Supplementary materials

3D-QSAR, molecular docking, and molecular dynamics simulation study of thieno[3,2-b]pyrrole-5- carboxamide derivatives as LSD1 inhibitors

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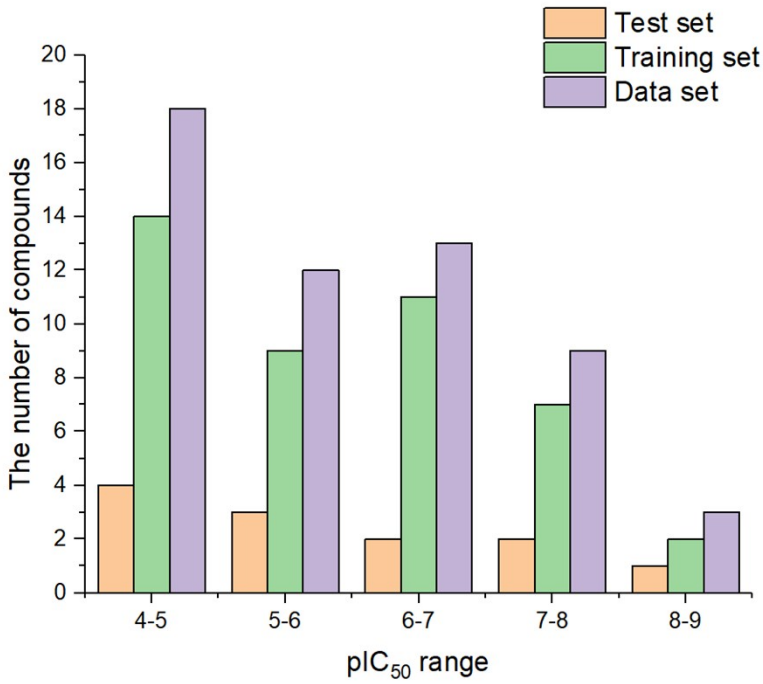

Fig. S1. 3D-QSAR Histogram of activity data distribution

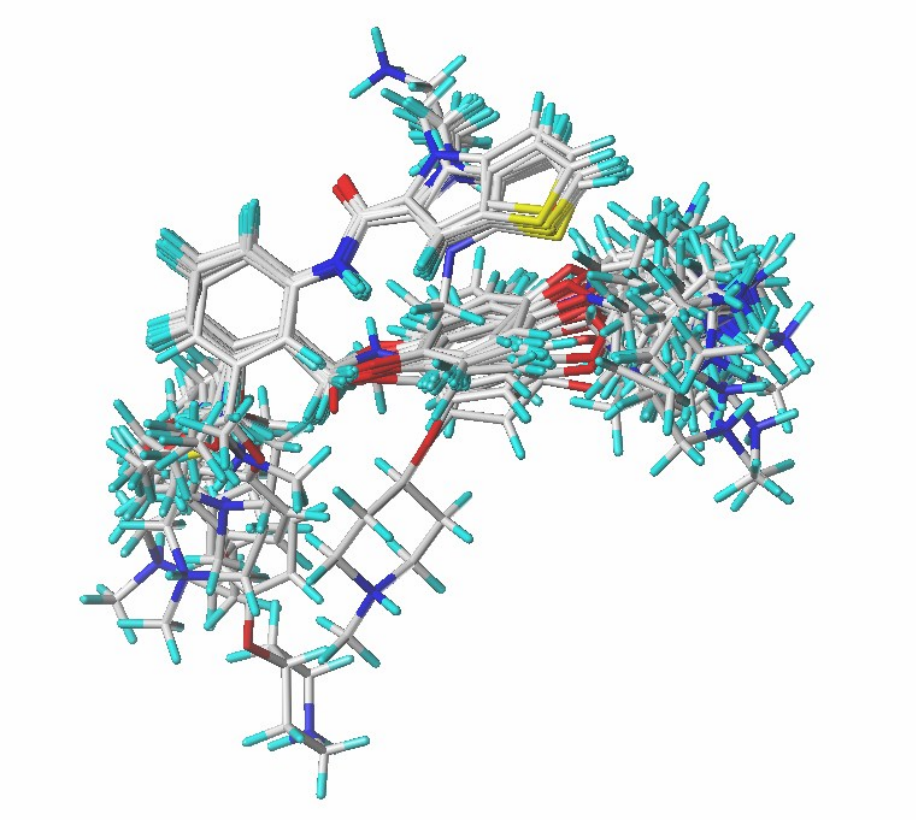

Fig S2. Docking-based alignment of training set compounds.

