

Structural and Quantitative Analysis of Polyfluoroalkyl Substances (PFASs) and para-phenylenediamines (PPDs) by Direct Analysis in Real Time and Ion Mobility and Mass Spectrometry (DART-IM-MS)

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Supplementary Information

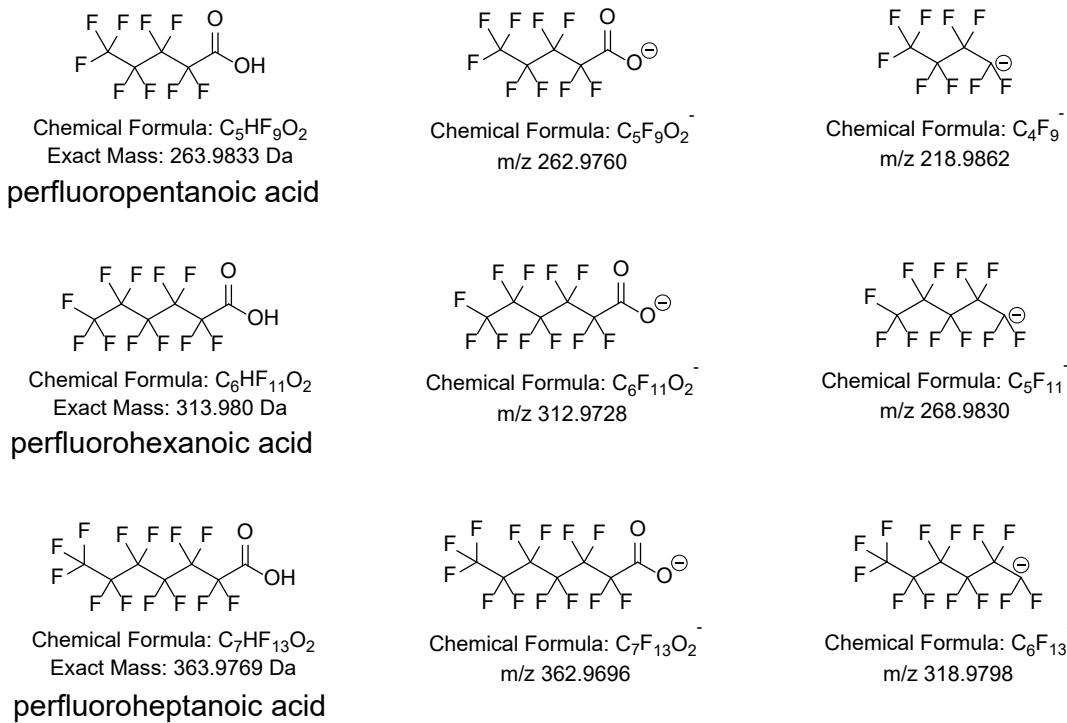


Figure S1: PFAS molecules studied and their $[M - H]^-$ and $[M - CO_2H]^-$ anions observed in negative ion mode DART-MS spectra: top, perfluoropentanoic acid (PFPA); center, perfluorohexanoic acid (PFHexA); bottom, perfluoroheptanoic acid (PFHepA). All quoted mass and m/z data are monoisotopic values.

