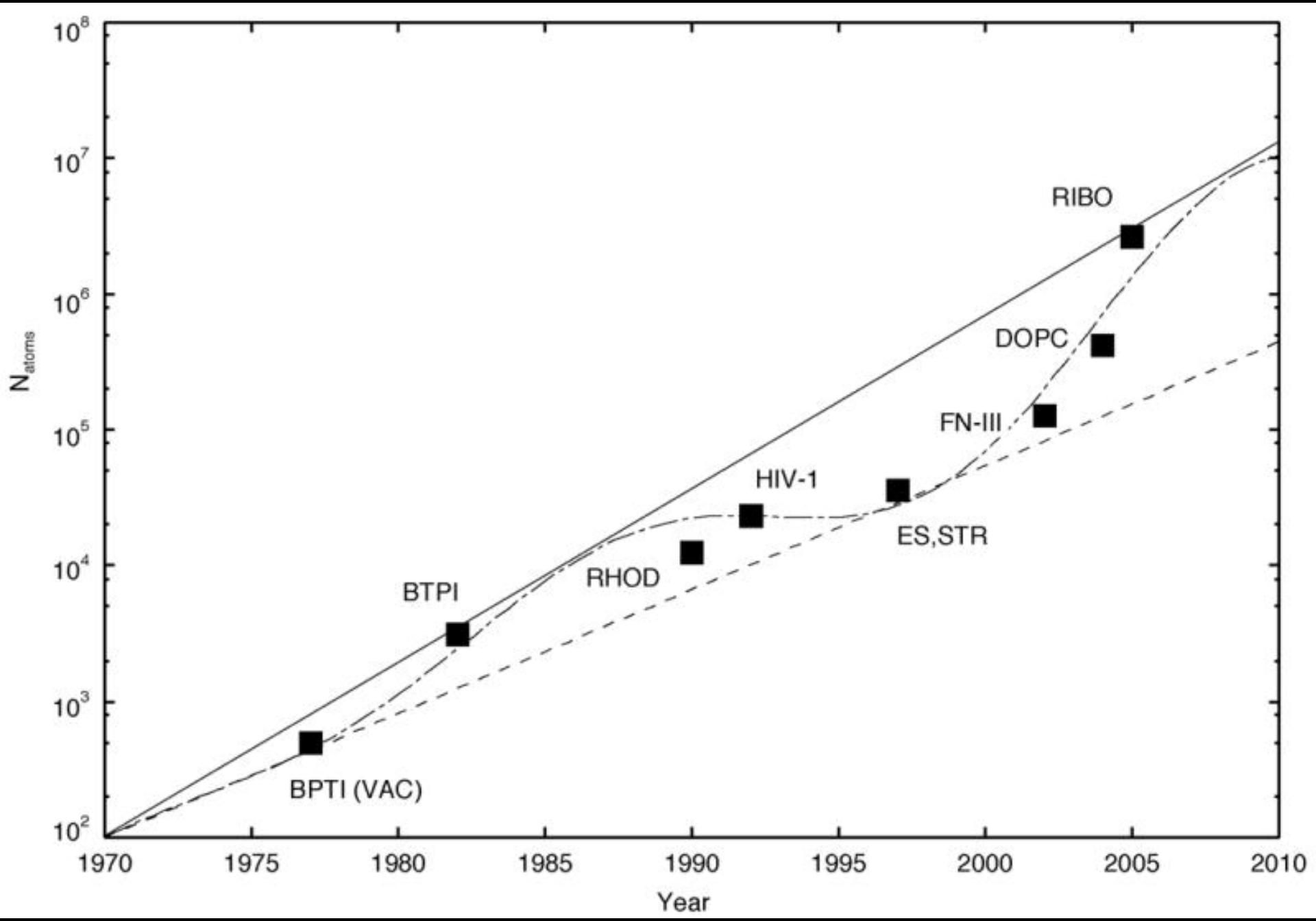
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10^7
10^6
10^5
10^4
10^3
10^2
N_{atoms}
1970
1975
1980
1985
1990
1995
2000
2005
2010
Year
RIBO
DOPC
FN-III
HIV-1
ES,STR
RHOD
BTPI
BPTI (VAC)

Simulations of Biomolecules Using Molecular Dynamics

Introduction

The first molecular dynamics simulation of a biomolecule was a simulation of bovine pancreatic trypsin inhibitor (BPTI) in 1977 [J. A. McCammon, B. R. Gelin, and M. Karplus, *Nature* **267,** 585 (1977)]. BPTI was chosen for simulation because it is relatively small (58 residues) and a high-resolution x-ray crystal structure was available at the time (Figure 1). The simulation was carried out in vacuum and was 9.2 ps in length.

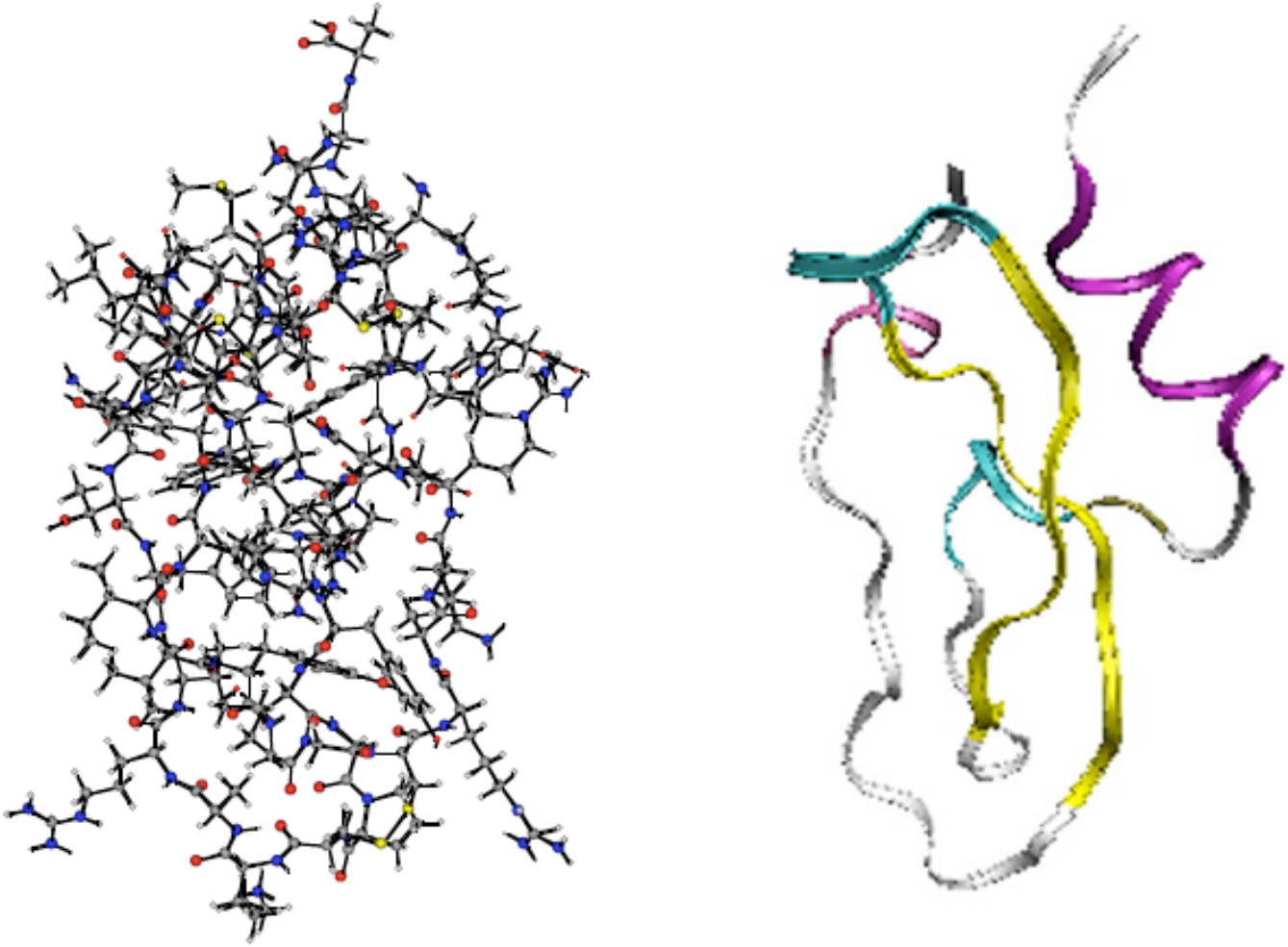
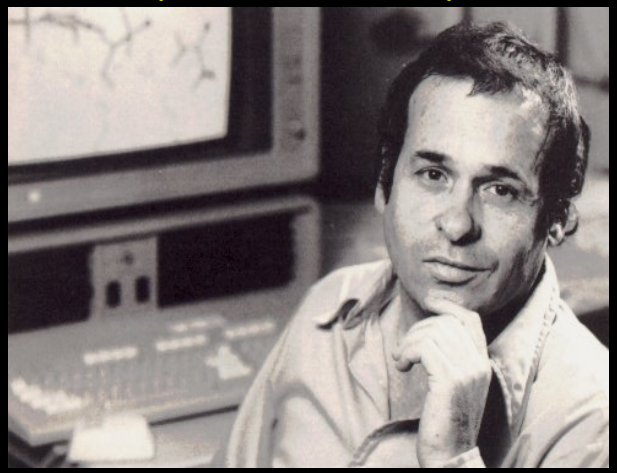


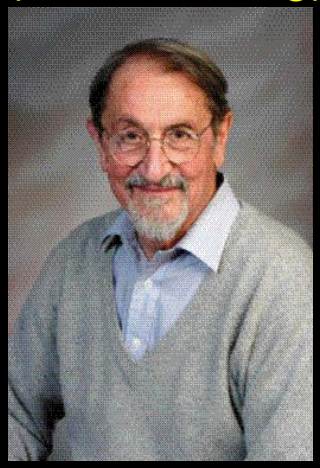
Figure 1. Atomic model and ribbon diagram of BPTI.

Arieh Warshel
(Sneior Lifson)



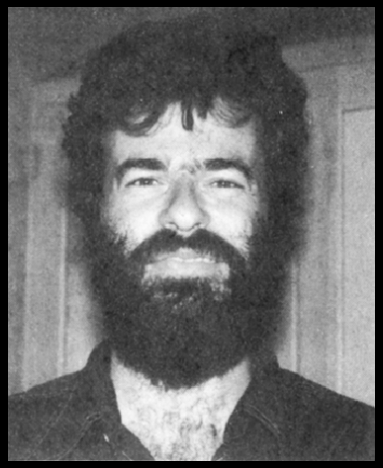
CFF (1967)
Consistent Force Field

Martin Karplus
(Linus Pauling)



CHARMM

Peter Kollman



AMBER (1981)

Klaus Schulten

NAMD

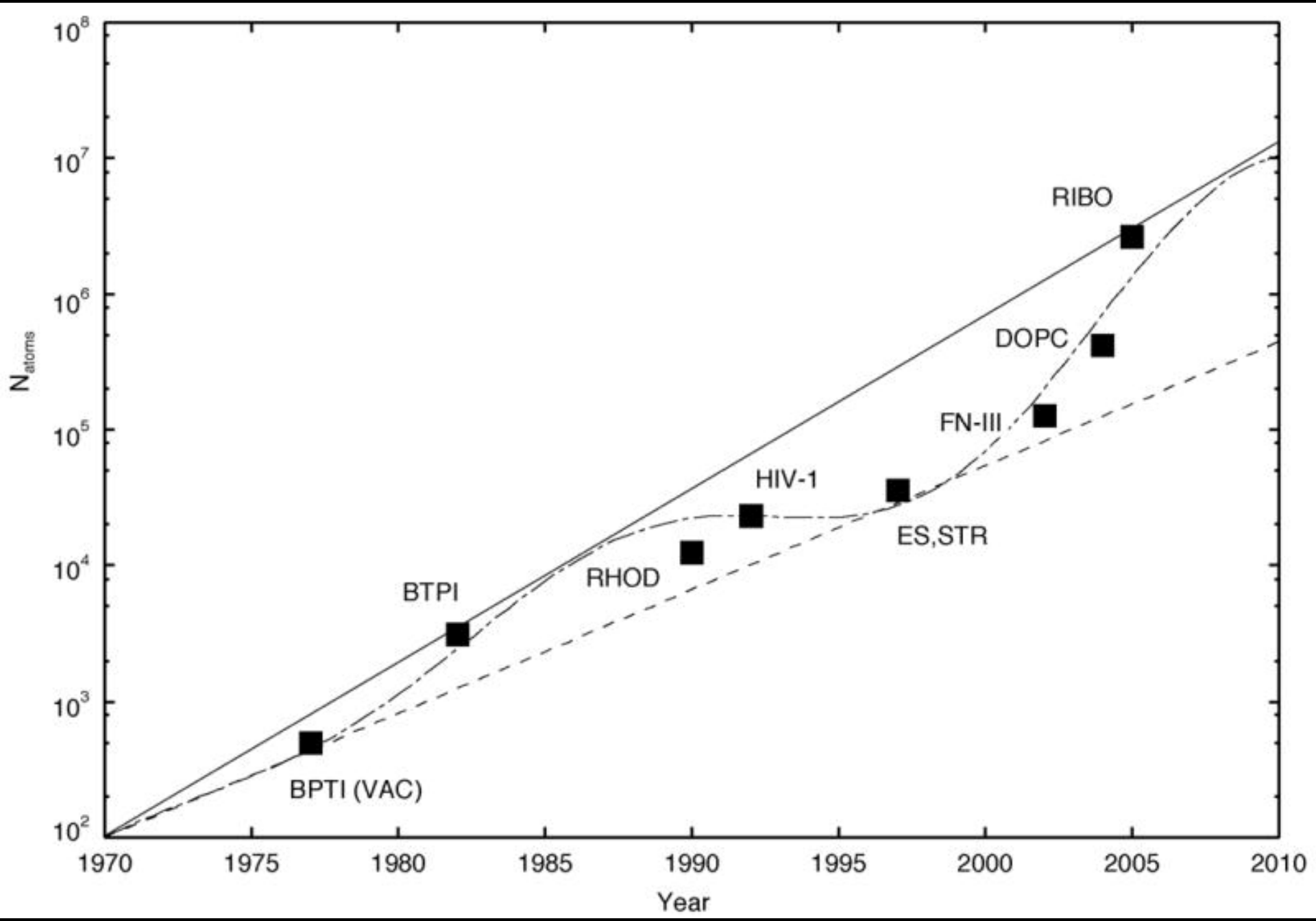
Michael Levitt
(John Kendrew)

Andy McCammon

Bruce Gellin

WEIZAC
GOLEM

BPTI (1977)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10^3
10^2
N_{atoms}
1970
1975
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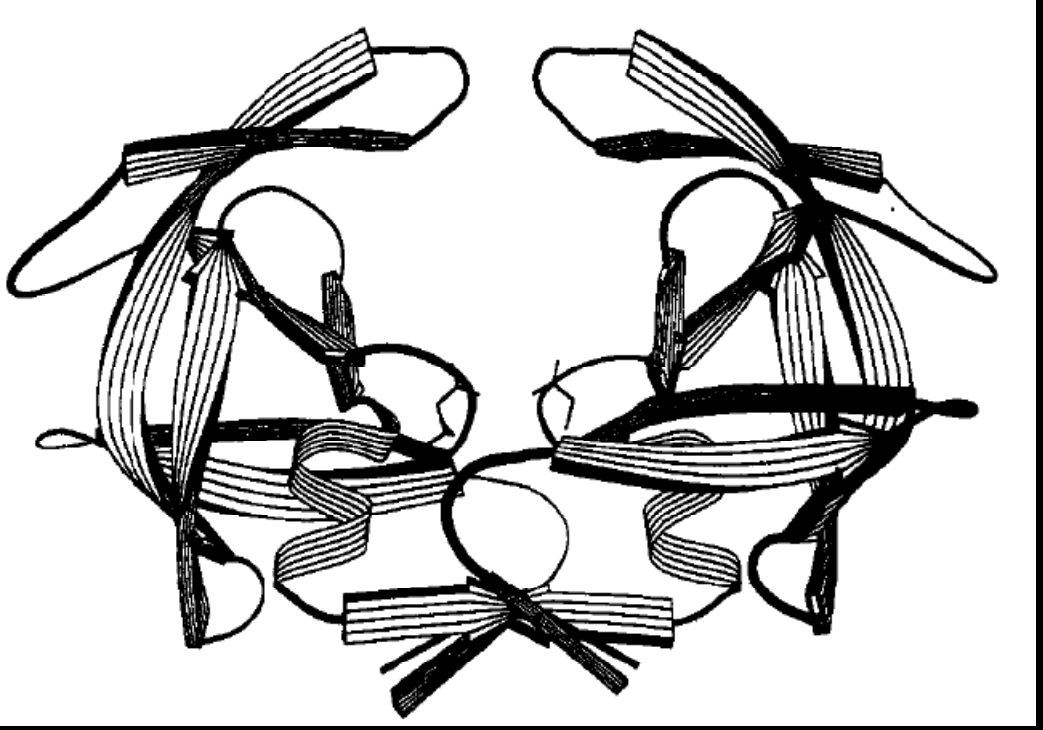
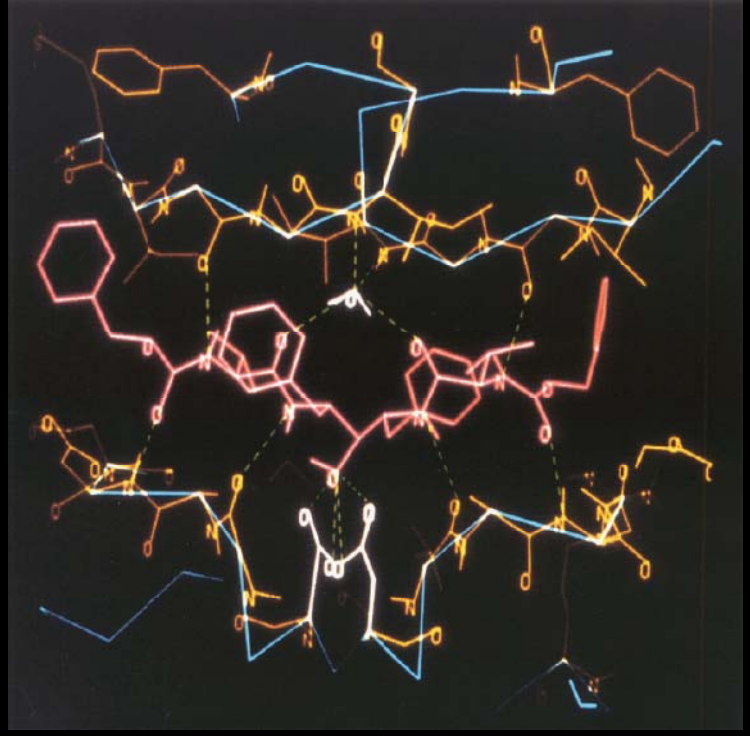
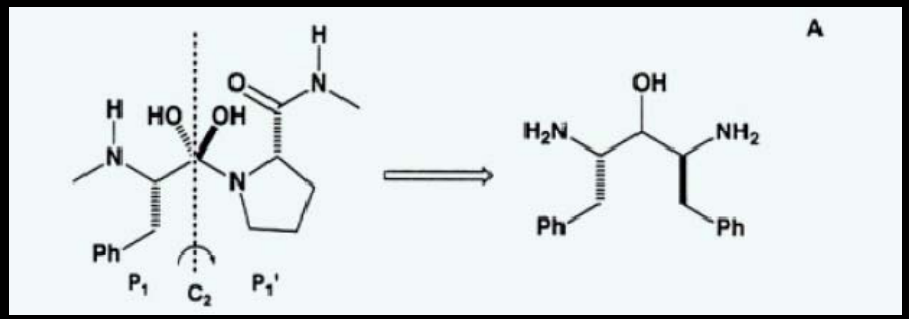
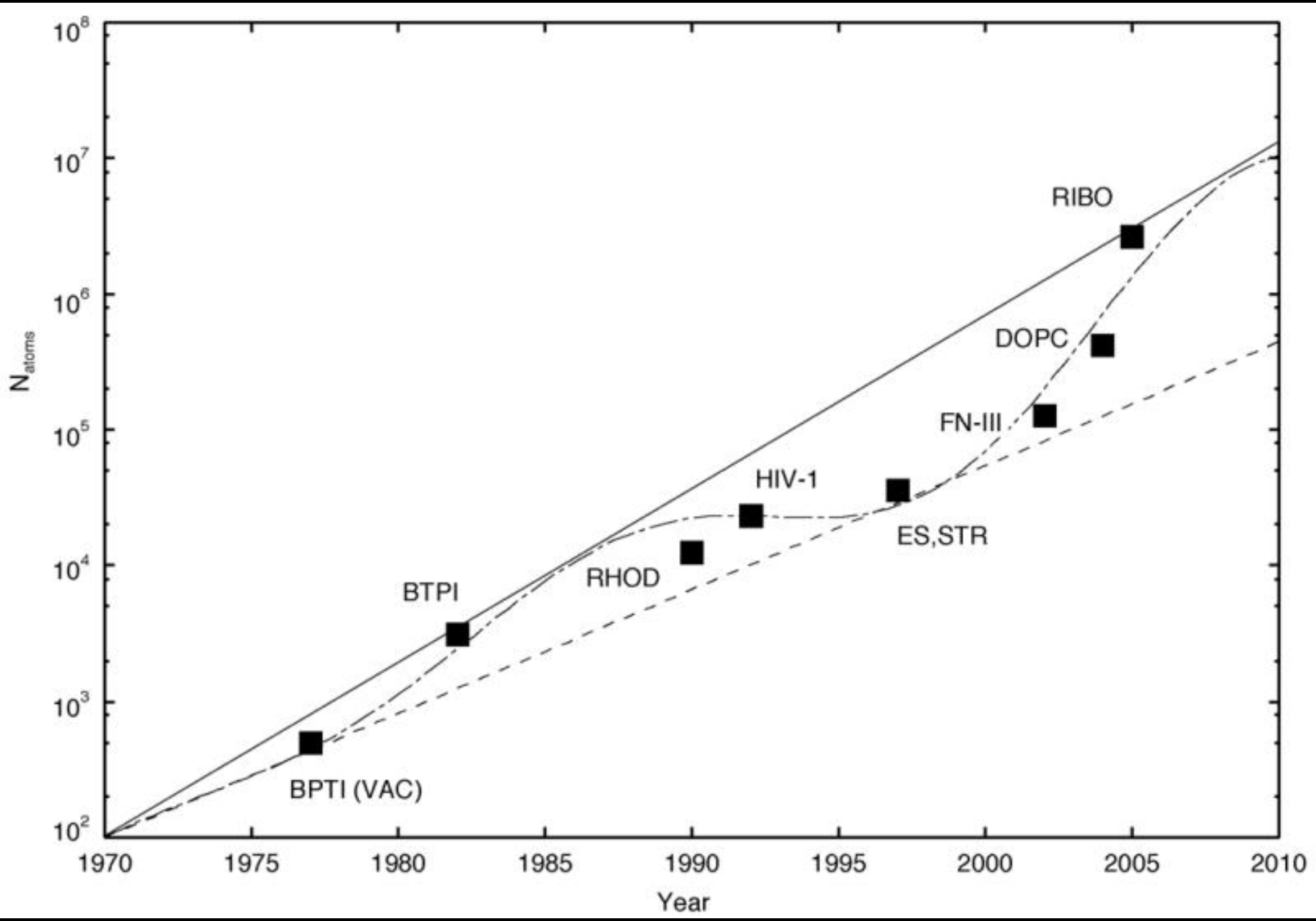
2010
Year
RIBO
DOPC
FN-III
HIV-1
ES,STR
RHOD
BTPI
BPTI (VAC)





