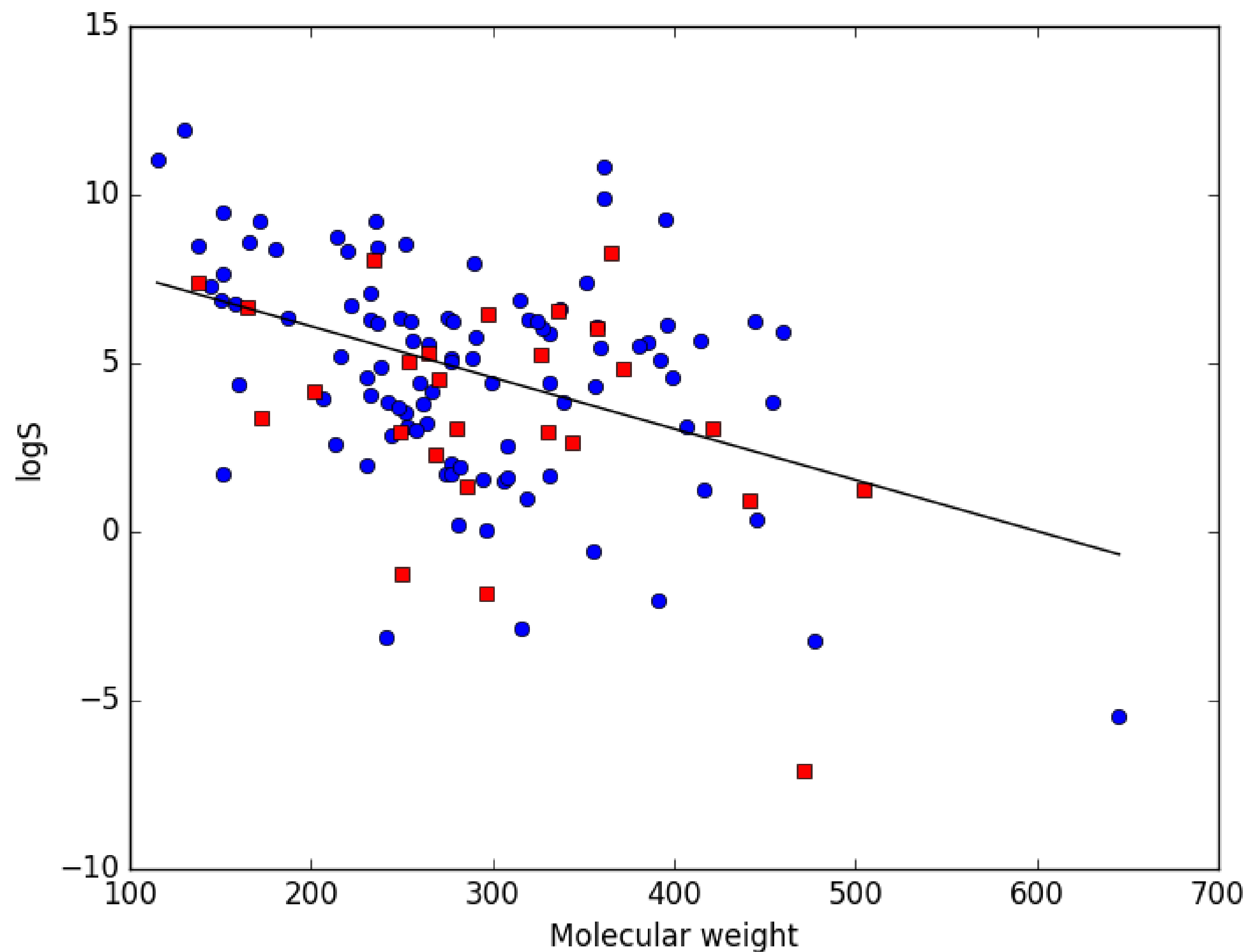


Historically informative descriptors [5]

- Molecular size or surface area - cost of forming cavity in water
- Octanol:water partition coefficient (P) - solubility relative to a non polar phase
- Melting point - higher means more stable solid
- Hydrogen bonding - favors water solubility
- Atom/group contributions
- Molecular connectivities

Molecular weight has some predictive power



From Ref [1]
Blue: training
Red: test
Black: predictions