Building your system

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Martinize
Insane
Backward
DAFT

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Martinize
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Vermouth/Martinize2

Polyply
TS2CG
Coby

…

Building your system

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Every simulation has a purpose

Every simulation has a start

starting structure

What to build?

- Resolution
- Organization
- Composition
- Components

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Atomistic dynamics?
Atomistic structure?

What to build?

- Resolution
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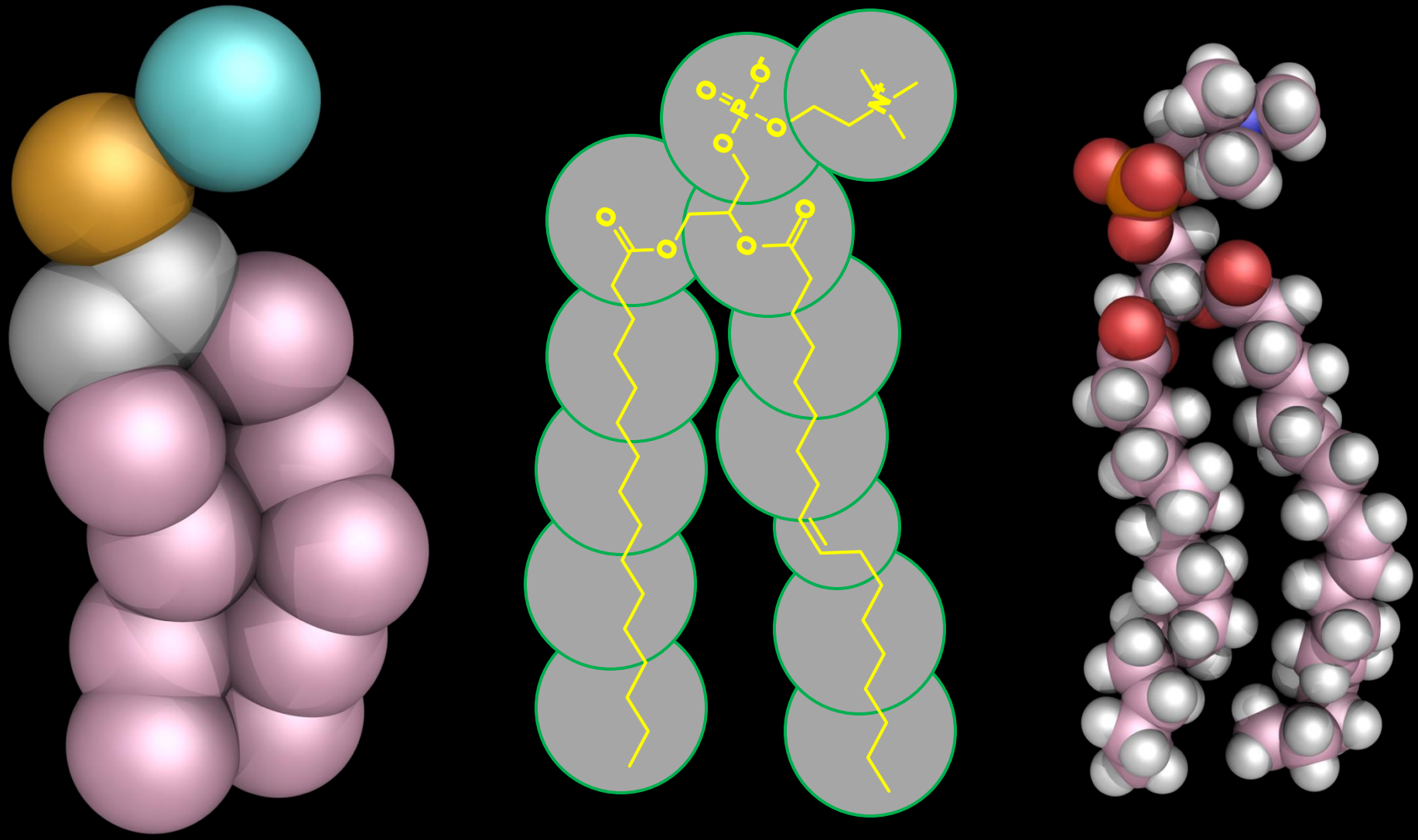
Atomistic dynamics?
Atomistic structure?

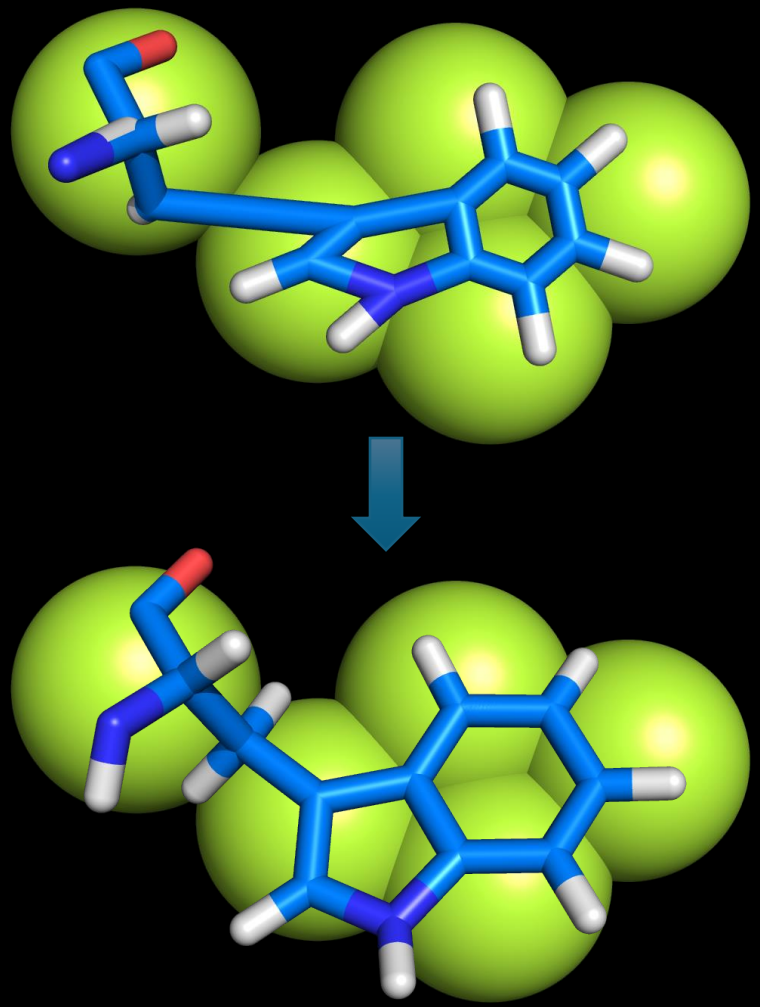
Coarse grain simulation
Backmapping

Backmapping



Backmapping

Tryptophan

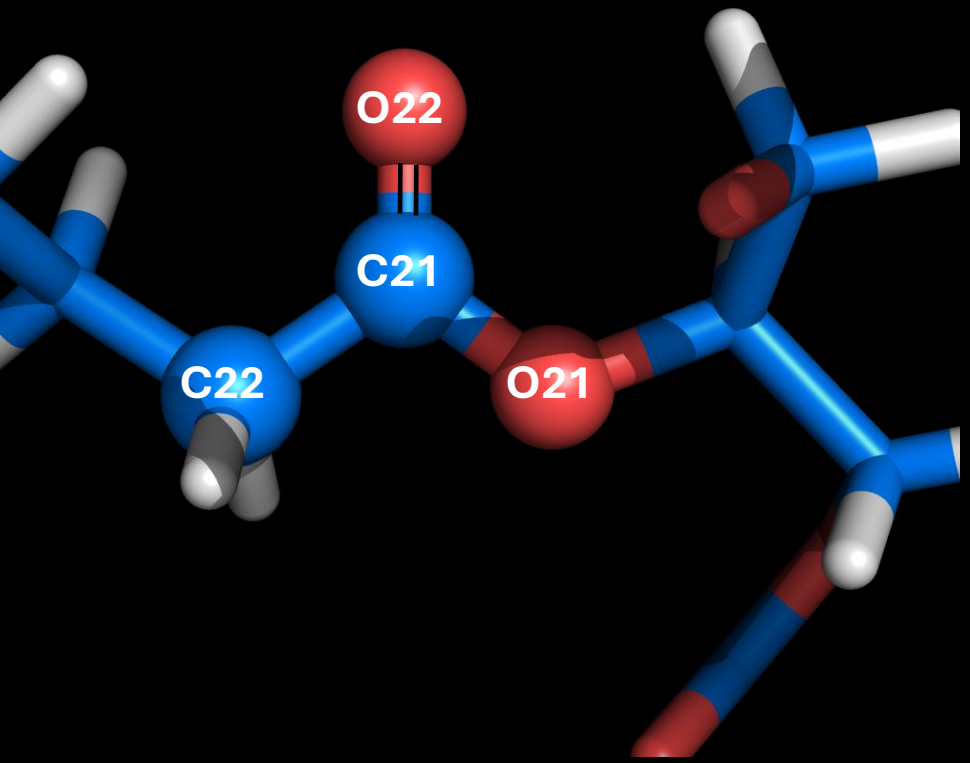


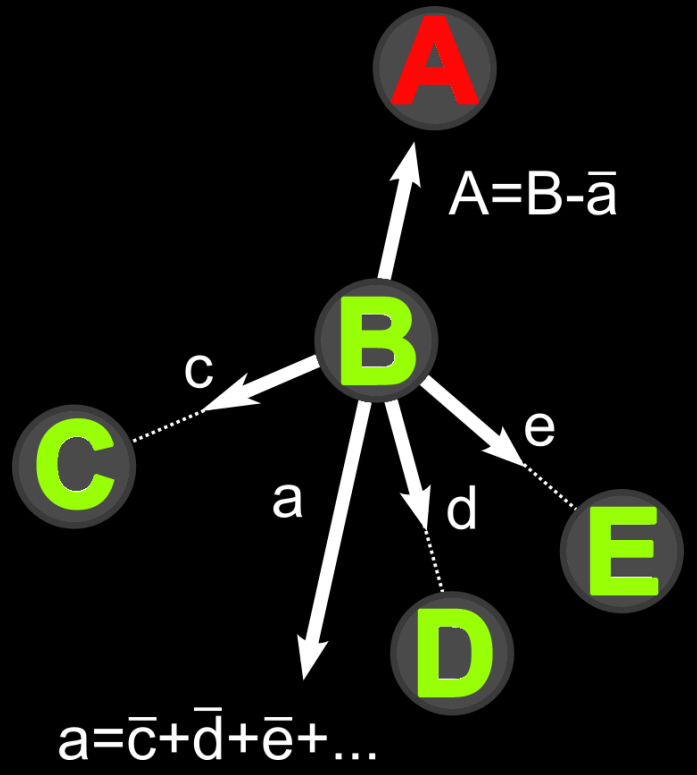
```
[ molecule ]
TRP

[ martini ]
BB SC1 SC2 SC3 SC4

[ mapping ]
charmm36

[ atoms ]
    1   N     BB
    2   HN    BB
    3   CA    BB
    4   HA    BB
    5   CB    SC1 BB
    6   HB1   SC1 BB
    7   HB2   SC1 BB
    8   CG    SC1 SC1 SC1 SC1 SC3 SC3
    9   CD1   SC1
   10   HD1   SC1
   11   NE1   SC2 SC1
   12   HE1   SC2
   13   CE2   SC2 SC2 SC3
   14   CD2   SC3 SC3 SC2
   15   CE3   SC3 SC3 SC4
   16   HE3   SC3
   17   CZ3   SC4 SC4 SC3
   18   HZ3   SC4
   19   CZ2   SC2 SC2 SC4
   20   HZ2   SC2
   21   CH2   SC4 SC4 SC2
   22   HH2   SC4
   23   C     BB
   24   O     BB
```

```
[ trans ]
CB   CG   CD2 CE2
HD1  CD1  NE1 CE2
HE1  NE1  CD1 CG
HE3  CE3  CD2 CE2
HZ2  CZ2  CE2 CD2
HZ3  CZ3  CE3 CD2
HH2  CH2  CZ3 CE3

[ chiral ]
CB   CA   N   C
HB1  CA   N   C
HB2  CA   N   C

[ chiral ]
HA   CA   N   CB   C
```

