thermoscientific



Thermo Scientific mzCloud Library for confident and accurate PFAS analysis

Global regulatory bodies are investigating for the prevalence of per- and polyfluoroalkyl substances (PFAS) compounds due to their toxicity, persistence and wide-spread use, especially as aqueous film forming foam (AFFF). PFASs are also used in a wide variety of industrial and household consumer products such as carpets and furniture, food packaging, cookware. Human exposure to PFAS residues has been implicated in the incidence of cancer, obesity, endocrine system disruption, and other adverse health effects. It is estimated that there are over 6000 possible PFAS compounds. Quantitation and screening for the prevalence of any of these compounds at low levels is especially challenging.

To assist you in delivering high quality identification of fluorochemicals, Thermo Fisher Scientific has produced a high-resolution, accurate-mass (HRAM) library of PFAS compounds to deliver ultimate confidence and confirmation in the data you report. What makes this library especially powerful is that it is 100% curated with real standards on state-of-the-art Orbitrap[™] technology. Though some libraries may have more compounds, these are based on estimated structures based on lower resolution QTOF instrumentation – lower quality data will give more errors and lower confidence in library searches.

About mzCloud

The current Thermo Scientific[™] mzCloud[™] library is capable of PFAS analysis with:

- 43 standards
- HRAM MSⁿ data on each standard in negative mode and 100% curated
- Highest possible quality for mass accuracy and spectral reproducibility with multiple energy levels
- Compound identification based on MS/MS or MSⁿ data
- Similarity searching based on MS/MS or MSⁿ data to find unknown PFAS compounds



mzCloud is a state-of-the-art mass spectral database that assists analysts in identifying compounds in areas such as:

- Life sciences
- Metabolomics
- Pharmaceutical research
- Toxicology
- Forensic investigations
- Environmental analysis
- Food control
- Various industrial applications

The library features a freely searchable collection of HRAM spectra using a new third generation spectra correlation algorithm.

Compound list:

Perfluorobutanoic acid Perfluoropentanoic acid Perfluorohexanoic acid Perfluorohepatoic acid Perfluorooctanoic acid Perfluorononanoic acid N-[{Heptadecafluorooctyl}sulfonyl} -glycine Sulfuramide Perfluorodecanoic acid Perfluorododecanoic acid Perfluorohexadecanoic acid Perfluorooctadecanoic acid Perfluorotetradecanoic acid Perfluorotridecanoic acid Perfluoroundecanoic acid Perfluoro-1-butanesulfonic acid

Perfluoro-1-decanesulfonic acid Perfluoro-1-hexanesulfonic acid Perfluoro-1-octanesulfonic acid N-Ethylperfluoro-1-octanesulfonamidoacetic acid N-Methylperfluoro-1octanesulfonamidoacetic acid Perfluorooctylsulfonamide Bisperfluorooctyl phosphate Bisperfluorodecyl phosphate Perfluorooctyl phosphate Perfluorodecyl phosphate 4:2 Fluorinated telomer sulfonate Perfluoro-1-butanesulfonamide Perfluoro-1-hexanesulfonamide N-(3-(Dimethylamino)propyl) tridecafluorohexanesulphonamide

Figure 1: Fast separation of PFAS compounds.



6:2 Fluorinated telomer sulfonate

8:2 Fluorinated telomer sulfonate

10:2 Fluorinated telomer sulfonate 11-Chlorohexadecafluoro-3oxanonane-1-sulfonate

2,2,3-Trifluoro-3-(1,1,2,2,3,3-hexafluoro-3-trifluoromethoxy-propoxy)-propionic acid

Perfluoro-1-dodecanesulfonate

Perfluoro-1-pentanesulfonate

9-Chlorohexadecafluoro-3-oxanonane-1-sulfonate

Hexafluoropropylene oxide dimer acid

Perfluoro-1-heptanesulfonate

Perfluoro-1-nonanesulfonate

N-EtFOSE

5-(1,1,2,2,3,3,3-heptafluoropropyl)-N-methyl-1,3,4-thiadiazol-2-amine

Find out more at www.thermofisher.com/PFAS

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