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

Peleg Bar Sapir<sup>1</sup> Under supervision of Prof. Maria Andrea Mroginski<sup>2</sup>

> <sup>1</sup>Freie Universität Berlin <sup>2</sup>Techniche Universität Berlin

February 14, 2018

#### Molecular Hydrophobicity Potential

Pelg Bar Sapir

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

Hydrophobicity and log F

Molecular Hydrophobicity

Potential

Gonoral fo

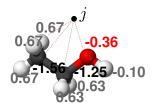
Force constants

Distance function

Surface

Solvent accesible surface

ntegration



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

#### Molecular Hydrophobicity Potential

Pelg Bar Sapir

Introduction

Hydrophobicity and log I

Molecular

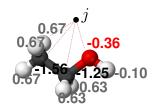
Potential

General form

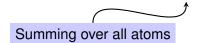
Force constants

Surface

Solvent accesible surface Evenly distributed points



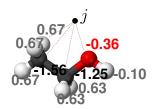
$$\mathsf{MHP}\left(\mathbf{x}'\right) = \sum_{i=1}^{k} \left[ \begin{array}{c|c} f_i \end{array} \cdot \left[ D\left(\mathbf{x} - \mathbf{x}'\right) \end{array} \right]$$



#### Molecular Hydrophobicity Potential

Pelg Bar Sapir

General form



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

# Summing over all atoms

Molecular Hydrophobicity Potential

Pelg Bar Sapir

Introduction

Hydrophobicity and log I

Molecular

Potential

General form

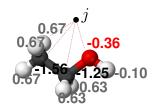
orce constants

Distance function

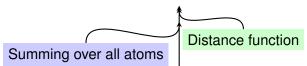
Surface

Evenly distributed points

Evenly distributed point: ntegration



$$\mathsf{MHP}\left(\mathbf{x}'
ight) = \sum_{i=1}^{k} \left[ egin{array}{c} f_i \end{array} \cdot \left[ D\left(\mathbf{x} - \mathbf{x}'
ight) \end{array} 
ight]$$



Molecular Hydrophobicity Potential

Pelg Bar Sapir

Introduction

Hydrophobicity and log I

Molecular

Potential

General form

orce constants

Distance func

Solvent accesible surface

Evenly distributed points Integration

◆母 ▶ ◆重 ▶ ◆重 ● 夕♀◎

## Force constants

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

Pelg Bar Sapir

troduction ydrophobicity a

olecular

ropnoblential

ial eral form

Force constants

tance function

olvent accesible surface venly distributed points

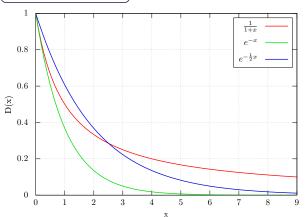
nly distributed points gration

# Audry form

## Exponential decay form

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

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



Molecular Hydrophobicity Potential

Pelg Bar Sapir

ntroduction

Hydrophobicity and log P

ydrophobicity otential

otential

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

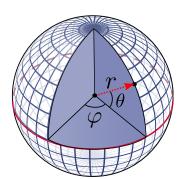
urface

Solvent accesible surface

Evenly distributed point ntegration

## Evenly distributed points

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



Molecular Hydrophobicity Potential

Pelg Bar Sapir

ntroduction

Hydrophobicity and log I

Molecular Hydrophobicity

Potential

General for

stance function

Sunace

Solvent acces

Evenly distributed points

Integration

## Integration

#### Molecular Hydrophobicity Potential

#### Pelg Bar Sapir

#### Introduction

Hydrophobicity and log

#### Molecular Jydrophobicity

Potential

#### Potential

General form Force constants

#### istance funct

Solvent accesible surface

#### Integration