Electronic Supplementary Material (ESI) for Analytical Methods.
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Supplementary Materials for

Machine Learning and Signal Processing assisted Differential Mobility Spectrometry (DMS) Data Analysis for Chemical Identification

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1. Dispersion plots of mixture of chemicals

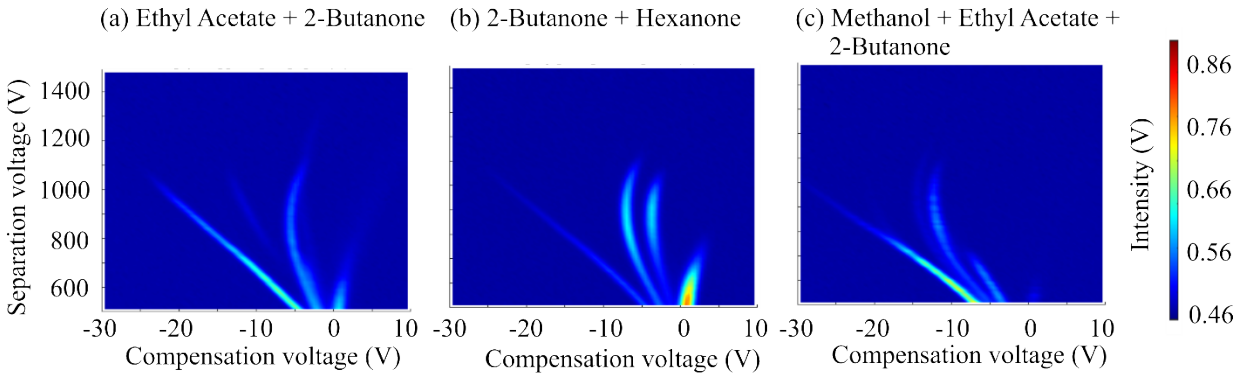

Figure S1: Dispersion plots of mixture of chemicals: (a) Ethyl Acetate + 2-Butanone, (b) 2-Butanone + Hexanone, and (c) Methanol + Ethyl Acetate + 2-Butanone.

2. Comparison of machine learning algorithms

Table S1: Comparison of different machine learning algorithms in identifying chemicals from the dispersion data of samples

	Approach	Reported prediction accuracy for testing data
Rajapakse et al. [1]	Partial least squared discriminant analysis	0-100% (performance varied depending on the mixture complexity)
Yeap et al. [2]	Support vector machine + Bag of visual words	~90 %
Li et al. [3]	Principal component analysis + support vector machine	66.7-80%
Li et al. [3]	Convolutional neural network	86.7 -100%
Current work	Convolutional neural network	~100 % (for the considered cases)

1. Rajapakse, M.Y., et al., *Automated chemical identification and library building using dispersion plots for differential mobility spectrometry.* Analytical Methods, 2018. **10**(35): p. 4339-4349.
2. Yeap, D., et al., *Machine vision methods, natural language processing, and machine learning algorithms for automated dispersion plot analysis and chemical identification from complex mixtures.* Analytical chemistry, 2019. **91**(16): p. 10509-10517.
3. Li, H., et al., *Identification of Specific Substances in the FAIMS Spectra of Complex Mixtures Using Deep Learning.* 2021. **21**(18): p. 6160.