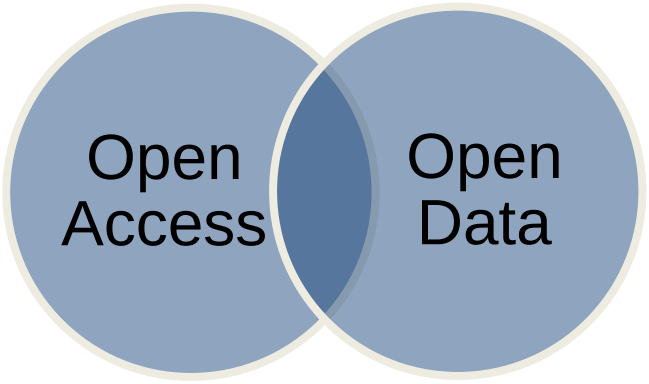
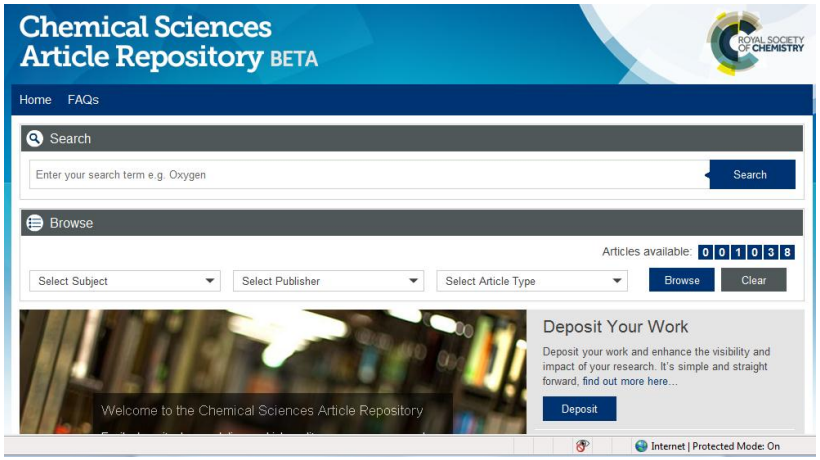
The Royal Society of Chemistry: Research Data and Community Initiatives

Serin Dabb
Executive Editor, Data

dabbs@rsc.org
@SerinDabb

- Literature alerting services
- Recently acquired ***MarinLit***
- **The Merck Index* *Online***





CDS National Chemical Database Service

ChemSpider
Search and share chemistry

Today

1. National Chemical Database Service
2. ChemSpider
3. Data Repository (in progress)
4. Data mining of Royal Society of Chemistry publications (in progress)

National Chemical Database Service

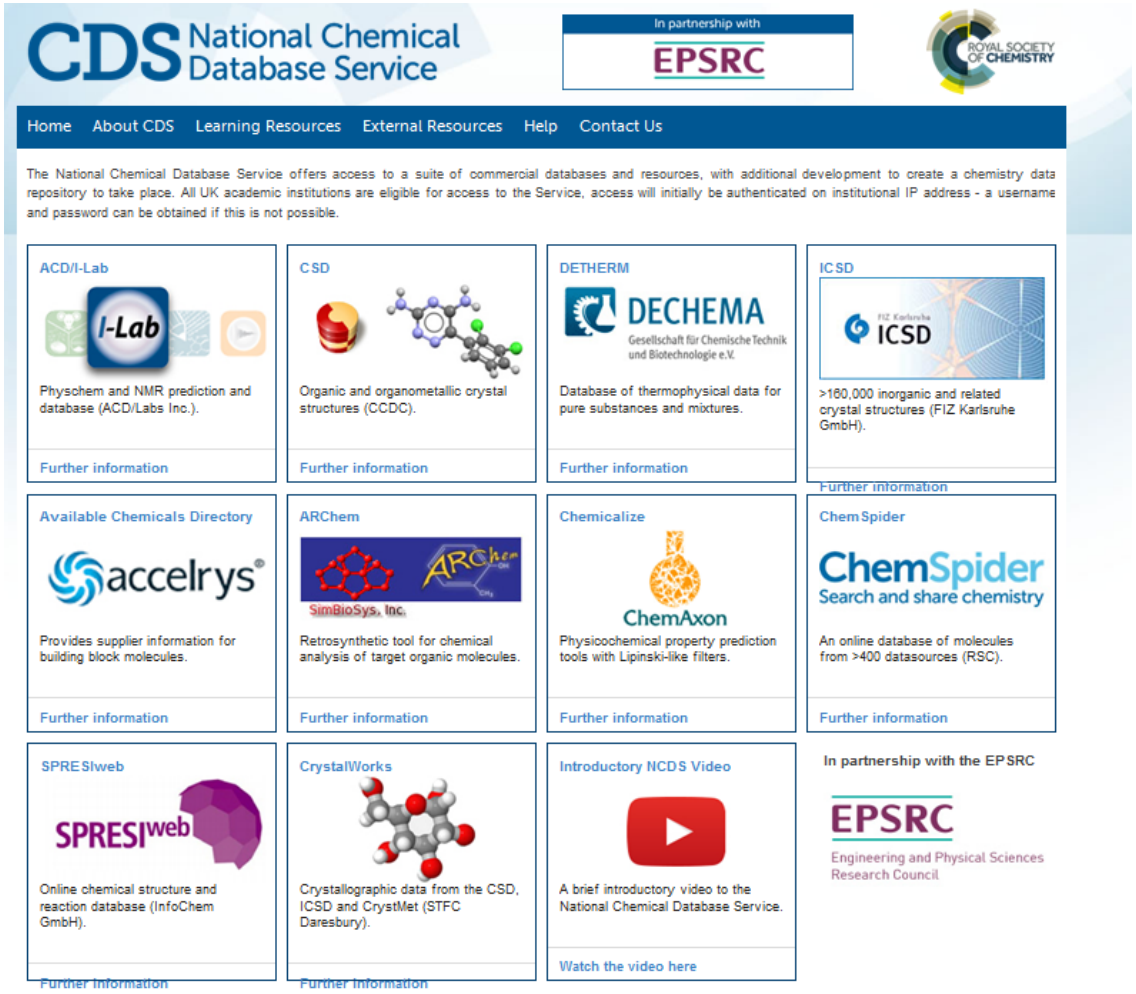
- An online collection of scientific resources and databases
- Hosted by the RSC,

 - funded by the EPSRC

Free for all UK academia

http://cds.rsc.org

@cds_rsc



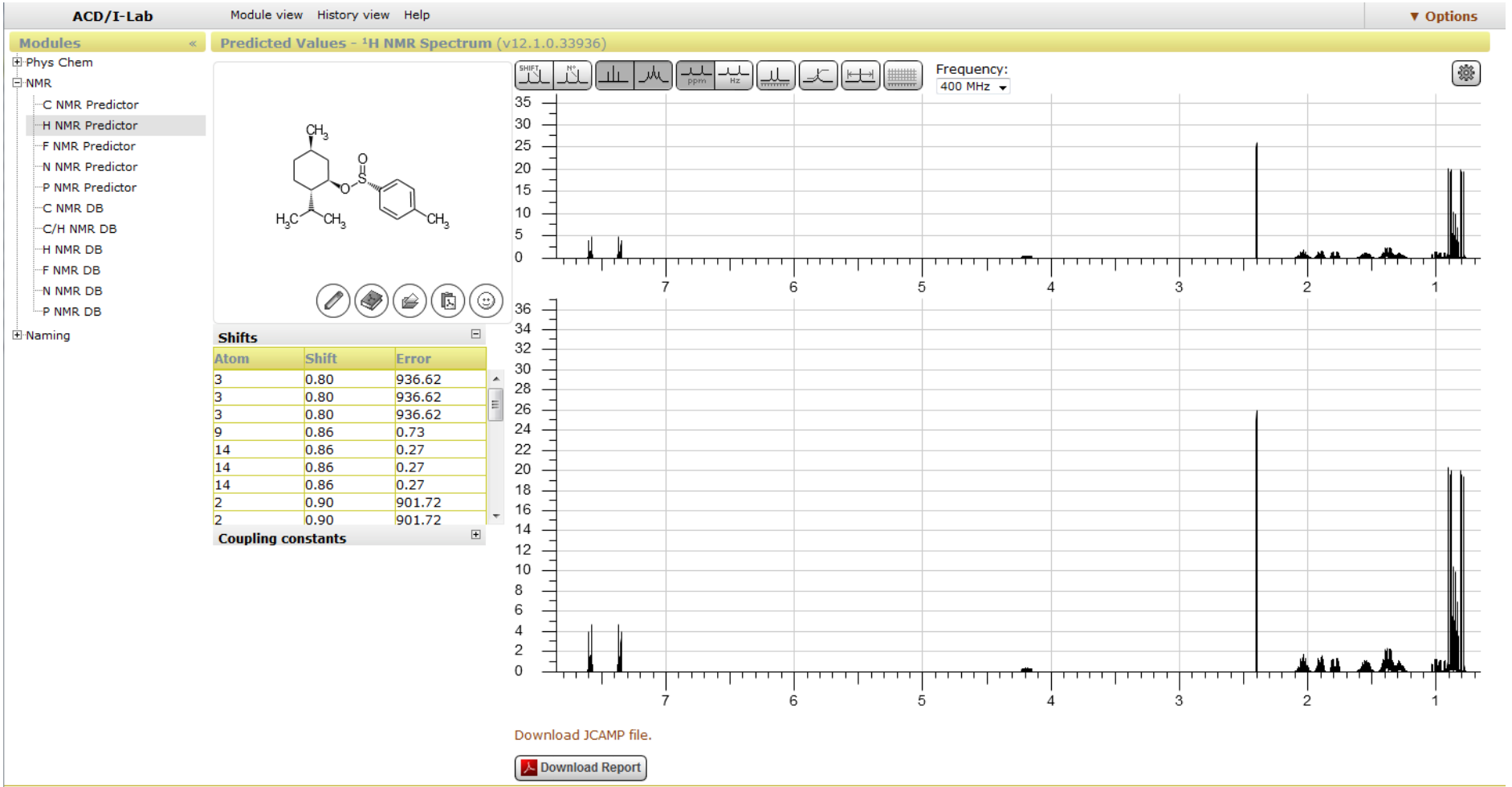
Predicts physicochemical properties, NMR spectra and chemical shifts

Also assesses prediction reliability and includes searchable content databases.

