MACAL

Stefan Ascher[*]

April 4, 2007

MACAL calculates the mass of an amino acid sequence with the following formula:

$$MH_z^+(S) = \frac{\sum\limits_{k=1}^{n} (S_k + M_{S_k}) + T_N + T_C}{z} \pm P$$

$MH_z^+(S)$ Mass of sequence S with charge z

n Length of sequence

S_k Mass of amino acid at position k in sequence S

M_{S_k} Mass of modification at amino acid S_k, fixed or variable

T_N Addition to N-Terminus

T_C Addition to C-Terminus

P Mass of a proton, added or substracted depending on the species

---

[*]stefan.ascher@i-med.ac.at