

Step 2: Working with available antigens

AbsolutNoLib (or Absolut)

```
./AbsolutNoLib listAntigens
```

Available antigens are named: PDBID_Chains, ex: 1FBI_X

```
./AbsolutNoLib info_antigens
```

```
./AbsolutNoLib info_antigen 1ADQ_A
```

```
./AbsolutNoLib info_filenames 1FBI_X
```

Download the structure files OR let 'single binding' (below recalculate them)

```
./AbsolutNoLib repertoire 1FBI_X SmallSetCDR3.txt 10
```

This creates the file 1FBI_XFinalBindings_Process_1_Of_1.txt

Absolut

```
./Absolut discretize
```

Step 2: Working with available antigens

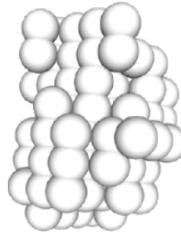


Step 3: High throughput annotation of CDRH3 sequences

```
./Absolut repertoire 1FBI ListCDR3s.txt NbThreads  
./Absolut repertoire 1FBI ListCDR3s.txt NbThreads prefixInResultFile  
.AbsolutNoLib repertoire 1FBI ListCDR3s.txt NbThreads  
mpieexec -n NbProcesses ./AbominationMPI repertoire 1FBI ListCDR3s.txt NbThreadsPerProc
```

Input 1: Antigen **structure ID** (inside the code)

1FBI_X



Input 2: Precalculated possible structures (200MB)

The file should be present in the folder of calculation

./AbsolutNoLib info_fileNames 1FBI_X

Input 3: **List of CDR3s** to 'structurally annotate'

1	CAGPSTTVYYYFDYW
2	CARAYYSNDYW
3	CARWDDYDDWFAYW
4	CARESSGGYGYW
5	CARYNYGPMDYW
...	

(optional) **Input 4:** **Tag** to be put in output filenames

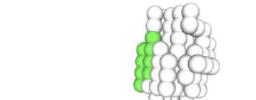
(optional) **Input 5:** **First** to **Last** lines to process

Output: Annotated Files

One file per process; Each CDR3 annotated with binding structures / energy

Ex: 1FBI_XFinalBindings_Process_2_Of_2.txt

CDR3	Slides (11 AA)	Best?	Slide	Energy	Structure
CARDIVTTWPYYAMDYW	CARDIVTTWPY	false	CARDIVTTWPY	-54.77	129120-DSLLRRDDSD
	ARDIVTTWPYY	false	ARDIVTTWPYY	-61.49	125152-UUUSURUDUD
	RDIVTTWPYYA	false	RDIVTTWPYYA	-54.07	141278-SLSSRRSDDSD
42881_03a	CARDIVTTWPYYAMDYW	false	DIVTTWPYYAM	-59.4	121119-RUSLLSDDUD
42881_03b	CARDIVTTWPYYAMDYW	false	DIVTTWPYYAM	-59.4	116959-USSDDDSRRLR
42881_04a	CARDIVTTWPYYAMDYW	false	IVTTWPYYAMD	-62.9	121055-USDDSRLRLR
42881_05a	CARDIVTTWPYYAMDYW	false	VTTWPYYAMDY	-64.95	137374-URDSRUURDU
42881_06a	CARDIVTTWPYYAMDYW	true	TTWPYYAMDYW	-65.09	141405-SSSDRRLRS
42882_00a	CARDKGAYSNSWYFDVW	false	CARDKGAYSNS	-47.55	137312-RULUUSUSDS
42882_01a	CARDKGAYSNSWYFDVW	true	ARDKGAYSNSW	-48.6	129120-DSLSDLSSL
...					



Temp. Output: Backup files with ongoing calculations, in case of crash (1/thread)

Ex: TemporaryBindingsFor5KN5_Ctest_t1_Part1_of_2.txt

Step 4: Extraction of structural features

AbsolutNoLib (or Absolut)

