# Total Synthesis of an *Isatis indigotica*-Derived Alkaloid using a Biomimetic Thio-Diels-Alder Reaction

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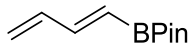
# SUPPORTING INFORMATION

## General Experimental Details

Commercially available reagents were used throughout without purification unless otherwise stated. Anhydrous solvents were used as supplied. Diethyl ether, tetrahydrofuran, dichloromethane, acetonitrile, 1,4-dioxane, dimethylformamide and toluene were dried using an LC Technology Solutions Inc. SP-1 solvent purification system under an atmosphere of dry nitrogen. Ether refers to diethyl ether. All reactions were routinely carried out in oven-dried glassware under a nitrogen atmosphere unless otherwise stated. Analytical thin layer chromatography was performed using silica plates and compounds were visualized at 254 and/or 360 nm ultraviolet irradiation followed by staining with either alkaline permanganate or ethanolic vanillin solution. Infrared spectra were obtained using a Perkin Elmer spectrum One Fourier Transform Infrared spectrometer as thin films between sodium chloride plates. Absorption maxima are expressed in wavenumbers ($cm^{-1}$). Melting points were recorded on an Electrothermal melting point apparatus and are uncorrected. NMR spectra were recorded as indicated on an NMR spectrometer operating at 400 MHz for $^{1}H$ nuclei and 100 MHz for $^{13}C$ nuclei. Chemical shifts are reported in parts per million (ppm) relative to the tetramethylsilane peak recorded as δ 0.00 ppm in $CDCl_3$/TMS solvent, or the residual acetone (δ 2.05 ppm), chloroform (δ 7.26 ppm), or DMSO (δ 2.50 ppm) peaks. The $^{13}C$ NMR values were referenced to the residual acetone (δ 29.9 ppm), chloroform (δ 77.1 ppm) or DMSO (δ 39.5 ppm) peaks. $^{13}C$ NMR values are reported as chemical shift δ and assignment. $^{1}H$ NMR shift values are reported as chemical shift δ, relative integral, multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet), coupling constant (*J* in Hz) and assignment. Assignments are made with the aid of DEPT 90, DEPT 135, COSY, NOESY and HSQC experiments. All experiments were conducted at 298 K. Conventional NMR tubes (5 mm diameter, Norell) using a sample volume of 500 μL were used. High resolution mass spectra were obtained by electrospray ionization in positive ion mode at a nominal accelerating voltage of 70 eV on a microTOF mass spectrometer.

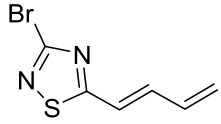
(*E*)-2-(Buta-1,3-dienyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**12**)




The *title compound* was prepared with slight modification to the procedure described by Morken and co-workers.[1] To a stirred solution of 2,2,6,6-tetramethylpiperidine (0.318 mL, 1.89 mmol) in THF (2 mL) at -5 °C was added *n*-butyllithium (1.29 M, 1.45 mL, 1.89 mL) dropwise. The resulting solution was stirred at -5 °C for 15 min before adding bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methane (500 mg, 1.89 mmol) as a solution in THF (3.75 mL). The solution was stirred for 10 minutes before being cooled to -78 °C, at which point it turned cloudy. Acrolein (0.105 mL, 1.56 mmol) was then added dropwise as a solution in THF (2 mL) and the resulting solution was stirred at -78 °C for 3 h. The solution was then warmed to room temperature, and quenched with methanol (10 mL) before being concentrated *in vacuo*. The crude material was then purified by flash chromatography on silica gel eluting with hexanes – ethyl acetate (95:5) to afford the *title compound* (154 mg, 0.855 mmol, 55 %) as colourless oil. $\delta_H$ (400 MHz, $CDCl_3$) 7.00 (1 H, dd, *J* 17.8, 10.4, CH), 6.41 (1 H, dtd, *J* 17.0, 10.2, 1.0, CH), 5.57 (1 H, d, *J* 18.1, CH), 5.38 (1 H, dd, *J* 16.9, 1.3, ½ x $CH_2$), 5.26 (1 H, dd, *J* 10.0, 1.1, ½ x $CH_2$), 1.28 (12 H, s, 4 x Me). $^1$H NMR data is in agreement with the literature.[1]

(1) Coombs, J. R.; Zhang, L.; Morken, J. P. *Org. Lett.* **2015**, *17*, 1708–1711.

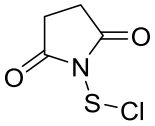
(*E*)-3-Bromo-5-(buta-1,3-dienyl)-1,2,4-thiadiazole (**13**)




To a sealed tube charged with 3-bromo-5-chloro-1,2,4-thiadiazole (**11**) (714.7 mg, 3.58 mmol), diene **12** (568 mg, 3.15 mmol) and potassium carbonate (539 mg, 3.90 mmol), was added 1,4-dioxane (26.1 mL) and water (2.9 mL) and the resulting mixture was degassed with nitrogen for 30 min before adding bis(di-*tert*-butyl(4-dimethylaminophenyl)phosphine)dichloropalladium(II) (115.5 mg, 0.163 mmol, 5 mol%). The mixture was sealed under nitrogen and heated to 80 °C for 24.5 h, before being cooled to room temperature, dried using $Na_2SO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by flash chromatography on silica gel eluting with petroleum ether – ethyl acetate (95:5) to afford the *title compound* (347 mg, 1.60 mmol, 51%) as an unstable yellow oil. $\nu_{max}/cm^{-1}$ (neat): 2921, 1621, 1594, 1454, 1348, 1265, 1216, 1097, 996, 924, 802; $\delta_H$ (400 MHz,

$CDCl_3$) 7.30 (1 H, ddd, *J* 15.8, 10.7, 0.98, C-CH=CH), 6.76 (1 H, dd, *J* 15.8, 1.0, C-CH), 6.53 (1 H, dtd, *J* 17.0, 10.4, 0.97, CH-CH=$CH_2$), 5.68 (1 H, dd, *J* 17.0, 0.97, ½ x $CH_2$), 5.57 (1 H, d, *J* 10.0, ½ x $CH_2$); $\delta_C$ (100 MHz, $CDCl_3$) 188.1 (C), 145.9 (C), 140.8 (CH), 135.1 (CH), 126.1 ($CH_2$), 120.1 (CH); complete characterisation could not be obtained due to stability issues.

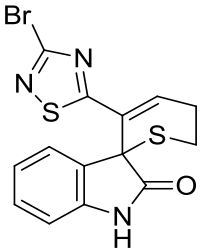
*N*-Chlorosulfenylsuccinimide (succNSCl)




The *title compound* was prepared with slight modification to the procedure described by Kaminskaya and co-workers.[2] To a round bottom flask charged with *N*-chlorosuccinimide (300 mg, 2.25 mmol), sulfur (72 mg, 2.25 mmol) and tetrabutylammonium iodide (42 mg, 0.113 mmol, 5 mol%) was added dichloroethane (4.5 mL), and the resulting mixture was heated to 70 °C for 24.5 h. Upon complete consumption of the starting material, the solution was cooled, and concentrated *in vacuo*. The crude material was washed with petroleum ether (15 mL) to provide the *title compound* (309 mg, 1.87 mmol, 83%) as a bright yellow semi-stable solid that was used without further purification. The *title compound* was found to be air and moisture sensitive, but could be stored under nitrogen, in a desiccator, in the dark, for several weeks with minimal degradation. M.p. 103.3-107.1 °C (lit. 73-74 °C)[2]; $\nu_{max}/cm^{-1}$ (neat): 3153, 3078, 1771, 1684, 1371, 1293, 1185, 848, 819; $\delta_H$ (400 MHz, $CDCl_3$) 2.76 (4 H, s, 2 x $CH_2$); $\delta_C$ (100 MHz, $CDCl_3$) 177.5 (C), 29.7 (2 x $CH_2$). Spectroscopic data is consistent with the literature.[3]

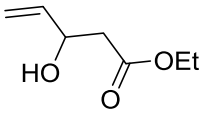
(2) Borovikova, G. S.; Levchenko, E. S.; Kaminskaya, E. I. *J. Org. Chem. USSR (Engl. Transl.);* **1986**, *22*, 86–92.
(3) Bombala, M. U.; Ley, S. V. *J. Chem. Soc., Perkin Trans. 1* **1979**, 3013-3016.

(±)-3'-(3-Bromo-1,2,4-thiadiazol-5-yl)-5',6'-dihydrospiro(indoline-3,2'-thiopyran)-2-one [(±)**15**]




A solution of oxindole (**14**) (24.7 mg, 0.186 mmol) and triethylamine (0.026 mL, 0.188 mmol) in dichloromethane (0.6 mL) was stirred at room temperature for 15 minutes before being transferred to a stirred solution of *N*-chlorosulfenylsuccinimide (33.6 mg, 0.203 mmol) in dichloromethane (0.6 mL) at -78 °C dropwise. The resulting solution was stirred for 10 minutes, then was warmed to -5 °C. Diene **13** (40 mg, 0.184 mmol) was then added as a solution in dichloromethane (0.3 mL). The solution was then warmed to room temperature and stirring continued for 1 h, before adding pyridine (0.066 mL, 0.559 mmol) dropwise to generate the dienophile **9**. The reaction mixture was stirred at room temperature for 15 h, before being diluted with dichloromethane (10 mL), and washed with water (4 x 5 mL). The organic layer was dried using $Na_2SO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by flash chromatography on silica gel, with dry loading, eluting with petroleum ether – ethyl acetate (3:1) to afford the *title compound* (13.9 mg, 0.0366 mmol, 20%) as a dark orange solid. M.p. 66.6-69.7 °C; HRMS [ESI, $(M + Na)^+$] found 401.9328, [$C_{14}H_{10}BrN_3OS_2 + Na^+$] requires 401.9341; $\nu_{max}/cm^{-1}$ (neat): 3200, 2929, 1703, 1616, 1471, 1444, 1227, 1205, 1177, 904, 728, 677; $\delta_H$ (400 MHz, acetone-$d_6$) 9.75 (1 H, br s, NH), 7.59 (1 H, t, *J* 4.4, C=CH-$CH_2$), 7.35 (1 H, ddd, *J* 7.8, 7.64, 1.2, ArH), 7.18 (1 H, d, *J* 7.4, ArH), 7.06 (1 H, d, *J* 7.5, ArH), 6.99 (1 H, ddd, *J* 7.6, 7.5, 1.0, ArH), 3.79 (1 H, ddd, *J* 13.7, 8.1, 6.7, ½ x $CH_2$), 2.92 – 2.88 (2 H, m, $CH_2$), 2.79 – 2.75 (1 H, m, ½ x $CH_2$); $\delta_C$ (100 MHz, acetone-$d_6$) 189.5 (C), 177.3 (C), 144.9 (C), 144.0 (C), 143.6 (C=CH-$CH_2$), 131.4 (CH), 128.7 (C), 127.5 (C), 126.1 (CH), 123.3 (CH), 111.4 (CH), 49.1 (C), 27.9 ($CH_2$), 22.2 ($CH_2$). The diene **13** was also recovered (10.4 mg, 0.0479 mmol, 26%).

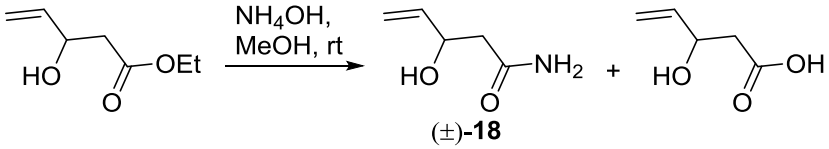
Ethyl-3-hydroxy-4-pentanoate




The *title compound* was prepared with slight modification to the procedure described by Zibuck and Streiber.[4] To a stirred solution of *N*,*N*-diisopropylamine (3.08 mL, 22.0 mmol) in THF (80 mL) at -78 °C was added freshly titrated *n*-butyllithium (13.33 mL, 1.65 M, 22 mmol) dropwise and the resulting solution was stirred for 15 minutes prior to the dropwise addition of dry ethyl acetate (1.95 mL, 20 mmol). The solution was stirred at -78 °C for 1 h, before adding acrolein (1.34 mL, 20 mmol) as a solution in THF (10 mL) dropwise. Stirring was continued for a further 15 minutes before being quenched with ammonium chloride (sat., 20 mL). The mixture was then warmed to room temperature and the volatiles were removed *in vacuo*. The aqueous residue was then extracted with diethyl ether (2 x 80 mL), and the organic extracts were washed with brine (40 mL), then were dried using $Na_2SO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by flash chromatography on silica gel eluting with petroleum ether – ethyl acetate (3:1) to afford the *title compound* (2.36 g, 16.4 mmol, 82%) as a pale yellow liquid. $\delta_H$ (400 MHz, $CDCl_3$) 5.88 (1 H, ddd, *J* 17.1, 10.5, 5.5, $CH_2$=CH), 5.31 (1 H, dt, *J* 17.2, 1.4, ½ x $CH_2$), 5.15 (1 H, dt, *J* 10.5, 1.3, ½ x $CH_2$), 4.56 – 4.51 (1 H, br m, CH), 4.17 (2 H, q, *J* 7.1, $CH_2$Me), 2.97 (1 H, br d, *J* 3.8, OH), 2.58 (2 H, dd, *J* 16.2, 4.1, ½ x $CH_2$), 2.51 (2 H, dd, *J* 16.2, 8.3, ½ x $CH_2$), 1.27 (3 H, t, *J* 7.1, Me). $^1$H NMR data is concordant with the literature.[4,5]

(4) Zibuck, R.; Streiber, J. M. *J. Org. Chem.* **1989**, *54*, 4717–4719.
(5) Crimmins, M. T.; Wang, Z.; McKerlie, L. A. *J. Am. Chem. Soc.* **1998**, *120*, 1747–1756.

3-Hydroxy-4-pentenamide [(±)-**18**]




(±)-**18**

To a stirred solution of ethyl-3-hydroxy-4-pentanoate (200 mg, 1.39 mmol) in methanol (6 mL) was added ammonium hydroxide (6 mL, 28 – 30% as $NH_3$) and the resulting solution was stirred at room temperature for 17 h, then was concentrated *in vacuo*. The crude material was then purified by flash chromatography on silica gel eluting with dichloromethane – methanol

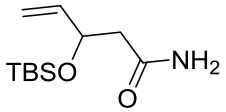
(10:1) to afford the *title compound* (87.7 mg, 0.762 mmol, 55%), along with 3-hydroxypent-4-enoic acid (18.1 mg, 0.156 mmol, 11%).

(±)-**18**, colourless amorphous solid; M.p. 80.1-83.4 °C (88-89 °C)[6]; HRMS [ESI, $(M + Na)^+$] found 138.0521, [$C_5H_9NO_2 + Na^+$] requires 138.0525; $\nu_{max}/cm^{-1}$ (neat): 3343, 1670, 1625, 1408, 1319, 1107, 1001, 924, 814, 667; $\delta_H$ (400 MHz, $CDCl_3$) 5.90 (2 H, br s + ddd, *J* 17.2, 10.6, 5.7, ½ x $NH_2$ + $CH_2$=CH), 5.53 (1 H, br s, ½ x $NH_2$), 5.33 (1 H, dt, *J* 17.2, 1.3, ½ x $CH_2$=CH), 5.17 (1 H, dt, *J* 10.6, 1.3, ½ x $CH_2$=CH), 4.57 – 4.52 (1 H, m, CH), 3.33 (1 H, br s, OH), 2.51 (1 H, dd, *J* 15.6, 3.3, ½ x $CH_2$), 2.41 (1 H, dd, *J* 15.6, 8.4, ½ x $CH_2$); $\delta_C$ (100 MHz, DMSO-$d_6$) 172.3 (C), 141.6 (CH), 113.1 ($CH_2$), 68.2 (CH), 43.1 ($CH_2$). NMR data is concordant with the literature.[6]

**3-Hydroxypent-4-enoic acid**, yellow oil; $\delta_H$ (400 MHz, $CDCl_3$) 5.91 (1 H, ddd, *J* 17.3, 10.6, 5.7, $CH_2$=CH), 5.34 (1 H, dt, *J* 17.3, 1.2, ½ x $CH_2$=CH), 5.20 (1 H, dt, *J* 10.3, 1.2, ½ x $CH_2$=CH), 4.60 – 4.55 (1 H, br m, CH), 2.69 – 2.56 (2 H, m, $CH_2$), 2 x OH not observed. $^1$H NMR data is concordant with the literature.[7]

(6) Knapp, S.; Gibson, F. S. *J. Org. Chem.* **1992**, *57*, 4802–4809.
(7) Sabitha, G.; Reddy, S. S. S.; Bhaskar, V.; Yadav, J. S. *Synthesis* **2010**, 1217–1222.

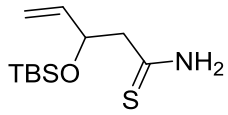
3-((*tert*-Butyldimethoxysilyl)oxy)pent-4-enamide [(±)-**19**]




To a stirred solution of β-hydroxyamide (±)-**18** (400 mg, 3.47 mmol) in dichloromethane (35 mL) was added imidazole (710 mg, 10.4 mmol) followed by *tert*-butyldimethylsilyl chloride (786 mg, 5.21 mmol) and the resulting solution was stirred at room temperature for 16 h. Following complete consumption of the starting material, the reaction mixture was diluted with dichloromethane (100 mL) and washed with water (2 x 50 mL). The organic layer was then dried using $Na_2SO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by flash chromatography on silica gel eluting with dichloromethane – methanol (9:1) to afford the *title compound* (779 mg, 3.40 mmol, 98%) as a colourless solid. M.p. 55.5-58.0 °C; HRMS [ESI, $(M + Na)^+$] found 252.1384, [$C_{11}H_{23}NO_2Si + Na^+$] requires 252.1390; $\nu_{max}/cm^{-1}$ (neat): 3390, 3155, 2929, 2857, 1671, 1624, 1405, 1253, 1107, 1002, 938, 918, 813, 778; $\delta_H$ (400

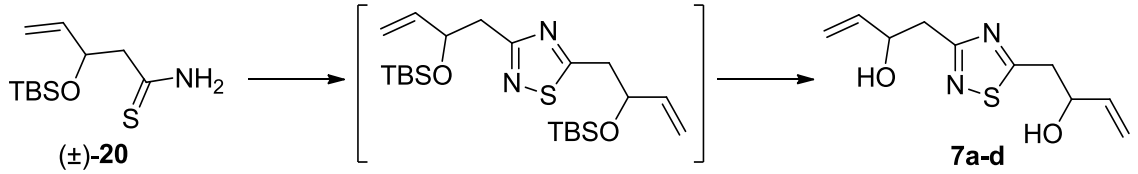
MHz, $CDCl_3$) 6.21 (1 H, br s, ½ x $NH_2$), 5.87 (1 H, ddd, *J* 17.0, 10.4, 5.5, $CH_2$=CH), 5.44 (1 H, br s, ½ x $NH_2$), 5.26 (1 H, dt, *J* 17.0, 1.5, ½ x $CH_2$=CH), 5.13 (1 H, dt, *J* 10.5, 1.5, ½ x $CH_2$=CH), 4.56 – 4.52 (1 H, m, CH), 2.45 (1 H, dd, *J* 14.6, 4.3, ½ x $CH_2$), 2.39 (1 H, dd, *J* 14.6, 6.2, ½ x $CH_2$), 0.91 (9 H, s, 3 x Me), 0.10 (3 H, s, Me), 0.08 (3 H, s, Me); $\delta_C$ (100 MHz, $CDCl_3$) 173.7 (C), 139.5 (CH), 115.1 ($CH_2$), 70.7 (CH), 44.5 ($CH_2$), 25.9 (3 x Me), 18.2 (C), -4.5 (Me), -5.0 (Me).

3-((*tert*-Butyldimethoxysilyl)oxy)pent-4-enethioamide [(±)-**20**]




To a stirred solution of amide (±)-**19** (90 mg, 0.392 mmol) in THF (3.9 mL) was added Lawesson's reagent (95.1 mg, 0.235 mmol) and the resulting solution was stirred at room temperature for 30 minutes before being concentrated *in vacuo*. The crude product was purified by flash chromatography on silica gel eluting with petroleum ether – ethyl acetate (3:1) to afford the *title compound* (82.4 mg, 0.334 mmol, 86%) as a colourless waxy solid. M.p. 74.4-78.6 °C; HRMS [ESI, $(M + Na)^+$] found 268.1163, [$C_{11}H_{23}NOSSi + Na^+$] requires 268.1162; $\nu_{max}/cm^{-1}$ (neat): 3314, 3111, 2929, 2858, 1648, 1450, 1407, 1252, 1051, 999, 920, 812, 779; $\delta_H$ (400 MHz, $CDCl_3$) 7.91 (1 H, br s, ½ x $NH_2$), 7.65 (1 H, br s, ½ x $NH_2$), 5.86 (1 H, ddd, *J* 17.1, 10.5, 5.5, $CH_2$=CH), 5.28 (1 H, dt, *J* 17.5, 1.4, ½ x $CH_2$=CH), 5.15 (1 H, dt, *J* 10.3, 1.5, ½ x $CH_2$=CH), 4.57 – 4.52 (1 H, m, CH), 2.94 (1 H, d, *J* 1.9, ½ x $CH_2$), 2.93 (1 H, d, *J* 3.0, ½ x $CH_2$), 0.90 (9 H, s, 3 x Me), 0.10 (3 H, s, Me), 0.08 (3 H, s, Me); $\delta_C$ (100 MHz, $CDCl_3$) 207.0 (C), 138.7 (CH), 115.8 ($CH_2$), 72.7 (CH), 52.8 ($CH_2$), 25.9 (3 x Me), 18.2 (C), -4.4 (Me), -4.9 (Me).

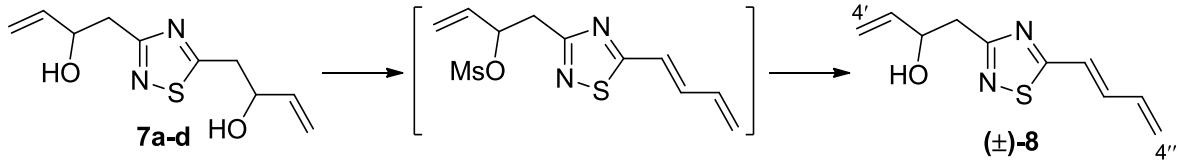
Insatindigothiadiazoles A-D (**7a-d**)




To a stirred solution of thioamide (±)-**20** (282 mg, 1.15 mmol) in dichloromethane (12 mL) was added phenyliodine(III) diacetate (PIDA) (371 mg, 1.16 mmol) and the resulting solution

was stirred at room temperature for 15 minutes before being diluted with dichloromethane (30 mL), and washed with water (2 x 15 mL). The organic layer was then dried using $Na_2SO_4$, filtered, and concentrated *in vacuo* to afford the crude disilylated thiadiazole. The crude material was dissolved in THF (8 mL) and tetrabutylammonium fluoride (1 M in THF, 1.56 mL, 1.56 mmol) was added dropwise. The resulting solution was stirred at room temperature for 6 h, with additional tetrabutylammonium fluoride (1 M in THF, 0.78 mL, 0.78 mmol) added after the first 3 h. The solution was then diluted with ethyl acetate (25 mL) and was washed with ammonium chloride (sat., 2 x 15 mL). The organic layer was then dried using $Na_2SO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by flash chromatography on silica gel eluting with petroleum ether – ethyl acetate (1:4) to afford the *title compounds* (64 mg, 0.266 mmol, 46%) as a colourless solid. M.p. 46.8-49.4 °C; HRMS [ESI, $(M + Na)^+$] found 249.0673, [$C_{10}H_{14}N_2O_2S + Na^+$] requires 249.0668; $\nu_{max}/cm^{-1}$ (neat): 3296, 2920, 1643, 1488, 1401, 1318, 1162, 1130, 999, 921, 843, 667; $^1H$ NMR and $^{13}C$ NMR see Tables S1 and S2.

