Topspin

Bruker NMR software for spectrometer control, data acquisition, processing, displaying and analysing.

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Free TopSpin processing software for academia

- https://www.bruker.com/service/support-upgrades/software-downloads/nmr/free-topspin-processing/free-topspin-download.html
- Register
- Download – current version 3.5 pl7 valid until 31.03.2019
- Topspin is a Java based software independent from the platform – Windows, Mac or Linux (ISO file contains all)
- Install – providing you have an appropriate permissions
- When running for the first time – prompt to configure as datastation – default 600 MHz spectrometer

How to start

- Browser window - right click – add new data directory
- Spectrum window – drag and drop
- Workflow tabs
- Flowbar
- Tool bar, Browser & Structure
- Main Topspin/Spectrum window
- Data Set Tabs
- Command line
- Acquisition info bar

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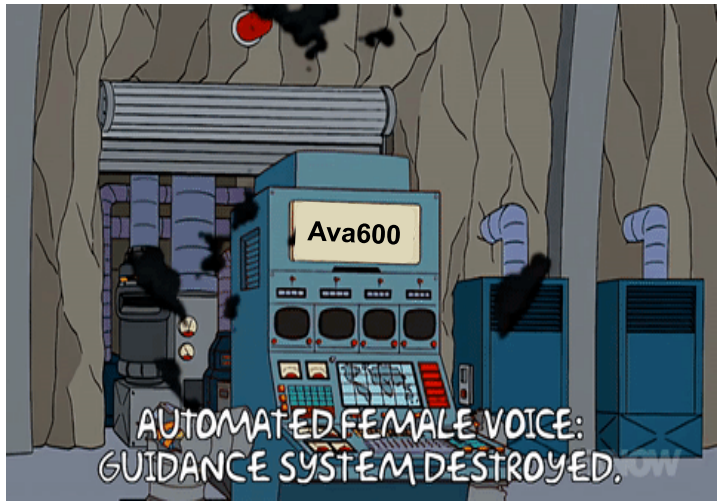

Databases & Prediction

- **ACD/I-Lab**
- https://cds.rsc.org/
- http://ilab.cds.rsc.org/?cdsrdr=1
- **Nmrdb.org**
- https://www.nmrdb.org/
- **Spectral Database for Organic Compounds SDBS**
- http://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi
- **nmrshiftdb2**
- https://nmrshiftdb.nmr.uni-koeln.de
- https://www.chem.wisc.edu/areas/reich/chem605/index.htm

Structure Elucidation

- Bruker:
- CMC-se Small Molecule Structure Elucidation
- CMC-assist Assisted NMR Data Interpretation …
- Mnova:
- Mnova Structure Elucidation
- Verify - Automatic confirmation of structure identity
- ACD:
- ACD/Structure Elucidator Suite
- Automated Structure Verification