

# D8 Structural Biology Solutions

## Latest Developments in Home-Lab Crystallography

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# D8 Structural Biology Solutions



The development of the new instrument platform was driven by –

- Providing the best data possible
- Improving usability and serviceability
- Minimal demands on services
- Strictest safety standards
- Modularity / expandability
- Providing a “future proof” platform



D8 VENTURE with TXS

# D8 VENTURE Configurations



## Core configuration

- HELIOS MX optic
- KAPPA goniometer
- PHOTON 100 CMOS-APS detector
- Radiation Safety enclosure
- PROTEUM2 Software
- Control PC

# D8 VENTURE Configurations



## Configuration options

- X-Ray Generator
  - IµS *high brilliance* microfocus ST
  - TXS microfocus RAG
  - METALJET liquid metal-jet
- Low-temperature device
  - KRYOFLEX II
  - Cryostream 700
  - COBRA
- Automated Sample Handling
  - ISX Stage for *in situ* crystallography
  - SCOUT

# Modern X-Ray Sources



- Highest performance
- Lowest maintenance



Generator	<b>I<math>\mu</math>S</b> <i>high-brilliance</i>	<b>TXS</b>	<b>METALJET</b>
Technology	Microfocus ST	Microfocus RAG	Liquid-metal jet
Wavelength, Å	1.54	1.54	1.34
Power, W	50	2500	200
Cooling	Air	Water	Air
Maintenance	Minimal	Low	Low



