Supplementary Materials: A Comparative Study of Molecular Structure, p*K*a, Lipophilicity, Solubility, Absorption and Polar Surface Area of Some Antiplatelet Drugs

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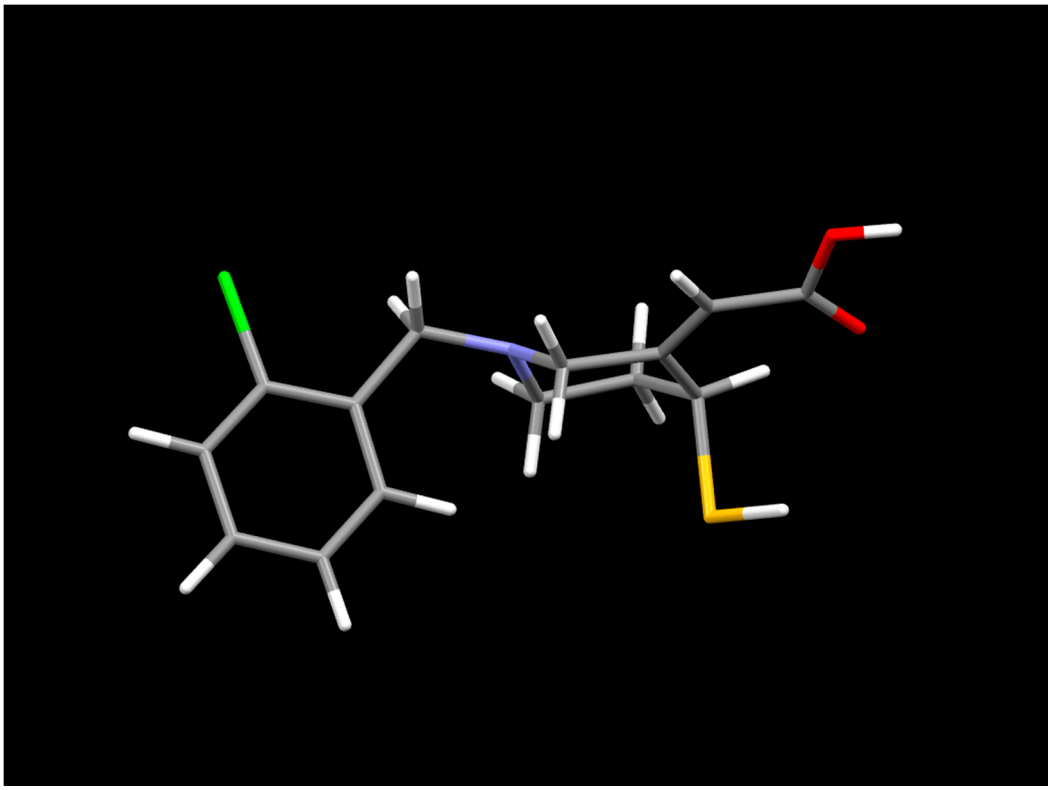
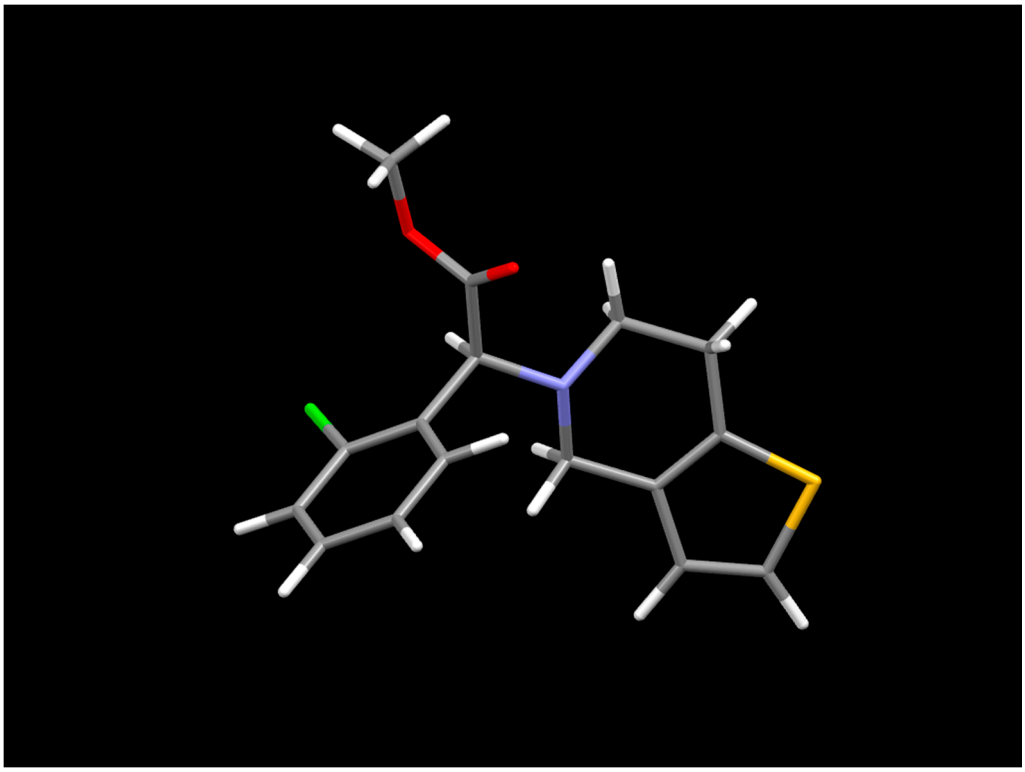
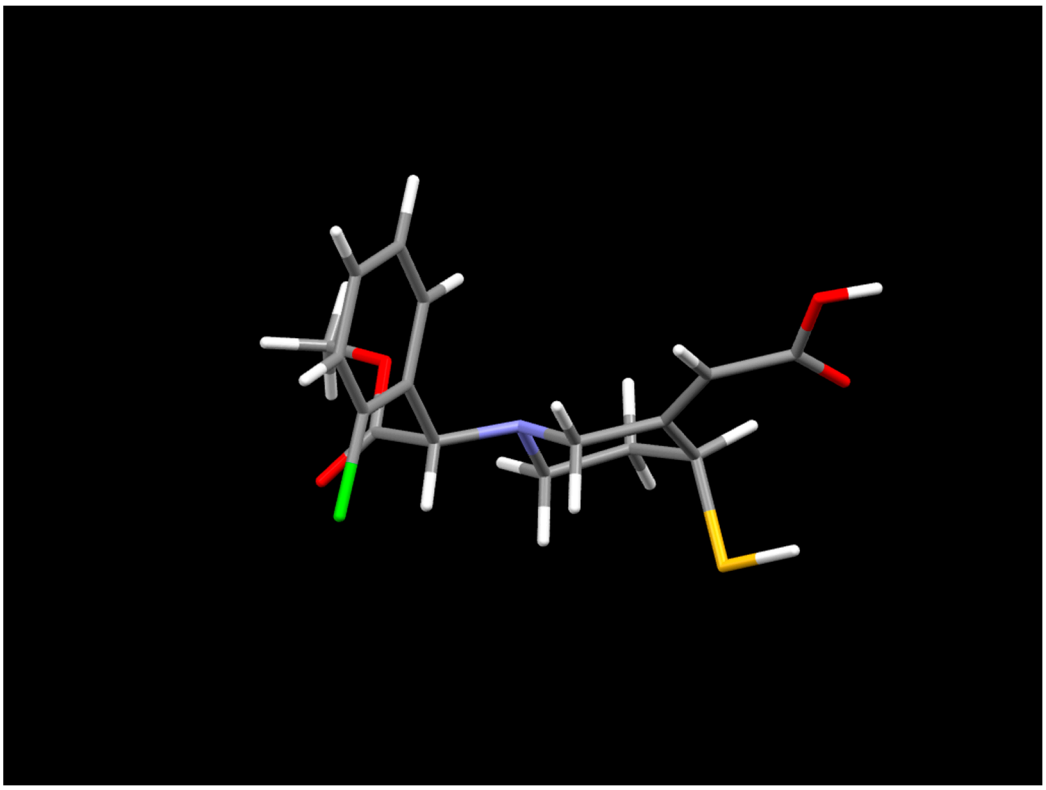
Overall shape of the ticlopidine computed at the Becke3LYP/6-311++G(d,p) level of theory.



