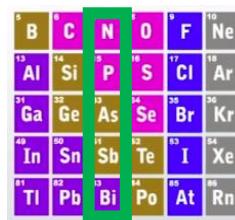




Pnictogen Bonding and Reversed Bilayer Vesicles

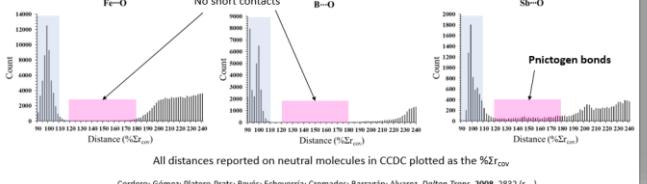
Olivia H. Villanueva, Shiva Moaven, Anthony F. Cozzolino

Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX

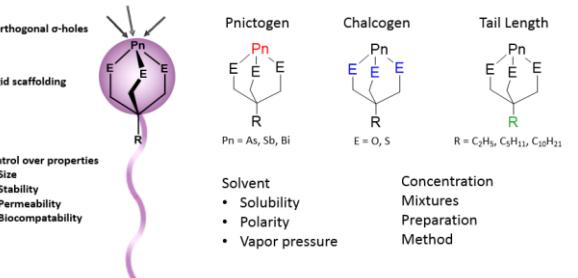


Pnictogen bonding (PnB)

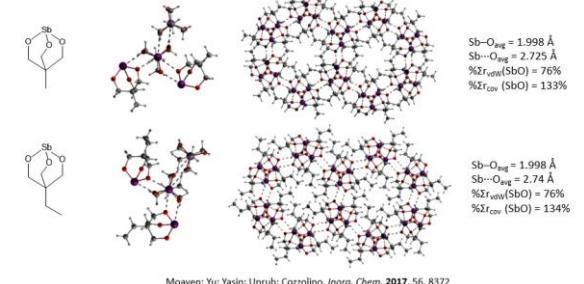
"The net attractive interaction between an electrophilic region [or regions] associated with a [pnictogen] atom in a molecular entity [PnB donor] and a nucleophilic region in another, or the same, molecular entity [PnB acceptor]" – adapted from IUPAC Halogen Bond



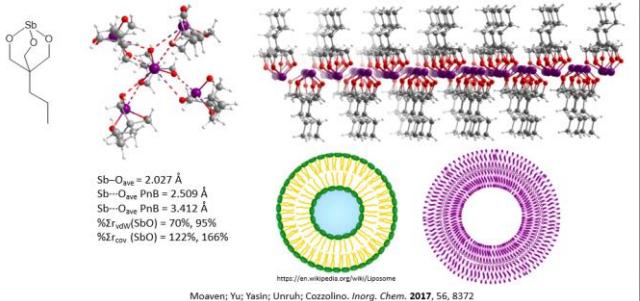
Design Consideration and Factors Investigated



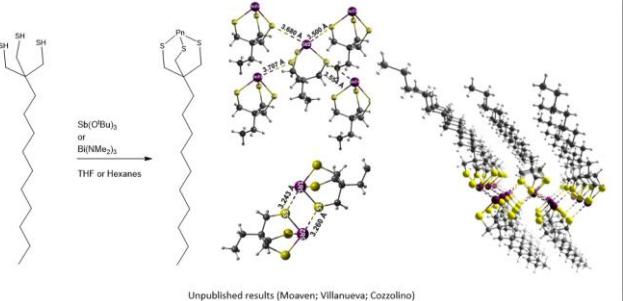
Self-Assembled Helical Columns



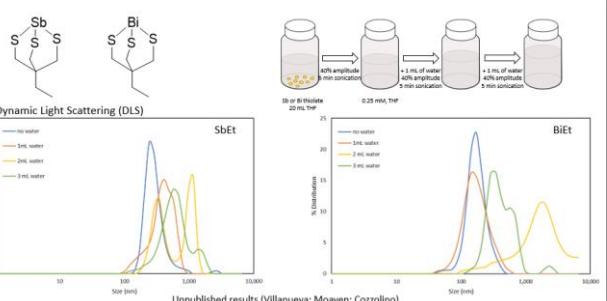
Self-Assembled Reversed Bilayer



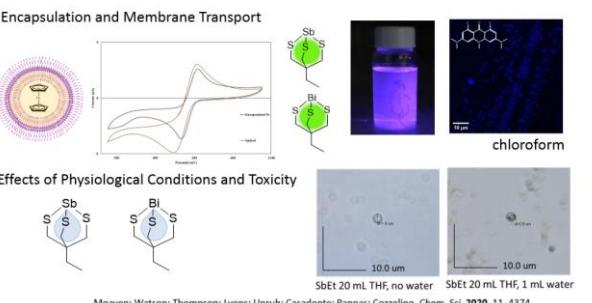
Increasing the Tail Length



Addition of Water Increases Particle Size



Future Work



Acknowledgements



Acknowledgements:

