

SUPPLEMENT

Ershov P.V., Yablokov E.O., Kaluzhskiy L.A., Mezentsev Yu.V., Gnedenko O.V., Konstantinov M.A., Toropygin I.Yu., Ivanov A.S. (2025) Glycyrrhizic acid: novel potential protein targets. Biomeditsinskaya Khimiya, 71(4), 270-282.

DOI: 10.18097/PBMCR1595

Table S1. Visualization of hydrogen and hydrophobic bonds between amino acid residues of the protein and chemical groups of glycyrrhizic acid.

Protein*	Amino acid residues of protein interacting with glycyrrhizic acid	Basic model parameters
Acox2	<p>ACOX2_RAT_P97562_prepared Glycyrrhizic acid_D (8)</p>	Rank score: -7,83109 dG (ккал/моль): -11,35330
Acr1c9	<p>1AFS_P Glycyrrhizic acid_D</p>	Rank score: -9,31565 dG (ккал/моль): -12,35497

Maoa	1O5W_P Glycyrrhizin_D_dimer	<p>Rank score: - 7,51663 dG (ккал/моль): - 10,68945</p>
Mat1a	P13444_METK1_RAT_1QM4_prepared Glycyrrhizic acid_D (1)	<p>Rank score: - 8,69516 dG (ккал/моль): - 12,13821</p>
Nalcn	7CU3_P glycyrrhizic acid_D	<p>Rank score: - 8,72160 dG (ккал/моль): - 13,76953</p>

* Acox2, peroxisomal acyl-coenzyme A oxidase 2; Akr1c9, 3-alpha-hydroxysteroid dehydrogenase; Maoa, monoamine oxidase A [flavin-containing]; Mat1a, S-adenosylmethionine synthase isoform type-1; Nalcn, sodium leak channel non-selective protein