Alex Sodt

BS Chem/Physics Univ. Washington 2000
2002 Q-Chem software developer
PhD 2007 Martin Head-Gordon (electronic structure)
2007-9 post-doc with Teresa Head-Gordon (biophysics)
2010-2015 post-doc with Richard Pastor@NIH (lipid biophysics)

Currently Principal Investigator NICHD/NIH

Eunice Kennedy Schriver National Institute of Child Health and Human Development

www.q-chem.com

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Q-Chem Forum:

iOpenShell
Center for computational studies of electronic structure

Q-Chem Employment Opportunities:

Research Associate in Computational Chemistry:

Q-Chem, Inc., is seeking a scientist for a research associate position at its main office in Pleasanton, CA. The successful candidate should have a Ph.D. in theoretical chemistry or a closely-related field, with significant programming experience (C++, Fortran). Duties will include implementation of novel features, algorithm development, and code maintenance. Previous experience as a developer of a quantum chemistry software package is highly desirable. Candidates must be legally authorized to work for a US company and willing to relocate to California. The initial contract will be for one year, renewable upon mutual consent.

Please send a CV to jobs@q-chem.com. Review of applications will commence on Jan. 25, 2016, and continue until the position is filled.

Q-Chem Inc., 6601 Owens Drive, Suite 105, Pleasanton, CA 94588

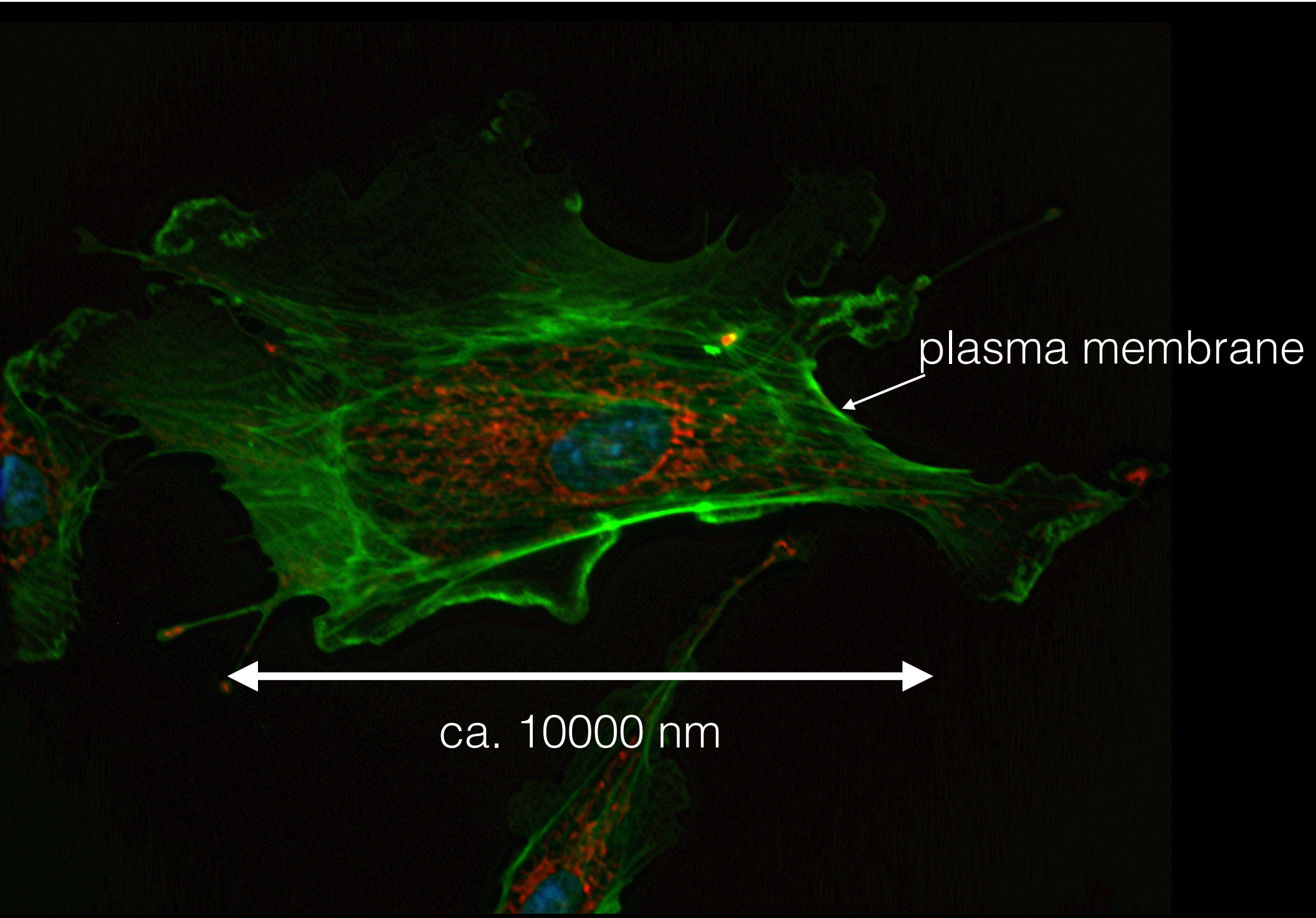
Internship Opportunity for Graduate Students and Postdocs:

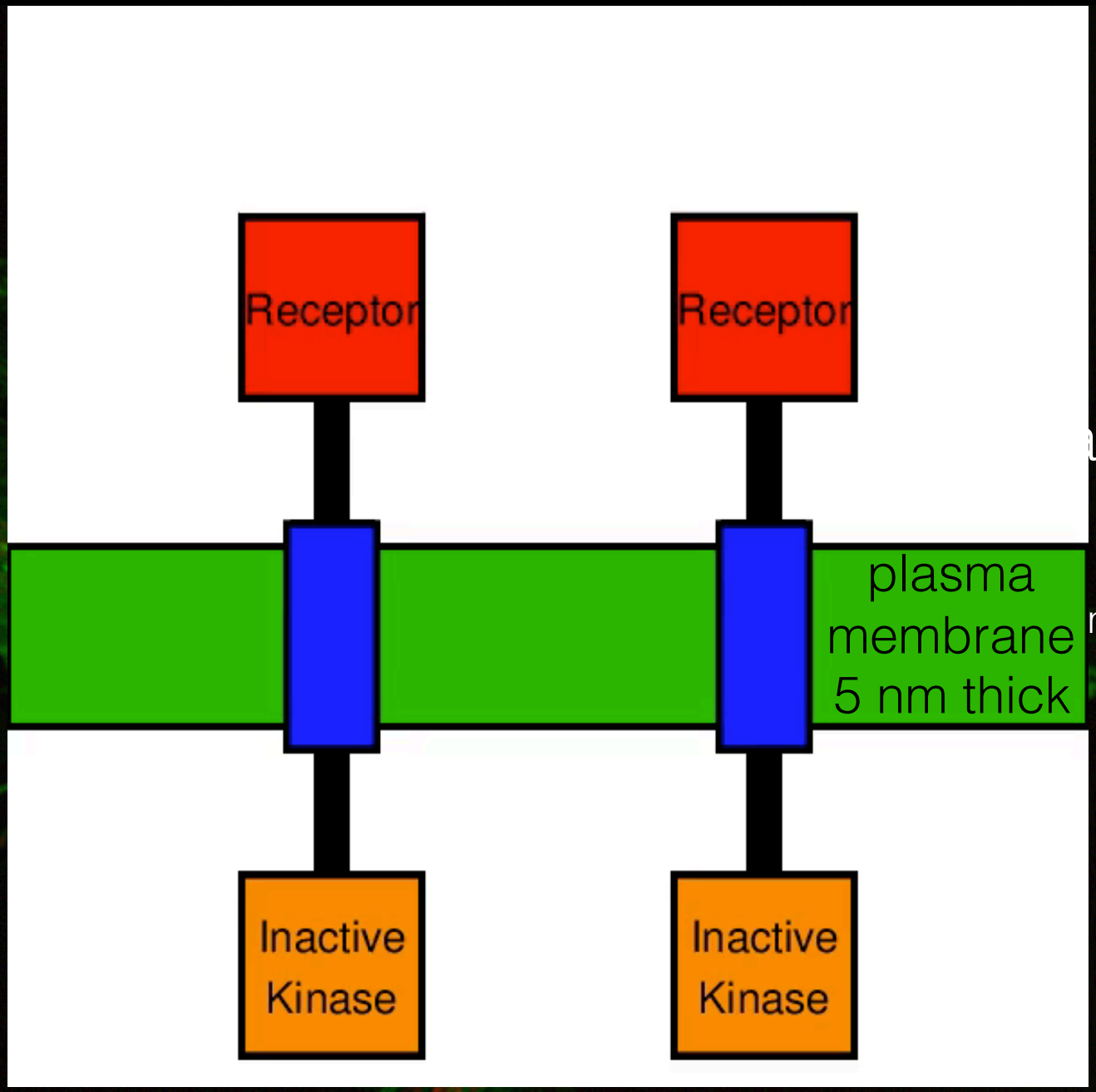
Q-Chem is announcing an internship program for graduate students and postdocs. The goal of the program is to accelerate the development of new capabilities and core infrastructure; to provide training to new generation of Q-Chem developers; and to help academic developers integrate new features into Q-Chem.

Two types of internships will be supported:

1. **Targeted internships aimed at specific developments initiated by Q- Chem, Inc.** In this case, Q-Chem will provide travel support (domestic airfare and ground transportation) and a stipend of $2,500 per month ($625 per week), to be used to cover local accommodation costs.

2. **Internships initiated by academic developers.** Q-Chem will provide 50% of travel support (domestic airfare and ground transportation) and a stipend of $1250 per month towards local expenses.

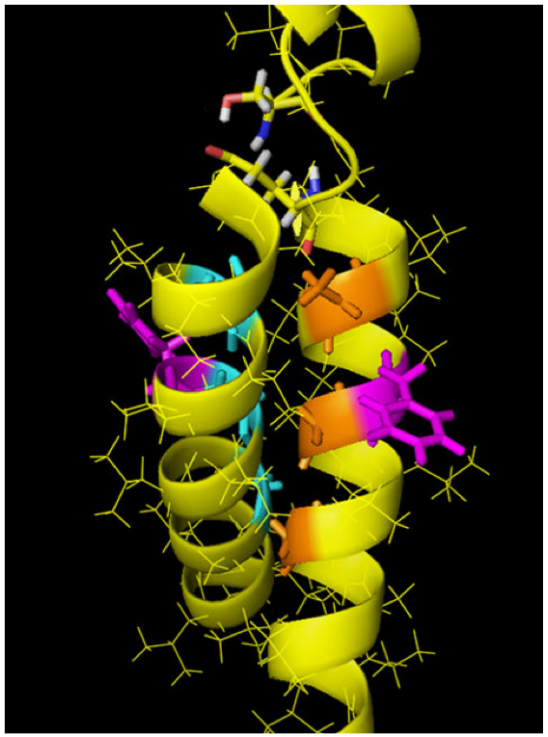

plasma membrane
ca. 10000 nm


Receptor
Receptor
plasma
membrane
5 nm thick
Inactive
Kinase
Inactive
Kinase

membrane

ms)

