



HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

Kemiallisten aseiden nopea ja kannettava kenttätesti

Rapid and Portable Infield Detection of Warfare Agents (weSAFE)

MATINE funding: €150,353; Project duration: 2 years; Start date: 01.03.2023

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OUR GOAL

To enable rapid, sensitive,
and easy fingerprint
detection of **warfare
agents** and **harmful
molecules**



NEED



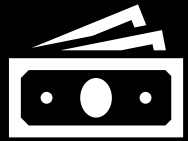
Chemical and biological
weapons:

lethal at **low**
concentration levels

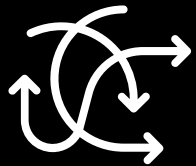
THE PROBLEM: CONVENTIONAL DETECTION METHODS



Slow



Expensive








Complex sample preparation

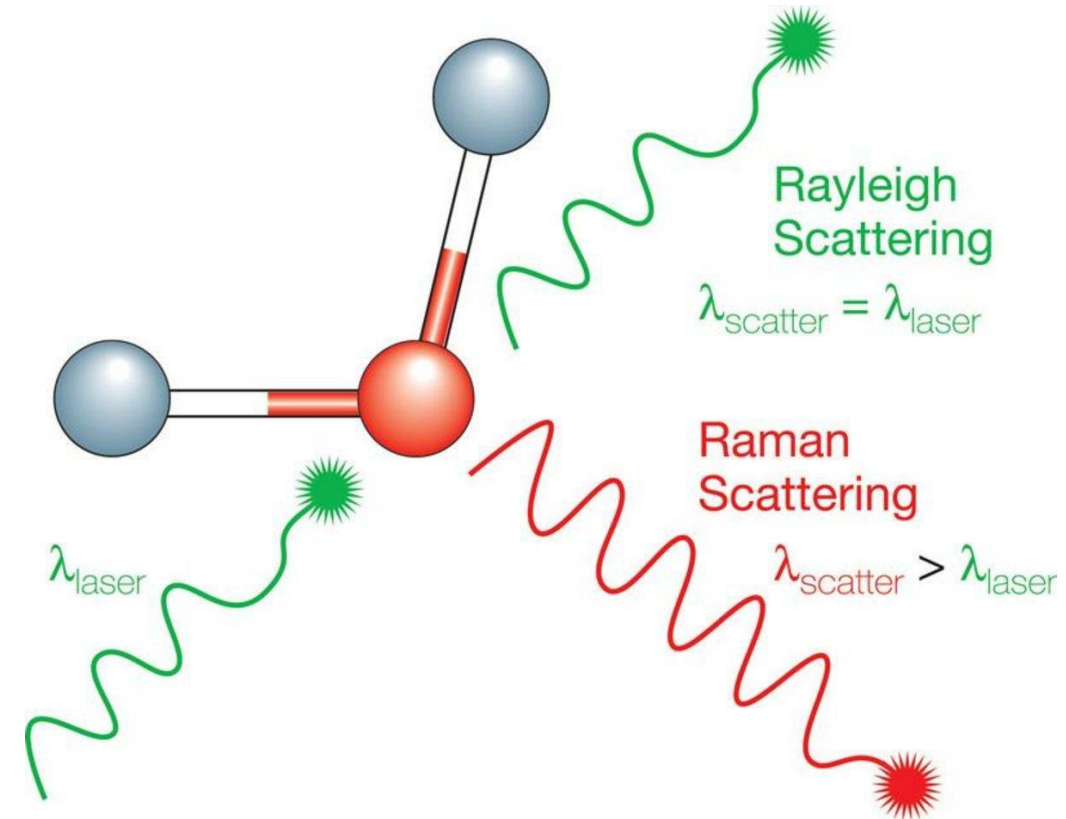
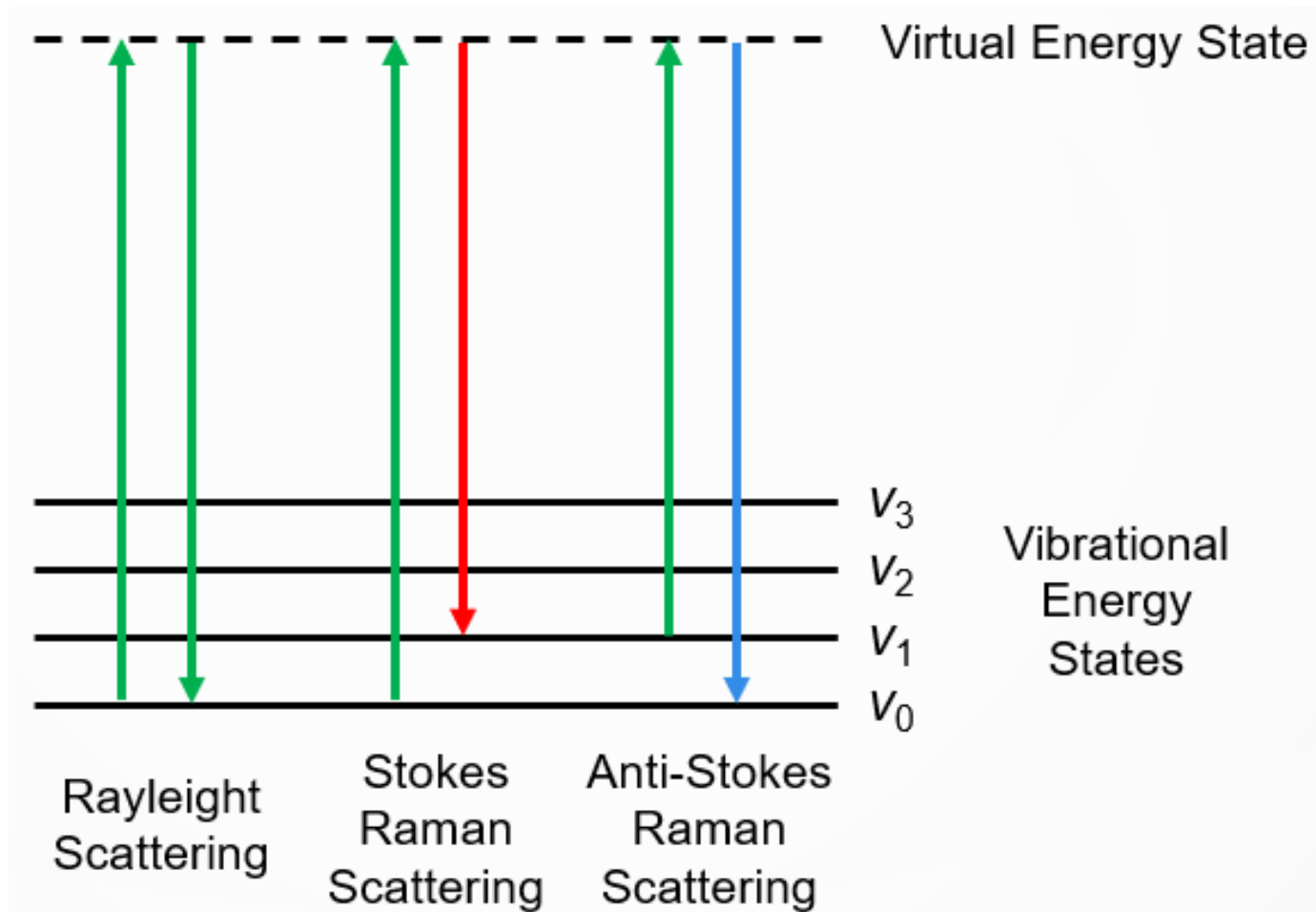


