



Mestrelab Research

chemistry software solutions

Allotrope Converter from Bruker NMR Data

Anna Codina, PhD Director, Pharmaceutical Business Unit



**Guy Desmarquets, PhD, Vice President, Business Development & Strategic
Partnership - MESTRELAB**

- **Work triggered by conversations and outcomes from the last Allotrope Connect Paris and other past meetings and strong collaborations between Bruker and Mestrelab and between Bruker/Mestrelab and the Allotrope founders**
- **Based on BI/Pfizer approach, i.e. matching their requirements, Mestrelab has implemented a professionally-developed, supported, commercial application :**
 - **Raw Data (FID's) and Processed Data (Spectra) in the Data Cubes**
 - **Proprietary-format vendor files in the Data Package**
 - **Meta data extracted leaf nodes in the Data Description,**

- **Prototype tested by BI with Pfizer involved. First feedback and bug fixing**
- **First version will be ready in command lines called by our automation system (Mgears) in a few weeks**
- **The tool will be continuously evolving based on Allotrope members requirements (yearly subscription)**

```
Microsoft Windows [Versión 10.0.17763.737]
(c) 2018 Microsoft Corporation. Todos los derechos reservados.

D:\ADF>java -jar b2adf-0.1.0.jar -h
b2adf 0.1.0 - Copyright (C) 2019 Mestrelab Research S.L.
usage: b2adf [-edc <mask>] [-edp <mask>] [-h] -i <dir_path> -o <file_path>
-edc <mask>      Exclude from Data Cube. Specifies which parts of
                  original data set will NOT be written to data cube. R -
                  Raw data; S - Spectral data; I - Imaginary part(s) of
                  spectra. Usage example: -edc RI
-edp <mask>      Exclude from Data Package. Specifies which parts of
                  original data set will NOT be written to data package.
                  It accepts the same values as the option -edc.
-h              Print this message.
-i <dir_path>    Bruker Input dataset.
-o <file_path>   Output Allotrope ADF file. Overwrites the file if it
                  exists.

D:\ADF>
```

- Java program executable by command line

ADF Explorer of 2D data

The screenshot displays the ADF Explorer software interface. On the left is a Tree View showing a hierarchical structure of data cubes and measures. The main area contains two 'Measure Graph' windows. The left graph shows a 2D heatmap with a color scale from 0.000 to 0.008. The right graph shows a 2D plot with a color scale from 2 to 10. Both graphs have a 'Copy Graph' button and checkboxes for 'Cross-Hair' and 'Logarithmic'. The status bar at the bottom indicates the number of points and resampling status for each graph.

Tree View:

- Y3515
 - Data Description
 - Data Cubes
 - EXP0013_FID_RAWDATA_11
 - EXP0013_PROC0001_SPC_1R
 - EXP0010_FID_RAWDATA_11
 - EXP0013_FID_RAWDATA_1R
 - EXP0010_PROC0001_SPC_1R
 - EXP0012_PROC0001_SPC_2RR
 - EXP0011_FID_RAWDATA_2I
 - EXP0011_FID_RAWDATA_2R
 - Measures
 - AFR_0001588
 - Measures
 - AFR_0001588
 - Dimensions
- Data Package
 - Y3515
 - 11
 - 13
 - 10
 - 12

Measure Graph [D:\ADF\test data\JOHN H\Y3515.adf] (Left):

