OXFORD INSTRUMENTS

X-Pulse Benchtop NMR

Modular, flexible system with NEW X-Spin integrated software

- Fully tuneable broadband NMR
- Variable temperature measurements
- Customisable and upgradable
- Comprehensive sample automation
- Compliance-ready for GxP and 21 CFR Part 11



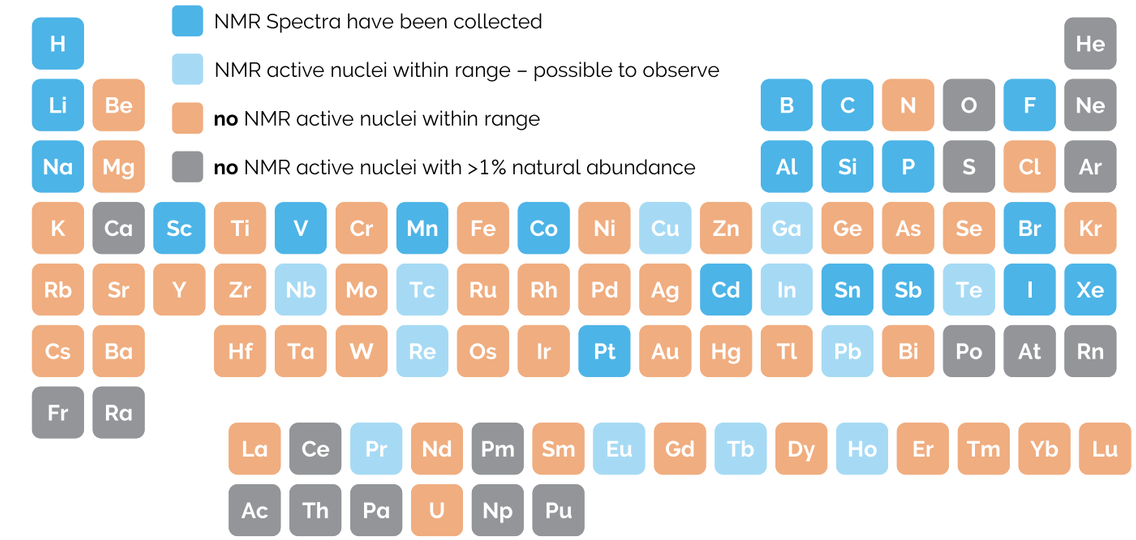
www.oxinst.com

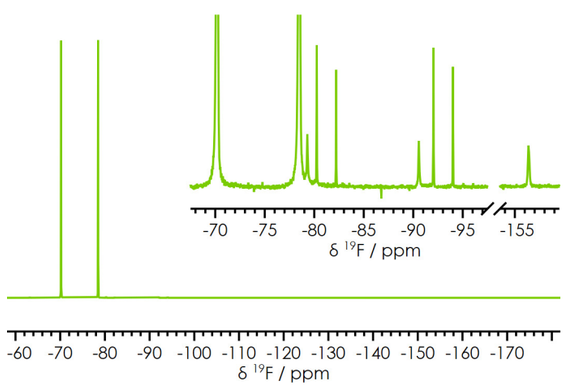
Introducing X-Pulse

X-Pulse is a revolutionary benchtop nuclear magnetic resonance (NMR) spectrometer that brings broadband NMR to the benchtop at 60 MHz or 90 MHz for the first time. X-Pulse is the ideal instrument for flexible chemical analysis, across a wide variety of applications, as it enables investigation of the largest number of nuclei without compromising performance.

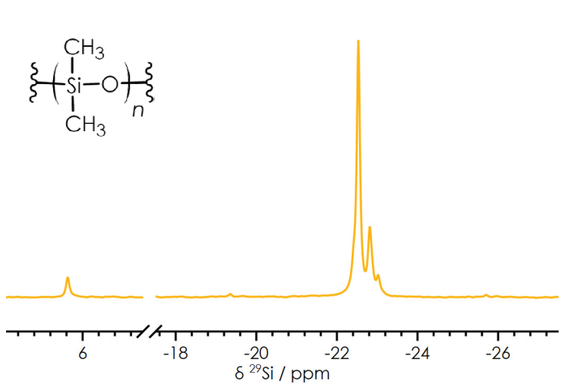
X-Pulse's unique features that will benefit your workflow:

- Broadband capability enables a large number of nuclei to be measured.
- A wide variable temperature range option of 0-60˚C allowing users to thoroughly investigate reaction kinetics or characterise electrolyte properties.
- The orientation of the diffusion gradient ensures accurate measurement, even in flow experiments.
- User exchangeable probes mean no compromise between versatility and sensitivity.
- User removeable probe means minimal machine downtime for breakages and spills.





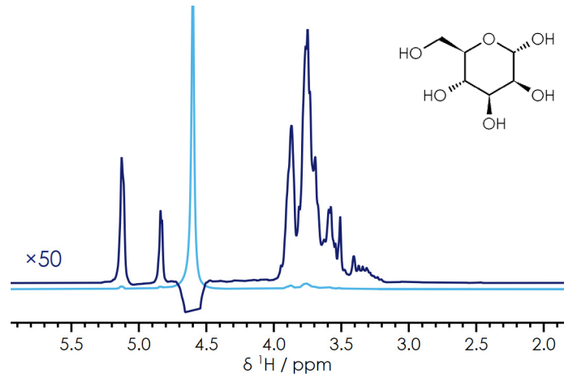
^{19}F NMR spectrum of Li-ion battery electrolyte, insert showing trace quantities of decomposition products.