# Modern X-Ray Sources

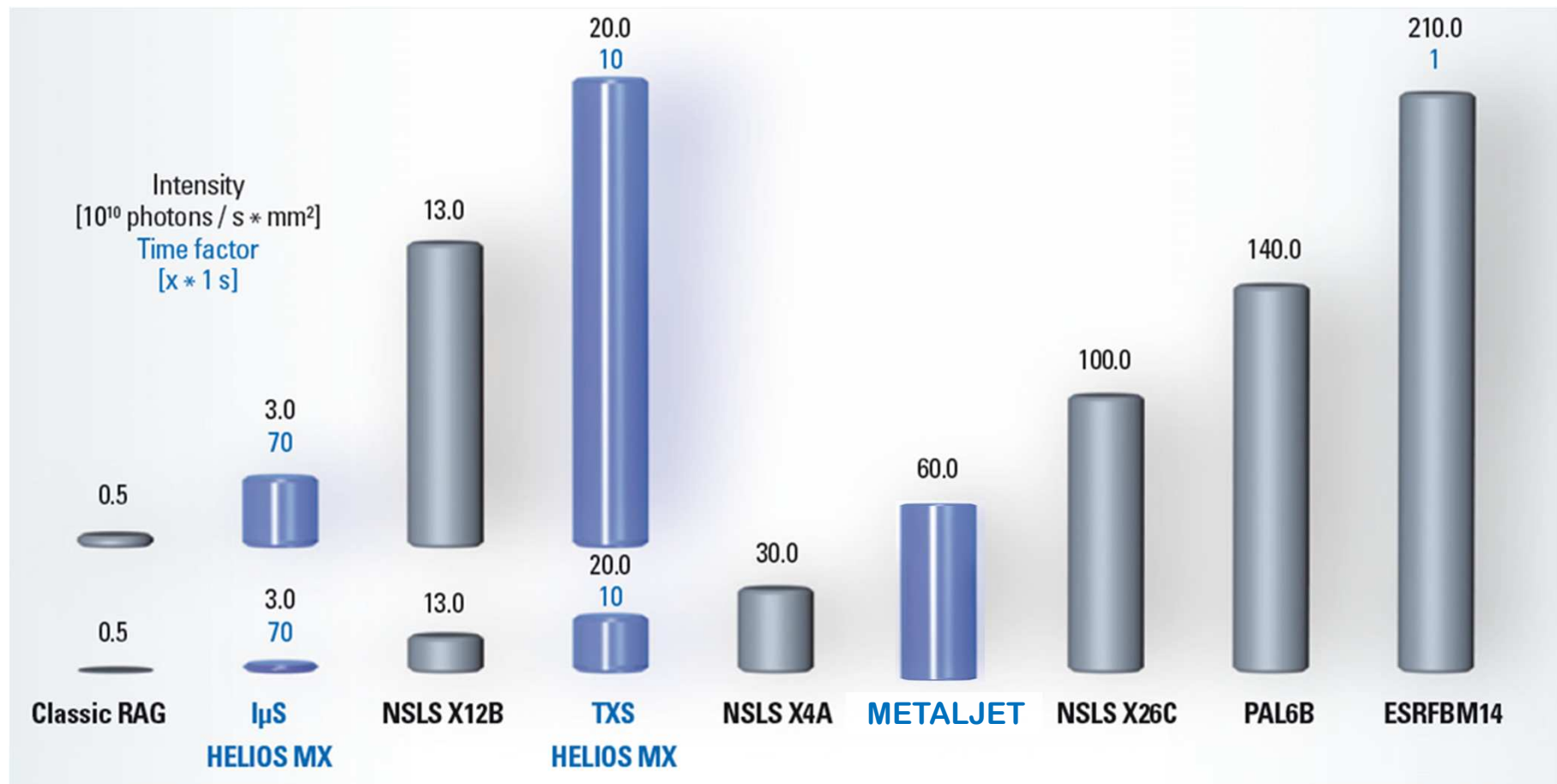


- Highest performance
- Lowest maintenance



Generator	I $\mu$ S <i>high-brilliance</i>	TXS	METALJET
Optics	HELIOS MX	HELIOS MX	HELIOS MX
Wavelength, Å	1.54	1.54	1.35
Spectral purity, % K $\alpha$	99.9%	99.9%	99.9%
Beam diameter, $\mu$ m	95	160	70
Divergence, mrad	1.0 – 7.6	1.0 – 7.6	1.0 – 7.6
Intensity, ph/mm <sup>2</sup> /s	$3.0 \times 10^{10}$	$1.6 \times 10^{11}$	$6.0 \times 10^{11}$

