

Reproducibility Made Easy: A Tool for Methodological Transparency and Efficient Standardized Reporting based on the proposed MRSinMRS Consensus.

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Abstract

Purpose:

Recent expert consensus publications have highlighted the issue of poor reproducibility in magnetic resonance spectroscopy (MRS) studies, mainly due to the lack of standardized reporting criteria, which affects their clinical applicability. To combat this, guidelines for minimum reporting standards (MRSinMRS) were introduced to aid journal editors and reviewers in ensuring the comprehensive documentation of essential MRS study parameters. Despite these efforts, the implementation of MRSinMRS standards has been slow, attributed to the diverse nomenclature used by different vendors, the variety of raw MRS data formats, and the absence of appropriate software tools for identifying and reporting necessary parameters. To overcome this obstacle, we have developed the REproducibility Made Easy (REMY) standalone toolbox. **Methods:**

REMY software supports a range of MRS data formats from major vendors like GE (p. file), Siemens (.twix, .rda, .dcm), Philips (.spar/.sdat), and Bruker (.method), facilitating easy data import and export through a user-friendly interface. REMY employs external libraries such as spec2nii and pymapVBVD to accurately read and process these diverse data formats, ensuring compatibility and ease of use for researchers in generating reproducible MRS research outputs. Users can select and import datasets, choose the appropriate vendor and data format, and then generate an MRSinMRS table, log file, and methodological documents in both Latex and PDF formats.

Results:

REMY effectively populated key sections of the MRSinMRS table with data from all supported file types. In the hardware section, it successfully read and filled in fields for Field Strength [T], Manufacturer Name, and Software Version, covering three of the five required hardware fields. However, it could not input data for RF coil and additional hardware information due to their absence in the files. For the acquisition section, REMY accurately read and populated fields for the pulse sequence name, nominal voxel size, repetition time, echo time, number of acquisitions/excitations/shots, spectral width [Hz], and number of spectral points, significantly contributing to the completion of the Acquisition fields of the table. Furthermore, REMY generates a boilerplate methods text section for manuscripts.

Conclusion:

This approach reduces effort and obstacles associated with writing and reporting acquisition parameters and should lead to the widespread adoption of MRSinMRS within the MRS community.

Abbreviations: MRS, MRSinMRS, ReproducibilityMadeEasy

1. Introduction

Magnetic resonance spectroscopy (MRS) is a non-invasive magnetic resonance imaging (MRI) method used to evaluate the metabolic profiles of tissues.^{1,2} Over the past four decades, the field of MRS progressed greatly in protocol development for metabolite acquisition, as well as

advancements in pre- and post-processing of data and metabolite quantification.²⁻⁶ These efforts have led to a plethora of MRS consensus papers that provide a platform for education and training, standardization, and addressing conflicting viewpoints (Table 1). The combined progress in technical innovations within the MRS field and the consensus achieved among experts aimed to promote MRS to clinical researchers and psychiatrists and to improve access to non-expert users.^{3,4,7-18} One particularly impactful consensus publication addressed the urgent need for standardized reporting criteria for MRS studies. The authors recognized that the enormous methodological heterogeneity in the field has contributed to a lack of reproducibility across different groups, sites, and techniques. Furthermore, they identified a lack of structured methods reporting, making it difficult to compare and integrate quantitative results. In fact, the majority of journals within the MRI field require study overview checklists for experimental setup details and participant characteristics, such as STARD¹⁹, CONSORT²⁰, PRISMA²¹, and STROBE²², however, these do not cover reporting standards for acquisition parameters and the technical details that are required for an MRI acquisition, including acquisition parameters necessary for MRS measurements. Consequently, comparing studies is difficult and may lead to inaccurate and inconsistent conclusions, contributing to the slow translation of MRS from the research setting to clinical applications.

To overcome the lack of information in publications, a checklist of minimum requirements for reporting MRS studies was developed - the Minimum Reporting Standards for in vivo Magnetic Resonance Spectroscopy (MRSinMRS).¹⁵ The objective was that, for clinical and research studies using MRS, authors should complete the provided table and attach it as a supplementary figure or appendix to their manuscript. This was intended to foster standardization and simplification of the review process and ensure that all critical parameters of data acquisition and analysis are appropriately reported. As a further step, the editors of 121 clinical journals were asked to consider implementing the MRSinMRS table as a requirement for publication, of which seven agreed and 12 are currently evaluating the proposal.²³

While the expert consensus papers have been widely cited in MRS publications (Table 1), the actual recommendations are not nearly as well implemented in practice. Research groups with long-established workflows experience the adoption of consensus practices as an inconvenience, often due to a lack of strong incentive, while researchers new to the MRS field may not yet have the necessary expertise or guidance to implement them. For example, the MRSinMRS consensus paper, published in 2021, has been cited 102 times to date, but only 43 references actually incorporated the MRSinMRS table, while the remaining 59 citations only acknowledged the paper (Figure 2). While the MRSinMRS table offers a practical solution for reporting methods, locating required parameters within DICOM headers or MRS raw files can be challenging, especially for beginners. This is primarily due to variations in MRS data formats and nomenclature across different vendors and the complex nature of the parameters themselves.⁹ Although MRS software developers have begun implementing the MRSinMRS checklist into their standard output tables, community members expressed a clear need for a user-friendly and easy-to-use standalone solution at the 2022 Magnetic Resonance Spectroscopy workshop in Lausanne, Switzerland.²⁴ Incorporating the MRSinMRS table provides editors, reviewers, and readers with a clear overview of the specific MRS methodology used in each study, while also

guaranteeing the availability of comprehensive details for those seeking to replicate an experiment or conduct meta-analyses based on the results. Moreover, the checklist (Figure 1) will establish a consistent format for presenting MRS information and offer journals less acquainted with MRS a coherent means of validating methods.

