

Abdelkrim Rachedi

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<http://emboss.bioinf.wits.ac.za/stad>
<http://www.bioinformers.co.uk>
<http://www.algeriansgate.co.uk>

Previously I was with the European Bioinformatics Institute, Hinxton, Cambridge, UK

Current teaching

I teach the following courses:

- Introduction to Bioinformatics (second year students / School of Molecular & Cell Biology)
- Structural Bioinformatics (honours students / School of Molecular & Cell Biology)
- Introductory Bioinformatics Techniques (honours students / School Molecular & Cell Biology)
- Introductory Bioinformatics Techniques (honours students / Schools of Human Genetics; and Molecular Medicine & Haematology.)
- Computational Molecular Biology (part of the course to honours students / School of Computer Science)

Admin

The set up and running of the Bioinformatics Journal Club, see Wits-Bioinformatics web site at <http://www.bioinf.wits.ac.za/bjc.html>

Research

Projects and Area of interest:

- See
- <http://www.bioinf.wits.ac.za/research.html>
 - <http://www.bioinf.wits.ac.za/services.html>

MSc and BSc Honors potential projects:

- Nucleic acids structural parameters, ligand binding sites and motifs^(a).
- Ligand binding modes in proteins; tapping into the roots of species drug binding selectivity^(b).
- Catalytic groupings of amino acids and their 3D arrangements in proteins; a study into understanding the biological function of proteins^(b).

(a) This project will expand on the BSc-Honors project [NALD database](#) (see next sections) studying nucleic acids, ligands, binding motifs, binding classes and disease links. The

project will investigate the possibility to create a platform for DNA/RNA targeted drug design.

- (b) Both of these projects draw on published work I have done before at the European Bioinformatics Institute, see [MSDsite: a database search and retrieval system for the analysis and viewing of bound ligands and active sites](http://www3.interscience.wiley.com/journal/109665397/abstract). see URL: <http://www3.interscience.wiley.com/journal/109665397/abstract>

Postgraduate and honours supervision:

- MSc - 2011: **Catalytic groupings of amino acids and their 3D arrangements in proteins; a study into understanding the biological function of proteins**
- BSc Honors - 2011: **Amino Acids and Structural Motifs in Protein-DNA Complexes.**
- BSc Honors - 2010: **Nucleic Acids Ligand Binding Motifs, Binding Classes & Disease Links.** (done)

Research output:

01. Abdelkrim Rachedi, Khuphukile Madida, (2011). **NALD: Nucleic Acids and Ligands Database; Ligand Binding Motifs, Binding Classes & Disease Links, 2nd ISCB Africa ASBCB Conference on Bioinformatics, March 9-11, 2011.**
02. Abdelkrim Rachedi, (2011). **Annotation of structural targets in South Africa; the STAD database, 2nd ISCB Africa ASBCB Conference on Bioinformatics, March 9-11, 2011.**
03. Khuphukile Madida, Abdelkrim Rachedi, (2010). **Ligand Types, Classes and Targets in the Nucleic Acids Complexes & Relations to South African Prevalent Diseases, Wits Faculty of Health Sciences Research Day, 22 September, 2010.**
04. Abdelkrim Rachedi, (2009). **STAD: Structural Targets Annotation Database, Proceedings for the Second Southern African Bioinformatics Workshop, 11th - 12th, Johannesburg, October 2009**
05. Shira Albeck, Pedro Alzari, Claudia Andreini, Lucia Banci, Ian Berry, Ivano Bertini, Christian Cambillau, Bruno Canard, Lester Carter, Serge Cohen, Jon Diprose, Orly Dym, Robert M Esnouf, C Felder, F Ferron, F Guillemot, R Hamer, M Jelloul, R.A Laskowski, S Longhi, R Lopez, C Luchinat, H Malet, C Mayo, T Mochel, L Moulinier, R J Morris, T Oinn, A Pajon, Y Peleg, A Perrakis, O Poch, J Prilusky, **A Rachedi**, R Ripp, A Rosato, I Silman, D I Stuart, J L Sussman, J-C Thierry, J D Thompson, J M Thornton, T Unger, B Vaughan, W Vranken, J D Watson, G Whamond, Z.R Yang and Kim Henrick. (2006) **SPINE Bioinformatics and data management aspects of high throughput structural genomics projects. Acta Cryst.** (Authors in alphabetical order, refer to the section "**3. SPINE Targets, Database and tools:**")
06. Golovin A., Dimitropoulos D., Oldfield T., **Rachedi A.** and Henrick (2005) **MSDsite: A Database Search and Retrieval System for the Analysis and Viewing of Bound Ligands and Active Sites. PROTEINS: Structure, Function, and Bioinformatics 58(1): 190-9.**
07. A. Golovin, T. J. Oldfield, J. G. Tate, S. Velankar, G. J. Barton, H. Boutselakis, D. Dimitropoulos, J. Fillon, A. Hussain, J. M. C. Ionides, M. John, P. A. Keller, E. Krissinel, P. McNeil, A. Naim, R. Newman, A. Pajon, J. Pineda, **A. Rachedi**, J. Copeland, A. Sitnov, S. Sobhany, A. Suarez-Uruena, J. Swaminathan, M. Tagari, S. Tromm, W. Vranken and K. Henrick (2004) **E-MSD: an integrated data resource for bioinformatics *Nucleic Acids Research*, 32 (Database issue), D211-D216.**

