

Delivering The Benefits of Chemical-Biological Integration in Computational Toxicology at the EPA

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U.S. Environmental Protection Agency, RTP, NC*

This work was reviewed by the U.S. EPA and approved for presentation but does not necessarily reflect official Agency policy.

*August 21-25, 2016
ACS Fall Meeting, Philadelphia, PA*

Who is NCCT?

- National Center for Computational Toxicology – part of EPA’s Office of Research and Development
- Research driven by EPA’s *Chemical Safety for Sustainability Research Program*
 - Develop new approaches to **evaluate the safety of chemicals**
 - Integrate advances in biology, biotechnology, chemistry, exposure science and computer science
- Goal - To identify **chemical exposures** that may disrupt biological processes and cause adverse outcomes.

Scientific leadership

<https://www.epa.gov/chemical-research/toxicity-forecasting>



Toxicity Forecasting

Advancing the Next Generation of Chemical Evaluation

EPA needs rapid and efficient methods to prioritize, screen and evaluate thousands of chemicals. EPA's Toxicity Forecaster (ToxCast) generates data and predictive models on thousands of chemicals of interest to the EPA. ToxCast uses high-throughput screening methods and computational toxicology approaches to rank and prioritize chemicals. In fact, EPA's Endocrine Disruption Screening Program (EDSP) is working to use ToxCast to rank and prioritize chemicals.



- ToxCast has data on over 1,800 chemicals from a broad range of sources including industrial and consumer products, food additives, and potentially "green" chemicals that could be safer alternatives to existing chemicals.
- ToxCast screens chemicals in over 700 high-throughput assays that cover a range of high-

Computational Toxicology Research Updates



Get ToxCast Updates

[sign up](#)

Our Bioassay Data

<https://www.epa.gov/chemical-research/downloadable-computational-toxicology-data>



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Downloadable Computational Toxicology Data

EPA's computational toxicology research efforts evaluate the potential health effects of thousands of chemicals. The process of evaluating potential health effects involves generating data that investigates the potential harm, or hazard of a chemical, the degree of exposure to chemicals as well as the unique chemical characteristics.

As part of EPA's commitment to share data, all of the computational toxicology data is publicly available for anyone to access and use.

High-throughput Screening Data

EPA researchers use rapid chemical screening (called high-throughput screening assays) to limit the number of laboratory animal tests while quickly and efficiently testing thousands of chemicals for potential health effects.

- [ToxCast Data](#): High-throughput screening data on thousands of chemicals.

Rapid Exposure and Dose Data

EPA researchers develop and use rapid exposure estimates to predict potential exposure for thousands of chemicals.

- [High-throughput toxicokinetics data](#): It is important to link the external dose of a chemical to an internal blood or tissue concentration. This process is called toxicokinetics. EPA researchers measure the critical factors that determine the distribution

Rapid Chemical Exposure and Dose Research

EPA is responsible for ensuring the safety of thousands of chemicals. Quantitative exposure data are available for only a small fraction of registered chemicals. This type of exposure data is needed to thoroughly evaluate chemicals for potential risks to humans, wildlife and ecosystems. EPA is developing innovative methods to develop exposure estimates for thousands of chemicals to better protect human health and the environment. These innovative methods are called rapid exposure and dose assessments.

Rapid Exposure Predictions

Rapid, also called high-throughput, exposure predictions or ExpoCast provide rapid exposure estimates for thousands of chemicals. ExpoCast quickly and efficiently looks at multiple routes of exposure to provide exposure estimates. ExpoCast uses and enhances two well-known exposure models to estimate chemical exposure.

- [› Farfield Exposure Models](#)
- [› Nearfield Exposure Models](#)

Evaluating High-throughput Exposure Predictions

EPA is currently evaluating the effectiveness of high-throughput exposure models

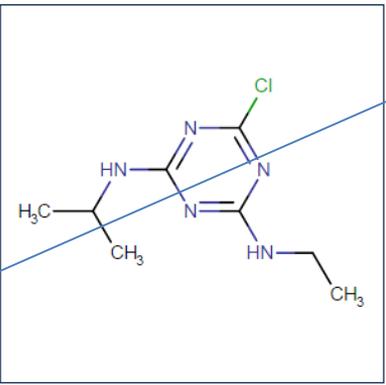


Pictured Above: Farfield Exposure Examples



- Aggregated Computational Toxicology Resource
- A warehouse of publicly available chemical toxicity data
- Aggregates data from >1000 public sources on >500,000 chemicals

ACToR Home Data Collections Search Assays Chemical Download Apps



Atrazine
 1912-24-9 | DTXSID9020112

InChi: InChi=1S/C8H14ClN5
 InChi Key: MXWJ/TOOROX
 SMILES: CCNC1=NC(Cl)=NC(NC(C)C)=N1
 Molecular Formula: C8H14Cl
 Molecular Weight: 215.69 g/l

Synonyms
Hazard
Acute Toxicity
Chronic Toxicity
Carcinogenicity
Genotoxicity
Developmental Toxicity
Reproductive Toxicity
Biomonitoring
Occurrence
Non-regulatory Risk Management
Regulatory Risk Management
Production and Release
In Vitro
Inherent Chemical Property
Use

Genotoxicity

Show Data Hide Data

- ▶  CheLIST combination of files from Method Validation Group
- ▶  DSSTox NTP BSI GeneTox Index
- ▶  DSSTox NTP BSI URL
- ▶  Genotoxicity Data In Vitro from EPA HPVIS
- ▶  NLM TOXNET CCRIS Data MSTU - MUTAGENICITY STUDIES

▼  Genotoxicity Data In Vitro from EPA HPVIS

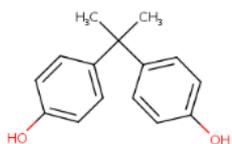
▼  Result Group:

Component Name	Value
Conclusion	Negative
Conclusion (GeneTox)	This study was judged to have given a negative result since the observed increase in the first experiment was not reproducible.
Dose Remarks	30 - 50 g/mL with activation20 - 40 g/mL without activation
Genotoxic Effect	Negative
GLP	No Data
Metabolic Activation	With and Without
Method/Guideline Followed	No Data
Program Flag	HPVIS
Reliability	2
Results Remarks	With metabolic activation: 50 g/mLWithout metabolic activation: None reported In the first test with metabolic activation an increase in the percentage of metaphases with chromosome aberrations from bisphenol A treated cultures was observed only at the top dose in the presence of cytotoxicity; 14% at 50 g/mL compared to 3% in controls. In these high-dose cultures it was stated that cell confluence was reduced by approximately 70%. In the second test no significant increases were observed in with metabolic activation; only 3% of cells at the highest dose had aberrations. No significant increases in aberrations were observed without metabolic activation with bisphenol A evidently being tested up to "toxic levels." The positive controls produced clear increases in chromosome aberrations.
Species	Mammalian Cell Line
Sponsor Name	General Electric Company - Plastics
Sponsored Chemical Result Type	72162-28-8
Strain	Chinese Hamster Ovary (CHO)

Justt, H., Brown, B.M., Rodgers, C., Anderson, B.E., Ressnick, M.A. and Zeiger, E. 1989. Chromosomal aberrations and sister chromatid exchange tests in Chinese hamster ovary. Environ. Mol. Mutagen. 14:165-187. As cited in the EU Risk Assessment. Data entered into the HPVIS extracted from the robust

Chemical: BISPENOL A

CASRN: 80-05-7



Export Use Data



Export Product Data



Chemical and Product Categories is a database containing information mapping >43,000 chemicals to a set of terms categorizing their usage or function.

Use Information:

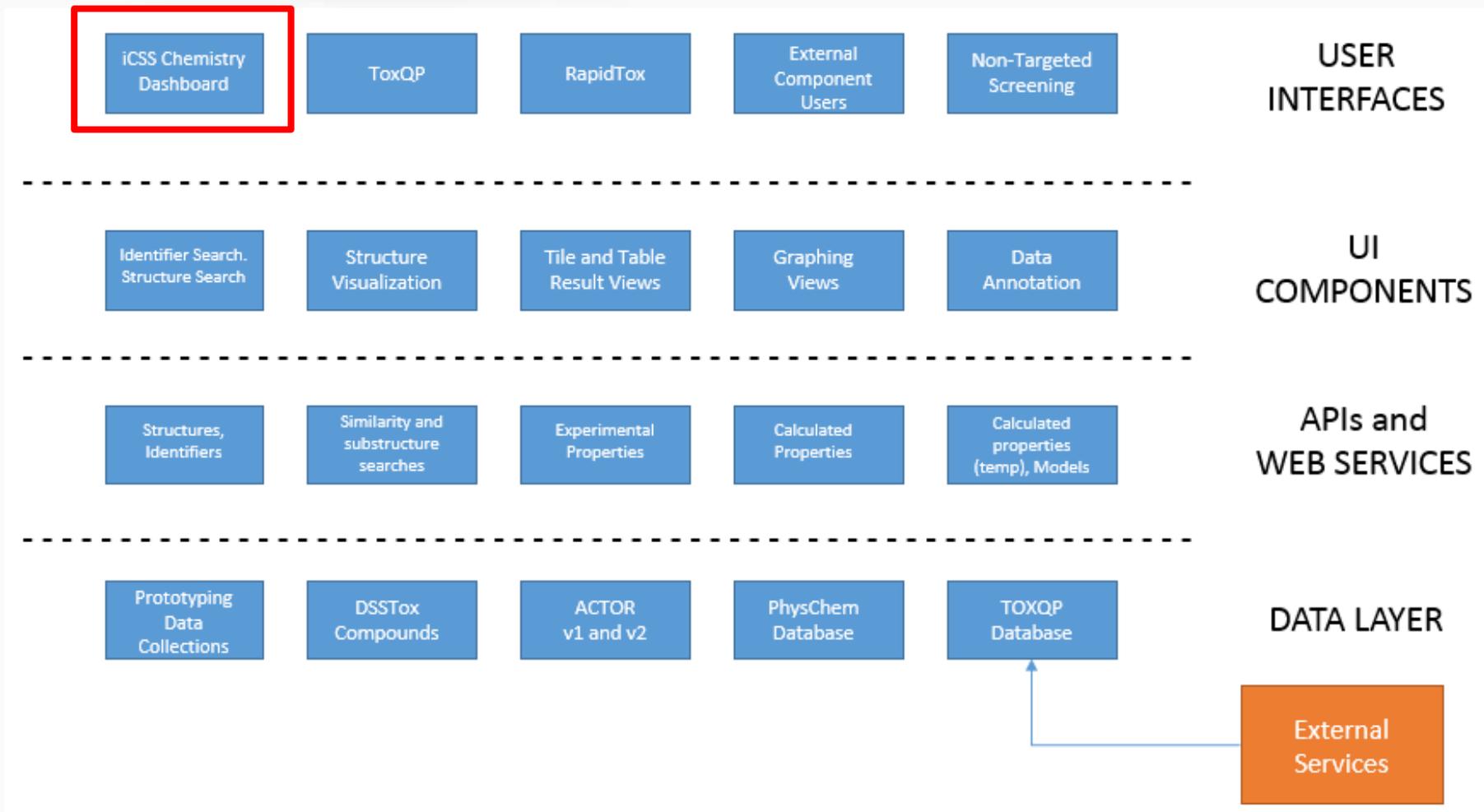
CPCat Description ▾	Source Description ▾	ACToR Data Set/List ▾	Source ▾	Class of Chemical Category ▾
consumer_use_ACToRUseDB	Consumer Use		ACToR UseDB	Use Categories
personal_care_ACToRUseDB	Personal Care Product		ACToR UseDB	Use Categories
industrial_manufacturing_ACToRUseDB	Chemical Industrial		ACToR UseDB	Use Categories
child_use detected	Consumer Products	The Danish EPA:Exposure of 2-year-olds to chemical substances in Consumer Products. This project included a survey of the products as well as chemical analyses and risk assessments of a number of selected products that 2 year-old children come into contact with throughout the course of a day. A total of 12 product groups were included in the survey phase. Selected products from 10 of these product groups were subsequently included in a screening phase and several problematic substances were subjected to quantitative analysis. A risk assessment was also performed for a number of problematic substances.	ACToR Data Sets and Lists	Use Categories
consumer_use detected	Consumer Products	TNO Nederlands Organisation for Applied Scientific Research:Hazardous Chemicals in Consumer Products:In this study 33 consumer products, including body care products, toys, textiles, deodorizers and cleaners, have been tested for the presence of bisphenol-A, alkylphenols and ethoxylates, phthalates, musks and organotin compounds.	ACToR Data Sets and Lists	Use Categories
child_use	Consumer Products:	(state of) Washington:Washington Childrens Safe Product Act (CSPA) Reporting Rule. List of chemical of high concern to children (CHCC)	ACToR Data Sets and	Use Categories