To address this need, we have developed the expandable base for an open-source standalone software application to enhance accessibility and streamline the reporting process for both novice and expert MRS researchers. This application automates the population of the hardware and acquisition portions of the MRSinMRS table using a single data file from an MRS study, and generates a corresponding methods section to be used in publications. Advantages of the application are evident in easy data input, using an intuitive graphical user interface (GUI) as shown in Figure 4, and freedom from any proprietary dependencies. Furthermore, it was implemented to facilitate extensions and incorporation of existing features in the future, making it a community-driven software.

MRSinMRS checklist			Always filled by RMY
Site (name or number)			Filled by RMY if filetype supports it
1. Hardware			Never filled by RMY
a. Field strength [T]	•		Features in development
b. Manufacturer			Features in development
c. Model (software version if available)			
d. RF coils: nuclei (transmit/receive), number of channels, type, body part			
e. Additional hardware			
2. Acquisition			
a. Pulse sequence			
b. Volume of interest (VOI) locations			
c. Nominal VOI size [cm3, mm3]			
d. Repetition time ($T_{\rm R}$), echo time ($T_{\rm E}$) [ms, s]			
e. Total number of excitations or acquisitions per spectrum			
In time series for kinetic studies			
i. Number of averaged spectra (NA) per time point			
ii. Averaging method (eg block-wise or moving average)			
iii. Total number of spectra (acquired/in time series)			
f. Additional sequence parameters (spectral width in Hz, number of spectral points,			
frequency offsets)			
If STEAM:, mixing time (T_{M})			
If MRSI: 2D or 3D, FOV in all directions, matrix size, acceleration factors, sampling			
method			
g. Water suppression method			
h. Shimming method, reference peak, and thresholds for "acceptance of shim" chosen			
i. Triggering or motion correction method (respiratory, peripheral, cardiac triggering,			
incl. device used and delays)			
3. Data analysis methods and outputs			
a. Analysis software			
b. Processing steps deviating from quoted reference or product			
c. Output measure (eg absolute concentration, institutional units, ratio), processing steps deviating from quoted reference or product)			
d. Quantification references and assumptions, fitting model assumptions			
4. Data quality a. Reported variables (SNR, linewidth (with reference peaks))			
b. Data exclusion criteria			
c. Quality measures of postprocessing model fitting (eg CRLB, goodness of fit, SD of			
residual)			
d. Sample spectrum			
a sample spectrum		I	

Figure 1. Minimum Reporting Standards for in vivo Magnetic Resonance Spectroscopy (MRSinMRS) checklist of required parameters for the publication of MRS studies, adopted from Lin et al. (2021.) A template Excel spreadsheet of this table can be found at:

<u>https://github.com/agudmundson/mrs_in_mrs</u> Highlighted in green are the fields that REMY always populates, in yellow fields that REMY populates if the filetype supports it, and in orange fields that REMY doesn't populate at this point.



Figure 2. Adoption and Utilization of the MRSinMRS Consensus in MRS Research. This figure illustrates the citation dynamics of the MRSinMRS consensus since its publication in 2021, highlighting a total of 102 citations. It differentiates between papers that merely cited the consensus (n=59) and those that actively integrated its reporting table into their methodology (n=43). The trend indicates an initial phase of citations without substantial adoption of the reporting table in 2021 and 2022. In contrast, 2023 marks a significant shift towards implementing the consensus framework, with 30 papers including the reporting table versus 20 that only cited the consensus. This trend signifies a growing commitment within the MRS research community towards enhancing research reproducibility through standardized reporting. REMY is anticipated to further streamline the reporting process, enabling researchers to automatically populate the table, thereby facilitating more efficient and accurate adherence to the consensus guidelines.

2. Methods

Here, we describe the development of a software suite termed "REproducibility Made EasY" (REMY). REMY is freely available for download from the GitHub repository <u>https://github.com/agudmundson/mrs_in_mrs;</u> the source code is open under a liberal BSD-3

license. REMY is designed as a standalone application to create the MRSinMRS table and a matching MRS methods section that can be used in publications. The Python-based (v. 3.11) application requires no programming experience, operating through an intuitive graphical user interface (GUI) built using Tkinter²⁵ (Figure 4). While REMY is available to run through the command line, executables were created using PyInstaller for Windows, macOS, and Linux. The application is operating-system (OS) agnostic, meaning it operates uniformly across platforms. As an open-source application, REMY is transparent, granting visibility into its underlying codebase.

2.1. Workflow Overview

REMY currently supports various commonly used MRS data formats, including GE pfiles (.7); Siemens DICOM (.ima), .rda, and Twix (.dat); Philips spar/sdat (.spar/.sdat); and Bruker Method (.method). To begin, users will select a dataset with a file explorer using the 'Import' button. Once selected, REMY will automatically update the outputs to export to this directory. Users can also select a different folder using the 'Export' button. Now that a dataset has been selected, users must select which vendor and which data format they have input using the dropdown menus. Finally, the 'Run' button exports and MRSinMRS table, log file, and text documents (Latex and PDF format) with a completed and referenced Methods section as shown in Figure 3. Once REMY has completed, the 'Run' button updates to read 'Completed.'

2.1.1. Data Reading

Beyond the standard codebase, necessary for the application execution, REMY also leverages spec2nii²⁹ and pymapVBVD (<u>https://github.com/wtclarke/pymapvbvd</u>) to read the various file formats. When reading Siemens data, REMY uses the 'pymapVBVD' function from spec2nii to read Twix and the 'multi_file_dicom' function from spec2nii to read dicom. For GE, the 'pfile' class and '_dump_struct' function are used to read pfiles. Philips spar/sdat is read using the read_spar function from spec2nii. REMY reads Bruker method files directly by parsing the text and uses the 'Dataset' class from brukerapi (<u>https://github.com/isi-nmr/brukerapi-python</u>, included with spec2nii).

