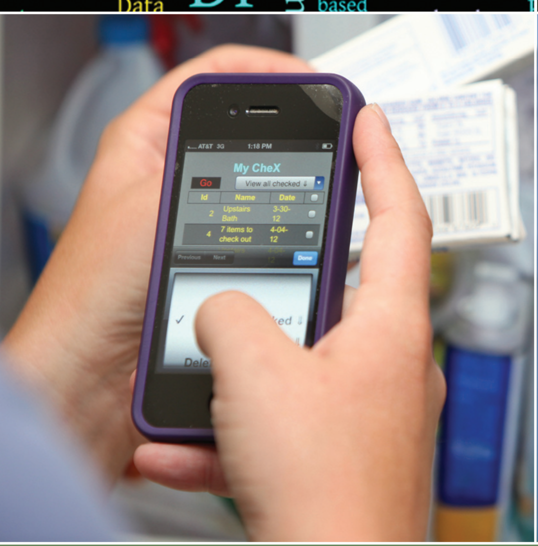
EPA/600/R13/041 | June 26-27, 2012 | Research Triangle Park, NC

EPA United States Environmental Protection Agency



Summary Report for Personal Chemical Exposure Informatics:

VISUALIZATION AND EXPLORATORY RESEARCH IN SIMULATIONS AND SYSTEMS (PerCEIVERS)

Office of Research and Development
US Environmental Protection Agency, Washington DC, 20460

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Summary Report for Personal Chemical Exposure Informatics:
VISUALIZATION AND EXPLORATORY RESEARCH IN SIMULATIONS AND SYSTEMS (PerCEIVERS)

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US Environmental Protection Agency, Washington DC, 20460

Disclaimer

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1.0
Introduction and Summary of Opening Remarks

Background, Purpose, Themes, and Topics of the Workshop

EPA Research Pathfinder Innovation Projects (PIPs), an internal competition for Agency scientists, was launched in 2010 to solicit innovative research proposals that would help the Agency to advance science for sustainability. In 2011, of the 117 proposals received from almost 300 scientists, 12 winners were awarded with seed funding to pursue their creative solutions to environmental and human health challenges. One of these projects was "Systems Reality Modeling Project, Step 1: Chemical Inventory." A team of nine scientists from the National Exposure Research Laboratory (NERL) and the National Center for Environmental Assessment (NCEA) (eight from NERL, one from NCEA) proposed to develop novel informatics and data curation approaches that both exposure assessment communities and proactive members of the public may use to become more aware of the chemicals present in our living space and lifestyle. This awareness is a component of "personal chemical exposure informatics."

A two-day workshop on Personal Chemical Exposure Informatics was held on June 26 and 27, 2012, at the US Environmental Protection Agency campus in Research Triangle Park, North Carolina. This report details the presentations and breakout group discussions to further advance this particular research field and identify gaps for additional efforts.

The three major topics in this workshop were:

1. Consumer product ingredient (chemical) informatics;
2. Real-time methods for monitoring human behavior/activity; and
3. Increasing chemical exposure awareness through motivational communication, curricula and participatory outreach development.

There was a diverse set of themes at this workshop that relates to personal chemical exposures informatics, including but not limited to:

- Exposure concepts: near-field and far-field sources
- Current consumer/personal exposure assessment models
- Household/consumer product ingredient (chemical) data-sources and open-access chemical information
- Human factors (activity and location pattern) data sources and survey methods
- Social media analysis and reporting methods for informing personal chemical exposure such as survey methods, data-mining, passive inquiry, and privacy/ethical considerations
- Data mining in support of Personal Chemical Exposure Informatics
- Gamification (application of game design thinking to non-game purposes) of exposure concepts and consumer product exposure modeling with emphasis on curriculum development for modeling processes and variables associated with personal exposure
- Personal informatics tools development for chemical exposures or "chemically-related" decision processes
- DIY community for tools/methods/apps development for monitoring personal chemical exposures – crowdsourcing initiatives and open-data exchange
- Novel data visualization/analytic representations (communications/outreach and rendering of information) for communities/consumers and educators/DIYers for personal chemical exposure awareness
- Data/effort sharing Personal Chemical Exposure and Personal Informatics (life-logging and life-streaming concepts)

Workshop Organization

A total of 27 presenters and 43 workshop participants attended (both physically and remotely) the PerCEIVERS workshop (Agenda see Appendix A). The presenters came from a variety of research disciplines/interests (i.e., exposure and dosimetry modeling) and types of organizations - i.e., private industry, non-profit organizations (creative arts, science advancement [e.g., SHODOR and NC Life & Science Museum], and academia), and government agencies (e.g., US EPA, USDA, NLM, and CPSC) - to discuss and explore strategies for filling gaps in data, modeling, and communication in the greater realm of personal chemical exposure informatics.

This workshop was held to stimulate development and promote collaboration on the use of ubiquitous computing devices (smartphones, tablets, notebooks) by individual modern consumers as a means to identify chemical exposures

Figure 1: Presentation Roster of title slides (overview) for PerCEIVERS 2012 of all presentations.

arising from their personal actions (activities and location) and the consumer products they use, as inspired by the Systems Reality pathfinder innovation project. [1]

Another objective of the workshop was to investigate personal chemical exposure informatics in the broader context of exposure types and sources. This context includes strategies for communicating personal chemical exposure awareness through a variety of venues: from product bar-code scanning, to activity/location (behavioral) recording via smart-journaling or passive network monitoring, to scenario exploration. Presenters and participants delved into the challenges of describing human-product-chemical systems and modeling their interactions in our everyday life.

There were seven sessions with a total of 27 presentations, of which 8 were performed remotely over multiple time-zones (Berlin Germany, North Carolina, and San Francisco). Streaming live-video was available, and Adobe Connect was used for remote slide-casting. All presentations were annotated on the fly and video-recorded for later analysis.

A full list of attendees and their biographical information, as well as the biographies of the presenters, can be found in Appendix B.

[1] Additional information:
(a) http://www.epa.gov/ord/sciencematters/june2011/pathfinder.htm
(b) http://www.epa.gov/ord/sciencematters/june2011/innovation.htm
(c) http://www.epa.gov/sciencematters/december2011/executivemessage.htm
(d) http://www.epa.gov/heasd/research/srm.html

2.0
Summary of Workshop Presentations

A list of presentation titles, presenter affiliations, and session chairs is available in Appendix A. In addition, the presentations can be viewed in their entirety in Appendix D.

The text from all 27 presentations was placed into many-eyes (www.many-eyes.com) to construct a visual synopsis of the PerCEIVERs workshop, providing a visual representation of the major themes of the workshop (see Figure below). The major themes have arbitrarily been colored:

- Red – Supporting exposure assessment (modeling and informatics/knowledge-based approaches)
- Blue- Understanding personal chemical exposure from the use of consumer products
- Green- Identifying information gaps pertaining to (a) chemical ingredients of products; (b) human time-location activity data; and
- Yellow: (c) product use information.

There were seven sessions in the workshop, and each session had three to five presentations.

1. Overview and innovation

In this session, Dr. Peter Preuss (EPA) presented the EPA Office of Research and Development's (ORD) innovation strategy and gave an overview of the Pathfinder Innovation Projects (PIPs). Dr. Michael-Rock Goldsmith (EPA) and Mr. Ryan Edwards (Shaw University Summer Research Internship 2011) gave an overview of the Systems Reality Modeling (SRM) project, which was one of the 12 awarded PIPs. The SRM project is a multi-part project that characterizes an individual's consumer product inventory, links consumer products to chemical ingredients, collects individual time/location activity patterns, and simulates personal chemical exposures. Ms. Madeline Reich (Shaw University Summer Research Internship 2012) used several case studies to demonstrate, as part of the SRM project, how social network analysis can be used to obtain human time-location activity patterns passively.

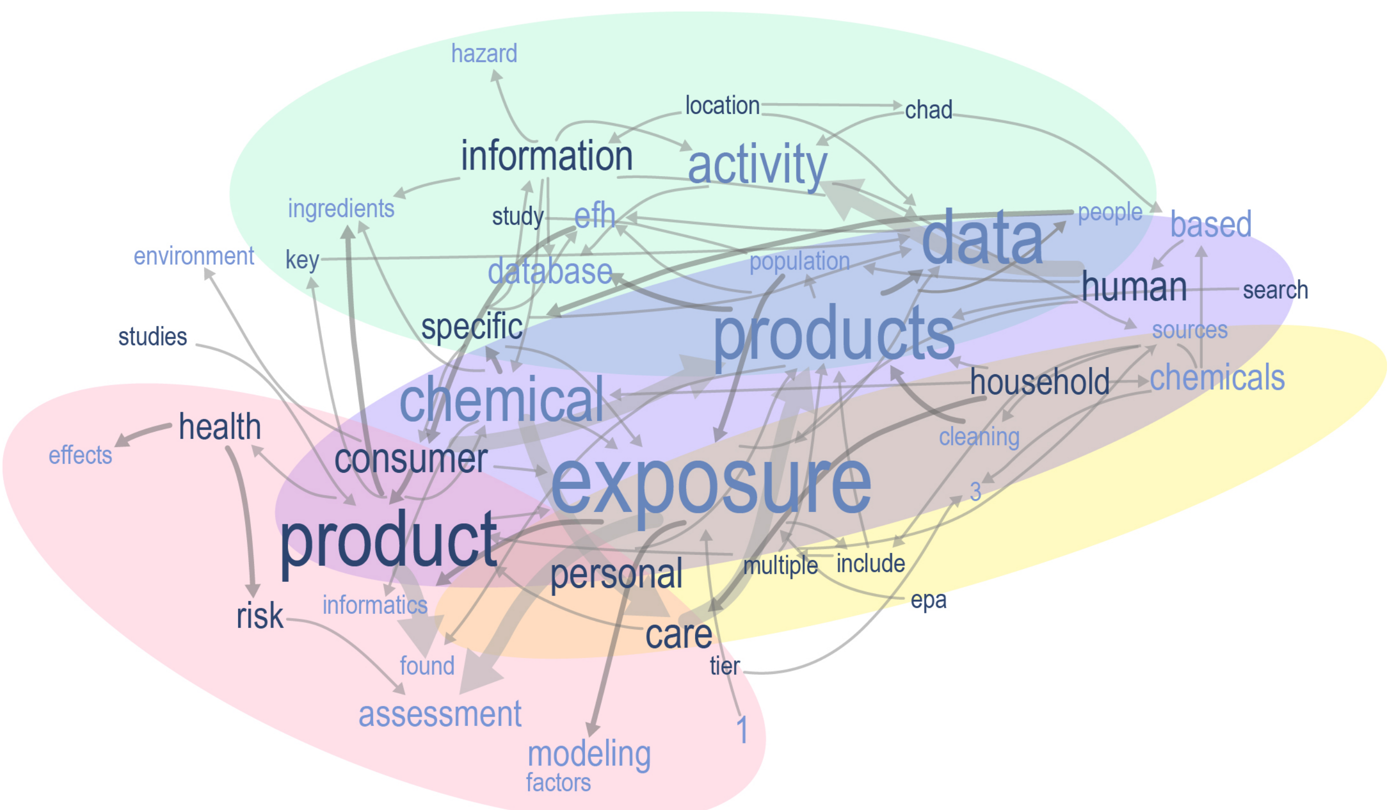

Figure 2: Phrasenet map of all text information from all presentations presented at PerCEIVERS 2012 (visualized in www.many-eyes.com, color for conceptual domains manually added.)

2. Exposure-based chemical prioritization

In this session, Dr. Elaine Cohen-Hubal (EPA) presented the basic concepts of exposure science, and the framework of ExpoCast™, which is a tool for chemical prioritization based on exposure potentials. Dr. John Wambaugh (EPA) presented an approach, in ExpoCastTM, which uses production volume to predict exposure potentials. Dr. Jade Mitchell-Blackwood (USDA) introduced a "Multi-Criteria Decision Modeling" framework for prioritizing chemicals for more targeted testing based on chemical properties and life cycle considerations.

3. Exposure factors and informatics

In this session, Dr. Linda Phillips (EPA) introduced the EPA's Exposure Factor Handbook and its Consumer Products Use Data. Dr. Kristin Isaacs (EPA) described the critical attributes of human activity patterns and their uses in exposure assessment and exposure modeling. She also presented current databases, tools, and projects on collecting and analyzing human activity pattern data. Dr. Deborah Bennett (University of California, Davis) presented her study on using bar code scanner and motion sensors to evaluate the use of personal and household care products with minimal burden to the study participants. Mr. Michael Keating described how smart phones can be used as a flexible research tool to conduct surveys, obtain micro-level location data, or collect data on air quality, physical activity, etc. Dr. Curry Guinn (The University of North Carolina at Wilmington) presented their autocoding program that maps the text of voice diaries to the EPA's Consolidated Human Activity Database (CHAD).

4. Consumer exposure models

In this session, Ms. Cathy Fehrenbacher gave an overview of the current exposure tools and models used by the EPA's Office of Pollution Prevention and Toxics (OPPT). Dr. Christina Cowan-Ellsberry (The Lifeline Group) presented the three types of information needed for exposure assessment: chemical-specific, product-specific, and people-specific information, as well as example sources for these data. She also introduced probabilistic models to estimate aggregate exposures. Selection of distributions for model parameters was also discussed.

5. Chemical information for consumer products

In this session, Dr. Antony Williams (Chemspider at Royal Society of Chemistry) gave an overview on the free chemical database, ChemSpider. Dr. Henry DeLima (householdproducts.nlm.nih.gov) introduced the Household Products Database which contains over 12,000 consumer products in nine product categories. Dr. Rogelio Tornero-Velez (EPA) presented the idea that human activities and chemical use patterns are not random events. Dr. Treye Thomas (US Consumer Product Safety Commission) gave an overview of the mission and the type of research conducted by the US Consumer Product Safety Commission.

6. Participatory methods and personal informatics

In this session, Dr. Bill Pease (GoodGuide.com) introduced a web-based platform (GoodGuide.com) that tracks the health, environment, and social aspects of products, brands and companies, for helping buyers to make purchase decisions. Mr. Michael Nagle (QuantifiedSelf.com and theSprouts.org) introduced the Quantified Self which is a collaboration of users and tool makers who are interested in self-tracking, such as exercise, diet, or sleep, using computers, phones, and other methods. Dr. Michael Breen (EPA) presented his research on using Microenvironment Tracker to record time and duration people spent in microenvironments for supporting exposure modeling. Ms. Shannon O'Shea (EPA) introduced the EPA's Community-Focused Exposure and Risk Screening Tool (C-FERST) which is a community mapping and assessment tool to support decision making.

7. Engaging the community for personal chemical exposure informatics: gamification, visual and computer models, electronic and live-action role play

In this session, George Scheer (elsewhere) presented on the artists in residence community and living museum known as 'elsewhere' (http://www.goelsewhere.org/), where the public and artists mingle (live action role play) and explore our relationships with everyday things. Dr. Benjamin Balak (Rollins College) discussed the current stasis of pedagogy in our school systems, and presented on his use of games to teach economics and game theory, how games enable so-called ADD kids to focus and learn for hours at a time, and the motivation for gamifying disciplines such as exposure science. Dr. Robert Panoff (Shodor) presented on the benefits of visual dynamic learning and agent based simulation approaches developed at Shodor (http://www.shodor.org/), and why computational chemistry needs to be within the reach of high school students. Bech Tench (Museum of Life and Science) spoke of the Experimonth sessions at the Durham museum; one monthly session involved exploration of prisoner's dilemma, another involved rhetorical analysis of texts among an online group to identify markers of learning (evidenced by changes in text sentiment).

3.0 Summary of Workshop Discussions and Outcomes

3.1 Breakout Discussions

The breakout sessions for PerCeivers mirrored the overall workshop themes (**see Appendix C**). A total of five themes (Themes A-E) with some intentionally open-ended questions were provided (see below) to the workshop participants to facilitate free discussion on these topics. A summary of the questions and discussions in each of the five ***Breakout Group Discussion Themes (A through E)*** are provided below. Additional web sites mentioned throughout the course of this exercise are provided in **Appendix E**.

THEME A.
Exposure factors informatics, e.g., real-time human factors

Discussion summary:

- How to make data available?
  - First, identify the information needed. For example, identify the important parameters needed to properly describe an exposure scenario.
  - A lot of data are available already. We may get those data from structured querying or asking around (e.g., manufacturer or marketing group)
  - One needs to be cautious about the accuracy of the acquired data. Also, these data often lack an estimate of variability.
  - Should we reward companies for being more open by providing data?
- How to conduct inventories and estimate exposures?
  - Linking products to exposure scenarios for estimating exposures.
  - Frequency and duration information needs to be collected, but it is difficult to collect such information for certain products.
  - How representative is a generic product that is linked to an exposure scenario?

THEME B.
Consumer/personal exposure modeling

Discussion summary:

- How to protect private information?
  - Not all "unprotected" information is public information. How do we identify which information we can use without consent?
  - There are many restrictions for government agencies to collect or use private information (e.g., Privacy Act of 1974), but those restrictions may not apply to other non-government agencies. Can government agencies still use the results of these findings?
  - How reliable are the data collected from social networks?
  - There are many methods to aggregate and anonymize data collected from individuals (e.g., Silent Spring study).
  - Do "observations" count as "surveys" (e.g., counting numbers of joggers in 10 min in different seasons)?
- What are the innovative methods to discover trends in human activity?
  - One use for aggregated and anonymized data is to discover trends of human activity over time, across populations for comparison.
  - The North Carolina Museum of Life and Science collects data from attendees to generate hypotheses for more targeted research.
  - Some example tools for discovering trends include Google, alpha engine, RADIANG, SPSS Text analytic, wikigroup, and concept maps.
  - PatientsLikeMe.com is a data-driven social networking site that collects disease, symptom, and treatment information from members.
  - Can Google popularity assessment be used to rank product use in a population? Currently, there are databases on products, but no analysis on ranking the uses of different products (e.g., by weight purchased per year?).
  - Challenges with collecting, curating, storing, searching, sharing, analyzing, and visualizing Big Data.

THEME C.
Chemical informatics for consumer products, i.e., consumer product chemical ingredient data sources, data mining, analytics, and visualization

Discussion summary:

- What categories of products are important in terms of data needs?
  - Articles, such as furniture, appliances, and non-household products (e.g., building materials)
  - Toys
- Are there any chemicals/products of emerging concern or lifestyle changes for which consumer use information does not exist?
  - Brominated flame retardants
  - Electronics (e.g., cellphones, tablets)
  - Nanomaterials

    - Lifestyle change: the advancement of technology makes people stay indoor longer.
- What can be done to make product/chemical information more easily attainable?
    - Voluntary vs. regulatory (State or Federal)? Purchase information from industries?
    - May get access to data through 3rd party certification groups (e.g., Green Guard)

THEME D.

Participatory methods and personal informatics tools, e.g., social media mining/analysis and reporting, DIY community

Discussion summary:

- When using personal monitoring or social media to gather consumer use data, what are the data biases (e.g., groups that have no access to/interest in social media)
    - The types of biases of interest depend on whether we are analyzing existing data or designing new studies
    - Targeting vs. self-selection
    - Lower socioeconomic classes are typically under-represented. For these classes, we may provide them access to technology (e.g., cellphones, internet access)
    - Older generations are typically under-represented when analyzing social media data.
    - App use varies widely by age ("App use" covers the number of apps, the identity of apps, and the categories of apps that are used by different age groups)
    - Based on the methods used, can we identify the population represented?
    - Can social media tell us what is really happening?
    - Is knowledge gained from old-fashioned surveys still applicable?
    - May be difficult to collect information from one individual for a long period of time. Sometimes, the best approach may be combining results from several people to represent one scenario.
- How to engage DIYers to develop an app or game to collect product/chemical use data and/or product/chemical inventories?
    - Government "challenges"
    - Look for those who are already at stake
    - Examples of PatientsLikeMe.com, QuantifiedSelf.com and curetogether.com. People like to compare themselves to others in a community.
    - Examples of shopper cards or loyalty programs.
- What are the elements to make a tool, game, or learning module ideal for combining consumer use data with household product inventories?
    - Pitch the tool, game or learning module as something fun or useful to the users, not as a way to get something from the users.
    - Fun, low burden, visual.
- Are there privacy concerns? What is the public health message that can be sent?
    - If the purpose is behavior modification, then it is "Big Brother".
        - "Opt in" vs. "Opt out"
    - Must consider biases
        - Aggregating data may be needed to protect privacy, but the utility of these data may be limited.

THEME E.

Data visualization and analytics for engagement and communication, e.g., gamification and computational simulations, novel data visualization/analytic representations, sharing personal chemical exposure informatics

Discussion summary:

- Need to provide incentives to motivate participation.
- A video of walking through the house may be a better survey than answering questions online.
- What is the best point of data collection (e.g., checkout line at the supermarket)?
- Forming groups to build the tool together.
- Government monitoring data, such as activity mapping or exposure factors, can be useful to parameterize the models.
- People generally want to know more about themselves, so setting goals or competing in a game will get them interested.
- One idea: scan the barcode of a product and the product becomes a character in a game. Players can fight against each other with their "products" and the most "toxic" one wins.

3.2 Workshop Outcomes

Introductions The opening session of the workshop introduced some of the newer areas of innovation at the US EPA related to the pathfinder innovation projects in ORD. The natural segue was to bring up the concept of systems reality modeling and how to model the various facets of personal chemical exposure using chemical ingredient profiles of everyday household products, to understanding or developing passive interrogation methods in order to capture human-activity patterns with unprecedented temporal-spatial resolution using geo-coded and seasonal big-data streams and clever data mining techniques. This introductory section brought forth the PIP innovation projects (Preuss), the SRM PIP1 (Goldsmith) and provided two excellent examples of sub-domains of this research performed by exceptionally gifted highschool students (Edwards & Reich).

Presentation Session 2 focused on different prioritization approaches on chemicals based on their exposure potentials. It was suggested that the most critical outcome would be a fundamental transformation in exposure science to realize the NRC vision for toxicity testing, in which human exposure information is critical for guiding the development and use of toxicity information. Two examples were provided to demonstrate the beginning of such a transformation. One example showed that despite very large uncertainties in the exposure estimates, it is still possible to isolate a group of chemicals with the highest predicted exposure potentials and target those chemicals for further assessment. The other example showed that a variety of exposure metrics ranging from physical-chemical properties to socioeconomic measures can be efficiently and intelligently combined to inform screening level risk estimates.

Presentation Session 3 considered various means of quantifying and characterizing the factors that drive exposure, particularly information technologies that may be used to support computational exposure sciences. The session began with a discussion of recent updates to EPA's Exposure Factor Handbook (EPA, 2011) with an emphasis on the handbook's Consumer Products Use Data. The critical attributes of human activity patterns and their uses in exposure assessment and exposure modeling were discussed, along with currently deployed tools and databases. Ongoing EPA projects aimed at improving the quality of EPA's data on human activity patterns were discussed, including better means of collecting and analyzing human activity information. Other informatics topics were covered, including a recently completed study that employed bar code scanners and motion sensors to estimate how personal and household care products are actually used. The study also endeavored to find methods that can reduce burdens on participants. Recruitment and retention of subjects and participants is crucial in light of the paucity of reliable use, habit, and practice data for products. Smart phones were discussed as promising research tools that may provide flexible means of conducting surveys, gathering finely-textured location data, and collecting co-incidental environmental and physiological information, e.g. air quality and physical activity, respectively. The session wrapped up with a discussion of operational program for autocoding i.e. mapping text of voice diaries to the EPA's Consolidated Human Activity Database (CHAD). Reference: U.S. EPA, 2011: Exposure Factors Handbook, National Center for Environmental Assessment, Office of Research and Development, EPA/600/R-09/052F

Presentation Session 4 outlined the current standard methods used for exposure assessments. The ideas of generic product categories and exposure scenarios were outline while commonly needed inputs for assessments such as production volume were catalogued. The need for extensive parameterization of exposure models was highlighted leading to the identification of the need for novel methods of data collection. Several possible solutions were detailed in the discussion afterward including the identification of trade organizations as potential data providers and greater public/private communication to enhance the collection of relevant consumer product use data.

Presentation Session 5 highlighted the use of extant and emerging technologies in chemical-based exposure risk assessments related to consumer products. It was widely recognized that chemical databases are important assets that can be readily utilized to ascertain chemical specific data. However, there is an important continued effort to reduce ambiguity in chemical structure-related data (i.e., incorrect stereoisomers). One method proposed was by adopting more open and definitive standards such as InChi codes – i.e., IUPAC's textual identifier for chemical substances. Furthermore, product categories and chemical composition data should be leveraged in chemical risk assessment to reduce the amount of chemical information required. However, existing databases are limited where information regarding articles such as furniture, appliances, and non-household products (e.g., building materials) are incomplete or nonexistent. It was proposed that industry or third party (i.e., NGO) collaboration would be a necessary means to elicit data on certain products and this topic was explored further within Breakout Theme C. Others recognized that human factors and specific use patterns can drive the need for identifying a subset of chemical substances (i.e., non-random, co-occurrence of chemicals) and thereby restrict the chemical information/testing/modeling requirement. Integrated testing of consumer products was highlighted as well demonstrating the clear need for chemical information in narrowing existing data gaps.

Presentation Session 6 explored participatory methods and personal informatics with the goal of developing an app for engaging the public to examine their personal chemical exposure to consumer products, and the option of giving exposure scientists access to their personal data. Good Guide is an example of a similar type of app, with years of point-of-purchase data that is possibly available to the Systems Realty research team. Another presentation demonstrated how GPS technology, which is often built into smart phones, can be used to characterize activity/location information. Another outcome from this session was a discussion of how to engage interest in an individual's own personal informatics, and ways to facilitate communication between the EPA and communities to effectively communicate accurate information (e.g. c-FERST).

Presentation Session 7 investigated applications in 'gamifying' problems, with the expectation that this approach may be useful in addressing the problems of engaging the community to learn about chemical exposures. Gamification is the application of game elements and game design techniques to help solve real-world problems. The main outcome was the discussion and suggestion of different gamification strategies, including role playing, computer simulation, and online social games. Formulating problems as games also has the benefit of engaging participants from diverse backgrounds who would otherwise not have participated.

Breakout Theme A discussed the use of innovative, social media-based methods for collecting exposure factor information. The outcome was an increased recognition by the attending EPA and academic scientists regarding the potential for the development of rapid, deployable, inexpensive, reproducible, and validated methods to collect, mine, analyze, and disseminate exposure factor data from social media data streams. Some of these methods have subsequently been demonstrated through the development of multiple EPA PIP3 proposals, as well as other proposed CSS research.

Breakout Theme B acknowledged the challenges, such as privacy concerns or issues with gathering data from a large population, in obtaining relevant chemical use and human behavior data needed for more detailed exposure modeling. Besides new ideas to tackle these challenges, another outcome was the awareness of multiple sources of databases that currently exist and may be used to refine our knowledge regarding chemical uses and human behaviors.

Breakout Theme C was primarily concerned with the accessibility and usability of data relating to consumer product ingredients and chemical informatics (i.e., from both sources of curated as well as raw data). Questions were raised about public sources of easily attainable ingredient information, portals for public/regulatory/industrial exchange about emerging concerns for emerging products, and product ingredient prioritization (i.e. prioritization based on actual consumption scaling). Data on articles such as furniture, appliances, non-household products (e.g., building materials) and toys (early life-stage) are not currently well documented, captured or consolidated. It was also mentioned that material additives, such as flame retardants or stain repellants (i.e. brominated flame retardants), components of commonplace objects (i.e. cellphones, tablets, and other consumer electronics), and nanomaterials have not received enough documentation, despite their ubiquitous use. There are several ways that lists of ingredients present in consumer products may be obtained. Participants discussed the differences in public access to data that is voluntarily disclosed vs. that which is mandatorily disclosed as a result of government regulation. They also discussed what types of data may be purchased directly from industry or via third parties (e.g. Green Guard).

Breakout Theme D discussed the use of participatory methods and personal informatics tools, rather than traditional monitoring methods, to obtain exposure information. The outcome was a greater awareness among participants of potential biases when relying on "ubiquitous" technology (e.g., cell phones, social media) to generate exposure information. For example, older segments of population and those within lower socioeconomic strata are likely to be underrepresented. With this knowledge, efforts should be made to increase representation of such individuals by providing access to technology, along with appropriate training. Another outcome from this discussion was a possible strategy for developing a platform for individuals to voluntarily provide information on their own habits as consumers. Such a platform should allow people to compare themselves to others in a community in a fun, low-burden, yet highly visual way. Moreover, the purpose should be behavior observation rather than modification, and privacy protection (through data aggregation) should be explicitly guaranteed.

Breakout Theme E discussed the variety of ways data visualization/analytics, aggregation, and sharing for the purpose of engagement and communication with the public could be accomplished (e.g., gamification and computational simulations, novel data visualization/analytic representations, and sharing personal chemical exposure informatics). Questions were discussed regarding how to engage the public on the issues of chemical exposure, motivate them to share or add to data efforts, encourage them to participate in games developed to emphasize the need for exposure research, and communicate to them the fundamental relationship between exposure and risk in a way that is understandable by the lay individual. One of the many discussion points on how to improve in these areas was the need to provide incentives to motivate participation (although specifics on how this would be implemented were not discussed). The capabilities of current technology can be harnessed in creative ways to provide information that is insufficiently captured by traditional approaches. Instead of performing a question-based survey to catalog consumer products in a home, a participant could take a video with their phone while walking through their house instead. The groups also discussed alternative points of data collection (e.g., the checkout line at the supermarket), or forming DIY and self-help interest groups to build tools that emphasize personal chemical exposure together. The group found that the concept of passive monitoring data, such as activity mapping or exposure factors, can be useful to parameterize the models. A concept of developing a game for informing oneself of household product dangers came to light - One idea: scan the barcode of a product and the product becomes a character in a game. Players can fight against each other with their "products", and the most "toxic" one wins. If young people play the game they might engage older family members to participate, raising awareness and expanding the domain of research.

Conclusions and Next Steps The workshop explored and highlighted a variety of extant technologies, methods and innovations from a variety of scientific and non-scientific disciplines that could be used to inform personal chemical exposure. The diversity of interests and expertise provided an unprecedented potential for innovative and collaborative opportunities for scientific and technological advancement, as well as outreach and community based involvement. Both within and outside the Agency, current efforts are underway to capitalize on the outcomes by developing and strengthening many of the innovative initiatives identified.

Examples include:

- **Data gap identification**: Article and household furnishing and materials as sources of exposure, as well as key additives added to such products (such as flame, stain, and water resistant additives added to many commercial articles and household goods).
- **Information accessibility** related to consumer product ingredients and constituents was a key area of interest, as the public and regulatory agencies alike would

like streamlined portals and dashboards that can give them ingredient and material composition through consolidated web-accessible databases.

- **Methods to capture "big data"** related to exposure factors and exposure modeling as a whole.
- **Approaches to more holistically integrate disparate datasets** related to exposure assessment calculations and models.
- **Methods to gamify** (developing a game that would inform the player about personal chemical exposures) **and develop platforms that engage communities** and individuals to compare exposure sources and "share" (for instance via social networks) their findings

Several of the highlighted outcomes are being developed further among workshop participants as complete research proposals that are currently being considered for funding (i.e., EPA Pathfinder Innovation Projects). The ideation process exploring the variety of topics within the workshop is anticipated to give rise to several manuscripts and other future collaborative initiatives for years to come.

Appendix A - Agenda

Personal chemical exposure informatics: visualization, user Experience, Research in Systems modeling and Simulations (PerCEIVERS)
ROOM C111C, US Environmental Protection Agency
Research Triangle Park, NC

Remote Call-in: 1-866-299-3188

Call-in Code: 919-541-1021

June 26-27, 2012

Day 1 – Tuesday, June 26, 2012 (8:30 am – 5:00 pm)

WebConference Link, Day 1: https://epa.connectsolutions.com/perceiversday1/

Session 1: Overview and Innovation – Chair: Linda Sheldon

8:30 – 8:45	*Welcome and Opening Remarks* – Peter Preuss, EPA Office of Research and Development (ORD) Chief Innovation Officer
8:45 – 9:05	*Personal Chemical Exposure Informatics* – Rocky Goldsmith, EPA National Exposure Research Laboratory (NERL)
9:05 – 9:20	*SRM stepping closer to the vision!*– Ryan Edwards, NCSU undergraduate/SHAW SRP
9:20 – 9:35	*Search Terms + Tweets = Exposure Informatics 2.0?* – Madeline Reich, SHAW SRP

Session 2: Exposure-Based Chemical Prioritization – Chair: Peter Egeghy, NERL US EPA

9:35 – 9:55	*Does exposure imitate art? Recent impressions* – Elaine Cohen-Hubal, EPA National Center for Computational Toxicology
9:55 – 10:10	*ExpoCast High Throughput Exposure Potential Prioritization* – John Wambaugh, EPA National Center for Computational Toxicology
10:10 – 10:25	From *Decision Analytics for Exposure Prioritization to dietary residue exposures* – Jade Mitchell-Blackwood, US Department of Agriculture, Food Safety and Inspection Service
10:25 – 10:45	***break***

Session 3: Exposure Factors and informatics – Chair: Dan Vallero, NERL US EPA

10:45 – 11:00	Exposure Factors Handbook Consumer Products Data- Linda Phillips, US EPA, NCEA
11:00 – 11:15	Human Activity Data in Exposure Assessment - Kristin Isaacs, US EPA, NERL
11:15 – 11:30	SUPERB and Passive sampling methods - Deborah Bennett, UC-Davis
11:30 – 11:45	Smartphones as a Flexible Research Tool: Lessons from Early Implementations and the Consumer Marketplace– Michael Keating, Research Triangle Institute
11:45 – 12:00	*Natural Language Processing and human activity patterns* – Curry Guinn, UNC Wilmington
12:00 – 1:15	***lunch*** (on your own, ***Lake Side Café*** recommended)

Session 4: Consumer Exposure Models - – Chair: Chris Grulke, NERL US EPA

1:15 – 1:30	*Consumer Exposure Assessment in a Regulatory Context under TSCA*– Cathy Fehrenbacher, EPA Office of Chemical Safety and Pollution Prevention

1:30 – 1:45 *Chemical Use: The Key to Near-Field Chemical Exposure Estimation*– Michael Jayjock, The Lifeline Group

1:45 – 2:00 *Probabilistic Exposure Assessments for Consumer Products* –Christina Cowan-Ellsberry, The Lifeline Group

Breakout Discussion Session I

Attendees will be assigned to breakout groups based on their interests and adequate coverage of themes

2:00 – 3:30 Breakout Group Discussion

Themes:

1. Exposure factors informatics, e.g., real-time human factors (Room C400A)

2. Consumer/personal exposure modeling (Room C111C)

3:30 – 3:45 Break (rapporteurs and chairs to prepare reports)

3:45 – 4:10 Presentation by rapporteurs (10 minutes each)

4:10 – 4:45 Joint Discussion

4:45 – 5:00 Preview of next day's meeting

5:00 Meeting adjourns (shuttle to return to hotel)

6:15 pm Option to meet for Dinner at "Mez Contemporary Mexican Restaurant" (5410 Page Road, Durham: (919) 941-1630)* Please note that this is self-purchase dinner. We have made reservations to accommodate up to 25 people.

