

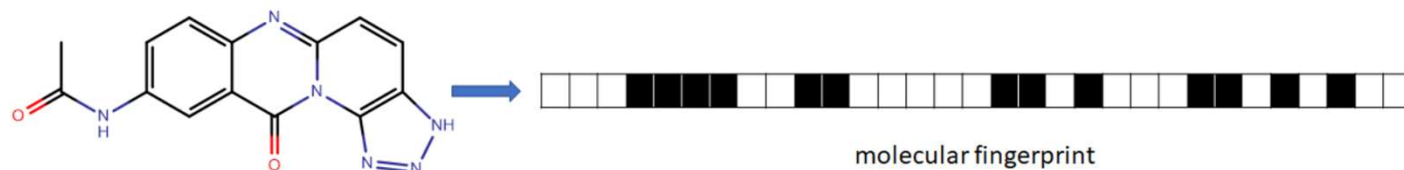
Hackathon Presentation

by

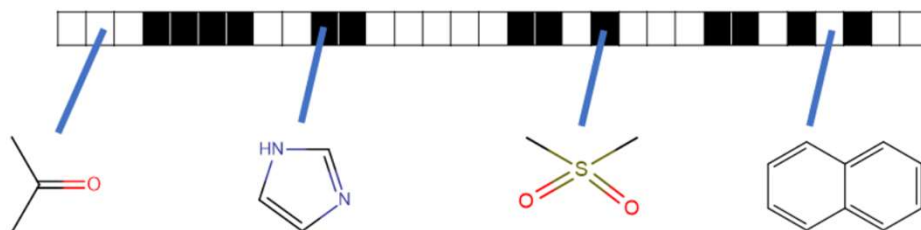
Odetocode

ML4Science,202

Computing Molecular Descriptors:

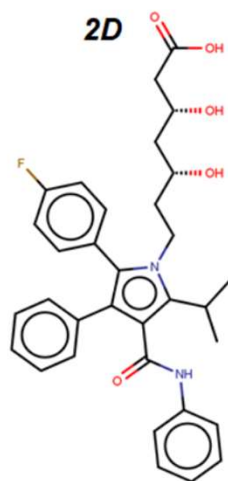


2D Fragment-based, keyed fingerprints: each bit position monitors the presence or absence of structural fragments, e.g. MACCS (166 bits)

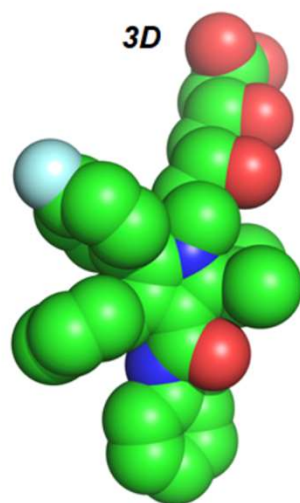


0D/1D

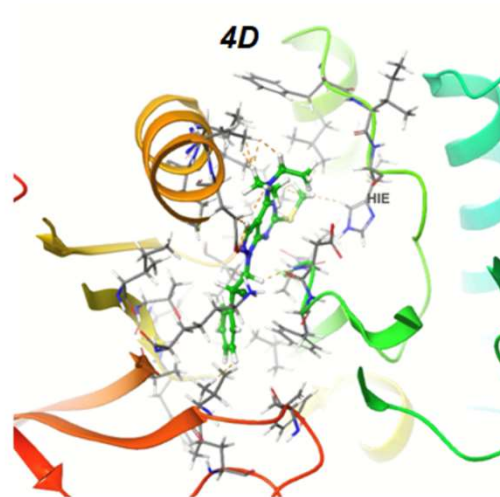
$C_{33}H_{35}FN_2O_5$



3D

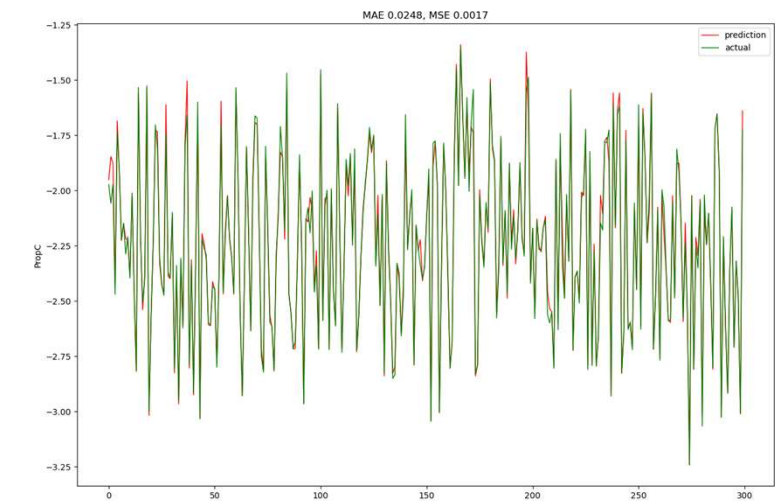
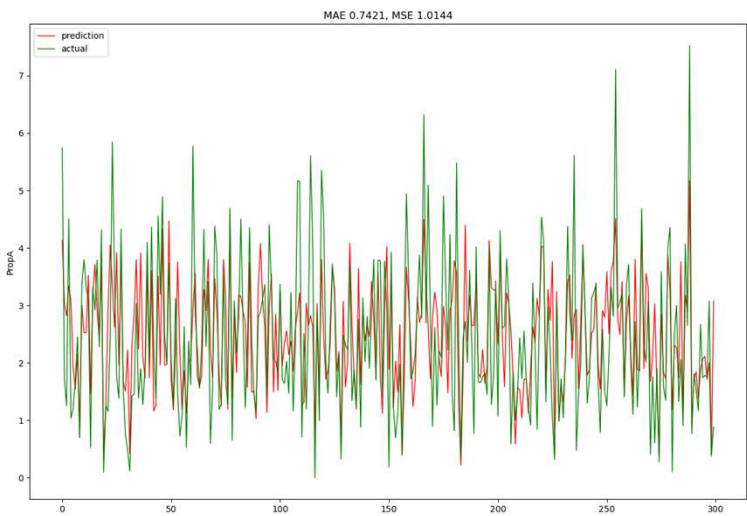


4D



RandomForestRegressor,RidgeCV

Train-split: 90%-10%, 5 CV



| R2 score (Train) | R2 score (Evaluation) |
|---------------------|--------------------------|
| 0.91 | 0.42 |
| 0.93 | 0.89 |
| 0.99 | 0.99 |
| 0.93 | 0.87 |

