

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

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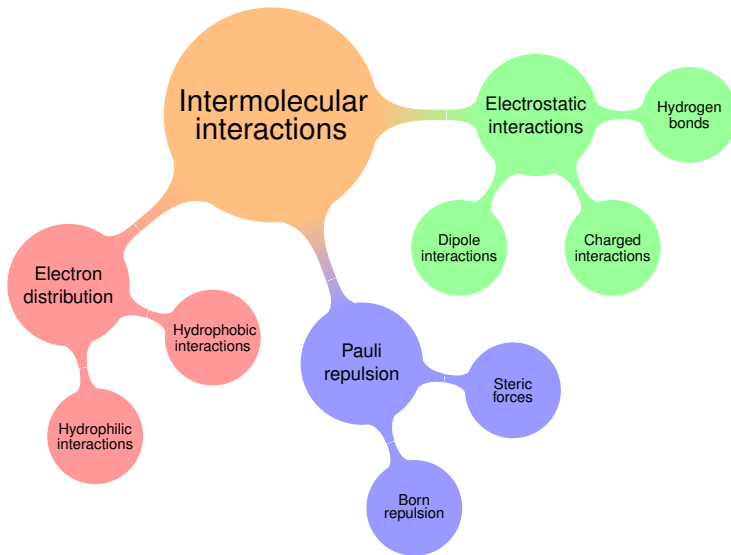
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# Hydrophobicity and log P



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

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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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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

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- ▶ Commonly used: water and octanol
- ▶ Can be measured at an **ionized** or **unionized** state
- ▶  $\log P_{\text{octanol/water}} = \log \left( \frac{[\text{solute}]_{\text{water}}}{[\text{solute}]_{\text{octanol}}} \right)$

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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
- ▶  $\log P_{\text{octanol/water}} = \log \left( \frac{[\text{solute}]_{\text{water}}}{[\text{solute}]_{\text{octanol}}} \right)$
- ▶ Hydrophobicity **increases** with the (common)  $\log P$

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# What is Molecular Hydrophobicity Potential (MHP)?

- By measuring the  $\log P$  of many (ca. 30,000) compounds[3]

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# What is Molecular Hydrophobicity Potential (MHP)?

- ▶ By measuring the  $\log P$  of many (ca. 30,000) compounds[3]
- ▶ Combining these values with a distance-depended decay function, a potential can be constructed.

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# What is Molecular Hydrophobicity Potential (MHP)?

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- ▶ By measuring the  $\log P$  of many (ca. 30,000) compounds[3]
- ▶ Combining these values with a distance-depended decay function, a potential can be constructed.
- ▶ This potential predicts the local  $\log P$  behaviour of fragments of a molecule.

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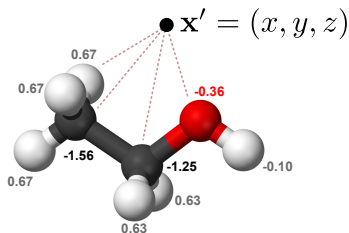
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# The MHP Formula

## Molecular Hydrophobicity Potential

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

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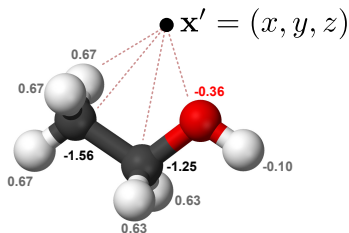
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Summing over all atoms

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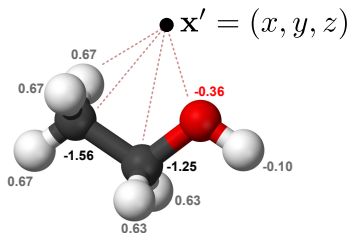
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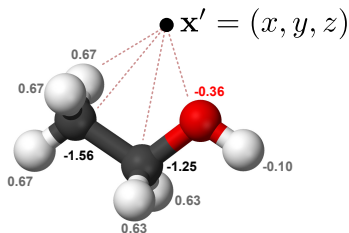
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# Force Constants - Carbon

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

Type	Description	$f_i$ value
<u>Carbon in:</u>		
1	CH <sub>3</sub> R	-1.5603
3	CHR <sub>3</sub>	-0.6681
7	CH <sub>2</sub> X <sub>2</sub>	-1.0305
13	RCX <sub>3</sub>	0.7894
17	=CR <sub>2</sub>	0.0383
24	R—CH—R	-0.3251
25	R—CR—R	0.1492
26	R—CX—R	0.1539