Dr. Daniel K. Unruh
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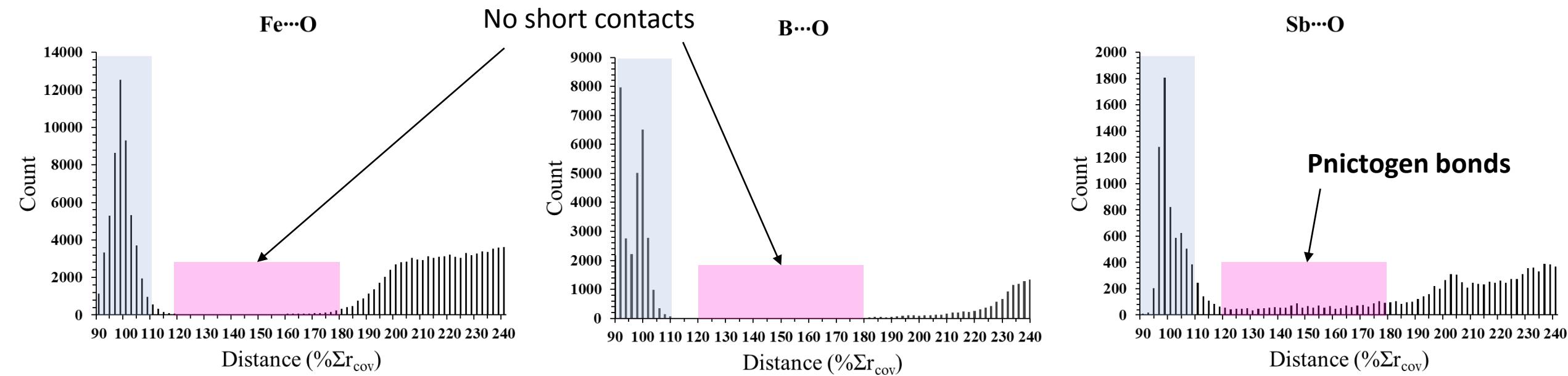
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Jason Yasin (UG)
Sarah S. Villareal (UG)
Fibronia Khalil (UG)
Jingze Yu (H)
Maythe Vega (H)



Pnictogen bonding (PnB)

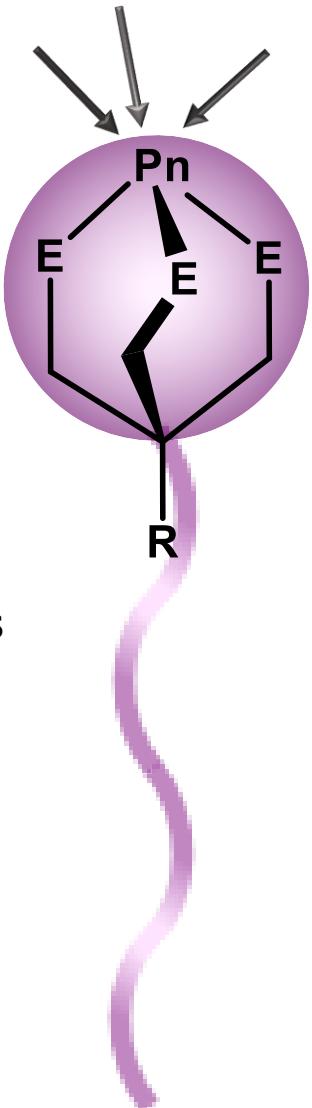
“The net attractive interaction between an electrophilic region [or regions] associated with a [pnictogen] atom in a molecular entity [PnB donor] and a nucleophilic region in another, or the same, molecular entity [PnB acceptor]” – adapted from IUPAC *Halogen Bond*



All distances reported on neutral molecules in CCDC plotted as the % Σr_{cov}

Design Consideration and Factors Investigated

3 orthogonal σ -holes

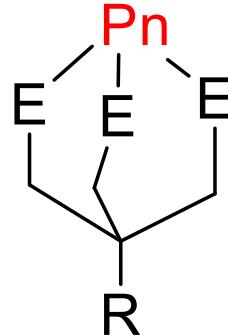


Rigid scaffolding

Control over properties

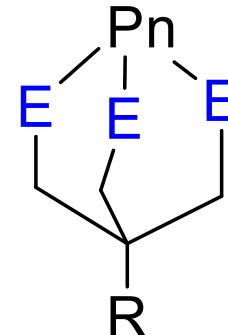
- Size
- Stability
- Permeability
- Biocompatibility

Pnictogen



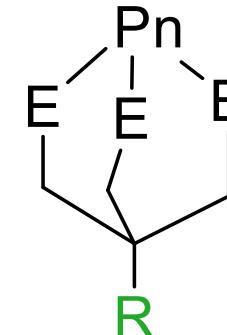
Pn = As, Sb, Bi

Chalcogen



E = O, S

Tail Length



R = C₂H₅, C₅H₁₁, C₁₀H₂₁

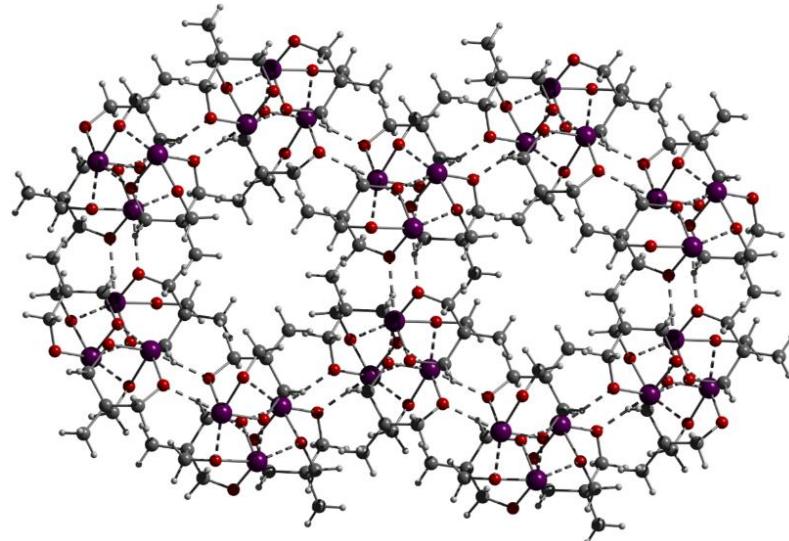
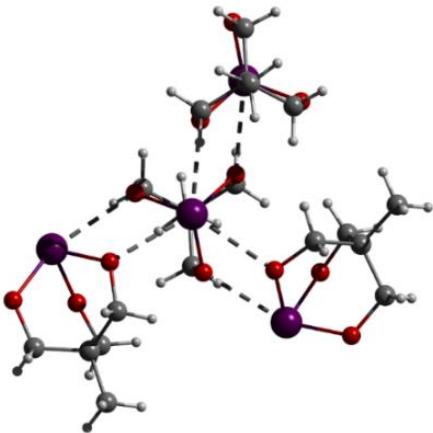
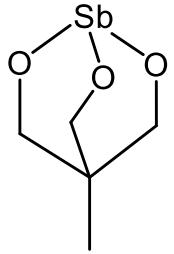
Solvent

