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

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February 18, 2018

## Molecular Hydrophobicity Potential

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Hydrophobicity and log P Partition Coefficient

# Hydrophob Potential

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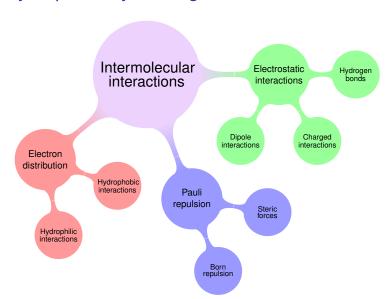
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# Definition

The ratio of concentrations of a compound in a mixture of two immiscible phases at equilibrium

# Molecular Hydrophobicity Potential

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# Definition

The ratio of concentrations of a compound in a mixture of two immiscible phases at equilibrium

Commonly used: water and octanol

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# Definition

The ratio of concentrations of a compound in a mixture of two immiscible phases at equilibrium

- Commonly used: water and octanol
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## Molecular Hydrophobicity Potential

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# Definition

The ratio of concentrations of a compound in a mixture of two immiscible phases at equilibrium

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## Molecular Hydrophobicity Potential

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# Definition

The ratio of concentrations of a compound in a mixture of two immiscible phases at equilibrium

- Commonly used: water and octanol
- Can be measured at an ionized or unionized state

$$\qquad \log P_{\text{octanol/water}} = \log \left( \frac{[\text{solute}]_{\text{water}}}{[\text{solute}]_{\text{octanol}}} \right)$$

ightharpoonup Hydrophobicity increases with the (common)  $\log P$ 

## Molecular Hydrophobicity Potential

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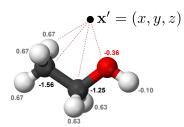
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$$\mathsf{MHP}\left(\mathbf{x}'\right) = \sum_{i=1}^{k} \left[ f_i \cdot D\left(\mathbf{x} - \mathbf{x}'_i\right) \right]$$

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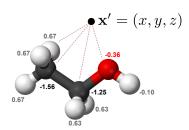
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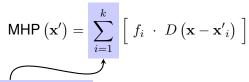
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Summing over all atoms

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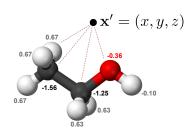
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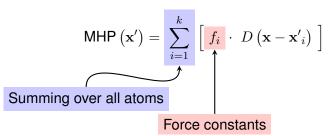
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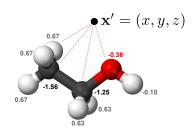
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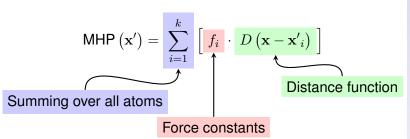
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# Force Constants - Carbon

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# **Carbon** atom contribution to hydrophobicity<sup>1</sup>

Type	Description	$f_i$ value
•	Carbon in:	
1	$\mathrm{CH_{3}R}$	-1.5603
3	$CHR_3$	-0.6681
7	$CH_2X_2$	-1.0305
13	$RCX_3$	0.7894
17	$=CR_2$	0.0383
24	RCHR	-0.3251
25	RCRR	0.1492
26	RCXR	0.1539

<sup>&</sup>lt;sup>1</sup>Source: Ghose et al, J. Phys. Chem. A 1998, 102, 3762-3772

# Force Constants - Hydrogen

**Hydrogen** atom contribution to hydrophobicity<sup>2</sup>

Type	Description	$f_i$ value
	Hydrogen attached to:	
46	$\overline{\mathrm{C_{sp^3}}$ , no $\mathrm{X}$ in $lpha$	0.7341
47	$ m C_{sp}^2$	0.6301
50	X	-0.1036
52	$\mathrm{C}_{\mathrm{sp}^3}$ , 1 X in $lpha$	0.6666
54	$C_{cm^3}$ . 3 X in $\alpha$	0.6338

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<sup>&</sup>lt;sup>2</sup>Source: Ghose et al, J. Phys. Chem. A 1998, 102, 3762-3772



# Force Constants - Oxygen

# **Oxygen** atom contribution to hydrophobicity<sup>3</sup>

Type	Description	$f_i$ value
	Oxygen in:	
56	Alcohol	-0.3567
57	Phenol, enol, carboxyl OH	-0.0127
58	Ketone	-0.0233
61	Nitro, N-oxides	1.0520
62	O-	-0.7941

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<sup>&</sup>lt;sup>3</sup>Source: Ghose et al, J. Phys. Chem. A 1998, 102, 3762-3772



