A scientific exploitation of FAIR NMR data associated with the mechanism of catalytic amidation reactions using boron reagents

The scenario: The topic is catalytic amidation reactions using boron containing reagents, and the study of the kinetics and mechanism using ^{11}B NMR. The ^{11}B nucleus is very broad and the spectrum often very noisy. Establishing an accurate chemical shift requires careful adjustment of the acquisition parameters. Being able to inspect these parameters and if necessary apply different, perchance better weighting functions to the FID is an important aspect of ^{11}B NMR analysis which requires access to the raw data files.

Initial Lead Discovery: In this example, the lead discovery is initiated directly from the metadata registered for data (rather than for a journal article) *via* the following sequence, which gradually becomes more specific.

1. Search query	Hits	Comment
https://commons.datacite.org/?query=titles.title:*amidation*	161	Keyword in title
https://commons.datacite.org/?query=titles.title:*amidation*+AND+titles.title:*catalytic*	2	Specific title
https://commons.datacite.org/?query=titles.title:*boron*+AND+titles.title:*catalysed*	20	Alternative keywords
hhttps://commons.datacite.org/?query=descriptions.description:*NMR*	17,978	General search for NMR
https://commons.datacite.org/?query=titles.title:*boron*+AND+titles.title:*catalysed*+AND+titles.title:*NMR*	1	NMR in title
Possible Discovery lead: 10.14469/hpc/2247		
https://commons.datacite.org/?query=subjects.subjectScheme:inchi+AND+subjects.subject:*C20H14B3F9N2O3*	1	Molecular formula
https://commons.datacite.org/?query=subjects.subjectScheme:inchikey+AND+subjects.subject:*BHYQUOWHUMNGMD-UHFFFAOYSA-N*	1	InChIkey
https://commons.datacite.org/?query=subjects.subjectScheme:inchikey+AND+subjects.subject:*BHYQUOWHUMNGMD-UHFFFAOYSA-N*+AND+descriptions.description:*11B*	1	InChI and Nucleus
https://commons.datacite.org/?query=media.media_type:chemical/x-mnpub*+AND+subjects.subjectScheme:inchikey+AND+subjects.subject:*BHYQUOWHUMNGMD-UHFFFAOYSA-N*+AND+descriptions.description:*11B*	1	Constrained for Raw NMR data
Discovery lead:**10.14469/hpc/2365**		

Metadata found for Hit:

The metadata for the final hit is displayed on the "landing page" for the hit and can be obtained in machine form as::

https://data.datacite.org/application/vnd.datacite.datacite+xml/10.14469/hpc/2365

Keyword	Value
inchi	InChI=1S/C20H14B3F9N2O3/c24-12-3-9(4-13(25)18(12)30)21-35-22(10-5-14(26)19(31)15(27)6-10)37-23(36-21,34-2-1-33)11-7-16(28)20(32)17(29)8-11/h3-8H,1-2,33-34H2/q-1
inchikey	BHYQUOWHUMNGMD-UHFFFAOYSA-N
NMR_Nucleus	11B
NMR_Pulse	1D
NMR_Solvent	CDCl3

NMR_temperature	298

Member of collection / collaboration	
DOI	**Description**
10.14469/hpc/2247	A mechanistic insight into the boron-catalysed direct amidation reaction. NMR spectra.

Member of collection / collaboration	
10.14469/hpc/1620	A mechanistic insight into the boron-catalysed direct amidation reaction

Associated DOIs		
Current dataset ...	**DOI**	**Description**
References	10.1021/acscatal.8b01708	Article: Extracting Knowledge from Data through Catalysis Informatics
References	10.1039/C7SC03595K	Article: Mechanistic insights into boron-catalysed direct amidation reactions
References	10.1021/acs.joc.8b00859	Article: An accessible Method for DFT Calculation of 11B NMR Shifts of Organoboron Compounds

Following the last of these discovery leads cites further data as Ref 16: 10.14469/hpc/3702 and the process can cycle again. In this example, this leads to data relating to the computational calculation of ^{11}B shifts using a quantum DFT based procedure, which provides a new entry point for ^{11}B NMR.

Summary

This example introduces an expanded metadata section introducing specific NMR parameters such as nucleus, solvent, pulse sequence, temperature etc (red text above). It is a very early implementation of this aspect and must now be regarded as obsolete, but it serves the purpose of illustrating how metadata might be used to locate raw NMR data with very specific characteristics.