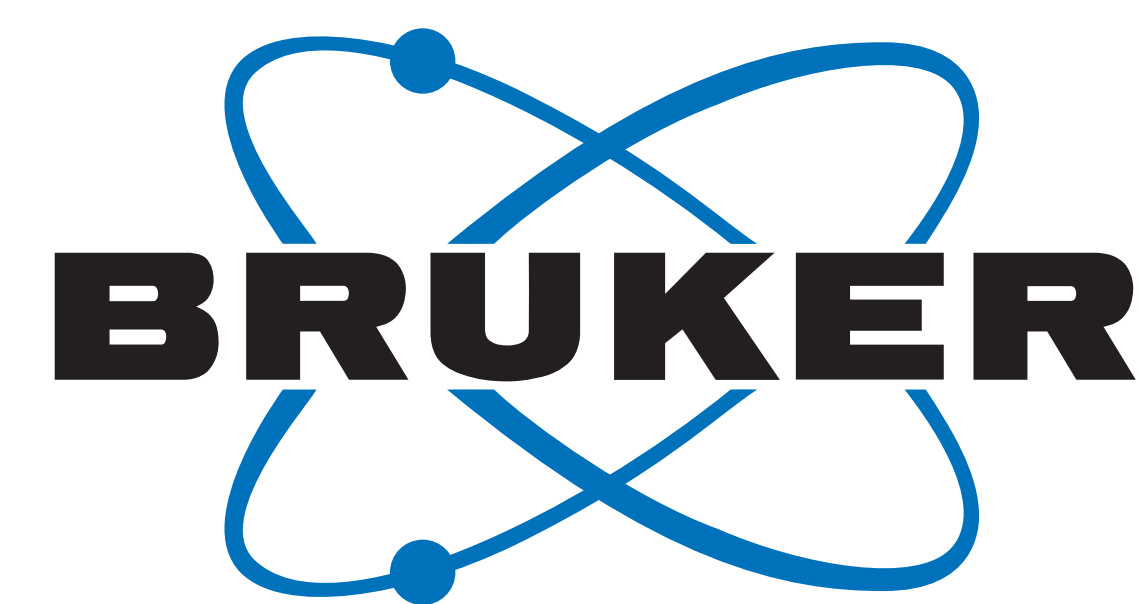


# Ultra-High-Field: Results from Bruker's First-of-a-Kind 1.3 GHz NMR Spectrometer



## Abstract

Bruker has developed and tested a 1.3 GHz (30.55 T) spectrometer, setting a new world record for high-resolution NMR. Tests were conducted using five different NMR probes, achieving high-resolution NMR at 1.3 GHz for the first time.

## Magnet Technology

The 1.3 GHz HTS/LTS hybrid magnet developed by Bruker is a groundbreaking achievement in superconducting magnet technology. Operating at a field strength of 30.55 T, this magnet is superconducting and functions in persistent mode, ensuring stable and continuous operation. The magnet has a 54 mm room-temperature bore, which is compatible with Bruker's BOSS3 room temperature shim system. This design allows the use of standard bore probes, making it versatile for various NMR applications.

Despite its higher field strength, the new 1.3 GHz magnet maintains the same physical dimensions and cryogen consumption as Bruker's 1.2 GHz magnets, with only a slightly increased stray field radius.

Achieving 1.3 GHz in such a compact form-factor was made possible by the qualification of a high-temperature superconductor with a new architecture which enables higher current densities than what could previously be reached. In addition, from a magnet design perspective, quench protection and force management were additional challenges that needed to be addressed successfully ahead of the first energization.

The first-of-a-kind 1.3 GHz magnet serves as an important proof-of-principle and validates the technology developments which enable this new chapter of ultra-high field NMR with even higher dispersion and resolution.



