Implementing Molecular Hydrophobicity Potential Measurment for the Analysis of Dynamic Biomolecular Interactions

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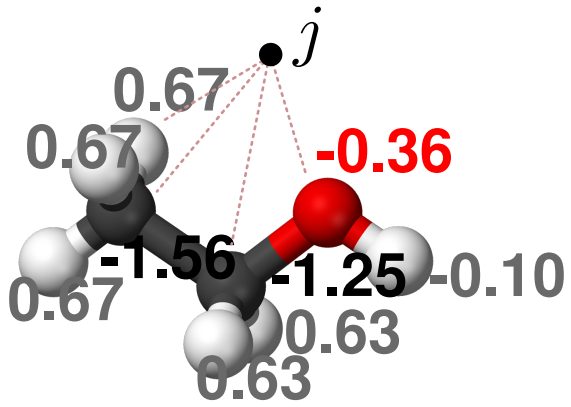
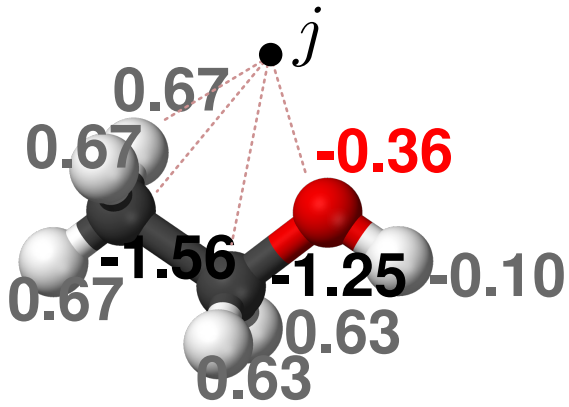
Outline

The MHP Formula



$$\text{MHP}\left(\mathbf{x}'\right) = \sum_{i=1}^{k} \left[f_i \cdot D\left(\mathbf{x} - \mathbf{x}'\right) \right]$$

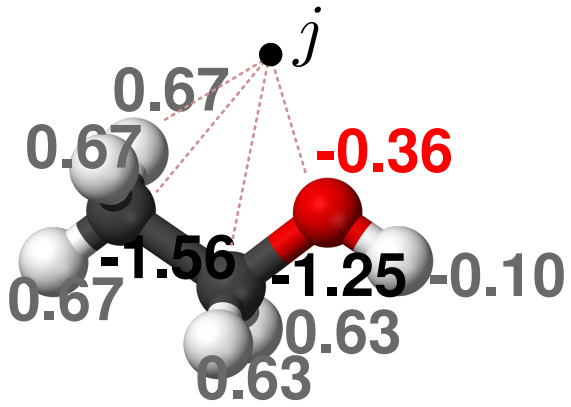
The MHP Formula



$$\text{MHP}\left(\mathbf{x}'\right) = \sum_{i=1}^{k} \left[f_i \cdot D\left(\mathbf{x} - \mathbf{x}'\right) \right]$$

Summing over all atoms

The MHP Formula

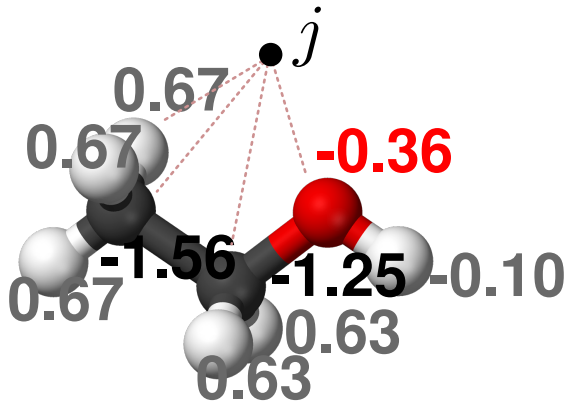


$$\text{MHP}\left(\mathbf{x}'\right) = \sum_{i=1}^{k} \left[f_i \cdot D\left(\mathbf{x} - \mathbf{x}'\right) \right]$$

Summing over all atoms

Force constants

The MHP Formula



$$\text{MHP}\left(\mathbf{x}'\right) = \sum_{i=1}^{k} \left[f_i \cdot D\left(\mathbf{x} - \mathbf{x}'\right) \right]$$

Summing over all atoms

Distance function

Force constants

Force constants

Type	Description	f_i value
	C in:	
3	$\mathrm{CHR_3}$	-0.6681
15	$=\mathrm{CH_2}$	-0.7866
36	$\mathrm{R{-}CH{-}X}$	-0.2405
	H attached to:	
45	$\mathrm{C_{sp^3}}$ having no X attached to next carbon	0.7341
46	$\mathrm{C_{sp^3}}, \mathrm{C_{sp^2}}$	0.6301
50	Heteroatom	-0.1036
52	$\mathrm{C_{sp^3}}$ having 1 X attached to next carbon	0.6666
	O in:	
56	Alcohol	-0.3567
58	Ketone	-0.0233
62	$\mathrm{O^-}$	-0.7941