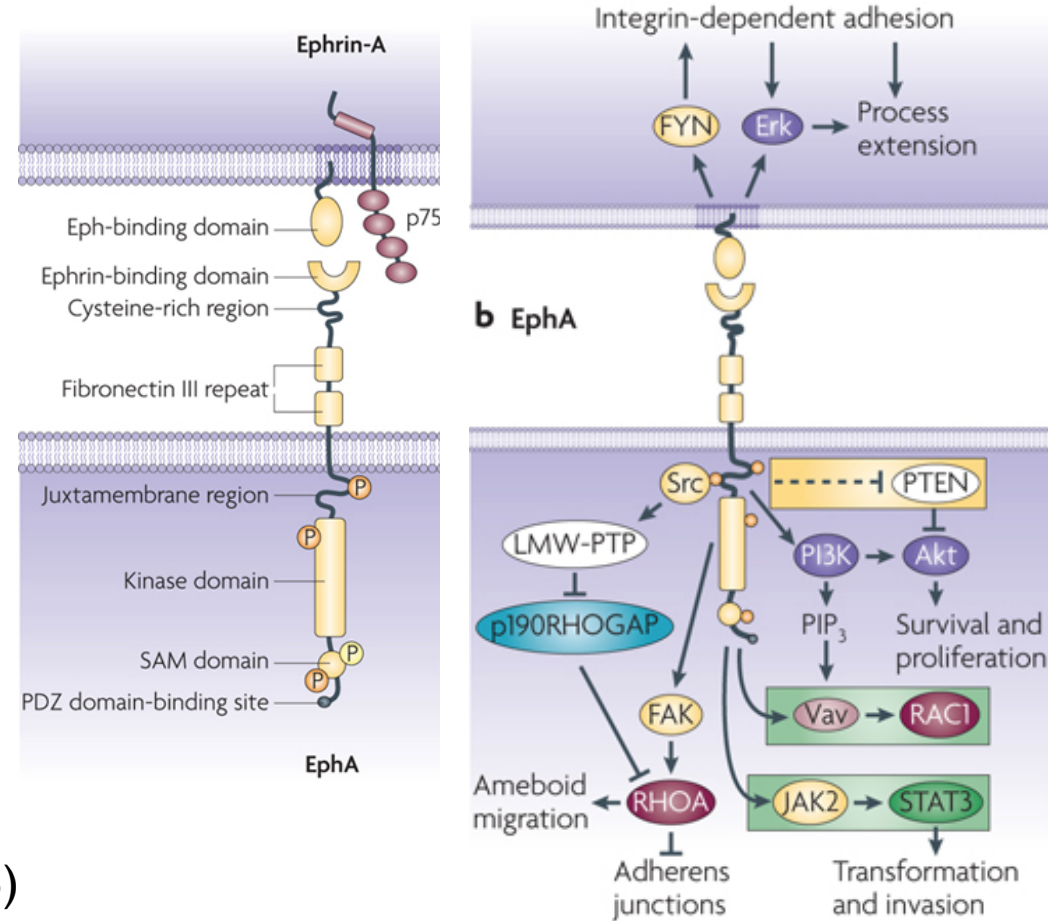
Simple system, carefully controlled: *transmembrane region, small bilayer patch*



EphA1, Zhang et al, Proteins **81** 365-376 (2013)

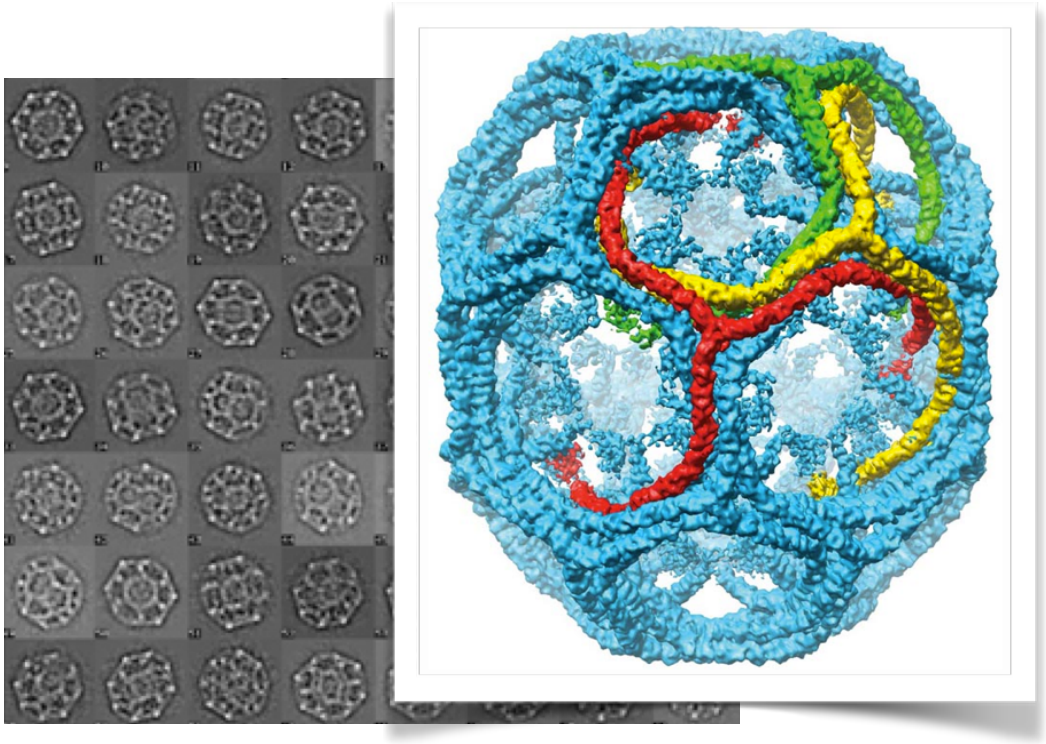
Bocharaov et al, J. Biol. Chem., **283**, 29385 (2008

Would like to do full system, in a realistic environment



Pasquale, Nat. Rev. Cancer, **10** 165 (2010)

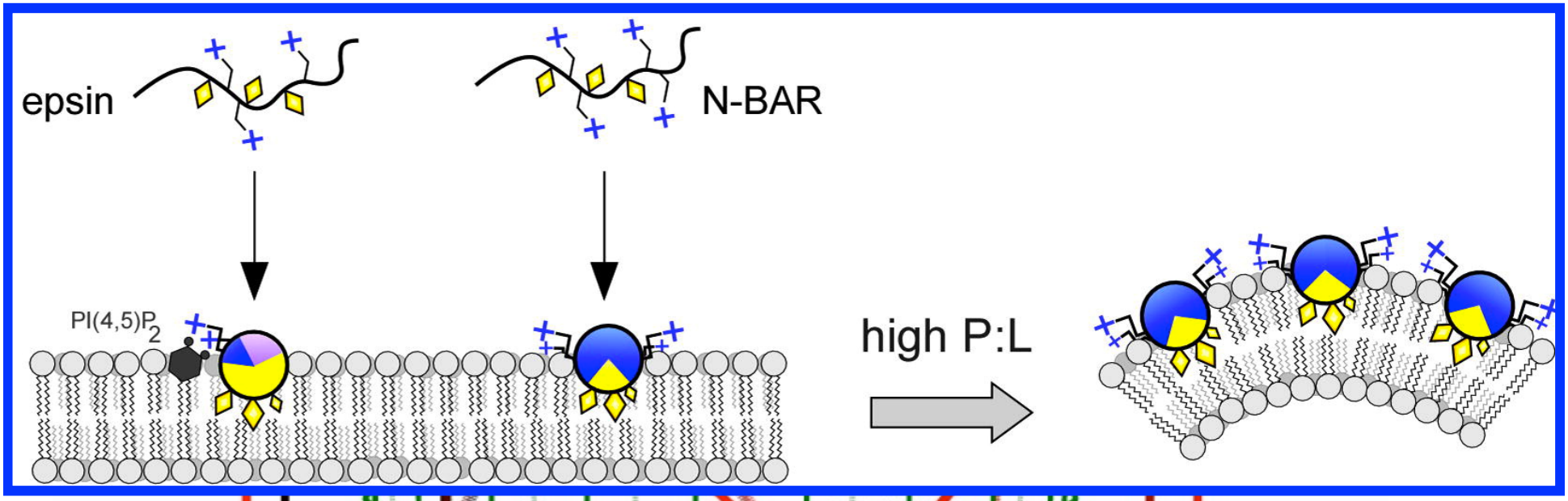
Transport of receptors from the membrane into the cell

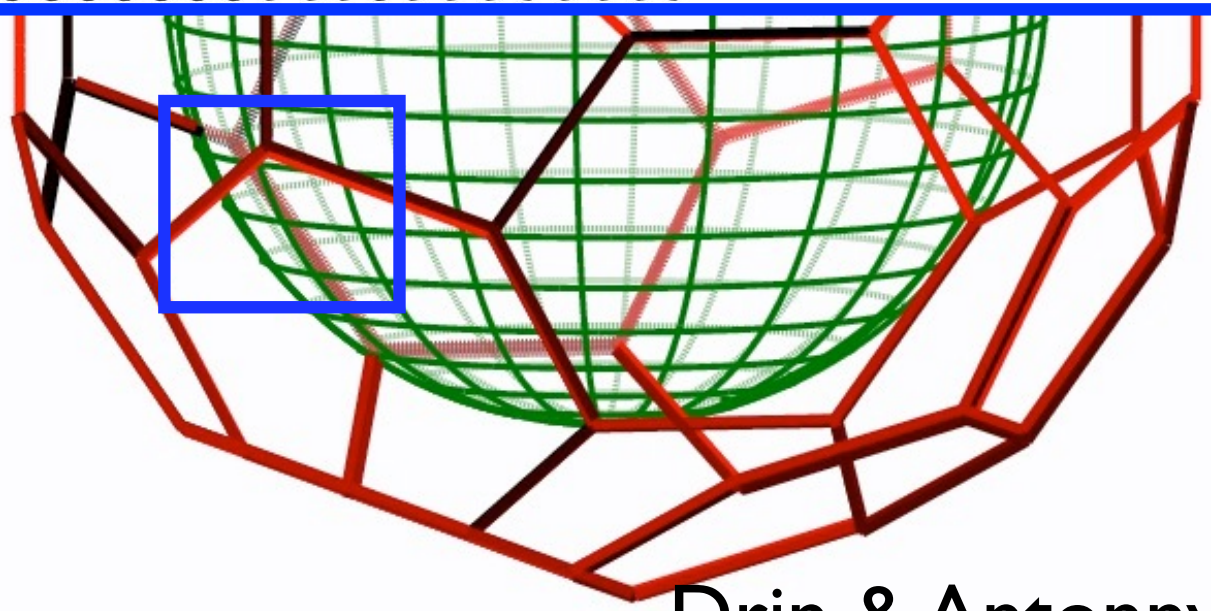


electron microscopy

Fotin et al, Nature **432** 573 (2004)

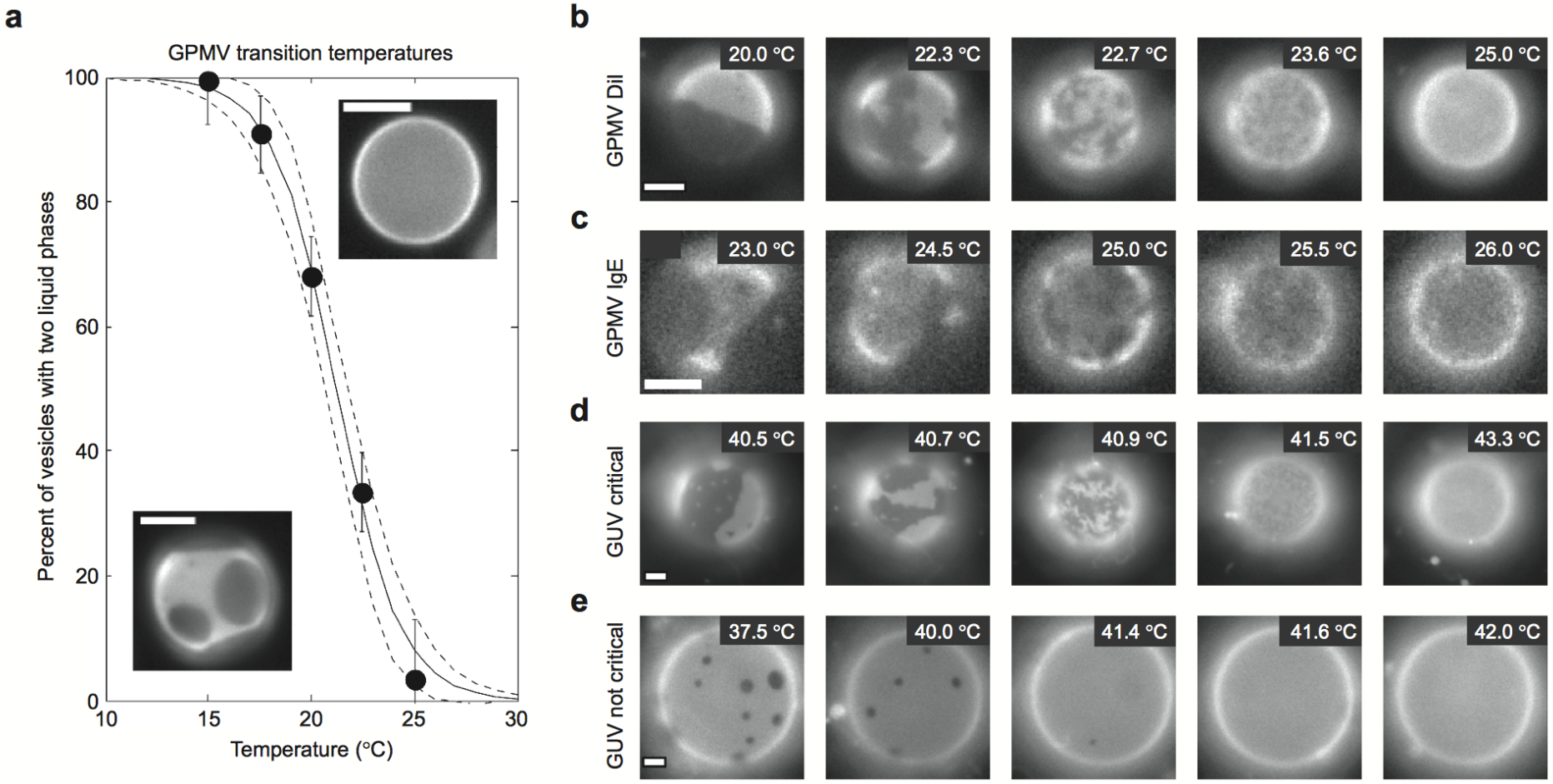
Protein-lipid curvature coupling





Drin & Antonny FEBS Letters
584 1840 (2010)