HIV proteáza




10^8
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10^4
10^3
10^2
N_{atoms}
1970
1975
1980
1985
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1995
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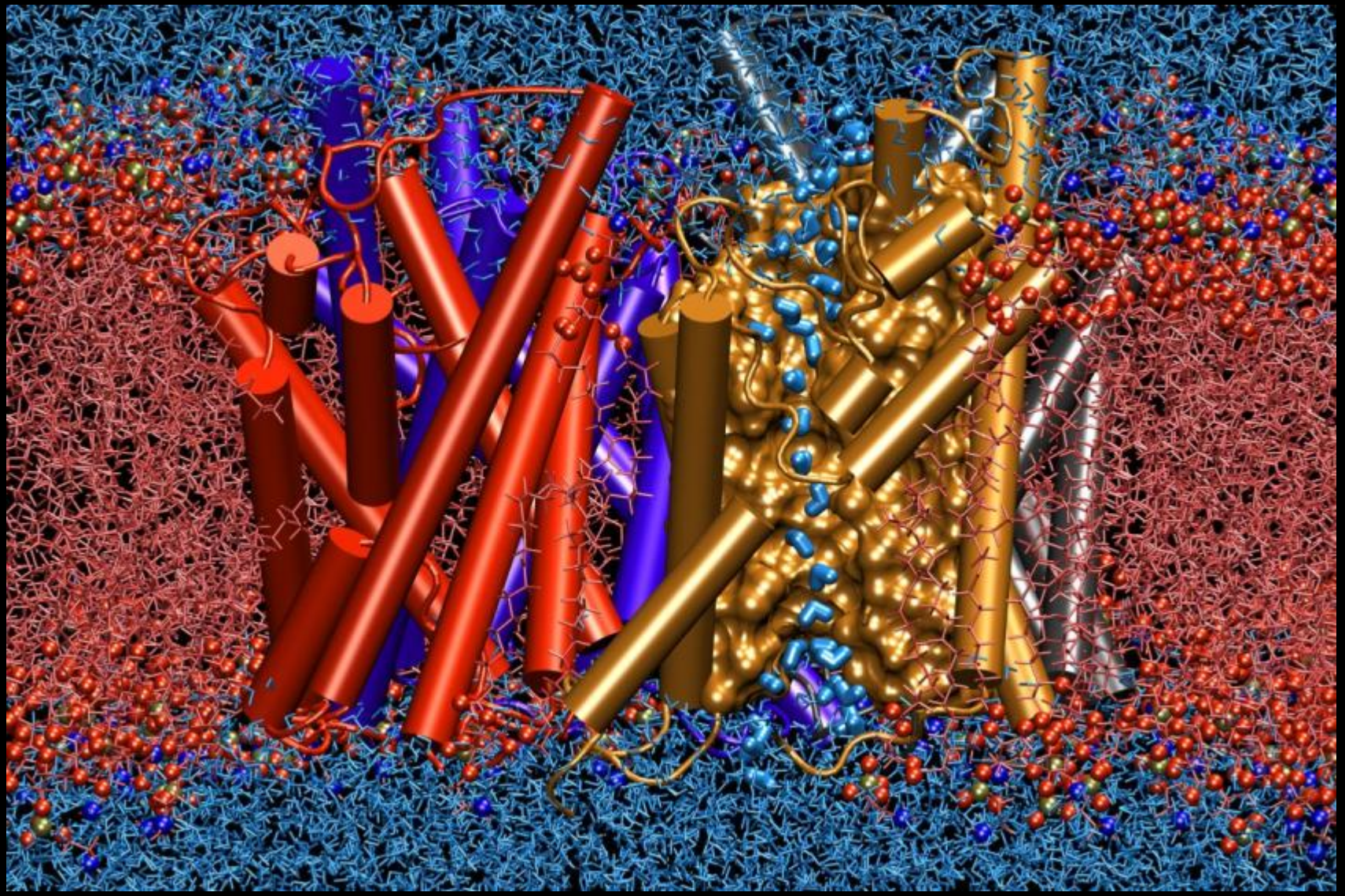
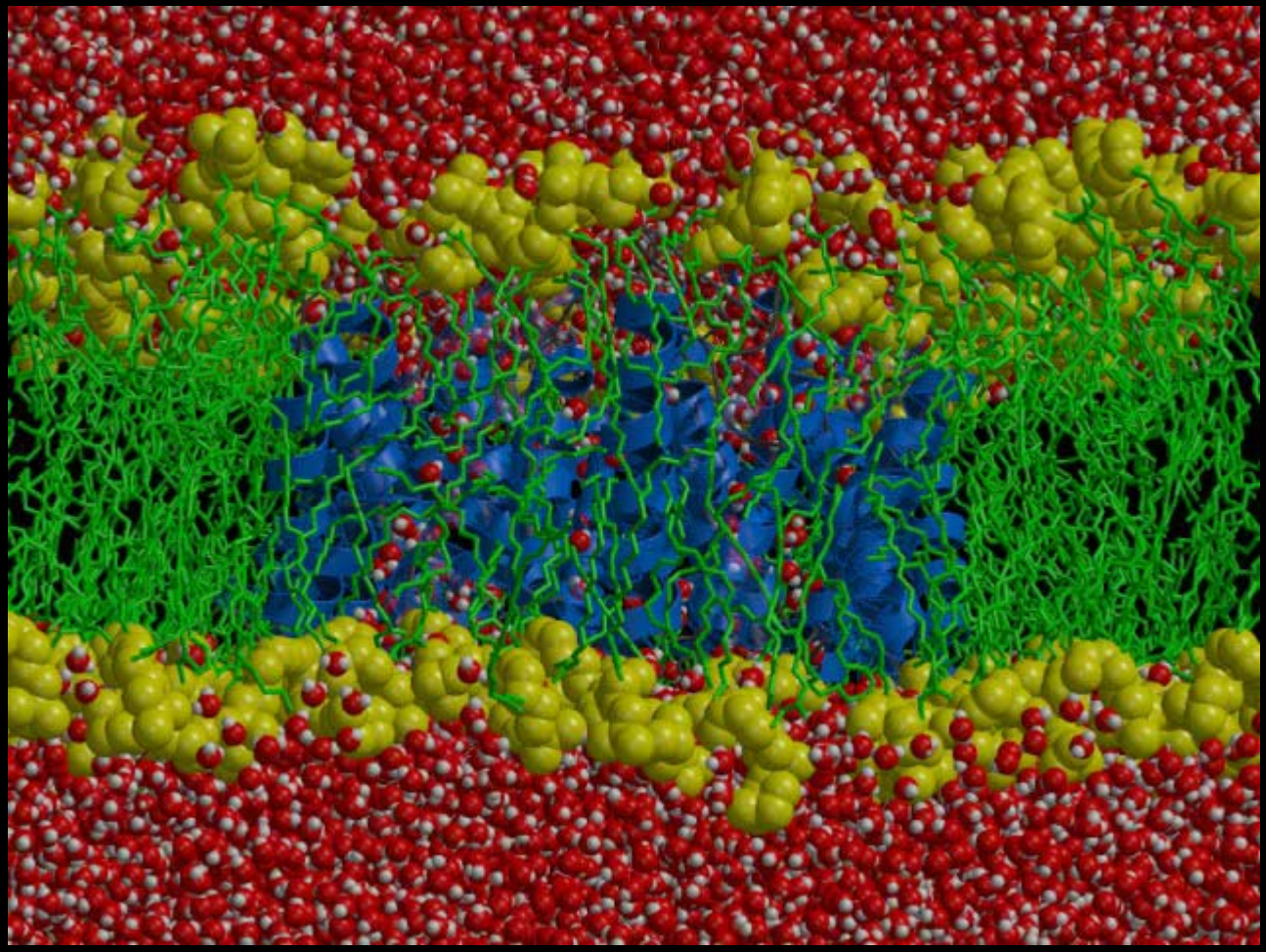
2005
2010
Year
RIBO
DOPC
FN-III
HIV-1
ES,STR
RHOD
BTPI
BPTI (VAC)

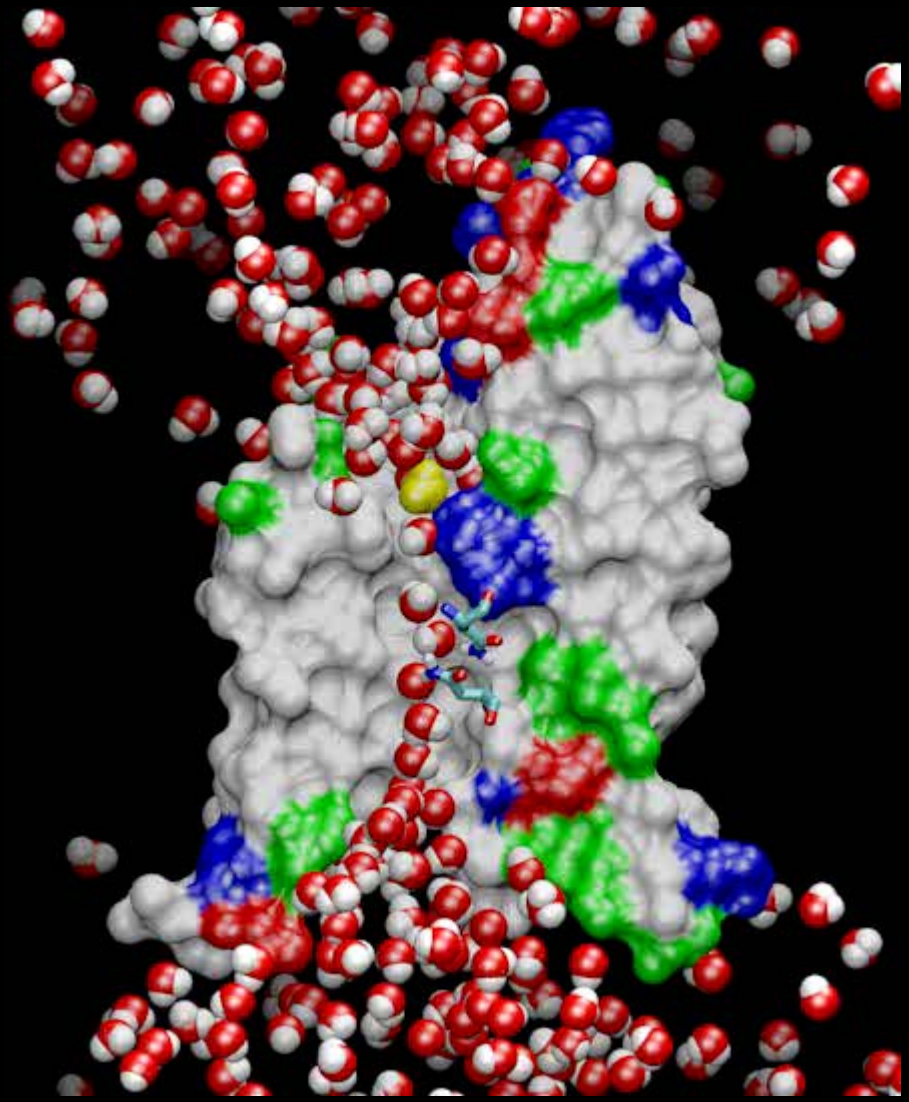
Structure, Dynamics, and Function of Aquaporins

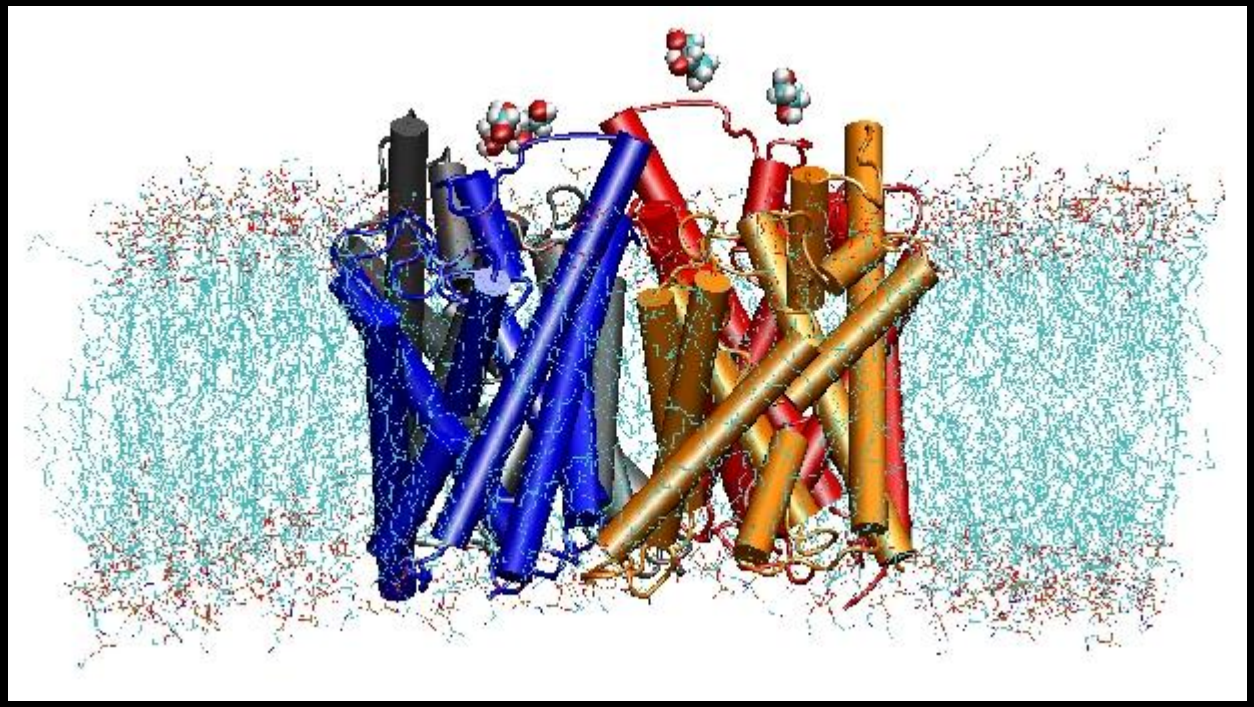


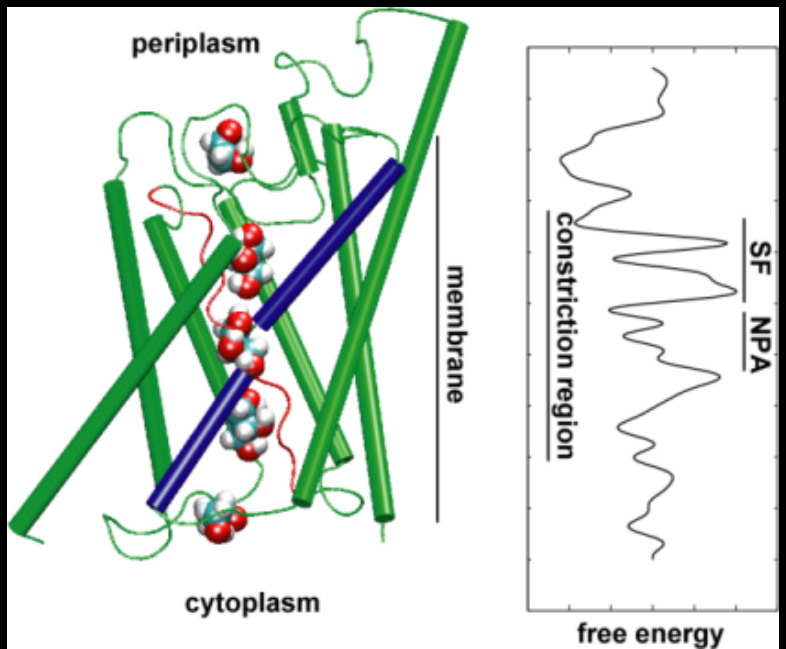
Structure, Dynamics, and Function of Aquaporins

