Publication of raw and curated NMR spectroscopic data for organic molecules

Christoph Steinbeck

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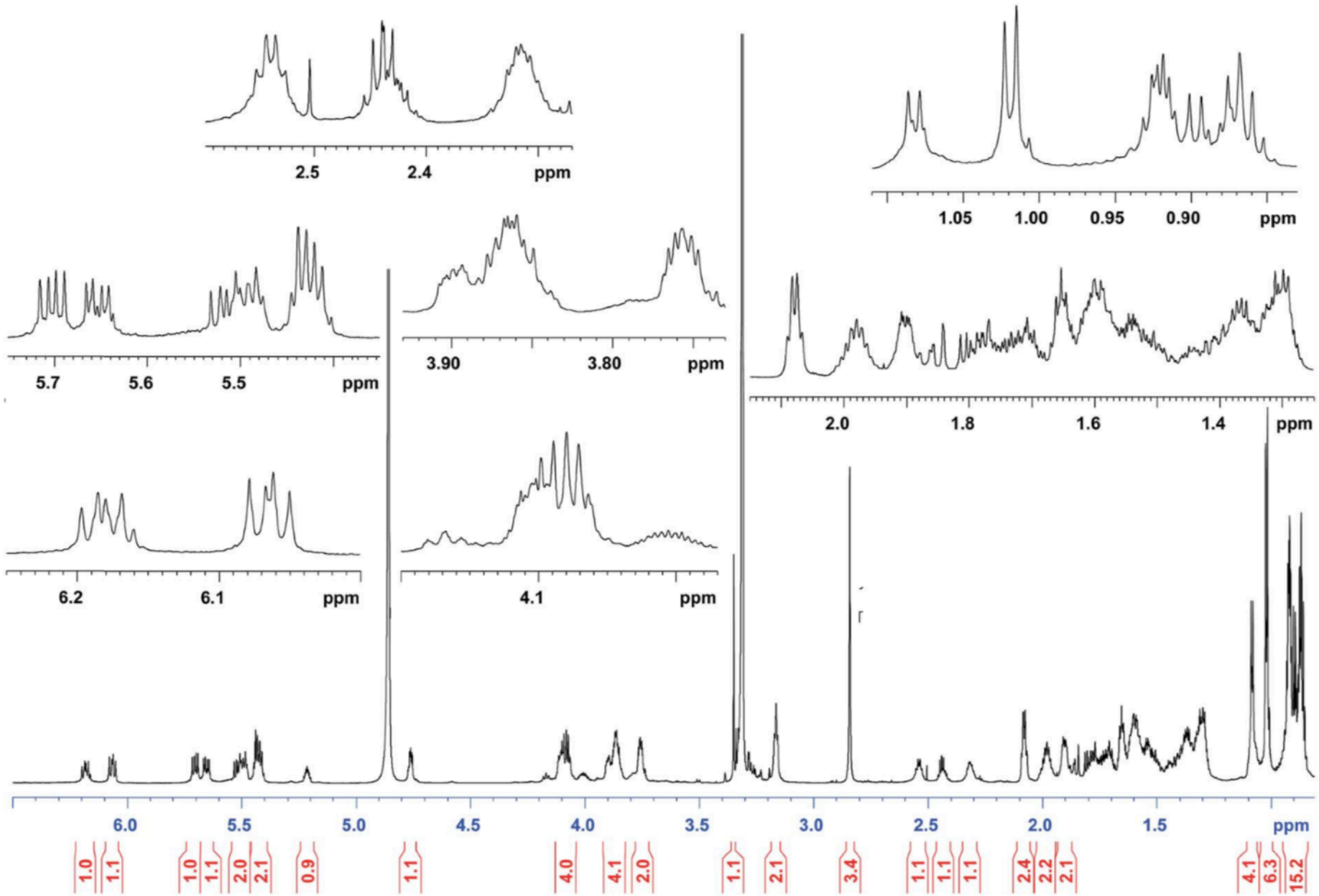
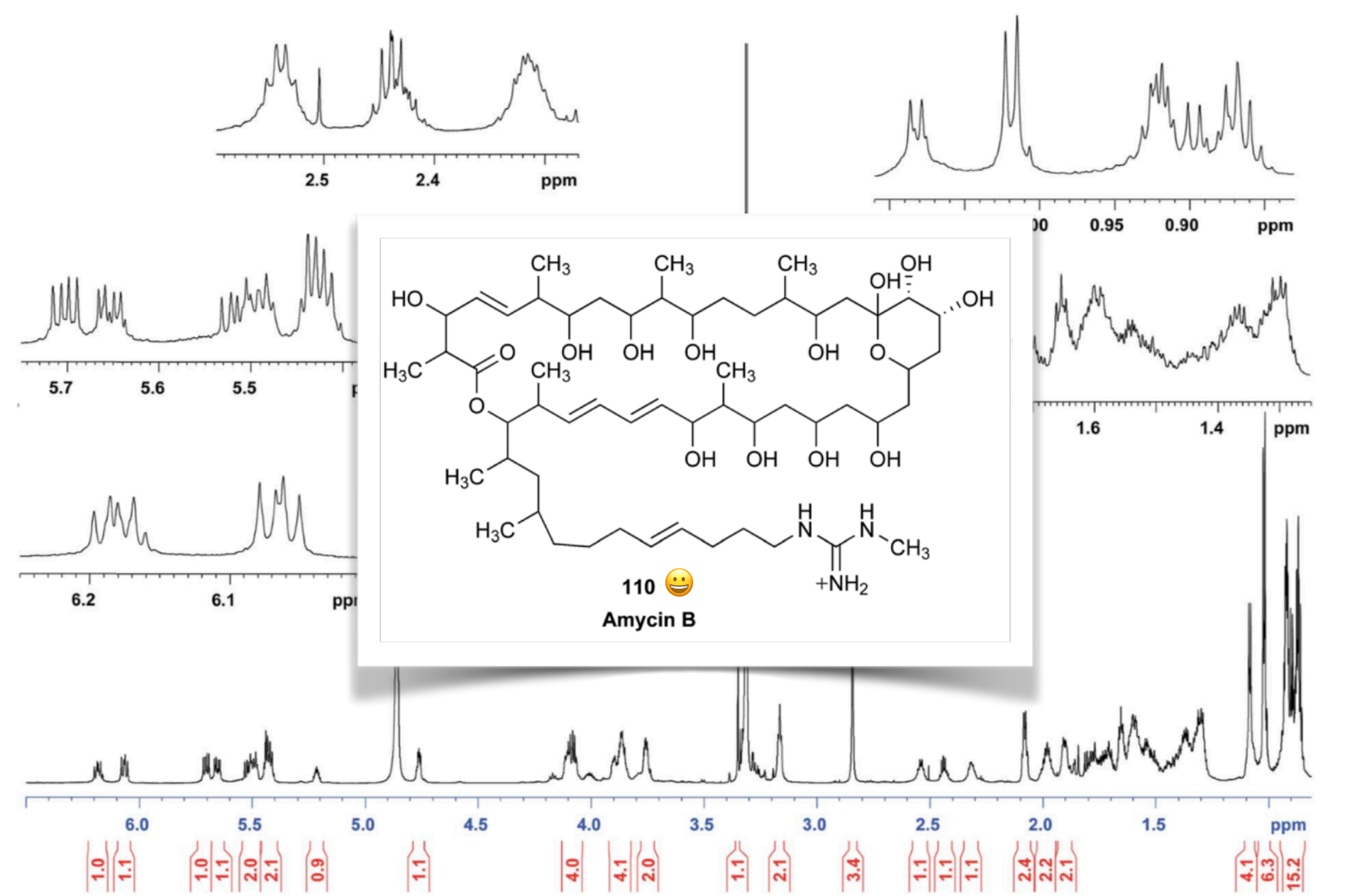


^{1}H NMR (900 MHz, methanol-d_4) spectrum for amycin B (**107**).



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Nuclear Magnetic Resonance (NMR) in Synthetic Organic Chemistry

2-(2-Iodo-2-phenylethoxy)isoindoline-1,3-dione (3aa). White solid: 90% yield (176 mg); mp = 135-136 °C. ^{1}H NMR (300.13 MHz, $CDCl_3$): δ = 7.85-7.68 (m, 4H), 7.54 (d, J = 7.4 Hz, 2H), 7.36-7.17 (m, 3H), 5.53 (dd, J_1 = 9.8 Hz, J_2 = 5.7 Hz, 1H), 5.00-4.88 (m, 1H), 4.71 (dd, J_1 = 10.7 Hz, J_2 = 5.7 Hz, 1H). ^{13}C NMR (75.47 MHz, $CDCl_3$): δ = 163.3, 139.8, 134.7, 128.9, 128.7, 128.6, 127.9, 123.7, 81.4, 25.2. ^{15}N NMR (40.56 MHz, $CDCl_3$): δ = -163.0. IR (KBr) ν(cm^{-1}): = 1731, 1720, 1465, 1192, 1138, 1127, 1114, 1081, 1020, 988, 875, 716, 696, 519. Anal. Calcd for $C_{16}H_{12}INO_3$: C, 48.88; H, 3.08; N, 3.56. Found: C, 48.73; H, 2.95; N, 3.56.

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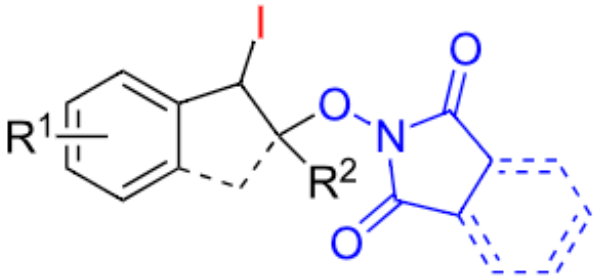

3xy:
3aa–ka, 3ab–db, 3fb, 3hb, 3kb

the first letter (x) stands for the employed vinyl arene **1a–k**, the second letter (y) - imide **2a,b**

Provides marginal evidence in experimental section that the reported structure is what we say it is.

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Keywords: *Litsea verticillata*; Lauraceae; Verticillatol; Sesquiterpene; (+)-5′-Demethoxyepiexcelsin; Lignan; Sesquiterpene; 2D NMR; Absolute structure; Anti-HIV activity; HOG.R5; Reporter cell line; Green fluorescent protein

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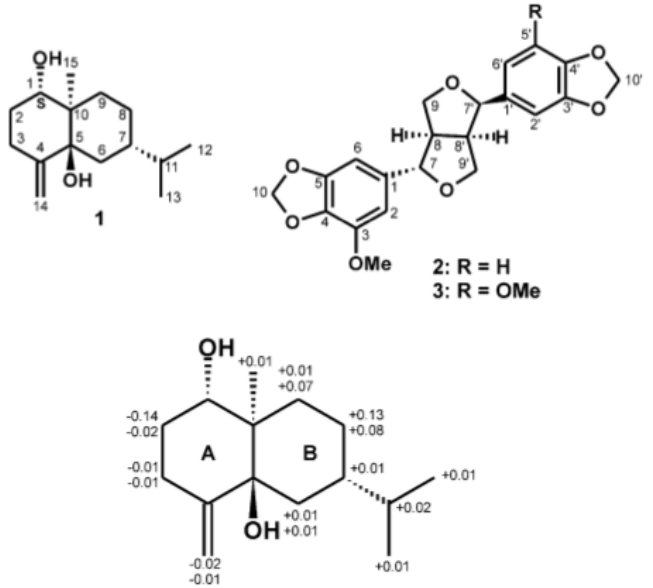

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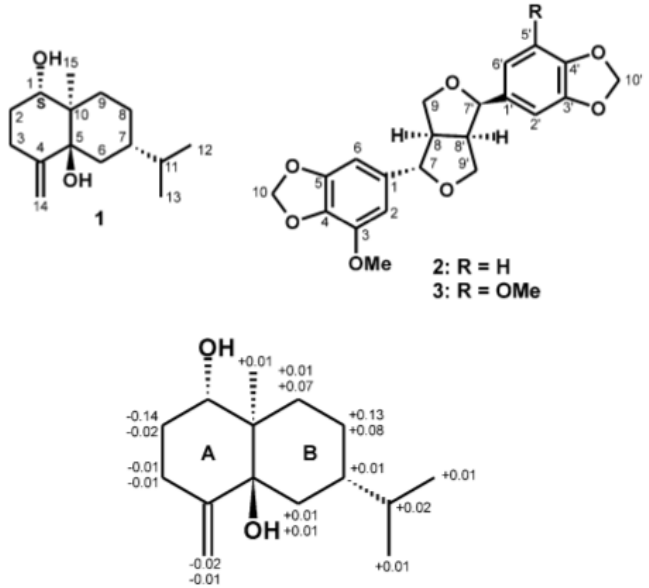