Backmapping

; ester group
[out]
O22 C21 O21 C22

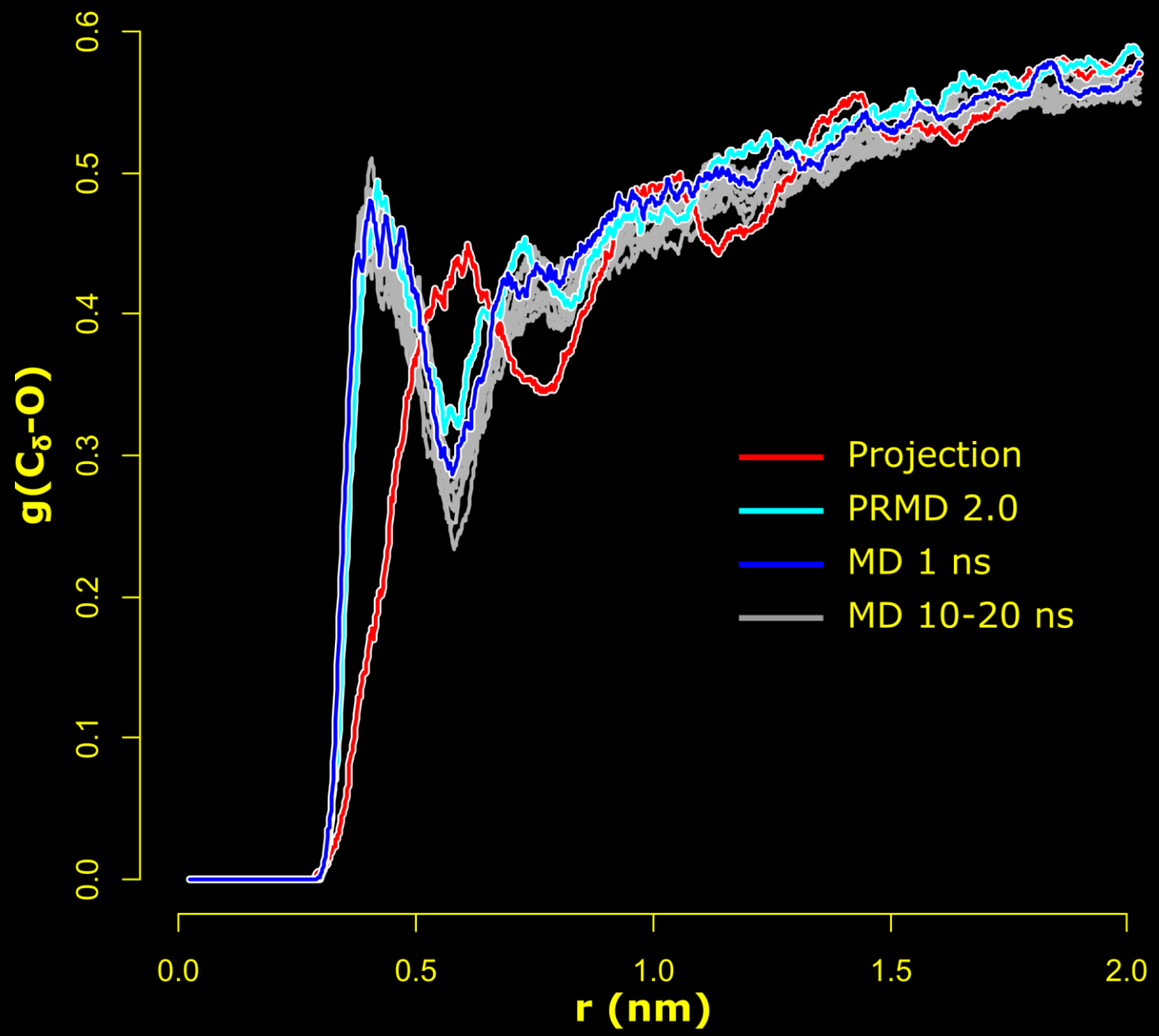




A, B, C, D, E atoms
a, b, c, d,e vectors
ā normalized vector

Backmapping

Solvent



What to build?

- Resolution
- Organization
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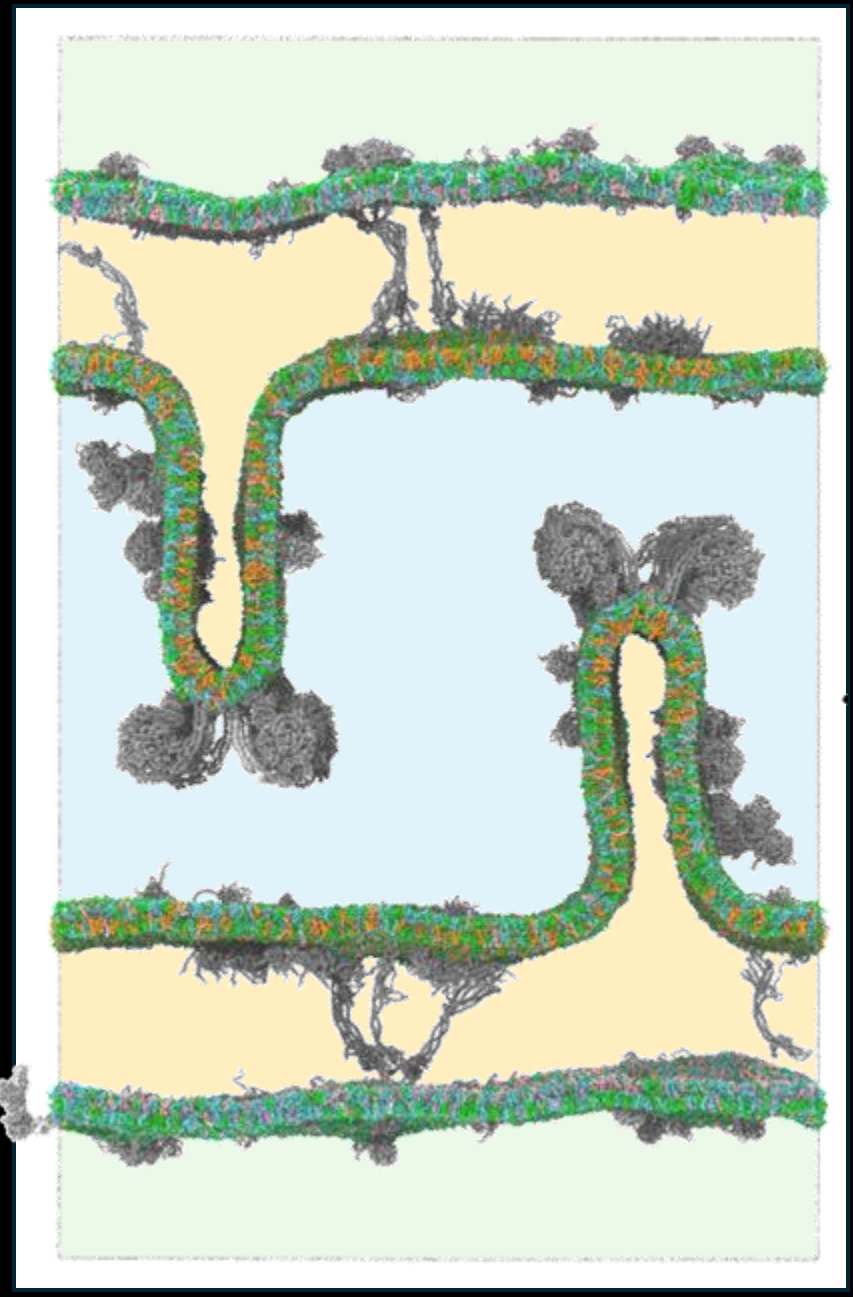
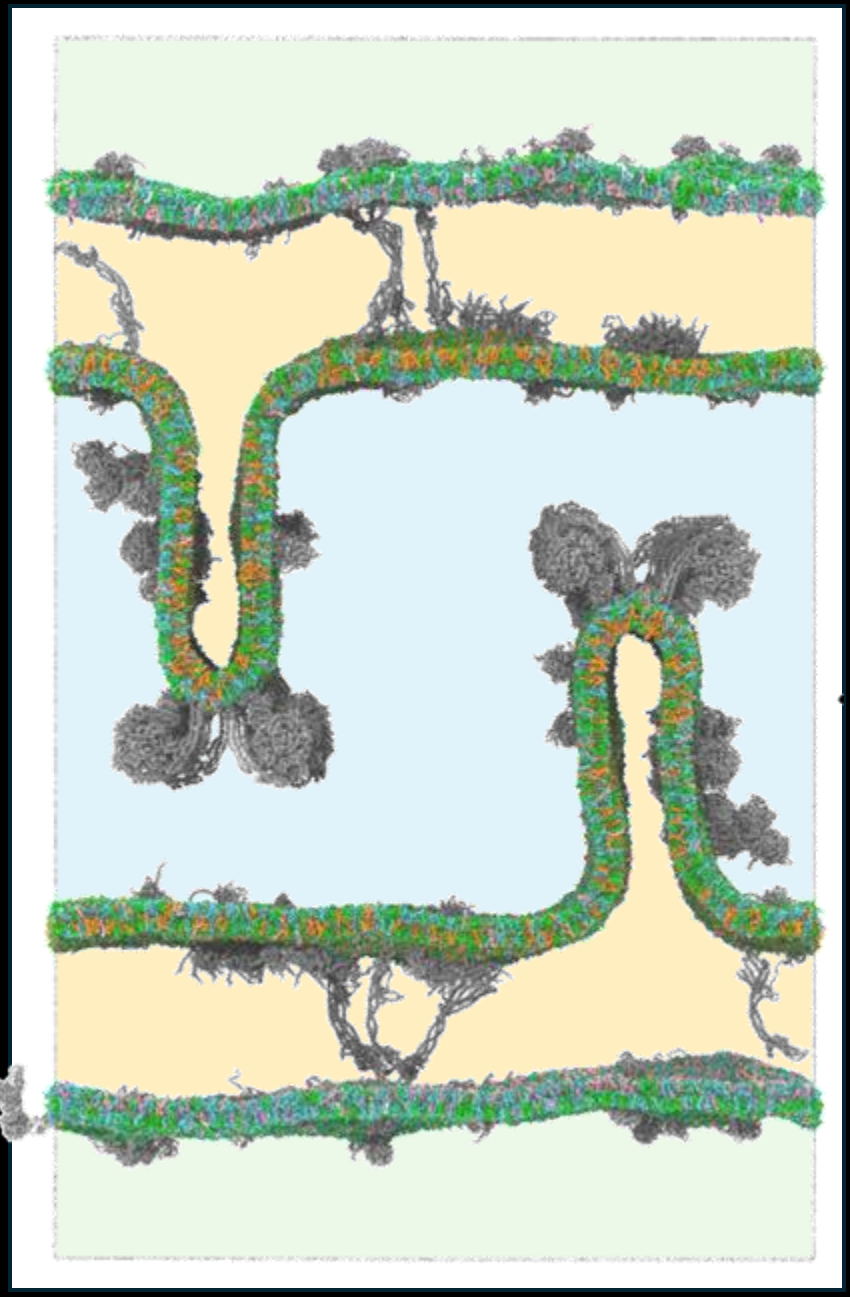
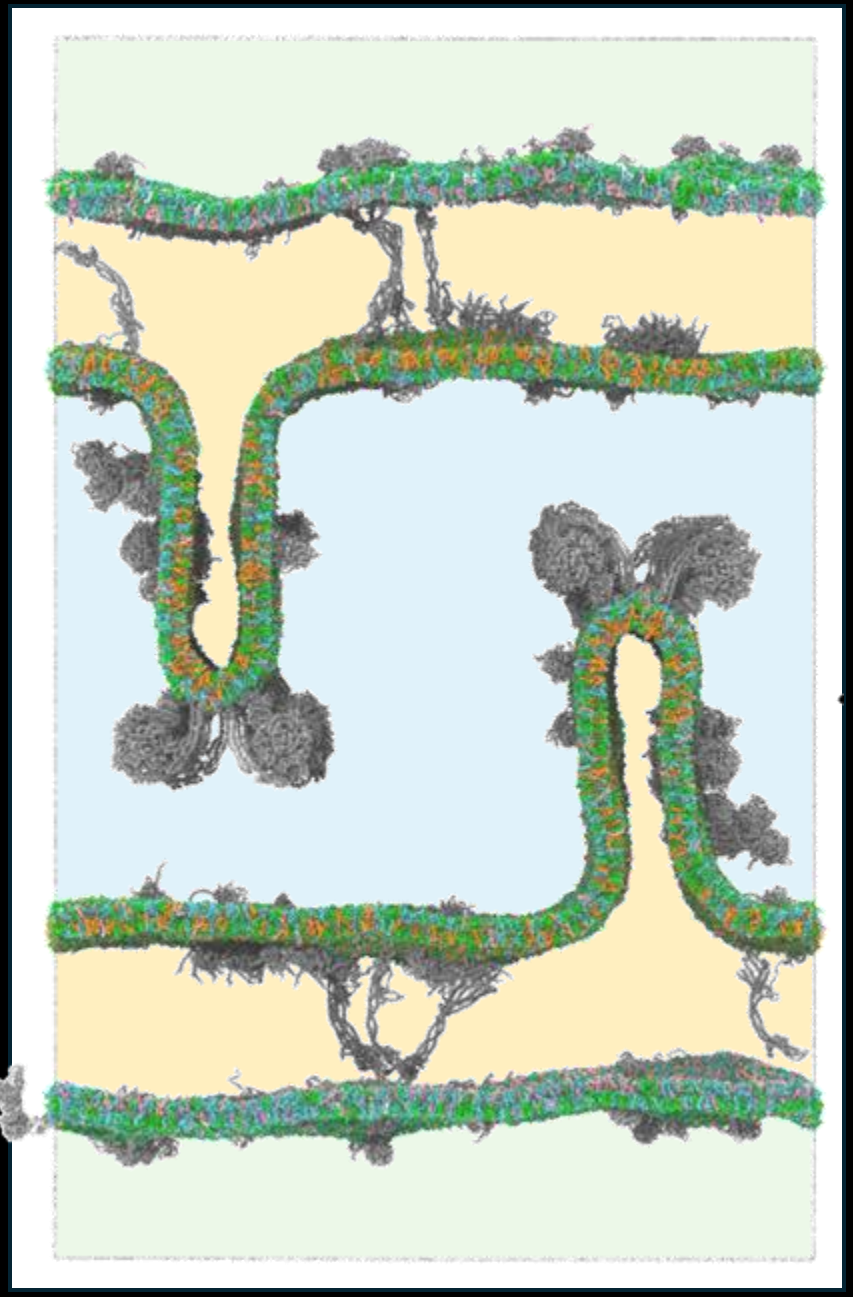


