



**STSM grantee (1<sup>st</sup> period):** Bianca Martinengo

**Project Title:** “Sustainable biocatalytic derivatization of antiparasitic natural lipids and Cashew Nut Shell Liquid (CNSL) derivatives using unspecific peroxygenase (UPOs) enzymes”

**Home institution:** University of Bologna – *Alma Mater Studiorum* (Prof.ssa Maria Laura Bolognesi)

**Host institution:** University College London (UCL) (Prof. Daniele Castagnolo)

The STSM has been carried out at UCL, Department of Chemistry, in the research laboratory of Dr. Castagnolo. The goal of this STSM was the derivatization of lipids, CNSL derivatives, and drug building blocks exploiting UPOs enzymes, with the aim of identifying and synthesising compounds with potential improved antiparasitic activity.

During the first part of the project, we managed to develop several biocatalytic reactions on model substrates, both fatty acid and aromatic heterocyclic compounds, bearing different unsaturated moieties using a panel of UPOs available in Dr. Castagnolo’s lab. All the compounds were treated with different UPOs at standard conditions; each biotransformation was monitored by GC-MS, to evaluate the formation of oxidation products, and by (chiral) HPLC to evaluate the enantio- and regioselectivity, and thus the most suitable biocatalysts for further investigations.

Based on preliminary outcomes, we started applying these procedures on CNSL derivatives, for the purpose of understanding the potential exploitation of UPOs in the derivatization of natural/waste products characterized by unsaturated pentadecyl alkyl side chains. Unfortunately, the experiments carried out using UPO enzymes on CNSL mixtures failed. More promising results were obtained using CAL-B – urea hydrogen peroxide (UHP) oxidative system. The reaction was scaled-up and the oxidative product was isolated and characterized by <sup>1</sup>H and <sup>13</sup>C NMR. Further investigations are required to find out more sustainable ways to functionalize the unsaturated chain of CNSL derivatives and if there is possibility to achieve highly stereoselective chemical transformations. Regarding follow-up experiments, we are evaluating the option of performing biological assays to test the antiparasitic potential of crude mixtures and isolated products after biocatalytic reactions, with the purpose of clarifying if the enzymatic derivatization may lead to improved antiparasitic potential.

Regardless of the results obtained, this STSM represented a great opportunity to join a dynamic and international research group at UCL. As expected, I had the opportunity here to learn deeply about Green Chemistry, biocatalysis and enzymatic reactions. Additionally, I acquired skills about techniques and instrument that I could not have acquired otherwise (i.e. set-up and work-up of enzymatic reaction, daily use of Normal Phase (NP) Chiral HPLC, NP and Reverse Phase (RP) HPLC, HPLC-MS, GC-MS).