

Stanford HTBC Small Molecule Library

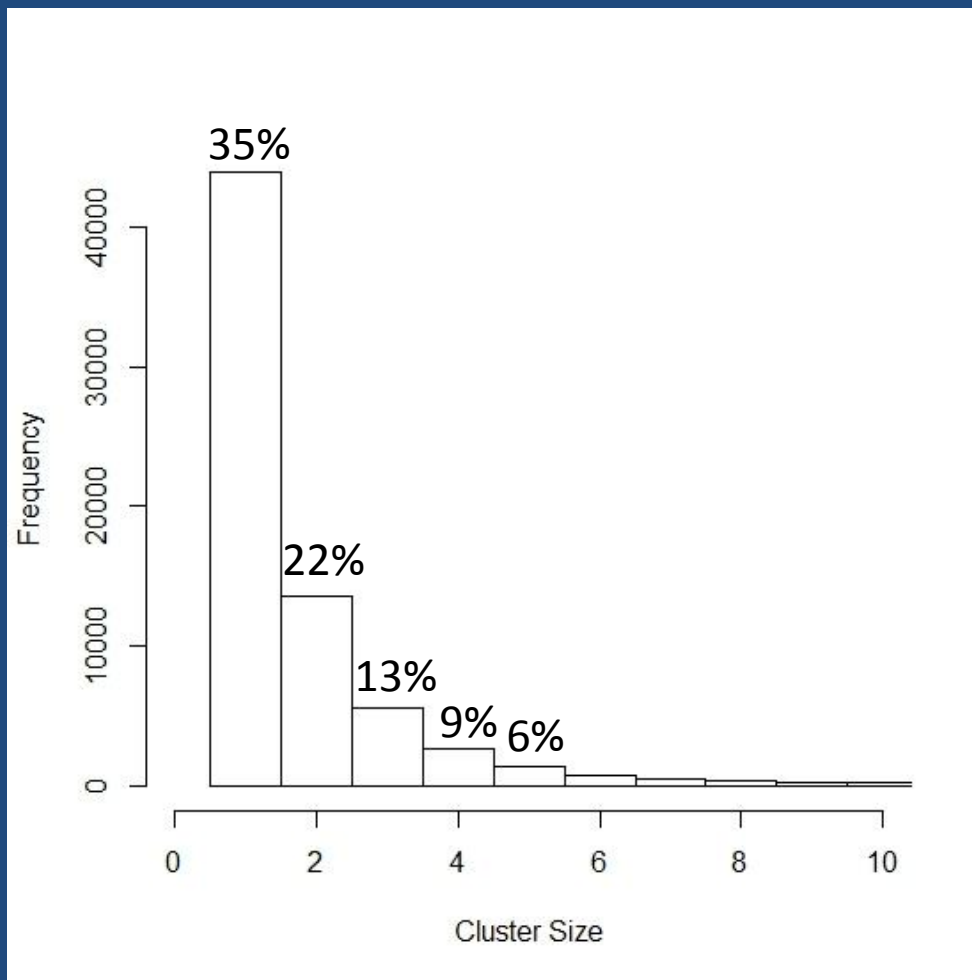
HTBC Small Molecule Library

>130,000 compounds

- Main Sources:
 - ChemDiv (50,000)
 - SPECS (30,000)
 - Chembridge (23,500)
- Smaller Libraries
 - FDA Approved Drug Library
 - NIH Clinical Collection and NCI DTP
 - LOPAC1280 and Biomol ICCB know bioactives
 - Microsource Spectrum

