

Supplementary data

PolyPhen-2 report for P30532 D398N (rs16969968)

Query

Protein Acc	Position	AA ₁	AA ₂	Description
P30532	398	D	N	Canonical; RecName: Full=Neuronal acetylcholine receptor subunit alpha-5; Flags: Precursor; Length: 468

Results

+ Prediction/Confidence

PolyPhen-2 v2.2.3r406

HumDiv

This mutation is predicted to be **BENIGN** with a score of **0.004** (sensitivity: **0.97**; specificity: **0.59**)

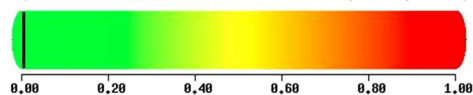
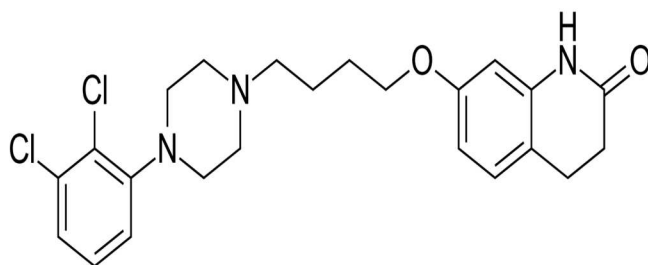


Fig. S1: PolyPhen-2 identifies the D398N mutation as benign with a score of 0.0004.

(a)



(b)

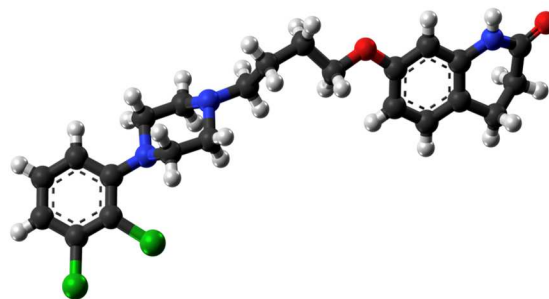


Fig. S2: (a) 2D and (b) 3D structure of Aripiprazole molecule, an atypical antipsychotic marketed as an antidepressant, selected as reference drug. (Clc4cccc(N3CCN(CCCCOc2ccc1c(NC(=O)CC1)c2)CC3)c4Cl)

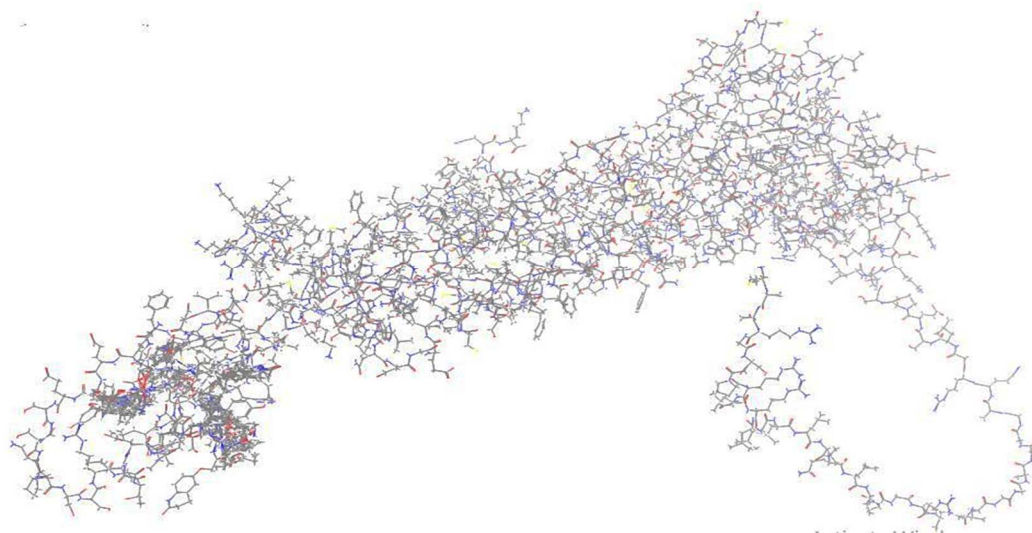


Fig. S3: 2D and 3D structural visualization of CHRNA5 docked with Aripiprazole (Reference compound) and selected ligands by Maestro.