Supplementary material (S1)

Amplification of LLM2 open reading frame (ORF) from *Priestia megaterium* PSA10 genome.

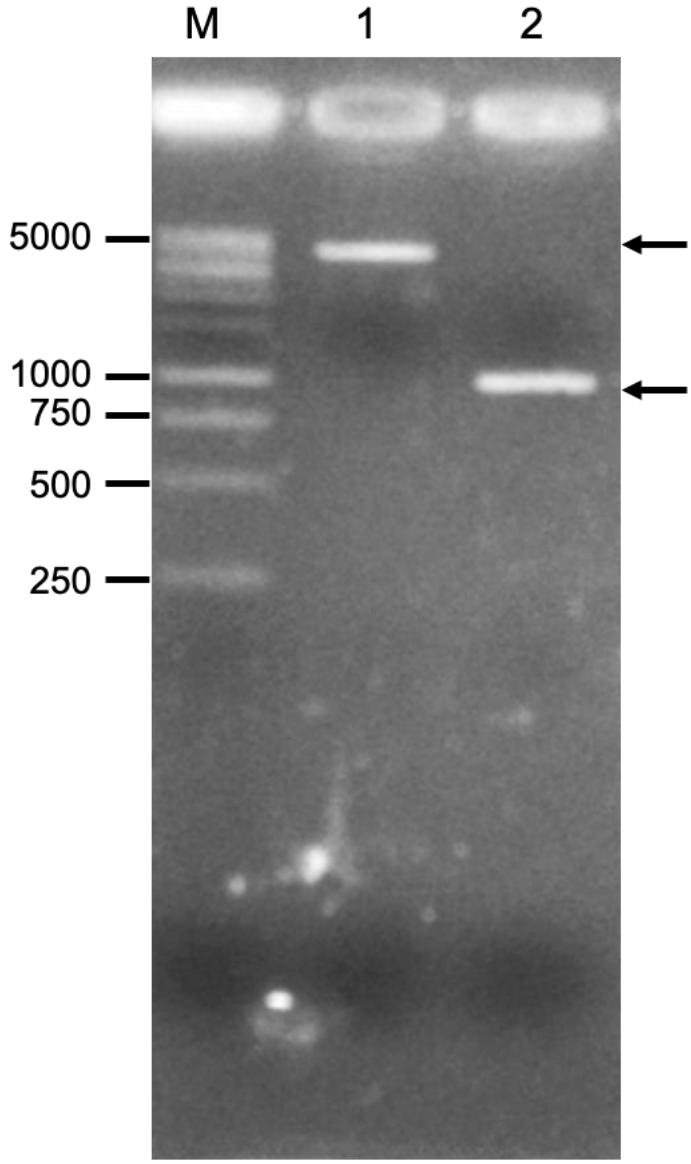


Figure S1. Amplified LLM2 open reading frame from *Priestia megaterium* PSA10 genome. The amplified ORF has a size of ±926 bp (indicated by lower arrow). The digested pET28a(+) are indicated by the upper arrow. Lane M: 1 kb ladder DNA marker; Lane 1. *Nco*I-*Bam*HI double digested pET28a(+); Lane 2. *Nco*I-*Bam*HI double digested *llm2* open reading frame.

Selection of positive clone was carried out by implementing colony PCR using the T7 promoter and T7 terminator primers.

