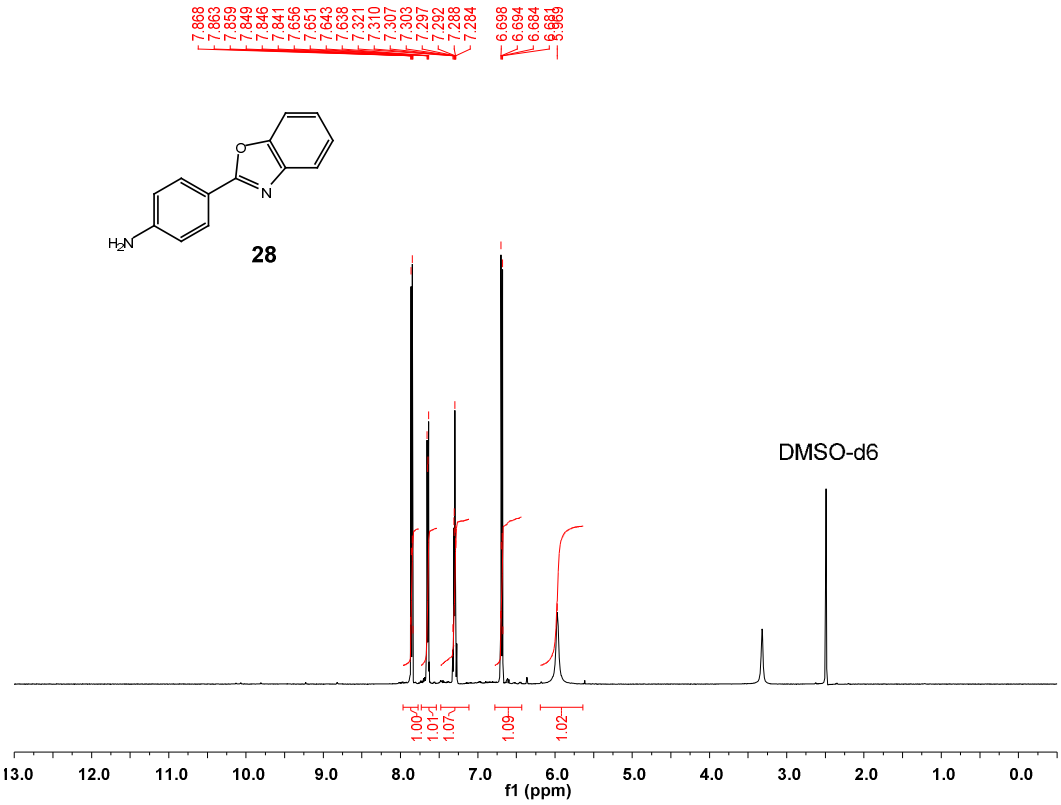
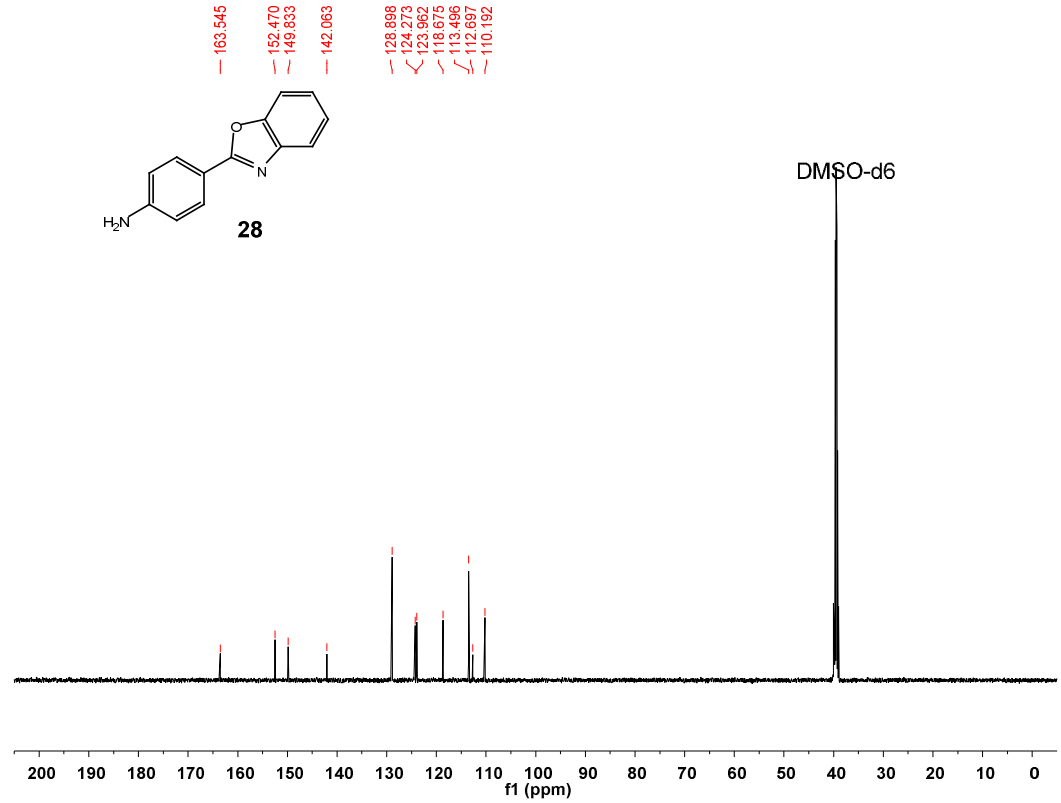
8.307
8.300
8.197
8.176
7.799
7.791
7.783
7.779
7.770
7.763
7.440
7.436
7.422
7.417
7.412
7.405
7.398
7.394
7.390
7.380
7.373
7.358
7.351
OH
N
N
O
26
DMSO-d6
1.28
1.00
1.03
1.92
3.07
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