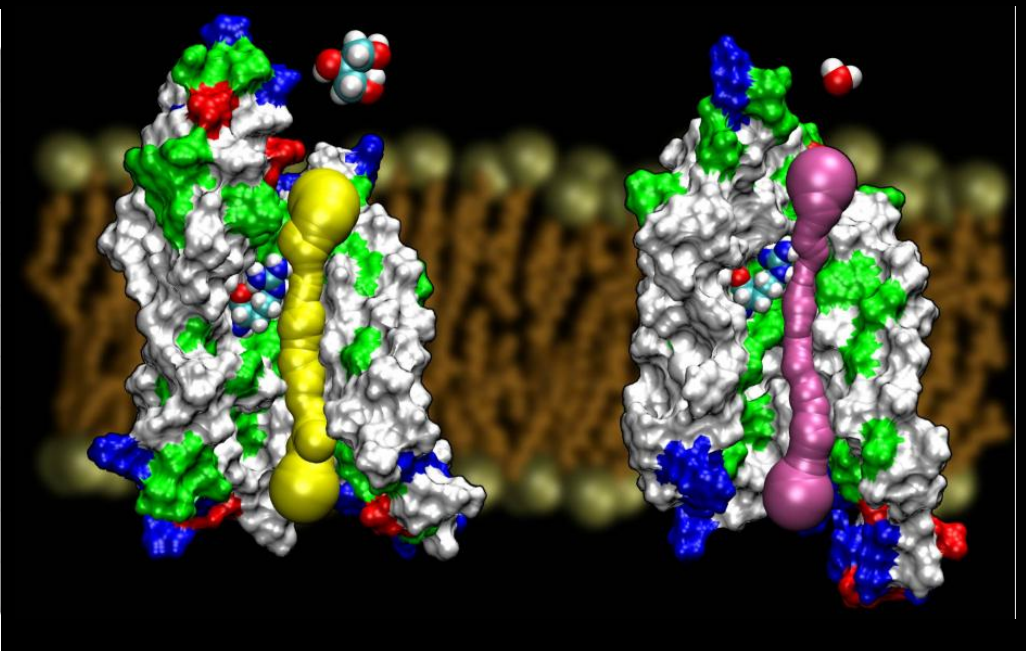


Structure, Dynamics, and Function of Aquaporins

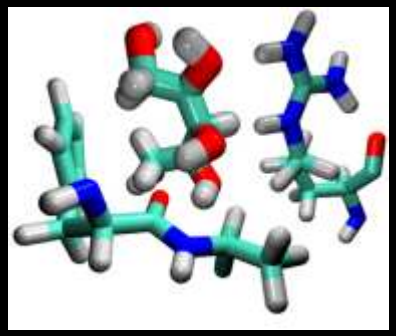


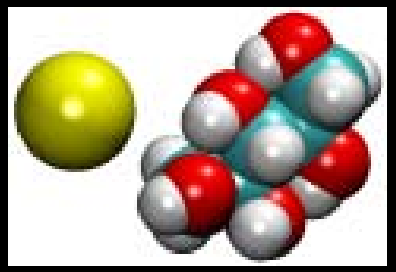


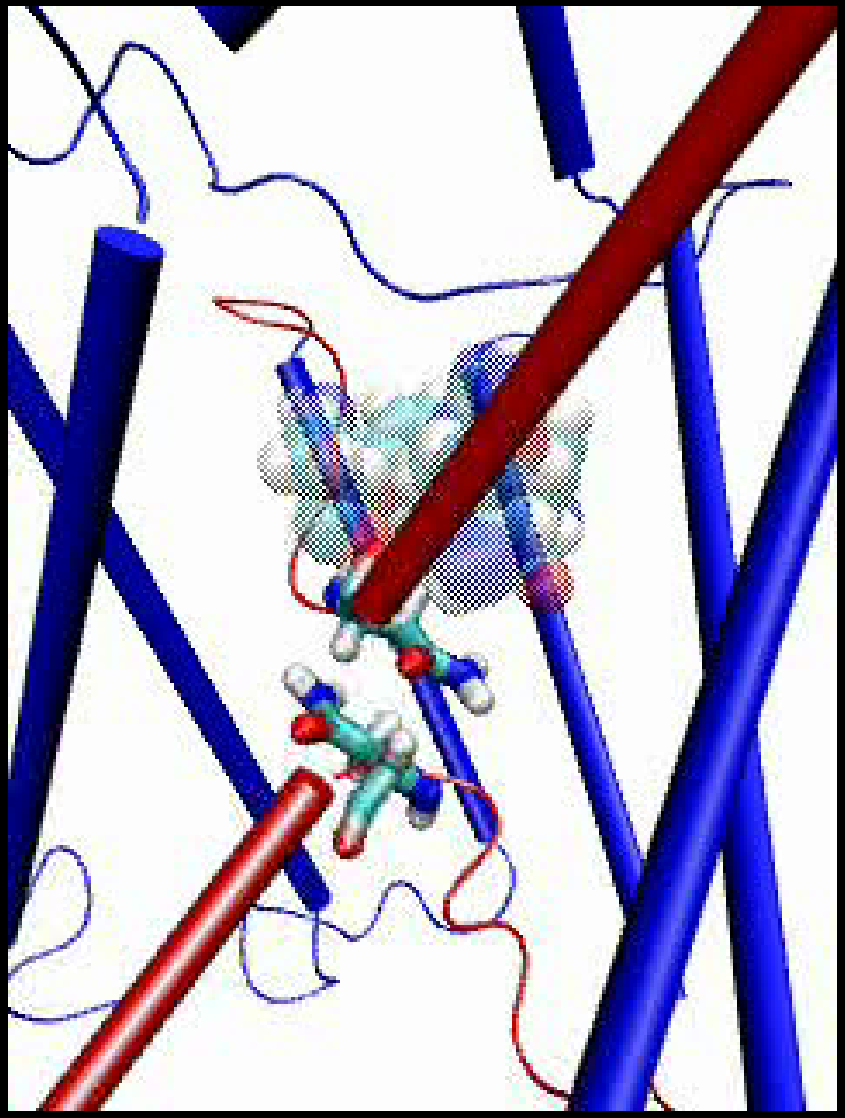

periplasm
membrane
cytoplasm
SF
NPA
constriction region
free energy



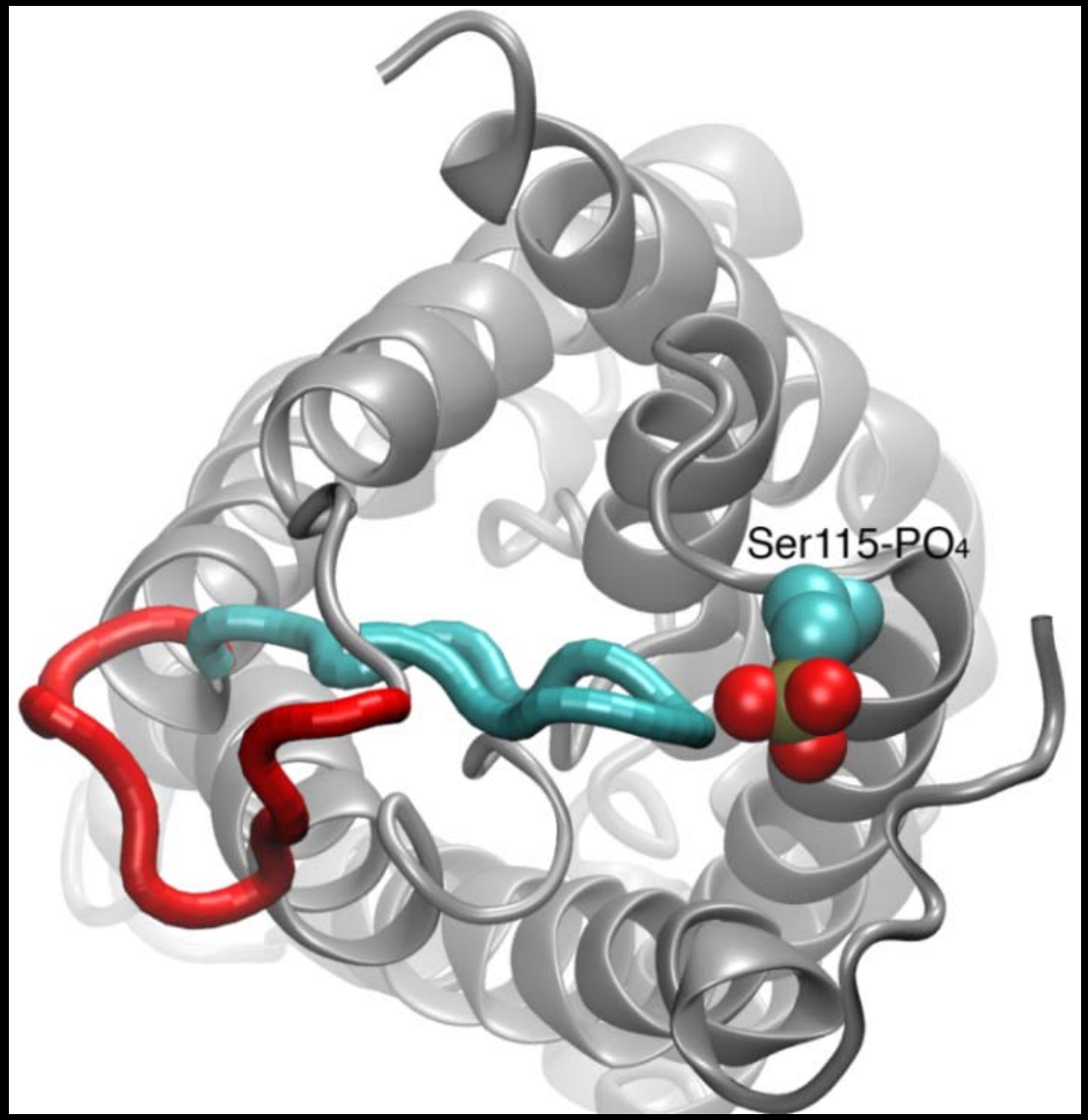
ribitol

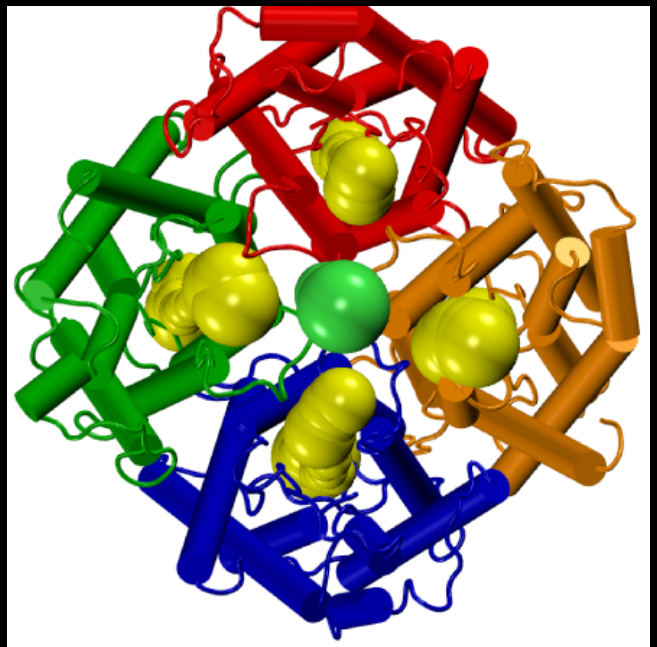


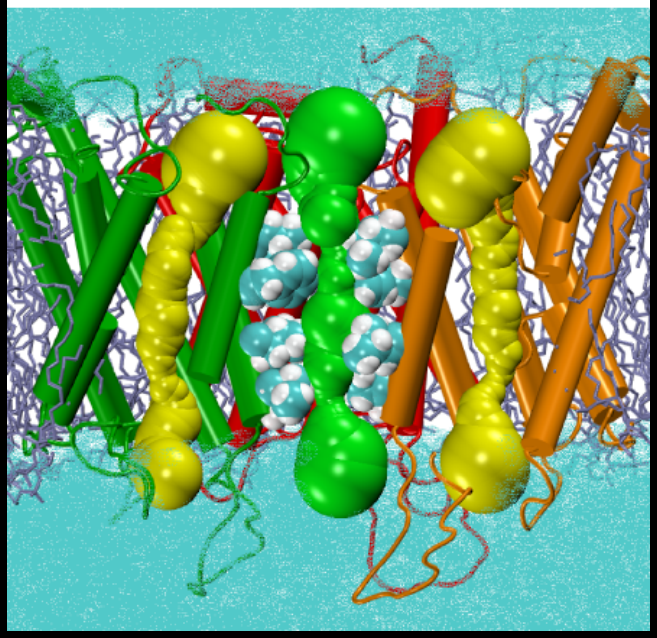


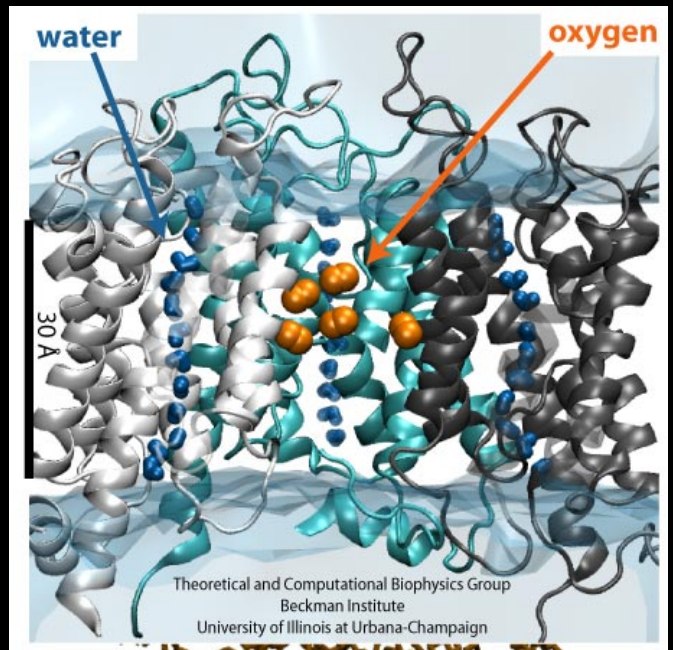


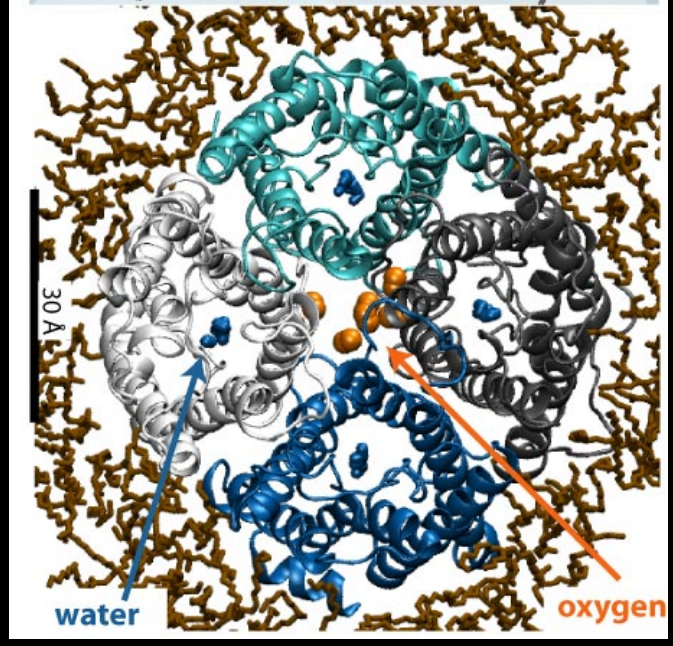
Structure, Dynamics, and Function of Aquaporins



