The Conformational Space of the Neurotransmitter Serotonin: How the Rotation of a Hydroxyl Group Changes All

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Electronic Supplementary Material

The supporting online material contains :

1. The tree diagram of the 14 most stable conformers of serotonin.

2. The rotationally resolved spectra of the electronic origins of the B, C and F conformers of serotonin.

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Supplementary Figure S1: Tree diagram of the 14 most stable conformers of serotonin. The name of each conformer arises from the position of the amino group (Gph, Gpy, Anti), given first and shown with their respective Newman projection, the orientation of the amino group group relative to the indole chromophore (up, out, ph or py) and the orientation of the hydroxyl group (*syn* and *anti*), given at the end of the name.



Supplementary Figure S2: Rovibronic spectrum of the electronic origin of the B conformer of serotonin along with a simulation using the best CMA-ES fit parameters, given in the full article.



Supplementary Figure S3: Rovibronic spectrum of the electronic origin of the C conformer of serotonin along with a simulation using the best CMA-ES fit parameters, given in the full article.



Supplementary Figure S4: Rovibronic spectrum of the electronic origin of the F conformer of serotonin along with a simulation using the best CMA-ES fit parameters, given in the full article.