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

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

Type	Description	$f_i$ value
	Hydrogen attached to:	
46	C <sub>sp</sub> <sup>3</sup> , no X in $\alpha$	0.7341
47	C <sub>sp</sub> <sup>2</sup>	0.6301
50	Heteroatom X	-0.1036
52	C <sub>sp</sub> <sup>3</sup> , 1 X in $\alpha$	0.6666
54	C <sub>sp</sub> <sup>3</sup> , 3 X in $\alpha$	0.6338

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

# Force Constants - Oxygen

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### 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 <sup>-</sup>	-0.7941

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

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

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

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

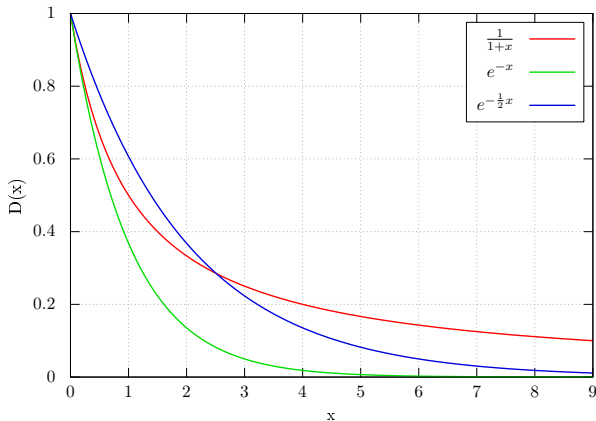
# Distance function

Audry form

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

Exponential decay form

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



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- ▶ The surface around a molecule accessible to solvent molecules

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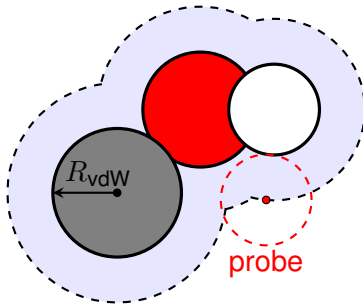
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- ▶ The surface around a molecule accessible to solvent molecules



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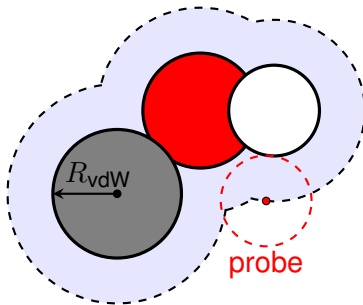
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- ▶ The surface around a molecule accessible to solvent molecules



(For water molecules usually  $r = 1.4$  [Å])

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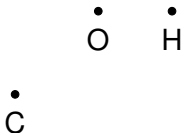
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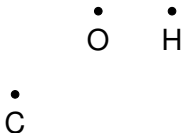
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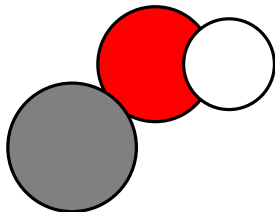
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# How to Create the Solvent Accessible Surface?



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

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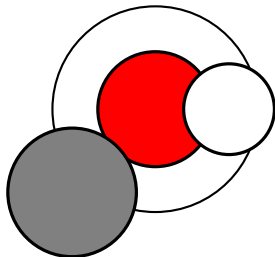
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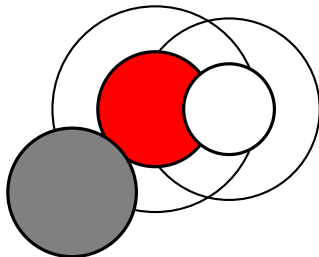
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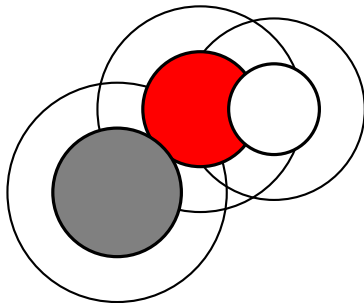
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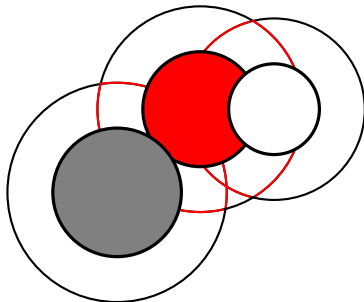
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1. Take all atoms with their vdW-radii
2. Create spheres around all atoms with  
 $R^i = R_{\text{vdw}}^i + R_{\text{probe}}$
3. Delete all points that are "buried" in other extended spheres (i.e.  $\Delta(p^i, c^j) \leq R^j + R_{\text{probe}}$ )

