

Supplementary files

Table S1. Cluster analysis of the SnocOBP7-ligand complexes based on the MD simulations trajectories.

System	Cluster	Number of frames	Occurrence (%)
S1	1	115	38.21
	2	78	25.91
	3	45	14.95
	4	26	8.64
	5	17	5.65
	6	10	3.32
	7	6	1.99
	8	3	1.00
	9	1	0.33
S2	1	119	39.53
	2	74	24.58
	3	44	14.62
	4	27	8.97
	5	19	6.31
	6	10	3.32
	7	6	1.99
	8	2	0.66
S10	1	199	66.11
	2	60	19.93
	3	26	8.64
	4	13	4.32
	5	3	1.00

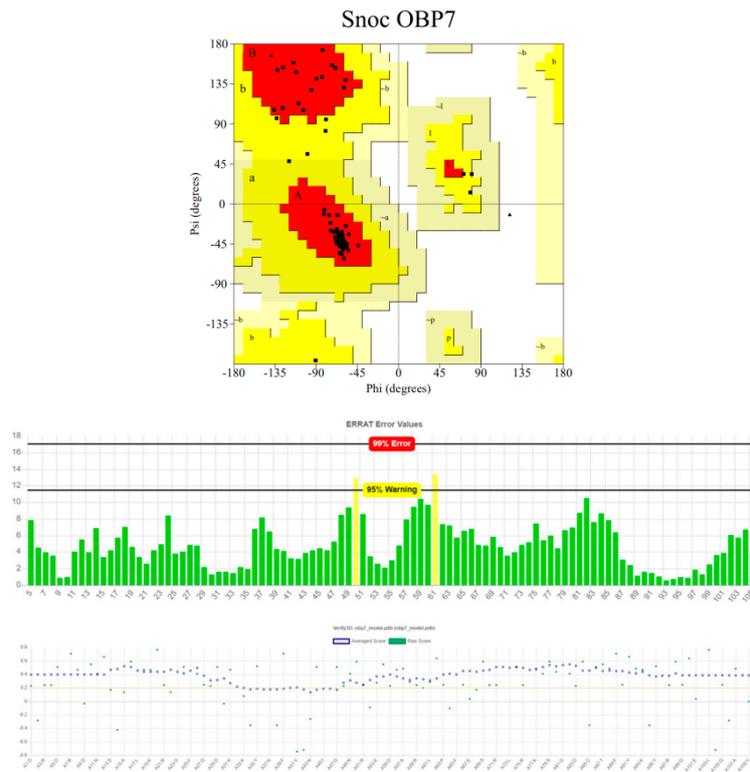


Figure S1. Ramachandran plot, ERRAT and Verify_3D result of SnocOBP7 model. (A): Ramachandran plot; (B): ERRAT; (C): Verify_3D.

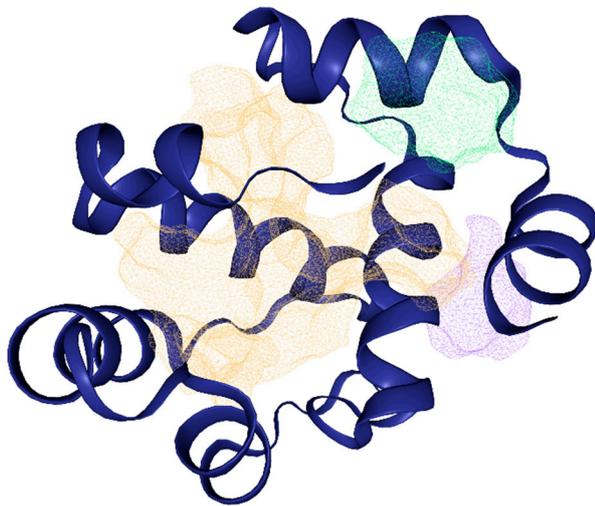


Figure S2. Predicted binding pocket of SnocOBP7.