Limited sensitivity, no fingerprint

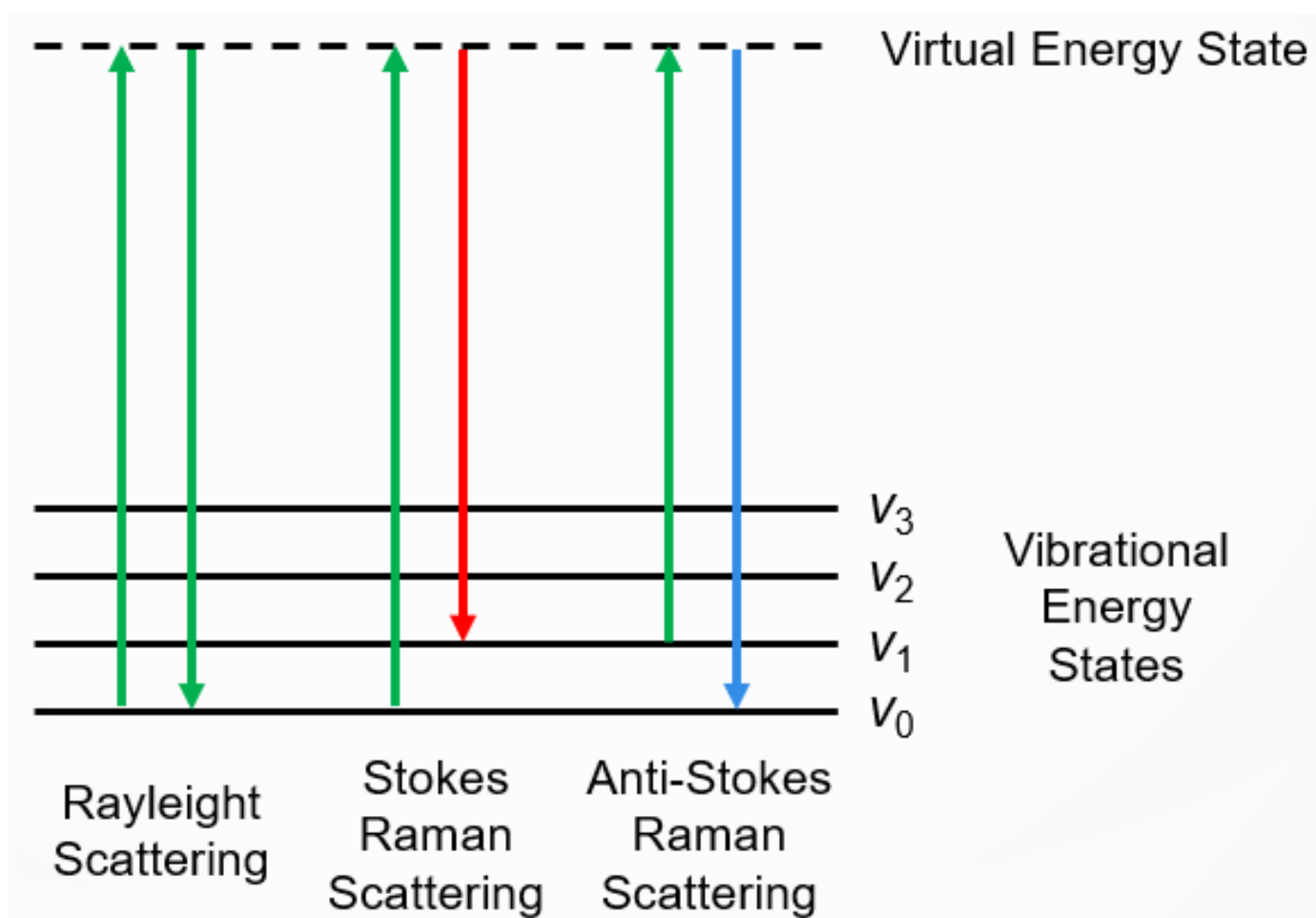
SOLUTION: SURFACE ENHANCED RAMAN SCATTERING (SERS)

-  **Sensitive:** detection at low concentration levels
-  **Rapid:** fast response times
-  **Easy to execute:** minimal sample preparation
-  **Portability:** in-field or remote (drone) based detection
-  **Precision:** fingerprint identification

RAMAN AND SURFACE ENHANCED RAMAN SCATTERING (SERS)



