MC_DNA:
A web server for the detailed study of the structure and dynamics of DNA and chromatin fibers

BioExcel Webinar Series

Presenter: Jürgen Walther
Host: Adam Carter

11th April, 2018

Partners

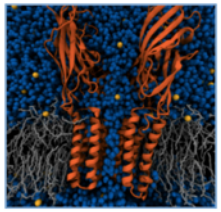
Funding

Horizon 2020
European Union Funding
for Research & Innovation

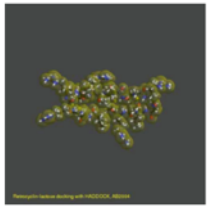
This webinar is being recorded

BioExcel Overview

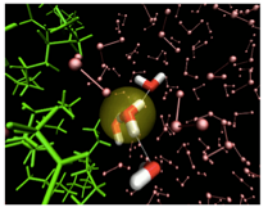
- **Excellence in Biomolecular Software**
  - Improve the performance, efficiency and scalability of key codes



MD simulations
/GROMACS/

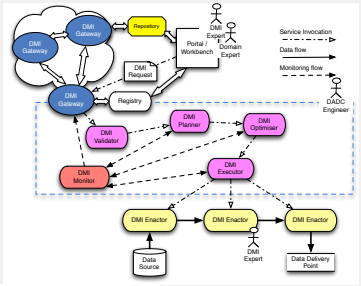


Docking
/HADDOCK/



QM/MM
/CPMD/

- **Excellence in Usability**
  - Devise efficient workflow environments with associated data integration



Key Workflows and Platforms

Galaxy PROJECT · Open PHACTS · COMPSs · Open for Innovation KNIME · Apache Taverna

- **Excellence in Consultancy and Training**
  - Promote best practices and train end users

Interest Groups

- Integrative Modeling IG
- Free Energy Calculations IG
- Hybrid methods for biomolecular systems IG
- Biomolecular simulations entry level users IG
- Practical applications for industry IG
- Training IG
- Workflows IG

Support platforms

http://bioexcel.eu/contact


Forums

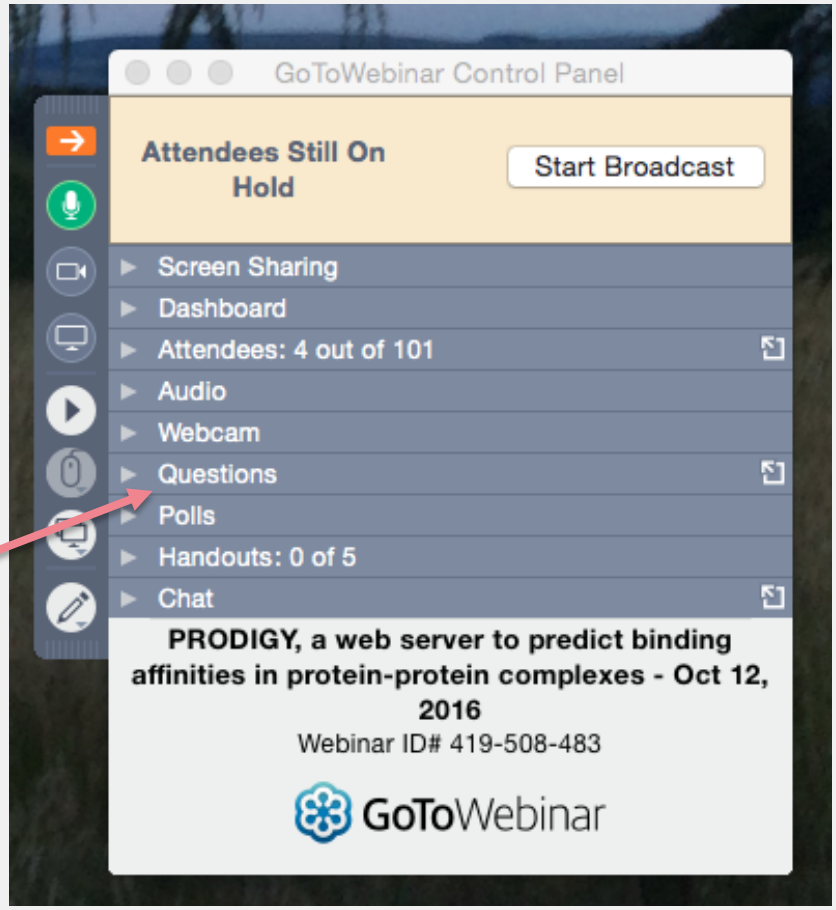
de Repositories
Cha hannel

Video annel


Audience Q&A session

Please use the **Questions** function in GoToWebinar application

Any other questions or points to discuss after the live webinar? Join the discussion the discussion at http://ask.bioexcel.eu.



Today's Presenter

Jürgen Walther, IRB Barcelona

Jürgen obtained his B.Sc. degree at the University of Würzburg in Physics. His final degree work was done in Astrophysics.

He did his master degree at the University of Texas at Austin (USA) in Physics with specialization in Biophysics, where he worked on refining a microscope technique involving light microscopy, TIRF fluorescence and optical trapping to visualize the movement of molecular motors walking along microtubules.

He is now working as a PhD student in Modesto Orozco's Molecular modeling and bioinformatics laboratory of at the Institute for Research in Biomedicine, Barcelona.
His main focus is to bridge known information of free DNA and of chromatin maintaining a high level of resolution in the theoretical models used. The application MC_DNA has been developed and integrated into a webserver. MC_DNA is a component of the Multiscale Genomics project where a unified view of the genome at all length scales from base-pair to chromosome in form of a webserver is developed.

A web server for the detailed study of the structure and dynamics of DNA and chromatin fibers.

Joint bioexcel-MuG webinar

Jürgen Walther – 11.04.2018

Partners

Funding

Horizon 2020
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for Research & Innovation

Outline

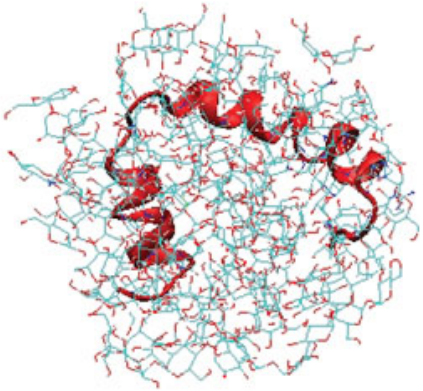
1. Introduction into Biomolecular Simulations

2. MC_DNA webserver

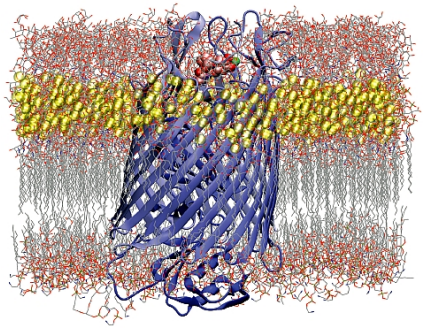
    - Method
    - Webpage
    - Input
    - Output
    - Analysis

Biomolecular simulations: A matter of…

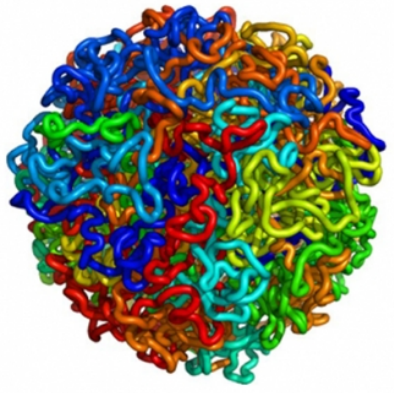
Size



Small peptides
~ 1.000 atoms

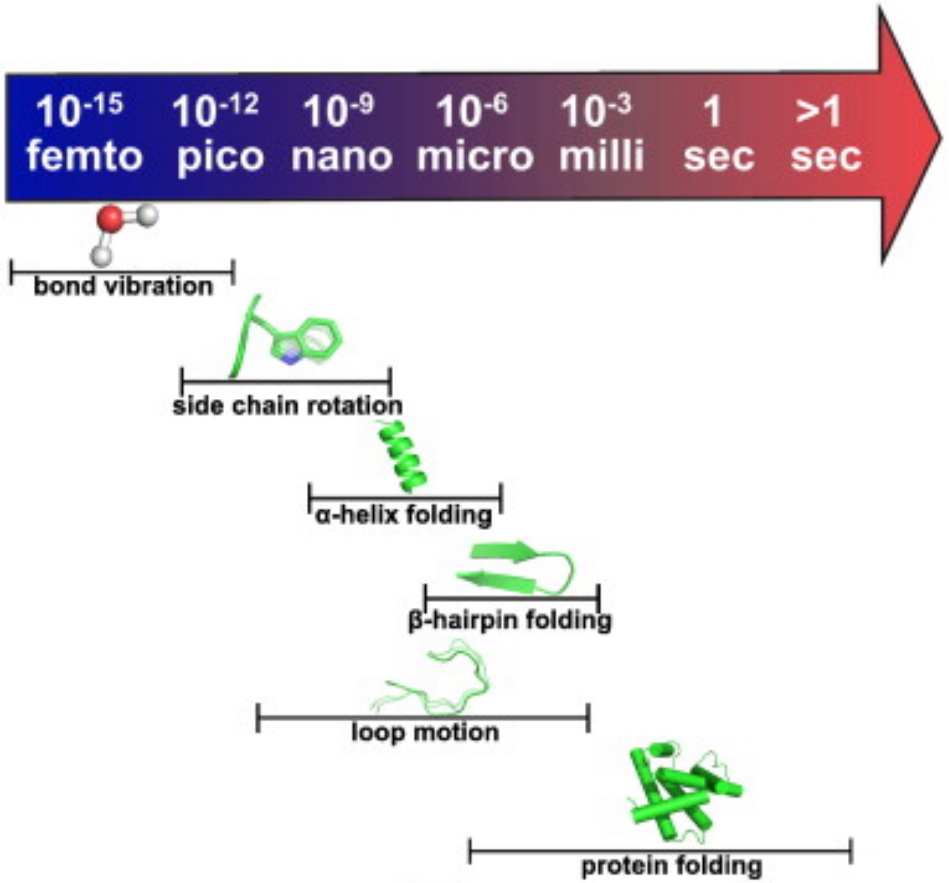


Macromolecular complexes
~ 50.000 to ~ 1.000.000 atoms



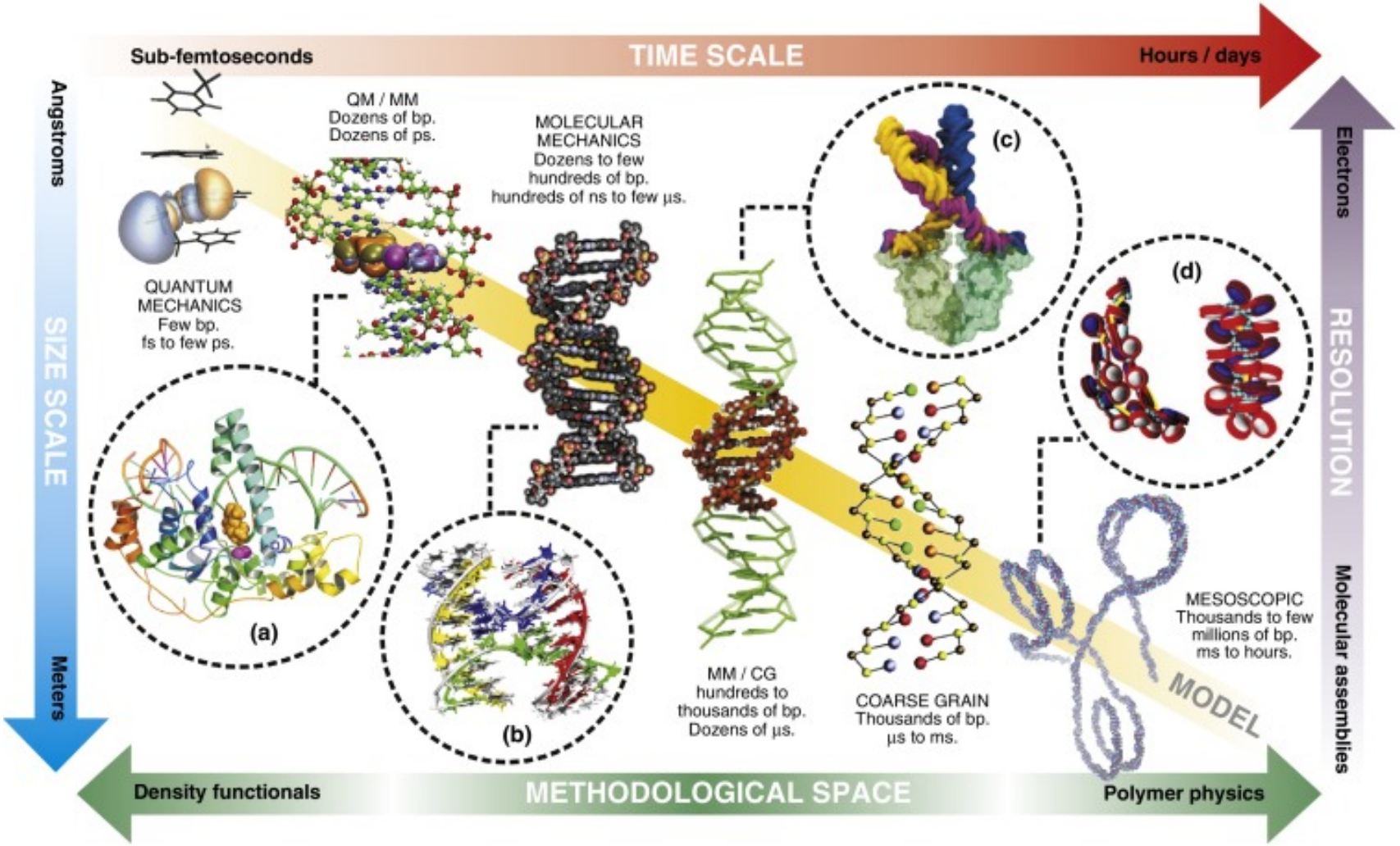
Human Genome
~ 10e+10 atoms

Time

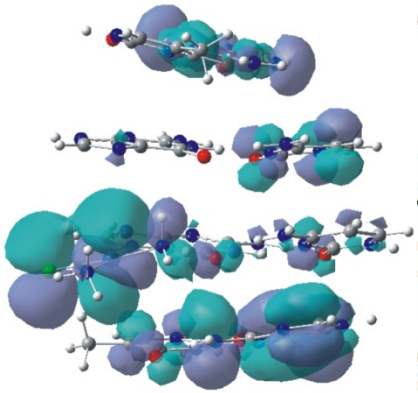


Werner et al. Adv Drug Deliv Rev. **2012**, 64: 323.

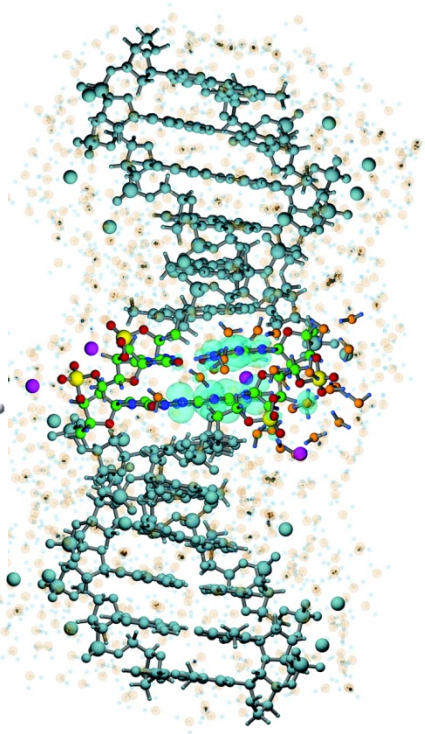
Biomolecular simulations: The big picture



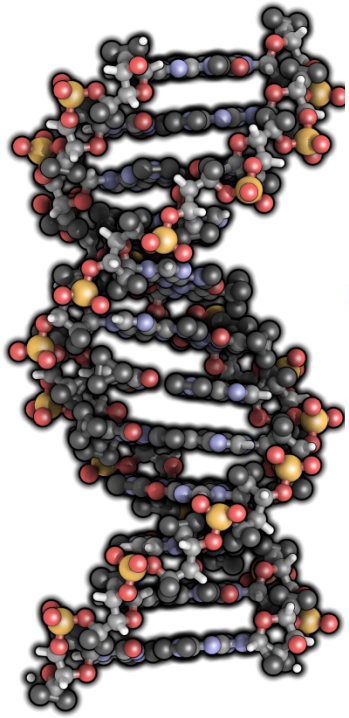
Biomolecular simulations: Models



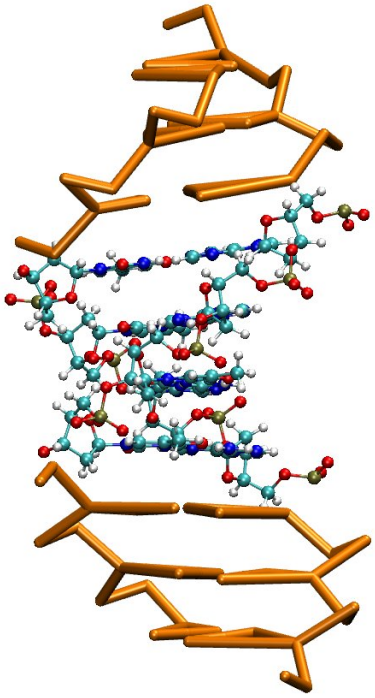
Quantum Mechanics
Dozens to hundreds of atoms
Few ps



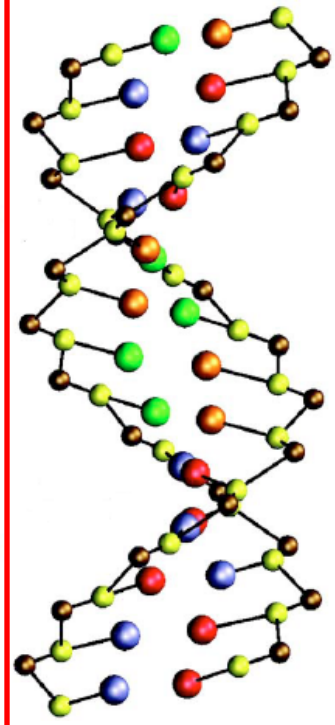
QM/MM
Dozens to thousands of atoms
Dozens of ps



Molecular Mechanics
Thousands to few millions of atoms
Hundreds of ns to few ms



MM/CG
few millions of "atoms"
Hundreds of μs to few ms



Coarse Grained
Several millions of "atoms"
Dozens of μs to ms

Biomolecular simulations: A multi-scale problem

Available online at www.sciencedirect.com
ScienceDirect
Current Opinion in Structural Biology

Multiscale simulation of DNA

Pablo D Dans[1,2], Jürgen Walther[1,2], Hansel Gómez[1,2] and Modesto Orozco[1,2,3]

DNA is not only among the most important molecules in life, but a meeting point for biology, physics and chemistry, being studied by numerous techniques. Theoretical methods can help in gaining a detailed understanding of DNA structure and function, but their practical use is hampered by the multiscale nature of this molecule. In this regard, the study of DNA covers a broad range of different topics, from sub-Angstrom details of the electronic distributions of nucleobases, to the mechanical properties of millimeter-long chromatin fibers. Some of the biological processes involving DNA occur in femtoseconds, while others require years. In this review, we describe the most recent theoretical methods that have been considered to study DNA, from the electron to the chromosome, enriching our knowledge on this fascinating molecule.

Addresses
[1] Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology, Baldiri Reixac 10-12, 08028 Barcelona, Spain
[2] Joint BSC-IRB Research Program in Computational Biology, Baldiri Reixac 10-12, 08028 Barcelona, Spain
[3] Department of Biochemistry and Molecular Biology, University of Barcelona, 08028 Barcelona, Spain

Corresponding author: Orozco, Modesto (modesto.orozco@irbbarcelona.org)

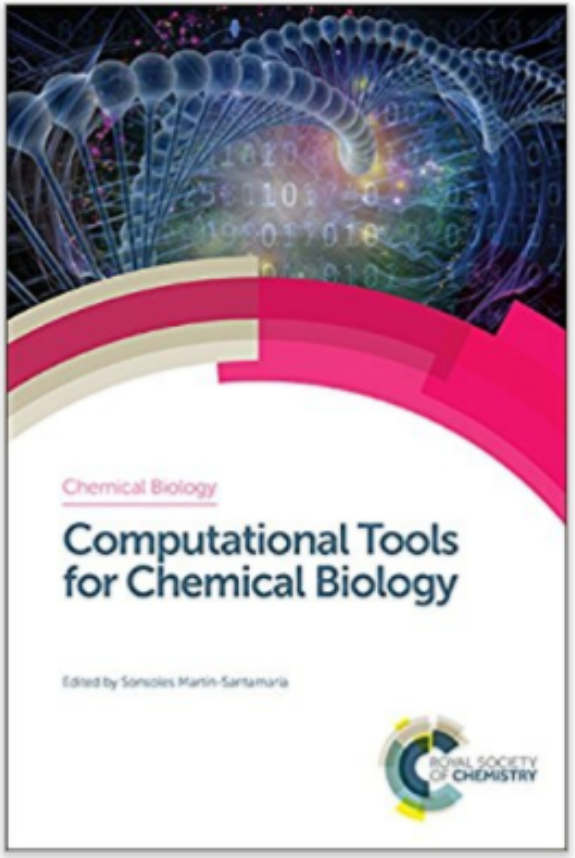
in the day time-scale (10^5 s); the local breathing of nucleobases occurs in the millisecond range (10^{-3} s), while electronic rearrangements take place in the sub-femtosecond time-scale ($<10^{-15}$ s).

