SuperNova

DRIVING X-RAY INNOVATION

The Measure of Confidence

Agilent Technologies

The Fastest, Most Intense Dual Wavelength Small Molecule System

The SuperNova from Agilent Technologies is the fastest, most intense dual wavelength X-ray diffraction system available today.

Our latest generation dual wavelength system, the SuperNova, builds upon the success of Agilent's Gemini, the world's first dual wavelength diffractometer.

The SuperNova brings together Agilent's specially developed high intensity molybdenum X-ray micro-focus source, the Mova, and the world's best selling high intensity copper X-ray micro-focus source, the Nova. Co-mounted on a single diffractometer platform alongside the fastest, highest performance CCD detectors, the SuperNova's X-ray sources provide up to 4x the intensity of traditional sealed tube systems and up to 3x the intensity of a 5kW rotating anode. Together this combination of high intensity and fast CCD enables fast data collection in both Mo and Cu experiments.

The fastest, most advanced diffractometer, the SuperNova is easy to use and fully automated, from data collection, through data reduction and processing, to structure solution and refinement using Agilent's AutoChem software.

The SuperNova is the ideal diffractometer for both modern crystallographic research and leading analytical service laboratories. Of the highest performance and versatility, the SuperNova can be applied to a wide range of specialist applications in both small molecule and protein crystallography.

