

Mode Forward Language English
Traversal property instance of
Root item OpenChrom
Iterations Unlimited
Size property Click to set

Build Tools ▾

OpenChrom



chromatography software

Mode
Undirected

Language
English

Traversal property
developer

Root item
OpenChrom

Iterations
Unlimited

Size property
Click to set

Build Tools ▾

OpenChrom



Lablicate

Mode Forward Language English
Traversal property instance of
Root item Lablicate
Iterations Unlimited
Size property Click to set

Build Tools ▾

Lablicate



business

Mode Reverse Language English

Traversal property writable file format

Root item Allotrope Data Format

Iterations Unlimited

Size property Click to set

Build

Tools ▾

OpenChrom



Allotrope Data Format



Data Analysis

This is the main perspective. Most of the work is performed here.

MALDI-TOF MS

Inspect and compare spectra

HPLC DAD

Look at full wavelength data

PCA

Used for principal component analysis

Demo

Load a demo chromatogram.

ADF

ADF (Allotrope Data Format)

ASM

ASM (Allotrope Simple Model)



Marketplace

Get commercial platform extensions.

PCR

Polymerase Chain Reaction (PCR)









Plug-in Installation



Install plug-ins to handle vendor file formats or extend the platform with additional features.

Filter

-  **Agilent OpenLab HPLC-UV/Vis** Lablicate Converter License Terms 
Reads *.dx files.
-  **Allotrope Data Format** Lablicate End User License 
Reads and writes *.adf files.
-  **Allotrope Data Format** Lablicate End User License 
Reads and writes *.asm files.

Cancel

Finish



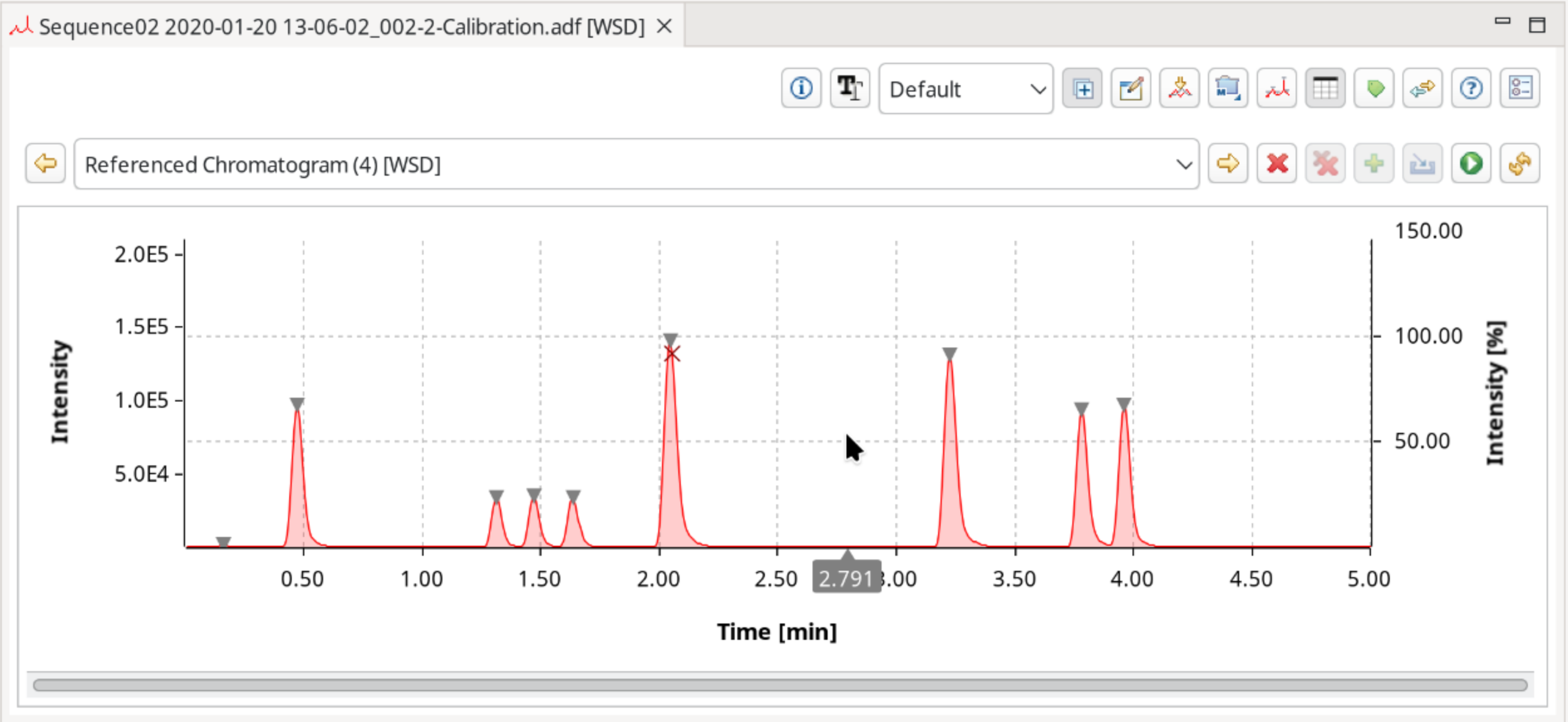
Data Project Explorer Sequences Peaks/Scans

Drives Home Workspace User Location

- ▼ Agilent
 - ▼ ADF
 - > Sequence02 2020-01-20 13-06-02_001-1-Blank.adf
 - > Sequence02 2020-01-20 13-06-02_002-2-Calibration.adf
 - > Sequence02 2020-01-20 13-06-02_003-3-Sample01.adf
 - > Sequence02 2020-01-20 13-06-02_004-4-Sample02.adf
 - > Sequence02 2020-01-20 13-06-02_005-5-QC.adf
 - > ASM
 - > ChemStation
- > MS
- > NMR

Select User Location

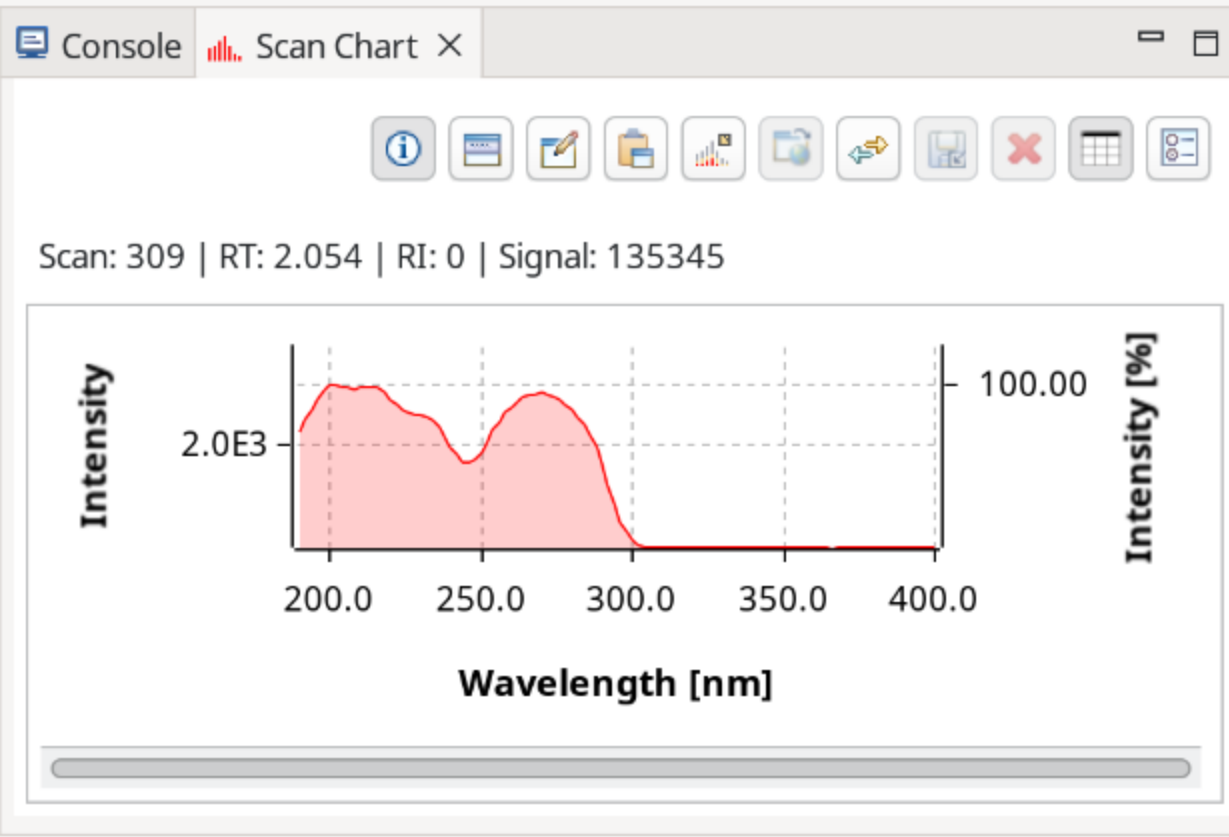
Open Selected Measurements



Edit History Targets

Edit History Events: 1

Description	Editor	Date
ADF export		Fri Oct 16 16



Feedback Scan Table ✕

Scan: 309 | RT: 2.054 | RI: 0 | Signal: 135345

Wavelength [nm]	Intensity	Intensity [%]
190.0	2232.2498	70.7546
192.0	2453.6138	77.7710
194.0	2690.3301	85.2741
196.0	2874.9934	91.1273
198.0	3037.8784	96.2902
200.0	3151.0102	100.0000

Signals: 106



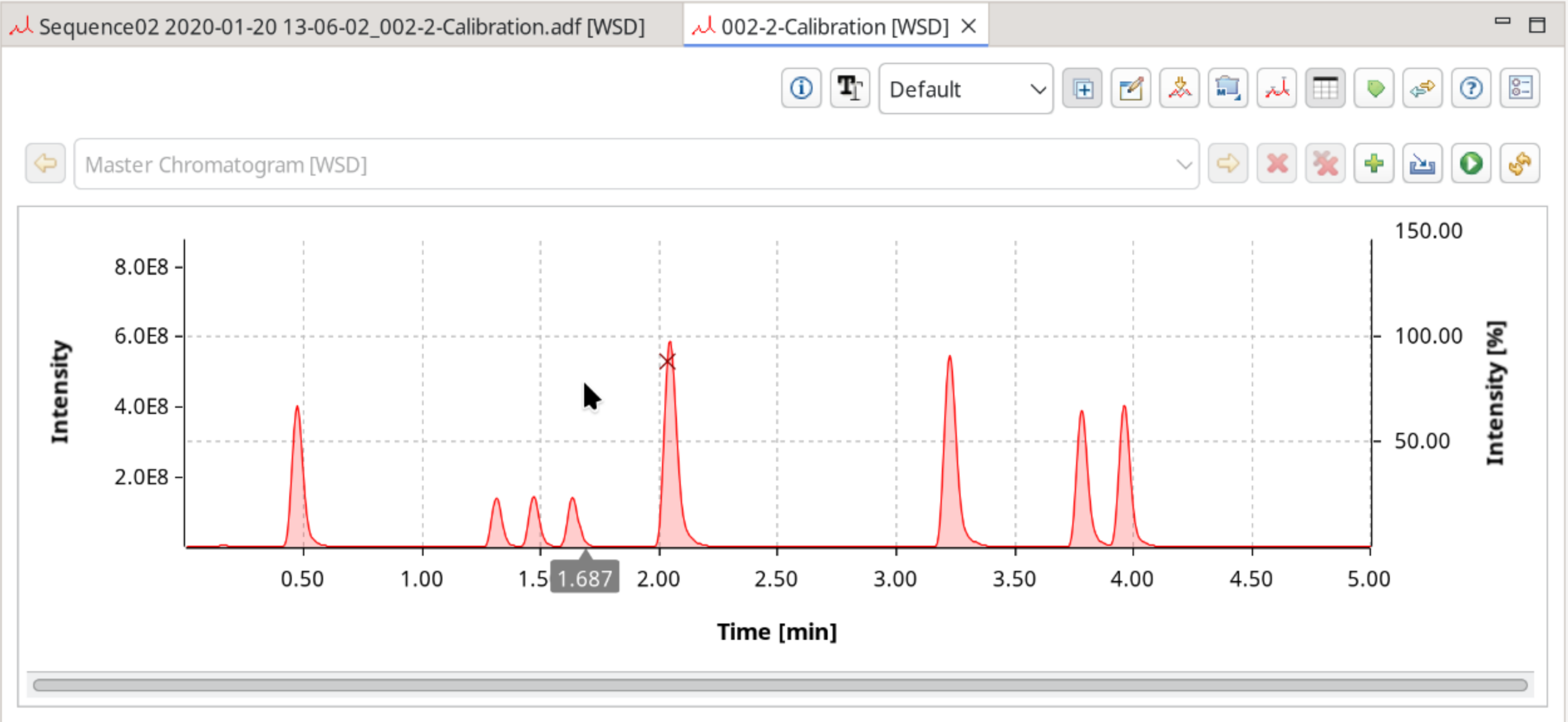
Data Project Explorer Sequences Peaks/Scans

