



## Solid State Analysis of Medicines

- Expand your analytical power with open access solid-state NMR

Characterization of drug substances and drug products is a critical need in the pharmaceutical industry. Solid state NMR spectroscopy (ssNMR) is an excellent analytical technique to characterize the solid forms of a drug substance to identify different crystalline and/or forms, monitor form conversion during Active Pharmaceutical Ingredient (API) scale up, detect low amounts of other forms (e.g. crystalline in amorphous), measure relaxation times for prediction of physicochemical stability, and guard intellectual property. Similarly, drug product is uniquely suited to characterization by ssNMR because excipients typically do not significantly interfere with the analysis, even at low levels of drug substance in the drug product.

Although traditionally in the hands of few specialists, recent advances have enabled the deployment of the technique to the walk-up lab. Instruments are today equipped with the new iProbe with automatic tuning and matching and magic angle adjustment; and sample changers driven by the same automation software used in liquid state NMR. Because of the new 'shuttle technology' the same sample changer can be used for both liquids and solids NMR, which enables to upgrade from liquids to solids for half the price of a Powder X-ray Diffraction (PXRD) instrument!

## User Benefits

- Identification and quantification of crystalline and amorphous content in APIs and formulated products
- Quantification of the amount of each form without the need for a standard
- Multiple attribute: multiple nuclei can be analyzed, providing several unique spectra for each form
- Unique to NMR, relaxation times:
  - identify peaks for different crystalline forms, as each relaxation time for a form is usually unique;
  - selectively enhance or remove different forms in a mixture of components, which can be useful for form identification and showing intellectual property infringement
  - predict both particle size and chemical degradation rates, especially in formulated products
- Selectivity: labelling of nuclei such as  $^{13}\text{C}$  and  $^{15}\text{N}$  can be used to enhance certain signals when sensitivity is a challenge, as well as avoiding peak overlap



## Features

- Automatic tuning, matching and magic angle setting
- RF-configuration:  $^1\text{H}$ - $^{19}\text{F}/^{31}\text{P}$ - $^{15}\text{N}$
- 4 mm rotors, up to 15 kHz MAS
- Builds on well established liquid state automation hardware/software
- Integrates into pharma workflows
- Remote access & analysis management
- State-of-the-art GxP

## Key Components

- iProbe CP-MAS and 4 mm rotors
- 400, 500 or 600 MHz magnet
- AVANCE III HD or AVANCE NEO console
- SamplePro (hr)-MAS or SampleCase Plus with MAS shuttles\*
- TS 4.1.3 and beyond (includes IconNMR)
- MAS3 pneumatic control unit

\*Requires AVANCE NEO Console

Service	Description	Status	Open access	Creator
<a href="#">NMR - 13C - CP.MAS</a>	cross-polarization to 13C	Active	Yes	Kristof Grohe
<a href="#">NMR - 13C - CP.CPPI</a>	cross-polarization and CH, CH2, CH3 editing	Active	Yes	Kristof Grohe
<a href="#">NMR - 13C - CP.MAS TOSS.NOS</a>	sideband suppression and non-quarternary carbon suppression after cross-polarization	Active	Yes	Kristof Grohe
<a href="#">NMR - 15N - HETCOR</a>	correlation between 1H and 15N with cross-polarization and 15N detection	Active	Yes	Kristof Grohe
<a href="#">NMR - 15N - CPMAS</a>	cross-polarization and 15N detection	Active	Yes	Kristof Grohe