ACD/I-Lab

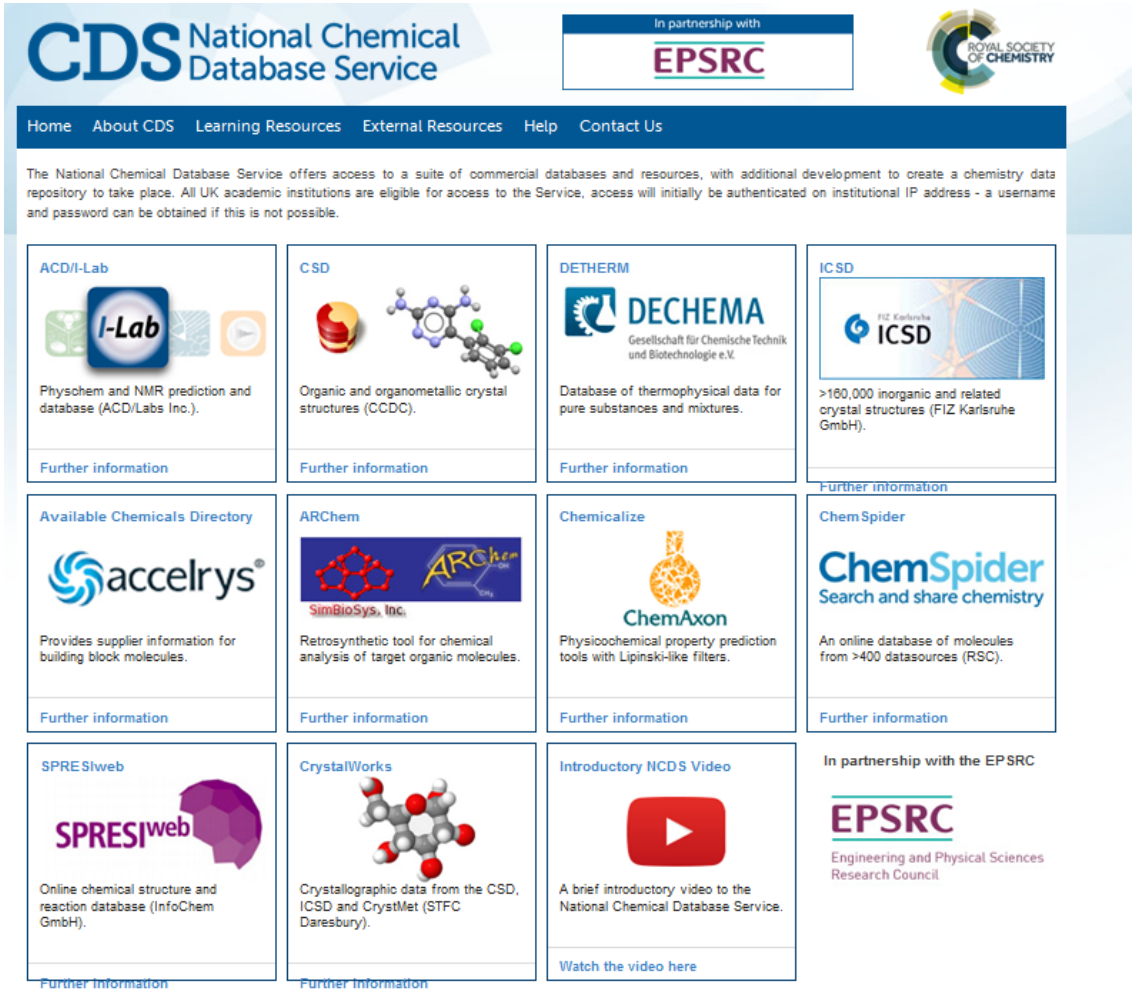
Physchem and NMR prediction and database (ACD/Labs Inc.).

Further information



Learning materials:
Videos
Factsheets
Worked examples

National Chemical Database Service



…..AND

A data repository for the UK academic community

New data policies

EPSRC-funded research data is a public good produced in the public interest and should be made freely and openly available with as few restrictions as possible in a timely and responsible manner.

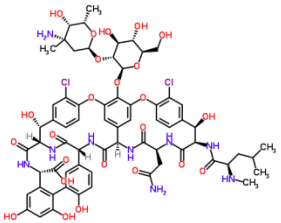
Institutional and project specific data management policies and plans should be in accordance with relevant standards and community best practice and should exist for all data. Data with acknowledged long term value should be preserved and remain accessible and useable for future research

EPSRC Policy Framework on Research Data

EPSRC

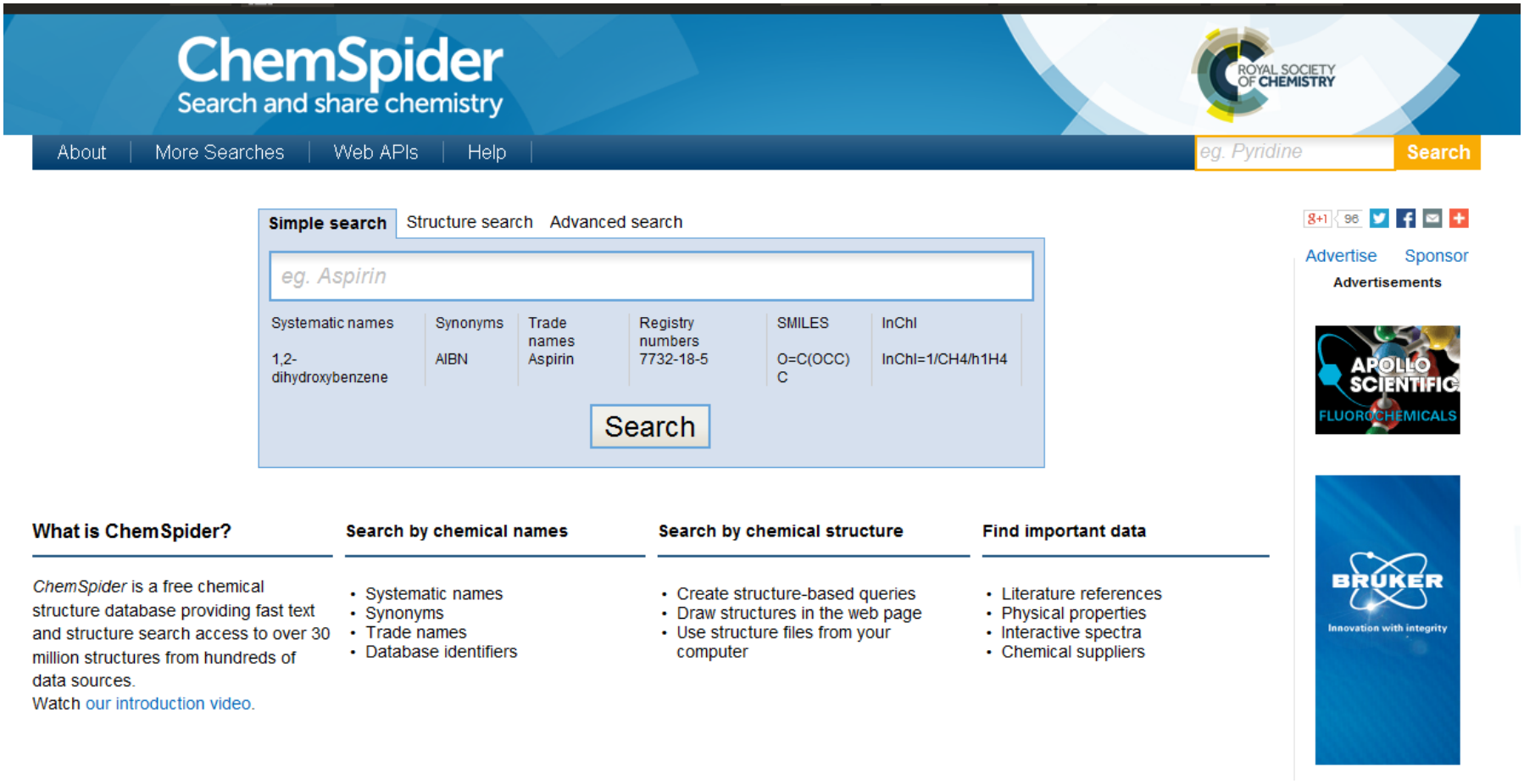
Engineering and Physical Sciences Research Council

ChemSpider
Search and share chemistry

Google + Wikipedia The Free Encyclopedia +  = Free to use

- 28 million structures
- Over 400 different data sources, including:
  - PubChem, ChEBI
  - GSK Malarial compounds
  - Chemical Suppliers Catalogues
  - Patents
  - RSC journals
- Physical properties, spectra, safety information and much more
- Access it anywhere there's internet

www.chemspider.com/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Search
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Structure search
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eg. Aspirin
Systematic names
1,2-dihydroxybenzene
Synonyms
AIBN
Trade names
Aspirin
Registry numbers
7732-18-5
SMILES
O=C(OCC)C
InChI
InChI=1/CH4/h1H4
Search
What is ChemSpider?
ChemSpider is a free chemical structure database providing fast text and structure search access to over 30 million structures from hundreds of data sources.
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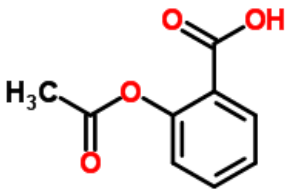

Cell 2D 3D Save Zoom

Aspirin

ChemSpider ID: **2157**

Molecular Formula: $C_9H_8O_4$

Average mass: 180.157394 Da

Monoisotopic mass: 180.042252 Da

▼ Systematic name

2-Acetoxybenzoic acid

▶ SMILES and InChIs

▶ Cite this record

Featured data source

The Merck Index *Online* has more data on this compound

Want to comment on this record?

