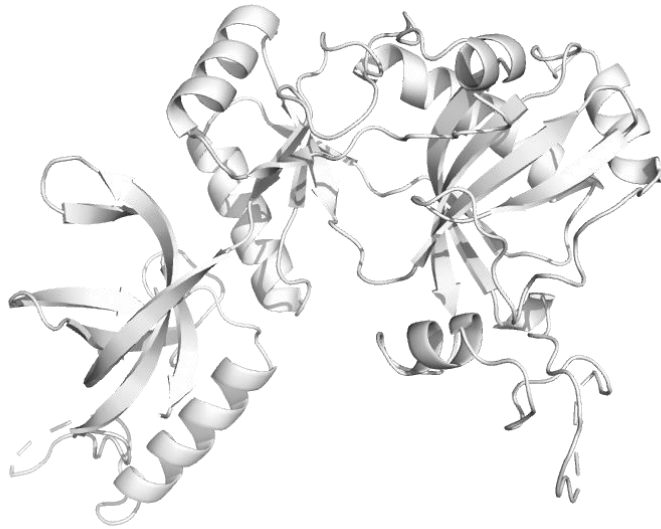


Work Report

贾宁欣

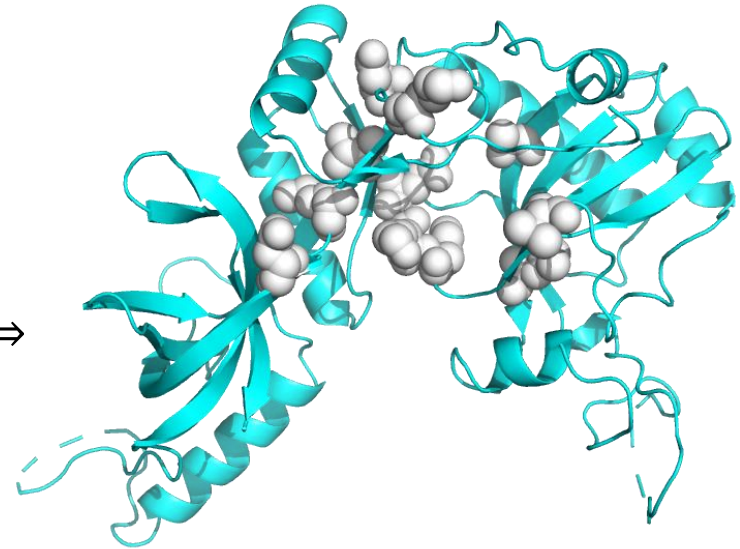
10-22-2021

Experiment Subject



Protein

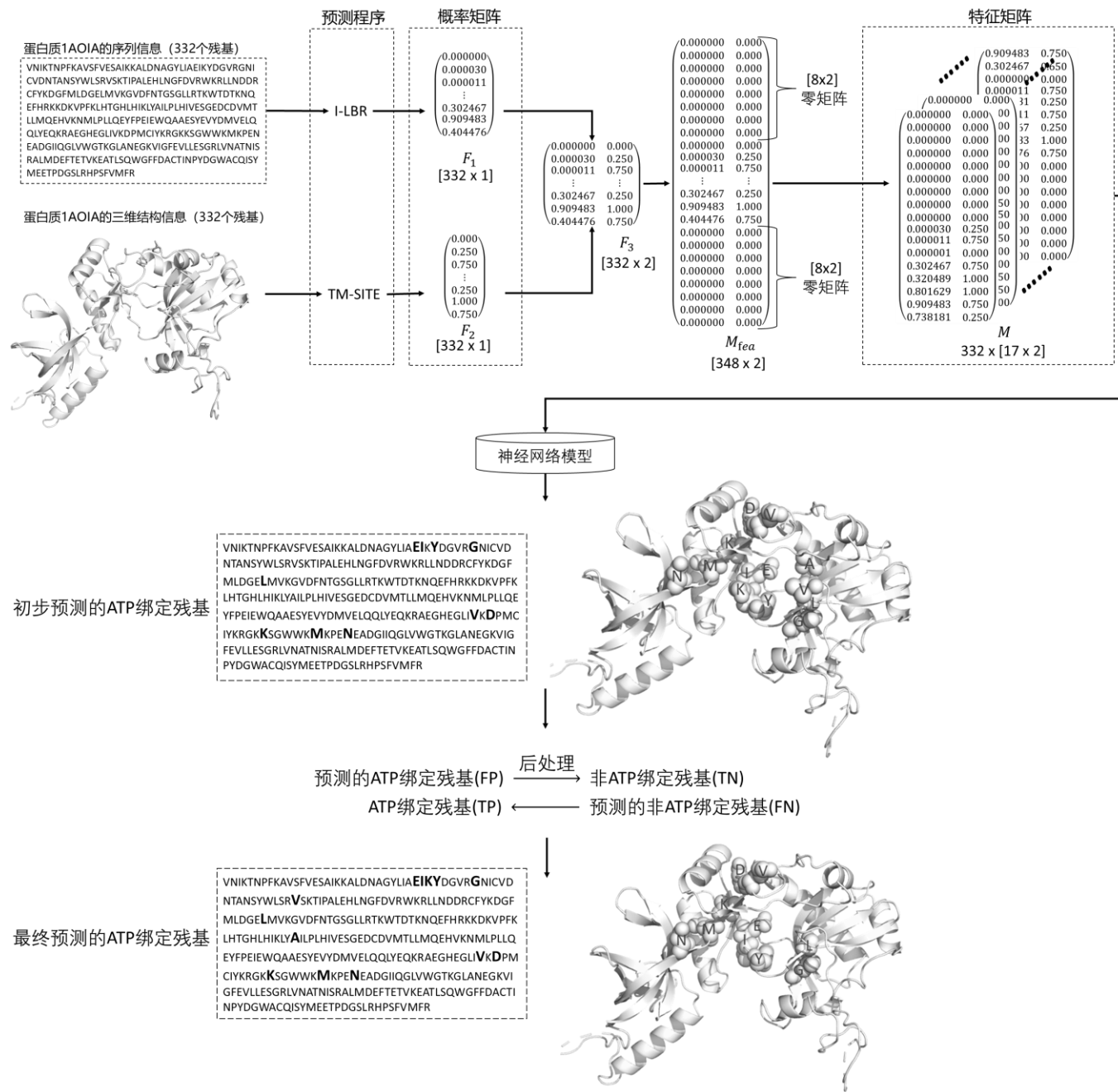
Predict
⇒



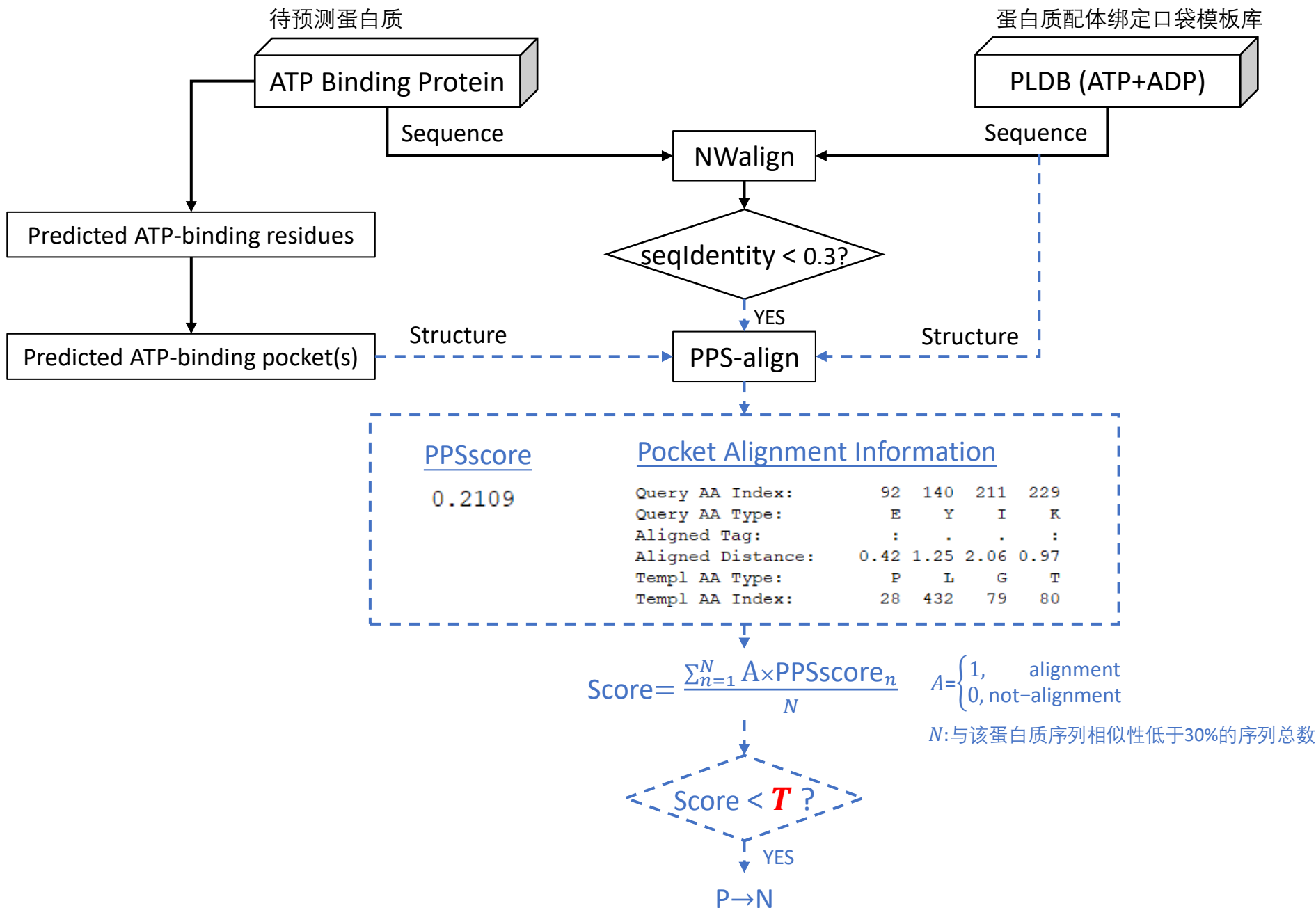
ATP-binding Residues

ABP -- ATP Binding Protein

Experiment Flow Chart



Postprocessing



Experiment Results -- Prediction

Table 1

Statistical composition of the two data sets used in this study.

Data set	N_{pro}^a	N_{pos}^b	N_{neg}^c	$PNratio^d$
PART-388	388	5657	142,086	1: 25.12
PART-TEST	41	674	14,159	1: 21.01

^a Number of proteins.

^b Number of ATP-binding residues.

^c Number of non-ATP-binding residues.

^d $PNratio = N_{pos} : N_{neg}$.

PART-388 and PART-TEST are two widely used benchmark data sets constructed in our previous work [].

#

A sliding window with size W (centered at the target residue) is utilized, and inspired by ATPint, we set $W = 17$ in this study.

Table 2

Performance of XXX based on different features and their combinations.

