

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

Peleg Bar Sapir¹

Under supervision of
Prof. Maria Andrea Mroginski²

¹Freie Universität Berlin

²Technische Universität Berlin

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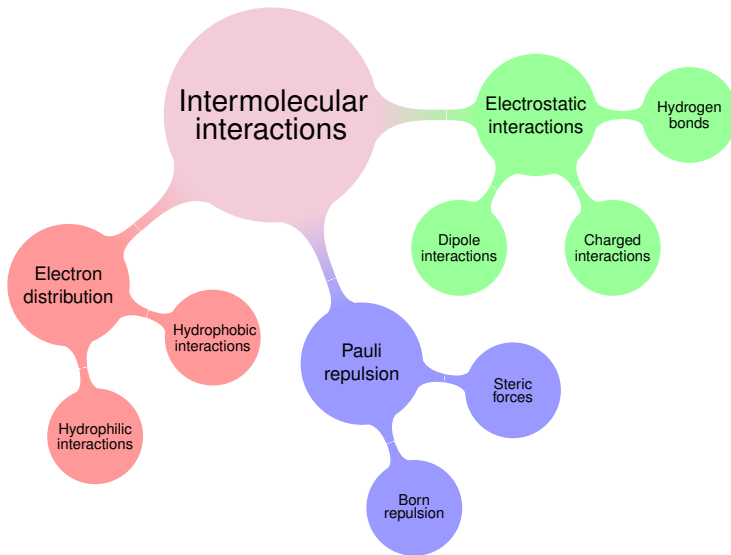
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The ratio of concentrations of a compound in a mixture of two immiscible phases at equilibrium

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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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- ▶ 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) compounds¹, single atoms can be assigned local "force" values.

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¹Ghose et al, J. Phys. Chem. A 1998, 102, 3762-3772

What is Molecular Hydrophobicity Potential (MHP)?

- ▶ By measuring the $\log P$ of many (ca. 30,000) compounds¹, single atoms can be assigned local "force" values.
- ▶ Combining these values with a distance-depended decay function, a potential can be constructed.

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- ▶ By measuring the $\log P$ of many (ca. 30,000) compounds¹, single atoms can be assigned local "force" values.
- ▶ 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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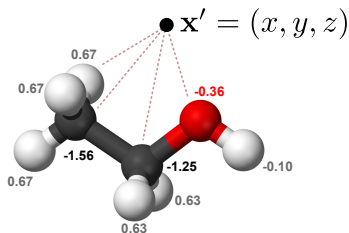
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¹Ghose et al, J. Phys. Chem. A 1998, 102, 3762-3772

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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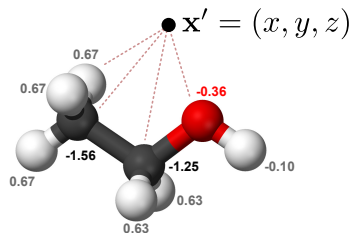
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Summing over all atoms

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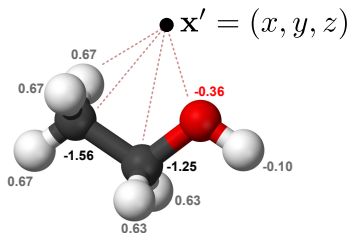
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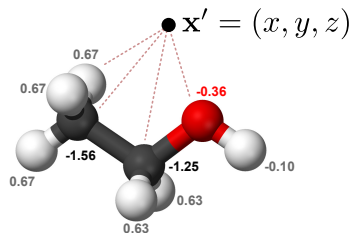
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$$\text{MHP}(\mathbf{x}') = \sum_{i=1}^k \left[f_i \cdot D(\mathbf{x} - \mathbf{x}'_i) \right]$$

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Force Constants - Carbon

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Carbon atom contribution to hydrophobicity²

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

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

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Hydrogen atom contribution to hydrophobicity³

Type	Description	f_i value
	Hydrogen attached to:	
46	C _{sp} ³ , no X in α	0.7341
47	C _{sp} ²	0.6301
50	Heteroatom X	-0.1036
52	C _{sp} ³ , 1 X in α	0.6666
54	C _{sp} ³ , 3 X in α	0.6338