- To interrogate chemical screening data from ToxCast and the Tox21 collaboration

The screenshot displays the EPA iCSS ToxCast Dashboard interface. The top navigation bar includes 'Home' and 'Export' buttons. The main content area is divided into several sections:

- Choose a view:** Radio buttons for 'Assays' and 'Chemicals' (selected).
- Database:** prod_dashboard_v2
- Dashboard:** v2
- Chemicals - 10:** A table listing chemicals with columns for CASRN, Chemical Name, and Chemical Class. The selected chemical is Bisphenol A (CASRN 80-05-7).
- Assays - 1091:** A table listing assay endpoints with columns for Assay Endpoint Name and Gene Symbol. The selected assay is ACEA_T47D_80hr_Positive, associated with the ESR1 gene.
- Filters - 0:** A table for filtering results.
- Chemical Activity Summary:** A scatter plot titled 'Active endpoints for 80-05-7'. The x-axis is 'AC50 (uM)' on a log scale from 0.001 to 100. The y-axis is 'Scaled Top of the Curve' from 0.0 to 9.7. A legend on the right lists various biological targets such as background measurement, cell adhesion molecules, cell cycle, cell morphology, cyp, cytokine, dna binding, esterase, gpcr, growth factor, hydrolase, ion channel, kinase, and lyase.

Our Developing Architecture



- Providing access to our “curated chemistry”
- Database of chemicals, mapped to identifiers, and tens of thousands of experimental physchem properties
- Predictive models and calculation details
- An integration hub for NCCT applications
- A link farm across 10s of EPA and Public websites

Our Latest Dashboard

<https://comptox.epa.gov>

An Integration Hub



>720,000 chemicals
>14 years of assembled data

CompTox Dashboard

- Bisphenol
- Bisphenol A
- Bisphenol A (BPA)
- BISPHENOL A ANHYDRIDE
- Bisphenol A bis(2-hydroxyethyl)ether
- Bisphenol A bis(2-hydroxyethyl ether) diacrylate
- Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
- Bisphenol A bis(2-hydroxy-3-methacryloxypropyl) ether
- Bisphenol A bis(2-hydroxy-3-methacryloyloxypropyl ether)

Help



Mutation Research/Fundamental and Molecular Mechanisms of Mutagenesis

Volume 499, Issue 1, 29 January 2002, Pages 27–52



Mutation Research Frontiers

Distributed structure-searchable toxicity (DSSTox) public database network: a proposal

Ann M. Richard^a,  , ClarLynda R. Williams^{a, b}

 [Show more](#)

[http://dx.doi.org/10.1016/S0027-5107\(01\)00289-5](http://dx.doi.org/10.1016/S0027-5107(01)00289-5)

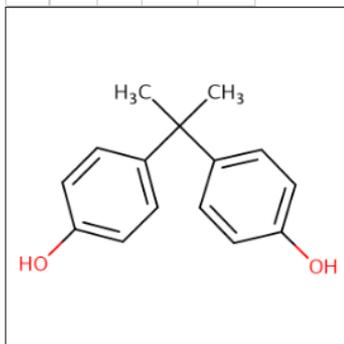
[Get rights and content](#)

Bisphenol A (Accessing DSSTox Data)

Bisphenol A

80-05-7 | DTXSID7020182

🔍 Searched by Approved Name: Found 1 result for 'bisphenol A'.



