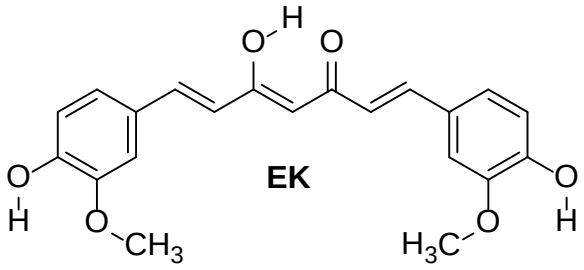
Scientific report

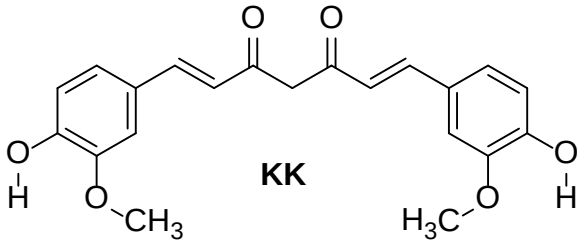
for STSM in Scuola Normale Supriore (Pisa, Italy), host: prof. Chiara Cappelli

of prof. Liudmil Antonov

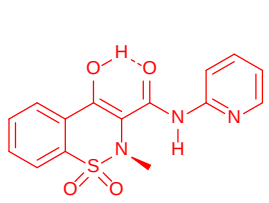
In the frame of two weeks project the following activities have been carried out:

1. Two-way transfer of knowledge between the host (Prof Chiara Cappelli, computational chemistry) and the guest (Prof Liudmil Antonov, experimental spectroscopy) in the field of solvent effect description in tautomeric systems. This includes a lecture given by the guest ("Tautomerism: a historical overview, methods for investigation and challenging cases to study", on Feb 4, 2019) as well as discussions with the host and members of her group (EMBEDLAB@SNS). The following aspects have been discussed: general aspects of the use of QM/MM in solvents effect description (with Prof. Cappelli), description of water on the tautomerism in curcumin and piroxicam (with Prof. Cappelli and Dr. Puglisi, postdoc), photochemical properties and proton transfer in polyphenols (with Mr. Sulejman Skoko, PhD student), tautomerism in theophylline, doxorubicin, ground and excited state proton transfer reactions as well as the possibility for use of AMBIT2 tautomeric structure generator (will Ms Sara Luz Gomez Maya, PhD student).
2. Dr Puglisi was provided a comprehensive review on the computational methodology for solvent effect description developed in EMBEDLAB@SNS.
3. A scientific paper based on the running collaboration between the host and the guest, dealing with the effect of water (by using non-polarizable and fully polarizable QM/MM approaches) on the absorption spectra of the keto-enol and diketo tautomers of curcumin (see the structures below) has been finalized and submitted to PCCP.





4. Calculations devoted to the water effect on the absorption and NMR spectra of the most stable tautomers of piroxicam (marked in red) has started and first results are expected after end of the visit.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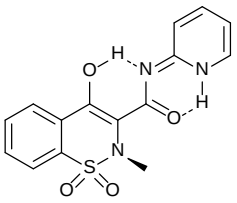
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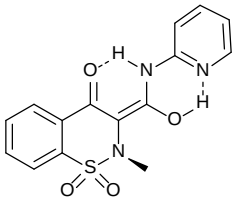
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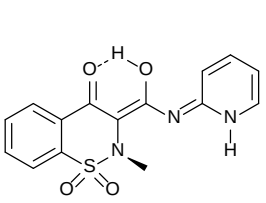
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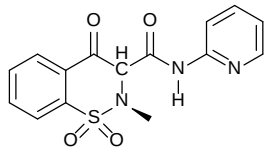
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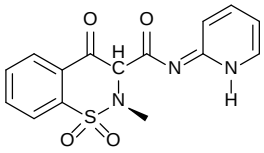
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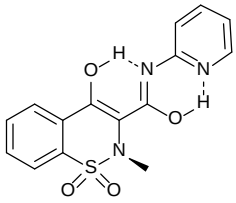
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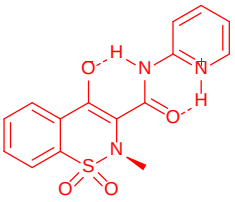
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Generally, the STSM has been very useful for both sides and has open opportunities for collaborative investigations in future.