

NMR Community Project Update

Boehringer Ingelheim & Pfizer

Bo Du (Pfizer)

Paul-James Jones (Boehringer Ingelheim)

Justin Van Duine (Pfizer)



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NMR Converter (Bruker to ADF) - Features

- PoC NMR converter feature-complete (BI-Pfizer collaboration)
- Compatible with all data (30+ years)
- No loss of information on conversion (reversible if needed; compatible with GxP)
- ADF implementation adds in desirable capabilities missing from Bruker formats
- Supports cutting-edge experiments (6D+)
- Complete leaf-node metadata intrinsically supports semantic search; data lake storage

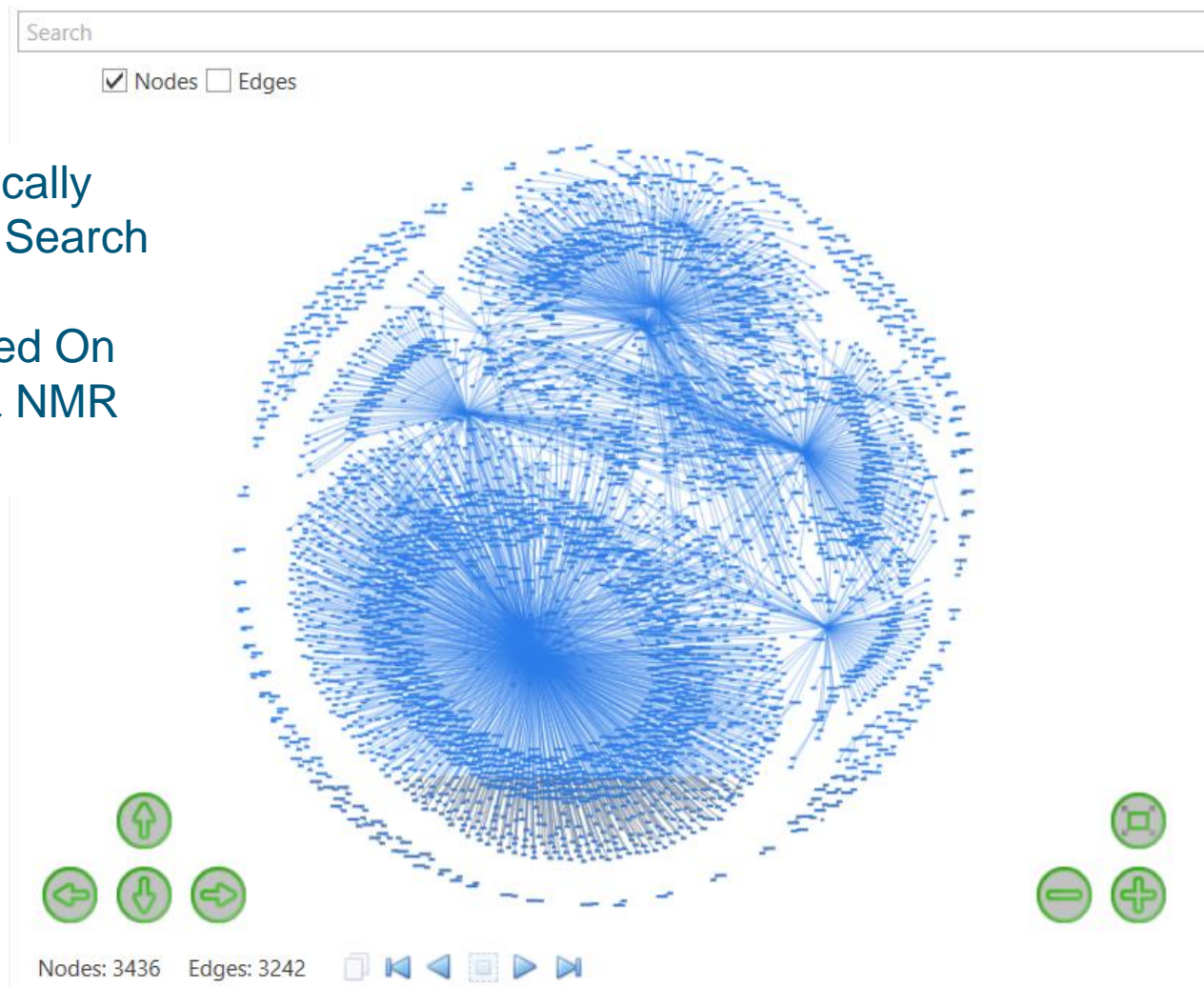
On-Going Activities

- Pfizer extending code to support multi-experiment sets within a single ADF (e.g. kinetics/reaction mechanism studies, qNMR, proof-of-structure, etc.)
- BI extending code to fully support latest version of Bruker TopSpin (v4.x)
- Currently in discussions with Bruker/MestreLab & others to produce commercial, enterprise version of BI/Pfizer PoC converter

