Investigation of beta-Amyloid-(1-42)-DMPC lipid-protein system in Alzheimer diseased cells by Raman Spectroscopy and Molecular Dynamics

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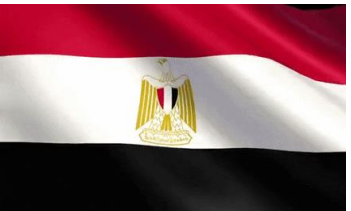
Conducted at: Department of Raman spectroscopy, FLNP, Joint Institute for Nuclear Research, Dubna, Moscow Region, Russia



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Outlines

Introduction

- ✓ Our project.
- ✓ Raman Spectroscopy &technicalities in Raman’s.
- ✓ Molecular dynamics &technicalities in MD.

Milestones in our work

Phase one

- ✓ P-L System prep-protocol.

Phase two

- ✓ Spectroscopic analysis.

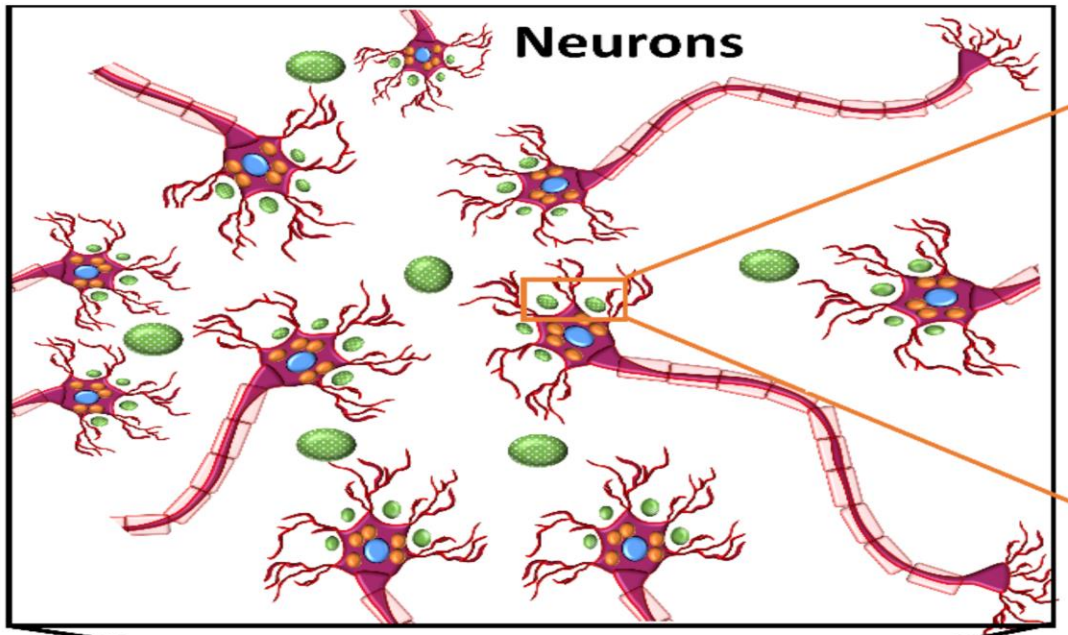
Phase three

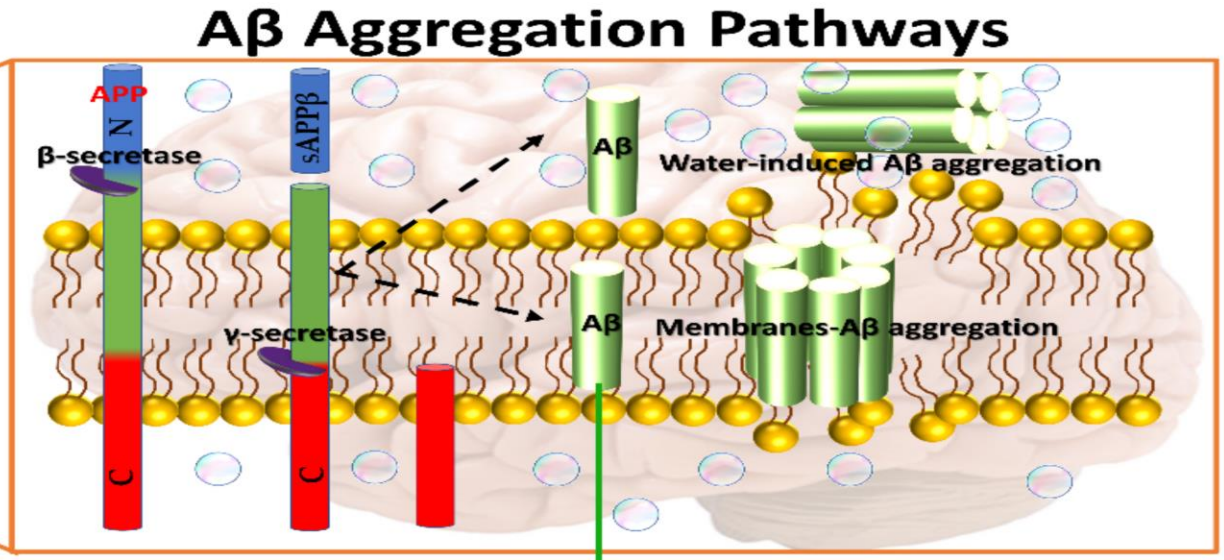
- ✓ P-L System MDS Investigation.
- ✓ Our work-flow in MDS.
- ✓ MDS production analysis.

