Supporting Information

semiaza-Bambusurils are Anion-Specific Transmembrane Transporters

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Table of Contents

1. General

All commercially available chemicals and solvents were purchased from commercial sources and used without further purification. Unless otherwise stated, all heated chemical reactions were performed in an oil bath. NMR spectra were recorded with AVIII400 Bruker spectrometers. ^{1}H and ^{13}C NMR spectra were performed in acetonitrile-d_3, or by using residual solvent signals (δ_H = 1.94 ppm, δ_C = 118.2 and 1.39 ppm) or DMSO-d_6 (δ_H = 2.50 ppm, δ_C = 39.5 ppm). Signal multiplicities use the following abbreviations or combinations thereof: *s*-singlet, *d*-doublet, *t*-triplet, *m*-multiplet and *b*-broad. Peak signals of the ^{13}C NMR spectra exhibiting quartet at 125.5, 122.3, 119.1 and 115.9 ppm, assigned for the CF_3 group in triflate anions, were omitted for clarity.

Mass spectrometry and high-resolution mass spectra (HRMS) were recorded with a Water Xevo G2 QTOF spectrometer (ESI-TOF, MeCN/H_2O 7:3 at a flow rate of 0.2 mL/min). Since all new semiaza-BUs, **3a-f**, are in the form of polyiminium triflate salts, neutralization of the compounds was performed by using the following protocol:

Elemental analysis: Determination of C, H, N, and S element amount (%) was performed using the Thermo Flash 2000 Organic Elemental Analyzer (Thermo Scientific, USA). Samples (2-4 mg) were mixed with vanadium (8-10 mg) and placed in tin crucible under flash combustion method (950 °C) using a constant flow of He gas at a rate of 140 ml/min, and oxygen gas flow at 250 ml/min for 5 seconds. The standards used during measurements were cysteine, 2,5-bis(5-tert-butyl-2-benzo-oxazol-2-yl) thiophene (BBOT), sulfanilamide, methionine and nicotinamide.

Melting points were measured on a Stuart SMP11 apparatus and are reported uncorrected. Samples were placed into a glass capillary (10 µl) and heated from 150 °C to 250 °C at a rate of 1 °C/min.

2. Synthetic procedures and characterization

***semithio*-BU[6], 1**.

The compound was synthesized according to the previously reported procedure but using tetraethylammonium chloride (Et_4NCl) as an anion template.[1]
^{1}H NMR (400 MHz, DMSO-d_6): δ = 5.60 (s, 12H, CH), 5.20 (s, 12H, CH_2), 3.30 (s, 36H, CH_3), 3.19 (q, J = 7.2 Hz, 16H, Et_4N^+), 1.15 (t, J = 7.2 Hz, 24H, Et_4N^+), ^{13}C NMR (100 MHz, DMSO-d_6) δ = 183.2 (C=S), 158.3 (C=O), 71.0 (CH), 51.8 (NCH_2N), 49.3 (NCH_2), 34.8 (12xCH_3), 7.6 (4xCH_3).

The chloride complex of *semithio*-BU[6], **1**, was used to synthesize **3a-c,** whereas the bromide complex of *semithio*-BU[6] was used as a starting material for synthesizing **3d-f**.

***semi-(methyl)sulfonium*-BU[6], 2**.

The compound was synthesized according to a previously reported procedure[2]; the crude purity was confirmed by ^{1}H NMR and then used for the next step without further purification.

General procedure for the synthesis of 3a-c.

To a suspended solution of **2** (500 mg, 0.24 mmol) in THF (50 mL), was added an alkyl amine of choice, *i.e.*, butyl (**a**), pentyl (**b**) or heptyl amine (**c**) (10 equiv., 2.4 mmol), and the reaction was reflux for 14 h. Then, the reaction mixture was cooled to room temperature, and the solvent was removed under reduced pressure. Finally, the remaining solid crude was washed and sonicated several times with a mixture of $CHCl_3$:diethyl ether (1:1) to afford N-(1,3-dimethyl-5-oxohexahydroimidazo[4,5-d]imidazol-2(1H)-ylidene)alkyl-1-aminium trifluoromethanesulfonate, **3a-c** respectively, as fine faint yellow powders.

General procedure for the synthesis of 3d-f.

To a suspended solution of **2** (500 mg, 0.24 mmol) in THF (50 mL), was added an alkyl amine of choice, *i.e.*, methylthioethyl (**d**), methylthiopropyl (**e**) or (4-methylthio)benzylamine (**f**) (10 equiv., 2.4 mmol). The reaction mixture was refluxed for 16 h and then cooled to room temperature. Then, diethyl ether (50 mL) was added, precipitating the crude product. After filtration, the solid crude was washed and sonicated several times with a mixture of $CHCl_3$:diethyl ether (1:1) to afford N-(1,3-dimethyl-5-oxohexahydroimidazo[4,5-d]imidazol-2(1H)-ylidene) thioalkyl-1-aminium trifluoromethanesulfonate, **3d,e**, and N-(1,3-dimethyl-5-oxohexahydroimidazo[4,5-d]imidazol-2(1H)-ylidene) thioaryl-1-aminium trifluoromethanesulfonate, **3f** respectively, as fine yellowish powders.

Because all semiaza-BU[4] derivatives, **3a-f** in the form of polyiminium triflate salt could not tolerate the standard conditions of mass spectroscopic analysis, high-resolution molecular mass (HRMS) could be achieved by subsequent neutralization reaction following the next procedure:

General procedure for the synthesis of 4a-f.

semiaza-BU[6] in the salt form (50 mg) and Amberlyst A26 resins (OH- form, 50 mg) were suspended in methanol (20 mL), and the mixture was stirred at room temperature for 15-20 min. After filtration, the clear yellowish filtrate was concentrated under reduced pressure to afford a yellowish powder of neutral *semiaza*-BU[6] **4a-f**, in quantitative yield (>95%).

***semiaza*-Bambus[6]uril, 3a and its free-anion form, 4a**:

Yellowish powder (0.40 g, 82%); m.p. 212-215 °C.

^{1}H NMR (400 MHz, acetonitrile-d_6): δ = 6.21 (s, 6H, NH), 5.8 (s, 12H, CH), 5.17 (s, 12H, CH_2), 3.42 (q, 12H, NCH_2), 3.30 (s, 36H, CH_3), 1.62 (m, 12H, CH_2), 1.39 (m, 12H, CH_2), 0.9 (t, 18H, CH_3) ppm. ^{13}C NMR (100 MHz, acetonitrile-d_6) δ = 160.38 (C=N$^+$HR), 158.97 (C=O), 73.96 (CH), 48.59 (NCH_2N), 44.62 (NCH_2), 35.06 (6xCH_2), 32.4 (12xCH_3), 19.84 (6xCH_2), 13.44 (6xCH_3) ppm.

CHN analysis (%) for **3a**: Calcd for $C_{71}H_{120}ClF_{15}N_{30}O_{21}S_5$: C, 38.58; H, 5.47; N, 19.01; Found: C, 38.12; H, 5.60; N, 18.90.

^{1}H NMR (400 MHz, acetonitrile-d_6) of **4a**: δ = 5.45 (s, 12H, CH), 5.02 (s, 12H, CH_2), 3.28 (t, 12H, NCH_2), 3.05 (s, 36H, CH_3), 1.45 (m, 12H, CH_2), 1.36 (m, 12H, CH_2), 0.90 (t, 18H, CH_3) ppm.

HRMS (TOF/ESI+), *m/z* calcd for **4a**: $C_{66}H_{114}N_{30}O_6$ 1422.9538; found: 1423.9610 $[M+H]^+$.

***semiaza*-Bambus[6]uril, 3b and its free-anion form, 4b**:

Yellowish powder (0.47 g, 85%); m.p. 220-222 °C

^{1}H NMR (400 MHz, acetonitrile-d_6): δ = 6.15 (s, 6H, NH), 5.77 (s, 12H, CH), 5.14 (s, 12H, CH_2), 3.37 (q, 12H, NCH_2), 3.28 (s, 36H, CH_3), 1.63 (m, 12H, CH_2), 1.33 (m, 24H, CH_2), 0.91 (t, 18H, CH_3) ppm. ^{13}C NMR (100 MHz, acetonitrile-d_6) δ = 160.36 (C=N$^+$HR), 158.9 (C=O), 73.85 (CH), 48.61 (NCH_2N), 44.81 (NCH_2), 35.06 (12xCH_3), 30.09 (6xCH_2), 28.72 (6xCH_2), 22.45 (6xCH_2), 13.78 (6xCH_3) ppm.

CHN analysis (%) for **3b**: Calcd for $C_{77}H_{132}ClF_{15}N_{30}O_{21}S_5$: C, 40.30; H, 5.80; N, 18.31. Found: C, 41.11; H, 6.05; N, 17.45.

^{1}H NMR (400 MHz, acetonitrile-d_6) of **4b**: δ = 5.59 (s, 12H, CH), 5.07 (s, 12H, CH_2), 3.34 (t, 12H, NCH_2), 3.17 (s, 36H, CH_3), 1.57 (m, 12H, CH_2), 1.32 (m, 24H, CH_2), 0.90 (t, 18H, CH_3) ppm.

HRMS (TOF/ESI+), *m/z* calcd for **4b**: $C_{72}H_{126}N_{30}O_6$ 1507.044; found: 1508.0555 $[M+H]^+$.

***semiaza*-Bambus[6]uril, 3c and its free-anion form, 4c**:

Yellowish powder (0.47 g, 80%); m.p. 233-235 °C.

^{1}H NMR (400 MHz, acetonitrile-d_6): δ = 6.07 (s, 6H, NH), 5.68 (bs, 12H, CH), 5.05 (bs, 12H, CH_2), 3.32 (bm, 12H, NCH_2), 3.20 (s, 36H, CH_3), 1.54 (bs, 12H, CH_2), 1.24 (bs, 48H, CH_2), 0.82 (bt, 18H, CH_3) ppm. ^{13}C NMR (100 MHz, acetonitrile-d_6) δ = 160.40 (C=N$^+$HR), 158.88 (C=O), 73.78 (CH), 48.60 (NCH_2N), 44.87 (NCH_2), 35.08 (12xCH_3), 31.97 (6xCH_2), 30.36 (6xCH_2), 30.21 (6xCH_2), 26.53 (6xCH_2), 22.84 (6xCH_2), 13.93 (6xCH_3) ppm.

CHN analysis (%) for **3c**: Calcd for $C_{89}H_{156}ClF_{15}N_{30}O_{21}S_5$: C, 43.40; H, 6.38; N, 17.06. Found: C, 42.70; H, 6.08; N, 17.81.

^{1}H NMR (400 MHz, acetonitrile-d_6) of **4c**: δ = 5.48 (s, 12H, CH), 5.04 (s, 12H, CH_2), 3.31 (t, 12H, NCH_2), 3.10 (s, 36H, CH_3), 1.49 (m, 12H, CH_2), 1.30 (m, 32H, CH_2), 0.89 (t, 18H, CH_3) ppm.

HRMS (TOF/ESI+),-*m/z* calcd for **4c**: $C_{84}H_{150}N_{30}O_6$ 1675.2355;-found: 1676.2433 [M+H].

***semiaza*-Bambus[6]uril, 3d and its free-anion form, 4d**:

Yellowish powder (0.49 g, 83%); m.p. 240-242 °C.

^{1}H NMR (400 MHz, acetonitrile-d_6): δ = 6.35 (s, 6H, NH), 5.89 (s, 12H, CH), 5.18 (s, 12H, CH_2), 3.64 (m, 12H, NCH_2), 3.34 (s, 36H, CH_3), 2.78 (t, 12H CH_2), 2.13 (s, 18H, SCH_3) ppm. ^{13}C NMR (100 MHz, acetonitrile-d_6) δ = 160.27 (C=N$^+$HR), 158.93 (C=O), 74.10 (CH), 48.60 (NCH_2N), 41.10 (NCH_2), 38.19 (12xCH_3), 33.68 (6xCH_2S), 14.59 (6xSCH_3);

CHN analysis(%) for **3d**: Calcd for $C_{65}H_{108}BrF_{15}N_{30}O_{21}S_{11}$: C, 33.03; H, 4.61; N, 17.78; S, 14.92. Found: C, 33.13; H, 4.16; N, 17.72; S, 15.22.

^{1}H NMR (400 MHz, acetonitrile-d_6) of **4d**: δ = 5.50 (s, 12H, CH), 5.05 (s, 12H, CH_2), 3.54 (t, 12H, NCH_2), 3.12 (s, 36H, CH_3), 2.63 (m, 12H, SCH_2), 2.11 (s, 18H, CH_3), ppm**.**

HRMS (TOF/ESI+), *m/z* calcd for **4d**: $C_{60}H_{102}N_{30}O_6S_6$ 1530.69; found: 1531.70 [M+H]$^+$.

***semiaza*-Bambus[6]uril, 3e and its free-anion form, 4e**:

Yellowish powder (0.49 g, 83%); m.p. 243-245 °C.

^{1}H NMR (400 MHz, acetonitrile-d_6): δ = 6.32 (s, 6H, NH), 5.86 (s, 12H, CH), 5.16 (s, 12H, CH_2), 3.54 (m, 12H, NCH_2), 3.32 (s, 36H, CH_3), 2.55 (t, 12H CH_2) 2.09 (s, 18H, SCH_3), 1.92 (m, 12H, CH_2) ppm. ^{13}C NMR (100 MHz, acetonitrile-d_6) δ = 160.56 (C=N$^+$HR), 158.92 (C=O), 74.06 (CH), 48.55 (NCH_2N C), 43.68 (NCH_2), 35.16 (12xCH_3), 30.84 (6xCH_2S), 29.32 (6xCH_2), 14.86 (6xSCH_3) ppm.

CHN analysis (%) for **3e**: Calcd for $C_{71}H_{120}BrF_{15}N_{30}O_{21}S_{11}$: C, 34.84; H, 4.94; N, 17.17; S, 14.41. Found: C, 34.83; H, 4.96; N, 17.20; S, 15.04.

^{1}H NMR (400 MHz, acetonitrile-d_6) of **4e**: δ = 5.45 (s, 12H, CH), 5.02 (s, 12H, CH_2), 3.38 (t, 12H, NCH_2), 3.05 (s, 36H, CH_3), 2.56 (t, 12H, SCH_2), 2.05 (s, 18H, CH_3), 1.72 (m, 12H, CH_2) ppm**.**

HRMS (TOF/ESI+), *m/z* calcd for **4e**: $C_{66}H_{114}N_{30}O_6S_6$ 1614.78; found: 1615.79 [M+H]$^+$.

***semiaza*-Bambus[6]uril, 3f and its free-anion form, 4f**:

Yellowish powder (0.45 g, 68%); m.p. 212-215 °C (decomp.).

^{1}H NMR (400 MHz, acetonitrile-d_6): δ = 7.31 (bs, 24H, CH), 5.76 (bs, 12H, CH), 5.08 (bs, 12H, CH_2), 4.09 (s, 12H, NCH_2), 3.28 (s, 36H, CH_3), 2.51 (s, 18H, SCH_3) ppm. ^{13}C NMR (100 MHz, acetonitrile-d_6) δ = 160.81 (C=N$^+$HR), 158.84 (C=O), 140 (6xSC_{aryl}), 135 (6xC_{aryl}), 128.25

(6xCH_{aryl}), 128.15 (6xCH_{aryl}), 73.95 (CH), 48.58 (NCH_2N), 47.48 (NCH_2), 35.05 (12xCH_3), 15.01 (6xSMe) ppm.

CHN analysis (%) for **3f**:. Calcd for $C_{95}H_{120}BrF_{15}N_{30}O_{21}S_{11}$: C, 41.71; H, 4.42; N, 15.36; S, 12.89. Found: C, 41.28; H, 4.43; N, 15.49; S, 12.79.

^{1}H NMR (400 MHz, DMSO-d_6) of **4f**: δ = 7.31 (bs, 12H, CH), 7.22 (bs, 12H, CH), 5.40 (s, 12H, CH), 5.05 (s, 12H, CH_2), 4.54 (s, 12H, NCH_2), 3.12 (s, 36H, CH_3), 2.45 (s, 18H, CH_3), ppm.

HRMS (TOF/ESI+), *m/z* calcd for **4f**: $C_{90}H_{114}N_{30}O_6S_6$ 1902.7862; found: 1903.7940 $[M+H]^+$.

3. NMR data

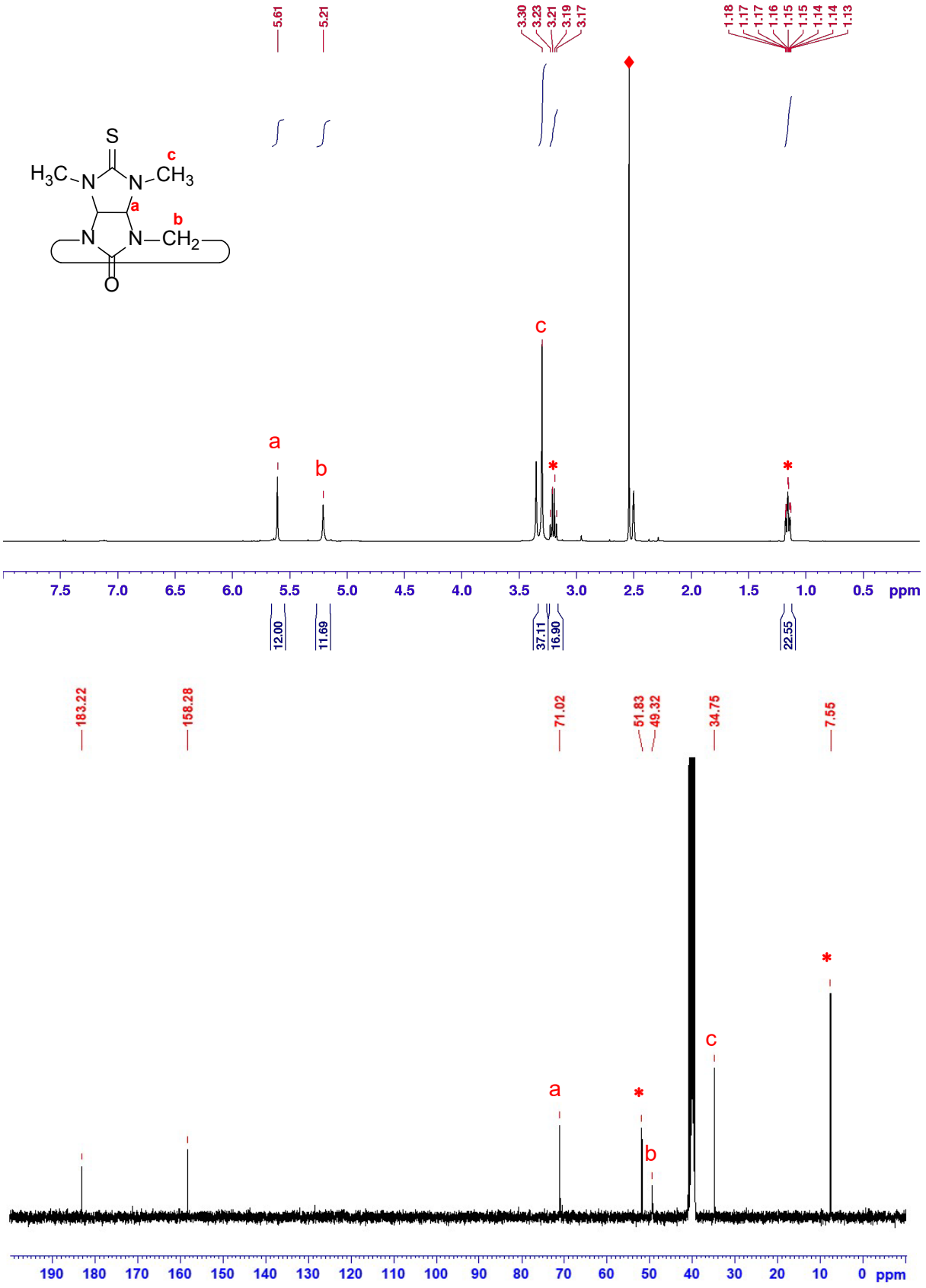

Fig. S1 ^{1}H NMR (400 MHz, DMSO-d_6) (*top*) and ^{13}C NMR (100 MHz, DMSO-d_6) (*bottom*) spectra of compound **1**. The asterisks refer to signals of Et_4NCl salt. The rhombi refer to guest DMSO molecules in the single crystal of **1**.

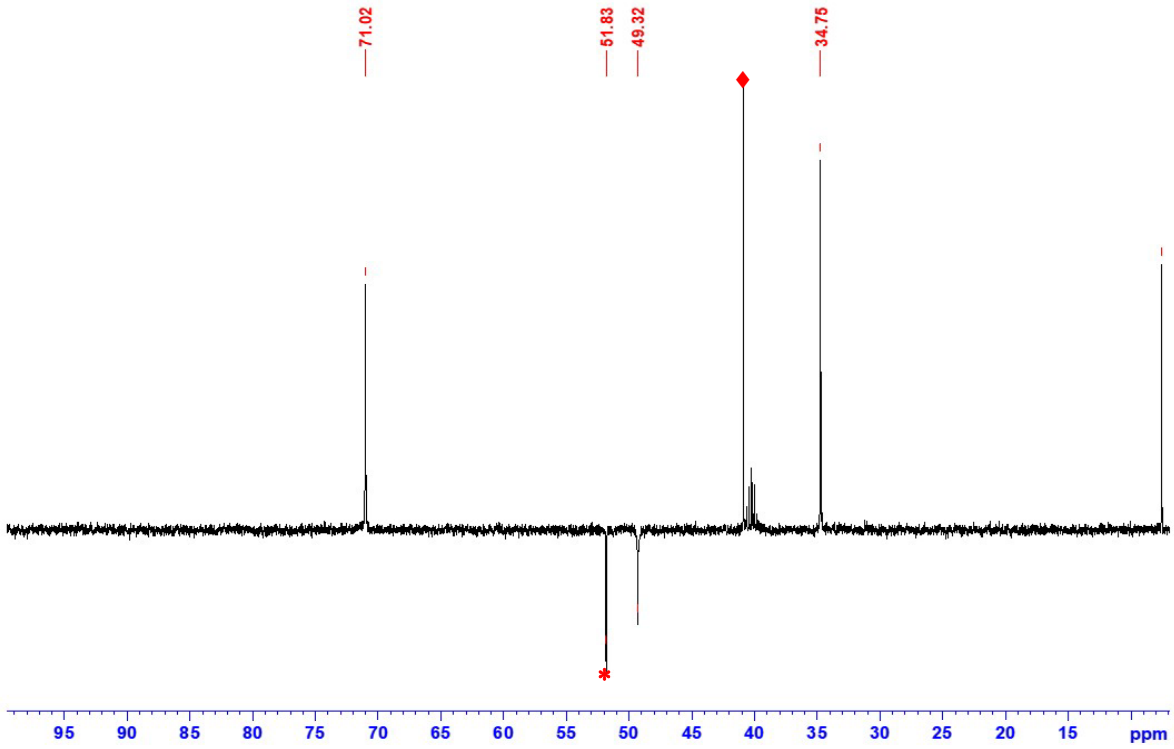

Fig. S2 Distortion less enhancement by polarization transfer (DEPT) spectrum of **1** (100 MHz, DMSO-d_6). The asterisks refer to signals of Et_4NCl salt. The rhombi refers to guest DMSO molecules in the single crystal of **1**.

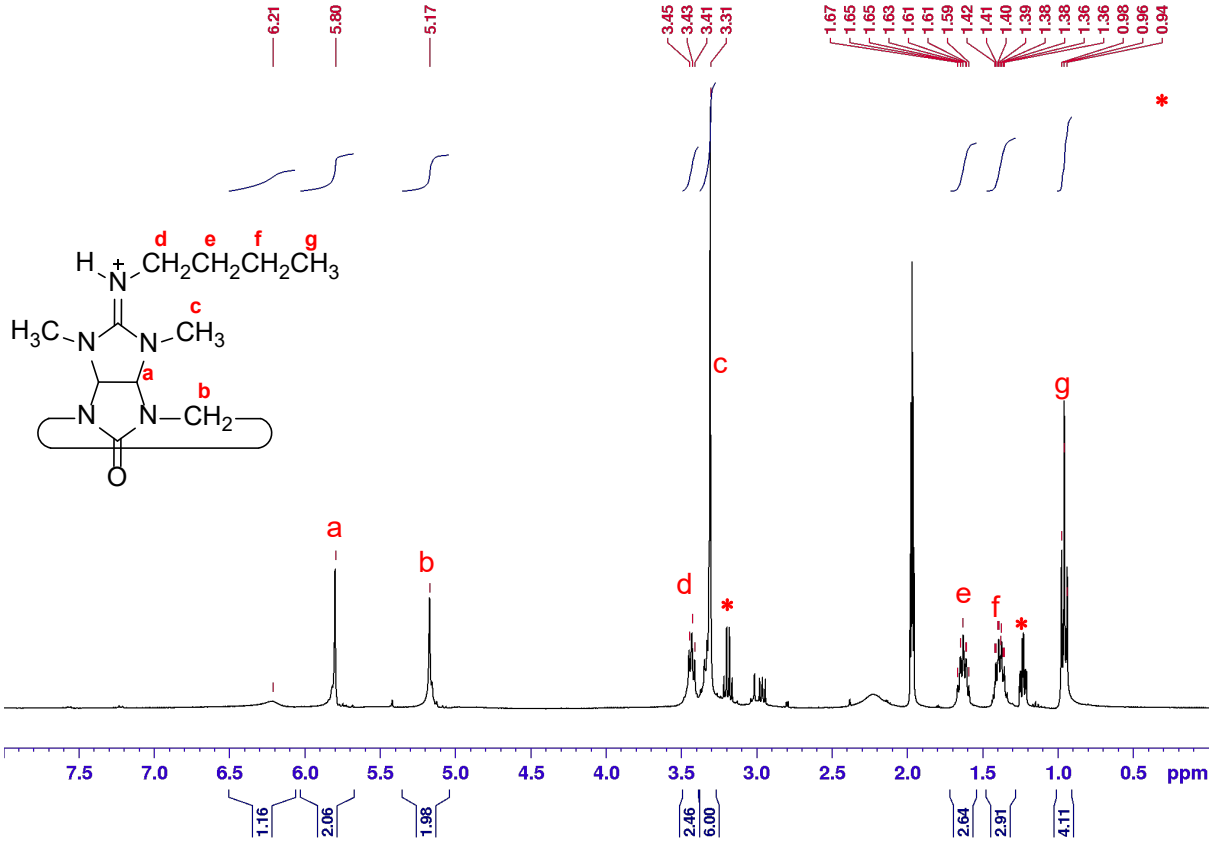

Fig. S3 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **3a**. The asterisks refer to signals of Et_4NCl salt, which was added to avoid signal broadening.

