

All data taken at Pacific Northwest National Laboratory (PNNL)

**Operators:** Jerome C. Birnbaum, Tyler O. Danby, Timothy J. Johnson, Molly Rose K. Kelly-Gorham, Rodica Lindenmaier, Tanya L. Myers

**SAMPLE CONDITIONS & PHYSICAL PROPERTIES**

Chemical name	L-Histidine
Chemical formula	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>
Synonyms	(S)-2-Amino-3-(4-imidazolyl)propionic acid
CAS number	71-00-1
Location of field sample	n/a
History of sample	n/a
Molecular Weight	155.15 g/mol
Melting Point	282 °C (dec.)
Boiling Point	n/a
Density (25° C)	1.24 g/cm <sup>3</sup>
Hardness, Mohs scale	n/a
Crystallography:	
Cell dimension	a = Å b = Å c = Å
Crystal system	
H-M symbol (point gr)	
Space group	
H-M symbol (space gr)	
Crystal habit	
Color	White
Diaphaneity	Sub-translucent to opaque
Particle size	10-600 µm (mean 70 µm)
Particle size assessment	Optical microscopy
Supplier	Sigma-Aldrich
Stated purity	≥ 99%
Date packed	20 April 2016      Weight: 1.146 grams
Synthesis method	n/a
Synthesis reference	n/a
Texture	Fine, rectangular crystalline needles
Physical state	Solid
Surface roughness	n/a
Elemental composition	n/a
Isotopic composition	n/a
Moisture content	n/a
Temperature of sample	25 ± 2 °C
Substrate	n/a

## INSTRUMENT PARAMETERS

### Tensor 37 FT-IR manufactured by Bruker Optics

External diffuse reflectance accessory	A 562-G integrating sphere
Sphere diameter	75 mm
Angle to normal incidence	14.8°
Sphere opening diameter	19 mm (entrance port)
Spectral range	7,500 to 600 $\text{cm}^{-1}$ saved; 7500 to 600 $\text{cm}^{-1}$ reported
Beamsplitter	Ge on KBr
Detector (dia. Det. Port in sphere)	2×2 mm, 60° field of view MCT (550; 0.9); 1 cm
Apodization function	Blackman-Harris 3-term
Aperture	6 mm
Coadded scans	2048
Scanner speed	40 kHz
Switch gain on	512 points
Low pass filter	Open
Scan technique	double-sided, forward-backward
Non-linear correction	On
High and low folding limit	15800.54-0.00 $\text{cm}^{-1}$
Phase resolution	32.00
Phase correction mode	Mertz
Zerofilling	4×
Wavenumber accuracy	$\pm 0.4 \text{ cm}^{-1}$
Spectral resolution	4 $\text{cm}^{-1}$
Accuracy verification	10/28/2015
Wavelength vetted on:	ICL polystyrene standard #0009-7394-0025A, thin film
Reflectance:	$\pm 2\%$ using SRS reflectance standards 50-010-DH27B-4878

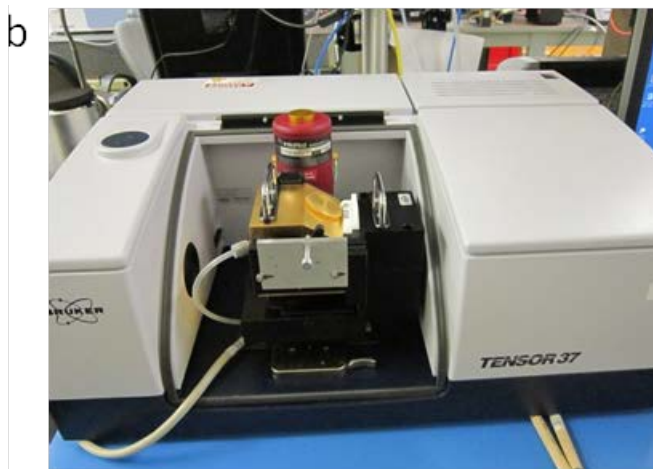
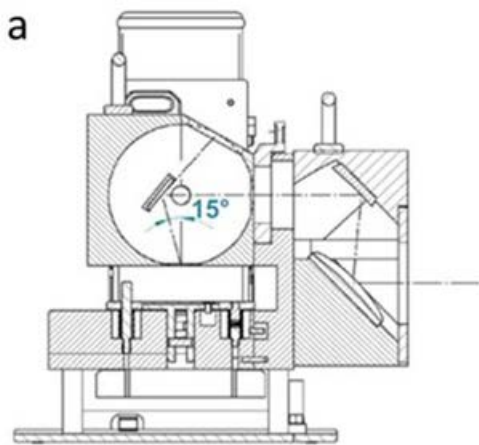


