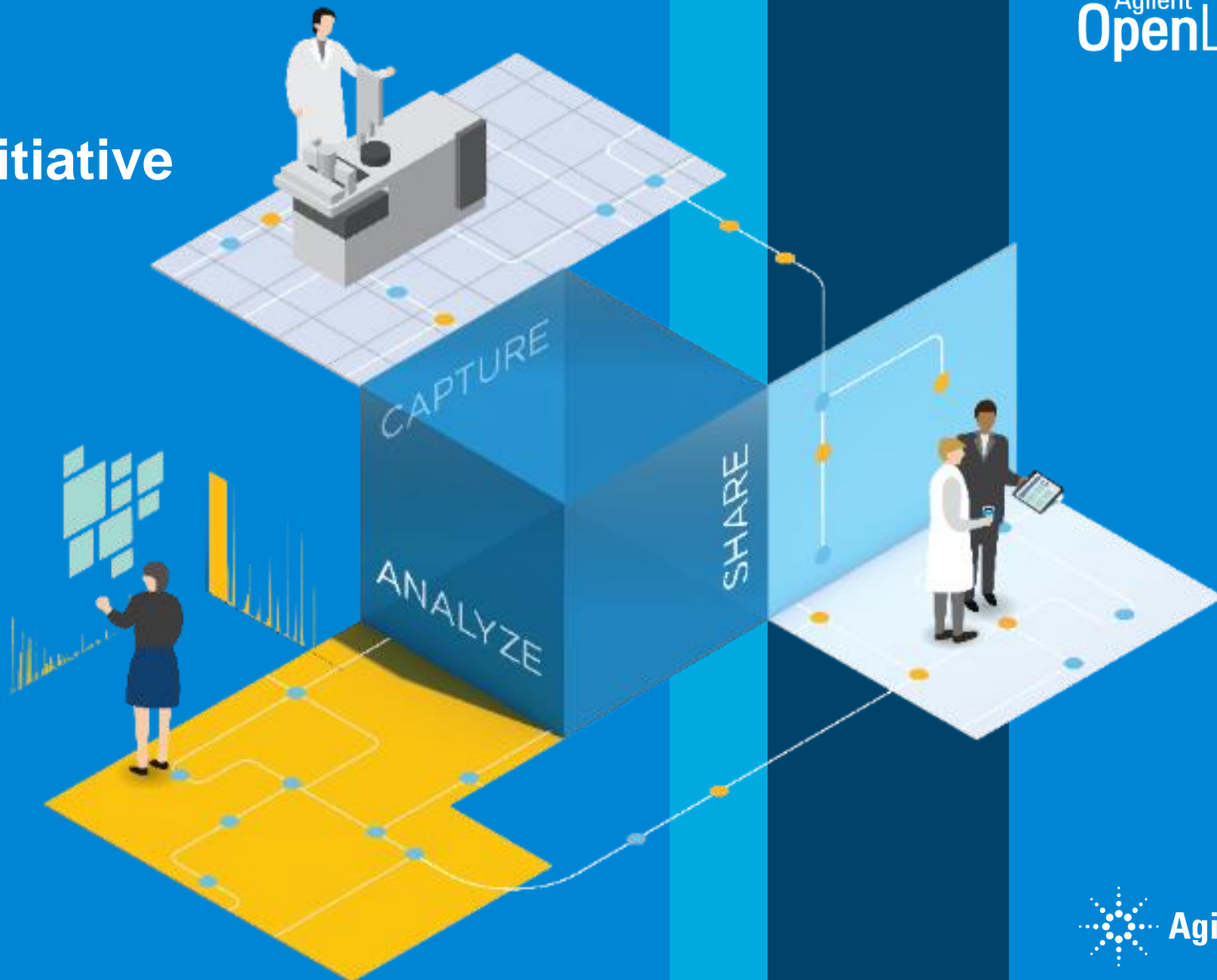


# Agilent Allotrope Initiative

Strategic Direction  
April 2018

*Jerry Hall*  
*Heiko Fessenmayr*  
Software & Informatics Division



# Agilent's Allotrope engagement



Agilent  
OpenLab

## Phase 0

**2014**

Joined Allotrope as Partner Member.