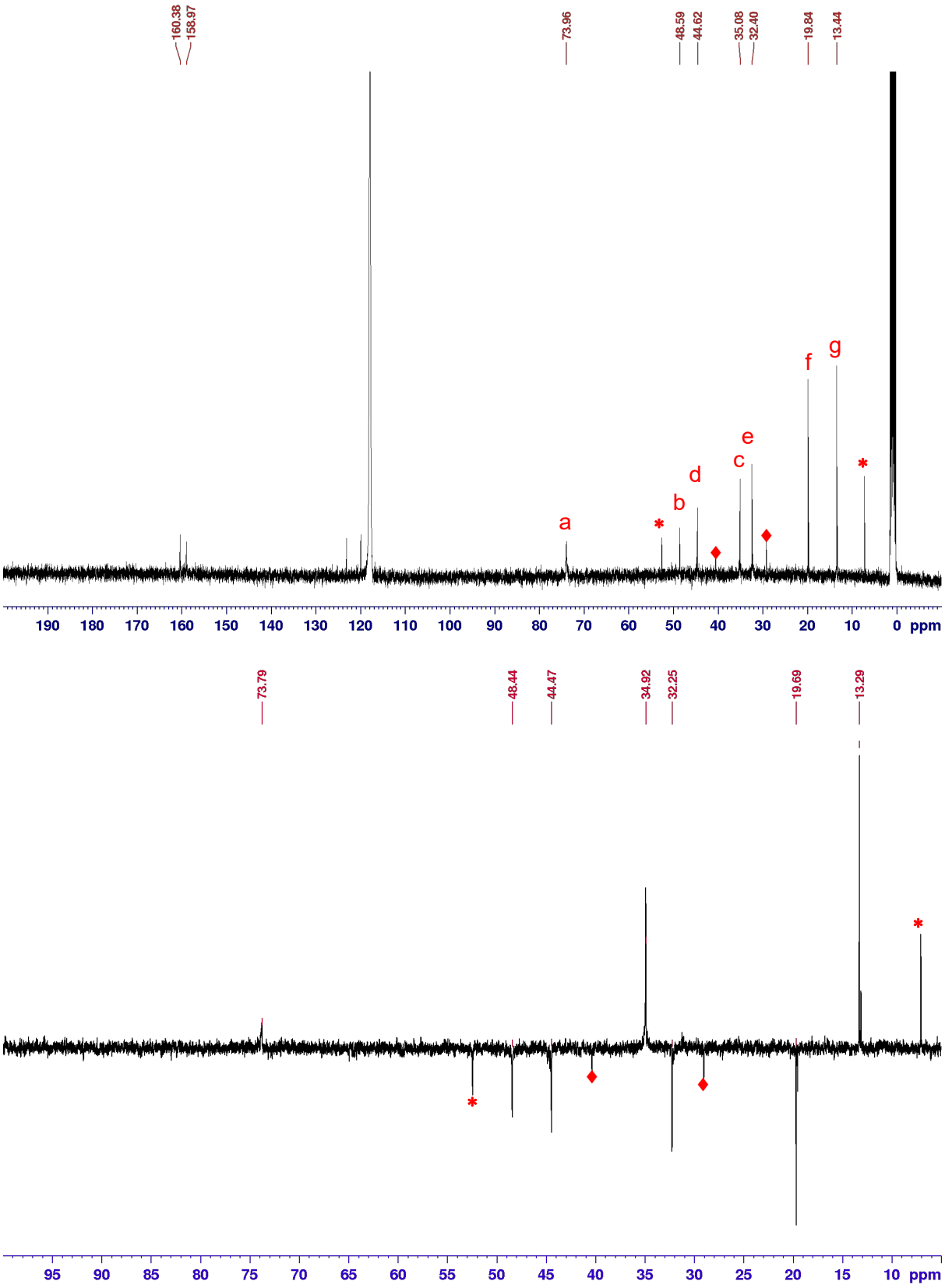

Fig. S4 NMR spectra of compound **3a**: *top* and *bottom*: ^{13}C NMR (100 MHz, acetonitrile-d_3) and DEPT experiment, respectively**.** The asterisks refer to signals of Et_4NCl salt. The rhombi refer to trace impurity of amine.

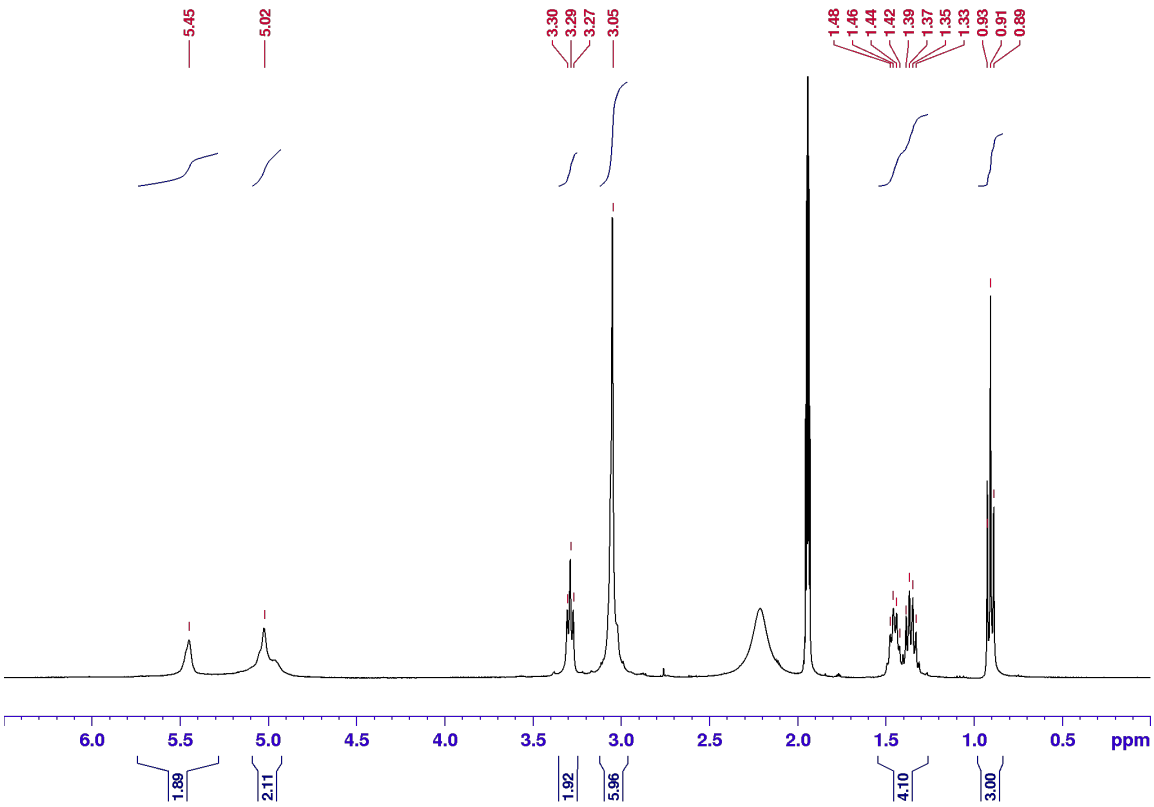

Fig. S5 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **4a**.

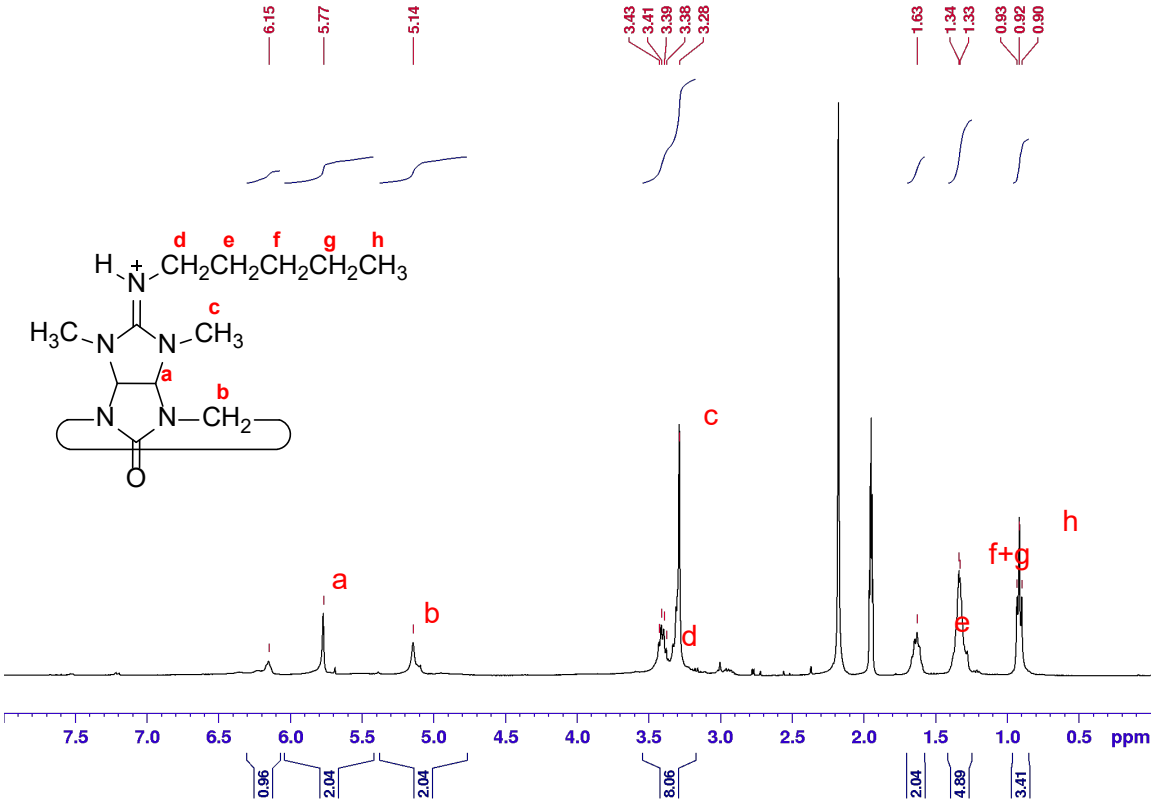

Fig. S6 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **3b.**

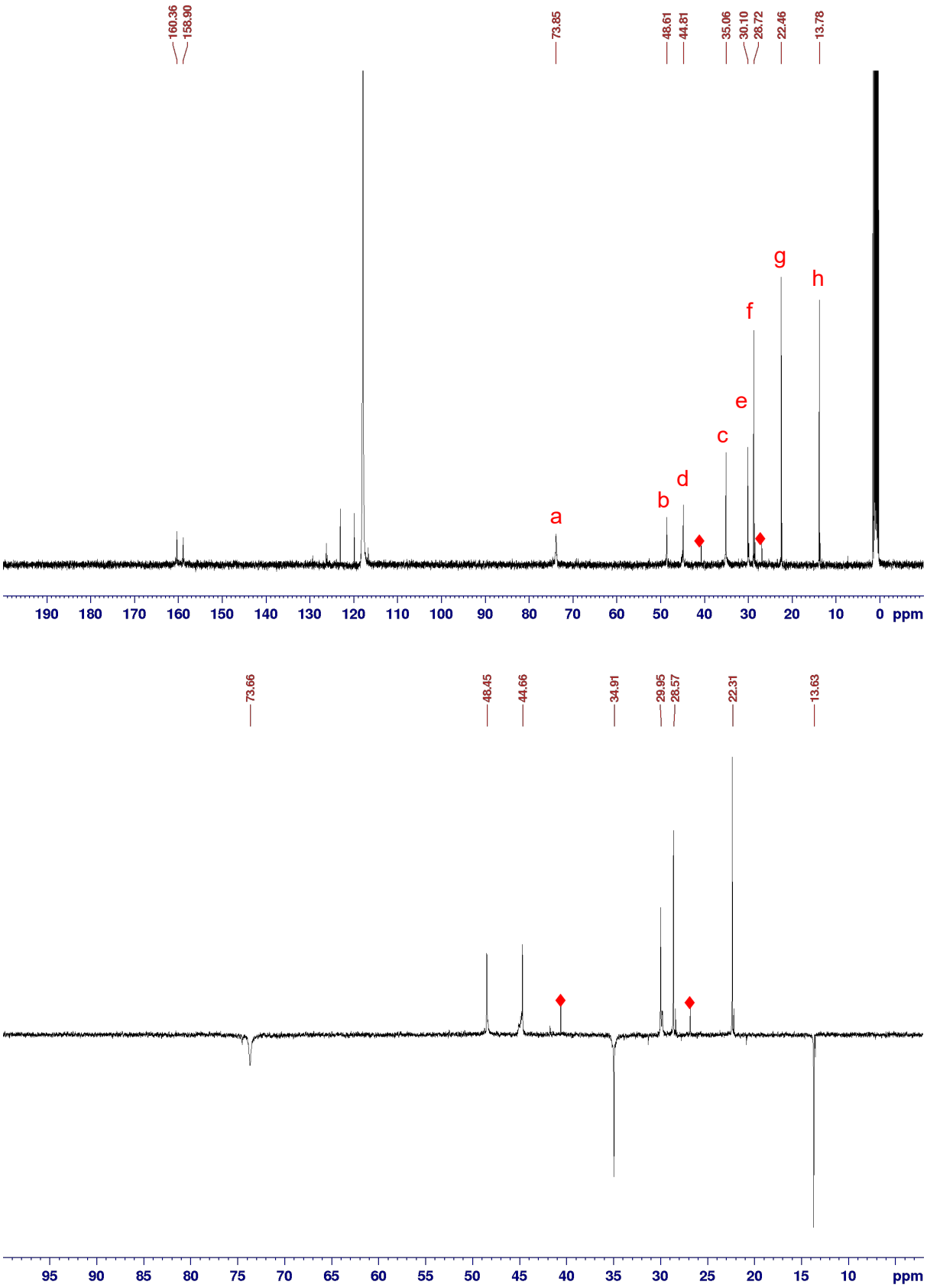

Fig. S7 NMR spectra of compound **3b**: *top* and *bottom*: ^{13}C NMR (100 MHz, acetonitrile-d_3) and DEPT experiment, respectively. The rhombi refer to trace impurity of amine.

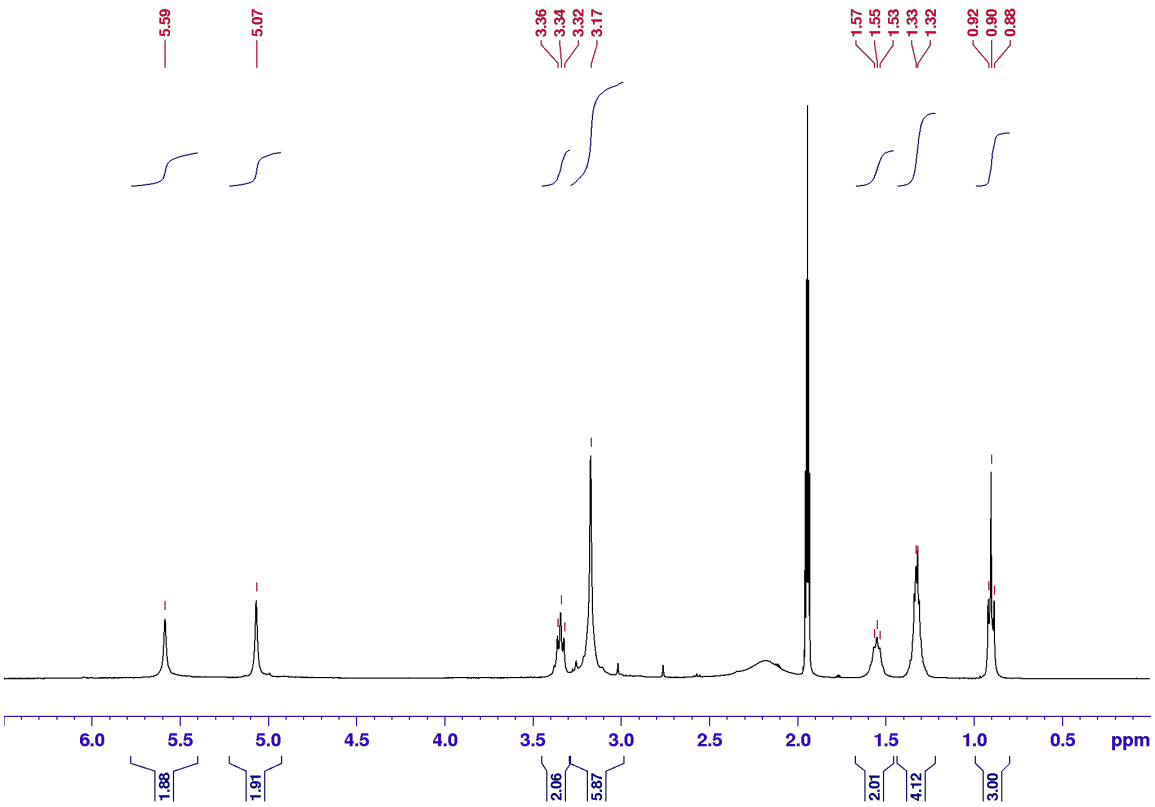

Fig. S8 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **4b**.

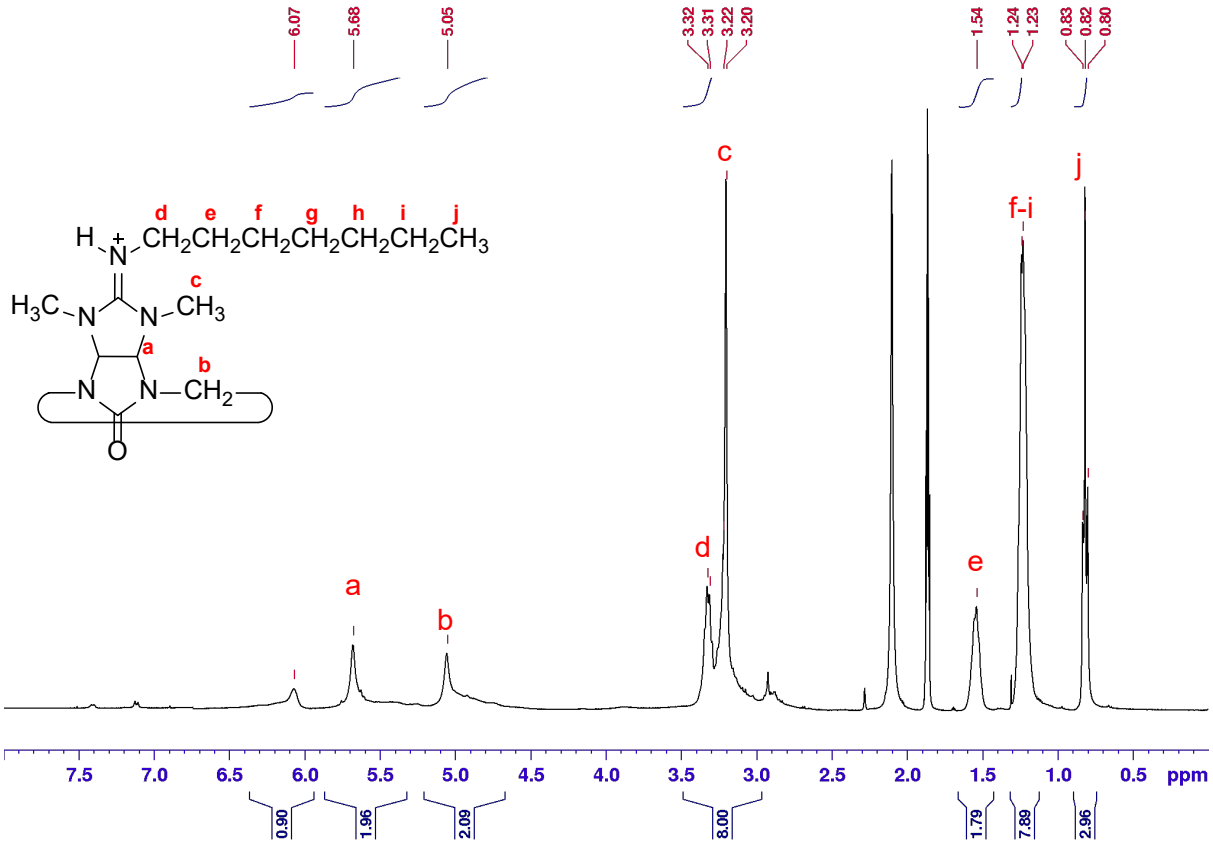

Fig. S9 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **3c**.

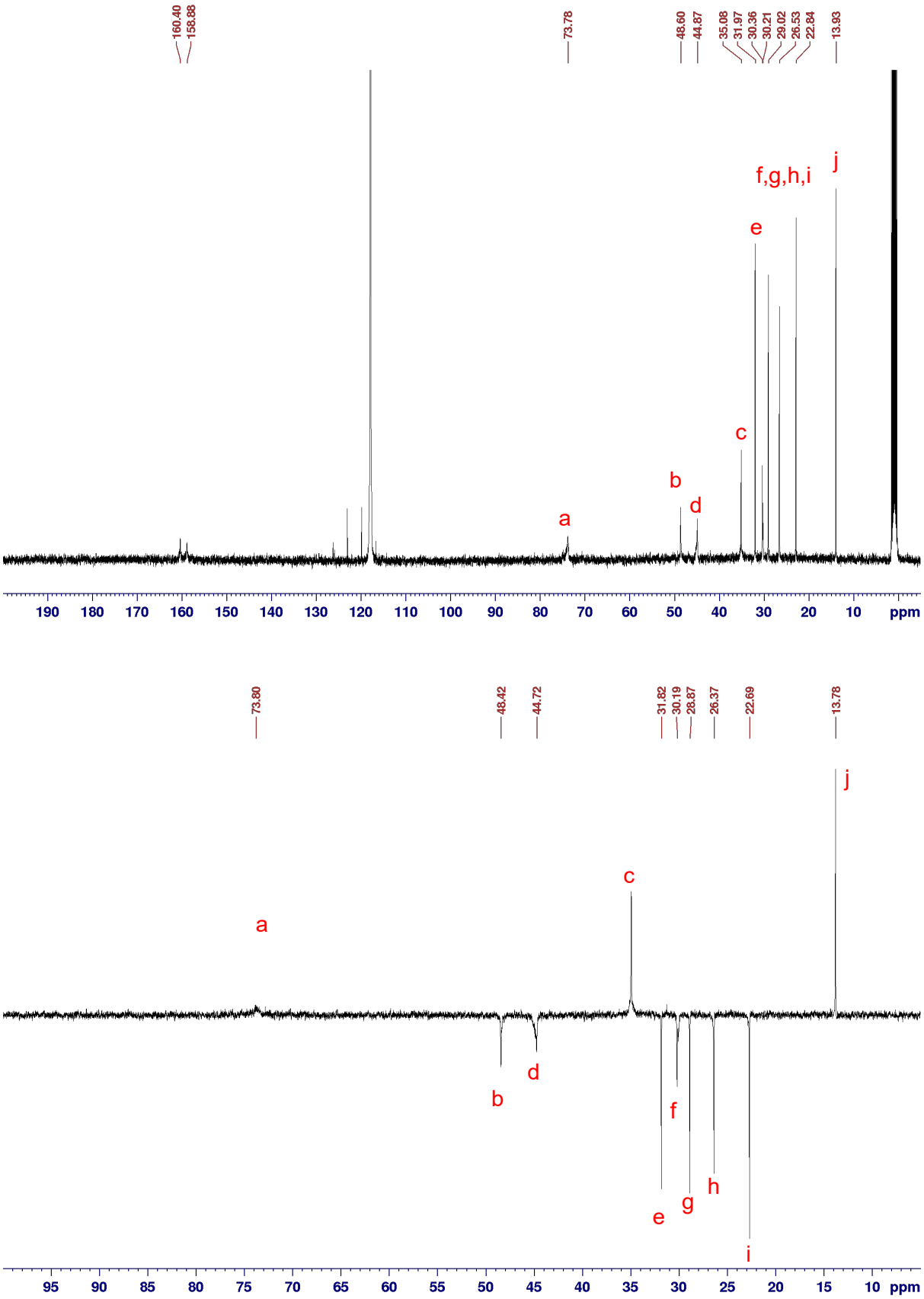

Fig. S10 NMR spectra of compound **3c**: *top* and *bottom*: ^{13}C NMR (100 MHz, acetonitrile-d_3) and DEPT experiment, respectively.

