CTD: a resource for predicting chemical-gene-disease networks

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Chemical landscape

- > 60,000
- ~2,000 added/year
- ~8,000 are carcinogens
- No toxicity data for ~40% of the 3,300 “high production volume” chemicals
- Full toxicity data for only 25% of chemicals in consumer products

Category	Size of Category	Estimate Mean Percent In the Select Universe
Pesticides and Inert Ingredients of Pesticides Formulations	3,350	10 24 2 26 38
Cosmetic Ingredients	3,410	2 14 10 18 56
Drugs and Excipients Used in Drug Formulations	1,815	18 18 3 36 25
Food Additives	8,627	5 14 1 34 46
Chemicals in Commerce: At Least 1 Million Pounds/Year	12,860	11 11 78
Chemicals in Commerce: Less than 1 Million Pounds/Year	13,911	12 12 76
Chemicals in Commerce: Production Unknown or Inaccessible	21,752	10 8 82

Complete Health Hazard Assessment Possible

Partial Health Hazard Assessment Possible

Minimal Toxicity Information Available

Some Toxicity Information Available (But Below Minimal)

No Toxicity Information Available

Crofton et al. Congenital Anomalies 2012; 52, 140–146

Many disorders are on the rise

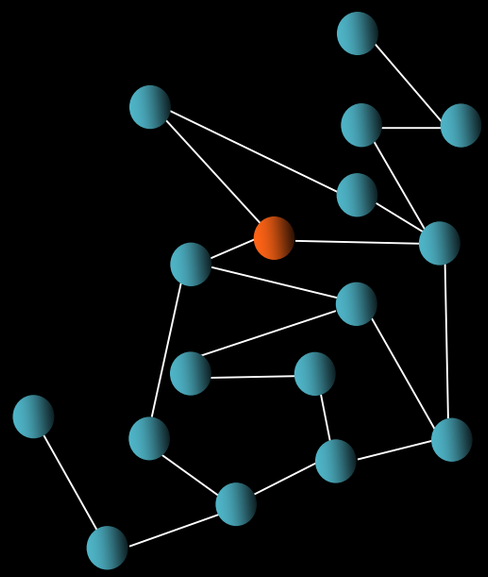
- Leukemia
- Cancers (Brain, breast, childhood)
- Asthma
- Fertility and full term pregnancies
- Birth defects
- Autism

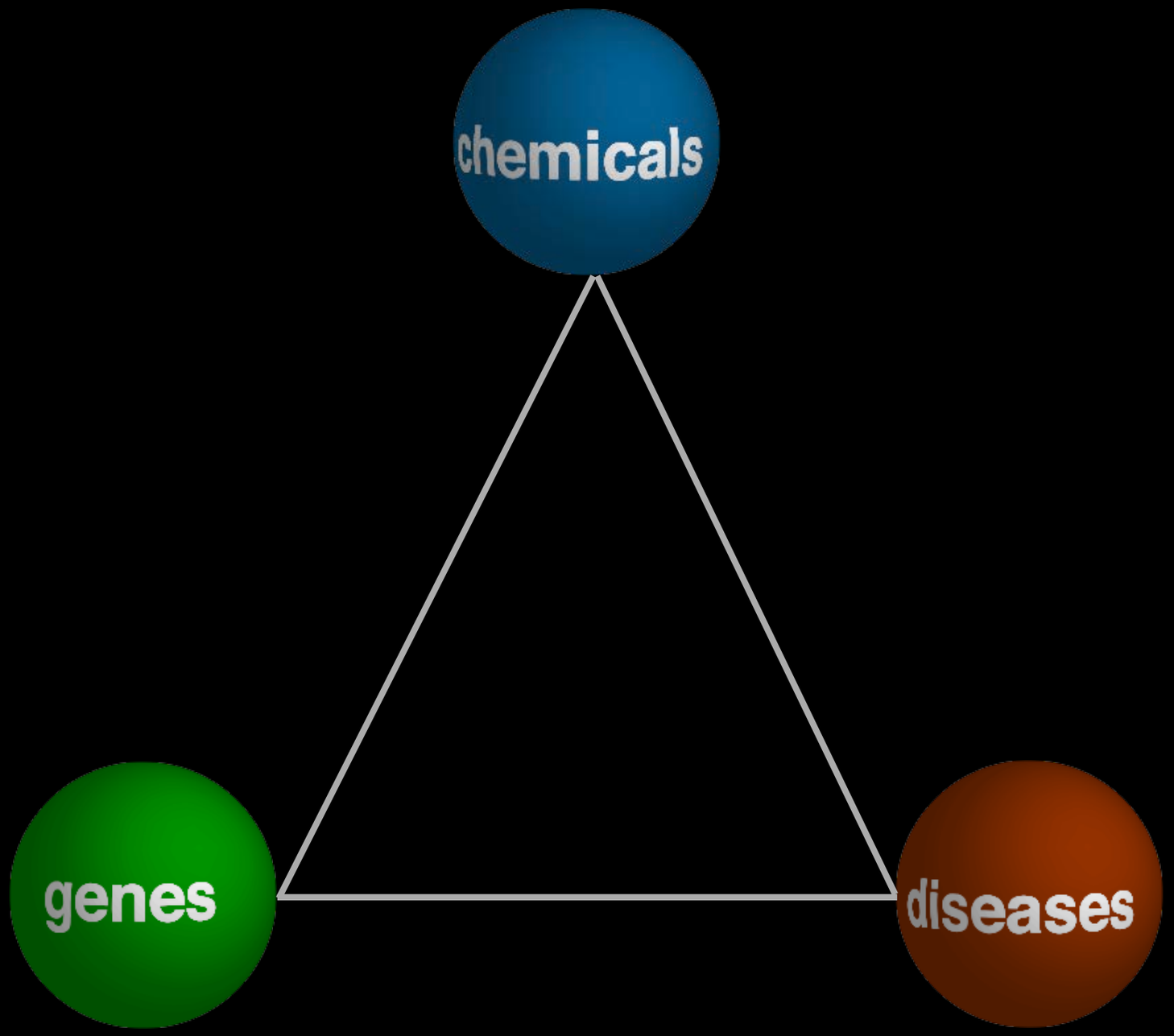
How does the environment affect our health?