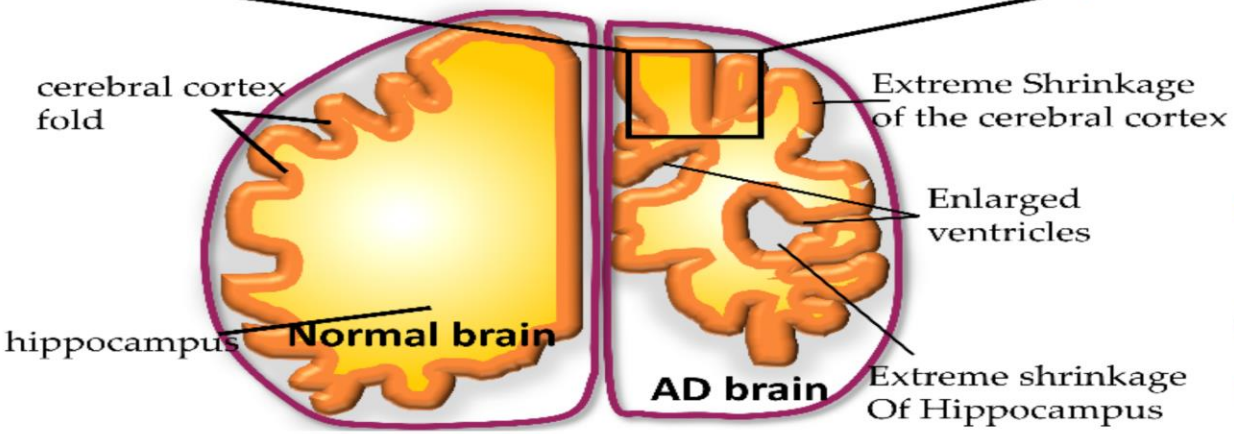
Project Team Acknowledgement

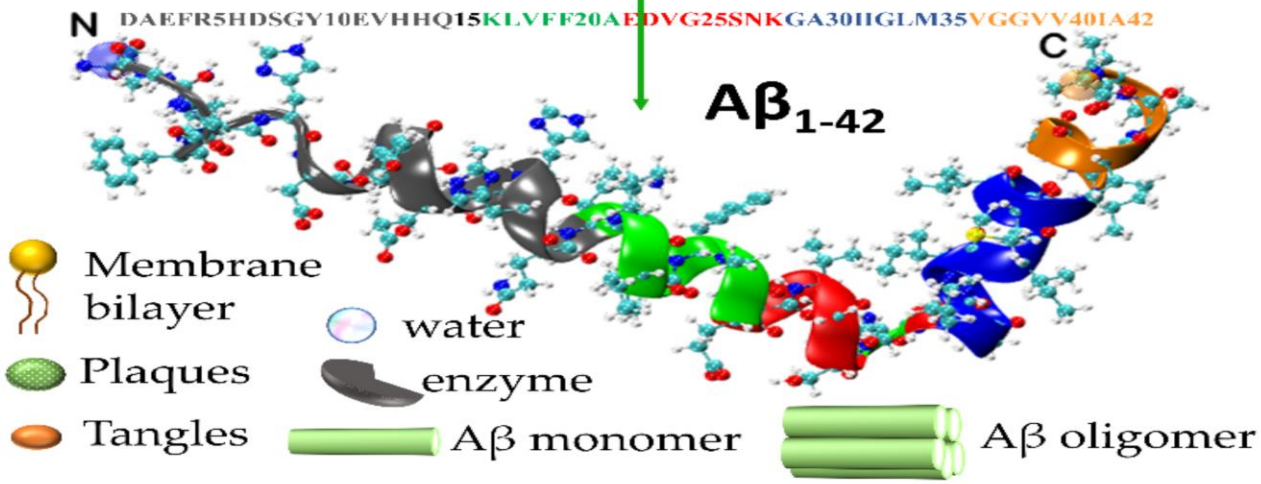
The Grand Scheme of Our Project

Beta-amyloid 1-42 → Neurons accumulations → peptide aggregation in the bilayer membrane → Alzheimer





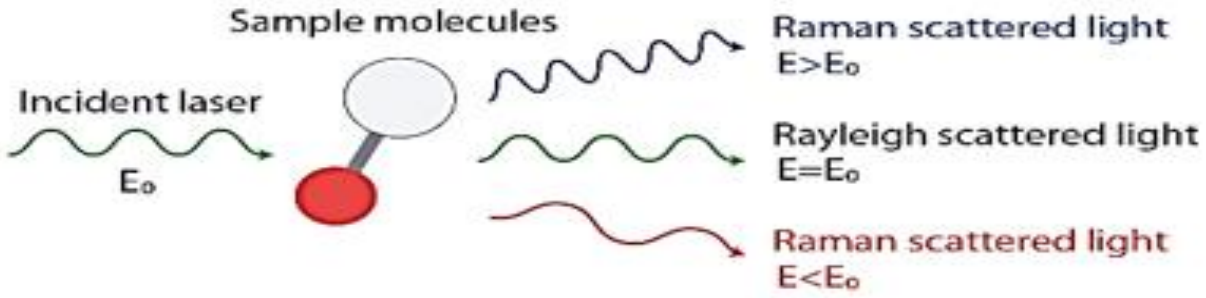




https://doi.org/10.3390/ijms221910798

The Raman effect

Phenomenon in physics and spectroscopy where light interacts with matter, causing a shift in its energy level and resulting in the scattering of light with different wavelengths.



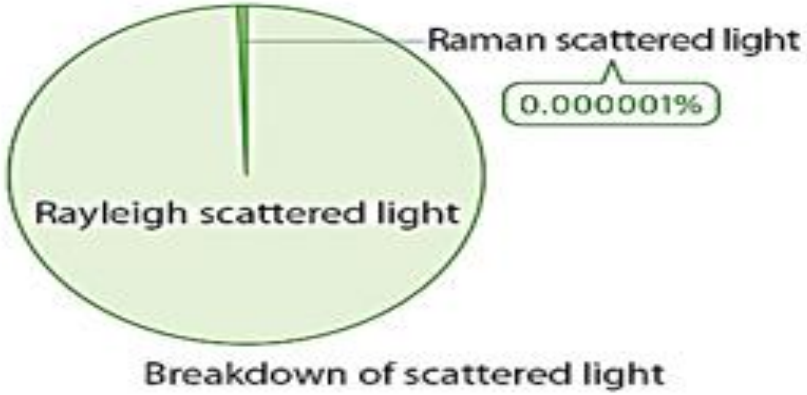
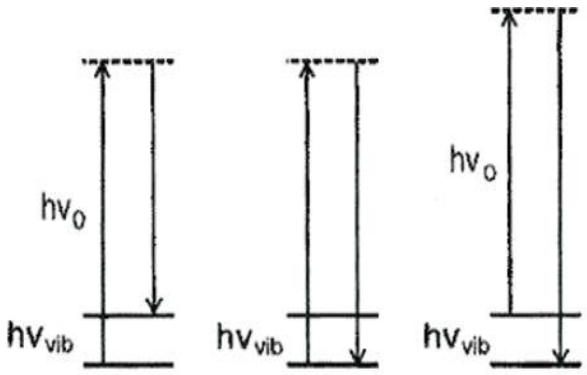
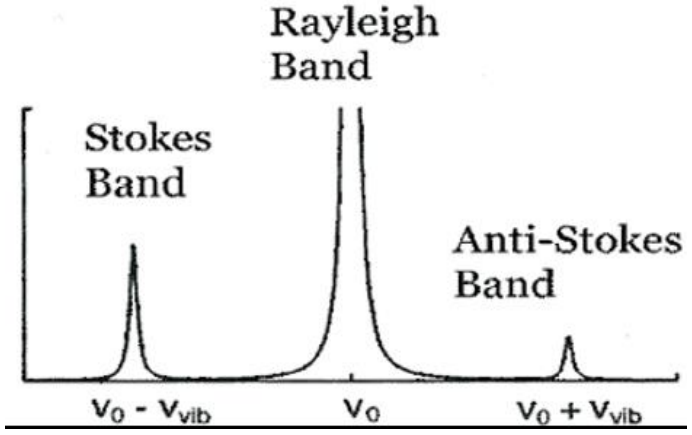


Diagram of the Rayleigh and Raman Scattering Processes



E0<Ev **&**E0=Ev **&**E0>Ev



E0<Ev **&**E0=Ev **&**E0>Ev

Raman spectra

Into Raman spectra:

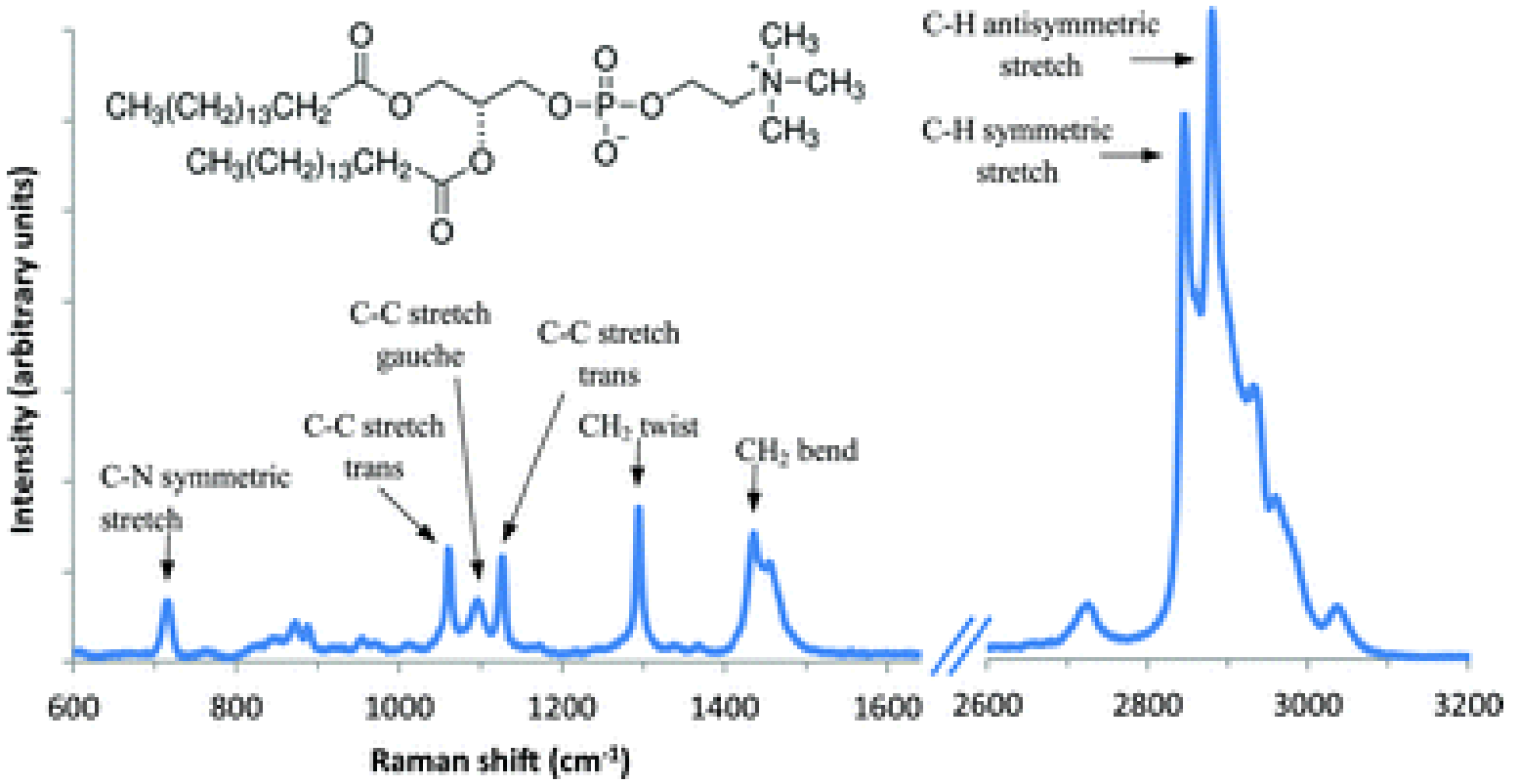
- ✓ Raman Shift:
- ✓ Vibrational Frequencies:
- ✓ Peak Intensity
- ✓ Bonds Between Atoms and Material Fingerprint

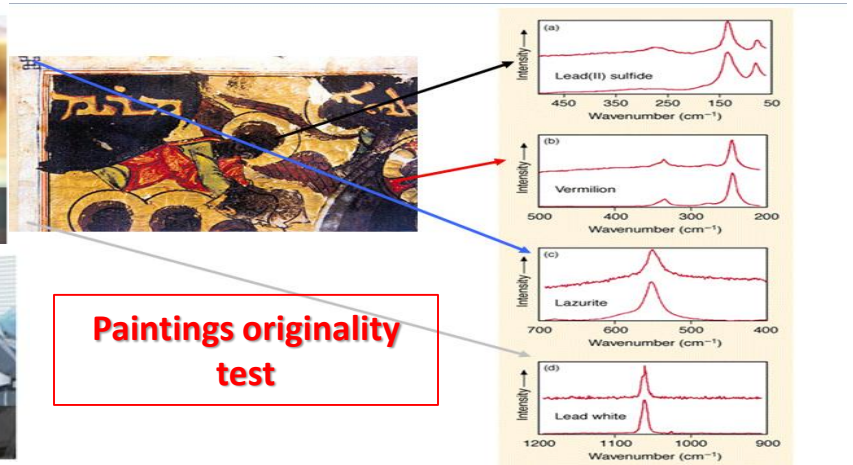
Raman spectra gives:

- ✓ Information about the molecular composition structure, and dynamics of materials
- ✓ Study solid, liquid and gaseous samples
- ✓ Fingerprint spectroscopy

Applications:

- ✓ Chemical analysis
- ✓ Material characterization
- ✓ Biomedical diagnostic
- ✓ Imaging: pharmaceutics, forensics, art, etc