08. Boutselakis, H., Copeland, J., Dimitropoulos, D., Fillon, J., Golovin, A., Henrick, K., Hussain, A., Ionides, J., John, M., Keller, P., Krissnel, E., McNeil, P., Naim, A., Newman, R., Oldfield, T., Pineda, J., **Rachedi, A.**, Sitnov, A., Sobhany, S., Suarez-Uruena, A., Swaminathan, J., Tagari, M., Tate, J., Tromm, S., Velankar, S. and Vranken, W., (2003) **E-MSD: the European Bioinformatics Institute Macromolecular Structure Database.** *Nucleic Acids Research*, **31**, 458-462

09. Abdelkrim Rachedi, Michael Rebhan and Hong Xue.
GABAagent: a system for integrating data on GABA receptors.
Bioinformatics. 2000 Apr;**16(4):301-12.**

10. Abdelkrim Rachedi, Michael Rebhan and Hong Xue.
Internet-based Integrated Retrieval Information System for GABA receptors.
Society for Neuroscience Abstracts. Vol.25, Part 2, page1809, Oct. 1999.

11. Khoo ASB, Balraj P, **Rachedi A**, Chin CN, Volpi L.
A novel complex mutation of the OTC (Ornithine Transcarbamylase) Gene in a Malaysian Pedigree. *Human Mutation*. 1999 Nov; 14(5): 448.

12. Khoo ASB, Balraj P, **Rachedi A**, Volpi L, Chin CN.
Clinical Correlation of a Novel Mutant Ornithine Transcarbamylase (OTCase) Homology Model. In Proceedings of the 10th National Biotechnology Seminar: Biotechnology towards the next millenium, pages 26-27. SIRIM Berhad, Malaysia, 27 & 28 October 1998.

13. Khoo ASB, Balraj P, **Rachedi A**, Volpi L, Tan SK, Lim PKC, Chin CN.
Molecular Genetic Investigations of a family with multiple early neonatal deaths.
In Abstracts of the First Scientific Seminar of the National Institutes of Health, Ministry of Health, Malaysia: Research in the New Millenium, Page 45. Kuala Lumpur, Malaysia, 30-31 October 1998.

14. **A. Rachedi**, C.E. Sansom, C.R. Groom, J. Thillet, R. Griffin & A.J. Geddes.
The Structure of Mouse Dihydrofolate Reductase in Ternary Complex with NADPH and the Lipophilic Antifolate, Methylbenzoprim. In Proceedings of the 9th National Biotechnology Seminar: Positioning National R & D in Biotechnology for Global Competitiveness, pages 96-102. Penang, Malaysia, 23-26 November 1997.

Patents

**Patent for “SYSTEM FOR USE IN MOLECULAR DRUG DESIGN”,
registration No. 2011/0168**

Software development

Databases:

NALD A database for Nucleic Acids and Ligands Database, (see Research output **01**).

URL: <http://embooss.bioinf.wits.ac.za/nald>

STAD A database for Structural Targets Annotation Database, (see Research output **02**).

URL: <http://embooss.bioinf.wits.ac.za/stad>

SPINE@EBI A database and package of software tools for searching and tracking structural targets in Europe. Project moved to stage two dealing with complex targets, (see Research output **05**).

GABAagent (search engine and e-mail alert database system for GABA receptors;

URL: <http://www.ust.hk/gaba> (see Research output **09**)

See also: http://www.ust.hk/~webopa/news/1999_News/news0527.pdf: HKUST Univ.'s press release about the GABAagent system.

Standalone applications:

RBPNM Rapid building of Protein/DNA Motifs in Standard 3D-Conformations.

URL: <http://www.bioinformers.co.uk/bscmpd/html/bsps>

VB Visual Biochemistry. Educational software for biochemistry. VB exists both as a windows application and as online e-book. The online version is a java applet with animated features that can be accessed from the URL: http://www.bioinformers.co.uk/bscmpd/html/VB_html

MtS Molecules to Study. Educational software for structural biochemistry.

URL: <http://www.bioinformers.co.uk/bscmpd/html/MtS/>

Web services (additional personal activity):

Bioinformers The BioInformers is a non-profit bioinformatics based server created on Feb.2006 The server is dedicated for Structural Genomics Informatics, GABA receptors & related drugs, Protein & DNAmotifs, Software tools including web based tools and educational bioinformatics.

URL: <http://www.bioinformers.co.uk/>

AlgeriansGate The Algerians Gate is a non-profit Server. The server is dedicated for Algeria's intellectual, scientific and cultural achievements. The AlgeriansGate provides Databases & Search utilities.

URL: <http://www.algeriansgate.co.uk/>

The AlgeriansGate hosts also **ASD** and **AWD** databases which are online search engines and databases dedicated for servicing the Algeria scientists and writers.

see <http://www.algeriansgate.co.uk/asd.html> and <http://www.algeriansgate.co.uk/awd.html>