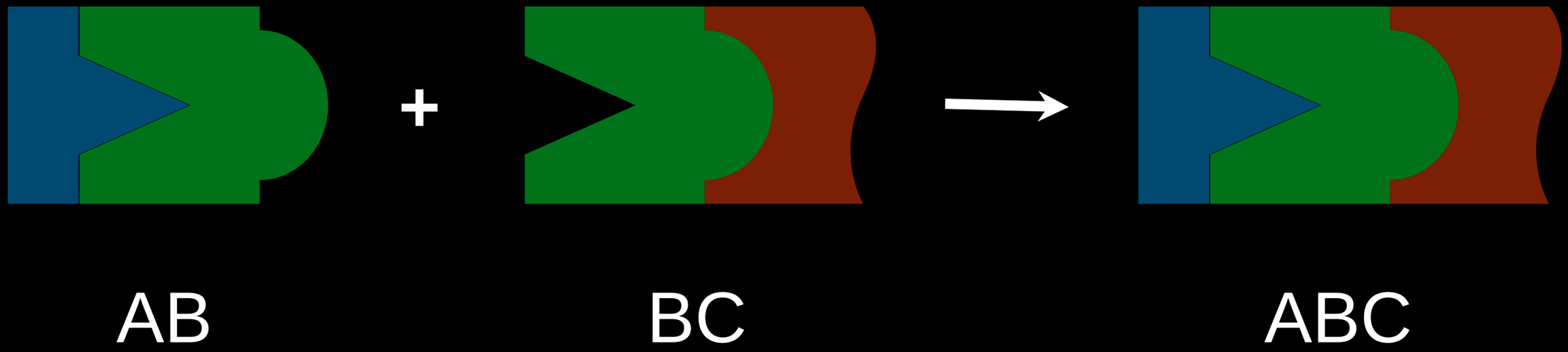
Environment
(chemicals)

Genes

Disease

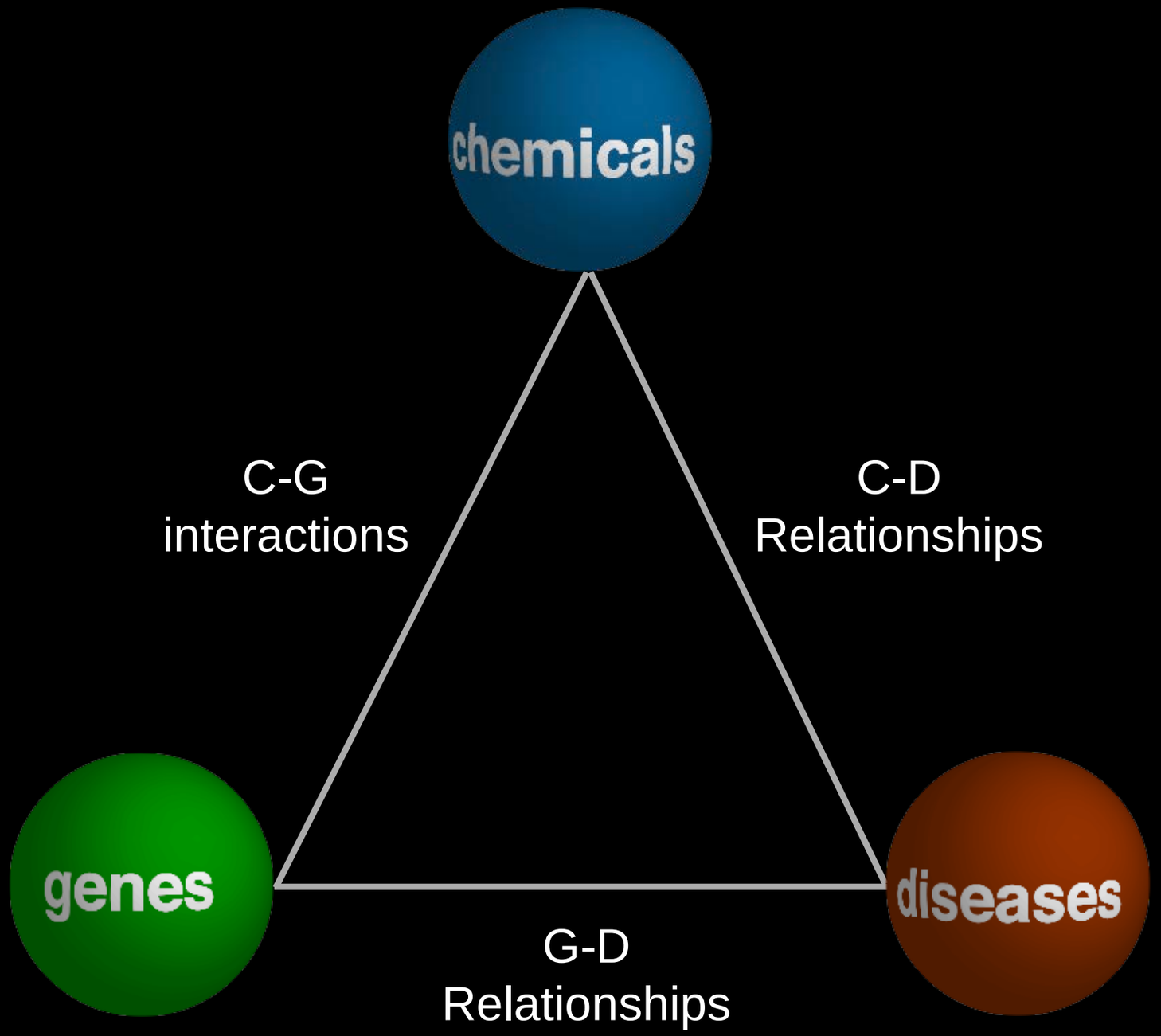



chemicals
genes
diseases



AB BC ABC

Evans and Rzhetsky, Science, 329:399 (2010)