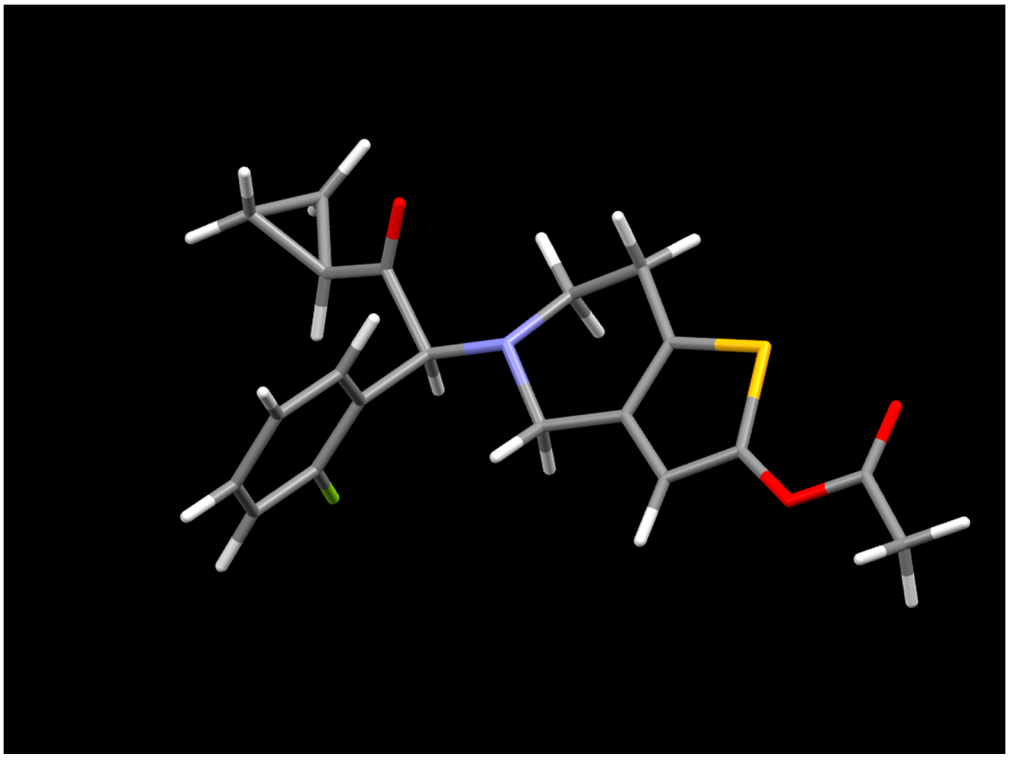
Overall shape of the ticlopidine metabolite computed at the Becke3LYP/6-311++G(d,p) level of theory.



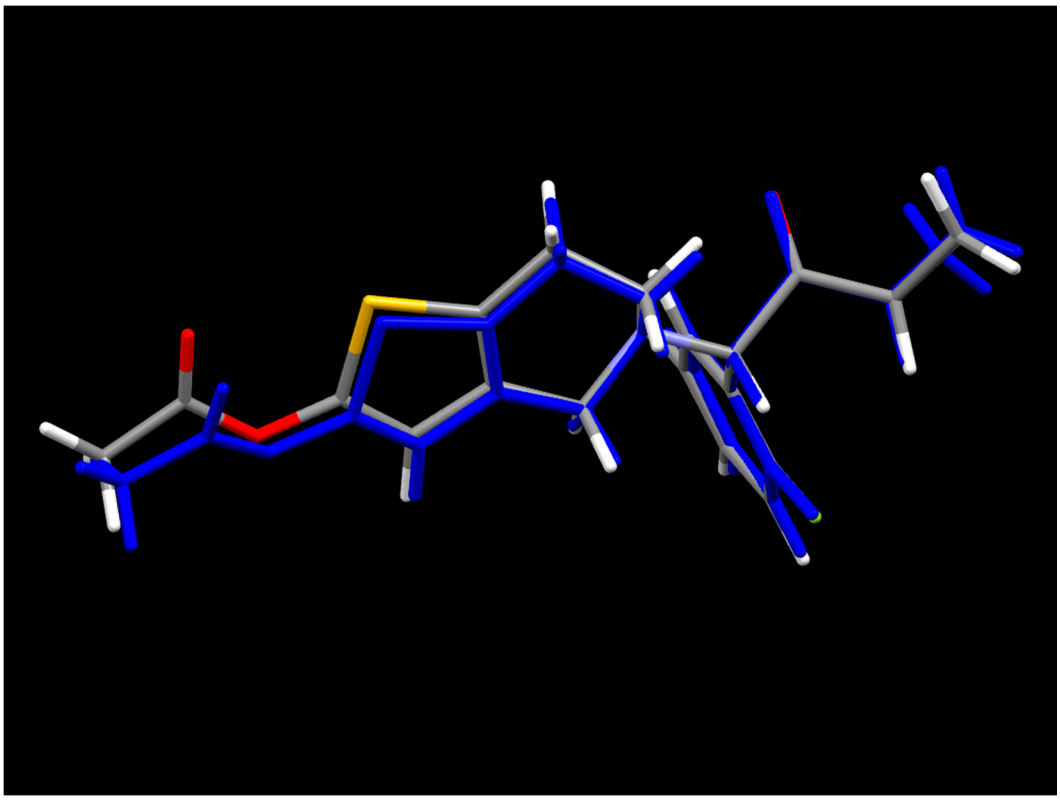
Overall shape of the clopidogrel computed at the Becke3LYP/6-311++G(d,p) level of theory.



