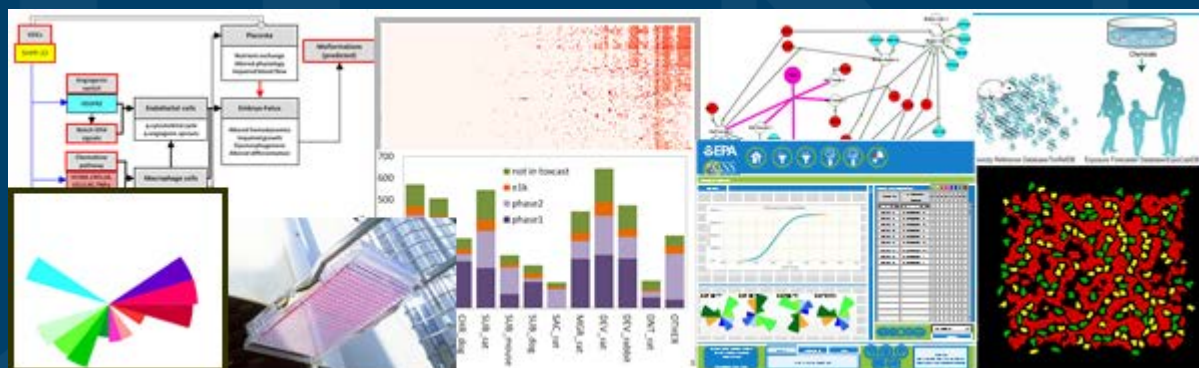


Overview of the CompTox Research Effort



ECHO Seminar
April 21, 2017

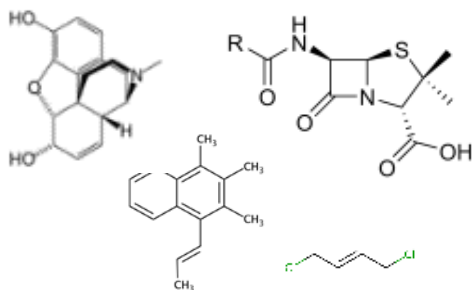
Russell Thomas
Director
National Center for Computational Toxicology

Outline

- Short overview of CompTox research effort
- Availability of research data
- Potential application to prioritizing for exposure monitoring

Understanding 'Why' We Need to Innovate In This Space...

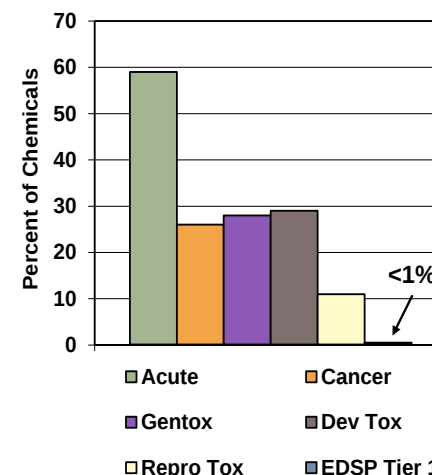
Number of Chemicals /Combinations



Ethics Concerns

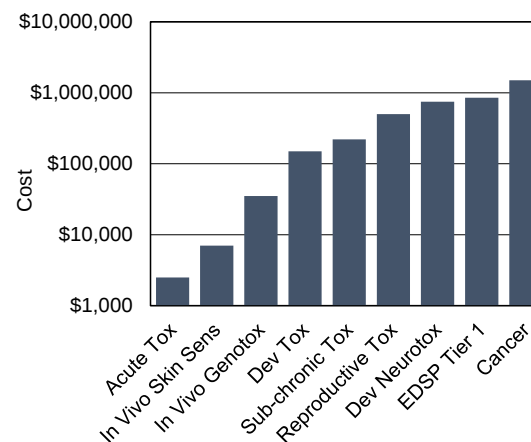


Lack of Data



Modified from Judson *et al.*, EHP 2010

Economics



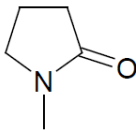
Risk Assessments Generally Contain a Standard Set of Components

EPA United States Environmental Protection Agency
EPA Document# 740-R1-5002 March 2015
Office of Chemical Safety and Pollution Prevention

TSCA Work Plan Chemical Risk Assessment

**N-Methylpyrrolidone:
Paint Stripper Use**

CASRN: 872-50-4



March 2015

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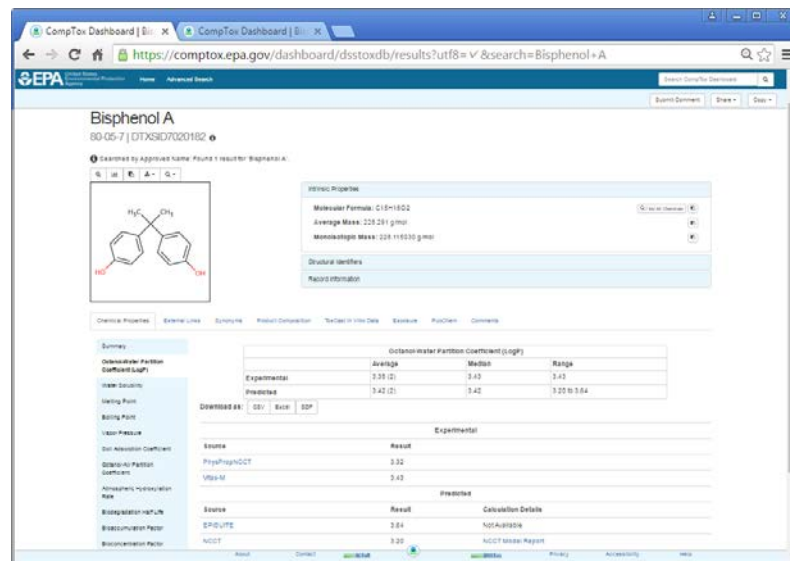
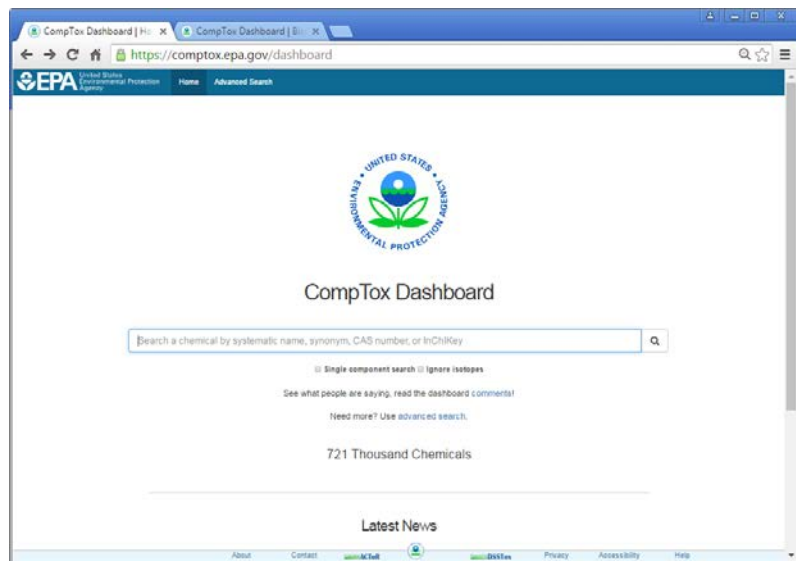
Phys Chem
Exposure
Hazard
Dose Response,
PK, and PODs

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Variability
Risk Summary
Uncertainty

New technologies and approaches will also have to cover these basic components

It All Starts With Chemistry...

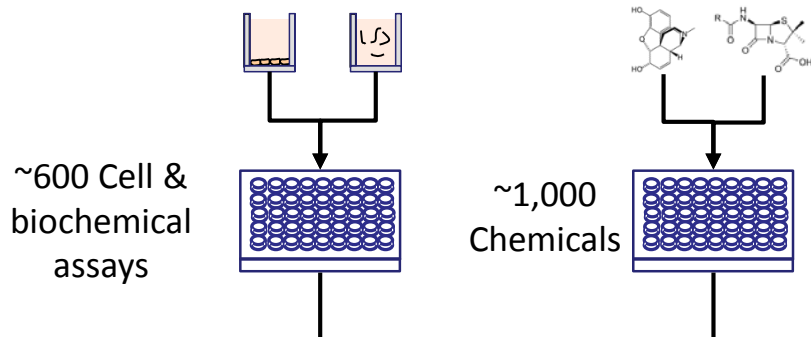


<https://comptox.epa.gov/dashboard>

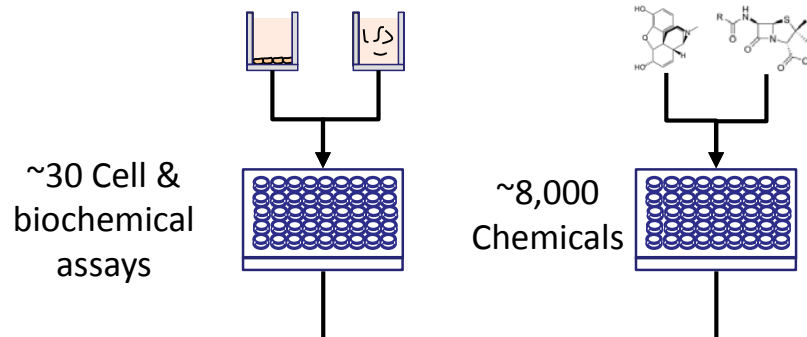
- Chemical structure database of >700,000 unique substances with QC flags to link chemical structure with names and identifiers
- Consensus QSAR models for a range of physical chemical properties, environmental fate, and hazard characteristics
- Comprehensive physical-chemical property database (experimental and predicted)

Adding the High-Throughput Hazard Screening Component

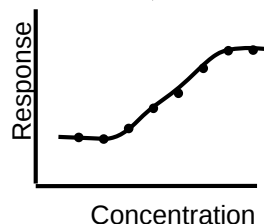
ToxCast



Tox21

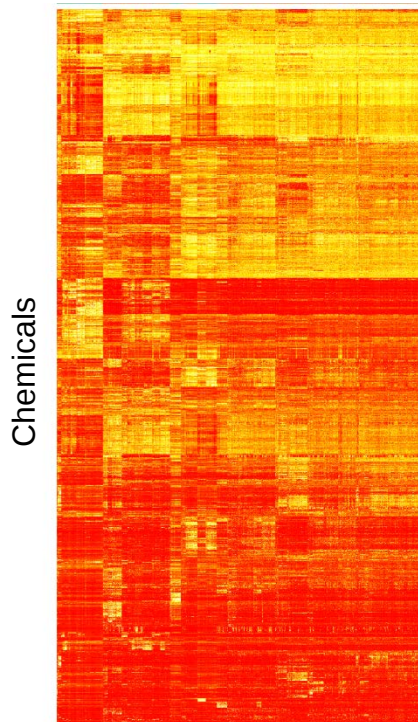


Set	Chemicals	Assays	Completion
ToxCast Phase I	293	~600	2011
ToxCast Phase II	767	~600	2013
ToxCast Phase III	1001	~100	Ongoing
E1K (endocrine)	880	~50	2013