chemicals
C-G
interactions
C-D
Relationships
genes
diseases
G-D
Relationships

chemicals
genes
diseases
5,896 Genes
163 Genes
57 curated
>1,000 inferred
Breast Cancer

Giving insight into how chemicals affect our health.

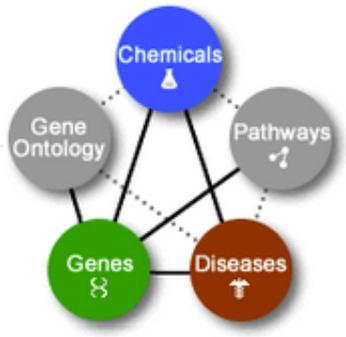
Comparative Toxicogenomics Database

Connec

CTD illum nental chemicals affect human health.
More...

Discov

1. What h associated with a gene/protein? (Example)
2. What h associated with a chemical? (Example)
3. What g ct with a chemical? (Example)
4. What c th a gene/protein? (Example)
5. What r hemical–gene/protein interaction? (Example)
6. What cellular functions (GO terms) are affected by a chemical? (Example)



16,241,275 TOXICOGENOMIC RELATIONSHIPS!

Keyword Search

All

Name, ID, author...

Search | Advanced searches

Updated Chemicals

(4-amino-1,4-dihydro-3-(2-pyridyl)-5-thioxo-1,2,4-triazole)copper(II) 2',3,3',4',5-pentachloro-4-hydroxybiphenyl 4-hydroxy-2-nonenal Cadmium Cadmium Chloride cadmium sulfate cobaltiprotoporphyrin cobaltous chloride Copper Copper Sulfate cupric chloride Cisplatin Ethanol Hydrogen Peroxide Iron lead acetate lead nitrate Lipopolysaccharides Mercuric Chloride Mercury Oxygen Streptozocin Tetradecanoylphorbol Acetate Tretinoin vinclozolin

Updated Diseases

Updated Genes

News

- *August 7, 2012*
  New data available!
- *July 19, 2012*
  You can now create custom similarity analyses for ChemComps and GeneComps!
- *May 8, 2012*
  Use our new Gene Set Enricher tool to find GO functional annotations or pathways that are enriched for a set of genes.
- *January 9, 2012*
  Use our new MyVenn tool to view relationships among your own data sets.
- *November 7, 2011*
  We have a new URL! http://ctdbase.org/
- *September 15, 2011*
  Exposure data is coming.
- *All changes...*

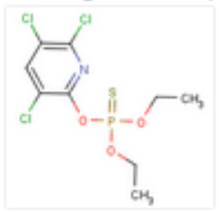
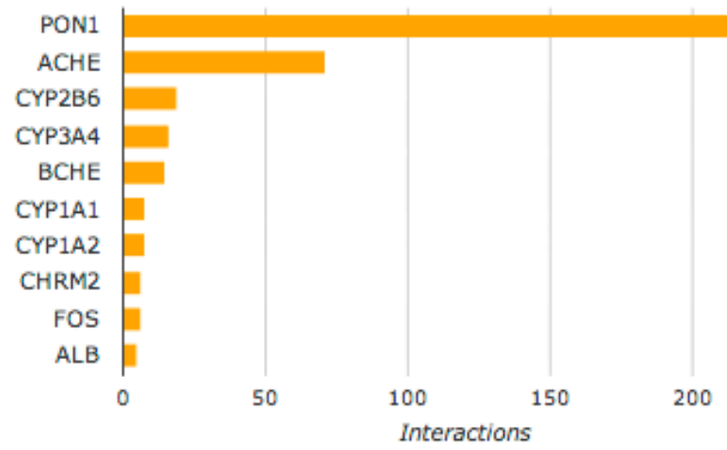
Subscribe to CTD's mailing list:
Email address Subscribe

Our Latest Publication

- Hirschman L, Burns GA, Krallinger M, Arighi C, Cohen KB, Valencia A, Wu CH, Chatr-Aryamontri A, Dowell KG, Huala E, Lourenço A, Nash R, Veuthey AL, Wiegers T, Winter AG.
  Text mining for the biocuration workflow.
  Database (Oxford). 2012 Apr 18;2012:bas020. Print 2012. [PMID:22513129]
- *All CTD publications...*

Chlorpyrifos

Basics | Interactions | Genes | Diseases | ChemComps | Pathways | GO | References | Links

Name	**Chlorpyrifos**
CAS Type 1 Name	Phosphorothioic acid, O,O-diethyl O-(3,5,6-trichloro-2-pyridinyl) ester
Equivalent Terms	Dursban · Lorsban
CAS Registry Number	2921-88-2
Definition	An organothiophosphate cholinesterase inhibitor that is used as an insecticide and as an acaricide.
Chemical Drawing	
MeSH® ID	D004390
Curator Note	*For additional curated data about phosphorus, please also see Phosphorus and its chemical descendants.*
Top Interacting Genes	