Drives Home Workspace User Location

- Agilent
 - ADF
 - Sequence02 2020-01-20 13-06-02_001-1-Blank.adf
 - Sequence02 2020-01-20 13-06-02_002-2-Calibration.adf
 - ACQRES.REG
 - CSlbk.ini
 - DAMETHOD.REG
 - INFO.MTH
 - RECALIB.MTH
 - rpthhead.txt
 - DAD1.UV**

Select User Location

Open Selected Measurements

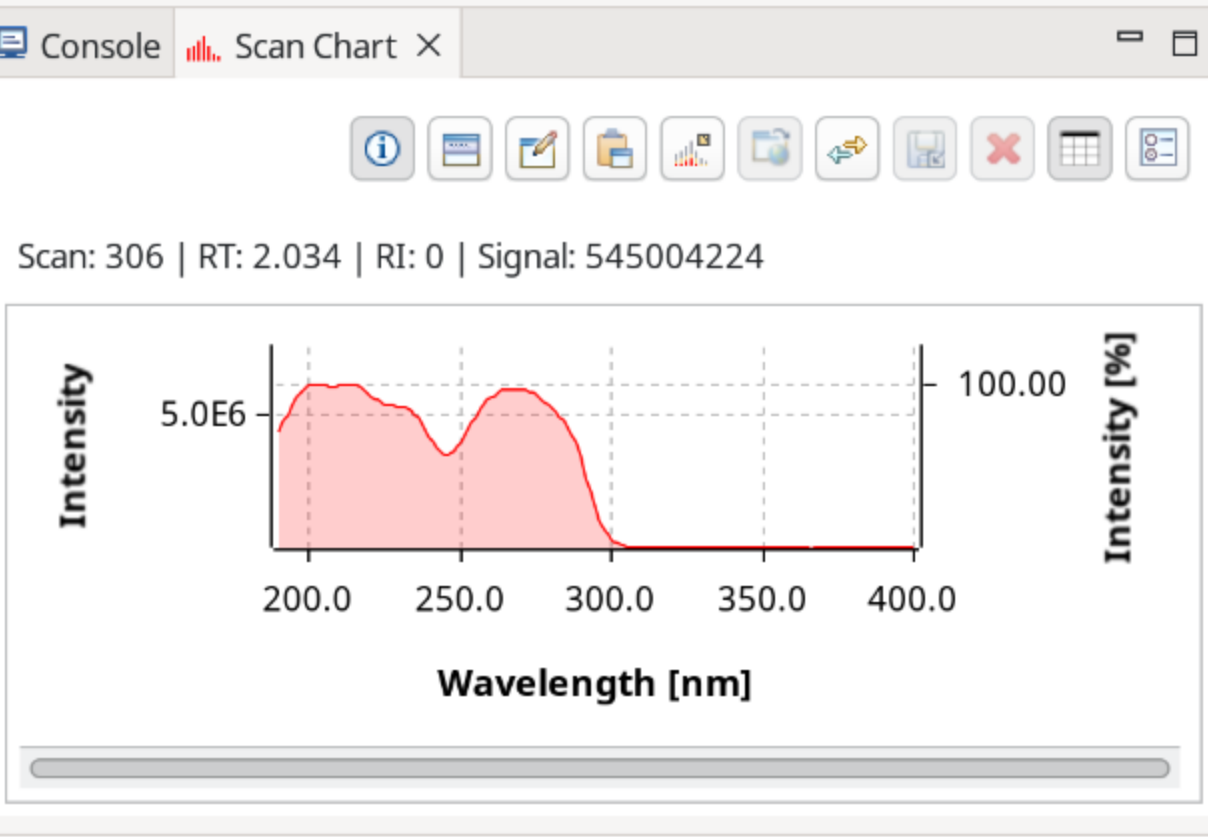


Edit History Targets Header Data X

Number Entries: 32 / 32

Name	Value
Barcode	
Barcode Type	
Batch Number	ColDescription)
Column	LC
Comment	IsHW
Data Name	

Table Miscellaneous Findings



Feedback Scan Table X

Scan: 306 | RT: 2.034 | RI: 0 | Signal: 545004224

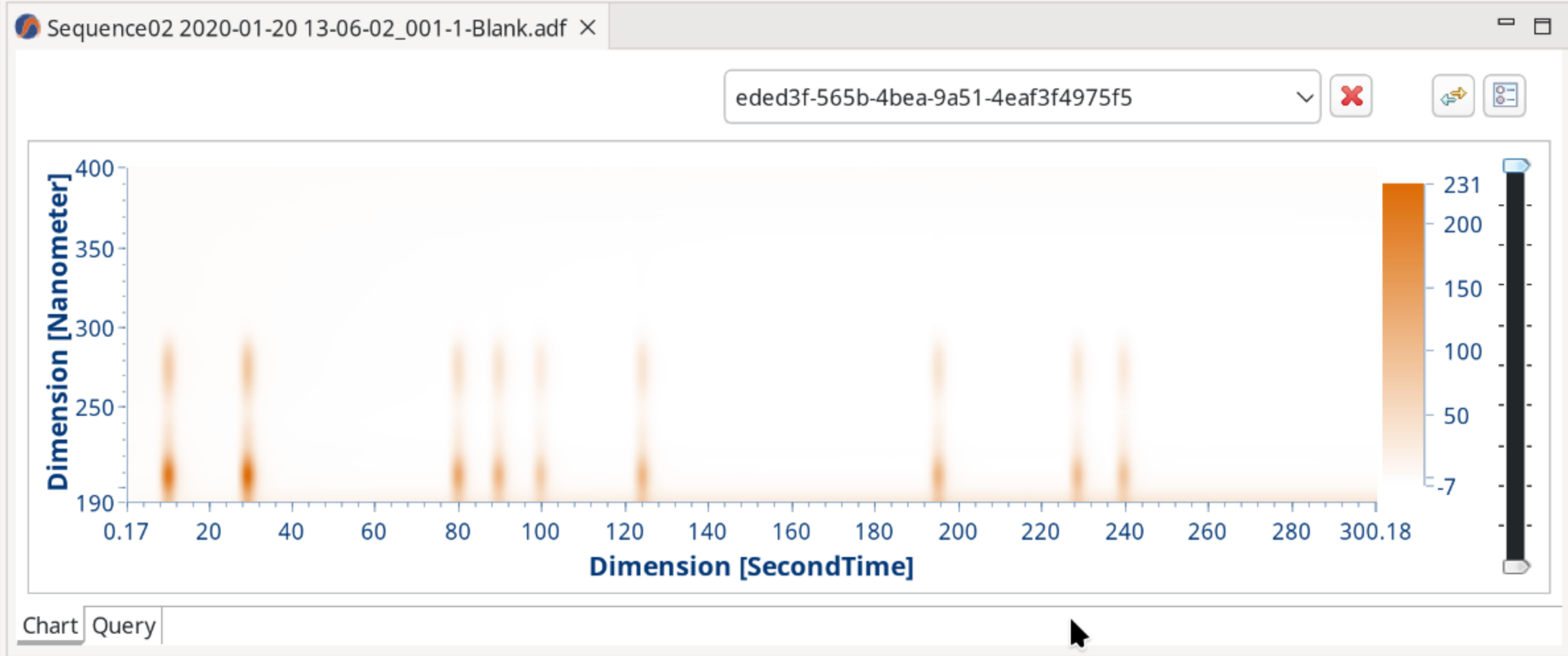
Wavelength [nm]	Intensity	Intensity [%]
190.0	4383841.0	71.5530
191.0	4587400.5	74.8755
192.0	4790960.0	78.1979
193.0	5030258.5	82.1038
194.0	5269557.0	86.0096
195.0	5440440.5	89.7040

Signals: 211



File Explorer

- ▼ HPLC-DAD
 - > ASM
 - ▼ Agilent
 - ▼ ADF
 - Sequence02 2020-01-20 13-06-02_001-1-Blank.adf
 - Sequence02 2020-01-20 13-06-02_002-2-Calibration.adf
 - Sequence02 2020-01-20 13-06-02_003-3-Sample01.adf
 - Sequence02 2020-01-20 13-06-02_004-4-Sample02.adf
 - Sequence02 2020-01-20 13-06-02_005-5-QC.adf
 - > ASM
 - > ChemStation
 - > MS



Data Package

- ▼ ChemStation
 - ▼ 001-1-Blank.D
 - ACQRES.REG
 - CSlbk.ini
 - ▼ DA.M
 - DAMETHOD.REG
 - INFO.MTH
 - RECALIB.MTH
 - rpthead.txt
 - DAD1.UV
 - DAD1A.ch
 - DAD1B.ch

Data Model Table **Data Model Graph**

Subject	Predicate	Object
2311c03b:17531d94069:-7cb8	type	globally unique identifier
2311c03b:17531d94069:-7cb8	identifies	urn:uuid:2e39b969-d8ca-4355-ac7a-a7e3c4e9d789
2311c03b:17531d94069:-7cb8	has value	311ea059-71cc-49c0-ba21-4ba5238183e1
2311c03b:17531d94069:-7cb9	type	chromatographic peak resolution using peak width at half-height
2311c03b:17531d94069:-7cb9	unit	Unitless
2311c03b:17531d94069:-7cb9	numeric value	2.1969453829144
2311c03b:17531d94069:-7cba	type	chromatographic peak resolution using baseline peak widths
2311c03b:17531d94069:-7cba	unit	Unitless
2311c03b:17531d94069:-7cba	numeric value	2.26994914940013
2311c03b:17531d94069:-7cbb	type	asymmetry factor measured at 5 % height
2311c03b:17531d94069:-7cbb	unit	Unitless



