


Methods, IPH, Günther

<p>GRID computing</p> <p><i>parallel data processing</i></p>	<p>Model: <i>SunFire X2250, Dell PE 1950, BL460c HP, Grid</i></p> <p>Unit and Room: <i>Rechenzentrum of the university</i></p> <p>Responsible: <i>Dr. Volker-H. Winterer, Rechenzentrum</i></p> <p>Further information: <i>http://www.bfg.uni-freiburg.de</i></p>	
<p>Short Description:</p> <p>The Black-Forest Grid is currently constituted of 760 Cores and 2GB RAM per Core.</p>	<p>Picture of the Equipment</p>	
<p>Available Experiments/Techniques:</p> <p>Ligand-based / structure-based compound screenings High throughput docking of compounds Molecular dynamics simulations of molecular interactions Prediction of binding affinities</p>		
<p>Special Equipment:</p> <p>Software, Molecular Modeling Platforms: Schrodinger, Inc. software suite Accelrys, Inc. software suite</p>		
<p>Measurements on the equipment are currently done by:</p>	<p><input type="checkbox"/> Students <input checked="" 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>Typical problems that may be solved with this instrument:</p>	<p><i>Identification of small molecules that come into question for drug leads. Prediction of binding affinities.</i></p>	