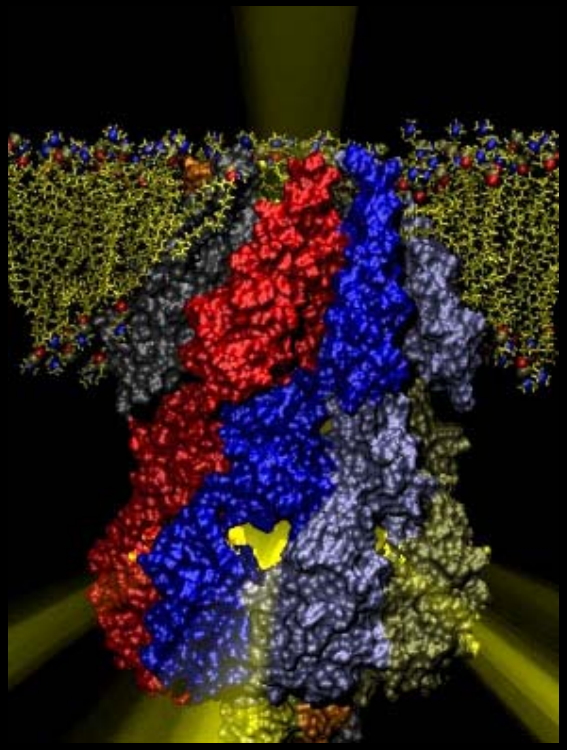


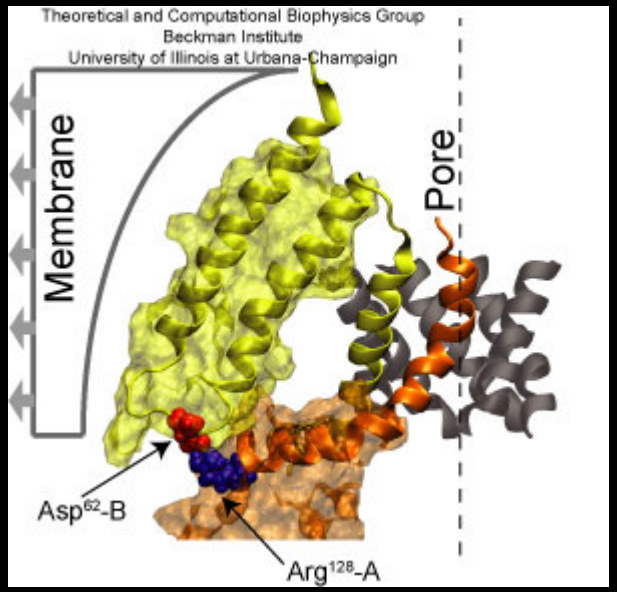


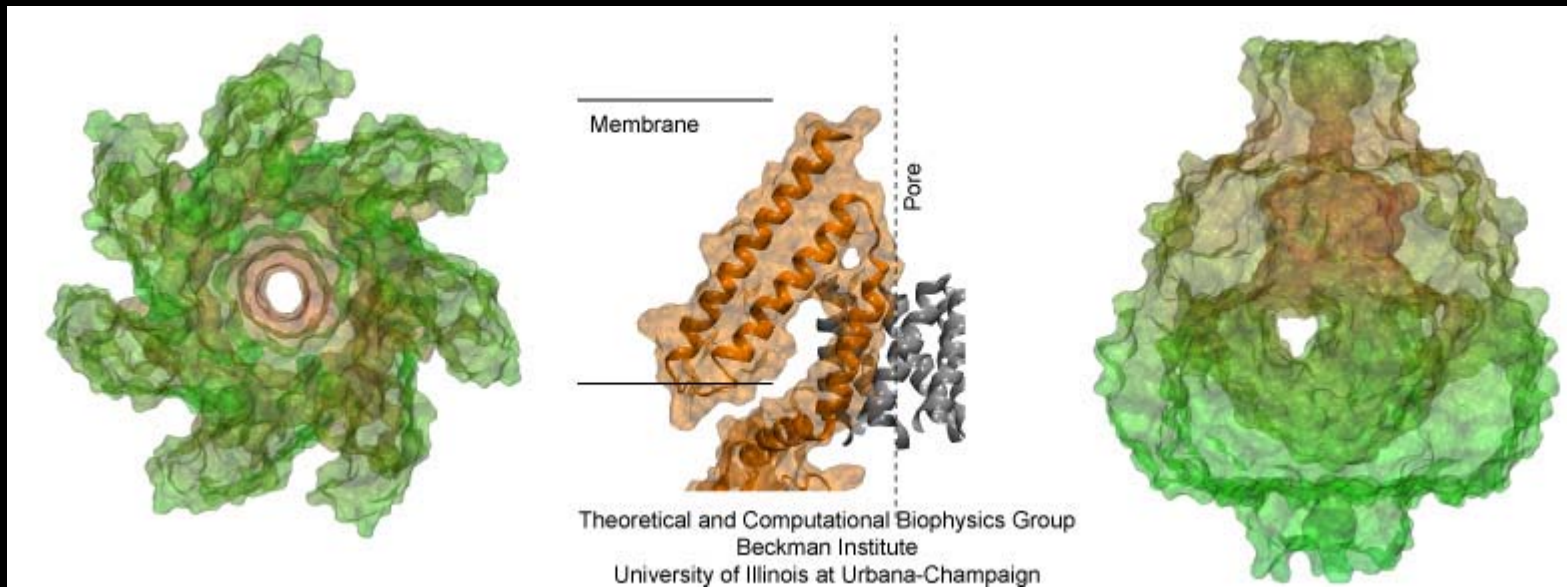

water
oxygen
30 Å
Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign


30 Å
water
oxygen

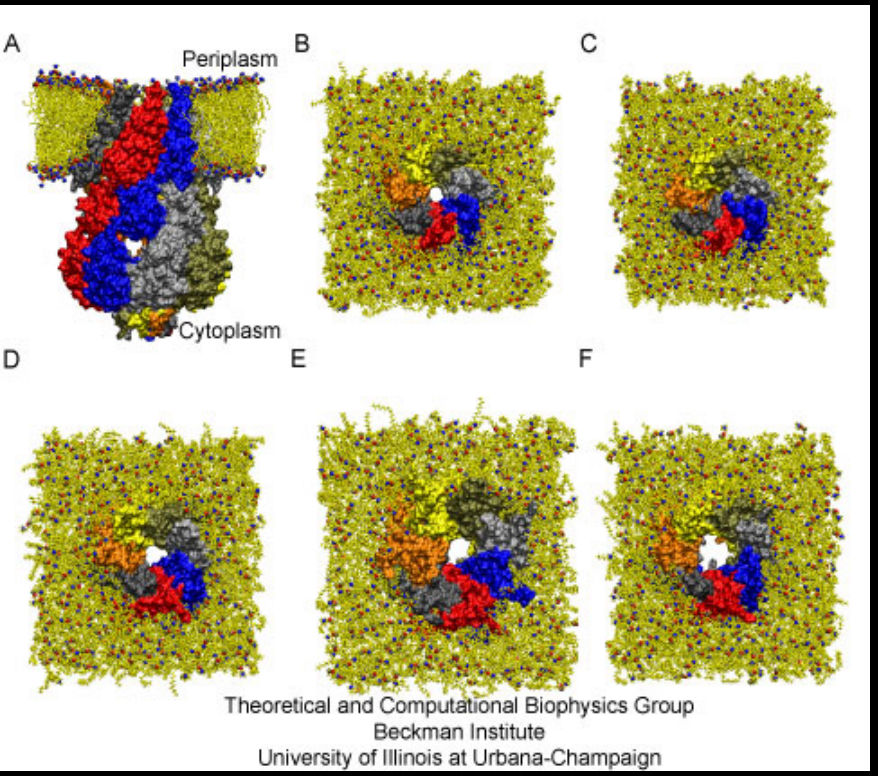
Mechanosensitive Channel MscS

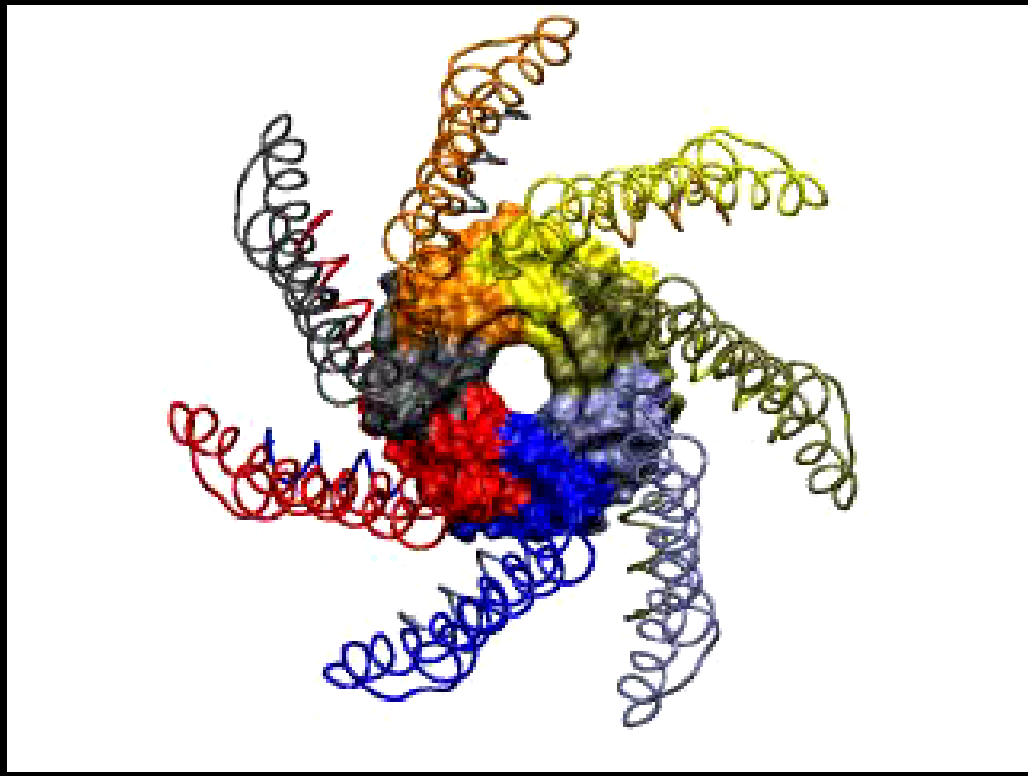




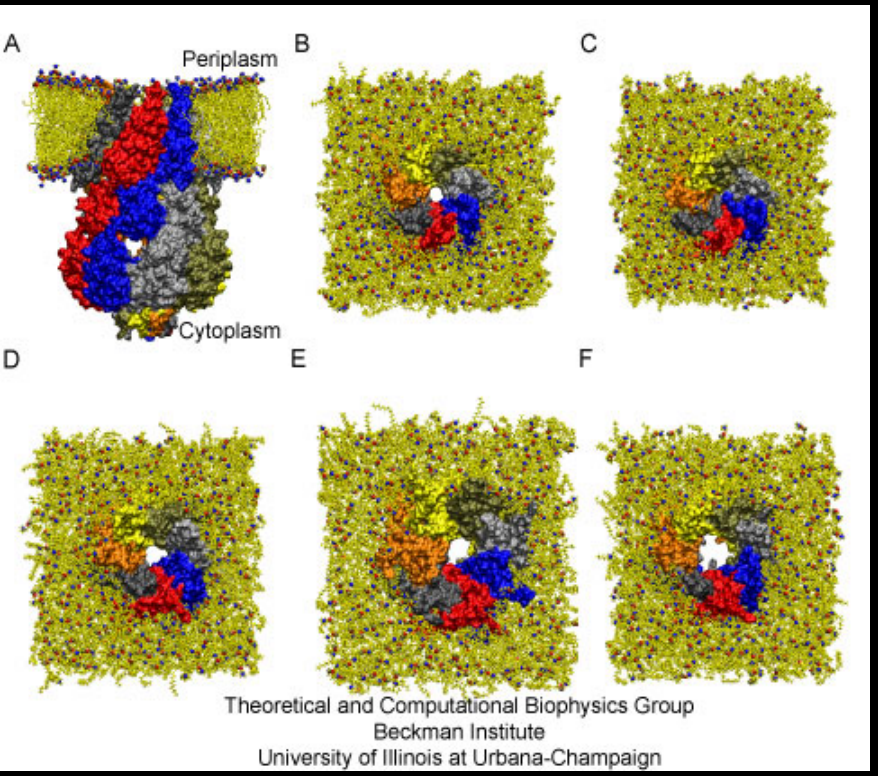


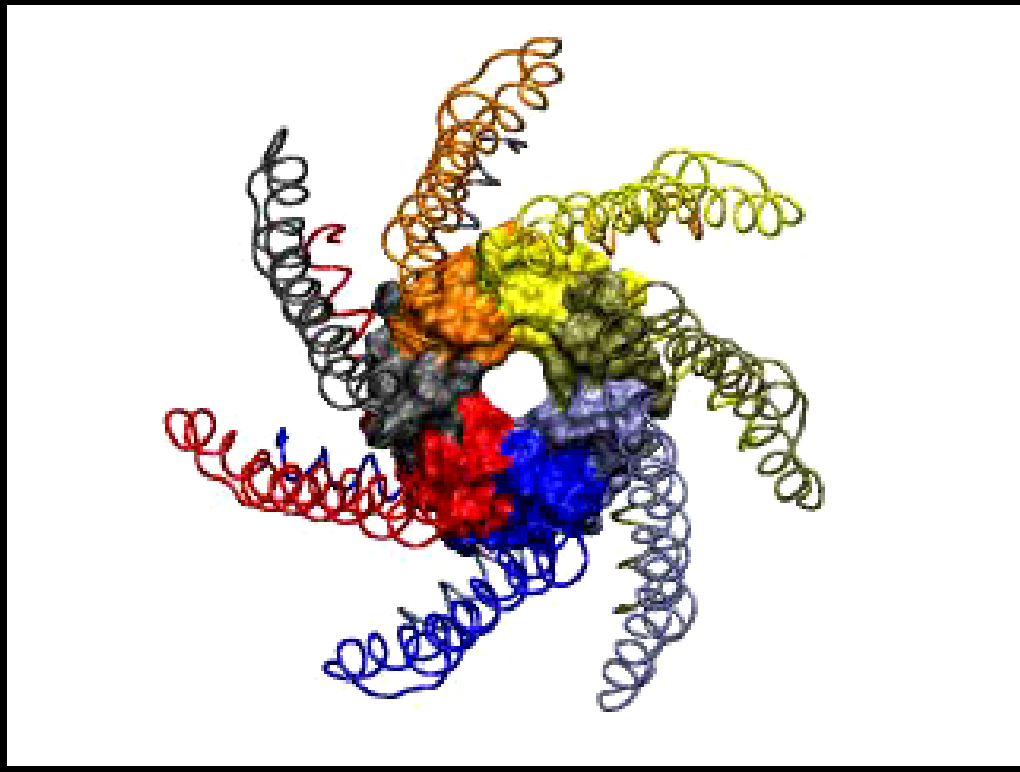
Mechanosensitive Channel MscS



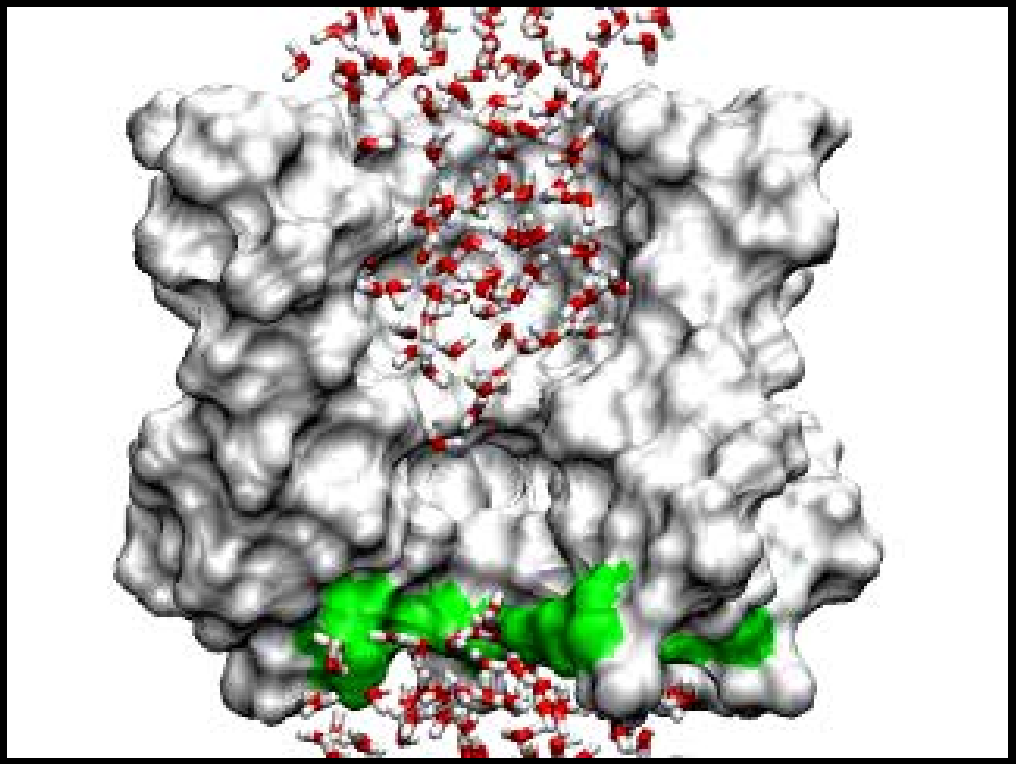


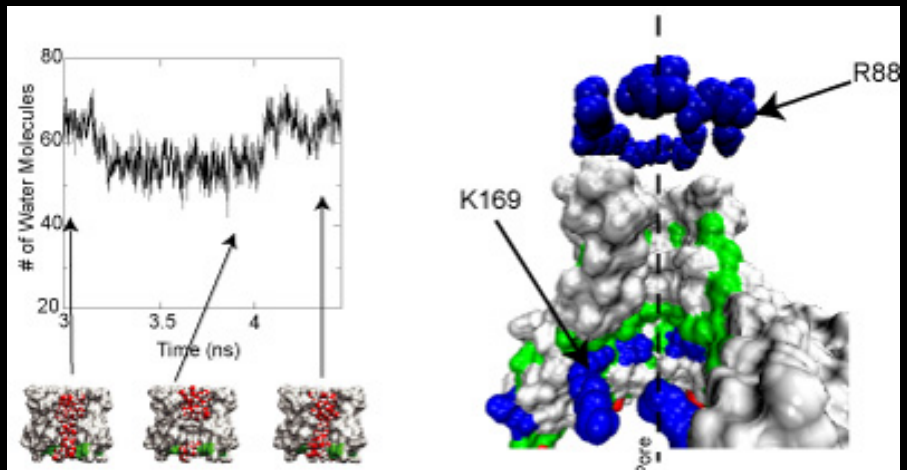
Mechanosensitive Channel MscS

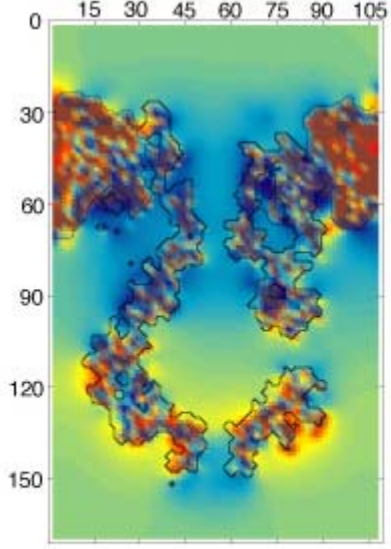




Mechanosensitive Channel MscS







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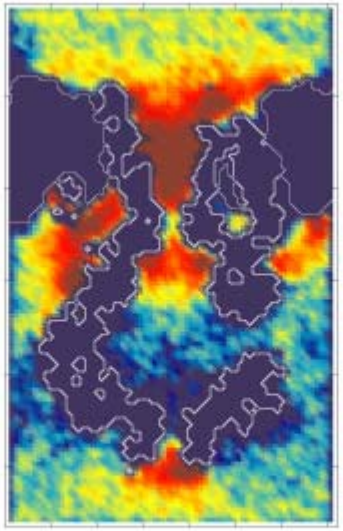

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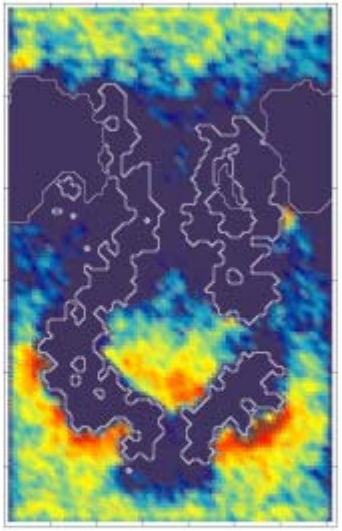

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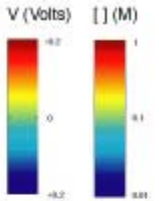

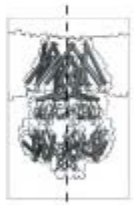

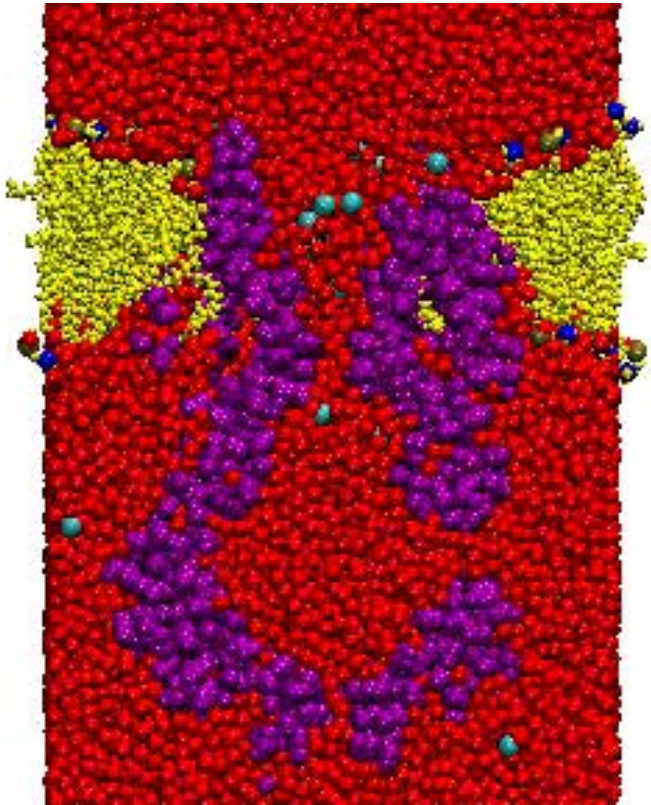

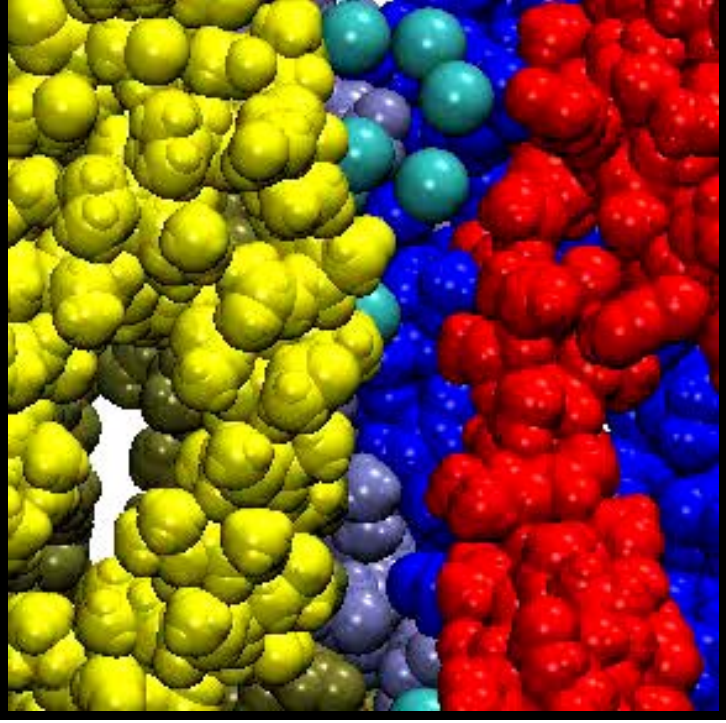

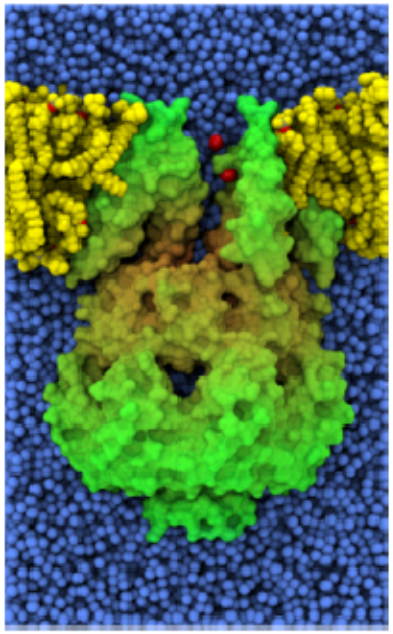

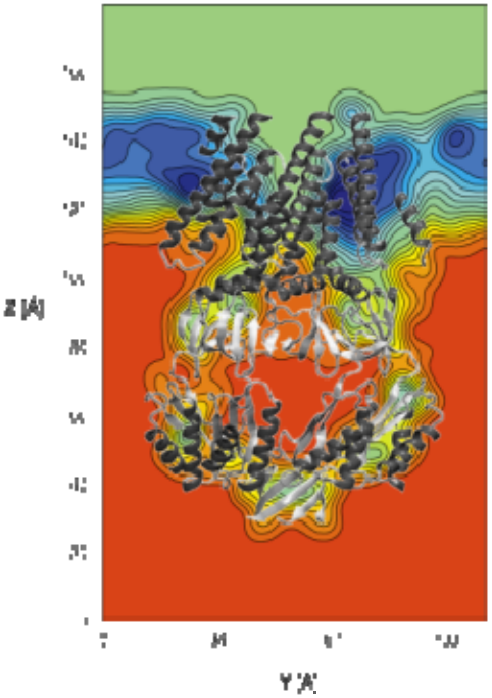
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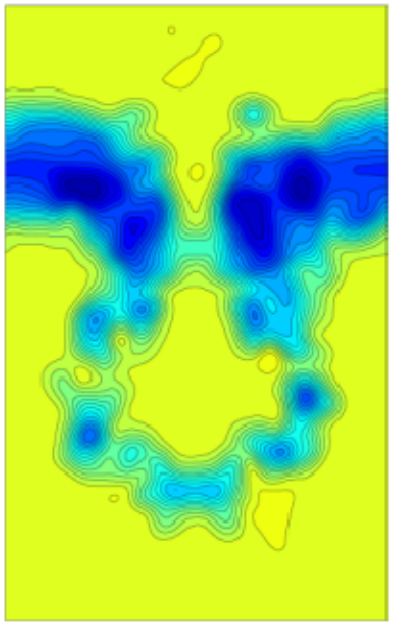
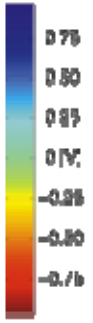
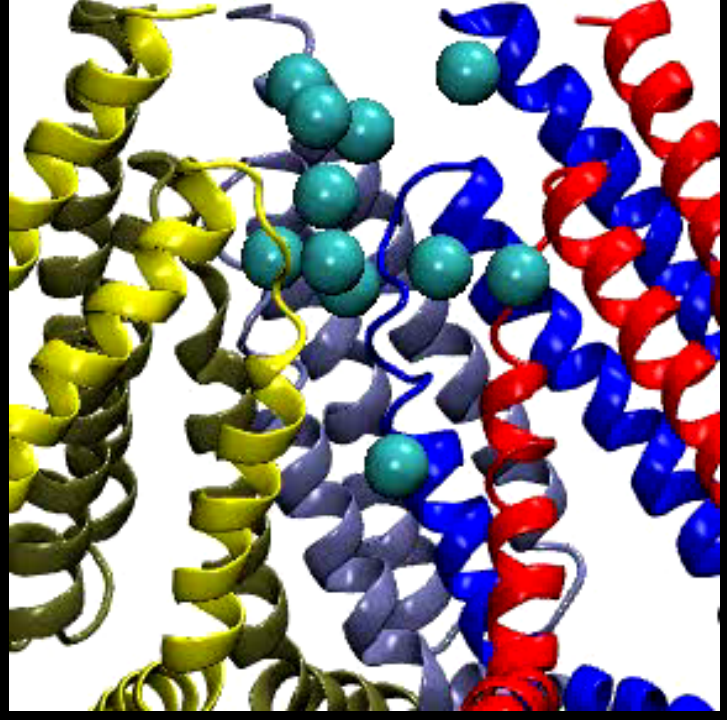
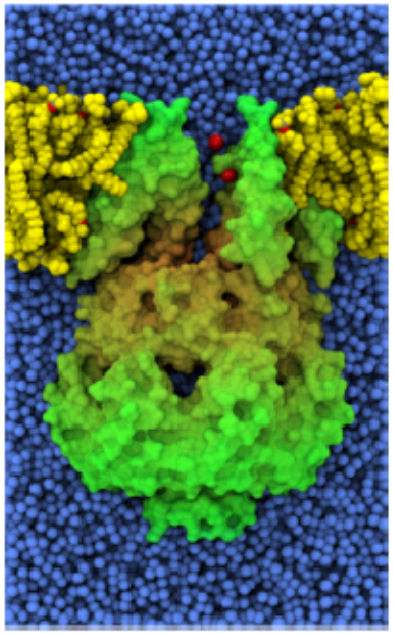
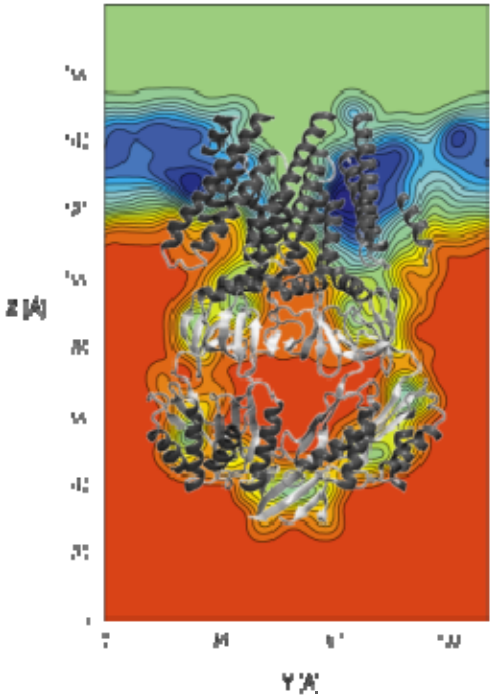
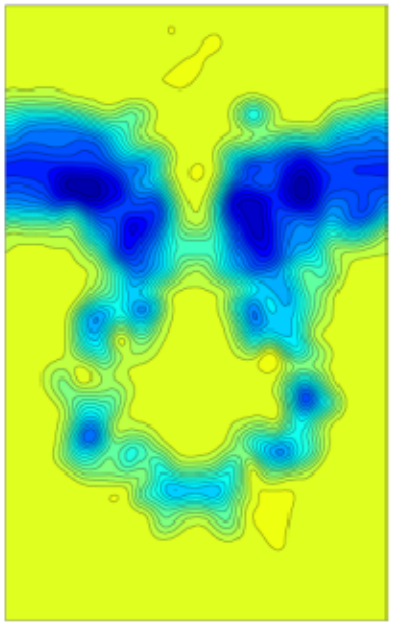