Ancestors

Top ↑

1. Chemicals ← Organic Chemicals ← Organophosphorus Compounds ← Organophosphates ← Organothiophosphates ← *Chlorpyrifos*
2. Chemicals ← Organic Chemicals ← Organophosphorus Compounds ← Organothiophosphorus Compounds ← Organothiophosphates ← *Chlorpyrifos*
3. Chemicals ← Organic Chemicals ← Sulfur Compounds ← Organothiophosphorus Compounds ← Organothiophosphates ← *Chlorpyrifos*

Descendants

Top ↑

Chlorpyrifos
- chlorpyrifos-methyl
- O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphate

Chlorpyrifos

Basics | Interactions | Genes | Diseases | ChemComps | Pathways | GO | References | Links

1–100 of 1,901 results.

First | Previous | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | Next | Last

	Interacting Chemical	Interacting Gene	Interaction	References	Organisms
1.	Chlorpyrifos	ABCA1A	Chlorpyrifos results in increased expression of ABCA1A mRNA	1	1
2.	Chlorpyrifos	ABCA1A	[Copper co-treated with Chlorpyrifos] results in increased expression of ABCA1A mRNA	1	1
3.	Chlorpyrifos	ABCA5	[Copper co-treated with Chlorpyrifos] results in decreased expression of ABCA5 mRNA	1	1
4.	Chlorpyrifos	ABCB1	Chlorpyrifos binds to ABCB1 protein	1	1
5.	Chlorpyrifos	ABCB1	Chlorpyrifos inhibits the reaction [ABCB1 protein results in increased export of Doxorubicin]	1	1
6.	chlorpyrifos-methyl			1	1
7.	chlorpyrifos-methyl		esults in increased transport	1	1
8.	Chlorpyrifos		NA	1	1
9.	Chlorpyrifos		NA	1	1
10.	Chlorpyrifos		expression of ABCF2 mRNA	1	1
11.	Chlorpyrifos		NA	1	1
12.	Chlorpyrifos	ABCG8	Chlorpyrifos results in increased expression of ABCG8 mRNA	1	1
13.	Chlorpyrifos	ABHD2B	[Copper co-treated with Chlorpyrifos] results in decreased expression of ABHD2B mRNA	1	1
14.	Chlorpyrifos	ABI3BP	Chlorpyrifos results in increased expression of ABI3BP mRNA	1	1
15.	Chlorpyrifos	ACACA	[Copper co-treated with Chlorpyrifos] results in increased expression of ACACA mRNA	1	1
16.	Chlorpyrifos	ACAT2	Chlorpyrifos results in increased expression of ACAT2 mRNA	1	1
17.	Chlorpyrifos	ACAT2	[Copper co-treated with Chlorpyrifos] results in increased expression of ACAT2 mRNA	1	1
18.	Chlorpyrifos	ACCN2	Chlorpyrifos results in decreased expression of ACCN2 mRNA	1	1
19.	Chlorpyrifos	ACE1	ACE1 gene mutant form results in decreased susceptibility to Chlorpyrifos	1	1
20.	Chlorpyrifos	ACE-1	ACE-3 protein inhibits the reaction [Chlorpyrifos results in decreased activity of ACE-1 protein]	1	1
21.	Chlorpyrifos	ACE-1	Chlorpyrifos results in decreased activity of ACE-1 protein	1	1
22.	Chlorpyrifos	ACE-2	ACE-3 protein inhibits the reaction [Chlorpyrifos results in decreased activity of ACE-2 protein]	1	1
23.	Chlorpyrifos	ACE-2	Chlorpyrifos results in decreased activity of ACE-2 protein	1	1
24.	Chlorpyrifos	ACE-3	ACE-3 protein inhibits the reaction [Chlorpyrifos results in decreased activity of ACE-1 protein]	1	1
25.	Chlorpyrifos	ACE-3	ACE-3 protein inhibits the reaction [Chlorpyrifos results in decreased activity of ACE-2 protein]	1	1

Chlorpyrifos

Basics | Interactions | Genes | Diseases | ChemComps | Pathways | GO | References | Links

1–100 of 1,167 results.

First | Previous | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | Next | Last

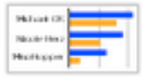
	Interacting Gene	Interactions	Organisms
1.	PON1	240	3
2.	ACHE	71	15
3.	CYP2B6	19	2
4.	CYP3A4	16	1
5.	BCHE	15	3
6.	CYP1A1	8	4
7.	CYP1A2	8	1
8.	CHRM2	6	2
9.	FOS	6	2
10.	ALB	5	1
11.	CYP2C19	5	1
12.	SOD1	5	3
13.	ABCB1	4	1
14.	ADRBK1	4	1
15.	AHR	4	3
16.	ATP2B2	4	2
17.	CAT	4	2
18.	CNR1	4	1
19.	DLG4	4	2
20.	GNRH1	4	2
21.	GRM2	4	2
22.	HSP70	4	3
23.	NCAM1	4	3
24.	NDUFB3	4	3
25.	NDUFB4	4	3
26.	NLGN2	4	2
27.	NR1I2	4	2
28.	NR1I3	4	2
29.	SEMA4F	4	3
30.	SNAPIN	4	3
31.	SYN2	4	2
32.	TNR	4	3

Chlorpyrifos

Basics | Interactions | Gene

These diseases are associate
(via a curated gene interacti

Disease categories [Show chart]



