

Supplementary Information

Targeted disruption of pi-pi stacking in Malaysian banana lectin reduces mitogenicity while preserving antiviral activity

Evelyn M. Covés-Datson^{1,2}, *Steven R. King*³, *Maureen Legendre*³, *Michael D. Swanson*^{4,12}, *Auroni Gupta*³,
*Sandra Claes*⁵, *Jennifer L. Meagher*⁶, *Arnaud Boonen*⁵, *Lihong Zhang*⁷, *Birte Kalveram*⁷, *Zoe Raglow*³,
*Alexander N. Freiberg*⁷, *Mark Prichard*⁸, *Jeanne A. Stuckey*^{6,9}, *Dominique Schols*⁵, *David M.*
Markovitz^{3,4,10,11*}

¹Medical Scientist Training Program, University of Michigan, Ann Arbor MI 48109; ²Department of Microbiology & Immunology, University of Michigan, Ann Arbor MI 48109; ³Department of Internal Medicine, Division of Infectious Diseases, University of Michigan, Ann Arbor MI 48109; ⁴Graduate Program in Immunology, University of Michigan, Ann Arbor MI 48109; ⁵Laboratory of Virology and Chemotherapy, Rega Institute for Medical Research, University of Leuven, 3000 Leuven, Belgium; ⁶Life Sciences Institute, University of Michigan, Ann Arbor MI 48109; ⁷Department of Pathology, University of Texas Medical Branch, Galveston TX 77555; ⁸University of Alabama Health Services Foundation Diagnostic Virology Laboratory, University of Alabama at Birmingham, Birmingham AL 35294; ⁹Department of Biological Chemistry, University of Michigan, Ann Arbor MI 48109; ¹⁰Cellular and Molecular Biology Program, University of Michigan, Ann Arbor MI 48109; ¹¹Cancer Biology Program, University of Michigan, Ann Arbor MI 48109; Present Address: Predictive and Clinical Immunogenicity, Merck and Co., Inc, Kenilworth NJ 07033

Material included:

Table S1

Table S1. Crystallography Data Collection and Refinement Statistics.

Data Collection	WT Malay BanLec	F84T Malay BanLec
PDBID	6OPR	6OQ0
Space Group	P4 ₃ 2 ₁ 2	P2 ₁ 2 ₁ 2 ₁
Unit Cell (Å)	52.526, 52.526, 221.307	79.247, 157.871, 204.101
Wavelength (Å)	0.9786	0.9786
Resolution (Å) ¹	1.51 (1.51 – 1.54)	1.80 (1.80 – 1.83)
R _{sym} ²	0.060 (0.414)	0.084 (0.662)
<I/σI> ³	20 (5)	10 (2)
Completeness (%) ⁴	99.5 (98.4)	99.8 (99.5)
Redundancy	14.0 (11.7)	7.1 (6.9)
Refinement		
Resolution (Å)	1.51	1.80
R-Factor ⁵	18.4	20.2
R _{free} ⁶	20.2	23.4
Protein atoms	2117	16861
Water Molecules	363	2240
Unique Reflections	49784	229852
R.m.s.d. ⁷		
Bonds	0.008	0.008
Angles	0.99	1.07
MolProbity Score (1)	0.92	0.93
Clash Score (1)	0.70	0.76

¹Statistics for highest resolution bin of reflections in parentheses.

² $R_{\text{sym}} = \frac{\sum_h \sum_j |I_{hj} - \langle I_h \rangle|}{\sum_h \sum_j I_{hj}}$, where I_{hj} is the intensity of observation j of reflection h and $\langle I_h \rangle$ is the mean intensity for multiply recorded reflections.

³Intensity signal-to-noise ratio.

⁴Completeness of the unique diffraction data.

⁵R-factor = $\frac{\sum_h | |F_o| - |F_c| |}{\sum_h |F_o|}$, where F_o and F_c are the observed and calculated structure factor amplitudes for reflection h .

⁶ R_{free} is calculated against a 5% random sampling of the reflections that were removed before structure refinement.

⁷Root mean square deviation of bond lengths and bond angles.

References

1. Chen, V. B., Arendall, W. B., Headd, J. J., Keedy, D. A., Immormino, R. M., Kapral, G. J., Murray, L. W., Richardson, J. S., and Richardson, D. C. (2010) *MolProbity*: all-atom structure validation for macromolecular crystallography. *Acta Crystallogr. Sect. D Biol. Crystallogr.* **66**, 12–21