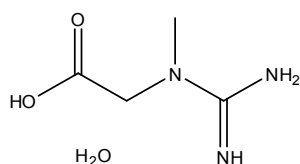
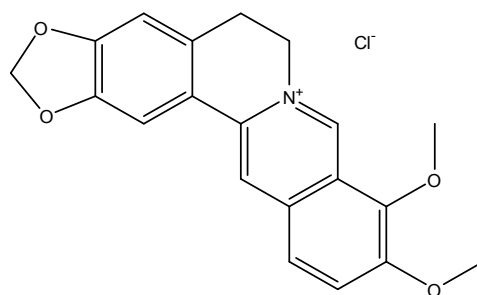


Tech Tip 0013 - *Hydrates and Salts*



Creatine hydrate



Berberine chloride

Many products in the ChromaDex® Phytochemical catalog are supplied in their hydrate or salt form. The main purpose of the addition of water or salts is to stabilize or increase the solubility of the parent chemical compound. Creatine hydrate and berberine chloride are such examples.

Chemical reference materials in the form of hydrates and salts are routinely used in quantitative analysis. Confusion is not uncommon when reporting the final values calculated with using such standards. The analyst must first determine if the end result will be reported as the hydrate or salt, or as the compound without the hydrate or salt. This determines how the initial calibration curve is generated.

Working with Hydrates

Hydrate, when used in a chemical name, indicates the substance contains water. This means there is a one-to-one ratio of a single molecule of water to a single molecule of compound such as in the creatine hydrate (C₄H₉N₃O₂•H₂O). Dihydrates and trihydrates are also known and defined as two molecules of water to one molecule of compound or three molecules of water to one molecule of compound respectively.

Example 1 – Determine the total amount of creatine in a sample.

The standard for creating the calibration curve is creatine hydrate, but creatine will be reported as the end result. The molecular weight of creatine hydrate is 149.15. The molecular weight of creatine is 131.13. The analyst must adjust the numbers in the calibration curve to match the compound without the hydrate. This is simply done by converting the actual weight of the standard by the percent creatine in the weighed out standard. Creatine is 87.92% w/w of creatine hydrate. So, 1 g of creatine hydrate would be equal to approximately 0.88 g of creatine. The adjusted value for creatine is then used to develop the calibration curve and the number generated by quantification will be in terms of creatine.

Example 2 – Determine the total amount of creatine hydrate in a sample.

Since the standard is creatine hydrate and the end result will be reported as creatine hydrate, no conversion is needed in the weight of the standard.

Working with Salts

Salts, such as chlorides, are used in a chemical name to indicate the substance contains a stabilizing ion such as Cl⁻ as in the compound berberine chloride (C₂₀H₁₈NO₄Cl). Many other salt forms exist: sulfate, nitrate, sodium, potassium, etc. Salts of a compound are commonly formed to generate a stable compound that is readily soluble in water or acid.

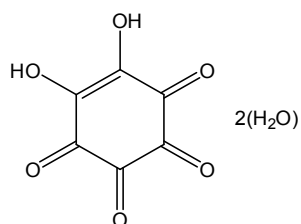
Example 3 – Determine the total amount of berberine in a sample.

The standard for creating the calibration curve is berberine chloride, but berberine will be reported as the end result. The molecular weight of berberine chloride is 371.81. The molecular weight of berberine is 336.36. The analyst must adjust the numbers in the calibration curve to match the compound without the chloride. This is simply done by converting the actual weight of the standard by the percent of berberine in the weighed out standard. Berberine is 90.47% w/w of berberine chloride. So, 1 g of berberine chloride would be equal to approximately 0.90 g of berberine. The adjusted value for berberine is then used to develop the calibration curve and the number generated by quantification will be in terms of berberine.

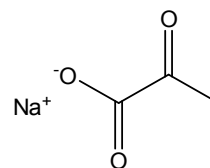
Example 4 - Determine the total amount of berberine chloride in a sample.

Since the standard is berberine chloride and the end result will be reported as berberine chloride, no conversion is needed in the weight of the standard.

Other examples of hydrates and salts include:



Rhodizonic acid dihydrate



Pyruvic acid sodium salt

Please contact your ChromaDex[®] Technical Sales Representative with any questions you may have.