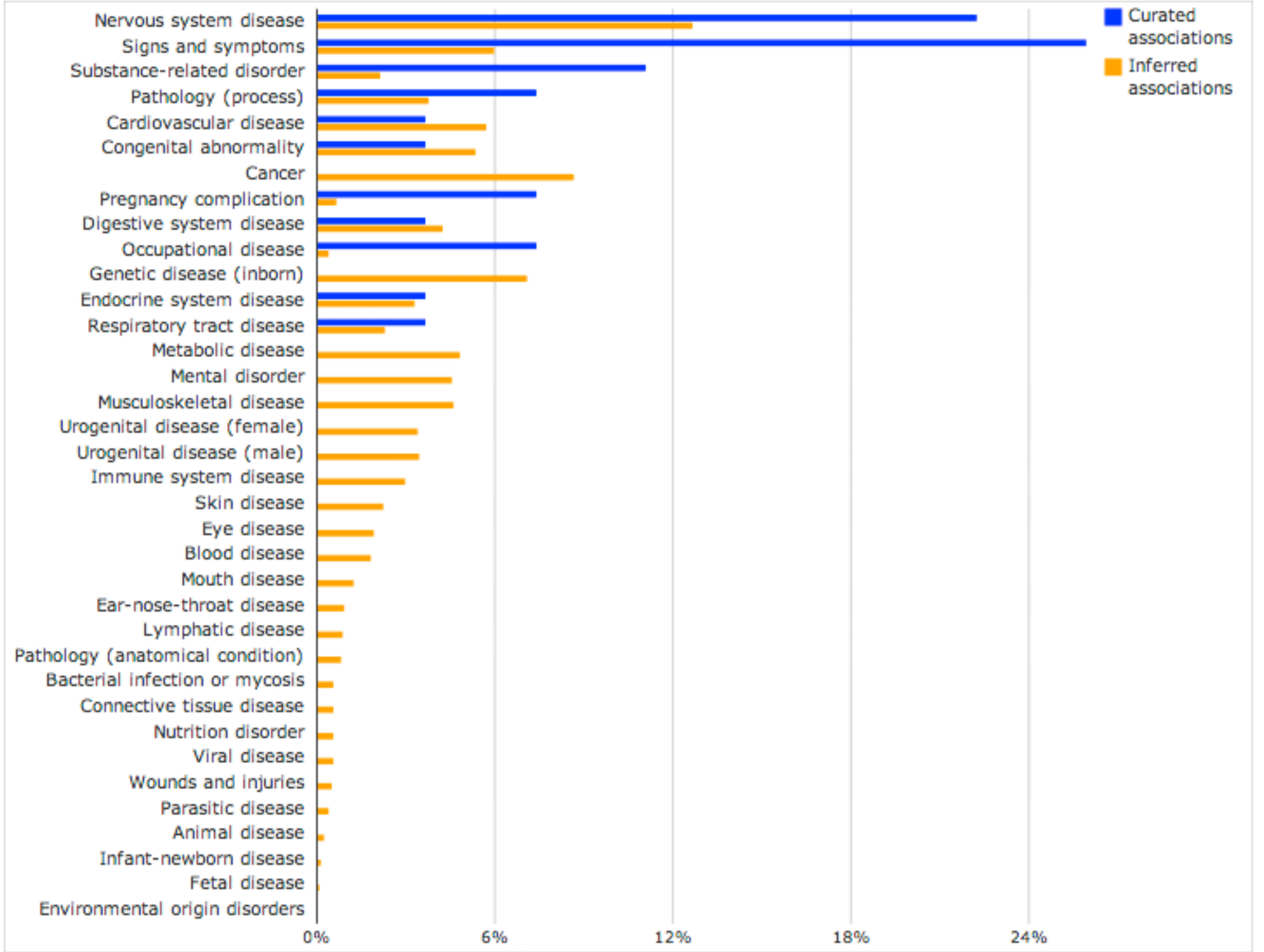
Filter by | Disease category: All categories

1–100 of 1,328 results.

First | Previous | 1 | 2 | 3 | 4 | 5

	Chemical	Disea					erences
1.	Chlorpyrifos	Nervous S Diseases					19
2.	Chlorpyrifos	Neurotoxi Syndrome					10
3.	Chlorpyrifos	Liver Dise					20
4.	Chlorpyrifos	Brain Dise					2
5.	Chlorpyrifos	Persian G Syndrome					2
6.	Chlorpyrifos	Weight Lo					3
7.	Chlorpyrifos	Fetal Deat					3
8.	O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphate	Poisoning					6
9.	O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphate	Hypotherr			1 gene: CNR1		2
10.	O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphate	Nervous System Diseases	M	GO	*2 genes:* ACHE · PNPLA6	3.09	4

Disease categories [Hide chart]

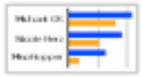


Chlorpyrifos

Basics | Interactions | Genes | Diseases | ChemComps | Pathways | GO | References | Links

These diseases are associated with *Chlorpyrifos* or its descendants. Each association is *curated* (M *marker/mechanism* and/or T *therapeutic*) and/or *inferred* (via a curated gene interaction).

Disease categories [Show chart]



Filter by | Disease category: All categories | Association type: All types | Filter

1–100 of 1,328 results.

