MOLECULAR DYNAMICS SIMULATION OF THE INTERACTION BETWEEN CHOLATES AND CHOLESTEROL

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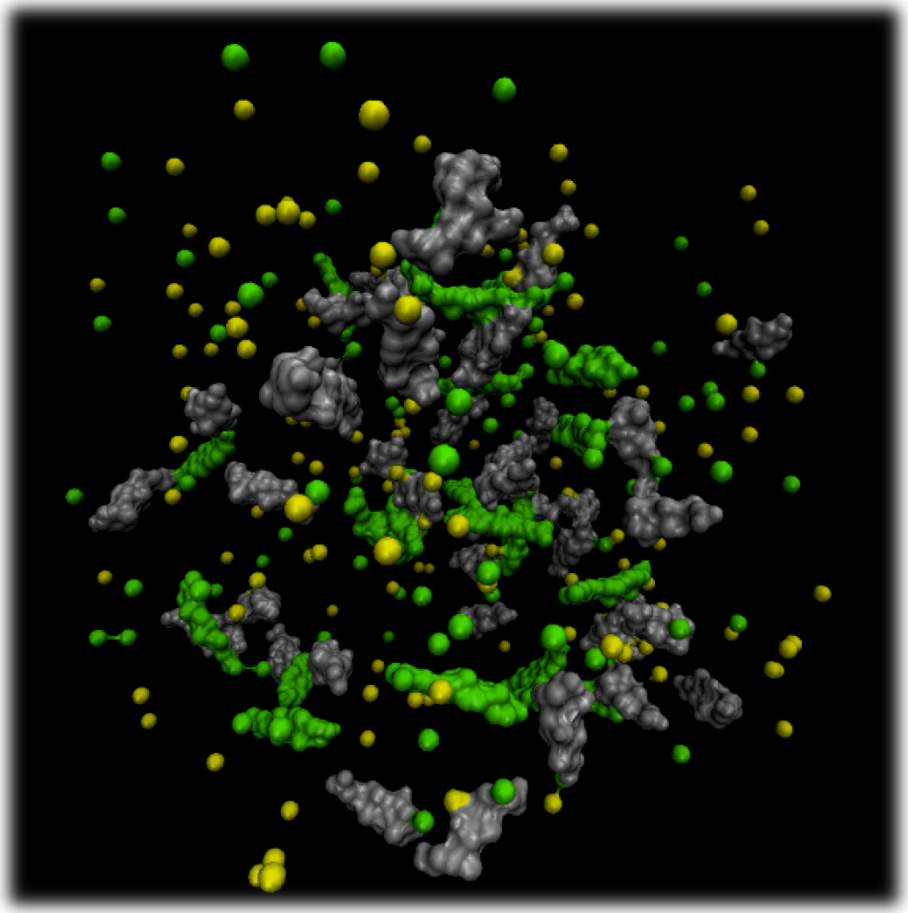
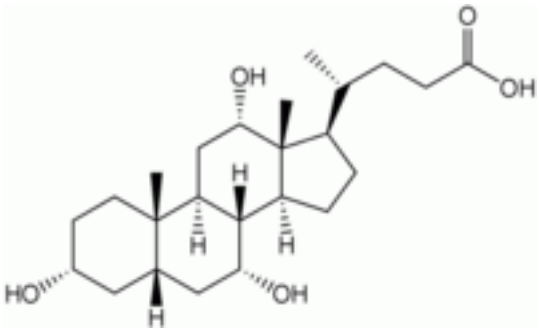
Background

- Molecular Dynamics
  - computer simulation technique
- Cholates
  - play an important role as solubilizers of cholesterol and fat-soluble vitamins