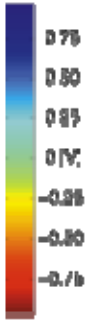




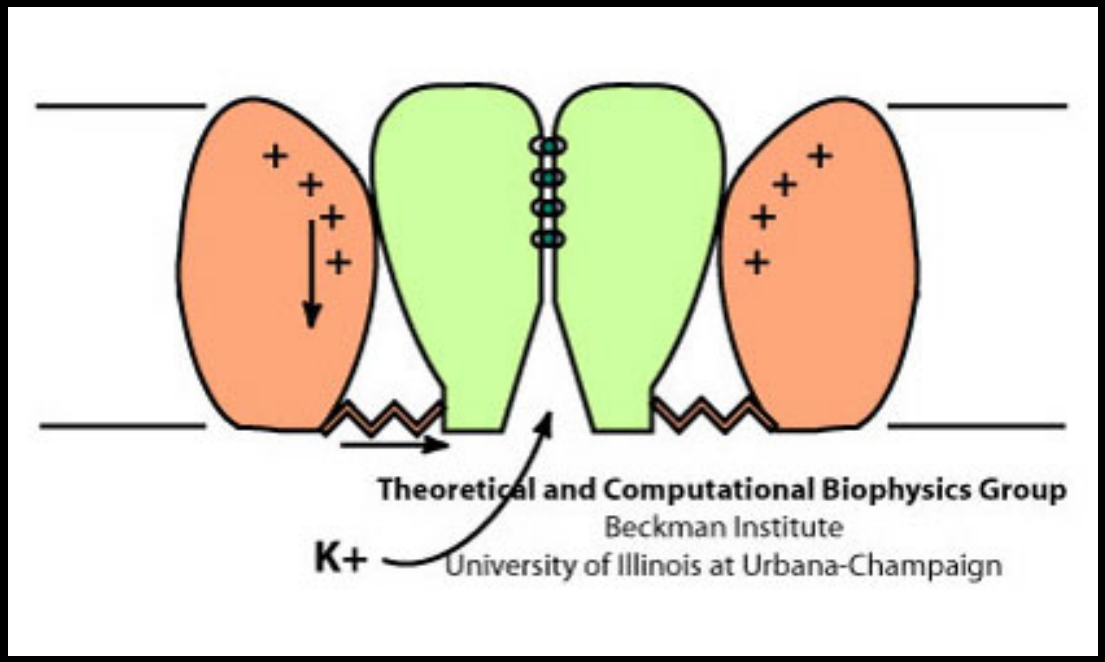


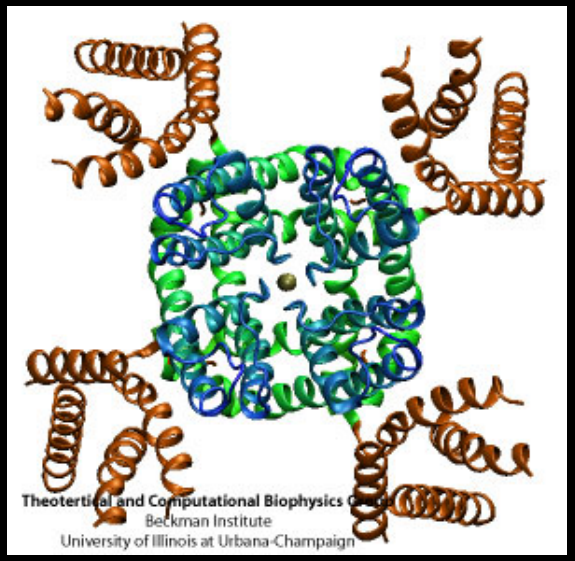

z [Å]
x [Å]

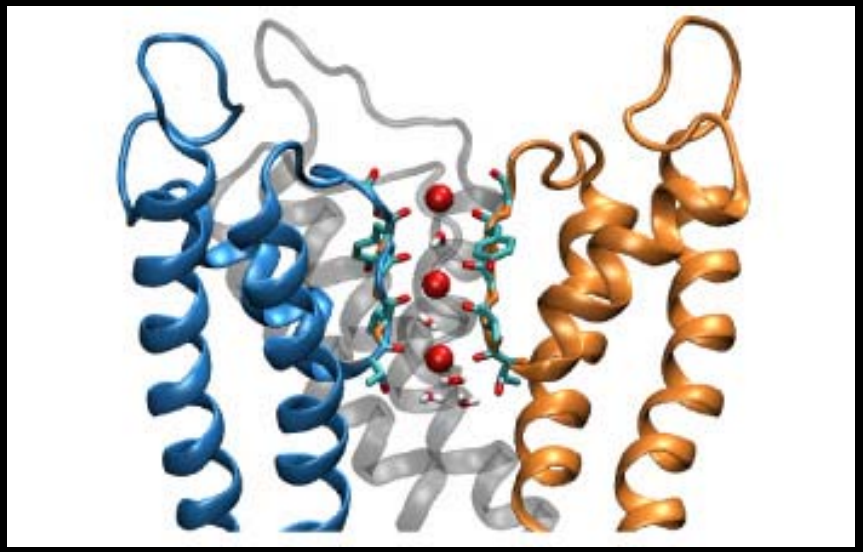




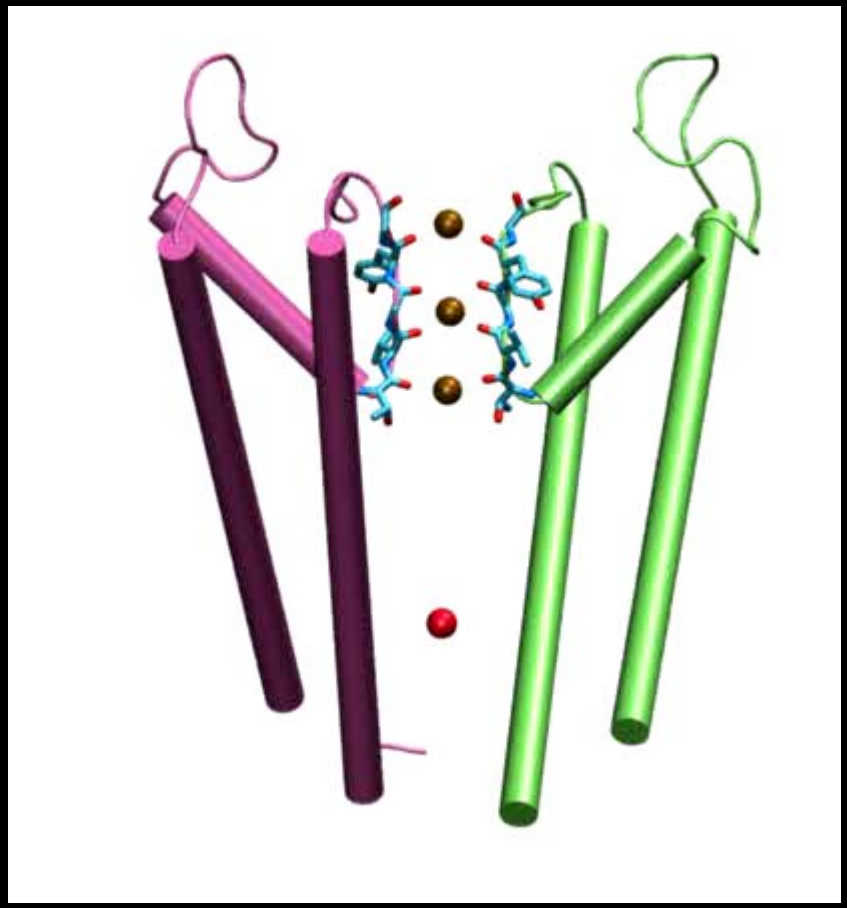
Potassium Channel

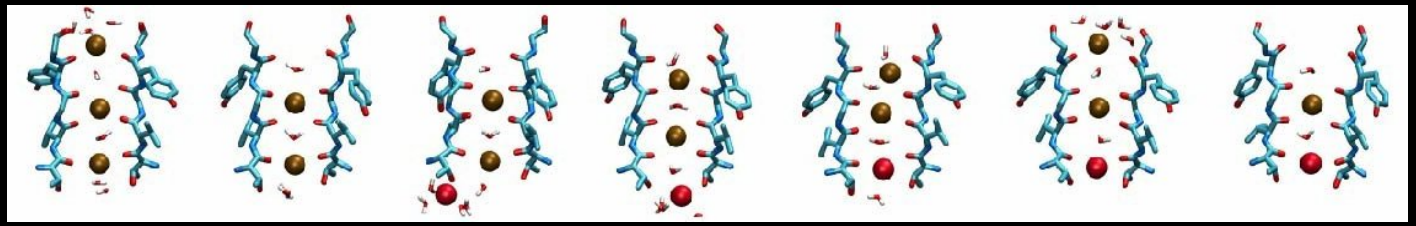




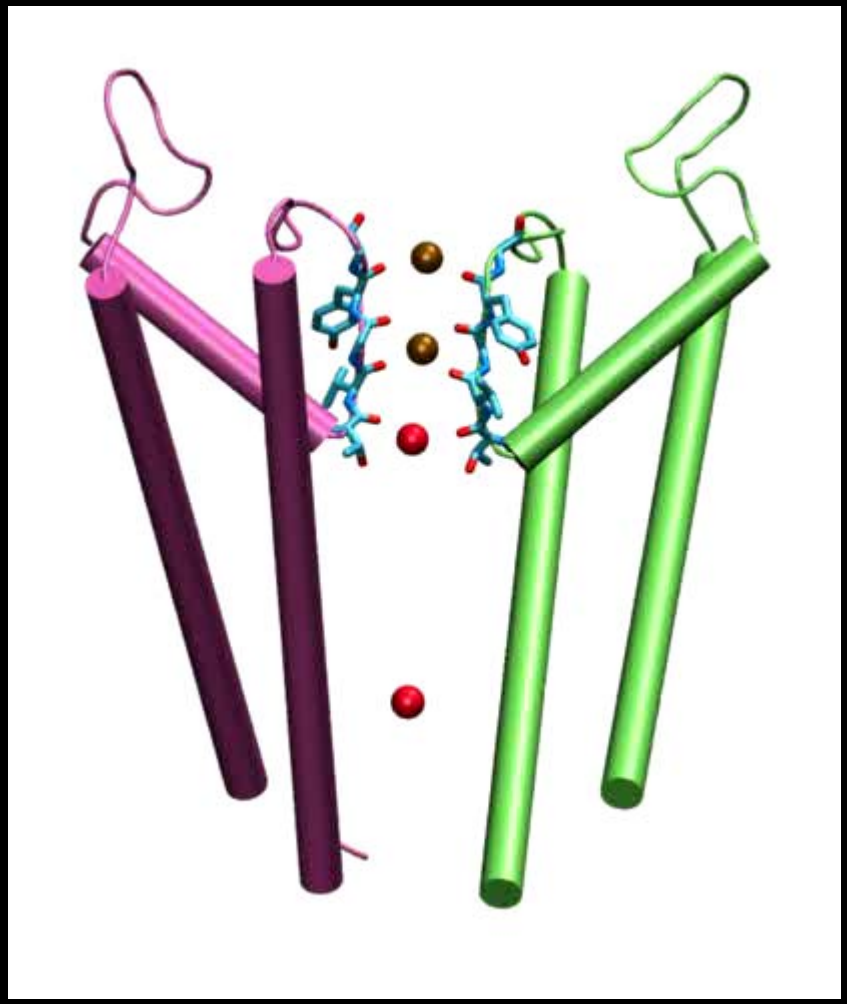


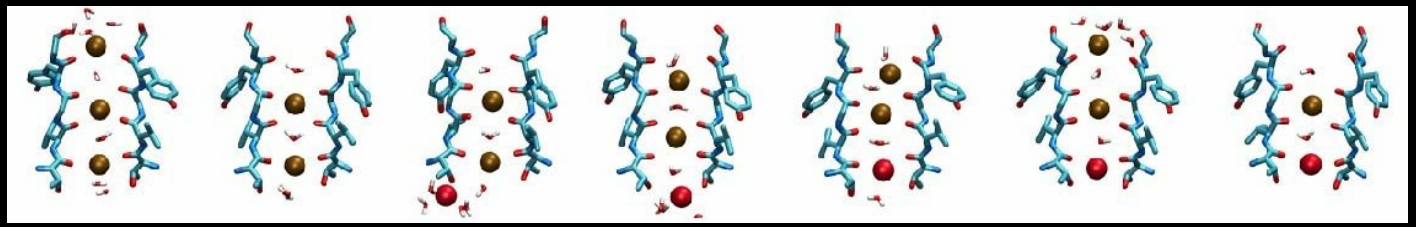
Potassium Channel



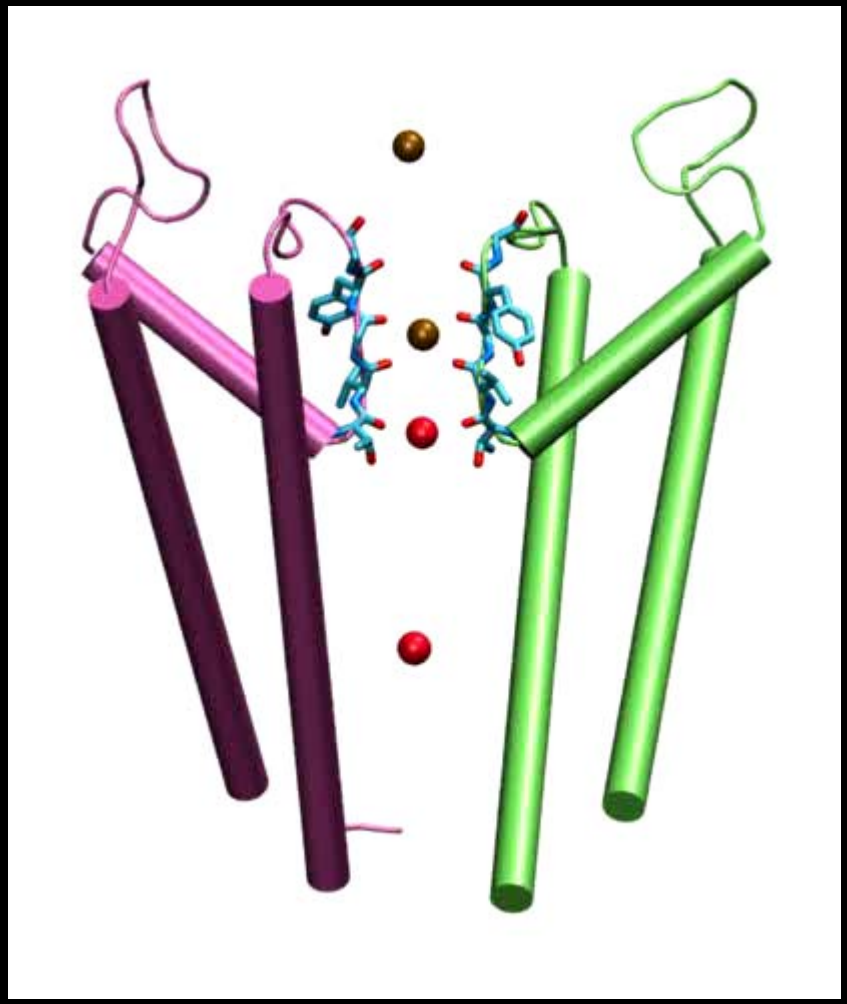


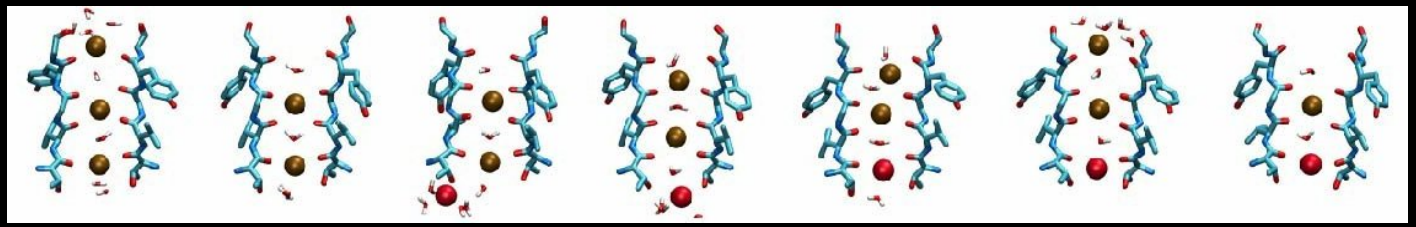
Potassium Channel

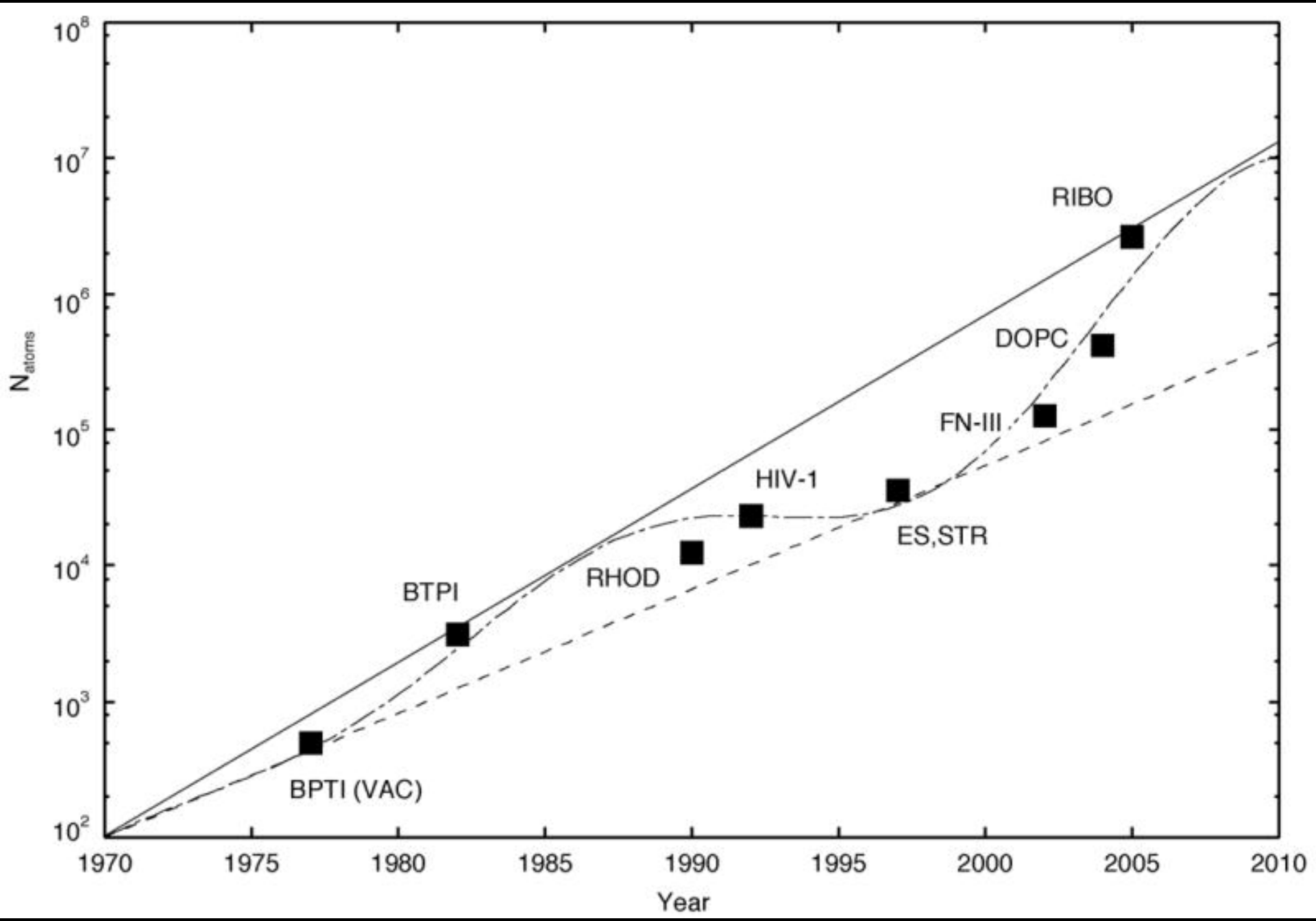




Potassium Channel






10^8
10^7
10^6
10^5
10^4
10^3
10^2
N_{atoms}
1970
1975
1980
1985
1990
1995
2000
2005
2010
Year
RIBO
DOPC
FN-III
HIV-1
ES,STR
RHOD
BTPI
BPTI (VAC)