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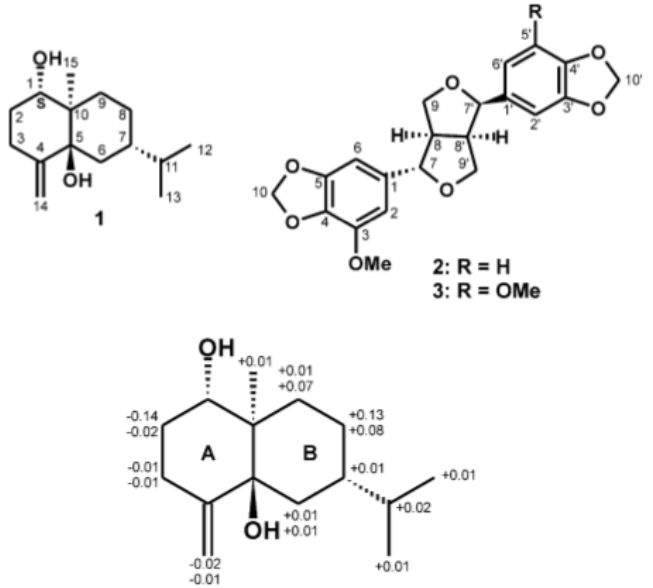

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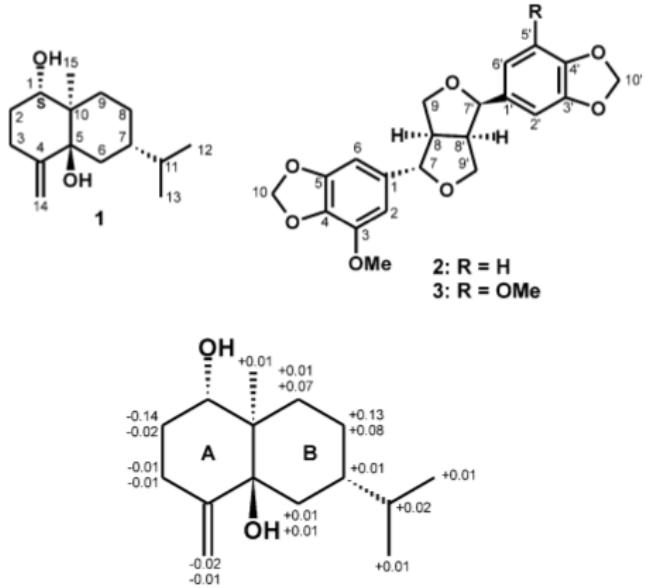

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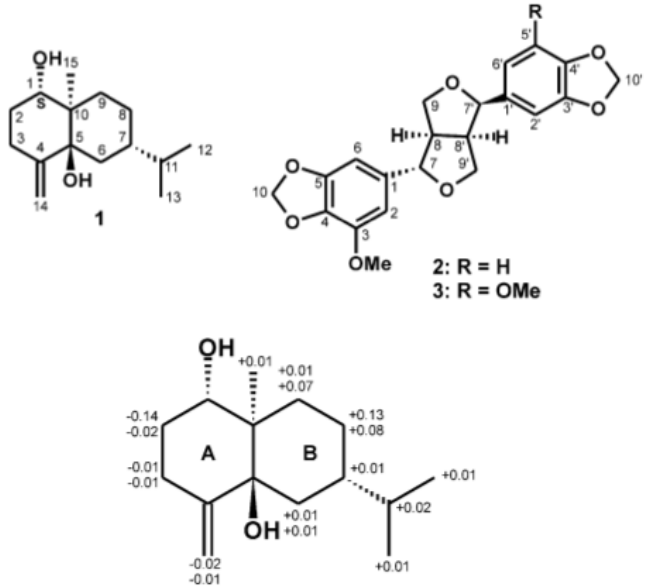

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Phys.chem. data

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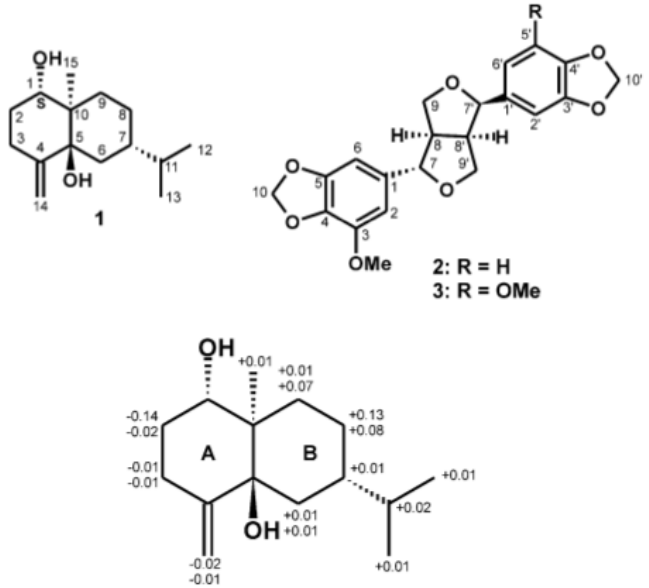

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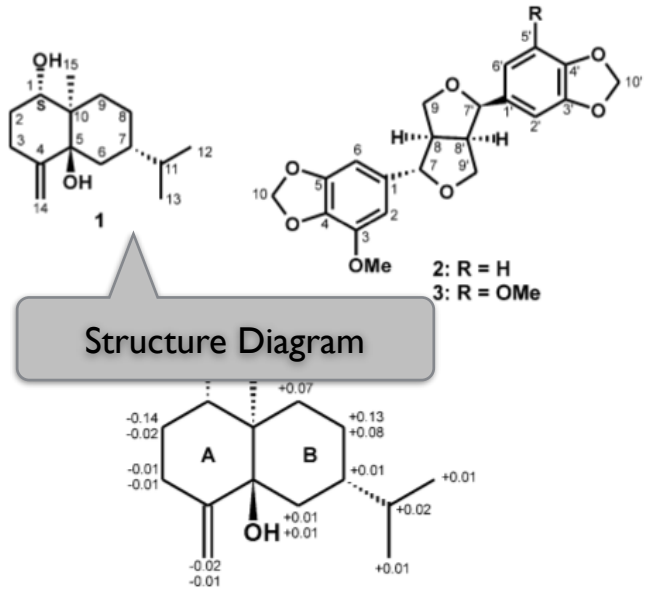

Structure Diagram

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The eudesmane sesquiterpenoid, verticillatol (**1**), as well as the lignan, (+)-5′-demethoxyepiexcelsin (**2**), and a known lignan, (+)-epiexcelsin (**3**), were isolated from *Litsea verticillata* Hance. Ligna… anti-HIV activity with an IC_{50} value of 16.4 μg/ml (42.… μM), while the known lignan **3** was inactive up to a … μg/ml (48.3 μM). Compound **1** demonstrated we… value of 34.5 …/ml (144.7 μM) while being devoid of cytotoxicity at 20 μg/ml. The structures were elu… NMR … solute configuration of the new sesquiterpenoid was determined by the generation of Mosher esters. © 2… All rights reserved.

Chemical Name

Chemical Class

Biol. Species

Biol. Activity

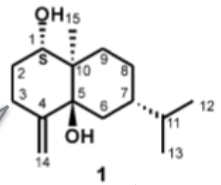
Keywords: Litsea verticillata; Lauraceae; Verticillatol; Sesquiterpene; (+)-5′-Demethoxyepiex… ne; 2D NMR; Absolute structure; Anti-HIV activity; HOG.R5; Reporter cell line; Green fluorescent protein

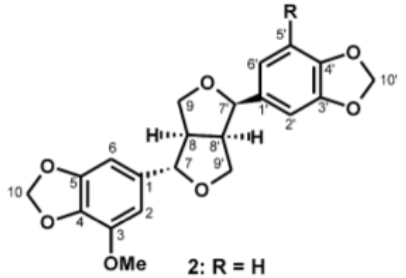
Phys.chem. data

3.6. *Verticillatol (1)*

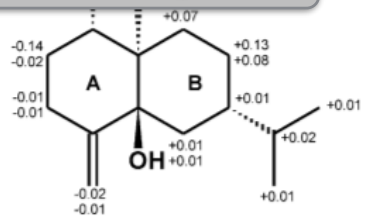
Colorless oil, $[\alpha]_D^{25}$ −41.2° ($CHCl_3$; *c* 0.13). IR ν_{max} (film): 3432, 2932, 2869, 101… d_5, *J* in Hz): δ 4.93, 4.87 (1H… *dd*, *J* = 11.5, 4.9, H-1β), 3.18 (1H, *td*, *J* = 13.6, 5.6, H-5α), 2.25 (1H, *m*, H-9β), 2.18 (1H, *m*, H-3β), 2.17 (1H, *m*, H-9α), 2.15 (1H, *m*, H-2β), 2.07 (1H, *m*, H-7), 1.99 (1H, *m*, 2α-H), 1.82 (1H, *dd*, *J* = 12.7, 2.7, H-6β), 1.70 (1H, *brt*, *J* = 12.7, H-6α), 1.70 (1H, *brt*, *J* = 12.7, H-8α), 1.43 (1H, *m*, H-11), 1.38 (1H, *m*, H-8β), 1.15 (3H, *s*, Me-15), 0.90, 0.89 (3H each, *d*, *J* = 6.0, Me-12 and-13). ^{13}C NMR (pyridine-d_5): δ 72.2 (*d*, C-1), 32.2 (*t*, C-2), 31.0 (*t*, C-3), 153.8 (*s*, C-4), 75.3 (*s*, C-5), 34.7 (*t*, C-6), 38.7 (*d*, C-7), 24.8 (*t*, C-8), 31.0 (*t*, C-9), 43.3 (*s*, C-10), 33.3 (*d*, C-11), 20.1 and 20.2 (each *q*, C-12 and C-13), 107.1 (*t*, C-14), 13.3 (*q*, C-15). EIMS: *m/z*

Atom Numbers





Structure Diagram



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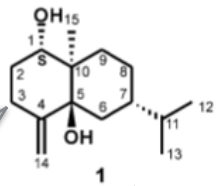
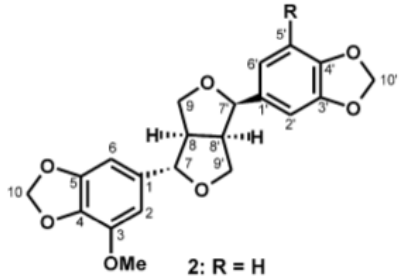
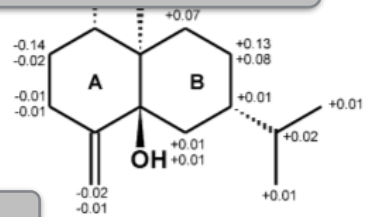




Structure Diagram



Spectral data

Hoang, V. D. et al., Phytochemistry 59, 325–329 (2002).

Nuclear Magnetic Resonance (NMR) in Natural Products Chemistry

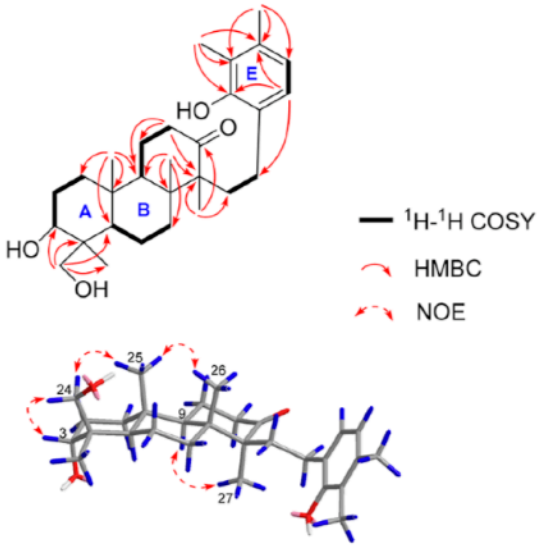


Figure 7. Selected HMBC, ^{1}H–^{1}H COSY, and NOE correlatio compound **6**.

Liu, F. et al., J. Nat. Prod., doi:10.1021/acs.jnatprod.7b01074

S8-1 expanded COSY Spectrum of libertellenone O (**1**) in $CDCl_3$.

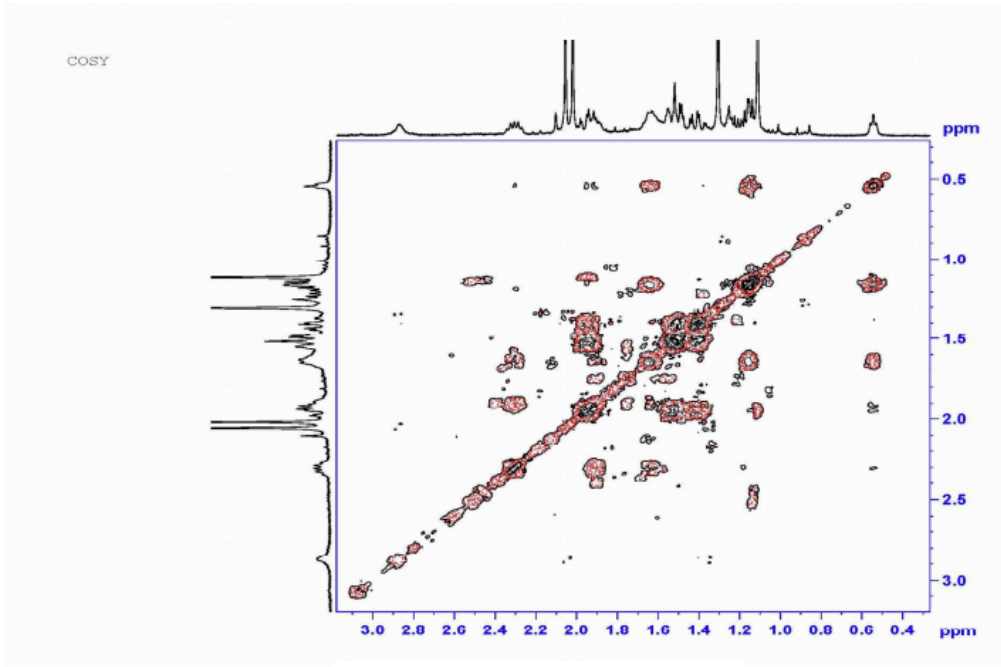


Image (!) from the supplemental information of *Nat. Prod.*, **2018**, *81* (7), pp 1553–1560

Bairoch's Lament

"It is quite depressive to think that we are spending millions in grants for people to perform experiments, produce new knowledge, hide this knowledge in often badly written text and then spend some more millions trying to second guess what the authors really did and found"

Bairoch A (2009) The future of annotation/biocuration. Nature Precedings doi:10.1038/npre.2009.3092.1.