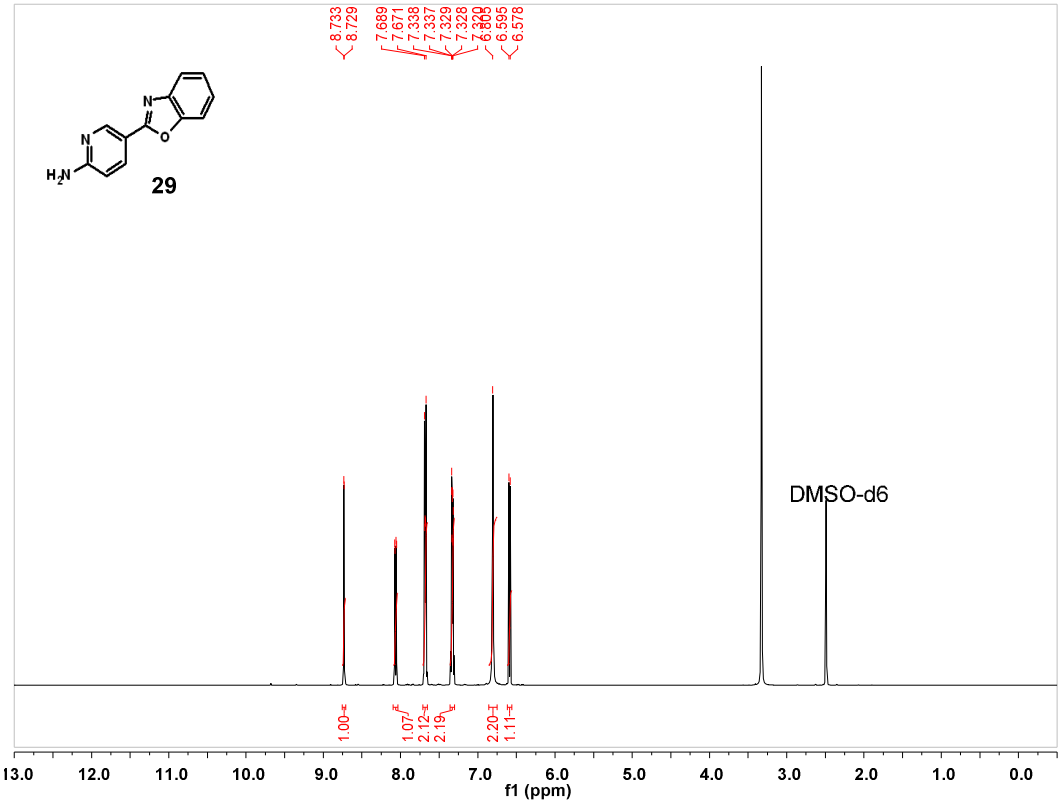

161.673
156.079
150.286
141.433
138.654
136.110
125.442
125.037
124.810
122.865
119.808
110.994
OH
N
N
O
26
DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

