

Compound	Protein	Free energy/(kcal/mol)
Dexamethasone	LAYN	-7.89
Dronabinol	LAYN	-6.39
Ethinylestradiol	LAYN	-7.28
Calcitriol	LAYN	-6.81
Cyclosporine	TNFAIP3	-13.08
Vincristine	TNFAIP3	-9.39
Withaferin A	TNFAIP3	-6.57
Ursodeoxycholic acid	TNFAIP3	-6.44

Supplementary Table.S3 Potential drug screening. The free energy of binding is less than -5, which indicates that the small molecular compound has a stable binding with the protein.