**Fig. 1:** The first-of-a-kind 1.3 GHz NMR magnet capitalizes on Bruker's well proven HTS/LTS hybrid technology.



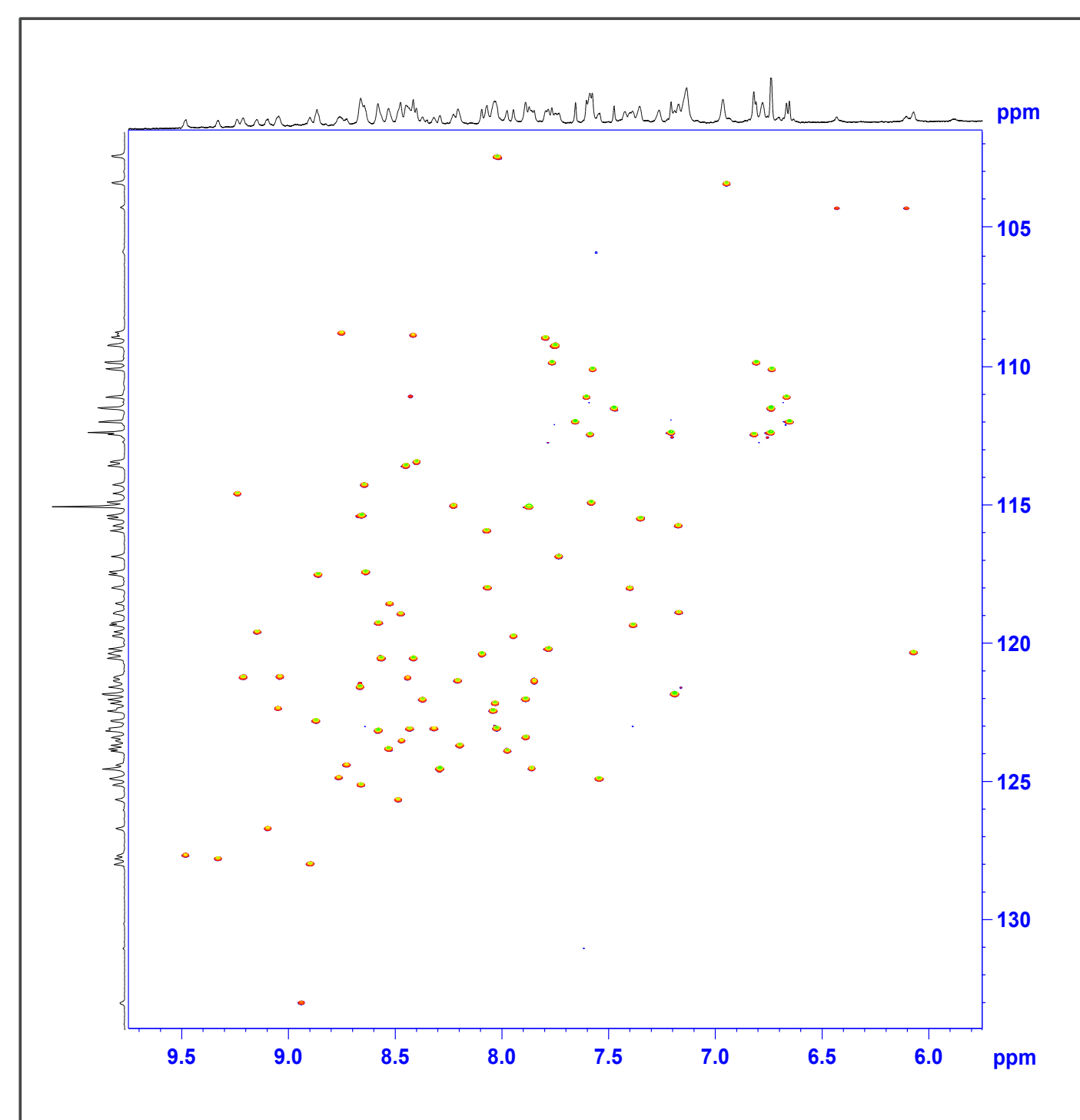
**Fig. 2:** Three of the NMR probes which were used for the first characterization of the 1.3 GHz spectrometer.

