

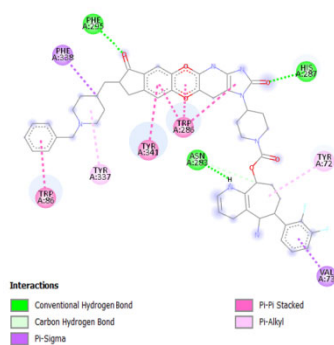
Investigation of cholinergic inhibition by donepezil-rimegepant hybrids in alzheimer's disease: An *in silico* study

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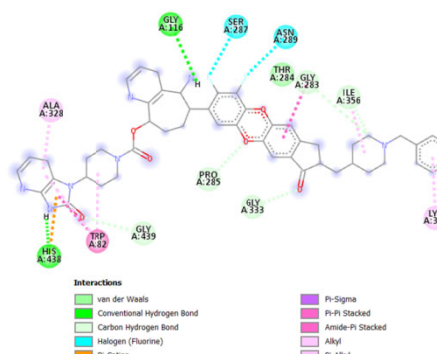
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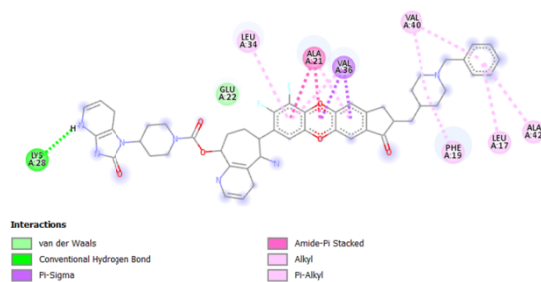
Supporting Data



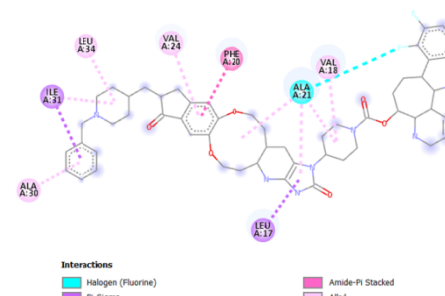
4EY7(DR5 Hybrid)



2Y1K(DR3 Hybrid)



2BEG(DR3 Hybrid)



1IYT(DR16 Hybrid)

Suppl. Fig. S1 — Other best interaction 2d plots

Supplementary Table

Suppl. Table S1 — Bioactive score of all the selected DR hybrids

hybrids	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
DR1	-3.03	-3.66	-3.58	-3.69	-3.02	-3.04
DR2	-3.01	-3.65	-3.58	-3.57	-2.99	-3.32
DR3	-2.79	-3.59	-3.54	-3.63	-2.69	-3.12
DR4	-2.79	-3.59	-3.54	-3.63	-2.69	-3.12
DR5	-2.79	-3.6	-3.54	-3.65	-2.69	-3.1
DR6	-2.79	-3.6	-3.54	-3.65	-2.69	-3.1
DR7	-3.21	-3.7	-3.65	-3.72	-3.25	-3.51
DR8	-3.23	-3.7	-3.65	-3.72	-3.24	-3.52
DR9	-2.91	-3.64	-3.54	-3.65	-2.83	-3.25
DR10	-2.88	-3.63	-3.55	-3.64	-2.83	-3.22
DR11	-3.21	-3.5	-3.57	-3.57	-2.79	-3.1
DR12	-2.79	-3.65	-3.58	-3.58	-2.65	-3.2
DR13	-3.01	-3.5	-3.59	-3.54	-2.63	-3.4
DR14	-2.89	-3.69	-3.65	-3.61	-2.61	-3.65
DR15	-3.02	-3.4	-3.54	-3.71	-2.79	-3.12
DR16	-3.04	-3.54	-3.61	-3.62	-2.63	-3.14
DR17	-3.01	-3.64	-3.58	-3.22	-2.99	-3.15
DR18	-2.79	-3.51	-3.61	-3.11	-3.68	-3.15
