

# ***Improving NMR Data Quality, Consistency, Standardization and Mining of Stored Analytical Information***

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# Enabling NMR Analytics

- We are striving to help extracting more value out of your NMR data with an offer supporting:
  - Data consistency
  - Data quality
  - Data standardization
  - Data Mining
  - Predictive science

# NMR Data Quality and Consistency

- Industrial R&D has evolved toward an open innovation model. The nature of the partners is very diverse. They are all generating huge amount of NMR data. Data transferring requires consistency with the data from internal sources. Following solutions can support transferability
- Intelligent Spectrometer
  - *Automated spectrometer performance validation*
- Smartly drive the spectrometer
  - *Software driven NMR experiment optimization*
- Improving Data Quality Prior to Standardization
  - *NMR methods sharing, spectrometer validation SOPs,..*

# Intelligent Spectrometer

- System Suitability Test (SST) will be run automatically at a frequency defined by the user
- Pass / Fail automatic report
- Can be set up to stop automation if SST fails
- Reliable ('does not forget to run before GxP experiment')
- User defined tests also possible
- Can follow SOPs

### Tests Definition (IconNMR configuration)

System Suitability Test (SST)   SST Standard Tests   SST User Tests

**<sup>1</sup>H Lineshape Humptest**

☒ Perform <sup>1</sup>H Lineshape Test

Sample Position

**Linewidths**

Linewidth at 0.55% of signal height <  Hz

Linewidth at 0.11% of signal height <  Hz

Resolution Halfwidth <  Hz

Left Plot Limit  ppm   Right Plot Limit  ppm

**<sup>1</sup>H Sensitivity Test**

☒ Perform <sup>1</sup>H Sensitivity Test

Sample Position

**Signal region**

Left limit  ppm   Right limit  ppm











**Noise region**

Left limit  ppm   Right limit  ppm

Noise delta  ppm   S/N >  :1

### Automatic Tests Acquisition (IconNMR)

Experiment Table

H...	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par
▼ 1		1 Queued	C:\Bruker\TopSpin4.0.1	SST_2017-09-15-14-39-06	1	Acetone	PROHUMP	★ 	
▼ 2		1 Queued	C:\Bruker\TopSpin4.0.1	SST_2017-09-15-14-39-06	2	CDCI3	PROSENS	★ 	
▼ 3		1 Queued	C:\Bruker\TopSpin4.0.1	SST_2017-09-15-14-39-06	3	CDCI3	C13SENS	★ 	
▼ 4		1 Queued							

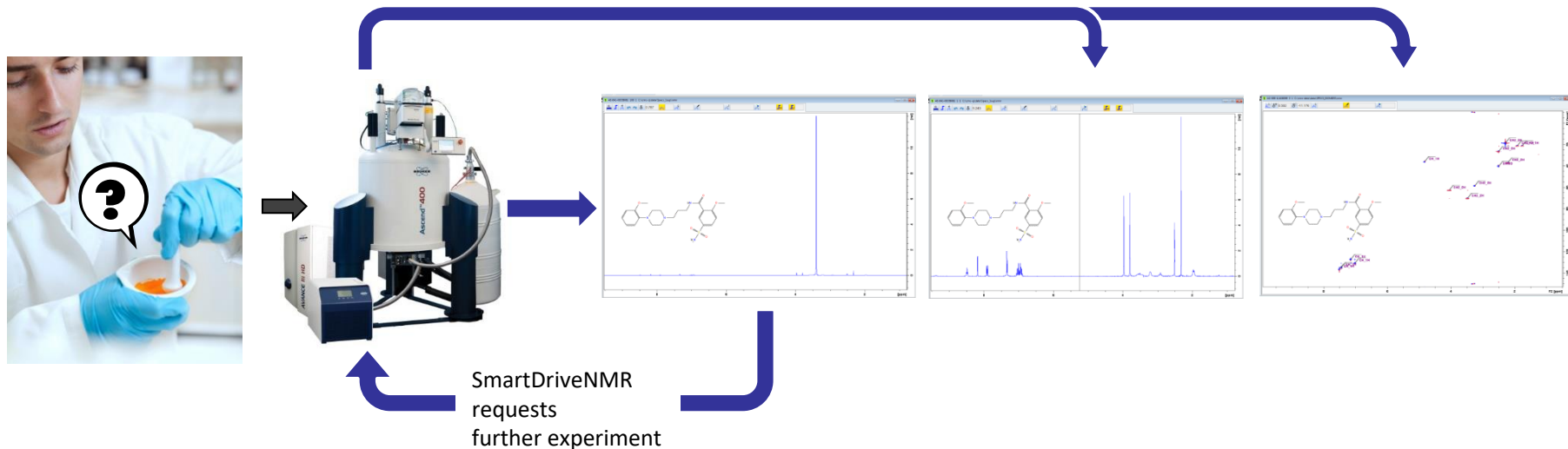
### Automatic Report Generation (IconNMR)

