



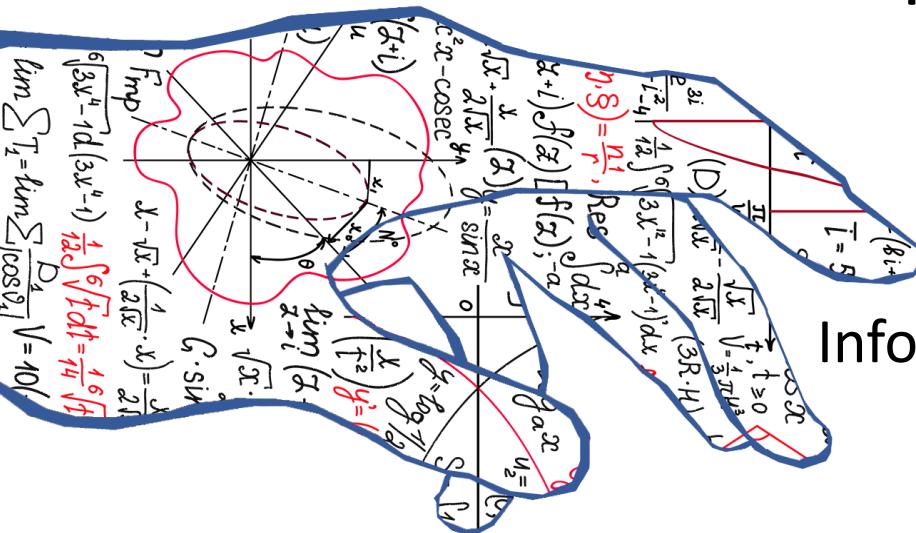
ITMO UNIVERSITY



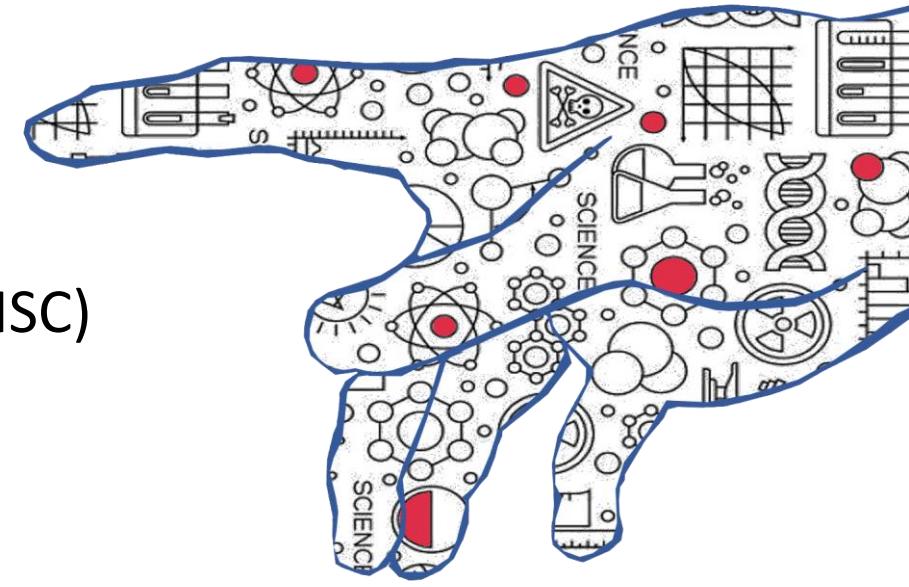
INFOCHEMISTRY SCIENTIFIC CENTER

Cheminformatics and synthetic biology: computational methods and projects

Prof. Sergey Shityakov

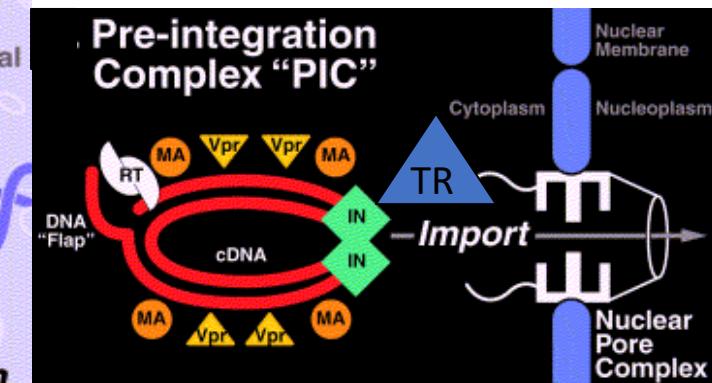
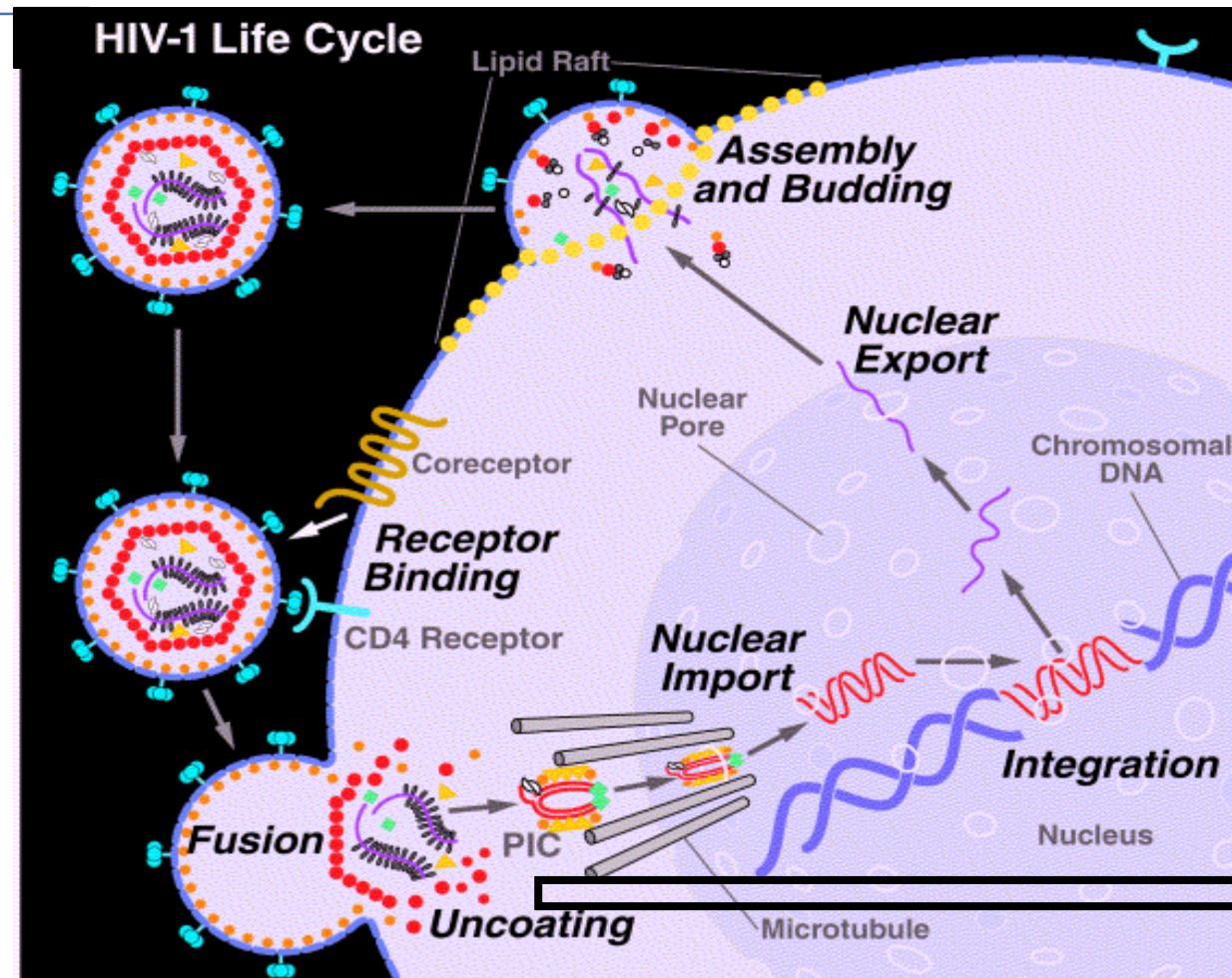


Infochemistry Scientific Center (ISC)
ITMO University
Saint-Petersburg, 2024





TR-SR1 and HIV-1 IN

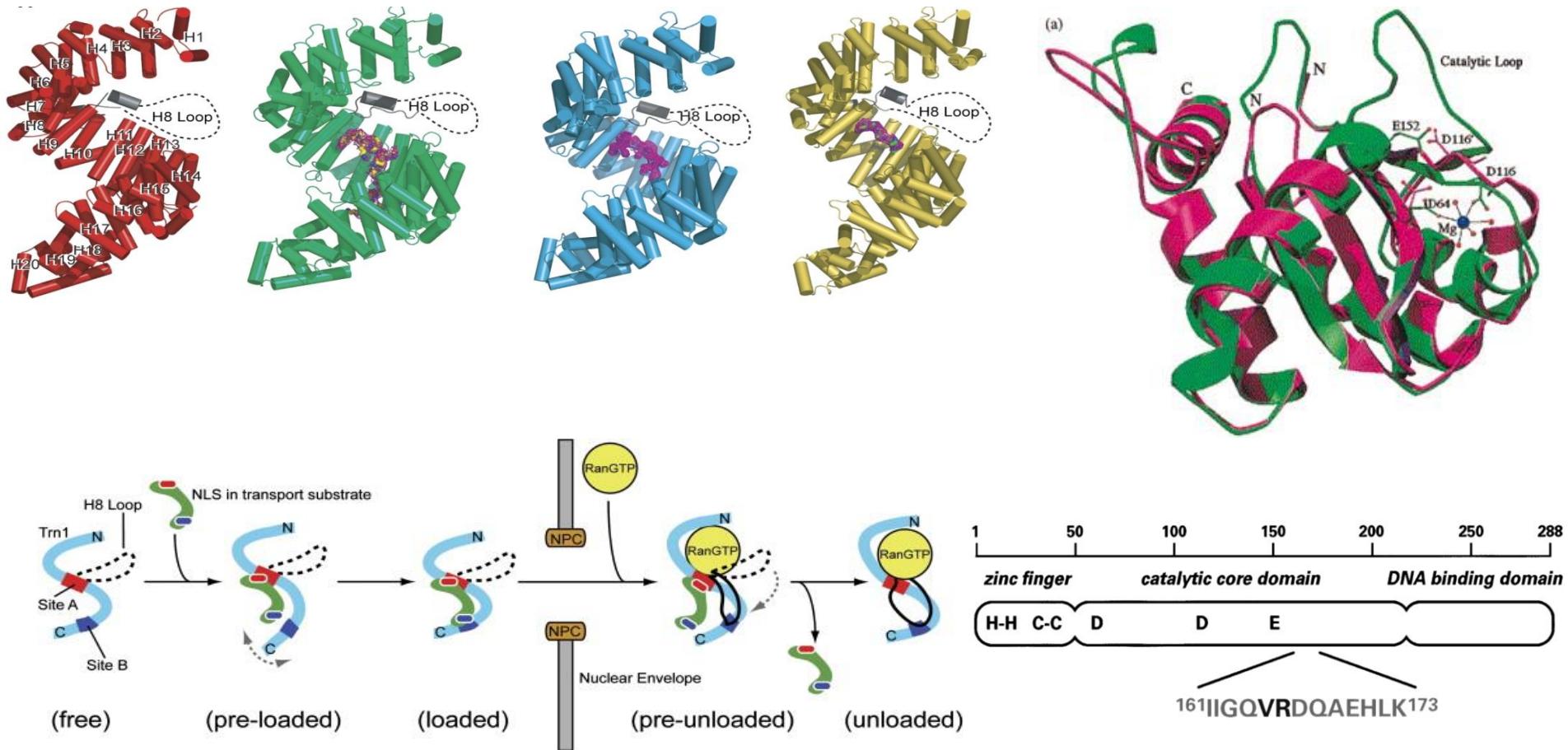
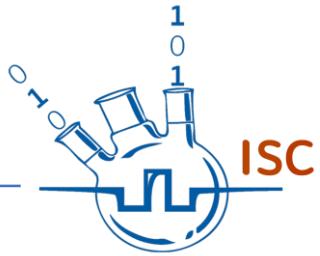


Sherman et al., Micro. Inf, 2002

IT'S MORE than a
UNIVERSITY



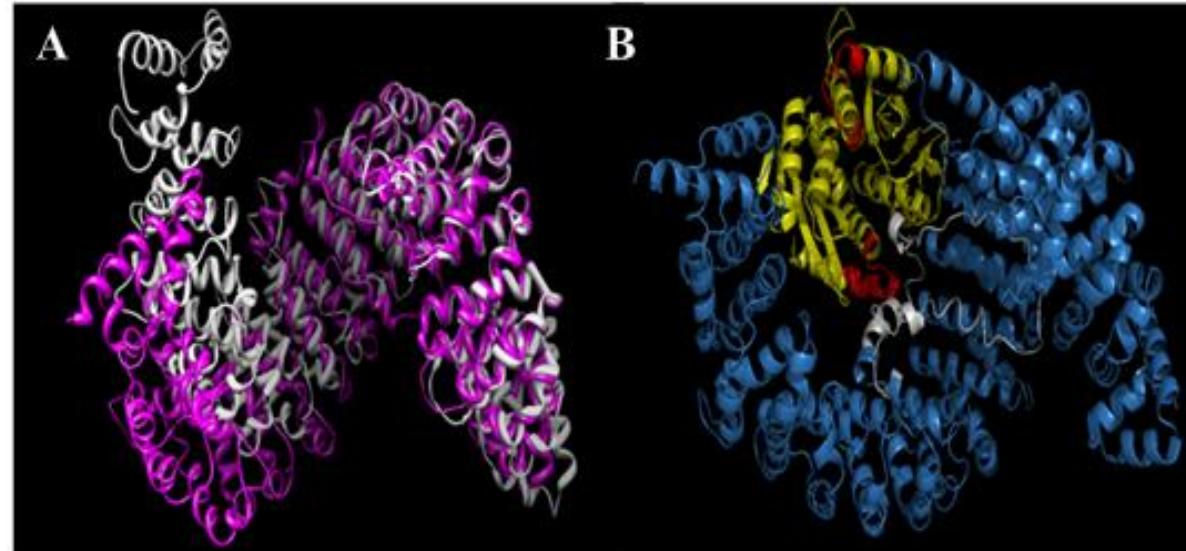
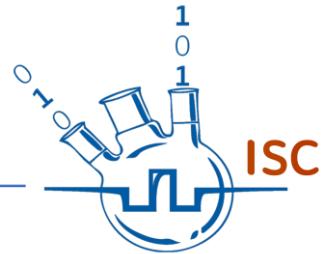
Structure of TR-SR1 and HIV-1 IN



Imasaki et al., Cell, 2007
ITMO more than a
UNIVERSITY



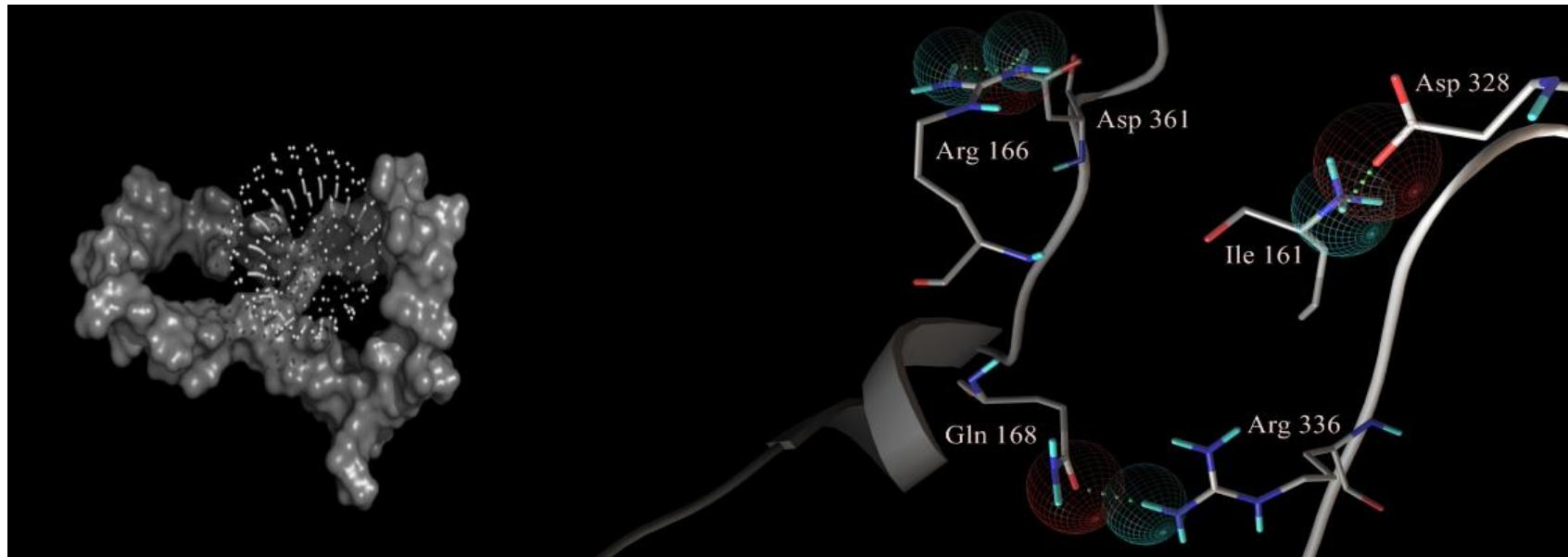
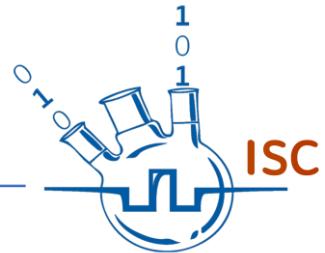
TR-SR1/SR2 3D superimposition and docking



Rank	Solution Number	Global Energy	Attractive VdW ¹	Repulsive VdW	ACE	HBE
1	6	-0.50	-20.21	15.78	3.71	0.00
2	3	-0.37	-39.79	29.36	4.69	-5.05
3	2	2.06	-1.72	0.00	0.12	-0.80
4	5	5.19	-22.87	9.68	-4.69	0.00
5	4	9.72	-25.44	19.09	6.44	-1.79
6	7	13.03	-6.27	0.14	4.51	0.00
7	1	14.98	-3.89	1.69	-1.13	0.00



Flexible docking of TR-SR2 H8-loop and HIV-1 IN NLS



donor 'NLS' \Rightarrow acceptor 'H8-loop'
residues in close contact

Ile 161 \Rightarrow Asp 332, Lys 334,
Ile 333, Asp 328
Gln 168 \Rightarrow Arg 336
His 171 \Rightarrow Ser 355
Val 165 \Rightarrow Arg 336
Arg 166 \Rightarrow Asp 361

donor 'H8-loop' \Rightarrow acceptor 'NLS'
residues in close contact

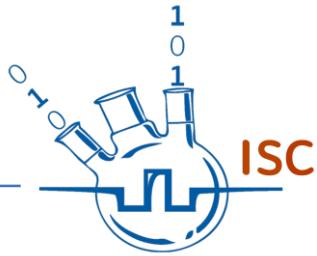
Lys 334 \Rightarrow Ile 161
Arg 336 \Rightarrow Gln 168 Val 165
Asp 361 \Rightarrow Arg 166
Asp 328 \Rightarrow Ile 161
Asp 332 \Rightarrow Ile 161
Ser 355 \Rightarrow His 171
Ile 333 \Rightarrow Ile 161

Shityakov et al., OJB, 2010

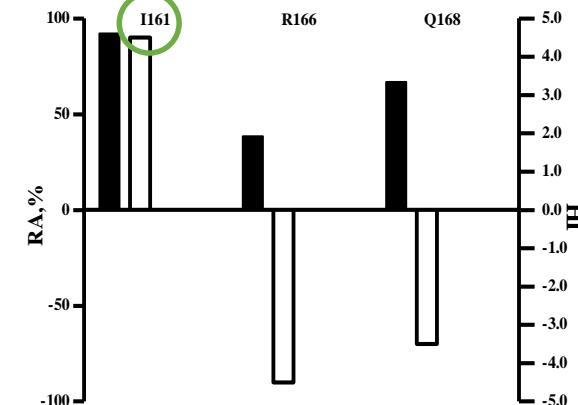
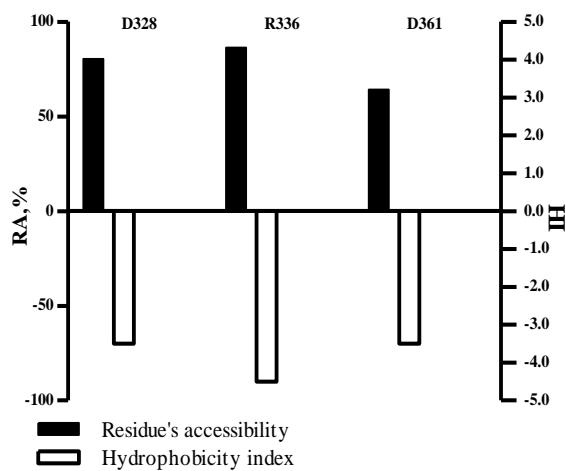
ITMO more than a
UNIVERSITY



The H8-loop of the TR-SR2 and the HIV-1 NLS



H8-loop	Area	Acc. (%)	HI	IN NLS	Area	Acc. (%)	HI
Asp 328	130.255	80.3	-3.5	Ile 161	157.887	92.2	4.5
Asp 332	106.409	65.6	-3.5	Val 165	71.374	48.0	4.2
Ile 333	111.333	65.0	4.5	Arg 166	93.843	38.5	-4.5
Lys 334	115.095	54.4	-3.9	Gln 168	125.090	66.9	-3.5
Arg 336	210.727	86.4	-4.5	His 171	127.643	66.6	-3.2
Ser 355	74.924	100.0	-0.8				
Asp 361	104.115	64.2	-3.5				

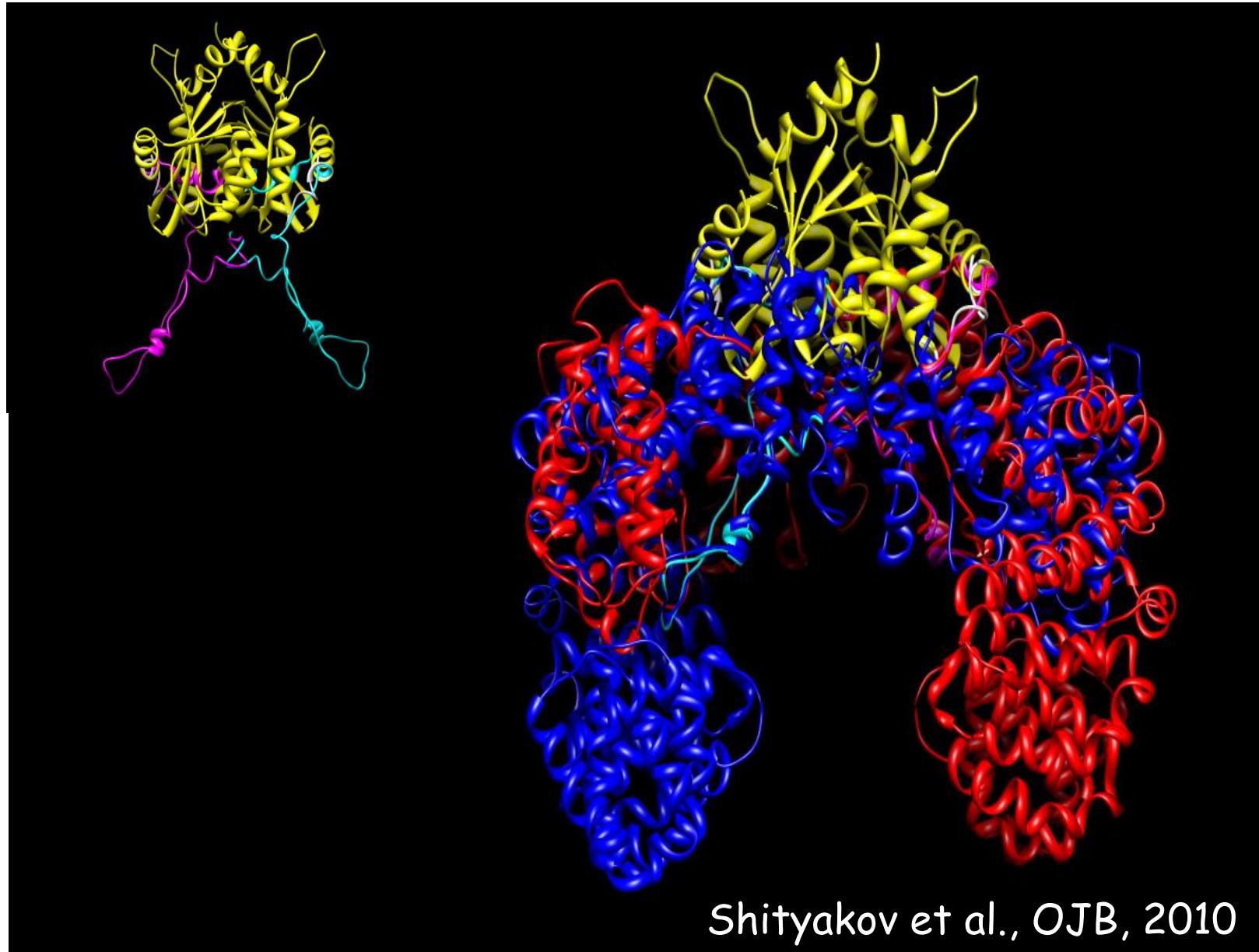
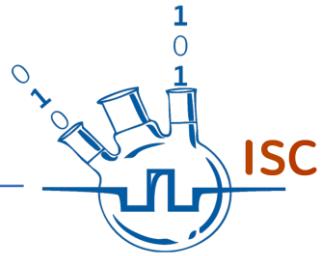


Shityakov et al., OJB, 2010

ITSMORE than a
UNIVERSITY



TR-SR1/SR2 3D superimposition and docking

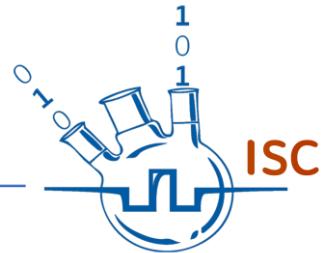


Shityakov et al., OJB, 2010

IT₃MOre than a
UNIVERSITY

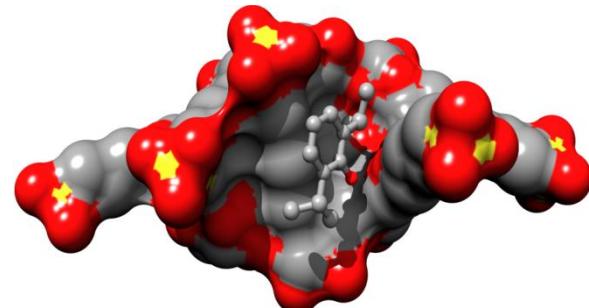


Screening of CD-formulated compounds

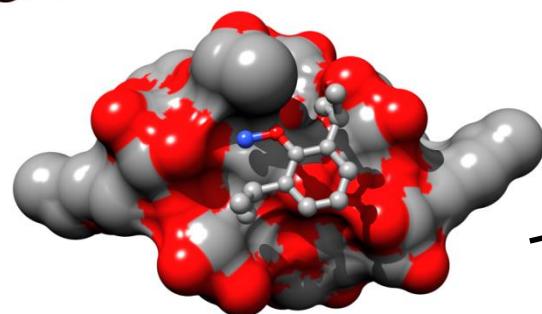
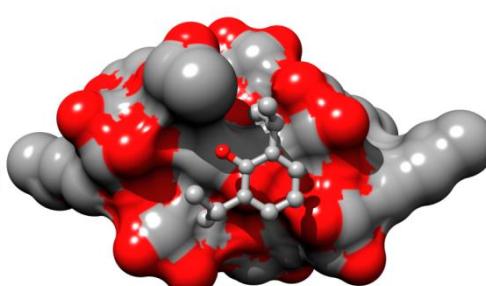


