

DFT study of regio- and stereoselective [3+2] cycloaddition between diazopropane and substituted chalcone derivatives and molecular docking of novel pyrazole derivatives as anti-Alzheimer's agents

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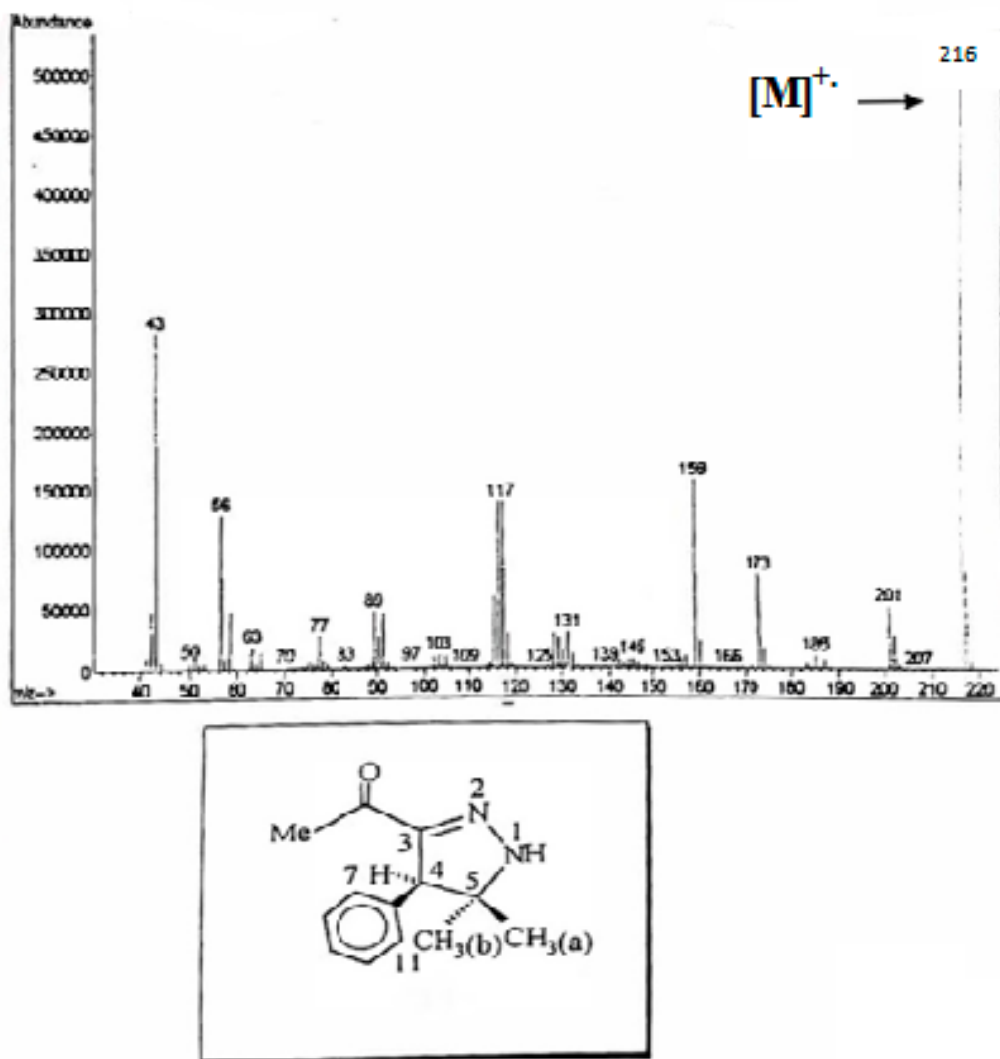


