Electronic Supplementary Information

# Coordinative flexibility in an acyclic bis(sulfonamide) ligand

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## S1. Discussion of the structure of hpsmsH

The molecular and intermolecular geometry requires the molecule to be a zwitterion: $SO_3^-$ and $NH^+$. There is no place for an H atom in the vicinity of the $SO_3^-$ group and there must be an H atom mediating the interaction between the N atoms of the pyridyl rings. This H atom was **not** evident in difference Fourier maps: it is placed in the most chemically reasonable position. The H atom of the phenol OH group was placed geometrically and allowed to rotate about the OH bond to the position of maximum electron density (AFIX 147 in SHELXL). The highest residual peak is associated with the chloroform molecule.

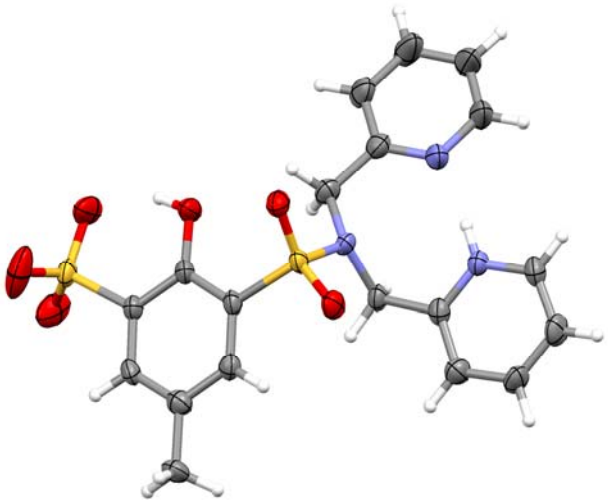

**Fig. S1.** Molecular structure of 2-hydroxy-3-(*N*,*N*-bis(2-pyridylmethyl)-sulfonamido)-5-methylbenzenesulfonic acid (hpsmsH) with displacement ellipsoids drawn at 50% probability for non-H atoms. The $CHCl_3$ molecule is not shown.

## S2. Geometry around N atoms

Deviation (Å) of the N atom from the plane defined by the three attached atoms (2 × C, 1 × S):

| | | | | |
|---|---|---|---|---|
| **bpsmpH** | N1 | 0.316 | N4 | 0.341 |
| **psmsp** | N1 | 0.271 | | |
| **1** | N1 (non-coord) | 0.220 | N4 (coord) | 0.479 |
| **2** | N1 (non-coord) | 0.058 | N4 (coord) | 0.467 |
| | N7 (non-coord) | 0.074 | N10 (coord) | 0.464 |
| **3** | N1 (non-coord) | 0.119 | N4 (coord) | 0.482 |
| **4** | N1 (non-coord) | 0.148 | N4 (coord) | 0.479 |
| **5** | N1 (non-coord) | 0.093 | N4 (coord) | 0.399 |
| **6** | N1 (coord) | 0.505 | N4 (coord) | 0.496 |
| **7** | N1 (coord) | 0.465 | N4 (coord) | 0.468 |
| **8** | N1 (coord) | 0.456 | N4 (coord) | 0.474 |