Computational Study of Resveratrol

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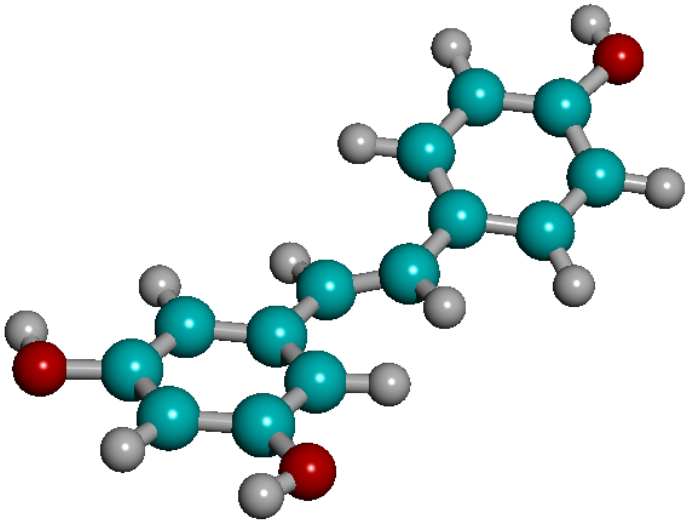
Resveratrol has many interesting and important properties ranging from being an anti-fungal agent in plants to a wine constituent thought to reduce heart disease.[1] Building on our previous work done on the related structures of stilbene and 4-nitro-4'-dimethylaminostilbene (DMANS), this study looks at the structural conformations and electronic properties of resveratrol.[2,3,4] The computational methods used in this study include, but not limited to, molecular dynamic simulations (AMBER 7 and HyperChem 6.0) and quantum chemical (Gaussian 98) in various degrees of solvation.



Trans-resveratrol

[1] Trela, B.C.; Waterhouse A.L. Resveratrol: Isomeric Molar Absorptivitives and Stability. *J. Agric. Food Chem.* **1996**, 44, 1253-1257.
[2] Soo Hoo, Yong; Barker, Beau; Smith, Jonathan M. "Spectroscopic and computational study of charge-transfer in 4-dimethylamino-4'-nitrostilbene", **2001**, American Chemical Society Fall National Meeting, Chicago.
[3] http://www.gustavus.edu/oncampus/academics/chem/pchem/44stilb/44stilb.html
[4] Morley, J. O. "Theoretical calculations of the structure of a donor-acceptor stilbene, azobenzene and related molecules". *Journal of Molecular Structure (Theochem)* **1995**, *340*.