Figure S1. Mass spectrum in EI mode of D2 compound

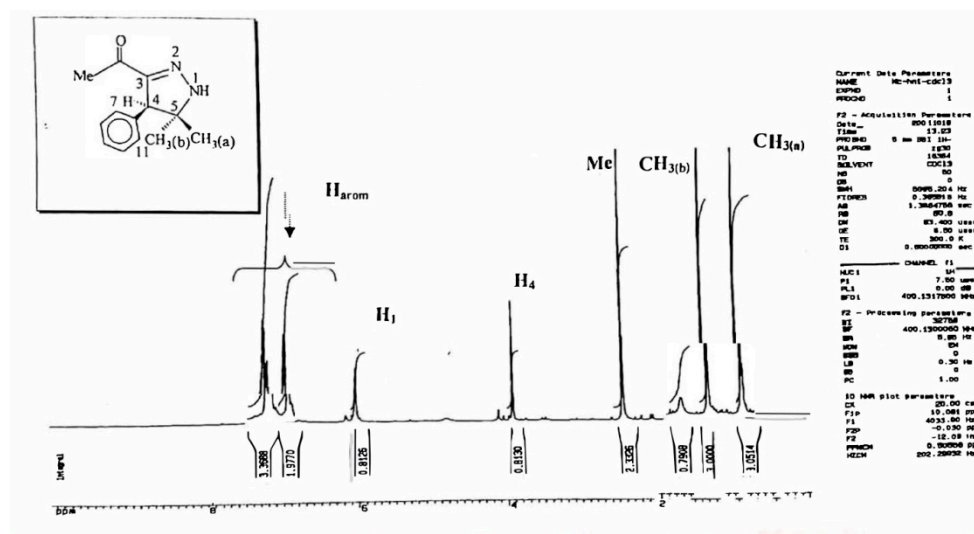


Figure S2. ¹H NMR spectrum((CDCl₃, 300MHz) of D2 compound

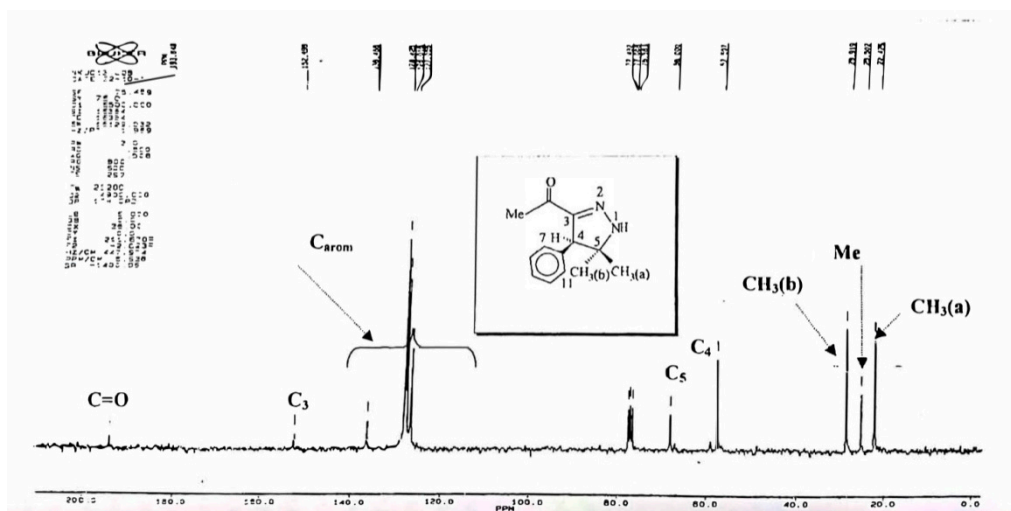


Figure S3. ^{13}C NMR spectra (CDCl_3 , 75MHz) of D2 compound

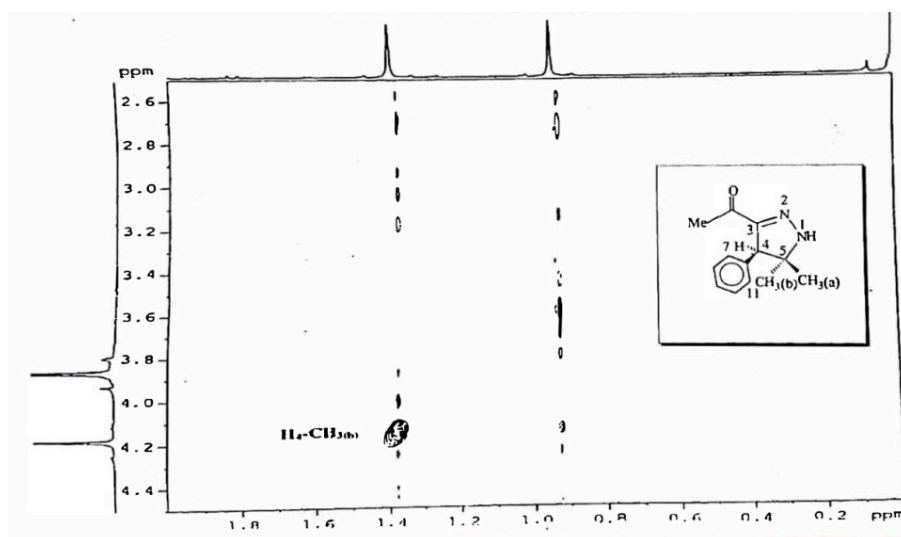


Figure S4. ^1H NMR-NOESY spectrum of D2 compound