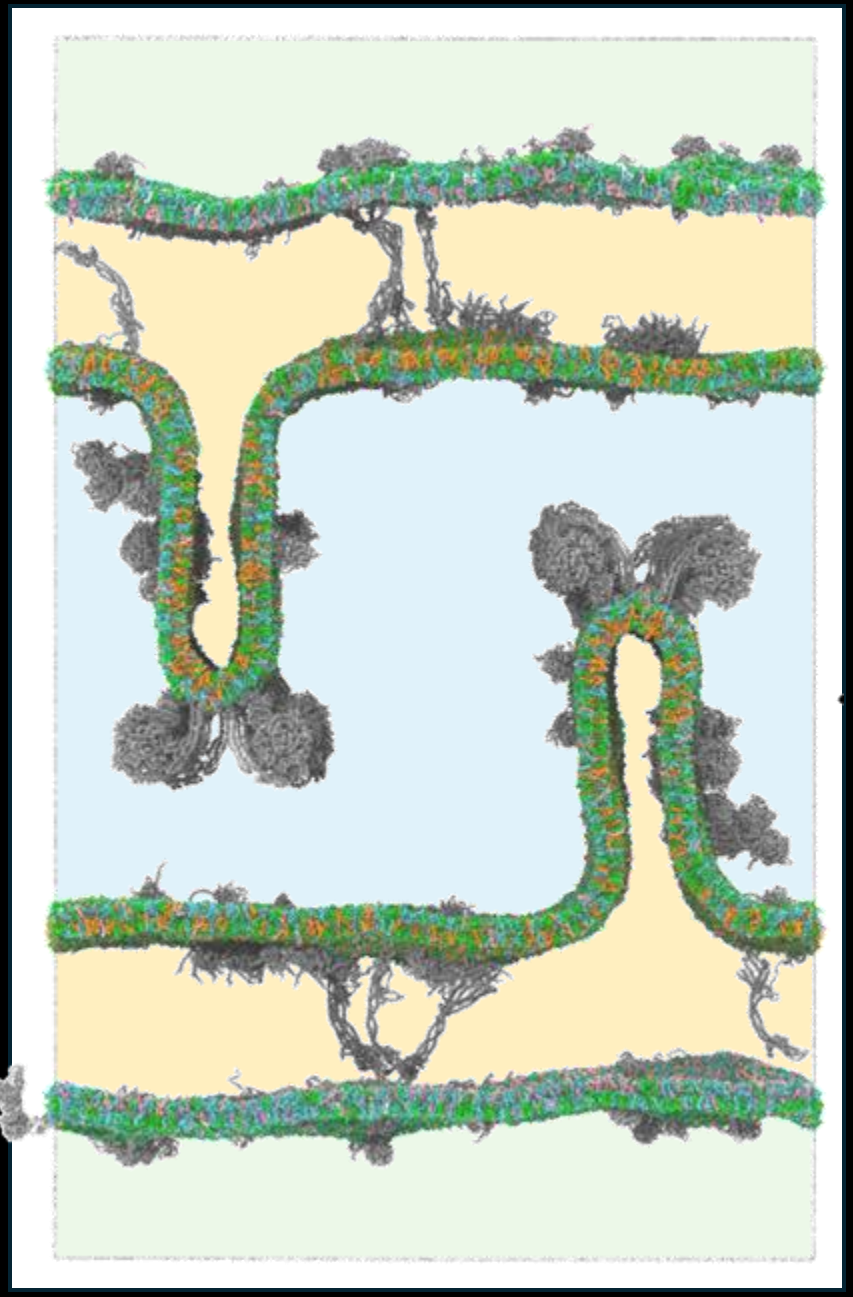


Relaxation time...



Relaxation time...

Given infinite time, any system will converge to its proper ensemble

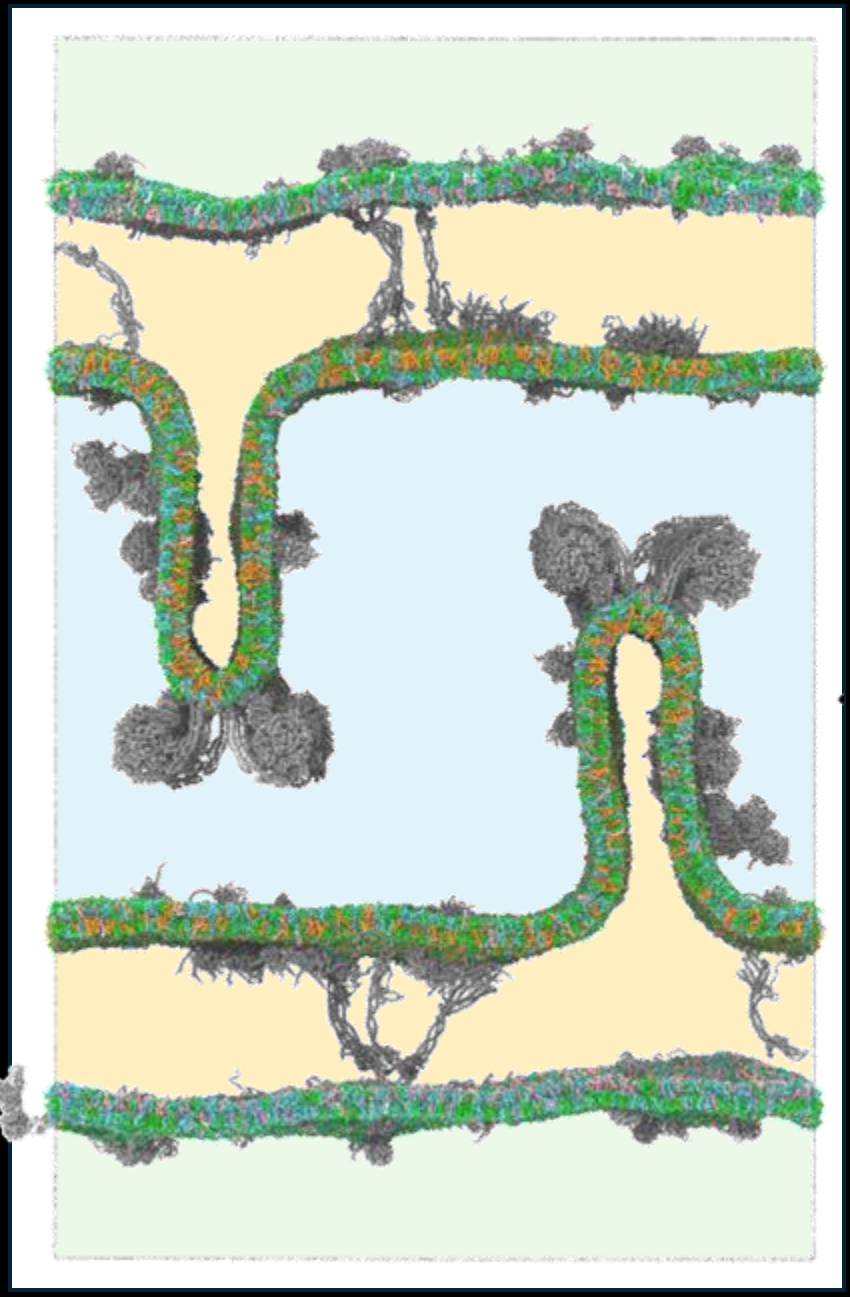


Relaxation time...