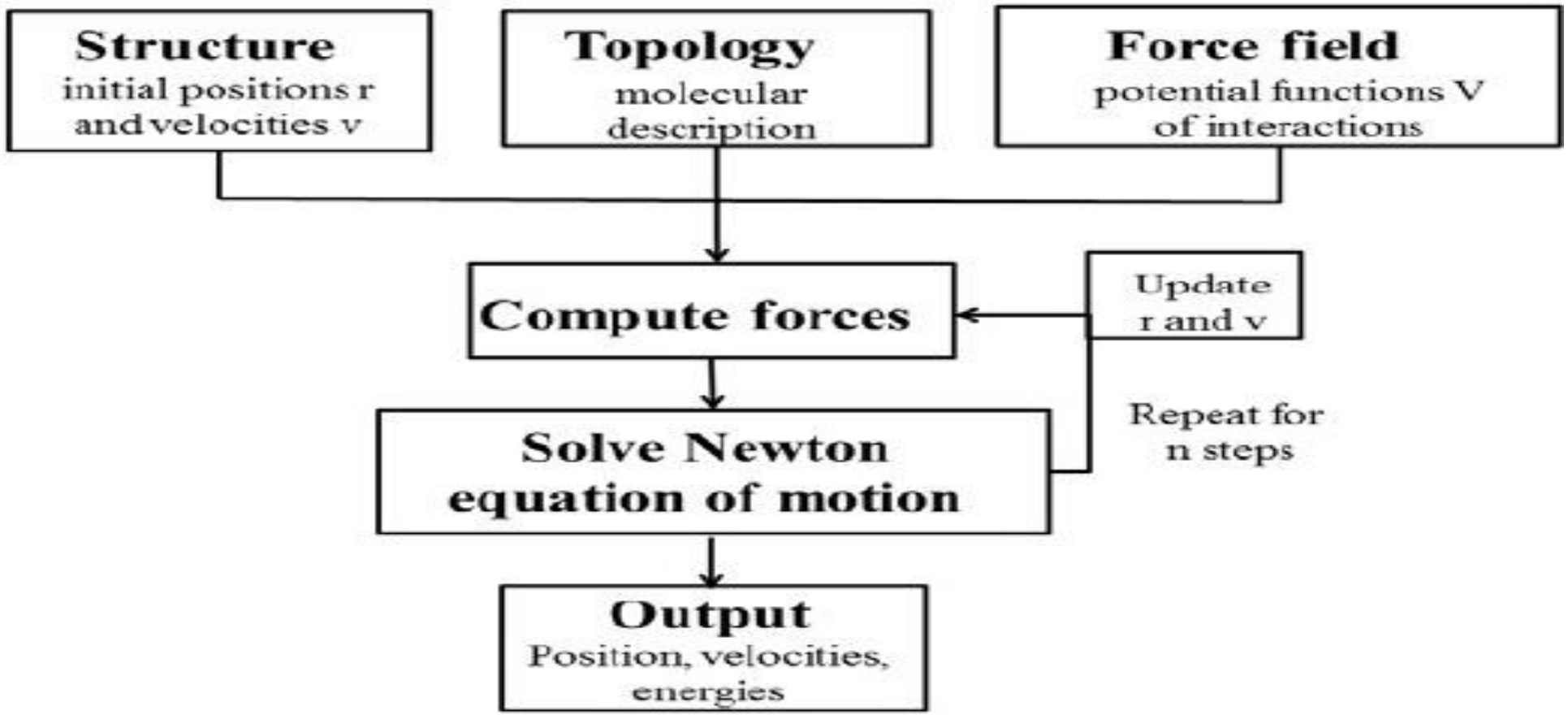




Paintings originality test

Molecular dynamics (MD)

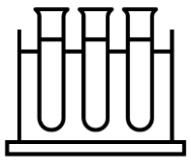
Molecular dynamics is a computational simulation technique used to study the motion and behavior of atoms and molecules over time. It involves solving the equations of motion for each particle in a system to investigate their positions, velocities, and interactions, providing insights into the dynamic properties and processes of molecular systems at the atomic level



For our Protein-Lipid complex: **MD will predict how every atom in a protein or p-L molecular system will move over time.**

Sonavane, Yogesh & Paajanen, Antti & Ketoja, Jukka & Paavilainen, Sami & Maloney, Thaddeus. (2014). Molecular dynamics simulation of functionalized nanofibrillar cellulose.

P-L System prep-protocol .



Lipids Preparation

Powder DMPC and dissolve it in Chloroform ($CHCL_3$)

Dissolved DMPC into the vial

Dry under argon

Dry under a vacuum for a few hours.

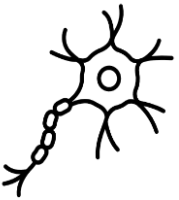
Get a final dried lipid film.

Aβ Preparation

Peptide dissolved in DMSO

Put on a vortex

Add buffer to a certain volume



Aβ precipitate at the bottom of the Eppendorf

Aβ-Lipids Complex Preparation

Aβ added to liposomes

Sample introduction to ultrasonic bath

P-L complex Purification from DMSO

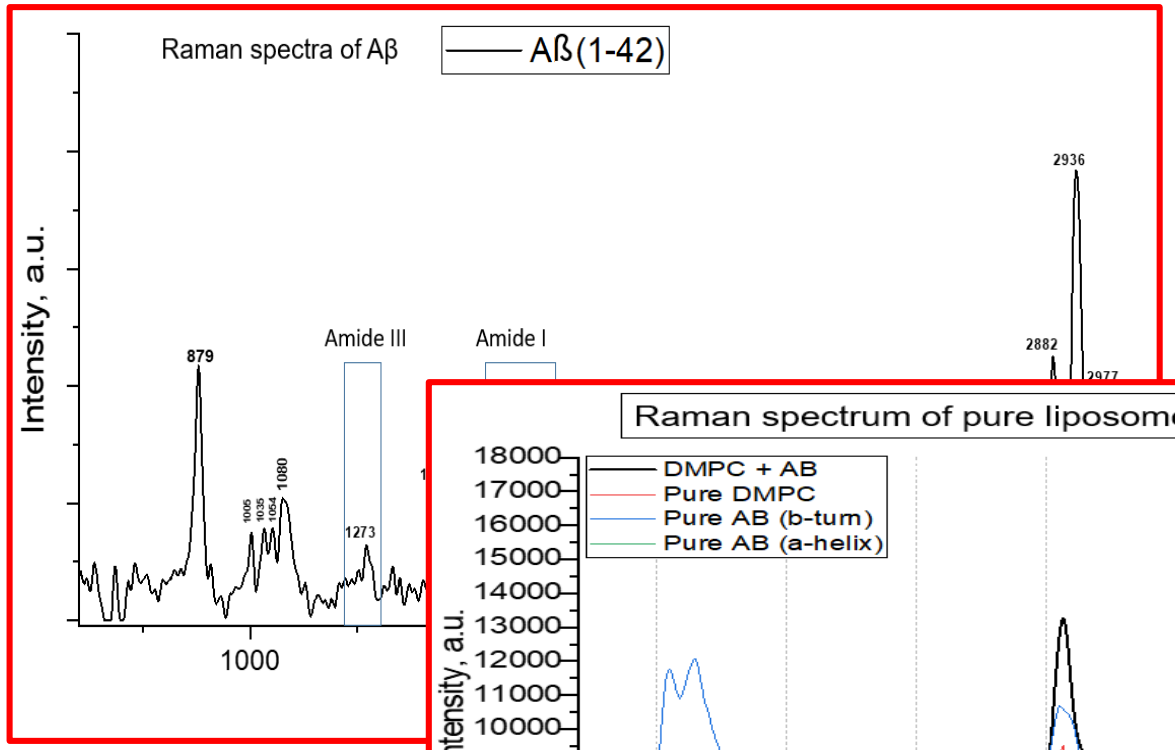
Complex centrifuge to settles to the bottom of Eppendorf

