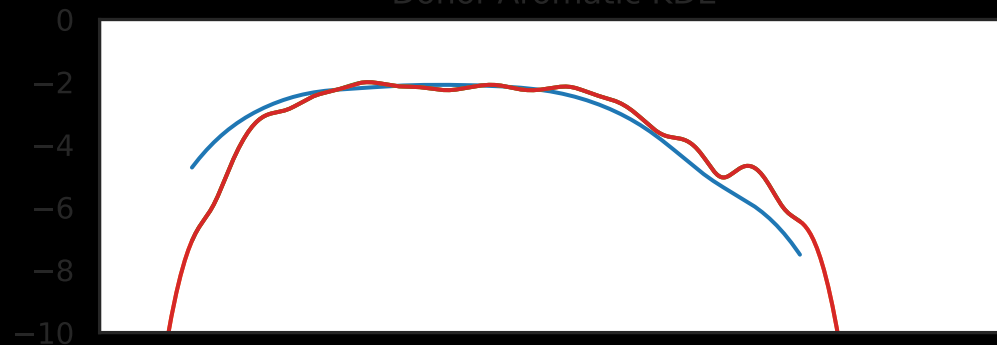


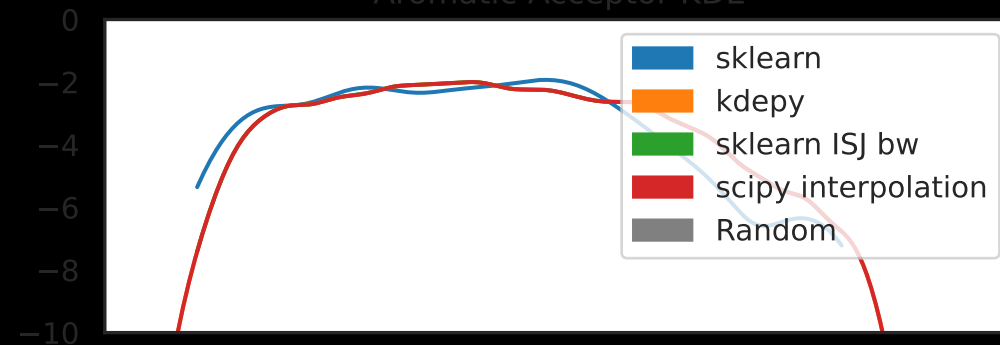
Mpro

Probability Density

Donor-Aromatic KDE

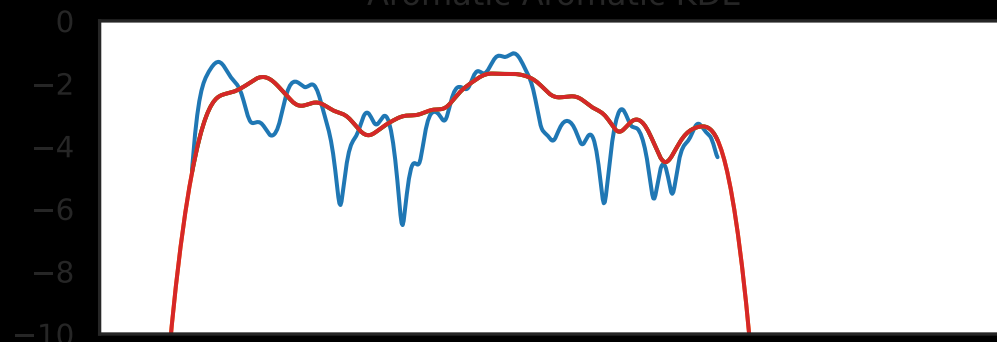


Aromatic-Acceptor KDE

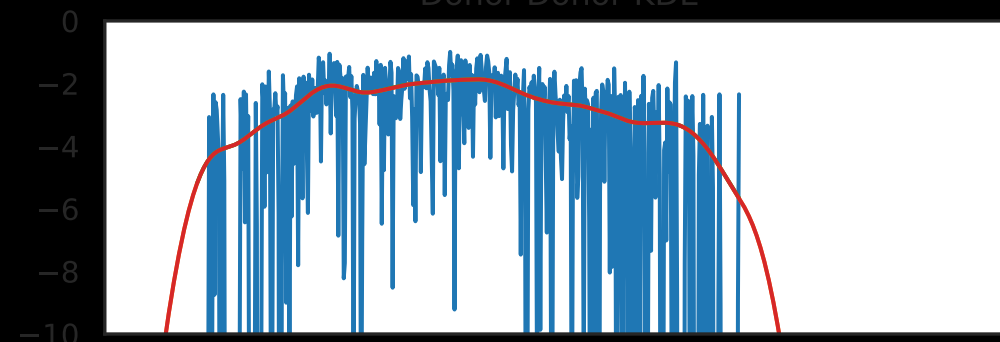


- sklearn
- kdepy
- sklearn ISJ bw
- scipy interpolation
- Random

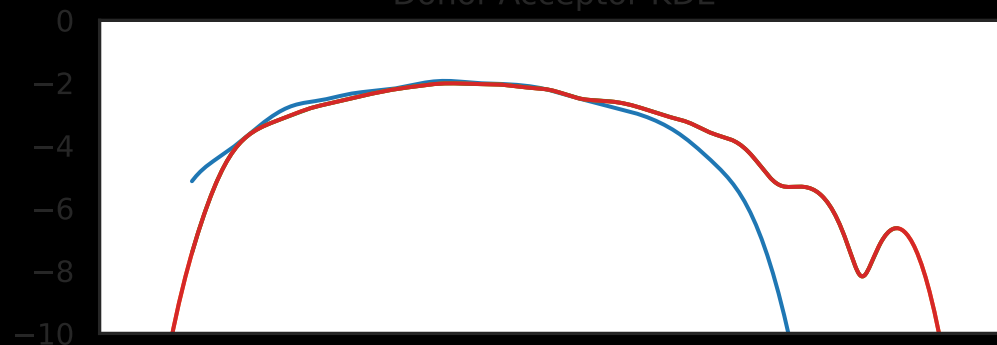
Aromatic-Aromatic KDE



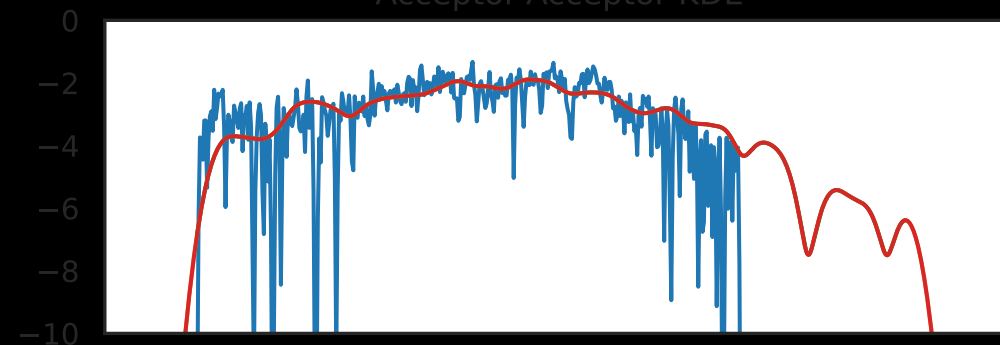
Donor-Donor KDE



Donor-Acceptor KDE



Acceptor-Acceptor KDE



Distance (angstrom)