

Additional file 1

Each entry in the amino acid index has information organized as:

H Accession number

D Data description

R LITDB entry number

A Author(s)

T Title of the article

J Journal reference

C Accession numbers of similar entries with the correlation coefficients of 0.8 (-0.8) or more (less).

I Amino acid index data in the following order

Ala Arg Asn Asp Cys Gln Glu Gly His Ile
Leu Lys Met Phe Pro Ser Thr Trp Tyr Val

// Index separator symbol

An example amino acid index is shown below.

H ANDN920101

D alpha-CH chemical shifts (Andersen et al., 1992)

R LIT:1810048b PMID:1575719

A Andersen, N.H., Cao, B. and Chen, C.

T Peptide/protein structure analysis using the chemical shift index
method: upfield alpha-CH values reveal dynamic helices and aL sites

J Biochem. and Biophys. Res. Comm. 184, 1008-1014 (1992)

C BUNA790102 0.949

I	A/L	R/K	N/M	D/F	C/P	Q/S	E/T	G/W	H/Y	I/V
	4.35	4.38	4.75	4.76	4.65	4.37	4.29	3.97	4.63	3.95
	4.17	4.36	4.52	4.66	4.44	4.50	4.35	4.70	4.60	3.95

//

Figure 1: A sample entry in the AAindex database