

spant

Wilson, Martin

DOI:
[10.21105/joss.03646](https://doi.org/10.21105/joss.03646)

License:
Creative Commons: Attribution (CC BY)

Document Version
Publisher's PDF, also known as Version of record

Citation for published version (Harvard):
Wilson, M 2021, 'spant: an R package for magnetic resonance spectroscopy analysis', *Journal of Open Source Software*, vol. 6, no. 67, 3646. <https://doi.org/10.21105/joss.03646>

[Link to publication on Research at Birmingham portal](#)

General rights

Unless a licence is specified above, all rights (including copyright and moral rights) in this document are retained by the authors and/or the copyright holders. The express permission of the copyright holder must be obtained for any use of this material other than for purposes permitted by law.

- Users may freely distribute the URL that is used to identify this publication.
- Users may download and/or print one copy of the publication from the University of Birmingham research portal for the purpose of private study or non-commercial research.
- User may use extracts from the document in line with the concept of 'fair dealing' under the Copyright, Designs and Patents Act 1988 (?)
- Users may not further distribute the material nor use it for the purposes of commercial gain.

Where a licence is displayed above, please note the terms and conditions of the licence govern your use of this document.

When citing, please reference the published version.

Take down policy

While the University of Birmingham exercises care and attention in making items available there are rare occasions when an item has been uploaded in error or has been deemed to be commercially or otherwise sensitive.

If you believe that this is the case for this document, please contact UBIRA@lists.bham.ac.uk providing details and we will remove access to the work immediately and investigate.

spant: An R package for magnetic resonance spectroscopy analysis

Martin Wilson¹

¹ Centre for Human Brain Health and School of Psychology, University of Birmingham, Birmingham, UK

DOI: [10.21105/joss.03646](https://doi.org/10.21105/joss.03646)

Software

- [Review](#) ↗
- [Repository](#) ↗
- [Archive](#) ↗

Editor: [Chris Hartgerink](#) ↗

Reviewers:

- [@joaomcteixeira](#)
- [@chartgerink](#)

Submitted: 09 August 2021

Published: 02 November 2021

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](https://creativecommons.org/licenses/by/4.0/)).

Summary

Magnetic Resonance Spectroscopy (MRS) allows the measurement of small molecules (metabolites) in the body without the use of harmful radiation. Based on the same basic principles and technology behind Magnetic Resonance Imaging (MRI), most modern MRI scanners are also capable of acquiring MRS — making the technique highly suited to a number of clinical applications ([Oz et al. \(2014\)](#)). Despite the success of MRS in the research environment, clinical translation has proven slow due to a number of technical and practical reasons, with challenges associated with reliable data processing and analysis having particular importance ([Wilson et al. \(2019\)](#)). The `spant` (SPectroscopy ANalysis Tools) package has been developed to: (1) provide open-source implementations of traditional and modern MRS processing and analysis techniques for routine analysis ([Near et al. \(2021\)](#)) and (2) aid the development, validation and comparison of new algorithms and analysis pipelines.

Statement of need

Traditional MRS analysis was dominated by the use of proprietary software, either supplied by scanner manufactures or offline tools such as LCMoDel ([Provencher \(1993\)](#)) and jMRUI ([Naressi et al. \(2001\)](#)). In more recent years there has been a steadily increasing trend toward the use of open-source methods — with some early examples including TARQUIN ([Reynolds et al. \(2006\)](#); [Wilson et al. \(2011\)](#)) and AQSES ([Pouillet et al. \(2007\)](#)). This trend is set to continue with the recent transition of LCMoDel to an open-source license, and an acceleration in the development of new open-source methods and packages such as Vespa ([Soher et al. \(2011\)](#)), Gannet ([Edden et al. \(2014\)](#)), FID-A ([Simpson et al. \(2017\)](#)), Osprey ([Oeltzschner et al. \(2020\)](#)), suspect ([Rowland \(2021\)](#)) and FSL-MRS ([Clarke et al. \(2021\)](#)). The availability of the MRSHub (<https://mrshub.org/>), a new community orientated software sharing and support platform, and the recent development of the NIFTI MRS file format ([Clarke & Wilson \(2021\)](#)), to aid data sharing and interoperability, are set to further enhance the ecosystem of open-source MRS analysis tools.

The vast majority of recently developed open-source MRS analysis tools have been written in either MATLAB or Python. Whilst all languages have strengths and weaknesses, R is particularly suited to the interactive exploration and batch processing of large and complex datasets — typical of MRS and neuroimaging studies. For example, the acquisition and storage of high dimensional datasets, including three spatial axes, chemical shift and coil axes are becoming more common for MRS. For a typical study, these scans may be acquired at multiple time-points for multiple participants split across one or more groups (e.g. control and treatment) - requiring both single subject and group level analyses.