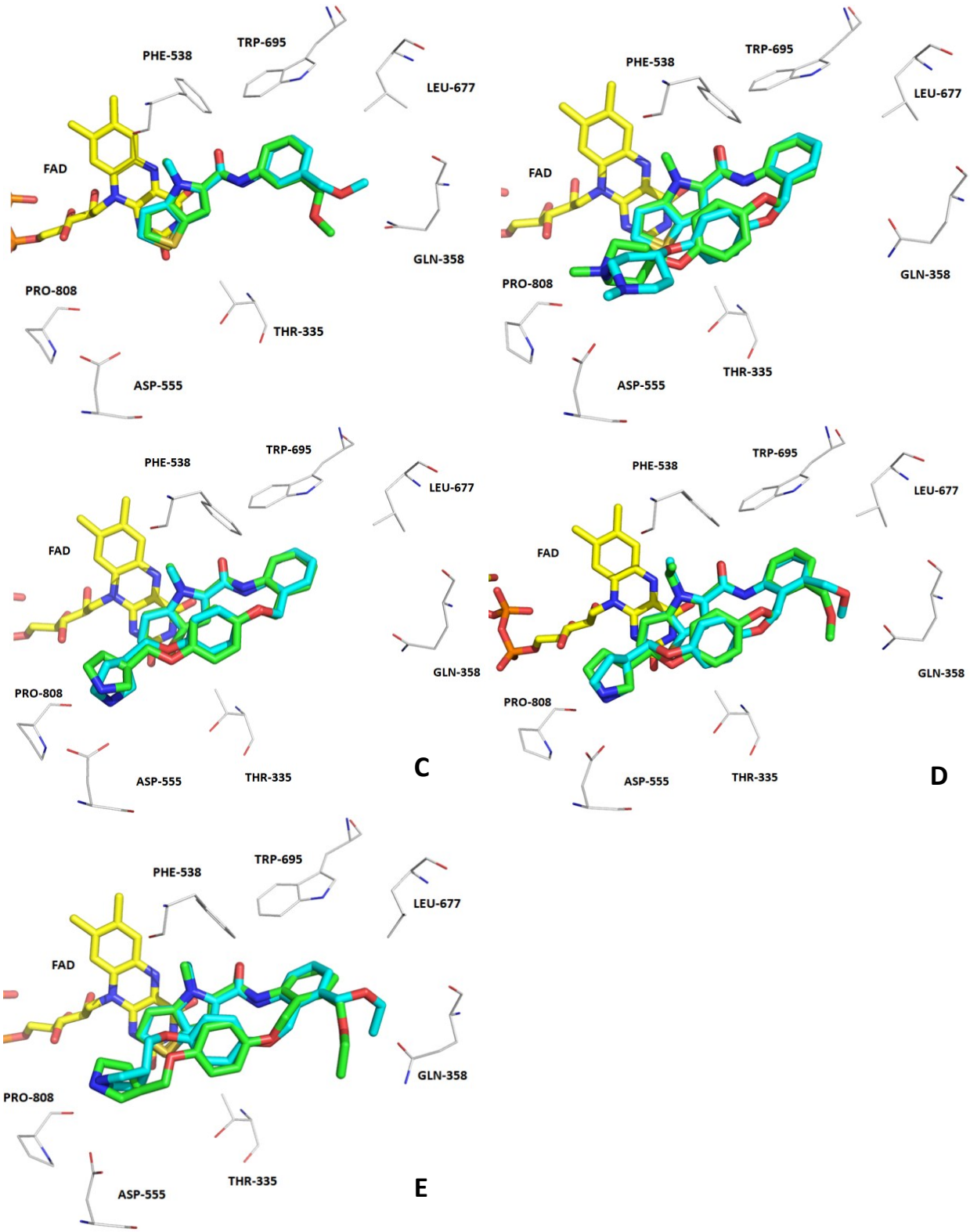

Fig. S3. Figures A, B, C, D, and E show the superposition of the crystal pose of the compounds (green) (PDB: 5LGN, 5LGT, 5LGU, 5LHH, 5LHI), and the docked pose of the compounds (cyan), respectively, and the FAD as a reference for orientation is shown in yellow.