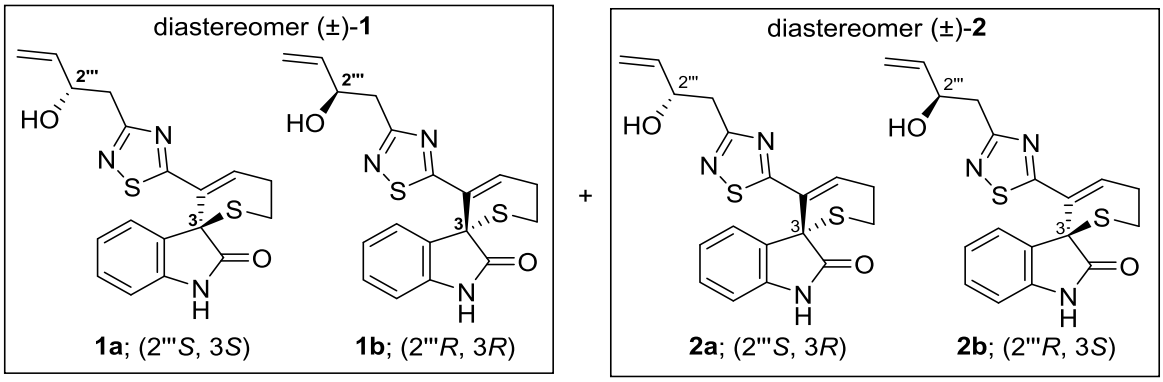
(*E*)-1-(5-(Buta-1,3-dien-1-yl)-1,2,4-thiadiazol-3-yl)but-3-en-2-ol [(±)-**8**]




To a stirred solution of insatindigothiadiazoles (**7a-d**) (62 mg, 0.274 mmol) in dichloromethane (2.3 mL) at 0 °C was added triethylamine (0.05 mL, 0.358 mmol) followed by methanesulfonyl chloride (0.646 M solution in dichloromethane, 0.44 mL, 0.284 mmol) dropwise. The reaction was warmed to room temperature for 15 minutes, then was cooled back to 0 °C and a second equivalent of triethylamine (0.05 mL, 0.358 mmol) was added. The reaction mixture was warmed to room temperature for 1 h, then diluted with ethyl acetate (20 mL), and washed with water (3 x 10 mL). The organic layer was then dried using $Na_2SO_4$, filtered, and concentrated *in vacuo* to afford crude mesylate, to which a mixture of THF-$H_2O$ (3:1, 4 mL) was added. The solution was heated to 40 °C for 2 h. Upon completion of the reaction, the solution was cooled to room temperature, diluted with ethyl acetate (25 mL) and washed with sodium bicarbonate (sat., 10 mL). The organic layer was then dried using $Na_2SO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by flash chromatography on silica gel eluting with petroleum ether – ethyl acetate (1:1) to afford the *title compound* (16.9 mg, 0.0811 mmol, 30%)

as a yellow oil, which was used immediately in the next step due to its observed instability. HRMS [ESI, $(M + Na)^+$] found 231.0566, [$C_{10}H_{12}N_2OS + Na^+$] requires 231.0563; $\delta_H$ (400 MHz, $CDCl_3$) 7.23 (1 H, ddd, *J* 15.5, 10.5, 0.9, Ar-CH=CH), 6.78 (1 H, d, *J* 15.9, Ar-CH=CH), 6.53 (1 H, dt, *J* 17.0, 10.3, CH=CH-CH=$CH_2$), 5.96 (1 H, ddd, *J* 17.4, 10.5, 5.5, CH=$CH_2$), 5.63 (1 H, dm, *J* 17.0, ½ x CH=$CH_2$(4")), 5.52 (1 H, dd, *J* 10.3, 1.0, ½ x CH=$CH_2$(4")), 5.34 (1 H, dt, *J* 17.0, 1.5, ½ x CH=$CH_2$(4')), 5.15 (1 H, dt, *J* 10.7, 1.3, ½ x CH=$CH_2$(4')), 4.68 – 4.63 (1 H, br m, CH-OH), 3.83 (1 H, br d, *J* 4.2, OH), 3.26 (1 H, dd, *J* 15.5, 3.5, ½ x $CH_2$), 3.13 (1 H, dd, *J* 15.5, 8.4, ½ x $CH_2$); $\delta_C$ (100 MHz, $CDCl_3$) 186.0 (C), 174.6 (C), 139.8 (CH), 139.4 (CH), 135.4 (CH), 124.9 (CH=$CH_2$), 121.0 (CH), 115.4 (CH=$CH_2$), 70.8 (CHOH), 40.0 ($CH_2$).

(±)-3'-(3-(2-Hydroxybut-3-en-1-yl)-1,2,4-thiadiazol-5-yl)-5',6'-dihydrospiro(indoline-3,2'-thiopyran)-2-one [(±)-**1** and (±)-**2**]



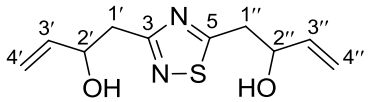

A solution of oxindole (**14**) (4.52 mg, 0.0340 mmol) and triethylamine (0.035 mL, 0.251 mmol) in dichloromethane (0.2 mL) was stirred at room temperature for 15 minutes before being transferred to a stirred solution of *N*-chlorosulfenylsuccinimide (6.1 mg, 0.0369 mmol) in dichloromethane (0.2 mL) at -78 °C dropwise. The resulting solution was stirred for 10 minutes, then was warmed to -5 °C. Diene [(±)-**8**] (7.0 mg, 0.0336 mmol) was added as a solution in dichloromethane (0.1 mL). The solution was warmed to room temperature and stirring continued for 1 h, before adding pyridine (0.01 mL, 0.124 mmol) dropwise to generate the dienophile **9**. The reaction mixture was stirred at room temperature for 69.5 h, before being diluted with dichloromethane (10 mL), and washed with water (4 x 5 mL). The organic layer was dried using $Na_2SO_4$, filtered, and concentrated *in vacuo*. The crude product was purified by preparative TLC eluting with petroleum ether – acetone (3:1) to afford the *title compound* (6.7 mg, 0.0181 mmol, 54%, 1:1 mixture of diastereomers) as an orange oil. The diastereomers were separated by preparative TLC eluting with petroleum ether – ethyl acetate (45:55) to

afford the natural product (±)-**1** (3.1 mg, 0.00835 mmol) as a yellow oil and its diastereomer (±)-**2** (3.2 mg, 0.00862 mmol) as a yellow oil.

(±)-**1**; HRMS [ESI, $(M + Na)^+$] found 394.0651, [$C_{18}H_{17}N_3O_2S_2 + Na^+$] requires 394.0654; $\nu_{max}/cm^{-1}$ (neat): 3227, 2926, 1702, 1617, 1472, 1320, 1180, 1105, 926, 748, 676; $^1H$ NMR and $^{13}C$ NMR see Tables S3 and S4.

(±)-**2**; HRMS [ESI, $(M + Na)^+$] found 394.0666, [$C_{18}H_{17}N_3O_2S_2 + Na^+$] requires 394.0654; $\nu_{max}/cm^{-1}$ (neat): 3228, 2923, 1703, 1617, 1472, 1320, 1180, 1105, 926, 749, 676; $^1H$ NMR and $^{13}C$ NMR see Tables S5 and S6.

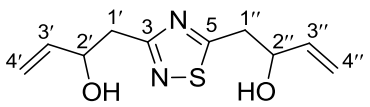
**Table S1.** $^{1}$H NMR comparison of natural **7a-d** (2:4:1:2)[8] with synthetic **7a-d** (1:1:1:1).




| H | Natural insatindigothiadiazoles (7a-d)[8] $\delta_H$ (acetone-$d_6$, 600 MHz) | Synthetic insatindigothiadiazoles (7a-d) $\delta_H$ (acetone-$d_6$, 400 MHz) | Δδ |
|---|---|---|---|
| **1'a** | 3.075/3.077 (dd, *J* 15.6, 6.0) | 3.08 – 3.06 (m/unresolved) | -0.01 |
| **1'b** | 3.047/3.051 (dd, *J* 15.6, 7.8) | 3.08 – 3.06 (m/unresolved) | +0.02 |
| **2'** | 4.652/4.654 (m) | 4.68 – 4.63 (m) | 0 |
| **3'** | 5.938/5.939 (ddd, *J* 17.4, 10.8, 5.4) | 5.99 – 5.91 (m) | +0.01 |
| **4'a** | 5.236/5.239 (ddd, *J* 17.4, 1.8, 1.2) | 5.25 (dm, *J* 17.0) | +0.01 |
| **4'b** | 5.004 (ddd, *J* 10.8, 1.8, 1.2) | 5.01 (dt, *J* 10.5, 1.6) | +0.01 |
| **1''a** | 3.373 (dd, *J* 15.6, 4.2) | 3.38 (dd, *J* 15.5, 4.0) | +0.01 |
| **1''b** | 3.213/3.216 (dd, *J* 15.6, 7.8) | 3.23 (dd, *J* 15.5, 8.0)/3.22 (dd, *J* 15.5, 8.1) | +0.01 |
| **2''** | 4.513 (m) | 4.55 – 4.50 | +0.01 |
| **3''** | 5.974/5.976 (ddd, *J* 17.4, 10.8, 5.4) | 6.03 – 5.94 (m) | +0.01 |
| **4''a** | 5.322/5.324 (ddd, *J* 17.4, 1.8, 1.2) | 5.33 (dm, *J* 16.8) | +0.01 |
| **4''b** | 5.100/5.101 (ddd, *J* 10.8, 1.8, 1.2) | 5.10 (dt, *J* 10.5, 1.6) | 0 |
| **2'-OH** | 4.177/4.182 (d, *J* 5.4) | 4.18 (d, *J* 5.0)/4.19 (d, *J* 4.9) | +0.01 |
| **2''-OH** | 4.697 (br d, *J* 4.8) | 4.70 (d, *J* 4.9) | 0 |

(8) Chen, M.-H.; Lin, S.; Wang, Y.-N.; Zhu, C.-G.; Li, Y.-H.; Jiang, J.-D.; Shi, J.-G. *Chin. Chem. Lett.* **2016**, *27*, 643–648.

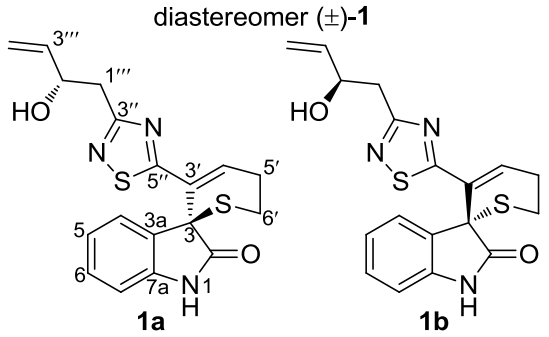
**Table S2.** $^{13}C$ NMR comparison of natural **7a-d** (2:4:1:2)[8] with synthetic **7a-d** (1:1:1:1).




| C | Natural insatindigothiadiazoles (7a-d)[8] $\delta_C$ (acetone-$d_6$, 150 MHz) | Synthetic insatindigothiadiazoles (7a-d) $\delta_C$ (acetone-$d_6$, 100 MHz) | Δδ |
|---|---|---|---|
| **3** | 173.76 | 173.80 | +0.04 |
| **5** | 188.77 | 188.81 | +0.04 |
| **1'** | 41.40/41.42 | 41.44/41.46 | +0.04 |
| **2'** | 71.44 | 71.37/71.49 | -0.01 |
| **3'** | 141.88 | 141.89/141.92 | +0.03 |
| **4'** | 144.04 | 114.09 | +0.05 |
| **1''** | 39.81 | 39.81/39.85 | +0.02 |
| **2''** | 71.00/71.02 | 71.04/71.06 | +0.04 |
| **3''** | 141.03/141.05 | 141.07/141.09 | +0.04 |
| **4''** | 115.25 | 115.29 | +0.04 |

(8) Chen, M.-H.; Lin, S.; Wang, Y.-N.; Zhu, C.-G.; Li, Y.-H.; Jiang, J.-D.; Shi, J.-G. *Chin. Chem. Lett.* **2016**, *27*, 643–648.

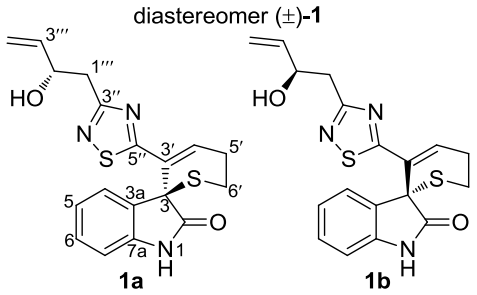
**Table S3.** [1]H NMR comparison of natural **1a**/**b**[9] with synthetic **1a/b**.




| H | Natural 1a/b[9] $\delta_H$ (acetone-$d_6$, 600 MHz) | Synthetic 1a/b $\delta_H$ (acetone-$d_6$, 400 MHz) | Δδ |
|---|---|---|---|
| **4** | 7.07 (dd, *J* 7.8, 1.2) | 7.08 (br d, *J* 7.4) | +0.01 |
| **5** | 6.90 (ddd, *J* 1.2, 7.2, 7.8) | 6.91 (ddd, *J* 1.0, 7.5, 7.5) | +0.01 |
| **6** | 7.24 (ddd, *J* 1.2, 7.2, 7.8) | 7.25 (ddd, *J* 1.1, 7.7, 7.7) | +0.01 |
| **7** | 6.99 (dd, *J* 7.8, 1.2) | 7.00 (d, *J* 7.6) | +0.01 |
| **4'** | 7.40 (dd, *J* 4.8, 4.2) | 7.41 (t, *J* 4.5) | +0.01 |
| **5'a** | 2.84 (m) | 2.87 – 2.83 (m) | +0.01 |
| **5'b** | 2.84 (m) | 2.87 – 2.83 (m) | +0.01 |
| **6'a** | 3.76 (ddd, *J* 13.8, 8.4, 6.6) | 3.77 (ddd, *J* 13.9, 7.8, 6.2) | +0.01 |
| **6'b** | 2.74 (ddd, *J* 13.8, 4.2, 3.6) | 2.75 (dt, *J* 13.4, 3.9) | +0.01 |
| **1'''a** | 2.88 (dd, *J* 14.4, 6.6) | 2.89 (dd, *J* 14.5 7.4) | +0.01 |
| **1'''b** | 2.79 (dd, *J* 14.4, 6.6) | 2.79 (unresolved) | 0 |
| **2'''** | 4.31 (m) | 4.34 – 4.29 (m) | +0.01 |
| **3'''** | 5.63 (ddd, *J* 16.8, 10.8, 5.4) | 5.64 (ddd, *J* 17.2, 10.6, 5.4) | +0.01 |
| **4'''a** | 4.98 (ddd, *J* 16.8, 1.8, 1.2) | 4.99 (dt, *J* 17.3, 1.8) | +0.01 |
| **4'''b** | 4.86 (ddd, *J* 10.8, 1.8, 1.2) | 4.87 (dt, *J* 10.5, 1.7) | +0.01 |
| **1-NH** | 9.68 (br s) | 9.67 (br s) | -0.01 |
| **2'''-OH** | 3.95 (d, *J* 4.2) | 3.94 (d, *J* 5.0) | -0.01 |

(9) Chen, M.; Lin, S.; Li, L.; Zhu, C.; Wang, X.; Wang, Y.; Jiang, B.; Wang, S.; Li, Y.; Jiang, J.; et al. *Org. Lett.* **2012**, *14*, 5668–5671.

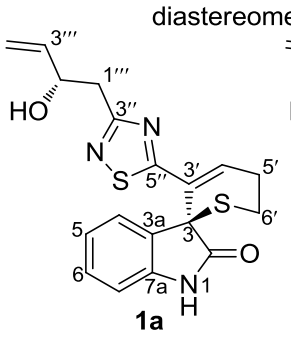
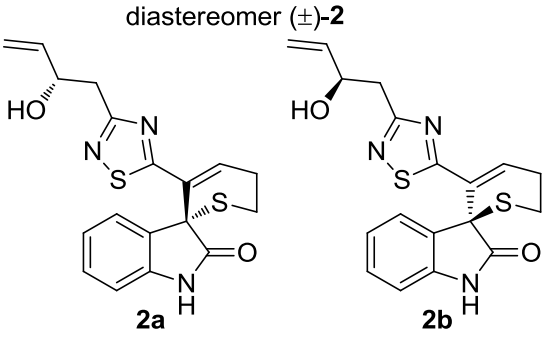
**Table S4.** $^{13}C$ NMR comparison of natural **1a/b**[9] with synthetic **1a/b**.




| C | Natural 1a/b[9] $\delta_C$ (acetone-$d_6$, 150 MHz) | Synthetic 1a/b $\delta_C$ (acetone-$d_6$, 100 MHz) | Δδ |
|---|---|---|---|
| **2** | 177.7 | 177.8 | +0.1 |
| **3** | 49.5 | 49.6 | +0.1 |
| **3a** | 130.3 | 130.4 | +0.1 |
| **4** | 125.2 | 125.3 | +0.1 |
| **5** | 122.9 | 122.9 | 0 |
| **6** | 130.5 | 130.5 | 0 |
| **7** | 110.9 | 111.0 | +0.1 |
| **7a** | 143.7 | 143.8 | +0.1 |
| **3'** | 128.6 | 128.7 | +0.1 |
| **4'** | 142.1 | 142.1 | 0 |
| **5'** | 27.8 | 27.8 | 0 |
| **6'** | 22.2 | 22.3 | +0.1 |
| **3''** | 174.1 | 174.2 | +0.1 |
| **5''** | 187.3 | 187.3 | 0 |
| **1'''** | 41.5 | 41.6 | +0.1 |
| **2'''** | 71.1 | 71.2 | +0.1 |
| **3'''** | 141.5 | 141.5 | 0 |
| **4'''** | 114.0 | 114.0 | 0 |

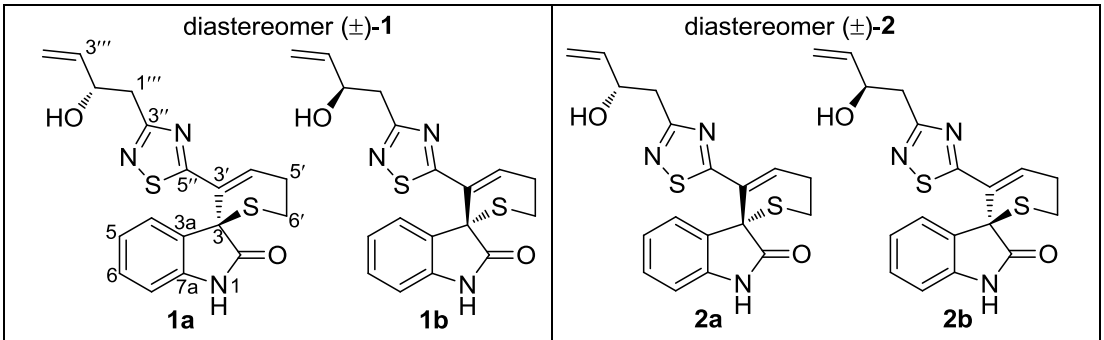
(9) Chen, M.; Lin, S.; Li, L.; Zhu, C.; Wang, X.; Wang, Y.; Jiang, B.; Wang, S.; Li, Y.; Jiang, J.; et al. *Org. Lett.* **2012**, *14*, 5668–5671.

**Table S5.** $^{1}$H NMR comparison of natural **1a/b**[9] with synthetic **2a/b**.

| | | | |
|---|---|---|---|
|  | |  | |
| **H** | **Natural 1a/b[9]**<br>**$\delta_H$ (acetone-$d_6$, 600 MHz)** | **Synthetic 2a/b**<br>**$\delta_H$ (acetone-$d_6$, 400 MHz)** | **Δδ** |
| **4** | 7.07 (dd, *J* 7.8, 1.2) | 7.09 (dd, *J* 7.5, 1.5) | +0.02 |
| **5** | 6.90 (ddd, *J* 1.2, 7.2, 7.8) | 6.92 (ddd, *J* 7.5, 7.5, 1.0) | +0.02 |
| **6** | 7.24 (ddd, *J* 1.2, 7.2, 7.8) | 7.27 (ddd, *J* 1.4, 7.7, 7.7) | +0.03 |
| **7** | 6.99 (dd, *J* 7.8, 1.2) | 7.02 (d, *J* 7.8) | +0.03 |
| **4'** | 7.40 (dd, *J* 4.8, 4.2) | 7.43 (t, *J* 4.4) | +0.03 |
| **5'a** | 2.84 (m) | 2.88 – 2.83 (unresolved) | +0.02 |
| **5'b** | 2.84 (m) | 2.88 – 2.83 (unresolved) | +0.02 |
| **6'a** | 3.76 (ddd, *J* 13.8, 8.4, 6.6) | 3.76 (ddd, *J* 14.0, 7.7, 6.3) | 0 |
| **6'b** | 2.74 (ddd, *J* 13.8, 4.2, 3.6) | 2.75 (dt, *J* 13.2, 4.0) | +0.01 |
| **1'''a** | 2.88 (dd, *J* 14.4, 6.6) | 2.88 – 2.83 (unresolved) | -0.02 |
| **1'''b** | 2.79 (dd, *J* 14.4, 6.6) | 2.83 – 2.77 (unresolved) | +0.01 |
| **2'''** | 4.31 (m) | 4.40 – 4.36 (m) | +0.07 |
| **3'''** | 5.63 (ddd, *J* 16.8, 10.8, 5.4) | 5.71 (ddd, *J* 17.3, 10.5, 5.5) | +0.08 |
| **4'''a** | 4.98 (ddd, *J* 16.8, 1.8, 1.2) | 5.11 (dt, *J* 17.2, 1.7) | +0.13 |
| **4'''b** | 4.86 (ddd, *J* 10.8, 1.8, 1.2) | 4.91 (dt, *J* 10.5, 1.7) | +0.05 |
| **1-NH** | 9.68 (br s) | 9.67 (br s) | -0.01 |
| **2'''-OH** | 3.95 (d, *J* 4.2) | 3.67 (br s) | -0.28 |

(9) Chen, M.; Lin, S.; Li, L.; Zhu, C.; Wang, X.; Wang, Y.; Jiang, B.; Wang, S.; Li, Y.; Jiang, J.; et al. *Org. Lett.* **2012**, *14*, 5668–5671.

**Table S6.** $^{13}C$ NMR comparison of natural **1a**/**b**[9] with synthetic **2a/b**.




| C | Natural 1a/b[9] $\delta_C$ (acetone-$d_6$, 150 MHz) | Synthetic 2a/b $\delta_C$ (acetone-$d_6$, 100 MHz) | Δδ |
|---|---|---|---|
| **2** | 177.7 | 177.7 | 0 |
| **3** | 49.5 | 49.6 | +0.1 |
| **3a** | 130.3 | 130.3 | 0 |
| **4** | 125.2 | 125.4 | +0.2 |
| **5** | 122.9 | 123.0 | +0.1 |
| **6** | 130.5 | 130.5 | 0 |
| **7** | 110.9 | 111.0 | +0.1 |
| **7a** | 143.7 | 143.8 | +0.1 |
| **3'** | 128.6 | 128.6 | 0 |
| **4'** | 142.1 | 142.1 | 0 |
| **5'** | 27.8 | 27.9 | +0.1 |
| **6'** | 22.2 | 22.3 | +0.1 |
| **3''** | 174.1 | 174.3 | +0.2 |
| **5''** | 187.3 | 187.2 | -0.1 |
| **1'''** | 41.5 | 41.4 | -0.1 |
| **2'''** | 71.1 | 71.3 | +0.2 |
| **3'''** | 141.5 | 141.6 | +0.1 |
| **4'''** | 114.0 | 114.2 | +0.2 |

(9) Chen, M.; Lin, S.; Li, L.; Zhu, C.; Wang, X.; Wang, Y.; Jiang, B.; Wang, S.; Li, Y.; Jiang, J.; et al. *Org. Lett.* **2012**, *14*, 5668–5671.

## DFT Calculations

### Computational Methods

DFT calculations were performed using the Gaussian 09 software package.[10] Geometry optimizations of starting materials, transition states and products were performed using the M06-2X[11] exchange-correlation functional and the 6-311G+(d,p) basis set. This level of theory was selected in order to account for dispersion effects, which are important in this context. All calculations employed tight convergence criteria and an ultrafine integration grid with symmetry turned off. Stationary points were characterised by normal mode vibrational frequency calculations. Transition states were further validated by performing intrinsic reaction coordinate (IRC) calculations. All calculations employed a polarizable continuum (PCM) model with dichloromethane as the solvent. Predicted free energy values were calculated as the sum of the electronic energy and the thermal correction to the Gibbs energy at 298.15 K. Gibbs free energy calculations were chosen in order to incorporate the effects of entropy on both barrier heights and reaction energies.


10. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

11. Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241.

## Calculated thio-Diels-Alder Reactions of 8 and 9

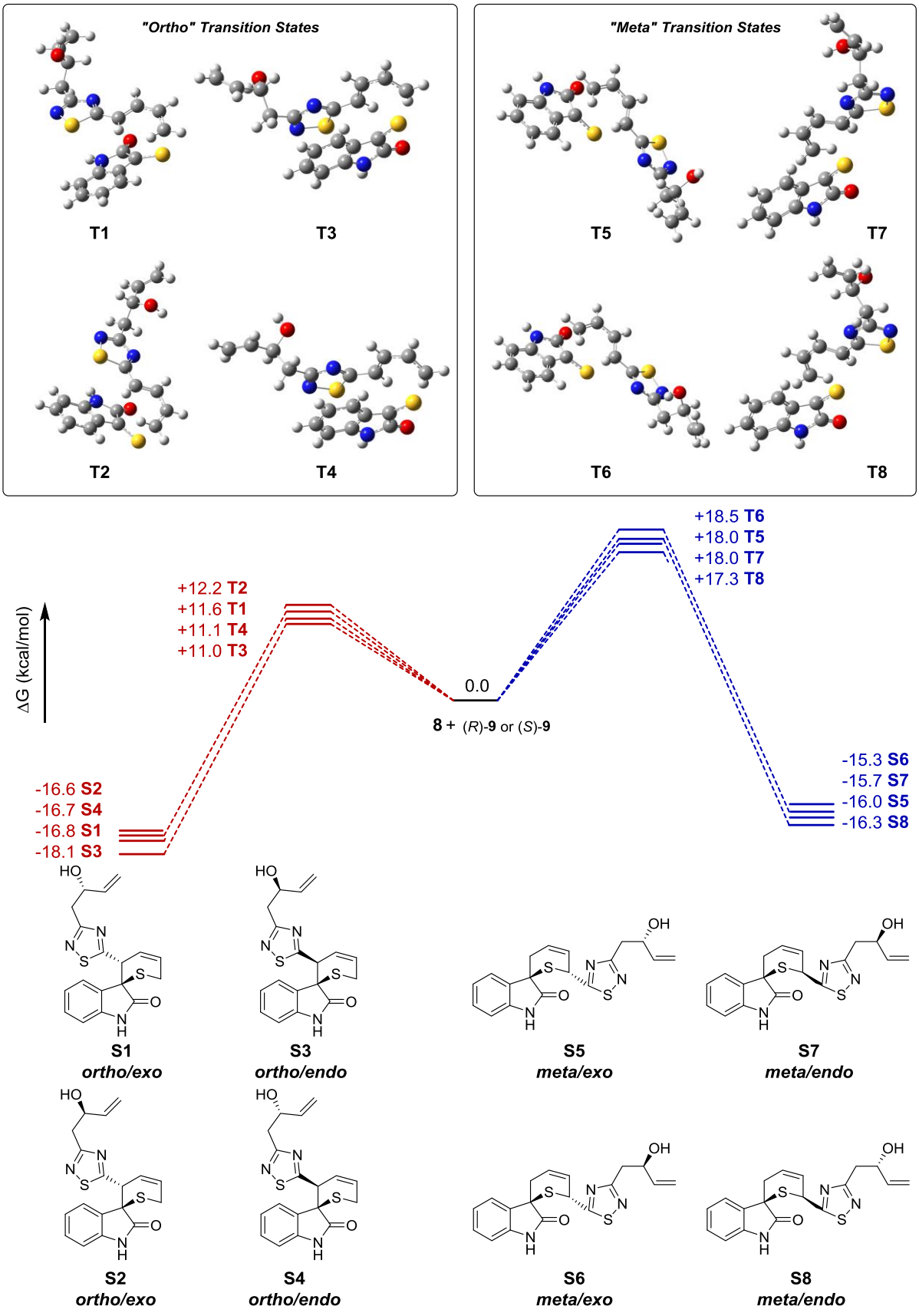



**Figure S1.** DFT computed Gibbs free energies and transition state structures for reaction of **8** and either (*R*)-**9** or (*S*)-**9**.

