Supplementary material

Exploring the interaction between *Salvia miltiorrhiza* and α-glucosidase: Insights from computational analysis and experimental studies

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Outline of the Supplementary material

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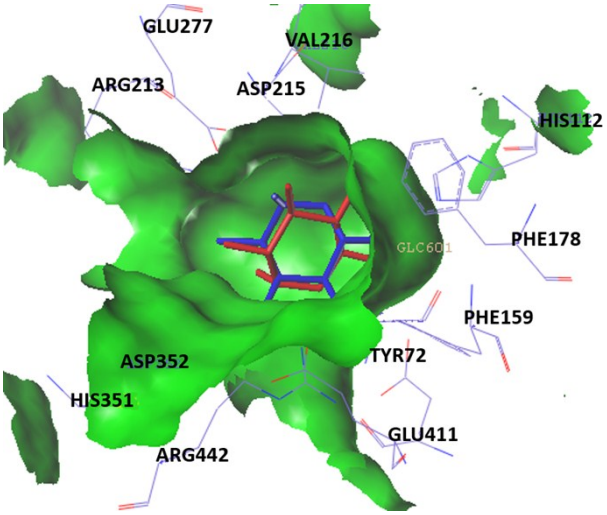

Fig. S1 Re-docking results of the original ligand α-D-glucose binding to α-glucosidase. Key residues are shown as stick models, and hydrogen bonds are labeled as yellow dashed lines. The cognate ligand appears in blue and the re-docking structure is colored in red.

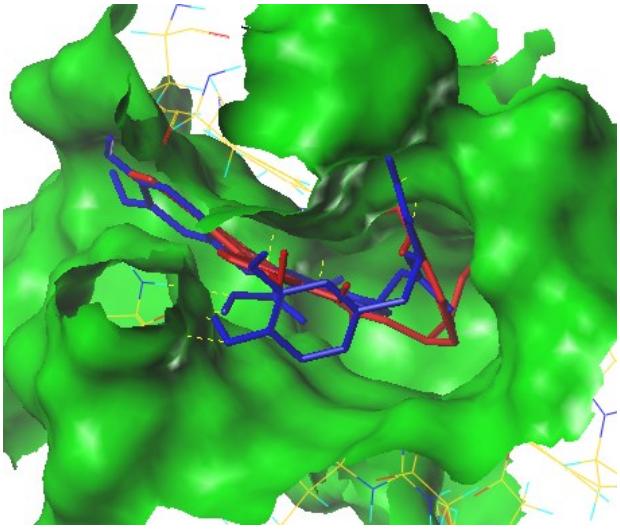

Fig. S2 View of superimposed docking conformations for the molecules binding to the active pocket of α-glucosidase. Key residues are shown as stick models, and hydrogen bonds are labeled as yellow dashed lines. Compounds SAC and LA are colored as red and blue, respectively.

Table S1 The list of chemicals identified in *Salvia miltiorrhiza* and their docking scores when binding to the active site of XO.

