

Applying 21st Century Toxicology to Green Chemical and Material Design

September 20-21, 2011

Washington, DC 20001

Suggested Reading and Related Links

Session 1

DeVito S and R. Garrett, Designing Safer Chemicals: Green Chemistry for Pollution Prevention, American Chemical Society, Washington. D.C.,1996.

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Sanderson, Katharine. Chemistry: It's not easy being green. Nature Vol 469. 6 January 2011.

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Schwarzman MR, Wilson MP. New Science for Chemicals Policy. Science Vol 326(5956) pp. 1065-1066. 20 November 2009.

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Session 2

Bus JS and Becker RA. Toxicity testing in the 21st century: A view from the chemical industry.

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Carney EW, Ellis AL, et al. Critical evaluation of current developmental toxicity testing strategies; a case of babies and their bathwater. Birth Defects Research Part B: Developmental and Reproductive Toxicology. 18 July 2011.

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Dahl JA, Maddux BL, Hutchison, JE. Toward Greener Nanosynthesis. Chemical Reviews Vol 107 pp. 2228-2269. 13 June 2007

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Greene N, Aleo MD, et al. Using an in vitro cytotoxicity assay to aid in compound selection for in vivo safety studies. Bioorganic & Medicinal Chemistry Letters Vol 20(17) pp. 5308-5312 1 September 2010

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<http://www.ncbi.nlm.nih.gov/pubmed/20553011>

Greene N and Naven R. Early Toxicity Screening Strategies. *Current Opinion Drug Discovery & Development* Vol 12(1) pp. 90-97. January 2009
<http://www.ncbi.nlm.nih.gov/pubmed/19152217>

Harper SL, Hutchison JE, Tanguay RL, et al. Systematic Evaluation of Nanomaterial Toxicity: Utility of Standardized Materials and Rapid Assays. *ACS Nano* Vol 5(6) pp. 4688-4697. 28 June 2011
<http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3124923/?tool=pubmed>

Hutchison JE. Greener Nanoscience: A Proactive Approach to Advancing Applications and Reducing Implications of Nanotechnology. *ACS Nano* Vol 2(3) pp.395-402. March 2008
<http://www.ncbi.nlm.nih.gov/pubmed/19206562> (abstract link)

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<http://www.ncbi.nlm.nih.gov/pubmed/18691886>

Judson RS, Huock KA, et al. *In Vitro* Screening of Environmental Chemicals for Targeted Testing Prioritization: The ToxCast Project. *Environmental Health Perspectives* Vol 118(4) pp. 485-492. April 2010
<http://ehp03.niehs.nih.gov/article/info:doi/10.1289/ehp.0901392>

Judson RS, Martin MT, et al. Analysis of Eight Oil Spill Dispersants Using Rapid, In Vitro Tests for Endocrine and Other Biological Activity. *Environmental Science & Technology* Vol 44(15) pp. 5679-5985. 1 August 2010
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<http://ehp03.niehs.nih.gov/article/fetchArticle.action?articleURI=info%3Adoi%2F10.1289%2Fehp.1002180>

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Sedykh A, Zhu H, et al. Use of *in Vitro* HTS-derived concentration-response data as biological descriptors improves the accuracy of QSAR Models of *in Vivo* Toxicity. *Environmental Health Perspectives* Vol 119(3) pp. 364-370 March 2011
<http://ehp03.niehs.nih.gov/article/info:doi/10.1289/ehp.1002476>

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Session 3

Adler S, Basketter D, Creton S, et al. Alternative (non-animal) methods for cosmetics testing: current status and future prospects – 2010. *Archives of Toxicology*. Vol 85(5) pp. 367-485. 1 May 2011

http://ihcp.jrc.ec.europa.eu/our_activities/alt-animal-testing/report_2010/fulltext.pdf

ASTM International. Standard Guide for Assessing the Environmental and Human Health Impacts of New Energetic Compounds. ASTM Designation: E 2552 – 08

<http://www.astm.org/Standards/E2552.htm>

Boobis AR, Cohen SM, Dellarco V, et al. IPCS framework for analyzing the relevance of a cancer mode of action for humans. *Critical Reviews in Toxicology*. Vol 36(10) pp. 781-792. Nov-Dec. 2006

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Daginnus K, Gottardo S, et al. A model-based prioritization exercise for the European water framework directive. *International Journal of Environmental Legislation and Public Health*. Vol 8(2) pp. 435-455. 1 February 2011.