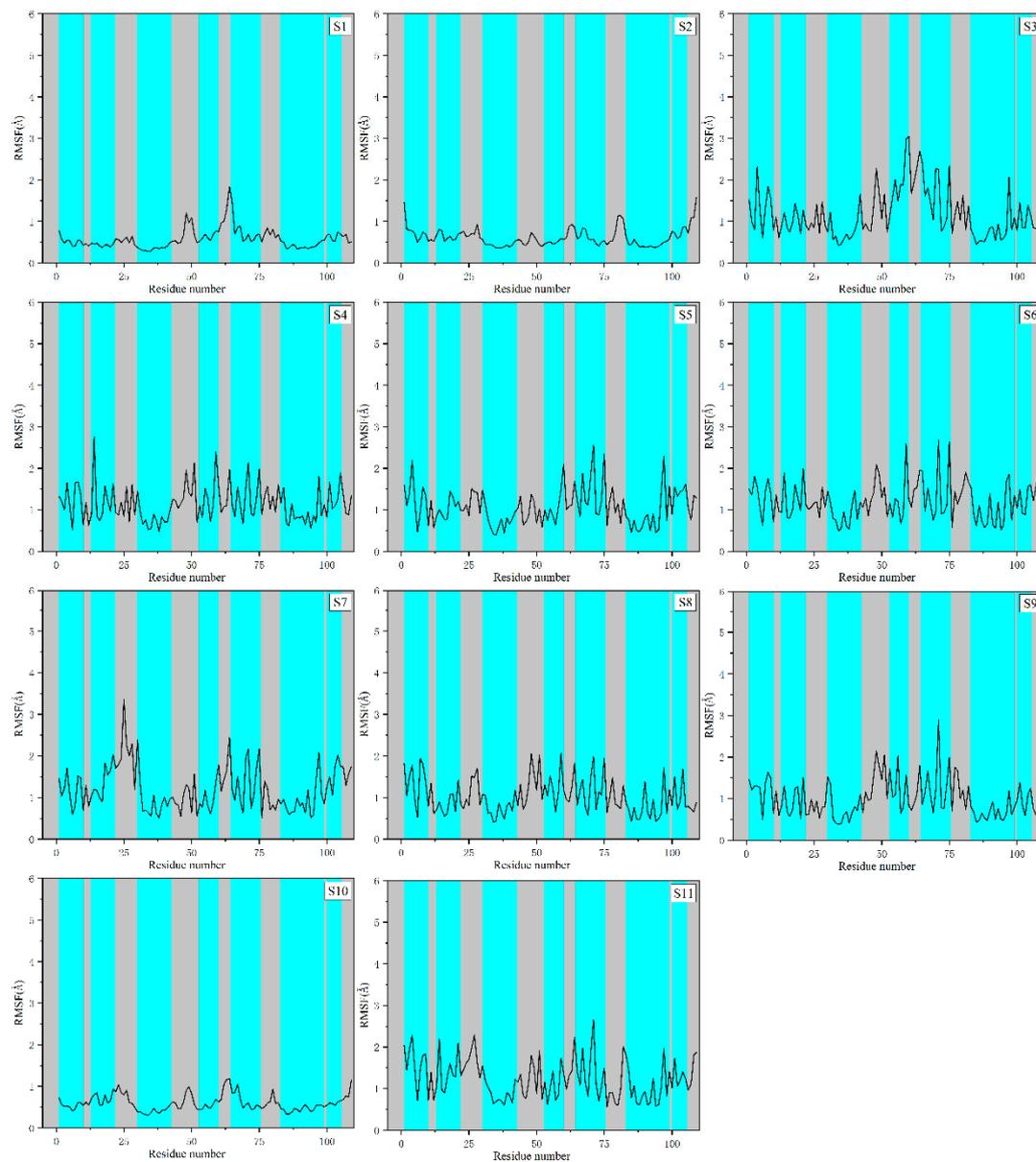


Figure S3. The root-mean-square fluctuation (RMSF) curve of the 11 systems. The secondary structure of the initial conformation of SnocOBP7 was calculated by DSSP. The background color determines the different structure types: the gray area represents the loop, and the blue represents the alpha helix. Refer to Table 1 for system specific information.