Table S1 Randomizations of biological activity for the Y-random test.

Random_1	Random_2	Random_3	Random_4	Random_5	Random_6	Random_7	Random_8	Random_9	Random_10
4.873	6.346	4.166	5.538	6.171	8.108	4.318	8.174	8.174	4.728
4.777	6.209	6.752	7.745	6.095	8.174	4.599	8.108	7.194	4.873
4.599	6.171	5.538	5.886	5.886	7.194	4.281	7.745	4.166	6.171
4.281	8.174	7.745	7.252	8.108	4.166	4.166	7.194	4.777	7.187
7.535	4.529	7.194	7.187	7.745	4.281	7.194	6.79	4.411	5.131
7.067	5.658	5.027	7.18	7.194	4.599	8.174	6.752	4.048	4.599
8.174	5.131	6.355	7.535	4.728	4.318	8.108	6.509	5.032	4.318
8.108	4.873	4.728	7.067	7.535	5.032	5.131	6.355	4.318	5.032
5.602	4.777	8.108	5.131	7.067	4.048	4.873	5.824	4.599	4.048
5.131	4.599	6.209	4.873	5.658	4.411	4.728	5.658	4.281	4.411
5.658	4.281	6.171	7.194	8.174	4.777	4.668	5.602	8.108	4.777
6.509	5.027	6.095	6.917	5.602	4.654	4.654	5.538	4.654	4.654
4.166	5.602	5.886	6.827	5.538	4.668	4.777	5.131	4.668	6.346
6.752	5.538	7.187	6.68	6.917	4.728	4.411	5.032	4.728	6.68
5.824	7.745	5.658	6.346	7.252	4.873	4.048	5.027	4.873	6.827
5.886	7.18	5.602	6.209	7.187	5.131	5.032	4.873	5.131	6.917
7.252	7.535	6.346	8.174	6.209	5.658	6.752	4.777	5.658	4.668
7.187	7.067	4.048	6.171	6.827	4.529	5.824	4.728	4.529	6.752
6.917	4.318	5.032	6.095	6.68	4.577	5.658	4.668	4.577	6.209
6.827	4.728	4.318	8.108	6.346	6.509	5.602	4.654	6.509	8.108
6.68	4.668	7.18	4.281	5.658	6.355	5.538	4.599	6.68	8.174
6.346	8.108	7.535	4.411	5.131	6.79	7.745	4.577	6.346	7.194
6.209	6.095	7.067	4.048	4.281	4.046	5.027	4.529	6.209	4.166
7.18	5.886	8.174	5.032	5.032	5.027	4.046	4.411	6.752	4.281
7.194	7.252	6.917	5.027	4.318	7.745	6.79	4.318	5.824	7.067

4.529	7.187	4.529	4.166	7.18	5.538	6.355	7.535	5.658	5.886
6.171	4.046	5.658	4.577	5.027	5.602	6.509	7.252	5.602	6.095
6.095	6.79	5.131	6.509	4.411	5.658	4.577	7.187	5.538	7.252
4.411	6.355	6.509	4.046	4.048	5.824	4.529	7.18	7.745	7.535
4.048	6.509	4.046	4.318	6.79	6.752	5.658	7.067	5.027	7.18
5.032	7.194	4.411	5.658	4.668	6.209	7.18	6.917	4.046	5.658
4.318	5.824	4.281	5.602	4.654	6.346	7.535	6.827	6.79	4.529
4.728	5.658	5.824	6.79	4.577	6.68	7.252	6.68	6.355	4.577
4.046	6.752	6.79	6.355	4.529	6.827	7.187	6.346	6.827	6.509
6.79	6.917	4.577	6.752	4.046	6.917	6.171	6.209	6.917	6.355
6.355	6.827	4.873	5.824	4.166	7.067	6.095	6.171	7.067	6.79
5.538	6.68	4.777	4.728	6.752	5.886	5.886	6.095	5.886	4.046
7.745	5.032	4.599	4.668	4.873	6.095	7.067	5.886	6.095	5.027
5.658	4.654	7.252	4.654	6.355	6.171	6.917	5.658	6.171	7.745
5.027	4.577	6.827	4.777	6.509	7.187	6.827	4.281	7.187	5.538
4.668	4.411	6.68	4.529	4.777	7.252	6.68	4.166	7.252	5.602
4.654	4.048	4.668	5.658	4.599	7.535	6.346	4.048	7.535	5.658
4.577	4.166	4.654	4.599	5.824	7.18	6.209	4.046	7.18	5.824