- Solubility
- Polarity
- Vapor pressure

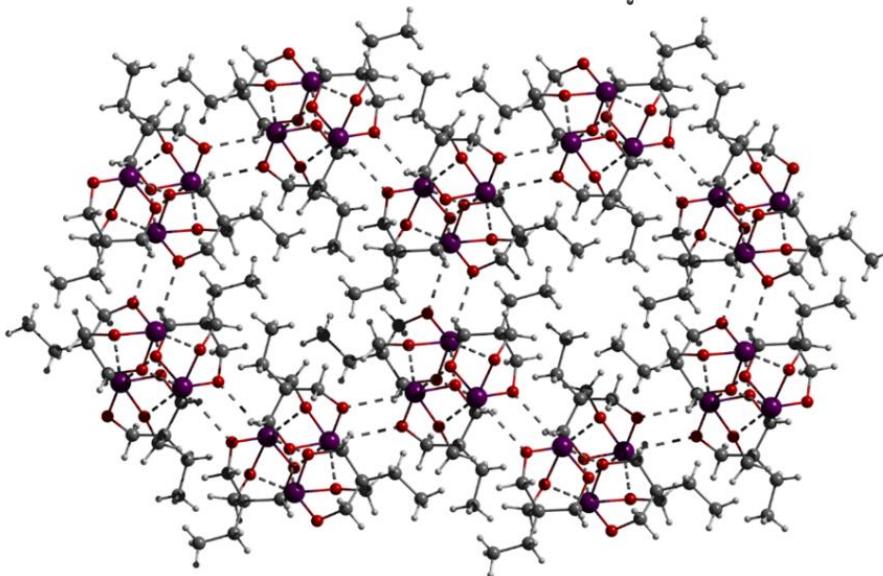
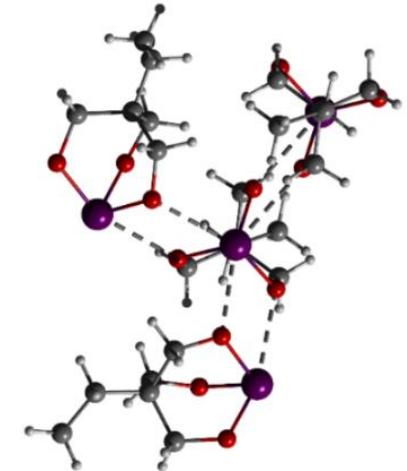
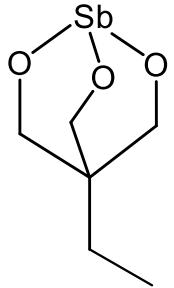
Concentration

- Mixtures
- Preparation
- Method

Self-Assembled Helical Columns

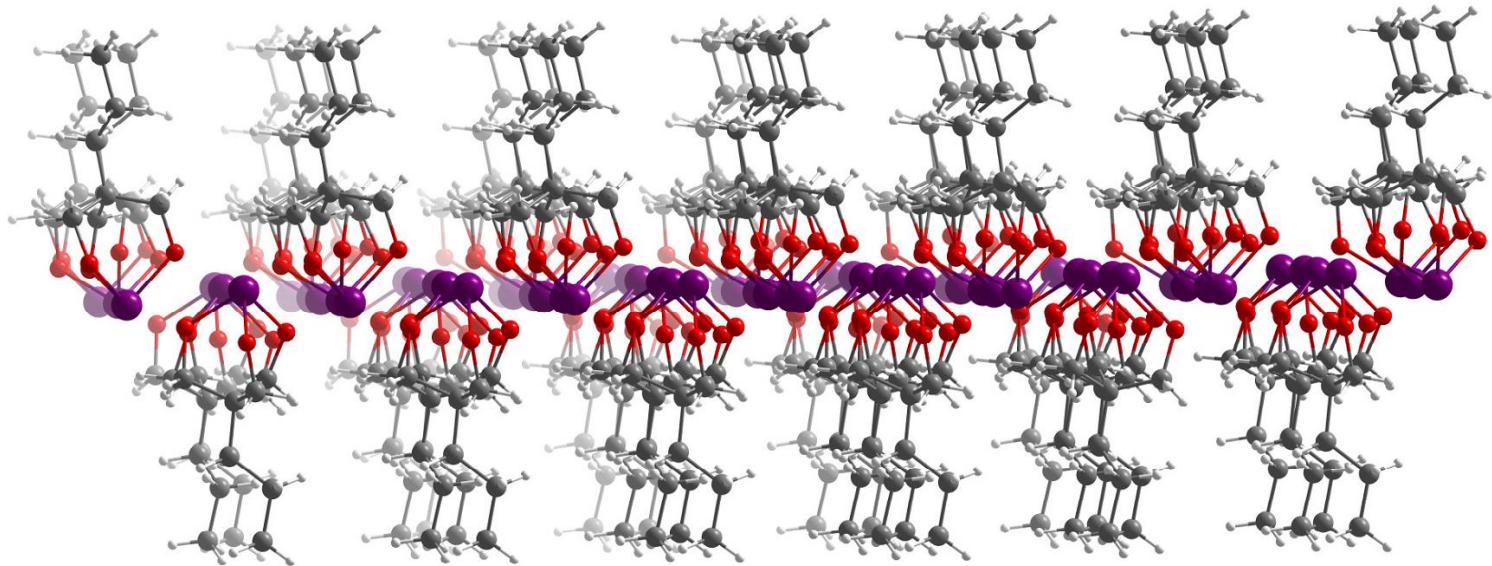
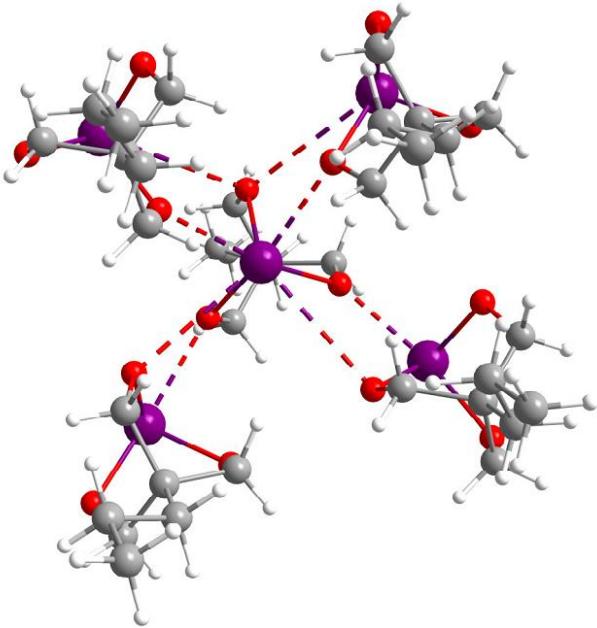
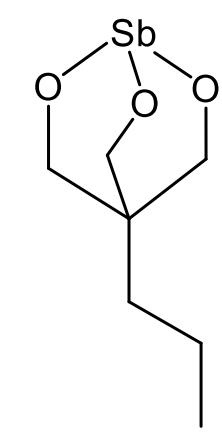