In silico screening of CD-formulated general anesthetics

Propofol/SBECD
 $\Delta G = -3.2 \text{ kcal/mol}$

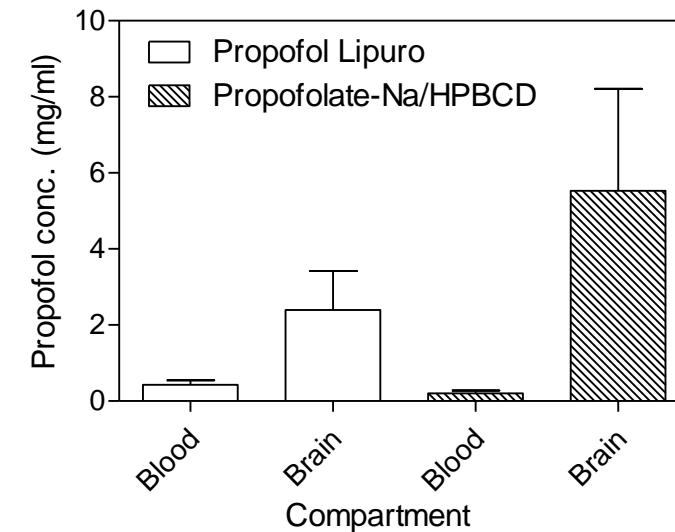


Propofol/HPBCD
 $\Delta G = -1.8 \text{ kcal/mol}$



$\Delta G = -1.4 \text{ kcal/mol}$
Propofolate-Na/HPBCD

in vivo BBB study

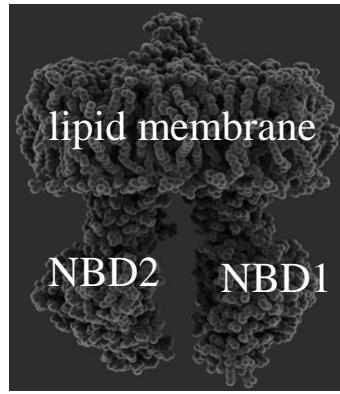


SBECD – sulfobutyl- β -cyclodextrin
HPBCD – hydroxypropyl- β -cyclodextrin

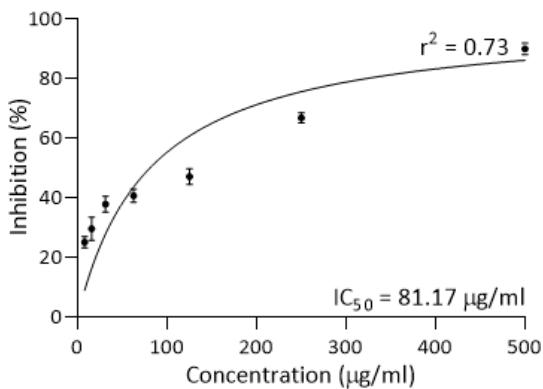


Screening of carbon nanoparticles as drug-delivery vectors

Model of P-gp transporter at the BBB (multidrug resistance)

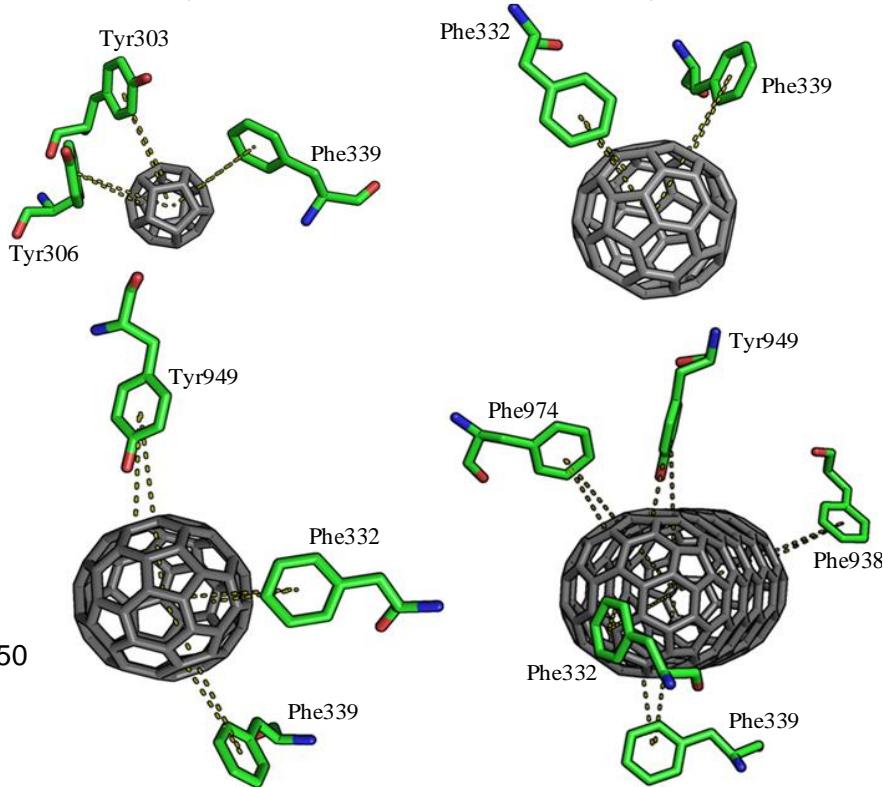


NBD – nucleotide-binding domain
in vitro BBB cell toxicity test



MWCNT – multi-walled carbon nanotube

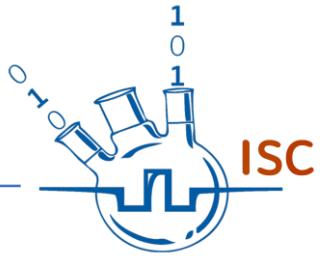
Geometric configuration of π - π stacking involved in P-gp interaction with carbon nanoparticles (fullerenes and nanotube)



Shityakov *et al.*, Int. J. Nanomedicine, 2013



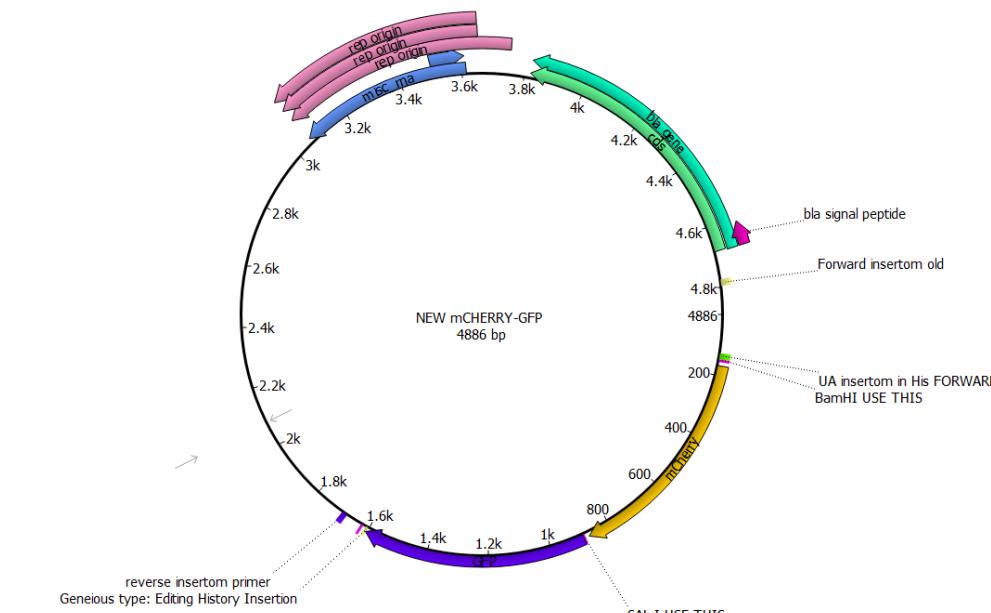
Synthetic biology collaboration



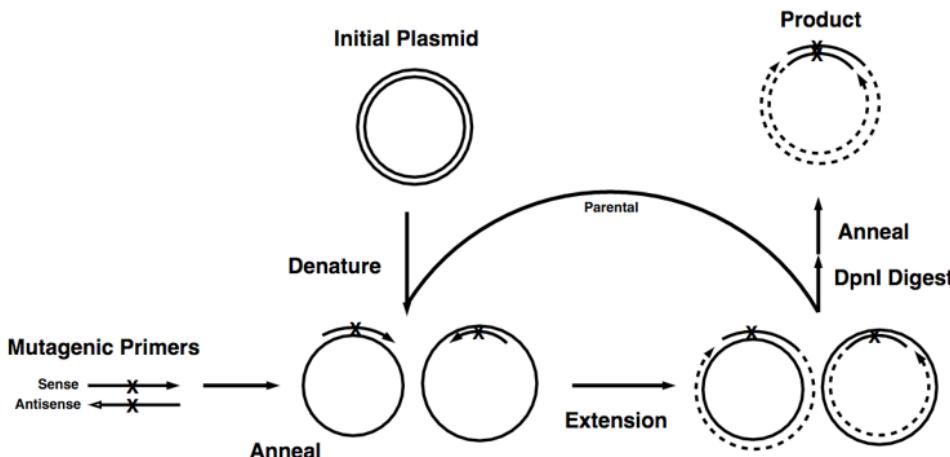
Prof. Thomas Dandekar



Dr. Elena Benkurova



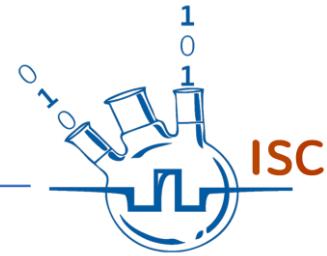
Site-directed mutagenesis



IT'S MOre than a
UNIVERSITY

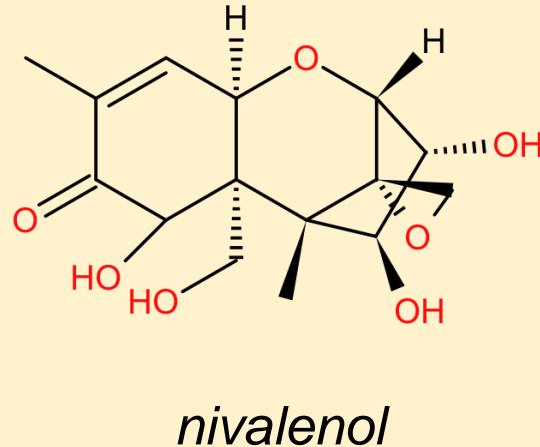


SCREENING DNA-APTAMERS TO NIVALENOL

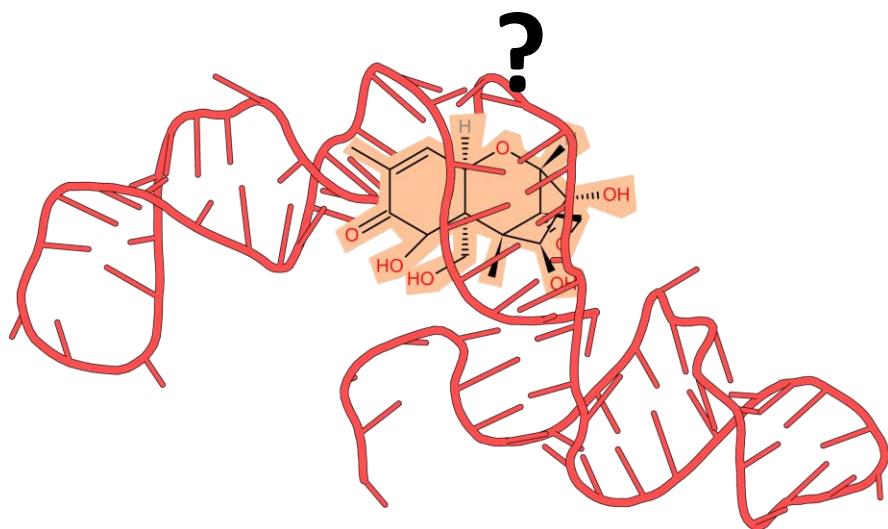


STARTING POINT:

- 10 rounds of selection from randomized library ($\sim 10^{15}$ sequences) were performed
- The last library was sequenced with Illumina platform
- The acquired library contains 3400 unique sequences



We need to select several sequences as most potent aptamers

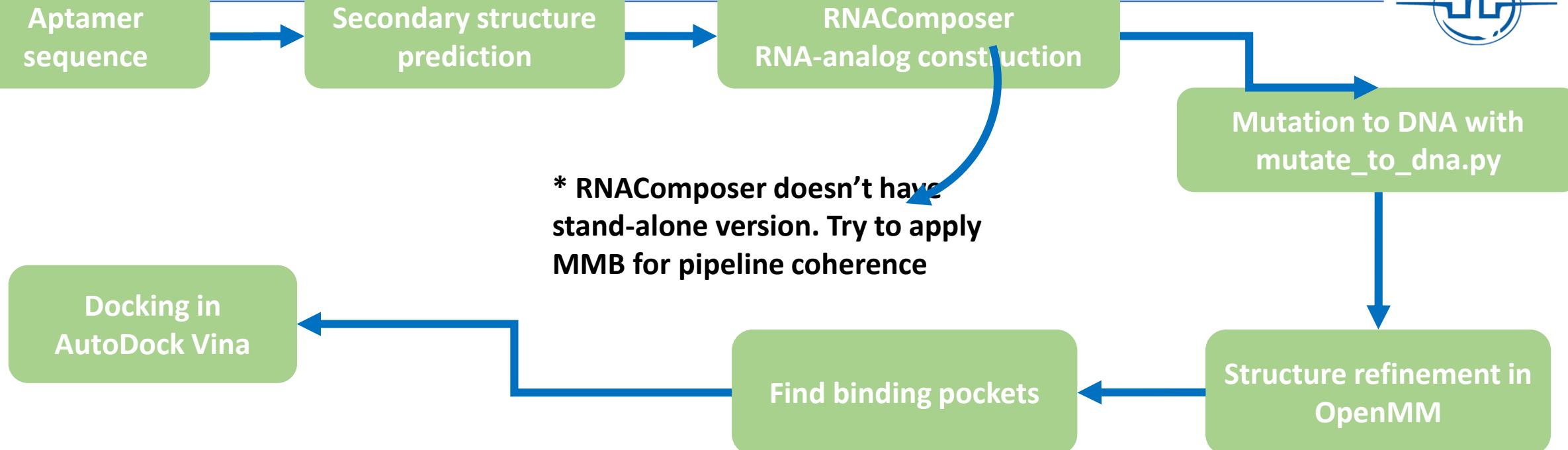
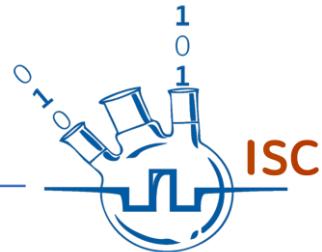


Roadmap:

1. Preliminary screening of the library based on 2d-structure analysis
2. Identification of several candidate sequences for a thorough modelling
3. Generation of DNA 3D-structure and *in silico* binding studies
4. Verification *in vitro*



"AptaFold" current progress



Model aptamer: ochratoxin A (OTA) binding sequence, simulated in following paper:

Article

An In-Silico Pipeline for Rapid Screening of DNA Aptamers against Mycotoxins: The Case-Study of Fumonisin B1, Aflatoxin B1 and Ochratoxin A

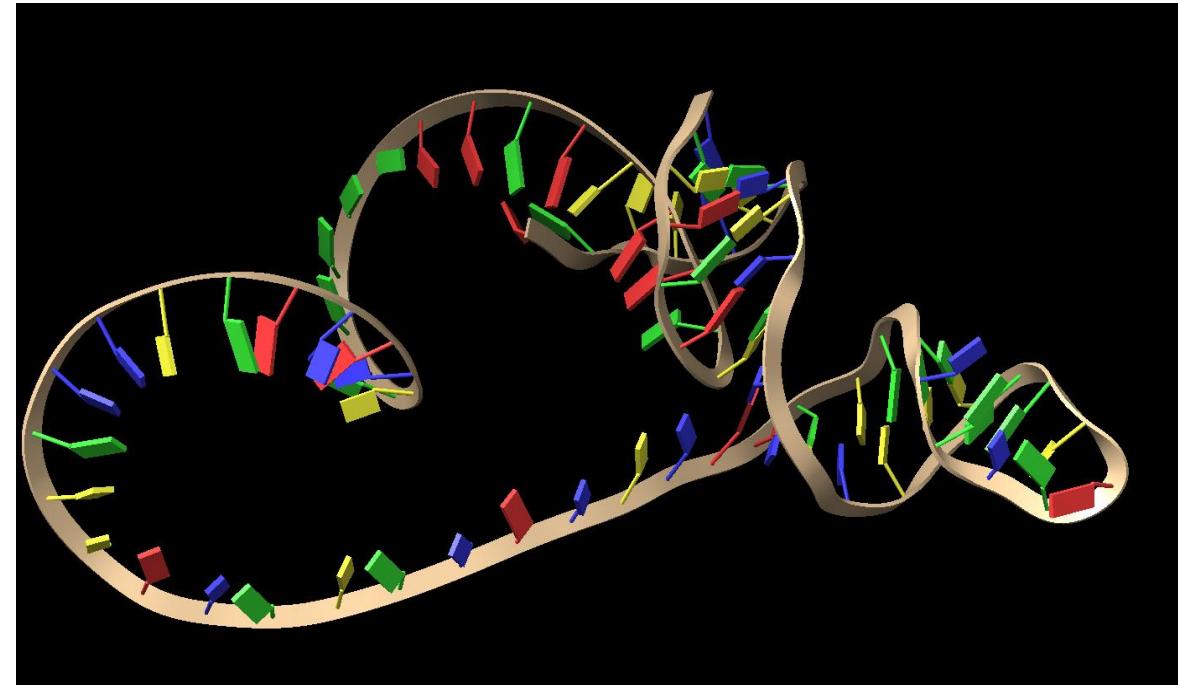
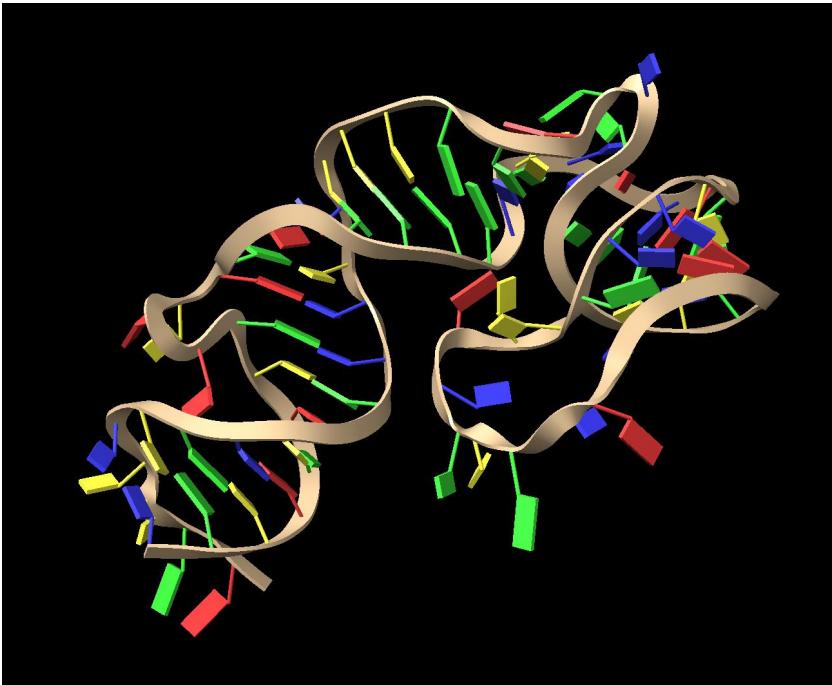
Fulvio Ciriaco ^{1,*}, Vincenzo De Leo ¹, Lucia Catucci ¹, Michelangelo Pascale ², Antonio F. Logrieco ², Maria C. DeRosa ³ and Annalisa De Girolamo ^{2,*}



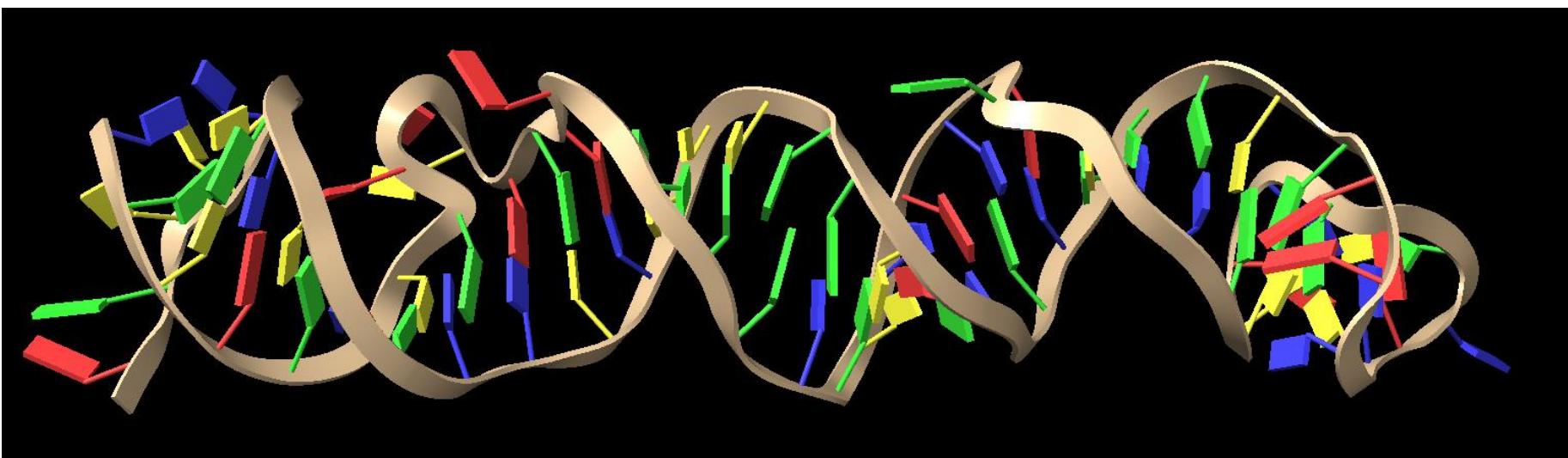
OTA-aptamer generation with several folding algorithms



