Table S1: Docking scores of the top 10 compounds from both libraries. The compounds chosen as potential candidate for further analysis are highlighted in yellow color.

Compound ID	Binding energy score (Kcal/mol)
MPD3 Library	
ZINC14781695	-10.7
ZINC95099417	-10.3
ZINC5854691	-10.3
ZINC1530850	-10.2
ZINC49015315	-10.2
ZINC85932323	-10
ZINC14713101	-10
ZINC148327405	-9.9
ZINC85996587	-9.9
NPACT Library	
ZINC14819291	-9.9
ZINC14727630	-9.7
ZINC14645641	-9.5
ZINC238741704	-9.3
ZINC95099258	-8.9
ZINC105487149	-8.7
ZINC96902284	-8.5
ZINC95099258	-8.3
ZINC257512858	-8.2
ZINC299817645	-8.2