Intrinsic Properties

Molecular Formula: C₁₅H₁₆O₂

🔍 Find All Chemicals

Average Mass: 228.291 g/mol



Monoisotopic Mass: 228.115030 g/mol



Structural Identifiers

Record Information

Chemical Properties

External Links

Synonyms

Product Composition

ToxCast in Vitro Data

Exposure

Analytical

PubChem

Comments

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Contact

Presented by ACToR



Presented by DSSTox

Privacy

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Physicochemical Properties

Summary

Octanol-Water
Partition Coefficient
(LogP)

Water Solubility

Melting Point

Boiling Point

Vapor Pressure

Soil Adsorption
Coefficient

Octanol-Air Partition
Coefficient

Atmospheric
Hydroxylation Rate

Biodegradation Half
Life

Bioaccumulation

Download as: [CSV](#) [Excel](#) [SDF](#)

Property	Average (Exp.)	Median (Exp.)	Range (Exp.)	Average (Pred.)	Median (Pred.)	Range (Pred.)	Result Unit
Octanol-Water Partition Coefficient (LogP)	3.38 (2)	3.43	3.43	3.42 (2)	3.42	3.20 to 3.64	-
Water Solubility	5.26e-04 (1)	5.26e-04	5.26e-04	2.22e-03 (2)	2.22e-03	7.56e-04 to 3.68e-03	mol/L
Melting Point	155 (7)	156	153 to 158	138 (2)	138	132 to 144	°C
Boiling Point	200 (1)	200	200	349 (2)	349	334 to 364	°C
Vapor Pressure	-	-	-	7.06e-08 (1)	7.06e-08	-	mmHg
Soil Adsorption Coefficient	-	-	-	2.92 (2)	2.92	2.74 to 3.10	-
Octanol-Air Partition Coefficient	-	-	-	8.39 (1)	8.39	-	-
Atmospheric Hydroxylation Rate	-	-	-	-10.4 (1)	-10.4	-	-
Biodegradation Half Life	-	-	-	15.1 (1)	15.1	-	days
Bioaccumulation Factor	-	-	-	173 (1)	173	-	-
Bioconcentration Factor	1.64 (1)	1.64 	1.64	82.0 (3)	82.0	1.38 to 173	-

Chemical Properties

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Data Downloads

Summary

Download as:

Property	Value	Median (Exp.)
Octanol-Water Partition Coefficient (LogP)		3.43
Water Solubility		5.26e-04
Melting Point		156
Boiling Point		200
Vapor Pressure		-
Soil Adsorption Coefficient		-
Octanol-Air Partition Coefficient	-	-
Atmospheric Hydroxylation Rate	-	-

Select/Deselect All
 Octanol-Water Partition Coefficient (LogP)
 Water Solubility
 Melting Point
 Boiling Point
 Vapor Pressure
 Soil Adsorption Coefficient
 Octanol-Air Partition Coefficient
 Atmospheric Hydroxylation Rate
 Biodegradation Half Life
 Bioaccumulation Factor
 Bioconcentration Factor

Data Download: Excel

A1 :    Property

	A	B	C	D	E	F	G	H
1	Property	Average (Exp.)	Median (Exp.)	Range (Exp.)	Average (Pred.)	Median (Pred.)	Range (Pred.)	Result Unit
2	Octanol-Water Partition Coefficient (LogP)	3.38 (2)	3.43	3.43	3.42 (2)	3.42	3.20 to 3.64	-
3	Water Solubility	5.26e-04 (1)	5.26E-04	5.26E-04	2.22e-03 (2)	2.22E-03	7.56e-04 to 3.68e-03	mol/L
4	Melting Point	155 (7)	156	153 to 158	138 (2)	138	132 to 144	°C
5	Boiling Point	200 (1)	200	200	349 (2)	349	334 to 364	°C
6	Vapor Pressure	-	-	-	7.06e-08 (1)	7.06E-08	-	mmHg
7	Soil Adsorption Coefficient	-	-	-	2.92 (2)	2.92	2.74 to 3.10	-
8	Octanol-Air Partition Coefficient	-	-	-	8.39 (1)	8.39	-	-
9	Atmospheric Hydroxylation Rate	-	-	-	-10.4 (1)	-10.4	-	-
10	Biodegradation Half Life	-	-	-	15.1 (1)	15.1	-	days
11	Bioaccumulation Factor	-	-	-	173 (1)	173	-	-
12	Bioconcentration Factor	1.64 (1)	1.64	1.64	82.0 (3)	82	1.38 to 173	-
13								
14								

Chemical Properties

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[Comments](#)

- NCCT_Model predictions built on curated data
- All chemicals in CompTox Dashboard pushed through all predictive models
- Predicted data made available, with detailed **MODEL REPORTS**

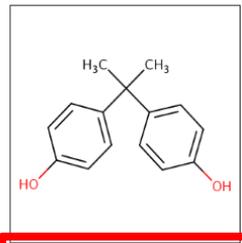
Predicted Data

Predicted

Source	Result	Calculation Details
EPISUITE	132 °C	Not Available
NCCT	144 °C	NCCT Model Report

NCCT Models: Melting Point

Bisphenol A
80-05-7 | DTXSID7020182



Model Results

Predicted value: 144 °C
 Global applicability domain: **Inside**
 Local applicability domain index: 0.91
 Confidence level: 0.65

Calculation Result for a chemical

Model Performance with full QMRF

Model Performance

QMRF

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Nearest Neighbors from Training Set