Overall shape of the clopidogrel metabolite computed at the Becke3LYP/6-311++G(d,p) level of theory.

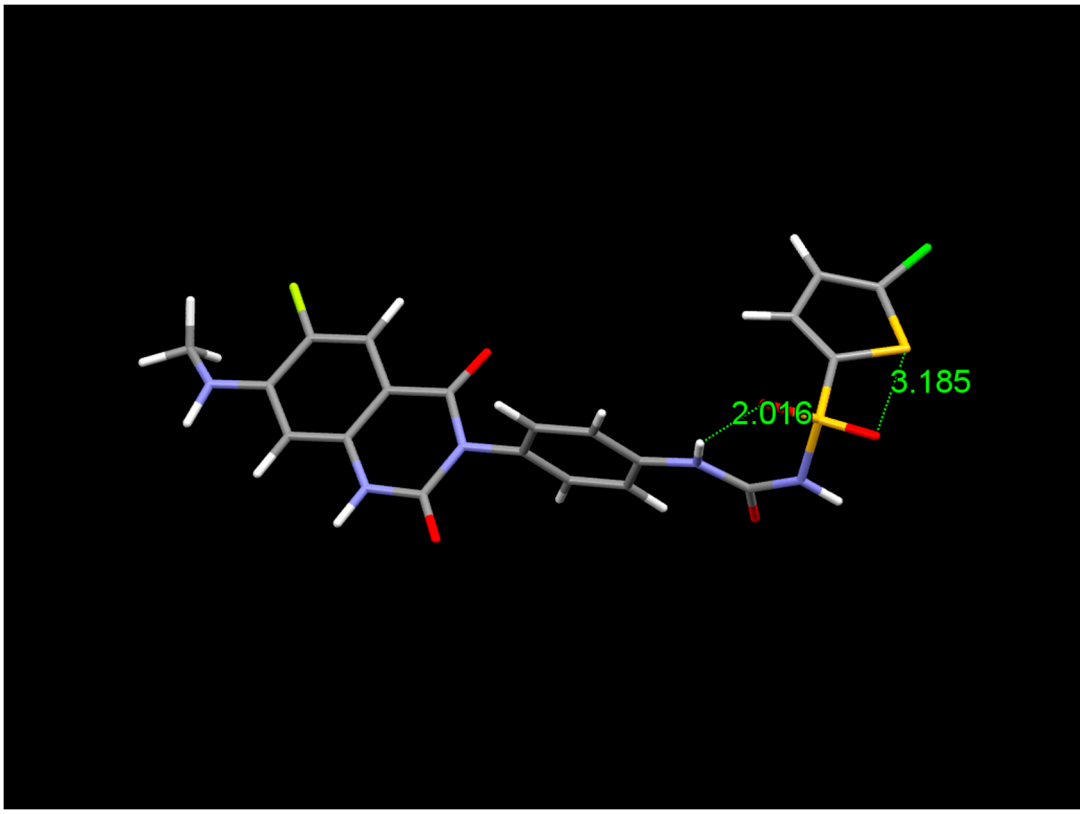


Overall shape of the prasugrel computed at the Becke3LYP/6-311++G(d,p) level of theory.