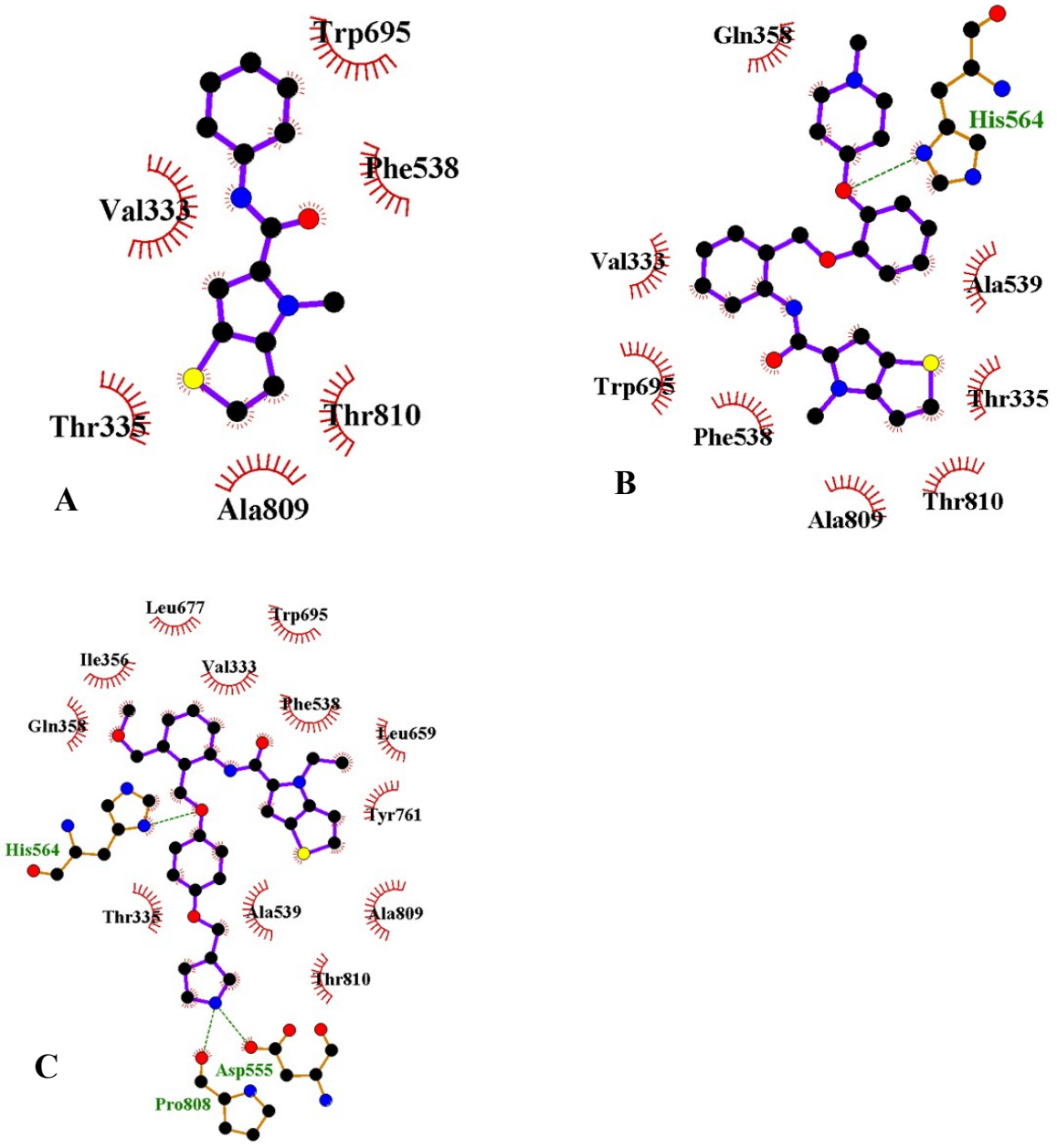

Fig. S4. 2D diagram of compounds **1** (A), **28** (B) and **54** (C). Purple solid line represents ligand bond. Brown solid line means non-ligand bond. Green dashed line is hydrogen bond. The red spoke arc represents residues with hydrophobic interaction with ligand. Carbon atoms, oxygen atoms, nitrogen atoms and sulfur atoms are shown in black, red, blue and yellow respectively.

