

Table 6 introduces the metabolites in the *E. coli* glycolysis pathway compiled in this work, together with public database identifiers, size and concentration. The radius of metabolites (R_{vdW}) can be approximated by a calculation method for the van der Waals volume (V_{vdW}) (Equation 3) [47]:

$$V_{\text{vdW}} = \left(\sum_i^{\text{atom nr}} V_{\text{vdW}_i} \right) - 5.92N_{\text{B}} - 14.7R_{\text{A}} - 3.8R_{\text{NR}}, \quad (3)$$

which accounts for the van der Waals volume for each atom (V_{vdW_i}), the number of bonds (N_{B}), the number of aromatic rings (R_{A}) and the number of non-aromatic rings (R_{NR}) in the molecule. Each radius can then be calculated using the geometric relation $V_{\text{vdW}} = \frac{4}{3}\Pi.R_{\text{vdW}}^3$. Data on the molecular structure of the metabolites can be automatically retrieved from chemical databases, such as PubChem [18] and CheBI [19].