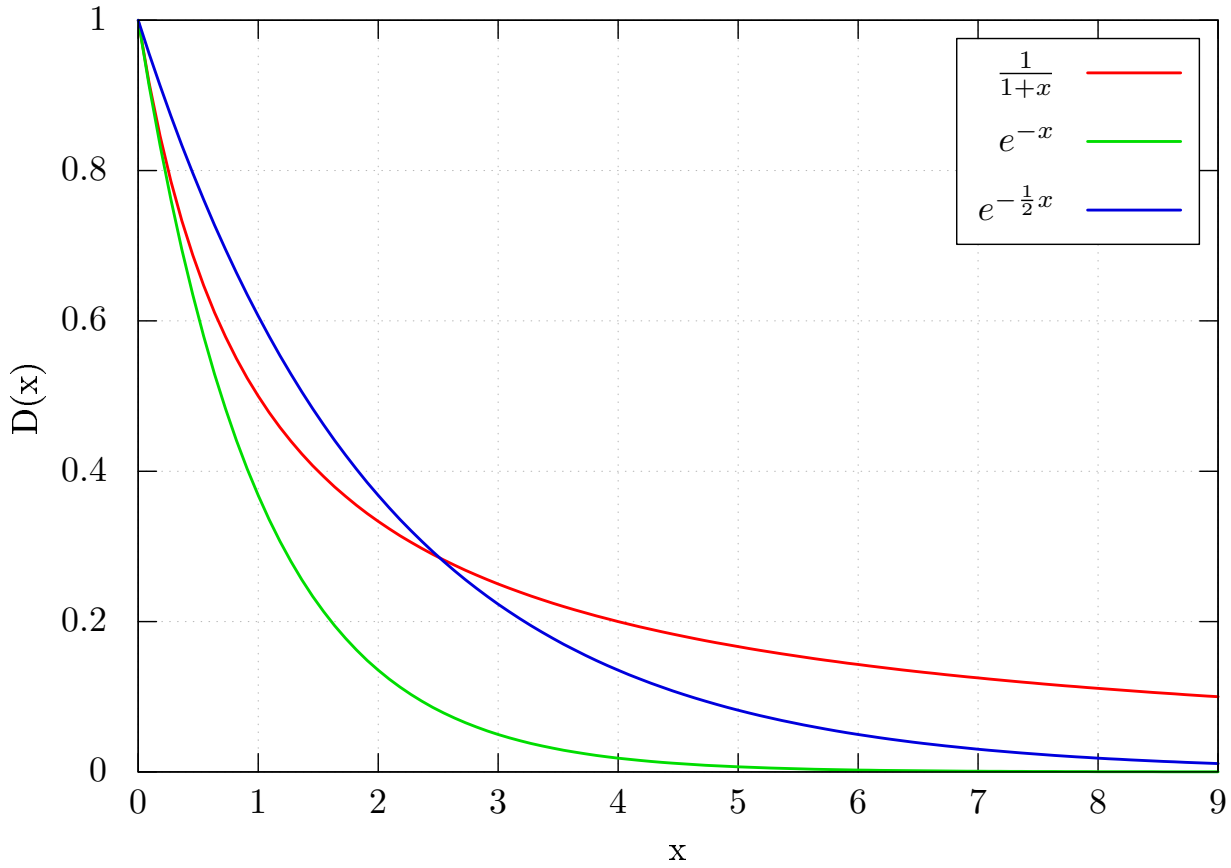
Distance function

Audry form

$$D(x) = \frac{1}{1+x}$$

Exponential decay form

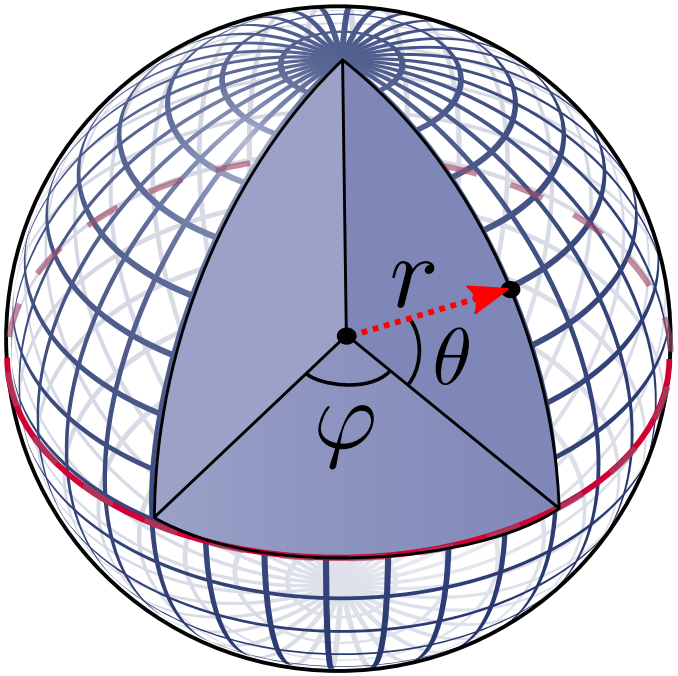
$$D(x) = e^{-\alpha x}$$



Solvent accesible surface

Evenly distributed points

How to distribute N points on a surface of a sphere?



Integration