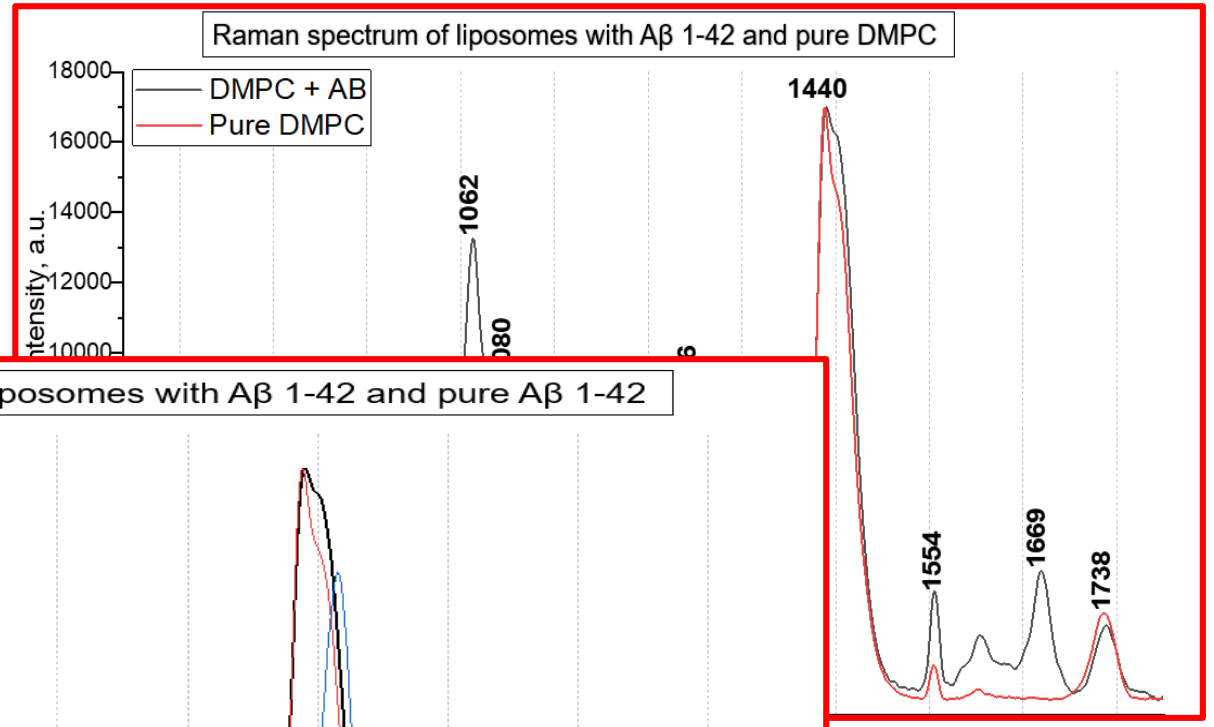
DMSO is pumped off

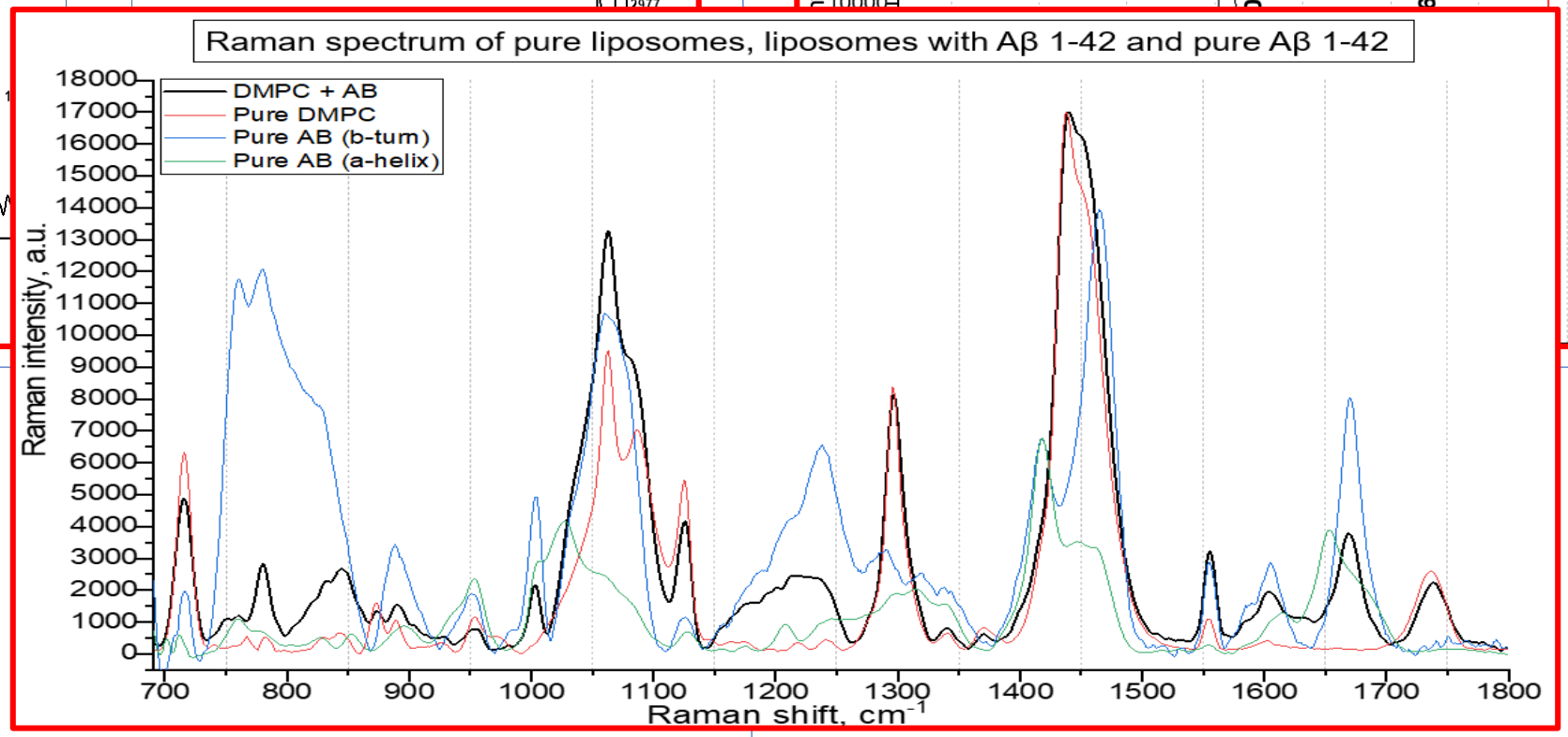
Ultrasonic stirring bath

P-L complex is Left to stabilize

Spectroscopic analysis Results

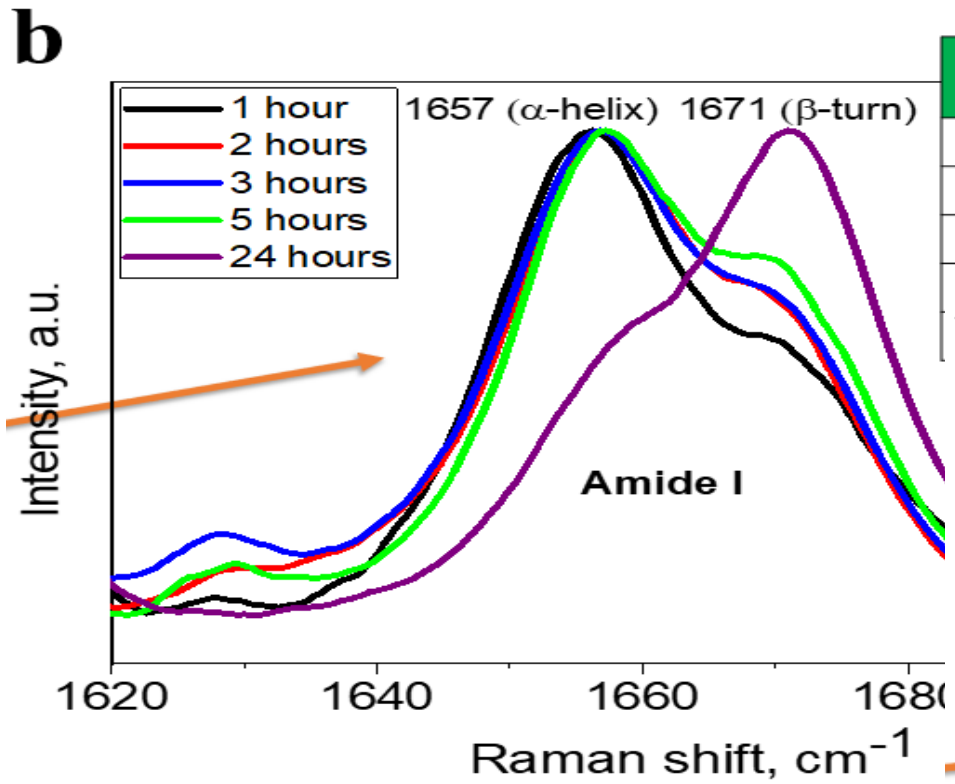




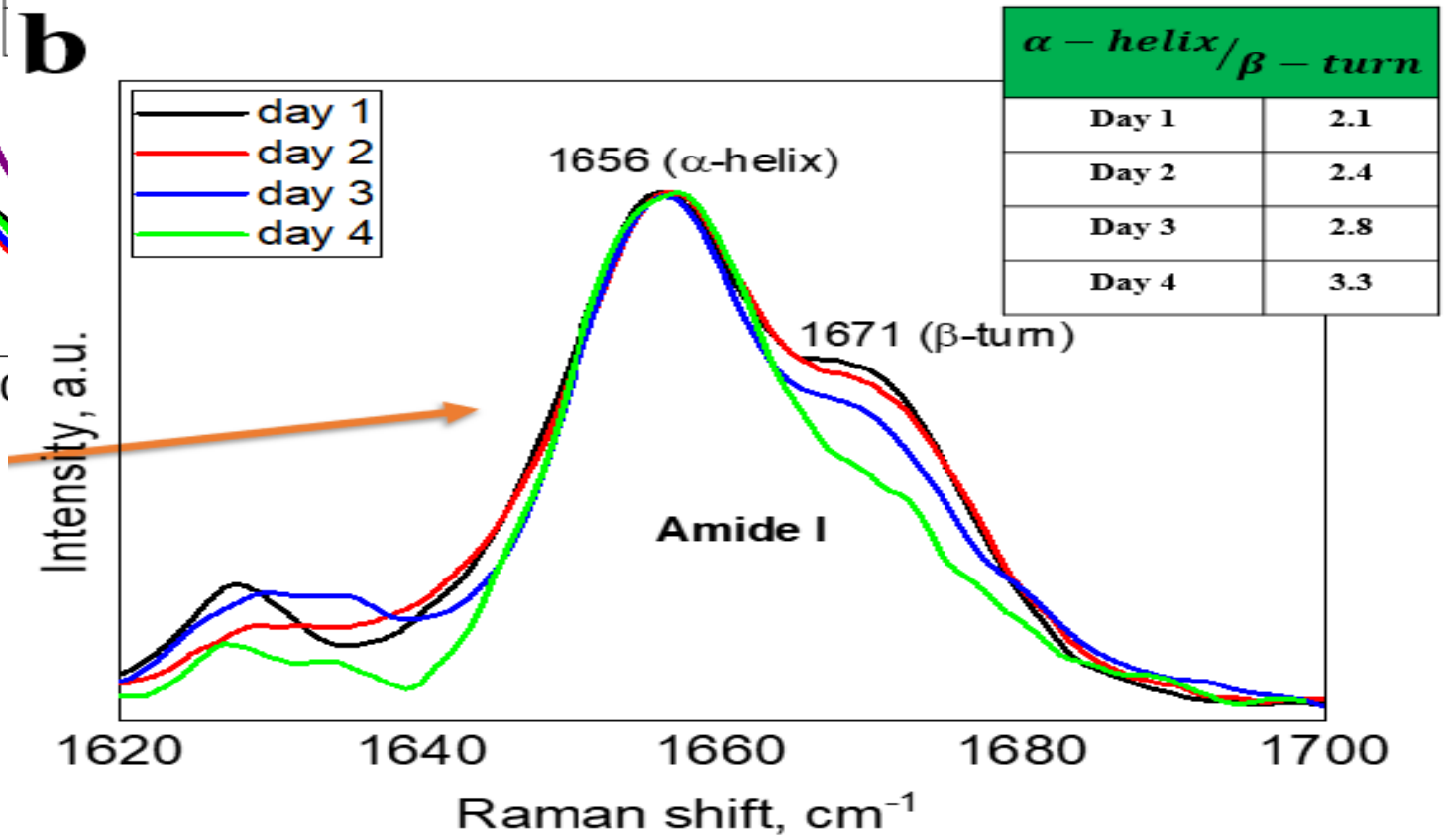


Artyom Shutikov, Ekaterina Demina, Yersultan Arynbek, Darya Zakrytnaya,Kahramon Mamatkulov1 and Grigory Arzumanyan. Department of Raman spectroscopy, FLNP, Joint Institute for Nuclear Research, Dubna, Moscow Region, Russia.

