Position probability matrix

$$PPM(\alpha) = \begin{array}{c c} & \begin{array}{ccc} 1 & 2 & m \end{array} \\ \begin{array}{c} A \\ R \\ n \end{array} & \begin{pmatrix} \alpha_{A1} & \alpha_{A2} & \alpha_{Am} \\ \alpha_{R1} & \alpha_{R2} & \alpha_{Rm} \\ \alpha_{n1} & \alpha_{n2} & \alpha_{nm} \end{pmatrix} \end{array} \tag{1}$$

Normalized inverted Shannon entropy for each alignment as conservation score

$$CS(m) = 1 - S(m) \tag{2}$$

$$S(m) = -\frac{\sum(\alpha_n * \log_2(\alpha_n))}{S_{max}} \tag{3}$$

Exchange probability

$$EP(m) = \begin{bmatrix} 0 & \alpha_{A1} * \beta_{R1} & \alpha_{A1} * \beta_{n1} \\ \alpha_{R1} * \beta_{A1} & 0 & \alpha_{R1} * \beta_{n1} \\ \alpha_{n1} * \beta_{A1} & \alpha_{n1} * \beta_{R1} & 0 \end{bmatrix} \tag{4}$$

Weighed exchange matrix (PAM, BLOSUM)

$$WEM = \begin{array}{c c} & \begin{array}{ccc} A & R & n \end{array} \\ \begin{array}{c} A \\ R \\ n \end{array} & \begin{pmatrix} 0 & i_{AR} & i_{An} \\ i_{RA} & 0 & i_{An} \\ i_{nA} & i_{nR} & 0 \end{pmatrix} \end{array} \tag{5}$$

Weighed exchange probability

$$WEP(m) = EP_m * WEM * \beta \tag{6}$$

where β is the influence of the matrix.

Subfamily specific residue (SSR) score of position m (ES_m)

$$SSR_{score}(m) = CS_m * EP_m * WEP_m \tag{7}$$