The `spant` package was developed to combine traditional and modern MRS data processing techniques with strengths of R, including: plotting/visualization, statistics, machine learning and data wrangling. Furthermore, `spant` may be used to conveniently combine MRS results with other imaging modalities, due to the availability of a wide range of R packages focused on image processing (Muschelli et al. (2019)) and support for the NIFTI data format (Whitcher et al. (2011); Clayden et al. (2021)). `spant` also supports the majority of common MR vendor data formats allowing complete pipelines to be developed, from raw time-domain samples to metabolite quantities derived from spectral fitting.

`spant` is part of the MRSHub, demonstrating its acceptance and interest from the MRS community. At the time of writing, `spant` has been used to develop and validate two new MRS spectroscopy analysis algorithms: RATS (Wilson (2019)) and ABfit (Wilson (2021)), and has also been used to study cancer (Franco et al. (2021)), Alzheimer's Disease (Montal et al. (2021)) and psychosis (Fisher et al. (2020)) — confirming its suitability for both MRS methods research and clinical studies.

Acknowledgements

Particular thanks go to Dr Jonathan D. Clayden and Dr Robert W. Cox for their work on the `RNifti` package (Clayden et al. (2021)) and NIFTI standard (<https://nifti.nimh.nih.gov/>) which have substantially expanded the capabilities of `spant`.

References

- Clarke, W. T., Stagg, C. J., & Jbabdi, S. (2021). FSL-MRS: An end-to-end spectroscopy analysis package. *Magn Reson Med*, 85(6), 2950–2964. <https://doi.org/10.1002/mrm.28630>
- Clarke, W. T., & Wilson, M. (2021). *NIFTI-MRS format specification*. <https://doi.org/10.5281/zenodo.5168794>
- Clayden, J., Cox, B., & Jenkinson, M. (2021). *RNifti: Fast R and C++ access to NIFTI images*. <https://CRAN.R-project.org/package=RNifti>
- Edden, R. A., Puts, N. A., Harris, A. D., Barker, P. B., & Evans, C. J. (2014). Gannet: A batch-processing tool for the quantitative analysis of gamma-aminobutyric acid-edited MR spectroscopy spectra. *J Magn Reson Imaging*, 40(6), 1445–1452. <https://doi.org/10.1002/jmri.24478>
- Fisher, E., Wood, S. J., Elsworth, R. J., Upthegrove, R., & Aldred, S. (2020). Exercise as a protective mechanism against the negative effects of oxidative stress in first-episode psychosis: a biomarker-led study. *Transl Psychiatry*, 10(1), 254. <https://doi.org/10.1038/s41398-020-00927-x>
- Franco, P., Huebschle, I., Simon-Gabriel, C. P., Dacca, K., Schnell, O., Beck, J., Mast, H., Urbach, H., Wuertemberger, U., Prinz, M., Hosp, J. A., Delev, D., Mader, I., & Heiland, D. H. (2021). Mapping of metabolic heterogeneity of glioma using MR-spectroscopy. *Cancers (Basel)*, 13(10). <https://doi.org/10.3390/cancers13102417>
- Montal, V., Barroeta, I., Bejanin, A., Pegueroles, J., Carmona-Iragui, M., Altuna, M., Benjam, B., Videla, L., Fernández, S., Padilla, C., Aranha, M. R., Iulita, M. F., Vidal-Piñero, D., Alcolea, D., Blesa, R., Lleó, A., & Fortea, J. (2021). Metabolite signature of Alzheimer's disease in adults with Down syndrome. *Ann Neurol*.

