

Example SI for Check AMM

A-level alert. The reported data should be reevaluated because it does not match the reported molecular formula. This conclusion is based on the recalculated mass error, which should be correct as long as the reported molecular formula is accurate, being larger than the mass error reported. It could suggest extraneous or missing atom(s) in the reported molecular formula.

- Example where correct accurate mass is **319.1329**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₃ **350.1111**; Found **350.1151**.
- Example where the molecular formula should be **C₂₁H₁₉O₃**, but there is an **extra O**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₄ 319. 1329; Found 319.1333.

B-level alert. The error is likely due to a typo in the reported molecular formula. Examples with invalid molecular formulas, for which no processing could be done by Check AMM, are also flagged under this alert.

- Example where the molecular formula has **unexpected capitalizations**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁**h₁₉O₃ 319.1329; Found 319.1333.**
- Example where the molecular formula has **unexpected notations**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉**o**₃ 319.1329; Found 319.1333.

C-level error. The reported mass calculation involved molecular weights instead of the accurate masses of the elements.

- Example where the accurate mass is **319.1329**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₃ **319.3746**; Found 319.1333.

D-level error. The errors are likely due to typos in the reported calculated and/or accurate mass.

- Example where the reported and measured accurate **masses differ in their integers**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₃ 3**2**9.1329; Found 3**1**9.1333.
- Example where the reported and measured accurate **masses have swapped digits**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₃ 319.**13**29; Found 319.**31**33.
- Example where the reported and measured **accurate masses differ only by one of their digits**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₃ 319.1**3**29; Found 319.1**2**29.

E-level alert. The reported accurate mass calculation involved adding H, Na, or K masses as 1, 23, and 39 respectively, instead of their accurate masses.

- Example where the accurate mass should be **319.1329**, but the **mass of H was added as 1**: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₃ **320.1334**; Found 319.1329.

F-level alert. The mass of an electron was not considered when calculating the accuracy mass. This flag is applied when the reported calculated accurate mass matches the accurate mass of the neutral molecule since compounds are converted to molecular ions by the mass spectrometer.

- Example where the **mass of the electron abstracted** was not considered: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₃ **319.1334**; Found 319.1329.

G-level alert. Not an input error.

- Example where there is no input error, but it is above the selected threshold in Check AMM: HRMS (ESI) m/z: [M + H]⁺ Cald for C₂₁H₁₉O₃ 319.1329; Found 319.1320.

Invalid format. The SI provided could not be processed due to unexpected inputs.

- Example: **HRMS ESI** m/z: calculated for C₂₁H₁₉O₃ found: 319.1320.