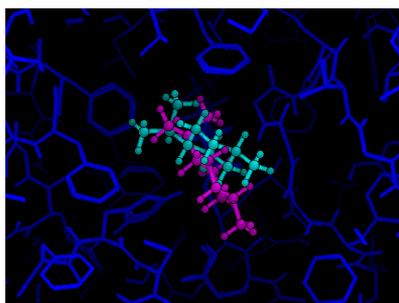


**Molecular Models for Real World Problems**



Diastereomeric Transitionstates in Enzyme

**CURRENT RESEARCH:**

Selectivity of Catalysts and Enzymes

Active Site Modeling and Drug Design

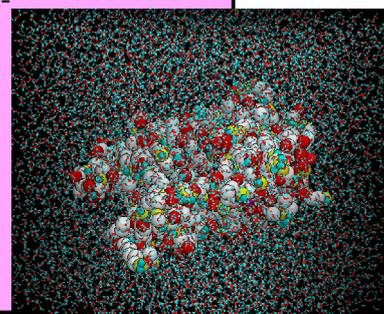
Model based Structure-Property Relations

Structures in Solution

Thermodynamic Properties

Visualization

$$\Delta H_{\text{vap}} = \frac{d \ln P}{dT} * RT^2$$



Proteindimer in Aqueous Solution

**MODEL GENERATION:**

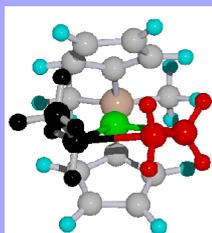
Analysis of Real World Problem

Reduction to the Relevant Phenomena

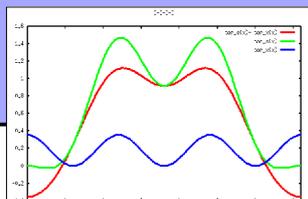
Formulation of the Questions to Answer

Implementation of Models and Methods

Derivation of Descriptors

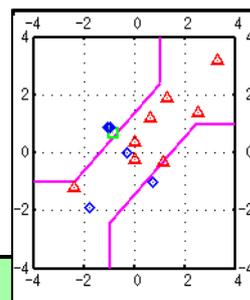


Transitionstate in Polymerisation



Tuning of Force Field Terms

**Enhancing Research Efficiency by Modeling Support for Experiments**



Exp. vs Cal. Selectivity

**MOLECULAR DESIGN:**

Finding Structure-Property Relations

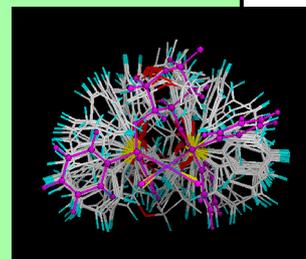
Model Validation

Automated Structure Generation

Virtual Screening

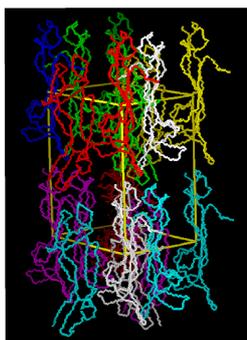
Predicting Improved Molecules

Validating Predictions



Best of ALL Geometries

**Unique Models for Unique Answers**



Proteindimers in Crystal

**PROTEIN MODELING:**

Converting X-ray Data to Geometries

Structure Analysis

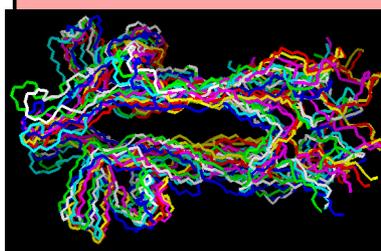
Structure Dynamics

Data Reduction

Active Site Models

Drug Design

Homology



Dynamics of Proteindimer in Solution

**COMPANY:**

Spun-off WWU Münster in 1992

3 Theoretical-Organic Chemists

**EXPERIENCE:**

Theoretical Chemistry

Problem Analysis

Model Generation

Software Implementation