During the last years we have witnessed the development of a wide repertoire of theoretical methods that aimed to reproduce the properties of DNA, either isolated or protein bound. Even if primitive, these methods allow researchers to consider the DNA at different resolution levels, and provide information of great value on the structure, dynamics, and interactions of this fascinating molecule. We will briefly summarize some of these most recent theoretical approaches, focusing our analysis on the contributions of the last three years, when the field has experienced a significant improvement.

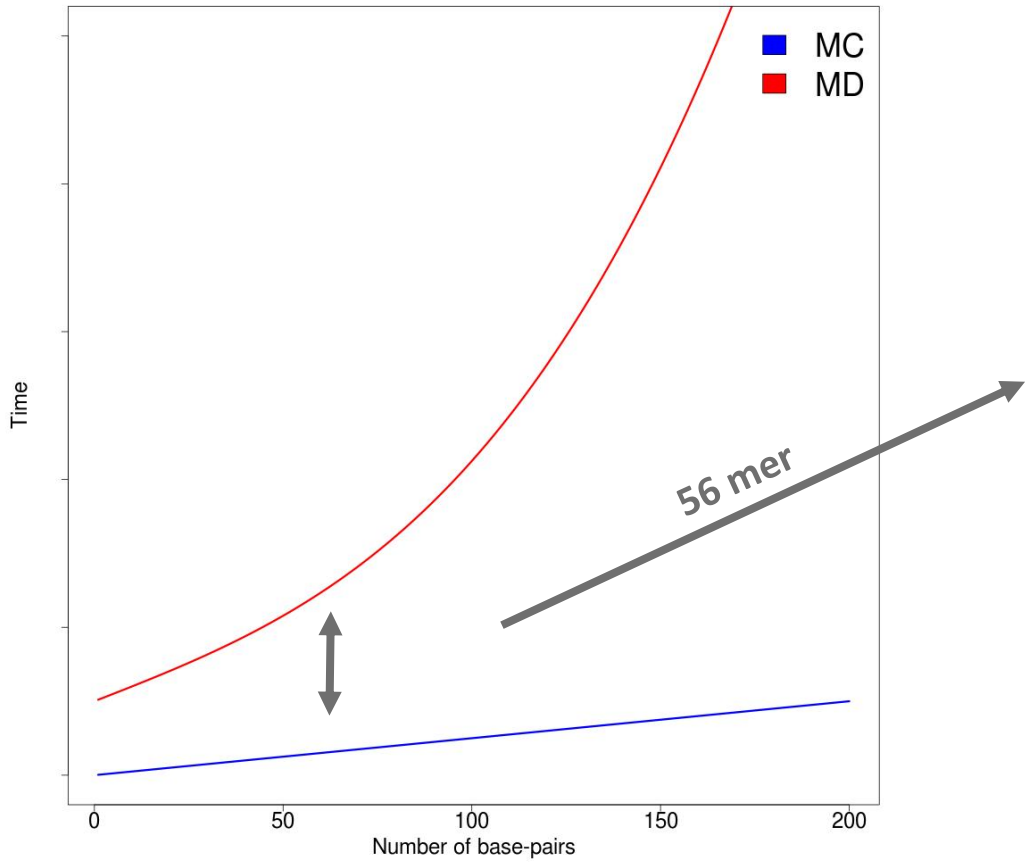
For the sake of simplicity, throughout this manuscript we will classify theoretical methods in four groups, according to their level of resolution (Figure 1): firstly, electronic, secondly, atomistic, thirdly, coarse grained, and lastly, mesoscopic. It is worth noting that moving in the resolution space means moving also in the methodological space, since the basic physical models underlying the

Multiscale simulation of DNA (2016)
PD Dans, J Walther, H Gómez, M Orozco
Current opinion in structural biology 37, 29-45

Molecular Modeling of Nucleic Acids (2017)
H Gómez, J Walther, L.Darré, I Ivani, PD Dans, M Orozco. In Computational Tools for Chemical Biology. RSC, ISBN: 1782627006

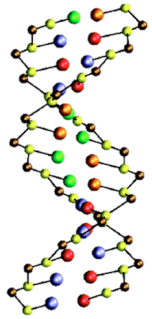


Calculation time: coarse-grained DNA (MC) vs atomistic DNA (MD) simulations



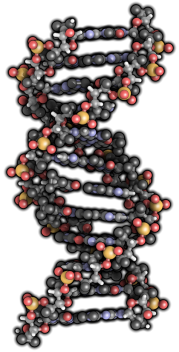
MC DNA

10K structures in 10 min (1 CPU)



vs

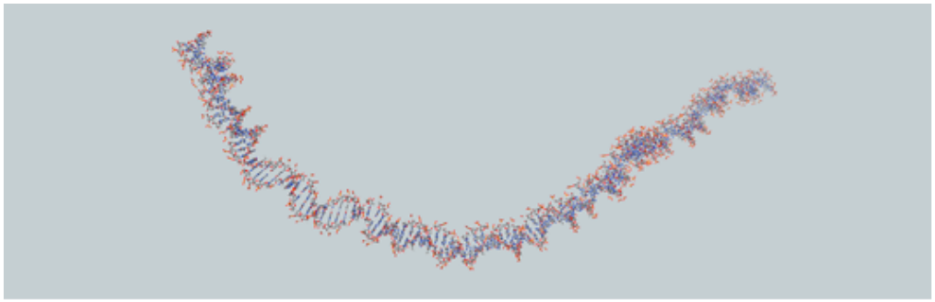
650,000 CPU hours in the MareNostrum supercomputer



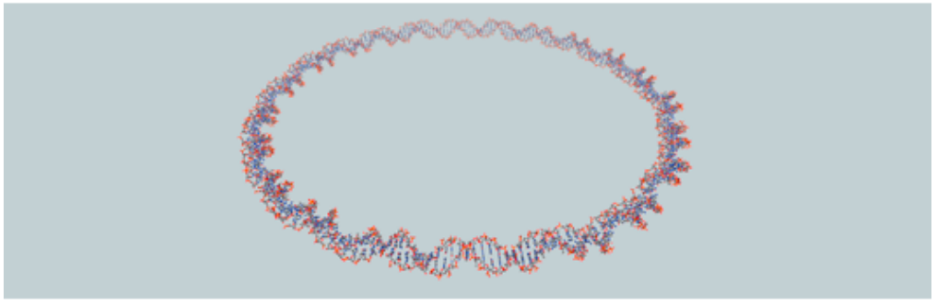
MC DNA

http://mmb.irbbarcelona.org/MCDNA/

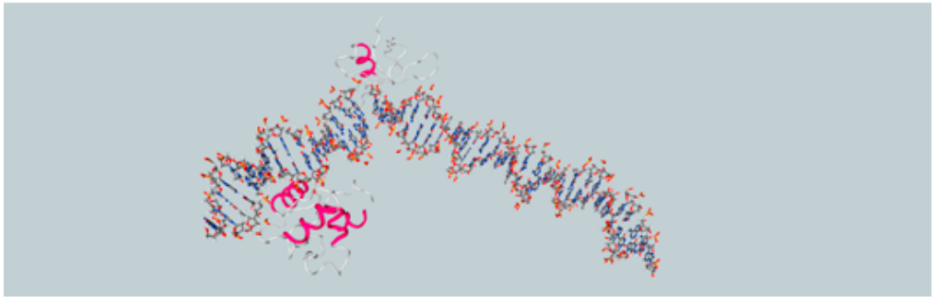
Free linear



Circular

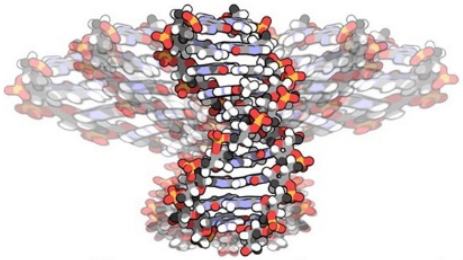


Protein-coated



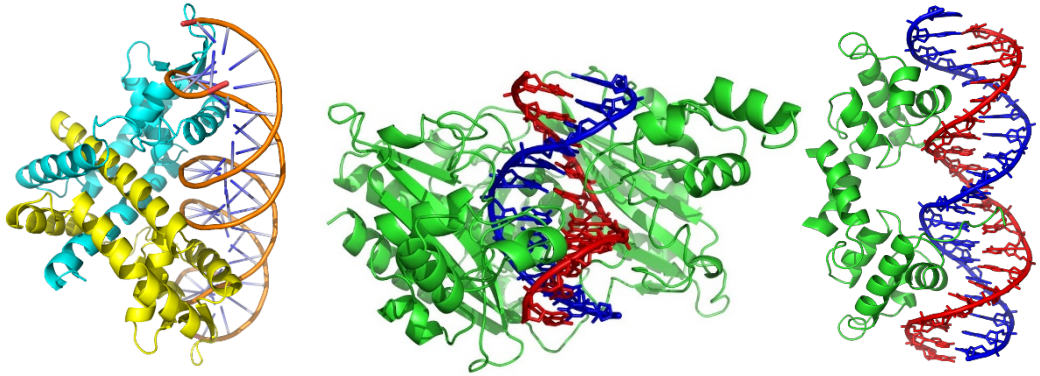
MC DNA

Dynamics of free linear DNA (MC_DNA)

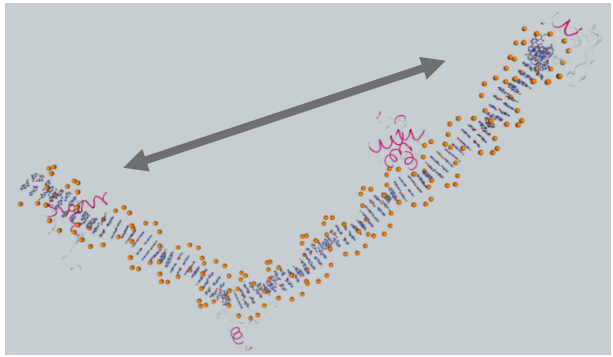


Distant contacts in a constrained environment (circular MC_DNA)

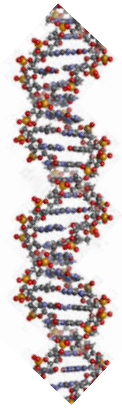
Accessibility of a protein-coated DNA fiber (MC_DNA + proteins)

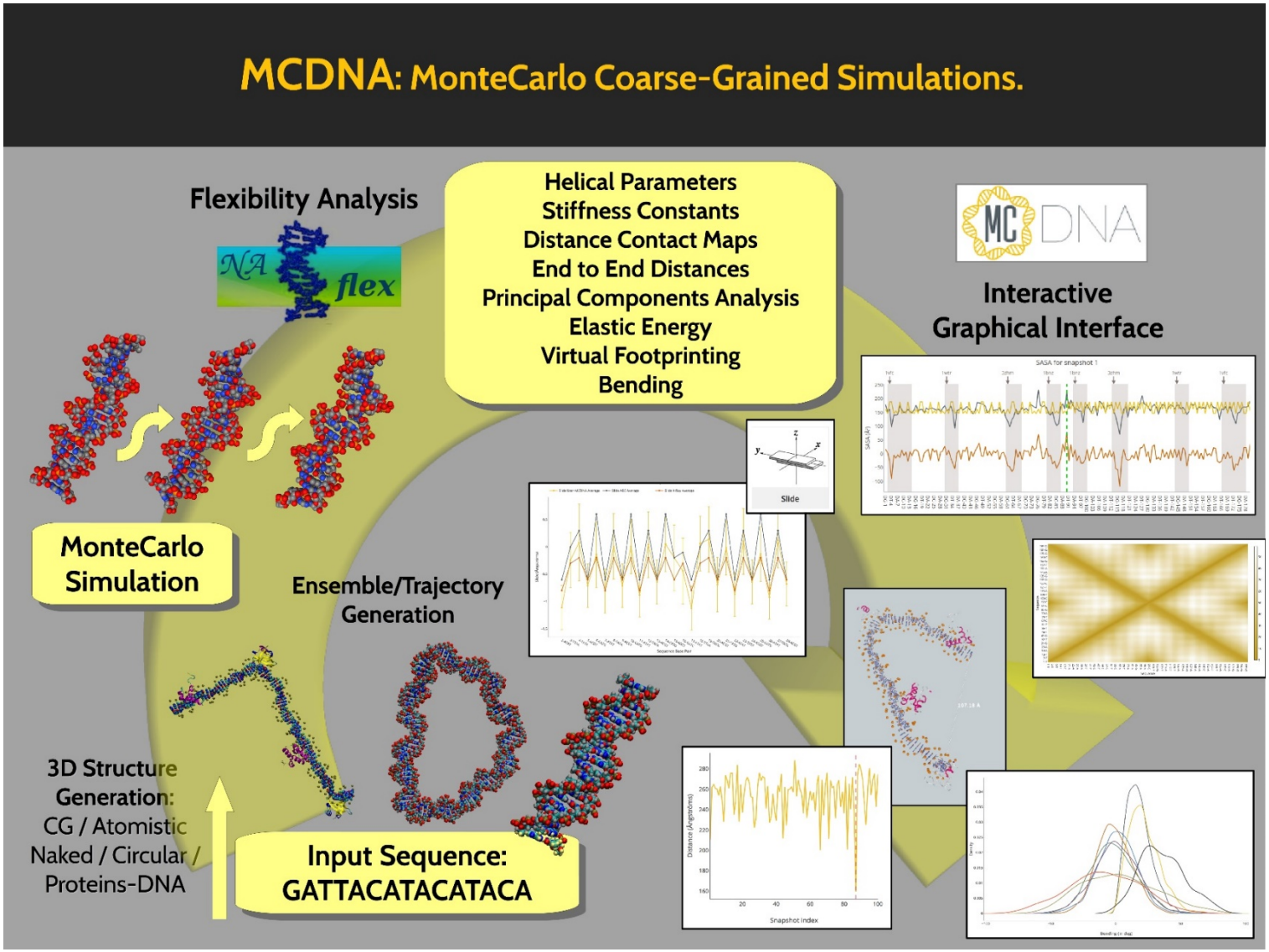


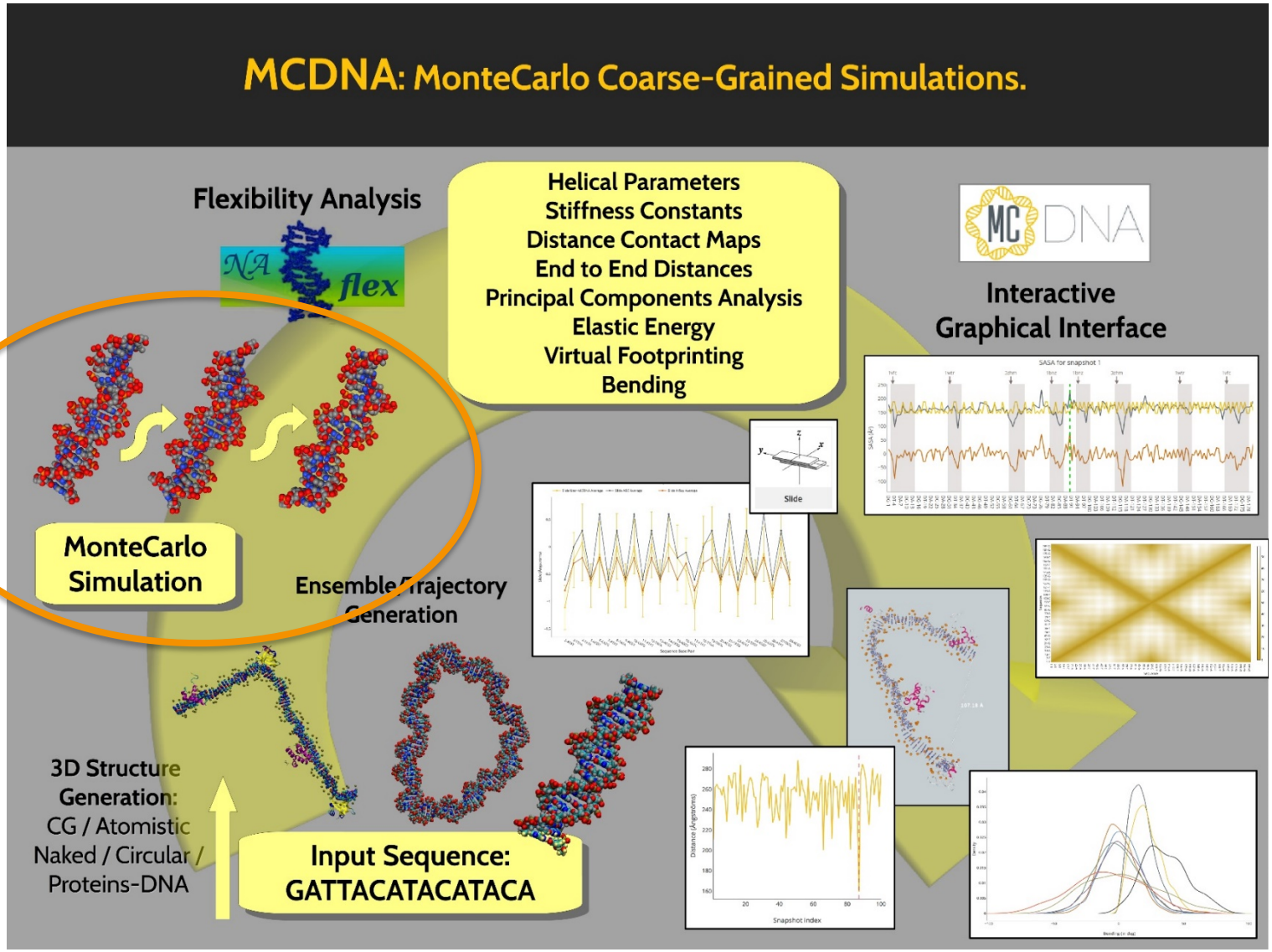
DNA-mediated protein-protein communication



Adopting bioactive conformation




MCDNA: MonteCarlo Coarse-Grained Simulations.
Flexibility Analysis
NA flex
Helical Parameters
Stiffness Constants
Distance Contact Maps
End to End Distances
Principal Components Analysis
Elastic Energy
Virtual Footprinting
Bending
MC DNA
Interactive Graphical Interface
MonteCarlo Simulation
Ensemble/Trajectory Generation
3D Structure Generation:
CG / Atomistic
Naked / Circular /
Proteins-DNA
Input Sequence:
GATTACATACATACA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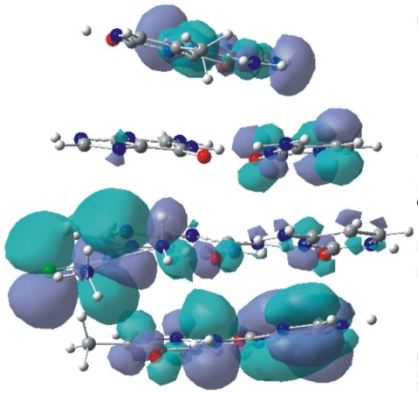
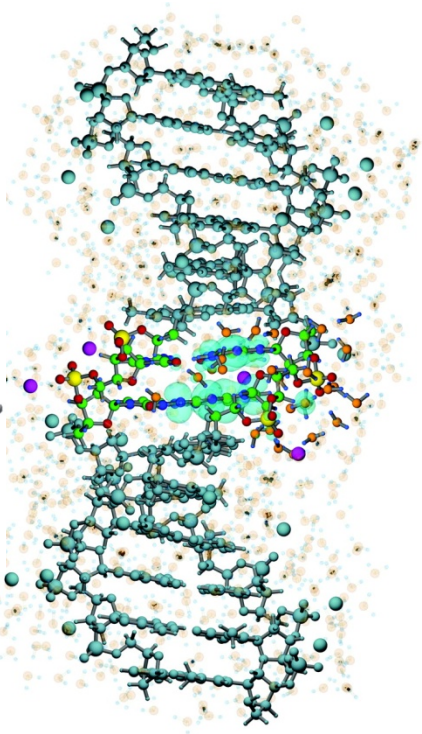
Interactive Graphical Interface
MonteCarlo Simulation
Ensemble Trajectory Generation
Slide
3D Structure Generation:
CG / Atomistic
Naked / Circular /
Proteins-DNA
Input Sequence:
GATTACATACATACA

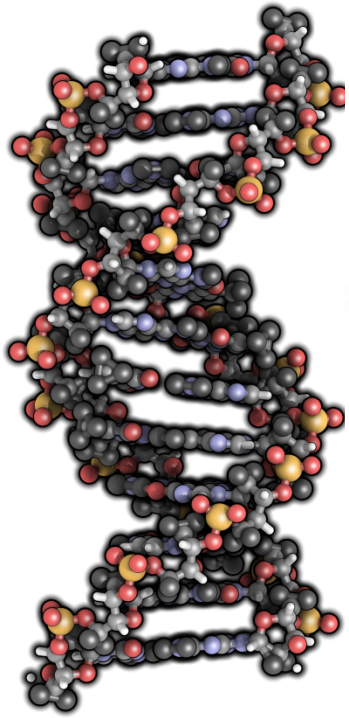
From molecular mechanics to coarse grained