# Modern microfocus X-ray sources and BM beamlines



# PHOTON 100 CMOS-APS Detector

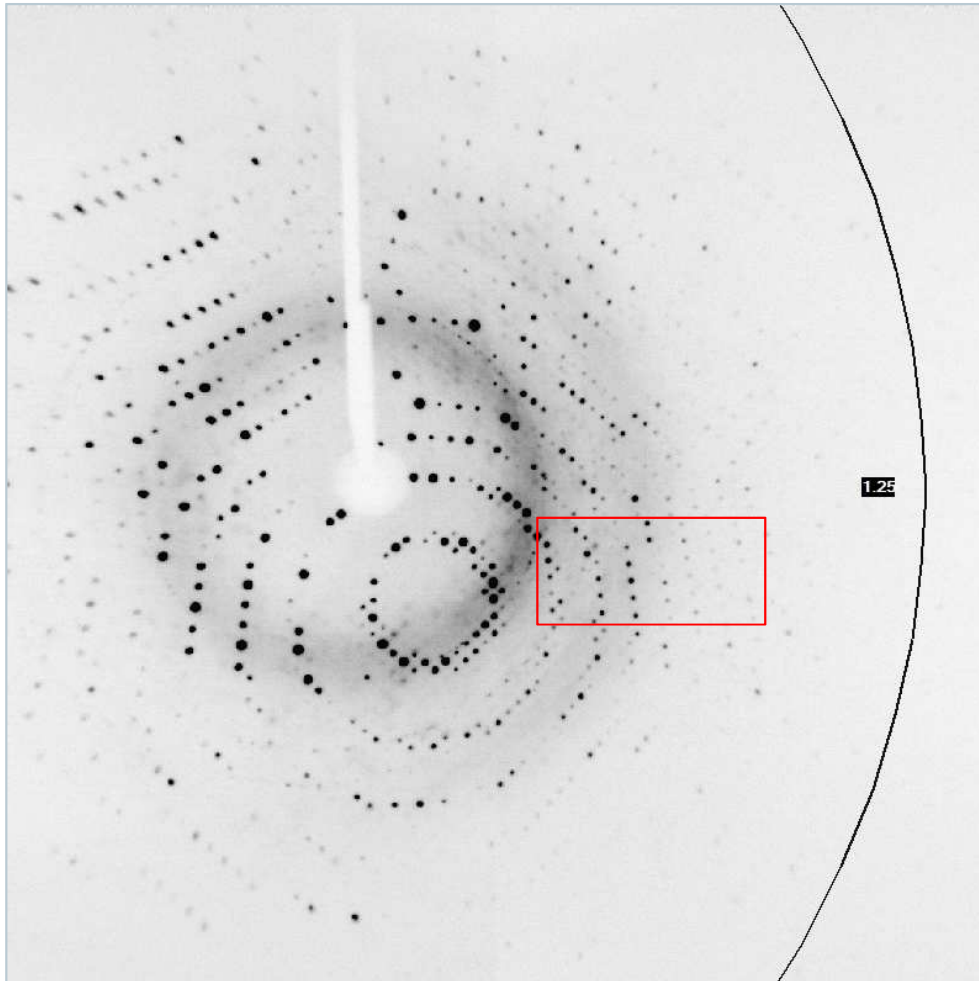


- First CMOS active pixel sensor for XRD
- Air cooled
- Large active area, 10,000 mm<sup>2</sup>
- Seamless, no gaps or dead areas
- Ideal point spread, 1 pixel (96  $\mu\text{m}$ )
- High sensitivity, near quantum limited
- Low noise
- No spatial distortion
- Shutterless data collection

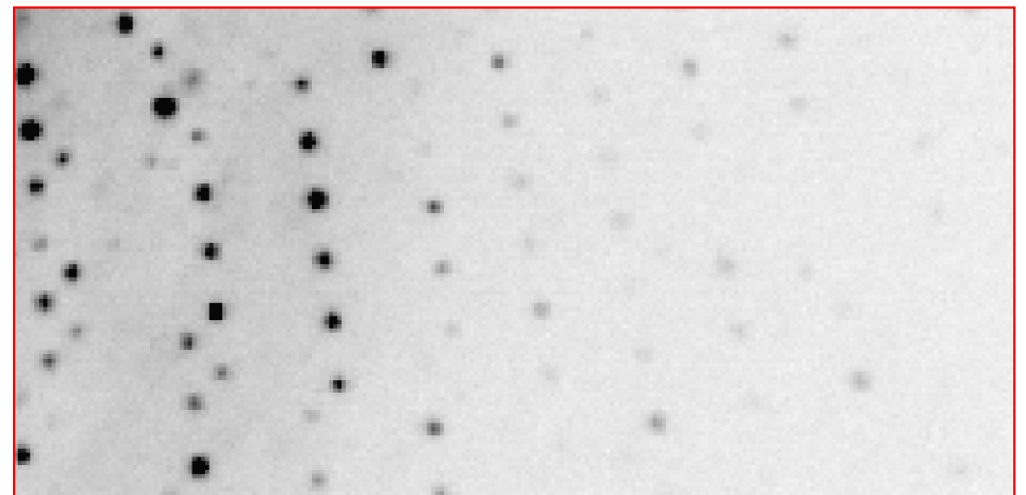


# PHOTON 100

## Superior data quality



- 2 second exposure
- Low, uniform background
- Full well capacity 5,000,000 e<sup>-</sup>
- PSF  $\approx$  1 pixel = 96  $\mu$ m
- Well-defined reflections
- No overloads