Day 2 – Wednesday, June 27, 2012 (8:30 am – 3:30 pm)

WebConference Link, Day 2: https://epa.connectsolutions.com/perceiversday2/

Session 5: Chemical Information for Consumer Products – Chair: Danny Chang, NERL US EPA

8:30-8:45 *ChemSpider—A crowdsourced community environment for hosting and validating chemistry data*– Antony Williams, Chemspider at Royal Society of Chemistry

8:45-9:00 *Household Products Database and tools for consumers*– Henry DeLima, DeLima Associates (with contributions from Pertti Hakkinen from the National Library of Medicine)

9:00-9:15 *Birds are Cool, Ecologists got it going on!* – Mike Tornero, EPA National Exposure Research Laboratory

9:15-9:30 *Human Exposure Assessment Strategies for Consumer Products* – Treye Thomas, US Consumer Product Safety Commission

Session 6: Participatory Methods and Personal Informatics - – Chair: Kathleen Holm, NERL US EPA

9:30-9:45 *Consumer Empowerment at point-of-purchase* – Bill Pease, GoodGuide.com

9:45-10:00 *Producing and Promoting Personal Informatics* – Michael Nagle, QuantifiedSelf.com and theSprouts.com

10:00-10:15 *GPS and Exposure Assessment for Individuals*– Michael Breen, EPA National Exposure Research Laboratory

10:15-10:30 *Getting Chemical Ideas and Information to Communities* – Shannon O'Shea and Brad Schultz, EPA National Exposure Research Laboratory

10:30-10:45 ***break***

Session 7: Engaging the community for personal chemical exposure informatics: Gamification, visual and computer models, electronic and live-action role play – Chair: Mike Tornero, NERL US EPA

10:45-11:00 *Teaching and learning about oneself through gaming:* Education 2.0 -Benjamin Balak, Rollins College

11:00-11:15 *Computational Thinking in Chemistry: Dynamic Variations for Visual Learning* -Robert Panoff, SHODOR

11:15-11:30 *Evidence of learning in online social environments* - Beck Tench, NC Life & Science Museum

11:30-11:45 Live-Action Role Play (*LARP) with every-day stuff* - George Scheer, Elsewhere Collaborative

11:45- 1:00 **lunch** (on your own, ***Lake Side Café*** recommended)

Breakout Discussion Session II

Attendees will be assigned to breakout groups based on their interests and adequate coverage of themes

1:00 – 2:30	Breakout Group Discussion
	Themes:
	1. Chemical informatics for consumer products, i.e., consumer product chemical ingredient data sources, data mining, analytics, and visualization (Room C300C)
	2. Participatory methods and personal informatics tools, e.g., social media mining/analysis and reporting, DIY community (Room C111C)
	3. Data visualization and analytics for engagement and communication, e.g., gamification and computational simulations, novel data visualization/analytic representations, sharing personal chemical exposure informatics (Room C111C)
2:30– 2:45	Break (rapporteurs and chairs to prepare reports)
2:45 – 3:00	Presentation by rapporteurs (*5 minutes each*)
3:00 – 3:30	Joint Discussion

Session 8: Summary and Closing

3:30 – 4:00	**Summary and Future Work**
4:00 – 4:15	Closing Comments - meeting adjourns

Appendix B
Workshop Attendees, Presenters Bios, and participant contact details

Presenter Biographies

Dr. Peter Preuss is the Chief Innovation Officer in the Office of Research and Development (ORD), US EPA. Dr. Preuss leads an interdisciplinary team charged with building an innovation infrastructure for science that will move US EPA forward on the path to sustainability. In their first year, Dr. Preuss and his team have already introduced several innovative ideas and approaches to ORD, including the use of collaborative platforms for research planning and competitive internal awards to promote high-risk, high-reward research. The team has established a cross agency innovation workgroup to help US EPA make effective use of open innovation challenges, prizes and awards delegated under the America Competes Act. Additionally, the team has launched an environmental pavilion on InnoCentive.com; a company that specializes in open source innovation for scientific and technical challenges. Currently Dr. Preuss and team are working closely with ORD's National Program Directors on high profile signature projects oriented around topics such as sustainable alternatives to toxic chemicals and net zero structures and communities. As his team endeavors to promote new air monitoring sensors and applications to enhance citizen science and citizen empowerment, Dr. Preuss continues to work to bring innovative science and technology research to the forefront of ORD's activities.

Dr. Michael-Rock ("Rocky") Goldsmith is a principal investigator and Physical Research Scientist in the Exposure Dose Research Branch (EDRB) of the National Exposure Research Laboratory (NERL) at the US EPA. Prior to joining the Agency in 2006, Rocky had worked in pharmaceutical, tobacco and explosives industries in R&D and product development, and completed his Ph.D. in theoretical chemistry at Duke University in 2005. Since 2006 he has been active in six (6) major themed areas of research that span molecular (1-3) and macroscale (4-6) modeling in support of modern risk assessment of environmental chemicals: (1) In silico / computational modeling: (a) approaches for parameter estimation to support the development of pharmacokinetic models, (b) screening-level and provisional forward and reverse dosimetry models, (c) model development for linking exposure to internal dose (tissue dose, or biomarkers of exposure), specifically for characterization of absorption, distribution metabolism and elimination (ADME). (2) Ongoing research on in silico chemical genomics methods to complement the IVIVE (in vitro to in vivo extrapolation) paradigm for systems modeling and toxicogenomics efforts in modern risk assessment (3) Bringing stereochemistry and its implications on quantitative risk assessment of racemates and effects research to the forefront of critical scientific awareness: misguided mixtures research (4) Development of low-burden, personal household chemical exposure informatics "apps" to better understand chemical exposure arising from the "things we expose ourselves to", coupled to comparative analytics to social streams of one's nearest neighbor for exposure scenario simulation using life simulation strategy engines. (5) The development of novel robust and rugged low-cost remote sensing technologies using in vivo assays, and (6) Quantitative mapping, visualization and modeling using uncommon medium and unconventional technology from 3D anaglyph images, PS3 desktop supercomputing, poster with a digital screen add-on, and tablet device (iPod Touch) household product scanning and actigraphy integration.

Mr. Ryan Edwards recently graduated Southeast Raleigh High School. He is in the honor roll, the national honors society, the Technology Student Association, and the FIRST robotics club. This past summer, he worked at the Environmental Protection Agency where he helped research the possible ways to monitor daily human exposure to various products and chemicals, and aided in the debugging and development of an MSDS database creation tool. He is an eagle scout, and a black belt, having participated in both activities for over ten years. After earning his black belt, he now acts as an instructor to both children and adults, and he sometimes helps out in the special needs classes. Ryan hopes to go into a career in robotics, and plans to go to North Carolina State University this coming fall. Besides building several robots with his robotics club, and participating in several engineering classes, Ryan has also participated in an independent study course where he researched humanoid robotics and constructed a robotic hand.

Ms. Madeline Reich is a rising senior at Fuquay Varina High School and is an Apprentice with the Shaw University and US Environmental Protection Agency's Research Apprenticeship Program. She is spending six weeks at the RTP Environmental Protection Agency to work on "Social Network Analysis for Personal Chemical Exposure Informatics" with her mentors Michael Goldsmith, Daniel Chang, and Chris Grulke.

Dr. Elaine Cohen Hubal is currently a senior scientist in US EPA's National Center for Computational Toxicology (NCCT). The NCCT has a mission to integrate modern computing and information technology with molecular biology to improve Agency prioritization of data requirements and risk assessment of chemicals. Dr. Cohen Hubal leads ExpoCast, the EPA research program in exposure science to support chemical prioritization and toxicity testing. Her primary research interests are in characterizing human exposure and developing approaches for using human exposure metrics to inform health studies and public health policy. The current focus of her research is on applying a systems approach to characterize complex relationships between environmental factors and health outcomes with an emphasis on vulnerable populations. Previously, she was Acting Associate Director for Human Exposure Modeling in the Human Exposure and Atmospheric Sciences Division of the US EPA's National Exposure Research Laboratory (NERL) where she worked to develop and direct NERL's human exposure modeling research program. Dr. Cohen Hubal has published in the areas of children's exposure and human health risk modeling. Dr. Cohen Hubal has served as an expert on a variety of scientific panels and committees including the Voluntary Children's Chemical Evaluation Program (VCCEP) Peer Consultation Panel and the Study Design Working Group for the National Children's Study. Currently, she serves as chair of the WHO IPCS working group on "Identifying Important Life Stages for Monitoring and Assessing Risks from Exposures to Environmental Contaminants." Dr. Cohen Hubal also serves as an associate editor for reviews for the Journal of Exposure Science and Environmental Epidemiology. Dr. Cohen Hubal received her Ph.D. and M.S. in Chemical Engineering from North Carolina State University and a B.S. in Chemical Engineering from Massachusetts Institute of Technology.

Dr. John Wambaugh is a Physical Scientist with the United States Environmental Protection Agency's National Center for Computational Toxicology (NCCT). His areas of active research include virtual tissues, high throughput exposure modeling, and biostatistics. He co-leads the EPA ExpoCast project team and is a member of the Virtual Liver and ToxCast teams. John's research on these projects focuses on predicting chemical effects in, and exposures to, humans using in vitro laboratory measurements and computer simulations. John Wambaugh received his Ph.D. in 2006 from Duke University (physics) for work in experimental non-equilibrium statistical mechanics; in particular how large-scale behaviors can depend on small-scale differences. John worked with Woodrow Setzer (EPA/NCCT) and Hugh Barton (Pfizer, formerly EPA/NCCT) as a post-doctoral researcher at the NCCT; studying the statistical analysis of biological models, with an emphasis on Bayesian methods and integrating multiple data types. He received his B.S. (physics) from the University of Michigan, Ann Arbor, obtained a M.S. (physics) from Georgia Institute of Technology, and a M.S. (computer science) from Duke University.

Dr. Jade Mitchell-Blackwood is currently a Risk Analyst with the USDA Food Safety Inspection Service. She works on hazard identification and prioritization of chemicals in food products. Earlier this year, Jade completed a post-doctoral fellowship in the National Exposure Research Laboratory (NERL) at the US EPA in Research Triangle Park, NC. She worked in exposure modeling research to develop innovative approaches to exposure-based prioritization of chemicals which fall under the Toxic Substance Control Act (TSCA) for rapid risk screening. Her interests in the project included informing the type, quantity and quality of data or information needed to prioritize chemicals based on exposure potential using statistical, mechanistic and decision models. Jade has a Ph.D. is in Environmental Engineering from Drexel University in Philadelphia, PA where she focused on decision making under high uncertainty for managing risks associated with bioaerosols of pathogenic agents.

Dr. Linda Phillips is an environmental biologist in EPA's National Center for Environmental Assessment, Exposure and Risk Characterization Group where she provides technical support to program offices and regions on topics related to exposure assessment and risk analysis. A primary focus of her work has been in support of NCEA's Exposure Factors Program which has produced documents such as the Child-specific Exposure Factors Handbook and the Exposure Factors Handbook. She is currently managing the development of a web-based toolbox to make exposure assessment tools more accessible to the user community.

Dr. Kristin Isaacs is a Research Physical Scientist in EPA's NERL. Her current research focuses on the development and evaluation of human exposure and dosimetry models and associated algorithms for use in risk assessment of air pollutants and chemicals. Her specific interests include development of physiology-based energy expenditure prediction methods and associated inhalation and dietary dose algorithms, monitoring and assessment of human activity patterns, development and evaluation of indoor chemical source-to-concentration models, and development and application of sensitivity analyses for exposure/dose models. She has 10 years' experience supporting EPA modeling research. She received her Ph.D. in Biomedical Engineering from Vanderbilt University in 2002, where her doctoral work involved development of visualization-based sensitivity analysis methods for physiological and pharmacokinetic models. She subsequently completed postdoctoral training in EPA's National Health and Environmental Effects Research Laboratory (NHEERL), focusing on the development and application of lung dosimetry models for particulate matter. From 2004-2010 she was an Environmental Project Scientist with Alion Science and Technology Inc., providing research and analysis support for a number of EPA models, including the Air Pollutant Exposure (APEX) model of the Office of Air Quality Planning and Standards (OAQPS) and NERL's Stochastic Human Exposure and Dose Simulation (SHEDS) models. She joined NERL in 2010. She has over a dozen publications in the Journal of Exposure Science and Environmental Epidemiology, Environmental Modelling and Software, Journal of Aerosol Medicine, Cellular and Biochemical Biophysics, and Journal of Pharmacokinetics and Pharmacology. She has also co-authored two chapters in the CRC Press Aerosols Handbook (2011).

Dr. Deborah Bennett is an associate professor in Environmental and Occupational Health in the Department of Public Health Sciences at the University of California, Davis. Dr. Bennett's research focuses on the fate, transport, and exposure of chemicals in both the indoor and multimedia environments within the context of both environmental risk assessment and environmental epidemiology. Her work utilizes both modeling and measurement techniques, bridging the gap between these two lines of inquiry. Current research interests include exposure to pesticides from indoor uses, relating environmental measures to biological measures for flame retardants, exposures and resulting risks from hazardous air pollutants, supporting exposure assessments in Autism studies, quantifying intake fraction values and measurement of exposures to agricultural workers. Dr. Bennett received her doctoral degree in mechanical engineering from UC Berkeley, worked as a scientist at the Lawrence Berkeley National Laboratory, and was a member of the faculty at the Harvard School of Public Health. She has served on both the EPA Science Advisory Board and the Science Advisory Panel and other EPA committees and was a US representative to OECD/UNEP Workshop on the use of Multimedia models. Dr. Bennett received the Early Career Award from the International Society of Exposure Assessment and was an EPA STAR Fellow.

Mr. Michael Keating, who joined RTI in 2008, is a survey manager in the Program on Digital Technology and Society. Mr. Keating has a broad range of survey research experience, including leadership of field, Web, and virtual data collection efforts; management of data collection field staff; data quality control; instrument development, programming, and testing; and creation of survey materials. His research interests focus on the use of new technologies in survey research and data collection, including crowdsourcing methodologies, smartphone panels, virtual world data collection methods, and cloud computing to improve field study efficiencies. His academic training is in political science.

Dr. Curry I. Guinn is an Associate Professor at the University of North Carolina Wilmington and formerly a Research Engineer at RTI International. Using pioneering spoken human-computer dialogue algorithms, Dr. Guinn has integrated advanced spoken dialogue capabilities in a variety of virtual reality-based applications. Dr. Guinn was co-Principal Investigator on a National Science Foundation grant leading the development of interactive virtual humans with emotions that affect their body and facial gestures, decision-making, and language generation. Dr. Guinn has led research in using both symbolic and statistical techniques in natural language parsing and understanding. Funded primarily by STRICOM's ACT II program, Dr. Guinn led the development of a system that allows military maintenance personnel to talk to a computerized assistant in a virtual reality environment during the diagnosis and repair of equipment. His work has been supported by research grants and contracts from U.S. Department of Defense, the National Science Foundation, National Institute of Justice, National Institute of Health, the Environmental Protection Agency, and commercial businesses such as IBM, Michelin, Lexxle, and John Deere. Dr. Guinn received his B.S. from Virginia Polytechnic Institute and State University, his M.S. and Ph.D. degrees from Duke University and is the author or co-author of 40 peer reviewed articles.

Ms. Cathy Fehrenbacher is the Chief of the Exposure Assessment Branch in the Office of Pollution Prevention and Toxics at the US Environmental Protection Agency in Washington, D.C. Cathy has a B.S. in Environmental Science from Lamar University in Texas, and a M.S. in Industrial Hygiene from Texas A&M University. She is a Certified Industrial Hygienist and has over 25 years of experience in various aspects of industrial hygiene, exposure assessment, and environmental fate and transport. She has authored or co-authored several publications and chapters on the use of modeling approaches for predicting inhalation and dermal exposure, and has given numerous presentations and lectures on EPA's programs, methods, and policies for assessing and managing chemical risks. She currently serves as co-chair of the OECD Exposure Assessment Task Force.

Dr. Michael A. Jayjock is a senior member of LifeLine Group's management team. Prior to joining LLG, he was the Senior Research and EHS Fellow and Manager, Risk Assessment, in the Toxicology Department of Rohm and Haas Company, where he has served in various technical positions since 1969. He has a Ph.D. in Environmental Engineering from Drexel University, Philadelphia, Pennsylvania, where he also received his Master of Science degree in Environmental Science and Occupational Health. Dr. Jayjock is a Fellow of the American Industrial Hygiene Association and Diplomat of the American Board of Industrial Hygiene (CIH). He has served on various committees of the American Industrial Hygiene Association: Committee on Exposure Assessment Strategies, Exposure Strategies Modeling Subcommittee, Exposure Strategies Expert System Subcommittee, Committee on Risk Assessment, and Low-Dose Estimation Task Group. Dr. Jayjock's principal research interest includes the development of better-estimating and more cost-efficient exposure models. He has expertise in such areas as exposure modeling and human exposure to environmental pollutants, human health risk assessment, and uncertainty analysis. He has published extensively in peer-reviewed publications and served from 1998-2003 as an Editorial Board Member for the American Industrial Hygiene Journal. He has made numerous technical presentations, including at the American Industrial Hygiene Conference, International Society of Exposure Assessment Conference, and the Air Toxics Monitoring Workshop to Support EPA's Integrated Urban Air Toxics Strategy. His wide service on advisory committees includes: US EPA - Office of Pollution Prevention & Toxics - Voluntary Children's Chemical Evaluation Program (VCCEP); Peer Consultation Panel on Flame Retardants, 2003; US EPA Science Advisory Board, Executive Committee, Human Health Research Strategy Panel, November 2002; US EPA Science Advisory Board Consultant 2001-2003 - Integrated Human Exposure Committee; US EPA Science Advisory Board Member 1998-2001 - Integrated Human Exposure Committee (IHEC); and National Research Council - National Academy of

Sciences, as a Member of the Committee to Review Risk Management in the DOE's Environmental Remediation Program, the Committee on Advances in Assessing Human Exposure to Airborne Pollutants, and the Committee on Toxicology - Subcommittee on Risk Assessment of Flame-Retardant Chemicals.

Dr. Christina E. Cowan-Ellsberry recently retired as a Principal Scientist in the Environmental Sciences and Human Safety Departments of The Procter & Gamble Company in Cincinnati, OH. Dr. Cowan-Ellsberry has worked in the area of environmental fate and risk assessment for over 30 years. While working in the environmental field, she conducted fate studies and developed models for predicting the fate of both inorganic and organic chemicals in the environment. Dr. Cowan-Ellsberry has also served as a technical representative for industry to the US EPA's Endocrine Disrupter's Priority Setting workshop, Environment Canada's "Categorization and Screening of the DSL" project, and numerous international panels including the OECD's Environmental Exposure Task Force, the OECD working group for developing an internationally harmonized classification scheme for hazardous to the Aquatic environment, and both the NAFTA Commission for Environmental Cooperation and the UNEP Criteria Expert Groups for developing the criteria and process for identifying candidate Persistent, Bioaccumulative and Toxic substances for international management which is now incorporated into the recently adopted Persistent Organic Pollutants protocol. For several years, she has been applying her exposure modeling expertise to improve human exposure assessment approaches and models for consumer products. She has been especially active in advancing the field of probabilistic and aggregate exposure assessment for humans by conducting research to understand and provide recommendations on how to conduct probabilistic and aggregate exposure assessments for consumer products. In addition, she was a key participant in several international activities such as the recent SDA compilation of habits and practices data for consumer product exposure which has greatly improved public access to these important data thereby improving consumer product exposure assessments. She has been a guest lecturer at several international universities and recently led a training session under UN sponsorship in Africa, gave testimony before the US Congress on TSCA reform in the area of Persistent, Bioaccumulative and Toxic substances and was a technical expert in the successful D5 Board of Review in Canada. She has also authored or co-authored over 60 scientific papers, 5 book chapters and 4 books and holds one US patent. She has been a member of SETAC for over 20 years and of ISES for over 10 years and served as ISES counselor from 2007 to 2009.

Dr. Antony Williams is the VP of Strategic Development at the Royal Society of Chemistry. He obtained his PhD from the University of London focused on Nuclear Magnetic Resonance and postdoc'ed at the National Research Council in Ottawa, Canada and ran the NMR Facility at Ottawa University. He was the NMR Technology Leader at the Eastman Kodak Company in Rochester then joined Advanced Chemistry Development (ACD/Labs) as their Chief Science Officer working on structure representation, nomenclature and analytical data handling. With a small team of passionate individuals interested in sharing chemistry data with the community he oversaw the development of the ChemSpider database as a hobby project. ChemSpider quickly developed into one of the community's primary online chemistry resources and was acquired by the Royal Society of Chemistry. He is the ChemConnector in the chemistry social network environment."

Mr. Henry DeLima is a mechanical engineer and owner of DeLima Associates, a management consulting firm founded in the San Francisco Bay area over 26 years ago. Henry has provided consulting services in the areas of energy and environmental health to commercial, institutional and federal government clients. Services in the environmental health area include authoring materials to aid primary care physicians in diagnosing and treating patients exposed to specific environmental toxins, developing medical management guidelines for first responders and emergency room physicians in treating victims of acute chemical incidents and developing databases of environmentally preferable construction products for EPA and DOD. Some of the products developed by DeLima Associates include the Household Products Database and the Dietary Supplements Database currently hosted by the National Library of Medicine.

Dr. Pertii (Bert) Hakkinen is the Senior Toxicologist and Toxicology and Environmental Health Science Advisor in the Division of Specialized Information Services, National Library of Medicine (NLM), (US) National Institutes of Health (NIH). He provides leadership on the development of new resources in toxicology, exposure science, risk assessment and enhancements to existing NLM resources in these fields. Dr. Hakkinen is the project leader for the Wireless Information System for Emergency Responders (WISER) and Chemical Hazards Emergency Medical Management (CHEMM) tools, represents NLM on various committees, and provides leadership for NLM's participation in national and international efforts in toxicology-, exposure-, and risk assessment-related information. He is an Adjunct Associate Professor in Biomedical Informatics and the co-director of a public health informatics course offered since 2009 at the Uniformed Services University of the Health Sciences (USUHS) in Bethesda, Maryland. Further, he is the Vice-chair of the Scientific Advisory Panel for the Mickey Leland National Urban Air Toxics Research Center (NUATRC) in Houston, Texas. During his career Dr. Hakkinen has held numerous leadership positions in the field of toxicology and risk assessment. Before joining the NIH in 2008, Dr. Hakkinen served for several years on the auxiliary staff of the European Commission (EC) at the EC's Institute for Health and Consumer Protection, Joint Research Centre, in Italy. He has also held positions with Toxicology Excellence for Risk Assessment (TERA) and Gradient Corporation in the US, and at the Procter and Gamble Company in the US and Japan. Dr. Hakkinen earned a B.A. in Biochemistry and Molecular Biology from the

University of California, Santa Barbara, and received his Ph.D. in Comparative Pharmacology and Toxicology from the University of California, San Francisco. Dr. Hakkinen is a member of the Society of Toxicology (SOT) and a charter member of the Society for Risk Analysis (SRA) and the International Society of Exposure Science (ISES). He is a co-editor and co-author of the latest edition of the Encyclopedia of Toxicology, and of the last two editions of the Information Resources in Toxicology book.

Dr. Rogelio (Mike) Tornero-Velez is a scientist with the National Exposure Research Laboratory of the US EPA. Dr. Tornero has led efforts within the Agency to couple probabilistic exposure models with physiologically-based pharmacokinetic models to investigate cumulative exposures to pyrethroids pesticides. He has adapted methods from the field of community ecology to investigate the co-occurrence of chemicals in the environment with anthropogenic origin. He received a Ph.D. in Environmental Sciences and Engineering from the University of North Carolina at Chapel Hill in 2001.

Dr. Treye A. Thomas is a toxicologist and leader of the Chemical Hazards Program team in the US Consumer Product Safety Commission's (CPSC) Office of Hazard Identification and Reduction. His duties include establishing priorities and projects to identify and mitigate potential health risks to consumers resulting from chemical exposures during product use. Dr. Thomas has conducted comprehensive exposure assessment studies of chemicals in consumer products and quantified the potential health risks to consumers exposed to these chemicals. Specific activities have included conducting exposure and/or health hazard assessments of flame retardant (FR) chemicals, combustion by-products, indoor air pollutants, and compounds used to pressure-treat wood. Dr. Thomas is the leader of the CPSC nanotechnology team, and is responsible for developing agency activities and policy for nanotechnology. Dr. Thomas has served as a CPSC representative on a number of nanotechnology committees including the ILSI/HESI Nanomaterial Environmental, Health, and Safety Subcommittee, the Federal NSET and NEHI sub-committees, and the International Council on Nanotechnology (ICON). Dr. Thomas received a Bachelor's degree in Chemistry from the University of California, Riverside, an MS in Environmental Health Sciences from UCLA, and a PhD in Environmental Sciences at the University of Texas, Health Science Center, Houston. He completed a post-doctoral fellowship in Industrial Toxicology at the Warner-Lambert Corporation (now Pfizer Pharmaceutical).

Dr. Bill Pease is Chief Scientist of GoodGuide, where he is responsible for the systems used to rate products and companies by their health, environmental and social impacts. Bill is an environmental scientist and has served on the faculty at the School of Public Health, University of California at Berkeley. Bill was also Director of Internet Projects at Environmental Defense Fund, where he created scorecard.org, the web's top-ranked site for localized environmental information. He has worked for Cal-EPA, the California Department of Health Services, and the Massachusetts Department of Environmental Management. His academic areas of interest include informatics and quantitative risk assessment. Bill holds a BA from Yale University, and an MS in Energy and Resources and a PhD in Environmental Health Sciences from the University of California, Berkeley. He was also a Rhodes Scholar at Oxford University in England.

Dr. Michael Nagle (@nagle5000) runs the Boston Quantified Self Meetup and is a co-founder of sprout, a non-profit in Somerville working to make science a cultural activity. He is fascinated by how people learn. While studying theoretical math at MIT, he began working to build environments that support sustainable inquiry for kids, and later, adults. If he didn't think education was in such vital need of renewal, he would probably be a hardcore mathematician and a softcore DJ.

Dr. Michael S. Breen is a Research Physical Scientist in the National Exposure Research Laboratory at the US Environmental Protection Agency (EPA). His research focuses on development of air pollution exposure models, integrated with novel personal sensor technologies, to improve exposure assessments for individuals in health studies. Dr. Breen is co-investigator for three near-road health studies assessing exposure to traffic-related air pollutants, one study with asthmatic children and two studies with a coronary artery disease cohort. Currently, he is developing three exposure models: Exposure Model for Individuals (EMI), GPS-based Microenvironment Tracker (MicroTrac) model, and Personal Exposure Index (PEI) model. He serves on various science steering committees and conference technical organizing committees, member of the EPA Ozone Integrated Science Assessment Review Team, and peer-reviewer for three journals. Dr. Breen received his Doctorate in Biomedical Engineering from Case Western Reserve University, Cleveland, Ohio, and joined EPA in 2005. He authored over 20 publications, holds two US patents, and received various scientific awards including the Sally Liu Outstanding New Researcher Award from the International Society of Exposure Science, the Biological Modeling Specialty Section Award from the Society of Toxicology, and the EPA Pathfinder Innovation Project Award.

Ms. Shannon O'Shea is a contractor in the EPA Office of Research and Development's Sustainable and Healthy Communities Research Program. Her primary focus is development of EPA's Community-Focused Exposure and Risk Screening Tool (C-FERST), including populating the tool with information and tracking and incorporating feedback from stakeholders and pilot end-users. Shannon received her undergraduate degree in Biological Sciences from NC State University and worked at Duke University in Molecular Biology prior to pursuing her M.S.P.H degree in Environmental Sciences and Engineering from UNC School of Public Health. At UNC Shannon studied Environmental Health and Toxicology and became interested in community-based research.

Professor Benjamin Balak is an Associate Professor of Economics at the Department of Economics at Rollins College, and is currently the Chairperson of the department. Professor Balak holds a PhD in economics from the University of North Carolina at Chapel Hill and, prior to that, studied abroad at the American University of Paris (FR) where he earned a BA in economics. He also holds a postgraduate diploma from the University of Kent at Canterbury (UK). Professor Balak's areas of interest include the history of economic thought, economic history, philosophy and ethics, and comparative economic systems and cultures.

Dr. Robert M. Panoff is founder and Executive Director of the Shodor Education Foundation (www.shodor.org), a non-profit education and research corporation in Durham, NC, dedicated to reform and improvement of mathematics and science education through computational and communication technologies. As PI on several National Science Foundation (NSF) and US Department of Education grants that explore interactions between technology and education, he develops interactive simulation modules that combine standards, curriculum, supercomputing resources and desktop computers. In recognition of Dr. Panoff's efforts in college faculty enhancement and curriculum development, the Shodor Foundation was named as a NSF Foundation Partner for the revitalization of undergraduate education. In 1998, Shodor established the Shodor Computational Science Institute, which was expanded with NSF funding in 2001 to become the National Computational Science Institute (www.computationalscience.org). Shodor's Computational Science Education Reference Desk (www.shodor.org/refdesk) serves as a Pathway portal of the National Science Digital Library. Dr. Panoff consults at several national laboratories and is a frequent presenter at NSF workshops on visualization, supercomputing, and networking. Dr. Panoff has served on the NSF advisory panel for Applications of Advanced Technology program, and is a founding partner of NSF-affiliated Corporate and Foundation Alliance. Dr. Panoff received his M.A. and Ph.D. in theoretical physics from Washington University in St. Louis, with both pre- and postdoctoral work at the Courant Institute of Mathematical Sciences at New York University. Wofford College awarded Dr. Panoff an honorary Doctor of Science degree in recognition of his leadership in computational science education.

Ms. Beck Tench is a simplifier, illustrator, story teller and technologist. Formally trained as a graphics designer at the University of North Carolina's School of Journalism and Mass Communication, she has spent her career elbow deep in web work of all sorts – from the knowledge work of information architecture and design to the hands dirty work of writing code and testing user experiences. Currently, she serves as Director for Innovation and Digital Engagement at the Museum of Life and Science in Durham, NC where she studies and experiments with how visitors and staff use technology to experience risk-taking, community-making and science in their everyday lives. Specialties: Visual Thinking, Informal Science Education, Data Visualization, Human Computer Interaction

Mr. George Scheer is co-founder and Collaborative Director of Elsewhere, a living museum and international residency program set within a former thrift store in Greensboro, NC. He is also a co-curator of Kulturpark, a project to animate an abandoned amusement park in East Berlin. His theoretical and artistic projects take place at the intersection of aesthetics and social change. George holds an MA in Critical Theory and Visual Culture from Duke University and a BA from the University of Pennsylvania in Political Communications. He is currently pursuing a PhD in Communication Studies and Performance at UNC-Chapel Hill. George's currents projects can be found online at elsewhereelsewhere.org and kulturpark.org

PerCEIVERS 2012 Workshop Attendees				
NAME	**TITLE**	**INSTITUTION**	**EMAIL ADDRESS**	**PHONE NUMBER**
Rocky Goldsmith	Research Physical Scientist	U.S. Environmental Protection Agency	goldsmith.rocky@epa. gov	919-541-0497
Antony Williams	VP of Strategic Development	Royal Society of Chemistry	williamsa@rsc.org	919-201-1516
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Benjamin Balak	Associate Professor	Rollins College	bbalak@rollins.edu	321-948-9803
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Appendix C
PerCEIVERS 2012 Break-Out Sessions

Group Assignments
We ask that you consider or think about some of these open breakout charge questions and can even jot down ideas for multiple sessions (even one's you don't think you will attend) that could potentially contribute to discussion.

For Day 1, we will have about 20 people in each group. Participants can choose their two preferences before the meeting, and we assign them to different groups based on their choices and # of people in each group.

For Day 2, we will have about 15 people in each group. Participants can choose their preferences before the meeting, and we assign them to different groups based on their choices and # of people in each group.

Breakout session charge questions For Day 1 and 2 and specific theme areas.
Same questions are asked in different groups, so that we can see different perspectives on the same issue.

Day 1

THEME A. (Room C400A)

Exposure factors informatics, e.g., real-time human factors

1. What is the best way to define activities related to consumer product use?
2. Are there any chemicals/products of emerging concern or lifestyle changes for which consumer use information does not exist?
3. What categories or products are most important in terms of data needs?

THEME B. (Room C111C)

Consumer/personal exposure modeling

1. What can be done to make product/chemical information more easily attainable?
2. What is the best way to define activities related to consumer product use?
3. How can household inventories best be used with activity information to estimate potential exposure?

Day 2

THEME C. (Room C300C)

Chemical informatics for consumer products, i.e., consumer product chemical ingredient data sources, data mining, analytics, and visualization

1. What can be done to make product/chemical information more easily attainable?
2. Are there any chemicals/products of emerging concern or lifestyle changes for which consumer use information does not exist?
3. What categories or products are most important in terms of data needs?

THEME D. (Room C111C)

Participatory methods and personal informatics tools, e.g., social media mining/analysis and reporting, DIY community

1. When using personal monitoring or social media to gather consumer use data, what are the data biases (e.g., groups that have no access/interest to social media)
2. 2. How to engage DIYers to develop an app or game to collect product/chemical use data and/or product/chemical inventories?
3. What are the elements to make a tool, game, or learning module ideal for combining consumer use data with household product inventories?
4. Are there privacy concerns? What is the public health message that can be sent?

Day 1	Chair	Rapporteur	Room location
A) Exposure factors	Kristin Isaacs	Dan Vallero	C400A
B) Exposure modeling	Cecilia Tan	Chris Grulke	C111C
Day 2			
C) Chemical informatics	Jade Mitchell-Blackwood	Dan Chang	C300C
D) Personal informatics tools	Mike Breen	Peter Egeghy	C111C
E) Engagement/Communication	Rocky Goldsmith	Kathleen Holm	C111C

THEME E. (Room C111C)

Data visualization and analytics for engagement and communication, e.g., gamification and computational simulations, noval data visualization/analytic representations, sharing personal chemical exposure informatics

1. What are the motivation factors for people to participate in product/chemical inventories or use survey/study?
2. How could the act of learning about one's exposures be "gamified"
3. Can LARP / technology assisted games co-exist with computer simulated environments such as Sims / Second life / Civilization or with agent-based models to engage the participant?
4. How could one visualize or make the visual imagery motivational and informative with regards to personal chemical exposures?

Appendix D
Workshop Presentation Material

PerCEIVERS
@ US-EPA in RTP-NC

Day I Presentations
– June 26, 2012

ORD Innovation

June 26th, 2012

Peter Preuss, PhD
Chief Innovation Officer
EPA Office of Research and Development

"What we can do -- what America does better than anyone else -- is **spark the creativity and imagination** of our people…

…In America, **innovation** doesn't just change our lives. It is how we make our living."

- President Barack Obama

3

Innovation at the EPA

"By coming together to **advance sustainability and innovation**, we will in turn enhance our security for decades to come."

- Administrator Jackson, EPA

"ORD must help **drive that innovation**, because in its absence, our mission cannot be achieved."

- Paul Anastas, EPA

4

ORD Innovation Strategy

Shifting from individual projects to a systematic approach

What?	How?
Support innovation at the bench in ORD laboratories *By fostering a dynamic work environment that rewards and recognizes creative problem solving*	• *Pathfinder Innovation Projects* • *Innovation in Research Plans* • *PeerOvation Awards* • *Apps and Sensors for Air Pollution (ASAP)*
Demonstrate the power of transdisciplinary research *Learning how to connect scientists in new ways and engage practitioners and users*	• *Within ORD (IdeaScale)* • *Federal Environmental Research Network* • *Design Labs* • *Apps and Sensors for Air Pollution (ASAP)*
Use open innovation to broaden network of environmental problem solvers *Bring in new ideas and creative solutions from external scientists and others*	• *InnoCentive and TopCoder challenges* • *Challenge.gov* • *Partnering with OSTP, NASA, HHS, DOD* • *Apps and Sensors for Air Pollution (ASAP)*
Showcase research that exemplifies the principles of Path Forward *Expand understanding of innovative research and sustainability*	• *Signature projects* • *Pathfinder Innovation Projects* • *Apps and Sensors for Air Pollution (ASAP)*

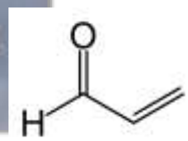
5

Pathfinder Innovation Projects (PIP): From Libraries to Pilot Facilities

6

EPA United States Environmental Protection Agency

Open Innovation



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EPA United States Environmental Protection Agency

Real-time Air Quality for Human Health

8

Workshops: Bringing Innovators Together

9

Creating an Innovative Research Culture

PeerOvations – peer-driven recognition for research and administrative innovation

Federal Environmental Research Network (FERN) – connecting ideas and experts across agencies

Interactive Educational Tools – Community-driven mobile tools for stormwater management decisions

10

Innovation Moving Forward

We believe that innovation in ORD will prosper with:

•**Visible leadership and commitment.** Consistent support from lab and center directors and the new National Program Directors, demonstrated by aligned resources and incentives, is a critical determinant of innovation success.

•**Design-thinking and experimentation.** An organization willing to experiment, test, and learn will be able to produce and sustain innovation over the long haul.

•**Smart risk taking.** Not all innovation activities will succeed, but we can still learn from, and benefit from, creative projects that don't achieve the anticipated results.