Spectroscopic analysis Results



$\alpha - helix/\beta - turn$	
1 hours	2.6
2 hours	2.3
3 hours	2.2
5 hours	1.6



$\alpha - helix/\beta - turn$	
Day 1	2.1
Day 2	2.4
Day 3	2.8
Day 4	3.3

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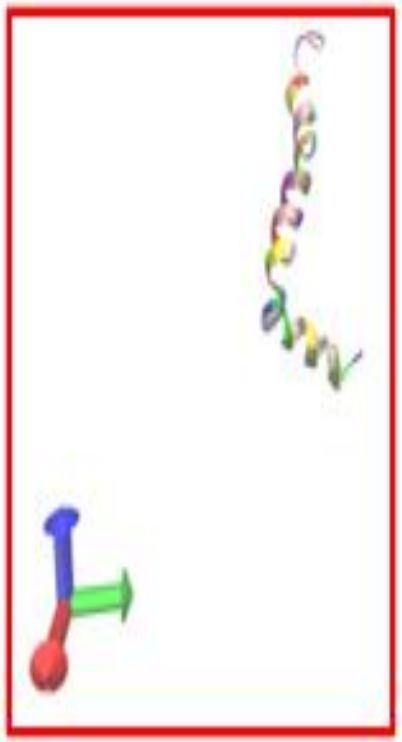
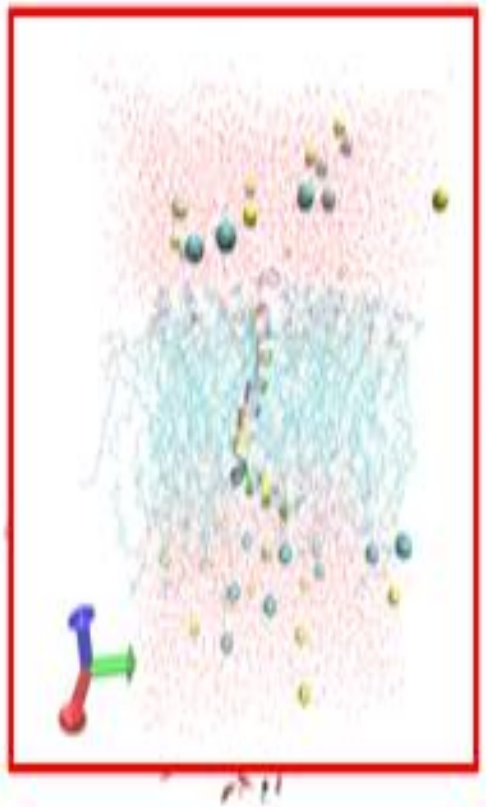
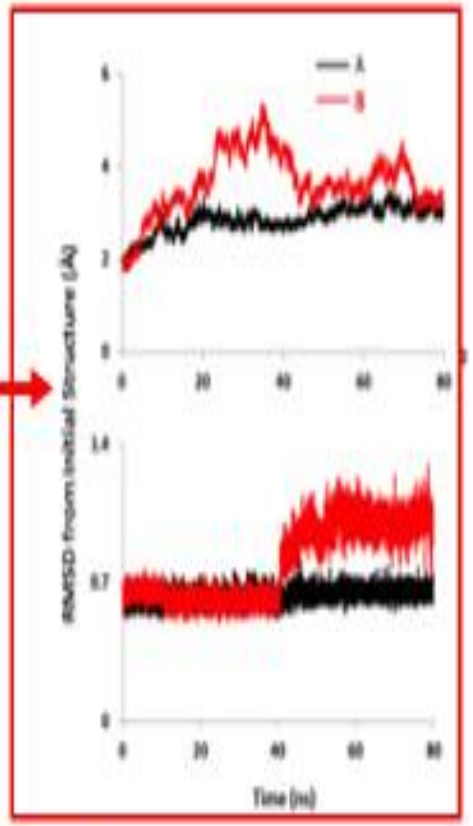
MD Workflow







