Matrix Representation

Three classes of matrices of order k ($k \in [-12,12]$) can be used in **MuLiMs-MCoMPAs software**, *specifically* Non-stochastic (NS), Simple-stochastic (SS) and Mutual Probability (MP) matrices.

1. Non-stochastic (NS) matrix

The codification of 3D information of the non-covalent interactions of the biomacromolecular (protein or peptide) structure is fulfilled through rules between pairs of atoms and the values of these rules are represented in the *two-tuples multimetric-(dis)similarity matrix* (M). When no normalizing procedure is performed over their elements, this matrix is denoted as *non-stochastic two-tuples multimetric-(dis)similarity matrix* ($_{ns}$M). The generalized expression of this matrix is the k^{th} *non-stochastic two-tuples multimetric-(dis)similarity matrix*, designated by $_{ns}M^{k}$ where superscript k indicates the power to which $_{ns}$M is raised. Thus, for k = 0, all coefficients $_{ns}m_{ij}^{0}$ corresponding to the matrix $_{ns}M^{0}$ have value 1; and for k = 1, the coefficients $_{ns}m_{ij}^{1}$ of the matrix $_{ns}M^{1}$, codify information about the interactions between two atoms. The formal definitions of these elements is shown below:

$$
{}_{\mathrm{ns}}m_{ij}^{1} = \begin{cases} D_{ij} & if\ i \neq j \\ D_{io} & i = j \\ 0 & otherwise \end{cases} \tag{1}
$$

where, D_{ij} is a (dis) similarity measure between two atoms, D_{io} is the Euclidean spatial distance between each atom i of the protein and the center o of the molecule. It should be noted that the diagonal entries could have assigned values different to zero values in order to achieve greater discrimination of the biomacromolecular structures.

2. Simple-stochastic (SS) matrix

The k^{th} *simple-stochastic two-tuples multimetric-(dis)similarity matrix* ($_{ss}$M^{k}), can be directly obtained from ($_{ns}$M^{k}). The coefficients of this matrix are computed as follows:

$$
{}_{ss}m_{ij}^{k} = \frac{{}_{ns}m_{ij}^{k}}{S_j} = \frac{{}_{ns}m_{ij}^{k}}{\sum_{j=1}^{n} {}_{ns}m_{ij}^{k}} \tag{2}
$$

where, ${}_{ns}m_{ij}^{k}$ are the elements of the k^{th} power of the matrix $({}_{ns}\mathrm{M}^{1})$.

3. Mutual probability (MP) matrix

The k^{th} *mutual probability two-tuples multimetric (dis)similarity matrix* ${}_{mp}\mathrm{M}^{k}$, can be obtained from ${}_{ns}\mathrm{M}^{k}$. The elements ${}_{mp}m_{ij}^{k}$ of this matrix are computed as follows:

$$ {}_{mp}m_{ij}^{k} = \frac{{}_{ns}m_{ij}^{k}}{S_{ij}} = \frac{{}_{ns}m_{ij}^{k}}{\sum_{i=1}^{n}\sum_{j=1}^{n} {}_{ns}m_{ij}^{k}} \quad \textbf{(3)} $$

where, ${}_{ns}m_{ij}^{k}$ are the elements of the k^{th} power of the matrix $({}_{ns}\mathrm{M}^{1})$.