MFold



RNAFold

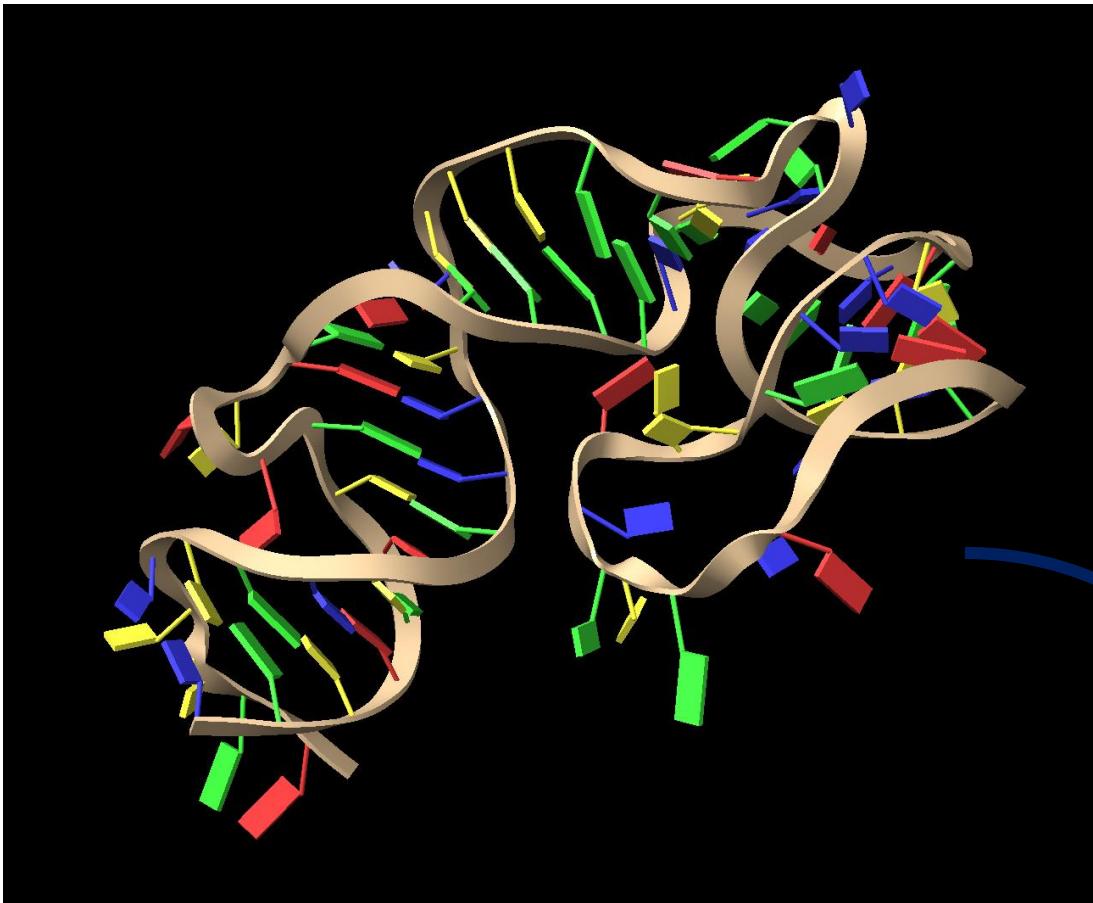
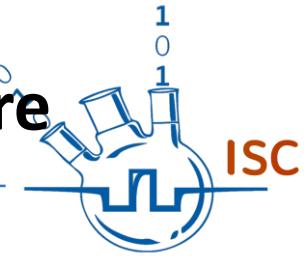


seqfold

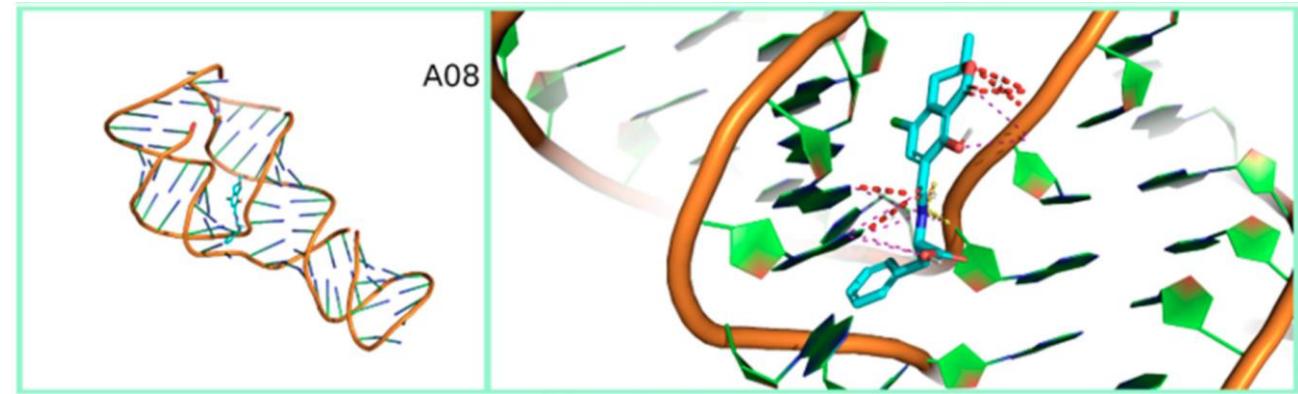
IT₃MOre than a
UNIVERSITY



Mfold has the best prediction compared to published structure



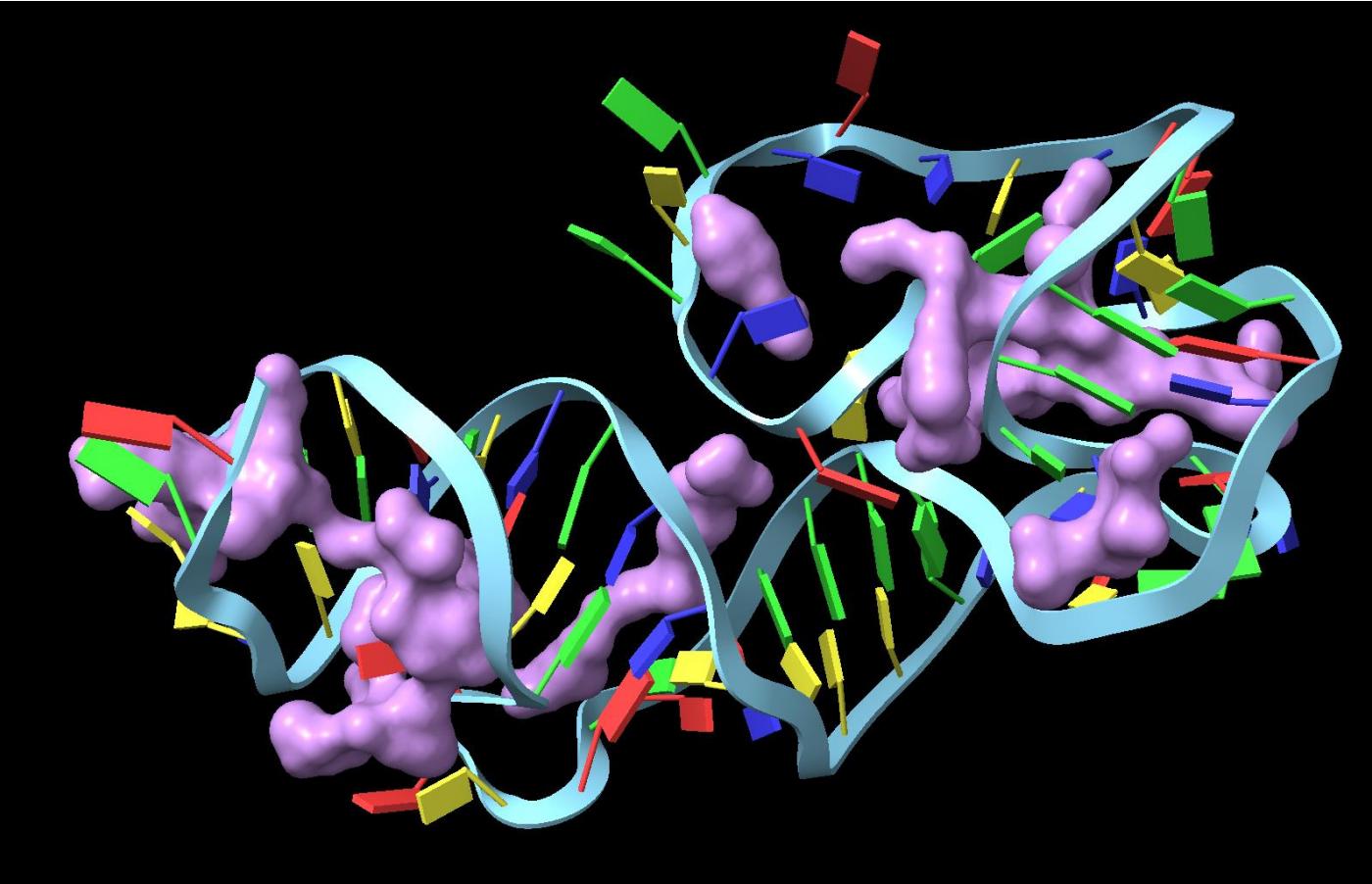
Published aptamer-target complex structure



- The structure was generated in RNAComposer and mutated to DNA with a custom python script
- Then the model was refined with OpenMM one-step simulation



Potential binding pockets are identified with *focket* tool

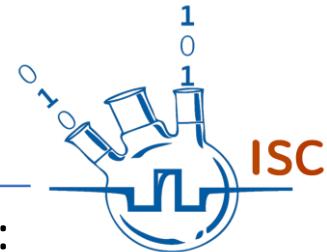


OTA-aptamer with pockets scanned by *focket* (pink surfaces)

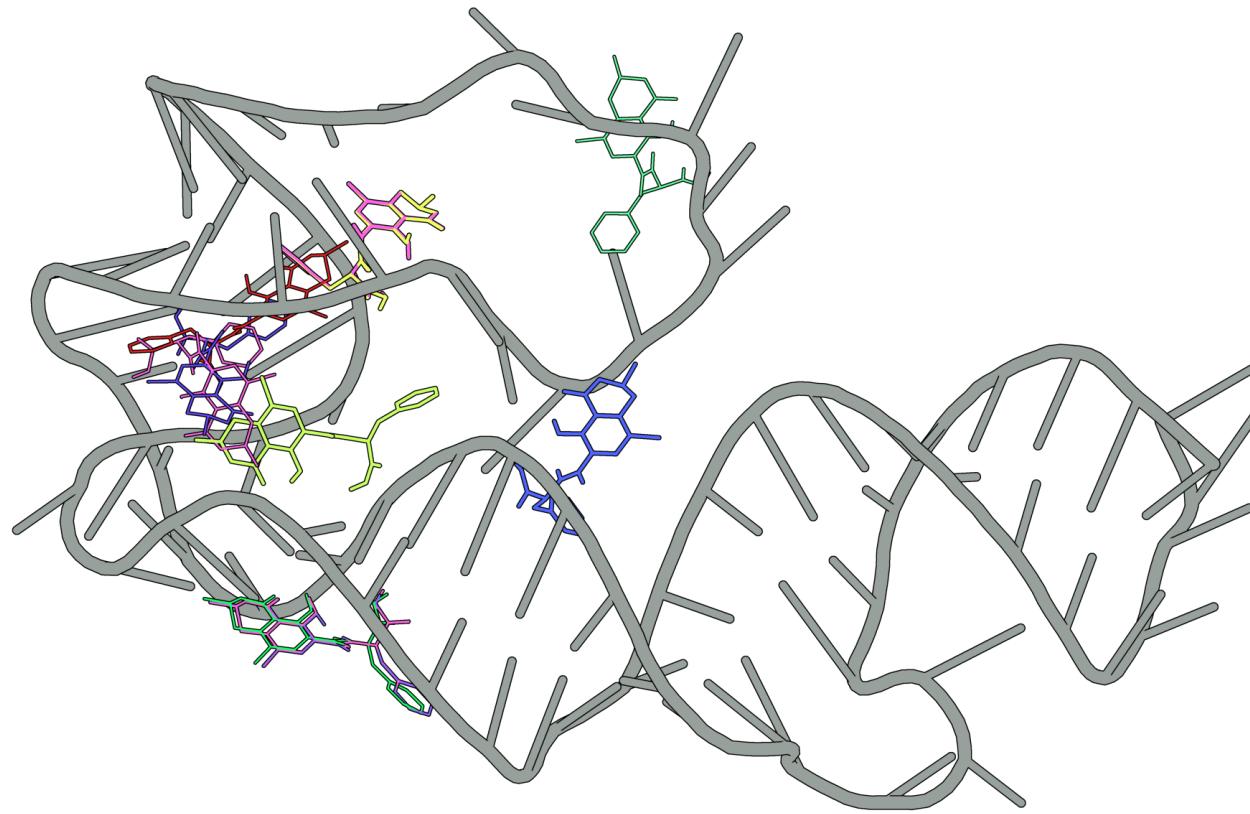
- Pockets are generated as groups of virtual atoms attributed to a particular group
- Coordinates for docking are defined as centroids of these groups
- In total 11 groups are defined for OTA-aptamer



AutoDock Vina for target docking

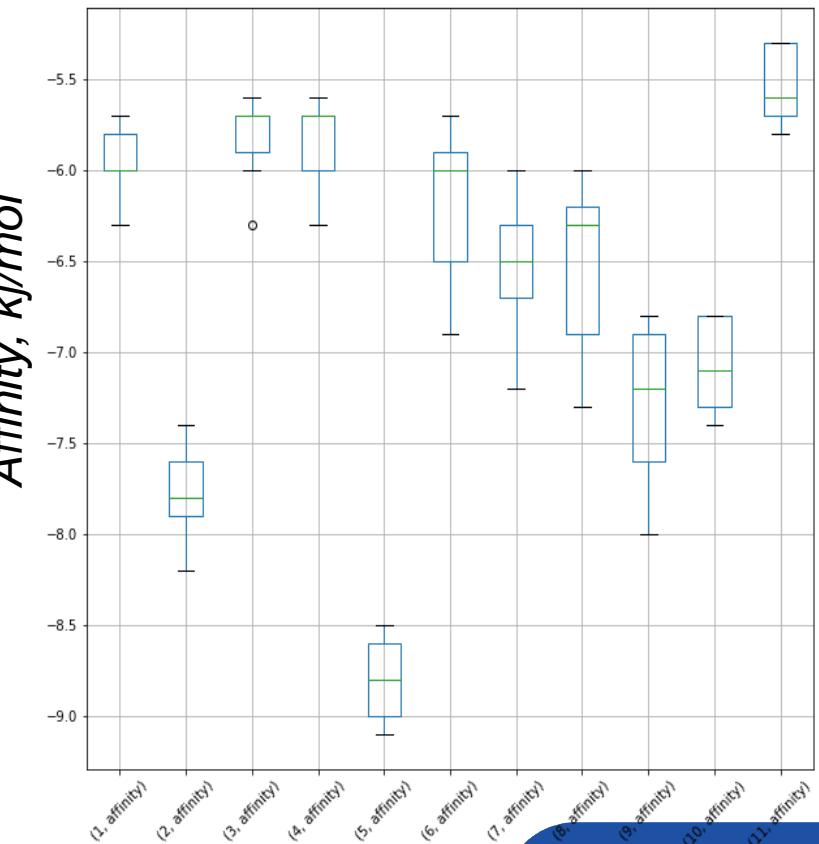


- AutoDock Vina was applied to predict OTA binding at 11 pockets with following box parameters:
--size_x 25 --size_y 25 --size_z 25 (size in Angstroms)



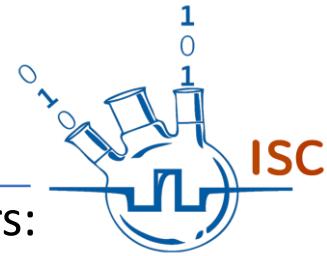
Visualization of best docking positions for each pocket. Some of them are closely overlapping

Energy box plot for each pocket

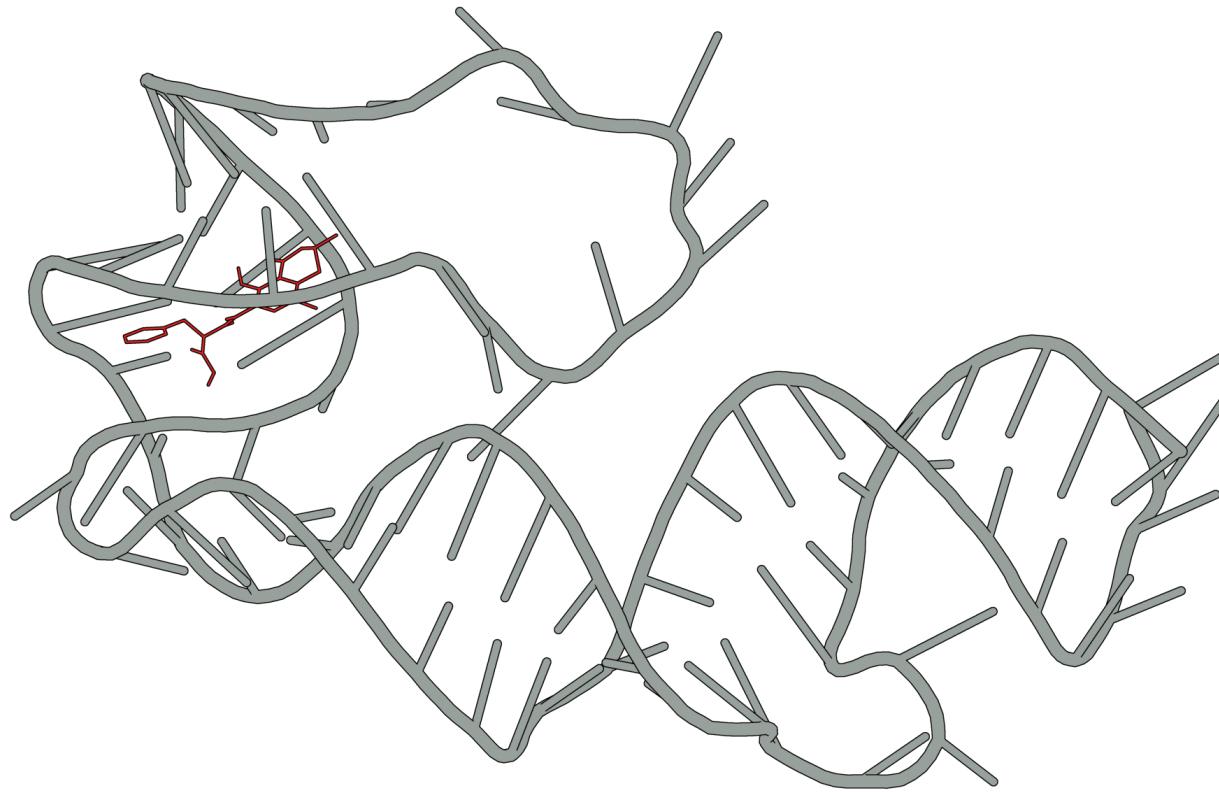




AutoDock Vina for target docking

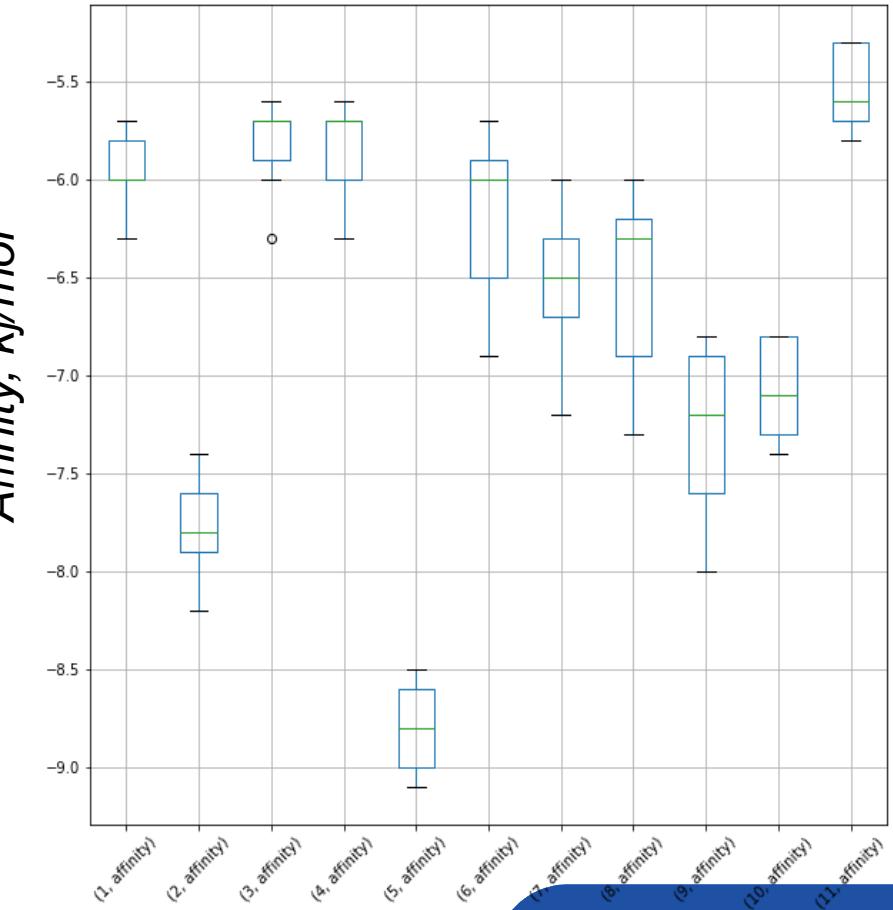


- AutoDock Vina was applied to predict OTA binding at 11 pockets with following box parameters:
--size_x 25 --size_y 25 --size_z



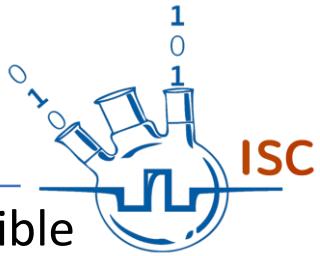
Visualization of best docking positions for pocket 5

Energy box plot for each pocket



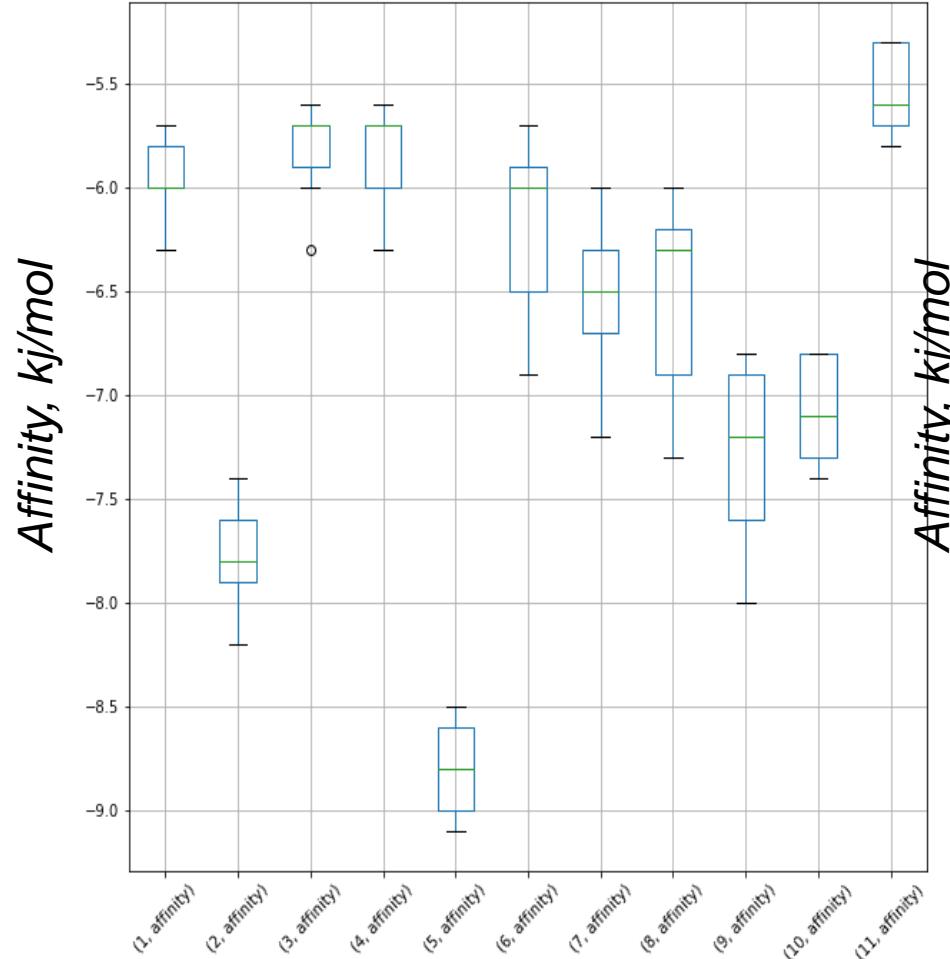


Reproducibility

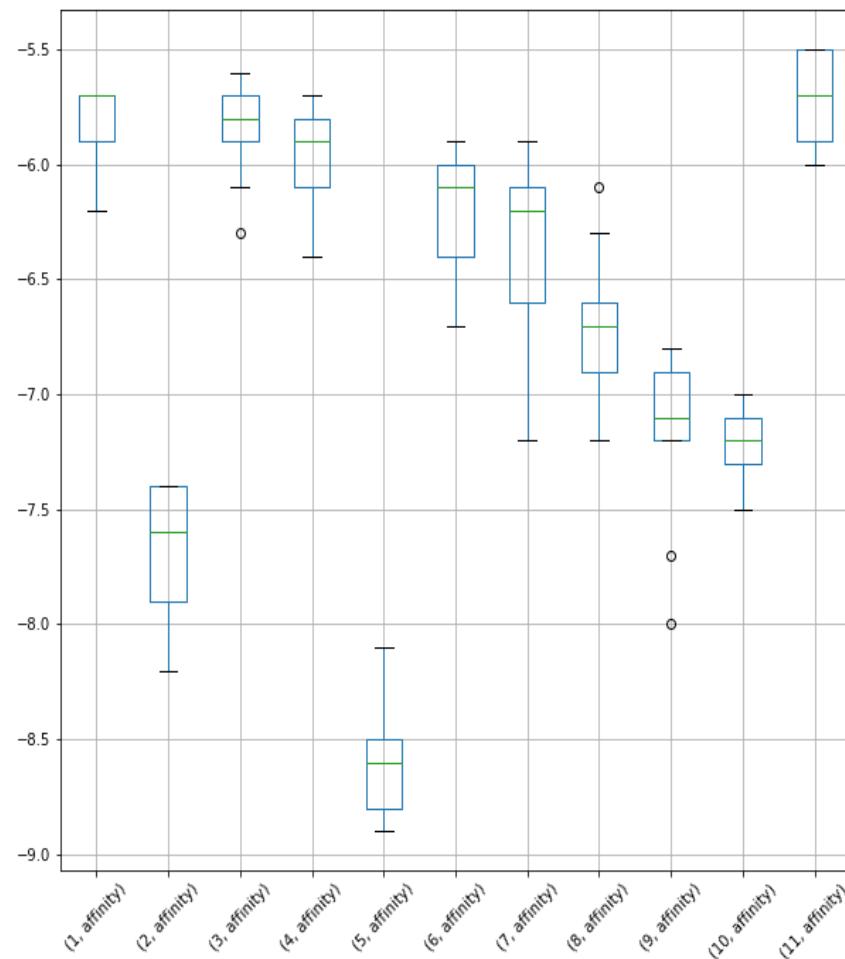


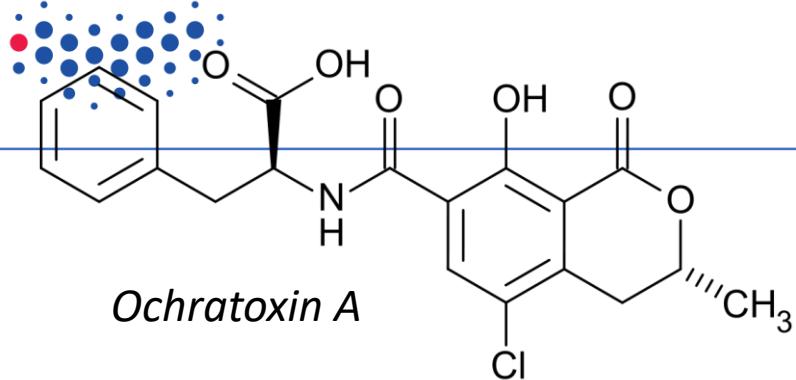
The analysis with AutoDock Vina was performed twice to check if the result is reproducible