First | Previous | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | Next | Last

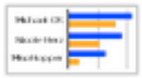
	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Chlorpyrifos	Nervous System Diseases	M	GO	*17 genes:* ABCB1 · ABCG2 · ACHE · ADRB2 · ATF3 · BDNF · CASP3 · CASP9 · FOS · GFAP · NGF · PENK · SEPP1 · SLC18A2 · SLC6A3 · SOD1 · TNF	7.77	19
2.	Chlorpyrifos	Neurotoxicity Syndromes	M	GO	*10 genes:* ABCB1 · BCHE · BCL2L1 · CCK · CYP3A5 · FOS · NFE2L2 · NQO1 · PON1 · TIMP3	5.04	10
3.	Chlorpyrifos	Liver Diseases	M	GO	*13 genes:* AHR · ALPL · BCL2L1 · CCK · CYP1A2 · HMOX1 · NQO1 · SC5DL · SERPINA1 · SOCS1 · SOD1 · TIMP3 · TNF	4.73	20
4.	Chlorpyrifos	Brain Diseases	M		*1 gene:* TH	3.96	2
5.	Chlorpyrifos	Persian Gulf Syndrome	M		*1 gene:* PON1	3.70	2
6.	Chlorpyrifos	Weight Loss	M	GO	*2 genes:* CRH · OXT	3.57	3
7.	Chlorpyrifos	Fetal Death	M	GO	*2 genes:* LPAR1 · OXT	3.31	3
8.	O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphate	Poisoning	M	GO	*2 genes:* ACHE · BCHE	3.10	6
9.	O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphate	Hypothermia	M		*1 gene:* CNR1	3.09	2
10.	O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphate	Nervous System Diseases	M	GO	*2 genes:* ACHE · PNPLA6	3.09	4

Chlorpyrifos

Basics | Interactions | Genes | Diseases | ChemComps | Pathways | GO | References | Links

These diseases are associated with *Chlorpyrifos* or its descendants. Each association is *curated* (M *marker/mechanism* and/or T *therapeutic*) and/or *inferred* (via a curated gene interaction).

Disease categories [Show chart]



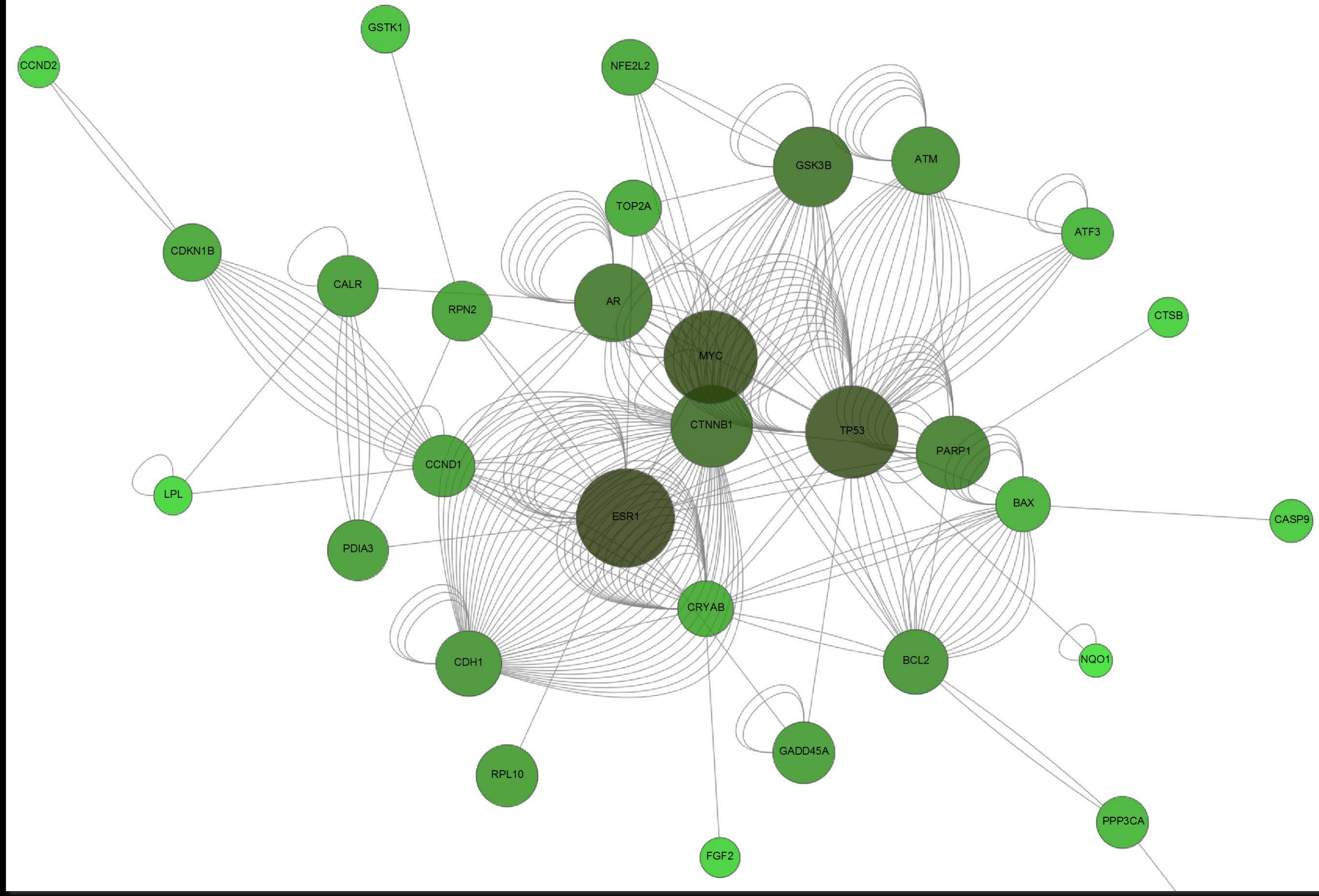
Filter by (Disease category: All categories; Animal disease; Bacterial infection or mycosis; Blood disease; Cancer) (Association type: All types; curated; inferred) Filter