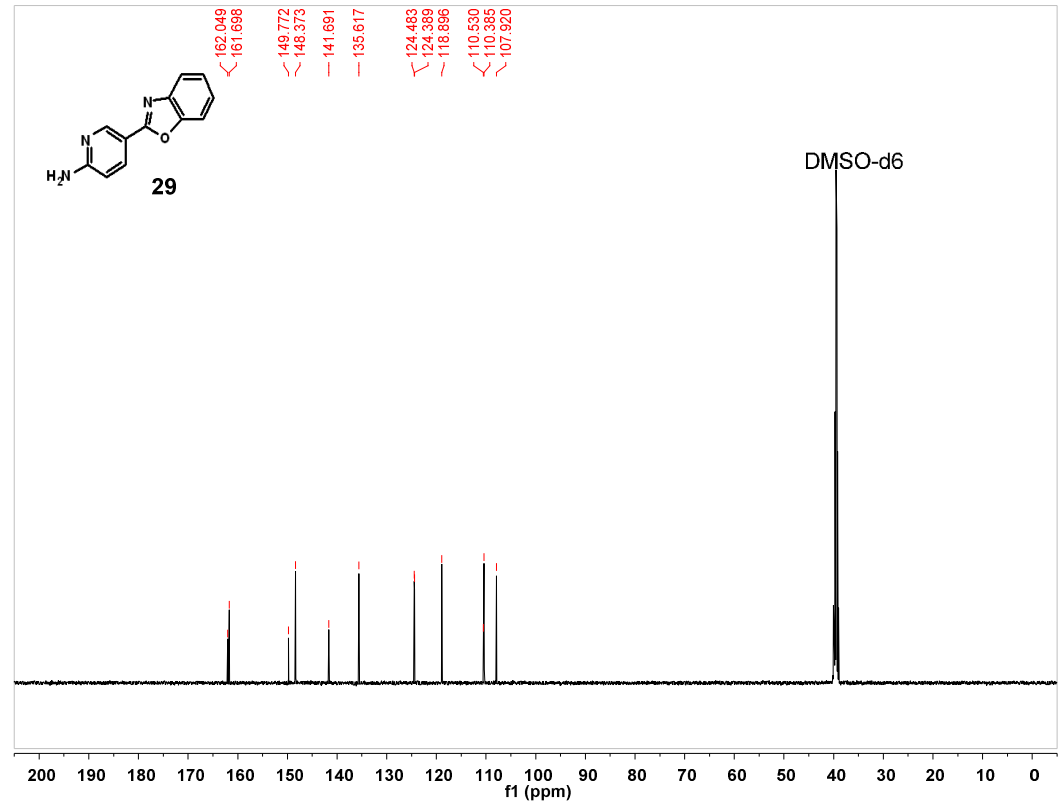

8.000
7.996
7.980
7.976
7.702
7.701
7.696
7.689
7.688
7.685
7.679
7.616
7.615
7.609
7.605
7.598
7.593
7.354
7.348
7.343
7.340
7.336
7.330
7.266
7.262
7.248
7.245
7.241
7.227
6.884
6.882
6.863
6.861
6.737
6.735
6.719
6.717
6.715
6.709
4.799
NH2
O
N
27
MeOD
0.94
0.96
0.97
1.84
1.17
0.97
1.05
2.09
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

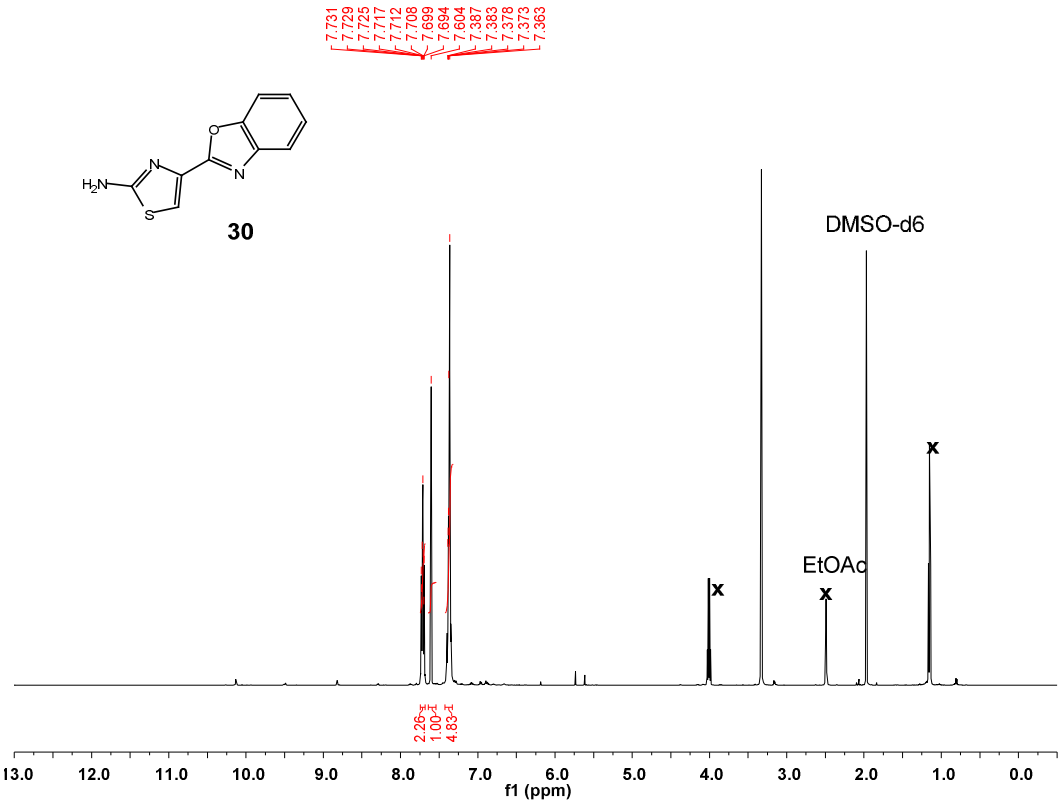

164.774
150.657
150.278
143.268
133.641
129.534
126.043
125.655
120.304
117.520
117.290
111.299
109.129
NH2
O
N
27
MeOD
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