First try



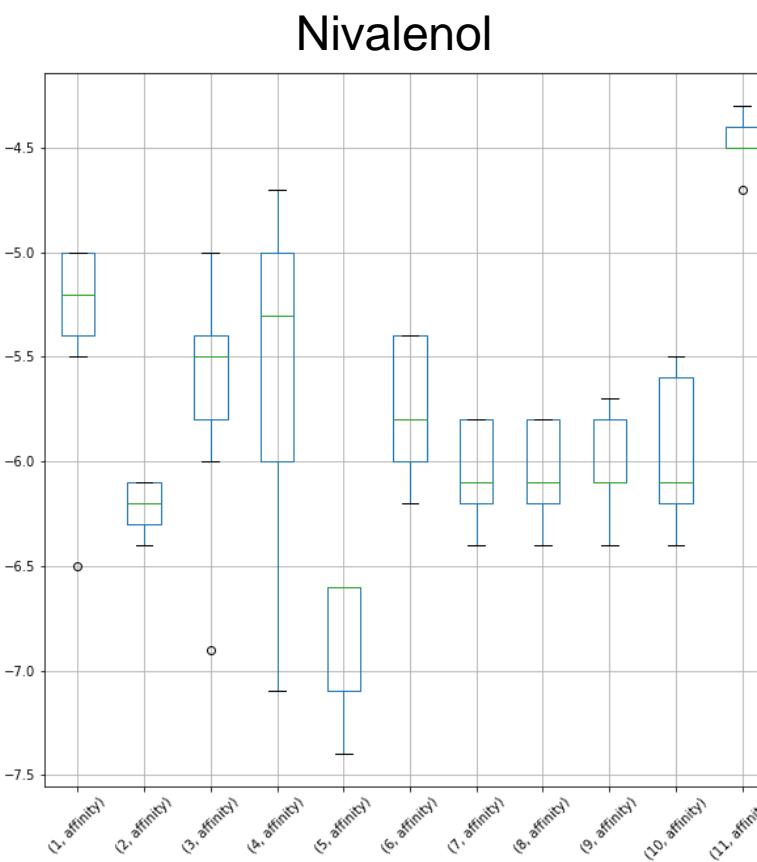
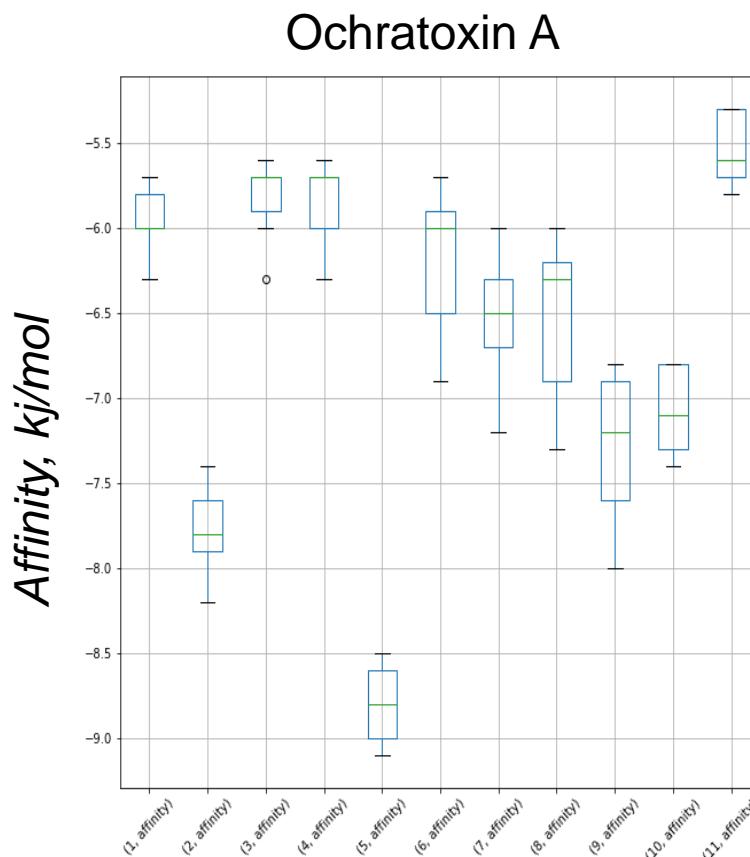
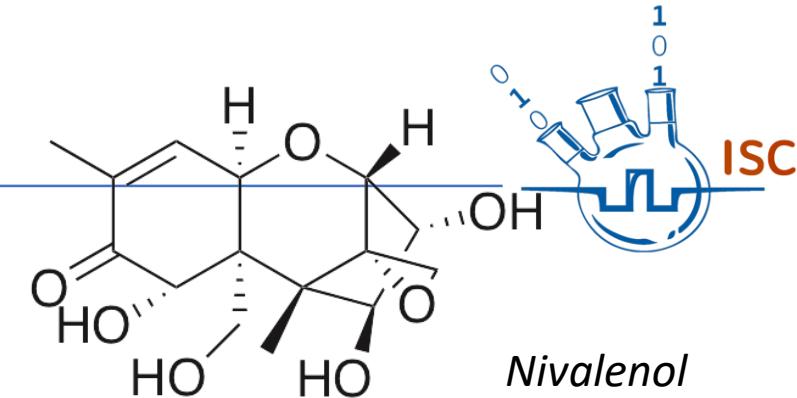
Second try





Docking with a control

The analysis was performed with molecule of nivalenol as negative control to compare results



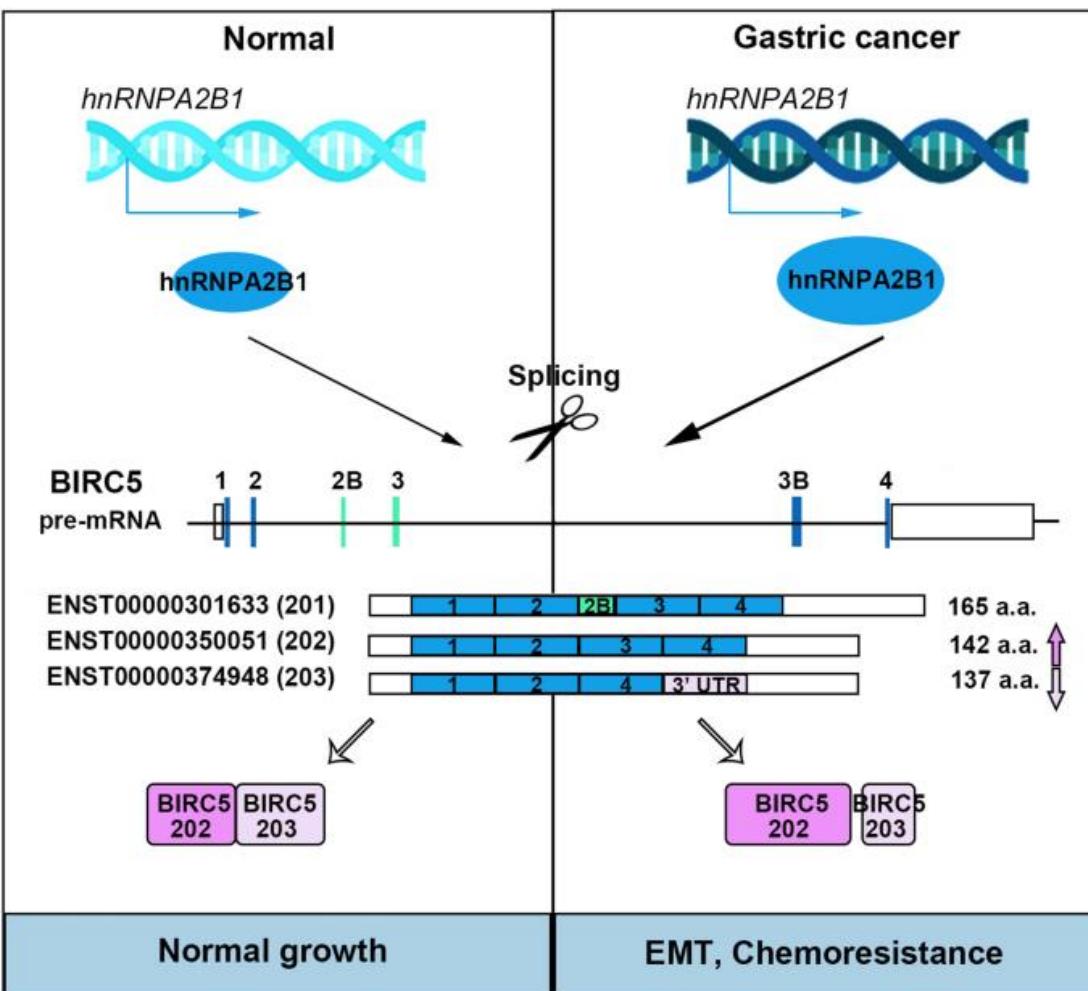
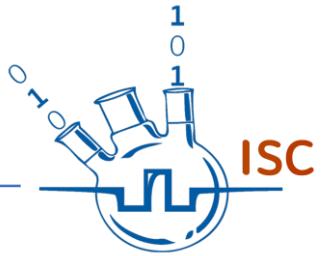
- Some similarity can be observed. For example pocket 5 has bigger affinity to nivalenol too
- However, all affinities to nivalenol are notably higher (in terms of energy)



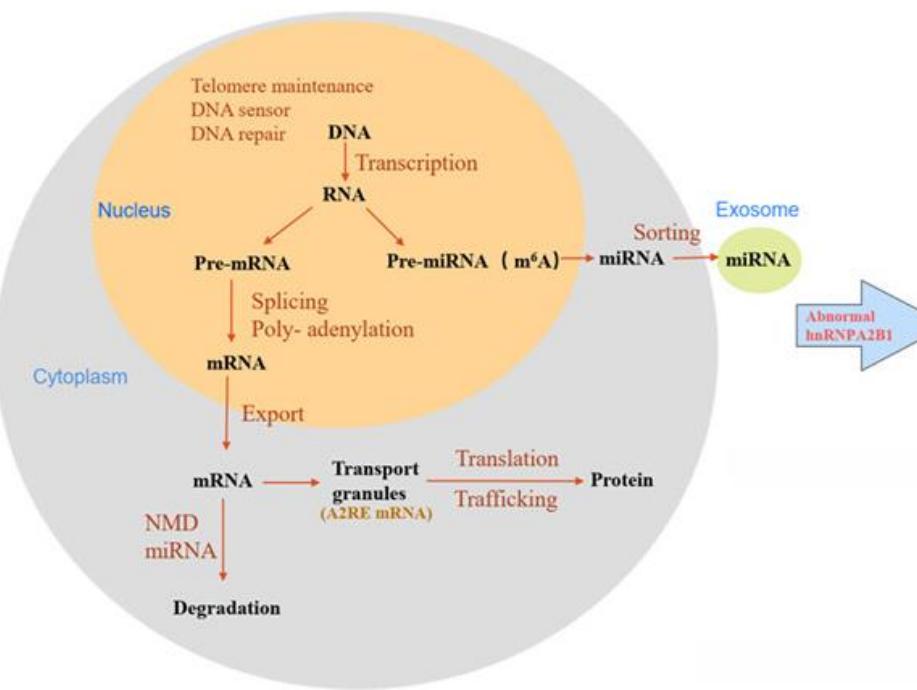
- **To date, the modeling procedure is established from primary aptamer sequence to aptamer-target models predicted by AutoDock Vina**
- Some steps in modeling procedure can be improved, for example: by evaluation of other pocket-searching programs etc.
- The next step would be approbation of MD simulation for the aptamer-target complex with highest affinity
- Then the algorithm can be applied to screen candidate aptamers from NGS data



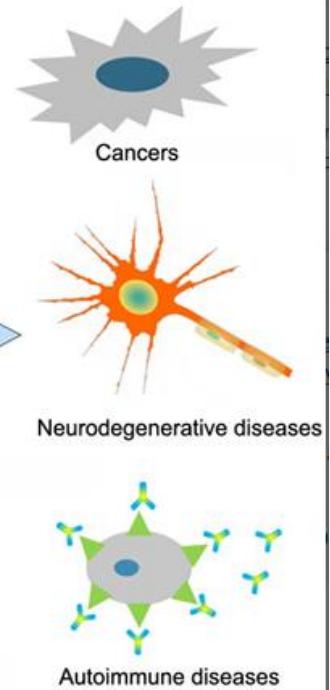
hnRNPA2/B1



hnRNPA2B1-mediated RNA metabolism: from beginning to end

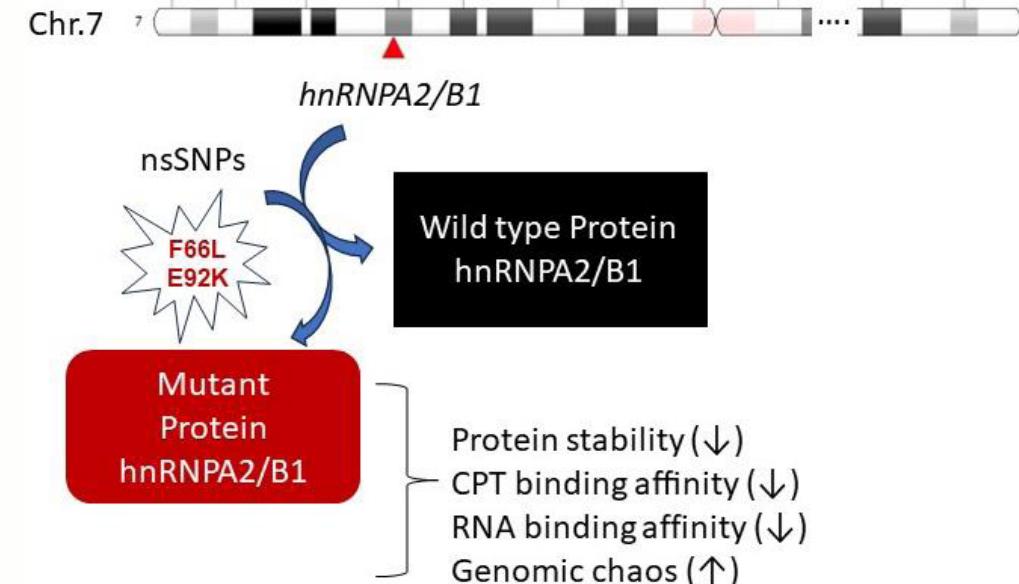
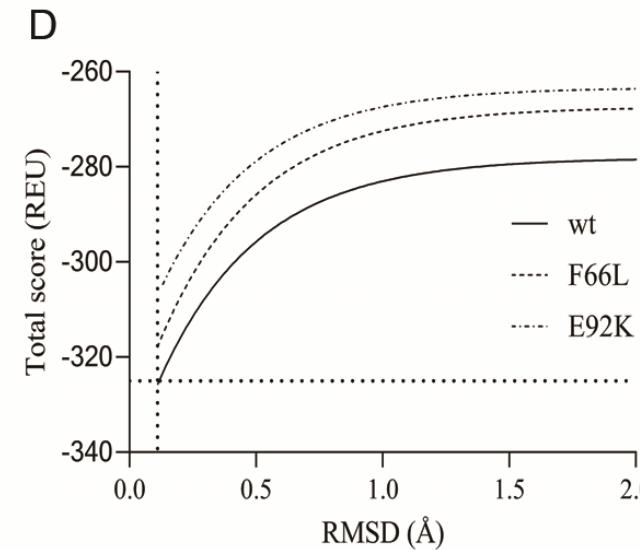
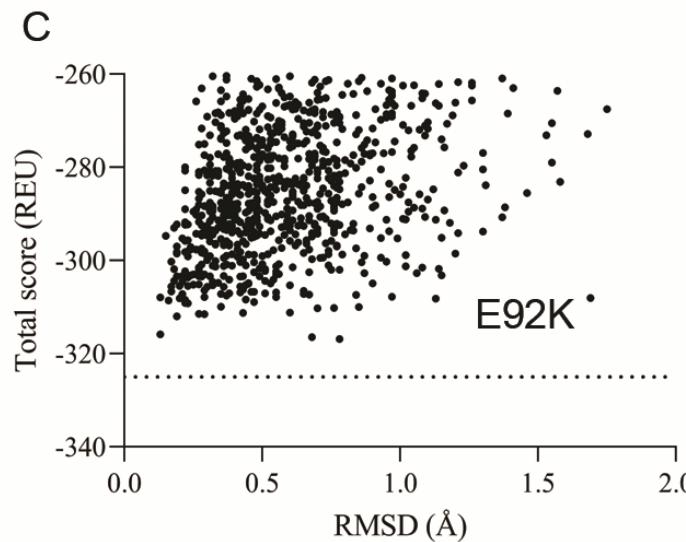
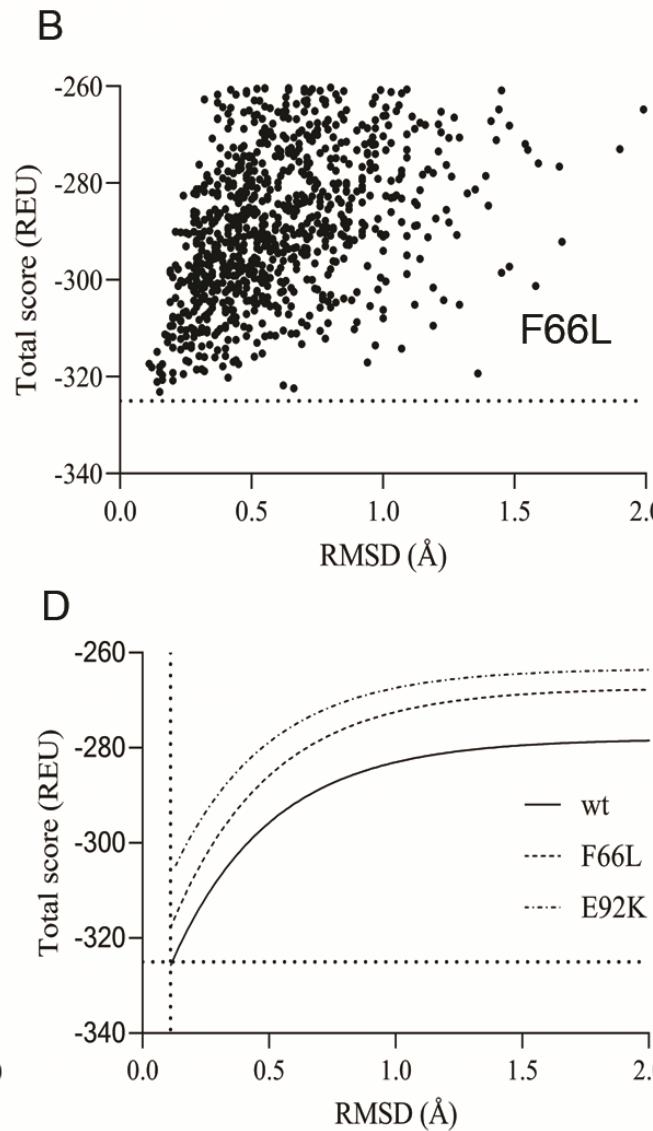
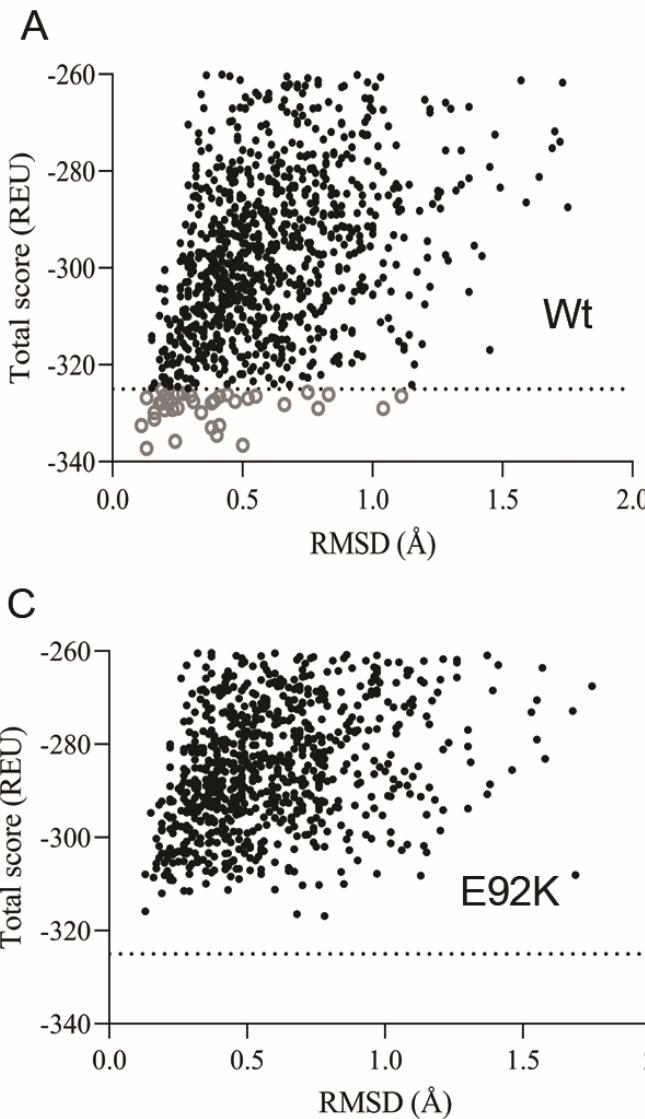
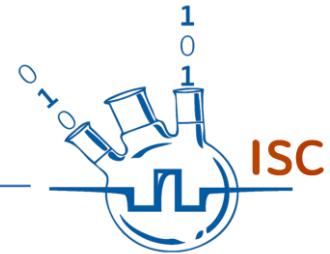


The diseases involved in hnRNPA2B1





SNP in hnRNPA2/B1





SNP in hnRNPA2/B1

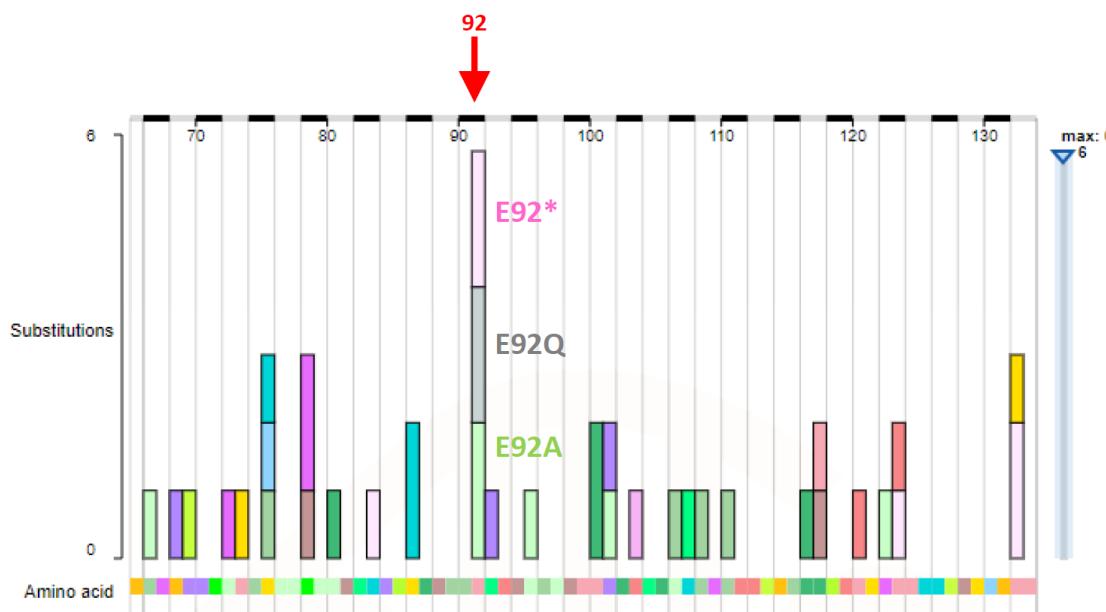
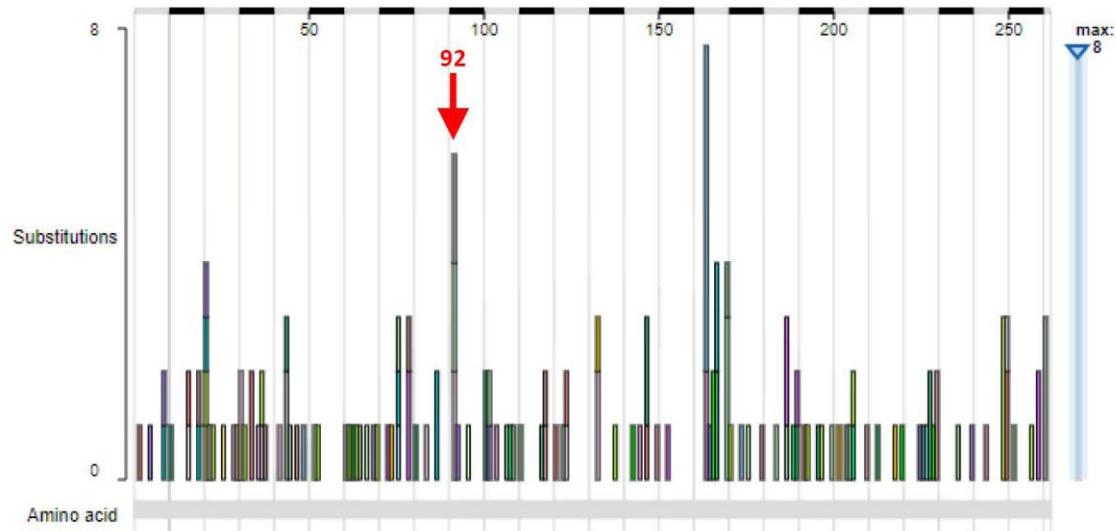
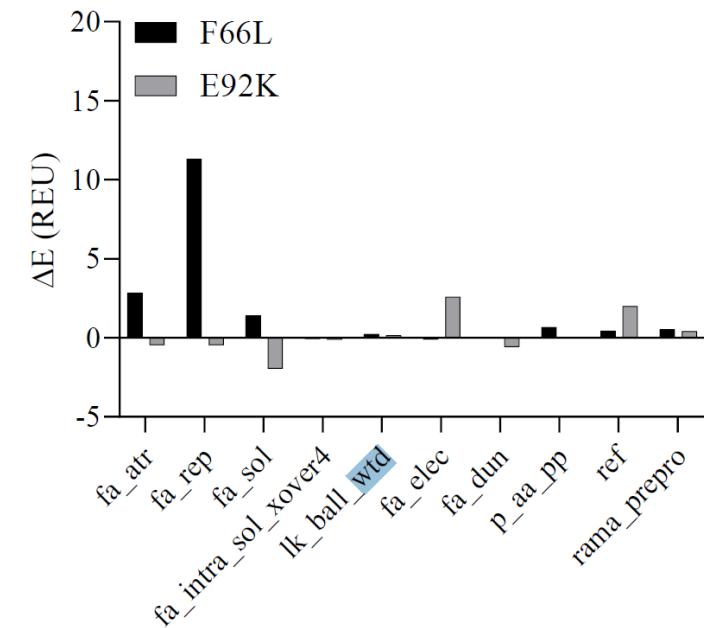


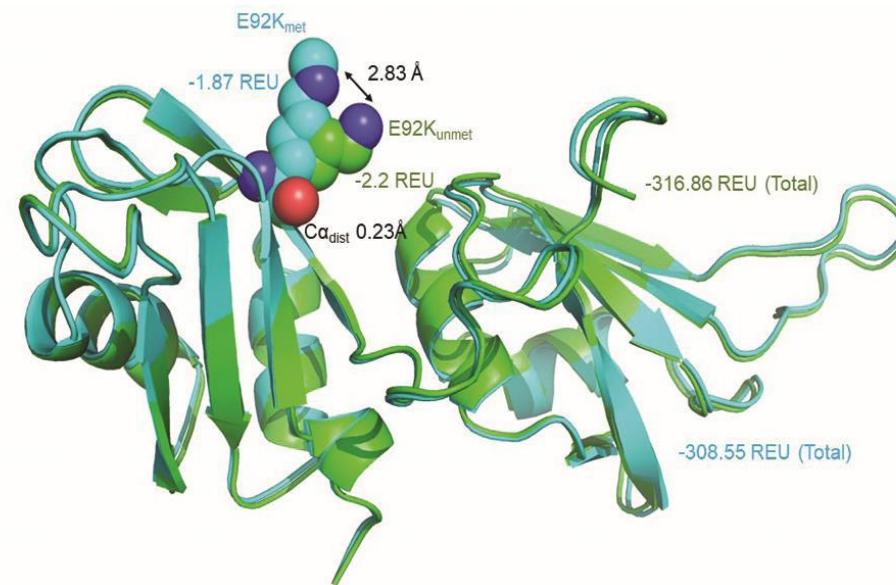
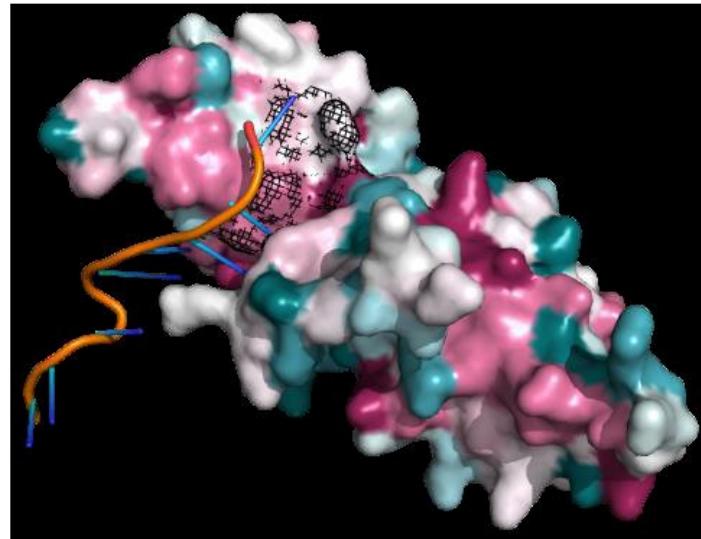
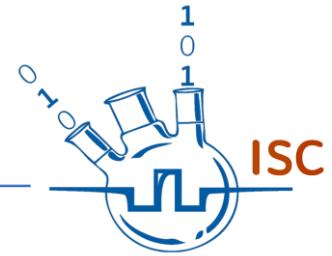
Table 1. Molsoft protein stability prediction

