Supporting Information

Synthesis and structure-activity relationships of suramin-derived $P2Y_{11}$ receptor antagonists with nanomolar potency

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4-Ethyl-3-nitro-benzoic acid was synthesized according to Fahim and Fleifel.[39]
Yield: 90.7%. Mp 187°C, Lit. 188-189°C.[23] ^{1}H NMR (DMSO-d_6): δ 8.35 (d, 1H, ar, J = 1.8 Hz), 8.15 (dd, 1H, ar, J = 7.8, 1.8 Hz), 7.66 (d, 1H, ar, J = 7.8 Hz), 2.89 (q, 2H, -CH_2-, J = 7.3 Hz), 1.23 (t, 3H, -CH_3, J = 7.3 Hz). IR ν_{max} (KBr, cm^{-1}): 2970, 2880, 2650, 2525, 1690, 1615, 1560, 1355, 1300, 850. TLC: R_f 0.74 (EM1). Anal. ($C_9H_9NO_4$) C, H, N.
4-Isopropyl-3-nitro-benzoic acid was synthesized according to Bryan and Foote.[40]
Yield: 90.4%. Mp 156°C, Lit. 157°C.[24] ^{1}H NMR (DMSO-d_6): δ 8.24 (s, 1H, ar), 8.15 (d, 1H, ar, J = 8.5 Hz), 7.78 (d, 1H, ar, J = 8.5 Hz), 3.29 (sep, 1H, -CH=, J = 6.9 Hz), 1.27 (d, 6H, 2x –CH_3-, J = 6.9 Hz). IR ν_{max} (KBr, cm^{-1}): 3420, 2980, 1690, 1615, 1535, 1415, 1385, 1355, 1290, 850. TLC: R_f 0.76 (EM1). Anal. ($C_{10}H_{11}NO_4$) C, H, N.
2-Nitro-biphenyl-4-carboxylic acid was synthesized according to Grieve and Hay, and Sala and Sargent.[41;42]
Yield: 75.7%. Mp 188-192°C, Lit. 191°C.[25] ^{1}H NMR (DMSO-d_6): δ 13-14 (br s, 1H, OH, ex), 8.42 (d, 1H, ar, J = 1.6 Hz), 8.26 (dd, 1H, ar, J = 8.0, 1.6 Hz), 7.72 (d, 1H, ar, J = 8.0 Hz), 7.37-7.56 (m, 5H, ar). IR ν_{max} (KBr, cm^{-1}): 2550-3450, 1695, 1610, 1555, 1530, 1500, 1420, 1285. TLC: R_f 0.44 (EM2). Anal. ($C_{13}H_9NO_4$) C, H, N.
4-(Methoxymethyl)-3-nitro-benzoic acid
4-(Bromomethyl)-benzoic acid was used to synthesize 4-(methoxymethyl)-benzoic acid according to Olson, and Harwood et al.[20;21] which was subsequently nitrated to 4-(methoxymethyl)-3-nitro-benzoic acid by a standard nitration method.[19] Yield: 76.4%. ^{1}H NMR (DMSO-d_6): δ 12.80 (br s, 1H, NH, ex), 9.10 (d, 1H, ar, J = 2.5 Hz), 8.64 (dd, 1H, ar, J = 7.5, 2.5 Hz), 7.74 (d, 1H, ar, J = 7.5 Hz), 4.82 (s, 2H, -CH_2-), 3.40 (s, 3H, -CH_3). TLC: R_f 0.51 (EM3). Anal. ($C_9H_9NO_5$) C, H, N.

General procedure for the synthesis of the benzoyl chloride derivatives 1g-1i.[22;23]
To a suspension of the nitro benzoic acid derivatives (100 mmol) in toluene (50 mL) and DMF (0.5 mL) an excess of thionylchloride (14.5 mL, 200 mmol) was added and stirred under reflux for approx. 2h until the reaction mixture turns into a clear and yellow solution. Excessive thionylchloride and toluene was removed under vacuum. The obtained products **1g-i** were dissolved in toluene and immediately used for the acylation reaction. Thus, no analytical data were obtained.

Nitro derivatives 3g-i and 6g-i.
8-(4-Chloro-3-nitrobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (3g).
3g was synthesized from **1g** and **2** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 94.2%. ^{1}H NMR (DMSO-d_6): δ 12.86 (br s, 1H, NH, ex), 9.42 (d, 1H, ar, J = 1.9 Hz), 8.76 (d, 1H, ar, J = 2.0 Hz), 8.63 (d, 1H, ar, J = 1.9 Hz), 8.44 (dd, 1H, ar, J = 8.4, 2.0 Hz), 8.11 (d, 1H, ar, J = 8.2 Hz), 8.04 (d, 1H, ar, J = 8.2 Hz), 7.97 (d, 1H, ar, J = 8.4 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 3100, 2340, 1660, 1605, 1520, 1470, 1370, 1290, 1235, 1190, 890. NaCl: 1.5%. H_2O: 13.5%. TLC: R_f 0.49 (EM3). Anal. ($C_{17}H_8ClN_2Na_3O_{12}S_3$) C, H, N.
8-(4-Methoxy-3-nitrobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (3h).
3h was synthesized from **1h** and **2** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 89.9%. ^{1}H NMR (DMSO-d_6): δ 12.74 (br s, 1H, NH, ex), 9.43 (d, 1H, ar, J = 2.5 Hz), 8.64 (d, 2H, ar, J = 2.5 Hz), 8.53 (dd, 1H, ar, J = 7.5, 2.5 Hz), 8.11 (d, 1H, ar, J = 8.8 Hz), 8.06 (d, 1H, ar, J = 8.8 Hz), 7.56 (d, 1H, ar, J = 8.9 Hz), 4.06 (s, 3H, -CH_3). NaCl: 2.4%. H_2O: 10.3%. TLC: R_f 0.52 (EM3). Anal. ($C_{18}H_{11}N_2Na_3O_{13}S_3$) C, H, N.
8-(4-(Methoxymethyl)-3-nitrobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (3i).
3i was synthesized from **1i** and **2** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 88.3%. ^{1}H NMR (DMSO-d_6): δ 12.88 (br s, 1H, NH, ex), 9.41 (d, 1H, ar, J = 2.5 Hz), 8.78 (d, 1H, ar, J = 2.5 Hz), 8.63 (d, 1H, ar, J = 2.5 Hz), 8.52 (dd, 1H, ar, J = 7.5, 2.5 Hz),

8.11 (d, 1H, ar, *J* = 7.5 Hz), 8.05 (d, 1H, ar, *J* = 7.5 Hz), 7.88 (d, 1H, ar, *J* = 7.5 Hz), 4.86 (s, 2H, -CH_2-), 3.42 (s, 3H, -CH_3). NaCl: 0.7%. H_2O: 7.8%. TLC: R_f 0.55 (EM3). Anal. ($C_{19}H_{13}N_2Na_3O_{13}S_3$) C, H, N.

8-(4-Chloro-3-(3-nitrobenzamido)-benzamido)naphthalene-1,3,5-trisulfonic acid trisodium salt (6g).

6g was synthesized from **4g** and **1a** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 22.9%. ^{1}H NMR (DMSO-d_6): δ 12.75 (br s, 1H, NH, ex), 10.77 (br s, 1H, NH, ex), 9.41 (d, 1H, ar, *J* = 1.8 Hz), 8.87 (d, 1H, ar, *J* = 1.8 Hz), 8.62 (d, 1H, ar, *J* = 1.8 Hz), 8.49 (dd, 2H, ar, *J* = 8.0, 1.8 Hz), 8.22 (d, 1H, ar, *J* = 2.0 Hz), 8.16 (dd, 1H, ar, *J* = 8.4, 2.0 Hz), 8.09 (d, 1H, ar, *J* = 8.2 Hz), 8.02 (d, 1H, ar, *J* = 8.2 Hz), 7.89 (t, 1H, ar, *J* = 8.0 Hz), 7.74 (d, 1H, ar, *J* = 8.4 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2340, 1640, 1580, 1520, 1455, 1415, 1330, 1240, 1185, 1075, 895. NaCl: 8.5%. H_2O: 16.1%. TLC: R_f 0.49 (EM3). Anal. ($C_{24}H_{13}ClN_3Na_3O_{13}S_3$) C, H, N.

8-(4-Methoxy-3-(3-nitrobenzamido)-benzamido)naphthalene-1,3,5-trisulfonic acid trisodium salt (6h).

6h was synthesized from **4h** and **1a** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 92.6%. ^{1}H NMR (DMSO-d_6): δ 12.61 (br s, 1H, NH, ex), 10.22 (br s, 1H, NH, ex), 9.42 (s, 1H, ar), 8.85 (s, 1H, ar), 8.64 (s, 1H, ar), 8.48 (d, 2H, ar, *J* = 7.5 Hz), 8.32 (s, 1H, ar), 8.21 (d, 1H, ar, *J* = 7.5 Hz), 8.10 (d, 1H, ar, *J* = 7.5 Hz), 8.05 (d, 1H, ar, *J* = 7.5 Hz), 7.89 (pt, 1H, ar, *J* = 7.5 Hz), 7.27 (d, 1H, ar, *J* = 7.5 Hz), 3.95 (s, 3H, -CH_3). NaCl: 0.7%. H_2O: 17.8%. TLC: R_f 0.52 (EM3). Anal. ($C_{25}H_{16}N_3Na_3O_{14}S_3$) C, H, N.

