Name	Keywords	Description	Language	Access mode : •Online (web server) •Link to download •Request to author	Reference	Contact
MolDesc	*Molecular descriptors*	SB&C Platform providing: Tool to compute molecular properties or ADMETox properties	Django, Docker, Python	Serveur web : https://sbc.icoa.fr http://moldesc.icoa.fr		**Institut de Chimie Organique et Analytique (ICOA)** pascal.bonnet@univ-orleans.fr
F2D	*Fragments* *Kinase inhibitors*	SB&C Platform providing: *in silico* fragment based drug design protocol to find new kinase inhibitors	Django, Docker, Python	Serveur web : https://sbc.icoa.fr http://frags2drugs.icoa.fr	To be published	**Institut de Chimie Organique et Analytique (ICOA)** pascal.bonnet@univ-orleans.fr
METAPREDICT	*ADMETox*	SB&C Platform providing: Tool to compute ADMETox properties based on QSAR models	Django, Docker, Python	Serveur web : https://sbc.icoa.fr http://metapredict.icoa.fr	To be published	**Institut de Chimie Organique et Analytique (ICOA)** pascal.bonnet@univ-orleans.fr
VSprep	*Database preparation*	A KNIME Workflow for the Preparation of Molecules for Virtual Screening	Knime and third party applications	On request	Gally, J.-M. ; Bourg, S. ; Fogha, J. ; Do Q.T. ; Aci-Sèche, S. ; Bonnet, P. VSPrep: A KNIME workflow for the preparation of molecular databases for virtual screening *Current Medicinal Chemistry* **2019**, 26, 1. Gally, J.-M. ; Bourg, S. ; Do Q.T. ; Aci-Sèche, S. ; Bonnet, P. VSPrep: A general KNIME workflow for the preparation of molecules for virtual screening *Molecular Informatics* **2017**, 36, 1700023.	**Institut de Chimie Organique et Analytique (ICOA)** pascal.bonnet@univ-orleans.fr
Kinomine	*Kinases* *Crystal structures* *Activity* *Selectivity*	SB&C Platform providing: A tool to search and extract chemical and biological kinase knowledge	Django, Docker, Python	Serveur web : https://sbc.icoa.fr http://kinomine.icoa.fr	To be published	**Institut de Chimie Organique et Analytique (ICOA)** pascal.bonnet@univ-orleans.fr
LEA3D	*de novo drug design* *virtual screening using functions such as: docking (PLANTS program), shape similarity (SENSAAS program) and/or molecular properties*	Outil de criblage virtuel et de design de petites molécules		Serveur web : https://chemoinfo.ipmc.cnrs.fr/LEA3D	Douguet D., e-LEA3D: a computational-aided drug design web server, *Nucleic Acids Res*., **2010**, 38, Suppl:W615-21. doi:10.1093/nar/gkq322	**Institut de Pharmacologie Moléculaire et Cellulaire (IPMC)** douguet@ipmc.cnrs.fr
SENSAAS	*Molecular alignment* *Molecular similarity* *Shape similarity*	Alignment moléculaire basé sur la forme 3D	Python3.7	Serveur web : https://chemoinfo.ipmc.cnrs.fr/SENSAAS Demande des codes sources aux auteurs	Douguet D. and Payan F., SENSAAS: Shape-based Alignment by Registration of Colored Point-based Surfaces, *Molecular Informatics*, **2020**, 8, 2000081. doi:10.1002/minf.202000081	**Institut de Pharmacologie Moléculaire et Cellulaire (IPMC)** douguet@ipmc.cnrs.fr

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@TOME V3	*Comparative modeling* *Ligand interactions*	A pipeline for comparative modeling of protein-ligand complexes		Serveur web : http://atome.cbs.cnrs.fr/ATOME_V3	Pons JL and Labesse G, *Nucleic Acids Research*, **2009**. doi:10.1093/nar/gkp368	**Centre de Biochimie Structurale (CBS)** labesse@cbs.cnrs.fr