feature	Thres	Sen(%)	Spe(%)	Acc(%)	Pre(%)	MCC	F1-sco	AUC
PSFM	0.14	55.93	98.93	96.97	71.27	0.616	0.627	0.844
TMSITE	0.32	63.35	99.05	97.43	76.11	0.681	0.691	0.917
ILBR	0.38	51.93	99.27	97.11	77.09	0.619	0.621	0.892
PSFM+ TMSITE	0.28	63.95	98.96	97.37	74.57	0.677	0.688	0.884
PSFM+ILBR	0.41	55.64	99.10	97.13	74.70	0.630	0.638	0.855
TMSITE+ILBR	0.34	66.02	99.17	97.67	79.18	0.711	0.720	0.932
PSFM+TMSITE+LIBR	0.56	63.50	99.04	97.42	75.89	0.681	0.691	0.889

Note: The best results are highlighted in bold type.

Experiment Results -- Prediction

Table 3

Performance comparison of XXX, S-SITEatp, TM-SITEatp, ATPseq, ATPbind and DeepATPseq over 5-fold cross-validation tests on PART-388.

Predictors	Sen(%)	Spe(%)	Acc(%)	Pre(%)	MCC	AUC
S-SITEatp ^a	69.88	94.47	93.53	33.47	0.455	N/A
TM-SITEatp ^a	73.64	95.29	94.46	38.37	0.507	N/A
ATPseq ^a	57.52	98.86	97.27	66.69	0.605	0.913
ATPbind ^a	64.04	98.88	97.55	69.57	0.655	0.932
DeepATPseq ^b	52.20	99.03	97.39	69.75	0.613	
XXX			待做			

^a Data excerpted from Ref. []. (ATPbind 2018)

