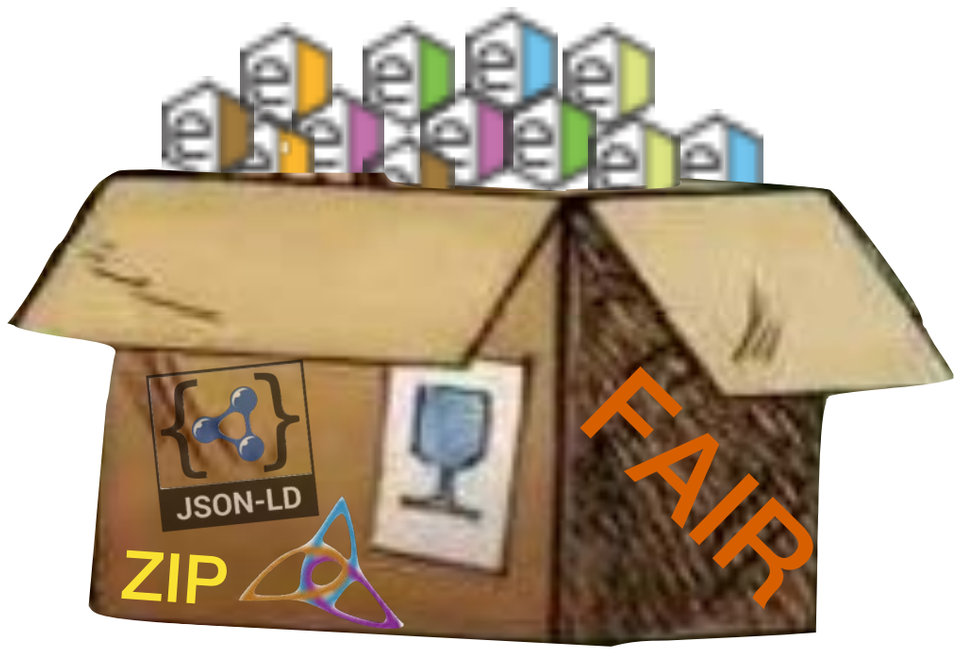
The CHEMeDATA initiative:
A step towards FAIR chemistry data



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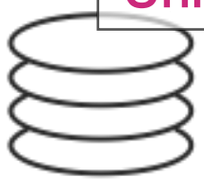
Researchers

University repository



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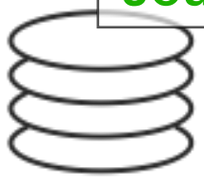

Researchers

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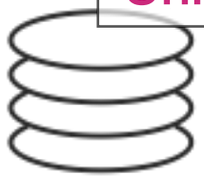

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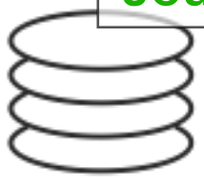

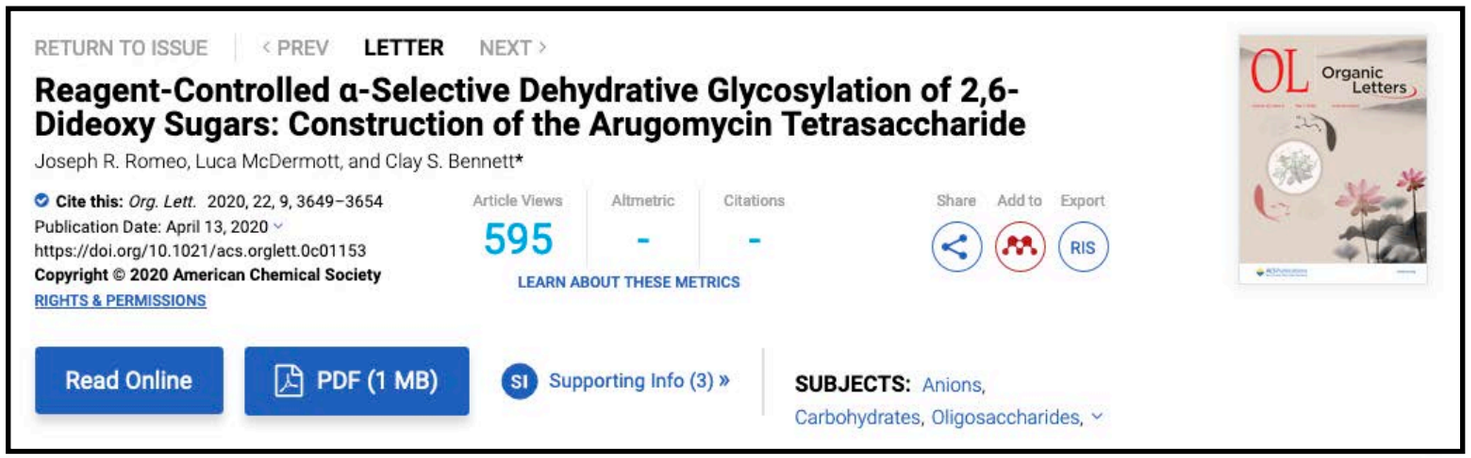
RETURN TO ISSUE | < PREV LETTER NEXT >

Reagent-Controlled α-Selective Dehydrative Glycosylation of 2,6-Dideoxy Sugars: Construction of the Arugomycin Tetrasaccharide

Joseph R. Romeo, Luca McDermott, and Clay S. Bennett*

Cite this: *Org. Lett.* 2020, 22, 9, 3649−3654
Publication Date: April 13, 2020
https://doi.org/10.1021/acs.orglett.0c01153
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SUBJECTS: Anions, Carbohydrates, Oligosaccharides,

OL Organic Letters

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.orglett.0c01153.