8-(4-(Methoxymethyl)-3-(3-nitrobenzamido)benzamido)naphthalene-1,3,5-trisulfonic acid trisodium salt (6i).

6i was synthesized from **4i** and **1a** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 92.5%. ^{1}H NMR (DMSO-d_6): δ 12.71 (br s, 1H, NH, ex), 10.58 (br s, 1H, NH, ex), 9.42 (d, 1H, ar, *J* = 2.5 Hz), 8.88 (s, 1H, ar), 8.64 (d, 1H, ar, *J* = 2.5 Hz), 8.51 (dd, 2H, ar, *J* = 7.5, 2.5 Hz), 8.17 (s, 2H, ar), 8.10 (d, 1H, ar, *J* = 7.5 Hz), 8.05 (d, 1H, ar, *J* = 7.5 Hz), 7.92 (t, 1H, ar, *J* = 7.5 Hz), 7.62 (d, 1H, ar, *J* = 7.5 Hz), 4.59 (s, 2H, -CH_2-), 3.28 (s, 3H, -CH_3). NaCl: 1.6%. H_2O: 15.9%. TLC: R_f 0.56 (EM3). Anal. ($C_{26}H_{18}N_3Na_3O_{14}S_3$) C, H, N.

Compounds **3a-f** and **6a-f** have been described by Nickel et al. but no analytical data have been given.[18] Analytical data of **3a** are given in Kassack et al.[16] Thus here, analytical data of **3b-f** and **6a-f** are presented.

8-(4-Methyl-3-nitrobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (3b).

Yield: 88.1%. ^{1}H NMR (DMSO-d_6): δ 12.81 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, *J* = 1.9 Hz), 8.67 (d, 1H, ar, *J* = 1.6 Hz), 8.62 (d, 1H, ar, *J* = 1.6 Hz), 8.38 (dd, 1H, ar, *J* = 8.2, 1.9 Hz), 8.08 (d, 1H, ar, *J* = 8.2 Hz), 8.03 (d, 1H, ar, *J* = 7.9 Hz), 7.65 (d, 1H, ar, *J* = 8.2 Hz), 2.60 (s, 3H, -CH_3). NaCl: 18.2%. H_2O: 15.0%. TLC: R_f 0.49 (EM3). Anal. ($C_{18}H_{11}N_2Na_3O_{12}S_3$) C, H, N.

8-(4-Ethyl-3-nitrobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (3c).

Yield: 95.0%. ^{1}H NMR (DMSO-d_6): δ 12.64 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, *J* = 1.8 Hz), 8.62 (m, 2H, ar), 8.41 (d, 1H, ar, *J* = 8.2 Hz), 8.09 (d, 1H, ar, *J* = 8.2 Hz), 8.03 (d, 1H, ar, *J* = 8.2 Hz), 7.70 (d, 1H, ar, *J* = 8.2 Hz), 2.93 (q, 2H, -CH_2-, *J* = 7.4 Hz), 1.27 (t, 3H, -CH_3, *J* = 7.4 Hz). IR ν_{max} (KBr, cm^{-1}): 3200, 2970, 1650, 1620, 1575, 1335, 1195, 1075, 1040, 840. NaCl: 9.3%. H_2O: 14.7%. TLC: R_f 0.52 (EM3). Anal. ($C_{19}H_{13}N_2Na_3O_{12}S_3$) C, H, N.

8-(4-Isopropyl-3-nitrobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (3d).

Yield: 80.1%. ^{1}H NMR (DMSO-d_6): δ 12.86 (br s, 1H, NH, ex), 9.41 (d, 1H, ar, *J* = 1.9 Hz), 8.62 (d, 1H, ar, *J* = 1.9 Hz), 8.49 (s, 1H, ar), 8.44 (d, 1H, ar, *J* = 8.2 Hz), 8.10 (d, 1H, ar, *J* = 8.2 Hz), 8.07 (d, 1H, ar, *J* = 8.2 Hz), 7.82 (d, 1H, ar, *J* = 8.2 Hz), 3.29 (sep, 1H, -CH=, *J* = 6.8 Hz), 1.32 (d, 6H, $(-CH_3)_2$, *J* = 6.8 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2960, 1660, 1640,

1530, 1340, 1230, 1195, 1075, 1045, 840. NaCl: 5.1%. H_2O: 12.3%. TLC: R_f 0.52 (EM3). Anal. ($C_{20}H_{15}N_2Na_3O_{12}S_3$) C, H, N.

8-(3-Nitro-4-phenylbenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (3e).
Yield: 82.9%. ^{1}H NMR (DMSO-d_6): δ 12.92 (br s, 1H, NH, ex), 9.41 (d, 1H, ar, J = 1.9 Hz), 8.68 (d, 1H, ar, J = 1.6 Hz), 8.63 (d, 1H, ar, J = 1.9 Hz), 8.51 (dd, 1H, ar, J = 8.1, 1.6 Hz), 8.11 (d, 1H, ar, J = 8.2 Hz), 8.07 (d, 1H, ar, J = 8.2 Hz), 7.74 (d, 1H, ar, J = 8.1 Hz), 7.40-7.58 (m, 5H, -C_6H_5). IR ν_{max} (KBr, cm^{-1}): 3450, 1670, 1620, 1550, 1525, 1505, 1355, 1325, 1225, 1190, 1170, 1040, 840. NaCl: 1.9%. H_2O: 14.8%. TLC: R_f 0.63 (EM4). Anal. ($C_{23}H_{13}N_2Na_3O_{12}S_3$) C, H, N.

8-(4-Fluoro-3-nitrobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (3f).
Yield: 89.6%. ^{1}H NMR (DMSO-d_6): δ 12.85 (br s, 1H, NH, ex), 9.41 (d, 1H, ar, J = 1.9 Hz), 8.86 (dd, 1H, ar, J = 7.4, 2.4 Hz), 8.63 (d, 1H, ar, J = 1.8 Hz), 8.57-8.60 (m, 1H, ar), 8.08 (d, 1H, ar, J = 8.2 Hz), 8.03 (d, 1H, ar, J = 8.2 Hz), 7.76 (dd, 1H, ar, J = 11.1, 8.7 Hz). ^{13}C NMR (DMSO-d_6): δ 162.7 (C-O), 157.3 (ar, C-F), 155.2 (ar, C-N), 143.0 (ar, C-N), 142.7 (ar, C-S), 141.3 (ar, C-S), 136.8 (ar, C-H), 136.0 (ar, C-C), 133.7 (ar, C-S), 132.8 (ar, C-H), 131.5 (ar, C-C), 127.0 (ar, C-H), 126.1 (ar, C-H), 125.0 (ar, C-H), 123.4 (ar, C-C), 123.1 (ar, C-H), 118.7 (ar, C-H). IR ν_{max} (KBr, cm^{-1}): 3440, 3100, 1665, 1615, 1530, 1485, 1360, 1325, 1235, 1075, 1040, 845. NaCl: 22.8%. H_2O: 18.0%. TLC: R_f 0.78 (EM3). Anal. ($C_{17}H_8FN_2Na_3O_{12}S_3$) C, H, N.

8-(3-(3-Nitrobenzamido)benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (6a).
Yield: 72.2%. ^{1}H NMR (DMSO-d_6): δ 12.67 (br s, 1H, NH, ex), 10.74 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, J = 1.9 Hz), 8.86 (pt, 1H, ar, J = 1.9 Hz), 8.61 (d, 1H, ar, J = 1.9 Hz), 8.46 (d, 1H, ar, J = 9.2 Hz), 8.44 (d, 1H, ar, J = 9.2, 2.2 Hz), 8.32 (s, 1H, ar), 8.07 (d, 2H, ar, J = 8.2 Hz), 8.01 (d, 1H, ar, J = 8.2 Hz), 7.98 (d, 1H, ar, J = 7.9 Hz), 7.85 (t, 1H, ar, J = 8.2, 7.9 Hz), 7.50 (t, 1H, ar, J = 8.2, 7.9 Hz). NaCl: 0.8%. H_2O: 15.9%. TLC: R_f 0.48 (EM3). Anal. ($C_{24}H_{14}N_3Na_3O_{13}S_3$) C, H, N.

8-(4-Methyl-3-(3-nitrobenzamido)-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (6b).
Yield: 68.8%. ^{1}H NMR (DMSO-d_6): δ 12.63 (br s, 1H, NH, ex),10.52 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, J = 2.2 Hz), 8.84 (pt, 1H, ar, J = 1.9 Hz), 8.60 (d, 1H, ar, J = 1.9 Hz), 8.49 (d, 1H, ar, J = 7.3 Hz), 8.44 (ddd, 1H, ar, J = 8.2, 1.3, 0.9 Hz), 8.00-8.06 (m, 4H, ar), 7.85 (t, 1H, ar, J = 8.2 Hz), 7.40 (d, 1H, ar, J = 8.2 Hz), 2.32 (s, 3H, -CH_3). NaCl: 79.4%. H_2O: 12.9%. TLC: R_f 0.52 (EM3). Anal. ($C_{25}H_{16}N_3Na_3O_{13}S_3$) C, H, N.

