Compounds	2D-structure	Bioavailability Radar for Druglikeness
25- hydroxycholest erol	H O H	FLEX BIZE INSATU POLAR INSOLU
Tyrphostinb46		FLEX FLEX NBATU FISOLU
Flufenamic acid		FLEX FLEX FLEX FOLAR FOLAR
Nortriptyline hydrochloride	HN	PLEX PLEX NEATU NBOLU
Piceatannol	но он	FLEX INSATU FOLAR
Retinol	H H H H H H H H H H H H H H H H H H H	FLEX NISATU FOLAT

## Supplemental Table SI: Bioavailability Radar showing the drug-likeness of the compounds



(LIPO = lipophilicity as XLOGP3; SIZE = size as molecular weight; POLAR = polarity as TPSA (topological polar surface area); INSOLU = insolubility in water by I og S scale; INSATU = insaturation as per fraction of carbons in the sp3 hybridization and FLEX = flexibility as per rotatable bonds]





The pink area in the radar displays the ideal range for each of the parameters including lipophilicity, molecular weight, polarity, solubility, saturation and flexibility

Compound name	Human Ether-a-go-go- related gene inhibition	Carcinogen	Acute oral toxicity	
25-hydroxycholesterol	Weak inhibitor	Non-carcinogen	Ш	
Tyrphostinb46	Weak inhibitor	Non-carcinogen	111	
Flufenamic acid	Weak inhibitor	Non-carcinogen	П	
Nortriptyline hydrochloride	Weak inhibitor	Non-carcinogen	111	
Piceatannol	Weak inhibitor	Non-carcinogen	111	
Retinol	Weak inhibitor	Non-carcinogen	111	
Tak-715	Weak inhibitor	Non-carcinogen	111	
Losmapimod	Weak inhibitor	Non-carcinogen		

# Supplemental Table S3: Toxicity analysis of compounds

Supplementary Files Potential therapeutic compounds against hypercholesterolemia: an in-silico analysis



Supplemental Figure S1: Root-mean-square fluctuation (RMSF) analysis. **a)** RMSF graph of TAK-715, **b)** Tyrphostin b46, **c)** Retinol, **d)** 25-hydroxycholesterol, **e)** Piceatannol, **f)** Losmapimod, **g)** Flufenamic acid, **h)** Nortriptyline hydrochloride. RMSF shows the flexibility of ligand and protein. High RMSF shows more vigorous ligand-receptor interactions which depicts that the receptor and ligand are moving a lot and have more fluctuations whereas low RMSF indicates that the interactions are less vigorous and the ligand and receptor are tightly bound to each other.