Leaf Node

Metadata Intrinsicly Supports Semantic Search

Literal Terms Based On Bruker Top Spin & NMR SME's



Demo: Pfizer Implementation ADF Browser Plug-in

Pfizer team:

Justin Van Duine

Nathan Reddy

Vijay Bulusu

James Silva

Bo Du

• Zifo Team:

Krishnan Somaskandan

Venkatesh Kannan

Mukhil Anand Asokarajan



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Demo: Pfizer Implementation: ADF Plug-in

- Implementation of ADF is critical to Pfizer's "Scientific Data Cloud (SDC) Strategy
- Partnered with Zifo to development a browser plug-in based on the ADF Viewer

SDC & Search

Scientific Data Cloud

ADF

ADF	<i>found in</i>	File Name
ADF	<i>found in</i>	File Extension

Pfizer Confidential: The computer system (including all software, electronic mail, and the network) you have accessed is for the sole use of Company-authorized users (including contractors, consultants, and Company employees) in their conduct of Company-related business. Anything created, obtained or retained on the system is the property of the Company. All persons accessing the system without, or in excess of their authority or otherwise inappropriately using the system are subject to disciplinary action including termination and/or criminal prosecution. The Company regularly monitors the system for maintenance and to investigate the activities of individuals suspected of improper usage. Monitoring includes the capture and retention of all electronic mail traffic in a repository in accordance with applicable legal rules. Anyone using the system consents to such monitoring. Any suspected misuse should immediately report to the locations Corporate Security representatives. System users are accountable for the use and security of their passwords.

SDC Search-Release 3.1 Elastic6.4 Build 01 05-Apr-2019

Search

38 results found for ADF. (0.03 seconds)


Advanced Filters Showing 1 to 10 of 38 Show 10 Per Page


00706125-0377-01_SEG2018-177_PDE4_4_2D-04-01-2019.adf Scientist Name : Foley,David Anthony File Size (MB) : 39.150 File Time Created : Tue Apr 02 11:44:43 EDT 2019	...
00706125-0400-01_SEG2019-83_Javier_Magano_OPRD_5_2D-04-01-2019.adf Scientist Name : Foley,David Anthony File Size (MB) : 18.929 File Time Created : Tue Apr 02 11:44:44 EDT 2019	...
00706361-0339_SEG2019-84_PF-07104665_HbS_YL600_8_2D-04-01-2019.adf Scientist Name : Nguyen,Bao File Size (MB) : 69.107 File Time Created : Tue Apr 02 11:44:45 EDT 2019	...
00711726-0112-1_10_1D-10-30-2018.adf Scientist Name : Ainsworth,Emma File Time Created : Tue Apr 02 11:44:46 EDT 2018	...
00705980-0514-02_10_1D-12-10-2018.adf Scientist Name : Jones,Ricky Anthony File Time Created : Tue Apr 02 11:44:47 EDT 2018	...
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 File Details

