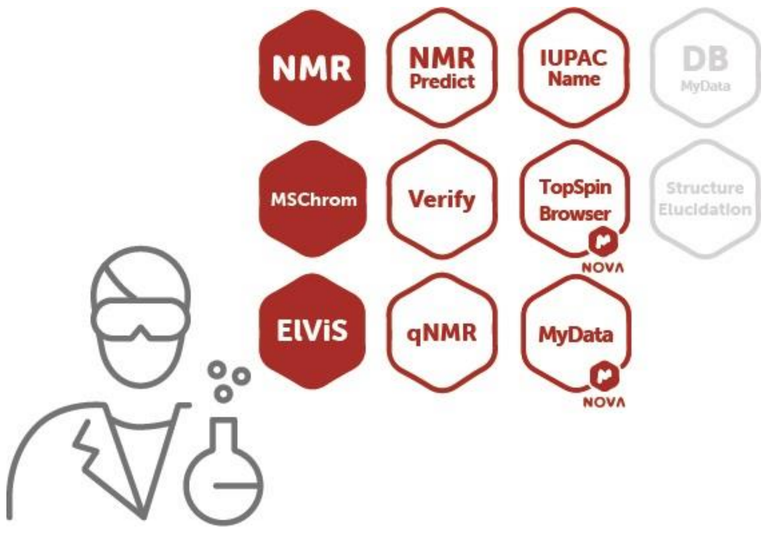
EUROMAR 2022

Bruker Chemist Suite

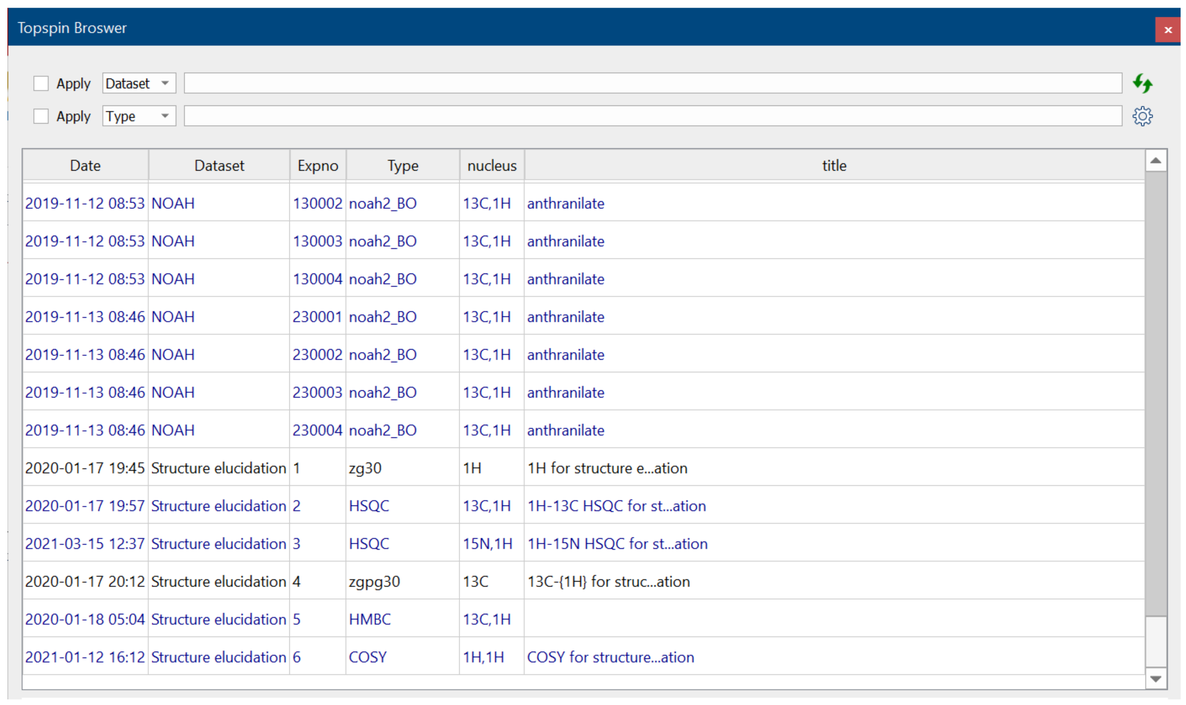
Processing, Analysis, Data Storage, and Reporting

NEW!