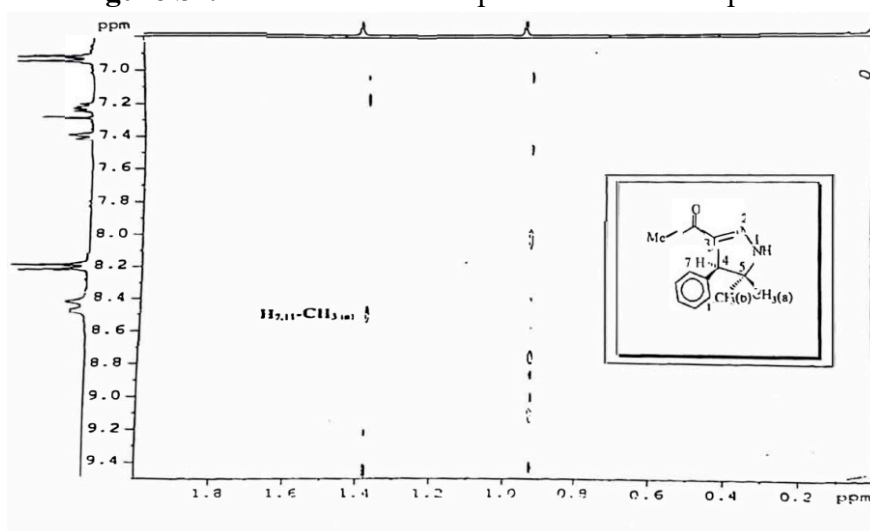


Figure S5. ^1H NMR-NOESY spectrum of D2 compound (0.2 - 1.8 ppm)

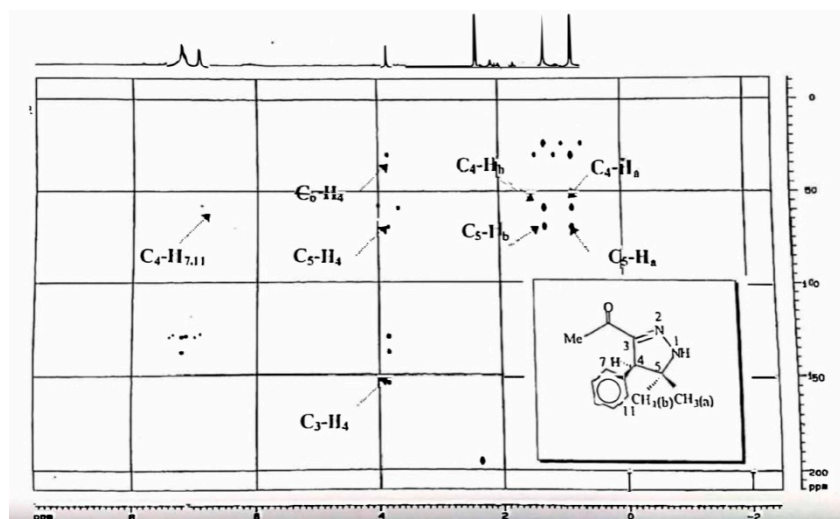


Figure S6. HMBC spectrum of D2 compound

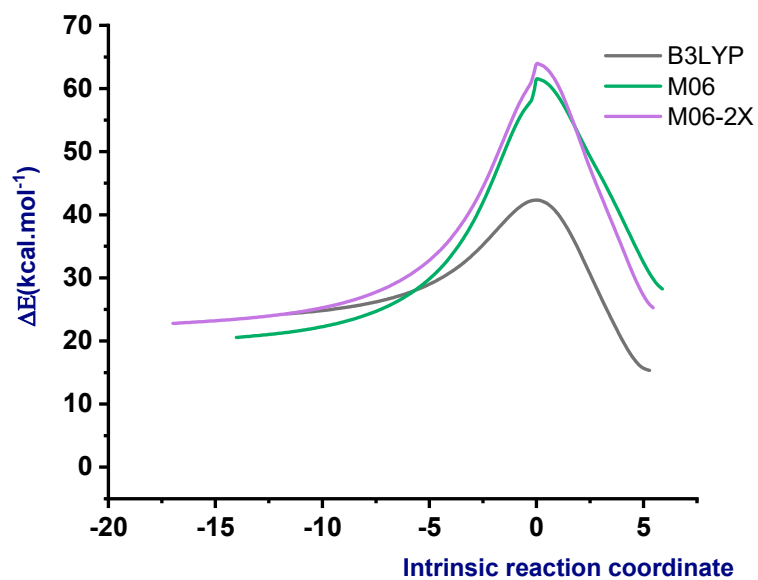


Figure S7. IRC plots of 1HP1 at B3LYP, M06 and M06-2X functional with 6-311+G(d, p) basis set.

