

Table 1: Tools for Structural Bioinformatics developed by the partners of WP3.

PIG	3D protein structural web service. It includes Geno3D, Modeome3D, MAGOS and SuMo.		PRABI-Gerland	http://pig-pbil.ibcp.fr		200 runs per month
Geno3D	automatic web server for protein molecular modelling		PRABI-Gerland	http://geno3d-pbil.ibcp.fr	Combet et al. (2002) <i>Bioinformatics</i> , 2002, 18, 213-214	1000 runs per month.
MAGOS	automated protein modelling coupled to the creation of a hierarchical and annotated Multiple Alignment of Complete Sequences		PRABI-Gerland	http://pig-pbil.ibcp.fr/magos/	Garnier et al. (2006) <i>Bioinformatics</i> , 2006, 22, 2164-2165	200 runs per months
MODEOME/MS 2PH	an interactive system for the integrated analysis of phenotypic consequences of missense mutations in proteins involved in human genetic diseases		PRABI-Gerland	http://modeome3d-pbil.ibcp.fr http://ms2phdb-pbil.ibcp.fr/Coordinator: David? Raphael ?	Friedrich et al. (2010) <i>Hum. Mutat.</i> , 2010, 31, 127-135	120 runs per months for MODEOME N.A. for MS2PH
Curves+	conformational analysis for nucleic acids		PRABI-Gerland	http://gbio-pbil.ibcp.fr/Curves_plus	Lavery et al., <i>Nucleic Acids Res.</i> 37 (2009) 5917-5929	236 runs per month.
ABC	database of DNA dynamics as a function of base sequence		PRABI-Gerland	http://gbio-pbil.ibcp.fr/ABC	Lavery R. et al., <i>Nucleic Acids Res.</i> 38 (2010) 299-313.	
Esript Endscript	generation of article-quality figures containing a large amount of information.		PRABI-Gerland	http://endscript.ibcp.fr	Gouet et al., (2003) <i>Nucleic Acids Res</i> 31 : 3320-3	9000 runs per months
SuMo	Similarities in arbitrary 3D structures or substructures of proteins		PRABI-Gerland	http://sumo-pbil.ibcp.fr	Jambon et al., <i>Bioinformatics</i> , 2005, 21:3929-3930	700 runs per month.
T-REKS	<i>ab initio</i> identification of the tandem repeats in proteins		ReNaBi-GS - CRBM	http://bioinfo.montp.cnrs.fr/?r=t-reks http://bioinfo.montp.cnrs.fr/?r=repeatDB ; http://bioinfo.montp.cnrs.fr/?p=profiles&r=profile	Jorda et al., 2009, <i>Bioinformatics</i> . 25(20):2632	
PRDB	Protein DataBase	Repeat	ReNaBi-GS - CRBM	http://bioinfo.montp.cnrs.fr/?p=profiles&r=profile	Jorda et al. 2010, <i>FEBS J</i> 277:2673	
e-LEA3D	Structure based screening		ReNaBi-GS - IPMC	http://bioinfo.ReNaBi-GS-IPMC.cnrs.fr/lea.html	Douguet, <i>Nucleic Acids Research</i> , 2010, 38, Suppl:W615-21	10 runs per month
HeliQuest	α -helix physicochemical properties and bank screening for similar segments		ReNaBi-GS - IPMC	http://heliquest.ReNaBi-GS-IPMC.cnrs.fr/	Drin et al., <i>Nature Structural & molecular biology</i> , 2007, 14(2), 138-46. Gautier et al., <i>Bioinformatics</i> . 2008 Sep 15;24(18):2101-2.	900 runs per month (analysis and screening)
Docking@grid	Flexible docking of small compounds		ReNaBi-NE - INRIA LILLE	http://dockinggrid.gforge.inria.fr/		
STRIP	Strategy for Interacting Sites Prediction		Aplibio - RPBS	http://biodev.cea.fr/strip/	Aucher et al. <i>Mol Cell Proteomics</i> (2010). In press	100 runs per month
VIRFAM	Remote Homology Detection of Viral Protein Families		Aplibio - RPBS	http://biodev.cea.fr/virfam/	Lopes et al. <i>Nucleic Acids Res.</i> (2010) 38(12):3952-62.	100 runs per month
SCOTCH	Scoring models of complexes using evolutionary data.		Aplibio - RPBS	http://biodev.cea.fr/scotch/	Madaoui et al. <i>PNAS</i> (2008) 105(22):7708-13.	
HMM-Kalign	Generating sub-optimal HMM alignments		Aplibio - RPBS	http://www-spider.cea.fr/Groups/hk3039/view.html	Becker et al., <i>Bioinformatics</i> . (2007) 23(22):3095-7.	
KAKSI	Assignment of protein secondary structures		Aplibio - MIGALE	http://genome.jouy.inra.fr/outils/mig/kaksi	Martin et al. <i>BMC Struct. Biol.</i> 2005	
GORV	prediction of protein secondary structures		Aplibio - MIGALE	http://gor.bb.iastate.edu	Sen et al. <i>Bioinformatics</i> 2005	

