Random initialization of the excitation-emission matrix fluorescence spectral variables in constraint fashion for subsequent multivariate curve resolution alternating least square analysis on a peculiarly designed calibration set: Simultaneous sensing of nine polycyclic aromatic hydrocarbons in water samples

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Polycyclic aromatic hydrocarbons (PAHs) are carcinogenic and mutagenic in nature therefore their sensing in water sample is an important analytical task. In the present work, a novel approach that is based on the random initialization of the excitation-emission matrix fluorescence (EEMF) spectral variables in constraint fashion for subsequent multivariate curve resolution alternating least Square (MCR-ALS) analysis is introduced for simultaneously sensing the complex dilute aqueous mixture of PAHs. The usefulness of the proposed analytical approach is successfully demonstrated by applying it intentionally on a calibration set that is peculiar in many senses. The peculiarity mainly arises because the designed (i) the calibration set consist of nine PAHS having significant spectral overlap, (ii) the concentration of each PAH in different samples are kept constant and (iii) any two samples differ only in the presence and absence of the PAHs. The proposed approach is found to make precise and accurate estimation of each of the nine PAHs without involving any pre-separation. In summary, the proposed approach provides a simple and cost-effective procedure for simultaneous sensing of several PAHs in water samples. The proposed approach could be very useful in developing countries.