No.	Compound name	Total score	Crash	Polar	Similarity	Cscore
107	Voglibose	9.2304	-1.8504	7.0369	0.733	4
101	Salvianolic acid A methyl ester	8.9762	-3.4979	4.7451	0.508	4
104	Miglitol	8.9406	-3.946	5.6308	0.724	3
61	Salviaflaside	8.256	-2.3649	7.5879	0.674	4
16	Danshenxinkun D	8.2025	-2.908	1.5773	0.576	5
39	Salvianolic acid A	8.0625	-4.8119	5.2313	0.461	5
6	Ailanthoidol	7.9983	-2.6038	1.7588	0.558	5
7	Ammonium-potassium lithospermate B	7.9471	-4.9875	5.2545	0.411	2
73	Salvinal	7.944	-1.849	1.1792	0.501	3
66	Salvianolic acid C	7.781	-1.3509	3.6274	0.416	2
21	Dimethyl lithospermate	7.7762	-2.4858	3.3555	0.306	1
54	Prolithospermic acid	7.5764	-1.602	4.1771	0.479	5
62	Salvianan	7.5739	-1.5589	0.0009	0.415	5
36	Lithospermic acid	7.4909	-4.7748	5.1816	0.385	3
38	Methyl rosmarinate	7.3039	-1.4381	4.4873	0.496	3
48	Monomethyl lithospermate	7.2932	-2.3384	5.1734	0.611	3
24	Ethyl lithospermate	7.2234	-3.2101	2.6722	0.309	1
67	Salvianolic acid D	7.0714	-1.6177	4.2302	0.563	2
108	DNJ	7.0843	-1.5381	7.2341	0.4472	3
98	Curcumin	7.0368	-3.3968	4.1913	0.485	5
98	Lithospermic acid dimethyl ester	6.9227	-2.5488	3.8819	0.576	2
105	Quercetin	6.9021	-0.5736	4.3644	0.495	2
63	Salvianen	6.7496	-1.6808	0.0019	0.419	5
69	Salvianolic acid F	6.7124	-1.0378	2.5665	0.518	4
71	Salvianolic acid I	6.7064	-1.9836	6.8996	0.545	4
75	Sibiriquinone A	6.6425	-1.3782	0.0001	0.442	4
82	Tanshindiol C	6.5428	-1.6438	3.2699	0.567	4
106	Resveratrol	6.5283	-0.8755	3.9377	0.552	4
88	Tanshinone IIB	6.4413	-3.2199	1.8774	0.465	5
31	Isosalvianolic acid C	6.3885	-1.2262	3.9306	0.566	2
2	1,2-Didehydromiltirone	6.3201	-4.7113	0.1113	0.442	5
11	Cryptoacetalide	6.1736	-1.2694	0	0.427	5
100	Salvianic acid A methyl ester	6.1606	-0.877	3.6551	0.519	5
43	Miltiodiol	6.1311	-2.1751	1.434	0.424	3
103	Acarbose	5.9797	-1.6866	2.5186	0.575	5
90	Trijuganone A	5.9083	-3.032	1.8776	0.256	4
85	Tanshinol B	5.8389	-0.9408	1.1286	0.552	4
80	Tanshindiol A	5.8366	-1.101	1.0835	0.576	2
72	Salvianolic acid J	5.7766	-2.2593	2.9293	0.566	3
96	16-Formyloxydanshenxinkun A	5.7497	-1.4903	1.1084	0.419	3