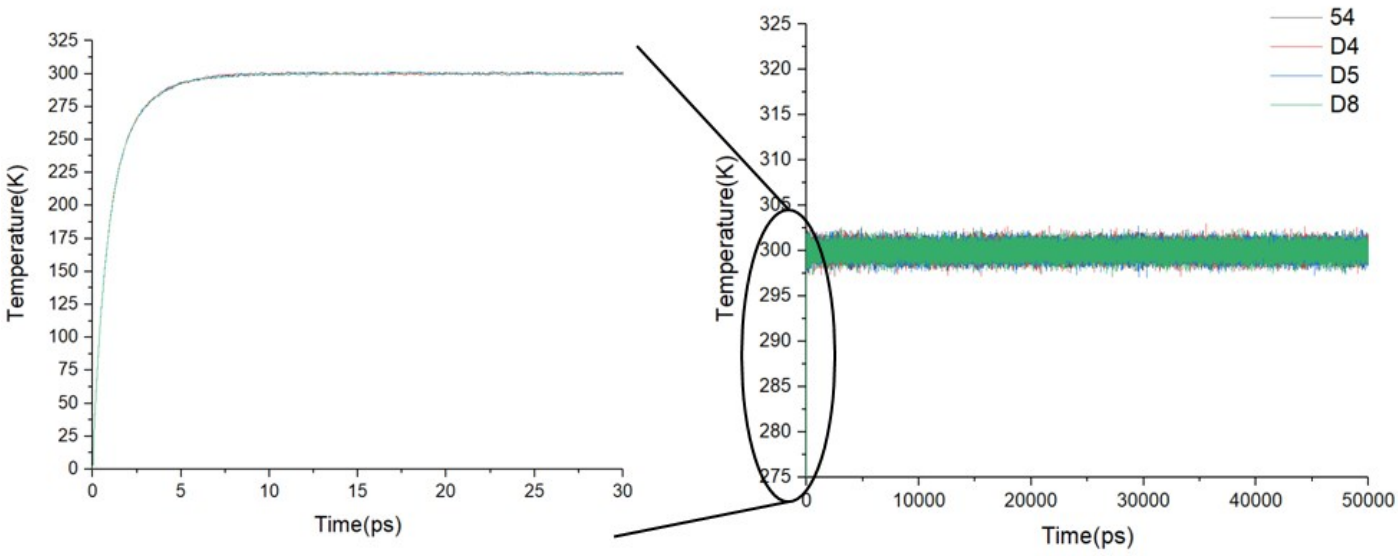

Fig. S5. Temperature fluctuation plot in MD.

