A Machine Learning Based Computer-aided Molecular Design/Screening Methodology for Fragrance Molecules

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Hightlights

- A computer-aided molecular design/screening method is developed for fragrance molecules.
- The odor of molecules are predicted using a data driven machine learning approach.
- A MILP/MINLP model is established and decomposition-based solution approach is applied for the design/screening.
- Case studies highlighting the effectiveness of the developed model are presented.