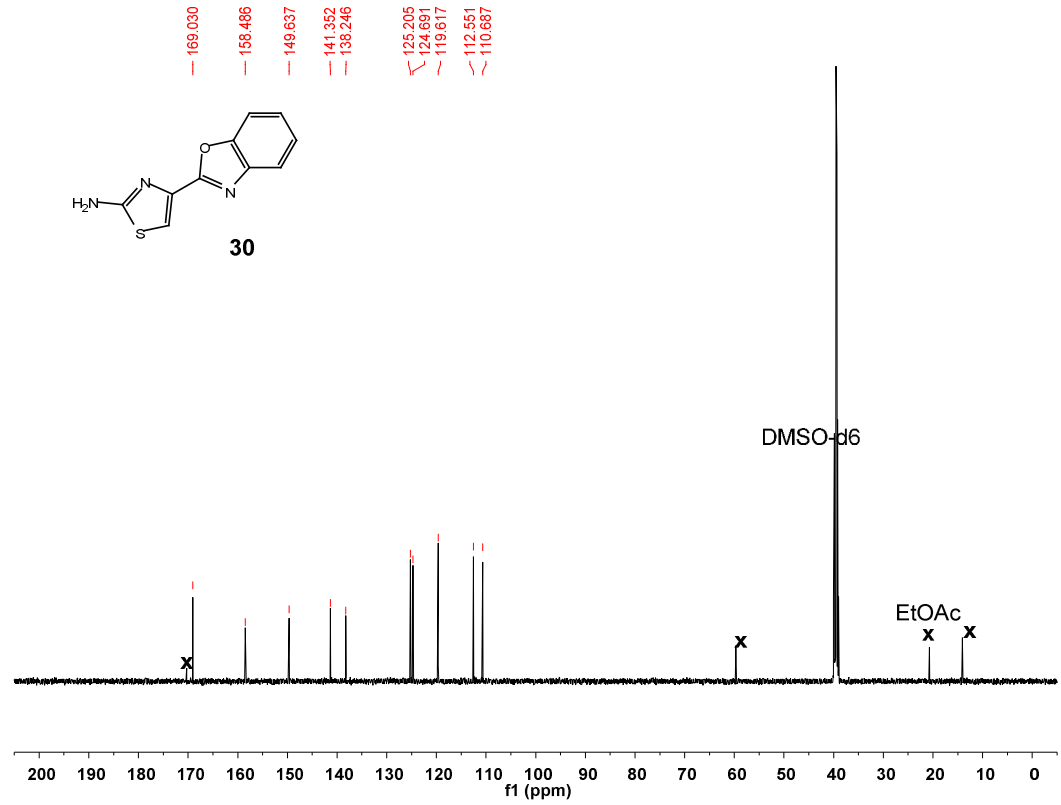

7.868
7.863
7.859
7.849
7.846
7.841
7.656
7.651
7.643
7.638
7.321
7.310
7.307
7.303
7.297
7.292
7.288
7.284
6.698
6.694
6.684
28
DMSO-d6
1.00
1.01
1.07
1.09
1.02
f1 (ppm)

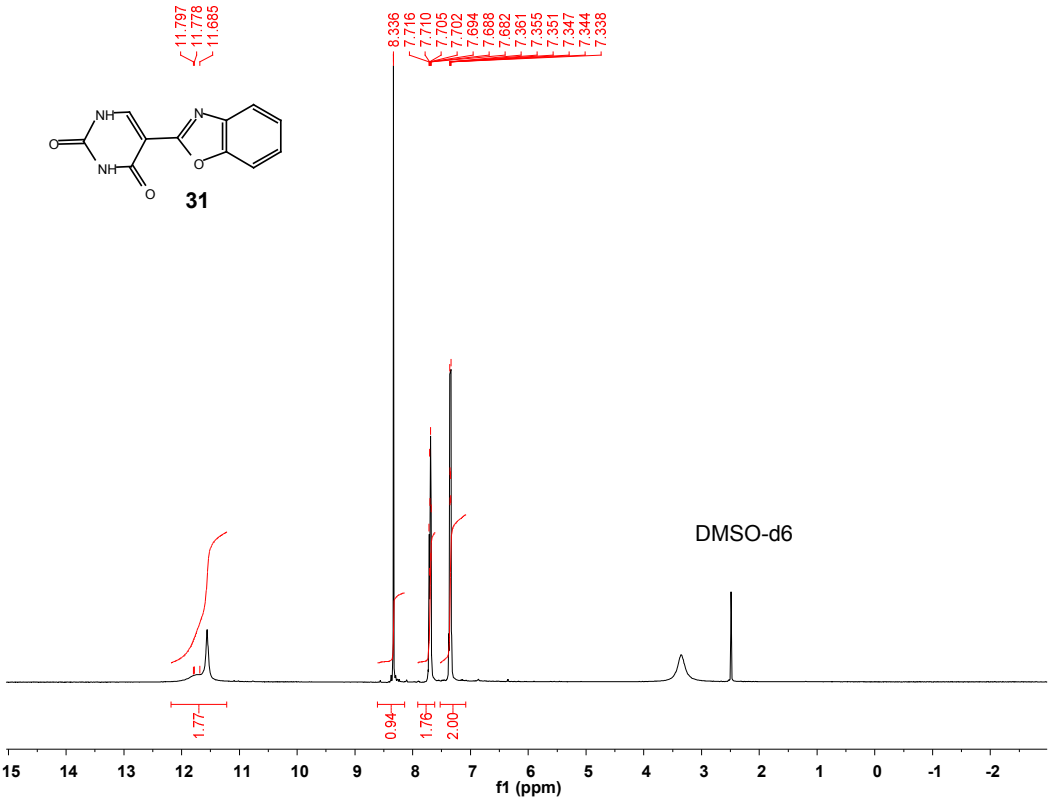

163.545
152.470
149.833
142.063
128.898
124.273
123.962
118.675
113.496
112.697
110.192
28
DMSO-d6
f1 (ppm)