2.1.2. Header Fields

When reading each file, REMY attempts to identify as many relevant fields as possible from the data header. Field strength, vendor, vendor software, pulse sequence, number of data points, TE, TR, spectral width, and voxel size are among the parameters commonly available for each vendor. While each header file uses unique nomenclature, REMY identifies, translates, and inputs these parameters into the generic MRSinMRS format and table.

2.1.3. Base Files

Included with REMY are a set of base files, each named MRSinMRS, that are used as a generic blueprint when generating the final outputs. The first of these files is the empty MRSinMRS table (.csv) that is read and populated throughout the execution process. Next, while LaTeX is not required to use REMY, all the necessary files to generate a LaTeX PDF are saved, including auxiliary document information (.aux), bibliography (.bbl), citations (.bib), control file (.bcf), and

bibliography log (.blg). These files are each copied over to the export directory and renamed to reflect the name of the dataset that was inputted.

2.1.4. Outputs

After completion, REMY will output a series of files to the export directory, each named after the input dataset. The first of which is a log file (.log) that includes detailed information about the runtime and notes whether any errors occurred. Next is the completed MRSinMRS table (.csv). If the users' system includes LaTeX, the necessary support files, LaTeX (.tex), and a text document (.pdf) will automatically be generated that now includes the information from the dataset.

It is increasingly recognized that the variability in data analysis methods among different vendor-proprietary pipelines and offline analysis tools cause substantial analytical variability, i.e., metabolite estimates are sensitive to the decisions made during pre-processing, modeling, and quantification.^{26–28} The MRSinMRS table therefore contains sections requiring details of data analysis procedures and data quality, that for now, is not automatically populated by REMY because it is not linked to a processing pipeline/software. However, when integrated into existing software packages, this functionality would be easily implemented in the future.³

2.1.5. Test datasets

For the development of the REMY, an initial single voxel spectroscopy (SVS) test dataset was used, consisting of 15 Siemens datasets including 8 twix (.dat), 3 DICOM (.ima) and 2 RDA (.rda) datasets, 8 Phillips .spar/.sdat datasets, 8 GE pfiles (.7) and 2 Bruker method files (PV 360 V1.1 and PV 360 V3.3). The initial test data came from 4 sites and was acquired at 3 field strengths (3T, 7T and 14T) with 6 different pulse sequences (STEAM, LASER, sLASER, PRESS, MEGA-PRESS and HERMES) ensuring a diverse test dataset covering the majority of SVS sequences (Supplementary Table 1).

After the application was developed, we performed a crash test using publicly available data from the Big GABA dataset (https://www.nitrc.org/projects/biggaba/). We randomly selected 15 PRESS datasets from 3 sites per vendor (i.e., 45 datasets per vendor) which contained GE (.7), Siemens Twix (.dat) and Philips (.spar/.sdat) files. We further expanded our crash test with spec2nii test data employing additional 4 GE (.7), 6 Philips (.spar/.sdat), 14 Siemens Twix, 2 Siemens DICOM (.ima), 3 RDA (.rda) and 2 Bruker (method) datasets to increase the diversity of sites and sequences included.



Figure 3. REMY Workflow. REMY supports multiple MRS data formats as input, including GE (.7), Siemens (.ima, .rda, .dat), Philips (.spar/.sdat), and Bruker (.method, .ser). Users initiate the process by importing a dataset, after which REMY looks for the necessary parameters in the header file of the data file, using spec2nii functionality. It then populates the hardware and acquisition parts of the MRSinMRS table, and creates documentation (in Latex and PDF formats) for the Methods section.

	Reproducibility Made Easy (RMY)									
Export a CSV acc	Reproducibilit	Ey Made Easy RS guidelines using MRS file headers								
Antonia S	Reproducibility M usnjar, Antonia Kaiser, G Aaron Gud	ianna Nossa, Dunja Simicic, and								
• •	-	, Bogner W, et al. netic Resonance Spectroscopy (MRSinMRS): 8iomedicine. 2021;34(5). doi:10.1002/nbm.44								
Import	/PATH/TO/IMPORT/File	2								
Export	/PATH/TO/EXPORT/Fil	e								
Select Vendor		First Select Vendor	\Diamond							
	Ru	n								

Figure 4. Reproducibility Made Easy User Interface. Single file import facilitates the table and methods section output at the location specified by the user.

Results

Initial test data

The application was tested using an initial SVS test dataset (Siemens twix (.dat) and DICOM (.ima), Phillips (.spar/.sdat), GE pfiles (.7) and Bruker (.method) files) with the aim of reading, and translating all the available hardware and acquisition parameters required in the MRSinMRS table. For the hardware section of the table, REMY successfully read Field strength [T], Manufacturer name, Software version, and nuclei from all the file types, therefore populating 4 of 5 required hardware fields from the MRSinMRS table. RF coil and additional hardware information were not present in any of the data files and therefore could not be inputted.

For the acquisition part of the table, pulse sequence name, nominal VOI size, TR, TE, total number of acquisitions or excitations per spectrum (NA), spectral width [Hz], and number of spectral points were successfully read from all file types populating an important part of the Acquisition fields of the MRSinMRS table. Necessary information on VOI anatomical location, WS method, transmit frequency offsets and shimming method could not be found in the majority of file types and as such was not automatically read. Therefore, the automatically generated methods section highlights all the necessary information that was not automatically populated in **bold**, indicating their importance and necessity for manual user input.

Crash test

List of parameters/fields that should have been filled: 1a, Field strength [T]; 1b, Manufacturer; 1c, Model; 1c, Software Version; 1d, Nuclei; 2a, Pulse Sequence; 2c, VOI Size; 2d, TR; 2d, TE; 2e, Total Number of Acquisitions (Total Excitations; NA); 2f, Spectral Width; and 2f, Number of Points. Supplementary Table 1 presents a comprehensive inventory of the datasets evaluated, along with the results of populating the necessary fields.