•**Creative empowerment.** Because innovation can come from anyone, it is essential that we empower people across ORD and be open to external ideas and processes.

•**Teams and partners.** ORD needs to become better at working across disciplines and with users and practitioners both in ORD and EPA, and with a variety of external partners.

•**Measurement and accountability.** We must strive to understand which ORD investments in innovation are yielding the greatest results, and continuously look for ways to improve ORD's innovation processes and infrastructure.

11

Social networking and Exposure Informatics: Systems Reality Modeling

Michael-Rock "Rocky" Goldsmith

Big Exposure Questions & Information Needs

Three big **questions** in personal chemical exposure informatics

1. What do we expose ourselves to everyday?
2. What chemicals are really in our products?
3. What product changes, or lifestyle changes could be modified to reduce exposures?

Two major data **requirements** essential for consumer product chemical exposure modeling**:**

1. Consumer product ingredients data
2. Human behavioral/action data (time/location/activity journals)

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Burden, passive interrogation, and personal informatics

- **Can we evaluate our product inventories in the context of others around us?**
  - require a means of reporting that is implemented everywhere (**ubiquitous), fast and dirty**
  - Need a mechanism of acquiring product data that is **ubiquitous and low burden**

- **Can we evaluate our activities and behaviors in the context of others?**
  - require a means of **rapidly assessing personal activities** (i.e. actigraphy)
  - Requires a means of **identifying and categorizing** local environmental human behavioral patterns in an unsupervised fashion. (NLP mining of social network feeds)

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Bigger Picture Questions:
How can we get real-time chemical ingredients or activity/location social/ behavioral data?

- **How can we capture "Real-life" like a "fly-on-the-wall"**
  - How does one obtain data to understand real systems in real-time
  - Dynamic updating of activity/location information at a specified geographic location
  - Twitter relationships
    - Big data that captures activity and location information and relateds to exposure assessment

- **How can we update and invigorate current data streams for activity/location information and how will this impact exposure models?**
  - directly update and renew CHAD-like activity/location data for studies that need to be geographically, life-stage, culturally, or gender segmented.
  - will translate on-line conversation and instances into relevant data for Exposure Modeling efforts such as CHAD or SHEDS?

How do we get required data elements for Modern Exposure Assessment?

•Require a vision of current data-streams and data needs

•Information model

•Chemical ingredients in products database

•Means to personally assess activities and to document them

- Creation of the Systems Reality Modeling (SRM) project
  - www.systemsreality.org

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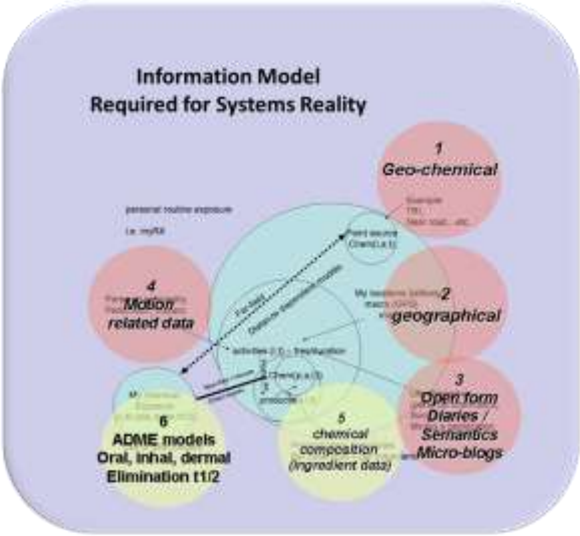
Mash-up of a variety of environmental, human, and chemical factors to perform personal chemical exposure informatics



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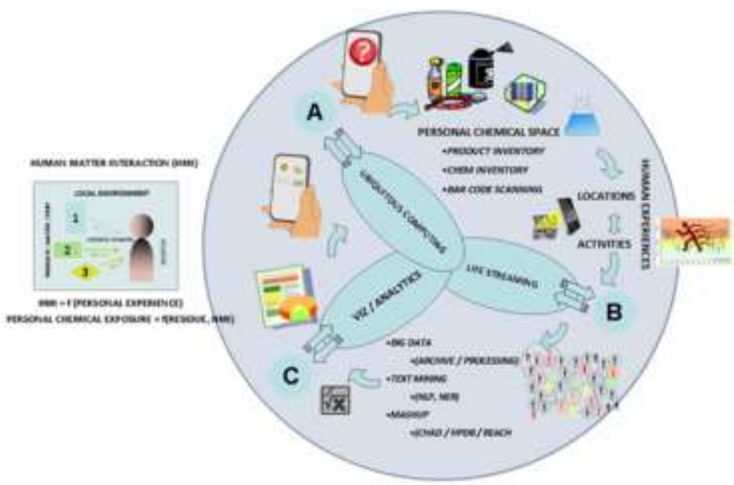
The Systems Reality Modeling workflow and Human Matter Interactions



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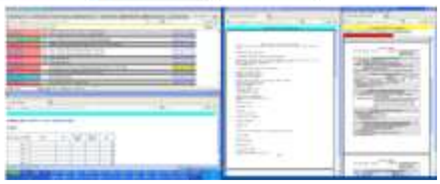
Our Consumer Product Chemical Ingredient inventory Interface

- >70% curation of 22K product High-market share consumer product MSDS inventory
- N-sampled, crowdsourced over 10 experts

- We enter chemical ingredient name, CAS#, link out to ACToR, and percent composition in a given product when available.



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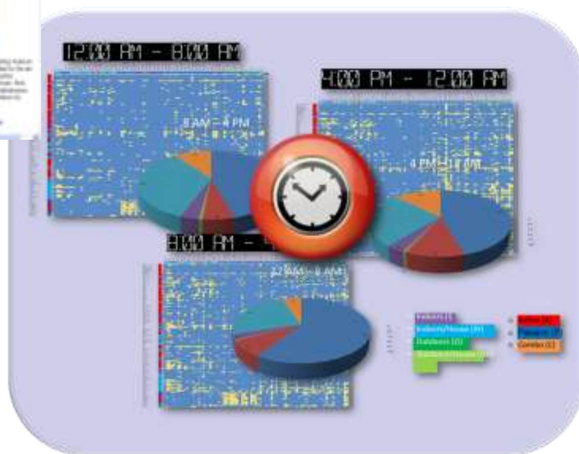
CHAD: provides context driven human behavior patterns

http://www.epa.gov/chadnet1/



- *Priors analysis on time-slot of activity relationships to locations*
- *Will provide first step for an intelligent exposure related journaling system.*

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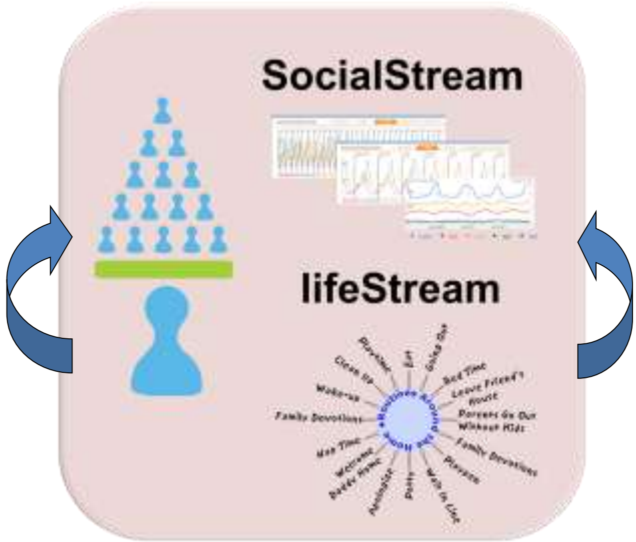
How does one relate to many? Converting spoken word into CHAD activity / location entries

Extrapolation From singleton To plurality of Exposure related events



NLP:(Natural Language Processing) Text-mining and search queries on micro-blogging to obtain "map" of exposure activities and locations

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Supporting NERL, program offices and CSS 2.3.1

Provides mechanism to wrap multiple required data-streams fore personal chemical exposure informatics into a ubiquitous, low-burden personal computing device; the smart-phone.

– **timely approaches based on devices that most people already own**, know how to use, lower-burden, and could reduce study attrition.
– This data **can feed into ExpoCast, CHAD, and SHEDs** while also
– filling a community based effort for personal chemical exposure informatics and **supporting CSS**!

Link to product page
Or www.systemreality.org

PREZI interactive Presentation:
http://goo.gl/yyPPc

System's Reality Modeling

Mark-up › Mining › Modeling

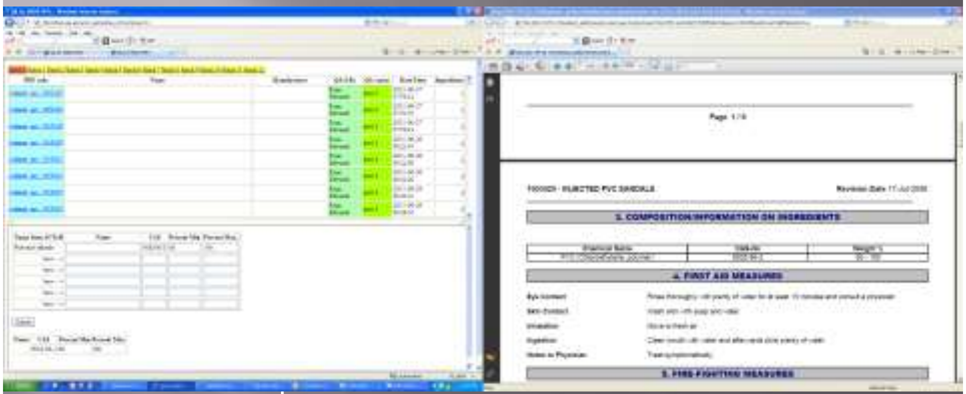
An EPA Pathfinder Innovation Project

Created by Ryan Edwards
Mentored by: Rocky Goldsmith

Project Outline

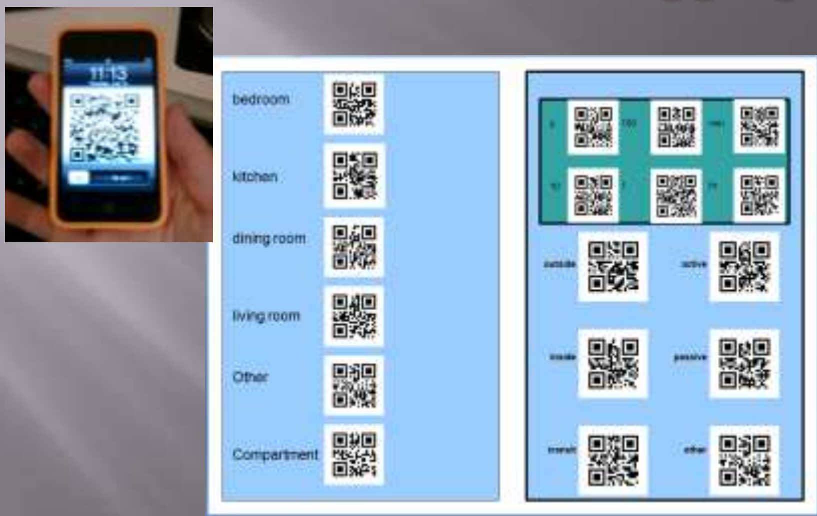
- Chemical Inventory (Mark up)
  - MSDS Database Design and Acquisition
  - Using Smartphone devices to scan product inventories and provide user with augmented reality of chemical exposures from personal products
- Data Mining
  - Move towards Integrating CHAD with social network streams
  - Capturing human activity patterns
- Computational Modeling
  - Simulating peoples daily activities used to explore personal chemical exposure scenarios

MSDS Manual Curation



Multi QR and UPC Code App Evaluation

Product Scanning: Microenvironment Tagging



Analyzing Human Activity Data

- CHAD (Consolidated Human Activity Database)
- Data taken from
  - 8 surveys
  - 123,542 entries
  - 21,723 subjects
  - Data taken by the top 25% by location
- Activity and Location Codes
- Natural Language Processor

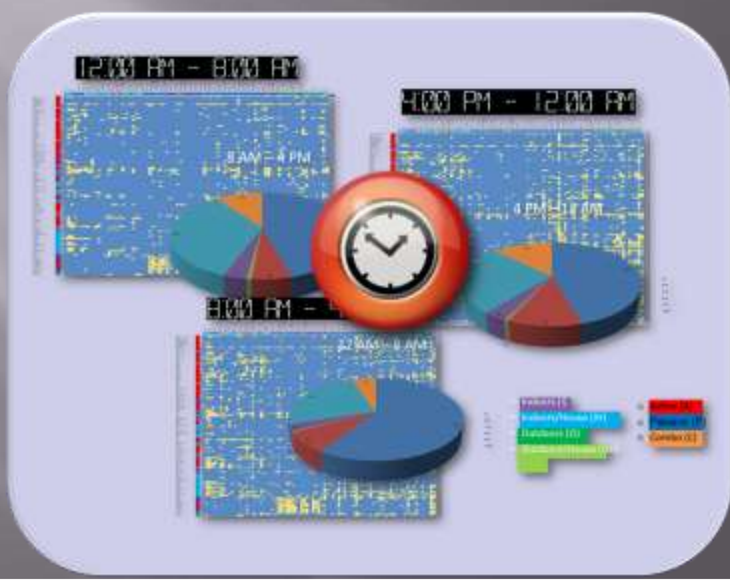
Example Diary Entry

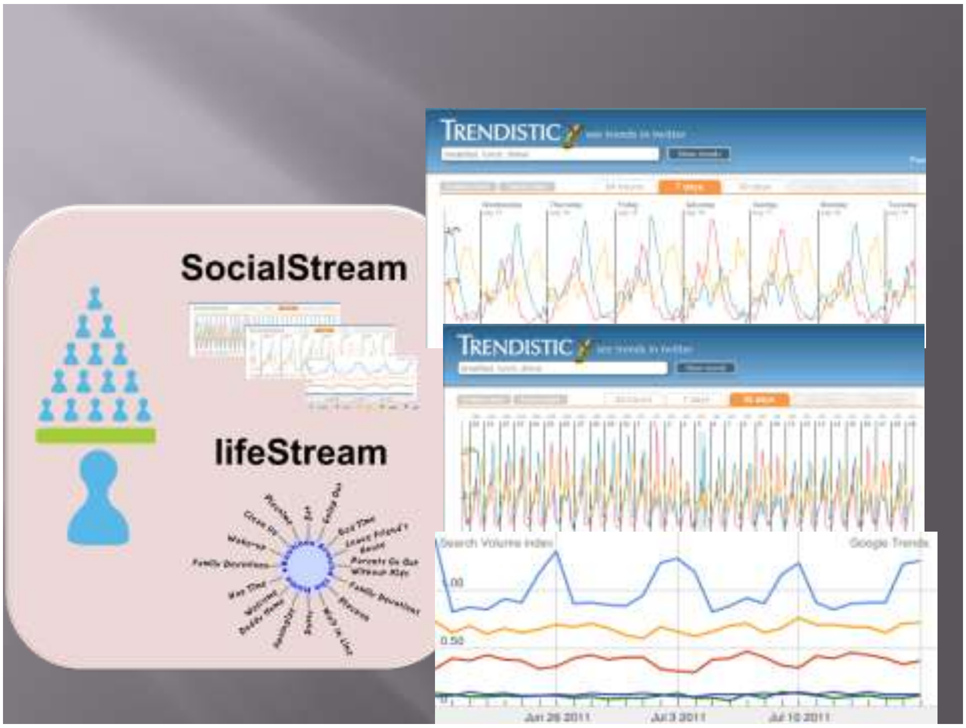
"In the kitchen about to make some eggs"

Location CHAD code: 30121 – Kitchen

Activity CHAD code: 11100 – Prepare and clean up food

Examining Activity Patterns





Sims3 for Agent-Based Human Modeling

- Character: Winston Smith
  - Traits: Handy, Natural cook, Neat, Friendly, Loves the outdoors,
  - Job: Office Drone

Future Work With the Sims

- Recording actions and locations
- Full AI
- Realistic worlds
- Possible Mods

Madeline Reich
SHAW University Summer Research Internship 2012

SEARCH TERMS +TWEETS = EXPOSURE INFORMATICS 2.0?

A bit about Maddie

- Rising Senior at FVHS
- Shaw University and the Environmental Protection Agency Research Apprenticeship Program
- Social Network Analysis for Personal Chemical Exposure Informatics

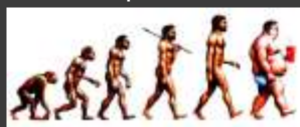
Identifying susceptible populations: SNA and search queries?

- Variables of interest
  - Geographic areas
  - Instances of disease related terms, weather, or human activities
  - Timelines
- Tools:
  - Google insights, Google maps
  - Twitter search, Twitter Maps
  - The Archivist
  - CDC, NOAA

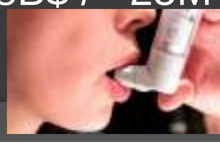
Disorders of interest

- **Migraines**, ~12B$ / ~75M people annually

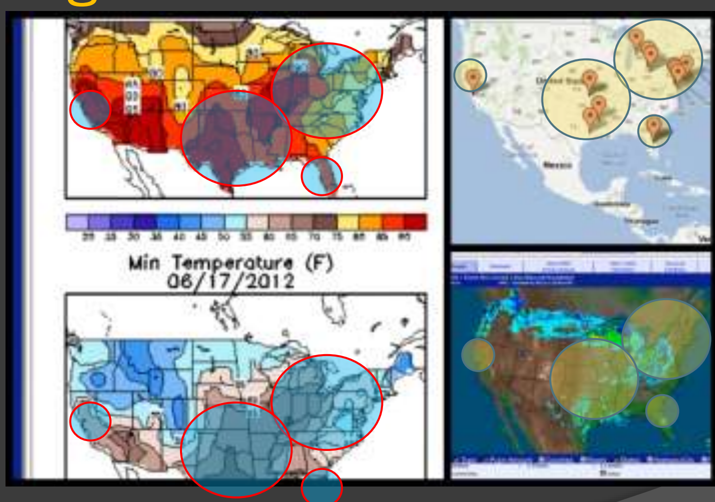
- **Obesity**, ~190B$ / ~111M people annually



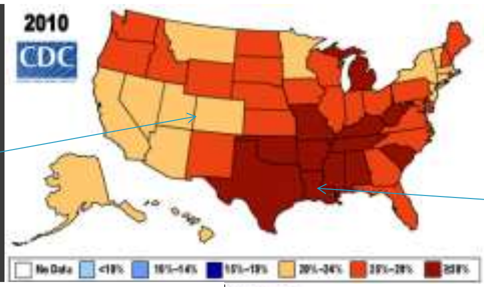
- **Asthma**, ~18B$ / ~25M people annually

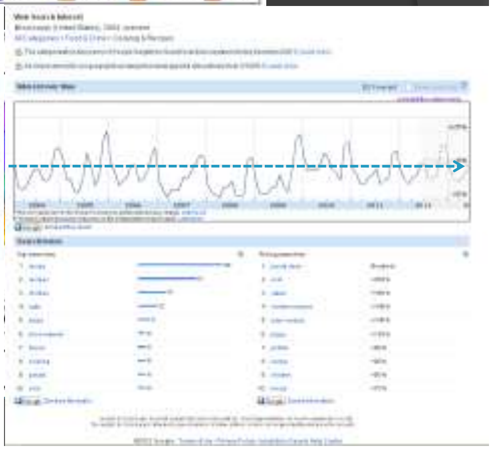


Migraines



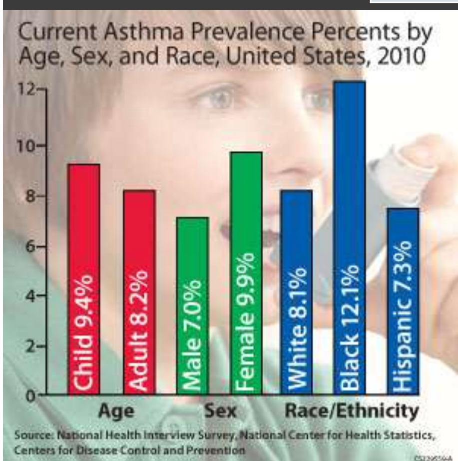
Obesity





Asthma

Age	13-17	18-25	26-34	35-44	45-54	55+
	20	18	8	4	0	0



C<A! ???

F>M !

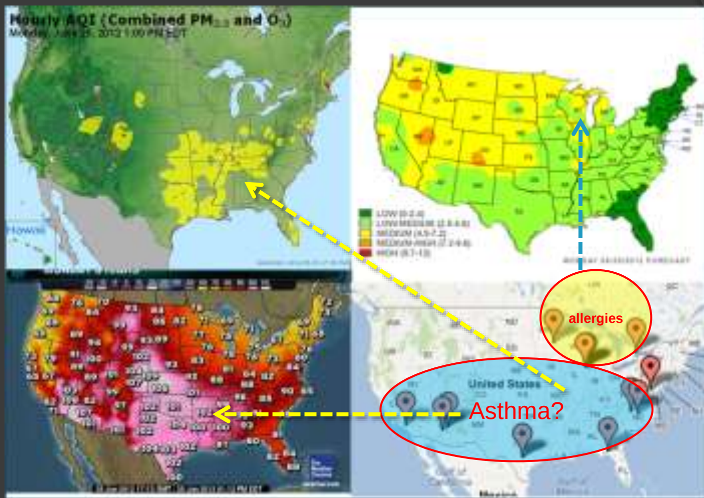
GENDER	Female	Male
	33	17

B>W>H!

Ethnicity	White	Black	Asian	Hispanic	Middle Eastern
	14	18	14	3	1

June 25th 2012

Air Quality index | Pollen.com pollen map



Temperature | Tweets for Asthma

Does Exposure Imitate Art? Recent Impressions

Renoir, *On the Terrace*, 1881

Personal Chemical Exposure Informatics: visualization, user experience, research in systems modeling and simulations.
June 26-27, 2012
Research Triangle Park, NC

Elaine Cohen Hubal
National Center for Computational Toxicology

Office of Research and Development
National Center for Computational Toxicology

Disclaimer.
Although this work was reviewed by EPA and approved for presentation, it may not necessarily reflect official Agency policy.

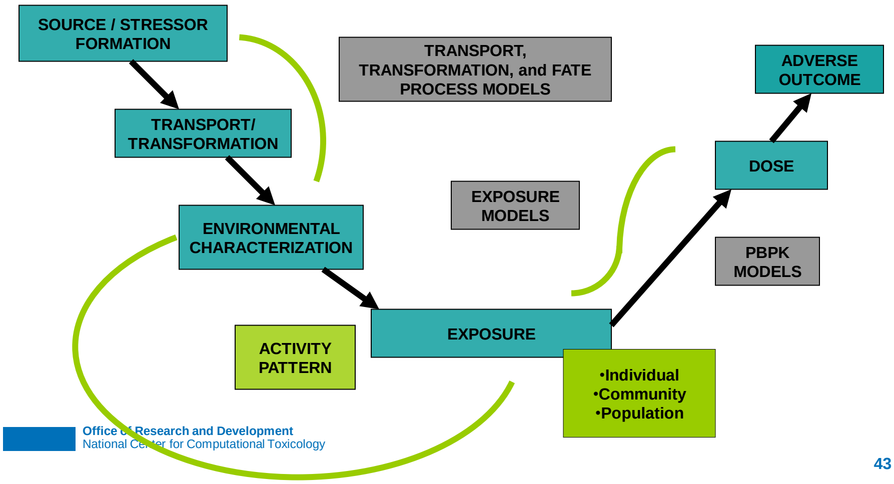
June 26, 2012

EPA United States Environmental Protection Agency

Exposure is the contact between a stressor and a receptor.

To assess exposure to a particular stressor we need to know

- **Properties of the stressor**
- **Sources, pathways, routes**
- **Pattern of exposure (magnitude, frequency, duration, location)**
- **Characteristics of receptor**



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National Center for Computational Toxicology

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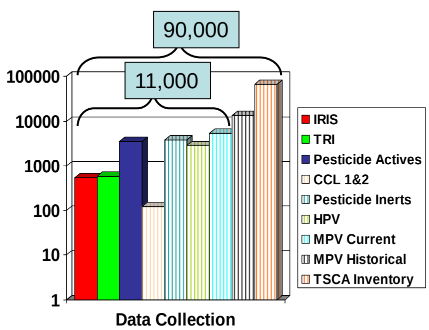
EPA United States Environmental Protection Agency

Context: Chemical Evaluation and Risk Assessment

Mandate: Assess Thousands of Chemicals

Need to develop methods to evaluate a large number of environmental chemicals for potential human-health risks



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National Center for Computational Toxicology

Richard Judson

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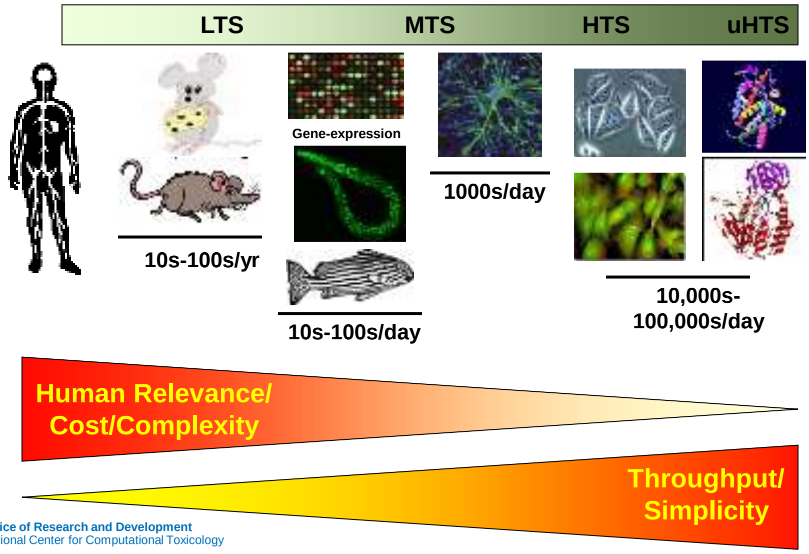
High-Throughput Screening Assays

batch testing of chemicals for pharmacological/toxicological endpoints using automated liquid handling, detectors, and data acquisition



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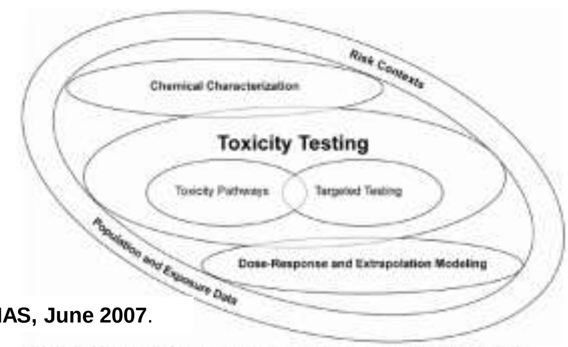
National Center for Computational Toxicology

Toxicity Testing in the Twenty-first Century: A Vision and a Strategy

- Key aspect of the NRC vision is that new tools are available to examine toxicity pathways in a depth and breadth that has not been possible
- An explosion of high-throughput-screening (HTS) data for *in vitro* toxicity assays will become available over the next few years ---- **Data are available now!**

How will this new toxicity information be *integrated with exposure information* to assess potential for real-world human health risk?



NAS, June 2007.

FIGURE 2-3 The committee's vision is a process that includes chemical characterization, toxicity testing, and dose-response and extrapolation modeling. At each step, population-based data and human exposure information are considered, as is the question of what data are needed for decision-making.

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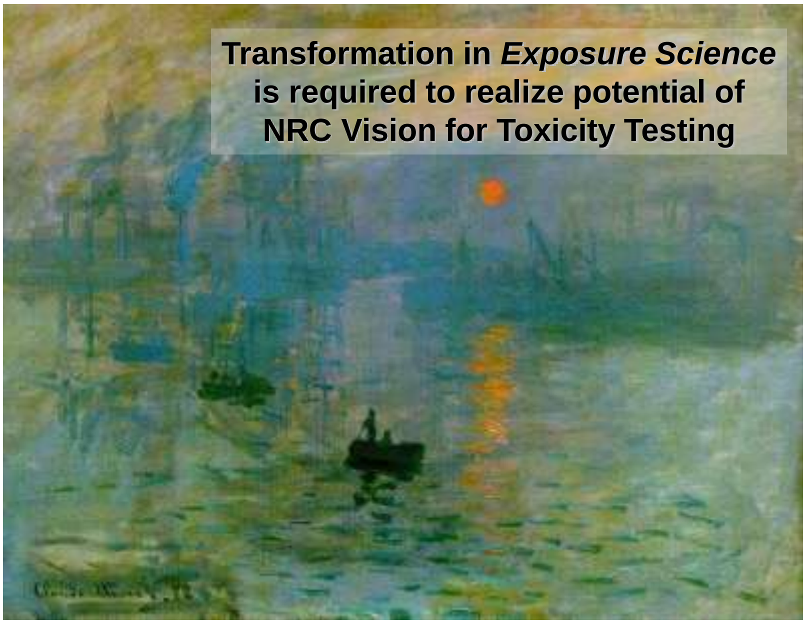
National Center for Computational Toxicology



Claude Monet, ***Impression,*** *soleil levant***,** 1872

United States Environmental Protection Agency

Does Exposure Imitate Art?

- System
  - Moved from studio out into modern world
  - Open compositions, realistic scenes
- Resolution
  - Exquisite detail (smoothly blended) of surrogate representation
  - Abstraction (distillation) of key determinants to address mechanism
  - Free brush strokes of pure color to emphasize vivid overall effects rather than details
- Determinants
  - Light (changing qualities)
  - Color (bright and varied)
  - Form (loose brush strokes)

Open System, Relevant Resolution

Jacques-Louis David, The Comtesse Vilain XIIII and Her Daughter (1816)

Pierre-Auguste Renoir, Le Moulin de la Galette, 1876

Key Determinants

Fragonard, The Swing, 1767

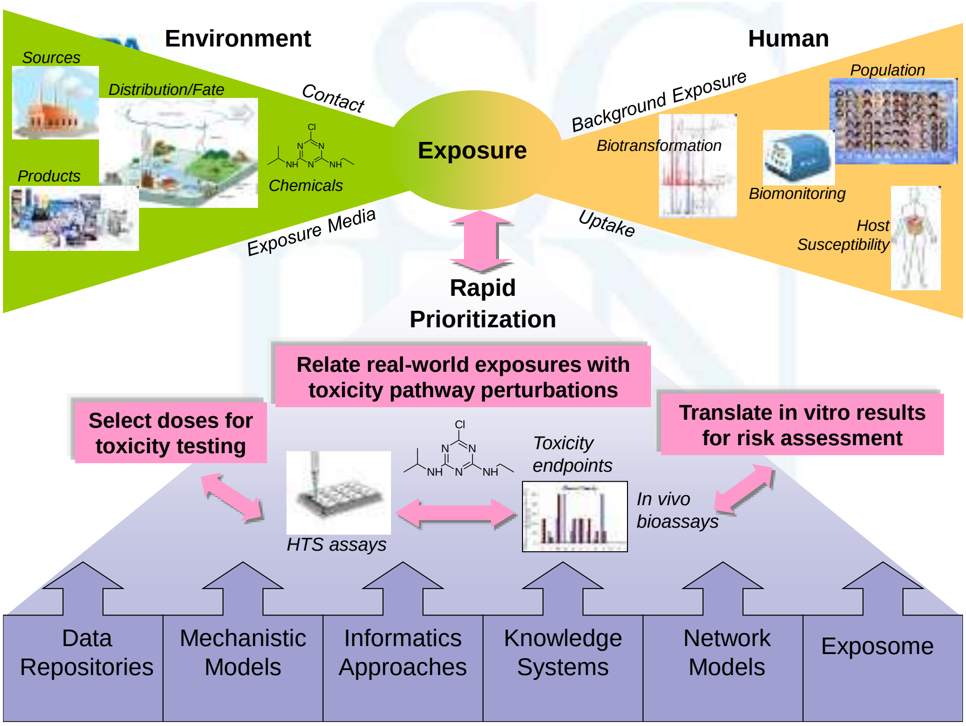
Renoir, The Swing (La Balançoire), 1876

Variability, Vulnerability and Life-stage Aspects Integral

Monet, Grainstacks 1890-1890

ExpoCast™: Exposure Science for Prioritization and Toxicity Testing

- Recognizes critical need for exposure information to inform
  - Chemical design and evaluation
  - Health risk management
- Goal
  - Advance characterization of exposure required to ***translate*** findings in computational toxicology to support exposure and risk assessment
  - **Together with ToxCast™ help EPA determine priority chemicals**
- Approach
  - **Mine and apply scientific advances and tools in a broad range of fields**
  - Develop novel approaches for evaluating chemicals based on potential for *biologically-relevant* human exposure



United States Environmental Protection Agency

ExpoCast: Recent Activities

- **Chemical Prioritization**
  - Incorporating and Linking Exposure Information into ACToR
  - ExpoCastDB
  - Integrated Chemical Prioritization Scheme
  - *Partnering to Develop Exposure Indices for Rapid Prioritization of Chemicals in Consumer Products*
  - High Throughput Exposure Estimates
  - *Rapid modeling of SVOC exposure in indoor environment*
  - *Intake Production Ratio*
- **Informing Design of Toxicity Testing**
  - Selecting Doses for ToxCast *In Vitro* Testing – Nanomaterials
  - Identify Priorities for Mixture Research - Modelinh Chemical Co-Occurrence
- **Translate in vitro Results for Risk Assessment**
  - *Combining ToxCast, Dosimetry and Exposure*
  - *ExpoDat2012: Exposure determinants for high throughput risk assessment*
- **Relate Real-World Exposures with Tox Pathway Perturbations**
  - *ExO: An Exposure Ontology*

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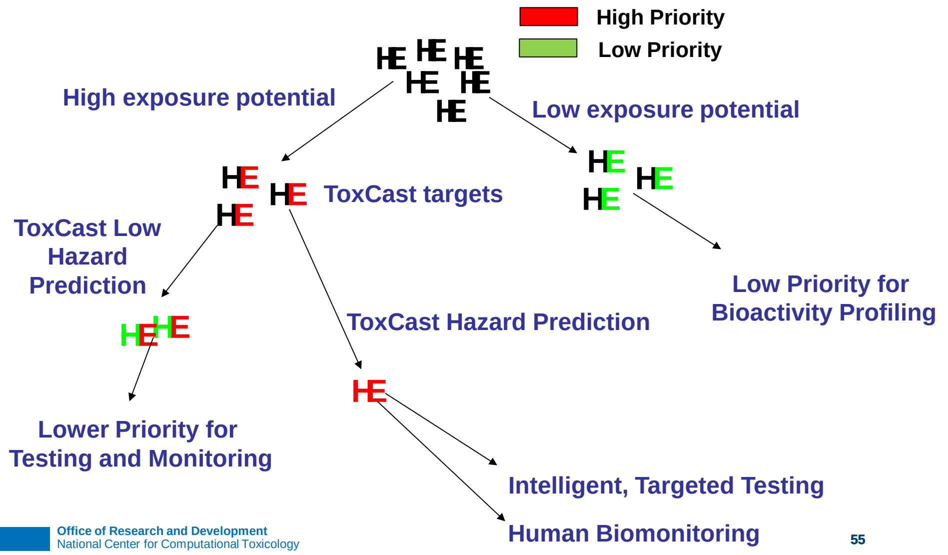
Prioritization: Using Hazard and Exposure Information



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Richard Judson

Knowledge Management and Decision Support Tools for CSS

- Data Management Warehouse (e.g., ACToR)
  - federate raw data generated by CSS/EPA and available in the public domain on: chemical structure, production, environmental fate, human use, ecological and health effects, **exposure,** etc.
- Ontologies for Interoperability
  - publicly available ontologies will be used to specify the semantics to integrate experimental data from multiple sources, as well as the inputs and outputs of diverse predictive tools (e.g. empirical models, pathway analysis, systemsmodels, etc.).
- Knowledge-based management system (KB):
  - Develop KB systems that use the above ontologies to acquire, organize, store and share the complex information flows across diverse CSS activities on chemical inherency, production, **exposure,** hazard, pathways and sustainability metrics.