Thanks to https://twitter.com/srp/status/1030192949802487809

Research Data Sharing is becoming the norm …

- … rather than the exception
- but some disciplines are a little more behind than others …

Why do we archive, curate and disseminate (raw) research data?

- **Data re-use** (including data use, reanalysis and repurposing)
- **Reproduction** of scientific results
  - For this we actually need to share the computational workflow for processing the data as well (see http://www.researchobject.org/)
- **Validation** of methods

Why people do not share data

- Fear of not being able to generate enough publications from their data
- Fear of being scooped by other researchers ("Research Parasites")
- Fear that one's own study is not replicable
- Fear to expose badly managed, flawed or inconsistent data
- Patient confidentiality
- Technical reasons

Smith, R. & Roberts, I. F1000Research 5, 781 (2016).

SCIENTIFIC DATA | DATA DESCRIPTOR OPEN

Metabolic differences in ripening of *Solanum lycopersicum* 'Ailsa Craig' and three monogenic mutants

Stephan Beisken, Mark Earll, Charles Baxter, David Portwood, Zsuzsanna Ament, Aniko Kende, Charlie Hodgman, Graham Seymour, Rebecca Smith, Paul Fraser, Mark Seymour, Reza M. Salek & Christoph Steinbeck

Affiliations | **Contributions** | **Corresponding authors**

Scientific Data **1**, Article number: 140029 | doi:10.1038/sdata.2014.29

Received 10 April 2014 | Accepted 06 August 2014 | Published online 16 September 2014

PDF | ISA tab | Citation | Reprints | Rights & permissions | Article metrics

Abstract

Abstract • **Background & Summary** • **Methods** • **Data Records** • **Technical Validation** • **Usage Notes** • **Additional information** • **References** • **Data Citations** • **Acknowledgements** • **Author information**

Application of mass spectrometry enables the detection of metabolic differences between groups of related organisms. Differences in the metabolic fingerprints of wild-type *Solanum lycopersicum* and three monogenic mutants, *ripening inhibitor* (*rin*), *non-ripening* (*nor*) and *Colourless non-ripening*...

Received: 22 January 2018 | Revised: 22 February 2018 | Accepted: 25 March 2018

DOI: 10.1002/mrc.4737

FEATURE ARTICLE RESEARCH ARTICLE

WILEY

NMReDATA, a standard to report the NMR assignment and parameters of organic compounds

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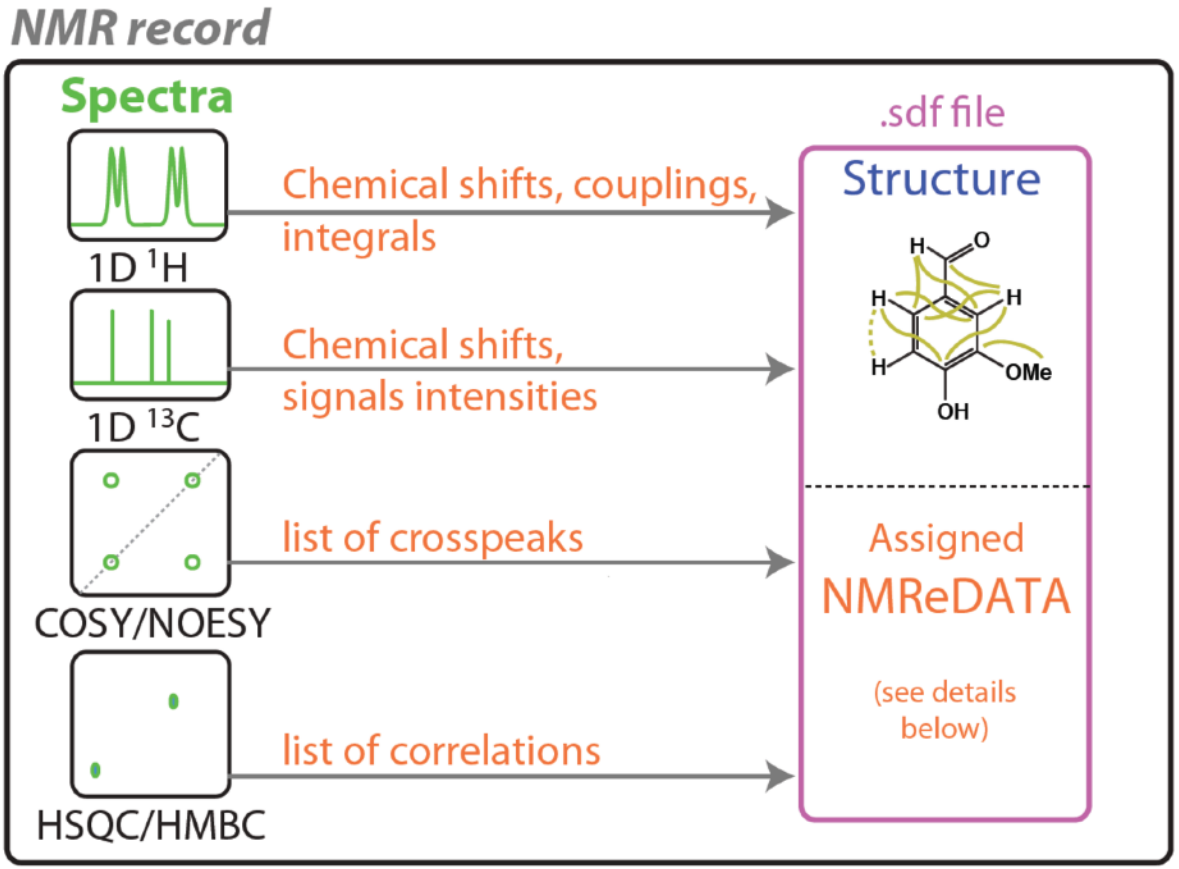
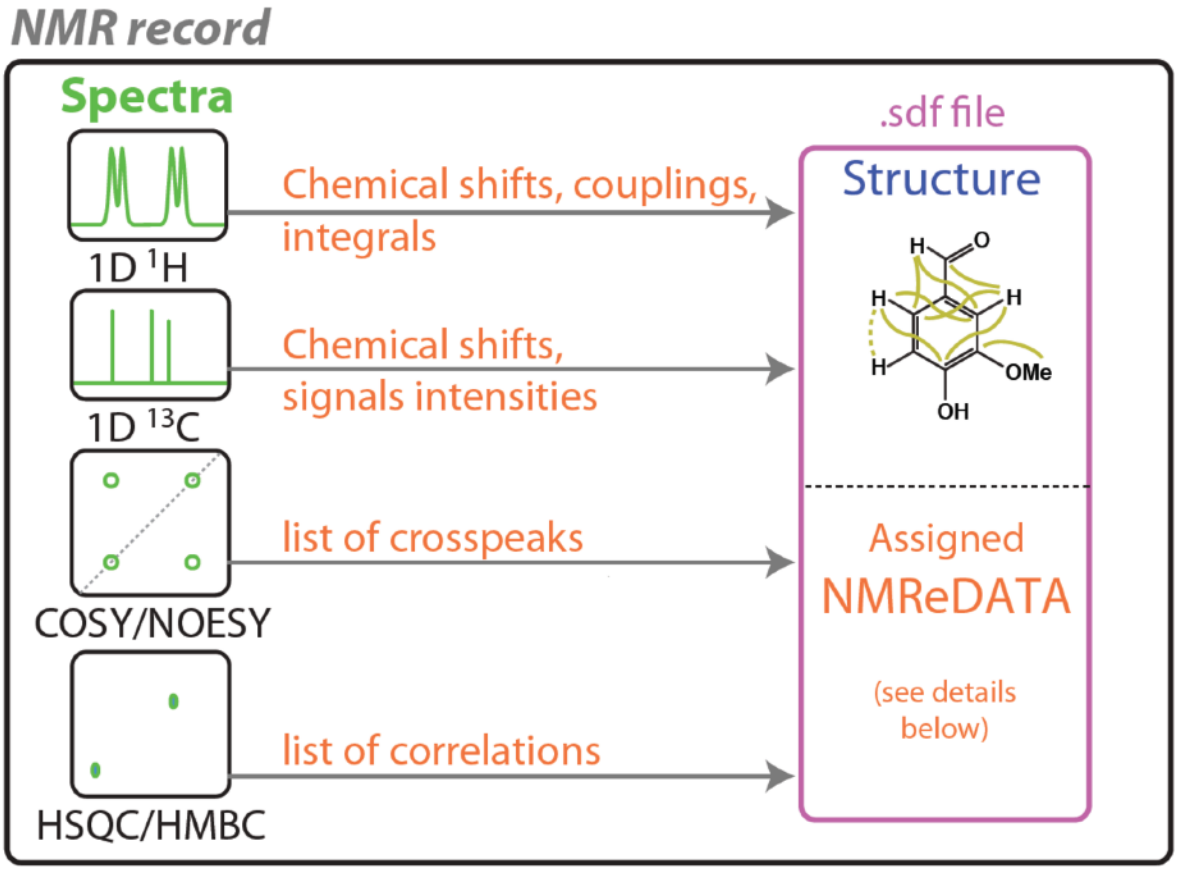
What is NMReData?



What is NMReData?

Machine-Readable Representation



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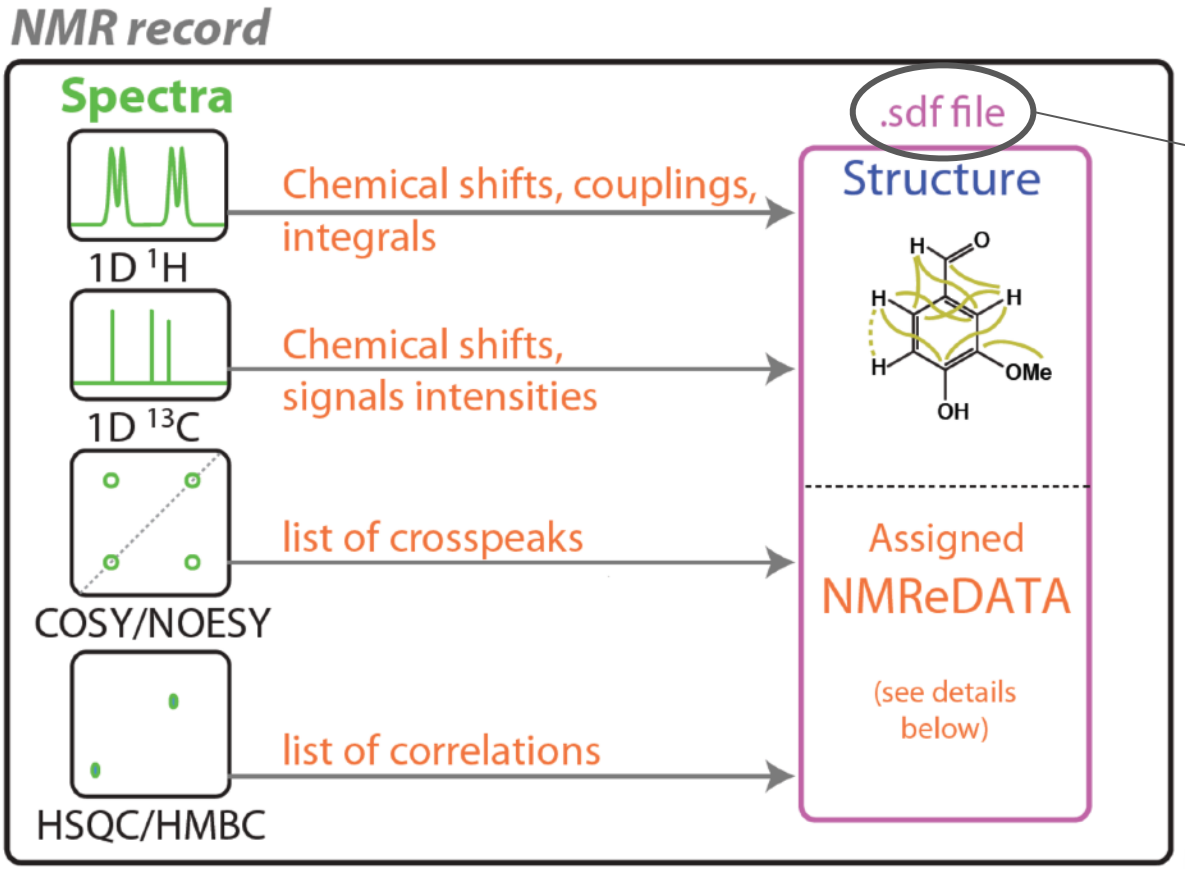

