SUPPORTING INFORMATION

Designer Dendrimers: Branched Oligosulfonimides with Controllable Molecular Architectures

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Experimental Section

Instruments and methods: Melting points were determined on a Büchi microscope heating unit and are uncorrected. NMR spectra were measured on Bruker AMX 300 or DRX 500 spectrometers. All chemical shifts are given in ppm with the solvent signals taken as internal standards; coupling constants are in hertz. EI mass spectra were obtained with Micromass Autospec Q spectrometer and MALDI mass spectra were recorded on a Micromass MALDI-Tof Spec E mass spectrometer equipped with an N_2 laser (337 nm). ESI mass spectra and MS/MS spectra were recorded on a Bruker APEX IV Fourier-transform ion-cyclotron-resonance (FT-ICR) mass spectrometer with an Apollo electrospray ion source equipped with an off-axis 70° spray needle.

Comment on dendrimer solubilities.

Oligosulfonimide dendrimers and dendrons of all generations bearing peripheral tosyl- and 2-naphthylsulfonyl groups exhibit very high solubilities in both polar aprotic and apolar aprotic (except for hexane) solvents. Their solubilities in DMF, THF, chloroform and benzene are in the range of 150-250 mg/mL. Nosyl-decorated branched sulfonimides show poor solubility in the above mentioned solvents at r.t. with the exception of 1st generation species as well as Janus-type dendrimers. The compounds with peripheral nitro-groups can be dissolved in hot THF and hot chloroform. All the above mentioned compounds have low or no solubility in methanol and ethanol. Oligosulfonimides bearing peripheral amino-groups are soluble in alcohols or mixtures of alcohols with either chlorinated solvents or benzene.

General synthetic procedures:

Persulfonylation of amines and sulfonamides with arylsulfonyl chlorides (preparation of compounds **2a, 3a, 4, 6a, 7, 9c, 10a, 11, 12a, 13a, b, 15a, b, 17a, b**): A mixture of a corresponding amine or sulfonamide, triethylamine (ca. fourfold molar excess per amino or sulfonamide group) and arylsulfonyl chloride (ca. threefold molar excess per amino or sulfonamide group) was stirred in dichloromethane at reflux for 2 to 24 hrs, dependently on the number of amino groups in a compound. Then the solvent was removed under reduced pressure and the residue was triturated with methanol. The solid precipitate was filtered through a glass filter and thoroughly washed with methanol. The resulting solid powders were dried in vacuum and then, if necessary, purified by chromatography on silica gel.

Persulfonylation of aromatic amines with arylsulfonyl chlorides (preparation of compounds **8a, 9a**): The procedure is fully analogous to the previous one with the exception of strict stoichiometric amount of the arylsulfonyl chloride added (two equivalents per amino group).

Reduction of nitro-derivatives with tin (II) chloride dihydrate (preparation of compounds **5b, 12b, 14**): A mixture of a nitro-compound and $SnCl_2 \cdot 2H_2O$ (four equivalents per nitro group) was boiled in a mixture of ethanol and concentrated hydrochloric acid (5 mL per gram of nitro-compound) for 5 hrs, cooled, and then poured onto ice. The pH was adjusted to 10 with 2 M aqueous NaOH, and the released amine was extracted with dichloromethane, dried over $MgSO_4$, and then evaporated to give corresponding amines as colorless solids.

Catalytic reduction of nitro-derivatives with H_2 (preparation of compounds **2b, 3b, 6b, 8b, 9d, 10b**): A nitro-compound was dissolved in a 2:1 mixture of benzene/ethanol. To this solution was added a catalytic amount of commercial 10% Pd/C that had been previously washed with ethanol. The resulting suspension was evacuated and the reaction flask was filled with H_2. This operation was repeated three times and the mixture was stirred for 24 hrs at room temperature under hydrogen pressure of 3 bar. Then the palladium catalyst was filtered off in a vacuum through a pad of Celite and rinsed with a 2:1 mixture of benzene/ethanol. The filtrates were combined and evaporated in vacuum to give a colorless solid. The yields of the catalytic hydrogenation are assumed quantitative.

General procedure for the Suzuki-Miyaura cross-coupling (preparation of compounds **18-20**): Aryl bromide (0.34 mmol, compounds **13b**, **15b** and **17b**) and benzene-1,4-bis(boronic acid)propane-1,3-diol diester (0.17 mmol) were dissolved in 10 mL of dry THF. A concentrated solution of $NaHCO_3$ in water (5 mL) was added to the reaction mixture and the system was degassed. Freshly prepared $Pd[P(p\text{-tolyl})_3]_3$ (10-14 mg) was added and the reaction mixture was allowed to stir at 80°C for 24 hrs under nitrogen atmosphere. Then 20 mL of water were added and the emulsion was taken up with 100 mL of dichloromethane. The organic layer was separated, washed with water and brine, dried over Mg_2SO_4 and evaporated. The brown viscous residue was chromatographed on silica gel column with hexane/ethylacetate (2:1) eluant.

N-*n*-octyl-4-nitrobenzenesulfonimide 2a: 1.0 g of octylamine **1** was used in the reaction. Recrystallized from methanol; yield 3.68 g (95%); m.p. 131-132 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.91 (t, $^{3}J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.27 (s, 10 H, CH_2), 1.71 (br. 2H, CH_2), 3.78 (m, 2 H, CH_2), 8.30 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 4 H, ArH), 8.46 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 4 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.05, 22.58, 26.45, 28.87, 29.07, 29.95, 31.66, 50.37, 124.45, 129.69, 145.05, 150.82 ppm; MS (EI, 80 eV): *m/z* = 499.11 $[M]^+$, 399.99 $[M - C_7H_{15}]^+$, 313.12 $[M - p\text{-}NO_2C_6H_4SO_2]^+$, 185.99 $[M - p\text{-}NO_2C_6H_4SO_2NC_8H_{17}]^+$; elemental analysis calcd (%) for $C_{20}H_{25}N_3O_8S_2$ (499.56): C 48.09, H 5.04, N 8.41, S 12.84; found C 48.26, H 5.08, N 8.27, S 13.02.

N-*n*-octyl-4-aminobenzenesulfonimide 2b: M.p. 149-150 °C; ^{1}H NMR (300 MHz, CD_3OD): δ = 0.93 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.27 (s, 10 H, CH_2), 1.61 (br. 2H, CH_2), 3.54 (m, 2 H, CH_2), 6.68 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 4 H, ArH), 7.52 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 4 H, ArH) ppm; MS (ESI pos., CH_3OH): *m/z* = 440.20 $[M+H]^+$ calcd monoisotopic peak ($^{12}C_{20}{}^{1}H_{30}{}^{14}N_3{}^{16}O_4{}^{32}S_2$) 440.16; 462.10 $[M+Na]^+$ ($^{12}C_{20}{}^{1}H_{29}{}^{14}N_3{}^{16}O_4{}^{32}S_2Na$) calcd monoisotopic peak 462.16.

N-*n*-octyl-4-(4-nitrobenzenesulfonimido)benzenesulfonimide 3a: 2.7 g of diamine **2b** were used in the reaction; yield 5.20 g (71%), m.p. 209-211 °C. ^{1}H NMR (300 MHz, $(CD_3)_2SO$): δ = 0.83 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.23 (s, 10 H, CH_2), 1.58 (br. 2H, CH_2), 3.81 (br, 2 H, CH_2), 7.50 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 8.02 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 8.14 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 8 H, ArH), 8.51 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 8 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $(CD_3)_2SO$): δ = 13.90, 22.01, 25.83, 28.33, 28.54, 31.14, 49.39, 125.14, 129.52, 130.04, 132.72, 137.55, 140.97, 142.47, 151.09 ppm; elemental analysis calcd (%) for $C_{44}H_{41}N_7O_{20}S_6$ (1180.22): C 44.78, H 3.50, N 8.31, S 16.30; found C 44.56, H 3.48, N 8.07, S 16.12.