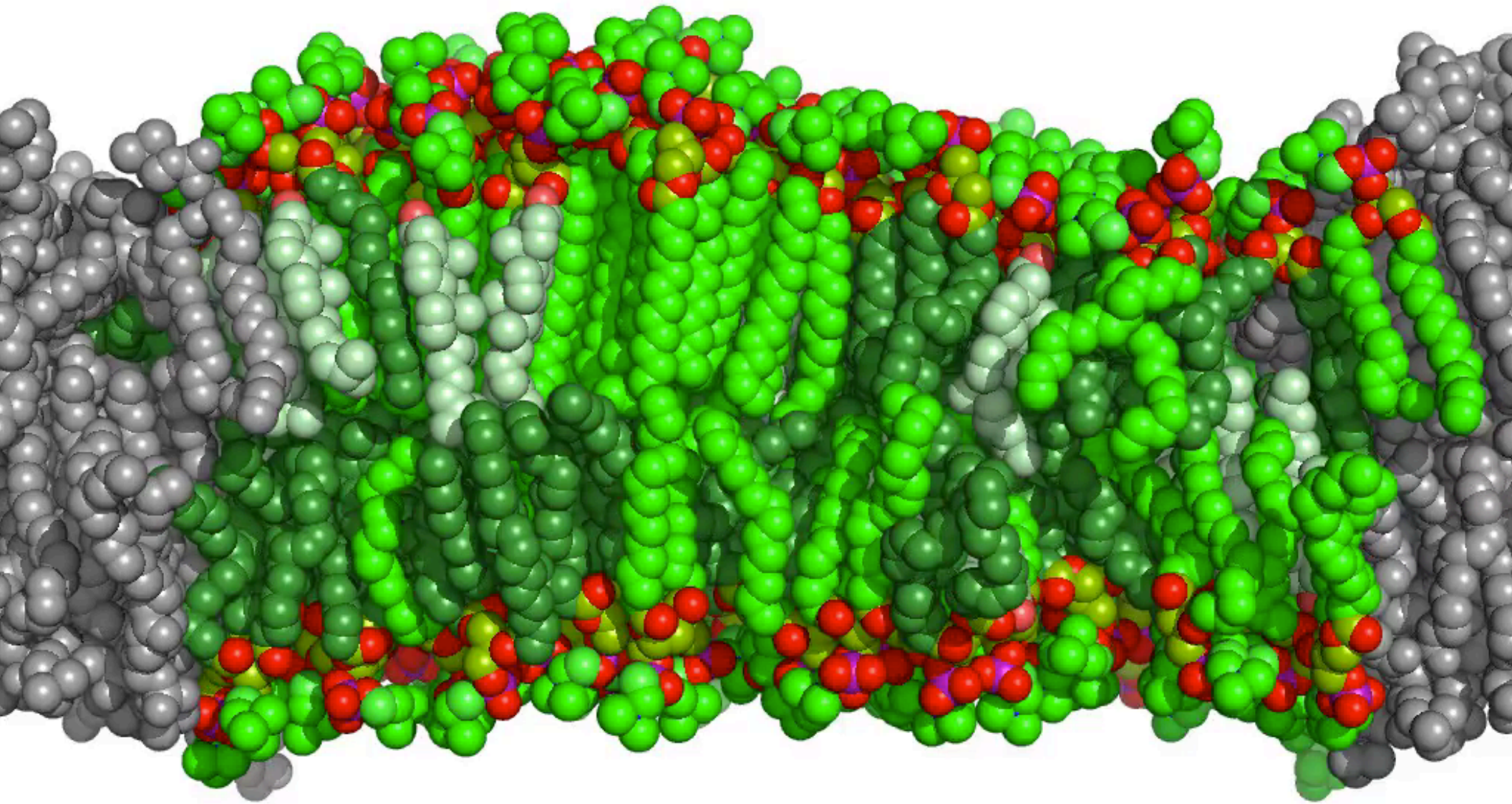
Modeling goals: lateral organization

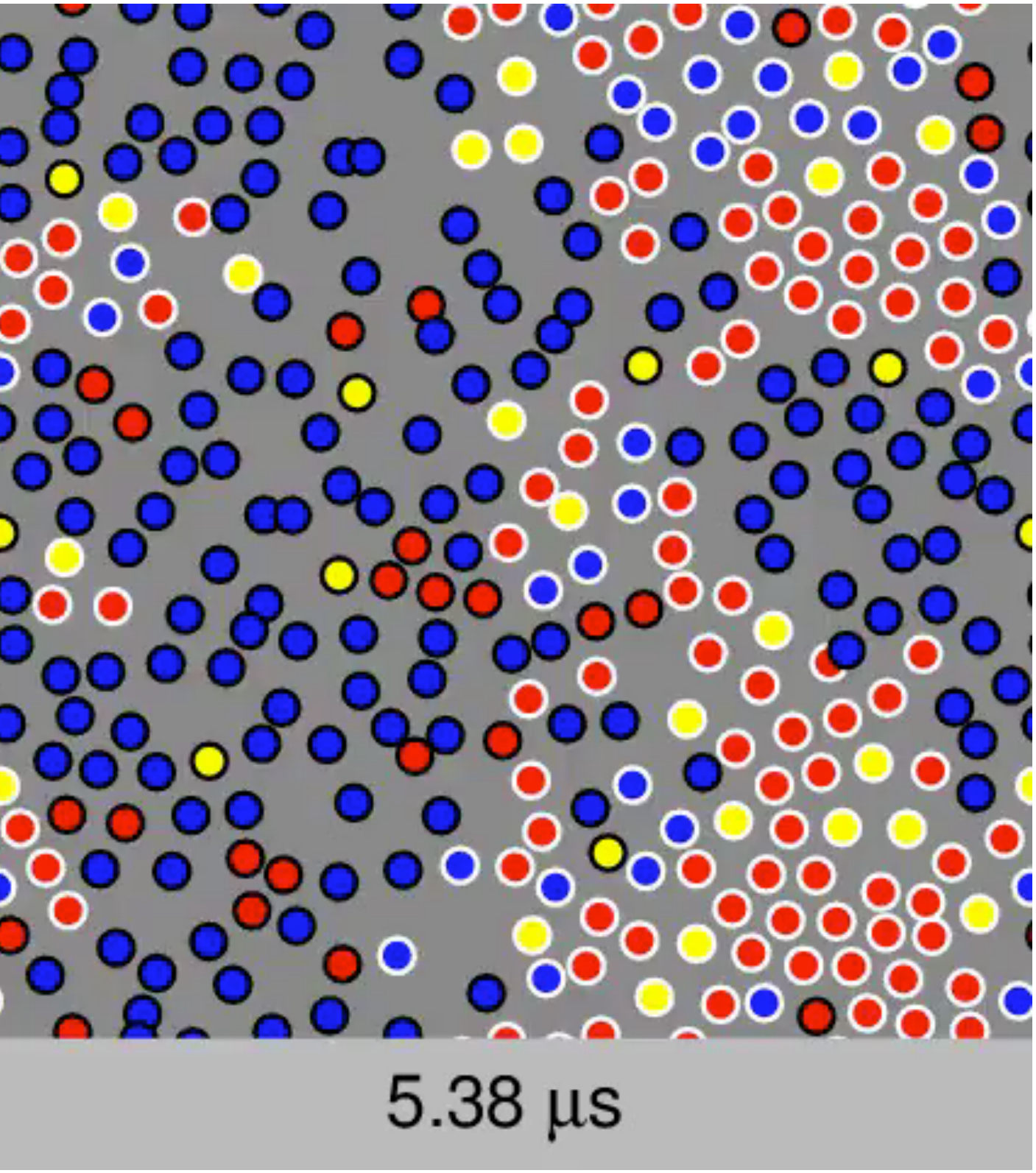


Veatch et al, ACS Chemical Biol, **3** 2008

Liquid ordered

Liquid disordered

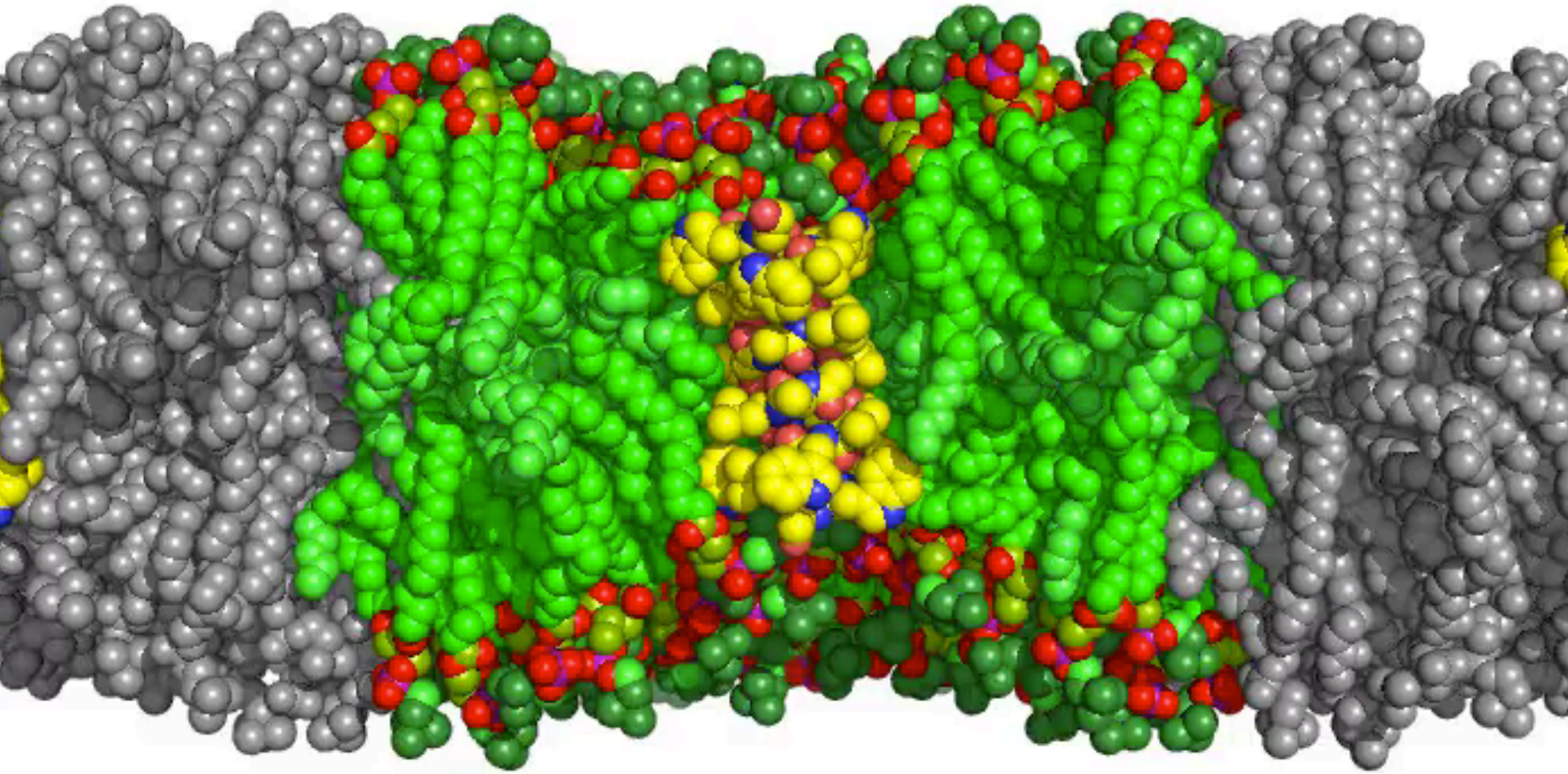




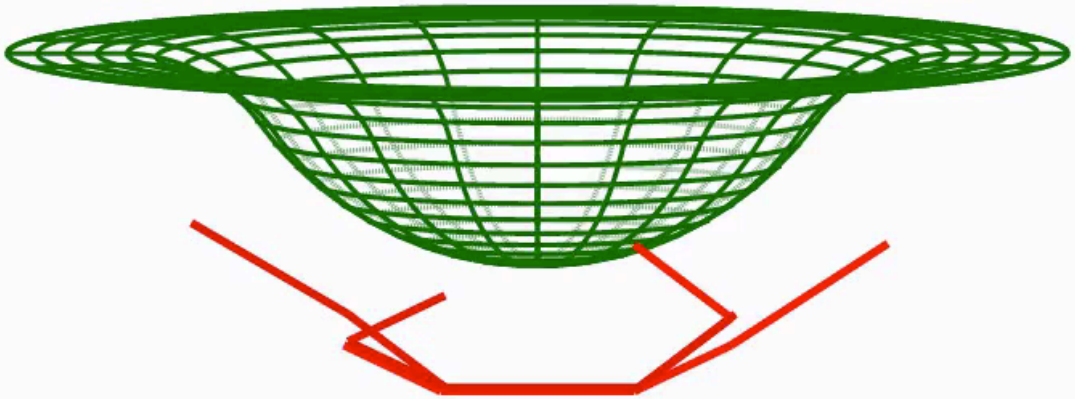
