Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000. This work was funded by the LDRD program.

Reducing the Global Danger of Weapons of Mass Destruction

NNSA Laboratory Directed Research & Development

innovation for our nation

Metabonomics for Detection of Nuclear Materials Processing

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What is the challenge?

▪ **Tracking Nuclear Materials production, especially covert operations, is a critical problem for nations worldwide. Model Additional Protocol now allows environmental sampling under certain conditions.**

▪ **Existing methodology relies heavily on isotope analysis. New methods that could detect chemical exposure, including chronic low level environmental exposure are desired.**

▪ **This project demonstrates the use of metabolic response (metabolic fingerprinting) within indigenous species as a possible tool for detection of specific chemical processing.**

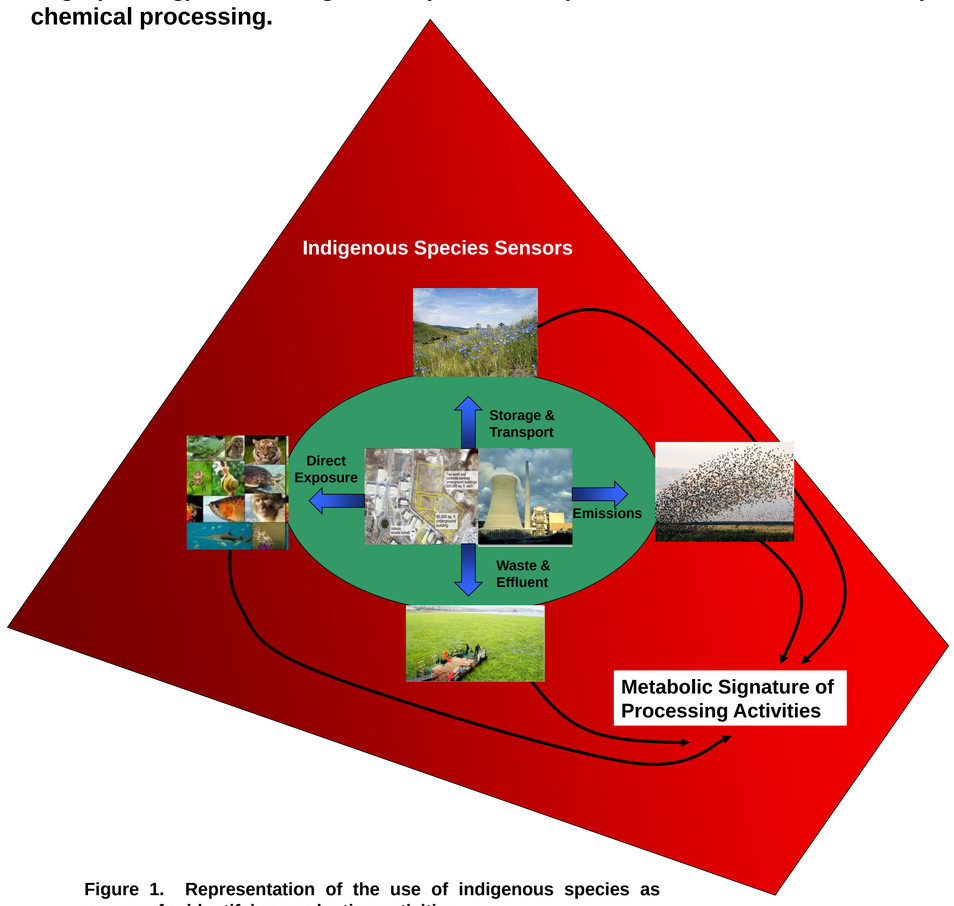

Figure 1. Representation of the use of indigenous species as sensors for identifying production activities.

What is our innovation?

In this project the metabolic response of different organisms monitoring nuclear magnetic resonance (NMR) spectroscopy is used to provide unique metabolic fingerprint that allows identification and tracking of exposure to chemicals used in nuclear materials processing activities.