Broad Success Derived from High-Throughput Screening Approaches

Group Chemicals by
Similar Bioactivity and
Predictive Modeling



Assays/Pathways

Provide Mechanistic
Support for Hazard ID



Carcinogenicity of perfluorooctanoic acid, tetrafluoroethylene, dichloromethane, 1,2-dichloropropane, and 1,3-propane sultone

In June, 2014, 20 experts from nine countries met at the International Agency for Research on Cancer (IARC, Lyon, France) to assess the carcinogenicity of perfluorooctanoic acid (PFOA), tetrafluoroethylene (TFE), dichloromethane (DCM), 1,2-dichloropropane (1,2-DCP), and with 1,2-DCP in this industry). The working group considered the rarity of cholangiocarcinoma, the very high relative risk, the young ages of the patients, the absence of non-occupational risk factors, and the intensity of the exposure as indications that the excess of metabolism of DCM does occur in strong evidence that DCM metabolism via glutathione-S-transferase T1 (GSTT1) leads to the formation of reactive metabolites, that GSTT1 activity is strongly associated with genotoxicity of DCM in vitro and in vivo, and that GSTT1-mediated metabolism of DCM does occur in



Carcinogenicity of tetrachlorvinphos, parathion, malathion, diazinon, and glyphosate

In March, 2015, 17 experts from 11 countries met at the International Agency for Research on Cancer (IARC, Lyon, France) to assess the carcinogenicity of the organophosphate pesticides tetrachlorvinphos, parathion, malathion, diazinon, and glyphosate (table). These assessments will be cell proliferation (hyperplasia in rodents). Tetrachlorvinphos is banned in the European Union. In the USA, it continues to be used on animals, including in pet flea collars. For parathion, associations with cancers in several tissues were observed in occupational studies. The insecticides malathion and diazinon were classified as "probably carcinogenic to humans" (Group 2A). Malathion is used in agriculture, public health, and residential insect control. It continues to be produced in substantial volumes throughout the world. There is limited evidence in

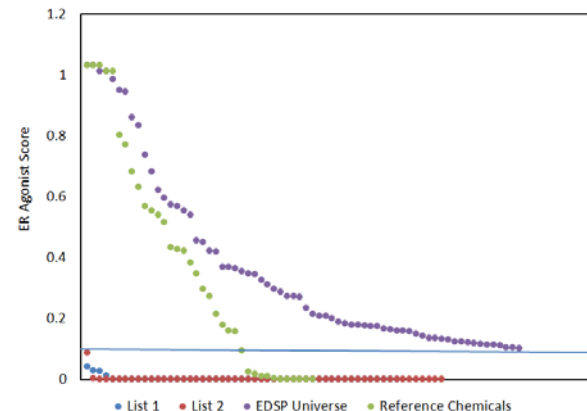


Carcinogenicity of lindane, DDT, and 2,4-dichlorophenoxyacetic acid

In June, 2015, 26 experts from 13 countries met at the International Agency for Research on Cancer (IARC, Lyon, France) to assess the carcinogenicity of the insecticides lindane and 1,1,1-trichloro-2,2-bis(4-chlorophenyl)ethane (DDT), and the herbicide 2,4-dichlorophenoxyacetic acid. Immunosuppressive effects that can operate in humans. The insecticide DDT was classified as "probably carcinogenic to humans" (Group 2A). DDT was used for the control of insect-borne diseases during World War 2; subsequently it was widely applied to eradicate blood or adipose taken in adulthood; however, the possible importance of early-life exposure to DDT remains unresolved. Studies on non-Hodgkin lymphoma and cancers of the liver and testis provided limited evidence in humans for the carcinogenicity of DDT.

IARC Monographs 110, 112, 113

Prioritization of Chemicals
for Further Testing



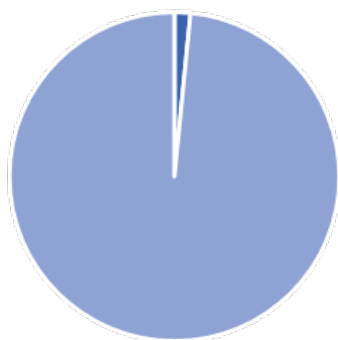
FIFRA SAP, Dec 2014

Selected Criticisms of ToxCast

- You don't include metabolism in your *in vitro* assays
- You don't measure my favorite endpoint
- You don't cover all of biological space
- *In vitro* assays are not normal biology
- Assay (x) in your battery did not get the right answer for my chemical
- My assay disagrees with your assay (x), so your approach is flawed
- You can't test my favorite chemicals because of limitations in your methods (e.g., solvents, high LogP)
- Your assay descriptions do not allow me to reproduce your results
- I get different answers when I analyze your data

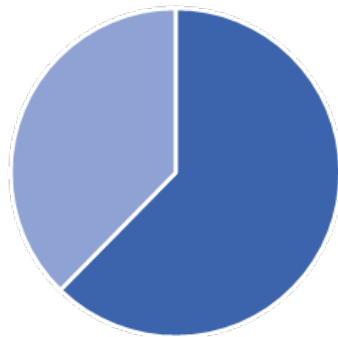
Beginning to Address Concerns for Increased Biological Coverage

Gene Coverage

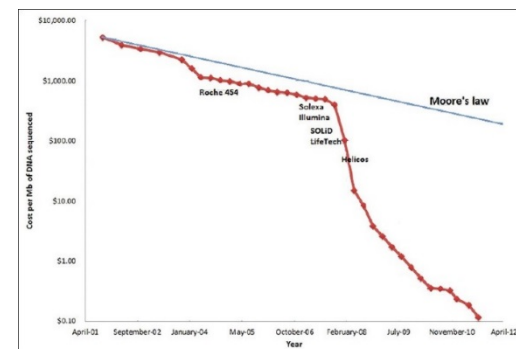


■ ToxCast
■ Not in ToxCast

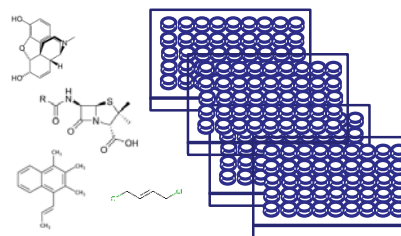
Pathway Coverage*



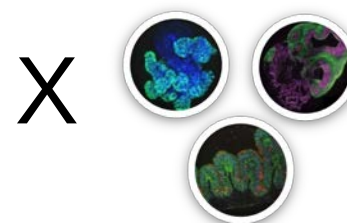
*At least one gene from pathway represented



Thousands of chemicals



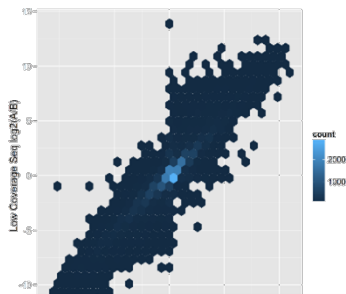
Multiple Cell Types



Requirements:

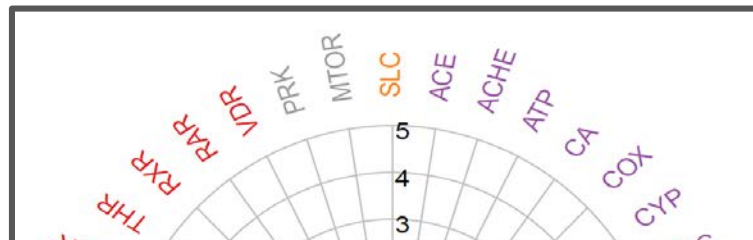
- Low cost
- Whole genome
- 384 well
- Automatable

Comparing Sequencing Platforms and Developing Analysis Approach



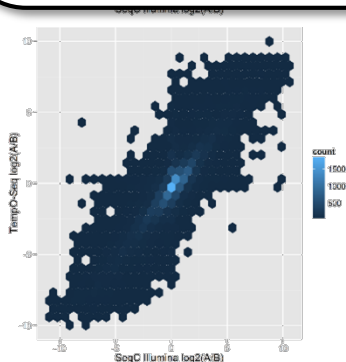
TruSeq
 r^2 0.74

MOA/MIE Analysis Pipeline



COMING SOON!

- Large scale screen of 1,000 chemicals (ToxCast I/II) in single cell type this summer
- Additional screens across multiple cell types/lines
- Additional reference chemicals and genetic perturbations (RNAi/CRISPR/cDNA)



Low Coverage
 r^2 0.83

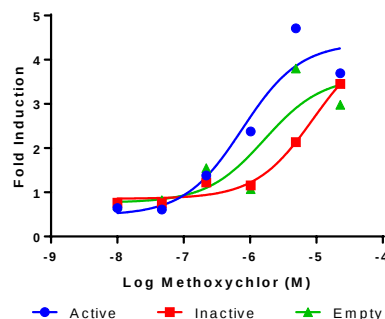


Currently capable of assigning to >40 MOAs/MIEs based on transcriptional responses

Beginning to Address Metabolic Competence

“Extracellular” Approach

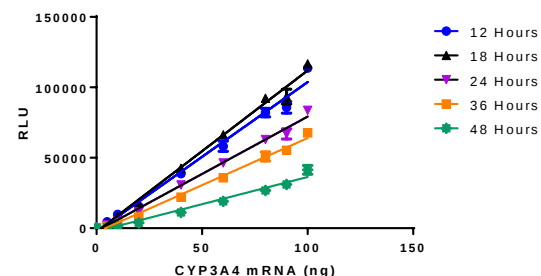
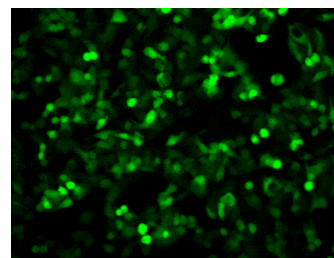
Chemicals metabolism in the media or
buffer of cell-based and cell-free assays



More closely models effects of hepatic
metabolism and generation of circulating
metabolites