N-*n*-octyl-4-(4-aminobenzenesulfonimido)benzenesulfonimide 3b: M.p. 145-147 °C; ^{1}H NMR (300 MHz, $(CD_3)_2SO$): δ = 0.85 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.23 (s, 10 H, CH_2), 1.53 (br. 2H, CH_2), 3.75 (br, 2 H, CH_2), 6.41 (br. 8 H, NH_2), 6.62 (d, $^{3}J_{H,\,H}$ = 8.8 Hz, 8 H, ArH), 7.27 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.34 (d, $^{3}J_{H,\,H}$ = 8.8 Hz, 8 H, ArH), 7.93 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH) ppm. MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 1082.16 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{44}{}^{1}H_{49}{}^{14}N_7{}^{16}O_{12}{}^{32}S_6Na$) 1082.17; 1098.14 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{44}{}^{1}H_{49}{}^{14}N_7{}^{16}O_{12}{}^{32}S_6K$) 1098.14.

Compound 4: 1 g of tetraaminoderivative **3b** was used for the reaction. The crude product was purified by column chromatography and then recrystallized from CH_2Cl_2/CH_3OH. R_f = 0.24 (silica gel, CH_2Cl_2); yield 1.22 g (57%); m.p. 151-155 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.88 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.27 (s, 10 H, CH_2), 1.69 (br. 2 H, CH_2), 2.47 (s, 24 H, CH_3), 3.71 (t, $^{3}J_{H,\,H}$ = 7.5 Hz, 2 H, CH_2), 7.19 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.24 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 8 H, ArH), 7.37 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 16 H, ArH), 7.81-7.84 (m, 24 H, ArH), 8.04 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.15, 21.83, 22.64, 26.59, 28.96, 29.15, 31.72, 50.29, 128.65, 129.46, 129.62, 129.99, 132.42, 132.63, 136.00, 138.61, 139.57, 140.24, 141.67, 145.83 ppm. MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 2330.21 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{100}{}^{1}H_{97}{}^{14}N_7{}^{16}O_{28}{}^{32}S_{14}K$) 2330.21; 2314.23 $[M+Na]^+$ calcd monoisotopic peak

($^{12}C_{100}{}^{1}H_{97}{}^{14}N_{7}{}^{16}O_{28}{}^{32}S_{14}Na$) 2314.24; elemental analysis calcd (%) for $C_{100}H_{97}N_7O_{28}S_{14}$ (2293.78): C 52.36, H 4.26, N 4.27, S 19.57; found C 52.32, H 4.60, N 4.13, S 18.95.

N-*n*-octyl-4-nitrobenzenesulfonamide 5a: *n*-octylamine (5 g, 39 mmol) and triethylamine (7 mL, 22 mmol) were dissolved in dry dichloromethane (200 mL). To the stirred mixture a solution of 4-nitrobenzenesulfonyl chloride (8.6 g, 39 mmol) in 60 mL of dry dichloromethane was added over a period of 10 min. The reaction mixture was allowed to stir for 20 min at room temperature and then the solvent was removed under reduced pressure. The viscous residue was triturated with 200 mL of methanol/water (5:1) and allowed to stand for 1 hr. Precipitated white flakes were filtered through a glass filter and thoroughly washed with 5% solution of hydrochloric acid and then with large amount of deionized water. The colorless crystalline solid was dried in vacuum resulting in 10.6 g (89%); m.p. 71-73 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.88 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.24 (s, 10 H, CH_2), 1.50 (br. 2 H, CH_2), 3.02 (m, 2 H, CH_2), 4.79 (t, $^{3}J_{H,\,H}$ = 6.0 Hz, 1 H, NH), 8.08 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 2 H, ArH), 8.39 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.04, 22.58, 26.45, 28.97, 29.07, 29.63, 31.68, 43.42, 124.41, 128.31, 146.03, 150.04 ppm. MS (EI, 80 eV): *m/z* = 314.12 $[M]^+$; elemental analysis calcd (%) for $C_{14}H_{22}N_2O_4S$ (314.40): C 53.48, H 7.05, N 8.91, S 10.20; found C 53.39, H 6.89, N 8.99, S 10.33.

N-*n*-octyl-4-aminobenzenesulfonamide 5b: 5 g of **5a** were used in the reaction. Yield 4.45 g (98%); m.p. 71-73 °C. ^{1}H NMR (300 MHz, CD_3OD): δ = 0.84 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.98 (s, 10 H, CH_2), 1.41 (br. 2 H, CH_2), 2.81 (m, 2 H, CH_2), 6.78 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.59 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, CD_3OD): δ = 13.03, 22.29, 26.29, 28.82, 28.88, 29.28, 31.55, 42.70, 121.52, 128.60, 138.22, 138.45 ppm; MS (EI, 80 eV): *m/z* = 284.14 $[M]^+$.

Compound 6a: 2 g of **5b** were used for the reaction. Yield 3.84 g (66%); m.p. 178-181 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.90 (t, $^{3}J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.28 (s, 10 H, CH_2), 1.73 (br. 2H, CH_2), 3.79 (t, $^{3}J_{H,\,H}$ = 7.5 Hz, 2 H, CH_2), 7.30 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 8.16 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 2 H, ArH), 8.18 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 4 H, ArH), 8.29 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 8.46 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 2 H, ArH), 8.48 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 4 H, ArH) ppm; NMR ^{13}C (75.47 MHz, $(CD_3)_2SO$): δ = 13.87, 22.01, 25.77, 28.28, 28.51, 29.44, 31.11, 49.87, 124.85, 125.14, 129.46, 129.51, 130.04, 132.80, 137.59, 140.96, 142.54, 143.96, 150.68, 151.11 ppm; MS (EI, 80 eV): *m/z* = 839.09 $[M]^+$, 653.13 $[M - p\text{-}NO_2C_6H_4SO_2]^+$, 525.99 $[M - p\text{-}NO_2C_6H_4SO_2NC_8H_{17}]^+$, 469.15 $[M - 2\ p\text{-}NO_2C_6H_4SO_2]^+$; elemental analysis calcd (%) for $C_{32}H_{33}N_5O_{14}S_4$ (839.89): C 45.76, H 3.96, N 8.34, S 15.27; found C 46.03, H 4.17, N 8.47, S 15.40.

Compound 6b: M.p. 125-128 °C; ^{1}H NMR (300 MHz, CD_3OD): δ = 0.90 (t, $^{3}J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.26 (br. 10 H, CH_2), 1.62 (br. 2H, CH_2), 3.62 (t, $^{3}J_{H,\,H}$ = 6.9 Hz, 2 H, CH_2), 6.66 (d, $^{3}J_{H,\,H}$ = 7.2 Hz, 6 H, ArH), 7.19 (d, $^{3}J_{H,\,H}$ = 8.1 Hz, 2 H, ArH), 7.43 (d, $^{3}J_{H,\,H}$ = 7.2 Hz, 4 H, ArH), 7.83 (d, $^{3}J_{H,\,H}$ = 8.1 Hz, 2 H, ArH) ppm; MS (EI, 80 eV): *m/z* = 749.20 $[M]^+$, 594.16 $[M - p\text{-}NH_2C_6H_4SO_2]^+$, 439.16 $[M - 2\ p\text{-}NH_2C_6H_4SO_2]^+$.