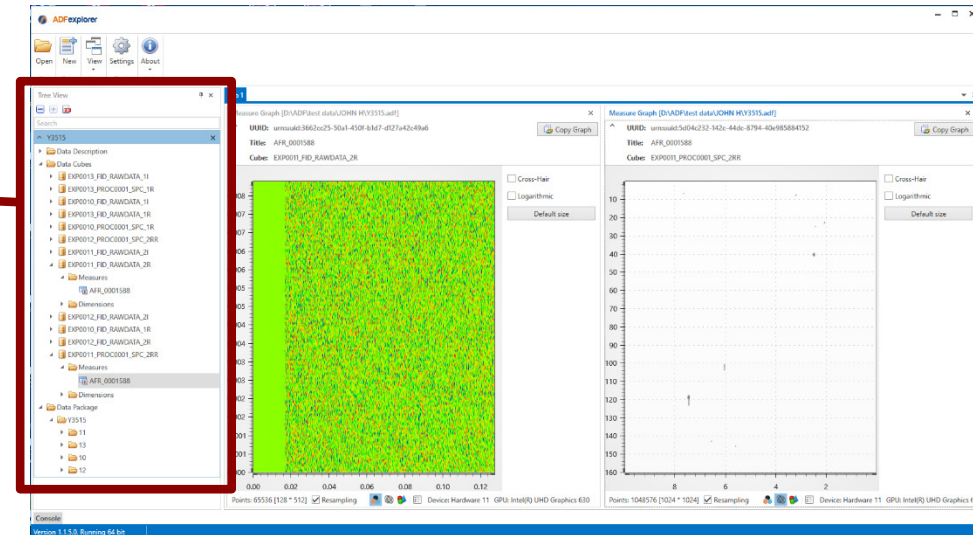
- UUID: urn:uuid:3662cc25-50a1-450f-b1d7-d127a42c49a6
- Title: AFR_0001588
- Cube: EXP0011_FID_RAWDATA_2R
- Points: 65536 [128 * 512] Resampling
- Device: Hardware 11 GPU: Intel(R) UHD Graphics 630

Measure Graph [D:\ADF\test data\JOHN H\Y3515.adf] (Right):

- UUID: urn:uuid:5d04c232-142c-44dc-8794-40e985884152
- Title: AFR_0001588
- Cube: EXP0011_PROC0001_SPC_2RR
- Points: 1048576 [1024 * 1024] Resampling
- Device: Hardware 11 GPU: Intel(R) UHD Graphics 630

Screen shots of the Tree View (ADF Explorer)

- ▶ Data Description
- ▶ Data Cubes
 - ▶ EXP0013_FID_RAWDATA_1I
 - ▶ EXP0013_PROC0001_SPC_1R
 - ▶ EXP0010_FID_RAWDATA_1I
 - ▶ EXP0013_FID_RAWDATA_1R
 - ▶ EXP0010_PROC0001_SPC_1R
 - ▶ EXP0012_PROC0001_SPC_2RR
 - ▶ EXP0011_FID_RAWDATA_2I
 - ▶ EXP0011_FID_RAWDATA_2R
 - ▶ Measures
 - ▶ AFR_0001588
 - ▶ Dimensions
 - ▶ EXP0012_FID_RAWDATA_2I
 - ▶ EXP0010_FID_RAWDATA_1R
 - ▶ EXP0012_FID_RAWDATA_2R
 - ▶ EXP0011_PROC0001_SPC_2RR
 - ▶ Measures
 - ▶ AFR_0001588
 - ▶ Dimensions
- ▶ Data Package
 - ▶ Y3515
 - ▶ 11
 - ▶ 13
 - ▶ 10
 - ▶ 12