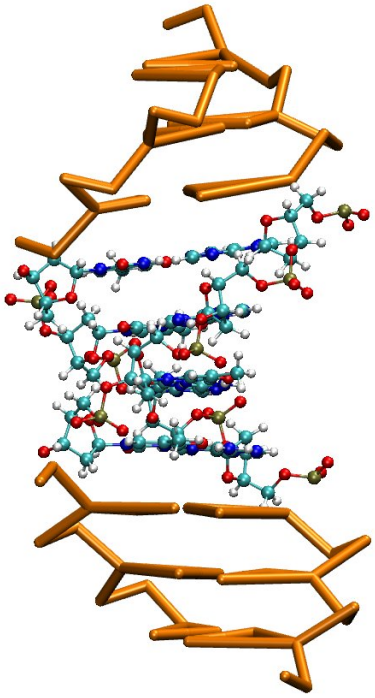
Quantum Mechanics
Dozens to hundreds of atoms
Few ps



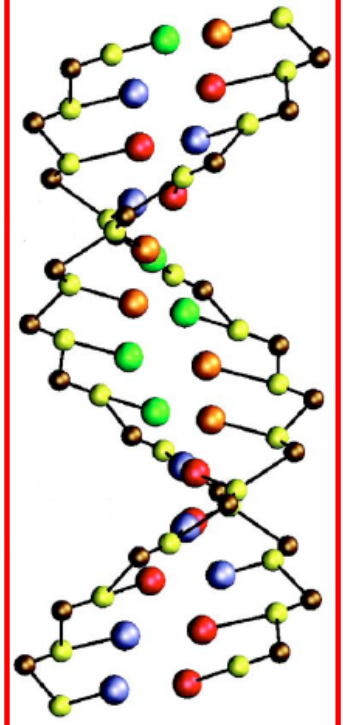
QM/MM
Dozens to thousands of atoms
Dozens of ps



Molecular Mechanics
Thousands to few millions of atoms
Hundreds of ns to few ms

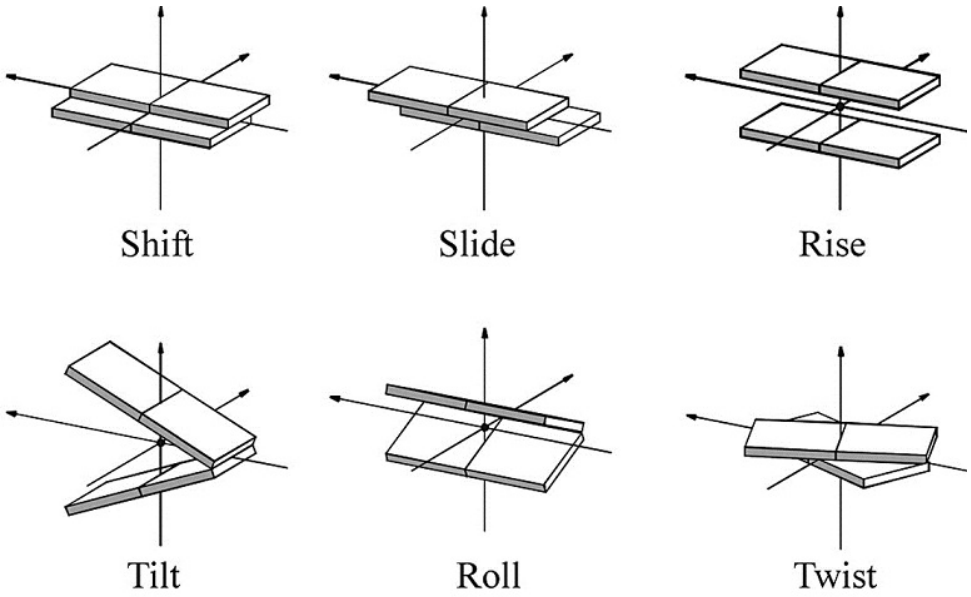


MM/CG
few millions of "atoms"
Hundreds of μs to (if) few ms

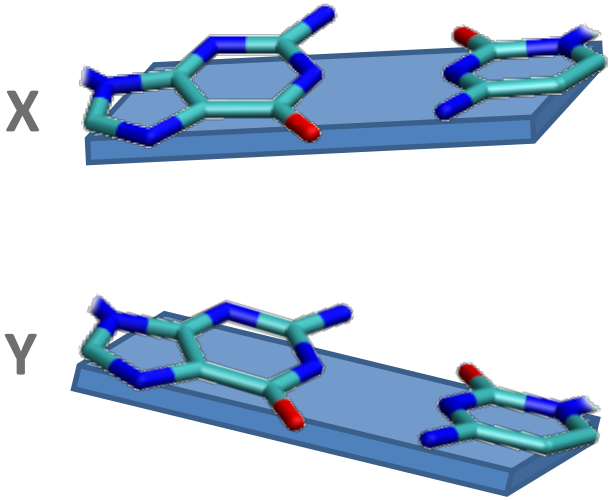


Coarse Grained
Several millions of "atoms"
Dozens of μs to ms

From cartesian to helical space



Base-pair step parameters (6)



Relative orientation and position between adjacent base-pairs

ABC database

x^0

Equilibrium values for each of the 136 unique tetranucleotides (taken as the average of a given helical parameter along time).

Pasi. NAR 2014

Obtaining the force constants from the covariance matrix in the helical space

Proc. Natl. Acad. Sci. USA
Vol. 95, pp. 11163–11168, September 1998
Biophysics

DNA sequence-dependent deformability deduced from protein–DNA crystal complexes

WILMA K. OLSON*†, ANDREY A. GORIN‡, XIANG-JUN LU*, LYNETTE M. HOCK*, AND VICTOR B. ZHURKIN†§

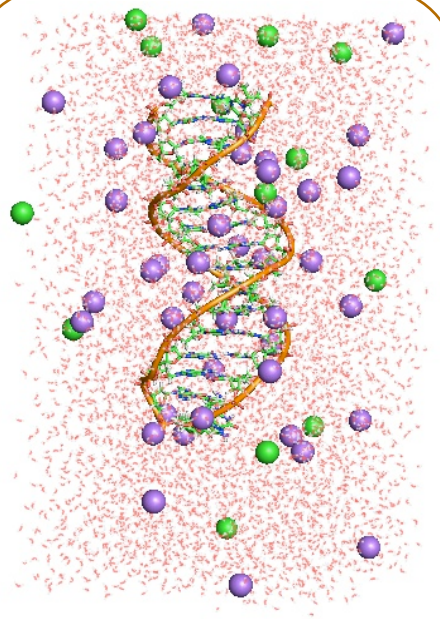
*Department of Chemistry, Rutgers University, New Brunswick, NJ 08903; ‡Sloan-Kettering Cancer Center, New York, NY 10021; and §National Cancer Institute, National Institutes of Health, Bethesda, MD 20892

Communicated by Donald M. Crothers, Yale University, New Haven, CT, June 30, 1998 (received for review April 13, 1998)

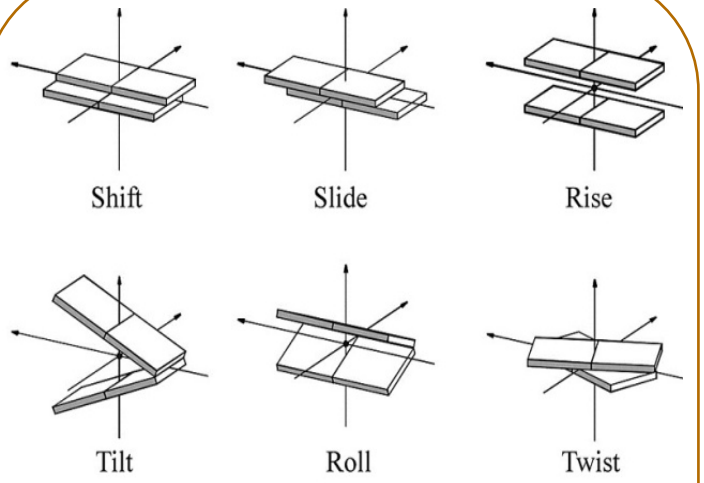
$$\mathrm{K}^{\mathrm{i}} = k_{\mathrm{B}} T C_{\mathrm{h}}^{-1} = \begin{bmatrix} k_{\mathrm{twist}} & k_{t-r} & k_{t-l} & k_{t-i} & k_{t-s} & k_{t-d} \\ k_{t-r} & k_{\mathrm{roll}} & k_{r-l} & k_{r-i} & k_{r-s} & k_{r-d} \\ k_{t-l} & k_{r-l} & k_{tilt} & k_{l-i} & k_{l-s} & k_{l-d} \\ k_{t-i} & k_{r-i} & k_{l-i} & k_{\mathrm{rise}} & k_{i-s} & k_{i-d} \\ k_{t-s} & k_{r-s} & k_{l-s} & k_{i-s} & k_{\mathrm{shift}} & k_{s-d} \\ k_{t-d} & k_{r-d} & k_{l-d} & k_{i-d} & k_{s-d} & k_{\mathrm{slide}} \end{bmatrix}$$

$$\mathrm{E}_{\mathrm{el}}^{\mathrm{i}} = \left(\mathrm{x_i} - \mathrm{x_i^0}\right)^{\mathrm{T}} \mathrm{K}^{\mathrm{i}} \left(\mathrm{x_i} - \mathrm{x_i^0}\right) \qquad \mathrm{x_i} \in \mathbb{R}^6, \mathrm{K_i} \in \mathbb{R}^{6\mathrm{x}6}$$

MC_DNA – The method: next-nearest neighbor model



All-atom MD simulations (parmbsc1)*



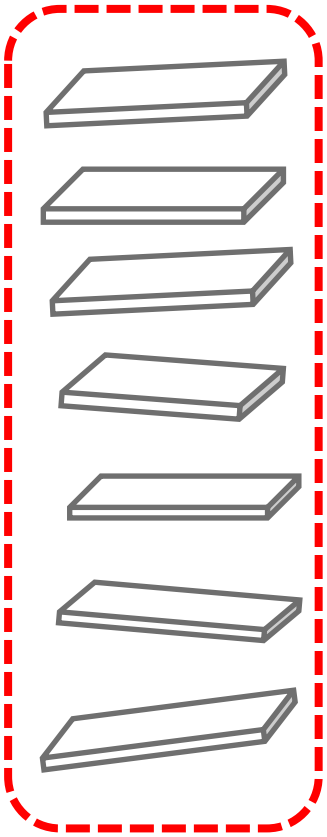
Elastic force constants $\mathbf{K^i}$ of bps i

bps parameters $\mathbf{x_i}$

bps equilibrium $\mathbf{x_i^0}$

$$E_{el}^{i} = \left(x_i - x_i^0\right)^T K^i \left(x_i - x_i^0\right)$$

Structure



Equilibrium structure built with x^0

Sequence-specific effects (NN model) included in elastic force constants K

MC_DNA – The method

Stochastic molecular simulation

Metropolis Monte Carlo

Randomly change helical parameters of random bp-step k

x_k -> $x_{k\,new}$

Calculate change in potential energy

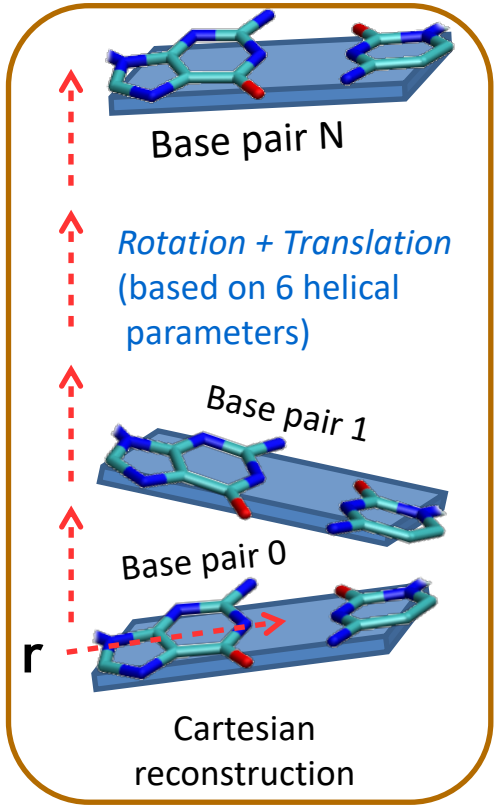
$$\Delta E = x_{k\,new}^T \, K \, x_{k\,new} - x_k^T \, K \, x_k$$

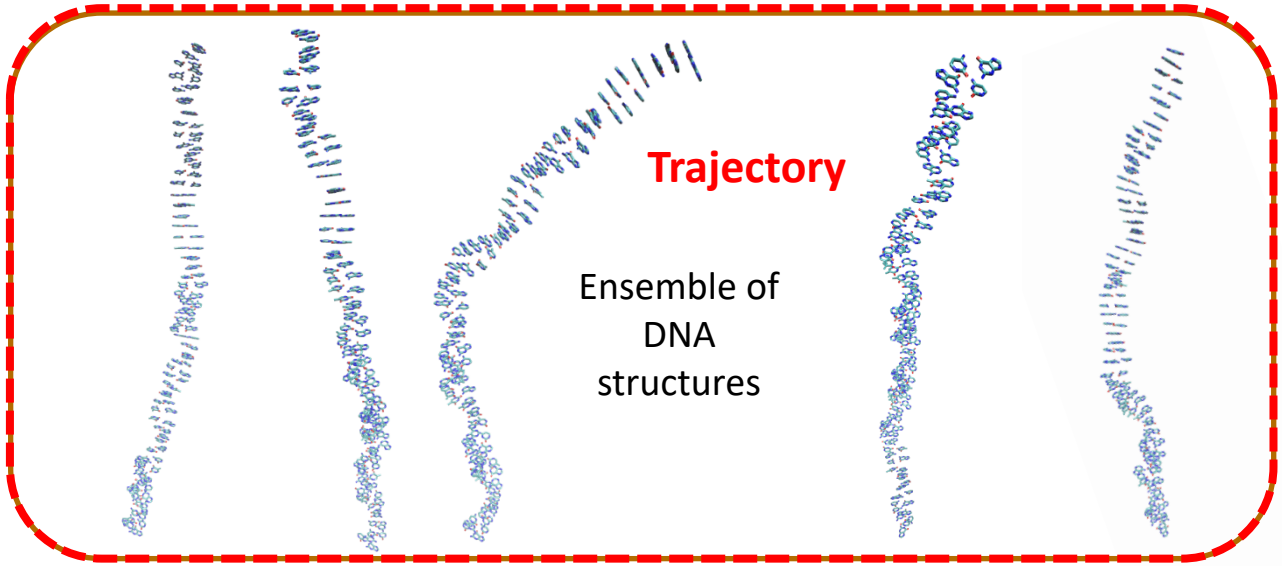
accept $x_{k\,new}$ keep x_k

yes no

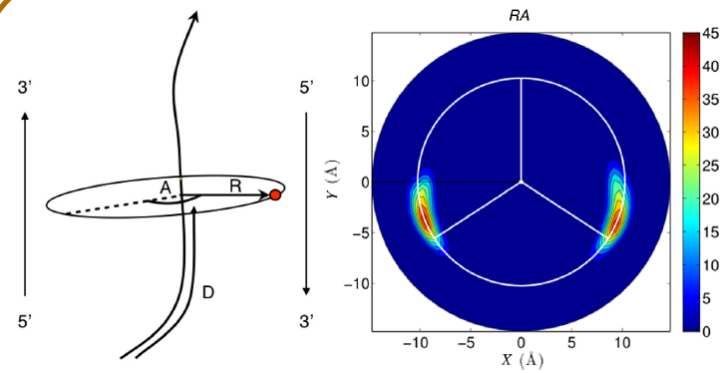
$\Delta E \geq 0$: $e^{-\Delta E/kT} > R$??

$\Delta E < 0$: accept $x_{k\,new}$

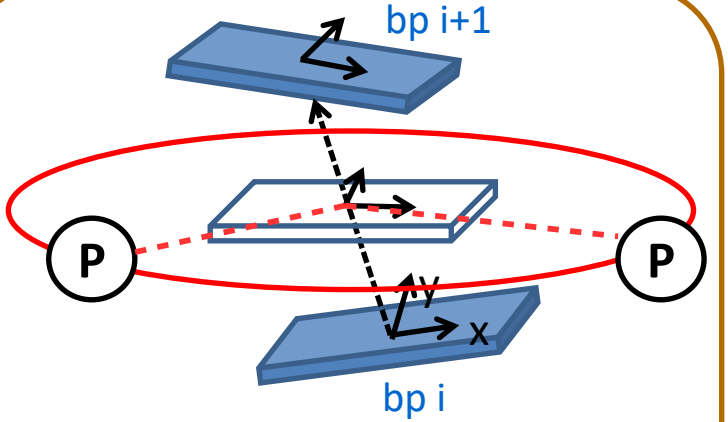




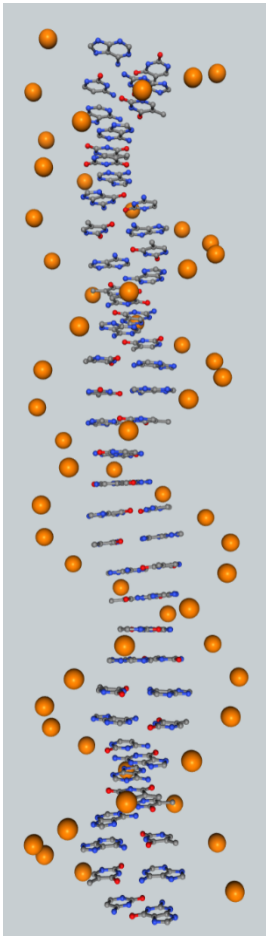
MC_DNA – Resolution



Phosphate position along helical axis**

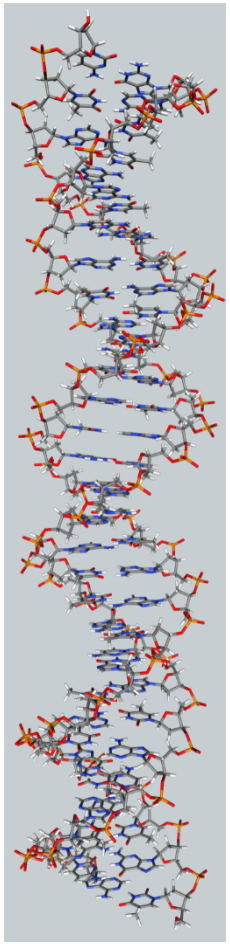


Phosphate reconstruction in MC_DNA



Coarse-grain

tleap*
+
minimization



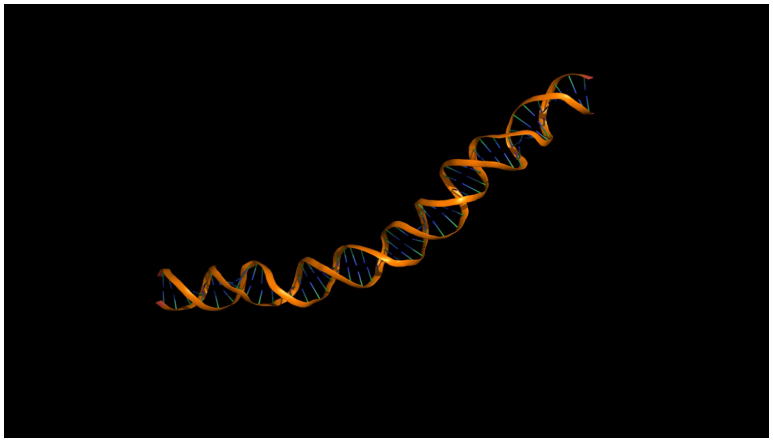
Atomistic

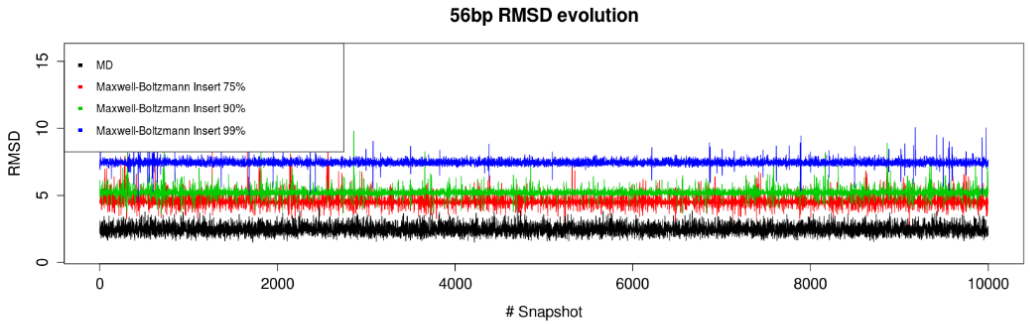
* Case et al., J. Comp. Chem., 2005

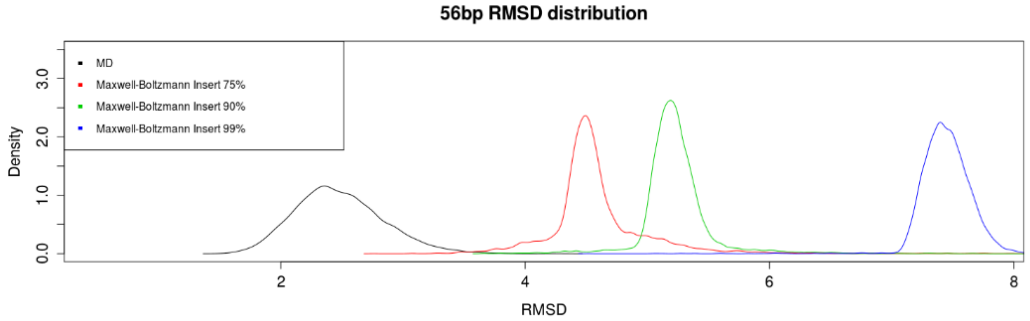
** Lavery et al., NAR, 2014

MC_DNA

Time-dependent pseudo trajectories



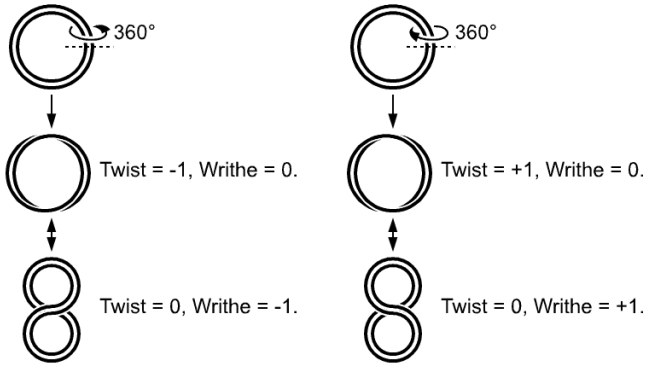




Circular MC_DNA

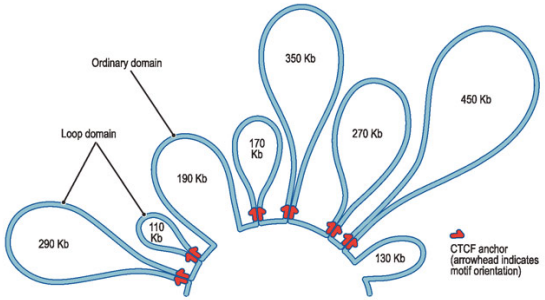
Mathematical background

Lk = Tw + Wr = const.



