Diastereoselective Synthesis of Piperidine Imino Sugars Using Aldol Additions of Metalated Bislactim Ethers to Threose and Erythrose Acetonides

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Supporting Information

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1. General methods.

All moisture-sensitive reactions were performed under an argon atmosphere using oven-dried glassware. Reagents and solvents were purchased and used without further purification unless otherwise stated. THF was distilled from sodium/benzophenone, CH_2Cl_2 was distilled from calcium hydride and Et_3N was distilled from sodium. Reactions were monitored by thin-layer chromatography carried out on 0.25 mm silica gel plates (60F-254) using UV light as visualizing agent and cerium sulfate/ammonium molybdate in 10% sulfuric acid or ninhydrin in a 3% HOAc/*n*-BuOH solution as developing agents. E. Merck Silica gel and RP-18 (both 230-400 mesh) were used for liquid chromatography separations and Dowex 50W-X8 resin (H^+ form, 100-200 mesh) was used for ion-exchange chromatography. Melting points are uncorrected. IR spectra were obtained as liquid film or as KBr pellets. Unless otherwise indicated, ^1H NMR and ^{13}C NMR spectra were recorded at 200 and 50 MHz, respectively, with broad-band ^1H decoupling at 25 °C. Chemical shifts are reported relative to internal $CDCl_3$ (δ 7.27) or to HOD in D_2O (δ 4.79) for ^1H, relative to internal $CDCl_3$ (δ 77.0) for ^{13}C. FABMS spectra were recorded using thioglycerol as a matrix. High resolution mass spectra were recorded using 3-nitrobenzylalcohol as a matrix. Optical rotations were taken at the Na_D-line. Multigram quantities of both enantiomers of 2,5-diethoxy-3-isopropyl-3,6-dihydropyrazine were obtained from Novartis kilo laboratory.

2. General procedures.

General procedure 1 for aldol addition. Method A. A solution of *n*-BuLi (1.2 equiv, 2.5 M in hexane) was added to a stirred solution of Schöllkopf˝s bislactim ether (1.2 equiv) in THF (10 mL/mmol) at −78 °C and the mixture was stirred for 1 h. Then, a 0.5 M solution of the additive ($ZnCl_2$, $SnCl_2$, $SnOTf_2$, Et_2AlCl, $MgBr_2{\cdot}OEt$, $Ti(O^iPr)_3Cl$ or $Ti(NEt_2)_3Cl$) in THF (1.2-2.4 equiv) was added dropwise. The mixture was stirred for 1 h, and a solution of aldehyde (1.0 equiv) in THF (2.5-4.0 mL/mmol) was added dropwise. After being stirred at −78 °C for 2 h, the reaction was quenched with

aqueous saturated NH_4Cl or $NaHCO_3$ solution. The crude reaction mixture was warmed to rt, and the solvent was removed in vacuo. The resulting material was diluted with water and extracted with ether. The combined organic layers were dried (Na_2SO_4) and evaporated, and the residue was purified by flash chromatography (silica gel, EtOAc/hexanes from 1:9 to 3:1 ratio) to yield the corresponding addition products. **Method B.** A solution of *n*-BuLi (3.0 equiv, 2.5 M in hexane) was added to a stirred solution of Schöllkopf´s bislactim ether (3.0 equiv) in THF (10 mL/mmol) at −78 °C and the mixture was stirred for 1 h. Then, a 0.5 M solution of the additive ($ZnCl_2$, $SnCl_2$, $MgBr_2{\cdot}OEt$, $Ti(O^iPr)_3Cl$, $Ti(NEt_2)_3Cl$ or TMSCl and $SnCl_4$) in THF (3.0-6.0 equiv) was added dropwise. The mixture was stirred for 1 h, and a solution of lactol (1.0 equiv) in THF (2.5-4.0 mL/mmol) was added dropwise. The reaction mixture was gradually warmed to 0 °C for 5-12 h, and the reaction was quenched with aqueous saturated NH_4Cl or $NaHCO_3$ solution and worked up as described in method A.

General procedure 2 for debenzylation: A solution of 4´-*O*-benzylated adduct in THF (20 mL/mmol) was stirred with 10% Pd/C (10% w/w) under H_2 (1 atm) for 6-12 h at rt. The catalyst was removed by filtration through a short pad of Celite, the filtrate was concentrated in vacuo and the residue was purified by flash chromatography to give the corresponding diol in an almost quantitative yield.

General procedure 3 for silylation: A solution of diol (1.0 equiv), DMAP (0.05 equiv) and Et_3N (1.3 equiv) in CH_2Cl_2 (16 mL/mmol) was treated with TBDPSCl (1.2 equiv) and the mixture was stirred at rt for 24 h. The solvent was removed in vacuo and the residue was purified by flash chromatography to yield the corresponding silylated product.

General procedure 4 for benzylation: A solution of aldol adduct (1.0 equiv) in THF (5 mL/mmol) was added to a stirred suspension of NaH (60% dispersion in mineral oil, 1.4 equiv) in THF (12 mL/mmol) at 0 °C. After 1 h, NBu_4I (0.35 equiv) and BnBr (1.4 equiv) were added, and the resulting solution was stirred at rt for 23 h. The reaction mixture was cooled to 0 °C and quenched by the addition of CH_3OH (3 mL/mmol). The solvents were removed in vacuo and the resulting material was diluted

with water and extracted with CH_2Cl_2. The combined organic layers were dried (Na_2SO_4) and evaporated and the residue was purified by flash chromatography to yield the corresponding benzylated product.

General procedure 5 for desilylation: Hydrated Bu_4NF (3.2 equiv) was added to a solution of 4´-*O*-silylated adduct (1.0 equiv) in THF (25 mL/mmol) at 0 ºC, and the mixture was stirred at rt for 2-4 h. The solvent was evaporated and the residue was purified by flash chromatography to give the corresponding diol.

General procedure 6 for mesylation: A solution of alcohol (1.0 equiv), Et_3N (2.0 equiv) and DMAP (0.17 equiv) in CH_2Cl_2 (15 mL/mmol) at 0 ºC was treated with MsCl (1.5 equiv) and the mixture was stirred for 30 min at rt. The solvent was evaporated and the residue was purified by flash chromatography to give the corresponding mesylate.

General procedure 7 for bislactim ether hydrolysis: A solution of bislactim ether (1.0 equiv) in EtOH (12 mL/mmol) or MeOH (30 mL/mmol) and 0.25 N HCl (2.0 equiv) was stirred at rt for 9 h. Then, the solution was diluted with water (10 mL/mmol) and concentrated to half its initial volume. The aqueous solution was made basic (pH~10) by the addition of $NaHCO_3$ followed by concentrated ammonia. The aqueous layer was extracted with CH_2Cl_2 (7 x 12 mL/mmol) and the combined organic layers were dried (Na_2SO_4) and evaporated. The crude was purified by flash chromatography to yield the corresponding amino ester.

General procedure 8 for cyclization of amino mesylate: Et_3N (2.0 equiv) was added to a solution of amino mesylate (1.0 equiv) in DMSO (12 mL/mmol) and the mixture was heated to 70 ºC for 2-3 h. The reaction mixture was cooled to rt, diluted with brine and extracted with EtOAc. The combined organic layers were dried (Na_2SO_4) and evaporated. The crude was purified by flash chromatography to give the corresponding pipecolate.

General procedure 9 for reduction of pipecolate: $LiEt_3BH$ (1 M in THF, 3.5 equiv or 4.5 equiv) was dropwise added to a solution of pipecolate (1.0 equiv) in THF (15 mL/mmol) at 0 °C and the

reaction mixture was stirred at this temperature for 3 h. The reaction mixture was quenched by the addition of aqueous saturated NH_4Cl solution, the solvents were removed in vacuo and the residue was diluted with water and extracted with EtOAc. The combined organic layers were dried (Na_2SO_4) and evaporated, and the crude piperidine was purified by flash chromatography or was directly subjected to the final deprotection step (see general procedure 10, Method B).

General procedure 10 for final deprotection: Method A: A solution of piperidine (1.0 equiv) in THF (20 mL/mmol) and 0.25 N HCl (5.0 equiv) was stirred with 10% Pd/C (10% w/w) under H_2 (1 atm) for 9-12 h at rt. The catalyst was removed by filtration through a short pad of Celite, the filtrate was concentrated in vacuo and the residue was diluted with 1% aqueous NH_3 solution and was evaporated again. The residue was purified by ion-exchange chromatography (Dowex 50W–X8, H^+ form, eluting with 1% aqueous NH_3 solution) followed by reversed-phase flash chromatography (RP-18, using H_2O as eluent) to give the corresponding imino sugar. **Method B:** Crude piperidine obtained according to general procedure 9 was passed through an ion-exchange column (Dowex 50W–X8, H^+ form, eluting with 1% aqueous NH_3 solution). The solvent was evaporated to give a residue which was further purified by reversed-phase flash chromatography (RP-18, using H_2O as eluent) to give the corresponding imino sugar.

General procedure 11 for oxidation: IBX (1.2 equiv) [*CAUTION: IBX has been reported to detonate upon heavy impact and heating over 200 ºC*] [1] in DMSO (3 mL/mmol) was added to a stirred solution of diol (1.0 equiv) in THF (3 mL/mmol) at 8 °C. The resulting mixture was stirred for 24 h at 8 °C and then was quenched with H_2O (8 mL/mmol). The mixture was filtered through Celite and the filter cake was washed with EtOAc and H_2O. The layers were separated and the aqueous phase was extracted with EtOAc. The combined organic layers were dried (Na_2SO_4) and evaporated and the residue was purified by flash chromatography to give starting diol and the corresponding lactol.

General procedure 12 for bislactim ether hydrolysis and cyclization by reductive amination: A solution of lactol (1.0 equiv) in EtOH (16 mL/mmol) and 0.25 N HCl (2.0 equiv) was stirred with 10%

Pd/C (10% w/w) under H_2 (1 atm) for 4 h at rt. The catalyst was removed by filtration through a short pad of Celite, the filtrate was made basic (pH~8) by the addition of $NaHCO_3$ and was concentrated to half its initial volume. The aqueous layer was extracted with CH_2Cl_2 (5 x 10 mL/mmol) and the combined organic layers dried (Na_2SO_4) and evaporated. The crude was purified by reversed-phase flash chromatography to yield the corresponding pipecolate.

3. Characterization data for new compounds.

Addition of (*S*)-15 to aldehyde 13a: Following the method A of the general procedure 1, reaction of (*S*)-**15** (1.77 g, 9.6 mmol) with **13a** (2.0 g, 8.0 mmol) using $SnCl_2$ as additive (1.82 g, 9.6 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:9 to 1:3 ratio), 2.26 g of a mixture of adducts **16a** and **17a** in a 57:43 ratio (65%). Separation of the diastereoisomers was accomplished by flash chromatography on silica gel, using EtOAc/hexanes (gradient from 1:5 to 1:3) as eluent.

(3*R*,6*S*,1´*R*,2´*S*,3´*S*)-3-[4-Benzyloxy-1-hydroxy-2,3-isopropylidenedioxybutyl]-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**16a**): Colorless oil; *Rf* = 0.56 (EtOAc/hexanes 1:3); $[\alpha]^{23}_D$ –2.2 (c 0.9, CH_2Cl_2); IR (film) ν 3447, 2940, 1706, 1240 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.68 (d, *J* = 6.8 Hz, 3H), 1.04 (d, *J* = 6.8 Hz, 3H), 1.43 (s, 3H), 1.44 (s, 3H), 2.21 (dsp, *J* = 6.8, 3.4 Hz, 1H), 2.79 (brd, *J* = 7.3 Hz, 1H), 3.63 (s, 3H), 3.65-3.70 (m, 2H), 3.73 (s, 3H), 3.98 (t, *J* = 3.4 Hz, 1H), 4.02-4.11 (m, 3H), 4.32-4.41 (m, 1H), 4.53/4.67 (AB system, *J* = 12.2 Hz, 2H), 7.27-7.39 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 16.7 (CH_3), 19.0 (CH_3), 27.0 (CH_3), 27.1 (CH_3), 31.7 (CH), 52.5 (CH_3), 56.9 (CH), 60.5 (CH), 70.8 (CH_2), 72.0 (CH), 73.5 (CH_2), 76.8 (CH), 79.1 (CH), 109.5 (C), 127.6 (CH), 128.3 (CH), 137.9 (C), 161.2 (C), 165.4 (C); FABMS (thioglycerol) *m/z* 435 (MH^+, 100). Anal. Calcd for $C_{23}H_{34}N_2O_6$: C, 63.57; H, 7.89; N, 6.45. Found: C, 63.91; H, 8.18; N, 6.09.

(3*R*,6*S*,1´*S*,2´*S*,3´*S*)-3-[4-Benzyloxy-1-hydroxy-2,3-isopropylidenedioxybutyl]-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**17a**): Colorless oil; *Rf* = 0.53 (EtOAc/hexanes 1:3); $[\alpha]^{23}_D$ –13.7 (c 1.0, CH_2Cl_2); IR (film) ν 3446, 2943, 1704, 1237 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.70 (d, *J* = 6.8 Hz, 3H), 1.06 (d, *J* = 6.8 Hz, 3H), 1.35 (s, 3H), 1.37 (s, 3H), 2.25 (dsp, *J* = 6.8, 3.4 Hz, 1H), 3.06 (d, *J* = 7.3 Hz, 1H),

3.62-3.65 (m, 2H), 3.69 (s, 3H), 3.70 (s, 3H), 3.73-3.83 (m, 1H), 3.98 (t, J = 3.4 Hz, 1H), 3.98-4.11 (m, 1H), 4.16-4.28 (m, 2H), 4.57/4.63 (AB system, J = 12.3 Hz, 2H), 7.25-7.36 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 16.6 (CH_3), 19.0 (CH_3), 26.7 (CH_3), 27.0 (CH_3), 31.8 (CH), 52.2 (CH_3), 52.6 (CH_3), 58.4 (CH), 60.8 (CH), 71.0 (CH_2), 73.5 (CH_2), 74.1 (CH), 77.8 (CH), 79.3 (CH), 109.4 (C), 127.7 (CH), 128.4 (CH), 137.8 (C), 160.8 (C), 165.3 (C); FABMS (thioglycerol) *m/z* 435 (MH^+, 100), 377 (MH^+-C_3H_6O, 70). Anal. Calcd for $C_{23}H_{34}N_2O_6$: C, 63.57; H, 7.89; N, 6.45. Found: C, 63.41; H, 7.89; N, 6.46.

Addition of (*S*)-15 to aldehyde 13b: Following the method A of the general procedure 1, reaction of (*S*)-**15** (166 mg, 0.9 mmol) with **13b** (299 mg, 0.75 mmol) using $SnCl_2$ as additive (171 mg, 0.9 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:9 to 1:3 ratio), 341 mg of a mixture of adducts **16b**/**17b**/**18b** in a 57:35:8 ratio (78%). Separation of the two major diastereoisomers (**16b** and **17b**) was accomplished by flash chromatography on silica gel, using EtOAc/hexanes (gradient from 1:6 to 1:2) as eluent. Compounds **16b** and **17b** were also prepared according to the general procedure 3: silylation of **16c** (1.10 g, 3.20 mmol) gave 1.82 g of **16b** (98%) while silylation of **17c** (800 mg, 2.32 mmol) gave 1.32 g of **17b** (98%).

(3*R*,6*S*,1´*R*,2´*S*,3´*S*)-3-[4-*tert*-butyldiphenylsilyloxy-1-hydroxy-2,3-isopropylidenedioxybutyl]-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**16b**): Colorless oil; *Rf* = 0.56 (EtOAc/hexanes 1:9); $[\alpha]^{20}_D$ –5.9 (c 0.9, CH_2Cl_2); IR (film) ν 3441, 2931, 1707, 1473, 1437 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.69 (d, J = 6.8 Hz, 3H), 1.06 (s, 9H), 1.06 (d, J = 6.8 Hz, 3H), 1.41 (s, 3H), 1.44 (s, 3H), 2.28 (dsp, J = 6.8, 3.4 Hz, 1H), 2.85 (d, J = 8.2 Hz, 1H), 3.62 (s, 3H), 3.73 (s, 3H), 3.79-3.88 (m, 2H), 3.99 (t, J = 3.4 Hz, 1H); 4.06-4.11 (m, 2H); 4.24-4.30 (m, 2H), 7.36-7.43 (m, 6H), 7.68-7.72 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.7 (CH_3), 19.1 (CH_3), 19.2 (C), 26.8 (CH_3), 27.1 (CH_3), 27.3 (CH_3), 31.7 (CH), 52.5 (CH_3), 52.6 (CH_3), 57.4 (CH), 60.5 (CH), 64.5 (CH_2), 72.0 (CH), 78.3 (CH), 78.8 (CH), 109.4 (C), 127.7 (CH), 129.7 (CH), 133.1 (C), 133.2 (C), 135.6 (CH), 161.3 (C), 165.4 (C); FABMS (thioglycerol) *m/z* 583 (MH^+, 36), 141 (100). Anal. Calcd for $C_{32}H_{46}N_2O_6Si$: C, 65.95; H, 7.96; N, 4.81. Found: C, 66.25; H, 8.16; N, 4.50.

(3*R*,6*S*,1′*S*,2′*S*,3′*S*)-3-[4-*tert*-butyldiphenylsilyloxy-1-hydroxy-2,3-isopropylidenedioxybutyl]-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**17b**): Colorless oil; *Rf* = 0.47 (EtOAc/hexanes 1:4); $[\alpha]^{20}_{D}$ −14.9 (c 1.2, $CHCl_3$); IR (film) ν 3441, 2934, 2858, 2362, 1701, 1238 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 0.72 (d, *J* = 6.8 Hz, 3H), 1.07 (s, 9H), 1.07 (d, *J* = 6.8 Hz, 3H), 1.35 (s, 3H), 1.37 (s, 3H), 2.29 (dsp, *J* = 6.8, 3.4 Hz, 1H), 2.88 (d, *J* = 7.8 Hz, 1H), 3.69 (s, 3H), 3.70 (s, 3H), 3.79-3.81 (m, 2H), 3.99 (t, *J* = 3.4 Hz, 1H); 4.04-4.08 (m, 2H); 4.14-4.16 (m, 1H), 4.27-4.29 (m, 1H), 7.36-7.47 (m, 6H), 7.66-7.72 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.7 (CH_3), 19.1 (CH_3), 19.2 (C), 26.8 (CH_3), 26.9 (CH_3), 27.1 (CH_3), 31.8 (CH), 52.2 (CH_3), 52.5 (CH_3), 58.5 (CH), 60.8 (CH), 64.6 (CH_2), 74.3 (CH), 76.8 (CH), 80.9 (CH), 109.3 (C), 127.7 (CH), 129.7 (CH), 133.1 (C), 135.6 (CH), 160.8 (C), 165.4 (C); FABMS (thioglycerol) *m/z* 583 (MH^+, 32), 141 (100). Anal. Calcd for $C_{32}H_{46}N_2O_6Si$: C, 65.95; H, 7.96; N, 4.81. Found: C, 66.12; H, 7.71; N, 4.61.

Addition of (*S*)-15 to lactol 13c: Following the method B of the general procedure 1, reaction of (*S*)-**15** (317 mg, 1.72 mmol) with **13c** (91 mg, 0.57 mmol) using $SnCl_2$ as additive (326 mg, 1.72 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:10 to 3:1 ratio), 122 mg of a mixture of adducts **16c**/**17c** in a 1:1 ratio (62%). Separation of the two diastereoisomers was accomplished by flash chromatography on silica gel, using EtOAc/hexanes (gradient from 1:2 to 3:1) as eluent. Compounds **16c** and **17c** were also prepared according to the general procedure 2: hydrogenation of **16a** (1.2 g, 2.76 mmol) gave 0.92 g of **16c** (97%) while hydrogenation of **17a** (0.9 g, 2.07 mmol) gave 0.67 g of **17c** (95%).

(3*R*,6*S*,1′*R*,2′*S*,3′*S*)-3-(1,4-dihydroxy-2,3-isopropylidenedioxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**16c**): Colorless oil; *Rf* = 0.60 (EtOAc/hexanes 3:1); $[\alpha]^{20}_{D}$ +1.5 (c 1.9, CH_2Cl_2); IR (film) ν 3404, 2957, 1691, 1235 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.66 (d, *J* = 6.8 Hz, 3H), 1.06 (d, *J* = 6.8 Hz, 3H), 1.41 (s, 3H), 1.43 (s, 3H), 2.31 (dsp, *J* = 6.8, 3.4 Hz, 1H), 2.65 (brd, *J* = 4,4 Hz, 1H), 3.69 (s, 3H), 3.70-3.82 (m, 3H), 3.74 (s, 3H), 4.02 (t, *J* = 3.4 Hz, 1H); 4.00-4.19 (m, 4H); ^{13}C NMR ($CDCl_3$) δ 16.4 (CH_3), 19.1 (CH_3), 26.9 (CH_3), 27.0 (CH_3), 31.3 (CH), 52.6 (CH_3), 52.9 (CH_3), 56.9 (CH), 60.4 (CH),

63.9 (CH_2), 73.5 (CH), 77.8 (CH), 80.6 (CH), 109.2 (C), 160.4 (C), 166.5 (C); FABMS (thioglycerol) *m/z* 345 (MH^+, 100). Anal. Calcd for $C_{16}H_{28}N_2O_6$: C, 55.80; H, 8.19; N, 8.13. Found: C, 55.98; H, 8.40; N, 7.89.

(3*R*,6*S*,1´*S*,2´*S*,3´*S*)-3-(1,4-dihydroxy-2,3-isopropylidenedioxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**17c**): Colorless oil; *Rf* = 0.42 (EtOAc/hexanes 3:1); $[\alpha]^{20}_D$ –24.1 (c 1.0, CH_2Cl_2); IR (film) ν 3438, 2945, 1706, 1235 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.71 (d, *J* = 6.8 Hz, 3H), 1.05 (d, *J* = 6.8 Hz, 3H), 1.33 (s, 3H), 1.36 (s, 3H), 2.28 (dsp, *J* = 6.8, 3.9 Hz, 1H), 2.71 (brs, 1H), 3.12 (brs, 1H), 3.70 (s, 3H), 3.72 (s, 3H), 3.60-3.80 (m, 3H), 3.99 (t, *J* = 3.6 Hz, 1H); 4.08-4.15 (m, 2H), 4.23 (t, *J* = 3.9 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 16.6 (CH_3), 18.9 (CH_3), 26.6 (CH_3), 26.9 (CH_3), 31.8 (CH), 52.2 (CH_3), 52.7 (CH_3), 58.2 (CH), 60.7 (CH), 63.3 (CH_2), 73.6 (CH), 77.7 (CH), 80.6 (CH), 109.1 (C), 160.6 (C), 165.7 (C); FABMS (thioglycerol) *m/z* 345 (MH^+, 100). Anal. Calcd for $C_{16}H_{28}N_2O_6$: C, 55.80; H, 8.19; N, 8.13. Found: C, 56.07; H, 8.00; N, 8.36.

Addition of (*R*)-12 to aldehyde (*S*,*S*)-19a: Following the method A of the general procedure 1, reaction of (*R*)-**12** (204 mg, 0.96 mmol) with (*S*,*S*)-**19a** (200 mg, 0.8 mmol) using $SnCl_2$ as additive (370 mg, 1.92 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:10 to 1:3 ratio), 240 mg of a mixture of adducts **21a/22a/23a** in a 65:31:3 ratio (65%). Separation of the diastereoisomers was accomplished by flash chromatography on silica gel, using EtOAc/hexanes (gradient from 1:6 to 1:3) as eluent.

(3*S*,6*R*,1´*R*,2´*R*,3´*S*)-3-[4-Benzyloxy-1-hydroxy-2,3-isopropylidenedioxybutyl]-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (**21a**): Colorless oil; *Rf* = 0.32 (EtOAc/hexanes 1:5); $[\alpha]^{25}_D$ +37.9 (c 1.9, CH_2Cl_2); IR (film) ν 3430, 1693, 1648, 1234, 1075 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.71 (d, *J* = 6.8 Hz, 3H), 1.05 (d, *J* = 6.8 Hz, 3H), 1.24-1.35 (m, 12H), 2.32 (dsp, *J* = 6.8, 3.5 Hz, 1H), 3.27 (d, *J* = 5.9 Hz, 1H), 3.47-3.53 (m, 1H), 3.70-3.79 (m, 1H), 3.91 (t, *J* = 3.5 Hz, 1H), 4.00-4.40 (m, 8H), 4.58 (s, 2H), 7.28-7.35 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 14.3 (CH_3), 16.5 (CH_3), 19.1 (CH_3), 25.4 (CH_3), 27.8 (CH_3), 31.3 (CH), 58.3 (CH), 60.5 (CH), 60.7 (CH_2), 68.8 (CH_2), 71.1 (CH), 73.8 (CH_2), 75.6 (CH), 76.8 (CH),

108.5 (C), 127.9 (CH), 128.0 (CH), 128.5 (CH), 137.2 (C), 160.4 (C), 165.0 (C); FABMS (thioglycerol) *m/z* 463 (MH^+, 49). Anal. Calcd for $C_{25}H_{38}N_2O_6$: C, 64.91; H, 8.28; N, 6.06. Found: C, 65.19; H, 8.59; N, 5.98

(3*S*,6*R*,1′*S*,2′*R*,3′*S*)-3-[4-Benzyloxy-1-hydroxy-2,3-isopropylidenedioxybutyl]-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (**22a**): Colorless oil; *Rf* = 0.20 (EtOAc/hexanes 1:4); $[\alpha]^{25}_D$ +5.7 (c 2.4, CH_2Cl_2); IR (film) ν 3448, 2978, 1696, 1238, 1093, 1036 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.70 (d, *J* = 6.8 Hz, 3H), 1.01 (d, *J* = 6.8 Hz, 3H), 1.23-1.33 (m, 6H), 1.37 (s, 3H), 1.47 (s, 3H), 2.25 (dsp, *J* = 6.8, 3.3 Hz, 1H), 2.73 (brd, *J* = 7.6 Hz, 1H), 3.61-3.79 (m, 2H), 3.95 (t, *J* = 3.3 Hz, 1H), 4.05-4.26 (m, 6H), 4.35-4.46 (m, 2H), 4.58 (s, 2H), 7.24-7.37 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 16.8 (CH_3), 19.0 (CH_3), 25.3 (CH_3), 27.6 (CH_3), 31.9 (CH), 57.4 (CH), 60.7 (CH), 60.8 (CH_2), 69.3 (CH_2), 70.0 (CH), 73.5 (CH_2), 75.8 (CH), 76.8 (CH), 108.3 (C), 127.6 (CH), 127.7 (CH), 128.3 (CH), 137.9 (C), 160.9 (C), 164.9 (C); FABMS (thioglycerol) *m/z* 463 (MH^+, 60). Anal. Calcd for $C_{25}H_{38}N_2O_6$: C, 64.91; H, 8.28; N, 6.06. Found: C, 65.22; H, 8.08; N, 5.84.

(3*R*,6*R*,1′*R*,2′*R*,3′*S*)-3-[4-Benzyloxy-1-hydroxy-2,3-isopropylidenedioxybutyl]-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (**23a**): Colorless oil; *Rf* = 0.48 (EtOAc/hexanes 1:5); $[\alpha]^{22}_D$ –46.6 (c 1.6, CH_2Cl_2); IR (film) ν 3465, 1696, 1646, 1233 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.75 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H), 1.28 (t, *J* = 7.0 Hz, 3H), 1.29 (t, *J* = 7.0 Hz, 3H), 1.40 (s, 3H), 1.46 (s, 3H), 2.25 (dsp, *J* = 6.8, 3.7 Hz, 1H), 2.46 (d, *J* = 7.2 Hz, 1H), 3.63 (dd, *J* = 9.8, 5.7 Hz, 1H), 3.83 (dd, *J* = 8.1, 4.2 Hz, 1H), 3.88 (dd, *J* = 5.9, 3.7 Hz, 1H), 4.04-4.50 (m, 8H), 4.54/4.68 (AB system, *J* = 11.9 Hz, 2H), 7.31-7.36 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 14.3 (CH_3), 17.1 (CH_3), 19.7 (CH_3), 25.6 (CH_3), 28.1 (CH_3), 31.0 (CH), 56.4 (CH), 60.3 (CH), 60.5 (CH_2), 60.6 (CH), 68.5 (CH), 68.7 (CH_2), 73.7 (CH_2), 76.1 (CH), 108.6 (C), 127.9 (CH), 128.4 (CH), 137.5 (C), 160.4 (C), 164.7 (C); FABMS (thioglycerol) *m/z* 463 (MH^+, 60). Anal. Calcd for $C_{25}H_{38}N_2O_6$: C, 64.91; H, 8.28; N, 6.06. Found: C, 65.10; H, 8.35; N, 5.90.

Addition of (*R*)-12 to lactol (*S*,*S*)-19c: Following the method B of the general procedure 1, reaction of (*R*)-**12** (796 mg, 3.75 mmol) with (*S*,*S*)-**19c** (200 mg, 1.25 mmol) using $SnCl_2$ as additive (1.42 g, 7.5 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:4 to 2:3 ratio), 414 mg of a mixture of adducts **21c**/**22c** in a 91:9 ratio (89%). The same reaction, using $Ti(NEt_2)_3Cl$ as additive (1.12 g, 3.75 mmol) gave, after flash chromatography, 363 mg of a mixture of adducts **21c**/**22c** in a 30:70 ratio (78%). The same reaction, using $MgBr_2{\cdot}OEt_2$ as additive (968 mg, 3.75 mmol) gave, after flash chromatography, 326 mg of a mixture of adducts **21c**/**22c**/**23c** in a 33:6:61 ratio (70%). Separation of the three diastereoisomers was accomplished by flash chromatography on silica gel, using EtOAc/hexanes (gradient from 1:4 to 3:1) as eluent. Compounds **21c**, **22c** and **23c** were also prepared according to the general procedure 2: hydrogenation of **21a** (610 mg, 1.32 mmol) gave 491 mg of **21c** (100%), hydrogenation of **22a** (305 mg, 0.66 mmol) gave 245 mg of **22c** (100%), while hydrogenation of **23a** (98 mg, 0.21 mmol) gave 79 mg of **23c** (100%).

(3*S*,6*R*,1´*R*,2´*R,3´S*)-3-(1,4-dihydroxy-2,3-isopropylidenedioxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**21c**): Colorless oil; *Rf* = 0.29 (EtOAc/hexanes 1:3); $[\alpha]^{26}_D$ +38.0 (c 1.6, CH_2Cl_2); IR (film) ν 3406, 1657, 1370, 1237 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.70 (d, *J* = 6.8 Hz, 3H), 1.03 (d, *J* = 6.8 Hz, 3H), 1.24-1.32 (m, 9H), 1.35 (s, 3H), 2.27 (dsp, *J* = 6.8, 3.3 Hz, 1H), 3.24 (brs, 1H), 3.40 (brd, *J* = 6.8 Hz, 1H), 3.69-3.95 (m, 2H), 3.92 (t, *J* = 3.3 Hz, 1H), 3.99-4.33 (m, 8H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 14.3 (CH_3), 16.7 (CH_3), 19.0 (CH_3), 25.0 (CH_3), 27.4 (CH_3), 31.9 (CH), 58.4 (CH), 60.6 (CH), 60.7 (CH_2), 60.9 (CH_2), 61.1 (CH_2), 70.5 (CH), 76.3 (CH), 77.5 (CH), 108.3 (C), 160.0 (C), 165.2 (C); FABMS (thioglycerol) *m/z* 373 (MH^+, 100). Anal. Calcd for $C_{18}H_{32}N_2O_6$: C, 58.05; H, 8.66; N, 7.52. Found: C, 57.72; H, 8.83; N, 7.34.

(3*S*,6*R*,1´*S*,2´*R*,3´*S*)-3-(1,4-dihydroxy-2,3-isopropylidenedioxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**22c**): Colorless oil; *Rf* = 0.31 (EtOAc/hexanes 1:3); $[\alpha]^{23}_D$ +25.8 (c 2.1, CH_2Cl_2); IR (film) ν 3442, 2983, 1665, 1462, 1369, 1239 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.72 (d, *J* = 6.8 Hz, 3H), 1.04 (d, *J* = 6.8 Hz, 3H), 1.25-1.34 (m, 6H), 1.36 (s, 3H), 1.50 (s, 3H), 2.28 (dsp, *J* = 6.8, 3.4 Hz, 1H), 2.96 (brs,

1H), 3.38 (brd, 1H), 3.79 (d, J = 5.4 Hz, 2H), 3.95 (t, J = 3.4 Hz, 1H), 4.07-4.28 (m, 7H), 4.36 (dd, J = 6.3, 3.9 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 14.2 (CH_3), 16.7 (CH_3), 19.0 (CH_3), 25.4 (CH_3), 27.5 (CH_3), 31.9 (CH), 57.1 (CH), 60.8 (CH), 61.1 (CH_2), 61.5 (CH_2), 70.0 (CH), 76.3 (CH), 77.6 (CH), 108.3 (C), 160.5 (C), 165.2 (C); FABMS (thioglycerol) *m/z* 373 (MH^+, 100). Anal. Calcd for $C_{18}H_{32}N_2O_6$: C, 58.05; H, 8.66; N, 7.52. Found: C, 57.80; H, 8.70; N, 7.30.

(3*R*,6*R*,1´*R*,2´*R*,3´*S*)-3-(1,4-dihydroxy-2,3-isopropylidenedioxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (**23c**): Colorless oil; *Rf* = 0.44 (EtOAc/hexanes 1:3); $[\alpha]^{21}_D$ –30.2 (c 2.2, CH_2Cl_2); IR (film) ν 3500, 2940, 1700, 1470, 1380, 1230 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 0.72 (d, J = 6.8 Hz, 3H), 1.09 (d, J = 6.8 Hz, 3H), 1.29 (t, J = 7.0 Hz, 6H), 1.39 (s, 3H), 1.47 (s, 3H), 2.13 (brs, 1H), 2.37 (dsp, J = 6.8, 3.4 Hz, 1H), 2.91 (brs, 1H), 3.81-3.99 (m, 3H), 4.12-4.41 (m, 8H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 14.3 (CH_3), 16.9 (CH_3), 19.5 (CH_3), 25.5 (CH_3), 27.9 (CH_3), 30.6 (CH), 56.0 (CH), 60.2 (CH), 60.7 (CH_2), 60.9 (CH_2), 68.7 (CH), 76.1 (CH), 77.5 (CH), 108.5 (C), 160.3 (C), 165.9 (C); FABMS (thioglycerol) *m/z* 373 (MH^+, 100). Anal. Calcd for $C_{18}H_{32}N_2O_6$: C, 58.05; H, 8.66; N, 7.52. Found: C, 57.71; H, 8.62; N, 7.13.

(3*S*,6*R*,1´*S*,2´*S*,3´*S*)-3-[1-benzyloxy-4-*tert*-butyldiphenylsilyloxy-2,3-isopropylidenedioxybutyl]-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (24b): Following the general procedure 4, benzylation of **14b** (1.5 g, 2.46 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:19 to 1:9 ratio), 1.29 g of **24b** (75%) as a colorless oil. *Rf* = 0.5 (EtOAc/hexanes 1:12); $[\alpha]^{24}_D$ +19.7 (c 1.1, CH_2Cl_2); IR (film) ν 2900, 1680, 1450, 1350, 1300, 1220, 1100 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 0.72 (d, J = 6.8 Hz, 3H), 1.05 (s, 9H), 1.08 (d, J = 6.8 Hz, 3H), 1.15 (t, J = 7.3 Hz, 3H), 1.35 (t, J = 7.3 Hz, 3H), 1.49 (s, 6H), 2.30 (dsp, J = 6.8, 3.9 Hz, 1H), 3.72-4.30 (m, 10H), 4.40-4.60 (m, 3H), 7.13-7.40 (m, 11H), 7.67-7.74 (m, 4H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 14.4 (CH_3), 16.5 (CH_3), 19.2 (C), 26.7 (CH_3), 27.5 (CH_3), 27.6 (CH_3), 31.3 (CH), 56.4 (CH), 60.4 (CH), 60.6 (CH_2), 64.2 (CH_2), 73.7 (CH_2), 74.9 (CH), 80.8 (CH), 81.3 (CH), 109.1 (C), 127.5 (CH), 127.8 (CH), 128.2 (CH), 129.4 (CH), 133.4

(C), 133.6 (C), 135.6 (CH), 138.0 (C), 161.5 (C), 163.7 (C); FABMS (thioglycerol) *m/z* 701 (MH^+, 51). Anal. Calcd for $C_{41}H_{56}N_2O_6Si$: C, 70.25; H, 8.05; N, 4.00. Found: C, 69.92; H, 8.21; N, 3.76.

(3*R*,6*S*,1′*R*,2′*S*,3′*S*)-3-[1-benzyloxy-4-*tert*-butyldiphenylsilyloxy-2,3-isopropylidenedioxybutyl]-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (25b): Following the general procedure 4, benzylation of **16b** (1.35 g, 2.32 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:19 to 1:9 ratio), 1.26 g of **25b** (81%) as a colorless oil. *Rf* = 0.35 (EtOAc/hexanes 1:9); $[\alpha]^{23}_D$ –30.4 (c 2.5, CH_2Cl_2); IR (film) ν 2942, 2861, 2361, 1701, 1240, 1104 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 0.65 (d, *J* = 6.8 Hz, 3H), 1.06 (d, *J* = 6.8 Hz, 3H), 1.06 (s, 9H), 1.46 (s, 3H), 1.48 (s, 3H), 2.29 (dsp, *J* = 6.8, 2.4 Hz, 1H), 3.43 (s, 3H), 3.64 (s, 3H), 3.81 (dd, *J* = 11.4, 5.4 Hz, 1H), 3.90-3.98 (m, 3H), 4.11 (dd, *J* = 11.5, 1.9 Hz, 1H), 4.28-4.37 (m, 2H), 4.50 (d, *J* = 11.5 Hz, 1H), 4.74 (d, *J* = 11.5 Hz, 1H), 7.21-7.44 (m, 11H), 7.71-7.75 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.5 (CH_3), 19.1 (CH_3), 19.2 (C), 26.8 (CH_3), 27.3 (CH_3), 27.4 (CH_3), 30.9 (CH), 52.2 (CH_3), 52.4 (CH_3), 56.5 (CH), 60.0 (CH), 65.1 (CH_2), 73.9 (CH_2), 78.2 (CH), 79.6 (CH), 81.1 (CH), 109.1 (C), 127.3 (CH), 127.6 (CH), 127.7 (CH), 128.1 (CH), 129.5 (CH), 133.5 (C), 133.6 (C), 135.6 (CH), 135.7 (CH), 138.7 (C), 161.0 (C), 164.2 (C); FABMS (thioglycerol) *m/z* 673 (MH^+, 87), 141 (100). Anal. Calcd for $C_{39}H_{52}N_2O_6Si$: C, 69.61; H, 7.79; N, 4.16. Found: C, 69.78; H, 8.03; N, 3.95.

(3*R*,6*S*,1′*S*,2′*S*,3′*S*)-3-[1-benzyloxy-4-*tert*-butyldiphenylsilyloxy-2,3-isopropylidenedioxybutyl]-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (26b): Following the general procedure 4, benzylation of **17b** (823 mg, 1.41 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes 1:10), 751 mg of **26b** (79%) as a colorless oil. *Rf* = 0.29 (EtOAc/hexanes 1:9); $[\alpha]^{23}_D$ –31.1 (c 2.2, CH_2Cl_2); IR (film) ν 2933, 2857, 2364, 1697, 1238, 1113 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 0.72 (d, *J* = 6.8 Hz, 3H), 1.06 (s, 9H), 1.09 (d, *J* = 6.8 Hz, 3H), 1.39 (s, 3H), 1.43 (s, 3H), 2.31 (dsp, *J* = 6.8, 3.2 Hz, 1H), 3.67-3.72 (m, 1H), 3.71 (s, 3H), 3.72 (s, 3H), 3.87 (dd, *J* = 11.4, 2.4 Hz, 1H), 3.91-3.99 (m, 3H), 4.44 (dd, *J* = 9.2, 7.0 Hz, 1H), 4.50 (dd, *J* = 3.90, 1.8 Hz, 1H), 4.50/4.67 (AB system, *J* = 11.5 Hz, 2H), 7.18-7.45 (m, 11H), 7.68-7.75 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.6 (CH_3), 19.1 (CH_3),

19.3 (C), 26.7 (CH_3), 27.2 (CH_3), 27.3 (CH_3), 31.3 (CH), 52.3 (CH_3), 52.5 (CH_3), 57.6 (CH), 60.4 (CH), 64.2 (CH_2), 73.6 (CH_2), 74.8 (CH), 81.9 (CH), 83.8 (CH), 109.1 (C), 127.5 (CH), 127.6 (CH), 127.6 (CH), 127.9 (CH), 128.3 (CH), 129.4 (CH), 129.5 (CH), 133.4 (C), 133.6 (C), 135.6 (CH), 135.7 (CH), 138.0 (C), 161.1 (C), 164.4 (C); FABMS (thioglycerol) *m/z* 673 (MH^+, 18), 141 (61), 214 (100). Anal. Calcd for $C_{39}H_{52}N_2O_6Si$: C, 69.61; H, 7.79; N, 4.16. Found: C, 69.46; H, 7.58; N, 3.99.

(3*S*,6*R*,1´*S*,2´*S*,3´*S*)-3-(1-benzyloxy-4-hydroxy-2,3-isopropylidenedioxybutyl)-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (24c): Following the general procedure 5, desilylation of **24b** (1.00 g, 1.43 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:6), 627 mg of alcohol **24c** (95%). Colorless oil; *Rf* = 0.35 (silica gel, EtOAc/hexanes 1:6); $[\alpha]^{23}_D$ +68.3 (c 5.0, CH_2Cl_2); IR (film) ν 3400, 2900, 1680, 1450, 1350, 1300, 1220, 1050 cm^{-1}; ^1H NMR ($CDCl_3$) δ 0.68 (d, *J* = 6.8 Hz, 3H), 1.05 (d, *J* = 6.8 Hz, 3H), 1.27 (t, *J* = 6.8 Hz, 3H), 1.30 (t, *J* = 6.8 Hz, 3H), 1.43 (s, 6H), 2.33 (dsp, *J* = 6.8, 3.4 Hz, 1H), 3.31 (brs, 1H), 3.69-3.87 (m, 2H), 3.90 (t, *J* = 3.4 Hz, 1H), 4.03-4.32 (m, 8H), 4.50/4.58 (AB system, *J* = 11.2 Hz, 2H), 7.20-7.37 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 14.3 (CH_3), 16.4 (CH_3), 19.1 (CH_3), 27.1 (CH_3), 31.2 (CH), 56.7 (CH), 60.3 (CH), 60.7 (CH_2), 61.1 (CH_2), 64.2 (CH_2), 74.2 (CH_2), 78.1 (CH), 78.9 (CH), 79.9 (CH), 108.8 (C), 127.7 (CH), 128.0 (CH), 128.3 (CH), 137.9 (C), 160.8 (C), 164.6 (C); FABMS (thioglycerol) *m/z* 463 (MH^+, 71). Anal. Calcd for $C_{25}H_{38}N_2O_6$: C, 64.91; H, 8.28; N, 6.06. Found: C, 65.23; H, 8.52; N, 5.99.

(3*R*,6*S*,1´*R*,2´*S*,3´*S*)-3-(1-benzyloxy-4-hydroxy-2,3-isopropylidenedioxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (25c): Following the general procedure 5, desilylation of **25b** (920 mg, 1.37 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes 1:6), 486 mg of alcohol **25c** (82%). Colorless oil; *Rf* = 0.50 (silica gel, EtOAc/hexanes 1:3); $[\alpha]^{23}_D$ +48.2 (c 1.4, CH_2Cl_2); IR (film) ν 3457, 2956, 1765, 1244 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 0.65 (d, *J* = 6.8 Hz, 3H), 1.09 (d, *J* = 6.8 Hz, 3H), 1.42 (s, 3H), 1.46 (s, 3H), 2.34 (dsp, *J* = 6.8, 3.1 Hz, 1H), 3.68 (s, 3H), 3.69 (s, 3H), 3.75-3.92 (m, 2H), 3.97-4.02 (m, 2H), 4.16 (dt, *J* = 3.8, 7.2 Hz, 1H), 4.24 (t, *J* = 3.1 Hz, 1H), 4.32 (t, *J* = 7.8 Hz, 1H), 4.52-4.57 (m, 1H), 4.55 (d, *J* = 11.2 Hz, 1H), 4.79 (d, *J* = 11.2 Hz, 1H), 7.26-7.35 (m, 5H);

^{13}C NMR (75 MHz, $CDCl_3$) δ 16.3 (CH_3), 19.2 (CH_3), 26.9 (CH_3), 27.0 (CH_3), 30.7 (CH), 52.4 (CH_3), 52.9 (CH_3), 56.9 (CH), 60.1 (CH), 64.7 (CH_2), 74.3 (CH_2), 78.1 (CH), 81.4 (CH), 82.3 (CH), 108.7 (C), 126.9 (CH), 127.5 (CH), 128.0 (CH), 128.1 (CH), 128.5 (CH), 138.4 (C), 160.2 (C), 166.4 (C); FABMS (thioglycerol) *m/z* 435 (MH^+, 63), 141 (100). Anal. Calcd for $C_{23}H_{34}N_2O_6$: C, 63.57; H, 7.89; N, 6.45. Found: C, 63.59; H, 8.06; N, 6.71.

(3*R*,6*S*,1´*S*,2´*S*,3´*S*)-3-(1-benzyloxy-4-hydroxy-2,3-isopropylidenedioxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (26c): Following the general procedure 5, desilylation of **26b** (626 mg, 0.93 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes 1:3), 375 mg of alcohol **26c** (93%). Colorless oil; *Rf* = 0.25 (silica gel, EtOAc/hexanes 1:3); $[\alpha]^{25}_D$ −17.2 (c 1.0, $CHCl_3$); IR (film) ν 3457, 2954, 1701, 1238, 1068 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.70 (d, *J* = 6.8 Hz, 3H), 1.06 (d, *J* = 6.8 Hz, 3H), 1.33 (s, 3H), 1.36 (s, 3H), 2.30 (dsp, *J* = 6.8, 3.2 Hz, 1H), 2.28-2.37 (m, 1H), 3.65-3.74 (m, 2H), 3.72 (s, 3H), 3.74 (s, 3H), 3.87-3.96 (m, 3H), 4.05 (dd, *J* = 8.5, 7.3 Hz, 1H), 4.43 (dd, *J* = 3.9, 2.3 Hz, 1H), 4.56 (d, *J* = 11.4 Hz, 1H), 4.72 (d, *J* = 11.4 Hz, 1H), 7.30-7.39 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.6 (CH_3), 19.1 (CH_3), 26.7 (CH_3), 27.0 (CH_3), 31.4 (CH), 52.4 (CH_3), 52.6 (CH_3), 57.0 (CH), 60.4 (CH), 63.8 (CH_2), 73.4 (CH_2), 76.9 (CH), 80.8 (CH), 82.4 (CH), 109.1 (C), 128.0 (CH), 128.3 (CH), 128.4 (CH), 137.4 (C), 160.9 (C), 164.8 (C); FABMS (thioglycerol) *m/z* 435 (MH^+, 100). Anal. Calcd for $C_{23}H_{34}N_2O_6$: C, 63.57; H, 7.89; N, 6.45. Found: C, 63.31; H, 7.61; N, 6.30.

(3*S*,6*R*,1´*S*,2´*S*,3´*S*)-3-(1-benzyloxy-2,3-isopropylidenedioxy-4-(methanesulfonyl)oxybutyl)-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (24d): Following the general procedure 6, mesylation of **24c** (600 mg, 1.3 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes 1:4), 701 mg of mesylate **24d** (100%). Colorless solid; m.p. 186-188 °C; *Rf* = 0.35 (silica gel, EtOAc/hexanes 1:4); $[\alpha]^{28}_D$ +29.8 (c 1.0, CH_2Cl_2); IR (KBr) ν 2970, 1695, 1352, 1300, 1238, 1176 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 0.69 (d, *J* = 6.8 Hz, 3H), 1.05 (d, *J* = 6.8 Hz, 3H), 1.27 (t, *J* = 7.3 Hz, 3H), 1.32 (t, *J* = 7.3 Hz, 3H), 1.43 (s, 3H), 1.44 (s, 3H), 2.33 (dsp, *J* = 6.8, 3.4 Hz, 1H), 2.97 (s, 3H), 3.93 (t, *J* = 3.4 Hz, 1H), 4.04-4.37 (m, 9H), 4.49-4.55 (m, 3H), 7.23-7.36 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 14.4 (CH_3), 16.4 (CH_3),

19.1 (CH_3), 26.9 (CH_3), 27.1 (CH_3), 31.4 (CH), 37.5 (CH_3), 56.5 (CH), 60.4 (CH), 60.7 (CH_2), 60.9 (CH_2), 70.9 (CH_2), 73.9 (CH_2), 76.6 (CH), 76.8 (CH), 79.8 (CH), 109.8 (C), 127.8 (CH), 128.1 (CH), 128.4 (CH), 137.9 (C), 160.8 (C), 164.6 (C); FABMS (thioglycerol) *m/z* 541 (MH^+, 56). Anal. Calcd for $C_{26}H_{40}N_2O_8S$: C, 57.76; H, 7.46; N, 5.18. Found: C, 57.75; H, 7.70; N, 5.03.

(3*R*,6*S*,1´*R*,2´*S*,3´*S*)-3-(1-benzyloxy-2,3-isopropylidenedioxy-4-(methanesulfonyl)oxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (25d): Following the general procedure 6, mesylation of **25c** (310 mg, 0.71 mmol) gave, after flash chromatography (silica gel, MeOH/CH_2Cl_2 1:50); 360 mg of mesylate **25d** (99%). Colorless solid; m.p. 76-79 °C; *Rf* = 0.2 (silica gel, MeOH/CH_2Cl_2 1%); $[\alpha]^{20}_D$ –44.5 (c 1.5, CH_2Cl_2); IR (KBr) ν 3854, 2934, 1698, 1355, 1246 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 0.68 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H), 1.48 (s, 3H), 1.49 (s, 3H), 2.33 (dsp, *J* = 6.8, 3.3 Hz, 1H), 3.06 (s, 3H), 3.68 (s, 3H), 3.69 (s, 3H), 4.00 (t, *J* = 3.4 Hz, 1H), 4.09 (dd, *J* = 7.3, 2.3 Hz, 1H), 4.14 (dd, *J* = 3.4, 2.5 Hz, 1H), 4.27-4.36 (m, 2H), 4.49-4.51 (m, 2H), 4.72 (d, *J* = 11.3 Hz, 1H), 4.82 (dd, *J* = 11.3, 1.8 Hz, 1H), 7.26-7.40 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.4 (CH_3), 19.1 (CH_3), 27.0 (CH_3), 27.1 (CH_3), 31.1 (CH), 37.7 (CH_3), 52.3 (CH_3), 52.7 (CH_3), 56.3 (CH), 60.2 (CH), 70.2 (CH_2), 73.9 (CH_2), 76.0 (CH), 78.2 (CH), 82.2 (CH), 110.0 (C), 127.5 (CH), 127.9 (CH), 128.2 (CH), 138.3 (C), 160.5 (C), 165.0 (C); FABMS (thioglycerol) *m/z* 513 (MH^+, 76), 141 (100). Anal. Calcd for $C_{24}H_{36}N_2O_8S$: C, 56.23; H, 7.08; N, 5.46. Found: C, 56.01; H, 7.22; N, 5.22.

(3*R*,6*S*,1´*S*,2´*S*,3´*S*)-3-(1-benzyloxy-2,3-isopropylidenedioxy-4-(methanesulfonyl)oxybutyl)-2,5-dimethoxy-3,6-dihydro-6-isopropylpyrazine (26d): Following the general procedure 6, mesylation of **26c** (331 mg, 0.76 mmol) gave, after flash chromatography (silica gel, MeOH/CH_2Cl_2 from 1:40 to 1:30 ratio), 375 mg of mesylate **26d** (96%). Colorless oil; *Rf* = 0.31 (silica gel, MeOH/CH_2Cl_2 2%); $[\alpha]^{20}_D$ –27.9 (c 1.0, $CHCl_3$); IR (film) ν 2953, 2250; 1698, 1226, 1189 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 0.70 (d, *J* = 6.8 Hz, 3H), 1.06 (d, *J* = 6.8 Hz, 3H), 1.32 (s, 3H), 1.37 (s, 3H), 2.30 (dsp, *J* = 6.8, 3.2 Hz, 1H), 2.95 (s, 3H), 3.72 (s, 3H), 3.74 (s, 3H), 3.92-4.06 (m, 4H), 4.16 (dd, *J* = 11.0, 6.5 Hz, 1H), 4.40-4.45 (m, 2H), 4.52 (d, *J* = 11.3 Hz, 1H), 4.72 (d, *J* = 11.3 Hz, 1H), 7.28-7.40 (m, 5H); ^{13}C NMR (75

MHz, $CDCl_3$) δ 16.6 (CH_3), 19.1 (CH_3), 26.8 (CH_3), 26.9 (CH_3), 31.5 (CH), 37.5 (CH_3), 52.4 (CH_3), 52.6 (CH_3), 57.0 (CH), 60.5 (CH), 70.7 (CH_2), 73.3 (CH_2), 75.4 (CH), 78.5 (CH), 82.3 (CH), 110.2 (C), 128.1 (CH), 128.3 (CH), 128.6 (CH), 137.4 (C), 160.7 (C), 164.8 (C); FABMS (thioglycerol) *m/z* 513 (MH^+, 100). Anal. Calcd for $C_{24}H_{36}N_2O_8S$: C, 56.23; H, 7.08; N, 5.46. Found: C, 56.47; H, 6.80; N, 5.63.

Ethyl (2*S*,3*S*,4*S*,5*S*)-2-Amino-3-benzyloxy-4,5-isopropylidenedioxy-6-(methanesulfonyl)oxy-hexanoate (27): Following the general procedure 7 hydrolysis of compound **24d** (700 mg, 1.29 mmol) in EtOH (21 mL) gave, after flash chromatography (silica gel, EtOAc/hexanes 4:1), 364 mg of amino ester **27** (65%) and 238 mg of compound **24d** (34%). The yield of compound **27** could be increased to 82% by resubjecting the recovered starting material to these hydrolytic conditions. Colorless oil; *Rf* = 0.61 (silica gel, EtOAc/hexanes 4:1); $[\alpha]^{27}_D$ –3.2 (c 1.3, CH_2Cl_2); IR (film) ν 3433, 1740, 1237 cm^{-1}; ^1H NMR ($CDCl_3$) δ 1.30 (t, *J* = 7.3 Hz, 3H), 1.43 (s, 6H), 2.99 (s, 3H), 3.67 (d, *J* = 1.5 Hz, 1H), 4.03-4.38 (m, 6H), 4.46-4.49 (m, 1H), 4.51/4.57 (AB system, *J* = 11.2 Hz, 2H), 7.28-7.41 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 26.9 (CH_3), 27.1 (CH_3), 37.5 (CH_3), 55.2 (CH), 61.4 (CH_2), 70.4 (CH_2), 73.9 (CH_2), 76.4 (CH), 77.2 (CH), 80.4 (CH), 109.9 (C), 128.1 (CH), 128.2 (CH), 128.5 (CH), 137.1 (C), 174.8 (C); FABMS (thioglycerol) *m/z* 432 (MH^+, 100). Anal. Calcd for $C_{19}H_{29}NO_8S$: C, 52.89; H, 6.77; N, 3.25; S, 7.43. Found: C, 53.10; H, 6.48; N, 3.26; S, 7.20.

Methyl (2*R*,3*R*,4*S*,5*S*)-2-Amino-3-benzyloxy-4,5-isopropylidenedioxy-6-(methanesulfonyl)oxy-hexanoate (28): Following the general procedure 7 hydrolysis of compound **25d** (336 mg, 0.65 mmol) in MeOH (20 mL) gave, after flash chromatography (silica gel, EtOAc/hexanes 4:1 to EtOAc), 219 mg of amino ester **28** (80%). Colorless solid; m.p. 89-90 °C; *Rf* = 0.51 (silica gel, EtOAc/hexanes 4:1); $[\alpha]^{26}_D$ –2.4 (c 1.1, CH_2Cl_2); IR (KBr) ν 3379, 2994, 1736, 1355, 1171 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 1.45 (s, 3H), 1.47 (s, 3H), 1.65 (s, 2H), 3.06 (s, 3H), 3.52 (d, *J* = 2.0 Hz, 1H), 3.64 (s, 3H), 4.07 (dd, *J* = 6.5, 2.1 Hz, 1H), 4.18-4.27 (m, 2H), 4.38-4.44 (m, 1H), 4.58/4.75 (AB system, *J* = 11.6 Hz, 2H), 4.69 (dd, *J* = 11.6, 2.1 Hz, 1H), 7.27-7.38 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 26.9 (CH_3),

27.0 (CH_3), 37.7 (CH_3), 52.2 (CH_3), 55.4 (CH), 70.0 (CH_2), 73.7 (CH_2), 75.8 (CH), 78.3 (CH), 79.2 (CH), 110.2 (C), 127.9 (CH), 128.1 (CH), 128.3 (CH), 137.7 (C), 174.6 (C); FABMS (thioglycerol) *m/z* 418 (MH^+, 100). Anal. Calcd for $C_{18}H_{27}NO_8S$: C, 51.79; H, 6.52; N, 3.36; S, 7.68. Found: C, 52.08; H, 6.80; N, 3.25; S, 7.93.

Methyl (2*R*,3*S*,4*S*,5*S*)-2-Amino-3-benzyloxy-4,5-isopropylidenedioxy-6-(methanesulfonyl)oxy-hexanoate (29): Following the general procedure 7 hydrolysis of compound **26d** (303 mg, 0.59 mmol) in MeOH (18 mL) gave, after flash chromatography (silica gel, EtOAc/hexanes 4:1 to EtOAc), 173 mg of amino ester **29** (70%). Colorless oil; *Rf* = 0.30 (silica gel, EtOAc/hexanes 4:1); $[\alpha]^{26}_D$ –21.6 (c 1.0, $CHCl_3$); IR (film) ν 3394, 2987, 1741, 1355, 1174 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 1.31 (s, 3H), 1.38 (s, 3H), 1.72 (brs, 2H), 2.99 (s, 3H), 3.72 (s, 3H), 3.93-3.96 (m, 2H), 4.01-4.06 (m, 1H), 4.10-4.14 (m, 1H), 4.21 (dd, *J* = 11.0, 6.2 Hz, 1H), 4.50 (dd, *J* = 11.0, 2.1 Hz, 1H), 4.57/4.71 (AB system, *J* = 11.3 Hz, 2H), 7.29-7.41 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 26.6 (CH_3), 26.8 (CH_3), 37.5 (CH_3), 52.0 (CH_3), 54.4 (CH), 70.2 (CH_2), 72.5 (CH_2), 74.1 (CH), 78.0 (CH), 81.6 (CH), 110.4 (C), 128.2 (CH), 128.3 (CH), 128.6 (CH), 136.9 (C), 172.6 (C); FABMS (thioglycerol) *m/z* 418 (MH^+, 100). Anal. Calcd for $C_{18}H_{27}NO_8S$: C, 51.79; H, 6.52; N, 3.36; S, 7.68. Found: C, 51.90; H, 6.30; N, 3.61; S, 7.44.