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Exposure Ontology, ExO: Definitions of Central Concepts

- **Exposure Stressor** - An agent, stimulus, activity, or event that causes stress or tension on an organism and interacts with an exposure receptor during an exposure event.
- **Exposure Receptor** - An entity (e.g., a human, human population, or a human organ) that interacts with an exposure stressor during an exposure event.
- **Exposure Event** - An interaction between an exposure stressor and an exposure receptor.
- **Exposure Outcome** - Entity that results from the interaction between an exposure receptor and an exposure stressor during an exposure event.

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Mattingly et al, EST, 2012

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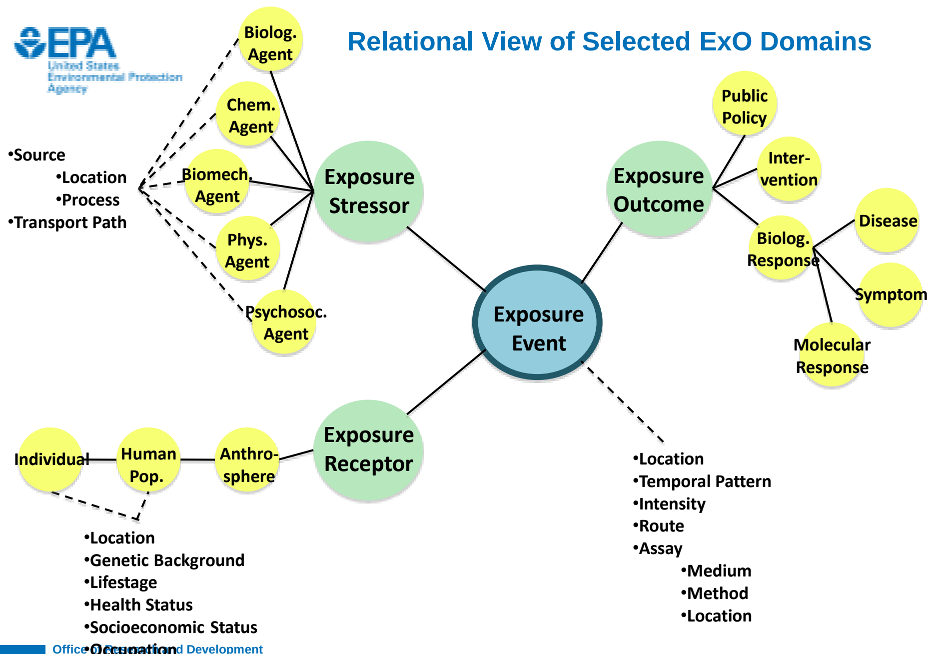
Relational View of Selected ExO Domains



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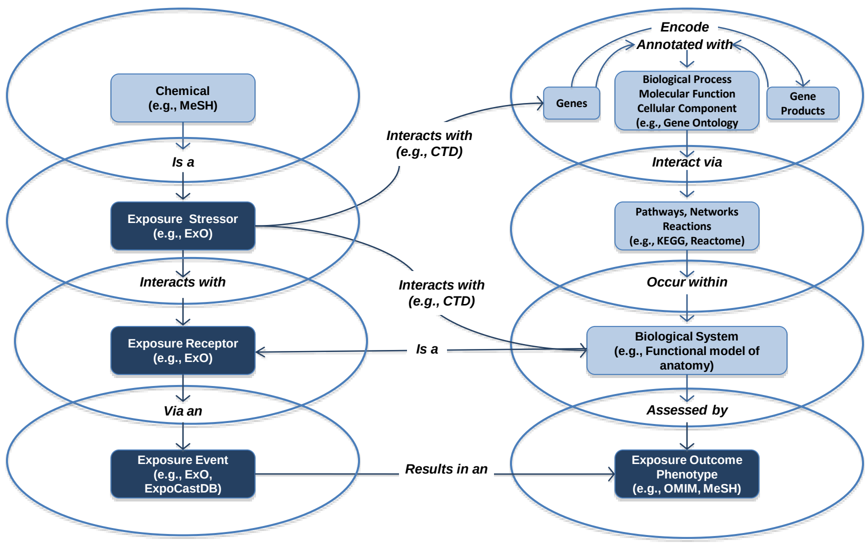
Mattingly et al, 2012, EST

High-level schematic of Exposure Ontology (ExO) integration within a broader biological context.



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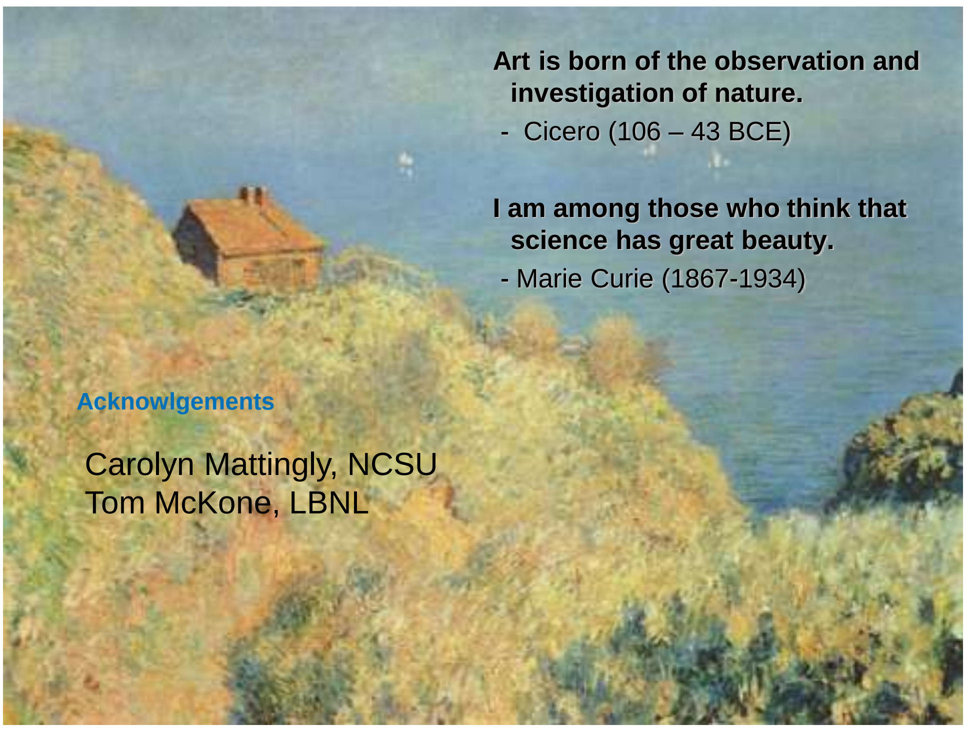
Mattingly et al, EST, 2012



ExpoCast:
High Throughput Exposure Potential Prediction

John Wambaugh
U.S. EPA, National Center for Computational Toxicology

Office of Research and Development

June 26, 2012

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

Introduction

Goal: There are thousands of chemicals, many without enough data for evaluation – working to provide a high-throughput exposure approach to use with the ToxCast chemical hazard identification.

TSCA21: Prioritization of ~500 Toxic Substances Control Act (TSCA) chemicals

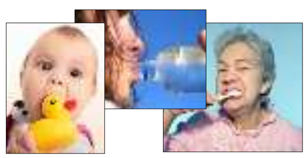
EDSP21: Prioritization of ~2000 Endocrine Disruptors Screening Program (EDSP) chemicals

OW21: Development of next chemical contaminants list (CCL)

Using fate and transport models to predict the contribution from manufacture and industrial use to overall exposure rapidly and efficiently

Applying and developing new high throughput models of consumer use and indoor exposure

Environmental Fate and Transport



Consumer Use and Indoor Exposure

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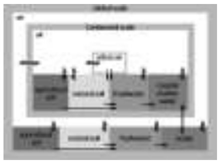
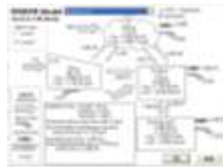
Exposure-related Models Amenable to High Throughput Operation

Exposure-based prioritization challenge identified two models capable of HT operation (RAIDAR and USEtox)

Harmonized chemical descriptors (EPI Suite)

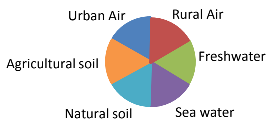
USEtox
Olivier Jolliet

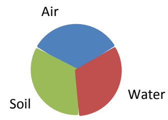




RAIDAR
Jon Arnot

Default release profiles needed (two variations used, either pesticidal or water)



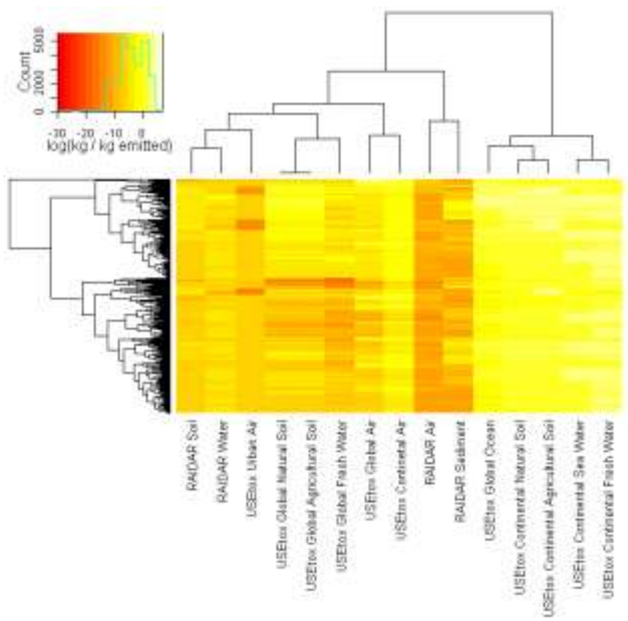


Predictions for 1678 Chemicals

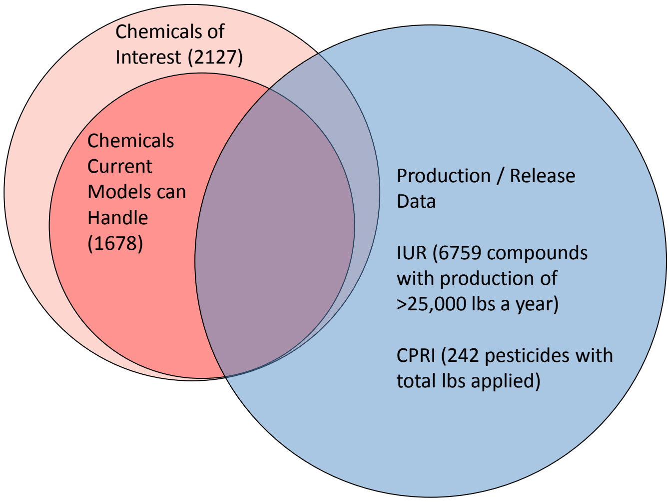
Models predict partitioning of >1600 chemicals into environmental media, and describe human interaction with that media

Use models like related high-throughput assays

How do we ground-truth these predictions?



Data Availability for Model Predictions and Ground-truthing

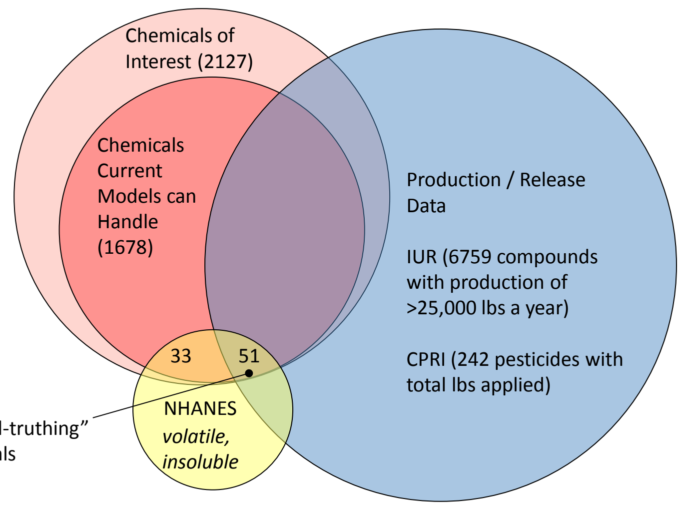


Data Availability for Model Predictions and Ground-truthing

Ground—truth with CDC NHANES urine data

Focusing on U.S. median initially

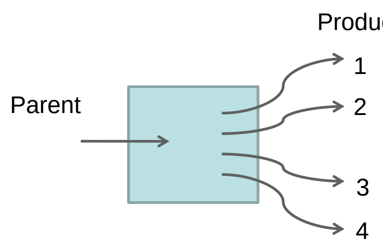
Capable of adding population variability, but will need consumer use models



Linking NHANES Urine Data and Exposure

Steady-state assumption

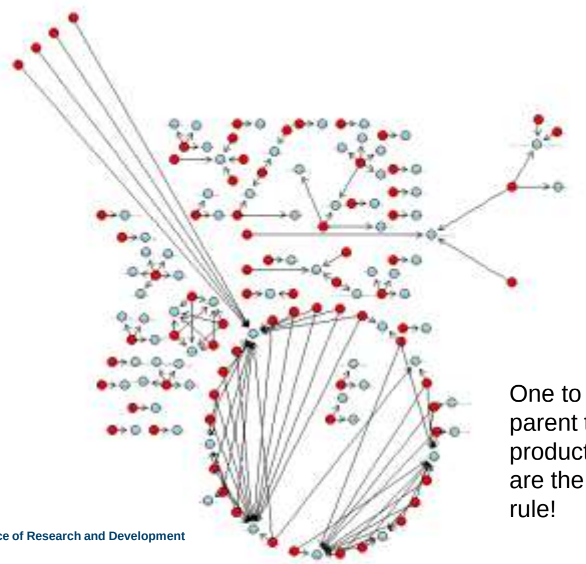
$$(\text{mg/kg/day})_i = \frac{1}{70\text{ kg}}\frac{\text{mg}_i}{\text{g}_{\text{creatine}}} * \frac{\text{g}_{\text{creatine}}}{\text{day}}$$



$$(\text{mg/kg/day})_0 = \text{MW}_0 \sum_i \phi_{0i} \frac{(\text{mg/kg/day})_i}{\text{MW}_i}$$

Lakind and Naiman (2008)

Stoichiometry of NHANES Parents and Metabolites



One to one mappings of parent to urinary products (metabolites) are the exception, not the rule!

Calibrate ExpoCast Predictions to CDC NHANES Data

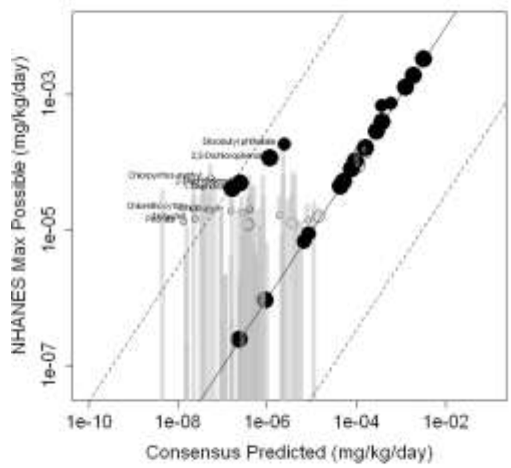
$$Y \sim b_1 + b_2 * N + m_2 \log(vu) + m_3 \log(vr)$$

Comparison between model predictions and biomonitoring data indicates positive correlation

Consumer use is critical: Compounds with near-field applications on average 11000x greater

Rigorous statistical analysis gives calibration of predictions

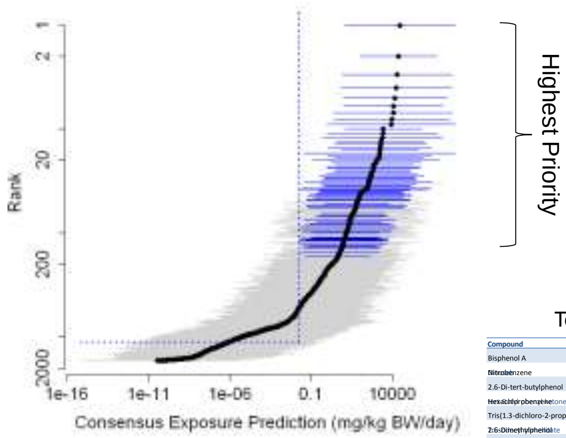
Same analysis gives uncertainty (confidence) in those predictions



Exposure Prioritization from ExpoCast

Uncertainty of prediction indicated by the horizontal confidence interval from the empirical calibration to the NHANES data

Horizontal dotted line indicates the fiftieth percentile rank and the vertical dotted line indicates the cutoff between overlapping top-half and lower half confidence intervals



Top Ten

Compound	CASRN
Bisphenol A	80-05-7
Nitrobenzene	98-95-3
2.6-Di-tert-butylphenol	128-39-2
Hexachlorobenzene	118-74-1
Tris(1.3-dichloro-2-propyl) phosphate	13674-87-8
2.6-Dimethylphenol	576-26-1
Octrizole	3147-75-9
Surinabant	288104-79-0
4-tert-Butylphenol	98-54-4
2.4-Di-tert-butylphenol	96-76-4
Potassium 2-ethylhexanoate	3164-85-0

Conclusions

- Production volume (a multiplicative factor in USEtox/RAIDAR predictions) is a primary determinant of predicted exposure
- Indoor/consumer use is a primary determinant
- Next steps:
  - HT models for exposure from consumer use and indoor environment
  - Use and evaluate these models as additional HT exposure assays

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U.S. E.P.A. Office of Research and Development ExpoCast Team

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The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

From *Decision Analytics for Exposure Prioritization to dietary residue exposures*

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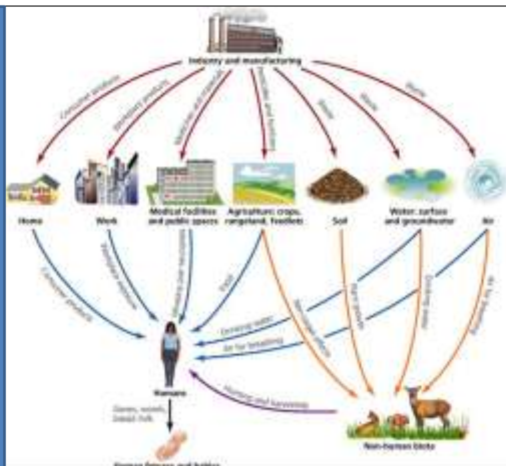
PerCEIVERS
Personal **C**hemical **E**xposure **I**nformatics: **v**isualization, user **E**xperience, **R**esearch in **S**ystems modeling and Simulations
U.S. EPA, Research Triangle Park, NC
June 26–27, 2012

Overview of Research/Work

Modeling approaches for multi-media, multi-pathway exposure screening for prioritization of chemicals

Chemical Safety for Sustainability

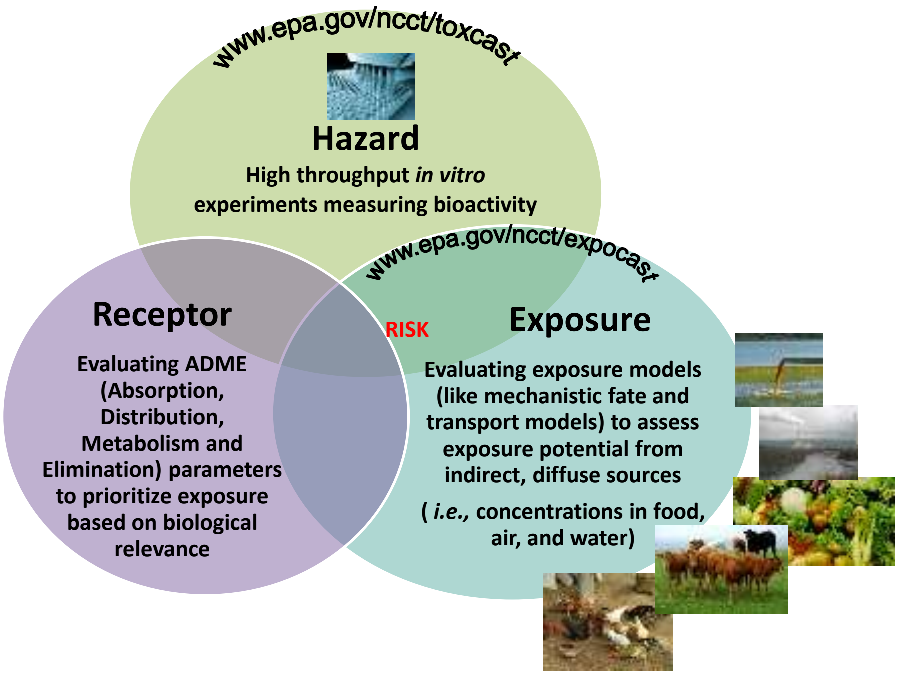
- Complementary exposure data for ranking chemicals for further testing
- Toxic Substance and Control Act (TSCA) Inventory
- Consumer products

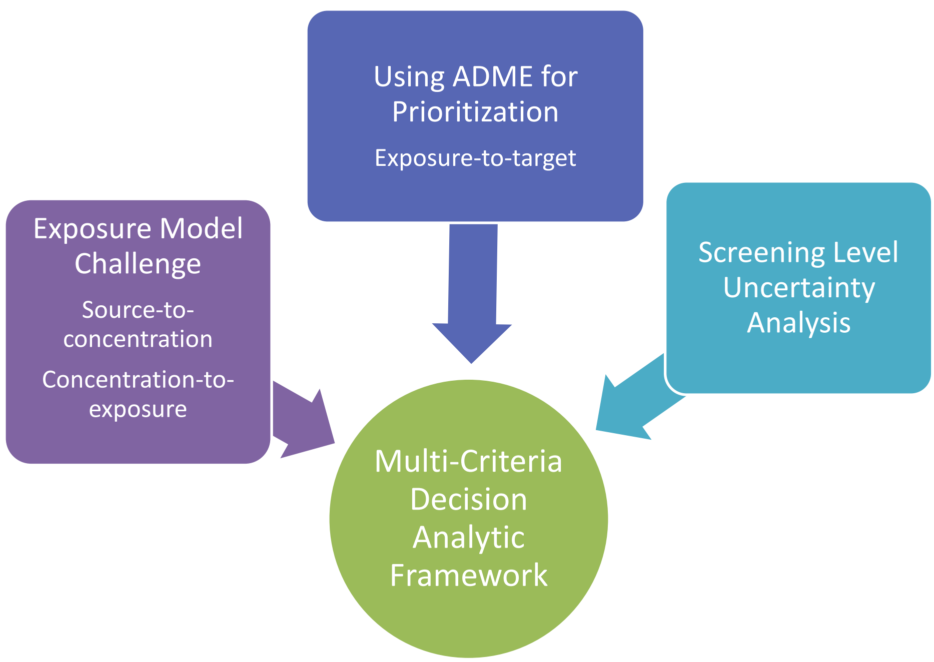


http://web.bryant.edu/~dlm1/sc372/readings/toxicology/toxicology.htm Dan L. McNally, Associate Professor, Department of Science and Technology, Bryant University, Smithfield, RI

National Residue Program

- Sampling of meat, poultry, and egg products
- Veterinary drugs
- Pesticides
- Environmental contaminants

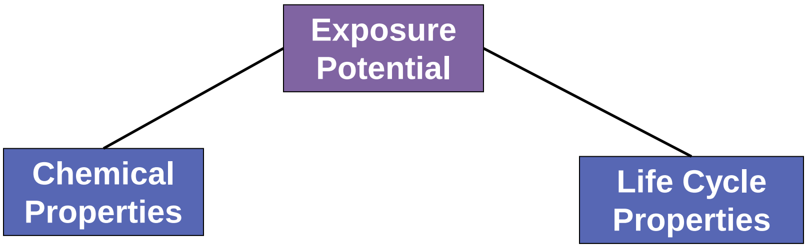

www.epa.gov/ncct/toxcast
Hazard
High throughput *in vitro* experiments measuring bioactivity
www.epa.gov/ncct/expocast
Receptor
Evaluating ADME (Absorption, Distribution, Metabolism and Elimination) parameters to prioritize exposure based on biological relevance
RISK
Exposure
Evaluating exposure models (like mechanistic fate and transport models) to assess exposure potential from indirect, diffuse sources
(*i.e.,* concentrations in food, air, and water)


Using ADME for Prioritization
Exposure-to-target
Exposure Model Challenge
Source-to-concentration
Concentration-to-exposure
Screening Level Uncertainty Analysis
Multi-Criteria Decision Analytic Framework

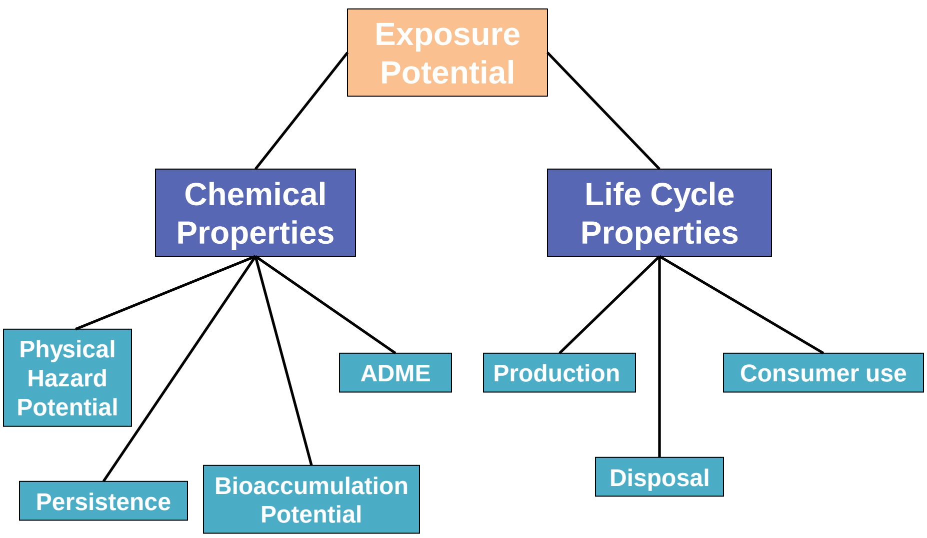
Multi-criteria Decision Modeling

Testing decision analytic approaches to:

- Integrate disparate data types (criteria and attributes)
- Overcome limitations of statistical or mechanistic models
- Provide a framework for value of information analysis
- Communicate results that are transparently and scientifically defensible



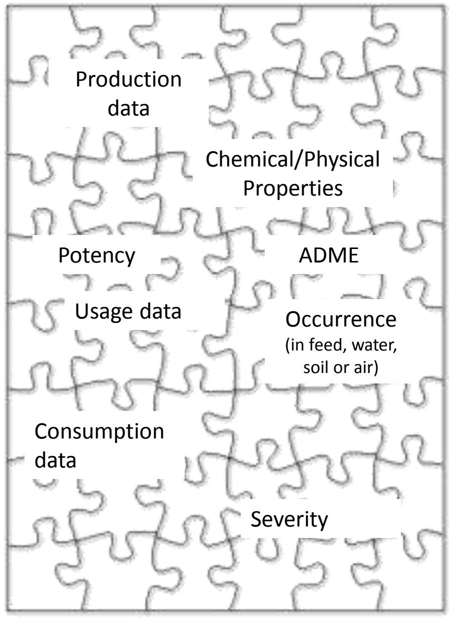
Multi-criteria Decision Modeling



Future FSIS Application

- Exposure and toxicity information for certain classes of chemicals, like veterinary drugs and pesticides are available
- Other classes, like many environmental contaminants, lack sufficient data

Criteria for ranking new hazards



United States Environmental Protection Agency

Exposure Factors Handbook: Consumer Products Data

Linda Phillips

U.S. EPA, ORD, NCEA

phillips.linda@epa.gov

Personal **C**hemical **E**xposure **I**nformatics: **v**isualization, user **E**xperience, **R**esearch in **S**ystems modeling and Simulations (***PerCEIVERS) Meeting***

June 26/27, 2012

History of the *Exposure Factors Handbook (EFH)*

- Precursor: *Development of Statistical Distributions or Ranges of Standard Factors Used in Exposure Assessment* - 1985
- EFH first published - 1989
- EFH updated - 1997
- Child-specific EFH - 2008
- EFH updated again - 2011
  http://cfpub.epa.gov/ncea/risk/recordisplay.cfm?deid=236252
- Highlights of the EFH - 2011
  http://cfpub.epa.gov/ncea/risk/recordisplay.cfm?deid=221023
- Toolbox (web-based) edition currently under development
- Related documents



Topics Covered in the 2011 *EFH*

- Executive Summary
- Introduction
- Variability and Uncertainty
- Food and Water Intake
- Mouthing Behavior
- Soil Ingestion
- Inhalation Rates
- Dermal Factors
- Body Weight
- **Consumer Products** (added in 1997)
- Activity Patterns
- Life Expectancy
- Building Characteristics



2011 Revision of the *EFH*

- Incorporated children's data from 2008 *Child-Specific EFH*
- Included data for other special populations (e.g., pregnant women)
- Improved organization and consistency on data presentation
- Expanded discussions on data limitations
- Enhanced selection criteria approach
- Added new data and analyses
  - **e.g., new consumer products data added**
- Developed new chapters/sections to address additional factors
- Revised recommendations

EPA-Expo-Box

(**EPA Expo**sure Assessment Tool **Box**)

Exposure Factors Module

- Currently under development
- Highlights of each factor
- Full detail for each factor
- Bookmarks for easy navigation
- Links to source references via HERO
- Spreadsheets in downloadable form
- Links to related resources
- Search capabilities (i.e., key words/topics)

EFH Consumer Products Data

Primary Data Sources/Surveys

- Cosmetic, Toiletry, and Fragrance Assoc. (1983)
- Westat (1987)
  - Household solvents
  - Household cleaning products
  - Interior painters survey
- Abt (1992) Methylene Chloride Survey
- EPA National Human Activity Patterns (1996)
- Bass et al. (2001) Household Pesticides
- Weegels and van Veen (2001) Household Products
- Loretz et al. (2005, 2008) Cosmetics
- Hall et al. (2007) Cosmetics
- Sathyanarayana et al. (2008) Baby Care Products

EFH Consumer Products Data

EFH Consumer Products Information Summaries

- Survey descriptions
  - study elements and scope
  - parameters (products, populations, and scale)
- Data tables
  - frequency
  - duration of use
  - amount of product used per event
- Limitations and Uncertainties
  - limited data (manufacturers data generally proprietary)
  - age of data (changes in uses over time)
- Recommended values **not provided** due to diversity of product types

Example of *EFH* Consumer Products Data

Table 17-40. Frequency of Use of Personal Care Products

Product Type	*N*	Average Number of Applications per Use Day[a]			
		Mean	SD	Min	Max
Hairspray (aerosol)	165[b]	1.49	0.63	1.00	5.36
Hairspray (pump)	162	1.51	0.64	1.00	4.22
Liquid Foundation	326	1.24	0.32	1.00	2.00
Spray Perfume	326	1.67	1.10	1.00	11.64
Body Wash	340	1.37	0.58	1.00	6.36
Shampoo	340	1.11	0.24	1.00	2.14
Solid Antiperspirant	340	1.30	0.40	1.00	4.00

[a] Derived as the ratio of the number of applications to the number of use days.
[b] Subjects who completed the study but did not report their number of applications were excluded.
N = Number of subjects (women, ages 18 to 65 years).
SD = Standard deviation.
Source: Loretz et al., 2006.

Use of *EFH* Consumer Products Use Data for Systems Reality Modeling

- Mapped EFH consumer product use data to NLM Household Products Database (HPD) product types
- Over 2,400 product types in 9 major HPD categories
- Identified EFH tables with relevant data on:
  - Amount used
  - Frequency of use
  - Duration of use
  - Total time exposed
  - Time exposed after use

Mapping of *EFH* Data to HPD Product Categories

CATEGORY	SUB-CATEGORY	PRODUCT	IN EFH? (yes=1; no=0)	REFERENCE TABLE: amount used	REFERENCE TABLE: frequency	REFERENCE TABLE: duration	REFERENCE TABLE: total time exposed	REFERENCE TABLE: time exposed after use	REFERENCE SOURCE
HOME MAINTENANCE	PAINT	INTERIOR LATEX GLOSS	1	Table 17-6 Table 17-15	Table 17-4 Table 17-14	Table 17-5 Table 17-13 Table 17-14 Table 17-23		Table 17-7	Westat 1987a Westat, 1987c Westat, 1987c US EPA, 1996
INSIDE THE HOME	LAUNDRY	SPOT REMOVER	1	Table 17-6	Table 17-4	Table 17-5 Table 17-28		Table 17-7	Westat 1987a US EPA, 1996
INSIDE THE HOME	CLEANER	TOILET BOWL	1	Table 17-37	Table 17-37	Table 17-37			Weegels and VanVeen, 2001
INSIDE THE HOME	CLEANER	TUB/TILE	1		Table 17-10	Table 17-11	Table 17-8 Table 17-9 Table 17-12		Westat, 1987b Westat, 1987b Westat, 1987b
PERSONAL CARE	EYE CARE/MAKEUP	CONTACT LENS CLEANER	0						
PERSONAL CARE	EYE CARE/MAKEUP	EYE MAKEUP REMOVER	1		Table 17-3				CTFA, 1983
PERSONAL CARE	EYE CARE/MAKEUP	EYE SHADOW	1	Table 17-52 Table 17-53	Table 17-3 Table 17-51				CTFA, 1983 Loretz et al., 2008 Loretz et al., 2008
PESTICIDES	INSECTICIDE	INSECT REPELLENT	1		Table 17-34 Table 17-35 Table 17-36	Table 17-30			US EPA, 1996 US EPA, 1996 Bass et al., 2001

Examples of New Consumer Product Use Data Not in 2011 EFH

- Just, et al. (2010) Urinary and air phthalate concentrations and self-reported use of personal care products among minority pregnant women in New York City. *J Expo Sci Environ Epidem* 20(7) 625-633.
- Wu, X. et al. (2010) Usage pattern of personal care products in California households. Food and Chemical Toxicology 48:3109–3119.
- Portland State University (PSU), Survey Research Lab (2011). Personal Care Products Survey. Available online at: http://www.oeconline.org/our-work/healthier-lives/whats-in-my-makeup-bag/personal-care-product-survey-report/
- Moran, R.E., et al. (2012) Frequency and longitudinal trends of household care product use. Atmospheric Environment 55: 417-424.

