



SMU

BROAD-SPECTRUM
ANTIBIOTIC GLASSES
CHARACTERIZATION
AND PURSUING
TUNABLE
SOLUBILITY

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WHAT ARE WE WORKING WITH?

Padda, I. S. Cef.
<https://www.ncbi.nlm.nih.gov/books/NBK560653/> (accessed Jul 15, 2021).

WHO List

Solubility

Crystal Structure

Cephalosporins

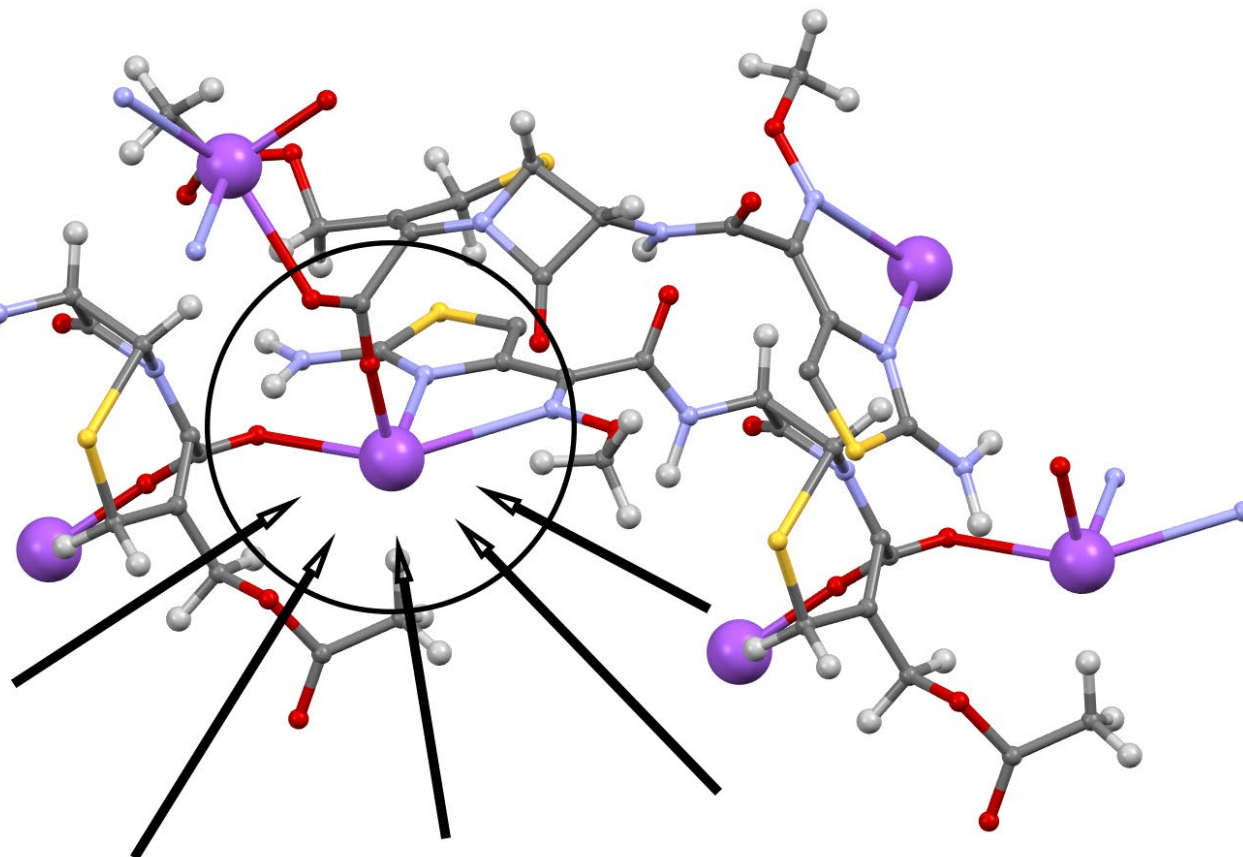
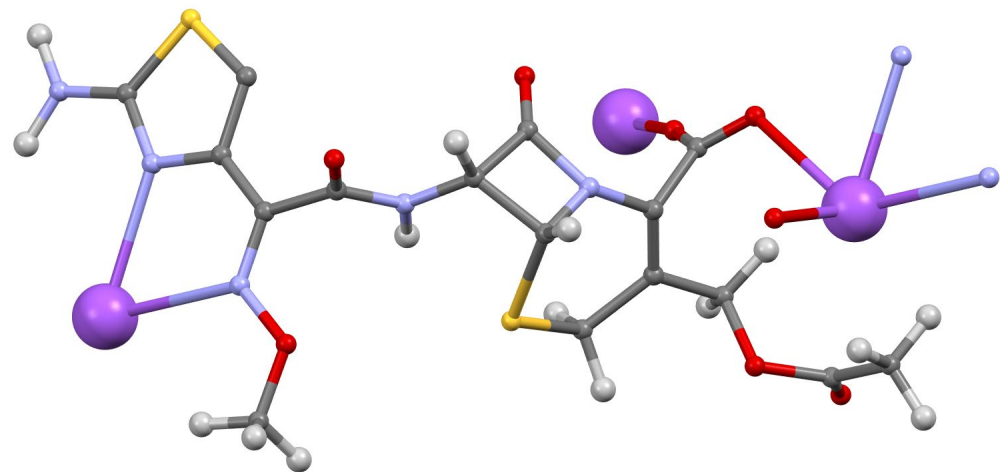
Compound X



