RICH CONFORMATIONAL LANDSCAPES OF MACROCYCLIC MUSKS BY BROADBAND ROTATIONAL SPECTROSCOPY: AN INSIGHT INTO THE MUSK SCENT MYSTERY

ECATERINA BUREVSCHI, DONATELLA LORU, M. EUGENIA SANZ, *Department of Chemistry, King's College London, London, United Kingdom*.

Musk odorants are key compounds in perfumery due to their warm, sensual and animalistic scent, and their fixative properties. Natural musks are macrocycles typically containing ketone or lactone functional groups. However, despite their widespread use, the molecular features conductive to musk smell are not clear. No experimental information is available on the conformations of macrocyclic musks and the structural elements determining their binding to odorant receptors. Here we present the study of several prototypical macrocyclic musks using broadband microwave spectroscopy in combination with quantum chemistry calculations. Their conformations have been identified and compared to start understanding the molecular determinants that lead to musk odour.