File Explorer

- Fall 2024
 - Data
 - Export
 - FT-IR
 - GC-FID
 - ADF
 - allotrope-rec-2023-09-gas-chromatography.adf
 - ASM
 - GC-MS
 - HPLC-DAD
 - ASM

allotrope-rec-2023-09-gas-chromatography.adf X

cf308-2ce1-11b2-80b8-c809a8720912

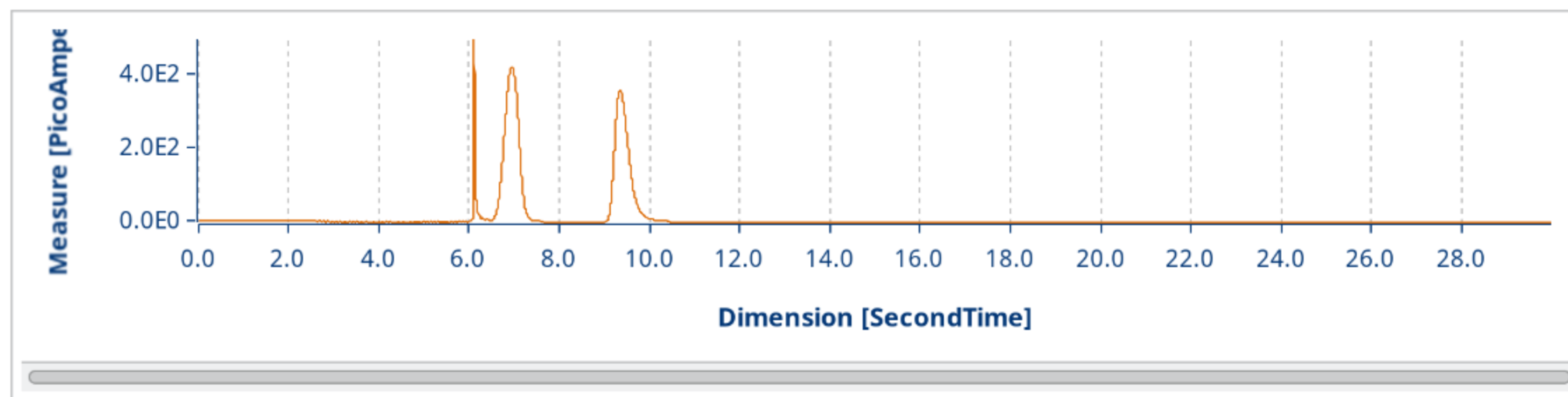
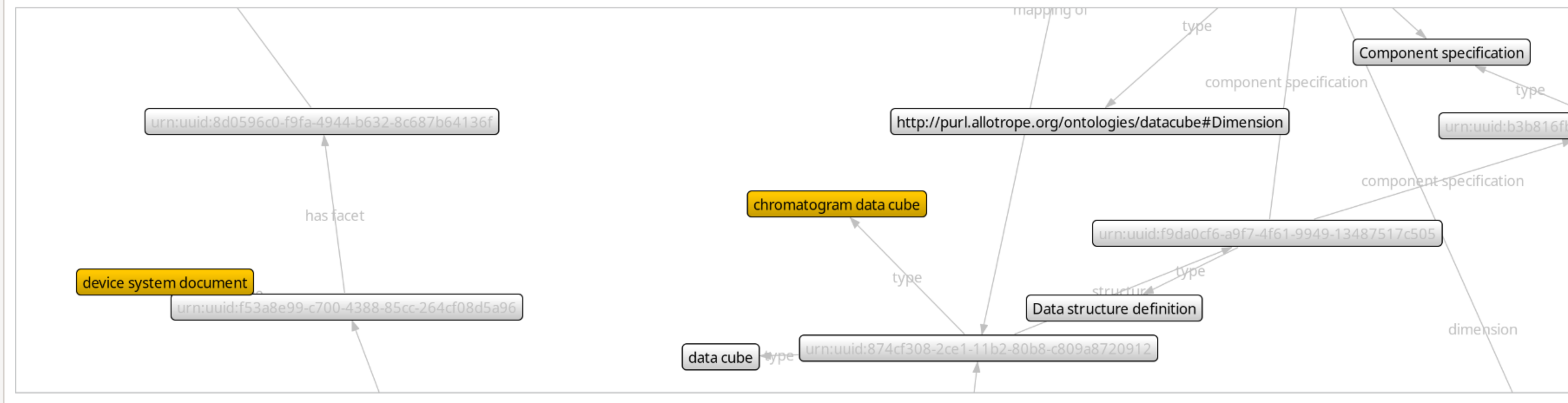


Chart Query

Data Model Table Data Model Graph





File Explorer

- ▼ HPLC-DAD
 - > ASM
 - ▼ Agilent
 - ▼ ADF
 - Sequence02 2020-01-20 13-06-02_001-1-Blank.adf
 - Sequence02 2020-01-20 13-06-02_002-2-Calibration.adf
 - Sequence02 2020-01-20 13-06-02_003-3-Sample01.adf
 - Sequence02 2020-01-20 13-06-02_004-4-Sample02.adf
 - Sequence02 2020-01-20 13-06-02_005-5-QC.adf
 - > ASM
 - > ChemStation
 - > MS
 - ▼ NMR

Sequence02 2020-01-20 13-06-02_003-3-Sample01.adf ×

```
PREFIX af-e: <http://purl.allotrope.org/ontologies/equipment#>
PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>

SELECT ?instance
WHERE {
  ?instance rdf:type af-e:AFE_0000224 .
}
```

Chart Query

Data Model Table | Data Model Graph

Subject	Predicate	Object
urn:uuid:203960b3-5c20-4c12-a2c0-79ac9135e0f7	has component	urn:uuid:3bd256cf-4198-49db-ace1-f2c948a042a2
urn:uuid:203960b3-5c20-4c12-a2c0-79ac9135e0f7	has component	urn:uuid:3df95ea4-8e7d-42a9-9733-3c0dd9bd64b4
urn:uuid:203960b3-5c20-4c12-a2c0-79ac9135e0f7	has component	urn:uuid:4ce74697-b773-4d4f-910c-1ff93da5d1a8
urn:uuid:203960b3-5c20-4c12-a2c0-79ac9135e0f7	has component	urn:uuid:46075b30-1a3e-410b-a96a-2d14421c9881
urn:uuid:203960b3-5c20-4c12-a2c0-79ac9135e0f7	has component	urn:uuid:41e00c04-a1ae-45a2-99c6-5fea79f1cd61
urn:uuid:203960b3-5c20-4c12-a2c0-79ac9135e0f7	type	high-performance liquid chromatograph

Console | Audit Trail

Messages

6 results.

File Explorer

- HPLC-DAD
 - ASM
 - Agilent
 - ADF
 - Sequence02 2020-01-20 13-06-02_001-1-Blank.adf
 - Sequence02 2020-01-20 13-06-02_002-2-Calibration.adf
 - Sequence02 2020-01-20 13-06-02_003-3-Sample01.adf
 - Sequence02 2020-01-20 13-06-02_004-4-Sample02.adf
 - Sequence02 2020-01-20 13-06-02_005-5-QC.adf
 - ASM
 - ChemStation
 - MS
 - NMR

Sequence02 2020-01-20 13-06-02_003-3-Sample01.adf

```

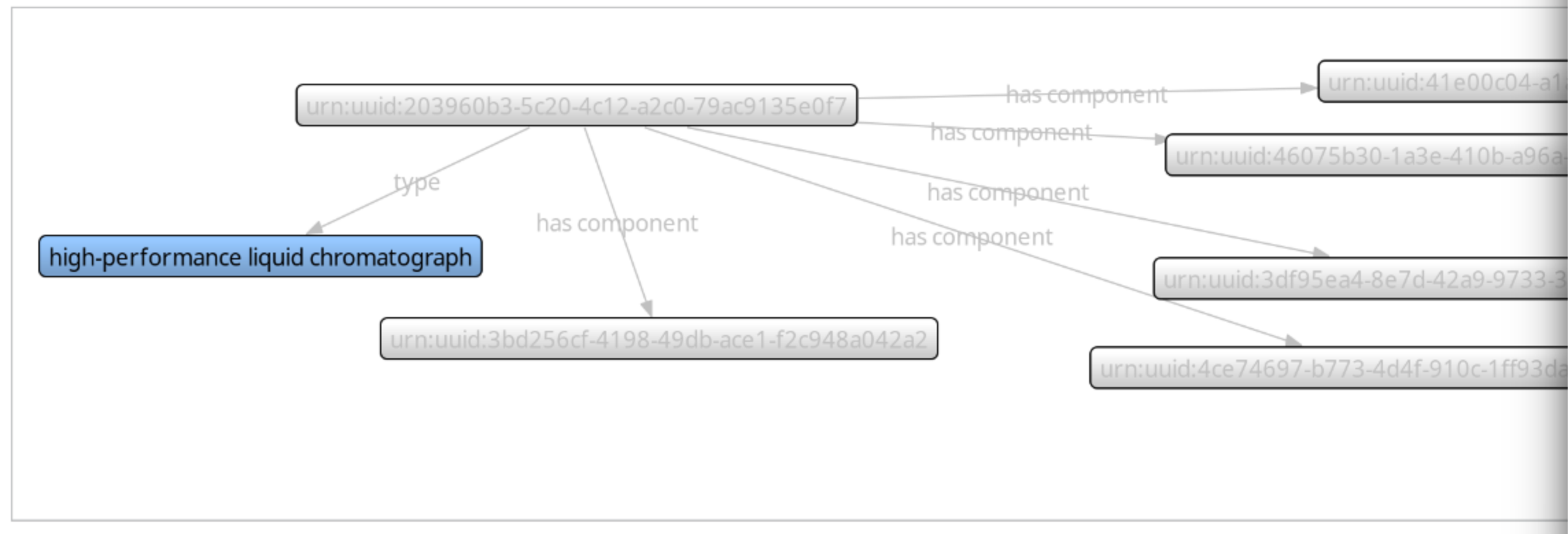
PREFIX af-e: <http://purl.allotrope.org/ontologies/equipment#>
PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>

SELECT ?instance
WHERE {
  ?instance rdf:type af-e:AFE_0000224 .
}

```

Chart Query

Data Model Table Data Model Graph



high-performance liquid chromatograph

(http://purl.allotrope.org/ontologies/equipment#AFE_0000224)

synonyms: HPLC system, high-performance liquid chromatography system

A high-performance liquid chromatograph is an instrument used for HPLC that is a technique in analytical chemistry used to separate the components in a mixture, to identify each component, and to quantify each component. It has pumps to pass a pressurized liquid solvent containing the sample mixture through a column filled with a solid adsorbent material. Each component in the sample interacts slightly differently with the adsorbent material, causing different flow rates for the different components and leading to the separation of the components as they flow out the column. [Wikipedia]

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defined in:

- <http://purl.allotrope.org/voc/afodomain/REC/2023/09/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2023/12/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2024/03/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2018/04/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2018/07/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2018/11/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2019/03/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2019/06/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2019/09/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2019/12/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2020/03/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2020/06/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2020/09/lc>
- <http://purl.allotrope.org/voc/afodomain/REC/2020/12/lc>



- ▼ Allotrope Connect
 - ▼ Fall 2024
 - ▼ Data
 - Export
 - > FT-IR
 - > GC-FID
 - > GC-MS
 - > HPLC-DAD
 - > MS
 - > NMR
 - > PCR

Select User Location

Open Selected Measurements

Name

Files: 0

Select data

Select files

Select items to process.

- ▼ Batch
 - ▼ Agilent
 - ▼ ChemStation
 - ▼ PARFUM MS
 - > 212 SEXY.D
 - > 24 FAUBOURG.D
 - > BLACK OPIUM.D
 - > POISON GIRL.D

Select User Location

Open Selected Measurements

Cancel

Finish

40.0 60.0 80.0 100.0 120.0

Ion [m/z]

Data Types: MSD Execute

profile

name

Description



No scan has been selected yet.