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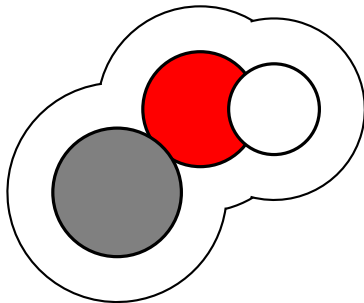
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1. Take all atoms with their vdW-radii
2. Create spheres around all atoms with  
 $R^i = R_{\text{vdw}}^i + R_{\text{probe}}$
3. Delete all points that are "buried" in other extended spheres (i.e.  $\Delta(p^i, c^j) \leq R^j + R_{\text{probe}}$ )
4.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

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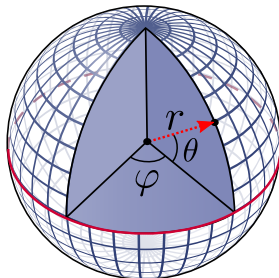
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How to distribute  $N$  points on a surface of a sphere?



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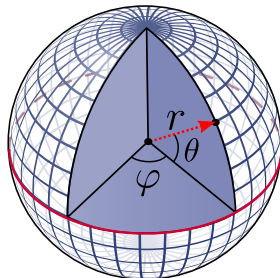
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How to distribute  $N$  points on a surface of a sphere?



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

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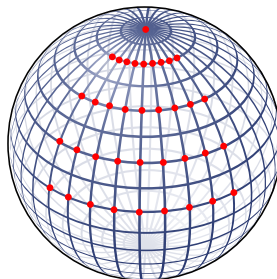
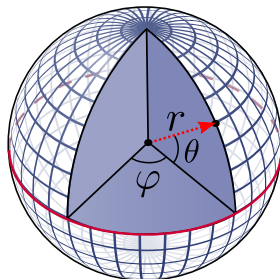
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$$\varphi_i = i \cdot \frac{2\pi}{N}$$
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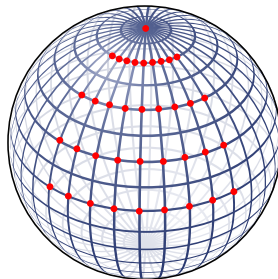
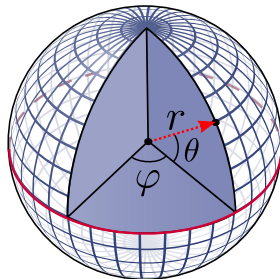
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# Evenly Distributed Points

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



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

► Points are not evenly distributed

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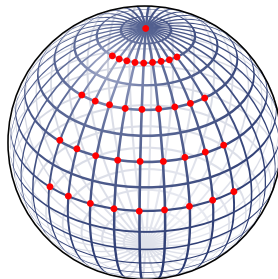
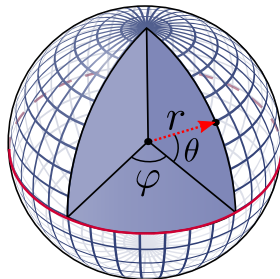
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# Evenly Distributed Points

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



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

- Points are not evenly distributed
- Several points overlap at poles

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Solution: **Vogel's method**

In 2 dimensions:

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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!)

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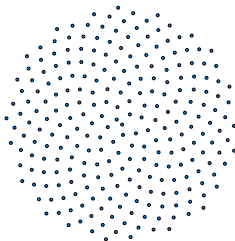


# Evenly Distributed Points

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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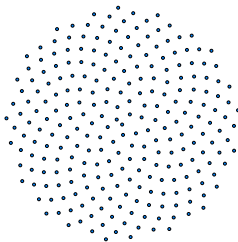
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# Evenly Distributed Points

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):

- ▶ 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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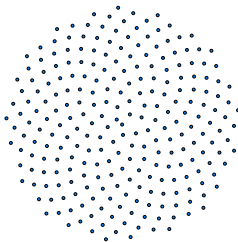
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Solution: **Vogel's method**