Nearest Neighbors from the Training Set

Bisphenol A
Measured: 153
Predicted: 144

4,4'-Propane-1,1'-diylidiphenol
Measured: 132
Predicted: 133

phenol, 4,4'-butylidenebis-
Measured: 137
Predicted: 142

Bisphenol B
Measured: 121
Predicted: 140

meso-Hexestrol
Measured: 187
Predicted: 157

Prediction Details and QMRF Report

Model Results

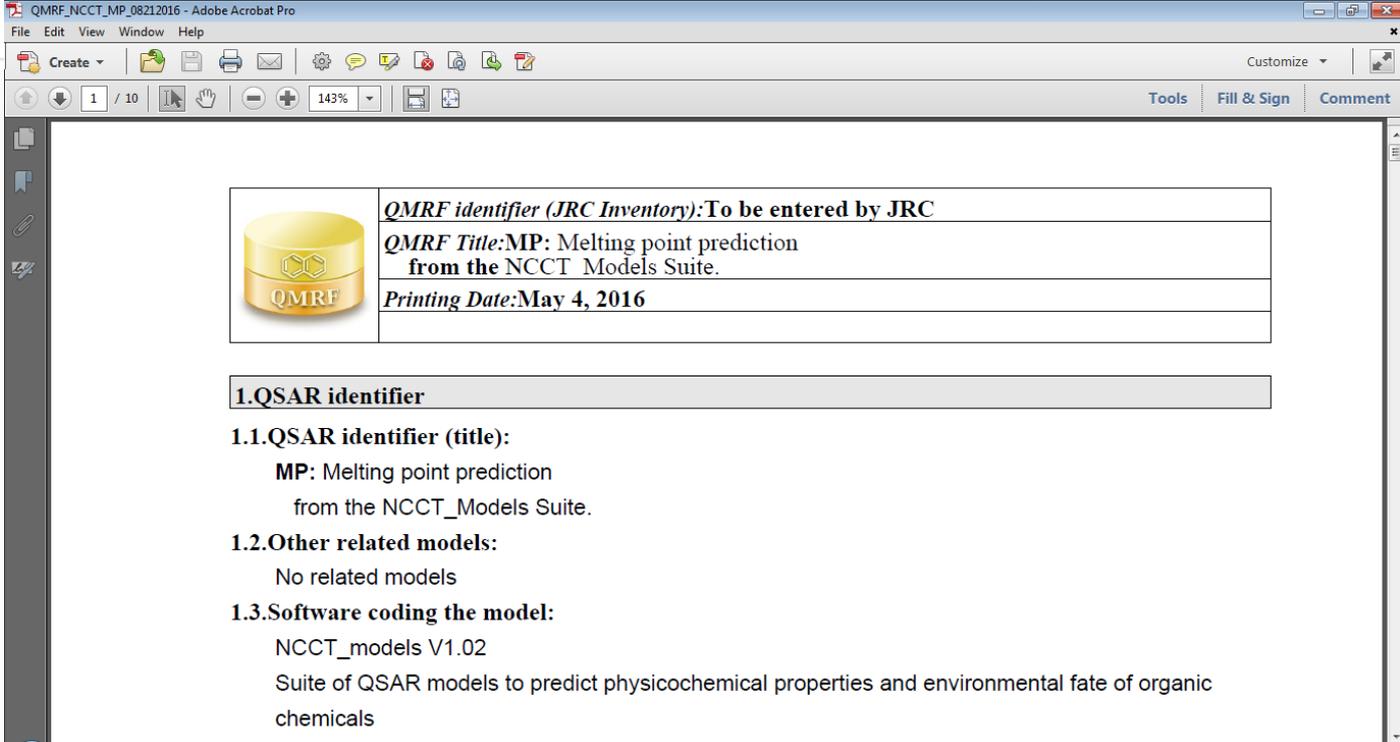
Predicted value: 144 °C

Global applicability domain: **Inside** ⓘ

Local applicability domain index: 0.91 ⓘ

Confidence level: 0.65 ⓘ

Applicability domain using the leverage approach. All training set space considered. More details in QMRF.



QMRF_NCCT_MP_08212016 - Adobe Acrobat Pro

File Edit View Window Help

Create [Icons]

1 / 10 [Navigation] 143% [Zoom] Tools Fill & Sign Comment

	QMRF identifier (JRC Inventory): To be entered by JRC
	QMRF Title: MP: Melting point prediction from the NCCT Models Suite.
	Printing Date: May 4, 2016

1. QSAR identifier

1.1. QSAR identifier (title):
MP: Melting point prediction from the NCCT_Models Suite.

1.2. Other related models:
No related models

1.3. Software coding the model:
NCCT_models V1.02
Suite of QSAR models to predict physicochemical properties and environmental fate of organic chemicals

External Links

Chemical Properties

External Links

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Comments

General

-  EPA Substance R...
-  NIST Chemistry ...
-  Household Produ...
-  PubChem
-  Chempider
-  CPCat
-  DrugBank
-  HMDB
-  Wikipedia
-  MSDS Lookup
-  ToxPlanet
-  ChemHat: Hazard...

Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  EDSP Dashboard
-  Gene-Tox
-  HSDB
-  ToxCast Dashboa...
-  LactMed
-  International Toxi...

Publications

-  Toxline
-  Environmental He...
-  NIEHS
-  National Toxicolo...
-  Google Books
-  Google Scholar
-  Google Patents
-  PubMed

Analytical

-  National Environ...
-  RSC Analytical A...

Prediction

-  Chemicalize
-  Proton NMR Predi...
-  Carbon-13 NMR ...
-  2D NMR HSQC/H...
-  ChemRTP Predictor