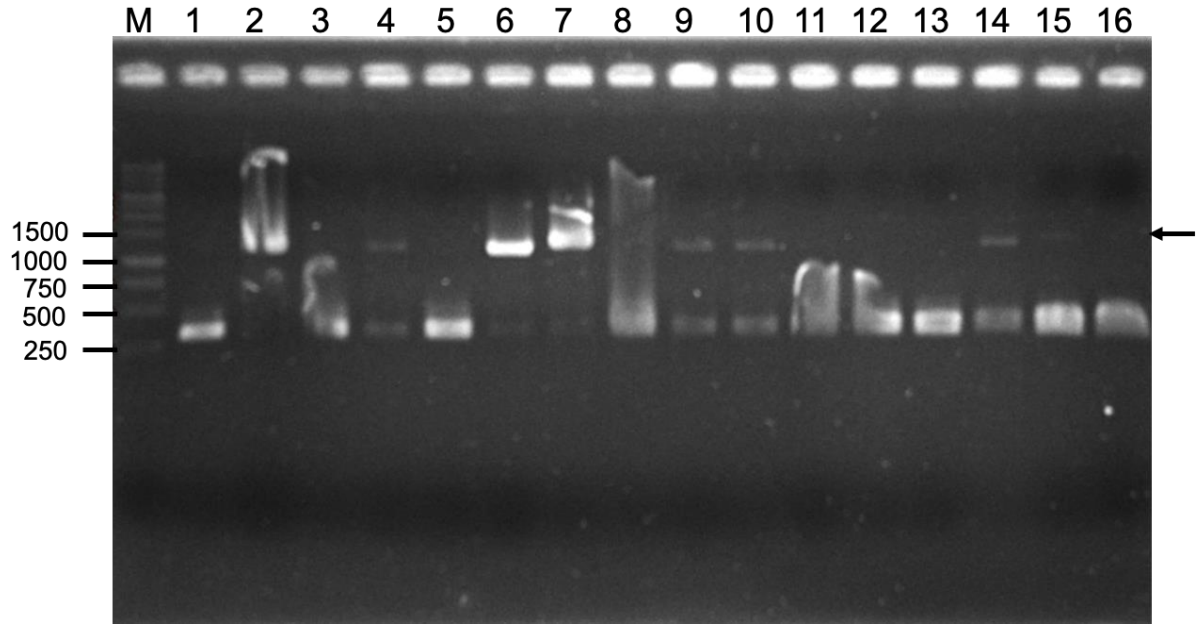


Figure S2. Visualization of colony PCR result to select the positive clone. The positive clones were indicated by showing band which has size ±1200 bp (indicated by arrow). Lane M: 1kb ladder DNA marker; Lane 1-16 are representation of the number selected colony grow on LB agar medium.

The selected positive cloned was then sequenced to check whether the llm2 was inserted in the correct orientation.

