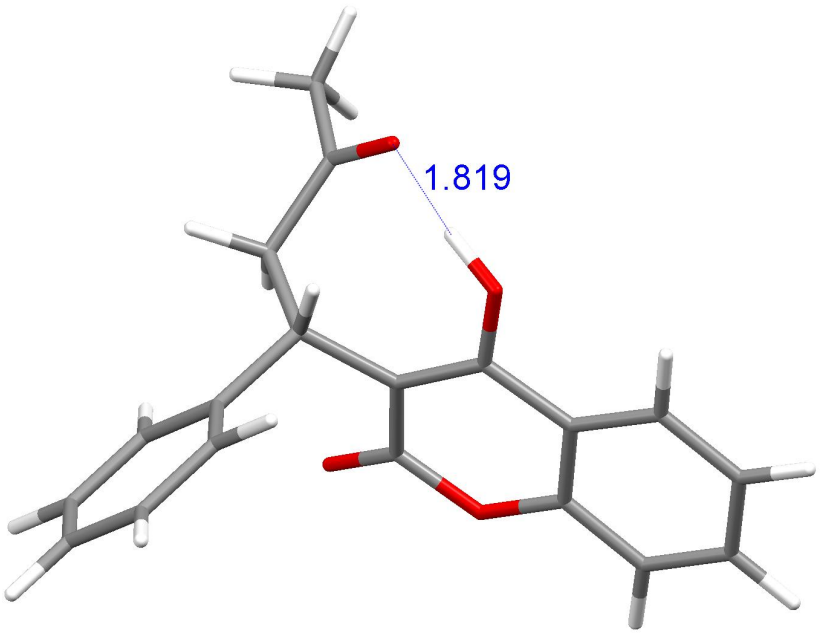
Electronic Supplementary Material (ESI) for RSC Advances

A comparative study of the molecular structure, lipophilicity, solubility, acidity, absorption and polar surface area of coumarinic anticoagulants and direct thrombin inhibitors

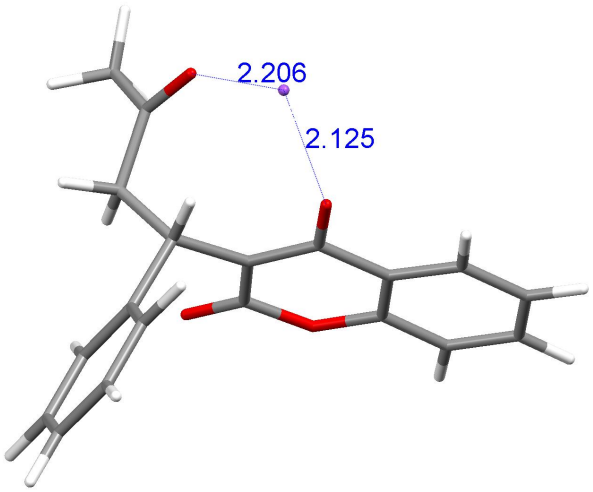
Milan Remko[a,b,*], Ria Broer[c], Anna Remková[b],

[a]*Comenius University in Bratislava, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Odbojarov 10, SK-832 32 Bratislava, Slovakia*
[b]*Center for Hemostasis and Thrombosis, Hemo Medika Bratislava, Šustekova 2, 851 04 Bratislava, Slovakia*
[c]*Department of Theoretical Chemistry, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands*