- Muschelli, J., Gherman, A., Fortin, J. P., Avants, B., Whitcher, B., Clayden, J. D., Caffo, B. S., & Crainiceanu, C. M. (2019). Neuroconductor: an R platform for medical imaging analysis. *Biostatistics*, 20(2), 218–239.
- Naressi, A., Couturier, C., Castang, I., Beer, R. de, & Graveron-Demilly, D. (2001). Java-based graphical user interface for MRUI, a software package for quantitation of in vivo/medical magnetic resonance spectroscopy signals. *Comput Biol Med*, 31(4), 269–286. [https://doi.org/10.1016/s0010-4825\(01\)00006-3](https://doi.org/10.1016/s0010-4825(01)00006-3)
- Near, J., Harris, A. D., Juchem, C., Kreis, R., Marjańska, M., Öz, G., Slotboom, J., Wilson, M., & Gasparovic, C. (2021). Preprocessing, analysis and quantification in single-voxel magnetic resonance spectroscopy: experts' consensus recommendations. *NMR Biomed*, 34(5), e4257. <https://doi.org/10.1002/nbm.4257>
- Oeltzschner, G., Zöllner, H. J., Hui, S. C. N., Mikkelsen, M., Saleh, M. G., Tapper, S., & Edden, R. A. E. (2020). Osprey: Open-source processing, reconstruction & estimation of magnetic resonance spectroscopy data. *J Neurosci Methods*, 343, 108827. <https://doi.org/10.1016/j.jneumeth.2020.108827>
- Oz, G., Alger, J. R., Barker, P. B., Bartha, R., Bizzi, A., Boesch, C., Bolan, P. J., Brindle, K. M., Cudalbu, C., Dinçer, A., Dydak, U., Emir, U. E., Frahm, J., González, R. G., Gruber, S., Gruetter, R., Gupta, R. K., Heerschap, A., Henning, A., ... Kauppinen, R. A. (2014). Clinical proton MR spectroscopy in central nervous system disorders. *Radiology*, 270(3), 658–679. <https://doi.org/10.1148/radiol.13130531>
- Poulet, J. B., Sima, D. M., Simonetti, A. W., De Neuter, B., Vanhamme, L., Lemmerling, P., & Van Huffel, S. (2007). An automated quantitation of short echo time MRS spectra in an open source software environment: AQSES. *NMR Biomed*, 20(5), 493–504. <https://doi.org/10.1002/nbm.1112>
- Provencher, S. W. (1993). Estimation of metabolite concentrations from localized in vivo proton NMR spectra. *Magn Reson Med*, 30(6), 672–679. <https://doi.org/10.1002/mrm.1910300604>
- Reynolds, G., Wilson, M., Peet, A., & Arvanitis, T. N. (2006). An algorithm for the automated quantitation of metabolites in in-vitro NMR signals. *Magn Reson Med*, 56(6), 1211–1219. <https://doi.org/10.1002/mrm.21081>
- Rowland, B. (2021). Suspect is a python package for processing MR spectroscopy data. In *GitHub repository*. GitHub. <https://github.com/openmrslab/suspect>
- Simpson, R., Devenyi, G. A., Jezard, P., Hennessy, T. J., & Near, J. (2017). Advanced processing and simulation of MRS data using the FID appliance (FID-A)-An open source, MATLAB-based toolkit. *Magn Reson Med*, 77(1), 23–33.
- Soher, B., Semanchuk, P., Todd, D., & Young, K. (2011). VeSPA: Integrated applications for RF pulse design, spectral simulation and MRS data analysis. *Proceedings of the 19th Annual Meeting of ISMRM, Montreal, Canada*, 1410.
- Whitcher, B., Schmid, V. J., & Thornton, A. (2011). Working with the DICOM and NIFTI data standards in R. *Journal of Statistical Software*, 44(6), 1–28. <https://doi.org/10.18637/jss.v044.i06>
- Wilson, M. (2021). Adaptive baseline fitting for ¹H MR spectroscopy analysis. *Magn Reson Med*, 85(1), 13–29. <https://doi.org/10.1002/mrm.28385>
- Wilson, M. (2019). Robust retrospective frequency and phase correction for single-voxel MR spectroscopy. *Magn Reson Med*, 81(5), 2878–2886. <https://doi.org/10.1002/mrm.27605>
- Wilson, M., Andronesi, O., Barker, P. B., Bartha, R., Bizzi, A., Bolan, P. J., Brindle, K. M., Choi, I. Y., Cudalbu, C., Dydak, U., Emir, U. E., Gonzalez, R. G., Gruber, S., Gruetter, R., Gupta, R. K., Heerschap, A., Henning, A., Hetherington, H. P., Huppi, P. S., ... Howe,

F. A. (2019). Methodological consensus on clinical proton MRS of the brain: Review and recommendations. *Magn Reson Med*, 82(2), 527–550. <https://doi.org/10.1002/mrm.27742>

Wilson, M., Reynolds, G., Kauppinen, R. A., Arvanitis, T. N., & Peet, A. C. (2011). A constrained least-squares approach to the automated quantitation of in vivo ^1H magnetic resonance spectroscopy data. *Magn Reson Med*, 65(1), 1–12. <https://doi.org/10.1002/mrm.22579>