Systems Biology-Informed Risk Assessment
Suggested Background Reading and Additional Information

June 14-15, 2012
Washington, DC

This is a list of suggested background material gathered by the meeting planning group and invited participants. Items deemed most important by the staff are asterisked.

General

* National Research Council. *Toxicity Testing in the 21st Century: A Vision and a Strategy*. Washington, DC: The National Academies Press, 2007.
http://www.nap.edu/catalog.php?record_id=11970

Kim Boekelheide

* Bhattacharya S, Zhang Q, et al. (June 2011) Toxicity testing in the 21st century: defining new risk assessment approaches based on perturbation of intracellular toxicity pathways. PLoS ONE Vol. 6(6) pp. 1-11
http://www.plosone.org/article/info:doi%2F10.1371%2Fjournal.pone.0020887

Ila Cote

*Environmental Protection Agency. (2011) Advancing the next generation of risk assessment: a NexGen program synopsis. www.epa.gov/risk/nexgen/docs/NexGen-Program-Synopsis.pdf

*Environmental Protection Agency (2011) Advancing the next generation (NexGen) of Risk Assessment: Public Dialogue Conference (Summary Report)
http://www.epa.gov/ncea/risk/nexgen/docs/NexGen-Public-Conf-Summary.pdf

* Barabasi Albert-Laszlo, Gulbahce Natali, Loscalzo Joseph. (2011 January) Network medicine: a network-based approach to human disease. Nat Rev Genet; 12(1): 56-68. Doi:10.1038/nrg2918
http://www.barabasilab.com/pubs/CCNR-ALB_Publications/201012-18_NatureRev-NetMedicine/201012-18_NatureRev-NetMedicine.pdf

Benzene-Related

*Smith MT, Zhang L, et al. (2011) Benzene, the exposome and future investigations of leukemia etiology. Chemico-Biological Interactions Vol. 192 pp. 155-159
http://superfund.berkeley.edu/pdf/353.pdf

*McHale CM, Zhang L, Smith MT. (2012 Feb) Current understanding of the mechanism of benzene-induced leukemia in humans: implications for risk assessment. Carcinogenesis; 33(2): 240-52. Epub 2011 Dec 12. http://www.ncbi.nlm.nih.gov/pubmed/22166497

McHale CM, Zhang L, Lan Q, et al. (2011 May) Global gene expression profiling of a population exposed to a range of benzene levels. Environmental Health Perspective; 119(5): 628-34. Epub 2012 Dec 13
http://ehp03.niehs.nih.gov/article/info%3Adoi%2F10.1289%2Fehp.1002546

Dean Jones

Jones DP, Park Y, Ziegler TR. (2012 April 23). Nutritional metabolomics: progress in addressing complexity in diet and health, Annual Reviews Nutr 32, in press
(This review outlines a general approach to operationalize the exposome and puts biomonitoring of environmental chemicals in the context of the broader metabolic profiling of nutritional and dietary metabolome, the metabolome related to the microbiome, and the pharmaceutical metabolome.) http://www.annualreviews.org/doi/abs/10.1146/annurev-nutr-072610-145159

* Park YP, Lee K, Soltow QA, Strobel FH, Brigham KL, Parker RE, Wilson ME, Sutliff RL, Mansfield KG, Wachtman LM, Ziegler TR, Jones DP (2012 May 16) High-performance metabolic profiling of plasma from seven mammalian species for simultaneous environmental chemical surveillance and bioeffect monitoring. Toxicology; 295(1-3): pp. 47-55.
(This study shows that high-resolution metabolomics can provide both chemical and bioeffect monitoring. The study also shows that some of the environmental chemicals found in humans are also found in laboratory animals.)
http://www.sciencedirect.com/science/article/pii/S0300483X12000492

Roede JR, Park Y, Li S, Strobel FH, Jones DP. 2012. Detailed mitochondrial phenotyping by high resolution metabolomics. PLoS ONE 2012; 7(3): e33020 PMCID: PMC3295783
(This study shows that environmental agents are present in mitochondria of laboratory animals.)
http://www.plosone.org/article/info%3Adoi%2F10.1371%2Fjournal.pone.0033020