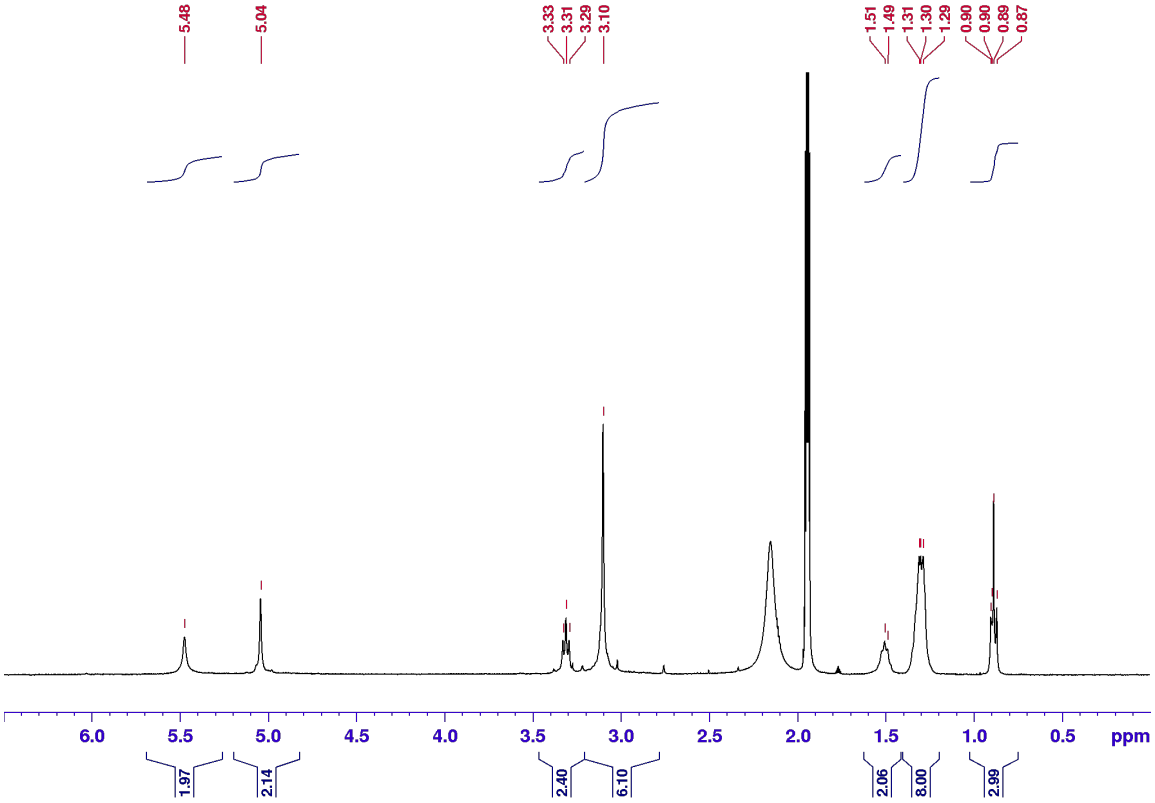

Fig. S11 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **4c**.

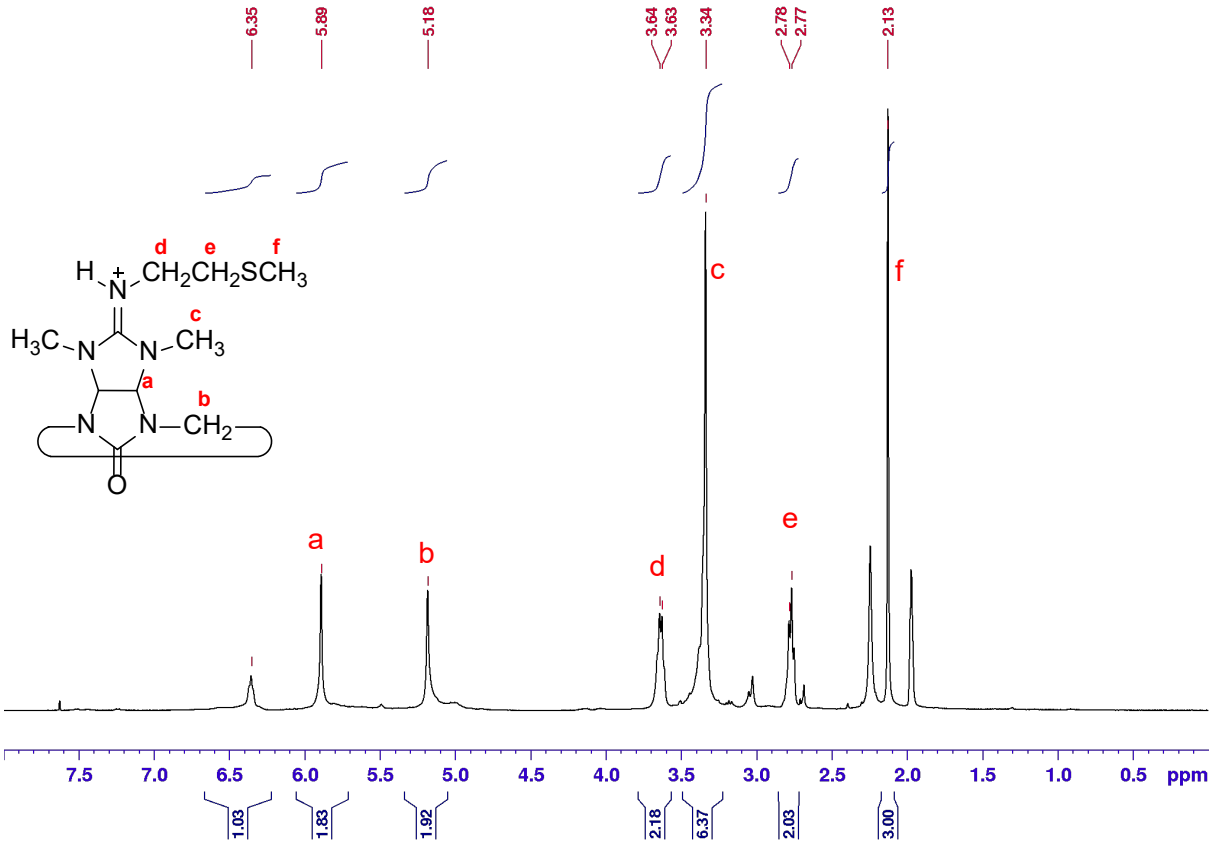

Fig. S12 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **3d**.

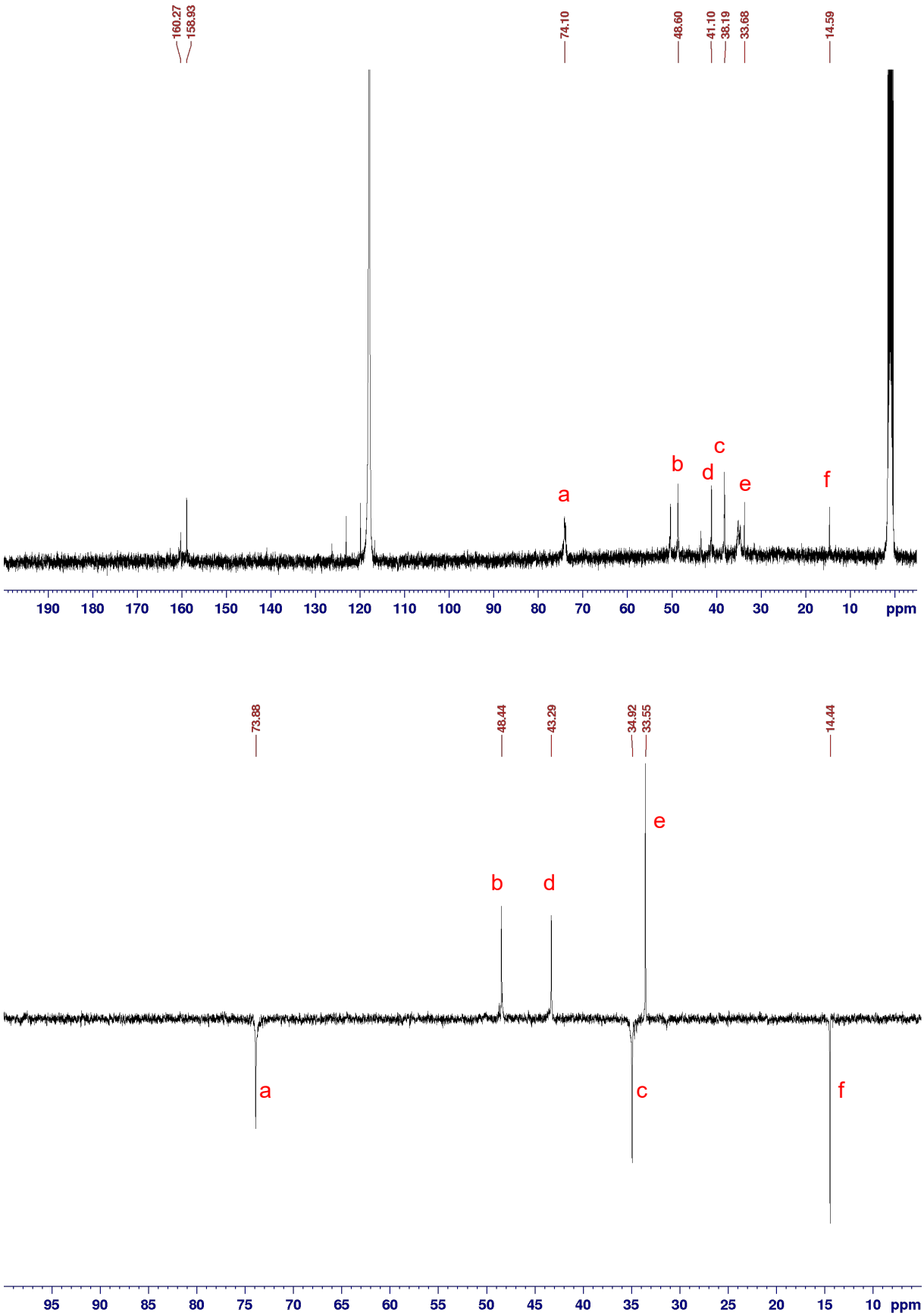

Fig. S13 NMR spectra of compound **3d**: *top* and *bottom*: ^{13}C NMR (100 MHz, acetonitrile-d_3) and DEPT experiment, respectively.

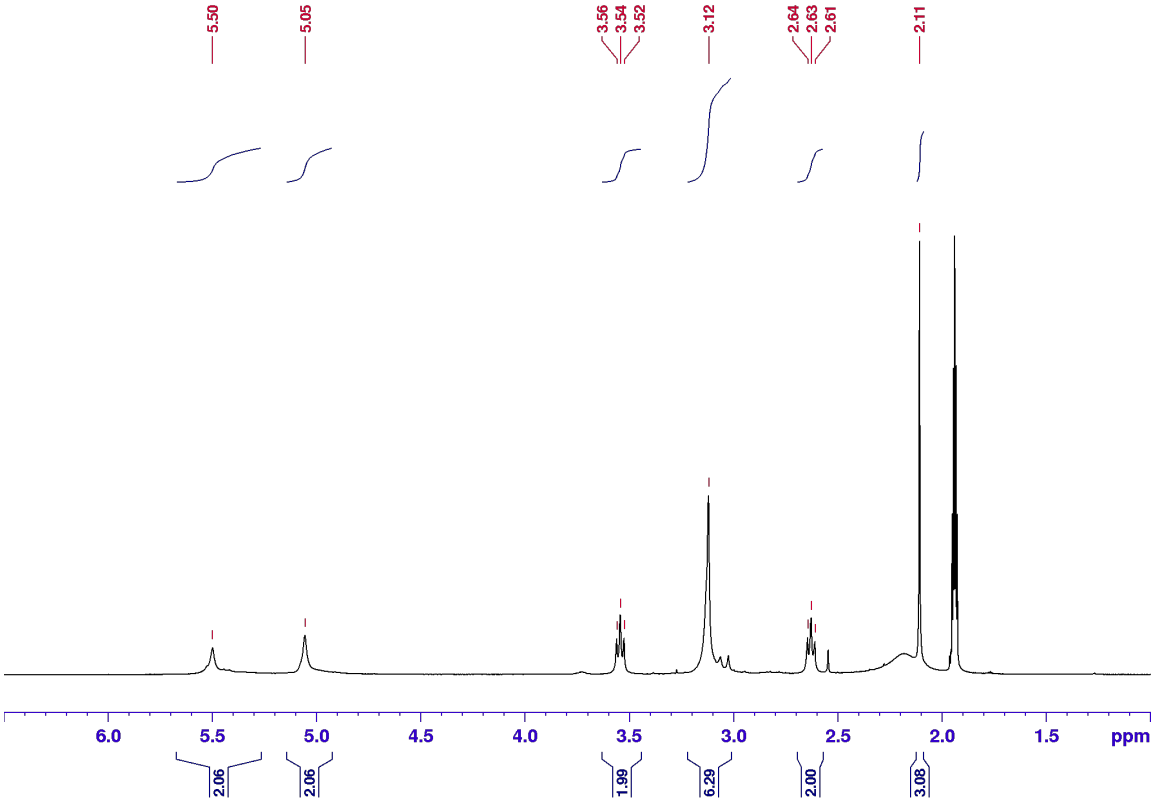

Fig. S14 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **4d**.

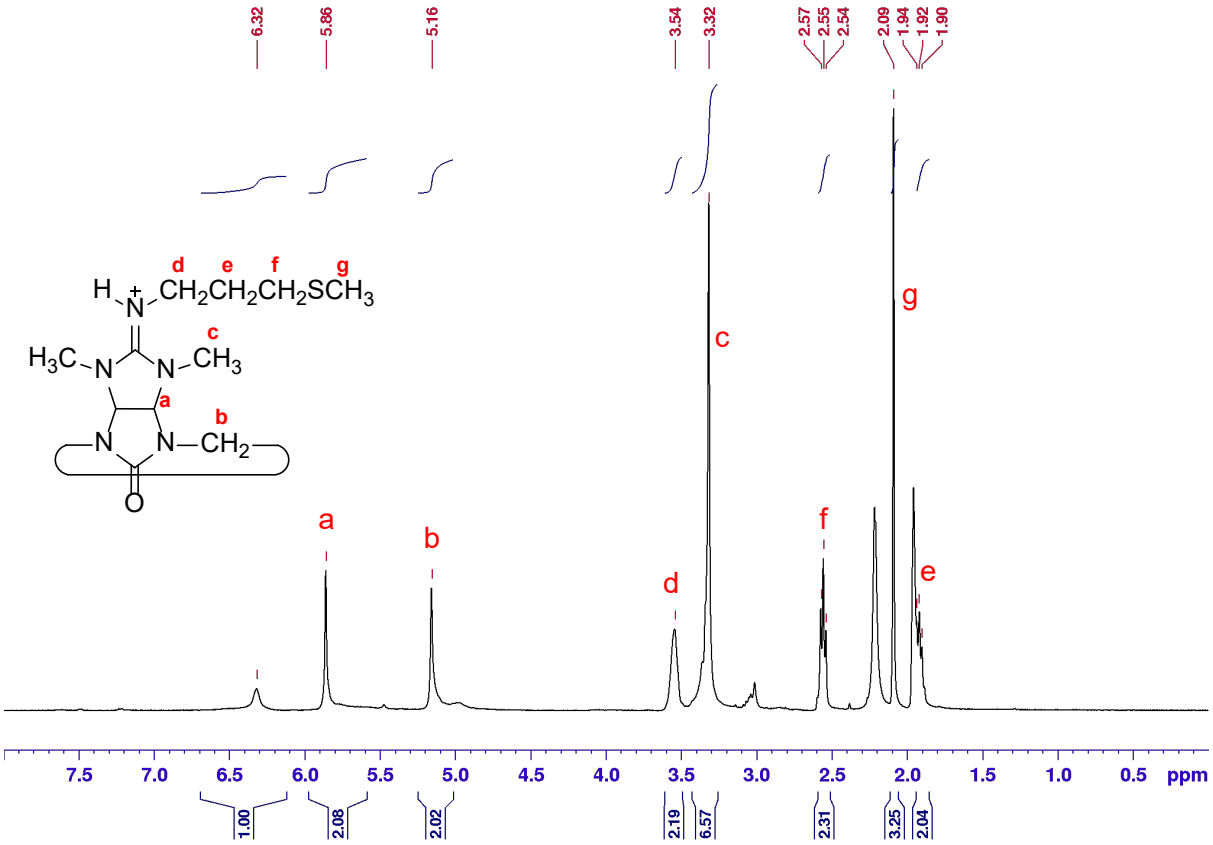

Fig. S15 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **3e**.

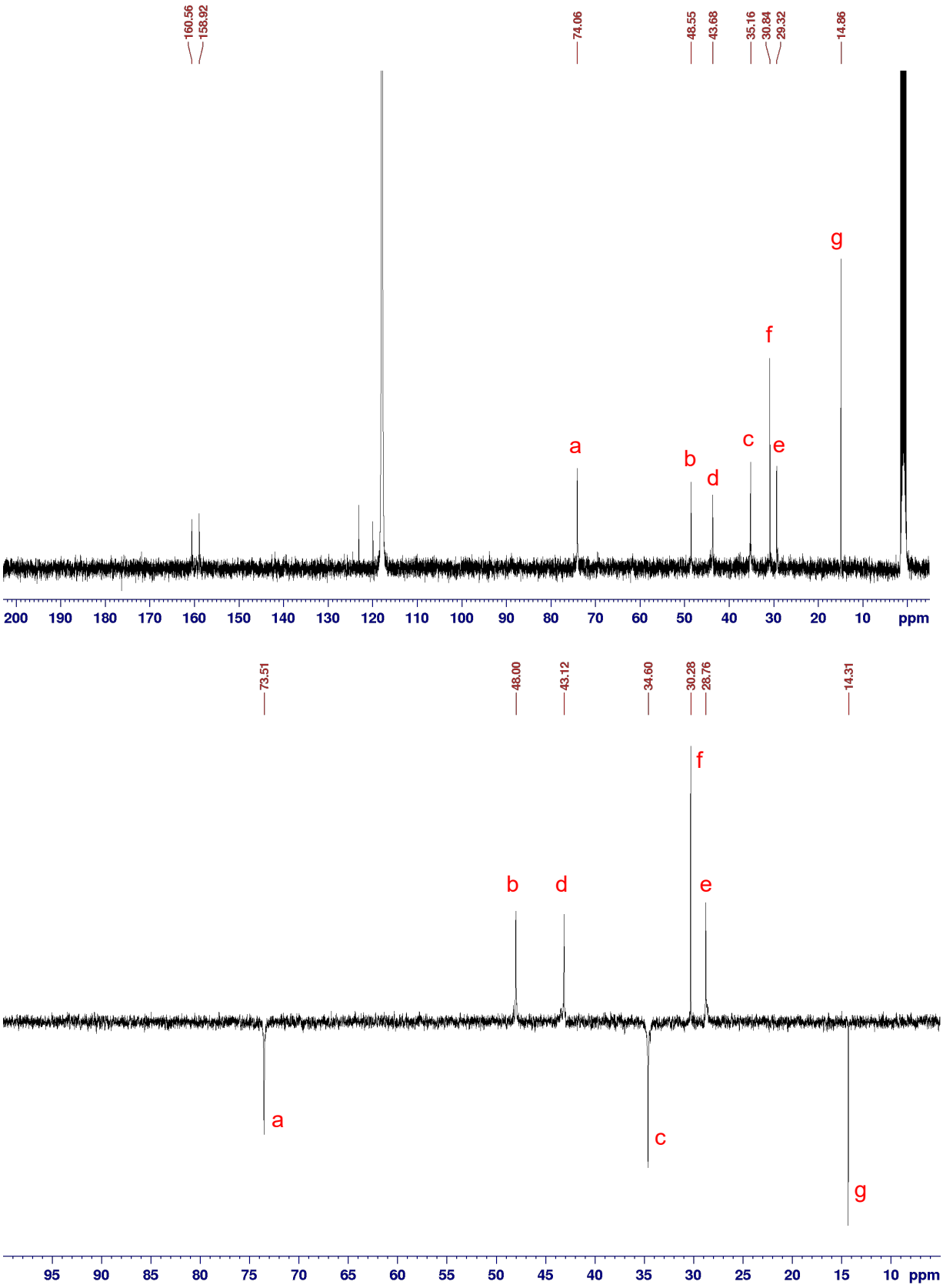

Fig. S16 NMR spectra of compound **3e**: *top* and *bottom*: ^{13}C NMR (100 MHz, acetonitrile-d_3) and DEPT experiment, respectively**.**

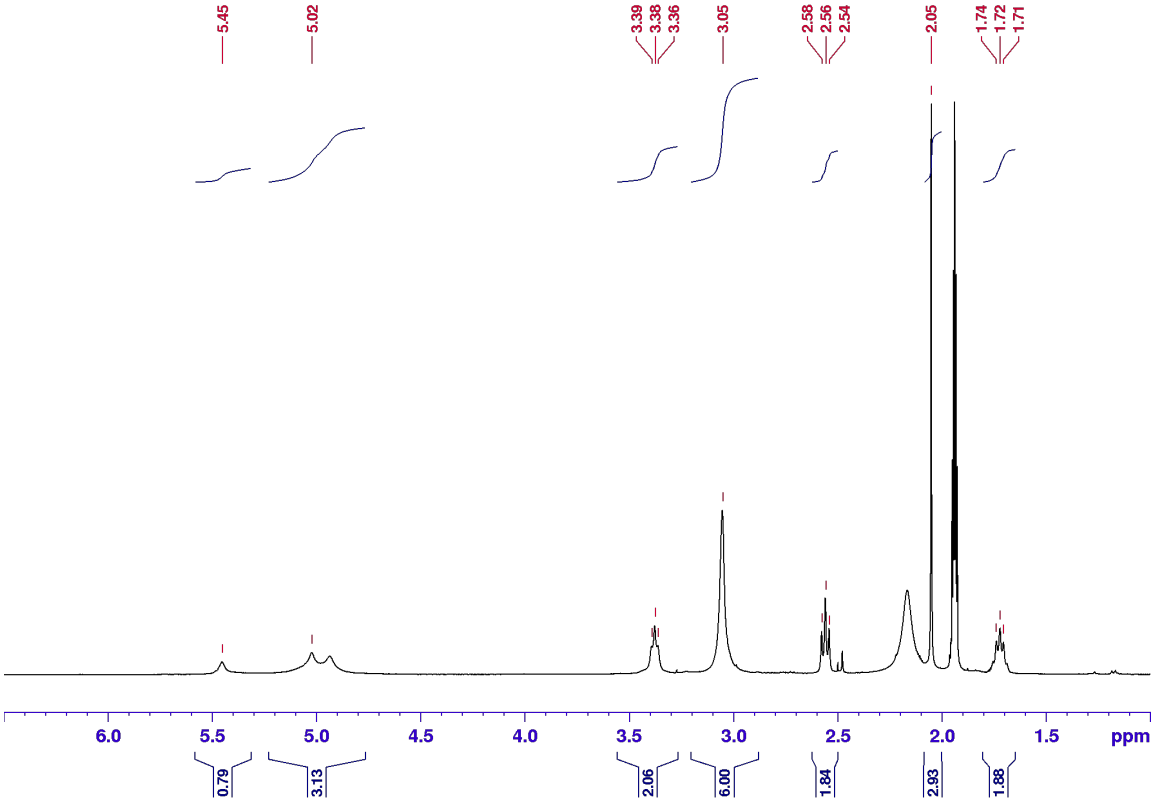

Fig. S17 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **4e**.

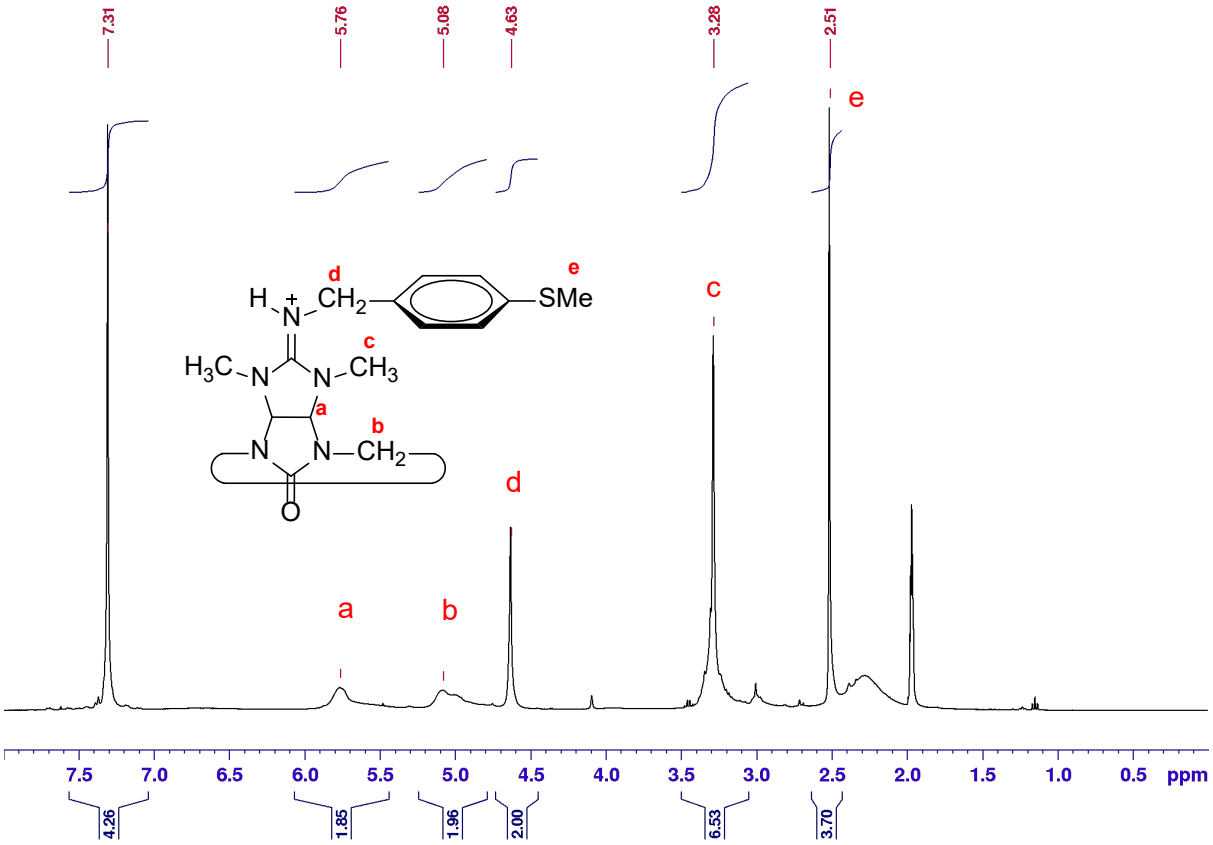

Fig. S18 ^{1}H NMR (400 MHz, acetonitrile-d_6) of compound **3f**.