## NMR Results

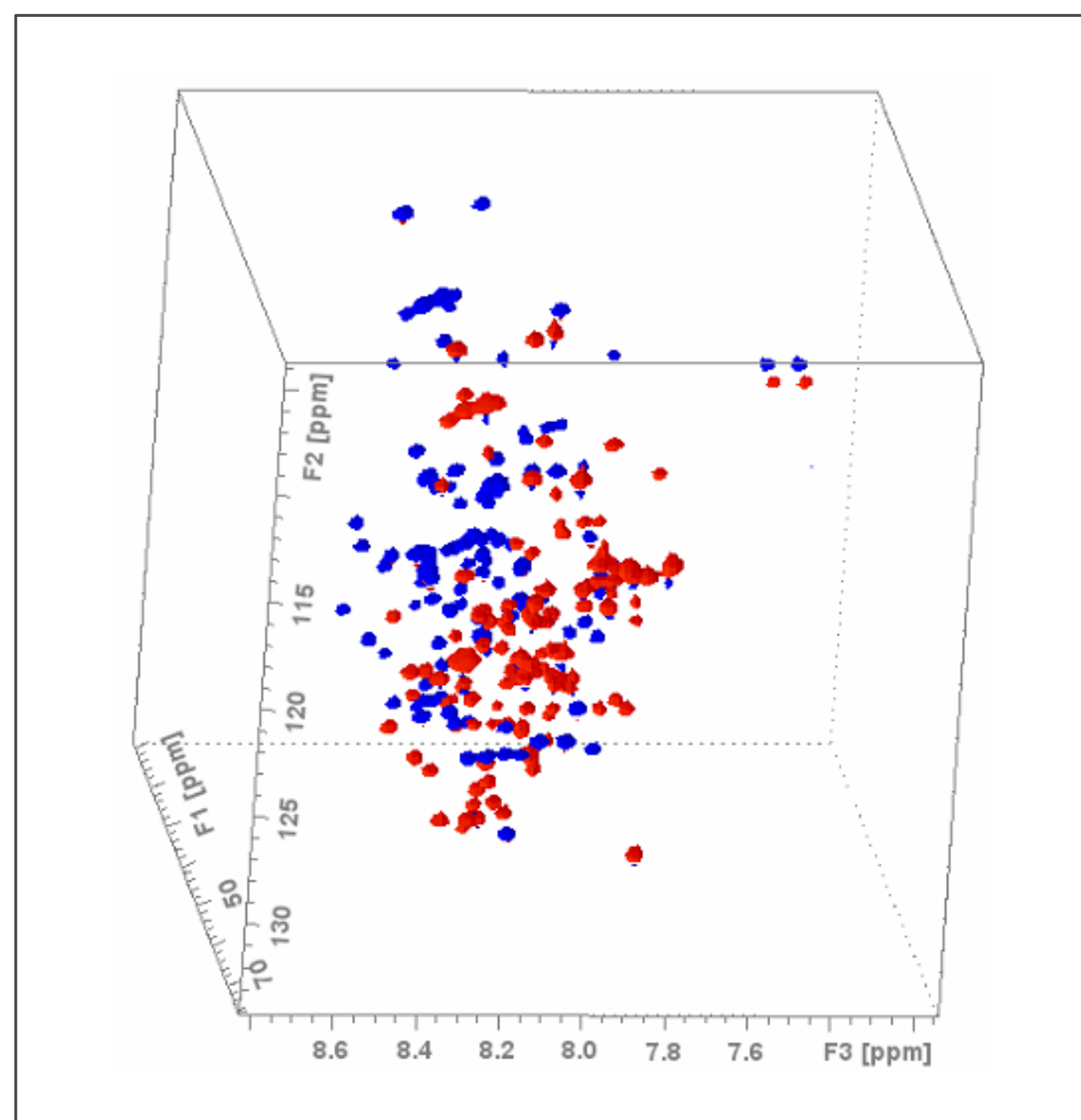
To test the capabilities of the 1.3 GHz spectrometer, five different NMR probes were utilized:

- **0.4 mm HCN Solid-State CPMAS Probe:** This probe is optimized for proton detection on biological systems. It was used to combine Bruker's record-breaking 160 kHz MAS technology with the world's highest field NMR magnet.
- **1.9 mm MAS Probe Optimized for Low-Gamma Detection:** This probe was used to characterize spectrometer performance on nuclei such as  $^{27}\text{Al}$ ,  $^{47/49}\text{Ti}$  or  $^{17}\text{O}$  and to demonstrate the benefits of UHF NMR for structure elucidation in material science, especially for quadrupolar or low-gamma nuclei.
- **3 mm TXI Probe:** This inverse detection probe features a Z-gradient and a  $^2\text{H}$  lock channel.
- **5 mm TXO CryoProbe:** This probe is also equipped with a Z-gradient and a  $^2\text{H}$  lock channel. The CryoProbe technology enhances sensitivity and resolution, making it suitable for detailed structural analysis. The probe is equipped with cold preamplifiers on all channels.
- **0.7 mm HCN Solid-State CPMAS Probe:** This probe was used to test UHF solid-state NMR applications at 1.3 GHz and at a spinning frequency of 111 kHz.