Human Activity Data in Exposure Assessment

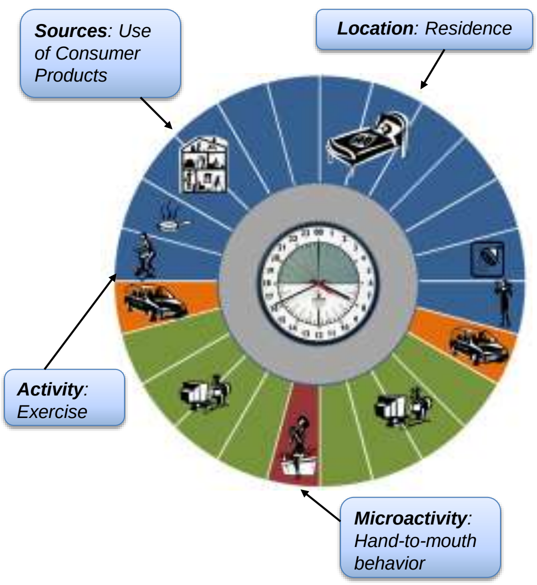
Kristin Isaacs, National Exposure Research Laboratory

PerCEIVERS Workshop, June 26, 2012

Office of Research and Development
National Exposure Research Laboratory

Human Activity Patterns in Exposure Assessment and Exposure Modeling

- Movement and activities of humans (receptor) in time and space
- Location→ microenvironment → pollutant concentrations
- Activity → energy expenditure → ventilation and/or caloric intake → intake dose
- Exposure-related activities or microactivities
- Pollutant-generating activities → microenvironmental sources



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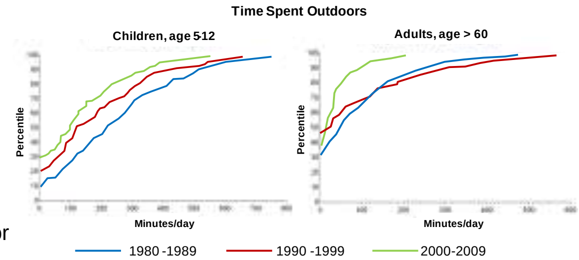
National Exposure Research Laboratory

Critical Attributes of Human Activity Data

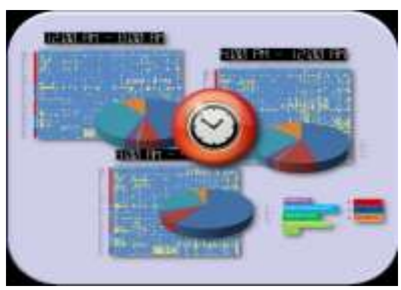
- **Longitudinal** Information
  - Quantification of mean behavior of individuals
  - Characterization of intra- and inter-individual variability
  - Temporal patterns in individuals (season, daytype)
  - Trends over time within individuals with growth and development or aging (change in lifestage)
- **Representative** Information
  - Age/Gender
  - Race
  - SES
  - Culture
  - Geography
- **Timely** Information
  - Population shifts in behavior

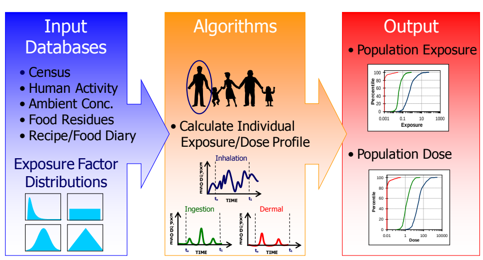
  due to societal changes



Current Databases and Tools

- NERL's Consolidated Human Activity Database (**CHAD**)
  - 41,600 real 24-hour human activity diaries
  - 19 studies 1980 – 2007
  - New data being added
- EPA's Exposure Models using CHAD
  - Based upon building a simulated population of people
  - Stochastic Human Exposure Simulations (SHEDS) Models (Multimedia chemicals, PM, Air Toxics)
  - Air Pollutants Exposure Model (APEX) - OAPQS
  - Screening-tier exposure models (SHEDS-Lite)

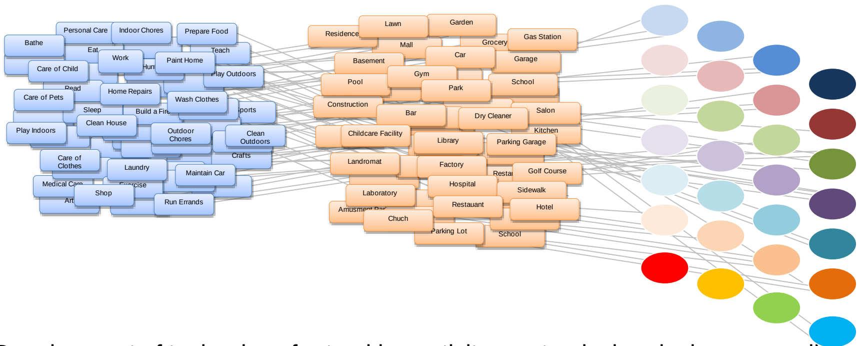




Human Activity Data and Personal Chemical Informatics

- Natural linkages between human activities and PCI
  - Locations /activities can drive contact with chemicals: Framework for modeling **Usage and Exposure**

CHAD Activities *CHAD Locations* *Chemical or Consumer Product Category*



- Development of technology for tracking activity can track chemical use as well

Current Projects to Address Human Activity and Potentially Chemical Exposures

- Collection of detailed human activity data is **burdensome**
- **Use of new technologies will be essential**
  - GPS (location) -MicroTrack
  - Accelerometry (activity level for intake dose)
  - Active collection
    - Smartphone methods for collection of data
- **Innovative data streams**
  - Social media
    - Natural language processing (NLP) of Twitter feed archives
    - Geographic component

Future Work

- Continue to rapidly update of CHAD to include detailed available human activity information on a minute-by-minute resolution for higher tier assessments
- Continue research into building longitudinal activity patterns from cross-sectional data
- Leveraging other public data and engaging the public – "**participatory sensing**"
- Energy expenditure (EE) research
  - Better characterization of EE for activities, ventilation, intake dose rates across life stage
  - Currently collaborating with exercise and obesity researchers CDC, NIH, NCI to build and curate a new database of individual EE measurements from academic and government labs across the U.S.
  - Linkage of average EE rates with dietary intake of food/chemicals
- Start to consider modeling paradigms for linking CHAD-type HA information with chemical use data in a meaningful way
- Isaacs.kristin@epa.gov

Passive Sampling Methods to Determine Personal and Household Care Product Use

Deborah Bennett[1], Xiangmei (May) Wu[1], Candice Teague[1]
Kiyoung Lee[3], Beate Ritz[2], Diana Cassady[1], Irva Hertz-Picciotto[1]

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[2] University of California, Los Angeles, Los Angeles, CA, U.S.A.
[3] Seoul National University, Seoul, Korea

STUDY GOALS

- **S**tudy of **U**se of **P**roducts and **E**xposure-**R**elated **B**ehaviors: SUPERB Study
- Pesticides, personal care products, household care products, food intake, time activity
- Multiple Tiers
  - Tier 1: Largest Tier collected 3 years of phone interviews
  - Tier 2: Internet based questionnaire every month
  - Tier 3: Home based passive methods
  - Tier 4: Environmental and biological samples
- Longitudinal changes

Background

- Traditionally, data has been collected through questionnaires, which is very time consuming for participants.
- Determining use of personal and household care products is of interest, both for use in epidemiology studies as well as in determining exposure for risk assessments.
- New sampling method is desired to minimize participants' effort.
- Identify products used and amount used.

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Study Population

- **453** families, children <6 yrs
  - Birth Certificate records
  - 22 Northern CA Counties
  - **30** families in Tier 3
- **152** households, adult >55 yrs
  - Probability sampling by number of housing units
  - 3 Central California counties, with high agricultural productivity
  - 17 individuals in Tier 3

Methods

- Bar codes readily found on consumer products quickly and reliably determine what products people used in their homes.
- Scan and weigh products at beginning and end of week. Mark scanned products.
- Determined the change in mass of the product over a one week period to assess the potential magnitude of exposure.
- Visit each home 4 times periods to capture longitudinal variability

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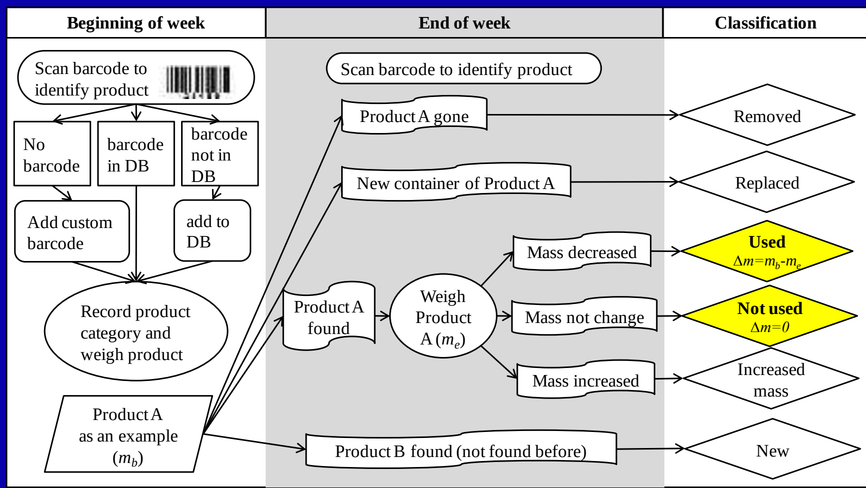
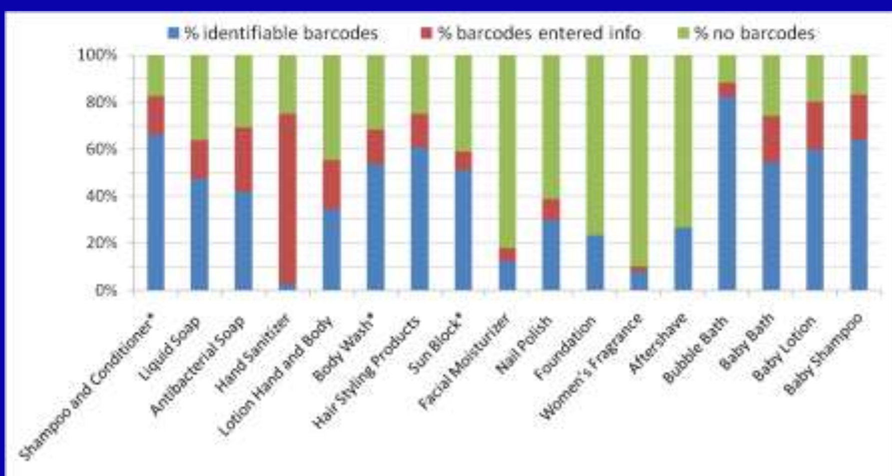
Sampling Procedure



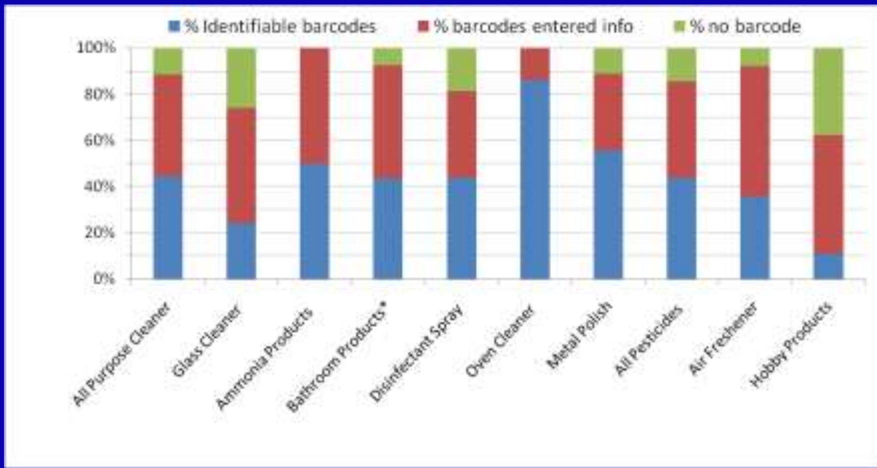
103

Frequency of identifiable barcodes, readable barcodes, and missing/illegible barcodes



104

Frequency of identifiable barcodes, readable barcodes, and missing/illegible barcodes



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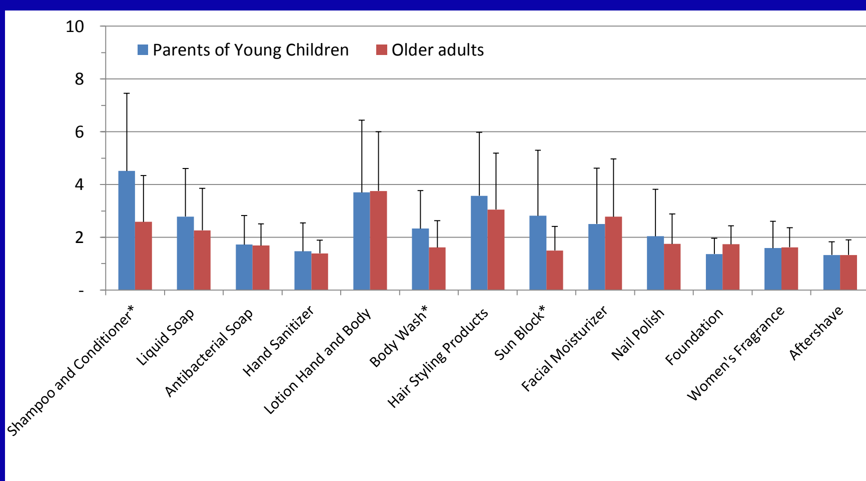
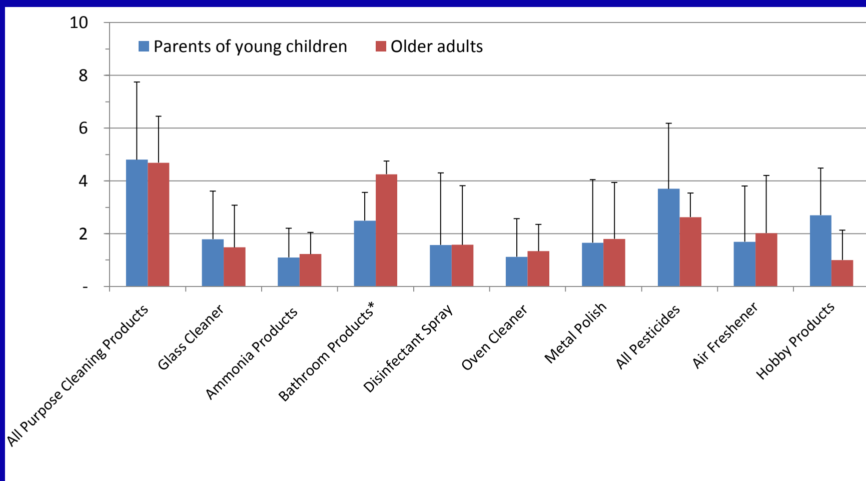
Number of product found per product category (Mean and STD)



106

Number of product found per product category (Mean and STD)



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Product Use Scenarios

- Used - Product found both times, and mass decreased
- Not Used - Product found both times, and mass the same
- Increased Mass - Product found both times, and mass increased
- Removed - Product found at beginning of week but not at end of week
- New - Product found only at end of week
- Rediscovered - Product found only at the end of the week, but had been seen before
- Replaced - Product found at the beginning and end of the week, but there was a new container at end of week

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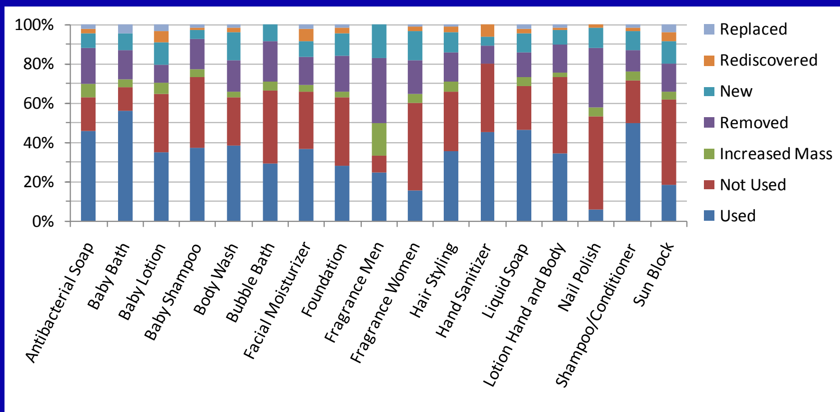
Personal Care Products

Percent of products that were used, not used, increased in mass, removed, new, rediscovered, or replaced during a week of observation



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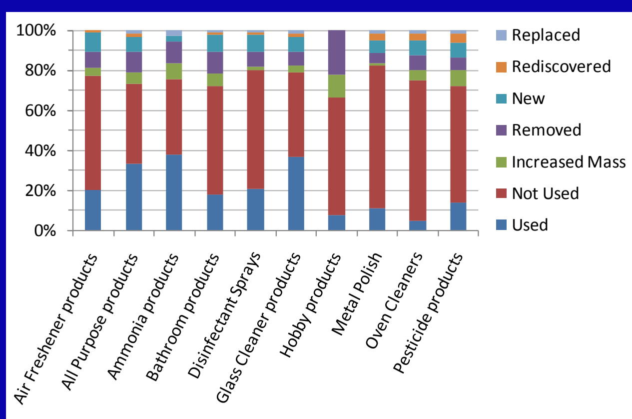
Household Care Products

Percent of products that were used, not used, increased in mass, removed, new, rediscovered, or replaced during a week of observation



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What about over 4 months?

Significant increases in the percent of products used for

- oven cleaning products (13.2 vs 4.5%)
- metal cleaning products (22.7 vs 10.7%)

Slight increases for

- bathroom products (22% from 17.8%)
- disinfectant sprays (23% from 20.6%)
- pesticides (15.5% from 13.9%)

However, the sum of the percent of products removed, new, and replaced increased to over 50%.

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Household Use Scenarios

For each category of products, scenarios with useable information:

- All products found, Used
- All products found, Not Used
- Not Owned

For those in the remaining groups, mass used was not quantifiable:

- Removed Only
- New Only
- Replaced Only
- Rediscovered Only
- Removed Plus
- Multiple Difficulties

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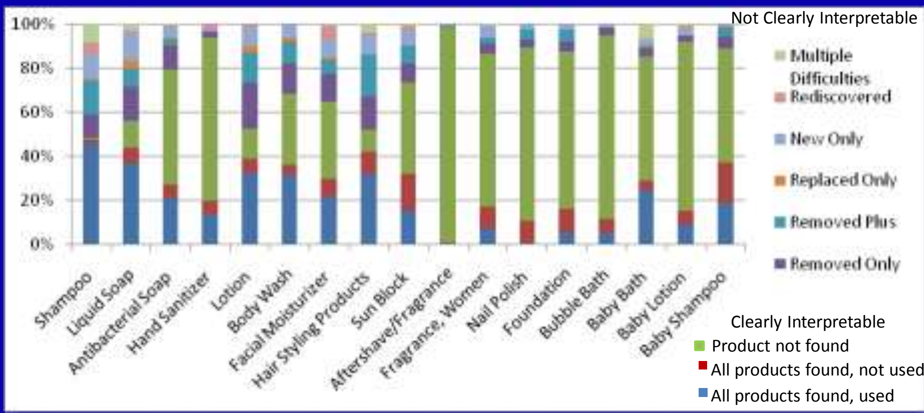
Household Use - Personal Care



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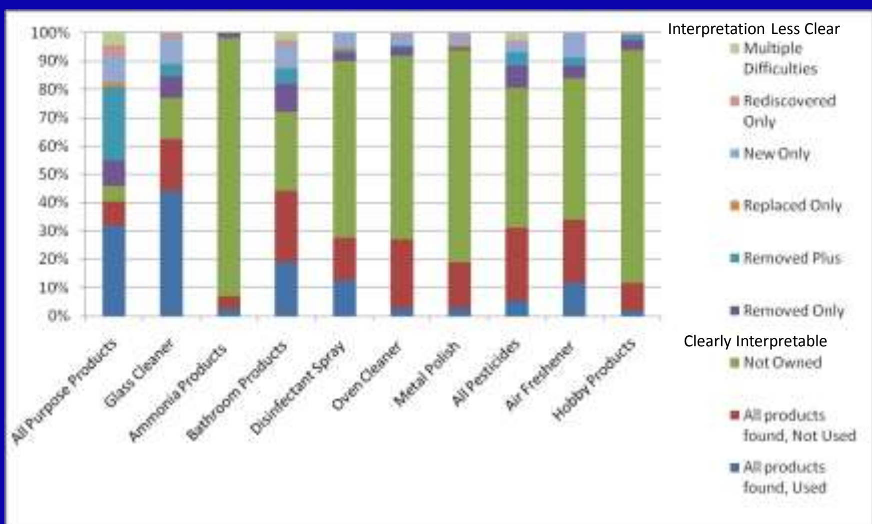
Household Use - Household Care



Calculating Mass Used

- Remember that we weighed all the products at the beginning and end of week
- Use these values to calculate mass used

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Mass (g) used in one week

	Households with young children		Households with older adults	
Product Type	Mean	Median	Mean	Median
Antibacterial Soap	22.3	12.9	28.2	18.1
Baby Bath	18.4	11.5	—	—
Baby Lotion	6.4	4.9	—	—
Baby Shampoo	16.6	11.0	—	—
Body Wash	47.1	25.8	21.2	14.4
Bubble Bath	42.1	30.1	83.8	83.8
Facial Moisturizer	8.8	3.7	6.2	3.6
Foundation	5.8	2.7	2.8	2.9
Fragrance Men	—	—	1.6	1.5
Fragrance Women	1.1	0.9	1.2	1.2
Hair Styling	25.9	12.4	11.9	10.6
Hand Sanitizer	6.5	4.0	1.9	1.6
Liquid Soap	43.9	25.5	24.2	12.7
Lotion Hand and Body	30.1	15.8	20.5	10.9
Nail Polish	1.3	1.3	3.9	3.9
Shampoo/Conditioner	64.5	48.2	49.4	28.3
Sun Block	8.4	5.7	9.3	1.4

Mass (g) used in one week

	Households with young children		Households with older adults	
Product Type	Mean	Median	Mean	Median
Air Freshener products	17.8	6.3	8.7	4.5
All Purpose products	126.4	75.9	59.0	24.4
Ammonia products	66.2	5.3	101.7	109.4
Bathroom products	88.6	21.7	35.4	18.7
Disinfectant Sprays	45.6	8.9	1.4	1.4
Glass Cleaner products	33.3	19.2	36.9	7.2
Hobby products	4.5	3.3	1.0	1.0
Metal Polish	9.9	2.0	12.0	5.0
Oven Cleaners	17.3	3.0	148.6	148.6
Pesticide products	35.9	21.8	18.7	16.1

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Single Use Mass

For shampoo and hand soap, we asked the participant to dispense the amount of each product they typically used onto a plastic sheet that they placed on their hand.

Individual use amount (g) and estimated number of uses per week

Product Type	location	Single Use Amount (g)			Uses per week based on Single Use Amount				
		Mean	Median	75th%	Mean	25th%	50th%	75th%	95th%
Liquid Soap	PYC	10.3	3.6	4.6	34.0	2.7	6.6	25.6	224.1
	OA	4.5	1.9	2.4	15.8	1.4	9.6	24.0	57.5
Shampoo/ Conditioner	PYC	40.8	6.8	57.5	11.2	1.7	6.0	16.8	34.5
	OA	7.6	3.8	13.3	10.0	2.2	8.2	14.9	24.2

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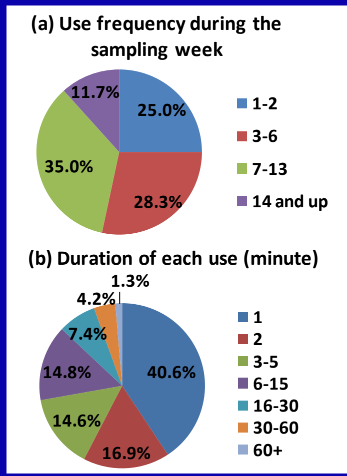
Motion Sensor to Record Use

Actical Accelerometers were strapped on two most frequently used products to record how often the product was moved.

- The use frequencies during different sampling weeks for each household were moderately consistent.
- The majority of the usage of cleaning products (92%) happened between 7am and 9pm, with peaks at mealtime, i.e., 8am, 12pm, 3pm, and 7pm.



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Conclusions and Future Directions

- The bar code scanner obtains actual products used the majority of the time relatively quickly.
- Participants store, but don't use, a large number of products. Participants could be asked to show staff which products are used.
- Instead of determining mass used, participants could be asked frequency of use.
- Overall, the use of bar code data and motion sensors are promising methods for evaluating use of personal and household care products with minimal burden to the participants.

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Questionnaire Household Cleaners

- Products: All purpose cleaner, Car cleaner, carpet cleaner, floor cleaner, glass cleaner, oven cleaner, polish, tub/shower cleaner, various types of air cleaners
- Cleaning Habits: Dry-mop, Wet-mop, sweep, and vacuum hard floors, vacuum carpets
- Frequency, correlations between product use, demographic differences
  - Frequency and Longitudinal Trends of Household Care Products Use, Atmospheric Environment, in press

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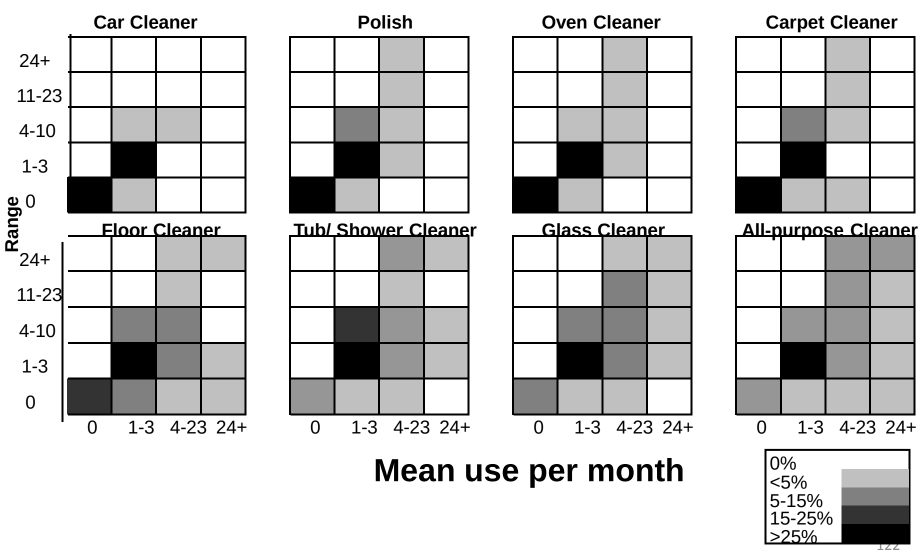
Longitudinal Consistency



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Personal Care Product Use

- Shampoo, Bath gel, body lotion, hand lotion, deodorant, liquid soap, waterless hand sanitizer, facial cleanser, facial moisturizer, mask, anti-aging cream, lip balm/lipstick, sunscreen hot/cool,
- Hair: dye, perm, spray, mousse
- Makeup: foundation, mascara, nail polish, fragrance
- Frequency, correlations, demographic differences, scented/unscented
- Wu X, **Bennett D.H.**, Ritz B., Frost J., Cassady D., Lee K. Hertz-Picciotto I. Usage Pattern of Personal Care Products in California Households. *Food and Chemical Toxicology*, 48(11): 3109-3119, 2010.

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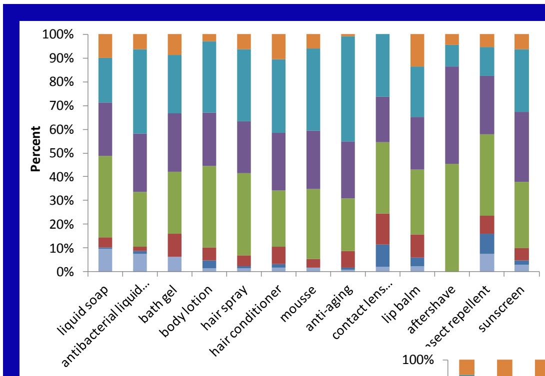
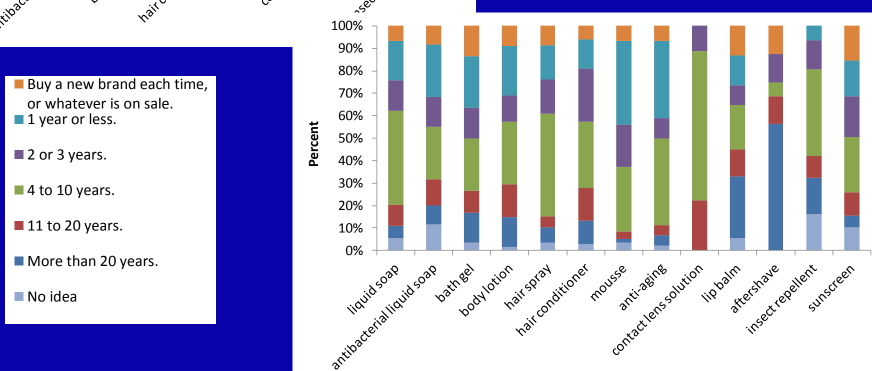
Brand Loyalty



(a) parents of young children in northern California

(b) older adults in central California



Acknowledgement

- The project was supported by United States Environmental Protection Agency (grant# RD-83154001-0).
- Many thanks to all the SUPERB participants.
- Special thanks to our field staff, Jessica Riley, Laura Gonzalez, Brianna Diaz and Karen Wagner.

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RTI International

RTI INTERNATIONAL

Smartphones as a Flexible Research Tool: Lessons from Early Implementations and the Consumer Marketplace

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PerCEIVERS 2012
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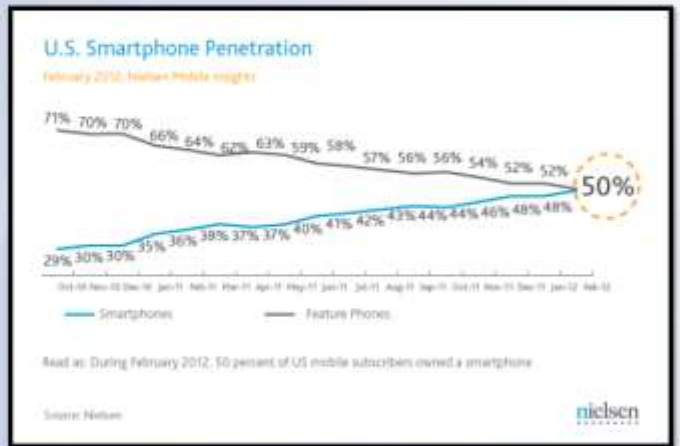
RTI International is a trade name of Research Triangle Institute

www.rti.org

RTI International

How fast is smartphone growth?



It's fast. *Really* fast.

Image: Neilson (2012). http://blog.nielsen.com/nielsenwire/online_mobile/smartphones-account-for-half-of-all-mobile-phones-dominate-new-phone-purchases-in-the-us/

RTI

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What technology is in a smartphone?

Samsung Galaxy Nexus

- 4.65 inch HD screen
- 5 megapixel camera
- Global positioning systems
- Accelerometer
- Bluetooth
- Access to fast data connections

RTI

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Questionnaire Administration

- Self-administration survey successes!
- High response rates.
- Promising usability.
- Journal entry is possible.
  - Text entry
  - Photo entry
- Be mindful of screen sizes...

Image: ZDNet http://www.zdnet.com/blog/btl/60-of-americans-would-give-up-alcohol-for-their-mobile-phones/20569

RTI

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Global Positioning Systems

- Capture micro-level location data
- Passive data collection opportunities
- Match location data with other data

Image: http://www.funnyphotos.net.au/images/multiple-gps-in-the-one-car1.jpg

GPS sensors should enhance data quality!

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Sensory Technology

- Bluetooth connection to sensory technology offers the possibility for collection of a rich set of data.
  - Indoor location
  - Air quality
- Accelerometers can track physical activity.

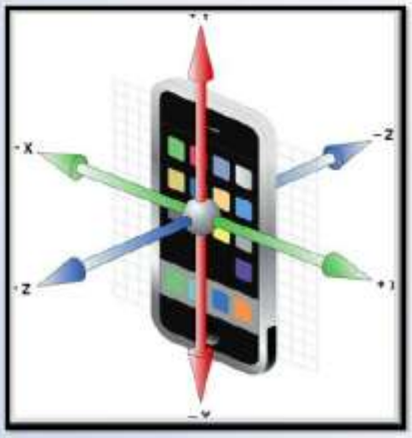

Image: http://iphonedevelopmentbits.com/wp-content/uploads/2010/06/device_axes.png

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Unanswered Questions

- Human subjects literature is still a work in progress.
- The privacy implications of personal data collection.
- Data security is a concern.

Image: http://info.synnex.com/pcw/blog/pcw/question.jpg

RTI

Natural Language Processing and Human Activity Patterns:

USING A SPOKEN DIARY AND HEART RATE MONITOR IN MODELING HUMAN EXPOSURE FOR EPA'S CONSOLIDATED HUMAN ACTIVITY DATABASE

Curry I. Guinn, UNC Wilmington

Daniel J. Rayburn Reeves, UNC Chapel Hill

Collecting Human Activity Data

- Purpose
  - To develop a method of generating an activity/location/time/energy expenditure database of sufficient detail to accurately predict human exposures and dose.
- To Evaluate
  - the use of digital voice recordings
  - the use of the ambulatory heart rate monitor
  - participant/instrumentation interactions
- To Develop
  - a protocol for automating the processing of voice recordings
  - an autocoding program that will be able to map the text of the diary entries to CHAD

Problems with Collecting Human Activity Data

- Recall Data
  - Failure to recollect many daily activities
  - Lack of detail
- Real-Time Paper Diaries
  - Increased number of reports/better detail
  - Burdensome
- Direct Observation
  - Greatest number of reports/most detail
  - Inefficient and expensive
- Platform for Solution
  - Audio diary using a digital voice recorder
  - Ambulatory Monitoring System that monitors heart rate and prompts subjects to provide diary entries when heart rate increases by a specified criterion level.

Database Sample

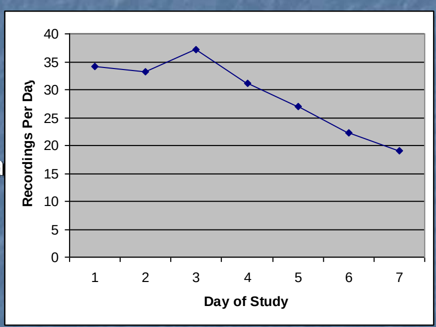
Time	Recorded Utterance	CHAD Location	CHAD Activity
8:57 AM	in the bedroom starting housework	30125 - Bedroom	11200 - Indoor chores
8:59 AM	carrying clothes to the laundry room	30128 - Utility room / Laundry room	11410 - Wash clothes
9:00 AM	the bedroom getting more clothes	30125 - Bedroom	11410 - Wash clothes
9:05 AM	loading the washing machine in the laundry room	30128 - Utility room / Laundry room	11410 - Wash clothes
9:06 AM	sitting down going to watch twenty minutes of Regis	30122 - Living room / family room	17223 - Watch TV
9:23 AM	I'm going to be brushing the dog in the family room	30122 - Living room / family room	11800 - Care for pets/animals

Subjects

ID	Sex	Occupation	Age	Education
1	F	Manages Internet Company	52	Some College
2	F	Grocery Deli Worker	18	Some College
3	M	Construction Worker	35	High School
4	F	Database Coordinator	29	Graduate Degree
5	F	Coordinator for Non-profit	56	Some College
6	M	Unemployed	50	High School
7	M	Retired	76	High School
8	M	Disabled	62	High School
9	M	Environment Technician	56	Graduate Degree

Voice Diaries

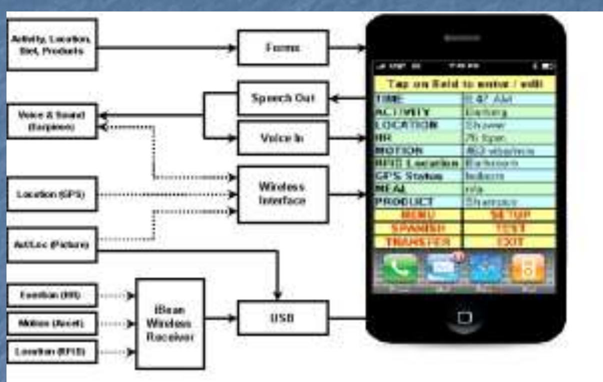
- Average: 29 entries/ "day"
- With average monitoring time of 8.56 hours, 3.39 recordings/hour
- First 3 days of trial: 34.44/ day
- Last 2 days of trial: 20.65/ day
- 1 out of 63 reporting periods data lost (1.6%)



Quality of Diary Entries

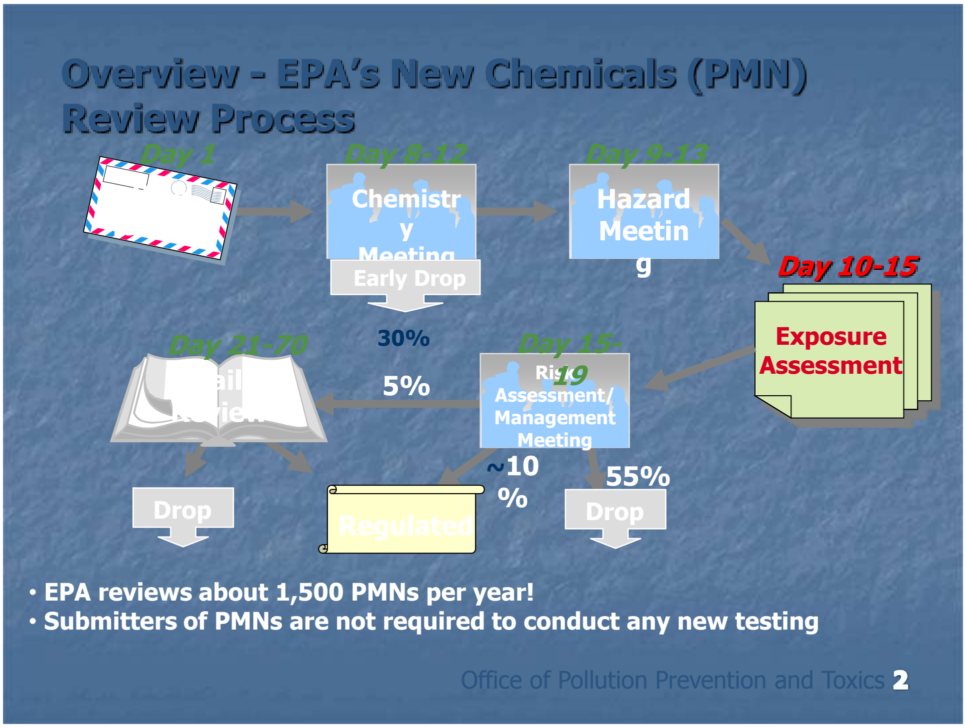
- Entry Length
  - 9.39 words average
- Some entries invalid because of length (subject failed to turn off recording)
  - 1/30 recordings (3%)
- Heart rate change and diary entry
  - Avg. of 28.8 beeps per day; 36.8% compliance
- Computer classification
  - 66% accuracy in activity; 76% in location
  - Significant improvements with less granular CHAD encodings

Time, Activity, Location, Exertion Data Gathering Platform



How do we fuse data from other sources (gps, beacons, heart rate monitor, etc.)?