**Sept 2015**

Agilent R&D started investigation

## Phase 1

**Nov 2015**

1st Agilent Integration project started:

*Prototype development of*

- *ChemStation2ADF export*

- *ECM ADF Filter*

**June 2016**

Installed prototype of

- CS2ADF Export
- ECM ADF Filter

in pharma company lab

Agilent was the **first software vendor** providing such prototypes

Offer prototypes as beta to all Allotrope members

## Phase 2

**Oct 2016 – End 2017**

Collaboration with 6 Allotrope members:



Enhanced prototype will support conversion of

- results metadata
- acquisition method parameter of standard LC
- Sequence export
- LC/MS-SQ rawdata
- auxiliary trace rawdata (pump pressure, oven temp, ..)

## Phase 3

*Commercialization*

**Since Jan 2018**

- Established Allotrope development team
- Developing 1<sup>st</sup> commercial version of ADFExport for ChemStation
- Further enhancement of ChemStation ADFExport prototype:
  - GC data export
  - Run logbook export
  - ADF audit trail
- Initial prototype for OpenLAB CDS
- Agilent GC experts now contribute to Chromatography working group
- Agilent MS experts proceed contributing to Mass Spec working group

# Beta Test Agreement Process



## BETA TEST AGREEMENT

Agilent Technologies [redacted] ("Agilent")

USER

[redacted]  
(Division)

[redacted]  
(Company Name)

[redacted]  
(Address)

[redacted]  
(Address)

Date: [redacted]

Date: [redacted]

By: [redacted]  
(Functional Mgr's Signature)

By: [redacted]  
(Authorized Signature)

[redacted]  
(Printed Name)

[redacted]  
(Printed Name)

[redacted]  
(Title)

[redacted]  
(Title)

EFFECTIVE DATE: [redacted]