Phillips .spar/.sdat - In total, 21 Philips .spar/.sdat datasets were tested, ranging from software versions 3.2.1/.2.1 to 5.1.7/1.7. The application achieved a 100% success rate in importing the data and extracting the targeted parameters, except for the model information, which is inaccessible from this file type. Consequently, we report a success rate of 91.6% in extracting all intended parameters.

Siemens twix (.dat) - 29 Siemens .dat datasets were tested, ranging from software version syngo MR B17 to E11. The application was 100% successful in reading in all 28 datasets and extracting the aimed parameters.

Siemens DICOM (.ima) - 2 Siemens .ima datasets were tested, ranging from MR B17 to E11. The application was 100% successful in reading in all datasets. The application was 100% successful in reading all datasets and 91.6% successful in extracting the aimed parameters (scanner model information missing).

Siemens RDA (.rda) - 3 Siemens .ima datasets were tested syngo MR B17 to XA31. The application was 100% successful in reading all datasets and extracting the aimed parameters.

GE pfiles (.7) - 19 GE pfiles (.7) were tested, ranging from software versions HD16 to MR24. The application was 100% successful in reading in all 19 datasets. It was 91.6% successful in

extracting the aimed parameters, extracting all the aimed parameters except the scanner model for 14 datasets (which is not available for this file type) and 83% successful for 5 datasets by failing to extract the number of spectral points in addition to the model. It's important to emphasize that the application reads GE pfiles for version 7 onwards, as supported by spec2nii since the parameter notation is drastically different in files before that version.

Bruker method files - 2 Bruker datasets were tested. The application was 100% successful in extracting the aimed parameters for these datasets, except for the scanner model information, which is inaccessible from this file type, leading to 91.6 % overall success rate. The data types that Bruker exports include ser and fid files; however, they are always accompanied by a method text file that contains all the necessary information for the MRSinMRS table. The nomenclature in the method files remains unchanged across versions (here tested PV6.0.1, PV 360 V1.1, PV 360 V3.3); therefore we chose to read this file type for our application.

MRSinMRS checklist		Methods provided by the automatic table tool
Site (name or number)		based on MRSinMRS reporting standards
1. Hardware		
a. Field strength [T]	2.89 T ·	Antonia Susnjar, Antonia Kaiser, Gianna Nossa, Dunja Simicic, Aaron Gudmundson
b. Manufacturer	Siemens	
c. Model (software version if available)	MAGNETOM Prisma	January 24, 2024
d. RF coils: nuclei (transmit/receive), number of channels, type, body part	64 ch, 1H	
e. Additional hardware		1 Methods
2. Acquisition		
a. Pulse sequence	PRESS	1.1 ¹ H-MRS Spectroscopy
b. Volume of interest (VOI) locations	ACC	1.1.1 Acquisition
c. Nominal VOI size [cm3, mm3]	40x25x27mm3	All scanning procedures were conducted using a Siemens MAGNETOM Prisma scanner equipped with a 64ch coil operating at 2.89 T. Before spectroscopy
d. Repetition time (T_R), echo time (T_E) [ms, s]	30/2000	data acquisition, a sequence for anatomical image anatomical image
e. Total number of excitations or acquisitions per spectrum	64	(info) was obtained for accurate MRS voxel placement and subsequent segmentation. MRS data were acquired utilizing the PRESS sequence in
In time series for kinetic studies		combination with WS method water suppression method. The following
i. Number of averaged spectra (NA) per time point		acquisition parameters were used: repetition time/echo time (TR/TE) of 2000
ii. Averaging method (eg block-wise or moving average)		ms/30 ms, and 64 transients recorded per acquisition of total number of acquisitions and a spectral width of 2000 kHz. The volume of interest (VOI
iii. Total number of spectra (acquired/in time series)		$=40 \times 25 \times 27$) was placed in ACC. The static magnetic field homogeneity
f. Additional sequence parameters (spectral width in Hz, number of spectral points, frequency offsets)	2000Hz, 2048 data points	was adjusted using BRAIN shimming method, the threshold for the acceptance of shim was set at thresholds using reference peak as the reference peak. For eddy current correction and quantification purposes,
If STEAM:, mixing time (T_{M})		number of averages transients of water-unsuppressed data were also acquired, using identical acquisition parameters.
If MRSI: 2D or 3D, FOV in all directions, matrix size, acceleration factors, sampling method		Note: !!! The positions in the text which could not be automatically filled using the table are highlighted in BOLD. Please fill in this information
g. Water suppression method		manually. !!! If you used multiple VOI or various VOI locations with the
h. Shimming method, reference peak, and thresholds for "acceptance of shim" chosen	BRAIN	same protocol, please change the text accordingly to include VOI specific information (both location and threshold for shim).
i. Triggering or motion correction method (respiratory, peripheral, cardiac triggering, incl. device used and delays)		 IF Diffusion: !!! If you use a diffusion weighted sequence, please include additional information: diffusion time (), b-values, number of transients per b-value and the diffusion direction.

Figure 5. Exported output from the REMY standalone application using a Siemens .twix MRS dataset. The first two sections of the table regarding data acquisition and hardware are populated, while data processing and quality need to be manually inputted by the researchers.