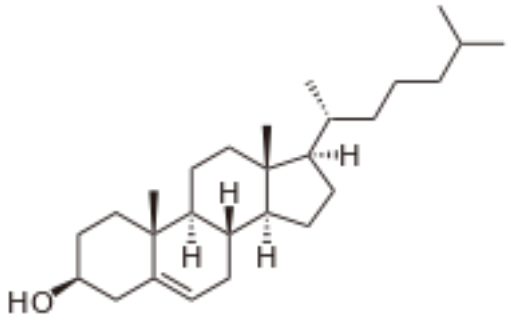


Structures

- Cholate



- Cholesterol



Purpose

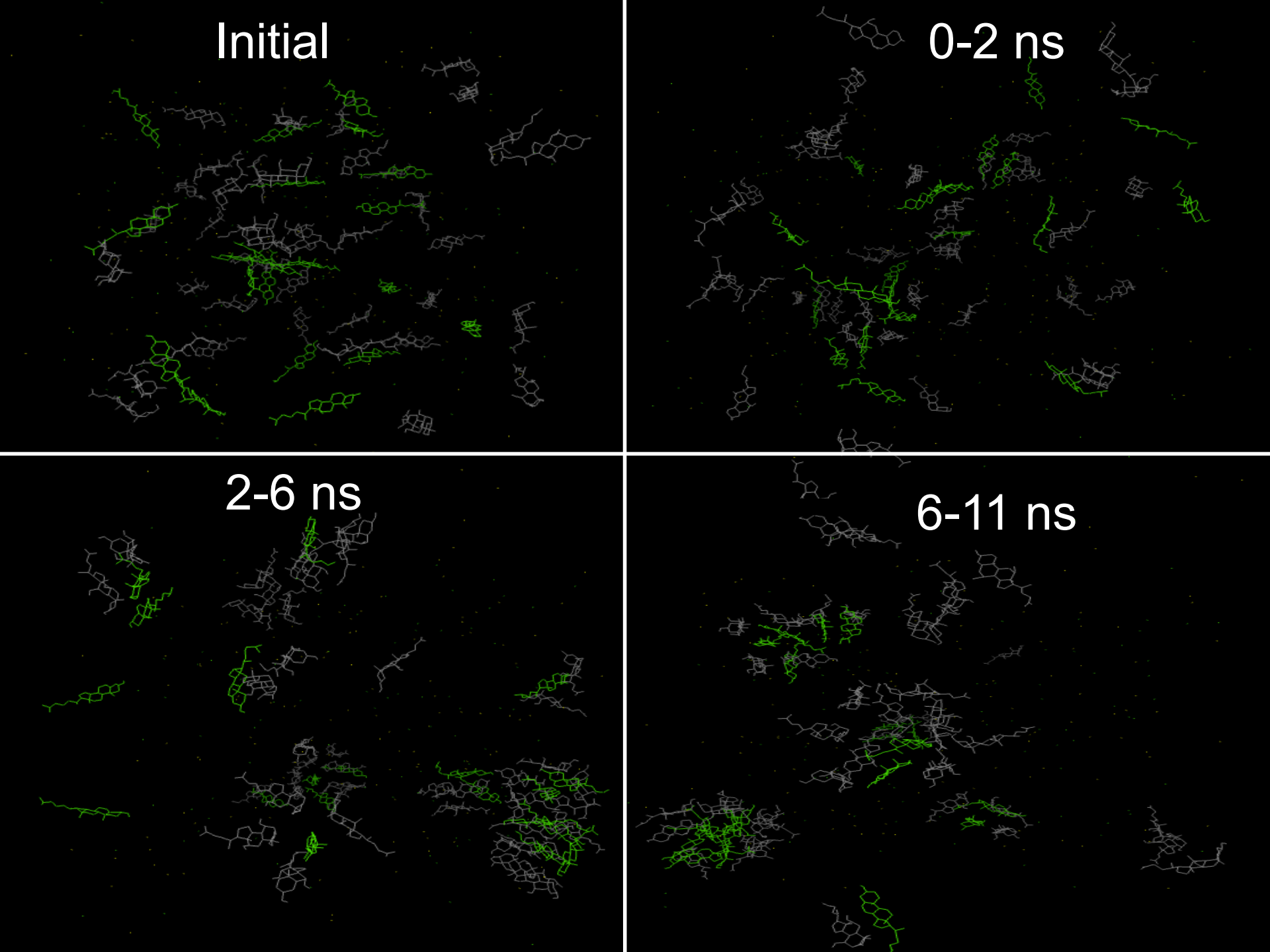
- Learn how to set up and run a MD simulation
- Analyze data using visual software