8-(4-Ethyl-3-(3-nitrobenzamido)-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (6c).
Yield: 97.4%. ^{1}H NMR (DMSO-d_6): δ 12.55 (br s, 1H, NH, ex), 10.55 (br s, 1H, NH, ex), 9.34 (s, 1H, ar), 8.81 (s, 1H, ar), 8.59 (s, 1H, ar), 8.44 (d, 2H, ar, J = 8.2 Hz), 8.08 (d, 1H, ar, J = 8.2 Hz), 8.00 (d, 2H, ar, J = 8.2 Hz), 7.95 (s, 1H, ar), 7.83 (t, 1H, ar, J = 8.2 Hz), 7.47 (d, 1H, ar, J = 8.2 Hz), 2.68 (q, 2H, -CH_2-, J = 7.5 Hz), 1.20 (t, 3H, -CH_3, J = 7.5 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 3090, 2960, 1660, 1570, 1525, 1415, 1350, 1330, 1255, 1195, 1075, 1040, 840. NaCl: 0.7%. H_2O: 15.3%. TLC: R_f 0.52 (EM3). Anal. ($C_{26}H_{18}N_3Na_3O_{13}S_3$) C, H, N.

8-(4-Isopropyl-3-(3-nitrobenzamido)-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (6d).
Yield: 73.7%. ^{1}H NMR (DMSO-d_6): δ 12.65 (br s, 1H, NH, ex), 10.53 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, J = 1.9 Hz), 8.85 (d, 1H, ar, J = 1.6 Hz), 8.59 (d, 1H, ar, J = 1.9 Hz), 8.45 (m, 2H, ar), 8.15 (dd, 1H, ar, J = 8.2, 1.6 Hz), 8.05 (d, 1H, ar, J = 8.2 Hz), 8.00 (d, 1H, ar, J = 8.2 Hz), 7.93 (d, 1H, ar, J = 1.6 Hz), 7.86 (t, 1H, ar, J = 8.0 Hz), 7.52 (d, 1H, ar, J = 8.2 Hz), 3.20 (m, 1H, -CH=), 1.21 (d, 6H, (-CH_3)$_2$, J = 6.8 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2960, 1640, 1520, 1420, 1340, 1300, 1195, 1075, 1040, 845. NaCl: 11.3%. H_2O: 12.5%. TLC: R_f 0.53 (EM3). Anal. ($C_{27}H_{20}N_3Na_3O_{13}S_3$) C, H, N.

8-(3-(3-Nitrobenzamido)-4-phenyl-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (6e).
Yield: 94.5%. ^{1}H NMR (DMSO-d_6): δ 12.77 (br s, 1H, NH, ex), 10.53 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, *J* = 1.9 Hz), 8.64 (s, 1H, ar), 8.61 (d, 1H, ar, *J* = 1.9 Hz), 8.40 (dq, 1H, ar, *J* = 8.0, 2.0, 1.0 Hz), 8.29 (dd, 1H, ar, *J* = 8.0, 1.5 Hz), 8.24 (dd, 1H, ar, *J* = 8.0, 1.6 Hz), 8.15 (d, 1H, ar, *J* = 1.6 Hz), 8.09 (d, 1H, ar, *J* = 8.2 Hz), 8.03 (d, 1H, ar, *J* = 8.2 Hz), 7.80 (t, 1H, ar, *J* = 8.0 Hz), 7.30-7.59 (m, 6H, 1 ar and -C_6H_5). IR ν_{max} (KBr, cm^{-1}): 3450, 1670, 1615, 1535, 1525, 1505, 1380, 1350, 1330, 1305, 1225, 1195, 1175, 1040, 850. NaCl: 1.3%. H_2O: 14.6%. TLC: R_f 0.70 (EM4). Anal. ($C_{30}H_{18}N_3Na_3O_{13}S_3$) C, H, N.

8-(4-Fluoro-3-(3-nitrobenzamido)-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (6f).
Yield: 97.8%. ^{1}H NMR (DMSO-d_6): δ 12.68 (br s, 1H, NH, ex), 10.73 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, *J* = 1.9 Hz), 8.85 (pt, 1H, ar, *J* = 2.0 Hz), 8.61 (d, 1H, ar, *J* = 1.9 Hz), 8.45-8.47 (m, 2H, ar), 8.28 (dd, 1H, ar, *J* = 7.6, 2.2 Hz), 8.17-8.20 (m, 1H, ar), 8.07 (d, 1H, ar, *J* = 8.2 Hz), 8.01 (d, 1H, ar, *J* = 8.2 Hz), 7.86 (t, 1H, ar, *J* = 8.2 Hz), 7.44 (dd, 1H, ar, *J* = 10.1, 8.5 Hz). ^{13}C NMR (DMSO-d_6): δ 164.3 (C-O), 163.6 (C-O), 158.8 (ar, C-N), 156.8 (ar, C-F), 148.0 (ar, C-C), 142.9 (ar, C-N), 142.3 (ar, C-S), 141.4 (ar, C-S), 135.3 (ar, C-H), 134.5 (ar, C-S), 134.3 (ar, C-H), 132.3 (ar, C-N), 131.5 (ar, C-C), 130.5 (ar, C-C), 127.8 (ar, C-H), 127.5 (ar, C-H), 126.9 (ar, C-H), 126.6 (ar, C-H), 125.9 (ar, C-H), 125.0 (ar, C-H), 123.4 (ar, C-C), 123.0 (ar, C-H), 115.8 (ar, C-H), 115.6 (ar, C-H). IR ν_{max} (KBr, cm^{-1}): 3440, 3100, 1665, 1610, 1535, 1490, 1350, 1330, 1230, 1200, 1045, 900. NaCl: 24.4%. H_2O: 18.1%. TLC: R_f 0.41 (EM3). Anal. ($C_{24}H_{13}FN_3Na_3O_{13}S_3$) C, H, N.

Synthesis of the amino derivatives 4g-i and 7g-i.

8-(3-Amino-4-chlorobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (4g).
3g (9.5 g, 15 mmol) were dissolved in water (80 mL). Under heavy stirring, a solution of iron(II) chloride x 4 H_2O (20.9 g, 105 mmol) in water (100 mL) was slowly added, rt, 6h. During the reaction, the pH was kept constant at 7.5 by automatic addition of a 0.5 N NaOH solution. At the end of the reaction, the pH was increased to pH 9.0. Precipitated iron(III) hydroxide was separated by filtration. The filtrate was neutralised to pH 7.0 with 1 N HCl and evaporated to dryness. Crude product was stirred in methanol (100 mL) for purification. The filtrate was evaporated to dryness to get **4g**. Yield: 8.0 g (88.9%). ^{1}H NMR (DMSO-d_6): δ 12.51 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, *J* = 1.9 Hz), 8.60 (d, 1H, ar, *J* = 1.9 Hz), 8.06 (d, 1H, ar, *J* = 8.2 Hz), 7.95 (d, 1H, ar, *J* = 8.0 Hz), 7.46 (d, 1H, ar, *J* = 1.7 Hz), 7.35 (dd, 1H, ar, *J* = 8.3, 1.7 Hz), 7.28 (d, 1H, ar, *J* = 8.3 Hz), 4.94 (br s, 2H, NH, ex). IR ν_{max} (KBr, cm^{-1}): 3440, 2340, 1655, 1620, 1570, 1520, 1480, 1420, 1325, 1220, 1190, 830. NaCl: 7.5%. H_2O: 14.1%. TLC: R_f 0.44 (EM3). Anal. ($C_{17}H_{10}ClN_2Na_3O_{10}S_3$) C, H, N.

8-(3-(3-Aminobenzamido)-4-chloro-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7g).
7g was synthesized from **6g** according to **4g**. Purification was done by stirring with methanol (450 mL) and cation exchange chromatography. Yield: 76.3%. ^{1}H NMR (DMSO-d_6): δ 12.74 (br s, 1H, NH, ex), 10.08 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, *J* = 1.8 Hz), 8.61 (d, 1H, ar, *J* = 1.8 Hz), 8.22 (d, 1H, ar, *J* = 2.0 Hz), 8.13 (dd, 1H, ar, *J* = 8.5, 2.0 Hz), 8.08 (d, 1H, ar, *J* = 8.2 Hz), 8.01 (d, 1H, ar, *J* = 8.2 Hz), 7.68 (d, 1H, ar, *J* = 8.5 Hz), 7.22-7.32 (m, 3H, ar), 6.91 (d, 1H, ar, *J* = 7.2 Hz), 5.30 (br s, 2H, NH, ex). IR ν_{max} (KBr, cm^{-1}): 3430, 1640, 1580, 1535, 1505, 1490, 1465, 1410, 1335, 1310, 1230, 1070, 890. NaCl: 29.2%. H_2O: 14.9%. TLC: R_f 0.47 (EM3). Anal. ($C_{24}H_{15}ClN_3Na_3O_{11}S_3$) C, H, N.

8-(3-Amino-4-methoxybenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (4h).
4h was synthesized from **3h** according to Kassack et al. and Nickel et al., rt, overnight.[16;18]
Yield: 90.6%. ^{1}H NMR (DMSO-d_6): δ 12.45 (br s, 1H, NH, ex), 9.43 (d, 1H, ar, *J* = 2.5 Hz),

8.65 (d, 1H, ar, *J* = 2.5 Hz), 8.09 (d, 1H, ar, *J* = 7.5 Hz), 8.03 (d, 1H, ar, *J* = 7.5 Hz), 7.51 (dd, 1H, ar, *J* = 7.5, 2.5 Hz), 7.39 (d, 1H, ar, *J* = 2.5 Hz), 6.92 (d, 1H, ar, *J* = 7.5 Hz), 4.88 (br s, 2H, NH, ex), 3.88 (s, 3H, -CH_3). NaCl: 6.0%. H_2O: 9.5%. TLC: R_f 0.45 (EM3). Anal. ($C_{18}H_{13}N_2Na_3O_{11}S_3$) C, H, N.

