

## SUPPLEMENTARY FILE FOR

### An Evolution-based DNA-binding Residues Predictor by Using Dynamic Query-driven Learning Scheme

Haiting Chai <sup>1</sup>, Jian Zhang <sup>1</sup>, Guifu Yang <sup>1,2,\*</sup>, Zhiqiang Ma <sup>1</sup>

<sup>1</sup>School of Computer Science and Information Technology, Northeast Normal University, Changchun, 130117, P.R. China

<sup>2</sup>Office of Informatization Management and Planning, Northeast Normal University, Changchun, 130117, P.R. China

\*Authors to whom correspondence should be addressed. Email: guifuyang.nenu@gmail.com (GFY)

The PDF file includes:

Table S1. The average position specific scores of twenty standard amino acids in our sample pool.

Table S2. Relative substitution possibilities of observed DBRs.

Table S3. Relative substitution possibilities of observed non-DBRs.

Table S4. Experimental results of DQPred-DBR on DNA\_T.

Table S5. Experimental results of DQPred-DBR on PDNA-41.

Figure S1. The distribution of DBRs- and non-DBRs-related CSP.

Figure S2. CSP of different substitution combinations.

Datasets with DNA-binding proteins with annotations based on the 3.5Å cut-off.

Supplementary Table S1. The average position specific scores of twenty standard amino acids in our sample pool.

	A	R	N	D	C	Q	E	G	H	I	L	K	M	F	P	S	T	W	Y	V
A	2.34	-1.18	-1.29	-1.56	-1.10	-0.82	-0.84	-0.76	-1.62	-1.18	-1.39	-0.76	-1.07	-2.08	-1.39	0.44	-0.27	-2.90	-1.78	-0.58
R	-1.29	3.98	-0.54	-1.38	-3.13	0.54	-0.14	-2.24	-0.50	-2.45	-2.09	1.62	-1.51	-2.68	-2.07	-0.78	-1.04	-2.99	-1.81	-2.28
N	-1.23	-0.35	3.78	0.62	-2.58	-0.10	-0.10	-0.82	0.04	-2.71	-2.76	-0.02	-1.98	-2.76	-1.86	0.33	-0.32	-3.42	-1.95	-2.43
D	-1.42	-1.11	0.83	4.13	-3.28	-0.08	1.35	-1.39	-0.89	-2.89	-3.12	-0.38	-2.53	-3.21	-1.59	-0.24	-0.94	-3.79	-2.54	-2.72
C	-0.85	-3.04	-2.76	-3.45	6.68	-2.76	-3.26	-2.86	-3.04	-1.39	-1.52	-2.85	-1.69	-2.45	-3.23	-1.30	-1.30	-3.21	-2.45	-1.11
Q	-0.85	0.59	-0.22	-0.38	-2.80	3.28	1.09	-1.88	-0.10	-2.24	-1.94	0.82	-1.01	-2.68	-1.56	-0.28	-0.72	-2.72	-1.65	-1.93
E	-0.85	-0.09	-0.13	1.15	-3.23	1.08	3.42	-1.82	-0.48	-2.52	-2.44	0.63	-1.85	-2.84	-1.39	-0.25	-0.78	-3.15	-1.96	-2.16
G	-0.33	-1.75	-0.36	-1.05	-2.73	-1.46	-1.46	4.26	-1.80	-3.34	-3.30	-1.19	-2.62	-3.12	-2.07	-0.32	-1.50	-3.18	-2.82	-2.85
H	-1.54	-0.36	0.06	-1.05	-2.83	-0.03	-0.40	-2.17	5.21	-2.59	-2.33	-0.59	-1.72	-1.49	-2.18	-0.85	-1.39	-2.47	0.47	-2.47
I	-1.27	-2.50	-2.89	-3.13	-1.57	-2.36	-2.66	-3.53	-2.78	3.28	1.29	-2.34	0.72	-0.26	-2.83	-2.07	-0.97	-2.67	-1.21	1.83
L	-1.47	-2.14	-2.98	-3.35	-1.71	-2.03	-2.57	-3.49	-2.55	1.41	2.98	-2.23	1.22	0.13	-2.87	-2.18	-1.27	-2.09	-0.99	0.57
K	-0.88	1.60	-0.21	-0.68	-2.91	0.71	0.52	-1.75	-0.72	-2.37	-2.21	3.26	-1.46	-2.75	-1.40	-0.32	-0.74	-3.06	-1.84	-2.04
M	-1.12	-1.53	-2.23	-2.74	-1.88	-1.04	-1.91	-2.89	-1.94	0.78	1.23	-1.43	3.74	-0.42	-2.65	-1.54	-0.96	-2.17	-1.10	0.22
F	-2.02	-2.63	-2.85	-3.42	-2.34	-2.63	-2.87	-3.32	-1.34	-0.15	0.26	-2.66	-0.19	4.73	-3.41	-2.29	-1.90	-0.06	2.07	-0.77
P	-0.84	-1.51	-1.47	-1.25	-2.90	-1.00	-0.81	-2.02	-1.83	-2.40	-2.46	-0.72	-2.28	-3.16	5.49	-0.67	-0.99	-3.63	-2.60	-2.07
S	0.27	-0.70	0.25	-0.43	-1.58	-0.30	-0.28	-0.73	-0.99	-2.12	-2.23	-0.25	-1.59	-2.44	-1.22	2.38	0.59	-3.04	-1.86	-1.72
T	-0.36	-0.94	-0.40	-1.11	-1.60	-0.72	-0.78	-1.83	-1.53	-1.06	-1.42	-0.61	-1.07	-2.14	-1.51	0.67	2.89	-2.95	-1.82	-0.66
W	-2.28	-2.35	-3.04	-3.48	-2.56	-1.95	-2.56	-2.83	-1.78	-1.91	-1.28	-2.41	-1.28	0.92	-3.46	-2.39	-2.16	8.41	1.55	-2.20
Y	-1.84	-1.84	-2.07	-2.87	-2.49	-1.70	-2.05	-3.09	0.62	-1.14	-0.91	-1.84	-1.01	2.13	-3.02	-1.84	-1.77	0.61	5.17	-1.26
V	-0.60	-2.24	-2.58	-2.87	-1.28	-1.97	-2.22	-3.03	-2.59	2.00	0.61	-1.98	0.25	-0.83	-2.46	-1.60	-0.49	-2.77	-1.27	2.74