$\text{Sb}-\text{O}_{\text{avg}} = 1.998 \text{ \AA}$
 $\text{Sb}\cdots\text{O}_{\text{avg}} = 2.725 \text{ \AA}$
 $\% \sum r_{\text{vdW}}(\text{SbO}) = 76\%$
 $\% \sum r_{\text{cov}} (\text{SbO}) = 133\%$

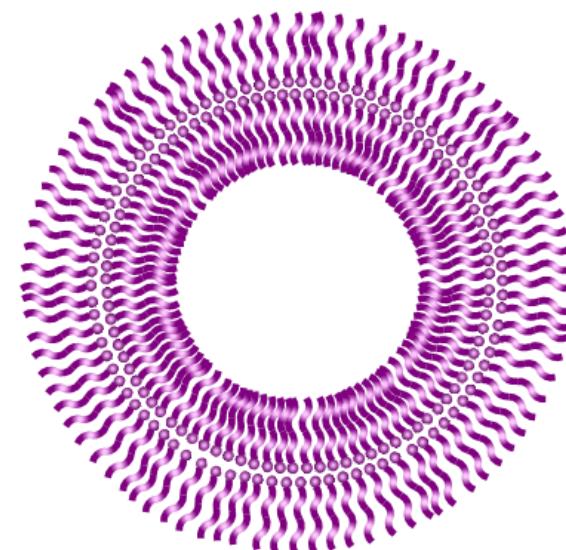
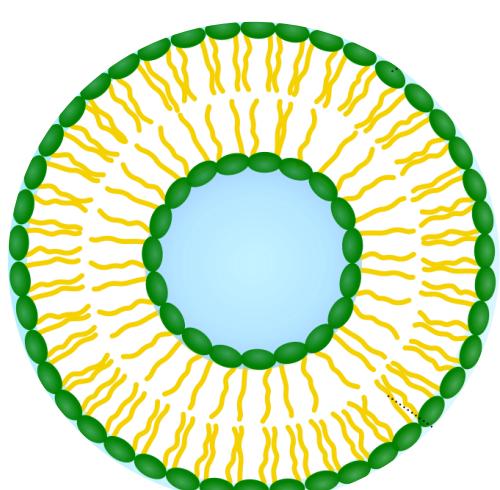


$\text{Sb}-\text{O}_{\text{avg}} = 1.998 \text{ \AA}$
 $\text{Sb}\cdots\text{O}_{\text{avg}} = 2.74 \text{ \AA}$
 $\% \sum r_{\text{vdW}}(\text{SbO}) = 76\%$
 $\% \sum r_{\text{cov}} (\text{SbO}) = 134\%$