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▶ **Names and Identifiers**

▶ **ChemSpider Searches**

▶ **Properties**

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▶ **Data Sources**

▶ **Wikipedia Article(s)**

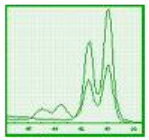
▶ **Patents**

▶ **RSC Databases**

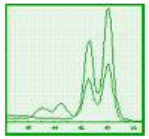
Spectra

Add

- Type: Infrared
  Comments: These data were collected from standards supplied by legitimate manufacturers or synthesized in forensic laboratories under controlled conditions. Supplied by John Meyers, Member of the ChemSpider Advisory Group.
  Approved: Yes
  Submitted by: Antony Williams



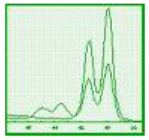
- Type: HNMR
  Associated Hyperlink: http://wwwchem.uwimona.edu.jm/spectra/JSpecView
  Comments: HNMR spectrum of Aspirin
  Approved: No
  Submitted by: Antony Williams



OPEN DATA

Download

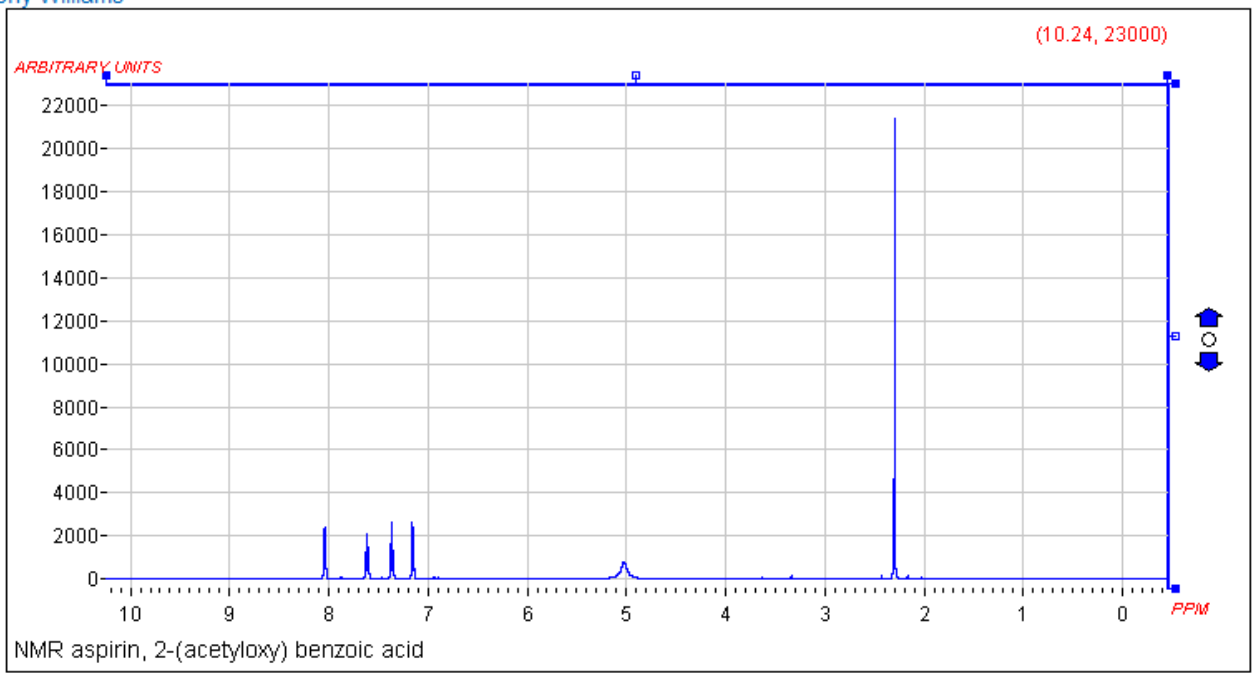
- Type: CNMR
  Associated Hyperlink: http://wwwchem.uwimona.edu.jm/spectra/JSpecView
  Comments: CNMR spectrum of aspirin
  Approved: No
  Submitted by: Antony Williams



OPEN DATA

Download

Type: HNMR
Associated Hyperlink: http://wwwchem.uwimona.edu.jm/spectra/JSpecView
Comments: HNMR spectrum of Aspirin
Approved: No
Submitted by: Antony Williams



NMR aspirin, 2-(acetyloxy) benzoic acid

OPEN DATA

Download

Adding and curating data

Adds quality and quantity…

- Users can comment for others to action
- Registered users can:
  Curate names
  Add links, spectra, and multimedia resources
- Depositors can add new compounds
- Curators and Master Curators assess and approve additions

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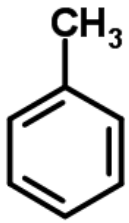
eg. Pyridine

Search term: **toluene** (Found by approved synonym)



2D 3D Save Zoom

toluene

ChemSpider ID: **1108**

Molecular Formula: C_7H_8

Average mass: 92.138397 Da

Monoisotopic mass: 92.062599 Da

Systematic name

Toluene

SMILES and InChIs

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The Merck Index *Online* has more data on this compound

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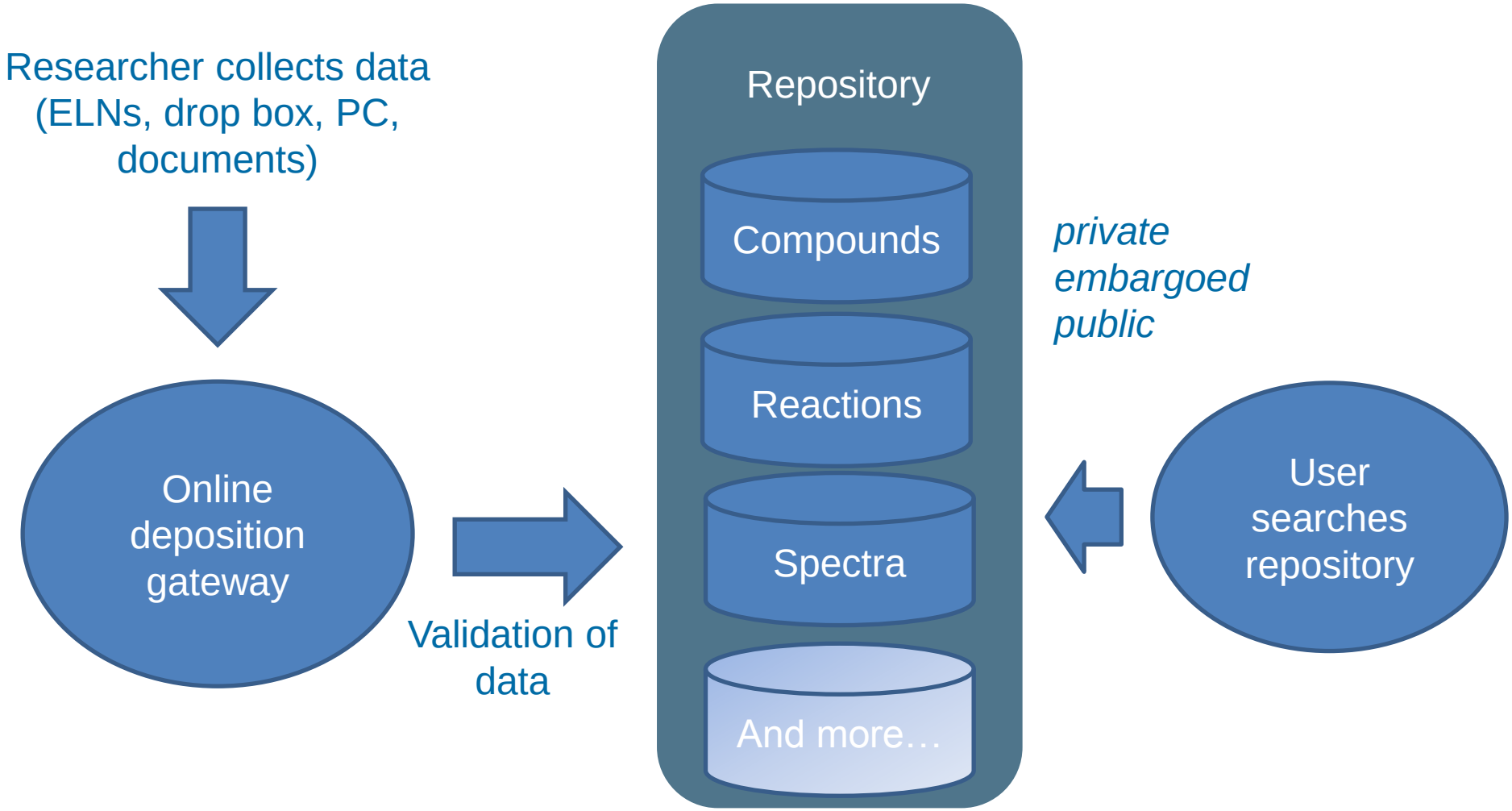
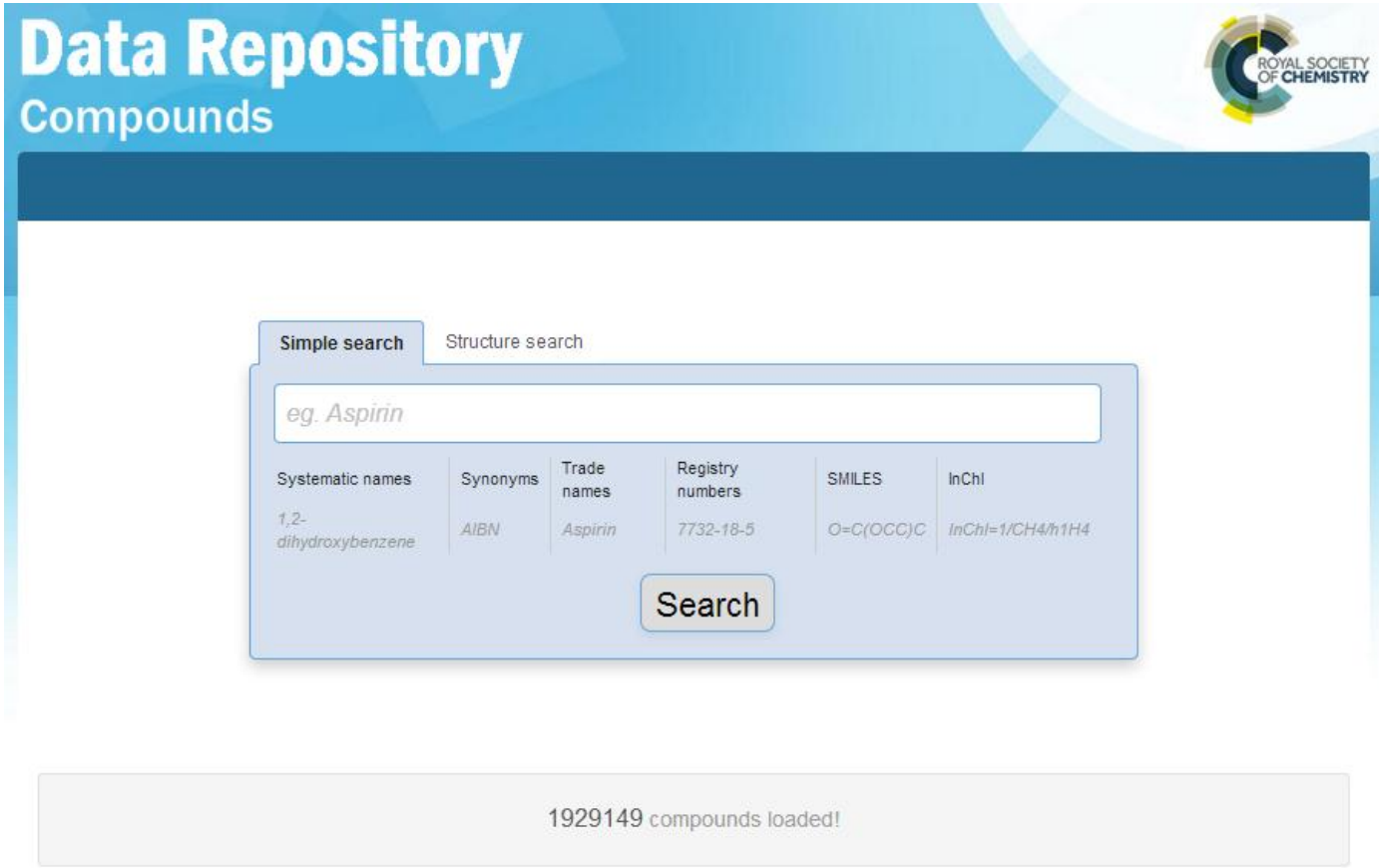
Identifier	Description
Image	Spectrum
CIF	Data source
Publication	DOI
PubMed ID	URL