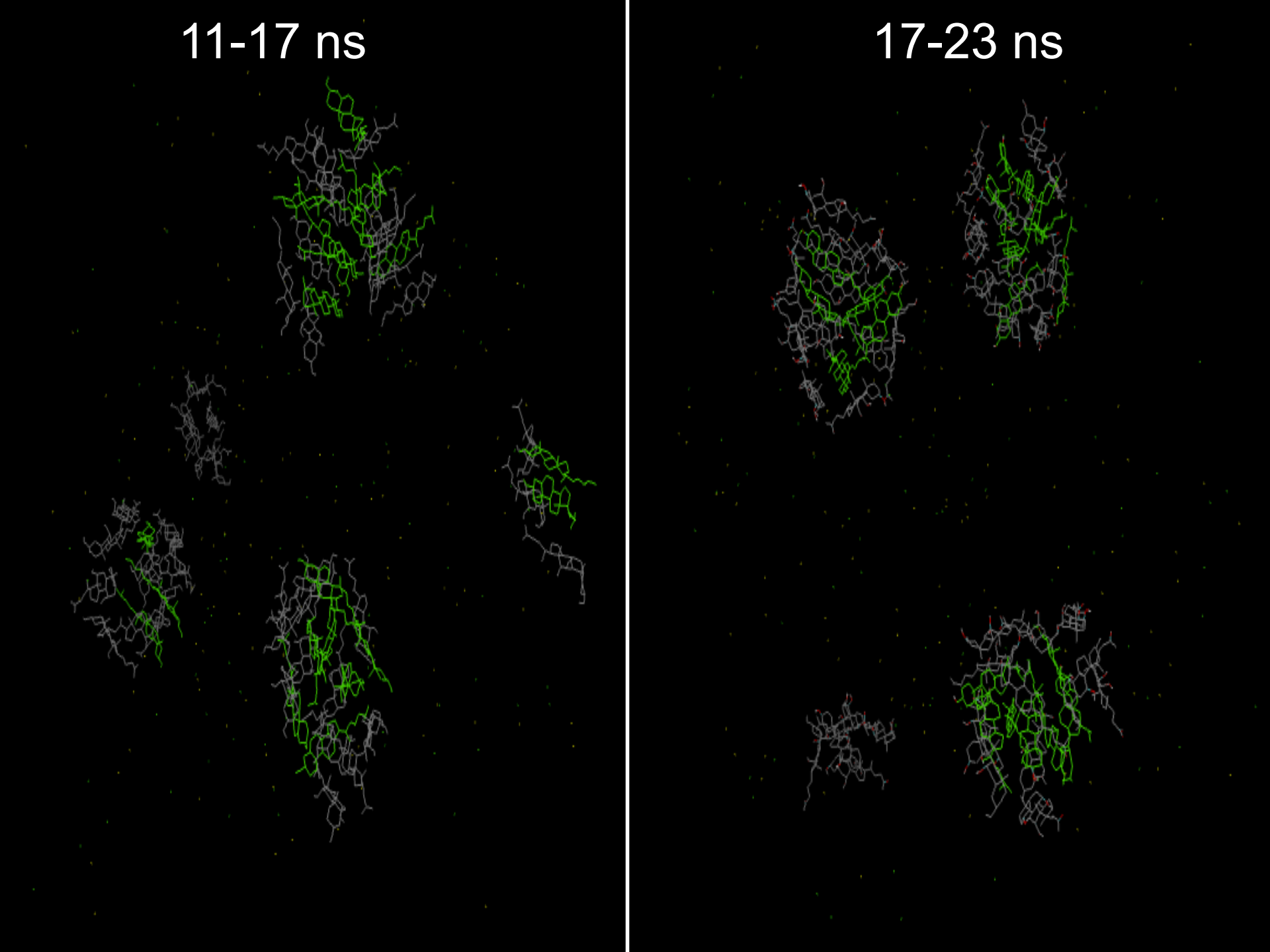
Motivation

- How many cholates aggregate together?
- How many cholesterol molecules are encapsulated?
- Shape of micelle