- Experimental details and characterization data (PDF)
- FAIR data, including the primary NMR FID files, for compounds **1**−**10** (ZIP)
- FAIR data, including the primary NMR FID files, for compounds **11**−**17**, **S3**, **S5**, and **S8** (ZIP)


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Journal publishers


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J'ESPÈRE QU'IL FAIT UN EFFORT POUR SES RANGEMENTS !... LA DERNIÈRE FOIS QUE J'AI OUVERT CETTE ARMOIRE, J'AI PRIS TOUT LE CONTENU...
ZIP


...SUR LA FIGURE !
BRRROMM
POUF
?!
ORROLOM
BRROM

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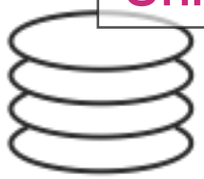

Journal publishers

File Information Tool Set (FITS)

Documentation and official code releases of the FITS and the FITS Web Service projects

Contact


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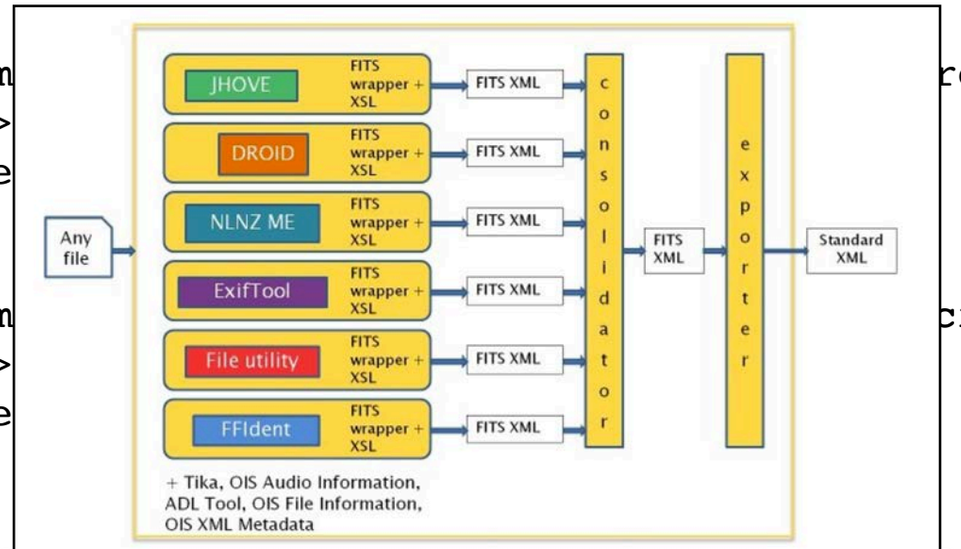
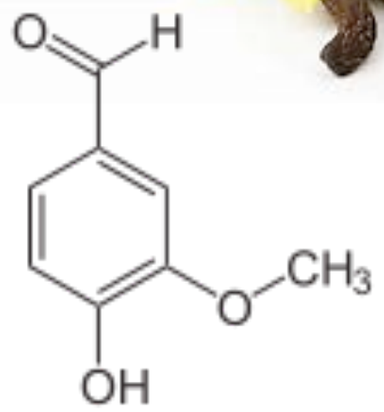
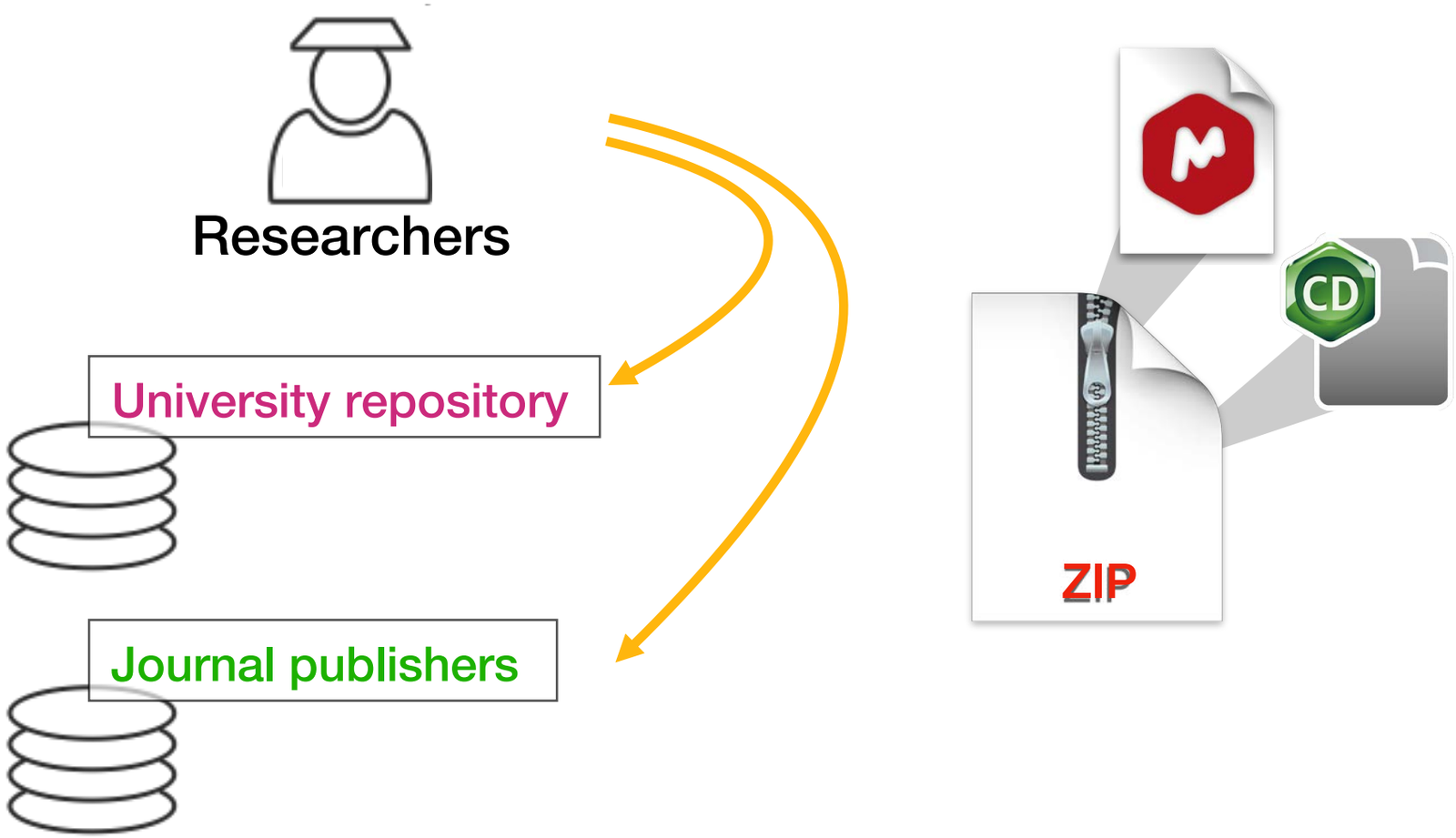