^{29}Si{^{1}H} DEPT NMR spectrum of a mixture of polysiloxanes.

Why Benchtop NMR Spectroscopy?

Benchtop NMR is a spectroscopic technique that provides structural and quantitative insights into liquid chemical samples. Minimal sample prep and its non-invasive, non-destructive nature make it perfect for complementing any existing analysis techniques. Benchtop NMR can easily be brought to the lab, and when coupled with a flow cell and X-Pulse broadband capabilities, provides real time monitoring of many nuclei within a sample.



^{1}H NMR spectra of Mannose in H_2O, without (light blue) and with (dark blue) WET solvent suppression.



Modular design: configured for today, flexible for tomorrow

Our X-Pulse system focuses on modularity, versatility, and upgradeability, meaning it can be tailored to your needs. For example, it can be easily coupled with a flow cell to monitor reactions in real time. Variable temperature capability can be added, and the unique user-exchangeable probe enables easy setup changes depending on your requirements, whether prioritising the highest signal-to-noise ratio (SNR) performance or multiple nuclei. It also provides easy access for cleaning.

1 BENCHTOP SYSTEM

Supports benchtop NMR acquisition, compact system, with broadband capability.



2 USER REMOVEABLE PROBE

Means minimal machine downtime for breakages and spills.

3 AUTOSAMPLING

To speed up analysis, X-Pulse can be fitted with a 25 position autosampler allowing 'hands free' analysis that reduces time spent in front of the instrument and maximises instrument use. Read more on page 8

4 INTEGRATED SOFTWARE SOLUTIONS

Choose from:

NEW X-SPIN SOFTWARE

Our acquisition software, X-Spin, is easy-to-use and suitable for all levels of operators from experts to infrequent users. Read more on page 12.

SPINFLOW SOFTWARE

Control setup and acquisition while retaining the depth and control required by experienced NMR users. Read more on page 10.

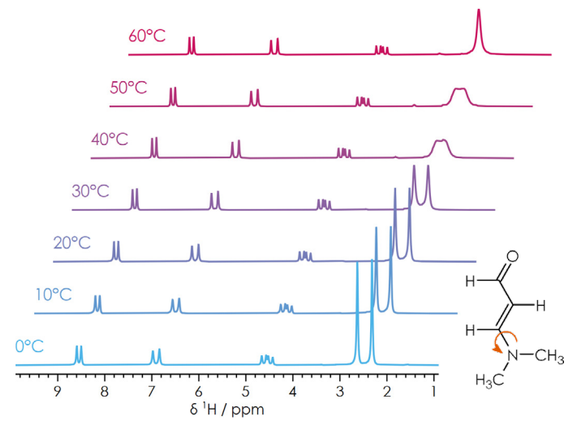
NEW

5 INSTALL AND QUALIFICATION PACKAGES

The X-Spin Compliance and Qualification Package helps regulated laboratories qualify their X-Pulse system and support GxP and 21 CFR Part 11 workflows. It includes IQ/OQ performed by a qualified engineer, PQ guidance and traceable certified standards. Combined with X-Spin's role-based access, secure user management and comprehensive audit trails, it provides a strong foundation for controlled, traceable NMR workflows.

6 VARIABLE TEMPERATURE (VT)

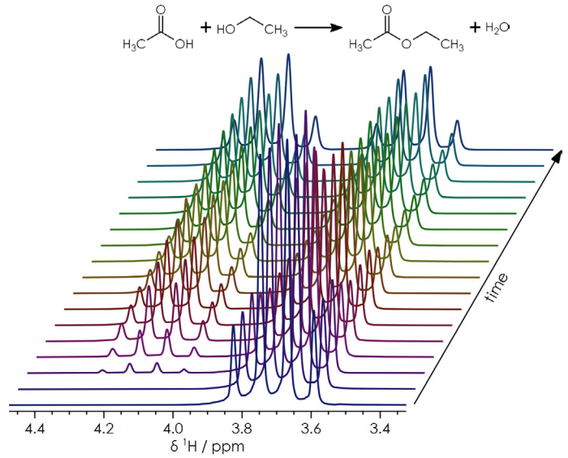
It is possible to combine the high sensitivity X-Pulse with the widest variable temperature (VT) range (0-60°C) available for a benchtop NMR spectrometer. This allows a comprehensive understanding of reaction kinetics, as well as enabling users to observe a wider range of reactions. The large temperature range also facilitates investigation of the behaviour of mixtures at different temperatures, for example, quantifying battery electrolyte performance over a range of temperatures, including below room temperature.



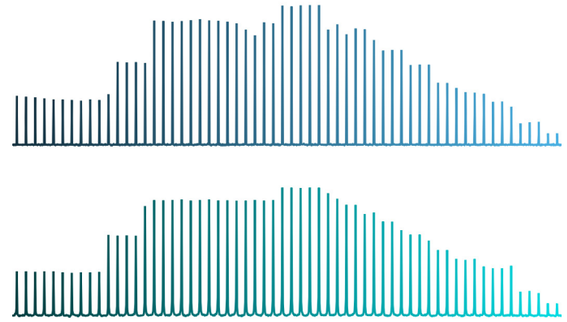
^{1}H spectra of 3-dimethylaminoacrolein at 0 to 60°C. As the temperature increases the two methyl signals coalesce into a single peak.