45 Years!!

Structure and pertaining information

- = sodium
- = carbon
- = oxygen
- = sulfur
- = nitrogen

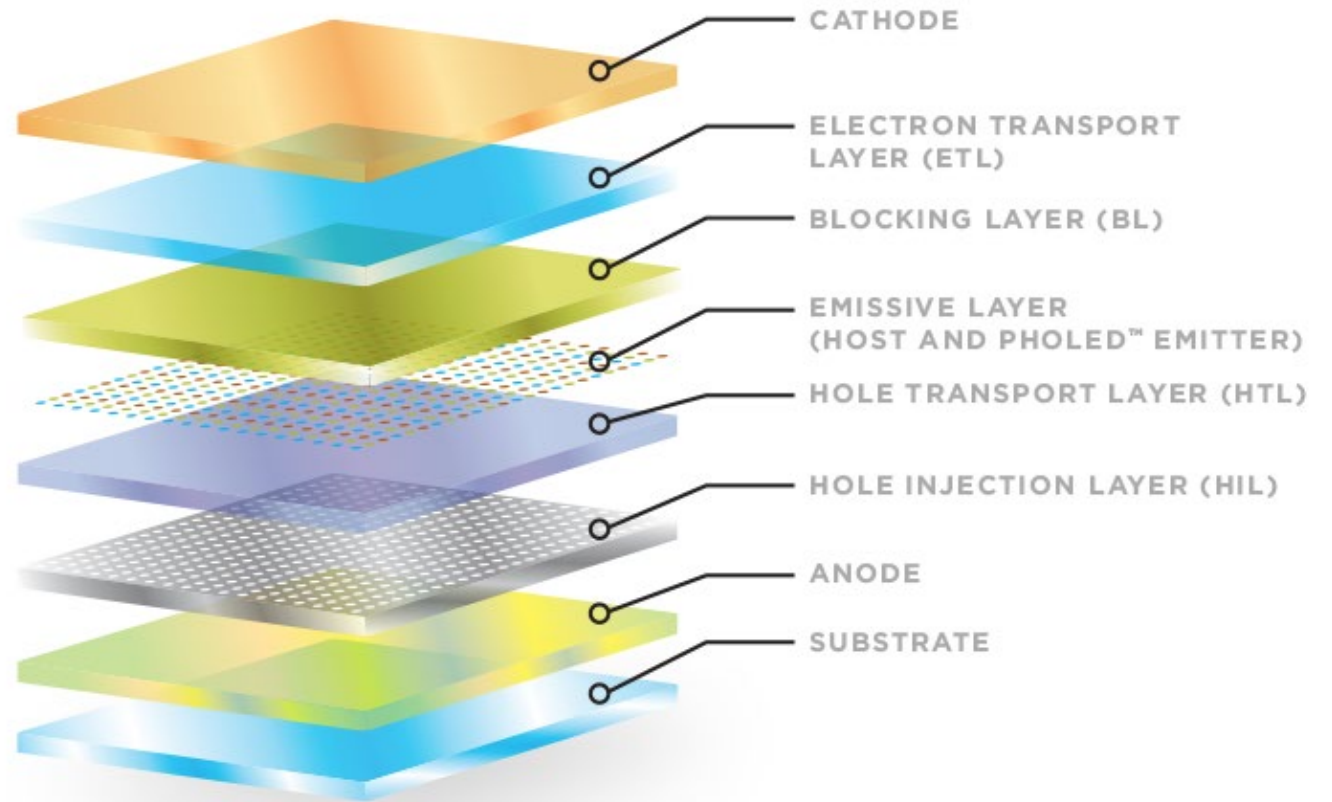


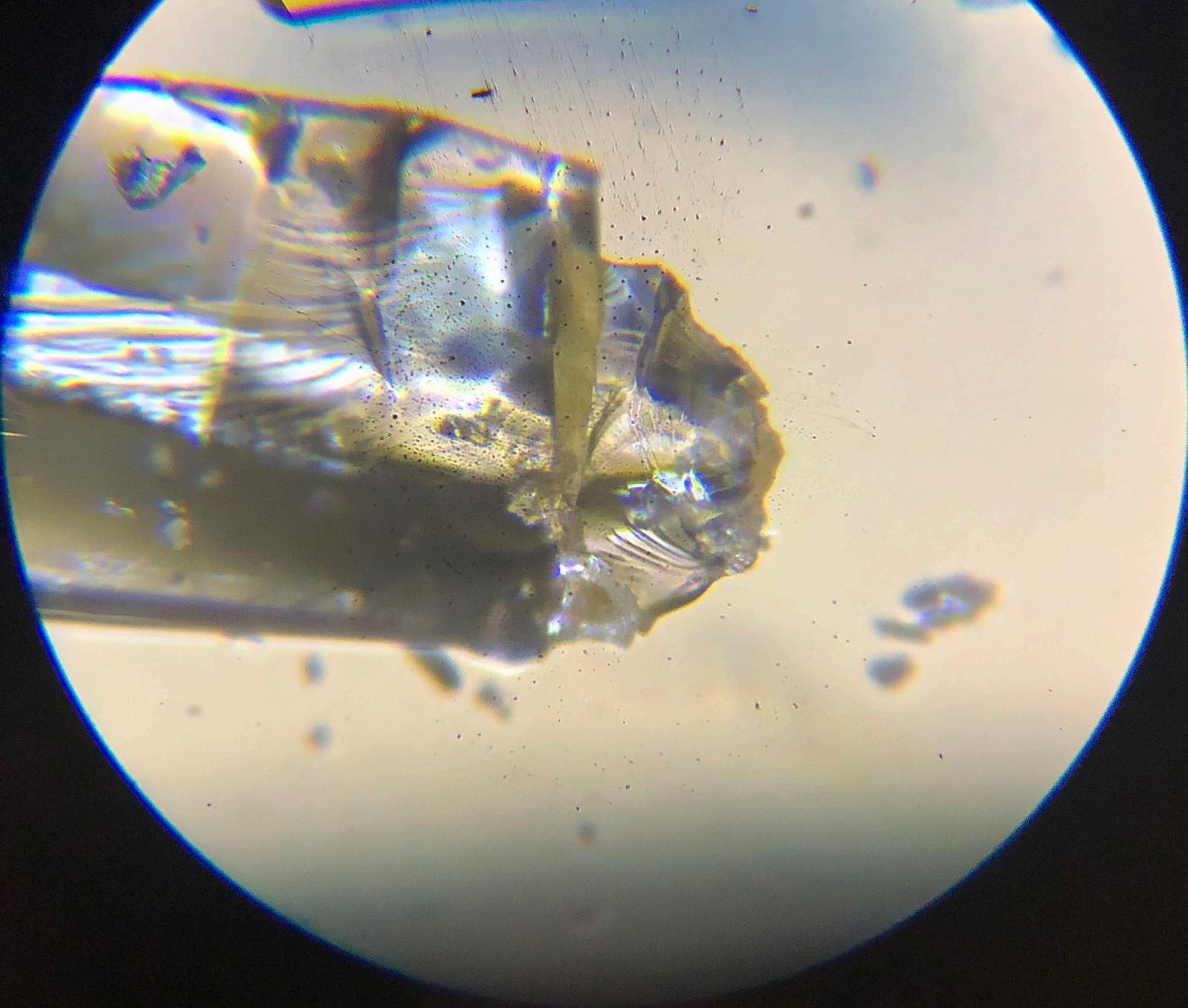
Possibilities for hypercoordination by small O-bearing solvents during crystallization