Structure *14*, 437–449, March 2006 DOI 10.1016/j.str.2005.11.014

Molecular Dynamics Simulations of the Complete Satellite Tobacco Mosaic Virus

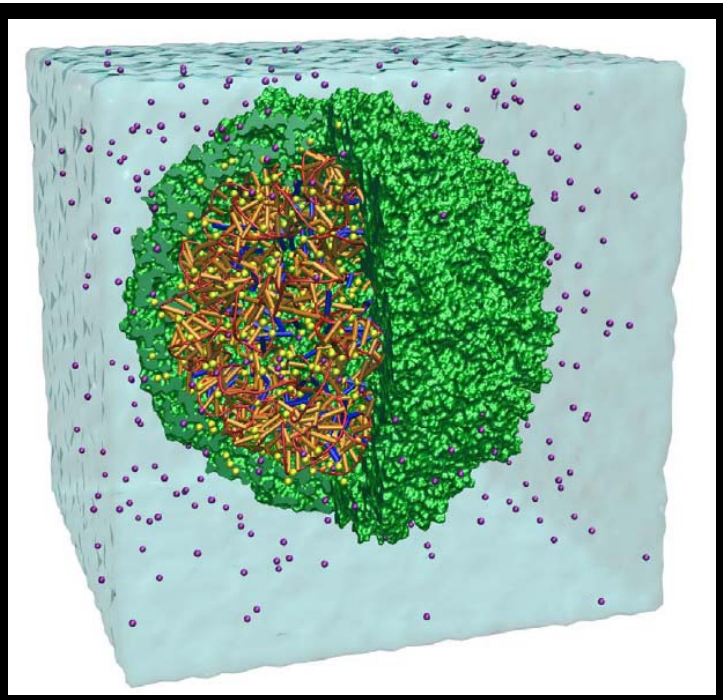
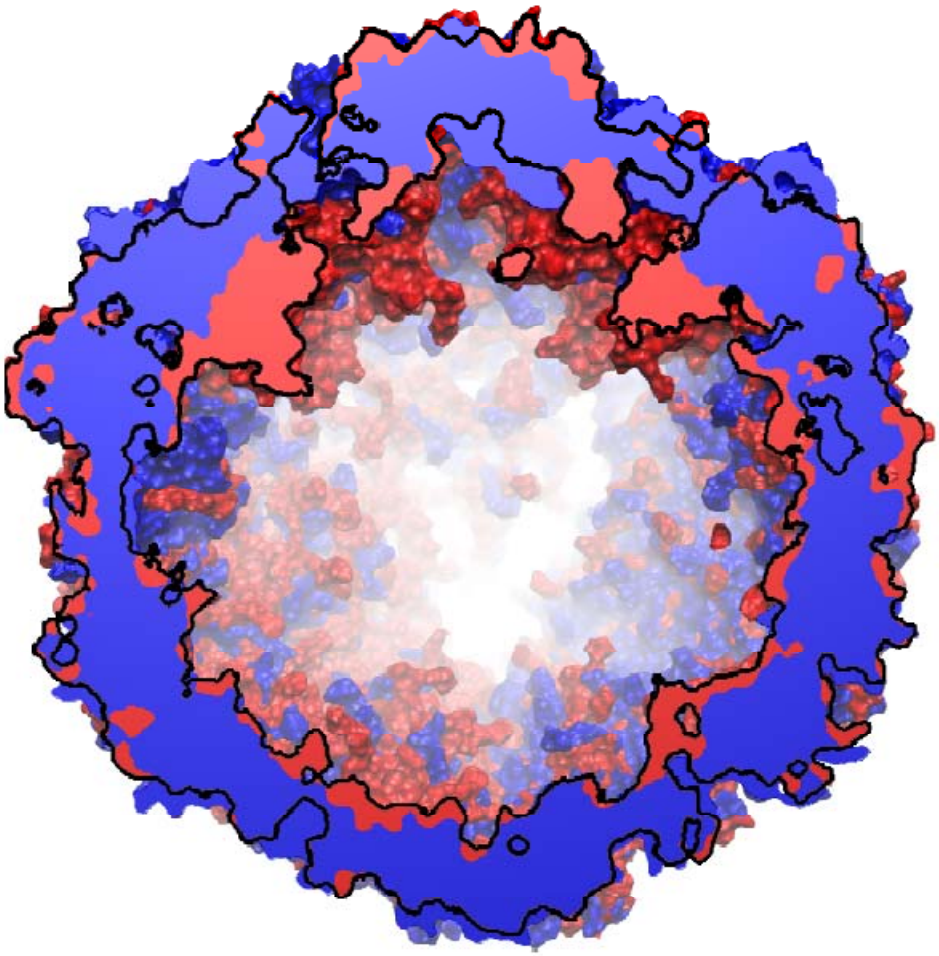
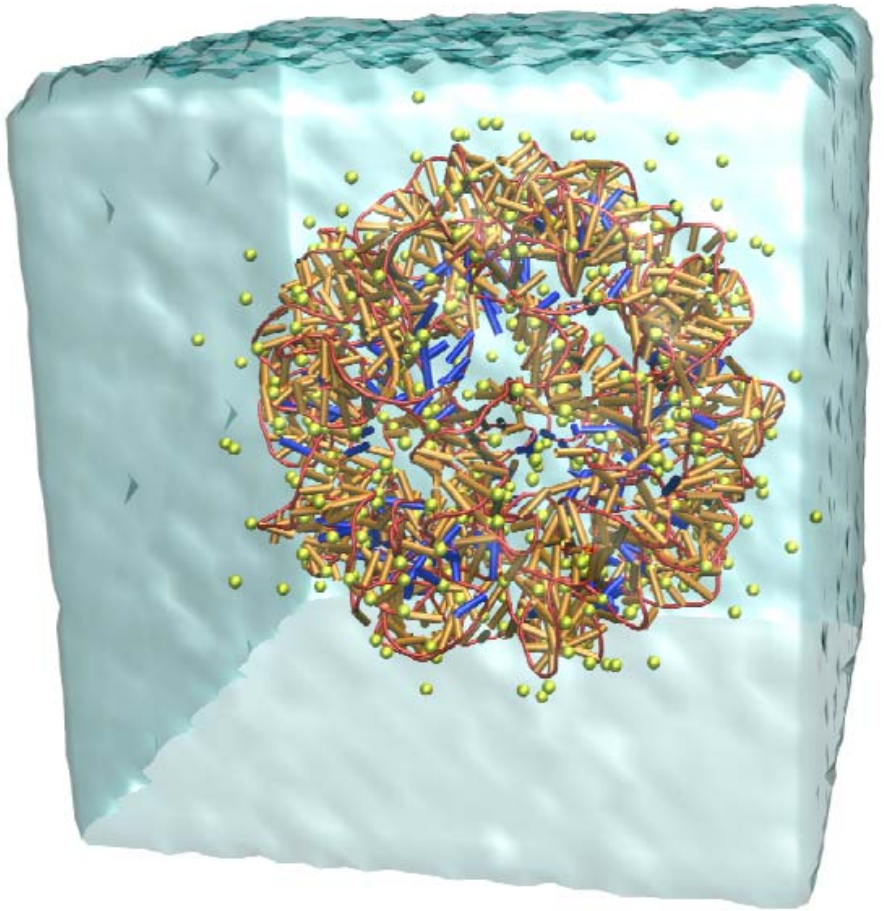
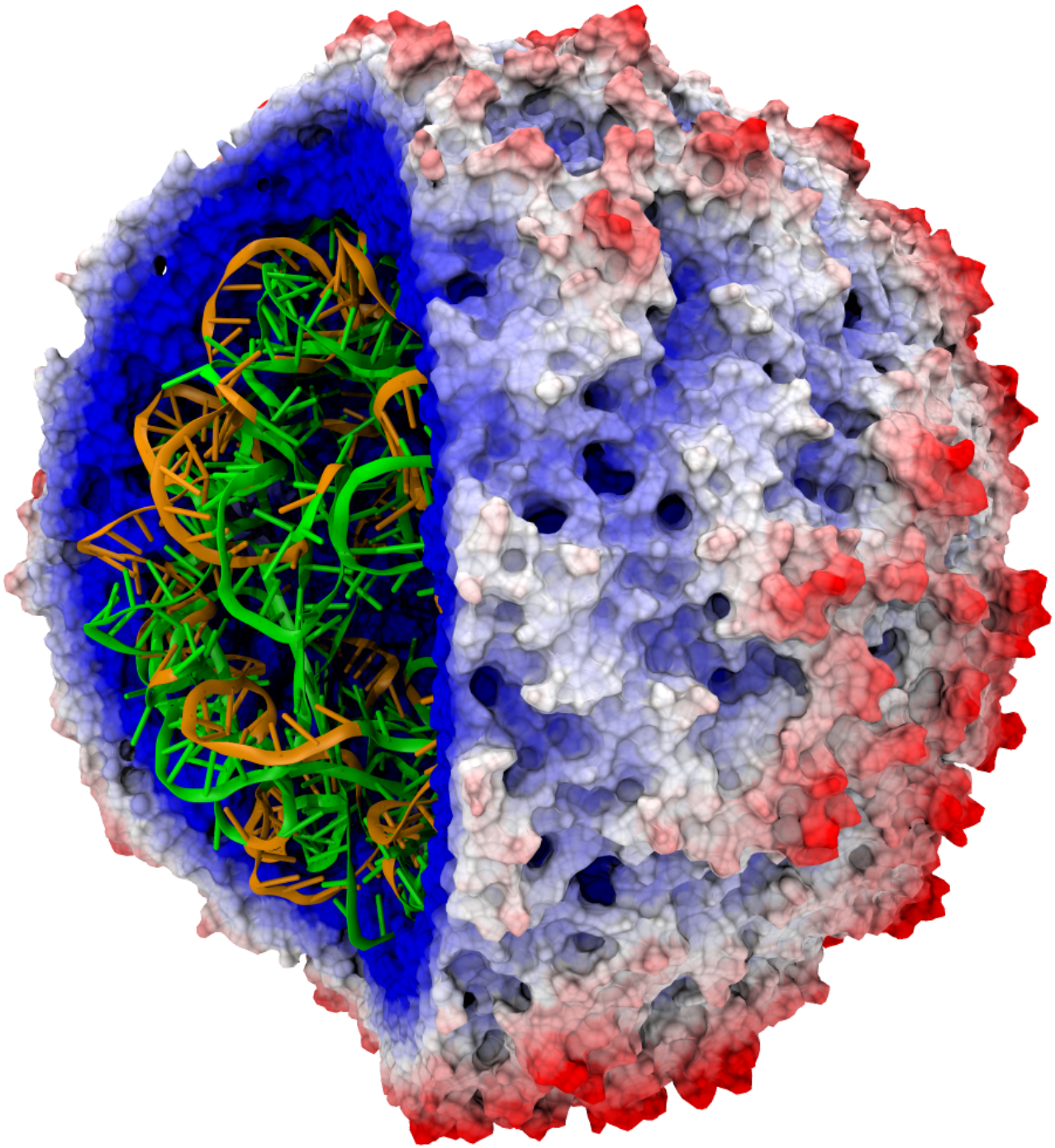


Table 1. Simulated Systems

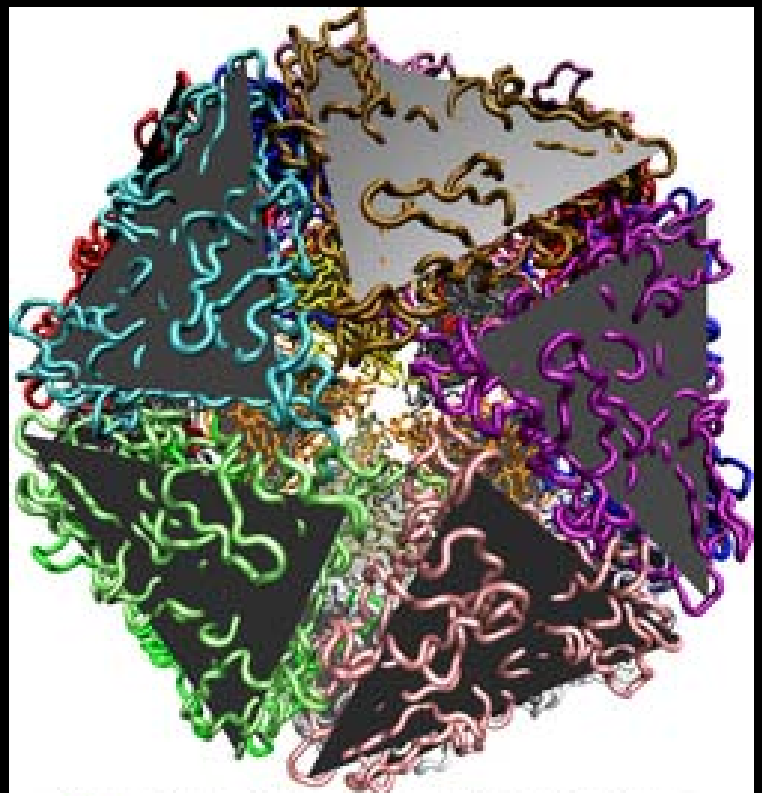
Name	Simulated System	Temperature (K)	Time (ns)	Atoms	System Size
simFULL	RNA/capsid assembly	298	13	1,066,628	220 Å × 220 Å × 220 Å
$simCAPSID_{310}$	Capsid alone	310	10	932,500	210 Å × 210 Å × 210 Å
$simCAPSID_{298A}$	Capsid alone	298	10	932,500	210 Å × 210 Å × 210 Å
$simCAPSID_{298B}$	Capsid alone	298	10	1,068,969	220 Å × 220 Å × 220 Å
simRNA	RNA alone	298	10	388,000	160 Å × 166 Å × 160 Å