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

Force Constants - Oxygen

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Oxygen atom contribution to hydrophobicity⁴

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

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

Force Constants - Various

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Various atom contribution to hydrophobicity⁵

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

⁵Source: Ghose et al, J. Phys. Chem. A 1998, 102, 3762-3772

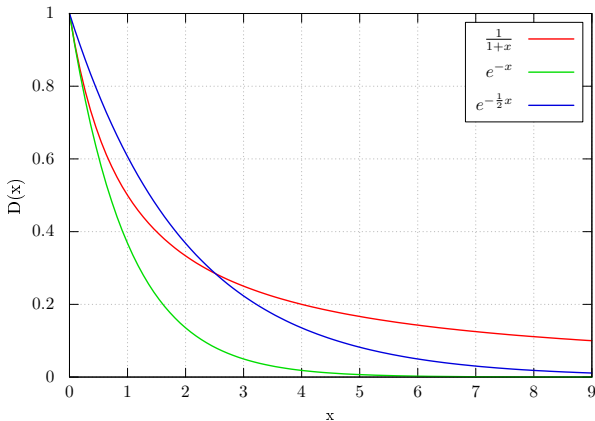
Distance function

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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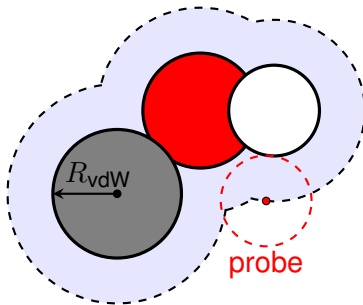
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Solvent Accessible Surface

- ▶ The surface around a molecule accessible to solvent molecules



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

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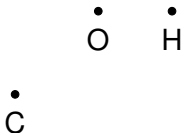
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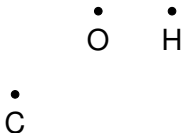
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1. Take all atoms with their vdW-radii

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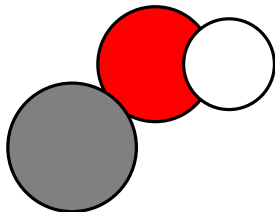
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How to Create the Solvent Accessible Surface?



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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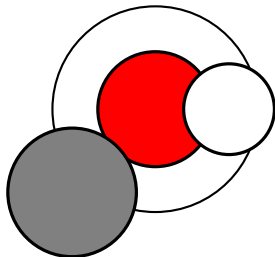
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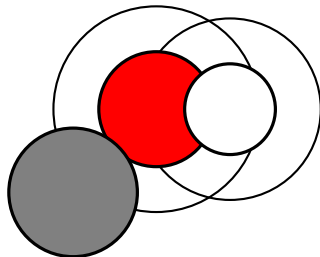
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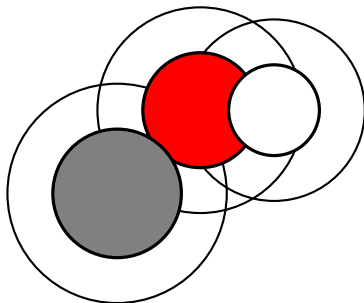
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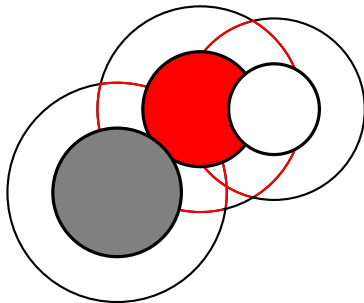
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How to Create the Solvent Accessible Surface?



1. Take all atoms with their vdW-radii
2. Create spheres around all atoms with
 $R^i = R_{\text{vdw}}^i + R_{\text{probe}}$
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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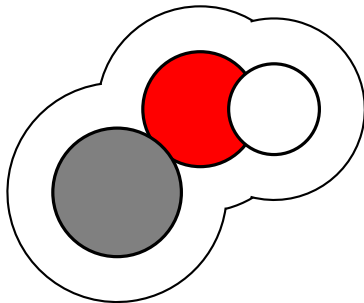
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How to Create the Solvent Accessible Surface?



