



*J. Serb. Chem. Soc.* **00(0)** S1-S4 (2026)

Journal of  
the Serbian  
Chemical Society

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Supplementary material

SUPPLEMENTARY MATERIAL TO  
***In silico* evaluation of phycobilins as multi-target anti-tubercular  
scaffolds: molecular docking, dynamic stability, ADMET, and  
mycobacterial sensitivity analysis**

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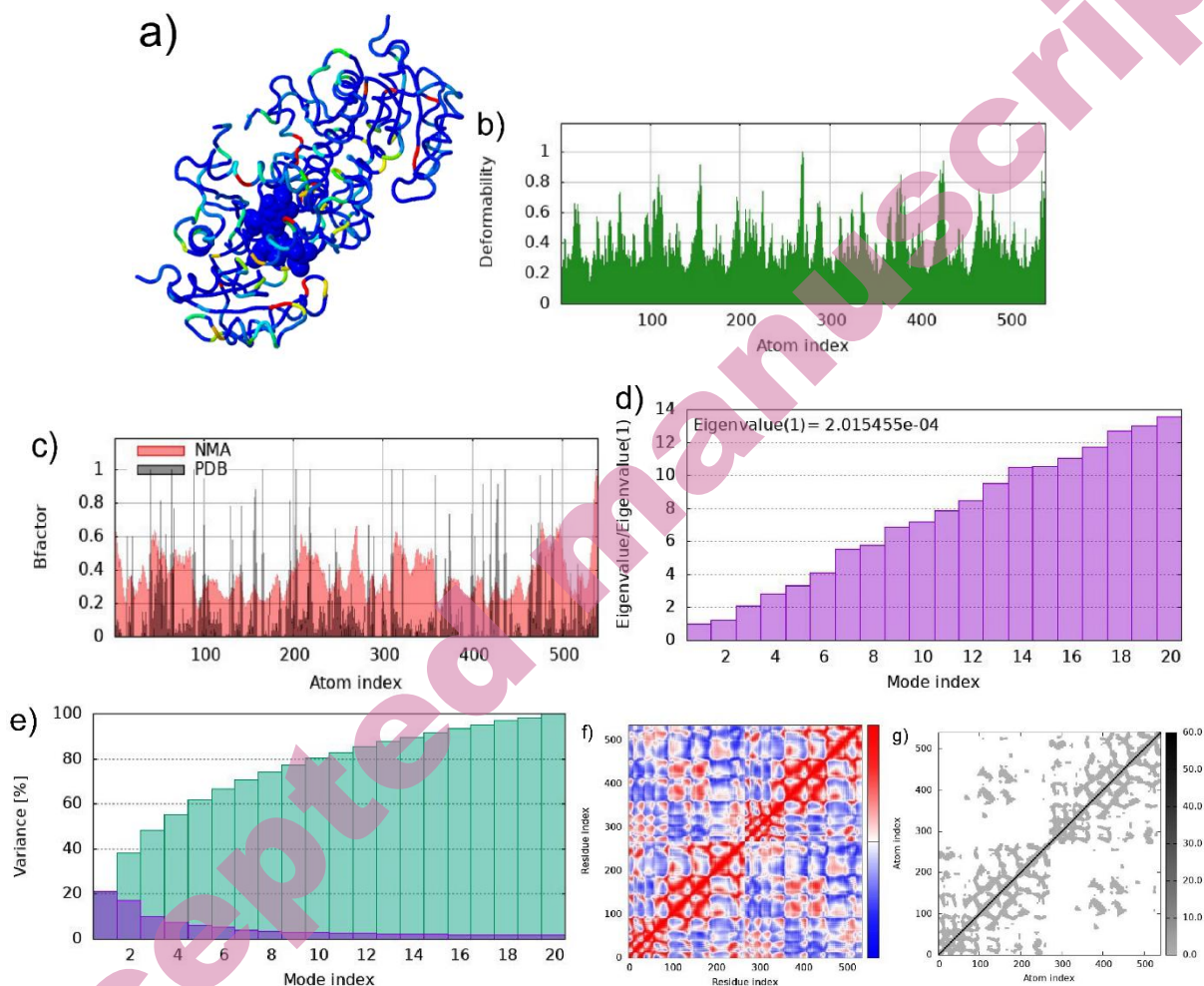


Fig. 1S. Normal mode analysis (NMA) of enoyl-acyl carrier protein reductase InhA (2NSD) with the phycocyanobilin structure and its dynamic behavior: a) Ligand bound in the binding pocket of the 2NSD protein. Blue: stable regions with low fluctuations; green and yellow: regions with moderate flexibility; orange and red: regions with high mobility; b) Deformability plot showing the flexibility of each residue, with peaks indicating regions of high deformability; c) Comparison of the normalized B-factors obtained from NMA (red) and from the crystal structure (black), indicating the reliability of the predicted atomic fluctuations; d) Eigenvalue associated with each normal mode, reflecting the stiffness of the motion; lower eigenvalues indicate greater deformability; e) The variance associated with normal modes (purple – individual; green – cumulative variances); f) Cross-correlation matrix of residue fluctuations, where red denotes correlated motions and blue denotes anti-correlated motions; g) Elastic network model showing pairwise atomic connections; darker regions represent stronger interactions.