Compound 7: 0.93 g of the triamine **6b** were used for the reaction.The product was purified by column chromatography. (R_f = 0.31, silica gel, CH_2Cl_2); Yield 1.41 g (70%). M.p. 135-137 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.88 (t, $^3J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.27 (s, 10 H, CH_2), 1.69 (br. 2 H, CH_2), 2.47 (s, 18 H, CH_3), 3.71 (t, $^3J_{H,\,H}$ = 7.5 Hz, 2 H, CH_2), 7.19 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.25 (d, $^3J_{H,\,H}$ = 8.7 Hz, 6 H, ArH), 7.37 (d, $^3J_{H,\,H}$ = 8.0 Hz, 4 H, ArH), 7.39 (d, $^3J_{H,\,H}$ = 8.0 Hz, 8 H, ArH), 7.81-7.85 (m, 16 H, ArH), 7.96 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 8.04 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.17, 21.84, 22.67, 26.64, 29.00, 29.20, 30.12, 31.77, 50.18, 128.15, 128.67, 129.11, 129.55, 129.63, 129.94, 130.01, 132.39, 132.53, 132.65, 136.04, 136.09, 138.51, 139.58, 139.61, 140.26, 140.86, 141.86, 145.74, 145.85 ppm; MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 1712.18 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{74}{}^1H_{75}{}^{14}N_5{}^{16}O_{20}{}^{32}S_{10}K$) 1712.18; 1696.194 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{74}{}^1H_{75}{}^{14}N_5{}^{16}O_{20}{}^{32}S_{10}Na$) 1696.21; elemental analysis calcd (%) for $C_{74}H_{75}N_5O_{20}S_{10}$ (1675.06): C 53.06, H 4.51, N 4.18, S 19.14; found C 52.87, H 4.60, N 3.83, S 19.28.

Compound 8a: 2 g of **5b** were used for the reaction. Recrystallized from dichloromethane/methanol; yield 1.92 g (42%); m.p. 242-244 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.90 (t, $^3J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.28 (s, 10 H, CH_2), 1.57 (br. 2H, CH_2), 3.09 (m, 2 H, CH_2), 4.74 (t, $^3J_{H,\,H}$ = 6.0 Hz, 1 H, NH), 7.23 (d, $^3J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.95 (d, $^3J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 8.18 (d, $^3J_{H,\,H}$ = 9.0 Hz, 4 H, ArH), 8.48 (d, $^3J_{H,\,H}$ = 9.0 Hz, 4 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $(CD_3)_2SO$): δ = 13.91, 22.04, 26.00, 28.50, 29.06, 29.89, 31.18, 42.59, 125.12, 128.04, 129.96, 132.33, 135.58, 142.72, 143.20, 151.05 ppm. MS (EI, 80 eV): *m/z* = 654.10 $[M]^+$, 463.97 $[M - C_8H_{17}NH]^+$, 284.27 $[M - 2\ p\text{-}NO_2C_6H_4SO_2]^+$; elemental analysis calcd (%) for $C_{26}H_{30}N_4O_{10}S_3$ (654.73): C 47.70, H 4.62, N 8.56, S 14.69; found C 47.48, H 4.68, N 8.41, S 14.87.

Compound 8b: M.p. 142-144 °C; ^{1}H NMR (300 MHz, $(CD_3)_2SO$): δ = 0.84 (t, $^3J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.20 (s, 10 H, CH_2), 1.33 (br. 2H, CH_2), 2.77 (m, 2 H, CH_2), 6.38 (s, 4 H, NH_2), 6.60 (d, $^3J_{H,\,H}$ = 7.2 Hz, 4 H, ArH), 7.15 (d, $^3J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.32 (d, $^3J_{H,\,H}$ = 7.2 Hz, 4 H, ArH), 7.72 (s, 1 H, NH), 7.78 (d, $^3J_{H,\,H}$ = 8.4 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $(CD_3)_2SO$): δ = 13.95, 22.06, 26.01, 28.50, 28.56, 29.00, 31.20, 42.59, 112.40, 122.41, 127.28, 130.33, 132.17, 138.01, 141.71, 154.35 ppm; MS (EI, 80 eV): *m/z* = 594.16 $[M]^+$, 439.16 $[M - p\text{-}NH_2C_6H_4SO_2]^+$, 284.27 $[M - 2\ p\text{-}NO_2C_6H_4SO_2]^+$.

Compound 9a: 2.5 g of diamine **8b** were used in the reaction. Purified by column chromatography (R_f = 0.32, silica gel, CH_2Cl_2); yield 2.70 g (48%); m.p. 157-159 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.83 (t, $^3J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.20 (s, 10 H, CH_2), 1.45 (br. 2H, CH_2), 2.95 (m, 2 H, CH_2), 4.39 (t, $^3J_{H,\,H}$ = 6.0 Hz, 1 H, NH), 7.08 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.23 (d, $^3J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.63-7.70 (m, 8 H, ArH), 7.74 (d, $^3J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.81 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.86-8.01 (m, 16 H, ArH), 8.43 (d, $^3J_{H,\,H}$ = 1.5 Hz, 4 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.17, 22.69, 26.58, 29.13, 29.17, 29.87, 31.79, 43.59, 122.82, 128.13, 128.15, 128.25, 129.70, 129.84, 129.86, 130.02, 130.91, 131.94, 132.33, 132.75, 135.60, 135.62, 137.27, 139.94, 140.05, 142.69 ppm; MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 1377.18 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{66}{}^1H_{58}{}^{14}N_4{}^{16}O_{14}{}^{32}S_7Na$) 1377.19; 1393.11 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{66}{}^1H_{58}{}^{14}N_4{}^{16}O_{14}{}^{32}S_7K$) 1393.16; elemental analysis calcd (%) for

$C_{66}H_{58}N_4O_{14}S_7$ (1355.64): C 58.47, H 4.31, N 4.13, S 16.56; found C 58.73, H 4.22, N 4.01, S 16.82.

Compound 9b: (R_f = 0.78, silica gel, CH_2Cl_2); yield 1.0 g (16%); m.p. 132-135 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.81 (t, $^3J_{H,H}$ = 6.9 Hz, 3 H, CH_3), 1.19 (m, 10 H, CH_2), 1.67 (m, 2H, CH_2), 3.69 (m, 2 H, CH_2), 7.11 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.24 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.57-7.69 (m, 10 H, ArH), 7.75 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.86-8.07 (m, 22 H, ArH), 8.44 (d, $^3J_{H,H}$ = 1.5 Hz, 4 H, ArH), 8.56 (d, $^3J_{H,H}$ = 1.5 Hz, 1 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.16, 22.65, 26.63, 28.99, 29.13, 30.03, 31.73, 50.06, 122.64, 122.81, 127.94, 128.01, 128.12, 128.46, 129.51, 129.75, 129.83, 129.97, 130.38, 130.90, 131.91, 131.96, 132.27, 132.79, 135.46, 135.58, 136.44, 138.27, 139.86, 140.07, 142.33 ppm; MS (ESI pos., CH_3OH): *m/z* = 1583.05 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{76}{}^1H_{64}{}^{14}N_4{}^{16}O_{16}{}^{32}S_8K$) 1583.17; 1567.18 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{76}{}^1H_{64}{}^{14}N_4{}^{16}O_{16}{}^{32}S_8Na$) 1567.20; elemental analysis calcd (%) for $C_{76}H_{64}N_4O_{16}S_8$ (1545.86): C 59.05, H 4.17, N 3.62, S 16.59; found C 59.26, H 4.21, N 3.68, S 16.56.

Compound 9c: 2 g of **9a** were used in the reaction. Purified by column chromatography (R_f = 0.73, silica gel, CH_2Cl_2); yield 1.52 g (68%); m.p. 149-151 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.83 (t, $^3J_{H,H}$ = 6.9 Hz, 3 H, CH_3), 1.19 (m, 10 H, CH_2), 1.67 (br. 2H, CH_2), 3.71 (m, 2 H, CH_2), 7.15 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.26 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.60-7.70 (m, 8 H, ArH), 7.77 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.87-8.04 (m, 18 H, ArH), 8.17 (d, $^3J_{H,H}$ = 9.0 Hz, 2 H, ArH), 8.36 (d, $^3J_{H,H}$ = 9.0 Hz, 2 H, ArH), 8.44 (d, $^3J_{H,H}$ = 1.5 Hz, 4 H, ArH) ppm; MS (ESI pos., CH_3OH): *m/z* = 1578.16 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{72}{}^1H_{61}{}^{14}N_5{}^{16}O_{18}{}^{32}S_8K$) 1578.14; 1562.16 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{72}{}^1H_{61}{}^{14}N_5{}^{16}O_{18}{}^{32}S_8Na$) 1562.17; elemental analysis calcd (%) for $C_{72}H_{61}N_5O_{18}S_8$ (1540.80): C 56.12, H 3.99, N 4.55, S 16.65; found C 55.98, H 4.20, N 4.41, S 16.62.

