Learned chemical perception of force field typing rules using Monte Carlo sampling
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- FORCE FIELDS (FF) GIVE THE ENERGY AND FORCES OF AN ATOMIC SYSTEM AS A FUNCTION OF THE COORDINATES.
- WE USE FF TO RUN MD OR MC SIMULATIONS.
- CONSIDERABLE HUMAN EXPERTISE IS REQUIRED FOR FF DEVELOPMENT.
- CHEMICAL PERCEPTION THROUGH ATOM TYPES (INDIRECT) CAN RELY ON EXPERT HUMAN INTUITION AND HAND-TWEAKING, CAN RESULT IN A POOR DATA STRUCTURE, AND CAN LEAD TO MANY REDUNDANT PARAMETERS.

BACKGROUND

WE DEVELOPED TWO TOOLS

SMARTY

SMIRKY

FRAGMENTS

SMARTY AND SMIRKY REPLACE HAND PICKED ATOM TYPES USING MONTE CARLO SAMPLING

INPUT

Molecule Sets

ATOM TYPES

PARAMETRIZED

INDIRECT

GOAL: BE ABLE TO LEARN CHEMICAL PERCEPTION OF MOLECULES WHILE SAMPLING OVER ATOM TYPES OR FRAGMENTS

METHODS

SMARTY AND SMIRKY RECOVER ALL ATOM TYPES AND FRAGMENTS OF AlkEthOH AND PhEthOH

WORKFLOW

PROPOSED ATOM TYPES OR FRAGMENTS ARE SCORED USING A BIPARTITE GRAPH

RESULTS

SMARTY

SMIRKY

100 % SUCCESS ON AlkEthOH AND PhEthOH SETS

SCORE AS A FUNCTION OF ITERATION

CONCLUSION

THIS STUDY DEMONSTRATES PROMISING RESULTS WHERE WE CAN REPLACE THE HUMAN EXPERT WITH AN AUTOMATED MACHINERY FOR SAMPLING DIRECT CHEMICAL PERCEPTION.

MiniDrugBank IS SIGNIFICANTLY MORE CHALLENGING FOR SMARTY AND SMIRKY

FREQUENCY OF SUCCESS FOR SMARTY/SMIRKY SIMULATIONS WITH AlkEthOH AND PhEthOH

CONSEQUENCES

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