Ion [m/z]	Intensity	Intensity [%]
-----------	-----------	---------------

Signals: --



No target data has been selected yet.

Veri	Rati	Name	CAS	Match Factor	Re
------	------	------	-----	--------------	----

Auto Chromatogram



Data Project Seque Peaks/

Drives Home Workspace User Location

- > FT-IR
- > GC-FID
- > GC-MS
 - > ADF
 - > ASM
- > Batch
 - > Agilent
 - > ChemStation
 - > PARFUM MS
 - > 212 SEXY.D
 - > 24 FAUBOURG.D

Select User Location

Open Selected Measurements

Batch Job Demo X

Name	Path
212 SEXY.D	/home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/
POISON GIRL.D	/home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/
24 FAUBOURG.D	/home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/
BLACK OPIUM.D	/home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/

Files: 4

Data Types: MSD Execute

Default Profile

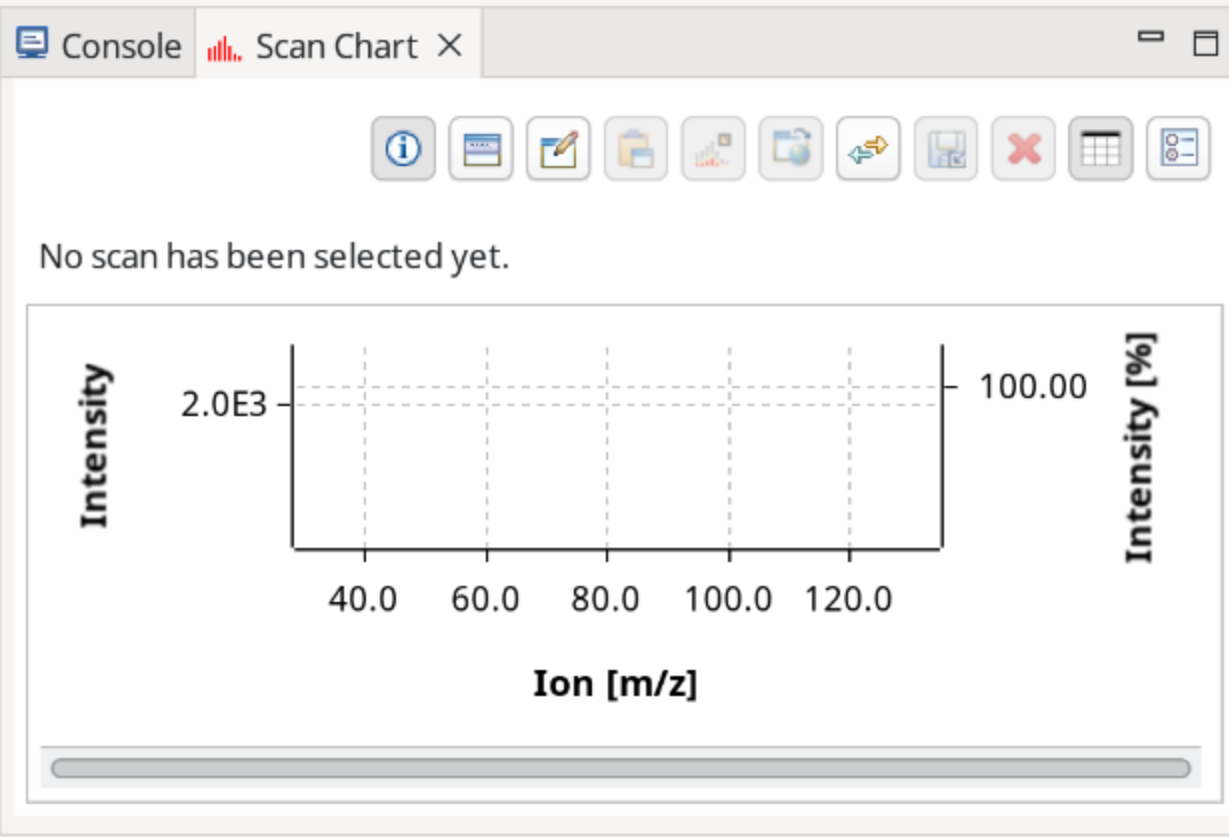
Name	Description
MCR-AR [Targeted]	A peak detector that first defines peak r
Peak Integrator Trapezoid	This extension point tries to implement a
High Pass Peaks	Keep the n-highest peaks
PBM	This plugin uses probability based mat
ASM GC-MS Chromatogram (*.json)	Reads and writes ASM chromatograms.

Edit History Targets X

No target data has been selected yet.

Veri	Rati	Name	CAS	Match Factor	Re
------	------	------	-----	--------------	----

Auto Chromatogram



Feedback Scan Table X

No scan has been selected yet.

Ion [m/z]	Intensity	Intensity [%]
-----------	-----------	---------------

Signals: --



Data Project Seque Peaks/

Drives Home Workspace User Location

- Data
 - Export
 - 212 SEXY.json
 - 24 FAUBOURG.json
 - BLACK OPIUM.json
 - POISON GIRL.json

Select User Location

Open Selected Measurements

Batch Job Demo x 212 SEXY.json [MSD]

Name	Path
212 SEXY.D	/home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Dat
POISON GIRL.D	/home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Dat
24 FAUBOURG.D	/home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Dat
BLACK OPIUM.D	/home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Dat

Files: 4

Data Types: MSD Execute

Default Profile

Name	Description
MCR-AR [Targeted]	A peak detector that first defines peak
Peak Integrator Trapezoid	This extension point tries to implement
High Pass Peaks	Keep the n-highest peaks
PBM	This plugin uses probability based ma
ASM GC-MS Chromatogram (*.json)	Reads and writes ASM chromatograms.

Type	Description	Message
✓ INFO	Peak Detector Targeted MCR-AR	262 peaks have been detected successfully.
✓ INFO	High Pass Peaks	The peak area is used to filter the peaks.
✓ INFO	Performance	13 ms/spectrum -> 50 spectra against the database (394054) took 651 ms
✓ INFO	ASM GC-MS Chromatogram (*.json)	Exported data to /home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/Export/POISON GIRL.json
✓ INFO	Batch Processor	Processing: /home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/GC-MS/Batch/Agilent/ChemStation/PARFUM MS/24 FAUBOURG.D completed
✓ INFO	Peak Detector Targeted MCR-AR	294 peaks have been detected successfully.
✓ INFO	High Pass Peaks	The peak area is used to filter the peaks.
✓ INFO	Performance	12 ms/spectrum -> 50 spectra against the database (394054) took 617 ms
✓ INFO	ASM GC-MS Chromatogram (*.json)	Exported data to /home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/Export/24 FAUBOURG.json
✓ INFO	Batch Processor	Processing: /home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/GC-MS/Batch/Agilent/ChemStation/PARFUM MS/BLACK OPIUM.D completed
✓ INFO	Peak Detector Targeted MCR-AR	217 peaks have been detected successfully.
✓ INFO	High Pass Peaks	The peak area is used to filter the peaks.
✓ INFO	Performance	13 ms/spectrum -> 50 spectra against the database (394054) took 651 ms
✓ INFO	ASM GC-MS Chromatogram (*.json)	Exported data to /home/mmailander/Dokumente/Allotrope Connect/Fall 2024/Data/Export/BLACK OPIUM.json

> Details

```
1 {
2   "$asm.manifest" : "http://purl.allotrope.org/manifests/gas-chromatography/REC/2024/09/gc-ms.tabular.manifest",
3   "gas chromatography aggregate document" : {
4     "gas chromatography document" : [ {
5       "analyst" : "Lic PA Groupe 1",
6       "measurement aggregate document" : {
7         "measurement document" : [ {
8           "sample document" : {
9             "description" : "",
10            "sample identifier" : "",
11            "written name" : "24 FAUBOURG"
12          },
13          "device control aggregate document" : {
14            "device control document" : [ {
15              "device type" : "mass selective detector",
16              "detection type" : "mass detection"
17            } ]
18          },
19          "detection type" : "mass detection",
20          "chromatogram data cube" : {
21            "label" : "MS1 data cube",
22            "cube structure" : {
23              "dimensions" : [ {
24                "@componentDatatype" : "double",
25                "concept" : "retention time",
26                "unit" : "s"
27              }, {
28                "@componentDatatype" : "double",
29                "concept" : "m/z",
30                "unit" : "m/z"
31              } ] ,
32              "measures" : [ {
33                "@componentDatatype" : "double",
34                "concept" : "intensity",
35                "unit" : "unitless"
36              } ]
37            },
38            "data" : {
106          }
107        },
108        "processed data aggregate document" : {
```



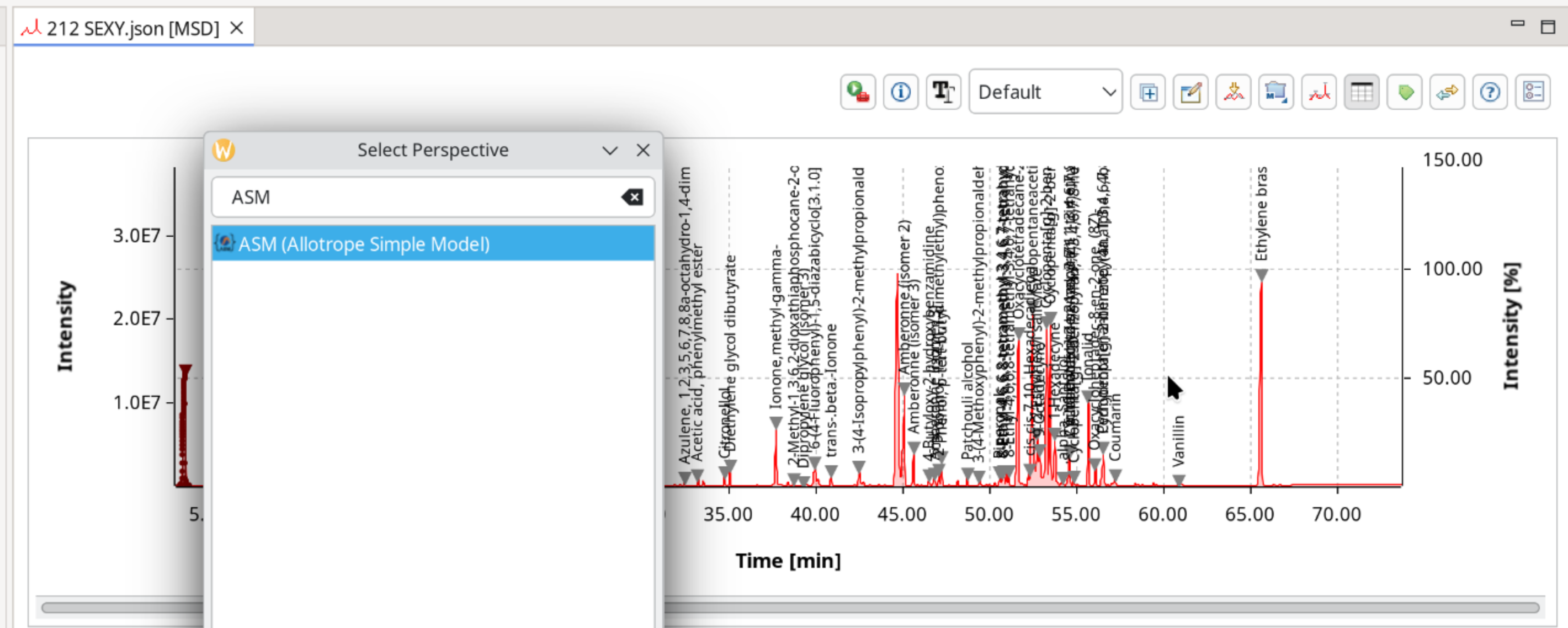

Data Project E Sequenc Peaks/Sc

Drives Home Workspace User Location

- Data
 - Export
 - 212 SEXY.json
 - 24 FAUBOURG.json
 - BLACK OPIUM.json
 - POISON GIRL.json
 - FT-IR
 - GC-FID
 - GC-MS
 - HPLC-DAD
 - MS