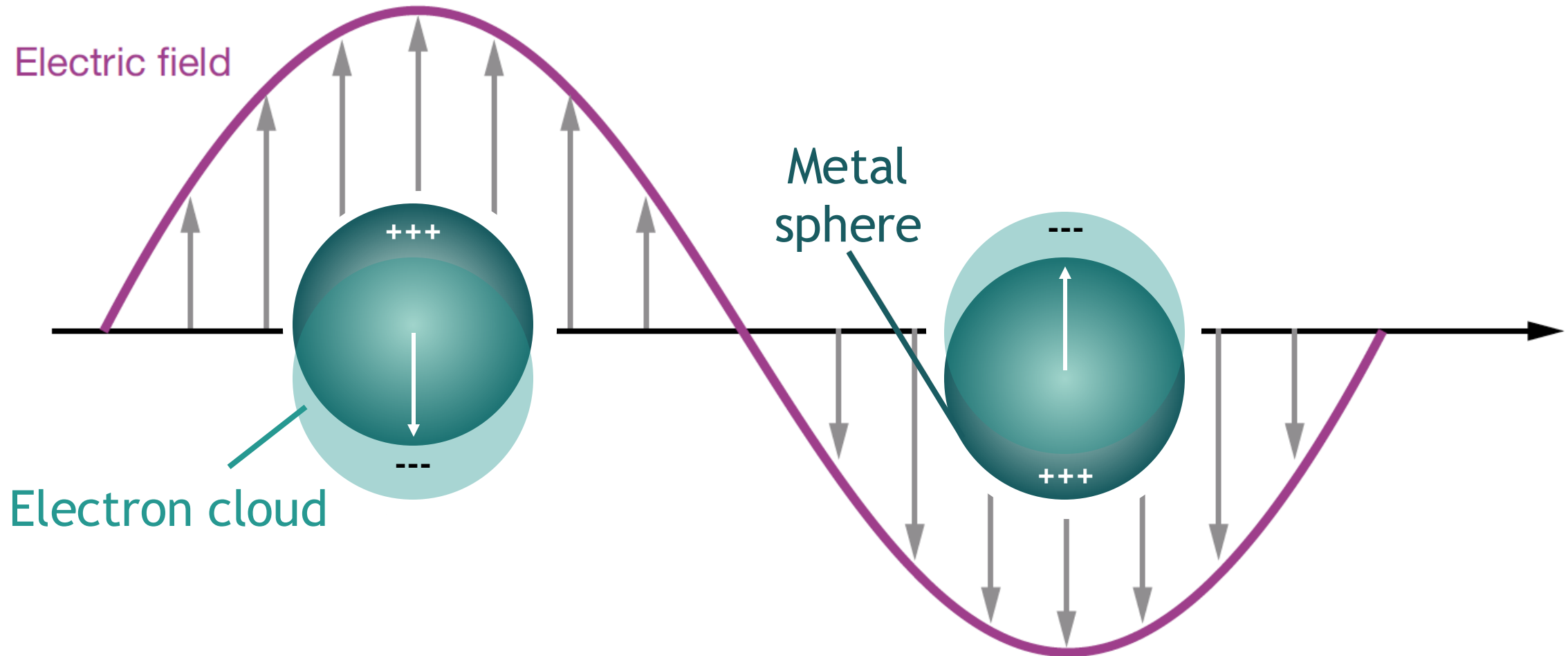
RAMAN AND SURFACE ENHANCED RAMAN SCATTERING (SERS)



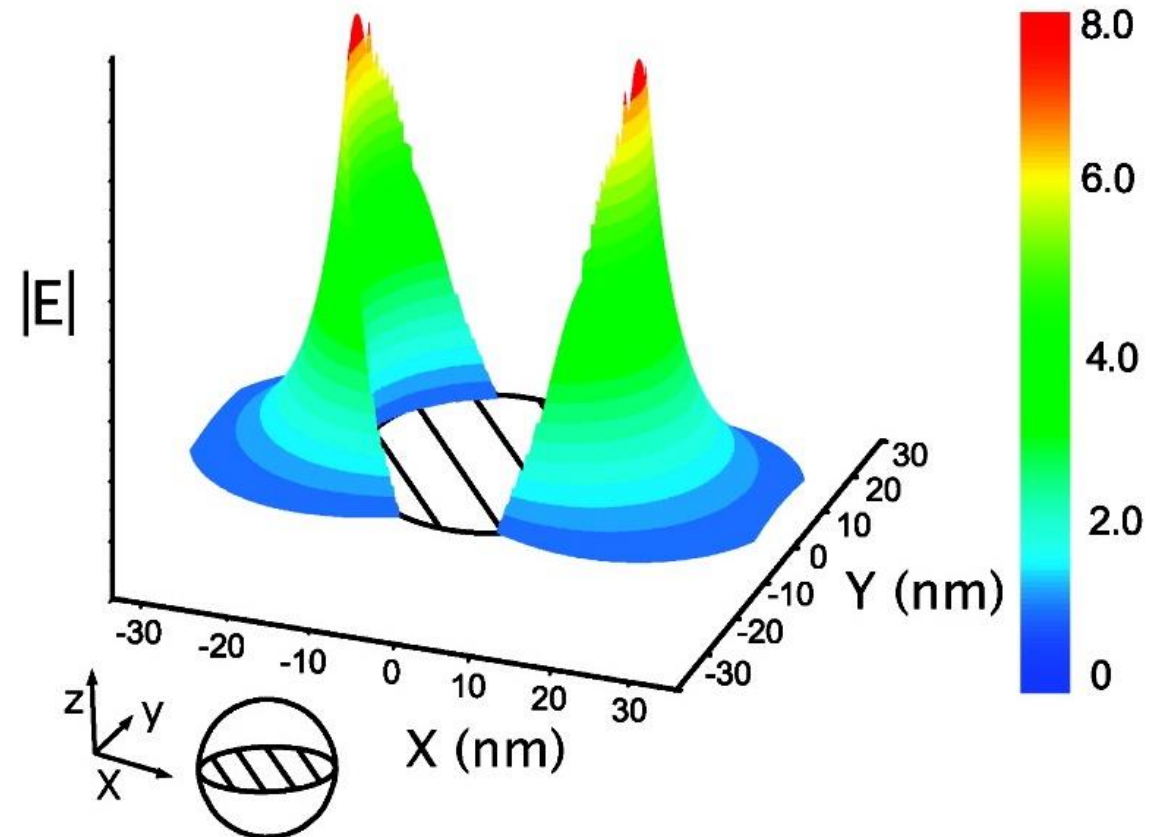
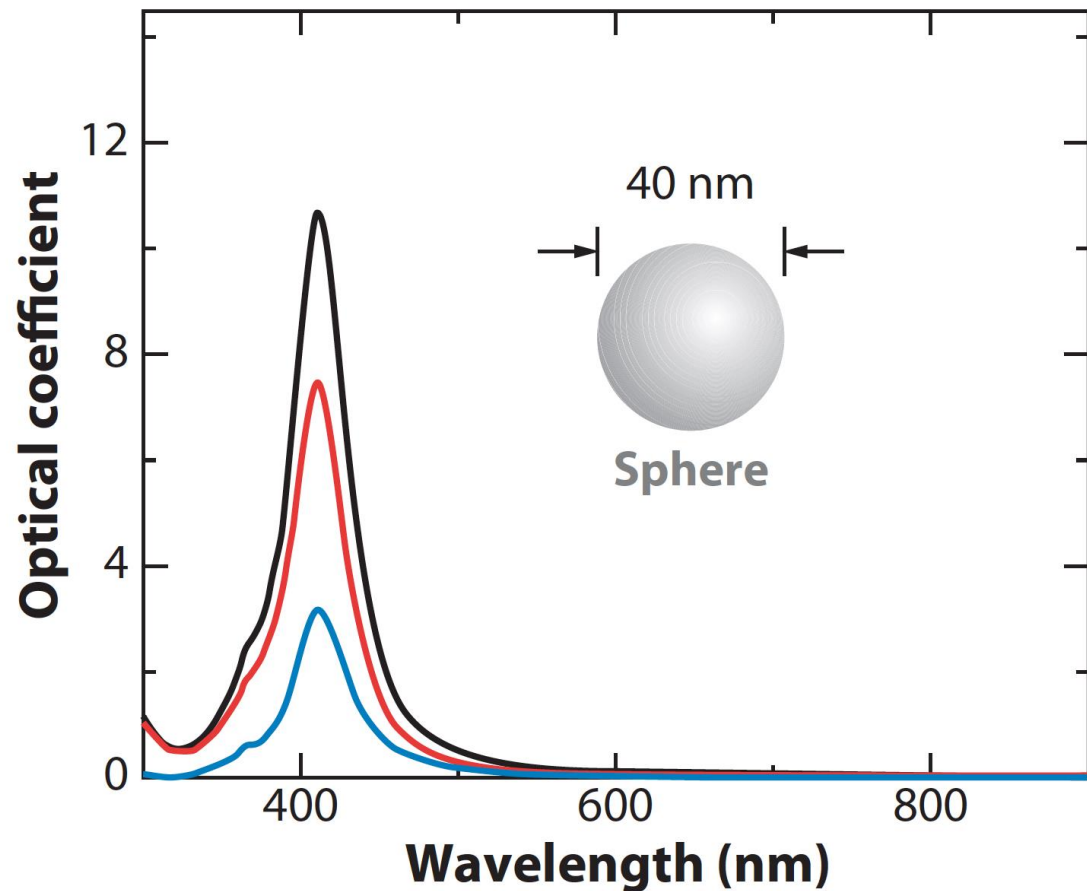
Signal positions determined by vibrational energy of molecule bonds

