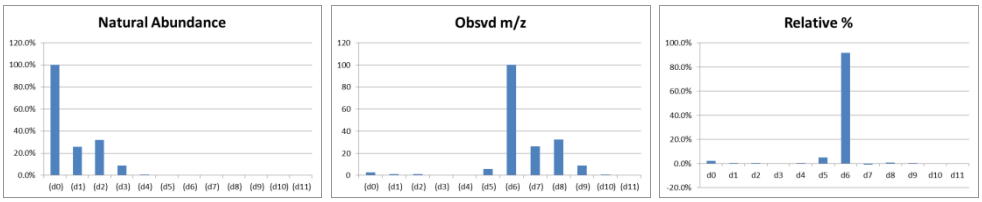
chemtos NEWS

MAY 18, 2022 VOLUME 22, NUMBER 1

Dear Sir/Madam,

It appears that the pandemic has finally become endemic, and we seem to have learned to live with and manage the disease! Hope you have a fantastic and productive Summer!

Let's discuss "isotopic purity" of a SIL (Stable-Isotope Labeled) compound. Each atom has a distribution of isotopes at natural abundance, for example carbon isotopes range from ^{8}C to ^{22}C, with major stable ones being ^{12}C at ~99% and ^{13}C at ~1%. (wiki) A molecule contains numerous types and number of atoms, each with their natural abundance distribution of isotopes. This translates to a distribution of isotopic masses for each molecule, which in a mass-spec detector is observed as a distribution of m/z. Presence of halogen atoms in a molecule usually widens the distribution. Now, when we replace natural abundance isotopes of atoms in a compound with heavier isotopes in order to synthesize the SIL compound, the expectation is that the m/z natural abundance distribution shifts to higher values without change – that would be 100% isotopic enrichment (or purity) of the SIL. In reality, the enrichment of the atomic isotopes within a molecule can vary and the natural abundance distribution is altered in the SIL as compared to natural abundance. The following is an example of SIL compound containing chlorine (and contained d0) that was analyzed for a client:



The isotopic purity can be estimated by fitting the observed m/z distribution with estimated natural abundance distribution to obtain relative % enrichment distribution. The Excel worksheet with the calculations can be found here ("save as" to download). Fill in observed m/z distribution for SIL and adjust d0 distribution to minimize negative relative % values. The Relative % distribution is the "Isotopic enrichment" distribution of the SIL compound – however, "isotopic purity" may be a little ambiguous and first requires proper definition that everyone can agree upon[1,2,3]!

Just a reminder that we at Chemtos have spent years optimizing our processes for accurate qNMR analysis using <5 mg of sample. We offer qNMR as analytical GLP re-certification service for $595 with turnaround time of 1-3 days. The process to submit sample for analysis is simple via a web submission form. NMR Services at Chemtos

A presentation that covers this discussion of CoA of organic compounds can be found here: https://www.chemtos.com/RefStd-CoA_discussion.pdf

"You guys are fantastic!" - 06/15/2021

"Thank you SO MUCH for your super-fast turnaround! " - 04/26/2022

"That was fast! Greatly appreciated!" – 03/18/2022

"the growing popularity of the qNMR technique you introduced us to. I have to say, since you educated us about its utility, it makes purity determinations MUCH easier." – 05/17/2022

Custom Synthesis of Ref Stds

With years of combined experience in varied chemical synthesis processes and isolation techniques, we have been able to synthesize and isolate compounds and metabolites at high purity, often in short time duration (typically less than 4 weeks). We find innovative ways to insert stable labels in the reference standards that we synthesize, even when others have struggled!

We are DEA licensed with quotas for manufacture of C-I through C-V compounds for use as analytical reference standards.

Analytical Services

Our standard GLP Certificate of Analysis includes (i) UV HPLC Purity assessment averaged over multiple absorbance wavelengths; (ii) LC-MS for confirmation of molecular weight; and (iii) Proton NMR analysis for molecular structure confirmation and residual protonated organic solvent determination. We also offer Quantitative proton NMR (qNMR) for potency value, KF titration for moisture content, Residue on Ignition for non-combustible inorganic salt content, Chiral HPLC and Optical Rotation analysis.

Catalog of in-stock Ref Stds

We carry a number of Certified Analytical Reference Standards in-stock (not for human consumption). All are accompanied by a comprehensive CoA that includes copies of the analytical data. We also offer DEA Exempt 1 ml solutions of analytical reference standards in flame sealed ampoules whose concentration has been confirmed using 2x quantitative proton NMR (qNMR) analysis.

Our web catalog can be found at Chemtos Web Catalog. Use of Search bar on top right is quite effective in finding compounds by name or CAS number or SMILES.

Please do not hesitate to contact us if we can be of any assistance in fulfilling your Certified Analytical Reference Standard or Compound Re-certification needs. We are at your service whenever you need us.

Sincerely,

Khalid Thakur

chemtos

Chemtos, LLC
16713 Picadilly Ct
Round Rock, TX 78664
Main: 512.686.4444