Automated Structure Verification by NMR

CMC-i™ Complete Molecular Confidence - Integrity

Only complete computational NMR spectral analysis provides a safe assessment of the consistency between a given structure and its ^{1}H NMR spectrum.

Finally overcoming tedious manual procedures, optimizing predicted spectral parameters to match experimental data using iterative spectral analysis is now possible in full automation.

Features

- Complete NMR spectral analysis yielding fully assigned spectra and highly accurate spectral parameters extracted from data, even for overlapping signals and strongly coupled spin systems
- Benefits from PERCH's highly sophisticated algorithms for predicting chemical shifts and couplings and optimizing them to match the experimental data using iterative quantum mechanical spectral analysis
- Extremely safe assessment of the consistency between a given structure and its ^{1}H NMR spectrum data based upon the quality of the fit and the similarity between predicted and actual spectral parameters, with optional use of HSQC information
- Accurate estimation of sample purity

Automated Consistency Analysis

Starting from the ^{1}H spectrum and the molecular structure with the optional use of HSQC information, ACA provides complete NMR spectral analysis in a fully automated fashion for the first time.

Extremely high selectivity and specificity are guaranteed because the analysis ensures that all NMR-parameters are self-consistent, while the quantum mechanical calculation deals with spectral overlap and higher order effects. Thus the "false positive rate" is remarkably small.

Complete Spectral Analysis

The probability of all reasonable shift assignments is ranked based on the distance between predicted and actual chemical shifts, weighted by the estimated prediction error and the compatibility with corresponding peak- and intensity information.

The pre-assigned solutions are then iterated by optimizing the predicted NMR-parameters to match the experimental data. A match index combines individual likelihoods of all assignments with the quality of the final fit. Solvent peaks are recognized and treated accordingly (no "dark regions").

Best Solution

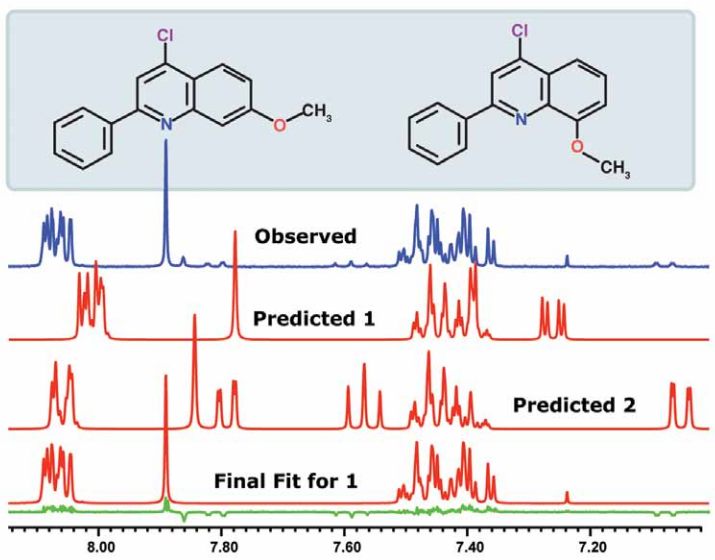
CMC-i is the solution even where first order analysis or pattern recognition fail. For example, it can still distinguish between the two isomers from the 1D proton spectrum alone (see figure 1).

CMC-i is available with TopSpin 3.0 as a separate license.

CMC-i

- Complete Analysis
- Full Automation (Analytical Profiler)
- High Selectivity (low false-positive)
- Includes Higher Order Spin Systems
- Includes Solvents
- Reliable Quantification (also with signal overlap)
- MW up to 500 (recommended)

Which structure is correct?



1) Match Index = 100.0
Total RMS = 6.7
Shift Similarity-% = 99.9
Coupling Similarity-% = 99.8
Highest local_RMS = 9.3 (H9)
R-factor(100*Calc/Obs) = 91.8
All chemical shifts are within range.
All J-couplings are within range.

2) Match Index = 0.0
Total RMS = 6.9
Shift Similarity-% = 94.7
Coupling Similarity-% = 0.2
Highest local RMS = 9.9 (H9)
R-factor(100*Calc/Obs) = 91.7
All chemical shifts are within range.
Following J-couplings are out of range:
J(H9,H16) found: 9.2, predicted: 7.3 +- 0.6 Hz
J(H9,H15) found: 2.8, predicted: 8.0 +- 0.9 Hz

Bruker BioSpin

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