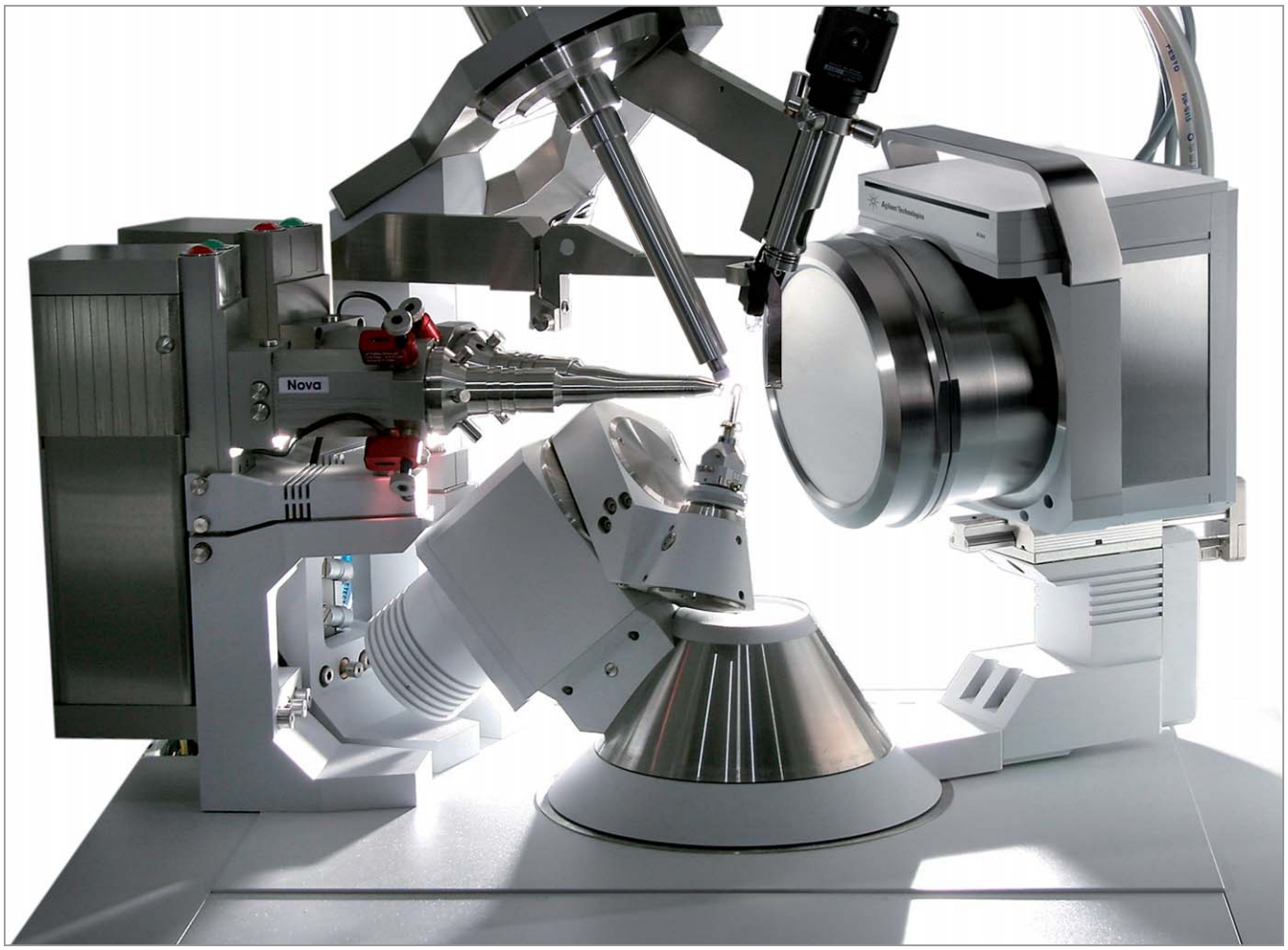
Kappa Goniometer

At the heart of the SuperNova is a high precision 4-circle kappa goniometer. Capable of supporting up to 2 Kg on the phi axis whilst maintaining a better than 10 micron sphere of confusion, the four goniometer axes are driven by high precision stepper motors and are fitted with both revolution and position optical encoder sensors for precision movement and accurate positioning. The extremely compact design of the two vertical X-ray sources gives the SuperNova goniometer an accessible range of angular resolution for both Mo and Cu wavelengths which is greater than any other commercially available diffractometer and significantly in excess of IUCr publication requirements.

The goniometer's theta (detector) arm incorporates a computer controlled and motorised sample to detector distance which has been designed to accept the complete range of Agilent fast CCD detectors including the 135 mm Atlas and the 92 mm Eos.

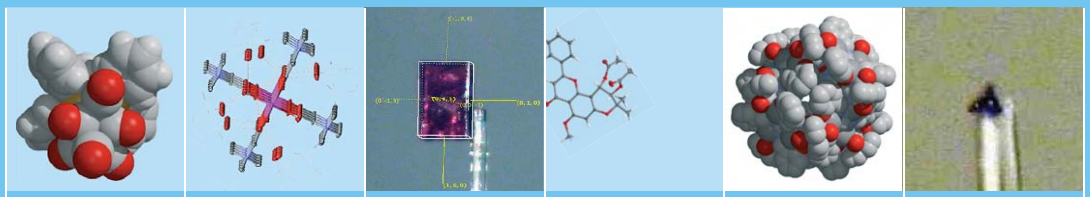
Optional Cryo-devices

With a very open geometry, the SuperNova's goniometer has been designed to accept all major open flow cryogenic sample environment devices including Agilent's liquid nitrogen cooling device (90-300K) and liquid helium device, Helijet (<10-100K).



View of the SuperNova goniometer, showing the co-mounted dual wavelength Nova (Cu) (left front) and the Mova (Mo) (left back) X-ray sources, the optional sample cooling device (top) and the Atlas CCD (right)

Applications



Service | Extended inorganics | Absorbing materials | Absolute structure | Macro-molecules | Small / weak crystals

Charge / electron density | Twinning | Quasi-crystals | High pressure | Incom-mensurate | Powder diffraction | Protein

The System

Compact and Self Contained

At 0.5 m^2, the SuperNova has the most compact footprint of any modern CCD diffractometer. Entirely self contained within a strikingly designed radiation proof and fully interlocked safety protection enclosure, the SuperNova comes complete with monitor and keyboard table and requires only an electricity supply and network connection (if available).

Housed atop the system and behind a lead-doped radiation protection window, the 4-circle kappa goniometer is illuminated by cool LED lighting which can be operated via switches on the system's front panel or remotely via software control.

Easy Sample Mounting

Sample mounting and alignment on the SuperNova is quick and easy using a dedicated video microscope of 120x magnification and sample illumination provided by focusing LEDs mounted astride the system beam stop. A software-enabled sample alignment assistant is built into Agilent's CrysAlis^{Pro} software, making crystal mounting even easier.

Based on the original Gemini design, the SuperNova's dual wavelength beam stop consists of two permanently co-mounted beam catchers orientated to catch both the Mo and Cu straight through X-ray beams. For ease of sample mounting, the whole beam stop assembly can be rotated out of the X-ray beam path and the CCD detector automatically driven away from the sample position providing greater access for the use of cryo-tools and for sample manipulation.