Structure determination by Nuclear Magnetic Resonnace

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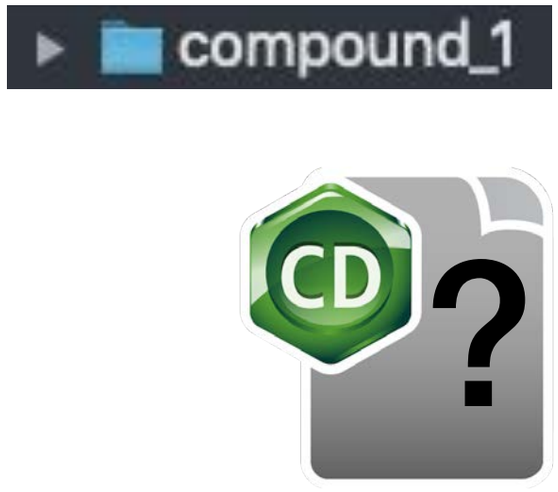
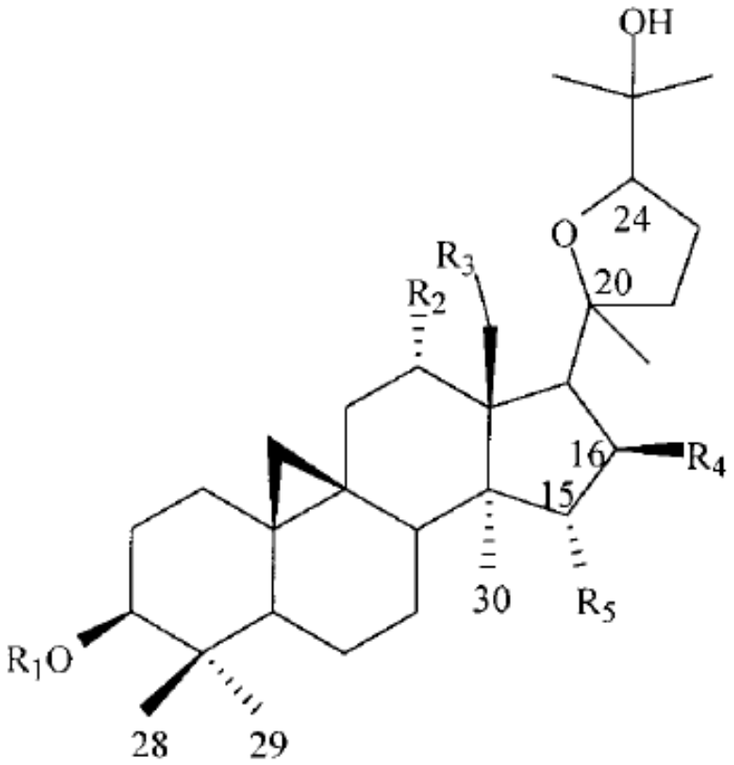

compound_1
CD
?

7.37
7.37
7.35
7.35
7.32
7.31
6.90
6.88
4.66
3.77
5 (d)
7.32
1 (dd)
7.36
2 (d)
6.89
9
9 (s)
3.77
6
5
1
2
1.00
1.03
1.00
0.99
3.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
f1 (ppm)