1–100 of 1,3

First | P | Next | Last

	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Chlorpyrifos	Prostatic Neoplasms		GO	*54 genes:* ACHE · ADRB2 · AR · ATF3 · ATM · BAX · CALR · CASP9 · CCND1 · CCND2 · CDH1 · CDH13 · CDKN1B · COMT · CRYAB · CSRP1 · CTNNB1 · CTSB · CYP1A1 · CYP3A4 · CYP3A5 · EIF3A · ESR1 · FGF2 · FGFR4 · GADD45A · GSK3B · GSTA1 · GSTK1 · GSTM1 · GSTM3 · GSTO1 · GSTT1 · IGF1 · IL6 · LPAR1 · LPL · MYC · NQO1 · PDIA3 · PENK · PON1 · PPP3CA · RNASE4 · RPL10 · RPN2 · SEPP1 · SLC12A2 · SOD2 · TGFA · TGFB1 · TNFSF10 · TOP2A · TP53	42.13	68
2.	Chlorpyrifos	Autistic Disorder		GO	*36 genes:* ADRB2 · AR · AVPR1A · BDNF · CACNA1C · CAT · CHRNA7 · CHRNB2 · COMT · DHCR7 · DLGAP2 · EGR2 · GPX1 · GRIA1 · GRIK2 · GRIN2A · GSTM1 · HTR1B · HTR1D · HTR2A · HTR5A · IGF1 · IL13 · IL6 · MEF2C · NRCAM · NTF3 · NTRK2 · OXT · OXTR · PON1 · ROBO2 · RPL10 · SLC6A4 · SLC6A8 · WNT2	35.71	46
3.	Chlorpyrifos	Carcinoma, Hepatocellular		GO	*41 genes:* ABCB1 · ACACA · AR · ATM · BCL2L1 · BTG2 · CCNA1 · CCND1 · CDH13 · CEBPA · CEBPB · COMT · CTNNB1 · CYP1A1 · CYR61 · ESR1 · FOS · GPC3 · GSTM1 · HSPA5 · IGF2R · IL6 · KRAS · MED1 · MYC · NFE2L2 · PDGFRL · PDIA3 · PRDX6 · PTK2 · SCD · SERPINA1 · SKP2 · SLIT2 · SOD2 · TGFA · TGFB1 · TH · TNFSF10 · TP53 · USP2	35.27	43
4.	Chlorpyrifos	Breast Neoplasms		GO	*51 genes:* ABCG2 · AHR · AR · ATM · BAG1 · BAX · CASP7 · CCND1 · CDH1 · CDKN1B · COMT · CTNNB1 · CYP1A1 · CYP2B1 · CYP2D6 · CYP3A4 · DKK1 · EDNRB · ESR1 · FGFR2 · FOS · GPX1 · GPX2 · GPX4 · HMOX1 · HP · HSP90AA1 · IGF1 · IGFBP5 · IL1B · IL6 · KDR · KIT · KRAS · KRT18 · LLGL1 · LPAR1 · MTDH · NOTCH1 · NQO1 · NRCAM · RGS2 · RRAD · SFRP5 · SOD2 · TGM2 · TNF · TNFSF10 · TOP2A · TP53 · WNT10B	32.71	63
5.	Chlorpyrifos	Schizophrenia		GO	*31 genes:* BDNF · CAMK2B · CELF2 · COMT · DLG1 · DRD2 · DRD4 · EIF5 · GABRB2 · GRIK2 · GRIK5 · GRIN2B · GRM2 · GSK3B · HP · HTR2A · HTR6 · HTR7 · IL1B · IL6 · KDR · NTF3 · NTRK1 · OXTR · RTN4 · SLC6A3 · SLC6A4 · TAC1 · TNF · TP53 · TPH1	30.05	31

PLoS One. 2012;7(11):e46524.


GSTK1
CCND2
NFE2L2
GSK3B
ATM
TOP2A
ATF3
CDKN1B
CALR
RPN2
AR
CTSB
MYC
CTNNB1
TP53
PARP1
CCND1
LPL
BAX
CASP9
ESR1
PDIA3
CRYAB
CDH1
BCL2
NQO1
GADD45A
RPL10
PPP3CA
FGF2