7 FLOW CELL

X-Pulse equipped with a flow cell makes real time reaction control and mechanistic studies straightforward. The flow cell itself is simple to install owing to X-Pulse's removable probe. In addition, X-Pulse features an external deuterium lock meaning reactions can be run and monitored without the need for expensive deuterated solvents. The orientation of the X-Pulse diffusion gradient will ensure accurate measurement, even whilst the sample is flowing, and the excellent stability of X-Pulse ensures the only variation you will see in the spectrum comes from the reaction itself



^{1}H spectra of the reaction of ethanol and acetic acid, monitored by flow NMR. As the reaction progresses, ethanol is consumed (quartet at 3.7 ppm) and ethyl acetate formed (quartet at 4.1 ppm).



^{7}Li (top) and ^{23}Na (bottom) quantitative NMR spectra, monitoring Li^{+} and Na^{+} concentration by flow NMR.

Modular. Flexible. Powerful.
Choose the modules that fit your research today and expand as your needs evolve.

Focus on applications

The X-Pulse has a wide variety of applications applicable to industry, academia, government and public-sector organisations, including:

STRUCTURAL ELUCIDATION OF SMALL MOLECULES

Determine chemical structures using one- and two-dimensional pulse sequences, alongside the using the multi-nuclear capability to analyse all nuclei of interest. Throughput can be maximised with the X-Auto autosampler.

PHARMACEUTICALS

Identify and quantify compounds both in research and development; or as simple, fast, and repeatable QC/QA measurements. Monitor reactions and processes, optionally using flow NMR. While compliance in a GLP environment is supported by the new X-Spin acquisition software.

INDUSTRIAL QA/QC

Perform reliable qualitative and quantitative analysis of reactants, intermediates and products. With the X-Spin acquisition software supporting compliance for GxP.

BATTERIES

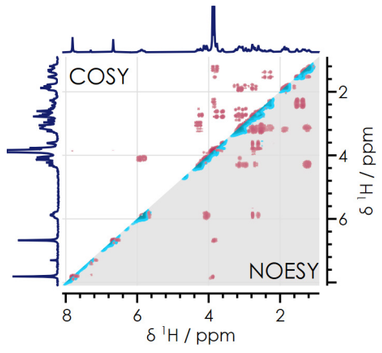
Qualitative and quantitative analysis of the composition of liquid electrolytes for QC/QA. Determine the products of electrolyte degradation and monitor these processes. Diffusion constants for charge carriers can be measured, to understand battery performance; with variable temperature measurement options.

CHEMICAL MANUFACTURING

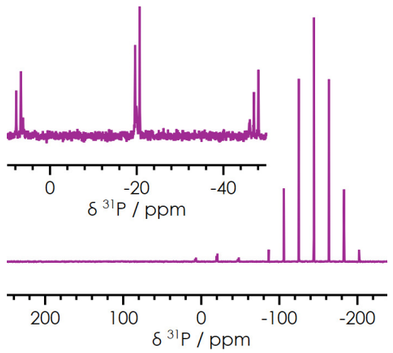
Perform robust QC/QA for the rapid analysis of samples, these measurements can be readily integrated into existing workflows and complement other techniques. Monitor reactions and processes in real time, with optional flow NMR for continuous analysis. Compliance in a GMP environment is supported by the new X-Spin software.

POLYMERS

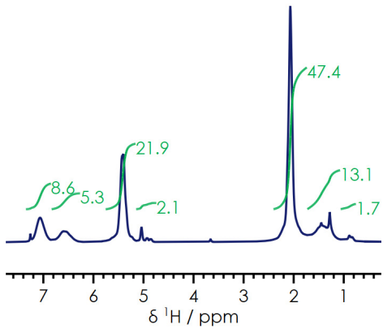
Composition and purity of polymers can be determined, and diffusion measurements used to obtain the average molecular weight. While polymerisation reactions may be monitored using flow NMR.



Two-dimensional ^{1}H-^{1}H spectra of Brucine; the COSY (top-left) shows through-bond couplings, and the NOESY (bottom-right) shows through-space interactions.



^{31}P NMR spectrum of Li-ion battery electrolyte, insert showing trace quantities of decomposition products.



^{1}H NMR spectrum of a block co-polymer, by integrating the signal regions the proportion of each block can be determined.

TEACHING NMR

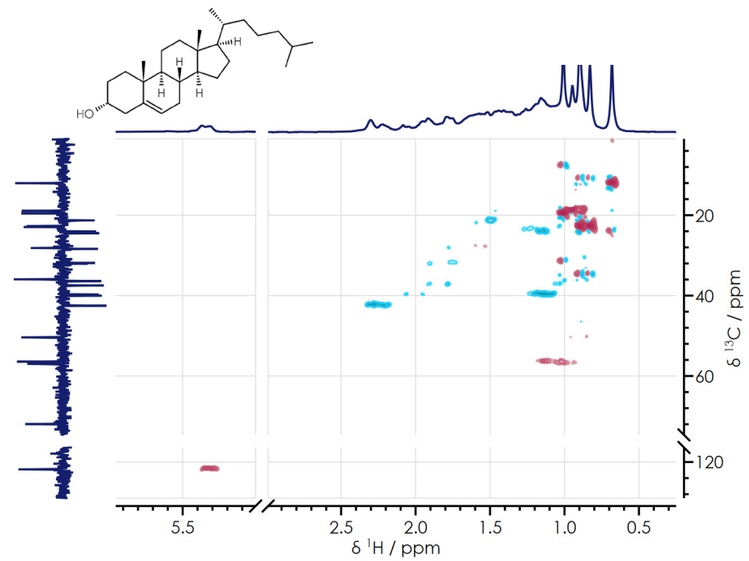
The X-Pulse can be used to teach fundamentals of NMR spectroscopy, engaging students by using examples containing a range of nuclei. Teaching of synthetic chemistry is supported by allowing students to acquire NMR spectra themselves as part of the lab session.

