The Electronic-Structure Informatics Web Platform for Discovery of Functional Molecules

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We will introduce our recently developed web platform for electronic-structure informatics (ESI). It is an emerging informatics in which electronic features of molecules are taken into account for machine learning studies predicting molecular properties and drug activity. Using this platform, machine learning (ML) can be easily applied even by non-experts of ML. In this presentation, we will show the capability of our ESI platform including application of the ESI database, evaluation of ESI descriptors using RDKit descriptors, i.e. without performing quantum chemistry calculations, and their use in regression modeling.