

DATE: 15 February 2019

TO: Thomas Blake

FROM: Eric Lucas and Bobby Brewer

SUBJECT: Calculations for Certificates of Analysis

This memo provides a summary of how molecular weights and isotopic purity were calculated for certificate of analyses. If you have any questions, please contact Bobby Brewer (brewerb@battelle.org; 614-424-7725) or Eric Lucas (lucasea@battelle.org; 614-424-7719).

The molecular weights of the acetylfentanyl-¹³C₆ was calculated using the following atomic weights:

Atom	Monoisotopic	Nat. abund. Avg.
C		12.011
H	1.0078250	1.00797
N	14.003074	14.0067
O	15.994915	15.9994
¹² C	12.000000	
¹³ C	13.003355	

The monoisotopic exact masses came from NIST at the following link: https://physics.nist.gov/cgi-bin/Compositions/stand_alone.pl. The natural abundance isotope-averaged masses are from the 1980 CRC Handbook of Chemistry and Physics and are a close match to the average values from the NIST website.

Isotopic purity is calculated by the ratio of the peak areas for the labeled material and the unlabeled material from the extracted ion chromatogram of the LC-MS/MS data. The quadrupole data uses a mass window of 0.5 Da (±0.25 Da). The extracted ion chromatogram is based on the sum for the mass window. Therefore, the extracted ion chromatogram for a selected mass (e.g., 329) includes the response for ±0.25 Da around the selected mass.