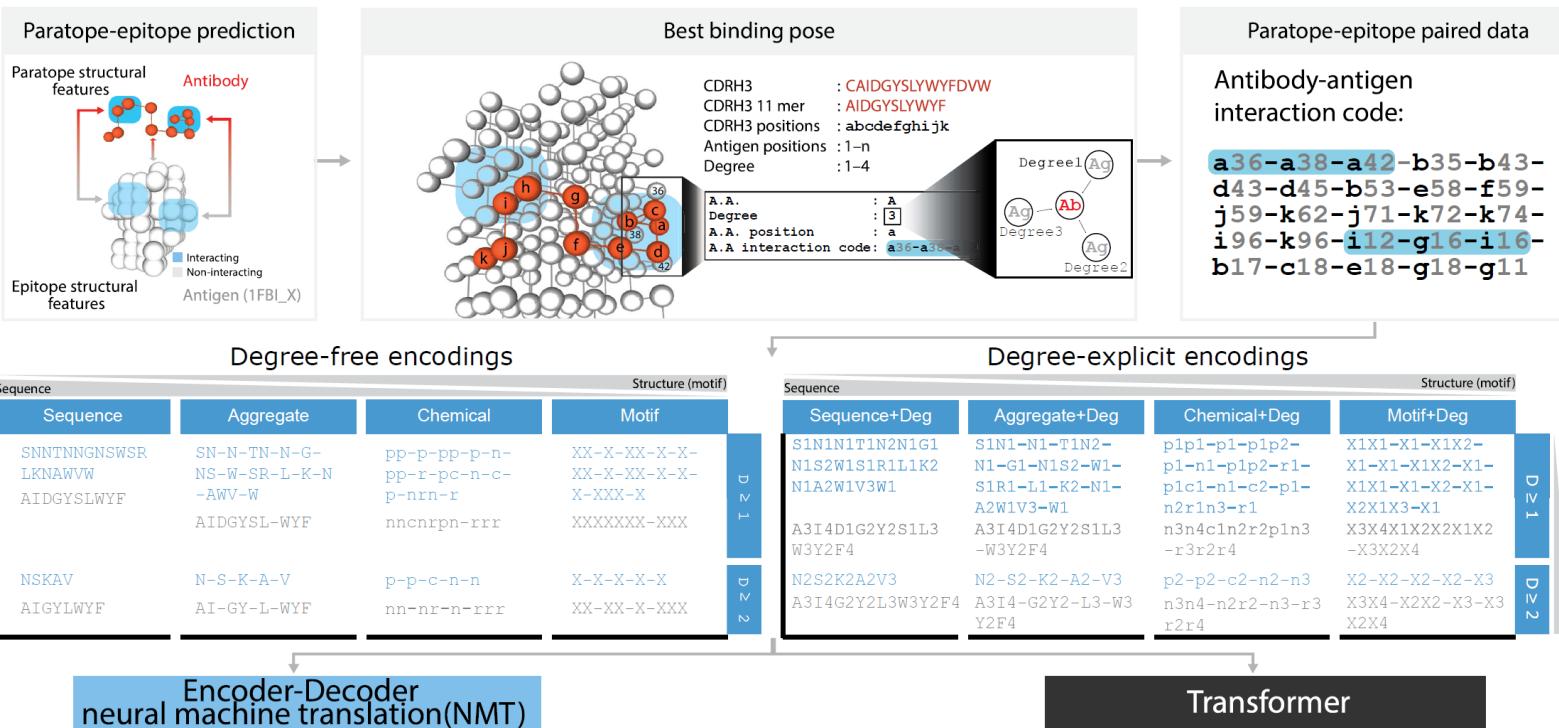
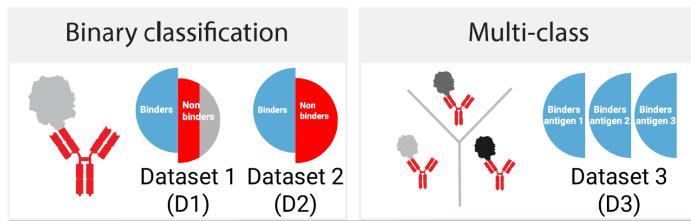
```
./AbsolutNoLib getFeatures 1FBI_X 1FBI_XFinalBindings_Process_1_Of_1.txt outputFeaturesFile.txt 1 true
```