Process, analyze, and report all spectroscopic data in one software solution with Bruker Chemist Suite: Bruker Chemist Suite is a collection of efficient tools for data management, processing, analysis and reporting of various types of analytical data. The software also provides powerful modules for quantification and purity determination, for generating an IUAPC name from a chemical structure and for NMR spectra prediction. It also helps with confirmation of chemical structure identity and structure verification.

Mnova TopSpin Browser



Date	Dataset	Expno	Type	nucleus	title
2019-11-12 08:53	NOAH	130002	noah2_BO	13C,1H	anthranilate
2019-11-12 08:53	NOAH	130003	noah2_BO	13C,1H	anthranilate
2019-11-12 08:53	NOAH	130004	noah2_BO	13C,1H	anthranilate
2019-11-13 08:46	NOAH	230001	noah2_BO	13C,1H	anthranilate
2019-11-13 08:46	NOAH	230002	noah2_BO	13C,1H	anthranilate
2019-11-13 08:46	NOAH	230003	noah2_BO	13C,1H	anthranilate
2019-11-13 08:46	NOAH	230004	noah2_BO	13C,1H	anthranilate
2020-01-17 19:45	Structure elucidation	1	zg30	1H	1H for structure e...ation
2020-01-17 19:57	Structure elucidation	2	HSQC	13C,1H	1H-13C HSQC for st...ation
2021-03-15 12:37	Structure elucidation	3	HSQC	15N,1H	1H-15N HSQC for st...ation
2020-01-17 20:12	Structure elucidation	4	zgpg30	13C	13C-{1H} for struc...ation
2020-01-18 05:04	Structure elucidation	5	HMBC	13C,1H	
2021-01-12 16:12	Structure elucidation	6	COSY	1H,1H	COSY for structure...ation

Fig. 1: Enhanced data browser to rapidly navigate and display NMR experiments but also to intuitively filter NMR datasets using multiple arguments (date and time, type, nucleus, dataset name and/or title information).

NMR
A professional way to visualize, process, analyze and report your 1D and 2D NMR data. Supports the specific NMR needs of analytical and organic chemists.

MSChrom
Process, analyze and report your LC-MS and GC-MS data from your different instruments.

NMR PREDICT
Calculates accurate and precise NMR chemical shifts using a novel procedure that combines several prediction engines.

ElViS
Visualize, process, analyze and report various electronic and vibrational spectroscopic techniques.

Verify
Automatic confirmation of structure identity based on NMR and/or LC/GC/MS data.

IUPAC Name
Generate the IUPAC name for your molecular structures.

qNMR
Quantitative NMR analysis made easy. For all qNMR concentration and purity determinations.

MyData
Store, search, and share analytical data.
A professional database with a very flexible data model for the efficiently shared storage of molecular structures and other data.

TopSpin Browser
Fast browsing through multiple dataset directories and NMR experiments and filter of NMR datasets created in TopSpin.

Features at a Glance

- One software suite and one graphical user interface to process analytical chemistry data (NMR, LC/GC-MS, UV-Vis, FT-IR, Raman)
- Powerful algorithms for prediction of NMR spectra as well as for automatic and assisted structure verification with a flexible scoring system
- Purity determination and quantification of 1D NMR data of various nuclei, in manual, assisted and automatic mode
- Easy storage in database and file access using DB MyData and TopSpin Browser
- Efficient reporting and reporting template

Conclusions

- Bruker Chemist Suite is an NMR centric set of plugins, exclusively offered to Bruker customers.
- Includes tools for processing other types of analytical data which may be useful for chemists:
  - MS, LC or GC or hyphenated (LC/MS or GC/MS) data
  - Optical and vibrational spectroscopies
- Helps chemists for NMR data interpretation (automatic or assisted), structure verification, quantification, chemical naming and data management.

Software