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Supporting information for article:

Structure of the adenylation–peptidyl carrier protein didomain of the *Microcystis aeruginosa* microcystin synthetase McyG

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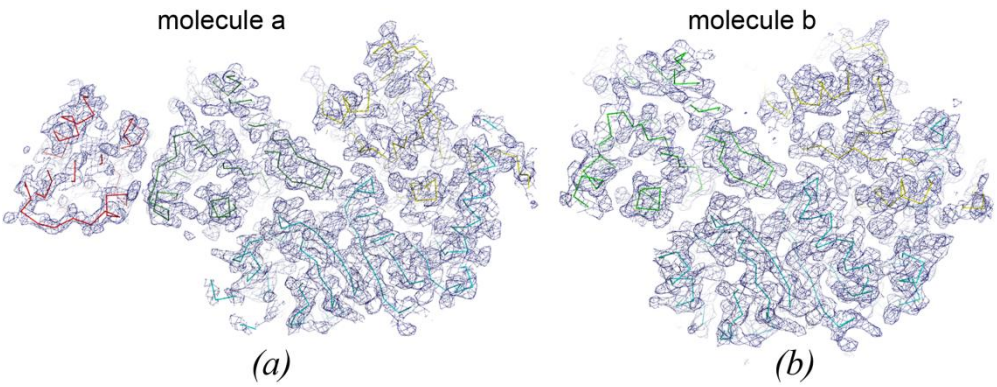

This figure shows the C-alpha trace of McyG A-PCP didomain

Table.S1. The catalytic constants of McyG A-PCP and mutants.

trans-cinnamate			
Enzyme	k_{cat} (min^{-1})	K_m (μM)	k_{cat}/K_m ($min^{-1}\cdot mM^{-1}$)
WT	0.1906±0.0057	10.15±1.34	18.79±1.80
V227T	0.3560±0.02	33.47±6.67	10.72±0.62
V227D	0.1485±0.0075	236.28±25.25	0.6424±0.1063
L-Phe			
Enzyme	k_{cat} (min^{-1})	K_m (μM)	k_{cat}/K_m ($min^{-1}\cdot mM^{-1}$)
WT	0.2074±0.0079	1079.01±105.31	0.1922±0.0026
V227T	0.043±0.005	1452.12±372.37	0.0287±0.0073
V227D	0.00473±0.0007	1146.27±459.36	0.0039±0.0003

Table S1 Activity assay of wild-type and mutants of McyG A domain towards trans-cinnamate and L-Phe. Adenylation activity was determined using a coupled continuous spectrophotometric assay for inorganic pyrophosphate (EnzChek Pyrophosphate Assay Kit; Invitrogen). Each reaction contained 50 mM Tris-Cl, pH 7.5, 1 mM $MgCl_2$, 1 mM ATP, 0.2 mM 2-amino-6-mecrapto-7-methylpurine ribonucleoside, 1 unit of purine nucleoside phosphorylase and 0.03 units of inorganic pyrophosphatase, 5 μM wild-type or mutants of

McyG A and varying concentrations of trans-cinnamate or L-Phe. Reaction was carried out at 30 °C and formation of 2-amino-6-mercapto-7-methylpurine was monitored at 360 nm.