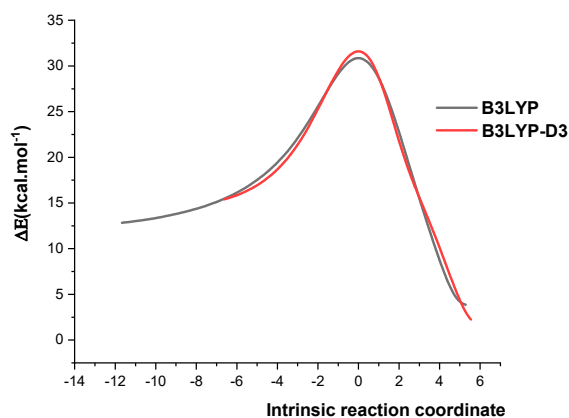


Figure S8. Computed IRC plots of the synthesis of 1HP1 at B3LYP and B3LYP-D3 functionals with 6-311+G(d, p) basis set

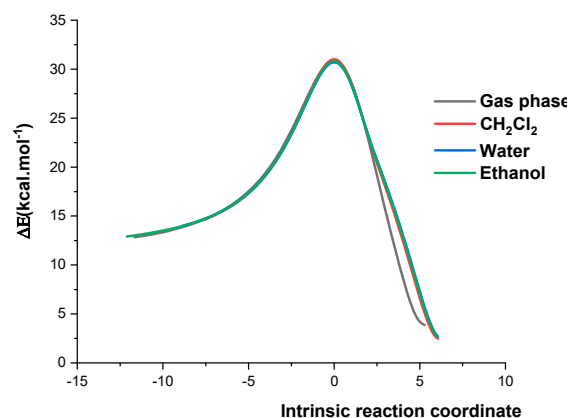


Figure S9. Computed IRC plots of the synthesis of 1HP1 at B3LYP/6-311+G(d, p) level with CPCM solvation model in three solvents: CH₂Cl₂, water and ethanol.