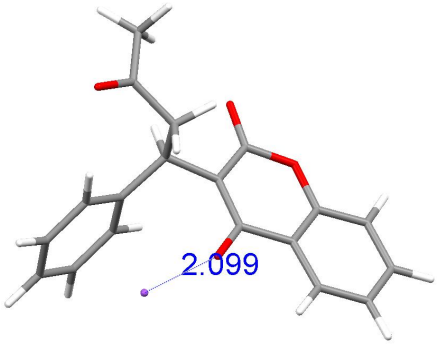
Supporting Material



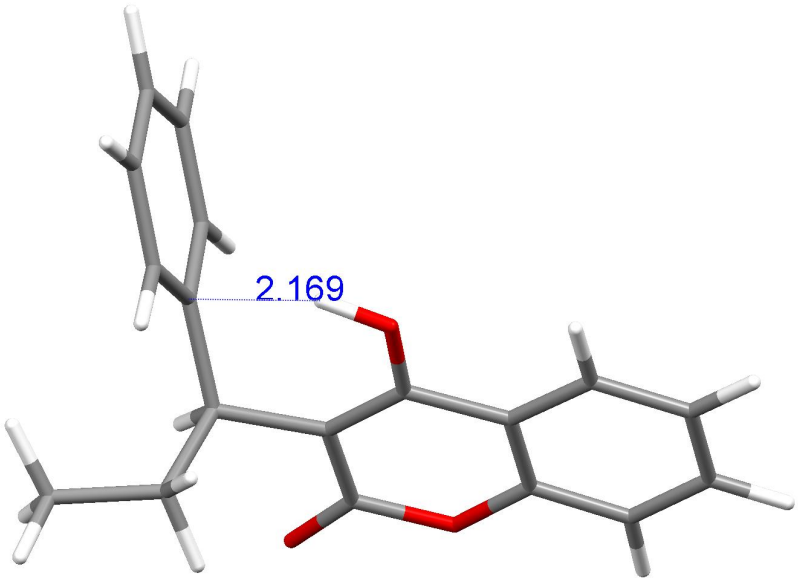
R-Warfarin, tautomer A



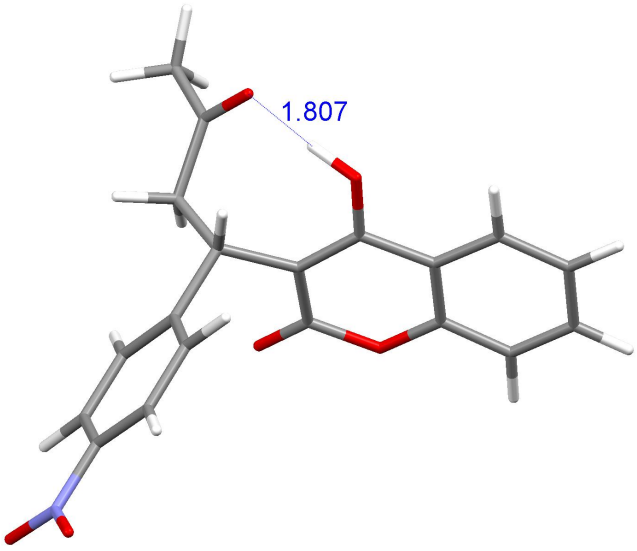
R-Warfarin sodium, tautomer A



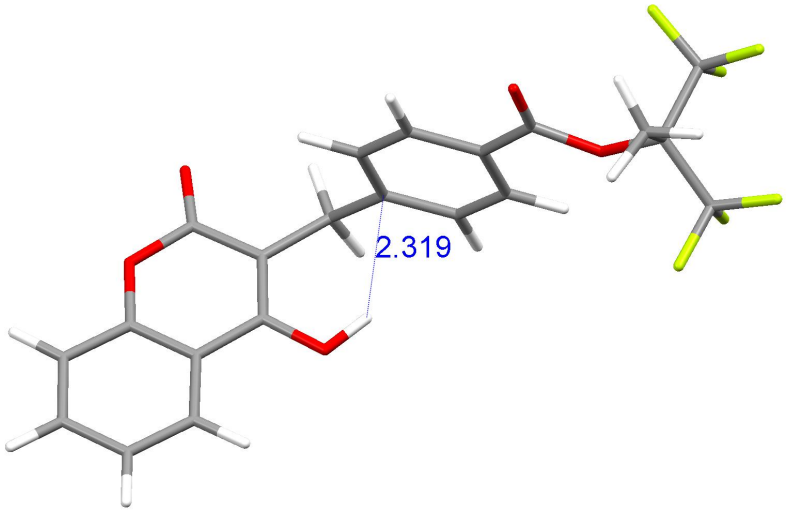
S-Warfarin sodium, tautomer A



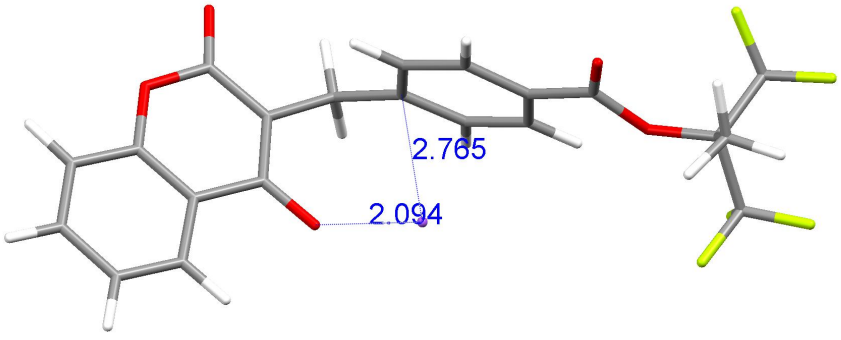
