

## COMPOUND DESIGN PROCESS - TO A BETTER START

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Molecule and formulation design is an information demanding activity, since all relevant knowledge is to be accessible within a single space and requires synchronized application of computational models to assist decision making on synthesis candidates. Our study aims to evaluate a software platform coping with this complexity (Marvin Live). The tool provides central management of innovative ideas and helps triage them based on predicted properties and available knowledge collected from a variety of sources. The calculated properties span physico-chemical descriptors, combined metrics, 3D overlay and modelling results, with the ability to check if they are compliant with local and international regulations. Use cases of rapid freedom to operate analysis by ultra-fast searching (MadFast Similarity Search) of exemplified structures from patents (SureChEMBL, ~17M entries) and opened access documents and databases in real time will be shown to ensure that designers can seamlessly exploit the chemical space around their ideas. The poster will walk through an example compound design cycle to obtain statistical results regarding performance as well as to demonstrate the suitability of the calculations.