Where does constrained DNA occur?

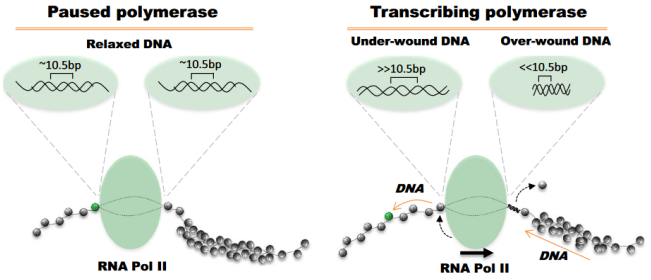
Plasmids, chromosomal bacterial DNA, DNA with robust anchor point (topological domains), RNAP



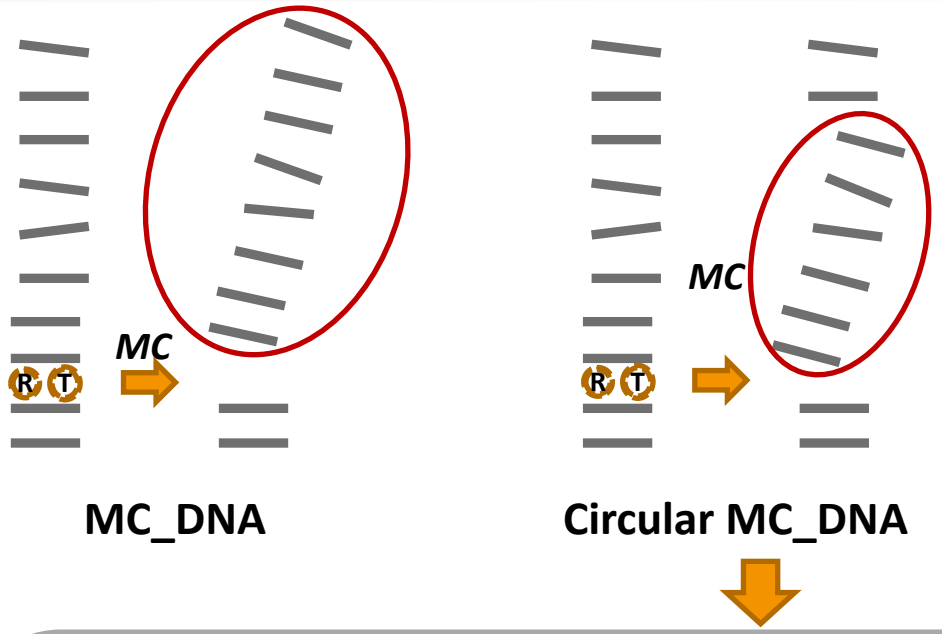
Effects of supercoiled DNA

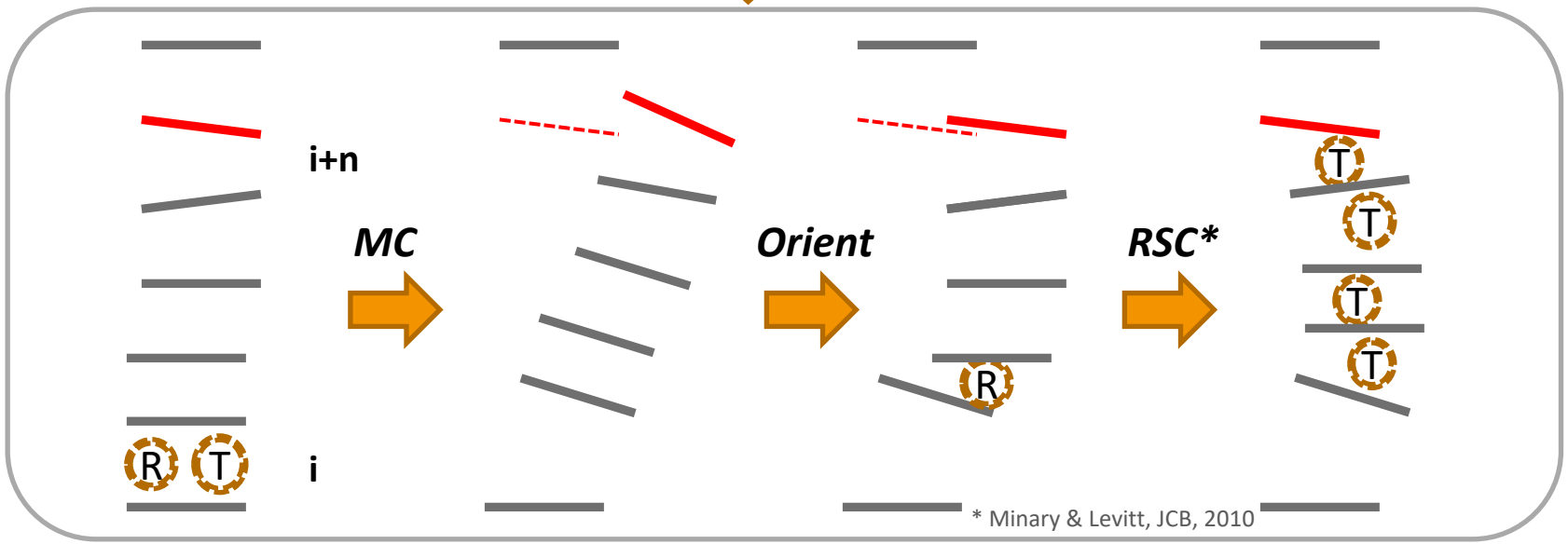
Distal sites are brought into close proximity
-> gene expression

DNA recognition by proteins

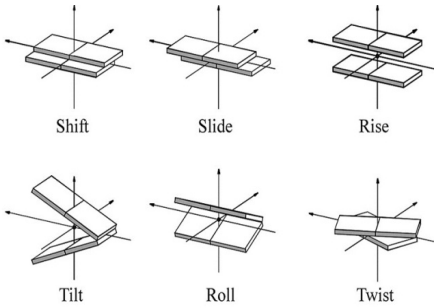


Circular MC_DNA
-
The method

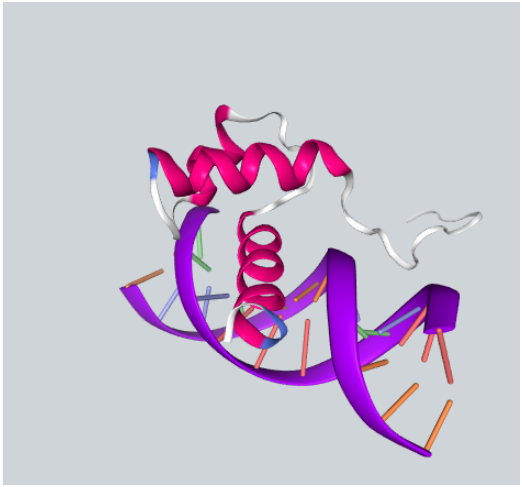




MC_DNA + Proteins: conformation of protein-bound DNA



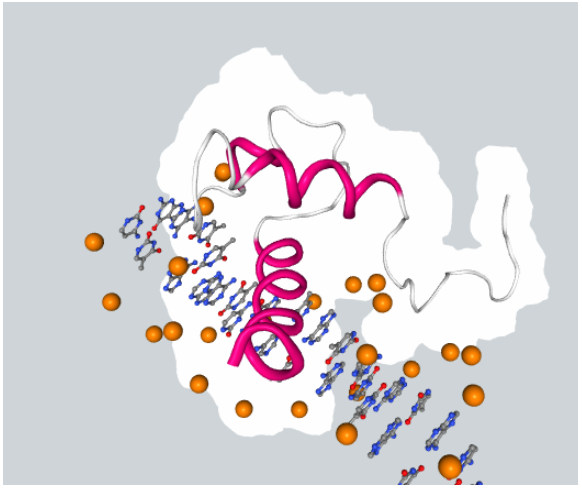
Protein-DNA complexes (Xray)



RCSB PDB PROTEIN DATA BANK

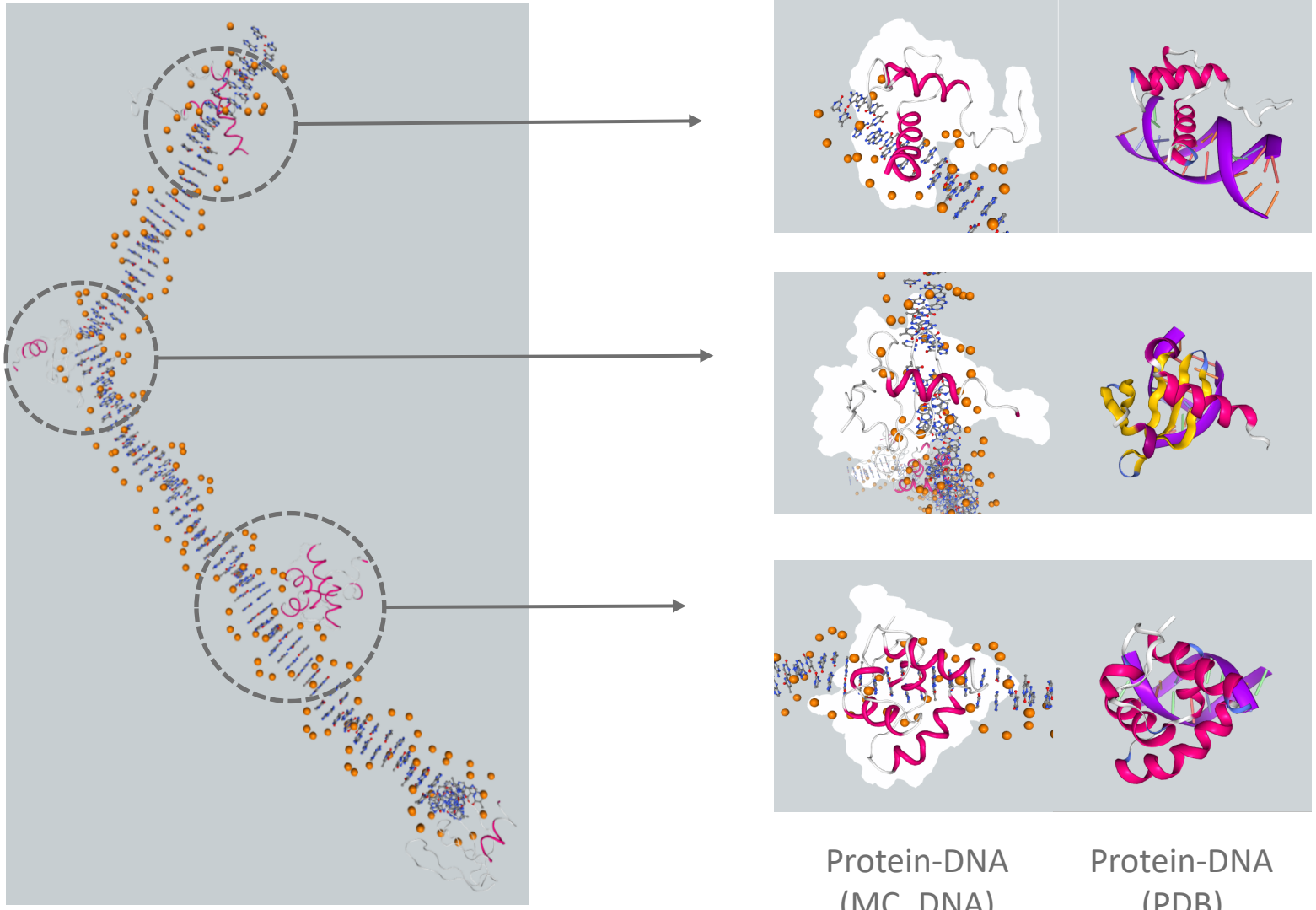
DNA conformation determined by Curves+ *

DNA adopts bioactive conformation (rigid)



MC DNA

MC_DNA + Proteins



Protein-DNA (MC_DNA)

Protein-DNA (PDB)

MC DNA

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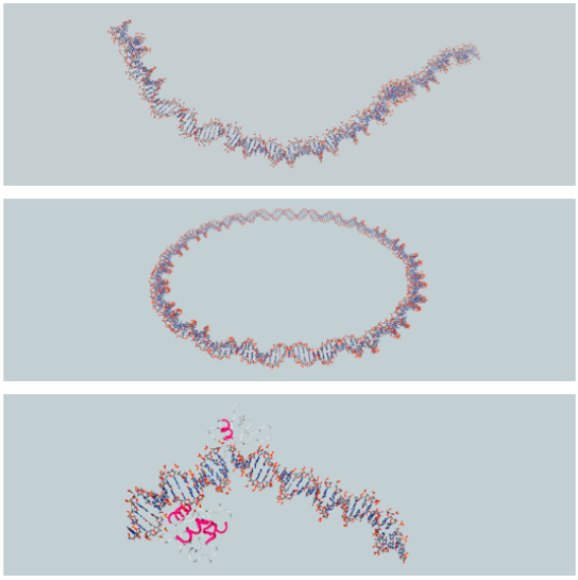
Welcome to MC DNA

Home

MC DNA



Thank you for visiting our website!!

The name of the webserver was inspired by the sampling method used to simulate DNA structures. MCDNA uses Monte Carlo sampling to obtain a set of representative DNA conformations at base pair step level accuracy. MCDNA provides an intuitive environment where in addition to simulations of unconstrained DNA MCDNA can simulate DNA in a constrained environment such as circular DNA and protein-DNA simulations while its performance exceeds common molecular dynamics simulations by several orders of magnitude.

Apart from the sequence it is possible to choose the resolution of the simulated DNA ('Coarse Grain' or 'Atomistic') and the type of operation to execute ('Create Structure' and 'Create Trajectory') which makes the webserver a flexible tool that can be tailored to the user's needs. Additionally, in the case of 'circular DNA' the amount of initial over- or undertwisting can be specified. In 'protein-DNA' the user can manually indicate the protein(s) to be superimposed onto the DNA at a given position in the sequence.

The graphical output of the simulations is complemented with a flexibility analysis done by Curves+ (backbone torsions, BI/BII, alpha/gamma, sugar puckering, grooves, axis base pair and inter base pair parameters), princial component analysis, contact matrix, bending and energy penalty calculations as well as individual analysis depending on the chosen simulation type (see more details in Help).

MCDNA is integrated in the Virtual Research Environment of the MuG project (https://www.multiscalegenomics.eu).

GUIDED TOUR

There is a complete Help section accessible through the main menu on the top of the page. But if you want to see a short introduction to this website, you can click the button below:

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MC DNA

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Welcome to MC DNA

Home

MC DNA

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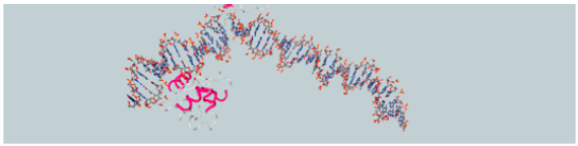

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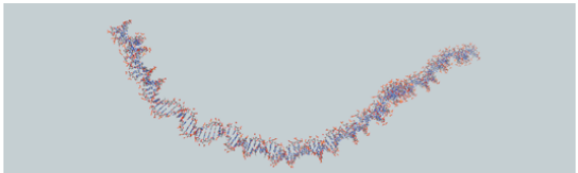

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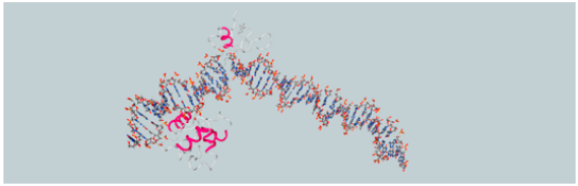
Home | Input data | Sample Inputs | Sample Outputs | Help

position in the sequence.



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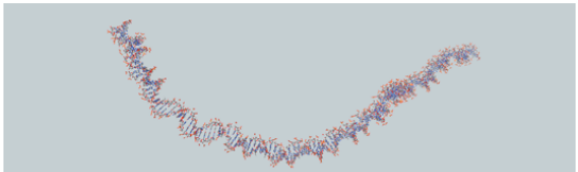
MC DNA



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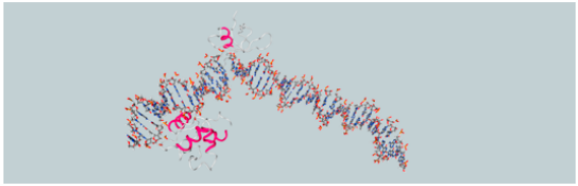

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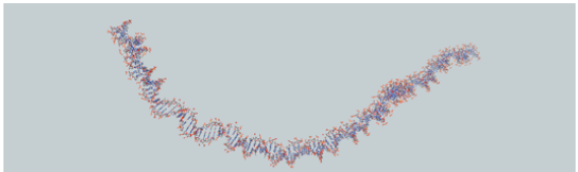

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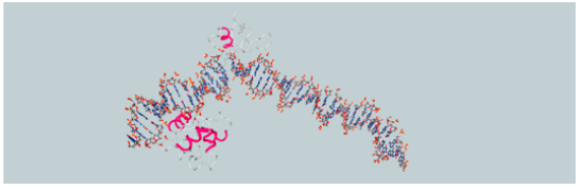

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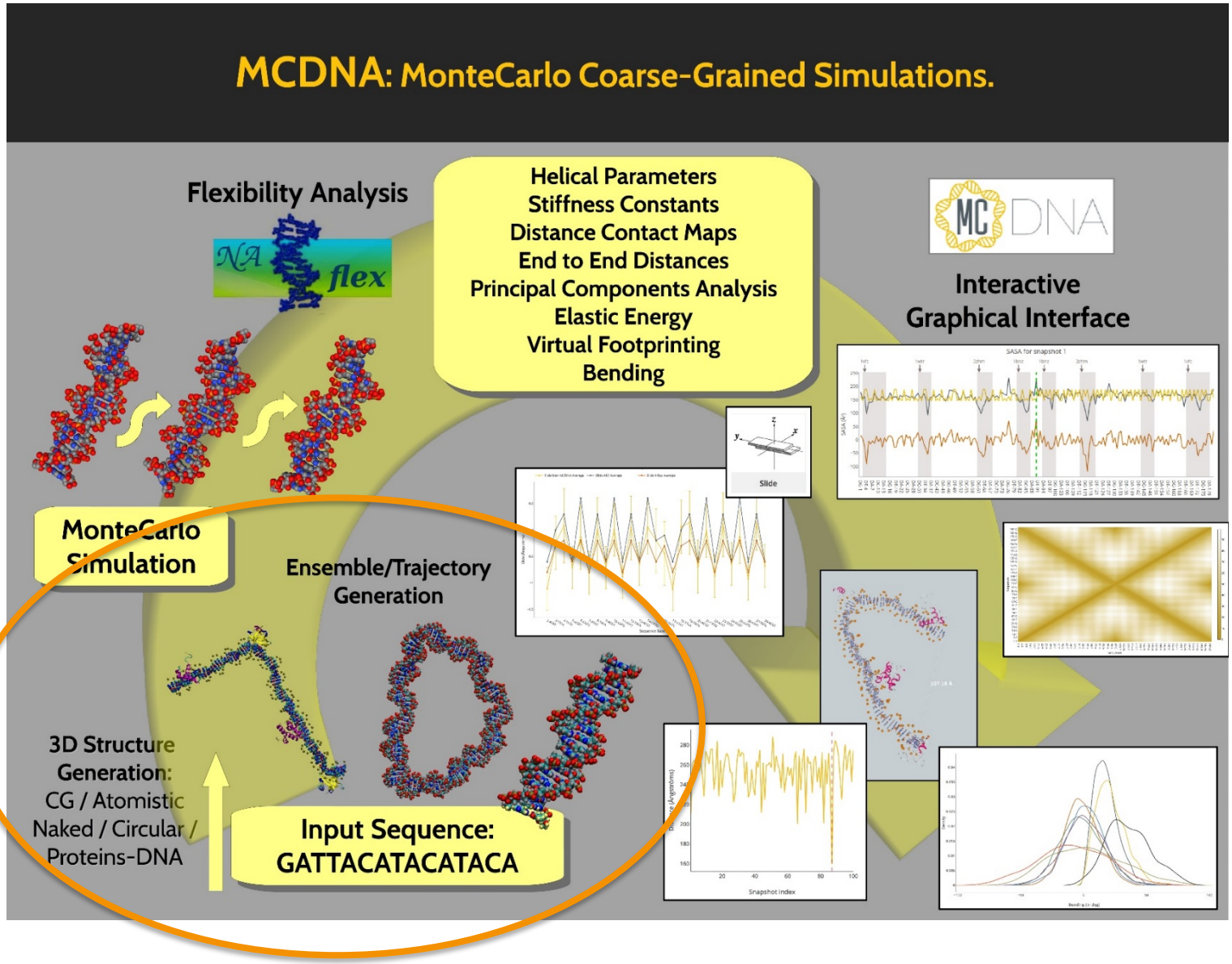

MCDNA: MonteCarlo Coarse-Grained Simulations.
Flexibility Analysis
NA flex
Helical Parameters
Stiffness Constants
Distance Contact Maps
End to End Distances
Principal Components Analysis
Elastic Energy
Virtual Footprinting
Bending
MC DNA
Interactive Graphical Interface
MonteCarlo Simulation
Ensemble/Trajectory Generation
3D Structure Generation:
CG / Atomistic
Naked / Circular /
Proteins-DNA
Input Sequence:
GATTACATACATACA
Slide
Snapshot index

Sample input – MC_DNA

INSERT YOUR INPUT DATA

All the form fields are mandatory except the *e-mail address* and *perform analysis*. If you provide your e-mail address, you will be notified once the job is finished. Disabling the analysis perform, the tool will calculate just the structure and / or the trajectory.

