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Title:	Relative stabilities and the spectral signatures of stacked and hydrogen-bonded dimers of serotonin
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	serotonin dimer conformer stability hydrogen bond and stacking absorption maxima
Issue Date:	2015
Publisher:	Taylor and Francis Ltd.
Citation:	Molecular Physics, 113(19)
Abstract:	The O–H...N hydrogen-bonded dimer of serotonin is shown to be more stable than the stacked dimer in its ground electronic state, by using the Møller–Plesset second-order perturbation theory (MP2) and the 6–31g** basis set. The vertical excitation energy for the lowest $\pi \rightarrow \pi^*$ transition for the monomer as well as the dimer is predicted by time-dependent density functional theory. The experimentally observed red shift of excitation wavelength on oligomerisation is explained in terms of the change in the HOMO–LUMO energy gap due to complex formation. The impact of dimer formation on the proton magnetic resonance spectrum of serotonin monomer is also examined.
Description:	Only IISERM authors are available in the record.
URI:	<a href="https://www.tandfonline.com/doi/full/10.1080/00268976.2015.1060365">https://www.tandfonline.com/doi/full/10.1080/00268976.2015.1060365</a> ( <a href="https://www.tandfonline.com/doi/full/10.1080/00268976.2015.1060365">https://www.tandfonline.com/doi/full/10.1080/00268976.2015.1060365</a> ) <a href="http://hdl.handle.net/123456789/2745">http://hdl.handle.net/123456789/2745</a> ( <a href="http://hdl.handle.net/123456789/2745">http://hdl.handle.net/123456789/2745</a> )
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