Self-Assembled Reversed Bilayer

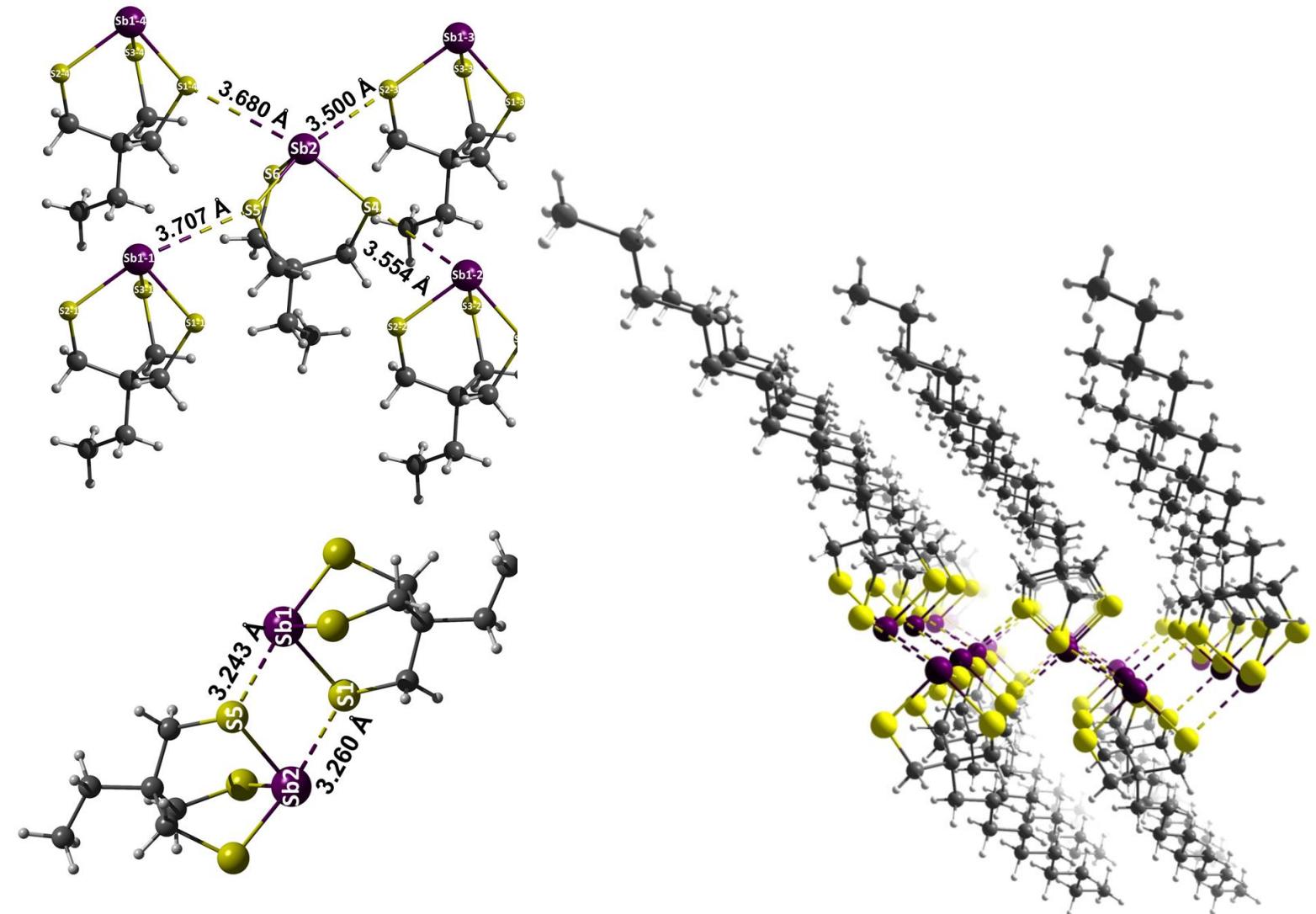
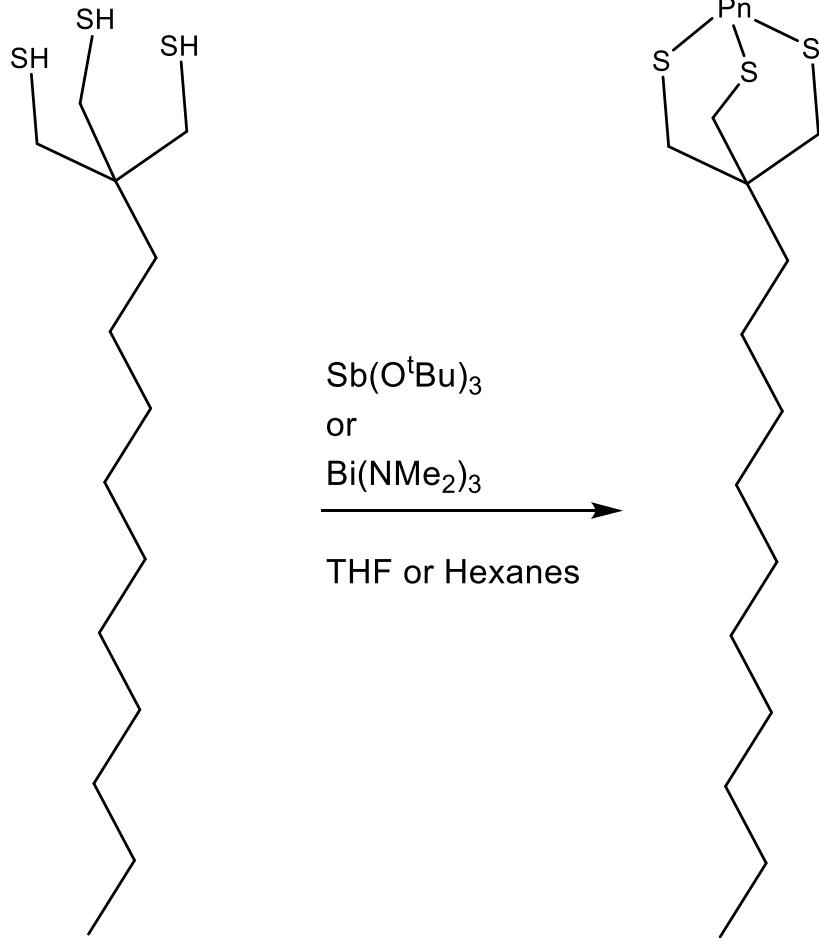


$Sb-O_{ave} = 2.027 \text{ \AA}$
 $Sb \cdots O_{ave} \text{ PnB} = 2.509 \text{ \AA}$
 $Sb \cdots O_{ave} \text{ PnB} = 3.412 \text{ \AA}$
 $\% \sum r_{vdW}(SbO) = 70\%, 95\%$
 $\% \sum r_{cov} (SbO) = 122\%, 166\%$



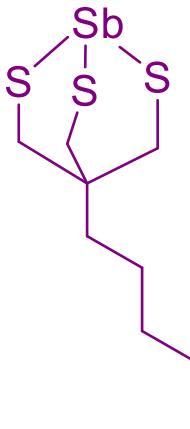
<https://en.wikipedia.org/wiki/Liposome>

