Subject: Re: Molecular Descriptors Tools (Free for non-commercial use)
Posted by Paul on Wed, 28 Sep 2022 18:01:01 GMT
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For organic compounds, Mordred is the best overall I have used. It's not been maintained for several years, so some tweaks to the freely available code are necessary (solutions are documented in the Issues tab on the Mordred Descriptor Github page). Mordred is mostly a convenient interface to descriptors calculated by RDKit, so that, too, is obviously an option (Mordred also makes sure implicit H atoms are presented correctly for calculations). Padel Descriptor and CDK Descriptor are free java interfaces to descriptors from CDK libraries. The other free program I've used that calculates a large number of descriptors is MOLD², free from the US FDA.GOV. In any case, users must
supply chemical logic (e.g., say you calculate a descriptor called "average ESP charge on a Q atom." Some programs may return no value for a molecule with no Q atoms, while others may incorrectly return a zero value.) Furthermore, validation is advisable, as descriptor values may vary between the programs, e.g., handling of implicit hydrogen atoms can cause differences. The adage "garbage in, garbage out" applies.

P.