Background

* Applications

Vallet-Regí, M.; Colilla, M.; González, B. Medical Applications of Organic–Inorganic Hybrid Materials within the Field of Silica-Based Bioceramics. *Chem. Soc. Rev.* 2011, 40 (2), 596–607.



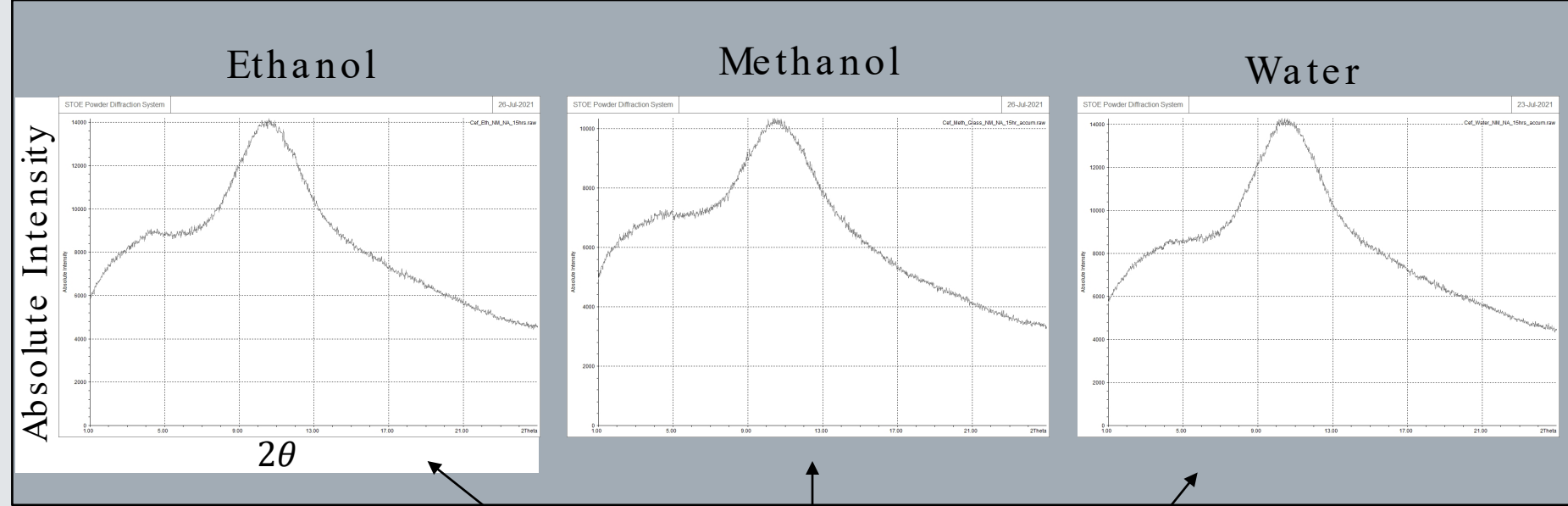


Formulation

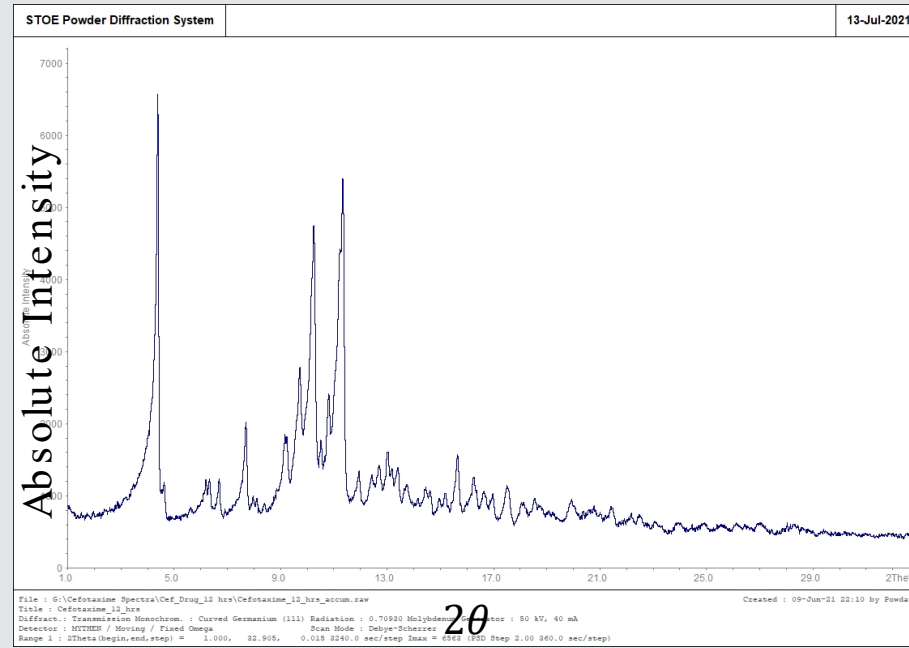
* Drug delivery –
drug stability

* Involves leaving
solvent systems
and drug systems
at room
temperature

Powder X-Ray Diffraction (PXRD)