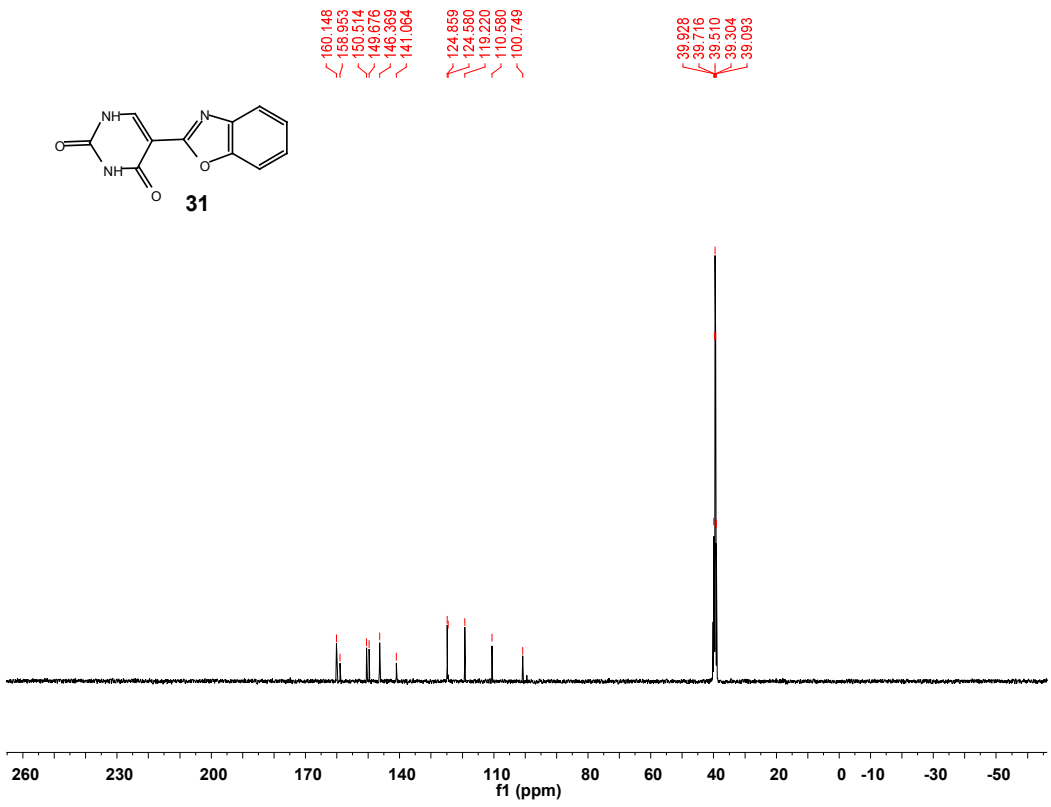

8.733
8.729
7.689
7.671
7.338
7.337
7.329
7.328
6.595
6.578
29
DMSO-d6
1.00
1.07
2.12
2.19
2.20
1.11
f1 (ppm)

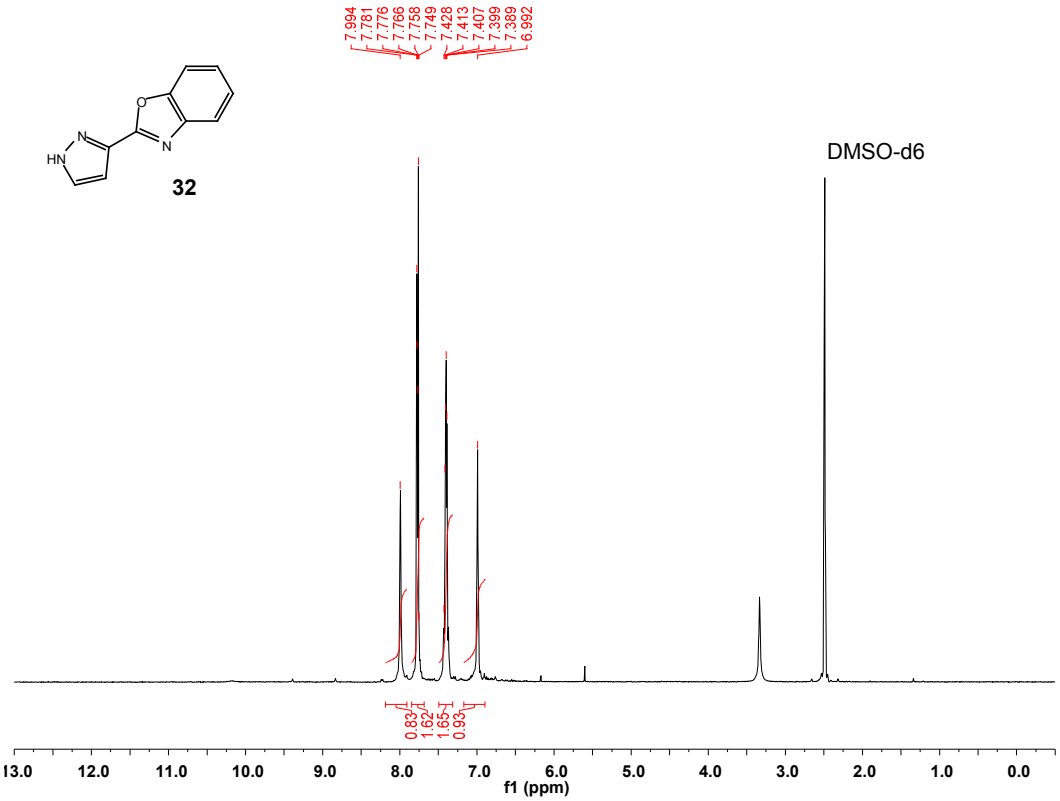

162.049
161.698
149.772
148.373
141.691
135.617
124.483
124.389
118.896
110.530
110.385
107.920
29
DMSO-d6
f1 (ppm)