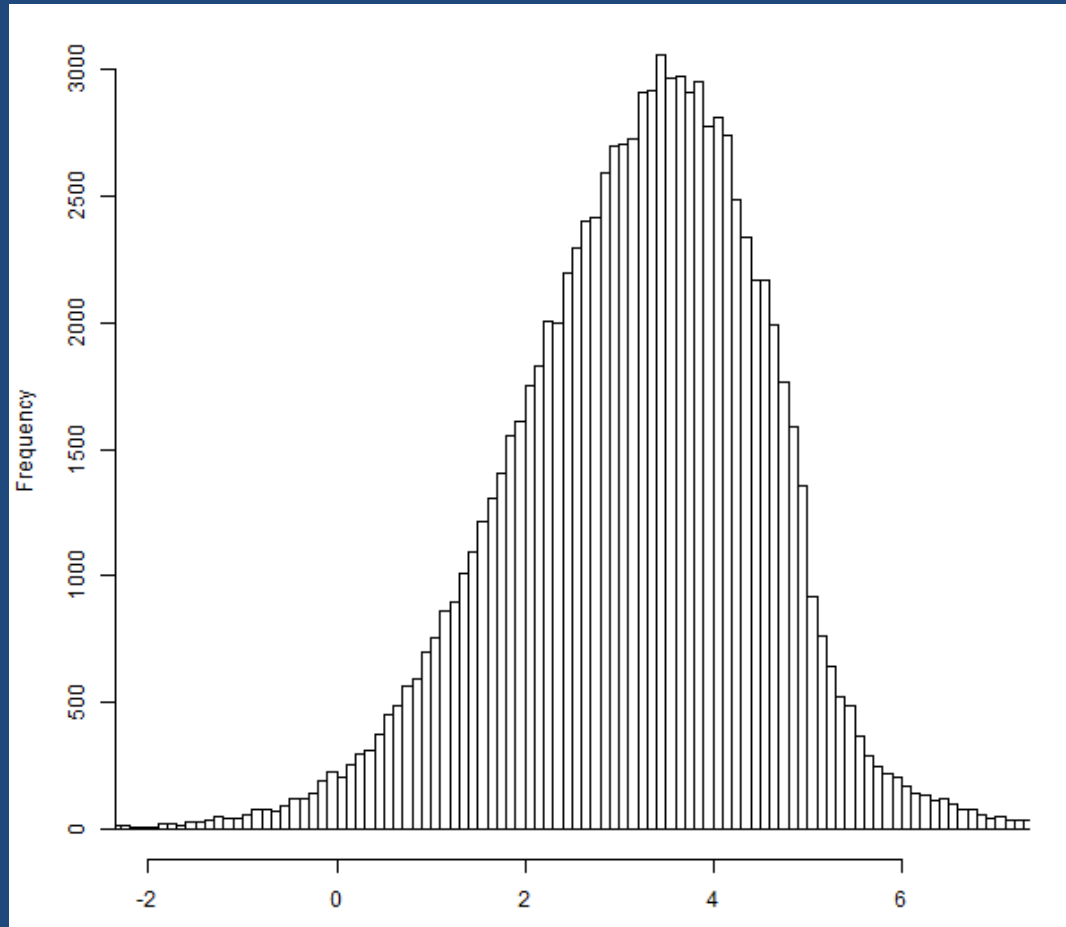
Details: <http://htbc.stanford.edu/compounds.html>

Clusters in Compound Library



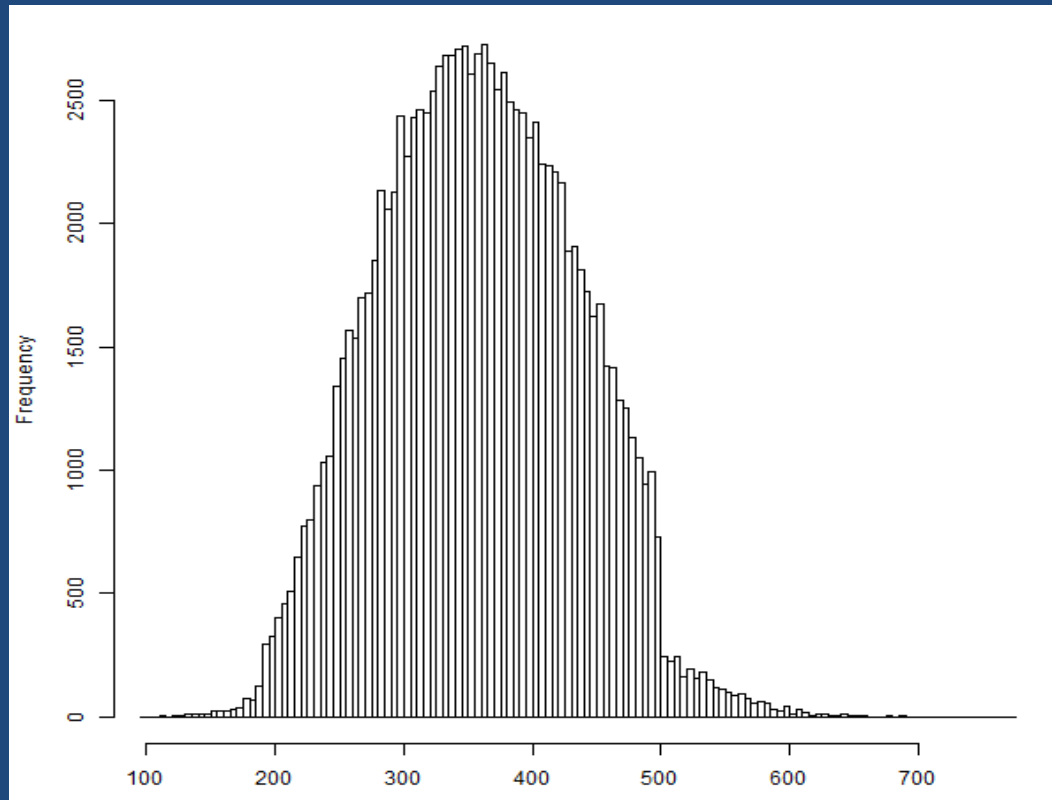
- FCF4 fingerprints
- Tanimoto similarity > 0.8
- Plot shows the distribution of cluster sizes
- Numbers are the % of the library that is in that group
- Largest cluster is 46 compounds