EDMON V3	*Nuclear hormone receptors endocrine-disrupting chemicals interactions*	Tool to estimate binding affinities		Serveur web : http://atome.cbs.cnrs.fr/ATOME_V3/SERVER/EDMon_v3.html	Delfosse et al., *PNAS*, **2012.** doi:10.1073/pnas.1203574109	**Centre de Biochimie Structurale (CBS)** labesse@cbs.cnrs.fr
CoSiAn	*2D and 3D molecular similarity*	Combinatorial similarity analysis		Serveur web : http://cosian.cbs.cnrs.fr		**Centre de Biochimie Structurale (CBS)** labesse@cbs.cnrs.fr
IChem **Shaper / Shaper2** **SiteAlign** **FuzCav** **FingerPrintLib** **pymolFP** **Fresno**	*Protein-ligand interactions* *Shape-based alignment of pharmacophore-annotated VolSite cavities* *Interaction fingerprints* *Scoring function*			Lien pour télécharger : http://bioinfo-pharma.u-strasbg.fr/labwebsite/download.html		**Laboratoire d'Innovation Thérapeutique (LIT)** rognan@unistra.fr
Chem-REST	*Chemical databases, REST protocole, Datasets for machine learning models*	Chemical Repository of Existing Structures and their computed properTies		Serveur web : https://chem-rest.pasteur.fr/		**Institut Pasteur - Structural Bioinformatics - Chemoinformatics and proteochemometric** olivier.sperandio@pasteur.fr
Frog **AMMOS** **MTiOpenScreen**	*Conformer generation* *Energy minimization of protein-ligands complexes* *Docking* *Virtual screening*	Services at RPBS Web Portal		Serveur web : https://bioserv.rpbs.univ-paris-diderot.fr/services.html#drugs-protein_inter	Labbé CM et al., MTiOpenScreen: a web server for structure-based virtual screening. *Nucleic Acids Res*. **2015,** 43(W1):W448-54. doi: 10.1093/nar/gkv306 Lagarde N et al., Online structure-based screening of purchasable approved drugs and natural compounds: retrospective examples of drug repositioning on cancer targets. *Oncotarget*. **2018** 17;9(64):32346-32361. doi: 10.18632/oncotarget.25966 Labbé CM et al., AMMOS2: a web server for protein-ligand-water complexes refinement via molecular mechanics. *Nucleic Acids Res.* **2017,** 45(W1):W350-W355. doi:10.1093/nar/gkx397	**Unité de Biologie Fonctionnelle et Adaptative (BFA)** pierre.tuffery@univ-paris-diderot.fr **Chimie médicinale et recherche translationnelle** maria.miteva@inserm.fr

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ISIDA **S4MPLE**	*Molecular descriptors* *QSPR model builder* *Generative Topographics Map (GTM)* *Flexible docking and peptide folding* *Reactivity analysis* *Prediction tools (physico-chemical properties, REACH endpoints)*	ISIDA Package is a suite of cheminformatics tools		Lien pour télécharger : https://complex-matter.unistra.fr/equipes-de-recherche/laboratoire-de-chemoinformatique/software-development/ Serveur web : https://complex-matter.unistra.fr/equipes-de-recherche/laboratoire-de-chemoinformatique/web-services/		**Laboratoire de Chémoinformatique** varnek@unistra.fr
FAF-Drugs4	*Drug design* *Free ADME-Tox Filtering Tool*	Préparation de chimiothèques	Python, C	Serveur web : http://fafdrugs4.mti.univ-paris-diderot.fr/	Lagorce D, Bouslama L, Becot J, Miteva MA, Villoutreix BO. *Bioinformatics*. **2017** Nov 15;33(22):3658-3660. doi:10.1093/bioinformatics/btx491	**NeuroDiderot** Bruno.villoutreix@inserm.fr