Click here to start the guided tour

Write or paste DNA sequence	GATTACATACATACAGATTACATACATACA
Tool	MC DNA
Resolution	Atomistic
Operations	× Create Structure × Create Trajectory
Number of structures	100
E-mail address	your@email.com
Perform analysis	✓ Enable / Disable Analysis

✔ Submit

Sample input – Circular MC_DNA

INSERT YOUR INPUT DATA

All the form fields are mandatory except the *e-mail address* and *perform analysis*. If you provide your e-mail address, you will be notified once the job is finished. Disabling the analysis perform, the tool will calculate just the structure and / or the trajectory.

Click here to start the guided tour

Write or paste DNA sequence	TCTCTCTCTCTCTCTTAAAGGTATACAAGAAAGTTTGTTGGTCTTTTTACCTTCC CGTTTCGCTCCAAGTTAGTATAAAAAAGCTGAACGAG
Tool	Circular MC DNA
Resolution	Atomistic
ΔLK	-1
Iterations per structure	25000000
Operations	× Create Structure × Create Trajectory
Number of structures	10
E-mail address	your@email.com
Perform analysis	✓ Enable / Disable Analysis

Sample input – MC_DNA + Proteins

INSERT YOUR INPUT DATA

All the form fields are mandatory except the *e-mail address* and *perform analysis*. If you provide your e-mail address, you will be notified once the job is finished. Disabling the analysis perform, the tool will calculate just the structure and / or the trajectory.

Click here to start the guided tour

Write or paste DNA sequence: GATTACATACATACAGATTACATACATACAGATTACATACATACAGATTACATACAT ACAGATTACATACATACAGATTACATACATACA

Tool: MC DNA + Proteins

Resolution: Atomistic

Proteins:

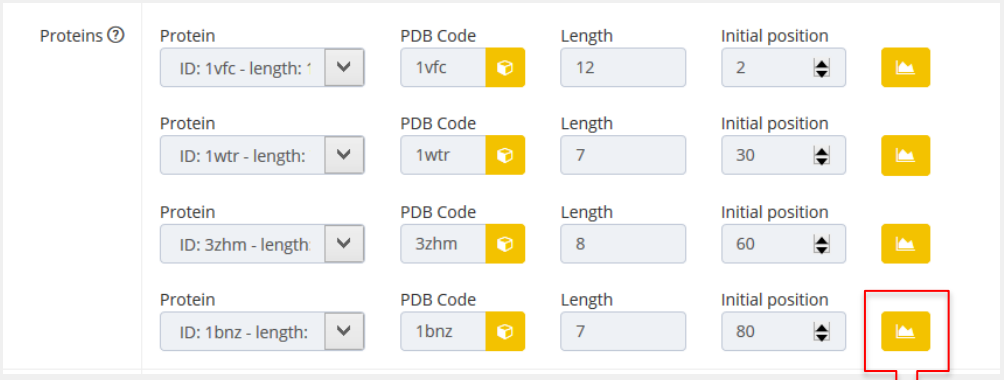
Protein	PDB Code	Length	Initial position
ID: 1vfc - length:	1vfc	12	2
ID: 1wtr - length:	1wtr	7	30
ID: 3zhm - length	3zhm	8	60
ID: 1bnz - length:	1bnz	7	80

Operations: × Create Structure × Create Trajectory

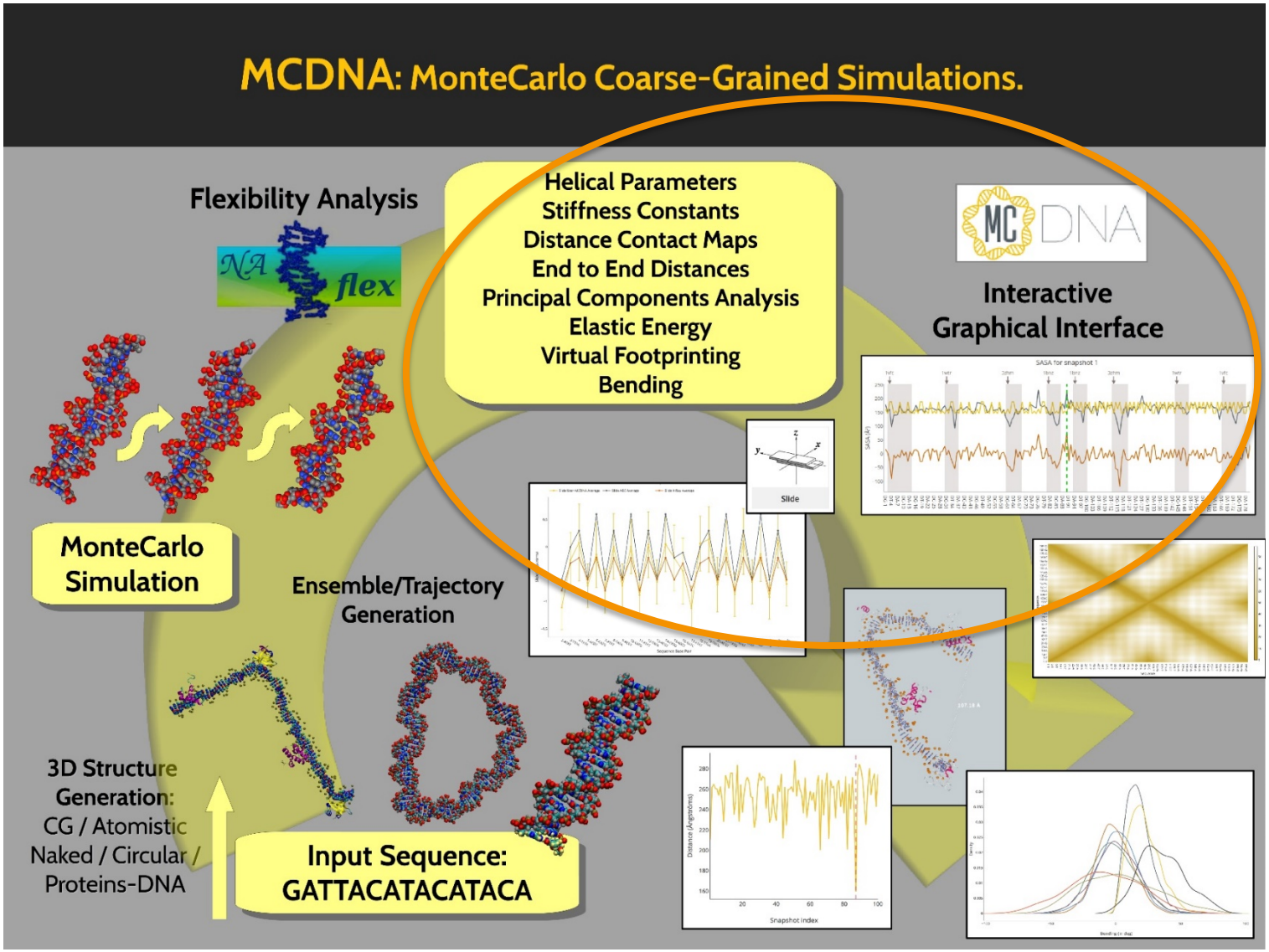
Number of structures: 50

E-mail address: your@email.com

Perform analysis: Enable / Disable Analysis



Protein affinity to bind to specific DNA sequence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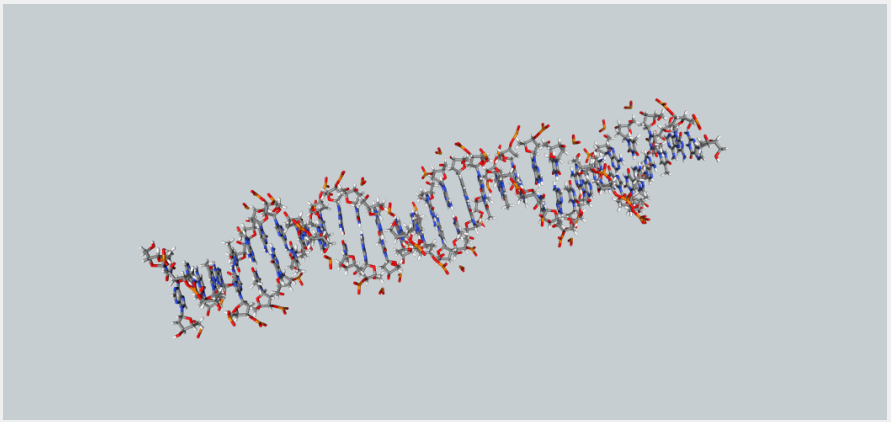
MonteCarlo Simulation
Ensemble/Trajectory Generation
3D Structure Generation:
CG / Atomistic
Naked / Circular /
Proteins-DNA
Input Sequence:
GATTACATACATACA

Summary | Structure Flexibility Analysis | Trajectory Flexibility Analysis

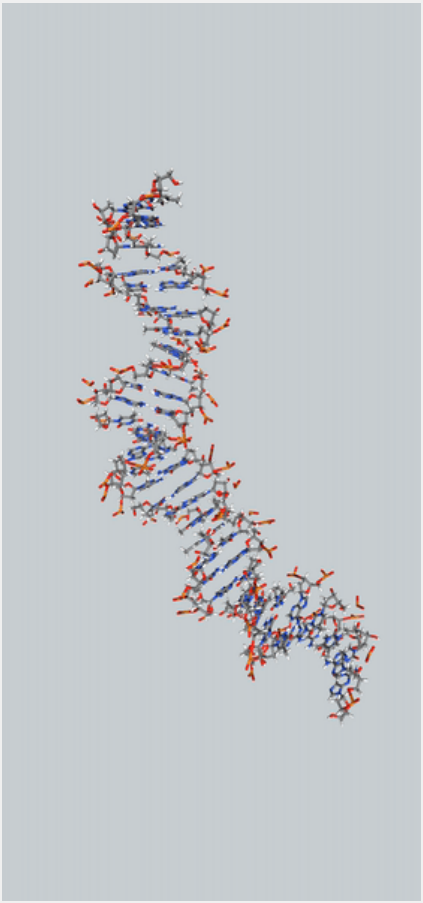
Download all summary in a compressed file

Selected Tool	MC DNA
Resolution	Atomistic
Operations	Create Structure, Create Trajectory
Number of Structures	100
Input sequence	GATTACATACATACAGATTACATACATACA

Structure



Trajectory



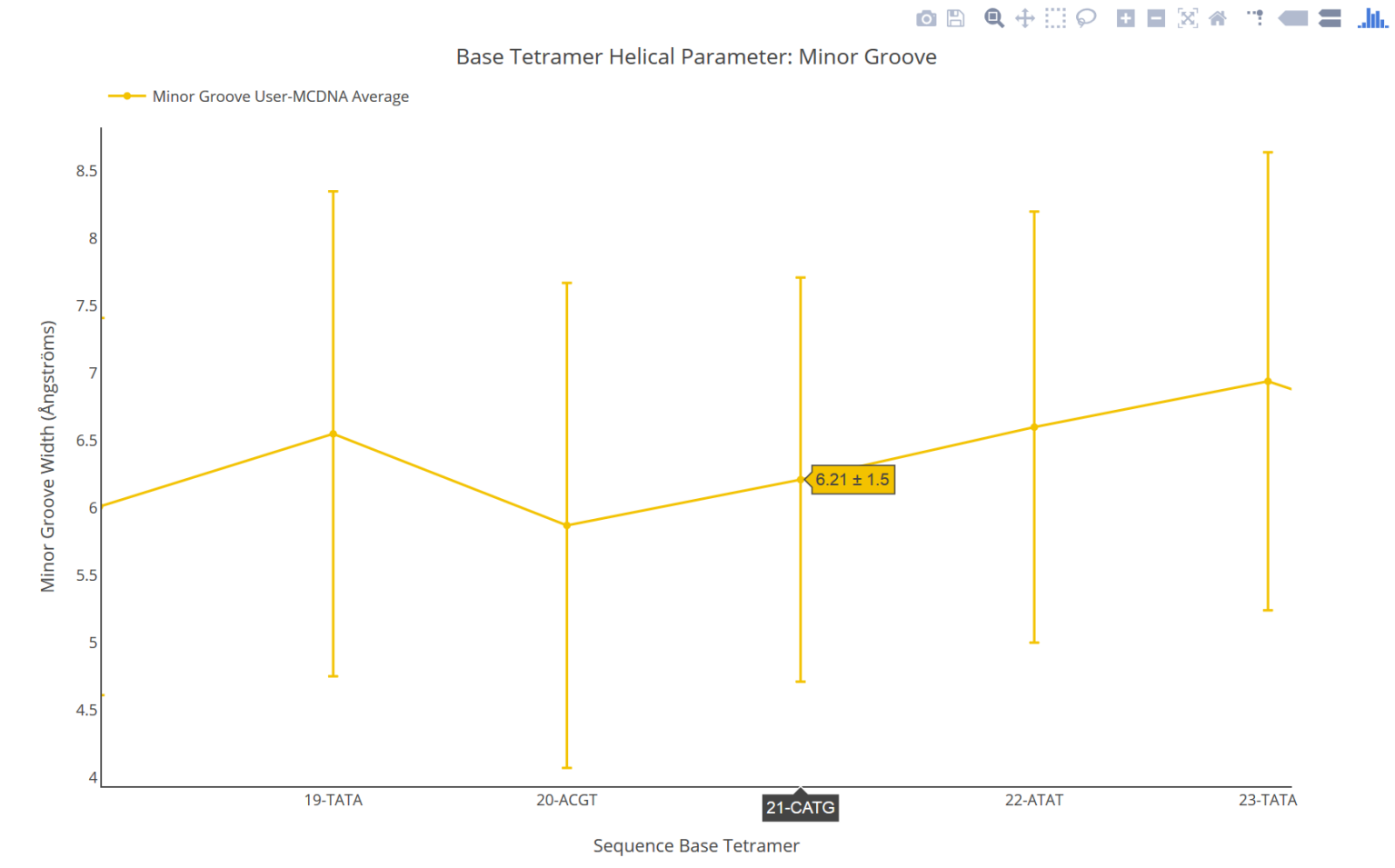
MC_DNA – Analysis Tools

Download all analysis in a compressed file

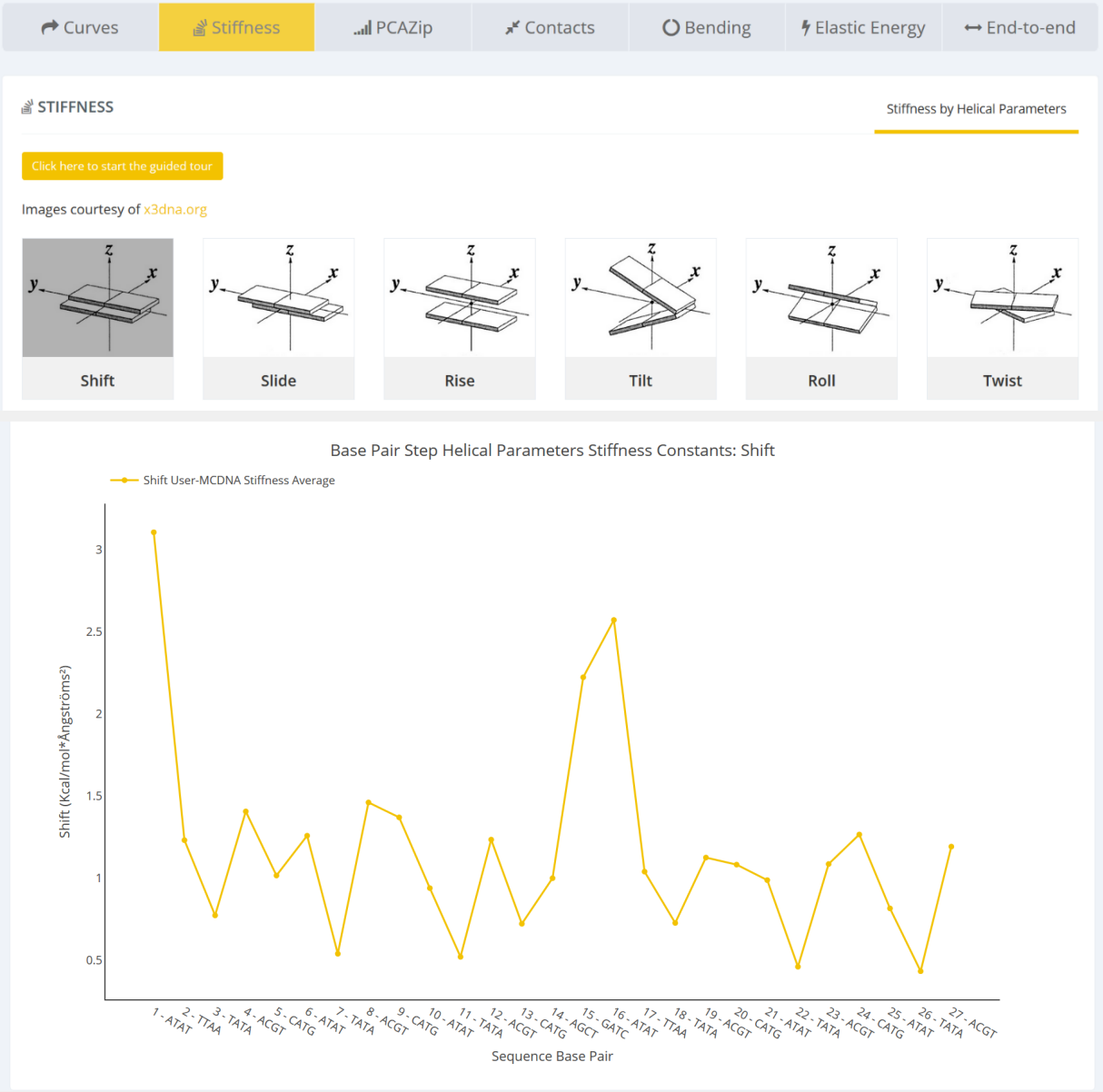
	MC_DNA CG		MC_DNA AA		Circular MC_DNA CG		Circular MC_DNA AA		MC_DNA + Proteins CG		MC_DNA + Proteins AA	
	Structure	Ensemble	Structure	Ensemble	Structure	Ensemble	Structure	Ensemble	Structure	Ensemble	Structure	Ensemble
Curves			X	X			X	X			X	X
Stiffness				X				X				X
PCAzip		X		X								
Contacts	X	X	X	X	X	X	X	X	X	X	X	X
Bending	X	X	X	X	X	X	X	X	X	X	X	X
Elastic Energy	X	X	X	X	X	X	X	X	X	X	X	X
End-to-End		X		X						X		X
SASA									X	X	X	X
Circular					X	X	X	X				