Options	Degree of analysis	1	2	3	1	2	3
	Include degree in motifs	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE
Input	ID_slide_Variant	3609351_01a	3609351_01a	3609351_01a	3609351_01a	3609351_01a	3609351_01a
	CDR3	CAIDGSLYWYFDVV	CAIDGSLYWYFDVV	CAIDGSLYWYFDVV	CAIDGSLYWYFDVV	CAIDGSLYWYFDVV	CAIDGSLYWYFDVV
	Best	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE
	Slide	AIDGSLYWYF	AIDGSLYWYF	AIDGSLYWYF	AIDGSLYWYF	AIDGSLYWYF	AIDGSLYWYF
	Energy	-90.78	-90.78	-90.78	-90.78	-90.78	-90.78
	Structure	137187-UDRUSUDRDU	137187-UDRUSUDRDU	137187-UDRUSUDRDU	137187-UDRUSUDRDU	137187-UDRUSUDRDU	137187-UDRUSUDRDU
	interactionCode	b0035a0036a0038a0042b0043d0043 b0035a0036a0038a0042b0043d0043 b0035a0036a0038a0042b0043d0043 b0035a0036a0038a0042b0043d0043 b0035a0036a0038a0042b0043d0043 b0035a0036a0038a0042b0043d0043 d0045b0053e0058f0059j0059k0062j0 d0045b0053e0058f0059j0059k0062j0 d0045b0053e0058f0059j0059k0062j0 d0045b0053e0058f0059j0059k0062j0 d0045b0053e0058f0059j0059k0062j0 d0045b0053e0058f0059j0059k0062j0 071k0072k0074i0096k0096i0102g010 071k0072k0074i0096k0096i0102g010 071k0072k0074i0096k0096i0102g010 071k0072k0074i0096k0096i0102g010 071k0072k0074i0096k0096i0102g010 071k0072k0074i0096k0096i0102g010 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110 6i0106b0107c0108e0108g0110					
	AGboundPositions	35-36-38-42-43-45-53-58-59-62-71-72-74-96-102-106-107-108-110	43-59-96-106-108	108	35-36-38-42-43-45-53-58-59-62-71-72-74-96-102-106-107-108-110	43-59-96-106-108	108
	hotspot_ID	1FBI_X_H1	1FBI_X_H1	1FBI_X_H1	1FBI_X_H1	1FBI_X_H1	1FBI_X_H1
	seqAGEpitope	S1N1N1T1N2N1G1N1S2W1S1R1L1K2 N1A2W1V3W1	N2S2K2A2V3	V3	SNNTNNNGNSWSRLKNAWVW	NSKAV	V
	seqABParatope	A3I4D1G2Y2S1L3W3Y2F4	A3I4G2Y2L3W3Y2F4	A3I4L3W3F4	AIDGSLWYF	AIGYLWYF	AILWF
	motifAGEpitope	X1X1--X1-X1X2--X1--X1X2--X1--X1X1--X1--X2--X1--X2X1X3--X1	X2--X2--X2--X2--X3	X3	XX-X-XX-X-X-XX-X-XX-X-X-X-XXX-X	X-X-X-X-X	X
	motifABParatope	X3X4X1X2X2X1X3--X3X2X4	X3X4--X2X2--X3--X3X2X4	X3X4--X3--X3--X4	XXXXXXXX-XXX	XX-XX-X-XXX	XX-X-X-X
	aggregatesAGEpitope	S1N1--N1--T1N2--N1--G1--N1S2--W1--S1R1--L1--K2--N1--A2W1V3--W1	N2--S2--K2--A2--V3	V3	SN-N-TN-N-G-NS-W-SR-L-K-N-AWV-W	N-S-K-A-V	V
	aggregatesABParatope	A3I4D1G2Y2S1L3--W3Y2F4	A3I4--G2Y2--L3--W3Y2F4	A3I4--L3--W3--F4	AIDGSL-WYF	AI-GY-L-WYF	AI-L-W-F
	chemicalAGEpitope	p1p1--p1p2--p1--n1--p1p2--r1--p1c1--n1--c2--p1--n2r1n3--r1	p2--p2--c2--n2--n3	n3	pp-p-pp-p-n-pp-r-pc-n-c-p-nrn-r	p-p-c-n-n	n
	chemicalABParatope	n3n4c1n2r2p1n3--r3r2r4	n3n4--n2r2--n3--r3r2r4	n3n4--n3--r3--r4	nnncnrpn-rrr	nn-nr-n-rrr	nn-n-r-r

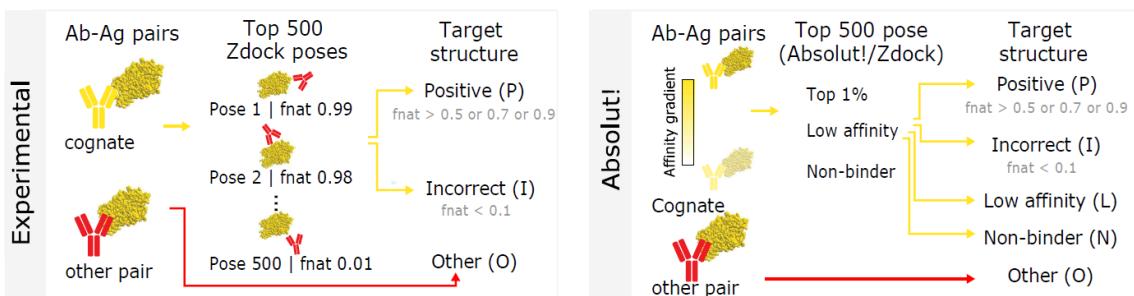
Visit the generated Absolut! database:

https://ns9999k.webs.sigma2.no/10.11582_2021.00063/projects/NS9603K/pprobert/AbsolutOnline/

