

Data curation: Calculated properties

1. Phase 1:

a. Curation of computationally determined properties of APIs

- ✓ Properties like molecular formula, number of rotatable bonds, Topological Polar Surface Area (TPSA), etc. in current versions are fetched from PubChem.
- ✓ For the missing entries we can calculate using RDKit.

b. Curation of experimentally determined properties of APIs

- ✓ Collect experimentally measured values for melting point, pKa, logD, solubility, enthalpy of fusion, and P_{eff} from various sources.
- ✓ The experimental data for these properties was either downloaded, fetched, scraped, or cleaned from different public sources /repositories.