Curves

Curves | Stiffness | PCAZip | Contacts | Bending | Elastic Energy | End-to-end



Stiffness


Curves
Stiffness
PCAZip
Contacts
Bending
Elastic Energy
End-to-end
STIFFNESS
Stiffness by Helical Parameters
Click here to start the guided tour
Images courtesy of x3dna.org
Shift
Slide
Rise
Tilt
Roll
Twist
Base Pair Step Helical Parameters Stiffness Constants: Shift
Shift User-MCDNA Stiffness Average
Shift (Kcal/mol*Ångströms²)
3
2.5
2
1.5
1
0.5
1 - ATAT
2 - TTAA
3 - TATA
4 - ACGT
5 - CATG
6 - ATAT
7 - TATA
8 - ACGT
9 - CATG
10 - ATAT
11 - TATA
12 - ACGT
13 - CATG
14 - AGCT
15 - GATC
16 - ATAT
17 - TTAA
18 - TATA
19 - ACGT
20 - CATG
21 - ATAT
22 - TATA
23 - ACGT
24 - CATG
25 - ATAT
26 - TATA
27 - ACGT
Sequence Base Pair

PCAzip

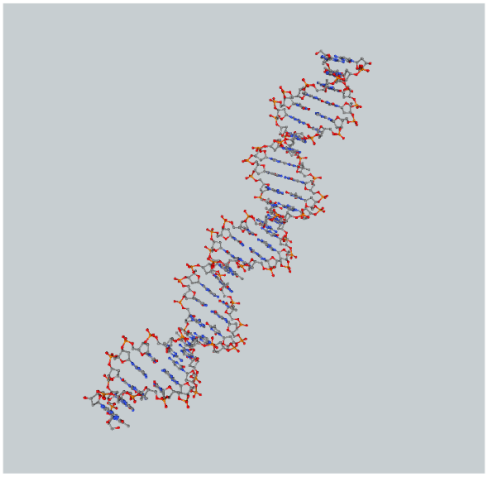
PCA TABLE

Search:

Animation Mode	Eigen value (Å²)	Collectivity index	Stiffness (kcal/(mol*Å²))
1	7787.68	0.72	0.07
2	5840.74	0.74	0.10
3	1961.09	0.69	0.30
4	1476.57	0.71	0.40
5	1011.08	0.73	0.58
6	851.27	0.65	0.70
7	620.27	0.70	0.96
8	373.04	0.66	1.59
9	317.20	0.64	1.87
10	243.93	0.72	2.44

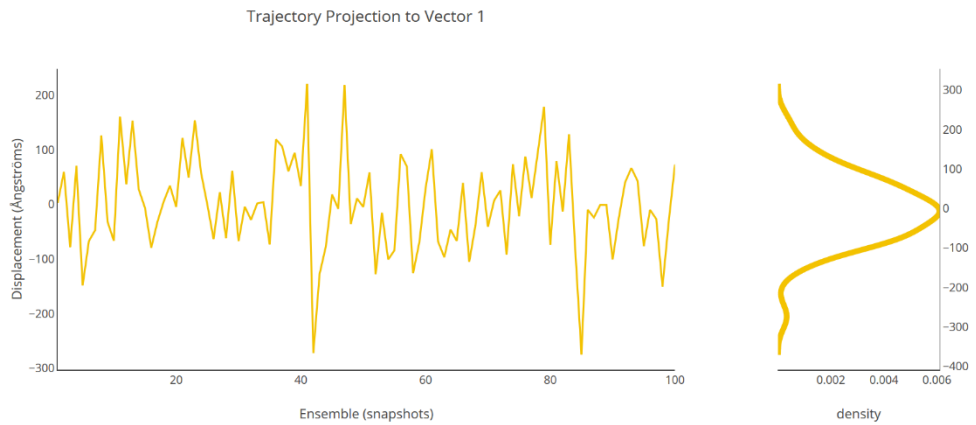
Showing 1 to 10 of 10 records

3D VIEW



Click here to view in full screen

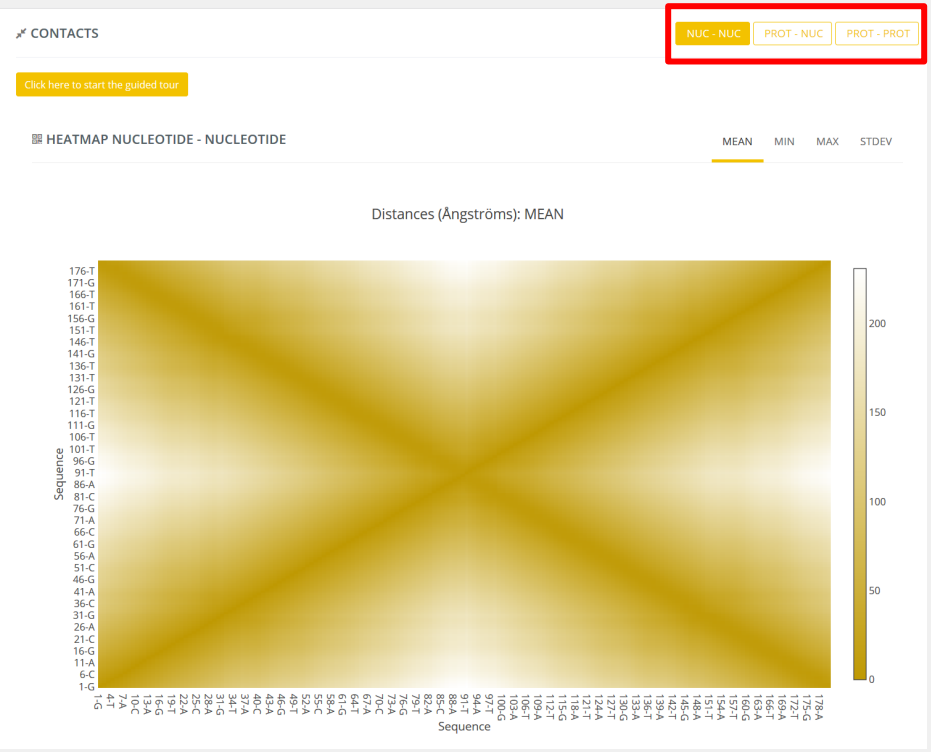
TRAJECTORY PROJECTION

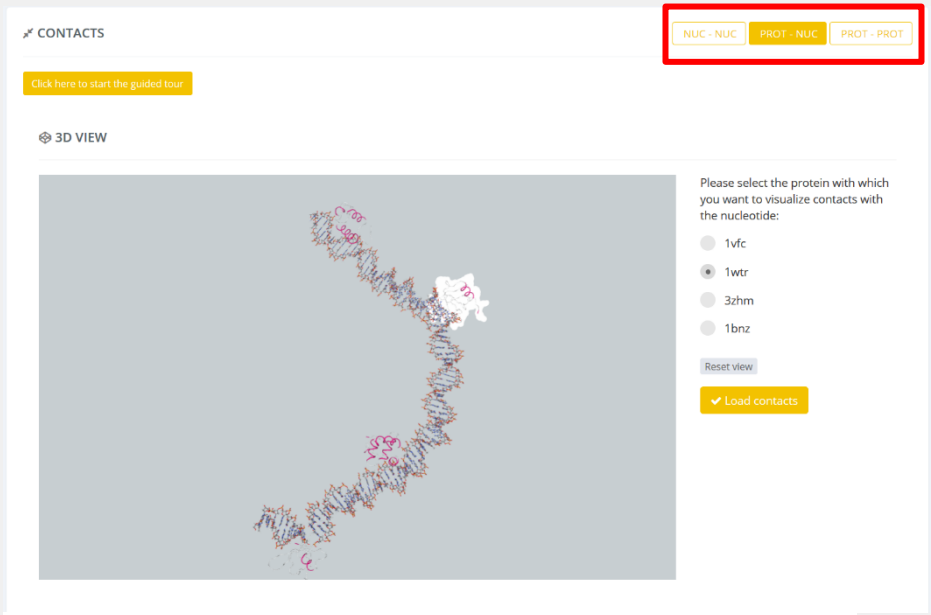


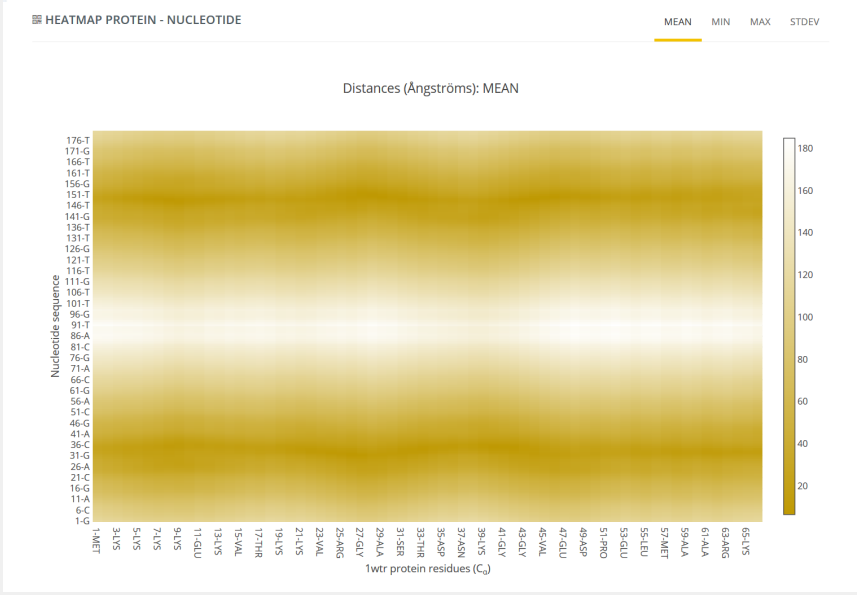
Contacts

DNA-protein

DNA-DNA

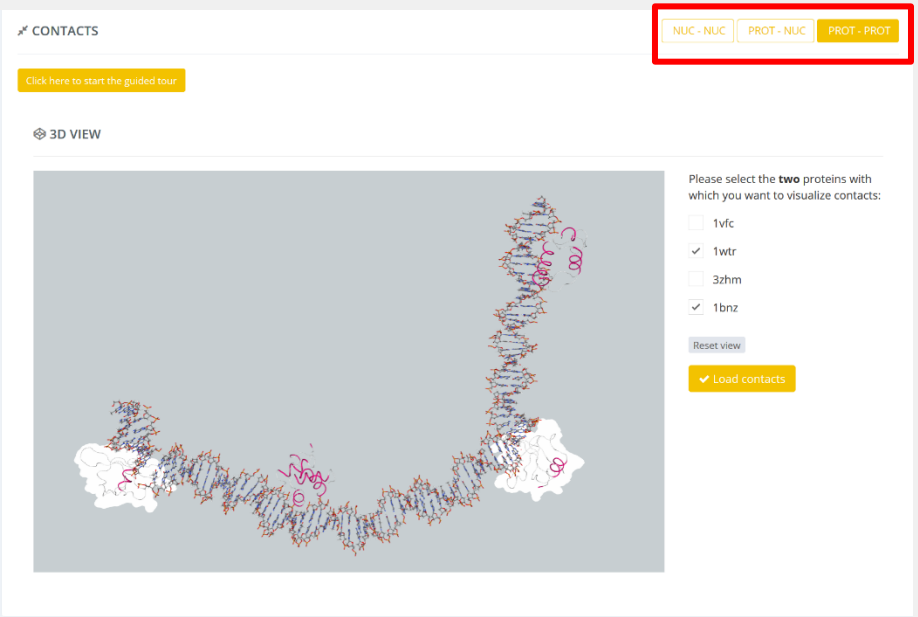




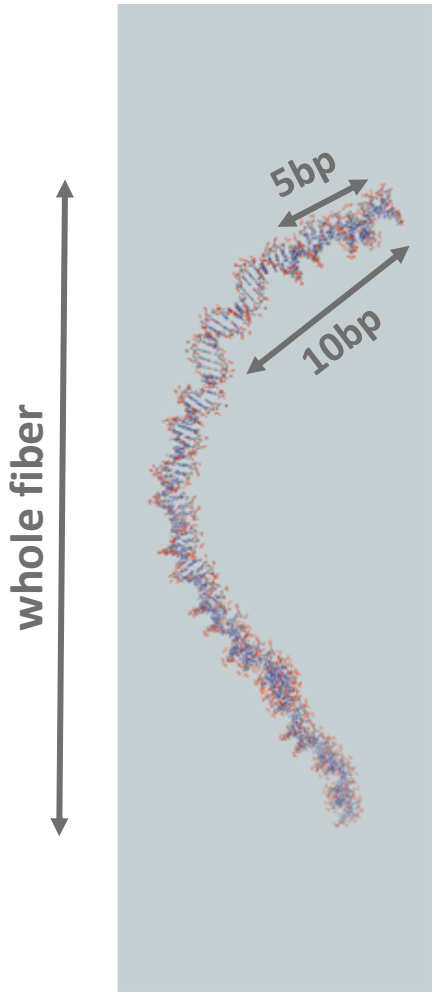


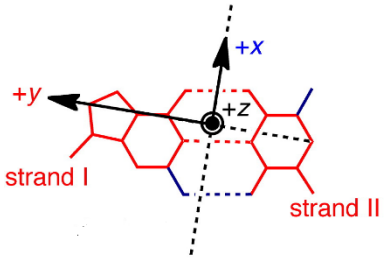
Contacts

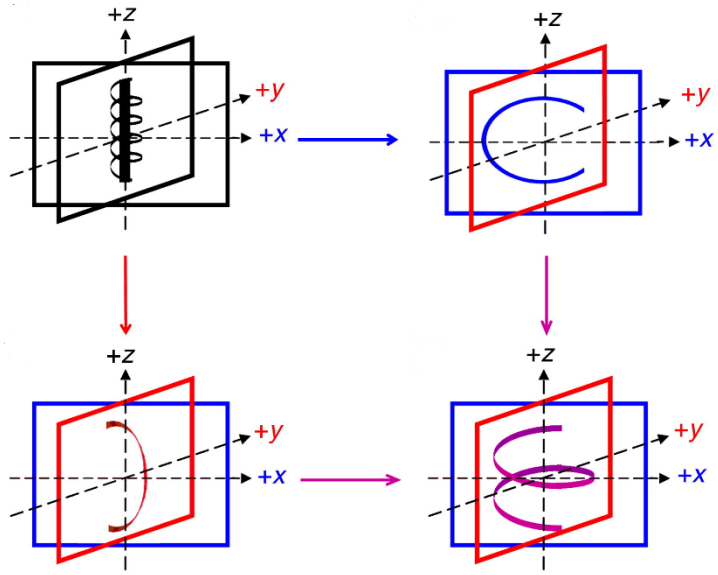
Protein-Protein



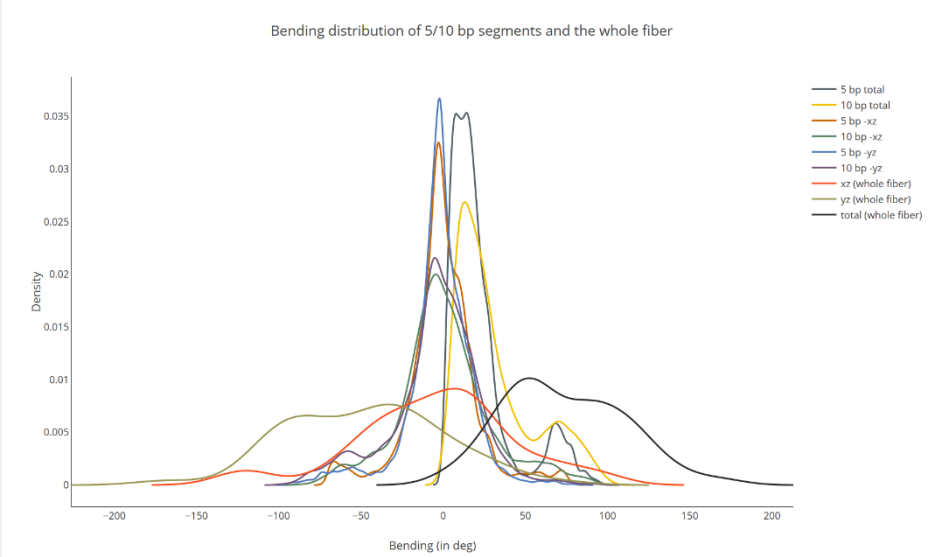
Bending

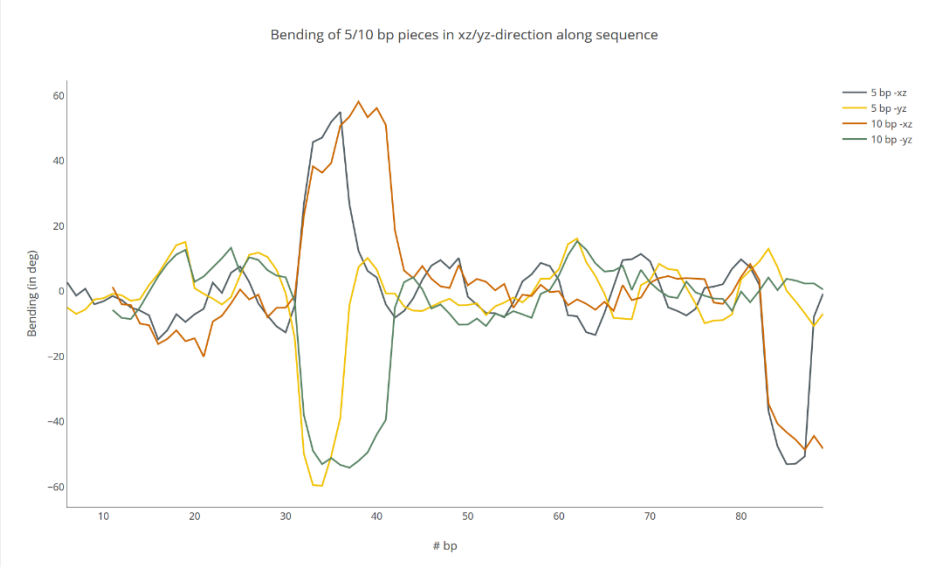


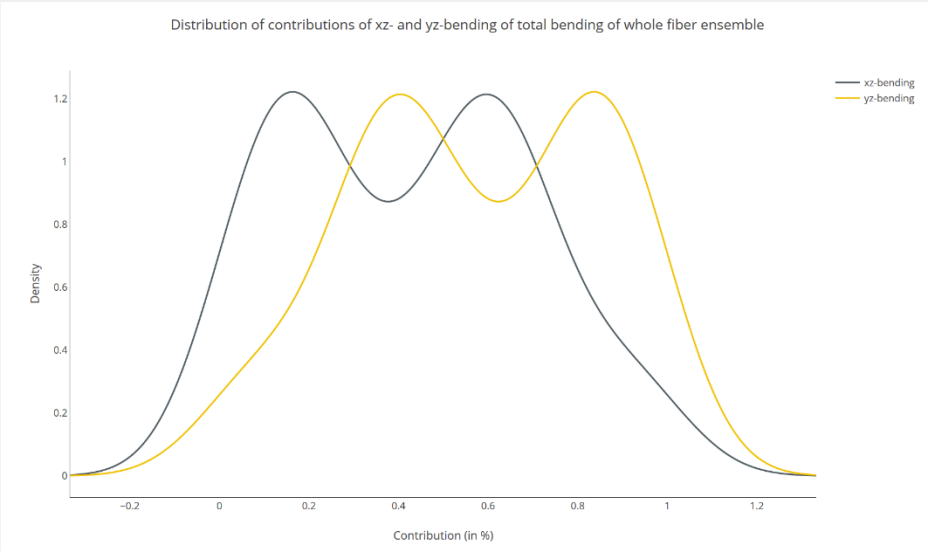


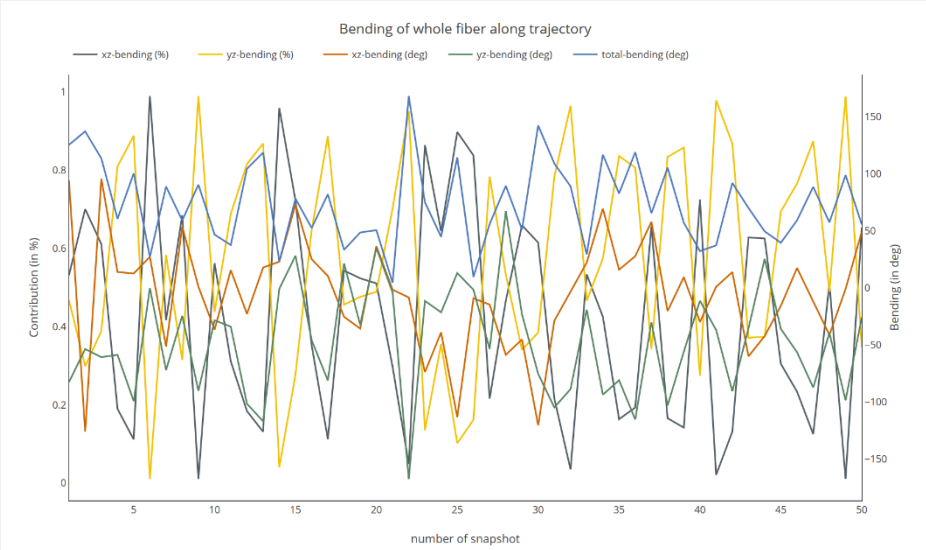


Segment	Bending Direction
5bp	xz plane
10bp	yz plane
whole fiber	absolute bending