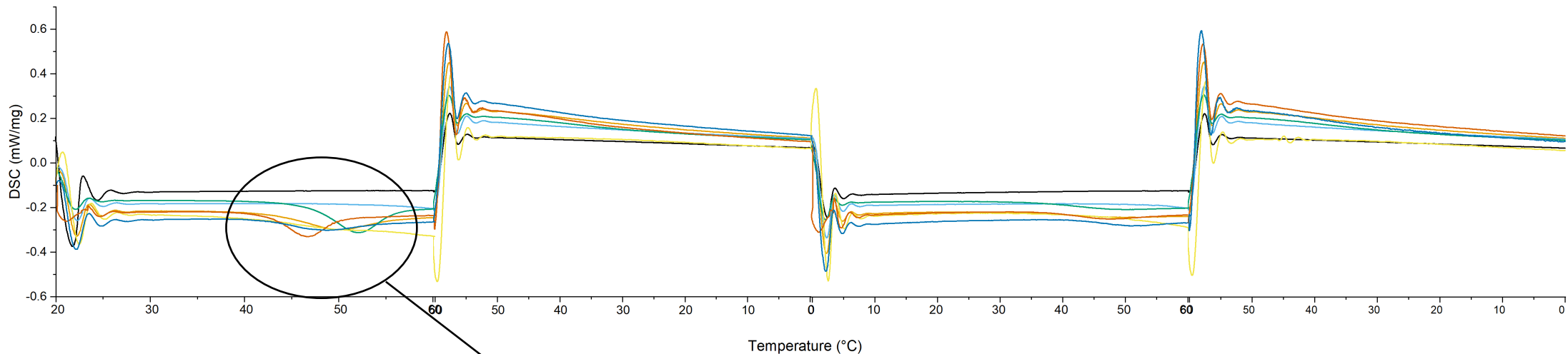


Glasses

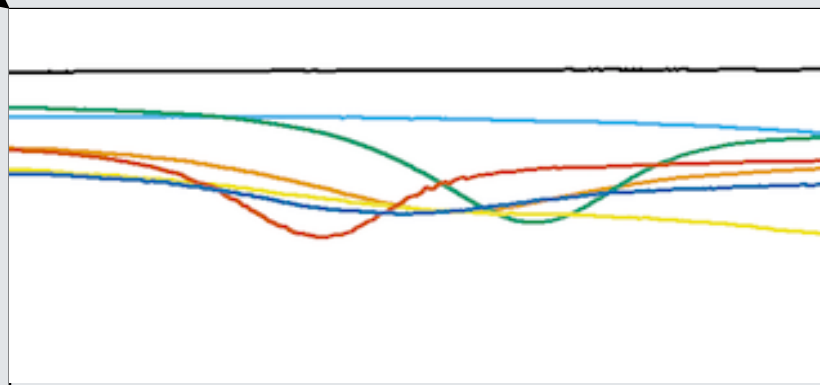


Drug

- Key Takeaways:
- Drug itself is crystalline
 - Glasses, even after milling, are amorphous (blobby and broad, no crystalline order)



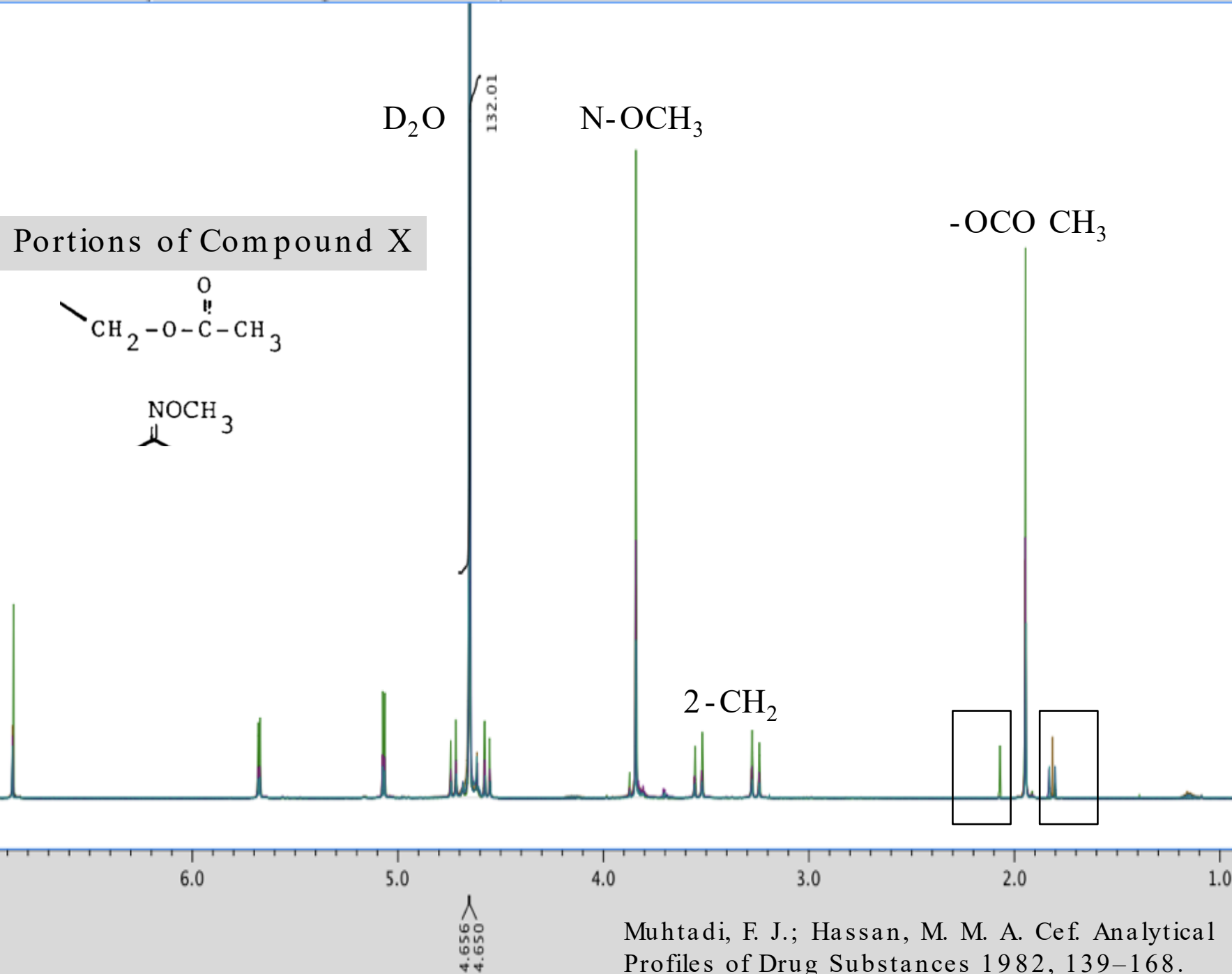
—	X	
—	X	Ethanol
—	X	Ethanol (Annealed)
—	X	Methanol
—	X	Methanol (Annealed)
—	X	Water
—	X	Water (Annealed)