Chemical Properties

External Links

Synonyms

Product Composition

ToxCast in Vitro Data

Exposure

PubChem

Comments

Found 83 synonyms

Legend: **Valid Synonyms** *Good Synonyms* *Other Synonyms*

 Copy all Synonyms

Bisphenol A

4,4'-(Propane-2,2-diyl)diphenol

phenol, 4,4'-(1-methylethylidene)bis-

BPA

4,4'-Propane-2,2-diylidiphenol

Phenol, 4,4'-(1-methylethylidene)bis-

80-05-7 Active CAS-RN

4-06-00-06717 Beilstein Registry Number

UNII-MLT3645I99 FDA Registry Number

(4,4'-Dihydroxydiphenyl)dimethylmethane

Over a million synonyms, different
levels of curation and validation

Chemical Properties

External Links

Synonyms

Product Composition

ToxCast in Vitro Data

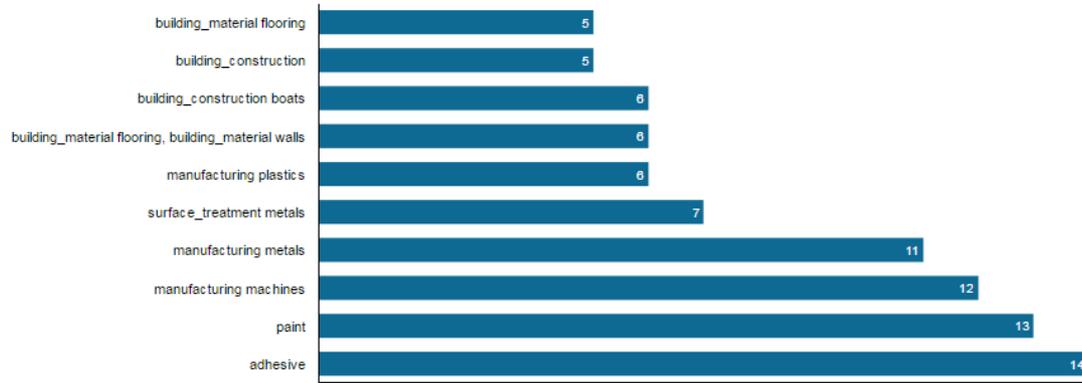
Exposure

PubChem

Comments

Functional Use and Composition (Integrating CPCat Data)

Frequent Uses and Functions



Download as: [CSV](#) [Excel](#)

Product Composition

Product	Percent Composition ↓	Manufacturer
BISPHENOL-A (BPA)	100%	GENERAL ELECTRIC COMPANY
EPOXY PASTE PIGMENTS, 3402-3408	<100%PPM	SYSTEM THREE RESINS
ISOPROPYLIDENEDIPHENOL, 99+%, 23965-8	99%+	ALDRICH CHEMICAL CO
BISPHENOL A (RESIN GRADE) (43106)	97.8%	SHELL OIL COMPANY
4,4-ISOPROPYLIDENEDIPHENOL, 97%, 13302-7	97%	ALDRICH CHEMICAL CO
ICO-PATCH EPOXY RESIN HARDENER, PART B	80%	INTERNATIONAL COATINGS CO
ADHESIVE-SCOTCH-WELD (R) 2216 B GRAY	72%	3M COMPANY
EPOCAST HARDENER 946, FPC 5000	45%	CIBA-GEIGY CORP
EPOLITE 1350 HANDENER	35-50	HEXCEL CORP, RESINS GROUP
EL CHEM NO 200 PRIMER PART B	22.5%	ELECTRO CHEMICAL ENGINEERING &

[Chemical Properties](#)

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[Product Composition](#)

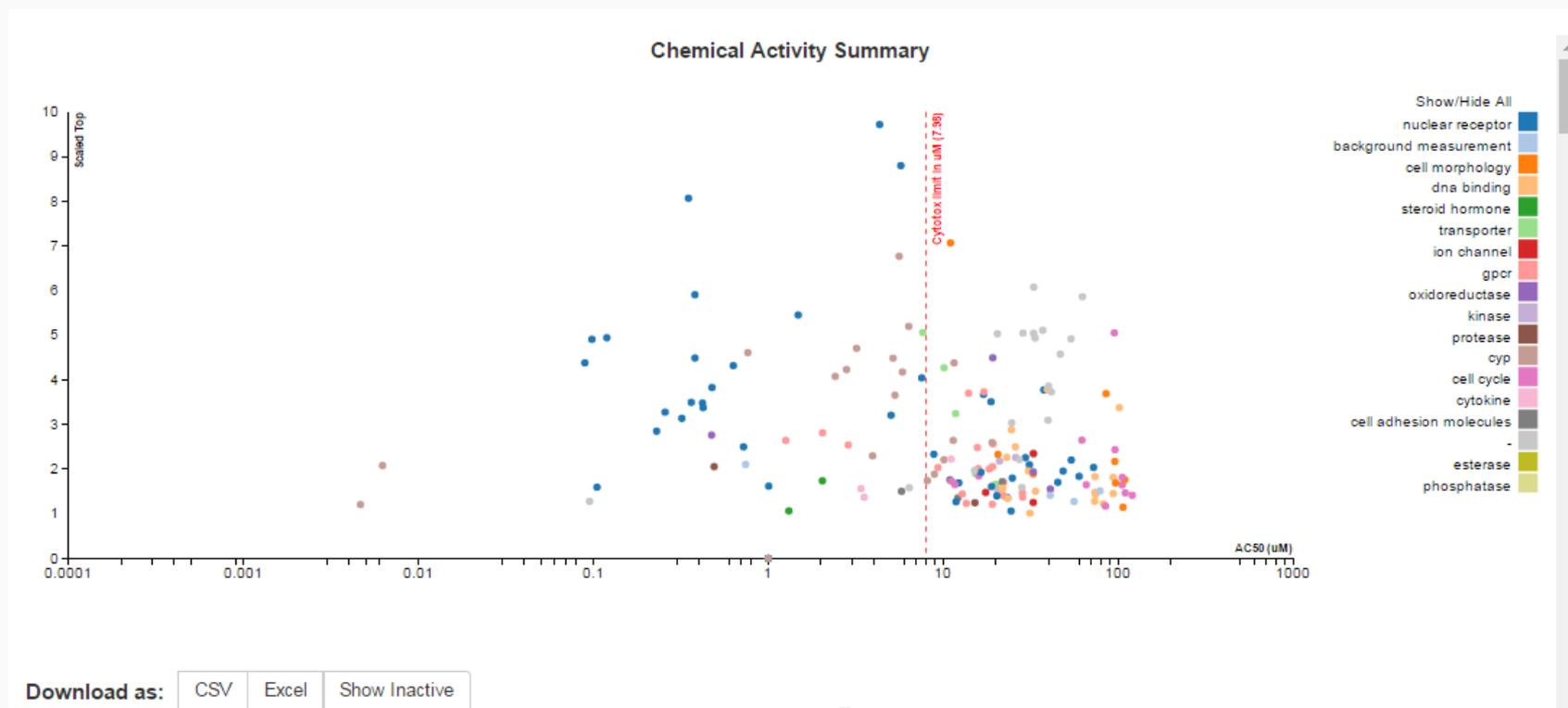
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Bioassay Screening Data (Integrating ToxCast Data)