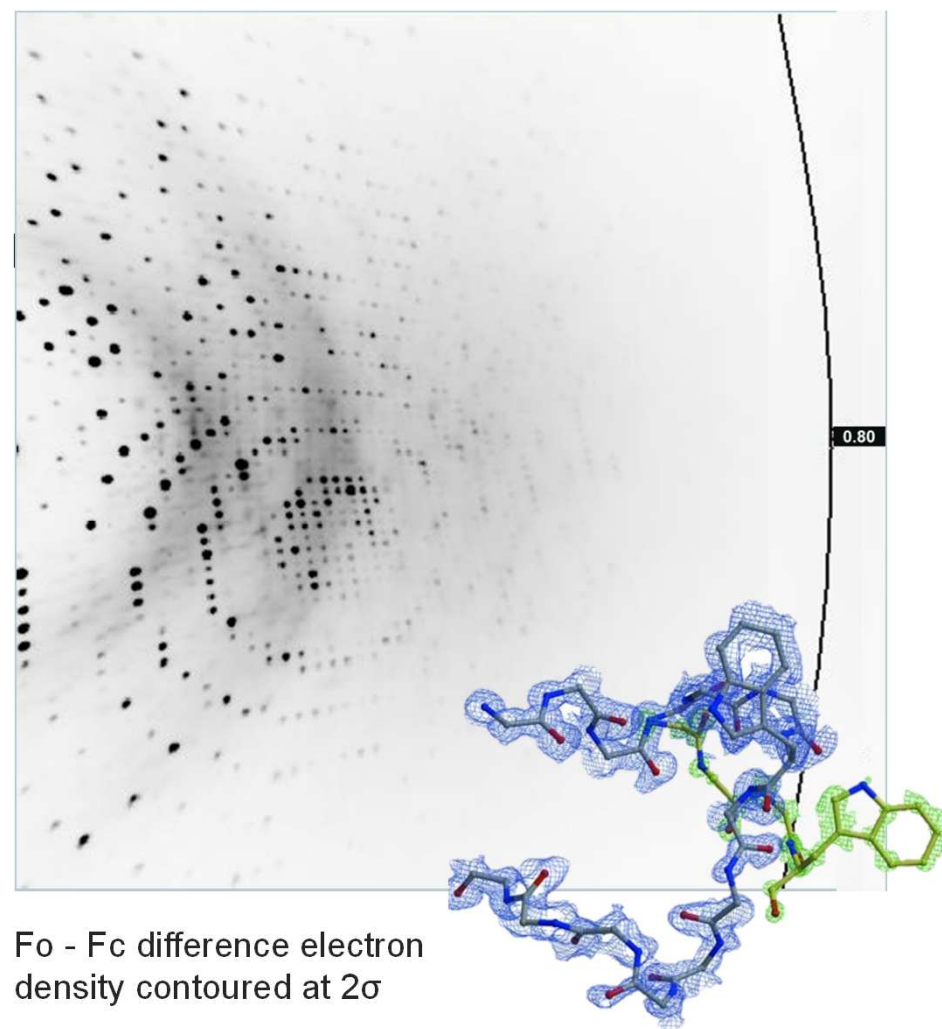


# D8 VENTURE with PHOTON 100

## High quality data to atomic resolution

- Well diffracting crystal with low-symmetry (P1)
- 5s/0.5°
- Full dataset collected in 30 minutes
- Comparison data collected at SLS PX II, ~2% to ~0.8 Å

Source	METALJET
Resolution [Å]	0.86 (0.96 – 0.86)
Completeness [%]	95.6 (91.6)
Redundancy	<b>5.8 (3.7)</b>
$\langle I/\sigma \rangle$	<b>10.45 (1.94)</b>
$R(\text{pim})$ [%]	2.15 (31.02)