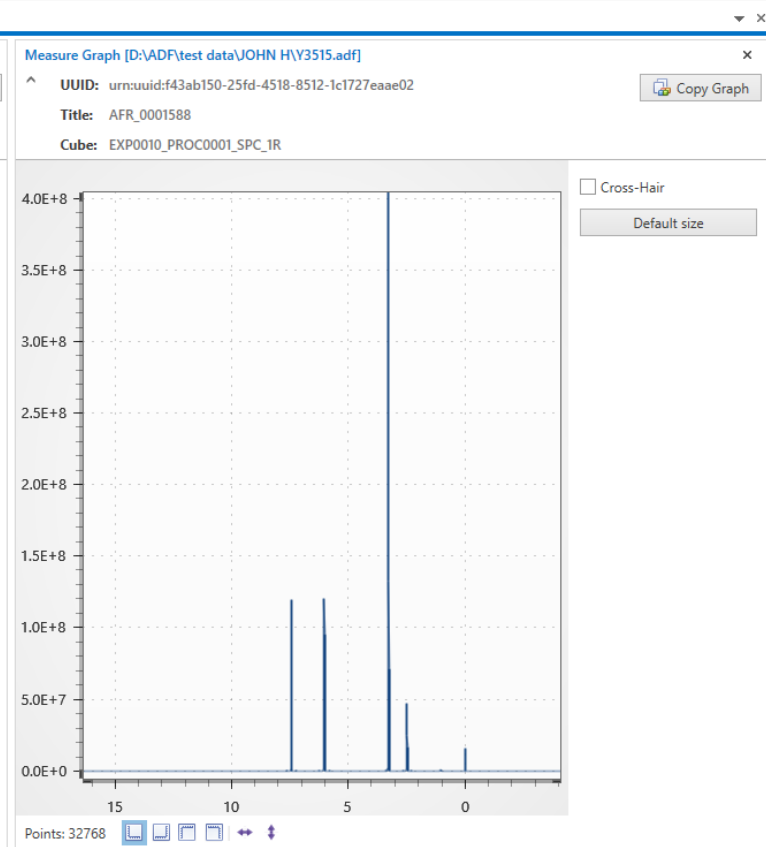
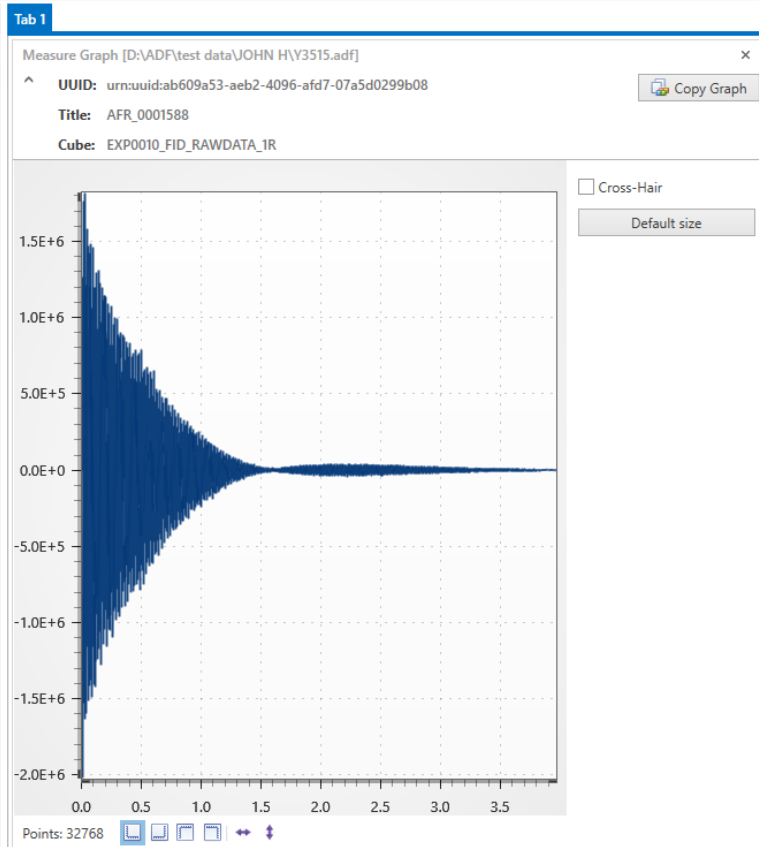
ADF Explorer

Open New View Settings About

File Tabs Views Tools Help

Tree View

- Y3515
 - Data Description
 - Data Cubes
 - EXP0013_FID_RAWDATA_11
 - EXP0013_PROC0001_SPC_1R
 - EXP0010_FID_RAWDATA_11
 - EXP0013_FID_RAWDATA_1R
 - EXP0010_PROC0001_SPC_1R
 - Measures
 - AFR_0001588
 - Dimensions
 - EXP0012_PROC0001_SPC_2RR
 - EXP0011_FID_RAWDATA_2I
 - EXP0011_FID_RAWDATA_2R
 - EXP0012_FID_RAWDATA_2I
 - EXP0010_FID_RAWDATA_1R
 - Measures
 - AFR_0001588
 - Dimensions
 - EXP0012_FID_RAWDATA_2R
 - EXP0011_PROC0001_SPC_2RR
- Data Package
 - Y3515
 - 11
 - 13
 - 10
 - 12