based on industry standard format

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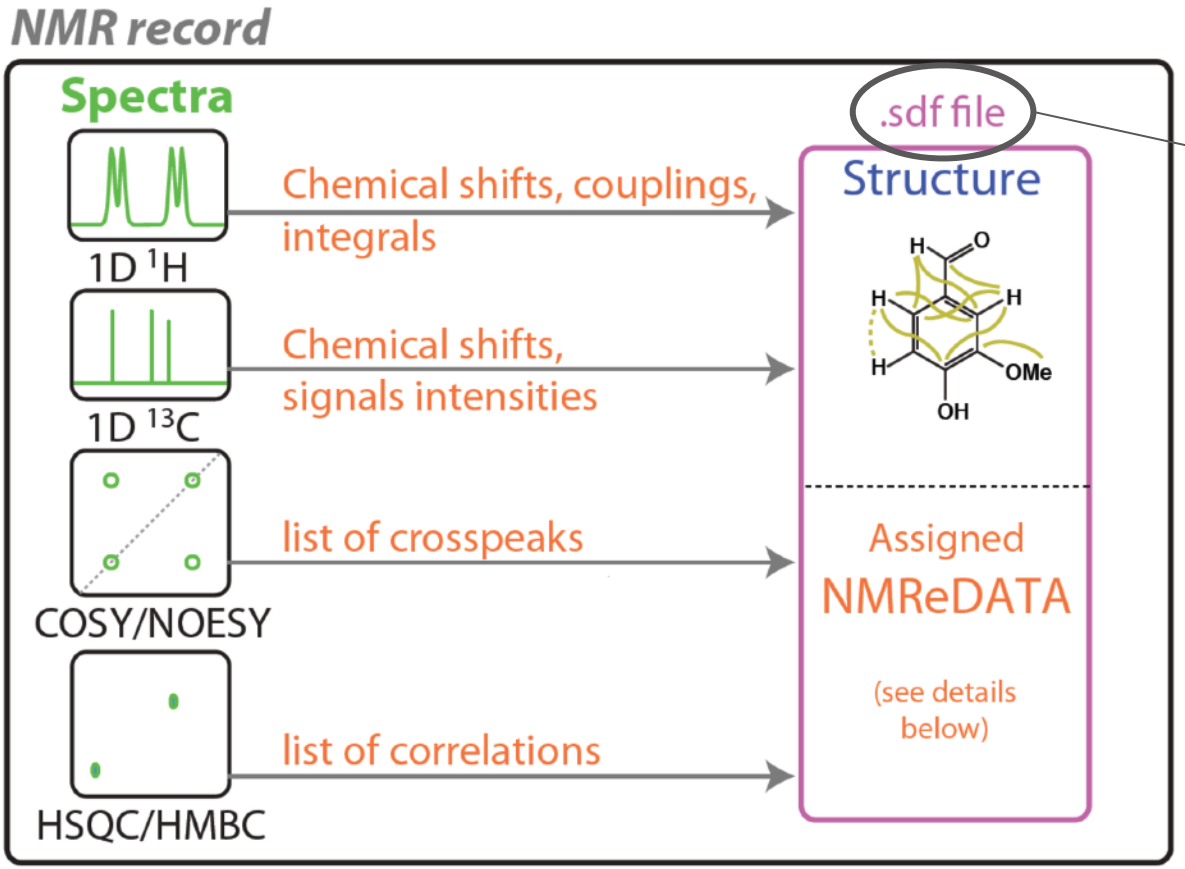

based on industry standard format

of

chemical Structure

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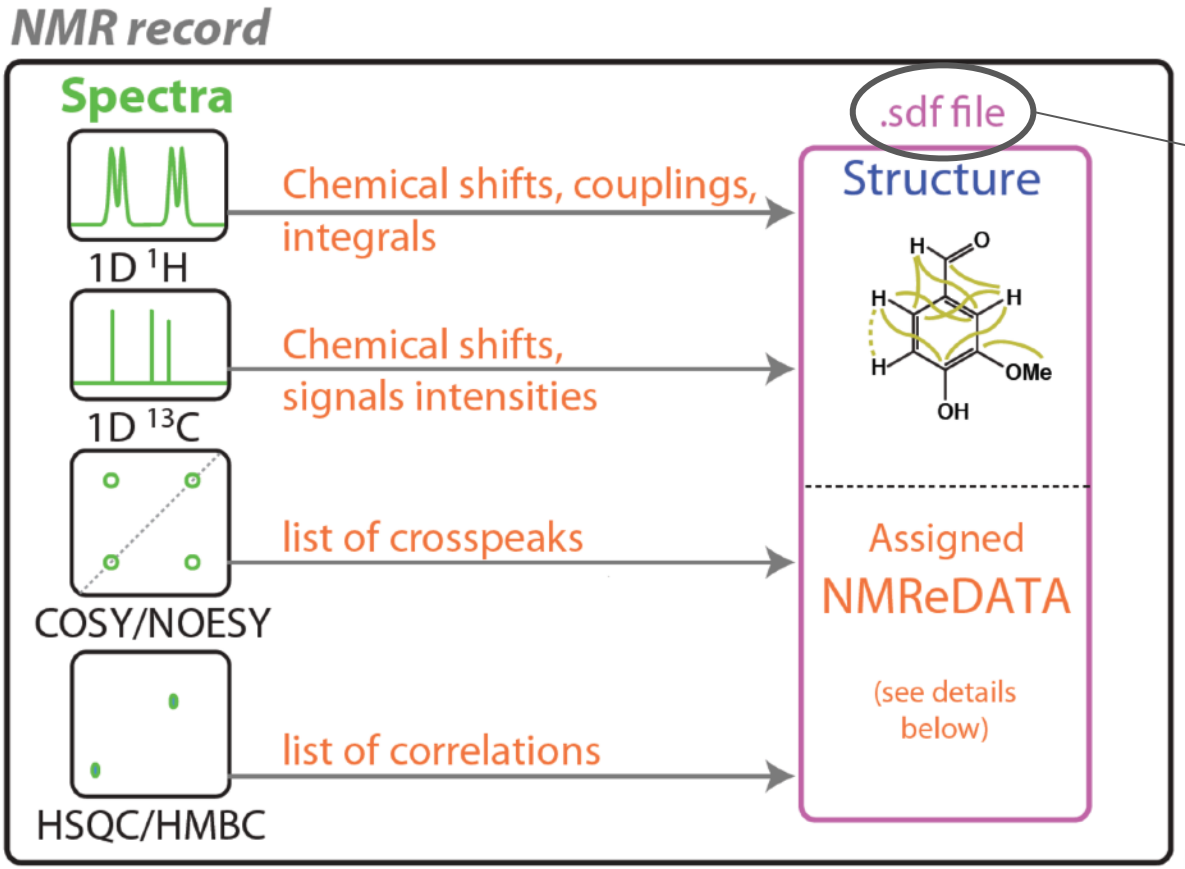

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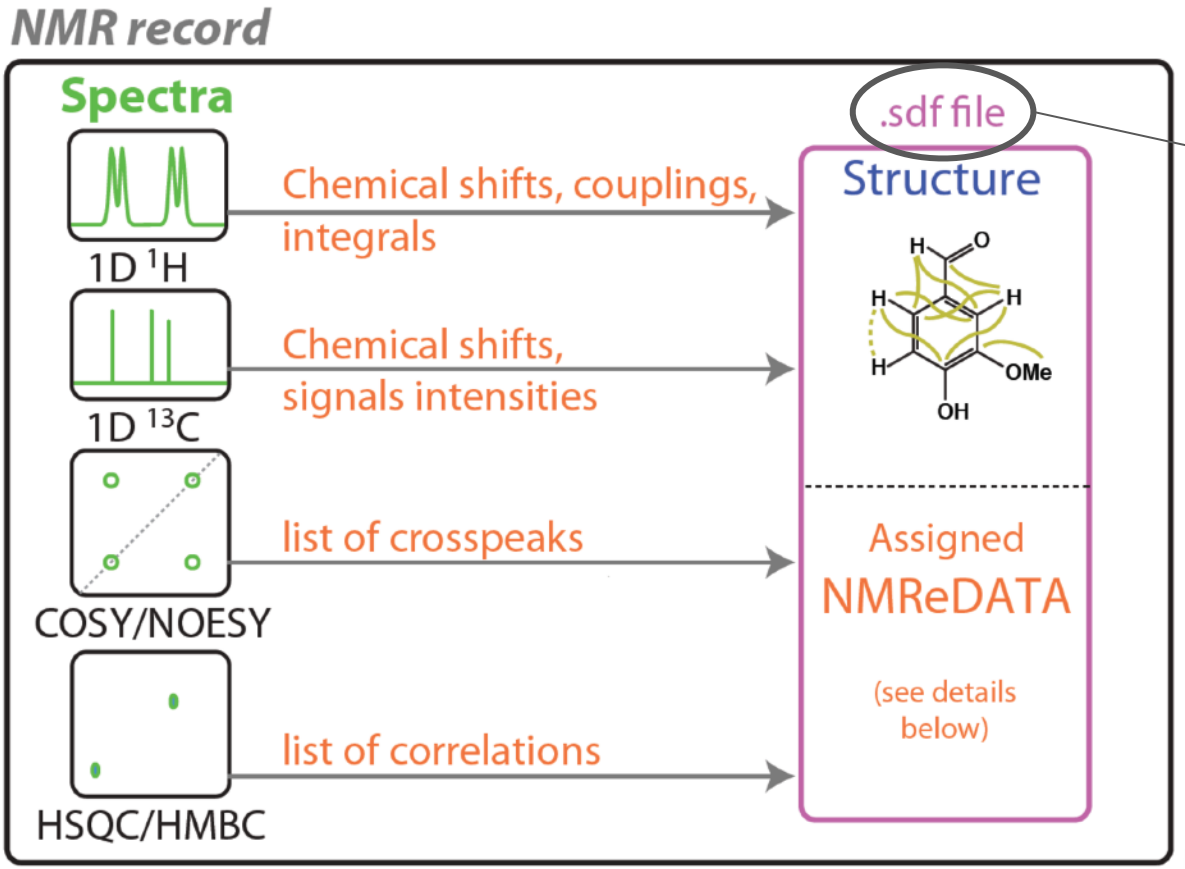

based on industry standard format

of chemical Structure

and assigned NMR Data

linked to the raw NMR Data

Why NMReData?

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- Improved **quality** of the NMR data for the community

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- Improved **quality** of the NMR data for the community
- Straightforward inclusion of NMR data in **reports** and articles

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- Easier **comparison** of dataset
- Improved **searchability** of NMR data
- Automatic **validation** by computational means (e.g. CASE)

How is NMReData supported?

- Support by major NMR software companies
- Mag. Res. Chem. will require submission of NMReData
  - Leads to raw NMR data becoming regularly available
  - More journals needed - how about Journal of Natural Products?
- I/O in NMRShiftDB2 available
- Broad support by software ecosystem crucial for enduring success
  - For updates see http://www.nmredata.org/wiki/Compatible_software

McAlpine, J. B. et al., Nat. Prod. Rep. 33, 1028 (2018).

Natural Product Reports

ROYAL SOCIETY OF CHEMISTRY

REVIEW

View Article Online
View Journal

Cite this: DOI: 10.1039/c7np00064b

The value of universally available raw NMR data for transparency, reproducibility, and integrity in natural product research†

James B. McAlpine, *[a] Shao-Nong Chen, [a] Andrei Kutateladze, [b] John B. MacMillan, [c] Giovanni Appendino, [d] Andersson Barison, [e] Mehdi A. Beniddir, [f] Maique W. Biavatti, [g] Stefan Bluml, [h] Asmaa Boufridi, [i] Mark S. Butler, [j] Robert J. Capon, [j] Young H. Choi, [k] David Coppage, [c] Phillip Crews, [c] Michael T. Crimmins, [l] Marie Csete, [m] Pradeep Dewapriya, [j] Joseph M. Egan, [n] Mary J. Garson, [o] Grégory Genta-Jouve, [p] William H. Gerwick, [qr] Harald Gross, [s] Mary Kay Harper, [t] Precilia Hermanto, [u] James M. Hook, [u] Luke Hunter, [u] Damien Jeannerat, [v] Nai-Yun Ji, [w] Tyler A. Johnson, [c] David G. I. Kingston, [x] Hiroyuki Koshino, [y] Hsiau-Wei Lee, [c] Guy Lewin, [f] Jie Li, [r] Roger G. Linington, [n] Miaomiao Liu, [i] Kerry L. McPhail, [z] Tadeusz F. Molinski, [aa] Bradley S. Moore, [qr] Joo-Won Nam, [ab] Ram P. Neupane, [ac] Matthias Niemitz, [ad] Jean-Marc Nuzillard, [ae] Nicholas H. Oberlies, [af] Fernanda M. M. Ocampos, [e] Guohui Pan, [ag] Ronald J. Quinn, [i] D. Sai Reddy, [b] Jean-Hugues Renault, [ae] José Rivera-Chávez, [ah] Wolfgang Robien, [ai] Carla M. Saunders, [aj] Thomas J. Schmidt, [ak] Christoph Seger, [al] Ben Shen, [ag] Christoph Steinbeck, [am] Hermann Stuppner, [al] Sonja Sturm, [al] Orazio Taglialatela-Scafati, [an] Dean J. Tantillo, [aj] Robert Verpoorte, [k] Bin-Gui Wang, [wao] Craig M. Williams, [o] Philip G. Williams, [ac] Julien Wist, [ap] Jian-Min Yue, [aq] Chen Zhang, [ar] Zhengren Xu, [ag] Charlotte Simmler, [a] David C. Lankin, [a] Jonathan Bisson [a] and Guido F. Pauli *[a]

McAlpine, J. B. et al., Nat. Prod. Rep. 33, 1028 (2018).

