Supplementary Materials

A Molecular Investigation of the Solvent Influence on Inter- and Intra-molecular Hydrogen Bond Interaction of Linamarin

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Table S1. Table summarizes the number of solvents molecules and the size of PBC box.

Solution system	Solvents	Linamarin	Total number	Box size (nm^3)
DCM &LINAMARIN	191	1	192	24.1724
WATER(TIP4P) & LINAMARIN	779	1	780	24.1724
DMSO & LINAMARIN	210	1	211	24.1724
MeOH	316	1	317	24.1724

Table S2. Summary of free energy contribution from each solvent.

	DCM	DMSO	methanol	water
State	ΔG_{solv}	ΔG_{solv}	ΔG_{solv}	ΔG_{solv}
0	0	0	0	0
1	1.499	1.907	1.778	1.919
2	3.292	5.242	4.446	7.839
3	2.798	6.53	4.586	13.201
4	1.037	5.861	3.486	14.697
5	-1.415	3.807	1.757	14.313
6	-4.258	0.845	-0.377	13.028
7	-7.355	-2.629	-2.794	11.27
8	-10.632	-6.428	-5.423	9.218
9	-14.045	-10.445	-8.209	6.964
10	-17.566	-14.626	-11.113	4.566
11	-19.32	-18.758	-14.255	-0.998
12	-21.001	-23.278	-17.965	-8.213
13	-22.682	-28.152	-22.664	-17.252
14	-24.318	-33.299	-28.869	-27.957

Coulomb:	-6.752	-18.673	-17.756	-32.523
vdWaals:	-17.566	-14.626	-11.113	4.566
TOTAL:	-24.318	-33.299	-28.869	-27.957