Discussion

REMY is a robust and convenient tool that enables researchers and clinicians to report essential MR hardware and acquisition parameters for MRS experiments. By automatically populating a standard table suggested by a consensus paper, sourced from a single MRS data file, the process facilitates straightforward study replication and streamlined method evaluation. Furthermore, the tool generates a methods section, simplifying the reporting process for researchers, which can help ensure the validity of the study setup and the interpretability of the results. The alternative requires a complete manual search for those parameters, and exporting and populating the table justified in the consensus paper.¹⁵ While our REMY tool populates the

hardware and acquisition sections of the MRSinMRS table from most data formats currently used (Figure 1), it cannot populate the other sections, and it is imperative for researchers to carefully fill those in manually after completing the analysis. This process can and should be automated as well; for example, the end-to-end analysis pipeline Osprey populates the data analysis methods and data quality sections in the MRSinMRS table with information generated by its built-in linear-combination modeling and quantification modules.²⁴ Leveraging the open-source and adaptable nature of REMY, we anticipate that other MRS analysis software developers may seamlessly integrate it into their pipelines. With straightforward modifications in the source code, the complete table generation process can be automated, further enhancing the ease and efficiency of MRS reporting.

While many have cited the MRSinMRS consensus paper, indicating the willingness of the MRS community to provide detailed methodological approaches, often the table is not included in neither the manuscript nor supplementary materials. A notable challenge in completing the table is the variation in parameter nomenclature among different scanner vendors, which can complicate the task of locating and reporting parameters. Additionally, given the inherent variations across vendors and software versions, we have established a detailed, frequently updated table on GitHub with software versions and datasets tested and implemented throughout REMY development. Other parameters like dynamics, transients, averages, and blocks also can be misconstrued as the same. In response, our application is equipped with a backend code that identifies the vendor and automates the population of parameters, mitigating the potential for human error. For instance, the total number of excitations or acquisitions per spectrum (2e) indicates how many single scans were recorded for the averaged spectrum. The subsequent fields 2e(i) - number of averaged spectra per time point (number of excitations per time point), 2e(ii) - averaging method and 2e(iii) total number of spectra, are required only for kinetic studies. By populating the table automatically, the confusion between terms has been successfully solved by REMY.

The substantial technical hurdle that may discourage researchers from using the REMY application, involving advanced coding, has been effectively addressed through the development of a user-friendly, extendable, standalone application. Note that for all vendors, the application successfully reads pulse sequence names; however, the sequences are often user modified and renamed for different studies. As such, the name that is given to the sequence and subsequently read by the application might not contain its original/true name and needs to be corrected by the user.

The application successfully translated the test data acquired with various MRS sequences to the output table and methods section as shown in Figure 5. Parameters that are used as a metric of success are field strength [T], manufacturer, model, software version, nuclei, pulse sequence, VOI size, TR, TE, NA, spectral width, and number of points. In cases where certain parameters are present in one data file format but absent in another, and consequently not filled in by REMY for the formats lacking this information, we interpret this as a failure or limitation in accurately reading and reporting parameters which has affected success rate measurement.

One major constraint of this project is its limited use for single voxel MRS, which inherently minimizes applicability across a broader spectrum, including multi-voxel MRS studies. However,

all code is openly available, to encourage the community to contribute to REMY and extend its usability to all possible MRS cases.

The rapid increase in development of available MRS processing software presents an opportunity for considerable advancement within the MRS field. As mentioned before, a drawback resides in the need for conclusive reporting of methods. We are actively strategizing to extend our outreach to software developers working on the development of MRS processing tools. The essence of our plan involves integrating our open-source application into existing tools, creating a partnership that simplifies reporting methods for the MRS scientists and eliminates an aspect of what can be perceived as "black box" processing. Although many MRS processing tools have taken steps to ensure transparency and logical checkpoints throughout their processing pipelines, the inclusion of MRSinMRS outputs and the completion of the third section in the table, pertaining to data analysis methods and outcomes, will further enhance the credibility of published research.

Furthermore, we provide a standardized and automatically filled methods section with adequate references. This not only establishes a standardized template, but also provides a concrete methodological framework that can be directly incorporated into publications. Given the increasing number of published MRS studies, we recognized a challenge within the field and provided a simple solution through our work. REMY as an application is a start to provide a valuable, easy-to-use, expandable resource for novice and expert MRS researchers.

Future Directions

Despite its current limitation to single voxel multinuclear MRS studies, the open-source nature of REMY invites contributions that could extend its applicability to other MRS applications. Moreover, the ability of REMY to be integrated into existing MRS processing tools promises further simplification of methodological reporting, increasing the transparency and credibility of MRS research. Additionally, to advance reporting in preclinical studies we will implement automatic population of the water suppression mode, and pulse bandwidth from the Bruker method file.

Lastly, the implementation of REMY could be refined, and the source code could be improved in accordance with community recommendations. For example, the future roadmap for REMY includes a demographics section that will be generated when researchers import all datasets of one study. The demographics section would provide the number of participants and, where available, gender, mean age, etc. This would be especially helpful for meta/mega-analyses. With the input of all datasets, REMY would highlight fields where the parameters, accidentally or deliberately, diverge across scans. In addition, after extraction is complete, the user would be presented with an editable list of the extracted parameters so that they can insert parameters that are typically not in headers (e.g., water suppression method) before the methods section is generated.

Conclusion

We developed the REMY application to boost the adoption of MRSinMRS consensus recommendations as a solution for insufficient MRS research reporting. By automating the population of the MRSinMRS table with essential study parameters from a single dataset,

REMY facilitates the replication of studies and evaluation of methodologies. Challenges such as the variation in parameter nomenclature across different scanner vendors and the technical hurdles associated with manual table completion have been effectively resolved. Additionally, by providing an automatically filled, standardized methods section with appropriate references, REMY sets a template that can be directly incorporated into publications, addressing the pressing need for standardized reporting in the growing body of MRS literature.

