

*Supplementary Material*

# Lipase-Catalyzed Synthesis, Antioxidant Activity, Antimicrobial Properties and Molecular Docking Studies of Butyl Dihydrocaffeate

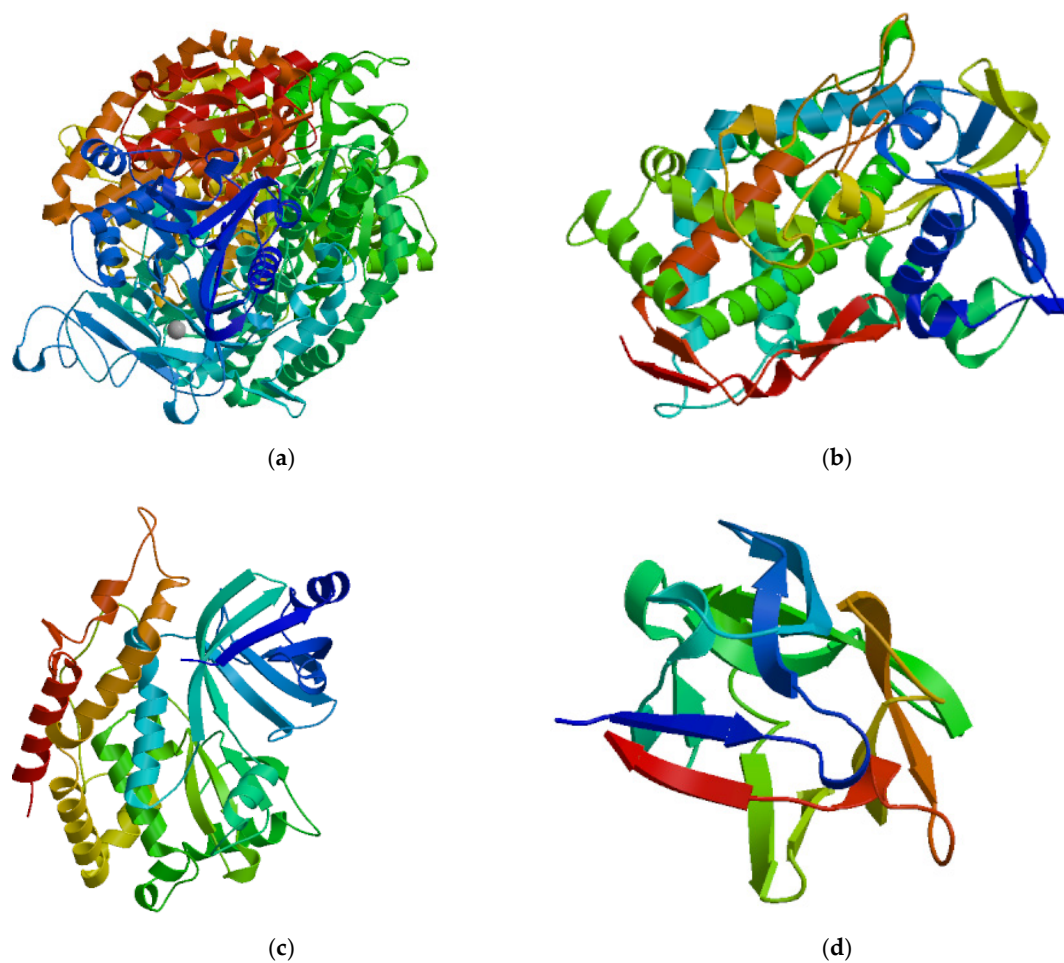
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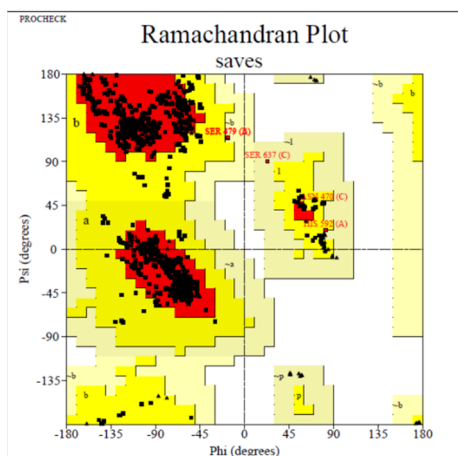
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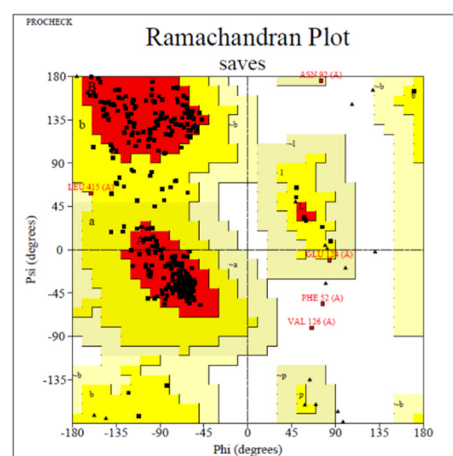
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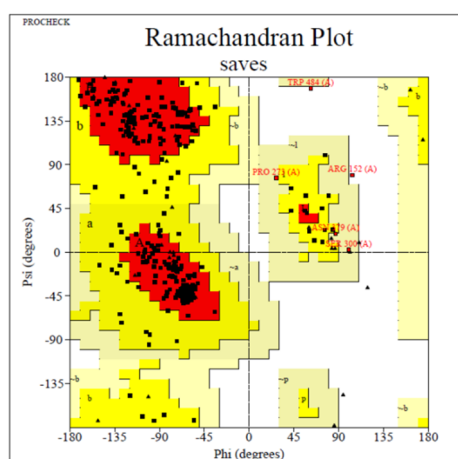
**Figure S1.** Structures of the modelled proteins (a) glutamine-fructose-6-phosphate transaminase, (b) 14- $\alpha$  sterol demethylase B, (c) invasin CotH3, (d) mucorin.



