1. Aim & motivation - Please explain the scientific and/or other motivation for the STSM and what scientific and/or other outcomes you aim to accomplish with the STSM. The tautomerism is a special case of isomerization which strongly depends on the environment. In most of the cases the interactions solute-solvent, that determine the tautomeric state of given organic molecule in solution, are specific and based on formation of intermolecular H-bonds.
Such kind of interactions is difficult to describe by using the standard at moment implicit solvation in the theoretical
calculations. The use of explicit solvent molecules in addition is not the best solution in the case of many possible
interaction sites in the studied tautomers and also from the viewpoint of computational costs. The theoretical
description of the tautomeric of Piroxicam (and other oxicams) is a typical example (RSC Adv., 2015,5, 31852-31860). One of the possibilities of handling the solvent as a continuum of many explicit solvent molecules is the use of the QM/MM approach which combines the accuracy and efficiency. Recently a new development in this
direction was done by Barone and Cappelli by implementing includes a fluctuating charge (FQ) approach to the MM
polarization. The protocol is calibrated against water, which allows a precise description of the equilibrium state and
spectral characteristics in aqueous solutions to be achieved. The aim of the current application is to provide 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. The guest will
earn practical knowledge about the possibilities of using QM/MM approach in the tautomeric research, while the host
will acquire information about the tautomeric processes and methods for their experimental study. The tautomeric
behavior of Piroxicam in water and the simulation of the optical and NMR spectra of the tautomers will be used as a
case study. We hope as a result of this visit collaborative ties to be established. 2. Proposed contribution to the
scientific objectives of the Action. The visit contributes the Action in two ways. From one side we will test the already
developed approach/code on a real tautomeric system, which could lead to improvement and could explain the
experimentally observed data for the tautomerism of Piroxicam in solution. On the other side we expect are result of
this visit a collaborative research to start in future based on the complimentary expertise of the host and guest. Techniques - Please detail what techniques or equipment you may learn to use, if applicable. There is a hope the
applicant to learn about the technology of the QM/MM simulations and to learn in longer perspective how to use the

code developed in Pisa. 4. Planning - Please detail the steps you will take to achieve your proposed aim. The overall visit is planned to be 14 days. The general steps include: a. Familiarization with the environment and computational facilities at the host institution – 2 days; b. Getting in depth with QM/MM and its developments by the host groups via discussions with the members of the group - 3 days; c. Transfer of knowledge from the guest by giving a lecture on the tautomerism and its experimental investigations – 1 day; d. Describbing the tautomeric state of Piroxicam and generating its spectral characteristics by using QM/MM/FQ – 7 days; e. Final discussion – 1 day;