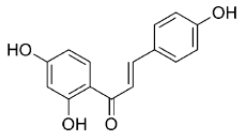
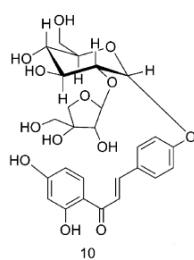
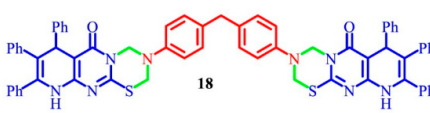
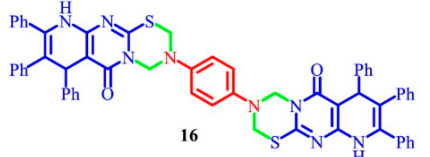
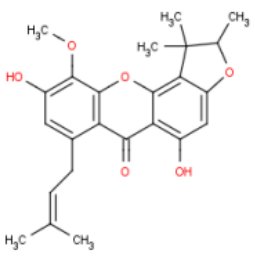
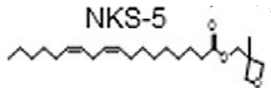
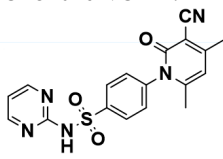
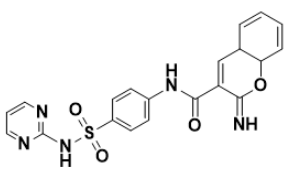
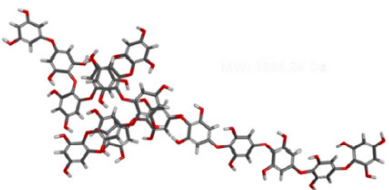


Table S2. Main therapeutic agents employed in in silico studies along with their respective chemical structures and/or formulas.

Study/ Year/ References	Class/Source	Main therapeutic agents used within in silico studies
Birari <i>et al</i> 2011., [32]	Flavonoids, Roots of <i>Glycyrrhiza glabra</i>	Isoliquiritigenin (7) ^a and Licuroside (10) ^a :  7
		 10
Coronado- Cáceres <i>et al.</i> , 2020 [33]	Peptides, Seeds of <i>Theobroma cacao</i> L	Cocoa (<i>Theobroma cacao</i> L.) peptide EEQR ^a
El-Korany <i>et al.</i> , 2020 [34]	Organic acid, <i>Aspergillus</i> <i>oryzae</i>	Kojic acid ^b
Yakaiah <i>et al.</i> , 2021 [35]	Heterocyclic Organic Compound, Seeds of <i>Myristica fragrans</i>	Tetrahydrofuran ^b
Elekofehinti <i>et</i> <i>al.</i> , 2020 [36]	Alkaloids, <i>Annona</i> <i>muricata</i> (Annonaceae)	Annonioside ^b and Annonaine ^b
Yaccoubi <i>et al.</i> , 2022 [37]	Tiadiazinona derivative, synthetic	Bis-fused thiadiazinones 16 ^a and 18 ^a  18  16
Fajriaty <i>et al.</i> , 2023 [38]	Phytochemicals, <i>Calophyllum soulattri</i>	Caloxanthone B ^a 
Khan <i>et al.</i> , 2023 [39]	Linoleic acid derivatives, synthetic	NKS-5 ^a : (9Z,12Z)-(3-methyloxetan-3-yl) methyl octadeca-9,12-dienoate  NKS-5

Lee <i>et al.</i> , 2008 [40]	Biarylpyrazolyl oxadiazole analogues, synthetic	43c ^a : 2-(4-((1H-1,2,4-triazol-1-yl)methyl)-5-(4-bromophenyl)-1-(2,4-dichlorophenyl)-1H-pyrazol-3-yl)-5-(1-(trifluoromethyl)cyclopropyl)-1,3,4-oxadiazole
Ghareb <i>et al.</i> , 2019 [41]	Benzenesulfonamide derivatives, synthetic	MS-13 ^a and MS-14 ^a : <div style="text-align: center;">  MSE-13 </div> <div style="text-align: center;">  MSE-14 </div>
Chen <i>et al.</i> , 2022 [42]	Short chain fatty acids (SCFAs), bacterial fiber fermentation	Butyrate ^b
Kang <i>et al</i> 2022 [43]	Florotanins, Algae <i>Ishige okamurae</i> (Yendo)	Ishophloroglucin A ^a <div style="text-align: center;">  </div>

^a Chemical structure and/or formula obtained in the original article

^b Chemical structure and/or formula not obtained in the original article