**PASS**

Summary of Achieved Specifications

Lineshape Test	PASS
linewidth at 0.55% of signal height:	(< 7Hz) 3.3Hz
linewidth at 0.11% of signal height:	(< 14Hz) 5.7Hz
lfwidth:	(< 0.7Hz) 0.34Hz
Experiment Directory:	C:\Bruker\TopSpin3\Sp6\hmrssu\SST_2016-10-16-13-16-58\1\data\1\1r
Sensitivity Test	PASS

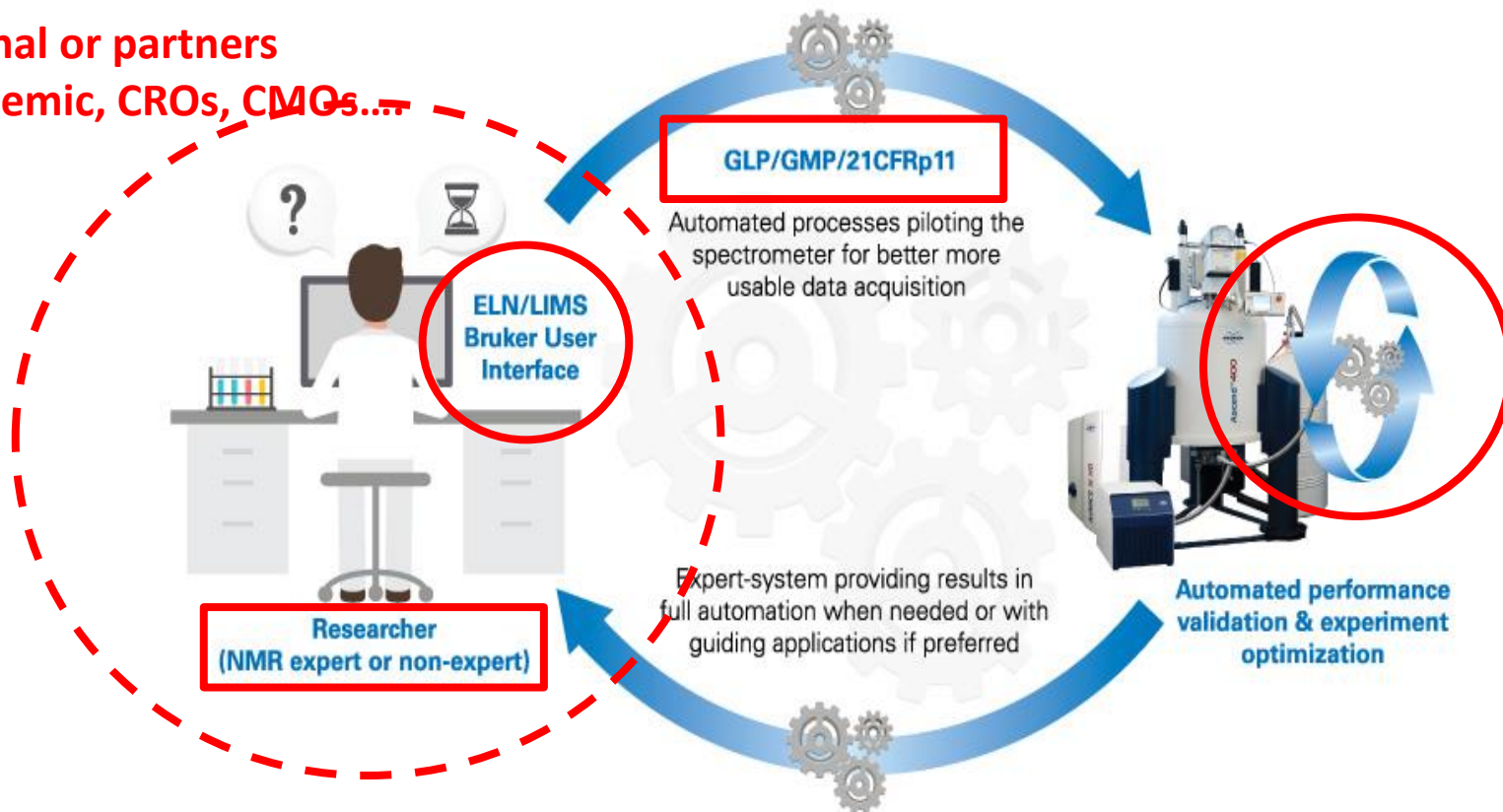
# Software driven NMR experiment optimization