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):

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

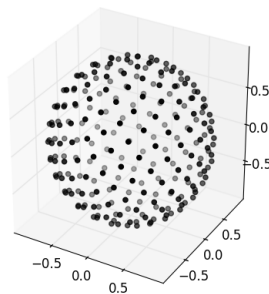


Image source: Marmakoide's Blog

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- ▶ Each atom's total surface area:

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

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# Integration

- ▶ Each atom's total surface area:

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

- ▶ The surface is represented by  $N$  points

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# Integration

- ▶ Each atom's total surface area:

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

- ▶ The surface is represented by  $N$  points

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

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- ▶ Each atom's total surface area:

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

- ▶ The surface is represented by  $N$  points

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

- ▶ In addition, each point has:  $\text{MHP}_j^a$

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# Integration

- ▶ Each atom's total surface area:

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

- ▶ The surface is represented by  $N$  points

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

- ▶ In addition, each point has:  $\text{MHP}_j^a$

Therefore, each atom has a total MHP of:

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

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- ▶ Written in **Python3**, utilizing **ProDy**

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# Program Specifications

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- ▶ Written in **Python3**, utilizing **ProDy**
- ▶ Heavy calculation written in **Cython**

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# Program Specifications

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- ▶ Written in **Python3**, utilizing **ProDy**
- ▶ Heavy calculation written in **Cython**
- ▶ Uses neighbor cells implementation for faster calculation

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

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- ▶ Written in **Python3**, utilizing **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

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- ▶ Input: PSF + PDB or DCD

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

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# Program Options

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

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# Program Options

- ▶ Input: PSF + PDB or DCD
- ▶ Subselection (optional): Atomic selection (like vmd)
- ▶ Number of points per atom (default: 64)
- ▶ Solvent probe radius (default:  $1.4\text{\AA}$ )

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- ▶ Input: PSF + PDB or DCD
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- ▶ Number of points per atom (default: 64)
- ▶ Solvent probe radius (default:  $1.4\text{\AA}$ )
- ▶ Cutoff distance for distance function (default:  $4\text{\AA}$ )

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- ▶ Input: PSF + PDB or DCD
- ▶ Subselection (optional): Atomic selection (like vmd)
- ▶ Number of points per atom (default: 64)
- ▶ Solvent probe radius (default:  $1.4\text{\AA}$ )
- ▶ Cutoff distance for distance function (default:  $4\text{\AA}$ )
- ▶ Frame range (if DCD)

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- By integrating and comparing to known  $\log P$  values, a correlation can be measured.

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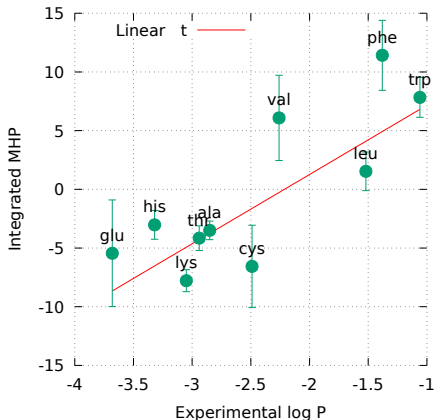
- ▶ By integrating and comparing to known  $\log P$  values, a correlation can be measured.
- ▶ A groups of amino acids of varying hydrophobicity where simulated and their MHP calculated.

# Validation via Known $\log P$ Values

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Validation in vacuum (5 frames per molecule)<sup>5</sup>,  $R^2 = 0.668$



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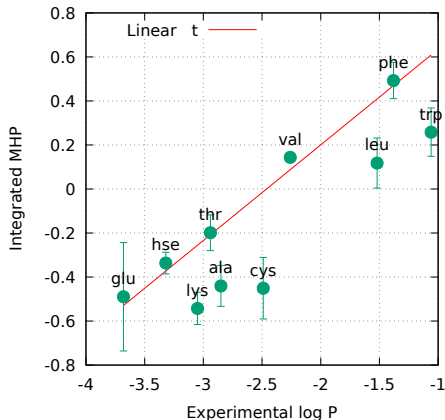
<sup>5</sup>MD simulation using NAMD, performed by Dr. Tillmann Utesch

# Validation via Known $\log P$ Values

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Validation in water + structural optimization (10 frames per molecule),  $R^2 = 0.748$