## Cartesian Coordinates (Å), Electronic Energies (*E*, Ha), and Thermal Corrections to Gibbs Free Energy ($G_C$, Ha)

### Reaction of 9 and 13

**9** $E$ = -835.972554, $G_C$ = 0.079840

| | | | |
|---|---|---|---|
| C | 1.29992600 | 0.73434200 | -0.01880000 |
| C | 2.27838900 | 0.36471800 | -0.94684000 |
| C | 2.19095400 | -0.81668600 | -1.68527100 |
| C | 1.08706500 | -1.62052900 | -1.46412700 |
| C | 0.09335600 | -1.26361600 | -0.53462200 |
| C | 0.19606800 | -0.08212600 | 0.19348700 |
| N | 0.75880800 | -2.84045300 | -2.06066600 |
| C | -0.42464100 | -3.33767900 | -1.57560600 |
| C | -0.91571500 | -2.30292300 | -0.53801000 |
| O | -0.96545500 | -4.36491300 | -1.89304600 |
| S | -2.28619200 | -2.45764000 | 0.30500400 |
| H | 1.40642000 | 1.65912100 | 0.53306800 |
| H | 3.13286000 | 1.01315900 | -1.10049400 |
| H | 2.95615100 | -1.08987000 | -2.40032100 |
| H | -0.57616900 | 0.18144700 | 0.90687900 |
| H | 1.31058000 | -3.31304200 | -2.76234100 |

**13** $E$ = -3313.405871, $G_C$ = 0.063139

| | | | |
|---|---|---|---|
| C | -0.23851900 | -4.16398000 | 1.26351600 |
| C | -2.62532000 | -5.67018700 | 2.37117400 |
| C | -1.16819200 | -3.68660200 | 2.10347200 |
| C | -2.44191200 | -4.34886900 | 2.39157500 |
| C | 1.02200700 | -3.47436800 | 1.04231800 |
| N | 1.40498800 | -2.36429100 | 1.63063600 |
| C | 2.63115700 | -2.03977600 | 1.15410000 |
| N | 3.23618300 | -2.77289800 | 0.27000900 |
| S | 2.21686000 | -4.04647800 | -0.06914400 |
| Br | 3.46919600 | -0.48164100 | 1.80308400 |
| H | -0.40447500 | -5.07864300 | 0.70426400 |
| H | -3.59350800 | -6.10319300 | 2.59019800 |
| H | -1.81106800 | -6.35506900 | 2.15885900 |
| H | -0.97906900 | -2.73585900 | 2.59398000 |
| H | -3.26586300 | -3.69864400 | 2.66966600 |

**TS1a** $E$ = -4149.387903, $G_C$ = 0.170054

| | | | |
|---|---|---|---|
| C | -0.76564100 | -0.21925900 | -0.00060400 |
| C | 0.15210900 | -0.51408400 | -1.00920600 |
| C | 0.04095400 | -1.67568200 | -1.77805600 |
| C | -1.01724000 | -2.52268100 | -1.50239700 |
| C | -1.95149900 | -2.24029800 | -0.48711100 |
| C | -1.82713800 | -1.08203600 | 0.26890700 |
| N | -1.33350600 | -3.75584200 | -2.08376300 |
| C | -2.43028400 | -4.33336200 | -1.48905300 |
| C | -2.88620700 | -3.35429500 | -0.44628100 |
| O | -2.90010200 | -5.42652300 | -1.74464800 |
| C | -1.07412300 | -4.74300100 | 1.22207900 |
| S | -4.28790200 | -3.52443400 | 0.39794100 |
| C | -3.91432600 | -5.39895200 | 1.58139800 |
| C | -1.79143200 | -4.40273400 | 2.33310300 |
| C | -3.13975800 | -4.77380000 | 2.54797100 |
| C | 0.20349800 | -4.12125700 | 0.95391900 |
| N | 0.64711500 | -3.03519000 | 1.55010300 |
| C | 1.83820700 | -2.71188800 | 0.99998000 |
| N | 2.36894800 | -3.42727700 | 0.05121800 |
| S | 1.31271700 | -4.67382300 | -0.25386500 |
| Br | 2.73886900 | -1.18200200 | 1.62934900 |
| H | -0.64510000 | 0.68378800 | 0.58479600 |
| H | 0.97511400 | 0.16491400 | -1.19786600 |
| H | 0.76222400 | -1.90878900 | -2.55193300 |
| H | -2.53813100 | -0.86809000 | 1.05893500 |
| H | -0.79878900 | -4.21134300 | -2.80963400 |
| H | -1.39386900 | -5.53259800 | 0.55201100 |
| H | -4.93739100 | -5.66553000 | 1.81814300 |
| H | -3.47300900 | -5.95050300 | 0.75853700 |
| H | -1.33401200 | -3.71897900 | 3.04058200 |
| H | -3.62607700 | -4.41709200 | 3.44841500 |

**TS1b** $E$ = -4149.384105, $G_C$ = 0.167503

| | | | |
|---|---|---|---|
| C | -0.82459900 | 1.19052800 | 0.56382000 |
| C | -1.38599600 | 0.12533200 | -0.14499600 |
| C | -0.59800600 | -0.90276600 | -0.66289700 |
| C | 0.77004700 | -0.82834200 | -0.45430700 |
| C | 1.34968600 | 0.23334200 | 0.26780100 |
| C | 0.54989000 | 1.24949700 | 0.78029400 |
| N | 1.77492100 | -1.70261700 | -0.86640200 |
| C | 3.02276700 | -1.29475100 | -0.43212600 |
| C | 2.77966400 | -0.01387000 | 0.32521900 |
| O | 4.06775200 | -1.87602300 | -0.62748000 |
| C | 3.19106600 | 1.19555000 | -2.10633000 |
| S | 3.94061600 | 0.72393000 | 1.23568800 |
| C | 4.25183200 | 2.66213400 | 0.18542100 |
| C | 4.52890400 | 1.39907400 | -1.91474700 |
| C | 5.04688000 | 2.12593600 | -0.82121400 |
| H | -1.46577500 | 1.97009000 | 0.95560800 |
| H | -2.45821300 | 0.09299300 | -0.29649800 |
| H | -1.03737300 | -1.72525400 | -1.21392600 |
| H | 0.99296000 | 2.05840900 | 1.35123800 |
| H | 1.62829600 | -2.56187700 | -1.37675900 |
| H | 3.20879900 | 2.90063600 | 0.01270200 |
| H | 5.22486300 | 0.88890000 | -2.57157900 |
| H | 6.12256100 | 2.14299900 | -0.68875600 |
| H | 2.44471500 | 1.77165600 | -1.57457900 |
| C | 2.69894200 | 0.32491600 | -3.15086000 |
| S | 1.03348300 | 0.26147500 | -3.60765100 |
| N | 3.42610500 | -0.52114300 | -3.84938200 |
| N | 1.32453300 | -0.92042800 | -4.73978300 |
| C | 2.60143600 | -1.17141200 | -4.70018400 |
| Br | 3.32734900 | -2.47210700 | -5.85297300 |
| H | 4.72334900 | 3.22604100 | 0.98108500 |

**TS2a** $E$ = -4149.374159, $G_C$ = 0.166627

| | | | |
|---|---|---|---|
| C | 0.80301700 | 0.65096800 | 0.04955300 |
| C | 2.14331600 | 0.26592500 | 0.08685200 |
| C | 2.51830400 | -1.07988200 | 0.06729900 |
| C | 1.50520700 | -2.02137900 | 0.01240800 |
| C | 0.15362400 | -1.64725100 | -0.02190600 |
| C | -0.20681400 | -0.30991600 | -0.00750000 |
| N | 1.59591500 | -3.41796600 | -0.01640100 |

| | | | |
|---|---|---|---|
| C | 0.36117600 | -4.01880100 | -0.08324100 |
| C | -0.64656000 | -2.87755400 | -0.06922800 |
| O | 0.14320600 | -5.20896700 | -0.13372500 |
| C | -0.83190700 | -3.30829500 | 2.23179600 |
| S | -2.18629500 | -3.02006700 | -0.67344700 |
| C | -3.55573800 | -3.29235700 | 1.31676800 |
| C | -1.70430700 | -2.30215600 | 2.56129200 |
| C | -3.02971200 | -2.27776300 | 2.09472600 |
| H | 0.54679600 | 1.70288900 | 0.06237900 |
| H | 2.91511200 | 1.02514600 | 0.12814400 |
| H | 3.56080100 | -1.37267900 | 0.09036900 |
| H | -1.25384600 | -0.02883300 | -0.04205900 |
| H | 2.45737200 | -3.94509000 | -0.02546900 |
| H | -1.17455800 | -4.28722800 | 1.91993000 |
| H | -3.16979000 | -4.30119800 | 1.38526100 |
| H | -1.32240800 | -1.41228600 | 3.04889700 |
| H | -3.61332100 | -1.37081100 | 2.21079100 |
| H | 0.20814500 | -3.24207700 | 2.53287800 |
| C | -4.89922500 | -3.16378400 | 0.75268700 |
| S | -5.76277100 | -4.48459600 | 0.05739100 |
| C | -6.76621900 | -2.31737000 | 0.08720500 |
| N | -7.06113700 | -3.51656000 | -0.31571200 |
| N | -5.57956600 | -2.04612700 | 0.68600300 |
| Br | -7.99884200 | -0.91746900 | -0.15894400 |

**TS2b** $E$ = -4149.373471, $G_C$ = 0.167284

| | | | |
|---|---|---|---|
| C | -2.53297200 | -0.62702300 | 1.35723200 |
| C | -2.95414200 | -1.79715400 | 0.72505600 |
| C | -2.06234100 | -2.83270100 | 0.43641200 |
| C | -0.73853000 | -2.65392500 | 0.79976300 |
| C | -0.30170000 | -1.48151600 | 1.43570400 |
| C | -1.19608300 | -0.46188700 | 1.71947000 |
| N | 0.34625100 | -3.52114300 | 0.63382100 |
| C | 1.50966400 | -3.00407500 | 1.15758700 |
| C | 1.14072200 | -1.62067200 | 1.67545500 |
| O | 2.58728500 | -3.55299200 | 1.19113800 |
| C | 1.71671000 | -0.68548400 | -0.40299700 |
| S | 2.05875400 | -0.83783200 | 2.81537200 |
| C | 3.08189600 | 0.92014200 | 1.54597800 |
| C | 3.08531300 | -0.65654600 | -0.32232400 |
| C | 3.75515600 | 0.12308000 | 0.63545000 |
| H | -3.25004000 | 0.15565600 | 1.57048800 |
| H | -3.99673700 | -1.91065500 | 0.45328000 |
| H | -2.39459600 | -3.74224200 | -0.04851500 |
| H | -0.85459200 | 0.43901700 | 2.21806500 |
| H | 0.29300300 | -4.44760200 | 0.23575000 |
| H | 1.22198100 | -1.37276100 | -1.08059100 |
| H | 2.10504100 | 1.33012300 | 1.32026000 |
| H | 3.66737000 | -1.37682600 | -0.88500100 |
| H | 4.82316300 | -0.02892100 | 0.76095900 |
| H | 1.10962000 | 0.13065400 | -0.03534400 |
| C | 3.78389300 | 1.65932600 | 2.59386600 |
| S | 5.30137600 | 1.19843200 | 3.28108200 |
| C | 4.19539100 | 3.15981300 | 4.08758200 |
| N | 5.29361800 | 2.50577000 | 4.31018000 |
| N | 3.30347400 | 2.74193900 | 3.15165500 |
| Br | 3.81522700 | 4.72059100 | 5.06612900 |

**16a** $E$ = -4149.435524, $G_C$ = 0.172634

| | | | |
|---|---|---|---|
| C | -1.72290000 | -0.01355900 | 0.01893600 |
| C | -1.09017100 | 0.06530800 | -1.22020200 |
| C | -0.98155400 | -1.04990100 | -2.05255900 |
| C | -1.51942400 | -2.23921900 | -1.59094800 |
| C | -2.14503100 | -2.33698100 | -0.34712400 |
| C | -2.26359000 | -1.22221000 | 0.46203100 |
| N | -1.54405400 | -3.49238400 | -2.22622700 |
| C | -2.12384000 | -4.45011500 | -1.45068600 |
| C | -2.58544700 | -3.76279200 | -0.14105800 |
| O | -2.21076200 | -5.63267200 | -1.69672200 |
| C | -1.86178700 | -4.50173300 | 1.04398100 |
| S | -4.41114000 | -3.89532800 | 0.00796300 |
| C | -4.57027000 | -4.81950500 | 1.59205800 |
| C | -2.38901000 | -4.06524900 | 2.38450500 |
| C | -3.68467300 | -4.22369500 | 2.63917300 |
| C | -0.37592200 | -4.30677600 | 0.92939100 |
| N | 0.28551800 | -3.34077600 | 1.50594800 |
| C | 1.59435900 | -3.45748500 | 1.15266800 |
| N | 1.99688500 | -4.41235500 | 0.37334900 |
| S | 0.65597100 | -5.31698500 | -0.01504700 |
| Br | 2.82536900 | -2.20021400 | 1.81901700 |
| H | -1.79856500 | 0.86968600 | 0.64055900 |
| H | -0.67782200 | 1.01098700 | -1.55091300 |
| H | -0.49724900 | -0.98755800 | -3.01907200 |
| H | -2.76618500 | -1.29169600 | 1.42005800 |
| H | -1.12690100 | -3.69680300 | -3.12385600 |
| H | -2.08121400 | -5.56401600 | 0.88269300 |
| H | -5.62556600 | -4.74610100 | 1.84851900 |
| H | -4.33361100 | -5.86885000 | 1.40506400 |
| H | -1.70380900 | -3.61241500 | 3.08966600 |
| H | -4.11936400 | -3.90206600 | 3.57856300 |

**16b** $E$ = -4149.433863, $G_C$ = 0.172024

| | | | |
|---|---|---|---|
| C | -0.20819600 | -0.48721600 | -0.37708800 |
| C | -0.60730700 | -1.81026700 | -0.55275300 |
| C | 0.32506400 | -2.83684800 | -0.71705900 |
| C | 1.66505500 | -2.48742000 | -0.70504800 |
| C | 2.07828100 | -1.16396300 | -0.54066000 |
| C | 1.14910000 | -0.15555700 | -0.36853200 |
| N | 2.78887600 | -3.30878600 | -0.85850200 |
| C | 3.96334500 | -2.60684000 | -0.78761800 |
| C | 3.57818900 | -1.10434200 | -0.67738200 |
| O | 5.07568900 | -3.07166600 | -0.82489700 |
| C | 3.98282500 | -0.36636800 | -2.01007500 |
| S | 4.37090000 | -0.31918200 | 0.77068500 |
| C | 5.54529700 | 0.85878700 | -0.02666100 |
| C | 5.47910000 | -0.30049700 | -2.17975200 |
| C | 6.20944100 | 0.27640400 | -1.23181600 |
| H | -0.95320200 | 0.28684600 | -0.24325100 |
| H | -1.66300300 | -2.05354400 | -0.55778300 |
| H | 0.01162100 | -3.86484000 | -0.84918200 |
| H | 1.47052700 | 0.87053600 | -0.22398800 |
| H | 2.76625700 | -4.31632200 | -0.93366300 |
| H | 4.98566900 | 1.76196300 | -0.27949300 |
| H | 5.92076800 | -0.76321300 | -3.05292100 |
| H | 7.29032900 | 0.31302100 | -1.30193700 |
| H | 3.57444000 | 0.64574100 | -1.90556600 |
| C | 3.31218400 | -1.02399900 | -3.18452700 |
| S | 1.79957000 | -0.52599200 | -3.84154000 |

| | | | |
|---|---|---|---|
| N | 3.79511200 | -2.06358400 | -3.80911500 |
| N | 1.82430000 | -1.73877100 | -4.97940600 |
| C | 2.91790600 | -2.40984800 | -4.79026100 |
| Br | 3.32034500 | -3.88806300 | -5.88177700 |
| H | 6.25923200 | 1.10898100 | 0.75595800 |

**17a** $E$ = -4149.432106, $G_C$ = 0.171102

| | | | |
|---|---|---|---|
| C | 0.16327800 | -0.14797100 | 0.11355100 |
| C | 1.40138300 | -0.50510300 | -0.41591200 |
| C | 1.74592700 | -1.84277700 | -0.61885600 |
| C | 0.81019800 | -2.80035200 | -0.26567600 |
| C | -0.43123000 | -2.45856700 | 0.27531900 |
| C | -0.76861800 | -1.13004600 | 0.45881700 |
| N | 0.90287100 | -4.19625700 | -0.37292500 |
| C | -0.22533200 | -4.82588000 | 0.06891800 |
| C | -1.19261200 | -3.72573300 | 0.57113200 |
| O | -0.42076700 | -6.01866000 | 0.10722800 |
| C | -1.40824100 | -3.97447000 | 2.08952700 |
| S | -2.76294400 | -3.80433800 | -0.37543800 |
| C | -3.97424100 | -4.08384200 | 1.01452700 |
| C | -2.48006500 | -3.09610000 | 2.66355800 |
| C | -3.70404800 | -3.13526500 | 2.14403800 |
| H | -0.08140100 | 0.89780200 | 0.25080100 |
| H | 2.11181800 | 0.26778200 | -0.68363400 |
| H | 2.70491500 | -2.11942100 | -1.03889300 |
| H | -1.74304800 | -0.86162400 | 0.85137800 |
| H | 1.69736300 | -4.69906900 | -0.74302000 |
| H | -1.67098200 | -5.03228300 | 2.20330200 |
| H | -3.84433100 | -5.12076300 | 1.33194600 |
| H | -2.23795300 | -2.41869800 | 3.47356800 |
| H | -4.50932600 | -2.49475600 | 2.48284700 |
| H | -0.45140100 | -3.81681900 | 2.58991100 |
| C | -5.33089900 | -3.91728600 | 0.40959500 |
| S | -6.23803000 | -5.21132500 | -0.27439700 |
| C | -7.14080500 | -3.00064900 | -0.31573200 |
| N | -7.48071100 | -4.19193000 | -0.70020300 |
| N | -5.95300400 | -2.77461800 | 0.30897800 |
| Br | -8.29798200 | -1.54862300 | -0.61319300 |

**17b** $E$ = -4149.437893, $G_C$ = 0.172178

| | | | |
|---|---|---|---|
| C | -0.47710000 | -1.15487400 | -1.05306700 |
| C | -0.61117700 | -2.13701700 | -0.07491000 |
| C | 0.48148100 | -2.56647400 | 0.68148600 |
| C | 1.70612300 | -1.97628400 | 0.42045000 |
| C | 1.85642300 | -0.99159700 | -0.55952400 |
| C | 0.76787100 | -0.56990900 | -1.30032400 |
| N | 2.94763600 | -2.22457200 | 1.01638500 |
| C | 3.94733100 | -1.47850700 | 0.45503900 |
| C | 3.29502900 | -0.54469000 | -0.58421000 |
| O | 5.12612400 | -1.54483000 | 0.72304400 |
| C | 3.96212900 | -0.62836100 | -1.95579300 |
| S | 3.30991200 | 1.16900200 | 0.08208500 |
| C | 5.08788200 | 1.56654200 | -0.04338700 |
| C | 5.25798500 | 0.11638600 | -2.10440200 |
| C | 5.74115400 | 1.05583800 | -1.29908700 |
| H | -1.34221200 | -0.84098800 | -1.62323000 |
| H | -1.58277100 | -2.58068800 | 0.10652400 |
| H | 0.37403400 | -3.33110500 | 1.44055900 |
| H | 0.87673400 | 0.20188700 | -2.05452500 |
| H | 3.12209200 | -2.91102400 | 1.73701700 |
| H | 4.12692000 | -1.68420800 | -2.19622600 |
| H | 5.07930000 | 2.66192500 | -0.08416600 |
| H | 5.83324400 | -0.13789600 | -2.98916100 |
| H | 6.68670500 | 1.52946200 | -1.55071900 |
| H | 3.25856400 | -0.25197400 | -2.70621100 |
| C | 5.87575000 | 1.21234300 | 1.19279600 |
| S | 7.49693100 | 0.62601700 | 1.13647200 |
| C | 6.45791600 | 0.99283200 | 3.25343000 |
| N | 7.59949200 | 0.58282200 | 2.79890300 |
| N | 5.45357200 | 1.36839600 | 2.41581100 |
| Br | 6.16196500 | 1.07768900 | 5.11260600 |

## Reaction of 8 and 9

**8** $E$ = -971.0546707, $G_C$ = 0.161944

| | | | |
|---|---|---|---|
| C | 1.71897400 | 0.46039700 | -3.17565800 |
| C | 2.94028100 | 1.58744200 | -0.63383000 |
| C | 3.02180500 | 0.51569800 | -2.86695700 |
| C | 3.58070800 | 1.31187900 | -1.77130400 |
| H | 1.94559600 | 1.20323800 | -0.43319600 |
| H | 3.71924000 | -0.05119800 | -3.47726300 |
| H | 4.59896700 | 1.66407000 | -1.90833400 |
| H | 0.99234700 | 1.05574400 | -2.63243500 |
| C | 1.21413500 | -0.37262400 | -4.25904600 |
| S | -0.46008300 | -0.42594800 | -4.68755900 |
| N | 1.92537700 | -1.15843200 | -5.02520100 |
| N | -0.17627300 | -1.51895700 | -5.90999500 |
| C | 1.10705300 | -1.77475600 | -5.93358300 |
| H | 3.40493100 | 2.18897600 | 0.13769700 |
| C | 1.69446000 | -2.72004000 | -6.93620500 |
| H | 2.13574100 | -3.57280800 | -6.41405000 |
| H | 0.89941000 | -3.08358000 | -7.58932700 |
| C | 2.77889700 | -2.04102700 | -7.77043000 |
| H | 3.57672200 | -1.69654600 | -7.10269800 |
| C | 3.34774300 | -2.98281200 | -8.79364300 |
| H | 2.63902200 | -3.36217100 | -9.52751200 |
| C | 4.62579800 | -3.34158100 | -8.83274200 |
| H | 5.33787400 | -2.96116000 | -8.10653900 |
| H | 5.00151800 | -4.02701700 | -9.58325500 |
| O | 2.15490400 | -0.92410200 | -8.39984300 |
| H | 2.81916200 | -0.46050200 | -8.91915100 |

**T1** $E$ = -1807.033400, $G_C$ = 0.266429

| | | | |
|---|---|---|---|
| C | -0.83409200 | 1.18836200 | 0.57642900 |
| C | -1.39016000 | 0.12493900 | -0.13882900 |
| C | -0.59745300 | -0.90078100 | -0.65479800 |
| C | 0.76903900 | -0.82525900 | -0.43810400 |
| C | 1.34341900 | 0.23491900 | 0.28990500 |
| C | 0.53950900 | 1.24847300 | 0.80047700 |
| N | 1.77786500 | -1.69793700 | -0.84321000 |
| C | 3.02353600 | -1.28483200 | -0.40810200 |
| C | 2.77429900 | -0.00830600 | 0.35023900 |
| O | 4.07044200 | -1.86554700 | -0.60230400 |
| C | 3.18149600 | 1.19795000 | -2.09324700 |
| S | 3.92695000 | 0.73936800 | 1.26428500 |
| C | 4.22268700 | 2.67308200 | 0.21047300 |
| C | 4.51566200 | 1.41268800 | -1.89151200 |
| C | 5.02328200 | 2.14317700 | -0.79524100 |
| H | -1.47828700 | 1.96632100 | 0.96661400 |
| H | -2.46138300 | 0.09196200 | -0.29724900 |

| | | | |
|---|---|---|---|
| H | -1.03239900 | -1.72157500 | -1.21184700 |
| H | 0.97846100 | 2.05699600 | 1.37523700 |
| H | 1.63835600 | -2.54451400 | -1.37590300 |
| H | 3.17785800 | 2.90203200 | 0.03507500 |
| H | 5.21868900 | 0.90858900 | -2.54539300 |
| H | 6.09856900 | 2.16985600 | -0.65972600 |
| H | 2.42810400 | 1.76486000 | -1.56124200 |
| C | 2.70335900 | 0.32740900 | -3.14829100 |
| S | 1.04143100 | 0.24978400 | -3.61338000 |
| N | 3.43571600 | -0.50498700 | -3.84782000 |
| N | 1.35274600 | -0.91778400 | -4.75079700 |
| C | 2.63909500 | -1.17941400 | -4.72750200 |
| H | 4.68858900 | 3.24500900 | 1.00373200 |
| C | 3.24359000 | -2.19163100 | -5.65139400 |
| H | 3.69616900 | -2.99302100 | -5.06216300 |
| C | 4.32075600 | -1.56244900 | -6.53311300 |
| H | 5.10858200 | -1.15099800 | -5.89189500 |
| C | 4.91217200 | -2.57314500 | -7.47449000 |
| O | 3.67972300 | -0.51173900 | -7.25294700 |
| H | 4.21465000 | -3.02373500 | -8.17822700 |
| C | 6.19683200 | -2.90962600 | -7.47893800 |
| H | 4.33731600 | -0.08238600 | -7.80893300 |
| H | 6.89733300 | -2.45884300 | -6.78239400 |
| H | 6.58948200 | -3.64623900 | -8.16993800 |
| H | 2.45714600 | -2.61687300 | -6.27688400 |