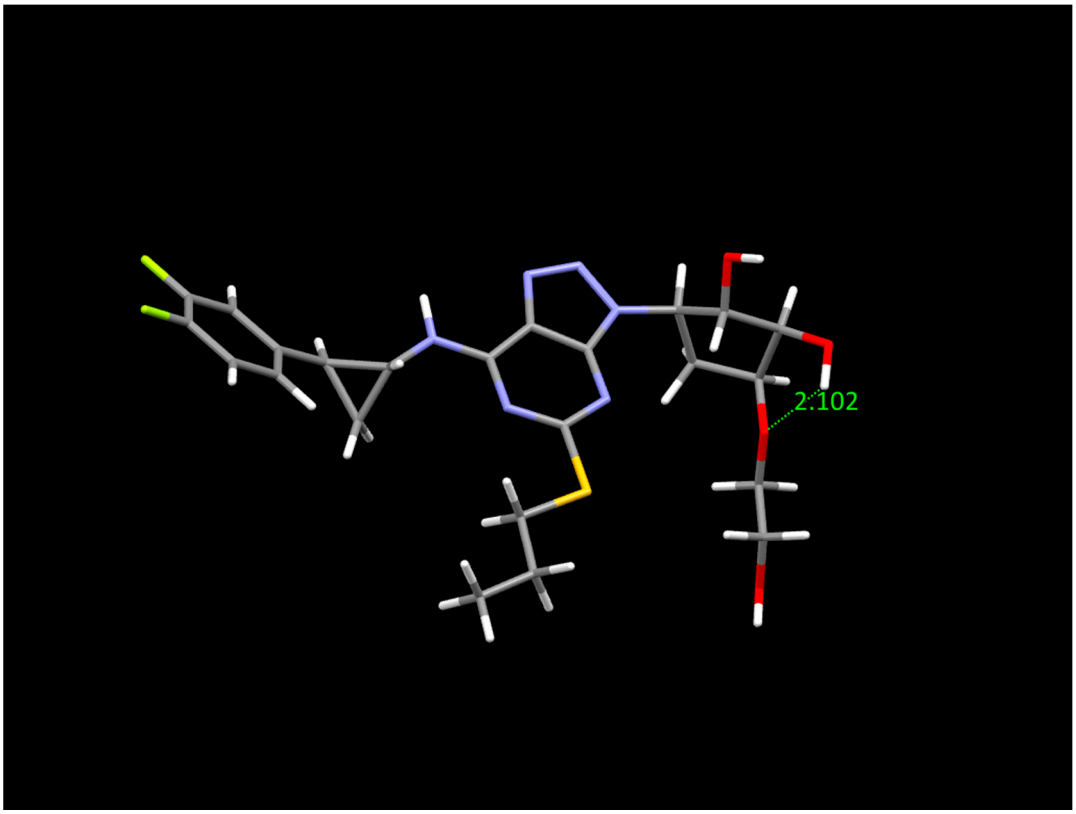


Molecular superimposition of the Becke3LYP-optimized molecular structure of prasugrel (color by connected atoms) and solid state prasugrel from [18] (blue).