Chart 1

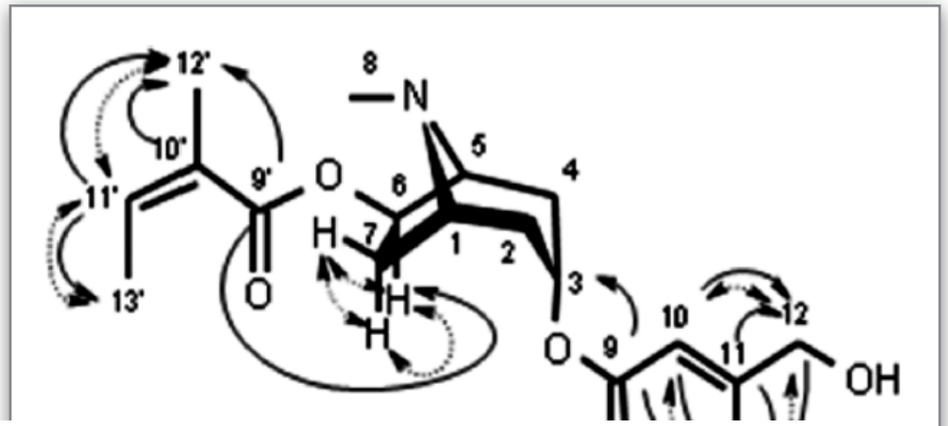


	R_1	R_2	R_3	R_4	R_5
1	Glc	H	OH	OH	H
2	Glc (1→6) glc	H	OH	OH	H
3	Xyl	H	OH	OAc	OAc
6	Xyl	H	H	OH	OAc
7	Xyl	OH	H	OH	OH

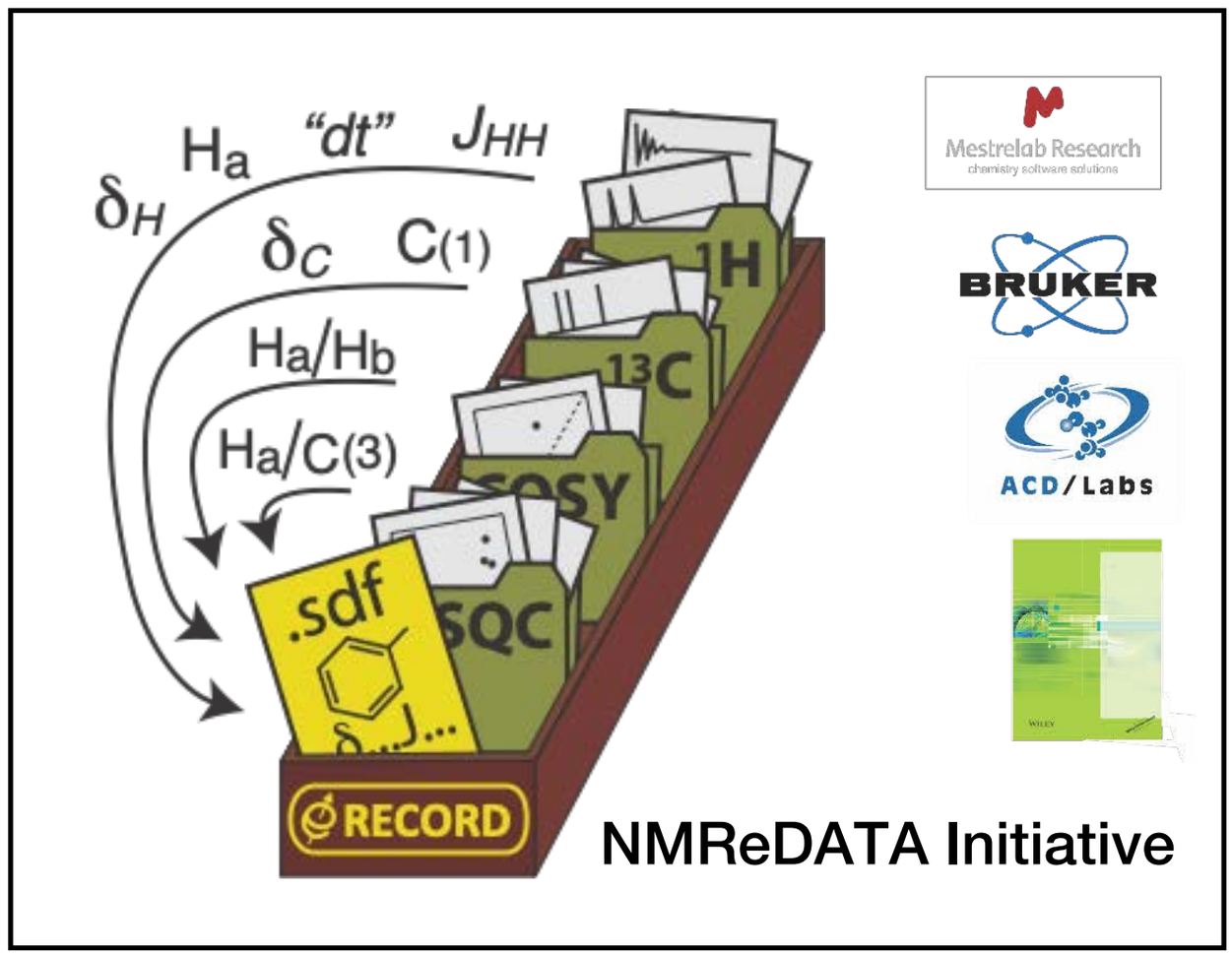
Table 1. NMR Spectroscopic Data (500 MHz, CD_3OD, δ in ppm) for Compounds **1**–**3** Obtained Using Capillary NMR