Compound 9d: M.p. 137-139 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.85 (t, $^3J_{H,H}$ = 6.9 Hz, 3 H, CH_3), 1.21 (m, 10 H, CH_2), 1.69 (br. 2H, CH_2), 3.63 (m, 2 H, CH_2), 6.75 (br. 2 H, NH_2), 7.12 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.27 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.61-7.70 (m, 8 H, ArH), 7.77 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.88-8.01 (m, 18 H, ArH), 8.46 (d, $^3J_{H,H}$ = 1.5 Hz, 4 H, ArH) ppm; MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 1532.19 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{72}{}^1H_{63}{}^{14}N_5{}^{16}O_{18}{}^{32}S_8Na$) 1532.19; 1548.22 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{72}{}^1H_{63}{}^{14}N_5{}^{16}O_{18}{}^{32}S_8K$) 1548.17.

Compound 10a: 850 mg of **9d** were used in the reaction. Purified by column chromatography (R_f = 0.25, silica gel, CH_2Cl_2); yield 750 mg (72%); m.p. 189-191 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.84 (t, $^3J_{H,H}$ = 6.9 Hz, 3 H, CH_3), 1.24 (m, 10 H, CH_2), 1.73 (br. 2H, CH_2), 3.73 (m, 2 H, CH_2), 7.17 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.22 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.28 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.62-7.71 (m, 8 H, ArH), 7.77 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.88-8.01 (m, 18 H, ArH), 8.13 (d, $^3J_{H,H}$ = 9.0 Hz, 4 H, ArH), 8.39 (d, $^3J_{H,H}$ = 9.0 Hz, 4 H, ArH), 8.46 (d, $^3J_{H,H}$ = 1.5 Hz, 4 H, ArH) ppm; MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 1902.16 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{84}{}^1H_{69}{}^{14}N_7{}^{16}O_{24}{}^{32}S_{10}Na$) 1902.15; 1918.04 $[M+K]^+$ calcd monoisotopic peak

($^{12}C_{84}{}^{1}H_{69}{}^{14}N_{7}{}^{16}O_{24}{}^{32}S_{10}K$) 1918.12; elemental analysis calcd (%) for $C_{84}H_{69}N_7O_{24}S_{10}$ (1881.13): C 53.63, H 3.70, N 5.21, S 17.05; found C 53.78, H 3.80, N 5.33, S 16.90.

Compound 10b: M.p. 140-142 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.85 (t, $^3J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.23 (m, 10 H, CH_2), 1.71 (br. 2H, CH_2), 3.65 (m, 2 H, CH_2), 6.64 (br. 4 H, NH_2), 7.14 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.22 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.27 (d, $^3J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.61-7.71 (m, 8 H, ArH), 7.77 (d, $^3J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.87-8.01 (m, 20 H, ArH), 8.46 (d, $^3J_{H,\,H}$ = 1.5 Hz, 4 H, ArH) ppm; MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 1842.19 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{84}{}^{1}H_{73}{}^{14}N_{7}{}^{16}O_{20}{}^{32}S_{10}Na$) 1842.20; 1858.19 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{84}{}^{1}H_{73}{}^{14}N_{7}{}^{16}O_{20}{}^{32}S_{10}K$) 1858.18.

Compound 11: 430 mg of **13b** were used in the reaction. Purified by column chromatography (R_f = 0.19, silica gel, CH_2Cl_2); yield 312 mg (54%); m.p. 214-215 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.84 (t, $^3J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.22 (m, 10 H, CH_2), 1.78 (br. 2H, CH_2), 3.73 (m, 2 H, CH_2), 7.15 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.17 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.20 (d, $^3J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.23 (d, $^3J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.58-7.68 (m, 8 H, ArH), 7.73 (d, $^3J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.80-7.95 (m, 24 H, ArH), 8.08 (d, $^3J_{H,\,H}$ = 9.0 Hz, 8 H, ArH), 8.37 (d, $^3J_{H,\,H}$ = 9.0 Hz, 8 H, ArH), 8.41 (d, $^3J_{H,\,H}$ = 1.5 Hz, 4 H, ArH) ppm; MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 2598.20 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{108}{}^{1}H_{85}{}^{14}N_{11}{}^{16}O_{36}{}^{32}S_{14}K$) 2598.09; 2582.12 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{108}{}^{1}H_{85}{}^{14}N_{11}{}^{16}O_{36}{}^{32}S_{14}Na$) 2582.11; elemental analysis calcd (%) for $C_{108}H_{85}N_{11}O_{36}S_{14}$ (2561.79): C 50.63, H 3.34, N 6.01, S 17.52; found C 50.38, H 3.16, N 5.93, S 17.38.

Compound 12a: 3 g of **5a** were used in the reaction. Recrystallized from methanol; yield 4.2 g (84%); m.p. 74-78 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.91 (t, $^3J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.26 (s, 10 H, CH_2), 1.69 (br. 2 H, CH_2), 3.74 (t, $^3J_{H,\,H}$ = 7.5 Hz, 2 H, CH_2), 7.76 (d, $^3J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.96 (d, $^3J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 8.27 (d, $^3J_{H,\,H}$ = 9.0 Hz, 2 H, ArH), 8.44 (d, $^3J_{H,\,H}$ = 9.0 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.08, 22.60, 26.48, 28.90, 29.08, 29.89, 31.68, 50.10, 124.34, 129.55, 129.67, 129.77, 132.60, 138.48, 145.55, 150.64 ppm; MS (EI, 80 eV): *m/z* = 534.03 $[M]^+$, 434.92 $[M - C_7H_{15}]^+$, 348.05 $[M - p\text{-}NO_2C_6H_4SO_2]^+$, 313.12 $[M - p\text{-}BrC_6H_4SO_2]^+$, 220.91 $[M - p\text{-}NO_2C_6H_4SO_2NC_8H_{17}]^+$, 185.99 $[M - p\text{-}BrC_6H_4SO_2NC_8H_{17}]^+$; elemental analysis calcd (%) for $C_{20}H_{25}BrN_2O_6S_2$ (533.46): C 45.03, H 4.72, Br 14.98, N 5.25, S 12.02; found C 44.93, H 4.65, Br 15.11, N 5.24, S 12.23.

Compound 12b: Yield 2.7 g (96%); m.p. 73-77 °C; ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ = 0.89 (t, $^3J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.25 (s, 10 H, CH_2), 1.66 (br. 2 H, CH_2), 3.67 (t, $^3J_{H,\,H}$ = 7.5 Hz, 2 H, CH_2), 5.81 (s, 2 H, NH_2), 6.76 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.64 (d, $^3J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.81 (d, $^3J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.87 (d, $^3J_{H,\,H}$ = 8.4 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $(CD_3)_2CO$): δ = 14.45, 23.36, 27.26, 27.31, 29.17, 29.89, 32.55, 50.05, 125.85, 128.89, 129.74, 130.71, 131.42, 133.16, 141.10, 155.07 ppm; MS (EI, 80 eV): *m/z* = 504.06 $[M]^+$, 346.05 $[M - p\text{-}NH_2C_6H_4SO_2NC_8H_{17}]^+$, 283.15 $[M - p\text{-}BrC_6H_4SO_2NC_8H_{17}]^+$, 220.91 $[M - p\text{-}NH_2C_6H_4SO_2NC_8H_{17}]^+$, 156.01 $[M - p\text{-}BrC_6H_4SO_2NC_8H_{17}]^+$.

