

Deep-Learning-Enabled Rapid Annotation of PFAS: Enhancing Nontargeted Screening through Spectral Encoding and Latent Space

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Abstract

Detecting PFAS is challenging due to their diverse chemical structures, lack of standards, complex sample matrices, and the need for sensitive equipment to measure trace levels. Background contamination and the sheer number of PFAS further hinder the development of a universal detection method. Liquid chromatography–high-resolution mass spectrometry (LC-HRMS) is the primary tool capable of analyzing PFAS in water, soil, and biological samples, and

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