

Supplementary Table 1. Binding energy of silybin with four different kinases and the relative rank of silybin among the drug leads screened from the FDA drug database. Column I, the four kinases targeted for virtual screening; Column II, PDB ID code of the crystal structure used as the receptor structure for each kinase during screening; Column III, the binding energy between silybin and the target kinase; Column IV, the binding rank of silybin among FDA drug leads obtained from virtual screening.

Kinase	PDB ID	Scoring Energy	Rank
BRAF	3OG7	-9.153	40
MEK1	3EQI	-9.076	22
ERK2	4ERK	-8.060	33
RSK1	2Z7R	-9.320	13