1.Starting Structure

Structure Check
Protonation State
Solvation
Adding Salts

2.Preparation of the Simulation System

Select Simulation Protocol

3. Simulation Run

Post-processing

4. Trajectory Analysis

MD analysis Results

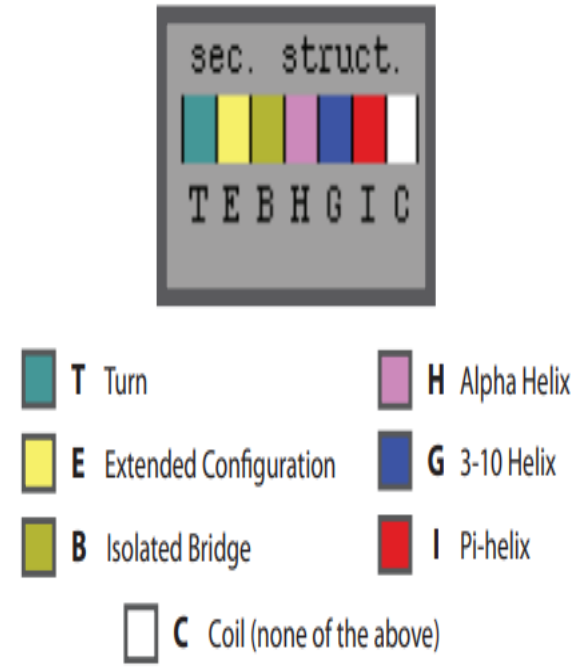
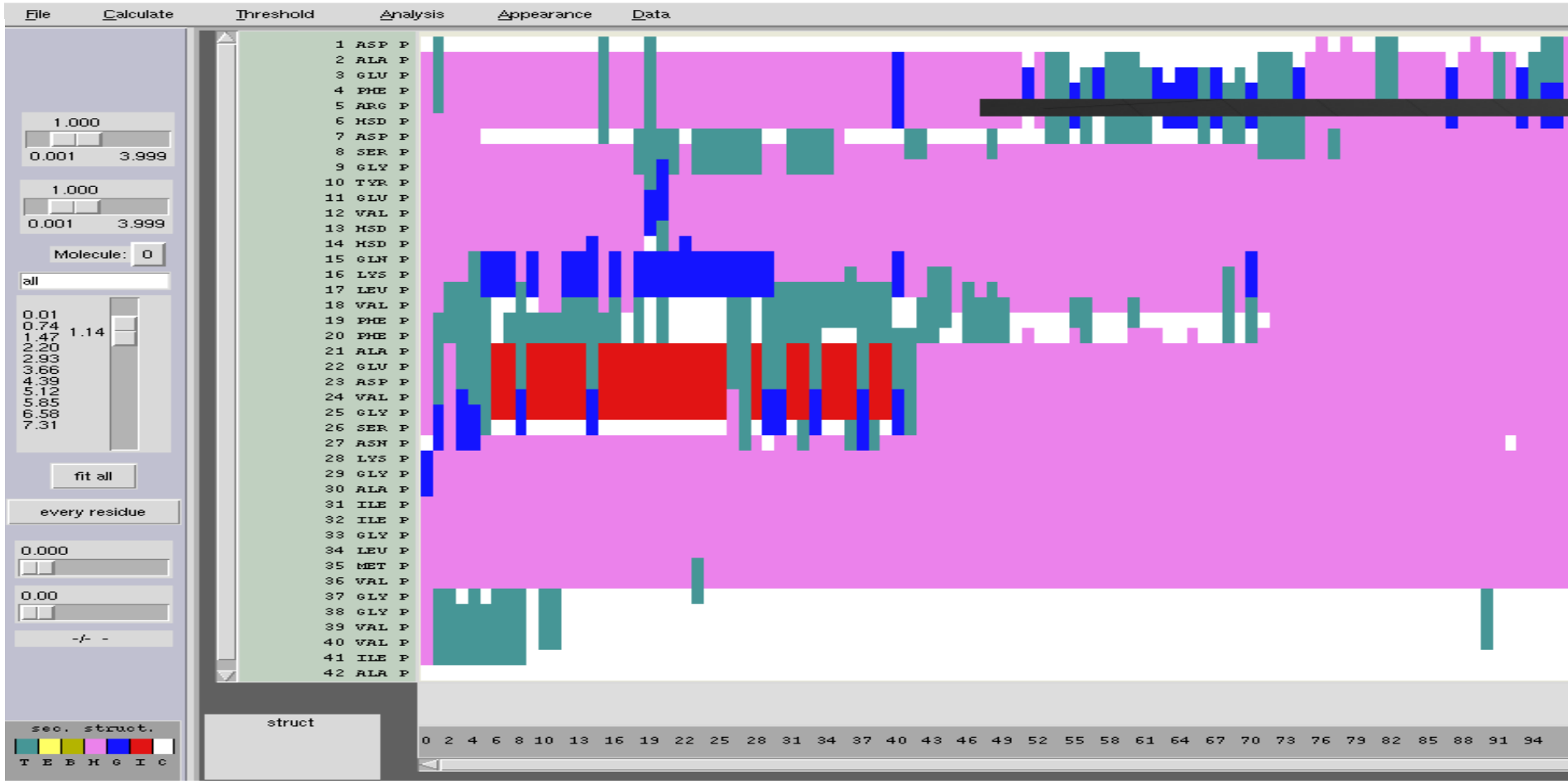


Figure 9: Color key for secondary structure plots.



Secondary structure analysis of peptide(1iyt) in liposome(lipid bilayer) during the 100ns.

