

NEXT GENERATION CB HAZARD PREDICTION AND CONSEQUENCE ASSESSMENT WITH MULTI-ECHELON DECISION SUPPORT APPLICATIONS

: Chemical Forensics Decision Support Via The Chemical Agents Reactions Database (card)

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The Chemical Agents Reactions Database (CARD) is a chemical structure/substructure-searchable database that contains over 3,000 key chemical reaction pathways (syntheses and decomposition) of selected chemical warfare agents, toxic industrial chemicals, pharmaceutical based agents, and explosives. CARD also compiles toxicological and physicochemical property data for numerous chemical threats encountered by first responders.

Under the direction of the Chemical Security Analysis Center (CSAC) of the U.S. Department of Homeland Security (DHS) Science and Technology Directorate (S&T), CARD was designed, developed, and deployed by SRC, Inc. This effort began in 2009, and 17 versions have been released and deployed on SIPRNet and will soon be available in an unclassified format to allow access for law enforcement organizations like the U.S. Customs and Border Protection (CBP), U.S. Coast Guard, Immigration and Customs Enforcement, Federal Bureau of Investigation (FBI), and the U.S. Secret Service. CARD undergoes continual maintenance to update data and introduce enhanced capabilities based on the most prominent and current emerging threat chemicals. CARD consists of a web application with a chemical substructure searching tool using Marvin JS and JChem Base (ChemAxon) that can query within the underlying database. CARD enables users to determine synthetic routes to known chemical agents, thus providing value to missions requiring chemical agent forensics. The database allows advanced queries to determine what combination of chemicals that might be found in the field could result in a synthetic route associated with toxic or hazardous chemicals. This capability can help facilitate identification of activities at a clandestine laboratory or validate sensor results from a sensitive site exploitation mission. In addition, CARD can facilitate identification of decontaminants that have been shown to be effective against known agents and the expected degradation products that one would expect.

CARD contains both unclassified and classified reaction sequences, which were extracted from source documents and presented as ChemDraw syntheses along with the appropriate preparation procedure and information on each chemical involved in the process. Reference documents associated with each reported reaction or chemical/toxicological data point are cited in the web application.

CARD serves as a centralized, vetted resource of reliable chemical threat data and supports the everyday missions of law enforcement with interdiction, prosecution, and reduction of drug proliferation. The system helps interagency users determine hazard and risk to personnel in the field and analysts to understand the true nature and origin of the illicit substance through forensic analyses conducted using CARD.

Thanks to DHS S&T CSAC and Battelle for many years of technical discussions and guiding the development of CARD as well as funding the launch of the web application.