SuperNova dual wavelength beam stop with focusing LED illumination

Inside the SuperNova cabinet base

Modular Design

Designed with ease of service and support in mind, the SuperNova has a modular construction with each major component being a self contained and easily exchangeable unit. Contained within the base of the SuperNova these units include:

- System control interface
- Embedded server computer
- Dual source X-ray generator
- X-ray generator chiller and
- CCD detector chiller

Embedded Server Computer

The SuperNova's embedded server computer handles everything from the automatic data collection, data storage and processing to automatic structure solution, refinement and structure report generation. Within the software, the machine control is separated from the crystallographic applications. As such, an optional second networked PC may be added for offline processing, remote access and experimental control of the SuperNova.

Integrated X-ray and CCD Cooling

The SuperNova's dual X-ray sources and CCD detector are cooled via two built in compact recirculating water chiller units of the peltier cooling design. Cooling water to the X-ray sources is cycled from the first chiller unit. The second identical chiller unit works on an isolated circuit and provides cooling to the CCD detector which is maintained at an operating temperature of -40°C.

Stylish design, Ultra Compact, Radiation Safe and Everything Inside

The complete SuperNova system including monitor / keyboard table

Mo & Cu X-ray Micro-sources

X-ray Sources

The SuperNova has been designed around two low power consumption yet high intensity X-ray micro-focus sources. Built in-house by Agilent Technologies, the Nova (Cu) and Mova (Mo) X-ray sources combine the latest in micro-focus X-ray tube technology with specially designed multi-layer X-ray optics. Of the orthogonal, double bounce design, these multi-layer optics achieve the efficient capture and focusing of X-rays into a high purity and well shaped X-ray beam. These low divergence (c.a. 4 mrad), high brilliance X-ray beams are arranged at a 21.5 degree offset to each other, such that both beams coincide at the centre of the goniometer where they are directed onto the crystal sample.

The SuperNova's two X-ray sources are powered from a single software controlled generator unit. This high voltage (50kV), low power consumption unit provides up to 50W of power to each X-ray source and provides virtually instantaneous switching between Mo and Cu wavelengths. Wavelength switching is completely automatic and can be initiated either by the click of a software icon or by queued Mo and Cu experiments which can be run automatically back to back.

When to Use Mo and Cu Wavelengths?

As the mainstay of small molecule chemical crystallography, Mo radiation is ideal for the study of crystals where absorption is a potential issue. Up to 10x higher scattering than Mo, Cu X-ray radiation is ideal for the study of many small, weakly diffracting crystals and is essential for the absolute structure determination of non-heavy atom samples and the study of proteins.

EXPERIMENT	Mo	Cu
Inorganic/Organometallic	✓	
Macro/Supramolecular		✓
Absolute structure (organic crystals)		✓
High pressure	✓	
Proteins		✓
Twins	✓	✓
Electron density	✓	
Small weak crystals		✓
Incommensurates	✓	✓
Heavily absorbing material	✓	
Quasi-crystals		✓
Powder	✓	✓

Dual Wavelength

For small molecule applications, the SuperNova's standard configuration provides co-mounted and interchangeable Mo and Cu high intensity X-ray sources. Each of these X-ray sources offers considerably higher X-ray intensities and significantly reduced diffuse background scatter than their traditional sealed tube counterparts. This makes them the perfect choice for the study of the most challenging, smallest, weakly diffracting crystals.

Mova micro-source

- Mo wavelength, 50W X-ray micro-focus source
- Multi-layer X-ray optic
- Up to 2.5x more intense than a standard Mo sealed tube with mono-capillary optic
- Approximately 200 micron beam size

Nova micro-source

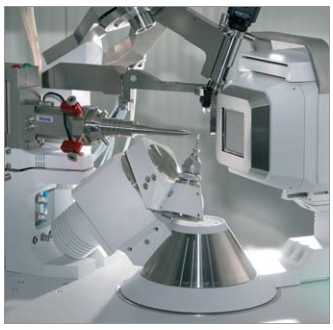
- Copper wavelength, 50W X-ray micro-focus source
- Multi-layer X-ray optic
- Up to 3x more intense than a 5kW rotating anode with optic
- Approximately 250 micron beam size

Single Wavelength

The SuperNova can also be configured with a single micro-focus X-ray source of either Mo or Cu wavelength then easily upgraded with the second source at a later date.