	1		**2**		**3**	
position	δ_C[a]	δ_H	δ_C[a]	δ_H	δ_C[a]	δ_H
1	61.4 CH	3.76 s	61.9	3.92 s	60.0[c]	4.02 s
2	33.7 CH_{endo}	2.34 s	33.4	2.39 br s		2.43 br s
	CH_{exo}	1.94 s		2.02 s		2.29–2.31 br s
3	64.3 CH	5.08, s	63.8	5.10 s	62.5[a]	5.14 s
4	32.3 CH_{endo}	2.38 br s	31.9	2.43 br s		
	CH_{exo}	2.14 s		2.22 s		
5	66.9 CH	3.63 s	67.4	3.79 s	66.0[c]	
6	76.5 CH	5.64 s	74.8	5.62 s	78.0[a]	
7	34.2 CH_{endo}	2.83 br s	34.3	2.88 s		
	CH_{exo}	2.38 br s		2.36 br s		
8	39.0 CH_3N	2.77 s	38.5	2.88 s	38.5[a]	
9	165.5[b] qC		165.5[b]			
10	112.4 CH	6.05 s	112.3	6.05 s	119.5[c]	
11	160.5[c] qC		160.7[c]		154.0[c]	
12	65.9 CH_2	4.10 s	65.8	4.11 s	174.0[c]	
	OH	3.33 s		3.36 s		
13	14.6 CH_3	2.11 s	14.7	2.11 s	14.6[a]	
9′	167.4[c] qC		166.3[b]		178.5[c]	
10′	127.3[c] qC/CH		114.8	5.74 s	115.5[c]	
11′	139.0 CH/qC	6.19 s	159.3[c]		157.0[a,c]	
12′	19.4 CH_3	1.91 s	19.3	2.19 s	19.0[c]	
13′	26.1 CH_3	2.01 s	26.3	1.95 s	26.2[c]	

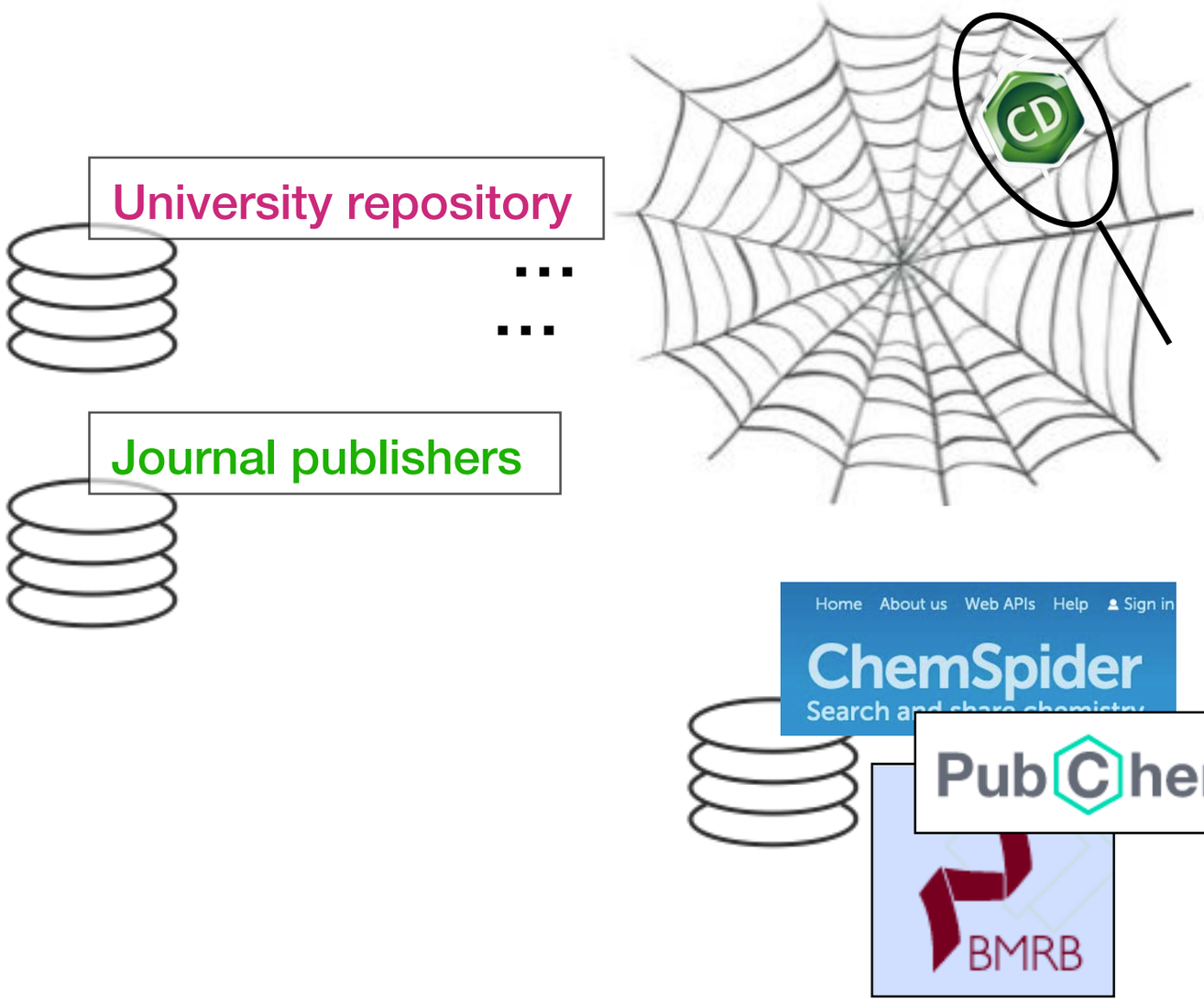
[a] Based on HSQC. [b] Based on standard ^{13}C NMR spec
$CDCl_3$ for the isomer mixture (isomer subfraction). [c] Bas