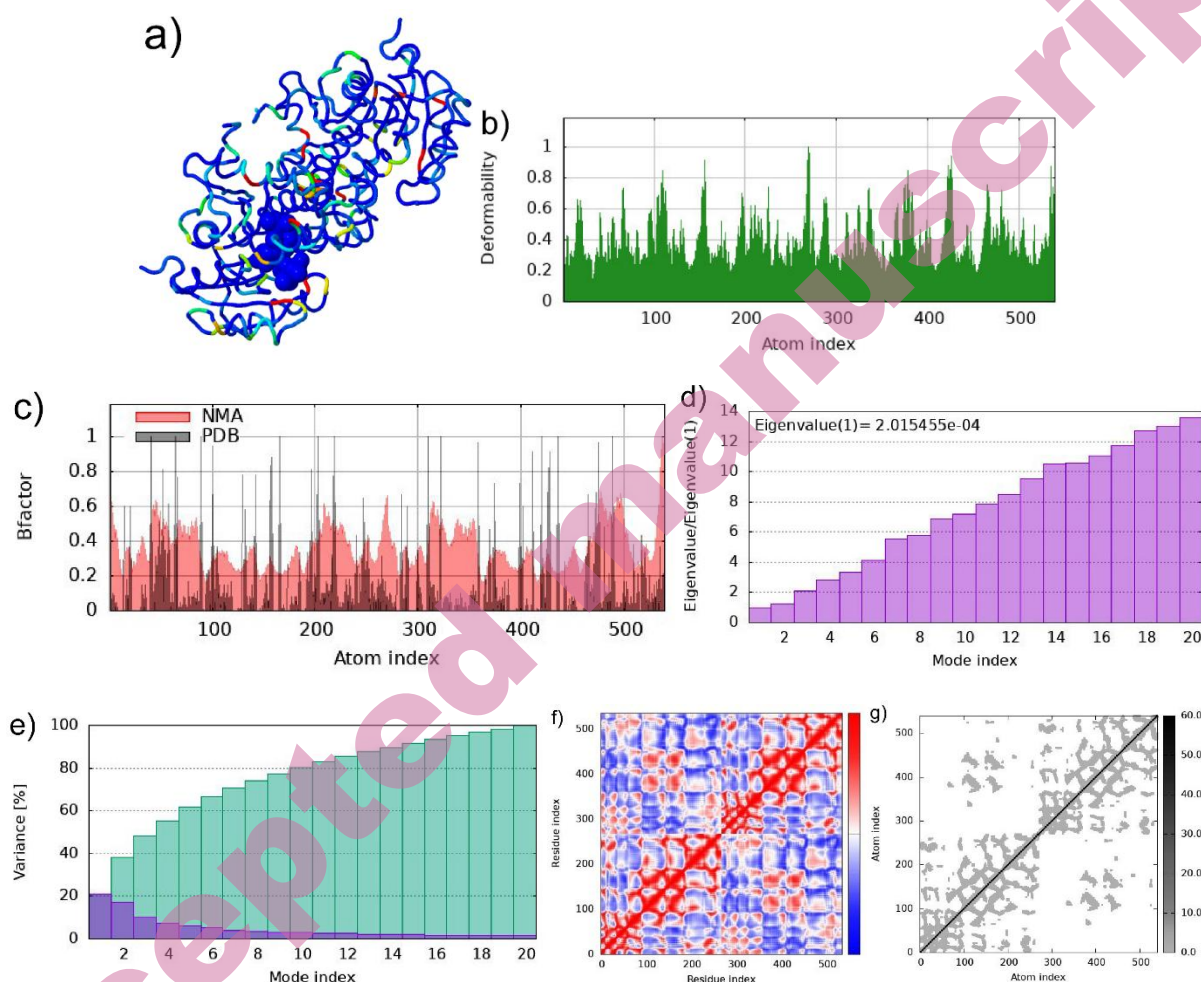


Fig. 2S. Normal mode analysis (NMA) of enoyl-acyl carrier protein reductase InhA (2NSD) with the phycoerythrobilin structure and its dynamic behavior: a) Ligand bound in the binding pocket of the 2NSD protein. Blue: stable regions with low fluctuations; green and yellow: regions with moderate flexibility; orange and red: regions with high mobility; b) Deformability plot showing the flexibility of each residue, with peaks indicating regions of high deformability; c) Comparison of the normalized B-factors obtained from NMA (red) and from the crystal structure (black), indicating the reliability of the predicted atomic fluctuations; d) Eigenvalue associated with each normal mode, reflecting the stiffness of the motion; lower eigenvalues indicate greater deformability; e) The variance associated with normal modes (purple – individual; green – cumulative variances); f) Cross-correlation matrix of residue fluctuations, where red denotes correlated motions and blue denotes anti-correlated motions; g) Elastic network model showing pairwise atomic connections; darker regions represent stronger interactions.