1. Take all atoms with their vdW-radii
2. Create spheres around all atoms with
 $R^i = R_{\text{vdw}}^i + R_{\text{probe}}$
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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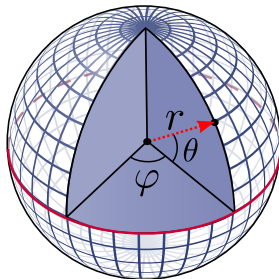
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How to distribute N points on a surface of a sphere?



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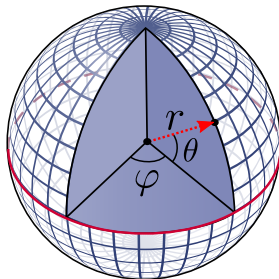
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How to distribute N points on a surface of a sphere?



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

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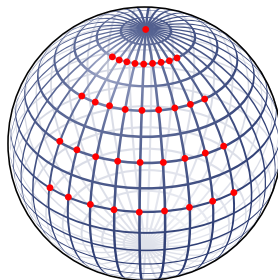
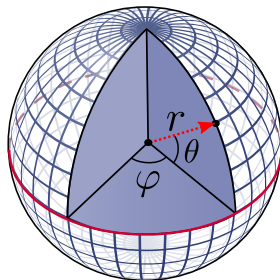
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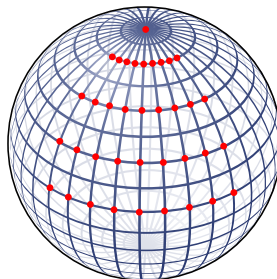
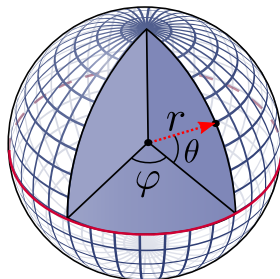
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Evenly Distributed Points

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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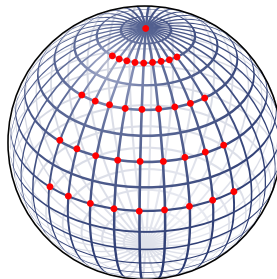
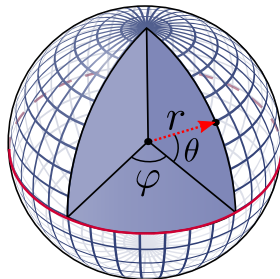
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Evenly Distributed Points

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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Solution: **Vogel's method**

In 2 dimensions:

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

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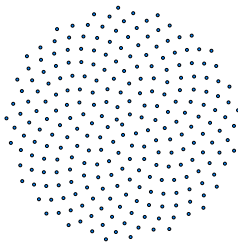
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Evenly Distributed Points

Solution: **Vogel's method**

In 2 dimensions:

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



In 3 dimensions (cylindrical coordinates):

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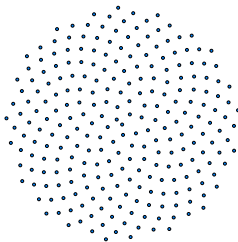
Thankyou

Evenly Distributed Points

Solution: **Vogel's method**

In 2 dimensions:

- ▶ Distances: $r_i = \sqrt{\frac{i}{N}}$
- ▶ Angle: $\theta_i = \varphi i$
(φ 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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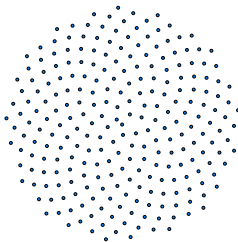
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Evenly Distributed Points

Solution: **Vogel's method**

In 2 dimensions:

- ▶ Distances: $r_i = \sqrt{\frac{i}{N}}$
- ▶ Angle: $\theta_i = \varphi i$
(φ 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:
 $\theta_i = \varphi i$, $\rho_i = \sqrt{1 - z_i^2}$