Increasing the Tail Length



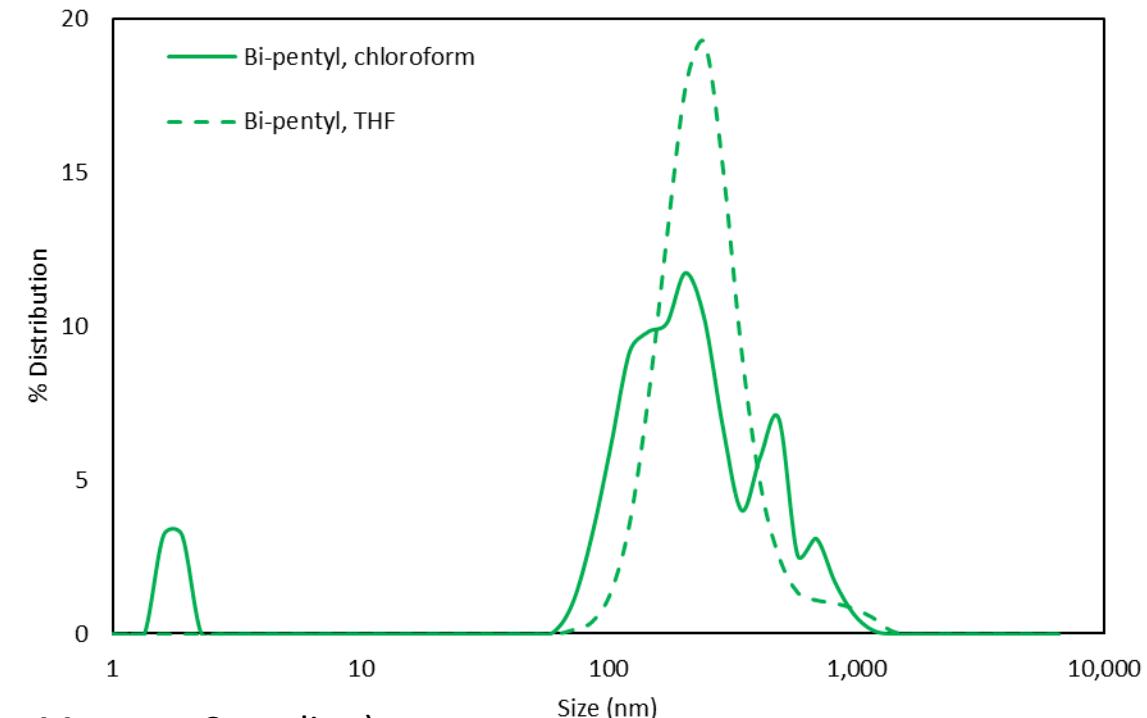
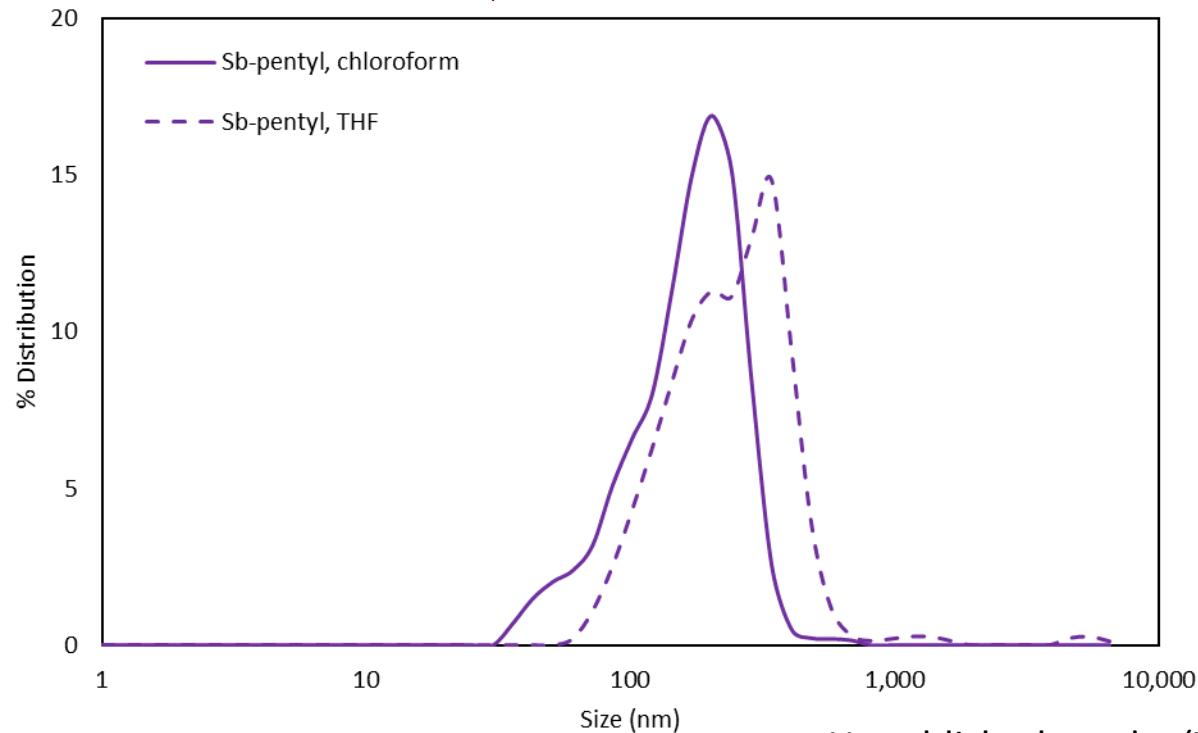
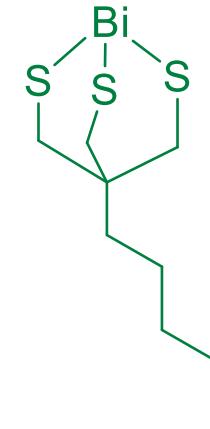
Unpublished results (Moaven; Villanueva; Cozzolino)

Varying Solvent or Pnictogen



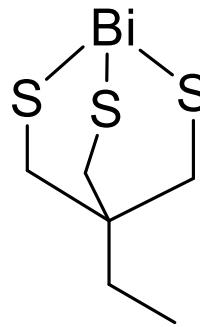
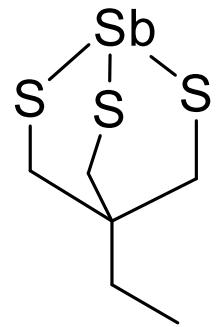
Average Vesicle Diameter (DLS)		
Pnictogen	Solvent	
	Chloroform	THF
Antimony	204.4 nm	344 nm
Bismuth	* nm	243 nm