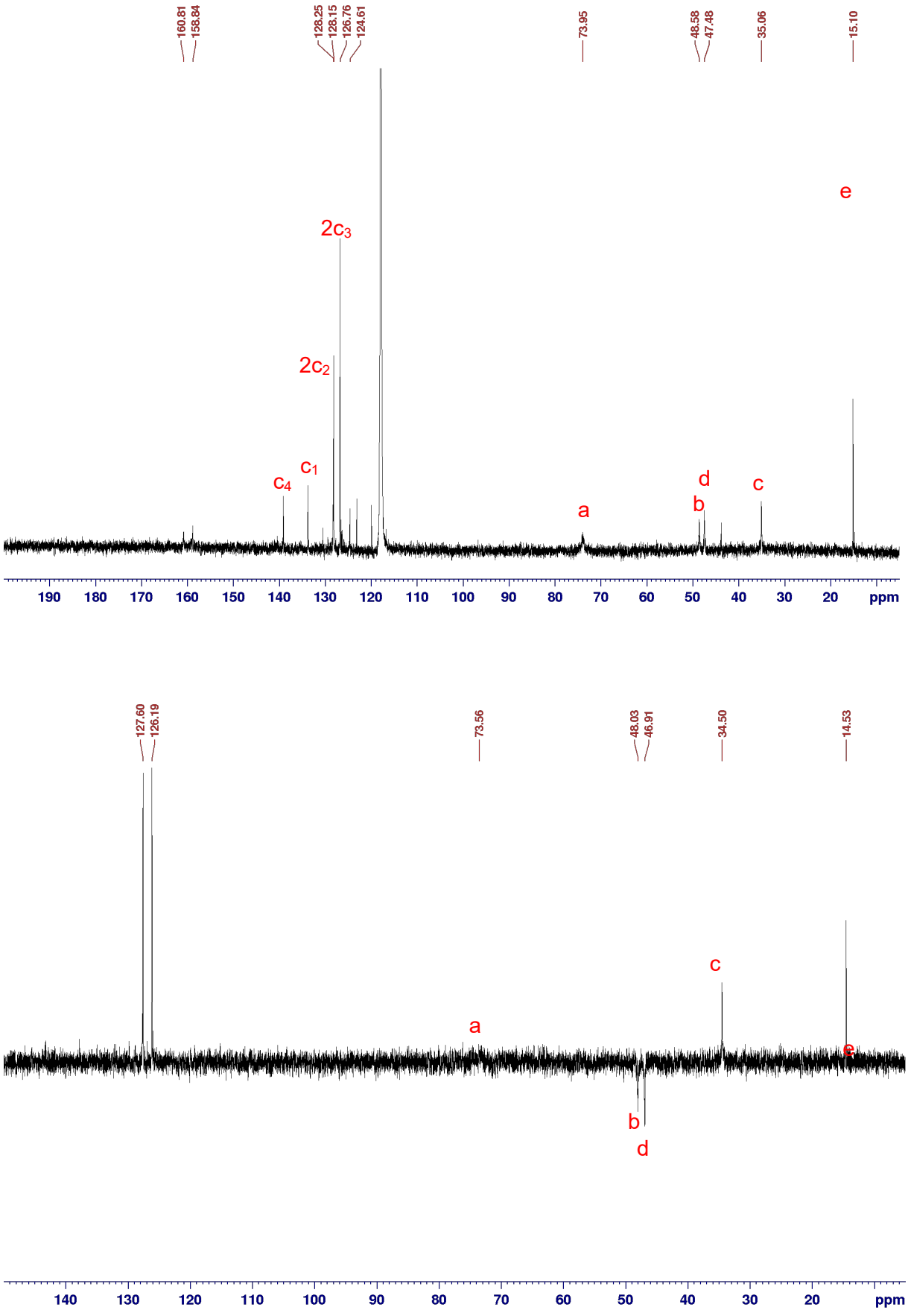

Fig. S19 NMR spectra of compound **3f**: *top* and *bottom*: ^{13}C NMR (100 MHz, acetonitrile-d_3) and DEPT experiment, respectively**.**

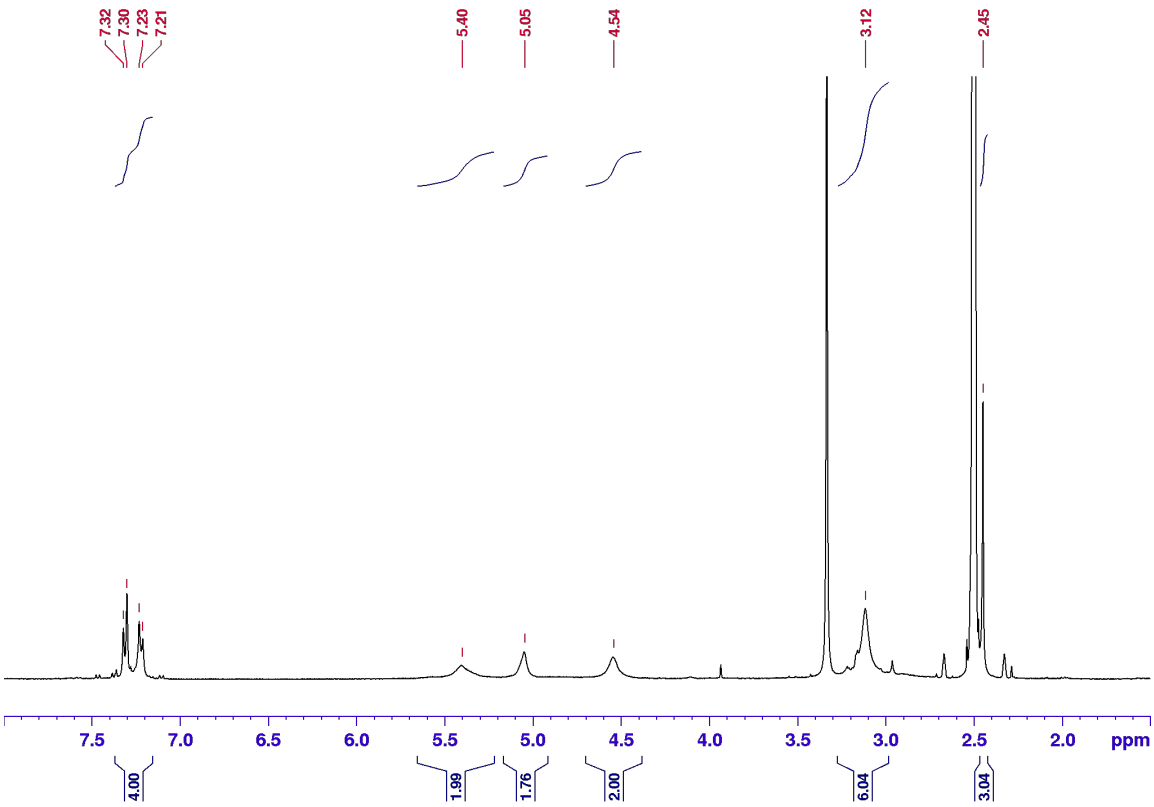

Fig. S20 ^{1}H NMR (400 MHz, DMSO-d_6) of compound **4f**.

4. X-ray crystallography

Crystals of *semithio*-BU[6] with tetraethylammonium chloride, **1** were obtained by standing a period in acetonitrile. A suitable single crystal was immersed in a drop of Paraton-N oil, mounted on a Bruker APEX II diffractometer, and kept at 200 (2) K during data collection. Data collection was performed by monochromatic Mo-K_α radiation (λ = 0.71073 Å) using φ and ω scans to cover the Ewald sphere. The crystal was kept Using Olex2; the structure was solved with the olex2.solve structure solution program, [3] using Charge Flipping and refined with SHELXL refinement package using Least Squares minimization.[4] Non-hydrogen atoms were refined with anisotropic displacement parameters (ADPs). The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Software used for molecular graphics: Mercury 2020.3.0.

CCDC 2111764 contains the supplementary crystallographic data for this study. This data can be obtained free of charge from the Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif. Pertinent crystallographic data and refinement parameters are summarized in Table S1.

Table S1: Crystallographic data for semi*thio*-BU[6]∗TEACl **1**.

Compound:	**1**
CCDC No.	2111764
empirical formula	$C_{42}H_{60}N_{24}O_6S_6$, $C_8H_{20}NCl$ (Et_4NCl), $C_4H_6N_2$ ($2\times CH_3CN$)
Mw	1437.30
crystal size (mm^3)	0.21 x 0.16 x 0.12
T (K)	200.15
crystal system	triclinic
space group	*P-1*
*a (*Å)	10.051(2)
b (Å)	13.150(3)
c (Å)	13.719(3)
α (°)	96.214(3)
β (°)	102.703(4)
γ (°)	95.675(5)
V ($Å^3$)	1744.3(7)
Z	1
$\rho_{calc.}$ ($g\ cm^{-3}$)	1.368
Final R indices ($I > 2\sigma(I)$) (all data)	$R_1 = 0.0611$ $R_1 = 0.1049$
Goodness-of-fit on F^2	1.029

5. Isothermal titration calorimetry (ITC):

ITC measurements were performed using Water's Nano ITC Low Volume Calorimeter (TA Instruments, USA) at 298 K in EtOH/acetonitrile (1:1). Data were obtained from each experiment consisting of 25 consecutive injections (2 μL each) of guest solutions of tetraethylammonium chloride (TEACl) (20-80 mM) into a fixed cylinder Hastelloy reaction cell (300 μL) charged with a solution of *semiaza*-BU[6], **4a-e** (8-13 mM).
All binding events were accompanied by the evolution or absorption of heat (a change in enthalpy, ΔH). In a single ITC experiment, a full thermodynamic characterization of the binding reactions was obtained, *i.e.*, the enthalpy (Δ*H*), entropy (Δ*S*), and overall Gibbs free energy (Δ*G*) of the reaction taking place in the calorimeter. The appropriate experimental design generates fundamental information about the molecular interactions driving the process and the binding constant (Ka). Data were analyzed using NanoAnalyze software v3.12.0

Each ITC titration figure includes calorimetric response as successive injections of the TEACl added to **4a-e** (upper panel) and integrated heat profiles of the calorimetric titration (lower panel) represent the enthalpy of complexation for each addition of anion. The solid line represents the best nonlinear independent fit of the experimental data.

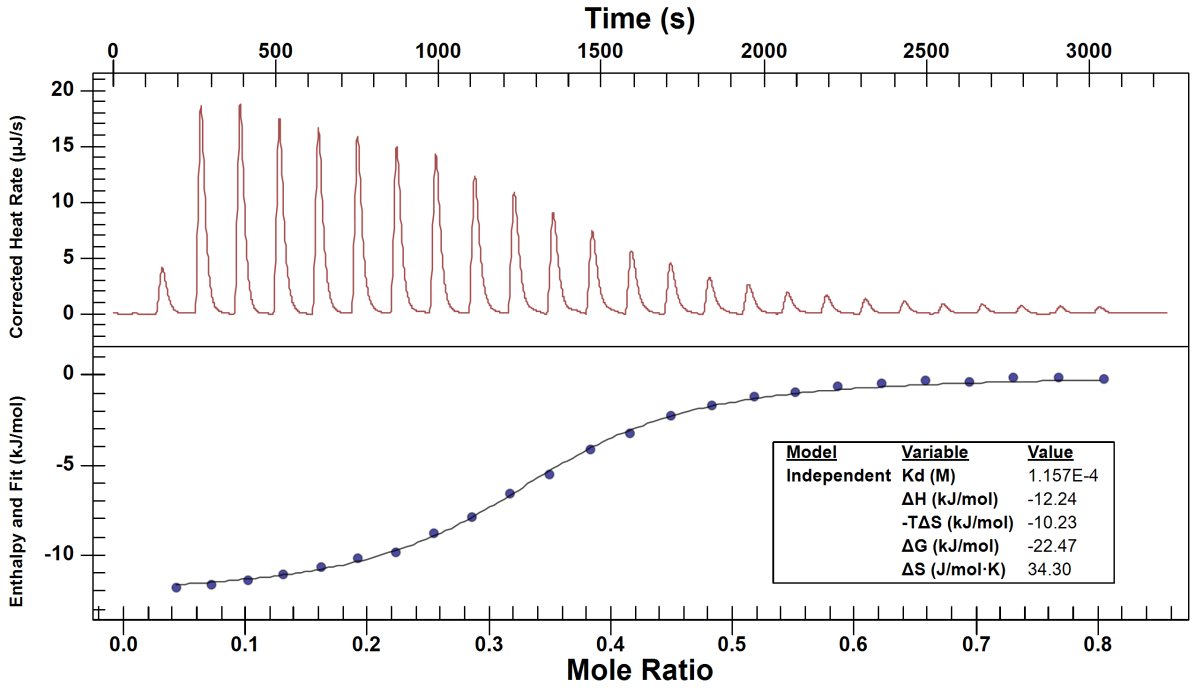

Fig. S21 ITC titration profile of host **4a** in solution (8 mM) of MeOH:$CHCl_3$ (1:1) mixture, with tetraethylammoniun chloride (TEACl) solution (20 mM) of the same solvent mixture at 298 K.

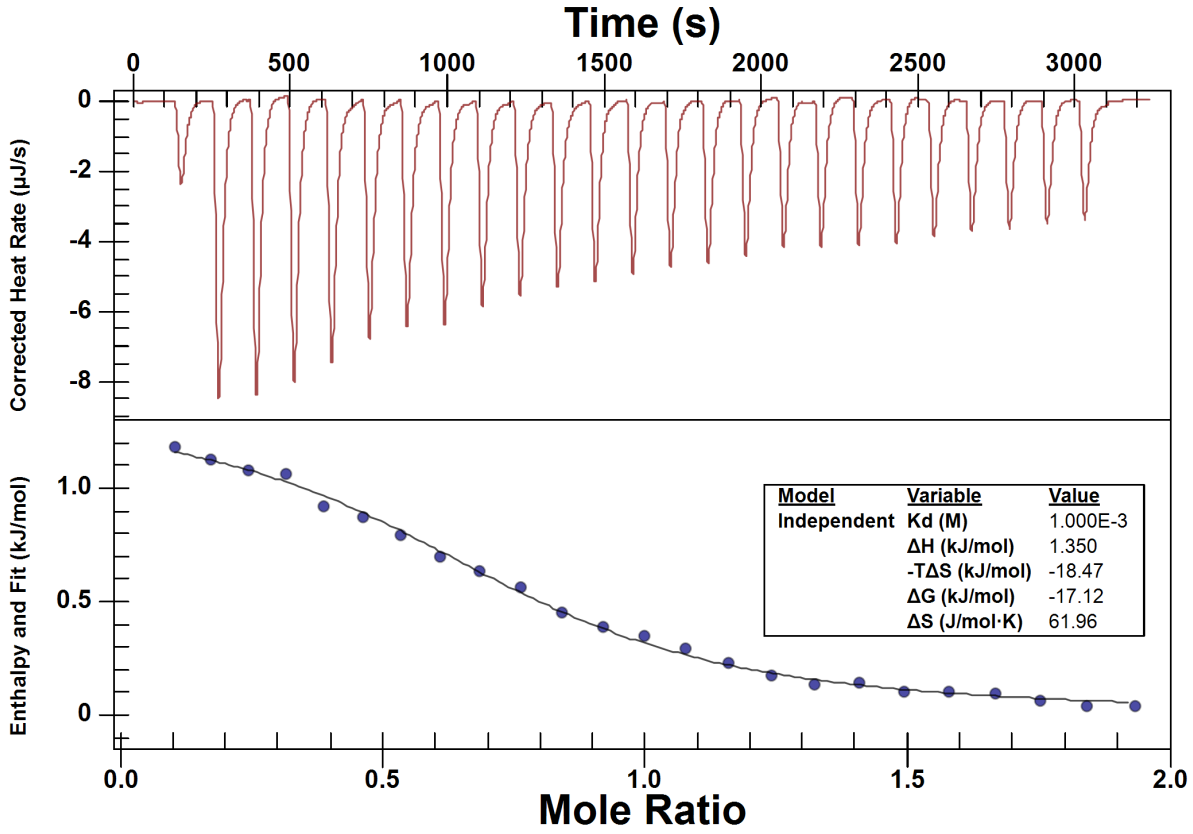

Fig. S22 ITC titration profile of host **4b** in solution (10 mM) of MeOH:$CHCl_3$ (1:1) mixture, with tetraethylammoniun chloride (TEACl) solution (60 mM) of the same solvent mixture at 298 K.

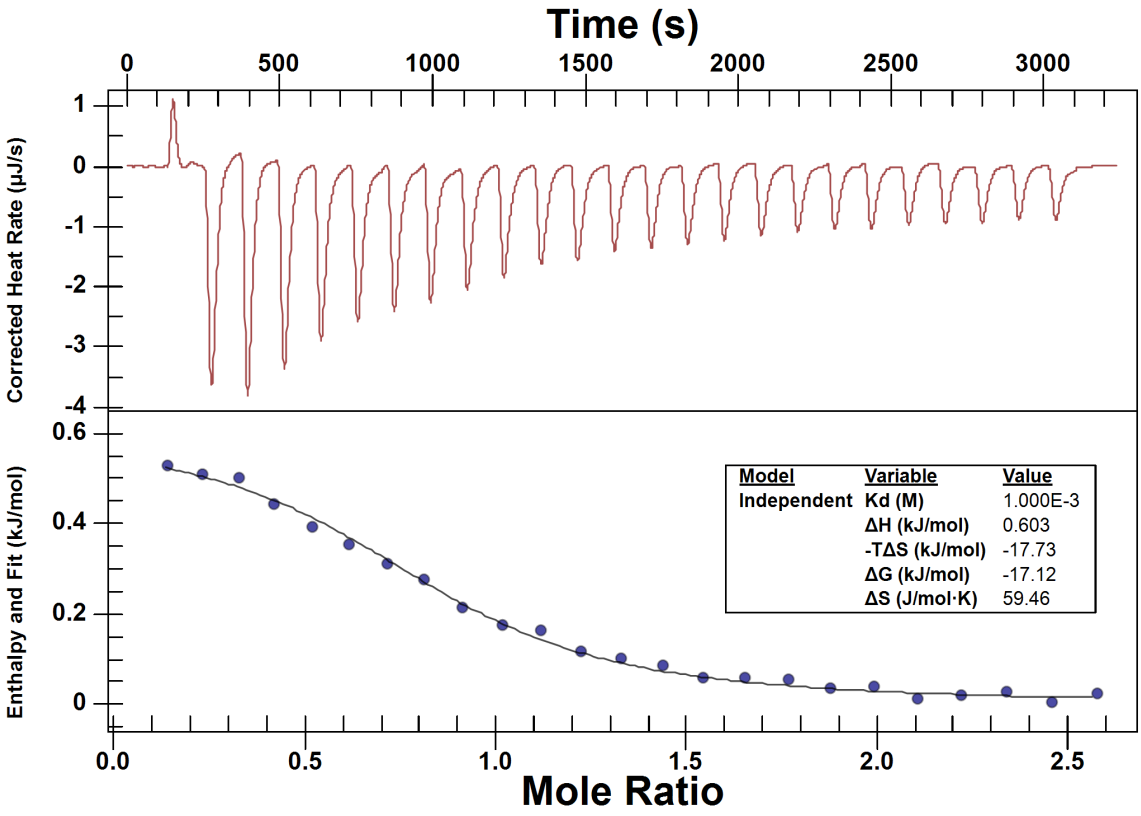

Fig. S23 ITC titration profile of host **4c** in solution (10 mM) of MeOH:$CHCl_3$ (1:1) mixture, with tetraethylammoniun chloride (TEACl) solution (80 mM) of the same solvent mixture at 298 K.

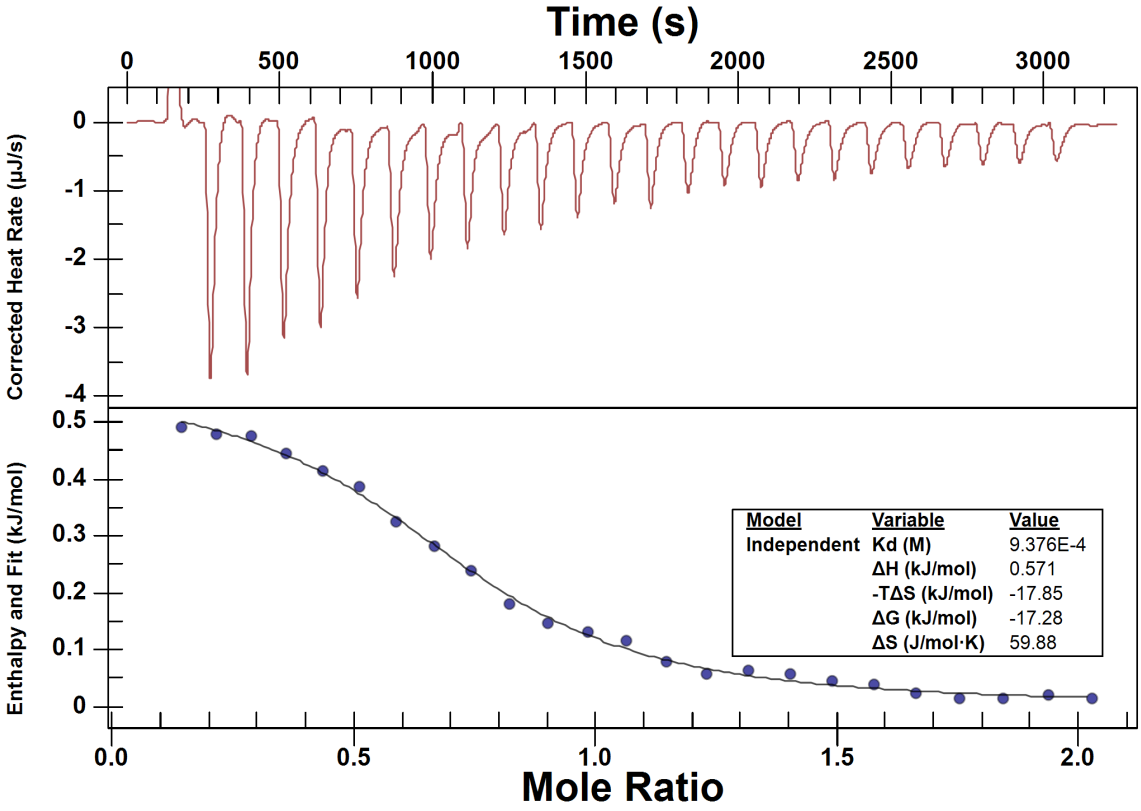

Fig. S24 ITC titration profile of host **4d** in solution (13 mM) of MeOH:$CHCl_3$ (1:1) mixture, with tetraethylammoniun chloride (TEACl) solution (80 mM) of the same solvent mixture at 298 K.