Ethyl (2*S*,3*S*,4*R*,5*S*)-3-benzyloxy-4,5-isopropylidenedioxypipecolate (30): Following the general the procedure 8, cyclization of **27** (300 mg, 0.7 mmol) gave, after flash chromatography (silica gel, MeOH/CH_2Cl_2 1:40), 199 mg of compound **30** (85%). Colorless oil; *Rf* = 0.35 (silica gel, MeOH/CH_2Cl_2 1:40); $[\alpha]^{24}_D$ +24.6 (c 2.3, CH_2Cl_2); IR (film) ν 3409, 2093, 1642 cm^{-1}; ^1H NMR ($CDCl_3$) δ 1.18 (t, *J* = 7.3 Hz, 3H), 1.45 (s, 3H), 1.46 (s, 3H), 2.69 (dd, *J* = 12.2, 10.7 Hz, 1H), 3.45 (dd, *J* = 12.2, 4.4 Hz, 1H), 3.48 (dd, *J* = 9.3, 1.9 Hz, 1H), 3.50 (d, *J* = 1.9 Hz, 1H), 3.94 (ddd, *J* = 10.7, 9.3, 4.4 Hz, 1H), 4.00-4.30 (m, 2H), 4.47 (t, *J* = 1.9 Hz, 1H), 4.57 (d, *J* = 11.2 Hz, 1H), 4.90 (d, *J* = 11.2 Hz, 1H), 7.25-7.35 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 14.1 (CH_3), 26.6 (CH_3), 26.8 (CH_3), 46.7 (CH_2), 61.2 (CH_2), 61.2 (CH), 71.4 (CH), 73.6 (CH_2), 76.4 (CH), 82.3 (CH), 109.4 (C), 127.6 (CH), 127.8 (CH),

128.3 (CH), 138.1 (C), 170.0 (C); FABMS (thioglycerol) *m/z* 335 (MH^+, 81). Anal. Calcd for $C_{18}H_{25}NO_5$: C, 64.46; H, 7.51; N, 4.18. Found: C, 64.52; H, 7.30; N, 4.26.

Methyl (2*R*,3*R*,4*R*,5*S*)-3-benzyloxy-4,5-isopropylidenedioxypipecolate (31): Following the general procedure 8, cyclization of **28** (152 mg, 0.36 mmol) gave, after flash chromatography (silica gel, MeOH/CH_2Cl_2 from 1:40 to 1:20 ratio), 107 mg of compound **31** (91%). Colorless solid; m.p. 79-80 °C; *Rf* = 0.45 (silica gel, MeOH/CH_2Cl_2 1:20); $[\alpha]^{26}_D$ –63.7 (c 1.0, CH_2Cl_2); IR (KBr) ν 3331, 2987, 1737, 1235, 1089 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.45 (s, 3H), 1.46 (s, 3H), 1.67 (brs, 1H), 3.12-3.20 (m, 1H), 3.29-3.37 (m, 2H), 3.70 (s, 3H), 3.83 (dd, *J* = 9.8, 6.6 Hz, 1H), 4.05 (d, *J* = 6.6 Hz, 1H), 4.08 (dd, *J* = 9.8, 8.5 Hz, 1H), 4.72/4.77 (AB system, *J* = 12.0 Hz, 2H), 7.26-7.35 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 26.7 (CH_3), 26.9 (CH_3), 44.0 (CH_2), 51.7 (CH_3), 57.7 (CH), 71.7 (CH_2), 75.9 (CH), 77.5 (CH), 78.9 (CH), 109.9 (C), 127.5 (CH), 128.2 (CH), 137.9 (C), 172.2 (C); FABMS (thioglycerol) *m/z* 322 (MH^+, 100). Anal. Calcd for $C_{17}H_{23}NO_5$: C, 63.54; H, 7.21; N, 4.36. Found: C, 63.34; H, 7.21; N, 4.32.

Methyl (2*R*,3*S*,4*R*,5*S*)-3-benzyloxy-4,5-isopropylidenedioxypipecolate (32): Following the general procedure 8, cyclization of **29** (132 mg, 0.32 mmol) gave, after flash chromatography (silica gel, MeOH/CH_2Cl_2 from 1:40 to 1:20 ratio), 91 mg of compound **32** (89%). Colorless oil; *Rf* = 0.51 (silica gel, MeOH/CH_2Cl_2 1:20), $[\alpha]^{25}_D$ –7.6 (c 1.0, $CHCl_3$); IR (film) ν 3352, 2984, 1739, 1231 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 1.44 (s, 3H), 1.48 (s, 3H), 1.97 (brs, 1H), 2.96 (t, *J* = 11.4 Hz, 1H), 3.31-3.37 (m, 2H), 3.76 (s, 3H), 3.86 (d, *J* = 2.1 Hz, 1H), 4.01 (ddd, *J* = 10.2, 9.6, 4.5 Hz, 1H), 4.62 (t, *J* = 2.1 Hz, 1H), 4.68 (d, *J* = 11.7 Hz, 1H), 4.92 (d, *J* = 11.7 Hz, 1H), 7.27-7.39 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 26.6 (CH_3), 26.7 (CH_3), 46.2 (CH_2), 52.4 (CH_3), 60.5 (CH), 71.1 (CH), 73.2 (CH_2), 76.0 (CH), 79.8 (CH), 109.0 (C), 127.6 (CH), 127.7 (CH), 128.4 (CH), 138.1 (C), 171.4 (C); FABMS (thioglycerol) *m/z* 322 (MH^+, 100). Anal. Calcd for $C_{17}H_{23}NO_5$: C, 63.54; H, 7.21; N, 4.36. Found: C, 63.86; H, 7.07; N, 4.50.

4-*O*-Benzyl-2,3-*O*-isopropylidene-1-deoxy-D-galactonojirimycin (33): Following the general procedure 9, reduction of **30** (91 mg, 0.27 mmol) with $LiEt_3BH$ (1 M in THF, 3.5 equiv) gave, after flash chromatography (RP-18, MeOH/H_2O 1:2), 67 mg of compound **33** (84%). Colorless solid; m.p. 117-119 °C; *Rf* = 0.15 (silica gel, MeOH/EtOAc 1:9); $[\alpha]^{26}_D$ +35.0 (c 2.2, CH_2Cl_2); IR (KBr) ν 3243, 2989, 2913, 1383, 1148, 1069 cm^{-1}; ^1H NMR ($CDCl_3$) δ 1.45 (s, 3H), 1.49 (s, 3H), 2.13 (brs, 2H), 2.63-2.74 (m, 2H), 3.36-3.49 (m, 2H), 3.63 (dd, *J* = 11.2, 4.9 Hz, 1H), 3.73 (dd, *J* = 11.2, 5.9 Hz, 1H), 3.94 (ddd, *J* = 10.3, 9.3, 4.4 Hz, 1H), 4.16 (brs, 1H), 4.60 (d, *J* = 11.2 Hz, 1H), 4.98 (d, *J* = 11.2 Hz, 1H), 7.29-7.38 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 26.7 (CH_3), 26.8 (CH_3), 47.7 (CH_2), 59.2 (CH), 63.9 (CH_2), 72.1 (CH), 73.7 (CH_2), 76.4 (CH), 82.8 (CH), 109.2 (C), 127.9 (CH), 128.1 (CH), 128.5 (CH), 138.0 (C); FABMS (thioglycerol) *m/z* 294 (MH^+, 100). Anal. Calcd for $C_{16}H_{23}NO_4$: C, 65.51; H, 7.90; N, 4.77. Found: C, 65.80; H, 7.82; N, 4.85.

4-*O*-Benzyl-2,3-*O*-isopropylidene-1-deoxy-L-idonojirimycin (34): Following the general procedure 9, reduction of **31** (88 mg, 0.27 mmol) with $LiEt_3BH$ (1 M in THF, 3.5 equiv) gave, after flash chromatography (RP-18, MeOH/H_2O 1:2), 69 mg of compound **34** (86%). Colorless solid; m.p. 97-98 °C; *Rf* = 0.33 (silica gel, MeOH/EtOAc 1:9); $[\alpha]^{25}_D$ –0.4 (c 0.9, CH_2Cl_2); IR (KBr) ν 3244, 2881, 1370, 1230, 1087 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.43 (s, 3H), 1.44 (s, 3H), 2.74 (dd, *J* = 12.7, 11.1 Hz, 1H), 3.11 (dd, *J* = 12.7, 4.4 Hz, 1H), 3.26 (ddd, *J* = 11.1, 9.0, 4.4 Hz, 1H), 3.33-3.37 (m, 1H), 3.56 (d, *J* = 9.2 Hz, 1H), 3.60 (d, *J* = 10.5 Hz, 1H), 3.80 (dd, *J* = 10.0 y 6.2 Hz, 1H), 3.82 (dd, *J* = 11.0 y 5.0 Hz, 1H), 4.64/4.81 (AB system, *J* = 12.1 Hz, 2H), 7.25-7.35 (m, 5H); ^{13}C NMR (125, MHz, $CDCl_3$) δ 26.7 (CH_3), 27.0 (CH_3), 42.2 (CH_2), 56.5 (CH), 57.7 (CH_2), 71.9 (CH_2), 76.8 (CH), 79.1 (CH), 80.0 (CH), 109.9 (C), 127.6 (CH), 127.7 (CH), 128.4 (CH), 138.1 (C); FABMS (thioglycerol) *m/z* 294 (MH^+, 100). Anal. Calcd for $C_{16}H_{23}NO_4$: C, 65.51; H, 7.90; N, 4.77. Found: C, 65.85; H, 7.80; N, 4.89.

4-*O*-Benzyl-2,3-*O*-isopropylidene-1-deoxy-L-altronojirimycin (35): Following the general procedure 9, reduction of **32** (68 mg, 0.20 mmol) with $LiEt_3BH$ (1 M in THF, 3.5 equiv) gave, after flash chromatography (RP-18, MeOH/H_2O 1:2), 49 mg of compound **35** (80 %). Colorless solid; m.p.

78-80 °C; *Rf* = 0.25 (silica gel, MeOH/AcOEt 1:9); $[\alpha]^{25}_D$ +31.4 (c 1.0, $CHCl_3$); IR (KBr) ν 3345, 2993, 2359, 1370, 1232; 1067 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 1.45 (s, 3H), 1.49 (s, 3H), 2.73 (dd, *J* = 12.9, 11.2 Hz, 1H), 3.18-3.27 (m, 1H), 3.23 (dd, *J* = 12.9, 4.4 Hz, 1H), 3.39-3.54 (m, 3H), 3.93-3.96 (m, 1H), 3.99 (ddd, *J* = 10.9, 9.6, 4.4 Hz, 1H), 4.62 (d, *J* = 11.6 Hz, 1H), 4.91 (d, *J* = 11.6 Hz, 1H), 7.28-7.37 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 26.7 (CH_3), 26.8 (CH_3), 44.0 (CH_2), 59.2 (CH_2), 60.0 (CH), 71.7 (CH), 73.1 (CH_2), 75.6 (CH), 80.1 (CH), 108.8 (C), 127.5 (CH), 127.7 (CH), 128.4 (CH), 138.7 (C); FABMS (thioglycerol) *m/z* 294 (MH^+, 100). HRMS (FAB) *m/z* 294.1700, $C_{16}H_{24}NO_4$ requires 294.1705.

(2*S*,3*S*,4*R*,5*S*)-Trihydroxypipecolic acid (36): Following the method A of the general procedure 10, final deprotection of **30** (61 mg, 0.18 mmol) gave 28 mg of compound **36** (88%). FABMS (thioglycerol) *m/z* 178 (MH^+, 100). Anal. Calcd for $C_6H_{11}NO_5$: C, 40.68; H, 6.26; N, 7.91. Found: C, 40.84; H, 6.41; N, 8.17. Treatment of **36** with HCl 1M (1 mL) followed by evaporation of the solvent afforded **36·HCl** in quantitative yield. Colorless solid; m.p. 169-171 °C; *Rf* = 0.48 (silica gel, BuOH/AcOH/H_2O 1:1:1); $[\alpha]^{26}_D$ +20.3 (c 1.3, H_2O); IR (film) ν 3400, 3306, 2960, 1716, 1282, 1087 cm^{-1}; ^1H NMR (D_2O) δ 2.70 (dd, *J* = 12.5, 11.4 Hz, 1H), 3.32 (dd, *J* = 12.5, 5.3 Hz, 1H), 3.51 (dd, *J* = 9.7, 3.0 Hz, 1H), 3.84 (ddd, *J* = 11.4, 9.7, 5.3 Hz, 1H), 4.10 (d, *J* = 1.8 Hz, 1H), 4.36 (dd, *J* = 3.0, 1.8 Hz, 1H); ^{13}C NMR (D_2O) δ 46.0 (CH_2), 61.0 (CH), 64.9 (CH), 68.7 (CH), 73.3 (CH), 169.6 (C).

(3*S*,6*R*,1´*S*,2´*S*,3´*S*)-3-(1-hydroxy-2,3-isopropylidenedioxy-4-oxobutyl)-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (37): Following the general procedure 11, oxidation of **20c** (590 mg, 1.58 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:4 to 2:3 ratio), 183 mg of starting diol **20c** (31%) and 375 mg of **37** (64%, 84% based on recovered starting material). Colorless oil; *Rf* = 0.60 (silica gel, EtOAc/hexanes 2:3); $[\alpha]^{27}_D$ –9.8 (final, c 2.8, CH_2Cl_2); IR (film) ν 3415, 2977, 2872, 1694, 1459, 1381, 1311, 1238, 1158, 1073, 1036 cm^{-1}; ^1H NMR ($CDCl_3$+D_2O, 2:1 mixture of anomers, Ha for protons of major isomer and Hi for protons of minor isomer) δ 0.70 (d, *J* = 6.8 Hz, 3Hi), 0.80 (d, *J* = 6.8 Hz, 3Ha), 1.00 (d, *J* = 6.8 Hz, 3Ha+3Hi), 1.30 (t, *J* = 6.8 Hz, 6Ha+6Hi), 1.34 (s,

3Ha), 1.41 (s, 3Hi), 1.53 (s, 3Ha), 1.56 (s, 3Hi), 2.10-2.30 (m, 1Ha+1Hi), 3.91-4.38 (m, 6Ha+6Hi), 4.53 (d, J = 5.9 Hz, 1Ha), 4.63 (dd, J = 6.1, 4.1 Hz, 1Hi), 4.76 (brs, 1Hi), 4.92-5.01 (m, 2Ha+1Hi), 5.23 (d, J = 4.4 Hz, 1Hi), 5.29 (s, 1Ha); ^{13}C NMR ($CDCl_3$) δ 14.2 (CH_3), 14.3 (CH_3), 16.8 (CH_3), 17.7 (CH_3), 18.9 (CH_3), 19.1 (CH_3), 24.5 (CH_3), 25.1 (CH_3), 26.1 (CH_3), 26.7 (CH_3), 32.2 (CH), 32.8 (CH), 57.0 (CH), 59.1 (CH), 60.5 (CH), 60.9 (CH_2), 61.0 (CH_2), 61.4 (CH_2), 61.6 (CH_2), 62.1 (CH), 79.5 (CH), 82.3 (CH), 82.7 (CH), 83.0 (CH), 87.1 (CH), 87.3 (CH), 98.5 (CH), 103.3 (CH), 112.3 (C), 112.7 (C), 160.0 (C), 160.8 (C), 165.6 (C); 169.2 (C); FABMS (thioglycerol) *m/z* 371 (MH^+, 100). HRMS (FAB) *m/z* 371.2166, $C_{18}H_{31}N_2O_6$ requires 371.2182. Anal. Calcd for $C_{18}H_{30}N_2O_6$: C, 58.36; H, 8.16; N, 7.56. Found: C, 58.57; H, 8.33; N, 7.30.

(3*S*,6*R*,1´*R*,2´*R*,3´*R*)-3-(1-hydroxy-2,3-isopropylidenedioxy-4-oxobutyl)-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (38): Following the general procedure 11, oxidation of **21c** (581 mg, 1.56 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:4 to 2:3 ratio), 181 mg of starting diol **21c** (31%) and 358 mg of **38** (62%, 82% based on recovered starting material). Colorless solid; m.p. 86-88 °C; *Rf* = 0.35 (silica gel, EtOAc/hexanes 1:4); $[\alpha]^{25}_D$ −18.6 (final, c 1.2, CH_2Cl_2); IR (film) ν 3409, 2983, 2945, 1693, 1254, 1070 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 0.77 (d, J = 6.8 Hz, 3H), 1.02 (d, J = 6.8 Hz, 3H), 1.28-1.37 (m, 9H), 1.49 (s, 3H), 2.22 (dsp, J = 6.8, 3.6 Hz 1H), 3.98-4.32 (m, 7H), 4.45 (d, J = 5.8 Hz, 1H), 4.95 (d, J = 2.5 Hz, 1H), 5.29-5.34 (m, 1H), 7.15 (brs, 1H); ^{13}C NMR ($CDCl_3$) δ 14.0 (CH_3), 14.1 (CH_3), 17.2 (CH_3), 19.0 (CH_3), 24.9 (CH_3), 26.4 (CH_3), 33.0 (CH), 57.8 (CH), 61.6 (CH_2), 61.8 (CH), 62.5 (CH_2), 81.0 (CH), 87.2 (CH), 88.1 (CH), 104.4 (CH), 111.9 (C), 159.9 (C), 167.4 (C); FABMS (thioglycerol) *m/z* 371 (MH^+, 100). Anal. Calcd for $C_{18}H_{30}N_2O_6$: C, 58.36; H, 8.16; N, 7.56. Found: C, 58.06; H, 8.45; N, 7.36.

(3*S*,6*R*,1´*S*,2´*R*,3´*R*)-3-(1-hydroxy-2,3-isopropylidenedioxy-4-oxobutyl)-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (39): Following the general procedure 11, oxidation of **22c** (600 mg, 1.61 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:4 to 2:3 ratio), 195 mg of starting diol **22c** (32%) and 400 mg of **39** (68%, 89% based on recovered starting material). Colorless

oil; *Rf* = 0.45 (silica gel, EtOAc/hexanes 1:4); $[\alpha]^{28}_{D}$ −15.8 (final, c 1.2, CH_2Cl_2); IR (film) ν 3115, 2977, 2810, 1717, 1208, 1078 cm^{-1}; ^1H NMR ($CDCl_3$, ca. 8:1 mixture of anomers, Ha for protons of major isomer and Hi for protons of minor isomer) δ 0.78 (d, *J* = 6.8 Hz, 3Hi), 0.80 (d, *J* = 6.8 Hz, 3Ha), 1.02 (d, *J* = 6.8 Hz, 3Ha+3Hi), 1.22-1.33 (m, 9Ha+6Hi), 1.38 (s, 3Hi), 1.46 (s, 3Ha), 1.56 (s, 3Hi), 2.10-2.26 (m, 1Ha+1Hi), 3.85-3.96 (m, 1Hi), 3.89 (dd, *J* = 4.6, 3.3 Hz, 1Ha), 4.06-4.23 (m, 6Ha+6Hi), 4.37 (dd, *J* = 6.8, 4.3 Hz, 1Hi), 4.43 (dd, *J* = 9.3, 3.4 Hz, 1Ha), 4.48-4.54 (m, 1Hi) 4.55 (d, *J* = 5.9 Hz, 1Ha), 4.84-4.90 (m, 1Hi), 4.91 (dd, *J* = 5.9, 2.9 Hz, 1Ha), 4.96-5.07 (m, 1Hi), 5.46 (s, 1Ha); ^{13}C NMR ($CDCl_3$, absorptions of major anomer) δ 14.0 (CH_3), 14.3 (CH_3), 17.6 (CH_3), 19.3 (CH_3), 24.7 (CH_3), 26.0 (CH_3), 31.9 (CH), 54.4 (CH), 61.3 (CH_2), 61.7 (CH), 80.5 (CH), 81.2 (CH), 85.6 (CH), 100.9 (CH), 112.1 (C), 161.6 (C), 165.3 (C); FABMS (thioglycerol) *m/z* 371 (MH^+, 100). Anal. Calcd for $C_{18}H_{30}N_2O_6$: C, 58.36; H, 8.16; N, 7.56. Found: C, 58.20; H, 8.30; N, 7.95.

(3*R*,6*R*,1′*R*,2′*R*,3′*R*)-3-(1-hydroxy-2,3-isopropylidenedioxy-4-oxobutyl)-2,5-diethoxy-3,6-dihydro-6-isopropylpyrazine (40): Following the general procedure 11, oxidation of **23c** (200 mg, 0.54 mmol) gave, after flash chromatography (silica gel, EtOAc/hexanes from 1:4 to 2:3 ratio), 58 mg of starting diol **23c** (20%) and 133 mg of **40** (67%, 86% based on recovered starting material). Colorless oil; *Rf* = 0.42 (silica gel, EtOAc/hexanes 1:4); ^1H NMR ($CDCl_3$ + D_2O 1.4:1 mixture of anomers, Ha for protons of major isomer and Hi for protons of minor isomer) δ 0.74 (d, *J* = 6.8 Hz, 3Hi), 0.77 (d, *J* = 6.8 Hz, 3Ha), 1.05 (d, *J* = 6.8 Hz, 3Hi), 1.08 (d, *J* = 6.8 Hz, 3Ha), 1.19-1.34 (m, 6Ha+9Hi), 1.41 (s, 3Ha), 1.52 (s, 3Hi), 1.56 (s, 3Ha), 2.27-2.38 (m, 1Ha+1Hi), 3.73-4.28 (m, 6Ha+6Hi), 4.54 (d, *J* = 5.9 Hz, 1Ha), 4.60 (dd, *J* = 5.9, 4.4 Hz, 1Hi), 4.79-4.81 (m, 1Ha), 4.82-4.86 (m, 1Hi), 4.92-5.00 (m, 1Ha+1Hi), 5.22 (dd, *J* = 11.2, 4.4 Hz, 1Hi), 5.28 (s 1Ha). FABMS (thioglycerol) *m/z* 371 (MH^+, 100). HRMS (FAB) *m/z* 371.2178, $C_{18}H_{31}N_2O_6$ requires 371.2182.

Ethyl (2*S*,3*S*,4*S*,5*R*)-3-hydroxy-4,5-isopropylidenedioxypipecolate ((–)-41): Following the general procedure 12, hydrolysis and reductive amination of **37** (150 mg, 0.40 mmol) gave, after flash chromatography (RP-18, from H_2O to MeOH/H_2O 3:7), 66 mg of compound (–)-**41** (67%). Colorless

solid; m.p. 87-89 °C; *Rf* = 0.36 (silica gel, BuOH/AcOH/H_2O 12:3:5); $[\alpha]^{25}_D$ −73.0 (c 1.5, CH_2Cl_2); IR (KBr) ν 3455, 2983, 2930, 2359, 1741, 1457, 1381, 1214, 1056 cm^{-1}; ^1H NMR ($CDCl_3$ + D_2O) δ 1.27 (t, *J* = 7.3 Hz, 3H), 1.36 (s, 3H), 1.53 (s, 3H), 2.97 (dd, *J* = 14.6, 3.4 Hz, 1H), 3.27 (d, *J* = 2.0 Hz, 1H), 3.41 (dd, *J* = 14.6, 1.5 Hz, 1H), 4.00-4.20 (m, 2H), 4.24 (q, *J* = 7.3 Hz, 2H), 4.73-4.82 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 14.1 (CH_3), 25.3 (CH_3), 25.9 (CH_3), 45.2 (CH_2), 59.7 (CH), 61.3 (CH_2), 65.6 (CH), 70.9 (CH), 74.2 (CH), 109.1 (C), 171.0 (C); FABMS (thioglycerol) *m/z* 246 (MH^+, 100). HRMS (FAB) *m/z* 246.1350, $C_{11}H_{20}NO_5$ requires 246.1341. Anal. Calcd for $C_{11}H_{19}NO_5$: C, 53.87; H, 7.81; N, 5.71. Found: C, 53.60; H, 7.72; N, 5.96.

Ethyl (2*R*,3*R*,4*R*,5*S*)-3-hydroxy-4,5-isopropylidenedioxypipecolate ((+)-41): Following the general procedure 12, hydrolysis and reductive amination of **40** (70 mg, 0.19 mmol) gave, after flash chromatography (RP-18, from H_2O to MeOH/H_2O 3:7), 31 mg of compound (+)-**41** (67%). Colorless solid; $[\alpha]^{22}_D$ +84.6 (c 1.1, CH_2Cl_2). ^1H NMR (D_2O) δ 1.31 (t, *J* = 7.3 Hz, 3H), 1.46 (s, 3H), 1.59 (s, 3H), 3.10 (dd, *J* = 15.6, 3.6 Hz, 1H), 3.33-3.45 (m, 1H), 3.60 (d, *J* = 1.8 Hz, 1H), 4.16-4.40 (m, 5H). Anal. Calcd for $C_{11}H_{19}NO_5$: C, 53.87; H, 7.81; N, 5.71. Found: C, 54.13; H, 7.69; N, 5.58.

Ethyl (2*S*,3*R*,4*R*,5*S*)-3-hydroxy-4,5-isopropylidenedioxypipecolate (42): Following the general procedure 12, hydrolysis and reductive amination of **38** (250 mg, 0.67 mmol) gave, after flash chromatography (RP-18, from H_2O to MeOH/H_2O 3:7), 84 mg of compound **42** (51%). Colorless solid; m.p. 164-166 °C; *Rf* = 0.50 (silica gel, BuOH/AcOH/H_2O 12:3:5); $[\alpha]^{26}_D$ +34.4 (c 0.7, MeOH); IR (KBr) ν 3445, 2937, 1631, 1419 cm^{-1}; ^1H NMR (D_2O) δ 1.26 (t, *J* = 7.0 Hz, 3H), 1.39 (s, 3H), 1.54 (s, 3H), 2.61 (dd, *J* = 14.0, 6.7 Hz, 1H), 2.96 (dd, *J* = 14.0, 4.9 Hz, 1H), 3.51 (d, *J* = 10.4 Hz, 1H), 4.06 (dd, *J* = 10.4, 3.6 Hz, 1H), 4.22 (q, *J* = 7.0 Hz, 2H), 4.34-4.44 (m, 1H), 4.57 (dd, *J* = 5.5, 3.6 Hz, 1H); ^{13}C NMR (125 MHz, D_2O) δ 14.7 (CH_3), 25.9 (CH_3), 27.7 (CH_3), 44.9 (CH_2), 58.8 (CH), 63.9 (CH_2), 68.4 (CH), 74.2 (CH), 76.1 (CH), 111.5 (C), 175.4 (C); FABMS (thioglycerol) *m/z* 246 (MH^+, 100). Anal. Calcd for $C_{11}H_{19}NO_5$: C, 53.87; H, 7.81; N, 5.71. Found: C, 53.90; H, 7.85; N, 5.68.

Ethyl (2*S*,3*S*,4*R*,5*S*)-3-hydroxy-4,5-isopropylidenedioxypipecolate (43): Following the general procedure 12, hydrolysis and reductive amination of **39** (250 mg, 0.67 mmol) gave, after flash chromatography (RP-18, from H_2O to MeOH/H_2O 3:7), 124 mg of compound **43** (75%). Colorless solid; m.p. 143-145 °C; *Rf* = 0.36 (silica gel, BuOH/AcOH/H_2O 12:3:5); $[\alpha]^{23}_D$ −17.5 (c 1.3, MeOH); IR (KBr) ν 3472, 2986, 1737, 1448 cm^{-1}; ^1H NMR (D_2O) δ 1.31 (t, *J* = 7.2 Hz, 3H), 1.45 (s, 3H), 1.58 (s, 3H), 2.76-2.85 (m, 1H), 3.12-3.30 (m, 1H), 3.85 (d, *J* = 3.3 Hz, 1H), 4.22-4.35 (m, 3H), 4.37-4.51 (m, 2H); ^{13}C NMR (D_2O) δ 14.4 (CH_3), 25.8 (CH_3), 27.7 (CH_3), 44.0 (CH_2), 58.0 (CH), 63.4 (CH_2), 68.0 (CH), 71.7 (CH), 76.3 (CH), 110.8 (C), 173.8 (C); FABMS (thioglycerol) *m/z* 246 (MH^+, 100). Anal. Calcd for $C_{11}H_{19}NO_5$: C, 53.87; H, 7.81; N, 5.71. Found: C, 54.01; H, 7.91; N, 5.68.

1-Deoxy-D-galactonojirimycin (3·HCl): Following the method A of the general procedure 10, final deprotection of **33** (36 mg, 0.12 mmol) gave 18 mg of 1-deoxy-D-galactonojirimycin (**3**) (90%). FABMS (thioglycerol) *m/z* 164 (MH^+, 100). Anal. Calcd for $C_6H_{13}NO_4$: C, 44.16; H, 8.03; N, 8.58. Found: C, 44.35; H, 7.97; N, 8.82. Treatment of **3** with HCl 1M (1 mL) followed by evaporation of the solvent afforded **3·HCl** in quantitative yield. Colorless solid; m.p. 243-245 °C (dec.); Rf = 0.42 (silica gel, BuOH/AcOH/H_2O 1:1:1); $[\alpha]^{24}_D$ +44.6 (c 0.9, H_2O), [lit.[2] $[\alpha]^{20}_D$ +46.1 (c 0.9, H_2O)]; IR (KBr) ν 3368, 3023, 2970, 1080 cm^{-1}; ^1H NMR (D_2O) δ 2.37 (dd, *J* = 12.7, 10.9 Hz, 1H), 2.75 (dt, *J* = 1.2, 6.5 Hz, 1H), 3.11 (dd, *J* = 12.7, 5.5 Hz, 1H), 3.45 (dd, *J* = 9.7, 3.0 Hz, 1H), 3.55-3.65 (m, 2H), 3.73 (ddd, *J* = 10.9, 9.7, 5.5 Hz, 1H), 3.98 (dd, *J* = 3.0, 1.2 Hz, 1H); ^{13}C NMR (D_2O) δ 49.9 (CH_2), 59.9 (CH), 62.3 (CH_2), 69.0 (CH), 70.1 (CH), 75.9 (CH).

1-Deoxy-D-allonojirimycin (4): According to general procedure 9, reduction of **42** (60 mg, 0.24 mmol) with $LiEt_3BH$ (1 M in THF, 4.5 equiv) and final deprotection following the method B of general procedure 10 gave, after flash chromatography 39 mg of 1-deoxy-D-allonojirimycin (98%). Colorless solid; m.p. 150-152 °C (dec.), [lit.[3] m.p. 149-150 °C]; *Rf* = 0.36 (silica gel, BuOH/AcOH/H_2O 12:3:5); $[\alpha]^{26}_D$ +30.5 (c 1.0, H_2O), [lit.[3] $[\alpha]^{25}_D$ +30.5 (c 0.15, H_2O)]; IR (KBr) ν 3401, 3319, 2878, 1254, 1042 cm^{-1}; ^1H NMR (D_2O) δ 2.71 (t, *J* = 11.7 Hz, 1H), 2.76 (ddd, *J* = 11.6, 5.5, 3.0 Hz, 1H), 2.89 (dd, *J* =

11.7, 5.2 Hz, 1H), 3.50 (dd, *J* = 11.0, 3.0 Hz, 1H), 3.66 (dd, *J* = 11.0, 5.5 Hz, 1H), 3.72 (ddd, *J* = 11.7, 5.2, 2.5 Hz, 1H), 3.83 (dd, *J* = 11.6, 3.0 Hz, 1H), 4.13 (brt, 1H); ^{13}C NMR (D_2O) δ 46.4 (CH_2), 57.2 (CH), 64.2 (CH_2), 71.0 (CH), 71.5 (CH), 74.2 (CH) [lit.[4]]; FABMS (thioglycerol) *m/z* 164 (MH^+, 100). Anal. Calcd for $C_6H_{13}NO_4$: C, 44.16; H, 8.03; N, 8.58. Found: C, 43.98; H, 8.00; N, 8.21.

1-Deoxy-L-altronojirimycin (*ent*-5): Following the method A of the general procedure 10, final deprotection of **35** (79 mg, 0.27 mmol) gave 41 mg of 1-deoxy-L-altronojirimycin *ent*-**5** (93%). Colorless oil; *Rf* = 0.10 (silica gel, BuOH/AcOH/H_2O 2:2:1); $[\alpha]^{25}_D$ –17.9 (c 1.6, H_2O), [lit.[4] $[\alpha]_D$ –21.0 (c 1.24, H_2O)]; IR (film) ν 3355, 1064, 959 cm^{-1}; ^{1}H NMR (500 MHz, D_2O) δ 2.82 (dd, *J* = 14.2, 2.6 Hz, 1H), 2.88 (ddd, *J* = 9.6, 4.6, 4.4 Hz, 1H), 3.00 (dd, *J* = 14.2, 1.9 Hz, 1H), 3.76-3.81 (m, 2H), 3.84 (dd, *J* = 9.6, 3.0 Hz, 1H), 3.90-3.94 (m, 1H), 3.95-3.96 (m, 1H); ^{13}C NMR (75 MHz, D_2O) δ 47.3 (CH_2), 58.5 (CH), 63.4 (CH_2), 68.8 (CH), 71.9 (CH), 73.3 (CH) [lit.[4]]. FABMS (thioglycerol) *m/z* 164 (MH^+, 100). HRMS (FAB) *m/z* 164.0924, $C_6H_{14}NO_4$ requires 164.0923. Anal. Calcd for $C_6H_{13}NO_4$: C, 44.16; H, 8.03; N, 8.58. Found: C, 44.30; H, 8.31; N, 8.65.

1-Deoxy-D-gulonojirimycin (6): According to the general procedure 9, reduction of **43** (79 mg, 0.32 mmol) with $LiEt_3BH$ (1 M in THF, 4.5 equiv) and final deprotection following the method B of general procedure 10 gave, after flash chromatography, 48 mg of 1-deoxy-D-gulonojirimycin (93%). Colorless solid; m.p. 148-150 °C, (lit.[5] m.p. 148-150 °C); *Rf* = 0.38 (silica gel, BuOH/AcOH/H_2O 12:3:5); $[\alpha]^{25}_D$ –13.9 (c 0.3, EtOH), [lit.[5] $[\alpha]^{20}_D$ –16.2 (c 0.3, EtOH)]; IR (KBr) ν 3350, 2900, 1050 cm^{-1}; ^{1}H NMR (D_2O) δ 3.17 (dd, *J* = 12.2, 11.3 Hz, 1H), 3.35 (dd, *J* = 12.2, 4.9 Hz, 1H), 3.57 (ddd, *J* = 8.4, 5.2, 1.8 Hz, 1H), 3.83 (dd, *J* = 12.2, 8.4 Hz, 1H), 3.94 (dd, *J* = 12.2, 5.2 Hz, 1H), 4.09 (dd, *J* = 4.6, 2.2 Hz, 1H), 4.16 (dd, *J* = 4.6, 1.8 Hz, 1H), 4.29 (ddd, *J* = 11.3, 4.9, 2.2 Hz, 1H) [lit.[4]]; ^{13}C NMR (D_2O) δ 47.0 (CH_2), 56.9 (CH), 63.9 (CH_2), 68.5 (CH), 72.1 (CH), 73.1 (CH); FABMS (thioglycerol) *m/z* 164 (MH^+, 100). Anal. Calcd for $C_6H_{13}NO_4$: C, 44.16; H, 8.03; N, 8.58. Found: C, 43.78; H, 7.67; N, 8.23.

1-Deoxy-L-idonojirimycin (*ent*-7·HCl): Following the method A of the general procedure 10, final deprotection of **34** (36 mg, 0.12 mmol) gave 18 mg of 1-deoxy-L-idonojirimycin *ent*-**7** (90%). FABMS

(thioglycerol) *m/z* 164 (MH^+, 100). HRMS (FAB) *m/z* 164.0924, $C_6H_{14}NO_4$ requires 164.0923. Anal. Calcd for $C_6H_{13}NO_4$: C, 44.16; H, 8.03; N, 8.58. Found: C, 43.92; H, 8.05; N, 8.38. Treatment of *ent*-**7** with HCl 1M (1 mL) followed by evaporation of the solvent afforded *ent*-**7·HCl** in quantitative yield. Colorless oil; *Rf* = 0.20 (silica gel, BuOH/AcOH/H_2O 12:3:5); $[\alpha]^{25}_D$ +8.7 (c 0.5, MeOH), [lit.[4] $[\alpha]^{25}_D$ +8.7 (c 0.56, MeOH)]; IR (film) ν 3267, 1057 cm^{-1}; ^1H NMR (300 MHz, D_2O) δ 3.38 (dd, *J* = 13.8, 3.3 Hz, 1H), 3.48 (dd, *J* = 13.6, 2.5 Hz, 1H), 3.63 (ddd, *J* = 7.8, 5.6, 1.6 Hz, 1H), 3.88-4.02 (m, 2H), 4.07-4.11 (m, 3H); ^{13}C NMR (75 MHz, CD_3OD) δ 46.6 (CH_2), 58.1 (CH), 60.3 (CH_2), 67.8 (CH), 68.7 (CH), 68.8 (CH); ^{13}C NMR (75 MHz, CD_3OD) δ 47.1 (CH_2), 58.3 (CH), 60.7 (CH_2), 67.9 (CH), 68.4 (CH), 69.3 (CH) [lit.[6]].

1-Deoxy-D-talonojirimycin (8): According to general procedure 9, reduction of (–)-**41** (50 mg, 0.20 mmol) with $LiEt_3BH$ (1 M in THF, 4.5 equiv) and final deprotection following the method B of general procedure 10 gave, after flash chromatography, 31 mg of 1-deoxi-D-talonojirimycin (95%). Colorless solid; m.p. 150-152 °C, [lit.[5] m.p. 150-151 °C]; *Rf* = 0.38 (silica gel, BuOH/AcOH/H_2O 12:3:5); $[\alpha]^{23}_D$ –21.7 (c 0.8, MeOH), [lit.[7] $[\alpha]^{25}_D$ –26.0 (c 1.0, MeOH)]; IR (KBr) ν 3434, 2900, 1050 cm^{-1}; ^1H NMR (D_2O) δ 3.26 (dd, *J* = 13.8, 1.8 Hz, 1H), 3.40 (dt, *J* = 1.6, 6.7 Hz, 1H), 3.52 (dd, *J* = 13.8, 3.0 Hz, 1H), 3.85 (t, *J* = 3.3 Hz, 1H), 3.87 (d, *J* = 6.7 Hz, 2H), 4.13-4.18 (m, 1H), 4.20-4.27 (m, 1H); ^{13}C NMR (D_2O) δ 49.9 (CH_2), 60.0 (CH), 62.3 (CH_2), 70.1 (CH), 70.2 (CH), 70.5 (CH) [lit.[8]]; FABMS (thioglycerol) *m/z* 164 (MH^+, 100). HRMS (FAB) *m/z* 164.0921, $C_6H_{14}NO_4$ requires 164.0923. Anal. Calcd for $C_6H_{13}NO_4$: C, 44.16; H, 8.03; N, 8.58. Found: C, 44.35; H, 8.31; N, 8.34.

4. Computational Methods.

Stationary points (reactant and transition state geometries) were optimized and characterized by frequency analysis using the Kohn-Sham formulation of the density functional theory with the hybrid exchange functional of Becke and the Lee, Yang, and Parr correlation functional (B3LYP) [9] and the cc-pVDZ basis set [10] with a small-core relativistic pseudopotential for Sn [11] (referred as B3LYP/cc-pVDZ-PP level). All reactants and products have positive defined Hessian matrices. Transition structures showed only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to motion along the reaction coordinate. All the energies reported are free energies and thus contain zero-point energy corrections (using frequencies scaled by 0.97)[12] and thermal and entropy effects at reaction temperature (195 or 273 K) and 1 atm pressure calculated at B3LYP/cc-pVDZ-PP level. Solvent effects were considered by reoptimizing the most significative gas-phase stationary points at B3LYP/cc-pVDZ-PP level using the self-consistent reaction field method [13] based on the polarizable continuum model of Tomasi´s group [14] (B3LYP(SCRF)/cc-pVDZ-PP level) with a permittivity of 7.52 for THF, the solvent used in experiments. Finally, single point energy calculations were computed at B3LYP/cc-pVTZ-PP for the gas-phase stationary points and at B3LYP(SCRF)/cc-pVTZ-PP level for the solution stationary points. All optimizations and frequency calculations reported in this article were performed using Gaussian03 program package.[15] cc-pVDZ-PP and cc-pVTZ-PP basis sets and ECP parameters for Sn were obtained from the Extensible Computational Chemistry Environment Basis Set Database, Version 02/02/06, as developed and distributed by the Molecular Science Computing Facility, Environmental and Molecular Sciences Laboratory which is part of the Pacific Northwest Laboratory, P.O. Box 999, Richland, Washington 99352, USA, and funded by the U.S. Department of Energy. The Pacific Northwest Laboratory is a multi-program laboratory operated by Battelle Memorial Institute for the U.S. Department of Energy under contract DE-AC06-76RLO 1830. Contact Karen Schuchardt for further information (https://bse.pnl.gov/bse/portal)

The conformational space accessible to the azaenolate moiety was sampled by considering three different rotamers for the isopropyl group (those with the tertiary carbon atom pointing to the metal atom, to the nucleophilic carbon atom or to the imidate moiety), two rotamers for each of the methoxy groups (directed to or opposite to the imidate nitrogen), and three rotamers for each of the tetrahydrofuran molecules coordinated to the lithium cation. For the glyceraldehyde and the erythrose acetonides, two different half-chair conformations for the dioxolane ring were considered. In addition, the two possible configurations at the tin(II) stereogenic centers (with tetrahedral or trigonal-bipyramidal environments) were generated and optimized for all the models reported.

SCHEME S1. Formation of dimer (**uA**)$_2$ from unsolvated tin(II) azaenolate (**uA**). Relative energies to **dA** in the gas-phase (at B3LYP/cc-pVTZ-PP level) are shown in parenthesis in kcal/mol. The hydrogen atoms are omitted for clarity except at chiral and reaction centers. Legend: carbon–grey, chlorine–ligth green, hydrogen–turquoise, nitrogen–blue, oxygen–red, tin–yellow.

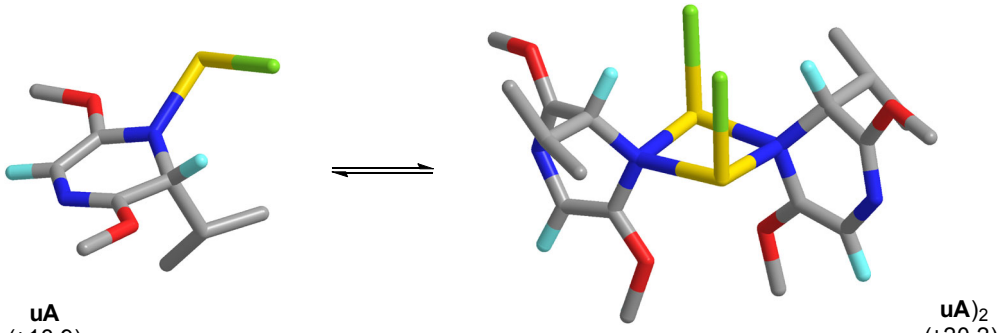


FIGURE S1. Felkin-Anh, modified-Cornforth and no-Anh models for azaenolate addition to D–glyceraldehyde acetonide.

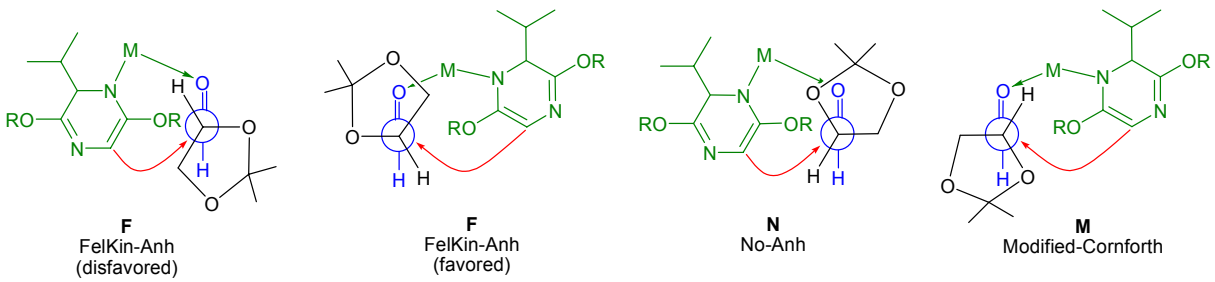


FIGURE S2. Representative chair-like starting geometries considered for TS location in the 3,6-trans-3,1′-anti-1′,2′-syn (**tas**) and 3,6-trans-3,1′-syn-1′,2′-anti (**tsa**) diastereomeric pathways for the rearrangement of **uADg** and **dADg**.

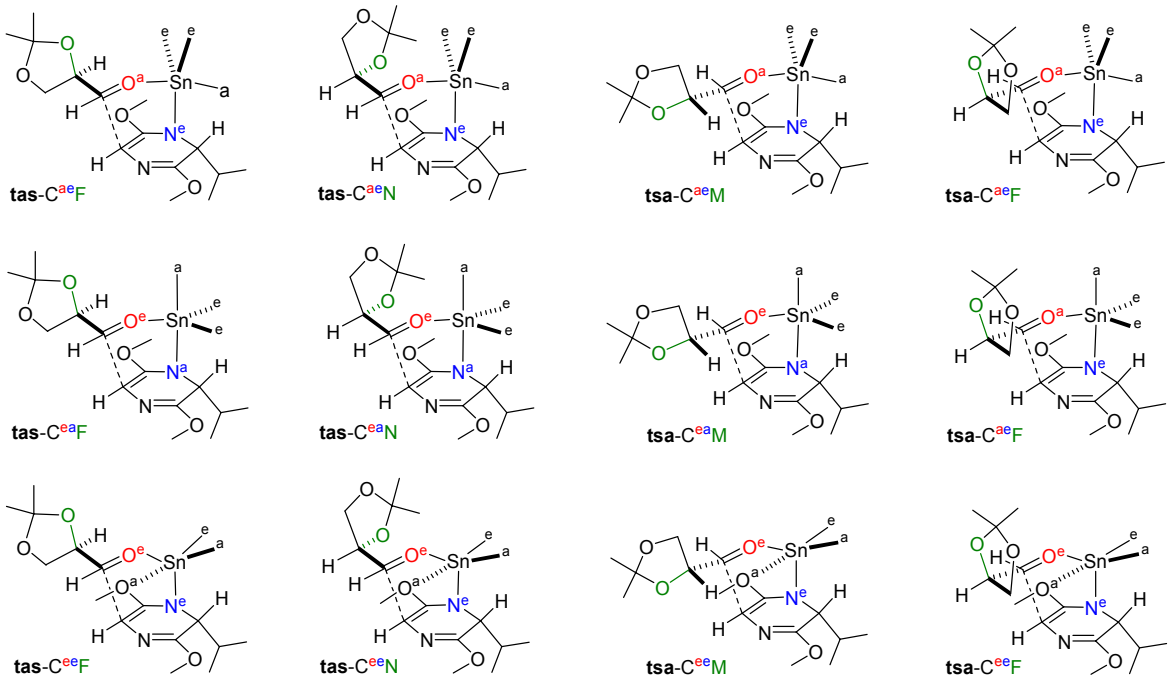


FIGURE S3. Chem3D representations of the most favored unsolvated TSs located (at B3LYP/cc-pVDZ-PP level) in the 3,6-cis diastereomeric pathways for the addition of unsolvated tin(II) azaenolate (**uA**) to D-glyceraldehyde acetonide (**Dg**). Relative energies to **utsa**-CM in the gas-phase (at B3LYP/cc-pVTZ-PP level) are shown in parenthesis in kcal/mol. Bond lengths are in Å. The hydrogen atoms are omitted for clarity except at chiral and reaction centers. Legend: carbon–grey, chlorine–ligth green, hydrogen–turquoise, nitrogen–blue, oxygen–red, tin–yellow.

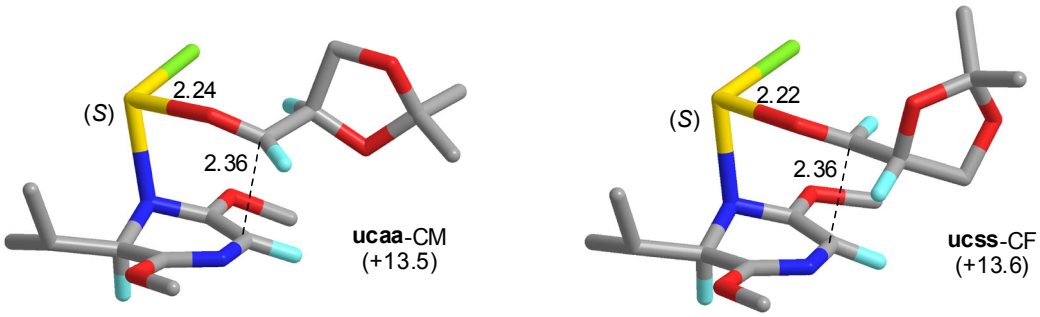


FIGURE S4. Chem3D representations of the most favored disolvated TSs located (at B3LYP/cc-pVDZ-PP level) in the 3,6-cis diastereomeric pathways for the aldol addition of disolvated tin(II) azaenolate (**dA**) to D-glyceraldehyde acetonide (**Dg**). Relative energies to **dtsa**-C^{ae}M in the gas-phase (at B3LYP/cc-pVTZ-PP level) are shown in parenthesis in kcal/mol. Bond lengths are in Å. The hydrogen atoms are omitted for clarity except at chiral and reaction centers. Legend: carbon–grey, chlorine–ligth green, hydrogen–turquoise, lithium–green, nitrogen–blue, oxygen–red, tin–yellow.

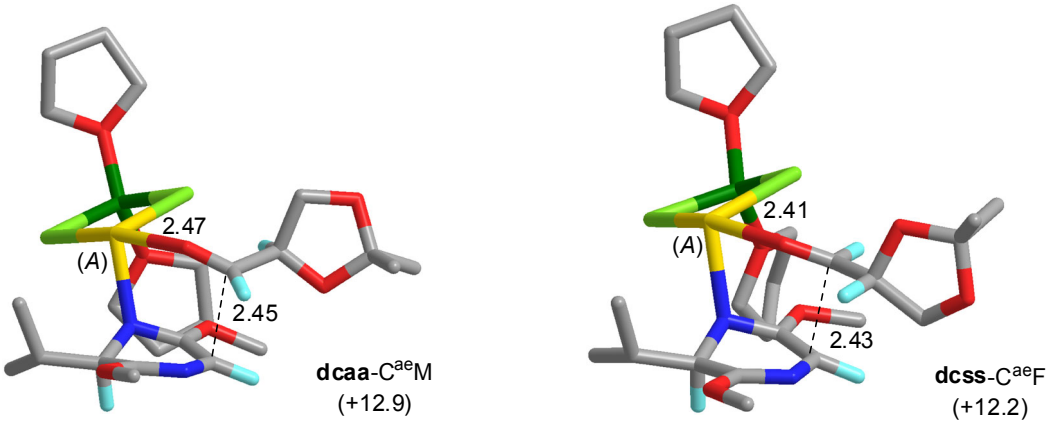
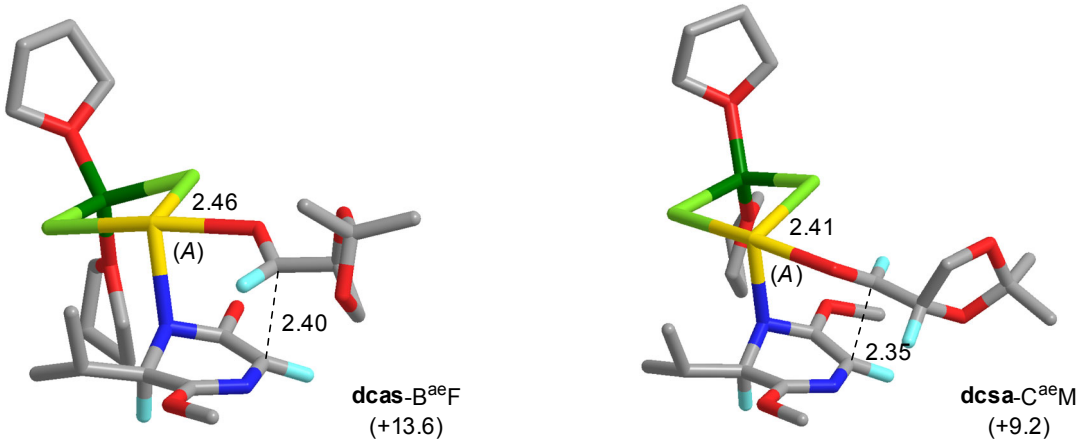


FIGURE S5. Chem3D representations of the most favored disolvated TSs located (at B3LYP/cc-pVDZ-PP level) in the 3,6-cis diastereomeric pathways for the aldol addition of disolvated tin(II) azaenolate (**dA**) to L-glyceraldehyde acetonide (**Lg**). Relative energies to **dtaa**-C^{ae}M in the gas-phase (at B3LYP/cc-pVTZ-PP level) are shown in parenthesis in kcal/mol. Bond lengths are in Å. The hydrogen atoms are omitted for clarity except at chiral and reaction centers. Legend: carbon–grey, chlorine–ligth green, hydrogen–turquoise, lithium–green, nitrogen–blue, oxygen–red, tin–yellow.



SCHEME S2. Selected geometries of tin(II) oxyanion **De** and intermediate complex **uADe** considered for TS location.

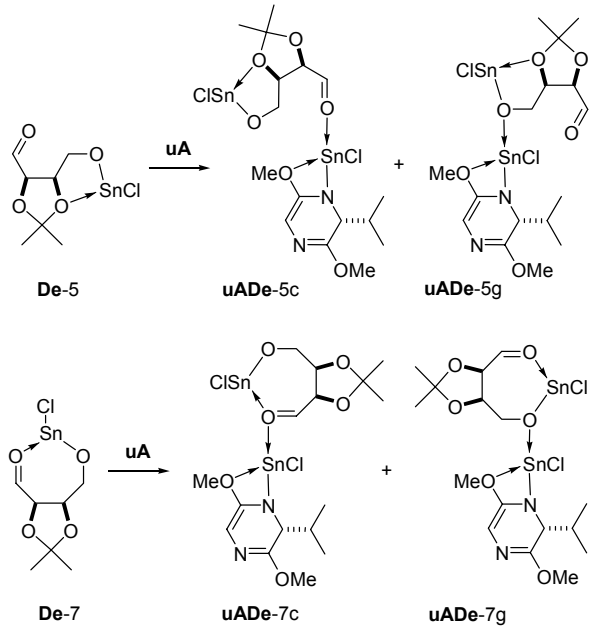


FIGURE S6. Chem3D representations of the most favored disolvated TSs located (at B3LYP/cc-pVDZ-PP level) in the 3,6-cis diastereomeric pathways for the aldol addition of unsolvated tin(II) azaenolate (**uA**) to D-erythrose acetonide (**De**). Relative energies to **utsa**–B7cg in the gas-phase (at B3LYP/cc-pVTZ-PP level) are shown in parenthesis in kcal/mol. Bond lengths are in Å. The hydrogen atoms are omitted for clarity except at chiral and reaction centers. Legend: carbon–grey, chlorine–ligth green, hydrogen–turquoise, lithium–green, nitrogen–blue, oxygen–red, tin–yellow.

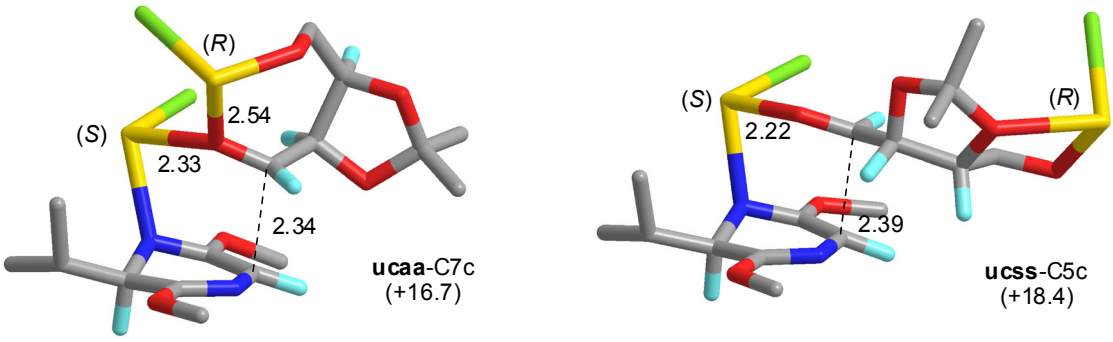


FIGURE S7. Chem3D representations of the most favored disolvated TSs located (at B3LYP/cc-pVDZ-PP level) in the 3,6-cis diastereomeric pathways for the aldol addition of unsolvated tin(II) azaenolate (**uA**) to L-erythrose acetonide (**Le**). Relative energies to **utaa**–B7cg in the gas-phase (at B3LYP/cc-pVTZ-PP level) are shown in parenthesis in kcal/mol. Bond lengths are in Å. The hydrogen atoms are omitted for clarity except at chiral and reaction centers. Legend: carbon–grey, chlorine–ligth green, hydrogen–turquoise, lithium–green, nitrogen–blue, oxygen–red, tin–yellow.

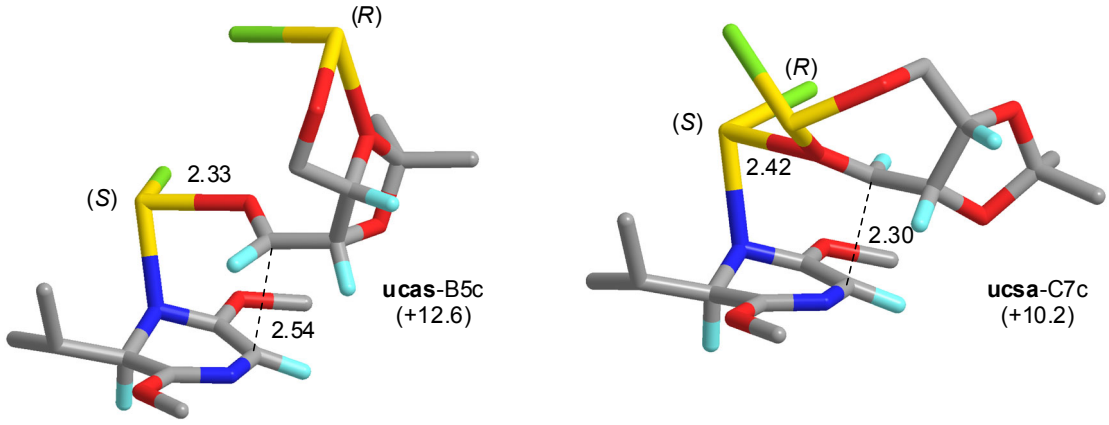


TABLE S1. Absolute energies (hartrees) and relative free energies (kcal/mol) in the gas phase calculated for intermediates located in the reaction of lithium azaenolate Li^{+}**15**$^{-}$ with $SnCl_2$ in the presence of three THF molecules.

	B3LYP/cc-pVDZ-PP			B3LYP/cc-pVTZ-PP	
model (*config*)	E_{SCF}	N_{imag}	E_{cor}[a]	E_{SCF}	G_{rel}
THF	-232.457947099	0	0.095336	-232.537239982	
$SnCl_2$	-1134.91861019	0	-0.016766	-1134.96376625	
$(THF)_3Li^{+}Cl^{-}$	-1165.29350183	0	0.313702	-1165.53293800	
$(THF)_3Li^{+}$**15**$^{-}$	-1316.94373805	0	0.531877	-1317.35702600	+24.7
uA	-1286.59998265	0	0.204498	-1286.81771728	+13.9
(**uA**)$_2$	-2573.21631334	0	0.425494	-2573.64183255	+20.2
dA (*A*)	-2219.45596955	0	0.422824	-2219.83556392	**0.0**
tA (*A*)	-2451.92247931	0	0.531324	-2452.37374750	+7.6

[a] Zero-point energy corrections with thermal and entropy effects at 195.15 K and 1.0 atm, scaled by 0.97.

