

Received January 8, 2021, accepted January 27, 2021, date of publication February 10, 2021, date of current version February 12, 2021.

Digital Object Identifier 10.1109/ACCESS.2021.3056955

Employing and Interpreting a Machine Learning Target-Cognizant Technique for Analysis of Unknown Signals in Multiple Reaction Monitoring

RYAN A. MCCARTHY^{id} AND ANANYA SEN GUPTA^{id}, (Member, IEEE)

Department of Electrical and Computer Engineering, The University of Iowa, Iowa City, IA 52242, USA
Iowa Technology Institute (ITI), The University of Iowa, Iowa City, IA 52242, USA

Corresponding author: Ryan A. McCarthy (ryan-mccarthy-1@uiowa.edu)

This work was supported in part by the University of Iowa through the Iowa Superfund Research Program under Grant NIEHS P42 ES 013661, in part by the National Science Foundation under Grant 1808463, and in part by the Center for Health Effects of Environmental Contamination (CHEEC).

• **ABSTRACT** The aim of this interdisciplinary work is a robust signal processing and autonomous machine learning framework to associate well-known (target) as well as any potentially unknown (non-target) peaks present within gas chromatography-mass spectrometry (GC/MS/MS) raw instrument signal. Particularly, this