8-(3-Amino-4-(methoxymethyl)-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (4i).

4i was synthesized from **3i** according to Kassack et al. and Nickel et al., rt, overnight.[16;18] Yield: 91.6%. ^{1}H NMR (DMSO-d_6): δ 12.47 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, *J* = 2.5 Hz), 8.61 (d, 1H, ar, *J* = 2.5 Hz), 8.06 (d, 1H, ar, *J* = 7.5 Hz), 7.98 (d, 1H, ar, *J* = 7.5 Hz), 7.37 (d, 1H, ar, *J* = 2.5 Hz), 7.34 (s, 1H, ar), 7.14 (d, 1H, ar, *J* = 7.5 Hz), 5.08 (br s, 2H, NH, ex), 4.39 (s, 2H, -CH_2-), 3.31 (s, 3H, -CH_3). NaCl: 0.9%. H_2O: 15.0%. TLC: R_f 0.48 (EM3). Anal. ($C_{19}H_{15}N_2Na_3O_{11}S_3$) C, H, N.

8-(3-(3-Aminobenzamido)-4-methoxy-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7h).

7h was synthesized from **6h** according to Kassack et al. and Nickel et al., rt, overnight.[16;18] Yield: 90.2%. ^{1}H NMR (DMSO-d_6): δ 12.58 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, *J* = 2.5 Hz), 9.21 (br s, 1H, NH, ex), 8.60 (d, 1H, ar, *J* = 2.5 Hz), 8.46 (d, 1H, ar, *J* = 2.5 Hz), 8.11 (dd, 2H, ar, *J* = 7.5, 2.5 Hz), 8.03 (d, 1H, ar, *J* = 2.5 Hz), 7.09-7.21 (m, 4H, ar), 6.77 (d, 1H, ar, *J* = 7.5 Hz), 5.35 (br s, 2H, NH, ex), 3.94 (s, 3H, -CH_3). NaCl: 0.9%. H_2O: 9.1%. TLC: R_f 0.46 (EM3). Anal. ($C_{25}H_{18}N_3Na_3O_{12}S_3$) C, H, N.

8-(3-(3-Aminobenzamido)-4-(methoxymethyl)-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7i).

7i was synthesized from **6i** according to Kassack et al. and Nickel et al., rt, overnight.[16;18] Yield: 86.4%. ^{1}H NMR (DMSO-d_6): δ 12.68 (br s, 1H, NH, ex), 9.92 (br s, 1H, NH, ex), 9.43 (d, 1H, ar, *J* = 2.5 Hz), 8.64 (d, 1H, ar, *J* = 2.5 Hz), 8.28 (s, 1H, ar), 8.11 (s, 1H, ar), 8.10 (d, 1H, ar, *J* = 7.5 Hz), 8.04 (d, 1H, ar, *J* = 7.5 Hz), 7.55 (d, 1H, ar, *J* = 7.5 Hz), 7.10-7.24 (m, 3H, ar), 6.80 (d, 1H, ar, *J* = 7.5 Hz), 5.38 (br s, 2H, NH, ex), 3.58 (s, 2H, -CH_2-), 3.34 (s, 3H, -CH_3). NaCl: 1.9%. H_2O: 12.9%. TLC: R_f 0.49 (EM3). Anal. ($C_{26}H_{20}N_3Na_3O_{12}S_3$) C, H, N.

Compounds **4a-f** and **7a-f** have been described by Nickel et al. but no analytical data have been given.[18] Analytical data of **4a** are given in Kassack et al.[16] Thus here, analytical data of **4b-f** and **7a-f** are presented.

8-(3-Amino-4-methyl-3-nitrobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (4b).

Yield: 95.6%. ^{1}H NMR (DMSO-d_6): δ 12.48 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, *J* = 1.9 Hz), 8.60 (d, 1H, ar, *J* = 1.9 Hz), 8.04 (d, 1H, ar, *J* = 8.2 Hz), 7.98 (d, 1H, ar, *J* = 8.2 Hz), 7.55 (d, 1H, ar, *J* = 7.6 Hz), 7.52 (s, 1H, ar), 7.13 (d, 1H, ar, *J* = 7.9 Hz), 4.91 (br s, 2H, NH, ex), 2.22 (s, 3H, -CH_3). NaCl: 24.6%. H_2O: 13.4%. TLC: R_f 0.37 (EM3). Anal. ($C_{18}H_{13}N_2Na_3O_{10}S_3$) C, H, N.

8-(3-Amino-4-ethylbenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (4c).

Yield: 82.3%. ^{1}H NMR (DMSO-d_6): δ 12.41 (br s, 1H, NH, ex), 9.36 (d, 1H, ar, *J* = 1.8 Hz), 8.59 (d, 1H, ar, *J* = 1.8 Hz), 8.03 (d, 1H, ar, *J* = 8.2 Hz), 7.96 (d, 1H, ar, *J* = 8.2 Hz), 7.32 (d, 1H, ar, *J* = 7.9 Hz), 7.28 (s, 1H, ar), 7.01 (d, 1H, ar, *J* = 7.9 Hz), 4.69 (br s, 2H, NH, ex), 2.50 (q, 2H, -CH_2-, *J* = 7.5 Hz), 1.15 (t, 3H, -CH_3, *J* = 7.5 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2960, 1635, 1570, 1535, 1420, 1330, 1195, 1065, 1040, 835. NaCl: 4.7%. H_2O: 16.4%. TLC: R_f 0.46 (EM3). Anal. ($C_{19}H_{15}N_2Na_3O_{10}S_3$) C, H, N.

8-(3-Amino-4-isopropylbenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (4d).

Yield: 90.6%. ^{1}H NMR (DMSO-d_6): δ 12.43 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, *J* = 2.0 Hz), 8.60 (d, 1H, ar, *J* = 2.0 Hz), 8.04 (d, 1H, ar, *J* = 8.2 Hz), 7.98 (d, 1H, ar, *J* = 8.2 Hz), 7.37 (dd, 1H, ar, *J* = 8.2, 1.6 Hz), 7.30 (d, 1H, ar, *J* = 1.6 Hz), 7.10 (d, 1H, ar, *J* = 8.2 Hz), 4.99 (br s,

2H, NH, ex), 2.98 (sep, 1H, -CH=, *J* = 6.8 Hz), 1.20 (d, 6H, $(-CH_3)_2$, *J* = 6.8 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2960, 1630, 1570, 1525, 1505, 1415, 1330, 1220, 1195, 1075, 1040, 840. NaCl: 5.2%. H_2O: 12.9%. TLC: R_f 0.48 (EM3). Anal. ($C_{20}H_{17}N_2Na_3O_{10}S_3$) C, H, N.

8-(3-Amino-4-phenylbenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (4e).
Yield: 93.2%. ^{1}H NMR (DMSO-d_6): δ 12.53 (br s, 1H, NH, ex), 9.39 (d, 1H, ar, *J* = 1.9 Hz), 8.61 (d, 1H, ar, *J* = 1.9 Hz), 8.07 (d, 1H, ar, *J* = 8.2 Hz), 7.99 (d, 1H, ar, *J* = 8.2 Hz), 7.33-7.54 (m, 7H, 2 ar and $-C_6H_5$), 7.08 (d, 1H, ar, *J* = 8.3 Hz), 4.91 (br s, 2H, NH, ex). IR ν_{max} (KBr, cm^{-1}): 3450, 1640, 1600, 1525, 1480, 1415, 1330, 1325, 1305, 1110, 1040. NaCl: 0.6%. H_2O: 15.4%. TLC: R_f 0.59 (EM4). Anal. ($C_{23}H_{15}N_2Na_3O_{10}S_3$) C, H, N.

8-(3-Amino-4-fluorobenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (4f).
Yield: 84.3%. ^{1}H NMR (DMSO-d_6): δ 12.45 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, *J* = 2.1 Hz), 8.60 (d, 1H, ar, *J* = 2.1 Hz), 8.04 (d, 1H, ar, *J* = 8.2 Hz), 7.96 (d, 1H, ar, *J* = 8.2 Hz), 7.46 (dd, 1H, ar, *J* = 9.0, 2.4 Hz), 7.36-7.39 (m, 1H, ar), 7.04 (dd, 1H, ar, *J* = 11.1, 8.7 Hz), 5.21 (br s, 2H, NH, ex). ^{13}C NMR (DMSO-d_6): δ 165.5 (C-O), 153.4 (C-F), 151.5 (ar, C-N), 142.7 (ar, C-N), 141.9 (ar, C-S), 141.5 (ar, C-S), 136.1 (ar, C-C), 134.7 (ar, C-S), 132.4 (ar, C-H), 131.4 (ar, C-C), 126.8 (ar, C-H), 125.8 (ar, C-H), 125.0 (ar, C-H), 123.4 (ar, C-C), 122.8 (ar, C-H), 116.9 (ar, C-H), 114.4 (ar, C-H). IR ν_{max} (KBr, cm^{-1}): 3440, 1620, 1540, 1510, 1425, 1370, 1235, 1200, 1165, 1125, 1045, 890. NaCl: 19.3%. H_2O: 10.9%. TLC: R_f 0.30 (EM3). Anal. ($C_{17}H_{10}FN_2Na_3O_{10}S_3$) C, H, N.