Soltow QA, Strobel FH, Mansfield KG, Wachtman L, Park Y, Jones DP (2011) High-performance metabolic profiling with dual chromatography-Fourier-transform mass spectrometry (DC-FTMS) for study of the exposome, Metabolomics, in press DOI: 10.1007/s11306-011-0332-1.
(This is a methods paper that includes measurement of environmental chemicals in a non-targeted platform. With new data extraction algorithms, >40,000 ions are detected by this method)
http://www.springerlink.com/content/97064253x0x3h17m/fulltext.pdf

Derek Knight

http://echa.europa.eu/ for information about the European Chemicals Agency.

http://www.seurat-1.eu/ for information about SEURAT-1. SEURAT-1 (Safety Evaluation Ultimately Replacing Animal Testing) will develop knowledge and technology building blocks required for the development of solutions for the replacement of current repeated dose systemic toxicity testing *in vivo* used for the assessment of human safety. The SEURAT-1 Research

Initiative is composed of six research projects, which started on 1 January 2011 and will run for five years. These projects will closely cooperate with a common goal and combine the research efforts of over 70 European universities, public research institutes and companies.

http://axlr8.eu/ for information about AXLR*. "AXLR8 is a coordination action funded by the European Commission Directorate General for Research & Innovation (Health Directorate; Advanced Therapies and Systems Medicine Unit) under the 7th European RTD Framework Programme Health Theme. AXLR8 will provide tools and opportunities for increased networking, information exchange, problem solving, strategic planning and collaboration among a variety of scientific disciplines and stakeholder groups with the goal to accelerate the transition to a toxicity pathway-based paradigm for chemical safety assessment. AXLR8 will act as a focal point for coordination among 3Rs research projects in Europe as well as internationally."

http://ihcp.jrc.ec.europa.eu/ for information about the Joint Research Centre Institute for Health and Consumer Protection.

Greg Paoli

* *Chapter 3 "The Design of Risk Assessments" pp. 65-92* of National Research Council. *Science and Decisions: Advancing Risk Assessment*. Washington, DC: The National Academies Press, 2009. http://www.nap.edu/openbook.php?record_id=12209&page=65

*Yokota F, Gray G, Hammitt JK, Thompson KM. Tiered chemical testing: A value of information approach. Risk Analysis 2004;24(6):1625-1639. http://onlinelibrary.wiley.com/doi/10.1111/j.0272-4332.2004.00555.x/pdf

Yokota F, Thompson KM. Value of information (VOI) analysis in environmental health risk management (EHRM). Risk Analysis 2004;24(3):635-650. http://onlinelibrary.wiley.com/doi/10.1111/j.0272-4332.2004.00464.x/pdf

Maurice Whelan

Andersen ME, Clewell HJ, Frederick CB. (1995) Contemporary Issues in Toxicology: Applying simulation modeling to problems in toxicology and risk assessment—a short perspective. Toxicology and Applied Pharmacology; Vol. 133(2), pp.181-187 http://www.ncbi.nlm.nih.gov/pubmed/7645013

James E. Bailey, "Mathematical Modeling and Analysis in Biochemical Engineering: Past Accomplishments and Future Opportunities", Biotechnology Progress (1998) http://onlinelibrary.wiley.com/doi/10.1021/bp9701269/abstract

*Organisation for Economic Co-operation and Development. (2012) Proposal for a template, and guidance on developing and assessing the completeness of adverse outcome pathways http://www.oecd.org/dataoecd/50/39/49963554.pdf

*Organisation for Economic Co-operation and Development. (2012) Draft: Collection of Working Definitions. http://www.oecd.org/dataoecd/50/38/49963576.pdf

