**YOUR REFERENCE:** CFJ\_ILP1x

**OUR REFERENCE:** UEAFIL\_LQ7MM

ANALYST COMMENTS:

Date: 09/02/2023

Dear Claire,

The sample above was solvated in MeCN and analysed by negative ion nanoelectrospray (nESI) on the Advion nanomate and Thermo LTQ Orbitrap XL.

Single- and double-charged ion envelopes incorporating multi-isotopic elements (in this case Mo) were yielded at ~ 561 2+ and 1364 1+. Theoretical isotopic profiles were generated to match these species, [M-TBA]+ for ions around m/z 1364 and [M-2TBA]2+ for the ions around m/z 561. The isotopic profile matches concur – this provides us with confidence that these ions represent the proposed species and must be used as your evidence of identity in this case.

Normally, we would then try to match the accurately measured m/z of the molecule’s monoisotopic ion (*i.e. the ion that includes the lowest m/z isotopes of all incorporated species, and the only ion that is* ***not*** *a mixture, 6 x 92Mo*) with the theoretical m/z value. Unfortunately, with molecules like this that incorporate multiple highly multi-isotopic elements (Mo, W) , it is often not possible to observe the monoisotopic ion in the envelope as it is just too weak. All ions above this monoisotopic ion are mixtures of isotopologues, i.e. contributions from all the isotopes from all the incorporated elements, and so their measurement is **not considered accurate**. The most abundant isotope, 98Mo x 6, has been selected to match for your information only. As explained above, mixtures cannot be measured accurately for identity verification – you’ll notice the problem as the generated theoretical isotope profile values do not match the LIST theoretical m/z values.

Please consider the data and get back to me if you have any questions or require further analysis.

Kind regards, Ann