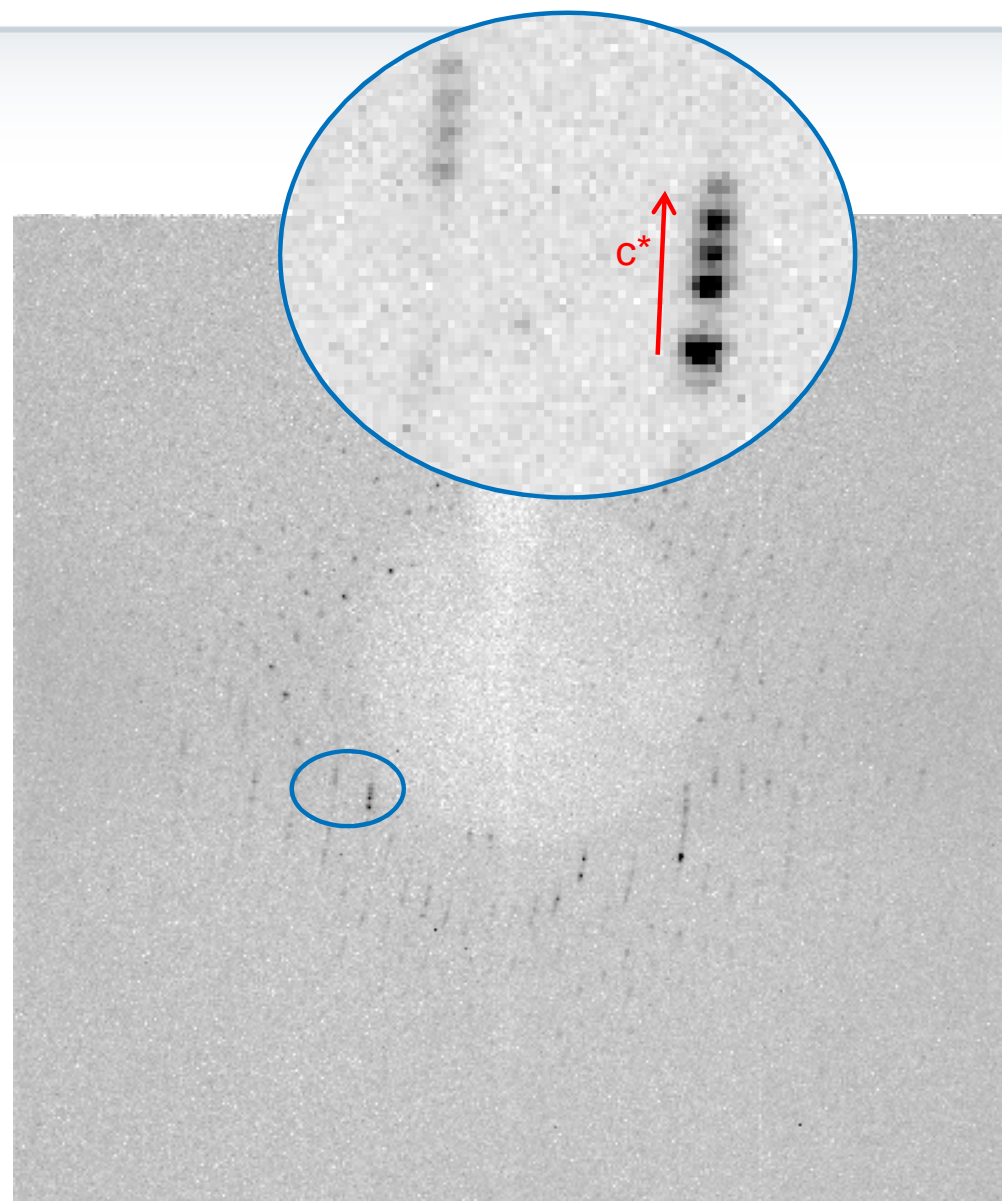
Fo - Fc difference electron density contoured at  $2\sigma$

# PHOTON 100

## Difficult crystals



- Large unit cell,  $c = 619 \text{ \AA}$
- Solvent content  $\sim 80\%$
- Very weak diffraction
- $DX = 150 \text{ mm}$ ,  $600 \text{ s}/0.25^\circ$
- Excellent PSF to resolve long axis
- High S/N
- Low noise