(Computational Modelling)

<http://www.mdpi.com/1660-4601/8/2/435/pdf>

European Commission: REACH Annex IV criteria defining absence of "significant toxicological effects"

(see section 2.2) http://ec.europa.eu/environment/chemicals/reach/pdf/4_Criteria%20Annex%20IV.pdf

European Commission Staff Working Paper. 4th Report on the implementation of the "Community Strategy for Endocrine Disrupters" a range of substances suspected of interfering with the hormone systems of humans and wildlife (COM (1999) 706). August 2011

(Endocrine Disrupters)

http://ec.europa.eu/environment/endocrine/documents/sec_2011_1001_en.pdf

Evans R, Kortenkamp A, et al. 2nd Interim report: (Part 1) State of the Science Assessment of Endocrine Disrupters

(Endocrine Disrupters)

http://ec.europa.eu/environment/endocrine/documents/summary_state_science.pdf

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Johnson Mark S, Cao Cheng J. Assessment of ESOH Impacts In Munitions Research, Development, Testing And Evaluation: Integration Of In Vitro Techniques Into A Phased Approach. Health Effects Research Program; Army Center for Health Promotion and Preventive Medicine

Johnson MS, Ruppert WH, et al. Assessing the Potential Environmental Consequences of a New Energetic Material: A Phased Approach. U.S. Army Center for Health Promotion and Preventative Medicine. December 2007

<http://www.dtic.mil/cgi-bin/GetTRDoc?Location=U2&doc=GetTRDoc.pdf&AD=ADA485448>

Paules RS, Aubrecht J, Corvi R, et al. Moving forward in human cancer risk assessment. Environmental Health Perspectives Vol 119(16). June 2011

(Toxicogenomics)

<http://ehp03.niehs.nih.gov/article/info%3Adoi%2F10.1289%2Fehp.1002735>

Workshop on Computational Chemistry and Systems Biology "Harnessing the Chemistry of Life: Revolutionising Toxicology" 5-7 July 2010.

(Computational Modelling)

http://ec.europa.eu/enterprise/epaa/2_activities/2_1_science/ws_comp_chem_final.pdf

Worth A, Lapenna S, et al. A Framework for assessing in silico Toxicity Predictions: Case Studies with selected Pesticides. JRC Scientific and Technical Reports. 2011.

(Computational Modelling)

<http://publications.jrc.ec.europa.eu/repository/bitstream/111111111/15717/1/lbna24705enc.pdf>

Related Links

CHEMBENCH <http://chembench.mml.unc.edu/>

Computational models predict nanoparticle toxicity. (Computational Modelling)

http://ihcp.jrc.ec.europa.eu/our_labs/computational_toxicology/computational-models-predict-nanoparticle-toxicity

EPA ToxCast: Screening Chemicals to Predict Toxicity Faster and Better

<http://www.epa.gov/ncct/toxcast/>

EPA Design for the Environment <http://www.epa.gov/dfe/index.htm>

Prospects for the use of computational methods in the toxicological assessment of chemicals in food.

(Computational Modelling)

http://ihcp.jrc.ec.europa.eu/our_activities/cons-prod-nutrition/computational-methods-toxicological-assessment-of-chemicals-in-food

Public consultation on the preliminary opinion concerning Toxicity and Assessment of Chemical Mixtures (Assessment of Chemical Mixtures)

http://ec.europa.eu/health/scientific_committees/consultations/public_consultations/scher_consultation_06_en.htm

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REACH Guidance on ITS and use of QSARs (2008)

http://guidance.echa.europa.eu/docs/guidance_document/information_requirements_en.htm

SEURAT-1. "Safety Evaluation Ultimately Replacing Animal Testing (SEURAT)". An EU FP-7 Research Initiative composed of six research projects, which started on 1 January 2011 and will run for five years. These projects closely cooperate with a common goal and combine the research efforts of over 70 European universities, public research institutes and companies. (Development of Alternative (non-animal) methods) <http://www.seurat-1.eu/>

The Use of Alternatives to Testing on Animals for the REACH Regulation 2011.

http://echa.europa.eu/publications/alternatives_test_animals_2011_en.asp

UN Globally Harmonized System of Classification and Labelling of Chemicals

http://live.unece.org/trans/danger/publi/ghs/ghs_rev03/03files_e.html