The most intense Mo & Cu X-ray Micro-sources

Co-mounted Nova (Cu) and Mova (Mo) X-ray Sources



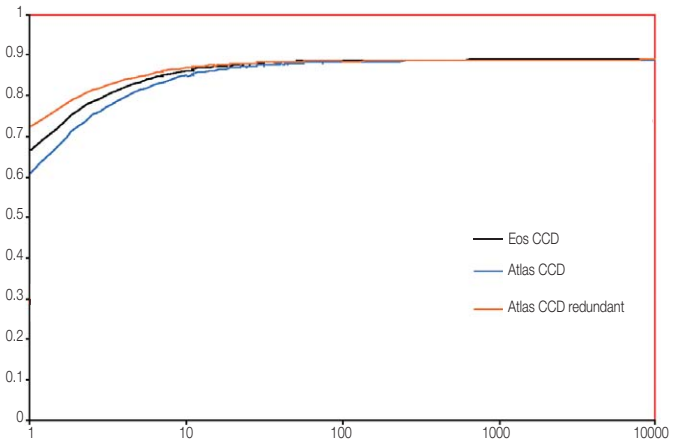
Single source SuperNova with Eos CCD

CCD detectors

Agilent Technologies, formerly as Oxford Diffraction, has been manufacturing and selling CCD detectors since 1992. As experts in CCD design and manufacture, with patented mounting technology, all our detectors are purpose built specifically for X-ray diffraction as part of a complete diffractometer system.

There are a number of key factors to consider when designing a modern CCD detector for today's experimental crystallographer. These factors should be considered as a whole rather than independently, since the detector is a collection of components and not just a CCD chip. The key factors are:

Speed –The 'frame to frame time' or 'duty cycle' is the actual time taken to read-out the CCD chip, digitise the data and write the data to the storage device. This cycle time is often significantly longer than the chip read-out time quoted by many manufacturers. For Agilent's Atlas and Eos detectors, the duty cycle is only 0.28 sec in 512 x 512 pixel mode, which is only 0.13 sec longer than the chip read-out time, making Agilent's CCDs the fastest CCD detectors currently available.



Comparison of Detective Quantum Efficiency (DQE)

Sensitivity – The ability to measure signal (reflections) above background is the Detective Quantum Efficiency (DQE) of the detector. As indicated by the plot of DQE versus the number of X-ray photons in a reflection, Agilent CCD detectors have a high DQE ranging from 0.6 to 0.85 (where the limit is 1.0) depending on strength of signal, and thus deliver outstanding sensitivity when measuring both strong and weak signals.

Gain – The conversion rate of X-ray photons to electrons is referred to as gain. Generally speaking the larger the gain figure the better, as this indicates a greater conversion of X-ray photons to electrons by the CCD. The Agilent Eos and Atlas with Mo gains of 330 and 180 e-/X-ray respectively are the highest currently available.

Precision – This relates to the precision of conversion of every X-ray image to a digital signal. Every image and every signal within that image is broken down into blocks of data 'bits'. The greater the number of hard wired bits (not software) the greater the number of blocks the data is digitised into and as a result the higher the precision of the data collected. At 18 bits hard wired, the Atlas and Eos are the highest precision CCD detectors currently available from any manufacturer.

Atlas

The Atlas CCD represents the optimum combination of large active area size (Ø135 mm) and detector sensitivity. The Atlas is the ideal choice of CCD for fast, high quality data collection using both Mo and importantly Cu radiation where small molecule data is typically sparsely spread within reciprocal space.

- Active area Ø135 mm
- Speed, 0.28 sec (duty cycle)
- Sensitivity, 40% higher
- Gain, 180 e-/X-ray (Mo)
- Precision, 18 bit (hard wired)
- Low noise

Eos

The Eos CCD combines the highest gain CCD (330 e-/X-ray) of any manufacturer with the highest precision and fastest duty cycle speed. The most sensitive CCD detector available today, the Eos is the best choice for single wavelength, molybdenum applications.

- Active area 92 mm diagonal
- Speed, 0.28 sec (duty cycle)
- Sensitivity, 40% higher
- Gain, 330 e-/X-ray (Mo)
- Precision, 18 bit (hard wired)
- Low noise

Dynamic Range – This describes a system's ability to measure strong and weak signals simultaneously on the same range. This is defined as the full well capacity over the total noise. For the Atlas and Eos the dynamic range is ≥50,000 and is equal to or higher than any other CCD detector.

Low Noise – The noise of a CCD detector is a combination of the read noise of the CCD chip, the combined noise of the detector electronics and the dark current noise. The dark current is typically insignificantly low and for routine small molecule crystallography, where exposure times are considerably <20 min, the dark current is so low it can be ignored. The noise of the detector then relates purely to the read noise and electronic noise. All Agilent detectors are built around low noise CCD chips and are optimised for very low noise electronics.

