AMINO ACIDS AND PEPTIDES (AAP) STRUCTURES, ENERGETICS AND SPECTROSCOPY (SES) DATABASE

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Derivation of structural, energetic, and spectroscopic properties for amino acids and polypeptide conformers from highly accurate theoretical approaches or mixed experimental-theoretical ones allows to set-up a database consistent with experiments $https://github.com/VibESLab/AAP\_SES\_DataBase$.

In this work, we present works towards the set-up of database, which will extend over purely computational databases available so far. Both semi-experimental and accurate theoretical data make a reliable reference and their combination allows an extensive benchmark exploration of DFT methodologies. In fact, the application of DFT for specific properties usually requires careful benchmarking, but the databases available in literature usually tend to focus on the DFT performance for the computation of atomic and molecular energies rather than on structural and spectroscopic parameters. In this work we focus on the structural and spectroscopic properties as well as conformational energies suggesting that desired accuracy can be obtained by means of dispersion-corrected double hybrid functionals (DHF).

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