8-(3-(3-Aminobenzamido)benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7a).
Yield: 84.3%. ^{1}H NMR (DMSO-d_6): δ 12.63 (br s, 1H, NH, ex), 10.20 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, *J* = 1.9 Hz), 8.61 (d, 1H, ar, *J* = 1.6 Hz), 8.31 (pt, 1H, ar, *J* = 2.0 Hz), 8.07 (d, 1H, ar, *J* = 8.2 Hz), 8.01 (d, 1H, ar, *J* = 8.2 Hz), 8.00 (dd, 1H, ar, *J* = 8.2, 1.6 Hz), 7.92 (d, 1H, ar, *J* = 7.9 Hz), 7.43 (t, 1H, ar, *J* = 7.9 Hz), 7.11-7.16 (m, 3H, ar), 6.75 (dd, 1H, ar, *J* = 7.9, 1.6 Hz), 5.27 (br s, 2H, NH, ex). NaCl: 0.7%. H_2O: 10.6%. TLC: R_f 0.42 (EM3). Anal. ($C_{24}H_{16}N_3Na_3O_{11}S_3$) C, H, N.

8-(3-(3-Aminobenzamido)-4-methylbenzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7b).
Yield: 85.3%. ^{1}H NMR (DMSO-d_6): δ 12.44 (br s, 1H, NH, ex), 9.87 (br s, 1H, NH, ex), 9.32 (d, 1H, ar, *J* = 1.9 Hz), 8.58 (d, 1H, ar, *J* = 1.9 Hz), 8.07 (d, 1H, ar, *J* = 7.9 Hz), 7.99 (dd, 1H, ar, *J* = 8.2, 3.2 Hz), 7.94 (s, 1H, ar), 7.92 (s, 1H, ar), 7.38 (d, 1H, ar, *J* = 7.9 Hz), 7.13-7.17 (m, 3H, ar), 6.77-6.78 (m, 1H, ar), 5.32 (br s, 2H, NH, ex), 2.27 (s, 3H, $-CH_3$). NaCl: 2.8%. H_2O: 16.2%. TLC: R_f 0.41 (EM3). Anal. ($C_{25}H_{18}N_3Na_3O_{11}S_3$) C, H, N.

8-(4-Ethyl-3-(3-aminobenzamido)-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7c).
Yield: 94.2%. ^{1}H NMR (DMSO-d_6): δ 12.55 (br s, 1H, NH, ex), 9.86 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, *J* = 1.9 Hz), 8.61 (d, 1H, ar, *J* = 1.9 Hz), 7.99-8.08 (m, 3H, ar), 7.92 (s, 1H, ar), 7.41 (d, 1H, ar, *J* = 8.2 Hz), 7.14-7.17 (m, 3H, ar), 6.73-6.78 (m, 1H, ar), 5.30 (br s, 2H, NH, ex), 2.70 (q, 2H, $-CH_2-$, *J* = 7.5 Hz), 1.19 (t, 3H, $-CH_3$, *J* = 7.5 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2980, 1640, 1570, 1520, 1480, 1325, 1190, 1075, 1040, 835. NaCl: 0.6%. H_2O: 14.1%. TLC: R_f 0.47 (EM3). Anal. ($C_{26}H_{20}N_3Na_3O_{11}S_3$) C, H, N.

8-(3-(3-Aminobenzamido)-4-isopropyl-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7d).
Yield: 90.9%. ^{1}H NMR (DMSO-d_6): δ 12.63 (br s, 1H, NH, ex), 9.89 (br s, 1H, NH, ex), 9.38 (d, 1H, ar, *J* = 2.0 Hz), 8.60 (d, 1H, ar, *J* = 2.0 Hz), 8.12 (dd, 1H, ar, *J* = 8.3, 1.6 Hz), 8.06 (d, 1H, ar, *J* = 8.2 Hz), 8.00 (d, 1H, ar, *J* = 8.2 Hz), 7.85 (d, 1H, ar, *J* = 1.6 Hz), 7.46 (d, 1H, ar, *J* = 8.3 Hz), 7.15 (m, 3H, ar), 6.75 (m, 1H, ar), 5.31 (br s, 2H, NH, ex), 3.24 (m, 1H, -CH=), 1.20 (d, 6H, $(-CH_3)_2$, *J* = 6.8 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2960, 1650, 1615, 1570, 1530, 1350, 1300, 1230, 1200, 1075, 1040, 835. NaCl: 11.8%. H_2O: 15.6%. TLC: R_f 0.44 (EM3). Anal. ($C_{27}H_{22}N_3Na_3O_{11}S_3$) C, H, N.

8-(3-(3-Aminobenzamido)-4-phenyl-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7e).
Yield: 87.3%. ^{1}H NMR (DMSO-d_6): δ 12.75 (br s, 1H, NH, ex), 9.80 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, *J* = 1.9 Hz), 8.62 (d, 1H, ar, *J* = 1.9 Hz), 8.20 (dd, 1H, ar, *J* = 8.0, 1.6 Hz), 8.11 (d, 1H, ar, *J* = 1.6 Hz), 8.09 (d, 1H, ar, *J* = 8.2 Hz), 8.03 (d, 1H, ar, *J* = 8.2 Hz), 7.31-7.54 (m, 6H, 1 ar and -C_6H_5), 7.07 (t, 1H, ar, *J* = 8.0 Hz), 7.02 (s, 1H, ar), 6.91 (d, 1H, ar, *J* = 8.0 Hz), 6.69 (dd, 1H, ar, *J* = 8.0, 2.0 Hz), 5.27 (br s, 2H, NH, ex). IR ν_{max} (KBr, cm^{-1}): 3450, 1670, 1640, 1530, 1505, 1445, 1330, 1040. NaCl: 1.6%. H_2O: 9.6%. TLC: R_f 0.60 (EM4). Anal. ($C_{30}H_{20}N_3Na_3O_{11}S_3$) C, H, N.
8-(3-(3-Aminobenzamido)-4-fluoro-benzamido)-naphthalene-1,3,5-trisulfonic acid trisodium salt (7f).
Yield: 99.5%. ^{1}H NMR (DMSO-d_6): δ 12.66 (br s, 1H, NH, ex), 10.01 (br s, 1H, NH, ex), 9.40 (d, 1H, ar, *J* = 1.9 Hz), 8.61 (d, 1H, ar, *J* = 1.9 Hz), 8.22 (dd, 1H, ar, *J* = 7.6, 2.2 Hz), 8.12-8.15 (m, 1H, ar), 8.06 (d, 1H, ar, *J* = 8.2 Hz), 8.01 (d, 1H, ar, *J* = 8.2 Hz), 7.38 (dd, 1H, ar, *J* = 10.1, 8.8 Hz), 7.12-7.17 (m, 3H, ar), 6.77 (dt, 1H, ar, *J* = 6.9, 1.9 Hz), 5.29 (br s, 2H, NH, ex). ^{13}C NMR (DMSO-d_6): δ 166.3 (C-O), 164.5 (C-O), 158.7 (ar, C-N), 156.7 (ar, C-F), 149.0 (ar, C-C), 142.9 (ar, C-N), 142.3 (ar, C-S), 141.4 (ar, C-S), 134.9 (ar, C-H), 134.3 (ar, C-S), 132.1 (ar, C-N), 131.5 (ar, C-C), 129.0 (ar, C-C), 127.7 (ar, C-H), 126.9 (ar, C-H), 125.9 (ar, C-H), 125.0 (ar, C-H), 123.4 (ar, C-C), 122.9 (ar, C-H), 117.2 (ar, C-H), 115.5 (ar, C-H), 115.4 (ar, C-H), 115.1 (ar, C-H), 113.4 (ar, C-H). IR ν_{max} (KBr, cm^{-1}): 3400, 3330, 1660, 1590, 1525, 1470, 1400, 1310, 1210, 1185, 1040. NaCl: 2.7%. H_2O: 6.0%. TLC: R_f 0.34 (EM3). Anal. ($C_{24}H_{15}FN_3Na_3O_{11}S_3$) C, H, N.