“Intracellular” Approach

Capable of metabolizing chemicals
inside the cell in cell-based assays

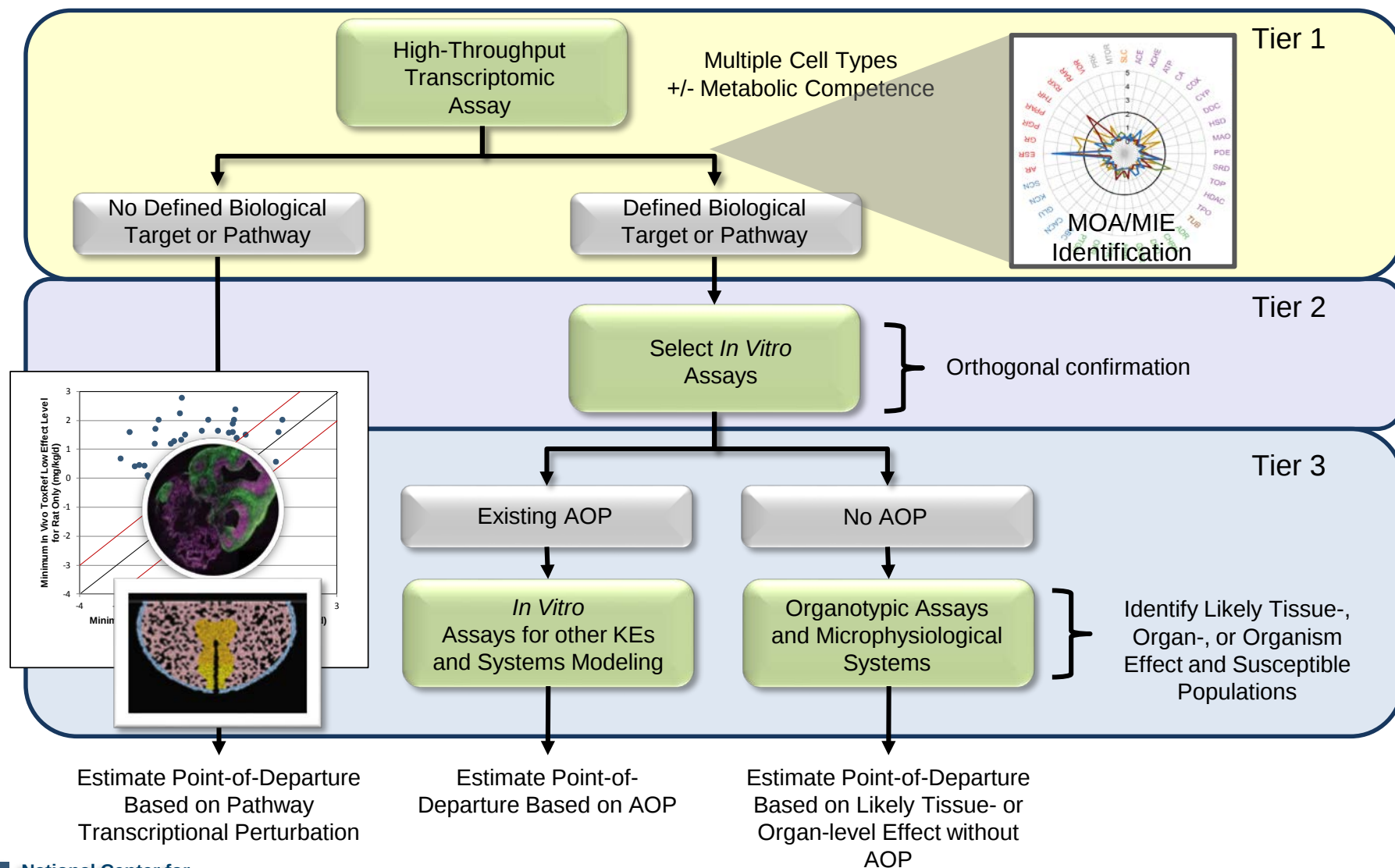


More closely models effects of target
tissue metabolism

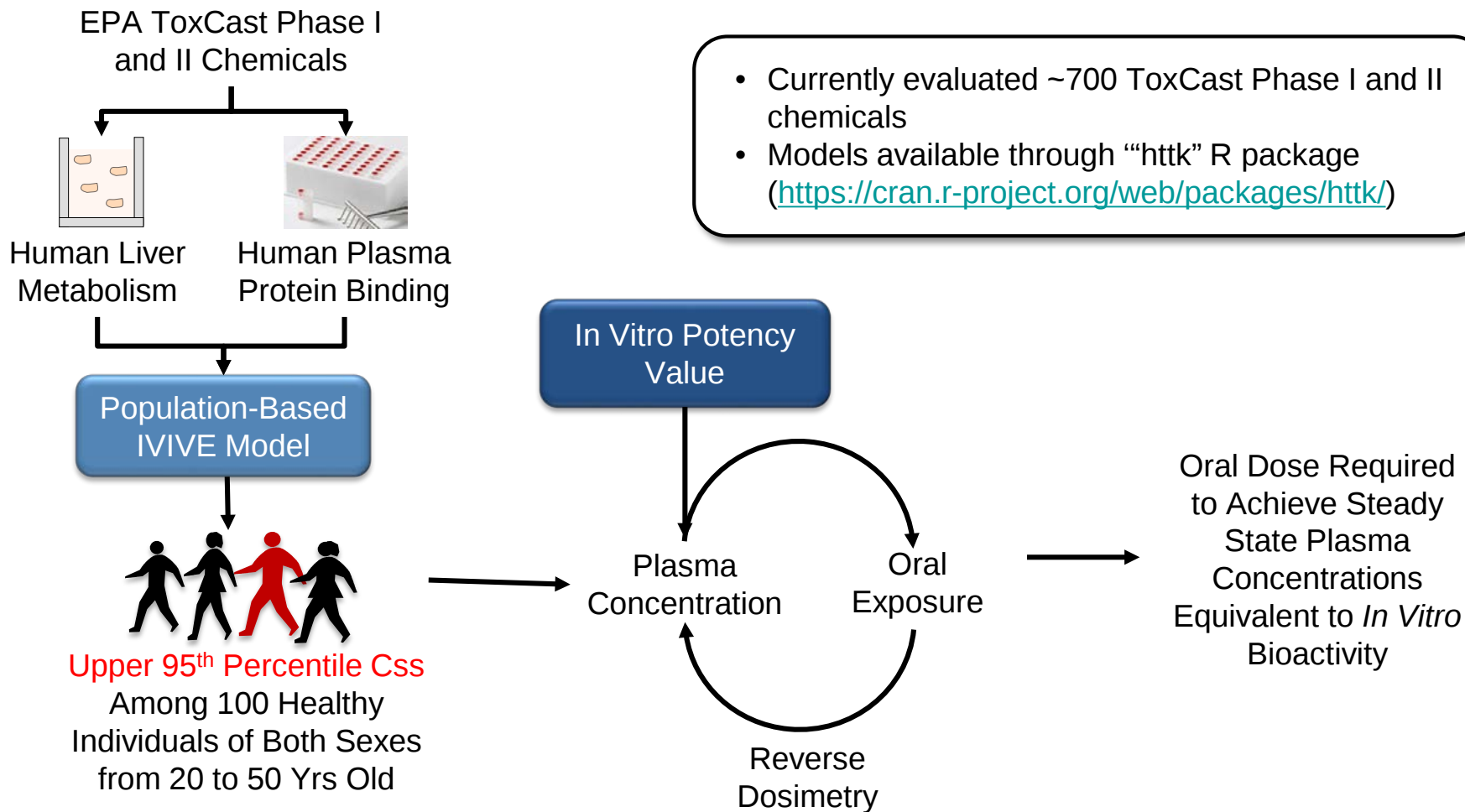
Integrated approach to model *in vivo*
metabolic bioactivation and detoxification

Collaboration with Unilever

Framework for Integrating Hazard Components...

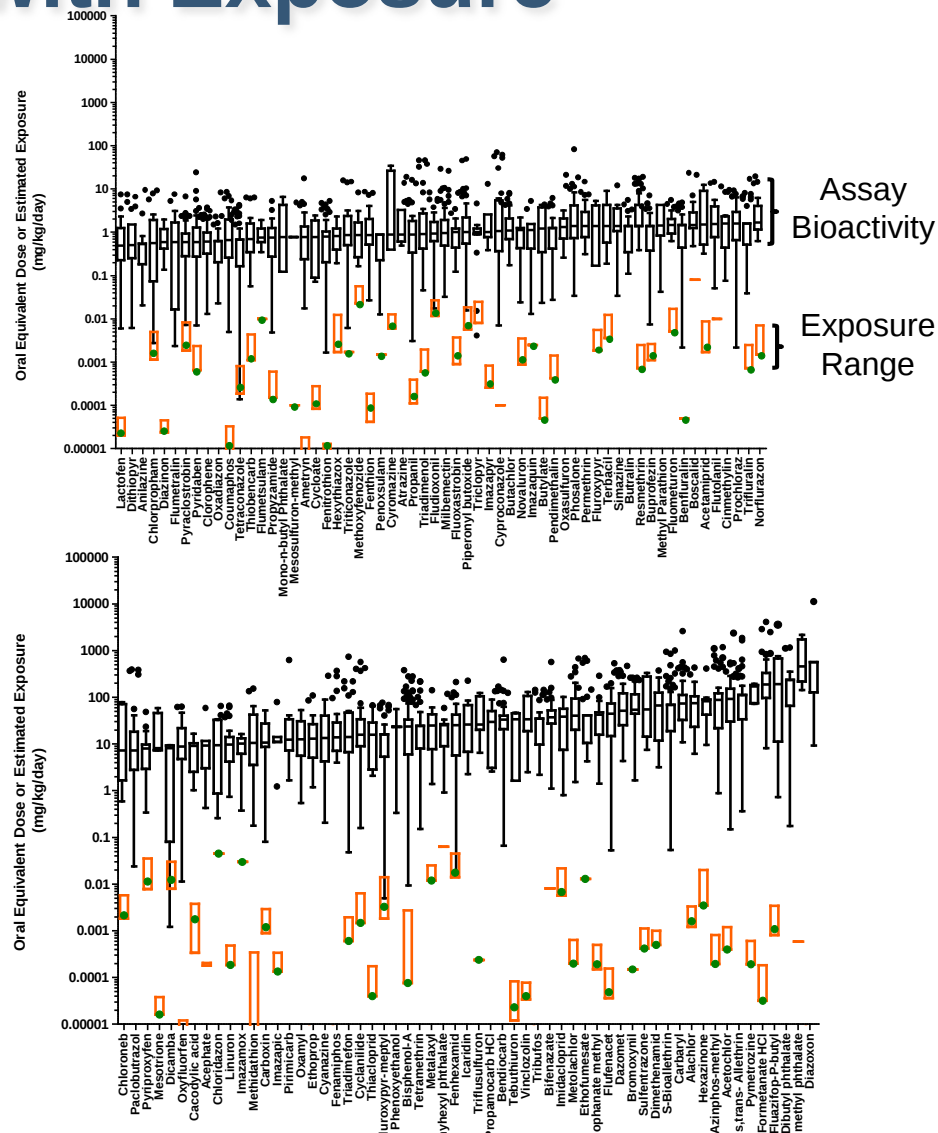
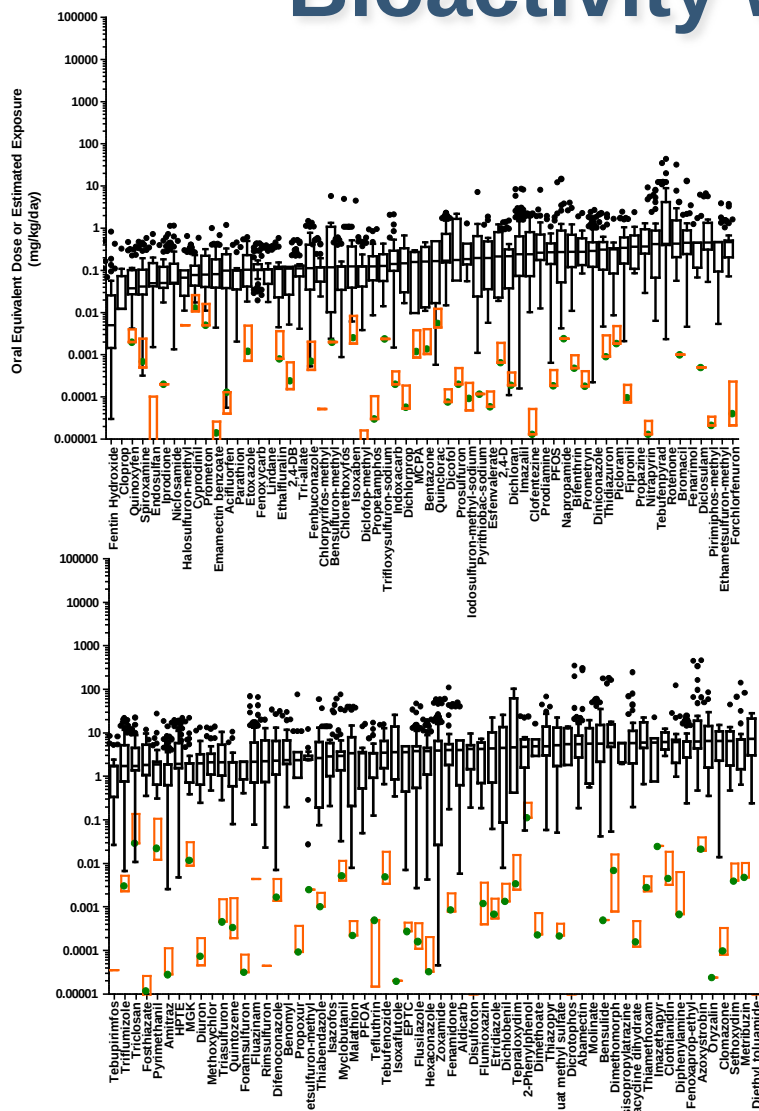