 Download File

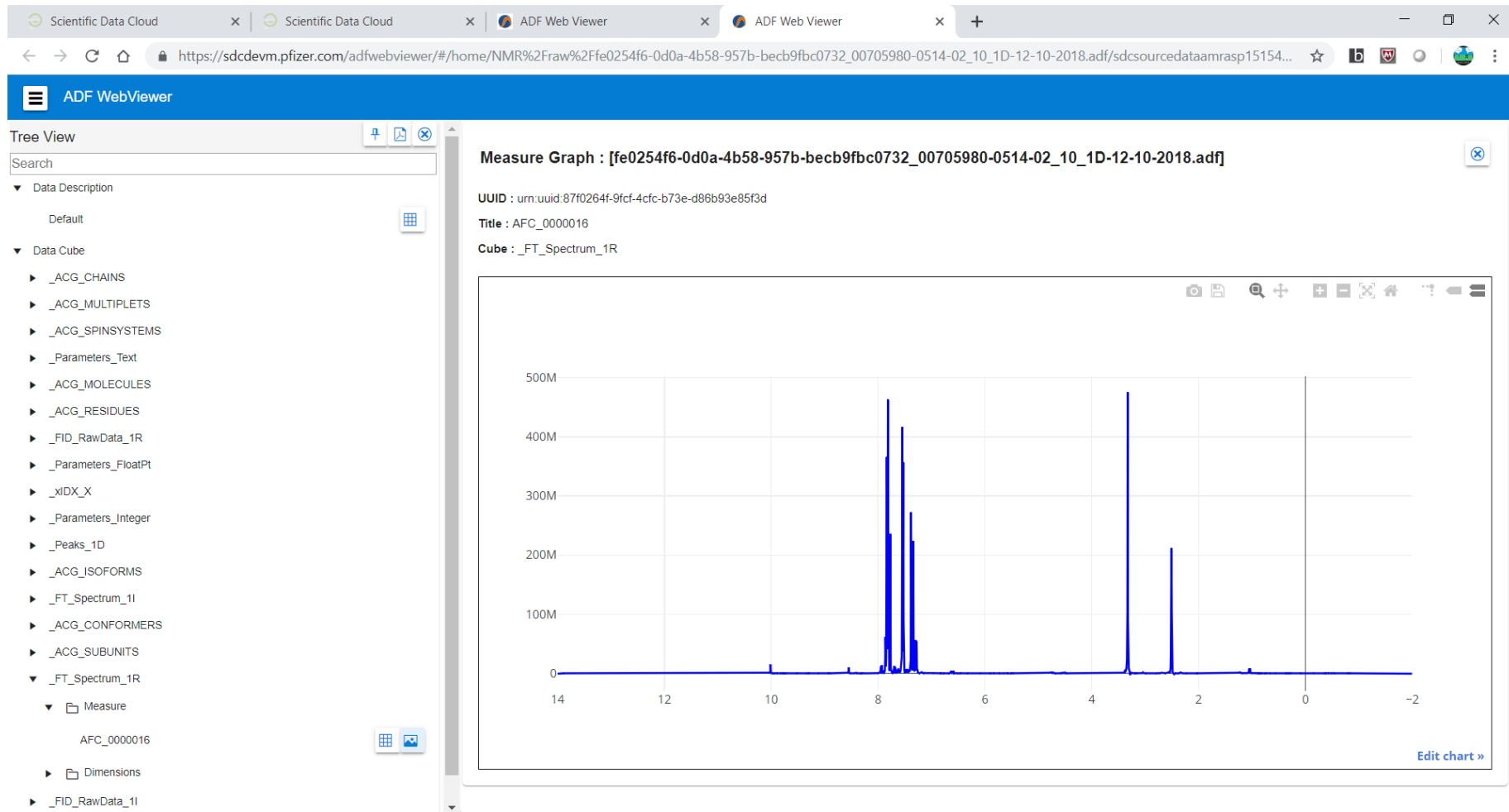
 View ADF

 File Details

 Download File

 View ADF

1D & 2D NMR Spectra Supported



Search

Scientific Data Cloud x Scientific Data Cloud x ADF Web Viewer x ADF Web Viewer x +

https://sdcdevm.pfizer.com/adfwebviewer/#/home/NMR%2Fraw%2Ffe0254f6-0d0a-4b58-957b-becb9fbc0732_00705980-0514-02_10_1D-12-10-2018.adf/sdcsourcedataamrasp15154...

ADF WebViewer

Tree View

Search

- Data Description
 - Default
- Data Cube
 - _ACG_CHAINS
 - _ACG_MULTIPLETS
 - _ACG_SPINSYSTEMS
 - _Parameters_Text
 - _ACG_MOLECULES
 - _ACG_RESIDUES
 - _FID_RawData_1R
 - _Parameters_FloatPt
 - _xIDX_X
 - _Parameters_Integer
 - _Peaks_1D
 - _ACG_ISOFORMS
 - _FT_Spectrum_11
 - _ACG_CONFORMERS
 - _ACG_SUBUNITS
 - _FT_Spectrum_1R
 - _FID_RawData_11
- Data Package

Data Description Table : [fe0254f6-0d0a-4b58-957b-becb9fbc0732_00705980-0514-02_10_1D-12-10-2018.adf]