* Inconclusive results from DLS measurements

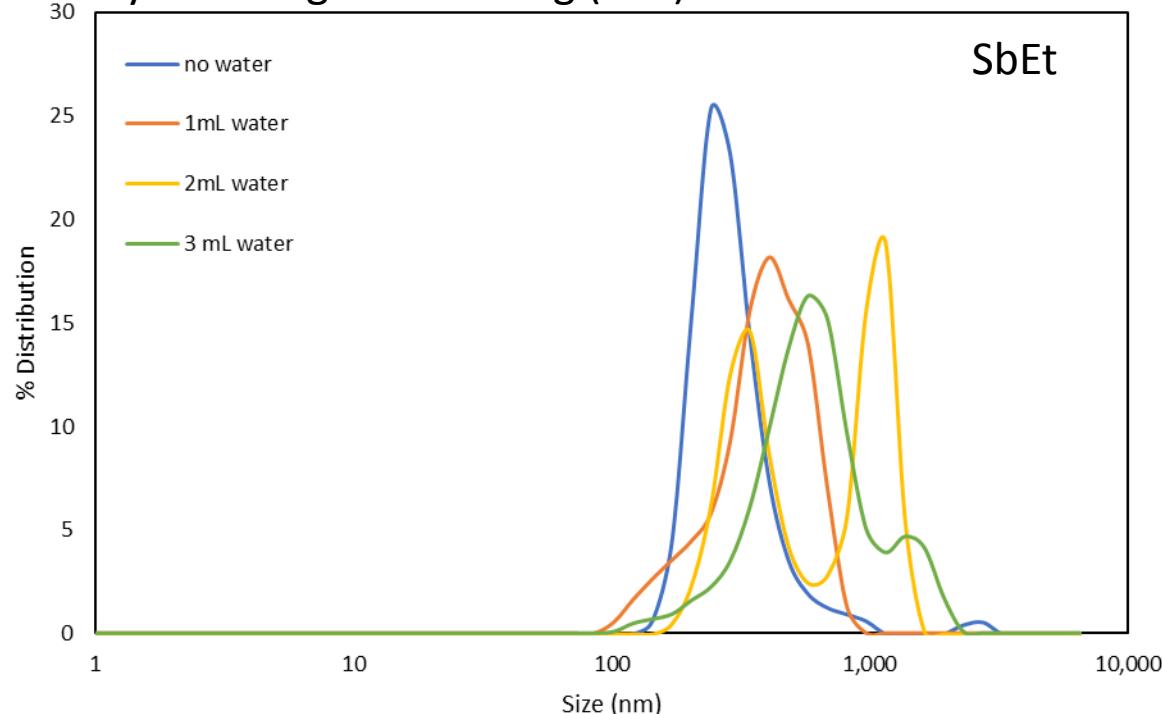


Unpublished results (Villanueva; Moaven; Cozzolino)

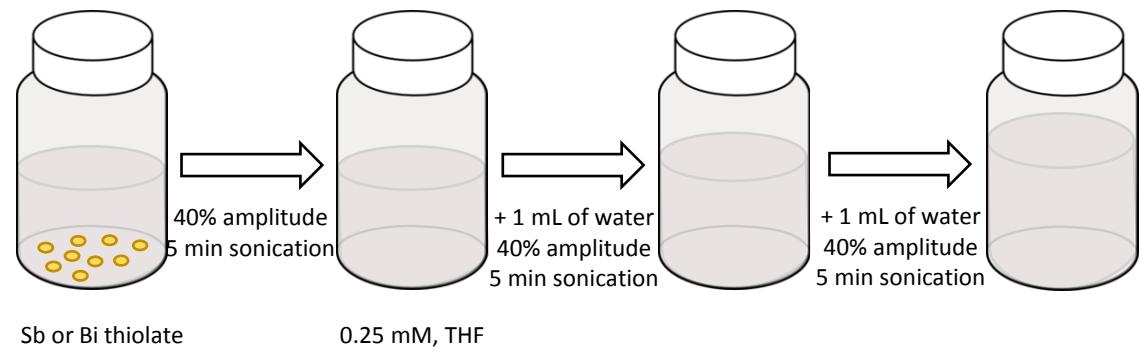
Addition of Water Increases Particle Size



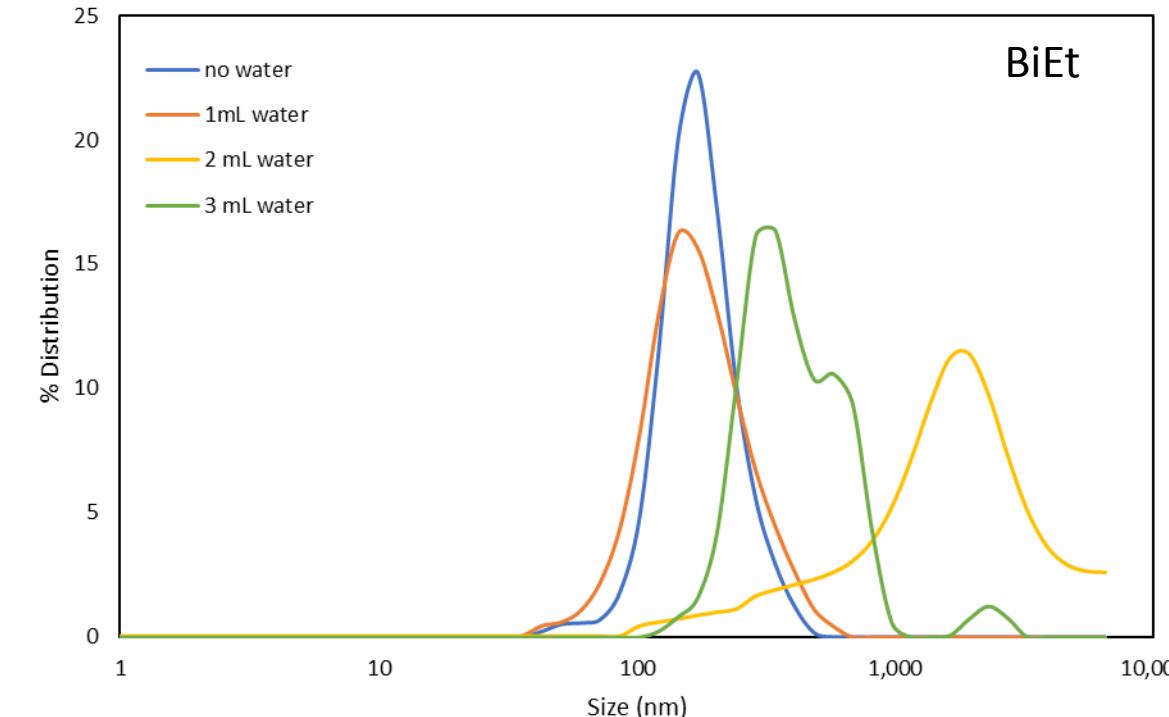
Dynamic Light Scattering (DLS)