# Comparison of PHOTON 100 with other detector technologies

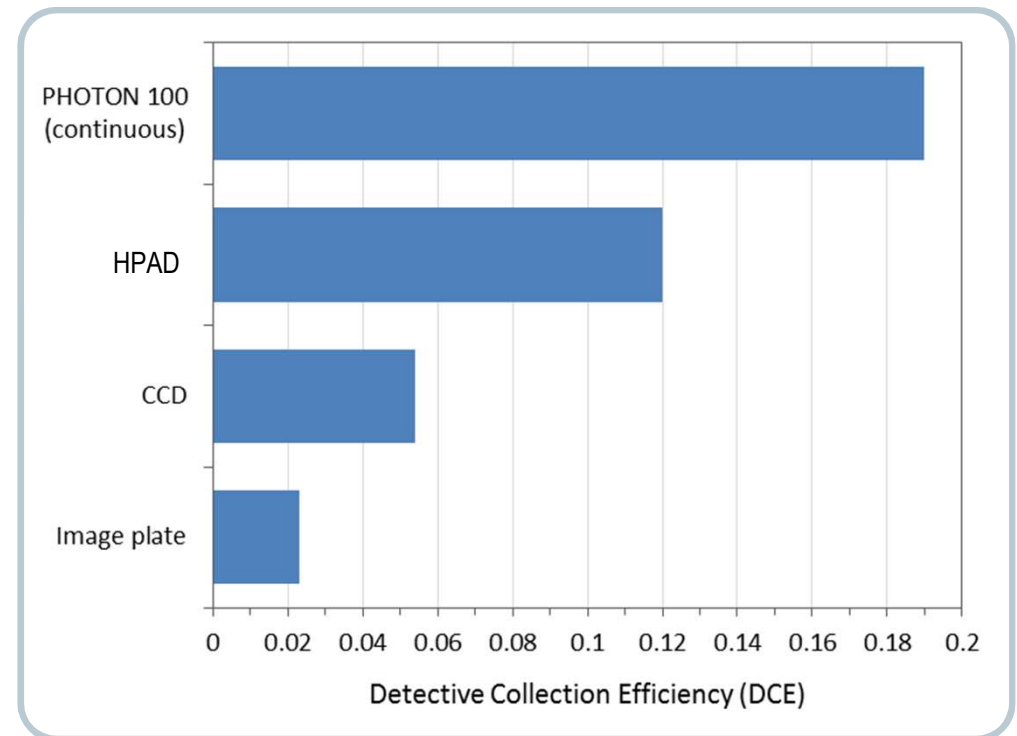


- Detective Collection Efficiency (DCE) quantifies the contribution of detector size, sensitivity, and readout speed on performance
- DCE is proportional to the “wall clock” time to achieve equivalent data statistics

$$DCE = \frac{\Omega}{4\pi} DQE (1 - f_{dead})$$

Diagram illustrating the components of the Detective Collection Efficiency (DCE) equation:

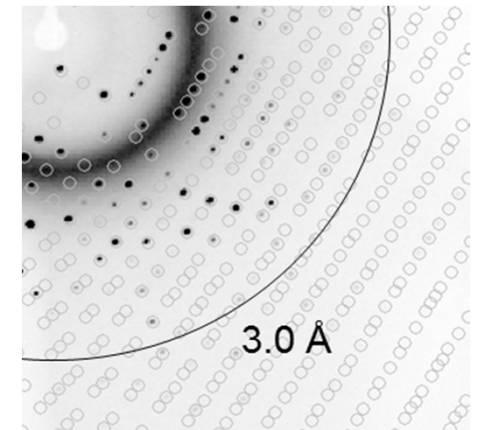
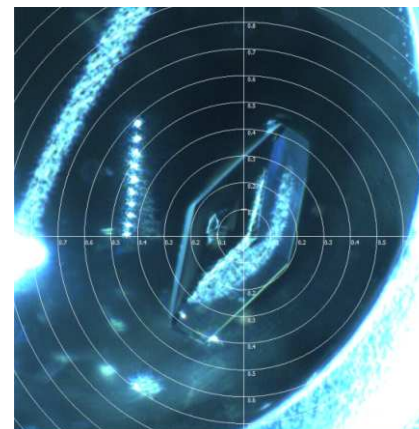
- $\frac{\Omega}{4\pi}$  is labeled "size" (solid angle).
- $DQE$  is labeled "sensitivity" (Detective Quantum Efficiency).
- $(1 - f_{dead})$  is labeled "speed" (dead time factor).



# D8 VENTURE with ISX Stage *in situ* crystallography



- Crystal screening and data collection in plates at RT
- Software controlled, motorized plate stage
- Compatible with all Bruker X-Ray sources
- Fast – less than 2 s well-to-well
- One-click centering
- Screen crystal immediately or add to a job queue for automated screening
- Collect up to 60 ° of data





# SCOUT

## Automated management of cryo-samples



- Compatible with KAPPA goniometer
- Uni-pucks
  - Compatible with most beamlines
  - Pin-in to minimize icing
  - 80 pin capacity in 5 pucks
- Fast sample exchange rate
- Extremely low failure rate
- TRACKER software
- Unique Instruction Sets
  - Automated sample mounting, centering and retrieval
  - Automated screening
  - Automated sorting
  - Automated data collection and processing

