

Dihydroquercetin in Obesity and Prediabetes: Case Report and Insights from Molecular Modeling

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Supplementary Materials

Table S1. Results of redocking and DHQ docking of unselected biological targets.

Biological target		Results of redocking		Affinity of DHQ stereoisomers, kcal/mol			
Name	PDB ID	Affinity, kcal/mol	RMSD	2R,3R	2S,3S	2S,3R	2R,3S
DYRK1A	6LN1	−6.154	2.342	−1.583	−3.241	−3.385	−3.186
PTP1B	1XBO	−5.080	3.323	−3.280	−3.241	−2.321	−3.301
SUR1	6JB3	−6.848	6.722	−6.595	−6.727	−6.775	−6.743
Glucokinase	3VF6	−7.351	5.104	−6.411	−6.004	−5.915	−6.173