# Force Constants - Various

# Various atom contribution to hydrophobicity<sup>4</sup>

Type	Description	$f_i$ value
66	Primary amine	-0.5427
67	Secondary amine	-0.3168
81	$\mathrm{F}$ attached to $\mathrm{C}_{\mathrm{sp^3}}$	0.4797
106	S  in  R-SH  (thiol)	1.0520
119	$P \text{ in } PR_3 \text{ (phosphine)}$	-0.7941

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<sup>&</sup>lt;sup>4</sup>Source: Ghose et al, J. Phys. Chem. A 1998, 102, 3762-3772



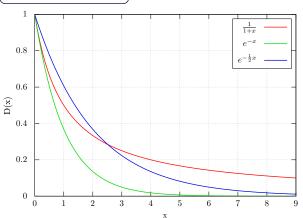
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# Audry form

# Exponential decay form

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

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



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# Solvent accesible surface

The surface around a molecule accesible to solvent molecules

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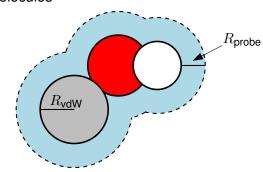
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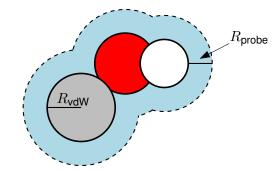
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# Solvent accesible surface

The surface around a molecule accesible to solvent molecules



For water molecules usually r = 1.4 |A|

## Molecular Hydrophobicity Potential

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1. Take all atoms with their vdW-radii

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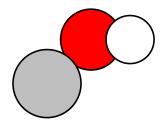
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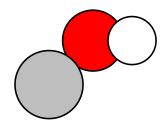
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- 1. Take all atoms with their vdW-radii
- 2. Create spheres around all atoms with  $R^i = R^i_{\text{vdw}} + R_{\text{probe}}$

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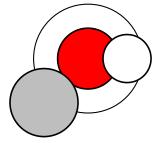
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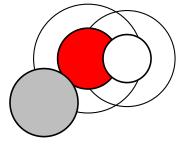
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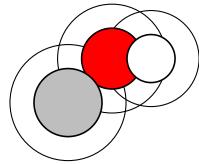
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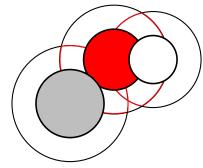
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- 1. Take all atoms with their vdW-radii
- 2. Create spheres around all atoms with  $R^i = R^i_{\text{vdw}} + R_{\text{probe}}$
- 3. Delete all points that are "burried" in other extended spheres (i.e.  $\Delta(p^i, c^j) \leq R^j + R_{\text{probe}}$ )

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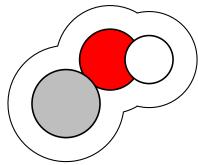
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- 2. Create spheres around all atoms with  $R^i = R^i_{\text{vdw}} + R_{\text{probe}}$
- 3. Delete all points that are "burried" in other extended spheres (i.e.  $\Delta(p^i, c^j) \leq R^j + R_{\text{probe}}$ )
- 4. The remaining surface is the solvent-accesible surface of the molecule

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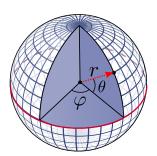
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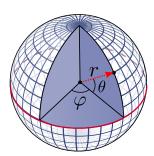
How to distribute *N* points on a surface of a sphere?



## Molecular Hydrophobicity Potential

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



$$\varphi_i = i \cdot \frac{2\pi}{N}$$
 
$$\theta_j = j \cdot \frac{\pi}{N}$$

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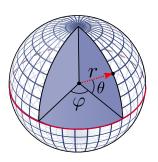
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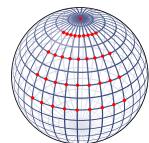
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# How to distribute N points on a surface of a sphere?







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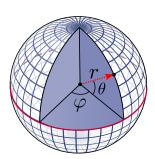
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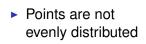


$$\varphi_i = i \cdot \frac{2\pi}{N}$$

$$\theta_j = j \cdot \frac{\pi}{N}$$





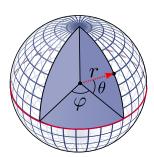


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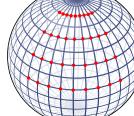
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How to distribute N points on a surface of a sphere?







$$\varphi_i = i \cdot \frac{2\pi}{N}$$
$$\theta_j = j \cdot \frac{\pi}{N}$$

$$\theta_j = j \cdot \frac{\pi}{N}$$

Points are not evenly distributed

Several points overlap at poles Pelg Bar Sapir

Solution: Vogel's method

In 2 dimensions:

# Molecular Hydrophobicity Potential

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Solution: Vogel's method

# In 2 dimensions:

▶ Distances:  $r_i = \sqrt{\frac{i}{N}}$ 

• Angle:  $\theta_i = \varphi i$ 

( $\varphi$  is the golden ratio!)