Protein	Chain	Residue	Wild-type	Mutant	ΔE_{mol}
Wt	A	66	Phe	Leu	1.33
Wt	A	92	Glu	Lys	0.18





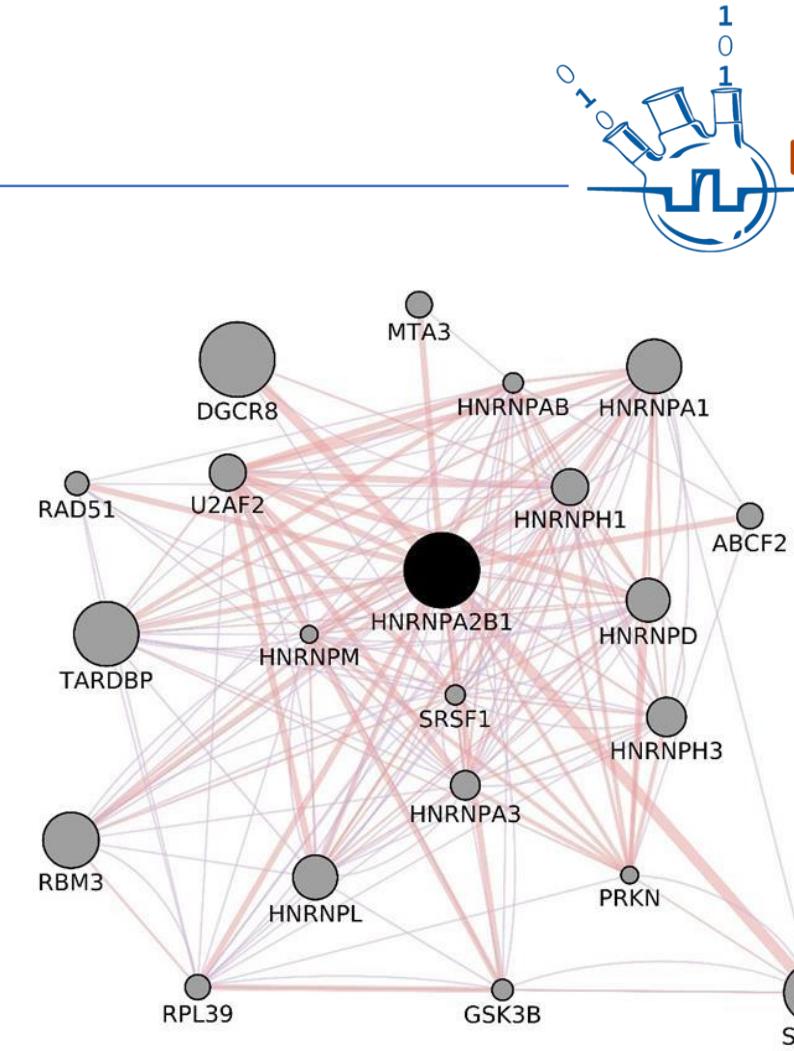
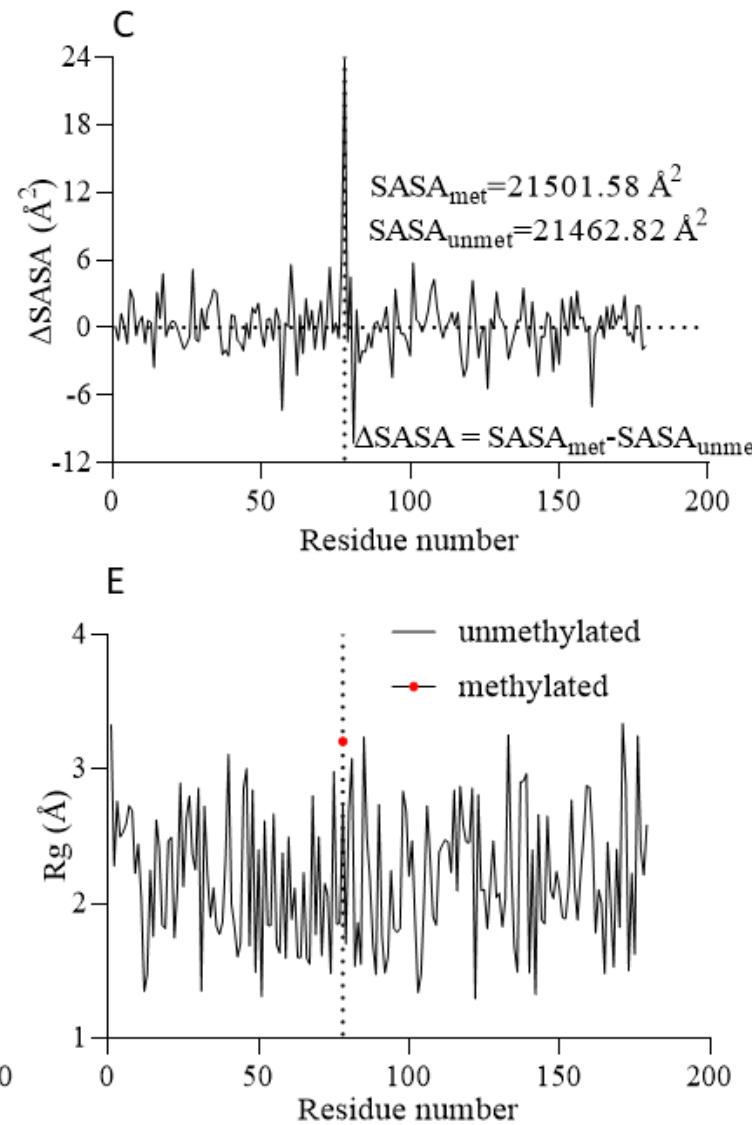
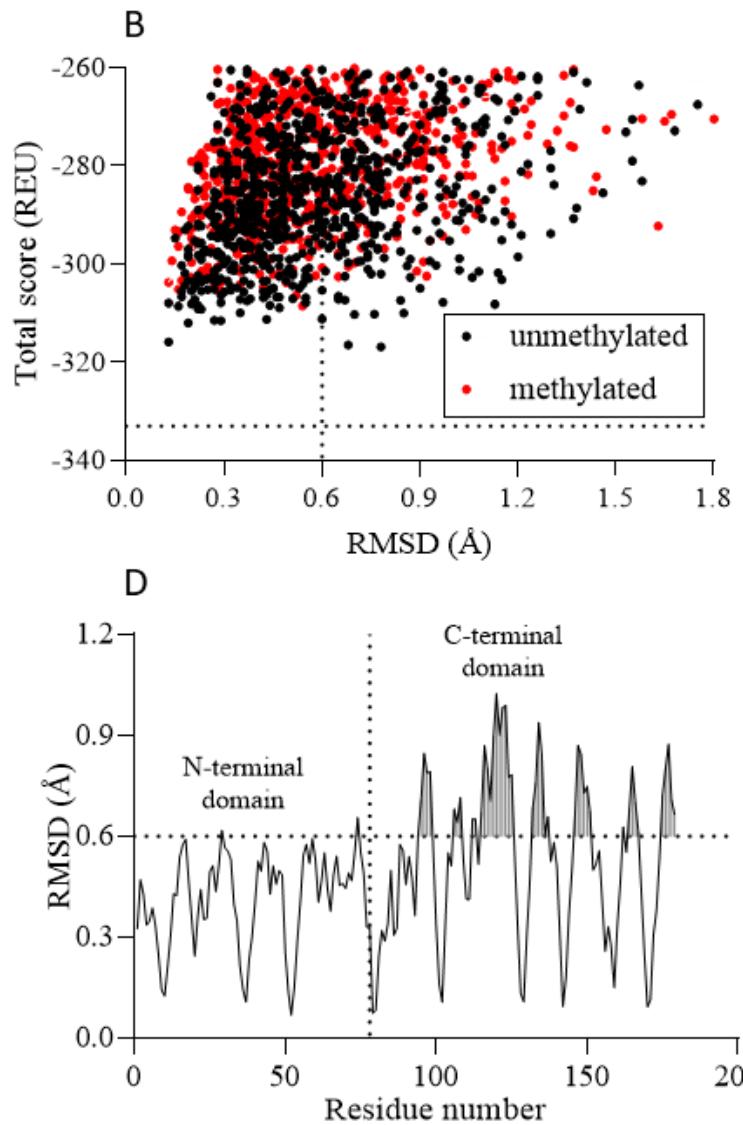
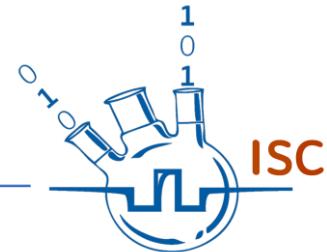
SNP in hnRNP A2/B1



ITSMOre than a
UNIVERSITY



SNP in hnRNPA2/B1





SNP in hnRNPA2/B1

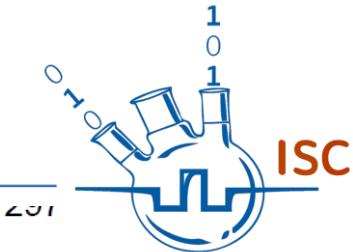


Table 2. Predicted posttranslational modifications and pathogenicity of the wild-type and substitution mutants of hnRNPA2/B1

Position	PTM scores	SNP type	MutPred2 score	SNP effect	PTMs
F66 (wt)	-	-	-	-	-
E92 (wt)	-	-	-	-	-
F66L	-	NS	0.877	Pathogenic	-
E92K	0.677	NS	0.779	Pathogenic	Methylation

NS, non-synonymous.

Table 3. Dihedral angle analysis of substitution
mutant E92K_{met} and E92K_{unmet}

Angle	Unmethylated	Methylated
φ	-131.98°	-131.95° ³⁰⁰
ψ	87.08°	161.87° ³⁰¹
ω	-176.31	87.13° ³⁰²
X1	-175.51	-175.51
X2	177.99	177.98° ³⁰³
X3	178.49	178.49° ³⁰⁴
X4	-177.33	-177.33° ³⁰⁵



SNP in hnRNPA2/B1

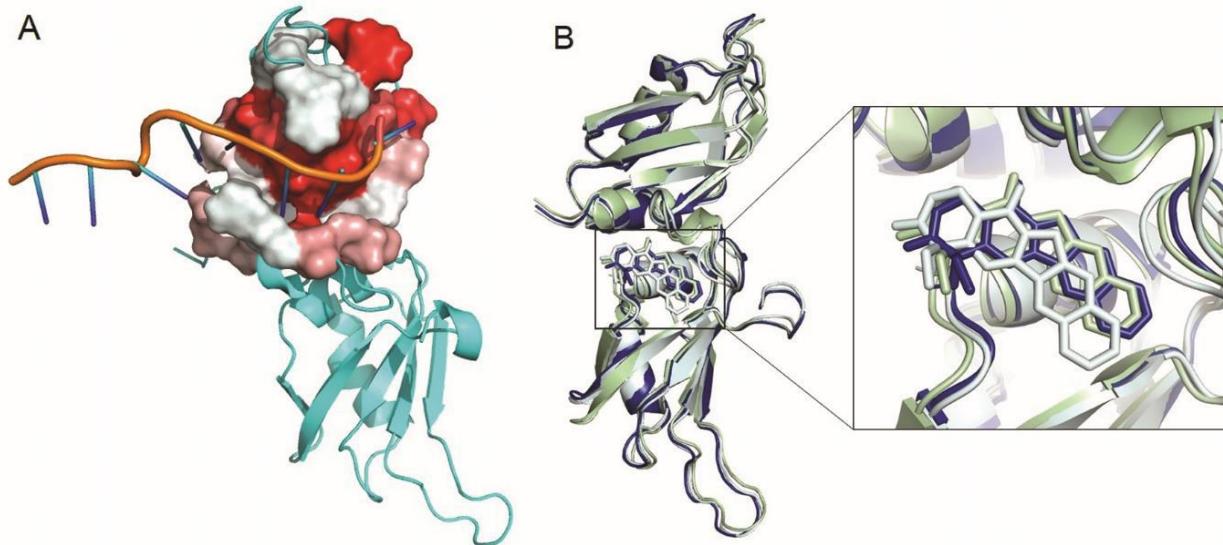
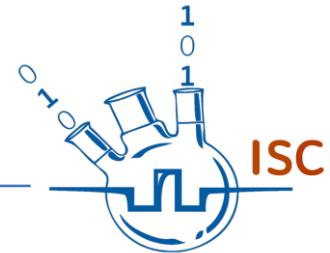
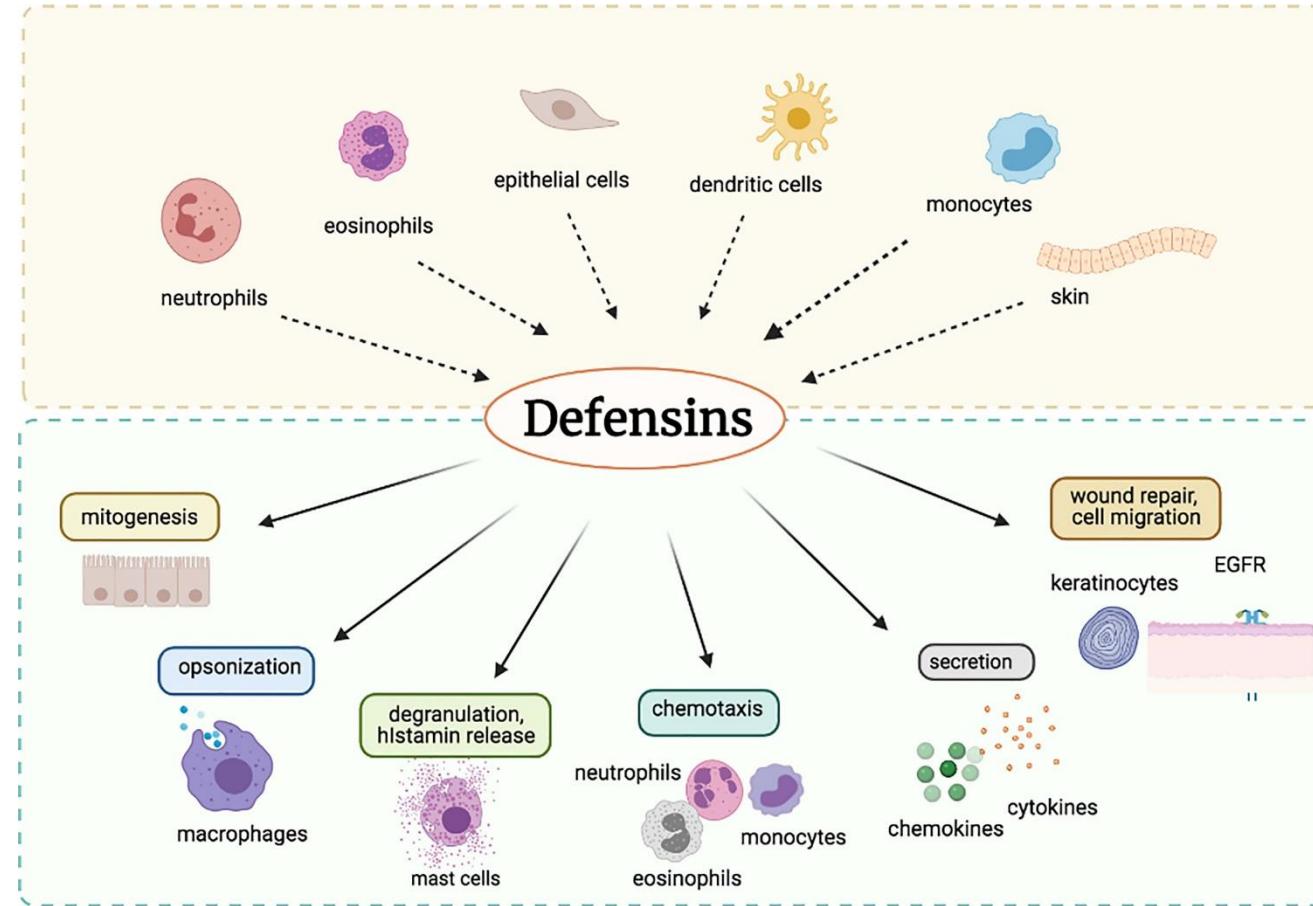
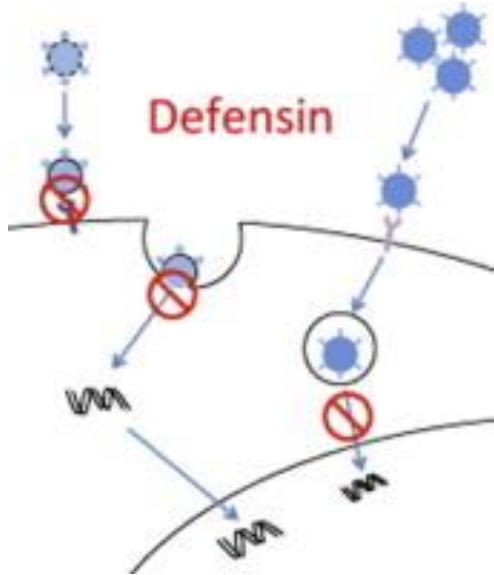
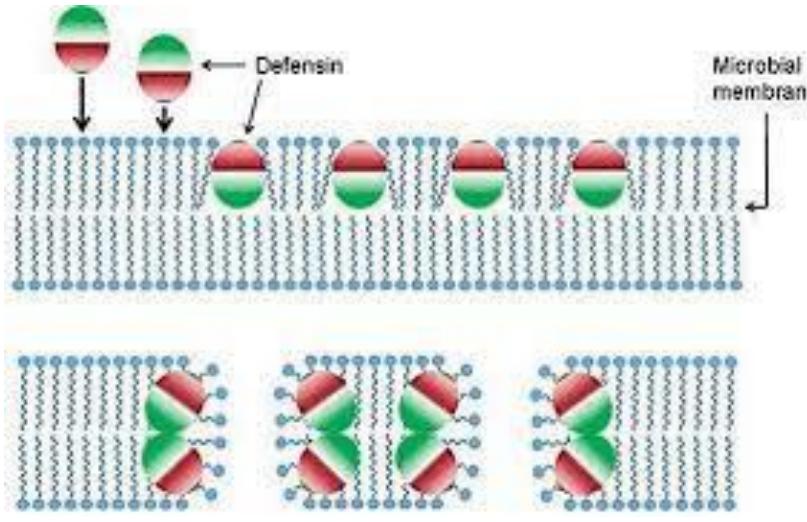


Table 4. Summary of molecular docking and structure-truncated MM/PB(GB)SA rescoring

Proteins	Total energy (kcal/mol)			
	FoldX protein-RNA docking	Protein-CPT docking	fastDRH*	
			GB	PB
Wt	-18.52	-9.55	-30.83 ± 4.54	-14.21 ± 11.50
F66L	-16.40	-9.41	-30.72 ± 3.77	-15.23 ± 12.17
E92K	-15.42	-8.23	-27.13 ± 4.35	-11.07 ± 11.18

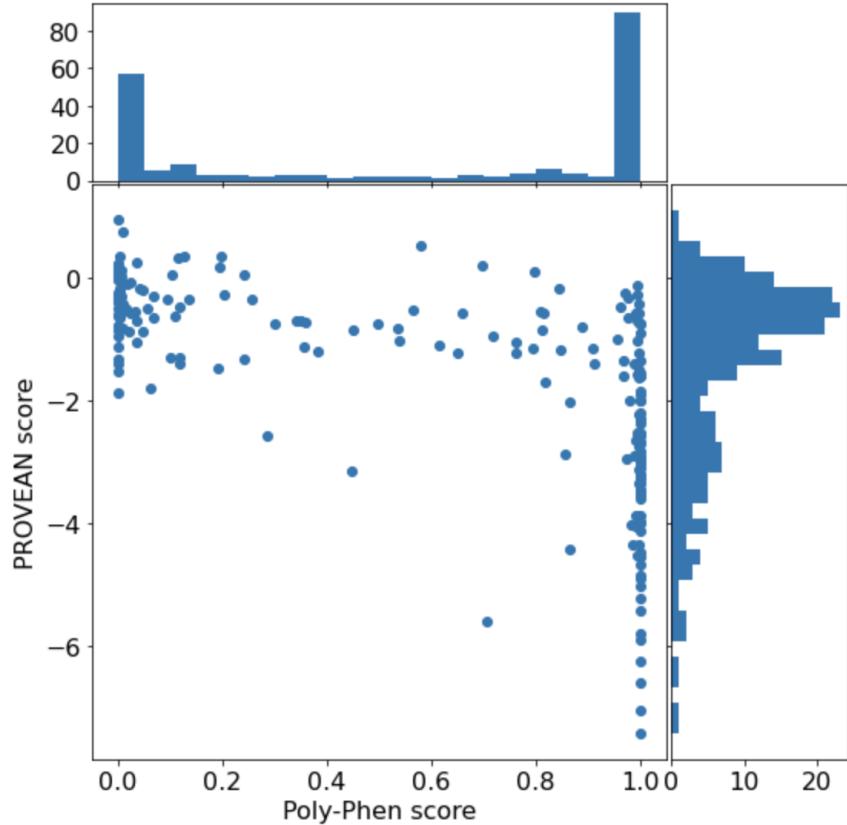
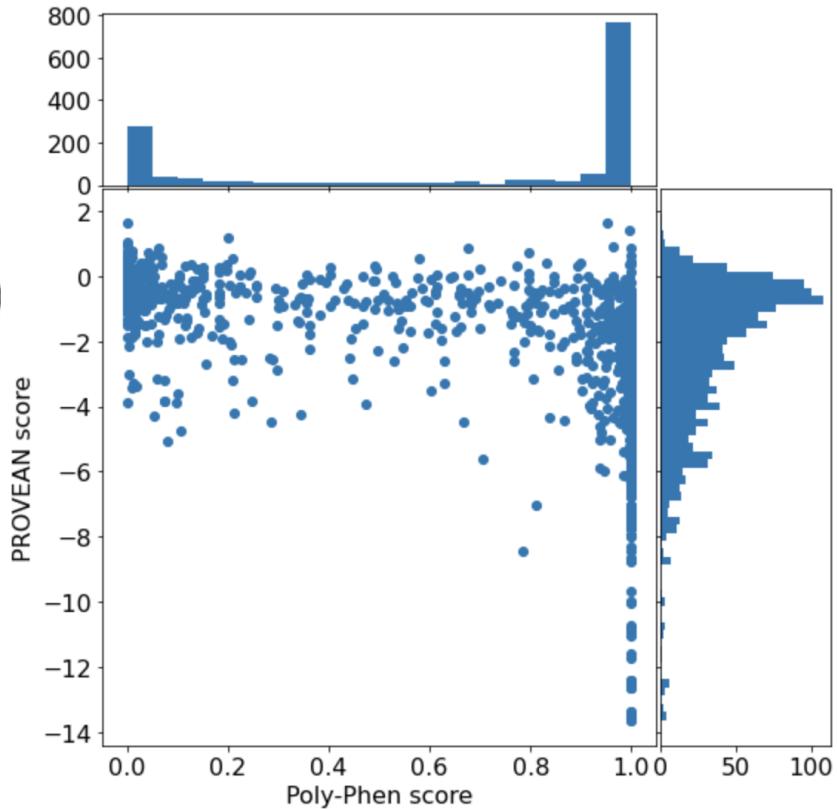
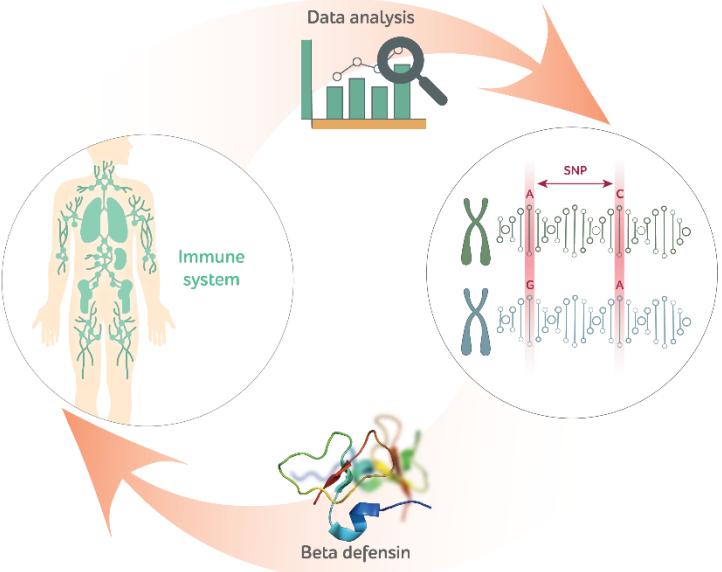
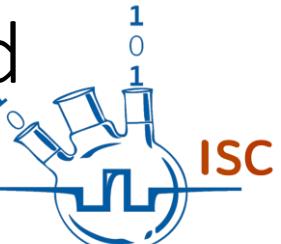