Author	Title	Cited
Oz et al.	Clinical proton MR spectroscopy in central nervous	613
(2014)	system disorders	
Mullins et al.	Current practice in the use of MEGA-PRESS	542
(2014)	spectroscopy for the detection of GABA	
Wilson et al.	Methodological consensus on clinical proton MRS of the	274
(2019)	brain: Review and recommendations	
Near et al.	Preprocessing, analysis and quantification in single-voxel	183
(2021)	magnetic resonance spectroscopy: experts' consensus	
	recommendations	
Lin et al.	Minimum reporting standards for in vivo magnetic	104
(2021)	resonance spectroscopy (MRSinMRS): experts'	
	consensus recommendations	
Cudalbu et al.	Contribution of macromolecules to brain 1H MR spectra:	83
(2021)	Experts' consensus recommendations	
Choi et al.	Spectral editing in 1H magnetic resonance spectroscopy:	71
(2021)	Experts' consensus recommendations	
Maudsley et al.	Advanced magnetic resonance spectroscopic	71
(2021)	neuroimaging: Experts' consensus recommendations	
Meyerspeer et al.	31 P magnetic resonance spectroscopy in skeletal	67
(2021)	muscle: Experts' consensus recommendations	
Kreis et al.	Terminology and concepts for the characterization of in	64
(2020)	vivo MR spectroscopy methods and MR spectra:	
	Background and experts' consensus recommendations	
Juchem et al.	B0 shimming for in vivo magnetic resonance	57
(2020)	spectroscopy	
Krššák et al.	Proton magnetic resonance spectroscopy in skeletal	40
(2020)	muscle: Experts' consensus recommendations	10
Andronesi et al.	Motion correction methods for MRS: experts' consensus	36
(2021)	recommendations	00
Tkac et al.	Water and lipid suppression techniques for advanced 1H	35
	MRS and MRSI of the human brain: Experts' consensus	33
(2021)	recommendations	
	recommenuations	

Lanz et al. (2021)	Magnetic resonance spectroscopy in the rodent brain:	12
	experts' consensus recommendations	

Table 1. Compilation of MRS consensus papers, along with their corresponding citation numbers. This table is a resource for any questions within the MRS field and the most updated list on published consensus in MRS.

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Author Contributions:

AS and AG contributed to the study conception. AS, AK and AG contributed to study design. AG has written the code and created the application. AK and DS have written code to generate the methods section with appropriate references. Material preparation, data collection and analysis were performed by AS, AK, GN, DS, and AG. The first draft of the manuscript was written by AS, AK, GN, DS, and AG. All authors provided feedback on earlier drafts of the manuscript and have read and approved the final version for submission.

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Supplementary Table 1. Evaluating datasets from Bruker, Philips, GE, and Siemens scanner vendors for the REMY application.