Synthesis of the urea derivatives 5g-i and 8g-i.
8,8'-(Carbonylbis(imino-3,1-(4-chlorophenylene)carbonylimino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (5g).
5g was synthesized from **4g** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 80.7%. ^{1}H NMR (DMSO-d_6): δ 12.65 (br s, 2H, NH, ex), 9.39 (s, 2H, ar), 9.22 (br s, 2H, NH, ex), 8.67 (s, 2H, ar), 8.62 (s, 2H, ar), 7.96-8.08 (m, 6H, ar), 7.61 (d, 2H, ar, *J* = 5.3 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2340, 1640, 1565, 1525, 1460, 1410, 1330, 1290, 1240, 1190, 1040, 830. NaCl: 4.9%. H_2O: 17.0%. TLC: R_f 0.22 (EM3). Anal. ($C_{35}H_{18}Cl_2N_4Na_6O_{21}S_6$) C, H, N.
8,8'-(Carbonylbis(imino-3,1-(4-methoxyphenylene)carbonylimino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (5h).
5h was synthesized from **4h** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 56.9%. ^{1}H NMR (DMSO-d_6): δ 12.29 (br s, 2H, NH, ex), 9.33 (d, 2H, ar, *J* = 2.5 Hz), 8.96 (br s, 2H, NH, ex), 8.68 (d, 2H, ar, *J* = 2.5 Hz), 8.57 (d, 2H, ar, *J* = 2.5 Hz), 8.01 (s, 4H, ar), 7.92 (d, 2H, ar, *J* = 7.5 Hz), 7.08 (d, 2H, ar, *J* = 7.5 Hz), 3.97 (s, 6H, 2 -CH_3). NaCl: 1.5%. H_2O: 17.1%. TLC: R_f 0.20 (EM3). Anal. ($C_{37}H_{24}N_4Na_6O_{23}S_6$) C, H, N.
8,8'-(Carbonylbis(imino-3,1-(4-(methoxymethyl)phenylene)carbonylimino))bis (naphthalene-1,3,5-trisulfonic acid) hexasodium salt (5i).
5i was synthesized from **4i** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 75.6%. ^{1}H NMR (DMSO-d_6): δ 12.62 (br s, 2H, NH, ex), 9.42 (d, 2H, ar, *J* = 2.5 Hz), 8.66 (br s, 2H, NH, ex), 8.63 (d, 2H, ar, *J* = 2.5 Hz), 8.32 (s, 2H, ar), 8.10 (d, 2H, ar, *J* = 7.5 Hz), 8.06 (s, 2H, ar), 8.02 (d, 2H, ar, *J* = 7.5 Hz), 7.49 (d, 2H, ar, *J* = 7.5 Hz), 4.58 (s, 4H, 2 -CH_2-), 3.30 (s, 6H, 2 -CH_3). NaCl: 12.1%. H_2O: 16.3%. TLC: R_f 0.17 (EM3). Anal. ($C_{39}H_{28}N_4Na_6O_{23}S_6$) C, H, N.
8,8'-(Carbonylbis(imino-3,1-phenylenecarbonylimino-3,1-(4-chlorophenylene)carbonyl-imino))-bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (8g).
8g was synthesized from **7g** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 76.4%. ^{1}H NMR (DMSO-d_6): δ 12.73 (br s, 2H, NH, ex), 10.29 (br s, 2H, NH, ex), 9.84 (br s, 2H, NH, ex), 9.41 (s, 2H, ar), 8.64 (s, 2H, ar), 8.01-8.21 (m, 8H, ar), 7.40-7.83 (m, 10H, ar).

ES-MS: calcd/found (m/z): 1334.9/1335.2 $[M-H]^-$, 1356.9/1357.2 $[M+Na-2H]^-$, 667.0/667.4 $[M-2H]^{2-}$. IR ν_{max} (KBr, cm^{-1}): 3460, 1650, 1585, 1525, 1485, 1460, 1415, 1340, 1305, 1220, 1075, 890. NaCl: 1.6%. H_2O: 11.9%. TLC: R_f 0.27 (EM3). Anal. ($C_{49}H_{28}Cl_2N_6Na_6O_{23}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-phenylenecarbonylimino-3,1-(4-methoxyphenylene) carbonylimino))-bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (8h).

8h was synthesized from **7h** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 89.2%. ^1H NMR (DMSO-d_6): δ 12.61 (br s, 2H, NH, ex), 9.56 (br s, 2H, NH, ex), 9.38 (d, 2H, ar, *J* = 2.5 Hz), 9.24 (br s, 2H, NH, ex), 8.62 (d, 2H, ar, *J* = 2.5 Hz), 8.39 (s, 2H, ar), 8.15 (d, 2H, ar, *J* = 7.5 Hz), 8.07 (d, 2H, ar, *J* = 7.5 Hz), 8.03 (d, 2H, ar, *J* = 7.5 Hz), 7.94 (s, 2H, ar), 7.85 (d, 2H, ar, *J* = 7.5 Hz), 7.63 (d, 2H, ar, *J* = 7.5 Hz), 7.46 (t, 2H, ar, *J* = 7.5 Hz), 7.22 (d, 2H, ar, *J* = 7.5 Hz), 3.97 (s, 6H, 2 -CH_3). ES-MS: calcd/found (m/z): 1327.0/1327.3 $[M-H]^-$, 1349.0/1349.3 $[M+Na-2H]^-$, 663.0/663.3 $[M-2H]^{2-}$. NaCl: 19.3%. H_2O: 15.2%. TLC: R_f 0.22 (EM3). Anal. ($C_{51}H_{34}N_6Na_6O_{25}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-phenylenecarbonylimino-3,1-(4-(methoxymethyl)phenylene) carbonylimino))-bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (8i).

8i was synthesized from **7i** according to Kassack et al. and Nickel et al., rt, 6h.[16;18] Yield: 88.8%. ^1H NMR (DMSO-d_6): δ 12.69 (br s, 2H, NH, ex), 10.16 (br s, 2H, NH, ex), 9.42 (br s, 2H, NH, ex), 9.35 (d, 2H, ar, *J* = 2.5 Hz), 8.64 (d, 2H, ar, *J* = 2.5 Hz), 8.26 (d, 2H, ar, *J* = 2.5 Hz), 8.02-8.16 (m, 8H, ar), 7.87 (d, 2H, ar, *J* = 7.5 Hz), 7.48-7.66 (m, 6H, ar), 4.59 (s, 4H, 2 -CH_2-), 3.35 (s, 6H, 2 -CH_3). ES-MS: calcd/found (m/z): 1355.1/1355.3 $[M-H]^-$, 1377.0/1377.2 $[M+Na-2H]^-$, 677.0/677.3 $[M-2H]^{2-}$. NaCl: 2.6%. H_2O: 15.8%. TLC: R_f 0.25 (EM3). Anal. ($C_{53}H_{38}N_6Na_6O_{25}S_6$) C, H, N.

Compounds **5a-f** and **8a-f** have been described by Nickel et al. but no analytical data have been given.[18] Analytical data of **5a** are given in Kassack et al.[16] Thus here, analytical data of **5b-f** and **8a-f** (except **8b** = suramin) are presented.

8,8'-(Carbonylbis(imino-3,1-(4-methylphenylene)carbonylimino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (5b).

Yield: 86.5%. ^1H NMR (DMSO-d_6): δ 12.51 (br s, 2H, NH, ex), 9.38 (d, 2H, ar, *J* = 1.9 Hz), 8.89 (br s, 2H, NH, ex), 8.61 (d, 2H, ar, *J* = 1.9 Hz), 8.35 (d, 2H, ar, *J* = 1.9 Hz), 8.05 (d, 2H, ar, *J* = 8.2 Hz), 8.03 (d, 2H, ar, *J* = 8.2 Hz), 7.86 (dd, 2H, ar, *J* = 8.2, 1.9 Hz), 7.26 (d, 2H, ar, *J* = 8.2 Hz), 2.39 (s, 6H, 2 -CH_3). NaCl: 34.1%. H_2O: 14.8%. TLC: R_f 0.13 (EM3). Anal. ($C_{37}H_{24}N_4Na_6O_{21}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-(4-ethylphenylene)carbonylimino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (5c).

Yield: 93.3%. ^1H NMR (DMSO-d_6): δ 12.55 (br s, 2H, NH, ex), 9.38 (d, 2H, ar, *J* = 1.9 Hz), 8.61 (d, 2H, ar, *J* = 1.9 Hz), 8.58 (br s, 2H, NH, ex), 8.30 (s, 2H, ar), 8.01-8.05 (m, 4H, ar),7.94 (d, 2H, ar, *J* = 8.2 Hz), 7.31 (d, 2H, ar, *J* = 8.2 Hz), 2.76 (q, 4H, 2 -CH_2-, *J* = 7.5 Hz), 1.27 (t, 6H, 2 -CH_3, *J* = 7.5 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2960, 1640, 1530, 1420, 1335, 1195, 1040, 840. NaCl: 10.5%. H_2O: 17.7%. TLC: R_f 0.17 (EM3). Anal. ($C_{39}H_{28}N_4Na_6O_{21}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-(4-isopropylphenylene)carbonylimino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (5d).