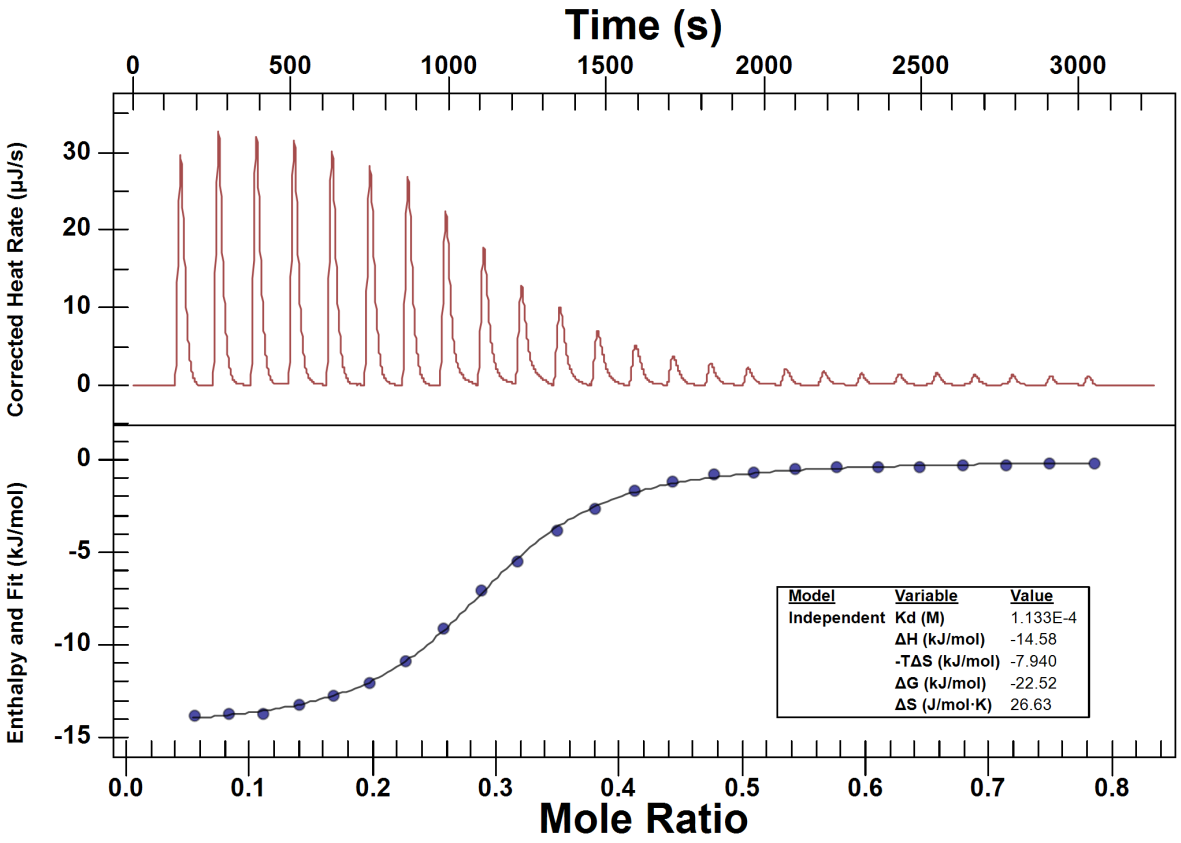

Fig. S25 ITC titration profile of host **4e** in solution (13 mM) of MeOH:$CHCl_3$ (1:1) mixture, with tetraethylammoniun chloride (TEACl) solution (30 mM) of the same solvent mixture at 298 K.

6. Chloride Transport experiments

Instruments

Fluorescence spectra were recorded with a Shimadzu RF-5301PC fluorimeter. All data from fluorescence studies were processed by OriginPro 2018 program. In addition, the pH measurements were recorded with a METTLER TOLEDO FiveEasyPlus FE28 pH meter.

6a. Vesicle preparation

EYPC LUVs (mean diameter 200 nm) loaded with the pH-sensitive HPTS (1 mM) fluorescence dye were prepared as follows:
In a clean, dry small round bottom flask, 3 mL of egg yolk phosphatidylcholine lipid (EYPC, 10 mg in $CHCl_3$) was dried by purging nitrogen gas with continuous rotation to form a thin transparent film of EYPC. The transparent film was kept in high vacuum for three hours to remove traces of $CHCl_3$ at room temperature. The resulting film was hydrated with 1 mL buffer (1 mM HPTS, 10 mM HEPES, 100 mM NaCl, pH = 7.0) for two hours at 40°C and subjected to freeze-thaw cycles (10 times). The resulting suspension was then extruded through a 0.22 µm pore-size polycarbonate membrane. Then, the extravesicular dyes were removed by gel filtration using Sephadex G-50 with buffer (10 mM HEPES, 100 mM NaCl, pH = 7.0). The obtained EYPC-LUV⊃HPTS vesicles were kept under 4°C and used within 24 hours.

6b. Chloride transporting activity studies across EYPC-LUV⊃HPTS

In a clean and dry fluorescent cuvette, 1950 µL of HEPES buffer (10 mM HEPES, 100 mM NaCl, pH = 8.0) was added, followed by the addition of 50 µL of EYPC-LUVs⊃HPTS to create the pH gradient between the extra and intravesicular system. The cuvette was placed in the fluorescence

instrument with slow stirring conditions. The time course of HPTS fluorescence emission intensity, F_t was observed at λ_{em} = 510 nm (λ_{ex} = 460 nm). Upon adding the anion carriers (**1** and **4a-f**, 1.25 μM**)**, the HPTS was immediately recorded. Finally, a solution of Triton X-100 (10 μL, 20% v/v) was added at t = 300 s to lyse vesicles to afford destruction of the pH gradient. For data analysis and comparison, time (X-axis) was normalized between the point of transporter addition, i.e., *t* = 0 s, and endpoint of the experiment, *i.e.*, the addition of Triton-X 100 at *t* = 300 s. Fluorescence intensities (*FI*) were normalized to fractional emission intensity using Eq. S1:

Eq. S1. $$I_F = \frac{F_t - F_0}{F_\infty - F_0}$$

where F_t = fluorescence intensity at a time *t*, F_0 = fluorescence intensity just after the transporter is added, and F_∞ = fluorescence intensity at saturation after complete leakage.

For chloride transport using the NMDG-Cl assay[5] see details in manuscript text.

6c. Cation selectivity assay

In a clean and dry fluorescent cuvette, 1950 μL of HEPES buffer (10 mM HEPES, 100 mM MCl, pH = 8.0; where M^+ = Li^+, Na^+, K^+, Rb^+, and Cs^+) was added followed by addition of 50 μL of EYPC-LUVs⊃HPTS at pH = 7.0, to generate the necessary pH gradient between the extra and intravesicular system. The cuvette was placed in the fluorescence instrument with slow stirring conditions. Then, a solution of **4c** in DMSO (0.25 μM) was injected into the suspended solution under gentle stirring conditions (at *t* = 0 s). Upon addition, HPTS emission was immediately monitored (510 nm) following excitation at 460 nm, and the transport activity was recorded for 300 s before 20 v/v-% of Triton X-100 (10 μL) was added to afford a maximum change in fluorescence intensity. For data analysis and comparison, time (X-axis) was normalized between the point of transporter addition, i.e., *t* = 0 s, and endpoint of the experiment, *i.e.*, the addition of Triton-X 100 at *t* = 300 s. Fluorescence intensities (*FI*) were normalized to fractional emission intensity using Eq. S1.

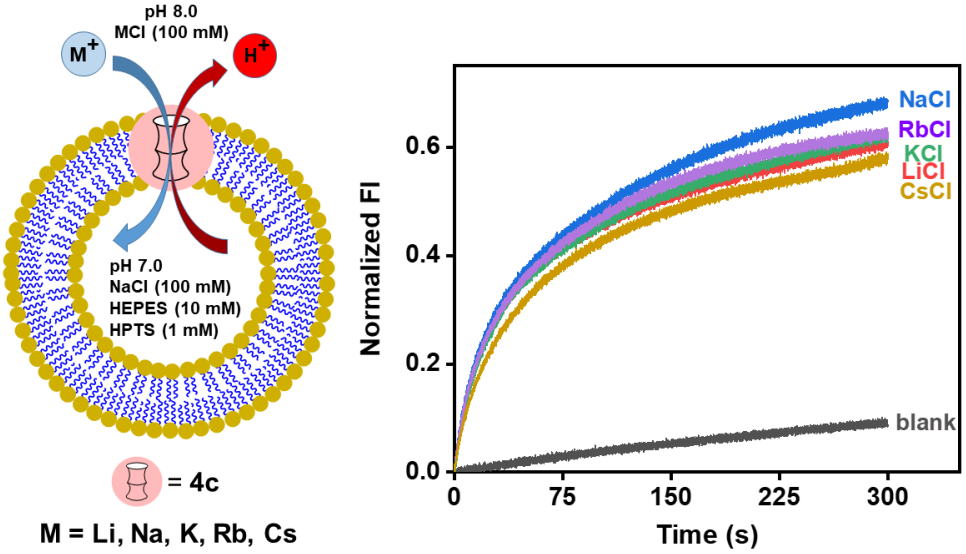

Fig. S26 *Left*: Schematic representation of the fluorescence-based cation selectivity assay. *Right*: Monitoring Cl^- transport activity of **4c** carrier (0.25 μM) following HPTS assay with various extravesicular chloride salts, *i.e.,* MCl (M = Li, Na, K, Rb and Cs). The fluorescence emission at 510 nm ($\lambda_{ex.}$ = 460 nm) was recorded for 300 s immediately after the addition of the carrier. All fluorescence curves are normalized, considering the starting point as zero fluorescence (FI = fluorescence intensity). A DMSO blank (grey) was used as a control.

6d. Hill plot analysis using SPQ assay[6].

Liposome preparation: Egg yolk L-α-phosphatidylcholine (EYPC, 10 mg, 13 μmol) was dissolved in $CHCl_3$ (3 mL) and dried with N_2 flow to form a thin lipid film. The resulting thin film was dried under high vacuum for 3 h. The lipid was then hydrated with $NaNO_3$ solution (1 mL, 200 mM) containing a chloride-sensitive dye 6-methoxy N-(3-sulfopropyl) quinolinium (SPQ) (0.5 mM) for two hours at 40°C followed by ten freeze-thaw cycles using liquid nitrogen and thermostat water bath. The resulting suspension was then extruded through 0.22 μm polycarbonate membrane before being purified by Sephadex G-50 to remove the extra vesicular dye using $NaNO_3$ solution (200 mM) as elute. The obtained vesicles were kept under 4 °C and used within 24 hours. The lipid concentration in each sample was 0.1 mM.

Fluorescent assay: The SPQ-containing LUV suspension (50 μL in 200 mM $NaNO_3$) was added to a NaCl solution (1.95 mL, 200 mM) to create an extravesicular chloride gradient. A solution of **4c** in DMSO (5 μL) at different concentrations was then injected into the suspension under gentle stirring. Upon addition of **4c**, the emission of SPQ was immediately monitored at 430 nm with excitation wavelength at 360 nm for 300 s. The time between adding the anion carriers and reading fluorescence intensities is less than 1 s. Finally, a solution of Triton X-100 (10 μL, 20% v/v) was added at t = 300 s to lyse vesicles to afford destruction of the chloride gradient. For data analysis and comparison, time (X-axis) was normalized between the point of transporter addition, i.e., t = 0 s, and endpoint of the experiment, *i.e.*, the addition of Triton-X 100 at t = 300 s. Fluorescence intensities (*FI*) were normalized to fractional emission intensity using Eq. S1.

Hill analysis: Fitting the fractional transmembrane activity I_{Cl^-} vs. carrier concentration (mol% compared to lipids) using the Hill equation $Y = 1/(1+ (EC_{50}/[C])^n)$ gave the Hill coefficient n and EC_{50} values.

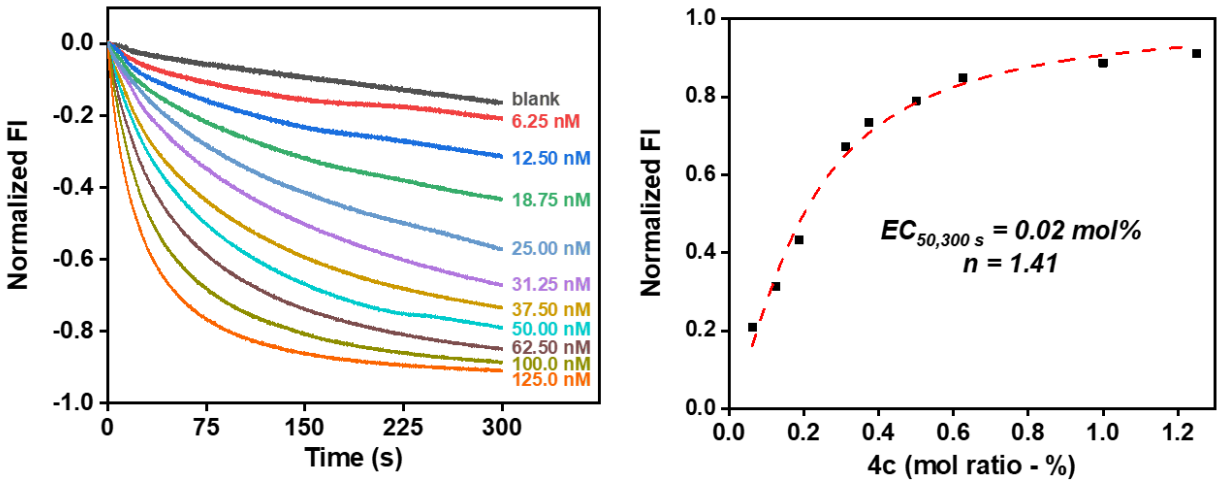

Fig. S27 SPQ assay for quantitative measurement of chloride transport with **4c**. *Left*: Normalized fluorescence intensity (FI) obtained by adding different concentrations of **4c**, and *Right:* Hill analysis of Cl^- transport facilitated by **4c**.[7]

Similar SPQ assay was performed to verify the transport seletivity of Cl^- over SO_4^{2-} :

Liposome preparation: Egg yolk L-α-phosphatidylcholine (EYPC, 10 mg, 13 μmol) was dissolved in $CHCl_3$ (3 mL) and dried with N_2 flow to form a thin lipid film. The resulting thin film was dried under high vacuum for 3 h. The lipid was then hydrated with $NaSO_4$ solution (1 mL, 100 mM) containing a chloride-sensitive dye 6-methoxy N-(3-sulfopropyl) quinolinium (SPQ) (0.5 mM) for two hours at 40°C followed by ten freeze-thaw cycles using liquid nitrogen and thermostat water bath. The resulting suspension was then extruded through 0.22 μm polycarbonate membrane before being purified by Sephadex G-50 to remove the extra vesicular dye using $NaSO_4$ solution (100 mM) as elute. The obtained vesicles were kept under 4 °C and used within 24 hours. The lipid concentration in each sample was 0.1 mM.

Fluorescent assay: The SPQ-containing LUV suspension (50 μL in 100 mM $NaSO_4$) was added to a NaCl solution (1.95 mL, 200 mM) to create an extravesicular chloride gradient. A solution of **4c** in DMSO (5 μL) at different concentrations was then injected into the suspension under gentle stirring. Upon addition of **4c**, the emission of SPQ was immediately monitored at 430 nm with excitation wavelength at 360 nm for 300 s. The time between adding the anion carriers and reading fluorescence intensities is less than 1 s. Finally, a solution of Triton X-100 (10 μL, 20% v/v) was added at t = 300 s to lyse vesicles to afford destruction of the chloride gradient. For data analysis and comparison, time (X-axis) was normalized between the point of transporter addition, i.e., *t* = 0 s, and endpoint of the experiment, *i.e.*, the addition of Triton-X 100 at *t* = 300 s. Fluorescence intensities (*FI*) were normalized to fractional emission intensity using Eq. S1.

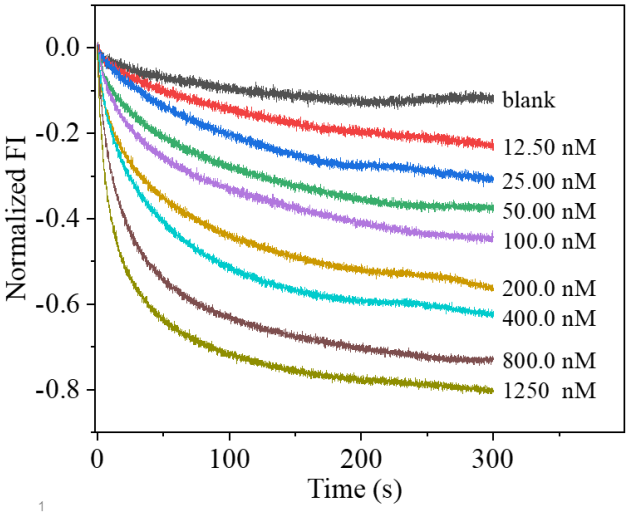

Fig. S28 SPQ assay following addition of different concentrations of **4c**. The changes in Normalized fluorescence intensity (FI) indicate that the tansport of sulphate anions by **4c** is significantly week.

6e. Anion selectivity following "dual gradient" type assay.

In a clean and dry fluorescent cuvette, 1950 μL of HEPES buffer (10 mM HEPES, pH = 6.4; 100 mM NaX, where X^- = Cl^-, Br^-, NO_3^-, and SO_4^{2-}) was added followed by addition of 50 μL of EYPC-LUVs⊃HPTS at pH = 7.0, to generate the necessary pH gradient between the extra and intravesicular system. First, the cuvette was placed in the fluorescence instrument with slow stirring conditions. Then, a solution of **4c** (50 nM) and FCCP (100 nM) in DMSO was injected into the suspended solution under gentle stirring conditions (at *t* = 0 s). Upon addition, HPTS emission was immediately monitored (510 nm) following excitation at 460 nm, and the transport activity was recorded for 300 s before 20 v/v-% of Triton X-100 (10 μL) was added to afford a maximum

change in fluorescence intensity. For data analysis and comparison, time (X-axis) was normalized between the point of transporter addition, i.e., t = 0 s, and endpoint of the experiment, *i.e.*, the addition of Triton-X 100 at t = 300 s. Fluorescence intensities (*FI*) were normalized to fractional emission intensity using Eq. S1.

6f. Anion selectivity following "anion gradient" assay.

Vesicle preparation: Anion gradient assays were conducted using POPC LUVs (mean diameter 200 nm) loaded with the pH-sensitive fluorescence dye HPTS (1 mM). The HPTS-loaded POPC LUVs were prepared as follows: a chloroform solution of POPC (10 mg) was evaporated in a round-bottom flask and the lipid film formed was dried under vacuum for at least 3 h. The resulting film was hydrated with 1 mL buffer solution (pH = 7.0) containing 1 mM HPTS, 10 mM HEPES and 100 mM NaCl for two hours at 40°C and subjected to freeze-thaw cycles (10 times). The resulting suspension was then extruded through a 0.22 μm pore-size polycarbonate membrane. Then, the extravesicular dyes were removed by gel filtration using Sephadex G-50 with buffer (10 mM HEPES, 100 mM NaCl, pH = 7.0). The obtained vesicles were kept under 4°C and used within 24 hours.

Fluorescent assay: The NaCl-containing vesicles were diluted using NaX (100 mM) external solutions to obtain $NaCl^{in}/NaX^{out}$ vesicles suspended in 2.0 mL samples containing 0.1 mM of POPC. No base pulse was added so no pH gradient was initially present. An anion transporter (added in 5 μL of DMSO) was added at time 0 to induce fluorecence intensity (FI^{in}) changes. The FI^{in} was monitored folloing the fluorescence response of HPTS (λ_{ex} = 460 nm, λ_{em} = 510 nm).

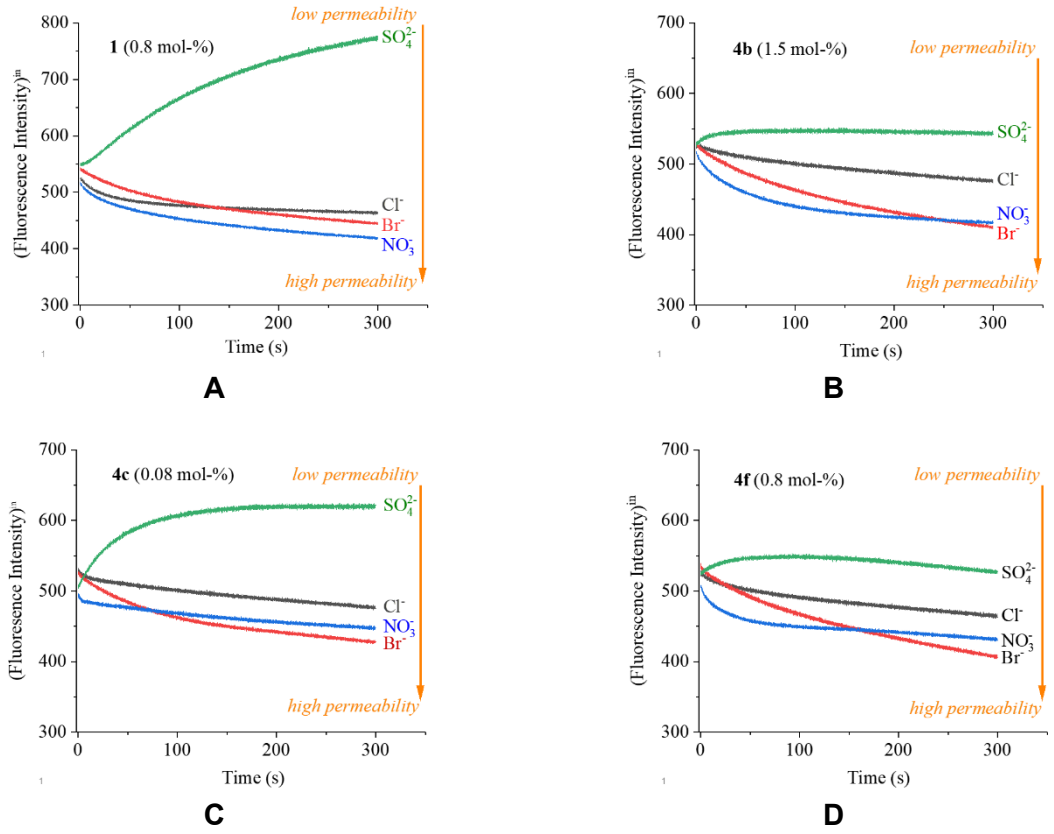

Fig. S29 Anion selectivity assays (**A-D**) with transpoters **1** and **4b,c,f** respectively, following anion gradient assay approach.

7. Lipophilicity determination

All calculations were carried out using the Gaussian 09 program. The initial structures of **4a-f** were such that their side-chains were oriented in a zigzag conformation. Structure optimizations were carried out in the gas phase, followed by water and octanol solvents, respectively, with the SMD model for the overall solvation effect. Lipophilicity was calculated in terms of the partition coefficient (Eq. 2):

Eq. 2. $$\text{clog } P = \frac{\Delta G(\text{water}) - \Delta G(\text{octanol})}{2.303RT}$$

The values of partition coefficients are calculated in an octanol-water mixture (Table S2).

Table S2: The partition coefficients (clog *P*) of *semiaza*-BU[6]l derivatives.

Compound	ΔG_{water} / Eh	$\Delta G_{octanol}$ / Eh	clog*P*
4a	-4673.224208	-4673.225311	0.5
4b	-4908.797849	-4908.802308	2.1
4c	-5379.940155	-5379.950400	4.7
4d	-6826.782670	-6826.774298	-3.8
4e	-7062.355274	-7062.358584	1.5
4f	-7976.193693	-7976.206772	6.0
1	-5788.396886	-5788.403541	3.1

DFT optimized the structures of **4a-f** and **1** using B97-D3B functional and 6-31g(d) basis set in the gas phase.