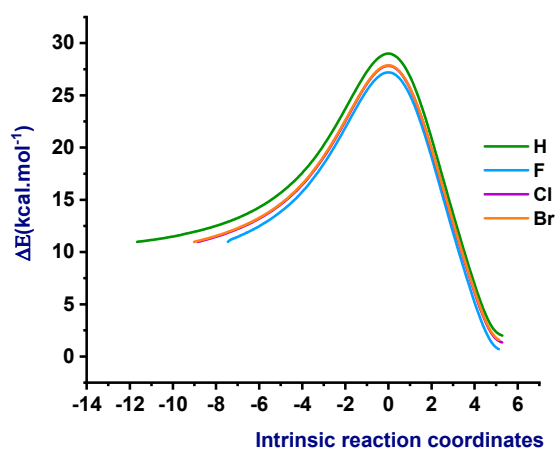


Figure S10. IRC plots as function of halogens at B3LYP level

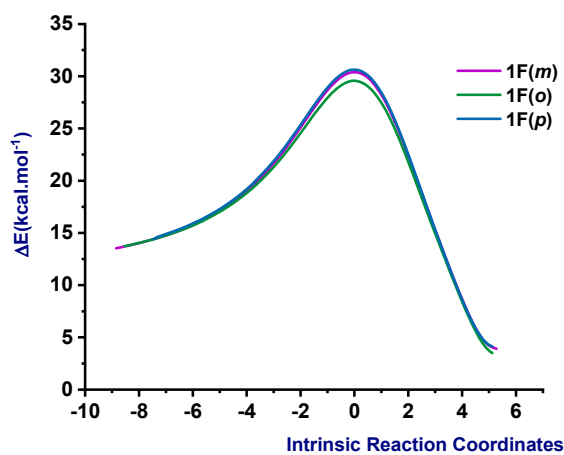


Figure S11. IRC plots of 1F(meta, ortho and para) pathways at B3LYP level

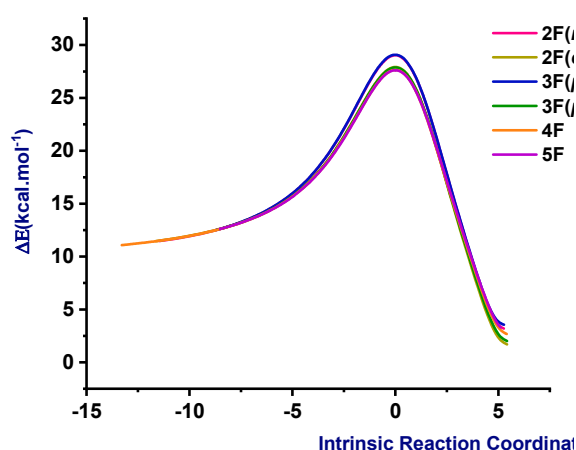


Figure S12. IRC plots of 2F, 3F, 4F and 5F pathways at B3LYP level

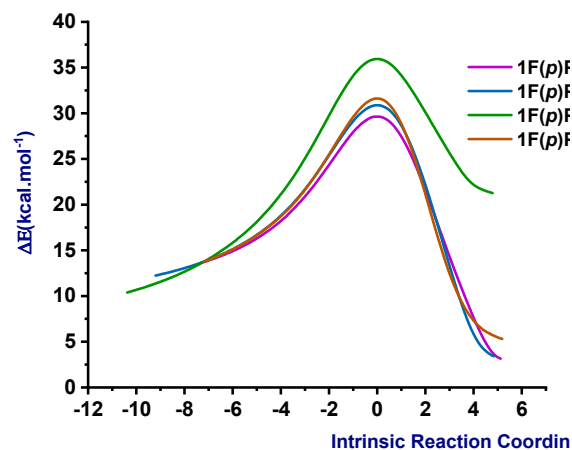
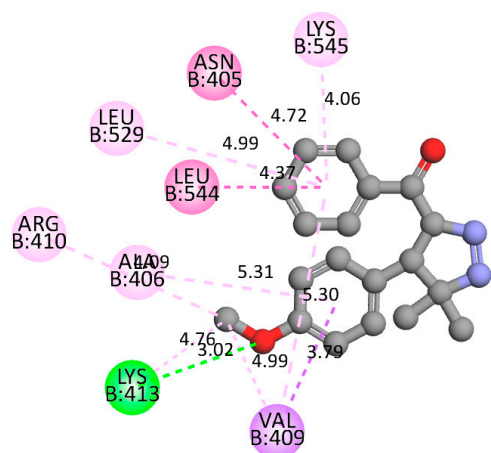
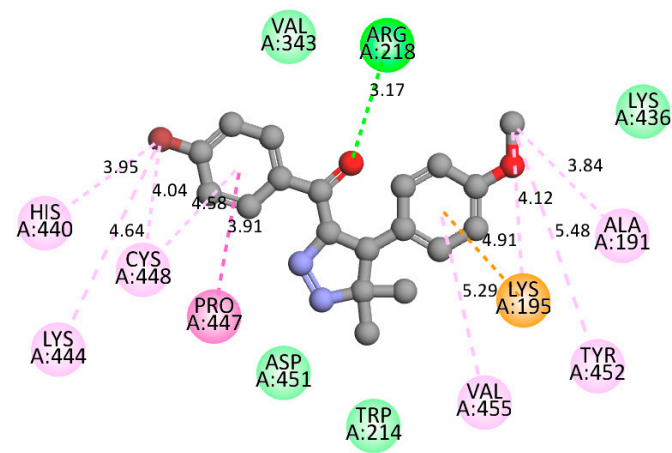


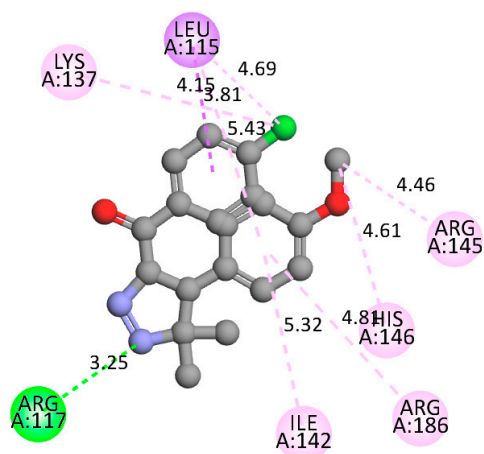
Figure S13. IRC plots of 1F(para) pathways at B3LYP level



