



# Soutenance de thèse

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## **Environment effects on chiral recognition : a spectroscopic study**

This work focuses on the study of chirality effects on the structure of cyclic dipeptides built on a diketopiperazine (DKP) ring with residues of identical (LL) or opposite (LD) chirality. The same systems are studied in different environments by means of optical spectroscopy coupled to quantum chemical calculations. The neutral molecules are isolated and cooled down to a few K in a supersonic expansion and characterized by UV and conformer-specific IR laser spectroscopy. The structure of the protonated systems, isolated in an ICR mass spectrometer, is determined by infrared multiple photon dissociation spectroscopy. Last, vibrational circular dichroism (VCD) is applied to the solid-state samples.

The studied systems possess an aromatic residue, either tyrosine (cyclo Tyr-Pro) or phenylalanine (cyclo Phe-Phe and Phe-His). The LD diastereomer is in most of the cases less stable and more flexible than LL. LL and LD differ from each other by weak interactions like NH... $\pi$  or CH... $\pi$  interactions. The most stable conformer usually corresponds to a structure with the aromatic chromophore folded over the DKP ring, the other part being extended. A dramatic effect of chirality is observed for some of the protonated dimers. Last, VCD experiments in the condensed phase show that the crystal phase of LPhe-DPhe formed by solid-state dehydration of the linear dipeptide is chiral due to synchronization of the transient chirality of the monomers.

**Vendredi 1<sup>er</sup> décembre 2017 à 14h30**

**Bât 210 – Amphi 1 (2<sup>ème</sup> étage)**

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*La soutenance sera suivie d'un pot auquel vous êtes chaleureusement conviés.*