

Step 1: Extract the files from the folder.

Step 2: Reproduce the results in Table 2 of the paper by running the following command:

python cal_metrics_from_pt.py

Methods	Vina Score(↓)		Vina Min (↓)		Vina Dock (↓)		High Affinity(↑)		QED(↑)		SA(↑)		Diversity(↑)	
	Avg.	Med.	Avg.	Med.	Avg.	Med.	Avg.	Med.	Avg.	Med.	Avg.	Med.	Avg.	Med.
liGAN	-	-	-	-	-6.33	-6.20	21.1%	11.1%	0.39	0.39	0.59	0.57	0.66	0.67
GraphBP	-	-	-	-	-4.80	-4.70	14.2%	6.7%	0.43	0.45	0.49	0.48	0.79	0.78
AR	-5.75	-5.64	-6.18	-5.88	-6.75	-6.62	37.9%	31.0%	0.51	0.50	<u>0.63</u>	<u>0.63</u>	0.70	0.70
Pocket2Mol	-5.14	-4.70	-6.42	-5.82	-7.15	-6.79	48.4%	51.0%	0.56	0.57	0.74	0.75	0.69	0.71
TargetDiff	-5.47	-6.30	-6.64	-6.83	-7.80	-7.91	58.1%	59.1%	0.48	0.48	0.58	0.58	0.72	0.71
DecompDiff	-5.67	-6.04	-7.04	-7.09	-8.39	-8.43	64.4%	71.0%	0.45	0.43	0.61	0.60	0.68	0.68
IRDiff	-6.03	-6.89	-7.27	-7.37	-8.42	-8.42	67.4%	72.7%	0.53	0.54	0.59	0.58	0.72	0.72
IPDiff	<u>-6.42</u>	<u>-7.01</u>	<u>-7.45</u>	<u>-7.48</u>	<u>-8.57</u>	<u>-8.51</u>	<u>69.5%</u>	<u>75.5%</u>	0.52	0.53	0.61	0.59	<u>0.74</u>	<u>0.73</u>
VFDiff	-7.37	-7.75	-8.18	-8.18	-8.77	-8.72	69.5%	75.5%	<u>0.54</u>	<u>0.55</u>	0.57	0.57	0.72	0.71
Reference	-6.36	-6.41	-6.71	-6.49	-7.45	-7.26	-	-	0.48	0.47	0.73	0.74	-	-

Step 3: You can visualize the protein-ligand complexes you want to examine by running the notebook.