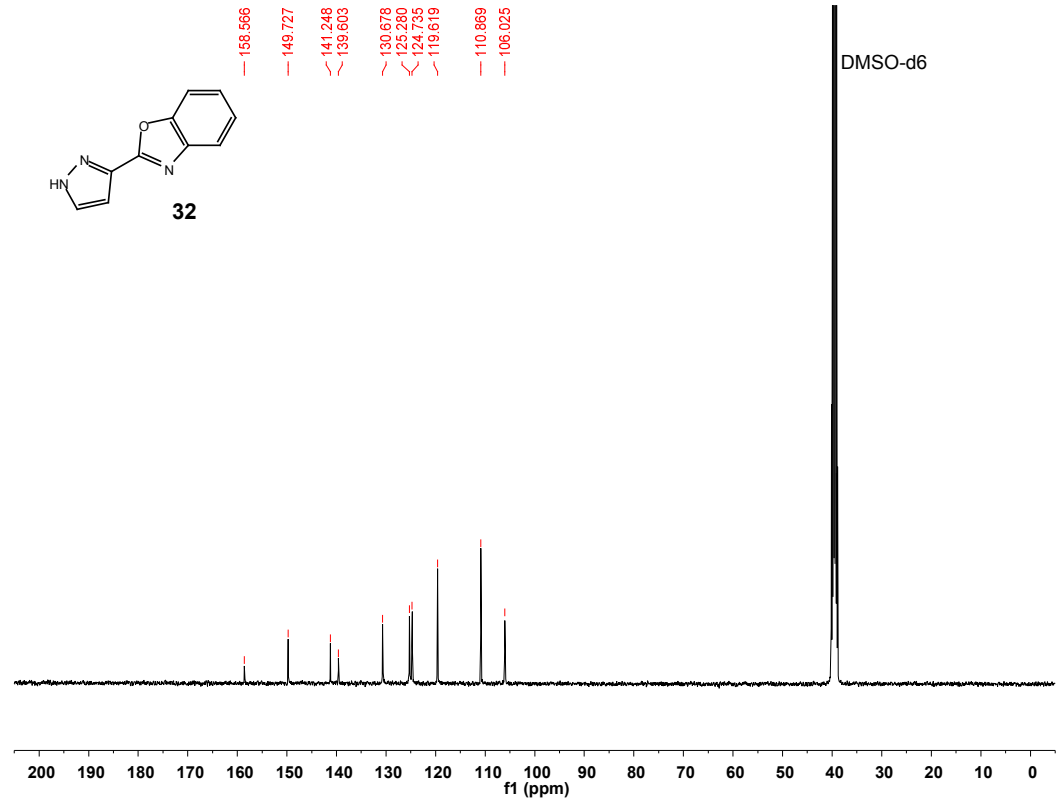

7.731
7.729
7.725
7.717
7.712
7.708
7.699
7.694
7.604
7.387
7.383
7.378
7.373
7.363
30
DMSO-d6
EtOAc
2.26
1.00
4.83
f1 (ppm)

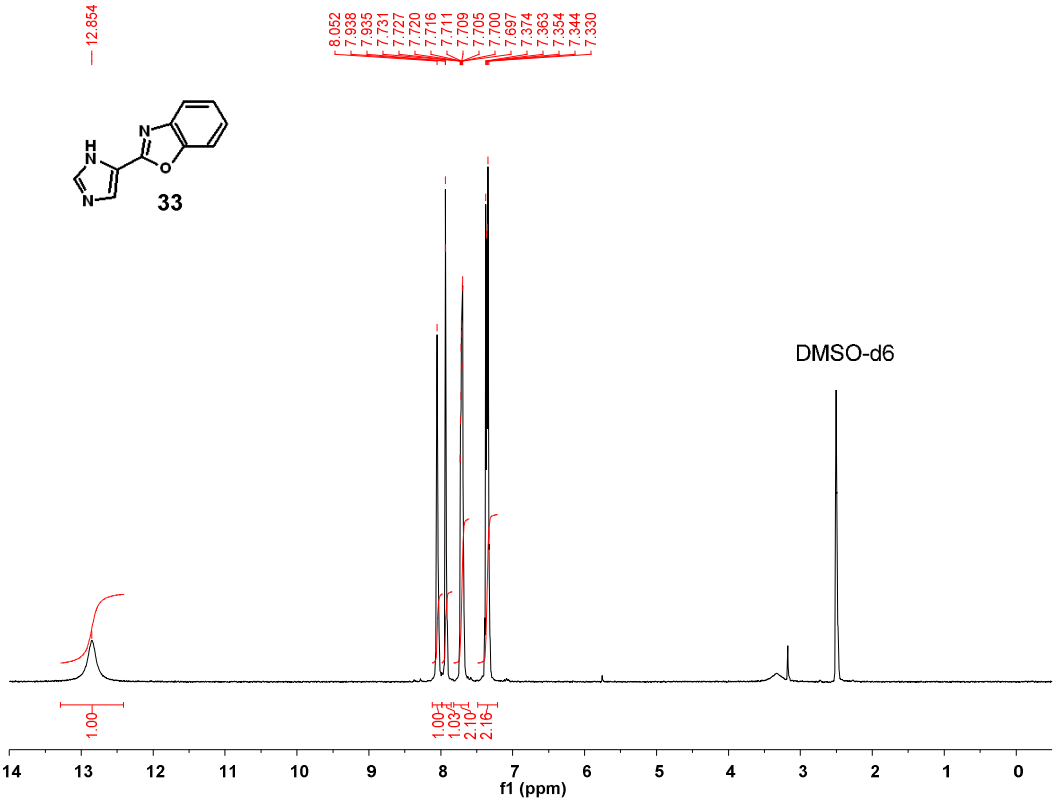

169.030
158.486
149.637
141.352
138.246
125.205
124.691
119.617
112.551
110.687
30
DMSO-d6
EtOAc
f1 (ppm)

