

**Table S2** The most 50 important CKSAAP encoding mRMR feature scores and their corresponding amino acid pairs are presented.

Ranks	Scores	Pairs	Ranks	Scores	Pairs
1	0.03	E×L	26	0.011	NxxxxW
2	0.018	A×××Y	27	0.011	G×××G
3	0.017	P×F	28	0.011	MxxxxxG
4	0.017	MF	29	0.011	K×Y
5	0.016	YxxxxV	30	0.011	PV
6	0.016	KD	31	0.01	AxxxxY
7	0.015	V×××V	32	0.01	K×K
8	0.015	G×××P	33	0.01	RxxxxF
9	0.014	DL	34	0.01	QxxxxE
10	0.014	ExxxxE	35	0.01	F××G
11	0.014	RI	36	0.01	MxxxxK
12	0.013	S×××H	37	0.01	TN
13	0.014	M××S	38	0.01	LV
14	0.014	GxxxxxE	39	0.01	IxxxxxA
15	0.013	D×A	40	0.01	G××xD
16	0.013	VF	41	0.01	MxxxxM
17	0.013	Y××xA	42	0.009	RK
18	0.012	P×xD	43	0.009	K××xV
19	0.012	LN	44	0.009	K××xD
20	0.012	TT	45	0.009	PE
21	0.012	K××xD	46	0.009	M×xL
22	0.011	GxD	47	0.009	Q×N
23	0.011	T×xD	48	0.009	D×V
24	0.011	EW	49	0.009	SM
25	0.011	P××xF	50	0.009	N××xT

For example, the feature 'ExL' represents a 1-spaced residue (any amino acid) pair of 'EL', where x stands for any amino acid. And the same representation was applied to other  $k$ -spaced residue pairs.