Adding the High-Throughput Toxicokinetic Component

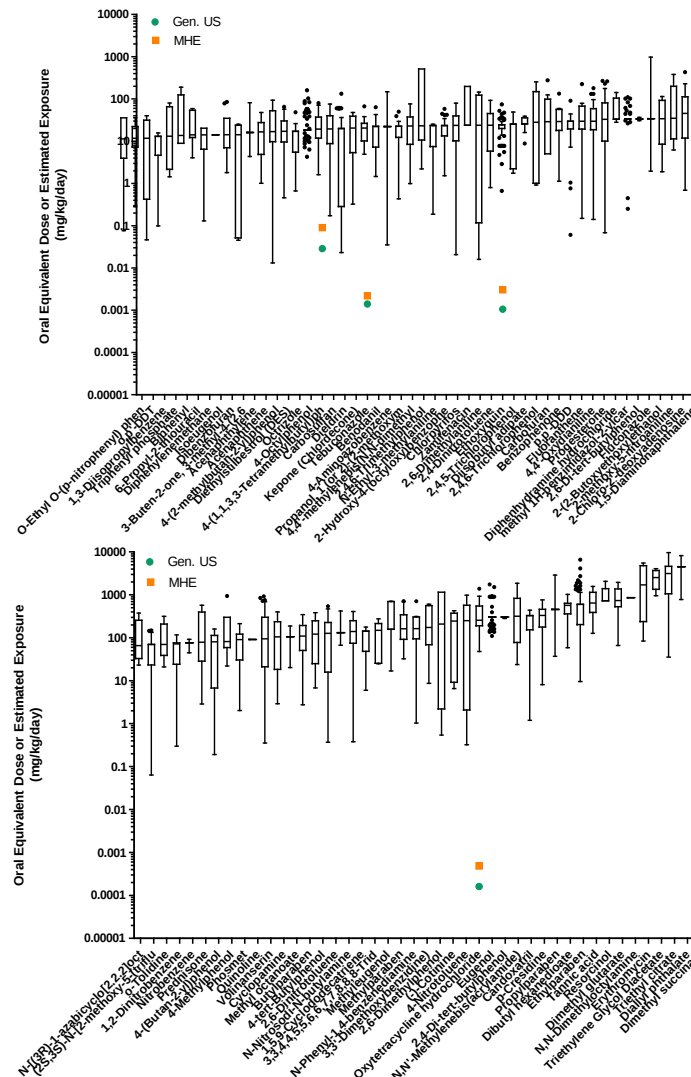
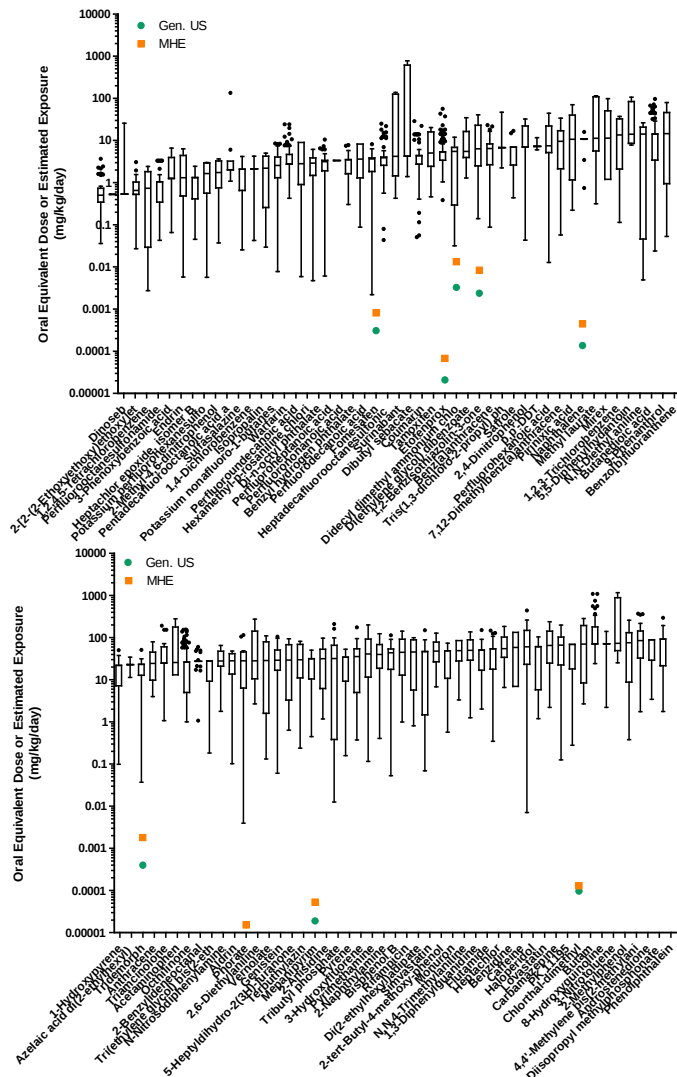


Retroff *et al.*, *Tox Sci.*, 2010
Wetmore *et al.*, *Tox Sci.*, 2012

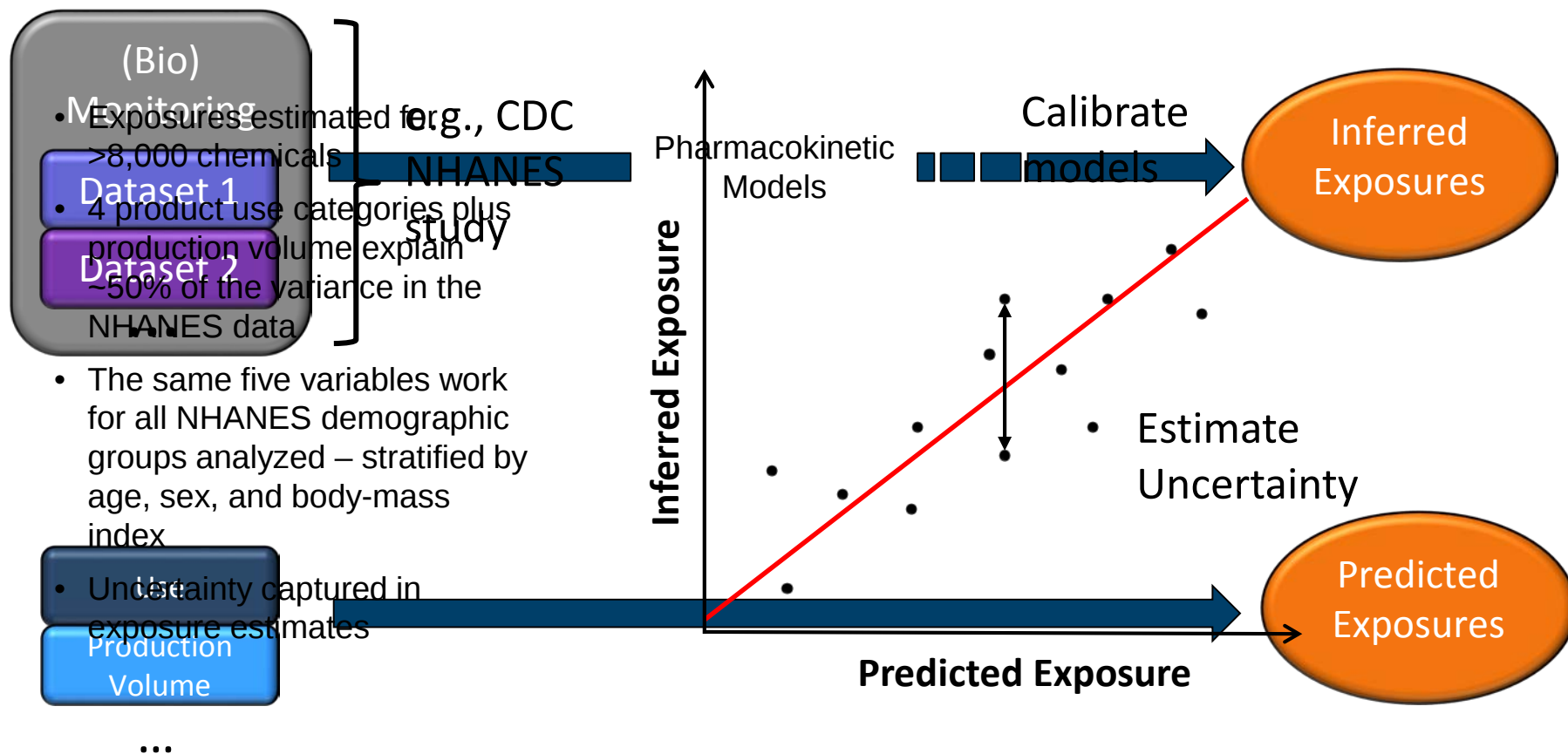
Comparing Dosimetry Adjusted Bioactivity with Exposure