**T2** $E$ = -1807.032656, $G_C$ = 0.266742

| | | | |
|---|---|---|---|
| C | -0.80167500 | 1.22019600 | 0.59190600 |
| C | -1.37879200 | 0.15031100 | -0.09649600 |
| C | -0.60363800 | -0.89026600 | -0.60942200 |
| C | 0.76696300 | -0.82311500 | -0.41705500 |
| C | 1.36244900 | 0.24290200 | 0.28497200 |
| C | 0.57593200 | 1.27166500 | 0.79227300 |
| N | 1.76148200 | -1.71044900 | -0.82575900 |
| C | 3.01770500 | -1.30181000 | -0.41767800 |
| C | 2.79203500 | -0.01226100 | 0.32634300 |
| O | 4.05603600 | -1.89449000 | -0.62101700 |
| C | 3.16722800 | 1.15649500 | -2.13996300 |
| S | 3.96543600 | 0.73789500 | 1.21103800 |
| C | 4.26403900 | 2.65592900 | 0.12153300 |
| C | 4.50675200 | 1.36188300 | -1.96602800 |
| C | 5.04106000 | 2.10326600 | -0.88969300 |
| H | -1.43254100 | 2.00995700 | 0.98014300 |
| H | -2.45282300 | 0.12406600 | -0.23605200 |
| H | -1.05507000 | -1.71623700 | -1.14533800 |
| H | 1.03127000 | 2.08533700 | 1.34665700 |
| H | 1.60624300 | -2.56408000 | -1.34255200 |
| H | 3.21811600 | 2.89112600 | -0.03795500 |
| H | 5.19320600 | 0.84272600 | -2.62561800 |
| H | 6.11886400 | 2.12156100 | -0.77420600 |
| H | 2.42918500 | 1.73766700 | -1.60185600 |
| C | 2.66176800 | 0.27610200 | -3.17330500 |
| S | 0.99304100 | 0.20902000 | -3.60993800 |
| N | 3.37526000 | -0.57316200 | -3.87521700 |
| N | 1.27202400 | -0.97491900 | -4.73476500 |
| C | 2.55771600 | -1.24848700 | -4.73213500 |
| H | 4.74920300 | 3.23396400 | 0.89863500 |
| C | 3.12284900 | -2.25197600 | -5.68994500 |
| H | 4.10284100 | -2.57586300 | -5.33106400 |
| C | 3.26492600 | -1.64878300 | -7.09821400 |
| H | 2.26901200 | -1.34046200 | -7.43263100 |
| C | 3.80319400 | -2.68070500 | -8.05392700 |
| O | 4.03056800 | -0.46079300 | -7.07120700 |
| H | 3.24777700 | -3.61524800 | -8.08444900 |
| C | 4.87630700 | -2.51642700 | -8.81798300 |
| H | 4.89047600 | -0.65645100 | -6.68137400 |
| H | 5.43651800 | -1.58798600 | -8.81512300 |
| H | 5.21852000 | -3.30414400 | -9.47806000 |
| H | 2.46709700 | -3.12313600 | -5.73884900 |

**T3** $E$ = -1807.036982, $G_C$ = 0.269004

| | | | |
|---|---|---|---|
| C | -0.76857800 | -0.20483800 | 0.02934300 |
| C | 0.12635600 | -0.47920500 | -1.00541700 |
| C | 0.00376300 | -1.63107700 | -1.78688400 |
| C | -1.04136700 | -2.48916300 | -1.49697200 |
| C | -1.95191500 | -2.22841000 | -0.45447900 |
| C | -1.81662600 | -1.07979800 | 0.31344900 |
| N | -1.37028600 | -3.71065000 | -2.09458000 |
| C | -2.44727500 | -4.30496200 | -1.48007300 |
| C | -2.88209800 | -3.34663200 | -0.41140300 |
| O | -2.91586400 | -5.39773900 | -1.74227700 |
| C | -1.02358800 | -4.75001700 | 1.19047100 |
| S | -4.26755900 | -3.53467700 | 0.45699500 |
| C | -3.85523400 | -5.41154700 | 1.62876200 |
| C | -1.70936100 | -4.41946000 | 2.32326100 |
| C | -3.05220600 | -4.79052200 | 2.57337900 |
| C | 0.25396700 | -4.13344300 | 0.89614100 |
| N | 0.72584600 | -3.06450300 | 1.48999200 |
| C | 1.91614100 | -2.71485500 | 0.92290000 |
| N | 2.39458500 | -3.44598500 | -0.05694400 |
| S | 1.32185500 | -4.67677300 | -0.35173800 |
| H | -0.64423800 | 0.69399200 | 0.62093300 |
| H | 0.93749600 | 0.21039500 | -1.20841300 |
| H | 0.70602300 | -1.84812100 | -2.58253700 |
| H | -2.51015100 | -0.88094100 | 1.12281200 |
| H | -0.84014500 | -4.16025000 | -2.82735400 |
| H | -1.36800900 | -5.52980800 | 0.52097900 |
| H | -4.87059700 | -5.67983600 | 1.89498600 |
| H | -3.43742300 | -5.95890200 | 0.79105500 |
| H | -1.23030000 | -3.74269700 | 3.02293400 |
| H | -3.51235400 | -4.43817700 | 3.48941600 |
| C | 2.65637400 | -1.52211600 | 1.43916500 |
| H | 3.53066200 | -1.33889400 | 0.81005800 |
| C | 3.09578400 | -1.72988100 | 2.89711600 |
| H | 2.19952600 | -1.92520300 | 3.49437200 |
| C | 3.76991400 | -0.48887400 | 3.41994100 |
| O | 3.88942200 | -2.89284100 | 3.02872900 |
| H | 3.19717200 | 0.42884500 | 3.30804200 |
| C | 4.97460200 | -0.45941500 | 3.97718800 |
| H | 4.66875200 | -2.79830600 | 2.46880800 |
| H | 5.55809700 | -1.36304100 | 4.11479000 |
| H | 5.40732600 | 0.47103500 | 4.32405800 |
| H | 2.00057000 | -0.64876100 | 1.38125100 |

**T4** $E$ = -1807.035641, $G_C$ = 0.267940

| | | | |
|---|---|---|---|
| C | -0.76714300 | -0.21486500 | 0.01621200 |
| C | 0.12779300 | -0.49590400 | -1.01641300 |
| C | 0.00221600 | -1.65027400 | -1.79408900 |
| C | -1.04638000 | -2.50348300 | -1.50257700 |
| C | -1.95902600 | -2.23447800 | -0.46393500 |

| | | | |
|---|---|---|---|
| C | -1.82016300 | -1.08404800 | 0.30036000 |
| N | -1.37890000 | -3.72636200 | -2.09572500 |
| C | -2.46040400 | -4.31327300 | -1.48196900 |
| C | -2.89455800 | -3.34836600 | -0.41927900 |
| O | -2.93289300 | -5.40522200 | -1.74146900 |
| C | -1.05156200 | -4.75393300 | 1.19386100 |
| S | -4.28582000 | -3.52446900 | 0.44284200 |
| C | -3.88742900 | -5.39316800 | 1.63346200 |
| C | -1.73661800 | -4.40862600 | 2.32283900 |
| C | -3.08185900 | -4.76960900 | 2.57417400 |
| C | 0.22823300 | -4.14575300 | 0.89296900 |
| N | 0.69864700 | -3.06566700 | 1.47020000 |
| C | 1.89005500 | -2.72693000 | 0.90234100 |
| N | 2.36916100 | -3.47732200 | -0.06467900 |
| S | 1.30030000 | -4.71169500 | -0.33868300 |
| H | -0.63901000 | 0.68442200 | 0.60604700 |
| H | 0.94034600 | 0.19118500 | -1.22172300 |
| H | 0.70470600 | -1.87257100 | -2.58812000 |
| H | -2.51416000 | -0.87969300 | 1.10794800 |
| H | -0.84897000 | -4.18129500 | -2.82532000 |
| H | -1.39949700 | -5.53877600 | 0.53204800 |
| H | -4.90496600 | -5.65265300 | 1.90013800 |
| H | -3.47162100 | -5.95027700 | 0.80120900 |
| H | -1.25459600 | -3.72743100 | 3.01615200 |
| H | -3.54136200 | -4.40612600 | 3.48620700 |
| C | 2.64864900 | -1.52248100 | 1.37564200 |
| H | 2.86325000 | -0.87165900 | 0.52556300 |
| C | 3.96702100 | -1.91730400 | 2.03972200 |
| H | 4.58063100 | -2.45868300 | 1.31000800 |
| C | 4.71332100 | -0.70887100 | 2.52958500 |
| O | 3.62705200 | -2.77800600 | 3.12426100 |
| H | 4.20021600 | -0.11491700 | 3.28375900 |
| C | 5.92161300 | -0.36534100 | 2.09862000 |
| H | 4.44106600 | -3.05673100 | 3.55512700 |
| H | 6.44033200 | -0.95794700 | 1.35103800 |
| H | 6.42913600 | 0.51642300 | 2.47169700 |
| H | 2.02785400 | -0.97428300 | 2.08678100 |

**T5** $E$ = -1807.023420, $G_C$ = 0.266620

| | | | |
|---|---|---|---|
| C | -2.49890900 | -0.55814200 | 1.32768700 |
| C | -2.94217800 | -1.72473100 | 0.70424800 |
| C | -2.07242800 | -2.78423600 | 0.43545500 |
| C | -0.74809200 | -2.63288100 | 0.80933800 |
| C | -0.28883400 | -1.46419400 | 1.43669500 |
| C | -1.16167700 | -0.42084200 | 1.70081800 |
| N | 0.31723200 | -3.52664100 | 0.66302900 |
| C | 1.48843600 | -3.03005000 | 1.19124900 |
| C | 1.14781500 | -1.63385400 | 1.68953100 |
| O | 2.55159300 | -3.60615400 | 1.24071300 |
| C | 1.75752900 | -0.73987800 | -0.41079300 |
| S | 2.07952700 | -0.84940500 | 2.81662200 |
| C | 3.11631600 | 0.88669200 | 1.53451600 |
| C | 3.12436400 | -0.72187700 | -0.31019900 |
| C | 3.78959300 | 0.06648200 | 0.64457200 |
| H | -3.19903800 | 0.24371500 | 1.52567100 |
| H | -3.98461300 | -1.81648400 | 0.42375000 |
| H | -2.42165900 | -3.69103400 | -0.04270700 |
| H | -0.80361900 | 0.47703100 | 2.19326900 |
| H | 0.24628900 | -4.45565400 | 0.27397500 |
| H | 1.26570300 | -1.43308200 | -1.08444800 |
| H | 2.14262800 | 1.29514100 | 1.29202400 |
| H | 3.70734300 | -1.45612800 | -0.85383800 |
| H | 4.85440500 | -0.09376600 | 0.78580500 |
| H | 1.15234900 | 0.08509600 | -0.06024700 |
| C | 3.81335100 | 1.64466600 | 2.57456000 |
| S | 5.34237700 | 1.21342600 | 3.25505700 |
| C | 4.20764900 | 3.18932100 | 4.06765700 |
| N | 5.31809200 | 2.52928700 | 4.27092000 |
| N | 3.32559300 | 2.72135000 | 3.12670000 |
| C | 3.88818800 | 4.43951000 | 4.82729300 |
| H | 2.99126000 | 4.27667000 | 5.43026800 |
| C | 3.63912000 | 5.61407300 | 3.88271100 |
| H | 2.78473200 | 5.37717700 | 3.23848900 |
| C | 3.35936600 | 6.87666900 | 4.64754800 |
| O | 4.82017800 | 5.74688300 | 3.09524500 |
| H | 4.16189000 | 7.21903500 | 5.29820900 |
| C | 2.22311700 | 7.55732300 | 4.55143700 |
| H | 4.69163700 | 6.47397300 | 2.47822500 |
| H | 1.42197200 | 7.22282800 | 3.89923700 |
| H | 2.05301900 | 8.46324500 | 5.12115600 |
| H | 4.72009000 | 4.67014500 | 5.49466100 |

**T6** $E$ = -1807.022627, $G_C$ = 0.266621

| | | | |
|---|---|---|---|
| C | -2.51504700 | -0.57255600 | 1.37158000 |
| C | -2.94886800 | -1.72747100 | 0.72032800 |
| C | -2.06852700 | -2.76870700 | 0.41709300 |
| C | -0.74335900 | -2.61138400 | 0.78563000 |
| C | -0.29361100 | -1.45422800 | 1.44064600 |
| C | -1.17685700 | -0.42897200 | 1.73870000 |
| N | 0.33150000 | -3.48816300 | 0.60811800 |
| C | 1.50015600 | -2.99192700 | 1.14194400 |
| C | 1.14661300 | -1.61389000 | 1.68020700 |
| O | 2.57102200 | -3.55505600 | 1.16852000 |
| C | 1.73215900 | -0.65403900 | -0.39371100 |
| S | 2.07593300 | -0.85227000 | 2.82485000 |
| C | 3.11456200 | 0.91714900 | 1.58148400 |
| C | 3.10004100 | -0.63966800 | -0.30727000 |
| C | 3.77641100 | 0.11994500 | 0.66285100 |
| H | -3.22327500 | 0.21513700 | 1.59583400 |
| H | -3.99217500 | -1.82440600 | 0.44485900 |
| H | -2.41041800 | -3.66653000 | -0.08281600 |
| H | -0.82562400 | 0.45997800 | 2.25181400 |
| H | 0.26874800 | -4.40728700 | 0.19484800 |
| H | 1.23287000 | -1.32635800 | -1.08286200 |
| H | 2.14066100 | 1.33655700 | 1.35945800 |
| H | 3.67634100 | -1.35852900 | -0.87784800 |
| H | 4.84204900 | -0.04716400 | 0.78905300 |
| H | 1.13124300 | 0.16028400 | -0.01235200 |
| C | 3.82405800 | 1.63960300 | 2.63769700 |
| S | 5.34548900 | 1.16829800 | 3.30542000 |
| C | 4.24288500 | 3.13999100 | 4.16770000 |
| N | 5.34255400 | 2.45447800 | 4.35428500 |
| N | 3.35325000 | 2.71117800 | 3.21754900 |
| C | 3.98280100 | 4.39711400 | 4.93837500 |
| H | 2.91299500 | 4.61869500 | 4.91206600 |
| C | 4.76683600 | 5.57888300 | 4.34093300 |
| H | 5.83239000 | 5.33210600 | 4.39068500 |
| C | 4.51632400 | 6.82784600 | 5.14398800 |
| O | 4.48688700 | 5.73470600 | 2.96423300 |
| H | 4.70066000 | 6.73446300 | 6.21171000 |

| | | | |
|---|---|---|---|
| C | 4.09317900 | 7.97956700 | 4.63720800 |
| H | 3.53785600 | 5.86522200 | 2.85455700 |
| H | 3.91842400 | 8.10032200 | 3.57385400 |
| H | 3.92154600 | 8.84019400 | 5.27214400 |
| H | 4.28209100 | 4.25785900 | 5.97853700 |

**T7** $E$ = -1807.023202, $G_C$ = 0.266437

| | | | |
|---|---|---|---|
| C | 0.76385800 | 0.66788400 | 0.06310400 |
| C | 2.10652500 | 0.29441300 | 0.12484300 |
| C | 2.49282400 | -1.04834200 | 0.11627000 |
| C | 1.48878400 | -1.99858200 | 0.04678500 |
| C | 0.13462000 | -1.63624300 | -0.01238500 |
| C | -0.23677600 | -0.30181700 | -0.00847400 |
| N | 1.59122100 | -3.39412000 | 0.02491600 |
| C | 0.36190700 | -4.00512300 | -0.06054700 |
| C | -0.65431100 | -2.87314100 | -0.06895900 |
| O | 0.15632100 | -5.19783900 | -0.11016200 |
| C | -0.86635700 | -3.29880500 | 2.24091500 |
| S | -2.18704300 | -3.02953400 | -0.68625100 |
| C | -3.58413900 | -3.31030600 | 1.28529700 |
| C | -1.75245500 | -2.29847300 | 2.54778200 |
| C | -3.07151200 | -2.28731900 | 2.06092100 |
| H | 0.49867000 | 1.71768300 | 0.06811700 |
| H | 2.87112600 | 1.06023000 | 0.17707700 |
| H | 3.53715700 | -1.33232300 | 0.15865300 |
| H | -1.28543400 | -0.02981400 | -0.06188300 |
| H | 2.45667400 | -3.91456300 | 0.03345900 |
| H | -1.19550900 | -4.28096000 | 1.92487000 |
| H | -3.18787400 | -4.31466700 | 1.36319900 |
| H | -1.38555900 | -1.40222800 | 3.03556700 |
| H | -3.66346800 | -1.38412400 | 2.16276700 |
| H | 0.16782000 | -3.22250500 | 2.55927700 |
| C | -4.92391700 | -3.19540800 | 0.70604100 |
| S | -5.77601100 | -4.53060600 | 0.02786200 |
| C | -6.81050800 | -2.34894000 | 0.01015000 |
| N | -7.07139000 | -3.57620600 | -0.36982800 |
| N | -5.61072600 | -2.08728300 | 0.61362100 |
| C | -7.82403300 | -1.26124300 | -0.16799900 |
| H | -7.32108800 | -0.29215000 | -0.12321800 |
| C | -8.90239000 | -1.33047100 | 0.92762200 |
| H | -9.39370000 | -2.30600900 | 0.85259500 |
| C | -9.92832700 | -0.24877500 | 0.71535700 |
| O | -8.32340700 | -1.30568800 | 2.21691000 |
| H | -10.37815500 | -0.22754000 | -0.27452800 |
| C | -10.28652900 | 0.64349300 | 1.63074900 |
| H | -7.80502600 | -0.49767200 | 2.30672900 |
| H | -9.86387800 | 0.63214000 | 2.62927800 |
| H | -11.02463800 | 1.40496000 | 1.41015900 |
| H | -8.29916800 | -1.35993900 | -1.14547900 |

**T8** $E$ = -1807.024011, $G_C$ = 0.266084

| | | | |
|---|---|---|---|
| C | 0.83811200 | 0.66148800 | 0.11759000 |
| C | 2.17410100 | 0.26053900 | 0.13467000 |
| C | 2.53316000 | -1.08845000 | 0.07289400 |
| C | 1.50897200 | -2.01645600 | -0.00359400 |
| C | 0.16126200 | -1.62640700 | -0.01721000 |
| C | -0.18311400 | -0.28595500 | 0.03918000 |
| N | 1.58286800 | -3.41212600 | -0.07536700 |
| C | 0.33982200 | -3.99573600 | -0.15488700 |
| C | -0.65305300 | -2.84549100 | -0.09628500 |
| O | 0.10893800 | -5.18152300 | -0.24585400 |
| C | -0.81017400 | -3.33867400 | 2.21063800 |
| S | -2.20488500 | -2.95222900 | -0.67369500 |
| C | -3.54664100 | -3.31443100 | 1.31503000 |
| C | -1.68544300 | -2.34573200 | 2.56739500 |
| C | -3.01535100 | -2.31663400 | 2.11077300 |
| H | 0.59406800 | 1.71545500 | 0.16282600 |
| H | 2.95490000 | 1.00937400 | 0.19314600 |
| H | 3.57232100 | -1.39380400 | 0.08036600 |
| H | -1.22706900 | 0.00765700 | 0.02010800 |
| H | 2.43785400 | -3.94865200 | -0.10798000 |
| H | -1.14998900 | -4.30993500 | 1.87289700 |
| H | -3.14910300 | -4.32063600 | 1.35223300 |
| H | -1.30458800 | -1.46539200 | 3.07310100 |
| H | -3.60268300 | -1.41585800 | 2.25305700 |
| H | 0.23187800 | -3.27414000 | 2.50500300 |
| C | -4.89972500 | -3.18424200 | 0.77007300 |
| S | -5.77204200 | -4.50784400 | 0.09196100 |
| C | -6.79835300 | -2.32138200 | 0.12753500 |
| N | -7.07499300 | -3.54111400 | -0.26021200 |
| N | -5.58259700 | -2.07350300 | 0.70853600 |
| C | -7.78051900 | -1.20451100 | -0.04685600 |
| H | -7.36165700 | -0.45863800 | -0.72714200 |
| C | -8.09882700 | -0.53061200 | 1.28643100 |
| H | -7.17497300 | -0.11375400 | 1.70340000 |
| C | -9.11350800 | 0.56380000 | 1.11272500 |
| O | -8.59832000 | -1.55732100 | 2.14017100 |
| H | -10.08344300 | 0.24815400 | 0.73287700 |
| C | -8.87674600 | 1.83835000 | 1.40071100 |
| H | -8.79753300 | -1.16764500 | 2.99715500 |
| H | -7.91259700 | 2.15720800 | 1.78519300 |
| H | -9.63117700 | 2.60309600 | 1.25857000 |
| H | -8.69523500 | -1.60392200 | -0.48766900 |

**S1** $E$ = -1807.083608, $G_C$ = 0.271342

| | | | |
|---|---|---|---|
| C | -1.14083400 | -0.71123900 | -0.57486500 |
| C | -1.39884000 | -2.05166800 | -0.85306900 |
| C | -0.36309900 | -2.96152400 | -1.07548400 |
| C | 0.93321100 | -2.47768000 | -1.01522100 |
| C | 1.20517800 | -1.13423700 | -0.75001200 |
| C | 0.17450700 | -0.24308600 | -0.52038200 |
| N | 2.13743800 | -3.16747500 | -1.19877200 |
| C | 3.23173000 | -2.35465100 | -1.06458900 |
| C | 2.69281100 | -0.91190900 | -0.85114900 |
| O | 4.38671900 | -2.70103400 | -1.11333500 |
| C | 3.03820400 | -0.02841100 | -2.10715800 |
| S | 3.37819200 | -0.17050400 | 0.67375500 |
| C | 4.47677100 | 1.15009000 | -0.00028400 |
| C | 4.52525100 | 0.17616600 | -2.24413100 |
| C | 5.19776900 | 0.72483400 | -1.23837200 |
| H | -1.96348000 | -0.03001400 | -0.39764600 |
| H | -2.42348400 | -2.40133400 | -0.89339000 |
| H | -0.56570700 | -4.00439100 | -1.28519000 |
| H | 0.38628000 | 0.79738700 | -0.29763500 |
| H | 2.21852900 | -4.16259700 | -1.35334500 |
| H | 3.85567900 | 2.02873400 | -0.18739100 |
| H | 5.01138900 | -0.17278300 | -3.14634800 |
| H | 6.27290300 | 0.85366500 | -1.28616300 |
| H | 2.54604000 | 0.93290400 | -1.91751100 |
| C | 2.43636500 | -0.63204600 | -3.34665900 |

| | | | |
|---|---|---|---|
| S | 0.94758700 | -0.12079500 | -4.04598000 |
| N | 2.96277000 | -1.62194600 | -4.00602000 |
| N | 1.05189100 | -1.26539300 | -5.24731600 |
| C | 2.15089400 | -1.94902000 | -5.06588500 |
| H | 5.16047600 | 1.38374700 | 0.81385000 |
| C | 2.54708100 | -3.06424100 | -5.98301300 |
| H | 2.55781200 | -4.00376200 | -5.42418600 |
| C | 3.93611000 | -2.82996500 | -6.57361700 |
| H | 4.66280300 | -2.76539600 | -5.75603500 |
| C | 4.32416700 | -3.94108900 | -7.50756300 |
| O | 3.86790500 | -1.58396600 | -7.26376300 |
| H | 3.68181600 | -4.07030400 | -8.37669300 |
| C | 5.37850200 | -4.72578100 | -7.31690300 |
| H | 4.73711800 | -1.39415500 | -7.63037800 |
| H | 6.02516000 | -4.59678600 | -6.45416000 |
| H | 5.62738200 | -5.52201600 | -8.00851400 |
| H | 1.81122100 | -3.14348700 | -6.78487200 |

**S2** $E$ = -1807.082746, $G_C$ = 0.270939

| | | | |
|---|---|---|---|
| C | -1.08830200 | -0.76154200 | -0.53642400 |
| C | -1.42440600 | -2.09760800 | -0.74271600 |
| C | -0.44489100 | -3.07208400 | -0.94630200 |
| C | 0.87631900 | -2.65688400 | -0.94164100 |
| C | 1.22593800 | -1.31940000 | -0.74716400 |
| C | 0.25106600 | -0.36352900 | -0.53624500 |
| N | 2.03776300 | -3.41694000 | -1.12717000 |
| C | 3.17627100 | -2.65844100 | -1.05320500 |
| C | 2.71903500 | -1.18145500 | -0.89911400 |
| O | 4.31024800 | -3.06683900 | -1.11056300 |
| C | 3.06969600 | -0.38528300 | -2.21225900 |
| S | 3.48828300 | -0.40437200 | 0.56600800 |
| C | 4.60533900 | 0.84522300 | -0.20454800 |
| C | 4.55910500 | -0.24462500 | -2.39444200 |
| C | 5.27710800 | 0.33139500 | -1.43655100 |
| H | -1.86865000 | -0.02911800 | -0.37267500 |
| H | -2.46693900 | -2.39241400 | -0.74104400 |
| H | -0.70883800 | -4.11091400 | -1.10139200 |
| H | 0.52387300 | 0.67310300 | -0.36885400 |
| H | 2.06379500 | -4.42174800 | -1.22904600 |
| H | 4.00639300 | 1.73250000 | -0.42079600 |
| H | 5.00805700 | -0.65649900 | -3.28917700 |
| H | 6.35435200 | 0.41869300 | -1.51851200 |
| H | 2.61742400 | 0.60321400 | -2.06829900 |
| C | 2.41767900 | -1.03517300 | -3.40287300 |
| S | 0.89075100 | -0.56622800 | -4.04622100 |
| N | 2.92673300 | -2.03935600 | -4.05701000 |
| N | 0.95350900 | -1.74436900 | -5.21351900 |
| C | 2.07179700 | -2.40749600 | -5.06643900 |
| H | 5.31849300 | 1.09847700 | 0.57787200 |
| C | 2.44614200 | -3.51069700 | -6.00661300 |
| H | 3.16198900 | -4.17334000 | -5.51345900 |
| C | 3.07470500 | -2.95002700 | -7.29495400 |
| H | 2.33447600 | -2.30093000 | -7.77416600 |
| C | 3.41876800 | -4.07544900 | -8.23478500 |
| O | 4.17327800 | -2.10914600 | -7.00580700 |
| H | 2.59695800 | -4.74809300 | -8.46926500 |
| C | 4.62150900 | -4.28207300 | -8.75727000 |
| H | 4.81058100 | -2.60367900 | -6.47751400 |
| H | 5.45080600 | -3.61519500 | -8.54918400 |
| H | 4.80745900 | -5.11917800 | -9.41908000 |
| H | 1.55796000 | -4.08971500 | -6.26466400 |