Unexpected computational technique:

Automated "structure-free" identification of domains by a hidden Markov model

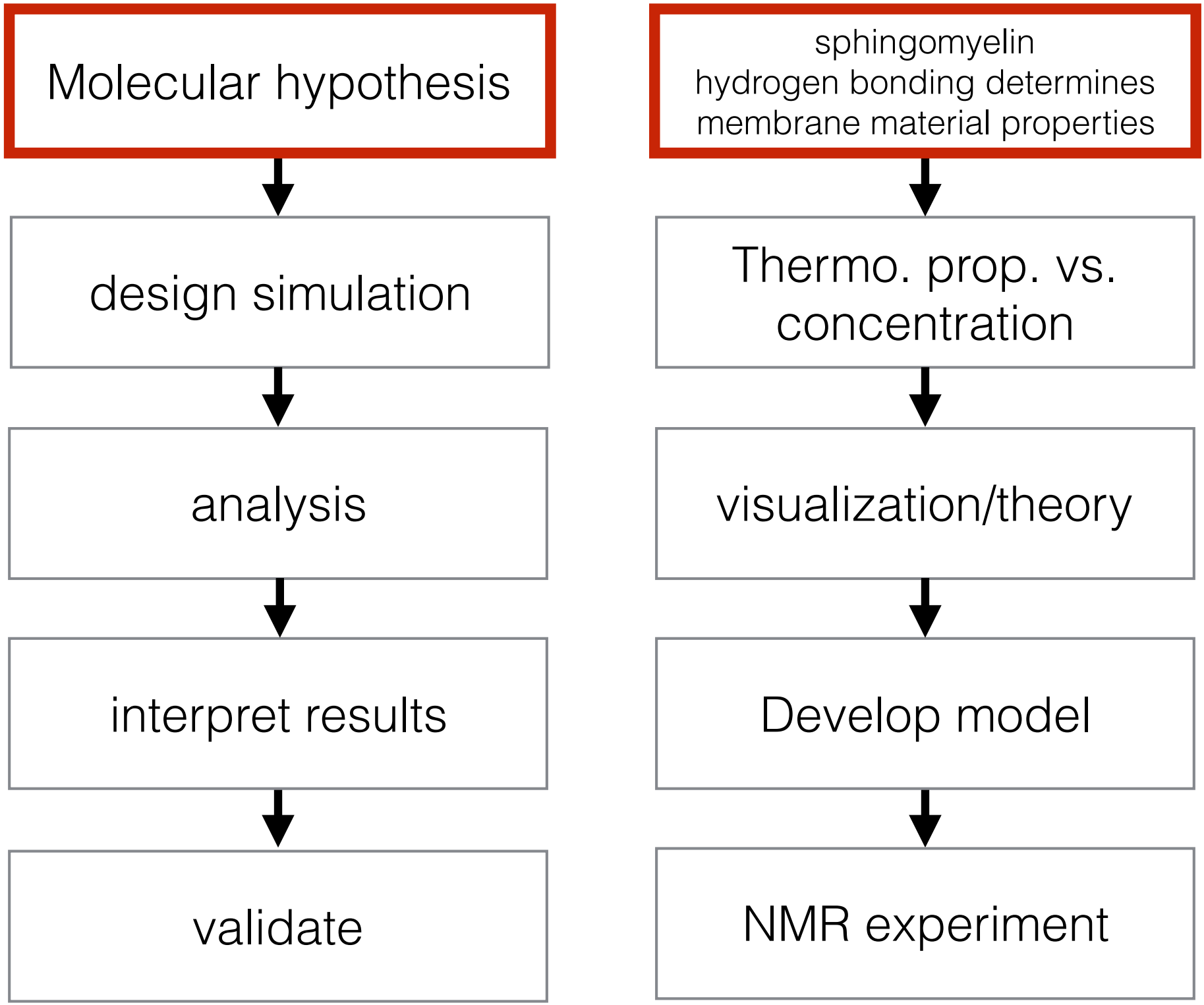
Material model of membrane deformation around a protein



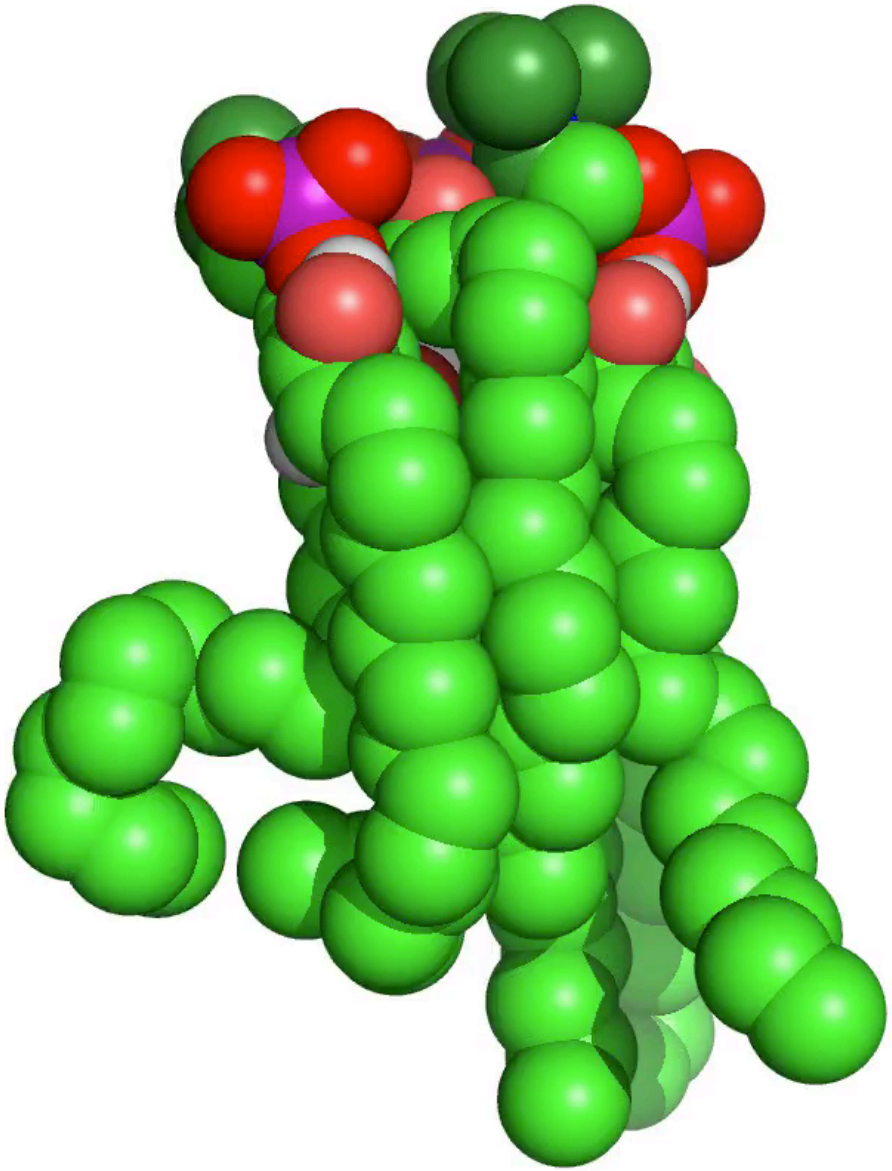
Membrane deformation energetics:

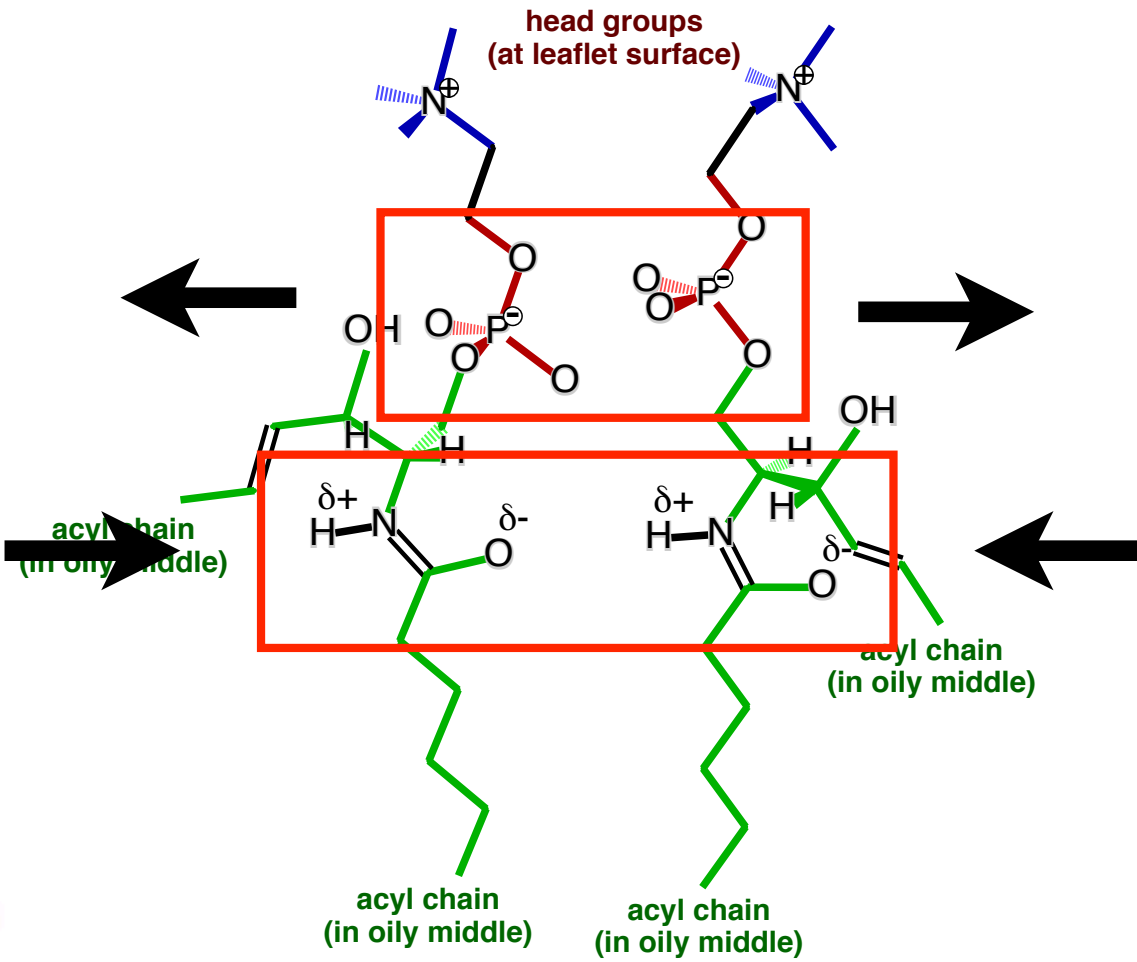


lipid composition: link of molecular property to model energy

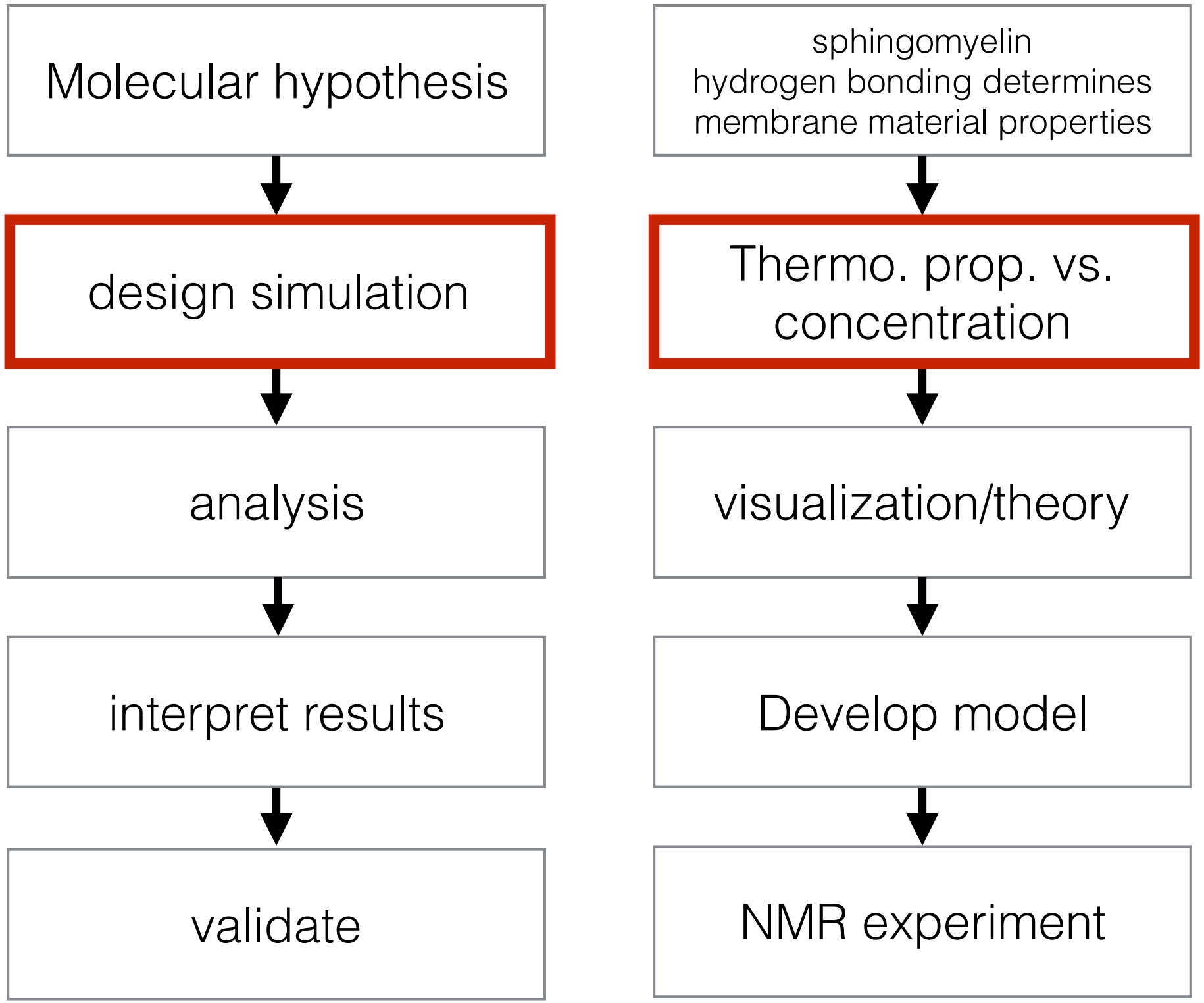

Molecular hypothesis
design simulation
analysis
interpret results
validate
sphingomyelin
hydrogen bonding determines
membrane material properties
Thermo. prop. vs.
concentration
visualization/theory
Develop model
NMR experiment

Sphingomyelin





Large positive spontaneous curvature


Molecular hypothesis
design simulation
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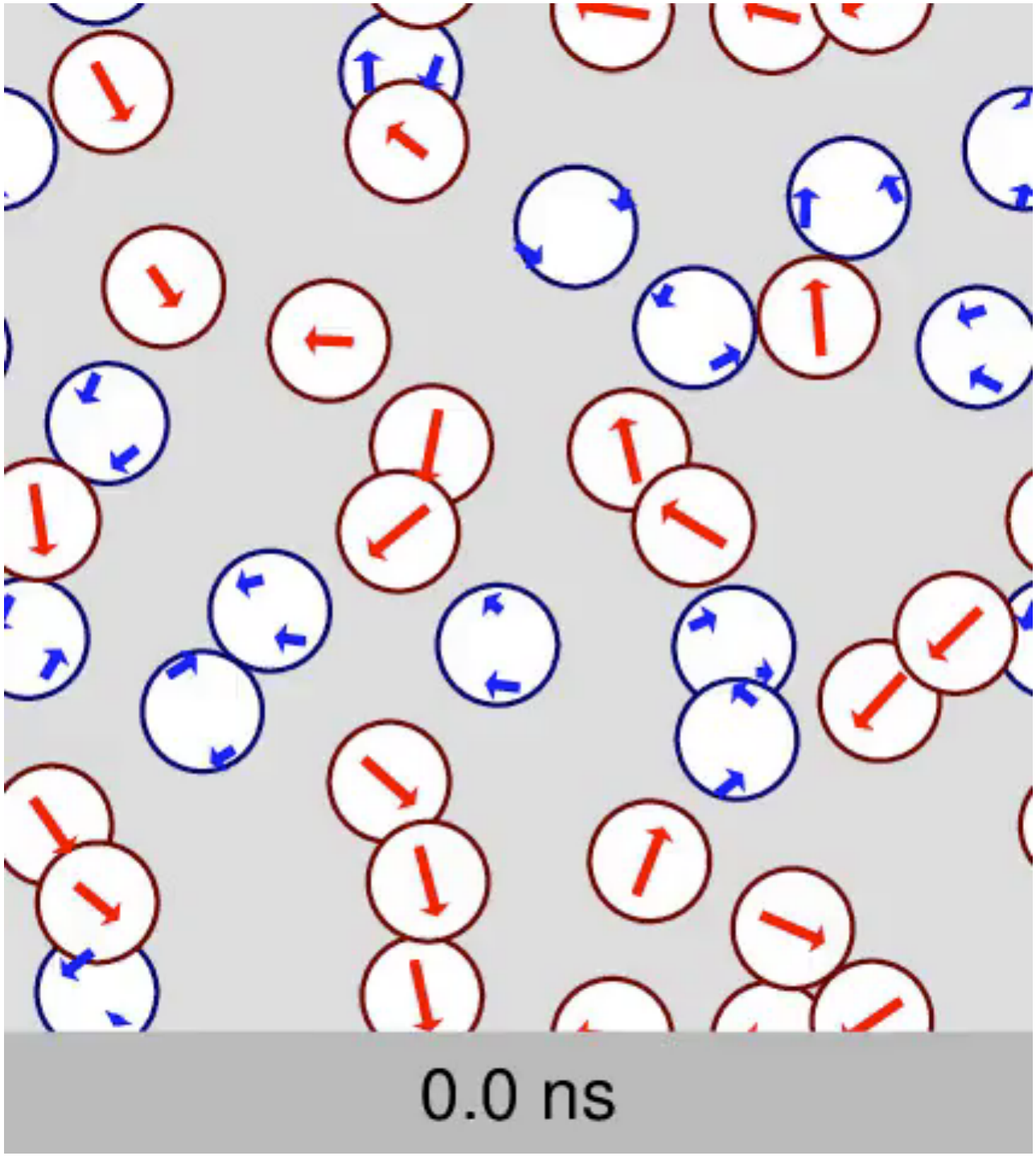
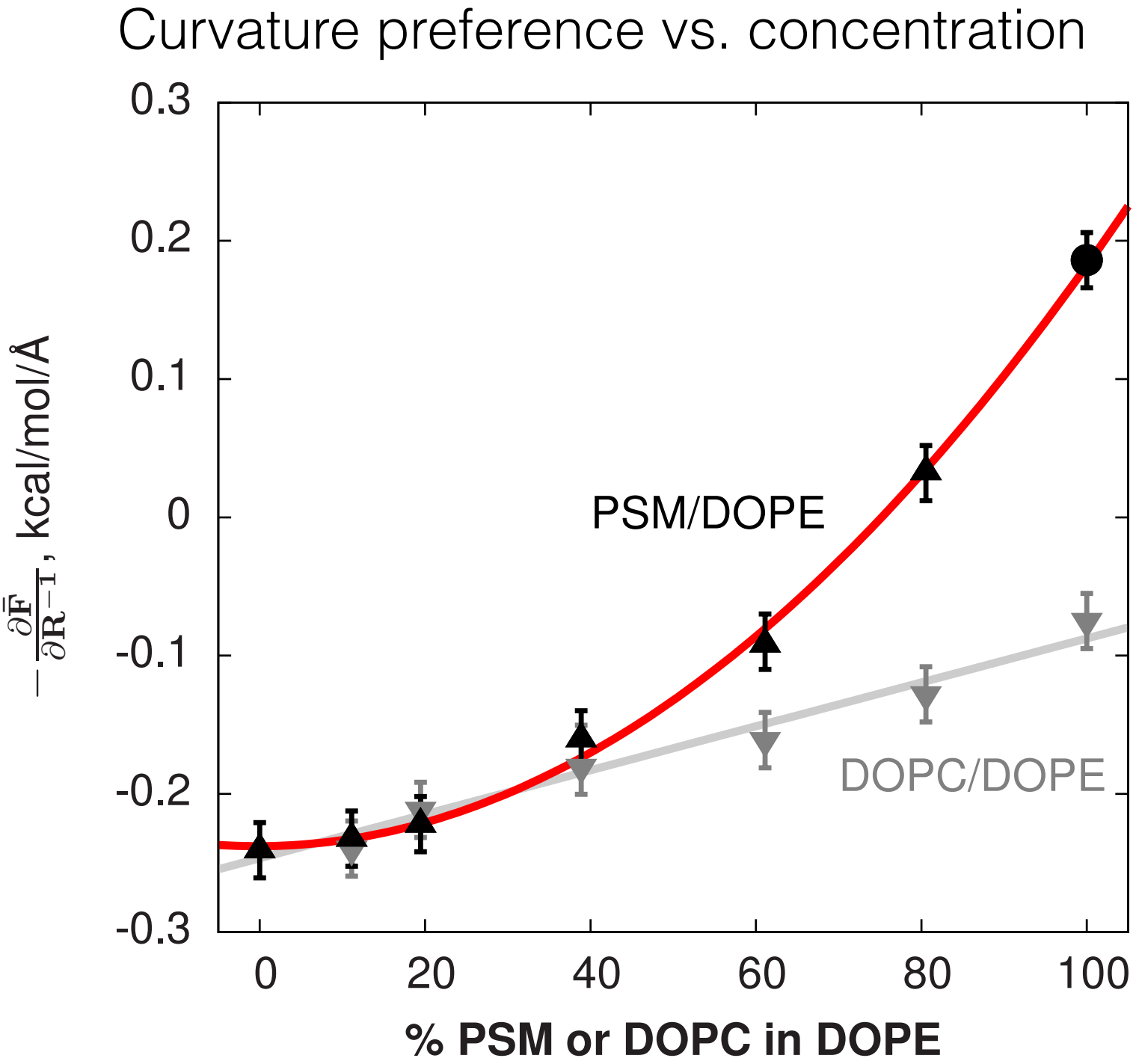
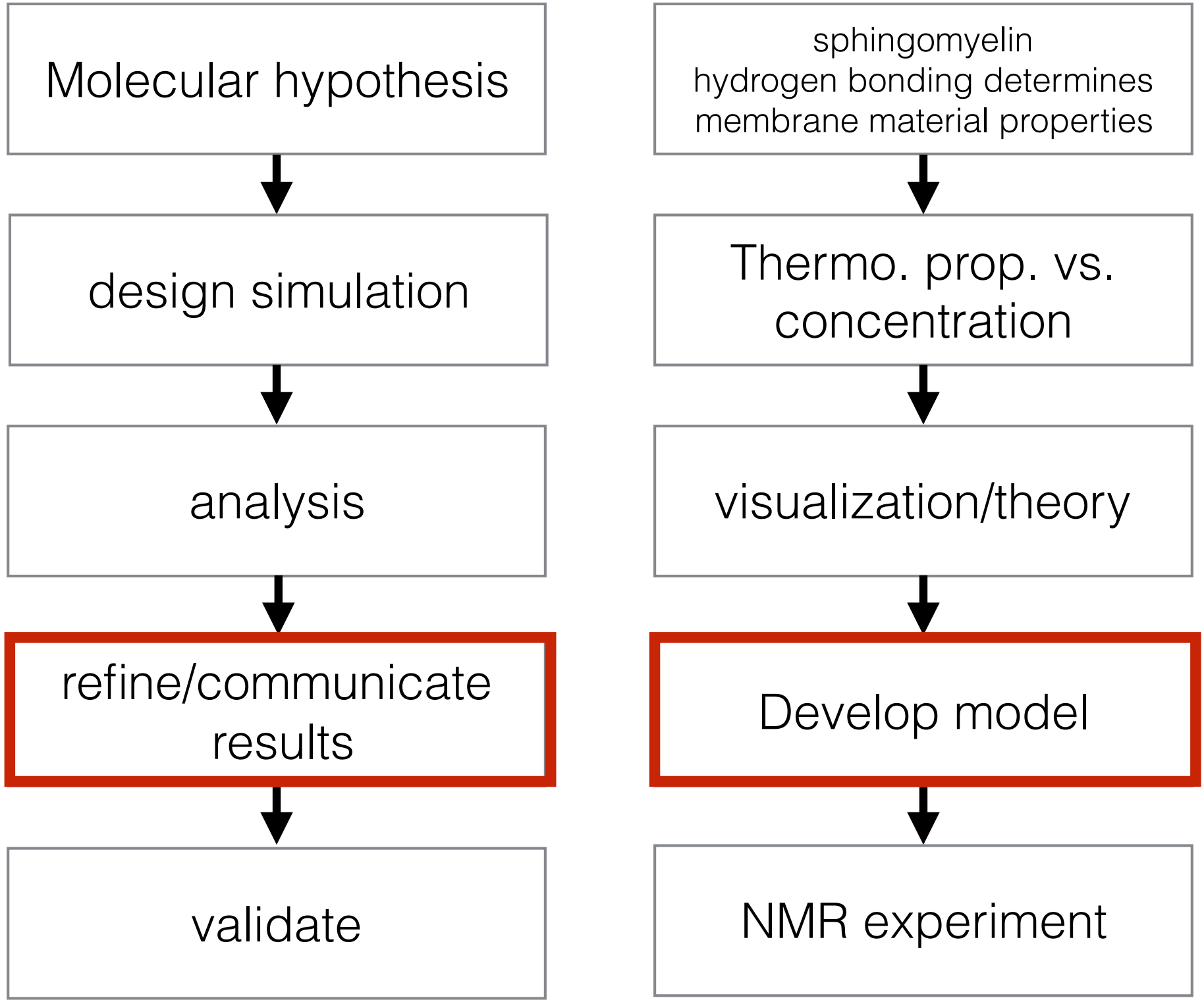
interpret results
validate
sphingomyelin
hydrogen bonding determines
membrane material properties
Thermo. prop. vs.
concentration
visualization/theory
Develop model
NMR experiment

