

INNOVATIONS IN NEXT GENERATION CB THREAT CHARACTERIZATION AND ASSESSMENT FOR DECISION SUPPORT

Earth's Field Nuclear Magnetic Resonance: A New Fieldable Spectroscopy For Organophosphate Detection

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There are millions of potential Organophosphorus (OP) chemical warfare agents (CWAs) due to the compositional flexibility of these nerve agents. Fieldable detection of CWAs is an on-going challenge that relies on reference library based analytical techniques, such as mass spectrometry and infrared spectroscopy. Nuclear magnetic resonance (NMR) is uniquely suited for structure determination, but the superconducting nature of the magnet prevents fielded analysis. In this study we turn to Earth's Field NMR (EFNMR), which has been made into a portable detector for OP CWAs. Until now, the spectral signatures of CWAs have not been thoroughly investigated using EFNMR. In this study, 30 CWA-relevant OP compounds were systematically studied to develop to EFNMR signature space of OP compounds. The compounds studied herein, are CWA surrogates, simulants, synthetic precursors, decomposition products, pesticides and NIH threat agents. EFNMR signatures for CWAs (including Novichoks) are reported for the first time using a combination of previously acquired high field NMR and insights gained from analysis of the EFNMR spectra. The results indicate that EFNMR provides a powerful analytical capability to distinguish the unique structure of OP compounds including CWAs. The spectral signatures are a diagnostic fingerprint of the molecular structure for virtually all OP CWAs, precursors, and hydrolysis products. The EFNMR signatures do not have background interferences, nor does it require a reference library making it an ideal candidate for fieldable analysis of known and unknown threats to protect the warfighter.