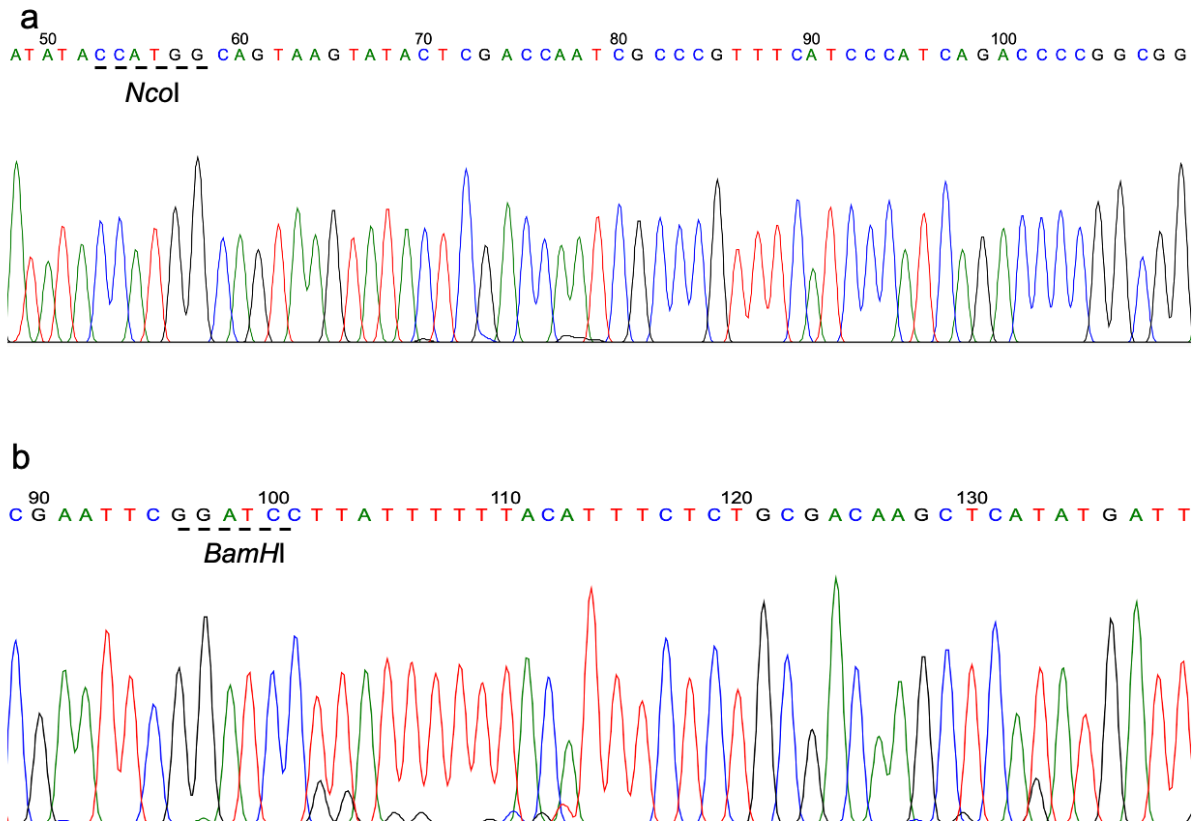


Figure S3. Sequencing of *llm2* cloned in pET28a(+) by using T7 promoter and T7 terminator primers. (a) Sequencing result when the T7 promoter used as primer, (b) Sequencing result when T7 terminator used as primer. The restriction site of *Nde*I and *Bam*HI are also indicated.

The model quality parameters of 3D structure of LLM2 from *Priestia megaterium* PSA10

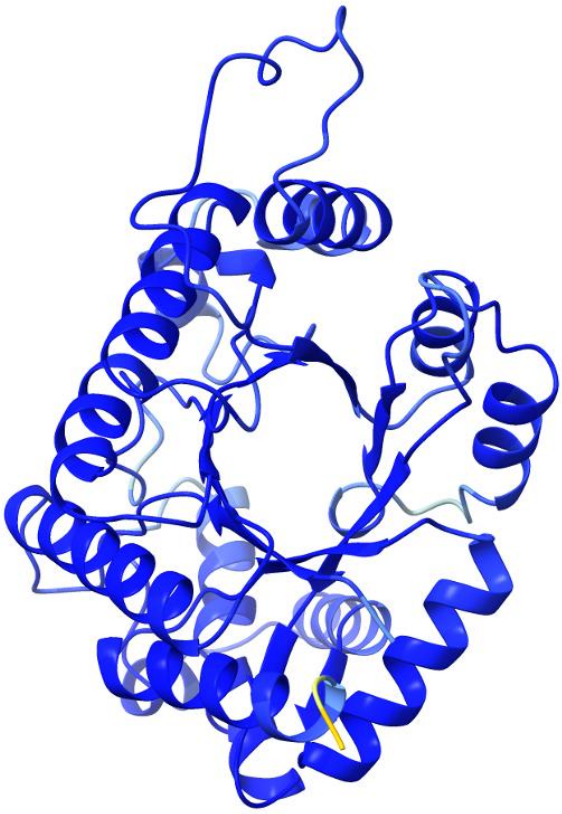


Figure S4. Structure of LLM2 from *Priestia megaterium* PSA10 predicted by AlphaFold2. Blue, light blue, and yellow colors indicate the high (pLDDT > 90), confident (90 > pLDDT > 70), and low (70 > pLDDT > 50) of pLDDT scores. pLDDT is a superposition free score that evaluates local distance difference of all atoms in model, including validation of stereochemical plausibility (Varadi et al., 2021; Jumper et al., 2020; Mariani et al., 2013)