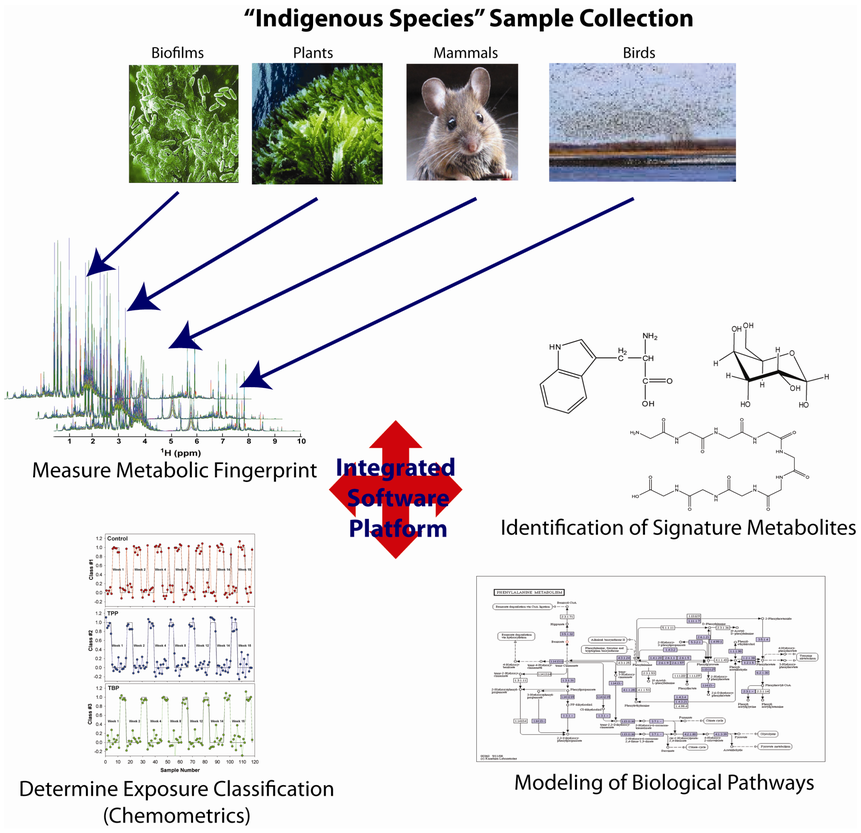

Figure 2. The metabonomics/metabolomic process for identifying chemical exposure.

What have we learned so far?

NMR spectroscopy in combination with chemometrics provides a method for detecting environmental exposure.

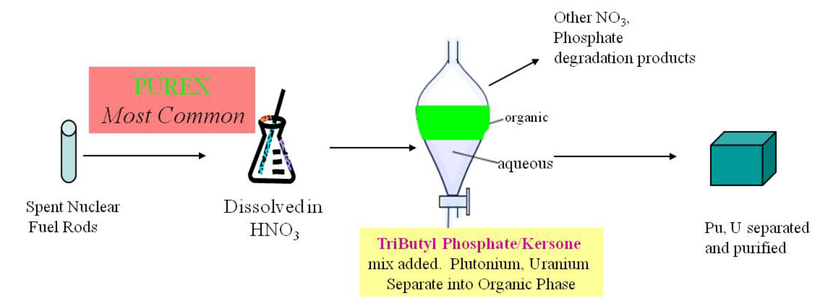

Figure 3. Schematic of the PUREX process from which we have targeted tributyl phosphate (TBP) as a signature of nuclear processing.