Distribution of cLogP



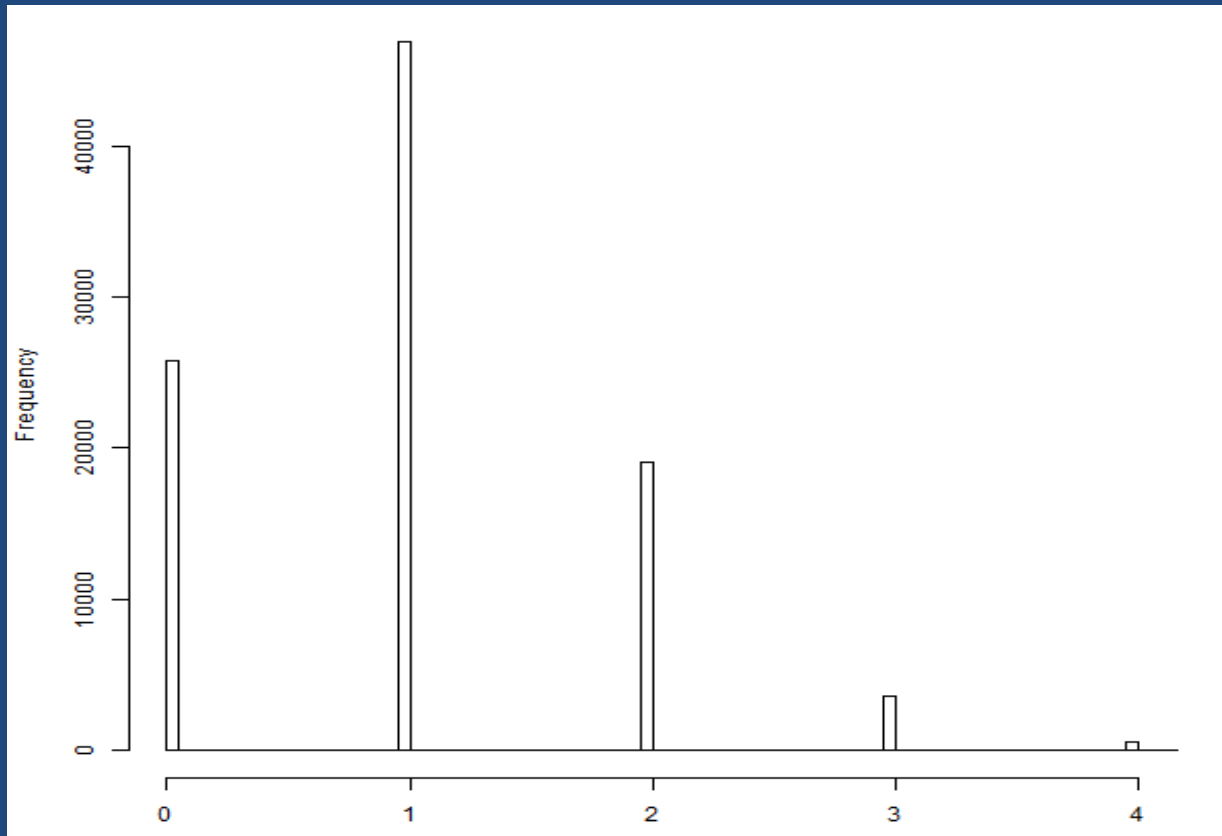
cLogP

Distribution of MW



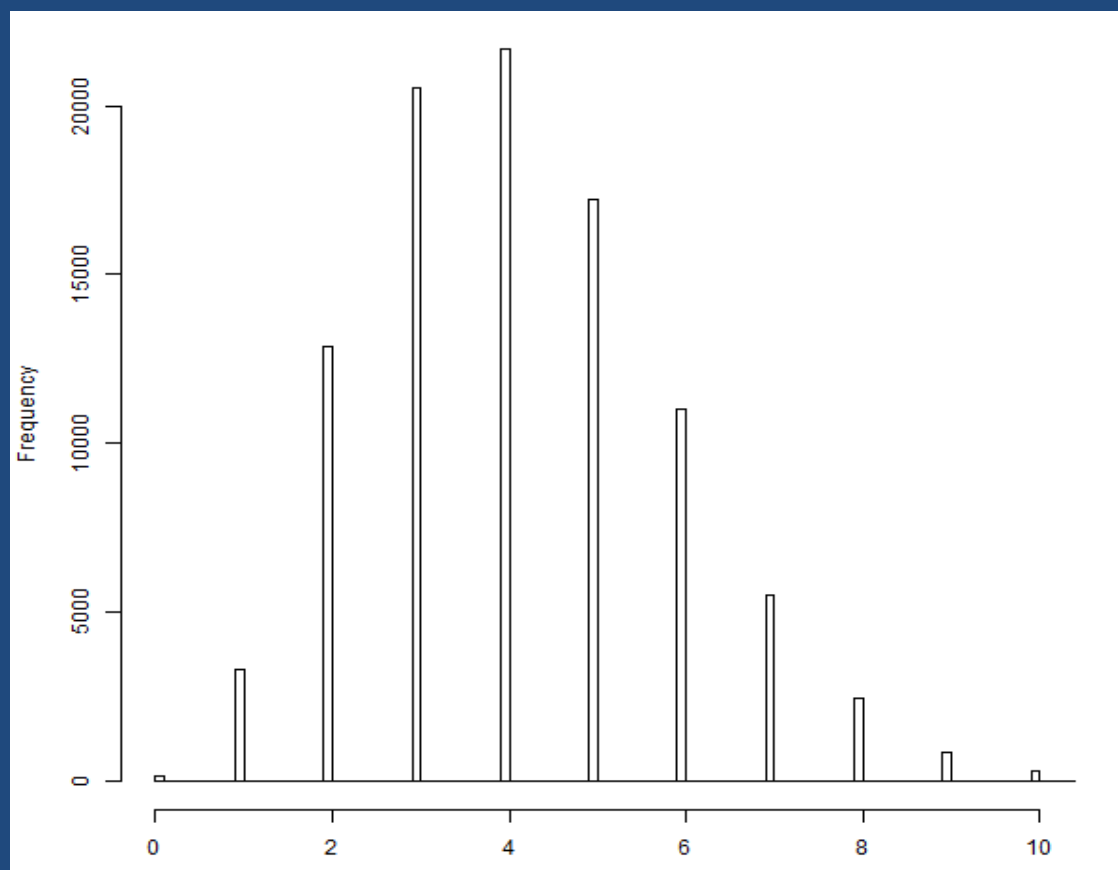
