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

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Molecular Hydrophobicity Potential

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ntroduction

Hydrophobicity and log P

Molecular Hydrophobicity Potential

Potential

Force constants

Distance function

Solvent accesible

Evenly distributed points

Integration

Outline

Introduction

Hydrophobicity and log P

Molecular Hydrophobicity Potential

Potential

General form

Force constants

Distance function

Surface

Solvent accesible surface

Evenly distributed points

Integration

Molecular Hydrophobicity Potential

Pelg Bar Sapir

ntroduction

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Molecular Hydrophobicity

Potential

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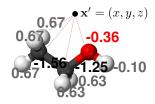
Force constants

Distance function

Surface

Solvent accesible surface

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

Molecular Hydrophobicity Potential

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Introduction

Hydrophobicity and log P

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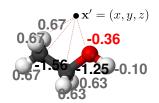
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General form

Distance function

Solvent accesible surface Evenly distributed points

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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

Molecular Hydrophobicity Potential

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Introduction

Hydrophobicity and log F

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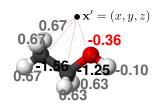
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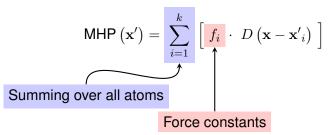
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Surface

Evenly distributed points





Molecular Hydrophobicity Potential

Pelg Bar Sapir

Introduction

Hydrophobicity and log F

Molecular Hydrophobi

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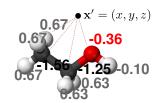
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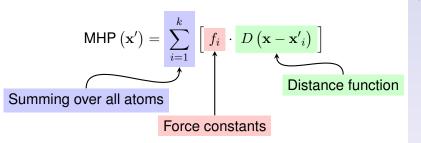
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Surface

Solvent accesible surface Evenly distributed points







Molecular Hydrophobicity Potential

Pelg Bar Sapir

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Hydrophobicity and log F

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Potential

General form

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Surface

Solvent accesible surface Evenly distributed points

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Force constants

Type	Description	f_i value
	C in:	
3	$\overline{\mathrm{CHR}}_3$	-0.6681
15	$=CH_2$	-0.7866
36	R-CH-X	-0.2405
	H attached to:	
45	$\mathrm{C}_{\mathrm{sp^3}}$, no X attached to next carbon	0.7341
46	$\mathrm{C_{sp^3}, C_{sp^2}}$	0.6301
50	Heteroatom	-0.1036
52	$\mathrm{C}_{\mathrm{sp^3}}$, 1 X attached to next carbon	0.6666
	<u>O in</u> :	
56	Alcohol	-0.3567
58	Ketone	-0.0233
62	0-	-0.7941

Molecular Hydrophobicity Potential

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General form
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Solvent accesible surface

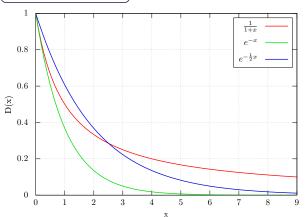
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Audry form

Exponential decay form

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

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



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Pelg Bar Sapir

ntroduction

Hydrophobicity and log P

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orce constants

Distance function

Solvent accesible surface

Solvent accesible surface

Molecular Hydrophobicity Potential

Pelg Bar Sapir

Introduction

Hydrophobicity and log F

Molecular Hydrophobicity

Potential

General form Force constant

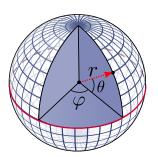
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Solvent accesible surface

Evenly distributed point ntegration

Evenly distributed points

How to distribute N^2 points on a surface of a sphere?



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ntroduction

Hydrophobicity and log

Molecular Hydrophobicity

Potential

General form Force constants

Distance function

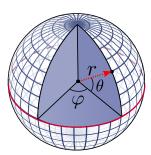
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Evenly distributed points

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How to distribute N^2 points on a surface of a sphere?



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

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Pelg Bar Sapir

ntroduction

Hydrophobicity and log

Molecular Hydrophobicity

Potential

General for

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Surface

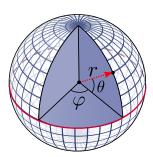
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Evenly distributed points

Integration

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How to distribute N^2 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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Hydrophobicity and log

Molecular Hydrophobicity

Potential

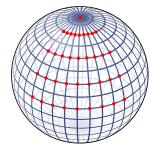
Force constants

Surface

Solvent accesible surface

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ntroduction

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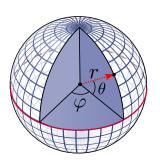
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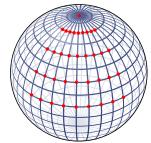
Solvent accesible surface

Evenly distributed points Integration

How to distribute N^2 points on a surface of a sphere?

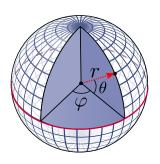




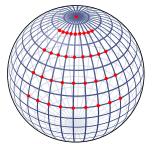


 $\varphi_i = i \cdot \frac{2\pi}{N}$ $\theta_j = j \cdot \frac{\pi}{N}$

Points are not evenly distributed How to distribute N^2 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

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:

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

Integration

Molecular Hydrophobicity Potential

Pelg Bar Sapir

Introduction

Hydrophobicity and log F

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Hydrophobicity Potential

Potential

General form Force constants

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urface

Solvent accesible surface Evenly distributed points

Integration