Natural Product Reports

ROYAL SOCIETY OF CHEMISTRY

REVIEW

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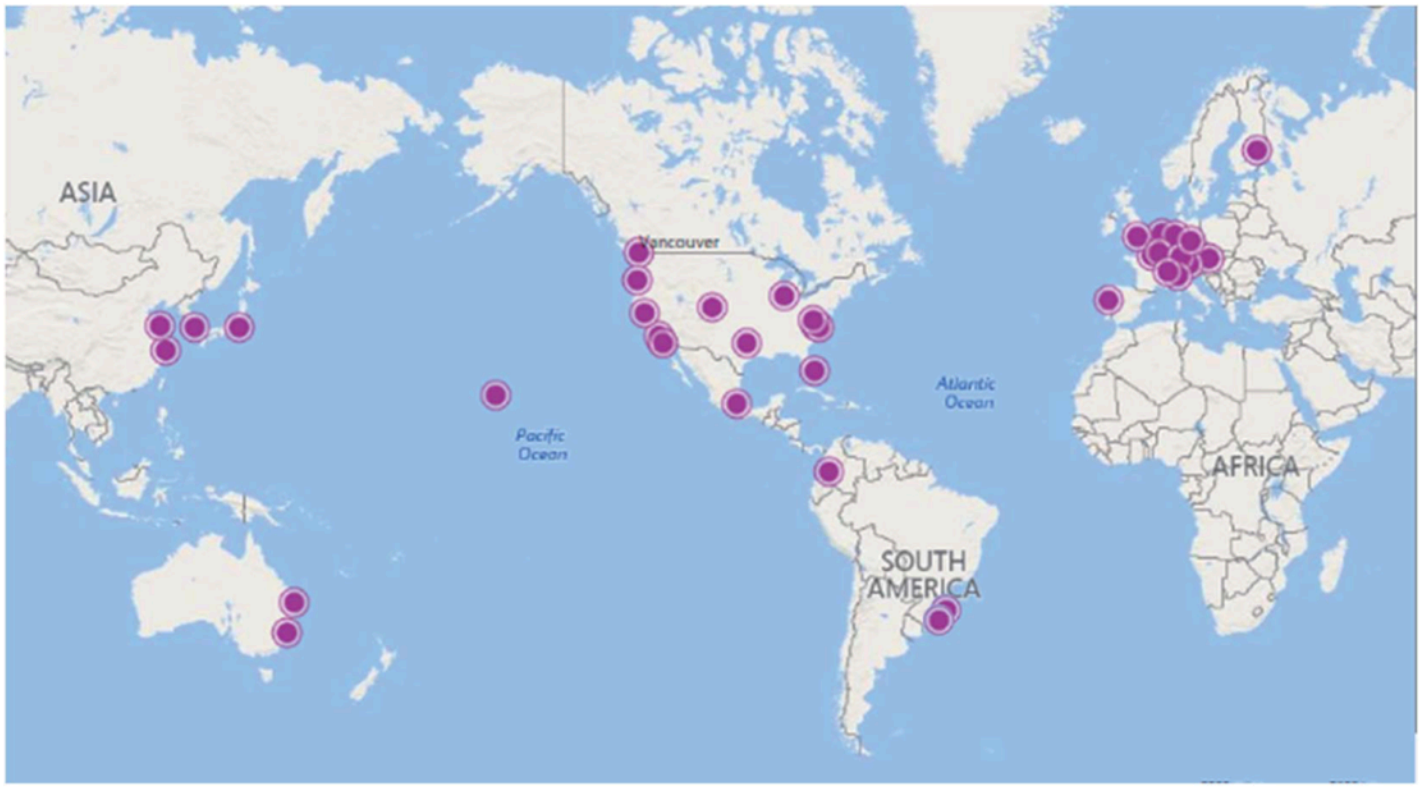
Check for updates

Cite this: DOI: 10.1039/c7np00064b

The value of universally available raw NMR data for transparency, reproducibility, and integrity in natural product research†



Why do we need a raw NMR Archive?

Natural Product Reports Review

1 Introduction
1.1 Preamble
1.2 Dimensionality and completeness
1.3 Human and machine processing of NMR data
1.4 Molecular transparency
1.5 Molecular topography
2 Introduction to the organization of this review
2.1 Rationale 1 – structure revisions
2.2 Rationale 2 – impurity detection and quantification
2.3 Rationale 3 – dereplication
2.4 Rationale 4 – enabling new methodology
2.5 Rationale 5 – other nuclei
2.6 Rationale 6 – data repositories
2.7 Rationale 7 – clinical applications
3 Structure revision
3.1 Incorrect ring closures: furan *vs.* pyrone ring systems
3.2 Incorrect ring closures: the lipopeptide arthrofactin
3.3 Incorrect ring closures: the case of aquatolide
3.4 The case of coibamide A
3.5 The structure of aldingenin B
3.6 Clearing the literature of blatantly incorrect natural product structures
3.7 Bredt's rule as a check on structure correctness
3.8 Correct analysis of coupling constants
3.9 Sulfones *vs.* sulfinates
3.10 Methylene signal assignments in the structural revision of aromin to montanacin D
3.11 The case of aglalactone
3.12 Diastereoisomers and rotamers
3.13 Data ambiguity
3.14 The importance of details
3.15 Structural instability leads to dynamic complexity
3.16 Acetogenins-the difficulty of configurational determination
3.17 Second order coupling patterns with first order look *vs.* "multiplets"
4 Impurity detection and quantification
4.1 Purification of thiotetronates

NIH Request for Information (RFI): Important Considerations for Potential Creation of an Open-Access Nuclear Magnetic Resonance (NMR) Data Repository

Notice Number: NOT-AT-17-015

Introduction

This Request for Information (RFI) seeks public comments on key points to consider regarding potential development of an open access repository and other resources to facilitate the deposit, sharing, and comparison of one- and two-dimensional nuclear magnetic resonance (NMR) data from natural products. For this purpose, "natural products" are defined as specialized metabolites and other small molecules from a variety of natural sources such as plants, fungi, bacteria, and marine organisms.

Response to this RFI is voluntary. Responders are free to address one or more of the items under "Information Requested." Instructions on how to respond are provided in "Submitting a Response." The deadline to submit your response is December 20, 2017.

Note: The deadline has passed and we are reviewing the input.

Submit a Response Online

Comments on the topic areas of this RFI may be submitted online.

The Raw NMR Archive

(…to be built)

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(…to be built)

- There is momentum for building a raw NMR data archive

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- Requirements:

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  - Stable funding and operation (EBI, NCBI, ELIXIR node, etc)

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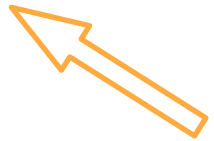

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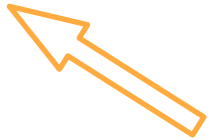
  - Ability to process, visualise and search 1D and 2D NMR data



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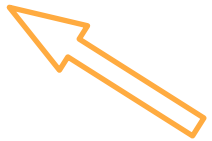
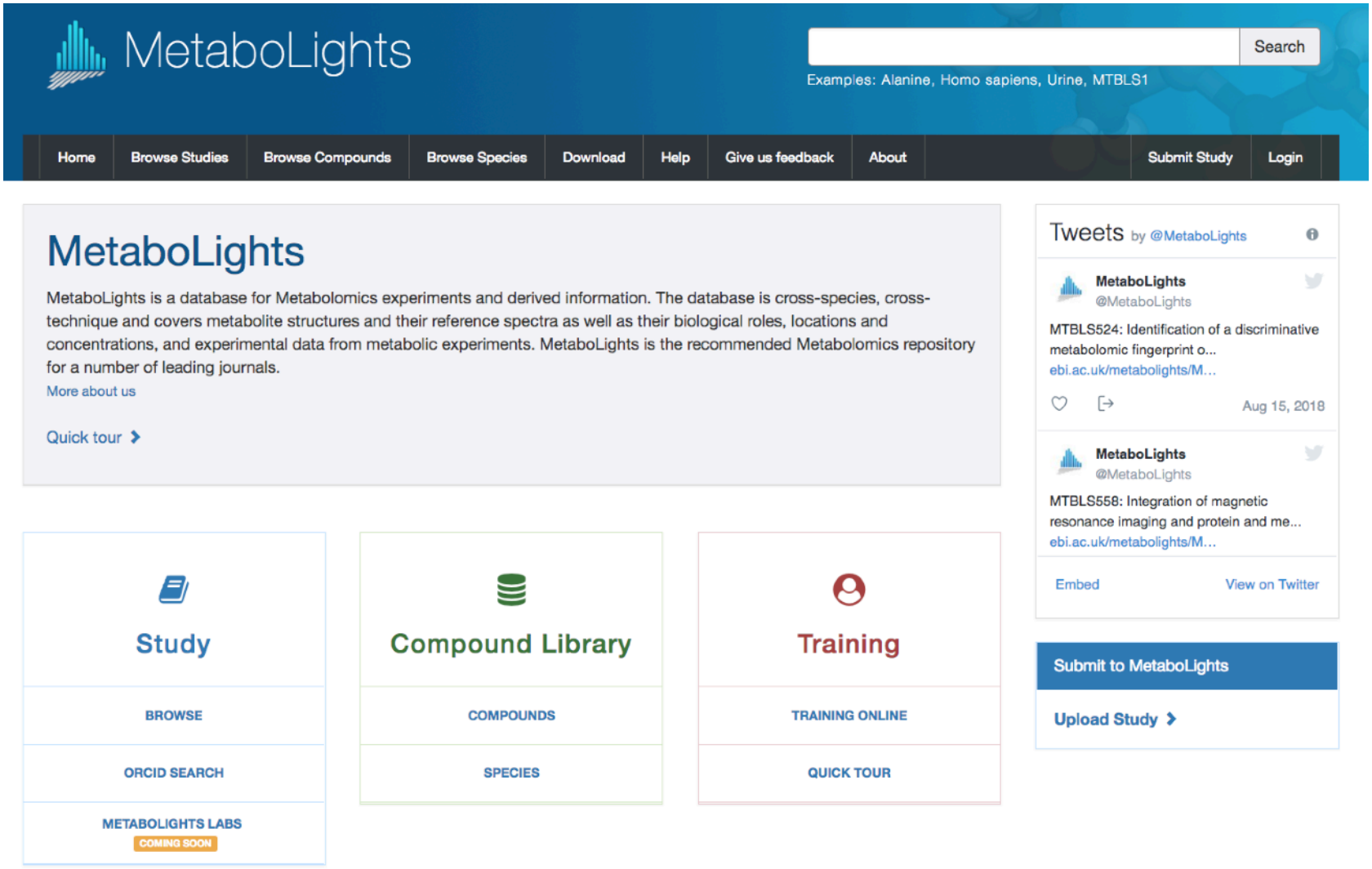
  - Framework for handling submissions of raw data and meta-data
  - Ability to process, visualise and search 1D and 2D NMR data
  - Total openness and support for the FAIR principle