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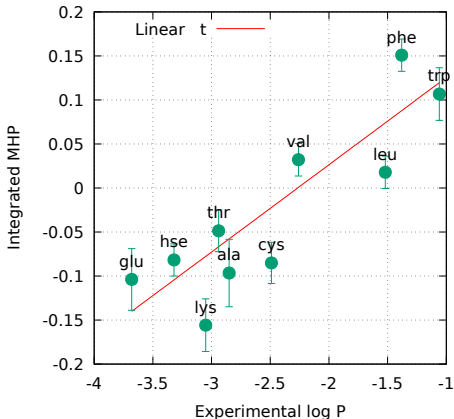


# Validation via Known $\log P$ Values

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Validation in water + structural optimization + SAS normalization  
(10 frames per molecule),  $R^2 = 0.760$



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# Validation via Known $\log P$ Values

- ▶ The validation shows a reasonable qualitative correlation to real data.

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# Validation via Known $\log P$ Values

- ▶ The validation shows a reasonable qualitative correlation to real data.
- ▶ Performed in water (with structural optimization), the results became more accurate.

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# Validation via Known $\log P$ Values

- ▶ The validation shows a reasonable qualitative correlation to real data.
- ▶ Performed in water (with structural optimization), the results became more accurate.
- ▶ The environment did not match experiments, which could affect the accuracy.

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# Validation via Known $\log P$ Values

- ▶ The validation shows a reasonable qualitative correlation to real data.
- ▶ Performed in water (with structural optimization), the results became more accurate.
- ▶ The environment did not match experiments, which could affect the accuracy.
- ▶ Amino acids are small molecules, each error becomes more significant.

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# Validation via Known $\log P$ Values

- ▶ The validation shows a reasonable qualitative correlation to real data.
- ▶ Performed in water (with structural optimization), the results became more accurate.
- ▶ The environment did not match experiments, which could affect the accuracy.
- ▶ Amino acids are small molecules, each error becomes more significant.
- ▶ Larger trajectories will sample conformational space better.

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# An Example System

An existing trajectory (100 frames) of a protein-membrane system<sup>6</sup> was analyzed.

- ▶ The peptide: OP-145, a Cathelicidin derivative with improved properties.

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<sup>6</sup>Trajectory provided by Dr. Alejandra de Miguel Catalina

# An Example System

An existing trajectory (100 frames) of a protein-membrane system<sup>6</sup> was analyzed.

- ▶ The peptide: OP-145, a Cathelicidin derivative with improved properties.
- ▶ The interaction mechanism pathway was studied by means of all-atom simulation.

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<sup>6</sup>Trajectory provided by Dr. Alejandra de Miguel Catalina



# An Example System

An existing trajectory (100 frames) of a protein-membrane system<sup>6</sup> was analyzed.

- ▶ The peptide: OP-145, a Cathelicidin derivative with improved properties.
- ▶ The interaction mechanism pathway was studied by means of all-atom simulation.
- ▶ The membrane used for the study consists of a mixture of two lipids, PG and PE, in agreement with experimental measurements.

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<sup>6</sup>Trajectory provided by Dr. Alejandra de Miguel Catalina

# A video of the system

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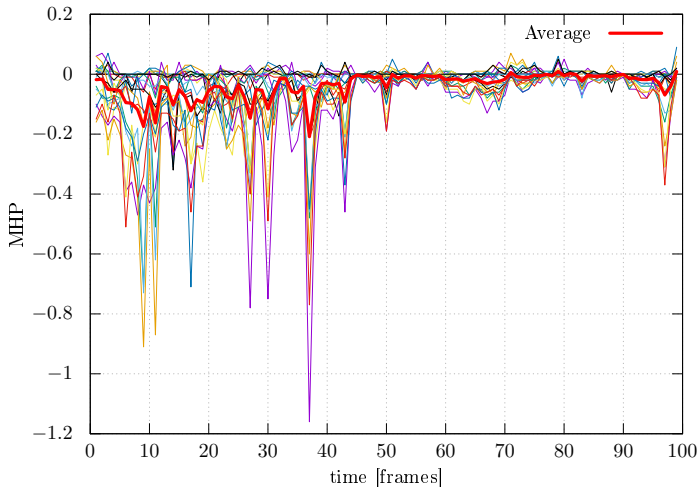
### Thankyou

