

Supplementary Materials: Regulation Efficacy and Mechanism of the Toxicity of Microcystin-LR Targeting Protein Phosphatase 1 via the Biodegradation Pathway

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Table S1. Molecular simulation parameters for the complexes of MCLR/MCLR biodegradation products and PP1.

Molecular simulation parameters	MCLR	Linearised MCLR	Glu ⁶ -Mdha ⁷ -Ala ¹ -Leu ² -MeAsp ³ -Arg ⁴	Adda ⁵ -Glu ⁶ -Mdha ⁷ -Ala ¹	Leu ² -MeAsp ³ -Arg ⁴	Glu ⁶ -Mdha ⁷ -Ala ¹	Adda ⁵
Combination energy (KJ/Mol)	- 4820.8 1	-4882.96	-4801.05	-4765.91	-4837.68	-4684.06	- 4764.6 3
Combination area (Å ²)	Total	743.51 85	752.4809	484.4441	608.3952	369.5579	359.80 27
	Ala ¹ →PP1	81.832 7	89.4847	78.9434	122.8509	--- ^a	129.6694 ---
	Leu ² →PP1	140.41 26	145.3441	130.2552	---	153.1681	---
	MeAsp ³ →PP1	66.469 1	77.7975	96.1365	---	159.0142	---
	Arg ⁴ →PP1	129.36 82	131.7525	138.4834	---	150.6687	---
	Adda ⁵ →PP1	351.83 4	359.5489	---	344.5371	---	359.80 27
	Glu ⁶ →PP1	194.09 55	195.9994	193.7585	176.8987	---	196.7631 ---
	Mdha ⁷ →PP1	137.24 25	131.8518	133.6010	142.2166	---	143.4255 ---
Active center exposure (Å ²)	Mn ¹²⁺ /Mn ²²⁺	120.76 28	120.7628	120.7628	120.7628	120.7628	120.76 28

	Mn ²⁺ + Asp ₆₄ +Asp ₉₂	446.68 81	440.0578	449.1638	446.8703	448.3228	445.0868	451.08 59
H-pi bonds (KJ/Mol)	Total	-2.1	-0.5	0	-0.6	0	0	0
	Trp₂₀₆ - Adda⁵	---	---	---	-0.6	---	---	---
	Ser₁₂₉ - Adda⁵	-1.4	---	---	---	---	---	---
	Asp₁₉₇ - Adda⁵	-0.7	-0.5	---	---	---	---	---
Ionic bonds (KJ/Mol)	Total	-74.4	-69.3	-32.6	-44.3	-69.8	-40.5	-1.5
	ASP₆₄ - Mn²⁺	-24.5	-24.3	---	-24.1	-24.5	-24.5	
	ASP₉₂ - Mn²⁺	-11.1	-11.2	---	-11.3	-10.9	-11.2	
	Arg₉₆ - MeAsp³	-17.2	-13.3	-14.3	-13.5	-15.5	---	---
	Asp₂₂₀ - Arg⁴	-7.3	-7.0	-6.7	---	-6.6	---	---
	Asp₁₉₇ - Adda⁵	-1.4	-1.8	---	-1.5	---	---	-1.5
	Glu₂₇₅ - Mdha⁷	-4.6	-11.7	-11.6	-7.4	---	-4.8	---
Hydrogen bonds (KJ/Mol)	Total	-48.5	-43.3	-36.0	-14.0	-37.6	-10.1	-2.2
	H₂O↔Toxins	-8.8	-3.8	-2.2	-3.5	---	-3.5	-2.2
	H₂O←Adda⁵	-2.8	---	---	---	---	---	-2.2
	H₂O→Arg⁴	-2.8	---	---	---	---	---	---
	H₂O→Glu⁶	-3.2	-3.8	-2.2	-3.5		-3.5	
	Asp₂₂₀←Arg⁴	-8.7	-10.2	-8.6	---	-9.1	---	---
	Glu₂₇₅←Mdha⁷	-0.5	-11.4	---	---	---	-0.5	---
	Arg₉₆→MeAsp³	-7.9	-12.2	-10.9	---	-9.8	---	---
	Arg₂₂₁→Arg⁴	-11.3	---	---	---	-0.7	---	---

^a --- no related parameter was detected.