nsSNPs in DEFB1 gene reveal impact on protein-ligand binding sites



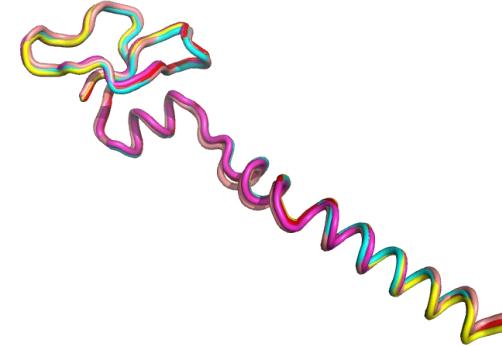
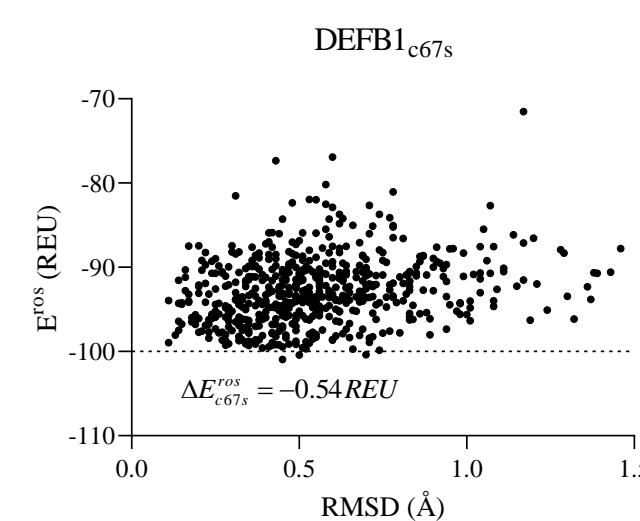
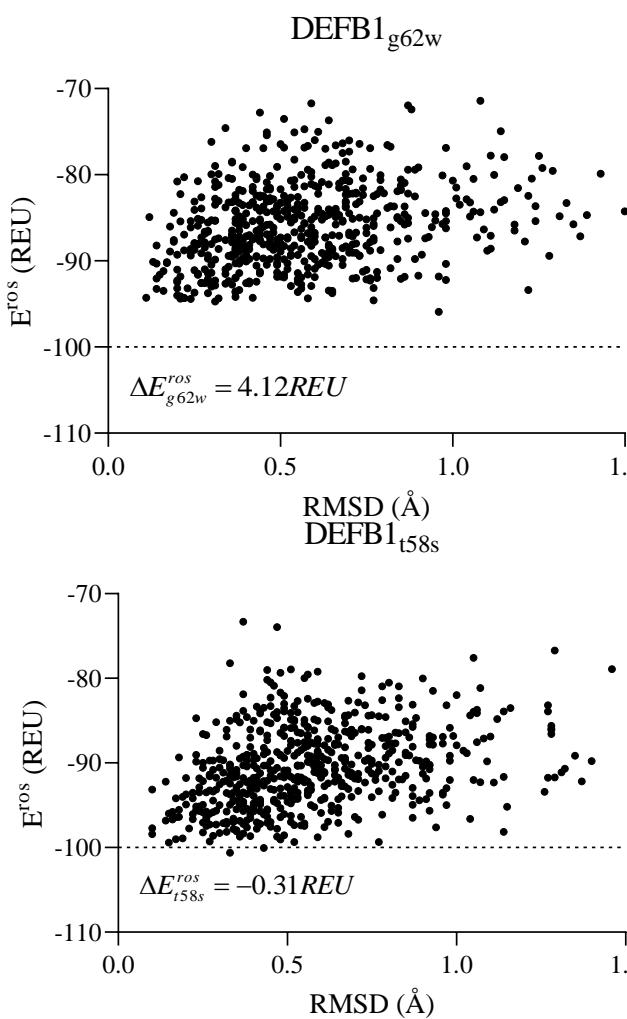
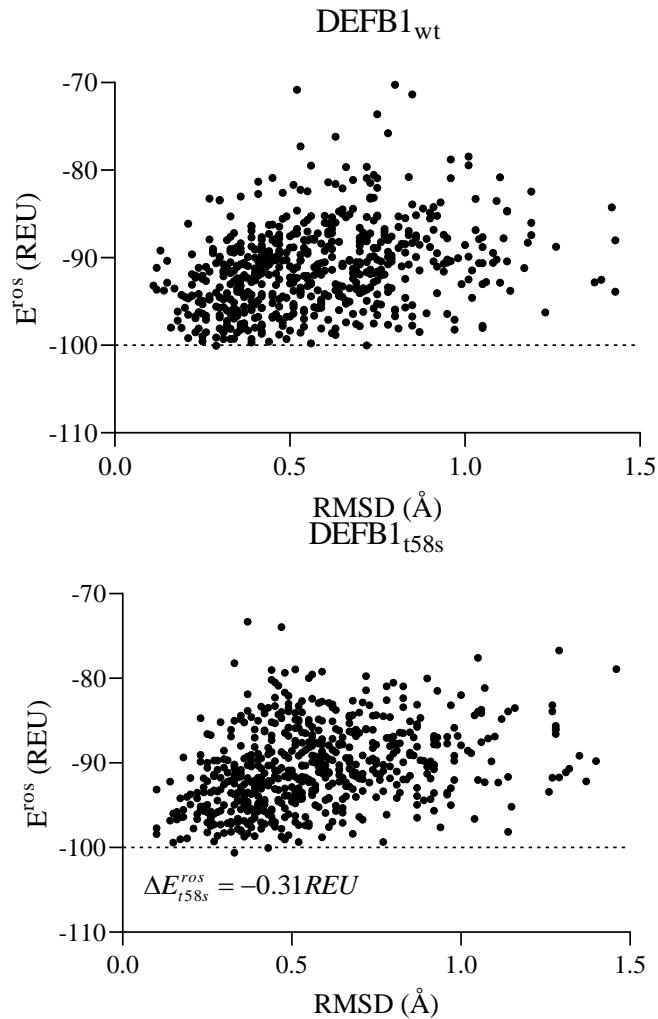


nsSNPs in DEFB1 gene reveal impact on protein-ligand binding sites



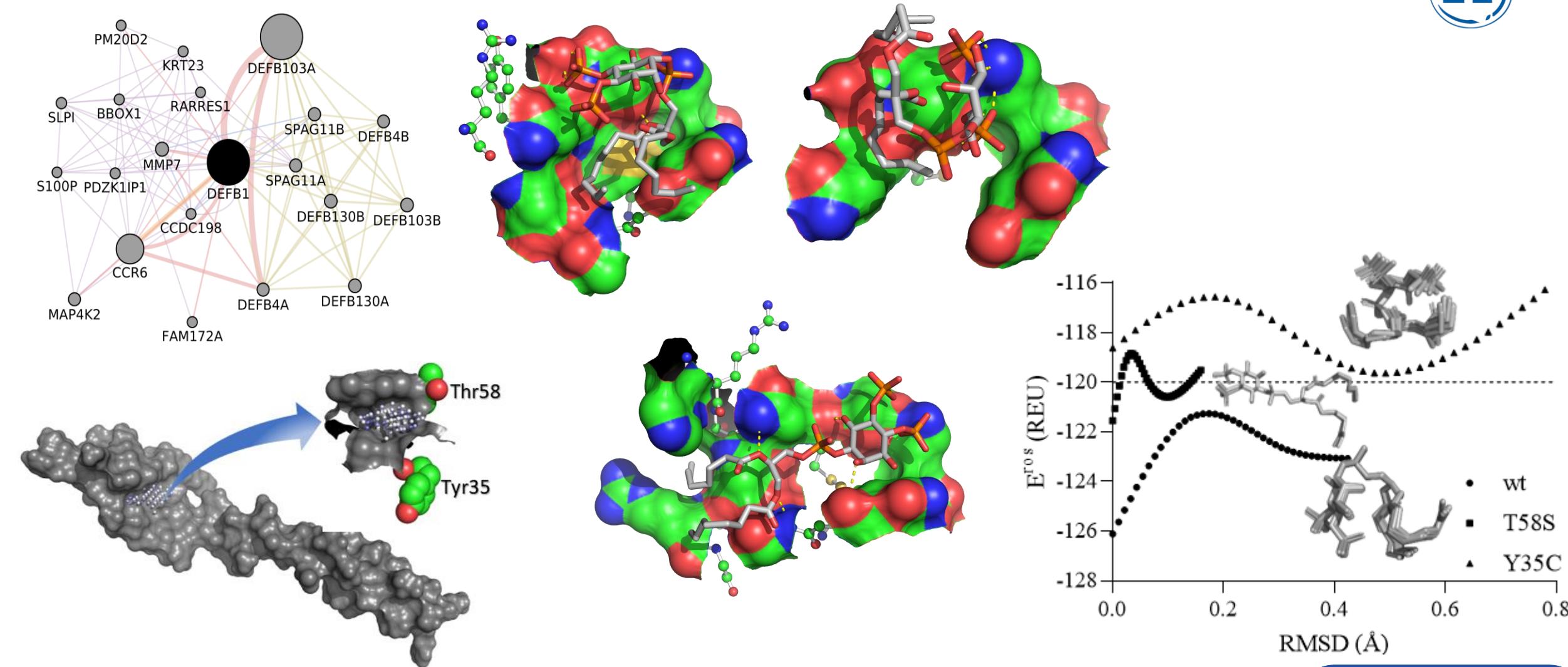
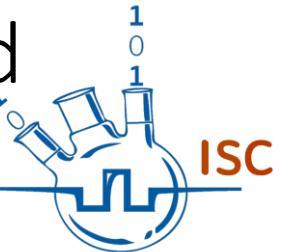


nsSNPs in DEFB1 gene reveal impact on protein-ligand binding sites



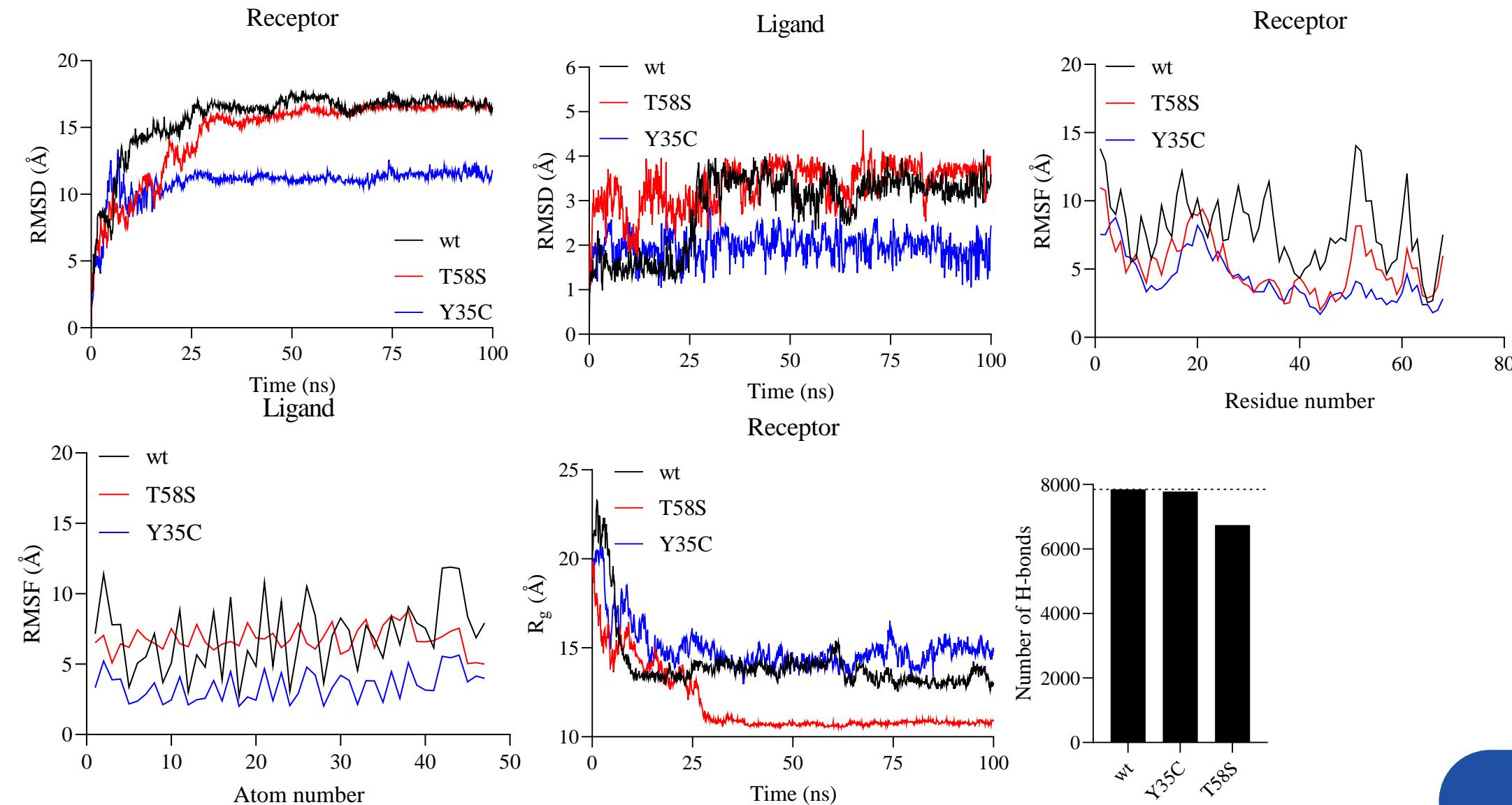


nsSNPs in DEFB1 gene reveal impact on protein-ligand binding sites



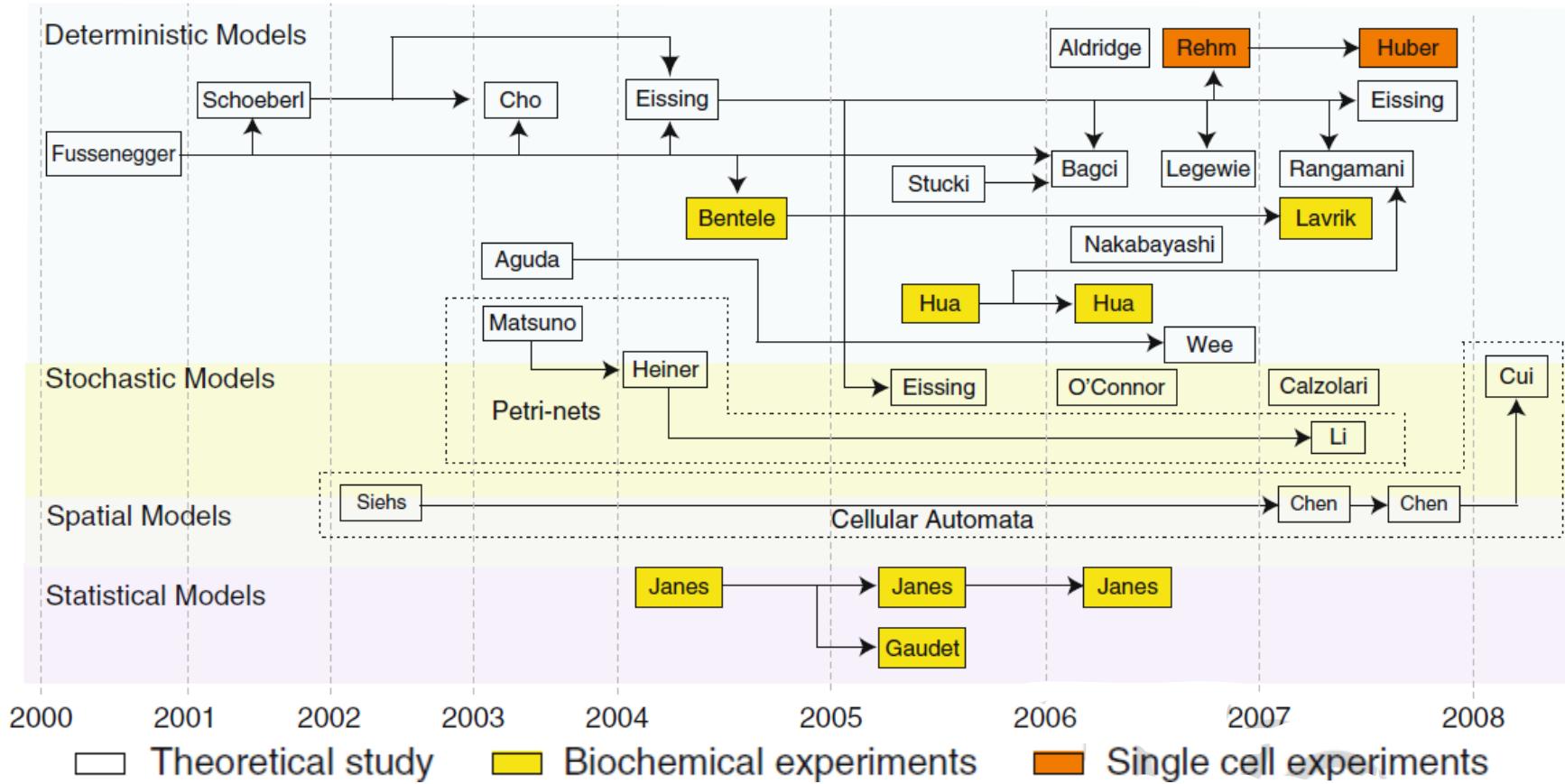
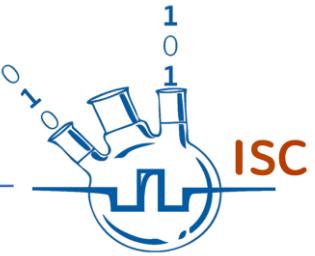


nsSNPs in DEFB1 gene reveal impact on protein-ligand binding sites



Cell death modelling



(From Huber, Bullinger and Rehm, Systems Biology Approaches to the Study of Apoptosis 2009)

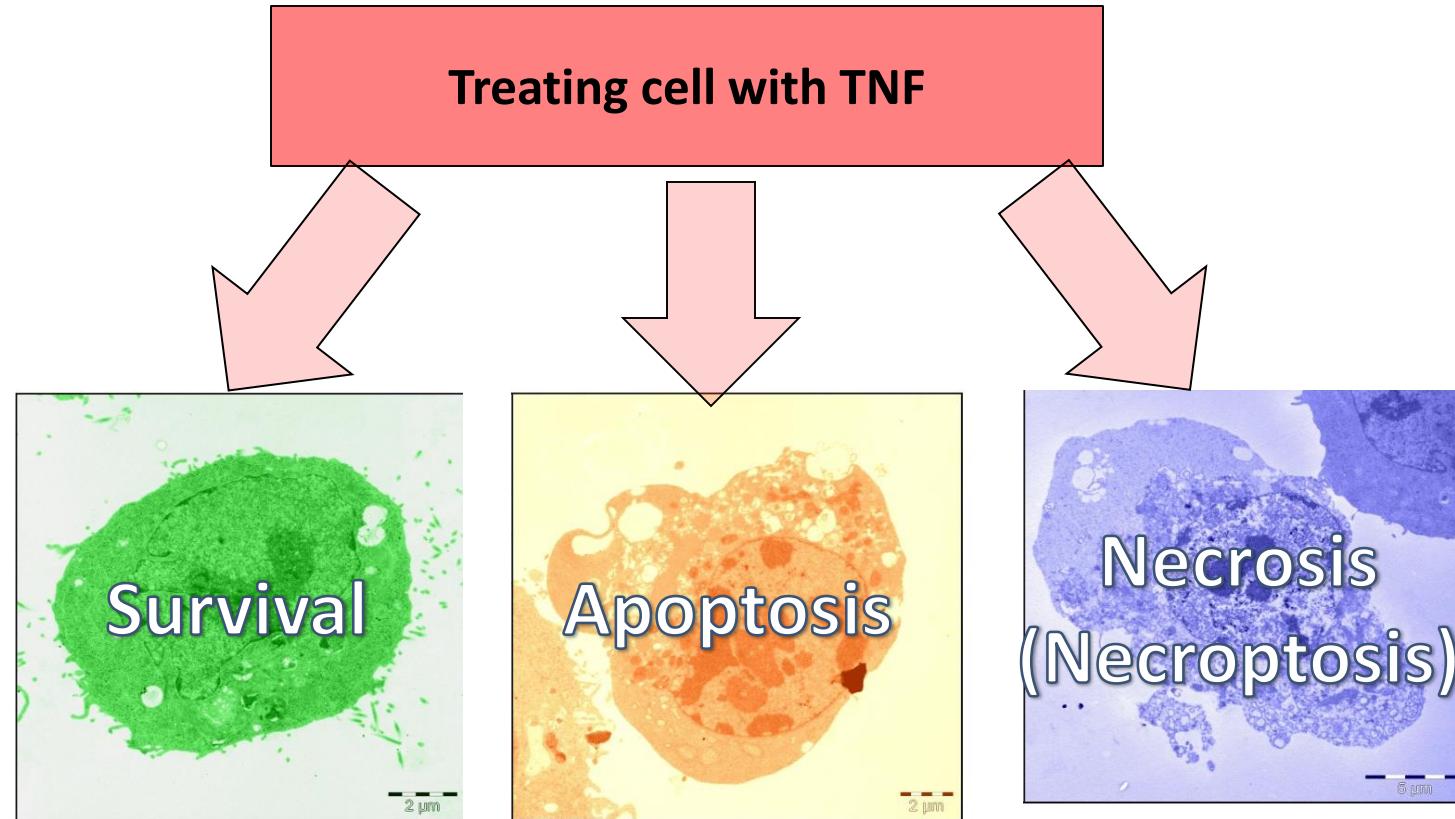
Cell Death Modalities

(From Galuzzi et al, Cell Death and Diff, 2007)





Apoptosis vs. Necrosis vs. Survival



OPEN ACCESS Freely available online

PLOS COMPUTATIONAL BIOLOGY

Mathematical Modelling of Cell-Fate Decision in Response to Death Receptor Engagement

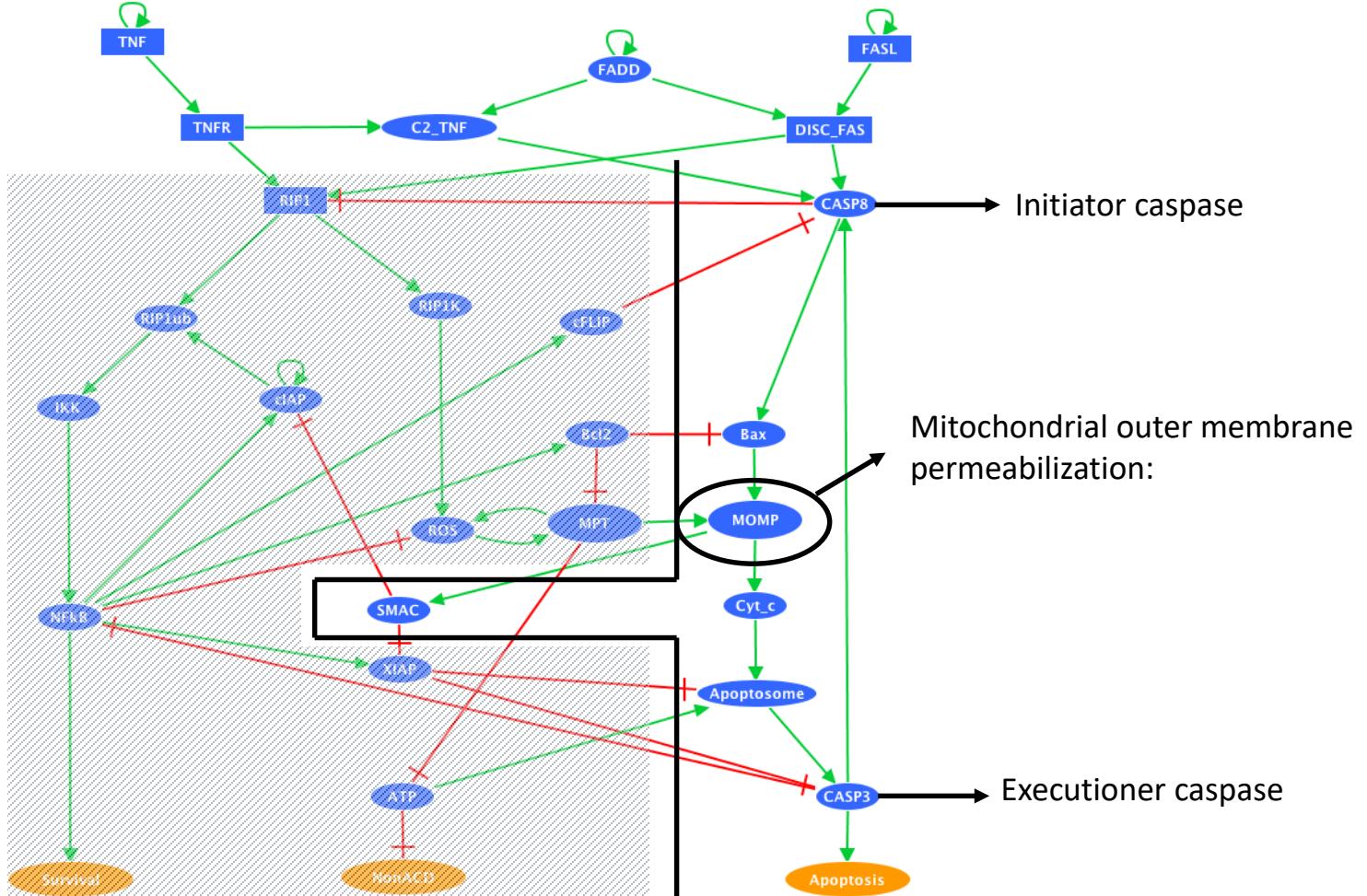
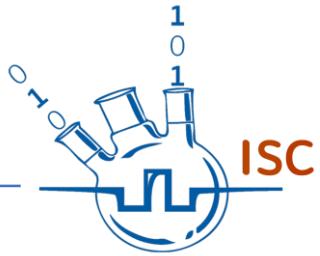
Laurence Calzone^{1,2,3*}, Laurent Tournier^{1,2,3}, Simon Fourquet^{1,2,3}, Denis Thieffry^{4,5}, Boris Zhivotovsky⁶, Emmanuel Barillot^{1,2,3†}, Andrei Zinov'yev^{1,2,3‡}

¹ Institut Curie, Paris, France, ² Ecole des Mines ParisTech, Paris, France, ³ INSERM U900, Paris, France, ⁴ TAGC – INSERM U928 & Université de la Méditerranée, Marseille, France, ⁵ CONTRAINTES Project, INRIA Paris-Rocquencourt, France, ⁶ Karolinska Institutet, Stockholm, Sweden

EMOre than a
NIVERSITY

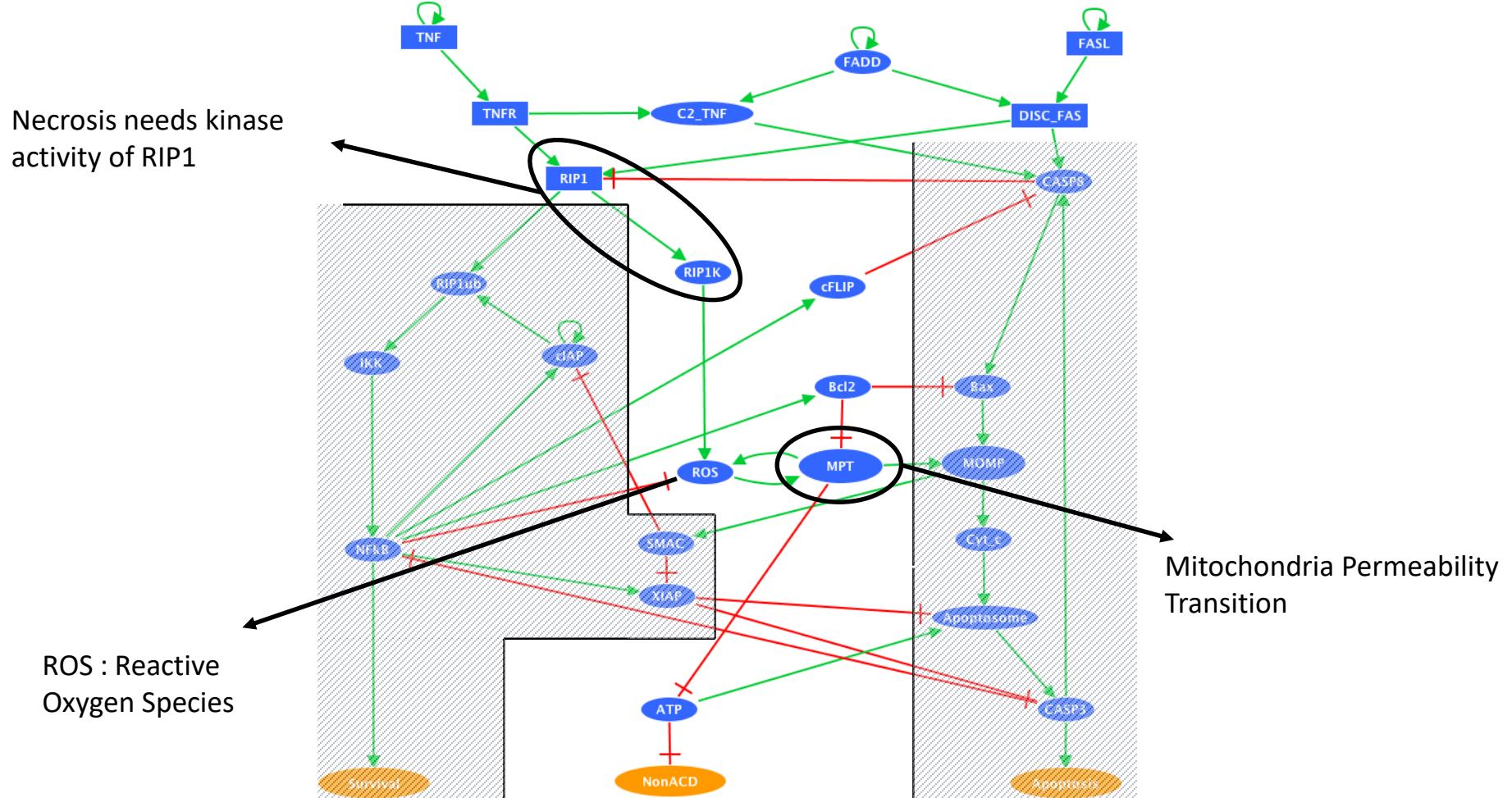
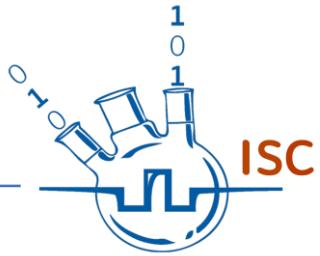