CrysAlis^{Pro} Software

The SuperNova comes complete with CrysAlis^{Pro}, Agilent's intelligent data collection and data processing software for small molecule and protein crystallography. Designed around an easy to use graphical user interface, CrysAlis^{Pro} can be operated under fully automatic, semi-automatic or completely manual control.

Automatic crystal screening

At the heart of CrysAlis^{Pro} are the automatic crystal screening, data collection and strategy software modules. For a typical crystal, a short pre-experiment lasting less than 5 minutes is recorded to evaluate the crystal quality. From the first frame of data, CrysAlis^{Pro} automatically evaluates the crystal quality and provides the user with information regarding the unit cell, intensity estimation by resolution range and suggested frame exposure times for the full data collection.

Fastest Strategy software

Following the pre-experiment, the sophisticated CrysAlis^{Pro} strategy software automatically calculates the optimal conditions for fast, high quality, complete data collection. No pre-defined strategies are used. Instead, all strategies are calculated based on the specific crystal orientation and unit cell. The user has complete control to optimise the strategy for a wide variety of targets including multiplicity, time and resolution. In addition, a series of restraints and constraints can be applied. The strategy calculations are extremely fast and efficient allowing the user to quickly adapt the data collection conditions with Mo or Cu radiation.

Experiments can also be designed to automatically collect data at multiple, user-defined temperatures (interfacing with any cryo- or heating device). The same facility can also be used to run back-to-back Cu and Mo experiments

Automatic and concurrent data reduction

Data reduction and processing initialise automatically with the start of data collection and employ intelligent routines which tune the parameters to give the best data quality. Since data reduction is concurrent with data collection, processed data are always available and accompanied by real time on-screen feedback of data quality and completeness.

Intelligent absorption correction

As part of the automatic data reduction and processing, an empirical absorption correction is applied to the data. If the user prefers, a range of alternative absorption approaches can be applied to the data including face indexation using a pre-recorded movie of the crystal recorded at the start of data collection.

Specialist crystallographic tools

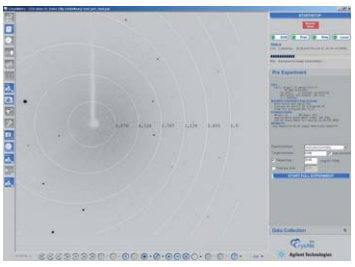
In addition to the automatic routines, CrysAlis^{Pro} provides hundreds of specialist tools and functions for dealing with non-standard and problematic crystals. These tools, which can be accessed either via the GUI or a command line interface which can be switched on/off at any time, include:

- Advanced unit cell finding
- Reciprocal space viewer
- Space group determination
- Twinning
- Incommensurates
- Remote device control (X-ray generators, Cryo-devices)
- Axial photos
- High pressure
- Powders
- Precession images

Compatibility and software licences

CrysAlis^{Pro} automatically outputs data in HKLF format and interfaces directly to OLEX2 , SHELX and third party data reduction packages including MOSFLM, DENZO and XDS. CrysAlis^{Pro} is provided under a multi-site, multi-user licence.

Crystal movie with overlayed absorption correction model



Main CrysAlis^{Pro} GUI

AutoChem Software

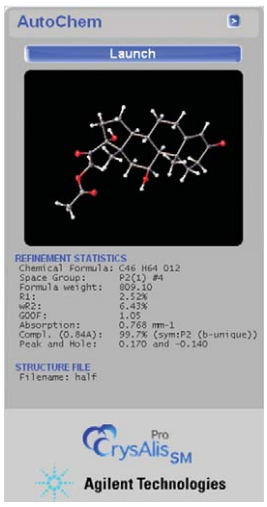
AutoChem is the ultimate in fully automatic structure solution and refinement programmes for chemical crystallography.

Developed exclusively for Agilent Technologies by the authors of OLEX2 (Durham University, UK), AutoChem adopts an entirely new approach to the automation of crystal structure determination and is seamlessly integrated into Agilent's CrysAlis^{Pro} software providing real time structure solution and refinement during data collection.

Since its launch in 2006, CrysAlis^{Pro} has provided automatic data collection and concurrent data reduction. Now using AutoChem, CrysAlis^{Pro} completes the crystal structure determination. AutoChem runs continuously throughout data collection providing the user with visual feedback within the main CrysAlis^{Pro} GUI. This feedback is presented in the form of an interactive 2-D model of the crystal structure alongside key refinement results including R factor, Goodness-of-fit and absolute structure parameter.