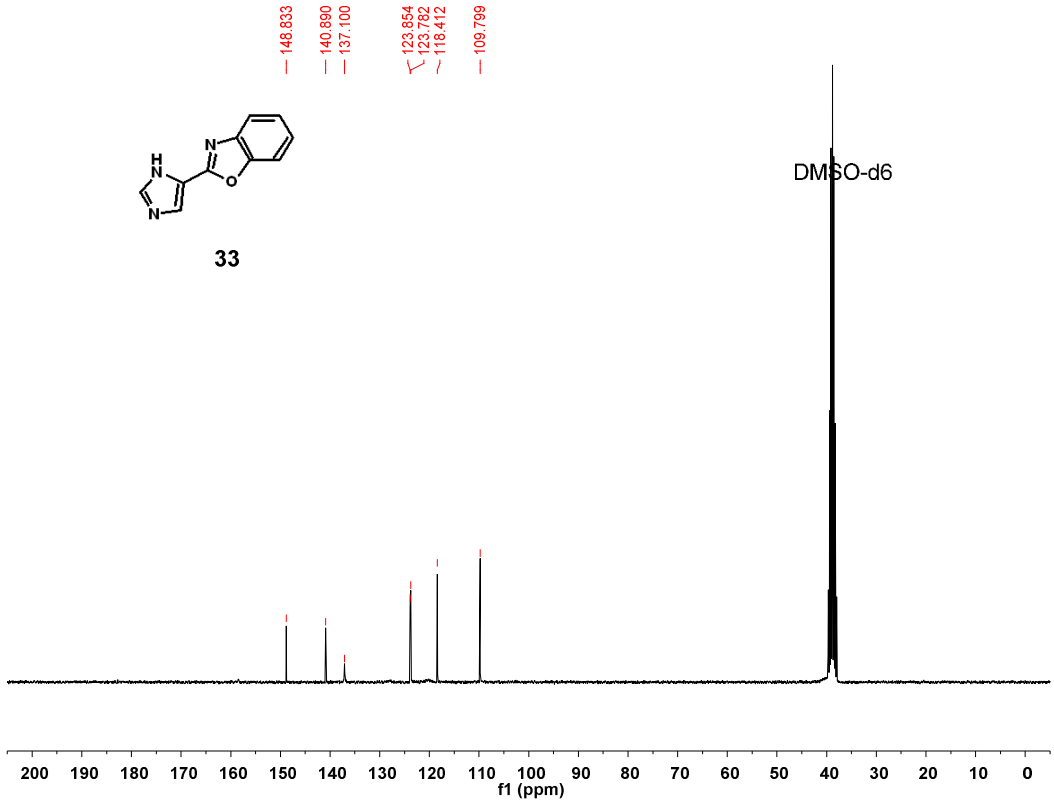

11.797
11.778
11.685
8.336
7.716
7.710
7.705
7.702
7.694
7.688
7.682
7.361
7.355
7.351
7.347
7.344
7.338
NH
O
NH
O
N
O
31
DMSO-d6
1.77
0.94
1.76
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