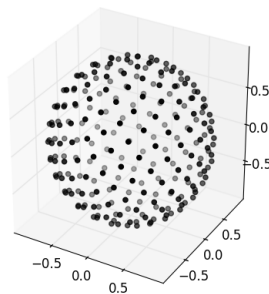


Image source: Marmakoide's Blog

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

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

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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\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\AA)
- ▶ Cutoff distance for distance function (default: 4\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\AA)
- ▶ Cutoff distance for distance function (default: 4\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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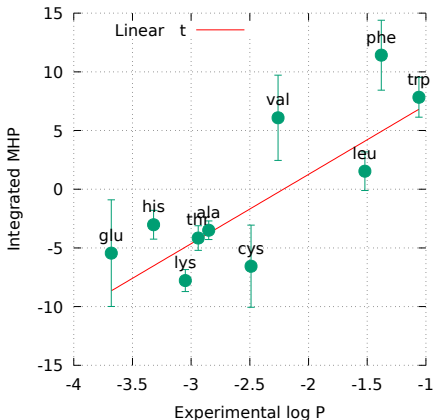
- ▶ By integrating and comparing to known $\log P$ values, a correlation can be measured.
- ▶ A groups of amino acids of varying hydrophobicity where simulated and their MHP calculated.

Validation via Known $\log P$ Values

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Validation in vacuum (5 frames per molecule)⁶, $R^2 = 0.668$



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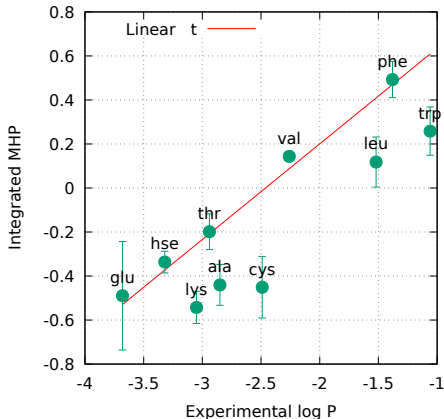
Thankyou

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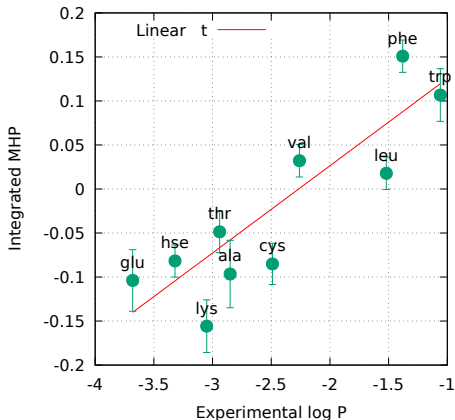
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Validation in water + structural optimization + SAS normalization
(10 frames per molecule), $R^2 = 0.760$



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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 existing trajectory (100 frames) of a protein-membrane system⁷ was analyzed.

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

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⁷Trajectory provided by Dr. Alejandra de Miguel Catalina

An Example System

An existing trajectory (100 frames) of a protein-membrane system⁷ 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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⁷Trajectory provided by Dr. Alejandra de Miguel Catalina

An Example System

An existing trajectory (100 frames) of a protein-membrane system⁷ 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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⁷Trajectory provided by Dr. Alejandra de Miguel Catalina

A video of the system

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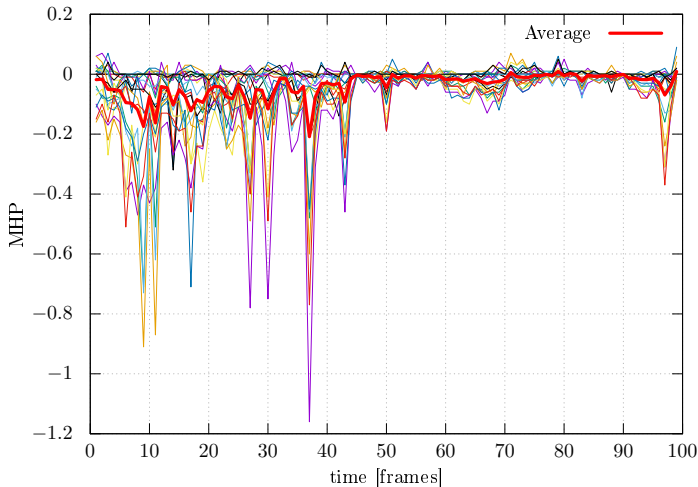
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MHP Change Over Time