Should the user wish to review the structure more closely or to control aspects of the structure solution, a full version of OLEX2 complete with AutoChem plugin can be launched at any time from within CrysAlis^{Pro}. Using OLEX2, the user is able to review all aspects of the refinement, step back to any stage of the process and apply changes as necessary.

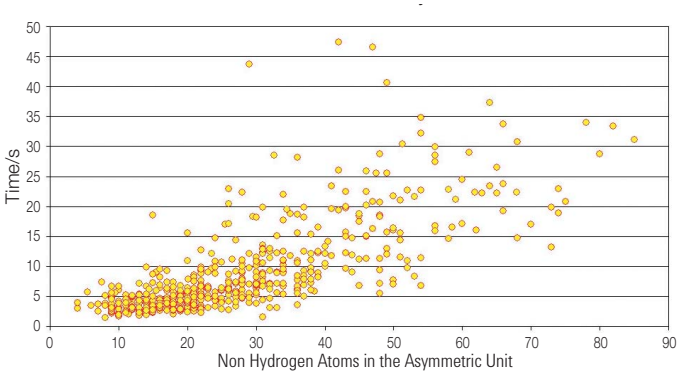
For standard crystal structures, AutoChem dramatically speeds up the process of structure solution, refinement and report generation. Developed using >2000 structures, AutoChem determined the majority of the tested routine structures in under 15 sec from solution to final report.



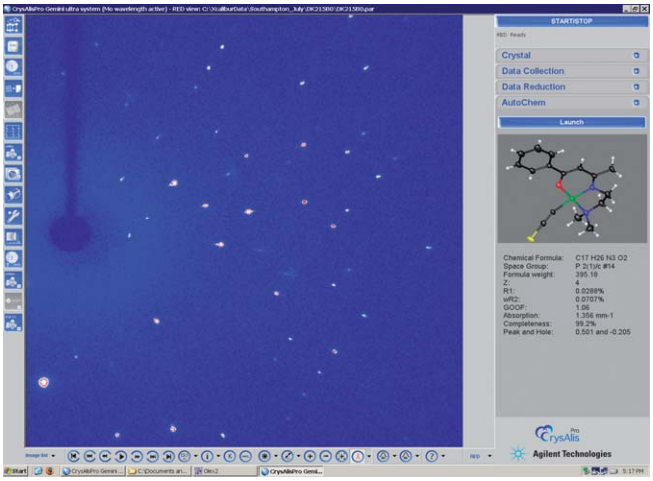
AutoChem Software

An intelligent programme, AutoChem selects the best method of structure solution, be it Patterson, direct methods or charge flipping. Using the speed and power of SMTBX[1] based refinement as standard but with options for SHELX, AutoChem refines the structure, accurately assigning atom types based on geometry. Atoms are modelled anisotropically where the data supports it and hydrogen atoms are included in calculated geometric positions. The structure is then re-labelled and refined to completion before a final html based structure report is generated.

- Fully automated structure solution, refinement and report generation
- Fully integrated with data collection software
- Developed using >2000 structures
- Majority of routine tested structures completed in under 15 sec
- Full user interaction and intervention possible at anytime
- AutoChem is exclusive to Agilent Technologies



Time for routine structure solution and refinement based on recent trials



CrysAlis^{Pro} with integrated AutoChem feedback panel

[1] Developed at Durham University in collaboration with CCTBX

SuperNova

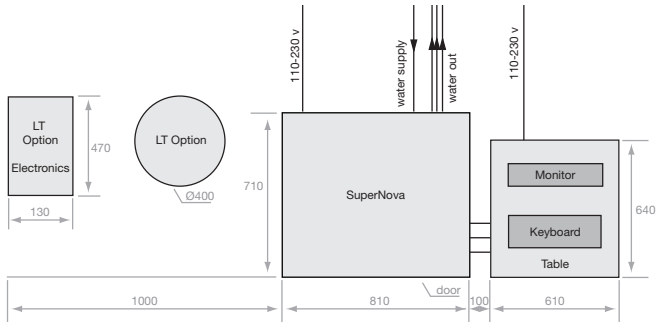
Technical Specifications

Environmental requirements

Power	230 / 110 V (switchable) ± 10% / 16 A fuse protected
Water supply	(where required) 2 l/min flow required / 3 - 5 bar gauge / 10 – 20 °C range / drain required
Relative Humidity	<80 % non-condensing
Weight loading	Able to bear system weight of 300 kg
Temperature	18 – 23 °C

Please refer to the system user manual for the most up to date and complete requirements.

Suggested system layout (in mm)



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