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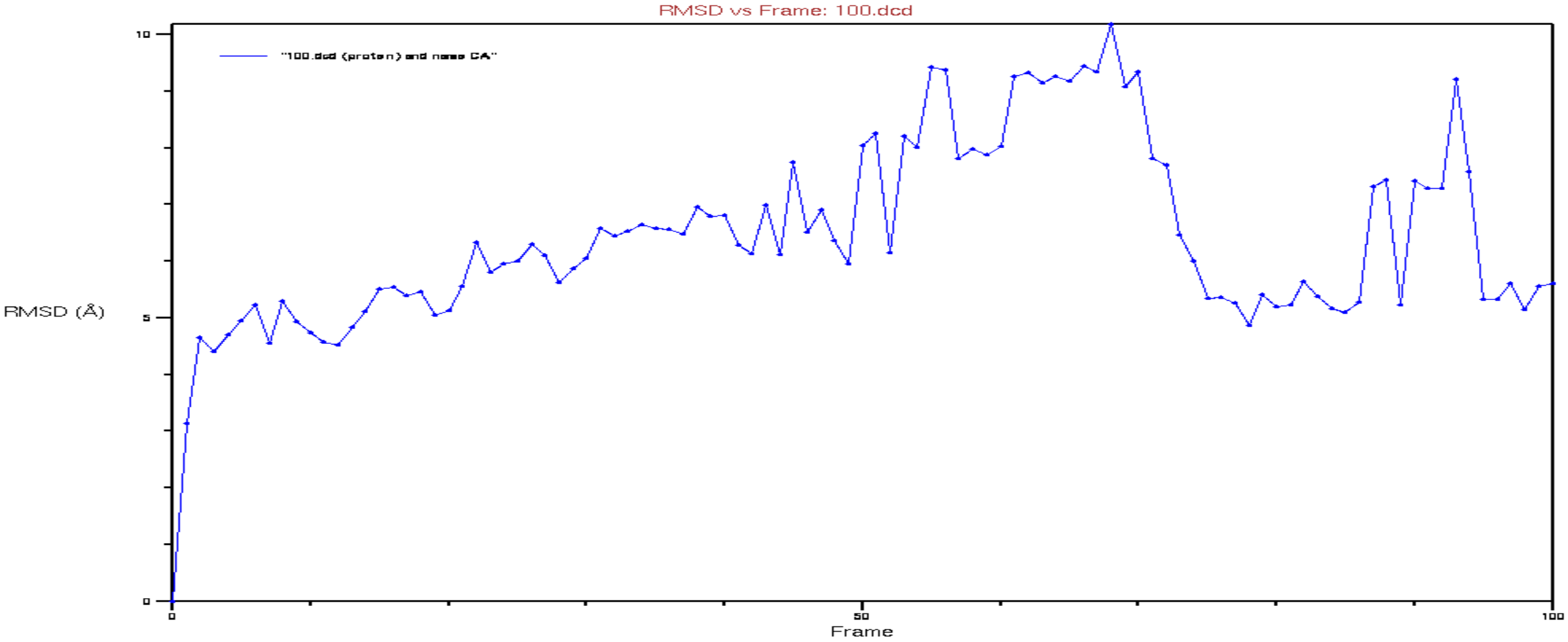
RMSD calculated by VMD



RMSD calculated by VMD

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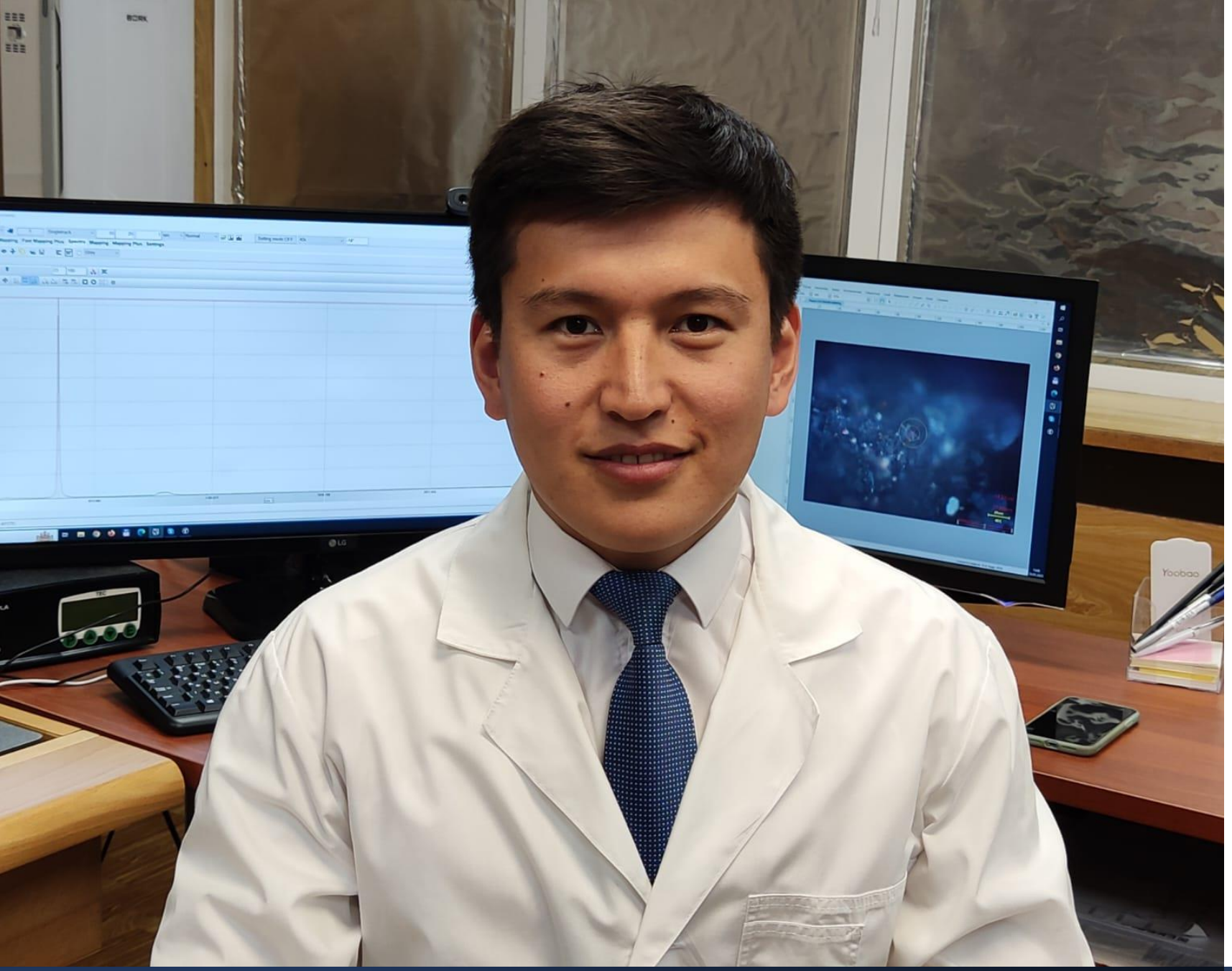

Yersultan Arynbek

Super-Supervision

- ✓ Showed Professionalism
- ✓ Helped through molecular dynamics
- ✓ Showed patience
- ✓ Metaphorically illustrated and represented every single concept with academic and scientific integrity.
- ✓ Committed to be present every single day.
- ✓ Taught me so many in Molecular dynamics
- ✓ Sacrificed his lunchbreaks to keep working and searching for solutions when any error first appeared .

Thank you! Raman Spectroscopy Department

Prof. ArZumanyan & Darya & Artyom & Kahramon

Thank you! Erina!

Thank you!