CHEMICAL RESEARCH

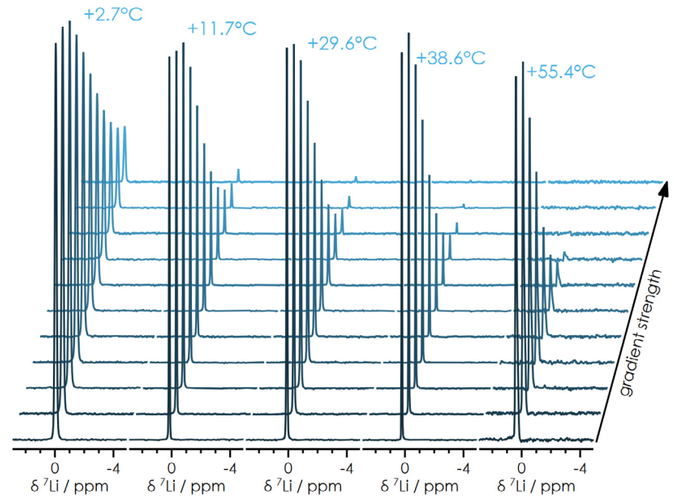
The X-Pulses' flexibility makes it ideal for multi-user labs and core instrument facilities, where there's a large variety of different requirements by end-users. Chemical reactions and processes can be monitored using a range of nuclei and pulse sequences, including by using flow NMR. Perform measurements at a range of temperatures using the variable temperature option. The new X-Spin acquisition software supports comprehensive user management for multi-user environments.

FUNDAMENTAL NMR RESEARCH

Pulse sequences for the X-Pulse are written in Python®, giving users the option to write their own sequences and run them as standard. Additionally, X-Pulse is highly modular and customisable (both hardware and software) therefore, can be integrated into a wide range of processes.



Two-dimensional ^{1}H-^{13}C HSQC spectrum of Cholesterol; identifying one-bond proton-carbon correlations, and distinguishing CH_3 & CH (red) from CH_2 (blue) centres.



^{7}Li PGSE NMR spectra of Li-ion battery electrolyte at 2 to 55°C. As the temperature increases the diffusion constant increases, resulting in greater signal attenuation as the gradient strength increases

X-Auto

Set up. Queue. Walk away.

X-Auto brings automated sample handling to the X-Pulse benchtop NMR platform. With 25 configurable sample positions, automated tube exchange and software controlled acquisition, X-Auto makes it easy to move from individual measurements to efficient, multi-sample NMR workflows. Whether you are screening samples in R&D, running routine quality control measurements or managing a busy teaching laboratory, X-Auto helps you spend less time managing samples and more time analysing results.

X-Auto can be fully controlled through X-Spin or SpinFlow that brings sample management and experiment setup into one intuitive workflow. Experiments can be added to individual samples, while predefined experiment queues can streamline repeated analysis. SpinFlow and X-Spin both provide automatic sample detection and live feedback on sample and experiment status.

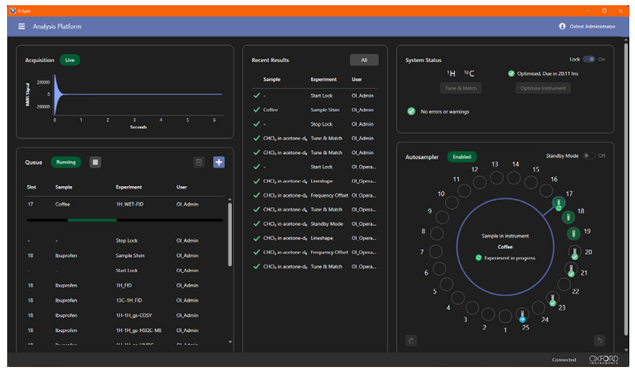
Highlighted features:

25 Sample positions – Automated sample exchange for up to 25 NMR tubes.

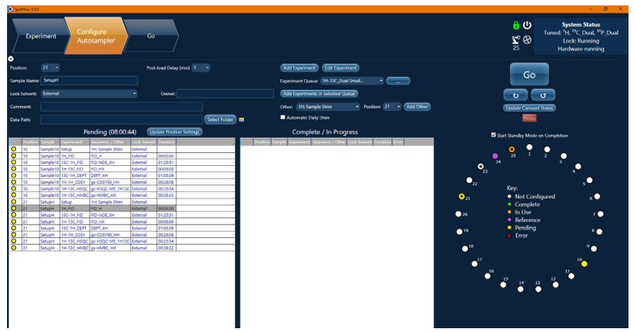
Multi-sample, multinuclear automation – Automate data acquisition across multiple samples and nuclei.