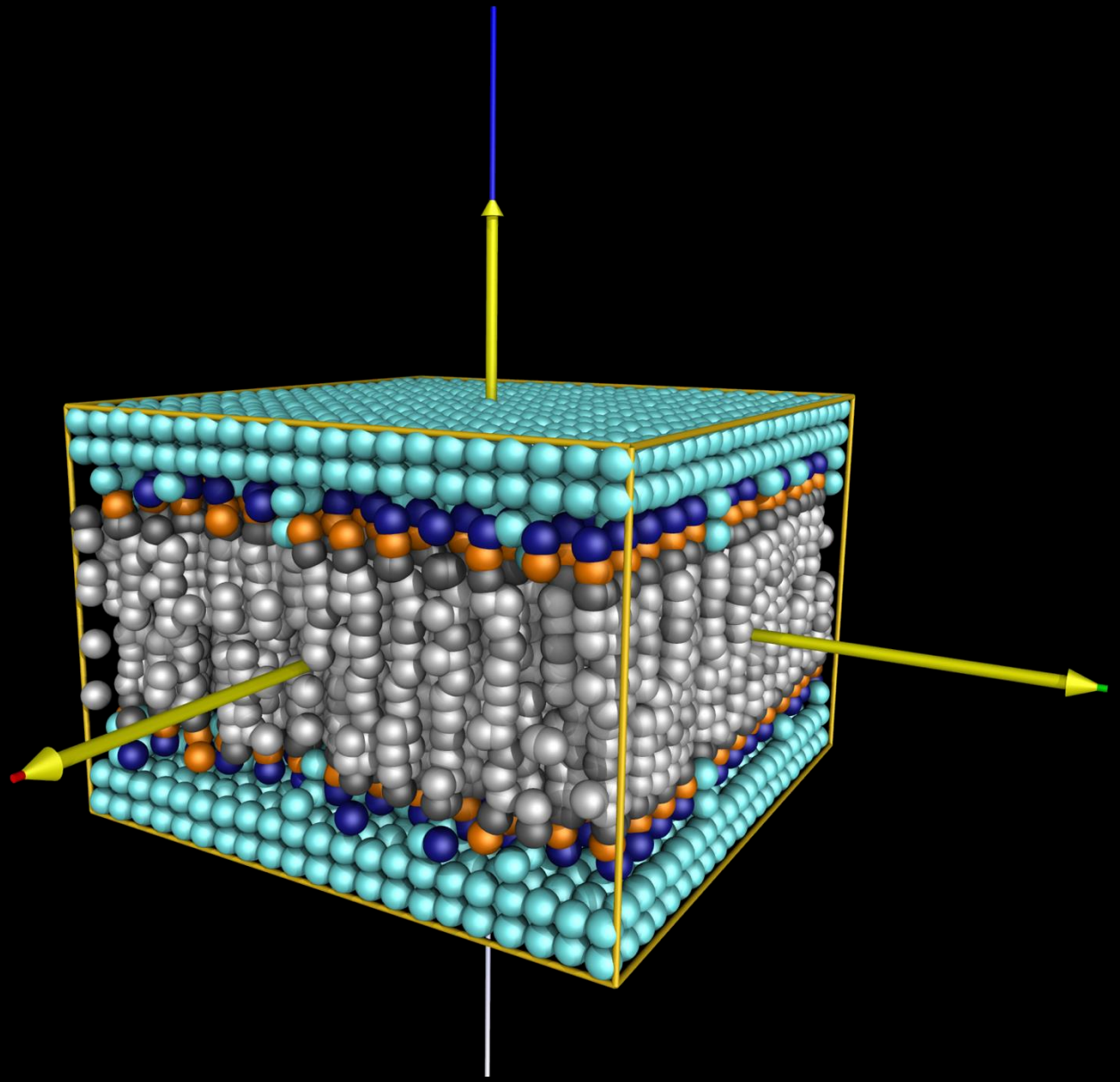
?

finite time

proper ensemble

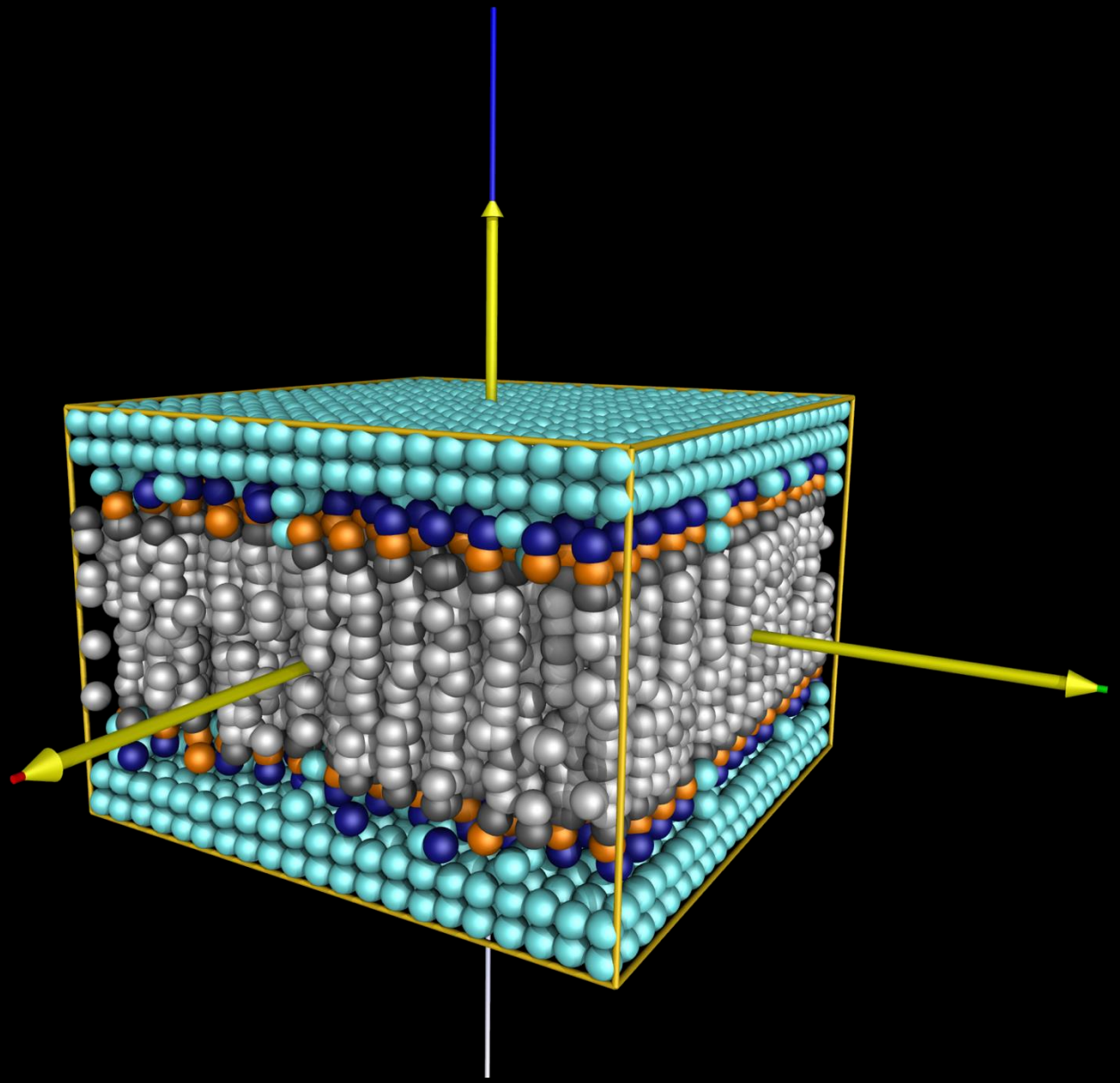


If there were a perfect solution, it wouldn’t be moving in simulation



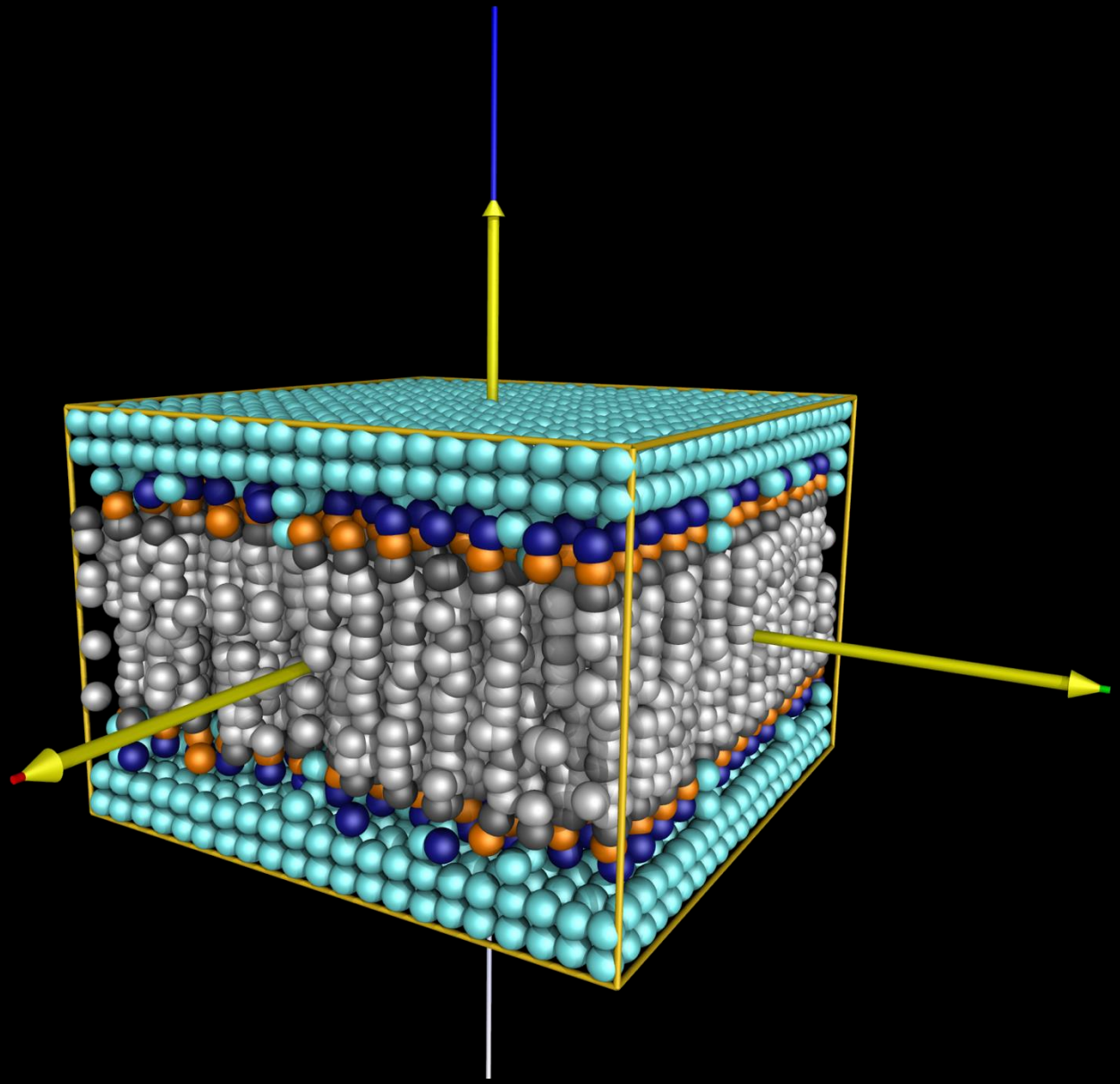
The insane philosophy:

