

**Supplementary Table S1. Summary of crystallographic analysis.**

	$\overset{\text{Semet}}{\text{A}}/\text{B56/C}$ crystal a*	$\overset{\text{Semet}}{\text{A}}/\text{B56}^{\text{Semet}}/\text{C}$	$\overset{\text{Semet}}{\text{A}}/\text{B56/C}$ crystal b
<b>Data collection</b>			
Space group	P2 <sub>1</sub> 3	P2 <sub>1</sub> 3	P2 <sub>1</sub> 3
Wavelength (Å)	0.9793	0.9793	0.9793
Resolution (Å) (outer shell)	50-3.7 (3.83-3.70)	50-3.75 (3.88-3.75)	50-3.5 (3.63-3.50)
Unique reflections	65390	61028	76332
Redundancy	8.5	7.6	4.4
R <sub>sym</sub> % (outer shell)**	16.1 (91.6)	16.5 (97.3)	11.8 (90.5)
I/σI (outer shell)	12.1 (2.2)	13.5 (1.9)	13.6 (1.4)
Complete (%) (outer shell)	98.8 (99.6)	94.4 (97.9)	97.5 (98.1)
<b>Phasing</b>			
Se sites found (expected)	25 (28)	39 (48) <sup>+</sup>	
Phasing power	1.22		
FOM (after DM)	0.87		
<b>Refinement</b>			
Resolution (Å)			20-3.5
R <sub>cryst</sub> / R <sub>free</sub> ***			25.7/31.5
Number of atoms			
Protein			19810
Microcystin			142
Metal (Mn <sup>++</sup> )			4
Water			0
Solvent content			76%
Model			
A/B56/C complexes per ASU			2
microcystin per complex			1
metal (Mn <sup>++</sup> ) per complex			2
B factors			
Protein			108.5
ligand / ion			83.8 / 75.7
water			N/A
TLS group per ASU			6
RMSD bond length (Å)			0.009
RMSD angle (°)			1.38
Ramachandran plot (%)			
most favored / additionally addowed / generously allowed / disallowed			81.2 / 17.3 / 1.5 / 0.0

\*  $\overset{\text{Semet}}{\text{A}}/\text{B56/C}$  : Selenomethionine-labeled structural A $\alpha$  subunit / B56 $\gamma$ 1 / catalytic C $\alpha$  subunit

\*\*  $R_{\text{sym}} = \sum_h |I_i(h) - \langle I(h) \rangle| / \sum_h I_i(h)$ , where  $I_i(h)$  is the  $i^{\text{th}}$  measurement of  $h$  and  $\langle I(h) \rangle$  is the mean of all measurements of  $I(h)$  for reflection  $h$ .

\*\*\* R<sub>free</sub> is R<sub>cryst</sub> calculated with only the test set (5%) of reflections. FOM, figure of merit.

<sup>+</sup>Total peaks in Se-anomalous difference map contoured at 5 $\sigma$  level. All 39 peaks corresponds to methionine position in our model.