**S3** $E$ = -1807.085264, $G_C$ = 0.271004

| | | | |
|---|---|---|---|
| C | -1.47812400 | -0.75009200 | -0.19350700 |
| C | -0.92448200 | -0.65659100 | -1.46895500 |
| C | -0.73816700 | -1.78862000 | -2.26422800 |
| C | -1.11657500 | -3.00826600 | -1.72901000 |
| C | -1.66167100 | -3.11936600 | -0.44881600 |
| C | -1.85844100 | -1.99018200 | 0.32388600 |
| N | -1.03806400 | -4.28210500 | -2.31525000 |
| C | -1.46705200 | -5.26298900 | -1.47202800 |
| C | -1.93194500 | -4.57392000 | -0.16490600 |
| O | -1.44177100 | -6.45661000 | -1.67311400 |
| C | -1.07571100 | -5.17773400 | 1.00782100 |
| S | -3.72431400 | -4.89357100 | 0.08143000 |
| C | -3.70849000 | -5.76337300 | 1.70386700 |
| C | -1.58825500 | -4.74688900 | 2.35576900 |
| C | -2.84532100 | -5.03335400 | 2.68253500 |
| C | 0.37467700 | -4.82702100 | 0.81554500 |
| N | 0.95704200 | -3.78361600 | 1.32919300 |
| C | 2.26990000 | -3.74679200 | 0.92664500 |
| N | 2.71501600 | -4.69701700 | 0.14756700 |
| S | 1.46467900 | -5.75121000 | -0.15322900 |
| H | -1.61837500 | 0.14579000 | 0.39825700 |
| H | -0.63772800 | 0.31312100 | -1.85792300 |
| H | -0.31684600 | -1.71620500 | -3.25914300 |
| H | -2.29917200 | -2.07217900 | 1.31094600 |
| H | -0.64612500 | -4.47948500 | -3.22555500 |
| H | -1.18512800 | -6.26321100 | 0.89730400 |
| H | -4.75259300 | -5.79331900 | 2.01034100 |
| H | -3.36709900 | -6.78789400 | 1.54279600 |
| H | -0.92375900 | -4.19618100 | 3.00916400 |
| H | -3.26826600 | -4.72316000 | 3.63117800 |
| C | 3.15849900 | -2.64440100 | 1.40822600 |
| H | 4.14275000 | -2.74956800 | 0.94622500 |
| C | 3.29476300 | -2.67368500 | 2.93875700 |
| H | 2.29338900 | -2.57444100 | 3.36923400 |
| C | 4.14465900 | -1.52205800 | 3.40669900 |
| O | 3.76510400 | -3.93164200 | 3.38082000 |
| H | 3.82330000 | -0.54217500 | 3.06123200 |
| C | 5.22090300 | -1.63852500 | 4.17517600 |
| H | 4.62478400 | -4.09797900 | 2.97692900 |
| H | 5.55224000 | -2.60224200 | 4.54573600 |
| H | 5.79575900 | -0.76813400 | 4.46708700 |
| H | 2.73712200 | -1.68260400 | 1.10328700 |

**S4** $E$ = -1807.083959, $G_C$ = 0.271871

| | | | |
|---|---|---|---|
| C | -2.83019700 | -0.48943000 | -0.19751100 |
| C | -2.32431900 | -0.38574300 | -1.49189800 |
| C | -2.13913600 | -1.51481100 | -2.29158700 |
| C | -2.47016600 | -2.74182400 | -1.74188500 |
| C | -2.96822200 | -2.86268700 | -0.44356000 |
| C | -3.16300400 | -1.73685000 | 0.33450000 |
| N | -2.38059600 | -4.01505400 | -2.32804200 |
| C | -2.75254300 | -5.00375600 | -1.46713500 |
| C | -3.19528900 | -4.32243600 | -0.14839000 |
| O | -2.69999900 | -6.19722200 | -1.66480800 |
| C | -2.29334100 | -4.90285700 | 1.00153000 |
| S | -4.97353100 | -4.68105400 | 0.14453000 |
| C | -4.89224800 | -5.56962800 | 1.75441500 |

| | | | |
|---|---|---|---|
| C | -2.78650800 | -4.49831500 | 2.36471000 |
| C | -4.02620400 | -4.82470100 | 2.71931300 |
| C | -0.86118900 | -4.50107900 | 0.77637200 |
| N | -0.30059700 | -3.44483000 | 1.29120700 |
| C | 0.99778900 | -3.35684200 | 0.85513400 |
| N | 1.45024500 | -4.27981300 | 0.04564800 |
| S | 0.23275100 | -5.37223500 | -0.23307600 |
| H | -2.96941900 | 0.40404500 | 0.39808300 |
| H | -2.07398100 | 0.58955600 | -1.89185700 |
| H | -1.75362400 | -1.43488800 | -3.30035300 |
| H | -3.56503900 | -1.82723700 | 1.33726700 |
| H | -2.01494100 | -4.20547400 | -3.25067800 |
| H | -2.36849600 | -5.99082800 | 0.88713900 |
| H | -5.92698800 | -5.63371000 | 2.08638300 |
| H | -4.52553300 | -6.58173300 | 1.57195400 |
| H | -2.12228900 | -3.93414100 | 3.00674600 |
| H | -4.43438800 | -4.53548200 | 3.68096100 |
| C | 1.88541500 | -2.23834800 | 1.31560200 |
| H | 2.30103500 | -1.71982900 | 0.44948000 |
| C | 3.03475100 | -2.76298200 | 2.17520100 |
| H | 3.62646500 | -3.46827200 | 1.57998600 |
| C | 3.91467100 | -1.64328400 | 2.65362500 |
| O | 2.43091000 | -3.44016200 | 3.27499000 |
| H | 3.42761300 | -0.89826900 | 3.28006800 |
| C | 5.20546900 | -1.54502500 | 2.35723200 |
| H | 3.13041900 | -3.79999600 | 3.82916300 |
| H | 5.69720600 | -2.28900200 | 1.73770700 |
| H | 5.81051800 | -0.72109700 | 2.71679500 |
| H | 1.28973600 | -1.53064600 | 1.89469800 |

**S5** $E$ = -1807.080466, $G_C$ = 0.269551

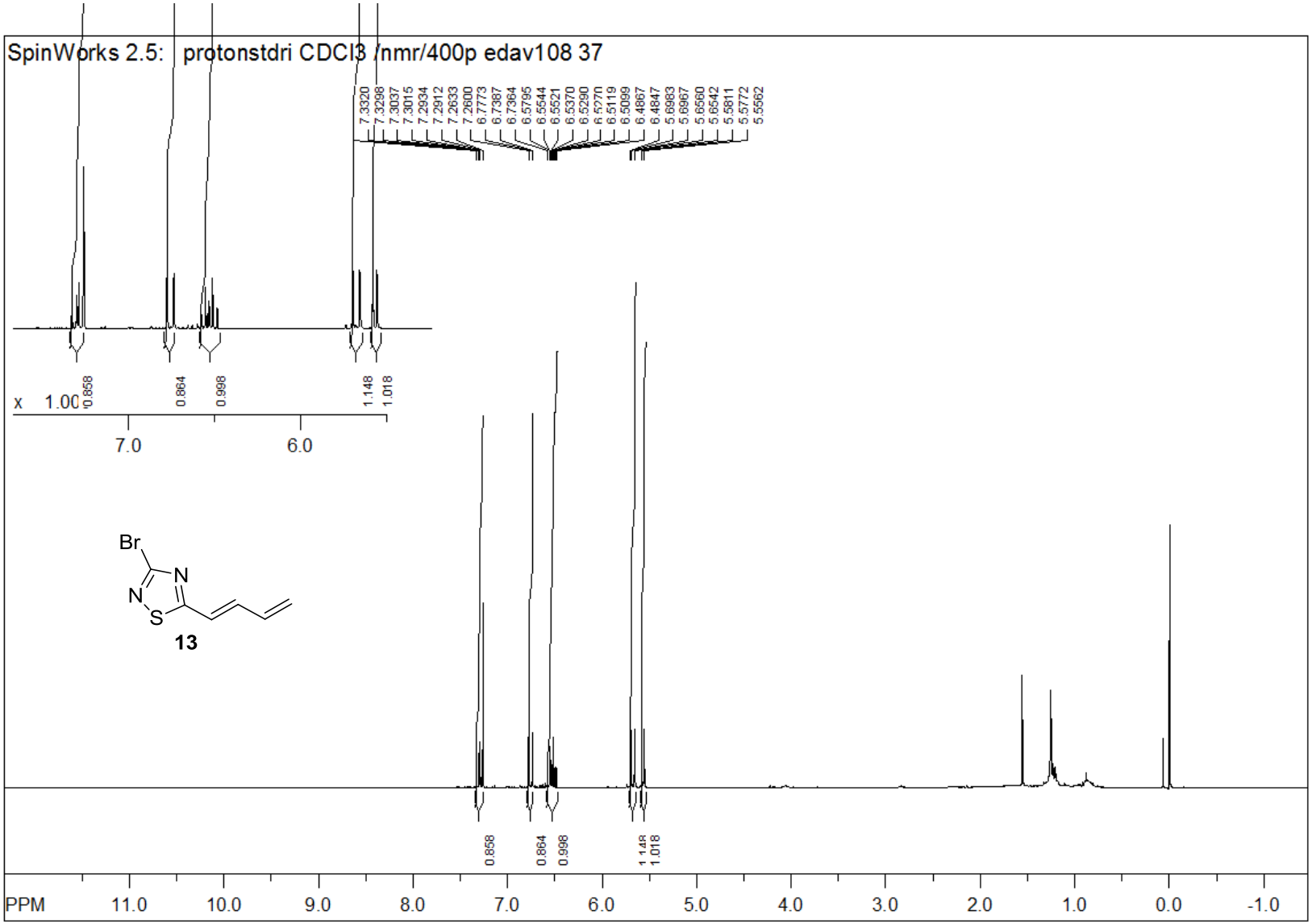
| | | | |
|---|---|---|---|
| C | -1.92764900 | -0.04436800 | -0.45953400 |
| C | -2.18189600 | -1.41126300 | -0.37083200 |
| C | -1.14354200 | -2.33762400 | -0.25639300 |
| C | 0.15011000 | -1.84370600 | -0.23720100 |
| C | 0.42036400 | -0.47726600 | -0.32933000 |
| C | -0.61462300 | 0.43262400 | -0.43629800 |
| N | 1.35661900 | -2.54758500 | -0.13161400 |
| C | 2.44620900 | -1.71899400 | -0.12823600 |
| C | 1.91475100 | -0.27421700 | -0.32147300 |
| O | 3.60040600 | -2.06278100 | -0.02735000 |
| C | 2.41603400 | 0.26858000 | -1.68565100 |
| S | 2.42955900 | 0.79505800 | 1.07445300 |
| C | 3.60158300 | 1.97950700 | 0.23413600 |
| C | 3.89730900 | 0.51015900 | -1.70409600 |
| C | 4.45668500 | 1.29881400 | -0.79274200 |
| H | -2.75233900 | 0.65240800 | -0.54107700 |
| H | -3.20512000 | -1.76694500 | -0.38689100 |
| H | -1.34175200 | -3.39977200 | -0.18414100 |
| H | -0.40883100 | 1.49639700 | -0.48807900 |
| H | 1.43698500 | -3.54855100 | -0.01994000 |
| H | 2.11781100 | -0.44192100 | -2.45902800 |
| H | 2.97475900 | 2.74628200 | -0.22631700 |
| H | 4.50294600 | 0.01361500 | -2.45218900 |
| H | 5.52690800 | 1.47432900 | -0.77072100 |
| H | 1.87197900 | 1.20076400 | -1.87587800 |
| C | 4.36375400 | 2.64157000 | 1.33729100 |
| S | 5.77369800 | 1.97723800 | 2.07904400 |
| C | 4.91082500 | 4.09130400 | 2.87547500 |
| N | 5.89470200 | 3.26823300 | 3.12136300 |
| N | 4.01974600 | 3.77364300 | 1.87686100 |
| C | 4.74218200 | 5.36783400 | 3.63960200 |
| H | 3.79929800 | 5.33685800 | 4.19160900 |
| C | 4.72464600 | 6.57614300 | 2.70493700 |
| H | 3.88500000 | 6.47372600 | 2.00810900 |
| C | 4.58677300 | 7.85822000 | 3.47629200 |
| O | 5.95752500 | 6.54211500 | 1.98960100 |
| H | 5.39059000 | 8.07260200 | 4.17812400 |
| C | 3.56918600 | 8.69864600 | 3.32873900 |
| H | 5.97180200 | 7.28345500 | 1.37630700 |
| H | 2.76783500 | 8.49192700 | 2.62571400 |
| H | 3.49908700 | 9.61356900 | 3.90512400 |
| H | 5.56172300 | 5.46350700 | 4.35367000 |

**S6** $E$ = -1807.079652, $G_C$ = 0.269894

| | | | |
|---|---|---|---|
| C | -1.13395000 | -0.16605200 | -0.46462100 |
| C | -1.40364100 | -1.53061100 | -0.38605700 |
| C | -0.37547800 | -2.47026500 | -0.28887200 |
| C | 0.92409200 | -1.99182800 | -0.27621000 |
| C | 1.20966500 | -0.62780000 | -0.35802200 |
| C | 0.18475000 | 0.29520300 | -0.44809900 |
| N | 2.12322500 | -2.71055200 | -0.18735100 |
| C | 3.22237100 | -1.89473400 | -0.18578400 |
| C | 2.70629000 | -0.44211300 | -0.35993400 |
| O | 4.37337900 | -2.25277900 | -0.09882900 |
| C | 3.20395700 | 0.10887100 | -1.72211400 |
| S | 3.24414200 | 0.60623100 | 1.04322600 |
| C | 4.42465100 | 1.78521300 | 0.20628400 |
| C | 4.68785100 | 0.33296000 | -1.74924700 |
| C | 5.26342800 | 1.10548300 | -0.83420400 |
| H | -1.95098800 | 0.54107300 | -0.53303700 |
| H | -2.43112900 | -1.87398300 | -0.39664900 |
| H | -0.58597600 | -3.53060200 | -0.22451800 |
| H | 0.40269500 | 1.35688000 | -0.49246400 |
| H | 2.19313900 | -3.71356100 | -0.08765700 |
| H | 2.89162100 | -0.58998200 | -2.50050700 |
| H | 3.80330100 | 2.56407100 | -0.24120000 |
| H | 5.28178600 | -0.16244300 | -2.50739700 |
| H | 6.33576800 | 1.26882600 | -0.82011600 |
| H | 2.66999200 | 1.04947300 | -1.89887500 |
| C | 5.20074300 | 2.42569500 | 1.31205500 |
| S | 6.63098500 | 1.76015500 | 2.00958300 |
| C | 5.75373600 | 3.83637800 | 2.88307600 |
| N | 6.75192000 | 3.01717100 | 3.08853400 |
| N | 4.85082400 | 3.53779000 | 1.89144700 |
| C | 5.62070100 | 5.10417600 | 3.66812400 |
| H | 4.58226500 | 5.44230800 | 3.62747000 |
| C | 6.53920100 | 6.20153500 | 3.10149500 |
| H | 7.57183000 | 5.84534900 | 3.17651200 |
| C | 6.39735100 | 7.46439200 | 3.90955200 |
| O | 6.31398200 | 6.39515200 | 1.71950800 |
| H | 6.54723200 | 7.34654000 | 4.98030100 |
| C | 6.10216500 | 8.65556200 | 3.40325100 |
| H | 5.38392400 | 6.61115900 | 1.58493200 |
| H | 5.96380000 | 8.79902200 | 2.33736600 |
| H | 6.00271700 | 9.52524100 | 4.04127400 |
| H | 5.88394000 | 4.91942500 | 4.71083700 |

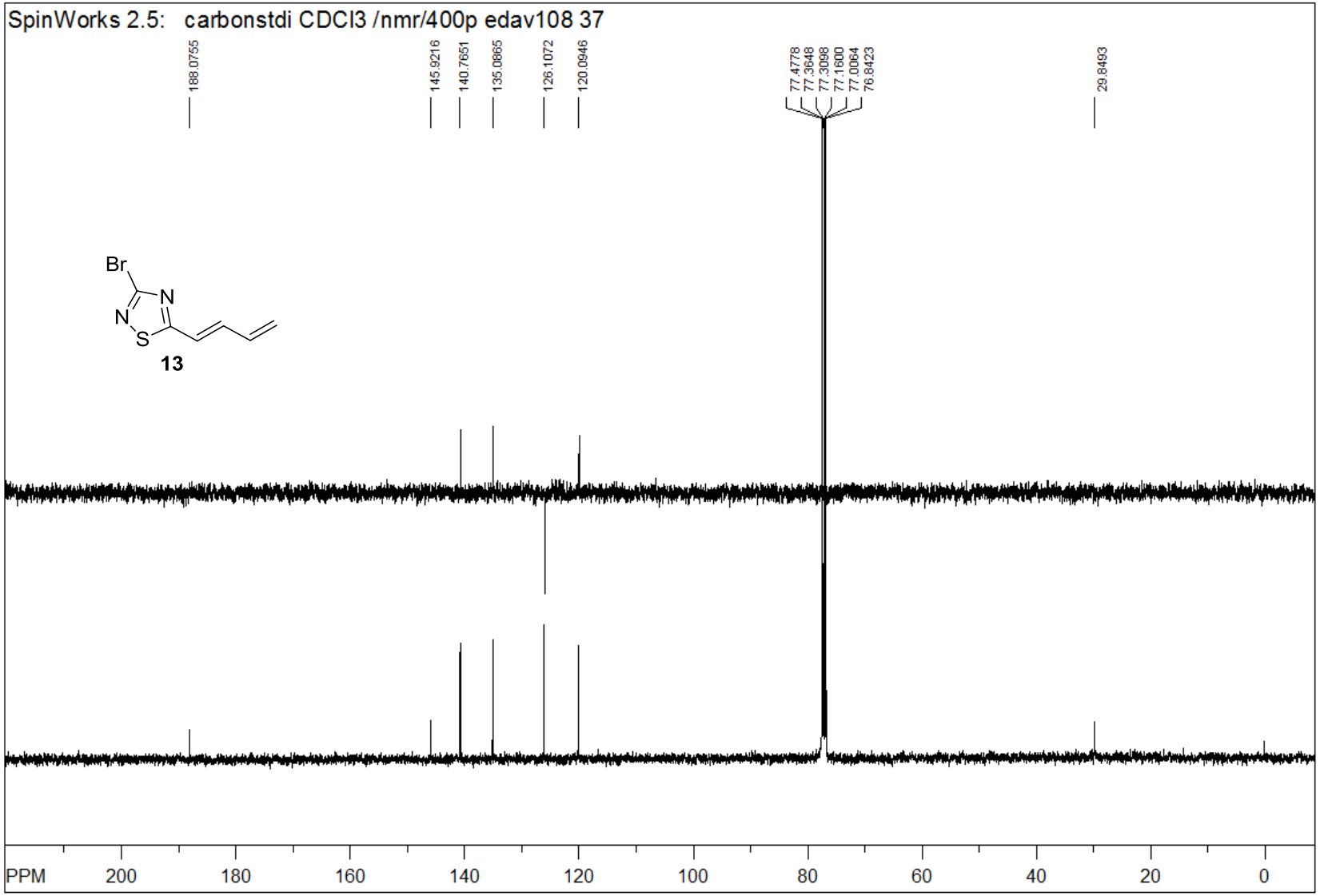
| **S7** | $E$ = -1807.081266, $G_C$ = 0.270742 | | |
|---|---|---|---|
| C | -1.81717300 | 0.45208200 | 0.17718700 |
| C | -0.57645600 | 0.16813600 | -0.38918200 |
| C | -0.17680500 | -1.14577200 | -0.64038800 |
| C | -1.06027500 | -2.15528000 | -0.29694800 |
| C | -2.30367400 | -1.88743800 | 0.28025300 |
| C | -2.69594500 | -0.58156000 | 0.51135600 |
| N | -0.90706000 | -3.54145500 | -0.44896900 |
| C | -1.99589700 | -4.23511000 | -0.00311400 |
| C | -3.00100600 | -3.19649400 | 0.55198800 |
| O | -2.13407200 | -5.43652600 | 0.00252000 |
| C | -3.17120900 | -3.49893200 | 2.06650900 |
| S | -4.58834900 | -3.31987200 | -0.36053500 |
| C | -5.75994700 | -3.67659300 | 1.04572900 |
| C | -4.26227800 | -2.67942600 | 2.68961300 |
| C | -5.49540100 | -2.75093600 | 2.19540500 |
| H | -2.10549500 | 1.48101400 | 0.35209700 |
| H | 0.09226700 | 0.98040000 | -0.64765800 |
| H | 0.78397400 | -1.36556300 | -1.08902300 |
| H | -3.67241300 | -0.36993200 | 0.93244000 |
| H | -0.09817100 | -3.99634400 | -0.84871500 |
| H | -3.39133200 | -4.56898600 | 2.15316900 |
| H | -5.58478300 | -4.71560700 | 1.33287400 |
| H | -4.02705700 | -2.01683800 | 3.51387600 |
| H | -6.31676300 | -2.15278500 | 2.57140800 |
| H | -2.20984000 | -3.31949600 | 2.55092300 |
| C | -7.13654700 | -3.53884600 | 0.47678000 |
| S | -8.04318900 | -4.85501300 | -0.16110800 |
| C | -9.00103500 | -2.63958600 | -0.21032000 |
| N | -9.30918000 | -3.86140000 | -0.56383100 |
| N | -7.78140500 | -2.41220100 | 0.37701700 |
| C | -9.97527400 | -1.51730800 | -0.39186700 |
| H | -9.43462500 | -0.56764200 | -0.37954000 |
| C | -11.03176300 | -1.52004700 | 0.72695800 |
| H | -11.56178900 | -2.47710900 | 0.68401300 |
| C | -12.01976500 | -0.40431200 | 0.51093400 |
| O | -10.42490800 | -1.48977500 | 2.00346200 |
| H | -12.48974700 | -0.38825500 | -0.46968500 |
| C | -12.32416300 | 0.52137800 | 1.41246900 |
| H | -9.86212700 | -0.70882600 | 2.05896700 |
| H | -11.88047900 | 0.51634900 | 2.40187800 |
| H | -13.03737000 | 1.30552000 | 1.18936500 |
| H | -10.47483900 | -1.61852800 | -1.35676800 |

| **S8** | $E$ = -1807.082074, $G_C$ = 0.270621 | | |
|---|---|---|---|
| C | -1.62042500 | 1.00838700 | 0.18380500 |
| C | -0.38954400 | 0.72571300 | -0.40422200 |
| C | -0.00512900 | -0.58598900 | -0.68858300 |
| C | -0.89344200 | -1.59478200 | -0.35570900 |
| C | -2.12695500 | -1.32841100 | 0.24292200 |
| C | -2.50434700 | -0.02437600 | 0.50688500 |
| N | -0.75500900 | -2.97864600 | -0.53973500 |
| C | -1.84495600 | -3.67196800 | -0.09602500 |
| C | -2.83272100 | -2.63681200 | 0.49536200 |
| O | -1.99476500 | -4.87185200 | -0.11570300 |
| C | -2.98396400 | -2.97097200 | 2.00529800 |
| S | -4.43386700 | -2.72583500 | -0.39685400 |
| C | -5.58858900 | -3.10025700 | 1.01875800 |
| C | -4.05717800 | -2.15382300 | 2.66153600 |
| C | -5.29773000 | -2.20162100 | 2.18328400 |
| H | -1.89708700 | 2.03583900 | 0.38439500 |
| H | 0.28328200 | 1.53740100 | -0.65370000 |
| H | 0.94791900 | -0.80454600 | -1.15400000 |
| H | -3.47351600 | 0.18680700 | 0.94466500 |
| H | 0.04383100 | -3.43189800 | -0.96097600 |
| H | -3.21402900 | -4.04034600 | 2.07199000 |
| H | -5.41985500 | -4.14683800 | 1.28109300 |
| H | -3.80303800 | -1.51105100 | 3.49583500 |
| H | -6.10690100 | -1.60192700 | 2.58248300 |
| H | -2.01370900 | -2.81201200 | 2.47909500 |
| C | -6.97235300 | -2.93774300 | 0.47359700 |
| S | -7.89383900 | -4.23017400 | -0.19498900 |
| C | -8.84352500 | -2.00966400 | -0.15713600 |
| N | -9.16402600 | -3.21652600 | -0.54367600 |
| N | -7.61287800 | -1.80739000 | 0.42004000 |
| C | -9.78405800 | -0.85585500 | -0.31822800 |
| H | -9.34310100 | -0.12303100 | -0.99881100 |
| C | -10.06281500 | -0.17699500 | 1.02153400 |
| H | -9.11845200 | 0.19772100 | 1.43259600 |
| C | -11.03126700 | 0.96091500 | 0.86466700 |
| O | -10.59802000 | -1.18699400 | 1.87383500 |
| H | -12.01564900 | 0.69157200 | 0.48639700 |
| C | -10.73919900 | 2.22055400 | 1.16736400 |
| H | -10.77494500 | -0.79384200 | 2.73413500 |
| H | -9.76043600 | 2.49297200 | 1.55066600 |
| H | -11.46100100 | 3.01849700 | 1.03895300 |
| H | -10.71746300 | -1.21785800 | -0.75218600 |