PSM

PE




Curvature preference vs. concentration
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
$-\frac{\partial \bar{F}}{\partial R^{-1}}$, kcal/mol/Å
PSM/DOPE
DOPC/DOPE
0
20
40
60
80
100
% PSM or DOPC in DOPE


Molecular hypothesis
design simulation
analysis
refine/communicate results
validate
sphingomyelin hydrogen bonding determines membrane material properties
Thermo. prop. vs. concentration
visualization/theory
Develop model
NMR experiment

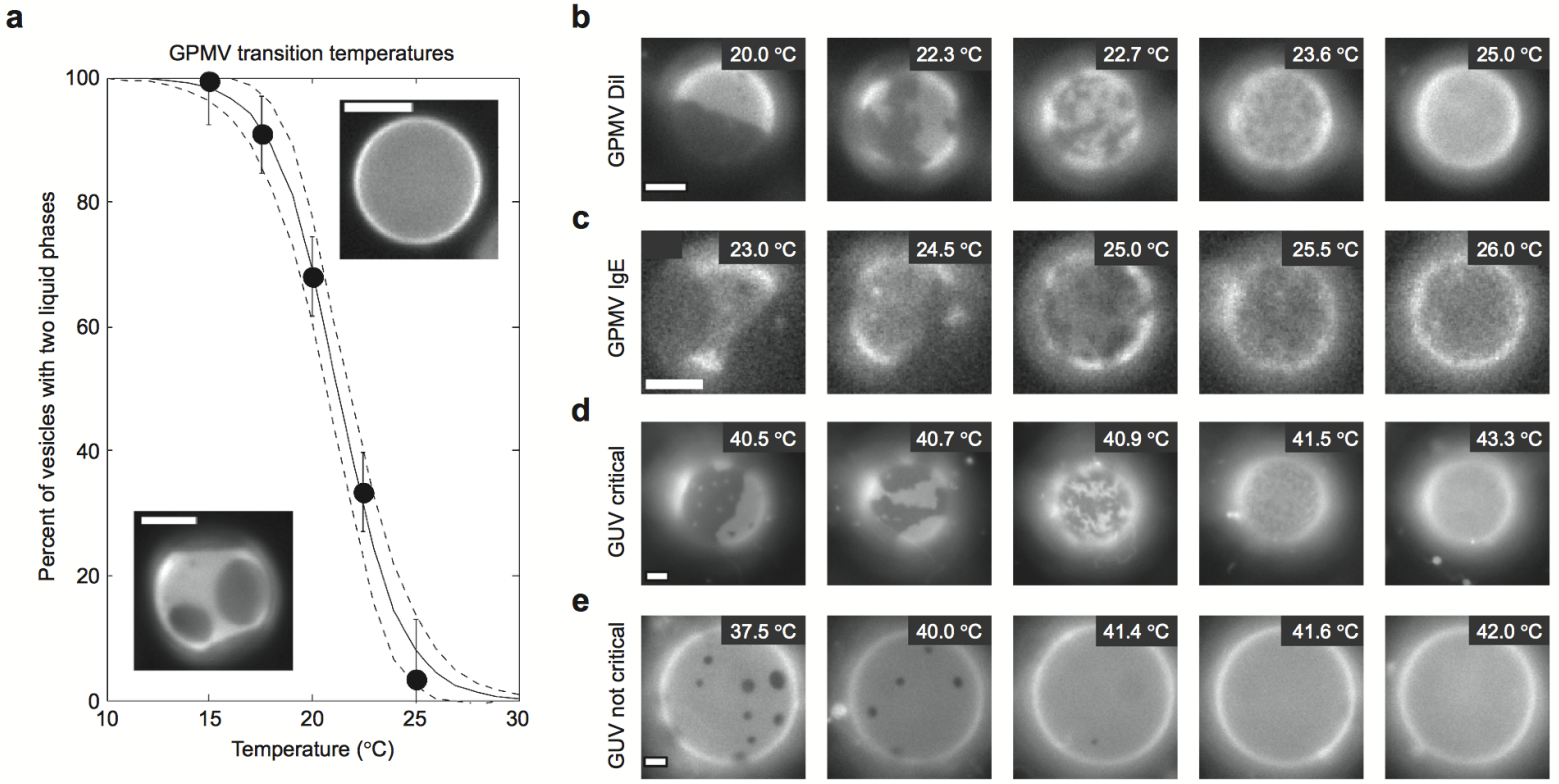
Model Development

Caveolae **(Enriched in sphingomyelin)**

Parton/Simons Nature Reviews, 2007

Model Development

sphingomyelin: favors ordered domains

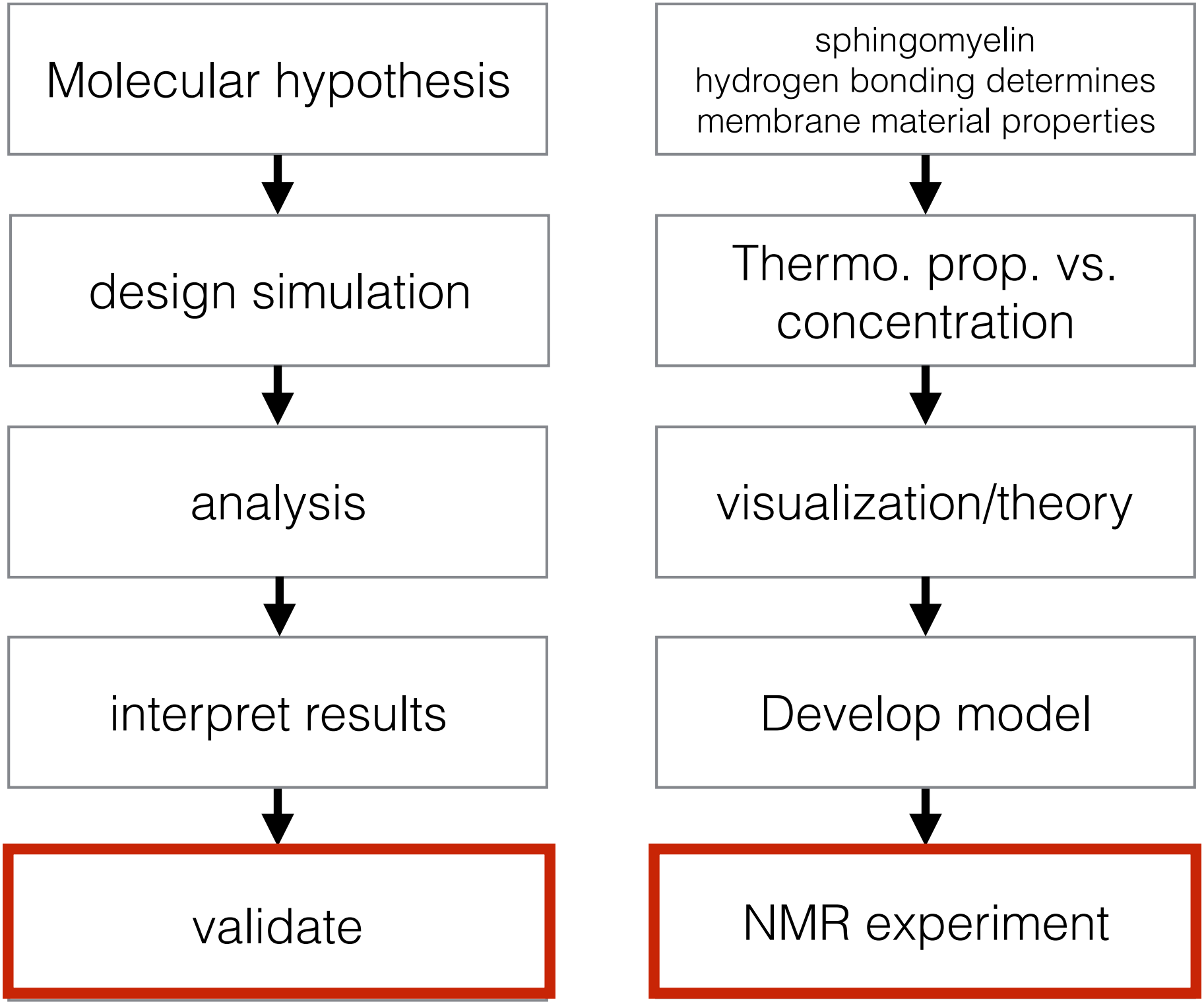


Veatch et al,
ACS Chemical Biol, **3** 2008

Mid-term goal:

Develop open-source membrane model
incorporating my theory/results (curvature, organization)
pluggable into systems biology/cell models

I will need:
creative coders with strong math background,
optimally: know how to develop with a group!