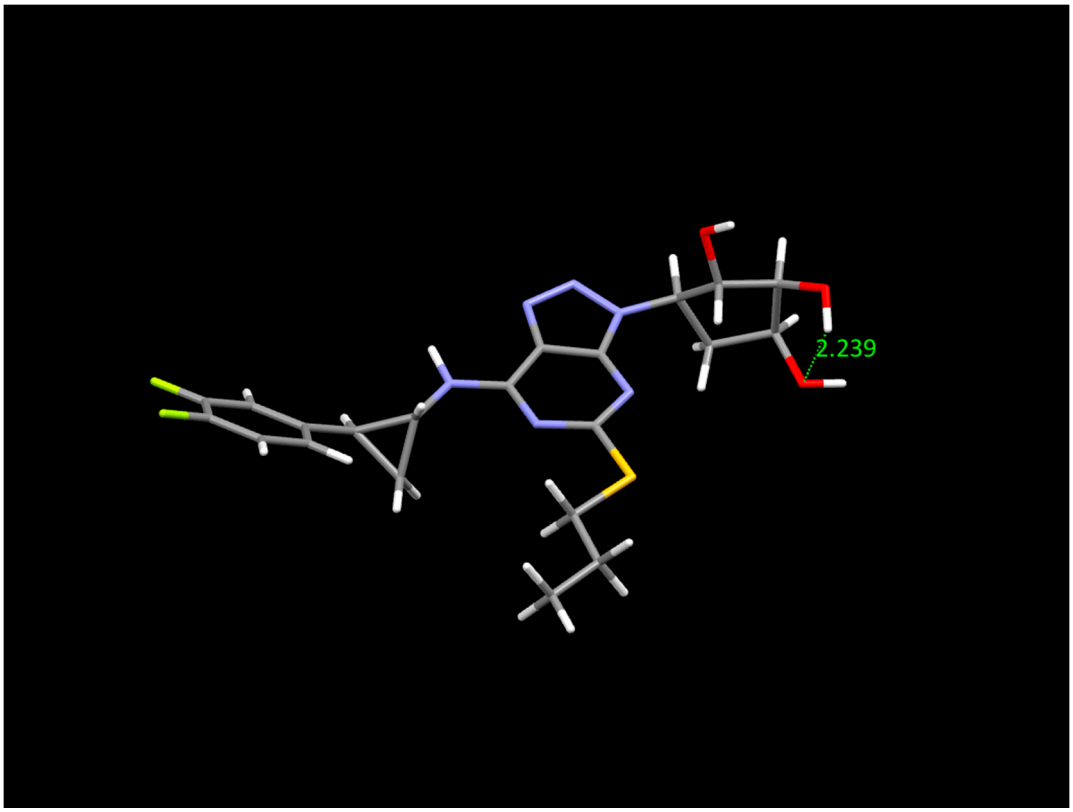
Overall shape of the prasugrel metabolite computed at the Becke3LYP/6-311++G(d,p) level of theory.



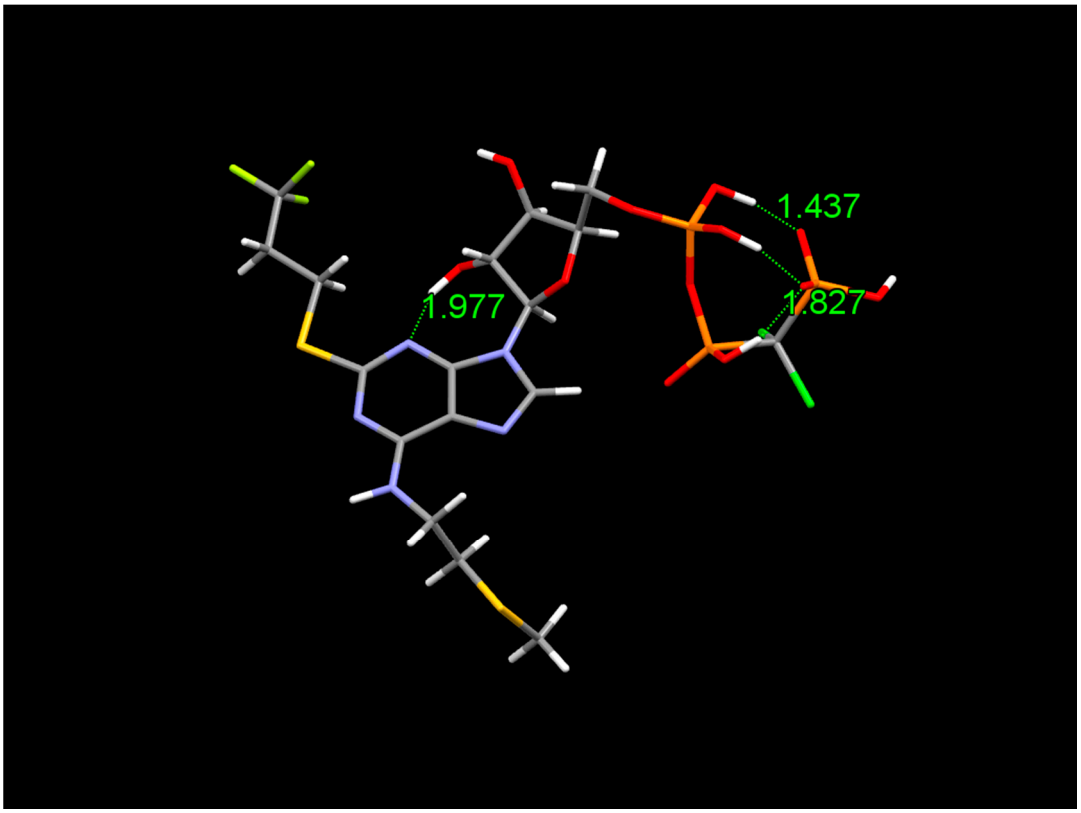
Overall shape of the elinogrel computed at the Becke3LYP/6-311++G(d,p) level of theory.