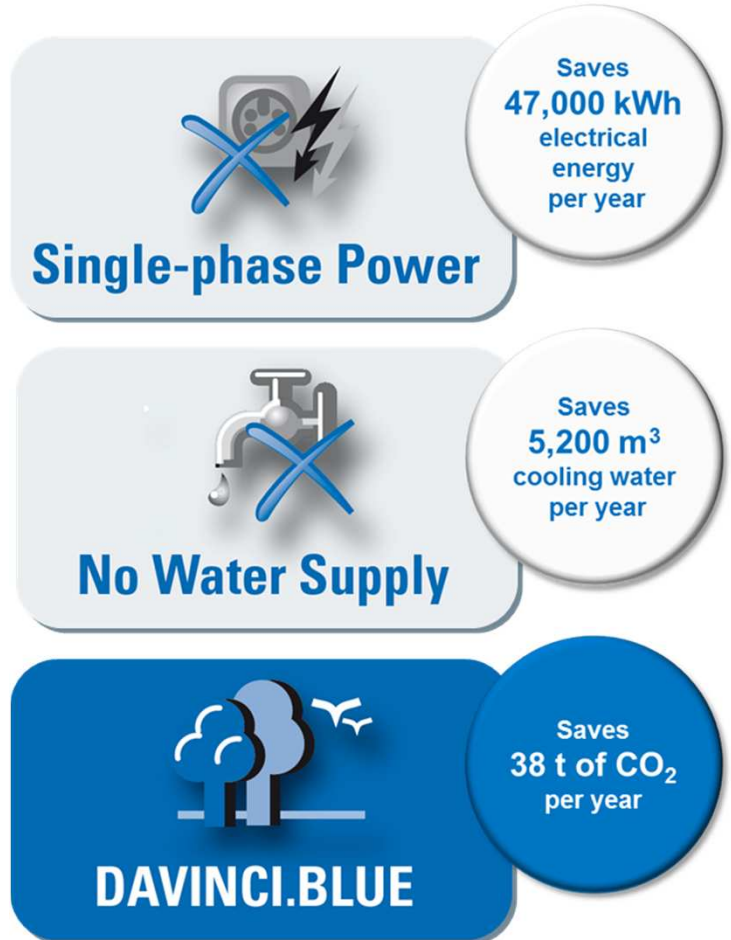


# D8 VENTURE

## Lowest running costs



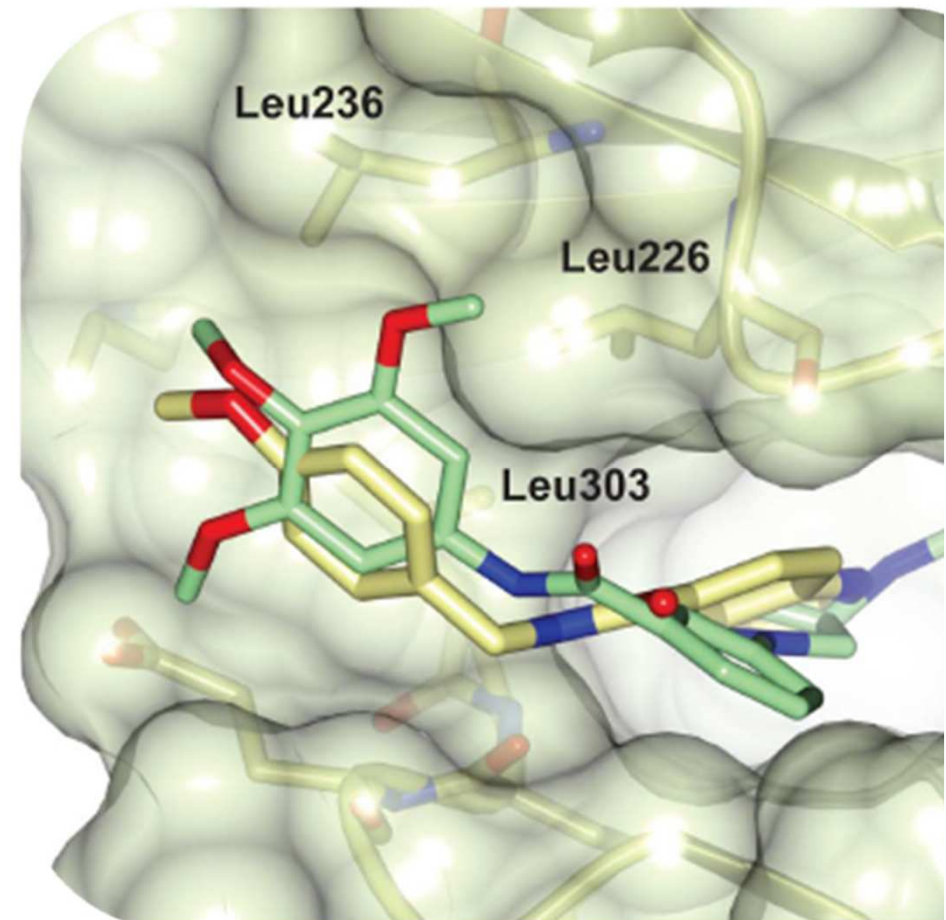
- METALJET and I $\mu$ S power consumption is less than 5% of 3 kW RAG
- PHOTON 100 operates at <5% power of a CCD detector
- Complete system runs on single-phase power
- Air-cooled sources
- Air-cooled PHOTON 100
- No external chillers
- No water supply required
- No gas purging