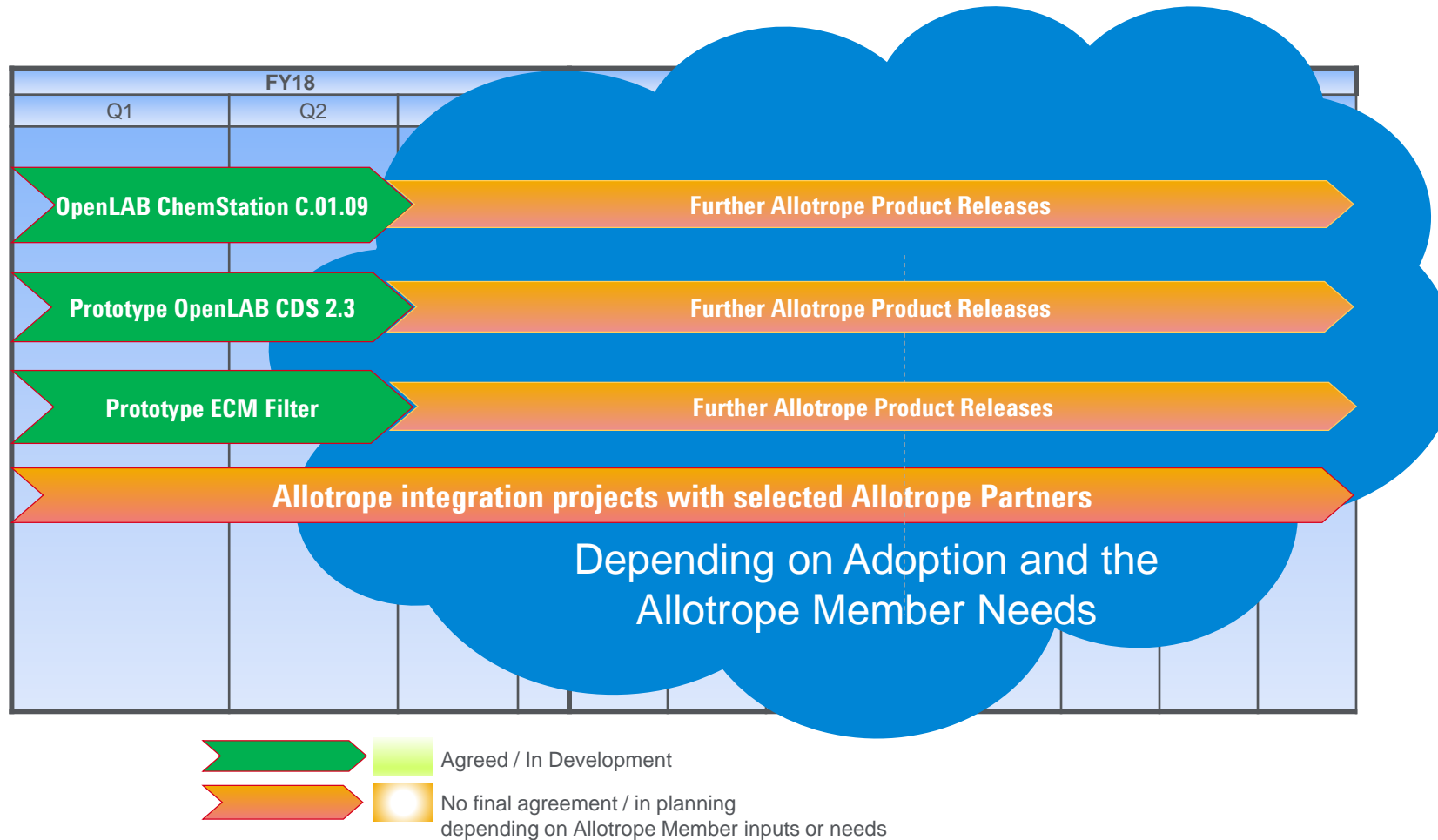
1. **Products.** Agilent shall provide to the undersigned User, at no charge to User, the following products and related technical information or documentation of Agilent (collectively the "Products"): [redacted].
2. **Term.** User shall be entitled to use the Products for [redacted] days after delivery of the Products by Agilent to User (the "Term"), unless this Agreement is terminated prior to that date pursuant to section 20 below.
3. **Location.** Agilent shall, at Agilent's expense, transport the Products to the following location of User (the "User Location"): [redacted].
4. **Installation.** The Products shall be installed at the User Location by User in accordance with the following requirements and conditions: [redacted].
5. **Use.** User shall use and test the Products during the Term for a minimum of [redacted] hours per week. User shall, at no charge to Agilent, provide Agilent with written status reports relating to such use and tests on forms and at intervals reasonably determined by Agilent.
6. **Restrictions on Use.** Regardless of the User Location, User shall not use the Products in any manner to produce, market, or support its own products; User's right to use the Products is

specifically limited to the right to test the Products as described in this Agreement. Further, the Products shall not be moved from the User Location. Agilent may inspect the Products at any time during the Term upon prior reasonable notice.