Raman effect is weak

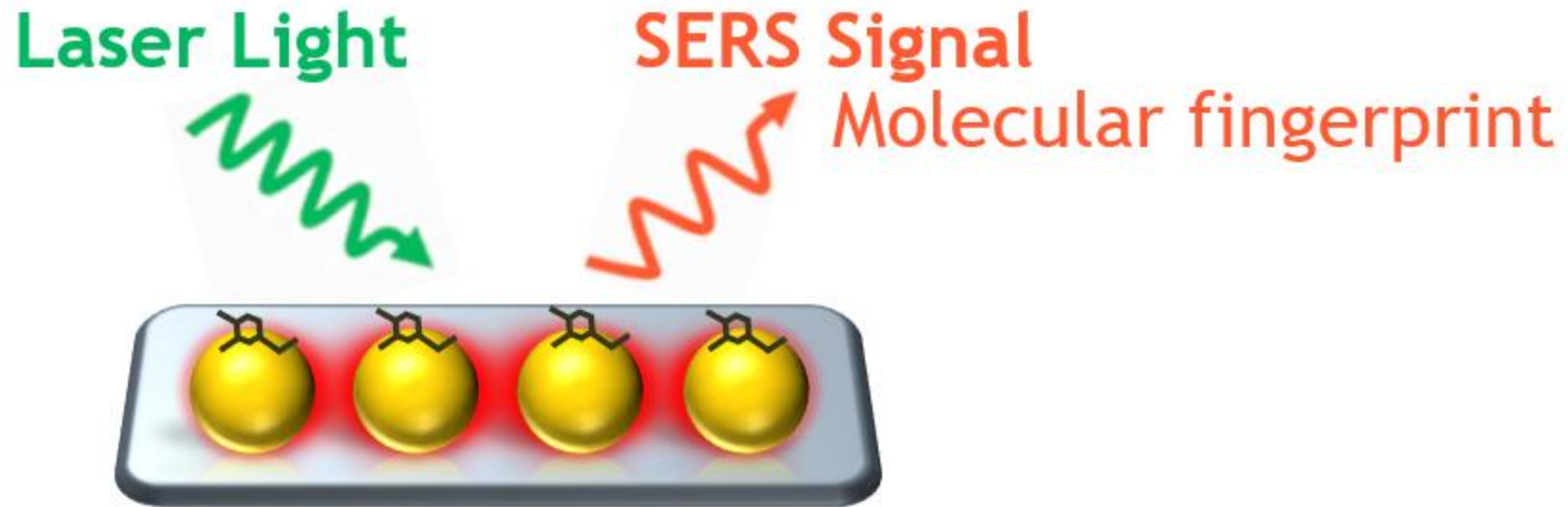
LOCALIZED SURFACE PLASMON RESONANCE (LSPR) EXCITATION



LOCALIZED SURFACE PLASMON RESONANCE (LSPR) EXCITATION



OUR GOAL: SUBSTRATES FOR SERS



Nanoparticle substrates

Target molecule from chemical or biological threat

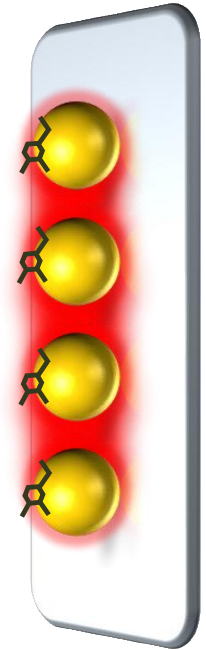
OUR GOAL: SUBSTRATES FOR SERS



**Photo of Portable
Raman Spectrometer**



**Portable Raman
Spectrometer
(commercial)**



**Designer
substrate**

GOALS: DETECTION OF CHEMICAL WARFARE AND BIOLOGICAL AGENTS



Nerve agents as chemical weapons

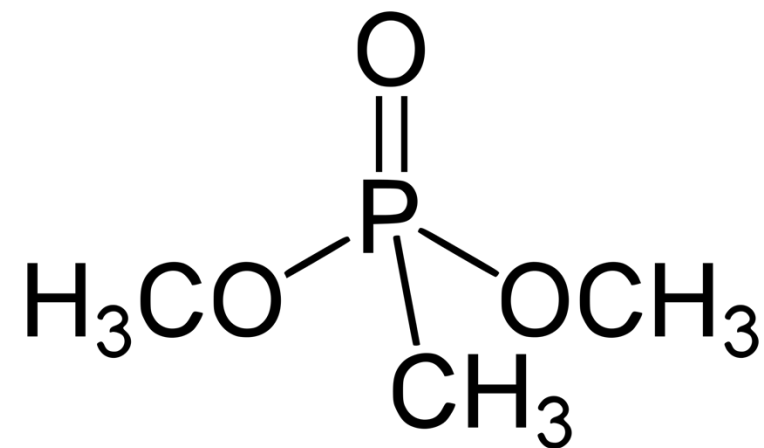


Anthrax as a biological weapon



TARGET MOLECULES

- Nerve agents **Tabun, Cyclosarin, Sarin (GB), Soman (GD), and VX**
- They are **highly toxic**
- Use herein simulant compounds that mimic the properties of these nerve agents
- **Dimethyl methylphosphonate (DMMP)**