ADF Explorer

Open New View Settings About
File Tabs Views Tools Help

Tree View

- exam1d_1Dsf
 - Data Description
 - Default
 - Data Cubes
 - NMR_EXP1_PROC1_FTSPECTRUM_11
 - NMR_EXP1_PROC1_FTSPECTRUM_1R
 - Measures
 - AFR_0001588
 - Dimensions
 - NMR_EXP1_FID_RAWDATA_11
 - NMR_EXP1_FID_RAWDATA_1R
 - Measures
 - AFR_0001588
 - Dimensions
 - Data Package
 - exam1d_1Dsf

Tab 3

Measure Graph [D:\ADF\NMRTestSuite\exam1d_1Dsf.adf] x

UUID: urn:uuid:42d1af82-9bb3-47b4-94ab-d3c6d65525e7
Title: AFR_0001588
Cube: NMR_EXP1_FID_RAWDATA_1R

Points: 32768

Measure Graph [D:\ADF\NMRTestSuite\exam1d_1Dsf.adf] x

UUID: urn:uuid:d2c57231-5547-43ab-bb28-67bf7b0ac6fb
Title: AFR_0001588
Cube: NMR_EXP1_PROC1_FTSPECTRUM_1R

Points: 32768

Data Description Table [D:\ADF\NMRTestSuite\exam1d_1Dsf.adf] x

Named Set: Default

Search

Subject Predicate Object

Drag a column header here to group by that column

| Subject | Predicate | Object |
|---|---|---|
| urn:uuid:f9554e6e-1c0f-4f70-b595-ee3... | http://www.w3.org/1999/02/22-rdf-synt... | http://purl.boehringer-ingenheim.com/o... |
| urn:uuid:f9554e6e-1c0f-4f70-b595-ee3... | http://purl.allotrope.org/ontologies/pro... | EXP0001-PROC0001 |
| urn:uuid:b317a431-963e-48de-8623-e7... | http://www.w3.org/1999/02/22-rdf-synt... | ACQTO--A1-E001 |
| urn:uuid:b317a431-963e-48de-8623-e7... | http://purl.obolibrary.org/obo/RO_0002... | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d... |
| urn:uuid:b317a431-963e-48de-8623-e7... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#MicroSecond |
| urn:uuid:b317a431-963e-48de-8623-e7... | http://qudt.org/schema/qudt#numericV... | -2.26890760309556 |
| urn:uuid:b4be55eb-30b6-4482-b5bb-c7... | http://www.w3.org/1999/02/22-rdf-synt... | AMP--A1-E001 |
| urn:uuid:b4be55eb-30b6-4482-b5bb-c7... | http://purl.obolibrary.org/obo/RO_0002... | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d... |
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| urn:uuid:385effa8-dd35-4357-91fa-12a... | http://www.w3.org/1999/02/22-rdf-synt... | AMP--A1-E002 |
| urn:uuid:385effa8-dd35-4357-91fa-12a... | http://purl.obolibrary.org/obo/RO_0002... | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d... |
| urn:uuid:385effa8-dd35-4357-91fa-12a... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:385effa8-dd35-4357-91fa-12a... | http://qudt.org/schema/qudt#numericV... | 100.0 |
| urn:uuid:629010ae-a7f9-4cca-a98b-080... | http://www.w3.org/1999/02/22-rdf-synt... | AMP--A1-E003 |
| urn:uuid:629010ae-a7f9-4cca-a98b-080... | http://purl.obolibrary.org/obo/RO_0002... | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d... |
| urn:uuid:629010ae-a7f9-4cca-a98b-080... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:629010ae-a7f9-4cca-a98b-080... | http://qudt.org/schema/qudt#numericV... | 100.0 |
| urn:uuid:a1aec90b-510c-4ad3-a1b3-1d... | http://www.w3.org/1999/02/22-rdf-synt... | AMP--A1-E004 |
| urn:uuid:a1aec90b-510c-4ad3-a1b3-1d... | http://purl.obolibrary.org/obo/RO_0002... | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d... |
| urn:uuid:a1aec90b-510c-4ad3-a1b3-1d... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:a1aec90b-510c-4ad3-a1b3-1d... | http://qudt.org/schema/qudt#numericV... | 100.0 |
| urn:uuid:7943f136-c1ab-46e5-84a9-116... | http://www.w3.org/1999/02/22-rdf-synt... | AMP--A1-E005 |
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| urn:uuid:7943f136-c1ab-46e5-84a9-116... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |

Count: 8331

Console

Version 1.1.5.0, Running 64 bit

ADF Explorer

Open New View Settings About
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Tree View

- exam1d_1DsF
 - Data Description
 - Default
 - Data Cubes
 - NMR_EXP1_PROC1_FTSPECTRUM_11
 - NMR_EXP1_PROC1_FTSPECTRUM_1R
 - NMR_EXP1_FID_RAWDATA_11
 - NMR_EXP1_FID_RAWDATA_1R
 - Data Package

Tab 1

Data Description Table [D:\ADF\NMRTestSuite\exam1d_1Ds.adf]

Named Set: Default

Search

Subject Predicate Object

Drag a column header here to group by that column

| Subject | Predicate | Object |
|---|---|--|
| urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d79f2cfe5 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | http://purl.boehringer-ingenheim.com/ontologies/NMR#bi-a-BIA_000001001 |
| urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d79f2cfe5 | http://purl.allotrope.org/ontologies/property#AFX_0000690 | EXP0001-PROC0001 |
| urn:uuid:b317a431-963e-48de-8623-e7e53df4f023 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | ACQTO--A1-E001 |
| urn:uuid:b317a431-963e-48de-8623-e7e53df4f023 | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d79f2cfe5 |
| urn:uuid:b317a431-963e-48de-8623-e7e53df4f023 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#MicroSecond |
| urn:uuid:b317a431-963e-48de-8623-e7e53df4f023 | http://qudt.org/schema/qudt#numericValue | -2.26890760309556 |
| urn:uuid:b4be55eb-30b6-4482-b5bb-c7bcb83030f6 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | AMP--A1-E001 |
| urn:uuid:b4be55eb-30b6-4482-b5bb-c7bcb83030f6 | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d79f2cfe5 |
| urn:uuid:b4be55eb-30b6-4482-b5bb-c7bcb83030f6 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:b4be55eb-30b6-4482-b5bb-c7bcb83030f6 | http://qudt.org/schema/qudt#numericValue | 100.0 |
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| urn:uuid:385effa8-dd35-4357-91fa-12a265e36e46 | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d79f2cfe5 |
| urn:uuid:385effa8-dd35-4357-91fa-12a265e36e46 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:385effa8-dd35-4357-91fa-12a265e36e46 | http://qudt.org/schema/qudt#numericValue | 100.0 |
| urn:uuid:629010ae-a7f9-4cca-a98b-0809f17af23a | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | AMP--A1-E003 |
| urn:uuid:629010ae-a7f9-4cca-a98b-0809f17af23a | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d79f2cfe5 |
| urn:uuid:629010ae-a7f9-4cca-a98b-0809f17af23a | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:629010ae-a7f9-4cca-a98b-0809f17af23a | http://qudt.org/schema/qudt#numericValue | 100.0 |
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| urn:uuid:a1aec90b-510c-4ad3-a1b3-1da5885e4247 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:a1aec90b-510c-4ad3-a1b3-1da5885e4247 | http://qudt.org/schema/qudt#numericValue | 100.0 |
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| urn:uuid:7943f136-c1ab-46e5-84a9-116e07bbae68 | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:f9554e6e-1c0f-4f70-b595-ee3d79f2cfe5 |
| urn:uuid:7943f136-c1ab-46e5-84a9-116e07bbae68 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |

Count: 8331

Console

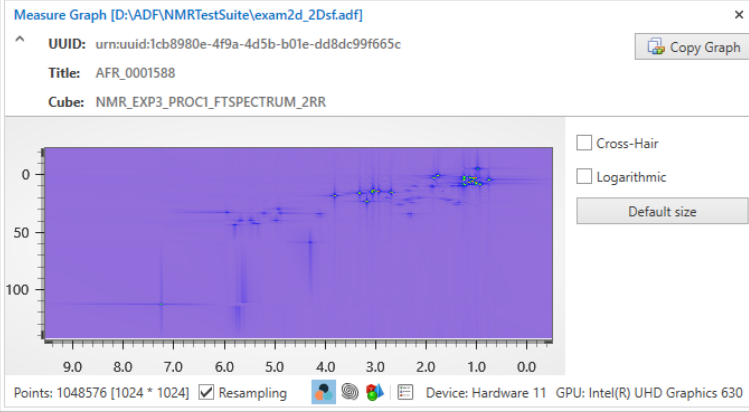
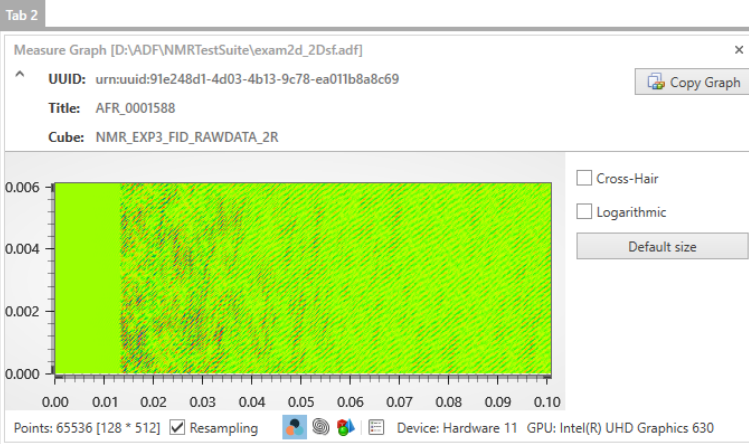
Version 1.1.3.0, Running 64 bit

ADF Explorer

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Tree View

- exam2d_2Dsf
 - Data Description
 - Default
 - Data Cubes
 - NMR_EXP3_PROC1_FTSPECTRUM_2RR
 - Measures
 - AFR_0001588
 - Dimensions
 - NMR_EXP3_FID_RAWDATA_2I
 - Measures
 - AFR_0001588
 - Dimensions
 - Data Package
 - exam2d_2Dsf



Data Description Table [D:\ADF\NMRTestSuite\exam2d_2Dsf.adf]