Chemical Properties

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Bioassay Screening Data (Integrating ToxCast Data)

Assay Name	Hit Call	Top	Scaled Top	AC50 ↓	log AC50	Intended Target Family
APR_Hepat_CellLoss_48hr_dn						
APR_HepG2_OxidativeStress_24h_up						
APR_HepG2_MitoMass_24h_dn						
APR_Hepat_DNADamage_48hr_up						
APR_HepG2_CellLoss_24h_dn						
APR_HepG2_OxidativeStress_72h_up						
ATG_HSE_CIS_up						
APR_Hepat_DNADamage_24hr_up						
APR_Hepat_CellLoss_24hr_dn						
APR_Hepat_Steatosis_24hr_up						
APR_HepG2_CellLoss_72h_dn						

APR_HepG2_OxidativeStress_72h_up

Assay Name: APR_HepG2_OxidativeStress_72h_up

Gene Symbol: null

Organism: human

Tissue: liver

Assay Format Type: cell-based

Biological Process Target: oxidative phosphorylation

Detection Technology: Fluorescence

Analysis Direction: positive

Intended Target Family: cell cycle

Description: Data from the assay component APR_HepG2_OxidativeStress_72hr was analyzed into 2 assay endpoints. This assay endpoint, APR_HepG2_OxidativeStress_72h_up, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of viability reporter, measures of protein for gain-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene . Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "cell cycle" intended target family, where the subfamily is "stress response".

[Chemical Properties](#)[External Links](#)[Synonyms](#)[Product Composition](#)[ToxCast in Vitro Data](#)[Exposure](#)[PubChem](#)[Comments](#)

Exposure Data – NHANES and ExpoCast Predictions

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

	Ages 6-11	Ages 12-19	Ages 20-65	Ages 65+	BMI > 30	BMI < 30	Repro. Age Females	Females	Males	Total
Minimum	3.80e-05	2.55e-05	2.79e-05	1.91e-05	2.38e-05	3.02e-05	2.83e-05	2.58e-05	2.94e-05	2.86e-05
Maximum	4.92e-05	3.38e-05	3.27e-05	2.31e-05	2.74e-05	3.30e-05	3.31e-05	3.03e-05	3.37e-05	3.08e-05
Mean	4.33e-05	2.93e-05	3.02e-05	2.10e-05	2.55e-05	3.16e-05	3.06e-05	2.80e-05	3.15e-05	2.97e-05

① Exposure Predictions (mg/kg-bw/day)

	Ages 6-11	Ages 12-19	Ages 20-65	Ages 65+	BMI > 30	BMI < 30	Repro. Age Females	Females	Males	Total
Median	6.30e-05	2.68e-05	2.05e-05	1.61e-05	1.69e-05	2.67e-05	1.11e-05	1.11e-05	3.89e-05	2.11e-05
95th Percentile	5.82e-03	2.00e-03	1.61e-03	2.18e-03	1.45e-03	2.26e-03	1.57e-03	9.09e-04	3.34e-03	2.00e-03



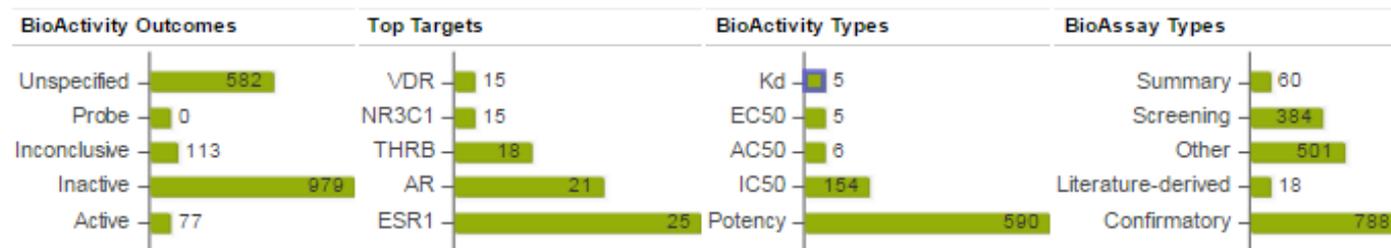
National Health and Nutrition Examination Survey

High-Throughput Models for Exposure-Based Chemical Prioritization in the ExpoCast Project

Environ. Sci. Technol., 2013, 47 (15), pp 8479–8488



Biological Activities



Structure	Substance SID	Activity			Compound Name	Bioassay Name
		Outcome	Type	Value [μ M]		
	312534041	Inactive			Bisphenol A	Screen for inhibitors of RMI FANCM (MM2) interaction [AID: 1159607 , Type: Other, PubMed ID: 26962873]
	144214049	Inconclu...	Potency	62.1889	Bisphenol A	qHTS assay for small molecule agonists of the p53 signaling pathway [AID: 651631 , Type: Confirmatory]
	144214049	Inactive	Potency		Bisphenol A	qHTS assay for small molecules that induce genotoxicity in human embryonic kidney cells expressing luciferase-tagged ATAD5 [AID: 651632 , Type: Confirmatory]
	144214049	Inconclu...	Potency	55.4259	Bisphenol A	qHTS assay for small molecule agonists of the p53 signaling pathway - cell viability [AID: 651633 , Type: Confirmatory]
	144214049	Inactive	Potency		Bisphenol A	qHTS assay for small molecules that induce genotoxicity in human embryonic kidney cells expressing...