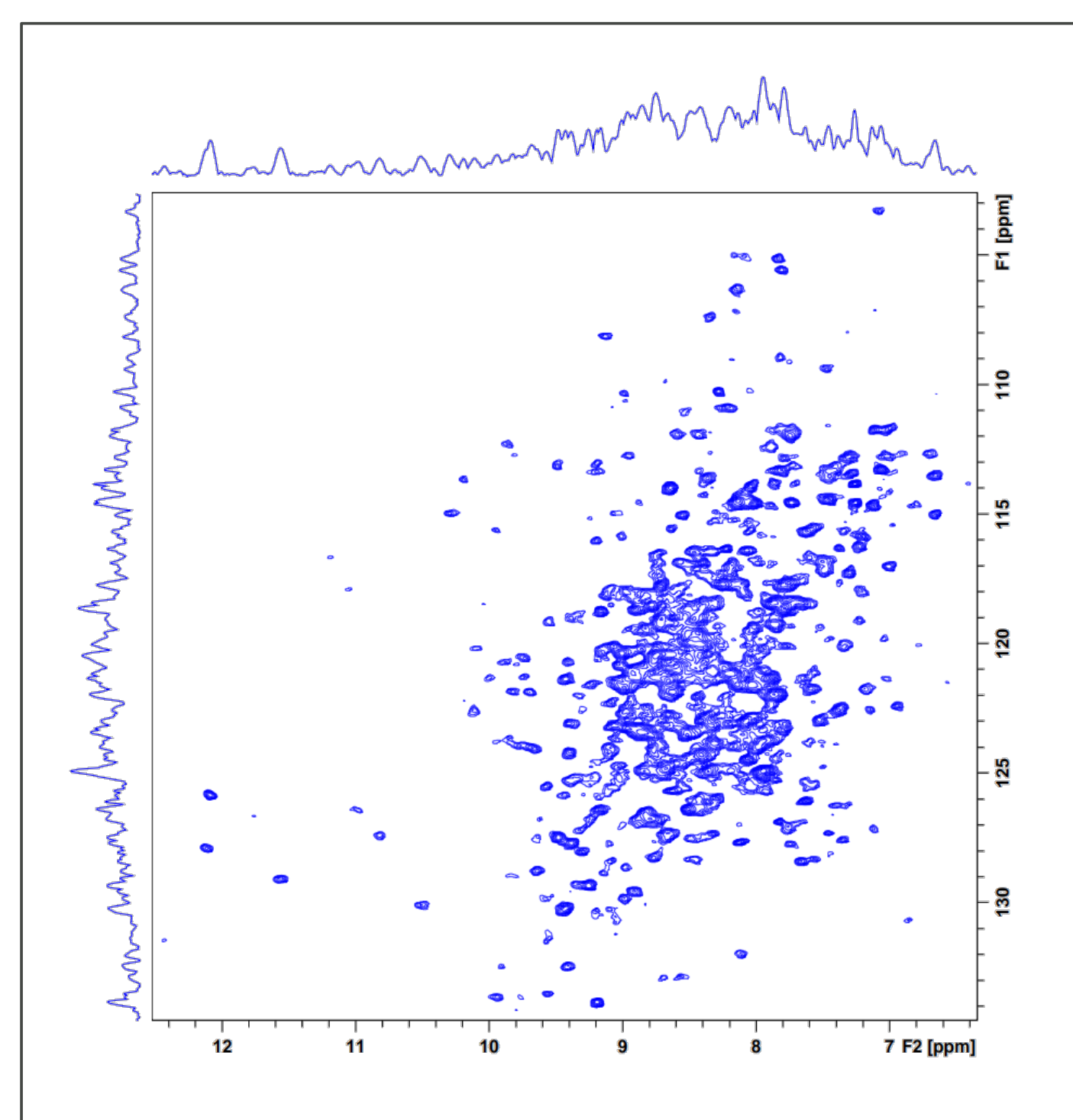
These probes were used to verify the practical applicability of the first-of-a-kind 1.3 GHz spectrometer with representative samples. A few of the resulting spectra are shown on the left in Figures 3 – 7.