Chemical Sciences Data Repository

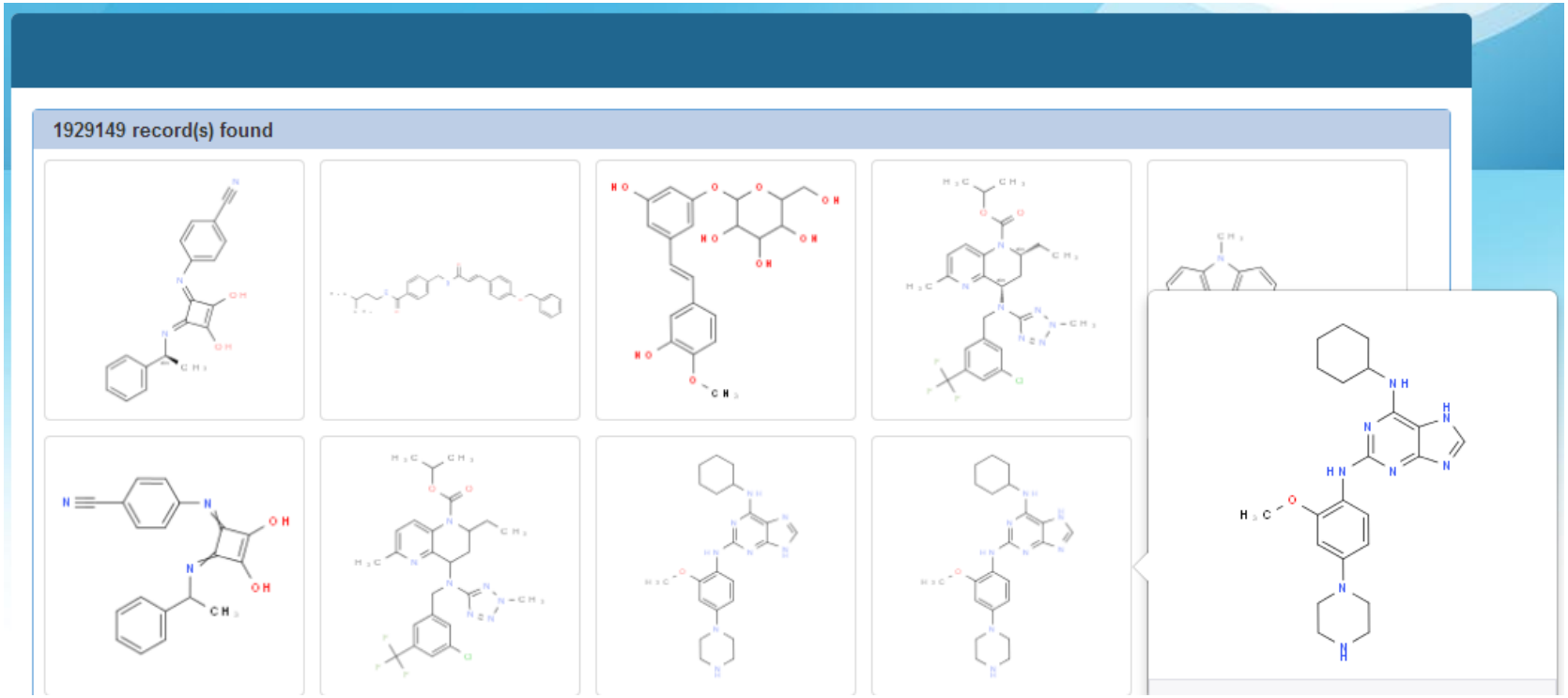
CDS National Chemical Database Service



Data Repository: Compounds

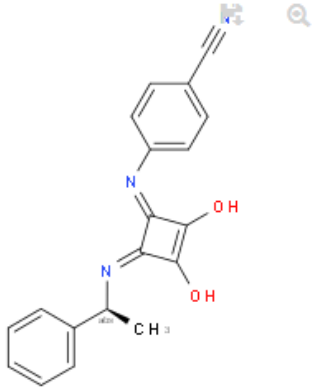


Data Repository: Compounds



Data Repository: Compounds

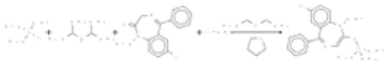
Compound Record



ID	1
Virtual	No
Molecular Formula	$C_{19}H_{15}N_3O_2$
Monoisotopic Mass	317.116425 Da
Molecular Weight	317.341309 Da
SMILES	C[C@H](/N=C1/C(=N/C2C=CC(=CC=2)C#N)/C(O)=C/1O)C1C=-CC=CC=1
Non Std. InChI	InChI=1/C19H15N3O2/c1-12(14-5-3-2-4-6-14)21-16-17(-19(24)18(16)23)22-15-9-7-13(11-20)8-10-15/h2-10,12,23-24H,1H-3/b21-16-,22-17-/t12-/m0/s1
Non Std. InChIKey	IQZAVINXCHHEGZ-CCTGVCNWNA-N
Std. InChI	InChI=1S/C19H15N3O2/c1-12(14-5-3-2-4-6-14)21-16-17-(19(24)18(16)23)22-15-9-7-13(11-20)8-10-15/h2-10,12,23-24H,1-H3/b21-16-,22-17-/t12-/m0/s1
Std. InChIKey	IQZAVINXCHHEGZ-CCTGVCNWSA-N
ChemSpider ID	28513355

Data Repository: Reactions

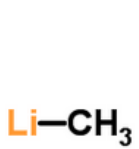
Reaction Record



ID	361532
RInChI	RInChI=0.02.1S////C6H15N/c1-5(2)7-6(3)4/h5-7H,1-4H3//CH3.Li/h1H3;///X/d-
RInChIKey Long	bSA-BEANN---UAOMVDZJSHZZME-UHFFFAOY-N-DVSDBMFJEQPWNO-UHFFFAOY-N--X
RInChIKey Short	bSA-BEANN-EANNATPGMB-BULSEIXIGJ-BIQAGPPMEE-NEANN-NEANN-NEANN

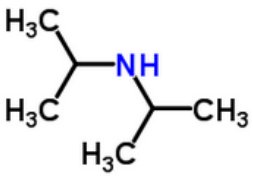
Reaction Components 7

1



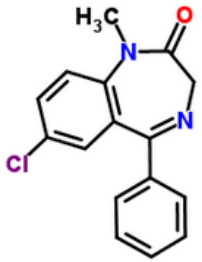
ID: 10915
Type: Reactant
ChemSpider ID: 10254338

2



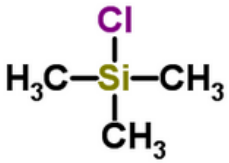
ID: 8290
Type: Reactant
ChemSpider ID: 7624