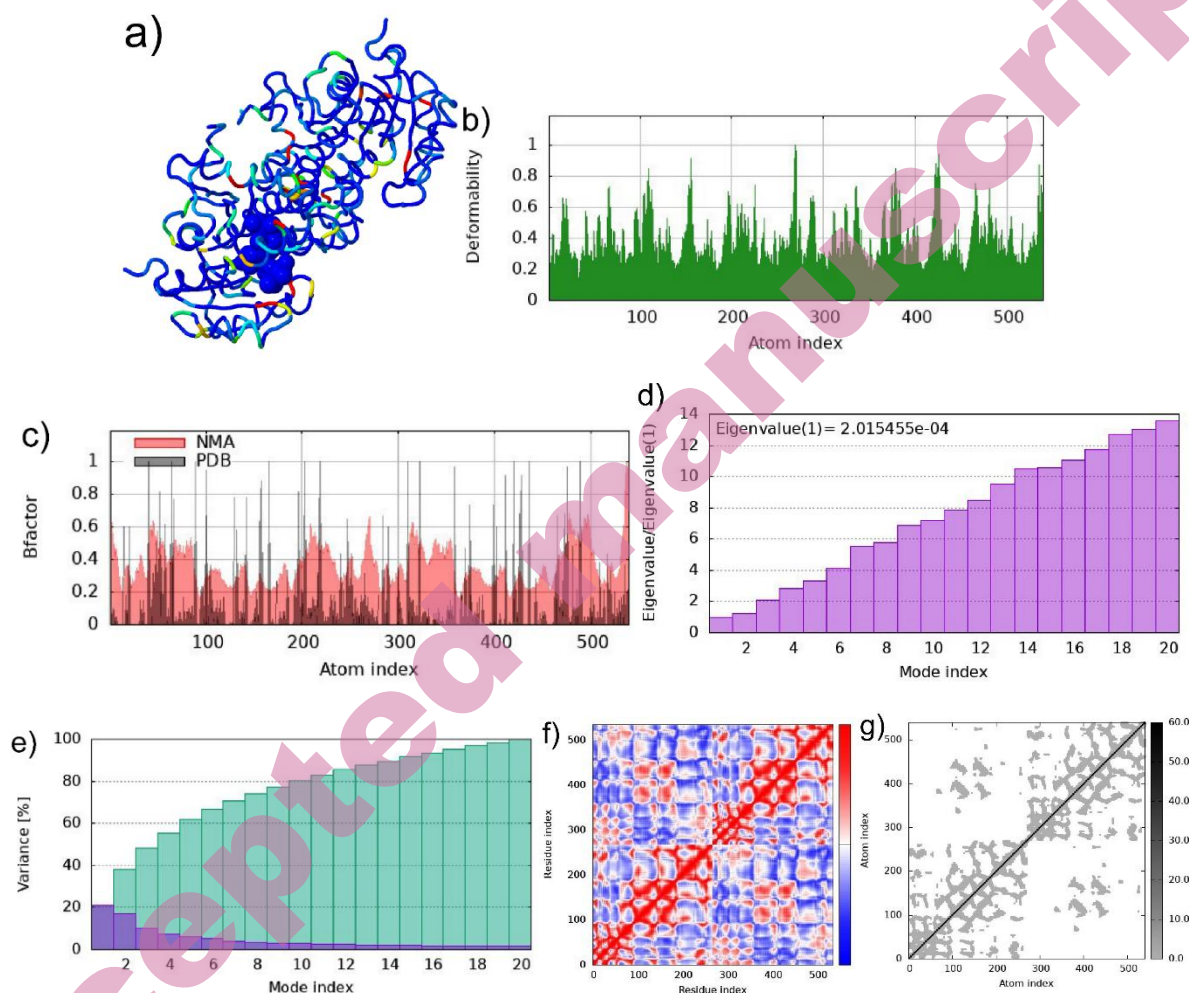


Fig. 3S. Normal mode analysis (NMA) of enoyl-acyl carrier protein reductase InhA (2NSD) with the phycourobilin structure and its dynamic behavior: a) Ligand bound in the binding pocket of the 2NSD protein. Blue: stable regions with low fluctuations; green and yellow: regions with moderate flexibility; orange and red: regions with high mobility; b) Deformability plot showing the flexibility of each residue, with peaks indicating regions of high deformability; c) Comparison of the normalized B-factors obtained from NMA (red) and from the crystal structure (black), indicating the reliability of the predicted atomic fluctuations; d) Eigenvalue associated with each normal mode, reflecting the stiffness of the motion; lower eigenvalues indicate greater deformability; e) The variance associated with normal modes (purple – individual; green – cumulative variances); f) Cross-correlation matrix of residue fluctuations, where red denotes correlated motions and blue denotes anti-correlated motions; g) Elastic network model showing pairwise atomic connections; darker regions represent stronger interactions.