Key Takeaways:

- Suggests T_g which points to glass
- The drug does not display this independently

Differential Scanning Calorimetry (DSC)



Proton Nuclear Magnetic Resonance

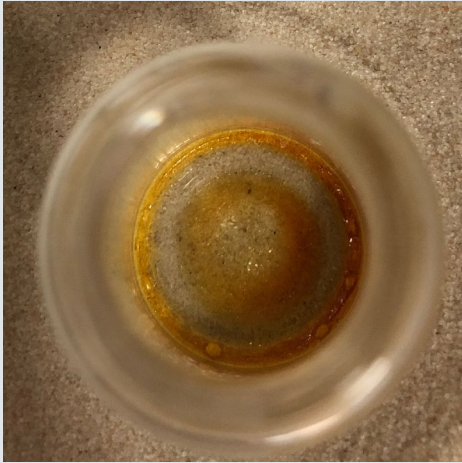
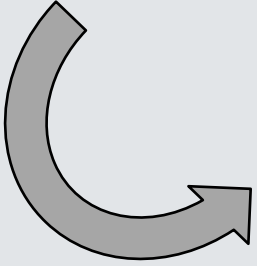
(^1H NMR)

Key Takeaways:

- Compound X is not changing (or changing very minimally) when placed into the glass and re-dissolved

Muhtadi, F. J.; Hassan, M. M. A. *Cef. Analytical Profiles of Drug Substances* 1982, 139–168.

Decomposed
Sample



Visual Test

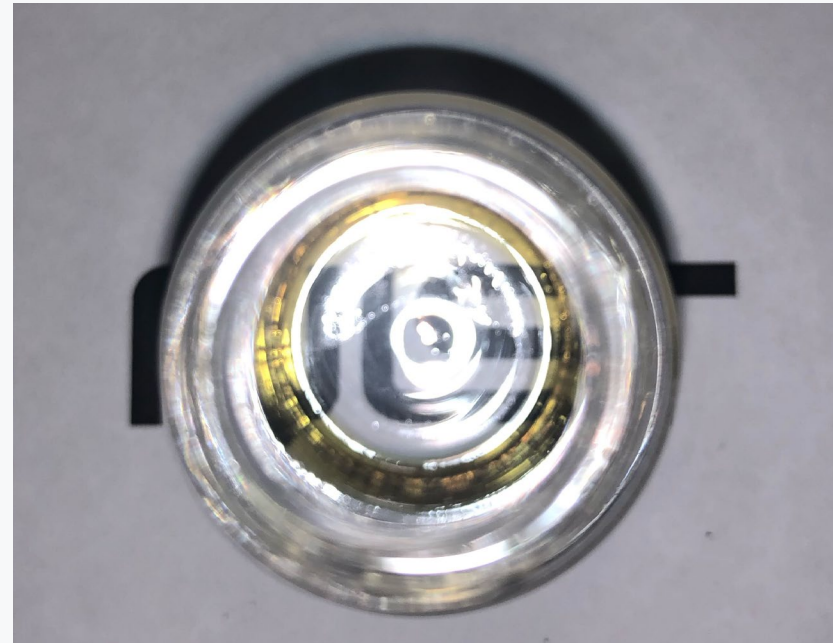
Key Takeaways:

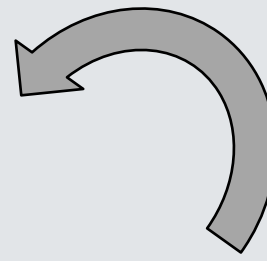
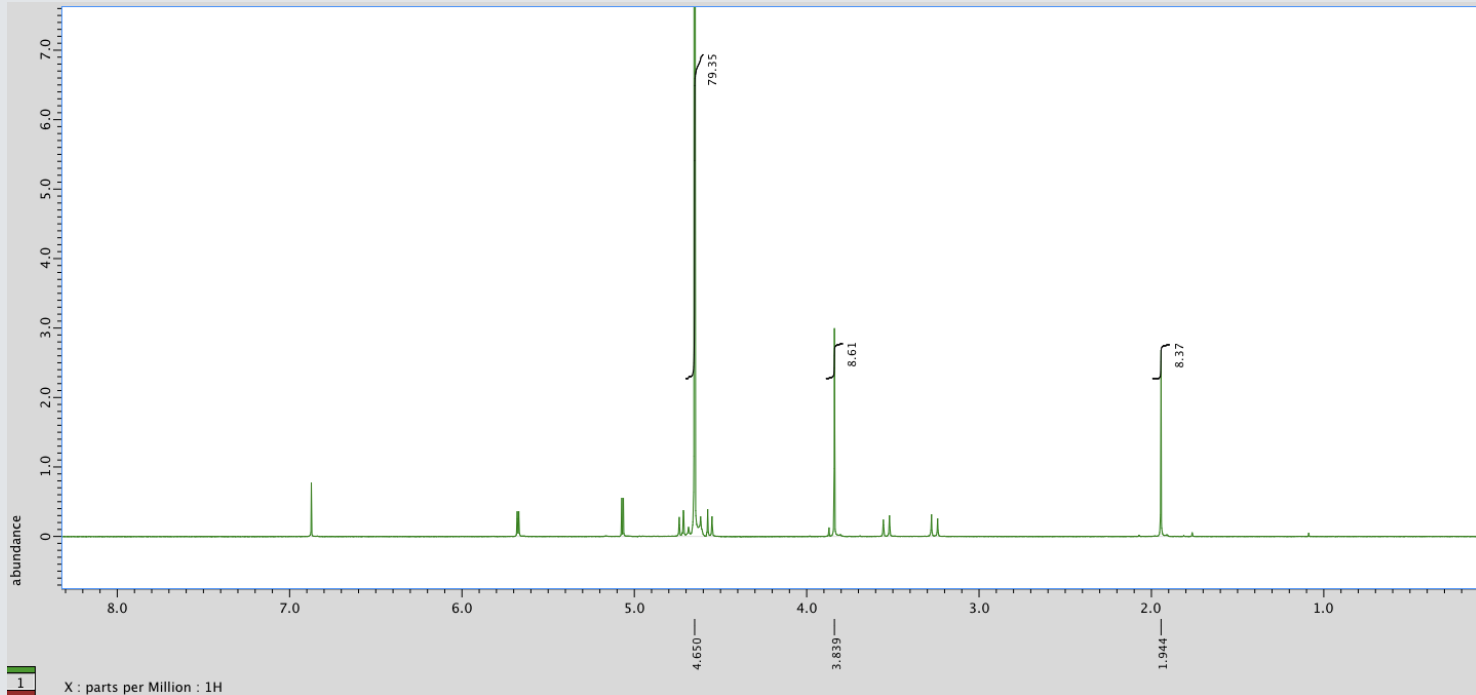
- Sample doesn't appear to be degrading when left in light for prolonged periods

One month
- light



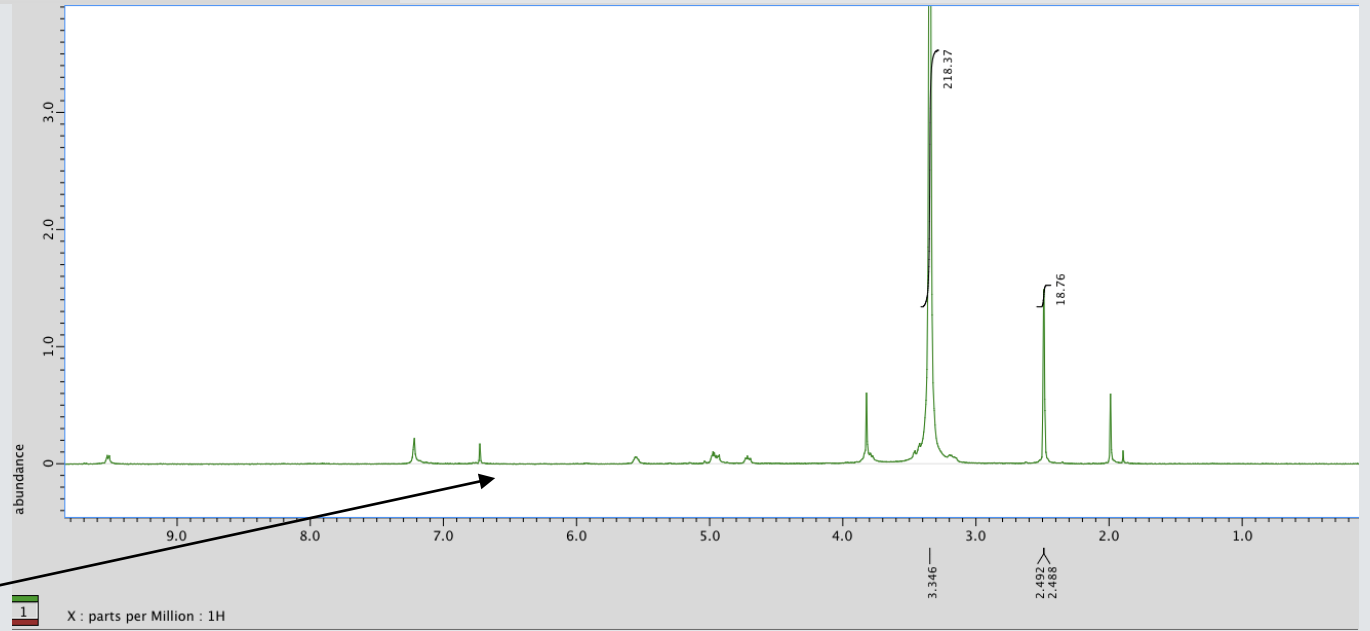
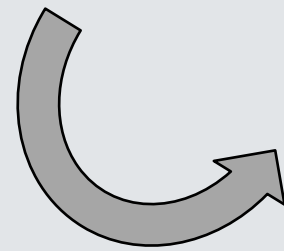
One month
- dark