Select User Location

Open Selected Measurements



Select Perspective

- ASM
- ASM (Allotrope Simple Model)

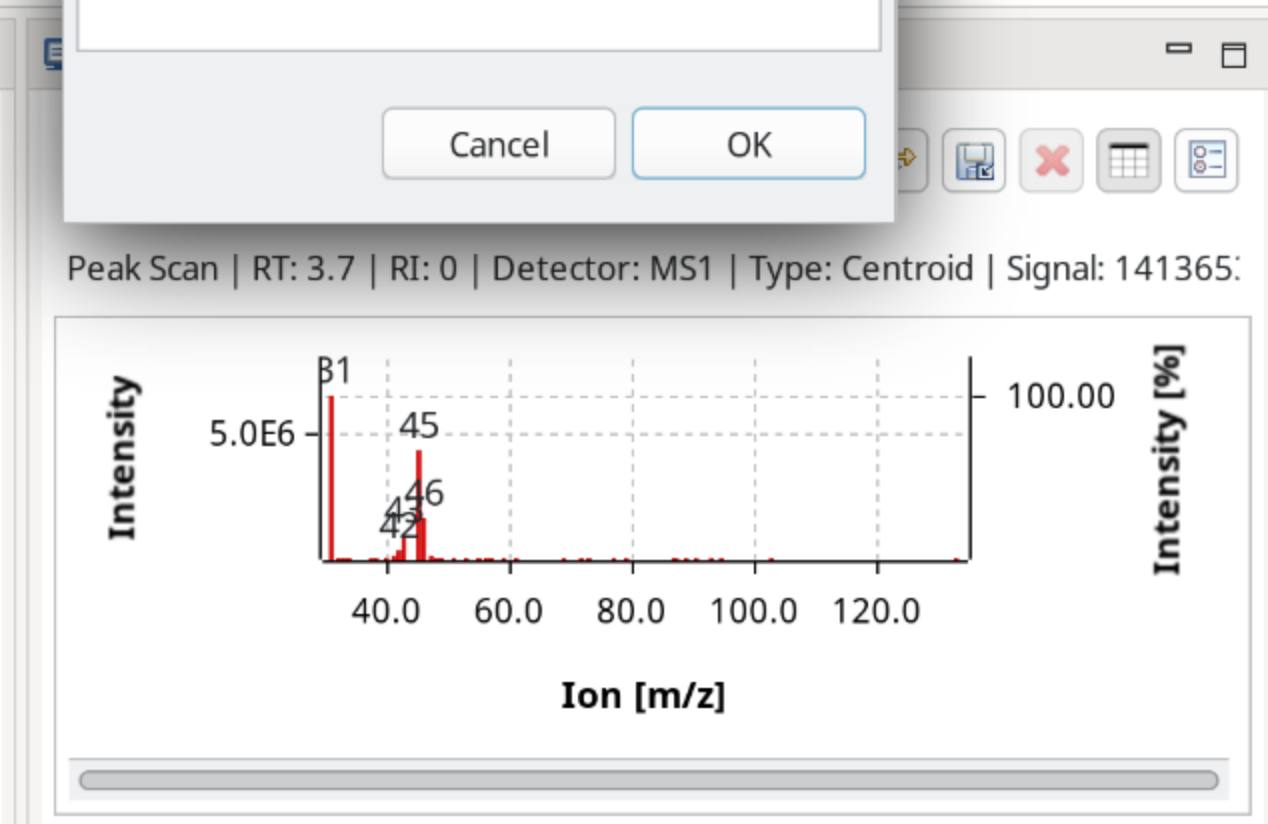
Cancel OK

Edit History Targets

Peak | Center RT: 3.7 | Center RI: 0 | Signal: 1226256323

Veri	Rati	Name	CAS	Match Factor	Re
				100.000	10

Auto Chromatogram



Feedback Scan Table

Peak Scan | RT: 3.7 | RI: 0 | Detector: MS1 | Type: Centroid | Signal: 141365:

Ion [m/z]	Intensity	Intensity [%]
31.2	6487109.5	100.0000
32.1	81263.1484	1.2527
33.1	18131.3164	0.2795
34.0	238.8329	0.0037
37.5	165.8839	0.0026
38.2	242.7602	0.0052

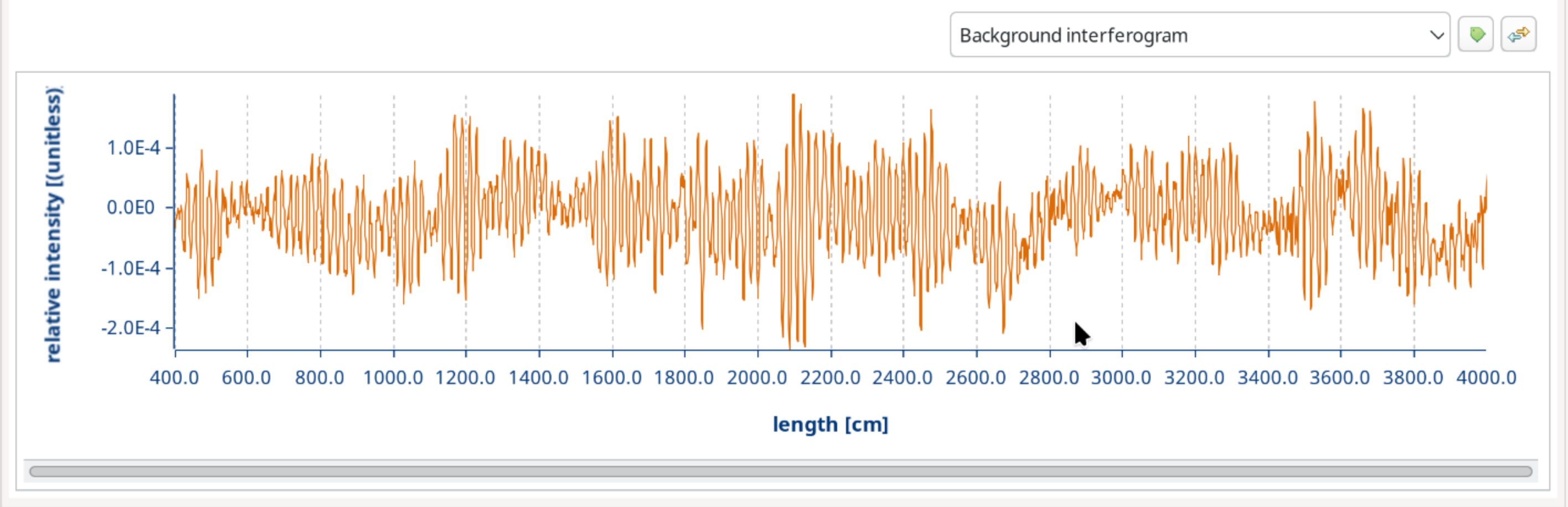
Signals: 36



File Explorer

- > Bilder
- > Daten
- ▼ Dokumente
 - ▼ Allotrope Connect
 - ▼ Fall 2024
 - ▼ Data
 - > Export
 - ▼ FT-IR
 - > ADF
 - ▼ ASM
 - allotrope-test-rec-2021-12-ftir.json
 - > GC-FID
 - > GC-MS
 - > HPLC-DAD
 - > MS
 - > NMR
 - > PCR
 - > Queries
 - > Slides
 - > Passwords
 - Downloads
 - > Entwicklung
 - Musik
 - > Nextcloud
 - > Schreibtisch
 - Videos
 - Vorlagen
 - Öffentlich

allotrope-test-rec-2021-12-ftir.json



Data Model Tree Data Model Graph

- ▼ Allotrope Simple Model
 - ▼ \$asm.manifest
 - <http://purl.allotrope.org/manifests/ftir/REC/2021/12/ftir.manifest>
 - ▼ analytical method identifier
 - AR-00000R0
 - ▼ analyst
 - Amgentoaks1
 - ▼ batch identifier
 - batch-number
 - ▼ detector type
 - DTGS (deuterated triglycine sulfate) KBr,MCT(Mercury cadmium telluride)
 - ▼ sample preparation description