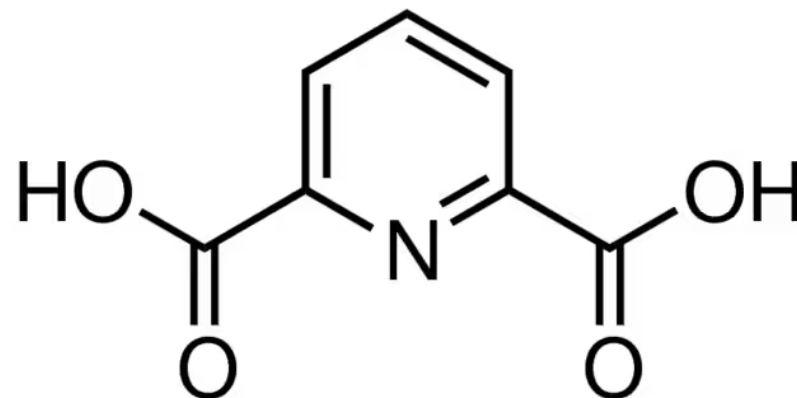
DMMP



TARGET MOLECULES

- **Biological threats**
- Anthrax as an example
- *Bacillus anthracis* bacteria
- DPA as a biomarker for *Bacillus anthracis*

DPA
2,6-Pyridinedicarboxylic acid





SERS MEASUREMENT

**All the results herein acquired
with a benchtop, portable
Raman instrument**

CORA 5001 BENCHTOP RAMAN

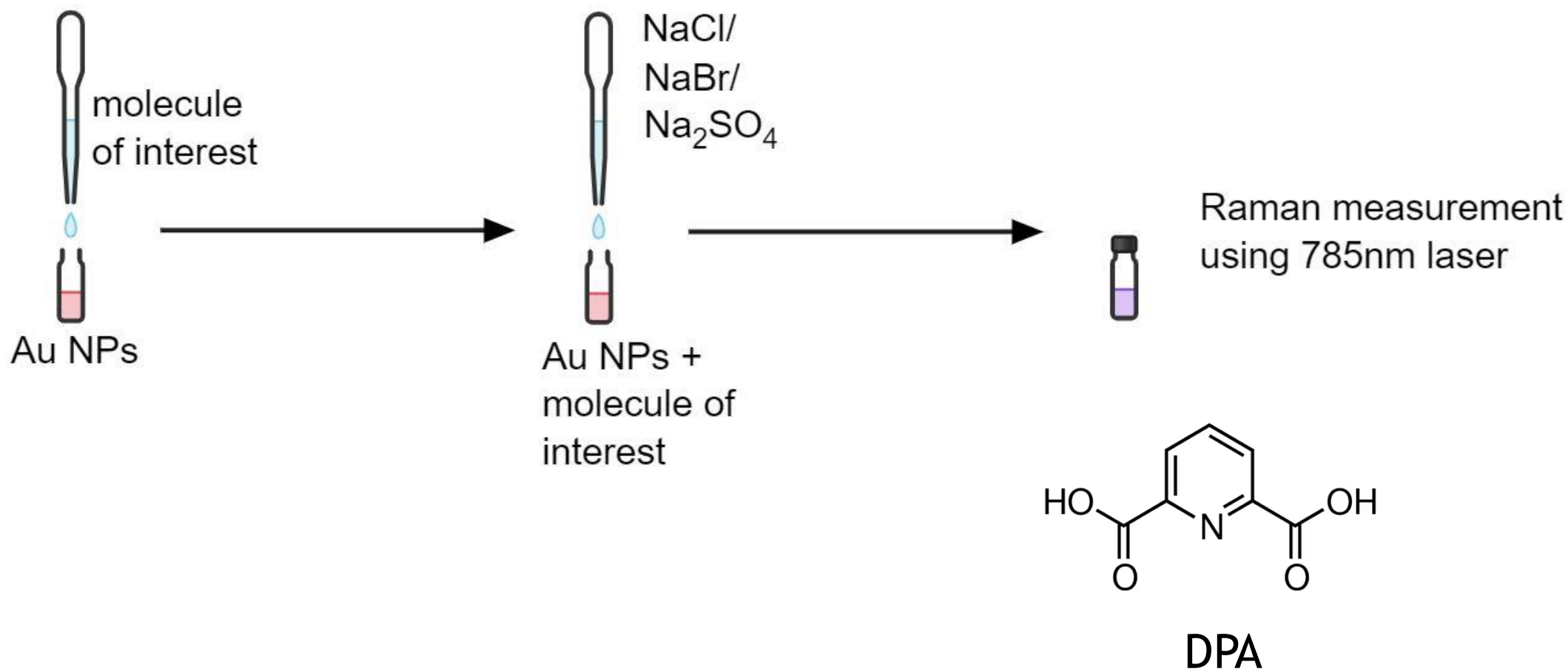


Establishing Effective Detection for DPA with Potential for Other Agents





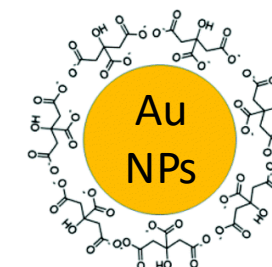
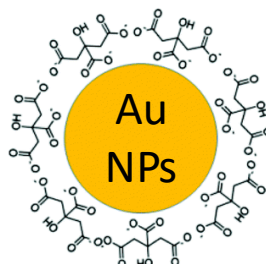
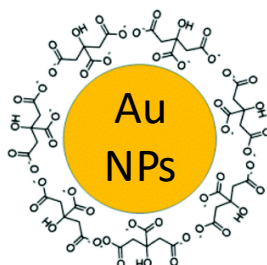
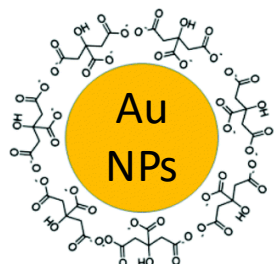
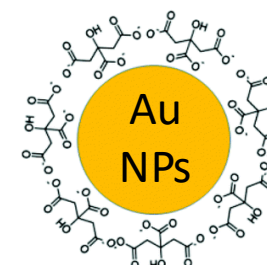
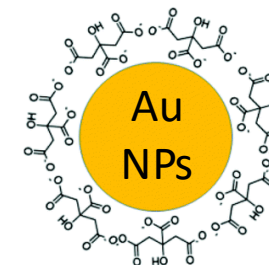
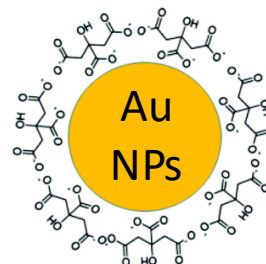
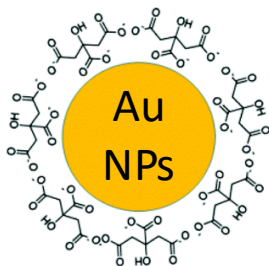
LIQUID PHASE DETECTION