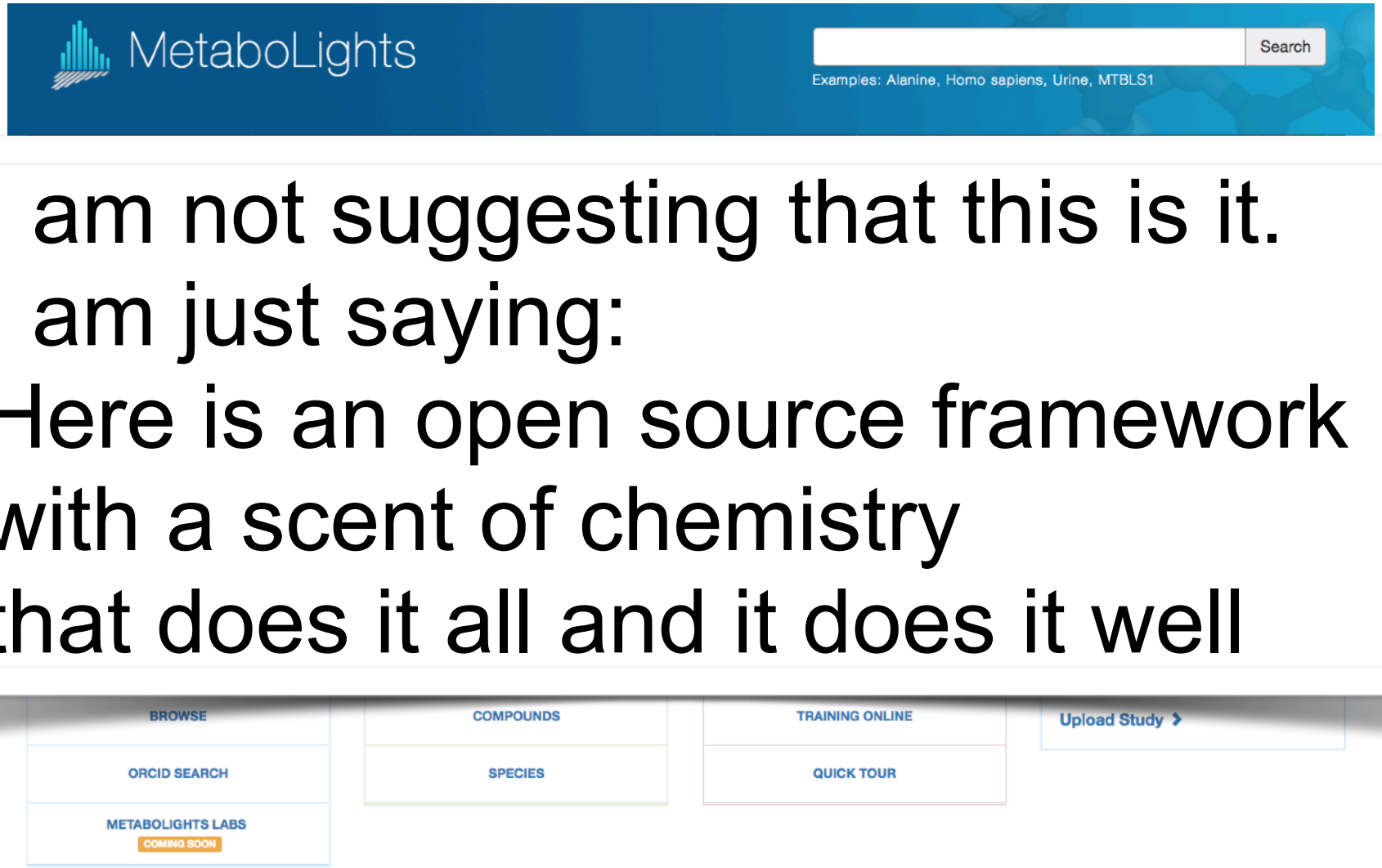


The Archive Framework



Lives at https://www.ebi.ac.uk/metabolights
or https://www.metabolights.org

The Archive Framework



I am not suggesting that this is it.
I am just saying:
Here is an open source framework
with a scent of chemistry
that does it all and it does it well

Lives at https://www.ebi.ac.uk/metabolights
or https://www.metabolights.org

Submitted ✓ — In curation ✓ — In review ✓ — Public ✓

MTBLS132: Absolute quantification of metabolites in tomato fruit extracts by fast 2D NMR (Tomato 700 MHz samples)

Abstract

Quantitative NMR metabolomics is a powerful tool to have access to valuable information on metabolism. Unfortunately, the quantitative analysis of metabolic samples is often hampered by peak overlap. Two-dimensional (2D) spectroscopy offers a promising alternative and quantitative results can be obtained provided that a calibration approach is employed. However, the duration of 2D NMR experiments is barely compatible with the metabolomic study of a large number of samples. This drawback can be circumvented by relying on "ultrafast" experiments capable of recording 2D spectra in a single-scan. While such experiments are not sensitive enough to match the concentrations of metabolic samples, a compromise can be reached by hybrid strategies capable of recording 2D NMR spectra of extracts in a few minutes only. The purpose of this study is to

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Authors: **Patrick GIRAUDEAU, Annick MOING, Mickael MAUCOURT, Catherine DEBORDE**

Contact Submitter

View Metabolites Assay | Download files | ORCID Claims | Reference this study

Release date: **11-Nov-2015**

Status: Public

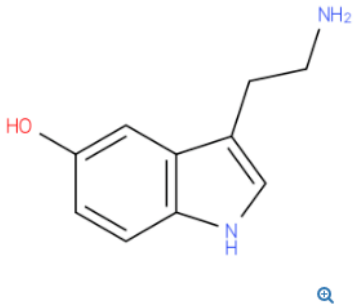
Study Design | Protocols | Samples | Assay | Files | Validation ✓ | Pathways

Show 10 entries

Search:

Protocol	Description
Sample Collection	Tomatoes (Solanum lycopersicum L. cv Moneymaker) were grown in a glass greenhouse in South-West of France in optimal commercial conditions as described previously [1]. The fruit were harvested at four different stages of development: 8, 21, 34 and 55 days post anthesis (DPA) on three different trusses (truss 5, 6, and 7). Eight DPA corresponds to the cell division stage, 21 DPA to the cell expansion stage, 34 DPA to the transition between cell expansion and ripening and 55 DPA to red-ripe fruit. Each biological replicate was made up of 4–5 fruits harvested on different plants. Three biological replicates, corresponding to the three different trusses, were used for each stage of the development. A quarter of the fruit pericarp from the equatorial zone was immediately frozen in liquid nitrogen. Fruit pericarp samples were ground in liquid nitrogen and stored at -80 °C until freeze-drying. An aliquot of fresh frozen powder was lyophilized and used for NMR analyses. Ref: [1] Biais, B., Bénard, C., Beauvoit, B., Colombié, S., Prodhomme, D., Ménard, G., et al. (2014). Remarkable reproducibility of enzyme activity profiles in tomato fruits grown under contrasting environments provides a roadmap for studies of fruit metabolism. Plant Physiology, 164, 1204–1221. doi: 10.1104/pp.113.231241. PMID:24474652
Extraction	Each extract was prepared from 40 mg (2 aliquots of 20 mg each) of lyophilized powder using a robotised Starlet platform (Hamilton, Villebon sur Yvette, France). The metabolic extraction was performed in four steps. After weighing 20 mg, 300 µl of EtOH/water (80/20, v/v) solution were added to each sample in a 1.1 ml Micronics tube, then the mixture was checked and put in a hot water bath at 80 °C during 10 min and finally placed in a centrifuge at 4,000 x g during 5 min. The supernatant was transferred into a 1.4 ml Micronics tube. The 1.1 ml Micronics tube containing the pellet was submitted to three other extraction steps: same solvent mixture, then EtOH/water (50/50, v/v), and pure Milli-Q water for the last step. The supernatants from the two aliquots and four steps were combined and evaporated to dryness using a vacuum evaporator (SpeedVac Savant, Asheville, USA). The dried extracts were titrated with KOD to pH 6 using a titration unit BTpH (Bruker Biospin, Rheinstetten, Germany) in 200 mM potassium phosphate buffer solution in D2O containing 2 mM EDTA. Then, trimethylsilyl [2,2,3,3-2H4] propionate sodium salt (TSP, 0.01% final concentration for chemical shift calibration) was added. Titrated extracts were frozen in liquid nitrogen and lyophilized during 12 h.

2D 3D



MOL | SMILES | InChIKey

MTBLC28790: Serotonin

Export | Upload Reference Spectra | ? Help

Chemistry | Biology | Pathways | Spectra | Reaction | Literature

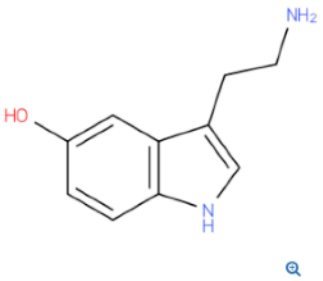
Compound Description

A primary amino compound that is the 5-hydroxy derivative of tryptamine.

Identification

IUPAC Names	thrombotonin
Molecular Formula	C10H12N2O
Mass	176.215
Monoisotopic Mass	176.095
Charge	0
InChI	InChI=1S/C10H12N2O/c11-4-3-7-6-12-10-2-1-8(13)5-9(7)10/h1-2,5-6,12-13H,3-4,11H2
InChIKey	QZAYGJVTTNCVMB-UHFFFAOYSA-N
SMILES	C1=CC(=CC=2C(=CNC12)CCN)O
Synonymns	3-(2-Aminoethyl)-1H-Indol-5-Ol
	3-(2-Aminoethyl)-1H-Indol-5-Ol
	5-HT
	5-Hydroxytryptamine
	Enteramine
	Serotonin

2D 3D



MOL | SMILES | InChIKey

MTBLC28790: Serotonin

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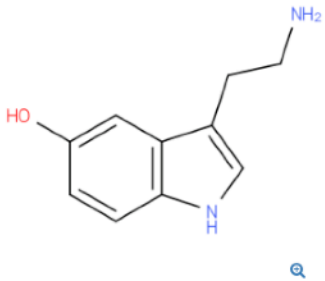
Chemistry | Biology | Pathways | Spectra | Reaction | Literature

Species

Homo sapiens	NCBI:9606 24136337 NCBI:9606 2580417 NCBI:9606 Geigy Scientific Tables, 8th Rev edition, pp. 165-177. Edited by Cornelius Lentner. NCBI:9606 Geigy Scientific Tables, 8th Rev edition, pp. 165-177. Edited by C. Lentner, West Cadwell, N.J.: Medical education Div., Ciba-Geigy Corp., Basel, Switzerland c1981-1992. MTBLS417 MTBLS417 MTBLS656
Paramuricea clavata	NCBI:317549 21939218
Triticum aestivum	MTBLS112
Pseudomonas putida	MTBLS319
Litoria verreauxii	MTBLS457 MTBLS457
Mus musculus	NCBI:10090 19425150 MTBLS216 MTBLS530 MTBLS292
Trypanosoma brucei	MTBLS49
Oryza sativa	MTBLS286 MTBLS286
Arabidopsis thaliana	MTBLS311
Human	MTBLS591
Homo sapiens (human)	MTBLS20 MTBLS20 MTBLS20

2D 3D



MOL | SMILES | InChIKey

MTBLC28790: Serotonin

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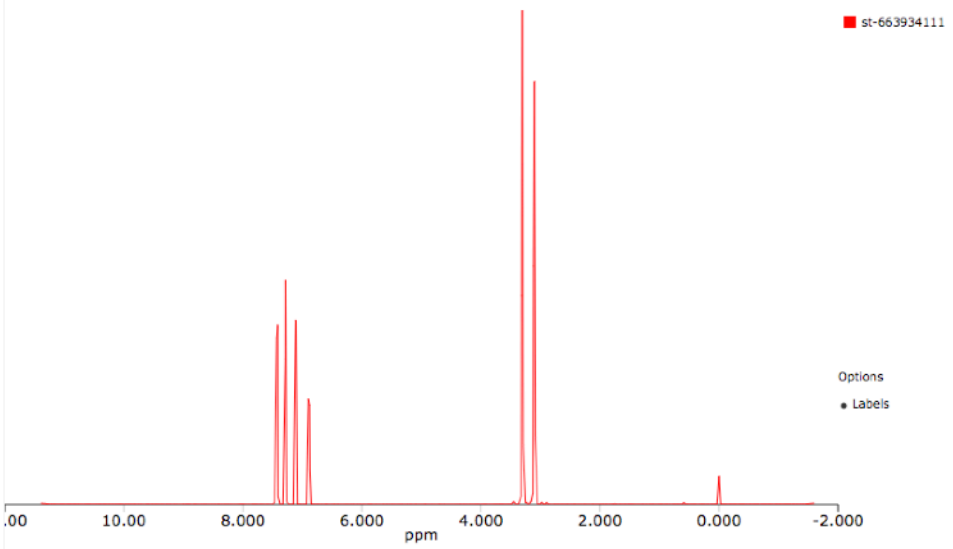
Chemistry | Biology | Pathways | Spectra | Reaction | Literature

NMR Spectra | MS Spectra

Select NMR spectra

BMSE (ID:000757) 1H 500 MHz - pH:7.4

Spectra Viewer



BMSE (ID:000757) 1H 500 MHz - pH:7.4

Species selection page

Find some direct links to some common model organisms and a wider list of all the organisms we have information about.