6.1 Optimized coordinates of **4a** ($C_{66}N_{30}H_{114}O_6$).

O	3.014922000	2.749158000	-3.627329000
O	1.087485000	5.317437000	1.085785000
O	0.988316000	1.100372000	4.975728000
N	-3.103614000	4.388330000	-2.842186000
N	-1.622708000	2.401623000	-3.018429000
N	0.785370000	2.045161000	-3.487910000
N	1.480507000	3.689470000	-2.135670000
N	-0.873494000	4.370011000	-2.178078000
N	6.100302000	2.447130000	1.919795000
N	3.850311000	1.976815000	2.364696000
N	1.798251000	3.337463000	2.102962000
N	2.519636000	3.797006000	0.034677000
N	4.400710000	2.266227000	0.151017000
N	-4.357040000	3.344324000	2.950842000
N	-2.166228000	2.997624000	2.261096000
N	-0.043126000	2.234487000	3.215328000
N	-0.962938000	0.330129000	3.954671000
N	-3.166079000	1.192728000	3.208576000
C	-2.009370000	3.743085000	-2.701487000
C	-0.290991000	2.149310000	-2.503665000
H	-0.306407000	1.244736000	-1.868804000
C	1.886744000	2.821258000	-3.139554000
C	0.109877000	3.427938000	-1.723173000

H	0.081265000	3.296710000	-0.628573000
C	-2.543441000	1.270171000	-2.897423000
H	-2.761919000	1.009943000	-1.843950000
H	-2.097548000	0.407519000	-3.401079000
H	-3.486898000	1.476801000	-3.398723000
C	0.869559000	1.023033000	-4.500514000
H	1.741749000	1.266733000	-5.114386000
H	-0.031334000	1.025881000	-5.124963000
C	2.442707000	4.380549000	-1.286089000
H	3.413387000	4.307623000	-1.787868000
H	2.159762000	5.429550000	-1.154681000
C	-0.859181000	5.760735000	-1.761320000
H	-0.159377000	6.344597000	-2.379743000
H	-0.551562000	5.844377000	-0.710555000
H	-1.873477000	6.151950000	-1.891855000
C	-4.319801000	3.846952000	-3.416534000
H	-4.850651000	4.678075000	-3.909348000
H	-4.139683000	3.099257000	-4.211288000
C	-5.244036000	3.264482000	-2.326630000
H	-5.521321000	4.076558000	-1.635636000
H	-4.678033000	2.538564000	-1.720396000
C	-6.502278000	2.584912000	-2.881526000
H	-6.207266000	1.783623000	-3.581298000
H	-7.085251000	3.310534000	-3.473375000
C	-7.378875000	1.990039000	-1.771849000
H	-7.713017000	2.770695000	-1.071021000
H	-6.816354000	1.241423000	-1.193540000
C	4.913020000	2.254364000	1.493422000
C	2.563539000	2.152620000	1.727703000
H	1.928369000	1.267408000	1.870190000
C	1.732604000	4.269344000	1.077098000
C	2.959844000	2.424075000	0.239661000
H	2.460516000	1.747457000	-0.471433000
C	4.013920000	2.163089000	3.800591000
H	4.976155000	1.728989000	4.090107000
H	3.194928000	1.661632000	4.327251000
H	4.022815000	3.232336000	4.071288000
C	4.848296000	1.170560000	-0.724901000
H	4.512806000	1.376292000	-1.748473000
H	4.462781000	0.183054000	-0.406319000
H	5.940471000	1.124357000	-0.719391000
C	0.850138000	3.370326000	3.208816000
H	1.371229000	3.354444000	4.171627000
H	0.291175000	4.307708000	3.109144000
C	7.178804000	2.821475000	1.017659000
H	7.569169000	3.792964000	1.368907000
H	6.849889000	2.980351000	-0.026117000
C	8.326774000	1.801374000	1.070139000
H	8.609401000	1.658545000	2.125701000
H	7.964356000	0.823664000	0.715914000
C	9.552000000	2.227589000	0.250497000
H	9.856753000	3.244190000	0.552904000
H	9.275722000	2.294775000	-0.815456000
C	10.739323000	1.269819000	0.416393000
H	10.466301000	0.245921000	0.122251000
H	11.072029000	1.236582000	1.465340000

C	-3.360914000	2.546758000	2.863972000
C	-1.144424000	2.001296000	2.266119000
H	-0.730238000	1.850793000	1.253227000
C	0.089420000	1.219725000	4.141837000
C	-1.829559000	0.725404000	2.853579000
H	-1.898760000	-0.107525000	2.135585000
C	-2.205091000	4.037121000	1.239668000
H	-2.405622000	3.624286000	0.233875000
H	-1.258927000	4.588286000	1.225888000
H	-3.020969000	4.717042000	1.500924000
C	-3.855122000	0.507680000	4.297493000
H	-3.484874000	0.825492000	5.286275000
H	-3.701565000	-0.571715000	4.184616000
H	-4.928883000	0.697151000	4.246140000
C	-5.688661000	2.972631000	3.391588000
H	-6.270376000	3.904603000	3.477303000
H	-5.696278000	2.527906000	4.404363000
C	-6.423359000	2.037446000	2.412810000
H	-5.839127000	1.113038000	2.277931000
H	-6.459350000	2.522155000	1.423959000
O	-3.014947000	-2.749015000	3.627167000
O	-1.087433000	-5.317313000	-1.085901000
O	-0.988330000	-1.100255000	-4.975851000
N	3.103530000	-4.388377000	2.842579000
N	1.622709000	-2.401578000	3.018499000
N	-0.785365000	-2.045087000	3.487857000
N	-1.480475000	-3.689400000	2.135607000
N	0.873518000	-4.369959000	2.178099000
N	-6.100337000	-2.447205000	-1.919799000
N	-3.850372000	-1.976786000	-2.364758000
N	-1.798261000	-3.337351000	-2.103052000
N	-2.519600000	-3.796919000	-0.034758000
N	-4.400735000	-2.266241000	-0.151059000
N	4.356996000	-3.344273000	-2.950926000
N	2.166199000	-2.997513000	-2.261205000
N	0.043106000	-2.234371000	-3.215448000
N	0.962951000	-0.330036000	-3.954824000
N	3.166062000	-1.192646000	-3.208692000
C	2.009352000	-3.743073000	2.701649000
C	0.291028000	-2.149253000	2.503653000
H	0.306488000	-1.244685000	1.868785000
C	-1.886747000	-2.821156000	3.139452000
C	-0.109822000	-3.427882000	1.723151000
H	-0.081174000	-3.296668000	0.628550000
C	2.543477000	-1.270153000	2.897486000
H	2.761957000	-1.009940000	1.844008000
H	2.097602000	-0.407487000	3.401138000
H	3.486928000	-1.476806000	3.398784000
C	-0.869574000	-1.022920000	4.500414000
H	-1.741776000	-1.266587000	5.114282000
H	0.031306000	-1.025752000	5.124883000
C	-2.442667000	-4.380475000	1.286000000
H	-3.413349000	-4.307556000	1.787774000
H	-2.159714000	-5.429474000	1.154589000
C	0.859184000	-5.760710000	1.761426000
H	0.159540000	-6.344578000	2.380026000

H	0.551338000	-5.844406000	0.710734000
H	1.873523000	-6.151879000	1.891766000
C	4.319650000	-3.847007000	3.417074000
H	4.850348000	-4.678094000	3.910110000
H	4.139420000	-3.099190000	4.211692000
C	5.244160000	-3.264745000	2.327289000
H	5.521625000	-4.076947000	1.636518000
H	4.678318000	-2.538939000	1.720772000
C	6.502262000	-2.585080000	2.882389000
H	6.207077000	-1.783716000	3.582002000
H	7.085114000	-3.310618000	3.474460000
C	7.379113000	-1.990328000	1.772845000
H	7.713377000	-2.771061000	1.072162000
H	6.816749000	-1.241741000	1.194346000
C	-4.913052000	-2.254407000	-1.493467000
C	-2.563583000	-2.152534000	-1.727782000
H	-1.928450000	-1.267295000	-1.870268000
C	-1.732581000	-4.269238000	-1.077199000
C	-2.959860000	-2.424008000	-0.239731000
H	-2.460556000	-1.747375000	0.471366000
C	-4.014010000	-2.163100000	-3.800649000
H	-4.976231000	-1.728969000	-4.090168000
H	-3.195011000	-1.661685000	-4.327337000
H	-4.022959000	-3.232355000	-4.071306000
C	-4.848377000	-1.170543000	0.724801000
H	-4.512820000	-1.376168000	1.748372000
H	-4.462985000	-0.183019000	0.406127000
H	-5.940560000	-1.124463000	0.719341000
C	-0.850168000	-3.370197000	-3.208925000
H	-1.371272000	-3.354316000	-4.171730000
H	-0.291210000	-4.307583000	-3.109271000
C	-7.178797000	-2.821505000	-1.017603000
H	-7.569028000	-3.793123000	-1.368646000
H	-6.849881000	-2.980107000	0.026216000
C	-8.326878000	-1.801542000	-1.070328000
H	-8.609474000	-1.658950000	-2.125931000
H	-7.964555000	-0.823729000	-0.716291000
C	-9.552101000	-2.227695000	-0.250657000
H	-9.856781000	-3.244369000	-0.552894000
H	-9.275863000	-2.294671000	0.815319000
C	-10.739473000	-1.270023000	-0.416775000
H	-10.466517000	-0.246053000	-0.122820000
H	-11.072143000	-1.237003000	-1.465741000
C	3.360890000	-2.546671000	-2.864078000
C	1.144404000	-2.001181000	-2.266239000
H	0.730224000	-1.850646000	-1.253348000
C	-0.089413000	-1.219628000	-4.141984000
C	1.829559000	-0.725309000	-2.853711000
H	1.898753000	0.107636000	-2.135734000
C	2.205021000	-4.037046000	-1.239816000
H	2.405557000	-3.624248000	-0.234007000
H	1.258840000	-4.588182000	-1.226049000
H	3.020887000	-4.716978000	-1.501083000
C	3.855216000	-0.507479000	-4.297454000
H	3.485218000	-0.825329000	-5.286315000
H	3.701463000	0.571890000	-4.184588000

H	4.929001000	-0.696759000	-4.245887000
C	5.688606000	-2.972662000	-3.391775000
H	6.270209000	-3.904687000	-3.477673000
H	5.696187000	-2.527794000	-4.404484000
C	6.423478000	-2.037695000	-2.412919000
H	5.839383000	-1.113214000	-2.277909000
H	6.459427000	-2.522521000	-1.424125000
C	7.840599000	-1.687508000	-2.885857000
H	8.424740000	-2.616049000	-3.001203000
H	7.787608000	-1.233673000	-3.890771000
C	8.571897000	-0.734505000	-1.933547000
H	8.653009000	-1.168591000	-0.926502000
H	8.033617000	0.220973000	-1.839218000
C	-7.840438000	1.687093000	2.885750000
H	-8.424664000	2.615570000	3.001209000
H	-7.787374000	1.233160000	3.890614000
C	-8.571681000	0.734128000	1.933357000
H	-8.652890000	1.168342000	0.926376000
H	-8.033304000	-0.221279000	1.838870000
H	11.596646000	1.580140000	-0.199203000
H	8.271355000	-1.493166000	2.179974000
H	9.588618000	-0.508478000	-2.286382000
H	-11.596802000	-1.580273000	0.198847000
H	-9.588357000	0.507939000	2.286218000
H	-8.271185000	1.492876000	-2.178827000

6.2 Optimized coordinates of **4b** ($C_{72}N_{30}H_{126}O_6$).

O	3.093174000	-3.088491000	3.224375000
O	1.107009000	-5.101317000	-1.737175000
O	0.923628000	-0.486727000	-5.127975000
N	-3.012059000	-4.772013000	2.283296000
N	-1.573058000	-2.798004000	2.744542000
N	0.833475000	-2.468277000	3.243181000
N	1.551812000	-3.861359000	1.645872000
N	-0.783072000	-4.614494000	1.640500000
N	6.067152000	-2.069160000	-2.328789000
N	3.804267000	-1.596784000	-2.686284000
N	1.780430000	-3.016412000	-2.548814000
N	2.528973000	-3.678582000	-0.546455000
N	4.393254000	-2.125531000	-0.527851000
N	-4.389040000	-2.973784000	-3.199462000
N	-2.181041000	-2.679796000	-2.537215000
N	-0.095871000	-1.827281000	-3.508810000
N	-0.998504000	0.166413000	-3.979287000
N	-3.187078000	-0.820419000	-3.366200000
C	-1.933155000	-4.089378000	2.242201000
C	-0.251969000	-2.446855000	2.262266000
H	-0.290301000	-1.459581000	1.766181000
C	1.954960000	-3.136132000	2.757601000
C	0.164979000	-3.589879000	1.302049000
H	0.107600000	-3.304978000	0.237920000
C	-2.519657000	-1.683139000	2.801202000
H	-2.753271000	-1.270686000	1.800990000
H	-2.091078000	-0.893657000	3.426246000
H	-3.453812000	-1.988670000	3.269173000

C	0.923093000	-1.572601000	4.367482000
H	1.805890000	-1.876316000	4.938249000
H	0.030898000	-1.658890000	4.998045000
C	2.509316000	-4.414200000	0.697202000
H	3.492030000	-4.365390000	1.178335000
H	2.258123000	-5.450890000	0.451884000
C	-0.748508000	-5.932430000	1.028948000
H	-0.100933000	-6.612423000	1.604834000
H	-0.363745000	-5.865618000	0.003385000
H	-1.771351000	-6.323891000	1.026974000
C	-4.258431000	-4.352650000	2.892121000
H	-4.769920000	-5.261060000	3.251222000
H	-4.128870000	-3.713829000	3.785686000
C	-5.177091000	-3.663822000	1.861862000
H	-5.328531000	-4.359723000	1.021280000
H	-4.657663000	-2.789419000	1.436653000
C	-6.528933000	-3.228187000	2.438609000
H	-6.367779000	-2.531809000	3.280829000
H	-7.048057000	-4.105798000	2.861883000
C	-7.436464000	-2.555555000	1.397443000
H	-7.558827000	-3.232039000	0.534278000
H	-6.933139000	-1.652350000	1.011646000
C	-8.813978000	-2.178710000	1.955511000
H	-9.445657000	-1.710445000	1.187626000
H	-8.721048000	-1.466216000	2.788596000
H	-9.343333000	-3.068138000	2.330890000
C	4.884432000	-1.949354000	-1.864567000
C	2.530823000	-1.864138000	-2.056307000
H	1.877874000	-0.980684000	-2.093447000
C	1.738003000	-4.050471000	-1.623927000
C	2.952934000	-2.287325000	-0.609938000
H	2.458920000	-1.696213000	0.177555000
C	3.950605000	-1.635159000	-4.136233000
H	4.892949000	-1.142350000	-4.395245000
H	3.107060000	-1.112817000	-4.599534000
H	3.990837000	-2.671968000	-4.510584000
C	4.854935000	-1.154125000	0.477303000
H	4.542200000	-1.496661000	1.471311000
H	4.458861000	-0.135835000	0.300927000
H	5.946277000	-1.098664000	0.456473000
C	0.807319000	-2.946837000	-3.632745000
H	1.307385000	-2.831354000	-4.599871000
H	0.257612000	-3.894702000	-3.613017000
C	7.165745000	-2.548989000	-1.505236000
H	7.553925000	-3.459947000	-1.994740000
H	6.860439000	-2.852445000	-0.486726000
C	8.310208000	-1.525367000	-1.442660000
H	8.511840000	-1.179220000	-2.468650000
H	7.983638000	-0.637829000	-0.877353000
C	9.591728000	-2.103587000	-0.827448000
H	9.867790000	-3.022617000	-1.373921000
H	9.397502000	-2.415904000	0.213484000
C	10.780224000	-1.131561000	-0.856682000
H	10.535094000	-0.236227000	-0.262960000
H	10.931616000	-0.779120000	-1.890717000
C	12.080057000	-1.755005000	-0.331991000

H	12.909915000	-1.033261000	-0.353646000
H	12.373383000	-2.624865000	-0.939895000
H	11.965503000	-2.102230000	0.706531000
C	-3.383943000	-2.189573000	-3.091874000
C	-1.158012000	-1.685934000	-2.496609000
H	-0.703949000	-1.625869000	-1.491510000
C	0.038352000	-0.702654000	-4.299069000
C	-1.863053000	-0.366202000	-2.941328000
H	-1.958896000	0.375594000	-2.132582000
C	-2.200510000	-3.789133000	-1.592522000
H	-2.363988000	-3.447540000	-0.554242000
H	-1.262093000	-4.350707000	-1.650226000
H	-3.033803000	-4.439244000	-1.873785000
C	-3.837438000	-0.083477000	-4.444397000
H	-3.349413000	-0.262812000	-5.416884000
H	-3.797930000	0.987530000	-4.211593000
H	-4.885642000	-0.375192000	-4.521421000
C	-5.722839000	-2.564146000	-3.598515000
H	-6.337927000	-3.477121000	-3.647106000
H	-5.743716000	-2.145549000	-4.623055000
C	-6.403193000	-1.578700000	-2.628459000
H	-5.779587000	-0.678280000	-2.519931000
H	-6.451262000	-2.042606000	-1.630546000
O	-3.093380000	3.088189000	-3.224329000
O	-1.106830000	5.101165000	1.737121000
O	-0.923721000	0.486594000	5.128013000
N	3.011781000	4.772072000	-2.283916000
N	1.572940000	2.797875000	-2.744807000
N	-0.833606000	2.468203000	-3.243420000
N	-1.551956000	3.860942000	-1.645843000
N	0.782826000	4.614473000	-1.641007000
N	-6.067067000	2.069508000	2.329033000
N	-3.804246000	1.596820000	2.686513000
N	-1.780344000	3.016360000	2.548937000
N	-2.528898000	3.678413000	0.546549000
N	-4.393219000	2.125430000	0.528015000
N	4.388874000	2.973699000	3.199731000
N	2.180994000	2.679666000	2.537113000
N	0.095940000	1.827293000	3.509056000
N	0.998312000	-0.166585000	3.979192000
N	3.186876000	0.820322000	3.366307000
C	1.932950000	4.089343000	-2.242654000
C	0.251869000	2.446724000	-2.262521000
H	0.290184000	1.459440000	-1.766465000
C	-1.955122000	3.135891000	-2.757666000
C	-0.165023000	3.589731000	-1.302275000
H	-0.107385000	3.304921000	-0.238137000
C	2.519606000	1.683060000	-2.801469000
H	2.753261000	1.270691000	-1.801251000
H	2.091073000	0.893527000	-3.426471000
H	3.453753000	1.988646000	-3.269469000
C	-0.923274000	1.572432000	-4.367637000
H	-1.806078000	1.876104000	-4.938411000
H	-0.031090000	1.658674000	-4.998219000
C	-2.509342000	4.413931000	-0.697173000
H	-3.492110000	4.365092000	-1.178200000

H	-2.258095000	5.450641000	-0.451985000
C	0.748583000	5.932237000	-1.029009000
H	0.101850000	6.612827000	-1.605131000
H	0.363003000	5.865247000	-0.003772000
H	1.771634000	6.323164000	-1.026136000
C	4.258260000	4.352625000	-2.892461000
H	4.769772000	5.260975000	-3.251679000
H	4.128845000	3.713603000	-3.785895000
C	5.176773000	3.664047000	-1.861907000
H	5.328022000	4.360118000	-1.021424000
H	4.657307000	2.789706000	-1.436638000
C	6.528748000	3.228334000	-2.438286000
H	6.367796000	2.531885000	-3.280479000
H	7.048022000	4.105888000	-2.861499000
C	7.435936000	2.555725000	-1.396800000
H	7.557890000	3.232160000	-0.533538000
H	6.932514000	1.652452000	-1.011280000
C	8.813717000	2.179016000	-1.954294000
H	9.445069000	1.710707000	-1.186159000
H	8.721220000	1.466599000	-2.787485000
H	9.343199000	3.068512000	-2.329336000
C	-4.884379000	1.949492000	1.864795000
C	-2.530786000	1.864078000	2.056525000
H	-1.877880000	0.980608000	2.093736000
C	-1.737868000	4.050335000	1.623956000
C	-2.952885000	2.287160000	0.610128000
H	-2.458877000	1.695997000	-0.177325000
C	-3.950589000	1.635222000	4.136463000
H	-4.892998000	1.142525000	4.395462000
H	-3.107099000	1.112803000	4.599770000
H	-3.990727000	2.672039000	4.510797000
C	-4.854871000	1.153610000	-0.476769000
H	-4.541254000	1.495283000	-1.470793000
H	-4.459610000	0.135169000	-0.299425000
H	-5.946268000	1.098932000	-0.456672000
C	-0.807303000	2.946836000	3.632915000
H	-1.307405000	2.831353000	4.600021000
H	-0.257584000	3.894698000	3.613194000
C	-7.165661000	2.549151000	1.505375000
H	-7.553956000	3.460123000	1.994756000
H	-6.860326000	2.852516000	0.486850000
C	-8.310002000	1.525388000	1.442829000
H	-8.511658000	1.179290000	2.468831000
H	-7.983279000	0.637853000	0.877606000
C	-9.591532000	2.103433000	0.827479000
H	-9.867949000	3.022244000	1.374136000
H	-9.397119000	2.416092000	-0.213315000
C	-10.779798000	1.131116000	0.856143000
H	-10.534360000	0.236065000	0.262117000
H	-10.931294000	0.778252000	1.890018000
C	-12.079682000	1.754457000	0.331451000
H	-12.909359000	1.032490000	0.352611000
H	-12.373360000	2.623972000	0.939679000
H	-11.964990000	2.102158000	-0.706894000
C	3.383814000	2.189459000	3.091978000
C	1.157898000	1.685866000	2.496671000

H	0.703670000	1.625812000	1.491652000
C	-0.038442000	0.702547000	4.299117000
C	1.862915000	0.366105000	2.941310000
H	1.958816000	-0.375652000	2.132533000
C	2.200635000	3.788766000	1.592158000
H	2.364381000	3.446944000	0.553988000
H	1.262180000	4.350305000	1.649539000
H	3.033801000	4.439027000	1.873458000
C	3.837337000	0.083113000	4.444246000
H	3.349503000	0.262320000	5.416856000
H	3.797630000	-0.987849000	4.211259000
H	4.885593000	0.374656000	4.521144000
C	5.722639000	2.564088000	3.598929000
H	6.337599000	3.477126000	3.648007000
H	5.743389000	2.145069000	4.623298000
C	6.403297000	1.579157000	2.628564000
H	5.779991000	0.678552000	2.519776000
H	6.451162000	2.043387000	1.630793000
C	7.805422000	1.176714000	3.101702000
H	8.443891000	2.074726000	3.168454000
H	7.740148000	0.774614000	4.128801000
C	8.488109000	0.133867000	2.205871000
H	8.572615000	0.532247000	1.181503000
H	7.845134000	-0.760435000	2.136063000
C	9.874217000	-0.272244000	2.721905000
H	9.810402000	-0.667417000	3.747568000
H	10.329183000	-1.047377000	2.091109000
H	10.557474000	0.590716000	2.740052000
C	-7.805179000	-1.175938000	-3.101763000
H	-8.444012000	-2.073725000	-3.168025000
H	-7.739784000	-0.774393000	-4.129072000
C	-8.487364000	-0.132318000	-2.206445000
H	-8.571881000	-0.530065000	-1.181830000
H	-7.844018000	0.761768000	-2.137262000
C	-9.873378000	0.274056000	-2.722516000
H	-10.327892000	1.049800000	-2.092145000
H	-9.809558000	0.668546000	-3.748445000
H	-10.557026000	-0.588606000	-2.739997000

6.3 Optimized coordinates of **4c** ($C_{84}N_{30}H_{150}O_6$).

O	2.584583000	-5.304429000	1.869504000
O	0.485140000	-4.925123000	-3.427562000
O	1.014461000	0.543268000	-5.024202000
N	-3.661744000	-5.458200000	0.457476000
N	-1.965217000	-4.109244000	1.677803000
N	0.435722000	-4.429680000	2.220332000
N	1.025797000	-5.054756000	0.150151000
N	-1.381042000	-5.495709000	-0.012891000
N	5.775904000	-1.790901000	-2.519894000
N	3.533193000	-1.665204000	-3.115204000
N	1.342746000	-2.753756000	-3.442430000
N	2.044775000	-4.166988000	-1.851378000
N	3.951679000	-2.772873000	-1.168247000
N	-4.760109000	-1.429707000	-3.596642000
N	-2.509414000	-1.796271000	-3.127570000

N	-0.311486000	-1.066839000	-3.962543000
N	-0.768511000	1.100376000	-3.628910000
N	-3.114249000	0.386075000	-3.296284000
C	-2.489487000	-5.023586000	0.713819000
C	-0.583405000	-3.818400000	1.360783000
H	-0.431756000	-2.724257000	1.317354000
C	1.472798000	-4.971589000	1.459912000
C	-0.315249000	-4.524714000	0.010116000
H	-0.351293000	-3.842007000	-0.856555000
C	-2.730667000	-3.000309000	2.243246000
H	-2.880783000	-2.171592000	1.525837000
H	-2.198587000	-2.620768000	3.122000000
H	-3.709170000	-3.339799000	2.580921000
C	0.661593000	-4.037589000	3.592301000
H	1.482031000	-4.662137000	3.960937000
H	-0.236735000	-4.209406000	4.195385000
C	1.926574000	-5.306619000	-0.967151000
H	2.899938000	-5.553538000	-0.529787000
H	1.567925000	-6.139411000	-1.581003000
C	-1.534362000	-6.411968000	-1.129801000
H	-0.760395000	-7.191132000	-1.080755000
H	-1.446541000	-5.896111000	-2.096456000
H	-2.525911000	-6.866457000	-1.042919000
C	-4.897837000	-5.073294000	1.110006000
H	-5.588693000	-5.928026000	1.022453000
H	-4.801013000	-4.880355000	2.194148000
C	-5.538154000	-3.867989000	0.392896000
H	-5.539680000	-4.086854000	-0.686618000
H	-4.897036000	-2.980037000	0.518694000
C	-6.965327000	-3.545765000	0.851868000
H	-6.974883000	-3.300983000	1.928239000
H	-7.594355000	-4.445149000	0.733894000
C	-7.583925000	-2.390847000	0.049571000
H	-7.451201000	-2.597427000	-1.026775000
H	-7.022235000	-1.462301000	0.253124000
C	-9.074785000	-2.158945000	0.331012000
H	-9.212661000	-1.840671000	1.379006000
H	-9.615707000	-3.115796000	0.225932000
C	4.556145000	-2.065533000	-2.250956000
C	2.214122000	-1.945349000	-2.608351000
H	1.679495000	-1.018382000	-2.337664000
C	1.210926000	-4.048973000	-2.962244000
C	2.521958000	-2.862866000	-1.391555000
H	1.978563000	-2.564182000	-0.478986000
C	3.788979000	-1.251835000	-4.484643000
H	4.796727000	-0.825923000	-4.517548000
H	3.049989000	-0.503910000	-4.792716000
H	3.741990000	-2.109426000	-5.177282000
C	4.354835000	-2.534150000	0.221594000
H	3.876167000	-3.287621000	0.855863000
H	4.076624000	-1.526224000	0.581333000
H	5.432782000	-2.648901000	0.334702000
C	0.428665000	-2.211055000	-4.440836000
H	0.972718000	-1.871264000	-5.328945000
H	-0.247280000	-3.028825000	-4.713829000
C	6.906481000	-2.243562000	-1.731676000