- ✓ Automated data processing and analysis
- ✓ Now including **long range H-C HMBC correlations**
- ✓ Spectra with **optimised quality**
- ✓ **Smart** – the spectrometer decided what experiment to run next
- ✓ Can follow **SOPs**

# Breaking the Barrier Resistance Toward NMR Enabling NMR-Related Collaborative Science

Internal or partners  
(academic, CROs, CMOs...)



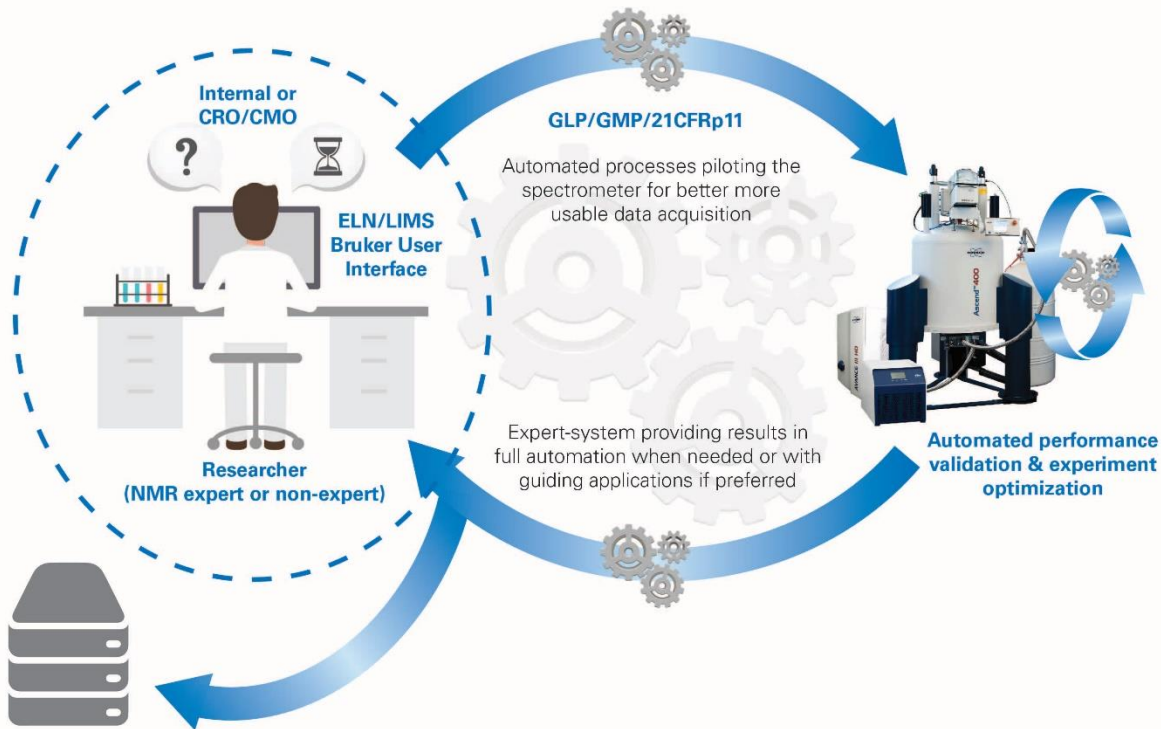
# Data Standardization: Allotrope Conversion

- We are developing a batch engine which can read all legacy Bruker data and convert them into a first version of ADF and store the file wherever the users wants us to store it. API for integration will be offered. We already have a customer minimum requirement and we are collecting some more with an ambition to offer a beta version in a few months
  - Batch version will be capable of transferring legacy data into ADF
  - Batch version can be used to convert data coming from other sources
  - Batch version will be called by Topspin to read ADF format in Topspin and write ADF format from TopSpin