3



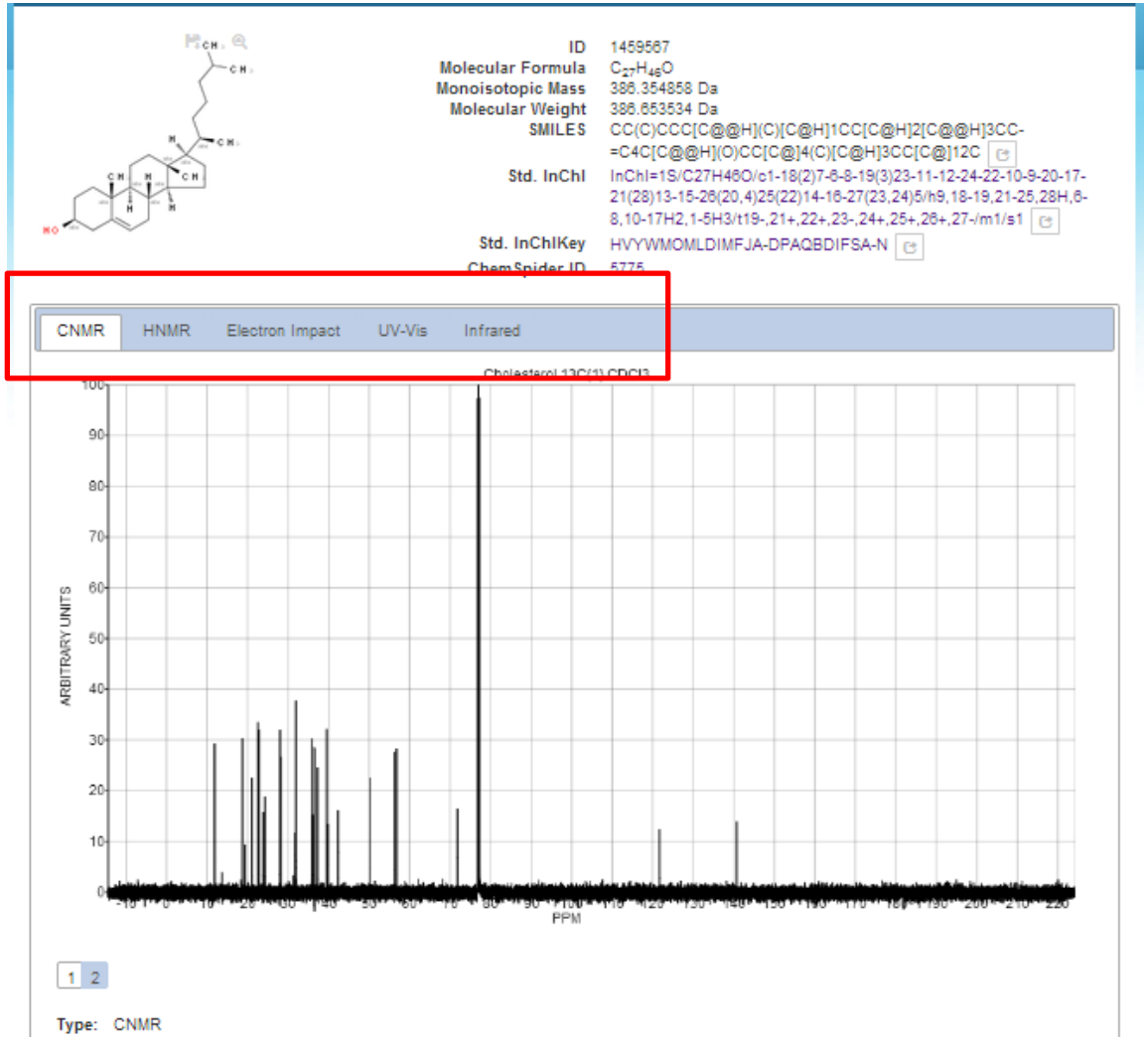
ID: 9876
Type: Reactant
ChemSpider ID: 2908

4

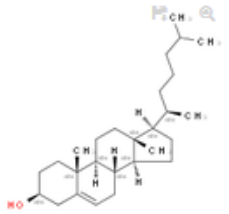


ID: 8205
Type: Reactant
ChemSpider ID: 6157

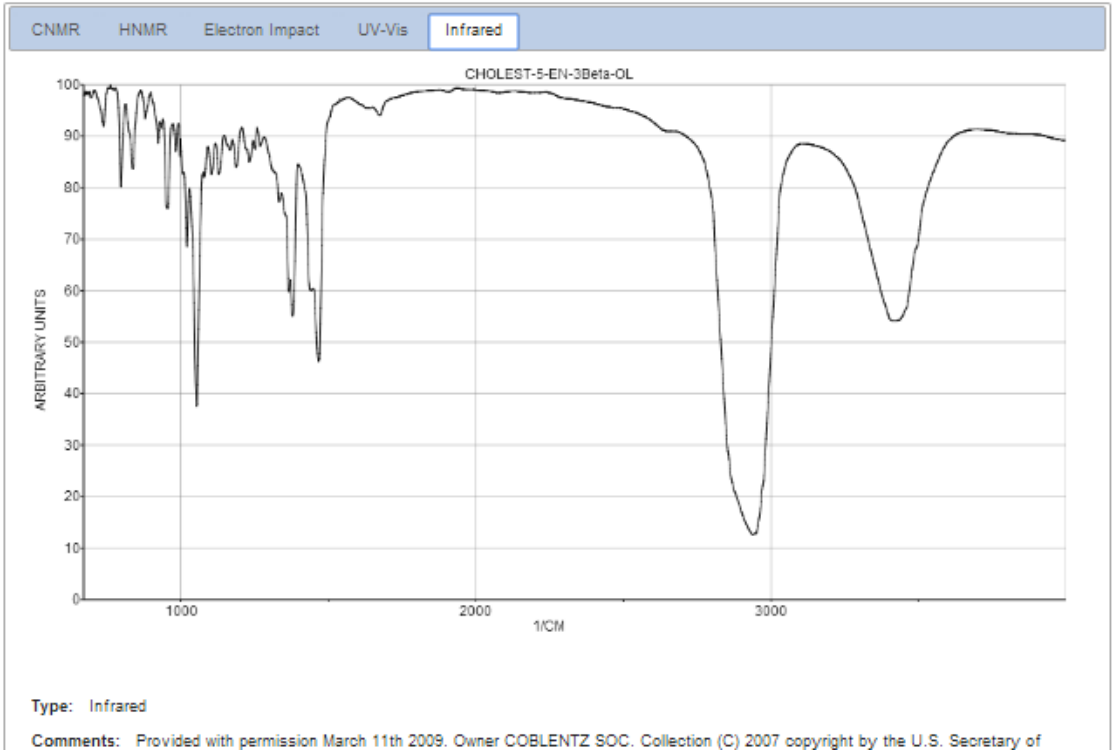
Data Repository: Spectra



Data Repository: Spectra



ID	1459567
Molecular Formula	$C_{27}H_{46}O$
Monoisotopic Mass	386.354858 Da
Molecular Weight	386.653534 Da
SMILES	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC-=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C
Std. InChI	InChI=1S/C27H46O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4)25(22)14-16-27(23,24)5/h9,18-19,21-25,28H,6-8,10-17H2,1-5H3/t19-,21+,22+,23-,24+,25+,26+,27-/m1/s1
Std. InChIKey	HVYWMOMLDIMFJA-DPAQBDIFSA-N
ChemSpider ID	5775



Type: Infrared

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ChemSpider SyntheticPages

Text

* *mandatory fields*

To link to another SyntheticPage, use [[xxx]] where xxx is the number of the SyntheticPage. To link some text in this way use the following [[xxx|text to be linked]], e.g. [[123|Page 123]]

* **Procedure or Transformation**

e.g. "Addition of 2-litioindole to tributyltin chloride" or "alkylation of zirconium tetrachloride with benzyl Grignard" or "Epoxidation of

* **Compound being made**

e.g. "2-indolylstannane", "Zirconium tetrabenzyl" or "Aromatic epoxides".

* **Chemicals Used (each on a different line)**

e.g. TBDMS-Cl, 97% (Sigma-Aldrich)

* **Procedure**

* **Author's Comments**

e.g.

- *Particular care should be taken when handling {name of reagent}*
- *This reaction has been performed with a range of alkenes, in our experience good yields were obtained for electron-rich alkenes, but using certain electron-poor alkenes as substrates (for example, acrylates) we obtained lower yields (40-50%)*
- *It is important to use freshly distilled tributyl tin hydride, we observed that there was only a small fall off in yield (<5%) if we*

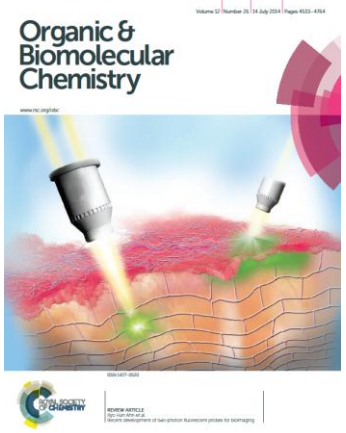
Lead Reference

e.g. S. Caddick, K. Aboutayab, K. Jenkins, R. I. West, J. Chem. Soc. Perkin Trans. 1, 1996, 675. DOI: 10.1039/P19960000675

Unanswered questions

- Level of curation from us
- Number of ‘required fields’
- Who can deposit? Who can have access (even if ‘private)?
- Standardisation of metadata
- What do people want to search on (properties? spectral features?)
- How does it link to the ESI?
- Should we assign DOIs for data?

Data mining of historic content



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TEMPO-mediated allylic C–H amination with hydrazones†

Xu Zhu and Shunsuke Chiba*

Cite this: *Org. Biomol. Chem.*, 2014, **12**, 4567

Received 23rd April 2014,
Accepted 10th May 2014

DOI: 10.1039/c4ob00839a

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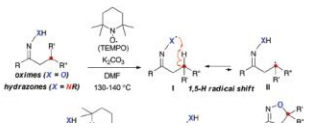
TEMPO-mediated reactions of alkenyl hydrazones afforded aza-heterocycles *via* sp³ C–H allylic amination. The transformation is featured by a sequence of remote allylic H-radical shift and allylic homolytic substitution with hydrazone radicals.

Development of methods for oxidative functionalization of sp³ C–H bonds that provide direct and step-economical approaches to construct functionalized organic structures has



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DOI: 10.1039/C4OB00839A (Communication) *Org. Biomol. Chem.*, 2014, **12**, 4567-4570

TEMPO-mediated allylic C–H amination with hydrazones†

Xu Zhu and Shunsuke Chiba *

Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore. E-mail: shunsuke@ntu.edu.sg; Fax: +65-67911961

Received 23rd April 2014 , Accepted 10th May 2014

First published on the web 13th May 2014

TEMPO-mediated reactions of alkenyl hydrazones afforded azaheterocycles *via* sp³ C–H allylic amination. The transformation is featured by a sequence of remote allylic H-radical shift and allylic homolytic substitution with hydrazone radicals.

Development of methods for oxidative functionalization of sp³ C–H bonds that provide direct and step-economical approaches to construct functionalized organic structures has been one the hottest trends in the area of synthetic organic chemistry.[1] To realize this goal in a regio- and chemo-selective manner, the use of organometallic intermediates as well as metal-carbene and -nitrene species with various transition-metal-catalysts has prevailed. On the other hand, free-radical mediated sp³ C–H bond functionalization by a remote H-radical shift[2] has been recognized for a long time as represented by the Hofmann–Löffler–Freytag reaction,[3] while the inherent violent chemical reactivity of the free radical species often renders these processes dyscontrol along with undesired side reactions such as fragmentation and intermolecular H-radical abstraction.

Our group has been interested in the use of stabilized O- and N-radicals derived from oximes and hydrazones, respectively, for remote sp³ C–H bond oxidation, and recently reported -sp³-C–H oxygenation and amination with oximes and hydrazones mediated by 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO) (Scheme 1).[4] In β-sp³-C–H oxygenation with oximes (X =

Electronic Supplementary Information

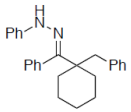
TEMPO-Mediated Allylic C-H Amination with Hydrazones

Xu Zhu and Shunsuke Chiba*

Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore.