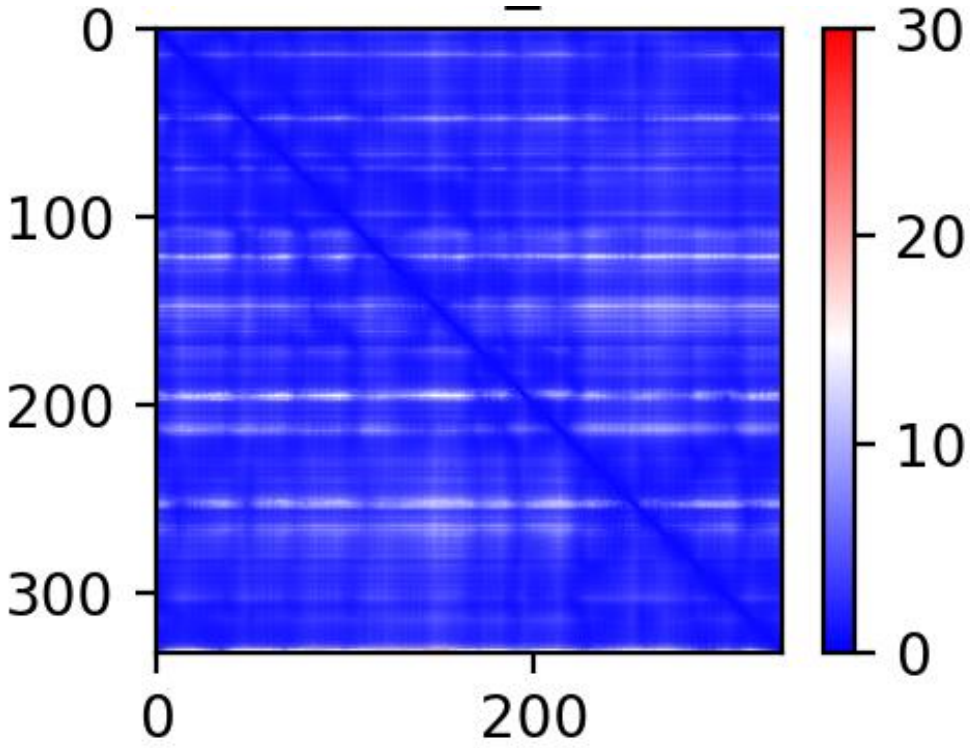


Figure S5. The diagram showing the predicted aligned error (PAE). The PAE (Predicted Aligned Error) indicates the expected distance error in residue x position, when the predicted and true structure are aligned on residue y (DeepMind, 2021).