S-Phenprocoumon, tautomer A



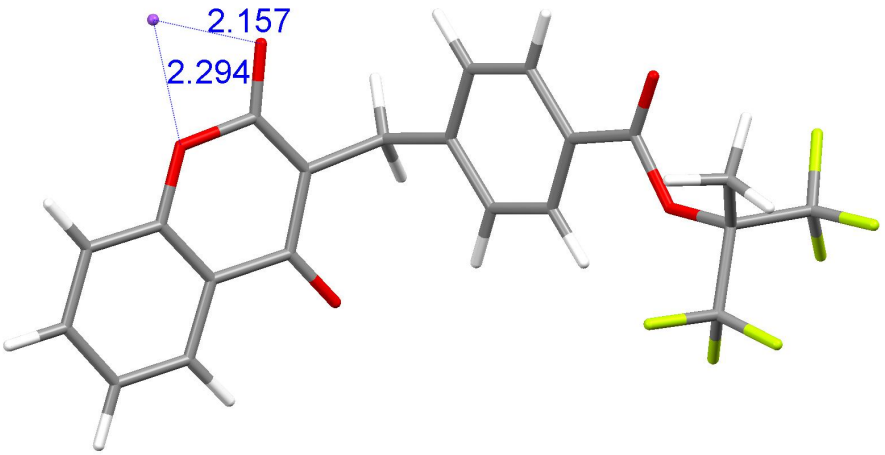
R-Acenocoumarol, tautomer A



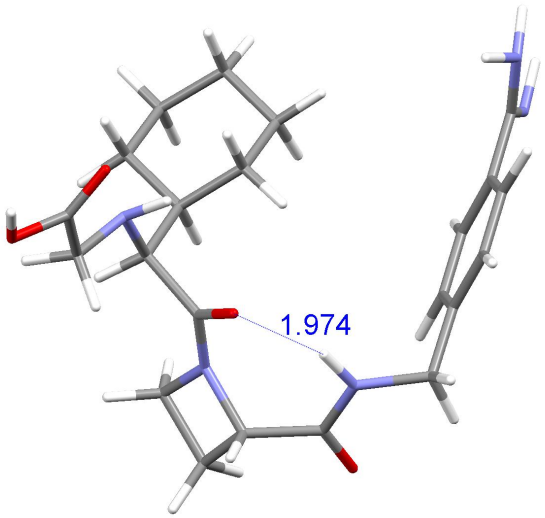
Tecarfarin, tautomer A



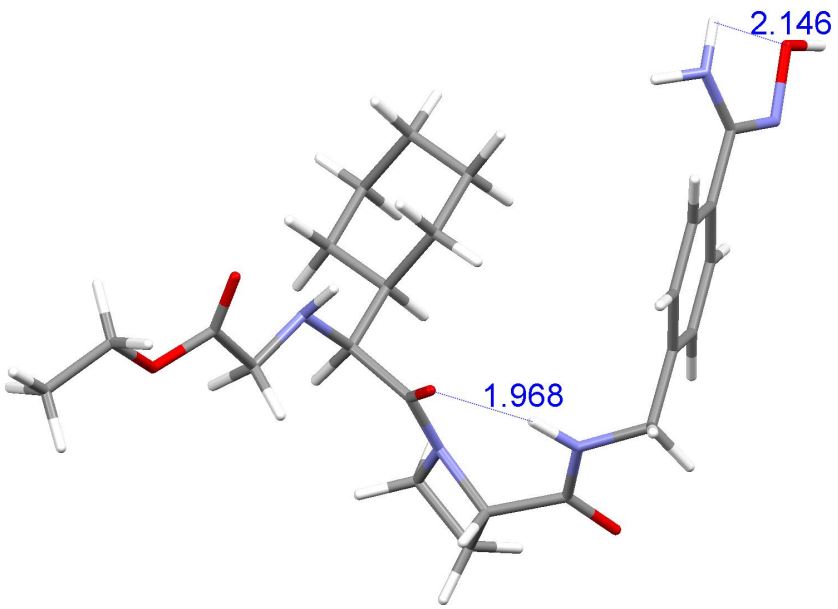
Tecarfarin sodium, tautomer A



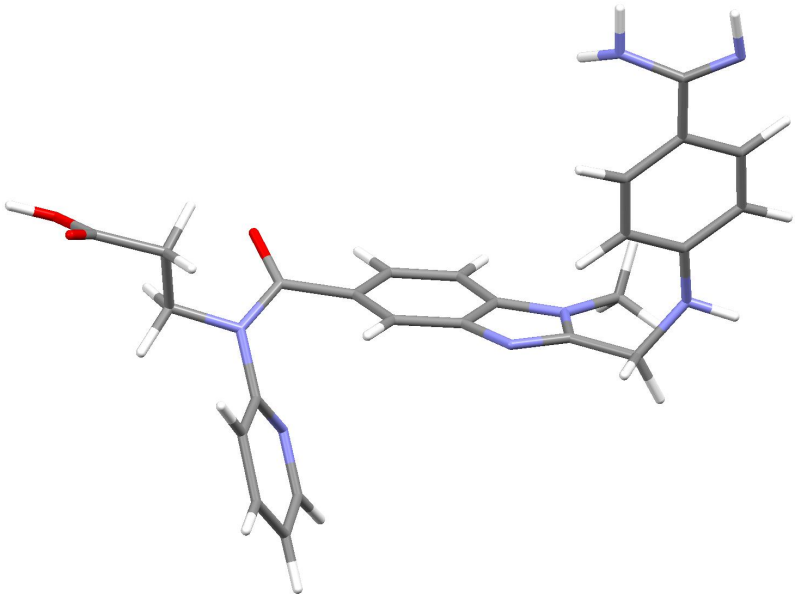
Tecarfarin sodium, tautomer B



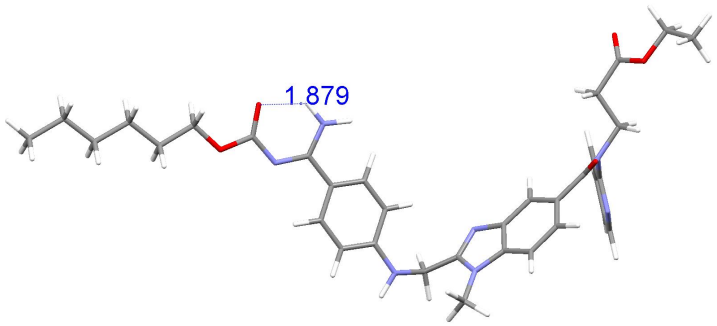
