Fragment-based Screening

● Simplifies fragment-based screening by NMR

Fragment screening in the pharmaceutical industry has become a widely applied method for the discovery of lead molecules. Weak binding affinities in the µM to mM range are a hallmark of fragments and appropriate screening methods are needed for the detection of binding ligands.

NMR-based Fragment Screening (Fragment-based Screening, FBS) is one of the most popular and reliable techniques and is used in more than 50% of screening campaigns.* However, data handling and analysis has been a bottleneck as many 1D ^{1}H or 1D ^{19}F spectra must be analyzed in parallel by the operator which can be a time consuming task.

Bruker now facilitates these tasks with a full Topspin based workflow solution.

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Benefits

- Greatly simplifies NMR-based fragment screening
- Seamless workflow from acquisition to data processing and analysis
- Automatic display of relevant data: screening experiment, reference spectra, compound IDs and cocktail composition
- Automatic recognition of standard NMR screening experiments
- Screening studies are organized and saved in projects
- Tracking of user's actions within a project
- On-the-fly automatic saving functionality
- Reporting in Microsoft Excel format
- Customization of both acquisition and analysis is implemented at various steps

Innovation with Integrity

NMR

The current workflow is cumbersome and typically involves manual data management, bookkeeping of experiment types, compound names and results. The FBS tool within Topspin streamlines this workflow allowing the user to focus on information content and data analysis. This reduces human error and increases the efficiency considerably, making NMR-based FBS superior to orthogonal methods.

Fragment Library
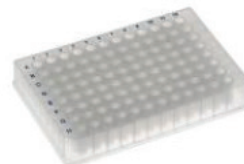
Experiments
(typical FBS screening experiments)

IconNMR
(automatically generates and runs experiments)

Automatic NMR parameter calibration and calculation

Automatic processing of NMR screening data

Data acquisition, processing and analysis with FBS tool in Topspin

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