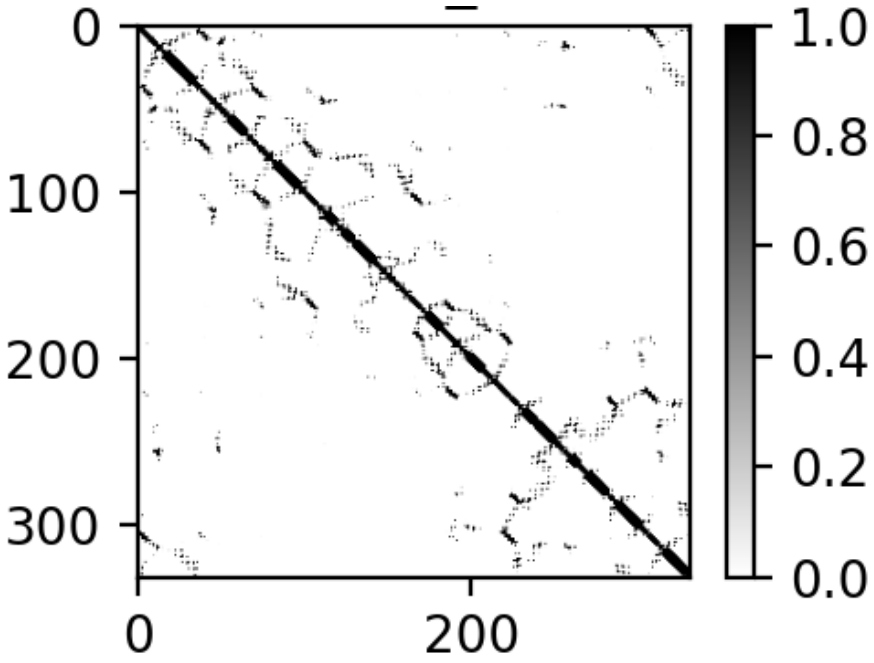
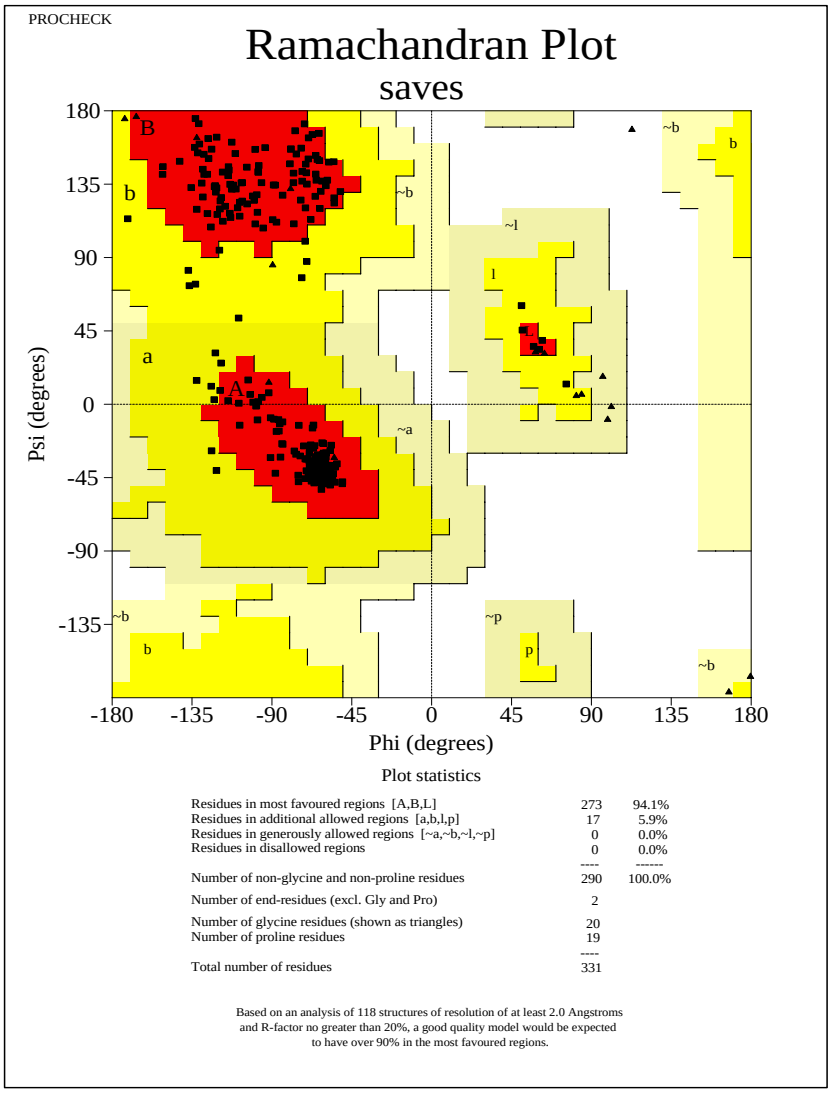


Figure S6. The diagram showing the predicted contact. The diagram shows the spatially close between two residues at certain distance threshold (8Å) (Adhikari and Cheng, 2018)



saves_01.ps

Fugure S7. Digaram showing the Ramachandran plot of the LLM2 model. Most of the residues are located at the favored regions.

