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# **farseernmr**

***Release 2.0.0-dev***

**FarSeer-NMR**

**Jan 31, 2020**



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## FARSEER-NMR



### Attention Attention Attention

We are currently rewriting Farseer-NMR towards **version 2**.

**Version 1** is still functional and working, though not much supported apart from minor bugs. You can download the latest stable version, v1.3.5, on the [releases tab](#), or visit the complete version 1 code and its documentation in [version 1 branch](#)) on GitHub.

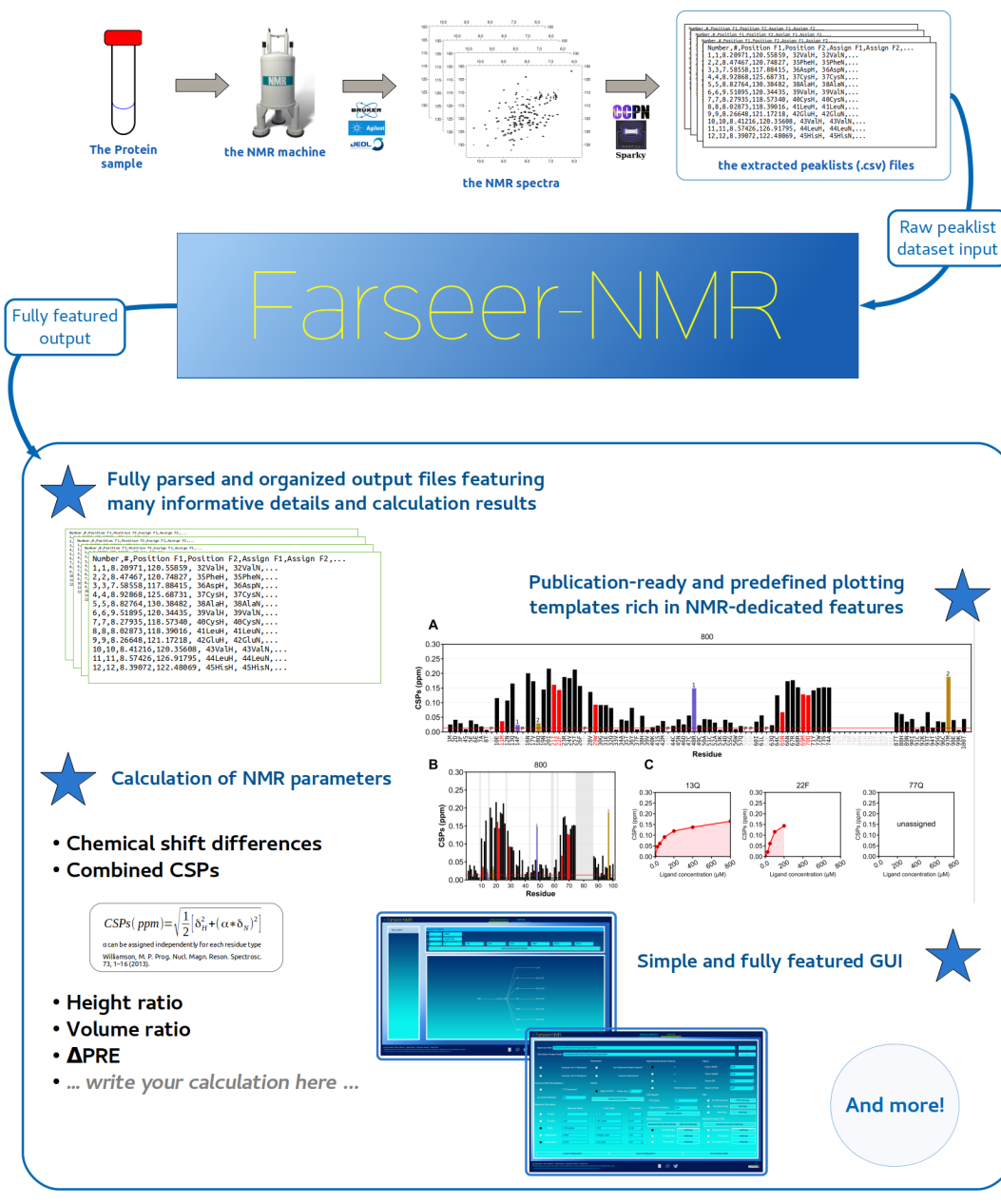
Our original publication is available at [JBioMolNMR](#)), cite us if you use Farseer-NMR for your research, regardless of which version you use.

Please note that the [master branch](#)) currently hosts the development of version 2, which is UNFINISHED software; again, please, refer to *version 1* for a stable and functional release.

Farseer-NMR runs purely on volunteer work without any official assigned funds. All help is welcomed, [engage with us](#))!