Supplementary Table S2. Relative substitution possibilities of observed DBRs.

	A	R	N	D	C	Q	E	G	H	I	L	K	M	F	P	S	T	W	Y	V
A	0.40	0.04	0.01	-0.27	-0.35	0.06	-0.26	0.39	-0.07	-0.39	-0.56	0.11	-0.22	-0.46	0.04	0.57	0.43	-0.14	-0.36	-0.16
R	-0.60	1.22	-0.43	-0.79	-0.55	-0.27	-0.73	-0.53	-0.33	-0.82	-0.68	0.15	-0.50	-0.68	-0.52	-0.39	-0.46	-0.23	-0.49	-0.74
N	-0.64	-0.25	1.31	-0.51	-0.54	-0.43	-0.72	-0.35	-0.13	-0.59	-0.72	-0.28	-0.41	-0.44	-0.48	-0.04	-0.09	-0.56	-0.38	-0.52
D	-0.39	-0.50	-0.13	0.71	-0.37	-0.48	-0.39	-0.03	-0.19	-0.50	-0.58	-0.65	-0.53	-0.38	-0.49	0.15	-0.26	-0.54	-0.25	-0.48
C	-0.01	0.89	1.38	0.48	-0.95	1.01	0.38	0.78	0.81	-0.67	-0.26	1.08	-0.00	0.20	0.70	0.70	0.57	0.61	0.87	-0.57
Q	-0.27	0.15	-0.29	-0.67	-0.45	1.16	-0.57	-0.31	-0.25	-0.67	-0.60	-0.12	-0.25	-0.65	-0.29	-0.18	-0.12	-0.29	-0.40	-0.28
E	-0.52	-0.11	-0.09	-0.22	-0.35	-0.22	0.58	-0.21	-0.15	-0.69	-0.69	-0.48	-0.48	-0.39	-0.42	-0.10	-0.44	-0.35	-0.44	-0.48
G	-0.23	-0.58	-0.54	-0.78	-0.48	-0.63	-0.92	1.05	-0.64	-0.87	-0.79	-0.64	-0.58	-0.60	-0.48	-0.18	-0.48	-0.25	-0.64	-0.70
H	-0.73	-0.46	-0.26	-0.83	-0.94	-0.64	-0.84	-0.57	1.84	-1.17	-1.09	-0.63	-0.90	-0.69	-0.83	-0.55	-0.62	-0.69	0.03	-1.10
I	-0.08	0.20	0.15	-0.04	-0.25	0.06	-0.19	0.16	-0.15	0.04	-0.59	0.08	-0.18	-0.41	0.11	0.25	0.30	-0.39	-0.39	-0.06
L	-0.01	0.38	0.23	-0.03	-0.35	0.44	-0.05	0.04	0.02	-0.68	-0.21	0.32	-0.02	-0.54	0.12	0.32	0.18	-0.34	-0.30	-0.42
K	-0.25	0.40	-0.30	-0.66	-0.29	-0.20	-0.61	-0.29	-0.29	-0.52	-0.52	0.90	-0.29	-0.53	-0.33	-0.15	-0.19	-0.30	-0.37	-0.40
M	0.20	0.37	0.34	0.02	-0.23	0.41	0.03	0.25	0.11	-0.62	-0.68	0.28	0.49	-0.23	0.14	0.35	0.31	0.01	-0.11	-0.39
F	-0.62	-0.42	-0.27	-0.47	-0.55	-0.44	-0.54	-0.39	0.05	-0.95	-0.93	-0.43	-0.82	0.73	-0.54	-0.35	-0.51	0.38	0.51	-0.94
P	-0.04	-0.16	-0.44	-0.73	-0.20	-0.33	-0.69	-0.19	-0.39	-0.48	-0.48	-0.35	-0.32	-0.43	0.43	0.10	-0.04	-0.25	-0.40	-0.42
S	0.09	-0.17	0.03	-0.50	0.05	-0.22	-0.56	0.19	-0.24	-0.42	-0.45	-0.17	-0.24	-0.39	-0.19	0.87	0.25	-0.29	-0.31	-0.30
T	-0.18	-0.19	-0.15	-0.57	-0.24	-0.28	-0.68	-0.18	-0.36	-0.48	-0.52	-0.17	-0.39	-0.61	-0.22	0.34	1.29	-0.39	-0.49	-0.34
W	-0.94	-0.54	-0.79	-0.91	-0.46	-0.74	-0.94	-0.41	-0.80	-1.23	-1.22	-0.90	-0.88	-0.41	-0.79	-0.61	-0.73	1.25	-0.23	-1.15
Y	-0.48	-0.14	-0.11	-0.50	-0.60	-0.31	-0.57	-0.34	0.33	-0.84	-0.85	-0.16	-0.60	0.08	-0.52	-0.26	-0.28	-0.05	1.06	-0.75
V	-0.07	0.48	0.20	-0.14	-0.42	0.32	-0.11	-0.06	-0.14	-0.41	-0.75	0.59	-0.15	-0.78	0.06	0.23	0.30	-0.50	-0.57	0.28

Supplementary Table S3. Relative substitution possibilities of observed non-DBRs.