^b Data excerpted from Ref. []. (DeepATPseq 2021)

Table 4

Performance comparison of XXX and other computational methods on the independent test data set.

Model	Sen(%)	Spe(%)	Acc(%)	Pre(%)	MCC	AUC
S-SITEatp ^a	67.51	92.65	91.51	30.41	0.416	N/A [#]
TM-SITEatp ^a	69.73	96.09	84.89	45.90	0.541	N/A
NsitePred ^a	46.74	97.70	95.39	49.22	0.456	0.852
TargetATPsite ^a	41.25	99.49	96.84	79.43	0.559	0.853
TargetS ^a	51.63	98.89	96.74	68.91	0.580	0.872
TargetSOS ^a	49.26	99.46	97.18	81.37	0.620	0.863
TargetNUCs ^a	46.88	99.66	97.26	86.81	0.627	0.856
ATPseq ^a	54.45	99.27	97.24	78.09	0.639	0.878
ATPbind ^a	62.31	98.85	97.19	72.04	0.656	0.915
DELIA ^b	62.17	98.67	97.01	69.03	0.640	
DELIA ^c				0.758	0.685	0.947
DeepATPseq ^b	57.42	99.22	97.32	77.71	0.655	
XXX	66.02	99.17	97.67	79.18	0.711	0.932

^a Data excerpted from Ref. []. (ATPbind 2018)

^b Data excerpted from Ref. []. (DeepATPseq 2021)

^c Data excerpted from Ref. []. (DELIA 2020)

[#] N/A, the corresponding value could not be computed.

Future Work

- 1、论文中配图;
- 2、后处理实验;