Bending distribution of 5/10 bp segments and the whole fiber
5 bp total
10 bp total
5 bp -xz
10 bp -xz
5 bp -yz
10 bp -yz
xz (whole fiber)
yz (whole fiber)
total (whole fiber)
Density
Bending (in deg)


Bending of 5/10 bp pieces in xz/yz-direction along sequence
5 bp -xz
5 bp -yz
10 bp -xz
10 bp -yz
Bending (in deg)
bp


Distribution of contributions of xz- and yz-bending of total bending of whole fiber ensemble
xz-bending
yz-bending
Density
Contribution (in %)

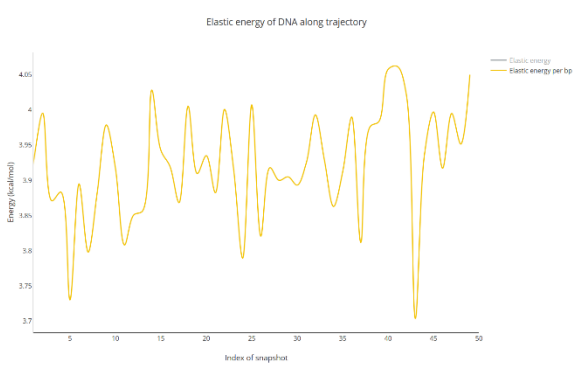

Bending of whole fiber along trajectory
xz-bending (%)
yz-bending (%)
xz-bending (deg)
yz-bending (deg)
total-bending (deg)
Contribution (in %)
Bending (in deg)
number of snapshot

Elastic Energy

Elastic energy of DNA

	Mean	SD
Elastic energy (kcal/mol)	348.82	7.16
Elastic energy per bp (kcal/mol)	3.92	0.08

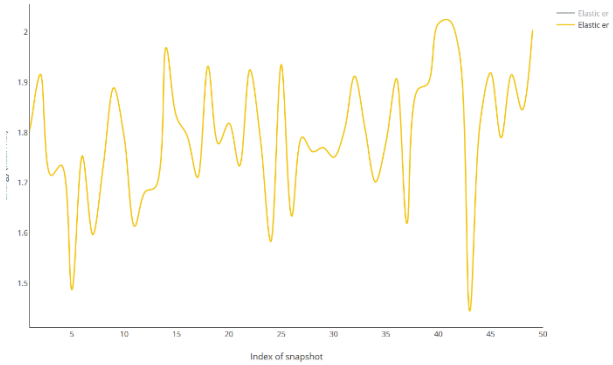
Elastic energy of DNA along trajectory



Elastic Energy of DNA not bound to a protein

	Mean	SD
Elastic energy (kcal/mol)	98.63	7.16
ic energy per bp (kcal/mol)	1.79	0.13

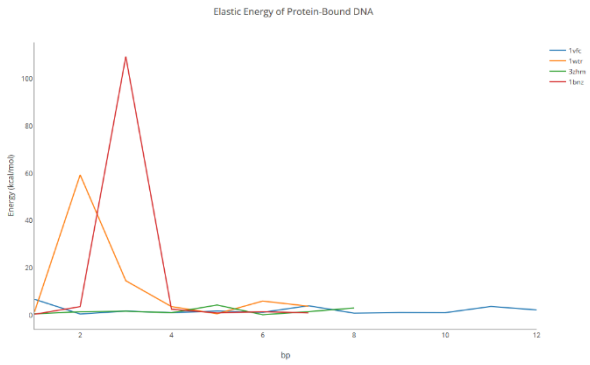
Elastic Energy of DNA not bound to a protein along trajectory

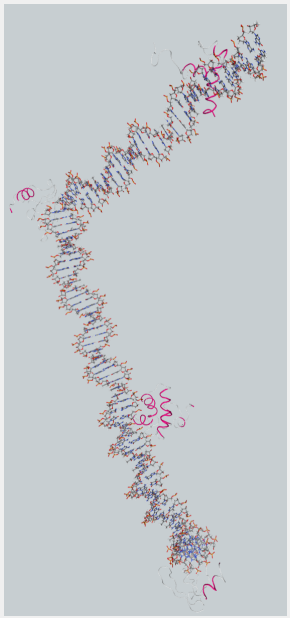


Elastic Energy of Protein-Bound DNA

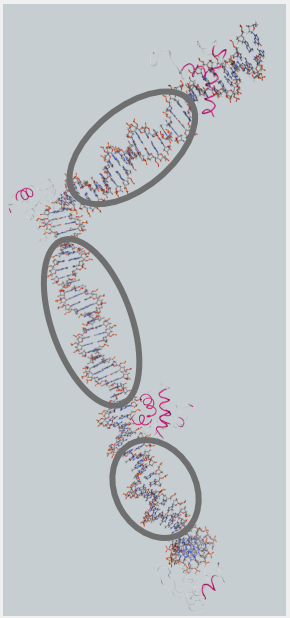
	Mean (kcal/mol)	SD (kcal/mol)
1VFC	2.21	1.81
1WTR	12.82	21.07
3ZDH	1.77	1.34
1BNZ	17.1	40.74

Elastic Energy of Protein-Bound DNA

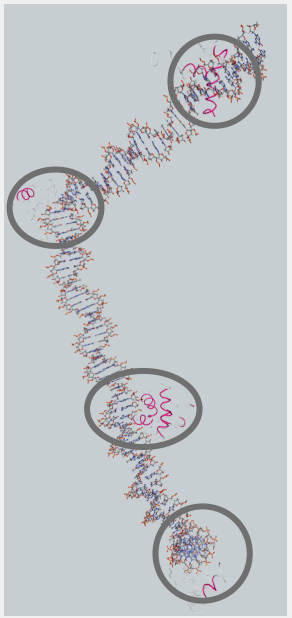




DNA



DNA not bound to protein



protein-bound DNA

Elastic energy of DNA

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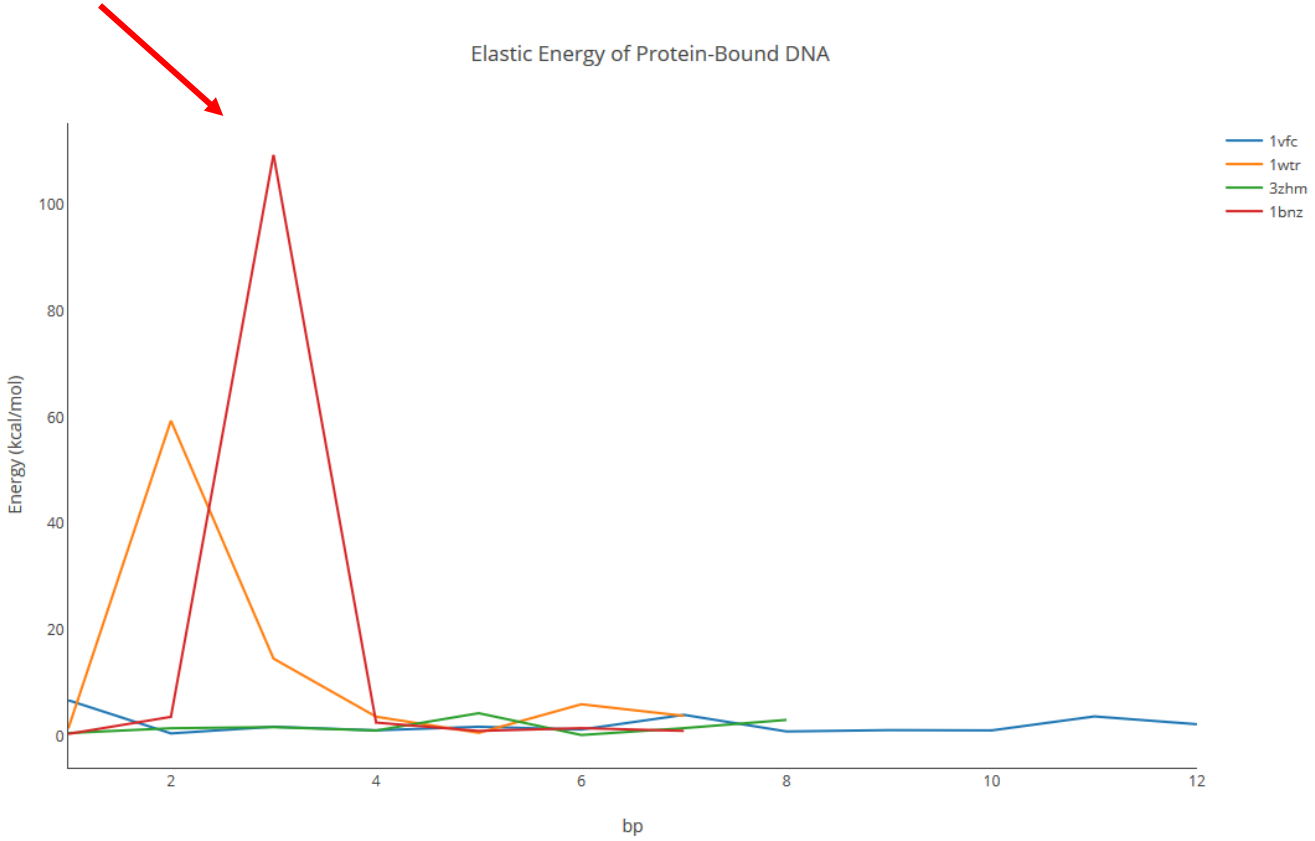


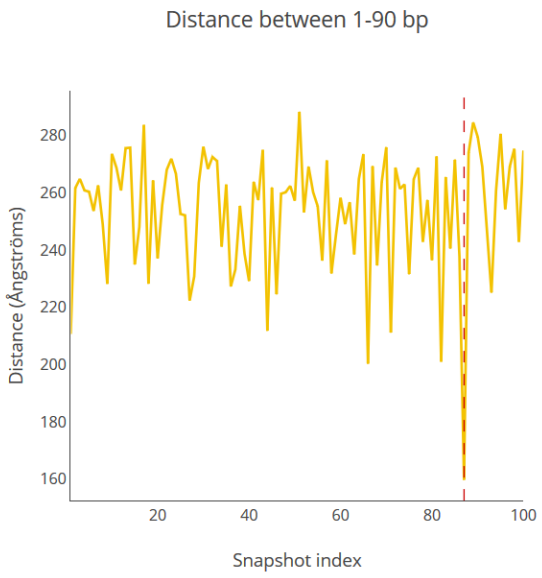
End-to-end distance

DISTANCES SELECTOR

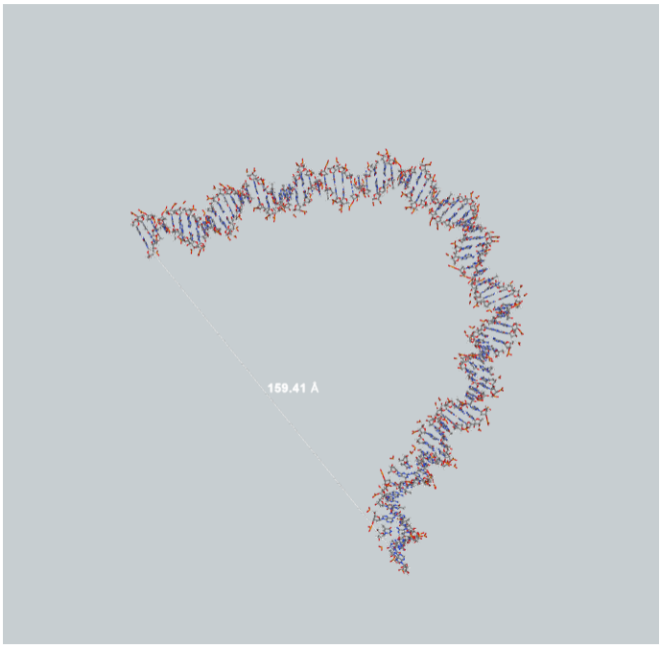
159.68Å 288.41Å

159.68 211.18 225.09 229.17 233.29 236.43 238.78 242.85 249.05 253.15 255.54 257.46 260.24 260.83 262 263.03 264.48 265.61 268.78 269.18 271.46 272.86 274.83 275.81 280.71

END-TO-END DISTANCES PLOT

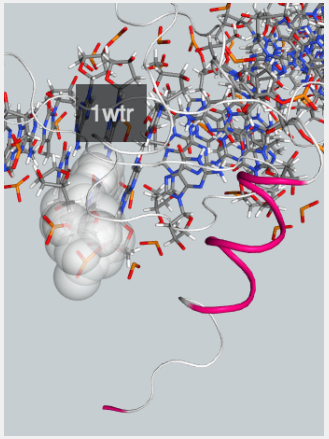


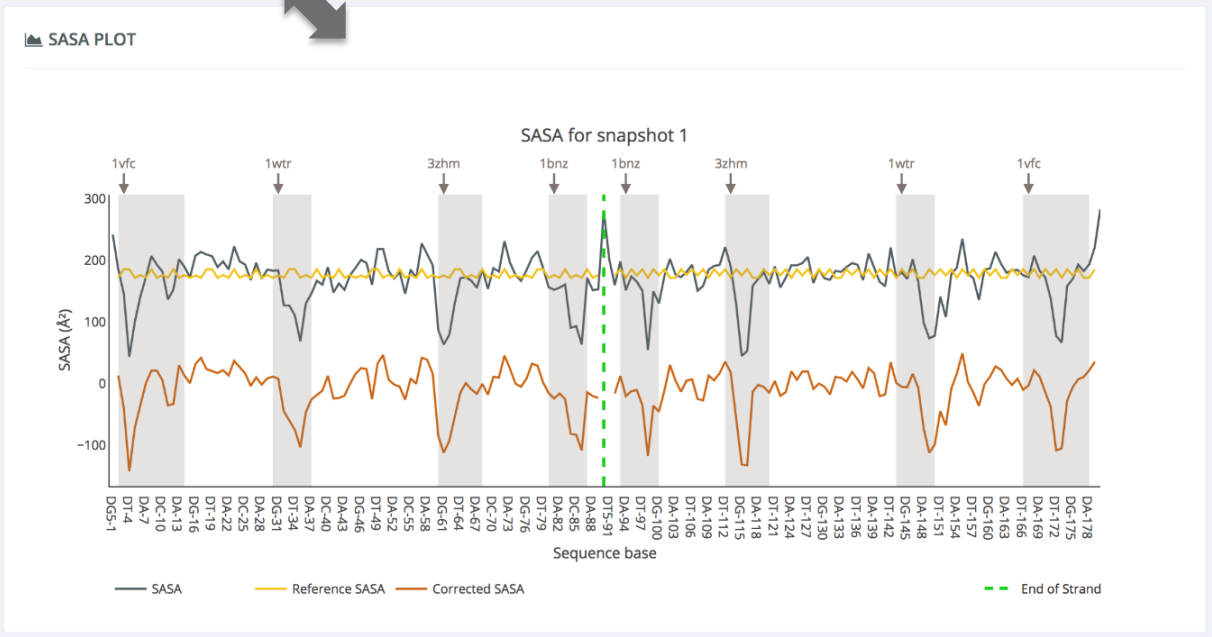
3D VIEW



Click here to view in full screen

Solvent accessible surface area (SASA)



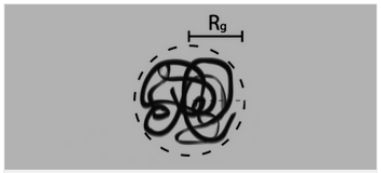


Circular parameters

CIRCULAR

Click here to start the guided tour

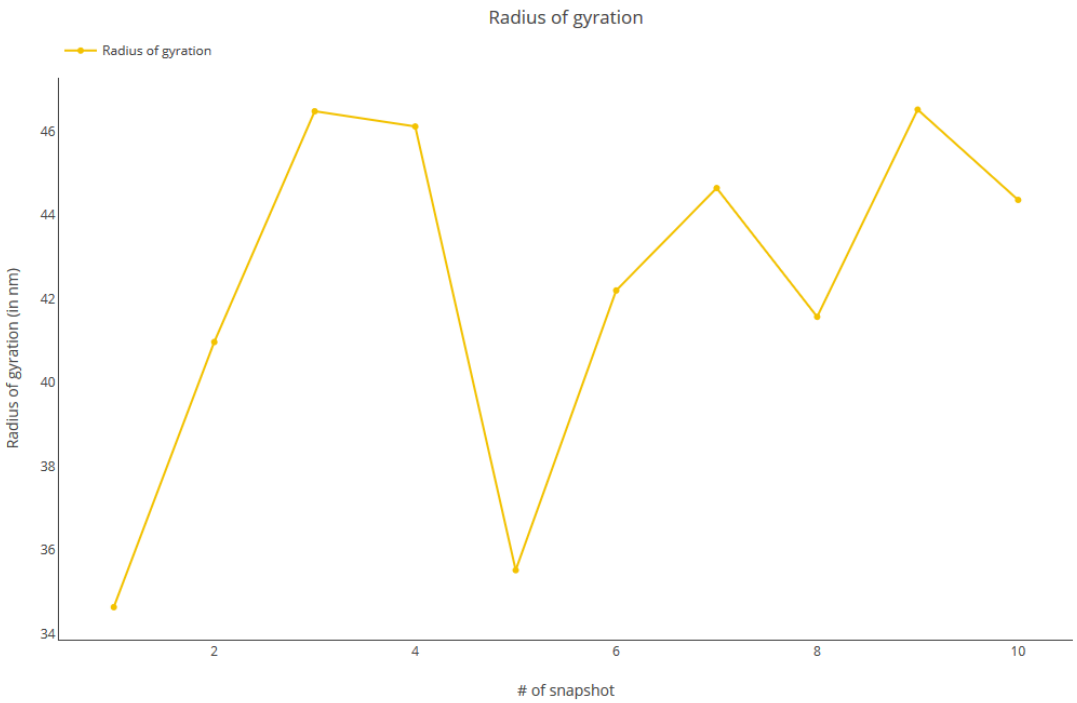
Images courtesy of *Danielle J. Mai, Christopher Brockman and Charles M. Schroeder* (Radius of Gyration) and *Guillaume Witz and Andrzej Stasiak* (Helical and Writhe).



Radius of Giration

Helical

Writhe

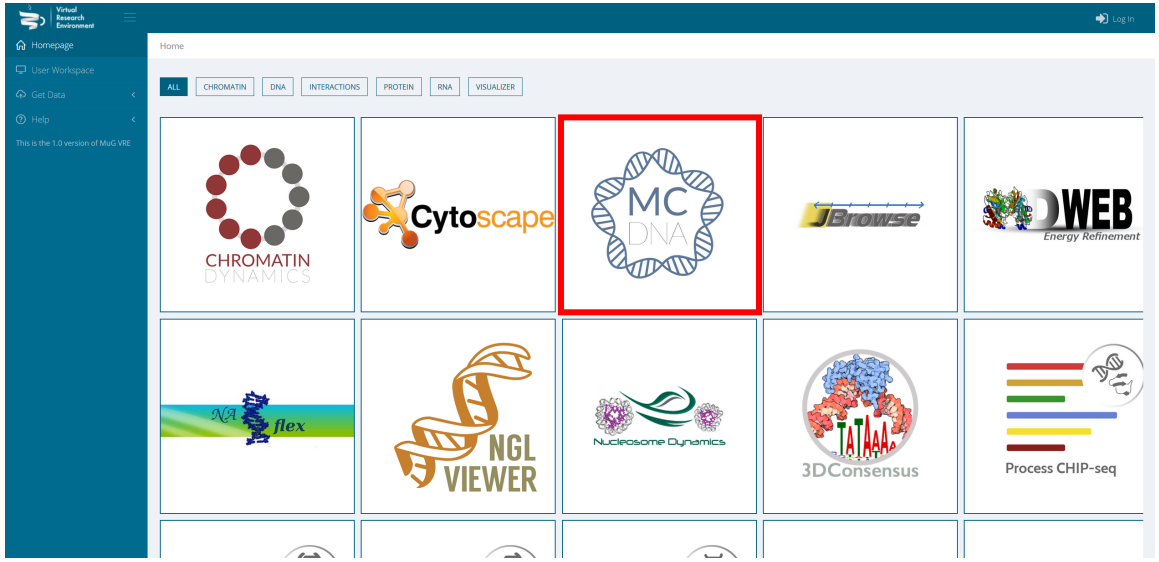


Multiscale Complex Genomics

http://multiscalegenomics.eu/MuGVRE/

What's MuGVRE?

The MuG Virtual Research Environment supports the expanding 3D/4D genomics community by developing tools to integrate the navigation in genomics data from sequence to 3D/4D chromatin dynamics data.