Compound 13a: 2.9 g of **12b** were used. Recrystallized from dichloromethane/methanol; yield 3.4 g (68%); m.p. 173-174 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.91 (t, $^{3}J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.27 (s, 10 H, CH_2), 1.70 (br. 2H, CH_2), 3.73 (t, $^{3}J_{H,\,H}$ = 7.6 Hz, 2 H, CH_2), 7.28 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.76 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.94 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 8.14 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 8.19 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 4 H, ArH), 8.48 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 4 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $(CD_3)_2SO$): δ = 13.90, 22.02, 25.75, 28.30, 28.48, 29.32, 31.11, 49.60, 125.15, 128.88, 129.42, 129.66, 130.04, 132.69, 132.75, 137.40, 138.10, 141.38, 142.54, 151.10 ppm; MS (EI, 80 eV): *m/z* = 874.02 $[M]^+$, 774.90 $[M - C_7H_{15}]^+$, 689.05 $[M - p\text{-}NO_2C_6H_4SO_2]^+$, 653.13 $[M - p\text{-}BrC_6H_4SO_2]^+$, 525.99 $[M - p\text{-}BrC_6H_4SO_2NC_8H_{17}]^+$; elemental analysis calcd (%) for $C_{32}H_{33}BrN_4O_{12}S_4$ (873.79): C 43.99, H 3.81, Br 9.14, N 6.41, S 14.68; found C 43.79, H 4.00, Br 8.89, N 6.30, S 14.74.

Compound 13b: 2.2 g of **12b** were used. Recrystallized from dichloromethane/methanol; yield 3.0 g (84%); m.p. 142-144 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.91 (t, $^{3}J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.28 (s, 10 H, CH_2), 1.69 (br. 2H, CH_2), 2.52 (s, 6 H, CH_3), 3.70 (t, $^{3}J_{H,\,H}$ = 7.5 Hz, 2 H, CH_2), 7.25 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.39 (d, $^{3}J_{H,\,H}$ = 7.5 Hz, 4 H, ArH), 7.75 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.84 (d, $^{3}J_{H,\,H}$ = 7.5 Hz, 4 H, ArH), 7.88 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 8.04 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.19, 21.86, 22.70, 26.63, 29.02, 29.20, 29.99, 31.80, 50.03, 128.70, 129.19, 129.35, 129.43, 129.76, 129.94, 132.46, 132.60, 136.15, 138.93, 139.44, 141.22 ppm; MS (EI, 80 eV): *m/z* = 810.08 $[M]^+$, 658.06 $[M - p\text{-}CH_3C_6H_4SO_2]^+$, 591.16 $[M - p\text{-}BrC_6H_4SO_2]^+$, 464.03 $[M - p\text{-}BrC_6H_4SO_2NC_8H_{17}]^+$; elemental analysis calcd (%) for $C_{34}H_{39}BrN_2O_8S_4$ (811.85): C 50.30, H 4.84, Br 9.84, N 3.45, S 15.80; found C 50.34, H 4.86, Br 9.93, N 3.43, S 15.96.

Compound 14: Yield 1.1 g (91%); m.p. 79-83 °C; ^{1}H NMR (300 MHz, CD_3OD): δ = 0.93 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.27 (s, 10 H, CH_2), 1.62 (br. 2H, CH_2), 3.54 (m, 2 H, CH_2), 6.68 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.28 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.60 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.75 (m, 6 H, ArH) ppm; MS (EI, 80 eV): *m/z* = 659.06 $[M]^+$, 439.16 $[M - p\text{-}BrC_6H_4SO_2]^+$, 311.01 $[M - p\text{-}NO_2C_6H_4SO_2NC_8H_{17}]^+$.

Compound 15a: 1 g of **14** was used in the reaction. Recrystallized from dichloromethane/methanol; yield 1.29 g (70%), m.p. 202-204 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.90 (t, $^{3}J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.26 (s, 10 H, CH_2), 1.70 (br. 2H, CH_2), 3.73 (m, 2 H, CH_2), 7.28 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.30 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.77 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.94 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 8.02 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 8.12 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 8.20, (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 2 H, ArH), 8.21 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 4 H, ArH), 8.49 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 2 H, ArH), 8.51 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 4 H, ArH) ppm; MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 1250.96 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{44}{}^{1}H_{41}{}^{79}Br^{14}N_6{}^{16}O_{18}{}^{32}S_6K$) 1250.96; 1234.98 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{44}{}^{1}H_{41}{}^{79}Br^{14}N_6{}^{16}O_{18}{}^{32}S_6Na$) 1234.99; elemental analysis calcd (%) for $C_{44}H_{41}BrN_6O_{18}S_6$ (1214.12): C 43.53, H 3.40, Br 6.58, N 6.92, S 15.85; found C 43.79, H 3.65, Br 6.55, N 7.11, S 15.81.

Compound 15b: 0.9 g of **14** was used in the reaction. Recrystallized from dichloromethane/methanol; yield 1.14 g (77%); m.p. 208-211 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.90 (t, $^{3}J_{H,\,H}$ = 6.9 Hz, 3 H, CH_3), 1.27 (s, 10 H, CH_2), 1.70 (br. 2H, CH_2), 2.52 (s, 9 H, CH_3), 3.71 (m, 2 H, CH_2), 7.20 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.22 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.37 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 6 H, ArH), 7.71 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 2 H, ArH), 7.75 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.82 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 4 H, ArH), 7.86 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.91 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 8.03 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.20, 21.89, 21.92, 22.72, 26.65, 29.04, 29.22, 31.81, 50.08, 128.75, 129.36, 129.53, 129.61, 129.80, 130.01, 130.10, 132.42, 132.58, 132.65, 135.72, 136.15, 138.89, 138.98, 139.88, 140.37, 141.64, 144.38, 145.81, 146.12 ppm. MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 1158.05 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{47}{}^{1}H_{50}{}^{79}Br^{14}N_3{}^{16}O_{12}{}^{32}S_6K$) 1158.05; 1142.07 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{47}{}^{1}H_{50}{}^{79}Br^{14}N_3{}^{16}O_{12}{}^{32}S_6Na$) 1142.08; elemental analysis calcd (%) for $C_{47}H_{50}BrN_3O_{12}S_6$ (1121.21): C 50.35, H 4.49, Br 7.13, N 3.75, S 17.16; found C 50.06, H 4.53, Br 7.30, N 3.69, S 17.30.

Compound 16: M.p. 142-144 °C; ^{1}H NMR (300 MHz, CD_3OD): δ = 0.93 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.29 (s, 10 H, CH_2), 1.66 (br. 2H, CH_2), 3.78 (m, 2 H, CH_2), 7.08 (d, $^{3}J_{H,\,H}$ = 8.8 Hz, 4 H, ArH), 7.31 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.67 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.74 (d, $^{3}J_{H,\,H}$ = 8.8 Hz, 4 H, ArH), 7.95 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 8.01 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH) ppm; MS (EI, 80 eV): *m/z* = 814.07 $[M]^+$.

Compound 17a: 1 g of **16** was used. Recrystallized from dichloromethane/methanol; yield 1.4 g (74%); m.p. 267-269 °C; ^{1}H NMR (500 MHz, $(CD_3)_2SO$): δ = 0.83 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.17 (s, 10 H, CH_2), 1.62 (br. 2H, CH_2), 3.77 (t, $^{3}J_{H,\,H}$ = 7.6 Hz, 2 H, CH_2), 7.44 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 7.50 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.70 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.92 (m, 6 H, ArH), 8.09 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH), 8.17 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 8 H, ArH), 8.53 (d, $^{3}J_{H,\,H}$ = 9.0 Hz, 8 H, ArH) ppm; elemental analysis calcd (%) for $C_{56}H_{49}BrN_8O_{24}S_8$ (1554.45): C 43.27, H 3.18, Br 5.14, N 7.21, S 16.50; found C 43.10, H 3.35, Br 5.19, N 7.52, S 16.74.