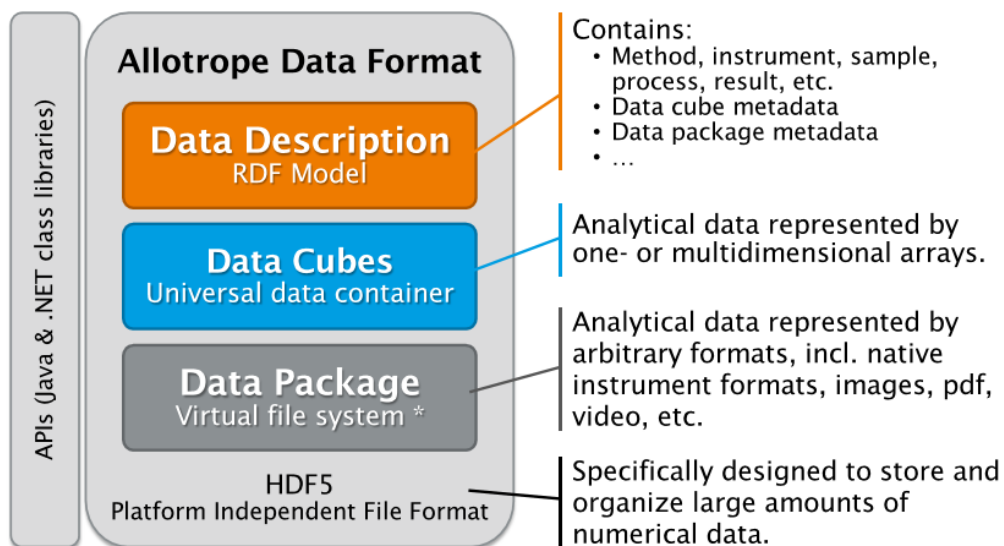
7. **Technical Support.** Agilent shall provide User with the following technical support during the Term: [redacted].
8. **Malfunctions.** Agilent shall respond as soon as practical to reported problems, but shall have no obligation to respond within a particular time frame. User shall report Product malfunctions to Agilent in accordance with the following procedures: [redacted].
9. **Title.** Agilent retains all right, title and interest to the Products, and shall be responsible for any personal property taxes assessed against the Products during the Term. User shall clearly identify all Products as the property of Agilent. The Products shall remain personal property and shall not become part of real property by annexation or otherwise. User shall not offer, loan, encumber, sell, or otherwise transfer the Products to any third party.
10. **Return of Products.** Upon the expiration of the Term or earlier termination of this Agreement, User shall promptly return the Products, and all copies whether supplied by Agilent or made by User, to Agilent at Agilent's expense.
11. **Disclaimer of Warranties.** USER ACKNOWLEDGES THAT THE PRODUCTS HAVE NOT COMPLETED AGILENT'S FULL QUALITY ASSURANCE PROGRAM AND MAY HAVE ERRORS OR DEFECTS. AGILENT MAKES NO EXPRESS OR IMPLIED WARRANTY OF ANY KIND WITH RESPECT TO THE PRODUCTS, AND SPECIFICALLY DISCLAIMS THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE.
12. **Future Availability.** While Agilent intends to commercially release the Products, Agilent reserves the right at any time not to release the Products or, even if released, to alter prices, features, specifications, capabilities, functions, release dates, general availability, or other characteristics of the Products.
13. **Limitation of Liability.** Agilent shall not be responsible for any loss or damage to User, its customers, or any other third parties caused by the Products or by Agilent's performance of this Agreement. AGILENT SHALL NOT BE LIABLE FOR ANY DIRECT, INDIRECT, SPECIAL, INCIDENTAL, OR CONSEQUENTIAL DAMAGES, WHETHER BASED ON CONTRACT, TORT OR ANY OTHER LEGAL THEORY, ARISING OUT OF ANY USE OF THE PRODUCTS OR ANY PERFORMANCE OF THIS AGREEMENT.
14. **Risk of Loss.** User shall be liable for all loss or damage to the Products while the Products are in the possession of User.

15. **Indemnity.** User shall defend, indemnify, and hold harmless Agilent from all claims, losses, costs, damages, expenses (including attorney's fees), and other liabilities arising out of User's use, operation, or possession of the Products, to the fullest extent permitted by law.
16. **Intellectual Property Rights.** All right, title, and interest to all intellectual property with respect to the Products, including that which may be or become protectable by patent, copyright, trademark, trade secret, or similar laws, shall remain exclusively with Agilent. No license or other right of any kind is granted by Agilent's furnishing the Products to User, except for the limited right to use and test the Products as expressly provided in this Agreement. User shall not use Agilent's copyrights, trademarks, trade names, or other intellectual property in any way.
17. **Confidentiality of Information.** Agilent regards all information pertaining to the Products to be of a proprietary and confidential nature. User shall protect the confidentiality of such information until such information becomes public by using the same degree of care, but not less than a reasonable degree of care, to prevent the unauthorized use, dissemination or publication of such information as Users uses to protect its own confidential information of a like nature. User shall not make public in any manner this Agreement or any reports or test results obtained pursuant to this Agreement.
18. **Alterations by User.** User shall not alter the Products. Any alterations made to or suggested for the Products by User shall be the exclusive property of Agilent, together with all rights therein.
19. **Assignment.** This Agreement is personal to User. User shall not assign or otherwise transfer any rights or obligations under this Agreement.
20. **Termination.** In the event that User fails at any time to comply with this Agreement, Agilent may terminate this Agreement immediately upon written notice to User. Further, either party may terminate this Agreement without cause on fifteen days prior written notice. The rights and responsibilities of the parties pursuant to sections 9, 10, 11, 12, 13, 14, 15, 16, 17 and 18 of this Agreement shall survive the expiration or earlier termination of this Agreement.
21. **Entire Agreement.** This Agreement contains the entire understanding and agreement of the parties relating to the subject matter hereof. Any representation, promise, or condition not explicitly set forth in this Agreement shall not be binding on either party. Any amendments to this Agreement shall be in writing and signed by the authorized representatives of each party.