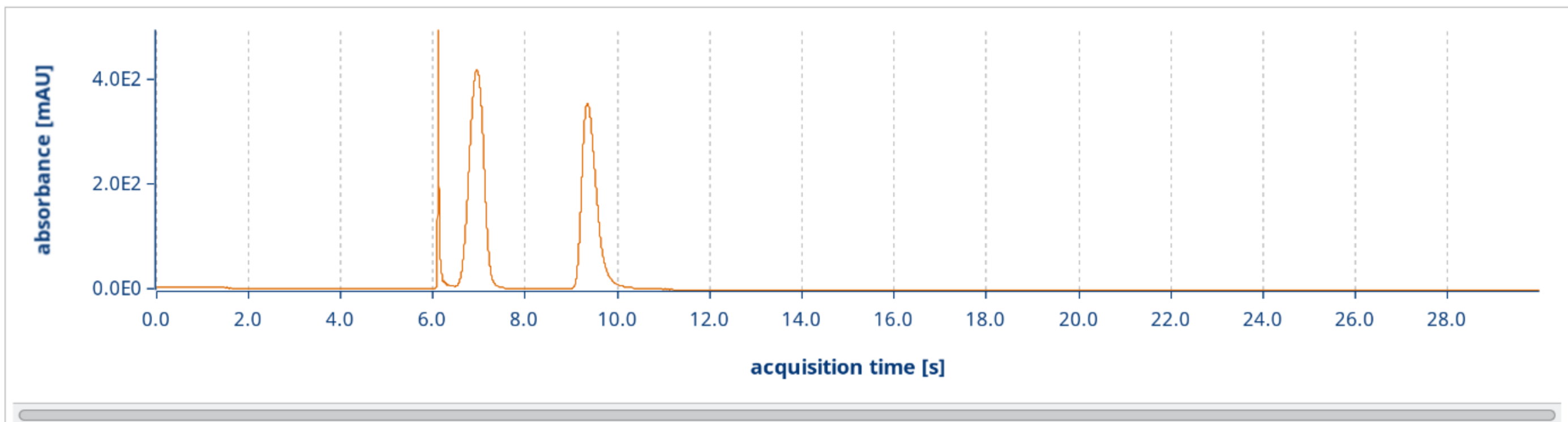


File Explorer

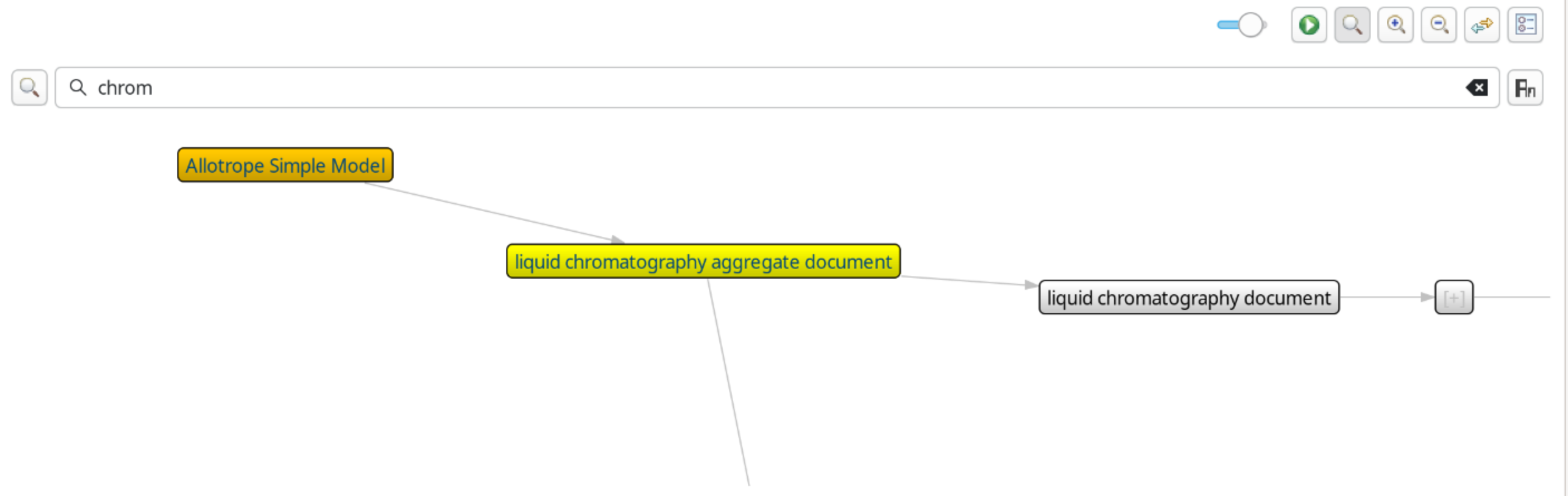
- > Bilder
- > Daten
- ▼ Dokumente
 - ▼ Allotrope Connect
 - ▼ Fall 2024
 - ▼ Data
 - > Export
 - > FT-IR
 - > GC-FID
 - > GC-MS
 - ▼ HPLC-DAD
 - ▼ ASM
 - allotrope-test-rec-2021-12-liquid-chro
 - allotrope-test-rec-2023-03-liquid-chro**
 - > Agilent
 - > MS
 - > NMR
 - > PCR
 - > Queries
 - > Slides
- > Passwords
- Downloads
- > Entwicklung
- Musik
- > Nextcloud
- > Schreibtisch
- Videos
- Vorlagen

allotrope-test-rec-2023-03-liquid-chromatography.json X

DAD1A chromatogram



Data Model Tree Data Model Graph





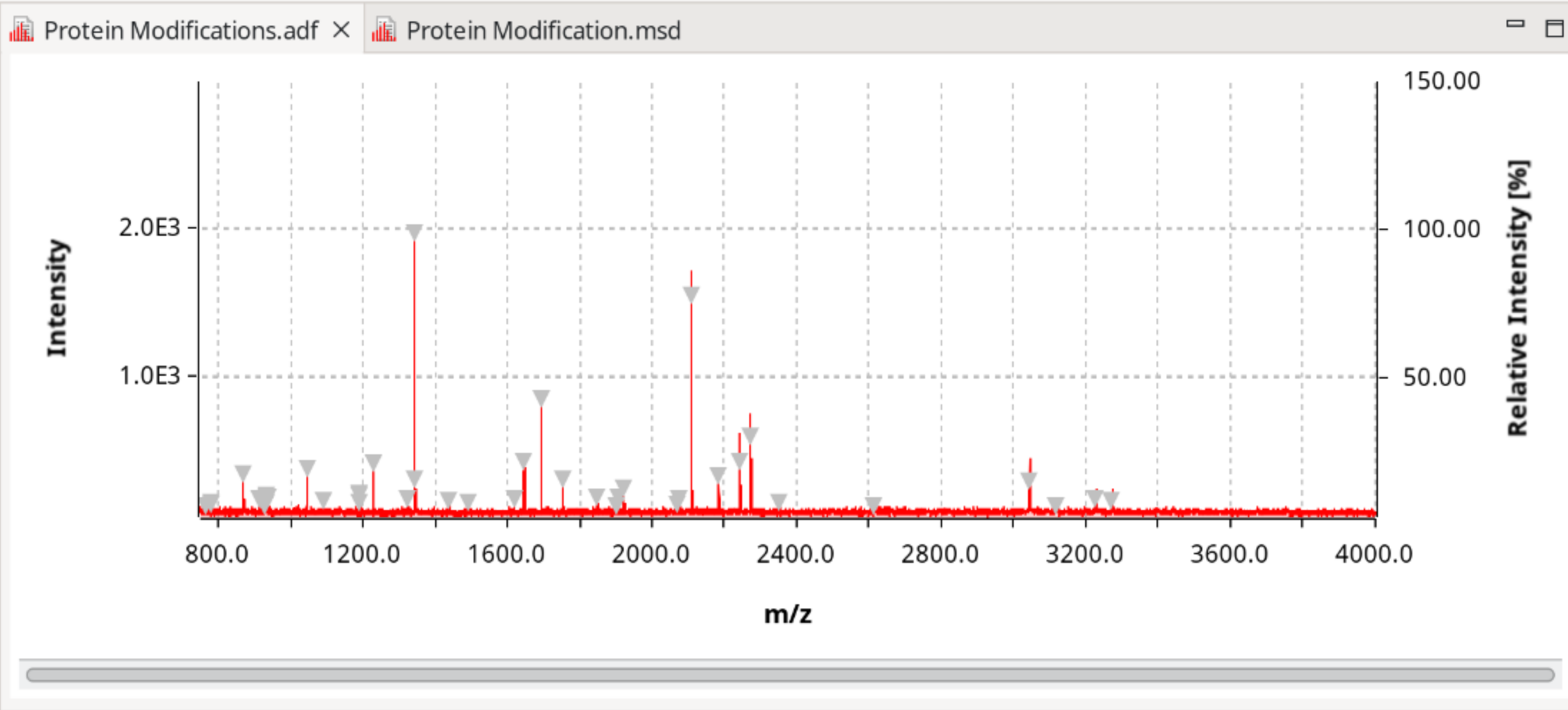
Mass Spectrum Fil Mass Spectrum H

Drives Home Workspace User Location

- Data
 - Export
 - 212 SEXY.json
 - 24 FAUBOURG.json
 - BLACK OPIUM.json
 - POISON GIRL.json
 - Protein Modifications.adf
 - Protein Modification.ms
 - FT-IR
 - GC-FID
 - GC-MS
 - HPLC-DAD
 - MS
 - ESI
 - MALDI TOF
 - Protein Modification.ms
 - NMR
 - PCR

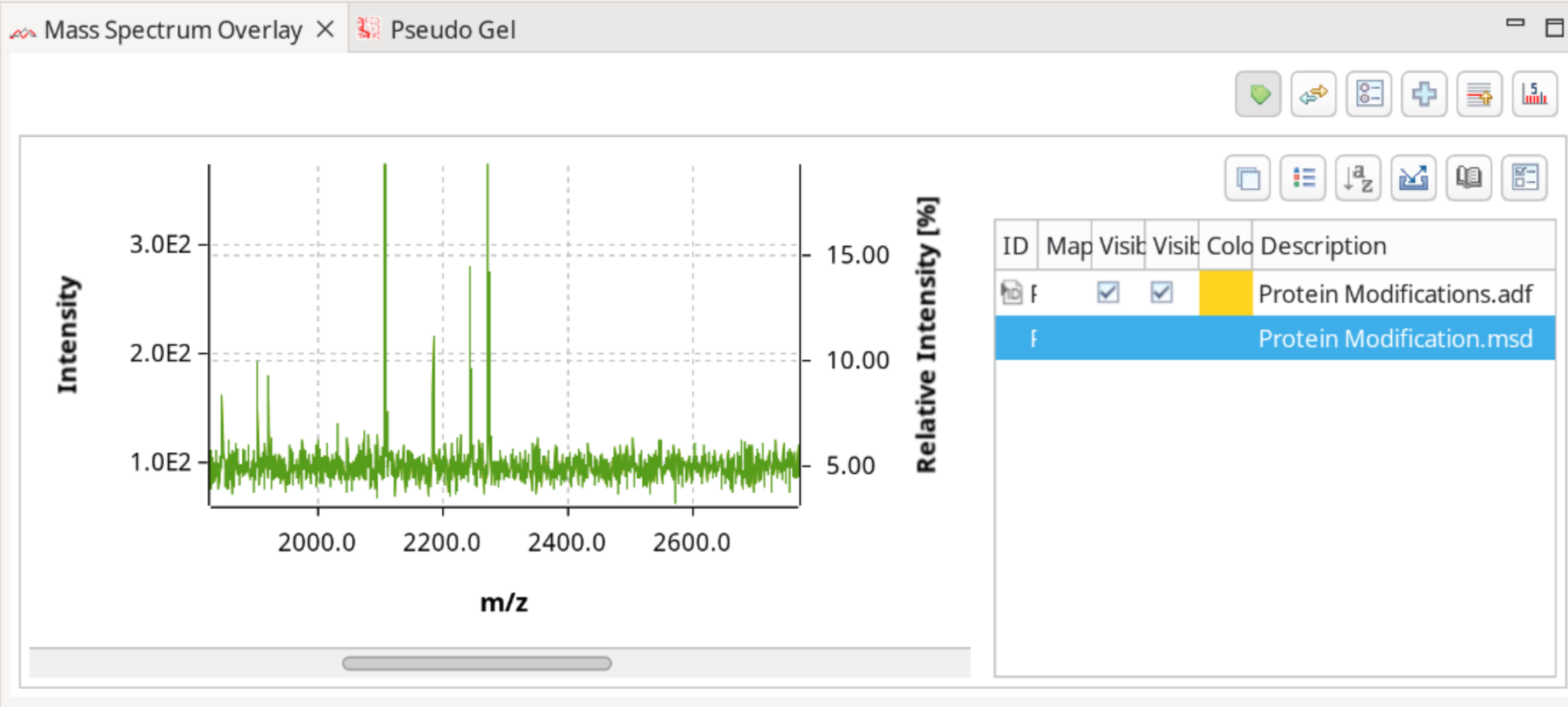
Select User Location

Open Selected Measurements



Mass Spectrum Peak List

m/z	abundance
870.46279	347
3043.54436	306
934.27241	206
1903.95275	189
2242.04368	431
1192.31229	221
3226.59515	185
1490.73675	162
930.25604	133
1044.59256	382
2272.18894	604
1093.53203	169
3271.60108	176
1751.89089	310
782.2952	157
2072.89622	183
1341.69648	316
933.2898	182
1342.70475	1956
2614.38139	132
1438.77659	170
1902.95519	135
2183.06605	341
1190.32269	209
3115.54447	132
940.44898	191
1227.50058	417
914.52138	182
1920.99041	256