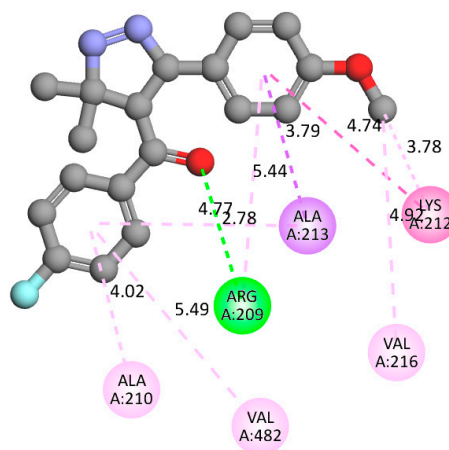
2D depiction of docking of ligand 1 in the active site of HSA (-8.3kcal/mol)



2D depiction of docking of ligand 2 in the active site of HSA (-8.6kcal/mol)



2D depiction of docking of ligand 3 in the active site of HSA (-7.8kcal/mol)

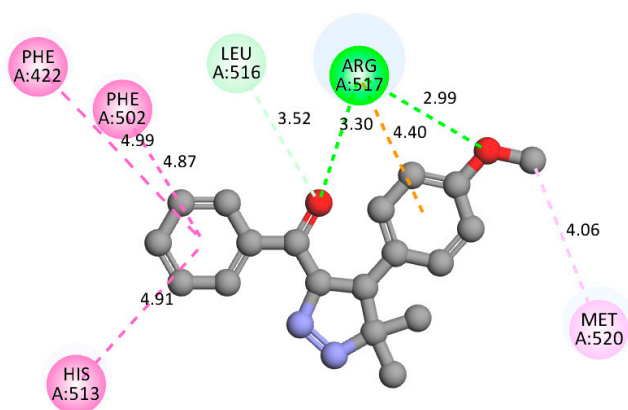


2D depiction of docking of ligand 4 in the active site of HSA (-8.5kcal/mol)

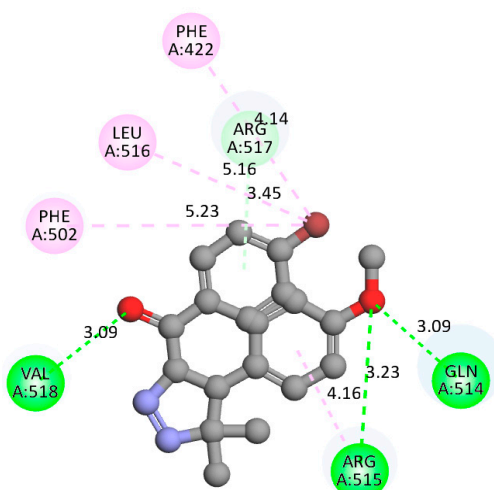
Interactions

■ Conventioanl Hydrogen Bond
 ■ Carbon Hydrogen Bond
 ■ Pi-Sigma
 ■ Amide-Pi Stacked
 ■ Pi-Cation
 ■ Alkyl, Pi-Alkyl

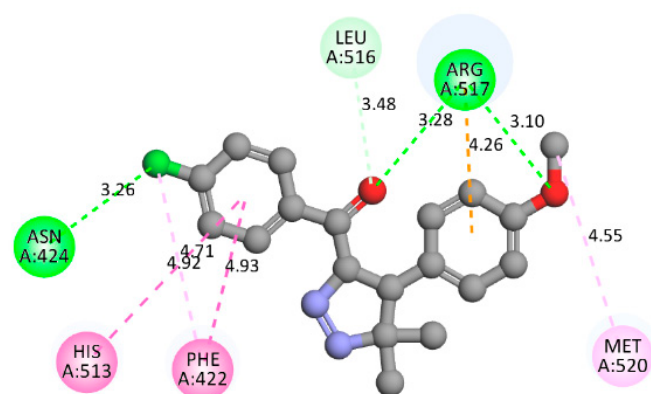
Figure S14. 2D depiction of docking of ligands 1HP1-4 in the active site of Human Serum Albumin



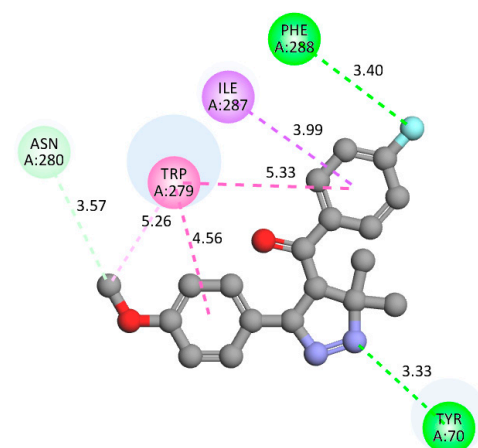
2D depiction of docking of ligand 1 in the active site of AChE