Daniel Krewski

*Sand S, Portier, CJ, Krewski D. (2011 Dec) A signal-to-noise crossover dose as the point of departure for health risk assessment. Environmental Health Perspective; 119(12): 1766-74. Epub 2011 Aug 3. http://ehp03.niehs.nih.gov/article/fetchArticle.action?articleURI=info%3Adoi%2F10.1289%2Fehp.1003327

*Krewski D, Westphal M, et al. (2011 April) New directions in toxicity testing. Annuarl Review of Public Health; 32: 161-78. http://papers.ssrn.com/sol3/papers.cfm?abstract_id=1810219

John Quackenbush

Culhane AC, Schroder MS, Sultana R, Picard SC, Martinelli EN, Kelly C, et al. GeneSigDB: a manually curated database and resource for analysis of gene expression signatures. Nucleic acids research. 2012;40(Database issue):D1060-6. Epub 2011/11/24. doi: 10.1093/nar/gkr901. PubMed PMID: 22110038; PubMed Central PMCID: PMC3245038. http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3245038/?tool=pubmed

Haibe-Kains B, Olsen C, Djebbari A, Bontempi G, Correll M, Bouton C, et al. Predictive networks: a flexible, open source, web application for integration and analysis of human gene networks. Nucleic acids research. 2012;40(Database issue):D866-75. Epub 2011/11/19. doi: 10.1093/nar/gkr1050. PubMed PMID: 22096235; PubMed Central PMCID: PMC3245161. http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3245161/

Mar JC, Matigian NA, Quackenbush J, Wells CA. attract: A method for identifying core pathways that define cellular phenotypes. PloS one. 2011;6(10):e25445. Epub 2011/10/25. doi: 10.1371/journal.pone.0025445. PubMed PMID: 22022396; PubMed Central PMCID: PMC3194807. http://www.plosone.org/article/info%3Adoi%2F10.1371%2Fjournal.pone.0025445

Mar JC, Wells CA, Quackenbush J. Defining an informativeness metric for clustering gene expression data. informatics. 2011;27(8):1094-100. Epub 2011/02/19. doi: 10.1093/informatics/btr074. PubMed PMID: 21330289; PubMed Central PMCID: PMC3072547. http://bioinformatics.oxfordjournals.org/content/early/2011/02/16/bioinformatics.btr074.short

McAdams HH, Shapiro L. Circuit simulation of genetic networks. Science. 1995;269(5224):650-6. PubMed PMID: 7624793. http://www.ncbi.nlm.nih.gov/pubmed/7624793

Other

*Gohlke JM and Portier CJ. (2007 September). The forest for the trees: A systems approach to human health research. Environmental Health Perspective; 115(9): 1261-1263 http://www.ncbi.nlm.nih.gov/pmc/articles/PMC1964909/

*Gohlke JM, Thomas R, Zhang Y, et al. (2009 May 5) Genetic and environmental pathways to complex diseases. BMC Systems Biology; 3:46 doi: 10.1186/1752-0509-3-46 http://www.biomedcentral.com/content/pdf/1752-0509-3-46.pdf

*Judson RS, Kavlock RJ, Setzer RW, et al. (2011 April 18) Estimating toxicity-related biological pathway altering doses for high-throughput chemical risk assessment. Chem Res Toxicol; 24(4): 451-62. Epub 2011 Mar 8. http://pubs.acs.org/doi/abs/10.1021/tx100428e

Parham F, Austin C, et al. (2009 December) Dose-response modeling of high-throughput screening data. J Biomol Screen; 14(10):1216-27. http://www.ncbi.nlm.nih.gov/pubmed/19828774

Thomas R, Gohlke JM, Stopper GF, et al. (2009) Choosing the right path: enhancement of biologically relevant sets of genes or proteins using pathway structure. Genome Biology; 10(4): R44. Epub 2009 Apr 24 http://genomebiology.com/2009/10/4/R44

Basketter, DA, Clewell H, et al. (2012) A roadmap for the development of alternative (non-animal) methods for systematic toxicity testing. ALTEX; 29(1): 3-91 http://www.ncbi.nlm.nih.gov/pubmed/22307314