

Sound Thermodynamic Properties Prediction for the Drug Design and Development in Pharmaceutical and Agrochemical Research Using COSMO-RS

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Thermodynamic property predictions are very often needed for drug design and development in pharmaceutical and agrochemical research. Most available prediction techniques are based on group contributions or increments, or at least on the recognition of certain functional groups, which often limits their applicability to compounds out of known classes. The quantum chemical based COSMO-RS method can well overcome such restrictions and it can provide a more fundamental – although not an ab initio – approach to thermodynamic properties of drugs and agrochemicals. The present state and current developments for COSMO-RS application in this area will be presented.