Table S1.The quality parameters of the LLM2 model structure

Parameters	Value (%)
pLDDT	96.6
pTMscore	93.6
Residues in	Value (%)
Most favored regions	94.1
Additional allowed regions	5.9
Generously allowed regions	0.0
Disallowed regions	0.0

Redocking of FMN in LuxA (3FGC)

Docking experiments were carried out by using AutoDock Vina ver. 1.1.2 (Trod et al., 2010)

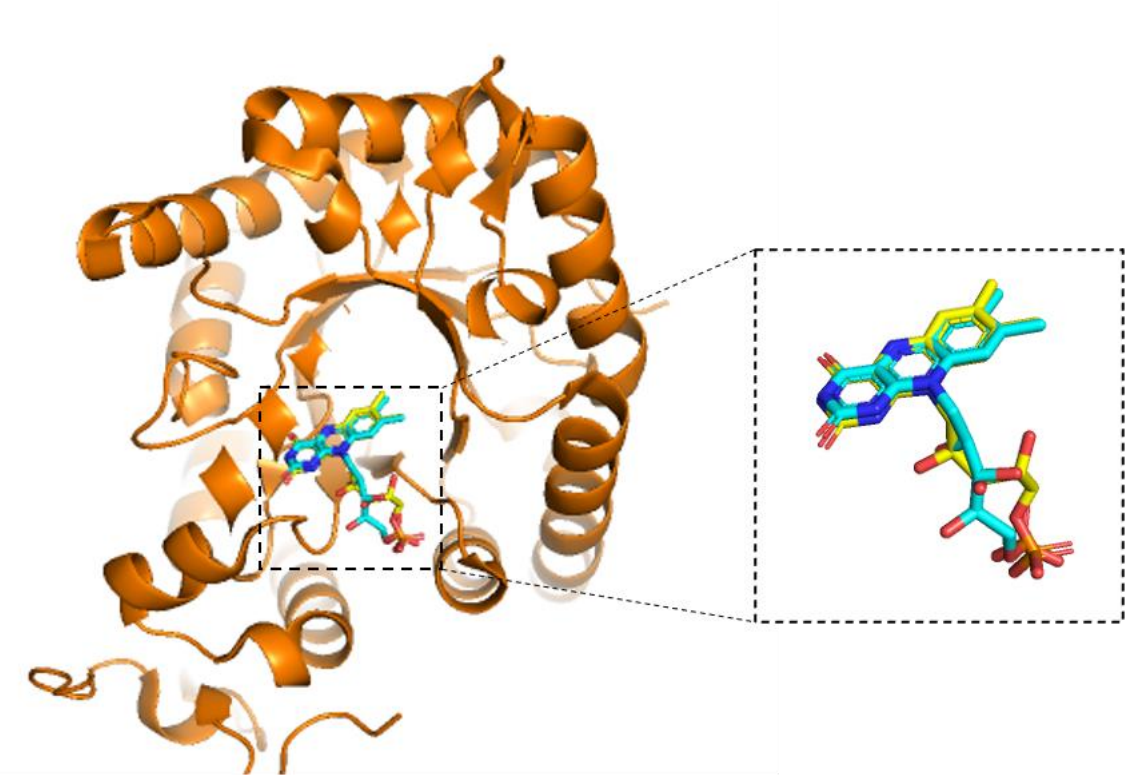


Figure S8. Redocking FMN in LuxA crystal structure (3FGC). The yellow color shown the crystal bound FMN and the redocking FMN was shown by cyan color.