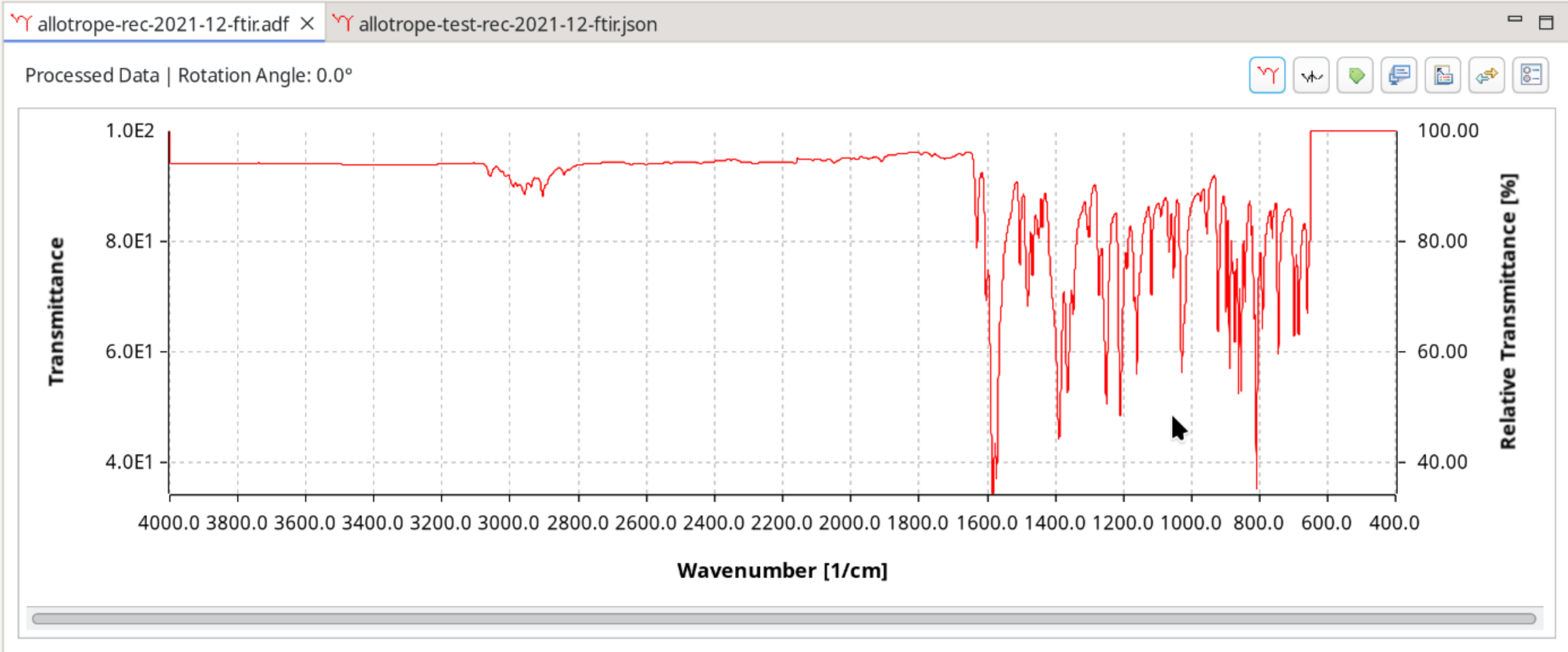
Data Projects Sequenc Peaks/Sc

Drives Home Workspace **User Location**

- ▼ Allotrope Connect
 - ▼ Fall 2024
 - ▼ Data
 - > Export
 - ▼ FT-IR
 - ▼ ADF
 - allotrope-rec-2021-12-ftir.adf
 - ▼ ASM
 - allotrope-test-rec-2021-12-ftir.json
 - > GC-FID
 - > GC-MS

Select User Location

Open Selected Measurements



Scan: 0 | RT: 0.0 | RI: 0 | Detector: MS1 | Type: Profile | Signal: 8196003

Veri	Rati	Name	CAS	Match Factor	Reverse Match	Match Factor D	Reverse

Auto Chromatogram

Type	Description	Message	Date	Proposed Solution

> Details



NMR Data Explorer Feedback

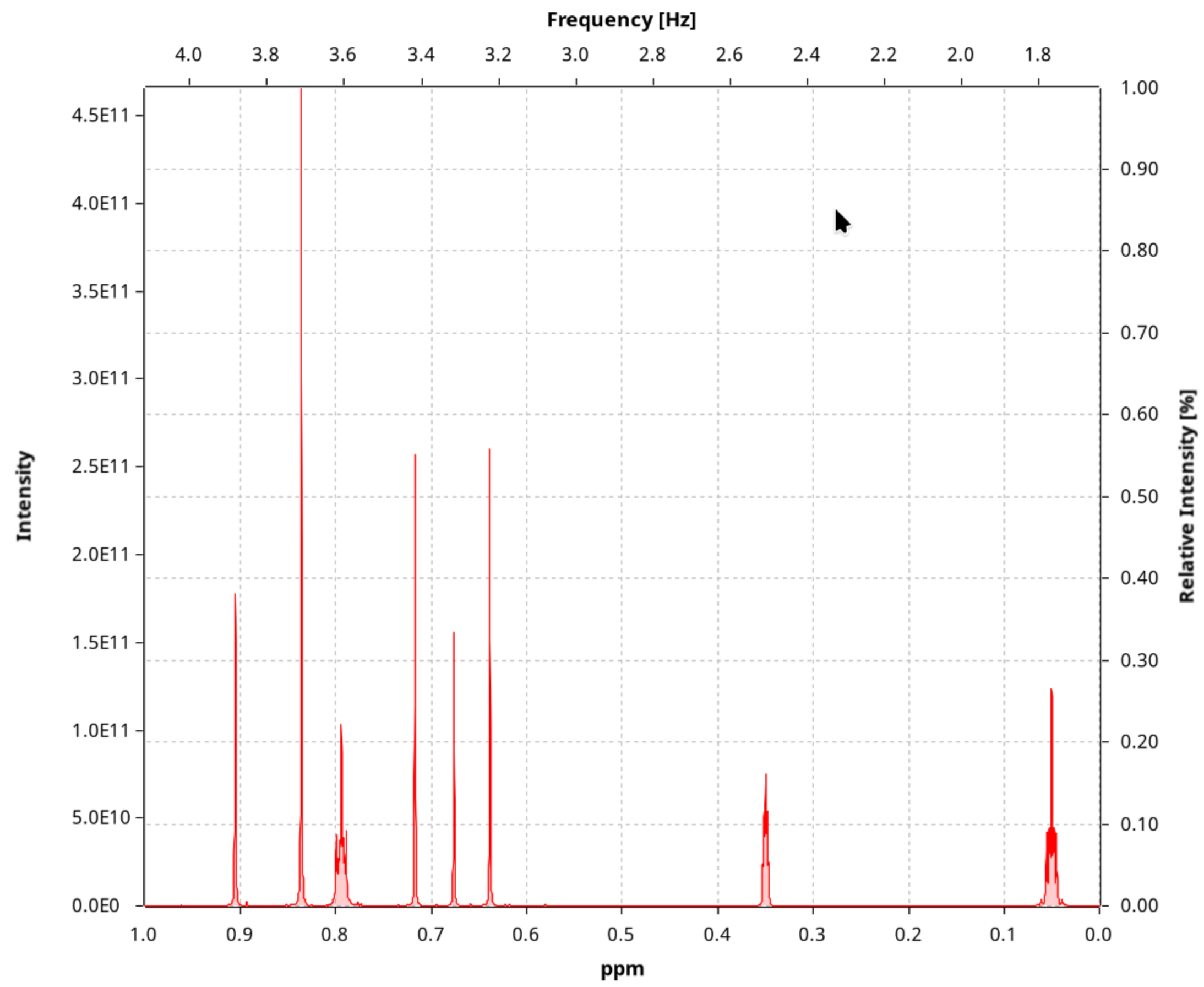
allotrope-rec-2022-03-qnmr.adf

Drives Home Workspace User Location

- Allotrope Connect
 - Fall 2024
 - Data
 - Export
 - FT-IR
 - GC-FID
 - GC-MS
 - HPLC-DAD
 - MS
 - NMR
 - ADF
 - allotrope-rec-2022-03-qnmr.adf
 - PCR
 - Queries
 - Slides

Select User Location

Open Selected Measurements



Measurements

Measurement Name	Value
------------------	-------



Data

Drives Home Workspace **User Location**

- MS
- NMR
- PCR
 - ASM
 - LightCycler
 - Food Virus.ixi**
- Queries

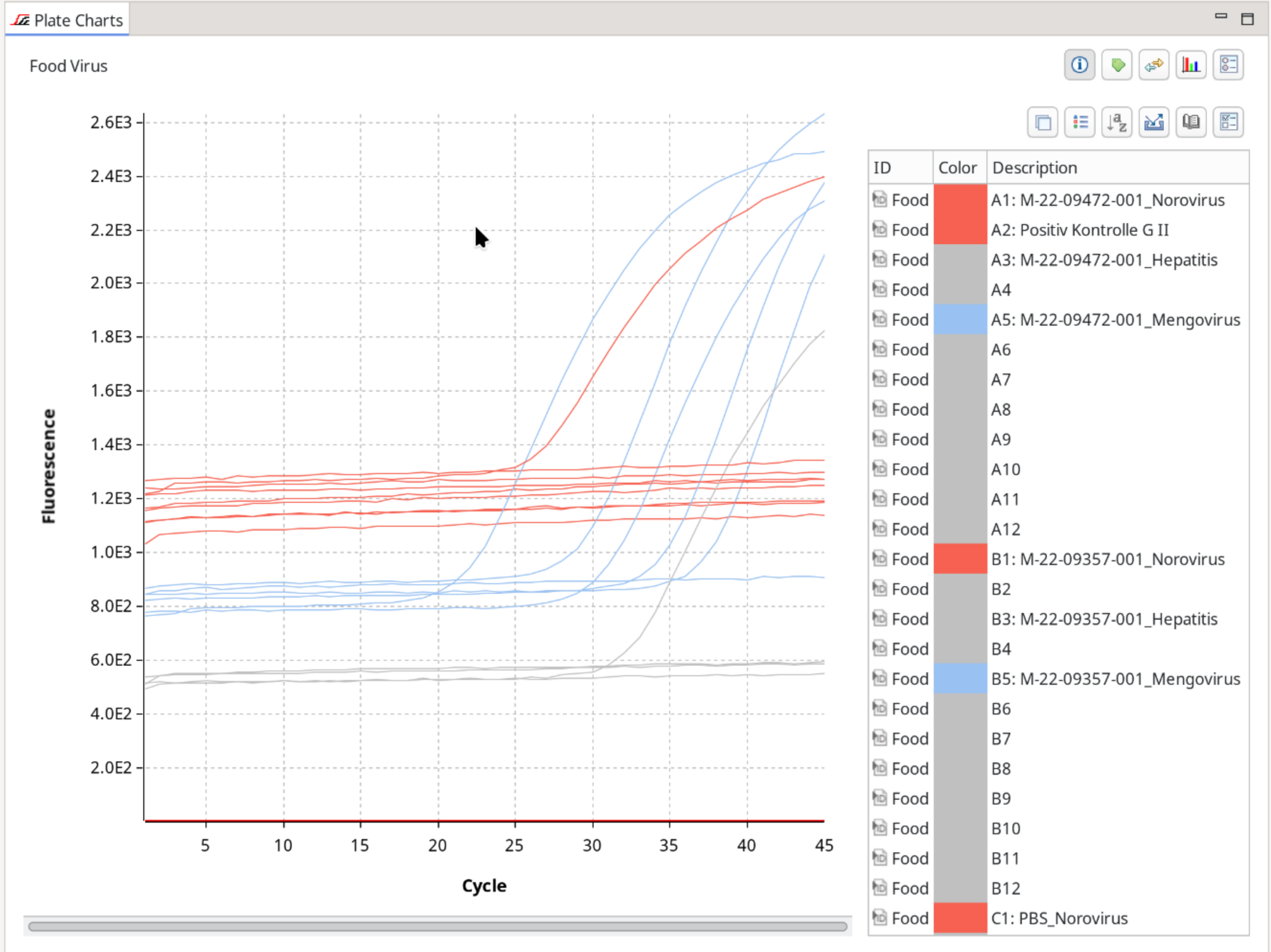
Select User Location

Open Selected Measurements

Food Virus.ixi

Wells: 96 All Subsets FAM

	1	2	3	4	5	6	7	8	9	10	11	12
A	A1	A2	A3	A4	A5	A6	A7	A8	A9	A1	A1	A1
B	B1	B2	B3	B4	B5	B6	B7	B8	B9	B1	B1	B1
C	C1	C2	C3	C4	C5	C6	C7	C8	C9	C1	C1	C1
D	D1	D2	D3	D4	D5	D6	D7	D8	D9	D1	D1	D1
E	E1	E2	E3	E4	E5	E6	E7	E8	E9	E1	E1	E1
F	F1	F2	F3	F4	F5	F6	F7	F8	F9	F1	F1	F1
G	G1	G2	G3	G4	G5	G6	G7	G8	G9	G1	G1	G1
H	H1	H2	H3	H4	H5	H6	H7	H8	H9	H1	H1	H1