MW

Distribution of Hydrogen Bond Donors



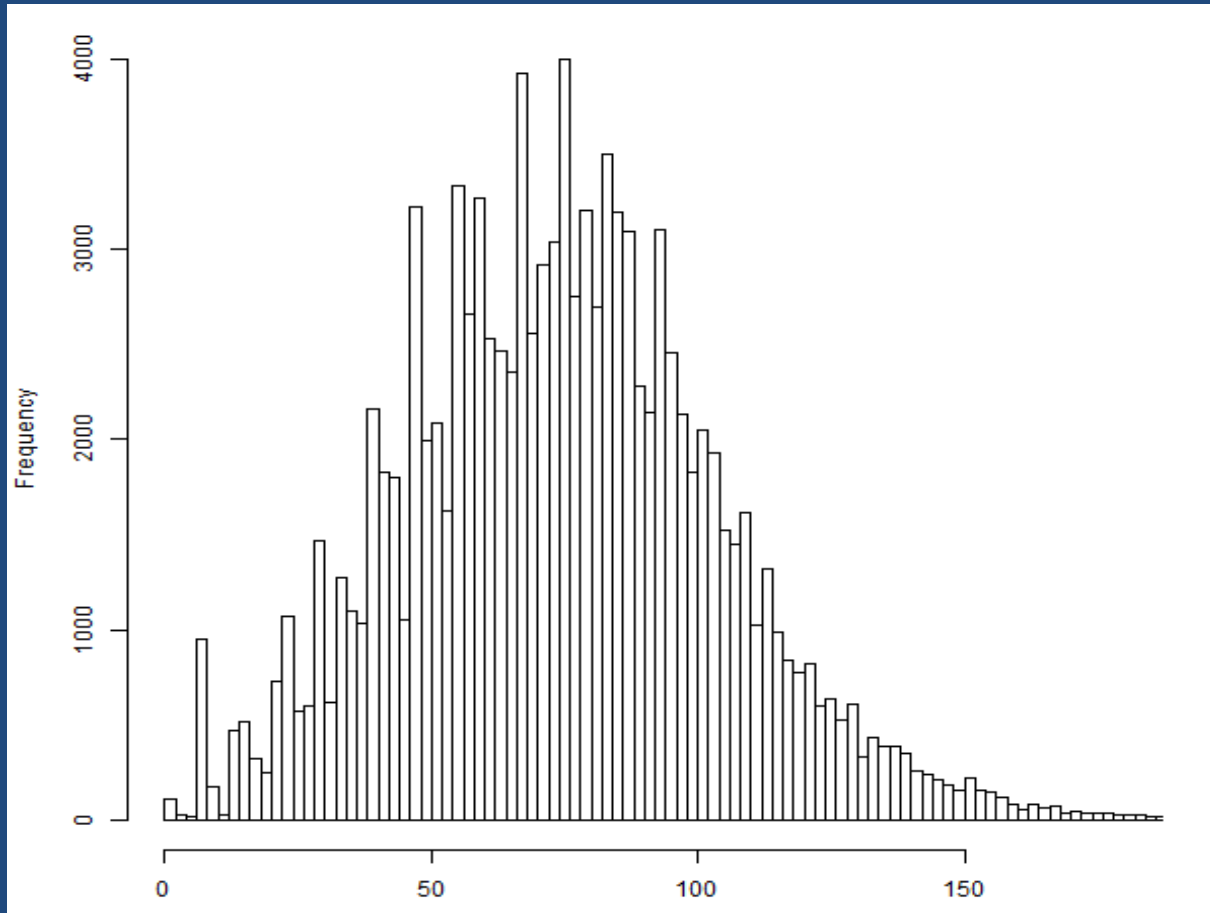
Number of Hydrogen Bond Donors