Yield: 87.6%. ^1H NMR (DMSO-d_6): δ 12.42 (br s, 2H, NH, ex), 9.38 (d, 2H, ar, *J* = 1.9 Hz), 8.60 (d, 2H, ar, *J* = 1.9 Hz), 8.58 (br s, 2H, NH, ex), 8.19 (s, 2H, ar), 7.98-8.07 (m, 6H, ar), 7.39 (d, 2H, ar, *J* = 8.2 Hz), 3.24 (sep, 2H, 2 -CH=, *J* = 6.7 Hz), 1.26 (d, 12H, 2 $(-CH_3)_2$, *J* = 6.7 Hz). IR ν_{max} (KBr, cm^{-1}): 3440, 2960, 1640, 1570, 1540, 1410, 1340, 1230, 1195, 1075, 1045, 840. NaCl: 8.5%. H_2O: 16.8%. TLC: R_f 0.15 (EM3). Anal. ($C_{41}H_{32}N_4Na_6O_{21}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-(4-phenylphenylene)carbonylimino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (5e).
Yield: 96.6%. ^{1}H NMR (DMSO-d_6): δ 12.66 (br s, 2H, NH, ex), 9.41 (d, 2H, ar, J = 1.9 Hz), 8.61 (d, 2H, ar, J = 1.9 Hz), 8.32 (d, 2H, ar, J = 1.6 Hz), 8.14 (br s, 2H, NH, ex), 8.08 (d, 2H, ar, J = 8.2 Hz), 8.02-8.04 (m, 4H, ar), 7.37-7.58 (m, 10H, 2 -C_6H_5), 7.34 (d, 2H, ar, J = 8.0 Hz). IR ν_{max} (KBr, cm^{-1}): 3450, 1660, 1600, 1535, 1325, 1315, 1295, 1040, 1020. NaCl: 0.7%. H_2O: 18.0%. TLC: R_f 0.30 (EM3). Anal. ($C_{47}H_{28}N_4Na_6O_{21}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-(4-fluorophenylene)carbonylimino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (5f).
Yield: 79.3%. ^{1}H NMR (DMSO-d_6): δ 12.58 (br s, 2H, NH, ex), 9.39 (d, 2H, ar, J = 1.9 Hz), 9.19 (br s, 2H, NH, ex), 8.74 (dd, 2H, ar, J = 8.2, 2.2 Hz), 8.61 (d, 2H, ar, J = 1.9 Hz), 8.06 (d, 2H, ar, J = 8.2 Hz), 8.03 (d, 2H, ar, J = 8.2 Hz), 7.98-8.01 (m, 2H, ar), 7.36 (d, 1H, ar, J = 8.5 Hz), 7.34 (d, 1H, ar, J = 8.5 Hz). ^{13}C NMR (DMSO-d_6): δ 164.9 (2 C-O), 155.1 (ar, 2 C-F), 153.2 (C-O), 152.1 (ar, 2 C-C), 142.8 (ar, 2 C-N), 142.1 (ar, 2 C-S), 141.4 (ar, 2 C-S), 134.5 (ar, 2 C-S), 132.5 (ar, 2 C-N), 131.4 (ar, 2 C-C), 127.1 (ar, 2 C-H), 126.9 (ar, 2 C-H), 125.9 (ar, 2 C-H), 125.0 (ar, 2 C-H), 123.3 (ar, 2 C-C), 122.9 (ar, 2 C-H), 122.0 (ar, 2 C-H), 114.7 (ar, 2 C-H). IR ν_{max} (KBr, cm^{-1}): 3440, 1610, 1520, 1475, 1420, 1330, 1200, 1065, 1045, 900. NaCl: 10.9%. H_2O: 17.4%. TLC: R_f 0.24 (EM3). Anal. ($C_{35}H_{18}F_2N_4Na_6O_{21}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-phenylenecarbonylimino-3,1-phenylenecarbonyl-imino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (8a).
Yield: 85.1%. ^{1}H NMR (DMSO-d_6): δ 12.63 (br s, 2H, NH, ex), 10.43 (br s, 2H, NH, ex), 9.60 (br s, 2H, NH, ex), 9.40 (d, 2H, ar, J = 1.9 Hz), 8.61 (d, 2H, ar, J = 1.9 Hz), 8.33 (s, 2H, ar), 8.08 (d, 2H, ar, J = 8.2 Hz), 8.04 (dd, 2H, ar, J = 8.2, 1.9 Hz), 8.02 (d, 2H, ar, J = 8.2 Hz), 7.98 (s, 2H, ar), 7.96 (d, 2H, ar, J = 7.9 Hz), 7.79 (dd, 2H, ar, J = 7.6, 1.9 Hz), 7.61 (d, 2H, ar, J = 7.6 Hz), 7.45 (dt, 4H, ar, J = 7.9, 4.4 Hz). ES-MS: calcd/found (m/z): 1267.0/1267.2 [M-H]$^-$, 1289.0/1289.4 [M+Na-2H]$^-$, 316.0/316.0 [M-4H]$^{4-}$. NaCl: 10.4%. H_2O: 15.3%. TLC: R_f 0.19 (EM3). Anal. ($C_{49}H_{30}N_6Na_6O_{23}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-phenylenecarbonylimino-3,1-(4-ethylphenylene)-carbonyl-imino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (8c).
Yield: 86.4%. ^{1}H NMR (DMSO-d_6): δ 12.55 (br s, 2H, NH, ex), 10.10 (br s, 2H, NH, ex), 9.39 (d, 2H, ar, J = 1.9 Hz), 8.61 (br s, 2H, NH, ex), 8.10 (d, 2H, ar, J = 1.9 Hz), 7.95-8.08 (m, 8H, ar), 7.94 (s, 2H, ar), 7.86 (d, 2H, ar, J = 8.2 Hz), 7.64 (d, 2H, ar, J = 8.2 Hz), 7.42-7.49 (m, 4H, ar), 2.71 (q, 4H, 2 -CH_2-, J = 7.5 Hz), 1.21 (t, 6H, 2 -CH_3, J = 7.5 Hz). ES-MS: calcd/found (m/z): 1323.1/1323.3 [M-H]$^-$, 1389.0/1389.3 [M+3Na-4H]$^-$, 661.0/661.3 [M-2H]$^{2-}$. IR ν_{max} (KBr, cm^{-1}): 3440, 1640, 1590, 1525, 1470, 1420, 1325, 1230, 1190, 1070, 1040, 835. NaCl: 14.5%. H_2O: 19.4%. TLC: R_f 0.35 (EM3). Anal. ($C_{53}H_{38}N_6Na_6O_{23}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-phenylenecarbonylimino-3,1-(4-isopropylphenylene) carbonylimino))-bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (8d).
Yield: 68.8%. ^{1}H NMR (DMSO-d_6): δ 12.64 (br s, 2H, NH, ex), 10.11 (br s, 2H, NH, ex), 9.44 (br s, 2H, NH, ex), 9.38 (d, 2H, ar, J = 1.9 Hz), 8.60 (d, 2H, ar, J = 1.9 Hz), 8.16 (d, 2H, ar, J = 8.0 Hz), 8.07 (d, 2H, ar, J = 8.2 Hz), 8.01 (d, 2H, ar, J = 8.2 Hz), 7.97 (s, 2H, ar), 7.88 (s, 2H, ar), 7.82 (d, 2H, ar, J = 8.3 Hz), 7.64 (d, 2H, ar, J = 8.3 Hz), 7.49 (d, 2H, ar, J = 8.0 Hz), 7.43 (d, 2H, ar, J = 8.3 Hz), 3.20 (m, 2H, 2 -CH=), 1.21 (d, 12H, 2 (-CH_3)$_2$, J = 6.8 Hz). ES-MS: calcd/found (m/z): 1351.1/1351.3 [M-H]$^-$, 1395.1/1395.3 [M+2Na-3H]$^-$, 675.1/675.3 [M-2H]$^{2-}$. IR ν_{max} (KBr, cm^{-1}): 3440, 2960, 1640, 1590, 1535, 1480, 1430, 1330, 1300, 1195, 1075, 1040, 840. NaCl: 10.7%. H_2O: 15.8%. TLC: R_f 0.22 (EM3). Anal. ($C_{55}H_{42}N_6Na_6O_{23}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-phenylenecarbonylimino-3,1-(4-phenylphenylene)carbonyl-imino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (8e).

Yield: 62.8%. ^{1}H NMR (DMSO-d_6): δ 12.76 (br s, 2H, NH, ex), 10.06 (br s, 2H, NH, ex), 9.41 (d, 2H, ar, J = 1.9 Hz), 8.99 (br s, 2H, NH, ex), 8.62 (d, 2H, ar, J = 1.9 Hz), 8.24 (dd, 2H, ar, J = 8.0, 1.6 Hz), 8.12 (d, 2H, ar, J = 1.6 Hz), 8.09 (d, 2H, ar, J = 8.2 Hz), 8.03 (d, 2H, ar, J = 8.2 Hz), 7.73-7.81 (m, 4H, ar), 7.31-7.56 (m, 16H, 6 ar and 2 -C_6H_5). ES-MS: calcd/found (m/z): 1419.1/1419.2 $[M-H]^-$, 1441.1/1441.2 $[M+Na-2H]^-$, 709.0/709.5 $[M-2H]^{2-}$. IR ν_{max} (KBr, cm^{-1}): 3450, 1660, 1525, 1505, 1470, 1225, 1150, 1040, 1020, 1005. NaCl: 2.5%. H_2O: 16.5%. TLC: R_f 0.18 (EM4). Anal. ($C_{61}H_{38}N_6Na_6O_{23}S_6$) C, H, N.

8,8'-(Carbonylbis(imino-3,1-phenylenecarbonylimino-3,1-(4-fluorophenylene)carbonyl-imino))bis(naphthalene-1,3,5-trisulfonic acid) hexasodium salt (8f).