2D depiction of docking of ligand 2 in the active site of AChE



2D depiction of docking of ligand 3 in the active site of AChE

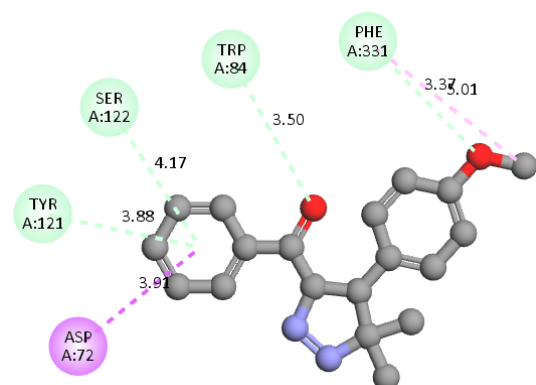


2D depiction of docking of ligand 4 in the active site of AChE

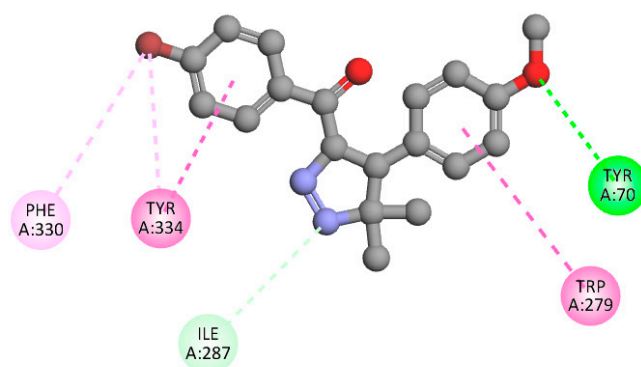
Interactions

- Conventioanl Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Donor Hydrogen
- Halogen (Fluorine)
- Alkyl, Pi-Alkyl
- Pi-Pi Stacked, Pi-Pi T Shaped, Amide-Pi Stacked
- Pi-Cation, Pi-Anion
- Pi-Sigma

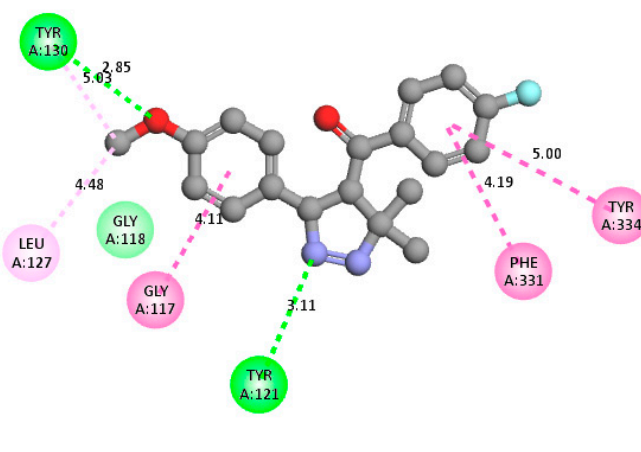
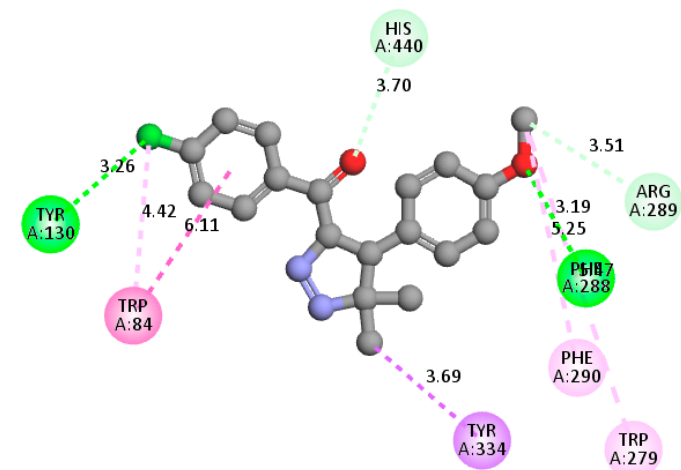
Figure S15. 2D depiction of docking of ligands 1HP1-4 in the active site of AChE (PDB ID: 1ACJ)