H	7.712348000	-2.502755000	-2.439454000
H	6.705621000	-3.163500000	-1.151006000
C	7.427361000	-1.121743000	-0.815020000
H	7.546092000	-0.220936000	-1.432739000
H	6.662673000	-0.870991000	-0.061284000
C	8.752968000	-1.450504000	-0.119067000
H	9.518114000	-1.681777000	-0.880228000
H	8.641015000	-2.363614000	0.491781000
C	9.243157000	-0.299081000	0.769962000
H	8.480682000	-0.090522000	1.537491000
H	9.320218000	0.620145000	0.164223000
C	10.591139000	-0.565902000	1.451059000
H	11.358905000	-0.759675000	0.681350000
H	10.522511000	-1.488536000	2.053890000
C	-3.597781000	-0.936462000	-3.390374000
C	-1.301016000	-1.083163000	-2.868867000
H	-0.822227000	-1.446880000	-1.941995000
C	0.081246000	0.220650000	-4.290243000
C	-1.734388000	0.411329000	-2.800221000
H	-1.707888000	0.824920000	-1.779948000
C	-2.713750000	-3.148489000	-2.632035000
H	-2.742393000	-3.187812000	-1.528420000
H	-1.918027000	-3.808426000	-2.996871000
H	-3.679770000	-3.494126000	-3.010743000
C	-3.543039000	1.480981000	-4.160249000
H	-2.921857000	1.544910000	-5.068736000
H	-3.474130000	2.427010000	-3.607231000
H	-4.578889000	1.327884000	-4.464271000
C	-5.972086000	-0.649214000	-3.776238000
H	-6.798994000	-1.370055000	-3.885259000
H	-5.950910000	-0.092882000	-4.733858000
C	-6.341511000	0.322465000	-2.637813000
H	-5.523687000	1.035952000	-2.463673000
H	-6.454980000	-0.250231000	-1.705231000
O	-2.264162000	3.803010000	-1.687249000
O	0.089267000	3.358931000	3.501330000
O	-0.801068000	-2.068115000	5.136725000
N	3.784486000	4.465351000	-1.037680000
N	2.263133000	2.675900000	-1.783277000
N	-0.154779000	2.893445000	-2.134435000
N	-0.580712000	3.635719000	-0.068682000
N	1.873371000	3.833624000	0.153494000
N	-5.427255000	1.313391000	3.250812000
N	-3.305453000	0.339269000	3.310023000
N	-1.045084000	1.317284000	3.599443000
N	-1.548824000	2.745498000	1.953599000
N	-3.717892000	1.736487000	1.533743000
N	4.927679000	-0.322944000	4.104346000
N	2.706682000	0.342568000	3.257762000
N	0.534184000	-0.457775000	4.084626000
N	0.976451000	-2.620607000	3.730757000
N	3.298176000	-1.855203000	3.442391000
C	2.754831000	3.715445000	-0.924481000
C	0.929474000	2.314669000	-1.348217000
H	0.833051000	1.216063000	-1.318807000
C	-1.129358000	3.480819000	-1.335944000

C	0.718132000	2.979903000	0.041650000
H	0.671980000	2.257862000	0.869690000
C	3.125457000	1.525618000	-2.089715000
H	3.209891000	0.821813000	-1.239631000
H	2.713649000	0.997772000	-2.955376000
H	4.130754000	1.856320000	-2.346068000
C	-0.422550000	2.511873000	-3.496775000
H	-1.234446000	3.154441000	-3.850455000
H	0.470184000	2.661508000	-4.114241000
C	-1.422496000	3.896951000	1.093971000
H	-2.405741000	4.191048000	0.710405000
H	-0.999028000	4.701932000	1.702178000
C	1.917592000	4.962857000	1.068304000
H	1.322429000	5.811794000	0.691489000
H	1.528810000	4.652813000	2.045406000
H	2.961824000	5.279500000	1.155755000
C	4.670105000	4.342262000	-2.185572000
H	4.909406000	5.359776000	-2.535505000
H	4.193840000	3.829522000	-3.042261000
C	5.986730000	3.630072000	-1.800973000
H	6.630603000	4.332162000	-1.249988000
H	5.756147000	2.817964000	-1.091515000
C	6.736897000	3.037287000	-3.001018000
H	6.101630000	2.263259000	-3.467266000
H	6.890949000	3.807112000	-3.776128000
C	8.085665000	2.407714000	-2.612465000
H	8.842375000	3.199427000	-2.480157000
H	7.983847000	1.922854000	-1.626834000
C	8.586541000	1.365030000	-3.621170000
H	7.838771000	0.555723000	-3.692492000
H	8.647363000	1.816641000	-4.626903000
C	-4.275078000	1.165058000	2.722063000
C	-1.988197000	0.571759000	2.765760000
H	-1.515802000	-0.375507000	2.465658000
C	-0.745631000	2.564560000	3.067922000
C	-2.280128000	1.545816000	1.573764000
H	-1.919774000	1.164046000	0.604748000
C	-3.484456000	-0.118001000	4.683174000
H	-4.509773000	-0.485968000	4.786750000
H	-2.768179000	-0.918023000	4.895872000
H	-3.340126000	0.705152000	5.403066000
C	-4.362929000	1.405235000	0.252539000
H	-3.943548000	2.044207000	-0.533777000
H	-4.226038000	0.344232000	-0.029236000
H	-5.435172000	1.602784000	0.319663000
C	-0.159925000	0.705250000	4.584755000
H	-0.720635000	0.374614000	5.464489000
H	0.559579000	1.482580000	4.866926000
C	-6.384819000	2.284951000	2.750988000
H	-6.635572000	2.941182000	3.603391000
H	-5.977310000	2.946877000	1.964039000
C	-7.691139000	1.629320000	2.271623000
H	-7.964075000	0.836983000	2.986461000
H	-7.527804000	1.126826000	1.302873000
C	-8.834185000	2.647699000	2.161463000
H	-9.033277000	3.064169000	3.164173000

H	-8.510688000	3.500326000	1.539428000
C	-10.131526000	2.065311000	1.587344000
H	-9.960937000	1.757197000	0.543409000
H	-10.392624000	1.144744000	2.136990000
C	-11.314878000	3.041606000	1.638936000
H	-11.535913000	3.292751000	2.691076000
H	-11.030040000	3.990445000	1.153951000
C	3.759602000	-0.551803000	3.637748000
C	1.508280000	-0.428043000	2.995726000
H	1.032204000	-0.068274000	2.067774000
C	0.134142000	-1.748192000	4.402823000
C	1.956249000	-1.917474000	2.920381000
H	1.941373000	-2.335043000	1.900608000
C	2.950748000	1.431828000	2.304808000
H	2.926078000	1.081509000	1.255081000
H	2.190711000	2.206812000	2.446509000
H	3.925570000	1.883762000	2.477199000
C	3.979310000	-3.015055000	3.991856000
H	3.604119000	-3.263040000	4.999277000
H	3.828326000	-3.876824000	3.331421000
H	5.043508000	-2.769337000	4.063637000
C	5.426059000	1.028747000	4.294383000
H	4.623207000	1.783926000	4.388465000
H	5.979241000	1.055265000	5.247344000
C	6.395605000	1.398487000	3.150314000
H	7.320032000	0.814028000	3.277673000
H	5.960937000	1.057661000	2.195392000
C	6.723800000	2.891664000	3.039182000
H	5.796848000	3.455173000	2.829029000
H	7.100370000	3.272970000	4.003888000
C	7.751241000	3.174236000	1.932702000
H	7.441881000	2.650071000	1.012269000
H	8.721000000	2.734021000	2.219081000
C	7.932105000	4.663059000	1.612537000
H	8.149988000	5.222272000	2.539493000
H	6.979073000	5.065537000	1.226824000
C	-7.632766000	1.089219000	-2.954115000
H	-8.485437000	0.390667000	-2.949111000
H	-7.574246000	1.488339000	-3.982620000
C	-7.918400000	2.258061000	-2.001291000
H	-7.911887000	1.902601000	-0.956956000
H	-7.097995000	2.993169000	-2.078515000
C	-9.258663000	2.946978000	-2.297378000
H	-9.331698000	3.147470000	-3.380855000
H	-10.082074000	2.250254000	-2.061398000
C	11.052826000	0.592639000	2.348104000
H	11.110883000	1.515367000	1.745296000
H	10.285547000	0.779896000	3.118876000
C	9.048421000	4.921877000	0.589614000
H	10.011057000	4.587770000	1.013473000
H	8.874975000	4.294293000	-0.299918000
C	9.948872000	0.762221000	-3.247314000
H	9.911997000	0.405972000	-2.204761000
H	10.717635000	1.553252000	-3.271640000
C	-9.464383000	4.260512000	-1.530942000
H	-9.338149000	4.075950000	-0.453090000

H	-8.669458000	4.971158000	-1.814308000
C	-12.583734000	2.497278000	0.967336000
H	-12.353126000	2.239469000	-0.080155000
H	-12.876820000	1.551821000	1.454084000
C	-9.706513000	-1.121385000	-0.607751000
H	-9.530835000	-1.431117000	-1.652147000
H	-9.185495000	-0.158634000	-0.484556000
C	-11.210192000	-0.929707000	-0.379358000
H	-11.625831000	-0.166520000	-1.053886000
H	-11.757829000	-1.868786000	-0.553739000
H	-11.416728000	-0.609104000	0.651914000
C	-13.755407000	3.486286000	1.007138000
H	-14.649386000	3.073394000	0.516681000
H	-14.026120000	3.737141000	2.044453000
H	-13.494324000	4.425926000	0.495945000
C	-10.837972000	4.894048000	-1.784778000
H	-10.977280000	5.121841000	-2.852980000
H	-11.647864000	4.213336000	-1.482271000
H	-10.960109000	5.831433000	-1.222032000
C	9.149093000	6.392538000	0.166159000
H	9.965734000	6.551218000	-0.553896000
H	8.213230000	6.729714000	-0.306379000
H	9.334583000	7.043432000	1.034737000
C	12.405652000	0.331769000	3.022618000
H	12.363704000	-0.567595000	3.656443000
H	13.196327000	0.172485000	2.273092000
H	12.709878000	1.176875000	3.657875000
C	10.363013000	-0.396078000	-4.163557000
H	9.628958000	-1.215423000	-4.113253000
H	10.424108000	-0.070134000	-5.213528000
H	11.344557000	-0.804434000	-3.880084000

6.4 Optimized coordinates of **4d** ($C_{60}N_{30}H_{102}S_6O_6$).

O	3.055371000	-2.885978000	3.517017000
O	1.637617000	-5.194827000	-1.449711000
O	1.344039000	-0.591526000	-4.844160000
N	-2.747076000	-4.765726000	2.656431000
N	-1.472974000	-2.648450000	2.658146000
N	0.885339000	-2.110887000	3.127977000
N	1.648570000	-3.833122000	1.906944000
N	-0.699967000	-4.500434000	1.574286000
N	6.553016000	-2.044814000	-1.869366000
N	4.294828000	-1.545914000	-2.212692000
N	2.374387000	-3.113563000	-2.222800000
N	2.924160000	-3.753121000	-0.142329000
N	4.850681000	-2.259999000	-0.105025000
N	-3.812720000	-3.544826000	-3.456385000
N	-1.644778000	-3.164730000	-2.710763000
N	0.457856000	-2.003352000	-3.212329000
N	-0.725373000	-0.198973000	-3.839131000
N	-2.849401000	-1.290154000	-3.159796000
C	-1.755457000	-4.015591000	2.344302000
C	-0.165881000	-2.296809000	2.133864000
H	-0.252795000	-1.391152000	1.509096000
C	1.979054000	-2.939155000	2.922417000

C	0.335484000	-3.534086000	1.336375000
H	0.454004000	-3.339892000	0.260637000
C	-2.492583000	-1.611824000	2.452704000
H	-2.747818000	-1.478928000	1.382921000
H	-2.103742000	-0.673582000	2.852680000
H	-3.406156000	-1.822745000	3.008274000
C	0.794113000	-1.202860000	4.247678000
H	1.669104000	-1.397655000	4.874991000
H	-0.121590000	-1.388111000	4.822941000
C	2.708662000	-4.448103000	1.108507000
H	3.615874000	-4.424948000	1.720511000
H	2.448680000	-5.480370000	0.858946000
C	-0.518861000	-5.911921000	1.280983000
H	0.103134000	-6.404526000	2.046586000
H	-0.036623000	-6.016835000	0.301653000
H	-1.507611000	-6.380828000	1.271971000
C	-3.828962000	-4.266080000	3.487854000
H	-4.193050000	-5.099629000	4.106633000
H	-3.505256000	-3.476776000	4.188378000
C	-4.995878000	-3.752541000	2.606362000
H	-5.616108000	-4.589225000	2.257227000
H	-4.587428000	-3.253853000	1.716941000
C	5.360713000	-1.964442000	-1.408026000
C	3.021158000	-1.930519000	-1.650875000
H	2.307802000	-1.096012000	-1.686705000
C	2.248892000	-4.138026000	-1.292502000
C	3.402943000	-2.379995000	-0.201928000
H	2.919519000	-1.769120000	0.575476000
C	4.472986000	-1.421975000	-3.656258000
H	5.346394000	-0.791789000	-3.847508000
H	3.583083000	-0.954164000	-4.089422000
H	4.639335000	-2.405366000	-4.125241000
C	5.327844000	-1.440254000	1.021290000
H	4.951043000	-1.871953000	1.955443000
H	4.984580000	-0.390131000	0.948028000
H	6.419929000	-1.444428000	1.058733000
C	1.461346000	-3.040750000	-3.357368000
H	2.007782000	-2.805633000	-4.275422000
H	0.997904000	-4.028817000	-3.449437000
C	7.635764000	-2.562844000	-1.049267000
H	8.097011000	-3.404758000	-1.589473000
H	7.306356000	-2.960896000	-0.073876000
C	8.702327000	-1.472425000	-0.857196000
H	9.184722000	-1.255637000	-1.821086000
H	8.229072000	-0.547668000	-0.501970000
C	-2.892878000	-2.697589000	-3.174034000
C	-0.753173000	-2.088138000	-2.387869000
H	-0.469713000	-2.115595000	-1.321521000
C	0.451200000	-0.908208000	-4.059169000
C	-1.537299000	-0.793365000	-2.780954000
H	-1.636634000	-0.066732000	-1.957682000
C	-1.603081000	-4.403450000	-1.934333000
H	-1.895447000	-4.232223000	-0.881867000
H	-0.597013000	-4.832288000	-1.960456000
H	-2.315214000	-5.097286000	-2.389027000
C	-3.698278000	-0.418696000	-3.972493000

H	-3.508388000	-0.547045000	-5.049952000
H	-3.491018000	0.622910000	-3.706397000
H	-4.758255000	-0.597734000	-3.771871000
C	-5.167626000	-3.165557000	-3.810719000
H	-5.679721000	-4.061859000	-4.188597000
H	-5.210059000	-2.425345000	-4.627316000
C	-5.943437000	-2.637825000	-2.586091000
H	-5.313857000	-1.940450000	-2.012615000
H	-6.215854000	-3.469248000	-1.920202000
O	-3.054932000	2.885990000	-3.516487000
O	-1.637348000	5.194474000	1.450392000
O	-1.344605000	0.590609000	4.844214000
N	2.747370000	4.765502000	-2.656429000
N	1.473270000	2.648240000	-2.658164000
N	-0.885104000	2.110430000	-3.127367000
N	-1.647837000	3.833137000	-1.906655000
N	0.700826000	4.499880000	-1.573294000
N	-6.553251000	2.045075000	1.868958000
N	-4.295173000	1.545657000	2.212247000
N	-2.374648000	3.113210000	2.222999000
N	-2.923698000	3.753123000	0.142446000
N	-4.850740000	2.260663000	0.104824000
N	3.812388000	3.544415000	3.458104000
N	1.644391000	3.164505000	2.712455000
N	-0.458359000	2.002617000	3.212574000
N	0.725164000	0.198518000	3.839714000
N	2.849213000	1.289832000	3.160676000
C	1.755915000	4.015263000	-2.344037000
C	0.166364000	2.296456000	-2.133539000
H	0.253520000	1.390797000	-1.508799000
C	-1.978579000	2.939034000	-2.921932000
C	-0.334898000	3.533698000	-1.335883000
H	-0.453696000	3.339293000	-0.260217000
C	2.492935000	1.611503000	-2.453545000
H	2.748306000	1.477936000	-1.383878000
H	2.104112000	0.673495000	-2.854103000
H	3.406436000	1.822852000	-3.009066000
C	-0.794130000	1.202405000	-4.247096000
H	-1.669157000	1.397359000	-4.874307000
H	0.121543000	1.387508000	-4.822457000
C	-2.707850000	4.448287000	-1.108218000
H	-3.614988000	4.425553000	-1.720347000
H	-2.447563000	5.480416000	-0.858420000
C	0.519734000	5.911368000	-1.279924000
H	-0.102105000	6.404065000	-2.045597000
H	0.037349000	6.016211000	-0.300663000
H	1.508497000	6.380238000	-1.270711000
C	3.828903000	4.266112000	-3.488465000
H	4.192647000	5.099830000	-4.107216000
H	3.504929000	3.476944000	-4.189021000
C	4.996241000	3.752463000	-2.607591000
H	5.616584000	4.589116000	-2.258589000
H	4.588203000	3.253592000	-1.718082000
C	-5.360927000	1.964681000	1.407662000
C	-3.021415000	1.930334000	1.650699000
H	-2.308101000	1.095797000	1.686421000

C	-2.248717000	4.137774000	1.292869000
C	-3.402961000	2.380167000	0.201814000
H	-2.919704000	1.769230000	-0.575640000
C	-4.473471000	1.421222000	3.655758000
H	-5.346921000	0.791010000	3.846724000
H	-3.583628000	0.953216000	4.088835000
H	-4.639820000	2.404460000	4.125060000
C	-5.328085000	1.441601000	-1.021912000
H	-4.950861000	1.873482000	-1.955810000
H	-4.985335000	0.391286000	-0.948994000
H	-6.420159000	1.446328000	-1.059588000
C	-1.461873000	3.040017000	3.357739000
H	-2.008519000	2.804595000	4.275588000
H	-0.998422000	4.028037000	3.450272000
C	-7.635850000	2.563699000	1.049024000
H	-8.096945000	3.405460000	1.589593000
H	-7.306301000	2.962145000	0.073843000
C	-8.702632000	1.473591000	0.856376000
H	-9.185313000	1.256597000	1.820076000
H	-8.229507000	0.548840000	0.500970000
C	2.892569000	2.697246000	3.175466000
C	0.753051000	2.087894000	2.388744000
H	0.470103000	2.115731000	1.322271000
C	-0.451638000	0.907478000	4.059450000
C	1.537175000	0.793076000	2.781675000
H	1.636585000	0.066582000	1.958287000
C	1.602828000	4.403382000	1.936236000
H	1.895206000	4.232274000	0.883749000
H	0.596799000	4.832297000	1.962378000
H	2.315017000	5.097067000	2.391071000
C	3.698259000	0.418176000	3.972989000
H	3.508793000	0.546500000	5.050523000
H	3.490725000	-0.623378000	3.706934000
H	4.758195000	0.597035000	3.771969000
C	5.167431000	3.165034000	3.811826000
H	5.679642000	4.061182000	4.189907000
H	5.210170000	2.424486000	4.628102000
C	5.942807000	2.637848000	2.586675000
H	5.312865000	1.941035000	2.012912000
H	6.215330000	3.469602000	1.921247000
C	-8.152911000	-1.320228000	-1.516455000
H	-8.911219000	-0.542726000	-1.671896000
H	-8.610003000	-2.193303000	-1.029939000
H	-7.368331000	-0.914588000	-0.864959000
C	-11.254604000	0.761094000	-0.017472000
H	-12.087782000	0.957395000	-0.703843000
H	-10.878082000	-0.255186000	-0.199058000
H	-11.617801000	0.838572000	1.016485000
C	-6.699105000	-1.592679000	2.087285000
H	-5.884995000	-1.238143000	1.439459000
H	-7.399714000	-2.203835000	1.502575000
H	-7.219807000	-0.712722000	2.482094000
C	11.254311000	-0.758994000	0.015821000
H	12.087673000	-0.954805000	0.702106000
H	11.617328000	-0.836749000	-1.018178000
H	10.877536000	0.257243000	0.197114000

C	8.152651000	1.321855000	1.515670000
H	8.609932000	2.195631000	1.030597000
H	8.910884000	0.544113000	1.670270000
H	7.368277000	0.917205000	0.863311000
C	6.699991000	1.592626000	-2.089702000
H	7.401526000	2.203424000	-1.505727000
H	5.886279000	1.238692000	-1.441055000
H	7.219769000	0.712276000	-2.484855000
S	-9.969273000	2.019269000	-0.355366000
S	-7.448720000	-1.744881000	-3.146840000
S	-6.021268000	-2.515144000	3.513223000
S	6.021318000	2.515275000	-3.515142000
S	9.969393000	-2.017424000	0.354411000
S	7.447971000	1.744147000	3.146486000

6.5 Optimized coordinates of **4e** ($C_{66}N_{30}H_{114}S_6O_6$).

O	-3.145782000	2.939884000	3.360797000
O	-1.160723000	5.101781000	-1.537280000
O	-0.934882000	0.626860000	-5.121242000
N	2.929165000	4.759731000	2.517690000
N	1.526917000	2.744752000	2.914971000
N	-0.876801000	2.353810000	3.384280000
N	-1.607495000	3.765868000	1.808221000
N	0.710648000	4.570398000	1.849422000
N	-6.101078000	2.260631000	-2.247001000
N	-3.867172000	1.663078000	-2.614796000
N	-1.822991000	3.040991000	-2.416005000
N	-2.570755000	3.629961000	-0.393326000
N	-4.449127000	2.099867000	-0.432663000
N	4.328301000	3.154628000	-3.203146000
N	2.139380000	2.792170000	-2.513430000
N	0.049407000	1.903121000	-3.433093000
N	1.025873000	-0.020879000	-4.033144000
N	3.194857000	0.964149000	-3.351504000
C	1.865081000	4.053237000	2.448321000
C	0.217649000	2.376478000	2.413189000
H	0.281514000	1.401659000	1.895935000
C	-2.005714000	3.014184000	2.903042000
C	-0.212190000	3.533011000	1.474913000
H	-0.134084000	3.277600000	0.404708000
C	2.490514000	1.645120000	2.983020000
H	2.763149000	1.253268000	1.984915000
H	2.056619000	0.838722000	3.582095000
H	3.403641000	1.958384000	3.486140000
C	-0.972637000	1.413635000	4.472926000
H	-1.867776000	1.685386000	5.039936000
H	-0.092110000	1.485717000	5.121143000
C	-2.568310000	4.330398000	0.869421000
H	-3.552850000	4.252454000	1.342959000
H	-2.331170000	5.377181000	0.654711000
C	0.665477000	5.894154000	1.249907000
H	0.013331000	6.563836000	1.832487000
H	0.279368000	5.832242000	0.224589000
H	1.684663000	6.295193000	1.250187000
C	4.187656000	4.328492000	3.090437000

H	4.719503000	5.228677000	3.438952000
H	4.079203000	3.682589000	3.981473000
C	5.056284000	3.636531000	2.016897000
H	5.232858000	4.351826000	1.200222000
H	4.488755000	2.803399000	1.576462000
C	6.389276000	3.109427000	2.553316000
H	6.224115000	2.393774000	3.375248000
H	7.006064000	3.934492000	2.943033000
S	7.287715000	2.271271000	1.185488000
C	8.851567000	1.864709000	2.036060000
H	9.495268000	1.375065000	1.295716000
H	8.679152000	1.173063000	2.871875000
H	9.347575000	2.774659000	2.401782000
C	-4.933894000	2.033710000	-1.783573000
C	-2.587758000	1.877862000	-1.973995000
H	-1.950141000	0.986482000	-2.054401000
C	-1.785123000	4.043332000	-1.458221000
C	-3.006425000	2.244750000	-0.509963000
H	-2.520263000	1.618851000	0.254400000
C	-4.005819000	1.758238000	-4.062422000
H	-4.963260000	1.307388000	-4.342244000
H	-3.178053000	1.224100000	-4.541336000
H	-4.009326000	2.808048000	-4.400879000
C	-4.921025000	1.037592000	0.476474000
H	-4.572122000	1.267334000	1.490809000
H	-4.566738000	0.032812000	0.180116000
H	-6.014120000	1.015911000	0.483148000
C	-0.866630000	3.016959000	-3.513470000
H	-1.377068000	2.924991000	-4.477653000
H	-0.326430000	3.969643000	-3.472910000
C	-7.169407000	2.721377000	-1.375232000
H	-7.507314000	3.696689000	-1.768516000
H	-6.847700000	2.897564000	-0.332930000
C	-8.361065000	1.749886000	-1.412770000
H	-8.646305000	1.597122000	-2.464391000
H	-8.052327000	0.773625000	-1.014902000
C	-9.548819000	2.296150000	-0.616114000
H	-9.783513000	3.324105000	-0.935589000
H	-9.314711000	2.314313000	0.459302000
S	-11.045867000	1.261705000	-0.885132000
C	-12.246042000	2.242270000	0.086017000
H	-13.216276000	1.733858000	0.018653000
H	-12.347816000	3.257458000	-0.322521000
H	-11.949908000	2.303360000	1.143210000
C	3.350806000	2.337787000	-3.080771000
C	1.147276000	1.765882000	-2.462842000
H	0.729799000	1.670899000	-1.444631000
C	-0.047777000	0.825438000	-4.289438000
C	1.874632000	0.476515000	-2.960873000
H	1.972601000	-0.300773000	-2.186825000
C	2.144211000	3.877865000	-1.539807000
H	2.301026000	3.507403000	-0.509543000
H	1.201915000	4.434174000	-1.586697000
H	2.975170000	4.540209000	-1.798556000
C	3.893264000	0.240008000	-4.408691000
H	3.457131000	0.440473000	-5.401423000