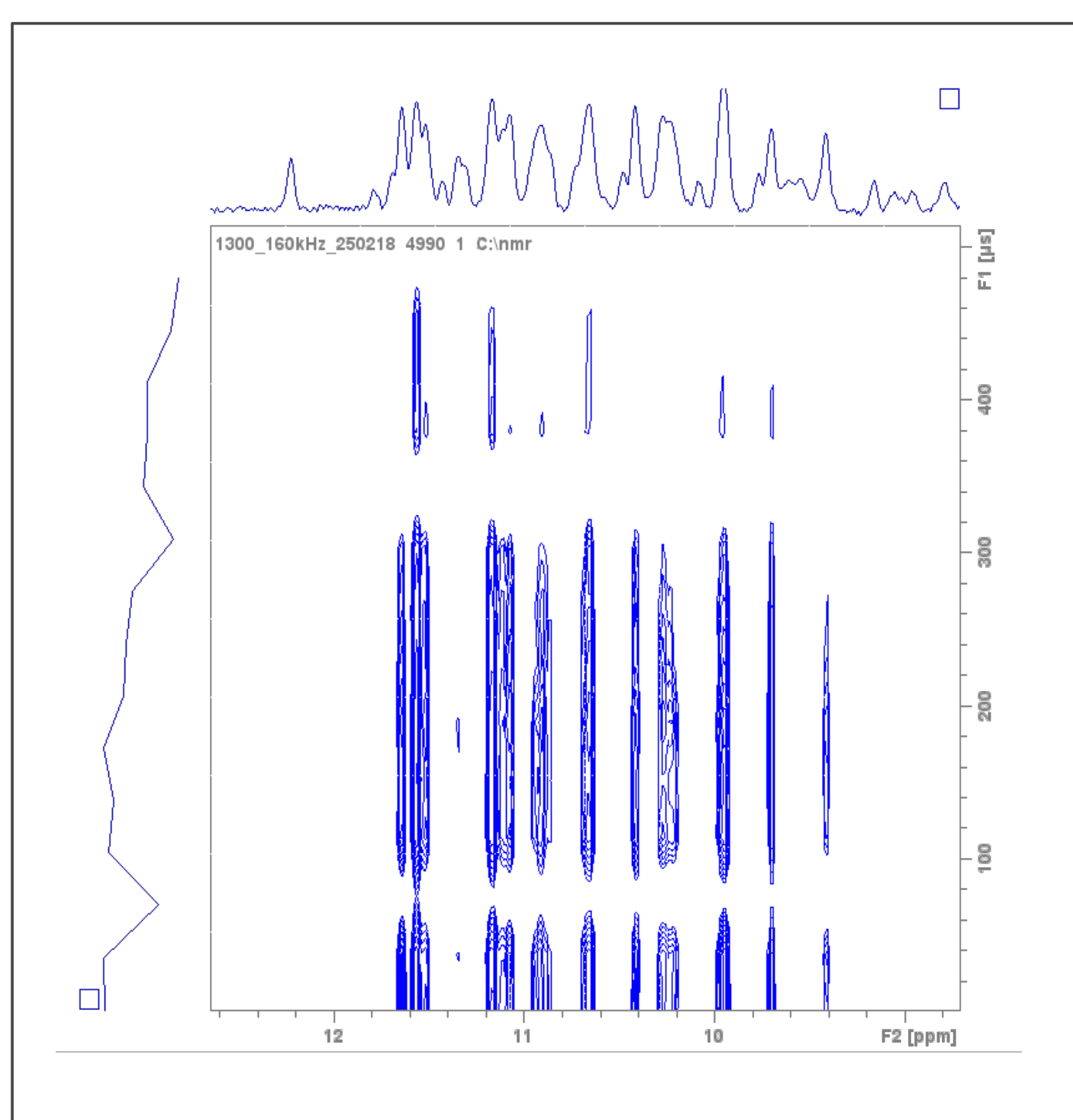
**Fig. 3:** 2D  $^1\text{H}$ - $^{15}\text{N}$  HSQC of ubiquitin in  $\text{H}_2\text{O}:\text{D}_2\text{O}$  (9:1), recorded with the 1.3 GHz 5 mm TXO CryoProbe.