If it’s good enough,
then it’s good enough



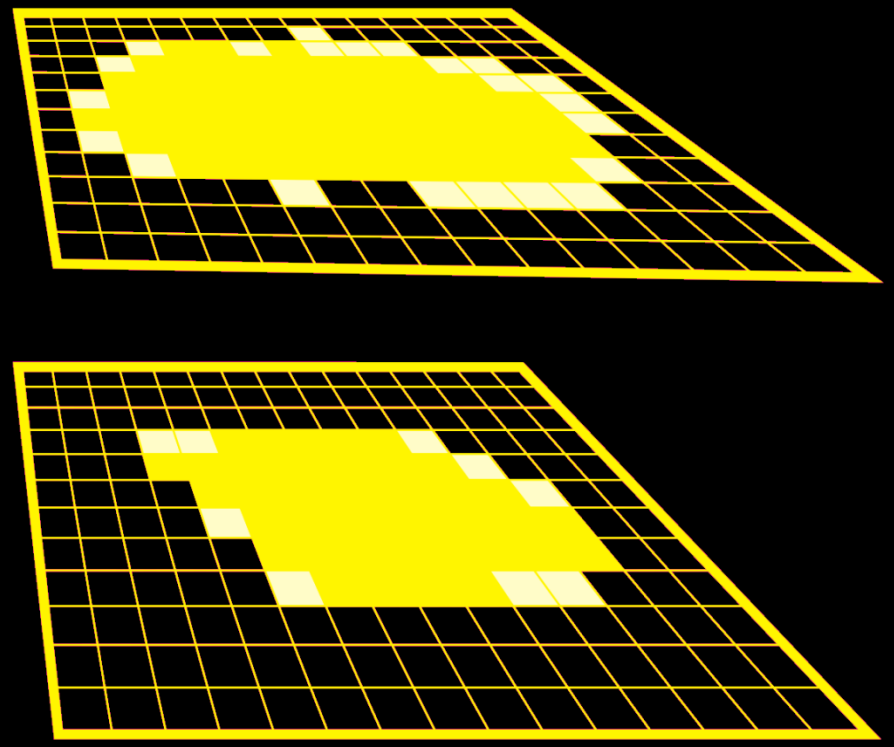
The insane philosophy:

As simple as possible
but not any simpler



The insane philosophy:

Whatever I can
get away with



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Whatever I can
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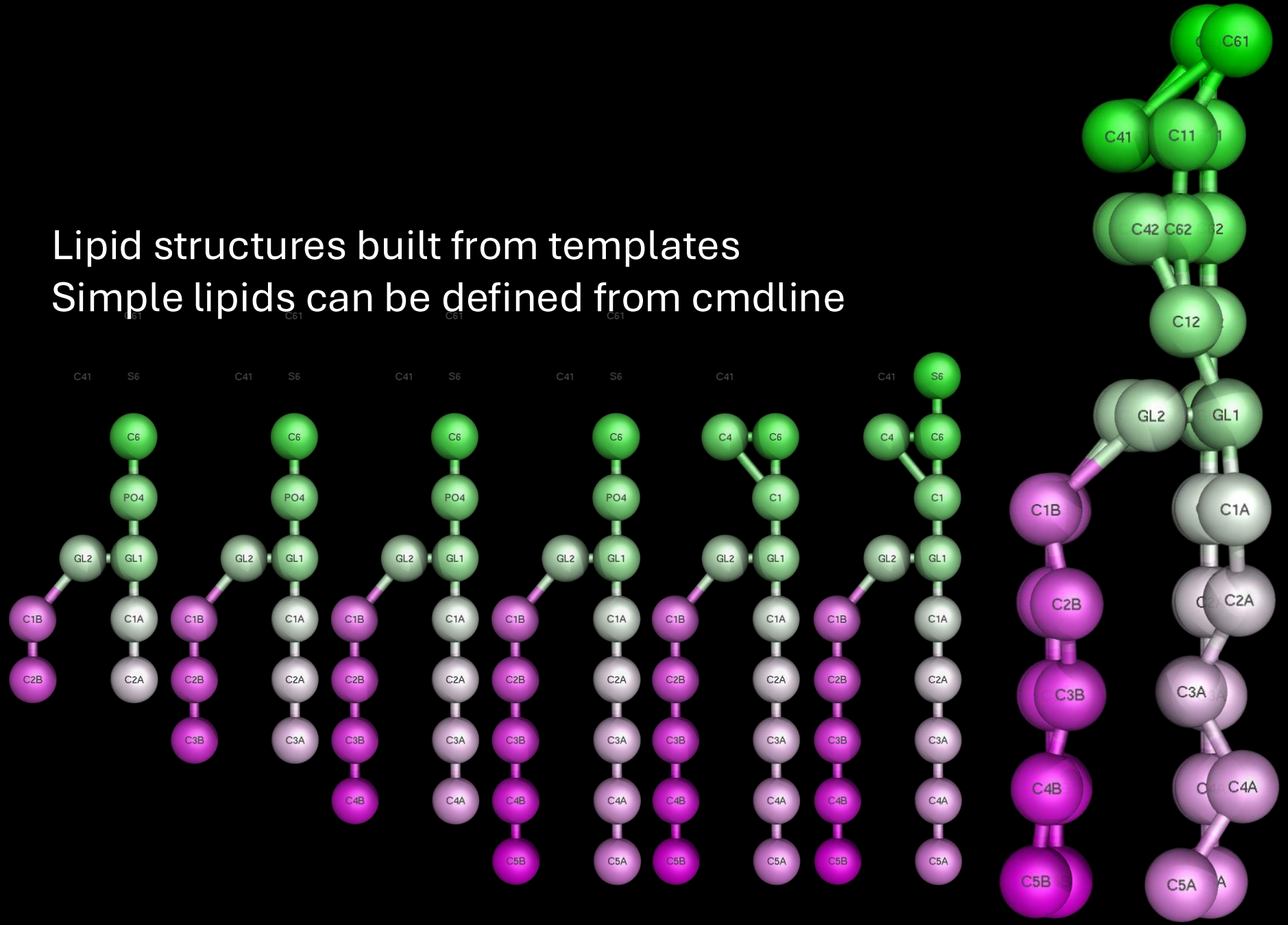
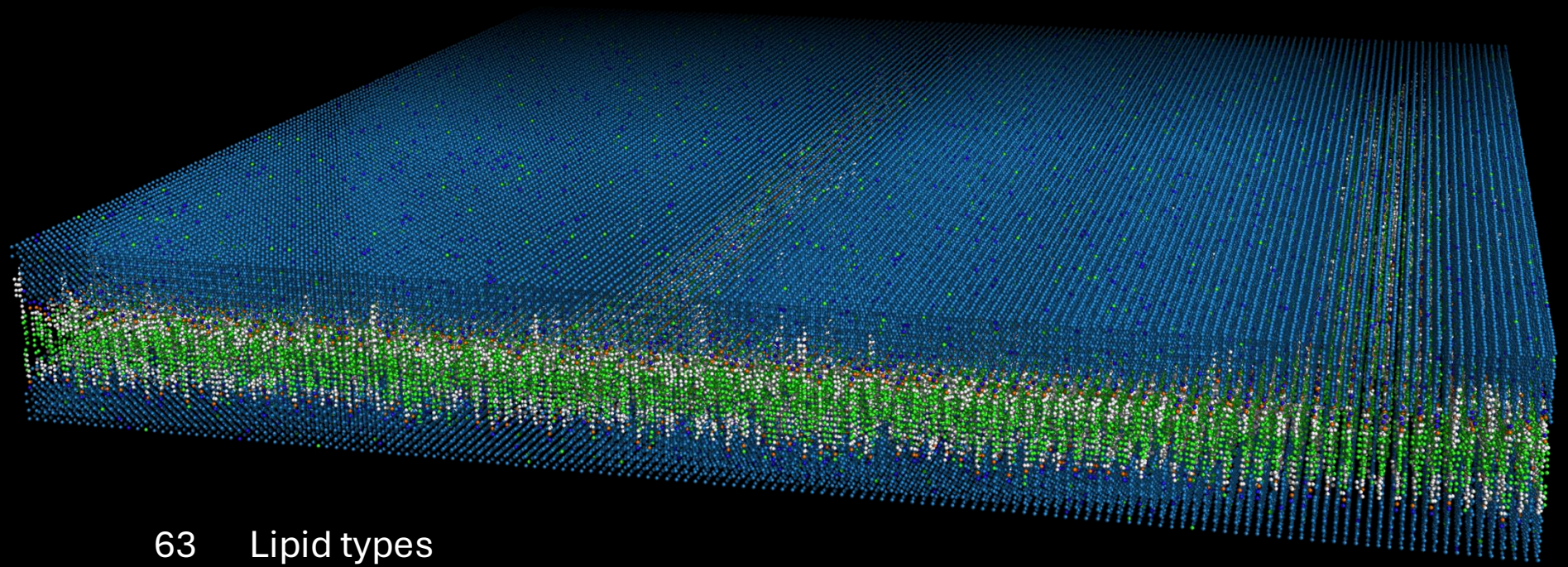
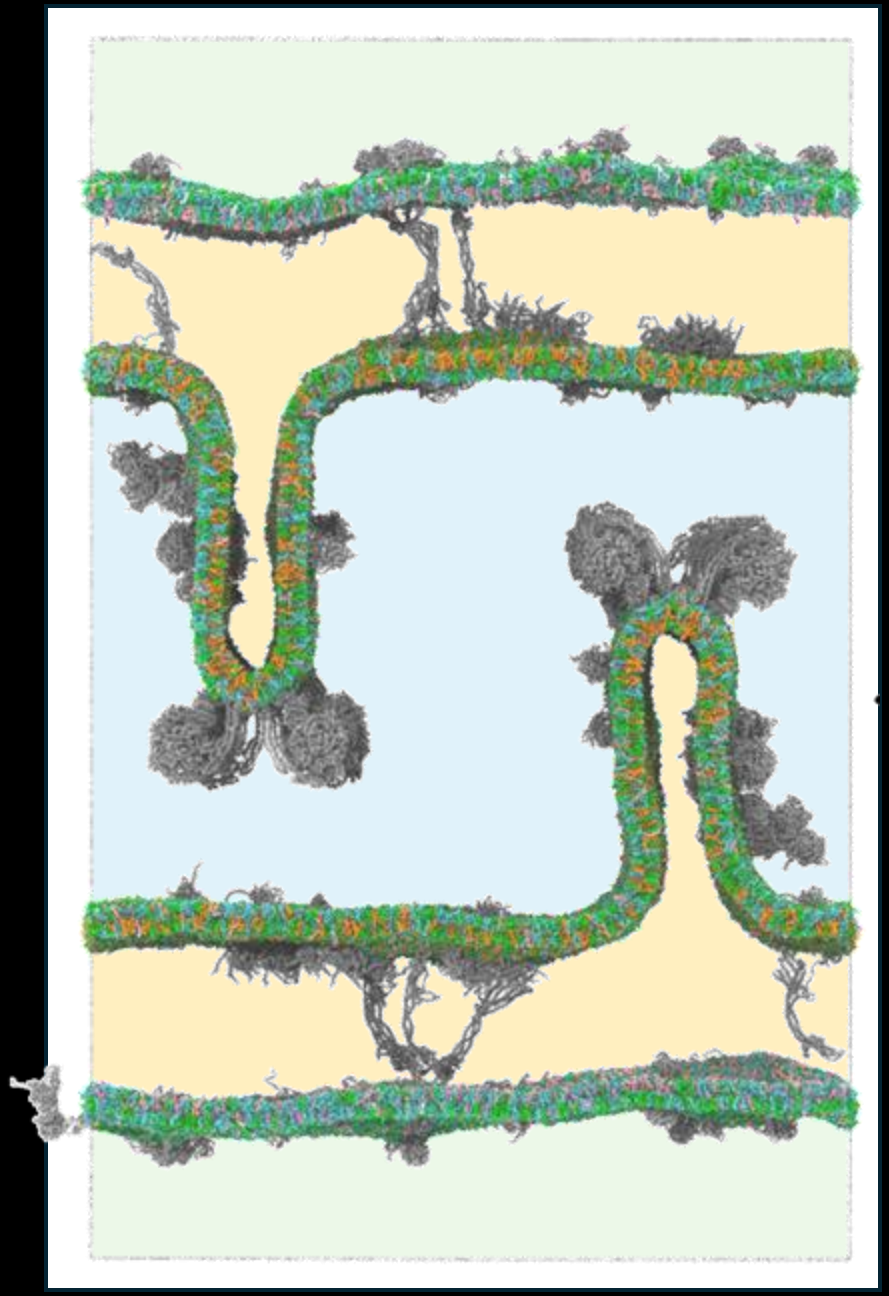
Lipid structures built from templates
Simple lipids can be defined from cmdline





