Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY MATERIAL

Table S1. $\Delta\Delta G_{binding}$ for the docking of Spx and Cpx with the OmpF protein using a docking box including the entire protein channel. Both protein models, 2OMF and 4KRA, were considered. The compound with the most stable binding energy (zwitterionic Cpx) was used as the reference for determining the $\Delta\Delta G_{binding}$ values.

Compound	**$\Delta\Delta G_{binding}$ / kcal·mol^{-1}**	
	2OMF	**4KRA**
Cpx zwitterionic	0.0	0.0
Spx zwitterionic	0.2	0.8
Cpx neutral	1.3	1.9
Spx negative	0.5	1.2
Spx neutral	0.9	2.2

Figure S1. Variation of the position of constriction zone residues in 4KRA and 2OMF structures. 4 KRA structure is represented in opaque and 2OMF is represented in translucent.

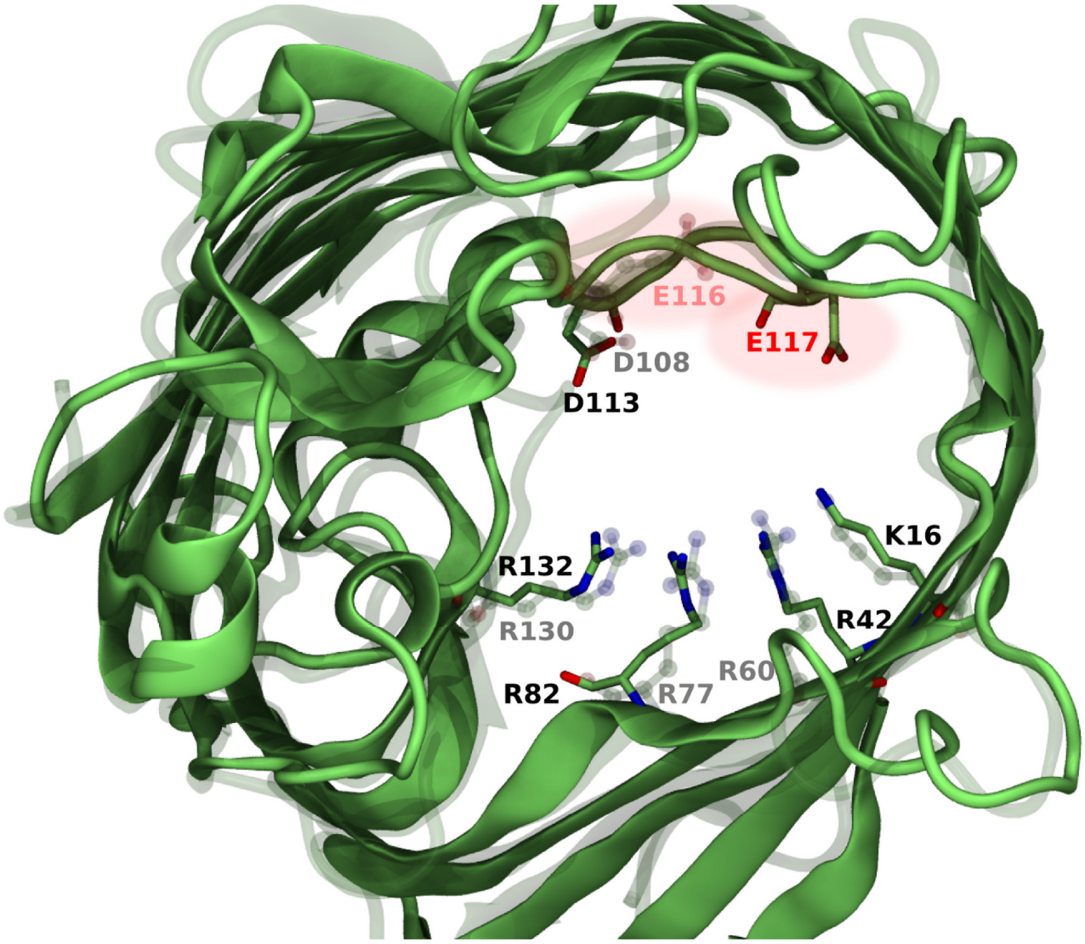

Figure S2. Comparison between the positions of the lowest energy rigid docking result of Cpx zwitterionic in the 4KRA structure and the x-ray position, RMSD = 4.95 Å. 4KRA structure and Cpx x-ray structure are represented in translucent and Cpx zwitterionic docking result is represented in opaque.