Virtual Research Environment: https://vre.multiscalegenomics.eu/home/

Horizon 2020
European Union Funding
For Research and innovation

Joint MuG-BioExcel workshop

Multi-resolution Nucleic Acids Simulations

22.06.2018 (Barcelona, Spain)

https://bioexcel.eu/events/multi-resolution-nucleic-acids-simulations-a-joint-mug-bioexcel-workshop/

co-located with the International Society of Quantum Biology and Pharmacology (ISQBP) President's meeting (19.-21.6.) in Barcelona (Spain)

Adam Hospital (Postdoctoral Fellow)

Back-end, Analysis

Molecular modeling and Bioinformatics group
IRB Barcelona, Spain

Genís Bayarri (Webdevelopper)

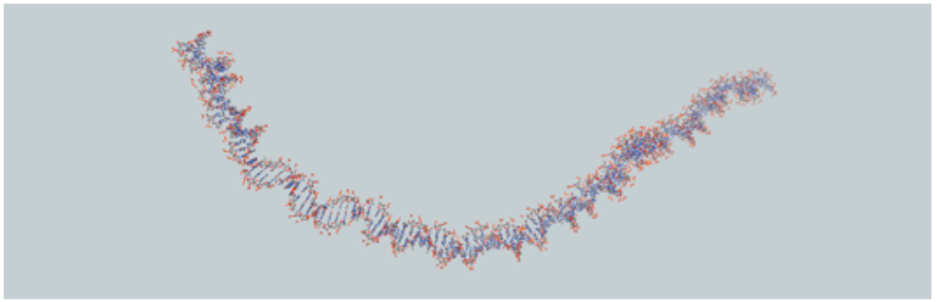
Webdesign, Front-end

Molecular modeling and Bioinformatics group
IRB Barcelona, Spain

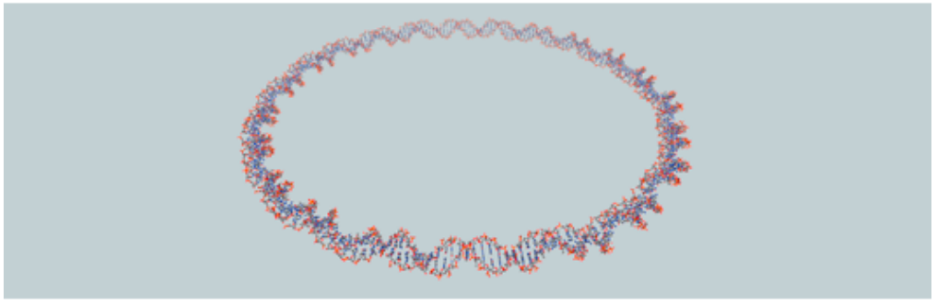
MC DNA

http://mmb.irbbarcelona.org/MCDNA/

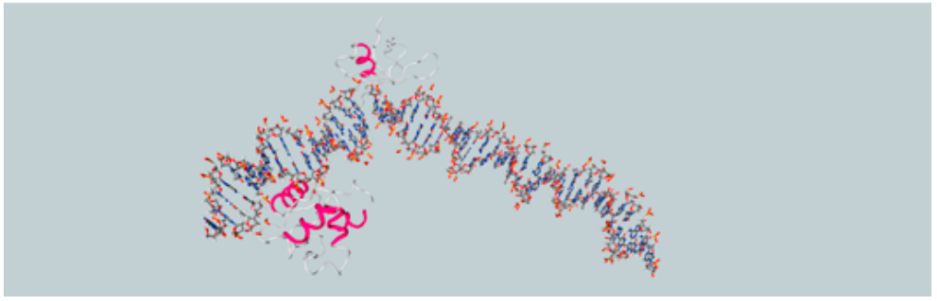
Free linear



Circular

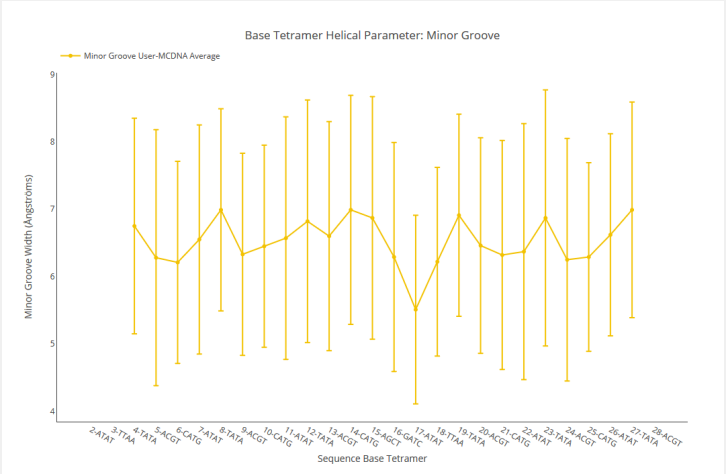


Protein-coated

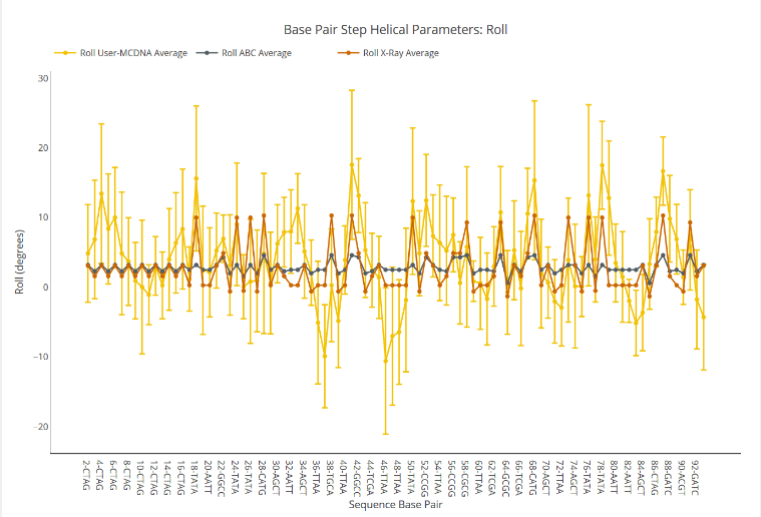


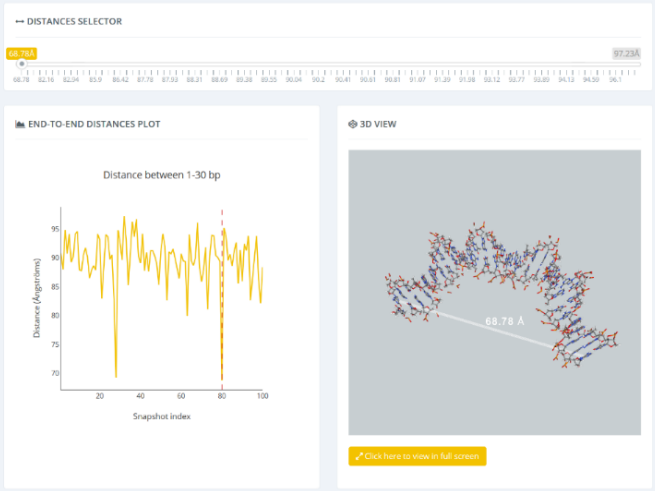
MC_DNA – Sample Output

MC_DNA

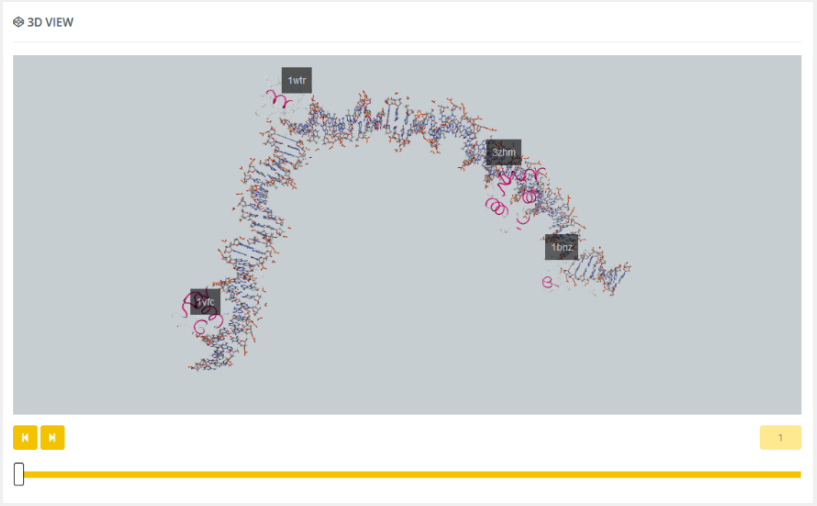


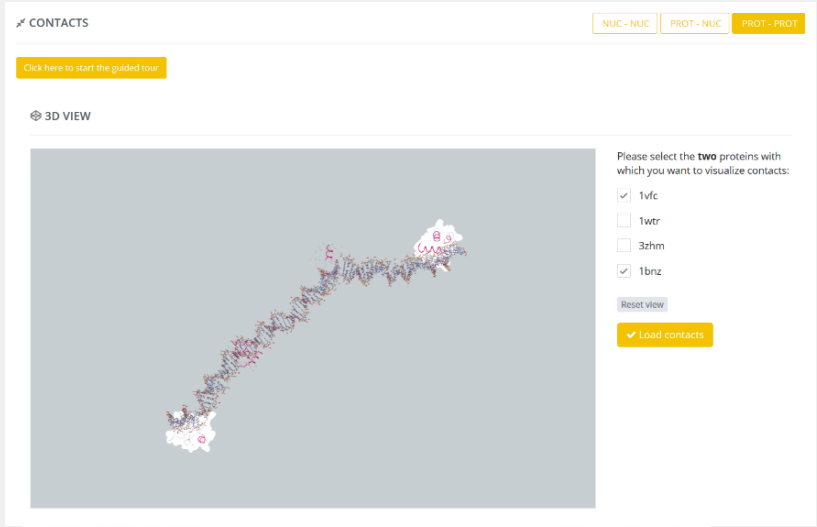
Circular MC_DNA

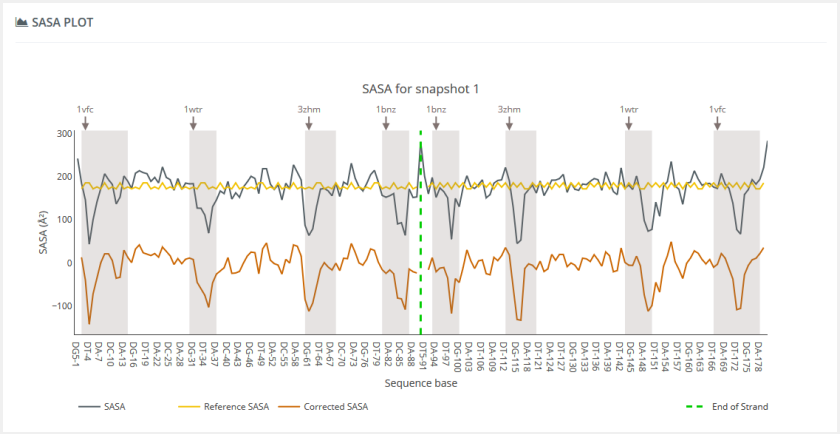


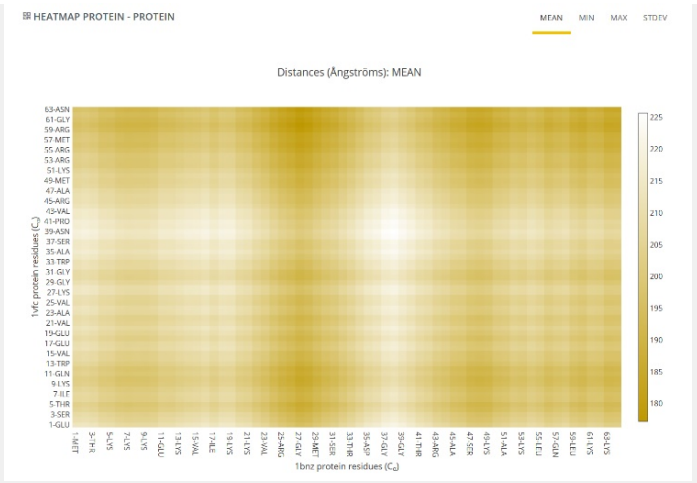


MC_DNA – Sample Output: MC_DNA + Proteins





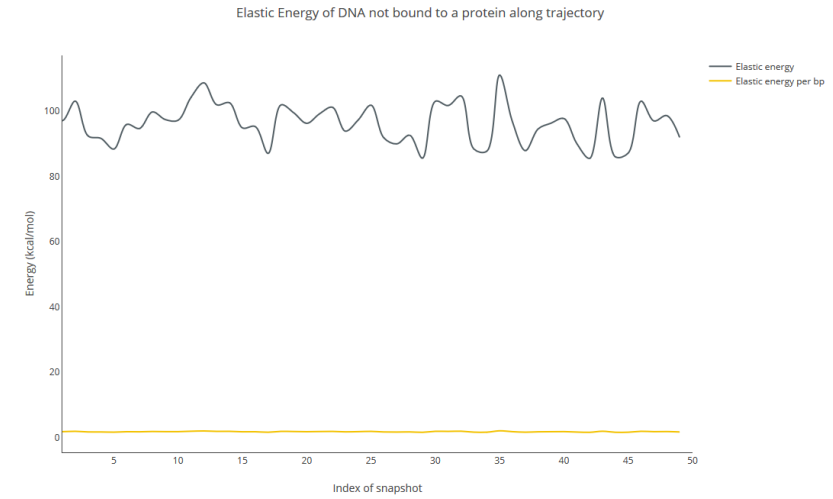




MC_DNA – Sample Output: MC_DNA + Proteins

Elastic Energy of DNA not bound to a protein

	Mean (kcal/mol)	SD (kcal/mol)
Total elastic energy (kcal/mol)	96.33	6.22
Total elastic energy per bp (kcal/mol)	1.75	0.11



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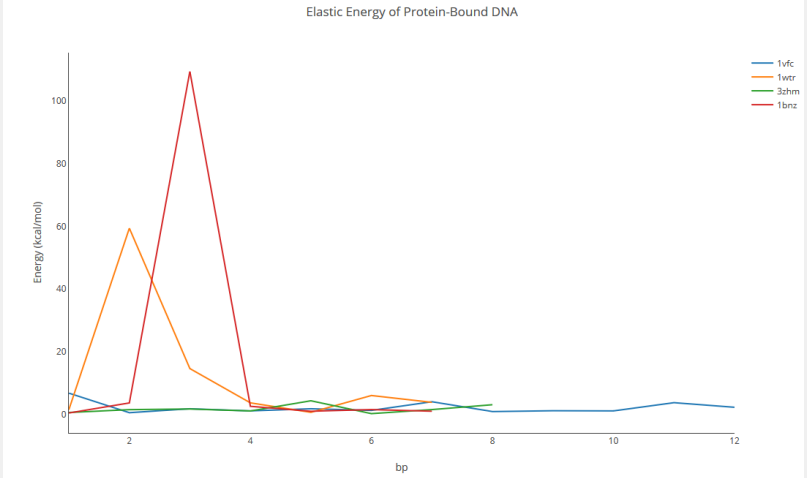
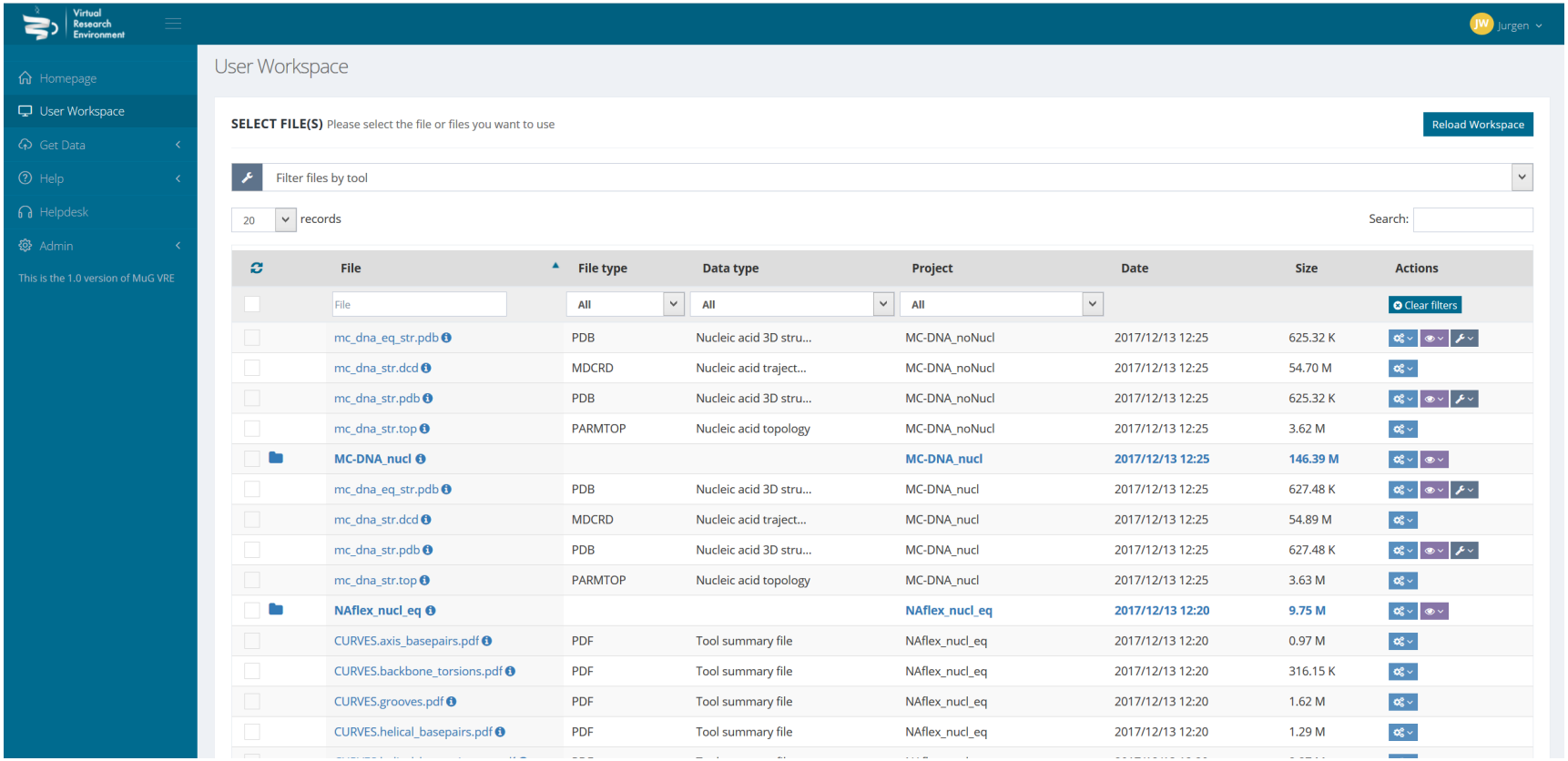


Multiscale Complex Genomics

https://vre.multiscalegenomics.eu/workspace/

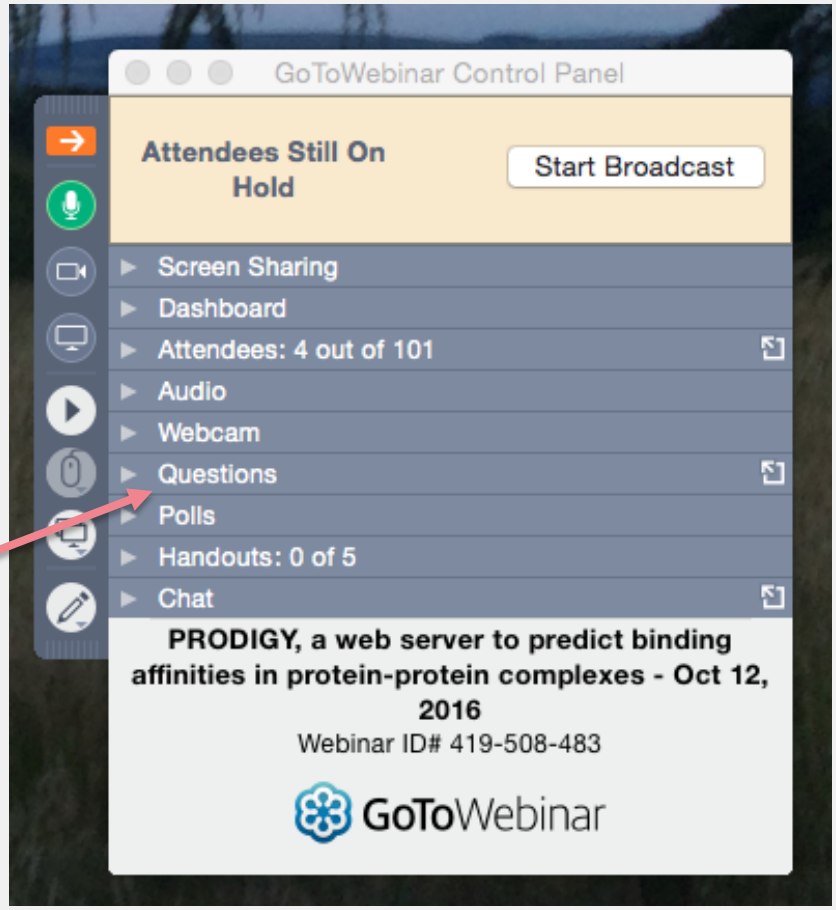


Horizon 2020
European Union Funding
For Research and innovation

Audience Q&A session

Please use the **Questions** function in GoToWebinar application

Any other questions or points to discuss after the live webinar? Join the discussion the discussion at http://ask.bioexcel.eu.



UPCOMING WEBINARS

http://bioexcel.eu/webinars

- **18th April**: *"Perspective on the Martini Force Field"*, Presenter: **Siewert-Jan Marrink,** University of Groningen
- **26 April**: *"Finding a trade-off between speed and accuracy in protein-ligand binding description"*, Presenter: **Walter Rocchia**, BiKi Technologies
- **10th May**: *"High-Confidence Protein–Ligand Complex Modeling by NMR Guided Docking Enables Early Hit Optimization"*, Presenter: **Andrew Proudfoot**, Novartis