2D depiction of docking of ligand 1 in the active site of AChE



2D depiction of docking of ligand 2 in the active site of AChE



2D depiction of docking of ligand 3 in the active site of AChE

2D depiction of docking of ligand 4 in the active site of AChE

Interactions

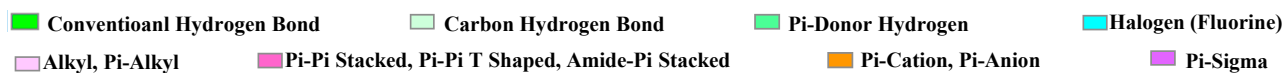
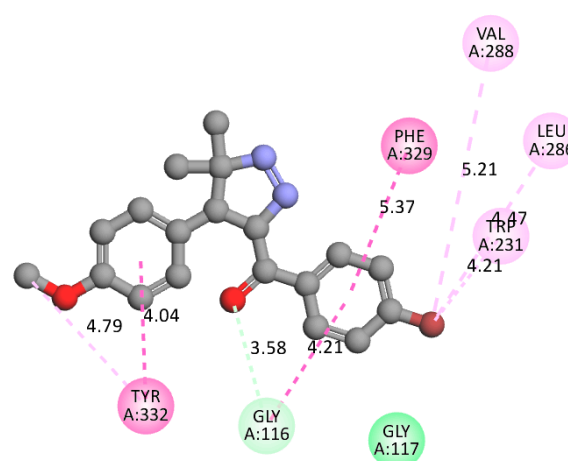
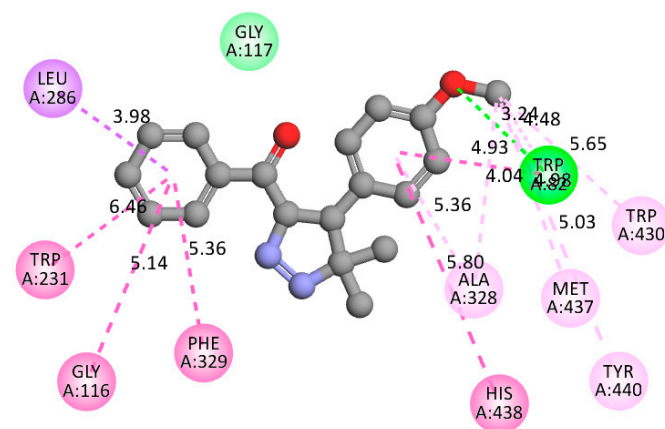
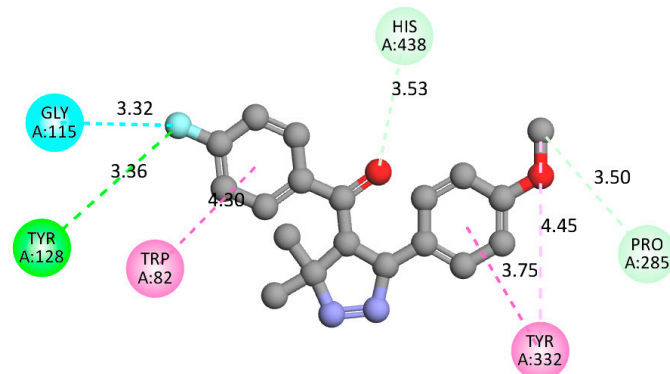
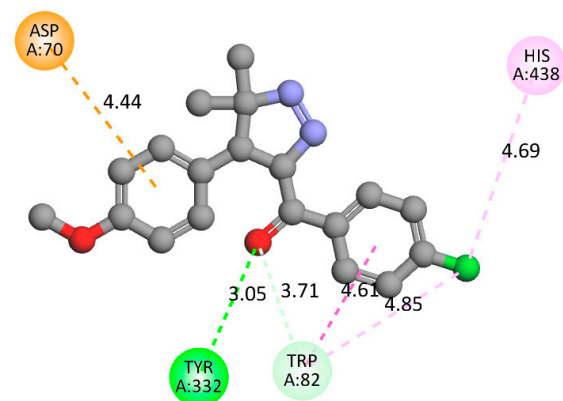


Figure S16. 2D depiction of docking of ligands 1HP1-4 in the active site of AChE (PDB ID: 1EVE)



2D depiction of docking of ligand 1 in the active site of BuChE

2D depiction of docking of ligand 2 in the active site of BuChE



2D depiction of docking of ligand 3 in the active site of BuChE

2D depiction of docking of ligand 4 in the active site of BuChE

Interactions

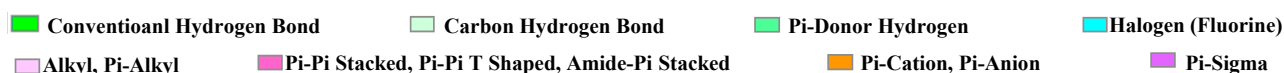


Figure S17. 2D depiction of docking of ligands 1HP1-4 in the active site of BuChE (PDB ID: 1P0I)