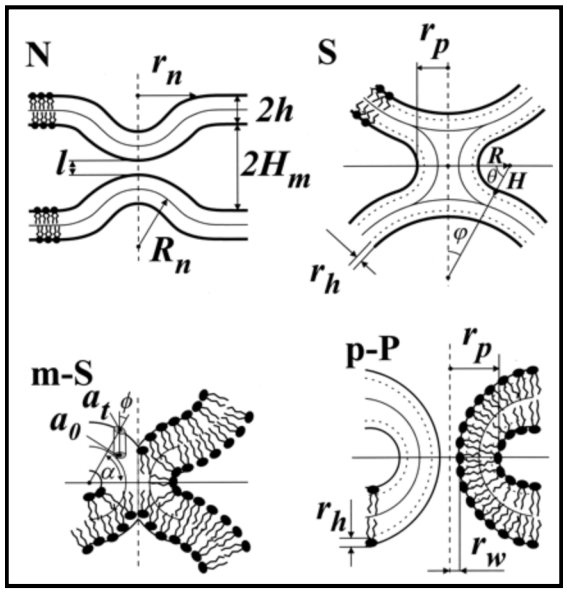

Molecular hypothesis
design simulation
analysis
interpret results
validate
sphingomyelin
hydrogen bonding determines
membrane material properties
Thermo. prop. vs.
concentration
visualization/theory
Develop model
NMR experiment

Faculty Search

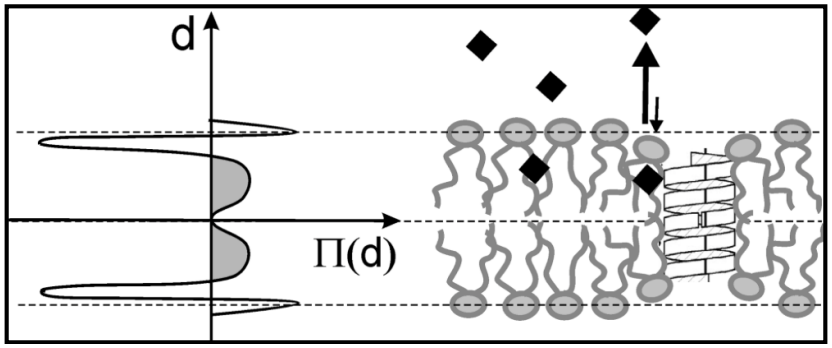
Was not given an interview at any of the research universities in the MD/DC area with multiple rounds of application:
Johns Hopkins,
U Maryland (main, Baltimore County),
American
U Delaware

Even after I got a K award (a baby R01)
I was still rejected.

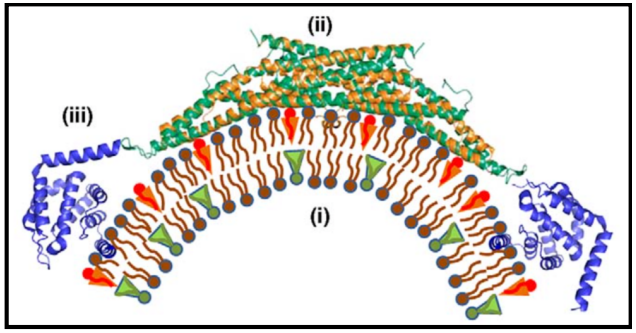
Where I was hired: My division at the NICHD includes:



Joshua Zimmerberg
Program Head,
Physical Biology
viral membrane fusion



Sergey Bezrukov
Chief, Section on Molecular Transport
membrane regulation of transport



Leonid Chernomordik
Chief, Section on Membrane Biology
membrane remodeling in biology

all experimentalists

Director

Dr. Francis Collins

previously le
humane genome project

my building!
(schd for demolition 2013)

~1200 Investigators
10% strong computational interest

Another American with Ebola will be flown to NIH in Bethesda

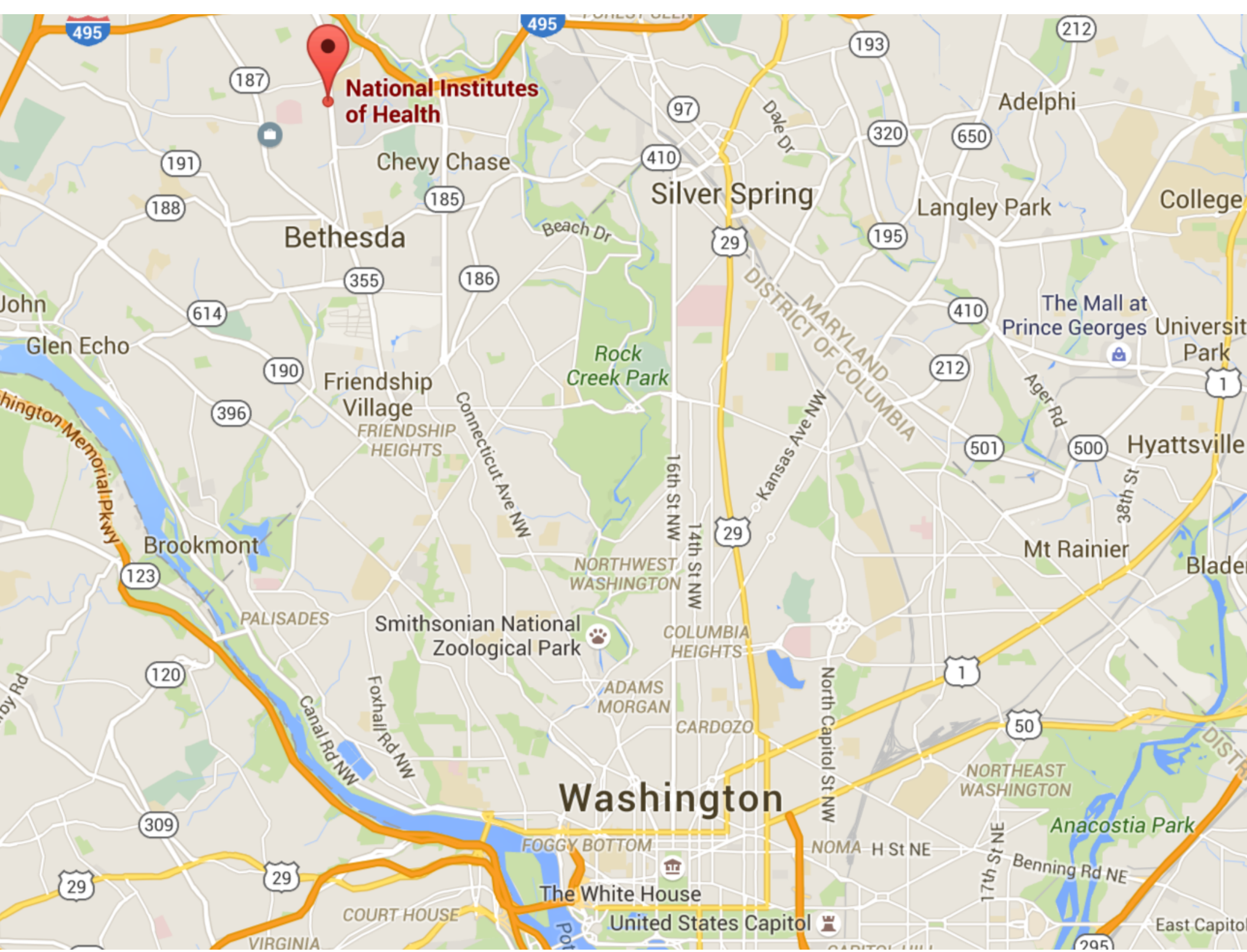
A | 99 | Save for Later | Reading List

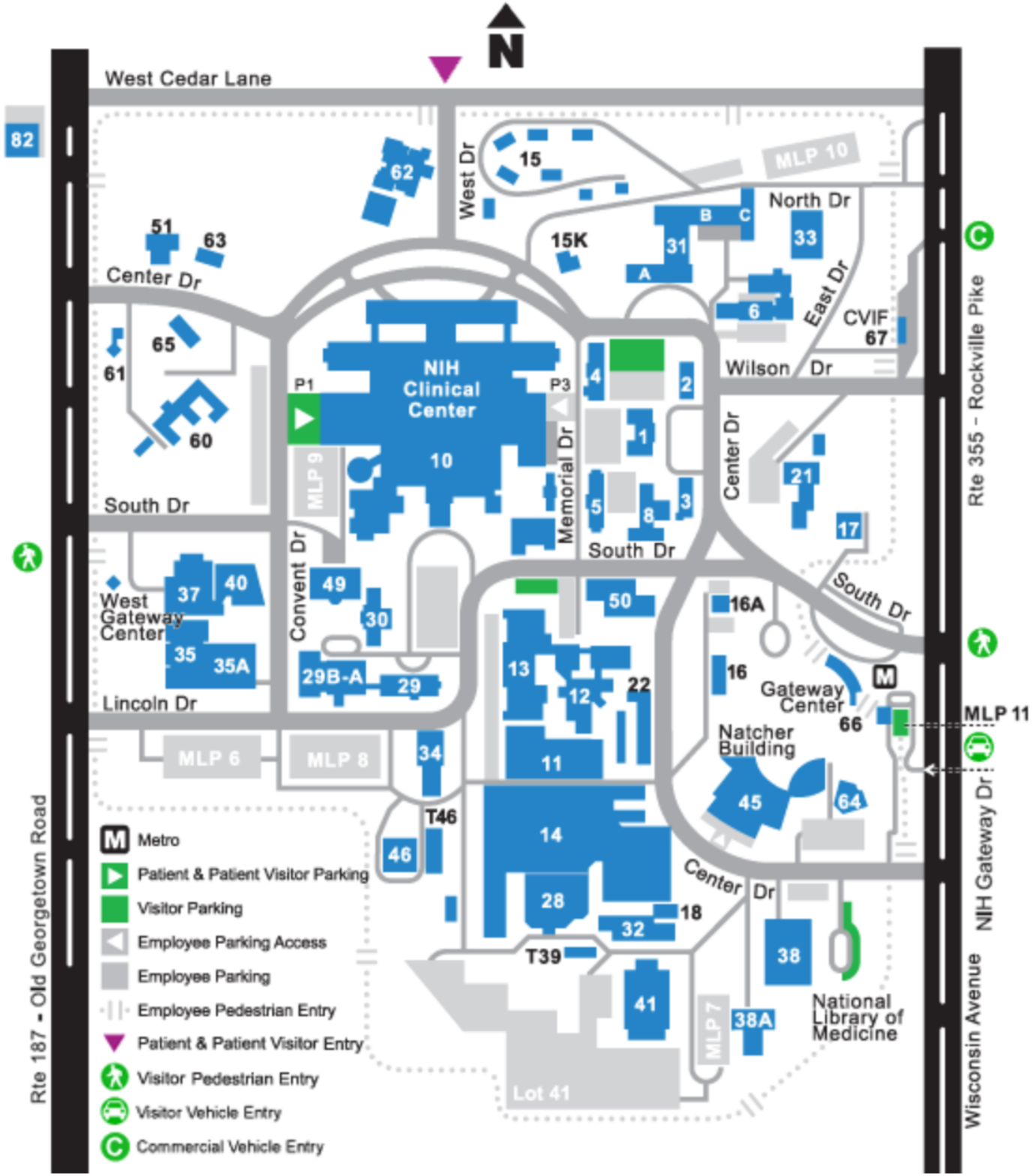
Alberto Cagigi is beginning the multi-step process of identifying antibodies against Ebola in samples from vaccinated volunteers at the National Institutes of Health in Bethesda, Md., on Feb. 4. (Cliff Owen/AP)