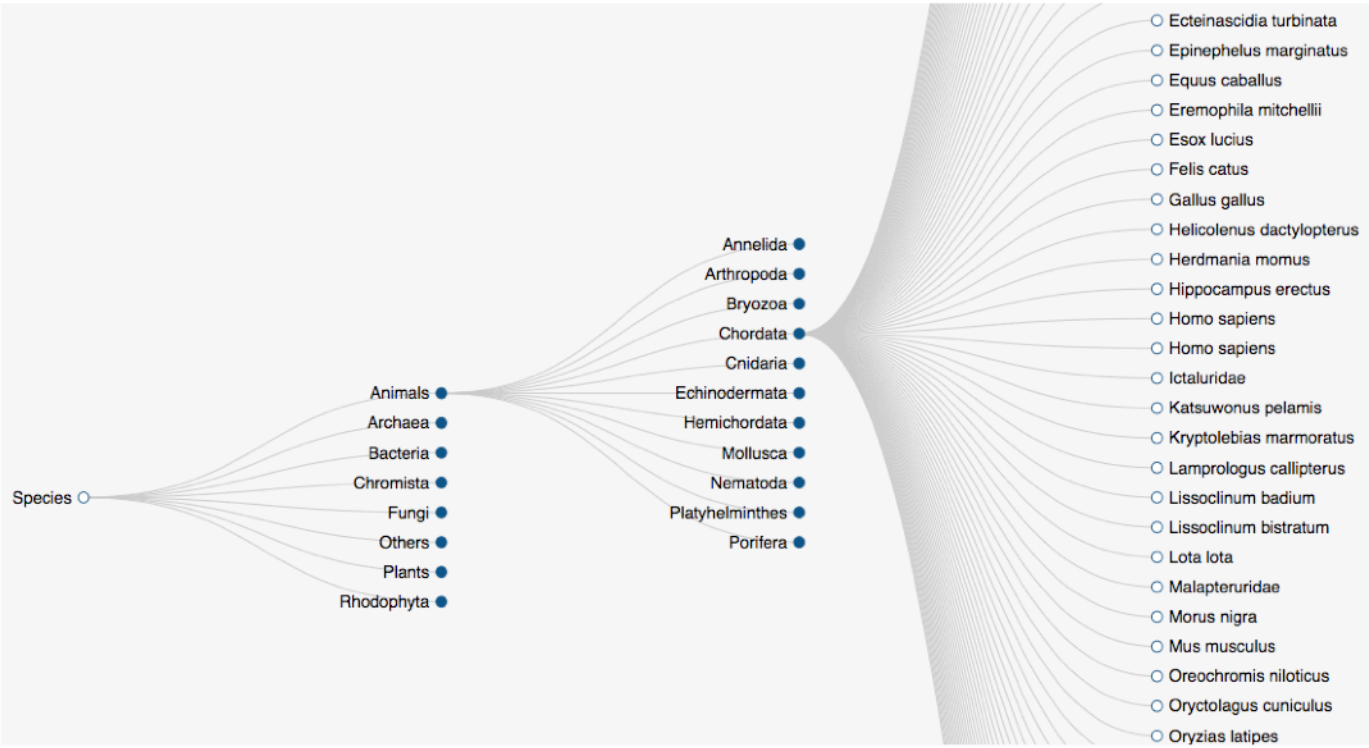
Taxonomy Search

Start typing the first 3 letters of the species name

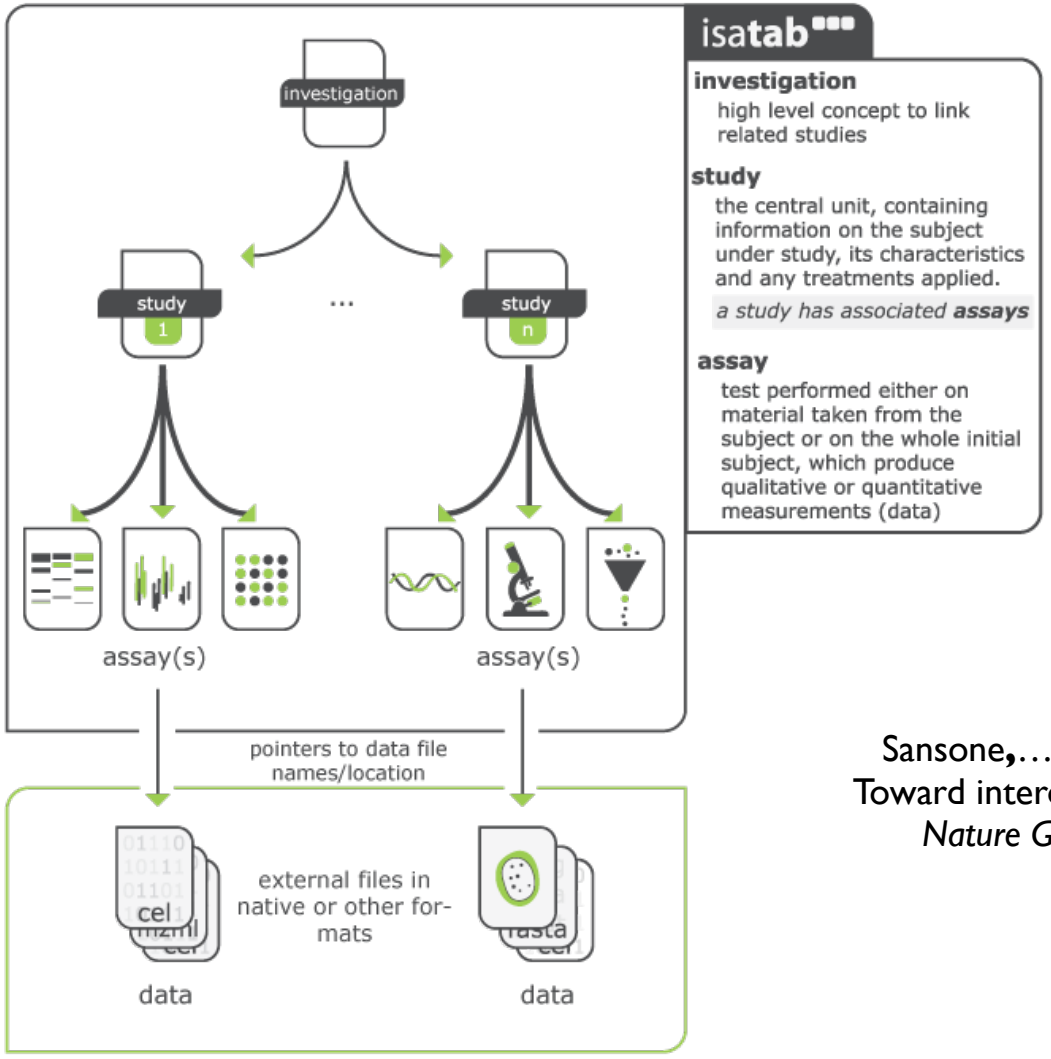
Model organisms

- Homo sapiens (Human)
- Mus musculus (Mouse)
- Arabidopsis thaliana (thale cress)
- Escherichia coli
- Saccharomyces cerevisiae (Baker's yeast)
- Caenorhabditis elegans

Taxonomy Browser (2820 species)

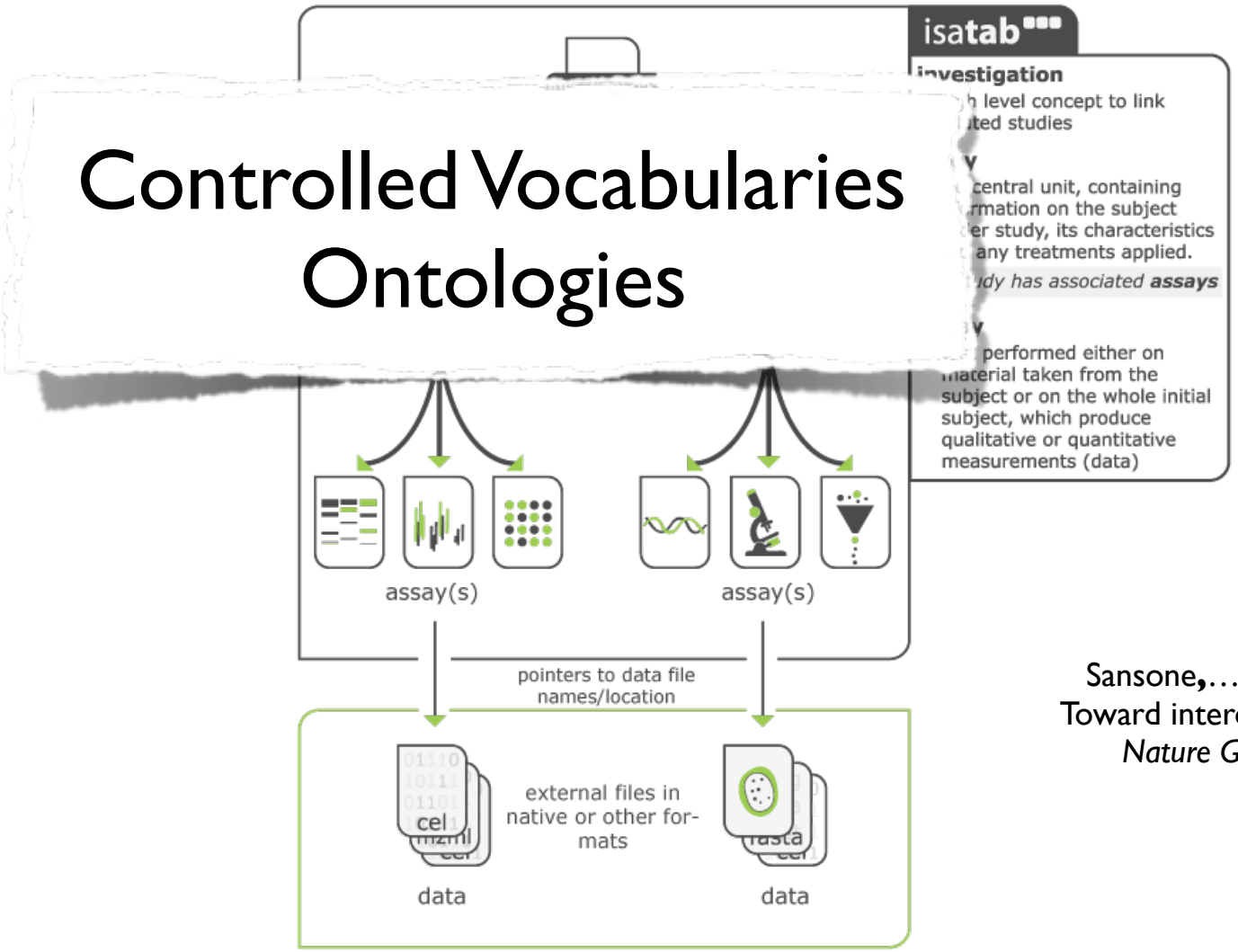


Data Submission to MetaboLights



Sansone, … Steinbeck et al. (2012)
Toward interoperable bioscience data.
Nature Genetics, 44, 121–126.

Data Submission to MetaboLights



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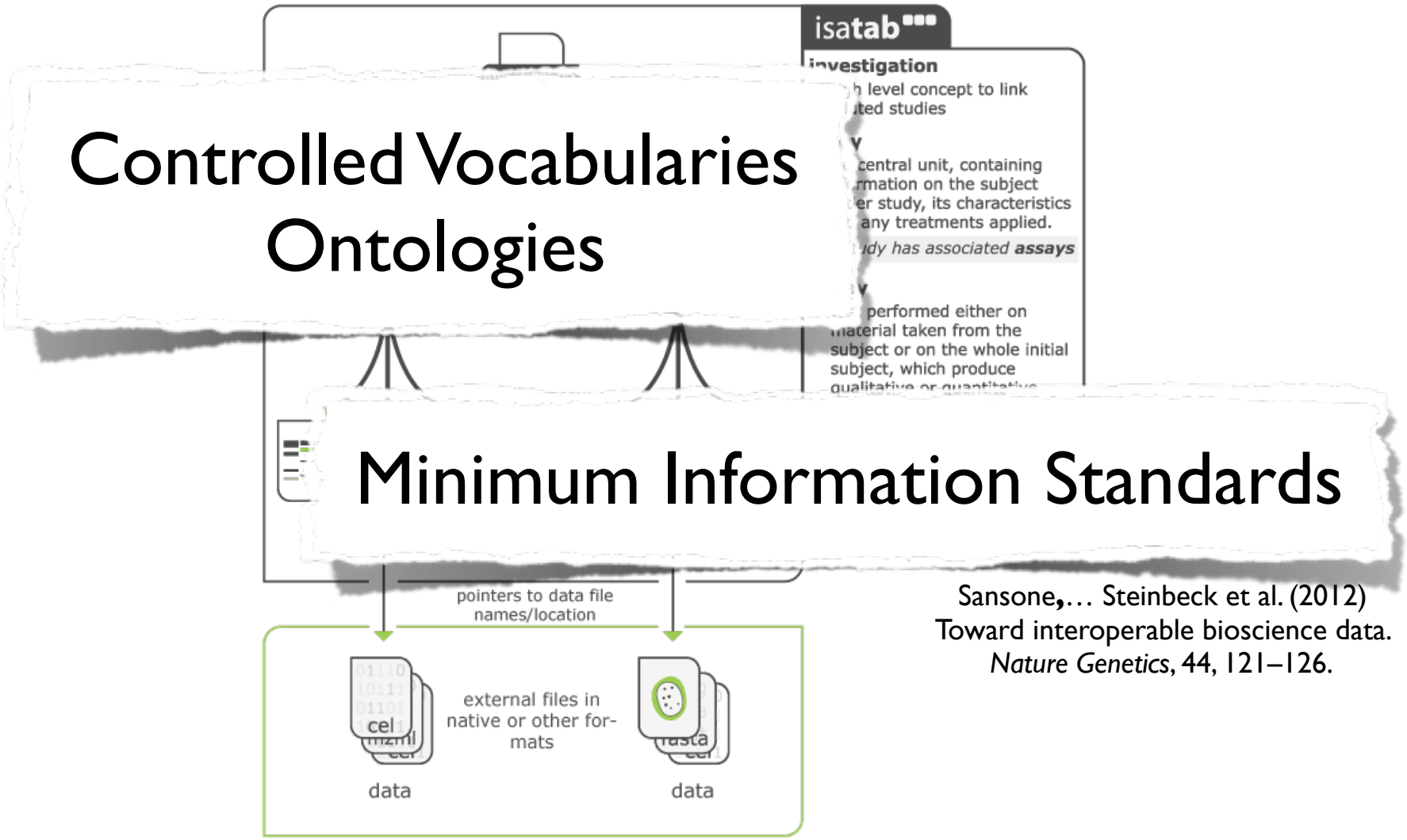


Sansone, … Steinbeck et al. (2012)
Toward interoperable bioscience data.
Nature Genetics, 44, 121–126.

STUDY ASSAYS

add new assay(s)

VIEW

metabolite profiling
NMR spectroscopy
Bruker
a_live_mtbl1_rms_metaboli...