Molecular
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MHP change over time for ARG-7



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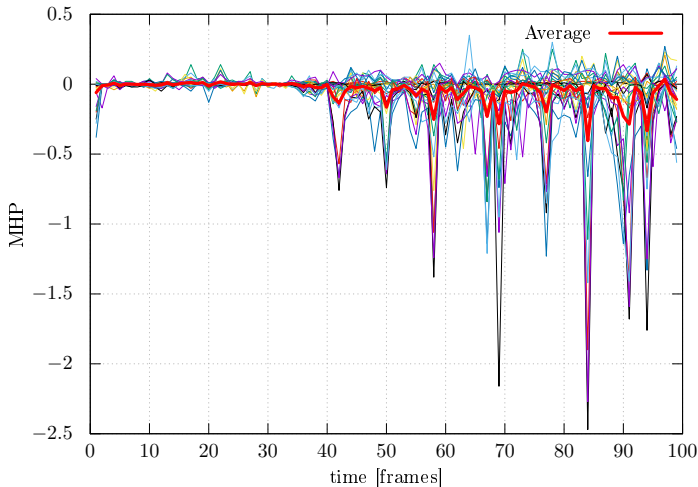
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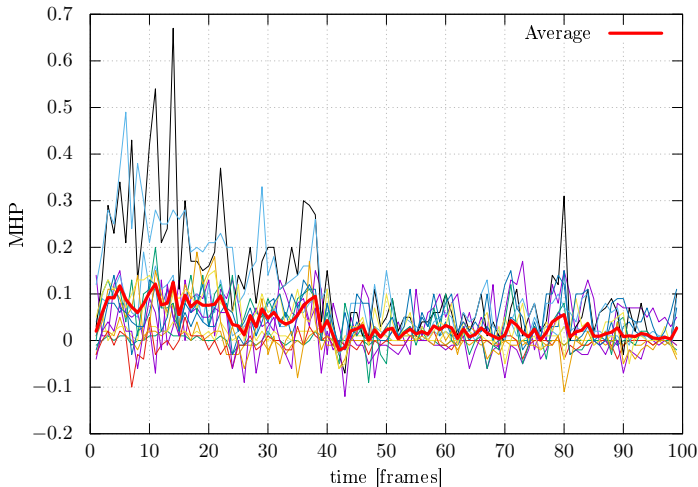
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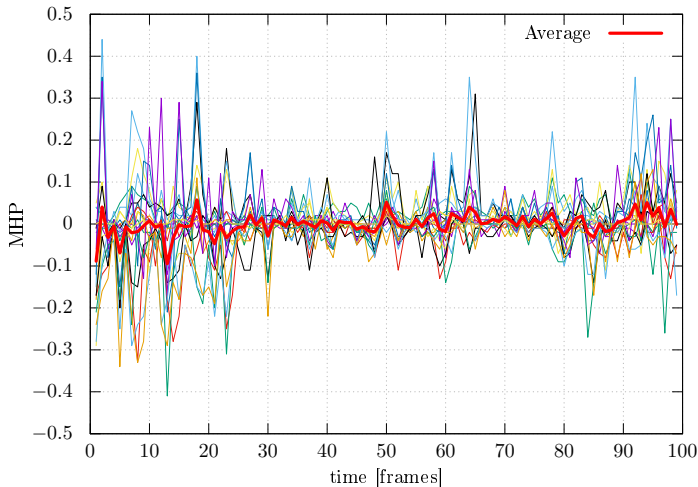
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- ▶ The validation shows a reasonable qualitative correlation to real data.

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- ▶ 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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- ▶ 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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- ▶ 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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MHP Change Over Time

- ▶ 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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