LIQUID PHASE DETECTION, DPA

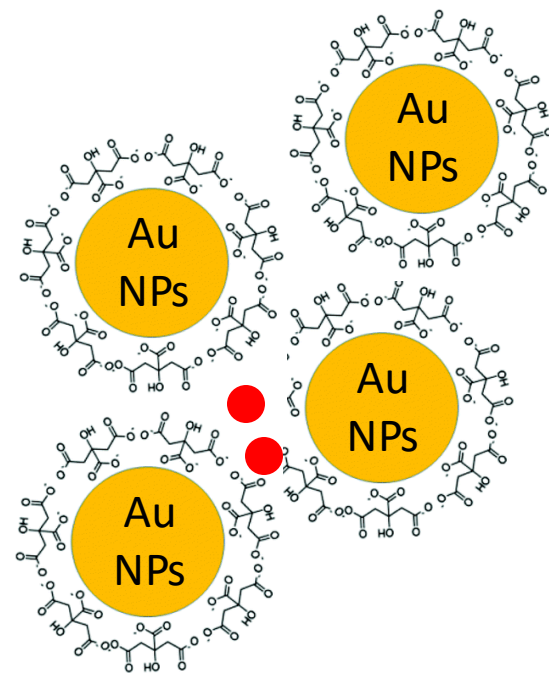
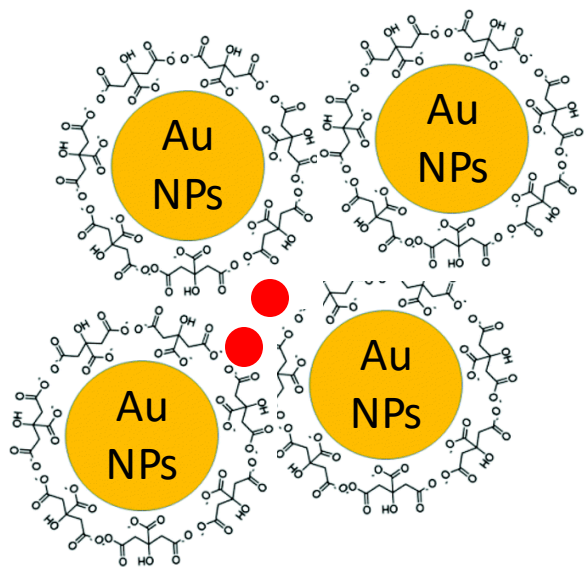
● = DMMP or DPA





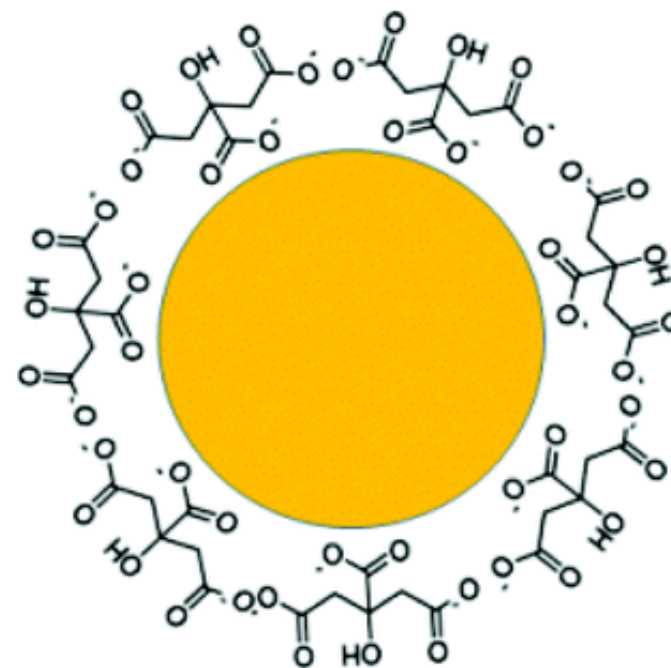
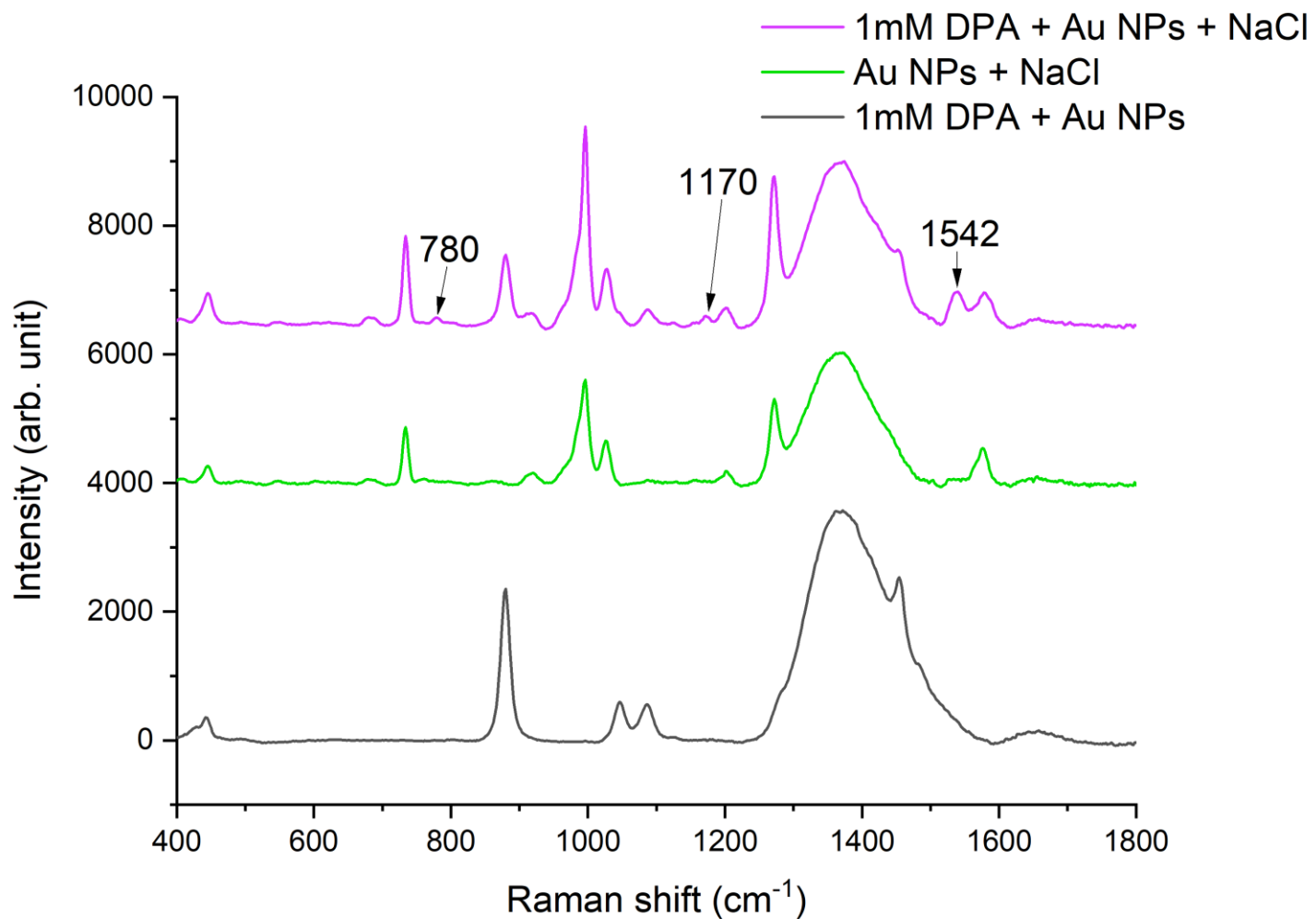
LIQUID PHASE DETECTION, DPA