How do we provide interactive prompts to the subject to improve reporting?



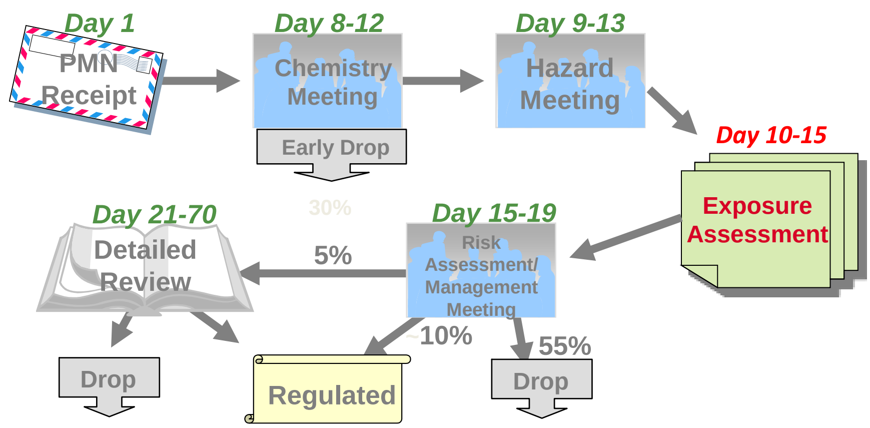
United States Environmental Protection Agency

Consumer Exposure Assessment for New Chemicals

Cathy Fehrenbacher, Chief
Exposure Assessment Branch
June 26, 2012

Office of Pollution Prevention and Toxics

Overview - EPA's New Chemicals (PMN) Review Process



- EPA reviews about 1,500 PMNs per year!
- Submitters of PMNs are not required to conduct any new testing

EPA Office of Pollution Prevention and Toxics | 2

OPPT's Exposure Tools and Models Include:

- Methods used by OPPT for exposure assessment, in the absence of, or to supplement data
- Computerized models and accompanying databases
- Default assumptions which can be modified by the user
- Online help and transparent guidance in using the models and databases
- Capability to address adults, children, and infant populations
- Some population and demographics data, and information on endangered species
- Some geospatial and graphing capabilities

EPA Office of Pollution Prevention and Toxics | 3

Application of OPPT's Models: workplace, home, community, environment (http://www.epa.gov/oppt/exposure/)







OPPT's Models for Consumer Exposure Assessment




- AMEM – chemical migration through polymers (under development)
- E-FAST – screening level modeling suite, includes Consumer Exposure Module
- MCCEM – higher tier consumer exposure
  - WPEM – wall paints
  - FIAM – formaldehyde in pressed wood products (new)

Consumer Exposure Data and Tools

- Consumer Product Scenarios
  - Developed in 1986; multi-volume set
  - Few were programmed into E-FAST; with user-defined scenario which is commonly used with the scenarios
  - Contain formulation data, weight fractions of functional components, exposure factors, use pattern, use conditions, frequency and duration, etc.
- Consumer Products Database
  - Confidential Business Information
  - Based on formulation-related data for consumer and commercial products available
  - Undergoing internal review

Future Directions

- Continue ongoing collaboration/coordination efforts – EPA, OECD, others
- Continue development of models, databases, tools
  - E-FAST redesign & redevelopment, IGEMS/CSM, ReachScan, AMEM
  - Consumer products database
- Importance of personal chemical exposure informatics
  - Data and tools to inform design, formulation, assessment and risk management
  - Transparency while protecting CBI
- Contributions to personal chemical exposure informatics
  - Unique set of data and tools for assessing consumer, general population, and environmental exposure to wide range of chemicals
  - Absence of data provides challenges
  - Assessment of nanomaterials
- Major issues or ideas that could/should be explored
  - CBI and other issues will be important
- Online contact method for further discussion

Chemical Use: The Key to Near-Field Chemical Exposure Estimation

Christina Cowan-Ellsberry
The LifeLine Group
Cincinnati, OH

Content

- Public Availability of Data
  - How to fill Chemical presence and Use gaps
  - Product use profile data

Necessary Information

Three types of information needed for exposure assessment

- Chemical Specific Information
  - Chemical properties
  - Chemical presence
  - Chemical fraction in product
- Product Specific Information
  - Use profile
- People Specific Information
  - demographics

Information = data, surrogate data, derivations, default values, assumptions

Necessary Information: Product Specific

Product Specific Information

- Use scenarios—how products are used by different people during different seasons and conditions
- Product co-uses and competitive uses
- Information applicable to many chemicals, so when product use profiles are constructed, much of the information is reusable across many chemicals
- Much of the information is publicly available

Sources of Information

- Publically available BUT
  - Not necessarily in final form required
    - This chemical is used in specific product at x%
    - Everyone uses 2 times per day etc.
  - Instead may need some interpretation and bringing together different parts of data
    - Chemical is used as fragrance in product, as emulsifier etc.
    - Type of product used in are face cream, body wash, etc.
- Publicly available information usually provides good initial listing of uses and potential products for consideration

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Chemical Specific Information

How are Chemicals Used in Products? Possible health concerns and tox reviews

- wikipedia.org
- product safety assessments (online) by manufacturer (i.e. Dow Chemical)
- government chemical and product reviews such as http://www.nicnas.gov.au/publications/information_sheets/existing_chemical_information_sheets

Characteristics of the chemical, sources, related information

- US Nat'l. Ctr for Biotechnology http://www.ncbi.nlm.nih.gov
- Forms, sources, links to other info sites http://www.chemindustry.com

Concentrations in products, possible substitutes, functions in products and use scenarios/profiles

- (example: Household Products Database http://hpd.nlm.nih.gov)
- European evaluations under REACh. 14,000 dossiers expected to be publicly available relatively soon
- The Cosmetic, Toiletry, and Fragrance Association (2006) International Cosmetic Ingredient Dictionary and Handbook, Washington DC, Ed Wenninger JA McEwan GN

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Necessary Information: Chemical Specific

- Chemical Specific Information
  - Hazard/toxicology information
  - Exposure related information
    - Physical/Chemical properties - Lipophilicity, size, vapor pressure, reactivity, etc.
    - Functionality because of its chemical properties - Surfactants, solvents, colorants, stabilizer, etc.
      - Considering competing chemicals and additional uses/products containing the chemical
    - Ranges of concentrations for functional ingredients
  - Usually readily publicly available – manufacturers discuss how chemical can be used and example products

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Example: Sodium Lauryl Sulfate

- Detergent surfactant function as a wetting agent, dispersing agent, emulsifying and/or foaming agent.
- Appears in a wide range of products because it is highly effective, relatively inexpensive, and especially useful for opaque, pearlescent or cream products, can be used in powdered or tablet product forms, provides high foam with good viscosity and is readily solubilized in cool water.
- Functionality determines both the product list and the likely concentration range in each product type within these two product categories. Even within a particular product type, the concentration range can vary considerably depending on the functionality required and the presence of other ingredients which serve the same or similar functionality

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Example: Sodium Lauryl Sulfate

- Heavy duty cleaning products where very effective removal of heavy grease and stains (e.g., heavy duty degreaser washes) is required the concentration of SLS can reach 50 %
- In less heavy duty cleaning products, such as carwashes, carpet cleaners, dish washing liquids, pet shampoos and upholstery cleaners; SLS is typically in the 3 to 30% range. In most household cleaners, SLS concentrations range from <1 to 5 percent.
- Product form can also determine the concentration range of SLS. For example, liquid laundry detergents and fabric softeners contain SLS at about 30% whereas the powder and tablet forms of these products may contain up to 93% SLS, which is then diluted in use.

Example: Sodium Lauryl Sulfate

- Depending on desired amount of lathering, the concentration in personal care products can also vary considerably. For example, a few hand soaps, body washes and shampoos can contain SLS in a wide range of concentrations up to 30 percent whereas most hand soaps contain 1 to 5% and face soaps 1 to 2.5% SLS. Notably, some children's toothpastes can contain up to 5 % SLS (Barkvol, 1989) because these products require more bubbles/foaming to make the tooth cleaning activity more fun. Shaving creams' concentrations range from 1 to 10% with the higher concentrations occurring in products that produce heavier and thicker foams or gels.

Example from One Website

Typical Face Cream Ingredient with Typical Concentration Ranges

Emulsifiers	2-6%
Emollients	10-35 %
Thickener	0.1-1%
Deionized Water	Q.S.
Preservatives	0.2-1 %
Humectants	1-8 %
Consistency factors	1-6%
Antioxidants	0.01-0.05%
UV filters	0.01-0.5%
Chelating Agents	0-0.02 %
Fragrance	0.1-1 %
Active agents	0.1-2%
Coloring agents	Q.S.
Aesthetic enhancers	0.1-5%

Chemical Information

- Physical/chemical properties define functionality
- Functionality defines how used in products and likely product forms
- Functionality defines concentration range in typical products
- Bring together the best information and make best initial judgment

Sources of Habits and Practices Data-US Data

Personal Care Product Council Studies:

- Exposure data for cosmetic products: Facial cleanser, hair conditioner, and eye shadow. Food Chemical Tox Loretz et al. 2008 vol:46 pg:1516
- Exposure data for personal care products: Hairspray, spray perfume, liquid foundation, shampoo, body wash, and solid antiperspirant. Food and Chem Tox Loretz et al., 2006 vol:44 pg:2008
- Exposure data for cosmetic products: lipstick, body lotion, and face cream. Food Chem Tox Loretz et al. 2005 vol:43 pg:279.

American Cleaning Institute–

- Global Exposure and Risk Screening Methods for Consumer Product Ingredients 2005 and updates

EPA Exposure Factors Handbooks – 1997 and updates

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Habits and Practices Data-Non-US

- COLIPA (European Cosmetics Association) Studies
  - SCCNFP/0321/02 and referenced in THE SCCP'S NOTES OF GUIDANCE FOR THE TESTING OF COSMETIC INGREDIENTS AND THEIR SAFETY EVALUATION
- Company marketing product will have data on
  - Other populations, sub-populations
  - Special product forms/use scenarios

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Other Product Forms

- Example, Azo and Benzidine dyes in temporary tattoos and skin paint
- Concentrations can range from 0.4 to 30 % and the area covered can range from quite small, for example children's hand stickers, to full torso body art (Louis Vuitton 2011, Chanel 2011).
- Concentration of the colorant in the product depends on the product formulation as well as the desired durability of the tattoo.

Necessary Information: People Specific

People Specific Information

- Morphometrics and physiological parameters (height/weight, breathing rates, etc)
- Age dependent activity profiles
- Demographic, econometric and ethnic activity-related influences (special subgroups)
- Once information is developed, useful for all subsequent analyses
- Independent of chemical but dependent on the product

Key Learnings

1. Information gathering, and initial use profiling requires 4 hours or less per chemical for most chemicals.
    1. Must have structured approach with stop points
2. Exposure scenarios for products are "reusable" across many chemicals, so efficiency increases as the process continues.
3. Needed information is increasingly available, spurred by other regulatory and private transparency initiatives, in organized public and commercial databases

Reference

Using publicly available information to create exposure and risk-based ranking of chemicals used in the workplace and consumer products

MICHAEL A. JAYJOCK, CHRISTINE F. CHAISSON, CLAIRE A. FRANKLIN, SUSAN ARNOLD, AND PAUL S. PRICE

Journal of Exposure Science and Environmental Epidemiology (2009) 19, 515–524

Probabilistic Exposure Assessments for Consumer Products

Christina Cowan-Ellsberry

The LifeLine Group

Cincinnati, OH

Outline

- Define different types of Probabilistic Exposure for consumer products
- Describe the sources of the Habits and Practices/Use data for products
  - Strengths and limitations
- Discuss some of the important things to consider when doing probabilistic exposure assessments
- Key Learnings

Data needed to Estimate Exposure

Habits and Practices or Use Data

- Amount /use
- Frequency of use/day
- Duration (continuous/intermittent; fraction of a lifetime)
- Method of application (e.g., rinse-off)
- Etc. - Modifying factors
- Body site(s) applied to

Demographic Data

- Size of area of application **or** Body Weight

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Probabilistic Exposure Assessment

- Individual Product Exposure
  - Variability in Use Patterns by age, gender, ethnicity etc.
    - 10% use 1 time per day, 30% use 2 times per day, etc.
- Aggregate Exposure
  - Include variability in non- and co-use patterns of individual products
- Population Exposure
  - Ensure that population or sub-population is correctly represented by Use Pattern data

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How are H&P/Use pattern data determined?

- Several sources
  - Focus Group Studies
  - Product Placement Studies
  - Market Research Surveys
- In all cases there is a lot of data collected, although not necessarily in form required
- Often need to combine data from several studies to get a complete picture of how the product is used.
- Need to recognize strengths and limitations of each source

Focus Group Studies

- Observe product handling under normal use conditions (e.g., for fragrance Products: Typical spray distances, Sites of exposure)
- Bottles are weighed before & after application (i.e., Amount applied per application (g))
- Deposition area determined by measurement of spread onto a paper collar applied to the preferred body target (i.e., Surface area (cm2) covered by product)
- Questionnaire to probe further (e.g., Number of sprays per application, Number of applications/site per day)

Limitations: Very costly, one time focus on product use, may not reflect actual use

Advantages: Personal observation, ask additional questions

Product Placement Studies

- Participant is given product, asked to use for set period of time, record when use, etc
  - For fragrance products: Number of sprays per application, number of applications per day, site of application
  - Bottles are weighed before & after time period to determine amount used over entire period
- Often coupled with information on how they like the product, demographics, etc.

Limitations: inaccurate/incomplete recording, other people may use product or participant may retain remaining product

Advantages: direct measurement of product amount used and frequency over multiple uses

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Market Research Surveys

Questionnaire - mail/internet/street/phone

- Target large numbers of consumers (> 1000)
- Include multiple countries, ethnic, economic groups to understand differences in use.

User Preferences and Use of Products

- Product Form: sprays, splash, parfum, etc. for fragrance products
- Frequency of use - daily, occasional, 1x, 2x + per day...
- Use with other products

Limitations: Recall is not perfect, bias in recording based on social acceptability of behavior, amount used data is missing

Advantages: large number of people can participate, multiple product use (co-use and non-use patterns)

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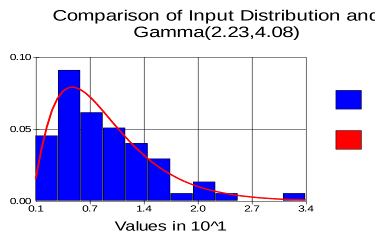
Individual Product Exposure

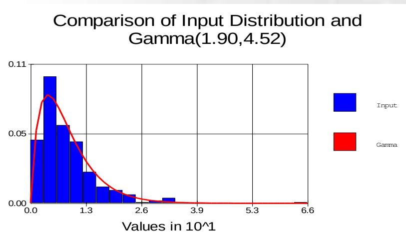
- Representing Habits and Practices data distribution
- Correlation between amount and frequency of use
- Choice of percentile of exposure
- Use patterns different for age, sex, ethnic group, etc.

Representing Data Distribution

- Appropriate statistical distributions for the habits and practices is critical. Use raw data as much as possible rather than force fit a statistical distribution

  1) fitted distributions may over-estimate high end users because they are continuous or user must determine where to truncate distribution; 2) raw data is often bi- or tri-modal; and 3) there is usually no "best fit" across all sub-sets of the data (e.g., Normal or Log-Normal is seldom the "best fit").





Correlation of Use Data

- For most products, data from several surveys will need to be combined since one survey may not contain data for all parts of the target population (e.g., non-users, age groups) nor data on both frequency of product use and amount used per application.
- If the frequency and amount used are positively correlated then the resulting exposure will be under estimated. However, data analysis for representative Beauty Care and Oral Care product studies where both frequency and amount have been measured shows that frequency of use and amount used per application are either negatively correlated or independent and none are positively correlated; therefore, exposure will be over-estimated for these products if independence is assumed when combining data from independent studies.
- Really important when looking at high-end exposure

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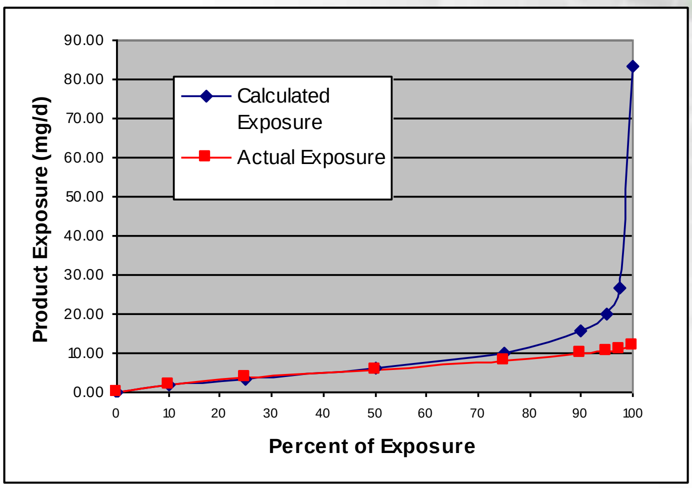
Example for Shampoo



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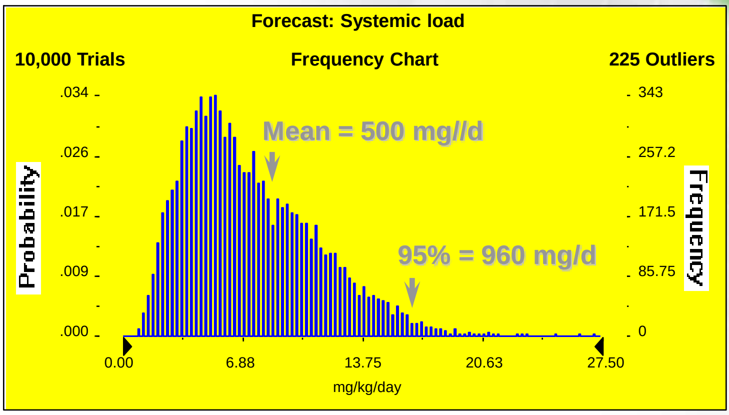
Monte Carlo Probabilistic Exposure Assessment



95th Percentile Deterministic Value was 1.93 gm/day

Aggregate Exposure

- Include non-use and co-use information
- Extent of ingredient use in that type of product

Aggregate Exposure Considerations

- Typical aggregate exposure assessment involves **adding** the exposures to the individual products – very conservative
  - Basic assumption of the additive approach is that a consumer uses all the product types frequently
- **Co-use and non-use** patterns of different product types are important determinants of exposure
  - If a person does not use a product or uses it very infrequently then this product will not contribute to aggregate exposure for that person

Extent that ingredient is used in a particular product type will vary
  - The extent of use will determine likelihood that person will come in contact with that ingredient when used that product type

Paraben	Added Exposure (mg/kg/d)
Methyl	1.25
Propyl	1.25
Ethyl	0.93
Butyl	0.47
Total	3.9

Probabilistic Aggregate Exposure

- For many products the percent of the population that are non-users can be very large.

Consumer Product	Approximate Percent of Population that are Non-Consumers
Toothpaste	2%
Conditioner	30 to 75% depending on M vs F
APDO	4%
Mouthwash	29 to 73%
Shampoo	< 5 to 50% depending on type of shampoo

Product Co-Use

Product co-use combination	Percent of participants
BC + BL + HL + FM + FC	27 %
BL + HL + FM + FC	16.9 %
BC + BL + HL + FC	5.5 %
BL + HL	6.6 %
BC + BL + HL + FM	4.7 %
BC + BL + HL	4.1 %
BL + HL + FM	4.5 %
Non-Use	31.3%

BC – body cream, BL-body lotion, HL – hand lotion, FM – facial moisturizer, and FC – facial cleanser.

Extent of Use Data: Methyl vs Ethyl Paraben Use

Percent of Product Formulations Containing Paraben

Products or Product Categories	Methyl	Propyl	Butyl	Ethyl
Eye make-up	35	34	3	0.2
Make-up	20	25	2	0.2
Skin Cleansing	62	51	8	2
Face, body and hand skin care	67	56	12	4
Moisturizing skin care	71	64	12	1
Night skin care	62	51	15	1
Across all formulations	28	24	3	0.8

Factor 71 *Factor 15.1*

**From Elder 1984. J. Amer. College of Toxic. 35:147-209.

Aggregate Exposure Summary

Paraben	Summed Aggregate Exposure (mg/kg-d)	Refined Estimate (mg/kg-d)
Methyl	1.25	0.56
Propyl	1.25	0.28
Ethyl	0.93	0.012 to 0.007
Butyl	0.47	0.003
Total	3.9	0.855

- ✓ Reduction in aggregate exposure by factor of 3 to 5 by applying refinements
  - ✓ Potentially larger if more products included

Cowan-Ellsberry and Robison. Regulatory Toxicology and Pharmacology 55 (2009) 321–329

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Population or Sub-Population Exposure

- Differences in use patterns by age, sex, ethnicity etc are very important and can be significant.
- Population exposure determined by estimating exposure sub-populations and then combine to calculate population exposure using census data
- Typically consumer surveys under represent young and old, and ethnic groups (e.g., African Americans, Hispanics) and focus on product users. If the survey population does not have the same demographics as the target population or data from several surveys are combined, exposure will need to be calculated as the weighted exposure by demographic group.
- Weighting can significantly modify (often reduce) exposure.

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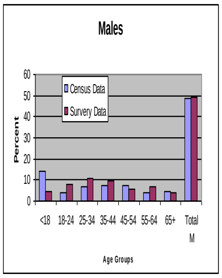
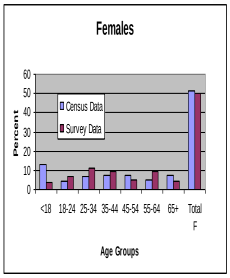
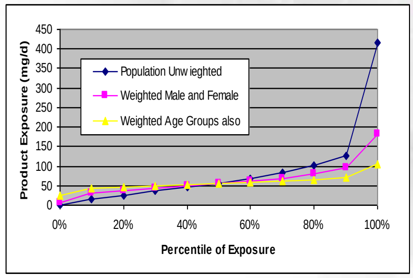
Example

- High-end aggregate exposure from multiple products is reduced by a factor >4x by proper weighting for gender and age. More detail more accuracy.





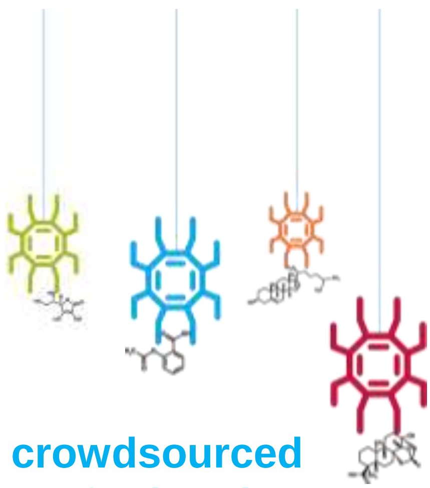


Key Learnings

- Consumer panels may not accurately reflect the general population or sub-population of interest
- Data on high-end frequency and consumption patterns are often less substantiated compared to average frequency and consumption. For example, when > x times per day use of product represents a significant percent of the responses.
- Co-use or non-use of products as well as extent of use of ingredient has an important impact on aggregate and population exposure estimates
- The higher the complexity of the model (i.e. the better exposure variability is reflected in the model) the more accurate the exposure estimate
- Probabilistic approaches to aggregation can result in a factor of 2 to 3 decrease in exposure compared to conventional additive approach

PerCEIVERS
@ US-EPA in RTP-NC

Day II Presentations
– June 27, 2012



RSC ChemSpider – A crowdsourced community environment for hosting and validating chemistry data

PERCEIVERS Meeting, June 2012

ChemSpider

- ***The Free Chemical Database***

- A central hub for chemists to source information
  - >26 million unique chemical records
  - Aggregated from >400 data sources
  - Chemicals, spectra, CIF files, movies, images, podcasts, links to patents, publications, predictions

- A central hub for chemists to deposit & curate data

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ChemSpider The free chemical database

We Want to Answer Questions

- Questions a chemist might ask…
  - What is the melting point of n-heptanol?
  - What is the chemical structure of Xanax?
  - Chemically, what is phenolphthalein?
  - What are the stereocenters of cholesterol?
  - Where can I find publications about xylene?
  - What are the different trade names for Ketoconazole?
  - What is the NMR spectrum of Aspirin?
  - What are the safety handling issues for Thymol Blue?

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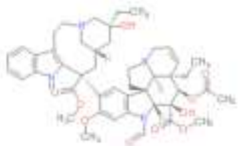
ChemSpider The free chemical database

I want to know about “Vincristine”



2D 3D Save Zoom

- 9 of 9 defined stereocentres

Vincristine

ChemSpider ID: **5758**

Molecular Formula: $C_{46}H_{56}N_4O_{10}$

Monoisotopic mass: 824.399644 Da

▼ Systematic name

(2α,2'β,3α,4α,5β,19β)-22-oxovincaleukoblastine

▶ SMILES and InChIs

Wikibox

Embed

Deprecate

Watch this record

Manage data slice

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Vincristine: Identifiers and Properties

▼ Names and Identifiers

Names and Synonyms | Database ID(s)

Validated by Experts, Validated by Users, Non-Validated,

(2'β)-22-Oxovincaleukoblastine

200-318-1 *[EINECS/ELINCS]*

22-Oxovincaleukoblastine

57-22-7 *[RN]*

vincaleukoblastine, 22-oxo-

vincaleukoblastine, 22-oxo-, (2'β)-

vincaleukoblastine, 22-oxo-, (3β,4'β)-

Vincristine *[Wiki]*

Vincristinum *[Latin]*

VIN

▼ Properties

Experimental data | Predicted - ACD/Labs | Predicted - ChemAxon

Data supplied by datasources and users.

- Experimental Physchem Properties
  - **Melting Point:** 218 - 220 C
- Miscellaneous
  - **Appearance:** solid
  - **Stability:** Stable, but may be heat sensitive. Incompatible with strongoxidizing agents.
  - **Toxicity:** IVN-RAT LD50 1300 mg kg-1, IPR-MUS LD50 5.2 mg kg-1
  - **Safety:** Safety glasses, gloves, good ventilation.

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Vincristine: Vendors and Sources

Chemical Vendors

Data Source	External ID(s)
Pharmlen	S-PTN3183
AvaChem Scientific	1011, 1011B
AOKChem	aokchem11421

Data Sources

Chemical Vendors | Biological Data | Publishers | Metabolism Data | Phys. Properties | Tox/Envir. Data | Natural Products | Data Aggregators | Safety Data | All Data Sources

Data Source	External ID(s)
ChemBank	NCI60_026703
DiscoveryGate	5978
LeadScope	LS-228
NIAID	002674
DrugBank	5978, APRD00495
Collaborative Drug Discovery	16374

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Vincristine: Patents

Patents

Google Patents | USPTO Granted | USPTO Applications | European Granted | European Applications | WO/PCT | Japanese Abstracts

powered by Google

Vincristine-containing product
US Pat. 5055449 - Nov 07, 1988 - Akzo N.V.
Vincristine is a mitosis-retarding Vinca alkaloid which is fairly effective in combating various types of cancer, particularly Hodgkins disease and other ...

Method of preparing vincristine
US Pat. 4375432 - Nov 16, 1981 - Eli Lilly and Company
METHOD OF PREPARING **VINCRISTINE** CROSS-REFERENCE This application is a continuation-in-part of my copending application Ser. No. 262836 filed May 12, 1981. ...

Process for the preparation of vincristine
US Pat. 4767855 - Jun 02, 1986 - P. F. Medicament
4767855 25 PROCESS FOR THE PREPARATION OF **VINCRISTINE** The present invention relates to a particularly effi- 5 cient process for the preparation of ...

Method of preparing vincristine
US Pat. 4303584 - Apr 02, 1980 - Eli Lilly and Company
Primary Examiner — Donald G. Daus Assistant Examiner — Diana G. Rivers Attorney, Agent, or Firm — James L. Rowe; Arthur R. Whale [57] ABSTRACT **Vincristine** ...

Synthetic vinblastine and vincristine derivatives
US Pat. 4144237 - Jun 13, 1977 - The United States of America as represented by the Department of Health, Education and Welfare ...

Vincristine: Articles

Articles

Links & Reference | RSC Journals | RSC Books | PubMed | MeSH Literature | Google Books

Print

Please click here to see full list of found articles.

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- Soysal T. Thrombotic Thrombocytopenic Purpura After Prophylactic Cefuroxime Axetil Administered in Relation to a Liposuction Procedure. , *Aesthetic Plast Surg* , 2011 Aug 19
- Hoster E. Update on the molecular pathogenesis and clinical treatment of mantle cell lymphoma: report of the 10th annual conference of the European Mantle Cell Lymphoma Network. , *Leuk Lymphoma* , 2011 Aug 18
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- Witzens-Harig M. Replacement of conventional doxorubicin by pegylated liposomal doxorubicin is a safe and effective alternative in the treatment of non-Hodgkin's lymphoma patients with cardiac risk factors. , *Ann Hematol* , 2011 Aug 18
- Kahl BS. VcR-CVAD induction chemotherapy followed by maintenance rituximab in mantle cell lymphoma: a Wisconsin Oncology Network study. , *Br J Haematol* , 2011 Aug 16
- Geskin L. Clonal T-Cell Receptor [gamma]-Chain Gene Rearrangements in Differential Diagnosis of Lymphomatoid Papulosis From Skin Metastasis of Nodal Anaplastic Large-Cell Lymphoma. , *Arch Dermatol* , Volume 147 , Issue 8 , 2011 Aug
- Suzuki O. [A case of Sjogren syndrome coexistent with MALT lymphoma occuring along the parotid gland and trachea]. , *Nihon Kokyuki Gakkai Zasshi* , Volume 49 , Issue 7 , 2011 Jul
- Goldman S. Efficacy of interstitial continuous vincristine infusion in a bioluminescent rodent intracranial tumor model. , *J Neurooncol* , 2011 Aug 14
- Finkler NJ. Metastatic choriocarcinoma in a viable intrauterine pregnancy treated with EMA-CO in the third trimester: a case report. , *J Reprod Med* , Volume 56 , Issue 7-8 , 2011 Jul-Aug

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Searches: The INTERNET

ChemSpider Searches

Search ChemSpider for:

- Records with the same molecular formula
- Compounds with the same skeleton
- Use this molecule in a structure search

Search external sites for this structure:

- Search Google Scholar (by synonym)
- Search Google for exact structure
- Search Google for structures with same skeleton

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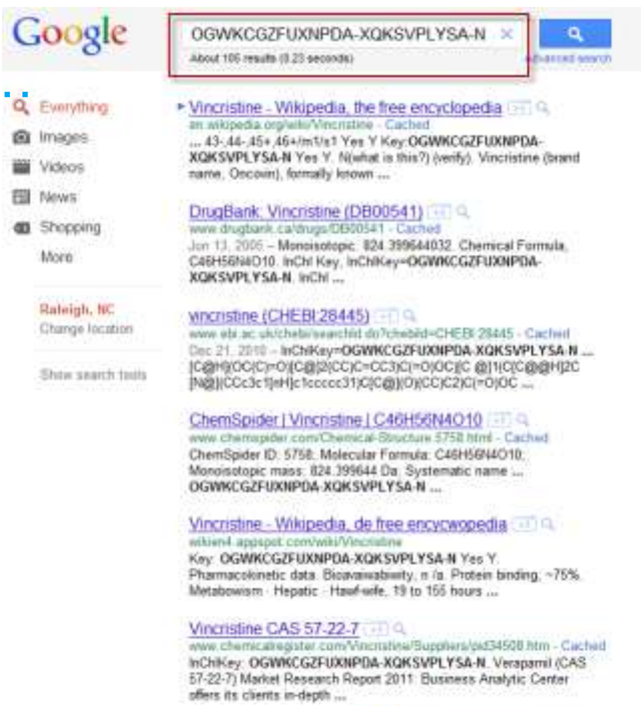
Validated Names for Searching…

And InChIs…



Chemistry Databases on the Internet

- Public databases are "trusted" as primary sources
- Trust is **granted without investigation** of the content
- Online data vary dramatically in quality!

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With Great Fanfare…

U.S. Department of Health and Human Services

NIH News

National Institutes of Health

National Human Genome Research Institute (NHGRI)

Embargoed for Release
Wednesday, April 27, 2011
2 p.m. EDT

Contact:
Geoff Spencer, NHGRI
301-402-0911

NIH researchers create comprehensive collection of approved drugs to identify new therapies for rare and neglected diseases

Researchers have begun screening the first definitive collection of thousands of approved drugs for clinical use against rare and neglected diseases. They are hunting for additional uses of the drugs hoping to find off-label therapies, for some of the 6,000 rare diseases that afflict 25 million Americans. The effort is coordinated by the National Institutes of Health's Chemical Genomics Center (NCGC).