# Agilent ADF Products - SID Roadmap for Allotrope



## Allotrope Data Format (ADF)



### Allotrope Mission

...development of a **comprehensive and innovative Framework...** ...for managing analytical data throughout its lifecycle.

### Marketing


- LC-UV rawdata and ChemStation files only. No LC-UV metadata due to delayed data model.
- Single Runs
- Automated post-run export
- Uploading to ECM by ECM Scheduler
- First release is “Research Use Only”
- Future development
  - Sequences
  - Localization
  - long-term archiving of calibrated results, no sample audit trail etc.
  - Manual export

Remark: ADF viewer (ADFExplorer) provided by Allotrope Foundation

- Established Allotrope development team in Waldbronn
- Developing 1<sup>st</sup> commercial version of ADFExport for ChemStation
- Further enhancement of ChemStation ADFExport prototype:
  - GC data export
  - Run logbook export
  - ADF audit trail
- Initial prototype for OpenLAB CDS
- Agilent GC SME (George Reiner) now contributes to Chromatography working group
- Agilent MS SME (Dave Peterson) proceed contributing to Mass Spec working group. Worked w/ Genentech on a prototype script to schedule their “ADF” archival system for LC-QTOF data.


# Refresher: Phase 1 & 2

**see poster**



# Agilent Allotrope Initiative

## OpenLAB ChemStation export into Allotrope format / OpenLAB ECM Allotrope search



**Agilent contact:**  
**Marketing:** Gerald Hall, Ralph Mueller  
**Technical:** Heiko Fessendenmayr

### Goal:

Export of **OpenLAB CDS ChemStation HPLC** results data into Allotrope ADF Format.

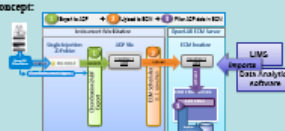
Upload of Allotrope ADF Files to **OpenLAB ECM** and search for ADF meta data

**Prototypes available**  
 Agilent offers prototypes to all Allotrope Members  
 For details contact [gerald.hall@agilent.com](mailto:gerald.hall@agilent.com)

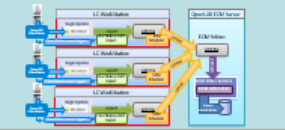
### Allotrope Initiative Phase-1

*w/ MerckMSD (Nov 2015 – Jan 2016)*


**Basic Concept:**



Deployed lab system prototype (OpenLAB ChemStation / OpenLAB ECM)



OpenLAB ECM able to search for ADF meta data




Allotrope ADF content example (high-level):


### Allotrope Initiative Phase-2

*w/ MerckMSD, Bayer, GSK, AbbVie (Dec 2017 – Dec 2017)*

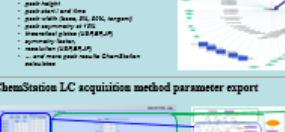
**ChemStation Sequence Export to Allotrope**




ChemStation Chromatogram, UV-spectra, Instr. signals: rawdata export




ChemStation peak results export



ChemStation LC acquisition method parameter export




ChemStation LC-MSD rawdata export (MS-spectra, TIC)



### Agilent: An engaged partner in the Allotrope Foundation

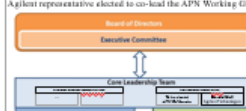
Agilent Allotrope Initiative:



