

TWELVE CONFORMERS OF 4-FLUOROTHREONINE UNVEILED BY LASER ABLATION ROTATIONAL SPECTROSCOPY

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Fluorinated amino acids are rare bio-organic compounds gaining great relevance in the pharmaceutical field. 4-fluorothreonine (4FT) is the only natural fluoro amino acid discovered so far. The fluorination of the methyl group significantly increases the complexity of the already intricate conformational panorama of threonine^a, making any conformational study even more challenging. Guided by state-of-the-art machine-learning methodologies^b and using a tandem of laser ablation rotational spectroscopies, up to twelve rotameric species have been discovered in the supersonic expansion of our experiments. These species have been ascribed to twelve of the thirteen low-energy predicted conformers based on rotational constants, nuclear quadrupole coupling constants, and dipole moment selection rules. These results again proved the potential of the laser ablation rotational spectroscopy techniques in structural studies of non-volatile solid biomolecules.

^aAlonso J. L., Pérez C., Sanz M. E., López J. C., Blanco S. *Phys Chem Chem Phys.* 2009 Jan 6;11(4):617–27

^bLeón I, Fusè M, Alonso ER, Mata S, Mancini G, Puzzarini C, et al. *J Chem Phys.* 2022;157(7).