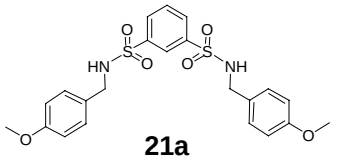
Compound 17b: 0.7 g of **16** was used. Purified by column chromatography (R_f = 0.39, silica gel, CH_2Cl_2); yield 0.9 g (72%), m.p. 127-129 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.90 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 3 H, CH_3), 1.26 (s, 10 H, CH_2), 1.72 (br. 2 H, CH_2), 2.50 (s, 12 H, CH_3), 3.72 (m, 2 H, CH_2), 7.15 (d, $^{3}J_{H,\,H}$ = 8.8 Hz, 2 H, ArH), 7.20 (d, $^{3}J_{H,\,H}$ = 8.8 Hz, 4 H, ArH), 7.33 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 8 H, ArH), 7.70 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 7.77 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.78 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 8 H, ArH), 7.82 (d, $^{3}J_{H,\,H}$ = 8.4 Hz, 2 H, ArH), 8.02 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 2 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.22, 21.91, 22.74, 26.66, 29.05, 29.23, 30.11, 31.81, 50.16, 128.75, 129.49, 129.55, 129.62, 129.68, 129.85, 130.07, 132.40, 132.70, 136.12, 138.53, 139.72, 140.30, 142.05, 145.89 ppm; MS (ESI pos., CH_3OH): *m/z* = 1467.18 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{60}{}^{1}H_{61}{}^{79}Br^{14}N_4{}^{16}O_{16}{}^{32}S_8K$) 1467.07; 1451.21 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{60}{}^{1}H_{61}{}^{79}Br^{14}N_4{}^{16}O_{16}{}^{32}S_8Na$) 1451.09; elemental analysis calcd (%) for $C_{60}H_{61}BrN_4O_{16}S_8$ (1430.57): C 50.37, H 4.30, Br 5.59, N 3.92, S 17.93; found C 50.26, H 4.42, Br 5.60, N 3.86, S 17.83.

Compound 18: 1 g of **13b** was used in the reaction. Recrystallized from chloroform/methanol; yield 820 mg (86%), m.p. 173-175 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.85 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 6 H, CH_3), 1.24 (s, 20 H, CH_2), 1.71 (br. 4 H, CH_2), 2.47 (s, 12 H, CH_3), 3.70 (t, $^{3}J_{H,\,H}$ = 7.5 Hz, 4 H, CH_2), 7.21 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.34 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 8 H, ArH), 7.74 (s, 4 H, ArH), 7.79 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 8 H, ArH), 7.81 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 8.03 (d, $^{3}J_{H,\,H}$ = 8.5 Hz, 4 H, ArH), 8.05 (d, $^{3}J_{H,\,H}$ = 8.5 Hz, 4 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.22, 21.91, 22.75, 26.74, 29.13, 29.27, 29.85, 30.20, 31.86, 50.06, 127.82, 128.27, 128.76, 128.97, 129.25, 129.98, 132.49, 136.23, 138.86, 139.39, 139.45, 139.66, 141.45, 145.72 ppm; MS (ESI pos., CH_3OH): *m/z* = 1577.30 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{74}{}^{1}H_{82}{}^{14}N_4{}^{16}O_{16}{}^{32}S_8K$) 1577.31; 1561.33 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{74}{}^{1}H_{82}{}^{14}N_4{}^{16}O_{16}{}^{32}S_8Na$) 1561.34; elemental analysis calcd (%) for $C_{74}H_{82}N_4O_{16}S_8$ (1539.98): C 57.71, H 5.37, N 3.64, S 16.66; found C 57.64, H 5.09, N 3.62, S 16.89.

Compound 19: 1 g of **15b** was used in the reaction. Recrystallized from chloroform/methanol; yield 730 mg (76%), m.p. 147-149 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.87 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 6 H, CH_3), 1.26 (s, 20 H, CH_2), 1.71 (br. 4 H, CH_2), 2.47 (s, 18 H, CH_3), 3.71 (t, $^{3}J_{H,\,H}$ = 7.5 Hz, 4 H, CH_2), 7.20 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.21 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.36 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 12 H, ArH), 7.73 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.74 (s, 4 H, ArH), 7.80 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 12 H, ArH), 7.90 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 8.04 (d, $^{3}J_{H,\,H}$ = 8.5 Hz, 4 H, ArH), 8.06 (d, $^{3}J_{H,\,H}$ = 8.5 Hz, 4 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.21, 21.90, 22.73, 26.72, 29.09, 29.25, 29.60, 30.14, 31.84, 50.06, 127.83, 128.27, 128.76, 128.99, 129.40, 129.62, 130.02, 130.11, 132.41, 135.75, 136.15, 138.75, 138.90, 139.42, 139.88, 140.39, 141.83, 145.82, 146.03, 146.11 ppm; MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 2195.31 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{100}{}^{1}H_{104}{}^{14}N_6{}^{16}O_{24}{}^{32}S_{12}K$) 2195.34; 2179.36 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{100}{}^{1}H_{104}{}^{14}N_6{}^{16}O_{24}{}^{32}S_{12}Na$) 2179.36; elemental analysis calcd (%) for $C_{100}H_{104}N_6O_{24}S_{12}$ (2158.70): C 55.64, H 4.86, N 3.89, S 17.82; found C 55.78, H 4.85, N 3.87, S 17.95.

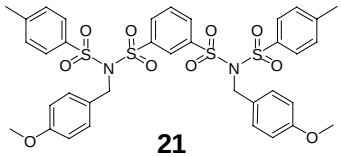
Compound 20: 800 mg of 17b were used in the reaction. Purified by column chromatography (R_f = 0.33, silica gel, CH_2Cl_2); yield 600 mg (78%), m.p. 177-179 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.87 (t, $^{3}J_{H,\,H}$ = 7.0 Hz, 6 H, CH_3), 1.26 (s, 20 H, CH_2), 1.72 (br. 4 H, CH_2), 2.48 (s, 24 H, CH_3), 3.72 (t, $^{3}J_{H,\,H}$ = 7.5 Hz, 4 H, CH_2), 7.19 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 7.22 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 8 H, ArH), 7.36 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 16 H, ArH), 7.77 (s, 4 H, ArH), 7.79 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 8 H, ArH), 7.80 (d, $^{3}J_{H,\,H}$ = 8.0 Hz, 16 H, ArH), 7.81 (d, $^{3}J_{H,\,H}$ = 8.7 Hz, 4 H, ArH), 8.07 (m, 8 H, ArH) ppm; ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 14.22, 21.91, 22.74, 26.73, 29.10, 29.26, 29.85, 30.18, 31.85, 127.86, 128.30, 128.76, 129.04, 129.59, 129.70, 132.39, 132.71, 136.13, 138.44, 139.37, 139.47, 139.74, 140.30, 142.25, 145.89 ppm. MS (ESI pos., CH_3OH/CH_2Cl_2): *m/z* = 2813.93 $[M+K]^+$ calcd monoisotopic peak ($^{12}C_{126}{}^{1}H_{126}{}^{14}N_8{}^{16}O_{32}{}^{32}S_{16}K$) 2813.36; 2797.95 $[M+Na]^+$ calcd monoisotopic peak ($^{12}C_{126}{}^{1}H_{126}{}^{14}N_8{}^{16}O_{32}{}^{32}S_{16}Na$) 2797.39; elemental analysis calcd (%) for $C_{126}H_{126}N_8O_{32}S_{16}$ (2777.42): C 54.49, H 4.57, N 4.03, S 18.47; found C 54.61, H 4.70, N 3.81, S 18.27.