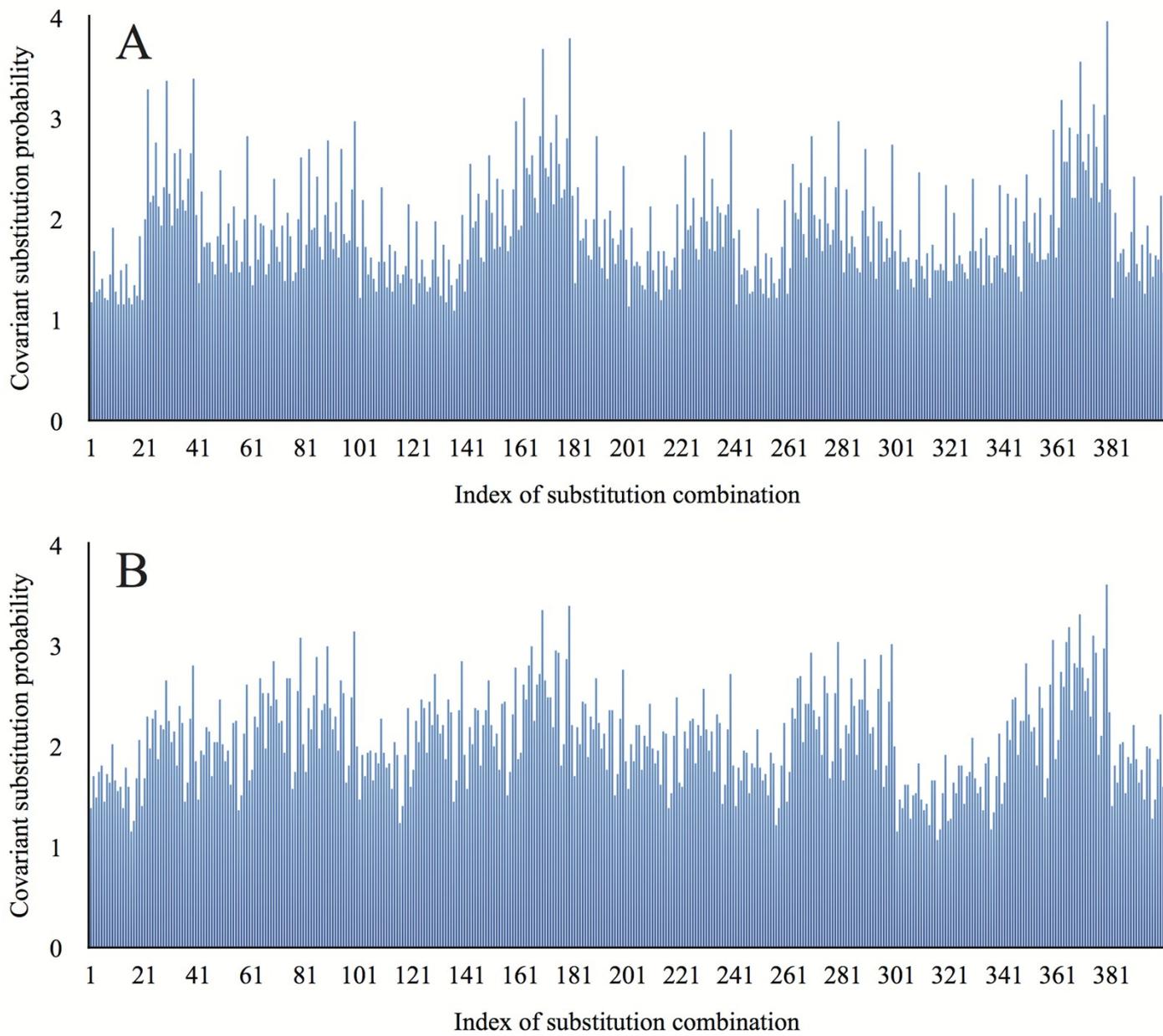
	A	R	N	D	C	Q	E	G	H	I	L	K	M	F	P	S	T	W	Y	V
A	-0.01	-0.00	-0.00	0.01	0.01	-0.00	0.01	-0.01	0.00	0.01	0.02	-0.00	0.01	0.01	-0.00	-0.02	-0.01	0.00	0.01	0.00
R	0.13	-0.26	0.09	0.17	0.12	0.06	0.16	0.11	0.07	0.17	0.15	-0.03	0.11	0.14	0.11	0.08	0.10	0.05	0.10	0.16
N	0.07	0.03	-0.14	0.06	0.06	0.05	0.08	0.04	0.01	0.06	0.08	0.03	0.04	0.05	0.05	0.00	0.01	0.06	0.04	0.06
D	0.01	0.02	0.00	-0.02	0.01	0.01	0.01	0.00	0.01	0.02	0.02	0.02	0.02	0.01	0.02	-0.00	0.01	0.02	0.01	0.02
C	-0.00	-0.02	-0.03	-0.01	0.02	-0.02	-0.01	-0.02	-0.02	0.02	0.01	-0.02	-0.00	-0.00	-0.02	-0.02	-0.01	-0.01	-0.02	0.01
Q	0.02	-0.01	0.02	0.06	0.04	-0.10	0.05	0.03	0.02	0.06	0.05	0.01	0.02	0.05	0.02	0.01	0.01	0.02	0.03	0.02
E	0.01	0.00	0.00	0.01	0.01	0.00	-0.01	0.00	0.00	0.02	0.02	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01
G	0.02	0.04	0.04	0.05	0.03	0.04	0.06	-0.07	0.04	0.06	0.05	0.04	0.04	0.04	0.03	0.01	0.03	0.02	0.04	0.05
H	0.09	0.05	0.03	0.10	0.11	0.08	0.10	0.07	-0.22	0.14	0.13	0.07	0.11	0.08	0.10	0.07	0.07	0.08	-0.00	0.13
I	0.00	-0.01	-0.00	0.00	0.01	-0.00	0.01	-0.00	0.00	-0.00	0.02	-0.00	0.00	0.01	-0.00	-0.01	-0.01	0.01	0.01	0.00