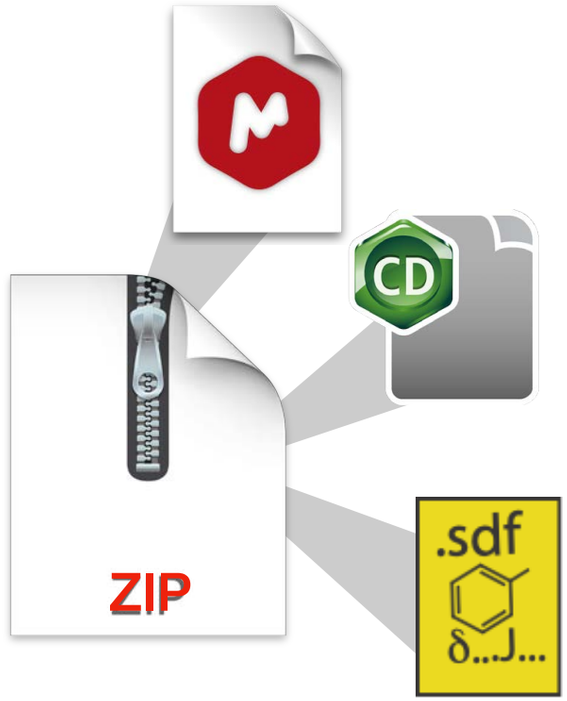


e (1): color-
(log ε) 220
92.4; EIMS
8 (12), 122
m/z 256 (62),
$/z$ 338.1973

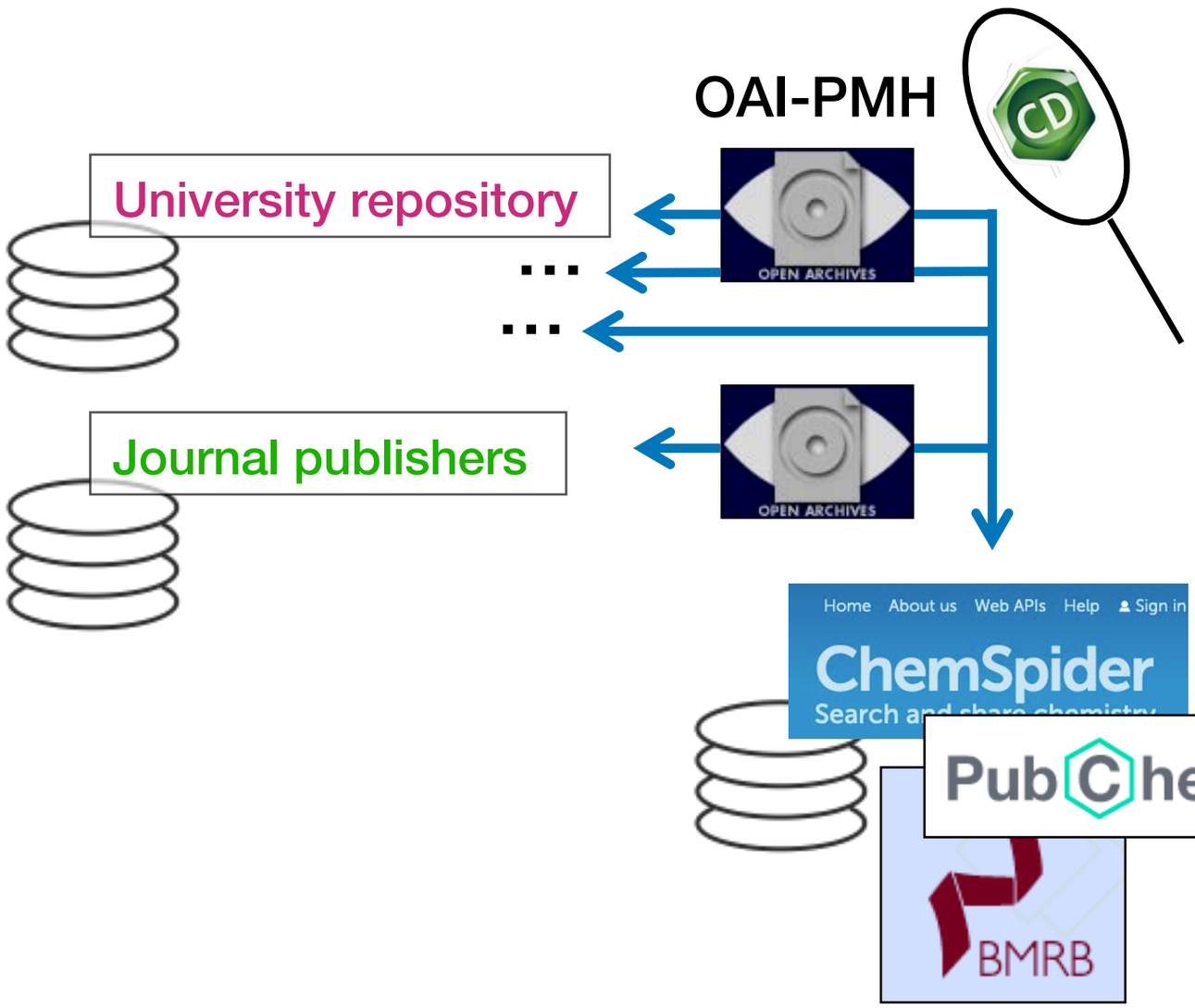


How can specialized databases find relevant data?