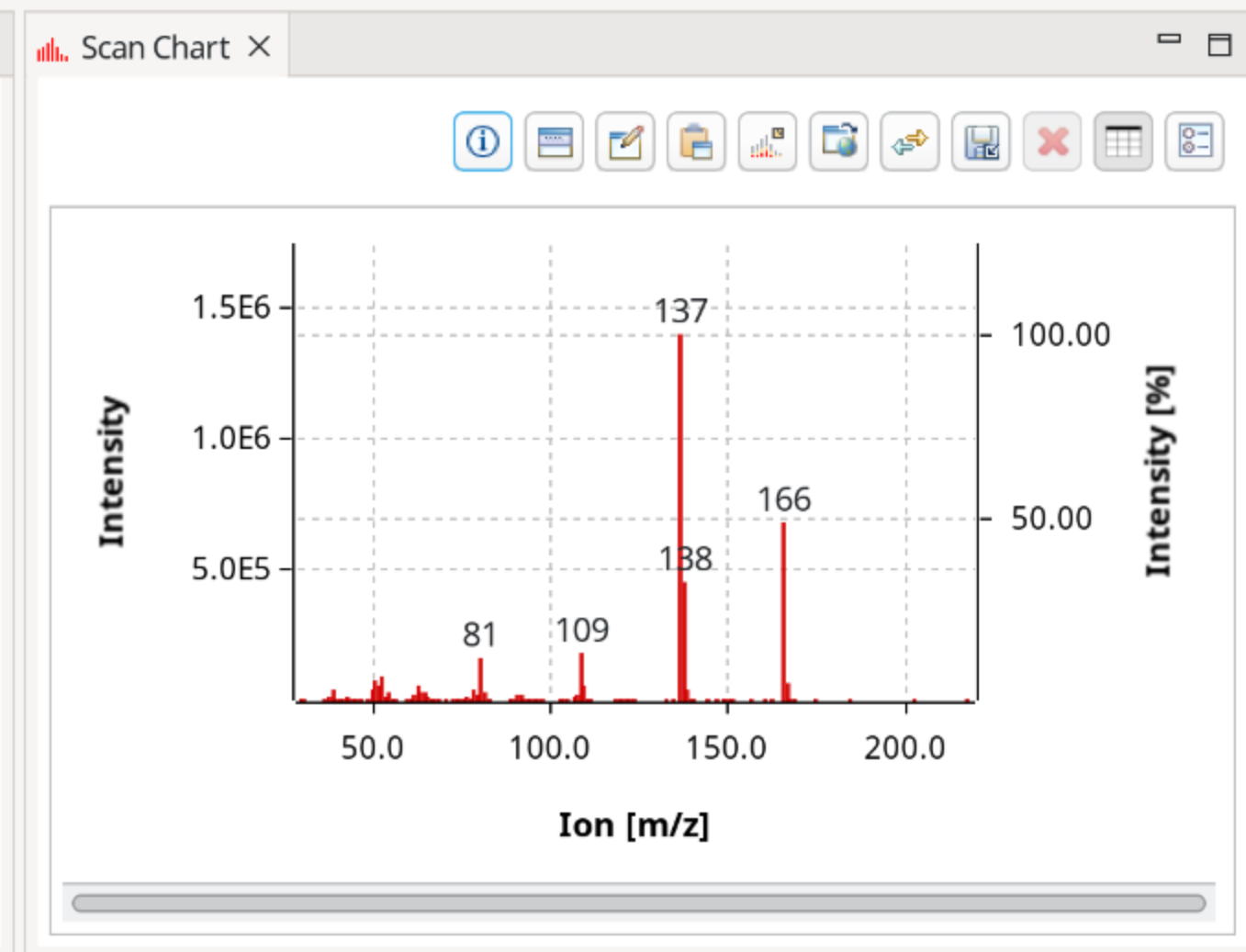
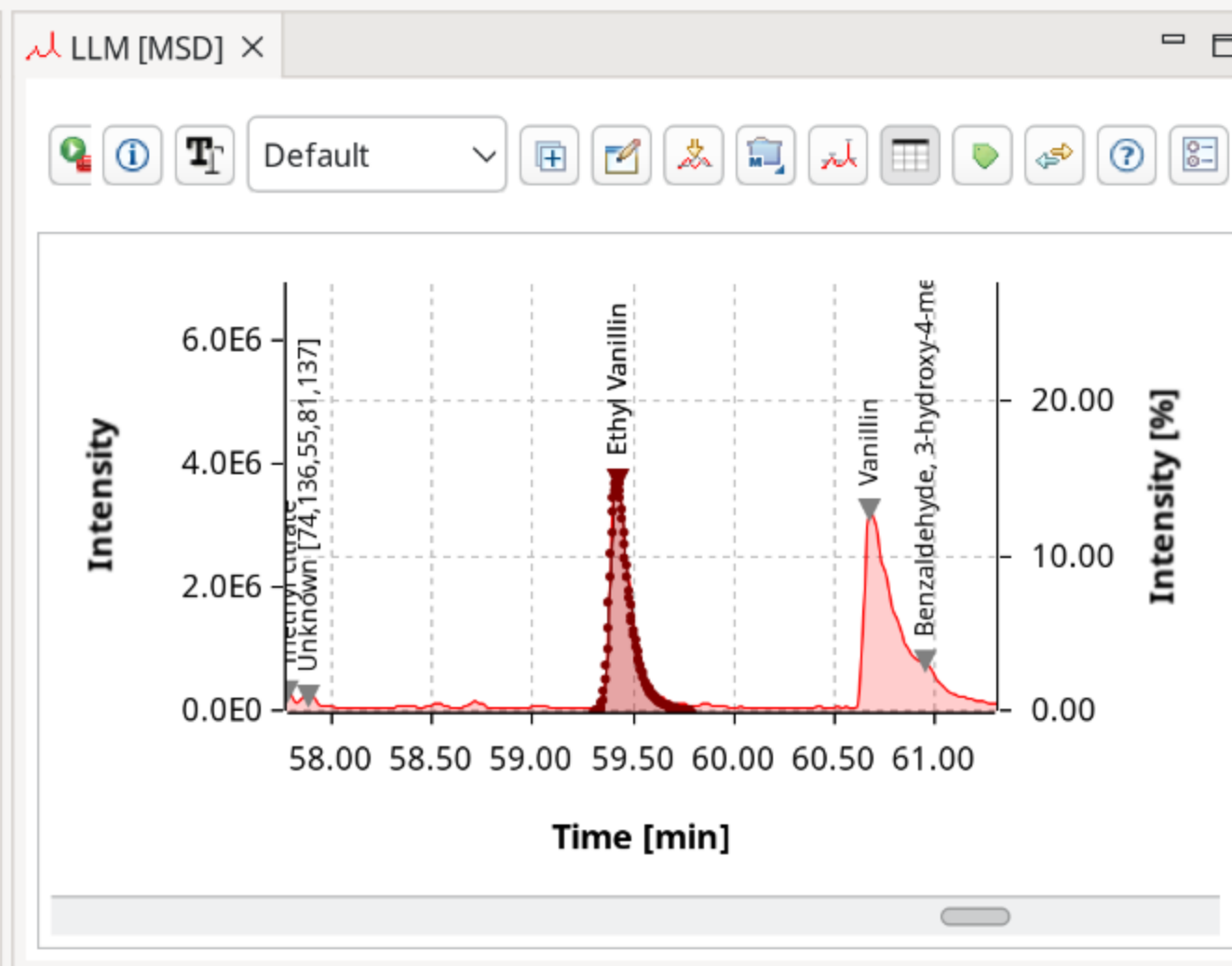




Chromatogram: LLM

Acti	Type	RT [min]	Area	S/N
<input checked="" type="checkbox"/>	PEAK	57.885	10809316	160.018
<input checked="" type="checkbox"/>	PEAK	59.426	266704202	2376.750
<input checked="" type="checkbox"/>	PEAK	60.676	303845619	2057.583
<input checked="" type="checkbox"/>	PEAK	60.948	40468427	512.974

Number Peaks: 4 / 100 | Scans: 0 / 0



Edit History Targets ×

Peak | Center RT: 59.426 | Center RI: 0 | Signal: 266704201

Veri	Rati	Name	CAS	Match Facto
		Ethyl Vanillin	121-32-4	95.400
<input type="checkbox"/>	<input checked="" type="checkbox"/>	Benzaldehyde, 4-ethoxy-3-	2539-53-9	92.800
<input type="checkbox"/>	<input checked="" type="checkbox"/>	Benzaldehyde, 4-(acetyloxy	72207-94-4	87.900
<input type="checkbox"/>	<input checked="" type="checkbox"/>	3,4-Dihydroxypropiopheno	7451-98-1	83.400
<input type="checkbox"/>	<input checked="" type="checkbox"/>	2,5-Dihydroxypropiopheno	938-46-5	83.100

Auto Chromatogram

Scan Explorer Feedback

Ask the AI agent

Citronellol ($C_{10}H_{20}O$) is a monoterpene, commonly featuring a long carbon chain with a hydroxyl group. When ionized, typically by Electrospray Ionization (ESI) or Electron Impact (EI) in a mass spectrometer, several fragmentation patterns can occur due to the cleavage of bonds in the molecule:

- m/z 69 (100%): This value represents the base peak and thus the most stable ion fragment. In monoterpenoids like citronellol, m/z 69 often corresponds to a $C_5H_9^+$ fragment, a common fragmentation product derived from the cleavage of the carbon chain.
- m/z 41 (79.446%): This is typically indicative of a $C_3H_5^+$ ion, which could arise from the cleavage and rearrangement of portions of the carbon backbone.
- m/z 67 (57.453%): This mass could represent a $C_5H_7^+$ ion, suggesting further fragmentation and loss of hydrogen atoms from the $C_5H_9^+$ fragment.
- m/z 81 (55.907%) and m/z 82 (54.803%): These ions suggest fragments that may contain the entire or parts of the alkene structure along with additional carbons and hydrogens, possibly a $C_6H_9^+$ and a $C_6H_{10}^+$ ion, respectively. $C_6H_{10}^+$ indicates the presence of an additional hydrogen, suggesting a hydrogen transfer or a less rearranged fragmentation pathway.
- m/z 55 (51.336%): This could be indicative of a $C_4H_7^+$ ion, suggesting a smaller alkyl chain fragment undergoing radical cation formation.



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Message the developers.



Data Analysis

This is the main perspective. Most of the work is performed here.

MALDI-TOF MS

Inspect and compare spectra

HPLC DAD

Look at full wavelength data

PCA

Used for principal component analysis

Demo

Load a demo chromatogram.

ADF

ADF (Allotrope Data Format)

ASM

ASM (Allotrope Simple Model)



Marketplace

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