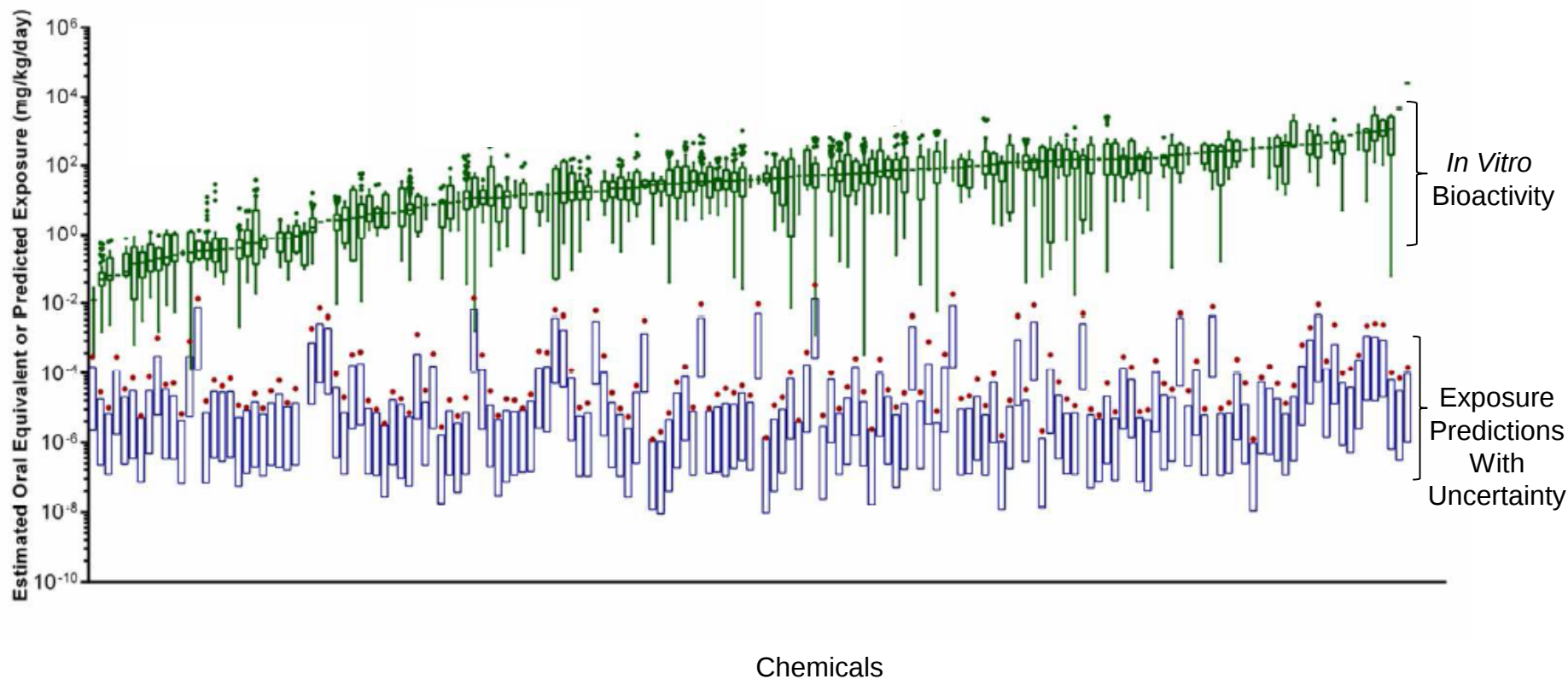
But, Exposure Information is Lacking on Most Chemicals



Adding the High-Throughput Exposure Component



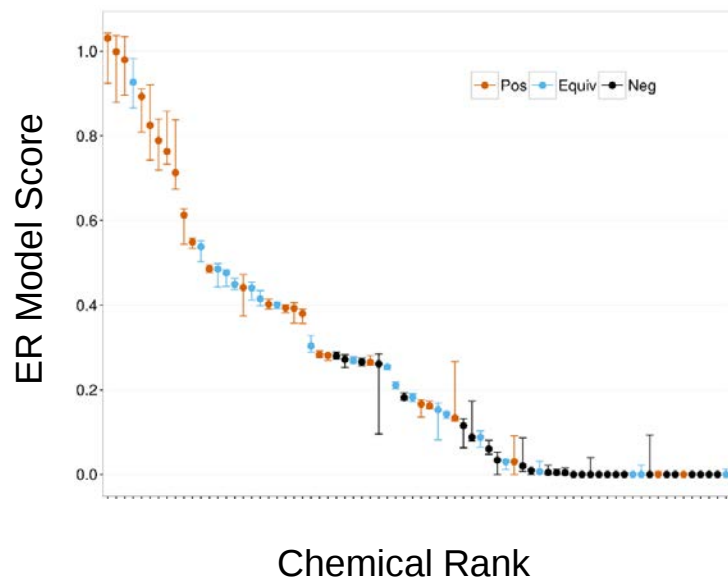
Comparing Bioactivity with Exposure Predictions for Risk Context



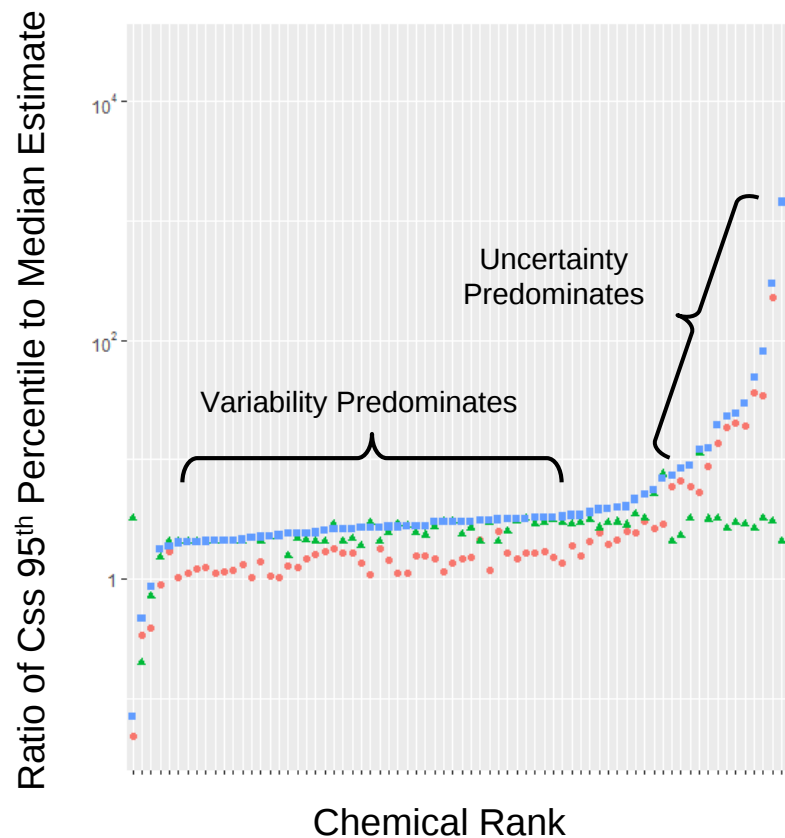
Wetmore et al., *Tox Sci.*, 2015

Adding in Uncertainty and Variability for PD and PK

Propagation of Experimental Uncertainty in Models of ER Potency



Propagation of Experimental Uncertainty in High-Throughput Toxicokinetic Estimates



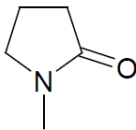
Covering All the Components of a 21st Century Risk Assessment

EPA United States Environmental Protection Agency
EPA Document# 740-R1-5002
March 2015
Office of Chemical Safety and
Pollution Prevention

TSCA Work Plan Chemical Risk Assessment

**N-Methylpyrrolidone:
Paint Stripper Use**

CASRN: 872-50-4



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Phys Chem

Exposure

Hazard

Dose Response,

PK, and PODs

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Variability

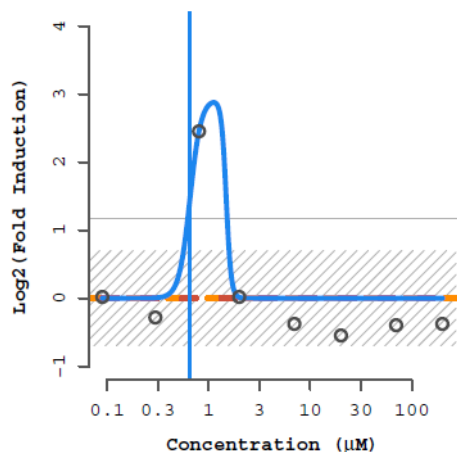
Risk Summary

Uncertainty

Outline

- Short overview of CompTox research effort
- Availability of research data
- Potential application to prioritizing for exposure monitoring

Regulatory Applications Require More Focus on Quality and Transparency



ASSAY: ARID117 (ATQ_Era_TRANS)

NAME: Thioglycolic acid
CHID: 26141 CASRN: 68-11-1
SPID(S): TX007664
L4ID: 420385

HILL MODEL (in red):
tp ga gw
val: 3.1e-11 -2.15 0.416
sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):
tp ga gw la lw
val: 2.93 -0.184 8 0.173 18
sd: 3.56 0.334 9.48 5.82 814

