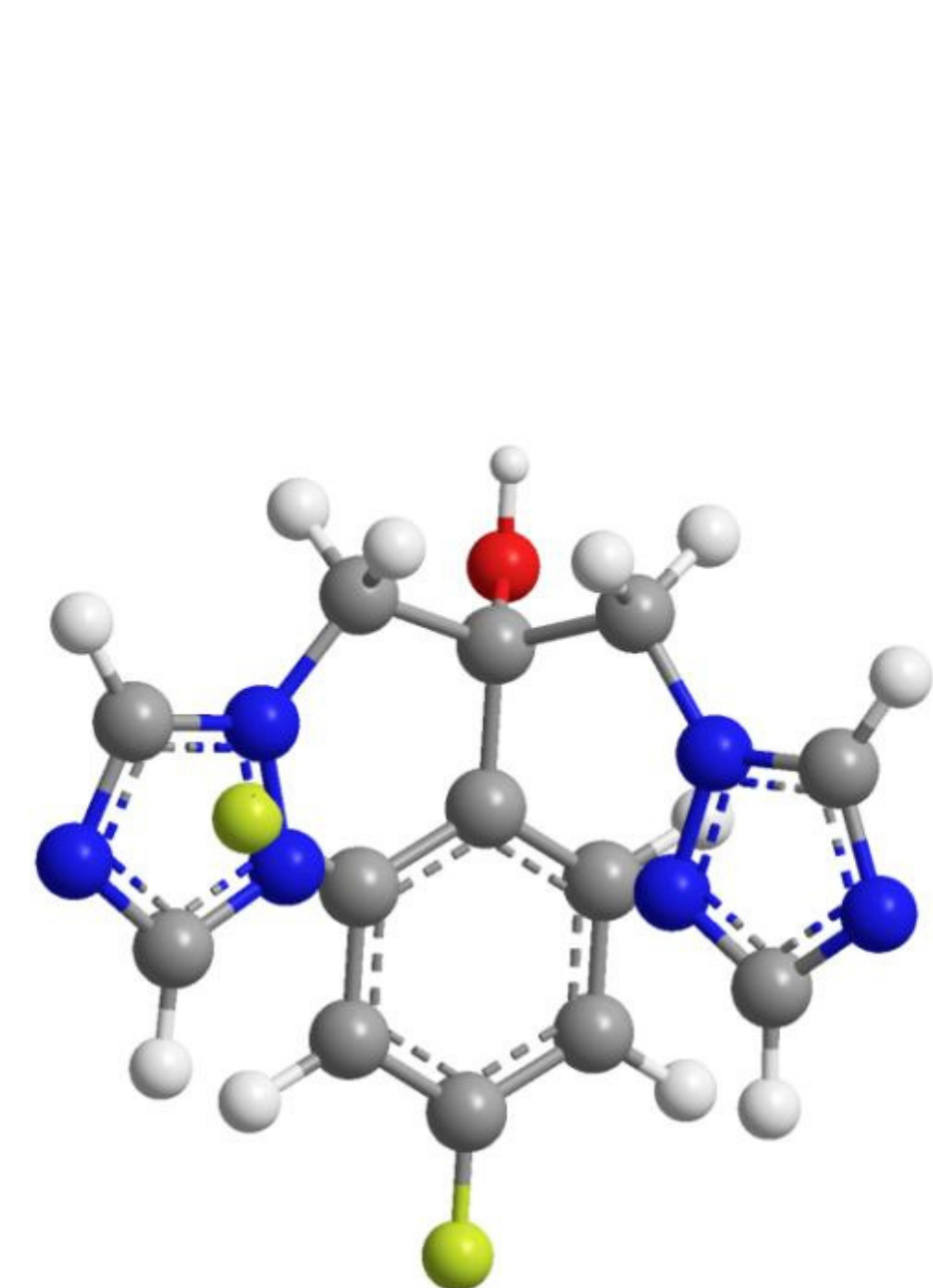
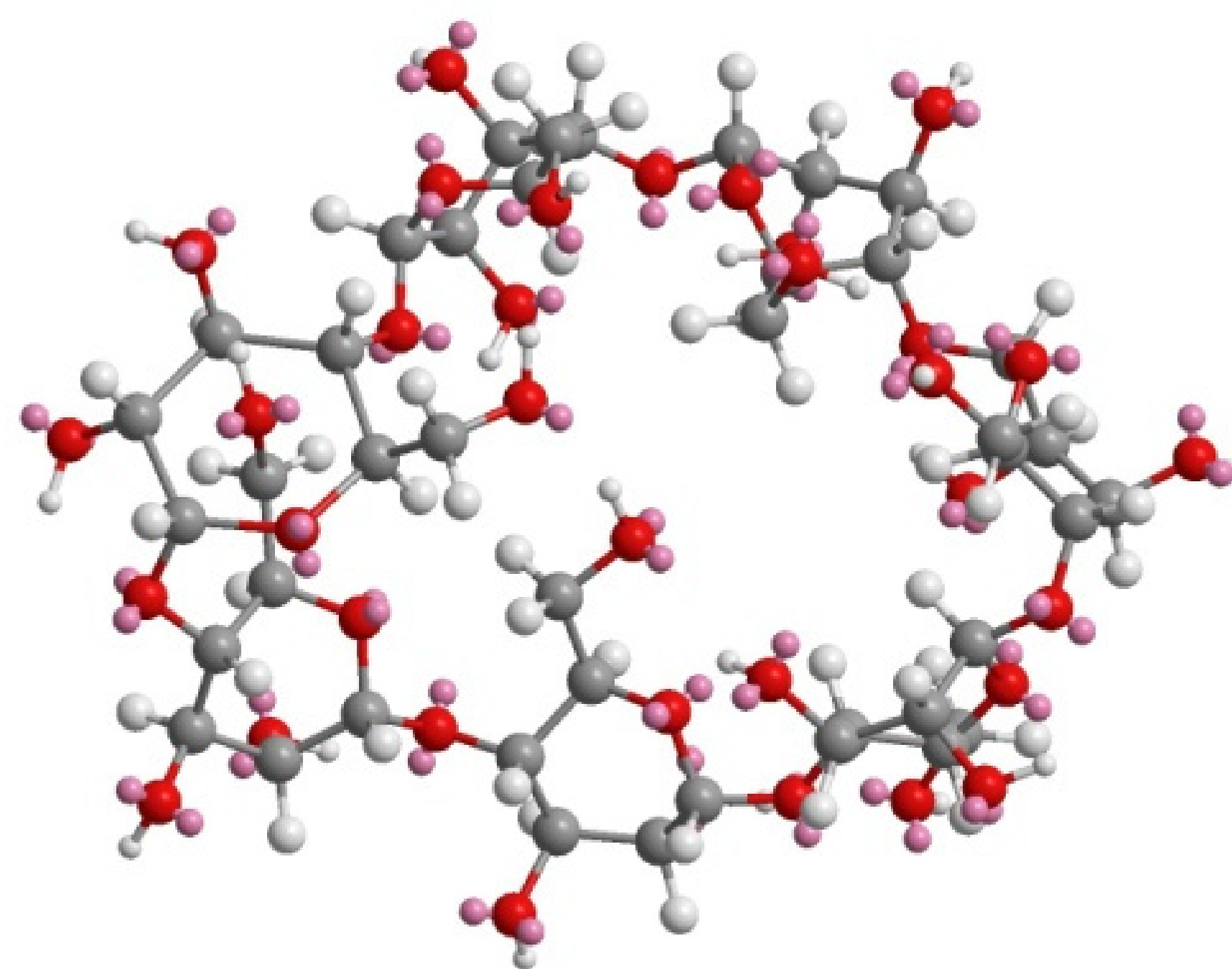
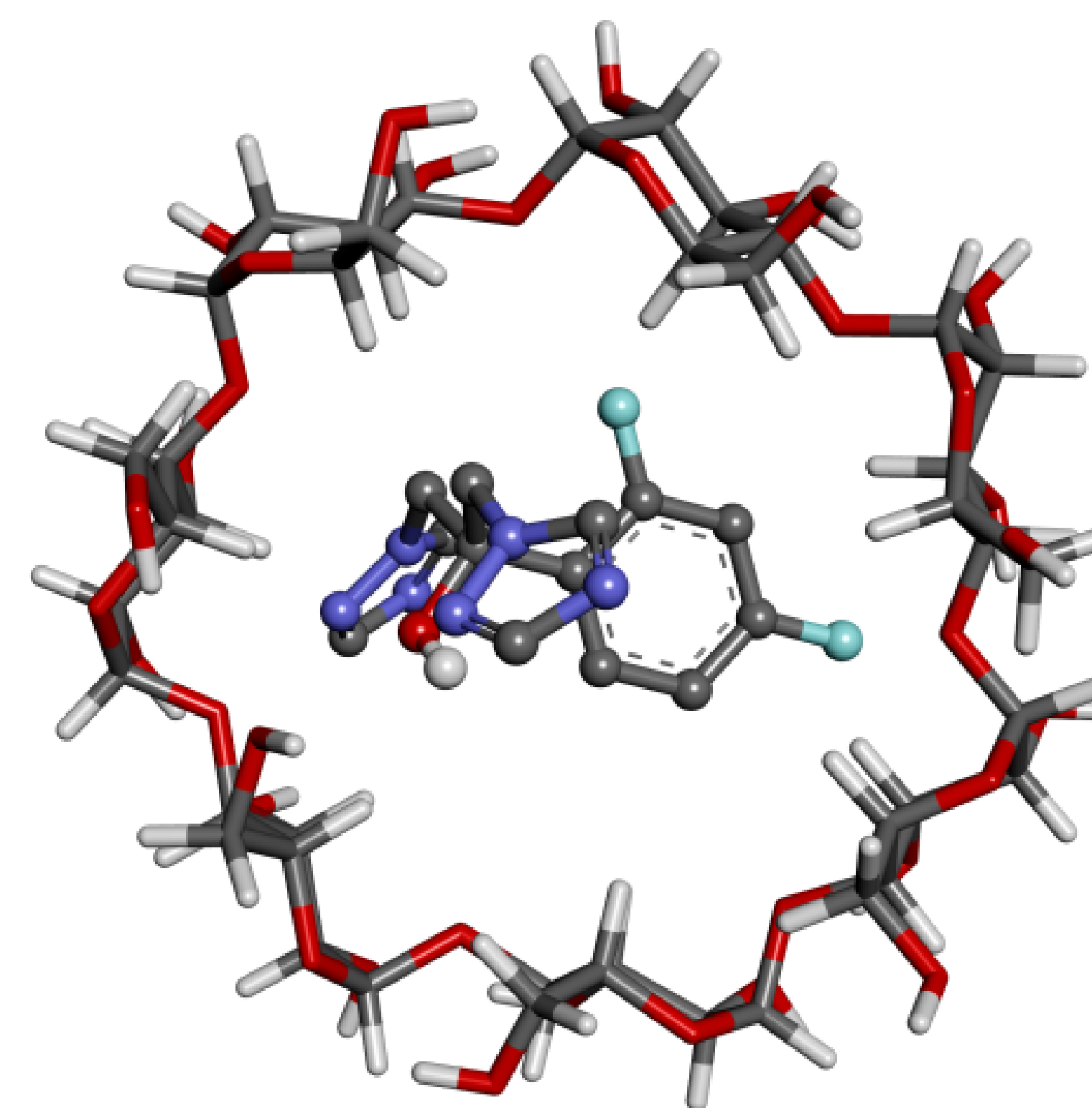




Fluconazole (FCZ)



β -Cyclodextrin (β -CD)



FCZ- β -CD1

Docking score:	-5.6 Kcal/Mol
Total energy:	-392504.76 Kcal/Mol
Heat formation:	7 2007 Kcal/Mol
HOMO-LUMO Gap:	0.359899 ev
Chemical potential (μ):	7.1273325 ev
Global hardness (η):	0.1799495 ev
Softness (S):	5.55711463
Global electrophilicity index (ω):	141.14757 ev