Figure 1: The Bruker 562-G integrating sphere (a) and Tensor 37 (b)

## Photographs of sample L-Histidine

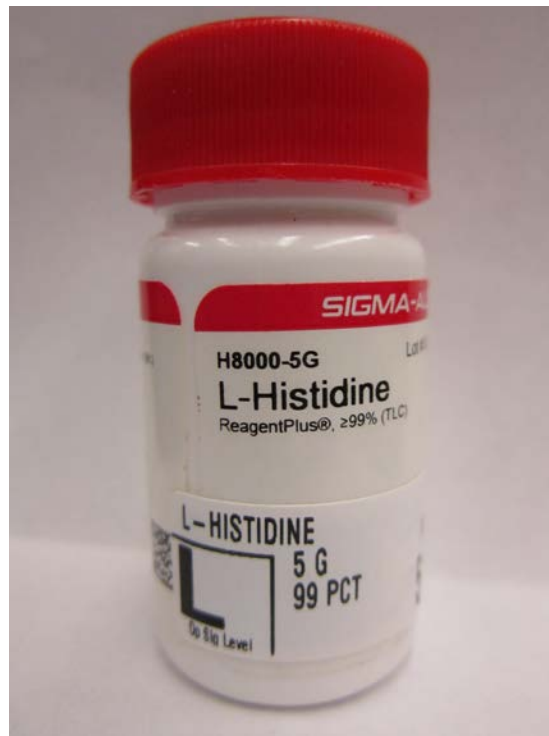


Figure 2: L-Histidine in Sigma-Aldrich container.



Figure 3: L-Histidine loaded in IR sample cup.

## PARTICLE SIZE PREPARATION AND CHARACTERIZATION

### Optical microscopy —

A Keyence VHX-1000 digital microscope with 16-bit resolution is used to provide photomicrographs of the various samples and particle sizes. Software included with the microscope differentiates the brightness and colors in the image and extracts the bright objects to produce a binary image. The software assumes all adjacent bright points are part of the same object then calculates the area for each of these objects. The area (A) is used to calculate the mean particle diameter (d) by assuming the particles are spherical and using the relationship  $d = \sqrt{4A/\pi}$ . Although the assumption of spherical particles is clearly not always valid, this procedure provides a reasonable estimate of the mean particle size.

