

Table S2

Grid Docking scores of acetylated compounds to the allosteric site, and of DNJ to the active site.

Molecule	Score	Site
NAC	-4,3342	Allosteric
NAG	-4,0682	Allosteric
NAS	-4,4576	Allosteric
MAL	-4,9417	Active Site
DNJ	-6,6378	Active Site