SbEt



Sb or Bi thiolate
20 mL THF

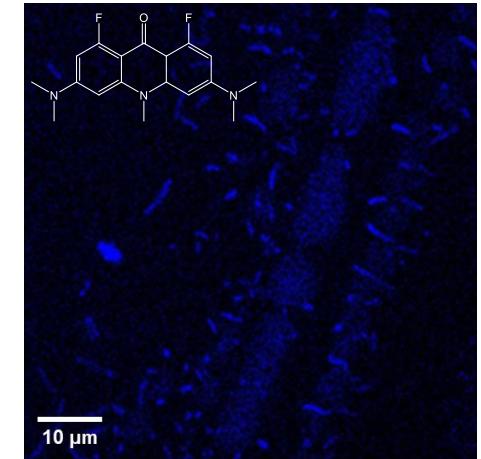
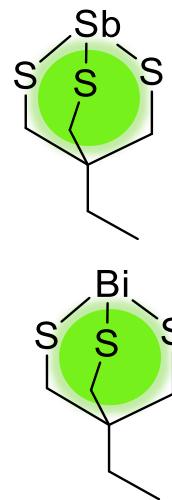
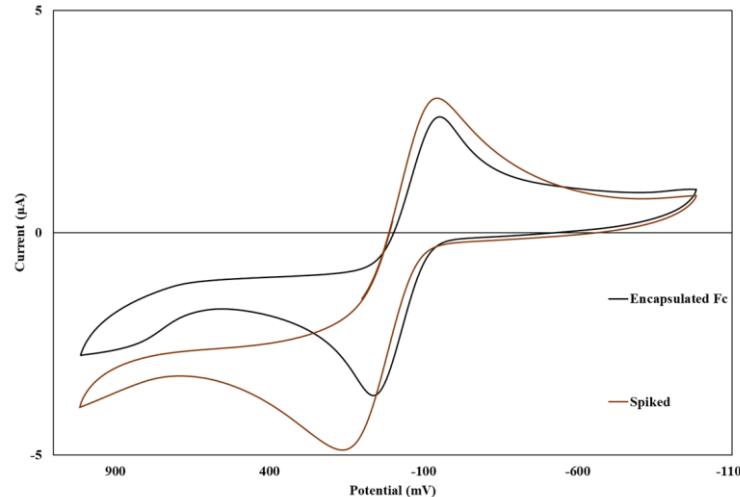
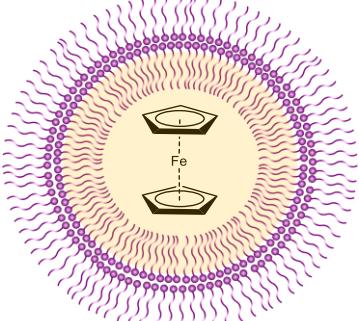


BiEt

Unpublished results (Villanueva; Moaven; Cozzolino)

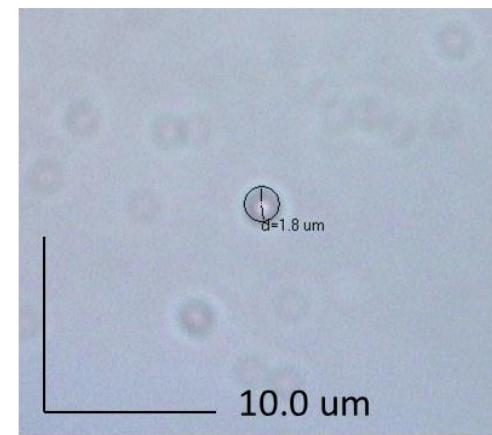
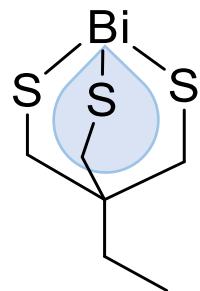
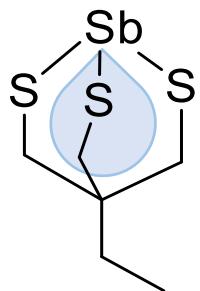
Future Work

Encapsulation and Membrane Transport

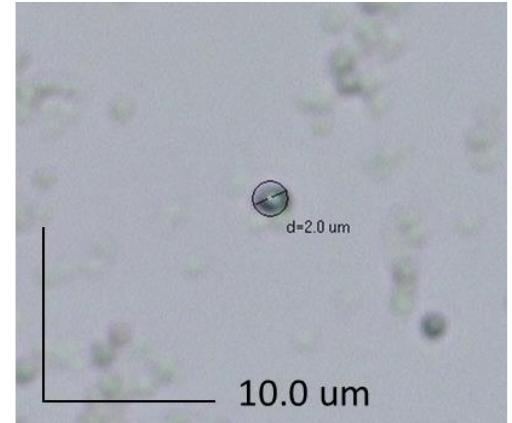


chloroform

Effects of Physiological Conditions and Toxicity



SbEt 20 mL THF, no water



SbEt 20 mL THF, 1 mL water

Acknowledgements



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