## **Supplementary Information**

Signal Peptide Prediction Using Machine Learning Approaches of Different Complexities

## Elias Kahl\*, Maximilian Mair\*, Julius Schlensok\* and Selin Türkoglu\*

\* all authors contributed equally.

TUM (Technical University of Munich) Department of Informatics, Bioinformatics & Computational Biology - i12, Boltzmannstr. 3, 85748 Garching bei München, Germany

## 2 Supplementary Information

AAindex ID(s)	Feature description	Original publication
KLEP840101	Net charge	Klein et al. (1984). Prediction of protein function from sequence properties. Discriminant
		analysis of a data base. Biochimica et biophysica acta, https://doi.org/10.1016/0167-
		4838(84)90312-1
KYTJ820101	Hydropathy index	Kyte & Doolittle (1982). A simple method for displaying the hydropathic character of a
		protein. Journal of molecular biology https://doi.org/10.1016/0022-2836(82)90515-0
RADA880108	Mean polarity	Radzicka et al. (1988). Comparing the polarities of the amino acids: side-chain distribution
		coefficients between the vapor phase, cyclohexane, 1-octanol, and neutral aqueous solution.
		Biochemistry https://doi.org/10.1021/bi00405a042
FAUJ880103	Normalized van der Waals	1
	volume	in biology and pharmacology. International journal of peptide and protein research
		https://doi.org/10.1111/j.1399-3011.1988.tb01261.x
MITS020101	Amphiphilicity index	Mitaku et al. (2002). Amphiphilicity index of polar amino acids as an aid in the
		characterization of amino acid preference at membrane-water interfaces. Bioinformatics
		(Oxford, England)
CHOP780201,	Normalized frequency of	, ,
CHOP780202,	alpha-helix, Normalized	amino acid sequence. Advances in enzymology and related areas of molecular biology
CHOP780203	frequency of beta-sheet,	https://doi.org/10.1002/9780470122921.ch2
	Normalized frequency of	
	beta-turn	
CHAM810101	Steric parameter	Charton (1981). Protein folding and the genetic code: an alternative quantitative model.
GU334030107	A	Journal of theoretical biology https://doi.org/10.1016/0022-5193(81)90377-5
CHAM830107	A parameter of charge transfer capability	Charton M. & Charton B. I. (1983). The dependence of the Chou-Fasman parameters on amino acid side chain structure. Journal of theoretical biology https://doi.org/10.1016/0022-
	Сарабініу	5193(83)90265-5
JANJ780101	Average accessible surface	` '
JANU / 80101	area	molecular biology https://doi.org/10.1016/0022-2836(78)90408-4
MEIH800103	Average side chain orientation	Meirovitch et al. (1980). Empirical Studies of Hydrophobicity. 1.
	angle	Effect of Protein Size on the Hydrophobic Behavior of Amino Acids.
	ungre	Macromoleculeshttps://doi.org/10.1021/ma60078a013
VELV850101	Electron-ion interaction	Veljković et al. (1985). Is it possible to analyze DNA and protein sequences by the
	potential	methods of digital signal processing?. IEEE transactions on bio-medical engineering
		https://doi.org/10.1109/TBME.1985.325549
WERD780101	Propensity to be buried inside	Wertz & Scheraga (1978). Influence of water on protein structure. An analysis of the
	. ,	preferences of amino acid residues for the inside or outside and for specific conformations
		in a protein molecule. Macromolecules https://doi.org/10.1021/ma60061a002
ZIMJ680105,	RF rank, Isoelectric point	Zimmerman et al. (1968). The characterization of amino acid sequences in proteins
ZIMJ680104		by statistical methods. Journal of theoretical biology https://doi.org/10.1016/0022-
		5193(68)90069-6

Table S1 . IDs of AAindex features which were used for creating the AAindex-encoding together with a short description which physicochemical property they represent and the original publication, from which the authors of AAindex collected the data. The values were parsed from the publicly available site at https://www.genome.jp/aaindex/