Named Set : Default

Drag a column header and drop it here to group by that column

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NMRParameters	http://www.pfizer.com/pharmsci/metadata/NMRPara...	3
NMRParameters	http://www.pfizer.com/pharmsci/metadata/NMRPara...	14
NMRParameters	http://www.pfizer.com/pharmsci/metadata/NMRPara...	14
NMRParameters	http://www.pfizer.com/pharmsci/metadata/NMRPara...	32768
NMRParameters	http://www.pfizer.com/pharmsci/metadata/NMRPara...	65536
NMRParameters	http://www.pfizer.com/pharmsci/metadata/NMRPara...	3
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NMR Spectra

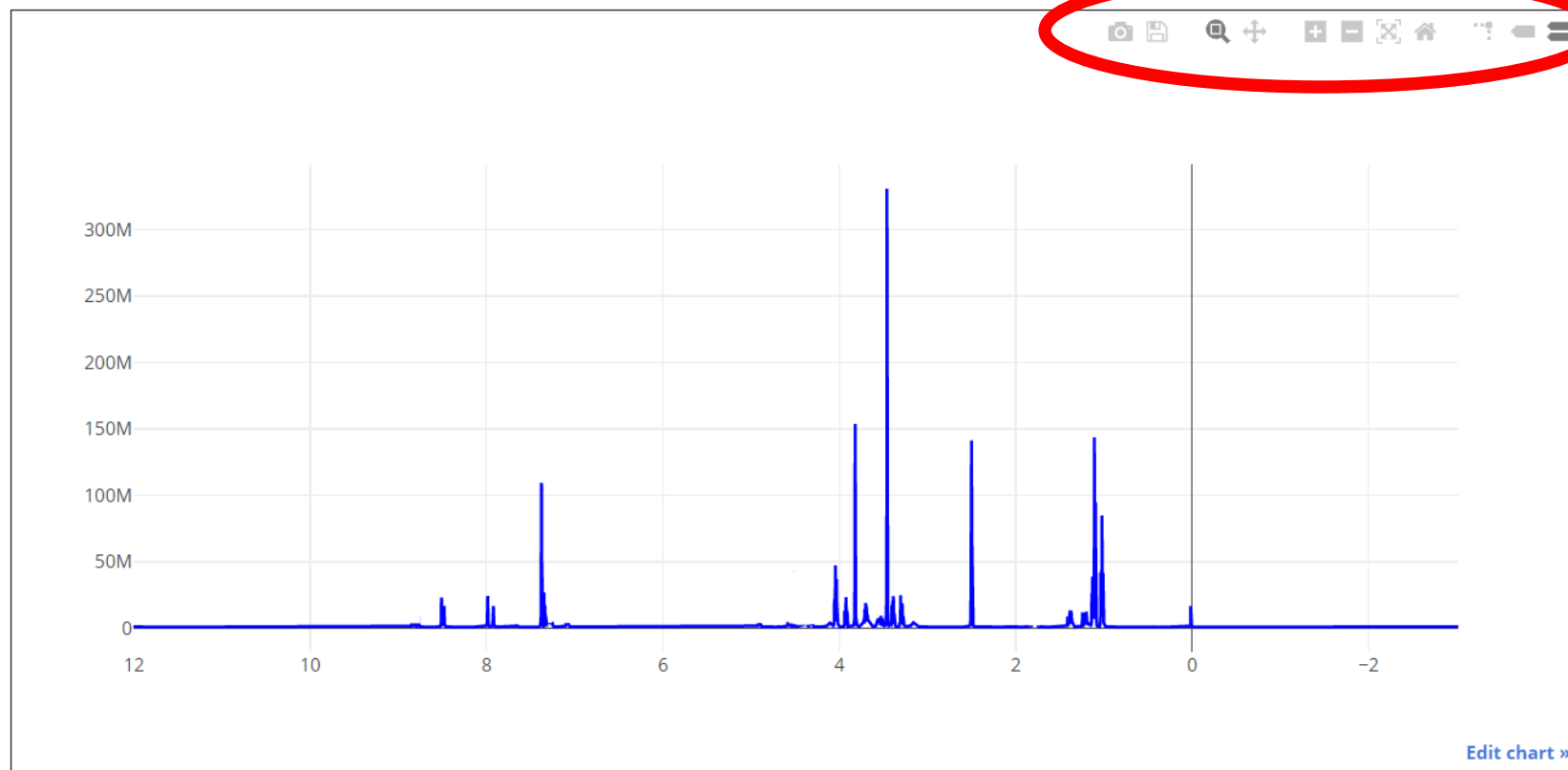
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Title : AFC_0000016

Cube : _FT_Spectrum_1R



[Edit chart »](#)