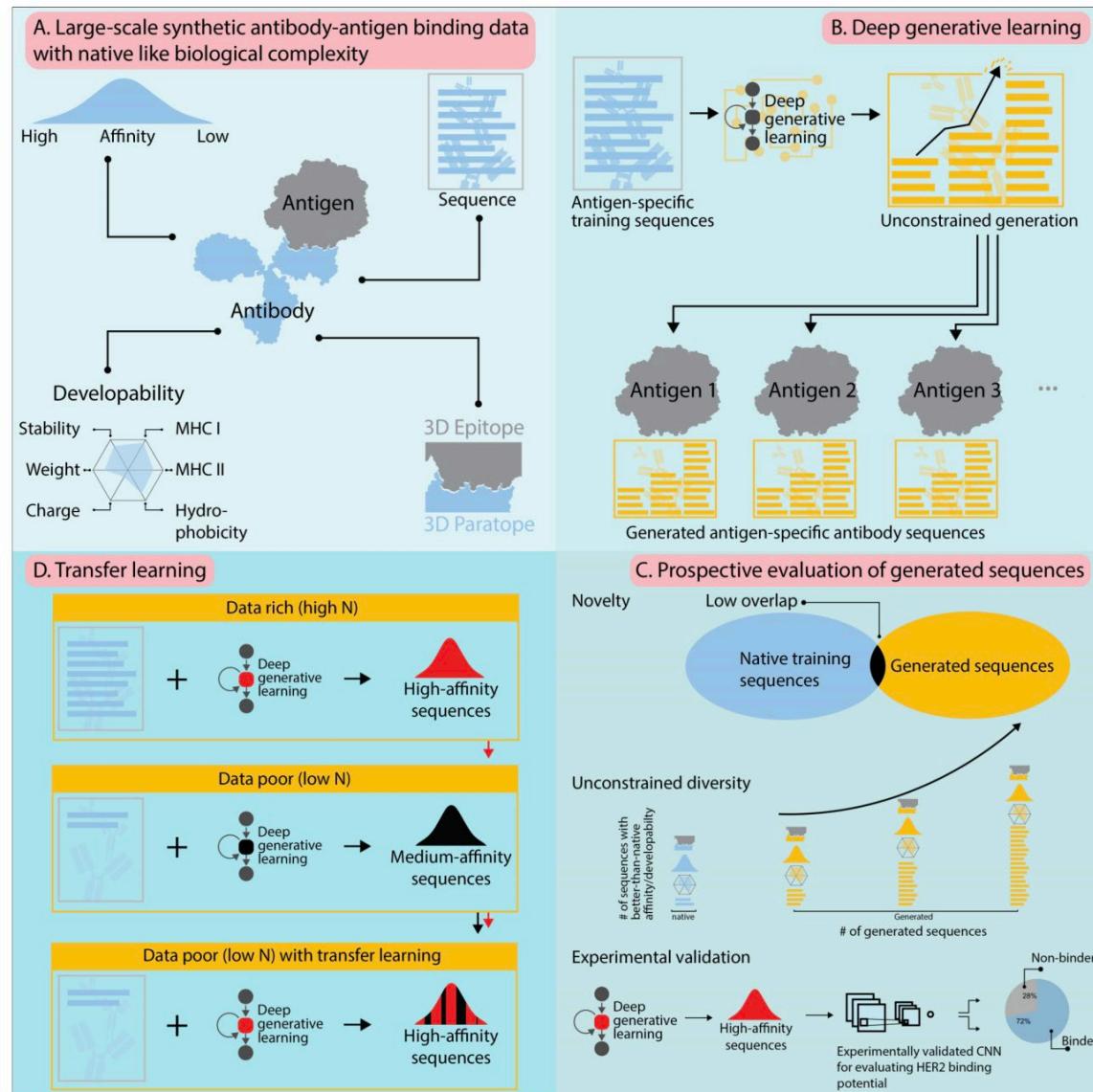
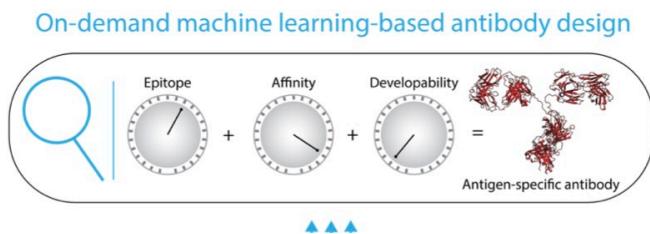
A Deep learning based paratope-epitope prediction



A Formulation of pose classification problems



Have used Absolut!: In silico proof of principle of machine learning-based antibody design at unconstrained scale



Have used Absolut!: AntBO: Towards Real-World Automated Antibody Design with Combinatorial Bayesian Optimisation

ANTBO: TOWARDS REAL-WORLD AUTOMATED ANTIBODY DESIGN WITH COMBINATORIAL BAYESIAN OPTIMISATION

A PREPRINT

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