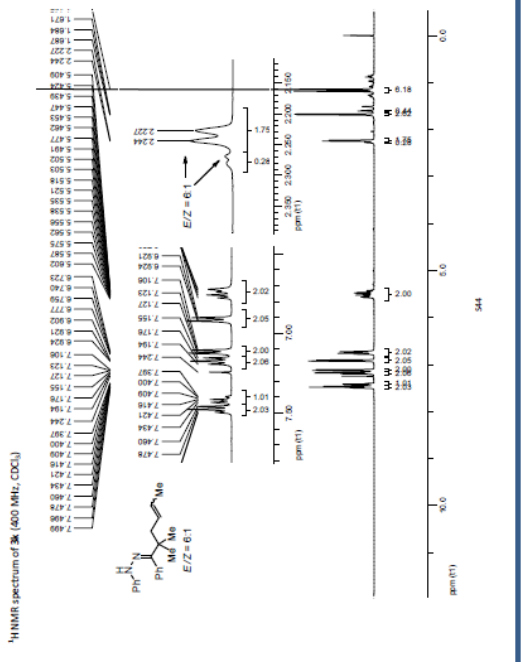
E-mail: shunsuke@ntu.edu.sg

(*Z*)-1-((1-Benzylcyclohexyl)(phenyl)methylene)-2-phenylhydrazine (3a):



68% yield as a yellow viscous liquid (single *Z*-isomer) from (1-benzylcyclohexyl)(phenyl)-methanone.[2]

IR (NaCl) 3337, 3053, 2934, 1647, 1601, 1503, 1452, 1308, 1265 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 1.19-1.35 (1H, m), 1.40-1.49 (4H, m), 1.53-1.56 (3H, m), 1.81-1.86 (2H, m), 2.99 (2H, s), 6.78 (1H, t, *J* = 8.0 Hz), 6.90-6.92 (5H, m), 7.17-7.26 (7H, m), 7.35-7.43 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.7, 26.0, 26.9, 34.4, 45.6, 112.5, 119.2, 125.9, 127.8, 128.39, 128.41, 129.0, 129.1, 131.1, 133.7, 138.9, 145.4, 151.5; ESIHRMS: Found: *m/z* 369.2333. Calcd for $C_{26}H_{29}N_2$: $(M+H)^+$ 369.2331.



Text Mining

The N-(β-hydroxyethyl)-N-methyl-N'-(2-trifluoromethyl-1,3,4-thiadiazol-5-yl)urea prepared in Example 6 , thionyl chloride (5 ml) and benzene (50 ml) were charged into a glass reaction vessel equipped with a mechanical stirrer , thermometer and reflux condenser .

The reaction mixture was heated at reflux with stirring , for a period of about one-half hour .

After this time the benzene and unreacted thionyl chloride were stripped from the reaction mixture under reduced pressure to yield the desired product N-(β-chloroethyl)-N-methyl-N'-(2-trifluoromethyl-1,3,4-thiaidazol-5-yl)urea as a solid residue

Results and discussion

Effect of pH of tyramine – oxalic acid eluent on retention behavior of mono- and divalent cations

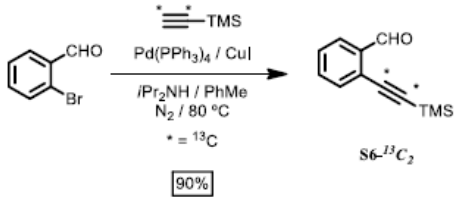
Since the silanol group on the surface of silica gel is a weakly acidic cation -exchanger, the cation -exchange capacity of a silica gel column is strongly influenced by the pH of the eluent . Hence, in order to separate common mono- and divalent cations (Li+, Na+, NH4+, K+, Mg2+ and Ca2+) on the Zorbax BP-SIL column in a reasonable time, the effect of the pH of 1 mmol dm−3 tyramine –0.2 mmol dm−3 oxalic acid as the eluent on the retention behavior of these cations was investigated. The pH of the eluent was adjusted with 1 mol dm−3 HNO3 .

Fig. 1 shows the relationship between the pH of the eluent and the retention volumes of the mono- and divalent cations . The retention volumes of these cations increased with increasing pH of the eluent . This is due mainly to an increase in the cation -exchange capacity of the Zorbax BP-SIL column by promoting the dissociation of the silanol group as a cation -exchanger. The retention volumes of the divalent cations markedly increased in comparison with those of the monovalent cations . This is because the retention volumes of divalent cations are strongly influenced by the cation -exchange capacity.9 Complete separation of the divalent cations and incomplete separation of the monovalent cations were achieved at pH ≥4.5. This indicated that oxalic acid acted as a complexing agent for the divalent cations .5,6

Effect of pH of 1 mmol dm−3 tyramine –0.2 mmol dm−3 oxalic acid as eluent on retention volumes of common mono- and divalent cations . Column, Zorbax BP-SIL (150 × 4.6 mm id); column temperature, 35 °C; eluent , 1 mmol dm−3 tyramine –0.2 mmol dm−3 oxalic acid . The pH of the eluent was adjusted with 1 mol dm−3 HNO3 . Flow rate, 1 ml min−1; detection, indirect UV at 265 nm; injection volume, 20 µl. Sample concentration, 0.2 mmol dm−3 for monovalent

Converting Text to Spectra

Scheme S13. Synthesis of **S6-$^{13}C_2$**

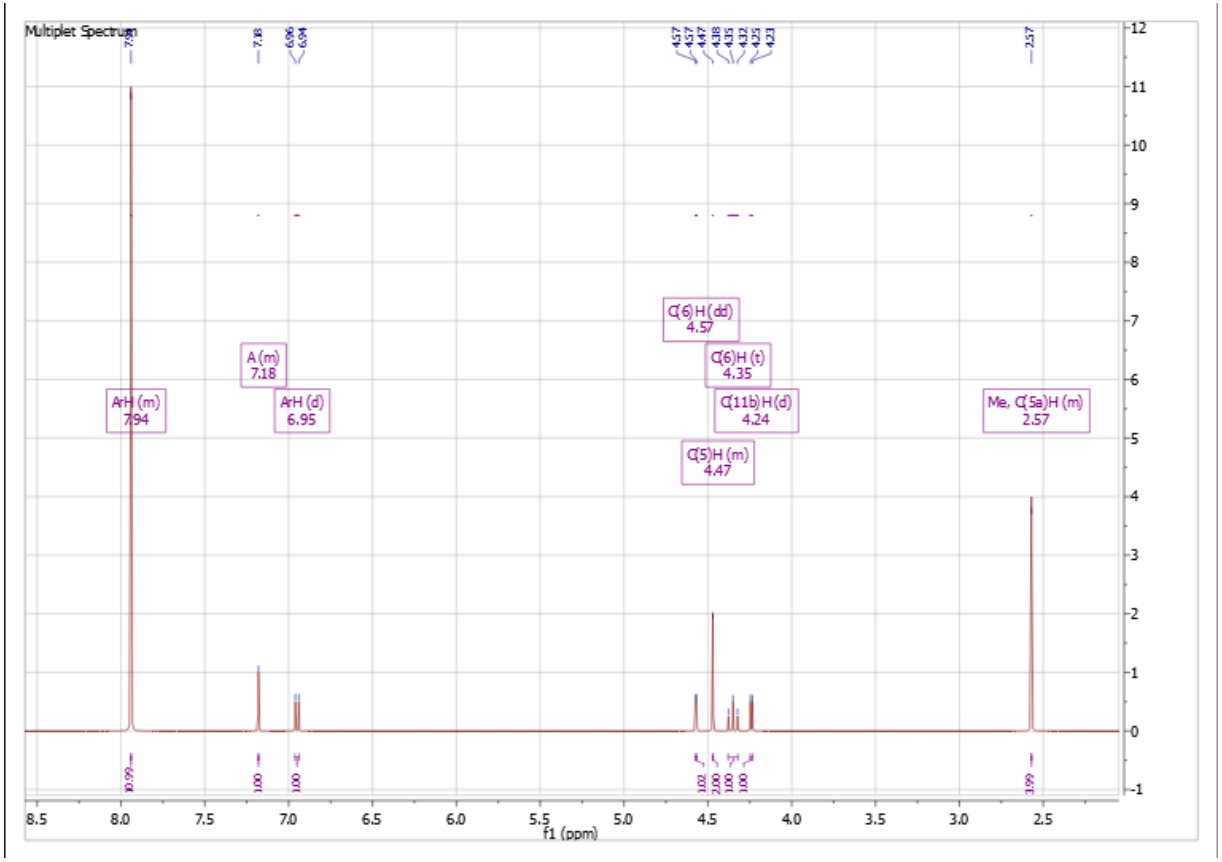


Synthesis of S6-$^{13}C_2$. 2-bromobenzaldehyde (0.526 g 2.84 mmol), CuI (5 mg, 0.028 mmol), and $Pd(PPh_3)_4$ (15 mg, 0.013 mmol) were loaded in a 25 mL Schlenk flask equipped with a magnetic stirrer. The flask was evacuated under dynamic vacuum to 150 mtorr and backfilled with N_2 three times. Anhydrous PhMe (3 mL) and anhydrous *i*Pr$_2$NH (1 mL) were added via cannula under N_2. The mixture was bubbled with N_2 for 20 min and trimethylsilylacetylene-$^{13}C_2$ (99% atom ^{13}C, 0.435 mL, 300 mg, 2.994 mmol) was added dropwise with stirring. The mixture was heated to 80 °C and stirred for 12 h, after which it was quenched with saturated NH_4Cl (*aq*), and extracted with CH_2Cl_2 (3 x 10 mL). The combined organic extracts were rinsed with saturated NH_4Cl (*aq*), water, and brine. The solution was dried over anhydrous $MgSO_4$, filtered over celite, and concentrated to dryness. The obtained dark residue was purified by column chromatography (SiO_2, 5% *v/v* THF/hexanes) to provide **S6-$^{13}C_2$** (0.554 g, 90% yield) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.56 (d, J_{CH} = 0.76 Hz, 1H), 7.91 (d, J = 7.95 Hz, 1H), 7.57 (m, J = 7.85, 1.71, 0.70 Hz, 1H), 7.54 (m, J = 7.75, 0.68 Hz, 1H), 7.43 (m, J = 7.75, 0.68 Hz, 1H), 0.28 (d, J_{CH} = 2.48 Hz, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 102.74 (d, J_{CC} = 136.2 Hz), 100.02 (d, J_{CC} = 136.3 Hz). EI-MS: calcd for $[C_{10}{}^{13}C_2H_{14}OSi]^+$ 204.09, found 203.15.