Non-Decomposed
Sample

Decomposed
Sample

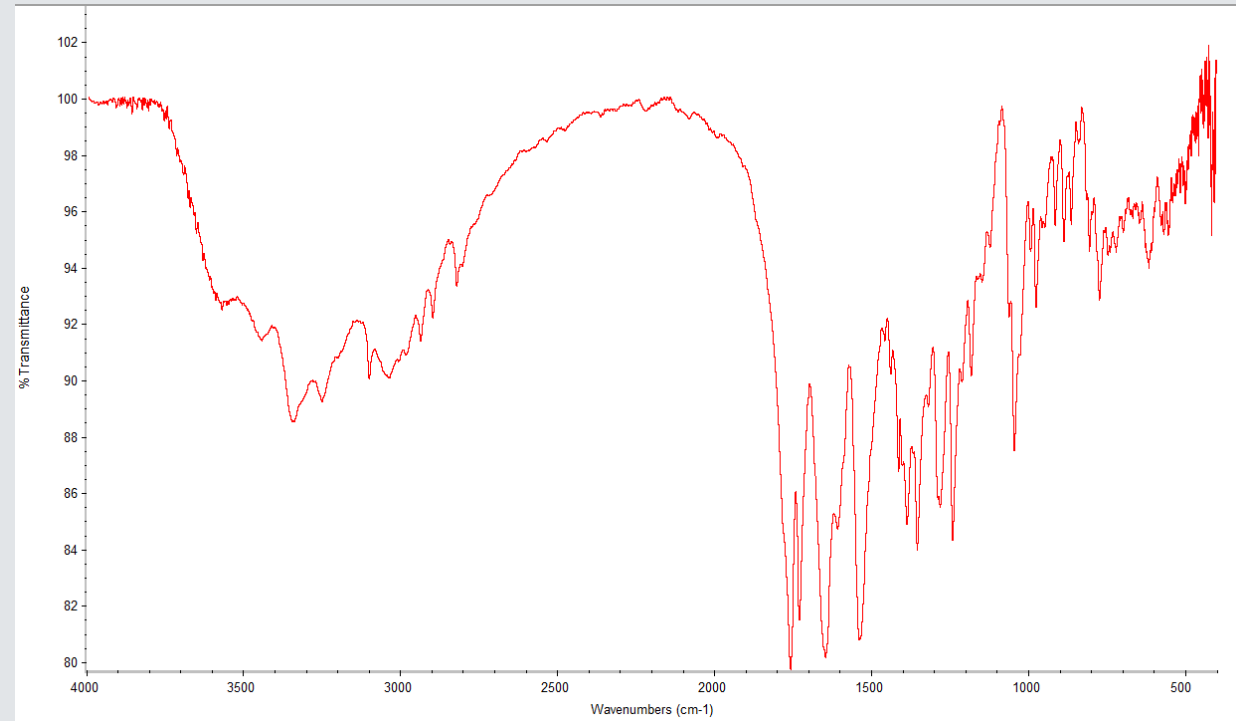


Preliminary IR (Infrared) Data

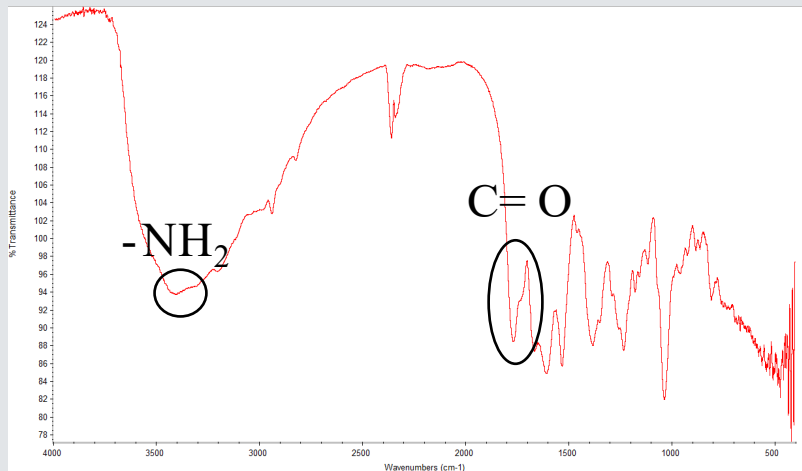
Key Takeaways:

- Compound X is not changing (or changing very minimally) when placed into the glass AND annealed