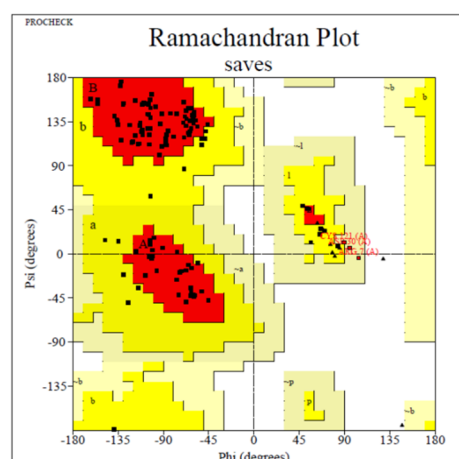
(a)



(b)



(c)



(d)

**Figure S2.** The Ramachandran's plots (PROCHECK) of the modelled proteins (a) glutamine-fructose-6-phosphate transaminase, (b) 14- $\alpha$  sterol demethylase B, (c) invasin Coth3, (d) mucorin.

**Table S1.** The estimated target-template alignment / predicted model quality indices.

|  | GFAT            | 14- $\alpha$ sterol<br>demethylase B | Invasin CotH3   | Mucorinic       |
|--|-----------------|--------------------------------------|-----------------|-----------------|
| SWISSPROT                              |                 |                                      |                 |                 |
| Template                               | 6r4g.1.A        | 4uhl.1.A                             | 5jd9.1.A        | 3pg0.1.A        |
| Sequence Identity (%)                  | 59.88           | 47.15                                | 19.92           | 32.09           |
| Coverage                               | 0.98            | 0.86                                 | 0.91            | 0.97            |
| Sequence Similarity                    | 0.48            | 0.43                                 | 0.31            | 0.37            |
| GMQE                                   | 0.83            | 0.67                                 | 0.59            | 0.68            |
| QMEANDisCo Global                      | 0.80 $\pm$ 0.05 | 0.70 $\pm$ 0.05                      | 0.56 $\pm$ 0.05 | 0.68 $\pm$ 0.07 |
| ERRAT                                  |                 |                                      |                 |                 |
| Overall Quality Factor                 | 95.02           | 92.31                                | 86.13           | 87.12           |
| PROCHECK                               |                 |                                      |                 |                 |
| Residues in Most Favoured Regions      | 91.70%          | 89.60%                               | 84.30%          | 82.50%          |
| Residues in Additional Allowed Regions | 7.90%           | 9.20%                                | 14.60%          | 15.10%          |
| Residues in Generously Allowed Regions | 0.40%           | 0.70%                                | 0.60%           | 2.40%           |
| Residues in Disallowed Regions         | 0.00%           | 0.50%                                | 0.60%           | 0.00%           |

Abbreviations: GFAT - glutamine-fructose-6-phosphate transaminase, GMQE - Global Model Quality Estimate