# Summary



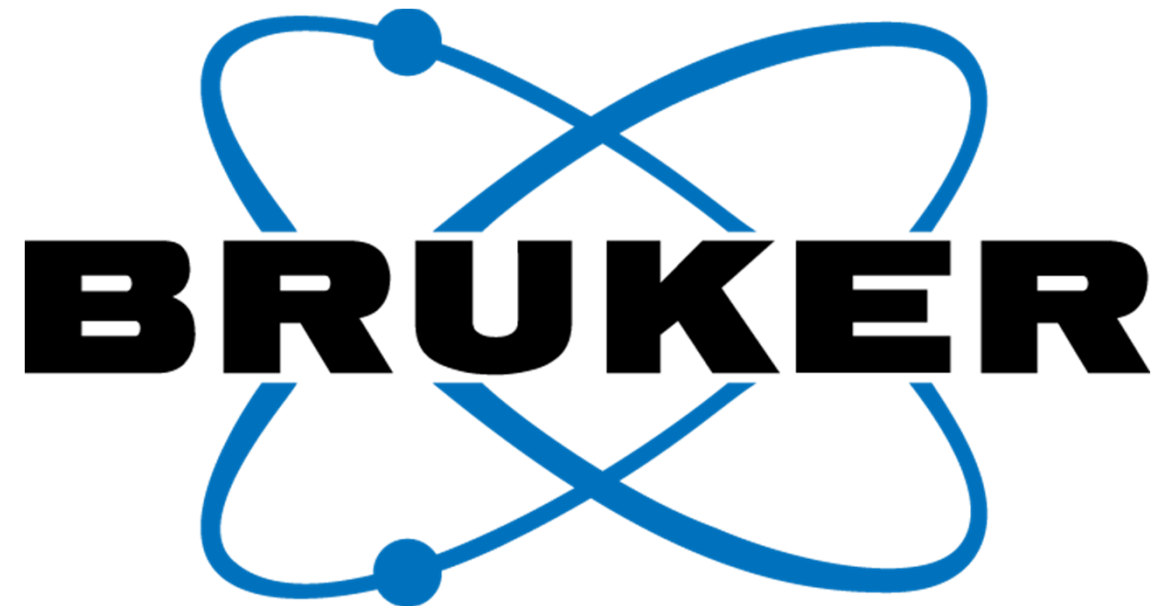
- The D8 systems are on a new platform designed for the next decade
- Highest performance
- Minimized maintenance
- Ease of use, robust
- Reduced utility consumption
- Automation
- Modularity
- 2<sup>nd</sup>-port options for TXS and METALJET
  - 2<sup>nd</sup> D8 SC-diffractometer
  - ISX Stage
  - PXRD
  - SAXS



## Further Information



- For further information, please contact Dr. Vernon Smith
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- Or the Bruker website, [www.bruker.com](http://www.bruker.com)
- Single-crystal XRD,  
<http://www.bruker.com/products/x-ray-diffraction-and-elemental-analysis/single-crystal-x-ray-diffraction.html>
- Structural Biology  
<http://www.bruker.com/industries/life-sciences/structural-biology.html>
- Details of local Bruker Offices can be found at  
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