STUDY DESIGN DESCRIPTORS

add a new design column

Field Name	design	design	design	design	design	design
Study Design Type	NCIT:Metabolo...	NCIT:Diabetes...	NCIT:Metabolic...	NCIT:Human S...	Urine global pr...	OBI:NMR spect...

+ New field to design descrip

STUDY PUBLICATIONS

add a new publication column | search for publication

Field Name	publication
Study PubMed ID	17190852
Study Publication DOI	http://dx.doi.or...
Study Publication Author List	Salek RM,Magu...
Study Publication Title	A metabolomic...
Study Publication Status	Published

search ontologies | view history | term definition

Recommended Ontologies | All Ontologies

Search for: diabetes type 2 | search

- MEDLINEPLUS - MedlinePlus Health Topics
- MESH - Medical Subject Headings
  - MESH:Diabetes Mellitus, Type 2
- NATPRO - Natural Products Ontology
- NCIT - National Cancer Institute Thesaurus
- NDFRT - National Drug File - Reference Terminology
- NIFSTD - Neuroscience Information Framework (NIF) Sta
- OMIM - Online Mendelian Inheritance in Man

filter

Term name: Diabetes Mellitus, Type 2

Service Provider: BioPortal

Source: http://data.bioontology.org/ontologies/MESH

definition: A subclass of DIABETES MELLITUS that is not INSULIN-responsive or dependent (NIDDM). It is characterized initially by INSULIN RESISTANCE and HYPERINSULINEMIA; and eventually by GLUCOSE INTOLERANCE; HYPERGLYCEMIA; and overt diabetes. Type II diabetes mellitus is no longer considered a disease

View in resource.

Selected term. (You can also enter freetext here): MESH:Diabetes Mellitus, Type 2 | Select Ontology Term

STUDY FACTORS

add a new factor column | select from previous factors...

Field Name	factor	factor
Study Factor Name	Gender	Metabolic synd...
Study Factor Type	NCIT:Gender	Mellitus, Type 2

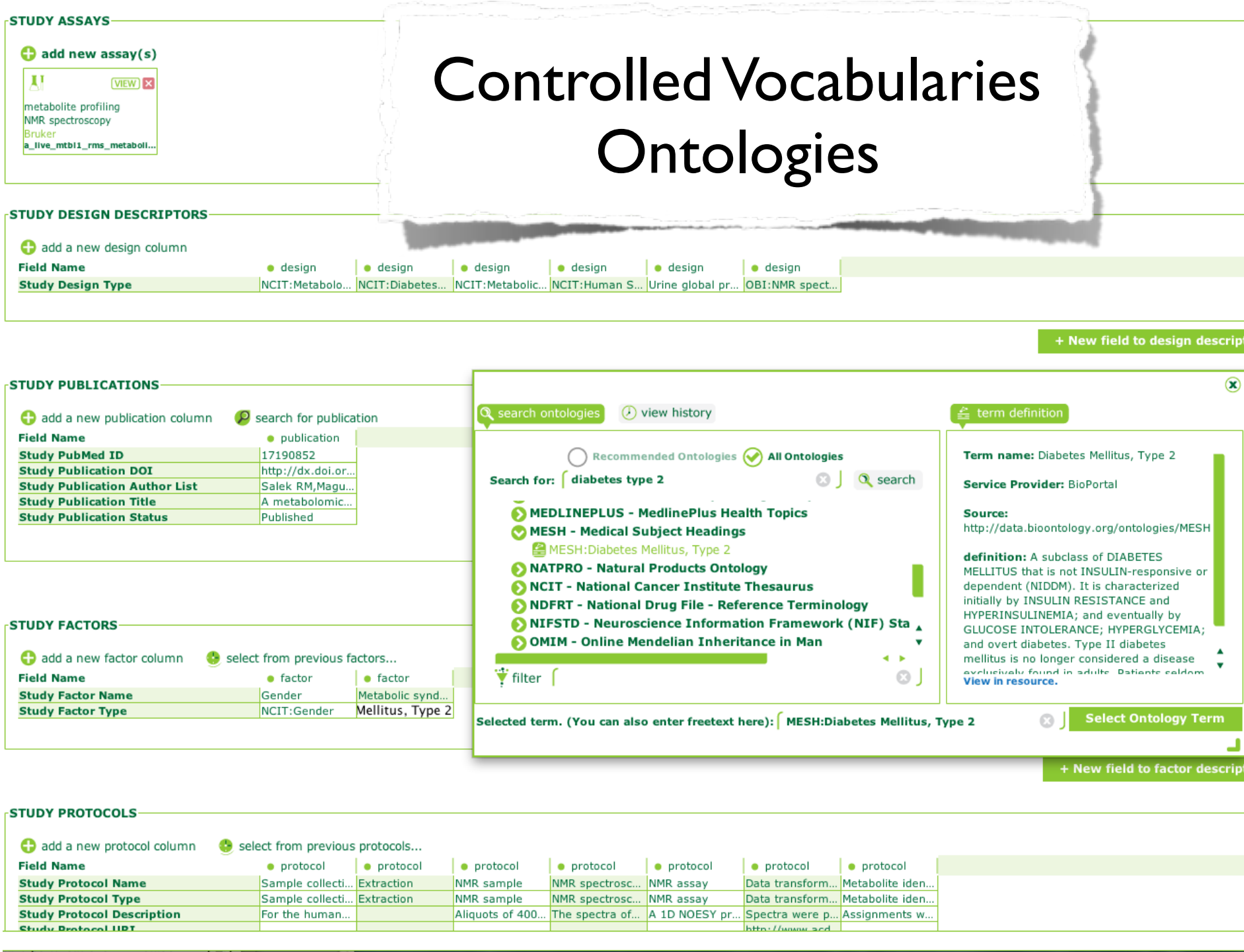
+ New field to factor descrip

STUDY PROTOCOLS

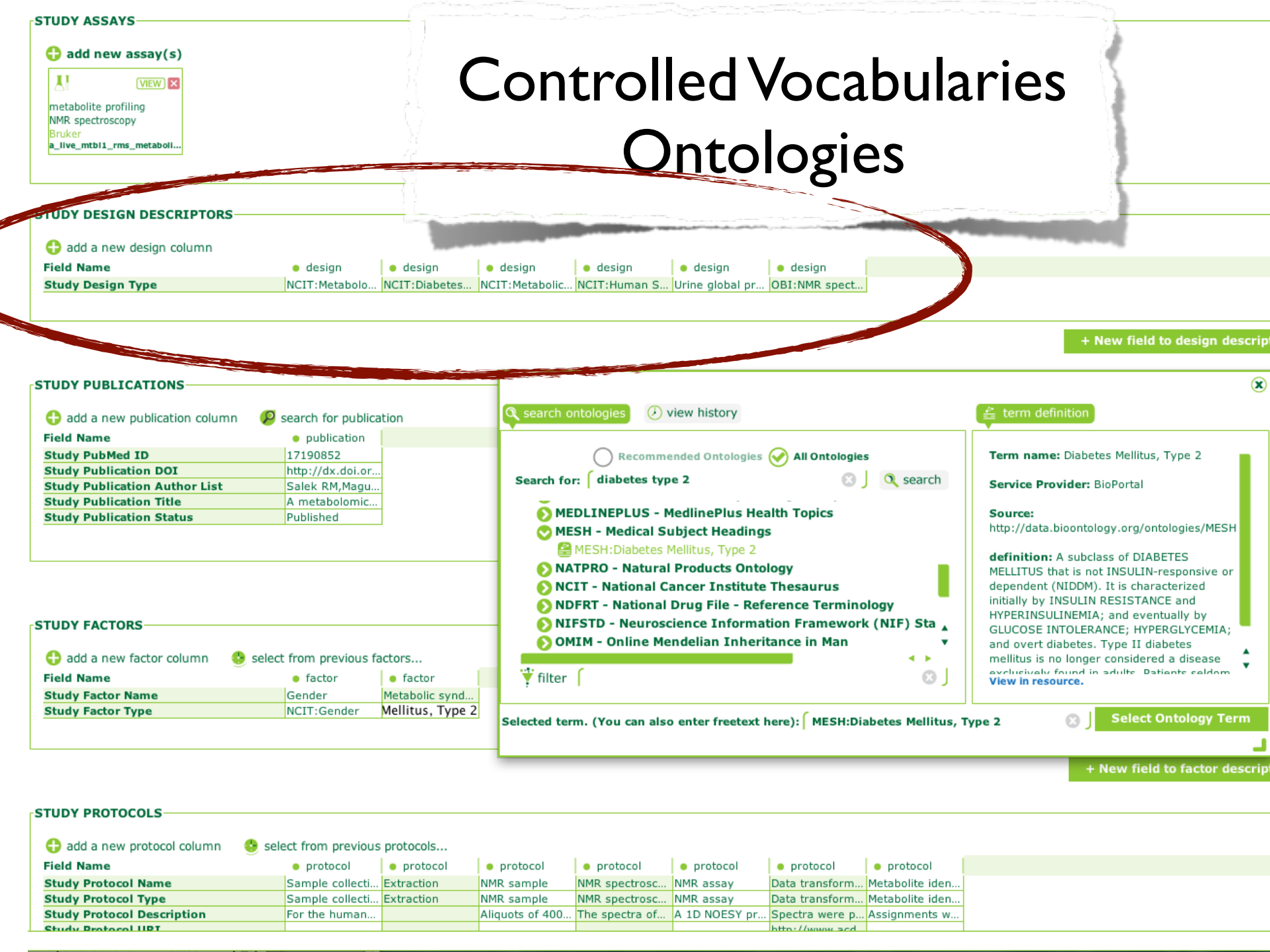
add a new protocol column | select from previous protocols...

Field Name	protocol	protocol	protocol	protocol	protocol	protocol	protocol
Study Protocol Name	Sample collecti...	Extraction	NMR sample	NMR spectrosc...	NMR assay	Data transform...	Metabolite iden...
Study Protocol Type	Sample collecti...	Extraction	NMR sample	NMR spectrosc...	NMR assay	Data transform...	Metabolite iden...
Study Protocol Description	For the human...		Aliquots of 400...	The spectra of...	A 1D NOESY pr...	Spectra were p...	Assignments w...
Study Protocol URI						http://www.acd	

Controlled Vocabularies Ontologies



Controlled Vocabularies Ontologies



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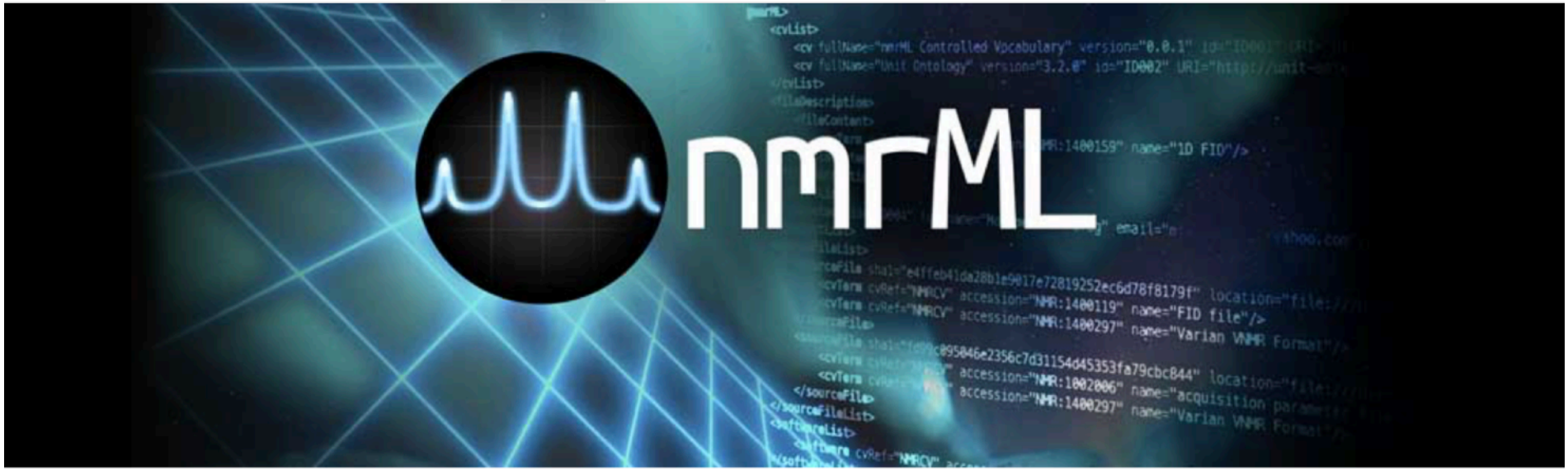

nmrML

nmrML is an open mark-up language for NMR data.

Learn more

View examples

nmrCV

nmrCV is an ontology for describing NMR experiments and acquisitions.

Learn more

Browse ontology

Converter

Use our web application to convert from different NMR data formats, to nmrML.

Convert your data

Validator

Use our web application to validate your nmrML instances.

Validate your data

Takeaways

- Global momentum for sharing raw and curated NMR data
- Open raw meta-data and data formats exist
- Open frameworks for meta-data handling exist
- Technical, chemistry-enabled archive frameworks available
- Editors' buy-in indispensable
- It could start right now (Figshare->DOI->Manuscript)

Stop clinging to your precious …

… and share your chemistry data!