Local-Fragment Formalism

In addition to ***total*** *algebraic indices* computed for the whole protein molecule, a **local-fragment** formalism can be developed. In this way, the matrix representations of the bio-macromolecular structures can be transformed to considerer information related with groups or amino acid-types belonging to a specific polypeptide fragment (*F*). So, these *local-fragment matrices* are used as matrix forms of the algebraic maps to compute the *local-fragment indices*. The amino acid-type fragments employed in this software are:

- Apolar (RAP)
- Polar positively charged (RPC)
- Polar negatively charged (RNC)
- Polar uncharged (RPU)
- Aromatic (ARO)
- Aliphatic (ALG)

Also we defined groups that include the amino acids that do not favor the folding and/or cannot be commonly found in proteins as part of α-helices or β-sheets (UFG), α-helices favoring amino acids (FAH), β-sheets favoring amino acids (FBS) and β-turns favoring amino acids (AFT). Additionally, groups composed of amino acids of the same kind (R amino acids) in the protein were defined, that is, 20 groups one per each natural α-amino acid, (e.g. F=Ala, F=Arg,…, F=Val). Table 1 shows the amino acidic composition of these local-fragments.

Table 1. Amino acidic composition of the local fragments pre-defined in the MuLiMs-MCoMPAs module of the ToMoCoMD-CAMPS software.

Local-Fragment	Amino acids
RAP[a]	PRO, ILE, ALA, VAL, LEU, PHE, TRP, MET.
RPC	LYS, HIS, ARG.
RNC	ASP, GLU.
RPU[d]	ASN, CYS, GLY, SER, THR, TYR, GLN.
ARO[e]	PHE, TYR, TRP.
ALG[f]	GLY, ALA, PRO, VAL, LEU, ILE, MET.
UFG[g]	GLY, PRO.
FAH[h]	ALA, CYS, LEU, MET, GLU, GLN, HIS, LYS.
FBS[i]	VAL, ILE, PHE, TYR, TRP, THR.
AFT[j]	GLY, SER, ASP, ASN, PRO.

[a:]Apolar; [b:]Polar positively charged; [c:]Polar negatively charged; [d:]Polar uncharged; [e:]Aromatic; [f:]Aliphatic; [g:]Unfolding amino acids; [h:]Helix favoring amino acids; [i:]Beta-sheets favoring amino acids; [j:]Beta-turn favoring amino acids