TABLE S2. Absolute energies (hartrees) and relative free energies (kcal/mol) in the gas phase calculated for selected intermediates and TSs in the addition of unsolvated tin(II) azaenolate (**uA**) to D-glyceraldehyde acetonide (**Dg**).

	B3LYP/cc-pVDZ-PP			B3LYP/cc-pVTZ-PP	
model [a]	E_{SCF}	N_{imag}	E_{cor} [b]	E_{SCF}	G_{rel}
Dg	-460.328023510	0	0.130692	-460.477703105	
uADg (*A*)	-1746.94666716	0	0.351370	-1747.30770701	
ucaa-CM (*S*)	-1746.92661837	1	0.352017	-1747.28530467	+13.5
ucss-CF (*S*)	-1746.92456421	1	0.351883	-1747.28494511	+13.6
utas-BF (*S*)	-1746.94101812	1	0.352628	-1747.30172168	+3.6
utas-BN (*S*)	-1746.94547700	1	0.352520	-1747.30608642	**+0.8**
utas-CF (*S*)	-1746.93510667	1	0.351464	-1747.29636058	+6.2
utas-CN (*S*)	-1746.94017156	1	0.352477	-1747.30074125	+4.1
utsa-BM (*S*)	-1746.93879472	1	0.351975	-1747.29901430	+4.9
utsa-CF (*S*)	-1746.94120455	1	0.351127	-1747.30184274	+2.6
utsa-CM (*S*)	-1746.94439965	1	0.351048	-1747.30583376	**0.0**
utsa-CM (*R*)	-1746.94310356	1	0.351835	-1747.30480839	+1.1

[a] Legend: **caa**–cis,anti,anti; **css**–cis,syn,syn; **tas**–trans,anti,syn; **tsa**–trans,syn,anti; B–boat-like; C–chair-like; F–Felkin-Anh; M–Cornforth; N–non-Anh; (*R*)–*R* configuration on Sn(II) stereogenic center.

[b] Zero-point energy corrections with thermal and entropy effects at 195.15 K and 1.0 atm, scaled by 0.97.

TABLE S3. Absolute energies (hartrees) and relative free energies (kcal/mol) in the gas phase calculated for selected intermediates and TSs in the addition of disolvated tin(II) azaenolate (**dA**) to D-glyceraldehyde acetonide (**Dg**).

	B3LYP/cc-pVDZ-PP			B3LYP/cc-pVTZ-PP	
model [a]	E_{SCF}	N_{imag}	E_{cor} [a]	E_{SCF}	G_{rel}
dADg	-2679.79534929	0	0.568468	-2680.31766559	
dcaa-C^{ae}M (*A*)	-2679.77343456	1	0.571096	-2680.29256665	+12.9
dcss-C^{ae}F (*A*)	-2679.77110534	1	0.568960	-2680.29157771	+12.2
dtas-B^{ae}F (*A*)	-2679.78409499	1	0.569522	-2680.30538876	+3.9
dtas-B^{ae}N (*A*)	-2679.79035353	1	0.571498	-2680.30988788	**+2.3**
dtas-C^{ae}F (*A*)	-2679.77843611	1	0.569066	-2680.30191289	+5.8
dtas-C^{ae}N (*A*)	-2679.78308675	1	0.569016	-2680.30482145	+3.9
dtsa-B^{ae}M (*A*)	-2679.78213112	1	0.569656	-2680.30329906	+5.3
dtsa-C^{ae}F (*C*)	-2679.78368530	1	0.569683	-2680.30534187	+4.0
dtsa-C^{ae}M (*A*)	-2679.78683781	1	0.568480	-2680.31053929	**0.0**
dtsa-C^{ae}M (*C*)	-2679.78835363	1	0.568885	-2680.31008175	+0.5
dtsa-C^{ea}M (*C*)	-2679.78641335	1	0.570224	-2680.30632392	+3.7

[a] Legend: **caa**–cis,anti,anti; **css**–cis,syn,syn; **tas**–trans,anti,syn; **tsa**–trans,syn,anti; B–boat-like; C–chair-like; F–Felkin-Anh; M–Cornforth; N–non-Anh; ae–axial-equatorial; ea–equatorial-axial; (*A*)–anticlockwise configuration on Sn(II) stereogenic center; (*C*)–clockwise configuration on Sn(II) stereogenic center.

[b] Zero-point energy corrections with thermal and entropy effects at 195.15 K and 1.0 atm, scaled by 0.97.

TABLE S4. Absolute energies (hartrees) and relative free energies (kcal/mol) in the gas phase calculated for selected intermediates and TSs in the addition of disolvated tin(II) azaenolate (**dA**) to L-glyceraldehyde acetonide (**Lg**).

	B3LYP/cc-pVDZ-PP			B3LYP/cc-pVTZ-PP	
model (*config*) [a]	E_{SCF}	N_{imag}	E_{cor} [a]	E_{SCF}	G_{rel}
dALg (*A*)	-2679.79278238	0	0.566614	-2680.31634221	
dcas-B^{ae}F (*A*)	-2679.76684954	1	0.568324	-2680.28642615	+13.6
dcsa-C^{ae}M (*A*)	-2679.77628380	1	0.571021	-2680.29622984	+9.2
dtaa-B^{ae}F (*A*)	-2679.78463222	1	0.570592	-2680.30565954	+3.0
dtaa-B^{ae}M (*A*)	2679.78355128	1	0.569331	-2680.30762304	+1.0
dtaa-C^{ae}F (*A*)	-2679.77860396	1	0.569278	-2680.30035057	+5.5
dtaa-C^{ae}M (*A*)	-2679.78634182	1	0.568895	-2680.30872155	**0.0**
dtaa-C^{ae}M (*C*)	-2679.78598497	1	0.569565	-2680.30689433	+1.6
dtss-B^{ea}F (*A*)	-2679.77092360	1	0.569171	-2680.29224566	+10.5
dtss-B^{ea}N (*S*)	-2679.77825006	1	0.569520	-2680.29806059	+7.1
dtss-C^{ae}F (*C*)	-2679.78310575	1	0.568668	2680.30569180	**+1.8**
dtss-C^{ae}N (*A*)	-2679.78110283	1	0.568607	2680.30328915	+3.2

[a] Legend: **caa**–cis,anti,anti; **css**–cis,syn,syn; **tas**–trans,anti,syn; **tsa**–trans,syn,anti; B–boat-like; C–chair-like; F–Felkin-Anh; M–Cornforth; N–non-Anh; ae–axial-equatorial; ea–equatorial-axial.

[b] Zero-point energy corrections with thermal and entropy effects at 195.15 K and 1.0 atm, scaled by 0.97.

TABLE S5. Total (hartrees) and relative (kcal/mol) free energies in THF solution (PCM method, ε=7.52) calculated for significative intermediates and TSs in the addition of disolvated tin(II) azaenolate (**dA**) to L-glyceraldehyde acetonide (**Lg**) or D-glyceraldehyde acetonide (**Dg**).

	B3LYP(SCRF)/cc-pVDZ-PP			B3LYP(SCRF)/cc-pVTZ-PP	
model [a]	*G*	N_{imag}	E_{cor} [a]	*G*	G_{rel}
dA (*A*)	-2219.429597	0	0.419072	-2219.807491	
Dg	-460.325194	0	0.130145	-460.475895	
dtas-B^{ae}N (*A*)	-2679.754574	1	0.569782	-2680.274497	+3.1
dtas-C^{ae}N (*A*)	-2679.753285	1	0.567943	-2680.273936	**+2.3**
dtsa-C^{ae}M (*A*)	-2679.754040	1	0.566978	-2680.276603	**0.0**
dtaa-C^{ae}M (*A*)	-2679.754845	1	0.566771	-2680.276474	**0.0**
dtss-C^{ae}F (*A*)	-2679.751572	1	0.567321	-2680.274758	**+1.4**

[a] Legend: **caa**–cis,anti,anti; **css**–cis,syn,syn; **tas**–trans,anti,syn; **tsa**–trans,syn,anti; B–boat-like; C–chair-like; F–Felkin-Anh; M–Cornforth; N–non-Anh; ae–axial-equatorial; ea–equatorial-axial.

[b] Zero-point energy corrections with thermal and entropy effects at 195.15 K and 1.0 atm, scaled by 0.97.

TABLE S6. Absolute energies (hartrees) and relative free energies (kcal/mol) in the gas phase calculated for selected intermediates and TSs in the addition of unsolvated tin(II) azaenolate (**uA**) to D-erythrose acetonide ((*R*,*R*)-**19c**).

	B3LYP/cc-pVDZ-PP			B3LYP/cc-pVTZ-PP	
model (*config*)[a]	E_{SCF}	N_{imag}	E_{cor}[a]	E_{SCF}	G_{rel}
(*R*)-**15**	-612.538844147	0	0.203046	-612.735449944	
(*R*,*R*)-**19c**	-574.877064201	0	0.154434	-575.062557220	
De (*R*)	-1248.95839077	0	0.138783	-1249.16471618	0.0
De-5 (*S*)	-1248.94294987	0	0.134265	-1249.15217104	+5.1
De-7 (*S*)	-1248.94656484	0	0.134811	-1249.15534518	+3.4
uADe (*S,R*)	-2535.59410867	0	0.348684	-2536.00821715	-12.8
ucaa-C7c (*S*,*R*)	-2535.54384743	1	0.347343	-2535.95986460	+16.7
ucss-C5c (*S*,*R*)	-2535.53706276	1	0.347364	-2535.95727411	+18.4
utas-B5c (*A*,*R*)	-2535.55870585	1	0.347096	-2535.97838553	+4.9
utas-B7c (*S*,*S*)	-2535.55647348	1	0.347826	-2535.97391720	+8.2
utas-C5c (*S*,*R*)	-2535.55286721	1	0.345808	-2535.97151690	+8.5
utas-C7 (*A*,*S*)	-2535.56009447	1	0.347852	-2535.97714790	+6.2
utas-C7c (*S*,*S*)	-2535.55827922	1	0.347910	-2535.97474497	+7.7
utas-C7g (*A*,*R*)	-2535.56716833	1	0.348504	-2535.98056703	**+4.5**
utsa-B5c (*A*,*S*)	-2535.55000114	1	0.344472	-2535.96966120	+8.8
utsa-B7cg (*A*,*R*)	-2535.57141161	1	0.347569	-2535.98604509	+0.4
utsa-B7cg (*A*,*S*)	-2535.57175316	1	0.347056	-2535.98623664	**0.0**
utsa-C5c (*S*,*R*)	-2535.56178897	1	0.346548	-2535.98193155	+2.4
utsa-C7c (*S*,*S*)	-2535.56566674	1	0.347984	-2535.98263703	+2.8

[a] Legend: **caa**–cis,anti,anti; **css**–cis,syn,syn; **tas**–trans,anti,syn; **tsa**–trans,syn,anti; B–boat-like; C–chair-like; 5–five-membered chelate; 7–seven-membered chelate; c–coordination of oxygen at carbonyl group of erythrose to Sn(II) azaenolate; g–coordination of oxygen at γ–position of erythrose to Sn(II) azaenolate.

[b] Zero-point energy corrections with thermal and entropy effects at 273.15 K and 1.0 atm, scaled by 0.97.

TABLE S7. Absolute energies (hartrees) and relative free energies (kcal/mol) in the gas phase calculated for selected intermediates and TSs in the addition of unsolvated tin(II) azaenolate (**uA**) to L-erythrose acetonide ((*S*,*S*)-**19c**).

	B3LYP/cc-pVDZ-PP			B3LYP/cc-pVTZ-PP	
model (*config*)[a]	E_{SCF}	N_{imag}	E_{cor}[a]	E_{SCF}	G_{rel}
uALe (*S*,*R*)	-2535.59242271	0	0.345786	-2536.00869333	-19.3
ucas-B5c (*S*,*R*)	-2535.54110245	1	0.346992	-2535.95909520	+12.6
ucsa-C7c (*S*,*R*)	-2535.54871244	1	0.348418	-2535.96434328	+10.2
utaa-B5c (*S*,*R*)	-2535.55464976	1	0.344500	-2535.97497601	+1.0
utaa-B7 (*R*,*S*)	-2535.55547431	1	0.346241	-2535.97416755	+2.6
utaa-B7c (*S*,*S*)	-2535.55712138	1	0.346195	-2535.97550005	+1.8
utaa-C5c (*S*,*R*)	-2535.55388512	1	0.345887	2535.97373451	+2.7
utaa-C7c (*S*,*R*)	-2535.56235905	1	0.347527	-2535.97963629	**0.0**
utaa-C7g (*S*,*S*)	-2535.56126955	1	0.348389	-2535.97677469	+2.3
utss-B5c (*R*,*S*)	-2535.54809269	1	0.346984	-2535.96612761	+8.1
utss-B7c (*S*,*S*)	-2535.55850525	1	0.349744	-2535.97287425	+5.6
utss-B7cg (*A*,*R*)	-2535.55959757	1	0.346833	-2535.97588115	**+1.9**
utss-B7g (*A*,*A*)	-2535.56149274	1	0.349502	-2535.97591749	+3.6
utss-C5c (*S*,*S*)	-2535.55500722	1	0.345579	-2535.97447129	+2.0
utss-C7c (*S*,*S*)	-2535.55843604		0.347585	-2535.97389412	+3.6

[a] Legend: **caa**–cis,anti,anti; **css**–cis,syn,syn; **tas**–trans,anti,syn; **tsa**–trans,syn,anti; B–boat-like; C–chair-like; 5–five-membered chelate; 7–seven-membered chelate; c–coordination of oxygen at carbonyl group of erythrose to Sn(II) azaenolate; g–coordination of oxygen at γ–position of erythrose to Sn(II) azaenolate.

[b] Zero-point energy corrections with thermal and entropy effects at 273.15 K and 1.0 atm, scaled by 0.97.

5. Cartesian coordinates of calculated structures.

For convenience, coordinates of all models reported (in the main text and the Supporting Information) are also available in xyz-format packed together into a single ZIP-archive.

THF

```
 E(RB+HF-LYP) =  -232.457947099
 Zero-point correction=                           0.112383 (Hartree/Particle)
 Thermal correction to Energy=                    0.115057
 Thermal correction to Enthalpy=                  0.115675
 Thermal correction to Gibbs Free Energy=         0.095336
 Sum of electronic and zero-point Energies=           -232.345564
 Sum of electronic and thermal Energies=              -232.342890
 Sum of electronic and thermal Enthalpies=            -232.342272
 Sum of electronic and thermal Free Energies=         -232.362611
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.000000    0.000000    0.000000
    2          8             0        0.000000    0.000000    1.432120
    3          6             0        1.346603    0.000000    1.919593
    4          6             0        2.242322   -0.311750    0.715944
    5          6             0        1.436654    0.311797   -0.432524
    6          1             0       -0.319595   -0.994503   -0.370530
    7          1             0       -0.732054    0.744249   -0.355732
    8          1             0        1.586206    0.994494    2.346259
    9          1             0        1.431922   -0.744272    2.728998
   10          1             0        3.257002    0.101448    0.818900
   11          1             0        2.329885   -1.402129    0.573016
   12          1             0        1.600822    1.402180   -0.466187
   13          1             0        1.685241   -0.101377   -1.421665
 ---------------------------------------------------------------------
```

$SnCl_2$

```
E(RB+HF-LYP) =  -1134.91861019
Zero-point correction=                           0.001702 (Hartree/Particle)
 Thermal correction to Energy=                    0.004268
 Thermal correction to Enthalpy=                  0.004886
 Thermal correction to Gibbs Free Energy=        -0.016766
 Sum of electronic and zero-point Energies=          -1134.916908
 Sum of electronic and thermal Energies=             -1134.914342
 Sum of electronic and thermal Enthalpies=           -1134.913724
 Sum of electronic and thermal Free Energies=        -1134.935377
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         17             0        1.857776   -0.920052    0.000000
    2         50             0        0.000000    0.625893    0.000000
    3         17             0       -1.857776   -0.920809    0.000000
 ---------------------------------------------------------------------
```

$(THF)_3Li^+15^-$

```
 E(RB+HF-LYP) =  -1316.94373805
 Zero-point correction=                           0.571585 (Hartree/Particle)
 Thermal correction to Energy=                    0.589530
 Thermal correction to Enthalpy=                  0.590148
 Thermal correction to Gibbs Free Energy=         0.531877
 Sum of electronic and zero-point Energies=          -1316.372154
 Sum of electronic and thermal Energies=             -1316.354208
 Sum of electronic and thermal Enthalpies=           -1316.353590
 Sum of electronic and thermal Free Energies=        -1316.411861
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        2.268596    1.961566   -1.001583
    2          6             0        1.008773    1.401773   -1.050718
    3          7             0        3.279359    1.266060   -0.320635
```

4	6	0	3.046837	0.045551	-0.015049
5	6	0	1.811055	-0.738603	-0.426136
6	8	0	3.925984	-0.684960	0.751184
7	7	0	0.679730	0.175645	-0.596549
8	6	0	2.051426	-1.667093	-1.667221
9	6	0	5.090960	0.010752	1.179753
10	3	0	-1.071596	0.040758	0.263956
11	6	0	2.951308	-2.863600	-1.327090
12	6	0	2.572920	-0.922466	-2.901814
13	8	0	-2.695907	0.053798	-0.890374
14	8	0	-1.313716	1.420713	1.709223
15	8	0	-1.344021	-1.697858	1.277171
16	6	0	-2.526864	0.086818	-2.326423
17	6	0	-3.990757	-0.497741	-0.564807
18	6	0	-2.124081	2.585017	1.408311
19	6	0	-0.102296	1.827557	2.399261
20	6	0	-1.118991	-2.983310	0.649994
21	6	0	-1.163257	-1.807619	2.709591
22	8	0	-0.121239	2.101945	-1.479959
23	6	0	0.082697	3.401416	-1.999993
24	6	0	-4.617587	-0.955327	-1.894537
25	6	0	-3.403325	-1.052981	-2.833267
26	6	0	0.010556	3.332054	2.171539
27	6	0	-1.463974	3.759169	2.135750
28	6	0	-1.098212	-3.306104	3.006266
29	6	0	-0.465150	-3.856181	1.719800
30	1	0	2.522095	2.953812	-1.366043
31	1	0	1.571891	-1.433050	0.403933
32	1	0	1.041881	-2.053706	-1.913684
33	1	0	5.670181	-0.706469	1.778818
34	1	0	4.828804	0.895001	1.785264
35	1	0	5.687111	0.361956	0.321025
36	1	0	2.560202	-3.433575	-0.466190
37	1	0	3.027775	-3.556588	-2.182320
38	1	0	3.968168	-2.534994	-1.061135
39	1	0	1.893521	-0.111117	-3.200264
40	1	0	2.682064	-1.612400	-3.756853
41	1	0	3.560666	-0.473390	-2.703986
42	1	0	-2.870417	1.064068	-2.714015
43	1	0	-4.596981	0.271681	-0.057073
44	1	0	-2.122807	2.725598	0.315345
45	1	0	-0.210505	1.583517	3.472648
46	1	0	-2.094194	-3.396326	0.331091
47	1	0	-1.999664	-1.290847	3.203365
48	1	0	-0.904689	3.773374	-2.311449
49	1	0	0.510613	4.089666	-1.247311
50	1	0	0.756944	3.387064	-2.875152
51	1	0	-5.167539	-1.902420	-1.791617
52	1	0	-5.324702	-0.196805	-2.267795
53	1	0	-2.884162	-2.017152	-2.703037
54	1	0	-3.669351	-0.946654	-3.895387
55	1	0	0.590735	3.833241	2.960306
56	1	0	-1.862667	3.854410	3.159901
57	1	0	0.733717	1.258230	1.968976
58	1	0	-3.154651	2.388240	1.745073
59	1	0	-1.630254	4.714932	1.616910
60	1	0	0.501934	3.521672	1.204713
61	1	0	-0.490511	-2.825550	-0.237865
62	1	0	-0.223119	-1.299343	2.986155
63	1	0	-0.514174	-3.528354	3.911251
64	1	0	-2.112196	-3.718064	3.143102
65	1	0	0.624965	-3.694417	1.727866
66	1	0	-0.653492	-4.928036	1.561075
67	1	0	-1.452547	-0.014787	-2.524198
68	1	0	-3.826098	-1.329608	0.139247

$(THF)_3Li^+Cl^-$

E(RB+HF-LYP) = -1165.29350183

Zero-point correction=	0.344738 (Hartree/Particle)
Thermal correction to Energy=	0.355853
Thermal correction to Enthalpy=	0.356471
Thermal correction to Gibbs Free Energy=	0.313702
Sum of electronic and zero-point Energies=	-1164.948764
Sum of electronic and thermal Energies=	-1164.937649
Sum of electronic and thermal Enthalpies=	-1164.937031

Sum of electronic and thermal Free Energies= -1164.979799

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.107102	0.191159	2.489639
2	3	0	0.032513	0.002965	0.258698
3	6	0	-0.174627	2.491439	-1.405955
4	6	0	-1.830272	2.269278	0.267158
5	6	0	-0.103365	3.747023	-0.543462
6	1	0	0.799246	2.035792	-1.633149
7	6	0	-1.501046	3.762766	0.098326
8	1	0	-2.863498	2.028466	-0.033652
9	1	0	0.116439	4.654194	-1.126277
10	1	0	-2.223801	4.250603	-0.576174
11	6	0	2.300692	-1.191357	-1.341657
12	6	0	2.937540	0.339952	0.352004
13	6	0	3.694382	-1.583363	-0.822675
14	1	0	1.553635	-1.988580	-1.201406
15	6	0	3.739947	-0.935735	0.570855
16	1	0	3.545434	1.127089	-0.133574
17	1	0	3.834722	-2.674154	-0.799779
18	1	0	3.229782	-1.565753	1.317076
19	1	0	-1.643612	1.899807	1.286799
20	1	0	-1.523107	4.296359	1.059371
21	1	0	0.674881	3.626779	0.227219
22	1	0	-0.717187	2.682497	-2.352395
23	1	0	2.311024	-0.901391	-2.405932
24	1	0	2.458579	0.727466	1.261921
25	1	0	4.763801	-0.739145	0.921921
26	1	0	4.480094	-1.157014	-1.467769
27	8	0	-0.911884	1.545242	-0.607485
28	8	0	1.869382	-0.055696	-0.548590
29	6	0	-1.391983	-2.530896	0.713901
30	6	0	-1.903063	-1.634371	-1.417519
31	6	0	-2.910181	-2.519650	0.586457
32	1	0	-0.977409	-3.540720	0.531595
33	6	0	-3.101389	-2.473892	-0.938877
34	1	0	-2.166500	-0.583515	-1.615949
35	1	0	-3.382983	-3.396133	1.053805
36	1	0	-3.051612	-3.491556	-1.359270
37	8	0	-0.940182	-1.635772	-0.334488
38	1	0	-1.429569	-2.054439	-2.321297
39	1	0	-4.062581	-2.033664	-1.242827
40	1	0	-3.316080	-1.612316	1.062617
41	1	0	-1.006312	-2.126623	1.660344

uA

E(RB+HF-LYP) = -1286.59998265
Zero-point correction= 0.231001 (Hartree/Particle)
Thermal correction to Energy= 0.239940
Thermal correction to Enthalpy= 0.240558
Thermal correction to Gibbs Free Energy= 0.204498
Sum of electronic and zero-point Energies= -1286.368982
Sum of electronic and thermal Energies= -1286.360043
Sum of electronic and thermal Enthalpies= -1286.359425
Sum of electronic and thermal Free Energies= -1286.395485

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.761605	1.923844	-0.278233
2	7	0	2.671892	0.938728	-0.689133
3	6	0	2.305889	-0.280680	-0.545102
4	8	0	3.072514	-1.313071	-0.955974
5	6	0	1.025922	-0.753326	0.120587
6	7	0	0.005115	0.303995	0.016379
7	6	0	0.474025	1.601383	0.022264
8	8	0	-0.553058	2.479049	0.262754
9	17	0	-2.013702	-2.277502	-0.875688
10	50	0	-2.103272	0.094844	-0.211083
11	6	0	-0.306081	3.867077	0.057982
12	6	0	1.314322	-1.238391	1.583860
13	6	0	4.321403	-0.971537	-1.566787
14	6	0	1.864082	-0.142785	2.506065

15	6	0	0.095348	-1.921003	2.210265
16	1	0	2.127835	2.948419	-0.276009
17	1	0	0.431792	4.247331	0.784452
18	1	0	0.057704	4.059995	-0.965481
19	1	0	-1.266784	4.373929	0.216338
20	1	0	2.099043	-2.005734	1.454183
21	1	0	4.793170	-1.926794	-1.829729
22	1	0	4.955471	-0.402929	-0.868737
23	1	0	4.160542	-0.356235	-2.465541
24	1	0	2.153115	-0.576004	3.477725
25	1	0	1.105542	0.632630	2.702982
26	1	0	2.750831	0.350552	2.080100
27	1	0	0.350708	-2.322824	3.204152
28	1	0	-0.282654	-2.745918	1.588670
29	1	0	-0.733023	-1.205057	2.360873
30	1	0	0.659464	-1.630403	-0.433509

$(uA)_2$

E(RB+HF-LYP) = -2573.21631334
Zero-point correction= 0.463126 (Hartree/Particle)
Thermal correction to Energy= 0.481697
Thermal correction to Enthalpy= 0.482315
Thermal correction to Gibbs Free Energy= 0.425494
Sum of electronic and zero-point Energies= -2572.753188
Sum of electronic and thermal Energies= -2572.734616
Sum of electronic and thermal Enthalpies= -2572.733998
Sum of electronic and thermal Free Energies= -2572.790820

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.217469	0.298327	1.703495
2	7	0	3.859083	0.999003	0.665894
3	6	0	3.570064	0.638682	-0.535312
4	8	0	4.128199	1.217707	-1.612471
5	6	0	2.616623	-0.494146	-0.890054
6	7	0	1.549174	-0.485315	0.154935
7	6	0	2.103575	-0.435849	1.451538
8	8	0	1.326625	-1.102206	2.358743
9	17	0	0.296626	2.001719	-2.247739
10	50	0	0.457534	1.740266	0.209940
11	6	0	1.715733	-1.034648	3.725741
12	6	0	3.421162	-1.815744	-1.131810
13	6	0	5.063661	2.272965	-1.360374
14	6	0	4.290514	-2.307460	0.035855
15	6	0	2.554621	-2.962780	-1.661641
16	6	0	-1.507314	0.755556	3.984264
17	8	0	-1.152876	0.886942	2.612760
18	6	0	-1.988473	0.311030	1.695406
19	6	0	-3.124190	-0.394204	1.939371
20	7	0	-1.497181	0.435887	0.377789
21	7	0	-3.800859	-1.035532	0.886902
22	6	0	-2.639959	0.589786	-0.571300
23	50	0	-0.423396	-1.766685	0.056945
24	6	0	-3.552652	-0.599383	-0.299341
25	6	0	-3.476900	1.906105	-0.431263
26	17	0	-0.655459	-1.677851	-2.406277
27	8	0	-4.116937	-1.138106	-1.393282
28	6	0	-2.637980	3.167723	-0.199511
29	6	0	-4.362012	2.078485	-1.675872
30	6	0	-4.981774	-2.260324	-1.179395
31	1	0	-4.433482	-3.086012	-0.700505
32	1	0	3.661159	0.392781	2.692764
33	1	0	2.712978	-1.483080	3.873476
34	1	0	1.732113	0.009560	4.081837
35	1	0	0.967888	-1.610030	4.286015
36	1	0	4.106834	-1.524579	-1.949603
37	1	0	5.405031	2.605624	-2.348389
38	1	0	5.908717	1.908782	-0.755749
39	1	0	4.580095	3.100514	-0.819021
40	1	0	4.926465	-3.140527	-0.307481
41	1	0	3.677048	-2.687761	0.868640
42	1	0	4.951985	-1.522089	0.429549
43	1	0	3.194676	-3.806243	-1.968131
44	1	0	1.936797	-2.663031	-2.518504

45	1	0	1.877398	-3.355582	-0.880549
46	1	0	2.126149	-0.240949	-1.839917
47	1	0	-0.725341	1.272573	4.554823
48	1	0	-2.484071	1.227917	4.185590
49	1	0	-1.551410	-0.306064	4.283133
50	1	0	-3.533868	-0.543612	2.936788
51	1	0	-2.229764	0.520805	-1.586510
52	1	0	-4.135134	1.782178	0.446268
53	1	0	-3.300376	4.044424	-0.110162
54	1	0	-1.949215	3.357585	-1.037898
55	1	0	-2.058821	3.116064	0.737806
56	1	0	-5.038650	2.939376	-1.551634
57	1	0	-4.974327	1.186821	-1.872701
58	1	0	-3.742752	2.261674	-2.570195
59	1	0	-5.330689	-2.555988	-2.176404
60	1	0	-5.828770	-1.983696	-0.532739

dA

E(RB+HF-LYP) = -2219.45596955
Zero-point correction= 0.462030 (Hartree/Particle)
Thermal correction to Energy= 0.479874
Thermal correction to Enthalpy= 0.480492
Thermal correction to Gibbs Free Energy= 0.422824
Sum of electronic and zero-point Energies= -2218.996726
Sum of electronic and thermal Energies= -2218.978882
Sum of electronic and thermal Enthalpies= -2218.978264
Sum of electronic and thermal Free Energies= -2219.035932

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.935206	0.549189	1.728904
2	7	0	2.974941	1.673909	0.882298
3	6	0	2.630020	1.502590	-0.336966
4	8	0	2.576812	2.546000	-1.218480
5	6	0	2.248307	0.185908	-0.992920
6	7	0	1.794643	-0.746313	0.046871
7	6	0	2.317453	-0.586737	1.300300
8	8	0	2.052776	-1.705910	2.060129
9	17	0	-1.013118	-0.965955	-1.919716
10	50	0	0.244081	-2.276291	-0.001228
11	6	0	2.116906	-1.577008	3.477948
12	6	0	3.402398	-0.357094	-1.896845
13	6	0	3.061853	3.797738	-0.732609
14	6	0	4.683353	-0.683893	-1.120477
15	6	0	2.935878	-1.559872	-2.723974
16	1	0	3.369340	0.664299	2.719087
17	1	0	3.159103	-1.439154	3.812662
18	1	0	1.501792	-0.730443	3.823168
19	1	0	1.725964	-2.517196	3.888780
20	1	0	3.620954	0.470325	-2.596822
21	1	0	2.985430	4.496937	-1.576197
22	1	0	4.107592	3.709439	-0.397113
23	1	0	2.464478	4.155530	0.121662
24	1	0	5.490468	-0.976971	-1.812530
25	1	0	4.519894	-1.522942	-0.424508
26	1	0	5.037335	0.177600	-0.532964
27	1	0	3.720603	-1.878639	-3.429433
28	1	0	2.027323	-1.330485	-3.303406
29	1	0	2.715510	-2.426223	-2.075289
30	1	0	1.399613	0.383672	-1.667743
31	17	0	-1.427866	-1.101870	1.699436
32	3	0	-1.976500	0.337228	-0.135467
33	6	0	-0.976915	3.117166	-0.796938
34	6	0	-0.660995	2.561462	1.433972
35	6	0	-1.003056	4.454113	-0.017875
36	1	0	0.000041	2.948304	-1.278579
37	6	0	-1.091172	4.026938	1.468214
38	1	0	-1.077001	1.934422	2.232901
39	1	0	-1.856766	5.083319	-0.309168
40	1	0	-2.126909	4.107973	1.834219
41	6	0	-4.802345	0.320168	0.759163
42	6	0	-4.592983	-0.095753	-1.571024
43	6	0	-6.133966	-0.224010	0.229452
44	1	0	-4.332167	-0.357462	1.489735

45	6	0	-5.706600	-0.987427	-1.033265
46	1	0	-5.000344	0.759257	-2.141979
47	1	0	-6.644649	-0.856697	0.969814
48	1	0	-5.303820	-1.979276	-0.770760
49	1	0	0.437751	2.452618	1.424880
50	1	0	-0.450437	4.633547	2.124985
51	1	0	-0.086157	5.028811	-0.216238
52	1	0	-1.771605	3.026422	-1.551151
53	1	0	-4.892181	1.322343	1.207416
54	1	0	-3.845913	-0.618340	-2.183779
55	1	0	-6.524002	-1.124653	-1.756325
56	1	0	-6.813328	0.602436	-0.037011
57	8	0	-1.201431	2.079961	0.183922
58	8	0	-3.916020	0.405337	-0.391856

dA, THF solution

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 Variational PCM results
 =======================
 <psi(f)|   H    |psi(f)>                    (a.u.) =   -2219.456604
 <psi(f)|H+V(f)/2|psi(f)>                   (a.u.) =   -2219.470765
 Total free energy in solution:
  with all non electrostatic terms          (a.u.) =   -2219.429597
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent               (kcal/mol) =      -8.89
 ---------------------------------------------------------------------
 Cavitation energy                        (kcal/mol) =      51.34
 Dispersion energy                        (kcal/mol) =     -26.67
 Repulsion energy                         (kcal/mol) =       1.16
 Total non electrostatic                  (kcal/mol) =      25.83
 ---------------------------------------------------------------------
 Zero-point correction=                           0.460394 (Hartree/Particle)
 Thermal correction to Energy=                    0.478530
 Thermal correction to Enthalpy=                  0.479148
 Thermal correction to Gibbs Free Energy=         0.419072
 Sum of electronic and zero-point Energies=          -2219.010371
 Sum of electronic and thermal Energies=             -2218.992235
 Sum of electronic and thermal Enthalpies=           -2218.991617
 Sum of electronic and thermal Free Energies=        -2219.051693
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.010227	0.635616	1.722929
2	7	0	2.941520	1.797865	0.925555
3	6	0	2.562419	1.651514	-0.288428
4	8	0	2.395300	2.715722	-1.126338
5	6	0	2.259140	0.334395	-0.984669
6	7	0	1.899792	-0.667865	0.026159
7	6	0	2.452377	-0.521577	1.268893
8	8	0	2.283453	-1.682791	1.991553
9	17	0	-0.943680	-1.017634	-1.921051
10	50	0	0.436928	-2.286571	-0.026242
11	6	0	2.408405	-1.610177	3.412816
12	6	0	3.425305	-0.087859	-1.937378
13	6	0	2.754866	3.997327	-0.603336
14	6	0	4.747536	-0.350147	-1.207228
15	6	0	3.026895	-1.289409	-2.801016
16	1	0	3.465501	0.740415	2.706751
17	1	0	3.455473	-1.423598	3.704835
18	1	0	1.763658	-0.816214	3.823046
19	1	0	2.093589	-2.589067	3.797993
20	1	0	3.567156	0.779335	-2.610456
21	1	0	2.582142	4.713681	-1.417334
22	1	0	3.813138	4.012077	-0.296221
23	1	0	2.140233	4.256176	0.273635
24	1	0	5.554732	-0.550958	-1.931376
25	1	0	4.666299	-1.228466	-0.545834
26	1	0	5.051856	0.510356	-0.590970
27	1	0	3.819722	-1.528782	-3.528604
28	1	0	2.096717	-1.099185	-3.360163
29	1	0	2.872428	-2.191069	-2.182088
30	1	0	1.380987	0.495823	-1.630476
31	17	0	-1.320845	-1.234202	1.706208
32	3	0	-2.037536	0.195482	-0.112435

33	6	0	-1.240613	3.030842	-0.778854
34	6	0	-0.946326	2.531995	1.470121
35	6	0	-1.410396	4.368015	-0.020439
36	1	0	-0.238483	2.945774	-1.230867
37	6	0	-1.506170	3.952616	1.468113
38	1	0	-1.332969	1.883033	2.267067
39	1	0	-2.309439	4.911156	-0.346609
40	1	0	-2.556097	3.941278	1.801262
41	6	0	-4.877298	0.162679	0.774289
42	6	0	-4.656127	-0.356298	-1.535073
43	6	0	-6.223613	-0.343480	0.244861
44	1	0	-4.453356	-0.503725	1.543645
45	6	0	-5.814585	-1.175702	-0.980013
46	1	0	-5.017563	0.495253	-2.140480
47	1	0	-6.771408	-0.923152	1.002495
48	1	0	-5.462575	-2.175153	-0.673098
49	1	0	0.158430	2.520370	1.500309
50	1	0	-0.943457	4.622352	2.135660
51	1	0	-0.544415	5.022616	-0.200492
52	1	0	-2.002318	2.860019	-1.553436
53	1	0	-4.928895	1.186677	1.176831
54	1	0	-3.928616	-0.933783	-2.121918
55	1	0	-6.627654	-1.301320	-1.710570
56	1	0	-6.859066	0.502524	-0.065128
57	8	0	-1.393757	1.985526	0.210626
58	8	0	-3.968000	0.156143	-0.364739

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tA

E(RB+HF-LYP) = -2451.92247931
Zero-point correction= 0.575641 (Hartree/Particle)
Thermal correction to Energy= 0.597018
Thermal correction to Enthalpy= 0.597636
Thermal correction to Gibbs Free Energy= 0.531324
Sum of electronic and zero-point Energies= -2451.346838
Sum of electronic and thermal Energies= -2451.325461
Sum of electronic and thermal Enthalpies= -2451.324843
Sum of electronic and thermal Free Energies= -2451.391155

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.802902	0.729666	0.159984
2	7	0	3.226216	1.569013	1.132175
3	6	0	2.064918	2.039195	0.872835
4	8	0	1.377497	2.796094	1.779534
5	6	0	1.317631	1.840337	-0.434712
6	7	0	1.692545	0.528351	-0.981264
7	6	0	3.018670	0.193138	-0.818016
8	8	0	3.375783	-0.801848	-1.696812
9	17	0	-1.653506	0.135080	-2.137427
10	50	0	0.448153	-1.252985	-1.214912
11	6	0	4.588483	-1.497241	-1.438725
12	6	0	1.530437	3.052856	-1.403165
13	6	0	2.046754	3.035811	3.018402
14	6	0	2.994318	3.347149	-1.759664
15	6	0	0.690144	2.908931	-2.676294
16	1	0	4.860330	0.504195	0.278066
17	1	0	0.240348	1.815521	-0.211116
18	1	0	4.648277	-2.294306	-2.192555
19	1	0	5.462292	-0.831877	-1.551060
20	1	0	4.583170	-1.937107	-0.428424
21	1	0	1.146613	3.922207	-0.834049
22	1	0	1.362726	3.653747	3.615986
23	1	0	3.000131	3.563019	2.854825
24	1	0	2.266291	2.088931	3.536873
25	1	0	3.056973	4.283414	-2.340271
26	1	0	3.423353	2.543773	-2.378886
27	1	0	3.625819	3.460889	-0.865779
28	1	0	0.793685	3.805528	-3.309942
29	1	0	-0.377408	2.760839	-2.454362
30	1	0	1.020653	2.037909	-3.264181
31	1	0	-0.936832	4.060559	1.659392
32	6	0	-1.944359	3.854915	2.052842
33	6	0	-3.027381	4.308790	1.062807
34	6	0	-2.173083	2.346461	2.116094

35	1	0	-2.034237	4.330732	3.040718
36	6	0	-3.036105	3.163210	0.051349
37	1	0	-2.809445	5.277682	0.590091
38	1	0	-4.005078	4.386002	1.567399
39	8	0	-2.675332	1.976893	0.802598
40	1	0	-2.936250	2.074423	2.867116
41	1	0	-1.256056	1.770560	2.300356
42	1	0	-2.289407	3.311693	-0.746820
43	1	0	-4.019107	2.991344	-0.413626
44	3	0	-2.563722	0.189081	0.046193
45	17	0	-0.861797	-1.056225	1.139908
46	8	0	-4.263319	-0.792120	0.069964
47	6	0	-4.517819	-1.858186	1.014913
48	6	0	-5.046541	-1.004699	-1.137837
49	6	0	-5.034987	-3.015717	0.167608
50	1	0	-3.574390	-2.065963	1.538823
51	1	0	-5.276850	-1.521275	1.745551
52	6	0	-5.866070	-2.277521	-0.892748
53	1	0	-5.673517	-0.115509	-1.310647
54	1	0	-4.339262	-1.107872	-1.975514
55	1	0	-5.620370	-3.740017	0.753069
56	1	0	-4.190681	-3.547756	-0.300598
57	1	0	-6.011233	-2.858791	-1.814900
58	1	0	-6.861125	-2.027936	-0.488947
59	1	0	2.066728	-1.076613	2.065706
60	6	0	2.512551	-2.076193	1.982803
61	8	0	2.204812	-2.602864	0.668293
62	6	0	1.952930	-3.093581	2.973853
63	1	0	3.609506	-1.976728	2.074782
64	6	0	1.846774	-3.996491	0.772700
65	6	0	2.155478	-4.412582	2.213892
66	1	0	0.880428	-2.905574	3.141432
67	1	0	2.470254	-3.065764	3.944671
68	1	0	0.770477	-4.106284	0.545693
69	1	0	2.419484	-4.564551	0.021594
70	1	0	1.504606	-5.228096	2.563173
71	1	0	3.202057	-4.749742	2.302697

Dg

E(RB+HF-LYP) = -460.328023510
Zero-point correction= 0.150893 (Hartree/Particle)
Thermal correction to Energy= 0.155535
Thermal correction to Enthalpy= 0.156153
Thermal correction to Gibbs Free Energy= 0.130692
Sum of electronic and zero-point Energies= -460.177131
Sum of electronic and thermal Energies= -460.172488
Sum of electronic and thermal Enthalpies= -460.171870
Sum of electronic and thermal Free Energies= -460.197332

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.078412	0.574813	0.349342
2	8	0	-3.021277	0.298745	-0.352896
3	6	0	-0.948428	-0.400731	0.679690
4	8	0	0.229302	0.318059	1.024414
5	6	0	1.200595	0.154200	-0.038344
6	8	0	0.510140	-0.500824	-1.098712
7	6	0	-0.534582	-1.266790	-0.513716
8	6	0	1.644928	1.521793	-0.532885
9	6	0	2.354350	-0.699891	0.486826
10	1	0	-1.957247	1.579956	0.830163
11	1	0	-1.276362	-1.005593	1.546009
12	1	0	-0.183937	-2.264209	-0.190938
13	1	0	2.364845	1.412848	-1.357914
14	1	0	2.121881	2.085492	0.282341
15	1	0	0.773685	2.084612	-0.897223
16	1	0	3.114612	-0.839395	-0.296636
17	1	0	1.991613	-1.689260	0.803689
18	1	0	2.822422	-0.213890	1.356037
19	1	0	-1.347546	-1.378766	-1.243459

Dg, **THF solution**

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Variational PCM results
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<psi(f)|   H    |psi(f)>                    (a.u.) =    -460.327106
<psi(f)|H+V(f)/2|psi(f)>                    (a.u.) =    -460.335107
Total free energy in solution:
 with all non electrostatic terms           (a.u.) =    -460.325194
-------------------------------------------------------------------
(Polarized solute)-Solvent              (kcal/mol) =      -5.02
-------------------------------------------------------------------
Cavitation energy                       (kcal/mol) =      17.94
Dispersion energy                       (kcal/mol) =     -12.37
Repulsion energy                        (kcal/mol) =       0.65
Total non electrostatic                 (kcal/mol) =       6.22
-------------------------------------------------------------------
Zero-point correction=                           0.150363 (Hartree/Particle)
Thermal correction to Energy=                    0.155008
Thermal correction to Enthalpy=                  0.155626
Thermal correction to Gibbs Free Energy=         0.130145
Sum of electronic and zero-point Energies=           -460.184744
Sum of electronic and thermal Energies=              -460.180100
Sum of electronic and thermal Enthalpies=            -460.179482
Sum of electronic and thermal Free Energies=         -460.204963
-------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
-------------------------------------------------------------------
   1          6             0       -2.070941    0.568088    0.362009
   2          8             0       -3.001693    0.315242   -0.371206
   3          6             0       -0.950434   -0.416448    0.684265
   4          8             0        0.232473    0.297924    1.035646
   5          6             0        1.196959    0.157386   -0.039161
   6          8             0        0.500113   -0.492650   -1.101295
   7          6             0       -0.533967   -1.275556   -0.509997
   8          6             0        1.624064    1.534744   -0.521230
   9          6             0        2.362199   -0.692828    0.464589
  10          1             0       -1.967494    1.558071    0.878895
  11          1             0       -1.284487   -1.024211    1.549016
  12          1             0       -0.167884   -2.267546   -0.189830
  13          1             0        2.338353    1.442415   -1.353554
  14          1             0        2.106268    2.091668    0.295879
  15          1             0        0.744790    2.096288   -0.869178
  16          1             0        3.117088   -0.814225   -0.327364
  17          1             0        2.010684   -1.689156    0.772542
  18          1             0        2.835416   -0.211876    1.334159
  19          1             0       -1.347148   -1.397866   -1.238579
-------------------------------------------------------------------
```

uADg (*A*)

```
E(RB+HF-LYP) =  -1746.94666716
Zero-point correction=                           0.384078 (Hartree/Particle)
Thermal correction to Energy=                    0.398098
Thermal correction to Enthalpy=                  0.398716
Thermal correction to Gibbs Free Energy=         0.351370
Sum of electronic and zero-point Energies=          -1746.562590
Sum of electronic and thermal Energies=             -1746.548569
Sum of electronic and thermal Enthalpies=           -1746.547951
Sum of electronic and thermal Free Energies=        -1746.595297
-------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
-------------------------------------------------------------------
   1          6             0       -1.404427   -1.669882    0.326380
   2          7             0       -1.329072   -1.637868    1.729133
   3          6             0       -0.157230   -1.680037    2.251846
   4          8             0        0.028877   -1.607309    3.588924
   5          6             0        1.158728   -1.808178    1.501818
   6          7             0        0.977620   -1.390635    0.101966
   7          6             0       -0.261999   -1.569524   -0.433632
   8          8             0       -0.219947   -1.466858   -1.794913
   9          6             0       -0.906997    1.118931    0.073213
  10          8             0       -0.135471    1.309641   -0.878045
  11          6             0       -2.348307    1.581688    0.054567
  12          8             0       -2.904637    1.601719   -1.245168
  13          6             0       -2.976566    2.971155   -1.724125
  14          8             0       -2.351795    3.763803   -0.715994
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15	6	0	-2.448243	3.060627	0.505413
16	17	0	2.735255	1.308543	1.162652
17	50	0	2.016026	0.238735	-0.963572
18	6	0	-1.455454	-1.383669	-2.510944
19	6	0	1.785672	-3.227568	1.654712
20	6	0	-1.146581	-1.484522	4.392532
21	6	0	0.925013	-4.339699	1.044488
22	6	0	3.209182	-3.249870	1.087017
23	6	0	-2.170713	3.114812	-3.004607
24	6	0	-4.449468	3.340712	-1.885951
25	1	0	-2.386443	-1.861487	-0.101455
26	1	0	-0.528377	0.758672	1.049232
27	1	0	-2.932673	0.916382	0.708403
28	1	0	1.858383	-1.101793	1.977242
29	1	0	-1.177373	-1.280399	-3.567825
30	1	0	-2.042439	-2.307964	-2.380139
31	1	0	-2.045999	-0.510607	-2.191927
32	1	0	1.847999	-3.394330	2.745397
33	1	0	-0.795038	-1.460970	5.431928
34	1	0	-1.825344	-2.336338	4.230036
35	1	0	-1.693583	-0.559203	4.149940
36	1	0	1.366755	-5.328143	1.252466
37	1	0	0.854544	-4.230147	-0.050192
38	1	0	-0.098164	-4.336439	1.452941
39	1	0	3.685543	-4.228865	1.257717
40	1	0	3.843268	-2.478431	1.554249
41	1	0	3.199738	-3.070535	-0.001251
42	1	0	-1.632349	3.390664	1.164610
43	1	0	-2.158725	4.167538	-3.324545
44	1	0	-2.617289	2.508248	-3.806595
45	1	0	-1.142182	2.777428	-2.822722
46	1	0	-4.544368	4.370586	-2.261907
47	1	0	-4.977451	3.266671	-0.923382
48	1	0	-4.936373	2.656555	-2.596957
49	1	0	-3.414402	3.232630	1.015779

dADg

E(RB+HF-LYP) = -2679.79534929
Zero-point correction= 0.614649 (Hartree/Particle)
Thermal correction to Energy= 0.637941
Thermal correction to Enthalpy= 0.638559
Thermal correction to Gibbs Free Energy= 0.568468
Sum of electronic and zero-point Energies= -2679.180701
Sum of electronic and thermal Energies= -2679.157409
Sum of electronic and thermal Enthalpies= -2679.156791
Sum of electronic and thermal Free Energies= -2679.226881

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.645242	-2.378770	-0.526825
2	7	0	-2.564882	-1.915316	0.801778
3	6	0	-1.389802	-1.772520	1.294848
4	8	0	-1.178073	-1.243744	2.531375
5	6	0	-0.107261	-2.168236	0.581672
6	7	0	-0.301357	-1.951800	-0.858328
7	6	0	-1.544244	-2.304193	-1.329094
8	8	0	-1.523332	-2.444046	-2.695865
9	6	0	-2.652476	1.269949	-1.021027
10	8	0	-2.240364	0.638085	-1.975253
11	6	0	-4.121543	1.587435	-0.806278
12	8	0	-4.244142	2.923802	-0.328316
13	6	0	-4.722815	2.905179	1.035504
14	8	0	-4.585201	1.556733	1.469536
15	6	0	-4.735664	0.726579	0.323539
16	17	0	0.721721	1.470696	-0.170017
17	50	0	0.584675	-0.381151	-2.106504
18	6	0	-2.776293	-2.429601	-3.372135
19	6	0	0.363894	-3.603270	0.991122
20	6	0	-2.341894	-0.828533	3.253381
21	6	0	-0.655997	-4.723779	0.745084
22	6	0	1.708469	-3.949710	0.343475
23	6	0	-3.824463	3.783247	1.892150
24	6	0	-6.186432	3.350214	1.053344
25	1	0	-3.624870	-2.699820	-0.873557

26	1	0	-1.960633	1.651605	-0.237207
27	1	0	-4.655047	1.466556	-1.762684
28	1	0	0.688459	-1.485053	0.913995
29	1	0	-2.541978	-2.438750	-4.445346
30	1	0	-3.372143	-3.326226	-3.127547
31	1	0	-3.346452	-1.521431	-3.117853
32	1	0	0.515395	-3.530403	2.086474
33	1	0	-1.980304	-0.502371	4.238024
34	1	0	-3.052066	-1.663142	3.362646
35	1	0	-2.853863	0.002529	2.742419
36	1	0	-0.286529	-5.667827	1.180819
37	1	0	-0.812615	-4.894163	-0.331453
38	1	0	-1.633278	-4.501638	1.198960
39	1	0	2.072129	-4.926881	0.702703
40	1	0	2.477107	-3.191934	0.558125
41	1	0	1.609913	-4.003511	-0.751942
42	1	0	-5.800362	0.520288	0.107859
43	1	0	-4.152801	3.753752	2.941999
44	1	0	-3.863693	4.823993	1.538313
45	1	0	-2.787053	3.425288	1.831613
46	1	0	-6.573752	3.353309	2.083677
47	1	0	-6.807598	2.673662	0.447482
48	1	0	-6.278917	4.363368	0.634249
49	1	0	-4.205017	-0.217716	0.514500
50	1	0	4.118596	3.398063	-2.579052
51	6	0	4.979526	3.464224	-1.893921
52	6	0	4.683300	4.441626	-0.746133
53	6	0	5.156081	2.148971	-1.143116
54	1	0	5.869023	3.738067	-2.480206
55	6	0	3.833039	3.591513	0.204920
56	1	0	4.155596	5.349905	-1.071496
57	1	0	5.621942	4.750516	-0.257072
58	8	0	4.198215	2.208855	-0.057105
59	1	0	6.173499	2.058884	-0.719399
60	1	0	4.928845	1.250765	-1.733560
61	1	0	2.753717	3.692562	0.007056
62	1	0	4.024016	3.808914	1.267818
63	3	0	2.934320	0.761026	0.322286
64	17	0	3.089210	-0.936407	-1.328617
65	8	0	3.054203	0.085179	2.141236
66	6	0	4.024993	-0.918071	2.523930
67	6	0	2.089704	0.285303	3.215129
68	6	0	3.386702	-1.667447	3.689652
69	1	0	4.225282	-1.543781	1.641894
70	1	0	4.960805	-0.414517	2.829167
71	6	0	2.603699	-0.547900	4.392048
72	1	0	2.036267	1.362809	3.433669
73	1	0	1.104688	-0.058526	2.863664
74	1	0	4.133057	-2.151018	4.336895
75	1	0	2.699861	-2.443103	3.314061
76	1	0	1.781646	-0.921740	5.019335
77	1	0	3.278122	0.047940	5.029454

ucaa-CM (*S*)

E(RB+HF-LYP) = -1746.92661837
Zero-point correction= 0.383867 (Hartree/Particle)
Thermal correction to Energy= 0.397267
Thermal correction to Enthalpy= 0.397885
Thermal correction to Gibbs Free Energy= 0.352017
Sum of electronic and zero-point Energies= -1746.542752
Sum of electronic and thermal Energies= -1746.529352
Sum of electronic and thermal Enthalpies= -1746.528734
Sum of electronic and thermal Free Energies= -1746.574602

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	7	0	0.000000	0.000000	1.404879
3	6	0	1.144057	0.000000	1.981835
4	8	0	1.258378	-0.043495	3.325500
5	6	0	2.450222	0.162582	1.216929
6	7	0	2.346464	-0.519472	-0.104074
7	6	0	1.190011	-0.175451	-0.724586
8	8	0	1.254343	-0.213289	-2.071929

9	6	0	-0.367234	-2.328428	-0.114730
10	8	0	0.716911	-2.845920	0.304979
11	6	0	-0.867036	-2.606571	-1.516968
12	8	0	-2.030309	-1.824196	-1.792493
13	6	0	-3.170329	-2.698918	-1.969829
14	8	0	-2.769531	-3.952668	-1.434881
15	6	0	-1.371168	-4.066358	-1.649445
16	17	0	2.477210	-3.144429	-2.785023
17	50	0	2.857148	-2.740839	-0.356924
18	6	0	0.193989	0.379669	-2.831699
19	6	0	3.749033	-0.071004	2.024522
20	6	0	0.033873	-0.128992	4.065023
21	6	0	3.930912	-1.446637	2.686865
22	6	0	4.983590	0.317698	1.199271
23	6	0	-4.331532	-2.174025	-1.141216
24	6	0	-3.496505	-2.803549	-3.460724
25	1	0	-0.912361	0.363442	-0.470178
26	1	0	-1.133550	-2.073584	0.635838
27	1	0	2.486499	1.246871	0.975109
28	1	0	0.526250	0.328441	-3.876256
29	1	0	-0.755071	-0.163787	-2.716410
30	1	0	0.057570	1.434181	-2.537537
31	1	0	3.659330	0.655369	2.850674
32	1	0	0.328157	-0.138856	5.122106
33	1	0	-0.513744	-1.048013	3.805269
34	1	0	-0.613353	0.734025	3.846928
35	1	0	4.723839	-1.383907	3.450538
36	1	0	4.249126	-2.222509	1.972368
37	1	0	3.013704	-1.787164	3.187281
38	1	0	5.892550	0.272069	1.820205
39	1	0	4.896798	1.340749	0.798951
40	1	0	5.129512	-0.357267	0.340854
41	1	0	-0.069681	-2.406508	-2.246872
42	1	0	-1.134186	-4.465466	-2.652061
43	1	0	-5.201489	-2.839935	-1.242373
44	1	0	-4.616377	-1.166540	-1.478290
45	1	0	-4.039018	-2.129440	-0.082777
46	1	0	-4.349994	-3.480748	-3.616776
47	1	0	-2.634530	-3.190887	-4.024270
48	1	0	-3.751259	-1.812680	-3.866042
49	1	0	-0.954375	-4.741753	-0.890714

ucss-CF (*S*)

E(RB+HF-LYP) = -1746.92456421
Zero-point correction= 0.383711 (Hartree/Particle)
Thermal correction to Energy= 0.397122
Thermal correction to Enthalpy= 0.397740
Thermal correction to Gibbs Free Energy= 0.351883
Sum of electronic and zero-point Energies= -1746.540853
Sum of electronic and thermal Energies= -1746.527442
Sum of electronic and thermal Enthalpies= -1746.526824
Sum of electronic and thermal Free Energies= -1746.572681

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	7	0	0.000000	0.000000	1.404156
3	6	0	1.142815	0.000000	1.985319
4	8	0	1.255114	-0.044173	3.328221
5	6	0	2.451707	0.178799	1.228927
6	7	0	2.356846	-0.480659	-0.101542
7	6	0	1.202902	-0.151059	-0.720155
8	8	0	1.283581	-0.177514	-2.065109
9	6	0	-0.311803	-2.328544	-0.224185
10	8	0	0.698892	-2.783781	0.402120
11	6	0	-1.665656	-2.421131	0.467349
12	8	0	-2.000744	-3.811403	0.588949
13	6	0	-2.953910	-4.162326	-0.436822
14	8	0	-3.173326	-2.970528	-1.194510
15	6	0	-2.831128	-1.874367	-0.357054
16	17	0	2.031085	-3.186242	-2.696935
17	50	0	2.781105	-2.754988	-0.370341
18	6	0	0.125003	0.094186	-2.848871
19	6	0	3.744599	-0.078545	2.037319

20	6	0	0.034735	-0.139170	4.072456
21	6	0	3.915968	-1.475178	2.656599
22	6	0	4.983718	0.325573	1.226387
23	6	0	-2.366191	-5.216421	-1.364379
24	6	0	-4.240766	-4.619700	0.249707
25	1	0	-0.887363	0.432894	-0.462270
26	1	0	-0.306406	-2.330160	-1.327443
27	1	0	2.491636	1.267731	1.009321
28	1	0	0.451706	0.016435	-3.892723
29	1	0	-0.676042	-0.640335	-2.669203
30	1	0	-0.255707	1.110871	-2.652057
31	1	0	3.655306	0.623794	2.883795
32	1	0	0.330785	-0.106442	5.128561
33	1	0	-0.483934	-1.084292	3.847870
34	1	0	-0.637140	0.697243	3.827974
35	1	0	4.703242	-1.441976	3.427823
36	1	0	4.237253	-2.226904	1.918091
37	1	0	2.993958	-1.829713	3.138746
38	1	0	5.892178	0.248737	1.844948
39	1	0	4.907816	1.363103	0.862615
40	1	0	5.119643	-0.320932	0.344901
41	1	0	-1.585750	-1.987596	1.472728
42	1	0	-3.670367	-1.579300	0.300256
43	1	0	-3.078402	-5.455516	-2.168800
44	1	0	-2.146804	-6.135753	-0.801497
45	1	0	-1.434499	-4.846792	-1.815843
46	1	0	-4.993192	-4.907299	-0.500263
47	1	0	-4.652740	-3.811647	0.872606
48	1	0	-4.037433	-5.483643	0.900204
49	1	0	-2.572933	-1.023781	-1.001365

utas-BN (*S*)

E(RB+HF-LYP) = -1746.94547700
Zero-point correction= 0.384410 (Hartree/Particle)
Thermal correction to Energy= 0.397829
Thermal correction to Enthalpy= 0.398447
Thermal correction to Gibbs Free Energy= 0.352520
Sum of electronic and zero-point Energies= -1746.561067
Sum of electronic and thermal Energies= -1746.547648
Sum of electronic and thermal Enthalpies= -1746.547030
Sum of electronic and thermal Free Energies= -1746.592957