● = DPA





LIQUID PHASE DETECTION, DPA





SOLID PHASE DETECTION, DPA

- The relationship between DPA concentration and anthrax spores is crucial: **DPA is a major component of Bacillus anthracis spores**
- **DPA is released** during spore germination, making it **an biomarker**
- **High sensitivity to low DPA levels** would enable early detection, essential for rapid intervention.



SOLID PHASE DETECTION, DPA

- **Low-level spore concentrations** typically range from **10 to 1,000 spores/mL** in environmental and clinical testing
- **10 spores/mL: approximately 0.1 nanomolar (nM)**
- **10 nM is 1.7 ppb or approximately 100 spores**
- For inhalation, the estimated infectious dose (ID_{50}), or dose that causes infection in 50% of exposed individuals, is around 2,500 to 10,000 spores.



SOLID PHASE DETECTION, DPA

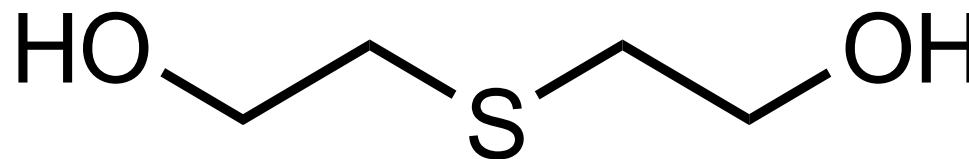
- **Final Optimization:** Enhance SERS substrate for even lower detection limits
- **Broader Applications:** Explore potential for other bacterial biomarker detections



MOLECULES OF INTEREST

- Mimics sulphur-based **mustard gases**
- Sulfur mustard is a type of chemical warfare agent that causes blistering of the skin

TDG
thiodiglycol

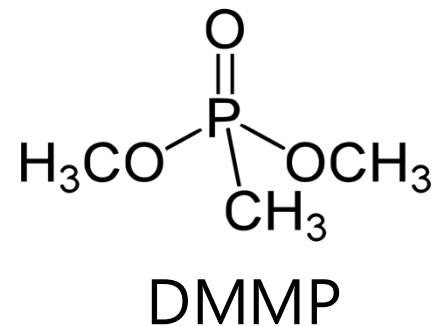
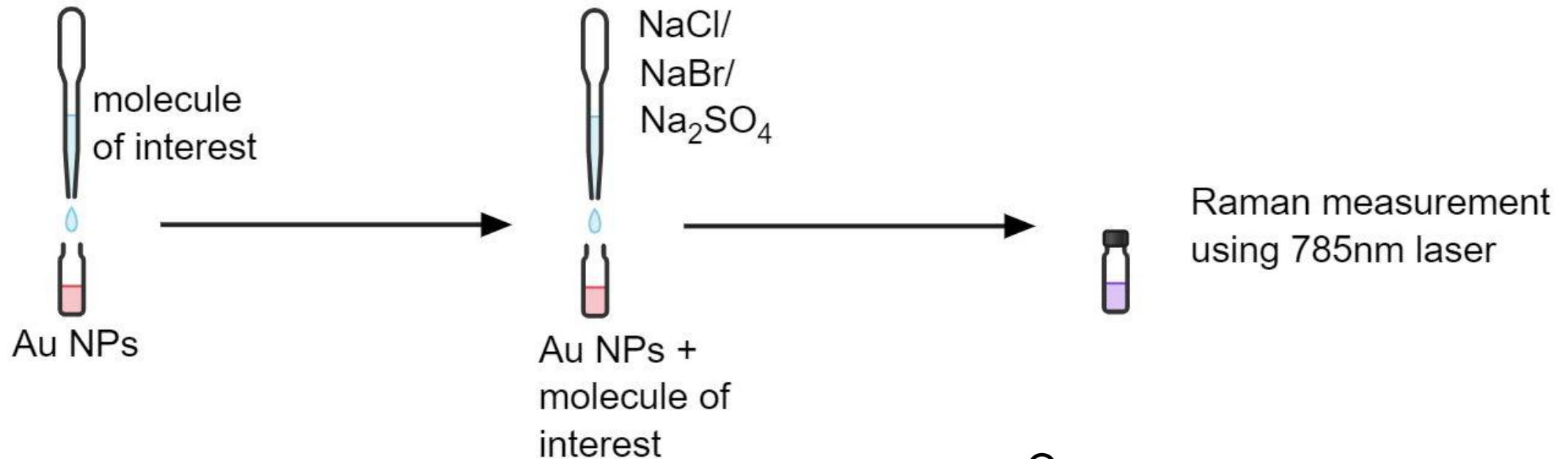