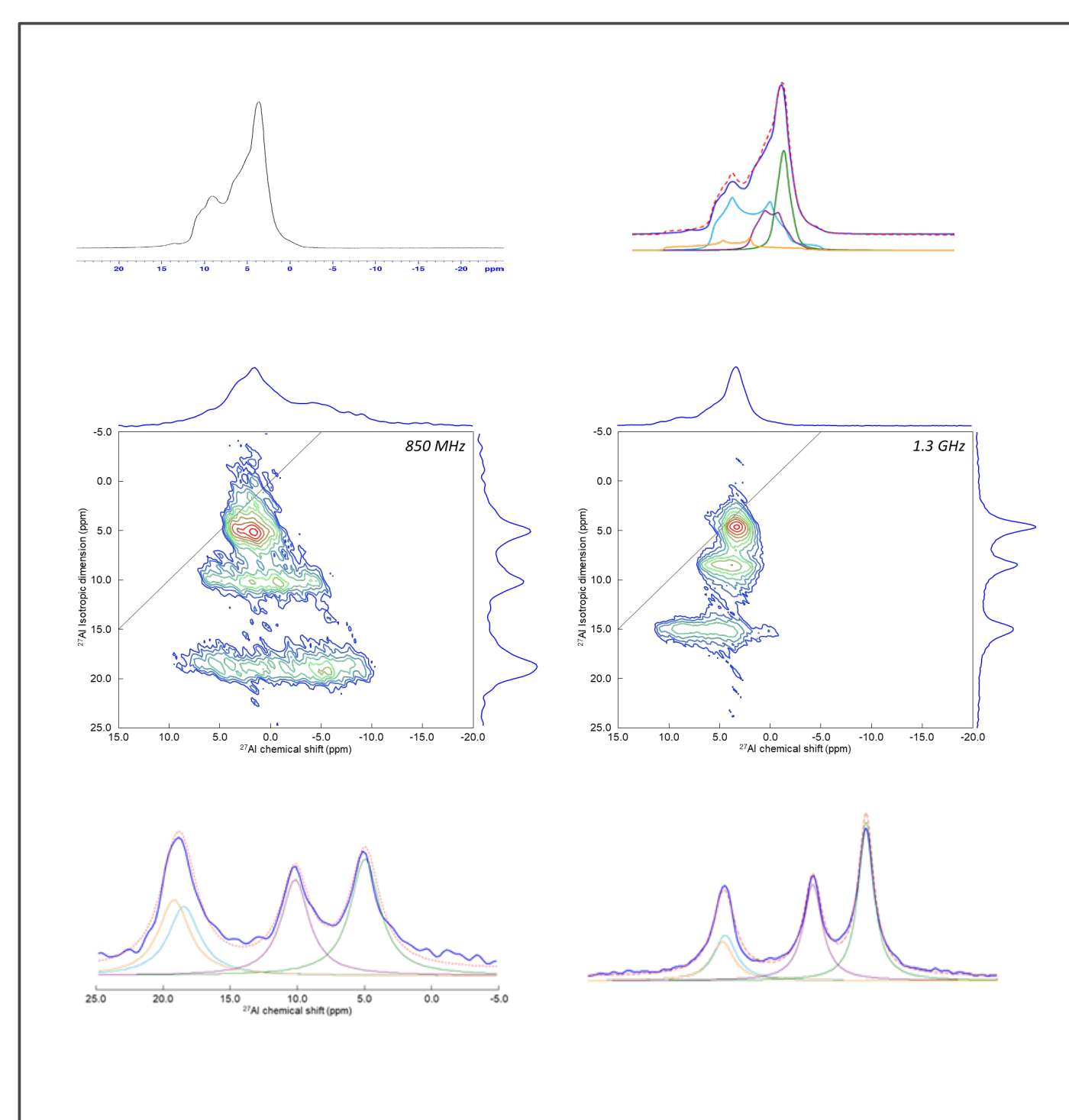
**Fig. 4:** BEST TROSY  $\text{HN}(\text{CO})\text{CaC}\beta$  correlation of  $\alpha$ -synuclein in  $\text{H}_2\text{O}:\text{D}_2\text{O}$  (9:1). Sample courtesy of CERM.



**Fig. 5:** 160 kHz solid-state NMR spectrum of fully protonated tryptophan synthase ( $2 \times 72$  kDa), one of the largest enzymes ever studied by solid-state NMR.



**Fig. 6:** Pseudo-2D  $^{15}\text{N}$  T2 experiment of deuterated and fully  $^1\text{H}$  back exchanged SH3. At 1.3 GHz, 2Ds can be used instead of 3Ds, leading to time savings of up to two orders of magnitude.



**Fig. 7:** Spectra of kyanite  $\text{Al}_2\text{SiO}_5$  (from top to bottom: 1D comparison with simulation; MQMAS 2D; MQMAS projection). UHF NMR leads to sharper lines and less spectral overlap.

## Conclusion

- Bruker has developed and built the first 1.3 GHz high-resolution NMR spectrometer.
- The magnet was successfully energized and homogenized and reached field multiple times.
- NMR tests were conducted with five different probes.
- This sets a new world record in high-resolution NMR.