OSS-HMM	prediction of protein secondary structures	Aplibio - MIGALE	http://genome.jouy.inra.fr/outils/mig/oss-hmm	Martin et al. BMC Struct. Biol. 2006	
VAST	3D structure comparisons	Aplibio - MIGALE	http://genome.jouy.inra.fr/outils/mig/vast	Gibrat et al. Curr. Opin. Struct. Biol. 1996	
FROST	Fold recognition	Aplibio - MIGALE	http://genome.jouy.inra.fr/frost	Marin et al. Proteins 2002	
ESAP	Loop Modeling	Aplibio - MIGALE	http://genome.jouy.inra.fr/logiciels/esap	Gibrat et al. Immunomethods 1992	
Hex, HexServer	rigid body protein docking using spherical polar FFTs	ReNaBi-NE - INRIA Nancy	http://hexserver.loria.fr	Ritchie, V. Venkatraman (2010), <i>Bioinformatics, In press</i> ; G. Macindoe et al., 2010, <i>Nucl. Acids Res.</i> , 38, W445-W449. Bresso et al., <i>In preparation</i> . Beaufrait et al., (2008), <i>J. Mol. Modeling</i> , 14, 135-48.; Ghemti et al., (2010), <i>J. Chem. Inf. Model.</i> , 50, 701-15.	1000 runs per month
PredIS3D	data mining prediction of protein interaction sites	ReNaBi-NE - INRIA Nancy	http://predis3d.loria.fr/	Mavridis et al., 2007, <i>J. Chem. Inf. Model.</i> , 47, 1787-1796.	
VSM-G	virtual screening manager for grids	ReNaBi-NE - INRIA Nancy	http://bioinfo.loria.fr/projects/vsm-g	Cantarel et al. (2009) <i>Nucleic Acids Res.</i> 37:D233-D238	150,000 pages per month
3D-Blast	sequence-independent protein shape comparison and classification	ReNaBi-NE - INRIA Nancy	http://3dblast.loria.fr	Miteva et al., <i>Nucleic Acids Res.</i> , (2005) 33:W372-5.	500 runs per month
CAZy	Carbohydrate-active enzymes database	ReNaBi-GS - Marseille	http://www.cazy.org	Papandreou et al., <i>Eur J Biochem.</i> 2004 ; 271(23-24):4762-8.	270 runs per month
PCE	Protein electrostatics	Aplibio - RPBS	http://bioserv.rpbs.univ-paris-diderot.fr/cgi-bin/portal.py?form=PCE-pot	Maupetit J et al., <i>Nucleic Acids Res.</i> 2006 34:W147-51.	500 runs per month
PFF	Protein Folding Fragments	Aplibio - RPBS	http://bioserv.rpbs.univ-paris-diderot.fr/PFF/	Saladin et al., <i>BMC Struct. Biol.</i> , 2009 9:27.	
SABBAC	Full structure from alpha carbon trace	Aplibio - RPBS	http://bioserv.rpbs.univ-paris-diderot.fr/SABBAC	Abraham et al., <i>Bioinformatics</i> 2008	260 runs per month
PTools	Protein docking	Aplibio - RPBS	In situ	Miteva et al., <i>Nucleic Acids Res.</i> 2006 ; 34:W738-44; Lagorce et al. <i>BMC Bioinformatics.</i> 2008	920 runs per month
swelfe	repeats in DNA sequences, amino-acid sequences or 3D structures.	Aplibio - RPBS	http://bioserv.Aplibio-RPBS.univ-paris-diderot.fr/cgi-bin/swelfe	Binisti et al., <i>Nucleic Acids Res.</i> 2005 ; 33:W320-3.; Autin et al., <i>Nucleic Acids Res.</i> 2007;35:W483-8	1700 runs per month
FAF-Drugs	ADME/tox	Aplibio - RPBS	http://mobyle.rpbs.univ-paris-diderot.fr/cgi-bin/portal.py?form=FAF-Drugs	Maupetit et al., <i>Nucleic Acids Res.</i> 2009 ; 37:W498-503.	300 runs per month
PPG/PMG	Online image/movie generation	Aplibio - RPBS	http://bioserv.rpbs.jussieu.fr/cgi-bin/PPG ; http://bioserv.rpbs.jussieu.fr/PMG.html	LeGuilloux et al., <i>BMC Bioinformatics.</i> 2009 Jun 2;10:168.; Schmidtke et al. <i>Nucleic Acids Res.</i> 2010;38:W582-9	Download / online
PEP-FOLD	Peptide de novo folding	Aplibio - RPBS	http://bioserv.rpbs.univ-paris-diderot.fr/PEP-FOLD	Leite Bohme et al., <i>Nucleic Acids Res.</i> 2007 ; 35:W568-72. Miteva et al., <i>Nucleic Acids Res.</i> 2010 ;38 :W622-7	10500 runs per month
fpocket/hpocket/mdpocket	Pocket identification in proteins	Aplibio - RPBS	http://bioserv.rpbs.univ-paris-diderot.fr/fpocket	Sperandio et al., <i>Nucleic Acids Res.</i> 2009 ;	50 runs per month
Frog/Frog2	Compound 3D generation	Aplibio - RPBS	http://bioserv.rpbs.univ-paris-diderot.fr		
wwLig-CSRre	Search for similar compounds	Aplibio - RPBS	http://bioserv.rpbs.univ-paris-		

diderot.fr/wwLigCSRre.html

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ExDynPept

molecular modeling
using experimental
data as constraints for
peptides

ReNaBi-NE-
Reims

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