Work in Progress: Environmental Fate, Transport and Toxicity

Applications Places System | 90 °F | Thu Jul 21, 4:21 PM | Jennifer Smith

RapidTox | Auramine hydrochloride - Mozilla Firefox

localhost:4040/dsstoxydb/results?exact=1&list_abbreviation=OPPINERTS&mass=0&search=Auramine+hydrochloride&single_component=0

EPA United States Environmental Protection Agency | Home | Chemistry Dashboard | Search Chemistry Dashboard

Submit Comment | Share | Copy

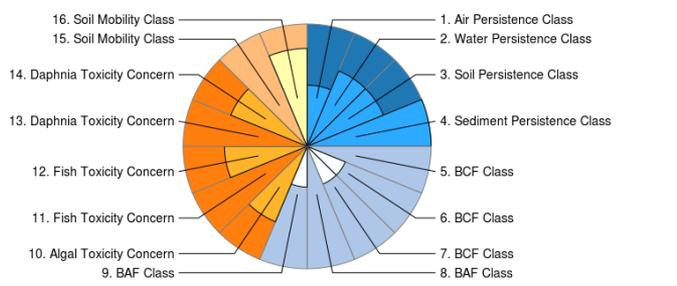
Chemical Properties | External Links | Synonyms | Product Composition | ToxCast in Vitro Data | Analytical | Toxicity Values | Similar Molecules | Exposure | Literature | PubChem | Comments

Predicted Hazards

Summary

- Toxicity
- EFate
- Ecotox
- Organ Toxicity

Predicted Hazards / Summary / Radial Plot



16. Soil Mobility Class
15. Soil Mobility Class
14. Daphnia Toxicity Concern
13. Daphnia Toxicity Concern
12. Fish Toxicity Concern
11. Fish Toxicity Concern
10. Algal Toxicity Concern
9. BAF Class

1. Air Persistence Class
2. Water Persistence Class
3. Soil Persistence Class
4. Sediment Persistence Class
5. BCF Class
6. BCF Class
7. BCF Class
8. BAF Class

■ Persistence ■ Bioaccumulation ■ Ecotox ■ Soil Mobility

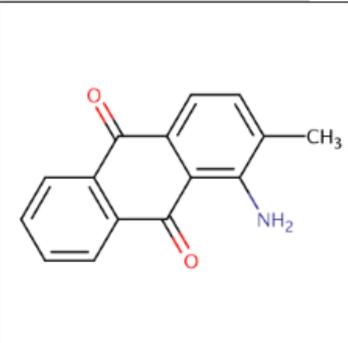
No.	Category	Model Name
1	Air Persistence Class	EPISUITE_Fugacity_3_air ⓘ
2	Water Persistence Class	EPISUITE_Fugacity_3_water ⓘ
3	Soil Persistence Class	EPISUITE_Fugacity_3_soil ⓘ
4	Sediment Persistence Class	EPISUITE_Fugacity_3_sediment ⓘ

localhost:4040/dsstoxydb/results?exact=1&list_abbreviation=OPPINERTS&mass=0&search=Auramine+hydrochloride&single_component=0#hazard-toxicity

RapidTox | Auramine h... | jsmith09@v2626umct... | icss-client - [/localdisk... | Google Hangouts - jen...

Work in Progress: Analog Identification and Similarity Search

3D     



Intrinsic Properties

Molecular Formula: C₁₅H₁₁NO₂

Average Mass: 237.257996 g/mol

Monoisotopic Mass: 237.078979 g/mol

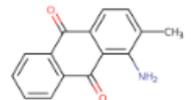
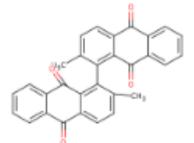
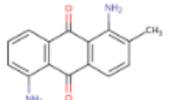
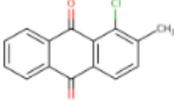
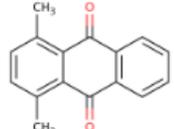
Structural Identifiers

Record Information

[Chemical Properties](#) [External Links](#) [Synonyms](#) [Product Composition](#) [ToxCast in Vitro Data](#) [Analytical](#) [Toxicity Values](#) **[Similar Molecules](#)**

[Exposure](#) [PubChem](#) [Comments](#)

Found 12 Similar Molecules
Searched with a similarity threshold of 0.6

 <p>1-Amino-2-methylanthraq... Similarity Index: 1.00</p>	 <p>[1,1'-Bianthracene]-9,9',1... Similarity Index: 0.75</p>	 <p>Anthraquinone, 1,5-diam... Similarity Index: 0.74</p>	 <p>9,10-Anthracenedione, 1... Similarity Index: 0.68</p>	 <p>9,10-Anthracenedione, 1... Similarity Index: 0.67</p>
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- NCCT has been delivering data, algorithms, models and software tools for a decade
- A new flexible architecture to support multiple both internal and external apps
- First iteration of CompTox dashboard supports chemistry based searches
- Future concept...



CompTox Dashboard

Chemicals	Products	Targets	Assays	Literature
-----------	----------	---------	--------	------------

Search a chemical by systematic name, synonym, CAS number, or InChIKey



Acknowledgements



Credit: the Research Triangle Foundation

*Kamel Mansouri
Chris Grulke
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Jeff Edwards
Matt Martin
John Wambaugh
Grace Patlewicz
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Kevin Crofton
Russell Thomas*