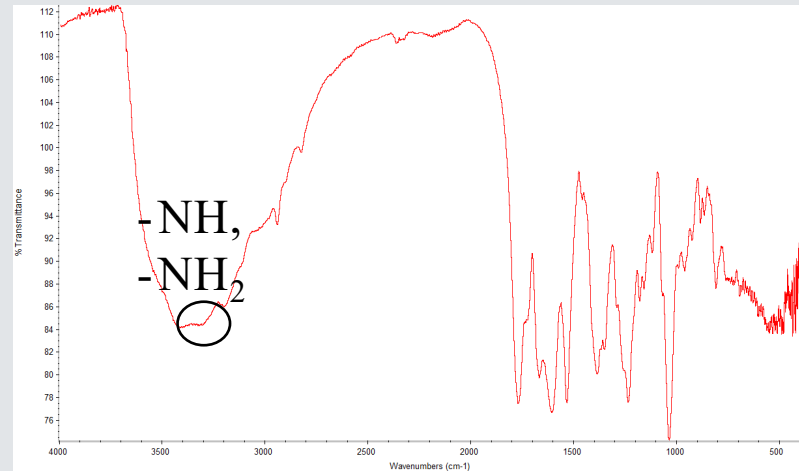
Drug



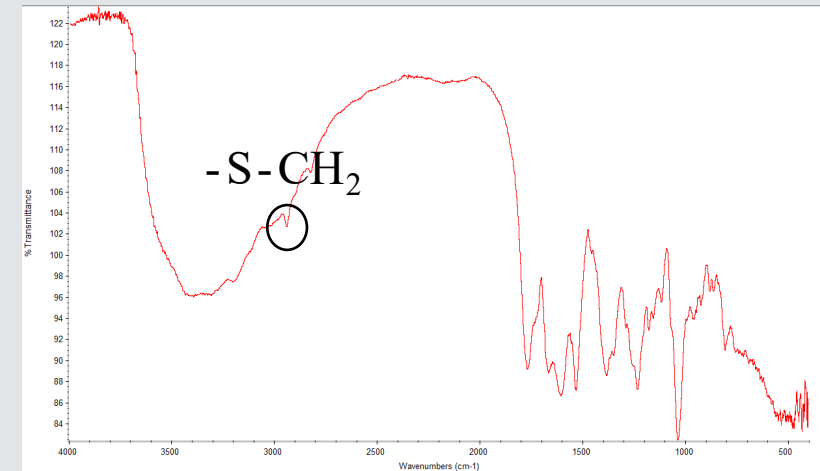
Ethanol Annealed



Water Annealed



Methanol Annealed



CONCLUSIONS AND FUTURE WORK

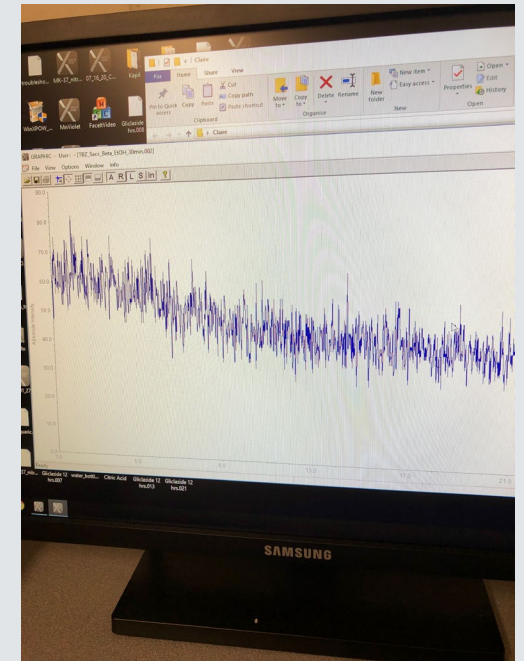
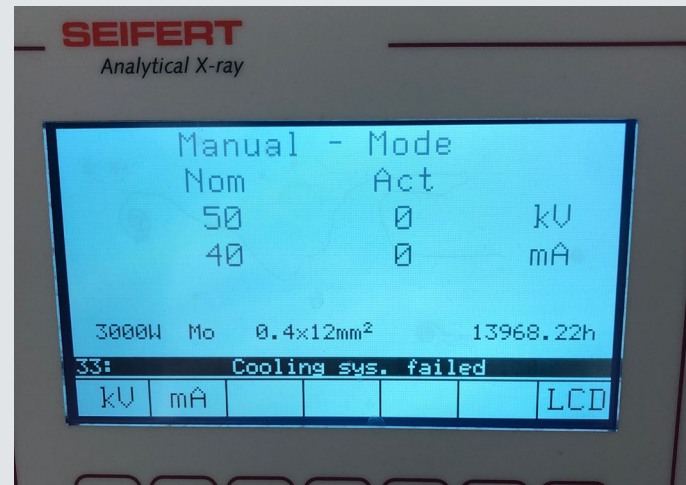
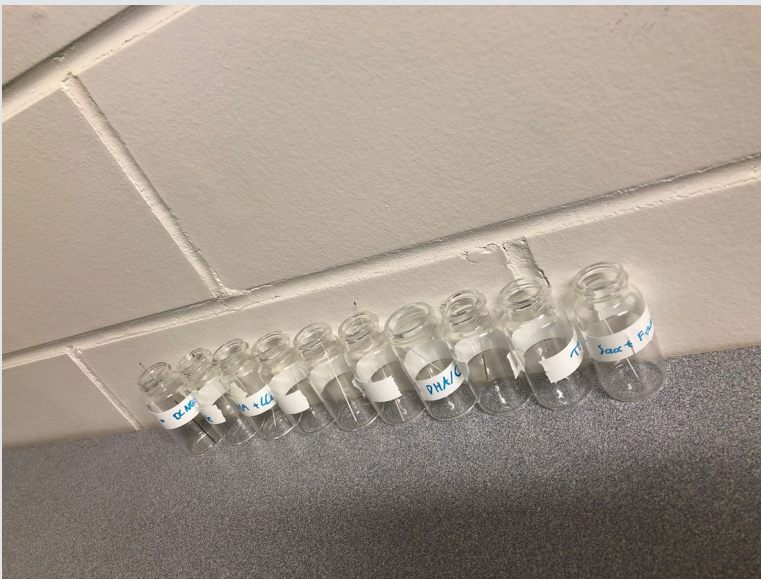
- Apply for beam time at NIST!
- Perform HPLC (High-Performance Liquid Chromatography)
- Perform IR and Raman on everything
- Optical properties
- Mill for different lengths of time to determine where re-crystallization occurs
- Thanks to Dr. Runčevski (PI), Dr. Brown (mentor), Dr. Klein (NIST), Dr. Toliver (SURF Director), Dr. Teixeira, Dr. Borchers, and Dr. Dura (OU Directors)

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NIST



Questions?