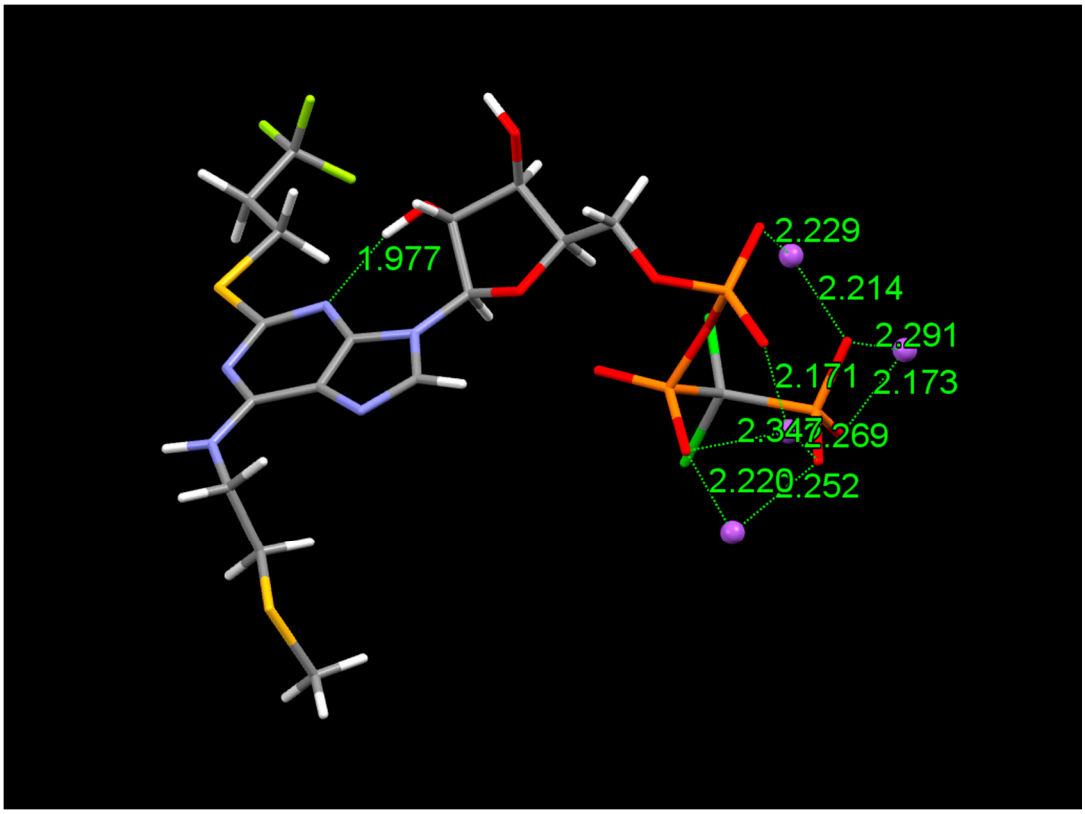
Overall shape of the ticagrelor computed at the Becke3LYP/6-311++G(d,p) level of theory (bond lengths are in Angstroms).



Overall shape of the ticagrelor metabolite computed at the Becke3LYP/6-311++G(d,p) level of theory (bond lengths are in Angstroms).



Overall shape of the cangrelor computed at the Becke3LYP/6-311++G(d,p) level of theory (bond lengths are in Angstroms).



Overall shape of the cangrelor tetrasodium computed at the Becke3LYP/6-311++G(d,p) level of theory (bond lengths are in Angstroms).

Figure S1. The geometries of the drugs studied. Molecule figures were generated using Mercury software (http://www.ccdc.cam.ac.uk/mercury/).