Melagatran



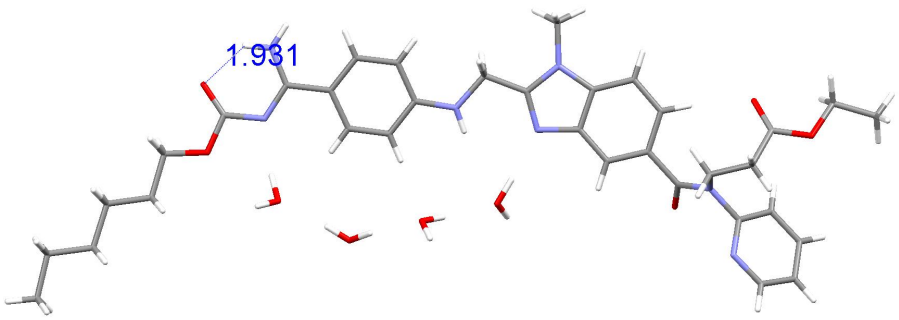
Ximelagatran



Dabigatran



Dabigatran etexilate



Dabigatran etexilate tetrahydrate, X-ray structure from ref. 24

Fig. 1A Overall shape of the most stable conformations of coumarinic anticoagulants and direct thrombin inhibitors (bond lengths are in Angstroms).