L	0.00	-0.01	-0.00	0.00	0.01	-0.01	0.00	-0.00	-0.00	0.01	0.00	-0.01	-0.00	0.01	-0.00	-0.01	-0.00	0.01	0.00	0.01
K	0.03	-0.06	0.04	0.09	0.04	0.03	0.08	0.04	0.04	0.07	0.07	-0.12	0.04	0.07	0.05	0.02	0.03	0.04	0.05	0.06
M	-0.01	-0.02	-0.02	-0.00	0.01	-0.02	-0.00	-0.01	-0.01	0.03	0.03	-0.01	-0.02	0.01	-0.01	-0.02	-0.01	-0.00	0.01	0.02
F	0.03	0.02	0.01	0.02	0.03	0.02	0.03	0.02	-0.00	0.04	0.04	0.02	0.04	-0.03	0.03	0.02	0.02	-0.02	-0.02	0.04
P	0.00	0.00	0.02	0.02	0.01	0.01	0.02	0.01	0.01	0.02	0.02	0.01	0.01	0.01	-0.01	-0.00	0.00	0.01	0.01	0.01
S	-0.01	0.02	-0.00	0.05	-0.00	0.02	0.06	-0.02	0.02	0.04	0.05	0.02	0.02	0.04	0.02	-0.09	-0.03	0.03	0.03	0.03
T	0.02	0.02	0.01	0.05	0.02	0.02	0.06	0.02	0.03	0.04	0.05	0.01	0.03	0.05	0.02	-0.03	-0.11	0.03	0.04	0.03
W	0.08	0.05	0.07	0.08	0.04	0.07	0.08	0.04	0.07	0.11	0.11	0.08	0.08	0.04	0.07	0.05	0.07	-0.11	0.02	0.10
Y	0.05	0.02	0.01	0.06	0.07	0.04	0.06	0.04	-0.04	0.10	0.10	0.02	0.07	-0.01	0.06	0.03	0.03	0.01	-0.12	0.08
V	0.00	-0.01	-0.00	0.00	0.01	-0.01	0.00	0.00	0.01	0.02	-0.01	0.00	0.02	-0.00	-0.01	-0.01	0.01	0.01	-0.01	-0.01

