Bioinformation

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$$\hat{H}o_j = \frac{1}{\hat{H}o_{sum}} \sum_{i=1}^{N} H_i^r \begin{cases} \left[1 - \frac{1}{2}\left(7\left(\frac{r_{ij}}{c}\right)^2 - 9\left(\frac{r_{ij}}{c}\right)^4 + 5\left(\frac{r_{ij}}{c}\right)^6 - \left(\frac{r_{ij}}{c}\right)^8\right)\right] & \text{for } r_{ij} \le c \\ \text{otherwise} & 0 \end{cases} \quad \text{(Equation 2)}$$

where $\hat{H}o_j$ - the empirical hydrophobicity attributed to *j*-th grid point being the result of hydrophobic interaction of side chains of individual $\hat{H}_i^r$ hydrophobicity. $\hat{H}o_{sum}$ - sum of all grid points hydrophobicity, which makes the distribution of empirical hydrophobicity standardized. The r_{ij} is the distance between *i*-th effective atoms and *j*-th grid point characterized by zero hydrophobicity. Each grid point collects the observed hydrophobicity $\hat{H}o_j$ from effective atoms localized closer than 9Å (cut-off distance for hydrophobic interaction according to Levitt **[11]**). More details concerning the presented model can be found in recently published papers. **[8, 9, 10]**