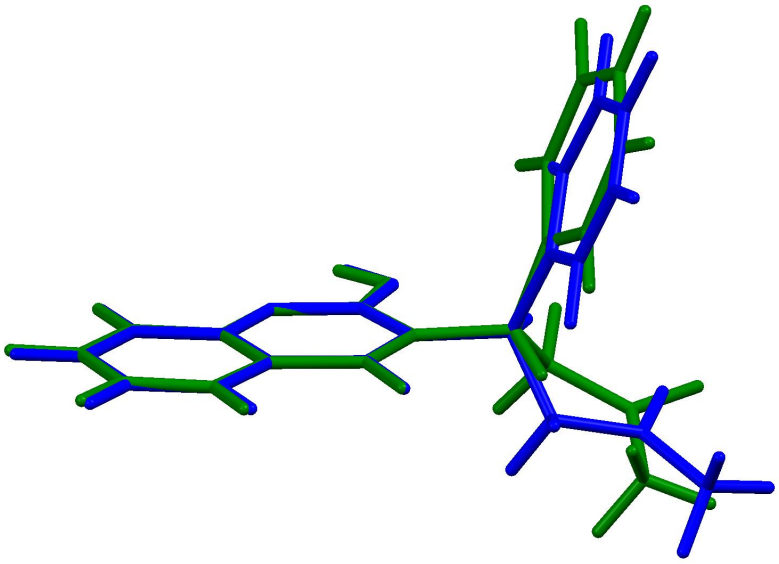


Fig. 2A Molecular superimposition of the *R*(+)-warfarin (blue) and *S*(–)-warfarin (green) from their cocrystals with human serum albumin myristate, PDB 1H9Z, 1HA2.

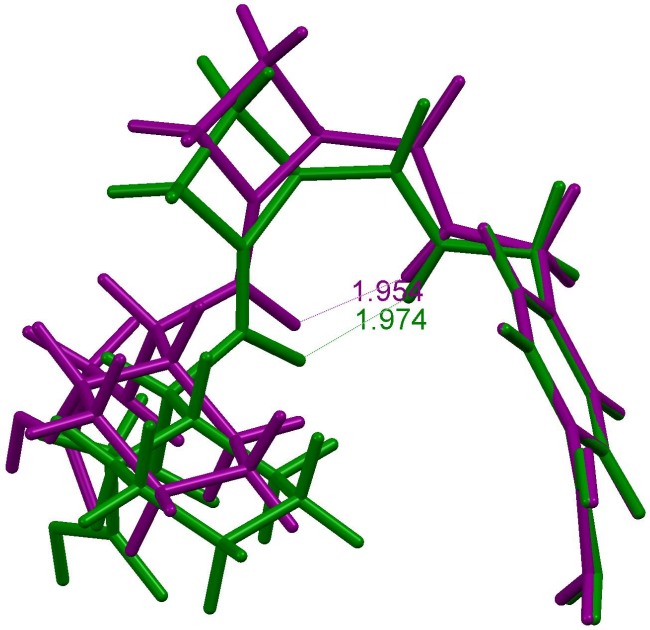


Fig. 3A Molecular superimposition of the DFT optimized melagatran (green) and in solution optimized melagatran (purple).

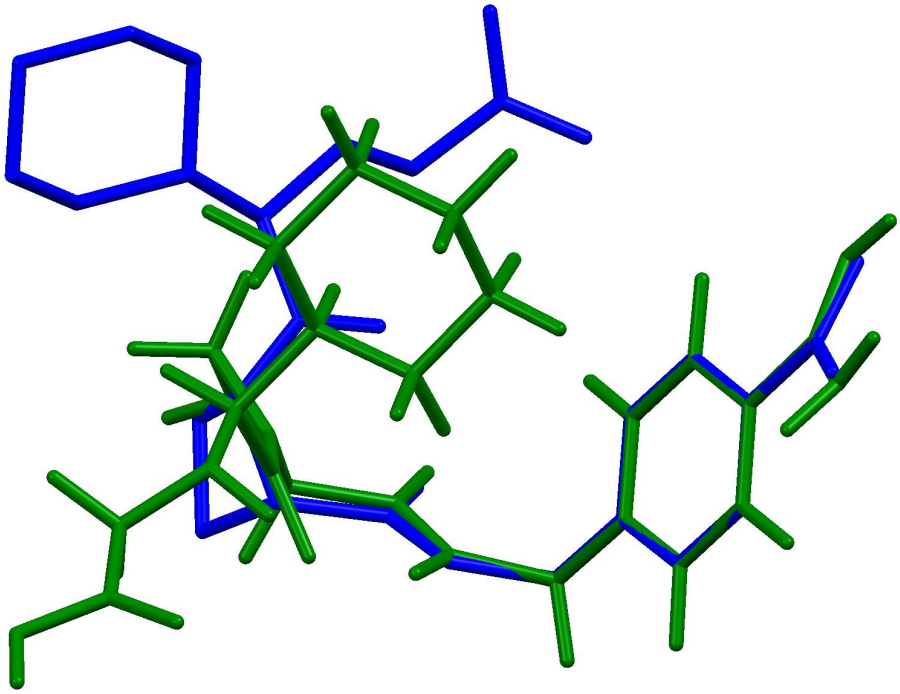


Fig. 4A Molecular superimposition of the DFT optimized melagatran (green) and melagatran from its cocrystal with thrombin (blue), PDB 1K1P.