Apoptosis



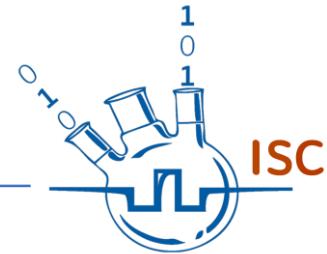


Necrosis





Boolean modeling



Назначить булеву функцію на узел

Example of CASP8

CASP8 = 0 when

DISC-Fas=0 and DISC-TNF=0 and CASP3=0

(equivalent to no external signals from death receptors
and no intracellular problems)

cFLIP=1

(equivalent to inhibition by the NFkB pathway)

CASP8 = 1 when

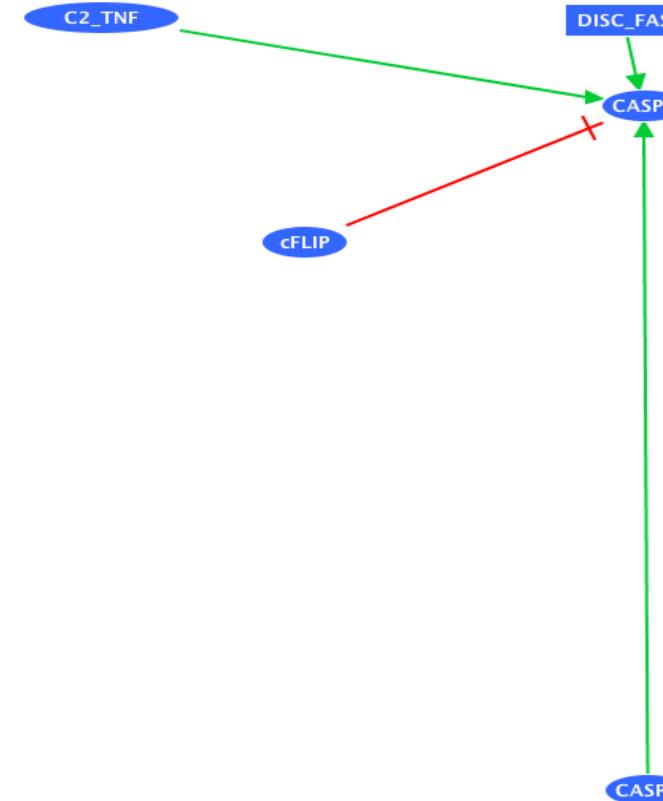
DISC-Fas=1 or/and DISC-TNF=1

(equivalent to signal from death receptors)

CASP3=1

(amplification signal, feedback activation)

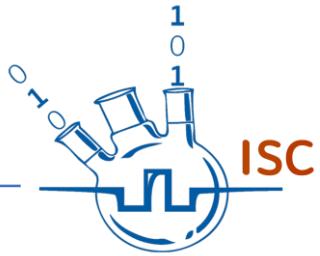
AND no cFLIP



One node = one species

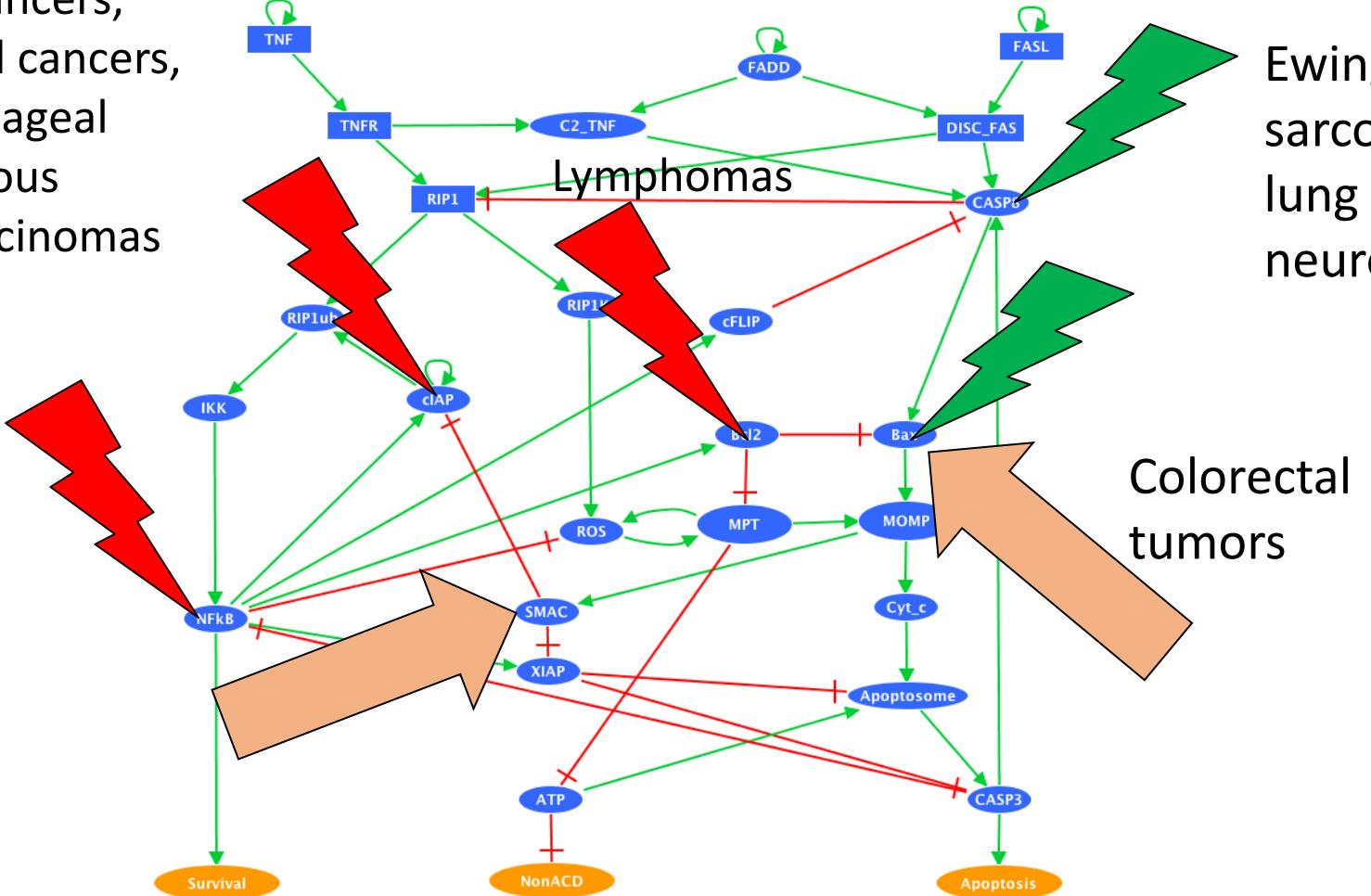


Target molecules in various tumors



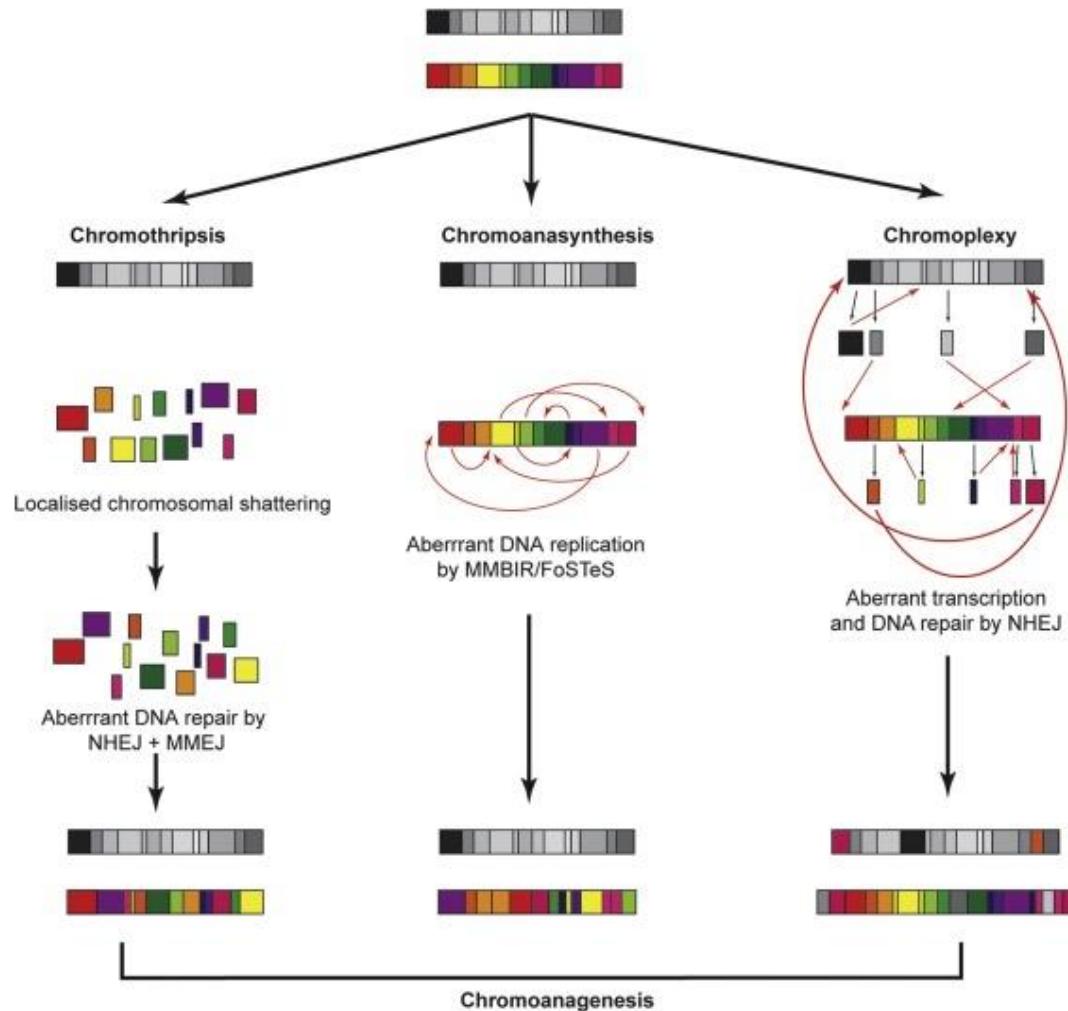
Lung cancers,
cervical cancers,
oesophageal
squamous
cell carcinomas

Lymphomas,
breast cancer





Genome chaos



Stress pathway

Cytokine deprivation
Intracellular damage

Oncogenes

BH3

Bcl-2

Bax

cyt C

Apaf-1

tBid

caspase-9

FADD

caspase-8

caspases 3, 6, 7

Apoptosis

Death receptor pathway

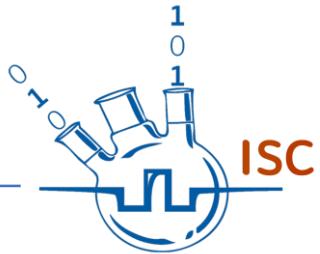
FasL, TNF α , TRAIL

Death receptors

ITSMORE than a
UNIVERSITY



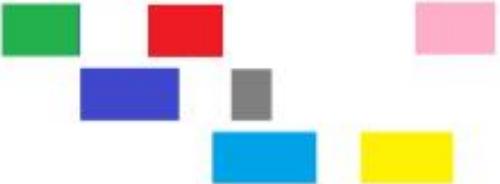
Genome chaos



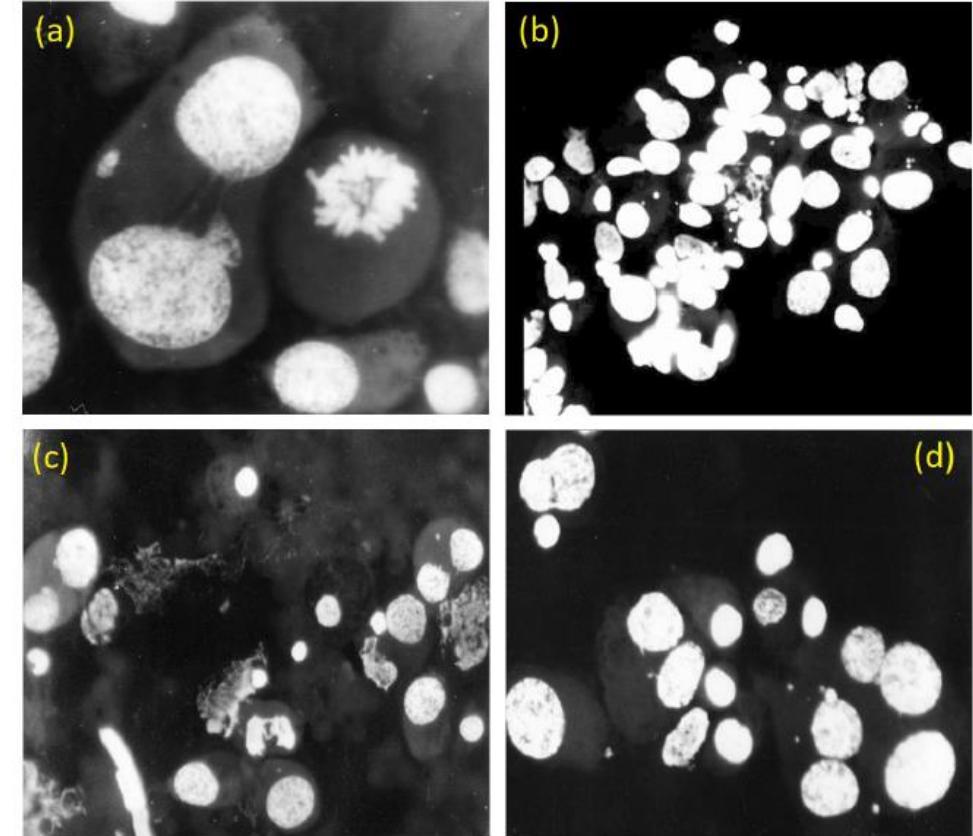
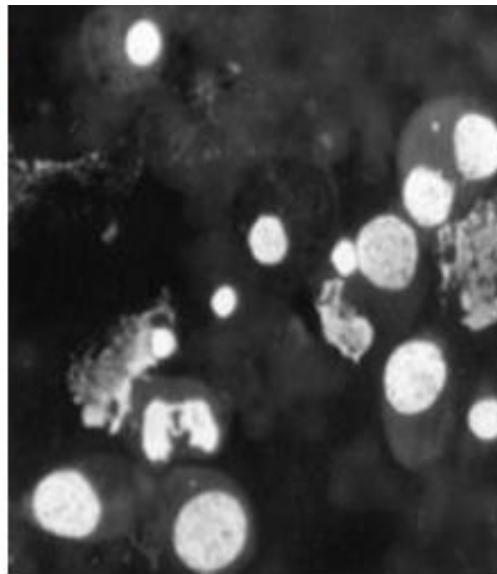
Normal chromosome



Chromothripsis

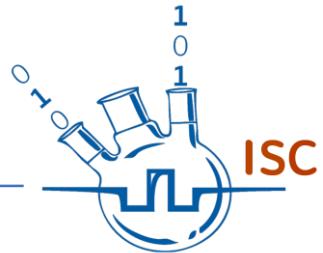


Altered chromosome





Genome chaos algorithm



```
gene_sequence = list("ATGGCGCACGCTGGGAGAACAGGGTACGATAA  
# Calculate the number of nucleotides  
num_nucleotides = len(gene_sequence)  
  
print("Number of Nucleotides:", num_nucleotides)  
  
import random  
  
# Mutation rate  
mutation_rate = 1.0e-4  
  
# Number of cell divisions  
num_divisions = 60  
  
# Initialize the gene sequence (as a list of characters, for example)  
gene_sequence = list("ATGGCGCACGCTGGGAGAACAGGGTACGATAACCAGGAGATAGTGATGAAGTACA  
  
# Function to apply mutations  
def apply_mutation(gene_sequence, mutation_rate):  
    mutated_sequence = []  
    for base in gene_sequence:  
        if random.random() < mutation_rate:  
            # Mutate the base (for simplicity, just change to a random base)  
            mutated_base = random.choice("ATCG")  
            mutated_sequence.append(mutated_base)  
        else:  
            mutated_sequence.append(base)  
    return mutated_sequence  
  
# Simulate cell divisions and mutations  
for _ in range(num_divisions):  
    gene_sequence = apply_mutation(gene_sequence, mutation_rate)  
  
# Print the mutated gene sequence  
mutated_gene = ''.join(gene_sequence)  
print("Mutated Gene Sequence:", mutated_gene)
```

```
# Genetic code dictionary  
genetic_code = {  
    "TTT": "F", "TTC": "F", "TTA": "L", "TTG": "L",  
    "CTT": "L", "CTC": "L", "CTA": "L", "CTG": "L",  
    "ATT": "I", "ATC": "I", "ATA": "I", "ATG": "M",  
    "GTT": "V", "GTC": "V", "GTA": "V", "GTG": "V",  
    "TCT": "S", "TCC": "S", "TCA": "S", "TCG": "S",  
    "CCT": "P", "CCC": "P", "CCA": "P", "CCG": "P",  
    "ACT": "T", "ACC": "T", "ACA": "T", "ACG": "T",  
    "GCT": "A", "GCC": "A", "GCA": "A", "GCG": "A",  
    "TAT": "Y", "TAC": "Y", "TAA": "*", "TAG": "*"  
    "CAT": "H", "CAC": "H", "CAA": "Q", "CAG": "Q",  
    "AAT": "N", "AAC": "N", "AAA": "K", "AAG": "K",  
    "GAT": "D", "GAC": "D", "GAA": "E", "GAG": "E",  
    "TGT": "C", "TGC": "C", "TGA": "*", "TGG": "W",  
    "CGT": "R", "CGC": "R", "CGA": "R", "CGG": "R",  
    "AGT": "S", "AGC": "S", "AGA": "R", "AGG": "R",  
    "GGT": "G", "GGC": "G", "GGA": "G", "GGG": "G",  
}  
  
# Function to translate a DNA sequence to a protein sequence  
def translate_dna_to_protein(dna_sequence):  
    protein_sequence = []  
    for i in range(0, len(dna_sequence), 3):  
        codon = dna_sequence[i:i + 3]  
        amino_acid = genetic_code.get(codon, 'X') # 'X' for unknown codons  
        protein_sequence.append(amino_acid)  
    return ''.join(protein_sequence)  
  
# Translate the reference and mutated sequences  
translated_reference_sequence = translate_dna_to_protein(reference_sequence)  
translated_mutated_sequence = translate_dna_to_protein(mutated_gene)  
  
print("Translated Ref Gene Sequence:", translated_reference_sequence)  
print("Translated Mut Gene Sequence:", translated_mutated_sequence)
```

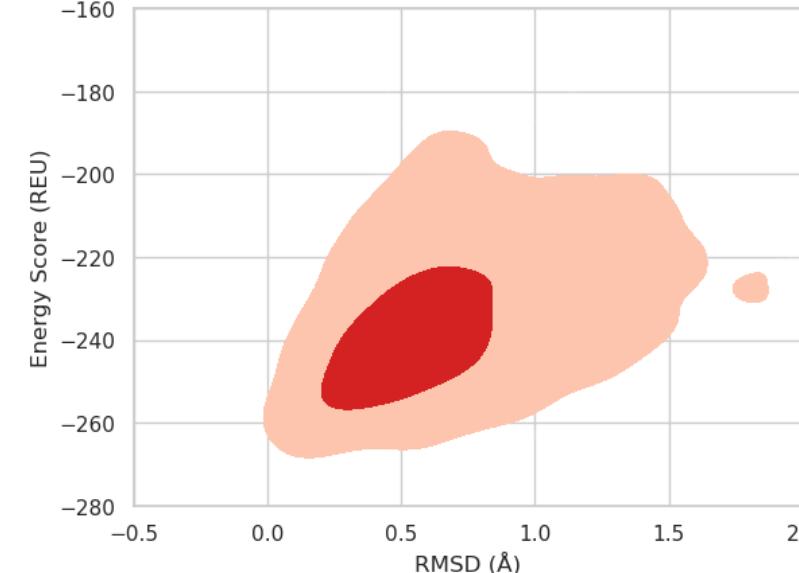
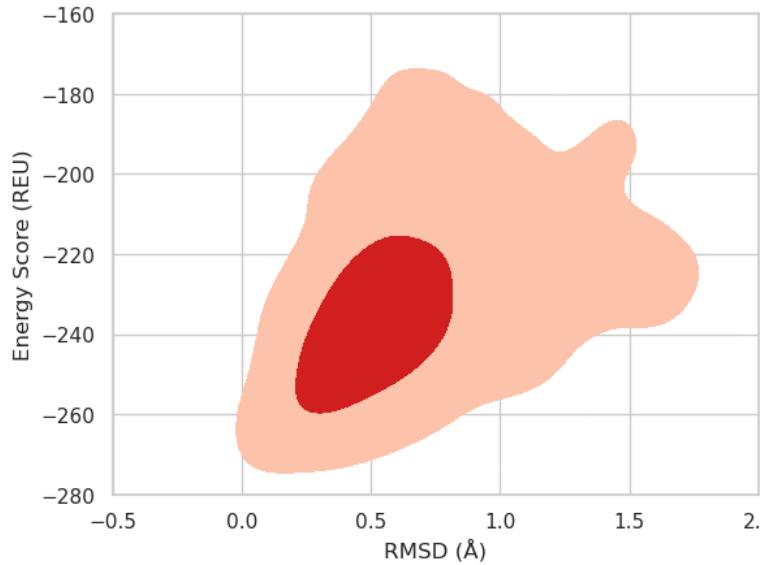
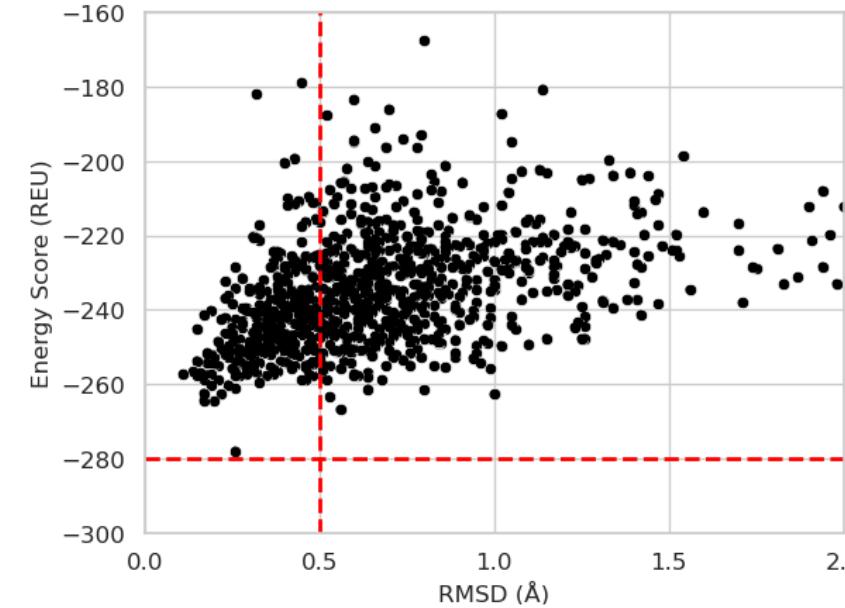
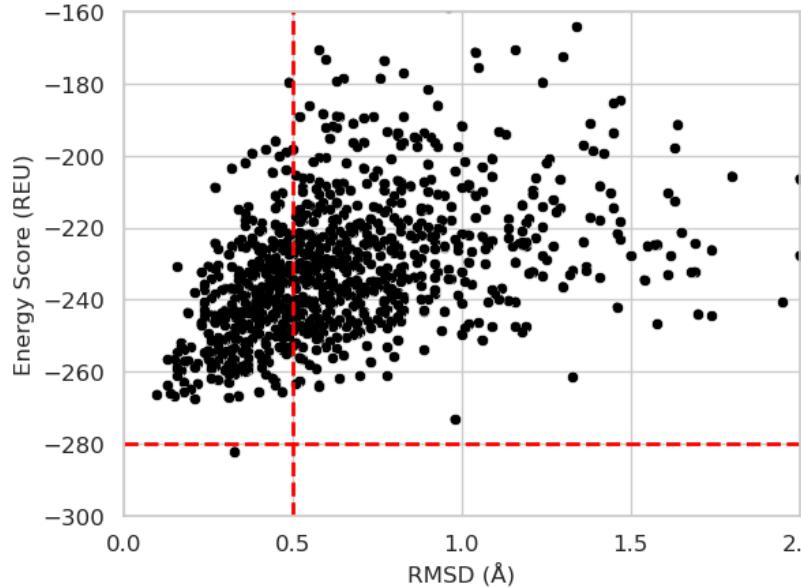
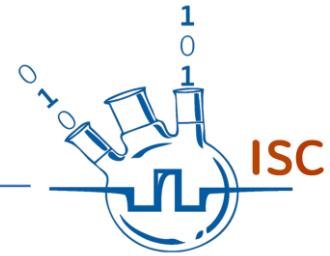
Protein Sequence 1: MAHAGRTGYDNREIVMKYIHYI
LTLRQAGDDFSRRYRRDFAEMSQLHLTPFTARGRFATVVEI
LFDFSWLSLKTLSSLALVGACITLGAYLGHK*