	CNST	HILL	GNLS
AIC:	20.14	26.14	17.79
PROB:	0.23	0.01	0.76
RMSE:	0.92	0.92	0.32

MAX_MEAN: 2.45 MAX_MED: 2.45 BMAD: 0.233

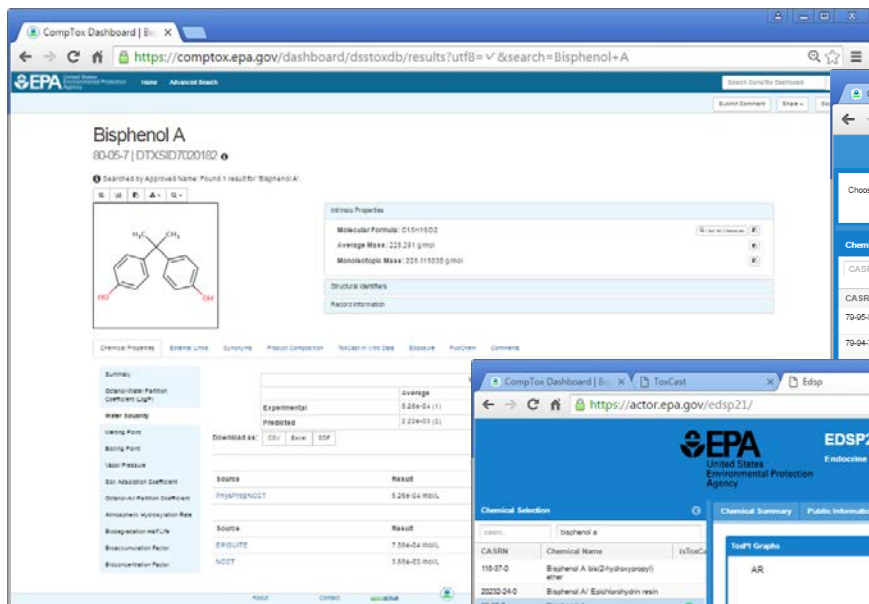
COFF: 1.17 HIT-CALL: 1 FITC: 50 ACTP: 0.77

FLAGS:

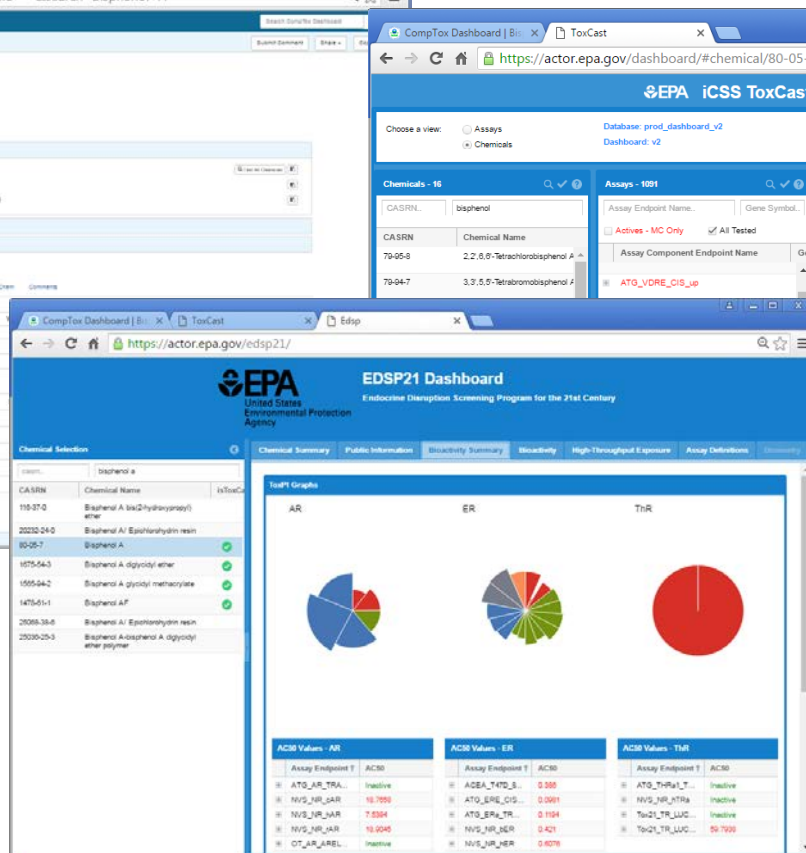
Only one conc above baseline, active
Borderline active

- Public release of Tox21 and ToxCast data on PubChem and EPA web site (raw and processed data)
- Publicly available ToxCast data analysis pipeline
 - Data quality flags to indicate concerns with chemical purity and identity, noisy data, and systematic assay errors
- Tox21 and ToxCast chemical libraries have undergone analytical QC and results publicly available
- Public posting of ToxCast procedures
 - Chemical Procurement and QC
 - Data Analysis
 - Assay Characteristics and Performance
- External audit on ToxCast data and data analysis pipeline
- Migrating ToxCast assay annotations to OECD 211 compliant format

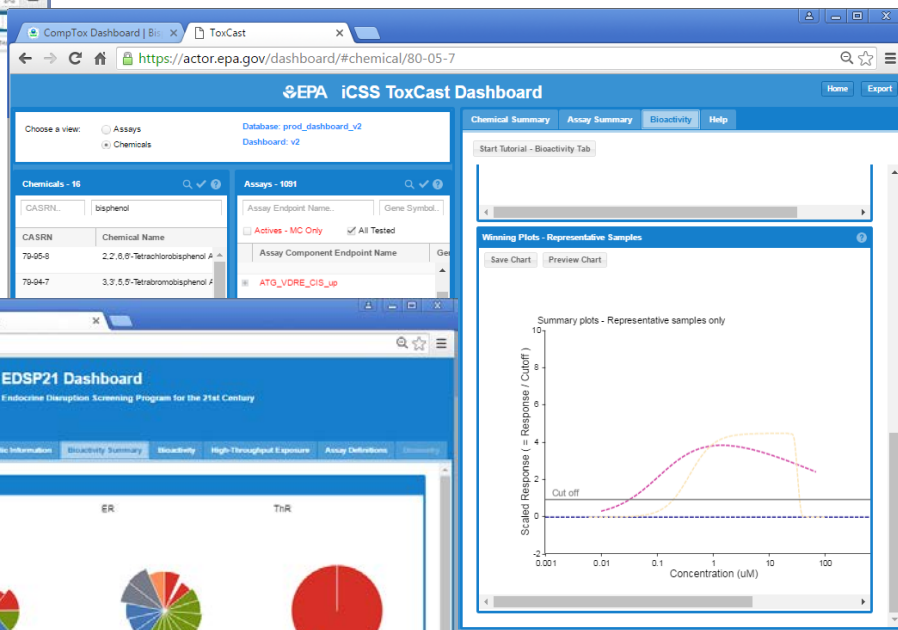
Effort to Provide Data Through Display and Decision Support Dashboards



Enhanced Chemistry
Dashboard
(<https://comptox.epa.gov/dashboard>)

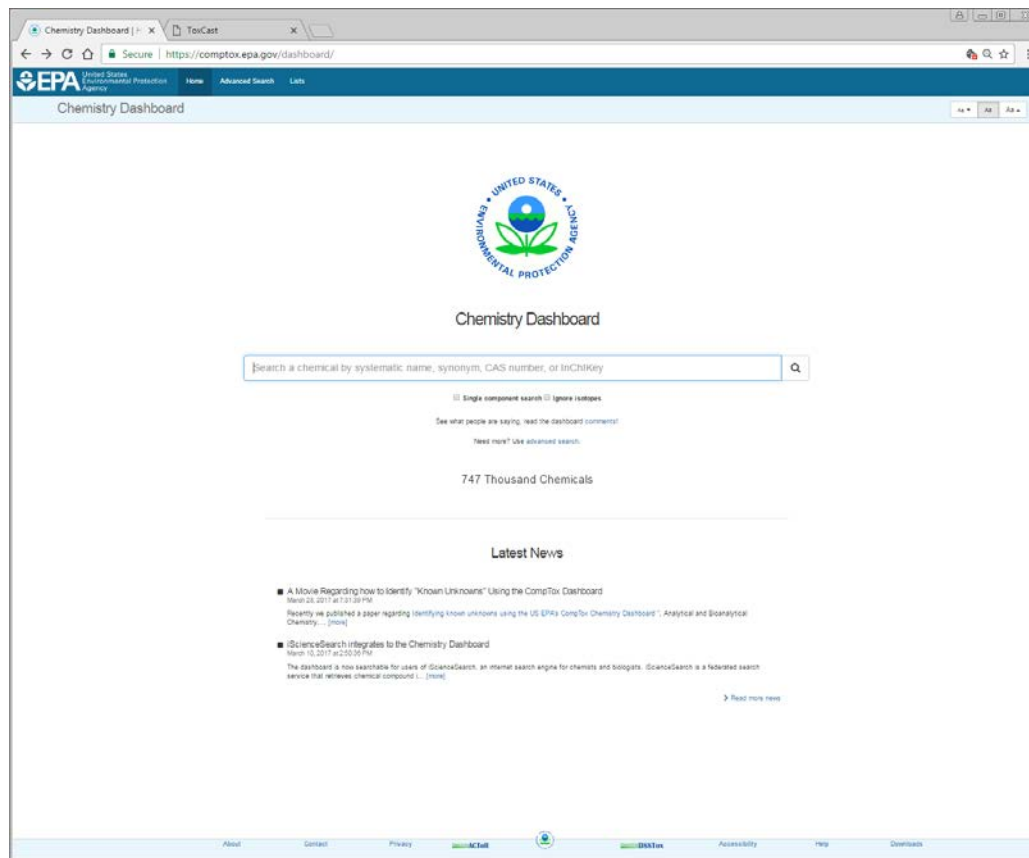


EDSP21 Dashboard
(<https://actor.epa.gov/edsp1>)



ToxCast Dashboard
(<https://actor.epa.gov/dashboard>)

Dashboard Allows Chemical Specific Queries or List Retrieval



Data Currently Organized and Presented as Simple Tabs



Chemical Properties Tab Builds on Chemistry Dashboard Foundation

Chemistry Dashboard | 1 x ToxCast x

Secure | <https://comptox.epa.gov/dashboard/dsstoxdb/results?utf8=✓&search=121-91-5>

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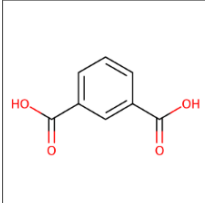
Search Chemistry Dashboard

Chemistry Dashboard Submit Comment Share Copy Aa Aa Aa

1,3-Benzenedicarboxylic acid
121-91-5 | DTXSID3021465

Searched by CAS-RN: Found 1 result for '121-91-5'.