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.108194	0.754388	-1.763479
2	7	0	-0.006371	-0.421826	-2.524190
3	6	0	0.802224	-1.378764	-2.243073
4	8	0	0.740046	-2.565258	-2.879853
5	6	0	1.907233	-1.357132	-1.199645
6	7	0	1.740154	-0.218958	-0.279187
7	6	0	1.056905	0.842860	-0.743832
8	8	0	1.226271	1.927245	0.049609
9	6	0	-1.313338	0.056823	0.106054
10	8	0	-0.835727	0.385973	1.233626
11	6	0	-2.635086	0.632754	-0.354169
12	8	0	-2.723129	2.039618	-0.156865
13	6	0	-3.882555	2.346146	0.652683
14	8	0	-4.693383	1.178102	0.593408
15	6	0	-3.817989	0.069784	0.483753
16	17	0	0.578315	-2.737191	1.715386
17	50	0	1.224722	-0.344992	1.928781
18	6	0	0.460485	3.113007	-0.210983
19	6	0	3.323715	-1.398745	-1.849474
20	6	0	-0.279120	-2.709564	-3.874235
21	6	0	3.621095	-0.166246	-2.711083
22	6	0	4.401023	-1.606596	-0.779551
23	6	0	-3.436565	2.652072	2.082834
24	6	0	-4.646632	3.486738	0.000679
25	1	0	-0.372116	1.637356	-2.182114
26	1	0	-1.034386	-0.908571	-0.350433
27	1	0	1.796278	-2.285745	-0.616157
28	1	0	0.763813	3.828909	0.563384
29	1	0	0.716518	3.520167	-1.202847
30	1	0	-0.618603	2.913908	-0.144959

31	1	0	3.311727	-2.287493	-2.504961
32	1	0	-0.157517	-3.722956	-4.276925
33	1	0	-0.160637	-1.956832	-4.668725
34	1	0	-1.278897	-2.587831	-3.428696
35	1	0	4.588572	-0.279292	-3.226929
36	1	0	3.678839	0.745186	-2.093514
37	1	0	2.848780	-0.006753	-3.481281
38	1	0	5.397672	-1.701790	-1.239978
39	1	0	4.212765	-2.518807	-0.189942
40	1	0	4.432825	-0.751803	-0.084152
41	1	0	-2.763525	0.401232	-1.424476
42	1	0	-4.351873	-0.745417	-0.022902
43	1	0	-4.314126	2.792048	2.732277
44	1	0	-2.832376	3.572056	2.102393
45	1	0	-2.814570	1.836149	2.476580
46	1	0	-5.550962	3.719333	0.582683
47	1	0	-4.942131	3.196140	-1.017134
48	1	0	-4.018373	4.388153	-0.049054
49	1	0	-3.471786	-0.280585	1.472623

utsa-CM (*S*)

E(RB+HF-LYP) = -1746.94439965
Zero-point correction= 0.383645 (Hartree/Particle)
Thermal correction to Energy= 0.397259
Thermal correction to Enthalpy= 0.397877
Thermal correction to Gibbs Free Energy= 0.351048
Sum of electronic and zero-point Energies= -1746.560755
Sum of electronic and thermal Energies= -1746.547141
Sum of electronic and thermal Enthalpies= -1746.546523
Sum of electronic and thermal Free Energies= -1746.593351

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	7	0	0.000000	0.000000	1.402835
3	6	0	1.145089	0.000000	1.982930
4	8	0	1.261660	0.050271	3.322083
5	6	0	2.493678	-0.075547	1.297957
6	7	0	2.383252	0.318149	-0.118853
7	6	0	1.206218	0.063714	-0.709734
8	8	0	1.274422	0.140837	-2.071057
9	6	0	-0.070894	2.334012	-0.405289
10	8	0	0.993099	2.796777	0.120740
11	6	0	-1.379899	2.556659	0.301666
12	8	0	-2.430305	1.942756	-0.443796
13	6	0	-3.610787	2.767249	-0.351234
14	8	0	-3.224177	3.938671	0.374270
15	6	0	-1.809524	4.033032	0.325569
16	17	0	4.251780	2.926886	1.270306
17	50	0	3.027579	2.397819	-0.800326
18	6	0	0.116084	-0.218180	-2.828681
19	6	0	3.174408	-1.465295	1.486900
20	6	0	0.048499	0.131700	4.077424
21	6	0	2.386209	-2.622792	0.862681
22	6	0	4.617309	-1.430154	0.969953
23	6	0	-4.055032	3.128449	-1.766486
24	6	0	-4.686349	2.048931	0.452848
25	1	0	-0.932796	-0.313032	-0.465254
26	1	0	-0.147544	2.206396	-1.500383
27	1	0	-1.317244	2.145935	1.324194
28	1	0	3.141107	0.657809	1.801664
29	1	0	0.409430	-0.124941	-3.881941
30	1	0	-0.177921	-1.259440	-2.617080
31	1	0	-0.738022	0.447145	-2.621089
32	1	0	3.202149	-1.617136	2.580826
33	1	0	0.354490	0.097874	5.130580
34	1	0	-0.621289	-0.707674	3.836717
35	1	0	-0.480169	1.073887	3.862993
36	1	0	2.855609	-3.587177	1.116916
37	1	0	2.367705	-2.545552	-0.237063
38	1	0	1.344556	-2.654208	1.221148
39	1	0	5.126587	-2.387034	1.169042
40	1	0	5.198186	-0.627225	1.451380
41	1	0	4.637929	-1.255625	-0.118002

42	1	0	-4.958990	3.755068	-1.734264
43	1	0	-4.275407	2.217836	-2.344235
44	1	0	-3.259275	3.684420	-2.284535
45	1	0	-5.561332	2.702696	0.587920
46	1	0	-4.291919	1.779997	1.443238
47	1	0	-5.004528	1.132069	-0.065434
48	1	0	-1.464945	4.568525	-0.581039
49	1	0	-1.457352	4.572016	1.214884

dcaa-C^{ae}M (*A*)

E(RB+HF-LYP) = -2679.77343456
Zero-point correction= 0.615187 (Hartree/Particle)
Thermal correction to Energy= 0.637382
Thermal correction to Enthalpy= 0.638000
Thermal correction to Gibbs Free Energy= 0.571096
Sum of electronic and zero-point Energies= -2679.158248
Sum of electronic and thermal Energies= -2679.136053
Sum of electronic and thermal Enthalpies= -2679.135435
Sum of electronic and thermal Free Energies= -2679.202338

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.976136	0.615486	1.188379
2	6	0	2.757662	-0.552282	-0.954304
3	7	0	3.673007	1.636356	0.520325
4	6	0	3.002173	2.691663	0.240215
5	8	0	3.531002	3.703039	-0.485174
6	6	0	1.602431	2.916220	0.789917
7	7	0	0.846771	1.633062	0.717692
8	6	0	1.586182	0.645921	1.291554
9	8	0	0.840959	-0.367947	1.819207
10	8	0	1.938612	0.161358	-1.565617
11	6	0	2.444852	-1.992586	-0.617456
12	8	0	3.464678	-2.552307	0.214267
13	6	0	3.869819	-3.834183	-0.316457
14	8	0	2.965621	-4.119996	-1.379280
15	6	0	2.496360	-2.878562	-1.880722
16	17	0	-1.218642	-1.433168	-0.614094
17	50	0	-0.339859	1.019564	-1.169110
18	6	0	1.513052	-1.335462	2.627892
19	6	0	0.883381	4.197512	0.319024
20	6	0	4.857654	3.497764	-0.979057
21	6	0	0.516630	4.269600	-1.170882
22	6	0	-0.328204	4.514203	1.207022
23	6	0	5.307619	-3.722302	-0.824402
24	6	0	3.696984	-4.905635	0.750384
25	17	0	-2.783412	1.813228	-0.083257
26	3	0	-3.240018	-0.453901	0.297739
27	8	0	-3.372286	-0.832482	2.211972
28	8	0	-4.767030	-1.059614	-0.766182
29	6	0	-3.297989	0.247090	3.176474
30	6	0	-2.816802	-2.042891	2.791487
31	6	0	-4.762647	-2.281154	-1.552701
32	6	0	-5.702154	-0.111587	-1.335109
33	6	0	-2.142581	-0.139598	4.090919
34	6	0	-2.332728	-1.661084	4.198333
35	6	0	-5.777730	-2.064240	-2.683116
36	6	0	-5.840347	-0.532800	-2.793756
37	1	0	-6.770884	-0.168262	-3.253304
38	1	0	3.590937	-0.103896	1.725820
39	1	0	3.831318	-0.285688	-0.948567
40	1	0	1.770981	3.087345	1.875507
41	1	0	0.729374	-2.014642	2.989037
42	1	0	2.260885	-1.909602	2.060914
43	1	0	2.001865	-0.846327	3.488678
44	1	0	1.639360	4.983677	0.489081
45	1	0	5.115237	4.413086	-1.527619
46	1	0	4.893475	2.622639	-1.646932
47	1	0	5.562398	3.328972	-0.150209
48	1	0	0.304221	5.314455	-1.452610
49	1	0	-0.402958	3.705718	-1.402806
50	1	0	1.332587	3.910988	-1.815267
51	1	0	-0.764480	5.487378	0.928182
52	1	0	-0.038365	4.568525	2.269615

53	1	0	-1.113786	3.750690	1.106175
54	1	0	1.455030	-2.073730	-0.141449
55	1	0	1.506176	-3.028245	-2.329457
56	1	0	5.647535	-4.688843	-1.226690
57	1	0	5.978200	-3.420276	-0.005856
58	1	0	5.379162	-2.965882	-1.620183
59	1	0	3.959628	-5.893572	0.342836
60	1	0	2.649193	-4.928287	1.082410
61	1	0	4.345993	-4.695475	1.613497
62	1	0	3.181930	-2.460589	-2.643174
63	1	0	-3.142812	1.176479	2.612491
64	1	0	-4.255032	0.303605	3.728598
65	1	0	-3.597752	-2.820639	2.803332
66	1	0	-1.993817	-2.370932	2.136905
67	1	0	-3.737476	-2.429767	-1.927018
68	1	0	-5.026135	-3.125164	-0.895151
69	1	0	-6.666293	-0.188059	-0.798522
70	1	0	-5.280297	0.892257	-1.188305
71	1	0	-2.182252	0.371855	5.064165
72	1	0	-1.186661	0.099660	3.598819
73	1	0	-3.102314	-1.898832	4.951157
74	1	0	-1.413646	-2.196669	4.478642
75	1	0	-5.467581	-2.556335	-3.616438
76	1	0	-6.765149	-2.465328	-2.400931
77	1	0	-4.989320	-0.148710	-3.379625

dcss-C^{ae}F (*A*)

E(RB+HF-LYP) = -2679.77110534
Zero-point correction= 0.614342 (Hartree/Particle)
Thermal correction to Energy= 0.636811
Thermal correction to Enthalpy= 0.637429
Thermal correction to Gibbs Free Energy= 0.568960
Sum of electronic and zero-point Energies= -2679.156764
Sum of electronic and thermal Energies= -2679.134294
Sum of electronic and thermal Enthalpies= -2679.133676
Sum of electronic and thermal Free Energies= -2679.202145

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.310587	0.658651	1.710659
2	6	0	2.332763	-0.954498	-0.106526
3	7	0	3.328308	1.433749	1.127641
4	6	0	2.956931	2.451934	0.444185
5	8	0	3.845723	3.232386	-0.211473
6	6	0	1.514452	2.939442	0.416308
7	7	0	0.597366	1.770328	0.441449
8	6	0	0.968332	0.892729	1.395191
9	8	0	-0.064893	0.133501	1.858897
10	8	0	1.954266	-0.242484	-1.059946
11	6	0	3.799447	-1.341801	-0.001971
12	8	0	3.941207	-2.537338	-0.788080
13	6	0	4.758243	-3.485459	-0.074989
14	8	0	5.237763	-2.801723	1.080750
15	6	0	4.303042	-1.773528	1.375991
16	17	0	-1.142518	-1.628030	-0.585092
17	50	0	-0.227769	0.701352	-1.460815
18	6	0	0.197130	-0.877671	2.824036
19	6	0	1.195764	4.046317	-0.612623
20	6	0	5.219224	2.842232	-0.133606
21	6	0	1.401434	3.683311	-2.091022
22	6	0	-0.199045	4.639407	-0.368899
23	6	0	3.899145	-4.690529	0.310831
24	6	0	5.956806	-3.861199	-0.935699
25	17	0	-2.809858	1.589408	-0.887871
26	3	0	-3.173699	-0.513563	0.064054
27	8	0	-3.618833	-0.307386	1.950839
28	8	0	-4.693656	-1.470138	-0.766952
29	6	0	-4.574897	-1.094618	2.695393
30	6	0	-3.315829	0.925872	2.664081
31	6	0	-4.579359	-2.832080	-1.266086
32	6	0	-5.615287	-0.721016	-1.597808
33	6	0	-5.084861	-0.180399	3.810556
34	6	0	-3.862397	0.712224	4.073464
35	6	0	-5.501114	-2.918538	-2.489967

36	6	0	-5.614365	-1.452003	-2.935196
37	1	0	-6.516721	-1.247214	-3.530057
38	1	0	2.604409	0.080190	2.585795
39	1	0	1.619624	-1.623947	0.409709
40	1	0	1.379441	3.441217	1.400175
41	1	0	-0.769765	-1.359023	3.017193
42	1	0	0.904552	-1.634425	2.449253
43	1	0	0.592836	-0.441421	3.757912
44	1	0	1.939247	4.828662	-0.382292
45	1	0	5.777171	3.612357	-0.681829
46	1	0	5.373953	1.855077	-0.596872
47	1	0	5.553514	2.791115	0.914105
48	1	0	1.413352	4.601561	-2.701380
49	1	0	0.581992	3.062339	-2.490916
50	1	0	2.351235	3.155916	-2.258261
51	1	0	-0.374058	5.496938	-1.038874
52	1	0	-0.304017	4.996992	0.668867
53	1	0	-0.996437	3.901072	-0.545738
54	1	0	4.407919	-0.532010	-0.432579
55	1	0	4.822265	-0.969542	1.912016
56	1	0	4.505891	-5.440906	0.840703
57	1	0	3.465788	-5.151566	-0.589490
58	1	0	3.070926	-4.380766	0.965852
59	1	0	6.616504	-4.554188	-0.391502
60	1	0	6.524887	-2.954611	-1.188171
61	1	0	5.622159	-4.344573	-1.865452
62	1	0	3.473807	-2.154376	2.004438
63	1	0	-5.358041	-1.432243	1.999923
64	1	0	-4.058758	-1.982432	3.103965
65	1	0	-2.230783	1.081875	2.606534
66	1	0	-3.819706	1.758724	2.146431
67	1	0	-3.521421	-3.002172	-1.518947
68	1	0	-4.868977	-3.526664	-0.460894
69	1	0	-6.617546	-0.735756	-1.129502
70	1	0	-5.246832	0.313015	-1.646290
71	1	0	-5.417990	-0.743920	4.694554
72	1	0	-5.931903	0.427942	3.452411
73	1	0	-3.126922	0.180744	4.700764
74	1	0	-4.113828	1.659928	4.571727
75	1	0	-5.091416	-3.578956	-3.268006
76	1	0	-6.492673	-3.306932	-2.204196
77	1	0	-4.732935	-1.154095	-3.525828

dtas-B^{ae}N (*A*), gas-phase

E(RB+HF-LYP) = -2679.79035353
Zero-point correction= 0.615755 (Hartree/Particle)
Thermal correction to Energy= 0.637944
Thermal correction to Enthalpy= 0.638562
Thermal correction to Gibbs Free Energy= 0.571498
Sum of electronic and zero-point Energies= -2679.174598
Sum of electronic and thermal Energies= -2679.152410
Sum of electronic and thermal Enthalpies= -2679.151792
Sum of electronic and thermal Free Energies= -2679.218855

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.493838	-2.056978	-0.037929
2	6	0	-2.502877	0.200061	0.697986
3	7	0	-1.755241	-2.569347	1.048938
4	6	0	-0.482786	-2.623759	0.913607
5	8	0	0.324251	-3.020979	1.932142
6	6	0	0.291645	-2.292916	-0.351021
7	7	0	-0.493150	-1.378343	-1.194387
8	6	0	-1.830653	-1.565909	-1.159095
9	8	0	-2.442570	-0.992288	-2.220115
10	8	0	-2.289010	0.985976	-0.251255
11	6	0	-3.828182	0.192895	1.449565
12	8	0	-4.955452	0.426183	0.616825
13	6	0	-5.417142	1.787701	0.788432
14	8	0	-4.515156	2.396887	1.709260
15	6	0	-3.891290	1.366904	2.451879
16	17	0	0.844260	1.202116	0.956858
17	6	0	-3.874511	-0.983581	-2.274219
18	6	0	0.742071	-3.596516	-1.088396

19	6	0	-0.330098	-3.368911	3.155551
20	6	0	-0.424840	-4.498702	-1.511764
21	6	0	1.642227	-3.277757	-2.286223
22	6	0	-5.320733	2.542100	-0.529102
23	6	0	-6.832985	1.736357	1.361328
24	50	0	-0.104026	0.833947	-1.503288
25	6	0	4.064385	4.917268	0.911782
26	6	0	3.855140	3.486973	1.428808
27	6	0	3.782974	4.779937	-0.592885
28	8	0	4.037753	2.610956	0.283706
29	6	0	4.355870	3.398771	-0.889124
30	3	0	3.075965	0.907164	0.169758
31	17	0	2.577486	0.334929	-2.043816
32	8	0	3.977963	-0.523490	1.139796
33	6	0	3.495366	-1.213816	2.326506
34	6	0	5.002511	-1.312087	0.489887
35	6	0	4.344412	-2.484127	2.447101
36	6	0	4.784419	-2.733816	0.996412
37	1	0	5.689140	-3.354155	0.915230
38	1	0	-3.548601	-2.326273	-0.060033
39	1	0	-1.659152	-0.203473	1.288905
40	1	0	1.211367	-1.767383	-0.053853
41	1	0	-4.127414	-0.448034	-3.198246
42	1	0	-4.259454	-2.015561	-2.335423
43	1	0	-4.308179	-0.466281	-1.406904
44	1	0	1.340565	-4.147113	-0.337808
45	1	0	0.467894	-3.672543	3.845796
46	1	0	-1.041038	-4.194872	2.998531
47	1	0	-0.885498	-2.508750	3.561391
48	1	0	-0.041186	-5.445603	-1.926248
49	1	0	-1.032301	-4.018943	-2.296287
50	1	0	-1.089251	-4.745804	-0.668918
51	1	0	2.014154	-4.208101	-2.746643
52	1	0	2.505932	-2.659381	-1.999727
53	1	0	1.085247	-2.716451	-3.052514
54	1	0	-3.940083	-0.775505	1.960324
55	1	0	-4.485365	1.080187	3.341186
56	1	0	-5.591455	3.598219	-0.378189
57	1	0	-6.005709	2.106130	-1.272290
58	1	0	-4.288551	2.476858	-0.897553
59	1	0	-7.226424	2.754809	1.500567
60	1	0	-6.835663	1.220788	2.333694
61	1	0	-7.500524	1.187383	0.679904
62	1	0	-2.904649	1.724062	2.780671
63	1	0	3.403160	5.638244	1.414057
64	1	0	5.105336	5.241032	1.075926
65	1	0	2.833941	3.323551	1.808820
66	1	0	4.578353	3.202597	2.210029
67	1	0	2.698289	4.790016	-0.788418
68	1	0	4.252222	5.571406	-1.195726
69	1	0	5.454499	3.435528	-1.012812
70	1	0	3.911143	2.889766	-1.754999
71	1	0	3.600117	-0.537390	3.189195
72	1	0	2.429199	-1.442611	2.178531
73	1	0	4.873473	-1.194211	-0.595781
74	1	0	5.996652	-0.925802	0.782482
75	1	0	3.771777	-3.319636	2.874909
76	1	0	5.224502	-2.308147	3.087702
77	1	0	3.977274	-3.219833	0.424719

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dtas-B^{ae}N (*A*), THF solution

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 Variational PCM results
 =======================
 <psi(f)|   H    |psi(f)>                    (a.u.) =   -2679.786797
 <psi(f)|H+V(f)/2|psi(f)>                   (a.u.) =   -2679.805691
 Total free energy in solution:
  with all non electrostatic terms          (a.u.) =   -2679.754574
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent              (kcal/mol) =     -11.86
 ---------------------------------------------------------------------
 Cavitation energy                       (kcal/mol) =      63.56
 Dispersion energy                       (kcal/mol) =     -32.83
 Repulsion energy                        (kcal/mol) =       1.35
 Total non electrostatic                 (kcal/mol) =      32.08
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Zero-point correction=	0.614244 (Hartree/Particle)
Thermal correction to Energy=	0.636533
Thermal correction to Enthalpy=	0.637151
Thermal correction to Gibbs Free Energy=	0.569782
Sum of electronic and zero-point Energies=	-2679.191447
Sum of electronic and thermal Energies=	-2679.169159
Sum of electronic and thermal Enthalpies=	-2679.168541
Sum of electronic and thermal Free Energies=	-2679.235909

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.629598	1.993460	0.073905
2	6	0	2.567381	-0.277859	0.761739
3	7	0	1.865762	2.507542	1.144644
4	6	0	0.596702	2.578028	0.974485
5	8	0	-0.236421	2.973162	1.967572
6	6	0	-0.148679	2.270218	-0.313590
7	7	0	0.654053	1.376428	-1.164779
8	6	0	1.990807	1.539970	-1.079946
9	8	0	2.627484	0.980896	-2.134979
10	8	0	2.345246	-1.044443	-0.208865
11	6	0	3.874596	-0.338787	1.540572
12	8	0	5.014389	-0.571126	0.721761
13	6	0	5.436555	-1.951996	0.846601
14	8	0	4.483114	-2.573983	1.708981
15	6	0	3.884812	-1.554721	2.493354
16	17	0	-0.879674	-1.211877	0.820199
17	6	0	4.062639	0.943795	-2.145581
18	6	0	-0.587284	3.589227	-1.030188
19	6	0	0.369287	3.295189	3.224398
20	6	0	0.587036	4.495433	-1.423125
21	6	0	-1.474896	3.294372	-2.242774
22	6	0	5.368965	-2.642906	-0.506798
23	6	0	6.831812	-1.967413	1.468693
24	50	0	0.283046	-0.840103	-1.542757
25	6	0	-5.193724	-4.288969	1.102700
26	6	0	-4.596782	-2.904207	1.371920
27	6	0	-4.528030	-4.684587	-0.224571
28	8	0	-4.243898	-2.359278	0.070216
29	6	0	-4.490350	-3.350306	-0.960512
30	3	0	-3.083556	-0.810822	-0.094935
31	17	0	-2.426639	-0.361945	-2.307182
32	8	0	-3.899485	0.661146	0.888118
33	6	0	-3.509335	1.222913	2.174331
34	6	0	-5.012807	1.408913	0.340278
35	6	0	-4.521695	2.335189	2.467489
36	6	0	-4.980612	2.751624	1.061754
37	1	0	-5.958554	3.255534	1.053040
38	1	0	3.689672	2.249420	0.086660
39	1	0	1.723829	0.137632	1.343862
40	1	0	-1.073610	1.739241	-0.043392
41	1	0	4.333787	0.427479	-3.075457
42	1	0	4.469401	1.968632	-2.166267
43	1	0	4.455649	0.394738	-1.278689
44	1	0	-1.194198	4.127475	-0.278327
45	1	0	-0.454924	3.588724	3.886993
46	1	0	1.086792	4.123092	3.112142
47	1	0	0.903876	2.424470	3.635668
48	1	0	0.211318	5.448812	-1.829933
49	1	0	1.208224	4.025921	-2.203484
50	1	0	1.237024	4.729981	-0.565307
51	1	0	-1.841640	4.233310	-2.689617
52	1	0	-2.342909	2.674029	-1.972491
53	1	0	-0.910773	2.745920	-3.013785
54	1	0	4.005970	0.603673	2.095809
55	1	0	4.479385	-1.326162	3.397971
56	1	0	5.614486	-3.710577	-0.397548
57	1	0	6.088178	-2.188393	-1.204876
58	1	0	4.352209	-2.537365	-0.907861
59	1	0	7.192770	-3.002296	1.571884
60	1	0	6.815291	-1.496666	2.463539
61	1	0	7.537203	-1.409359	0.834184
62	1	0	2.883831	-1.892975	2.799684
63	1	0	-4.987199	-4.993610	1.921809

64	1	0	-6.286925	-4.220251	0.975696
65	1	0	-3.675248	-2.962012	1.976325
66	1	0	-5.300917	-2.213193	1.861732
67	1	0	-3.503681	-5.054957	-0.049802
68	1	0	-5.086489	-5.453428	-0.779104
69	1	0	-5.459209	-3.128781	-1.444488
70	1	0	-3.689747	-3.262128	-1.708194
71	1	0	-3.521361	0.417957	2.925930
72	1	0	-2.482467	1.608830	2.078750
73	1	0	-4.869448	1.474556	-0.748389
74	1	0	-5.952596	0.863785	0.546532
75	1	0	-4.073965	3.160386	3.040632
76	1	0	-5.375047	1.941691	3.044391
77	1	0	-4.240419	3.421169	0.592862

dtas-C^{ae}N (*A*), THF solution

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 Variational PCM results
 =======================
 <psi(f)|   H    |psi(f)>                    (a.u.) =   -2679.775987
 <psi(f)|H+V(f)/2|psi(f)>                   (a.u.) =   -2679.801232
 Total free energy in solution:
  with all non electrostatic terms          (a.u.) =   -2679.753285
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent               (kcal/mol) =     -15.84
 ---------------------------------------------------------------------
 Cavitation energy                        (kcal/mol) =      62.69
 Dispersion energy                        (kcal/mol) =     -34.12
 Repulsion energy                         (kcal/mol) =       1.52
 Total non electrostatic                  (kcal/mol) =      30.09
 ---------------------------------------------------------------------
 Zero-point correction=                           0.613230 (Hartree/Particle)
 Thermal correction to Energy=                    0.635851
 Thermal correction to Enthalpy=                  0.636469
 Thermal correction to Gibbs Free Energy=         0.567943
 Sum of electronic and zero-point Energies=          -2679.188004
 Sum of electronic and thermal Energies=             -2679.165383
 Sum of electronic and thermal Enthalpies=           -2679.164765
 Sum of electronic and thermal Free Energies=        -2679.233291
---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -3.292114    2.006338    0.131813
    2          6             0       -3.224976    0.232024   -1.274107
    3          7             0       -2.887451    2.945262   -0.848696
    4          6             0       -1.628641    3.127968   -0.988738
    5          8             0       -1.130239    3.940425   -1.947613
    6          6             0       -0.525603    2.533867   -0.133662
    7          7             0       -1.025641    1.431089    0.704186
    8          6             0       -2.330026    1.427899    0.982530
    9          8             0       -2.629330    0.585666    2.006788
   10          8             0       -1.993689   -0.050256   -1.412387
   11          6             0       -4.226460   -0.803282   -0.788176
   12          8             0       -3.695222   -1.631202    0.245664
   13          6             0       -4.230633   -2.969465    0.099369
   14          8             0       -4.992797   -2.955379   -1.112636
   15          6             0       -4.558821   -1.837171   -1.878206
   16         17             0        1.362072   -0.301799   -1.473975
   17         50             0       -0.516508   -0.786241    0.318180
   18          6             0       -3.967868    0.539870    2.509876
   19          6             0        0.179682    3.640720    0.713496
   20          6             0       -2.077325    4.573047   -2.815126
   21          6             0       -0.762144    4.307550    1.723788
   22          6             0        1.432312    3.090092    1.402004
   23          6             0       -3.067640   -3.950944   -0.001196
   24          6             0       -5.178691   -3.278139    1.250518
   25          6             0        5.732392   -3.992515   -0.418932
   26          6             0        4.429392   -4.515759   -1.040760
   27          6             0        5.497570   -2.482850   -0.412361
   28          6             0        3.388775   -3.584356   -0.423163
   29          8             0        4.066929   -2.312684   -0.242490
   30          3             0        3.118513   -0.669403    0.196504
   31         17             0        1.783341   -0.798410    2.127502
   32          8             0        4.452574    0.746690    0.076103
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33	6	0	5.124164	1.372320	1.200464
34	6	0	4.837773	1.401518	-1.163131
35	6	0	5.648944	2.702087	0.666307
36	6	0	5.978450	2.349759	-0.791957
37	1	0	6.948427	1.828287	-0.850116
38	1	0	-4.335024	2.097401	0.442885
39	1	0	-3.673470	0.951319	-1.985470
40	1	0	0.232564	2.127909	-0.821329
41	1	0	-3.922751	-0.091851	3.406199
42	1	0	-4.310983	1.549640	2.787583
43	1	0	-4.657793	0.087066	1.785275
44	1	0	0.494373	4.404704	-0.020470
45	1	0	-1.484348	5.185652	-3.506322
46	1	0	-2.774573	5.203701	-2.241602
47	1	0	-2.662158	3.822681	-3.370156
48	1	0	-0.256741	5.151179	2.221925
49	1	0	-1.071194	3.596130	2.507163
50	1	0	-1.672505	4.700533	1.242065
51	1	0	1.959814	3.891523	1.945802
52	1	0	2.132288	2.652970	0.671913
53	1	0	1.174544	2.295867	2.119513
54	1	0	-5.156112	-0.301728	-0.457720
55	1	0	-3.449422	-4.979434	-0.091041
56	1	0	-2.431418	-3.887226	0.894499
57	1	0	-2.451999	-3.723815	-0.884167
58	1	0	-5.641745	-4.266343	1.105837
59	1	0	-5.975580	-2.520976	1.293770
60	1	0	-4.633269	-3.281963	2.206066
61	1	0	-3.659214	-2.072999	-2.476922
62	1	0	-5.378712	-1.531609	-2.543350
63	1	0	6.631935	-4.270928	-0.987913
64	1	0	5.844111	-4.368754	0.611776
65	1	0	4.229683	-5.573082	-0.812160
66	1	0	4.451046	-4.395724	-2.137008
67	1	0	5.795864	-2.020894	-1.370542
68	1	0	6.008849	-1.959413	0.409542
69	1	0	3.050720	-3.942997	0.564800
70	1	0	2.510125	-3.411175	-1.062037
71	1	0	4.393911	1.468753	2.016995
72	1	0	5.948498	0.714742	1.531817
73	1	0	5.128696	0.626935	-1.889549
74	1	0	3.958646	1.940291	-1.554675
75	1	0	6.517874	3.065831	1.234447
76	1	0	4.859983	3.470895	0.709304
77	1	0	6.019656	3.226695	-1.454899

dtsa-C^{ae}M (*A*), gas-phase

E(RB+HF-LYP) = -2679.78683781
Zero-point correction= 0.614673 (Hartree/Particle)
Thermal correction to Energy= 0.637278
Thermal correction to Enthalpy= 0.637896
Thermal correction to Gibbs Free Energy= 0.568480
Sum of electronic and zero-point Energies= -2679.172165
Sum of electronic and thermal Energies= -2679.149560
Sum of electronic and thermal Enthalpies= -2679.148942
Sum of electronic and thermal Free Energies= -2679.218358

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.007907	1.278263	0.824174
2	6	0	-2.927785	-0.896052	-0.115419
3	7	0	-2.907753	2.006386	-0.373025
4	6	0	-1.729270	2.323850	-0.762479
5	8	0	-1.512760	2.959945	-1.935060
6	6	0	-0.443997	2.093699	0.006695
7	7	0	-0.619822	1.012972	0.991439
8	6	0	-1.855482	0.882758	1.503093
9	8	0	-1.868889	0.091366	2.619575
10	8	0	-1.827575	-0.933554	-0.714609
11	6	0	-4.213103	-0.737143	-0.893112
12	8	0	-5.318490	-0.682147	0.011932
13	6	0	-6.446705	-1.339295	-0.592350
14	8	0	-5.968300	-1.930949	-1.805729
15	6	0	-4.549794	-1.972558	-1.740380

16	17	0	1.533430	-0.511479	-1.490276
17	50	0	0.229640	-1.074156	0.707351
18	6	0	-3.101505	-0.060592	3.323852
19	6	0	0.088631	3.418809	0.636053
20	6	0	-2.662856	3.227842	-2.739554
21	6	0	-0.839188	4.004029	1.707551
22	6	0	1.508535	3.226749	1.178230
23	6	0	-6.946612	-2.414288	0.369926
24	6	0	-7.515645	-0.316032	-0.957855
25	6	0	6.002101	-3.860919	0.180049
26	6	0	5.912589	-2.371769	-0.160698
27	6	0	4.950493	-4.470808	-0.758864
28	8	0	4.549417	-2.146107	-0.593812
29	6	0	3.852374	-3.411751	-0.723253
30	3	0	3.561621	-0.505041	-0.205643
31	17	0	2.650111	-0.476575	1.934794
32	8	0	4.759462	0.982584	-0.587656
33	6	0	4.861822	1.597489	-1.898377
34	6	0	5.311668	1.862690	0.424747
35	6	0	5.726116	2.844553	-1.703554
36	6	0	5.421319	3.228858	-0.247548
37	1	0	4.460561	3.764237	-0.181688
38	1	0	6.198573	3.858965	0.209005
39	1	0	-3.992724	1.272485	1.286519
40	1	0	-3.060783	-1.379526	0.874763
41	1	0	-4.157393	0.171265	-1.516200
42	1	0	0.310150	1.768889	-0.725791
43	1	0	-2.874052	-0.695243	4.189968
44	1	0	-3.472551	0.918457	3.670428
45	1	0	-3.877094	-0.540309	2.704459
46	1	0	0.131528	4.132296	-0.207258
47	1	0	-2.293616	3.787893	-3.608574
48	1	0	-3.405664	3.818827	-2.181706
49	1	0	-3.139609	2.289293	-3.064862
50	1	0	-0.472775	4.991667	2.033486
51	1	0	-0.876194	3.354848	2.597492
52	1	0	-1.867792	4.133800	1.335159
53	1	0	1.904215	4.173072	1.583881
54	1	0	2.190588	2.880038	0.384918
55	1	0	1.528995	2.470263	1.977900
56	1	0	-7.813149	-2.938891	-0.060188
57	1	0	-7.244950	-1.963382	1.328849
58	1	0	-6.149741	-3.147713	0.564240
59	1	0	-8.346867	-0.804619	-1.488855
60	1	0	-7.083482	0.453298	-1.614004
61	1	0	-7.908612	0.169130	-0.051708
62	1	0	-4.191584	-2.902694	-1.256981
63	1	0	-4.144995	-1.921241	-2.759891
64	1	0	7.014091	-4.263920	0.028288
65	1	0	5.717895	-4.030196	1.231306
66	1	0	6.588969	-2.099301	-0.990032
67	1	0	6.121077	-1.714747	0.697519
68	1	0	5.355135	-4.573937	-1.779559
69	1	0	4.591903	-5.457049	-0.429986
70	1	0	3.192244	-3.541269	0.152501
71	1	0	3.234591	-3.362957	-1.630634
72	1	0	5.298587	0.862728	-2.592173
73	1	0	3.843898	1.844661	-2.243239
74	1	0	4.639998	1.834330	1.294260
75	1	0	6.303791	1.477582	0.723721
76	1	0	5.480587	3.637003	-2.425404
77	1	0	6.794499	2.596893	-1.818947

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dtsa-C^{ae}M (*A*), THF solution

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 Variational PCM results
 =======================
 <psi(f)|   H    |psi(f)>                    (a.u.) =   -2679.783117
 <psi(f)|H+V(f)/2|psi(f)>                   (a.u.) =   -2679.805490
 Total free energy in solution:
  with all non electrostatic terms          (a.u.) =   -2679.754040
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent              (kcal/mol) =     -14.04
 ---------------------------------------------------------------------
 Cavitation energy                       (kcal/mol) =      64.91
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 Dispersion energy                        (kcal/mol) =     -34.05
 Repulsion energy                         (kcal/mol) =       1.43
 Total non electrostatic                  (kcal/mol) =      32.29
 ------------------------------------------------------------------
 Zero-point correction=                            0.613077 (Hartree/Particle)
 Thermal correction to Energy=                     0.635786
 Thermal correction to Enthalpy=                   0.636404
 Thermal correction to Gibbs Free Energy=          0.566978
 Sum of electronic and zero-point Energies=           -2679.192413
 Sum of electronic and thermal Energies=              -2679.169703
 Sum of electronic and thermal Enthalpies=            -2679.169085
 Sum of electronic and thermal Free Energies=         -2679.238512
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -3.047792    1.521595    0.596941
    2          6             0       -3.079262   -0.713741   -0.189940
    3          7             0       -2.849585    2.154121   -0.643129
    4          6             0       -1.636213    2.358850   -1.004370
    5          8             0       -1.328003    2.880519   -2.211554
    6          6             0       -0.401515    2.106053   -0.161950
    7          7             0       -0.689209    1.123051    0.896696
    8          6             0       -1.951613    1.110379    1.358263
    9          8             0       -2.061806    0.414121    2.528940
   10          8             0       -1.953077   -0.870307   -0.728877
   11          6             0       -4.315843   -0.525540   -1.055464
   12          8             0       -5.479136   -0.408920   -0.231897
   13          6             0       -6.310536   -1.579085   -0.408543
   14          8             0       -5.504359   -2.521161   -1.112484
   15          6             0       -4.607288   -1.766687   -1.921232
   16         17             0        1.465600   -0.729105   -1.351005
   17         50             0       -0.016079   -1.053749    0.789546
   18          6             0       -3.336190    0.382071    3.181952
   19          6             0        0.202169    3.438250    0.382814
   20          6             0       -2.419666    3.154818   -3.096337
   21          6             0       -0.728249    4.182907    1.348158
   22          6             0        1.573872    3.187746    1.018166
   23          6             0       -6.652910   -2.167088    0.951603
   24          6             0       -7.548937   -1.191067   -1.218124
   25          6             0        5.198759   -4.393910   -0.833256
   26          6             0        4.099015   -3.522403   -0.231503
   27          6             0        6.465523   -3.615243   -0.449391
   28          8             0        4.596558   -2.159338   -0.315578
   29          6             0        6.014230   -2.166378   -0.626408
   30          3             0        3.492839   -0.601410    0.026442
   31         17             0        2.438385   -0.570410    2.136321
   32          8             0        4.601160    0.955008   -0.336403
   33          6             0        4.860484    1.547828   -1.637174
   34          6             0        5.306613    1.694118    0.698316
   35          6             0        6.009620    2.530127   -1.416973
   36          6             0        5.767691    2.986671    0.029363
   37          1             0        4.967955    3.744665    0.064956
   38          1             0        6.663173    3.407329    0.510239
   39          1             0       -4.046915    1.621700    1.019256
   40          1             0       -3.284573   -1.101015    0.827846
   41          1             0       -4.185730    0.381165   -1.665600
   42          1             0        0.356720    1.672144   -0.830614
   43          1             0       -3.186602   -0.201446    4.099149
   44          1             0       -3.662445    1.403083    3.439617
   45          1             0       -4.105522   -0.097418    2.555953
   46          1             0        0.344539    4.071523   -0.513121
   47          1             0       -1.971868    3.612487   -3.987894
   48          1             0       -3.142318    3.841666   -2.629521
   49          1             0       -2.944716    2.224924   -3.367443
   50          1             0       -0.302099    5.166015    1.608068
   51          1             0       -0.859747    3.620517    2.287134
   52          1             0       -1.724707    4.354475    0.910474
   53          1             0        2.020747    4.133080    1.368439
   54          1             0        2.269546    2.723726    0.300646
   55          1             0        1.489959    2.503500    1.876944
   56          1             0       -7.277279   -3.065688    0.832841
   57          1             0       -7.206260   -1.432824    1.555671
   58          1             0       -5.728521   -2.444932    1.478379
   59          1             0       -8.199836   -2.066484   -1.366335
   60          1             0       -7.261729   -0.794444   -2.203646
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61	1	0	-8.118146	-0.411416	-0.689429
62	1	0	-3.712965	-2.372752	-2.120102
63	1	0	-5.070645	-1.477534	-2.882825
64	1	0	5.179730	-5.419865	-0.436927
65	1	0	5.094561	-4.443420	-1.930165
66	1	0	3.919945	-3.763739	0.830952
67	1	0	3.144082	-3.567846	-0.775598
68	1	0	6.730815	-3.809015	0.603419
69	1	0	7.336415	-3.858688	-1.075904
70	1	0	6.147074	-1.823645	-1.668124
71	1	0	6.521084	-1.460656	0.048739
72	1	0	5.097004	0.738387	-2.345006
73	1	0	3.942960	2.058758	-1.976462
74	1	0	4.613954	1.841986	1.539026
75	1	0	6.162939	1.086142	1.041903
76	1	0	5.995846	3.354876	-2.144739
77	1	0	6.980338	2.012888	-1.498795

dALg (*A*)

E(RB+HF-LYP) = -2679.79278238

Zero-point correction=	0.614224	(Hartree/Particle)
Thermal correction to Energy=	0.637700	
Thermal correction to Enthalpy=	0.638318	
Thermal correction to Gibbs Free Energy=	0.566614	
Sum of electronic and zero-point Energies=	-2679.178558	
Sum of electronic and thermal Energies=	-2679.155082	
Sum of electronic and thermal Enthalpies=	-2679.154464	
Sum of electronic and thermal Free Energies=	-2679.226168	

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.704269	-2.418323	-0.165159
2	6	0	-2.698186	0.974152	-0.480398
3	7	0	-2.512087	-1.870647	1.117684
4	6	0	-1.298829	-1.696468	1.495208
5	8	0	-0.984688	-1.085163	2.671073
6	6	0	-0.081742	-2.143458	0.702345
7	7	0	-0.399458	-2.015633	-0.725928
8	6	0	-1.677487	-2.391983	-1.064507
9	8	0	-1.778439	-2.606055	-2.418430
10	8	0	-2.476718	0.560407	-1.602374
11	6	0	-4.095926	1.026056	0.119549
12	8	0	-4.101937	1.842443	1.287911
13	6	0	-4.793132	3.078478	0.992840
14	8	0	-5.072646	3.046731	-0.405439
15	6	0	-5.134254	1.680380	-0.795508
16	17	0	0.767134	1.427136	-0.366636
17	50	0	0.370545	-0.529951	-2.149605
18	6	0	-3.086298	-2.597628	-2.982402
19	6	0	0.423083	-3.552688	1.159015
20	6	0	-2.087955	-0.615070	3.452583
21	6	0	-0.617050	-4.679342	1.086040
22	6	0	1.698382	-3.953235	0.410190
23	6	0	-3.871366	4.258070	1.264788
24	6	0	-6.081792	3.119196	1.813695
25	17	0	2.923718	-1.086463	-1.634984
26	3	0	2.996269	0.678623	-0.056785
27	8	0	3.311720	0.140923	1.788477
28	8	0	4.244445	2.091619	-0.513796
29	6	0	2.429590	0.449402	2.908057
30	6	0	4.238333	-0.907020	2.159861
31	6	0	5.214806	2.734547	0.344561
32	6	0	4.081334	2.846618	-1.743005
33	6	0	2.951126	-0.377934	4.085995
34	6	0	3.620397	-1.570933	3.386480
35	6	0	5.844880	3.844763	-0.498787
36	6	0	4.701667	4.211476	-1.456922
37	1	0	5.044826	4.716194	-2.371650
38	1	0	-6.727797	2.265925	1.558081
39	1	0	-3.708521	-2.760742	-0.404754
40	1	0	-3.668630	-3.476088	-2.654006
41	1	0	-3.621815	-1.673359	-2.710025
42	1	0	-2.948201	-2.647727	-4.071085
43	1	0	0.678356	-3.409287	2.227922

44	1	0	-1.647778	-0.206194	4.372184
45	1	0	-2.778539	-1.439453	3.690093
46	1	0	-2.649892	0.167430	2.917861
47	1	0	-0.208737	-5.595096	1.546762
48	1	0	-0.874394	-4.918986	0.042579
49	1	0	-1.546921	-4.420751	1.614030
50	1	0	2.097114	-4.903294	0.803320
51	1	0	2.483381	-3.186180	0.491012
52	1	0	1.493081	-4.087235	-0.663192
53	1	0	0.739510	-1.444477	0.920649
54	1	0	-1.880436	1.317759	0.191657
55	1	0	-4.350190	-0.010170	0.400271
56	1	0	-6.141384	1.252984	-0.635920
57	1	0	-4.376030	5.202247	1.009707
58	1	0	-2.961936	4.167169	0.653846
59	1	0	-3.587746	4.283214	2.327355
60	1	0	-6.633303	4.050964	1.615837
61	1	0	-5.850674	3.062567	2.888127
62	1	0	-4.866919	1.602211	-1.857892
63	1	0	2.465900	1.535182	3.085648
64	1	0	1.403338	0.168590	2.626039
65	1	0	4.353931	-1.575657	1.294326
66	1	0	5.218628	-0.452807	2.397410
67	1	0	4.688393	3.138664	1.227081
68	1	0	5.939323	1.977708	0.682740
69	1	0	4.609107	2.315293	-2.553961
70	1	0	3.006949	2.879174	-1.972077
71	1	0	2.140859	-0.675289	4.767017
72	1	0	3.695915	0.191786	4.666510
73	1	0	2.865581	-2.311860	3.078122
74	1	0	4.369392	-2.079568	4.011013
75	1	0	6.191462	4.689059	0.114916
76	1	0	6.707799	3.455907	-1.064105
77	1	0	3.971487	4.866818	-0.954068

dcas-B^{ae}F (*A*)

E(RB+HF-LYP) = -2679.76684954
Zero-point correction= 0.614751 (Hartree/Particle)
Thermal correction to Energy= 0.637190
Thermal correction to Enthalpy= 0.637808
Thermal correction to Gibbs Free Energy= 0.568324
Sum of electronic and zero-point Energies= -2679.152099
Sum of electronic and thermal Energies= -2679.129659
Sum of electronic and thermal Enthalpies= -2679.129041
Sum of electronic and thermal Free Energies= -2679.198525

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.422896	1.364888	1.564735
2	6	0	2.658610	-0.840996	0.649032
3	7	0	3.330417	1.937038	0.658130
4	6	0	2.846779	2.428892	-0.423576
5	8	0	3.650316	2.873808	-1.415591
6	6	0	1.348801	2.624262	-0.648797
7	7	0	0.603984	1.500693	-0.014760
8	6	0	1.073404	1.235710	1.217954
9	8	0	0.157226	0.606032	1.990984
10	8	0	1.544959	-1.411927	0.649028
11	6	0	3.800476	-1.447311	1.466908
12	8	0	4.229537	-2.614315	0.742779
13	6	0	5.528303	-2.368735	0.166113
14	8	0	5.798380	-0.988188	0.386315
15	6	0	5.079533	-0.607135	1.557733
16	17	0	-1.788959	-1.727895	0.860282
17	50	0	-0.184767	-0.581404	-0.891806
18	6	0	0.544458	0.040123	3.242205
19	6	0	0.952241	2.983188	-2.095739
20	6	0	5.058623	2.691416	-1.224203
21	6	0	1.142740	1.855955	-3.119457
22	6	0	-0.462212	3.574738	-2.158497
23	6	0	5.477151	-2.617058	-1.334381
24	6	0	6.552041	-3.255260	0.879152
25	17	0	-2.585586	0.517563	-1.796310
26	3	0	-3.607919	-0.378905	0.110094

27	8	0	-4.099323	1.011064	1.365383
28	8	0	-5.174851	-1.487259	-0.316517
29	6	0	-5.378868	1.275974	1.978776
30	6	0	-3.177520	2.108204	1.623955
31	6	0	-5.330268	-2.811862	0.265301
32	6	0	-5.708781	-1.478472	-1.664158
33	6	0	-5.341708	2.749471	2.384146
34	6	0	-3.852826	2.950061	2.704619
35	6	0	-6.026928	-3.666939	-0.801065
36	6	0	-5.672340	-2.936805	-2.105760
37	1	0	-6.373943	-3.147971	-2.926244
38	1	0	6.275368	-4.314966	0.772979
39	1	0	2.764276	1.293159	2.597899
40	1	0	2.969236	-0.204966	-0.202600
41	1	0	3.414453	-1.772281	2.445444
42	1	0	1.096421	3.530018	-0.054492
43	1	0	0.864801	0.826947	3.946307
44	1	0	-0.353324	-0.461296	3.623601
45	1	0	1.342565	-0.703840	3.113155
46	1	0	1.660751	3.782720	-2.369978
47	1	0	5.531323	3.073509	-2.138176
48	1	0	5.301853	1.627499	-1.074242
49	1	0	5.408321	3.254957	-0.345104
50	1	0	1.071197	2.260216	-4.142624
51	1	0	0.358890	1.084948	-3.039337
52	1	0	2.127898	1.374745	-3.020994
53	1	0	-0.692784	3.910275	-3.183000
54	1	0	-0.553126	4.449824	-1.492894
55	1	0	-1.224614	2.837433	-1.868292
56	1	0	5.645128	-0.857790	2.474930
57	1	0	5.211895	-3.665167	-1.536891
58	1	0	6.455859	-2.404146	-1.790570
59	1	0	4.721261	-1.964773	-1.793916
60	1	0	6.587292	-3.018723	1.953093
61	1	0	7.555162	-3.103283	0.451945
62	1	0	4.908546	0.473782	1.500885
63	1	0	-6.168856	1.032694	1.252305
64	1	0	-5.494762	0.617493	2.859062
65	1	0	-2.210781	1.677379	1.918546
66	1	0	-3.042235	2.669001	0.684307
67	1	0	-4.323284	-3.182869	0.513005
68	1	0	-5.915792	-2.720979	1.194292
69	1	0	-6.743878	-1.089110	-1.639197
70	1	0	-5.077796	-0.806300	-2.261955
71	1	0	-6.008451	2.968200	3.231254
72	1	0	-5.640267	3.388152	1.536437
73	1	0	-3.620537	2.553995	3.707358
74	1	0	-3.537386	4.003082	2.670823
75	1	0	-5.684486	-4.711746	-0.779906
76	1	0	-7.118955	-3.664877	-0.648747
77	1	0	-4.656263	-3.204070	-2.438586

dcsa-C^{ae}M (*A*)

E(RB+HF-LYP) = -2679.77628380
Zero-point correction= 0.615437 (Hartree/Particle)
Thermal correction to Energy= 0.637597
Thermal correction to Enthalpy= 0.638215
Thermal correction to Gibbs Free Energy= 0.571021
Sum of electronic and zero-point Energies= -2679.160847
Sum of electronic and thermal Energies= -2679.138687
Sum of electronic and thermal Enthalpies= -2679.138069
Sum of electronic and thermal Free Energies= -2679.205263

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.582004	0.576599	1.457011
2	6	0	2.399387	-0.871093	-0.385090
3	7	0	3.402618	1.501352	0.795357
4	6	0	2.829152	2.557146	0.344475
5	8	0	3.493555	3.473270	-0.391332
6	6	0	1.390820	2.893158	0.701448
7	7	0	0.583377	1.643255	0.644019
8	6	0	1.186987	0.688531	1.391207
9	8	0	0.333364	-0.234279	1.910983

10	8	0	2.021417	-0.097972	-1.300649
11	6	0	3.851090	-1.315036	-0.327217
12	8	0	4.050206	-2.181146	0.793361
13	6	0	4.443383	-3.486872	0.324266
14	8	0	4.110277	-3.515710	-1.058050
15	6	0	4.242025	-2.187072	-1.542134
16	17	0	-1.059110	-1.540099	-0.738519
17	50	0	-0.191238	0.848086	-1.424809
18	6	0	0.873458	-1.259010	2.744653
19	6	0	0.782012	4.150565	0.045911
20	6	0	4.854044	3.166642	-0.711464
21	6	0	0.623709	4.130604	-1.482072
22	6	0	-0.539970	4.531683	0.727782
23	6	0	3.615125	-4.546755	1.033965
24	6	0	5.948723	-3.664417	0.539784
25	17	0	-2.817888	1.635413	-0.794460
26	3	0	-3.111645	-0.530441	0.030998
27	8	0	-3.449430	-0.454965	1.940379
28	8	0	-4.621877	-1.485803	-0.807364
29	6	0	-4.397109	-1.224743	2.707651
30	6	0	-2.944285	0.661141	2.730508
31	6	0	-4.495904	-2.843772	-1.312560
32	6	0	-5.548856	-0.739889	-1.635227
33	6	0	-4.754900	-0.350902	3.909255
34	6	0	-3.436423	0.399144	4.153358
35	6	0	-5.417201	-2.932581	-2.536670
36	6	0	-5.541122	-1.465058	-2.975837
37	1	0	-6.444465	-1.264656	-3.570709
38	1	0	6.514119	-2.889561	0.000382
39	1	0	3.089650	-0.090580	2.151090
40	1	0	1.638580	-1.856372	2.224340
41	1	0	1.318057	-0.823801	3.656745
42	1	0	0.025724	-1.901294	3.014500
43	1	0	1.522193	4.938069	0.272518
44	1	0	5.224262	4.025993	-1.285313
45	1	0	4.911569	2.246259	-1.313907
46	1	0	5.449145	3.023520	0.203378
47	1	0	0.467068	5.158072	-1.851016
48	1	0	-0.262983	3.557669	-1.800337
49	1	0	1.514822	3.730288	-1.987159
50	1	0	-0.917277	5.487874	0.329813
51	1	0	-0.408840	4.649450	1.816497
52	1	0	-1.310436	3.764456	0.557171
53	1	0	1.441297	3.155893	1.780504
54	1	0	1.675799	-1.533931	0.121633
55	1	0	4.485159	-0.419047	-0.245446
56	1	0	5.278246	-1.971249	-1.863282
57	1	0	3.892837	-5.549419	0.675726
58	1	0	2.548738	-4.380013	0.825890
59	1	0	3.785436	-4.500212	2.119864
60	1	0	6.274805	-4.651626	0.178060
61	1	0	6.192076	-3.577501	1.609471
62	1	0	3.568392	-2.054131	-2.398895
63	1	0	-5.250742	-1.464705	2.055935
64	1	0	-3.918585	-2.169908	3.025017
65	1	0	-1.852083	0.680585	2.620198
66	1	0	-3.360960	1.589825	2.308129
67	1	0	-3.436840	-3.003299	-1.568395
68	1	0	-4.778581	-3.545030	-0.510711
69	1	0	-6.551160	-0.765157	-1.167612
70	1	0	-5.189218	0.297549	-1.676855
71	1	0	-5.092904	-0.941884	4.773358
72	1	0	-5.555665	0.358437	3.641949
73	1	0	-2.726415	-0.244819	4.699200
74	1	0	-3.564059	1.328320	4.727777
75	1	0	-5.002886	-3.587103	-3.317278
76	1	0	-6.405788	-3.329261	-2.251951
77	1	0	-4.661266	-1.158488	-3.564458

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dtaa-C^{ae}M (*A*), gas-phase

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E(RB+HF-LYP) =  -2679.78634182
Zero-point correction=                           0.614749 (Hartree/Particle)
Thermal correction to Energy=                    0.637321
Thermal correction to Enthalpy=                  0.637939
Thermal correction to Gibbs Free Energy=         0.568895
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Sum of electronic and zero-point Energies= -2679.171593
Sum of electronic and thermal Energies= -2679.149021
Sum of electronic and thermal Enthalpies= -2679.148403
Sum of electronic and thermal Free Energies= -2679.217447

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.093540	1.624524	0.524821
2	6	0	-3.112303	-0.211493	-1.020717
3	7	0	-2.865457	2.564198	-0.499237
4	6	0	-1.645135	2.821327	-0.785216
5	8	0	-1.311586	3.645131	-1.805910
6	6	0	-0.422654	2.313961	-0.044007
7	7	0	-0.751007	1.110312	0.737809
8	6	0	-2.023883	1.005918	1.161981
9	8	0	-2.161422	0.032180	2.116071
10	8	0	-1.913484	-0.397508	-1.315226
11	6	0	-3.912715	-1.304216	-0.337634
12	8	0	-5.175478	-0.825293	0.126007
13	6	0	-6.213677	-1.761081	-0.243511
14	8	0	-5.544316	-2.880033	-0.819945
15	6	0	-4.310790	-2.407422	-1.338231
16	17	0	1.585598	-0.236568	-1.658422
17	50	0	0.004820	-0.969472	0.290110
18	6	0	-3.384940	-0.024234	2.856335
19	6	0	0.211826	3.450568	0.819540
20	6	0	-2.394845	4.177925	-2.569919
21	6	0	-0.698100	3.926001	1.958211
22	6	0	1.587324	3.033227	1.347811
23	6	0	-7.139481	-1.086201	-1.255201
24	6	0	-6.941668	-2.239881	1.004273
25	17	0	2.301785	-0.749033	1.828273
26	3	0	3.446480	-0.661856	-0.212522
27	8	0	4.825639	0.727054	-0.339295
28	8	0	4.367978	-2.360362	-0.515019
29	6	0	4.937014	1.661349	-1.445706
30	6	0	5.405612	1.302124	0.862658
31	6	0	3.885908	-3.611307	0.049655
32	6	0	5.712703	-2.530678	-1.002104
33	6	0	5.880988	2.761270	-0.959929
34	6	0	5.601493	2.784191	0.550450
35	6	0	5.053756	-4.602946	-0.057534
36	6	0	6.279239	-3.682644	-0.178458
37	1	0	7.141092	-4.167246	-0.660639
38	1	0	-6.222801	-2.698971	1.698052
39	1	0	-4.103014	1.601693	0.930402
40	1	0	-3.581200	0.946220	3.342261
41	1	0	-4.239503	-0.297983	2.219346
42	1	0	-3.229949	-0.792904	3.625075
43	1	0	0.350108	4.291935	0.116234
44	1	0	-1.934018	4.819055	-3.332774
45	1	0	-3.077454	4.761903	-1.932613
46	1	0	-2.974289	3.369928	-3.044016
47	1	0	-0.257690	4.803331	2.460413
48	1	0	-0.825730	3.138047	2.718165
49	1	0	-1.696687	4.213629	1.592700
50	1	0	2.049054	3.852089	1.925198
51	1	0	2.266014	2.771996	0.519449
52	1	0	1.512957	2.148997	1.999566
53	1	0	0.324620	2.037689	-0.803339
54	1	0	-3.716338	0.534870	-1.572296
55	1	0	-3.330521	-1.735188	0.495930
56	1	0	-3.597045	-3.240967	-1.368566
57	1	0	-7.948691	-1.771589	-1.550031
58	1	0	-6.579566	-0.793634	-2.155930
59	1	0	-7.581776	-0.177763	-0.819274
60	1	0	-7.700871	-2.990220	0.736357
61	1	0	-7.439723	-1.396679	1.505554
62	1	0	-4.426014	-1.997341	-2.360150
63	1	0	5.312178	1.111859	-2.322574
64	1	0	3.930057	2.046405	-1.676845
65	1	0	4.716407	1.103003	1.695720
66	1	0	6.368612	0.797225	1.060522
67	1	0	3.587750	-3.403282	1.088334
68	1	0	2.997185	-3.932735	-0.515716