Protein Sequence 2: MAHAWRTGYDNREIVMKYIHYI
LTLRQAGDDFSRRYRRDFAEMSQLHLTPFTARGRFATVVEI
LFDFSWLSLKTLSSLALVGACITLGAYLGHK*

Sequence Identity: 99.58%

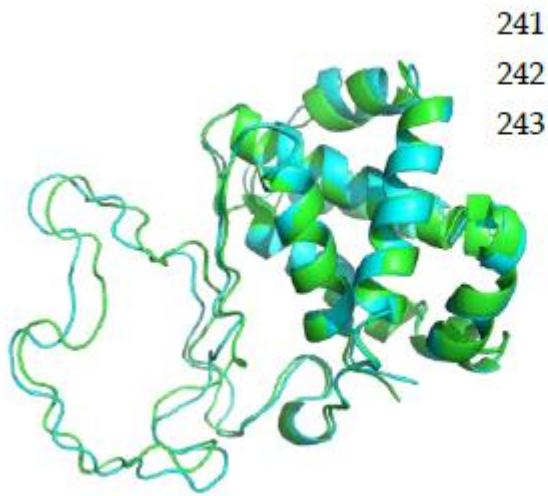
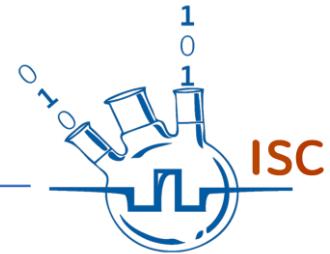


Genome chaos

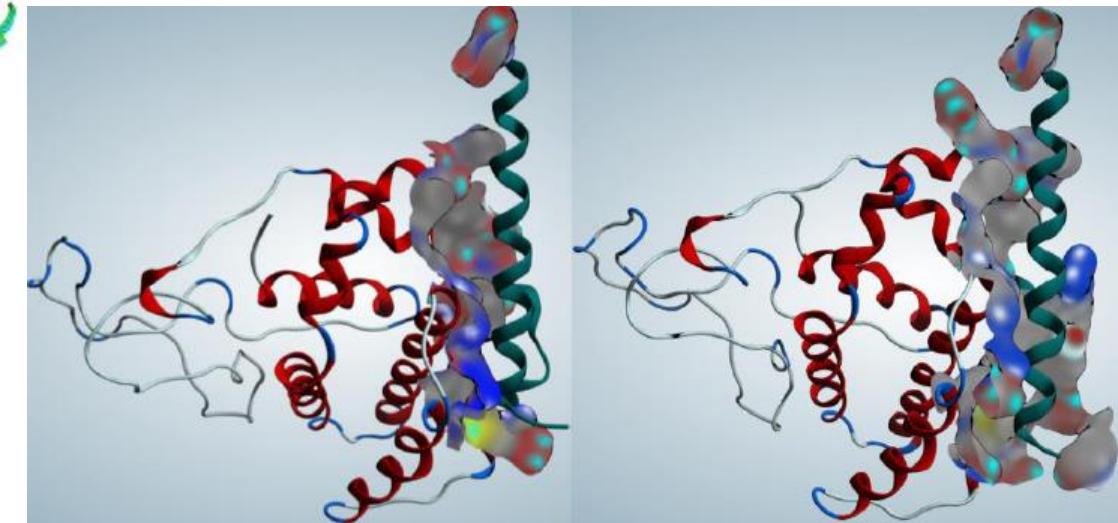
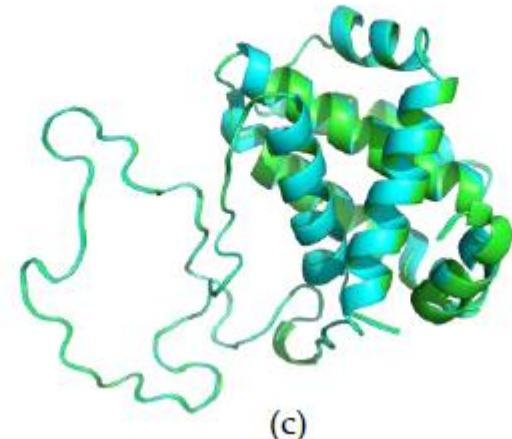
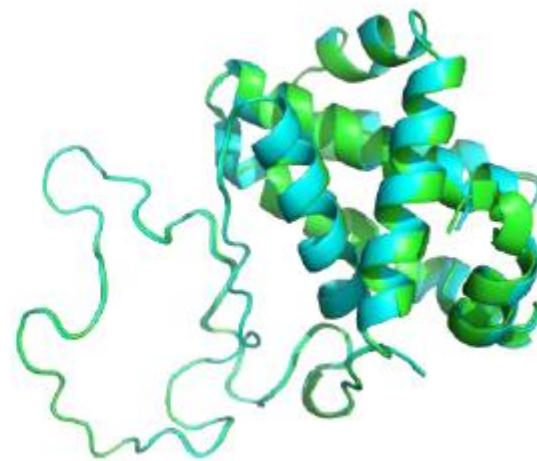




Genome chaos (BCL-2/BH3 interaction)



(a)



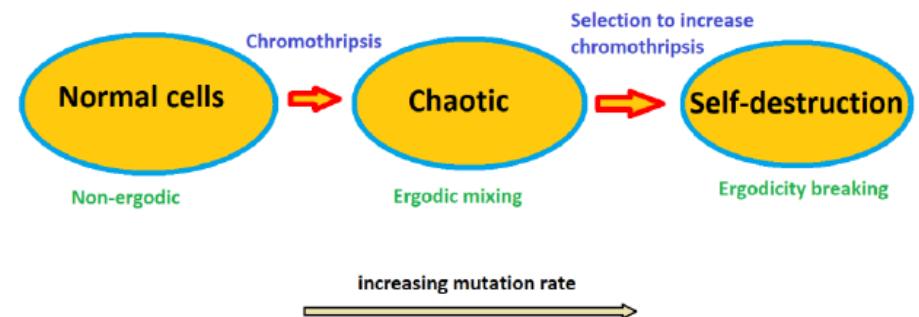
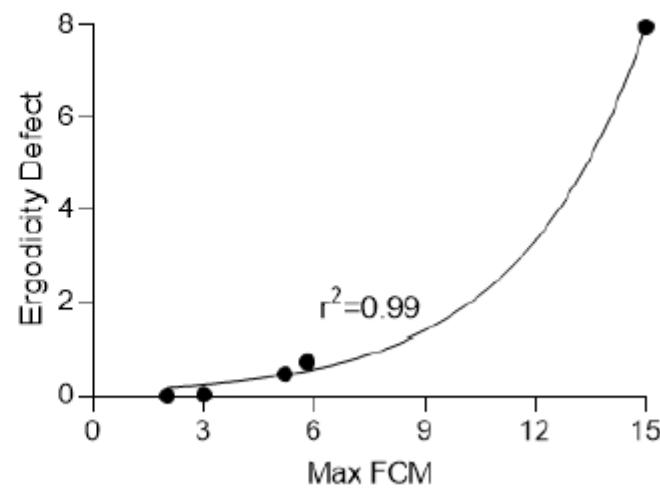
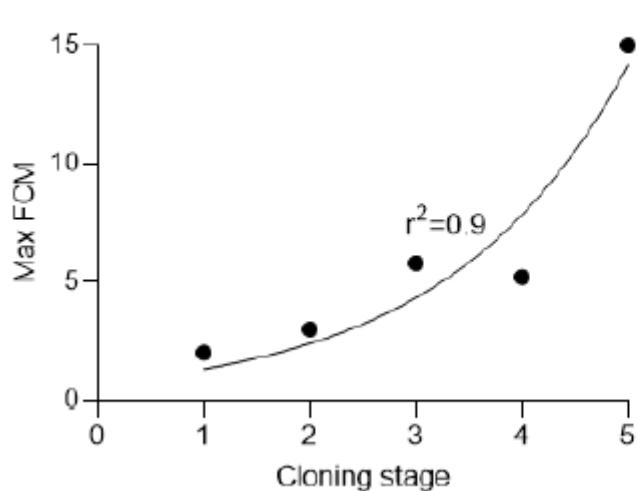


Genome chaos



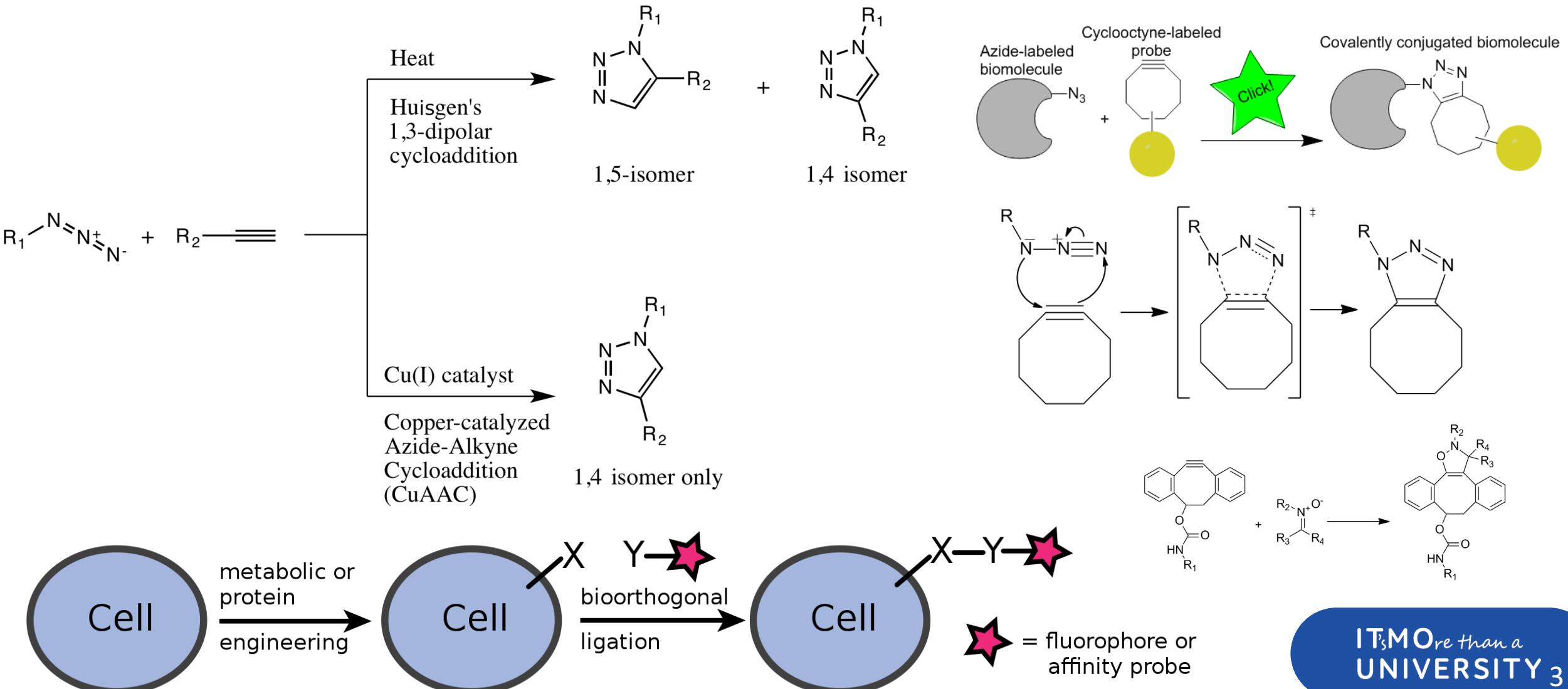
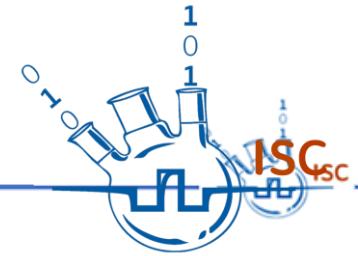
Table 1. Changes of observed minimum, average, and maximum FCM and calculated effective mutation rate and ergodicity defect at different stages of the selection for increasing FCM.

Stage	Clones	Min FCM	Average FCM	Max FCM	Effective mutation rate, $\times 10^{-4}$	Ergodicity defect
0	48	0.0	0.6	2.0	6.99	0
1	50	0.0	0.8	3.0	8.99	0.03
2	52	0.0	1.7	5.8	17.98	0.74
3	48	0.0	1.6	5.2	16.98	0.48
4	47	1.0	4.7	15.0	47.95	7.96





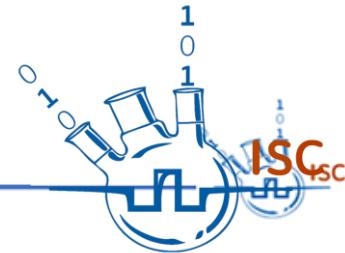
Click reaction and orthogonal chemistry



IT₃MOre than a
UNIVERSITY 3



NuroClick software



Home / Browse / Science & Engineering / Chemistry / AutoClickChem



AutoClickChem

Brought to you by: jdurrant

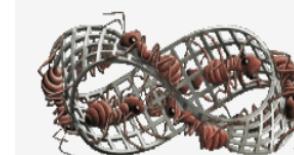
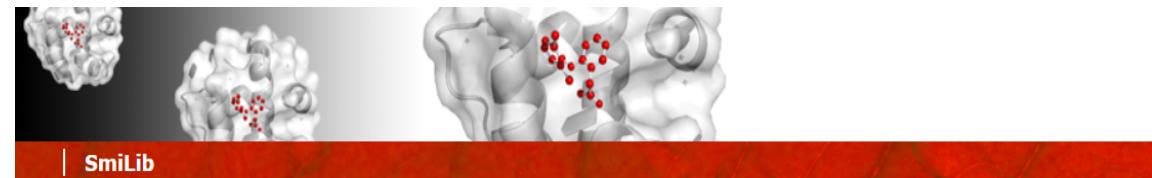
★★★★★ 1 Review

Downloads: 1 This Week

Last Update: 2014-06-03

[Download](#) [Get Updates](#) [Share This](#)

Windows | Mac | Linux



SmiLib v2.0



SmiLib v2.0

SmiLib is a free, platform independent software tool for rapid combinatorial library enumeration in the flexible and portable SMILES notation. SmiLib enumerates combinatorial libraries at rates of approximately 9,000,000 molecules per minute on fast computers.

If you wish to publish results obtained with SmiLib, please cite:

A. Schüller, V. Hähnke, G. Schneider; SmiLib v2.0: A Java-Based Tool for Rapid Combinatorial Library Enumeration, *QSAR & Combinatorial Science* **2007**, 3, 407-410.

Copyright © 2006-2008, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany. All rights reserved. Use is subject to [license terms](#).

Current version: 2.0 rc4. A convenience method to run SmiLib as a Java library from within your own Java projects was added. Please see the [change log](#) for a list of program modifications.

- [Run SmiLib](#)
- [User Manual](#)
- [API Documentation](#)
- [Download](#)
- [Contact](#)

Disclaimer

© 2013 Andreas Schüller |
Webdesign: Michael Meissner
[Webmaster](#)

Run SmiLib

SmiLib is available as a Java Web Start graphical user interface program.

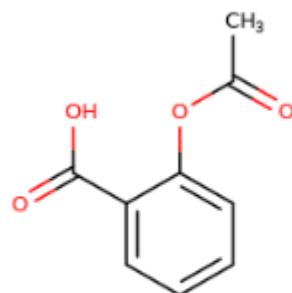
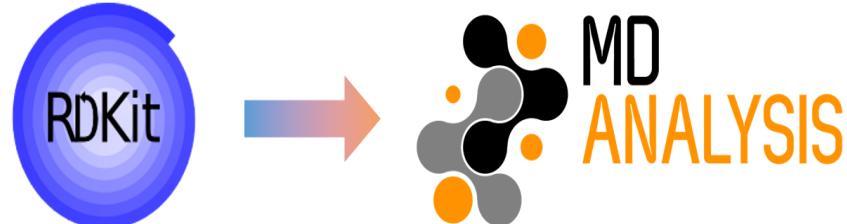
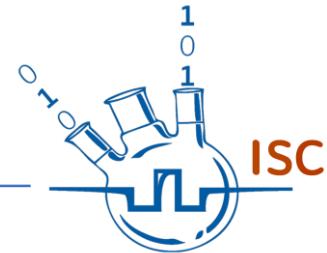
[Click here to start SmiLib](#)

Java Runtime Environment (JRE) is needed to run SmiLib.

IT'sMOre than a
UNIVERSITY 3



NuroClick software

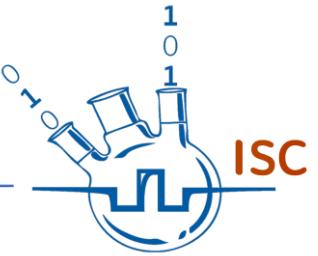


Compound

SMILES notation



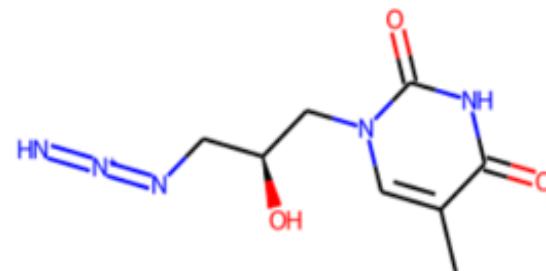
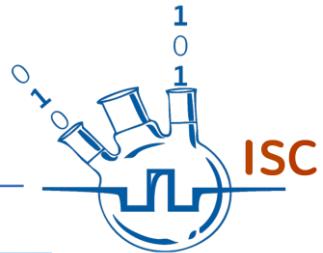
SMILES feature matrix



How it works?

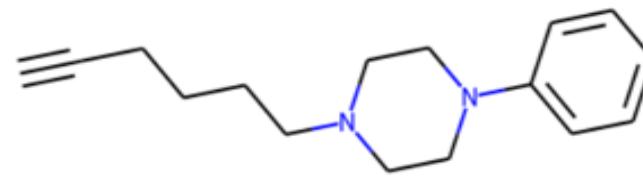


Step 1: reagents upload



C1=CC=C(C=C1)C(=O)N=[N+]=[N-]
C1=CC=C2C(=C1)C(=CN2)C(=O)N=[N+]=[N-]
CC(=O)N[C@H]([C@H]([C@H]([C@H](O)C(=O)N=[N+]=[N-])C(=O)OC
CCOC(=O)C(CCCN=[N+]=[N-])CC=C(C)C

Upload azides

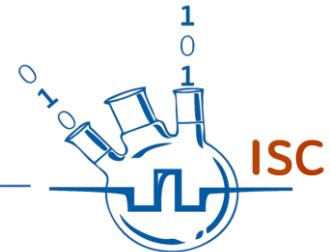


COC(=O)C1=CC=C(C=C1)C#CC2CCNCC2
C#CC(C(=O)NCCOCCOCC(=O)O)N
CC(C)(C)OC(=O)CCOCCC#C
C#CCOC1=CC=C(C=C1)N2C(=O)NNC2=O
C#CCOCCOCCOCCOCCSSCCOCCOCCOCC
#C

Upload alkynes



Step 2: click reaction initiation



100%

Starting library generation...

Irrelevant reagents: [N-]=[N+]=NC(=O)c1ccccc1 and C#CCOCCOCOCOCSSCCOCOCOCOCOC#C

Irrelevant reagents: [N-]=[N+]=NC(=O)c1[nH]c2cccc12 and C#CCOCCOCOCOCOCSSCCOCOCOCOC#C

Irrelevant reagents: COC(=O)[C@H](N=[N+]#[N-])[C@H](NC(C)=O)OC and C#CCOCCOCOCOCSSCCOCOCOCOC#C

Irrelevant reagents: CCOC(=O)C(CC=C(C)C)CCN=[N+]=[N-] and C#CCOCCOCOCOCSSCCOCOCOCOC#C

=====

Finished library generation!

Time: 00:00:02.

32 compounds were generated from 5 alkynes and 4 azides.

12 1,4-isomers and 12 1,5-isomers.

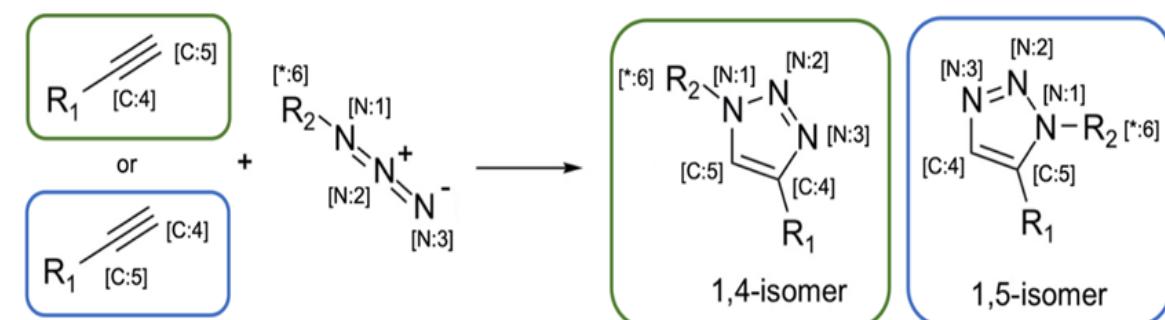
Warning: 8 molecules of 32 were generated from internal alkynes and could not be assigned 1,4/1,5 isometry.

Failed to construct 4 molecules.

[Get reaction products](#)

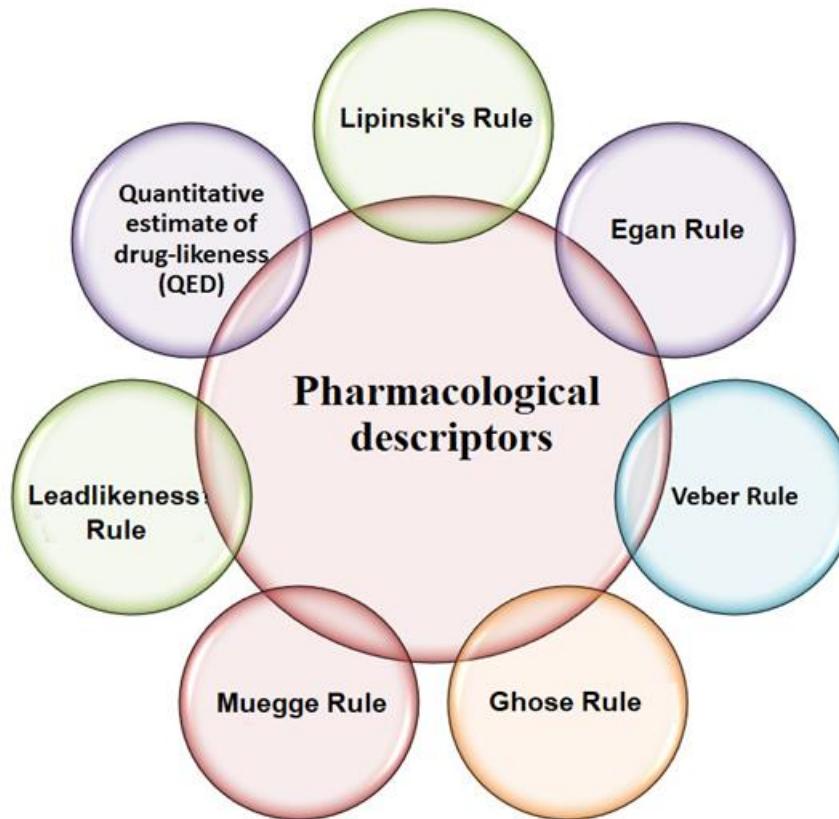
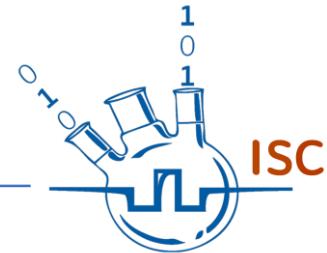
[Back](#)

[Next](#)





Step 3: PK/PD descriptor calculation



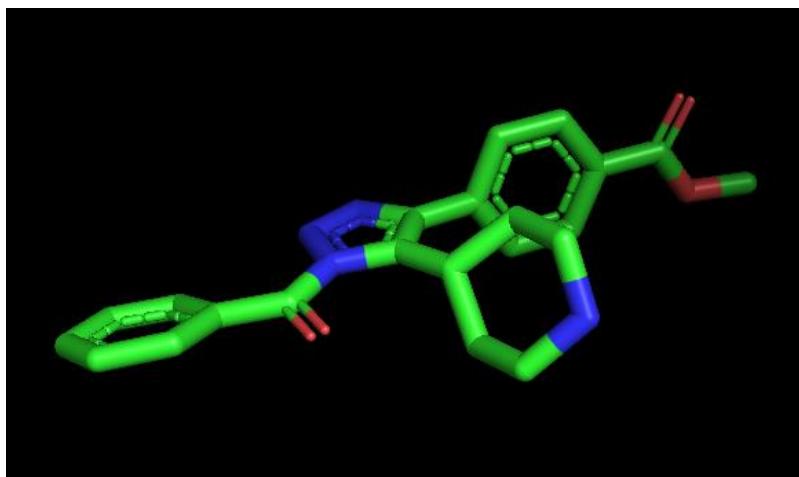
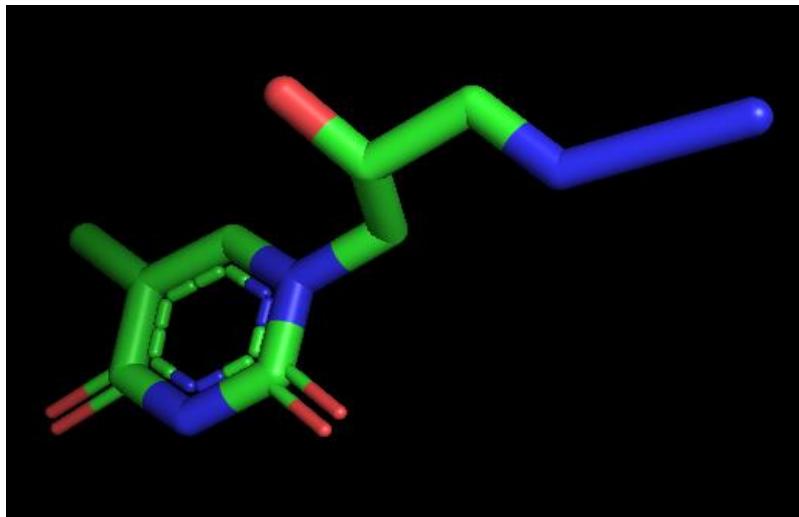
Select physical properties:

- Molecular weight (g/mol) from to
- Heavy atoms from to
- Aromatic heavy atoms from to
- Fraction Csp3 from to
- Rotatable bonds from to
- H-bond acceptors from to
- H-bond donors from to
- Molar refractivity from to
- TPSA from to

Back Next



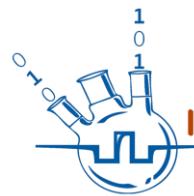
Step 4: save the results



Convert products to other formats:

- cml - Chemical Markup Language
- d2s - Text/Office Document
- dna - DNA Sequence
- fasta - FASTA (Automatic recognition)**
- fasta:dna - FASTA (DNA sequence)
- fasta:peptide - FASTA (peptide sequence)
- fasta:rna - FASTA (RNA sequence)
- gout - Gaussian Output Format
- inchi - InChI
- mol - MDL Molfile
- mol2 - Tripos Mol2

Back Next



Thank you for your attention