Test dataset Dataset Acquisition Bruker		Field Strength	Туре	Nucleus	Protocol	Software	TR	TE	sw	Nuber of Acquistions (NA)	Points	AP_Size	LR_Size	CC_Size
1 SVS	Bruker	14.08	Method	1H	User:jm_phcyc_rep_STEAM	ParaVision 360 V1.1;	4000	3	7142.857	2	4096	6.5	4	3.6
2 SVS	Bruker	14.08	Method	1H	Bruker:STEAM	ParaVision 360 V3.3;	4000		7142.857	16	4096	10	2	10
GE	Dianes	11.00	menou		Diateroficient	1 44 1 500 1 500 1 5.5,	1000	5	/112.00/	10	1050	10	~	10
1 SVS	GE	3	PFile	1H	OsLASER	26.0020008	2000	144	2500	64	2048	20	20	20
2 SVS	GE	3	PFile	1H	OsLASER	26.0020008	2000		2500	64	2048	20	20	20
3 SVS	GE	3	PFile	1H	OsLASER	26.0020008	2000		2500	64	2048	20	20	20
4 SVS	GE	3	PFile	1H	OsLASER	26.0020008	2000		2500	64	2048	20	20	20
5 SVS	GE	3	PFile	1H	OsLASER	26.0020008	2000	35	2500	64	2048	20	20	20
6 SVS	GE	3	PFile	1H	OsLASER	26.0020008	2000	35	2500	64	2048	20	20	20
7 SVS	GE	3	PFile	1H	hbcd	30.0	2000	80	2000	56	2048	20	20	20
8 SVS	GE	3	PFile	1H	hbcd	30.0	2000	35	2000	32	2048	20	20	20
Philips														
1 SVS	Philips	3	SDAT/SPAR	1H	SV_PRESS_45_ws	5.4.1 / .4.1	2000	45	2000	64	2048	30	15	10
2 SVS	Philips	3	SDAT/SPAR	1H	SV_PRESS_45_ws	5.4.1 / .4.1	2000	45	2000	64	2048	30	15	10
3 SVS	Philips	7	SDAT/SPAR	1H	MRS_dACC	3.2.1 / .2.1	5000	36	4000	64	2048	30	20	15
4 SVS	Philips	7	SDAT/SPAR	1H	MRS_dACC	3.2.1 / .2.1	5000	36	4000	64	2048	30	20	15
5 SVS	Philips	7	SDAT/SPAR	1H	MRS hippo	3.2.1 / .2.1	5000	36	4000	128	2048	30	20	15
6 SVS	Philips	7	SDAT/SPAR	1H	MRS_hippo	3.2.1 / .2.1	5000	36	4000	128	2048	30	20	15
7 SVS	Philips	7	SDAT/SPAR	1H	PreS_sLASER_3600	5.1.7 / .1.7	3600	36	3000	64	1024	25	18	18
8 SVS	Philips	7	SDAT/SPAR	1H	PreS sLASER 3600	5.1.7 / .1.7	3600	36	3000	64	1024	25	18	18
Siemens														
1 SVS	Siemens	2.89	Twix	1H	ISIS	syngo MR E11	4	0.0002	10000	8	1024	20	20	20
2 SVS	Siemens	6.98	IMA	1H	emi_adi_SPECIAL_trigger_TE		6500	16	8000	2	2048	20	20	25
3 SVS	Siemens	6.98	IMA	31P	LX_ISIS3D_130	syngo MR B17	3000	0.35	12004.80192	16	2048	55	20	25
4 SVS	Siemens	6.98	Twix	31P	LX_ISIS3D_130	syngo MR B17	3000	0.35	12004.80192	16	2048	20	55	25
5 SVS	Siemens	6.98	IMA	31P	LX_ISIS3D_120	syngo MR B17	3000		12004.80192	16	2048	55	20	25
6 SVS	Siemens	6.98	Twix	31P	LX_ISIS3D_120	syngo MR B17	3000	0.35	12004.80192	16	2048	20	55	25
7 SVS	Siemens	2.89	Twix	1H	SLASER_rDLPFC_4GABA	syngo MR E11	2000	35	5000	32	2048	30	30	30
8 SVS	Siemens	2.89	Twix	1H	LESS ACC 96avg TE35 4GA		3000	35	5000	32	2048	30	30	30
9 SVS	Siemens	2.89	Twix	1H	S WIP TE68 64avg bw DEL		2000	68	5000	64	2048	30	30	30
10 SVS	Siemens	2.89	Twix	1H	ACC MEGA SLASER 4GA		2000	68	5000	64	2048	30	30	30
11 SVS	Siemens	2.89	Twix	1H	IERMES GABA GSH 4GAB		2000	80	5000	128	2048	30	30	30
12 SVS	Siemens	2.9	RDA	1H	eja_svs_mpress_pre	syngo MR E11	2000	68	3703.703704	144	2048	22	22	22
13 SVS	Siemens	2.9	RDA	1H	eja svs mpress pre	syngo MR E11	2000	68	3703.703704	144	2048	22	22	22
Crash test data GE - big PRESS	aset													
G4_P														
1 SVS	GE	3	PFile	1H	PROBE-P	24	2000		5000	64	4096	30	30	30
2 SVS	GE	3	PFile	1H	PROBE-P	24	2000		5000	64	4096	30	30	30
3 SVS	GE	3	PFile	1H	PROBE-P	24	2000		5000	64	4096	30	30	30
4 SVS	GE	3	PFile	1H	PROBE-P	24	2000		5000	64	4096	30	30	30
5 SVS	GE	3	PFile	1H	PROBE-P	24	2000	35	5000	64	4096	30	30	30
G6_P														
1 SVS	GE	3	PFile	1H	PROBE-P	16	2000		2000	64		30	30	30
2 SVS	GE	3	PFile	1H	PROBE-P	16	2000		2000	64		30	30	30
3 SVS	GE	3	PFile	1H	PROBE-P	16	2000		2000	64		30	30	30
4 SVS	GE	3	PFile	1H	PROBE-P	16	2000		2000	64		30	30	30
5 SVS	GE	3	PFile	1H	PROBE-P	16	2000	35	2000	64		30	30	30
G8_P														
1 SVS	GE	3	PFile	1H	jpress	24	2000		2000	64	2048	30	30	30
2 SVS	GE	3	PFile	1H	jpress	24	2000		2000	64	2048	30	30	30
3 SVS	GE	3	PFile	1H	jpress	24	2000		2000	64	2048	30	30	30
4 SVS	GE	3	PFile	1H	jpress	24	2000		2000	64	2048	30	30	30
5 SVS	GE	3	PFile	1H	jpress	24	2000	35	2000	64	2048	30	30	30
Siemens - big GABA														
S1_P	0.				BBEGG		0000		4000		00.15			
1 SVS	Siemens	2.89	Twix	1H	PRESS_mid_parietal	syngo MR B17	2000		4000	64	2048	30	30	30
2 SVS	Siemens	2.89	Twix	1H	PRESS_mid_parietal	syngo MR B17	2000		4000	64	2048	30	30	30
3 SVS	Siemens	2.89	Twix	1H	PRESS_mid_parietal	syngo MR B17	2000		4000	64	2048	30	30	30
4 SVS	Siemens	2.89	Twix	1H	PRESS_mid_parietal	syngo MR B17	2000		4000	64	2048	30	30	30
5 SVS	Siemens	2.89	Twix	1H	PRESS_mid_parietal	syngo MR B17	2000	35	4000	64	2048	30	30	30
S5_P	C ¹	2.00				AR DIF	2007		1000		20.45	20		20
1 SVS	Siemens	2.89	Twix	1H	press	syngo MR B17	2000		4000	64	2048	30	30	30
2 SVS	Siemens	2.89	Twix	1H	press	syngo MR B17	2000		4000	64	2048	30	30	30
3 SVS	Siemens	2.89	Twix	1H	press	syngo MR B17	2000		4000	64	2048	30	30	30
4 SVS	Siemens	2.89	Twix	1H	press	syngo MR B17	2000		4000	64	2048	30	30	30
5 SVS	Siemens	2.89	Twix	1H	press	syngo MR B17	2000	35	4000	64	2048	30	30	30
S6_P														
1 SVS	Siemens	2.89	Twix	1H	svs_se_TE35_2.5x2.5x3	syngo MR B17	2000		4000	64	2048	30	30	30
2 SVS	Siemens	2.89	Twix	1H	svs_se_TE35_2.5x2.5x4	syngo MR B17	2000		4000	64	2048	30	30	30
3 SVS	Siemens	2.89	Twix	1H	svs_se_TE35_2.5x2.5x5	syngo MR B17	2000		4000	64	2048	30	30	30
	Siemens	2.89	Twix	1H	svs se TE35 2.5x2.5x6	syngo MR B17	2000	35	4000	64	2048	30	30	30
4 SVS 5 SVS	Siemens	2.89	Twix	1H	svs se TE35 2.5x2.5x7	syngo MR B17	2000	35	4000	64	2048	30	30	30