LM



Wikipedia
Isophthalic acid is an organic compound with the formula C₆H₄(CO₂H)₂. This colourless solid is an isomer of phthalic acid and terephthalic acid. ... Read more

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

Record Information

Chemical Properties Env. Fate/Transport Synonyms External Links Toxicity Values (Beta) Exposure Bioassays Similar Molecules (Beta) Literature Comments

Summary

Download as: TSV Excel SDF

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	1.66 (1)	1.46 (4)	1.66 to 1.66	1.46	1.66	1.21 to 1.78	-
Water Solubility	6.02e-04 (1)	1.53 (4)	6.02e-04 to 6.02e-04	1.53	6.02e-04	1.46e-02 to 6.02	mol/L
Density	-	1.45 (1)	-	1.45	-	-	g/cm ³
Melting Point	305 (7)	210 (3)	67.0 to 348	210	67.0 to 348	127 to 278	°C
Boiling Point	-	333 (3)	-	333	-	319 to 351	°C
Surface Tension	-	70.3 (1)	-	70.3	-	-	dyn/cm
Vapor Pressure	-	8.20e-07 (3)	-	8.20e-07	-	1.55e-07 to 2.12e-06	mmHg
LogKow: Octanol-Air	-	7.84 (1)	-	7.84	-	-	-
Henry's Law	-	9.98e-11 (1)	-	9.98e-11	-	-	atm-m ³ /mole
Index of Refraction	-	1.62 (1)	-	1.62	-	-	-
Molar Refractivity	-	40.1 (1)	-	40.1	-	-	cm ³
pKa Acidic Apparent	-	3.53 (1)	-	3.53	-	-	-
Molar Volume	-	114 (1)	-	114	-	-	cm ³
Polarizability	-	15.9 (1)	-	15.9	-	-	Å ³

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Data “Layers” Allow User Interaction with Underlying Models and Data

Chemistry Dashboard | 1 x ToxCast x

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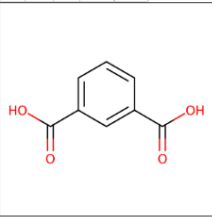
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1,3-Benzenedicarboxylic acid

121-91-5 | DTXSID3021485

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Summary

LogP: Octanol-Water

Water Solubility

Density

Melting Point

Boiling Point

Surface Tension

Vapor Pressure

LogK_{ow}: Octanol-Air

Henry's Law

Index of Refraction

Molar Refractivity

pK_a Acidic Apparent

Molar Volume

Polarizability

Download as: TSV Excel SDF

LogP: Octanol-Water			
	Average	Median	Range
Experimental	1.00 (1)	1.00	1.00
Predicted	1.40 (4)	1.40	1.21 to 1.70

Experimental

Source	Result
PhysPropNCCT	1.00

Predicted

Source	Result	Calculation Details	QMRF
EPISUITE	1.70	Not Available	Not Available
OPERA	1.21	OPERA Model Report	Available
NICEATM	1.33	Not Available	Available
ADCDLabs	1.50	Not Available	Not Available

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Data “Layers” Allow User Interaction with Underlying Models and Data

Chemistry Dashboard | x Chemistry Dashboard | x ToxCast

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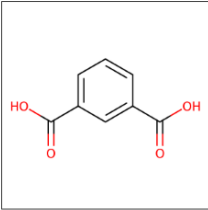
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Chemistry Dashboard

Save Report

OPERA Models: LogP: Octanol-Water

1,3-Benzenedicarboxylic acid
121-91-5 | DTXSID3021485



Model Results

Predicted value: 1.21
Global applicability domain: [inside](#)
Local applicability domain index: 0.79
Confidence level: 0.04

Model Performance



Weighted KNN model

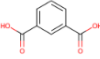
4-And CV (ZFN)		Training (ZFN)		Test (ZFN)	
Q2	R/IDE	R2	R/IDE	R2	R/IDE
0.88	0.69	0.86	0.67	0.88	0.78

CMRF

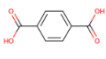
Nearest Neighbors from the Training Set



Phthalic acid
Measured: 0.73
Predicted: 1.18



1,3-Benzenedicarboxylic acid
Measured: 1.05
Predicted: 1.21



Terephthalic acid
Measured: 2.00
Predicted: 1.23



2-Hydroxyphenylacetic acid
Measured: 0.85
Predicted: 0.03e-01



Benzoic acid, 4-hydroxy-
Measured: 0.75
Predicted: 0.03e-01

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Environmental Fate, and Transport

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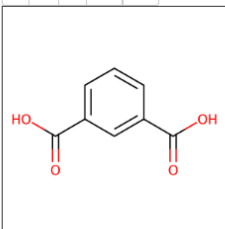
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1,3-Benzenedicarboxylic acid

121-91-5 | DTXSID3021485

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Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

Record Information

Chemical Properties Env. Fate/Transport Synonyms External Links Toxicity Values (Beta) Exposure Bioassays Similar Molecules (Beta) Literature Comments

Summary

Download as: TSV Excel SDF

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
Soil Adsorp. Coeff.	-	21.5 (2)	-	21.5	-	11.9 to 31.1	L/kg
Atmos. Hydroxylation Rate	-	1.98e-11 (1)	-	1.98e-11	-	-	cm ³ /molecule*sec
Biodeg. Half-Life	-	4.53 (1)	-	4.53	-	-	days
Fish Biotrans. Half-Life (Km)	-	1.12e-01 (1)	-	1.12e-01	-	-	days
Bioaccumulation Factor	-	4.84 (1)	-	4.84	-	-	-
Bioconcentration Factor	-	3.25 (4)	-	3.25	-	7.55e-01 to 4.84	-

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Quantitative *In Vivo* Toxicity Values Assembled From Multiple Sources

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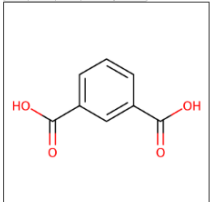
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1,3-Benzenedicarboxylic acid
121-91-5 | DTXSID3021485

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Q ID I A Q



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Exposure Limit

Point Of Departure

Regulatory Toxicity Value

Exposure Descriptor

Effect Level

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Point Of Departure

Grouping ID	Priority	Type	Subtype	Value	Units	Study Type	Exposure Route	Study Duration	Species	Media	Details	Source
303871	3	NOAEL	-	10.0	mg/m3	developme...	inhalation	developme...	rat	-	HPVIS Det...	HPVIS
310310	3	NOAEL	-	10.0	mg/m3	repeat dos...	inhalation	repeat dose	rat	-	HPVIS Det...	HPVIS
310311	3	NOAEL	-	0.5	% diet	repeat dos...	oral	repeat dose	rat	-	HPVIS Det...	HPVIS
310312	3	LOAEL	-	800	mg/kg-day	repeat dos...	oral	repeat dose	rat	-	HPVIS Det...	HPVIS
310313	3	NOAEL	-	250	mg/kg-day	repeat dos...	oral	repeat dose	rat	-	HPVIS Det...	HPVIS

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Sources include EPA and public sources

Integration of Exposure Data

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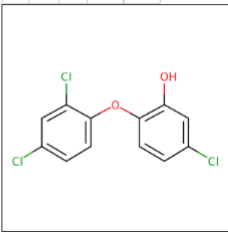
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Chemistry Dashboard

Triclosan

3380-34-5 | DTXSID5032498

Searched by Approved Name: Found 1 result for 'Triclosan'.



Wikipedia

Triclosan, similar in its uses and mechanism of action to triclocarban, is an antibacterial and antifungal agent found in consumer products, including toothpaste, soaps, detergents, toys, and surgical cleaning treatments. Its efficacy as an antimicrobial agent, the risk of antimicrobial resistance, and its possible role in disrupted hormonal development remain controversial. Additional research seeks to understand its potential effects on organisms and environmental health. Triclosan... Read more

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Chemical Weight Fraction (Beta)

Product Use Categories (Beta)

Chemical Functional Use (Beta)

Monitoring Data

Exposure Predictions

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Chemical Weight Fractions ⓘ

Product Name	Specific/Generic	Product Use Category	Reported Functional Use	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source	Product Date
antonio banderas ...	Specific	personal care: de...	-	0.001	0.01	MSDS	Retail Product Cat...	-
arm and hammer e...	Specific	personal care: de...	-	-	-	Ingredients List	DrugStore.com	-
armani code for m...	Specific	personal care: de...	-	-	-	Ingredients List	DrugStore.com	-
aromasense body...	Specific	personal care: bo...	-	0.0	0.0005	MSDS	Retail Product Cat...	-
dead sea essentia...	Specific	personal care: fac...	-	-	-	Ingredients List	DrugStore.com	-
dead sea essentia...	Specific	personal care: fac...	-	-	-	Ingredients List	DrugStore.com	-
dial complete liqui...	Specific	personal care: ha...	-	-	-	MSDS	Retail Product Cat...	2008-05-15
dr. snapz insect b...	Specific	personal care: bit...	-	-	-	MSDS	Retail Product Cat...	-
english leather cla...	Specific	personal care: de...	-	0.001	0.01	MSDS	Retail Product Cat...	2007-09-06
heno de pravia de...	Specific	personal care: de...	-	0.001	0.01	MSDS	Retail Product Cat...	-
heno de pravia tal...	Specific	personal care: bo...	-	0.001	0.001	MSDS	Retail Product Cat...	-
high school musio...	Specific	personal care: fra...	-	0.0015	0.0015	MSDS	Retail Product Cat...	-
insect bite 300ct 1	Specific	pesticides: insect...	-	0.0025	0.0025	MSDS	Retail Product Cat...	-
insect bite relief a...	Specific	pesticides: insect...	-	-	-	MSDS	Retail Product Cat...	-

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Integration of Exposure Data

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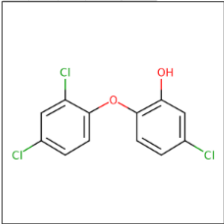
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Triclosan
3380-34-5 | DTXSID5032488

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LM



Wikipedia

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Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

Record Information

Chemical Properties Env. Fate/Transport Synonyms External Links Toxicity Values (Beta) Exposure Bioassays Similar Molecules (Beta) Literature Comments

Chemical Weight Fraction (Beta)

Product Use Categories (Beta) Download as: TSV Excel

Chemical Functional Use (Beta)

Monitoring Data

Exposure Predictions

Product Use Categories (PUCs)

Product Use Category	Product Name	Source	Product Date
personal care: deodorant	antonio banderas - blue seduction for men deso...	Retail Product Categories/Walmart	-
personal care: deodorant	arm and hammer essentials deodorant with natu...	DrugStore.com	-
personal care: deodorant	armani code for men alcohol free deodorant stic...	DrugStore.com	-
personal care: body oil	aromasense body oil rose petals 1	Retail Product Categories/Walmart	-
personal care: face mask	dead sea essentials by ahava mud mask cham...	DrugStore.com	-
personal care: face mask	dead sea essentials by ahava spa facial mud m...	DrugStore.com	-
personal care: hand soap	dial complete liquid hand soap 1	Retail Product Categories/Walmart	2006-05-15
personal care: bite relief	dr. snapp insect bite relief 1	Retail Product Categories/Walmart	-
personal care: deodorant	english leather classic deodorant 2007 holiday 1	Retail Product Categories/Walmart	2007-09-06
personal care: deodorant	heno de pravia deodorant 1	Retail Product Categories/Walmart	-
personal care: body powder	heno de pravia talcum powder 1	Retail Product Categories/Walmart	-
personal care: fragrance	high school musical all for one body spray 1	Retail Product Categories/Walmart	-
pesticides: insecticide	insect bite 300ct 1	Retail Product Categories/Walmart	-
pesticides: insecticide	insect bite relief applicator 1	Retail Product Categories/Walmart	-
personal care: fragrance	jovan white musk for women cologne body spra...	DrugStore.com	-

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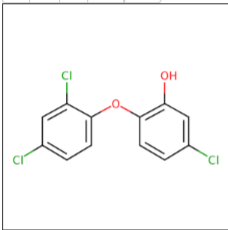
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Triclosan

3380-34-5 | DTXSID:5032498

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Wikipedia

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Product Use Categories (Beta)

Chemical Functional Use (Beta)

Monitoring Data

Exposure Predictions

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Collected Data on Functional Use

Harmonized Functional Use	Reported Functional Use	Source	Access Date
ubiquitous	Antimicrobial Agents	SpecialChem Polymer Additives	2014-12-30
ubiquitous	PRESERVATIVE	CosIng (EU)	2014-07-16
ubiquitous	ANTIMICROBIAL	ACToR UseDB	2014-05-01
ubiquitous	Biocide	American Cleaning Institute	-
ubiquitous	DEODORANT	CosIng (EU)	2014-07-16
-	antibacterial agent	Proctor & Gamble	-
-	oral care agent	Unilever	2015-07-17
-	oral care agent	Unilever	2015-07-17

Predicted Probability of Associated Functional Use

There are no predicted probabilities of associated functional use available.

