

iMRSAPred: Improved Prediction of Anti-MRSA Peptides using Pysicochemical and Pairwise Contact Energy Properties of Amino Acids

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Supplementary Files

Supplementary Table T1. The derived values of five physicochemical properties of 20 AAs [2].

Amino Acid	Irreplaceability	Rigidity	Flexibility	Hydrophilicity	Hydrophobicity
A	0.52	-1.33	-3.10	-0.50	0.62
C	1.12	-1.51	0.95	-1.00	0.29
D	0.77	-0.20	0.42	3.00	-0.90
E	0.76	-0.36	2.00	3.00	-0.74
F	0.86	2.87	-0.46	-2.50	1.19
G	0.56	-1.09	-2.74	0.00	0.48
H	0.94	2.26	-0.22	-0.50	-0.04

I	0.65	-1.74	0.42	-1.80	1.38
K	0.81	-1.82	3.95	3.00	-1.50
L	0.58	-1.74	0.42	-1.80	1.06
M	1.25	-1.74	2.48	-1.30	0.64
N	0.79	-0.20	0.42	0.20	-0.78
P	0.61	1.97	-2.40	0.00	0.12
Q	0.86	-0.36	2.00	0.20	-0.85
R	0.60	1.16	3.06	3.00	-2.53
S	0.64	-1.51	0.95	0.30	-0.18
T	0.56	-1.64	-1.33	-0.40	-0.05
V	0.54	-1.64	-1.33	-1.50	1.08

W	1.82	5.91	-1.00	-3.40	0.81
Y	0.98	2.71	-0.67	-2.30	0.26

Supplementary Table T2. The residue pairwise content energy matrix (RCEM) properties [1].

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	-1.65	-2.83	1.16	1.8	-3.73	-0.41	1.9	-3.69	0.49	-3.01	-2.08	0.66	1.54	1.2	0.98	-0.08	0.46	-2.31	0.32	-4.62
C	-2.83	-39.58	-0.82	-0.53	-3.07	-2.96	-4.98	0.34	-1.38	-2.15	1.43	-4.18	-2.13	-2.91	-0.41	-2.33	-1.84	-0.16	4.26	-4.46
D	1.16	-0.82	0.84	1.97	-0.92	0.88	-1.07	0.68	-1.93	0.23	0.61	0.32	3.31	2.67	-2.02	0.91	-0.65	0.94	-0.71	0.90
E	1.8	-0.53	1.97	1.45	0.94	1.31	0.61	1.3	-2.51	1.14	2.53	0.2	1.44	0.1	-3.13	0.81	1.54	0.12	-1.07	1.29
F	-3.73	-3.07	-0.92	0.94	-11.25	0.35	-3.57	-5.88	-0.82	-8.59	-5.34	0.73	0.32	0.77	-0.4	-2.22	0.11	-7.05	-7.09	-8.80
G	-0.41	-2.96	0.88	1.31	0.35	-0.2	1.09	-0.65	-0.16	-0.55	-0.52	-0.32	2.25	1.11	0.84	0.71	0.59	-0.38	1.69	-1.90
H	1.9	-4.98	-1.07	0.61	-3.57	1.09	1.97	-0.71	2.89	-0.86	-0.75	1.84	0.35	2.64	2.05	0.82	-0.01	0.27	-7.58	-3.20
I	-3.69	0.34	0.68	1.3	-5.88	-0.65	-0.71	-6.74	-0.01	-9.01	-3.62	-0.07	0.12	-0.18	0.19	-0.15	0.63	-6.54	-3.78	-5.26
K	0.49	-1.38	-1.93	-2.51	-0.82	-0.16	2.89	-0.01	1.24	0.49	1.61	1.12	0.51	0.43	2.34	0.19	-1.11	0.19	0.02	-1.19
L	-3.01	-2.15	0.23	1.14	-8.59	-0.55	-0.86	-9.01	0.49	-6.37	-2.88	0.97	1.81	-0.58	-0.6	-0.41	0.72	-5.43	-8.31	-4.90
M	-2.08	1.43	0.61	2.53	-5.34	-0.52	-0.75	-3.62	1.61	-2.88	-6.49	0.21	0.75	1.9	2.09	1.39	0.63	-2.59	-6.88	-9.73
N	0.66	-4.18	0.32	0.2	0.73	-0.32	1.84	-0.07	1.12	0.97	0.21	0.61	1.15	1.28	1.08	0.29	0.46	0.93	-0.74	0.93
P	1.54	-2.13	3.31	1.44	0.32	2.25	0.35	0.12	0.51	1.81	0.75	1.15	-0.42	2.97	1.06	1.12	1.65	0.38	-2.06	-2.09
Q	1.2	-2.91	2.67	0.1	0.77	1.11	2.64	-0.18	0.43	-0.58	1.9	1.28	2.97	-1.54	0.91	0.85	-0.07	-1.91	-0.76	0.01
R	0.98	-0.41	-2.02	-3.13	-0.4	0.84	2.05	0.19	2.34	-0.6	2.09	1.08	1.06	0.91	0.21	0.95	0.98	0.08	-5.89	0.36
S	-0.08	-2.33	0.91	0.81	-2.22	0.71	0.82	-0.15	0.19	-0.41	1.39	0.29	1.12	0.85	0.95	-0.48	-0.06	0.13	-3.03	-0.82
T	0.46	-1.84	-0.65	1.54	0.11	0.59	-0.01	0.63	-1.11	0.72	0.63	0.46	1.65	-0.07	0.98	-0.06	-0.96	1.14	-0.65	-0.37
V	-2.31	-0.16	0.94	0.12	-7.05	-0.38	0.27	-6.54	0.19	-5.43	-2.59	0.93	0.38	-1.91	0.08	0.13	1.14	-4.82	-2.13	-3.59
W	0.32	4.26	-0.71	-1.07	-7.09	1.69	-7.58	-3.78	0.02	-8.31	-6.88	-0.74	-2.06	-0.76	-5.89	-3.03	-0.65	-2.13	-1.73	-12.39
Y	-4.62	-4.46	0.9	1.29	-8.8	-1.9	-3.2	-5.26	-1.19	-4.9	-9.73	0.93	-2.09	0.01	0.36	-0.82	-0.37	-3.59	-12.39	-2.68

1. Dosztanyi, Z., et al., *The pairwise energy content estimated from amino acid composition discriminates between folded and intrinsically unstructured proteins*. Journal of molecular biology, 2005. **347**(4): p. 827-839.
2. Arif, M., M. Hayat, and Z. Jan, *iMem-2LSAAC: A Two-level Model for discrimination of Membrane Proteins And Their Types by extending the notion of SAAC into Chou's Pseudo Amino Acid Composition*. Journal of Theoretical Biology, 2018.