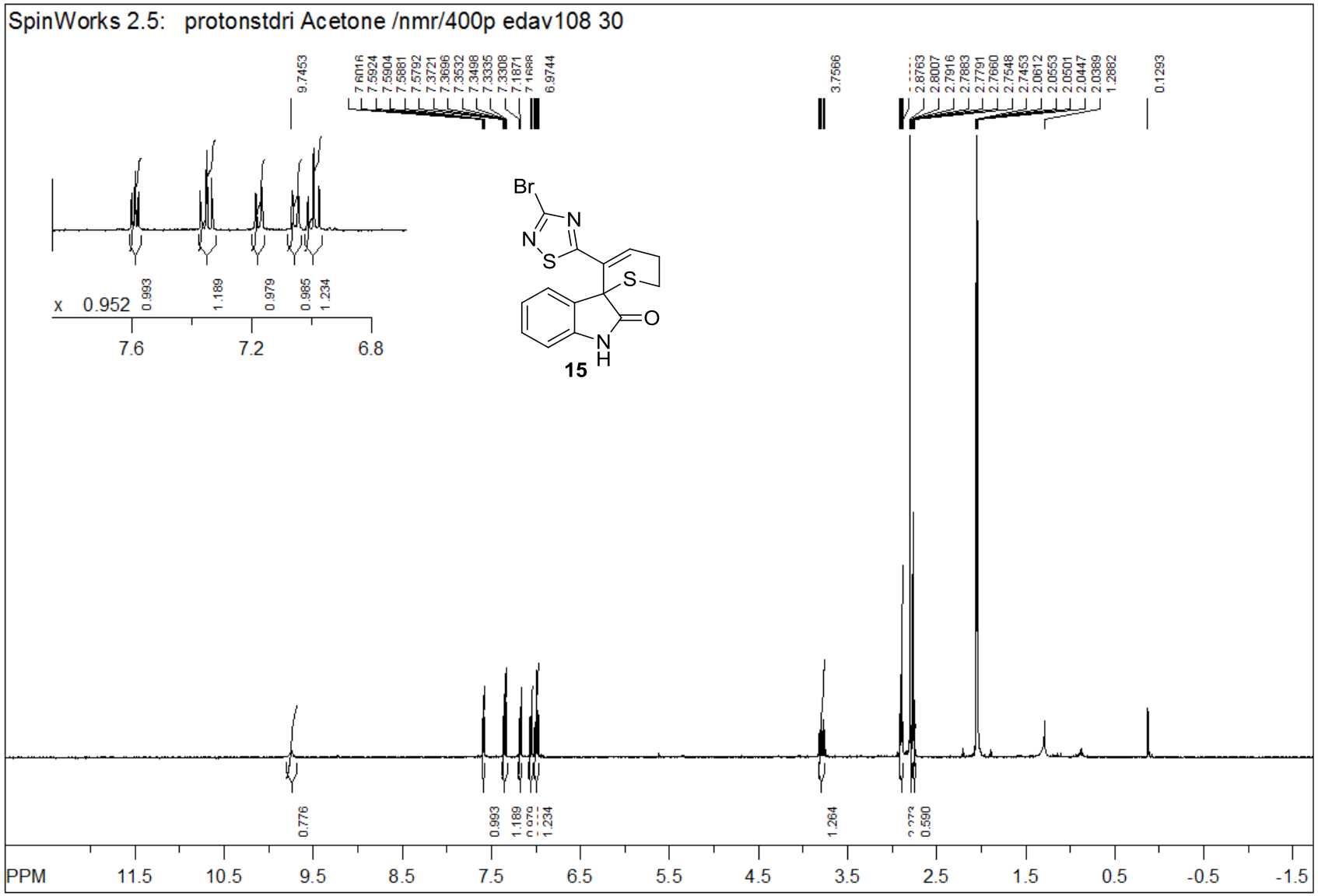

file: \\nmr\400plus\data\edav108\nmr\ED203.20\10\fid expt: <zg30>
transmitter freq.: 399.892099 MHz
time domain size: 32768 points
width: 8169.93 Hz = 20.430348 ppm = 0.249327 Hz/pt
number of scans: 30

freq. of 0 ppm: 399.890013 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 220.451 ppm/cm: 0.55128



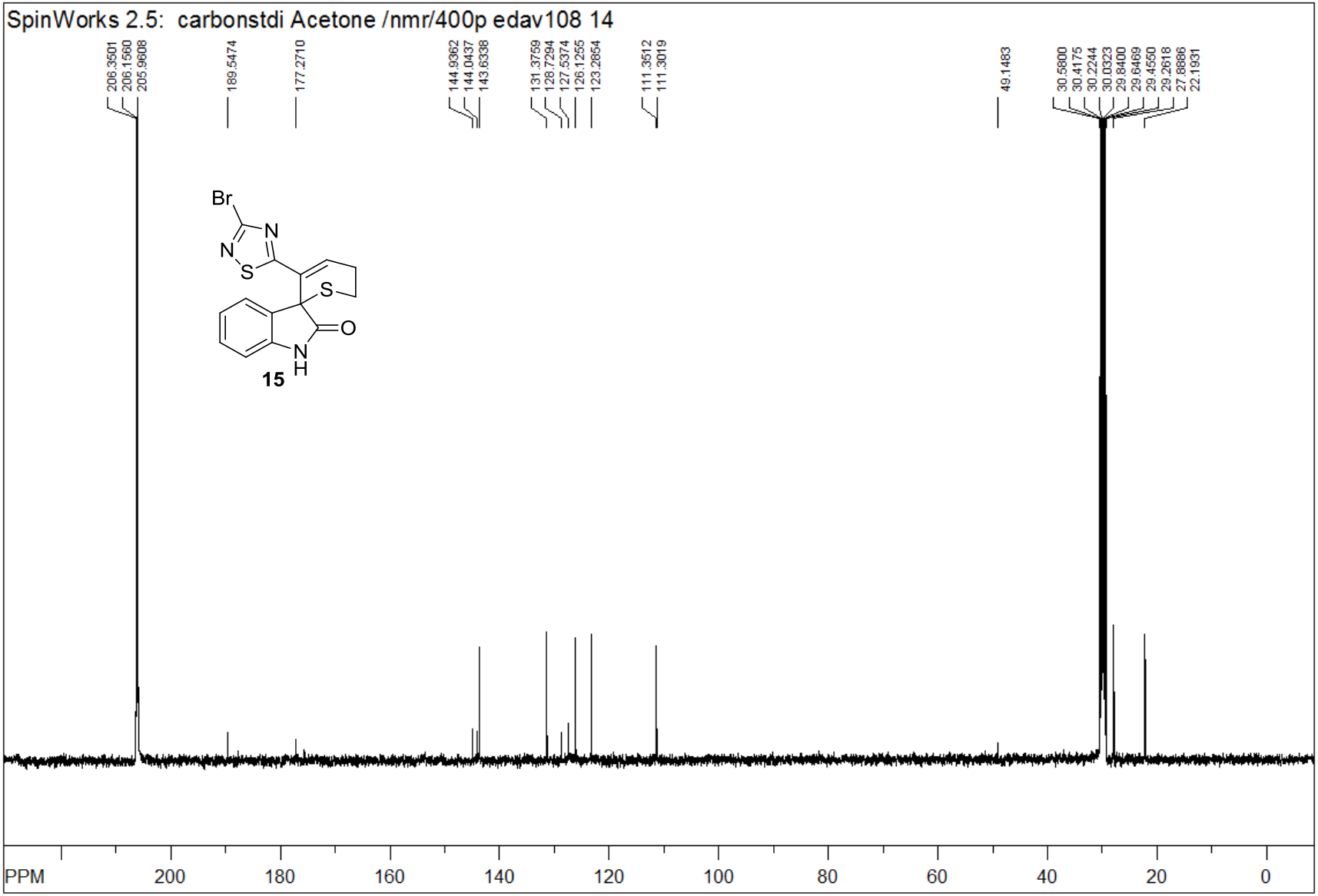

file: Z:\data\edav108\nmr\ED203.20\11\fid expt: <zgpg30>
transmitter freq.: 100.563482 MHz
time domain size: 65536 points
width: 24038.46 Hz = 239.037682 ppm = 0.366798 Hz/pt
number of scans: 1200

freq. of 0 ppm: 100.552406 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 920.868 ppm/cm: 9.15708



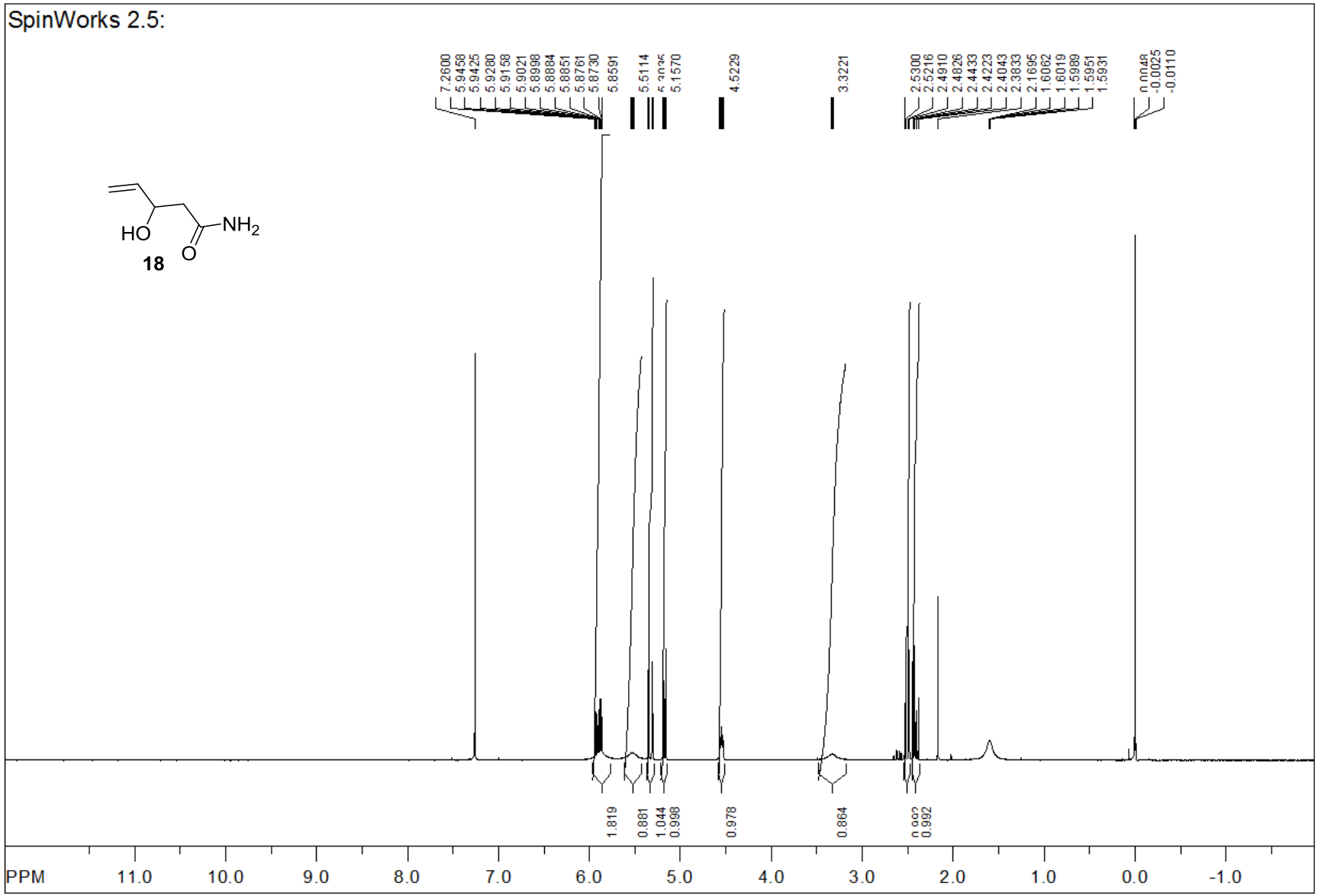

file: \\nmr\400plus\data\edav108\nmr\ED218.1_prod\10\fid expt: <zg30>
transmitter freq.: 399.892099 MHz
time domain size: 32768 points
width: 8169.93 Hz = 20.430348 ppm = 0.249327 Hz/pt
number of scans: 40

freq. of 0 ppm: 399.890010 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 234.816 ppm/cm: 0.58720



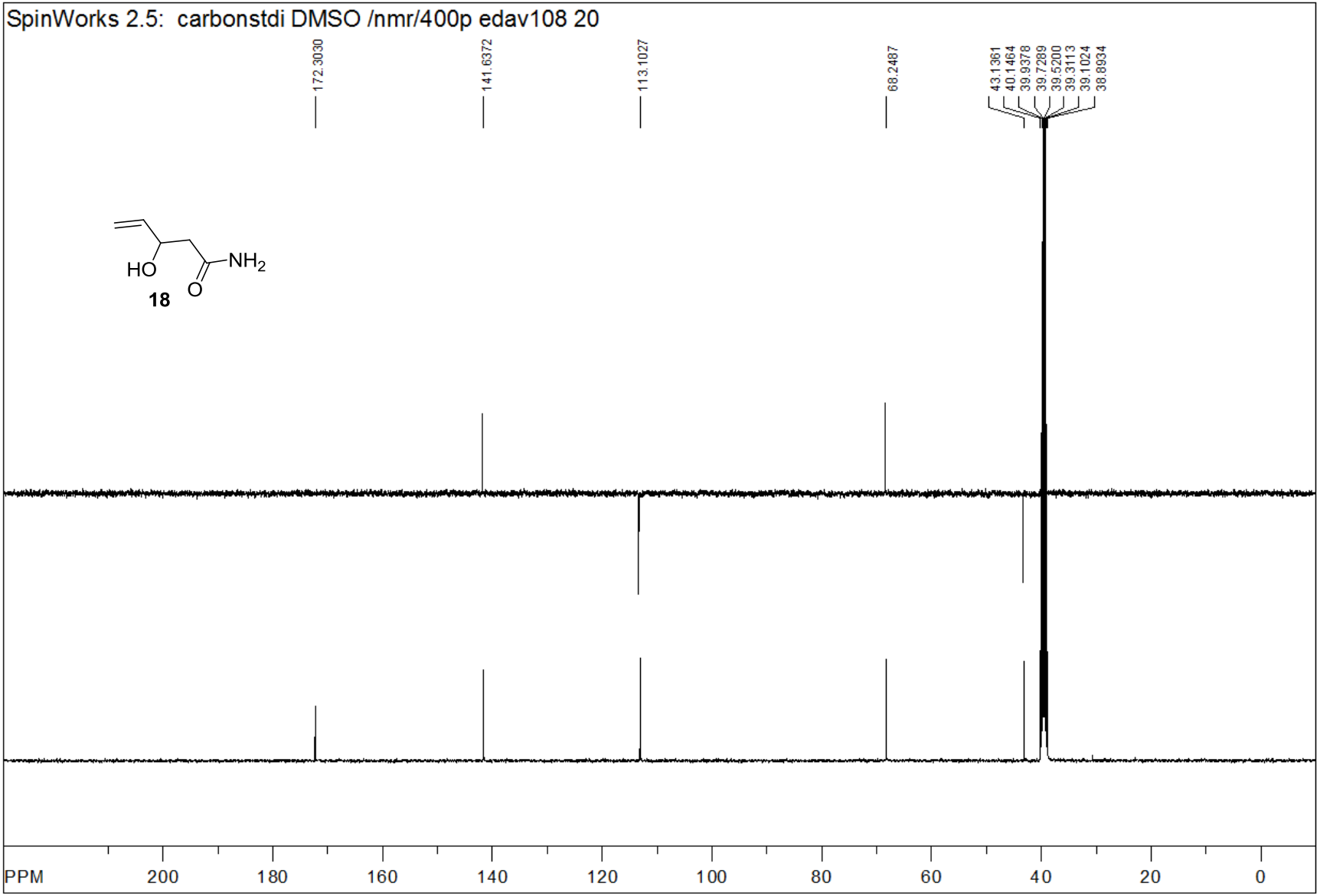

file: Z:\data\edav108\nmr\ED218.0\21\fid expt: <zgpg30>
transmitter freq.: 100.563482 MHz
time domain size: 65536 points
width: 24038.46 Hz = 239.037682 ppm = 0.366798 Hz/pt
number of scans: 1200

freq. of 0 ppm: 100.552330 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 961.538 ppm/cm: 9.56151



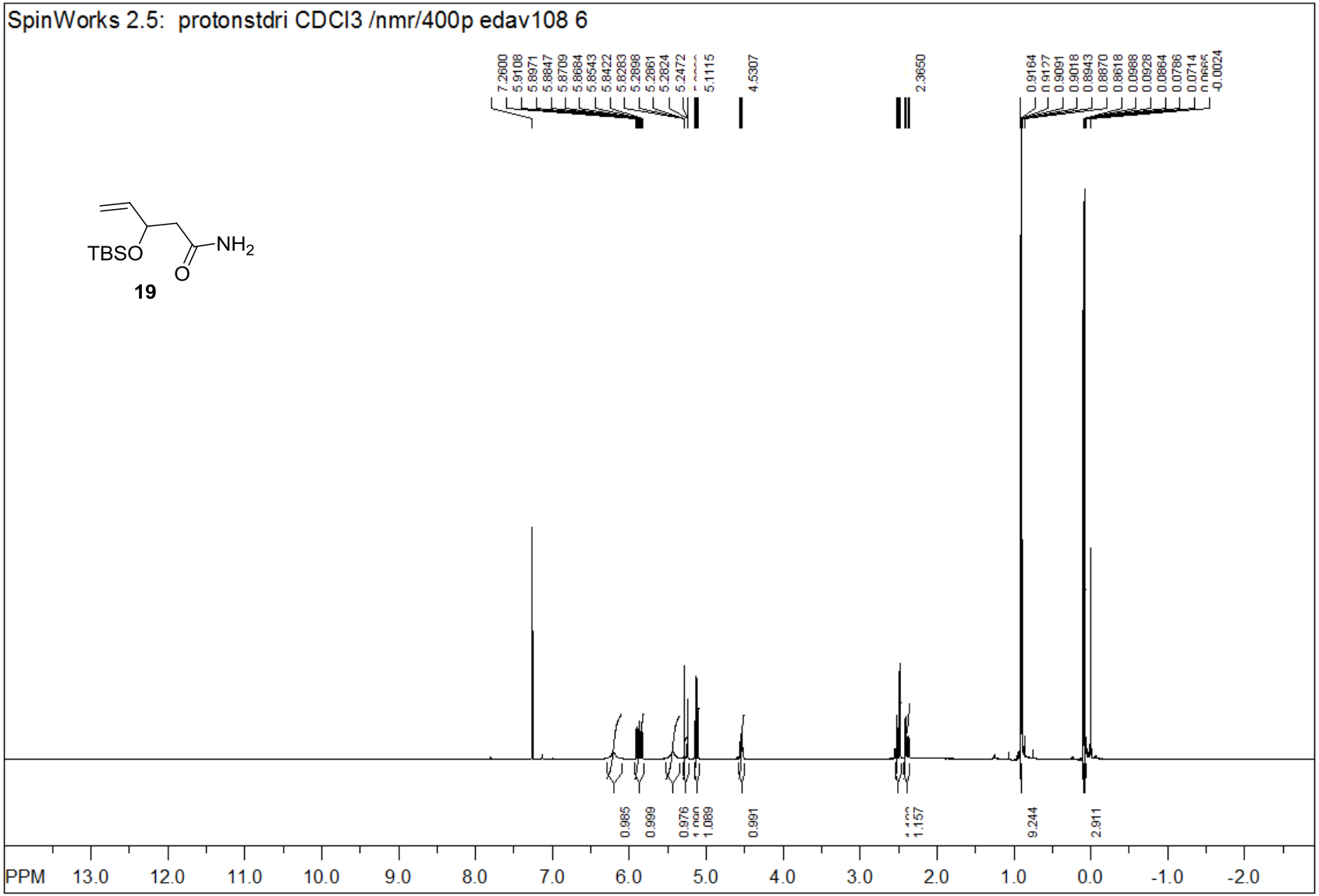

file: Y:\data\edav108\nmr\ED232.1_spot1\1\fid expt: <zg30>
transmitter freq.: 400.132001 MHz
time domain size: 32768 points
width: 8012.82 Hz = 20.025443 ppm = 0.244532 Hz/pt
number of scans: 50

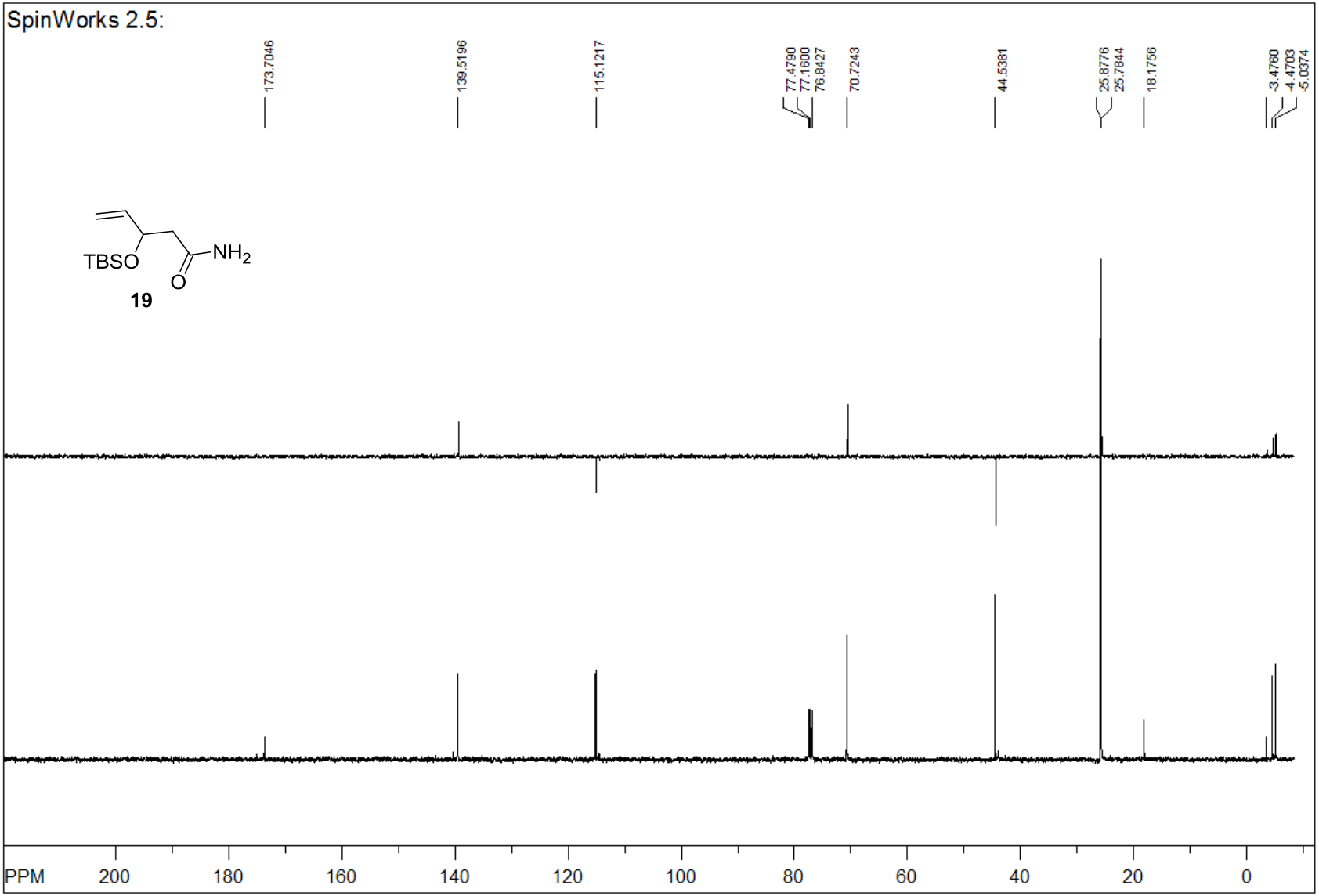
freq. of 0 ppm: 400.130010 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 230.468 ppm/cm: 0.57598




file: Z:\data\edav108\nmr\ED232.2\21\fid expt: <zgpg30>
transmitter freq.: 100.563482 MHz
time domain size: 65536 points
width: 24038.46 Hz = 239.037682 ppm = 0.366798 Hz/pt
number of scans: 2000