Simple workflow control – Manage X-Auto directly through X-Spin or SpinFlow.

Intelligent sample management - Automatic sample detection and live sample and experiment status help make running experiment queues straightforward.



Screen shot of X-Spin with Autosampler



Screen shot of SpinFlow Autosampler

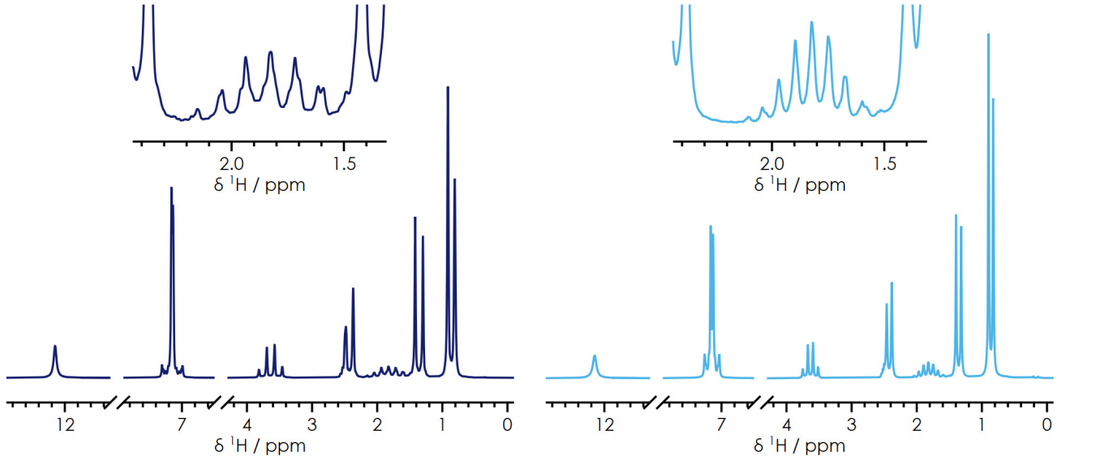


Spotlight on X-Pulse 90

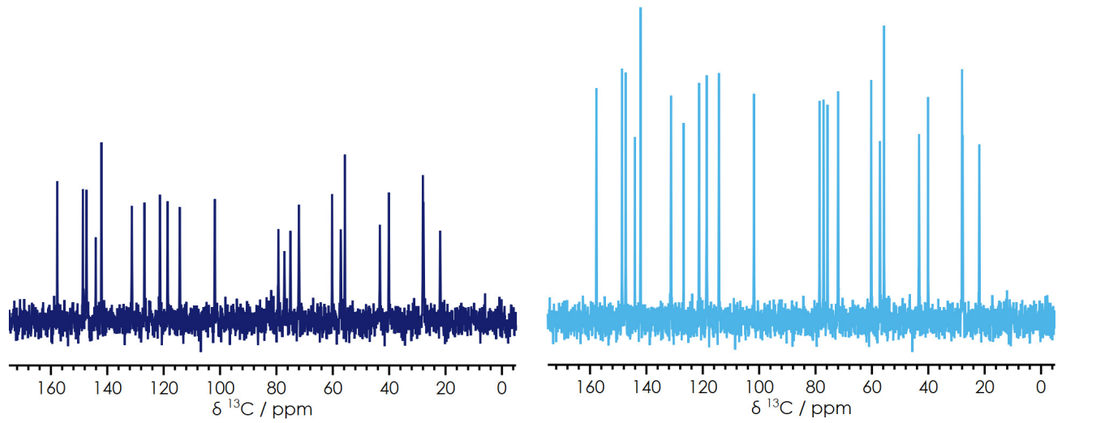
The Power of 90 MHz Performance

With a magnetic field of 90 MHz (2.1 T) X-Pulse 90 allows users to separate challenging peak overlaps and positively identify compounds of interest in samples. The increased spectral dispersion means that a peak that is hard to distinguish with a lower magnetic field is now separated and easily identifiable.

The increased sensitivity of X-Pulse 90 also enables detection and accurate measurement of molecules with a lower concentration, such as mass limited samples or when dealing with active pharmaceutical ingredients (APIs). The increased sensitivity and peak separation also enable much faster 2D experiments, even on larger molecules.