Challenges and insights on DMMP Detection



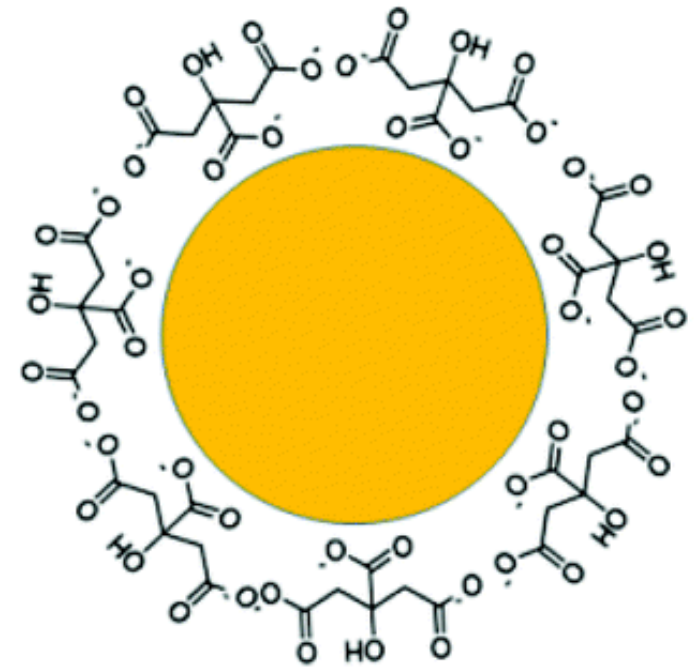
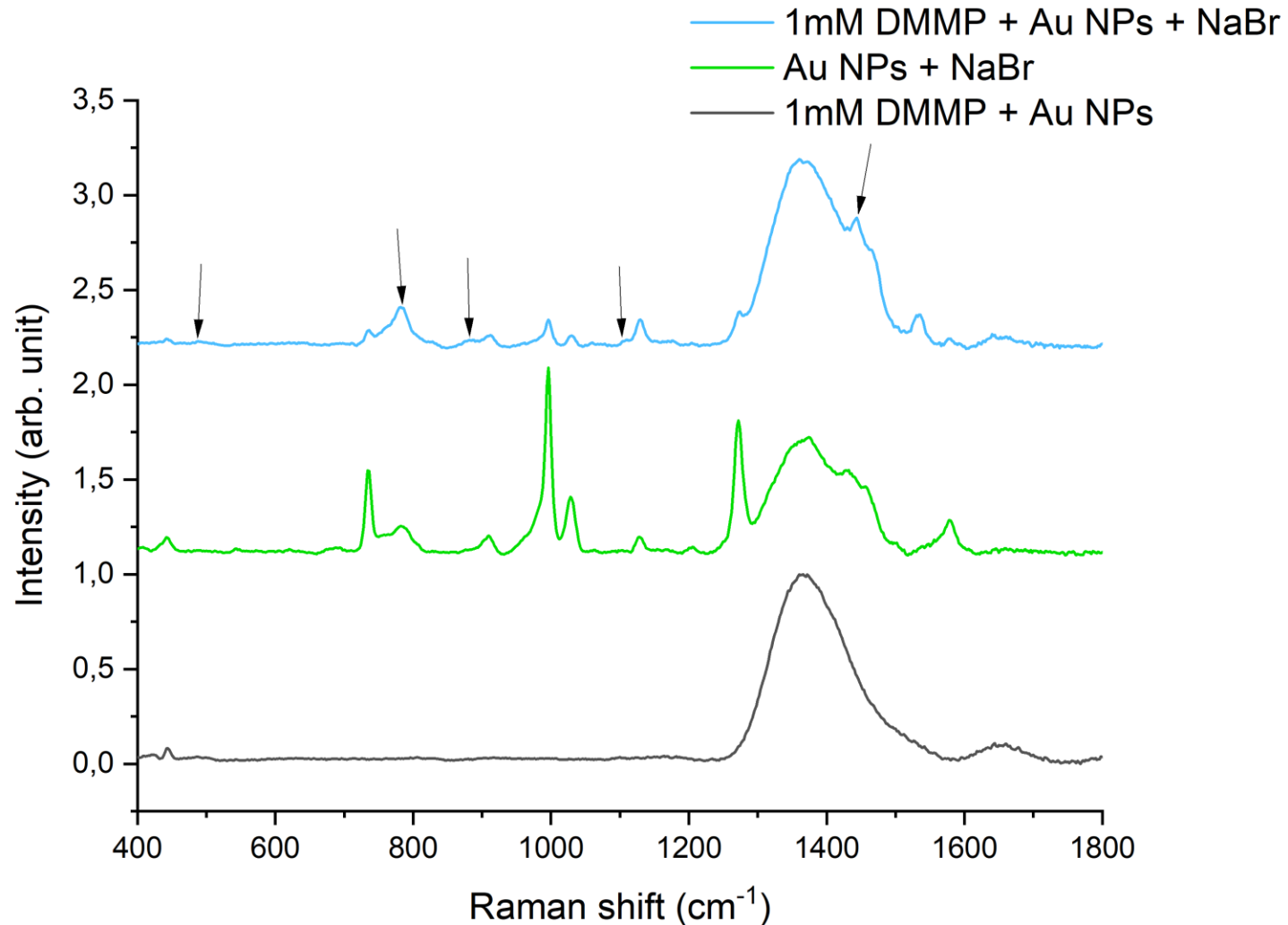


SERS MEASUREMENTS FROM LIQUID PHASE, DMMP





SERS MEASUREMENTS FROM LIQUID PHASE, DMMP





KEY TAKEAWAYS AND FUTURE DIRECTIONS

Significant Achievement

- Successfully demonstrated sensitive detection of DPA, a critical biomarker for anthrax spores, and TDG (marker for mustard gas)

Key Insights from DMMP Trials

- Identified challenges in achieving consistent signal enhancement, guiding future substrate and functionalization improvements



KEY TAKEAWAYS AND FUTURE DIRECTIONS

Next Steps

- For DMMP, explore alternative aggregation strategies and surface modifications to boost detection sensitivity

Impact

- Potential to enable rapid, in-field detection of both chemical and biological threats



PROJECT ORGANIZATION

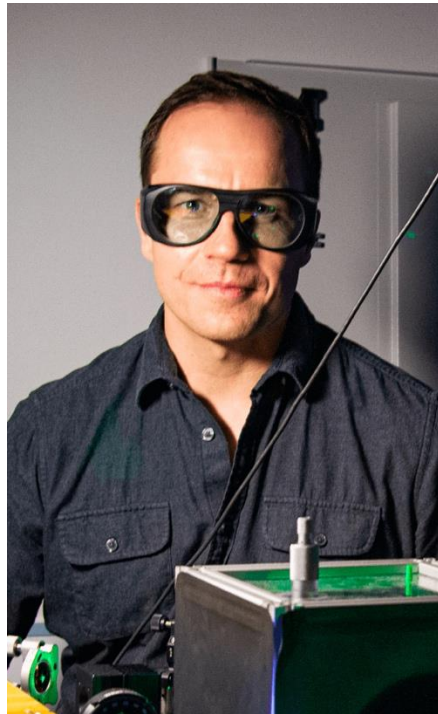
WP	Tasks / Months	3	6	9	12	15	18	21	24
1	Synthesis inorganic nanorattles	M1							
1	Characterization of SERS performances	M2							
2	SERS detection from the liquid phase			M3					
3	SERS detection from the gas phase			M4					
4	SERS detection using portable equipment			M5					
4	Prototype for infield detection							M6	

OUR TEAM



**Pedro Camargo, P.I.
(PC), UH**

Nanomaterials,
plasmonics, and SERS



**Markku Vainio
(MV), UH**

Molecular
Spectroscopy



**Hanna Hakulinen
(HH), VERIFIN**

Warfare agents
and analytical chemistry



**Matti Kuula
(MK), VERIFIN**

Portable Raman
applications



**Flavia da Silva
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Nanomaterials
and SERS