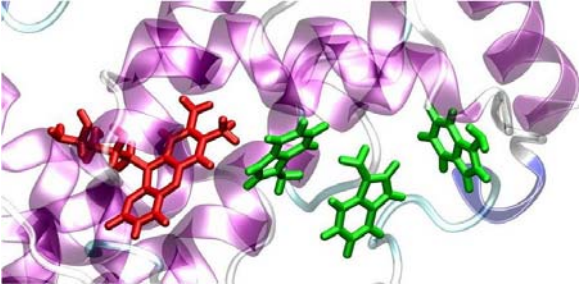


Methods, IPC, Koslowski

<p style="text-align: center;">Amber</p> <p style="text-align: center;"><i>Molecular dynamics</i></p>	<p>Model: Unit and Room: Responsible: Further information:</p>	<p><i>Version 10</i> <i>Physical Chemistry, various</i> <i>Prof. Thorsten Koslowski</i> <i>www.theochem.uni-freiburg.de</i></p>
<p>Short Description:</p> <p>Amber 10 molecular dynamics package with various extensions</p> <p>Available Experiments/Techniques:</p> <p>Molecular dynamics in a variety of ensembles, thermodynamic integration methods</p>	<p style="text-align: center;">Picture of the Equipment</p> 	
<p>Special Equipment:</p> <p>Extension to combined quantum mechanics - classical mechanics simulations</p>		
<p>Measurements on the equipment are currently done by:</p>	<p><input type="checkbox"/> Students <input type="checkbox"/> Students after Introduction <input checked="" type="checkbox"/> Students after extensive training <input checked="" type="checkbox"/> Trained scientific service personal</p>	
<p>Recent Publications, where this instrument was important (optional): Give citation</p>	<p>J. Phys. Chem. B 112, 16935 (2008), PCCP 7, 4039 (2005) (invited article)</p>	
<p>Typical problems that may be solved with this instrument:</p>	<p><i>Direct simulation of electron transfer, free energy surfaces for reactions</i></p>	