### Attention Attention Attention

## Farseer-NMR: a software suite for automatic treatment, analysis and plotting of large and multivariable datasets of bioNMR peaklists



A Python written, multi-platform and fully community-driven suite to analyse datasets of **peaklist files** extracted from multivariable series of Biomolecular Nuclear Magnetic Resonance (NMR) experiments.

With Farseer-NMR, you have:

- Automatic analysis of large and multivariable NMR **peaklist files** datasets
- Peaklist parsing and treatment

- Identification of `_missing_` and `_unassigned_` residues
- Automatic calculation of NMR parameters
- Comprehensive organization of the output
- Large suite of publication-ready plotting templates
- Full traceability via [Markdown](#)) formatted log file.

You can read now through the **contents** bellow.





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### 2.1 Installation

To install FarSeer-NMR version 2: ...

### 2.2 Usage

To use FarSeer-NMR version 2...

### 2.3 Contributing

Contributions are welcome, and they are greatly appreciated! Every little bit helps, and credit will always be given. You can contribute from the scope of an user or as a core Python developer.

#### 2.3.1 Reporting and Requesting

##### Bug reports

When [reporting a bug](#) please use one of the provided issue templates if applicable, otherwise just start a blank issue and describe your situation.

##### Documentation improvements

FarSeer-NMR could always use more documentation, whether as part of the official FarSeer-NMR docs, in docstrings, or even on the web in blog posts, articles, and such. Write us a [documentation issue](#) describing what you would like to see improved in the documentation, and if you can do it just [Pull Request](#) your proposed updates.

## Feature requests and feedback

The best way to send feedback is to file an issue at <https://github.com/Farseer-NMR/FarSeer-NMR/issues/new/choose> using the *feature* template.

If you are proposing a feature:

- Explain in detail how it would work.
- Keep the scope as narrow as possible, to make it easier to implement.
- Remember that this is a volunteer-driven project, and that code contributions are welcome :)

## 2.3.2 Code Development

To contribute to the development of *FarSeer-NMR*:

1. Fork the FarSeer-NMR repository.
2. Clone your fork to your local machine:

```
git clone https://github.com/YOUR-USER-NAME/FarSeer-NMR.git <destination folder>
```

3. Set up a new Python environment for the development of FarSeer-NMR so that the development version does not conflict with the production installation.

3.1 If you use Anaconda as your Python package manager do:

```
conda env create -f requirements_conda.yml
```

3.2 If you are using PyPI as your package manager follow [this instructions](#).

4. Remember to activate the new environment before proceeding to the installation, with Anaconda: `conda activate farseernmrdev`.
5. Install FarSeer-NMR in the development mode, from within your fork folder:

```
python setup.py develop
```

This ensures that the FarSeer-NMR version running in your development environment is the source in your git folder.

6. *FarSeer-NMR* relies on `tox` to orchestrate testing environments, ensuring correct collaborative development, install `tox`:

```
# with Anaconda
conda install -c conda-forge tox

# with PyPI
pip install tox
```

5. Create a branch for local development:

```
git checkout -b name-of-your-bugfix-or-feature
```

5.1 Now you can make your changes locally.

6. When you're done making changes run all the checks and docs builder with `tox` one command:

```
tox
```

6.1. If all tests pass you are set to go :-))

7. Commit your changes and push your branch to your *FarSeer-NMR* fork on GitHub:

```
git add .
git commit -m "Your detailed description of your changes."
git push origin name-of-your-bugfix-or-feature
```

8. Submit a pull request through the [GitHub website](#).

9. To keep you fork repository updated with the main repository latest changes:

```
# move to the master branch
git checkout master

# add a reference to the upstream repository
# this is the main FarSeer-NMR repository
# you only have to do this once
git remote add upstream https://github.com/Farseer-NMR/Farseer-NMR

# fetch the latest code from the main repository
git fetch upstream

# merge those changes to your master branch
git pull upstream master

# push to you online repository the new changes
# so that your fork synchronizes with the main
git push origin master
```

10. To continue developing a new feature just repeat from steps 5.

## Pull Request Guidelines

If you need some code review or feedback while you're developing the code just make a pull request.

For merging, you should:

1. Include passing tests (run `tox`)<sup>1</sup>.
2. Update documentation when there's new API, functionality etc.
3. Add a note to `CHANGELOG.rst` about the changes.
4. Add yourself to `AUTHORS.rst`.

## Tips

You can run individual test environment with `tox`, for example, to test lint:

```
tox -e check
```

to test documentation:

```
tox -e docs
```

to perform coverage-reported tests:

<sup>1</sup> If you don't have all the necessary python versions available locally you can rely on Travis - it will [run the tests](#) for each change you add in the pull request.

It will be slower though ...

```
tox -e py38
```

### 2.3.3 Continuous Integration

This project follows Continuous Integration (CI) good practices (let us know if something can be improved). As referred in the previous section, testing environment is provided by `tox`. All `tox` testing environments run on `Travis-CI`; there, we check for code style, code quality, documentation, tests and test coverage. If you want to know more, `tox` testing configuration is defined in the `tox.ini` file.

