

# Aurélien GROSDIDIER

## Personal Details

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<b>Address:</b>	Av. Secrétan, 20 1005 Lausanne Switzerland	<b>Nationality:</b>	French
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## Research Experience

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2007-present **PostDoc Project:** Improvement of EADock, development of SwissDock, an online workbench for molecular docking

2002-2007 **PhD Project:** Evolutionary algorithms (EA) in bioinformatics/molecular modeling @ [SIB](#)  
**EADock:** Design of a new molecular modeling docking algorithm. Application in drug-design, rational and fragment-based drug-design ([O. Michielin](#), MD-PhD)  
Expression data analysis, multiple sequence alignment ([C. Notredame](#), PhD)  
Object-oriented design and implementation of the [Jeep](#) evolutionary framework and [wrappers](#) around common tools (CHARMM, Modeler, Anolea)

2000-2001 **Internship:** Distribution of the [Swiss-Model](#) pipeline over a network @ GWER  
Implementation and evaluation of a distributed [Swiss-Model](#) pipeline using [CORBA](#), GlaxoSmithKline Experimental Research SA (A. Diemand, N. Guex)

1999-2000 **Internship:** Interaction between proteins and heparan sulfates @ [IBS](#) / [CERMAV](#)  
*In vitro/silico*, [design/implementation of a database](#) ([H. Lortat-Jacob](#), [A. Imberty](#))

1998-1999 **Internship:** Interaction between SDF-1 and heparan sulfates @ [IBS](#) / [CERMAV](#)  
Wet-lab, molecular modeling ([H. Lortat-Jacob](#), [A. Imberty](#))

1997-1998 **Internship:** Characterization of the pharmacophore of calcium channel inhibitors (School of Pharmacy, Grenoble, Prof. M. Cussac)

## Professional Experience

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2000-present **Supervision:** Technical director of [Antesis Interactive](#)  
Network infrastructure design, deployment and security ([DGA](#)), web-based distributed document management systems ([CNES](#)), supervision of technical courses

2003-2005 **Supervision:** President of [Antesis.org](#), an association promoting on-demand linux LiveCDs

## Education

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- 2002-2007 PhD Student @ Swiss Institute of Bioinformatics, Molecular Modeling Group  
2000-2001 Master Degree in Bioinformatics, University of Geneva (Switzerland)  
1995-2007 School of Pharmacy - Research, Joseph Fourier University (Grenoble - France)  
Certificate in Structural Chemistry, Molecular Modeling and Biotechnology  
1994-1995 Baccalaureate, specialization in physics, mention AB (Die - France)

## Skills

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- Computer Science: System administration: Linux/MacOSX/\*BSD/Win32  
Configuration, deployment, usage and administration of OpenLDAP
- Software: EADock / CHARMM / Modeler / Sybyl  
Chimera / VMD / Molmol  
Common sequence-related tools and resources
- Software Design: Object-oriented design and implementation, design patterns, UML modeling  
Programming languages: Java/PHP/Perl/C/C++/shell scripting
- Productivity: HPC: Cluster design, deployment and monitoring (SGE,LSF,Torque/MAUI)  
Grid computing: Condor, BOINC, xgrid
- Data Management: Common SQL engines (MySQL/PostgreSQL)  
R statistical package  
Design and implementation of integrated web-based user interfaces
- Languages: French: Mother tongue  
English: Fluent, spoken and written
- Things I forgot: <http://www.google.com/search?q=aurelien+grosdidier>

## Publications

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1. Grosdidier A., Zoete V., and Michielin O., **Blind docking of 260 protein-ligand complexes with EADock 2.0**, *J Comput Chem*, *accepted for publication*
2. Chodanowski P., Grosdidier A., Feytmans E., and Michielin O., **Local alignment refinement using structural assessment**, *PLoS ONE*. 2008 Jul 9;3(7):e2645.
3. Rochat B., Zoete V., Grosdidier A., von Grünigen S., Marull M., Testa B. and Michielin O., **In Vitro Biotransformation of Imatinib by CYP1A1 and CYP1B1: Could it Play a Role in Tumor-Specific Drug Metabolism and Disposition?**, *Biopharm Drug Dispos*. 2008 Mar;29(2):103-18.
4. Feige JN., Gelman L., Rossi D., Zoete V., Métivier R., Tudor C., Anghel SI., Grosdidier A., Lathion C., Engelborghs Y., Michielin O., Wahli W. and Desvergne B., **The endocrine disruptor monoethyl-hexyl-phthalate is a selective peroxisome proliferator-activated receptor gamma modulator that promotes adipogenesis**, *J Biol Chem*. 2007 Jun 29;282(26):19152-66. Epub 2007 Apr 27
5. Grosdidier A., Zoete V., and Michielin O., **EADock: docking of small molecules into protein active sites with a multiobjective evolutionary optimization**, *Proteins*, 2007, Jun 1;67(4):1010-25.
6. Zoete V., Grosdidier A., and Michielin O., **Peroxisome proliferator-activated receptor**

structures: Ligand specificity, molecular switch and interactions with regulators, *Biochim Biophys Acta*. 2007 Aug;1771(8):915-25. Epub 2007 Jan 18. Review.

7. Michalik L., Zoete V., Krey G., Grosdidier A., Gelman L., Chodanowski P., Feige JN., Desvergne B., Wahli W., and Michielin O., **Combined simulation and mutagenesis analyses reveal the involvement of key residues for PPARalpha helix 12 dynamic behavior.** *J. Biol. Chem.*, Jan 2007; 10.1074/jbc.M610523200
8. Li C., Grosdidier A., Crambert G., Horisberger JD., Michielin O., and Geering K., **Structural and functional interaction sites between Na,K-ATPase and FXYD proteins.** *J Biol Chem*. 2004 Sep 10;279(37): 38895-902
9. O'Sullivan O., Zehnder M., Higgins D., Bucher P., Grosdidier A., and Notredame C., **APDB: a novel measure for benchmarking sequence alignment methods without reference alignments.** *Bioinformatics* 2003 19: 215i-221i
10. Lortat-Jacob H., Grosdidier A., Imberty A., **Structural diversity of heparan sulfate binding domains in chemokines.** *Proc Natl Acad Sci U S A*. 2002 Feb 5;99(3): 1229-34
11. Sadir R., Baleux F., Grosdidier A., Imberty A., Lortat-Jacob H. **Characterization of the Stromal Cell-derived Factor-1-Heparin Complex** *J. Biol. Chem*. 2001 276: 8288-8296

## Conferences

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1. Aurélien Grosdidier, Vincent Zoete and Olivier Michielin, **EADock, docking small molecules into protein active sites with a multiobjective framework**, [ISQBP'06](#), best poster award

## References

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[O. Michielin](#), [C. Notredame](#), N. Guex, [H. Lortat-Jacob](#), [A. Imberty](#), [E. Drouet](#)