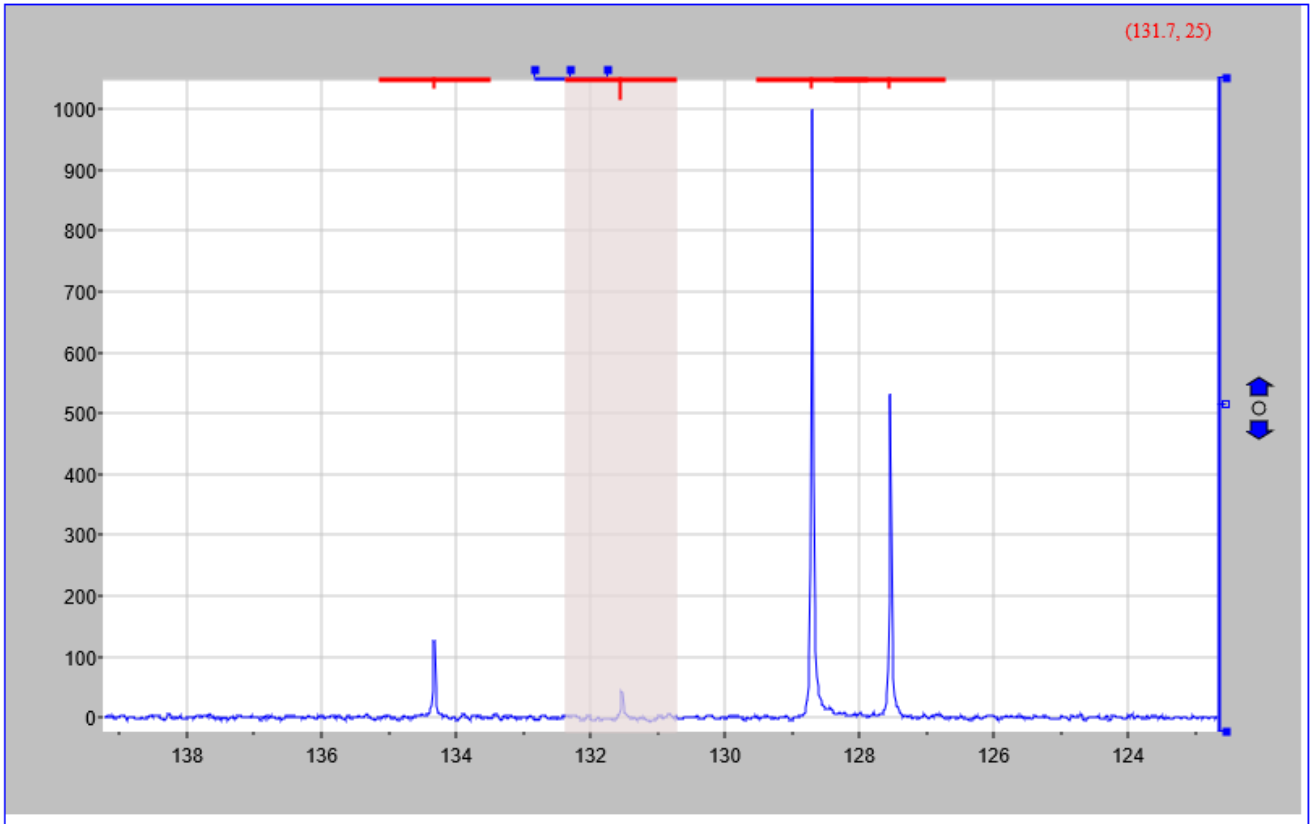
```
1H NMR (CDCl3, 400 MHz): δ = 2.42 (s, 3H, Me), 2.60 (s, 1H, C(5a)H), 4.16 (t, 1H, Jb = 10.4 Hz, C(6)H), 4.33 (d, 1H, J =
13C NMR (CDCl3, 100 MHz): δ = 14.41 (CH3), 29.51 (CH, benzylic methane), 30.12 (CH, benzylic methane), 66.20 (CH2), 68.52
1H NMR (CDCl3, 400 MHz): δ = 2.57 (m, 4H, Me, C(5a)H), 4.24 (d, 1H, J = 4.8 Hz, C(11b)H), 4.35 (t, 1H, Jb = 10.8 Hz, C(6)
13C NMR (CDCl3, 100 MHz): δ = 14.12 (CH3), 30.11 (CH, benzylic methane), 30.77 (CH, benzylic methane), 66.12 (CH2), 68.49
1H NMR (CDCl3, 400 MHz): δ = 2.12 (m, 1H, C(5a)H), 4.42–4.62 (m, 5H), 6.92–8.06 (m, 18H, ArH)
13C NMR (CDCl3, 100 MHz): δ = 30.75 (CH, benzylic methane), 31.09 (CH, benzylic methane), 66.64 (CH2), 68.00 (CH2), 117.3
1H NMR (CDCl3, 400 MHz): δ = 2.58 (m, 2H, C(6)H), 2.98 (dd, J = 7.2 Hz, 1H, C(1)H), 3.62 (q, 1H, C(10b)H), 4.37 (m, 2H, C
13C NMR (CDCl3, 100 MHz): δ = 29.93, 31.55, 35.71, 65.24, 67.87, 118.31, 123.29, 123.93, 124.10, 129.34 (ArC)
1H NMR (CDCl3, 400 MHz): δ = 2.52 (m, 1H, C(6)H), 4.38 (t, 1H, C(14a)H), 4.56 (m, 4H, Me & C(14)H), 6.92–8.15 (m, 12H, Ar
13C NMR (CDCl3, 100 MHz): δ = 29.22, 29.70, 66.07, 103.31, 115.29, 116.73, 117.81, 120.53, 121.49, 122.72, 122.99, 124.03
1H NMR (CDCl3, 400 MHz): δ = 2.39 (s, 3H, Me), 2.60 (s, 1H, C(5a)H), 4.04 (m, 2H, C(6)H & C(11b)H), 4.22 (s, 2H, C(5)H),
```

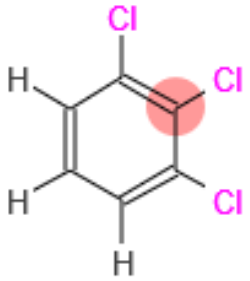
1H NMR (CDCl3, 400 MHz):

δ = 2.57 (m, 4H, Me, C(5a)H), 4.24 (d, 1H, J = 4.8 Hz, C(11b)H), 4.35 (t, 1H, Jb = 10.8 Hz, C(6)H), 4.47 (m, 2H, C(5)H), 4.57 (dd, 1H, J = 2.8 Hz, C(6)H), 6.95 (d, 1H, J = 8.4 Hz, ArH), 7.18–7.94 (m, 11H, ArH)



Visualisation of spectra



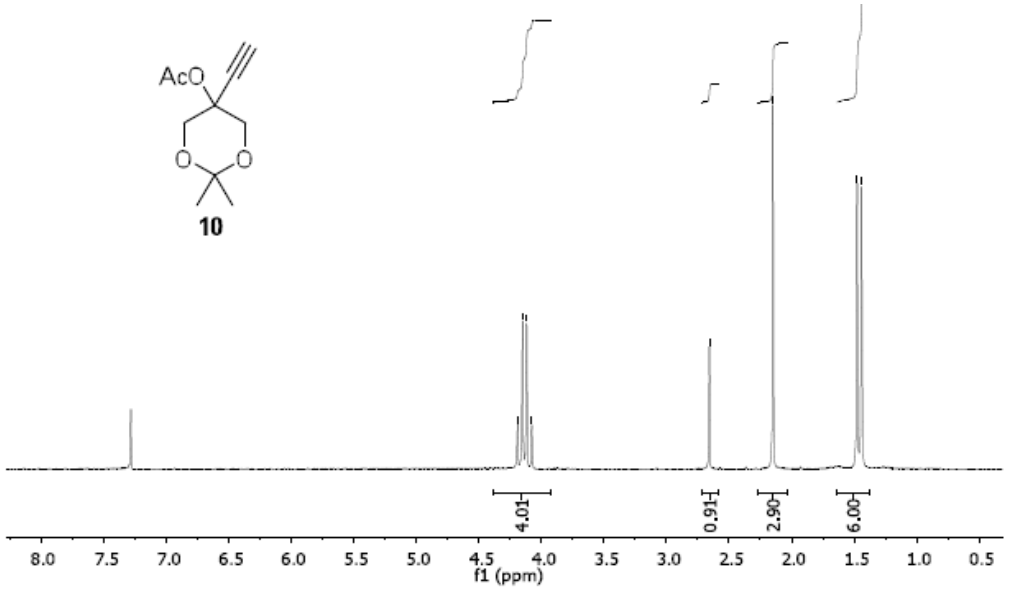


- Javascript viewer with JMol

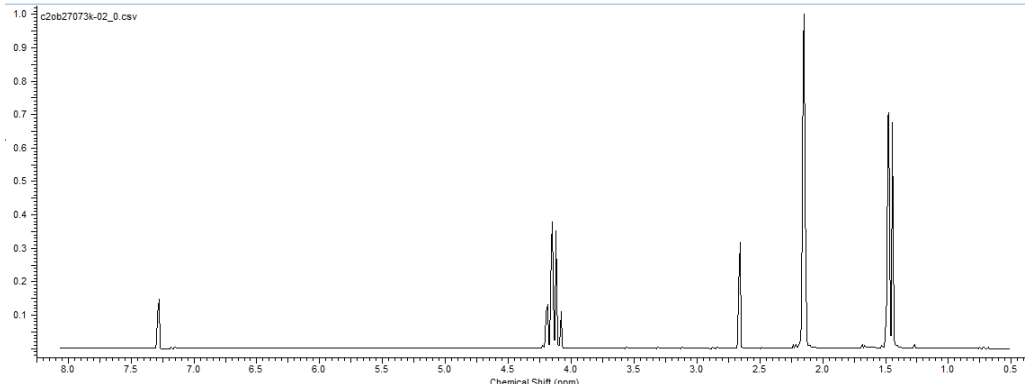
Figure Spectra into “Real Spectra”?