63	Lipid types
19280	Lipids
292221	Water molecules
9294	Ions
523616	Particles
16	Seconds



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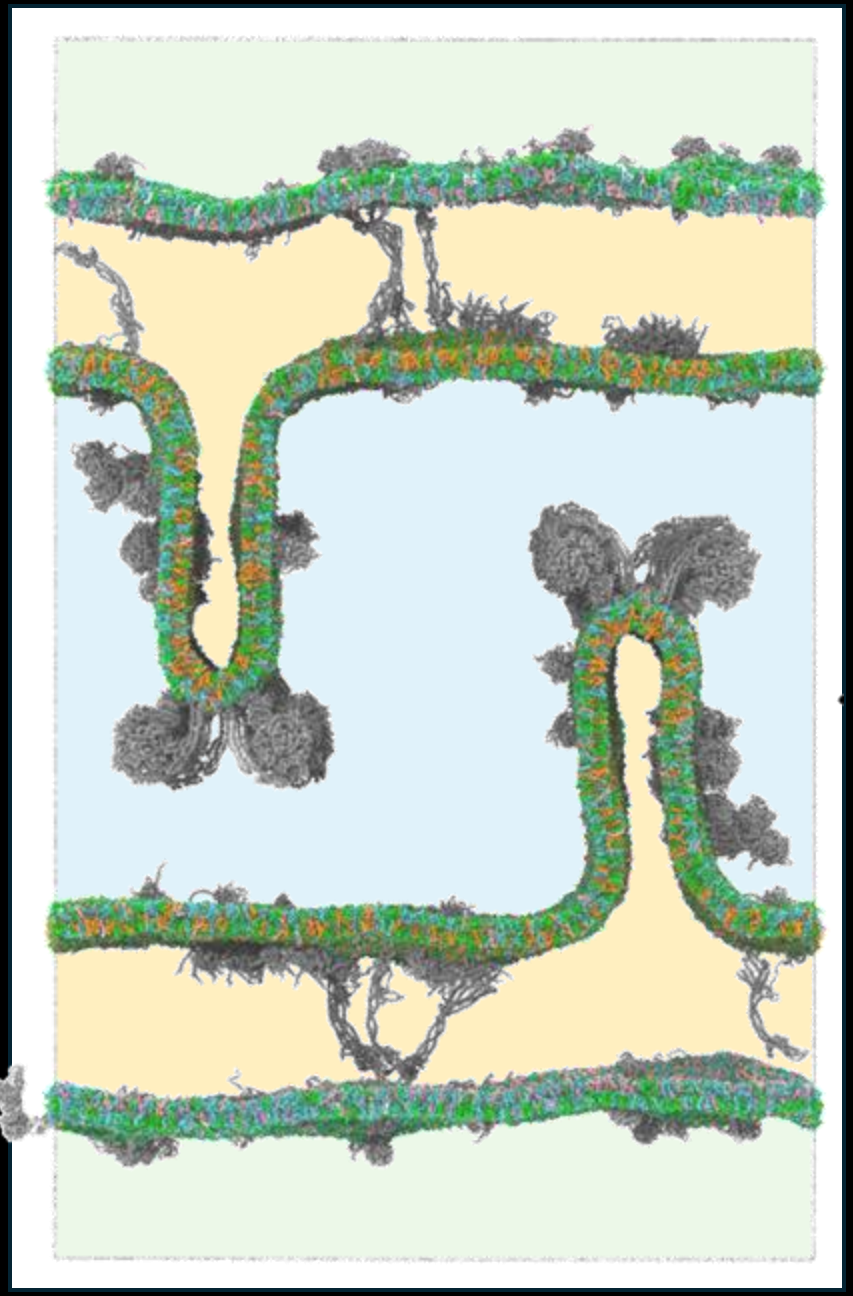

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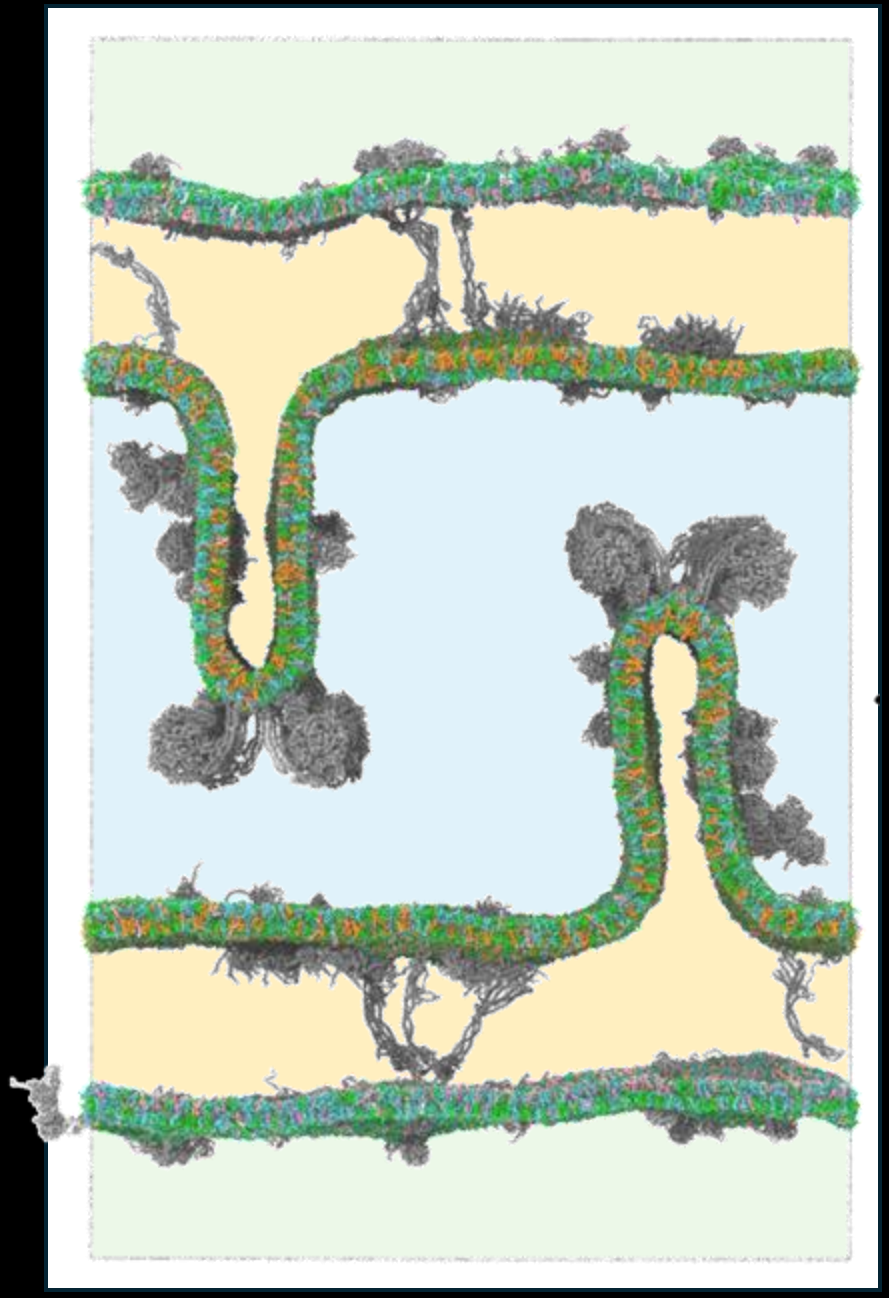