Named Set: Default

Search

Subject Predicate Object

Drag a column header here to group by that column

| Subject | Predicate | Object |
|--|--|--|
| urn:uuid:41d7ba3a-4f06-4c50-83bb-4... | http://www.w3.org/1999/02/22-rdf-sy... | http://purl.boehringer-igelheim.com... |
| urn:uuid:41d7ba3a-4f06-4c50-83bb-4... | http://purl.lallotrope.org/ontologies/p... | EXP0003-PROC0001 |
| urn:uuid:d30bf13e-c157-41c8-a2e3-a... | http://www.w3.org/1999/02/22-rdf-sy... | ACQTO--A2-E001 |
| urn:uuid:d30bf13e-c157-41c8-a2e3-a... | http://purl.obolibrary.org/obo/RO_00... | urn:uuid:41d7ba3a-4f06-4c50-83bb-4... |
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| urn:uuid:2b4eab69-2ac9-4fbe-b2b4-a... | http://www.w3.org/1999/02/22-rdf-sy... | AMP--A2-E001 |
| urn:uuid:2b4eab69-2ac9-4fbe-b2b4-a... | http://purl.obolibrary.org/obo/RO_00... | urn:uuid:41d7ba3a-4f06-4c50-83bb-4... |
| urn:uuid:2b4eab69-2ac9-4fbe-b2b4-a... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:2b4eab69-2ac9-4fbe-b2b4-a... | http://qudt.org/schema/qudt#numeri... | 100.0 |
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| urn:uuid:e316cce7-5ac6-4592-93ac-5... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:e316cce7-5ac6-4592-93ac-5... | http://qudt.org/schema/qudt#numeri... | 100.0 |
| urn:uuid:fcee1004-9d0d-4f4e-a94f-98... | http://www.w3.org/1999/02/22-rdf-sy... | AMP--A2-E003 |
| urn:uuid:fcee1004-9d0d-4f4e-a94f-98... | http://purl.obolibrary.org/obo/RO_00... | urn:uuid:41d7ba3a-4f06-4c50-83bb-4... |
| urn:uuid:fcee1004-9d0d-4f4e-a94f-98... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
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| urn:uuid:27e60837-faa3-4885-8d1e-a... | http://www.w3.org/1999/02/22-rdf-sy... | AMP--A2-E004 |
| urn:uuid:27e60837-faa3-4885-8d1e-a... | http://purl.obolibrary.org/obo/RO_00... | urn:uuid:41d7ba3a-4f06-4c50-83bb-4... |
| urn:uuid:27e60837-faa3-4885-8d1e-a... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:27e60837-faa3-4885-8d1e-a... | http://qudt.org/schema/qudt#numeri... | 100.0 |
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| urn:uuid:053c1f00-ada6-447a-8c31-bf... | http://purl.obolibrary.org/obo/RO_00... | urn:uuid:41d7ba3a-4f06-4c50-83bb-4... |
| urn:uuid:053c1f00-ada6-447a-8c31-bf... | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |

Count: 16638



Tree View

Search

- exam2d_2Dsf
- Data Description
 - Default
- Data Cubes
- Data Package

Tab 1

Data Description Table [D:\ADF\NMRTestSuite\exam2d_2Dsf.adf]

Named Set: Default

Search

Subject Predicate Object

Drag a column header here to group by that column

| Subject | Predicate | Object |
|---|---|--|
| urn:uuid:41d7ba3a-4f06-4c50-83bb-4aa73f1679a1 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | http://purl.boehringer-ingenheim.com/ontologies/NMR#bi-a-BIA_000001001 |
| urn:uuid:41d7ba3a-4f06-4c50-83bb-4aa73f1679a1 | http://purl.allotrope.org/ontologies/property#AFX_0000690 | EXP0003-PROC0001 |
| urn:uuid:30bf13e-c157-41c8-a2e3-ad16542cf3a8 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | ACQT0--A2-E001 |
| urn:uuid:30bf13e-c157-41c8-a2e3-ad16542cf3a8 | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:41d7ba3a-4f06-4c50-83bb-4aa73f1679a1 |
| urn:uuid:30bf13e-c157-41c8-a2e3-ad16542cf3a8 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#MicroSecond |
| urn:uuid:30bf13e-c157-41c8-a2e3-ad16542cf3a8 | http://qudt.org/schema/qudt#numericValue | 1000000.0 |
| urn:uuid:2b4eab69-2ac9-4fbc-b2b4-a930fd58a439 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | AMP--A2-E001 |
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| urn:uuid:2b4eab69-2ac9-4fbc-b2b4-a930fd58a439 | http://qudt.org/schema/qudt#numericValue | 100.0 |
| urn:uuid:e316cce7-5ac6-4592-93ac-5eaec2c7ae78 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | AMP--A2-E002 |
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| urn:uuid:e316cce7-5ac6-4592-93ac-5eaec2c7ae78 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:e316cce7-5ac6-4592-93ac-5eaec2c7ae78 | http://qudt.org/schema/qudt#numericValue | 100.0 |
| urn:uuid:fcee1004-9d0d-4f4e-a94f-98d0e58f9ea4 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | AMP--A2-E003 |
| urn:uuid:fcee1004-9d0d-4f4e-a94f-98d0e58f9ea4 | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:41d7ba3a-4f06-4c50-83bb-4aa73f1679a1 |
| urn:uuid:fcee1004-9d0d-4f4e-a94f-98d0e58f9ea4 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:fcee1004-9d0d-4f4e-a94f-98d0e58f9ea4 | http://qudt.org/schema/qudt#numericValue | 100.0 |
| urn:uuid:27e60837-faa3-4885-8d1e-ab45942f651c | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | AMP--A2-E004 |
| urn:uuid:27e60837-faa3-4885-8d1e-ab45942f651c | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:41d7ba3a-4f06-4c50-83bb-4aa73f1679a1 |
| urn:uuid:27e60837-faa3-4885-8d1e-ab45942f651c | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |
| urn:uuid:27e60837-faa3-4885-8d1e-ab45942f651c | http://qudt.org/schema/qudt#numericValue | 100.0 |
| urn:uuid:053c1f00-ada6-447a-8c31-bfe8db0145e9 | http://www.w3.org/1999/02/22-rdf-syntax-ns#type | AMP--A2-E005 |
| urn:uuid:053c1f00-ada6-447a-8c31-bfe8db0145e9 | http://purl.obolibrary.org/obo/RO_0002350 | urn:uuid:41d7ba3a-4f06-4c50-83bb-4aa73f1679a1 |
| urn:uuid:053c1f00-ada6-447a-8c31-bfe8db0145e9 | http://qudt.org/schema/qudt#unit | http://qudt.org/vocab/unit#Percent |




