

1 Article

2 Investigation on the enzymatic profile of mulberry 3 alkaloids by enzymatic study and molecular docking

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19 **Table S1.** The docking scores of the small compounds with HPA based on the consensus score function

Name	1-DNJ	DAB	FA	acarbose	miglitol
LigScore1	0.97	3.28	2.01	5.54	2.51
LigScore2	2.72	4.01	3.61	6.17	3.79
PLP1 (-)	-8.59	33.97	12.67	111.96	39.16
PLP2 (-)	0.44	26.86	14.08	90.63	29.9
Jain	-1.38	-0.50	0.64	1.97	-0.88
PMF (-)	87.00	95.57	81.95	255.24	108.46
PMF04 (-)	55.15	66.12	57.78	184.30	73.03
Surflex_score (-)	5.91	4.59	3.80	12.89	4.81
Glide_score (-)	4.21	4.01	4.12	7.81	3.96
D_score (-)	91.53	82.14	79.27	236.36	91.32
G_score (-)	166.82	114.49	103.48	373.11	209.9
Chemscore (-)	9.92	10.91	10.76	1.96	3.19

20 **Table S2.** The docking scores of the small compounds with NtSI based on the consensus score function

Name	1-DNJ	DAB	FA	acarbose	miglitol
LigScore1	4.07	4.14	1.27	4.22	4.35
LigScore2	3.46	3.92	3.57	4.20	3.89
PLP1 (-)	43.84	24.92	21.50	43.93	22.98
PLP2 (-)	54.69	22.91	29.88	47.90	28.36
Jain	2.12	-0.25	-0.46	0.92	0.67
PMF (-)	150.38	117.87	128.52	76.46	153.88

PMF04 (-)	99.88	95.81	88.76	74.83	124.19
Surflex_score (-)	5.63	6.68	5.21	4.51	3.74
Glide_score (-)	5.79	5.52	5.07	4.50	4.74
D_score (-)	124.47	126.81	102.47	137.78	186.63
G_score (-)	158.96	216.12	176.39	218.56	195.31
Chemscore (-)	25.41	22.73	25.57	13.36	17.56

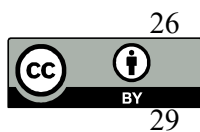
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22**Table S3.** The docking scores of the small compounds with NtMGAM based on the consensus score function

Name	1-DNJ	DAB	FA	acarbose	miglitol
LigScore1	6.34	3.88	3.78	5.06	5.26
LigScore2	5.77	4.29	4.67	4.22	5.05
PLP1 (-)	87.36	43.05	59.42	76.55	73.77
PLP2 (-)	82.44	49.05	66.83	82.48	79.96
Jain	7.07	3.88	5.15	1.54	4.70
PMF (-)	216.77	122.69	133.49	189.19	181.70
PMF04 (-)	162.02	79.41	88.82	151.09	124.81
Surflex_score (-)	8.34	6.20	6.62	2.62	7.57
Glide_score (-)	6.83	5.03	5.92	3.44	6.34
D_score (-)	103.40	78.95	97.88	140.40	118.45
G_score (-)	159.21	130.84	132.87	165.96	188.16
Chemscore (-)	3.28	4.24	5.78	-3.84	1.29

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24**Table S4.** The docking scores of the small compounds with CtMGAM based on the consensus score function

Name	1-DNJ	DAB	FA	acarbose	miglitol
LigScore1	5.35	3.83	4.77	6.25	5.51
LigScore2	5.43	4.51	4.48	6.56	5.11
PLP1 (-)	69.08	44.11	43.58	103.28	65.07
PLP2 (-)	79.15	47.92	53.08	91.38	73.52
Jain	6.68	2.32	3.38	2.85	6.91
PMF (-)	155.25	124.66	129.64	270.66	167.16
PMF04 (-)	103.07	78.60	79.04	201.80	112.31
Surflex_score (-)	7.82	6.55	5.74	12.05	5.92
Glide_score (-)	6.53	5.61	5.60	7.31	6.09
D_score (-)	112.50	90.42	99.30	232.24	122.12
G_score (-)	146.63	116.41	216.10	351.48	201.89
Chemscore (-)	6.10	8.90	5.20	-3.20	3.24

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