Distribution of Hydrogen Bond Acceptors



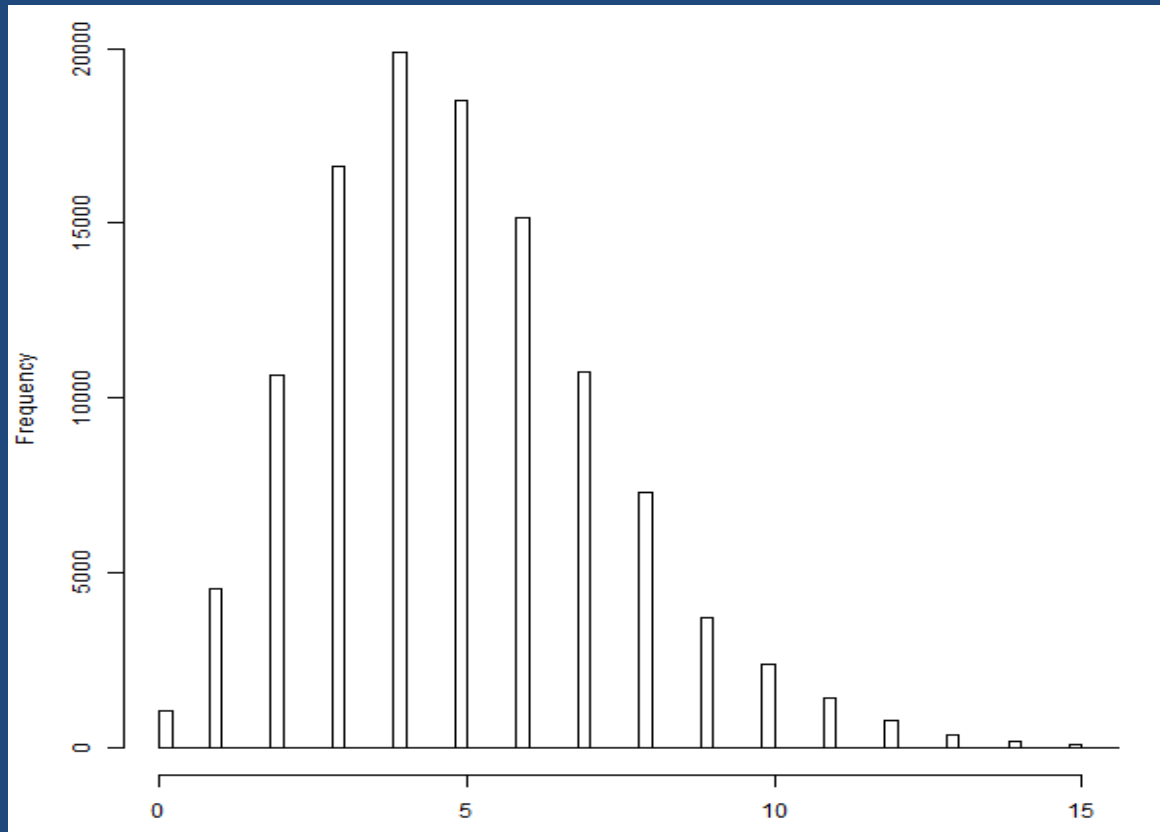
Number of H-Bond Acceptors