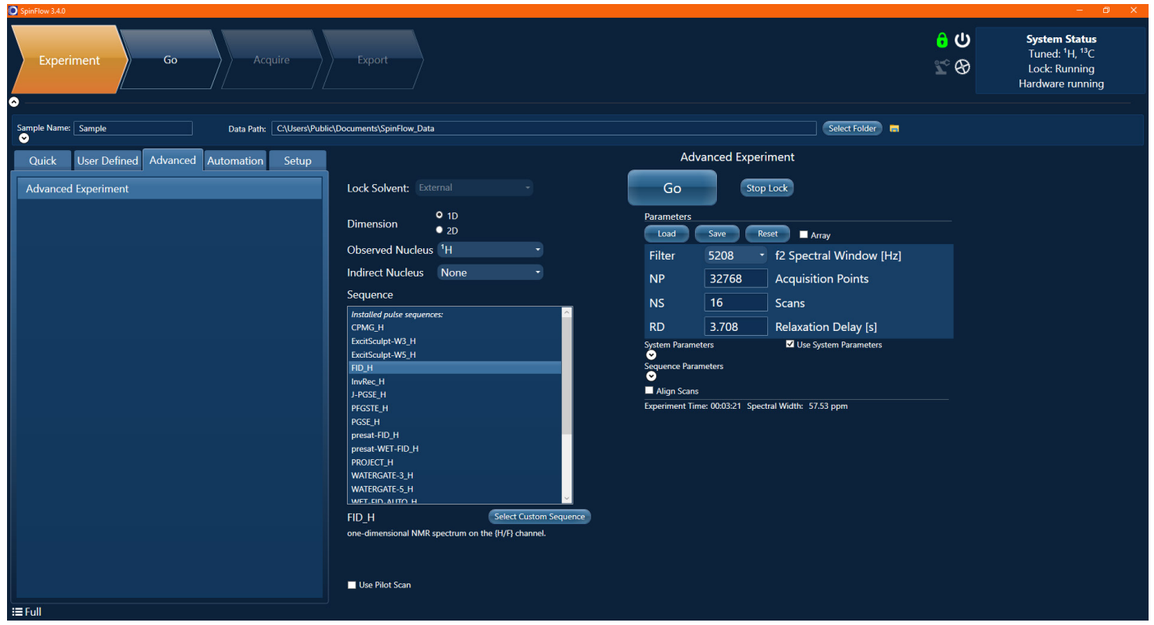
A comparison of Ibuprofen ^{1}H NMR spectra on X-Pulse 60 (left) and X-Pulse 90 (right), the zoomed in sections highlight the improved signal dispersion at the higher field.



A comparison of Quinine $^{13}C[^{1}H]$ spectra on X-Pulse 60 (left) and X-Pulse 90 (right), showing the improved sensitivity at the higher field.

SpinFlow software

From routine spectra to advanced NMR workflows



Powerful acquisition control. Flexible workflows. Built to adapt.

SpinFlow guides users through X-Pulse setup and acquisition while retaining the depth and control required by experienced NMR users.

- Quick experiments for routine measurements
- User defined experiments for repeatable workflows
- Advanced access to 1D, arrayed and 2D experiments
- Customisable parameters, saved methods and experiment queues

Simple when required. Advanced when the experiment demands it.

Accessible by design

Basic View presents Quick, User Defined and Automation workflows for straightforward operation

Advanced control

Full View enables access to installed 1D, arrayed and 2D experiments, available nuclei and customisable parameters

Optimise and reuse

Save parameter sets, array lists and optimised advanced experiments for repeatable acquisition or later use in a queue.

A broad experiment toolkit

Routine and quantitative

Standard 1D acquisition, inversion recovery, CPMG/PROJECT relaxation and PGSE/PFGSTE diffusion measurements

Selective and structural

Signal-suppression methods and 2D experiments including COSY, TOCSY, NOESY and *J*-Resolved

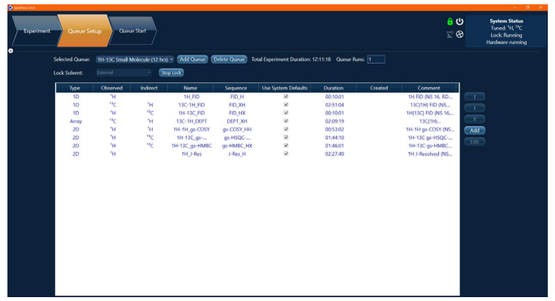
Heteronuclear capability

Experiments such as HMBC, HMQC, HSQC and HETCOR where supported by the X-Pulse configuration

Additional or updated pulse sequences can be supplied through Oxford Instruments Support, with support available for new sequence development.

Build and adapt **workflows around your chemistry**

Queue, repeat and adjust acquisition for reaction monitoring, flow NMR and automation





Pending (19:16:47)

	Experiment	Sequence / Other	Duration
	Event	Loop start	10
	Setup	1H: Sample Shim	
	1H_FID	FID_H	00:00:40
	FID_XH	FID_XH	00:21:43
	Event	Time Delay	00:05:00
	1H_FID	FID_H	00:00:40
	FID_XH	FID_XH	00:21:43
	Event	Loop end	
	1H_FID	FID_H	00:05:00
	13C-1H_FID	FID-NOE_XH	01:25:51
	1H-13C_FID	FID_HX	00:05:00
	13C-1H_DEPT	DEPT_XH	01:05:09
	1H-1H_COSY	gs-COSY90_HH	00:26:06
	1H-13C_HSQC	gs-HSQC-ME_1H13C	00:51:49
	1H-13C_HMBC	gs-HMBC_HX	00:26:22
	Event	Loop start	10
	Setup	1H: Sample Shim	
	1H_FID	FID_H	00:00:40
	Event	Time Delay	00:05:00
	1H_FID	FID_H	00:00:40
	Event	Time Delay	00:05:00
	1H_FID	FID_H	00:00:40
	Event	Loop end	

From predefined queues to live adaptation

Experiment Queue automates a predefined series. Sample Queue adds the ability to insert, reorder and adjust pending actions as the study develops.

