Electronic Supplementary Information

Thiophosphorylated bis-thioureas for competitive bulk liquid membrane transport of some metal ions

Maria G. Babashkina,*[a] Damir A. Safin,[a] Koen Robeyns,[a] Anna Brzuszkiewicz,[b] Henryk Kozlowski[b] and Yann Garcia[a]

[a] *Institute of Condensed Matter and Nanosciences, MOST - Inorganic Chemistry, Université Catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium. Fax: +32(0) 1047 2330; Tel: +32(0) 1047 2831; E-mail: maria.babashkina@ksu.ru*

[b] *Faculty of Chemistry, University of Wroclaw, F. Joliot-Curie Str. 14, 50383, Wroclaw, Poland.*

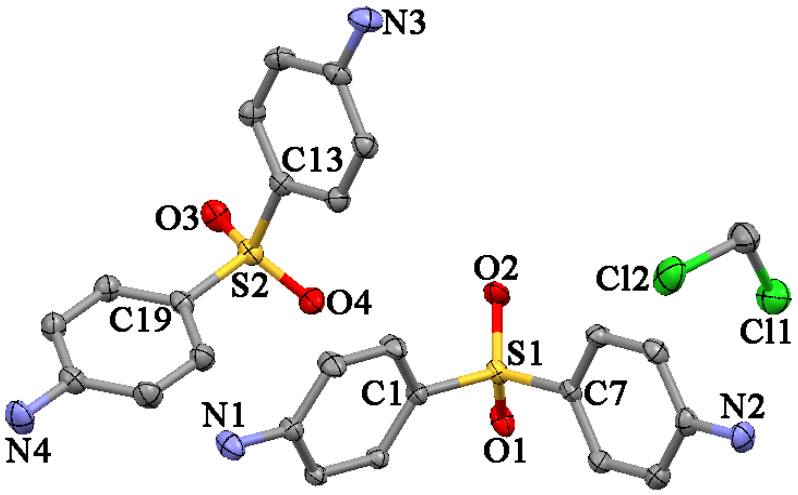

Fig. S1 Molecular structure of **2(4-aminophenylsulfone)·CH_2Cl_2**. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms were omitted for clarity.

Table S1 Selected bond lengths (Å) and bond angles (°) for **2(4-aminophenylsulfone)·CH_2Cl_2**

Bond lengths					
S(1)–O(1)	1.458(2)	S(1)–C(1)	1.748(2)	N(1)–C(4)	1.353(3)
S(1)–O(2)	1.442(2)	S(1)–C(7)	1.748(2)	N(2)–C(10)	1.372(3)
S(2)–O(3)	1.458(2)	S(2)–C(13)	1.748(2)	N(3)–C(16)	1.375(3)
S(2)–O(4)	1.444(2)	S(2)–C(19)	1.752(2)	N(4)–C(22)	1.360(3)
Bond angles					
O(1)–S(1)–O(2)	117.42(9)	O(2)–S(1)–C(7)	108.13(9)	O(3)–S(2)–C(19)	107.39(9)
O(1)–S(1)–C(1)	108.14(9)	C(1)–S(1)–C(7)	106.56(9)	O(4)–S(2)–C(13)	107.71(9)
O(1)–S(1)–C(7)	108.21(9)	O(3)–S(2)–O(4)	117.98(9)	O(4)–S(2)–C(19)	107.46(9)
O(2)–S(1)–C(1)	107.89(9)	O(3)–S(2)–C(13)	107.16(9)	C(13)–S(2)–C(19)	108.89(9)

Table S2 Selected hydrogen bond lengths (Å) and angles (°) for **2(4-aminophenylsulfone)·CH_2Cl_2**

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
N(1)–H(1B)···O(3)#1	0.86	2.13	2.962(3)	164
N(1)–H(1C)···O(2)#2	0.86	2.21	3.005(3)	155
N(2)–H(2B)···O(1)#3	0.86	2.28	3.086(3)	156
N(3)–H(3B)···O(3)#3	0.86	2.24	3.053(3)	157
N(3)–H(3C)···O(1)#4	0.86	2.54	3.216(3)	136
N(4)–H(4B)···O(1)#1	0.86	2.60	3.333(3)	144
N(4)–H(4C)···O(4)#1	0.86	2.16	3.014(3)	171

Symmetry transformations used to generate equivalent atoms: #1 $-x$, $1/2+y$, $3/2-z$; #2 $1-x$, $1/2+y$, $3/2-z$; #3 $1+x$, y, z; #4 x, $3/2-y$, $-1/2+z$