

Chemical Formula Syntax

The chemical formula syntax supported by MassMatrix is explained by the following rules.

Rule 1: Normal chemical formulas for chemical compounds are supported.

Methane: CH₄ (or CHHHH if you prefer)

Water: H₂O or HHO

Rule 2: parentheses are supported for repeating units in the formula.

Glucose: (CH₂O)₆ equivalent to C₆H₁₂O₆

Rule 3: Nested parentheses ARE NOT SUPPORTED.

CH₃((CH₂CHOH)₂)₅CH₃ IS NOT ACCEPTABLE.

Rule 4: Negative numbers are supported.

CH₅H⁻¹ equivalent to CH₄.

Rule 5: amino acid residues (3-letter abbr. or 1-letter abbr.) are supported, but HAVE TO BE SURROUNDED BY CURLY BRACKETS.

Glycine residue: {G} = {Gly} = C₂H₃NO

Aspartic acid residue: {Asp} = {D} = C₄H₅NO₃

Glycine amino acid: H{G}OH = H{Gly}OH = C₂H₅NO₂

Aspartic acid: H{Asp}OH = H{D}OH = C₄H₇NO₄

Rule 6: "{amino acid sequence}" cannot be nested in a "()" for repeated sequence. But "()" can be used inside "{}".

A peptide with a sequence of GGAEDGGAED: H{GGAEDGGAED}OH =

H{(GGAED)₂}OH

NOTE: H{(GGAED)₂}OH IS NOT ACCEPTABLE.

NOTE: {G₂} IS NOT ACCEPTABLE EITHER. {(G)₂} is acceptable and equal to {GG}.

Rule 7: Only the following isotopes for Hydrogen, Oxygen, Nitrogen and Carbon are accepted.

²H: D

³H: T

¹³C: C(13)

¹⁸O: O(18)

¹⁵N: N(15)

Lysine labeled with six ²H: C₆H₆D₆N₂O

Arginine labeled with six ¹³C and four ¹⁵N: C(13)₆H₁₂N(15)₄O

For more information, please contact support@massmatrix.bio