69	1	0	5.687717	-2.780640	-2.079758
70	1	0	6.233891	-1.571734	-0.870943
71	1	0	5.686225	3.723809	-1.454878
72	1	0	6.930872	2.483951	-1.152831
73	1	0	4.676854	3.343706	0.762725
74	1	0	6.417101	3.230257	1.138184
75	1	0	5.102732	-5.278549	0.808609
76	1	0	4.955386	-5.222359	-0.963881
77	1	0	6.593936	-3.320007	0.813990

dtaa-C^{ae}M (*A*), THF solution

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 Variational PCM results
 ======================
 <psi(f)|   H    |psi(f)>                    (a.u.) =   -2679.781758
 <psi(f)|H+V(f)/2|psi(f)>                   (a.u.) =   -2679.803832
 Total free energy in solution:
  with all non electrostatic terms          (a.u.) =   -2679.754845
 ---------------------------------------------------------------------
 (Polarized solute)-Solvent              (kcal/mol) =     -13.85
 ---------------------------------------------------------------------
 Cavitation energy                       (kcal/mol) =      63.60
 Dispersion energy                       (kcal/mol) =     -34.33
 Repulsion energy                        (kcal/mol) =       1.47
 Total non electrostatic                 (kcal/mol) =      30.74
 ---------------------------------------------------------------------
 Zero-point correction=                           0.612997 (Hartree/Particle)
 Thermal correction to Energy=                    0.635743
 Thermal correction to Enthalpy=                  0.636361
 Thermal correction to Gibbs Free Energy=         0.566771
 Sum of electronic and zero-point Energies=          -2679.190785
 Sum of electronic and thermal Energies=             -2679.168038
 Sum of electronic and thermal Enthalpies=           -2679.167420
 Sum of electronic and thermal Free Energies=        -2679.237011
  ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -3.084752    1.708794    0.368283
    2          6             0       -3.142359   -0.241836   -1.028757
    3          7             0       -2.804701    2.565076   -0.716503
    4          6             0       -1.570383    2.752840   -1.000681
    5          8             0       -1.187865    3.481252   -2.075457
    6          6             0       -0.378868    2.253416   -0.204751
    7          7             0       -0.765779    1.130053    0.665048
    8          6             0       -2.048271    1.104078    1.072578
    9          8             0       -2.235066    0.214657    2.095222
   10          8             0       -1.942542   -0.484476   -1.295558
   11          6             0       -3.980704   -1.250816   -0.270124
   12          8             0       -5.233485   -0.696174    0.129116
   13          6             0       -6.292033   -1.646687   -0.141553
   14          8             0       -5.640553   -2.826879   -0.614798
   15          6             0       -4.400360   -2.422987   -1.178744
   16         17             0        1.590968   -0.469084   -1.540830
   17         50             0       -0.104998   -1.014739    0.389449
   18          6             0       -3.476754    0.250792    2.814903
   19          6             0        0.301094    3.424205    0.574016
   20          6             0       -2.234431    4.004042   -2.900216
   21          6             0       -0.594811    4.024872    1.663820
   22          6             0        1.652476    2.986143    1.146449
   23          6             0       -7.213940   -1.057464   -1.207301
   24          6             0       -7.016365   -1.991761    1.151038
   25         17             0        2.171536   -0.792908    2.023072
   26          3             0        3.459739   -0.646843    0.036659
   27          8             0        4.712409    0.835304   -0.046210
   28          8             0        4.492818   -2.237137   -0.364760
   29          6             0        5.160190    1.475870   -1.271712
   30          6             0        5.298462    1.498108    1.106588
   31          6             0        3.897322   -3.549324   -0.553260
   32          6             0        5.938892   -2.351908   -0.305550
   33          6             0        6.285031    2.421490   -0.852766
   34          6             0        5.866165    2.810664    0.572847
   35          6             0        5.049957   -4.460654   -0.966663
   36          6             0        6.228372   -3.848268   -0.195769
   37          1             0        7.210822   -4.112849   -0.614065
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38	1	0	-6.300663	-2.394897	1.882251
39	1	0	-4.100371	1.755450	0.758364
40	1	0	-3.646815	1.259802	3.225571
41	1	0	-4.325769	-0.040984	2.179619
42	1	0	-3.360603	-0.466038	3.638297
43	1	0	0.484331	4.203398	-0.189051
44	1	0	-1.731928	4.551926	-3.707894
45	1	0	-2.888235	4.678613	-2.325216
46	1	0	-2.851663	3.189975	-3.311717
47	1	0	-0.120300	4.918692	2.101582
48	1	0	-0.761864	3.303633	2.480501
49	1	0	-1.578271	4.325896	1.268519
50	1	0	2.147645	3.825274	1.663307
51	1	0	2.326595	2.627996	0.351688
52	1	0	1.528820	2.160986	1.865180
53	1	0	0.362916	1.885440	-0.929815
54	1	0	-3.716287	0.469652	-1.652407
55	1	0	-3.423146	-1.630823	0.604701
56	1	0	-3.702082	-3.270189	-1.141481
57	1	0	-8.035661	-1.755658	-1.428724
58	1	0	-6.656599	-0.860856	-2.135439
59	1	0	-7.641850	-0.106422	-0.855670
60	1	0	-7.792582	-2.748875	0.961225
61	1	0	-7.496149	-1.095388	1.571456
62	1	0	-4.516301	-2.094532	-2.229756
63	1	0	5.480004	0.691287	-1.974848
64	1	0	4.305985	2.019266	-1.710710
65	1	0	4.509811	1.620676	1.862485
66	1	0	6.092779	0.849730	1.518605
67	1	0	3.446017	-3.868829	0.402635
68	1	0	3.104896	-3.454898	-1.310349
69	1	0	6.362063	-1.921297	-1.230389
70	1	0	6.298868	-1.769676	0.556017
71	1	0	6.376804	3.282147	-1.531637
72	1	0	7.251083	1.889626	-0.837308
73	1	0	5.082876	3.585993	0.546540
74	1	0	6.699973	3.182876	1.186306
75	1	0	4.860314	-5.513517	-0.710730
76	1	0	5.223342	-4.393221	-2.053866
77	1	0	6.203377	-4.167950	0.859385

dtss-C^{ae}F (*C*)

E(RB+HF-LYP) = -2679.78310575
Zero-point correction= 0.614514 (Hartree/Particle)
Thermal correction to Energy= 0.637089
Thermal correction to Enthalpy= 0.637707
Thermal correction to Gibbs Free Energy= 0.568668
Sum of electronic and zero-point Energies= -2679.168592
Sum of electronic and thermal Energies= -2679.146017
Sum of electronic and thermal Enthalpies= -2679.145399
Sum of electronic and thermal Free Energies= -2679.214437

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.491652	-1.243265	1.131444
2	6	0	2.392363	0.987893	0.076469
3	7	0	3.346255	-1.788944	0.155625
4	6	0	2.789542	-2.368166	-0.840936
5	8	0	3.504642	-2.875396	-1.870865
6	6	0	1.300703	-2.608406	-1.005837
7	7	0	0.521155	-1.663176	-0.185003
8	6	0	1.107671	-1.281232	0.965169
9	8	0	0.223823	-0.780627	1.872993
10	8	0	1.844324	0.710279	-1.008984
11	6	0	3.889428	1.249054	0.112077
12	8	0	4.046758	2.649779	-0.171666
13	6	0	5.048182	3.205180	0.702525
14	8	0	5.582746	2.107067	1.439443
15	6	0	4.589928	1.091311	1.461736
16	17	0	-1.215551	1.709858	0.262254
17	50	0	-0.411437	-0.048890	-1.503581
18	6	0	0.722753	-0.274455	3.104200
19	6	0	0.921756	-4.101791	-0.757692
20	6	0	4.924276	-2.725750	-1.799162

21	6	0	1.174161	-4.553049	0.686006
22	6	0	-0.526721	-4.370825	-1.179832
23	6	0	4.383164	4.222108	1.630626
24	6	0	6.169756	3.806064	-0.134194
25	17	0	-2.972394	-1.092640	-1.223235
26	3	0	-3.387335	0.657345	0.263727
27	8	0	-4.690776	1.943226	-0.422204
28	8	0	-4.062381	-0.094804	1.933356
29	6	0	-5.152855	1.902450	-1.795106
30	6	0	-4.692740	3.315973	0.056516
31	6	0	-5.276833	-0.873797	1.824677
32	6	0	-3.135446	-0.757620	2.841140
33	6	0	-4.889588	3.303617	-2.334080
34	6	0	-5.207912	4.172888	-1.107402
35	6	0	-4.873600	-2.290528	2.217892
36	6	0	-3.848882	-2.023942	3.331599
37	1	0	-3.148211	-2.858132	3.481500
38	1	0	5.784578	4.628909	-0.754428
39	1	0	2.944193	-1.086246	2.109447
40	1	0	1.803765	1.416520	0.910869
41	1	0	4.366974	0.646288	-0.676212
42	1	0	1.067907	-2.416612	-2.070429
43	1	0	1.423585	0.562194	2.950538
44	1	0	-0.152838	0.092004	3.654761
45	1	0	1.224082	-1.064798	3.689416
46	1	0	1.591978	-4.679211	-1.420202
47	1	0	5.321589	-3.230423	-2.689280
48	1	0	5.322490	-3.186063	-0.881489
49	1	0	5.207796	-1.661256	-1.804268
50	1	0	0.998166	-5.636996	0.783527
51	1	0	0.493422	-4.041452	1.385801
52	1	0	2.208868	-4.350666	1.005625
53	1	0	-0.783971	-5.433053	-1.035542
54	1	0	-0.689151	-4.128181	-2.243124
55	1	0	-1.230183	-3.761181	-0.591555
56	1	0	5.085593	0.119183	1.574159
57	1	0	3.903275	5.017733	1.041030
58	1	0	5.128388	4.674624	2.302732
59	1	0	3.607473	3.735252	2.240593
60	1	0	6.593602	3.032235	-0.789958
61	1	0	6.967461	4.194672	0.517250
62	1	0	3.882211	1.238557	2.301695
63	1	0	-4.602298	1.098240	-2.302084
64	1	0	-6.232586	1.662738	-1.804568
65	1	0	-5.330324	3.375583	0.952833
66	1	0	-3.657753	3.571777	0.335507
67	1	0	-6.036782	-0.457184	2.511996
68	1	0	-5.640473	-0.785061	0.790875
69	1	0	-2.216774	-0.982408	2.278737
70	1	0	-2.895680	-0.057510	3.657566
71	1	0	-5.510819	3.543967	-3.209434
72	1	0	-3.830054	3.407452	-2.619238
73	1	0	-6.296119	4.328235	-1.023012
74	1	0	-4.726438	5.161090	-1.136749
75	1	0	-5.728914	-2.896735	2.551325
76	1	0	-4.395091	-2.791443	1.361773
77	1	0	-4.363545	-1.836515	4.288617

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dtss-C^{ae}F (A), THF solution

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---------------------------------------------------------------------
Variational PCM results
=======================
<psi(f)|   H    |psi(f)>                    (a.u.) =   -2679.777590
<psi(f)|H+V(f)/2|psi(f)>                    (a.u.) =   -2679.801869
Total free energy in solution:
 with all non electrostatic terms           (a.u.) =   -2679.751572
---------------------------------------------------------------------
(Polarized solute)-Solvent              (kcal/mol) =     -15.24
---------------------------------------------------------------------
Cavitation energy                       (kcal/mol) =      64.25
Dispersion energy                       (kcal/mol) =     -34.11
Repulsion energy                        (kcal/mol) =       1.42
Total non electrostatic                 (kcal/mol) =      31.56
---------------------------------------------------------------------
Zero-point correction=                          0.612894 (Hartree/Particle)
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Thermal correction to Energy=	0.635666
Thermal correction to Enthalpy=	0.636284
Thermal correction to Gibbs Free Energy=	0.567321
Sum of electronic and zero-point Energies=	-2679.188977
Sum of electronic and thermal Energies=	-2679.166205
Sum of electronic and thermal Enthalpies=	-2679.165587
Sum of electronic and thermal Free Energies=	-2679.234550

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.025549	1.560610	0.836083
2	6	0	-3.108823	-0.695094	0.147270
3	7	0	-2.917307	2.157468	-0.436775
4	6	0	-1.734622	2.336376	-0.895378
5	8	0	-1.516022	2.822536	-2.137064
6	6	0	-0.437174	2.090692	-0.148274
7	7	0	-0.651461	1.184609	0.992379
8	6	0	-1.868209	1.201270	1.542337
9	8	0	-1.891249	0.557256	2.747837
10	8	0	-1.958370	-0.922763	-0.314062
11	6	0	-4.271716	-0.570602	-0.823418
12	8	0	-4.674283	-1.917683	-1.143313
13	6	0	-6.113671	-2.011136	-1.102871
14	8	0	-6.585925	-0.674322	-0.937369
15	6	0	-5.556041	0.054648	-0.278975
16	17	0	1.364469	-0.860787	-1.195497
17	50	0	0.038502	-1.007488	1.061253
18	6	0	-3.088719	0.591183	3.529776
19	6	0	0.235925	3.437105	0.265315
20	6	0	-2.672886	3.109489	-2.930781
21	6	0	-0.595445	4.248545	1.265921
22	6	0	1.655622	3.196775	0.787263
23	6	0	-6.524322	-2.893185	0.076829
24	6	0	-6.619745	-2.533556	-2.439804
25	6	0	4.119083	-3.526081	-0.116411
26	6	0	5.220675	-4.406572	-0.700620
27	8	0	4.592260	-2.161216	-0.273902
28	6	0	6.481979	-3.594127	-0.372852
29	6	0	6.006469	-2.159964	-0.601135
30	3	0	3.485055	-0.594862	0.024906
31	17	0	2.584847	-0.379641	2.199568
32	8	0	4.513869	0.910397	-0.653888
33	6	0	5.292187	1.827377	0.160928
34	6	0	4.617885	1.277313	-2.056627
35	6	0	5.598920	3.013777	-0.749242
36	6	0	5.715520	2.338630	-2.123924
37	1	0	6.704837	1.863869	-2.234303
38	1	0	-6.233139	-3.546978	-2.624233
39	1	0	-3.969271	1.738013	1.352636
40	1	0	-3.387932	-1.042636	1.162490
41	1	0	-3.915846	-0.064155	-1.734504
42	1	0	0.252187	1.597342	-0.850088
43	1	0	-3.917201	0.054439	3.039903
44	1	0	-2.841513	0.091493	4.474927
45	1	0	-3.393969	1.631361	3.728547
46	1	0	0.305721	4.017710	-0.673293
47	1	0	-2.291116	3.513890	-3.877042
48	1	0	-3.321186	3.844897	-2.429488
49	1	0	-3.258475	2.194997	-3.114015
50	1	0	-0.131659	5.233755	1.438103
51	1	0	-0.656344	3.736632	2.240317
52	1	0	-1.622513	4.421139	0.905519
53	1	0	2.149954	4.153394	1.025304
54	1	0	2.270761	2.667898	0.041880
55	1	0	1.644572	2.576271	1.696939
56	1	0	-5.658347	1.116345	-0.536867
57	1	0	-6.079236	-3.894713	-0.024530
58	1	0	-7.619853	-2.994416	0.117271
59	1	0	-6.176333	-2.458837	1.026288
60	1	0	-6.281168	-1.867880	-3.246827
61	1	0	-7.720035	-2.570013	-2.444576
62	1	0	-5.625569	-0.059328	0.820522
63	1	0	3.965998	-3.722703	0.959395
64	1	0	3.153904	-3.610717	-0.637378
65	1	0	5.224213	-5.414794	-0.260676

66	1	0	5.097737	-4.504619	-1.792289
67	1	0	6.769059	-3.740351	0.681866
68	1	0	7.345121	-3.850939	-1.004745
69	1	0	6.121855	-1.856112	-1.656780
70	1	0	6.511216	-1.421289	0.039675
71	1	0	4.693972	2.080018	1.048056
72	1	0	6.216123	1.314933	0.485023
73	1	0	4.844592	0.369594	-2.637132
74	1	0	3.640449	1.670772	-2.383388
75	1	0	6.512550	3.546051	-0.445838
76	1	0	4.761819	3.731094	-0.741209
77	1	0	5.570511	3.031815	-2.965615

De (*R*)

E(RB+HF-LYP) = -1248.95839077
Zero-point correction= 0.176579 (Hartree/Particle)
Thermal correction to Energy= 0.188374
Thermal correction to Enthalpy= 0.189239
Thermal correction to Gibbs Free Energy= 0.138783
Sum of electronic and zero-point Energies= -1248.781812
Sum of electronic and thermal Energies= -1248.770017
Sum of electronic and thermal Enthalpies= -1248.769152
Sum of electronic and thermal Free Energies= -1248.819607

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.557922	-1.760729	0.821180
2	8	0	-0.787192	-1.656329	0.723381
3	6	0	1.289002	-0.431869	1.158091
4	8	0	0.633534	0.640021	0.447379
5	6	0	1.678458	1.474151	-0.130729
6	8	0	2.714042	0.561220	-0.450095
7	6	0	2.660880	-0.542981	0.458935
8	6	0	2.547324	-1.871730	-0.310966
9	8	0	1.157944	-2.126125	-0.448328
10	17	0	-2.928338	0.915603	1.006642
11	50	0	-1.475364	-0.222909	-0.609408
12	6	0	1.172517	2.111718	-1.412059
13	6	0	2.126256	2.500426	0.909661
14	1	0	0.832357	-2.528940	1.578667
15	1	0	1.309919	-0.212835	2.234731
16	1	0	3.522057	-0.513308	1.145699
17	1	0	3.043653	-2.682784	0.260113
18	1	0	3.000381	-1.803450	-1.308688
19	1	0	1.969797	2.729553	-1.850295
20	1	0	0.900246	1.334777	-2.140250
21	1	0	0.304882	2.757310	-1.210819
22	1	0	2.484315	2.006138	1.824833
23	1	0	2.949963	3.104910	0.501857
24	1	0	1.291595	3.164620	1.178281

uADe (*S*,*R*)

E(RB+HF-LYP) = -2535.59410867
Zero-point correction= 0.408755 (Hartree/Particle)
Thermal correction to Energy= 0.437979
Thermal correction to Enthalpy= 0.438844
Thermal correction to Gibbs Free Energy= 0.348684
Sum of electronic and zero-point Energies= -2535.185354
Sum of electronic and thermal Energies= -2535.156130
Sum of electronic and thermal Enthalpies= -2535.155265
Sum of electronic and thermal Free Energies= -2535.245425

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.154988	1.815809	0.921391
2	7	0	2.477215	2.552792	-0.068152
3	6	0	1.984215	1.893634	-1.048738
4	8	0	1.234084	2.491842	-2.013775
5	6	0	2.163396	0.402518	-1.279216
6	7	0	2.303585	-0.254725	0.029917
7	6	0	3.000413	0.463715	0.978484

8	8	0	3.390864	-0.359587	2.009612
9	17	0	0.135426	-2.708756	-1.360837
10	50	0	1.074308	-1.784710	0.940906
11	6	0	3.885416	0.257092	3.193049
12	6	0	3.316191	0.114303	-2.296250
13	6	0	1.055449	3.905806	-1.875467
14	6	0	4.694823	0.624119	-1.855996
15	6	0	3.379222	-1.372423	-2.662056
16	1	0	3.734563	2.387048	1.642976
17	1	0	4.844737	0.767306	3.000967
18	1	0	3.161698	0.986082	3.595925
19	1	0	4.044603	-0.553230	3.916611
20	1	0	3.020864	0.676975	-3.202150
21	1	0	0.506820	4.224544	-2.771929
22	1	0	2.027936	4.417923	-1.814527
23	1	0	0.478348	4.137331	-0.966452
24	1	0	5.424358	0.485900	-2.671530
25	1	0	5.065992	0.066593	-0.981256
26	1	0	4.677727	1.693223	-1.595880
27	1	0	4.147425	-1.547422	-3.432917
28	1	0	2.416893	-1.743220	-3.046126
29	1	0	3.645105	-1.982077	-1.782753
30	1	0	1.245782	0.022298	-1.753474
31	6	0	-2.491965	0.989648	1.576760
32	6	0	-1.746695	2.324635	1.825921
33	6	0	-1.420384	-0.107598	1.817592
34	6	0	-0.326497	1.901248	2.228715
35	8	0	-0.439590	0.517311	2.622199
36	1	0	0.357115	2.027633	1.376025
37	1	0	0.067516	2.444108	3.097403
38	50	0	-2.127478	-1.090775	-1.096540
39	17	0	-3.540193	-2.501703	0.362309
40	8	0	-2.925860	1.061294	0.217093
41	8	0	-1.772339	2.992081	0.566809
42	8	0	-0.848573	-0.557464	0.612181
43	1	0	-1.813374	-0.953620	2.402341
44	1	0	-3.354089	0.835737	2.241581
45	1	0	-2.236261	2.938777	2.599220
46	6	0	-2.838423	2.458575	-0.202004
47	6	0	-2.461779	2.530210	-1.670101
48	1	0	-3.214408	2.019738	-2.288592
49	1	0	-2.417975	3.584121	-1.981808
50	1	0	-1.471420	2.082759	-1.833746
51	6	0	-4.165185	3.149754	0.112798
52	1	0	-4.098434	4.217850	-0.142451
53	1	0	-4.981532	2.693994	-0.466773
54	1	0	-4.413848	3.065137	1.181388

ucaa-C7c (*S*,*R*)

E(RB+HF-LYP) = -2535.54384743

Zero-point correction=	0.406054	(Hartree/Particle)
Thermal correction to Energy=	0.435086	
Thermal correction to Enthalpy=	0.435951	
Thermal correction to Gibbs Free Energy=	0.347343	
Sum of electronic and zero-point Energies=	-2535.137794	
Sum of electronic and thermal Energies=	-2535.108762	
Sum of electronic and thermal Enthalpies=	-2535.107897	
Sum of electronic and thermal Free Energies=	-2535.196505	

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.010549	-2.361718	1.216329
2	7	0	-0.643692	-1.808168	2.326544
3	6	0	-1.865635	-1.457663	2.168140
4	8	0	-2.570859	-0.906608	3.176648
5	6	0	-2.674589	-1.726154	0.904561
6	7	0	-1.783171	-1.783024	-0.284181
7	6	0	-0.632330	-2.426681	-0.042540
8	8	0	-0.061333	-2.953366	-1.141529
9	6	0	1.016834	-0.338613	0.535129
10	8	0	0.034877	0.376164	0.055417
11	6	0	2.198821	-0.687262	-0.334099
12	8	0	3.011928	-1.649513	0.339511
13	6	0	4.306995	-1.069146	0.647834

14	8	0	4.155183	0.321490	0.439839
15	6	0	3.189892	0.499305	-0.589508
16	6	0	2.688509	1.941911	-0.608652
17	8	0	2.095941	2.360619	0.600228
18	17	0	0.280087	-0.698914	-3.404020
19	50	0	-1.466975	0.007690	-1.778401
20	6	0	1.036285	-3.867907	-1.005166
21	6	0	-3.960475	-0.872973	0.765359
22	6	0	-1.878398	-0.728832	4.419817
23	6	0	-3.778647	0.652750	0.790962
24	6	0	-4.806934	-1.324187	-0.432690
25	6	0	4.620057	-1.307447	2.116690
26	6	0	5.354732	-1.672501	-0.289967
27	1	0	3.573769	2.575651	-0.804588
28	1	0	0.894043	-2.956001	1.439796
29	1	0	1.216090	-0.255416	1.612348
30	1	0	-3.058654	-2.761351	1.037152
31	1	0	1.250943	-4.205772	-2.026462
32	1	0	1.926177	-3.386642	-0.576311
33	1	0	0.737171	-4.729386	-0.384875
34	1	0	-4.526174	-1.126720	1.677590
35	1	0	-2.616251	-0.297896	5.107871
36	1	0	-1.020707	-0.050049	4.294707
37	1	0	-1.505154	-1.692664	4.797293
38	1	0	-4.759352	1.139969	0.916843
39	1	0	-3.355672	1.053814	-0.144460
40	1	0	-3.141007	0.972792	1.627217
41	1	0	-5.788799	-0.824993	-0.416776
42	1	0	-4.978986	-2.412370	-0.418926
43	1	0	-4.330183	-1.079435	-1.395480
44	1	0	1.848273	-1.080087	-1.299057
45	1	0	3.646353	0.316455	-1.583428
46	1	0	5.596243	-0.868527	2.371622
47	1	0	4.650560	-2.385834	2.331581
48	1	0	3.848033	-0.835554	2.740417
49	1	0	6.343826	-1.235730	-0.084460
50	1	0	5.098033	-1.478987	-1.342048
51	1	0	5.412281	-2.762285	-0.147844
52	1	0	2.014970	2.051263	-1.480397
53	50	0	0.119644	2.607869	0.962222
54	17	0	-0.686037	3.214715	-1.341335

ucss-C5c (*S*,*R*)

E(RB+HF-LYP) = -2535.53706276

Zero-point correction=	0.406580	(Hartree/Particle)
Thermal correction to Energy=	0.435441	
Thermal correction to Enthalpy=	0.436306	
Thermal correction to Gibbs Free Energy=	0.347364	
Sum of electronic and zero-point Energies=	-2535.130483	
Sum of electronic and thermal Energies=	-2535.101622	
Sum of electronic and thermal Enthalpies=	-2535.100757	
Sum of electronic and thermal Free Energies=	-2535.189698	

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.275770	0.517123	1.816059
2	7	0	-1.507977	1.837751	1.393521
3	6	0	-2.683350	2.121012	0.968109
4	8	0	-2.996115	3.360335	0.536168
5	6	0	-3.864002	1.161458	1.027063
6	7	0	-3.392098	-0.245849	0.954283
7	6	0	-2.291631	-0.457230	1.699843
8	8	0	-2.190048	-1.721209	2.147060
9	6	0	-0.376341	-0.265663	-0.255263
10	8	0	-1.374183	-0.146118	-1.038075
11	6	0	0.686752	0.807583	-0.395833
12	8	0	1.248044	0.665964	-1.711804
13	6	0	2.476287	1.356231	-1.715016
14	8	0	3.021266	1.117735	-0.370663
15	6	0	1.921506	0.777732	0.534561
16	6	0	2.317208	-0.526670	1.231210
17	8	0	3.579768	-0.356482	1.827922
18	17	0	-1.890113	-3.443302	-0.439054
19	50	0	-3.194782	-1.427367	-1.047287

20	6	0	-1.029223	-2.144668	2.860545
21	6	0	-5.057090	1.537102	0.114930
22	6	0	-1.954279	4.341606	0.573138
23	6	0	-4.757249	1.672817	-1.386672
24	6	0	-6.260607	0.619649	0.369634
25	6	0	3.375281	0.738165	-2.768456
26	6	0	2.297859	2.865556	-1.892177
27	1	0	1.580629	-0.751799	2.022581
28	1	0	-0.463706	0.401874	2.534965
29	1	0	-0.100601	-1.260988	0.122418
30	1	0	-4.268790	1.282455	2.055642
31	1	0	-1.221722	-3.187593	3.138209
32	1	0	-0.128018	-2.103843	2.231415
33	1	0	-0.880246	-1.537971	3.769293
34	1	0	-5.331699	2.546294	0.464932
35	1	0	-2.426362	5.283846	0.267643
36	1	0	-1.144194	4.077362	-0.125008
37	1	0	-1.531780	4.424699	1.585679
38	1	0	-5.588763	2.199472	-1.883169
39	1	0	-4.665875	0.696810	-1.890310
40	1	0	-3.838603	2.246109	-1.574108
41	1	0	-7.142362	0.980574	-0.183426
42	1	0	-6.521939	0.584173	1.439486
43	1	0	-6.065513	-0.415147	0.045887
44	1	0	0.171053	1.775814	-0.303406
45	1	0	1.856073	1.575851	1.290684
46	1	0	4.370104	1.208682	-2.757920
47	1	0	2.928638	0.902227	-3.760257
48	1	0	3.482819	-0.339390	-2.594074
49	1	0	3.273537	3.371438	-1.841497
50	1	0	1.653661	3.290225	-1.108608
51	1	0	1.841545	3.073275	-2.871698
52	1	0	2.307146	-1.361116	0.501186
53	50	0	5.121661	0.153666	0.581165
54	17	0	5.087144	-1.881063	-0.826828

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utas-C7g (*A*,*R*)

E(RB+HF-LYP) = -2535.56716833
Zero-point correction= 0.406668 (Hartree/Particle)
Thermal correction to Energy= 0.435624
Thermal correction to Enthalpy= 0.436489
Thermal correction to Gibbs Free Energy= 0.348504
Sum of electronic and zero-point Energies= -2535.160500
Sum of electronic and thermal Energies= -2535.131545
Sum of electronic and thermal Enthalpies= -2535.130680
Sum of electronic and thermal Free Energies= -2535.218664

1	6	0	0.340282	-2.266831	1.223980
2	7	0	1.112498	-1.806294	2.300075
3	6	0	2.095457	-1.030159	2.030346
4	8	0	2.834641	-0.454342	3.000367
5	6	0	2.620659	-0.682642	0.646433
6	7	0	1.575483	-0.931697	-0.358511
7	6	0	0.654063	-1.864221	-0.074413
8	8	0	-0.006477	-2.293382	-1.189042
9	6	0	-1.366199	-0.602004	1.788577
10	8	0	-0.677399	0.445162	1.944492
11	6	0	-2.663124	-0.572020	1.009395
12	8	0	-3.110034	-1.852752	0.582549
13	6	0	-4.305060	-1.596711	-0.175974
14	8	0	-4.134166	-0.282782	-0.735335
15	6	0	-2.946367	0.332124	-0.206418
16	6	0	-1.932799	0.403287	-1.355569
17	8	0	-0.659933	0.982837	-1.022610
18	17	0	-2.188548	3.550546	0.890106
19	17	0	2.418689	2.195142	-1.561592
20	50	0	1.067115	0.192033	-2.239759
21	50	0	-0.061744	2.251663	0.702448
22	6	0	2.416770	-0.699124	4.348484
23	6	0	-0.802922	-3.481671	-1.090555
24	6	0	3.959618	-1.434686	0.353778
25	6	0	3.808729	-2.960469	0.359093
26	6	0	4.602052	-0.948804	-0.950105
27	6	0	-5.535640	-1.599726	0.732080
28	6	0	-4.413944	-2.621624	-1.295187

29	1	0	-4.476654	-3.640582	-0.883943
30	1	0	-0.273225	-3.145297	1.413590
31	1	0	-1.164542	-3.678146	-2.108107
32	1	0	-0.182866	-4.327368	-0.751438
33	1	0	-1.652811	-3.325140	-0.413146
34	1	0	4.624603	-1.148504	1.188059
35	1	0	3.116156	-0.137727	4.980740
36	1	0	2.458569	-1.774053	4.582647
37	1	0	1.384507	-0.347970	4.499289
38	1	0	4.792760	-3.443216	0.243911
39	1	0	3.176117	-3.299452	-0.478385
40	1	0	3.361566	-3.329361	1.295545
41	1	0	5.595454	-1.406250	-1.085727
42	1	0	4.721461	0.145186	-0.966817
43	1	0	3.993575	-1.236297	-1.825670
44	1	0	2.860994	0.392193	0.636742
45	1	0	-1.345488	-1.344818	2.599430
46	1	0	-3.350031	-0.206083	1.809525
47	1	0	-3.203607	1.346411	0.123363
48	1	0	-1.770393	-0.618041	-1.739160
49	1	0	-2.414637	0.991877	-2.156083
50	1	0	-5.416542	-0.889371	1.563064
51	1	0	-5.705622	-2.604868	1.147210
52	1	0	-6.422607	-1.296152	0.156665
53	1	0	-3.544874	-2.552092	-1.962946
54	1	0	-5.321192	-2.426685	-1.885501

utsa-B7cg (*A*,*S*)

E(RB+HF-LYP) = -2535.57175316
Zero-point correction= 0.406052 (Hartree/Particle)
Thermal correction to Energy= 0.435204
Thermal correction to Enthalpy= 0.436068
Thermal correction to Gibbs Free Energy= 0.347056
Sum of electronic and zero-point Energies= -2535.165701
Sum of electronic and thermal Energies= -2535.136549
Sum of electronic and thermal Enthalpies= -2535.135685
Sum of electronic and thermal Free Energies= -2535.224697

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.254380	2.967490	0.259085
2	7	0	1.399557	2.371447	1.527037
3	6	0	0.393726	1.713954	1.980416
4	8	0	0.440173	1.067113	3.160324
5	6	0	-0.960239	1.569566	1.304485
6	7	0	-0.843763	1.857306	-0.138506
7	6	0	0.094695	2.766020	-0.476984
8	8	0	-0.138347	3.271687	-1.718345
9	6	0	2.190305	1.169903	-1.321302
10	8	0	1.262244	0.859435	-2.101994
11	6	0	2.737417	0.268338	-0.229343
12	8	0	3.955064	-0.252671	-0.789492
13	6	0	4.314254	-1.381522	0.009038
14	8	0	3.083891	-1.869566	0.571227
15	6	0	1.993985	-1.009934	0.204753
16	6	0	1.130850	-1.740538	-0.838046
17	8	0	-0.248434	-1.345353	-0.798823
18	17	0	-3.304938	-0.934097	-0.589189
19	17	0	-1.290275	-2.231313	2.356548
20	50	0	-1.072218	0.444044	-1.875452
21	50	0	-1.671106	-2.839847	-0.000232
22	6	0	0.811565	4.160832	-2.303070
23	6	0	-2.033016	2.449724	2.023993
24	6	0	1.655877	1.158962	3.909497
25	6	0	-1.715991	3.950104	1.983048
26	6	0	-3.439346	2.169622	1.486449
27	6	0	4.924680	-2.434008	-0.906313
28	6	0	5.245671	-0.972018	1.149964
29	1	0	1.538763	-1.614604	-1.853837
30	1	0	1.949827	3.776265	0.037588
31	1	0	2.911756	1.948669	-1.629889
32	1	0	2.953757	0.882266	0.661061
33	1	0	-1.273703	0.523446	1.432658
34	1	0	0.381387	4.464423	-3.265671

35	1	0	0.956304	5.051011	-1.669567
36	1	0	1.779344	3.665946	-2.475992
37	1	0	-1.995690	2.118649	3.077318
38	1	0	1.456562	0.642677	4.856641
39	1	0	1.930566	2.210416	4.083867
40	1	0	2.482560	0.663934	3.375395
41	1	0	-2.439422	4.507716	2.600034
42	1	0	-1.786643	4.345596	0.956403
43	1	0	-0.707812	4.173556	2.367139
44	1	0	-4.188003	2.747644	2.052615
45	1	0	-3.698982	1.103386	1.561896
46	1	0	-3.521518	2.460664	0.426633
47	1	0	1.377930	-0.838133	1.100498
48	1	0	5.166014	-3.340820	-0.332274
49	1	0	5.847309	-2.051676	-1.368546
50	1	0	4.212601	-2.694794	-1.702200
51	1	0	5.431517	-1.831836	1.811067
52	1	0	4.790276	-0.171023	1.751196
53	1	0	6.206994	-0.612061	0.752957
54	1	0	1.202999	-2.814607	-0.584772

uALe (*S*,*R*)

E(RB+HF-LYP) = -2535.59242271
Zero-point correction= 0.408087 (Hartree/Particle)
Thermal correction to Energy= 0.437652
Thermal correction to Enthalpy= 0.438517
Thermal correction to Gibbs Free Energy= 0.345786
Sum of electronic and zero-point Energies= -2535.184336
Sum of electronic and thermal Energies= -2535.154771
Sum of electronic and thermal Enthalpies= -2535.153906
Sum of electronic and thermal Free Energies= -2535.246636

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.796897	2.320187	1.008172
2	7	0	-2.933325	1.500155	2.144679
3	6	0	-2.963690	0.234499	1.951915
4	8	0	-3.027433	-0.647376	2.977280
5	6	0	-2.953980	-0.470879	0.602906
6	7	0	-2.317853	0.412780	-0.386741
7	6	0	-2.460317	1.765676	-0.186292
8	8	0	-2.095505	2.441174	-1.334682
9	17	0	-0.570702	-2.569310	-1.346005
10	50	0	-0.912509	0.010658	-1.966636
11	6	0	-1.844566	3.838807	-1.233040
12	6	0	-4.384025	-0.964024	0.211318
13	6	0	-3.028726	-0.089640	4.291730
14	6	0	-5.400019	0.171594	0.037751
15	6	0	-4.344343	-1.861567	-1.029648
16	1	0	-2.931046	3.389460	1.157451
17	1	0	-2.777024	4.388561	-1.021255
18	1	0	-1.104490	4.049866	-0.444474
19	1	0	-1.451268	4.151213	-2.209304
20	1	0	-4.702838	-1.585355	1.068276
21	1	0	-3.072285	-0.945011	4.978340
22	1	0	-3.897693	0.571554	4.438773
23	1	0	-2.115354	0.500607	4.467462
24	1	0	-6.408559	-0.239794	-0.134532
25	1	0	-5.145844	0.802257	-0.830006
26	1	0	-5.446600	0.820402	0.925854
27	1	0	-5.346489	-2.263123	-1.252043
28	1	0	-3.656244	-2.711135	-0.898859
29	1	0	-4.018134	-1.295093	-1.919712
30	1	0	-2.331520	-1.372755	0.712072
31	1	0	6.472378	1.116143	1.066223
32	6	0	5.551802	0.580709	1.343233
33	6	0	4.481519	0.797576	0.276732
34	1	0	5.206533	0.957999	2.317674
35	1	0	5.780286	-0.490198	1.449685
36	8	0	3.262625	0.120240	0.703043
37	8	0	4.127772	2.165113	0.168695
38	6	0	4.875711	0.300392	-1.103870
39	6	0	2.327312	1.078017	1.202610
40	6	0	3.007393	2.447512	1.002555

41	1	0	5.767418	0.842092	-1.452101
42	1	0	4.050284	0.490334	-1.804264
43	1	0	5.106702	-0.774984	-1.082737
44	6	0	1.057366	1.146822	0.302423
45	1	0	2.074059	0.827630	2.240592
46	6	0	1.971692	3.249191	0.213598
47	1	0	3.320099	2.940512	1.938069
48	8	0	1.253887	2.285417	-0.547304
49	1	0	1.302220	3.794041	0.909281
50	1	0	2.439263	3.963464	-0.476846
51	50	0	1.855307	-1.921649	-0.162127
52	17	0	1.080631	-2.109055	2.167616
53	8	0	0.864948	0.031534	-0.500782
54	1	0	0.167929	1.324446	0.939043

ucas-B5c (*S*,*R*)

E(RB+HF-LYP) = -2535.54110245
Zero-point correction= 0.406619 (Hartree/Particle)
Thermal correction to Energy= 0.435526
Thermal correction to Enthalpy= 0.436391
Thermal correction to Gibbs Free Energy= 0.346992
Sum of electronic and zero-point Energies= -2535.134484
Sum of electronic and thermal Energies= -2535.105577
Sum of electronic and thermal Enthalpies= -2535.104712
Sum of electronic and thermal Free Energies= -2535.194110

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.235591	1.438093	1.924772
2	7	0	-2.528501	2.488067	1.042034
3	6	0	-3.309900	2.217714	0.057506
4	8	0	-3.626502	3.150225	-0.867353
5	6	0	-4.010111	0.871656	-0.104001
6	7	0	-3.122193	-0.202854	0.406350
7	6	0	-2.582357	0.124501	1.607883
8	8	0	-2.241195	-0.949474	2.338473
9	6	0	-0.141533	0.731336	0.672967
10	8	0	-0.095016	-0.515708	0.543628
11	6	0	0.933976	1.477834	1.445714
12	8	0	1.441973	0.726840	2.541683
13	6	0	2.711570	0.135440	2.213879
14	8	0	2.988230	0.589253	0.862204
15	6	0	2.195175	1.768667	0.600455
16	6	0	2.084261	1.918195	-0.919542
17	8	0	3.370785	1.835312	-1.478868
18	17	0	-1.716334	-3.646191	0.633540
19	50	0	-1.716089	-1.606343	-0.740166
20	6	0	-1.504692	-0.779792	3.550155
21	6	0	-4.659055	0.616919	-1.484129
22	6	0	-3.040339	4.444871	-0.696415
23	6	0	-3.718716	0.657286	-2.698797
24	6	0	-5.495459	-0.670260	-1.468489
25	6	0	2.620674	-1.380239	2.210728
26	6	0	3.759719	0.688383	3.173503
27	1	0	3.487899	0.428641	4.207377
28	1	0	-1.895663	1.729700	2.917684
29	1	0	-0.749510	1.356897	-0.004278
30	1	0	0.501109	2.415639	1.823371
31	1	0	-4.869872	0.918604	0.600979
32	1	0	-2.092954	-0.206286	4.286546
33	1	0	-1.337340	-1.796218	3.927248
34	1	0	-0.538390	-0.285809	3.368922
35	1	0	-5.357216	1.463381	-1.602514
36	1	0	-3.435033	5.058781	-1.515817
37	1	0	-1.941514	4.388048	-0.750883
38	1	0	-3.315428	4.870855	0.280433
39	1	0	-4.313686	0.676450	-3.626751
40	1	0	-3.068747	-0.230474	-2.762584
41	1	0	-3.081752	1.553230	-2.694950
42	1	0	-6.060312	-0.774177	-2.408624
43	1	0	-6.217316	-0.673147	-0.636097
44	1	0	-4.868075	-1.569522	-1.357525
45	1	0	2.719629	2.646446	1.018271
46	1	0	1.412647	1.137387	-1.324997

47	1	0	1.641086	2.905432	-1.150140
48	1	0	2.377135	-1.733476	3.223798
49	1	0	3.585338	-1.822283	1.916991
50	1	0	1.837152	-1.706791	1.516590
51	1	0	3.817637	1.784063	3.097786
52	1	0	4.749608	0.261049	2.953113
53	50	0	4.394736	0.088383	-1.156445
54	17	0	2.674226	-1.480287	-1.965736

ucsa-C7c (*S*,*R*)

E(RB+HF-LYP) = -2535.54871244
Zero-point correction= 0.406571 (Hartree/Particle)
Thermal correction to Energy= 0.435432
Thermal correction to Enthalpy= 0.436297
Thermal correction to Gibbs Free Energy= 0.348418
Sum of electronic and zero-point Energies= -2535.142141
Sum of electronic and thermal Energies= -2535.113281
Sum of electronic and thermal Enthalpies= -2535.112416
Sum of electronic and thermal Free Energies= -2535.200294

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.326192	-1.623081	1.851681
2	7	0	-0.213763	-0.554043	2.580636
3	6	0	-1.473020	-0.337637	2.457622
4	8	0	-2.083772	0.662321	3.122855
5	6	0	-2.404433	-1.253451	1.677226
6	7	0	-1.675476	-1.858441	0.530999
7	6	0	-0.468755	-2.314594	0.899779
8	8	0	-0.018597	-3.342281	0.162028
9	6	0	1.185277	-0.415089	0.093065
10	8	0	0.159731	0.287948	-0.302356
11	6	0	2.339828	0.194179	0.867116
12	8	0	3.244079	-0.859847	1.204458
13	6	0	4.484276	-0.695009	0.464375
14	8	0	4.220097	0.313170	-0.497395
15	6	0	3.244829	1.179918	0.065525
16	6	0	2.590808	2.036084	-1.011393
17	8	0	1.698419	2.929025	-0.378055
18	17	0	0.241937	-2.113022	-2.762042
19	50	0	-1.542836	-0.829742	-1.610439
20	6	0	1.264483	-3.908160	0.449792
21	6	0	-3.813650	-0.690621	1.371049
22	6	0	-1.266281	1.454301	3.995124
23	6	0	-3.880322	0.632439	0.593907
24	6	0	-4.701258	-1.763871	0.725905
25	6	0	4.818829	-1.982474	-0.273145
26	6	0	5.580412	-0.272763	1.443702
27	1	0	5.321610	0.675561	1.936968
28	1	0	1.239689	-2.050225	2.261269
29	1	0	2.061183	-3.150459	0.432105
30	1	0	1.251547	-4.403054	1.435372
31	1	0	1.437953	-4.650267	-0.338283
32	1	0	-4.224970	-0.477677	2.372676
33	1	0	-1.953681	2.154319	4.485940
34	1	0	-0.502814	2.004336	3.423159
35	1	0	-0.757570	0.817288	4.733800
36	1	0	-4.908232	1.029190	0.627809
37	1	0	-3.632184	0.518884	-0.473997
38	1	0	-3.220781	1.396958	1.028962
39	1	0	-5.737209	-1.400936	0.634200
40	1	0	-4.717160	-2.688761	1.324713
41	1	0	-4.349246	-2.033287	-0.282424
42	1	0	-2.606410	-2.094359	2.376009
43	1	0	1.451976	-1.268503	-0.544545
44	1	0	1.955901	0.664868	1.785607
45	1	0	3.705188	1.867161	0.801199
46	1	0	3.381250	2.611815	-1.525343
47	1	0	2.105365	1.398338	-1.773054
48	1	0	5.756363	-1.860617	-0.835933
49	1	0	4.016908	-2.227149	-0.983891
50	1	0	4.943067	-2.811594	0.439197
51	1	0	6.536408	-0.144261	0.913830
52	1	0	5.706092	-1.038751	2.223701

53	50	0	-0.269619	2.622909	-0.019324
54	17	0	-1.132276	2.291051	-2.372816

utaa-C7c (*S*,*R*)

E(RB+HF-LYP) = -2535.56235905
Zero-point correction= 0.406702 (Hartree/Particle)
Thermal correction to Energy= 0.435698
Thermal correction to Enthalpy= 0.436563
Thermal correction to Gibbs Free Energy= 0.347527
Sum of electronic and zero-point Energies= -2535.155657
Sum of electronic and thermal Energies= -2535.126661
Sum of electronic and thermal Enthalpies= -2535.125796
Sum of electronic and thermal Free Energies= -2535.214832

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.432312	1.927607	1.329561
2	7	0	-0.963860	1.102350	2.328787
3	6	0	-2.021475	0.437601	2.031540
4	8	0	-2.574778	-0.429299	2.887733
5	6	0	-2.806215	0.523372	0.735403
6	7	0	-2.030658	1.205888	-0.317600
7	6	0	-1.070730	2.045283	0.080072
8	8	0	-0.609736	2.827642	-0.933989
9	6	0	0.982129	0.348278	0.339270
10	8	0	0.228827	-0.446762	-0.372486
11	6	0	2.110485	1.081012	-0.345110
12	8	0	2.584328	2.126669	0.494319
13	6	0	3.996170	2.272280	0.267592
14	8	0	4.454551	0.967876	-0.048405
15	6	0	3.391390	0.190697	-0.601199
16	6	0	3.463724	-1.202077	0.045993
17	8	0	2.668676	-2.128649	-0.648596
18	17	0	0.978517	-2.614350	2.299758
19	17	0	-2.489924	-1.915283	-1.757835
20	50	0	-1.192844	0.154459	-2.126732
21	50	0	0.839711	-2.892264	-0.176277
22	6	0	0.156615	4.000738	-0.609143
23	6	0	-4.203437	1.182423	0.953188
24	6	0	-1.884596	-0.647578	4.132047
25	6	0	-4.113395	2.633351	1.440089
26	6	0	-5.066698	1.066700	-0.307852
27	6	0	4.642272	2.720621	1.567576
28	6	0	4.262044	3.230670	-0.897614
29	1	0	3.763034	2.884379	-1.815982
30	1	0	0.290909	2.668416	1.665418
31	1	0	-0.405296	4.634119	0.096039
32	1	0	1.135896	3.736111	-0.187181
33	1	0	0.284626	4.534981	-1.559252
34	1	0	-4.673158	0.579064	1.749413
35	1	0	-2.508849	-1.358876	4.686459
36	1	0	-1.780906	0.297158	4.686114
37	1	0	-0.887740	-1.070576	3.941042
38	1	0	-5.116325	3.018768	1.684572
39	1	0	-3.689130	3.290348	0.662615
40	1	0	-3.491200	2.727786	2.344893
41	1	0	-6.080790	1.454403	-0.119004
42	1	0	-5.158066	0.020896	-0.641345
43	1	0	-4.634934	1.650952	-1.137034
44	1	0	-2.993066	-0.509577	0.405500
45	1	0	1.141132	0.057913	1.385779
46	1	0	1.747370	1.480549	-1.310697
47	1	0	3.524763	0.062732	-1.690045
48	1	0	4.525408	-1.507514	-0.011724
49	1	0	3.211995	-1.130697	1.121450
50	1	0	5.734340	2.768360	1.446380
51	1	0	4.402111	2.000476	2.361740
52	1	0	4.275700	3.716155	1.858869
53	1	0	5.342498	3.280417	-1.099199
54	1	0	3.901084	4.243934	-0.662487

utss-B7cg (*A*,*R*)

E(RB+HF-LYP) = -2535.55959757
Zero-point correction= 0.405740 (Hartree/Particle)
Thermal correction to Energy= 0.434747
Thermal correction to Enthalpy= 0.435609
Thermal correction to Gibbs Free Energy= 0.346833
Sum of electronic and zero-point Energies= -2535.153858
Sum of electronic and thermal Energies= -2535.124850
Sum of electronic and thermal Enthalpies= -2535.123988
Sum of electronic and thermal Free Energies= -2535.212765

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.642661	1.460312	-0.271946
2	7	0	2.508039	1.152684	1.092515
3	6	0	1.429490	1.545022	1.666437
4	8	0	1.194767	1.318498	2.976547
5	6	0	0.274888	2.274573	1.006085
6	7	0	0.344190	2.166346	-0.470988
7	6	0	1.601645	2.100695	-0.955062
8	8	0	1.887874	2.515332	-2.209750
9	6	0	1.995412	-0.306936	-1.915515
10	8	0	0.806172	-0.075240	-2.311273
11	6	0	2.300885	-1.658520	-1.324023
12	8	0	3.510497	-1.655255	-0.595815
13	6	0	3.531699	-2.861665	0.168082
14	8	0	2.149887	-3.211871	0.381695
15	6	0	1.288285	-2.369596	-0.395206
16	6	0	0.481394	-1.524914	0.601154
17	8	0	-0.745680	-0.977768	0.093729
18	17	0	-3.241017	0.831828	0.840165
19	17	0	-3.504648	-2.289390	-1.180020
20	50	0	-1.112285	0.608197	-1.428786
21	50	0	-2.635045	-1.646143	1.043934
22	6	0	0.871358	3.111998	-3.016843
23	6	0	0.168815	3.751617	1.499058
24	6	0	2.240214	0.688771	3.726058
25	6	0	1.391560	4.601134	1.133773
26	6	0	-1.132713	4.397293	1.011780
27	6	0	4.199172	-2.561822	1.501180
28	6	0	4.213201	-3.991876	-0.603844
29	1	0	5.267947	-3.744108	-0.796620
30	1	0	3.663469	1.514921	-0.649702
31	1	0	2.825761	0.179072	-2.451123
32	1	0	2.410575	-2.296710	-2.233651
33	1	0	-0.646001	1.777573	1.347322
34	1	0	0.203617	3.745114	-2.415265
35	1	0	1.401333	3.716331	-3.765172
36	1	0	0.285706	2.336889	-3.538905
37	1	0	0.122178	3.673641	2.599804
38	1	0	1.906187	0.708664	4.771062
39	1	0	3.189495	1.232043	3.606542
40	1	0	2.388064	-0.350838	3.394247
41	1	0	1.318303	5.597157	1.599930
42	1	0	1.467526	4.753630	0.044628
43	1	0	2.332079	4.140483	1.476772
44	1	0	-1.239246	5.414483	1.422140
45	1	0	-2.013392	3.811159	1.318614
46	1	0	-1.147526	4.474412	-0.087436
47	1	0	0.595293	-2.998099	-0.978758
48	1	0	0.237700	-2.213212	1.431164
49	1	0	1.119865	-0.731962	1.011700
50	1	0	5.269384	-2.351309	1.354883
51	1	0	4.097042	-3.423361	2.177129
52	1	0	3.729662	-1.676415	1.951292
53	1	0	3.709361	-4.167650	-1.566203
54	1	0	4.166869	-4.925319	-0.023003

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FIGURE S8. ^{1}H NMR (200 MHz, D_2O) for compound **3**•HCl.

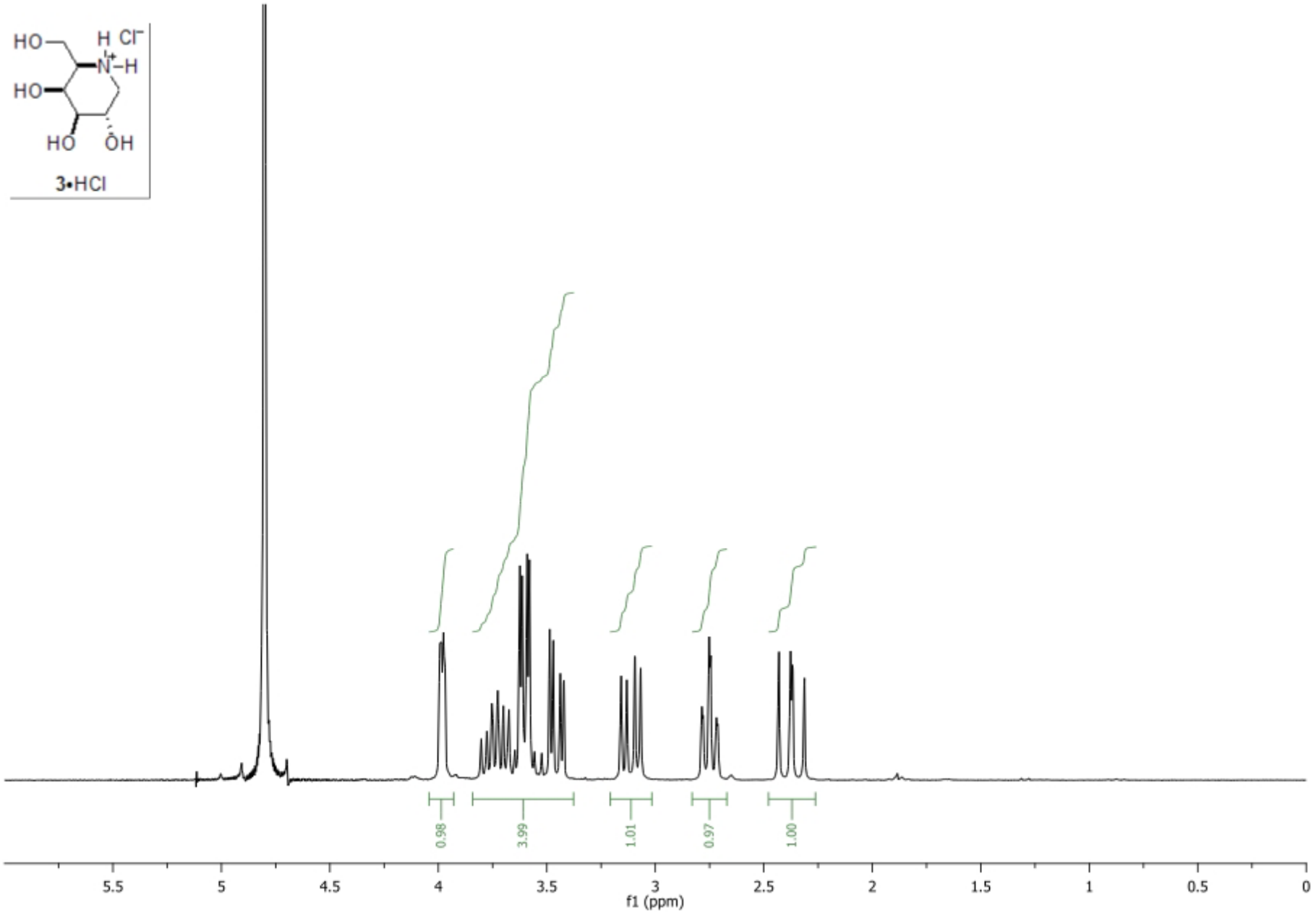

FIGURE S9. ^{1}H NMR (200 MHz, D_2O) for compound **4**.

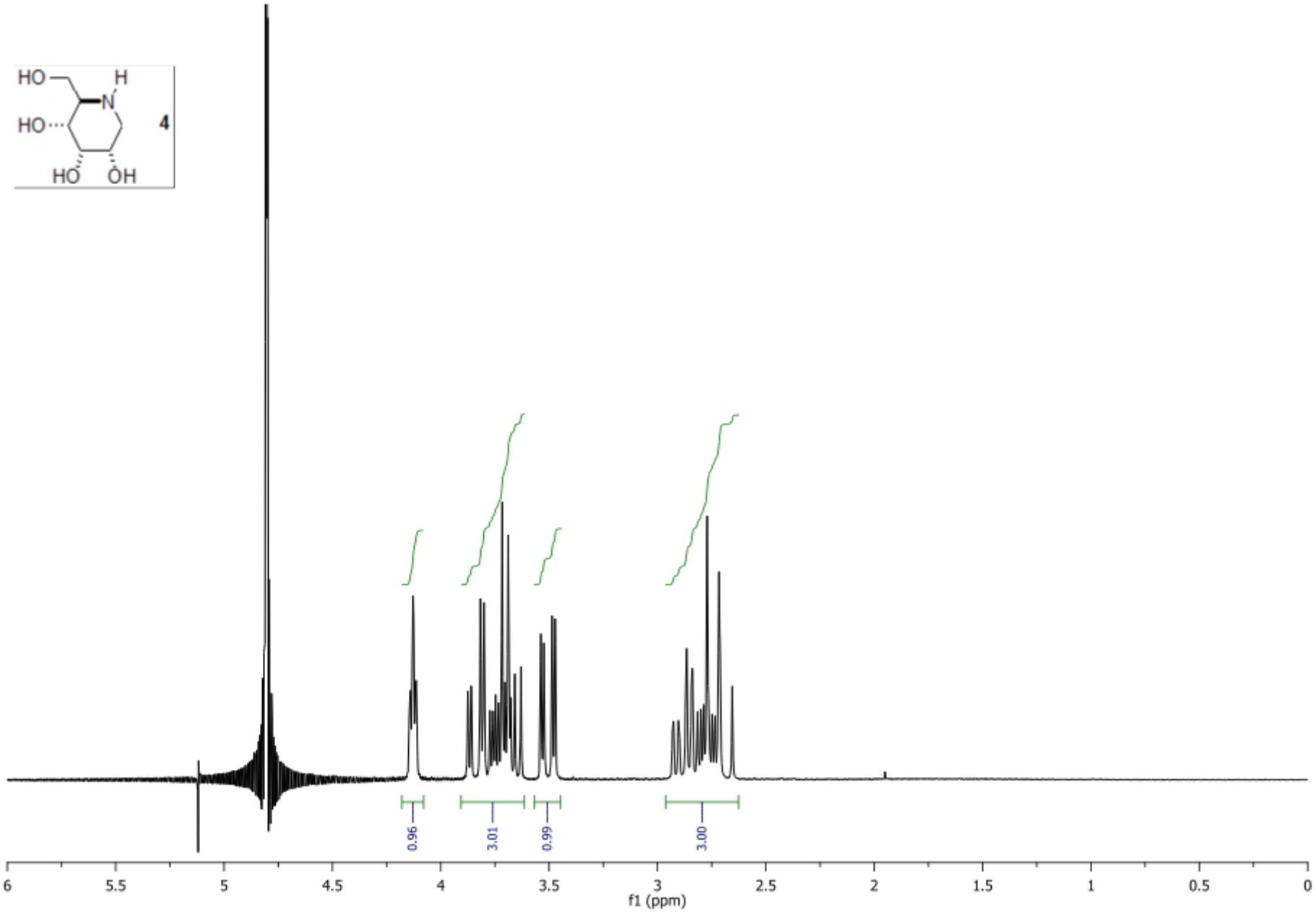

FIGURE S10. ^{1}H NMR (500 MHz, D_2O) for compound *ent*-**5**.