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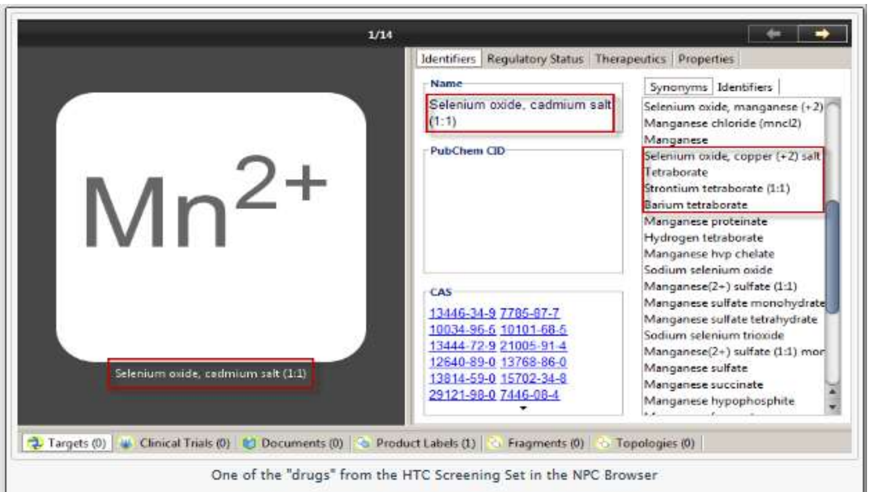
NPC Browser



One of the "drugs" from the HTC Screening Set in the NPC Browser

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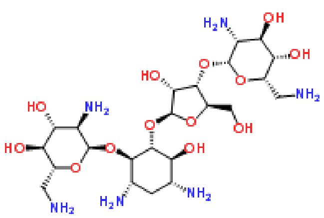

2D 3D Save Zoom

- 19 of 19 defined stereocentres

Neomycin

ChemSpider ID: **8075**

Molecular Formula: $C_{23}H_{46}N_{6}O_{13}$

Monoisotopic mass: 614.312286 Da

Systematic name

(1R,2R,3S,4R,6S)-4,6-diamino-2-{[3-O-(2,6-dia
idopyranosyl)-β-D-ribofuranosyl]oxy}-3-hydroxy
dideoxy-α-D-glucopyranoside

SMILES and InChIs

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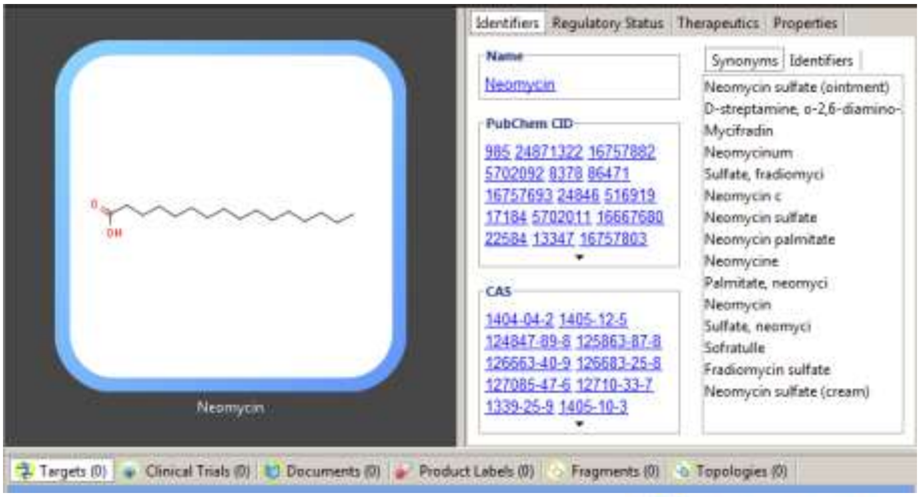
NPC Browser



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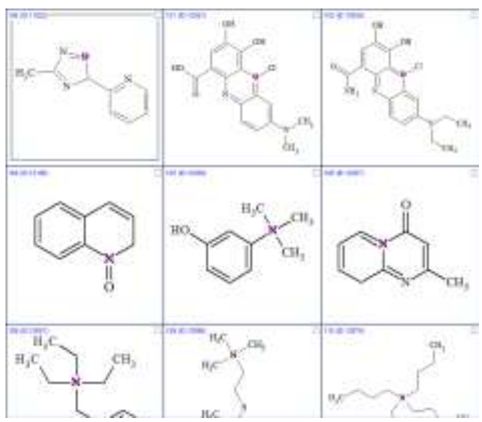
ChemSpider
The free chemical database

PHYSPROP Database

The freely downloadable database under the EPI Suite prediction software

Very Basic filters suggest data quality issues



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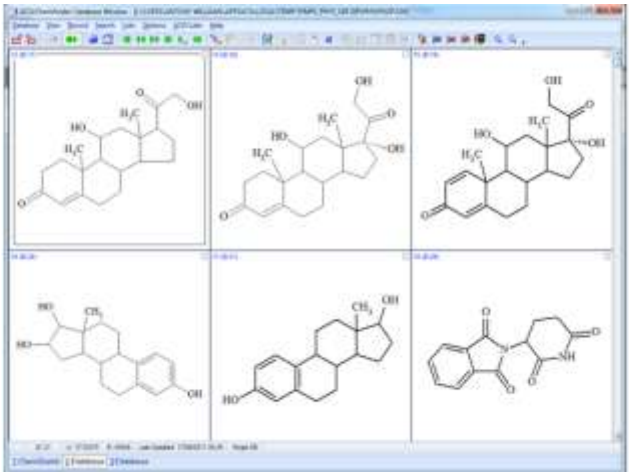
ChemSpider
The free chemical database

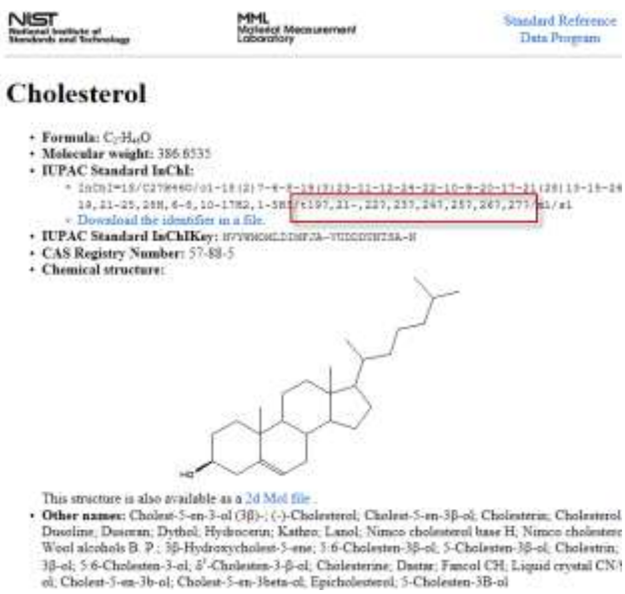
The Stereochemistry challenge.
12500 chemicals with "missed" stereo



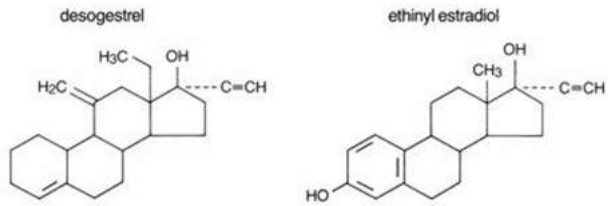
RSC | Advancing the Chemical Sciences

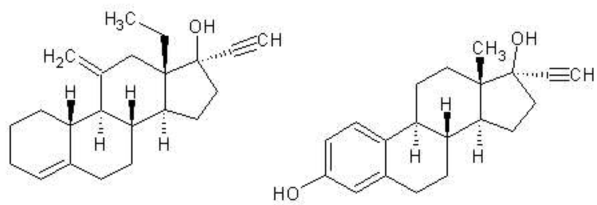
ChemSpider The free chemical database

NIST Webbook



FDA’s DailyMed





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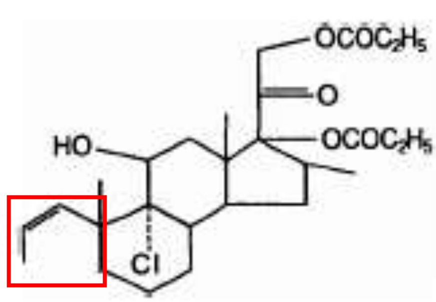
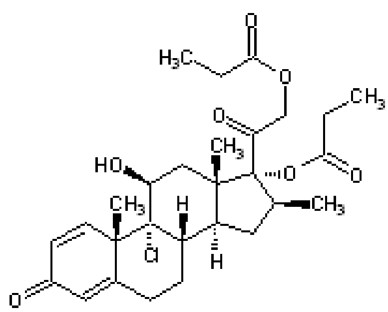
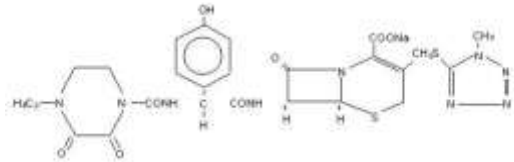
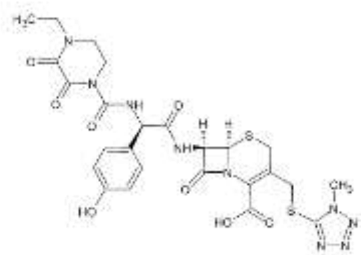




FDA's DailyMed





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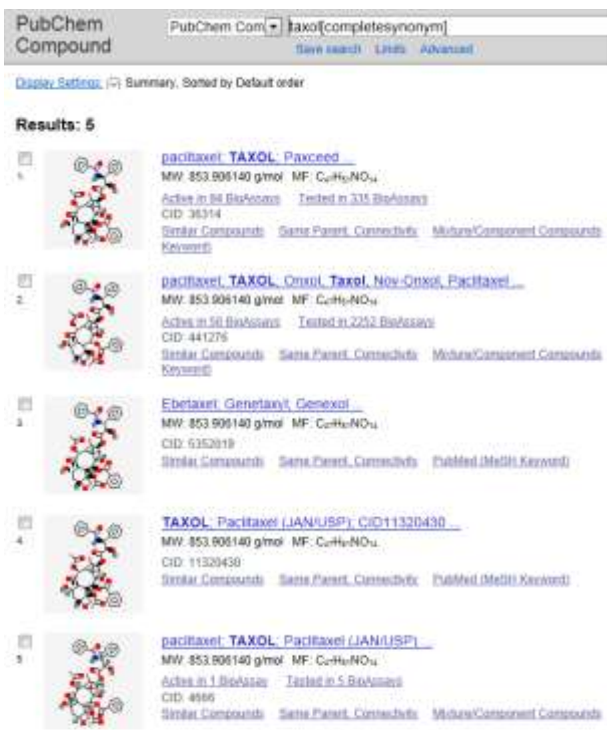
ChemSpider The free chemical database

PubChem



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Crowdsourced "Annotations"

- Users can add
  - Descriptions/Syntheses/Commentaries
  - Links to PubMed articles
  - Links to articles via DOIs
  - Add spectral data
  - Add Crystallographic Information Files
  - Add photos
  - Add MP3 files
  - Add Videos

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ChemSpider The free chemical database

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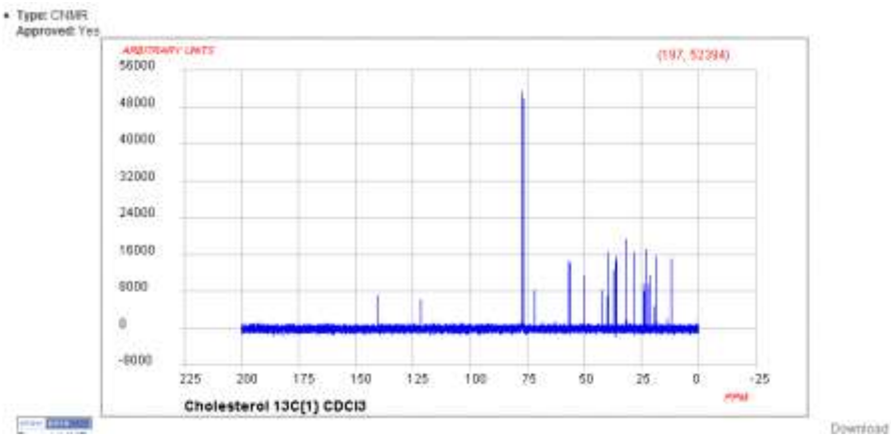
ChemSpider The free chemical database

Community Contribution to ChemSpider



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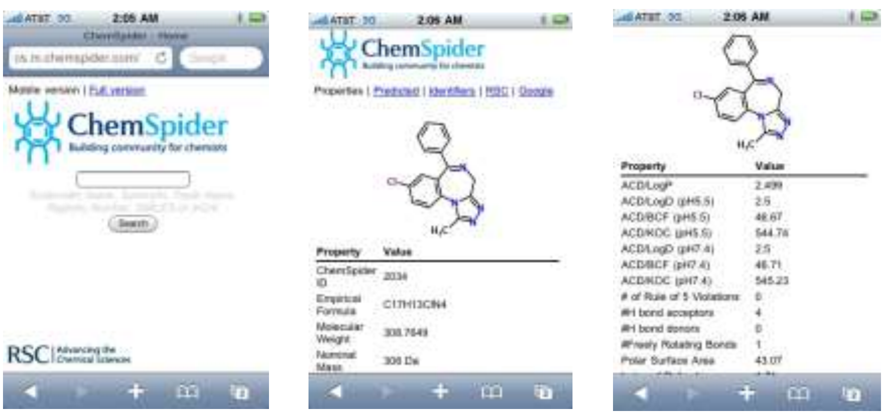
ChemSpider
The free chemical database

Structure Database Lookup



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ChemSpider
The free chemical database

SciMobileApps.com

Future of Chemistry on the Web?

- Public compound databases federate & build a linked environment of validated data!
- Data validation needs are **not** ignored
- **Public-Private** databases can be linked
- **Open Data** proliferate

RSC | Advancing the Chemical Sciences

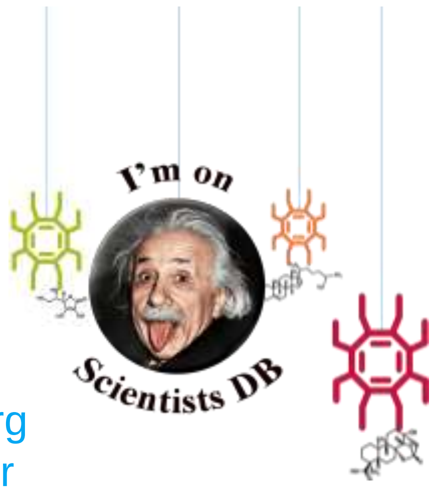
ChemSpider The free chemical database

Conclusions

- ChemSpider is a FREE resource for the community
- Grows daily with new data
- Concerned about data quality!
- Crowdsourced and algorithmic curation is working
- API is available to access data

- Anybody interested in depositing data?
- Any interest in accessing API?

Thank you



Email: williamsa@rsc.org
Twitter: ChemConnector
Personal Blog: www.chemconnector.com
SLIDES: www.slideshare.net/AntonyWilliams

Household Products Database
and tools for consumers

Presentation at:

Personal chemical exposure informatics: visualization, user Experience, Research in Systems modeling and Simulations (PerCEIVERS)

U.S. Environmental Protection Agency
Research Triangle Park, NC
June 26-27, 2012

Henry DeLima

DeLima Associates • 1227 Providence Terrace • McLean • Virginia • 22101 • 703-448-9653

Pertti Hakkinen, PHD

Acting Head, Office of Clinical Toxicology • National Library of Medicine, National Institutes of Health • 6707 Democracy Blvd. Suite 510 • Bethesda • Maryland • 20892 • 301-827-4222
and
Adjunct Associate Professor in Biomedical Informatics • Uniformed Services University of the Health Sciences • F. Edward Hébert School of Medicine

Household Products Database

Overview

- Background
- What's in it?
- How do we select Brands for inclusion?
- Sources for Brands-Specific Data
- Target Audience
- Site Statistics
- Proposed Enhancements

Household Products Database

Background

- **Sponsor: Centers for Disease Control & Prevention**

- **Objective: Develop and maintain a brands-specific consumer product database with:**
  - List of ingredients
  - Acute and chronic health effects
  - First aid information
  - Safe handling and disposal procedures

- **Launched: In 2001 by National Library of Medicine**
  Consumers' 24/7 global online gateway into NLM's databases: 30,000 page views/day

Household Products Database- 062612 35

Household Products Database

What's in it?

- **For each of over 12,000 Consumer Products in 9 Product Categories:**
  - Product Image & Description
  - Manufacturer Information
  - Ingredients from Labels and Safety Data Sheets
  - Properties and Data for Individual Ingredients from NLM's Suite of Databases
  - Health Effects for Product
  - First Aid Guidance

Household Products Database- 062612 36

Household Products Database

How do we Select Brands?

- **Selection of Brands**
  - Major Manufacturers and Market Share for Each Subcategory
  - Shelf Presence in Stores
  - Consumer Requests through National Library of Medicine
  - Unsolicited Requests from Manufacturers
  - Brand Highlighted by Media

Household Products Database- 062612

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Household Products Database

Where do we get Brand Information?

- **Data Sources (Established, On-going Process)**
  - Labels of Products
  - Manufacturer's Web Sites
  - Safety Data Sheets obtained directly from Manufacturers
  - Manufacturers' Health & Safety / Regulatory Affairs Offices
  - Manufacturers' Customer Service Agents

Household Products Database- 062612

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Household Products Database

Target Audiences

- **Consumers**
  - To identify the chemicals in products
  - To determine the health effects of product ingredients
  - To try to avoid brands that have some ingredients
  - To contact emergency health line
  - To have access to brand-specific First-Aid and risk management information
- **Researchers**
  - To help with design and conduct human exposure studies and risk assessments
- **Government Regulatory Agencies**
  - To identify additional chemicals to watch, and for possible regulation
  - To determine compliance with occupational and environmental laws
- **Physicians, and Hospital Emergency Departments**
  - To identify chemicals in products used by patients
  - To determine the health effects of product ingredients
  - To contact the product manufacturers for patient management information

Household Products Database

Site Statistics

- **Average Daily Page Views: >30,000**
  - Household Products Database (http://hpd.nlm.nih.gov)
  - Consumer Product Information Database (www.whatsinproducts.com)
- **Top Search Terms**
  - Ingredients
  - Safety Data Sheets
- **Rankings of Users by Country**
  - USA: 1
  - Canada: 2
  - EU (Combined): 4
  - UK: 6
  - Germany: 8

Household Products Database

Current and Proposed Enhancements

- **Global Taxonomy of Product Categories and Products**
  - Product Categories and Subcategories are based on U.S. Practices
  - Propose Alternate Categories to be Compatible with E.U. and Other Product Nomenclature
- **Include Products that contain Nanomaterials/nanoparticles:**
  - Identify specific ingredients present in nanoform
  - NLM has MOU's with CPSC and EPA relevant to this
- **Identify Products That Comply With Environmental Standards**
  - Allow Users to Search Products that Comply with Government-endorsed Environmental Standards such as EPA's DfE and ECO Labels in Europe
- **Provide Links for Worldwide Information Relevant to Product Subcategories**
  - Examples of Information Sources: RIVM, BfR, AFSSET, KTL, EC-DG/JRC
  - Web Sites, Reports, and Peer-reviewed publications
  - Provide search strategies, e.g., for a product category, for using NLM's PubMed database
- **Provide Educational Module(s) for Consumers and Others**
  - Alternative Products and Proper Use, Storage and Disposal of Products

Household Products Database- 062612

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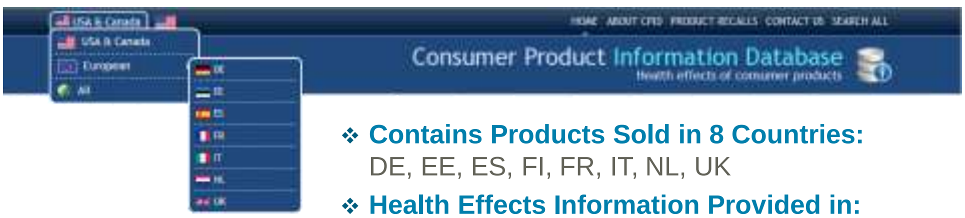
Household Products Database

In Progress: Pilot EU-Version of Database



- **Contains Products Sold in 8 Countries:** DE, EE, ES, FI, FR, IT, NL, UK
- **Health Effects Information Provided in:** Country-Specific Languages
- **Chemicals Classifications Provided for Each Ingredient**
  - Hazard Symbols, Risk and Safety Phrases (67/548/EEC)
  - Hazard and Precautionary Statements and Pictograms (GHS)
  - **S**ubstances of **V**ery **H**igh **C**oncern (SVHCs) Identified
- **Chemical Property Links to HSDB, Toxnet, ECHA-Chem, Etc.**
- **Safety Data Sheets provided for all Products (except Cosmetics)**
- **Product Ingredients can be Compared between Countries**

Household Products Database- 062612

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Entropy in Personal Chemical Informatics

(or why Birds are cool, Ecologists got it going on!)

PerCEIVERS June 27, 2012

Mike Tornero
EPA National Exposure Research Laboratory

The 2nd law of thermodynamics states that the universe tends towards higher entropy *

* **entropy:** the quantitative measure of disorder in a system

Image: http://delong.typepad.com/sdj/2009/11/why-the-universe-looks-the-way-it-does.html

"Life, contrary to the general tendency dictated by the 2nd law, decreases or maintains its entropy by feeding on negative entropy"

-Erwin Schrödinger

"I'd look for an entropy reduction, since this must be a general characteristic of life"

-James Lovelock on a theoretical life detection system for NASA

Limits of Predictability in Human Mobility

Chaoming Song,[1,2] Zehui Qu,[1,2,3] Nicholas Blumm,[1,2] Albert-László Barabási[1,2,*]

A range of applications, from predicting the spread of human and electronic viruses to city planning and resource management in mobile communications, depend on our ability to foresee the whereabouts and mobility of individuals, raising a fundamental question: To what degree is human behavior predictable? Here we explore the limits of predictability in human dynamics by studying the mobility patterns of anonymized mobile phone users. By measuring the entropy of each individual's trajectory, we find a 93% potential predictability in user mobility across the whole user base. Despite the significant differences in the travel patterns, we find a remarkable lack of variability in predictability, which is largely independent of the distance users cover on a regular basis.

When it comes to the emerging field of human dynamics, there is a fundamental gap between our intuition and the current modeling paradigms. Indeed, although we rarely perceive any of our actions to be random, from the perspective of an outside observer who is unaware of our motivations and schedule, our activity pattern can easily appear

18 19 FEBRUARY 2010 VOL 327 SCIENCE

Defined 3 measures of entropy

(E1) Number of cell phone towers triggered (Number of nodes visited)

(E2) + Time spent @ tower (+ Probability of visiting a node)

(E3) + Sequence of towers (+ Order of visiting nodes)

Entropy: E3<E2<E1 and E3 gives 93% predictability

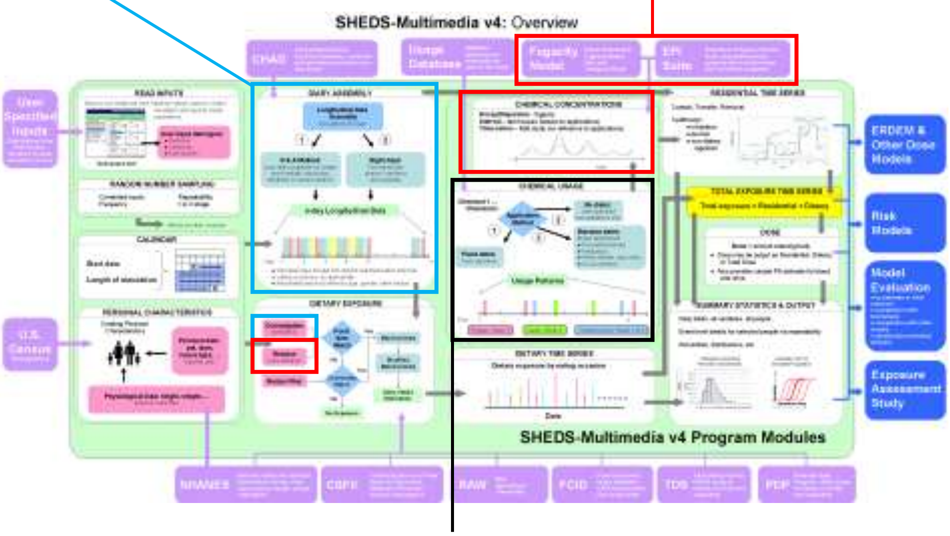
Entropy is a measure of predictability in activity
Activity is essential to exposure model

Exposure ~ f (Activity, Chemical Residue)

Entropy?
e.g., consider the problem of reconstructing long-term diets from 2-day dietary assessments

Activity/ entropy

Chemical property/ distribution

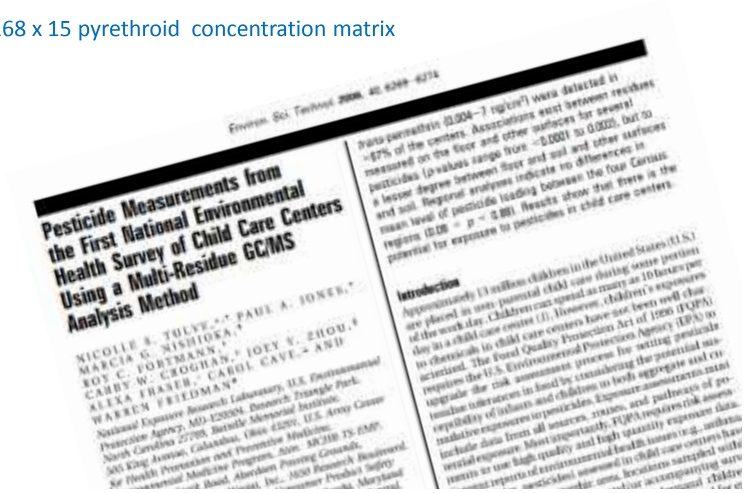


Chemical Usage Patterns... entropy measure? Source: Dr. Valerie Zartarian

Tulve et al. 2006. *Environ. Sci. Technol., 40, 6269-6274*

- National Survey of pesticide residues in child care centers
- 168 child care centers
- Surface wipe samples from indoor surfaces

Consider subset 168 x 15 pyrethroid concentration matrix


Environ. Sci. Technol. 2006, 40, 6269–6274

Pesticide Measurements from the First National Environmental Health Survey of Child Care Centers Using a Multi-Residue GC/MS Analysis Method

Introduction

A Community Ecology Model of Species Co-occurrence

Sites →

Species ↓

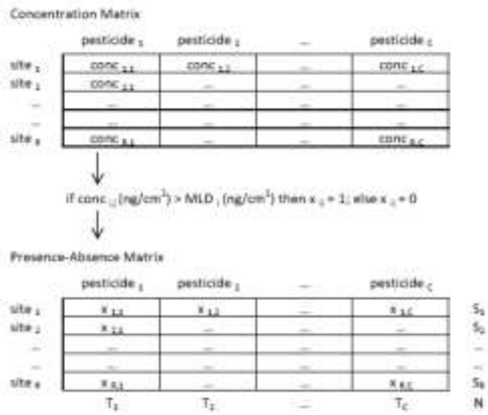
	Cuba	Hispanolia	Jamaica	Puerto Rico	Guadeloupe	Martinique	Dominica	St Lucia	Barbados	St Vincent	Grenada	Antiqua	St Croix	Grand Cayman	St Kits	Barbuda	Montserrat	St Martin	St Thomas	
Carduelis dominicensis	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**1**
Loxia leucoptera	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**1**
Volatina jacarina	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	**1**
Sprophilia nigrricolis	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	**1**
Melopyrha nigra	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	**2**
Loxigilla portoricensis	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**1**
Loxigilla violacea	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**2**
Loxigilla noxis	0	0	0	0	1	1	1	1	1	1	1	1	0	0	1	1	1	1	0	**12**
Melanospiza richardsoni	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	**1**
Tiara olivacea	1	1	1	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	**5**
Tiara bicolor	0	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1	1	1	1	**17**
Tiara canora	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**1**
Loxipasser anoxanthus	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**1**
Saltator albicollis	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	**4**
Torreornis inexpectata	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**1**
Ammodramus savannarum	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**3**
Zonotrichia capensis	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	**1**
	4	**7**	**5**	**4**	**3**	**3**	**3**	**4**	**2**	**2**	**4**	**2**	**1**	**2**	**2**	**2**	**2**	**2**	**1**	**55**

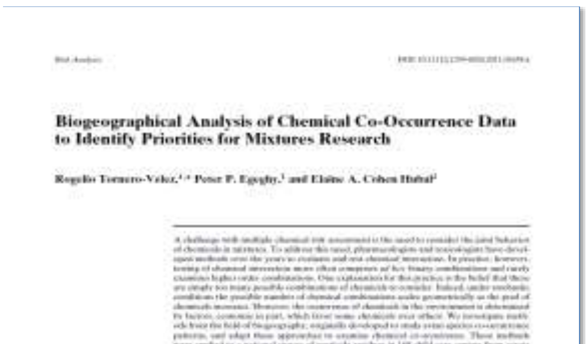
3-way mixture

Initial Dilemma: Apparent loss of information

Environmental; surface loading (ng/cm2) → presence/absence (0,1)

Community Ecology; species abundance (X) → presence/absence (0,1)

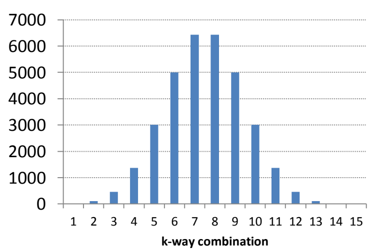




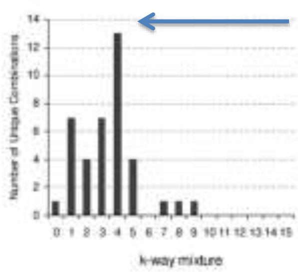
Biogeographical Analysis of Chemical Co-Occurrence Data to Identify Priorities for Mixtures Research

Rogelio Tornero-Velez, Peter P. Egeghy, and Elaine A. Cohen Hubal

random, abiotic



structured, birdlike



Randomize observed matrix according to null model of interest

decreasing entropy

decreasing entropy

Table 1. Nine null models based on the observed presence/absence matrix

	Colums Equally likely	Columns Proportional	Column Sums Fixed
Rows Equally Likely	**Sim 1** P(Xij)=1/RC Constraint: N	**Sim 6** P(Xij)=Tj/NR Constraint: N	**Sim 3** P(Xij)=1/R Constraint: Tj
Rows Proportional	**Sim 7** P(Xij)=Si/NC Constraint: N	**Sim 8** P(Xij)=SiTj/N2 Constraint: N	**Sim 5** P(Xij)=Si/N Constraint: Tj
Rows Sums Fixed	**Sim 2** P(Xij)=1/C Constraint: Si	**Sim 4** P(Xij)=Tj/N Constraint: Si	**Sim 9** P(Xij)=[Markov process] Constraint: Si,Tj

Adapted from Gotelli et al. (2000). Each entry gives the abbreviation for the null model, and a formula for calculating the probability of occupancy for the first cell in the matrix, P(Xij); N= total occurences, R= number of rows, C=number of columns, Si= sum of i-th row, Tj= sum of j-th column

Birdlike!

Co-Occurrence Pattern in Tulve's Child Care Center data shows structure like West Indian Finch Matrix

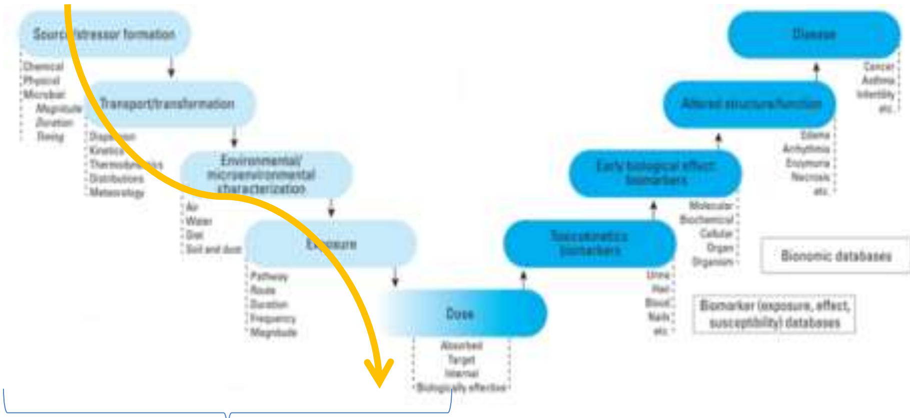
Biogeographical Analysis of Chemical Co-Occurrence Data 7

Table II. Null Model Analyses on the Child Center and West Indian Finch Matrices

	Child Care Center (CCC) Matrix 15 species × 168 sites		CCC Matrix, Lumped 12 species × 168 sites		West Indian Finch Matrix 17 species × 19 sites	
	CHECKER	COMBO	CHECKER	COMBO	CHECKER	COMBO
Observed	34	39	20	35	91	10
Null 1	7.21**	101.53**	8.76**	65.61**	70.78**	18.57**
Null 8	35.91	61.91**	21.70	46.33**	51.00**	17.18**
Null 9	34.99	42.78*	19.67	35.41	89.44	15.14**

Note: To remove the effect of structuring due to co-occurring isomers, "CCC matrix, lumped" combines three species pairs, *cis-/trans*-allethrin, *cis-/trans*-permethrin, and pyrethrins I and II into three single species (allethrin, permethrin, and pyrethrins). The CHECKER index is the number of species forming checker patterns, and has a theoretical range of 0 to $R(R-1)/2$, where R = number of rows (species). The COMBO index is the total number of unique combinations, and has a theoretical range of 0 to 2^{r}, yet is bounded by the number of sites (168). The expected indices are based on 5,000 simulations. **p-value < 0.001, *p-value < 0.05.

Consider 'life-like', entropy-reducing ecological patterns



Social-Biological ?

What are Emerging Behaviors, Activities, and Consumer Patterns leading to chemical exposures ?

Adapted: LioyPJ. Exposure science: a view of the past and milestones for the future. Environ Health Perspect. 2010 Aug;118(8):1081-90.

HUMAN EXPOSURE ASSESSMENT STRATEGIES FOR CONSUMER PRODUCTS

Treye A. Thomas, Ph.D.
U.S. Consumer Product Safety Commission
Office of Hazard Identification and Reduction
Bethesda, MD

June 26-27, 2012

This report was prepared by CPSC staff; it has not been reviewed or approved by, and may not necessarily reflect the views of, the Commission.

U.S. Consumer Product Safety Commission

- Independent regulatory agency (1973)
- Thousands of products in and around the home
- Generally, food, drugs, cosmetics, medical devices, pesticides, automobiles not included
- Does include child-resistant packaging for household chemicals, drugs, and cosmetics
- Staff of ~540; budget of $118 M
- 5 Commissioners appointed by President

CPSC National Product Testing & Evaluation Center

- New, modern lab-office location - 5 Research Place, Rockville, MD
- 63,000 sq ft (32,000 sq ft of laboratory testing space vs 13,000 at old site)
- Lease Awarded & Design Initiated May 2009
- Construction started April 2010
- Moved in and Operational May 2011
- ~75 Engineers, Scientists, and Support Staff

CPSC National Product Testing & Evaluation Center Testing Areas


Toy Test Lab


Children's Products Lab


Pool and Spa Products Lab


Impact Lab (Bike Helmets)


General Product Test Lab


Outdoor Power Sports Lab


Electrical Products Test lab


Chemistry Lab


Combustion Products Test Lab


Modern Conference Space


Machine Shop


Flammability/Fire Test Lab

Federal Hazardous Substances Act (FHSA)

- Risk-based
  - Considers toxicity, exposure, and bioavailability
  - Human experience takes precedence over animal data
  - Includes acute and chronic effects
  - Includes reasonably foreseeable misuse
    - Mouthing by children
- Does not require specific testing for chronic hazards

Chronic Hazard Guidelines

- Released in 1992
- Provide guidance in assessing risks from acute and chronic hazards
  - Carcinogenicity, neurotoxicity, and reproductive/developmental toxicity
  - **Exposure**
    - **Consider all sources of information**
  - Bioavailability
  - Acceptable daily intake (ADI)
    - Route-specific exposure limits
      - Inhalation
    - Establishing limits for susceptible populations
  - Risk assessment
  - Acceptable risk

Guidelines - Exposure Assessment

- Field data preferred
  - Pollutant levels in indoor air
- Laboratory data
  - Emission or migration data
  - Supplemented with mathematical models
- No available exposure data
  - Surrogate chemical
  - Theoretical model

Consumers

- Best estimate of "typical consumer" (50th percentile)
  - Upper (95th percentile) and lower bound (5th percentile) screening
  - Demographics
    - Variation in use patterns
    - Frequency of use
  - Time activity patterns
    - More time spent indoors
      - Especially among children

Data Gaps for Exposures from Consumer Products

- Product formulations
- Product release and residue data
  - Variation by chemical and product
- Frequency and duration of use of product
- The proportion of the population using product
- Scope of uses associated with products
- Secondary chemical by-products of health concern
  - Diversity of products
    - Matrices (*e.g.*, plastic, textile, household chemicals)
    - Variations within a product class
    - Coatings and paints

Considerations for Exposure Assessment

- Consumer environment
  - Housing types
    - Size and configuration
    - Ventilation
    - Sinks
      - Carpets, furnishings

Chemical Fate in the Indoor Environment

- Ambient air concentrations
- Form of the compound released
  - Gas
  - Particulate
- Chemical transformations???
  - Concentrations of reactive compounds
  - Photolysis
  - Effects of by-products
- Deposition and sequestration
- Absorption and re-release
- Removal mechanisms
  - Ventilation
    - Seasonal variation
  - Air cleaning devices

Estimating Exposure by Route

- Inhalation
  - Direct monitoring
    - Available "validated" methods
    - Collection efficiency
  - Modeling
  - **Surrogate data**
- Ingestion
  - Extraction with simulated saliva or gastric juices
  - Hand-to-mouth activity
    - Concentrations on hands
    - Removal efficiency

Estimating Exposure by Route

- Dermal
  - Quantify material leaching from product
  - Estimating amount of substance in contact with skin
  - Surface area of skin contacted
  - Duration, frequency of contact, thickness of liquid interfacial layer
  - Hand wipes (*e.g.,* CCA validation study)

Surveillance Data Bases

- Injury and Potential Injury Incident Data (IPII)
- Death Certificates (DTHS)
- In-Depth Investigations (INDP)
- National Electronic Injury Surveillance System (NEISS)

Overview/History

- National sample of 96 hospitals from all U.S. hospitals with at least 6 beds and 24-hour emergency service.
- Each hospital reports information on emergency treatments to CPSC.
- Hospital coder enters data in local PC and transmits the data to CPSC over the internet.
- System collects ~ 400,000 product-related injury reports each year.
  – (~ 300,000 non-CPSC injury reports each year).
- Multi-level system.
- Supports CPSC and other agencies.