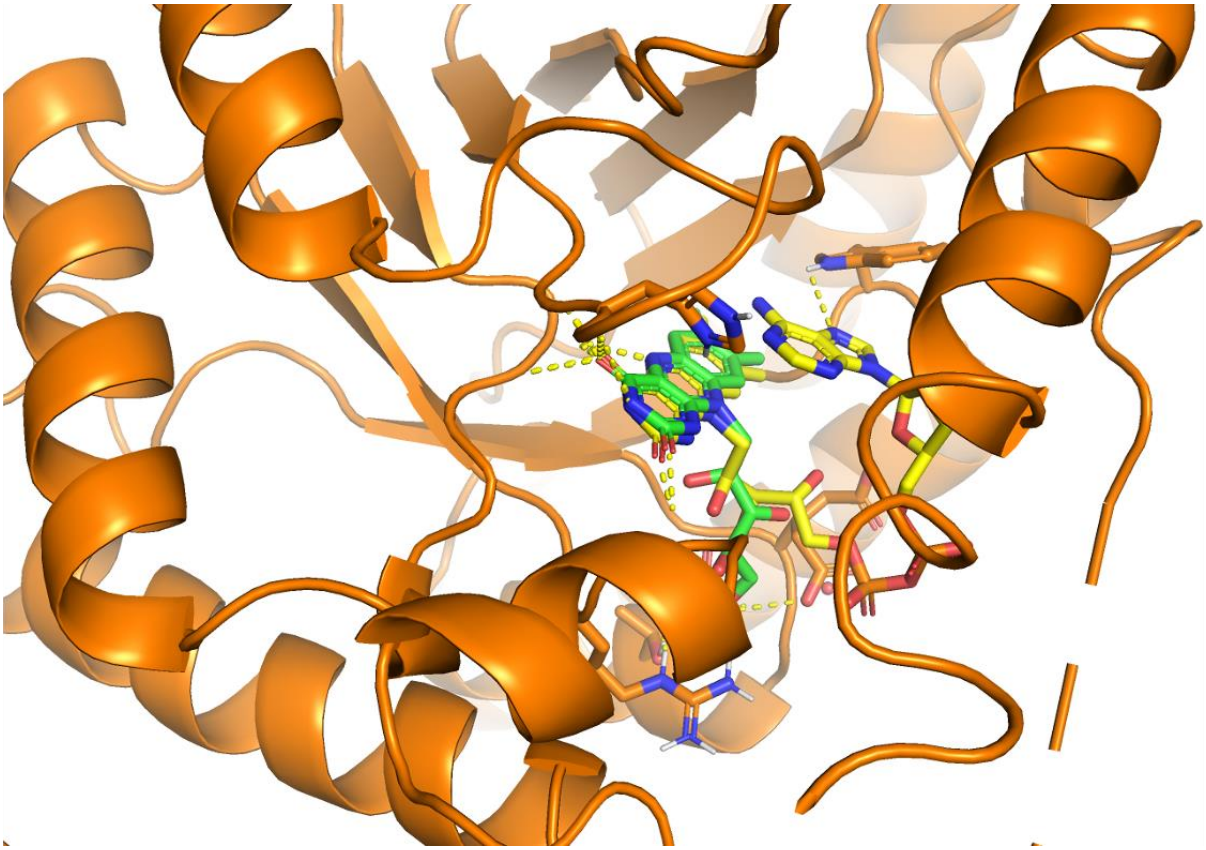


Figure S6. The superposition of the FMN and FAD binding mode on. LuxA (3FGC). The FMN and FAD were shown by the green and yellow color.

References

Adhikari, B and Cheng, J. (2016). Protein Residue Contacts and Prediction Methods. *Methods Mol Biol* 1415:463–476. https://doi.org/10.1007/978-1-4939-3572-7_24

DeepMind. 2021. https://www.deepmind.com/publications/enabling-high-accuracy-protein-structure prediction-at-the-proteome-scale

Mariani, V, Biasini, M, Barbato, A, and Schwede, T. (2013). lDDT: a local superposition-free score for comparing protein structures and models using distance difference tests. *Bioinformatics 29*(21): 2722–2728. https://doi.org/10.1093/bioinformatics/btt473

Trott, O. and Olson, AJ. 2010. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading, J Comp Chem 31:455-461. https://doi.org/10.1002/jcc.21334.

Varadi, M, Anyango, S, Deshpande, M, Nair, S, et al. 2022. AlphaFold Protein Structure Database: massively expanding the structural coverage of protein-sequence space with high-accuracy models, *Nucleic Acids Res*, 50(D1):D439–D444, https://doi.org/10.1093/nar/gkab1061