Yield: 86.3%. ^{1}H NMR (DMSO-d_6): δ 12.67 (br s, 2H, NH, ex), 10.27 (br s, 2H, NH, ex), 9.40 (s, 2H, ar), 9.24 (br s, 2H, NH, ex), 8.62 (s, 2H, ar), 8.24 (dd, 2H, ar, J = 7.9, 2.1 Hz), 8.16-8.19 (m, 2H, ar), 8.07 (d, 2H, ar, J = 8.2 Hz), 8.02 (d, 2H, ar, J = 8.2 Hz), 7.98 (s, 2H, ar), 7.82 (d, 2H, ar, J = 8.2 Hz), 7.63 (d, 2H, ar, J = 7.9 Hz), 7.43 (dt, 4H, ar, J = 9.5, 7.9 Hz). ^{13}C NMR (DMSO-d_6): δ 165.6 (2 C-O), 164.4 (2 C-O), 158.8 (C-O), 156.8 (ar, 2 C-F), 152.8 (ar, 2 C-N), 142.9 (ar, 2 C-N), 142.3 (ar, 2 C-S), 141.4 (ar, 2 C-S), 140.1 (ar, 2 C-C), 134.8 (ar, 2 C-C), 134.3 (ar, 2 C-S), 132.1 (ar, 2 C-N), 131.4 (ar, 2 C-C), 129.1 (ar, 2 C-H), 127.7 (ar, 2 C-H), 127.0 (ar, 2 C-H), 125.9 (ar, 2 C-H), 125.0 (ar, 2 C-H), 123.4 (ar, 2 C-C), 123.0 (ar, 2 C-H), 121.7 (ar, 2 C-H), 121.3 (ar, 2 C-H), 118.0 (ar, 2 C-H), 115.6 (ar, 2 C-H), 115.5 (ar, 2 C-H). ES-MS: calcd/found (m/z): 1303.0/1303.4 $[M-H]^-$, 1325.0/1325.3 $[M+Na-2H]^-$, 673.0/673.2 $[M+2Na -4H]^{2-}$. IR ν_{max} (KBr, cm^{-1}): 3440, 2940, 1640, 1610, 1540, 1470, 1425, 1325, 1225, 1195, 1075, 1040, 840. NaCl: 7.6%. H_2O: 15.4%. TLC: R_f 0.34 (EM3). Anal. ($C_{49}H_{28}F_2N_6Na_6O_{23}S_6$) C, H, N.

Elemental analysis data (CHN).

		C		H		N	
compd	formula	calcd[a)]	found	calcd[a)]	found	calcd[a)]	found
3a	$C_{17}H_9N_2Na_3O_{12}S_3$	30.6	30.5	2.4	2.4	4.2	4.3
3b	$C_{18}H_{11}N_2Na_3O_{12}S_3$	24.6	24.5	2.6	2.7	3.2	3.4
3c	$C_{19}H_{13}N_2Na_3O_{12}S_3$	28.2	28.1	3.1	2.9	3.5	3.4
3d	$C_{20}H_{15}N_2Na_3O_{12}S_3$	31.2	31.3	3.3	3.1	3.6	3.8
3e	$C_{23}H_{13}N_2Na_3O_{12}S_3$	34.2	34.2	3.2	3.1	3.5	3.6
3f	$C_{17}H_8FN_2Na_3O_{12}S_3$	21.0	20.8	2.4	2.0	2.9	2.9
3g	$C_{17}H_8ClN_2Na_3O_{12}S_3$	27.5	27.4	2.6	2.5	3.8	3.8
3h	$C_{18}H_{11}N_2Na_3O_{13}S_3$	30.1	29.9	2.7	2.3	3.9	3.9
3i	$C_{19}H_{13}N_2Na_3O_{13}S_3$	32.5	32.6	2.7	2.7	4.0	4.0
4a	$C_{17}H_{11}N_2Na_3O_{10}S_3$	32.4	32.4	2.7	2.8	4.4	4.6
4b	$C_{18}H_{13}N_2Na_3O_{10}S_3$	24.2	24.2	2.6	2.8	3.1	3.1
4c	$C_{19}H_{15}N_2Na_3O_{10}S_3$	30.5	30.5	3.8	3.6	3.7	3.7
4d	$C_{20}H_{17}N_2Na_3O_{10}S_3$	32.5	32.3	3.7	3.6	3.8	3.6
4e	$C_{23}H_{15}N_2Na_3O_{10}S_3$	36.1	35.8	3.7	3.6	3.7	3.6
4f	$C_{17}H_{10}FN_2Na_3O_{10}S_3$	25.0	25.1	2.2	2.4	3.4	3.5
4g	$C_{17}H_{10}ClN_2Na_3O_{10}S_3$	26.9	27.1	2.8	2.7	3.7	3.8
4h	$C_{18}H_{13}N_2Na_3O_{11}S_3$	30.7	30.7	2.9	2.8	4.0	3.9
4i	$C_{19}H_{15}N_2Na_3O_{11}S_3$	31.4	31.4	3.7	3.7	3.9	3.8
5a	$C_{35}H_{20}N_4Na_6O_{21}S_6$	30.4	30.3	3.1	3.0	4.0	4.2
5b	$C_{37}H_{24}N_4Na_6O_{21}S_6$	21.0	21.0	2.2	2.2	2.6	2.8
5c	$C_{39}H_{28}N_4Na_6O_{21}S_6$	28.3	28.3	3.5	3.2	3.4	3.3
5d	$C_{41}H_{32}N_4Na_6O_{21}S_6$	30.1	30.0	3.7	3.6	3.4	3.5
5e	$C_{47}H_{28}N_4Na_6O_{21}S_6$	35.0	34.6	3.7	3.6	3.5	3.6
5f	$C_{35}H_{18}F_2N_4Na_6O_{21}S_6$	25.8	25.6	2.8	2.5	3.4	3.5
5g	$C_{35}H_{18}Cl_2N_4Na_6O_{21}S_6$	26.9	26.9	3.0	2.8	3.6	3.6
5h	$C_{37}H_{24}N_4Na_6O_{23}S_6$	30.0	30.0	3.5	3.8	3.7	3.4
5i	$C_{39}H_{28}N_4Na_6O_{23}S_6$	27.5	27.5	3.3	3.1	3.3	3.3
6a	$C_{24}H_{14}N_3Na_3O_{13}S_3$	33.5	33.7	3.4	3.4	4.9	5.1
6b	$C_{25}H_{16}N_3Na_3O_{13}S_3$	7.4	7.4	0.7	0.9	1.0	1.1
6c	$C_{26}H_{18}N_3Na_3O_{13}S_3$	35.2	35.0	3.8	3.4	4.7	4.8
6d	$C_{27}H_{20}N_3Na_3O_{13}S_3$	33.2	33.1	3.3	3.2	4.3	4.4
6e	$C_{30}H_{18}N_3Na_3O_{13}S_3$	38.3	38.1	3.5	3.3	4.5	4.5
6f	$C_{24}H_{13}FN_3Na_3O_{13}S_3$	24.3	24.3	2.6	2.4	3.5	3.7
6g	$C_{24}H_{13}ClN_3Na_3O_{13}S_3$	29.4	29.3	3.0	3.0	4.3	4.3
6h	$C_{25}H_{16}N_3Na_3O_{14}S_3$	32.8	32.9	3.7	3.8	4.6	4.8

6i	$C_{26}H_{18}N_3Na_3O_{14}S_3$	33.9	33.8	3.7	3.6	4.6	4.6
7a	$C_{24}H_{16}N_3Na_3O_{11}S_3$	37.2	37.3	3.3	3.1	5.4	5.6
7b	$C_{25}H_{18}N_3Na_3O_{11}S_3$	34.9	34.7	3.9	3.6	4.9	4.9
7c	$C_{26}H_{20}N_3Na_3O_{11}S_3$	37.3	37.1	4.0	3.9	5.0	5.0
7d	$C_{27}H_{22}N_3Na_3O_{11}S_3$	33.1	33.1	3.8	3.5	4.3	4.4
7e	$C_{30}H_{20}N_3Na_3O_{11}S_3$	42.0	42.0	3.4	3.3	4.9	4.9
7f	$C_{24}H_{15}FN_3Na_3O_{11}S_3$	37.4	37.5	2.6	2.5	5.4	5.5
7g	$C_{24}H_{15}ClN_3Na_3O_{11}S_3$	24.1	24.1	2.4	2.4	3.5	3.6
7h	$C_{25}H_{18}N_3Na_3O_{12}S_3$	37.7	37.7	3.3	3.1	5.3	5.3
7i	$C_{26}H_{20}N_3Na_3O_{12}S_3$	36.5	36.5	3.8	3.7	4.9	4.9
8a	$C_{49}H_{30}N_6Na_6O_{23}S_6$	31.9	31.9	3.2	3.0	4.6	4.7
8c	$C_{53}H_{38}N_6Na_6O_{23}S_6$	30.1	30.1	3.7	3.7	4.0	4.2
8d	$C_{55}H_{42}N_6Na_6O_{23}S_6$	33.4	33.4	3.7	3.5	4.3	4.4
8e	$C_{61}H_{38}N_6Na_6O_{23}S_6$	38.4	38.3	3.8	3.5	4.4	4.5
8f	$C_{49}H_{28}F_2N_6Na_6O_{23}S_6$	32.0	32.1	3.1	3.5	4.6	4.6
8g	$C_{49}H_{28}Cl_2N_6Na_6O_{23}S_6$	34.7	34.7	3.0	3.2	5.0	5.3
8h	$C_{51}H_{34}N_6Na_6O_{25}S_6$	28.7	28.8	3.0	3.0	3.9	4.0
8i	$C_{53}H_{38}N_6Na_6O_{25}S_6$	35.1	35.1	3.8	3.5	4.6	4.8

[a] calculated CHN data include NaCl- and H_2O-content of the respective compound.