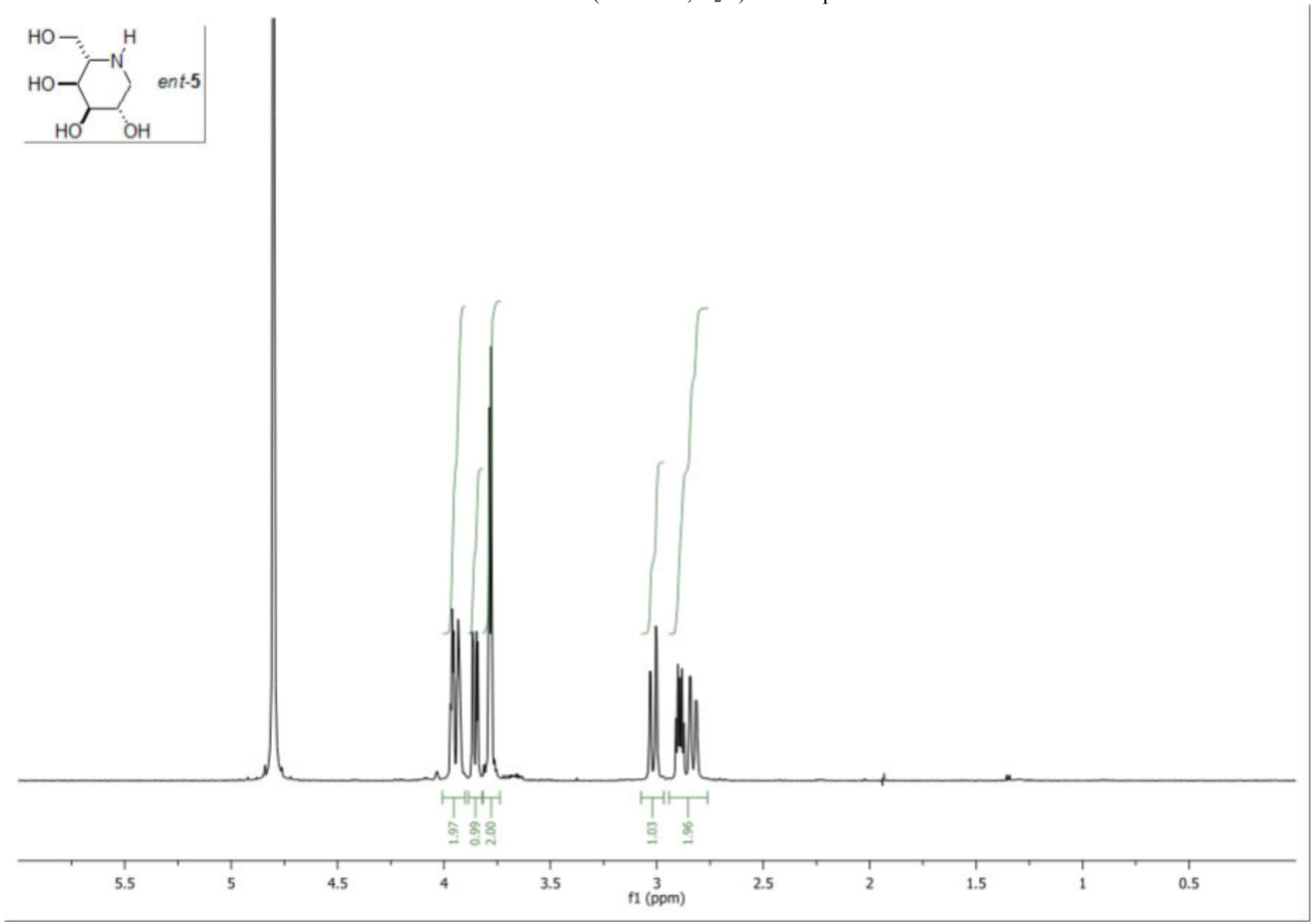

FIGURE S11. ^{1}H NMR (200 MHz, D_2O) for compound **6**.

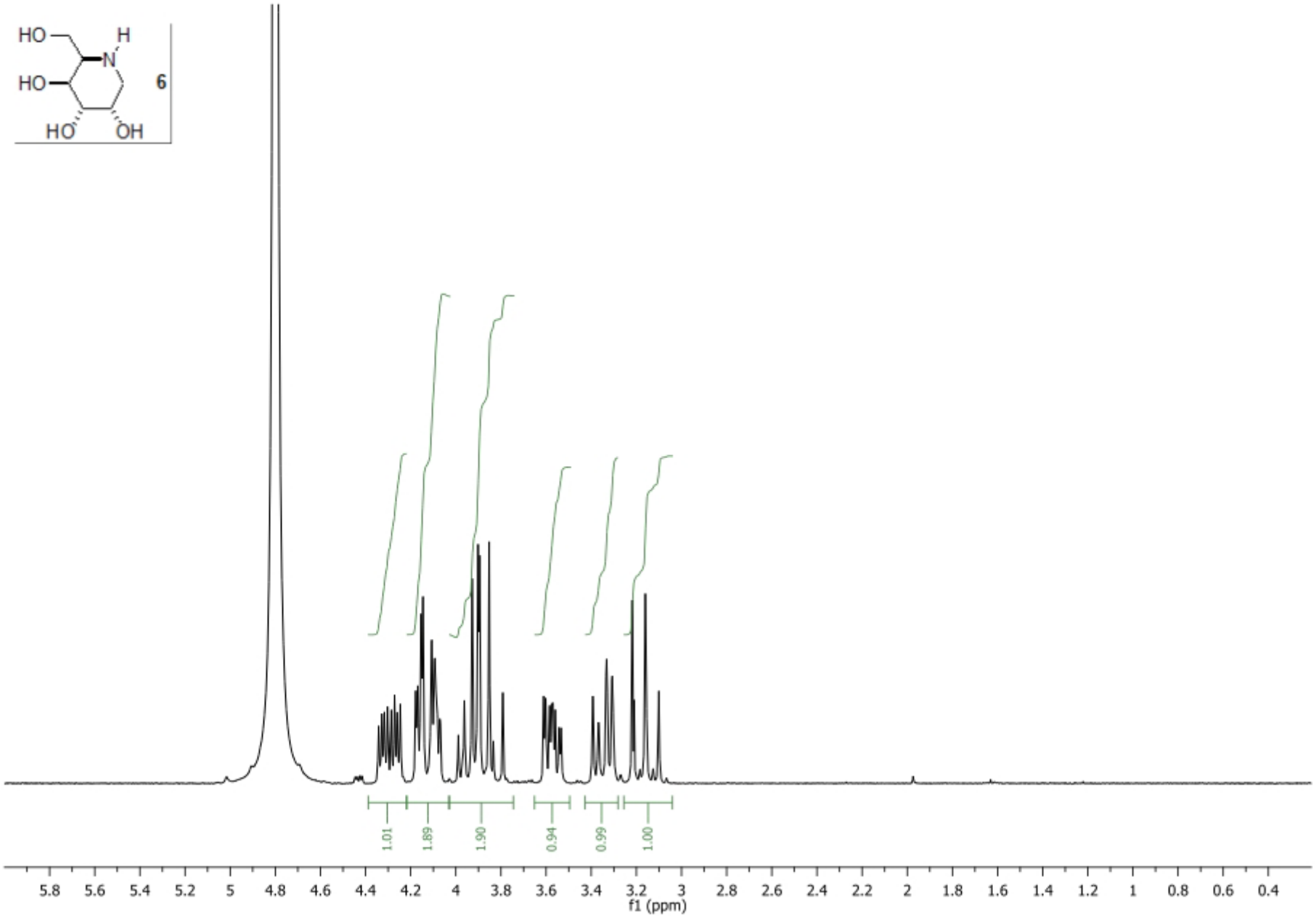

FIGURE S12. ^{1}H NMR (300 MHz, D_2O) for compound *ent*-**7**•HCl.

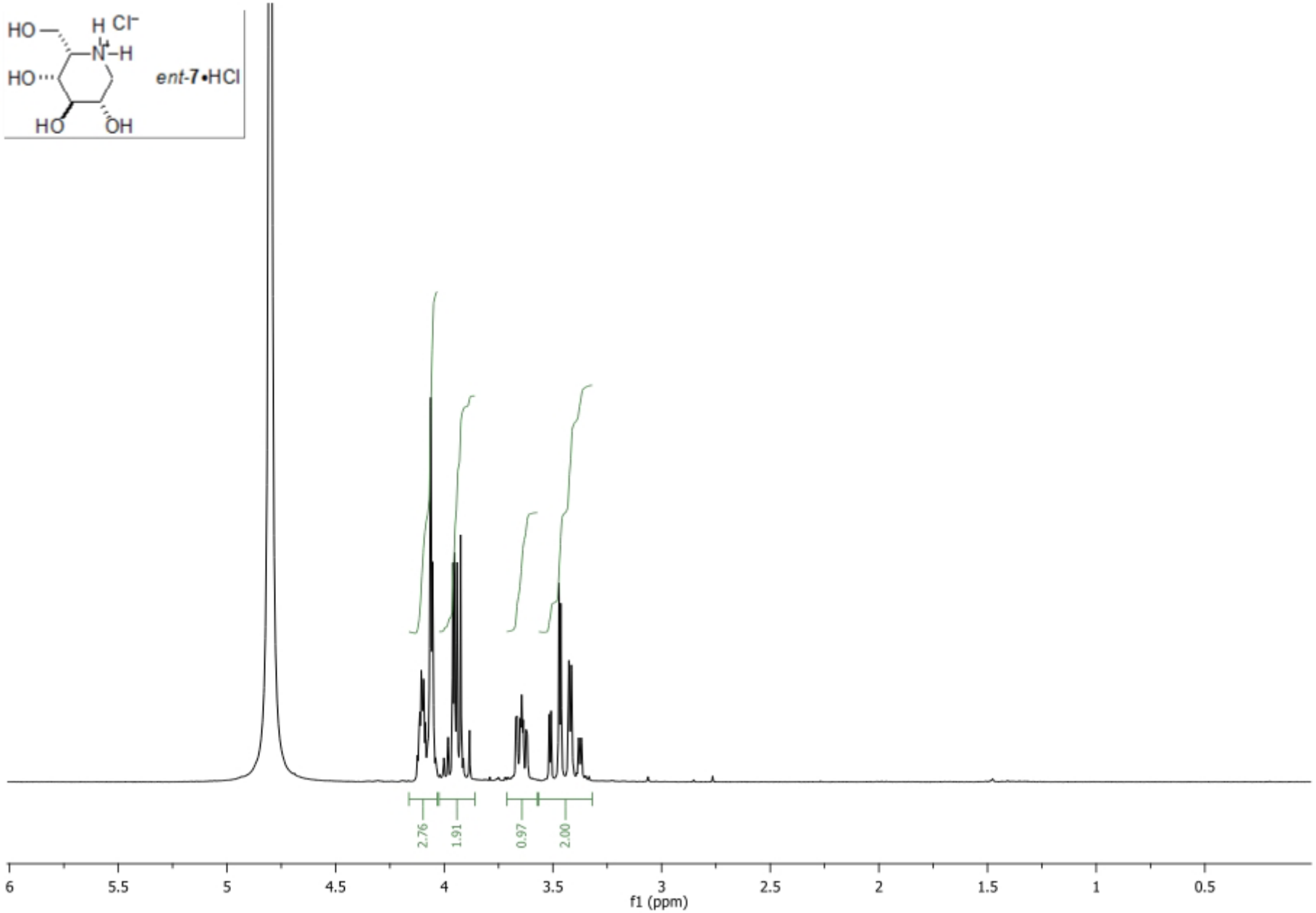

FIGURE S13. ^{1}H NMR (200 MHz, D_2O) for compound **8**.

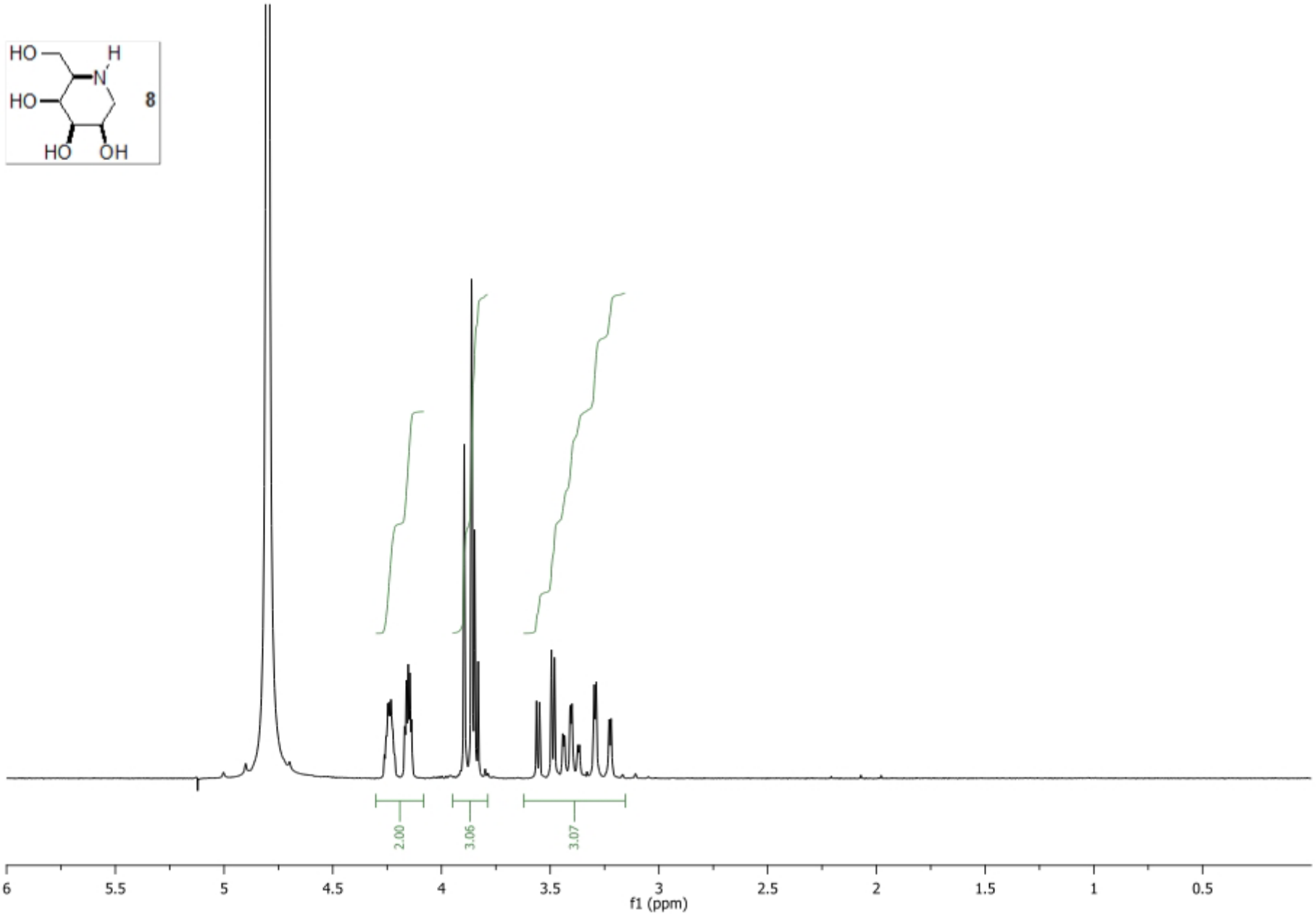

FIGURE S14. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **14a**.

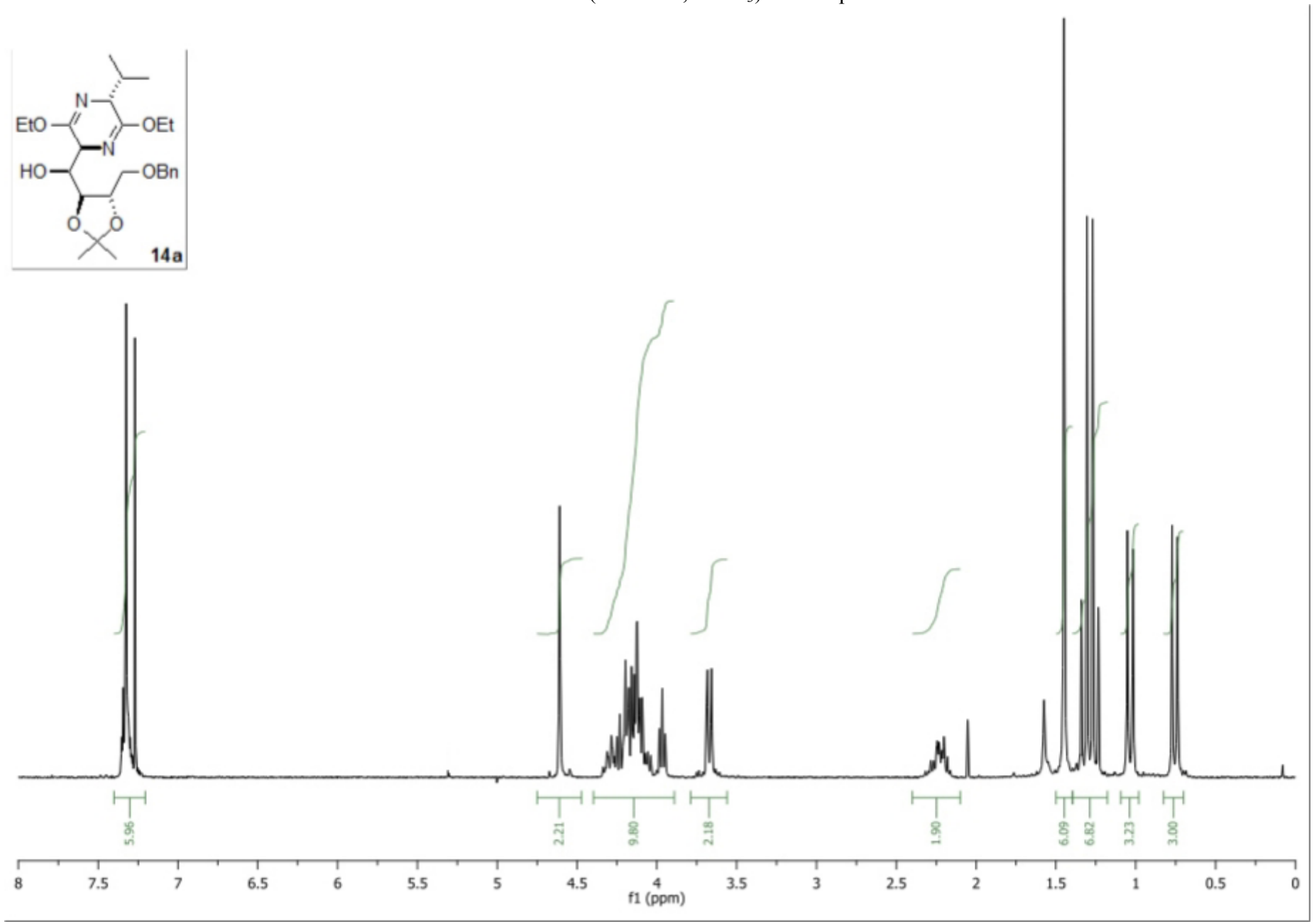

FIGURE S15. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **14b**. Prepared by silylation of **14c** following the general procedure 3.

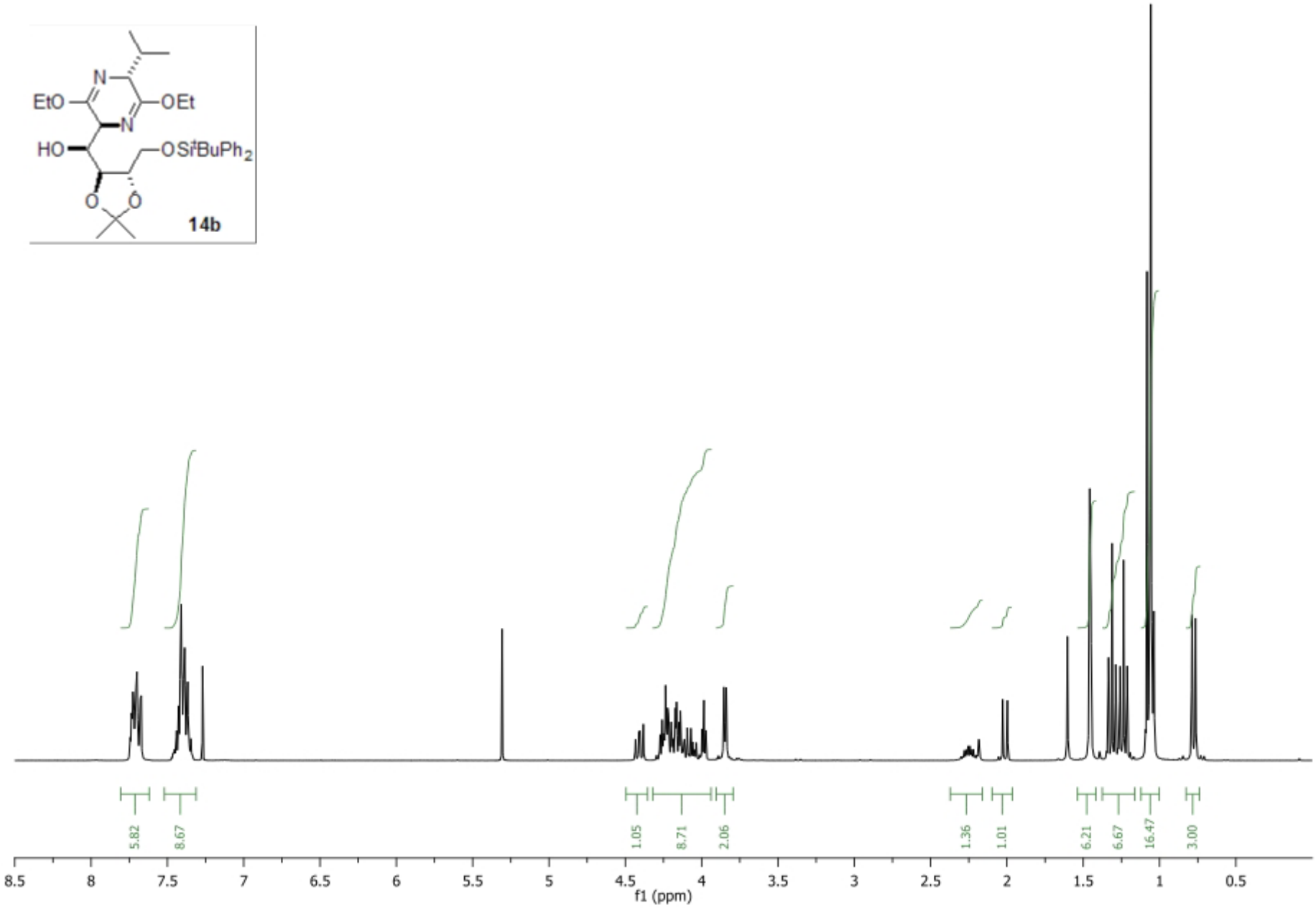

FIGURE S16. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **14c**. Prepared by debenzylation of **14a** following the general procedure 2.

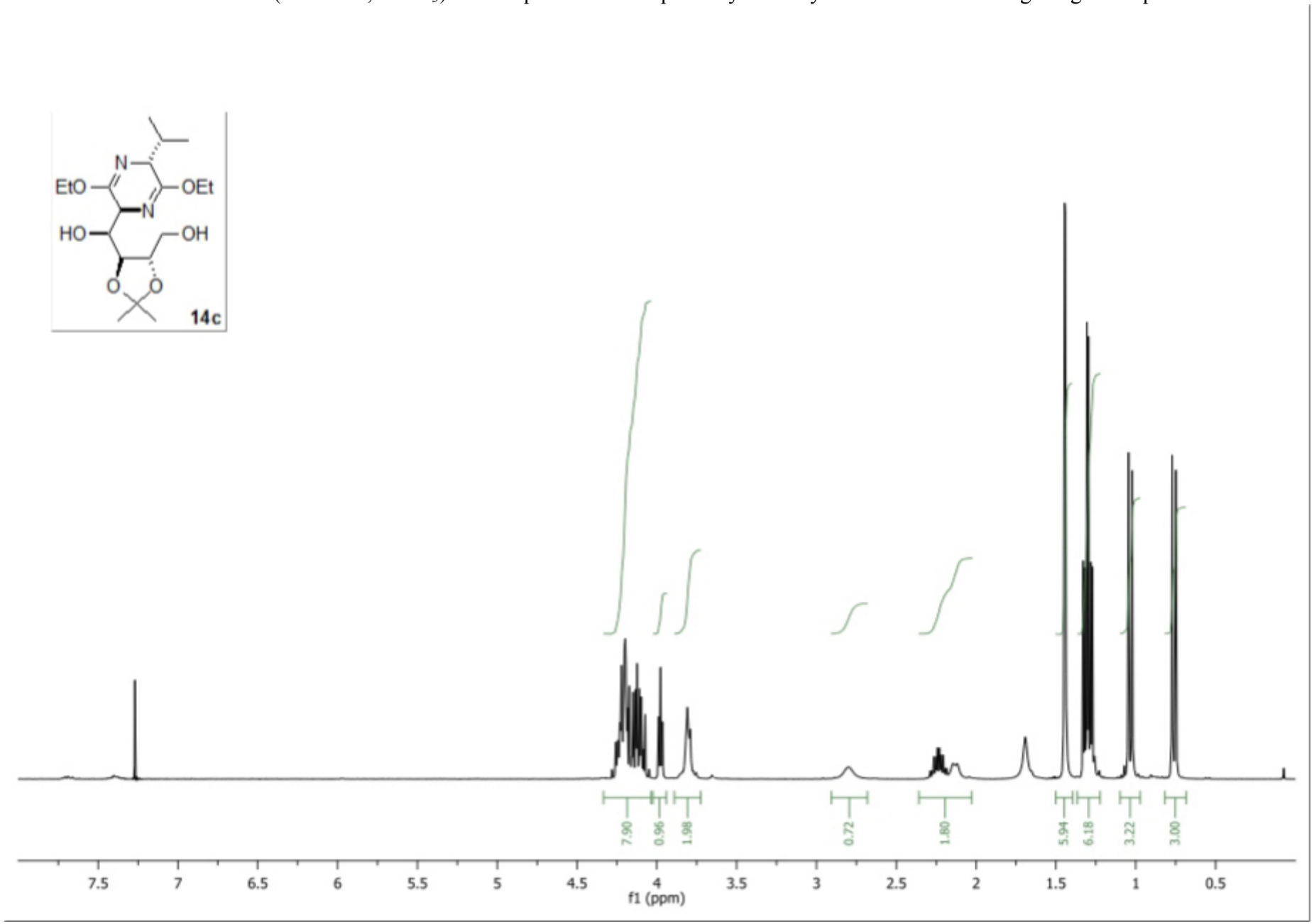

FIGURE S17. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **16a**.

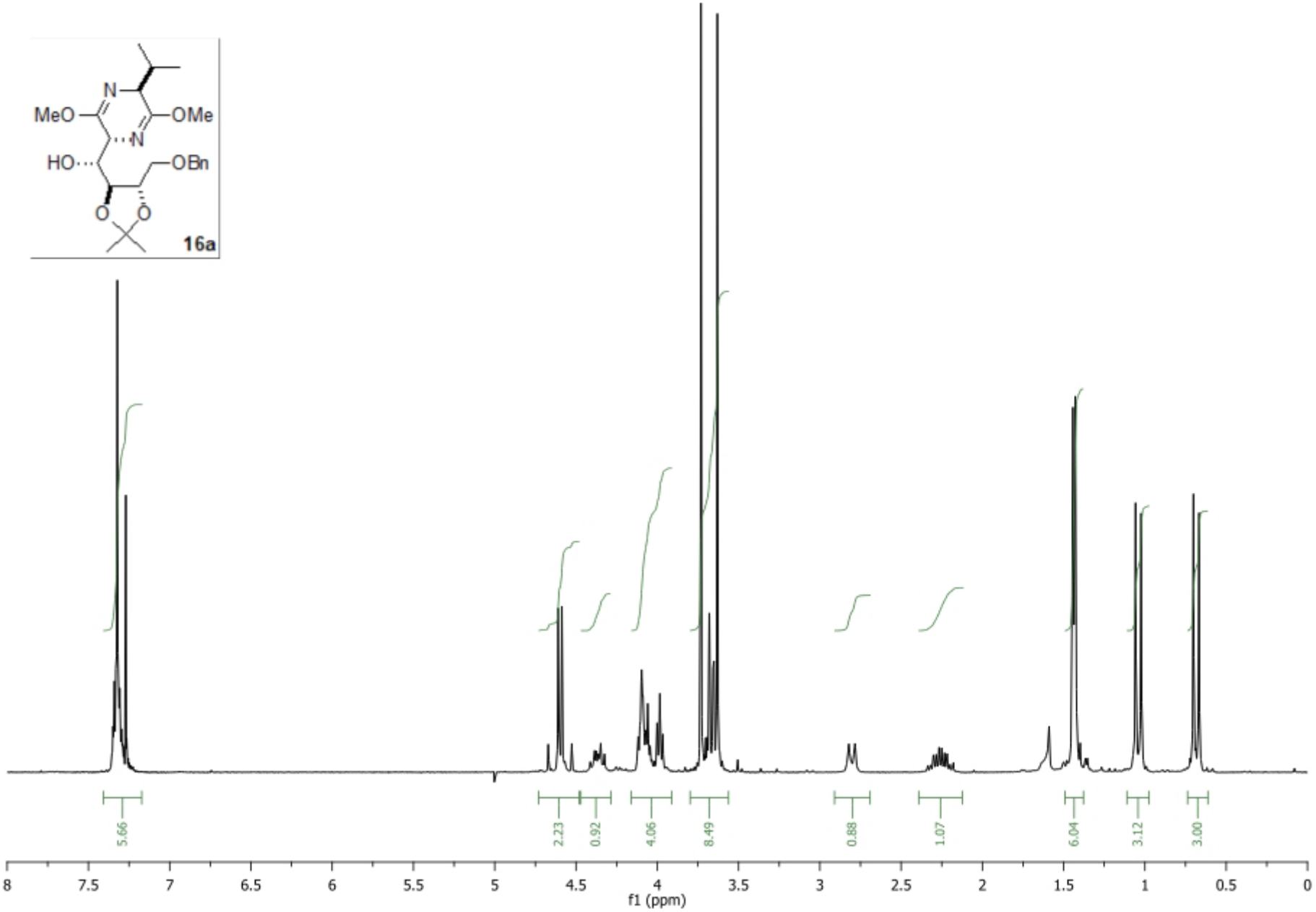

FIGURE S18. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **16b**. Prepared by addition of $SnCl^{+}$**15**$^{-}$ to **13b** following method A of the general procedure 1.

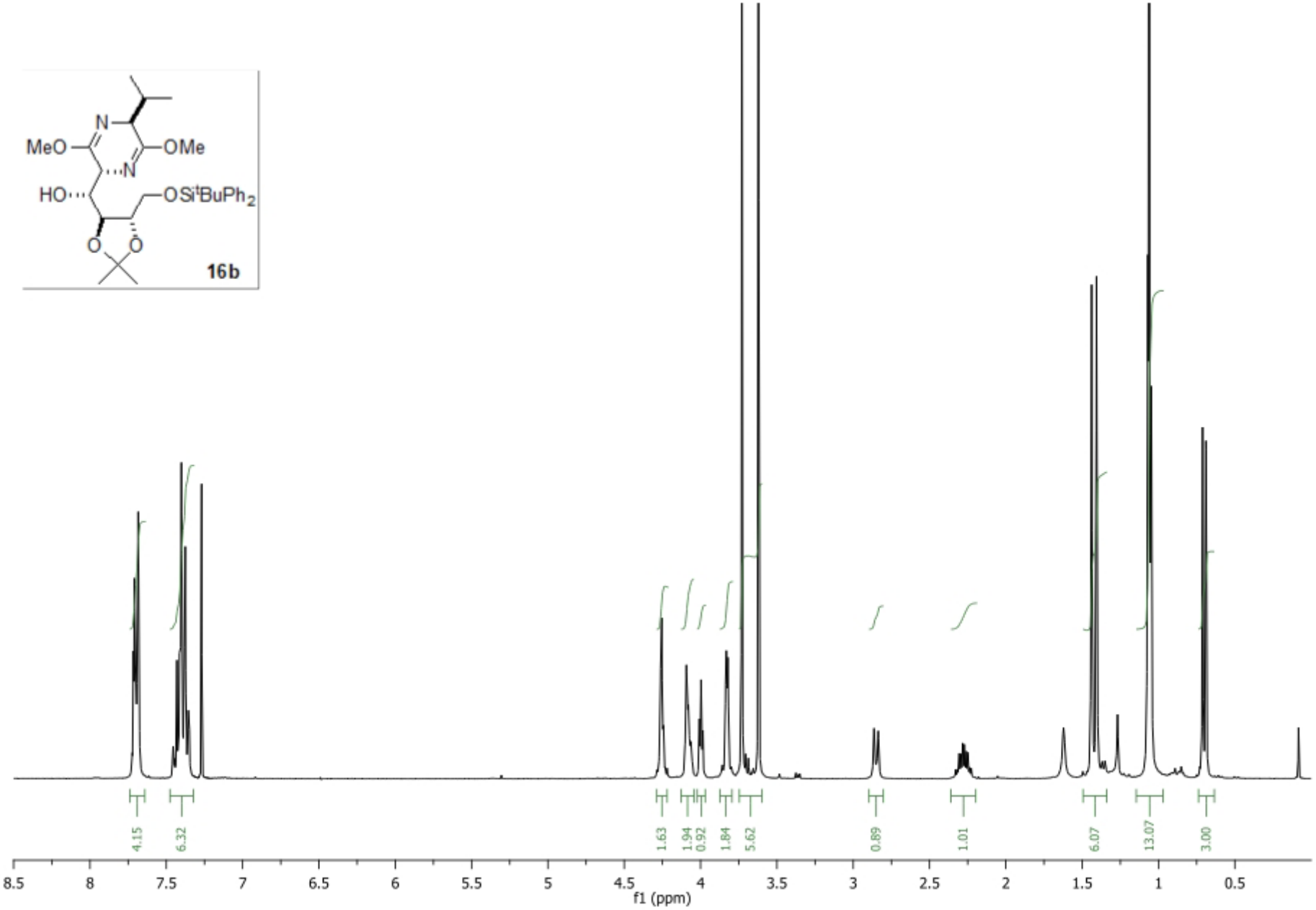

FIGURE S19. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **16c**. Prepared by hydrogenation of **16a** following the general procedure 2.

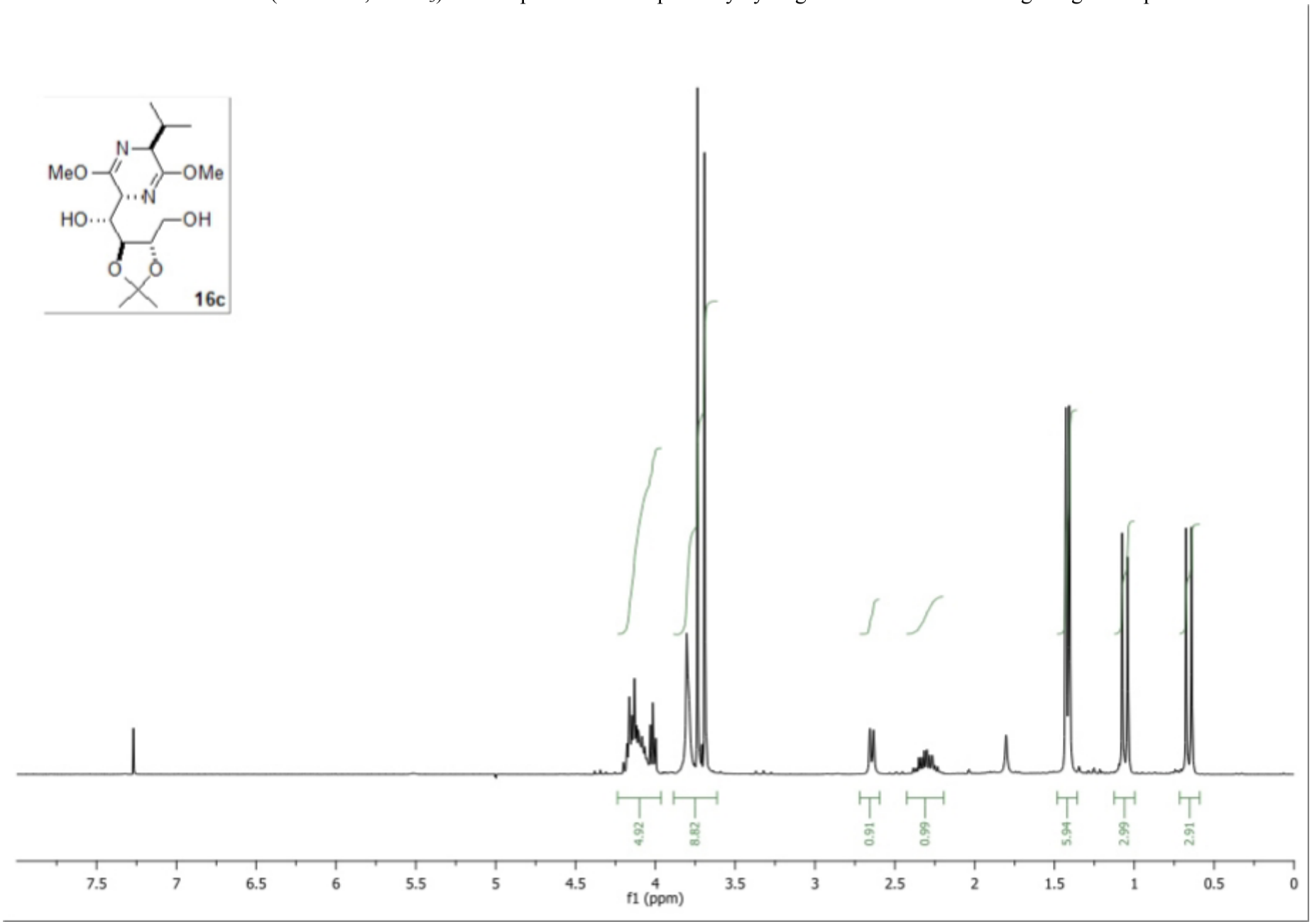

FIGURE S20. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **17a**.

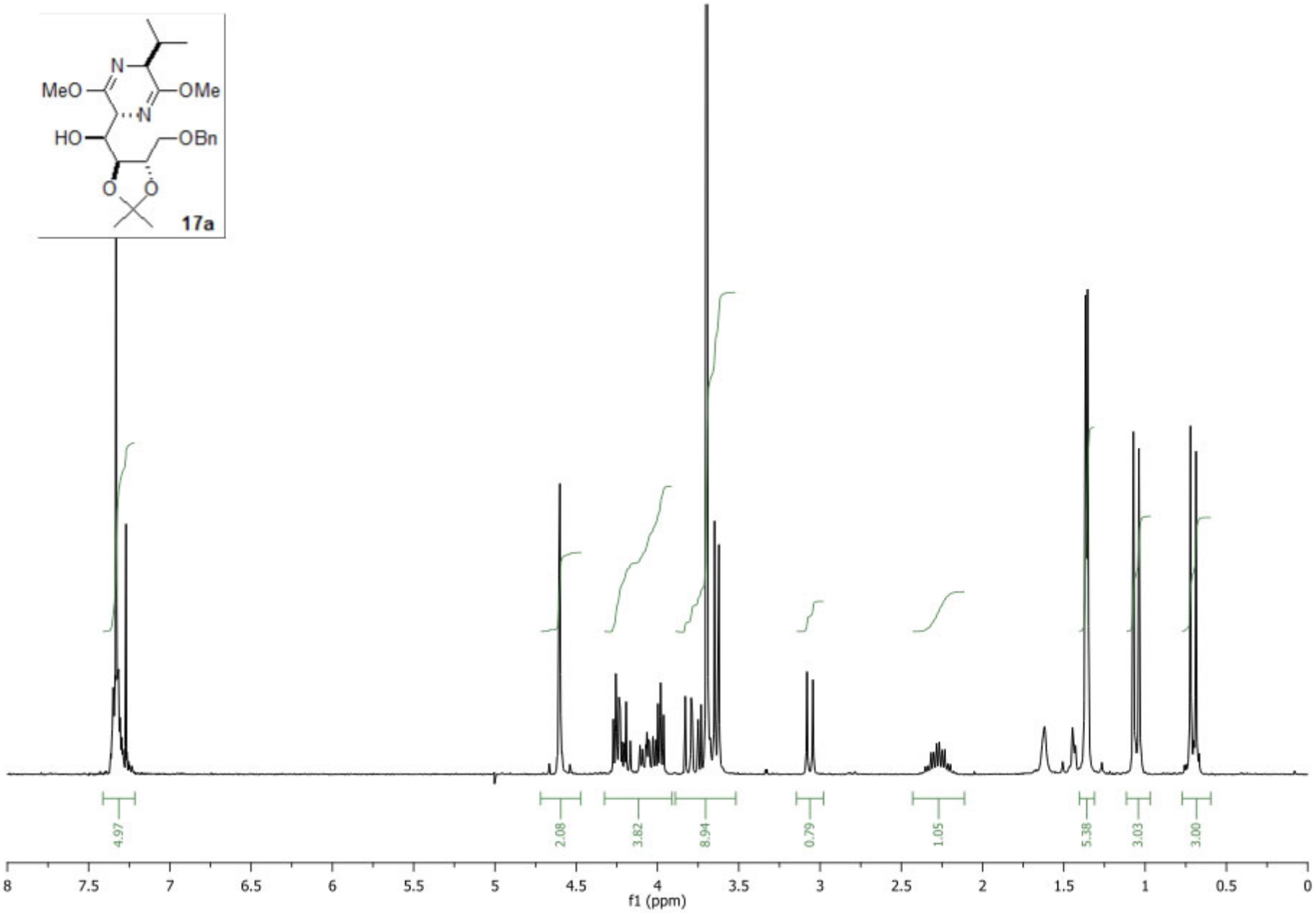

FIGURE S21. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **17b**. Prepared by addition of $SnCl^{+}$**15**$^{-}$ to **13b** following method A of the general procedure 1.

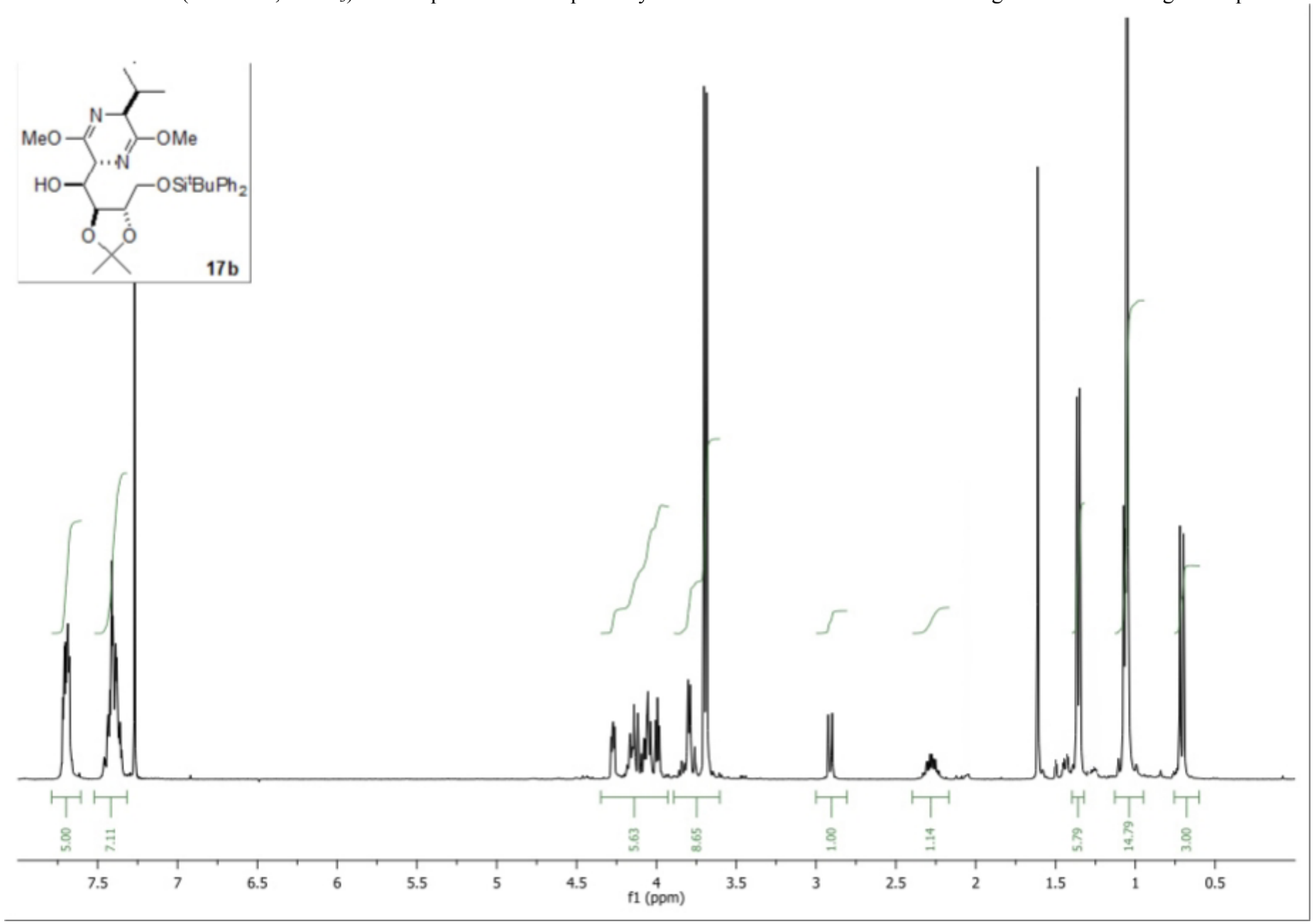

FIGURE S22. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **17c**. Prepared by hydrogenation of **17a** following the general procedure 2.

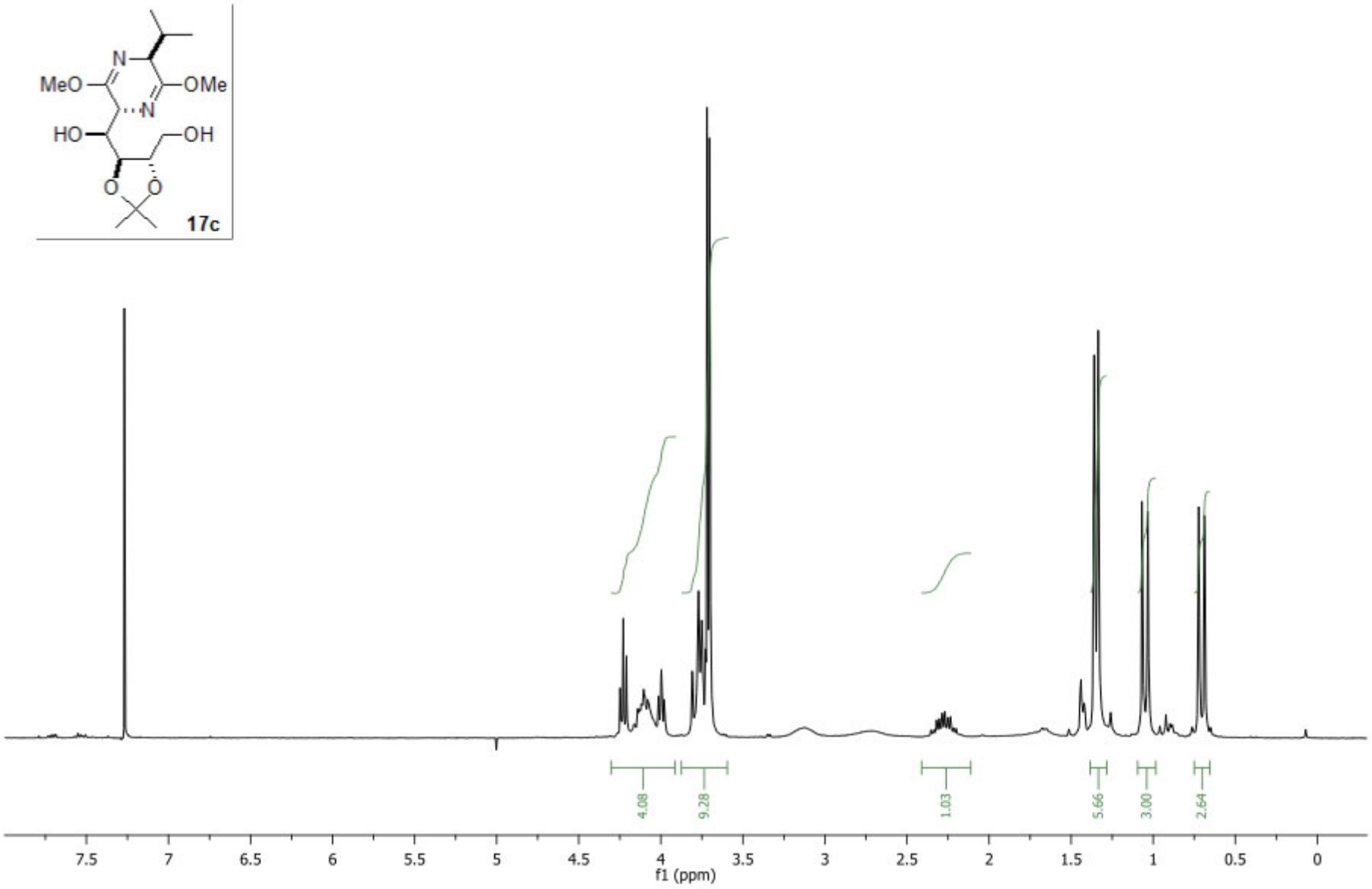

FIGURE S23. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **20a**.

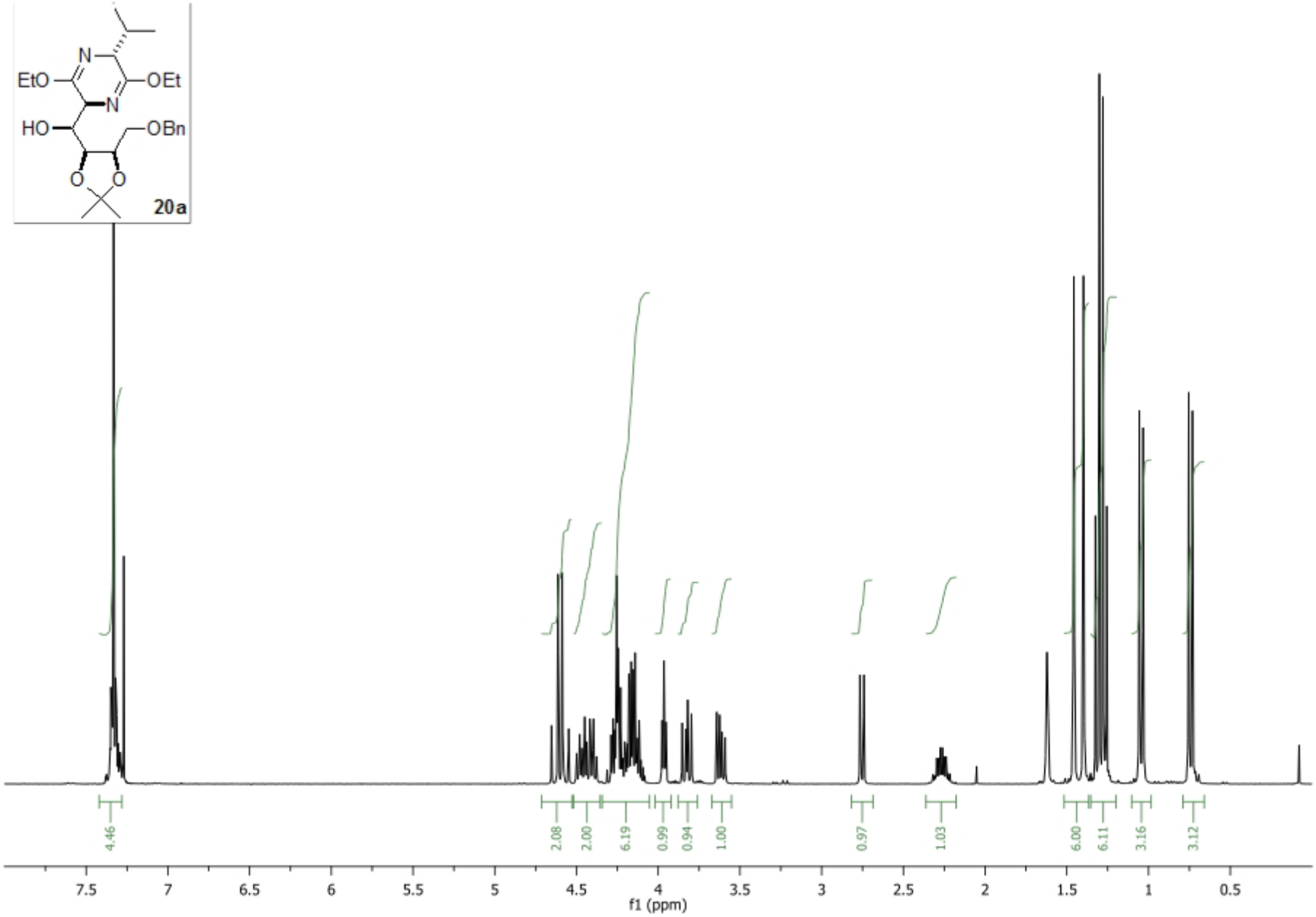

FIGURE S24. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **20c**. Prepared by addition of $SnCl^{+}\mathbf{12}^{-}$ to (*R*,*R*)-**19c** following method B of the general procedure 1.

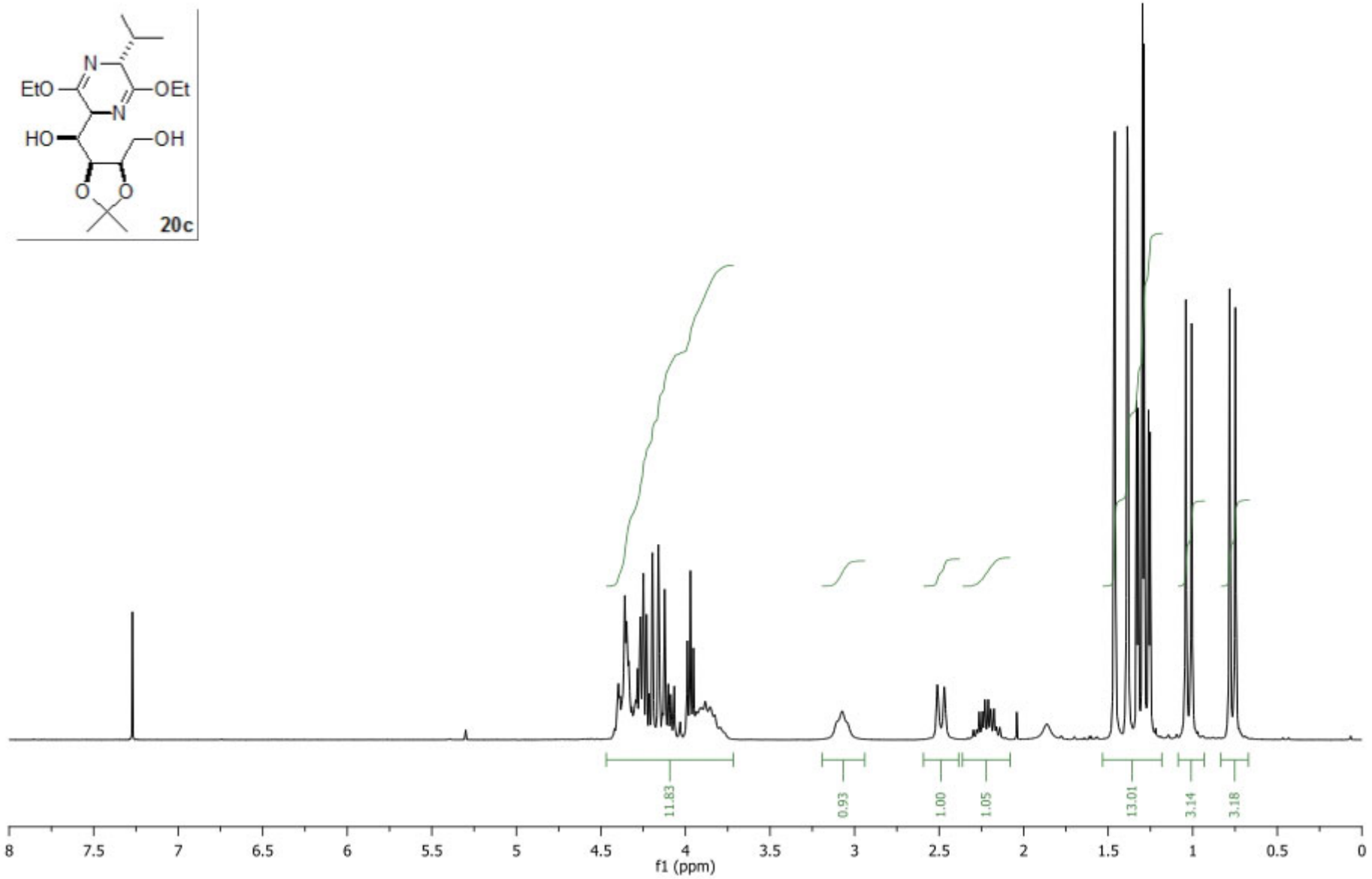

FIGURE S25. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **21a**.

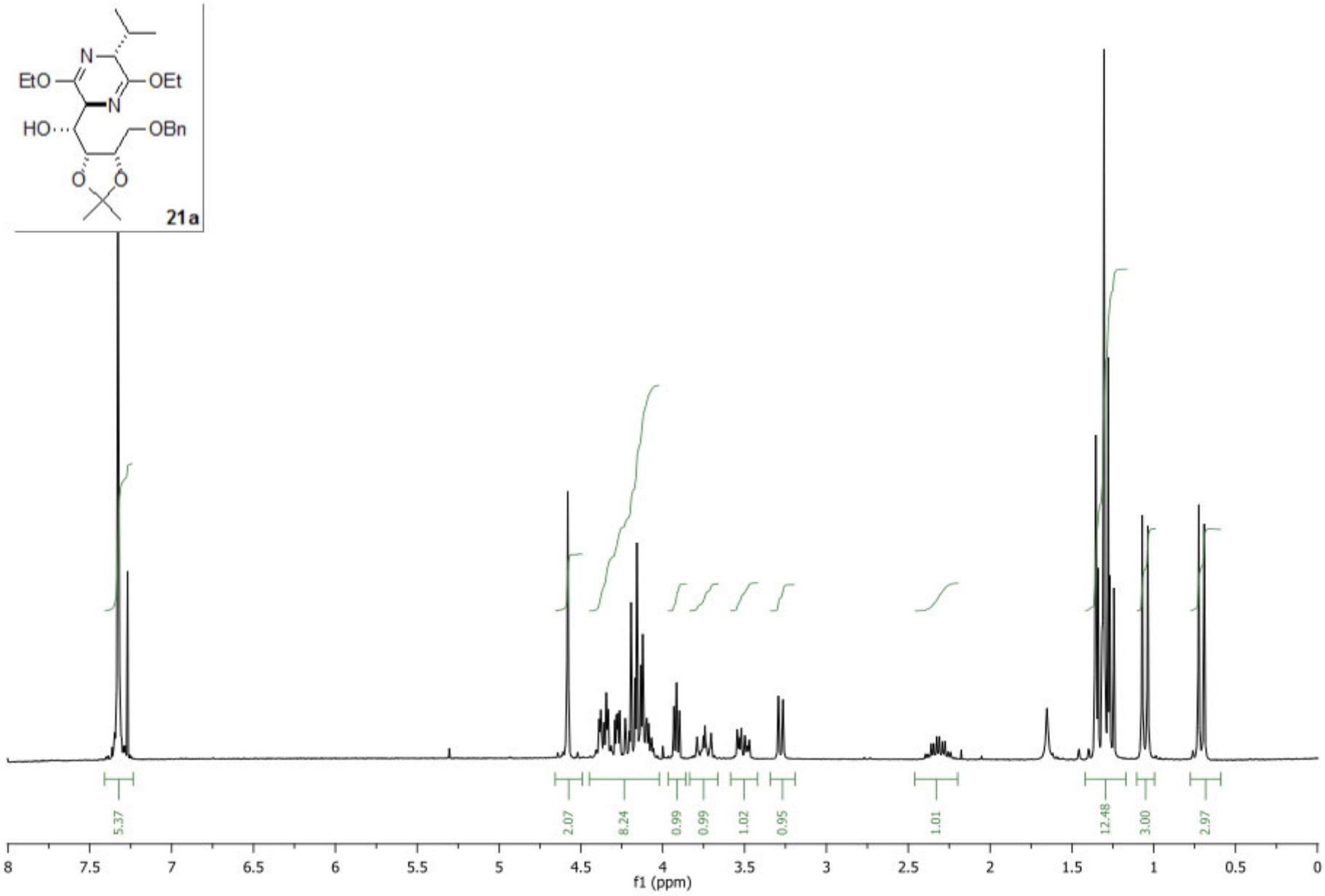

FIGURE S26. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **21c**. Prepared by addition of $SnCl^{+}$**12**$^{-}$ to (*S*,*S*)-**19c** following method B of the general procedure 1.