- We are turning text into structures
- We are turning text into spectra
- And we are turning figures into spectra

Turn “Figures” Into Data

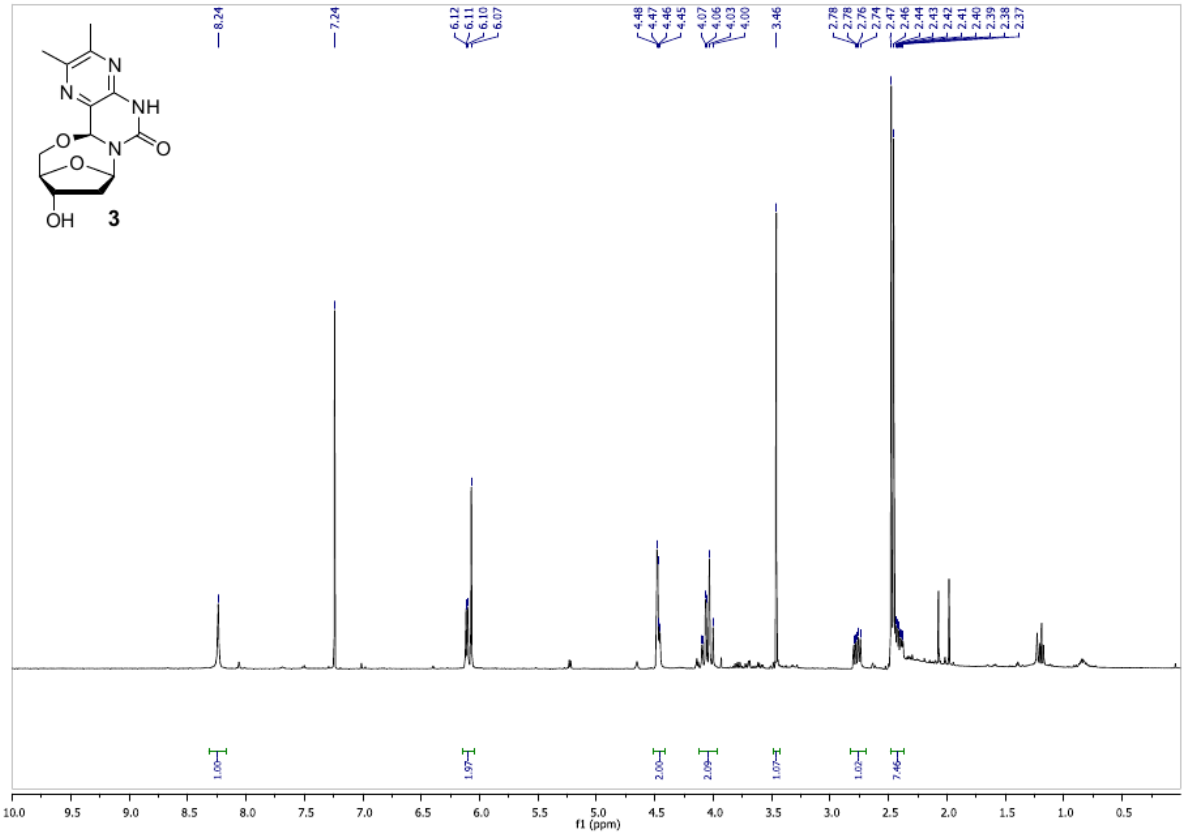


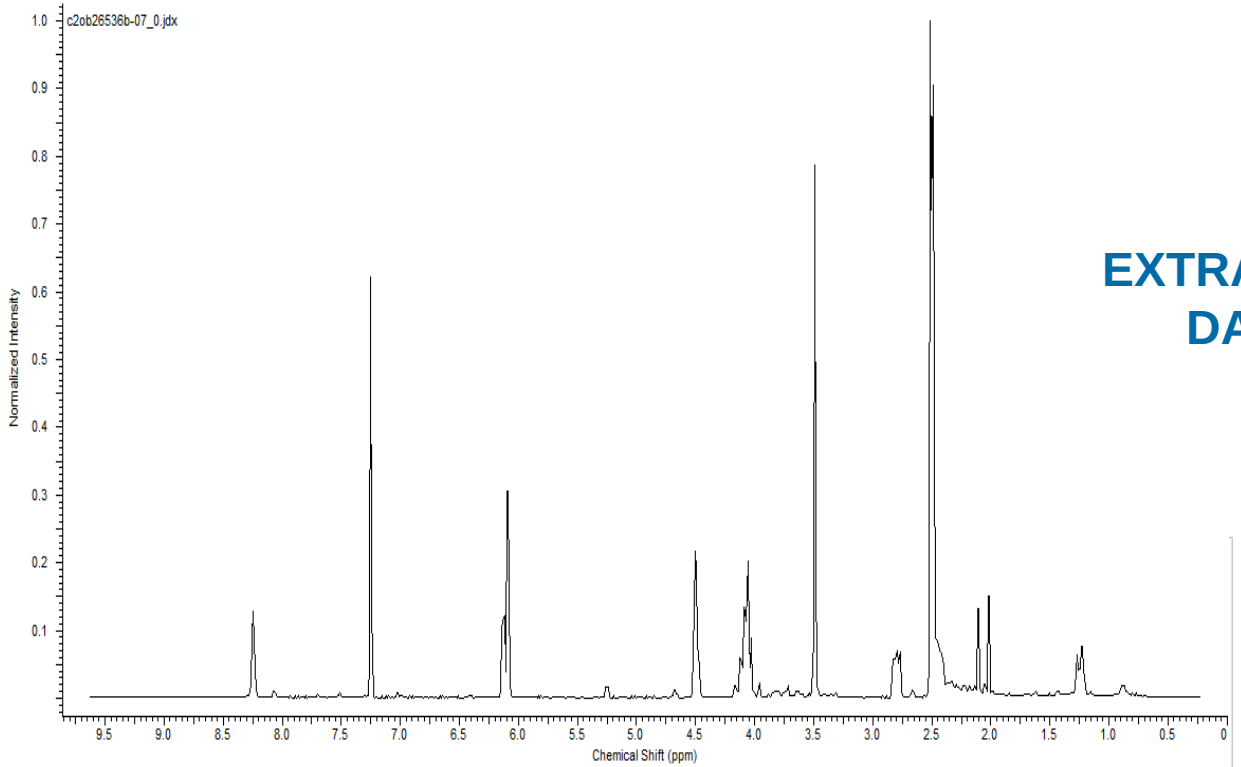
- Figure



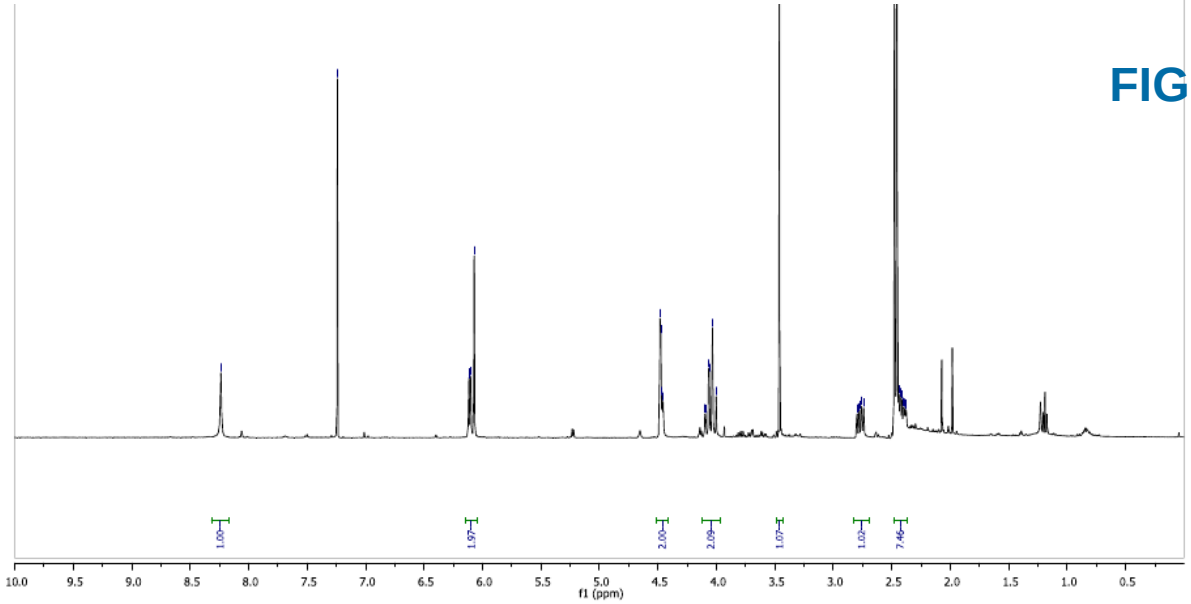
- Extracted Data

NMR-spectra





EXTRACTED DATA



FIGURE

Progress: Figures - Spectra

- Validation tests performed with William Brouwer. Good enough to proceed with larger test set
- Ready to run process across larger collection
- Focus on 21st century articles only for now

Example

- Input : 74 supplementary data documents/ 3444 pages
  - 1151 spectra
    - > 80% of peaks extracted to within 1-2 decimal places (ppm)

Acknowledgments

- Bill Brouwer (Penn State) – Plot2Txt Development
- Carlos Cobas and Santi Dominguez
- Bob Hanson and Bob Lancashire for Jmol/JSpecView Javascript version
- Leah McEwan and Will Dichtel
- ACD/Labs – Provider of spectroscopy tools

Royal Society of Chemistry eScience team:

Antony Williams, Colin Batchelor, Peter Corbett, Ken Karapetyan and Valery Tkachenko

Contact me: dabbs@rsc.org

Questions for you

- **Will you deposit your NMR spectra with ChemSpider?**
- **Would you like to be involved in future trials of the data repository?**
- **Feedback on ChemSpider or the National Chemical Database Service**?

- Are there any repositories or data banks members of your community currently use?
- What incentives would you need to deposit data?
- What functionality in a repository would you want (for example, searching capabilities)?
- How is your institution currently handling research data management? What plans are being put in place?