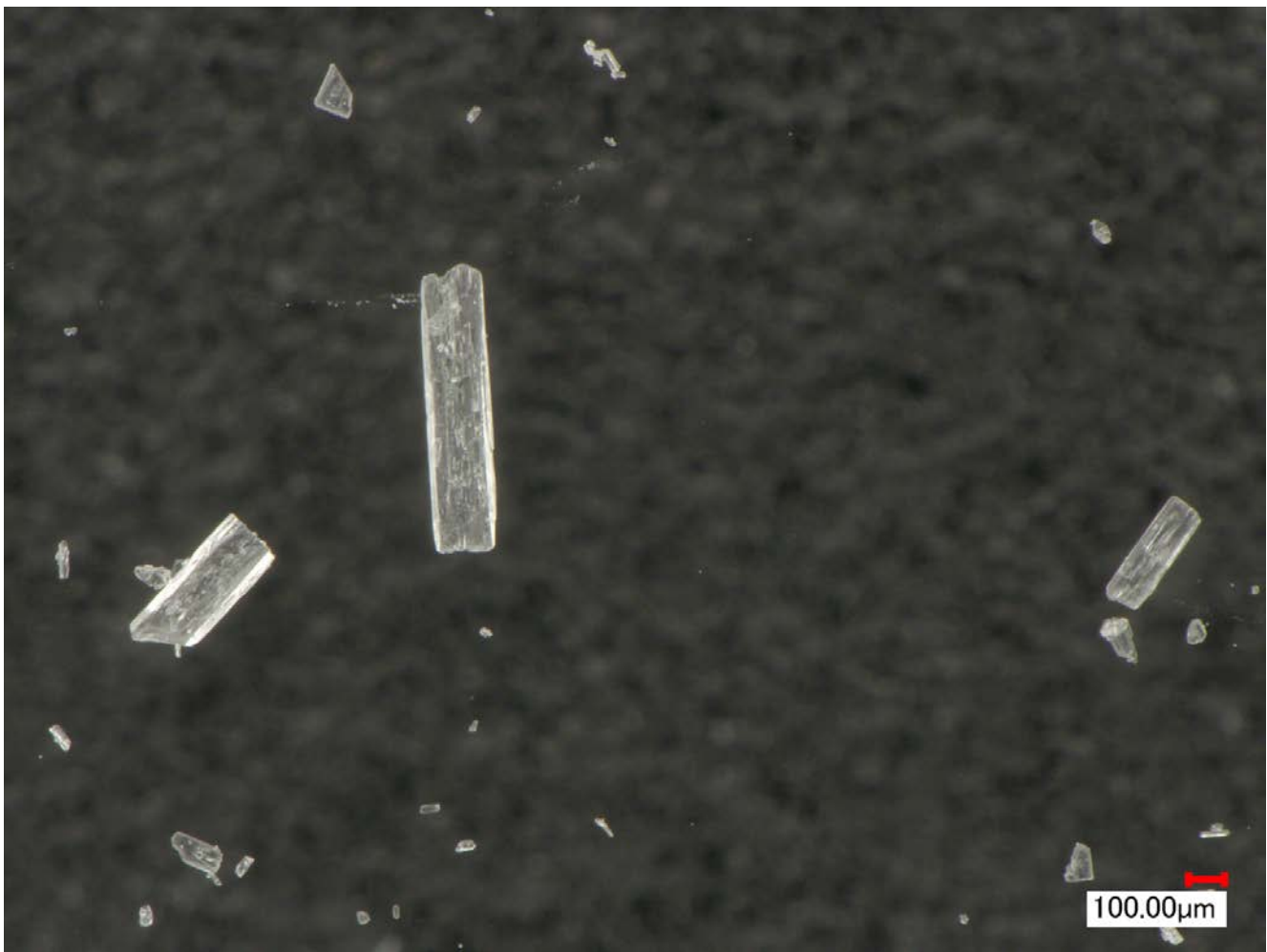


Figure 4: Photomicrograph of L-Histidine.

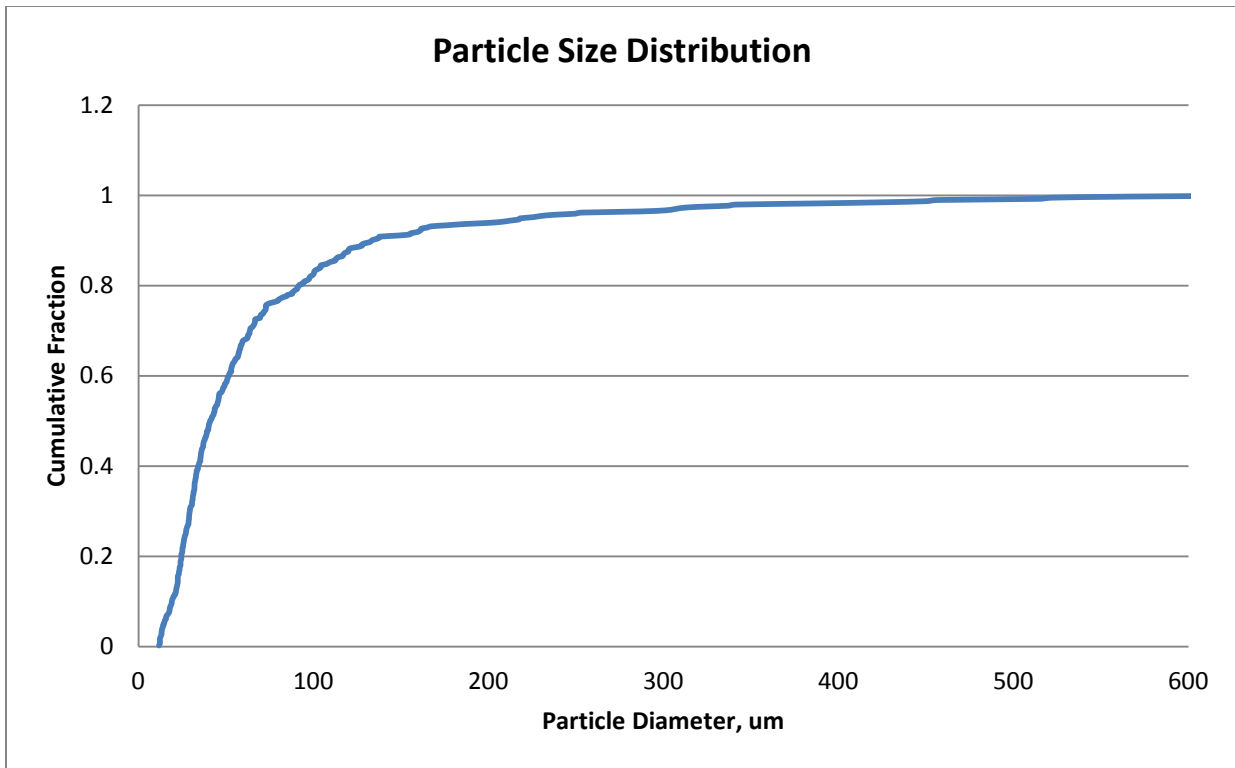


Figure 5: Particle size distribution of L-Histidine.