System Methodology

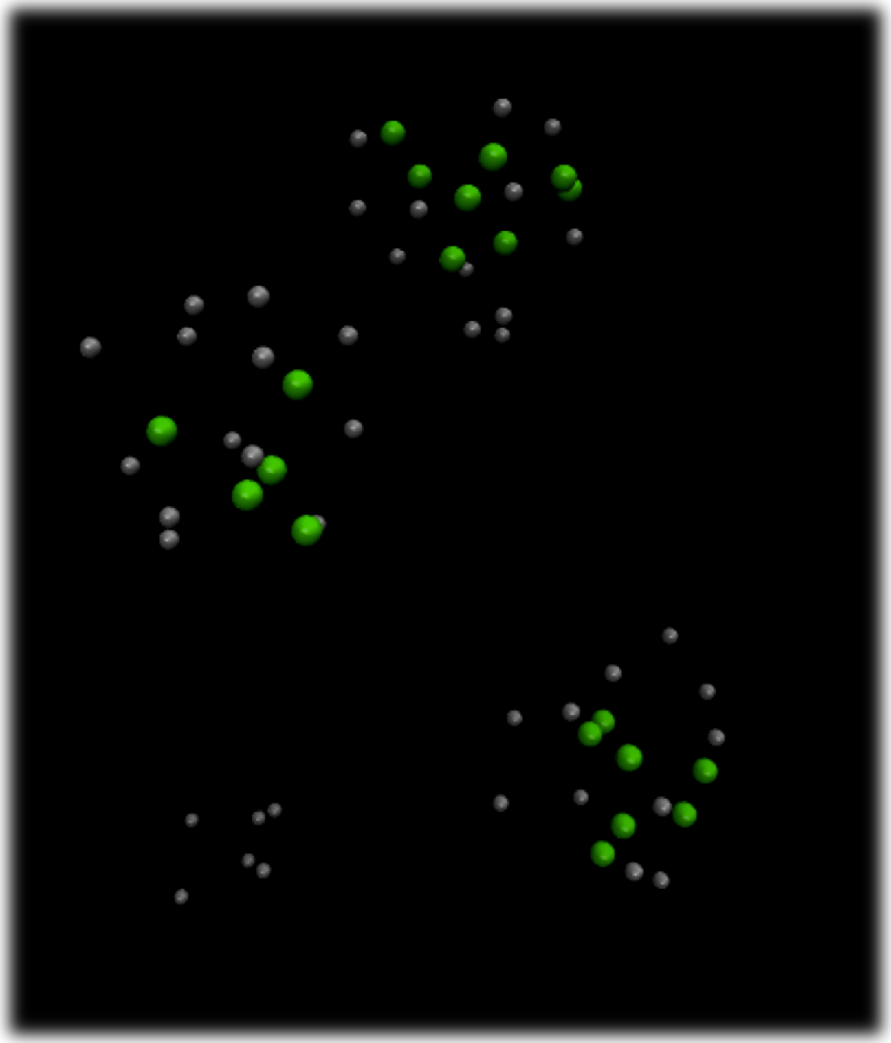
- Gather structures
  - Cholesterol (20), cholates (42), ions (226), water (3200)
- Set up system to be simulated
  - Packmol
- Energy minimization/Equilibration
  - GROMACS
- Run simulation
  - Queen Bee
- Analyze data
  - VMD, Grace