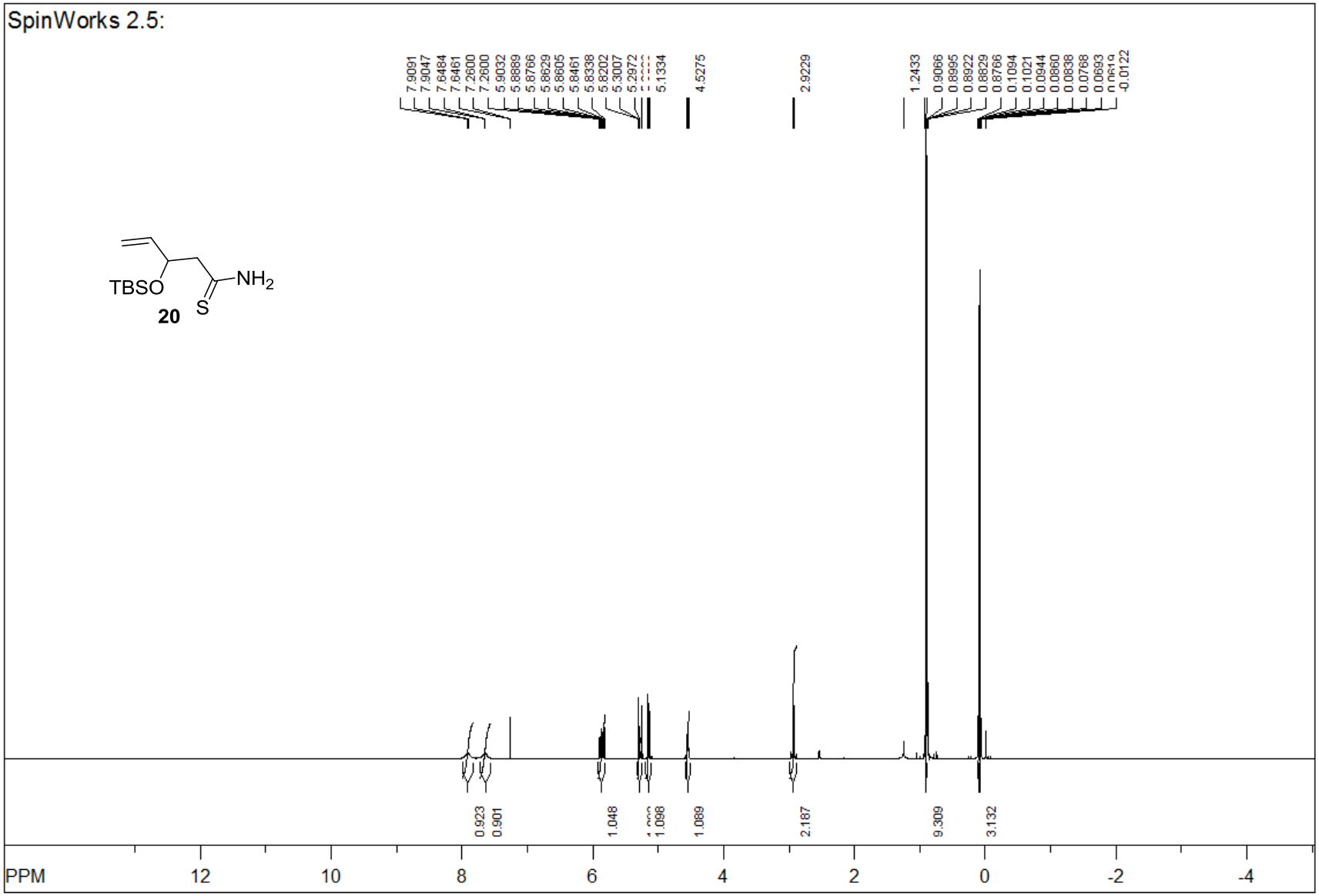
freq. of 0 ppm: 100.552469 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 961.538 ppm/cm: 9.56151


SpinWorks 2.5: protonstdri CDCl3 /nmr/400p edav108 6
TBSO
NH2
O
19
PPM 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 -1.0 -2.0
file: Z:\data\edav108\nmr\ED239.0\20\fid expt: <zg30>
transmitter freq.: 399.892099 MHz
time domain size: 32768 points
width: 8169.93 Hz = 20.430348 ppm = 0.249327 Hz/pt
number of scans: 30
freq. of 0 ppm: 399.890013 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 272.360 ppm/cm: 0.68108



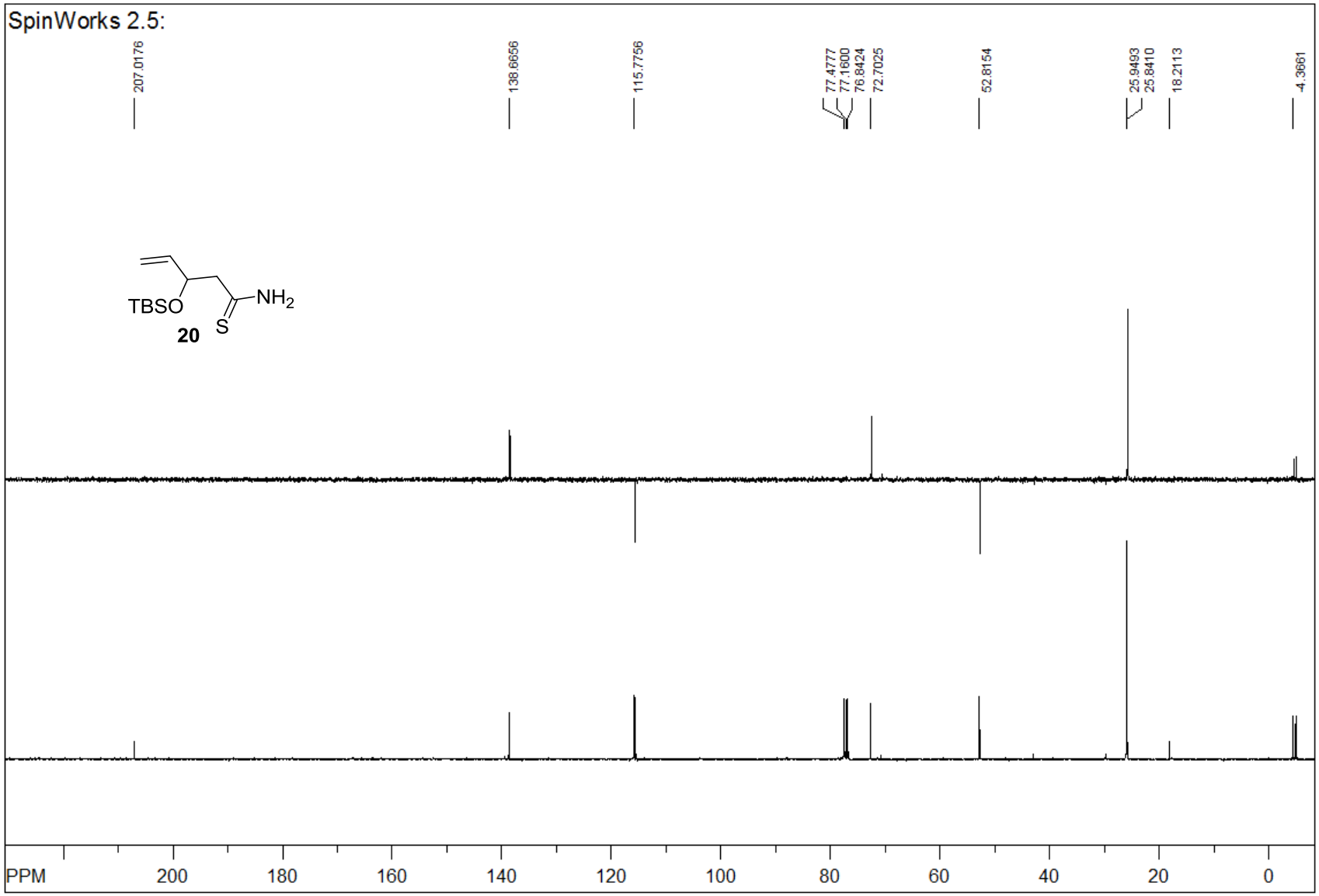

file: Y:\data\edav108\nmr\ED239.0\3\fid expt: <zgpg>
transmitter freq.: 100.623937 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.894068 ppm = 0.366798 Hz/pt
number of scans: 66

freq. of 0 ppm: 100.612758 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 932.416 ppm/cm: 9.26635



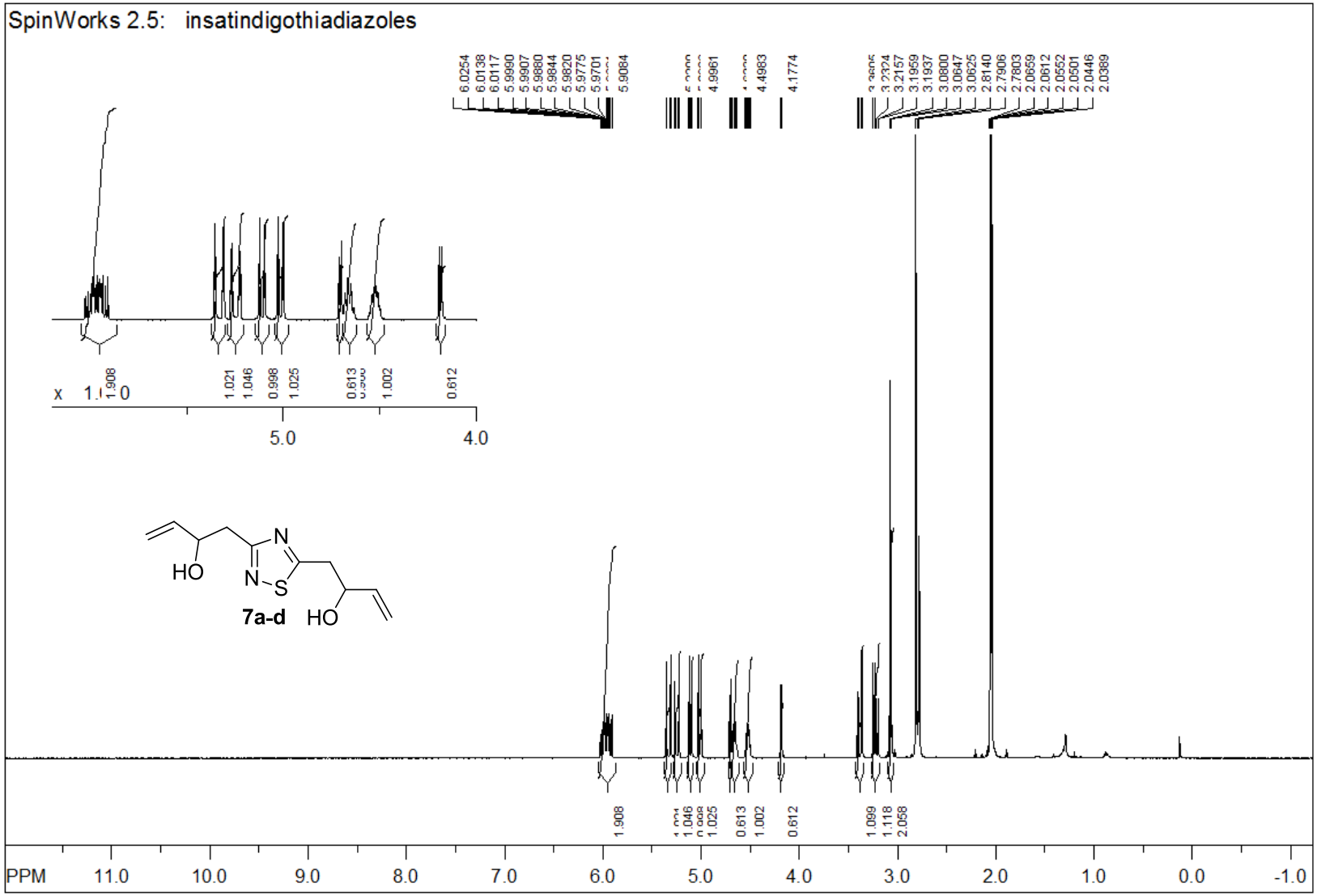

file: Y:\data\edav108\nmr\ED236.5\1\fid expt: <zg30>
transmitter freq.: 400.132001 MHz
time domain size: 32768 points
width: 8012.82 Hz = 20.025443 ppm = 0.244532 Hz/pt
number of scans: 20

freq. of 0 ppm: 400.130010 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 320.513 ppm/cm: 0.80102



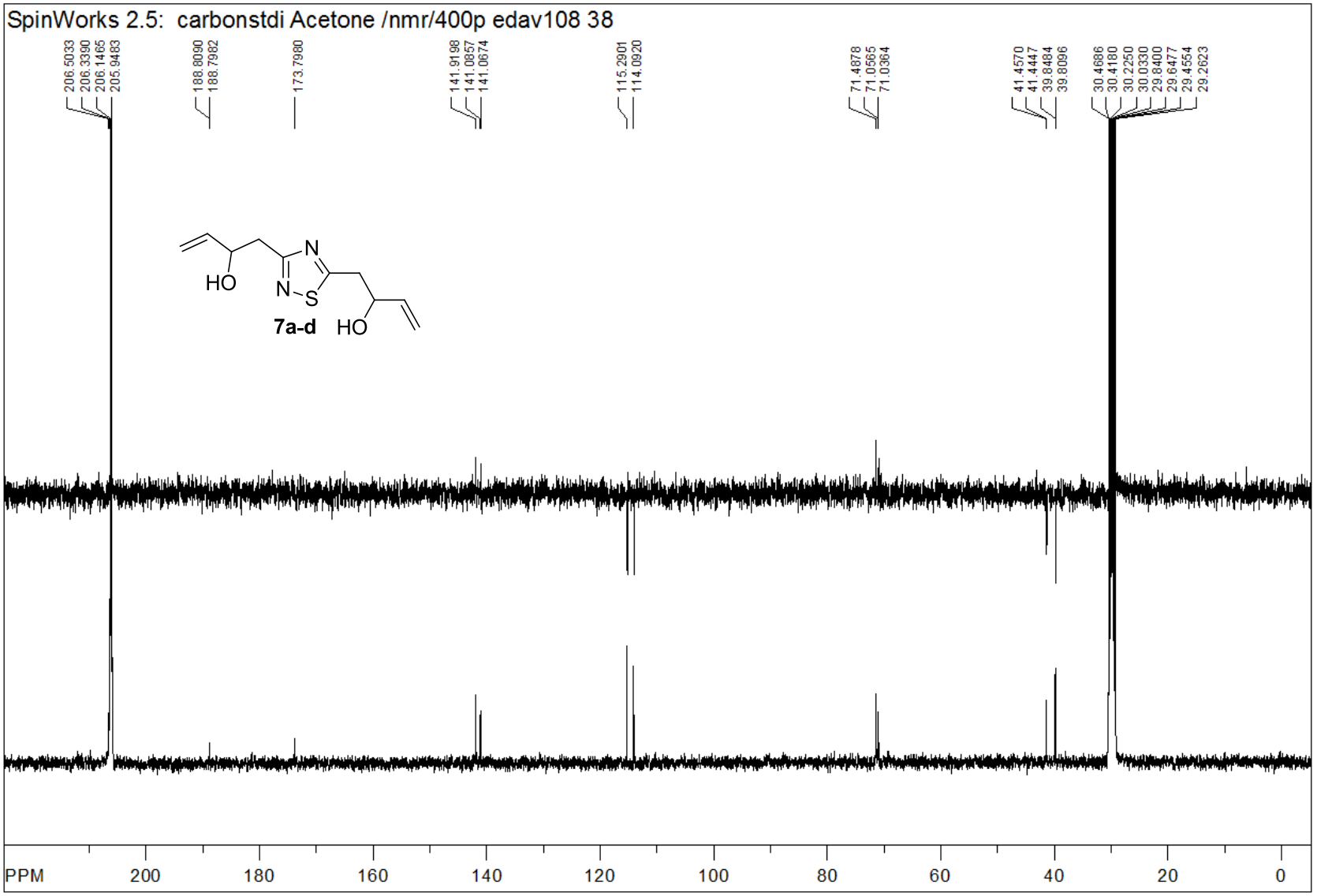

file: Y:\data\edav108\nmr\ED236.5\2\fid expt: <zgpg>
transmitter freq.: 100.623937 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.894068 ppm = 0.366798 Hz/pt
number of scans: 600

freq. of 0 ppm: 100.612756 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 961.538 ppm/cm: 9.55576



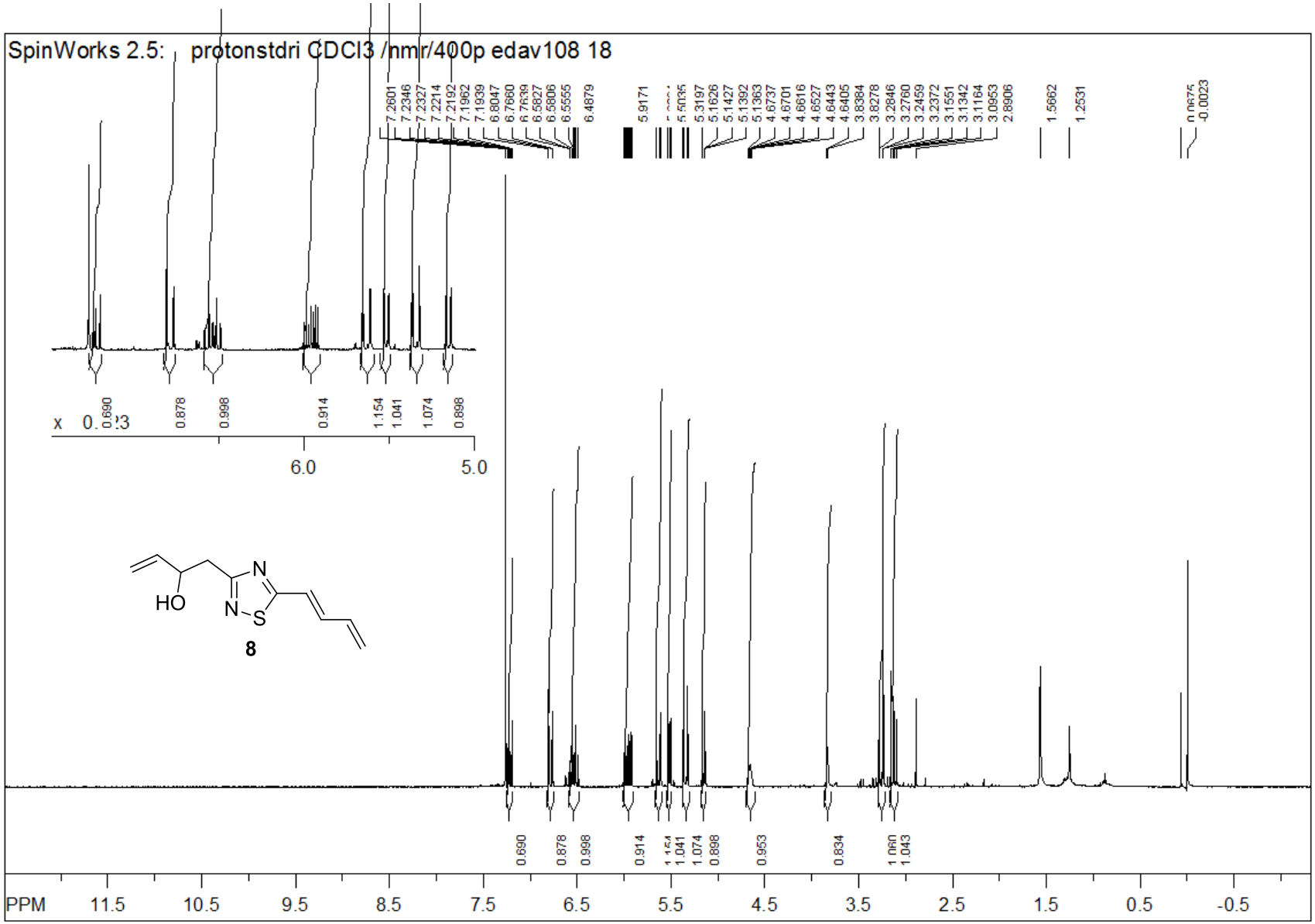

file: \\nmr\400plus\data\edav108\nmr\ED240.0\10\fid expt: <zg30>
transmitter freq.: 399.892099 MHz
time domain size: 32768 points
width: 8169.93 Hz = 20.430348 ppm = 0.249327 Hz/pt
number of scans: 60

freq. of 0 ppm: 399.890010 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 212.802 ppm/cm: 0.53215



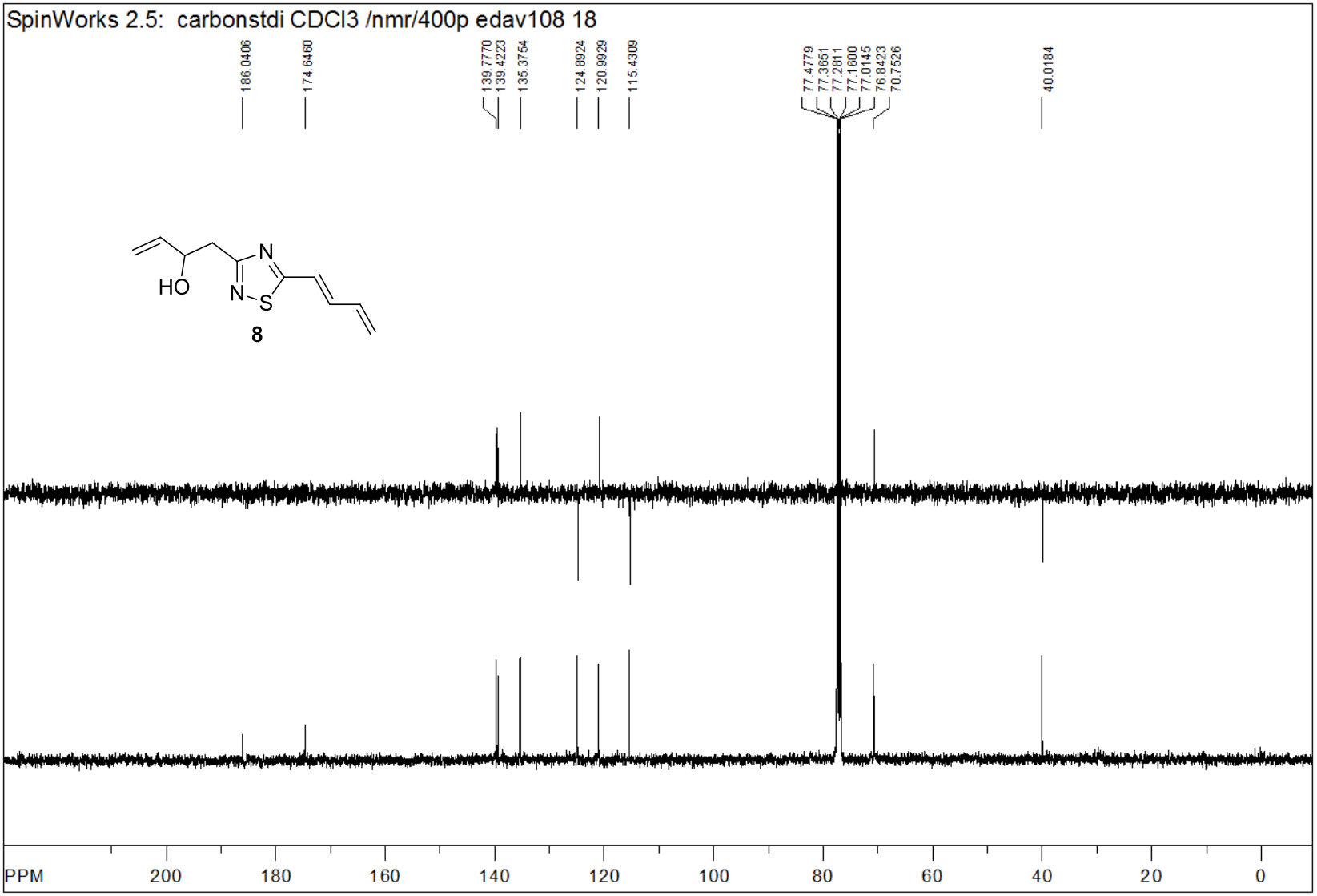

file: Z:\data\edav108\nmr\ED240.0\11\fid expt: <zgpg30>
transmitter freq.: 100.563482 MHz
time domain size: 65536 points
width: 24038.46 Hz = 239.037682 ppm = 0.366798 Hz/pt
number of scans: 3000

freq. of 0 ppm: 100.552329 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 925.889 ppm/cm: 9.20701



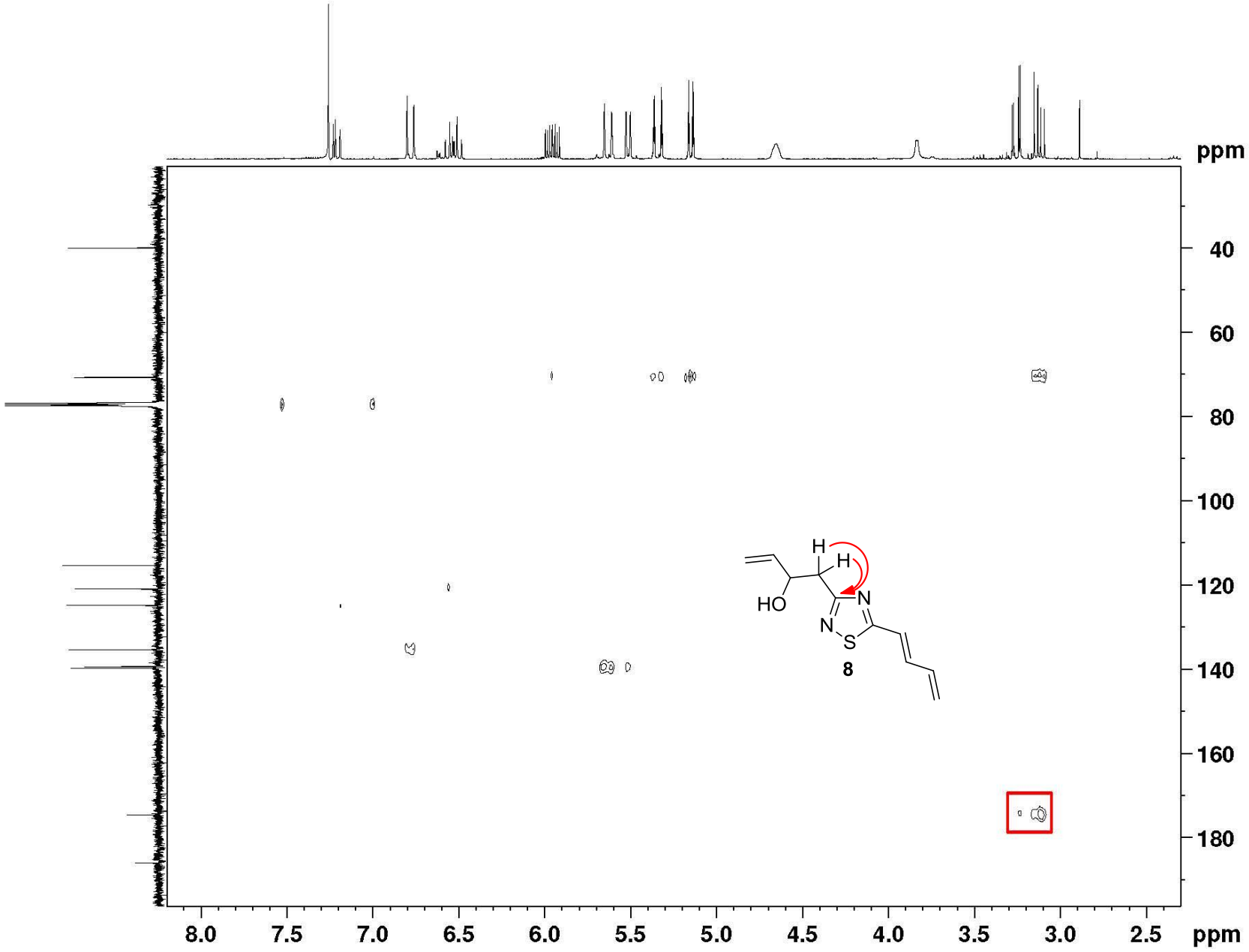

file: \\nmr\400plus\data\edav108\nmr\ED242.0_spot1\10\fid expt: <zg30>
transmitter freq.: 399.892099 MHz
time domain size: 32768 points
width: 8169.93 Hz = 20.430348 ppm = 0.249327 Hz/pt
number of scans: 40