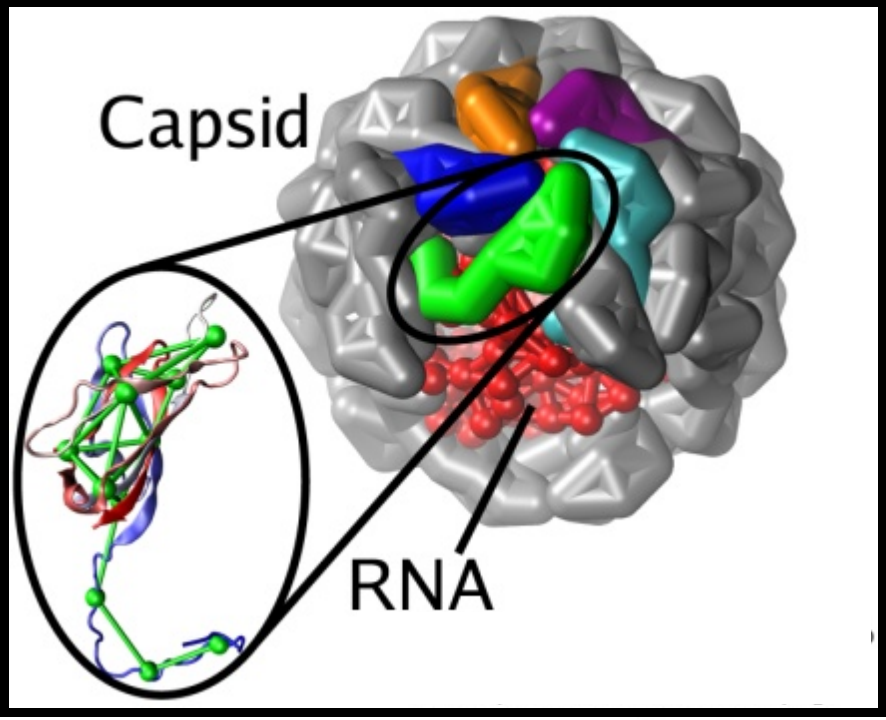


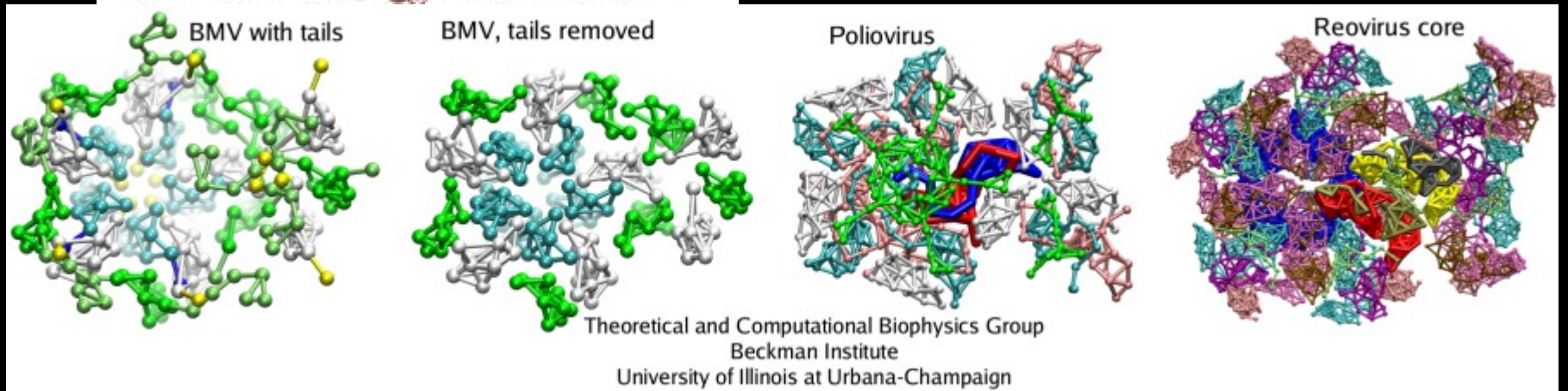


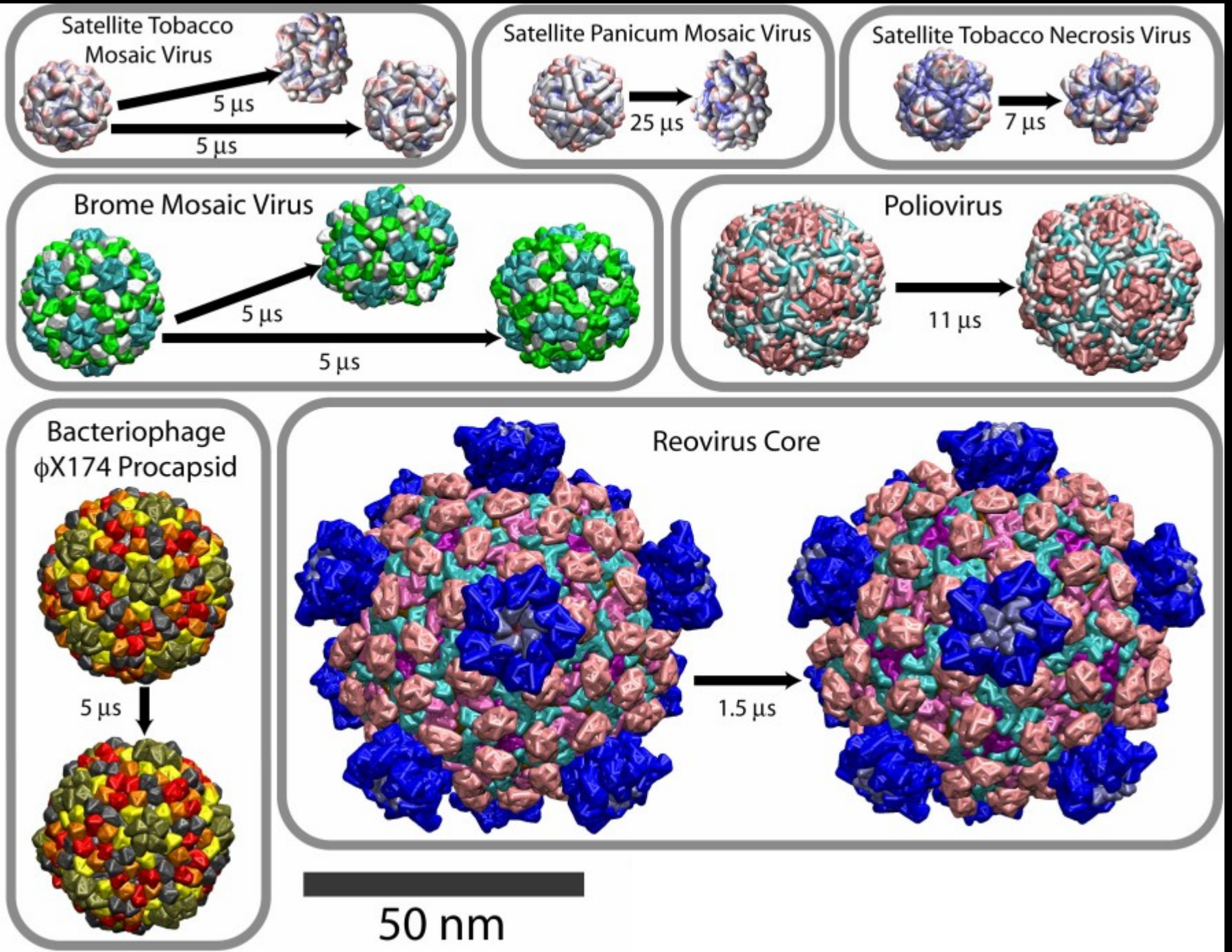


Viruses

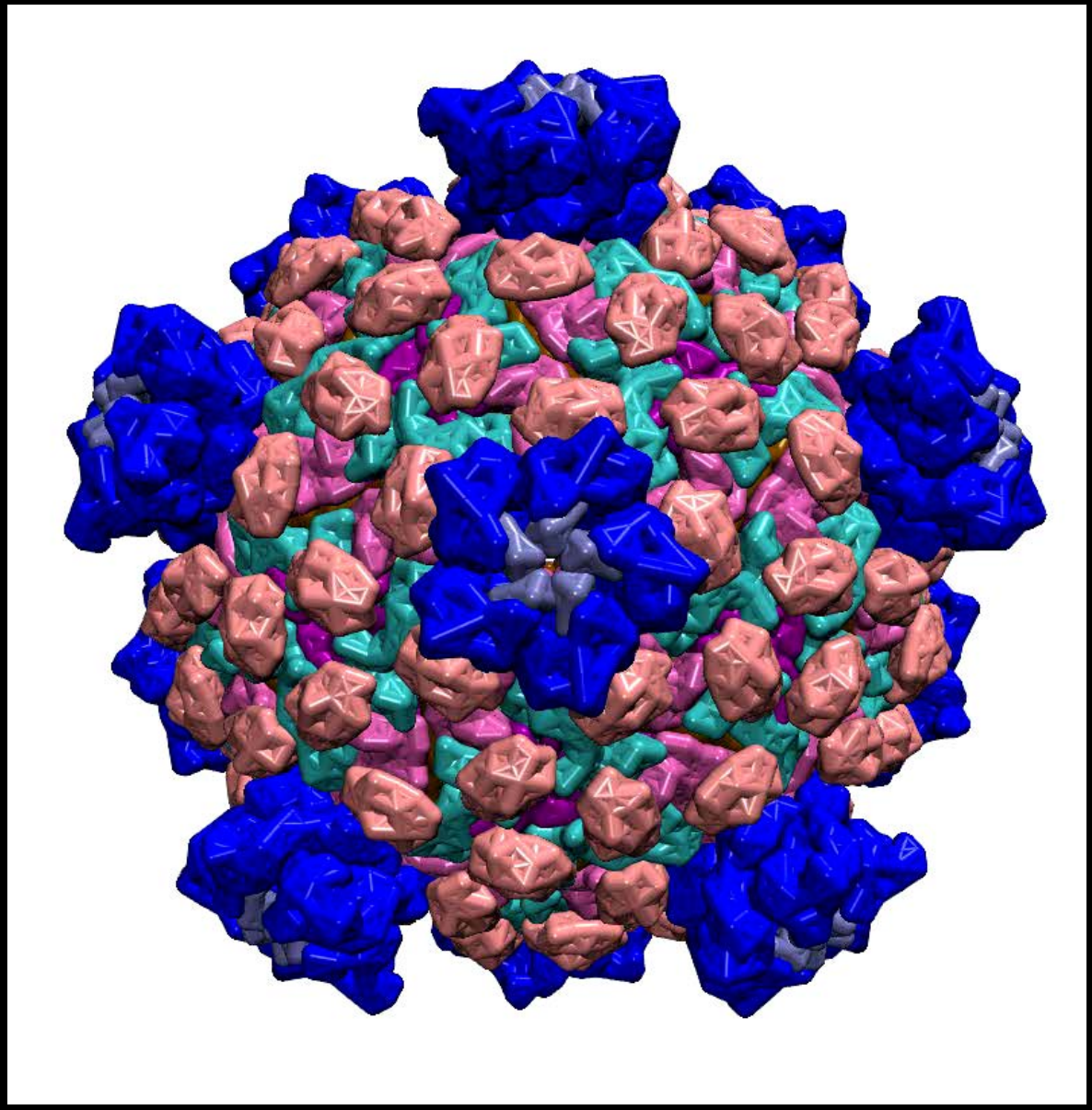


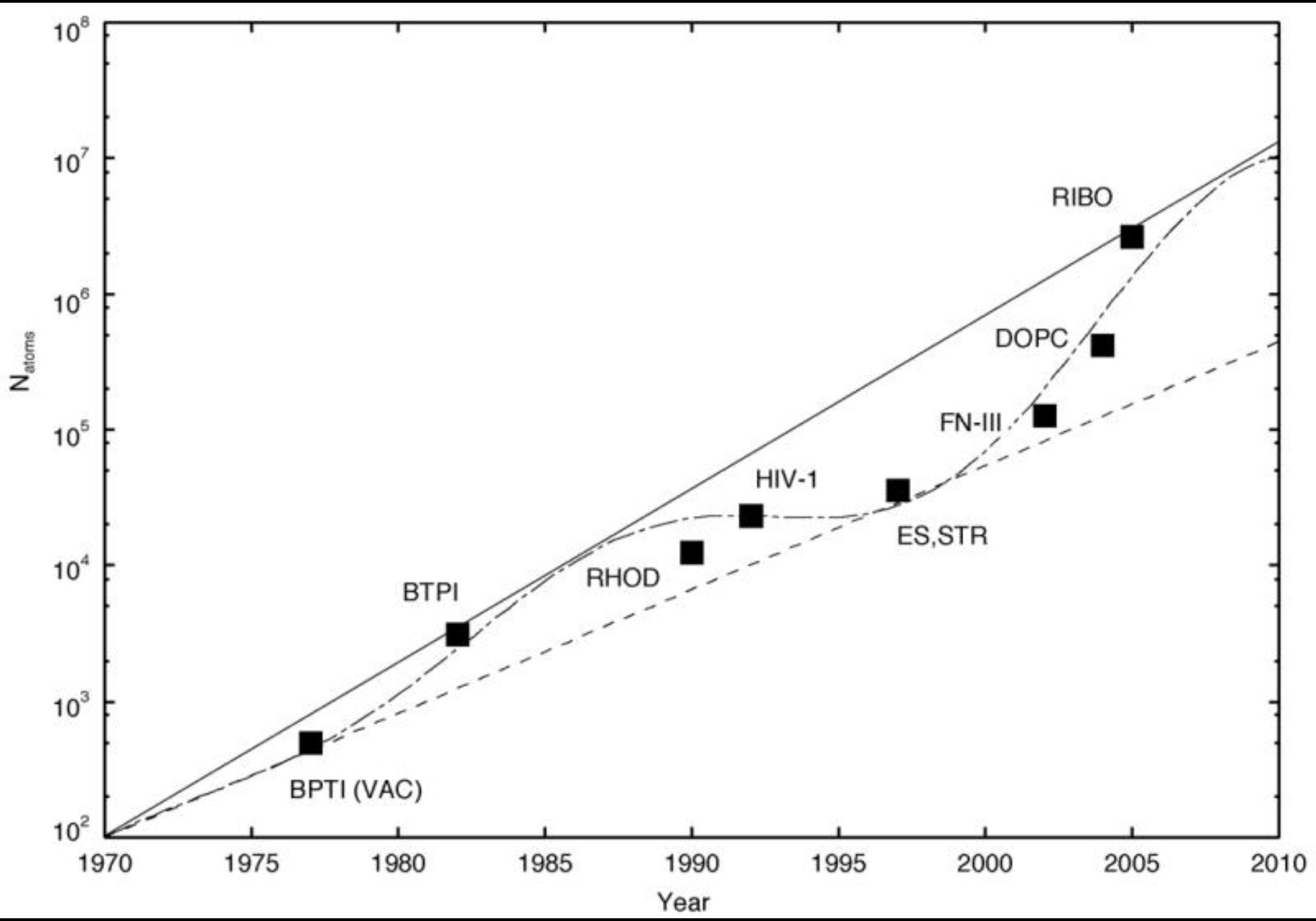

Capsid
RNA

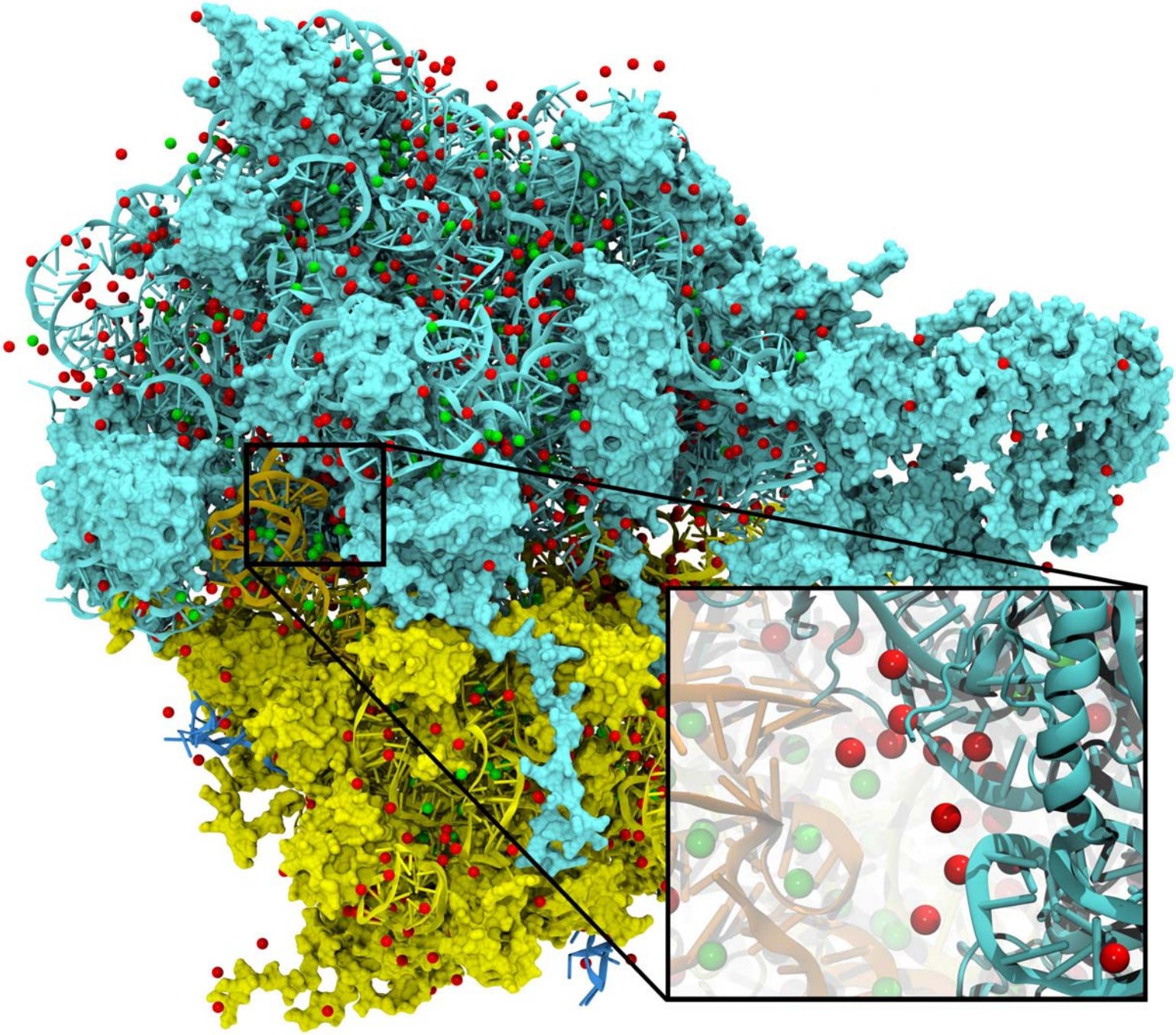

BMV with tails
BMV, tails removed
Poliovirus
Reovirus core
Theoretical and Computational Biophysics Group
Beckman Institute
University of Illinois at Urbana-Champaign


Satellite Tobacco Mosaic Virus
5 µs
5 µs
Satellite Panicum Mosaic Virus
25 µs
Satellite Tobacco Necrosis Virus
7 µs
Brome Mosaic Virus
5 µs
5 µs
Poliovirus
11 µs
Bacteriophage ϕX174 Procapsid
5 µs
Reovirus Core
1.5 µs
50 nm

Viruses




10^8
10^7
10^6
10^5
10^4
10^3
10^2
N_{atoms}
1970
1975
1980
1985
1990
1995
2000
2005
2010
Year
RIBO
DOPC
FN-III
HIV-1
ES,STR
RHOD
BTPI
BPTI (VAC)



Biophysical Journal Volume 92 June 2007 3817–3829

Refinement of the AMBER Force Field for Nucleic Acids: Improving the Description of α/γ Conformers

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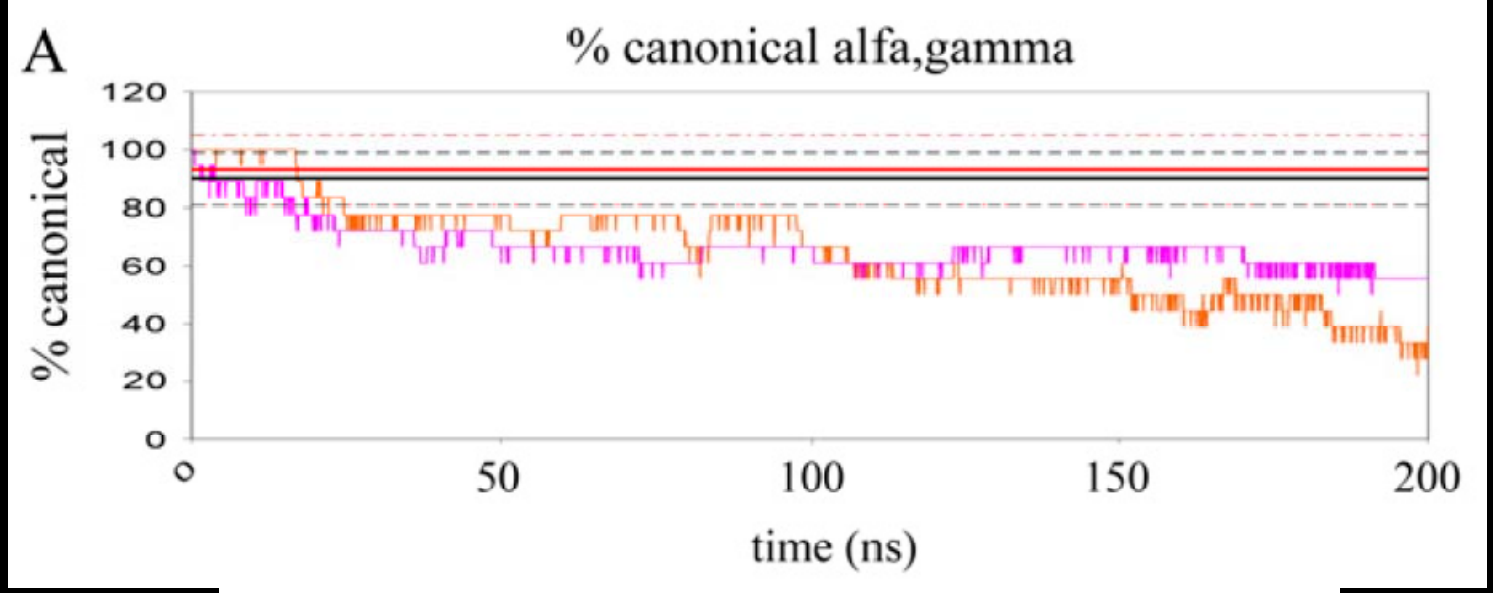
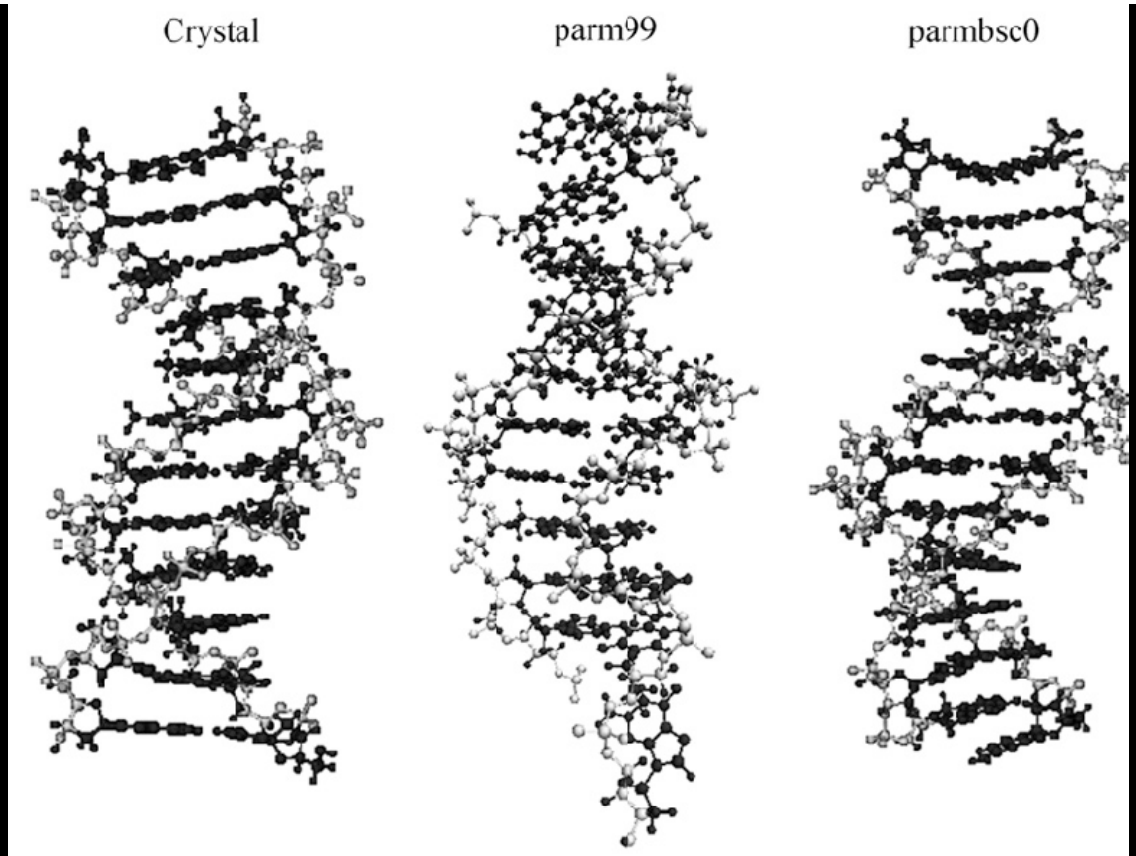
*Molecular Modeling and Bioinformatics Unit, Institut de Recerca Biomèdica & Instituto Nacional de Bioinformática, Parc Científic de Barcelona, Barcelona 08028, Spain; †Computational Biology Program, Barcelona Supercomputer Centre, Edifici Torre Girona, Barcelona 08028, Spain;

Sequence	Family	Length, ns
$D(CGCGAATTCGCG)_2$	B-DNA duplex DD	2×200
$d(T_{10}\cdot A_{10}\text{-}T_{10})$	Triplex PS	10
$d(C_{10}\cdot G_{10}\text{-}G_{10})$	Triplex APS	10
$d(T_{10}\cdot A_{10}\text{-}A_{10})$	Triplex APS	10
$d(GGGG)_4$	G-DNA PS	10
$d(GGGG)_4$	G-DNA APS	10
$d(CGCGCGCGCG)_2$	Z-DNA duplex	10
$d(CGCGAATTCGCG)_2$	A-DNA duplex	10
$d(T_{10}\cdot A_{10}\text{-}T_{10})$	A-DNA triplex	10
$d(ATATATATATAT)_2$	Hoogsteen duplex	10
r(UUCGGGCGCC)·d(GGCGCCCGAA)	DNA·RNA hybrid (PDB code 1FIX)	10
$r(CGCGAAUUCGCG)_2$	RNA duplex DD	10
r(GCGAGAGUAGG)·r(CCGAUGGUAGU)	RNA duplex (NDB code URL064)	10
r(CGCGGCACCGUCCGCGGAACAAACGG)	RNA pseudoknot (NDB code UR0004)	10
Nottingham dataset	B-DNA	38×3
Nottingham dataset	A-DNA	36×3
Nottingham dataset	Z-DNA	6×3
d(CCATGCGCTGAC)·d(GTCAGCGCATGG)	Pathological B-DNA	25


A
% canonical alfa,gamma
% canonical
120
100
80
60
40
20
0
0
50
100
150
200
time (ns)


Crystal
parm99
parmbsc0

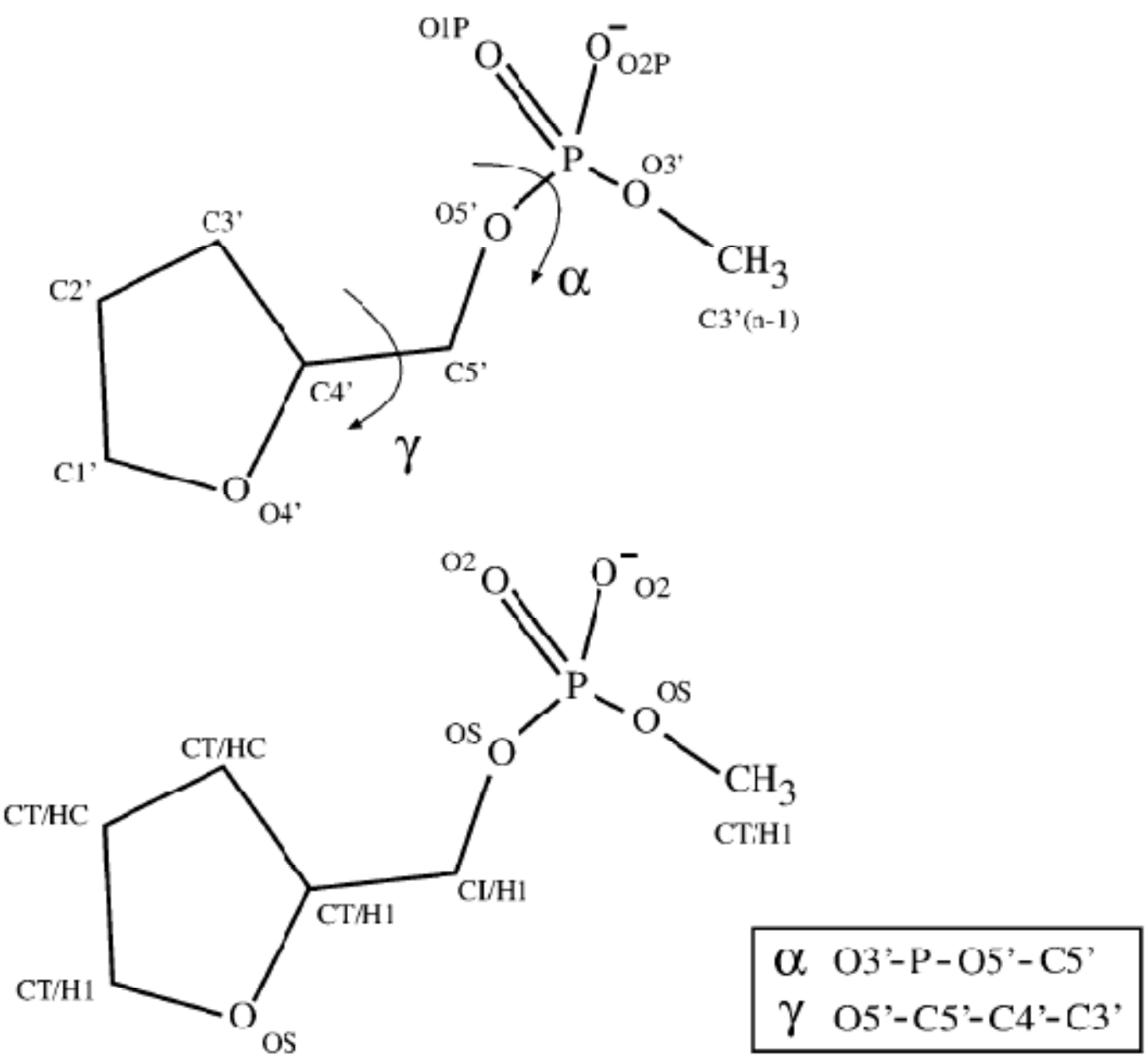
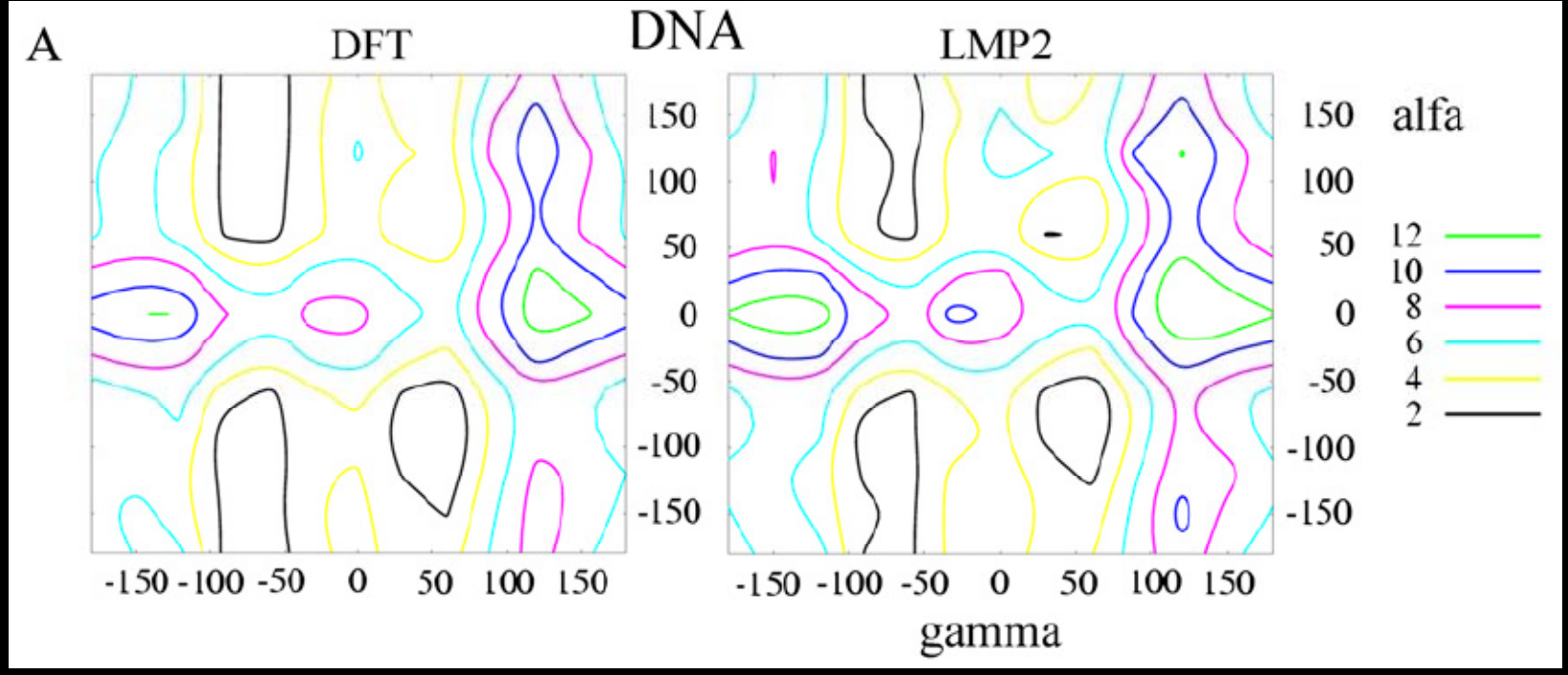
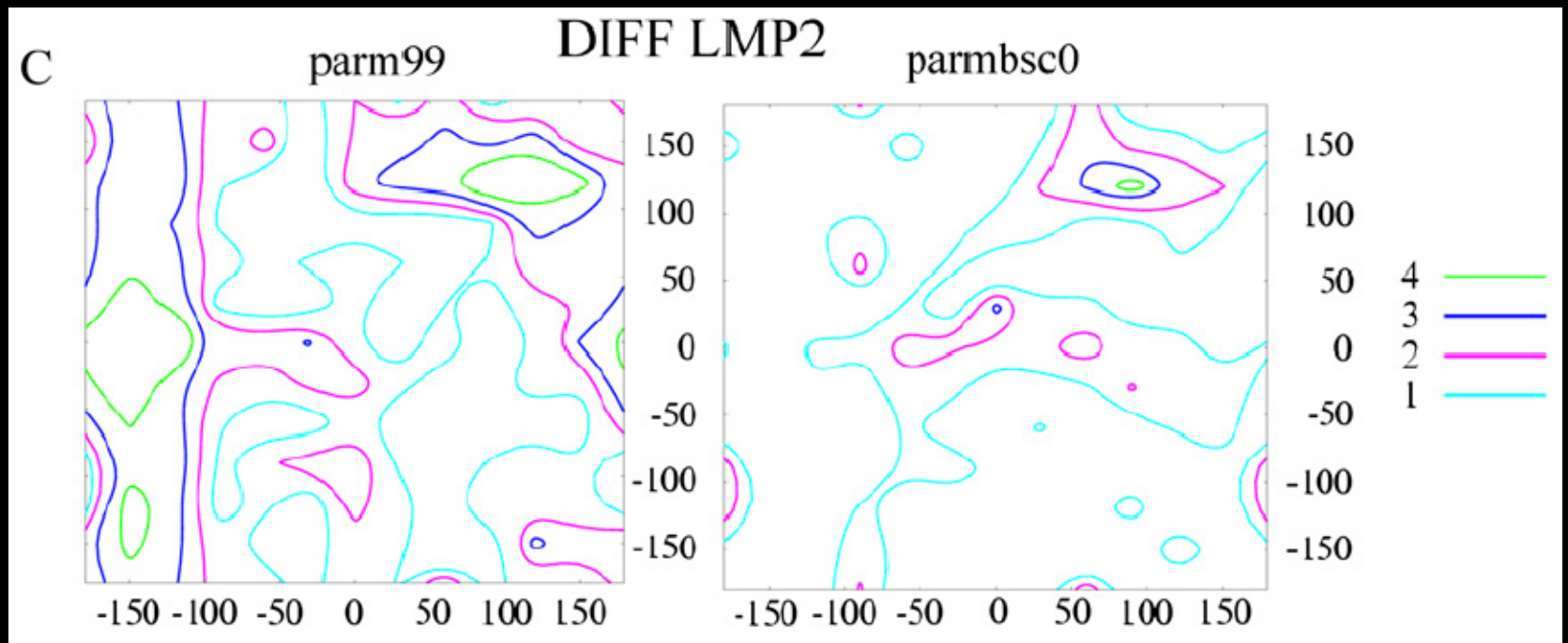