## 2.4 Citing

Thanks for using Farseer-NMR!

If you are using Farseer-NMR, or any of its components, to analyze your NMR peaklist data, **please cite our original article**:

Teixeira, J.M.C., Skinner, S.P., Arbesú, M., Breeze, A.L., Pons, M. **J Biomol NMR** (2018) 71:1, 1-9. DOI [10.1007/s10858-018-0182-5](https://doi.org/10.1007/s10858-018-0182-5)

### 2.4.1 Publications citing Farseer-NMR

- Miguel Arbesú, Miquel Pons. Integrating disorder in globular multidomain proteins: Fuzzy sensors and the role of SH3 domains. Archives of Biochemistry and Biophysics 2019, 677, 108161 <https://doi.org/10.1016/j.abb.2019.108161>.
- Luca Mureddu, Geerten W. Vuister. Simple high-resolution NMR spectroscopy as a tool in molecular biology. The FEBS Journal 2019, 286, issue 11, p2035 <https://doi.org/10.1111/febs.14771>.
- Teixeira, J.M.C.; Fuentes, H.; Bielskutė, S.; Gairi, M.; Žerko, S.; Koźmiński, W.; Pons, M. The Two Isoforms of Lyn Display Different Intramolecular Fuzzy Complexes with the SH3 Domain. Molecules 2018, 23, 2731. <https://doi.org/10.3390/molecules23112731>
- Arbesú, M.; Iruela, G.; Fuentes, H.; Teixeira, J.M.C.; Pons, M. Intramolecular fuzzy interactions involving intrinsically disordered domains. Front. Mol. Biosci. 2018, 5, 39. DOI [10.3389/fmolb.2018.00039](https://doi.org/10.3389/fmolb.2018.00039)
- Arbesú, M. et al. (2017) The Unique Domain Forms a Fuzzy Intramolecular Complex in Src Family Kinases. Structure 25, 630–640.e4. [10.1016/j.str.2017.02.011](https://doi.org/10.1016/j.str.2017.02.011)
- Marimon, O. et. al. (2016). An oxygen-sensitive toxin–antitoxin system. Nature Communications, 7, 13634. <https://doi.org/10.1038/ncomms13634>
- Bijlmakers, M.-J., et.al. (2015) A C2HC zinc finger is essential for the RING-E2 interaction of the ubiquitin ligase RNF125. Scientific Reports, 6, 29232. <https://doi.org/10.1038/srep29232>

Farseer-NMR on Google Citations)

## 2.5 Authors

All time complete authors contribution list..

### 2.5.1 Version 2 (under development)

### 2.5.2 Version 1

Version 1 development cycle spans from initial implementations to JBioNMR publication.

- Joao MC Teixeira
- Simon P Skinner
- Miguel Arbesu
- Miquel Pons
- Alexander L. Breeze

## 2.6 Acknowledgments

The Farseer-NMR Project wants to acknowledge to following people for their contributions to the project:

- Susana Barrera-Vilarmau ([ORCID 0000-0003-4868-6593](https://orcid.org/0000-0003-4868-6593)): beta-tester, data provider, plot suggestions.
- Jamie Ferrar, [Artistic Systems](https://twitter.com/artisticsystems): for providing the UI branding.
- [João P.G.L.M. Rodrigues](https://github.com/JoaoRodrigues): for all the years of coding discussions and mentorship, and in particular for the help in setting the Farseer-NMR organization profile on GitHub.
- Héctor Fuentes: intensive beta-tester, specially for the Windows version.
- **To all the users and participants of the Farseer-NMR workshops, thanks for your feedback, opinions, testing, interest and**
  - [Micael Silva (Nova University of Lisbon)](https://www.researchgate.net/profile/Micael\_Silva)
  - [Wouter Elings (Leiden University)](https://www.universiteitleiden.nl/en/staffmembers/wouter-elings#tab-1)

## 2.7 License

The entire Farseer-NMR project is distributed with no liability and is licensed under the [GPL-3.0](https://www.gnu.org/licenses/gpl-3.0.en.html).

<a href="https://www.gnu.org/licenses/gpl-3.0.en.html"></a>

## 2.8 Versioning

This project follows strictly [Semantic Versioning 2.0](#) for version control.

## 2.9 Changelog

### 2.9.1 v2

- *under development*
- added configuration files for CI and deployment
- configured tox.ini
- configured Travis-CI multiplatform, multi Python CI #316

### 2.9.2 v1

- For list of v1 releases visit [project releases](#).
- Latest v1 release hosted in [version1](#) branch.

### 2.9.3 v0

- pre-publication no JBioNMR, changes not tracked in detail.

## 2.10 FarSeer-NMR Library Documentation

## INDICES AND TABLES

- `genindex`
- `modindex`
- `search`