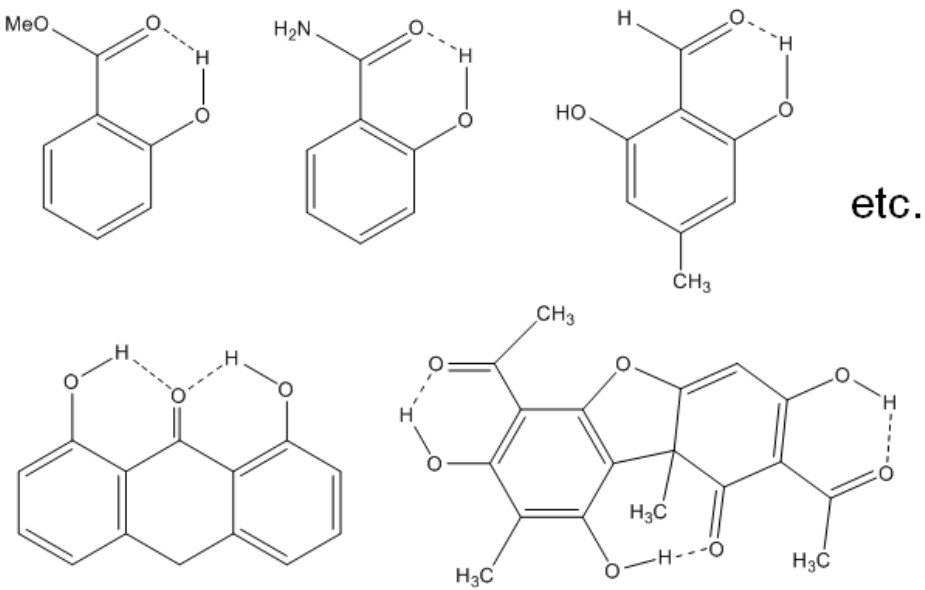
Computer Chemistry:

Hydrogen bonding



Dithranol Usnic Acid

”Computer Chemistry” is today an indispensable tool in the solution of chemical problems. Modern molecular modelling procedures contribute to the solution of complex problems in current chemistry and bio-chemistry [1]. But the phenomenon *hydrogen bonding* still causes theoretical difficulties. It is well known that hydrogen bonds play a fundamental role in chemistry and in molecular biology, f. inst. in *DNA*, *proteins*, and *carbohydrates*; but they are difficult to model. In general, accurate theoretical descriptions of hydrogen-bonded structures require the application of advanced and time-consuming quantum chemical calculational procedures [2].

The aim of the proposed project is to investigate if simpler and less expensive models based on so-called semi-empirical procedures can describe a *series* of several compounds with *intra-molecular hydrogen bonds* between carbonyl and hydroxy groups, *i.e.*, containing the structural element >C=O···H–O–. This group of compounds includes pharmaceutical drugs and biologically active substances like Dithranol, Usnic Acid, a.o. The project is a continuation of recent research at NSM [2] and can use the facilities in NSMs ”PC-lab” using the software package ”HyperChem”©.

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[1] J. Spanget-Larsen, *dansk kemi* **91**, 25-26 (2010).
[2] J. Spanget-Larsen, B.K.V. Hansen, P.E. Hansen, *Chem. Phys.* **389**, 107-115 (2011);
P.E. Hansen, J. Spanget-Larsen, *J. Mol. Struct.* **1018**, 8-13 (2012).