

## *Supporting Information*

### **Phosphonated Calixarene as a “Molecular Glue” for Protein Crystallization**

Jimi M. Alex,<sup>a</sup> Martin L. Rennie,<sup>a</sup> Stefano Volpi,<sup>b</sup> Francesco Sansone,<sup>b</sup> Alessandro Casnati,<sup>b</sup>  
and Peter B. Crowley\*,<sup>a</sup>

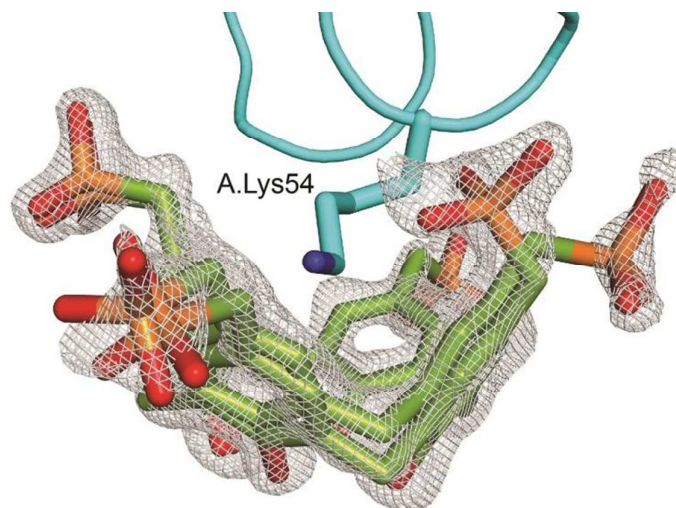
<sup>a</sup>School of Chemistry, National University of Ireland Galway, University Road, Galway,  
Ireland

<sup>b</sup>Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Università  
degli Studi di Parma, Viale delle Scienze 17/A, 43124 Parma, Italy

**Correspondence:** peter.crowley@nuigalway.ie      +353 91 49 24 80

#### **KEYWORDS**

assembly, cytochrome *c*, lysine recognition, patchy particle, X-ray crystallography



**Figure S1.**  $2F_o - F_c$  map (at 1.5 Å resolution and contoured to 1.0  $\sigma$ ) showing the electron density at A.Lys54, requiring two **pmclx<sub>4</sub>** conformers.

**Table S1.** X-ray data collection, processing and refinement statistics for cyt *c* - **pmclx<sub>4</sub>**<sup>a</sup>

Data collection	
Light source	APS
Beamline	24-ID-C
Wavelength (Å)	0.97910
Space group	<i>P</i> 1 2 <sub>1</sub> 1
Cell constants	<i>a</i> = 28.79 Å, <i>b</i> = 79.90 Å, <i>c</i> = 47.73 Å <i>α</i> = <i>γ</i> = 90°, <i>β</i> = 93°
Resolution (Å)	47.46-1.50 (1.55-1.50)
No. of unique reflections	34591 (3452)
Multiplicity	5.5 (5.4)
<i>I</i> / <i>σ</i> ( <i>I</i> )	18.7 (5.1)
Completeness (%)	99.2 (99.4)
<i>R</i> <sub>meas</sub> <sup>b</sup> (%)	6.1 (37.6)
<i>R</i> <sub>pim</sub> <sup>c</sup> (%)	2.6 (15.8)
Half-set correlation coefficient (CC <sub>1/2</sub> )	0.999 (0.966)
Solvent content (%)	46.7
Refinement	
<i>R</i> <sub>work</sub> (%)	0.1707
<i>R</i> <sub>free</sub> (%)	0.2012
rmsd bonds (Å)	0.0113
rmsd angles (°)	1.6080
Number of molecules in asymmetric unit	
protein	2
<b>pmclx<sub>4</sub></b>	3
water	281
Average B-factor (Å <sup>2</sup> )	20.6
Ramachandran analysis <sup>d</sup>	
% residues in favoured regions	98.0
% residues in allowed regions	100.0
PDB code	5NCV

<sup>a</sup>Values in parentheses correspond to the highest resolution shell; <sup>b</sup> $R_{\text{meas}} = \frac{\sum_{hkl} \nu(n/n-1) \sum_i |I_i(hkl) - \langle I(hkl) \rangle|}{\sum_{hkl} \sum_i I_i(hkl)}$ ; <sup>c</sup> $R_{\text{pim}} = \frac{\sum_{hkl} \nu(1/n-1) \sum_{i=1}^n |I_i(hkl) - \langle I(hkl) \rangle|}{\sum_{hkl} \sum_i I_i(hkl)}$ ; <sup>d</sup>Calculated in MolProbity.