## THREAT AGENT DEFEAT MODELING AND TESTING USING WMD SIMULANTS

# Nuclear Magnetic Resonance At Low Magnetic Fields For Signature Detection Of Chemical Warfare Agents (CWAS) And Emerging Threats

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Rapid detection, identification, and forensic characterization of CWAs and Emerging Threats are critically important for the protection and health of the warfighter and for attribution. Three revolutionary, portable, low power, low cost, and cryogen-free NMR devices have been developed at LANL for rapidly detecting and identifying hazardous chemicals and emerging threats. One device, called SEDONA (SpEctroscopic Detection Of Nerve Agents), operates at a ~350 mT magnetic field and scans bottles and reports the presence of a nerve agent in less than 10 seconds. This system identifies G and A agents with no false positives or false negatives. The other two devices are Earth's-Field Resonance Detection and Evaluation (ERDE) devices (JOUSTER and FLOWSTER) which are NMR instruments that detect and quantitate the components of a mixture, identify a separated complex and its purity, and/or identify an unknown whether an organic or inorganic metal or metal complex. Operating at 50 μT (Earth's magnetic field), chemical shift data is significantly reduced and unimportant; however, the J-couplings between nuclei are retained and exquisitely observed because they are independent of the magnetic field. The observed signal line shapes are very narrow at Earth's field; consequently, richer coupling information is obtained for compound identification. Since the observed NMR frequencies at Earth's field are only ~4-6 kHz, simultaneous excitation and detection is allowed; consequently, LANL's ERDE devices detect, quantitate, characterize, and identify the structure and bonding of an NMR active nuclei in a single experiment. These three devices are paradigm shifts in signature detection capabilities and open new realms of measurement signatures for detection and identification of emerging threats.

Nuclear Magnetic Resonance properties, such as relaxation and spin density, at low magnetic fields from Earth's field to mT magnetic fields have been demonstrated as effective methods to distinguish threat materials without the need for large and uniform magnetic fields. However, these methods generally require prior knowledge and look-up tables with their associated issues to identify threat materials. Because of the combination of multi-modal NMR signatures that includes relaxation, spin densities, and the spectroscopic measurement of J-coupling with multiple hetero-nuclei detection (e.g., 1H, 19F, 31P, 14,15N) our new, quite powerful, and spectroscopic methods identify threats at low magnetic fields without the requirement for look-up tables. These devices have been recognized and received R&D100 Awards in Analytical Chemistry in 2020 (SEDONA) and in 2021 (ERDE) with ERDE also receiving a Silver Market Disruption award.

In this talk we will present past and ongoing work using NMR signatures at low magnetic fields to identify chemical threat materials, with a focus on liquids. We will showcase our efforts with SEDONA as a chemical threat detector for nerve agents with a high throughput (~10 sec) as well as our efforts with ERDE to utilize hetero-nuclear J-coupling at low magnetic fields for the detection and subsequent identification of chemical threats such as CWAs, other organophosphorus materials, and related emerging threats. Our work addresses the latest developments in the use of low magnetic field NMR for solving real, practical problems in National Security.