Count: 16638

- **The BI/Pfizer implementation of the Allotrope leaf nodes dramatically simplified the converter.**
- **It has allowed great progress quickly and the development of a first draft more easily**
- **The leaf nodes approach has allowed Mestrelab to develop a proof of concept which is usable and providing value right away then allowing time to develop the cross-vendor ontologies for those parts where it makes sense.**
- **Users already have ADF file they can store, use, mine while development of ontologies are made in parallel**
- **Stepwise approach delivering value upfront to build on it**

- Please help us defining the most optimal next development steps:
- The audience can use any smartphone (Android) or iphone or tablet of computer to interactively participate to the poll:

 Respond at **PollEv.com/guydesmarque712**

 Text **GUYDESMARQUE712** to **22333** once to join,



Do you believe what is covered already in the converter is good enough for a first commercial version



Yes I want to start as soon as possible, I will update my saved files with the new converter from time

No I definitely want to see more capabilities

Maybe, don't know yet, need to discuss with you and see more details

to time

Start the presentation to see live content. Still no live content? Install the app or get help at PollEv.com/app





What is the most urgent next step, regarding raw data conversion?



A

Make the converter available in manual mode in the acquisition software

B

Convert the data on the fly right after the data are being acquired in automation

C

Both are equally urgent

D

None / Other

What is the next step in converting analyzed /results data to ADF




Peaks and
multiplets list

Assignments
(linking
chemical
structure to a
spectrum)

Quantification
results

Others

Adding
analyzed
data is not
needed



Are you considering converting legacy data and what is your time line

Yes, as soon as possible/available

Yes, in the coming 2 years (with a more advanced version of the converter)

Yes, in 2 to 5 years (when the converter will be very mature)

No



Where are you going to place the converted data?



A

A data Lake or equivalent NoSQL system

B

An SQL archiving system, an SDMS, a DB (Oracle or MySQL or PostgreSQL,..)

C

Other

What do you intend to do with the data stored as ADF files?

| A | B | C | D |
|-----------|-------------------------------------|------------------------------------|----------|
| Archiving | Read to other software for analysis | Interface with mining capabilities | Other |

Thank you for your help:

- *Paul-James Jones* (Boehringer Ingelheim)
- *Justin Van Duine* (Pfizer)
- *Bo Du* (Pfizer)
- *Nikolay Larin* (Mestrelab)
- *Felipe Seoane* (Mestrelab)

We are available the rest of the day, this evening and tomorrow at anytime, please feel free to connect with us if you are interested to discuss any further the current capabilities and your expectations for developing the converter. You can also send us an email to book an appointment at a specific time

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thank
you