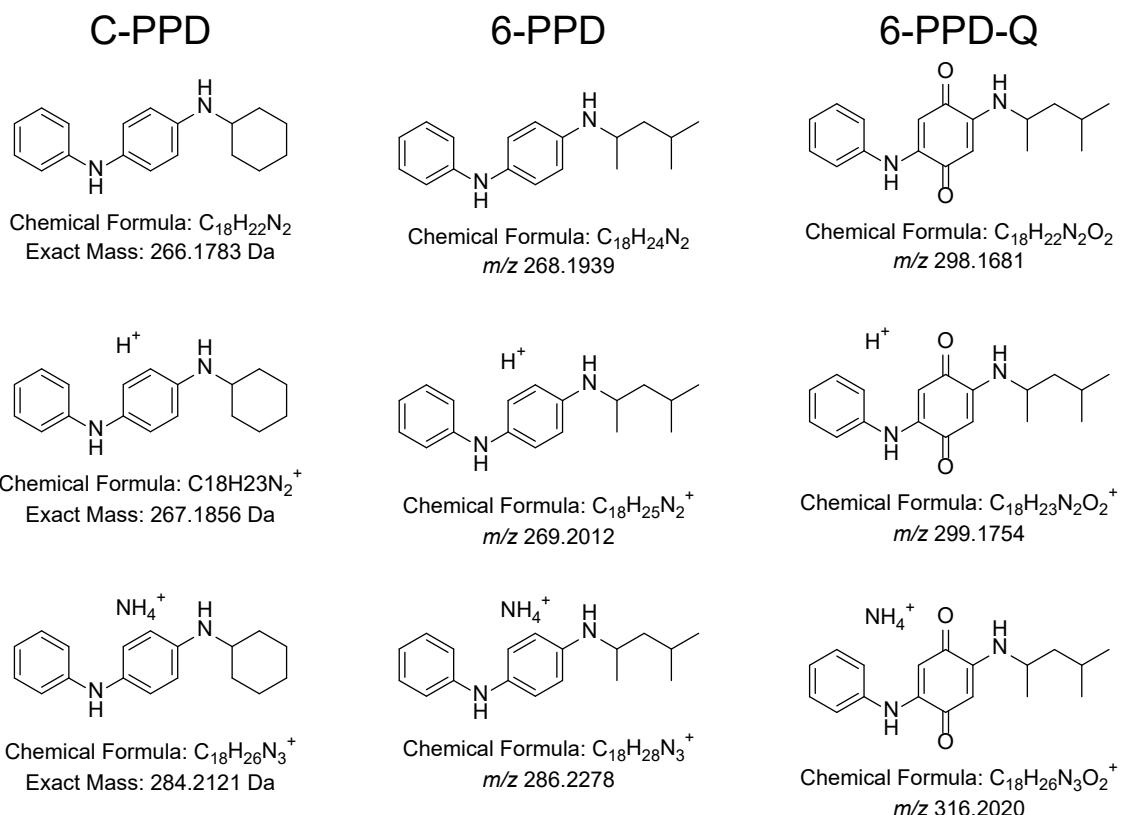


Figure S2: PPD molecules studied and their $[M + H]^+$ and $[M + NH_4]^+$ ions observed in positive ion mode DART-MS spectra: left, N-cyclohexyl-N'-phenyl-p-phenylenediamine (C-PPD); center, N-(1,3-dimethyl)-N'-phenyl-p-phenylenediamine (6-PPD); right, 6-PPD quinone). All quoted mass and m/z data are monoisotopic values.

Compound	Ion Structure	
Lactic Acid		Chemical Formula: $C_3H_7O_3^+$ m/z 91.0390
Caprolactam		Chemical Formula: $C_6H_{12}NO^+$ m/z 114.0913
Myristic Acid		Chemical Formula: $C_{14}H_{29}O_2^+$ m/z 229.2162
Palmitic Acid		Chemical Formula: $C_{16}H_{33}O_2^+$ m/z 257.2475
Oleic Acid		Chemical Formula: $C_{18}H_{35}O_2^+$ m/z 283.2632
Stearic Acid		Chemical Formula: $C_{18}H_{37}O_2^+$ m/z 285.2788
Cholestadiene		Chemical Formula: $C_{27}H_{45}^+$ m/z 369.3516
Bis(ethylhexyl Phthalate)		Chemical Formula: $C_{24}H_{39}O_4^+$ m/z 391.2843

Figure S3: Identified background ions from adventitious compounds in the atmosphere, which were used as internal calibrants for PFAS and PPD mass analysis. All quoted m/z data are monoisotopic values.



Figure S4: The QuickStrip DART sample plate which can hold up to 12 samples that are successively moved into the DART ion source at a preset speed.



Figure S5: The DART-SVP JumpShot ionization source attached to the timsTOF Pro 2 Bruker Q/ToF mass spectrometer.

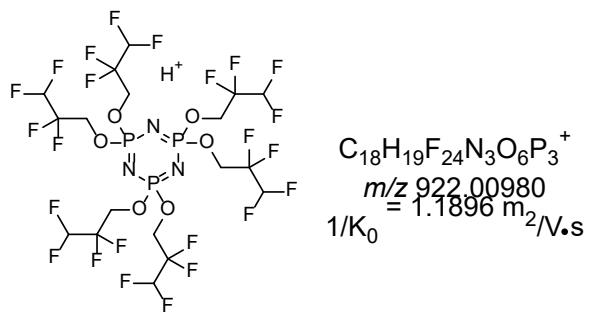
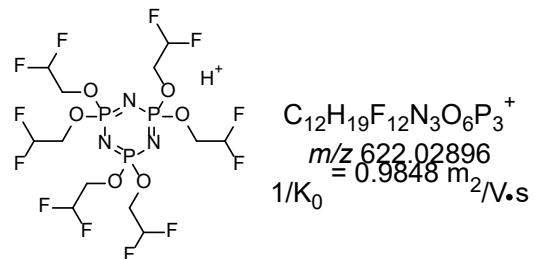
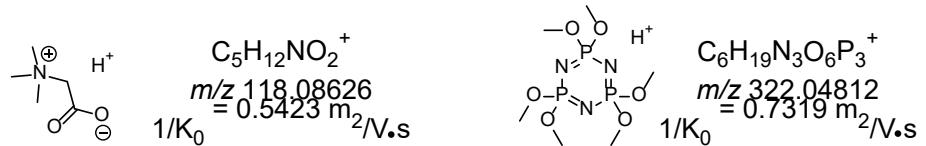


Figure S6: Agilent tune mix ions used for mass and ion mobility calibration.