# Data Mining

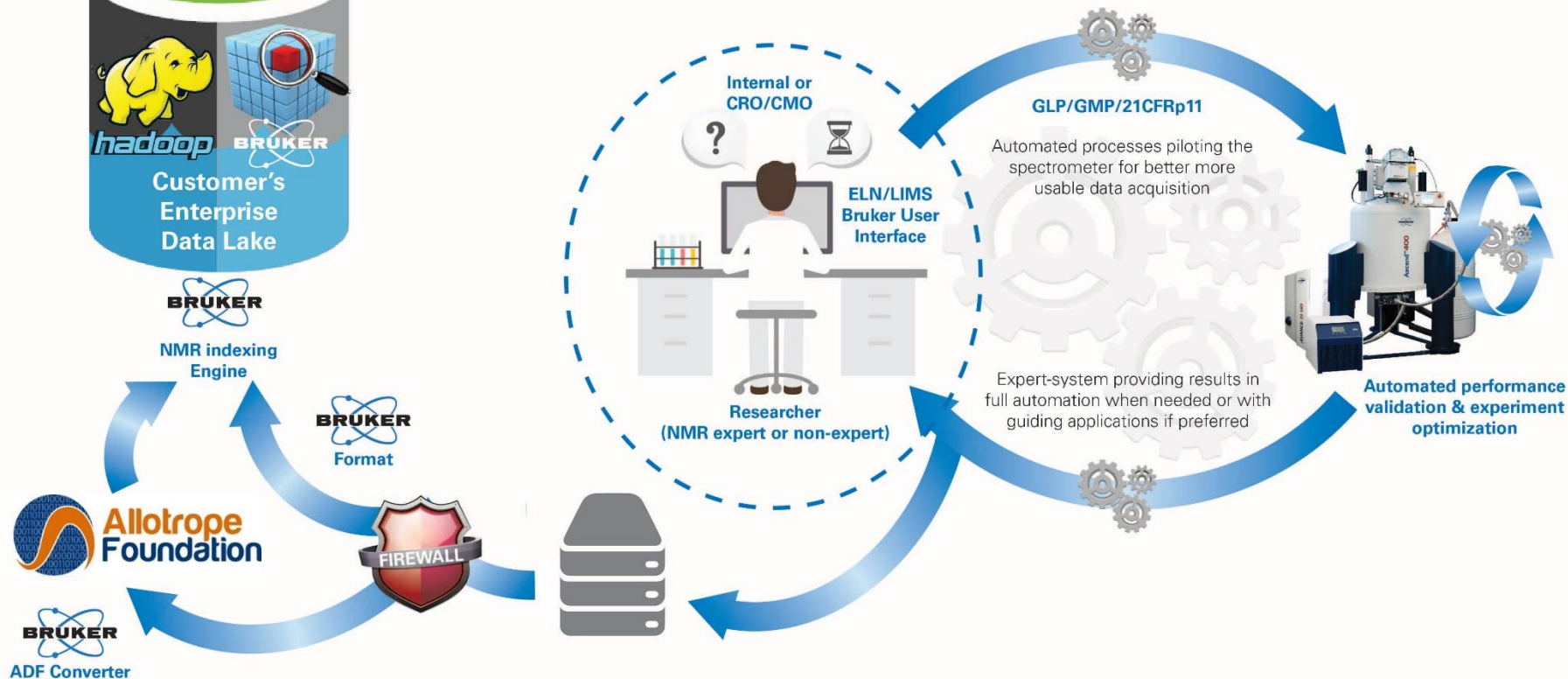
- Give value to Data Lake (as a service) by:
  - Offering indexing/structured engines for NMR related information (multiplicity, chemical shifts, distance between peaks,...) which can for example analyze and abstract information from spectrum at the time of conversion or export from TopSpin
  - Offering mining engines to extract data, based on NMR information:
    - Spectrum search
    - Sub spectrum and specific pattern search
    - Chemical shifts, multiplicity,... search
  - API and Integration capabilities





Impurities  
Extractables  
Leachables  
...  
Predictive  
Tools  
QC  
Regulatory  
Audits

# Bruker Professional Services



## Conclusion

- Bruker Magnetic resonance can offer a global approach working pre and post acquisition, interacting with the spectrometer and providing data consistency and integrity to match the current trend toward open innovation.
- Aiming to be part of a collaborative informatics ecosystem, our Informatics strategy is focused around:
  - Integration with third parties informatics (ELN or LIMS)
  - Data standardization
  - Data mining integrated in environments matching today's industrial IT roadmap
  - Assist Bruker users being compliant with GxP and 21CFR11
  - ....