Distribution of Polar Surface Area



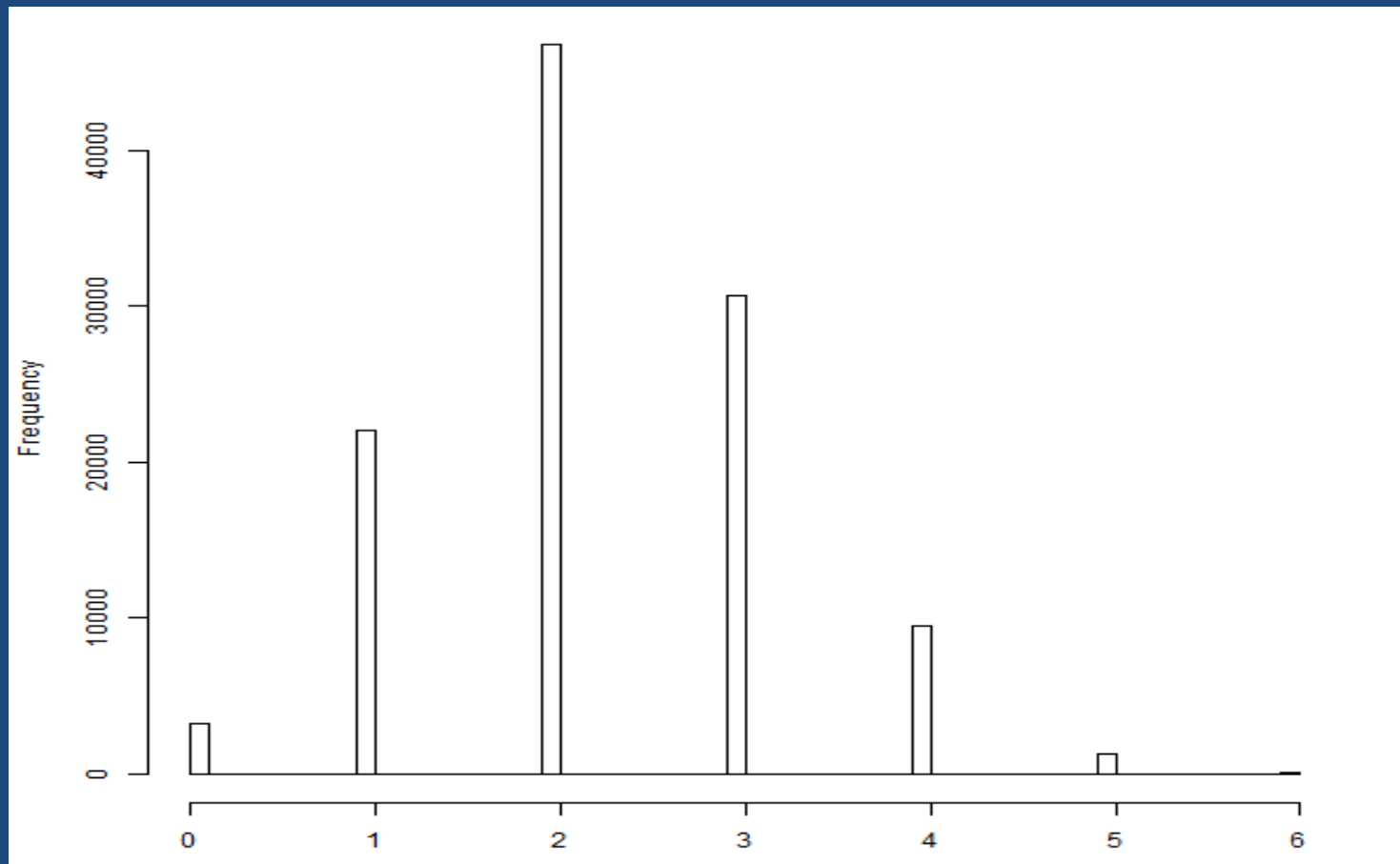
Polar Surface Area

Distribution of Number of Rotatable Bonds