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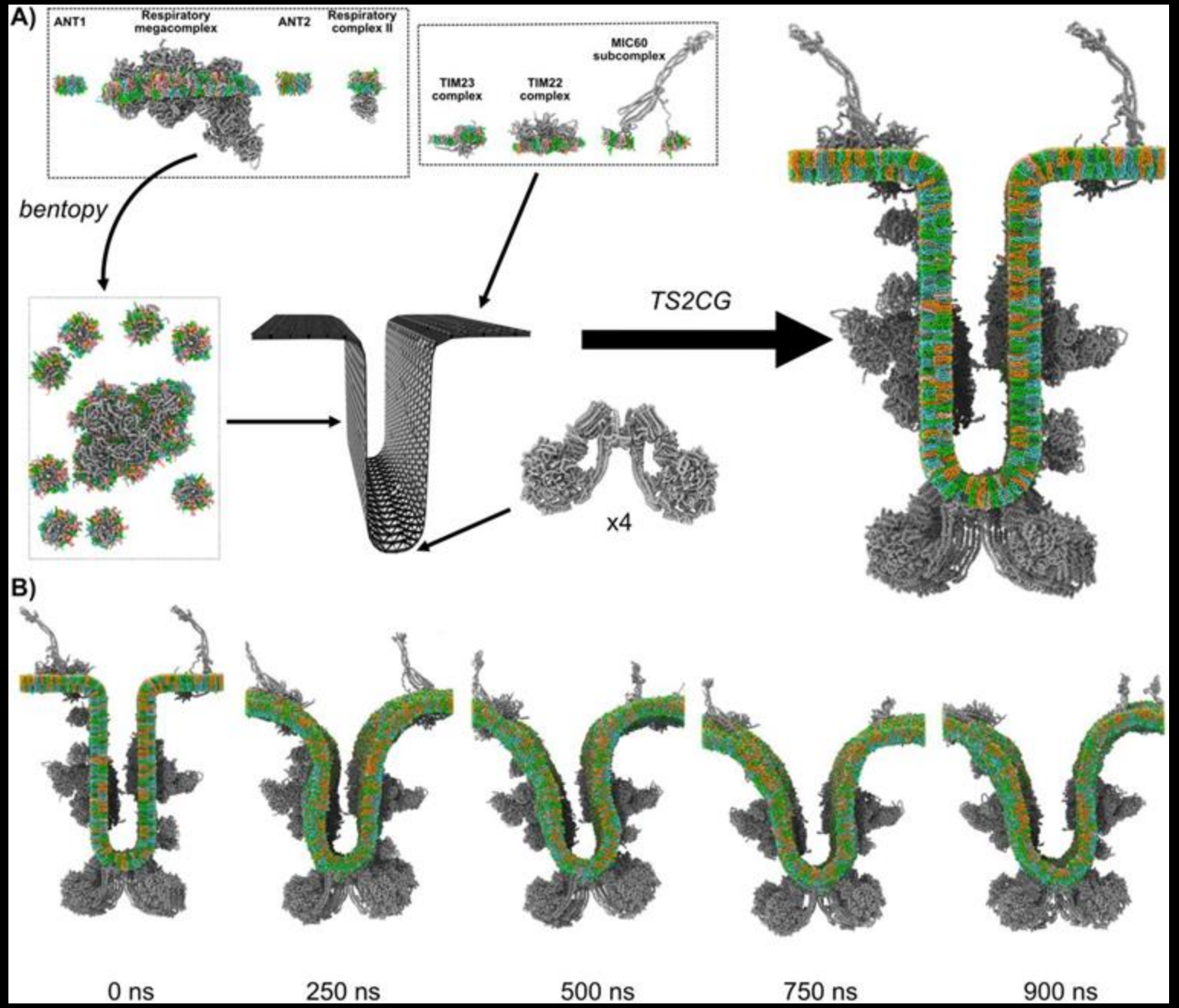
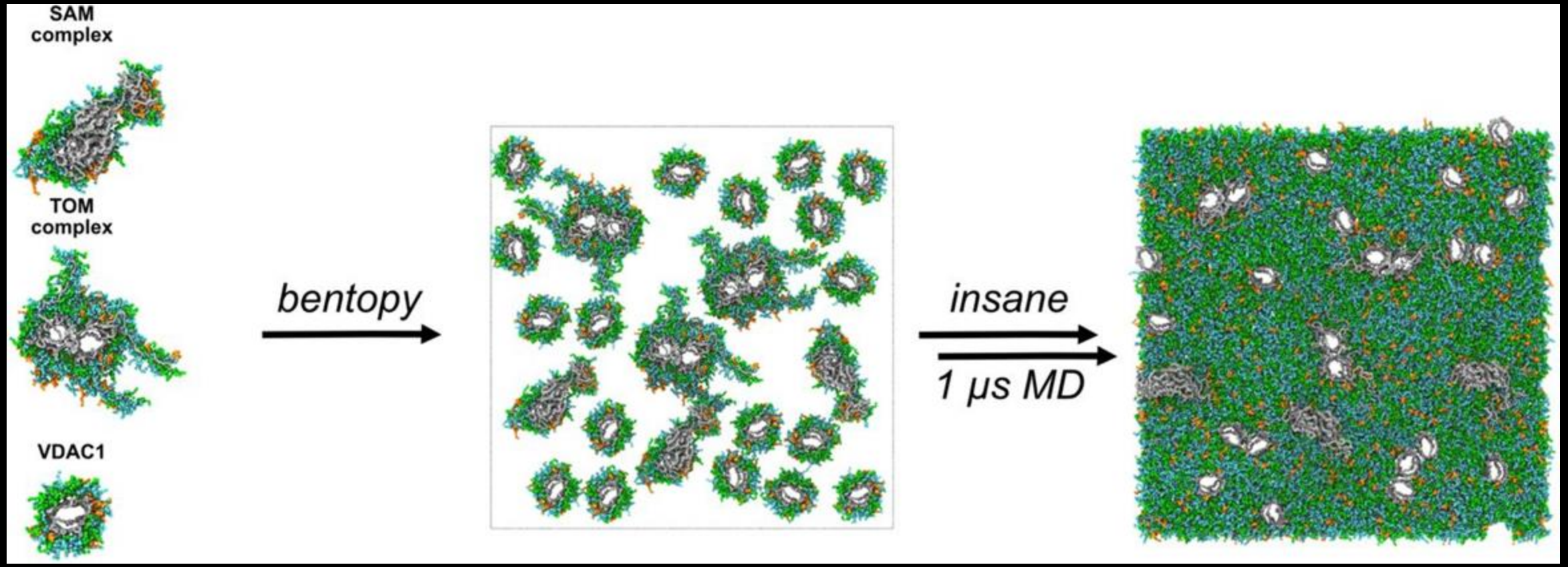

A)
ANT1
Respiratory megacomplex
ANT2
Respiratory complex II
TIM23 complex
TIM22 complex
MIC60 subcomplex
bentopy
TS2CG
x4
B)
0 ns
250 ns
500 ns
750 ns
900 ns


SAM complex
TOM complex
VDAC1
bentopy
insane
1 μs MD

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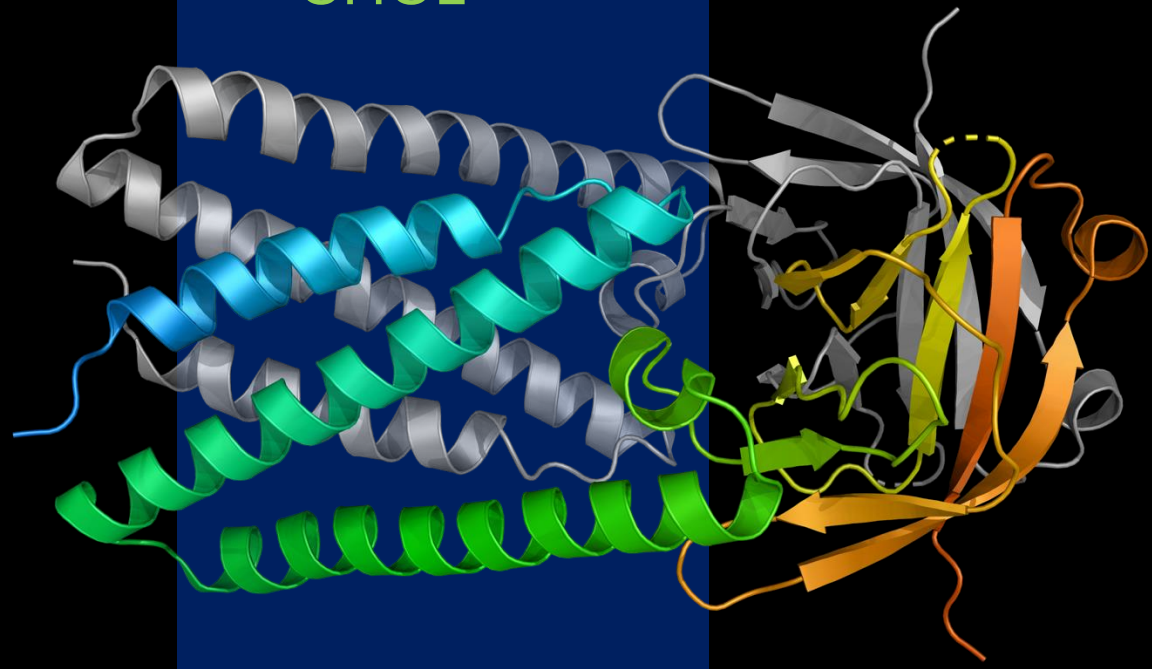
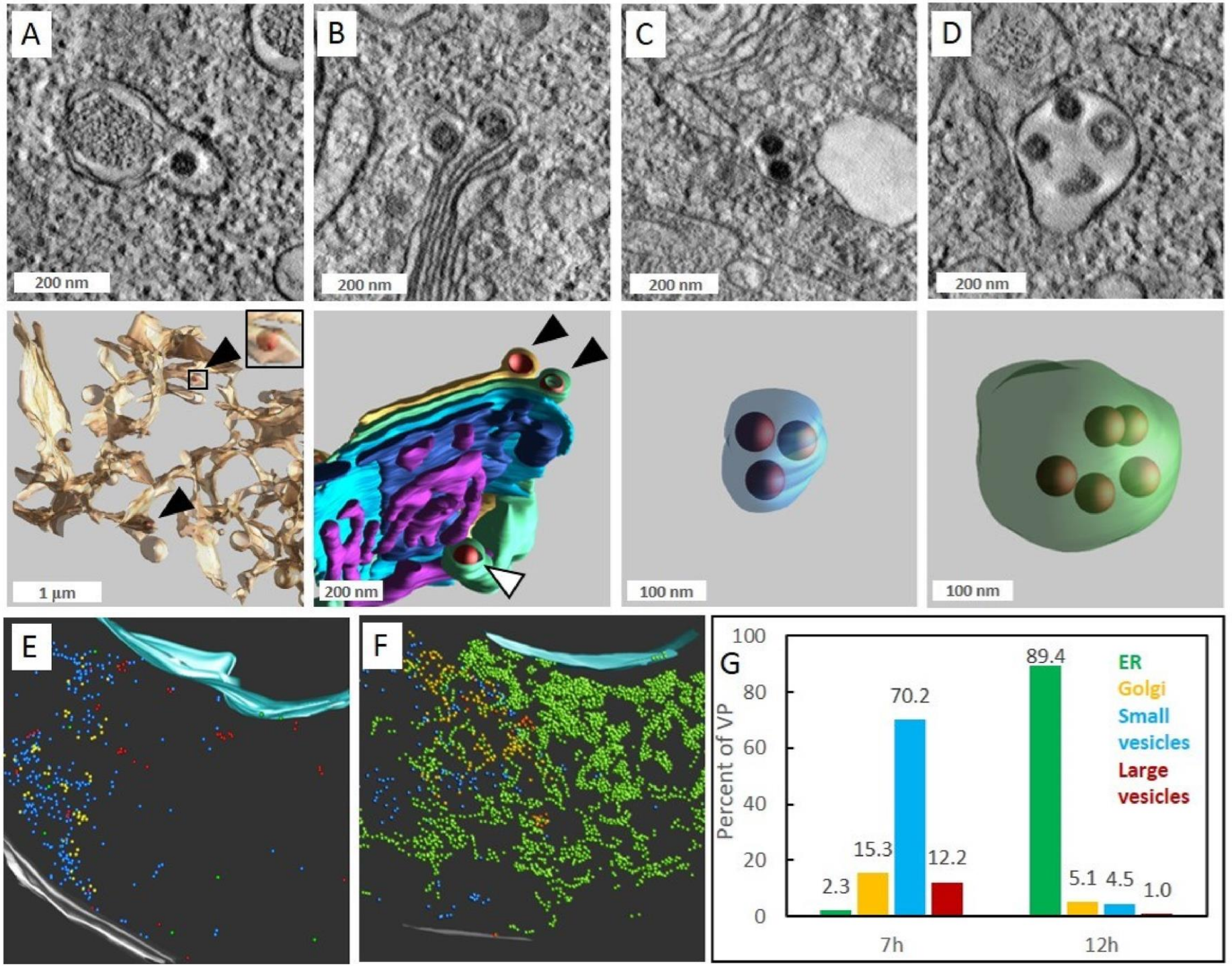
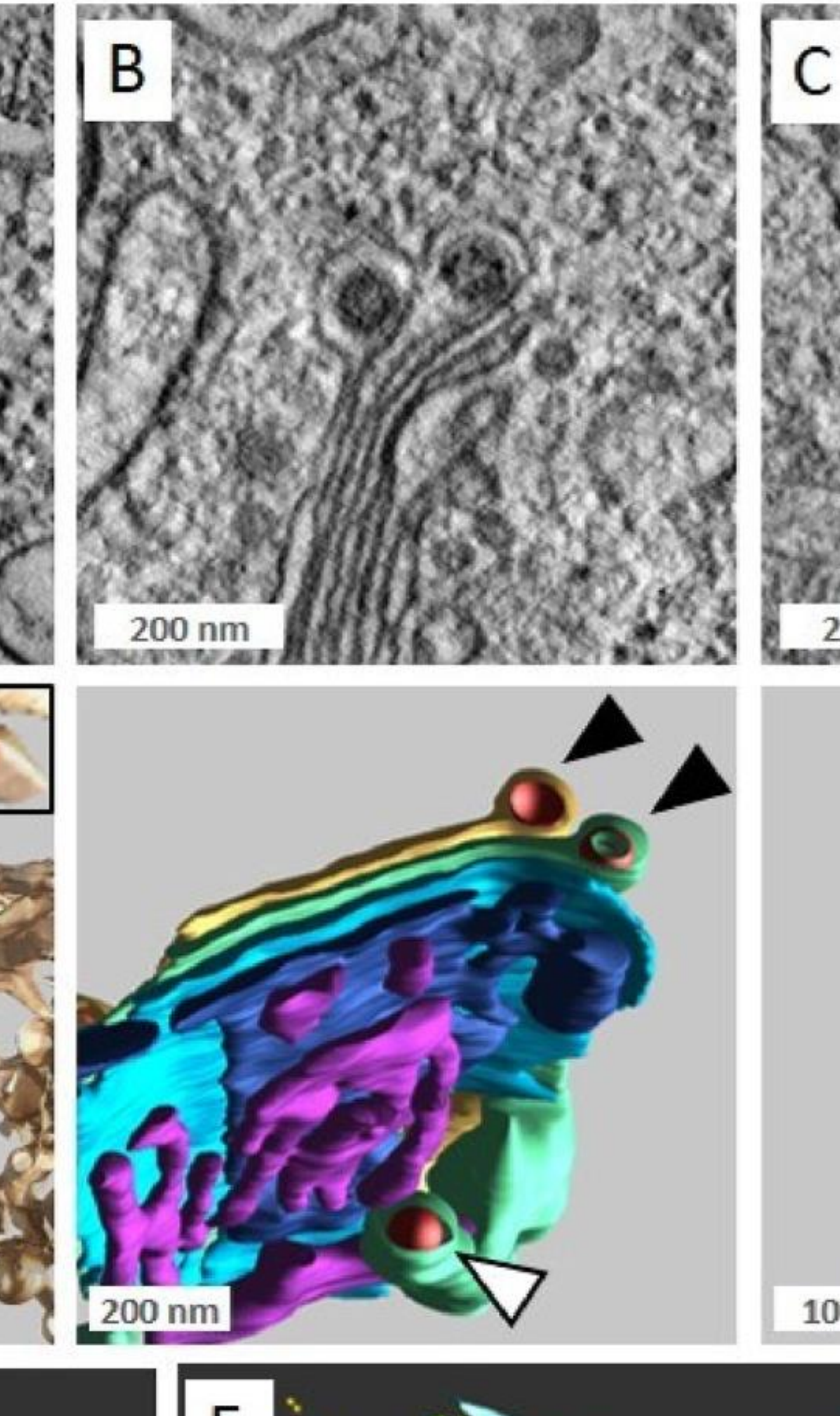
Martini 3
5 μs