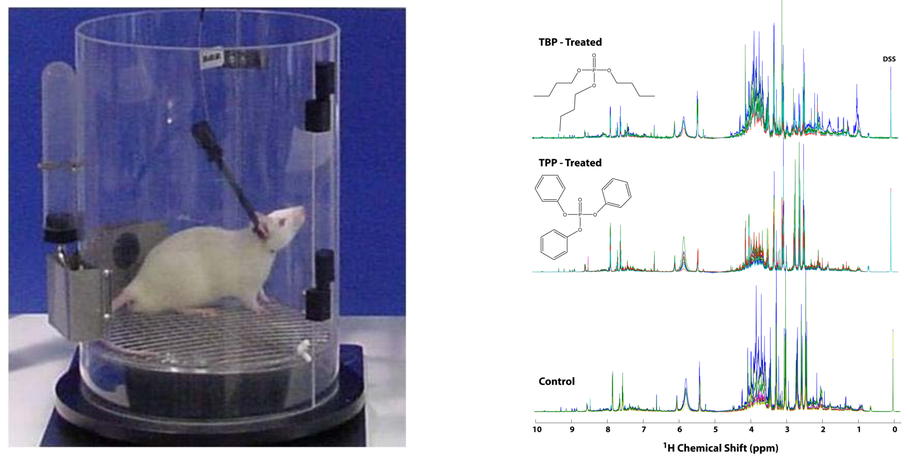

Figure 4. The experiment involved the exposure of rats to different doses of TBP followed by collection of the urine and subsequent NMR and chemometric analyses. In addition control animals and animals exposed to the common industrial chemical triphenyl phosphate (TPP) were also evaluated.

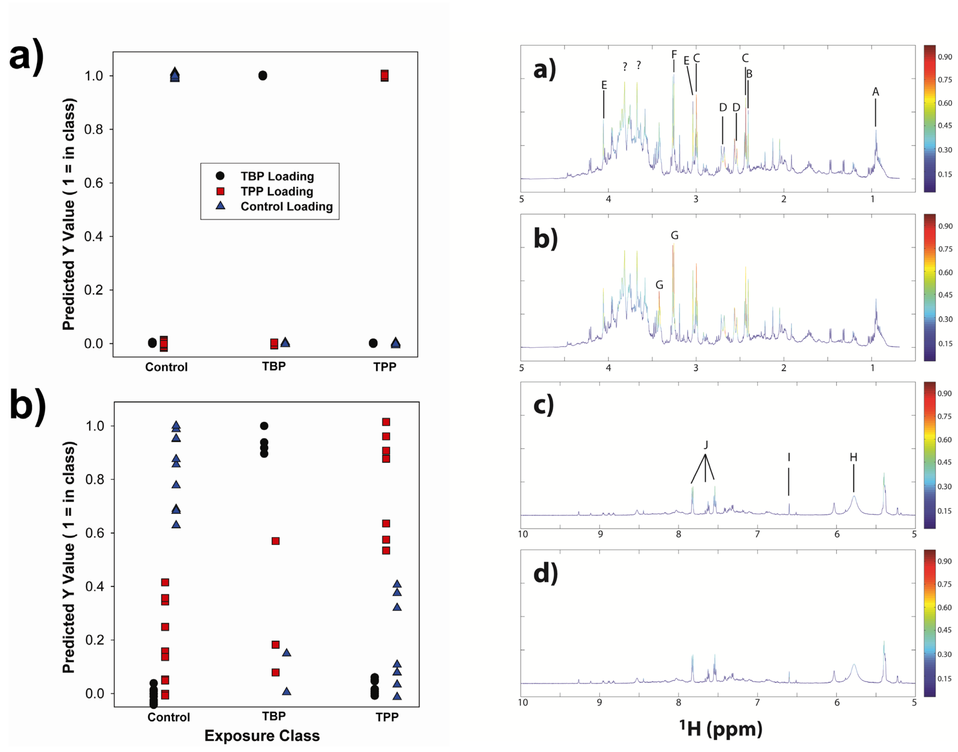

Figure 5. Classification results (Left) clearly identify TBP exposure from control and other background phosphate exposure. New chemometric tools (right) such as Orthogonal Partial Least Squares Discriminate Analysis (O-PLSDA) combined with Variable Importance in Projection (VIP) score weighting, provide the spectral signature responsible for this exposure classification.

Why is this important for our nation?

• Detection of covert nuclear materials processing facilities is of paramount importance to keeping our country safe.

• Metabolic profiling allows indigenous species, such as plants, animals or microbes to be used as sensors. Our approach allows hundreds of possible sensors, if not more, are always available to provide monitoring data.

• The method of metabolic profiling can be extended or applied to other chemicals of interest.

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