Philips - big GABA														
P1 P														
1 SVS	Philips	3	spar/sdat	1H	PRESS_PAR	5.1.7 ; .1.7 ;	2000	35	2000	64	2048	30	30	30
2 SVS	Philips	3	spar/sdat	1H	PRESS_PAR	5.1.7 ; .1.7 ;	2000	35	2000	64	2048	30	30	30
3 SVS	Philips	3	spar/sdat	1H	PRESS_PAR	5.1.7 ; .1.7 ;	2000	35	2000	64	2048	30	30	30
4 SVS	Philips	3	spar/sdat	1H	PRESS_PAR	5.1.7 ; .1.7 ;	2000	35	2000	64	2048	30	30	30
5 SVS	Philips	3	spar/sdat	1H	PRESS PAR	5.1.7 ; .1.7 ;	2000	35	2000	64	2048	30	30	30
P3 P														
1 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
2 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
3 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
4 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
5 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
P6 P														
1 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
2 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
3 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
4 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
5 SVS	Philips	3	spar/sdat	1H	PRESS PAR 35	3.2.2 ; .2.2 ;	2000	35	2000	64	2048	30	30	30
0.00			opuroun				2000				2010			
spec2nii test set														
GE- svMRS														
1 SVS	GE	3	PFile	1H	PROBE-P	24	2000	270	5000	16	4096	25	20	30
2 SVS	GE	3	PFile	1H	PROBE-P	24	2000	270	5000	16	4096	25	20	30
3 SVS	GE	3	PFile	1H	PROBE-P	24	2000	270	5000	16	4096	25	20	30
4 SVS	GE	3	PFile	1H	PROBE-P	24	2000	270	5000	16	4096	25	20	30
Siemens	-													
1 FID	Siemens	2.89	Twix	13C	fid_13C_360dyn_hyper_TR1000	syngo MR E11	1000	0.35	12004.80192	10	2048		quistion (ne	
2 SVS	Siemens	2.9	Twix	1H	HERC	syngo MR E11	2000	80	2000	224	1024	23	30	23
3 SVS	Siemens	6.98	Twix	1H	special_brain_withOVS_32Ch_	syngo MR B17	6500	9	8000	32	2048	20	20	20
4 SVS	Siemens	6.98	DICOM	1H	svs_se_Tra_sat	syngo MR B17	960	30	2000	2	512	20	30	40
5 SVS	Siemens	6.98	Twix	1H	svs_se_T>C15.0>S10.0_10	syngo MR B17	600	30	2000	2	512	30	20	40
6 SVS	Siemens	6.98	Twix	1H	svs_se_S>C10>S5_10	syngo MR B18	600	30	2000	2	512	30	20	40
7 SVS	Siemens	6.98	Twix	1H	svs_se_C>T15>S10_10	syngo MR B18	600	30	2000	2	512	30	20	40
8 SVS	Siemens	6.98	Twix	1H	svs_se_Tra_sat	syngo MR B18	960	30	2000	2	512	30	20	40
9 SVS	Siemens	2.89	DICOM	1H	svs_se_iso_tra_sat	syngo MR E11	860	33	2399.808015	16	512	25	30	20
10 SVS	Siemens	2.89	Twix	1H	svs_se_t>c15>s10_R10	syngo MR E11	600	33	2399.808015	16	512	30	25	20
11 SVS	Siemens	2.89	Twix	1H	svs_se_s>c10>t5_R10	syngo MR E11	600	33	2399.808015	16	512	30	25	20
12 SVS	Siemens	2.89	Twix	1H	svs_se_c>t15>s10_R10	syngo MR E11	600	33	2399.808015	16	512	30	25	20
13 SVS	Siemens	2.89	Twix	1H	svs_se_iso_tra_sat	syngo MR E11	860	33	2399.808015	16	512	30	25	20
14 SVS	Siemens	2.9	RDA	1H	svs_se_30	syngo MR XA20	2000	30	2399.808015	80	1024	20	20	20
15 SVS	Siemens	2.9	RDA	1H	svs_se_30	syngo MR XA20	2000	30	2399.808015	80	1024	20	20	20
16 SVS	Siemens	2.89	Twix	1H	svs_se_iso_tra_sat	syngo MR E11	860	33	2399.808015	16	512	30	25	20
17 SVS	Siemens	2.89	Twix	1H	svs se iso tra sat	syngo MR E11	860	33	2399.808015	16	512	30	25	20
18 SVS	Siemens	2.89	Twix	1H	svs se iso tra sat	syngo MR E11	860	33	2399.808015	16	512	30	25	20
19 SVS	Siemens	2.9	RDA	1H	svs_se_30_ala	syngo MR XA31	2000	30	2399.808015	80	1024	20	20	20
Philips		~												
1 SVS	Philips	3	spar/sdat	1H	HERC_ACC	5.4.0 ; .4.0 ;	2000	80	2000	320	2048	35	30	25
2 SVS	Philips	3	spar/sdat	1H	HYPER	5.7.1 ; .7.1 ;	2000	80	2000	256	2048	24	40	24
3 SVS	Philips	3	spar/sdat	1H	SV_PRESS_sh	5.5.2 ; .5.2 ;	2000	30	5000	64	2048	15	15	15
4 SVS	Philips	3	spar/sdat	1H	SV_PRESS_sh	5.5.2 ; .5.2 ;	2000	30	5000	64	2048	30	15	15
5 SVS	Philips	3	spar/sdat	1H	SV_PRESS_sh	5.5.2 ; .5.2 ;	2000	30	5000	64	2048	20	20	20
6 SVS	Philips	3	spar/sdat	1H	SV_PRESS_sh	5.5.2 ; .5.2 ;	2000	30	5000	64	2048	15	15	15
Bruker						-		-						
1 SVS	Bruker	9.4	Method	1H	Bruker:STEAM	ParaVision 6.0.1;	2500	3	4401.408451	16	2048	10	10	10
2 SVS	Bruker	9.4	Method	1H	Bruker:STEAM	ParaVision 6.0.1;	2500	3	4401.408451	16	2048	10	10	10