



SmartFormula Manually

Lower formula:

Upper formula:

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. Collect adducts

Adducts, neg.

Measured m/z Tolerance: ppm Charge:

Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma
708.45221	1	C ₄₈ H ₅₈ N ₃ O ₂	100.00	708.45235	0.20	-0.43	13.1

Automatically locate monoisotopic peak Maximum number of formulae

Check rings plus double bonds Minimum Maximum

Filter H/C element ratio Minimum H/C: Maximum H/C:

Estimate carbon number Generate immediately