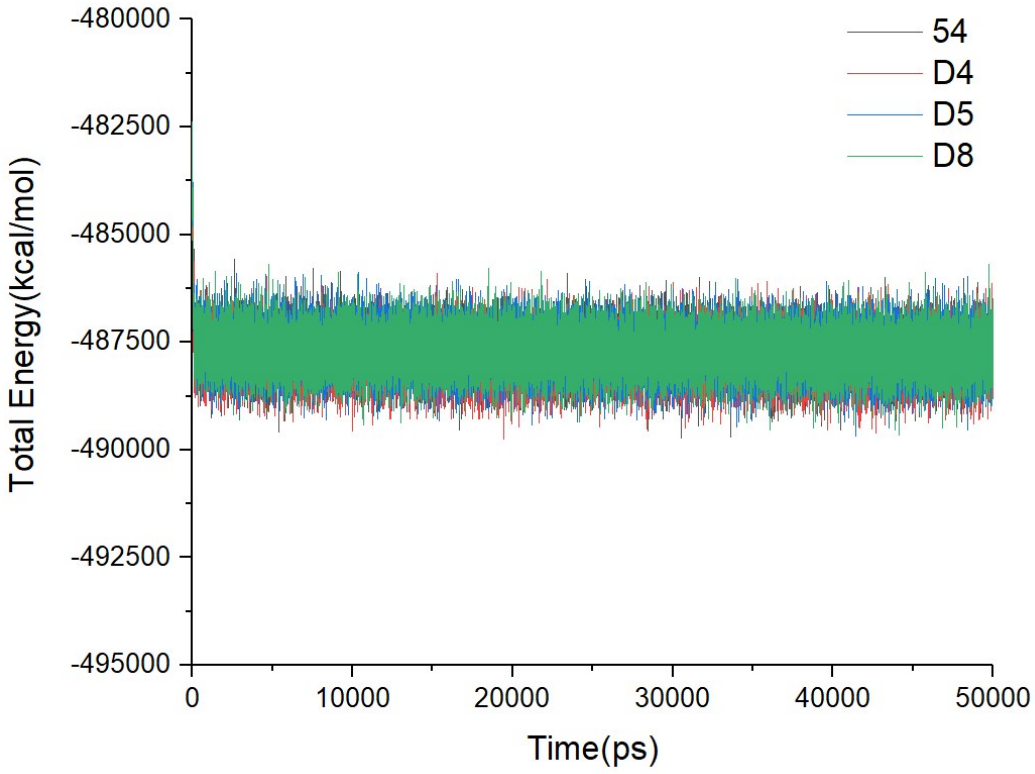

Fig. S6. Total energy fluctuation plot in MD.

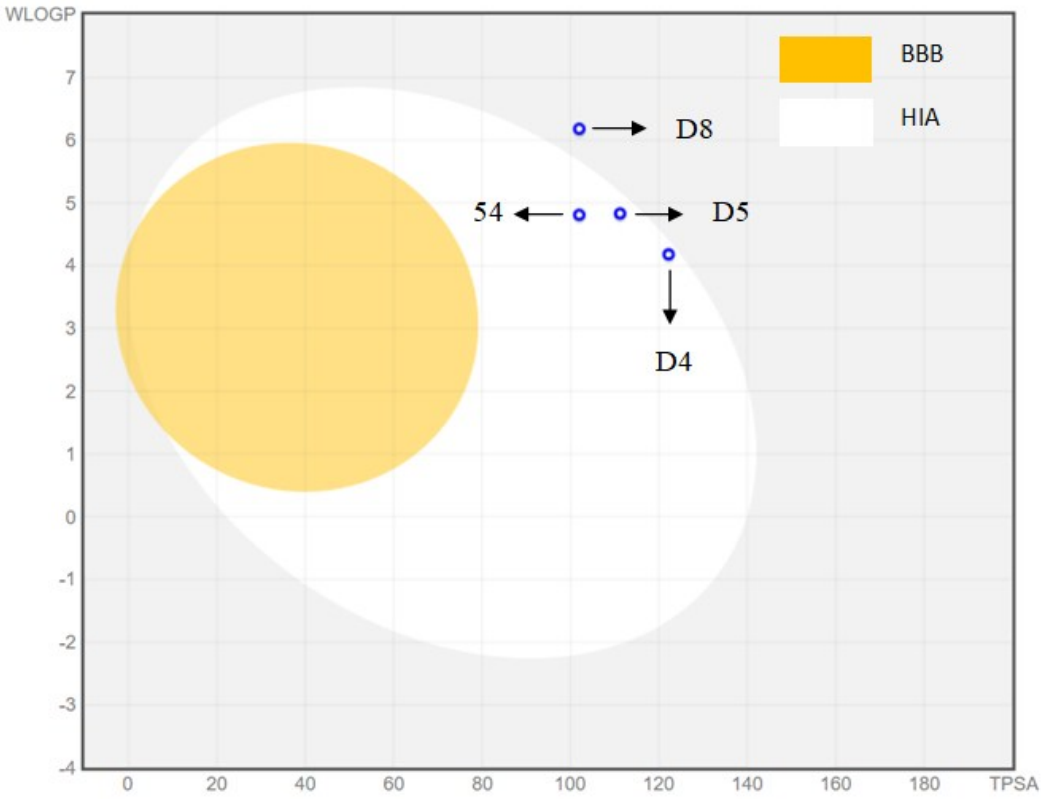

Fig. S7. BOILED-Egg model plot.