Compound 21a: To a stirred solution of 4-methoxybenzylamine (1.05 g, 7.6 mmol) and triethylamine (2mL) in dry dichloromethane (30 mL) a solution of benzene-1,3-disulfonyl chloride (1 g, 3.6 mml) in dichloromethane (10 mL) was added. The reaction mixture was stirred at room temperature for 2 hs. Then the solvent was removed under reduced pressure and the solid residue was recrystallized from dichloromethane/methanol affording 1.60 g (93%) of colorless crystalline solid. M.p. 158-160 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.77 (s, 6 H, OCH_3), 4.12 (d, $^3J_{H,H}$ = 6.0 Hz, 4 H, NCH_2Ar), 5.19 (t, $^3J_{H,H}$ = 6.0 Hz, 2 H, NH), 6.78 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.11 (d, $^3J_{H,H}$ = 8.7 Hz, 4 H, ArH), 7.58 (t, $^3J_{H,H}$ = 9.0 Hz, 1 H, ArH), 7.97 (d, $^3J_{H,H}$ = 9.0 Hz, 2 H, ArH), 8.28 (d, $^3J_{H,H}$ = 9.0 Hz, 2 H, ArH) ppm. EI-MS: m/z = 476.11 $[M]^+$. $C_{22}H_{24}N_2O_6S_2$ (476.57): calcd. C 55.45, H 5.08, N 5.88, S 13.46; found C 55.46, H 4.98, N 5.69, S 13.40.



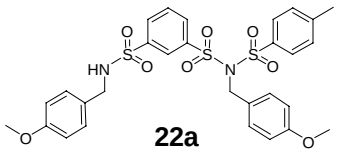
21a

Compound 21: To a vigorously stirred suspension of **21a** (1 g, 2.1 mmol) and Cs_2CO_3 (2 g) in acetonitrile (30 mL) a solution of tosyl chloride (1 g, 5.2 mmol) in acetonitrile (5 mL) was added. The reaction mixture was stirred at room temperature for 2 hs. Then cesium salts were filtered through a paper filter and the solvent was removed under reduced pressure. The viscous residue was triturated with methanol resulting in white powder, which was recrystallized from methanol/dichloromethane. Yield 1.45 g (88%); m.p. 172-173 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.45 (s, 3 H, CH_3), 3.81 (s, 6 H, OCH_3), 4.89 (s, 4 H, NCH_2Ar), 6.80 (d, $^3J_{H,H}$ = 8.0 Hz, 4 H, ArH), 7.30 (m, 8 H, ArH), 7.49 (t, $^3J_{H,H}$ = 8.4 Hz, 1 H, ArH), 7.71 (d, $^3J_{H,H}$ = 8.0 Hz, 4 H, ArH), 7.98 (d, $^3J_{H,H}$ = 8.4 Hz, 2 H, ArH), 8.14 (s, 1 H, ArH) ppm. $C_{36}H_{36}N_2O_{10}S_4$ (784.94): calcd. C 55.09, H 4.62, N 3.57, S 16.34; found C 55.06, H 4.54, N 3.66, S 16.16.



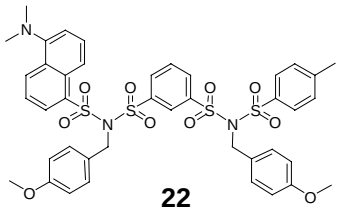
21

Compound 22a: To a vigorously stirred suspension of **21a** (2 g, 4.2 mmol) and Cs_2CO_3 (1.4 g, 4.2 mmol) in acetonitrile (30 mL) a solution of tosyl chloride (0.8 g, 4.2 mmol) in acetonitrile (5 mL) was added dropwise. The reaction mixture was stirred at room temperature for 2 hs. Then cesium salts were filtered through a paper filter and the solvent was removed under reduced pressure. The viscous residue was subjected to a column chromatography (silica gel, CH_2Cl_2, R_f = 0.18); yield 1.13 g (43%), m.p. 118-120 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.45 (s, 3 H, CH_3), 3.80 (s, 3 H, OCH_3), 3.81 (s, 3 H, OCH_3), 4.11 (d, $^3J_{H,H}$ = 6.0 Hz, 2 H, NCH_2Ar), 4.82 (t, $^3J_{H,H}$ = 6.0 Hz, 1 H, NH), 4.89 (s, 2 H, NCH_2Ar), 6.78 (d, $^3J_{H,H}$ = 8.0 Hz, 2 H, ArH), 6.84 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.11 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.34 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.39 (d, $^3J_{H,H}$ = 8.7 Hz, 2 H, ArH), 7.53 (m, 1 H, ArH), 7.80 (s, 1 H, ArH), 7.85 (d, $^3J_{H,H}$ = 8.0 Hz, 2 H, ArH), 7.94 (d, $^3J_{H,H}$ = 9.0 Hz, 1 H, ArH), 8.00 (d, $^3J_{H,H}$ = 9.0 Hz, 1 H, ArH) ppm. EI-MS: m/z = 630.12 $[M]^+$. $C_{29}H_{30}N_2O_8S_3$ (630.75): calcd. C 55.22, H 4.79, N 4.44, S 15.25; found C 55.16, H 4.54, N 4.65, S 15.17.



22a

Compound 22: To a vigorously stirred suspension of **22a** (1 g, 1.6 mmol) and Cs_2CO_3 (2 g) in acetonitrile (30 mL) a solution of dansyl chloride (1 g, 3.7 mmol) in acetonitrile (5 mL) was added. The reaction mixture was stirred at room temperature for 2 hs. Then cesium salts were filtered through a paper filter and the solvent was removed under reduced pressure. The solid residue was triturated with methanol resulting in a yellow powder, which was recrystallized from methanol/dichloromethane.Yield 1.17 g (85%), m.p. 165-166 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.45 (s, 3 H, CH_3), 2.99 (s, 6 H, $N(CH_3)_2$), 3.78 (s, 6 H, OCH_3), 4.89 (s, 2 H, NCH_2Ar), 5.11 (s, 2 H, NCH_2Ar), 6.70 (d, $^3J_{H,H}$ = 6.0 Hz, 2 H, ArH), 6.78 (d, $^3J_{H,H}$ = 6.0 Hz, 2 H, ArH), 7.29-8.38 (m, 18 H) ppm. MS (ESI pos., CH_3OH/CH_2Cl_2): m/z = 902.175 $[M+K]^+$, 886.201 $[M+Na]^+$. $C_{41}H_{41}N_3O_{10}S_4$ (864.04): calcd. C 56.99, H 4.78, N 4.86, S 14.84; found C 56.74, H 4.86, N 4.84, S 15.06.



22

Cartesian coordinates of the B3LYP/6-31G(d) optimized structures

Format:
{Atom} {X} {Y} {Z}

Molecule A

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H	4.6479865	-1.2799499	1.9385790
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Molecule B

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H	2.9642345	0.9296809	1.5497188
H	2.4025044	0.6111145	-0.0943236
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H	-1.9034987	-2.0032290	-2.3505283
C	-1.8545764	0.1539861	-2.5103832
C	-1.4676392	1.3453810	-1.8690738
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C         3.9655055   -0.7297902    0.5607806
H         4.7853923   -0.1074802    0.1865388
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Anion C''

