

nonresponse, and non-coverage. Standard errors of the weighted estimates of the quantile regression parameters were estimated with bootstrap. Quantile regression provides the trends in the overall data distribution. Quantile regression not only allows us to systematically evaluate patterns in extreme phthalate exposure over time but also allows us to estimate central tendency of phthalate exposure more robustly using the median. The analysis shows that there were significant decreasing trends in daily intake of DBP, BBP, and DEHP both at the median and at the 95th percentile over the period 2005-2012. Daily intake of DiBP increased at the median but not at the 95th percentile. Daily intake of DINP increased both at the median and at the 95th percentile. Specifically, daily intake of DEHP has declined since the 2005/2006 survey, and, by the 2011/2012 survey were approximately 15% the levels measured in the 2005/2006 survey for the 95th percentile. Given DEHP has been identified as the major driver for risk in multiple cumulative risk assessments (CRA) conducted with phthalates, the decrease has a significant impact on the CRA of phthalates conducted by the CHAP. Trends may be reflective of an industry move towards safer phthalates.

PS 496 High-Throughput Exposure Modeling of Semi-Volatile Chemicals in Articles of Commerce

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Chemical components of consumer products and articles of commerce such as carpet and clothing are key drivers of exposure in the near-field environment. These chemicals include semi-volatile organic compounds (SVOCs), some of which have been shown to alter endocrine functionality. SVOCs have the potential to accumulate in the indoor environment at high rates, which is correlated with high indoor exposures although it is not well quantified. The ExpoCast project is developing a model that predicts steady-state gas-phase concentrations (y_o) of 871 ToxCast Phase I and II chemicals based on their physicochemical properties such as logP, vapor pressure, Henry's law, boiling point, and molecular weight. These chemicals are currently limited to those found in the indoor environment as per their respective chemical use categories found in the ACToR database. The 74 chemical training set for this model is based on emissions data found in over 32 flooring materials (Wilke et al., 2004), including a natural and synthetic floor coverings, and adhesives. A linear regression yielded R² - and p- values of approximately 0.3 and 2.0E-12, respectively, with logP and vapor pressure being the most significant predictors for y_o . An indoor exposure prediction model (Little et al., 2012) was subsequently utilized in order to evaluate the robustness of the y_o predictor for chemicals lacking analytical data. For a given SVOC, exposure calculations depend on y_o and the surface area of its source material. In order to evaluate the indoor exposure model, high-throughput exposure predictions in were then compared with available oral equivalence values calculated from ToxCast high throughput screening assay data, available for 271 chemicals. Results show that both the y_o and indoor exposure models tend to over-predict their respective values. Future work using Monte Carlo based uncertainty analyses and chemical domain of applicability testing are being pursued to better calibrate the model and reduce uncertainty. This abstract does not necessarily reflect EPA policy.

PS 497 A High-Throughput Exposure Estimation Tool Incorporating ADME Processes

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EPA's Chemical Safety for Sustainability (CSS) research program has been developing new ways to prioritize chemicals used in consumer products and articles. Prioritization is being addressed from both a toxicity potential (i.e. ToxCast) and exposure potential (i.e. ExpoCast) standpoint. Combining these approaches will form the basis for improved methods for risk-based prioritization of chemicals found in consumer products and articles. The ultimate objective is to identify potentially problematic chemicals before they reach the marketplace or are used as ingredients in products wherein their use would lead to undesirable exposures. Currently, screening-level models, such as the Exposure & Fate Assessment Screening Tool (E-FAST) and the Stochastic Human Exposure and Dose Simulation-High Throughput (SHEDS-HT) model, are used to screen near-field chemical exposures across exposure pathways (inhalation, skin contact, dietary and non-dietary ingestion) for differing exposure scenarios. Model evaluation via comparison with biomonitoring data, however, requires information on absorption and clearance from the body (i.e., metabolic biotransformation). This tool allows for the incorporation of the pharmacokinetics that occur after chemical uptake in the body to estimate internalized dose allowing for better comparison of toxicity and exposure estimates. This is accomplished by incorporating robust methods for

route- and chemical-specific dose predictions considering absorption, distribution, metabolism, and excretion (ADME). The tool considers exposures from consumer products and articles accounting for product formulation and use; physical-chemical properties, such as partitioning coefficients; and user demographic information, exposure factors, activity patterns, and use profiles. The tool indicates products likely to be in specific microenvironments, along with the ways people contact chemicals in these products and articles, allowing better screening and ranking of exposure in a high throughput environment.

