

example_SI

Date: 2024-12-11, Threshold: 0 ppm, Score: 1/11 (9%)

A Level Alerts: 2 (18%), B-E Level Alerts: 7 (64%), F Level Alerts: 1 (9%) G Level Alerts: 1 (9%), # of Invalid Inputs: 1

Page Number	Reported Molecular Formula	Reported Calculated Exact Mass	Reported Measured Exact Mass	Mass Error Reported (ppm)	Recalculated Exact Mass	Mass Error Recalculated (ppm)	Alert Level	Molecular Ion Type	Comments
1	C21H19O3	350.1111	350.1151	11.4	319.1329	88491.5	A	cation	Found mass matches erroneous formula, recheck data and/or look for extraneous or missing atom(s) in the reported molecular formula.
1	C21H19O4	319.1329	319.1333	1.3	335.1278	50118.6	A	cation	Found mass matches erroneous formula, recheck data and/or look for extraneous or missing atom(s) in the reported molecular formula.
1	C21h19O3	319.1329	319.1333	1.3	N/A	N/A	B	cation	Invalid molecular formula. Check for capitalizations, notations (i.e. 0's mistaken for O's), or any other typographical errors.
1	C21H19O3	319.1329	319.1333	1.3	2169.8905	5799323.4	B	cation	Potential invalid molecular formula. Check for capitalizations, notations (i.e. 0's mistaken for O's), or any other typographical errors.
1	C21H19O3	319.3746	319.1333	756.1	319.1329	1.3	C	cation	The molecular weight (319.3746) was calculated, not the accurate mass (319.1329).
1	C21H19O3	329.1329	319.1333	31333.6	319.1329	1.3	D	cation	The reported and measured accurate masses differ in their integers.
1	C21H19O3	319.1329	319.3133	565	319.1329	565	D	cation	The calculated mass and the measured mass appear to be transposed by two digits.
1	C21H19O3	319.1329	319.1229	31.3	319.1329	31.3	D	cation	The calculated mass might contain a typo.
1	C21H19O3	320.1334	319.1329	3135.1	319.1329	0	E	cation	It appears that the accurate mass was generated by calculating the accurate mass for the neutral molecule C21H19O3 (319.1334) and adding +1.0000 => 320.1334.
2	C21H19O3	319.1334	319.1329	1.6	319.1334	1.6	F	cation	The reported mass was calculated not taking into account the mass of the electron.
2	C21H19O3	319.1329	319.132	2.8	319.1329	2.8	G	cation	Above selected threshold.

Page Number	Reported Molecular Formula	Reported Calculated Exact Mass	Reported Measured Exact Mass	Mass Error Reported (ppm)	Recalculated Exact Mass	Mass Error Recalculated (ppm)	Alert Level	Molecular Ion Type	Comments
2	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	The SI provided could not be processed due to unexpected inputs.