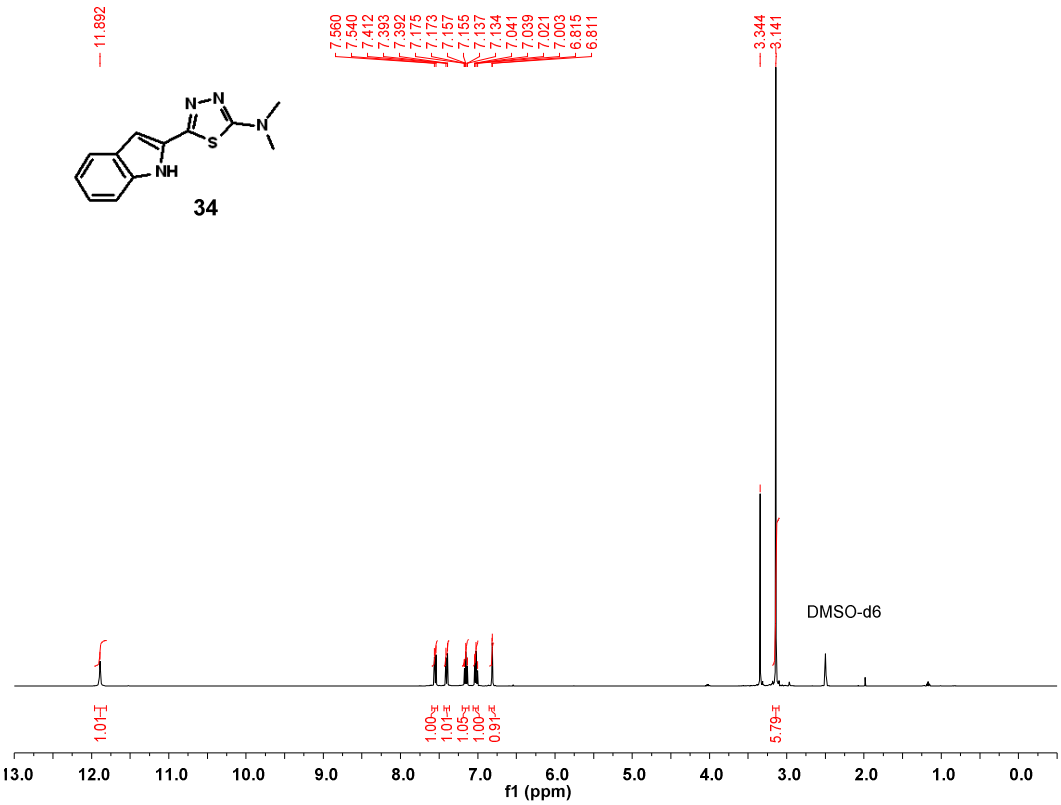

160.148
158.953
150.514
149.676
146.369
141.064
124.859
124.580
119.220
110.580
100.749
39.928
39.716
39.510
39.304
39.093
NH
O
NH
O
N
O
31
260 230 200 170 140 110 80 60 40 20 0 -10 -30 -50
f1 (ppm)

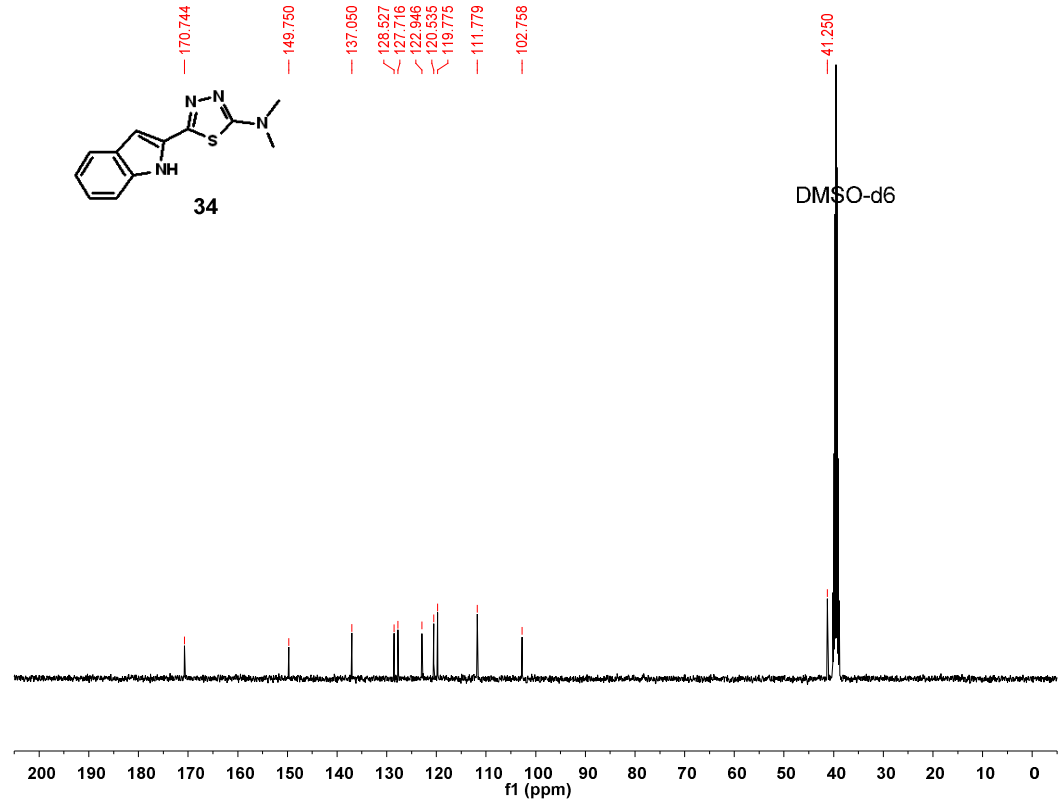

7.994
7.781
7.776
7.766
7.758
7.749
7.428
7.413
7.407
7.399
7.389
6.992
DMSO-d6
32
0.83
1.62
1.65
0.93
f1 (ppm)


158.566
149.727
141.248
139.603
130.678
125.280
124.735
119.619
110.869
106.025
DMSO-d6
32
f1 (ppm)


12.854
8.052
7.938
7.935
7.731
7.727
7.720
7.716
7.711
7.709
7.705
7.700
7.697
7.374
7.363
7.354
7.344
7.330
33
DMSO-d6
1.00
1.00
1.03
2.10
2.16
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


148.833
140.890
137.100
123.854
123.782
118.412
109.799
33
DMSO-d6
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


11.892
7.560
7.540
7.412
7.393
7.392
7.175
7.173
7.157
7.155
7.137
7.134
7.041
7.039
7.021
7.003
6.815
6.811
3.344
3.141
N
N
S
N
NH
34
DMSO-d6
1.01
1.00
1.01
1.05
1.00
0.91
5.79
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


170.744
149.750
137.050
128.527
127.716
122.946
120.535
119.775
111.779
102.758
41.250
N
N
S
N
NH
34
DMSO-d6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)