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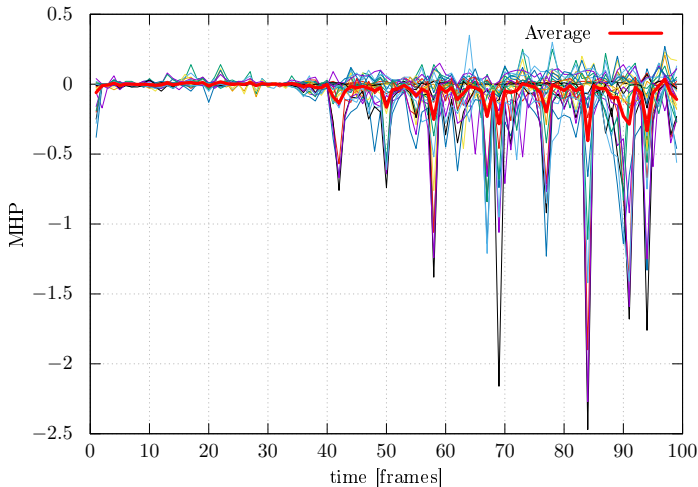
Thankyou

# MHP Change Over Time

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## MHP change over time for ARG-24



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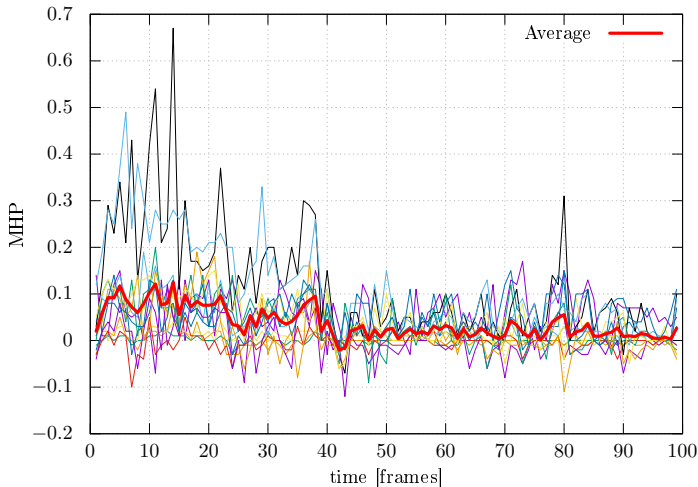
### Thankyou

# MHP Change Over Time

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## MHP change over time for PRO-22



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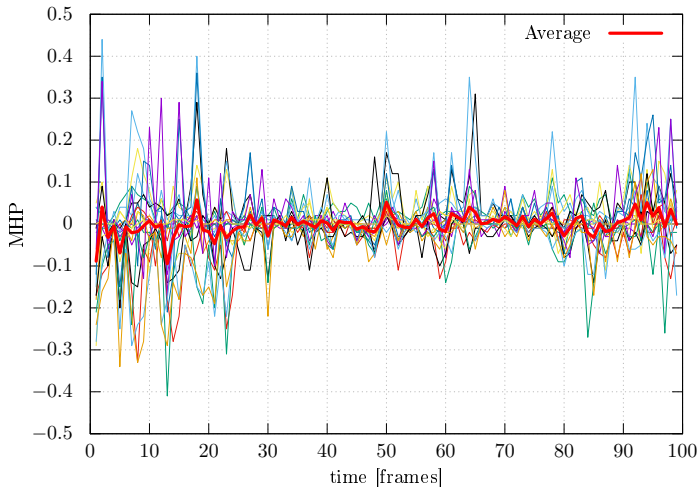
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# MHP Change Over Time

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## MHP change over time for LYS-3



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- ▶ We again get qualitative correlation to expected results (i.e. interior Hydrophobic).

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- ▶ We again get qualitative correlation to expected results (i.e. interior Hydrophobic).
- ▶ The amino acid residues have the correct hydrophobicity.

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# MHP Change Over Time

- ▶ We again get qualitative correlation to expected results (i.e. interior Hydrophobic).
- ▶ The amino acid residues have the correct hydrophobicity.
- ▶ Observing changes in MHP of fragments of interest is possible.

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# MHP Change Over Time

- ▶ We again get qualitative correlation to expected results (i.e. interior Hydrophobic).
- ▶ The amino acid residues have the correct hydrophobicity.
- ▶ Observing changes in MHP of fragments of interest is possible.
- ▶ More systems could (and should!) be analyzed using this method.

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# Thank You for Your Attention!

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