Consumer Product Safety Improvement Act of 2008

- Signed into law in August 2008
- http://www.cpsc.gov/cpsia.pdf
- Sec. 212. Establishment of a Public Consumer Product Safety Information Database.

Searching for Incidents and Recalls

Thank you

- CPSC Website
  - www.cpsc.gov
- Incident reports and recalls
  - www.saferproducts.gov
- Chronic Hazard Guidelines
  - http://www.cpsc.gov/BUSINFO/chronic.pdf

What is GoodGuide?

- Web-based platform that tracks the health, environmental and social aspects of products, brands and companies – covering over 175,000 products from 5,000 companies
- Tools that deliver this information at the point of purchase – changing the buying decisions of consumers, retailers and institutional purchasers

GoodGuide

74 Confidential

Scan a Bar Code –> Instant Shopping Advice

75 Confidential

GoodGuide.

Detailed Information about Product Ingredients, their Potential Health Hazards & Regulatory Status

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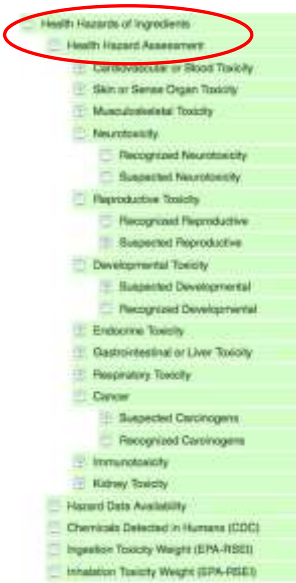
GoodGuide.

Product Health Ratings – Personal Care



Categorize ingredients by level of health concern based on:
1) Number of recognized & suspected health effects
2) Relative toxic potency
3) Detection in US population
4) Adequacy of toxicity data set

Assign product scores by counting ingredients by level of concern:
0 - 1 High concern
2 - 4 Medium concern
5 - 8 Low concern
10 No ingredients of concern

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GoodGuide

Categorizing Chemicals by Level of Concern

- GoodGuide's classification system combines data from hazard identification, potency estimation and exposure assessment
  - Improves on simpler classification systems that are hazard only
- Twelve health effects are tracked, with strength of hazard identification reflected in suspected vs recognized list of hazards
- GoodGuide is not making its own expert judgment that chemical x causes health effect y
- Health effect lists are compiled from authoritative scientific and regulatory sources
  - Scientific sources include IARC, NTP, medical and toxicology texts and review articles
  - Regulatory sources include CalEPA, EPA IRIS, EU CLP
- Health effects are not identified based on single or controversial scientific reports – available scientific data must be reviewed by a scientific or regulatory 3rd party that then publishes a hazard identification
  - Different approach than EWG or other NGOs

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GoodGuide

Modifying Screening-level Ratings with Better Data

- Presence of “bad actor” ingredients in a product is a warning signal
- To further evaluate whether there is a potential health risk, need:
  - % ingredient in formulation
  - Exposure potential from typical product use
  - These data are often not available from public sources
- Rating system can adjust product scores to suppress an ingredient when data indicate the ingredient is unlikely to pose a health risk because it is
  - present below a regulatory threshold, or
  - present in a product category unlikely to result in significant exposure
- Pre-empts criticism of hazard-based scoring by challenging manufacturer to provide the data required for risk assessment
- Example safe use determination:
  - Ethyl acetate is "known to be neurotoxic in man"
  - Ethyl acetate is used as a solvent in nail care cosmetics
  - Low % formulations and product category usage does not result in the high doses required to elicit neurotoxicity

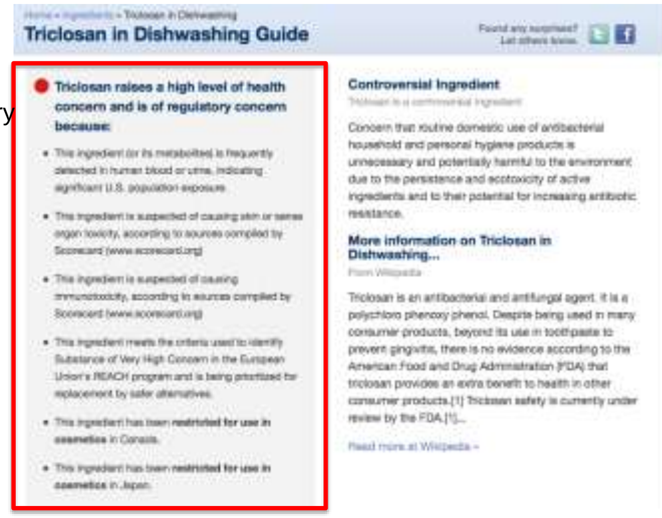
GoodGuide

Backing Up Our Health Ratings

GoodGuide

Ingredient Profiles

Scientific & Regulatory Basis for Level of Concern



Controversy Status

3rd-Party Online Resources

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GoodGuide.

Handling Data Gaps

- Ingredient lists are essential input to health ratings for personal care & household chemical products
- We acquire ingredient lists from manufacturer websites, and also operate a process for manufacturers to provide product ingredient lists to us directly using data submission templates
- Parsing tools break lists into ingredients and flag generic ingredient strings
- Ingestion tools match specific ingredients to GoodGuide chemical records

- Rating framework includes an “Ingredient Disclosure” node to address data gaps:
  - Failure to disclose any ingredients is heavily penalized
  - Incomplete disclosure using generic terms that prevent hazard assessment is subject to scaled penalty:
    - Tier I High Potential Hazard generic terms cap score at 4
    - Tier II Low Potential Hazard generic terms cap score at 8
    - Tier III fragrance generic terms cap score at 6

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GoodGuide.

Purchase Analyzer – Acquiring a Consumer's Entire Product History

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GoodGuide

Relevance to Personal Exposure Informatics

- Comprehensive catalogue of current consumer products, their ingredients and other attributes relevant to assessing health risk
- Capacity to acquire personal product purchase histories for consumers
- Distribution platform that engages over 1 million consumers per month who are interested in health impacts of consumer products

- Key data required to integrate exposure considerations into health ratings are unavailable:
  - Limited characterization of exposure potential associated with specific categories of consumer products
  - Manufacturers generally unwilling to disclose ingredient percent formulations, so impossible to assess compliance with safety benchmarks
  - Essentially no data available on actual exposures experienced by consumers under different use scenarios

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GoodGuide

Increasing Consumer Ease of Use : Augmented Reality App

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GoodGuide

The Quantified Self & Chemical Sensing

Michael Nagle
http://www.thesprouts.org
@nagle5000

What is the Quantified Self?

Quantified Self

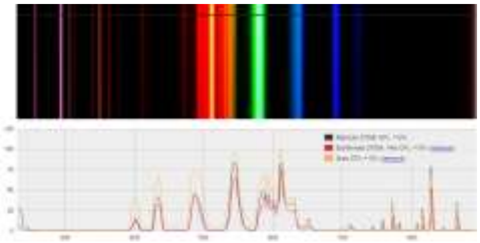
Example 1: Verifying Hypotheses

Example 2:
Identifying Causes

Sensing Chemicals 1:
Portland Smells

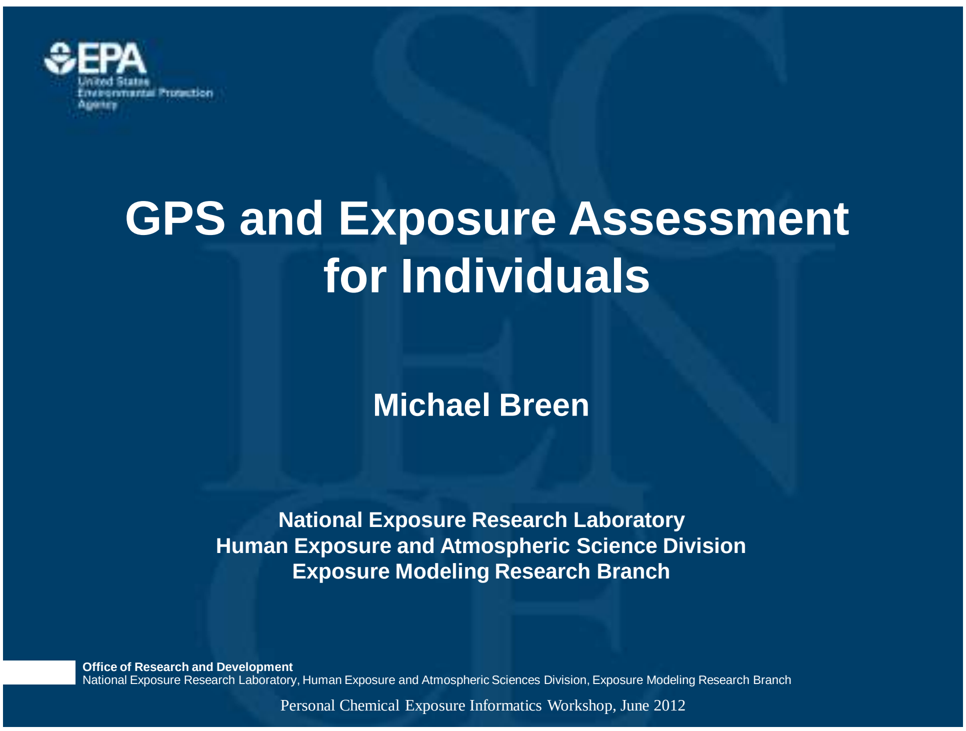
Sensing Chemicals 2: Asthamapolis

Sensing Chemicals 3: Public Laboratory

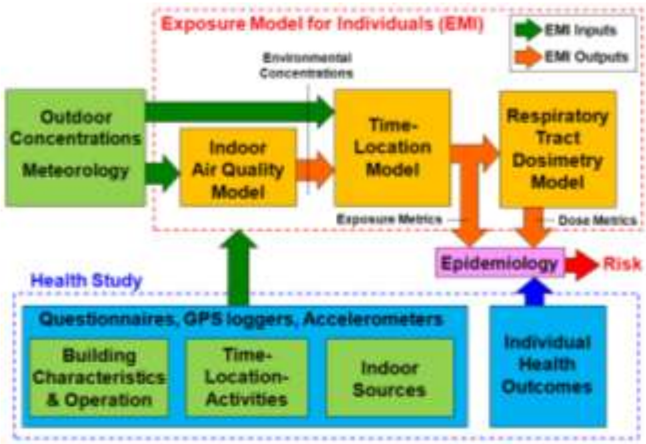


Thank you!

- Drop me a line if you have questions :: nagle@thesprouts.org

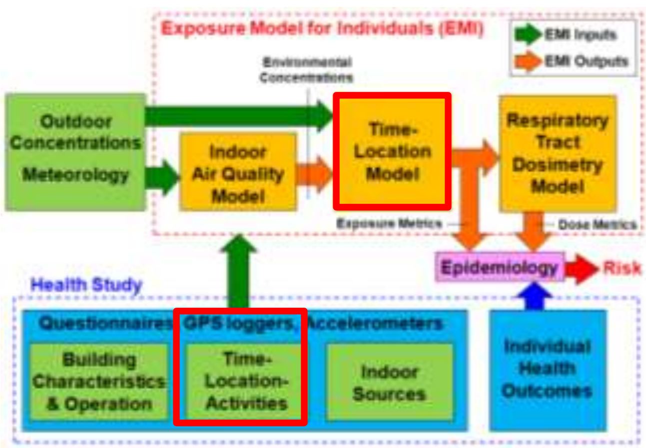


Exposure Model for Individuals (EMI)



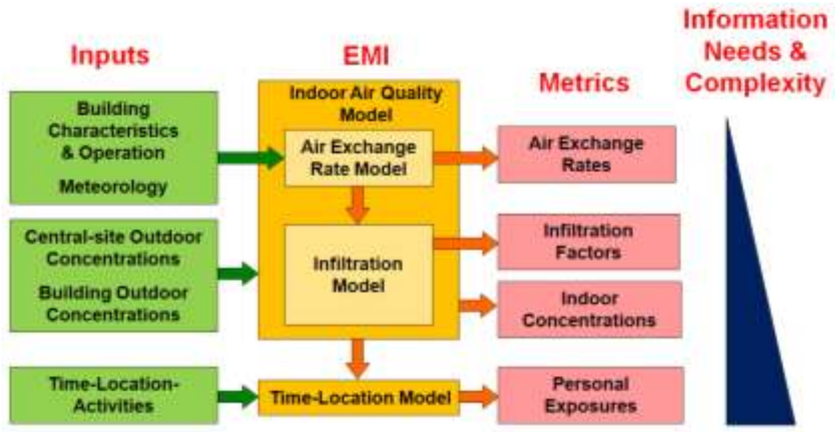
EMI Web site: www.epa.gov/heasd/emi

Exposure Model for Individuals (EMI)



EMI Web site: www.epa.gov/heasd/emi

Tiered EMI Metrics



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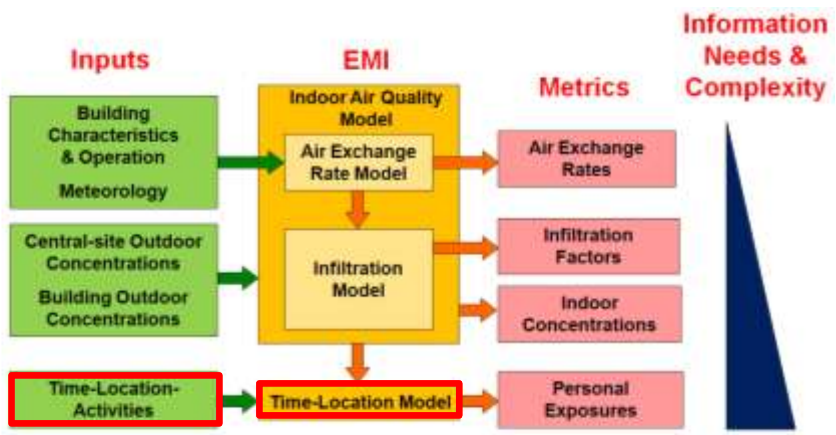
EMI Web site: www.epa.gov/heasd/emi

Tiered EMI Metrics



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EMI Web site: www.epa.gov/heasd/emi

Microenvironment Tracker (MicroTrac)

Qstarz GPS Travel Recorder
(BT-Q1000XT)

- Addresses critical need to develop exposure metrics for health studies:
  - Estimation of time spent in various microenvironments
- Classification algorithm to estimate time-of-day and duration in microenvironments (in-transit, home, school, work) based on:
  - Position and speed timelines from GPS data loggers
  - Marked boundaries of buildings using Google Earth
- Potential to reduce challenges with diaries (participant burden, inaccuracies, missing data)
- Ability to use smartphone GPS data

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Google Earth: Marked Boundaries

School | Home | Work

100

Classification Algorithm: Microenvironments

1. Home-indoors
2. Home-outdoors
3. Work/School-indoors
4. Work/School-outdoors
5. Other-indoors
6. Other-outdoors
7. In-transit

101

Classification Algorithm: Home

Home

GPS positions, Building boundaries

↓

Position within 50m radius of residence? — No → Continue …

↓ Yes

Position within residential boundary? — No → Done: Home-outdoors

↓ Yes

Done: Home-

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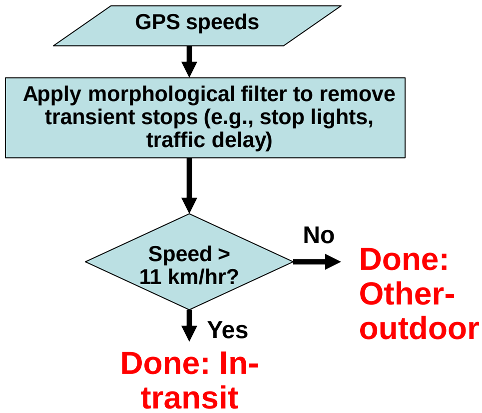
Classification Algorithm: In-transit

In-transit



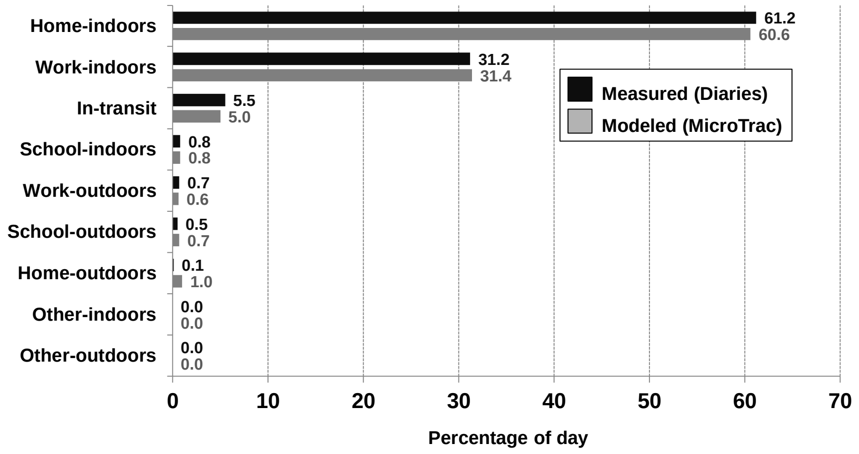
MicroTrac Pilot Study

- Collected GPS data for 24 hr workday (5 sec sampling time)
- Created diaries by marking "waypoints" with GPS loggers when changing microenvironments
- Evaluated MicroTrac estimates with diaries

EPA United States Environmental Protection Agency

MicroTrac Evaluation for Participant 1

24 hr dataset (17,280 samples): processing time = 36 sec



EPA United States Environmental Protection Agency

Summary of MicroTrac

- Evaluating feasibility from pilot study with concurrent GPS and diary data
- Limitations:
  - GPS spatial resolution (~3m)
  - Possible spatial errors near large buildings and dense clusters of trees (multipath errors)
- Small, lightweight, and low cost GPS devices have potential to address challenges with diaries
- Using smartphone GPS data, MicroTrac allows for real-time determination of microenvironment to support personal exposure APPs

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Getting Chemical Information to Communities

The EPA's Community-Focused Exposure and Risk Screening Tool (C-FERST)

Shannon O'Shea, Andrew Geller, Brad Schultz, and Valerie Zartarian

CFERSTMail@epa.gov

PerCEIVERS workshop | RTP, NC | June 27, 2012

What is C-FERST?

C-FERST is a community mapping and assessment tool to inform environmental public health decisions

What does C-FERST do?

- Enhances access to info for community decision-making
- Provides venue for technical assistance, science communication, collaborations
- Assists with identification and prioritization of community environmental health issues
- Fosters sustainable and healthy communities

Conceptual Framework

Innovative,
high quality science

User-friendly
interface and readouts

✓modeled local exposures
✓guidance on local measurements
✓cumulative risk science
✓other info useful to communities

❑ Follow community guidance; access info
❑ Map multimedia human exposures and risks
❑ Learn best practices in other communities
❑ Generate community reports for risk ranking

Assess Cumulative Exposure/Risk in Communities

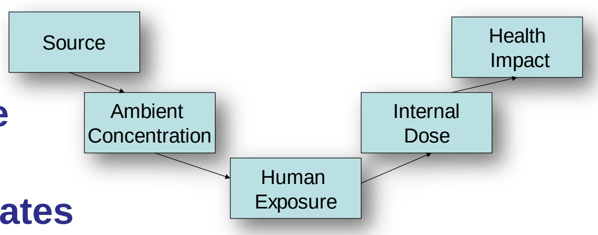
Prioritize environmental issues within a given community

Compare information across locations

Inform and assess impact of sustainable solutions, decisions, adaptive management strategies, and other actions

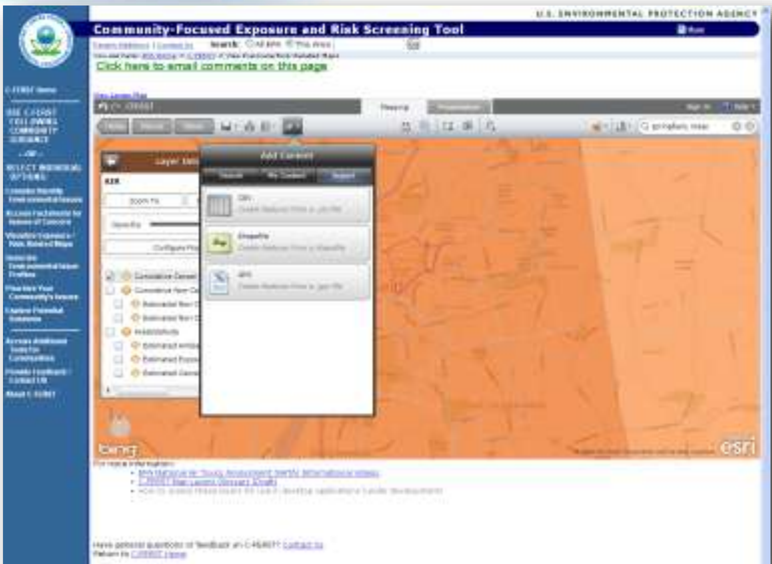
Structure of Estimates & Indicators in C-FERST

- **Ambient concentrations**
- **Human exposure estimates**
- **Biomarker estimates**
- **Risks/Health impacts**
  - **Cancer, Asthma, Early neurotoxicity effects, etc.**



Data Metrics	Your Community: ZIP Code 27704	Durham County, NC	North Carolina	National Average	Data Info/Notes*
Environmental Concentration Estimates (μg/m³)					
Outdoor Air - Acetaldehyde	2.3	2.3	2.2	1.9	NATA 2005
...others collapsed as a default...					
Human Exposure Estimates (mg/day or μg/m³ avg)					
Outdoor Air - Acetaldehyde **(μg/m³ annual avg)**	1.8	1.8	1.7	1.5	NATA 2005
Aggregate Childhood Lead (GM μg/dL in blood)	TBD	TBD	TBD	Available	
...others collapsed as a default...					
Health Risk Estimates (in One Million)					
Cumulative Air Toxics Cancer Risk	40.4	42.9	39.4	49.8	NATA 2005
Cumulative Air Toxics Non-Cancer Respiratory Risk†	1.2	1.4	1.2	2.3	NATA 2005
Cumulative Air Toxics Non-Cancer Neurological Risk†	0.03	0.04	0.04	0.06	NATA 2005
Outdoor Air - Acetaldehyde **	3.9	4	3.7	3.3	NATA 2005
Outdoor Air - Arsenic	0.8	0.9	0.8	1.3	NATA 2005
Outdoor Air - Benzene	3.9	4.8	4.6	7.4	NATA 2005
Outdoor Air - Butadiene **	1.1	1.5	1	1.9	NATA 2005
Outdoor Air - Chromium **	0.6	0.7	0.7	1.4	NATA 2005
Outdoor Air – Formaldehyde **	22.9	23.7	21.5	22.5	NATA 2005
Outdoor Air - Naphthalene **	0.6	0.7	0.6	2.3	NATA 2005
Outdoor Air - PAH **	0.6	0.7	0.8	1.5	NATA 2005
Indoor radon excess lung cancer mortality	N/A	N/A	N/A	Avail (PI)	NRRRA
Excess hospitalizations due to PM2.5	N/A	Available	Available	Available	BenMAP
Excess mortality due to PM2.5	N/A	Available	Available	available	BenMAP
Excess mortality due to ozone	N/A	Available	Available	available	BenMAP

† These values are expressed as a Hazard Quotient.
***see clarifying metadata for approach description*



Using C-FERST with Community Assessment Guidance

- CARE Roadmap
- PACE-EH
- EJ Toolkit
- HIA roadmap
- Tribal assessment roadmap
- Community-Cumulative Assessment Tool

Future Plans

- Cumulative exposure and risk science
  - Community-level exposures: lead, radon, ETS
  - Pathways: fish consumption, near-roadway
  - Effects: lung cancer, asthma, early neurotoxicity
  - **Measurements: citizen science, community sensors, etc.**
- Integrate with other programs and tools
- Sustainability and risk management aspects
- Continue to refine, incorporate feedback and broaden use of tool for community applications
- Peer review for public release via website

Acknowledgements

- **C-FERST Development Team**
  - Collaborators in ORD (NERL, OSP, SHC program)
  - CARE collaborators (regional project officers, community grantees)
  - EPA Region 1 GIS and Technical Team
  - EPA Office of Environmental Information (OEI), National Computing Center (NCC) and contractors
- **Other Contributors**
  - EPA Office of Environmental Justice (OEJ) & EJ Coordinators
  - EPA Regions & Program Offices
  - National EPA-Tribal Science Council & Tribal Partners
- **EPA/ORD Management for C-FERST Support**

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George Scheer - Director

Elsewhere @ elsewhereelsewhere.org
Greensboro, NC
Calling in from Berlin, Germany

http://www.youtube.com/watch?NR=1&feature=endscreen&v=eTHTnbqeLss

Prof. Benjamin Balak

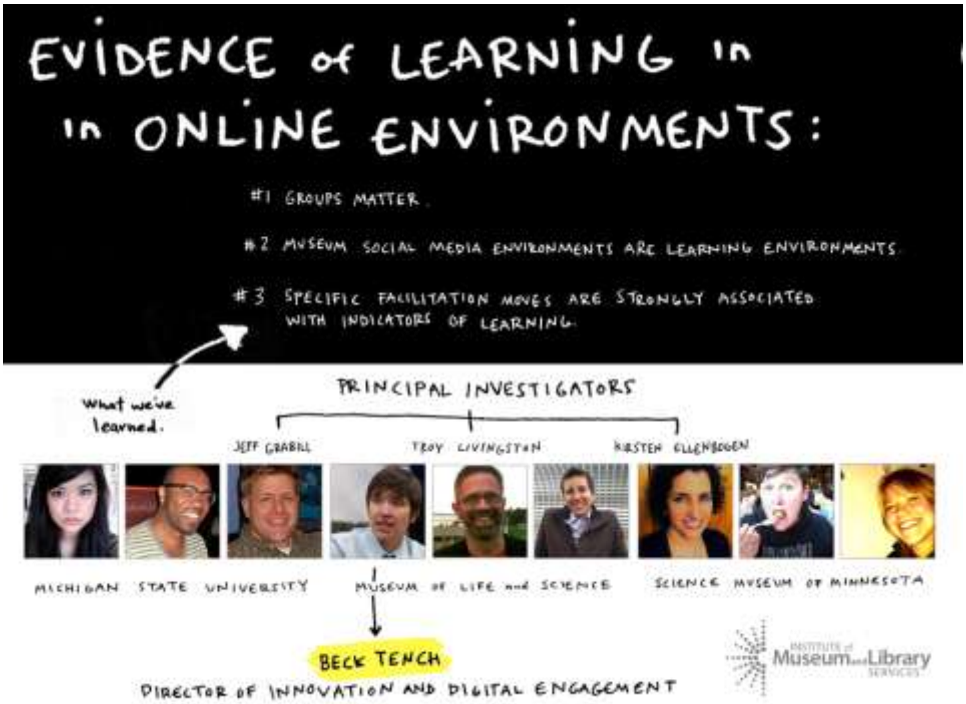
Rollins College, Florida

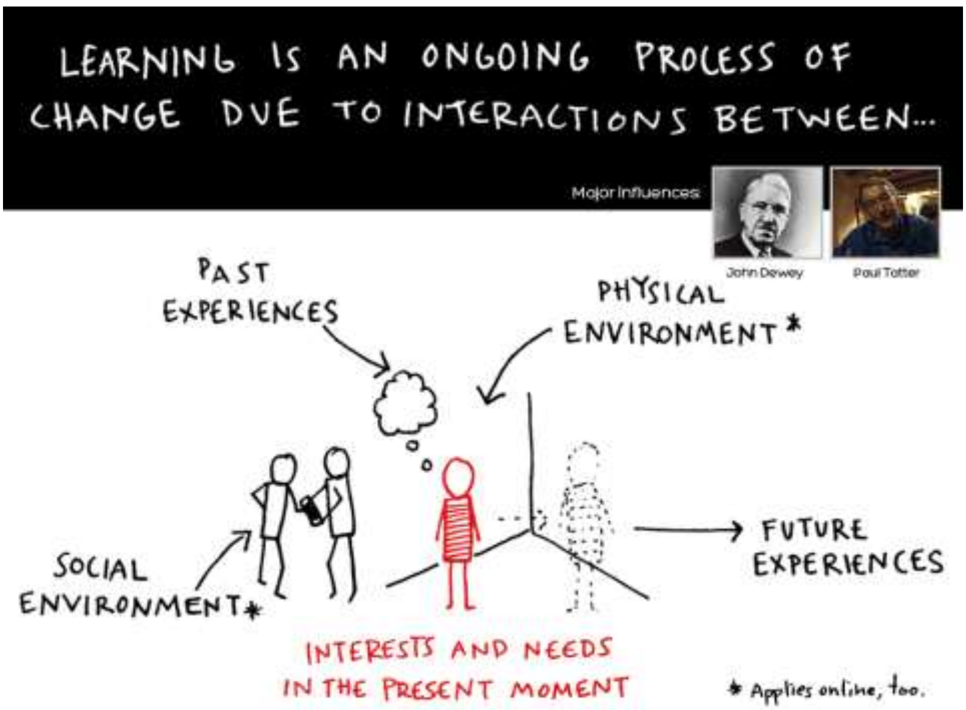
Balak presented aspects of his technologically-enhanced pedagogy in a session titled, "Engaging the community for personal chemical exposure informatics: Gamification, visual and computer models, electronic and live-action role play," participated in breakout sessions, and is working on a video game to gamify personal exposure.

Dr. Robert Panoff

SHODOR – Computational Science Non-Profit

http://www.shodor.org/talks/ct-chem/


EVIDENCE of LEARNING in
in ONLINE ENVIRONMENTS:
#1 GROUPS MATTER.
#2 MUSEUM SOCIAL MEDIA ENVIRONMENTS ARE LEARNING ENVIRONMENTS.
#3 SPECIFIC FACILITATION MOVES ARE STRONGLY ASSOCIATED WITH INDICATORS OF LEARNING.
What we've learned.
PRINCIPAL INVESTIGATORS
JEFF GRABILL
TROY LIVINGSTON
KIRSTEN ELLENBOGEN
MICHIGAN STATE UNIVERSITY
MUSEUM OF LIFE AND SCIENCE
SCIENCE MUSEUM OF MINNESOTA
BECK TENCH
DIRECTOR OF INNOVATION AND DIGITAL ENGAGEMENT
Museum and Library


LEARNING IS AN ONGOING PROCESS OF CHANGE DUE TO INTERACTIONS BETWEEN...
Major Influences:
John Dewey
Paul Totter
PAST EXPERIENCES
PHYSICAL ENVIRONMENT*
SOCIAL ENVIRONMENT*
FUTURE EXPERIENCES
INTERESTS AND NEEDS IN THE PRESENT MOMENT
* Applies online, too.


Claim
Construction of a connection between ideas or people
Invitation development
{ explanations, claims... }
Change in action, thinking, or values
Change in action, thinking, or values
Change in action, thinking, or values
Change in action, thinking, or values
"The thing that has struck me hardest during this whole month is that 'everyones a little bit racist' and it is how you undertstand that racism and how you relate it back to the world around you that is the real lesson."


THE MUSEUM of LIFE + SCIENCE PRESENTS:
EXPERIMONTH: MOOD
The mood of the community for all of April:
YOU + YOUR MOOD RATINGS (PRIVATE)
EVERYONE (PUBLIC)
Today:
This Week:
Mondays So Far:
Today's Featured Post
GENDER AND MOOD
EXPERIMONTH: MOOD COMPLIANCE
Experimonth: Text your mood 1 (low) to 10 (high).


Change
Other change move
Sympathy or empathy that shows a change in thought or feeling
Change in action, thinking or values
Use of technical or scientific concepts or language
Learning Discourse
Articulation of a shared role
Articulation of a shared experience
Articulation of a role
Change in action, thinking or values
Citation of authority
Citation of evidence
Claim
On Task Response (Must be 1st code)
Other discourse environment move
Explanations
Invocation of place
Invocation of education
Invocation of status
Use of values
Use of affect
Use of technology to achieve a purpose
Facilitation
Introducing new ideas
Suggest follow-up actions
Invitation connection
Invitation development
Demonstrate sympathy or empathy
Demonstrate respect for perspective or identity
Construction of connection between ideas or people*
Redirection
Provocation
Other
Other
Other


QUALITIES OF "GROUPNESS":
FACILITATION
THE RIGHT TECH
SHARED PURPOSE
SHARED EXPERIENCES
WRITING MATTERS

REFERENCES → NCMLS.ORG/EPA

Appendix E
WWW resources and URLs of interest

This table provides links to non-EPA web sites that provide additional information and resources. EPA cannot attest to the accuracy of information on that non-EPA page. Providing links to a non-EPA Web site is not an endorsement of the other site or the information it contains by EPA or any of its employees. The links are accurate as of May 21, 2013.

Name	URL	consumer product data	product use data	product ingredient data	human activity data	chemical data	exposure models	open symptoms data	social archiving	infoveillance	chemical genomics data	exposure related data, models or frameworks
EXPOCAST	http://www.epa.gov/ncct/expocast/											x
TOXCAST	http://www.epa.gov/ncct/toxcast/					x					x	
ACTOR	http://actor.epa.gov					x					x	
RAIDAR	http://www.trentu.ca/academic/aminss/envmodel/models/RAIDAR100.html						x					x
USETOX	http://www.usatox.org/						x					x
EPISUITE	http://www.epa.gov/oppt/exposure/pubs/episuite.htm					x						x
SYSTEMSREALITY	www.systemsreality.org	x					x					x
EXPOSURE FACTORS HANDBOOK	http://cfpub.epa.gov/ncea/risk/recordisplay.cfm?deid=236252	x	x		x							
CHAD: CONSOLIDATED HUMAN ACTIVITY DATABASE	http:www.epa.gov/chadnet1/chad_2003.html				x							
GOOGLE INSIGHTS	www.google.com/insights/								x	x		
CHEMSPIDER	www.chemspider.com					x						
CHEMICALIZE	http://www.chemicalize.org					x						
GOODGUIDE	http://www.goodguide.com	x	x	x								
AMEM	http://www.epa.gov/oppt/exposure/						x					
E-FAST	http://www.epa.gov/oppt/exposure/	x	x				x					
MCCEM	http://www.epa.gov/oppt/exposure/						x					
HOUSEHOLD PRODUCT DATABASE	http://hpd.nlm.nih.gov	x	x	x								
WHAT'S IN PRODUCTS	http://www.whatinsproducts.com	x	x	x								
SKIN DEEP	http://www.ewg.org/skindeep/	x	x	x								
SPROUTS	http://www.thesprouts.com							x				

Name	URL	consumer product data	product use data	product ingredient data	human activity data	chemical data	exposure models	open symptoms data	social archiving	infoveillance	chemical genomics data	exposure related data, models or frameworks
QUANTIFIED SELF	http://www.quantifiedself.com							x				
CURETOGETHER	http://www.curetogether.com							x				
PATIENTS LIKE ME	http://www.patientslikeme.com							x				
TWEET ARCHIVIST	http://www.tweetarchivist.com/archivist-desktop/								x	x		
CONSEXPO	http://www.rivm.nl/en/Topics/Topics/C/ConsExpo	x	x	x								x
COMPARATIVE TOXICOGENOMICS DATABASE	ctdbase.org										x	