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Integration of Exposure Data

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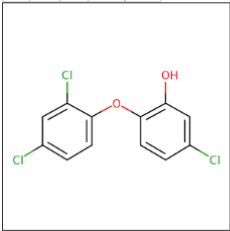
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Chemical Weight Fraction (Beta) Download as: TSV Excel

Product Use Categories (Beta)

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Monitoring Data

Exposure Predictions

1 National Health and Nutrition Examination Survey (NHANES) Inferences (mg/kg-bw/day)

	Ages 6-11	Ages 12-19	Ages 20-45	Ages 65+	BMI > 30	BMI < 30	Repro. Age Females	Females	Males	Total
Lower 95th Limit	1.55e-04	1.15e-04	1.94e-04	7.30e-05	1.29e-04	1.99e-04	1.77e-04	1.60e-04	1.73e-04	1.61e-04
Upper 95th Limit	2.59e-04	1.60e-04	2.74e-04	1.60e-04	1.75e-04	2.43e-04	2.45e-04	2.34e-04	2.39e-04	2.14e-04
Median	2.20e-04	1.39e-04	2.31e-04	1.09e-04	1.50e-04	2.20e-04	2.10e-04	1.90e-04	2.03e-04	1.97e-04

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Identifying Perturbed Pathways

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Chemistry Dashboard

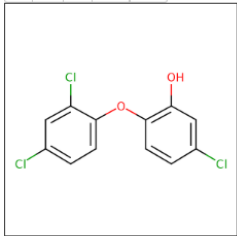
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Triclosan

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Presence in Lists

Record Information

Chemical Properties Env. Fate/Transport Synonyms External Links Toxicity Values (Beta) Exposure Bioassays Similar Molecules (Beta) Literature Comments

ToxCast

PubChem

Chemical Activity Summary

Download as: TSV Excel Show: Inactive Background

Assay Name	Hit Call	Top	Scaled Top	AC50	log AC50	Intended Target Family
TOX21_AR_BIA_Agonist_ratio	ACTIVE	87.8	2.09	84.4	1.93	nuclear receptor

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Show/Hide All

- nuclear receptor
- cell cycle
- cyp
- background measurement
- dna binding
- transporter
- gpcr
- oxidoreductase
- protease
- kinase
- cytokine
- cell adhesion molecules
- protease inhibitor
- growth factor
- misc protein
- cell morphology
- phosphatase

Displaying Similar Chemicals

Chemistry Dashboard | T x ToxCast x

Secure | <https://comptox.epa.gov/dashboard/dsstoxdb/results?utf8=✓&search=triclosan>

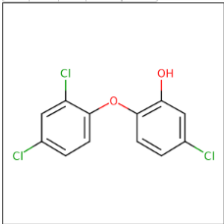
EPA United States Environmental Protection Agency Home Advanced Search Lists Search Chemistry Dashboard

Chemistry Dashboard Submit Comment Share Copy Aa Ab Aa

Triclosan
3380-34-5 | DTXSID502498

Searched by Approved Name: Found 1 result for 'triclosan'.

LM



Wikipedia

Triclosan, similar in its uses and mechanism of action to triclocarban, is an antibacterial and antifungal agent found in consumer products, including toothpaste, soaps, detergents, toys, and surgical cleaning treatments. Its efficacy as an antimicrobial agent, the risk of antimicrobial resistance, and its possible role in disrupted hormonal development remain controversial. Additional research seeks to understand its potential effects on organisms and environmental health. Triclosan... [Read more](#)

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

Record Information

Chemical Properties Env. Fate/Transport Synonyms External Links Toxicity Values (Beta) Exposure Bioassays Similar Molecules (Beta) Literature Comments

Similar Molecules
Searched with a similarity threshold of 0.9

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Properties Chemicals

						
Similarity Value		1	1	1	1	1
Log _P : Octanol-Water	Experimental	-	-	-	-	-
	Predicted	5.58	4.45	5.49	4.28	5.15
Water Solubility	Experimental	-	-	-	-	-
	Predicted	0.000113	0.00355	0.000152	0.0182	0.000352
Density	Experimental	-	-	-	-	-
	Predicted	-	-	-	-	-
Melting Point	Experimental	-	-	-	-	-
	Predicted	132	92.4	121	78.9	111
Boiling Point	Experimental	-	-	-	-	-
	Predicted	370	347	402	324	354

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Beginning to Fold In Literature Mining Capabilities

Chemistry Dashboard | ToxCast

Secure | <https://comptox.epa.gov/dashboard/dsstoxdb/results?utf8=✓&search=triclosan>

EPA United States Environmental Protection Agency

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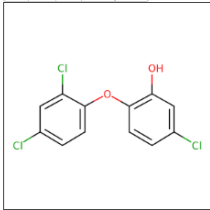
Chemistry Dashboard

Triclosan

3380-34-5 | DTXSID5032498

Searched by Approved Name: Found 1 result for 'triclosan'.

LM



Wikipedia

Triclosan, similar in its uses and mechanism of action to triclocarban, is an antibacterial and antifungal agent found in consumer products, including toothpaste, soaps, detergents, toys, and surgical cleaning treatments. Its efficacy as an antimicrobial agent, the risk of antimicrobial resistance, and its possible role in disrupted hormonal development remain controversial. Additional research seeks to understand its potential effects on organisms and environmental health. Triclosan... Read more

Intrinsic Properties

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Google Scholar

Abstract Sifter

PubChem Articles

PubChem Patents

Select Term:

Embryo and embryonic development

Retrieve Articles 51 Articles (out of 51)

Add additional query terms to filter abstracts:

embryo fetus development

Edit the Query Before Retrieving Articles

("3380-34-5" OR "Triclosan" OR "Triclosan") AND (embryo OR Embryonic Structures OR fetus OR Embryonic and Fetal Development)

Search and Count

embryo	fetus	devel...	Total	PMID	PubYr	Title
5	0	2	5	28334872	2017	Effects of 4-MBC and triclosan in embryos of the frog <i>Pelophylax perezi</i> .
5	0	1	4	28236114	2017	Methyltriclosan and triclosan impact embryonic development of <i>Danio rerio</i> and <i>Paracentrotus lividus</i> .
4	0	5	9	26103003	2017	Effects of sub-lethal teratogen exposure during larval development on egg laying and egg quality in adult <i>Caenorhabditis elegans</i> .
0	1	0	1	28108710	2017	Univariate predictors of maternal concentrations of environmental chemicals: The MIREC study.
2	0	0	2	28073982	2017	Urinary triclosan concentrations and early outcomes of in vitro fertilization-embryo transfer.

Record: 1 of 51

Title: Effects of 4-MBC and triclosan in embryos of the frog *Pelophylax perezi*.

Abstract: The widespread and increasing use of personal care products (PCPs) have led to environmental contamination by substances included in these products. These substances have been detected in aquatic compartments and shown to cause adverse effects on non-target aquatic organisms. In this work toxicity of the antimicrobial triclosan (TCS) and of the UV-filter 3-(4-methylbenzylidene) camphor (4-MBC) was assessed in the embryos of *Pelax* frog *Pelophylax perezi*. Lethal and sub-lethal parameters were evaluated in *Pelax* in Gosner stage 49 exposed to 0.0015-1.5 mg/l of 4-MBC and 0.25-2.50 mg/l of TCS during 144 h. Survival, malformations, length and hatching were evaluated as apical endpoints. Biomarkers of neurotoxicity, oxidative stress, energy metabolism and estrogenicity were determined at the biochemical level through the activities of cholinesterase (ChE), catalase (CAT), glutathione S-transferase (GST), lactate dehydrogenase (LDH) and levels of lipid peroxidation (LPO) and vitellogenin (Vtg). *Pelax* exposure to 4-MBC led to few developmental malformations (up to 3%) and a GST induction at 0.015 mg/l. Triclosan exposure reduced survival, delayed hatching (at 72 h) and *Pelax* induced malformations. In addition ChE was inhibited in the highest concentrations tested and GST and LDH were induced at 0.75 mg/l. The LOEC registered for TCS in *Pelax* frogs. Overall, our study showed that TCS might exert adverse effects on *P. perezi* early life stages, but only at four orders of magnitude above the concentrations found in environment. Furthermore, our results highlight the need to assess PCPs toxicity at different levels of biological organization.

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Outline

- Short overview of CompTox research effort
- Availability of research data
- Potential application to prioritizing for exposure monitoring

Integrating Different Components for Prioritization

RapidTox | Home

comptox.zn.epa.gov/dashboard/rapidtox/

United States
Environmental Protection
Agency

Home

CompTox Dashboard ▾

Hazard

Human Health

Dev Tox

☒ *In Vivo*

Repro Tox

☒ *In Vivo*

Cancer

☒ *In Vivo*

Literature

☒ *Male reproduction*

☒ *Female reproduction*

☒ *Embryo or embryonic development*

Endocrine

Estrogen Agonist

☒ *In Vitro*

☒ *QSAR*

Androgen Agonist

☒ *In Vitro*

☒ *QSAR*

Androgen Antagonist

☒ *In Vitro*

☒ *QSAR*

Exposure

CPCat

☒ *Present in Children's Products*

☒ *Pesticide Home Use*

☒ *Present in Consumer Products*

Physical Chemical Properties

☒ *Appropriate mass range*

☒ *Exclude polymers*

Prioritize

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Help

Thank You for Your Attention!

Tox21 Colleagues:

NTP Crew

FDA Collaborators

NCATS Collaborators

EPA Colleagues:

NERL

NHEERL

NCEA

Collaborators:

Unilever



EPA's National Center for Computational Toxicology