- Combine different experiment types, including arrays and 2D experiments
- Repeat queues at pre-set intervals for reaction monitoring or flow NMR
- Insert time delays, loops and supported setup actions
- Move, duplicate, add or remove pending items
- Use Sample Queue with or without X-Auto
- Automatically export spectra to your chosen processing software or workflow

Flexible enough for experiments that evolve

Interleave and repeat

Combine nuclei and experiment types, then control the acquisition cadence using queue repeats, loops and delays

Respond to new information

Add a targeted experiment, including a 2D measurement, when reaction progress reveals an intermediate or new analytical question

Scale the workflow

Run dynamic queues on a single sample or coordinate measurements across multiple samples with X-Auto

X-Spin software

X-Spin is the next-generation NMR acquisition platform for Oxford Instruments benchtop NMR spectroscopy systems. Combining an intuitive user experience with flexible method control, secure user management and automation support, X-Spin simplifies NMR workflows while improving productivity in both research and regulated laboratories.

From reaction monitoring and structure verification in chemistry research to analytical development, process monitoring and quality control in pharmaceutical environments, X-Spin helps laboratories acquire reliable NMR data quickly and consistently.

Unlock the full potential of your X-Pulse benchtop NMR spectrometer with X-Spin, the next-generation acquisition software designed to make NMR workflows simpler, faster and more consistent. Combining an intuitive user experience with flexible method control, secure user management and automation support, X-Spin is suitable for both research and regulated laboratory environments.

X-Spin makes routine operation accessible to users with different levels of NMR experience. Preconfigured experiment parameters and automated shim routines help occasional users begin their analyses quickly, without requiring every operator to become an NMR expert. For more experienced users, X-Spin provides full control over acquisition parameters, together with the ability to save and recall experimental methods to support consistent workflows and laboratory standard operating procedures.

KEY BENEFITS

SIMPLIFIED EXPERIMENT SETUP

Load experiment templates and use preset parameters for rapid, walk-up analysis.

RELIABLE OPTIMISATION

Automated shim routines optimise line shape for standard samples and users' own samples, while Tune and Match helps ensure the system performs optimally for each sample.

FLEXIBLE EXPERIMENTAL CONTROL

Adjust acquisition parameters and save or recall methods to meet routine and advanced analytical needs.

AUTOMATION-READY

Integration with the X-Auto autosampler supports automated sample handling, queue management and unattended operation for greater laboratory efficiency.

QUALIFICATION AND COMPLIANCE SUPPORT

X-Spin provides secure user management, role-based access, and comprehensive audit trails that automatically record user actions. It supports **IQ, OQ,** and **PQ** activities, alongside workflows designed to support **21 CFR Part 11** and **GxP** requirements, helping laboratories integrate NMR into established quality and compliance frameworks.



From acquisition to chemical and molecular insight

Advanced experiment builder

Allows full customisation of NMR experiments, saving them for future use.

Predefine your experiments

Saved templates, allow users to acquire spectra with a minimum of effort.

Queue multiple (pre-saved) experiments

On multiple samples use the X-Auto Autosampler to maximise throughput.



Specifications

		X-Pulse 90 1H/19F Only	X-Pulse 90 Broadband	X-Pulse 60 1H/19F Only	X-Pulse 60 Broadband
Operating Frequency | Magnetic Field strength		90.45 (±0.75) MHz | 2.1 (±0.017) T		59.7 MHz | 1.4 T	
Peak Width (20% Chloroform in acetone-d_6) at 50% height		< 0.35 Hz		< 0.35 Hz	
Peak Width (20% Chloroform in acetone-d_6) at 0.55% height		< 15 Hz		≤ 10 Hz	
^{1}H (Proton) Sensitivity (1% Ethyl Benzene, single scan)		≥ 320:1 SNR	≥ 240:1 SNR	≥ 200:1 SNR	≥ 140:1 SNR
Pulsed Field Gradients		3D (x, y, z) gradients for coherence selection, ≥ 0.5 T/m diffusion (z) gradient (perpendicular to sample tube)			
Available Nuclei:		^{1}H, ^{19}F	^{1}H, ^{19}F Freely Tuneable from ^{29}Si to ^{31}P (19% - 41% of ^{1}H) includes: ^{7}Li, ^{11}B, ^{13}C, ^{23}Na, ^{27}Al, ^{29}Si, ^{31}P, ^{45}Sc, ^{51}V, ^{55}Mn, ^{59}Co, ^{81}Br, ^{99}Tc, ^{119}Sn, ^{121}Sb, ^{129}Xe, ^{195}Pt, ^{207}Pb	^{1}H, ^{19}F	^{1}H, ^{19}F Freely Tuneable from ^{29}Si to ^{31}P (19% - 41% of ^{1}H) includes: ^{7}Li, ^{11}B, ^{13}C, ^{23}Na, ^{27}Al, ^{29}Si, ^{31}P, ^{45}Sc, ^{51}V, ^{55}Mn, ^{59}Co, ^{81}Br, ^{99}Tc, ^{119}Sn, ^{121}Sb, ^{129}Xe, ^{195}Pt, ^{207}Pb
Lock		External ^{2}H (Deuterium) lock			
Sample Temperature Range (VT Probe)		0°C to 60°C		0°C to 65°C	
Compatible Sample Tubes		5 mm diameter, 7" minimum length 8" minimum length with X-Auto autosampler 4 mm diameter with Variable Temperature			
Dimensions:	**Magnet**	39 × 54 × 45 cm			
	Electronics	26 × 52 × 37 cm			
	X-Auto (added height)	44 cm			
	Mobile Workstation	129 × 66 × 97 cm			
Weight:	**Magnet**	115 kg		159 kg	
	Electronics	22 kg		22 kg	
	X-Auto	9 kg		9 kg	
Acquisition Software		Oxford Instruments SpinFlow 3.4 (or later) Oxford Instruments X-Spin 1.2 (or later)			
Pulse Sequences		X-Pulse comes with a wide range of pulse sequences pre-programmed, including, but not limited to: • One-dimensional NMR Spectra (FID)‡ with the option of single or multiple solvent suppression available using presaturation, WET or WATERGATE. • T_1 measurements using Inversion Recovery (InvRec.)‡ • T_2 measurements using CPMG or PROJECT.‡ • Diffusion measurements using Pulsed-field Gradient Spin Echo (PGSE) or Pulsed-Field Gradient STimulated Echo (PFGSTE).‡ • Gradient-selective homo- and hetero-nuclear two-dimensional NMR Spectra, including: COSY, TOCSY, NOESY, HSQC-ME, HMBC, HMQC. • Other one- & two-dimensional NMR Spectra, include: DEPT, INEPT, J-Resolved, HSQC & HETCOR. • Non-uniform sampling (NUS) available for two-dimensional (2D) sequences. • Pulse sequences written in Python®. Users can write their own sequences and run them in SpinFlow as standard. • Additional sequences are available on request. ‡ available for all nuclei, with or without decoupling			
Processing Software		SciY Mnova 17 (or later)			
PC		Windows 11 Desktop PC, 24" Widescreen Monitor			