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H        -3.2769273    2.4390518   -2.8626504
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C        -1.4073492    1.4674567   -2.4408311
H         0.5663717    0.7155313   -2.0162680
C        -0.0511279    1.5986178   -2.1369184
S        -2.1120234   -0.1728262   -2.6185694
O        -3.3921989   -0.0794324   -3.3376319
O        -1.0494073   -1.0461081   -3.1351211
N        -2.5500851   -0.5430583   -1.0166807
H        -3.2951191   -1.2367448   -1.0802953
C         3.3280623    0.3488573    2.2805356
H         3.2146223    0.8222647    3.2705073
H         2.6011986    0.8663688    1.6167818
S         1.8271301   -1.5841840    3.0674080
O         1.8633714   -3.0560900    3.2324754
O         1.4111463   -0.7796272    4.2545540
N         3.1219388   -1.0905087    2.3204168
C        -0.7982958   -2.0426709   -0.0606929
H        -1.0002392   -2.7779440   -0.8350778
C        -1.5171903   -0.8380259   -0.0465632
C        -1.2597074    0.1155026    0.9425145
H        -1.8397116    1.0344918    0.9487833
C        -0.2862991   -0.1289296    1.9119002
H        -0.0987440    0.5848671    2.7074523
C         0.4416524   -1.3232474    1.8962281
C         0.1755071   -2.2779007    0.9056430
H         0.7378234   -3.2062427    0.9179350
C         4.7358619    0.6298785    1.7481067
H         4.9335225    1.7095370    1.6819832
H         5.4865026    0.1762007    2.4056833
H         4.8618348    0.1903729    0.7513911
---End of file---
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Anion C'

```
---Begin of file---
C        -2.2886954    3.8279279   -2.3768634
H        -1.9076670    4.8405221   -2.2629118
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C        -3.6548868    3.5767313   -2.2482137
H        -4.3416946    4.3920919   -2.0318273
H        -5.2052784    2.0744453   -2.2974343
C        -4.1402765    2.2727621   -2.3965033
H        -3.6248299    0.2089091   -2.7871435
C        -3.2628720    1.2255134   -2.6703439
C        -1.8937977    1.4826959   -2.7950818
H        -0.3392453    2.9519762   -2.7640141
C        -1.4045833    2.7803911   -2.6513015
S        -0.7587360    0.1052334   -3.1491534
O        -1.3144130   -0.5529579   -4.3461573
O         0.5824419    0.7334417   -3.2835301
N        -0.9498073   -0.9095860   -1.9082622
C         3.6892410   -1.9136763    2.9191228
H         4.3213462   -1.1364893    3.3729826
H         3.4887012   -1.6049941    1.8876223
S         1.3919973   -0.6323283    3.5613177
O         0.3772047   -0.9337983    4.5858465
O         2.2253629    0.5771689    3.7088619
N         2.3884230   -2.0310105    3.5927880
H         2.4822322   -2.2797674    4.5785833
C        -0.7199311   -1.6974071    0.3042466
H        -1.4355336   -2.4608606    0.0133989
C        -0.3510182   -0.7409419   -0.6946141
C         0.5860499    0.2601113   -0.2953404
H         0.9177583    0.9899919   -1.0225797
C         1.1003793    0.2923635    0.9914266
H         1.8075893    1.0650128    1.2776375
C         0.7158492   -0.6651307    1.9418062
C        -0.2058968   -1.6673317    1.5828146
H        -0.5119511   -2.4066119    2.3173763
C         4.4014000   -3.2648185    2.9262917
H         5.3611439   -3.1942486    2.4014333
H         4.6062625   -3.6017819    3.9510057
H         3.7881348   -4.0264777    2.4347159
---End of file---
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Molecule C

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---Begin of file---
C        -1.6537999    4.0093995   -2.7856483
H        -1.0574963    4.9170459   -2.7915008
C        -3.0439595    4.0827891   -2.6912504
H        -3.5310048    5.0511417   -2.6191598
H        -4.8970261    2.9769795   -2.6237291
C        -3.8148998    2.9159148   -2.6923657
H        -3.7859232    0.7585995   -2.7945031
C        -3.1982771    1.6706102   -2.7850379
C        -1.8044022    1.6121416   -2.8662422
H         0.0562128    2.6860367   -2.9591706
C        -1.0222364    2.7672567   -2.8766078
S        -1.0017692    0.0180965   -3.0374414
O        -1.6890061   -0.7548061   -4.0741903
O         0.4423706    0.2464410   -3.0681587
N        -1.4451957   -0.8060340   -1.6076617
H        -1.8592067   -1.6952987   -1.8723237
C         3.9305476   -1.4414019    2.7908370
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H         4.3585635   -0.6506035    3.4206121
H         3.6681213   -0.9861349    1.8297734
S         1.4153541   -0.9009287    3.6464349
O         0.5585706   -1.5822425    4.6232756
O         1.9206020    0.4553280    3.9004580
N         2.6886110   -1.9858971    3.3707631
H         2.8383626   -2.4859430    4.2475071
C        -0.7494952   -1.9674295    0.3926240
H        -1.2876524   -2.8447816    0.0423412
C        -0.7190631   -0.8060224   -0.4000995
C        -0.0293122    0.3253963    0.0571621
H        -0.0062816    1.2322080   -0.5342415
C         0.6302457    0.2876674    1.2826831
H         1.1604178    1.1593949    1.6502786
C         0.5958012   -0.8709384    2.0578837
C        -0.1023252   -1.9995027    1.6197148
H        -0.1358164   -2.8930829    2.2339248
C         4.9338680   -2.5709840    2.5748017
H         5.8495770   -2.1785968    2.1201733
H         5.2115970   -3.0434396    3.5250746
H         4.5198420   -3.3418372    1.9175329
---End of file---
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Molecule D

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---Begin of file---
C         4.1661008   -3.5624217    0.8932358
H         5.1443432   -3.6253329    1.3605757
C         3.2809332   -4.6406242    0.9689880
H         3.5734864   -5.5435654    1.4976974
H         1.3416676   -5.4100583    0.4159350
C         2.0241179   -4.5667194    0.3640548
H         0.6805025   -3.3411301   -0.8126790
C         1.6429441   -3.4116745   -0.3182459
C         2.5388199   -2.3410322   -0.3765656
H         4.4705242   -1.5492871    0.1551463
C         3.8017215   -2.3988375    0.2167024
S         2.0451727   -0.8668361   -1.2658161
O         3.2355718   -0.1762410   -1.7533076
O         0.9492213   -1.2260906   -2.1634124
S         2.2300797    1.2038309    0.9706237
O         1.4060610    1.3905699    2.1624023
O         3.5681818    0.6258361    1.0480155
N         1.3012496    0.1583152   -0.0645724
C        -6.3359456   -1.8933993    0.3584856
H        -7.2168958   -1.3082947    0.0588013
H        -6.2694566   -1.8541317    1.4474854
S        -4.6836911    0.2471612    0.3794092
O        -5.1737862    1.2693060   -0.5560062
O        -5.0489961    0.2849687    1.7980845
N        -5.0825932   -1.3099094   -0.1716451
H        -5.0753830   -1.2927414   -1.1921096
C        -0.8890196    0.8538219   -0.9227185
H        -0.3876581    1.3510274   -1.7453813
C        -0.1315428    0.1792689    0.0402930
C        -0.7586543   -0.4681383    1.1134151
H        -0.1528660   -0.9647193    1.8626941
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C        -2.1455014   -0.4469043    1.2197128
H        -2.6459345   -0.9283601    2.0528457
C        -2.8921843    0.2152719    0.2422232
C        -2.2792036    0.8722013   -0.8242998
H        -2.8843167    1.3998544   -1.5532545
C         1.4825946    5.0024765   -0.2022923
H         0.8015289    5.8022306    0.0734885
C         1.4176627    3.7800431    0.4672469
H         0.7066126    3.6129164    1.2685328
C         2.3063400    2.7670926    0.0996520
C         3.2567385    2.9443887   -0.9094840
H         3.9280203    2.1356982   -1.1733421
C         3.3062613    4.1722884   -1.5674283
H         4.0385927    4.3288256   -2.3539669
C         2.4224385    5.1967145   -1.2164875
H         2.4693410    6.1510497   -1.7336741
C        -6.4643377   -3.3353247   -0.1248308
H        -7.3738673   -3.7871696    0.2853827
H        -6.5322368   -3.3889754   -1.2183695
H        -5.6033112   -3.9309153    0.1940972
---End of file---
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