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

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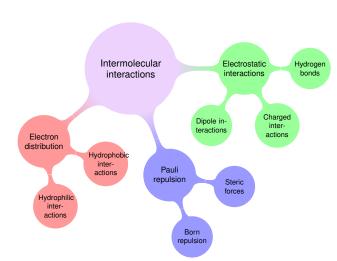
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# Hydrophobicity and log P



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Hydrophobicity and log P

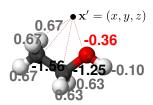
# Partition Coefficient

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

#### Molecular Hydrophobicity Potential

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## Partition Coefficient



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

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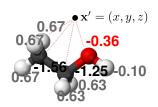
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$$\mathsf{MHP}\left(\mathbf{x}'\right) = \sum_{i=1}^{k} \left[ f_i \cdot D\left(\mathbf{x} - \mathbf{x}'_i\right) \right]$$

Summing over all atoms

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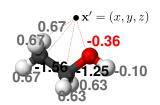
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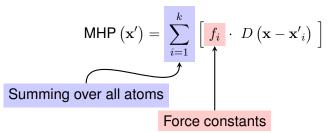
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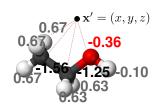
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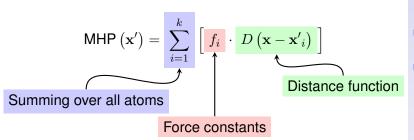
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# Force Constants - Carbon

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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 hydrophobicity4

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

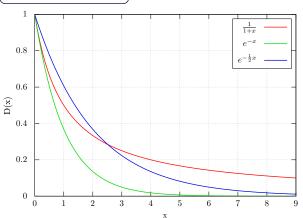


# Audry form

# 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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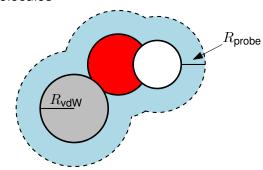
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# Solvent accesible surface

The surface around a molecule accesible to solvent molecules



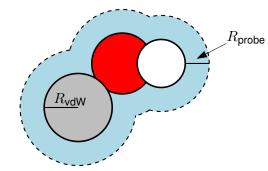
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#### Solvent accesible surface

# Solvent accesible surface

 The surface around a molecule accesible to solvent molecules



For water molecules usually  $r=1.4~{
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Take all atoms with their vdW-radii

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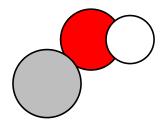
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1. Take all atoms with their vdW-radii

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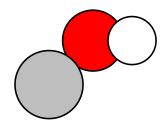
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- 1. Take all atoms with their vdW-radii
- 2. Create spheres around all atoms with  $R^i = R^i_{\text{vdw}} + R_{\text{probe}}$

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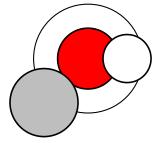
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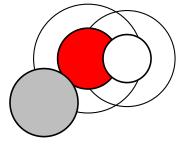
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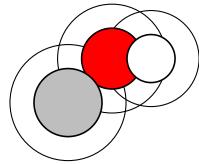
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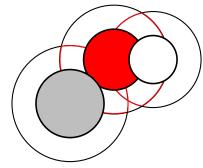
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- 1. Take all atoms with their vdW-radii
- 2. Create spheres around all atoms with  $R^i = R^i_{\text{vdw}} + R_{\text{probe}}$
- 3. Delete all points that are "burried" in other extended spheres (i.e.  $\Delta(p^i, c^j) \leq R^j + R_{\text{probe}}$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

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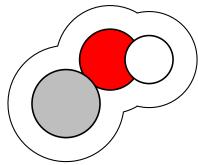
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- 2. Create spheres around all atoms with  $R^i = R^i_{\text{vdw}} + R_{\text{probe}}$
- 3. Delete all points that are "burried" in other extended spheres (i.e.  $\Delta(p^i, c^j) \leq R^j + R_{\text{probe}}$ )
- 4. The remaining surface is the solvent-accesible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

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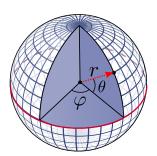
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How to distribute *N* points on a surface of a sphere?

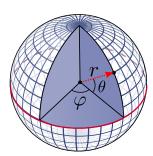


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Evenly distributed points

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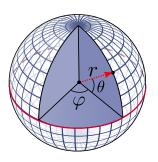
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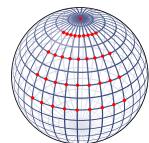
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## How to distribute N points on a surface of a sphere?







$$\varphi_i = i \cdot \frac{2\pi}{N}$$
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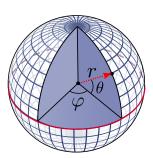
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How to distribute N points on a surface of a sphere?



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

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Points are not evenly distributed Pelg Bar Sapir

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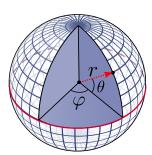
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How to distribute N points on a surface of a sphere?

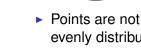


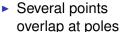
$$i\cdot\frac{2\pi}{N}$$

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

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







evenly distributed

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Evenly distributed points

Solution: Vogel's method

In 2 dimensions:

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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

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# Evenly distributed points

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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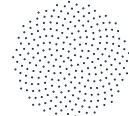
Solution: Vogel's method

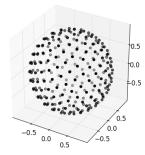
## In 2 dimensions:

- ▶ Distances:  $r_i = \sqrt{\frac{i}{N}}$
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# In 3 dimensions (cylindrical coordinates):

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





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► 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

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

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

▶ The surface is represented by *N* points

## 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
- ▶ Meaning: each point has  $V_j^a = \frac{4\pi}{N} \left( R_{\text{vdW}}^i + R_{\text{probe}} \right)^2$

## Molecular Hydrophobicity Potential

## Pelg Bar Sapir

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- ▶ In addition, each point has: MHP<sup>a</sup><sub>i</sub>

## Molecular Hydrophobicity Potential

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- In addition, each point has: MHP<sup>a</sup><sub>i</sub>

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

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Hydrophobicity and log P Partition Coefficient

## Molecular Hydrophobicity

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## Potential

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Distance function

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### Results

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

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- Uses neighbor cells implementation for faster calculation

## Molecular Hydrophobicity Potential

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- Written in Python3, utylizing ProDy
- Heavy calculation written in Cython
- Uses neighbor cells implementation for faster calculation
- Uses PSF, PDB and DCD files

## Molecular Hydrophobicity Potential

## Pelg Bar Sapir

## **Program Specifications**

- 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

## Pelg Bar Sapir

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► Input: PSF + PDB or DCD

## Molecular Hydrophobicity Potential

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### Molecular Hydrophobicity Potential

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

## Molecular Hydrophobicity Potential

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## Result

Validation via Known log | Values



- ► 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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## olecular ydrophobicity

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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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## Potential

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## Result

Validation via Known log p Values



- ► Input: PSF + PDB or DCD
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- 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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Force Constants

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## Resul

Validation via Known log p Values



- Input: PSF + PDB or DCD
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- Solvent probe radius (defalt: 1.4Å)
- Cutoff distance for distance function (default: 4Å)
- Frame range (if DCD)

### Molecular Hydrophobicity Potential

Pelg Bar Sapir

**Program Specifications** 

# Validation via Known $\log P$ Values

## Molecular Hydrophobicity Potential

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### Molecular Hydrophobicity Potential

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## Molecular Hydrophobicity Potential

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