Supplementary Table S4. Experimental results of DQPred-DBR on DNA\_T.

Model	Similarity Threshold	SN (%)	SP (%)	ACC (%)	MCC	AUC
Universal	N/A	57.8	84.3	81.7	0.311	0.809
	90%	60.5	87.4	84.8	0.374	0.821
	80%	61.1	87.8	85.3	0.385	0.832
Dynamic	70%	61.5	87.7	85.2	0.385	0.831
	<b>60%</b>	<b>61.9</b>	<b>87.7</b>	<b>85.2</b>	<b>0.388</b>	<b>0.835</b>
	50%	61.6	87.7	85.2	0.386	0.833
	40%	60.8	87.9	85.3	0.384	0.831

Supplementary Table S5. Experimental results of DQPred-DBR on PDNA-41.

Model	Similarity Threshold	SN (%)	SP (%)	ACC (%)	MCC	AUC
Universal	N/A	48.7	88.9	86.4	0.267	0.790
	90%	49.5	89.5	87.0	0.281	0.795
	80%	50.1	89.9	87.5	0.292	0.799
Dynamic	70%	50.7	90.9	88.4	0.312	0.803
	60%	51.1	90.8	88.3	0.313	0.804
	<b>50%</b>	<b>51.6</b>	<b>90.8</b>	<b>88.3</b>	<b>0.316</b>	<b>0.808</b>
	40%	50.9	90.8	88.3	0.312	0.803



Supplementary Figure S1. The distribution of (A) DBRs- and (B) non-DBRs-related CSP.



Supplementary Figure S2. CSP of different substitution combinations.











PSYLTIQOPGGKAQFGGORGEJMVEWALEAYGAHTIQLMELTJKSDIDHGRNAAYAEAIKHPGDEVPSPVFSFRVLKEQLQALALDVTQLEDKNPVDIFEGALKSR  
FVQKRNKGehGvDKRrEVEVLRAEKLjGLvP0K1PEIQQELKFQkGvVLYLdGt1GEPHe4PvVQGMJFHkL1HmVdEDNKHAKS1G

28e\_B Embryo in Sample point and PDNA-312

MNKGQRHKIRENTNEIETQDELVDMKLQDGKVYQTAVTSRDIKEHLHVKPVTNGSYKSL Embody in Sample pool and PDNA-512

2gb/s Embedded in Sample pool and PDNA-S12

11  
2vib\_A  
Antibody in Sample pool and PDNA-512





























































