Tool facilitating harvesting in database using OAI-PMH



The Open Archives Initiative Protocol for Metadata Harvesting

Protocol Version 2.0 of 2002-06-14
Document Version 2015-01-08
http://www.openarchives.org/OAI/2.0/openarchivesprotocol.htm

Previous protocol version: Protocol Version 1.1 of 2001-07-02
Instructions for migrating from Version 1.1 to 2.0
Implementation Guidelines

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

PROJECT DETAILS

DEVELOPMENT OF A STANDARD FOR FAIR DATA MANAGEMENT OF SPECTROSCOPIC DATA

Project No.:	2019-031-1-024
Start Date:	18 March 2020
End Date:	
Division Name:	Committee on Publications and Cheminformatics Data Standards
Division No.:	024

TASK GROUP CHAIR

Robert M. Hanson
Damien Jeannerat

MEMBERS

Mark Archibald
Ian Bruno
Stuart Chalk
Antony Davies
Jeffrey Lang
Henry Rzepa

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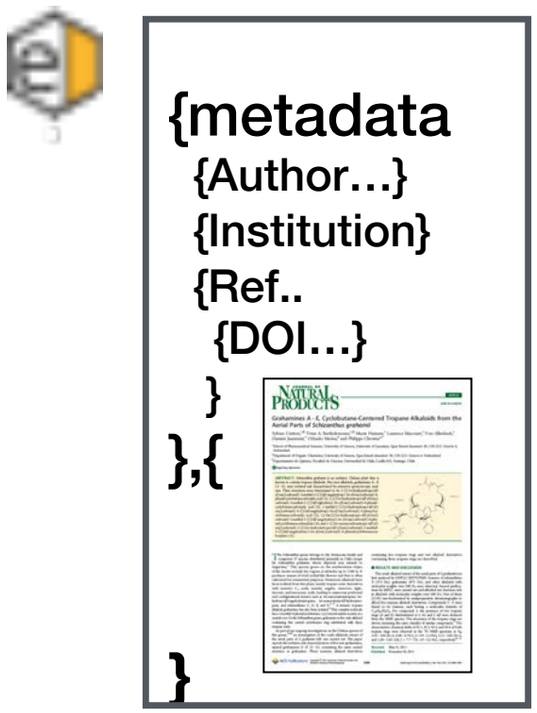
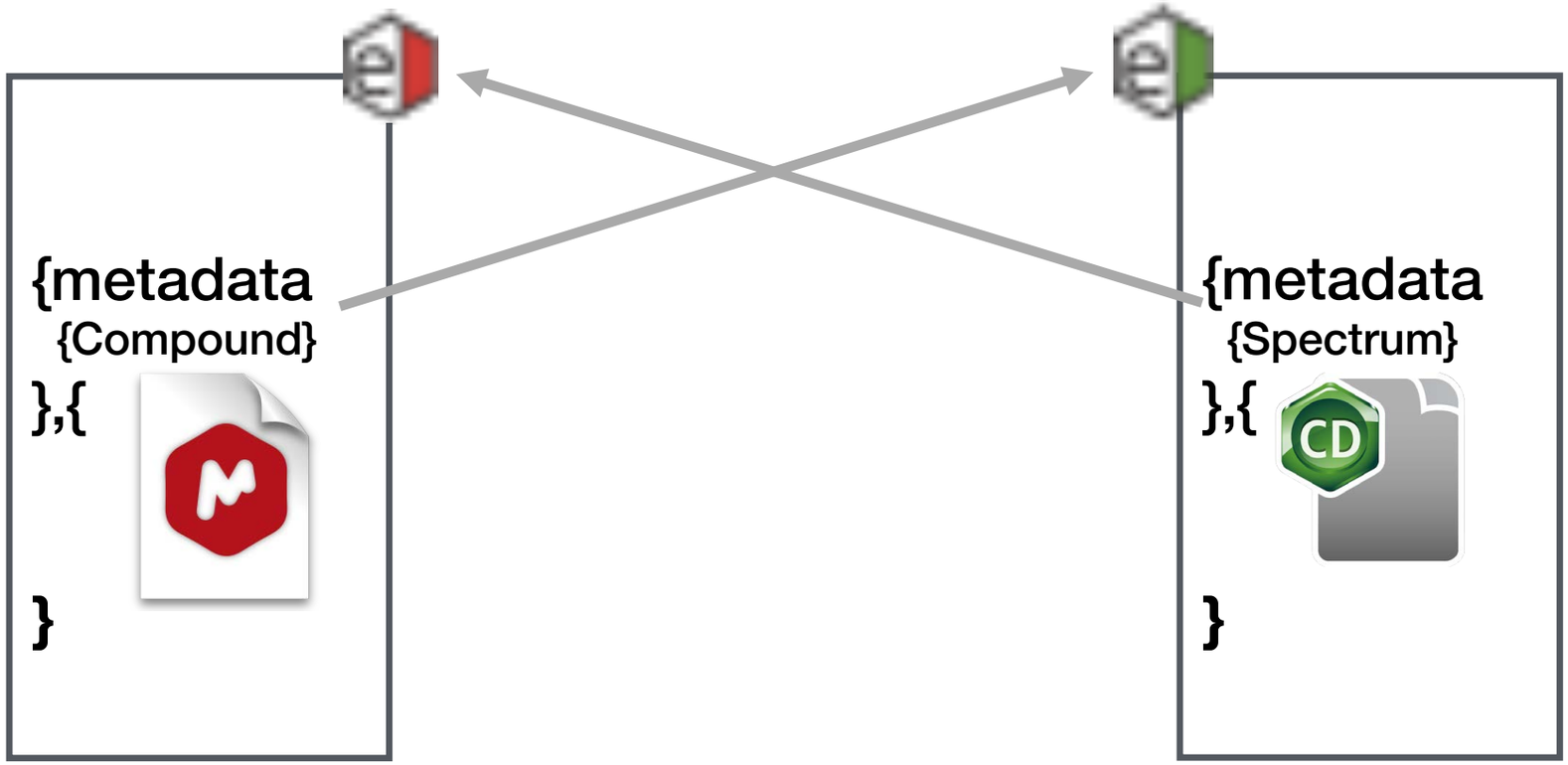
Digital entities and digital identifyers