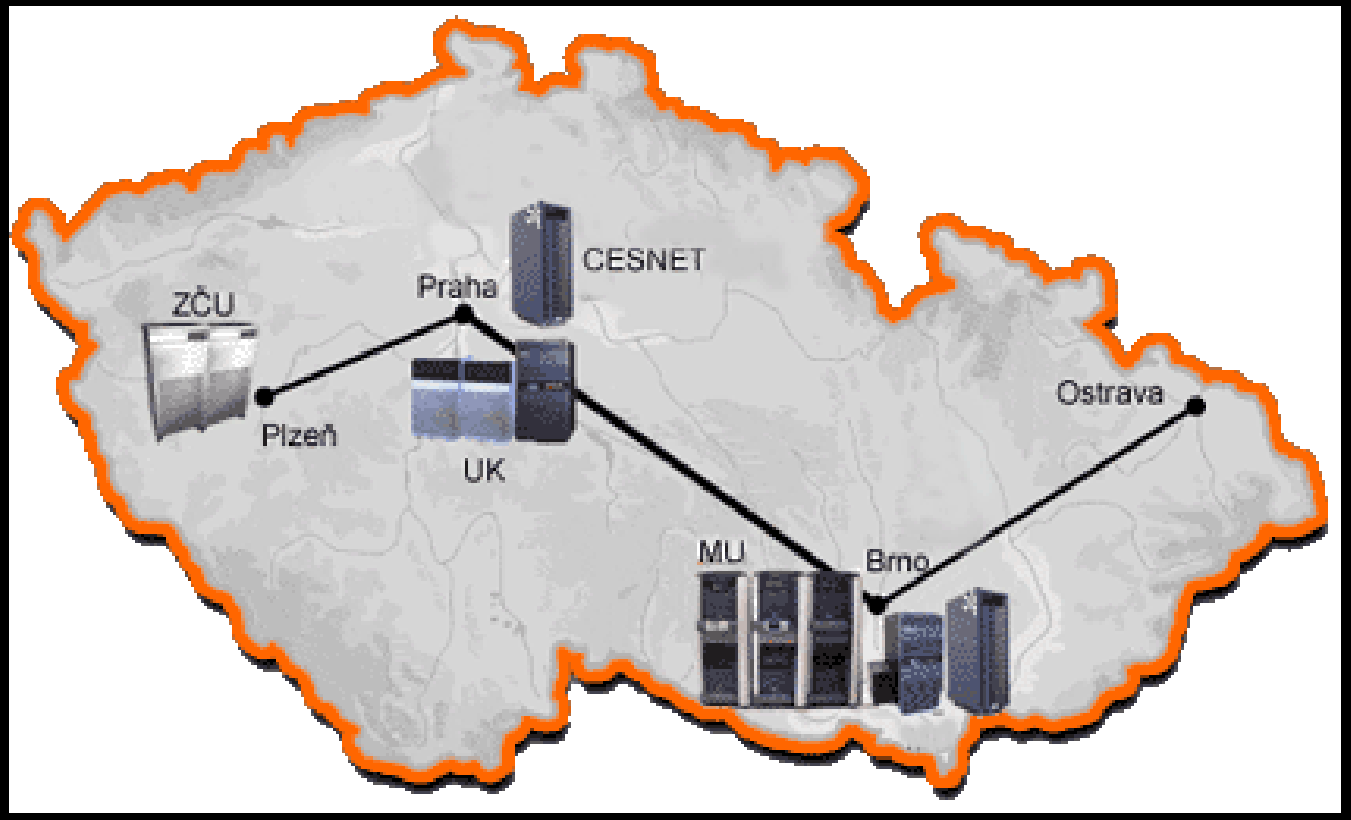
FIGURE 1 Schematic representation of the molecular model used to parameterize α and γ torsions. The atom-type definition is also displayed.


A
DFT
DNA
LMP2
150
100
50
0
-50
-100
-150
-150 -100 -50 0 50 100 150
alfa
12
10
8
6
4
2
gamma


C
parm99
DIFF LMP2
parmbsc0
150
100
50
0
-50
-100
-150
-150 -100 -50 0 50 100 150
4
3
2
1

Hardware

NIC Juelich
Barcelona …



1994 Superpočítačová centra Praha, Brno, Ostrava, Plzeň
1996 Metacentrum
1999 výzkumný záměr Cesnet
2004 EGEE grid

Metacentrum MU + UK
52 MU + 60 UK MIPS SGI Origin2000, Power Challenge
192 Pentium III, IV PC clustery

Coupled Clusters

MFF UK – Fyzikální sekce

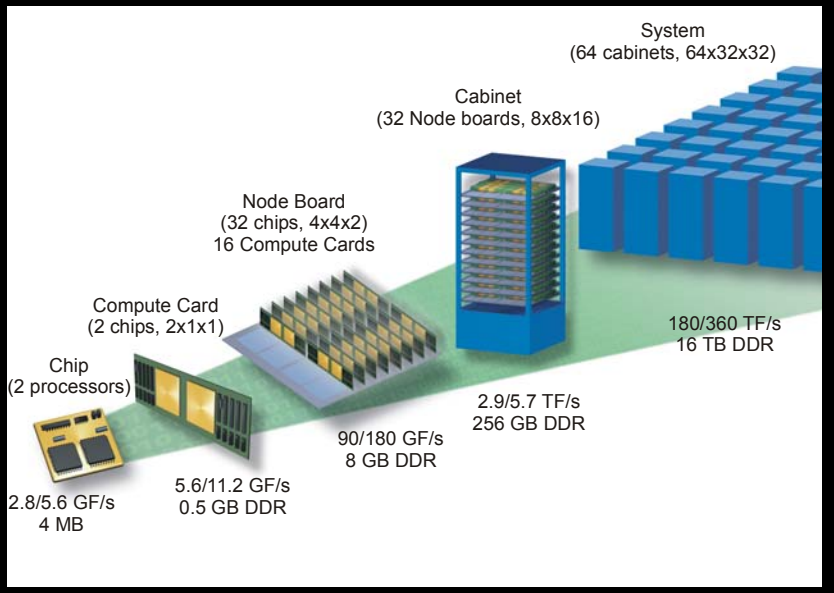
prof. RNDr. L. Skála DrSc. KCHF

Celkem: 100 procesorů (Opteron)

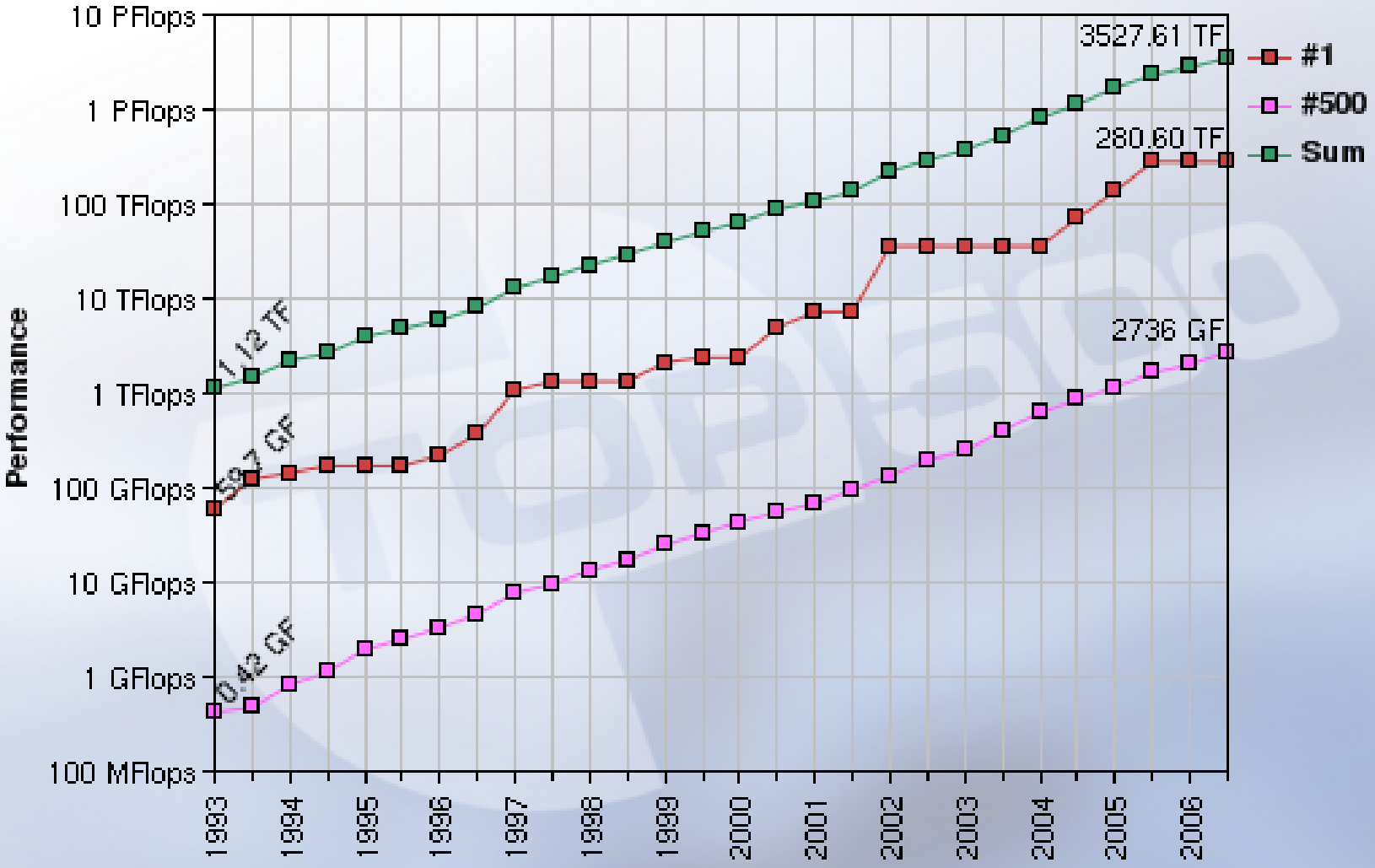
NAMD: 40 procesorů (MPI)

http://quantum.karlov.mff.cuni.cz/cc/

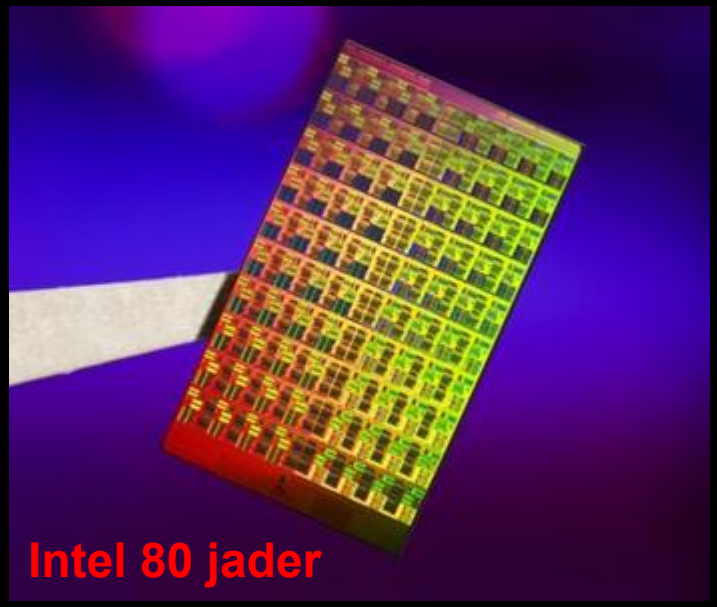
IBM Blue Gene 130.000 procesorů



Performance Development

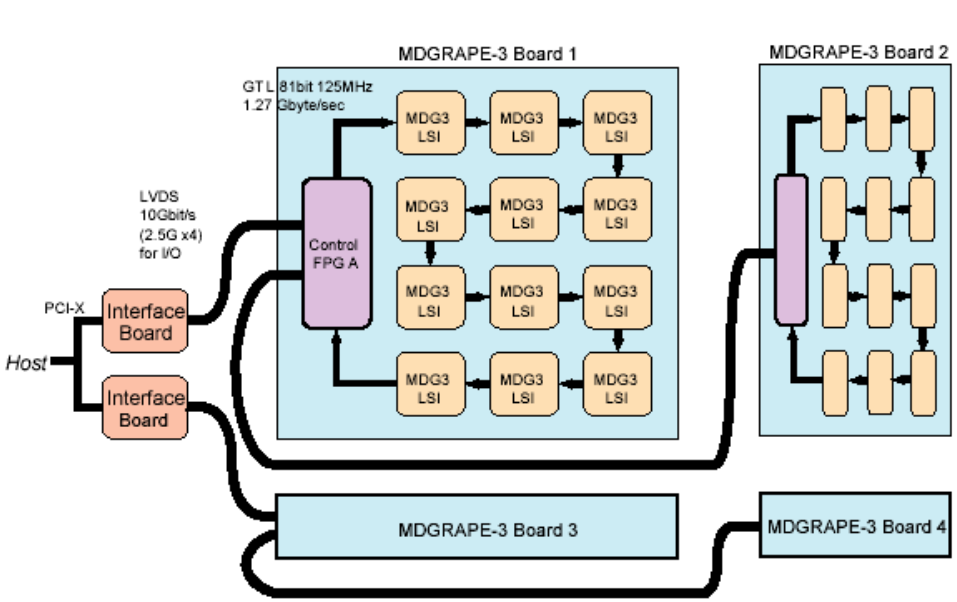


ASCI Red 10.000 procesorů



MDGRAPE 3

MDGRAPE 3



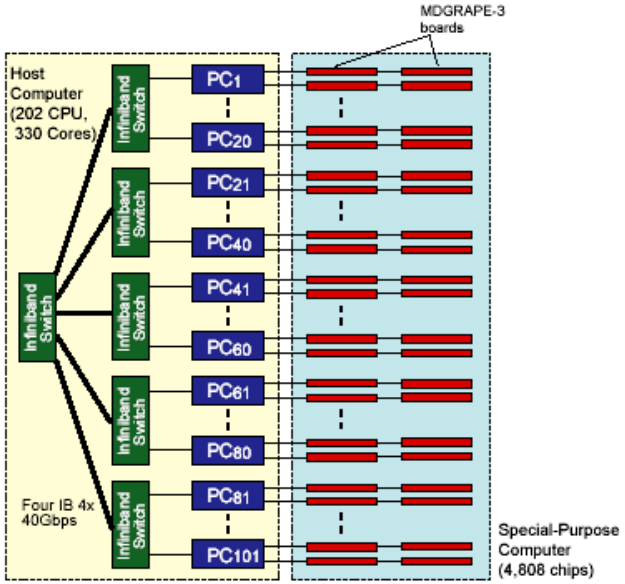


Figure 1. Block diagram of the MDGRAPE-3 board, which has 12 MDGRAPE-3 chips connected in a daisy-chain and an FPGA (left). Block diagram of the MDGRAPE-3 system, which is consisted of the PC cluster with 101 nodes and 402 MDGRAPE-3 boards (right).

System	Peak speed (Gflops)	Cost/speed ($/Gflops)	Power/speed (Watt/Gflops)	Size/speed (liter/Gflops)
MDGRAPE-3	1,000,000	**9**	**0.2**	**0.03**
Blue Gene/L	360,000	280	4	0.3
PC (Pentium D 3.0GHz)	12	80	25	3

Table 1. Advantages of MDGRAPE-3 against general-purpose computers. The MDGRAPE-3 is superior to general-purpose computers in all of the three points which are cost/speed, power/speed, and size/speed as underlined.

Number of atoms	3,339	4,953	13,101
Without MDGRAPE-3 card (sec)	346.73	844.52	9231.70
With MDGRAPE-3 card (sec)	6.38	7.33	34.31
Acceleration	**54**	**115**	**269**

Table 3. Performance of the MDGRAPE-3 card

GPU – NVIDIA – CUDA (Compute Unified Device Architecture)

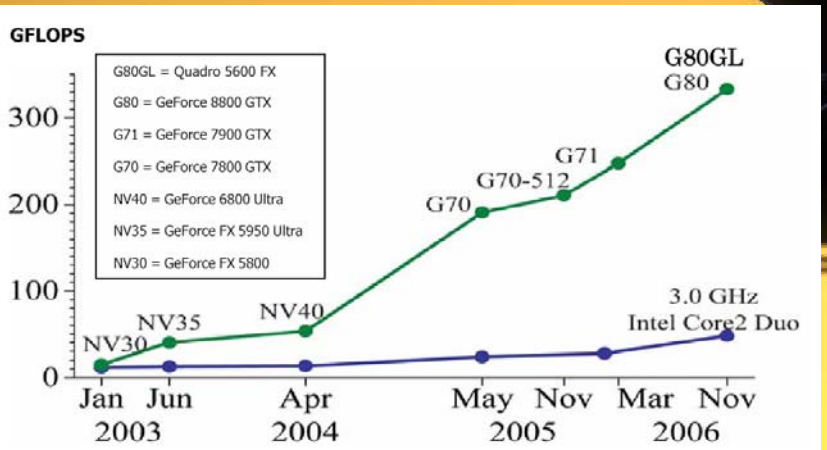


Figure 1-1. Floating-Point Operations per Second for the CPU and GPU

Accelerating Molecular Modeling Applications with Graphics Processors

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