

$$\hat{H}t_j = \frac{1}{\hat{H}t_{\text{sum}}} \exp\left(\frac{-(x_j - \bar{x})^2}{2\sigma_x^2}\right) \exp\left(\frac{-(y_j - \bar{y})^2}{2\sigma_y^2}\right) \exp\left(\frac{-(z_j - \bar{z})^2}{2\sigma_z^2}\right) \quad (\text{Equation 1})$$

where: $\hat{H}t_j$ denotes the hydrophobicity for j -th grid point (x_j, y_j, z_j) , the $(\bar{x}, \bar{y}, \bar{z})$ - the origin of coordinate system $(0,0,0)$ and $\sigma_x, \sigma_y, \sigma_z$ - the ellipsoid size ($\frac{1}{3}$ of the maximum length along each axis, respectively). The coefficient $\hat{H}t_{\text{sum}}$ (sum of hydrophobicity values attributed to all grid points) makes the $\hat{H}t_j$ standardized (the sum of $\hat{H}t_j$ over all grid points equal to 1.0).