POPC
POPE
POPS
POPI
CDL2
CHOL




A
200 nm
B
200 nm
C
200 nm
D
200 nm
1 µm
200 nm
100 nm
100 nm
E
F
G
Percent of VP
100
80
60
40
20
0
2.3
15.3
70.2
12.2
89.4
5.1
4.5
1.0
7h
12h
ER
Golgi
Small vesicles
Large vesicles


B
200 nm
C
200 nm
10

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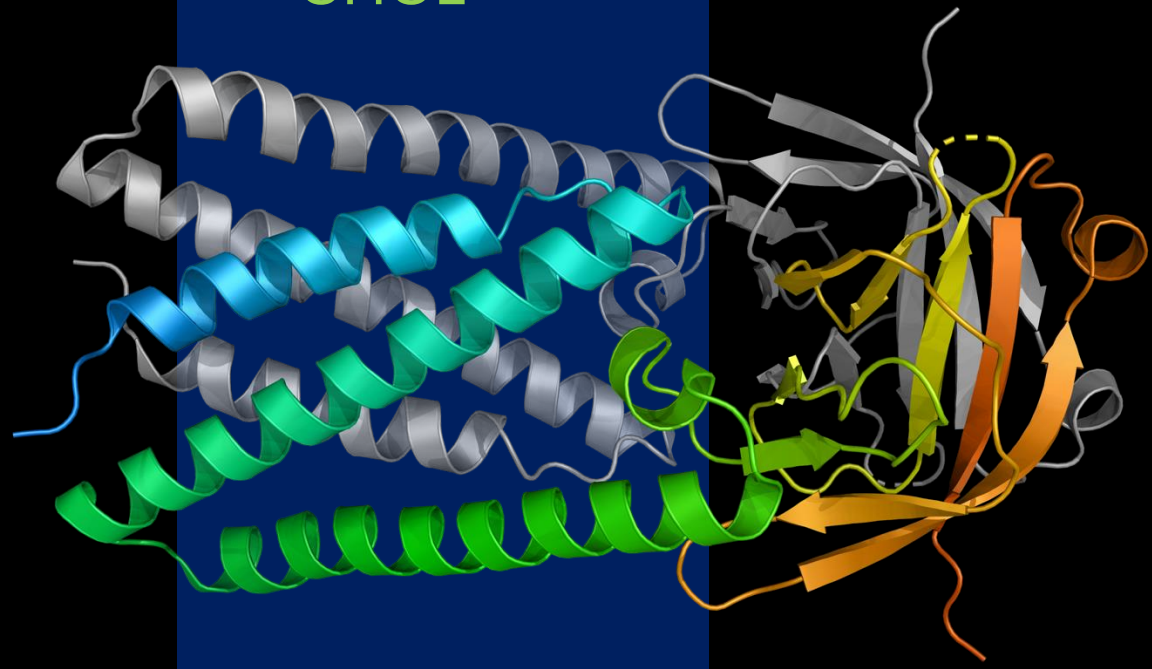
Martini 3
5 μs

POPC
POPE
POPS
POPI
CDL2
CHOL



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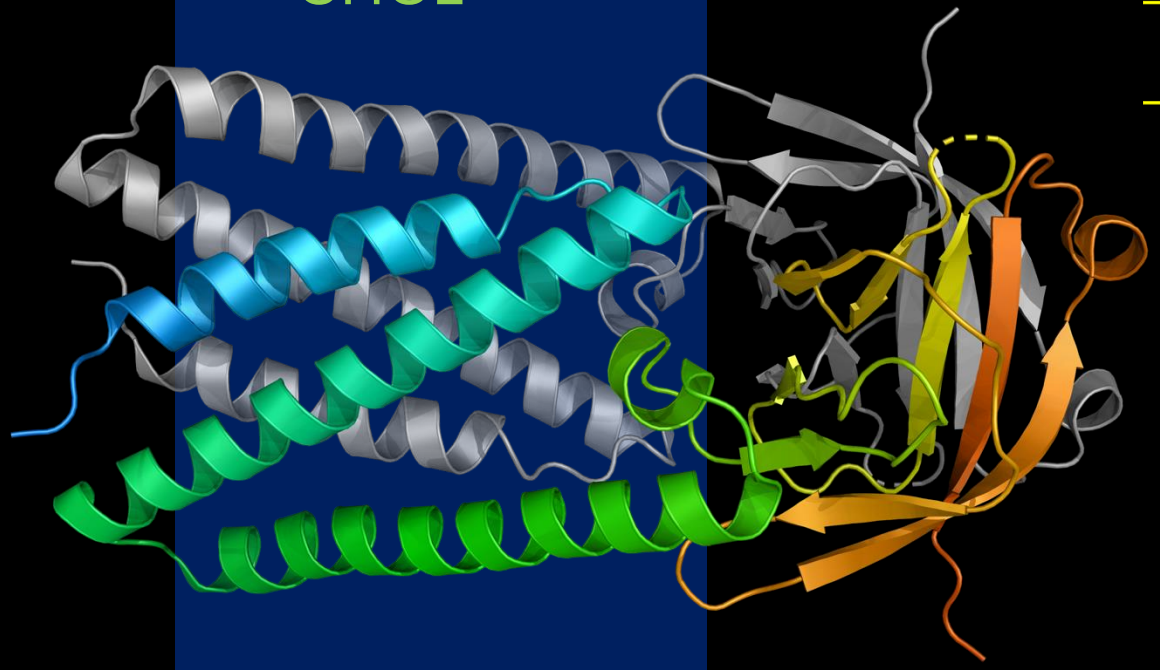
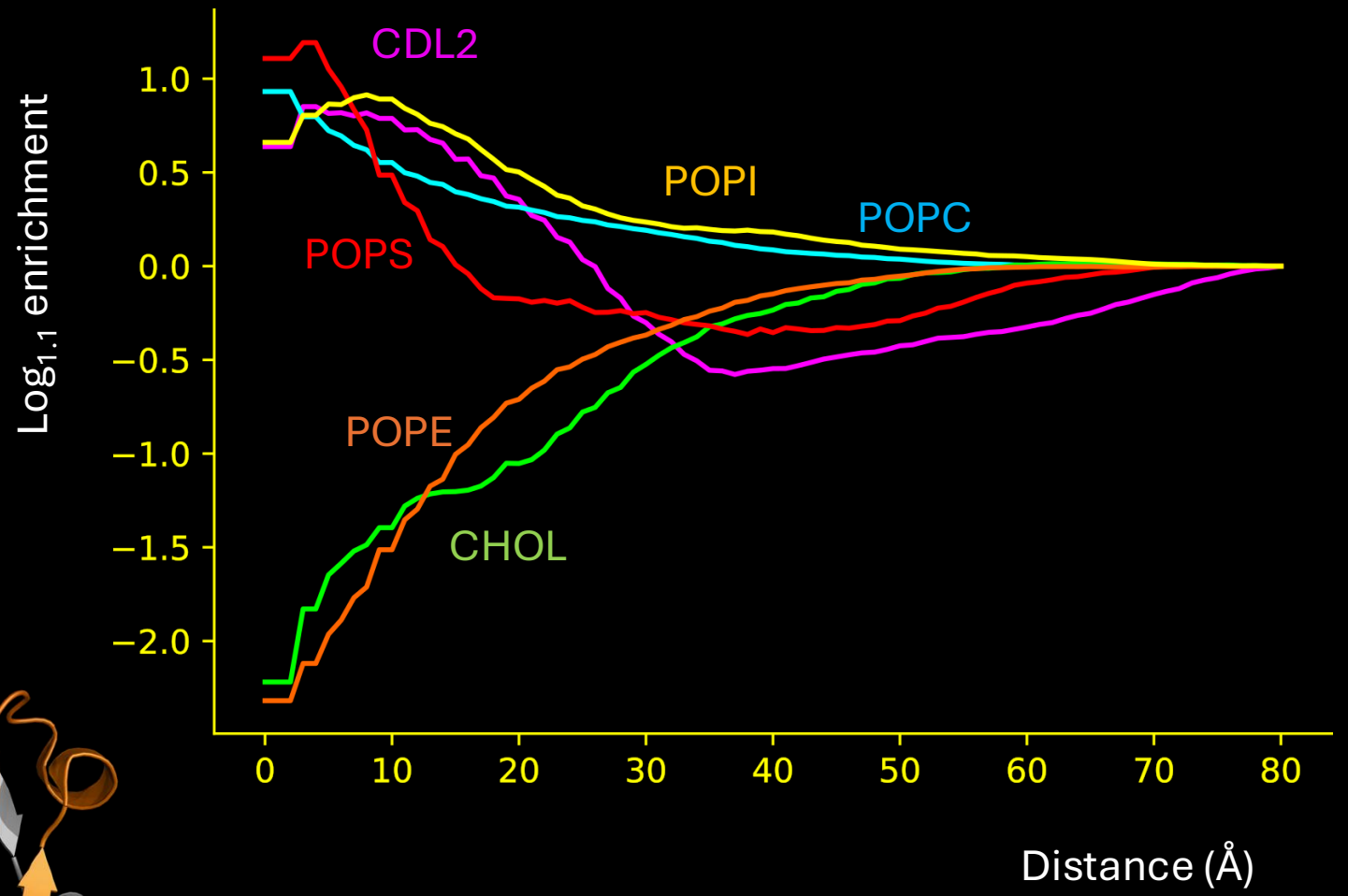
5 μs

POPC
POPE
POPS
POPI
CDL2
CHOL





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