This short communication presents a generic mathematical programming formulation for Computer-Aided Molecular Design (CAMD). A given CAMD problem, based on target properties, is formulated as a Mixed Integer Linear/Non-Linear Program (MILP/MINLP). The mathematical programming model presented here, which is formulated as an MILP/MINLP problem, considers first-order and second-order molecular groups for molecular structure representation and property estimation. It is shown that various CAMD problems can be formulated and solved through this model.
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