Number of Rotatable Bonds

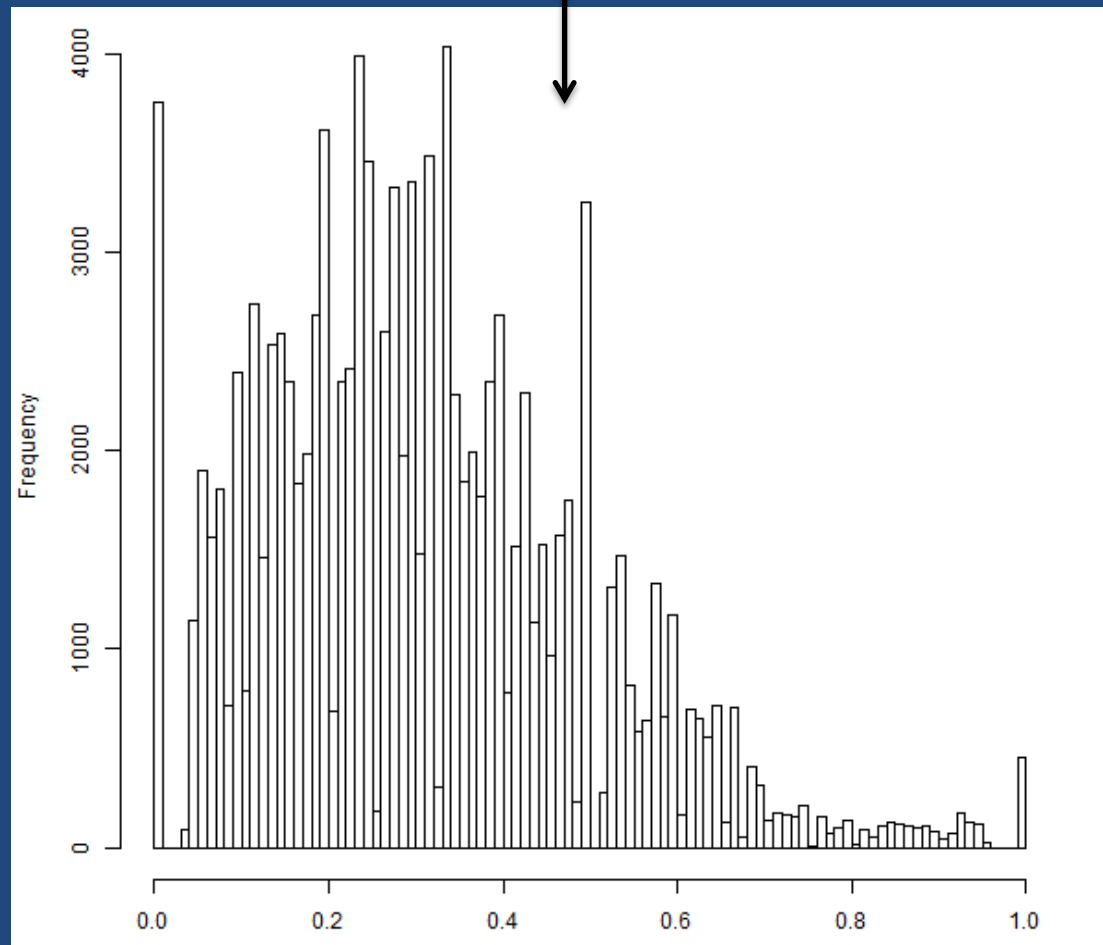
Distribution of Number of Aromatic Rings