81	Tanshindiol B	5.7423	-1.2897	2.1997	0.503	4
52	Nor-salvioxide	5.7076	-0.9472	0.9102	0.39	3
19	Dihydroisotanshinone II	5.6842	-1.3973	0.9662	0.389	5
10	Carnosol	5.6734	-3.5497	2.6861	0.492	4
60	Rosmarinic acid	5.6697	-2.1794	5.2282	0.453	3
58	Przewaquinone B	5.6638	-0.4572	1.3714	0.495	3
23	Epidanshenspiroketallactone	5.6557	-2.5258	0.1439	0.138	4
14	Danshenxinkun B	5.6346	-1.9321	1.431	0.472	3
5	15,16-Dihydrotanshinone I	5.6313	-2.6326	3.1371	0.538	3
3	1,2-Dihydrotanshinone I	5.6035	-1.6549	0.958	0.322	5
32	Isotanshinone I	5.5694	-0.3056	0.0147	0.393	4
59	Przewaquinone C	5.5014	-1.6211	1.9732	0.526	5
13	Danshenxinkun A	5.4955	-1.571	2.4696	0.55	4
57	Przewaquinone A	5.4724	-1.4571	0.1178	0.454	4
15	Danshenxinkun C	5.46	-1.5292	2.4481	0.224	4
102	Salvianolic acid C methyl ester	5.4299	-1.5386	4.0003	0.394	4
64	Salvianic acid A (danshensu)	5.3959	-0.7189	4.845	0.649	4
34	Isotanshinone IIB	5.373	-2.1601	0.8953	0.218	3
76	Sibiriquinone B	5.3441	-2.545	0.0001	0.446	4
79	Tanshinaldehyde	5.327	-2.9892	0.7836	0.395	5
94	3-Hydroxymethylenetanshinquinone	5.3007	-1.8257	2.124	0.291	4
26	Formyltanshinone	5.2819	-1.6515	0.9186	0.393	4
84	Tanshinol A	5.2725	-0.4297	1.2488	0.542	4
18	Dihydroisotanshinone I	5.2523	-2.6567	0.8773	0.203	4
87	Tanshinone IIA	5.2427	-2.0109	0.259	0.385	4
41	Methylene tanshinquinone	5.151	-0.7186	0.0118	0.409	3
30	Isoimperatorin	5.0987	-1.3398	0.9851	0.36	3
91	Trijuganone B	5.0285	-0.2997	0.0009	0.412	4
95	Tetrahydrotanshinone	5.0285	-0.2997	0.0009	0.412	4
8	Baicalin	5.0011	-3.073	5.9734	0.66	4
27	Hydroxytanshinone IIA	4.9756	-2.0615	0.3938	0.393	5
25	Ferruginol	4.8877	-4.4314	1.3545	0.465	4
49	Neocryptotanshinone	4.8806	-2.8158	0.9913	0.453	3
29	Isoferulic acid	4.8188	-0.4525	2.3006	0.488	3
9	Caffeic acid	4.8035	-0.4582	4.9008	0.447	3
20	Dihydrotanshinone I	4.8021	-3.5857	1.1615	0.217	5
74	Salviolone	4.7673	-1.8622	0.0055	0.367	4
78	Sugiol	4.7634	-3.7825	1.4158	0.467	4
83	Tanshinlactone	4.703	-0.4827	0	0.392	4
33	Isotanshinone IIA	4.701	-3.5621	0.0228	0.402	5
70	Salvianolic acid G	4.4879	-0.9263	1.0917	0.649	4
1	1,2,5,6-Tetrahydrotanshinone I	4.397	-0.6718	0.0016	0.418	5
51	Neosalvianen	4.316	-2.7495	0.0305	0.335	4
12	Cryptotanshinone	4.283	-3.0168	0.0895	0.44	4

56	Protocatechuic aldehyde	4.1276	-0.1525	3.5784	0.489	4
86	Tanshinone I	4.1219	-2.6882	1.2504	0.188	4
68	Salvianolic acid E	4.0632	-8.2318	6.0663	0.381	2
44	Miltionone I	4.0115	-1.8124	0.0003	0.412	1
55	Protocatechuic acid	4.0066	-0.4866	3.7967	0.715	5
22	Epicryptoacetalide	3.9486	-2.6758	0.001	0.206	5
45	Miltionone II	3.9373	-3.2175	0.0862	0.429	5
42	Methylenedihydrotan-shinquinone	3.7928	-2.0524	0	0.375	5
47	Miltirone	3.7842	-2.975	0	0.362	1
53	Nortanshinone	3.7414	-1.6023	0.0385	0.466	5
28	Isocryptotanshinone	3.3603	-4.2606	1.0126	0.399	5
97	Isosalvianolic acid C methyl ester	3.0371	-8.0513	1.0158	0.562	4
4	1-Ketoisocryptotanshinone	2.9538	-1.8968	0	0.443	5
77	Stigmasterol	2.725	-6.6141	0.9919	0.361	2
17	Daucosterol	2.6813	-8.1387	4.2069	0.644	4
50	Neo-przewaquinone A	2.4038	-1.1388	0.009	0.173	2
46	Miltipolone	1.6387	-4.0017	1.3989	0.167	2
40	Methyl tanshinonate	1.6309	-2.2041	0.0278	0.174	1
93	β-Sitosterol	0.036	-8.9396	1.1385	0.358	2
35	Lithospermate B	-0.214	-11.2344	2.1619	0.423	2
89	Tigogenin	-0.8191	-8.5743	0.5828	0.308	1
65	Salvianolic acid B	-2.7032	-11.6938	2.7613	0.458	2
92	Ursolic acid	-5.6972	-16.1459	0.5263	0.298	1
37	Magnesium lithospermate B	-95.3961	-100.6939	0.4175	0.547	2