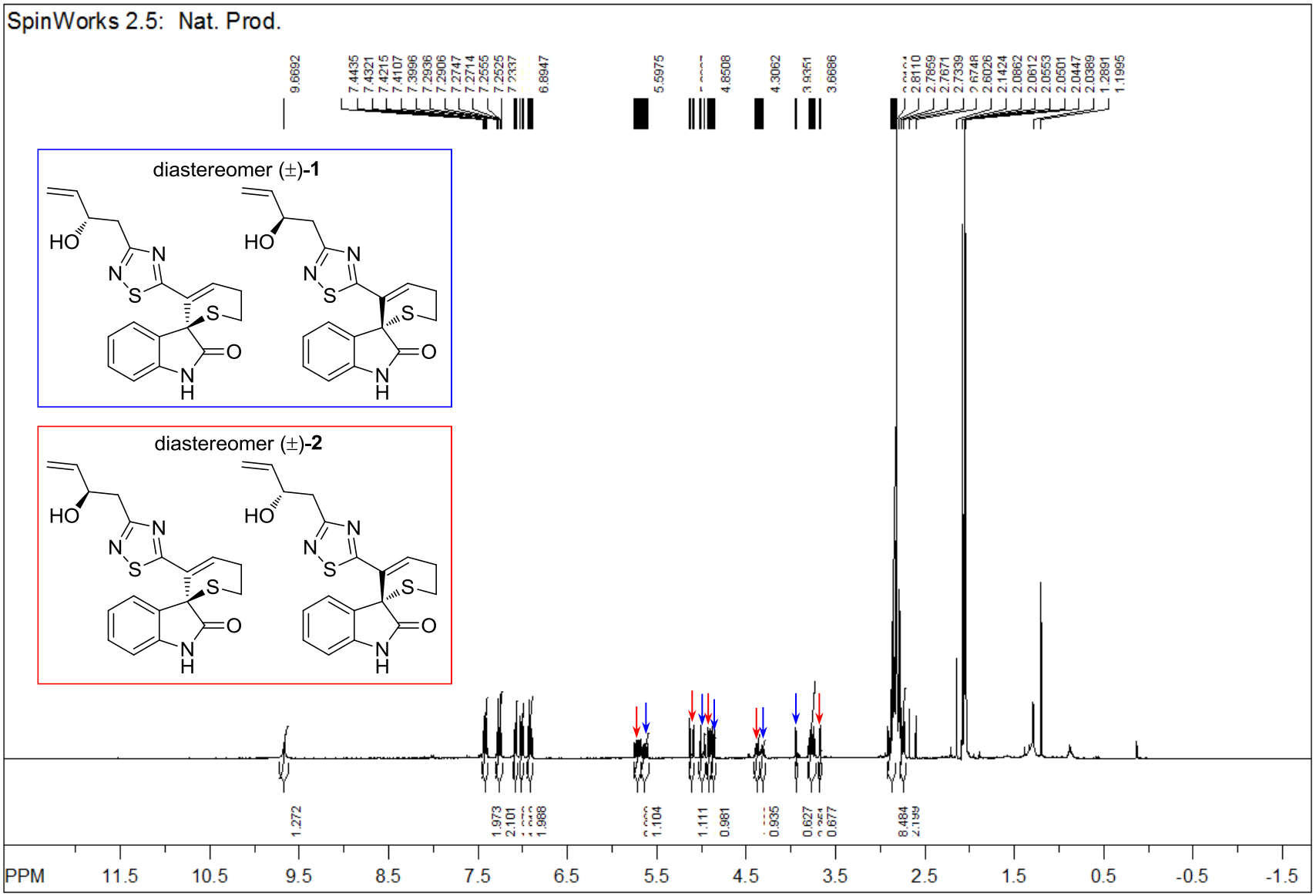
freq. of 0 ppm: 399.890013 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 222.475 ppm/cm: 0.55634




file: Z:\data\edav108\nmr\ED242.0_spot1\12\fid expt: <zgpg30>
transmitter freq.: 100.563482 MHz
time domain size: 65536 points
width: 24038.46 Hz = 239.037682 ppm = 0.366798 Hz/pt
number of scans: 3000

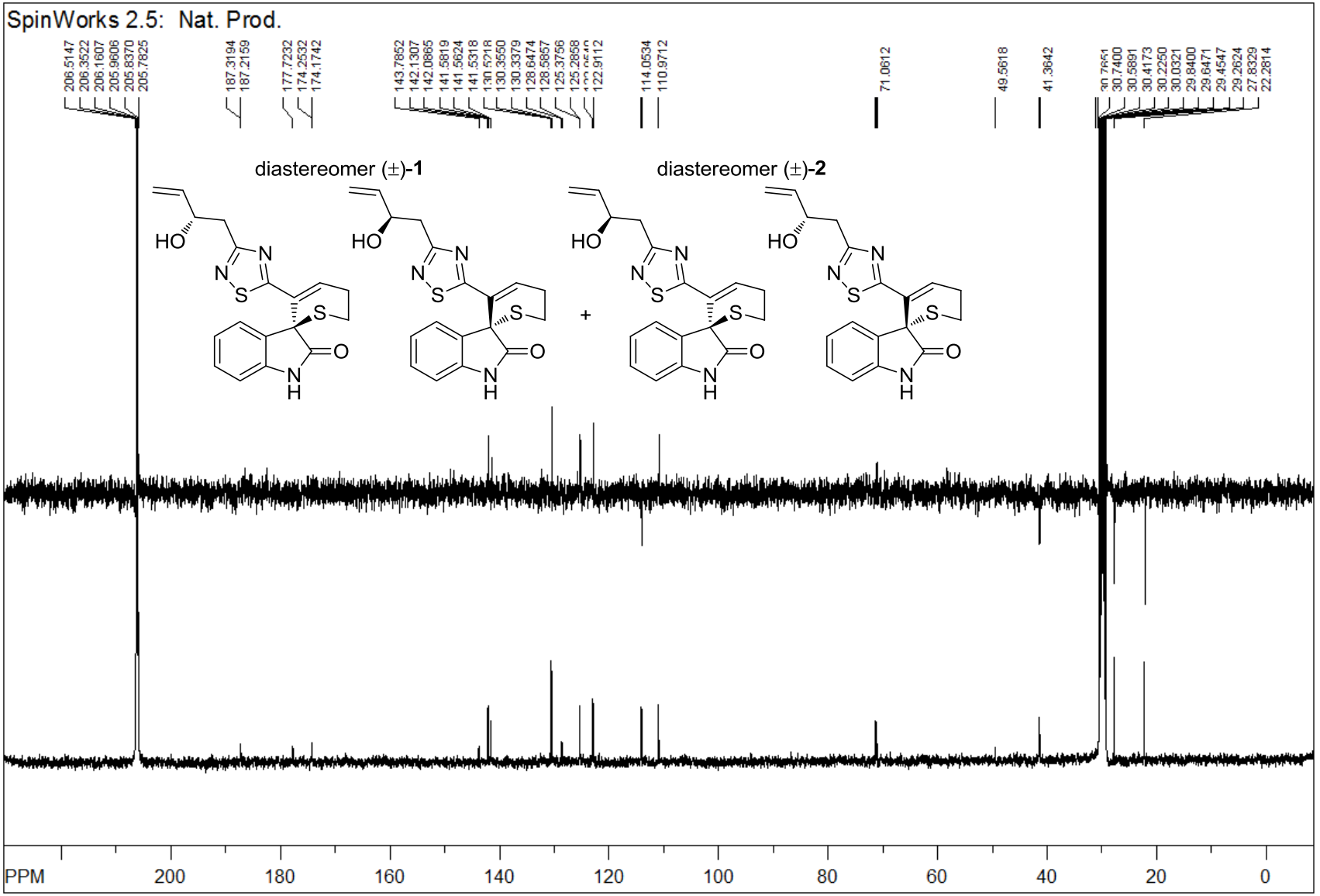
freq. of 0 ppm: 100.552406 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 961.538 ppm/cm: 9.56151


ppm
40
60
80
100
120
140
160
180
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
H
H
HO
N
N
S
8



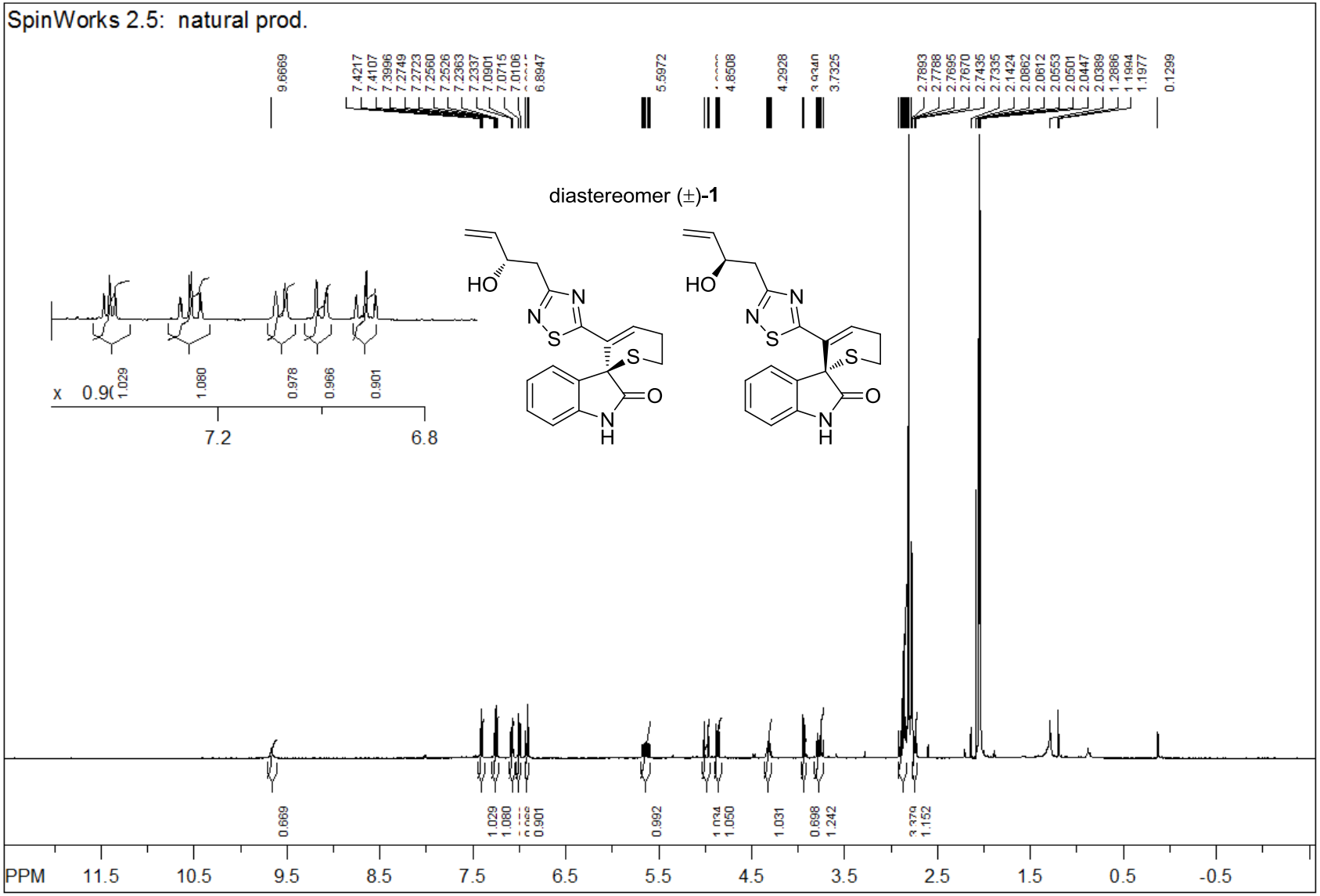

file: Z:\data\edav108\nmr\ED243.2\10\fid expt: <zg30>
transmitter freq.: 399.892099 MHz
time domain size: 32768 points
width: 8169.93 Hz = 20.430348 ppm = 0.249327 Hz/pt
number of scans: 50

freq. of 0 ppm: 399.890010 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 233.874 ppm/cm: 0.58484



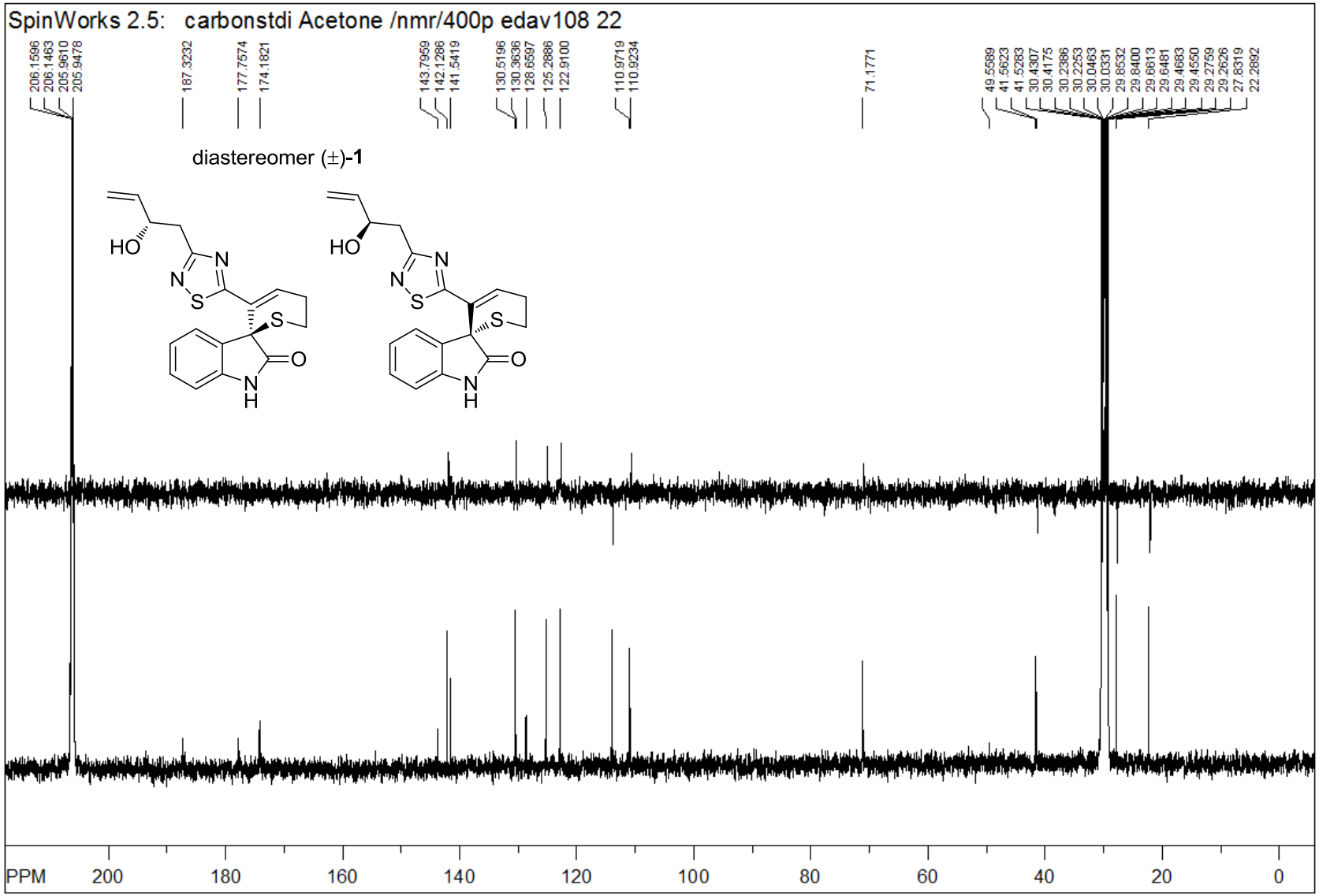

file: Z:\data\edav108\nmr\ED243.2\21\fid expt: <zgpg30>
transmitter freq.: 100.563482 MHz
time domain size: 65536 points
width: 24038.46 Hz = 239.037682 ppm = 0.366798 Hz/pt
number of scans: 5000

freq. of 0 ppm: 100.552330 MHz
processed size: 32768 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 961.538 ppm/cm: 9.56151



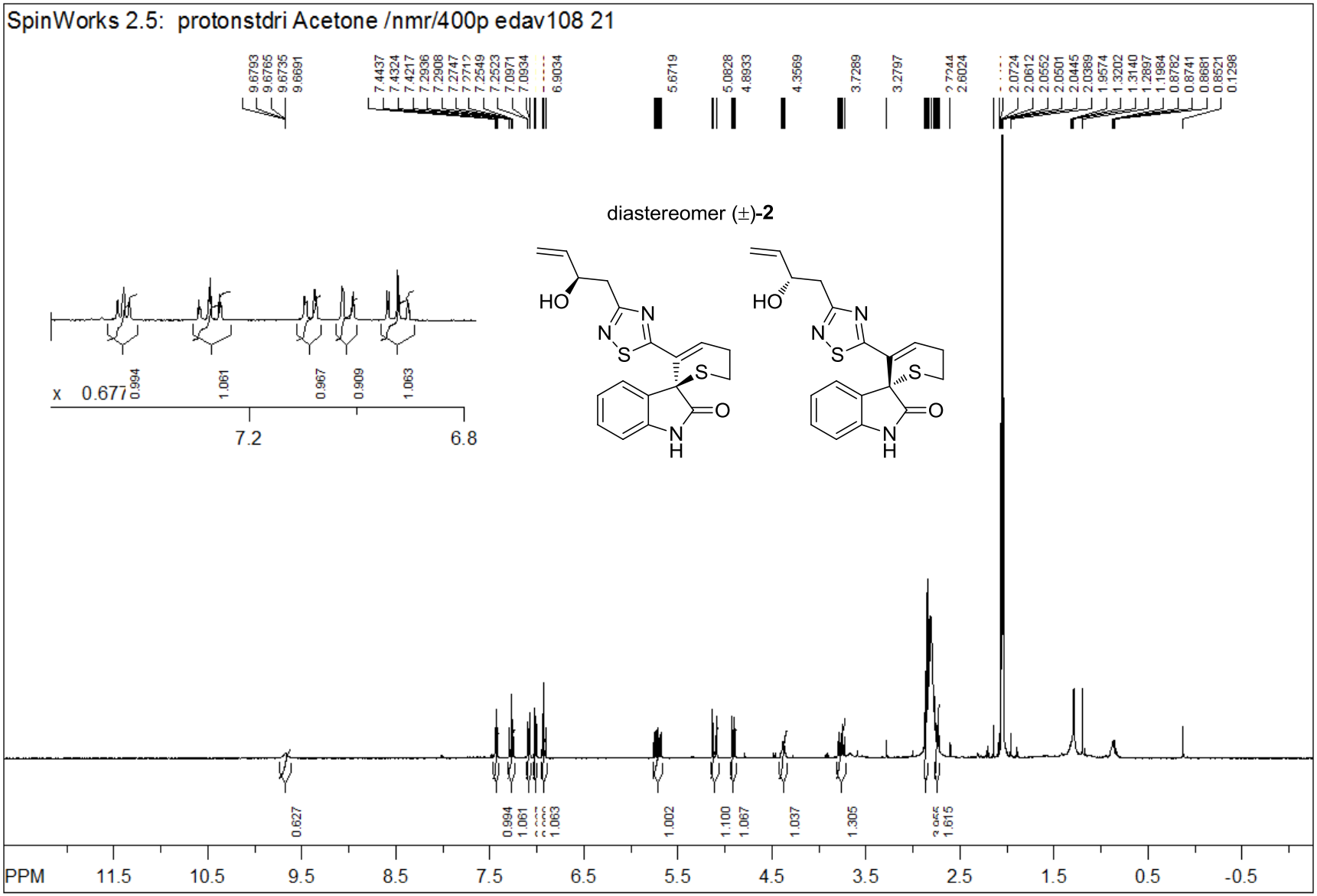

file: \\nmr\400plus\data\edav108\nmr\ED243_diast2\10\fid expt: <zg30>
transmitter freq.: 399.892099 MHz
time domain size: 32768 points
width: 8169.93 Hz = 20.430348 ppm = 0.249327 Hz/pt
number of scans: 60

freq. of 0 ppm: 399.890010 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 225.601 ppm/cm: 0.56415



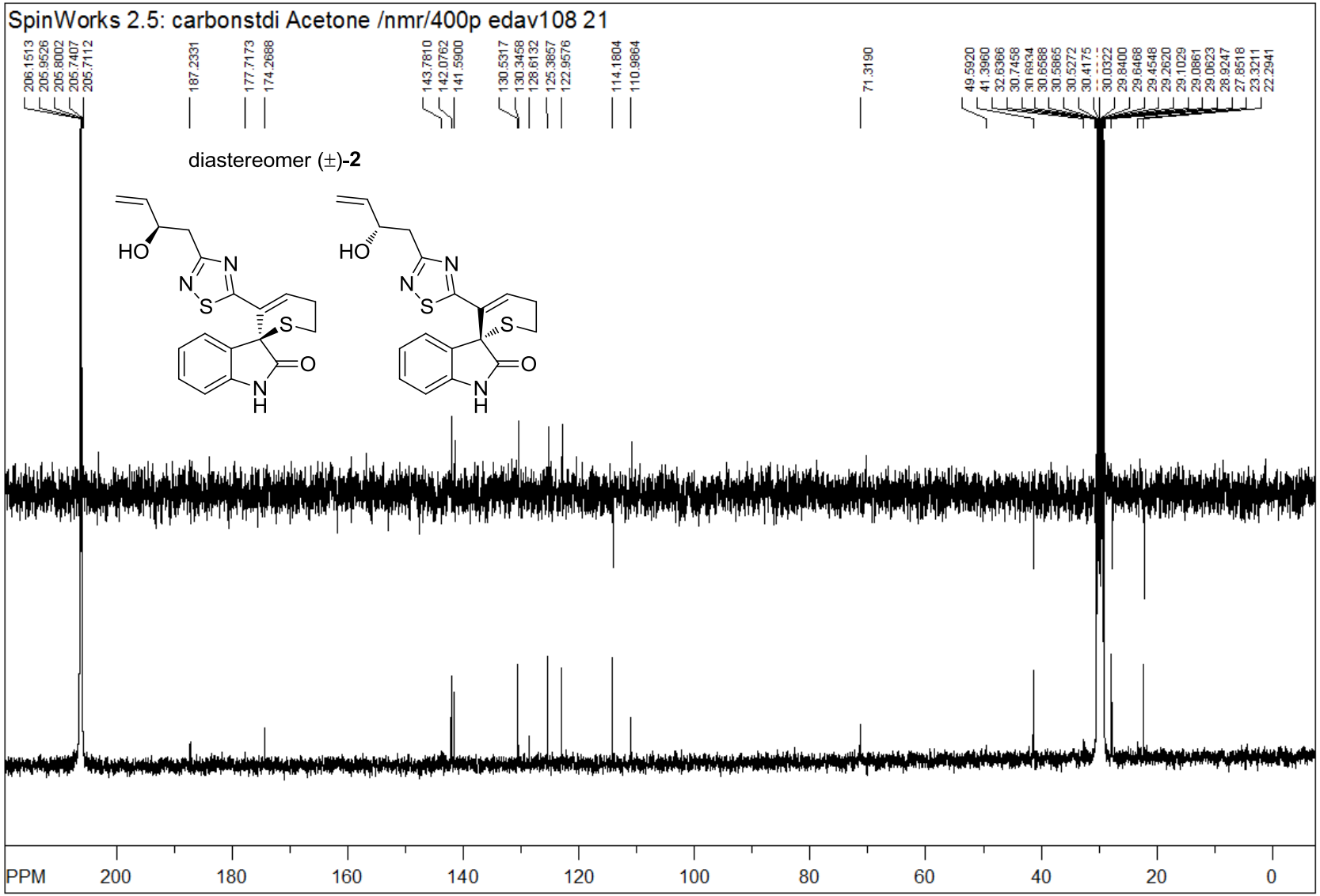

file: Z:\data\edav108\nmr\ED243_diast2\12\fid expt: <zgpg30>
transmitter freq.: 100.563482 MHz
time domain size: 65536 points
width: 24038.46 Hz = 239.037682 ppm = 0.366798 Hz/pt
number of scans: 7500

freq. of 0 ppm: 100.552329 MHz
processed size: 32768 complex points
LB: 2.000 GB: 0.0000
Hz/cm: 899.277 ppm/cm: 8.94238




file: \\nmr\400plus\data\edav108\nmr\ED243_diast1\10\format.temp expt: <zg30>
transmitter freq.: 399.892099 MHz
time domain size: 32768 points
width: 8169.93 Hz = 20.430348 ppm = 0.249327 Hz/pt
number of scans: 60

freq. of 0 ppm: 399.890010 MHz
processed size: 16384 complex points
LB: 0.000 GB: 0.0000
Hz/cm: 222.623 ppm/cm: 0.55671




file: Z:\data\edav108\nmr\ED243_diast1\21\fid expt: <zgpg30>
transmitter freq.: 100.563482 MHz
time domain size: 65536 points
width: 24038.46 Hz = 239.037682 ppm = 0.366798 Hz/pt
number of scans: 8000

freq. of 0 ppm: 100.552328 MHz
processed size: 32768 complex points
LB: 2.000 GB: 0.0000
Hz/cm: 911.328 ppm/cm: 9.06221