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Combining *in vitro* and *in silico* techniques: A complex case of metabolite structural assignment

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Liquid chromatography coupled to mass spectrometry (LC-MS) is undoubtedly the most widely used tool for metabolite identification. Despite of its extensive use, there are cases where LC-MS fully automated analyses are not sufficient to predict or to explain a metabolic profile. In this context, we will describe a study where the presence of multiple stereogenic centres and the possibility of epimerization can lead to unexpected chemical transformations. Through a combination of mass spectrometry, synthetic work, deuterium exchange studies and computational predictions we were able to solve a complicated puzzle and to elucidate the dynamic behavior of our metabolites in solution.

Biography

Paolo Schiavini has completed his Bachelor and Master's degree in Chemistry at "Università degli studi di Pavia", in Italy. At the age of 24 he moved to Montreal to pursue a PhD in Chemistry at McGill University under the supervision of Nicolas Moitessier and Karine Auclair. He is currently working on several areas at the interface between chemistry and biochemistry, including computer-aided drug design, drug metabolism and biocatalysis.

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