

Supporting Information

Table 1: The docking scores of compounds under study.

Ligand	MolDock Score	Rerank Score	Docking Score	Similarity Score
Carmofur	-108.067	-92.2914	-244.096	-127.506
Cinanserin	-111.377	-88.7229	-340.577	-226.815
Disufiram	-114.695	-91.6716	-182.858	-69.1153
Ebselen	-83.4664	-70.8063	-227.042	-144.338
HCQ	-120.2526	-68.9812	-228.544	-205.621
PX12	-72.3937	-53.3872	-180.616	-108.38
Shikonin	-104.243	-96.9656	-252.378	-149.258
TDZD	-84.0822	-67.7829	-228.997	-139.174
Tideglusib	-102.159	-69.0901	-350.229	-242.841