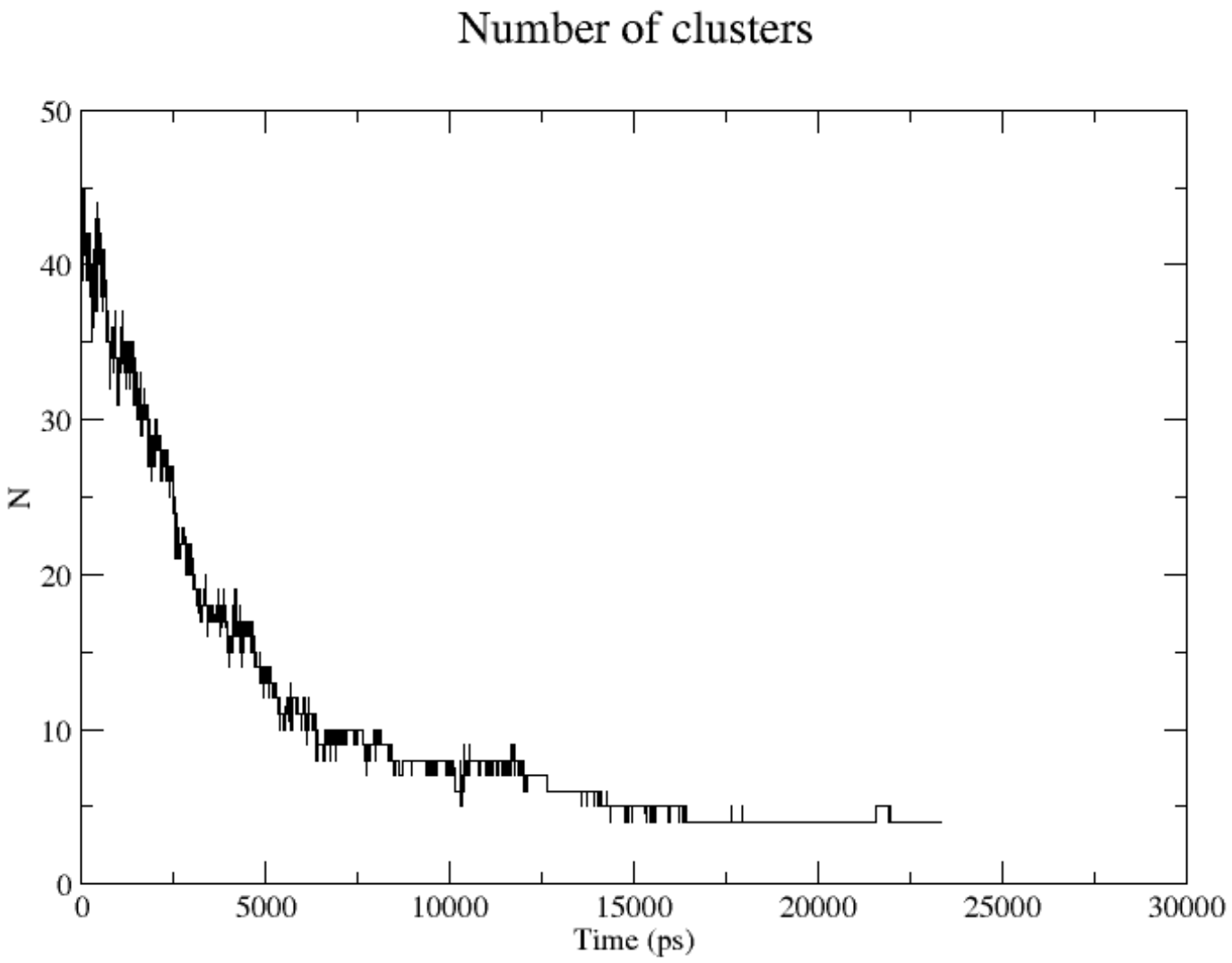

Initial
0-2 ns
2-6 ns
6-11 ns


11-17 ns
17-23 ns

Analysis

- Four micelles of cholates
  - 6,11,12,13
- Cholesterol
  - 5, 7, 8
- Spherical




Number of clusters
N
Time (ps)
0
10
20
30
40
50
0
5000
10000
15000
20000
25000
30000

Acknowledgements

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QUESTIONS?