H	3.832456000	-0.833843000	-4.196049000
H	4.947514000	0.519970000	-4.426107000
C	5.678458000	2.787607000	-3.585001000
H	6.252732000	3.723958000	-3.670666000
H	5.729335000	2.317654000	-4.585658000
C	6.378210000	1.887109000	-2.546792000
H	5.823691000	0.944237000	-2.436717000
H	6.350618000	2.387977000	-1.570040000
O	3.145806000	-2.940077000	-3.360789000
O	1.160527000	-5.101847000	1.537251000
O	0.935024000	-0.626896000	5.121225000
N	-2.929233000	-4.759622000	-2.517792000
N	-1.526876000	-2.744733000	-2.915122000
N	0.876874000	-2.353808000	-3.384289000
N	1.607444000	-3.765909000	-1.808224000
N	-0.710699000	-4.570400000	-1.849532000
N	6.101150000	-2.261137000	2.246967000
N	3.867294000	-1.663435000	2.614853000
N	1.822954000	-3.041130000	2.416035000
N	2.570664000	-3.630104000	0.393338000
N	4.449159000	-2.100138000	0.432694000
N	-4.328407000	-3.154503000	3.203451000
N	-2.139465000	-2.792216000	2.513696000
N	-0.049370000	-1.903178000	3.433154000
N	-1.025747000	0.020877000	4.033182000
N	-3.194789000	-0.964135000	3.351846000
C	-1.865115000	-4.053186000	-2.448435000
C	-0.217640000	-2.376479000	-2.413265000
H	-0.281515000	-1.401663000	-1.896006000
C	2.005730000	-3.014263000	-2.903034000
C	0.212140000	-3.533024000	-1.474972000
H	0.133992000	-3.277631000	-0.404769000
C	-2.490444000	-1.645084000	-2.983288000
H	-2.763131000	-1.253169000	-1.985223000
H	-2.056497000	-0.838737000	-3.582394000
H	-3.403545000	-1.958358000	-3.486452000
C	0.972776000	-1.413634000	-4.472930000
H	1.867931000	-1.685389000	-5.039913000
H	0.092263000	-1.485693000	-5.121169000
C	2.568185000	-4.330536000	-0.869415000
H	3.552743000	-4.252684000	-1.342931000
H	2.330939000	-5.377295000	-0.654712000
C	-0.665649000	-5.894100000	-1.249889000
H	-0.013397000	-6.563837000	-1.832290000
H	-0.279721000	-5.832115000	-0.224506000
H	-1.684836000	-6.295135000	-1.250333000
C	-4.187751000	-4.328345000	-3.090437000
H	-4.719646000	-5.228519000	-3.438907000
H	-4.079369000	-3.682446000	-3.981491000
C	-5.056292000	-3.636381000	-2.016827000
H	-5.232710000	-4.351622000	-1.200071000
H	-4.488775000	-2.803171000	-1.576523000
C	-6.389400000	-3.109421000	-2.553099000
H	-6.224396000	-2.393825000	-3.375113000
H	-7.006197000	-3.934558000	-2.942649000
S	-7.287677000	-2.271163000	-1.185228000

C	-8.851747000	-1.864944000	-2.035556000
H	-9.495356000	-1.375236000	-1.295172000
H	-8.679593000	-1.173417000	-2.871522000
H	-9.347708000	-2.775022000	-2.401022000
C	4.933967000	-2.034100000	1.783591000
C	2.587845000	-1.878058000	1.974072000
H	1.950315000	-0.986619000	2.054543000
C	1.785000000	-4.043436000	1.458218000
C	3.006451000	-2.244929000	0.510013000
H	2.520324000	-1.618959000	-0.254312000
C	4.005977000	-1.758625000	4.062474000
H	4.963454000	-1.307841000	4.342274000
H	3.178251000	-1.224459000	4.541423000
H	4.009438000	-2.808443000	4.400910000
C	4.921092000	-1.037865000	-0.476436000
H	4.572004000	-1.267489000	-1.490735000
H	4.566992000	-0.033062000	-0.179948000
H	6.014191000	-1.016354000	-0.483293000
C	0.866630000	-3.017057000	3.513524000
H	1.377094000	-2.925098000	4.477694000
H	0.326384000	-3.969716000	3.472988000
C	7.169414000	-2.721819000	1.375070000
H	7.507484000	-3.697074000	1.768354000
H	6.847546000	-2.898100000	0.332838000
C	8.360976000	-1.750218000	1.412388000
H	8.646432000	-1.597487000	2.463957000
H	8.052093000	-0.773953000	1.014641000
C	9.548612000	-2.296351000	0.615447000
H	9.783372000	-3.324341000	0.934753000
H	9.314312000	-2.314388000	-0.459933000
S	11.045675000	-1.261907000	0.884370000
C	12.245691000	-2.242153000	-0.087300000
H	13.215914000	-1.733715000	-0.019973000
H	12.347598000	-3.257456000	0.320924000
H	11.949352000	-2.302954000	-1.144451000
C	-3.350840000	-2.337743000	3.081065000
C	-1.147318000	-1.765964000	2.462990000
H	-0.729926000	-1.671040000	1.444740000
C	0.047872000	-0.825478000	4.289470000
C	-1.874606000	-0.476554000	2.961011000
H	-1.972639000	0.300678000	2.186918000
C	-2.144385000	-3.877975000	1.540147000
H	-2.301090000	-3.507553000	0.509852000
H	-1.202169000	-4.434410000	1.587132000
H	-2.975456000	-4.540178000	1.798895000
C	-3.892905000	-0.240104000	4.409298000
H	-3.456232000	-0.440365000	5.401832000
H	-3.832525000	0.833749000	4.196536000
H	-4.947052000	-0.520422000	4.427253000
C	-5.678581000	-2.787323000	3.585119000
H	-6.253034000	-3.723599000	3.670390000
H	-5.729547000	-2.317684000	4.585926000
C	-6.378031000	-1.886414000	2.547064000
H	-5.823432000	-0.943552000	2.437363000
H	-6.350306000	-2.387015000	1.570179000
C	-7.826501000	-1.593685000	2.943125000

H	-8.401241000	-2.531151000	3.001946000
H	-7.868285000	-1.109478000	3.932443000
S	-8.636172000	-0.496304000	1.710822000
C	-10.303673000	-0.422496000	2.452186000
H	-10.295743000	0.109165000	3.414396000
H	-10.937825000	0.110306000	1.734219000
H	-10.707131000	-1.434900000	2.595077000
C	7.826631000	1.594377000	-2.943008000
H	8.401355000	2.531843000	-3.001959000
H	7.868326000	1.110108000	-3.932303000
S	8.636444000	0.497086000	-1.710716000
C	10.303953000	0.423514000	-2.452083000
H	10.938207000	-0.109156000	-1.734108000
H	10.296102000	-0.108193000	-3.414271000
H	10.707247000	1.435975000	-2.595020000

6.6 Optimized coordinates of **4f** ($C_{90}N_{30}H_{114}S_6O_6$).

O	2.841592000	-0.346779000	5.166020000
O	-1.058583000	3.759870000	4.634906000
O	-0.949767000	5.181429000	-0.911416000
N	-1.231330000	-1.809621000	3.456350000
N	-1.575854000	-0.058416000	4.891305000
N	0.768625000	0.681405000	4.822345000
N	1.123383000	-1.336623000	3.925725000
N	-2.936075000	-1.937716000	5.219294000
N	2.194922000	4.750207000	1.723439000
N	3.190152000	3.027602000	2.803154000
N	1.067527000	2.958365000	4.060584000
N	-0.058507000	4.210825000	2.572453000
N	4.516440000	4.812413000	1.706678000
N	-3.481962000	1.316320000	-0.569332000
N	-3.486379000	2.296586000	1.494547000
N	-1.668882000	3.797555000	0.822906000
N	-1.834416000	3.047564000	-1.281347000
N	-5.554202000	1.442412000	0.484333000
C	-2.005110000	-1.344757000	4.571281000
C	-0.455095000	0.379947000	4.095359000
H	-0.722883000	1.243627000	3.471842000
C	-0.113610000	-0.903857000	3.286863000
H	0.049660000	-0.718518000	2.212774000
C	1.705890000	-0.340323000	4.691653000
C	-3.252101000	-3.325767000	4.905286000
H	-2.371378000	-3.873060000	4.520880000
C	-1.954151000	-2.095413000	2.204530000
H	-2.812761000	-2.737822000	2.401385000
H	-1.276973000	-2.628257000	1.532701000
H	-2.324037000	-1.176541000	1.709023000
C	-1.977913000	0.636873000	6.101221000
H	-2.955730000	0.246009000	6.399655000
H	-2.040931000	1.713269000	5.897747000
H	-1.260248000	0.466397000	6.920609000
C	1.792925000	-2.579114000	3.609671000
H	1.131412000	-3.428514000	3.816037000
H	2.680225000	-2.625228000	4.247662000

C	1.163099000	2.039755000	5.178728000
H	2.194949000	1.978876000	5.539962000
H	0.516243000	2.439858000	5.965762000
C	3.439941000	4.208691000	2.060431000
C	1.778236000	2.732086000	2.796694000
H	1.610379000	1.694100000	2.457411000
C	1.133932000	3.783423000	1.856257000
H	0.828989000	3.365539000	0.883027000
C	-0.118502000	3.659867000	3.846523000
C	5.847347000	4.299777000	1.988548000
H	5.977777000	4.009577000	3.047334000
C	2.096121000	5.915987000	0.856054000
H	2.227712000	6.841669000	1.435216000
H	1.107372000	5.926769000	0.383955000
H	2.875779000	5.882090000	0.083487000
C	4.091371000	1.874209000	2.881166000
H	5.081506000	2.176343000	3.219132000
H	4.203276000	1.354471000	1.915565000
H	3.694036000	1.182613000	3.630106000
C	-1.267039000	4.673674000	1.901504000
H	-1.116349000	5.661611000	1.454837000
H	-2.044733000	4.731584000	2.670776000
C	-4.297948000	1.681494000	0.507092000
C	-2.126438000	2.428723000	0.993293000
H	-1.424753000	1.875918000	1.638088000
C	-2.159847000	1.869124000	-0.466846000
H	-1.404519000	1.090123000	-0.661634000
C	-1.436937000	4.126970000	-0.502954000
C	-4.080956000	0.972761000	-1.852691000
H	-4.806121000	0.165708000	-1.711236000
H	-3.297925000	0.644544000	-2.541337000
H	-4.603519000	1.834561000	-2.298260000
C	-3.610404000	1.865160000	2.895696000
H	-4.629535000	2.024969000	3.253302000
H	-2.940625000	2.474855000	3.511871000
H	-3.357135000	0.800544000	3.030556000
C	-6.450808000	1.957622000	1.500439000
H	-6.081349000	2.910428000	1.929189000
O	-2.010489000	1.012018000	-4.705787000
O	1.691948000	-3.101108000	-3.777269000
O	0.637942000	-4.404151000	1.729273000
N	1.623110000	2.746865000	-2.853716000
N	2.472502000	0.860053000	-3.828376000
N	0.139299000	0.182494000	-4.289499000
N	-0.654015000	1.858606000	-3.010188000
N	3.465558000	2.886114000	-4.469833000
N	-2.121483000	-3.628990000	-1.270127000
N	-2.780644000	-2.422312000	-3.044583000
N	-0.425784000	-2.117153000	-3.722887000
N	0.246959000	-3.339450000	-1.956499000
N	-4.052288000	-4.405847000	-2.291723000
N	4.293555000	-1.671253000	1.494696000
N	3.793718000	-2.337764000	-0.635461000
N	1.557218000	-3.053892000	0.060675000
N	2.146502000	-2.684931000	2.200607000
N	5.986242000	-2.806181000	0.331853000

C	2.600497000	2.256605000	-3.766220000
C	1.200342000	0.426578000	-3.301880000
H	1.323401000	-0.467295000	-2.676087000
C	0.701682000	1.677934000	-2.516508000
H	0.689361000	1.525345000	-1.424799000
C	-0.952213000	1.028467000	-4.080577000
C	3.449056000	4.348176000	-4.521745000
H	2.438148000	4.754273000	-4.333642000
C	2.062612000	3.552939000	-1.708738000
H	1.231502000	4.172894000	-1.357937000
H	2.427929000	2.912274000	-0.883491000
H	2.881863000	4.208324000	-2.000658000
C	3.090444000	0.125422000	-4.926486000
H	4.137110000	0.435181000	-5.002161000
H	3.030640000	-0.947308000	-4.711570000
H	2.591699000	0.338340000	-5.886149000
C	-1.481363000	3.003907000	-2.693287000
H	-0.961567000	3.947094000	-2.907296000
H	-2.368778000	2.919860000	-3.329852000
C	-0.137649000	-1.165079000	-4.787871000
H	-0.987924000	-1.071960000	-5.468042000
H	0.728737000	-1.557443000	-5.325583000
C	-3.092430000	-3.551830000	-2.274013000
C	-1.477242000	-1.895673000	-2.720702000
H	-1.541147000	-0.821986000	-2.494164000
C	-1.014725000	-2.745279000	-1.494528000
H	-0.798155000	-2.144104000	-0.597651000
C	0.619836000	-2.884691000	-3.210099000
C	-5.123120000	-4.395537000	-3.267110000
H	-4.764889000	-4.230642000	-4.300011000
C	-2.088370000	-4.762010000	-0.358423000
H	-1.863526000	-5.699986000	-0.891466000
H	-1.323544000	-4.593172000	0.406262000
H	-3.069750000	-4.866509000	0.119340000
C	-3.451893000	-1.984974000	-4.260955000
H	-3.175173000	-2.598833000	-5.133732000
H	-4.536571000	-2.010740000	-4.122386000
H	-3.163236000	-0.947207000	-4.461902000
C	1.228394000	-3.922993000	-1.056918000
H	0.851542000	-4.854255000	-0.622994000
H	2.123007000	-4.126753000	-1.657859000
C	4.803334000	-2.317911000	0.364632000
C	2.526460000	-1.963762000	-0.033874000
H	2.087077000	-1.111614000	-0.574537000
C	2.850729000	-1.632303000	1.463278000
H	2.486732000	-0.649800000	1.800398000
C	1.373774000	-3.488466000	1.368280000
C	5.022432000	-1.740964000	2.755271000
H	6.031750000	-1.346674000	2.594279000
H	4.502855000	-1.136306000	3.505856000
H	5.107909000	-2.778872000	3.117191000
C	4.087285000	-1.687600000	-1.925370000
H	5.118134000	-1.890979000	-2.217050000
H	3.412086000	-2.089179000	-2.686926000
H	3.971319000	-0.591571000	-1.858236000
C	6.405742000	-3.591439000	-0.815360000

H	5.561420000	-4.183052000	-1.222125000
H	-3.531579000	-3.810142000	5.856806000
H	6.549728000	5.130964000	1.820223000
H	3.710220000	4.619518000	-5.558705000
H	-5.553472000	-5.411308000	-3.273462000
H	-6.534776000	1.247598000	2.345022000
H	6.734442000	-2.934039000	-1.639322000
C	6.270392000	3.147052000	1.083787000
C	7.287721000	2.267201000	1.481158000
C	7.707052000	1.215033000	0.659424000
C	7.111916000	1.024077000	-0.601674000
C	6.073503000	1.890644000	-0.999919000
C	5.667717000	2.937055000	-0.166899000
H	7.765922000	2.399745000	2.454975000
H	8.501201000	0.557127000	1.005372000
H	5.601324000	1.767405000	-1.976188000
H	4.887274000	3.617701000	-0.498635000
C	7.561004000	-4.517752000	-0.474698000
C	7.933018000	-4.792107000	0.850421000
C	8.990590000	-5.658713000	1.135231000
C	9.711705000	-6.276739000	0.093820000
C	9.348971000	-6.002015000	-1.237301000
C	8.285840000	-5.131946000	-1.506995000
H	7.383883000	-4.308387000	1.657004000
H	9.260447000	-5.861845000	2.173158000
H	9.888092000	-6.452511000	-2.068529000
H	8.019258000	-4.928758000	-2.547627000
C	4.431728000	5.018582000	-3.572957000
C	5.723782000	4.503086000	-3.372709000
C	6.590086000	5.077104000	-2.440158000
C	6.185513000	6.193282000	-1.679725000
C	4.912533000	6.744360000	-1.908299000
C	4.053205000	6.157761000	-2.844148000
H	6.031511000	3.611843000	-3.919510000
H	7.566486000	4.627120000	-2.260504000
H	4.576569000	7.617535000	-1.352512000
H	3.056316000	6.581420000	-2.987963000
C	-4.401820000	-3.494194000	3.919055000
C	-4.499514000	-4.664157000	3.148306000
C	-5.539755000	-4.848218000	2.230955000
C	-6.511093000	-3.844677000	2.054918000
C	-6.410511000	-2.661031000	2.815444000
C	-5.375207000	-2.496419000	3.739120000
H	-3.744625000	-5.446167000	3.260095000
H	-5.588629000	-5.772304000	1.657474000
H	-7.142075000	-1.864387000	2.668357000
H	-5.295060000	-1.573559000	4.313913000
C	-6.263519000	-3.424149000	-2.975716000
C	-7.445604000	-3.518567000	-3.732967000
C	-8.548697000	-2.711441000	-3.451019000
C	-8.488360000	-1.761455000	-2.411118000
C	-7.294271000	-1.623780000	-1.682258000
C	-6.203995000	-2.462010000	-1.955976000
H	-7.516151000	-4.264309000	-4.529039000
H	-9.474809000	-2.831681000	-4.014531000
H	-7.210805000	-0.884803000	-0.886469000

H	-5.307918000	-2.386945000	-1.340877000
C	-7.844498000	2.191998000	0.937054000
C	-8.949377000	2.289019000	1.801871000
C	-10.235195000	2.505672000	1.305905000
C	-10.450032000	2.634192000	-0.082684000
C	-9.346706000	2.567919000	-0.949327000
C	-8.062720000	2.344849000	-0.437786000
H	-8.805989000	2.171614000	2.878966000
H	-11.083120000	2.546843000	1.991533000
H	-9.476189000	2.651769000	-2.025316000
H	-7.216406000	2.255123000	-1.116856000
S	11.048333000	-7.357167000	0.572101000
S	7.640047000	-0.217451000	-1.766163000
S	7.325417000	6.829961000	-0.468951000
S	-12.138182000	2.822998000	-0.621783000
S	-9.952172000	-0.791549000	-2.084943000
S	-7.890280000	-3.993718000	0.943292000
C	-7.303164000	-5.235347000	-0.261581000
H	-6.284115000	-4.996332000	-0.589086000
H	-7.349534000	-6.253212000	0.147082000
H	-7.976102000	-5.155935000	-1.123356000
C	-12.009154000	2.673488000	-2.436791000
H	-13.040682000	2.680705000	-2.809971000
H	-11.466770000	3.521689000	-2.874279000
H	-11.527427000	1.729008000	-2.719276000
C	-9.970591000	-0.740315000	-0.254323000
H	-10.938936000	-0.309017000	0.024885000
H	-9.877752000	-1.755234000	0.148143000
H	-9.176819000	-0.096320000	0.136392000
C	11.603231000	-8.058152000	-1.017645000
H	12.021673000	-7.286599000	-1.677250000
H	12.392551000	-8.777990000	-0.768462000
H	10.785587000	-8.585246000	-1.526329000
C	8.801870000	-1.228553000	-0.786837000
H	9.689113000	-0.651328000	-0.497627000
H	8.292901000	-1.643781000	0.091547000
H	9.110848000	-2.056154000	-1.435790000
C	6.213381000	7.713023000	0.685969000
H	6.829469000	7.966523000	1.557993000
H	5.826019000	8.643148000	0.250210000
H	5.392623000	7.051847000	0.996484000

6.7 Optimized coordinates of **1** ($C_{42}N_{24}H_{60}S_6O_6$).

N	1.987377000	2.988288000	10.027573000
C	3.084678000	3.085019000	9.082075000
H	3.416380000	4.023792000	8.990238000
N	4.164031000	2.151214000	9.329198000
C	5.026917000	2.252801000	10.491626000
H	5.879339000	1.806262000	10.306562000
H	4.593446000	1.823749000	11.259713000
H	5.190672000	3.196845000	10.696171000
C	4.261314000	1.209414000	8.380778000
S	5.426361000	0.027203000	8.317605000
N	3.270744000	1.388635000	7.466587000
C	3.328028000	0.836234000	6.123826000

H	2.424641000	0.803200000	5.745348000
H	3.701379000	-0.068564000	6.158612000
H	3.897251000	1.403042000	5.563066000
C	2.463526000	2.560073000	7.764360000
H	2.506559000	3.239999000	7.032451000
N	1.094829000	2.253213000	8.144229000
C	0.826559000	2.585190000	9.431332000
O	-0.264914000	2.540456000	9.980124000
C	0.045072000	1.875265000	7.223081000
H	0.344335000	1.085824000	6.705457000
H	-0.755082000	1.609489000	7.742096000
N	-0.322831000	2.916582000	6.304994000
C	-0.920797000	4.189733000	6.676236000
H	-0.409558000	4.641984000	7.406754000
N	-2.339648000	4.107383000	6.978184000
C	-2.863973000	3.453237000	8.147012000
H	-3.689792000	3.899493000	8.428087000
H	-2.204221000	3.500423000	8.870572000
H	-3.053961000	2.515229000	7.938293000
C	-3.095392000	4.687759000	6.037555000
S	-4.770860000	4.799405000	6.067054000
N	-2.298192000	5.194752000	5.078838000
C	-2.764059000	5.973932000	3.955927000
H	-2.060398000	6.593940000	3.674852000
H	-3.560730000	6.480858000	4.218914000
H	-2.987760000	5.374670000	3.212887000
C	-0.887277000	4.996419000	5.376610000
H	-0.405015000	5.864745000	5.489319000
N	-0.203841000	4.111979000	4.449618000
C	0.129524000	2.917782000	5.023179000
O	0.733205000	2.012129000	4.467568000
C	0.198284000	4.442353000	3.109918000
H	-0.591930000	4.768906000	2.611775000
H	0.517505000	3.619023000	2.661867000
N	1.235472000	5.440066000	3.043128000
C	2.609335000	5.267889000	3.470307000
H	2.672492000	4.996391000	4.430416000
N	3.391547000	4.401329000	2.607600000
C	3.432253000	2.965729000	2.780142000
H	3.575783000	2.536334000	1.911869000
H	2.582795000	2.658442000	3.161402000
H	4.166166000	2.729933000	3.386819000
C	4.322972000	5.088882000	1.923001000
S	5.398954000	4.403508000	0.843226000
N	4.255810000	6.393308000	2.240254000
C	5.089396000	7.439052000	1.689235000
H	5.302473000	8.090418000	2.389141000
H	4.611348000	7.887802000	0.960109000
H	5.918568000	7.047237000	1.342761000
C	3.221817000	6.668143000	3.221235000
H	3.595568000	7.068714000	4.057504000
N	2.113247000	7.434929000	2.697628000
C	0.959034000	6.716166000	2.643778000
O	-0.133548000	7.136612000	2.304262000
C	2.092832000	8.889312000	2.603426000
H	2.890722000	9.189716000	2.101108000

H	1.292140000	9.166804000	2.092759000
N	2.076481000	9.544052000	3.887050000
C	0.979180000	9.447321000	4.832549000
H	0.647478000	8.508548000	4.924385000
N	-0.100173000	10.381125000	4.585425000
C	-0.963059000	10.279539000	3.422997000
H	-1.815481000	10.726078000	3.608062000
H	-0.529587000	10.708590000	2.654910000
H	-1.126814000	9.335495000	3.218452000
C	-0.197456000	11.322926000	5.533846000
S	-1.362503000	12.505137000	5.597018000
N	0.793115000	11.143704000	6.448036000
C	0.735830000	11.696105000	7.790798000
H	1.639217000	11.729140000	8.169275000
H	0.362479000	12.600904000	7.756011000
H	0.166607000	11.129297000	8.351557000
C	1.600332000	9.972266000	6.150264000
H	1.557299000	9.292340000	6.882173000
N	2.969029000	10.279127000	5.770394000
C	3.237299000	9.947150000	4.483292000
O	4.328772000	9.991884000	3.934499000
C	4.018787000	10.657075000	6.691542000
H	3.719523000	11.446516000	7.209166000
H	4.818940000	10.922850000	6.172527000
N	4.386689000	9.615758000	7.609629000
C	4.984655000	8.342607000	7.238387000
H	4.473417000	7.890355000	6.507869000
N	6.403506000	8.424957000	6.936440000
C	6.927831000	9.079102000	5.767611000
H	7.753650000	8.632846000	5.486536000
H	6.268079000	9.031917000	5.044051000
H	7.117819000	10.017111000	5.976331000
C	7.159251000	7.844580000	7.877068000
S	8.834719000	7.732935000	7.847569000
N	6.362050000	7.337587000	8.835786000
C	6.827917000	6.558407000	9.958696000
H	6.124256000	5.938399000	10.239771000
H	7.624588000	6.051482000	9.695710000
H	7.051618000	7.157669000	10.701737000
C	4.951135000	7.535921000	8.538013000
H	4.468874000	6.667594000	8.425304000
N	4.267699000	8.420361000	9.465005000
C	3.934334000	9.614558000	8.891444000
O	3.330654000	10.520210000	9.447055000
C	3.865574000	8.089987000	10.804705000
H	4.655788000	7.763434000	11.302849000
H	3.546353000	8.913317000	11.252756000
N	2.828386000	7.092274000	10.871495000
C	1.454523000	7.264451000	10.444316000
H	1.391366000	7.535948000	9.484207000
N	0.672311000	8.131011000	11.307023000
C	0.631605000	9.566610000	11.134482000
H	0.488075000	9.996005000	12.002754000
H	1.481063000	9.873897000	10.753221000
H	-0.102308000	9.802407000	10.527804000
C	-0.259114000	7.443457000	11.991622000

S	-1.335096000	8.128831000	13.071397000
N	-0.191952000	6.139032000	11.674369000
C	-1.025538000	5.093288000	12.225388000
H	-1.238615000	4.441922000	11.525483000
H	-0.547490000	4.644538000	12.954514000
H	-1.854710000	5.485103000	12.571862000
C	0.842041000	5.864196000	10.693388000
H	0.468290000	5.463625000	9.857119000
N	1.950611000	5.097411000	11.216995000
C	3.104824000	5.816174000	11.270845000
O	4.197406000	5.395728000	11.610362000
C	1.971027000	3.643028000	11.311197000
H	1.173136000	3.342624000	11.813515000
H	2.771718000	3.365536000	11.821864000

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