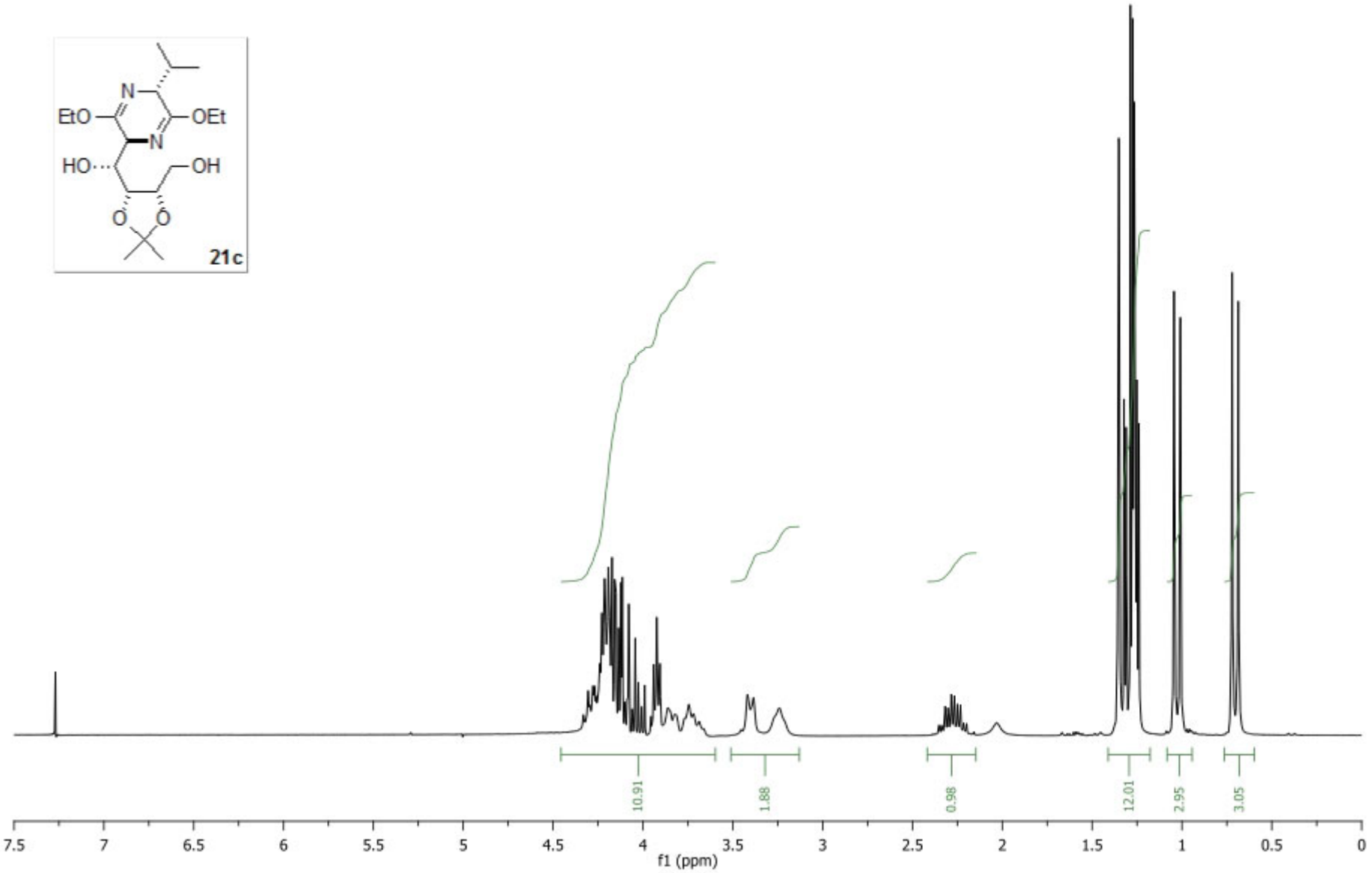

FIGURE S27. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **22a**.

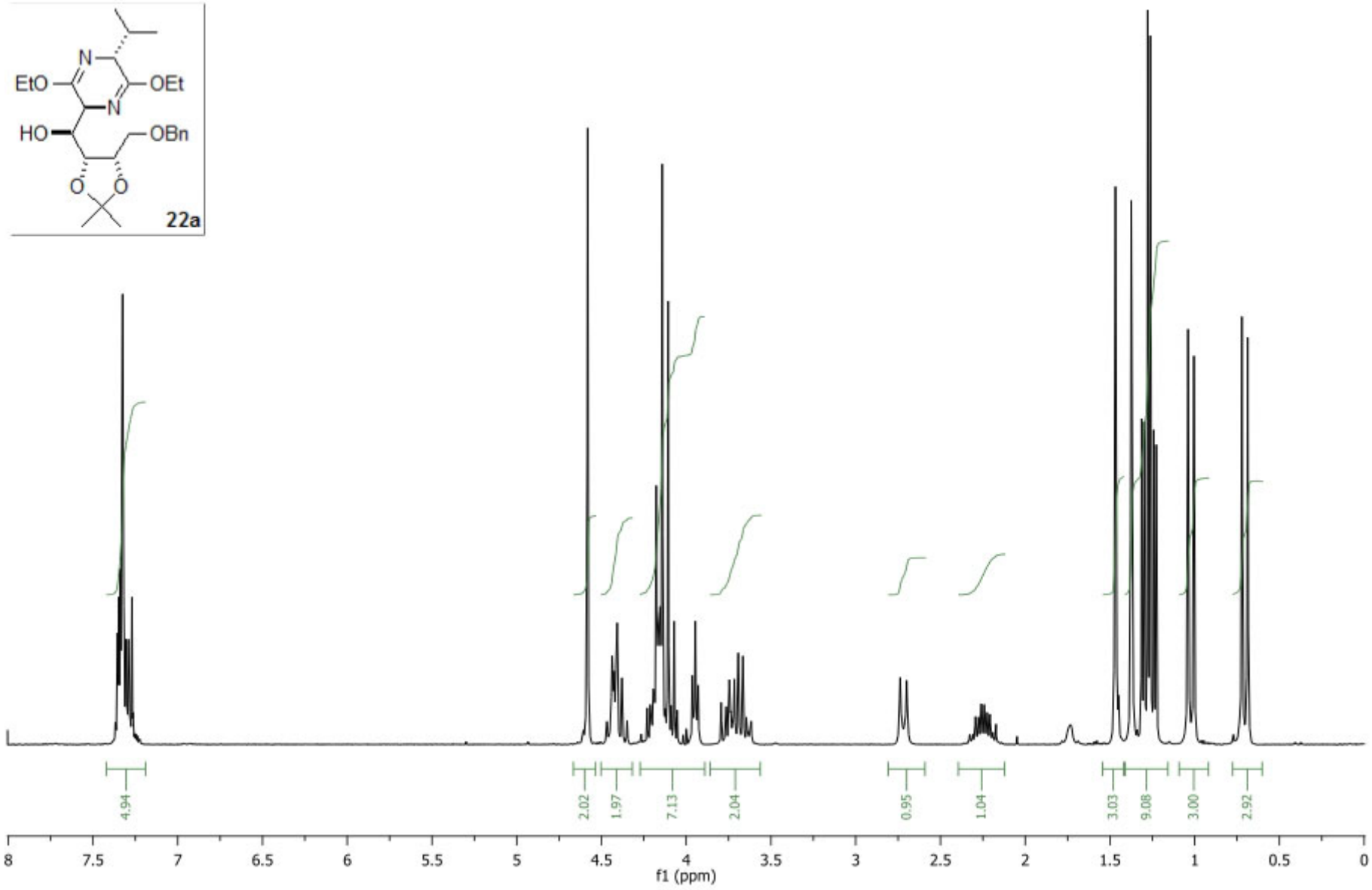

FIGURE S28. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **22c**. Prepared by addition of $(Et_2N)_3Ti^{+}$**12**$^{-}$ to (*S*,*S*)-**19c** following method B of the general procedure 1.

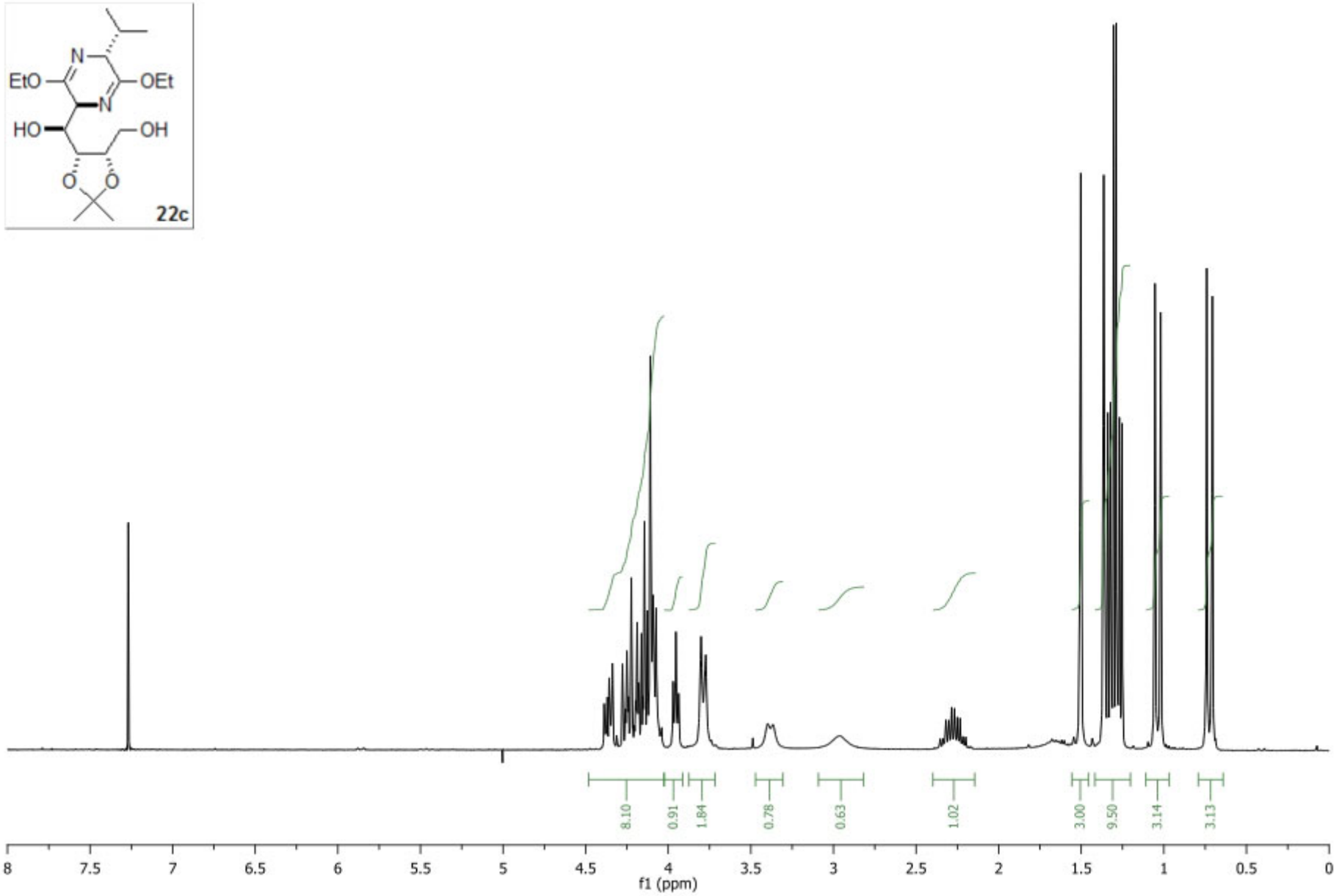

FIGURE S29. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **23a**.

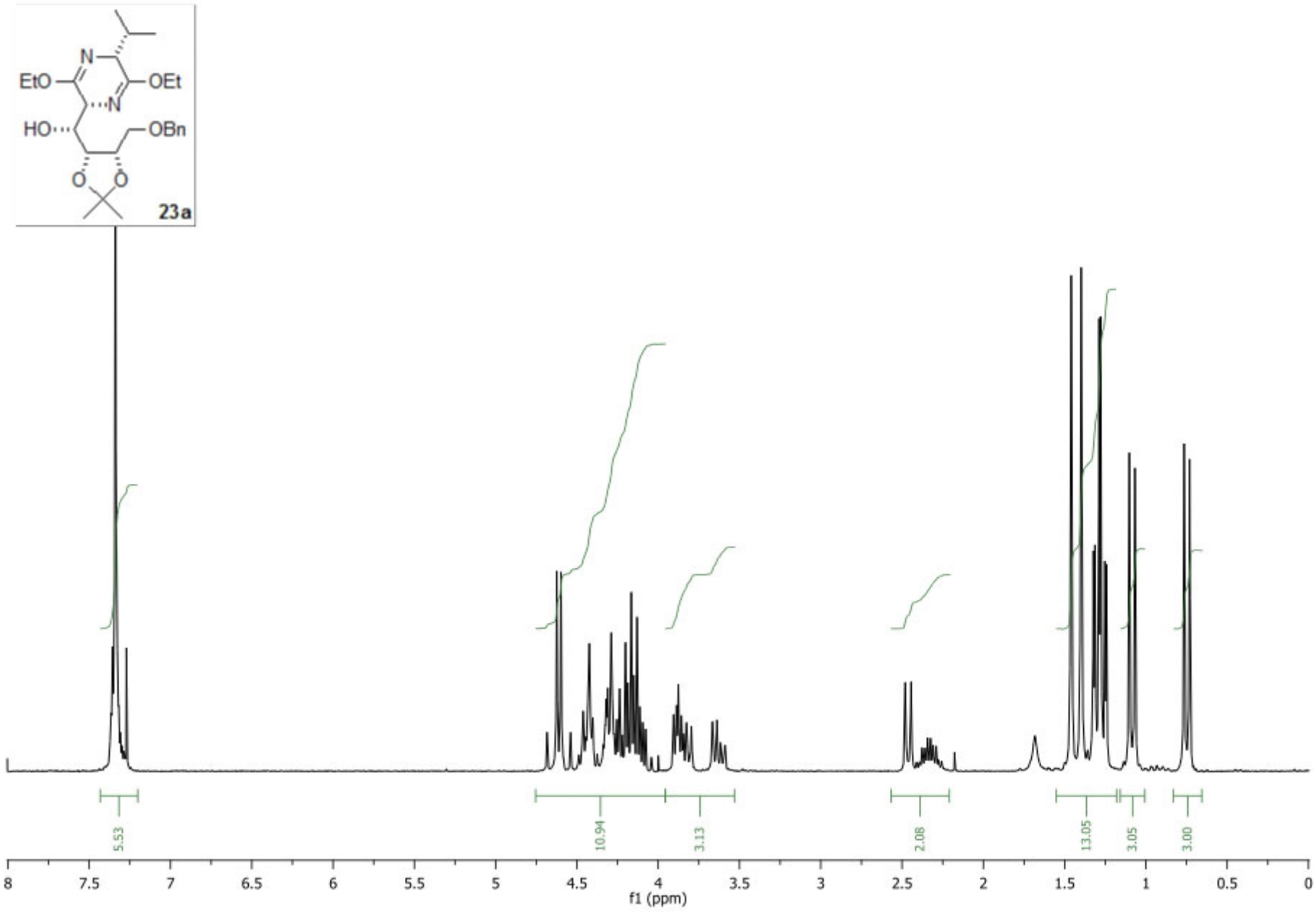

FIGURE S30. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **23c**. Prepared by addition of $MgBr^{+}$**12**$^{-}$ to (*S*,*S*)-**19c** following method B of the general procedure 1.

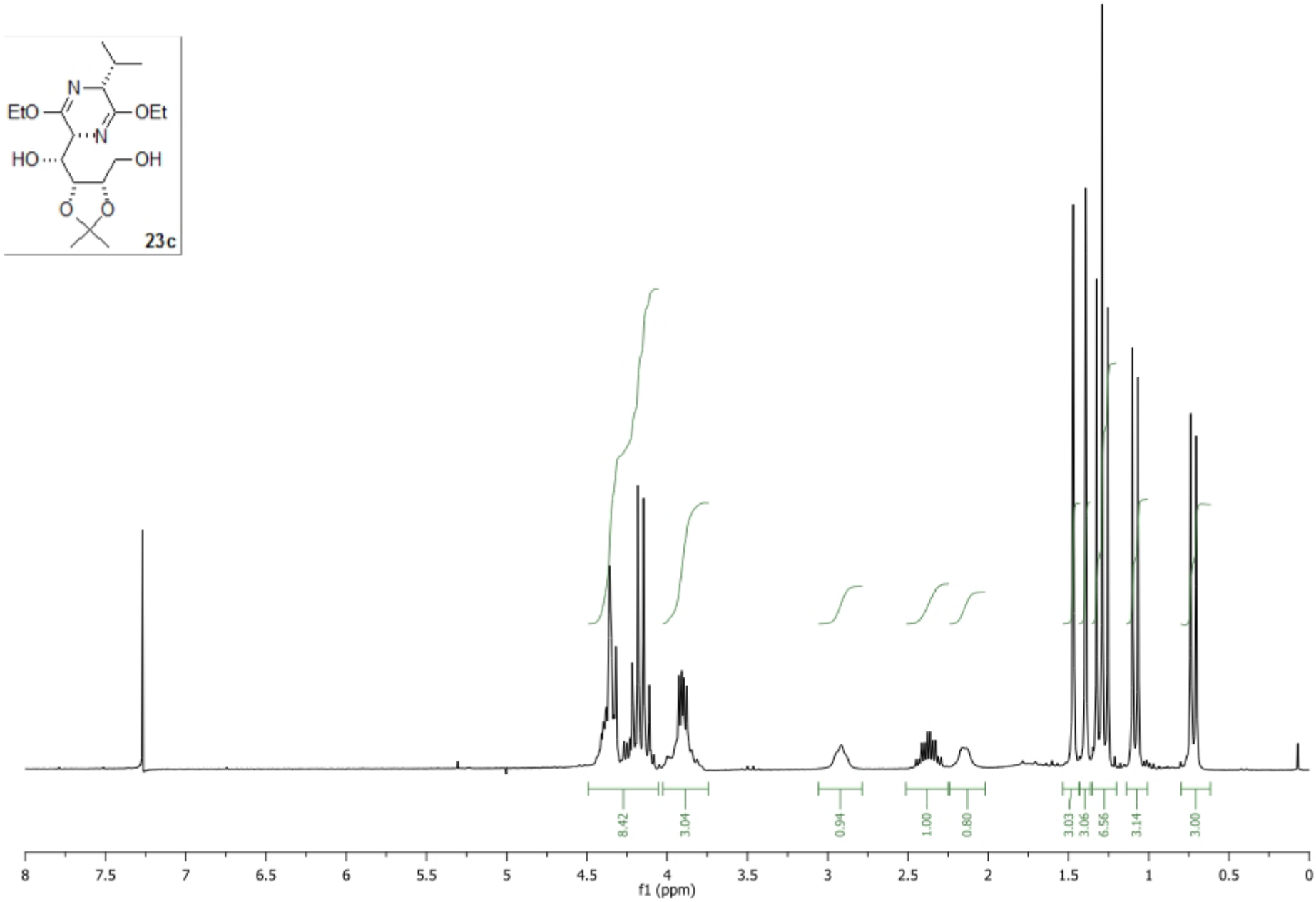

FIGURE S31. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **24b**.

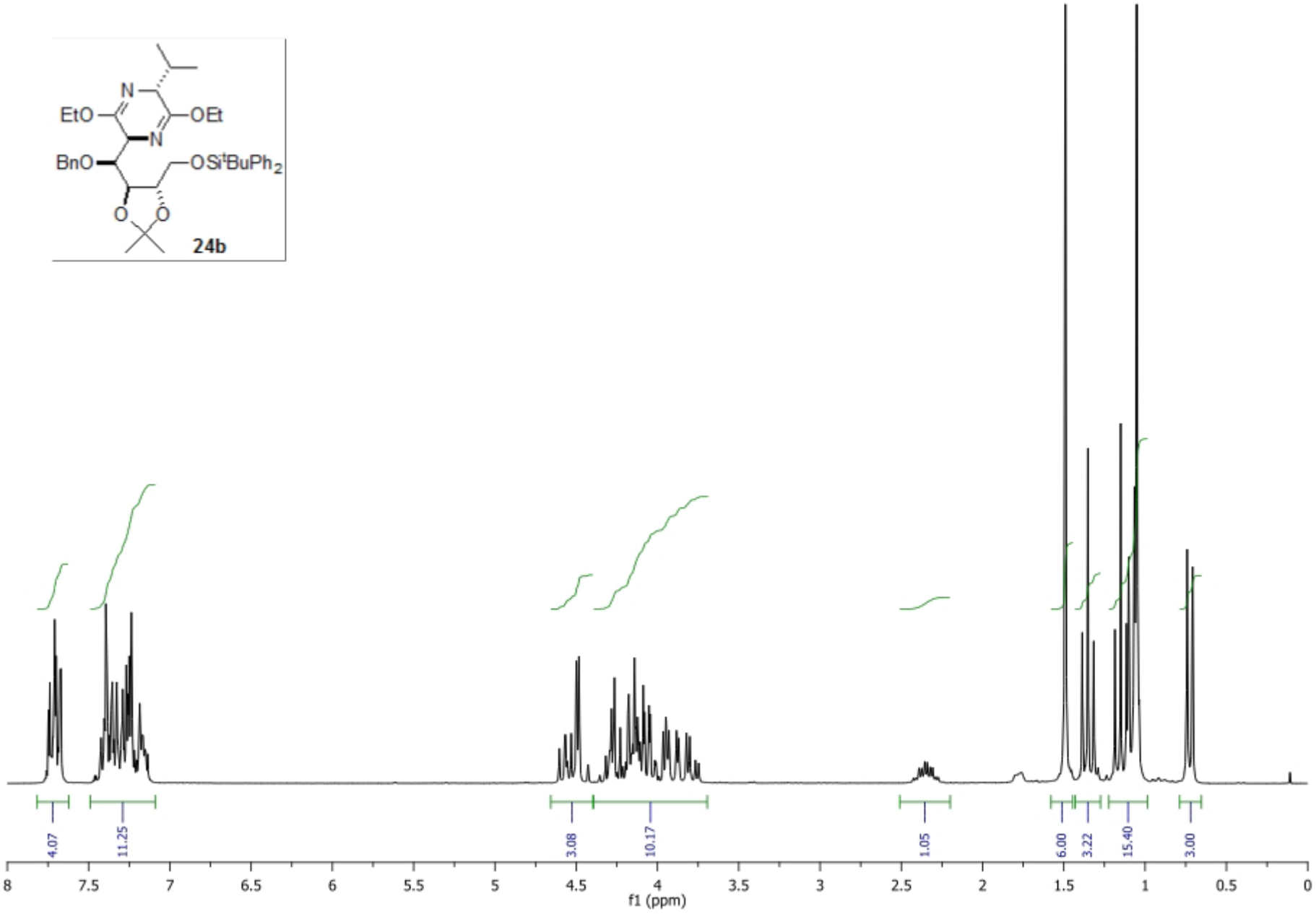

FIGURE S32. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **24c**.

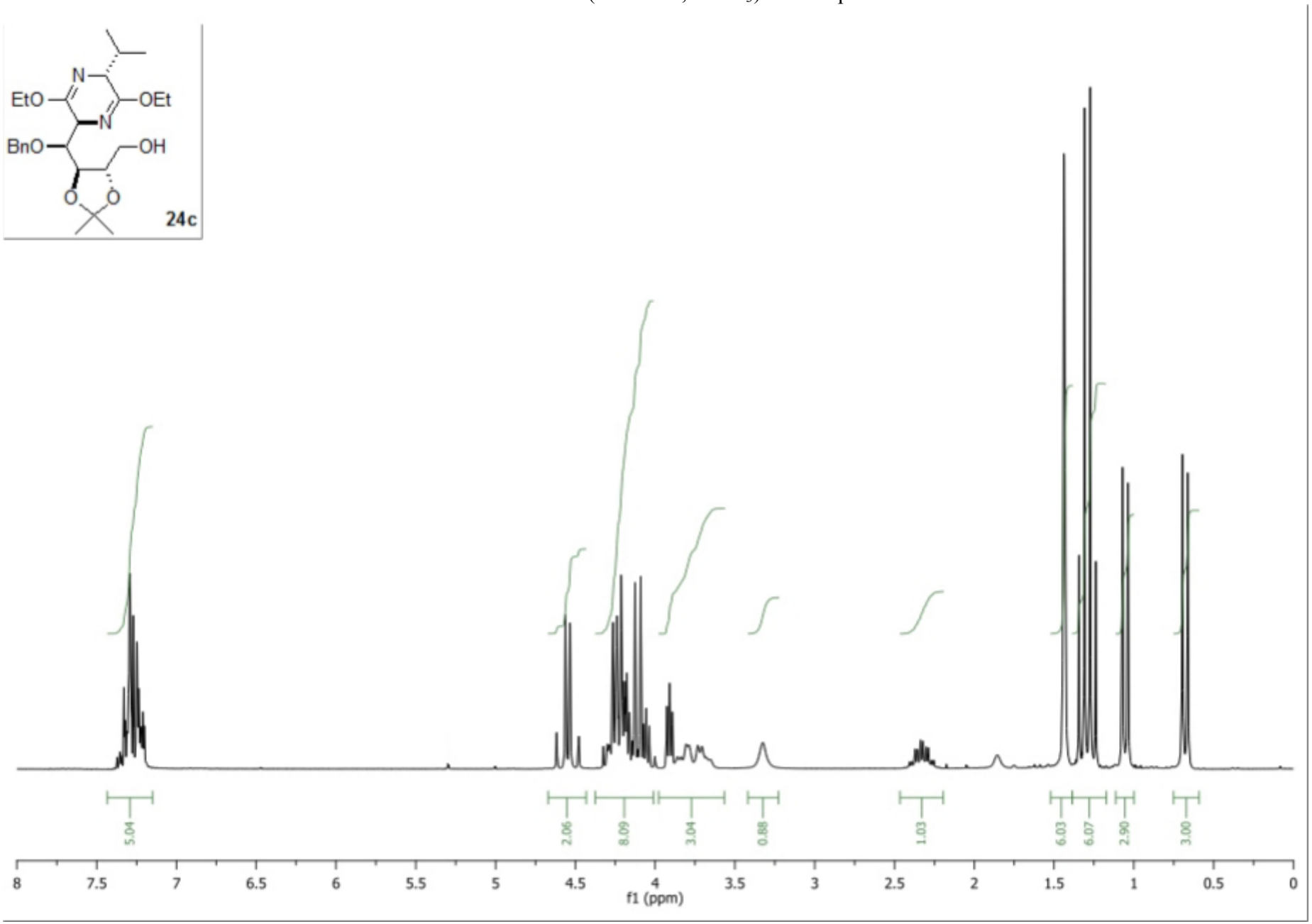

FIGURE S33. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **24d**.

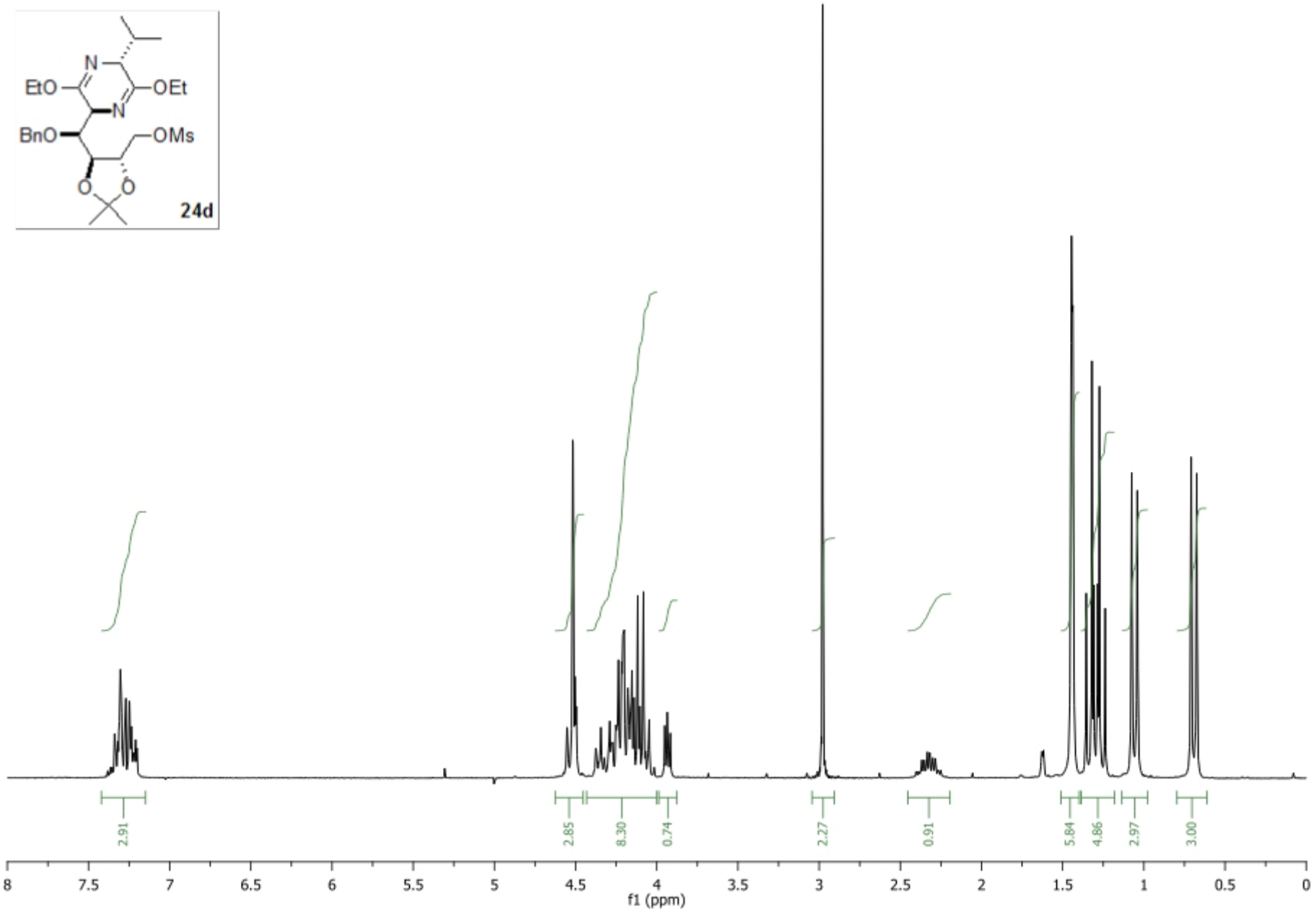

FIGURE S34. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **25b**.

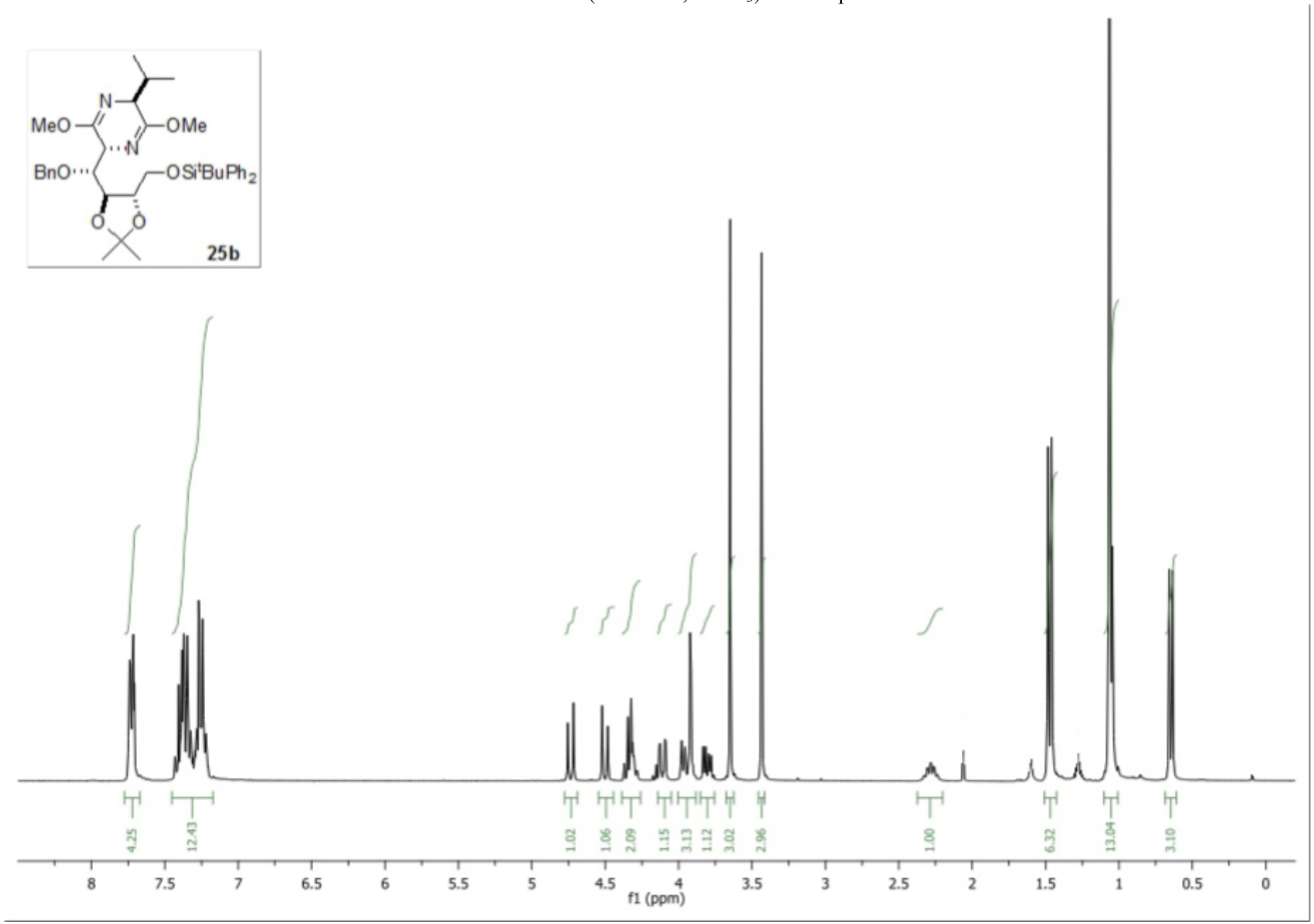

FIGURE S35. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **25c**.

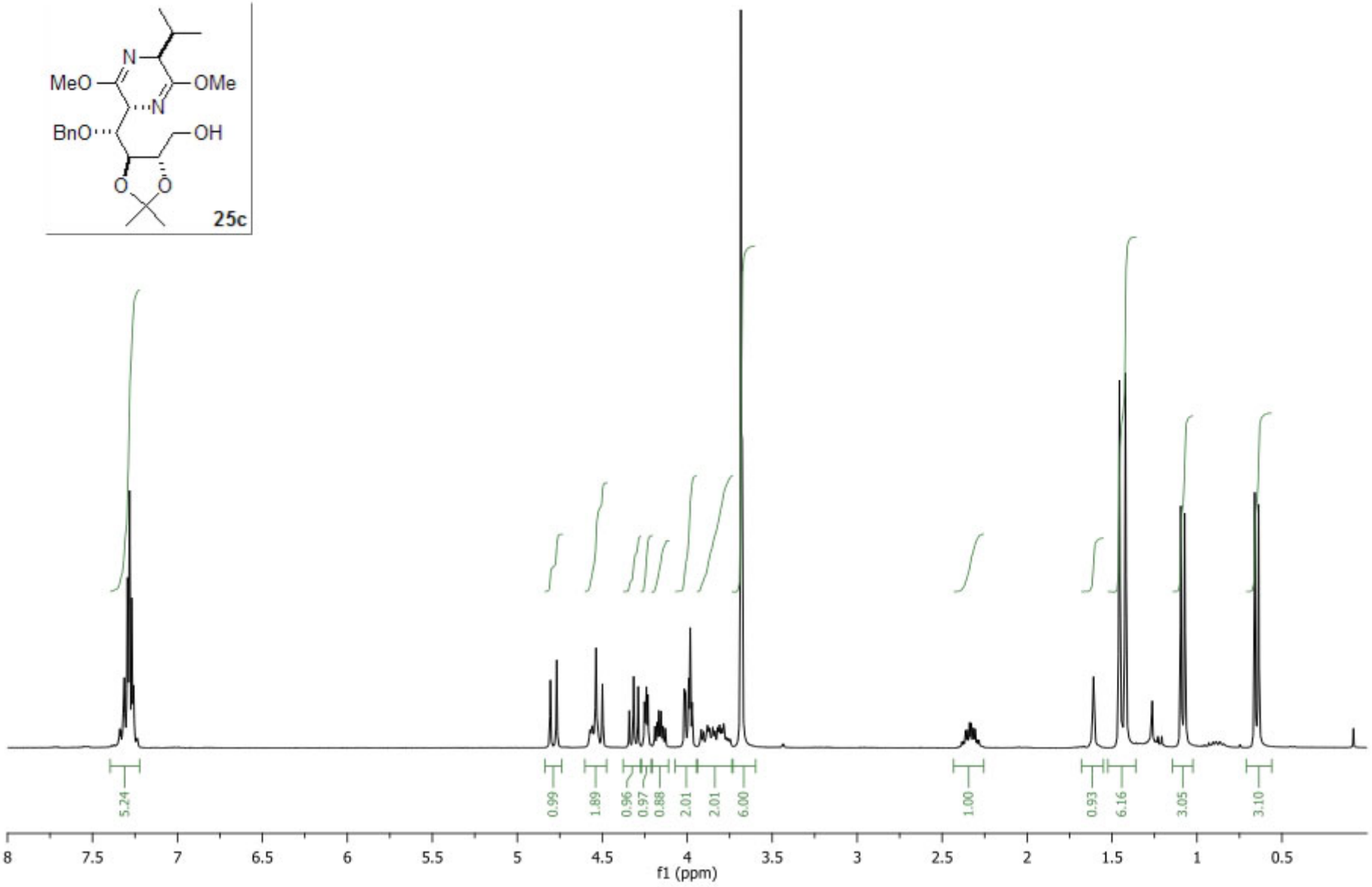

FIGURE S36. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **25d**.

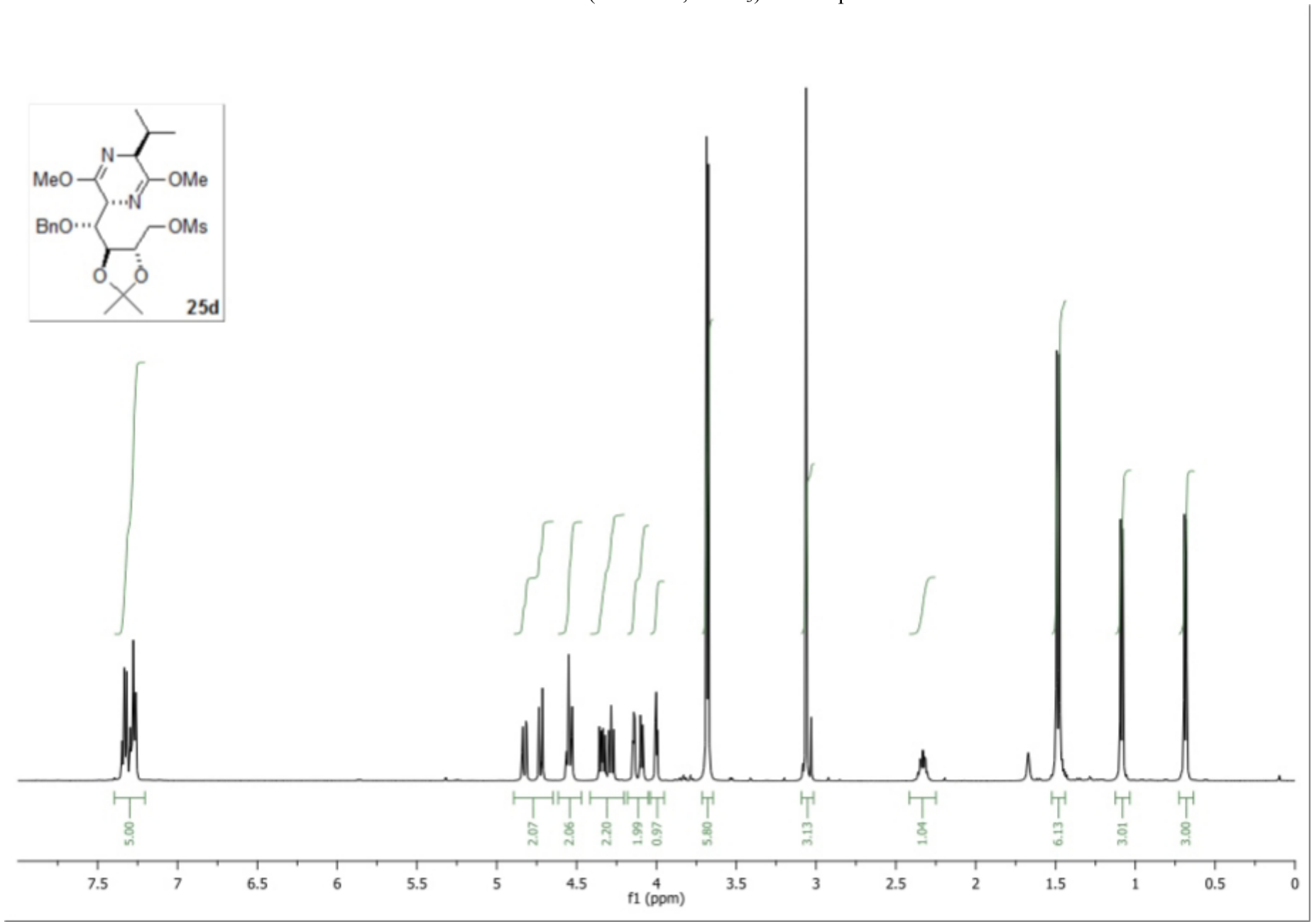

FIGURE S37. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **26b**.

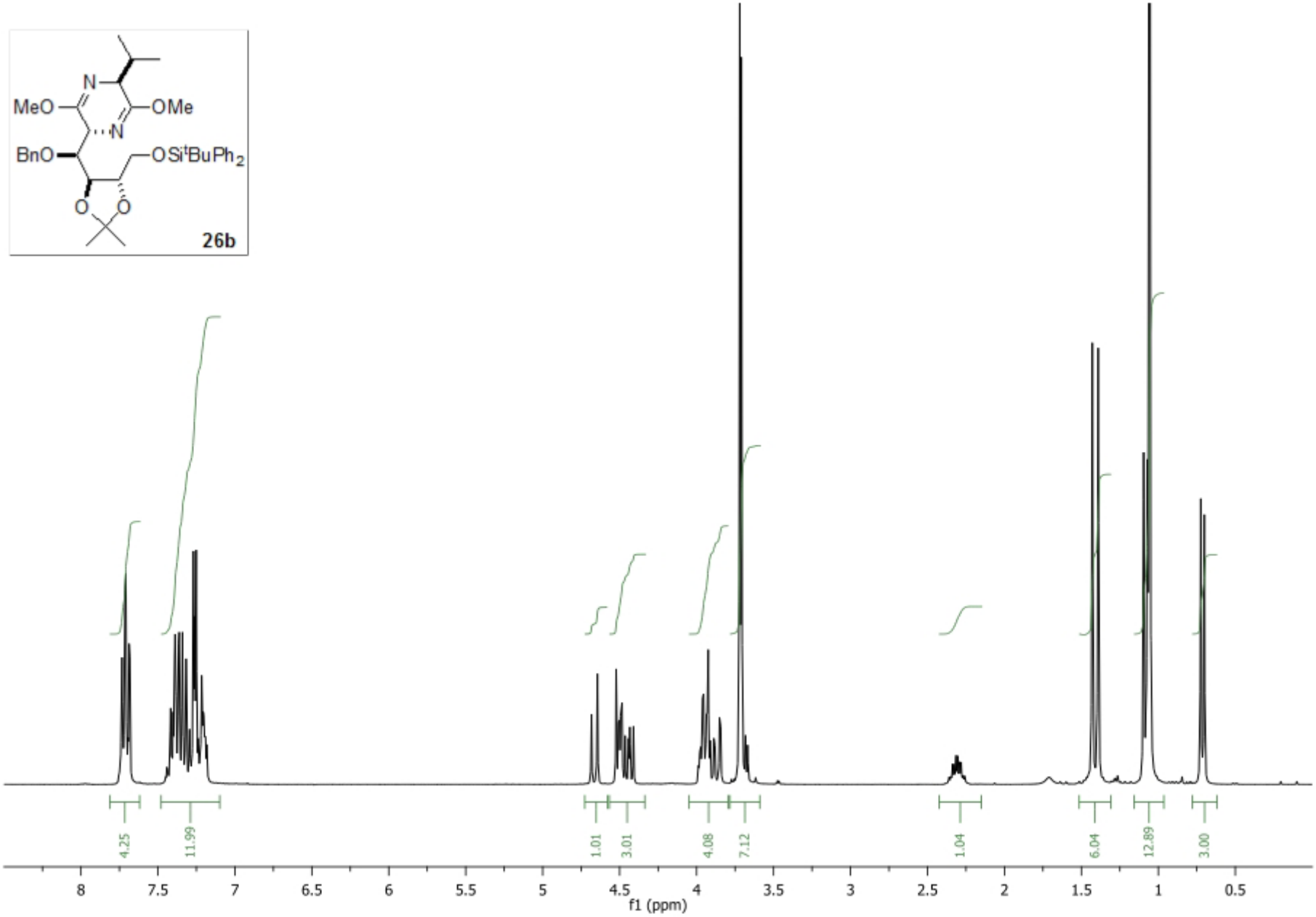

FIGURE S38. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **26c**.

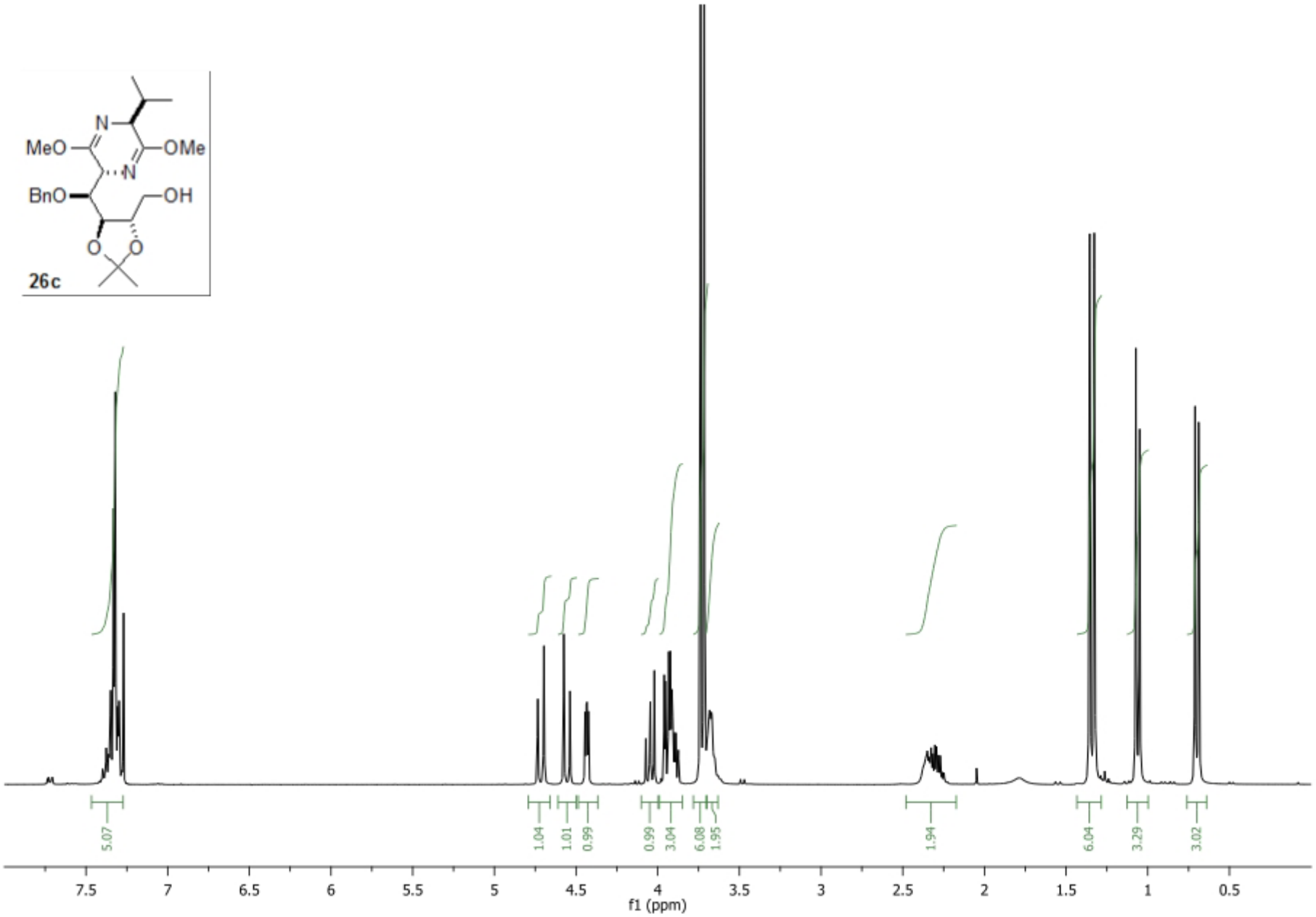

FIGURE S39. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **26d**.

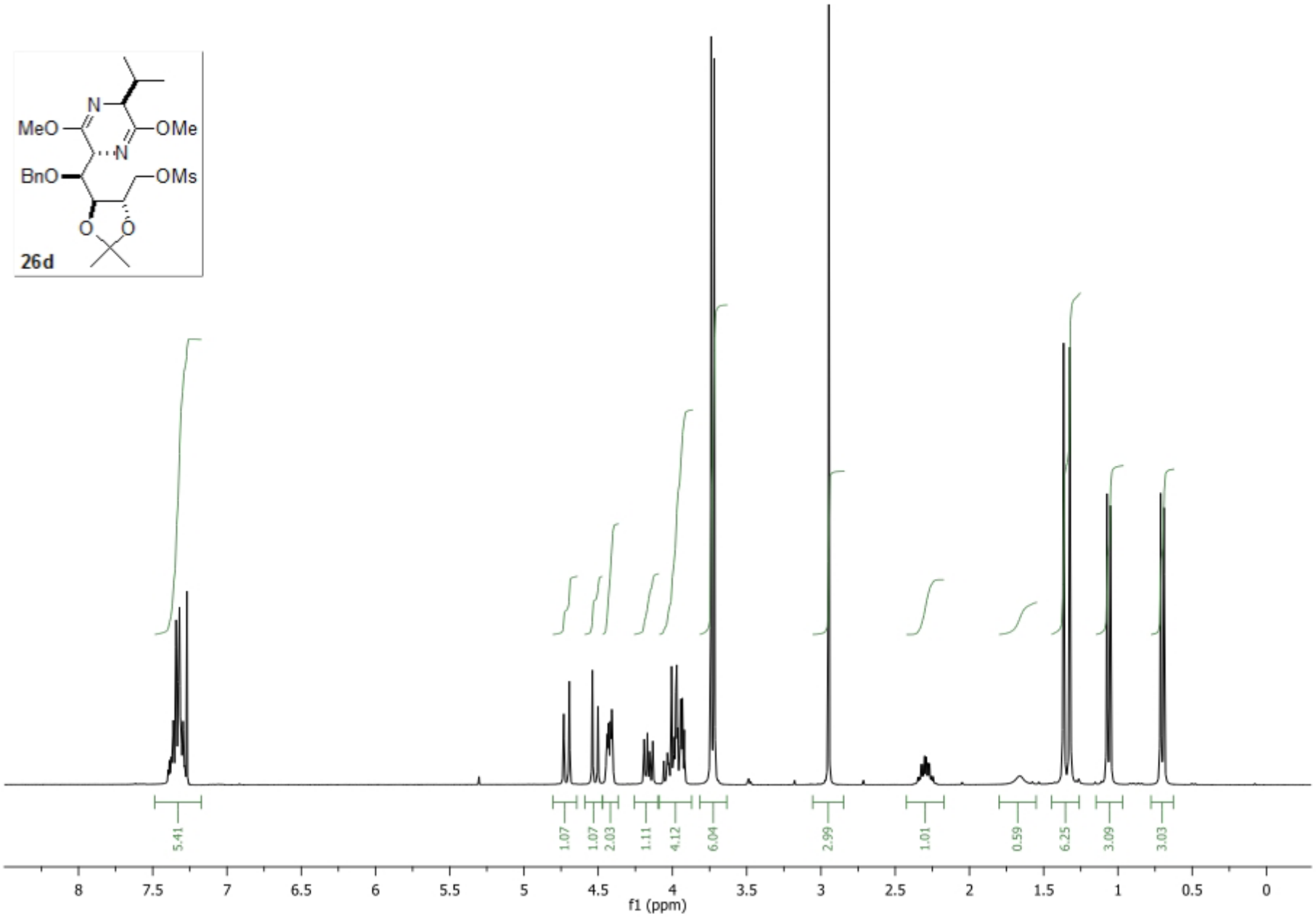

FIGURE S40. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **27**.

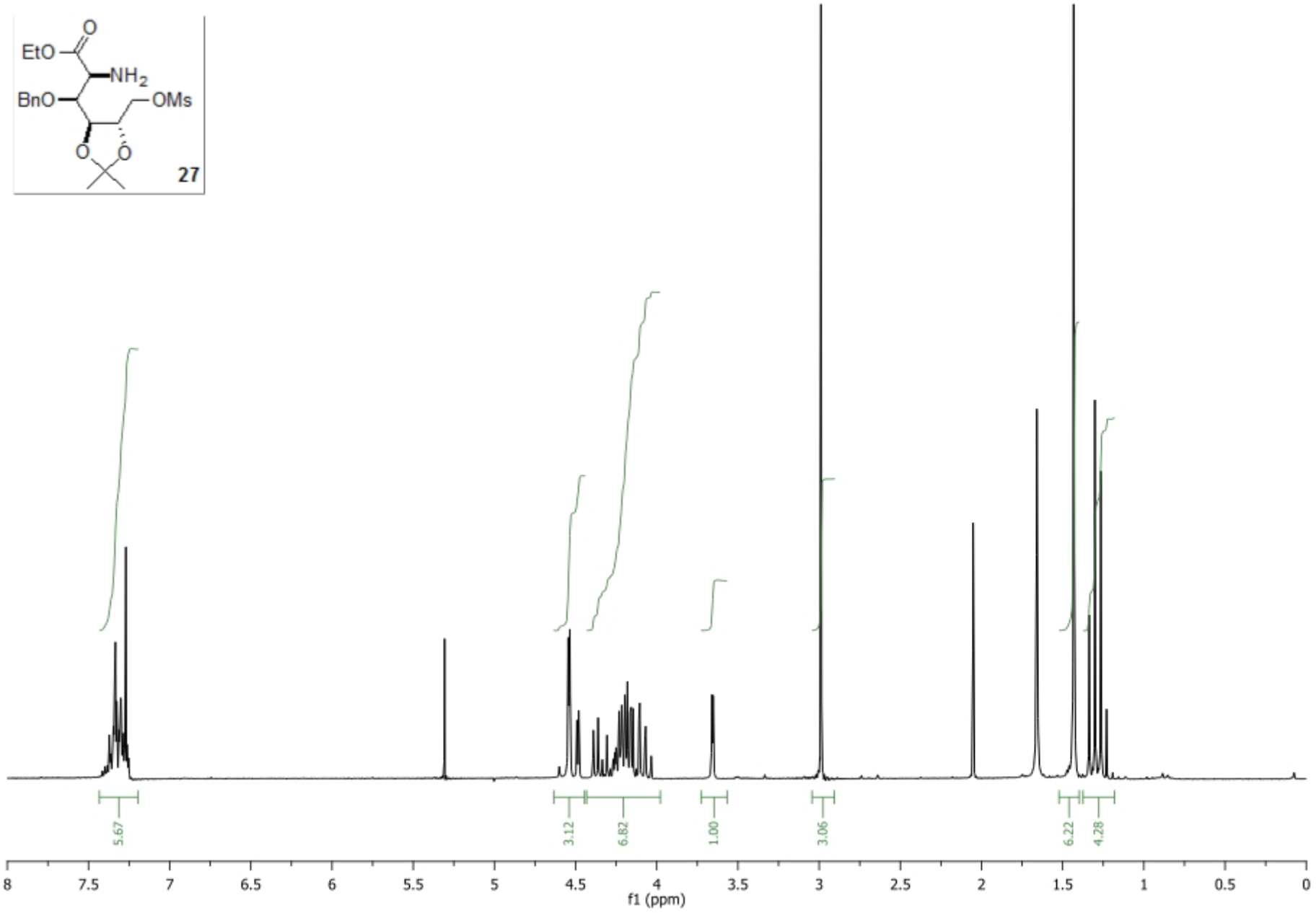

FIGURE S41. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **28**.