By Julie Zauzmer March 12, 2015 Follow @JulieZauzmer

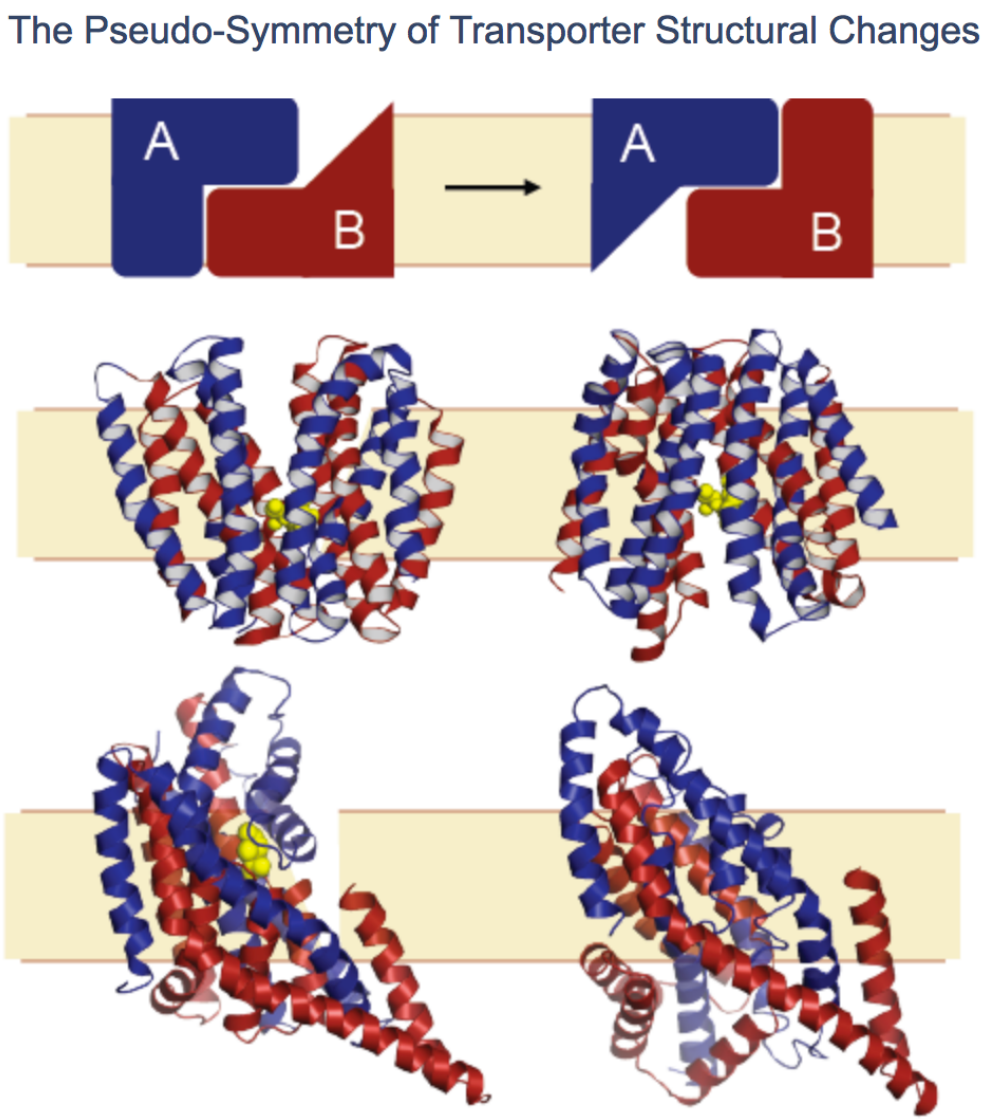
An American health-care worker has come down with Ebola and will be transported to the National Institutes of Health in Bethesda for treatment, NIH announced in a news release on Thursday.

Most Read


National Institutes of Health
Chevy Chase
Bethesda
Silver Spring
Adelphi
Langley Park
College
Glen Echo
Friendship Village
FRIENDSHIP HEIGHTS
Rock Creek Park
The Mall at Prince Georges
Hyattsville
Brookmont
PALISADES
Smithsonian National Zoological Park
NORTHWEST WASHINGTON
COLUMBIA HEIGHTS
ADAMS MORGAN
CARDOZO
Mt Rainier
NORTHEAST WASHINGTON
Anacostia Park
Washington
FOGGY BOTTOM
NOMA
The White House
United States Capitol
COURT HOUSE
VIRGINIA
Connecticut Ave NW
16th St NW
14th St NW
Kansas Ave NW
North Capitol St NW
Foxhall Rd NW
Canal Rd NW
Beach Dr
Dale Dr
Ager Rd
38th St
Benning Rd NE
MARYLAND
DISTRICT OF COLUMBIA
Washington Memorial Pkwy
495
187
191
188
185
97
410
193
212
320
650
195
355
186
614
190
396
501
500
123
120
309
29
50
1


N
West Cedar Lane
82
West Dr
15
MLP 10
North Dr
62
51
63
Center Dr
15K
B
C
31
A
33
East Dr
6
CVIF
67
65
61
NIH
Clinical
Center
10
P1
P3
4
2
1
Wilson Dr
Center Dr
60
MLP 9
Memorial Dr
5
8
3
21
South Dr
17
South Dr
Convent Dr
49
50
16A
37
40
West
Gateway
Center
30
35
35A
29B-A
29
13
12
22
16
Gateway
Center
M
66
MLP 11
Lincoln Dr
MLP 6
MLP 8
34
11
Natcher
Building
45
64
T46
46
14
Center Dr
28
18
32
38
T39
41
MLP 7
38A
National
Library of
Medicine
Lot 41
Rte 187 - Old Georgetown Road
Rte 355 - Rockville Pike
NIH Gateway Dr
Wisconsin Avenue
M Metro
Patient & Patient Visitor Parking
Visitor Parking
Employee Parking Access
Employee Parking
Employee Pedestrian Entry
Patient & Patient Visitor Entry
Visitor Pedestrian Entry
Visitor Vehicle Entry
C Commercial Vehicle Entry

Lucy Forrest



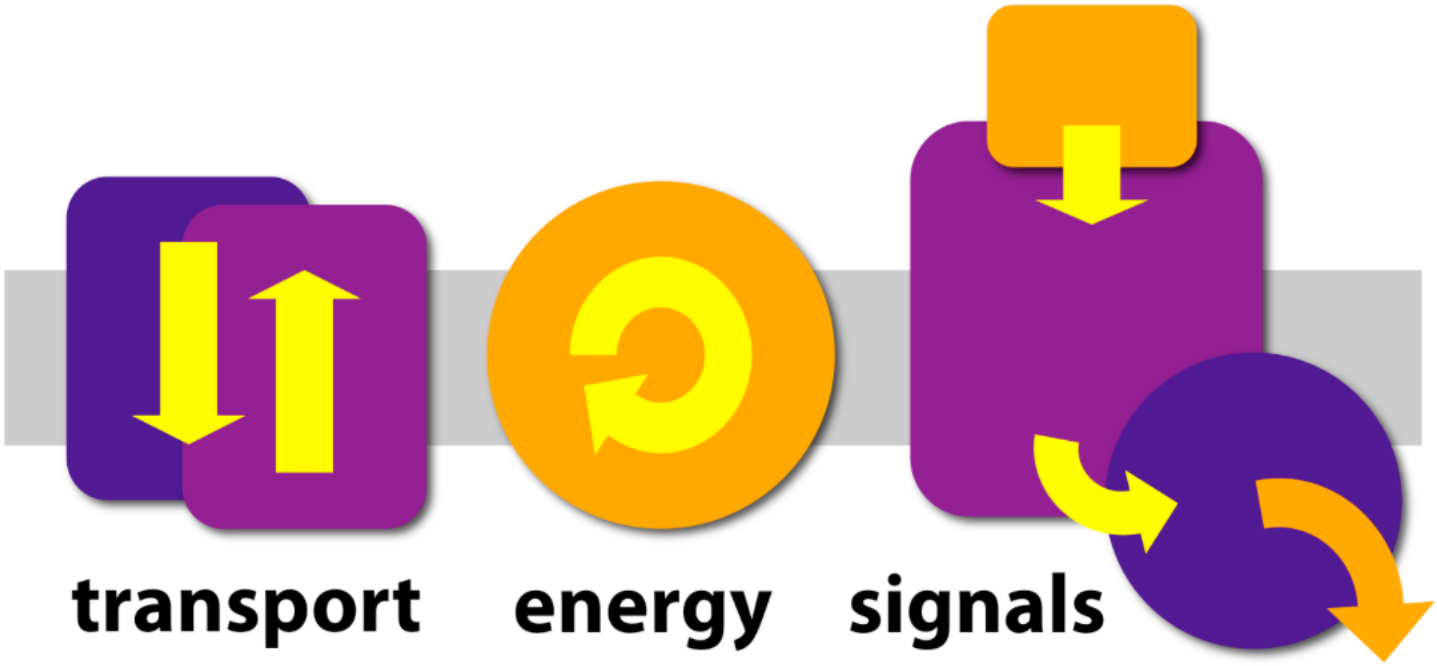
Relating structure/
sequence
to mechanism

AlignMe
software

http://
www.bioinfo.mpg.de/
AlignMe/faq.html

https://neuroscience.nih.gov/ninds/Faculty/Profile/lucy-forrest.aspx

Jose Faraldo-Gomez



Specific channel function
free energy methodology

http://www.faraldolab.org

Robert Best

- Balance of secondary structure in forcefields.
- Modeling protein folding kinetics using reduced diffusion to capture off-path dynamics.
- Protein folding mechanisms

Part of chemical physics lab including
Attila Szabo
Ad Bax (NMR)

http://spin.niddk.nih.gov/best/home.html

Computation at the NIH

Partition	FreeNds	FreeCPUs	Per-Node Resources Cores	CPUs	Mem	Disk
norm*	0/310	2542/7754	16	32	124g	800g
unlimited	0/14	0/234	16	32	124g	800g
niddk	26/86	1168/2736	16	32	124g	800g
ibfdr	39/191	1248/6112	16	32	61g	800g
ibqdr	2/102	64/3264	16	32	30g	400g
ibqdr	38/99	1216/3168	16	32	61g	400g
gpu	12/14	164/168	12	12	45g	600g
gpu	0/20	96/608	16	32	124g	800g
gpu	0/4	16/112	16	32	124g	800g

Biowulf

ca. 5000 cores
for Pastor/Brooks labs

http://www.lobos.nih.gov

Opportunities now

https://www.training.nih.gov/programs/sip

Summer internships: high school/undergrad/grad

EDUCATION LEVEL COMPLETED		MONTHLY STIPEND
HIGH SCHOOL	Before Graduation	$1,740
	After Graduation	$1,940
UNDERGRADUATE	After 1 year	$2,040
	After 2 years	$2,140
	After 3 years or >	$2,240
GRADUATE	Less than 1 year	$2,340
	After 1 year	$2,660
	After 2 years	$2,960
	After 3 years or >	$3,160

Opportunities now

https://www.training.nih.gov/programs/postbac_irta

Application is probably equivalent to grad school.
You must convince an NIH PI to offer you a job, probably with a convincing personal appeal.

POSTBACCALAUREATE IRTA STIPEND RANGES FOR ALL AREAS - Discretionary for Montana (RML-NIAID)

YEARS OF EXPERIENCE	INITIAL STIPEND	SECOND YEAR
0-1 year	$27,700	$29,700
1-2 years	$29,700	$31,000

Anxieties during a long job search

Could I work on a problem I was not obsessed with?
Had I become dependent on my obsession to do things others couldn't do?

Could I work in a group?
I've developed a lone-wolf short-term focused coding strategy

Could I accept a solution that wasn't correct, but that worked