

# TopSolids-BIO™

## ● Solid State NMR Wizard for Structural Biology

TopSolids is a new, easy-to-use software package for solid state NMR, facing today's challenge of solving the structure of insoluble proteins.

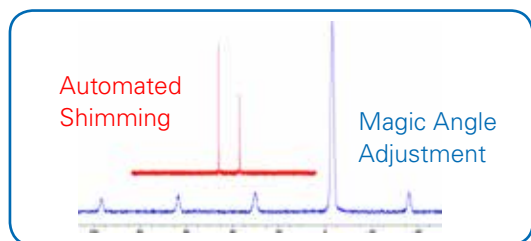
The software wizard provides step-by-step guidance for setting up even the most demanding experiments. As well as saving time, TopSolids also enables non-experts to run advanced solid state NMR experiments. All optimization parameters are stored in memory, so experiments can be queued to acquire the data necessary to access the 3D fold of your protein.

### Features

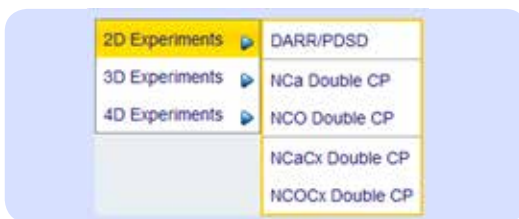
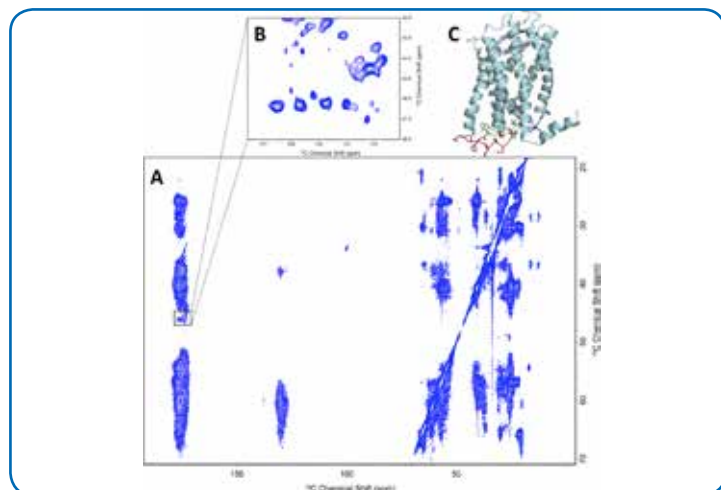
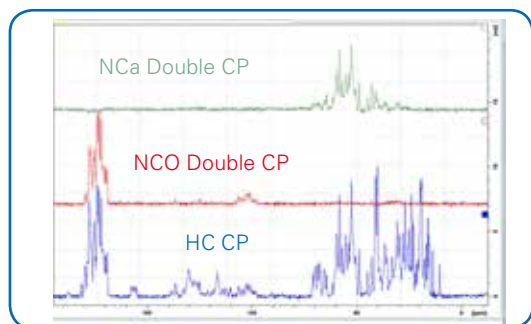
- Step-by-step guidance through spectrometer set-up
- Guided magic angle adjustment
- Very fast automatic pulse parameter calibration with adamantane
- Automated probe shimming
- Fast, automated experiment set-up on amino acids and polypeptides
- Automated parameter fine-tuning for proteins
- Automatic digital record-keeping
- Full library of backbone assignment experiments amenable to modern NUS sampling schemes
- Seamless integration with Bruker AVANCE™ III and III HD spectrometers

## Guided Set-up with TopSolids

TopSolids guides you through the optimization process for basic set-up on standard samples, as well as direct set-up on biological samples. The basic set-up menu includes magic angle setting, automatic fast pulse parameter measurements on  $^{13}\text{C}$  and  $^1\text{H}$  and automatic shimming. This process takes less than 15 minutes. The second stage of basic set-up is conducted with either enriched glycine or a small polypeptide. Setup for  $^{13}\text{C}$  and  $^{15}\text{N}$  takes less than 30 minutes and provides all required parameters for the most demanding experiments.

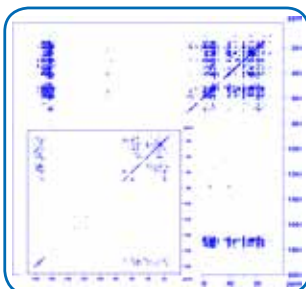


TopSolids helps you set up the spectrometer for your sample faster than ever before. Following the wizard's step-by-step instructions results in spectrometer performance rivaling any expert. The results of the set-up for your protein sample are automatically recorded in an easily readable document.

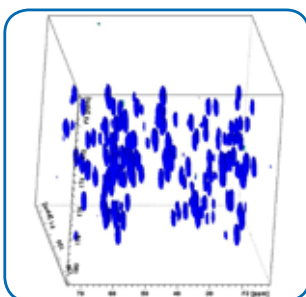


TopSolids provides protocols for all standard experiments used in backbone assignment projects. 3D DCP, triple CP and 4D triple CP experiments are available as well as 2D experiments.

TopSolids offers a complete selection of 1D to 4D cross polarization based double and triple resonance homo- and heteronuclear correlation experiments for backbone assignment. Following the wizard's recommendation, you can then check the appropriate experiments and queue them up. TopSolids takes care of running the experiments, automatically populating the required spectrometer settings for each experiment.



CC correlation experiment using a GB1 sample, 100ms CC mixing and 50ms mixing (inner spectrum). After acquisition, the full range of TopSpin processing tools can be used to prepare the data for analysis.



NCOCx 3D experiment run with TopSolids using a GB1 sample, 50ms CC mixing.

A: Two-dimensional  $^{13}\text{C}/^{13}\text{C}$  spin-exchange spectrum obtained with a 150 msec PDS mix time on a 2 mg sample of uniformly  $^{13}\text{C}/^{15}\text{N}$  labeled CXCR1 in DMPC liposomes at 293 K. The spinning rate was 15 kHz.  
 B: Expanded region containing the glycine resonances.  
 C: Three-dimensional structure of CXCR1, a G-protein coupled receptor with 350 residues, determined by rotationally aligned solid state NMR (Park et al (2012), Nature 491, 779-783).  
 Courtesy of Dr. Sang Ho Park, Dr. Anna De Angelis and Prof. Stan Opella.

## Workflow

### Assisted Spectrometer Set-up

1. Create a Project



2. Set Up Using Standards

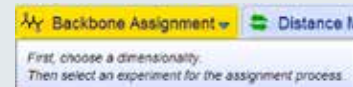


3. Fine-tuning on Biosample

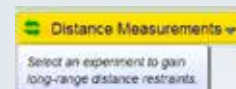


Standard Parameter sets

4. Backbone Assignment



5. Distance Measurements



6. Reliable Results and Reporting