Accessories	Description and Features
X-Auto Autosampler	X-Auto is a 25 position, instrument mounted, autosampler for the X-Pulse Benchtop NMR spectrometer. It includes: • Automated sample exchange for up to 25 NMR tubes • X-Auto sample holders • Fully controlled from the SpinFlow / X-Spin software interface • Automate data acquisition across multiple samples and nuclei
Flow Cell & System	Complete flow NMR system for X-Pulse Benchtop NMR spectrometer. Enabling the monitoring or reactions and processes as they happen. The full flow system includes: • Glass flow cell, OD 4.0 mm, ID 2.6 mm • Masterflex® Ismatec-Miniflex peristaltic pump (or equivalent) • PTFE tubing & PEEK connectors • Recommended flow rate from 0.1 - 8 ml/min
Variable Temperature	X-Pulse can be coupled with a gas variable temperature system to produce sample temperatures between 0°C and 60°C. The full gas-VT system comes with the following: • 4 mm NMR tubes (pack of 25) for use with gas-VT • JULABO® CORIO CD-600F recirculating thermal bath (or equivalent) for temperature control of the gas supply • Tubing, adapters, and insulation for any system modifications required Requires source of temperature controlled dry gas with a flow rate up to 20 L/min
Mobile Workstation	A workstation designed to bring X-Pulse to where you need it most. Includes: • Access hole pre-aligned to allow for use of gas variable temperature or flow system add-ons • Convenient height to allow easy sample loading, as well as tuning & matching • Dedicated space for magnet, electronics, and PC • Space for an uninterruptible power supply (UPS) if required, supplied by the end-user.
Additional Probes	The X-Pulse Benchtop NMR spectrometer has a user-removeable / user-exchangeable probe, additional probes can be purchased for the instrument. A ^{1}H/^{19}F only (high SNR) probe purchased with a X-Pulse Broadband Benchtop NMR spectrometer allows for the X-Pulse to be swapped between its Broadband and ^{1}H/^{19}F only configurations with the corresponding differences in capability / performance.

The **X-Auto Autosampler**, **Flow Cell & System**, and **Variable Temperature** accessories can all be used on the same X-Pulse instrument, however they cannot be used at the same time.

Environmental specifications	The following environmental requirements are necessary for the installation, operation, and performance of the instrument within specification, and are the responsibility of the purchaser: • Room temperature: 16°C to 26°C • Temperature stability <±0.5°C/hour and humidity < 90% • Power: 100 V-240 V, 50/60 Hz • Source of clean, dry compressed air/nitrogen for instruments with variable temperature option • Free from sources of magnetic interference e.g. pumps, magnetic stirrer plates, other magnetic instruments etc. • Free from sources of radio frequency interference (e.g. FM Transmitter stations < 100 meters away)

Service options

COMPLIANCE SERVICES

IQ, OQ and PQ provide structured, documented evidence that your X-Pulse is installed correctly, operates as intended and performs consistently for its intended use, helping to accelerate readiness, reduce internal validation effort, strengthen audit preparedness, lower compliance risk and establish a reliable baseline for ongoing maintenance, change control and requalification.

SERVICE PLANS

Our range of X-Pulse service plans offer flexible levels of protection to match your operational priorities and budget, combining annual preventative maintenance with remote technical support and on-site response to help maximise uptime, sustain dependable performance and control service costs throughout the instrument lifecycle. Selected plans add parts coverage, applications expertise and training, giving your team faster access to specialist support, and the confidence that your X-Pulse, and team, are supported for long-term success.

Order today

Need more information? At Oxford Instruments we are committed to finding the correct solution for you. With a dedicated team of technical advisors, we are able to offer you one-to-one guidance and technical support on all products.

To request more information please see: **nmr.oxinst.com/x-pulse-90**

Our Benchtop NMR systems are manufactured at our facility in High Wycombe, UK, and we have offices and support centres located worldwide.

Oxford Instruments,
High Wycombe, UK

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Original document in English

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XPULSE-BR-1126-R1

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