

Multi-AOP: A Lightweight Multi-View Deep Learning Framework for Antioxidant Peptide Discovery

Jianxiu Cai,^{1,2,†} Xinpo Lou,^{1,3,†} Chak Fong Chong,^{1,2} Deepa Alex,⁴
Joel P. Arrais,^{2,*} Yapeng Wang,^{1,*} Shirley W. I. Siu^{1,3,*}

¹Faculty of Applied Sciences,
Macao Polytechnic University, Rua de Luís Gonzaga Gomes, Macau SAR, China

²Department of Informatics Engineering,
University of Coimbra, Paço das Escolas, Coimbra, Portugal

³Centre for Artificial Intelligence Driven Drug Discovery,
Macao Polytechnic University, Rua de Luís Gonzaga Gomes, Macau SAR, China

⁴BioMyne-Biotech Innovation and Engineering Ltd

[†]These authors contributed equally to this work.

^{*}To whom correspondence should be addressed;

E-mail: jpa@dei.uc.pt; yapengwang@mpu.edu.mo; shirleysiu@mpu.edu.mo.

Table S1: Abbreviation of peptide feature descriptors

Abbreviation	Descriptor Full Name
AAC	Amino Acid Composition
CTD-C	Composition
CTD-D	Transition
CTD-T	Distribution
CTriad	Conjoint Triad
DDE	Dipeptide Deviation from Expected Mean
GAAC	Grouped Amino Acid Composition
DPC	Di-Peptide Composition
GDPC	Grouped Di-Peptide Composition
GTPC	Grouped Tri-Peptide Composition
KSCTriad	k-Spaced Conjoint Triad
QSOrder	Quasi-sequence-order

Table S2: Ablation study of Multi-AOP across the three benchmark datasets

Dataset	Model	Accuracy	Precision	Sensitivity	Specificity	MCC
AnOxPePred dataset	xLSTM	0.7879	0.7957	0.7526	0.8093	0.5755
	MPNN	0.7473	0.7462	0.7185	0.7871	0.4935
	Multi-AOP	0.8043	0.8226	0.7556	0.8493	0.6086
AnOxPP dataset	xLSTM	0.9375	0.9483	0.9257	0.9537	0.8754
	MPNN	0.8703	0.8489	0.9009	0.8396	0.7420
	Multi-AOP	0.9684	0.9835	0.9528	0.9839	0.9373
AOPP dataset	xLSTM	0.8804	0.9168	0.8366	0.9359	0.7637
	MPNN	0.8201	0.8400	0.7855	0.854	0.6418
	Multi-AOP	0.9043	0.9646	0.8396	0.9690	0.8156