PS 498 Development of a Computational Model Describing and Extrapolating Salivary Acinar Cell *In Vitro* Pesticide Transport

C. Timchalk, T. J. Weber and J. N. Smith. Pacific Northwest National Laboratory, Richland, WA.

The use of saliva as a biomonitoring matrix has potential to significantly advance quantitative dosimetry as an integral component of epidemiology. A major limitation has been an inability to predict which chemicals are readily cleared in saliva at levels that can be quantified from occupationally relevant exposure levels. In order to predict clearance, an *in vitro* mechanistic cellular computational model of salivary pesticide transport has been developed and will enable extrapolation of experimental results obtained from *in vitro* cell based systems to humans. This mechanistic cellular transport model has been developed describing basolateral, cellular, and apical compartments. Pesticides are distributed among these compartments by diffusion and active uptake and efflux by cells. The model was coded in acslX using ordinary differential equations. The model was parameterized with a kinetic (0, 1, 2, and 3 hr, 40 µg/mL) experiment and validated with a dose-dependent (9, 18, and 36 µg/mL, 4 hr) experiment using chlorpyrifos as an initial test pesticide in a Transwell *in vitro* rat salivary acinar cell system. The resulting model simulations fit the data reasonably well, and fit parameters suggest that chlorpyrifos is transported across basolateral and apical cell membranes by passive diffusion. Diffusion coefficients were consistent across chlorpyrifos concentrations tested, suggesting no dose-dependent differences in transport at concentrations tested. Mechanistic parameters from this model will be integrated into pharmacokinetic models to identify ideal chemical candidates for saliva biomonitoring. This experimental and modeling strategy will be further used to evaluate a broader range of pesticides with varying physical and chemical properties. Once established, this approach can be exploited for biomonitoring without the need to conduct more challenging *in vivo* saliva clearance studies.

PS 499 Development of an *In Vitro* Screening Assay for Noninvasive Biomonitoring

T. J. Weber, J. N. Smith and C. Timchalk. Health Impacts and Exposure Science, Pacific Northwest National Laboratory, Richland, WA.

The use of saliva as a biomonitoring matrix has the potential to significantly advance quantitative dosimetry as an integral component of epidemiology. A major limitation has been an inability to identify which chemicals are readily cleared in saliva, at levels that can be quantified. To address this limitation, we have undertaken efforts to develop a primary salivary gland epithelial cell model that can be used for chemical transport studies *in vitro*. Western blot analysis detected expression of alpha amylase and aquaporin 5 protein, suggesting that primary cells were acinar in origin. Cells strongly expressed the tight junction protein ZO-1 at points of cell-cell contact. A time-dependent increase in tight junction formation was confirmed by monitoring transepithelial electrical resistance (routinely reached > 2500 Ω/cm²). When resistance values were > 2000 Ω/cm², lucifer yellow transport from apical to basolateral chambers was approximately 0.1%/hr (acceptable standards are < 2%/hr). These data demonstrate excellent tight junction formation. We have demonstrated that the insecticide chlorpyrifos can be quantified in saliva at concentrations that are less than but parallel blood levels. Results from the Transwell assay using primary salivary gland epithelial cells indicate that chlorpyrifos transports by diffusion with transport rates that are linear among doses tested. Lucifer yellow was included in transport studies and was clearly disproportional to chlorpyrifos transport. These experiments establish the feasibility of utilizing an *in vitro* cell based uptake/clearance assay coupled with pharmacokinetic modeling as a novel chemical screening strategy to identify ideal chemical candidates for saliva biomonitoring. This approach will be further evaluated using a broader range of pesticides with varying physical and chemical properties. Once established this approach can be exploited for biomonitoring. Supported by CDC/NIOSH grant R01 OH008173.