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Solution: Vogel's method

# In 2 dimensions:

- ▶ Distances:  $r_i = \sqrt{\frac{i}{N}}$
- Angle:  $\theta_i = \varphi i$ ( $\varphi$  is the golden ratio!)

In 3 dimensions (cylindrical coordinates):

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# In 2 dimensions:

▶ Distances: 
$$r_i = \sqrt{\frac{i}{N}}$$

• Angle: 
$$\theta_i = \varphi i$$
  
( $\varphi$  is the golden ratio!)

# In 3 dimensions (cylindrical coordinates):

▶ Distances: 
$$z_i = \left(1 - \frac{1}{N}\right) \left(1 - \frac{2i}{N-1}\right)$$

► Angles:

$$\theta_i = \varphi i, \ \rho_i = \sqrt{1 - z_i^2}$$

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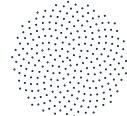
# In 2 dimensions:

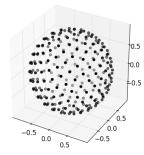
▶ Distances: 
$$r_i = \sqrt{\frac{i}{N}}$$

• Angle:  $\theta_i = \varphi i$ ( $\varphi$  is the golden ratio!)

# In 3 dimensions (cylindrical coordinates):

- ▶ Distances:  $z_i$  =  $\left(1-\frac{1}{N}\right)\left(1-\frac{2i}{N-1}\right)$
- Angles:  $\theta_i = \varphi i, \ \rho_i = \sqrt{1 - z_i^2}$





### Molecular Hydrophobicity Potential

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Evenly distributed points

► Each atom's total surface area:  $V^a = 4\pi \left(R_{\text{vdW}}^a + R_{\text{probe}}\right)^2$ 

$$V^a = 4\pi \left( R_{\text{vdW}}^a + R_{\text{probe}} \right)^2$$

### Molecular Hydrophobicity Potential

# Pelg Bar Sapir

► Each atom's total surface area:  $V^a = 4\pi \left(R_{\text{vdW}}^a + R_{\text{probe}}\right)^2$ 

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▶ The surface is represented by N points

### Molecular Hydrophobicity Potential

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Therefore, each atom has a total MHP of:

$$\mathsf{MHP}^a = \frac{4\pi}{N} \sum_{j=0}^M \mathsf{MHP}^a_j$$

### Molecular Hydrophobicity Potential

## Pelg Bar Sapir

Written in Python3, utylizing ProDy

### Molecular Hydrophobicity Potential

# Pelg Bar Sapir

### Introduction

Hydrophobicity and log P Partition Coefficient

# Molecular Hydrophobicity

Vhat is it?

## Potential

General form

Force Constants

Distance function

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#### Program Specifications

#### Results

Validation via Known log | Values

- Written in Python3, utylizing ProDy
- Heavy calculation written in Cython

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- Uses neighbor cells implementation for faster calculation
- ▶ Uses PSF, PDB and DCD files

### Molecular Hydrophobicity Potential

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### Program Specifications

### Result

Validation via Known log | Values

- Written in Python3, utylizing ProDy
- Heavy calculation written in Cython
- Uses neighbor cells implementation for faster calculation
- Uses PSF, PDB and DCD files
- Generates a PDB output, MHP values in beta column

### Molecular Hydrophobicity Potential

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► Input: PSF + PDB or DCD

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Validation via Known log Values

- ► Input: PSF + PDB or DCD
- Subselection (optional): Atomic selection (like vmd)

### Molecular Hydrophobicity Potential

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### Results

Validation via Known log

- ► Input: PSF + PDB or DCD
- Subselection (optional): Atomic selection (like vmd)
- ▶ Number of points per atom (default: 64)

### Molecular Hydrophobicity Potential

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### Resul

Validation via Known log Values

- ► Input: PSF + PDB or DCD
- Subselection (optional): Atomic selection (like vmd)
- Number of points per atom (default: 64)
- ► Solvent probe radius (defalt: 1.4Å)

### Molecular Hydrophobicity Potential

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## Result

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- Subselection (optional): Atomic selection (like vmd)
- Number of points per atom (default: 64)
- ► Solvent probe radius (defalt: 1.4Å)
- ► Cutoff distance for distance function (default: 4Å)

### Molecular Hydrophobicity Potential

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- ► Input: PSF + PDB or DCD
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- Number of points per atom (default: 64)
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- ► Cutoff distance for distance function (default: 4Å)
- ► Frame range (if DCD)

#### Molecular Hydrophobicity Potential

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### Result

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# An Example System

### Molecular Hydrophobicity Potential

# Pelg Bar Sapir