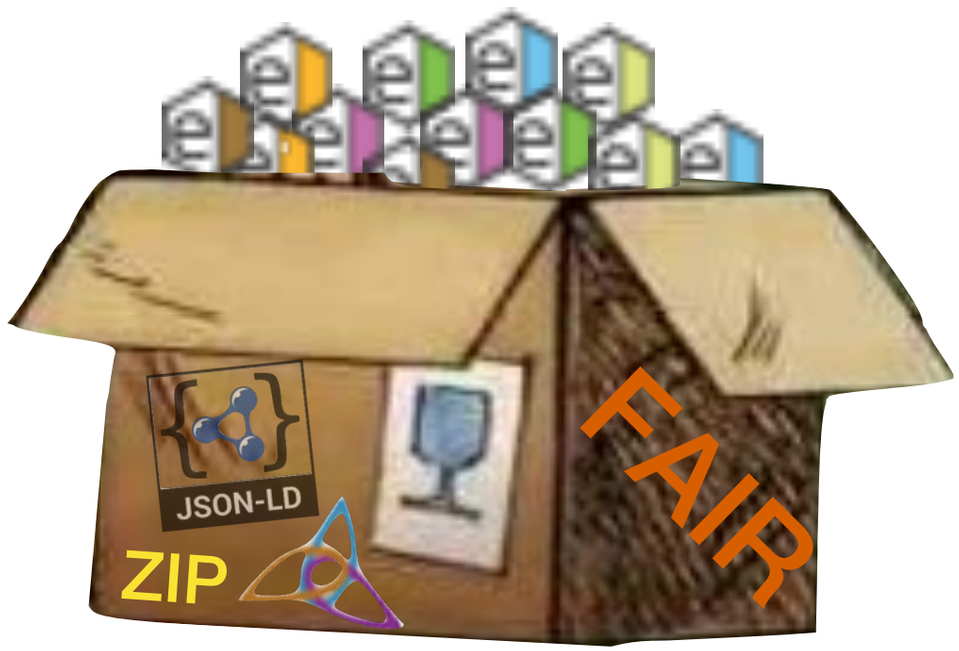
Books (ISBN)
Articles (DOI)

Other data …





The CHEMeDATA initiative:
A step towards FAIR chemistry data

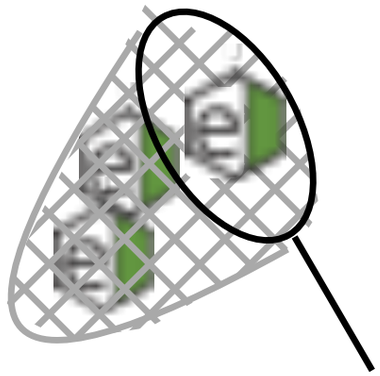


Dr. Damien Jeannerat

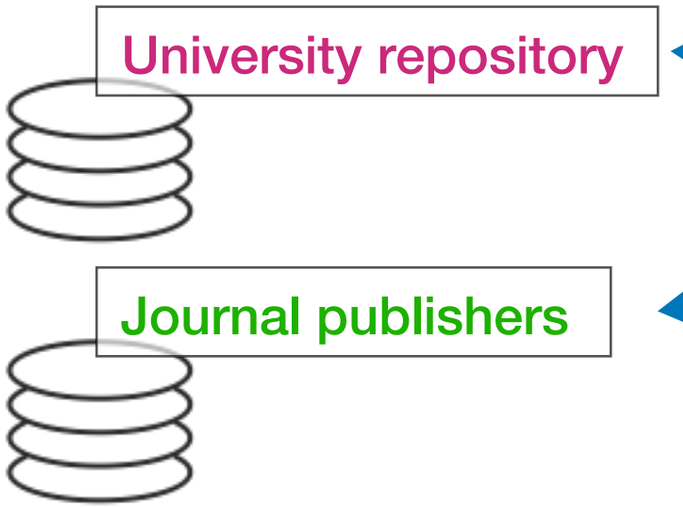
e-Research group / DLCM

CHEMeDATA

1) ***Define*** chemistry objects
2) ***Find*** them in repositories (to visualize…)
3) Convert them into ***open formats***
4) ***Registry*** of chemistry data
5) ***Web platform*** for crowd-sourced generation and curation of chemistry data



FAIR



IUPAC

Bob Hanson
Leah McEwen
Greg Banik
Dave Davidson …

Programmers

Angel Herraez
Julien Wist
Luc Patiny …

NMReDATA

Nils Schlörer
Stefan Kuhn
Jean-Marc Nuzillard
… *+ many more*

Paul Trevorrow (Wiley)

e-Research

Pierre-Yves Burgi
Hughues Cazeaux
… and DLCM/e-research team

Recommendation

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

FAIR Chemical Data
Publishing Guidelines Workshop
Chemical Structures and Spectra

NSF OAC – Award No. 1838958
1838960

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