Number of Aromatic Rings

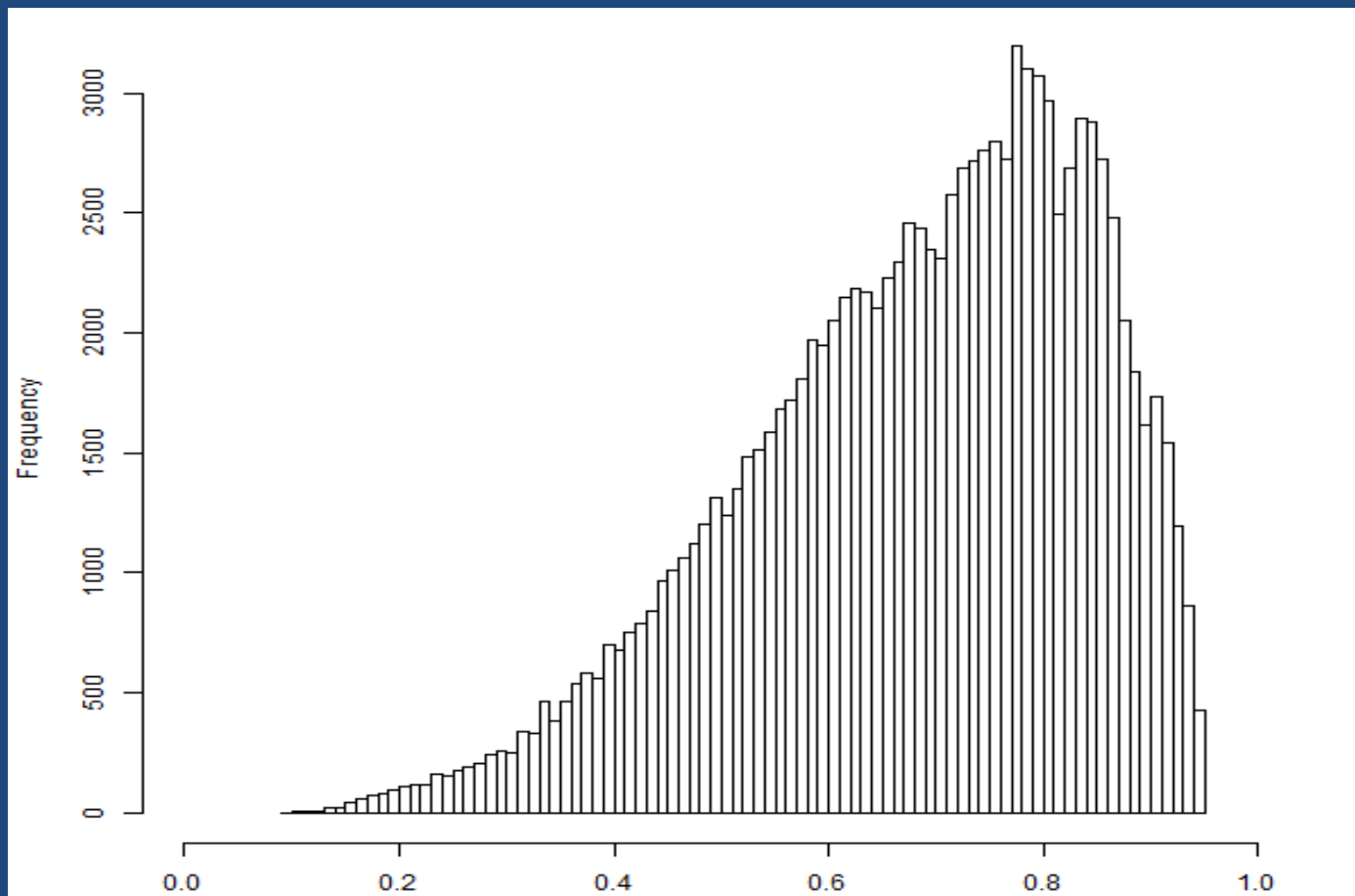
Fraction of SP3 Carbon

Mean for Drugs



Fsp3

Distribution of QED



QED, a measure of “Chemical Beauty”
Bickerton et al, 2012 Nature Chemistry