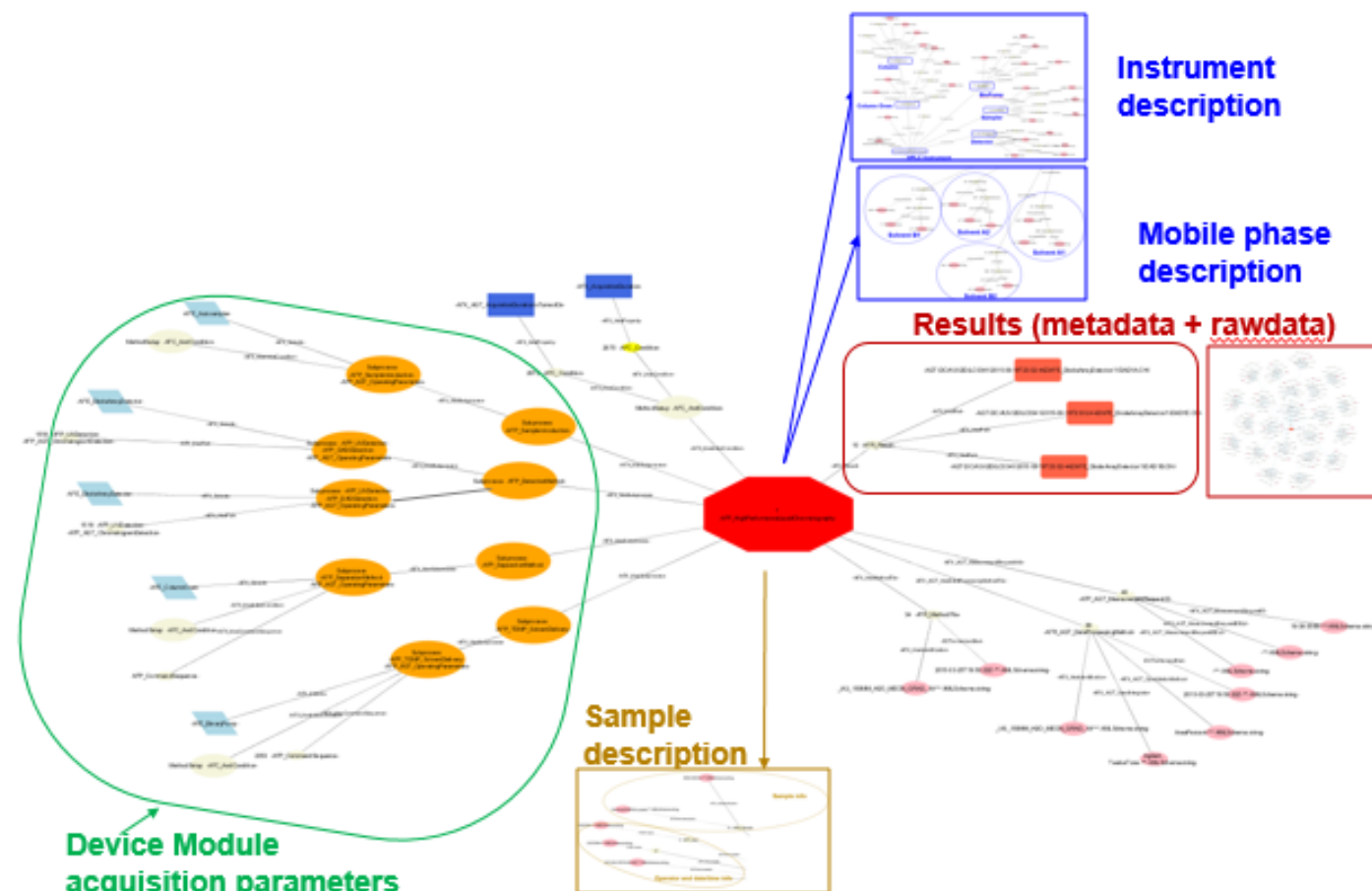
Agilent is an active partner in many workshops:

Workshop	Topic	Agilent Role
APN (APN) WS	Agilent	Agilent
MSD WS	Agilent	Agilent
Genomics WS	Agilent	Agilent
Mass Spec WS	Agilent	Agilent
ADP WS	Agilent	Agilent
Certification Support WS	Agilent	Agilent

Agilent representative elected to co-lead the APN Working Group



## OpenLab ChemStation prototype can write today ....



# A demo tells more than thousand slides ...

- ADF Export ChemStation export for LC data
  - Run Logbook
  - ADF Audit Trail
- ADF Export ChemStation export for GC data
- ADFExport for OpenLAB CDS
- Search ADF data and launch ADF Explorer from within OpenLAB ECM
- Prototype: OpenLAB ECM server-side conversion of ChemStation data

# Demos...



Thank you!