

Bioconda packaging of the Regulatory Sequence Analysis Tools (RSAT)



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Project links

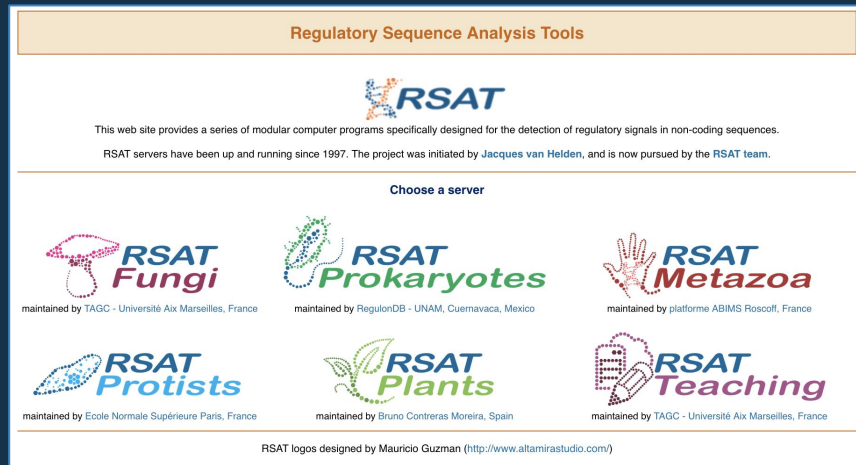
- RSAT: <http://rsat.eu/>
- Biohackathon project: <https://goo.gl/5VhtEK>



Background information

Regulatory Sequence Analysis Tools (RSAT)

- A software suite for the analysis of regulatory motifs in nucleic sequences.
- A 20-year project, supported by an international team
- Access: <http://rsat.eu/>
- Access and usage
 - **6 Web servers**: Metazoa, Plants, Fungi, Prokaryotes, Protists + Teaching (all taxa)
 - 51 Web-interfaced tools
 - ~10,000 queries / month (2017)
 - **Web services** (SOAP/WSDL)
 - ~8,000 queries / month (2017)
 - Downloadable **stand-alone** version
 - 234 downloads in 2017
 - **Virtual machine** on the cloud of the Institut Français de Bioinformatique (IFB)
- Downloadable from <http://teaching.rsat.eu/>
 - Tar archive with the tools
 - Virtual machine (ova, 10Gb)



Nguyen NTT, Contreras-Moreira B, Castro-Mondragon JA, Santana-Garcia W, Ossio R, Robles-Espinoza CD, Bahin M, Collombet S, Vincens P, Thieffry D, van Helden J, Medina-Rivera A, Thomas-Chollier M. **RSAT 2018: regulatory sequence analysis tools 20th anniversary**. Nucleic Acids Res. 2018 Jul 2;46(W1):W209-W214. [doi:10.1093/nar/gky317](https://doi.org/10.1093/nar/gky317). PMID: [29722874](https://pubmed.ncbi.nlm.nih.gov/29722874/)

Difficulties for RSAT installation

- Multiple languages
 - ~250 `perl` scripts + ~40 `python` scripts + 7 C/C++ compile tools
- Multiple library dependencies
 - `Perl`, `python`, `R` libraries
 - Installing these libraries requires some admin intervention (must be available to Apache user)
- Package segmentation
 - The current `tarball` includes tools + data (motif databases + demo datasets) -> a bit heavy
- Automatisations of the installation
 - Installation is managed via `bash`, `make` and some manual steps
- Portability
 - Some dependencies are hard to install on some platforms (e.g. Mac OS X)
 - The names of the packages required for dependencies vary between package managers (`apt-get`, `yum`, `brew`, ...).
 - Install scripts are based on `apt-get`, and package names are different in other package managers

Goals of the hacking project

<https://goo.gl/gkYYNc>

Goal and expected outcome

- **General goal of the hacking project**
 - Facilitate RSAT diffusion by enabling its installation via conda
- **Expected results** at the end of the hackathon
 - A git repository with the conda packaging scripts and metadata.
 - Be able to install the components of RSAT with simple conda commands, in a first time in a custom channel
 - `conda install -c rsat rsat-core` ## Install the core tools for command-line use
 - `conda install -c rsat rsat-data` ## Install RSAT data (motif databases)
 - `conda install -c rsat rsat-web` ## Install a local instance of the RSAT Web server
 - After testing, the packages will be submitted to bioconda (during or after biohackathon).

Post-biohackathon perspectives

- **RSAT deployment** on IFB *National Network of Computing Resources* (NNCR)
 - New appliance on the federation of clouds, via Biosphere (<https://biosphere.france-bioinformatique.fr/>)
 - Federation of clusters, for command-line access
 - Transfer some persistent Web servers (RSAT Fungi, Teaching) on IFB-core-cluster
- **Create Docker/singularity containers**
 - Will be greatly facilitated by conda packaging

Hack organisation

Organisation of the hacking project

- Duration: 2 hacking days (Tue 13 + Wed 14 Nov)
- Project representation at the biohackathon
 - [Jacques van Helden](#) head and main developer of the RSAT project
- Invited resource people and associated expertise
 - [Loic Gouarin](#) conda packaging
 - [Aurélien Naldi](#) conda packaging + bioinformatics analysis of genetic regulation
- **Any additional expertise and contribution from biohackers is welcome !**
 - Don't hesitate to propose your help via the biohackathon gitter
 - <https://gitter.im/bh2018paris/06-Bioconda-RSAT>

Steps and tasks

- Presentation of RSAT structure to conda expert.
- Identification of existing conda resources for the dependencies (Perl, python, R libraries).
 - Packaging of the other dependencies
- Evaluating if some reorganisation of the code is required for conda porting.
- Conda packaging in custom channel (conda -c rsat)
 - the core tools (stand-alone Unix commands).
 - RSAT data (motif databases, demo datasets, ...).
 - Installation of RSAT Web server and Web services (requires prior installation of an Apache server).
- Testing of the conda packages on different OS
 - Linux distributions via VMs on the IFB cloud
 - Mac OS X
- Submission of the conda packages to bioconda

Contact and links

- Contact
 - Jacques.van-Helden@univ-amu.fr
- Links related to the project
 - RSAT Portal: <http://rsat.eu/>
 - Biohackathon project: <https://goo.gl/5VhtEK>