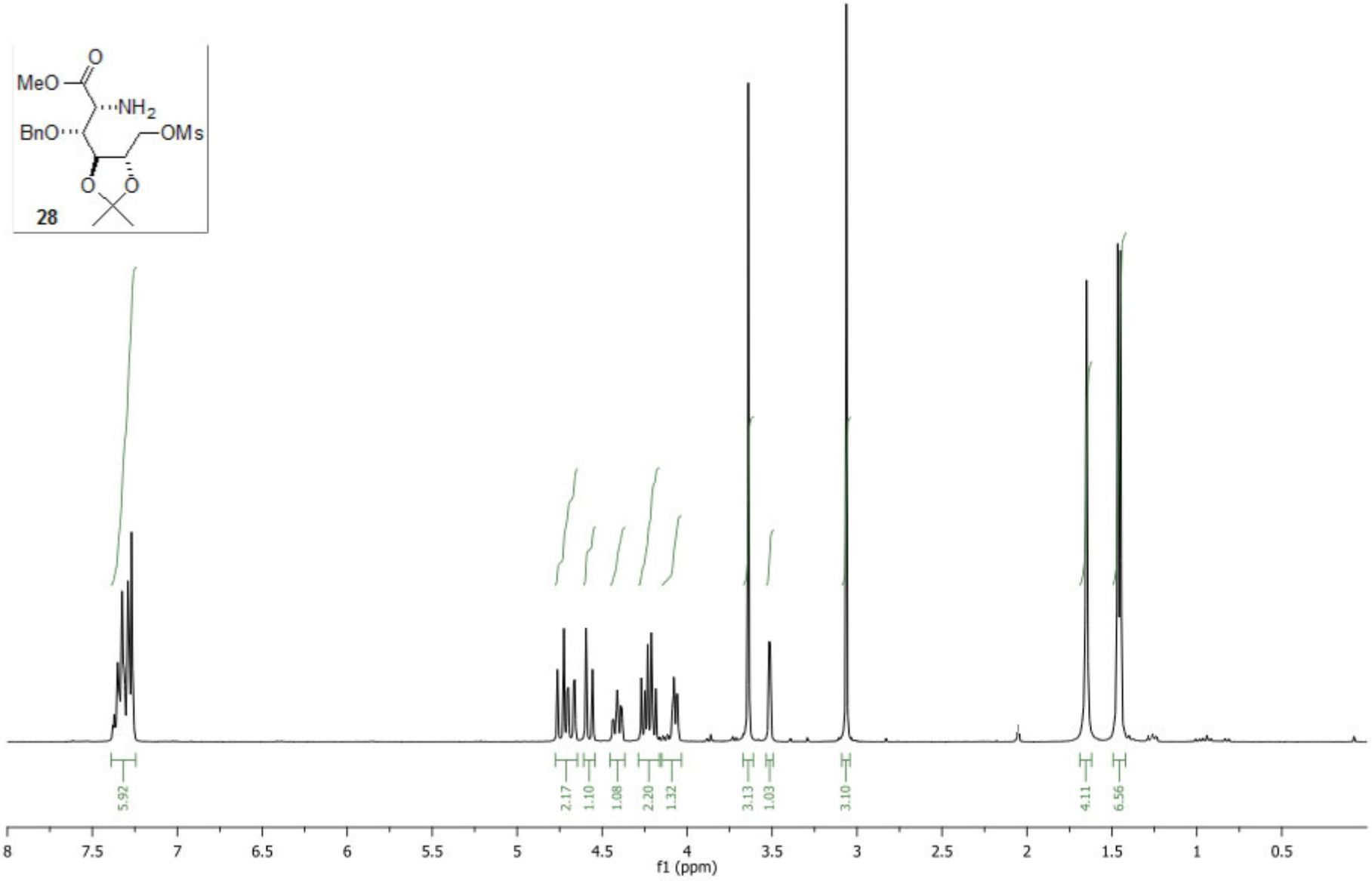

FIGURE S42. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **29**.

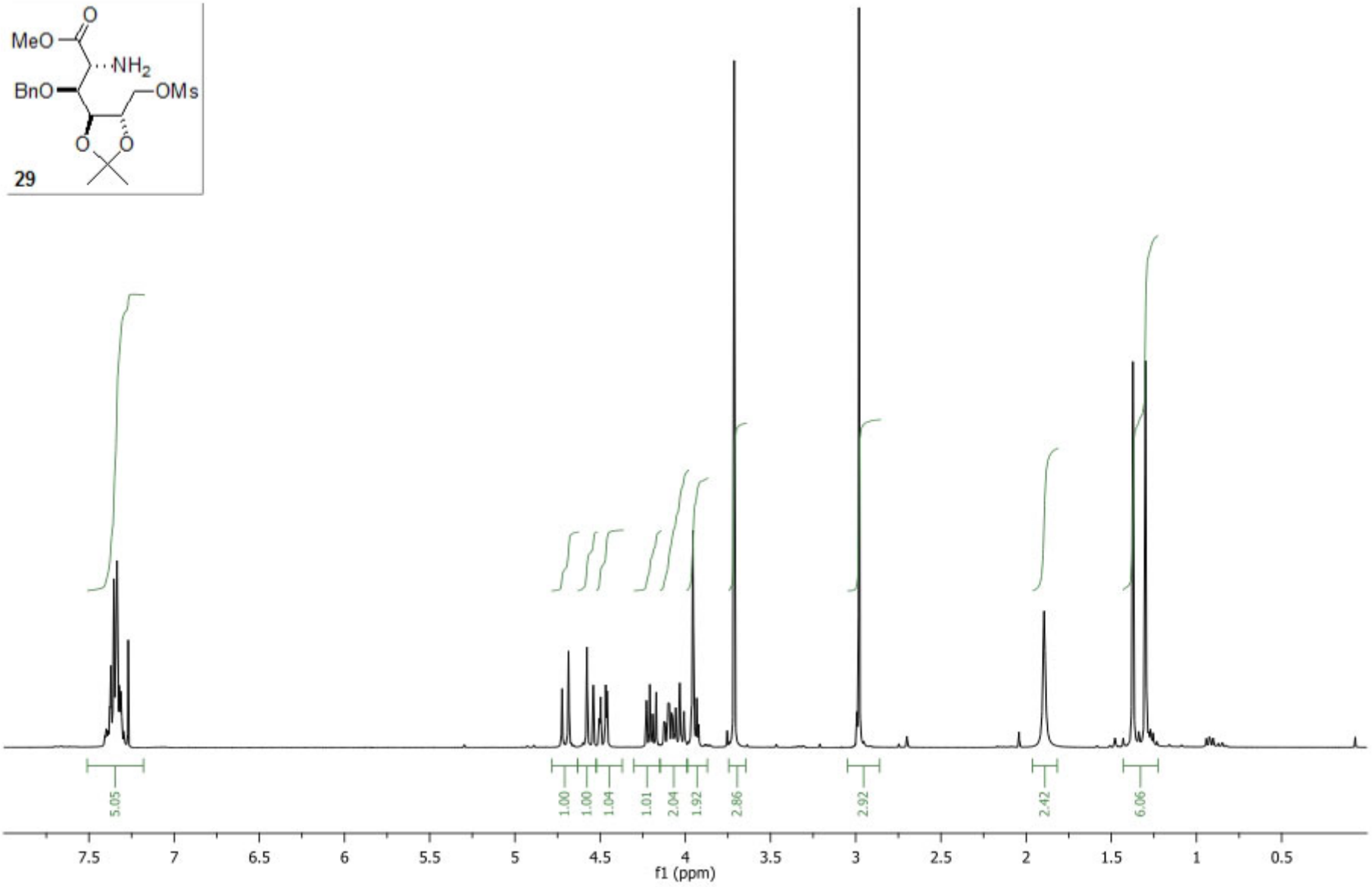

FIGURE S43. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **30**.

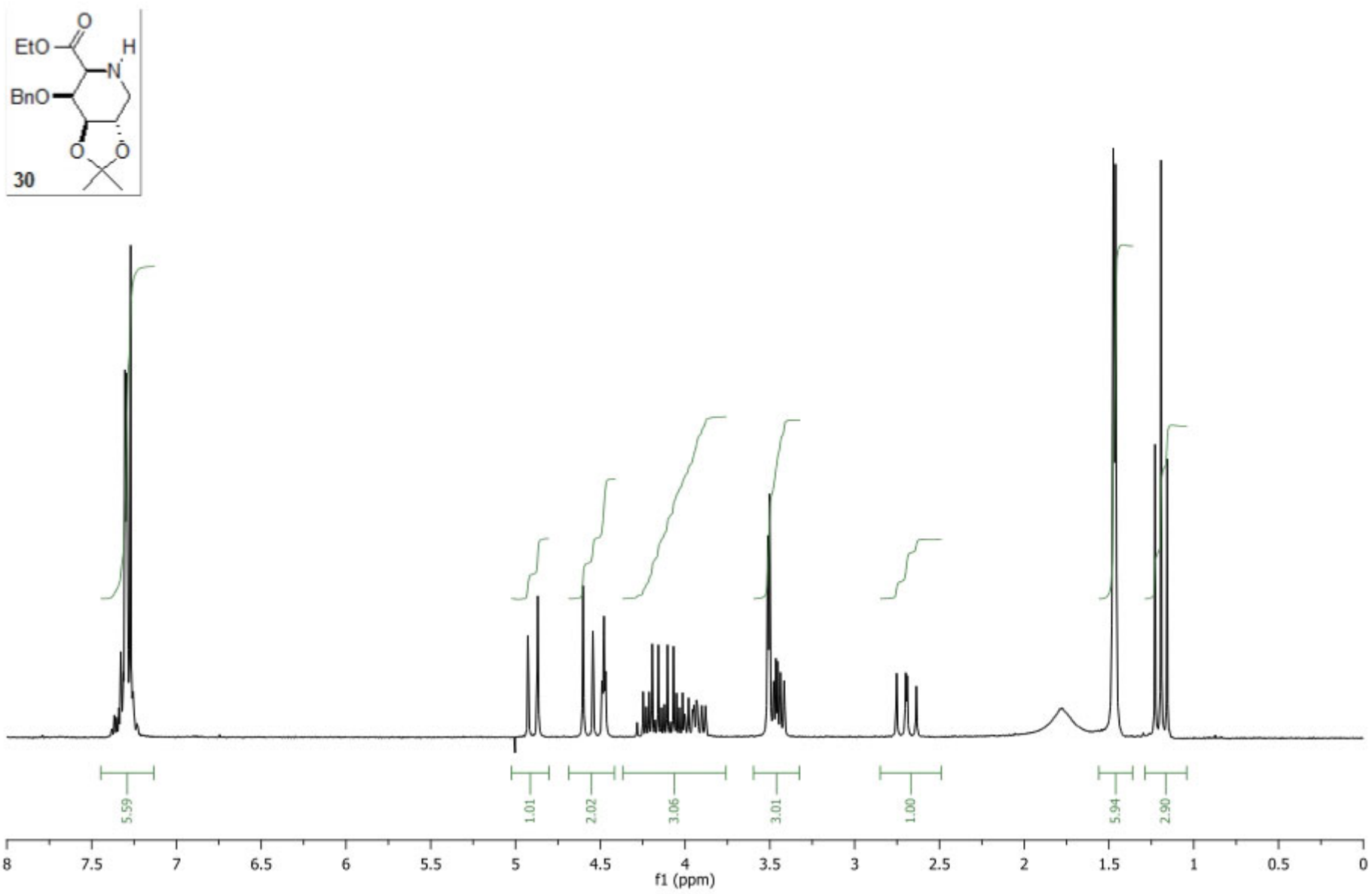

FIGURE S44. ^{1}H NMR (500 MHz, $CDCl_3$) for compound **31**.

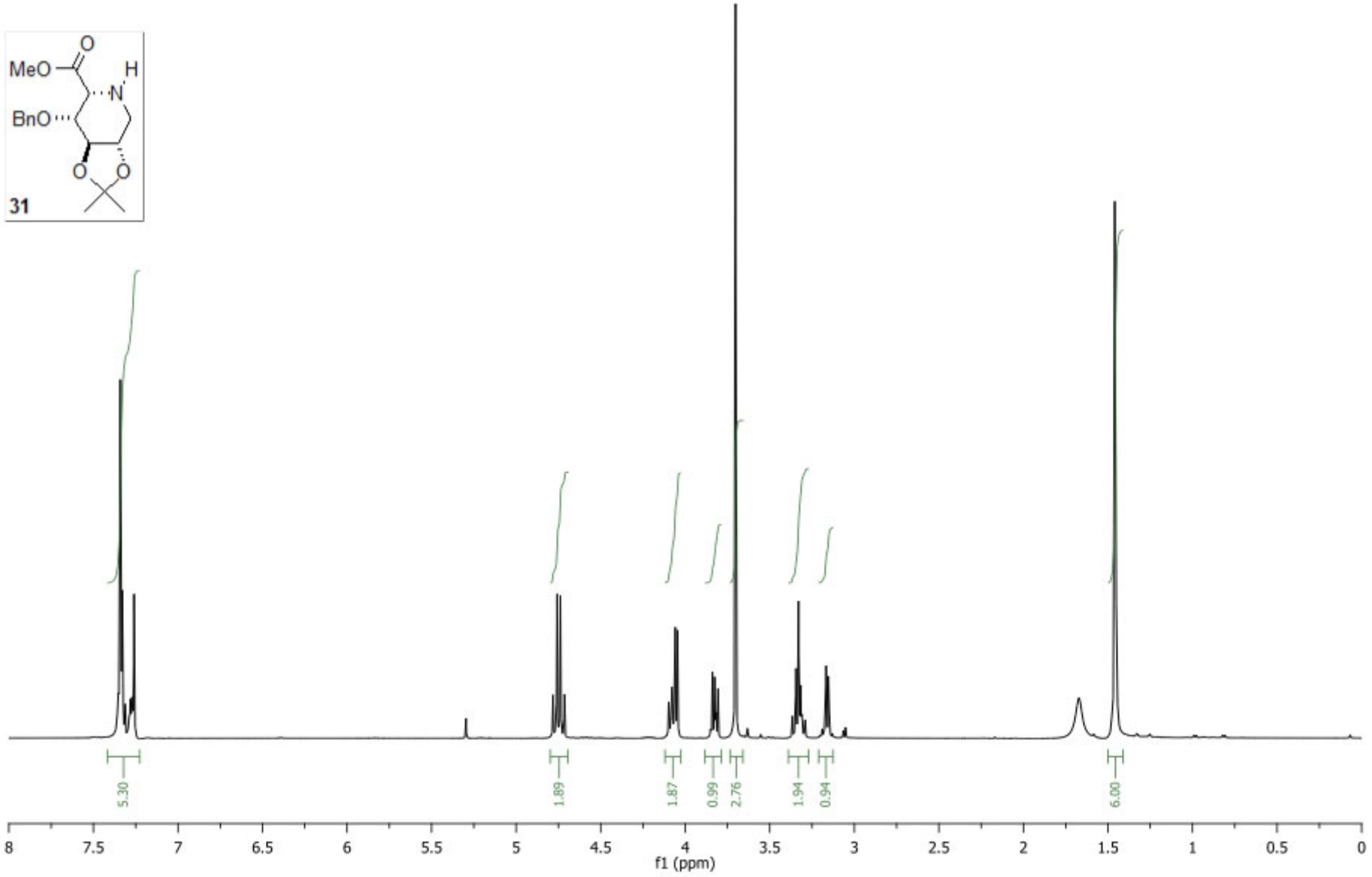

FIGURE S45. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **32**.

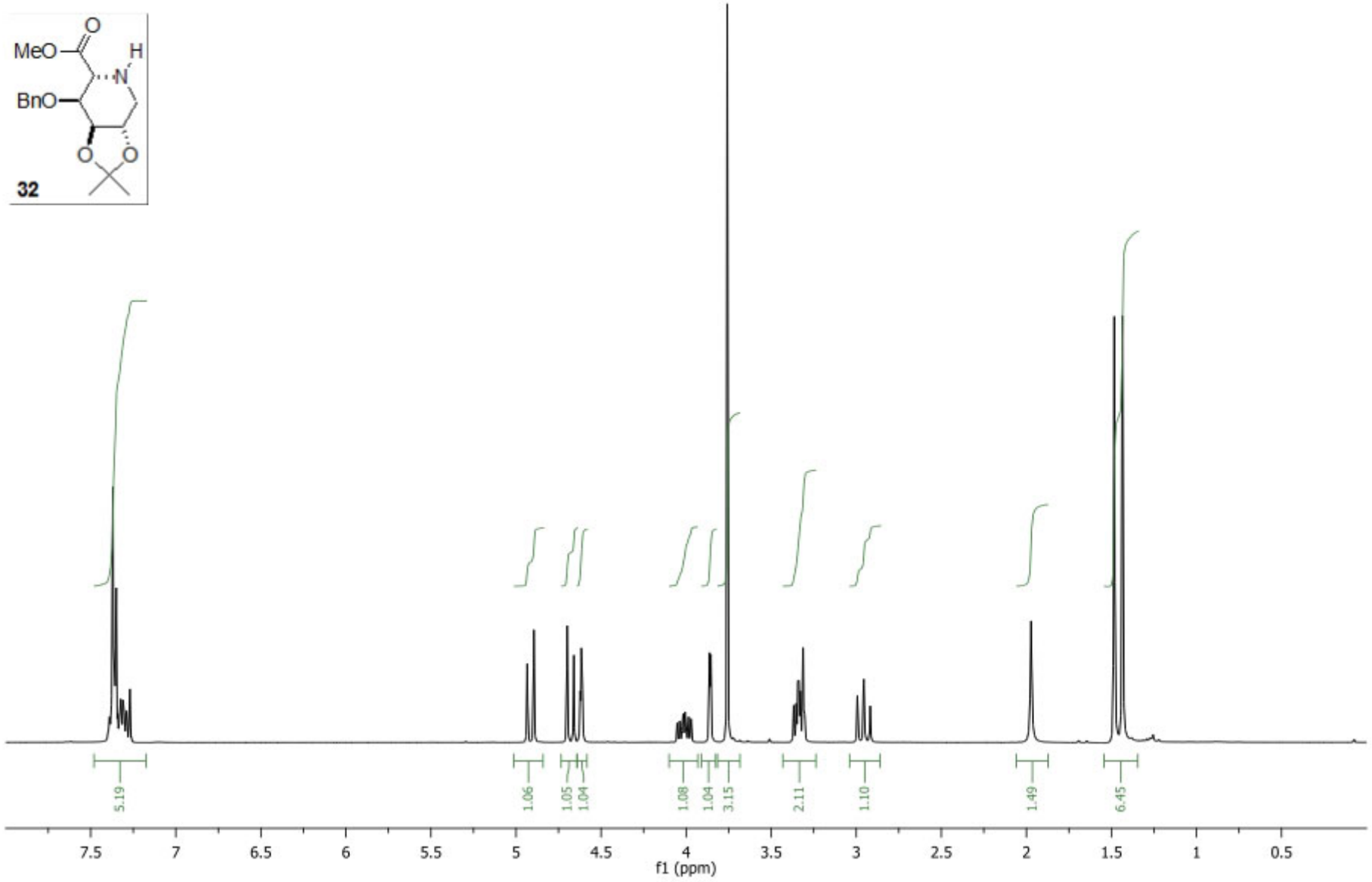

FIGURE S46. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **33**.

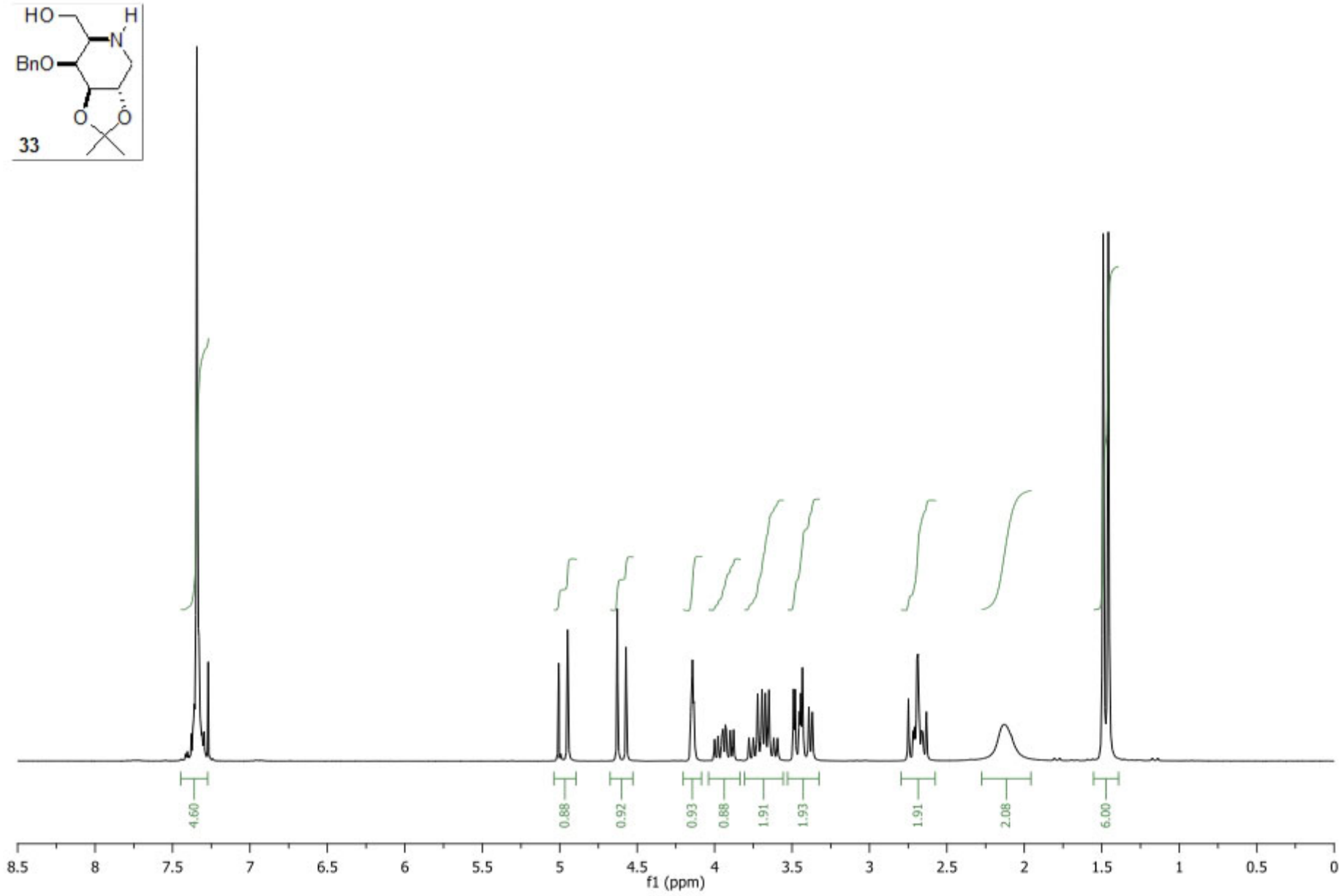

FIGURE S47. ^{1}H NMR (500 MHz, $CDCl_3$) for compound **34**.

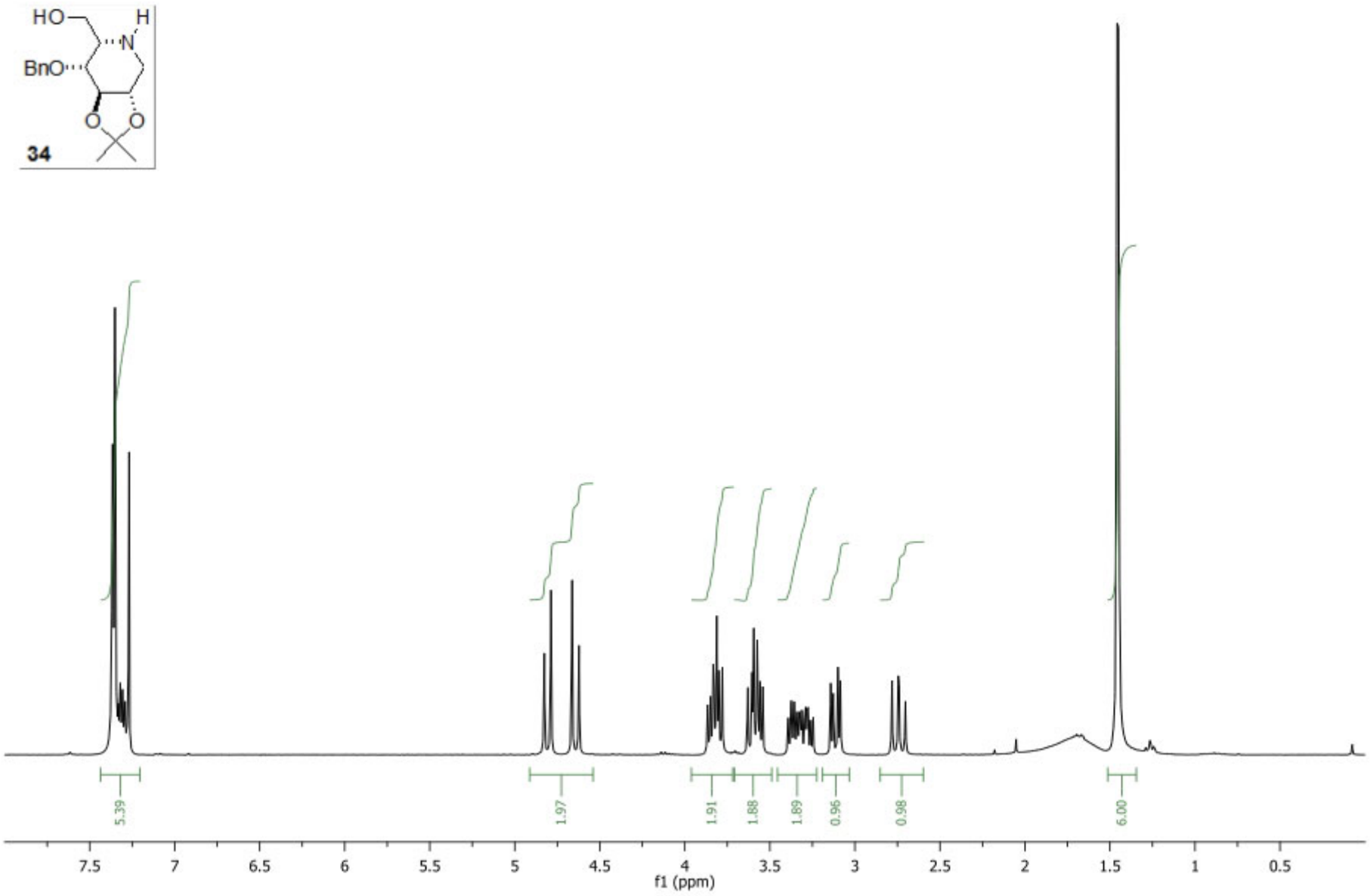

FIGURE S48. ^{1}H NMR (300 MHz, $CDCl_3$) for compound **35**.

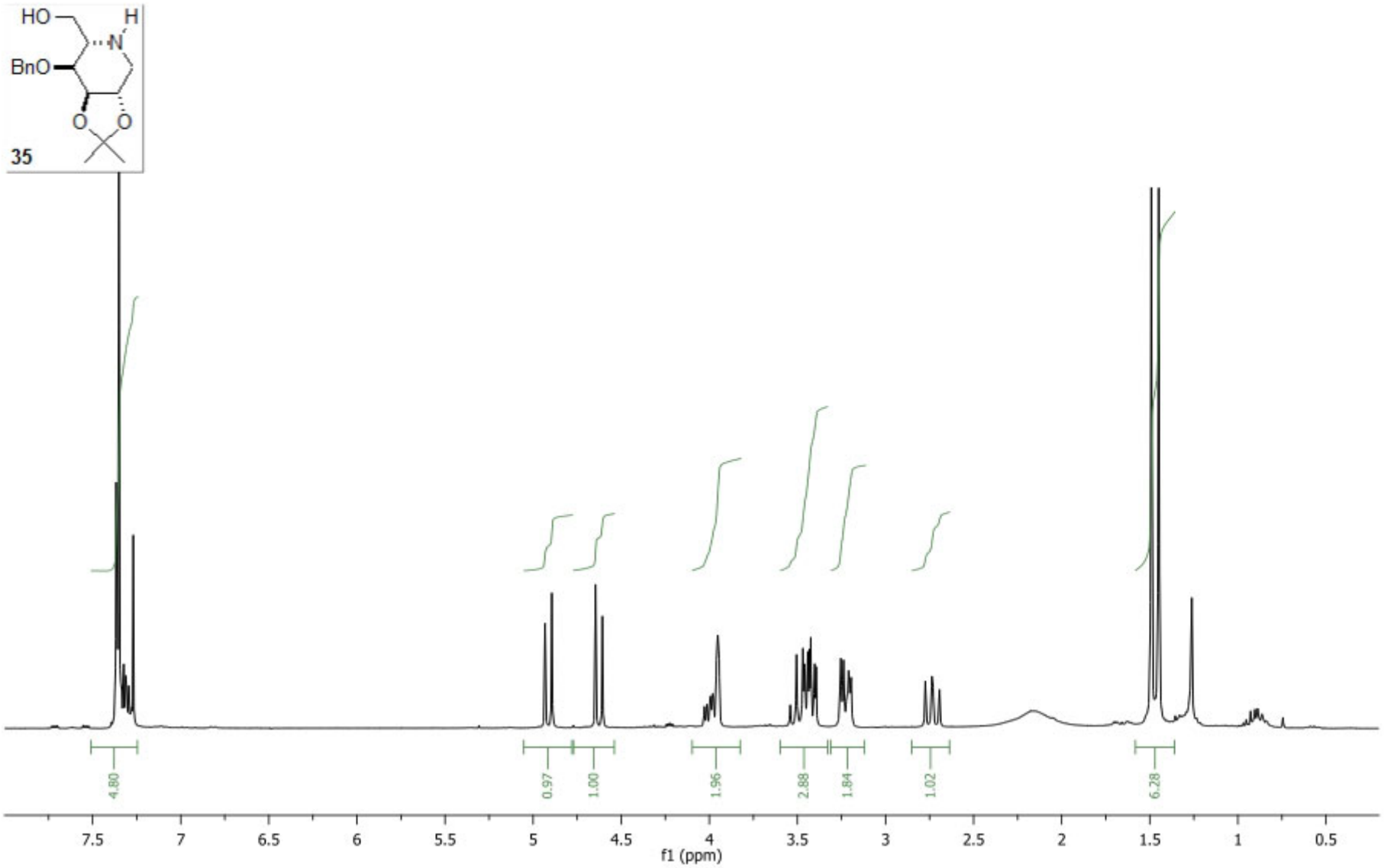

FIGURE S49. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **36**•HCl.

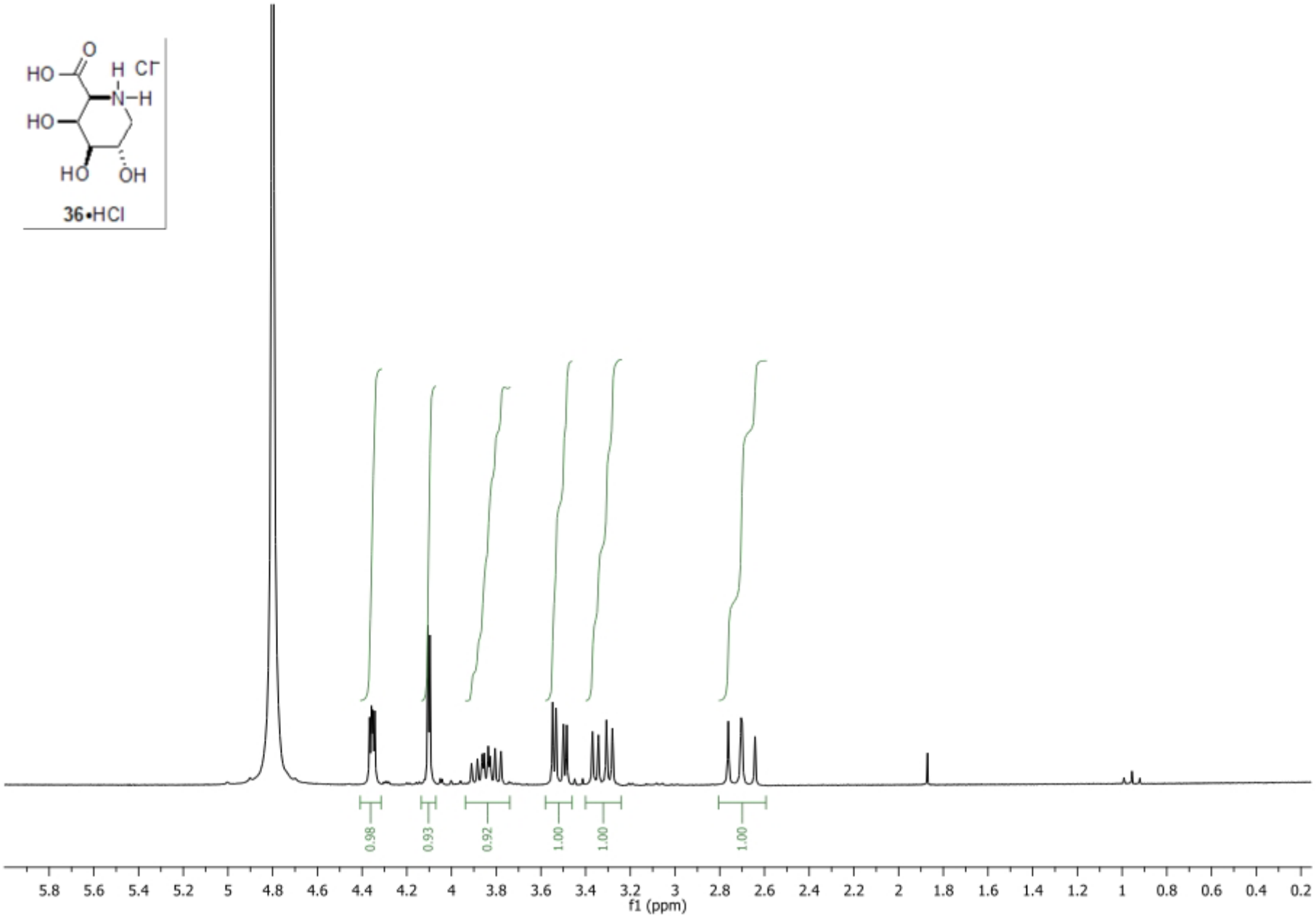

FIGURE S50. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **37**.

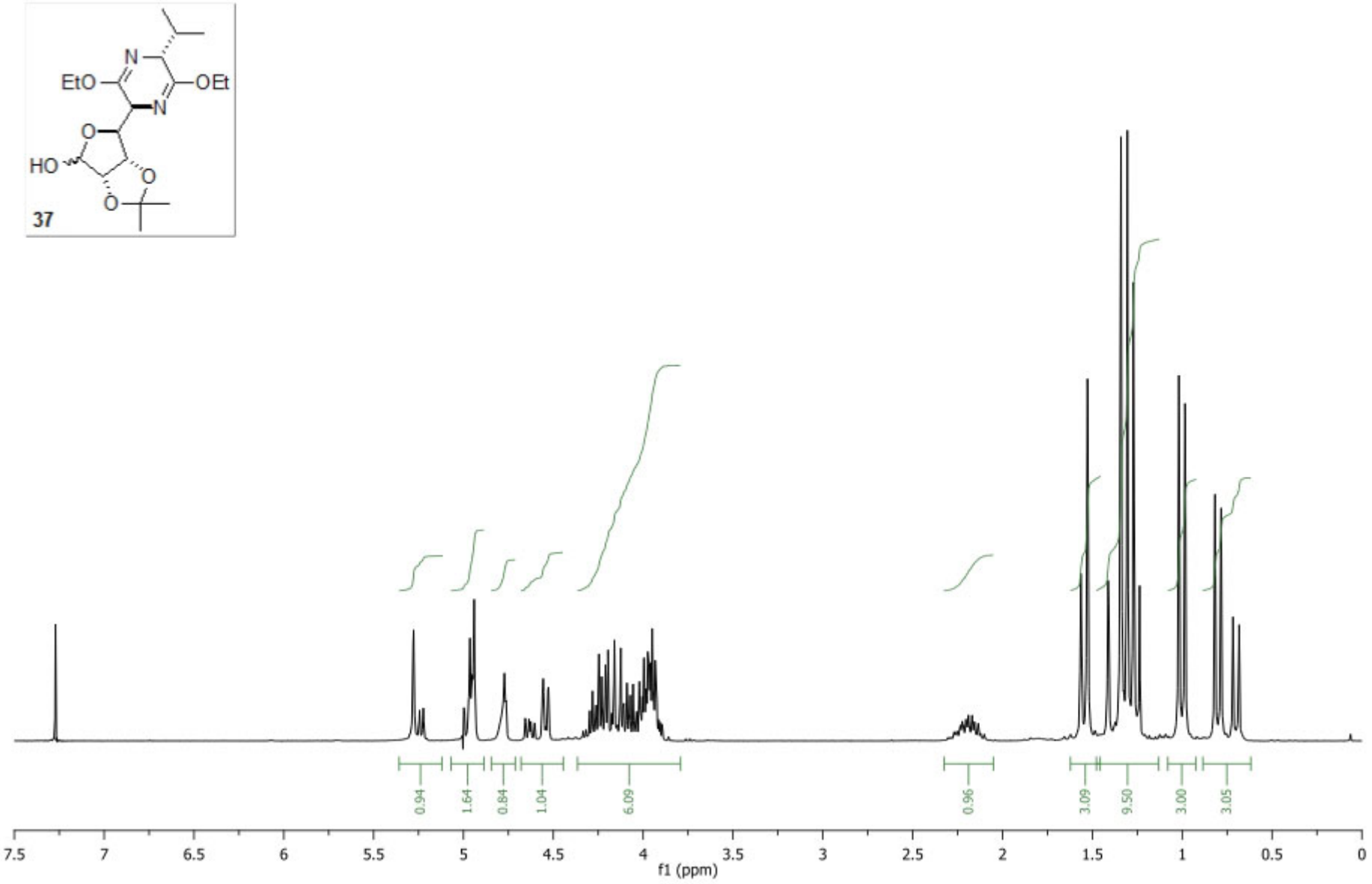

FIGURE S51. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **38**.

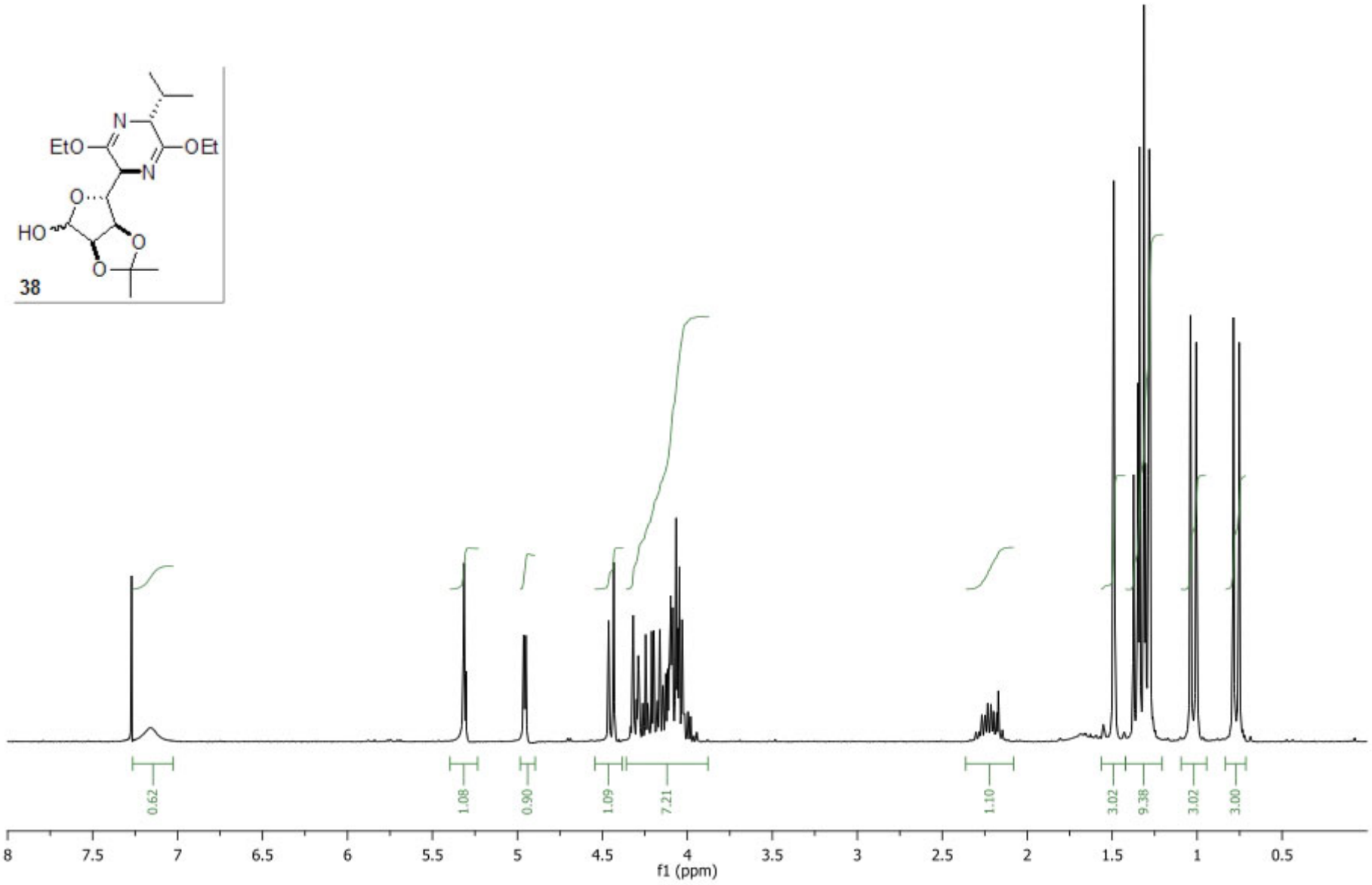

FIGURE S52. ^{1}H NMR (200 MHz, $CDCl_3$) for compound **39**.

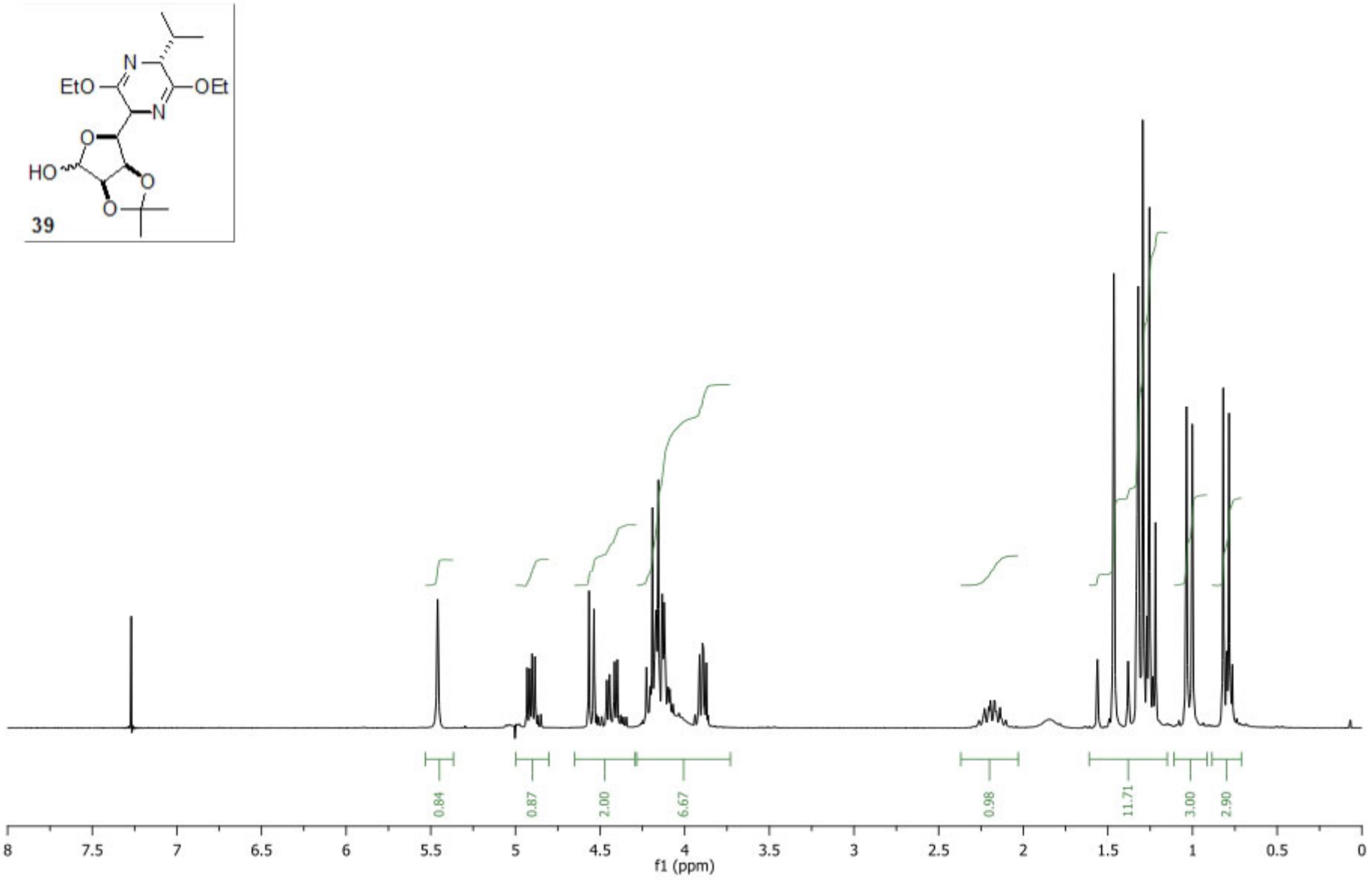

FIGURE S53. ^{1}H NMR (200 MHz, $CDCl_3$+D_2O) for compound **40**.

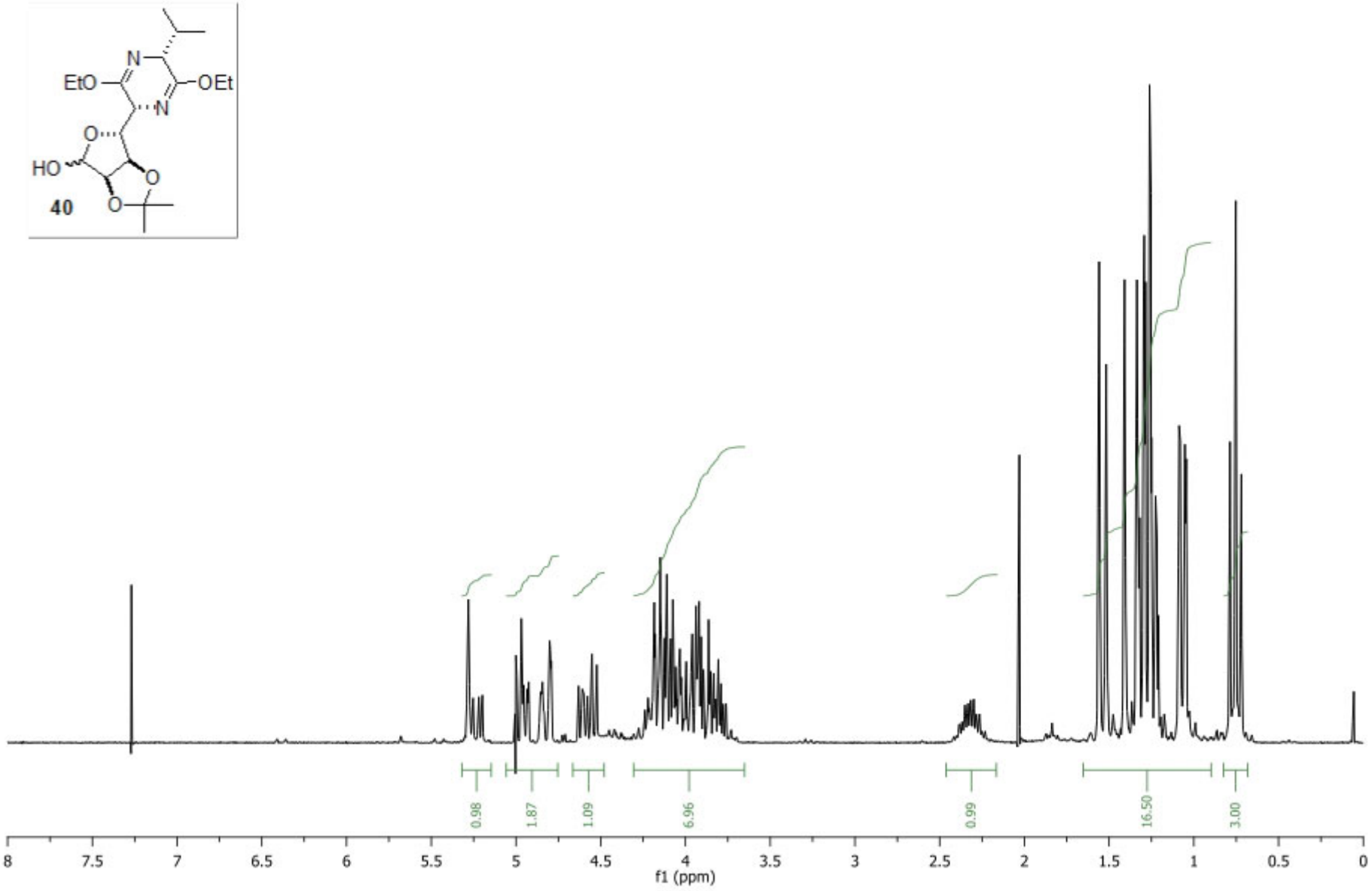

FIGURE S54. ^{1}H NMR (200 MHz, $CDCl_3$+D_2O) for compound (–)-**41**.

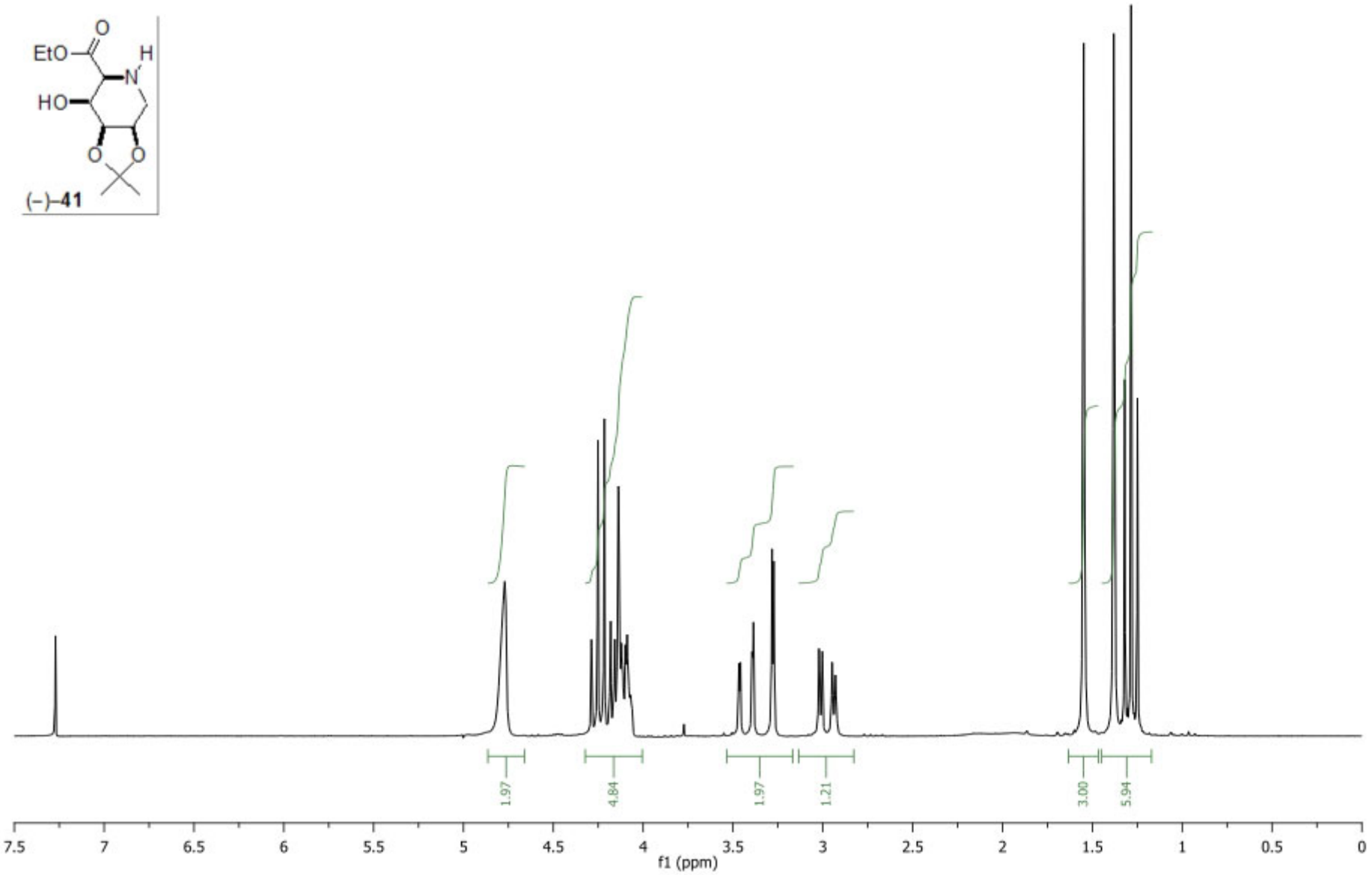

FIGURE S55. ^{1}H NMR (200 MHz, D_2O) for compound (+)-**41**.

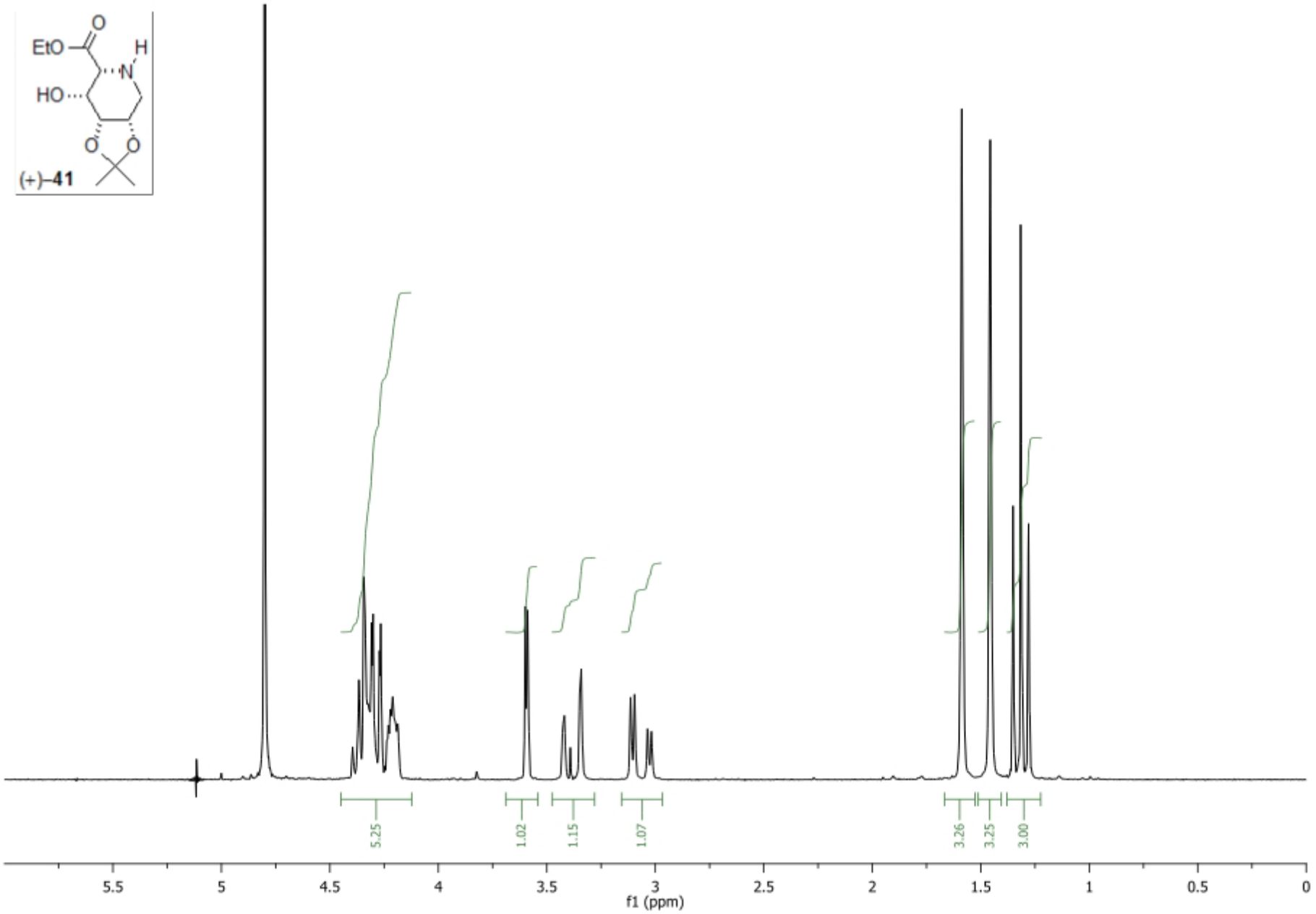

FIGURE S56. ^{1}H NMR (200 MHz, D_2O) for compound **42**.

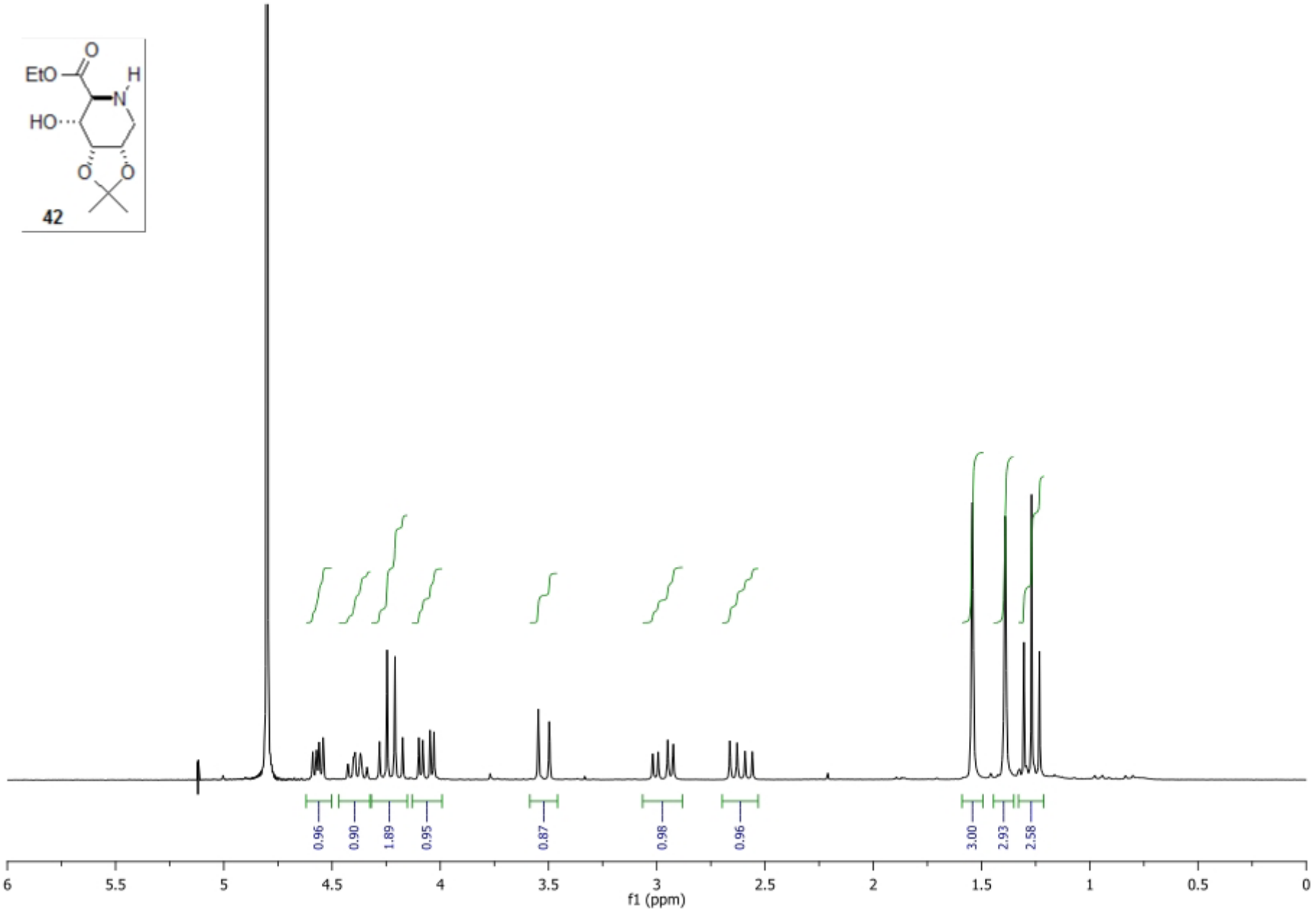

FIGURE S57. ^{1}H NMR (200 MHz, D_2O) for compound **43**.