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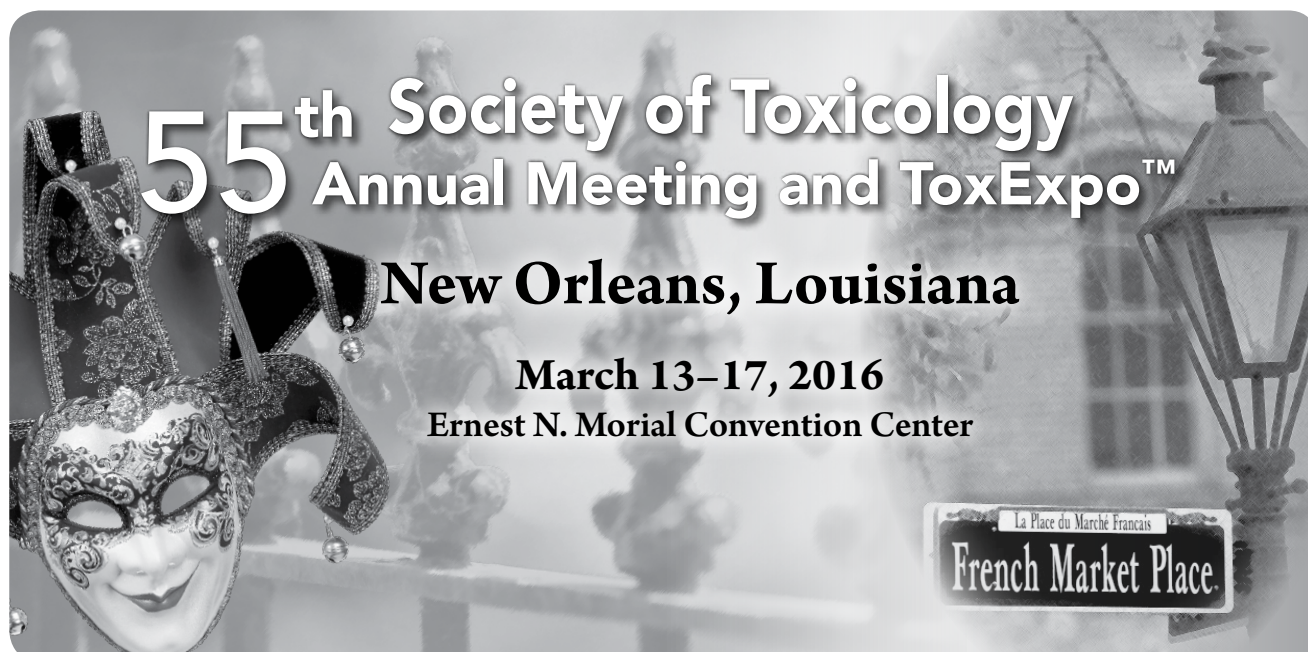
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Preface

This issue is devoted to the abstracts of the presentations for the Continuing Education courses and scientific sessions of the 54th Annual Meeting of the Society of Toxicology, held at the San Diego Convention Center, March 22–26, 2015.

An alphabetical Author Index, cross referencing the corresponding abstract number(s), begins on page 529.

The issue also contains a Keyword Index (by subject or chemical) of all the presentations, beginning on page 553.

The abstracts are reproduced as accepted by the Scientific Program Committee of the Society of Toxicology and appear in numerical sequence.

Scientific Session Types:

EC Education-Career
Development Sessions

FS Featured Sessions

IS Informational Sessions

PL Platform Sessions

PS Poster Sessions

RI Regional Interest Session

R Roundtable Sessions

S Symposium Sessions

W Workshop Sessions

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