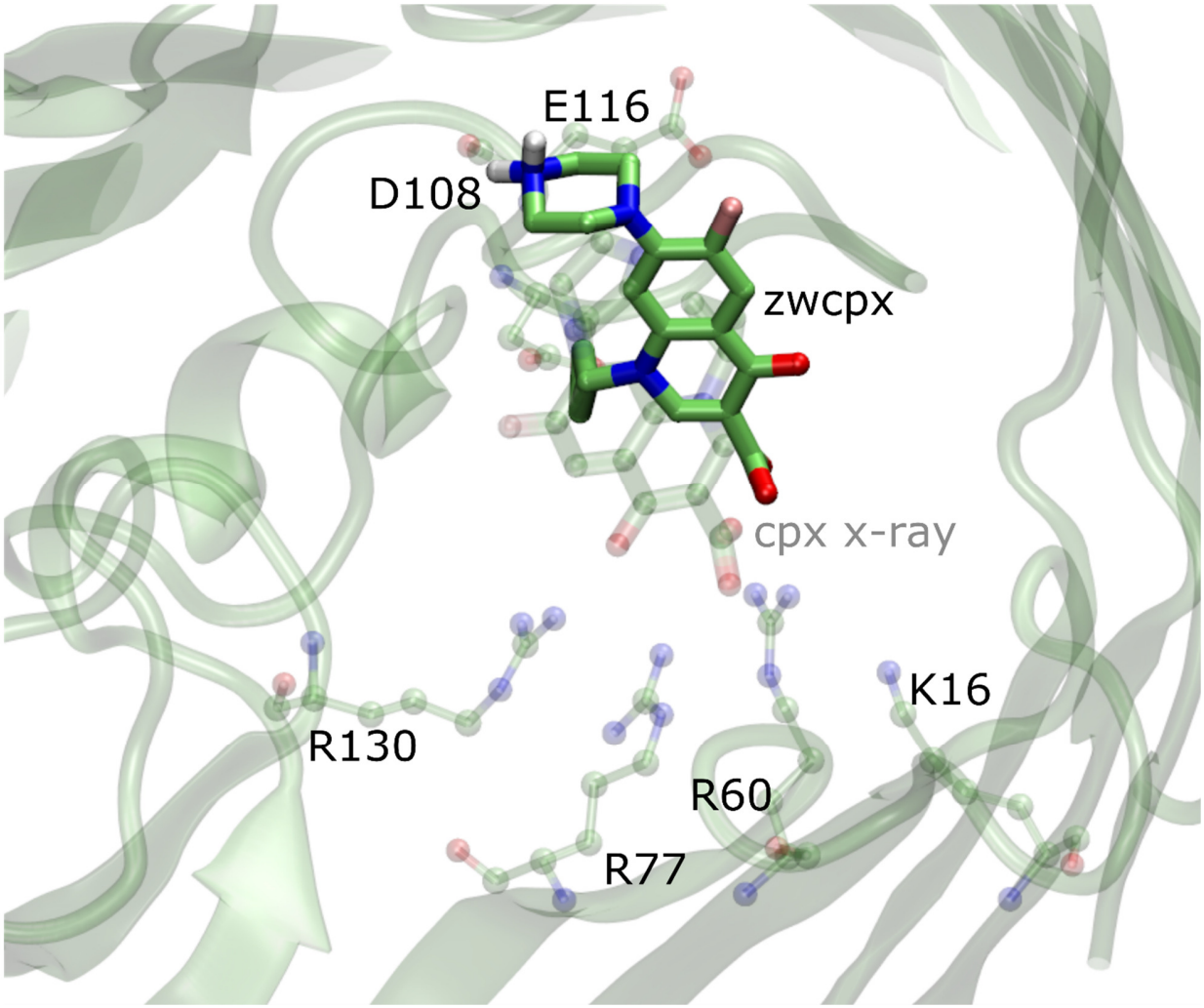

Figure S3. Comparison between the lowest binding free energy flexible docking pose of Cpx zwitterionic in the 4KRA OmpF structure with: (A) Cpx zwitterionic rigid docking pose, RMSD = 4.03 Å, and (B) Cpx x-ray, RMSD = 4.12 Å. The 4KRA rigid structure, Cpx zwitterionic rigid docking pose and x-ray Cpx structures are represented in translucent and Cpx zwitterionic flexible docking pose is represented in opaque. An RMSD of the constriction zone residues before and after flexibilization was also determined and it is 2.06 Å.