Chlorpyrifos

Basics | Interaction

These chemicals hav

Filter by interaction typ

- ☑ *increases*
- ☑ *decreases*
- ☐ *affects (degree unspeci*

all (unfiltered)
activity
binding
expression

Pathway view of top

Met
cyp
Chlorodiph
de
Methyl
C
pentabromodiph
P
Chlor
Plar
alpha-hexachlorocy
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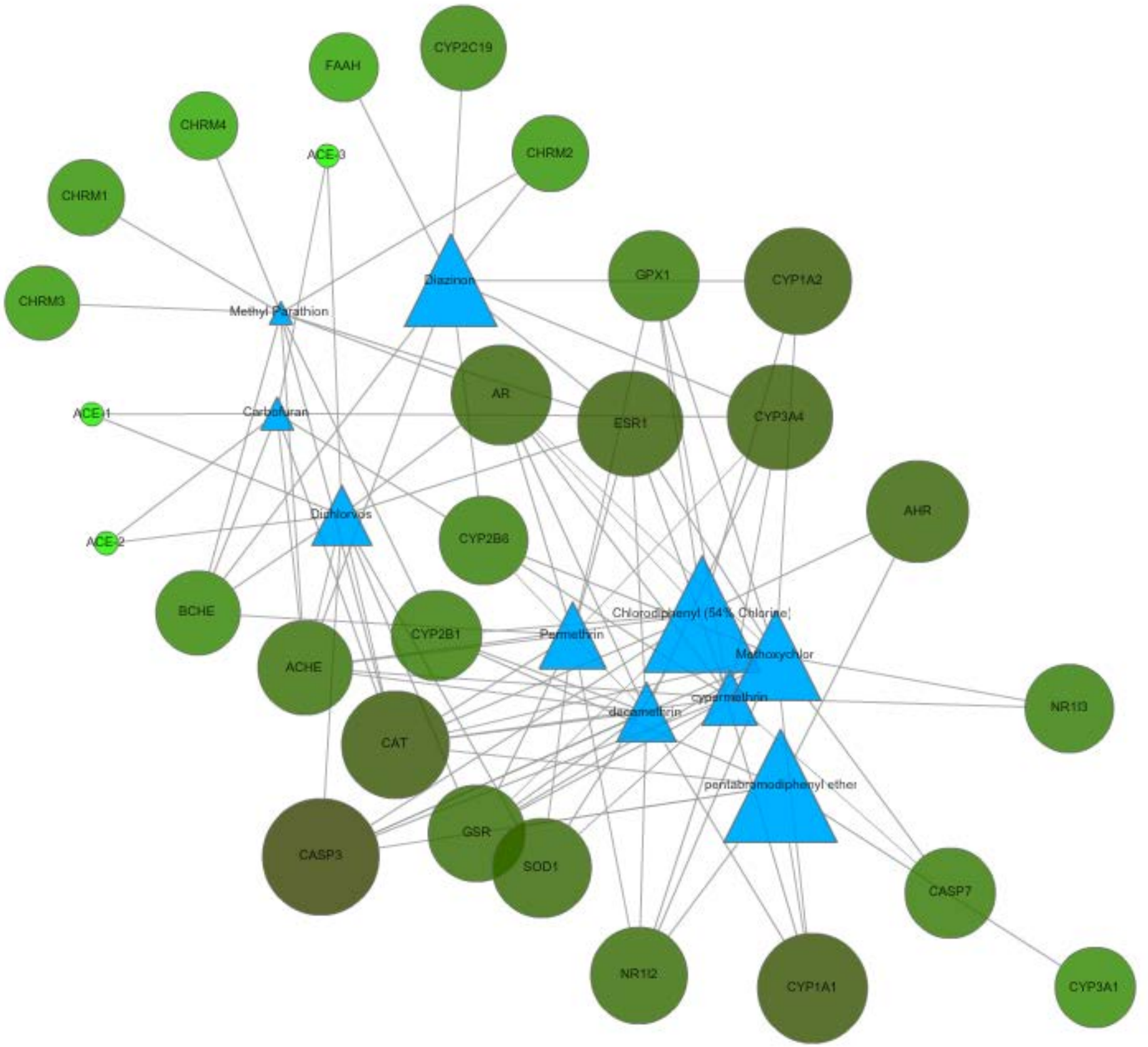


Download: CSV | Excel | XML | TSV

Pathway view of top 10 Comps: XGMML

Chlorpyrifos

Basics | Interactions | Genes | Diseases | ChemComps | **Pathways** | GO | References | Links

These pathways are enriched significantly among genes that interact with *Chlorpyrifos* or its descendants. We show only terms with a corrected p-value less than 0.01.

1–100 of 109 results.

First | Previous | 1 | 2 | Next | Last

	Pathway	Pathway ID	P-value	Corrected P-value	Annotated Genes	Genome Frequency
1.	Metabolism	REACT:111217	1.57e-84	4.64e-82	167	1362/34680 genes: 3.93%
2.	Signal Transduction	REACT:111102	6.89e-69	2.03e-66	162	1614/34680 genes: 4.65%
3.	Neuroactive ligand-receptor interaction	KEGG:04080	1.36e-63	4.01e-61	80	326/34680 genes: 0.94%
4.	Pathways in cancer	KEGG:05200	8.72e-51	2.57e-48	70	332/34680 genes: 0.96%
5.	Huntington's disease	KEGG:05016	1.25e-45	3.70e-43	53	189/34680 genes: 0.54%
6.	Alzheimer's disease	KEGG:05010	1.27e-42	3.73e-40	49	172/34680 genes: 0.50%
7.	Neuronal System	REACT:13685	1.27e-41	3.76e-39	58	281/34680 genes: 0.81%
8.	Metabolic pathways	KEGG:01100	7.25e-39	2.14e-36	106	1207/34680 genes: 3.48%
9.	Glutamatergic synapse	KEGG:04724	2.45e-36	7.24e-34	40	131/34680 genes: 0.38%
10.	MAPK signaling pathway	KEGG:04010	6.82e-35	2.01e-32	52	281/34680 genes: 0.81%
11.	Parkinson's disease	KEGG:05012	7.87e-35	2.32e-32	39	132/34680 genes: 0.38%
12.	Melanogenesis	KEGG:04916	1.01e-34	2.98e-32	36	106/34680 genes: 0.31%
13.	Calcium signaling pathway	KEGG:04020	2.48e-31	7.32e-29	41	182/34680 genes: 0.52%
14.	Axon guidance	KEGG:04360	9.94e-31	2.93e-28	36	133/34680 genes: 0.38%
15.	Oxidative phosphorylation	KEGG:00190	3.57e-28	1.05e-25	34	133/34680 genes: 0.38%
16.	Immune System	REACT:6900	4.36e-28	1.29e-25	84	1044/34680 genes: 3.01%
17.	Disease	REACT:116125	2.10e-27	6.20e-25	73	812/34680 genes: 2.34%
18.	Amyotrophic lateral sclerosis (ALS)	KEGG:05014	5.84e-27	1.72e-24	24	54/34680 genes: 0.16%
19.	Glutathione metabolism	KEGG:00480	5.84e-27	1.72e-24	24	54/34680 genes: 0.16%
20.	Developmental Biology	REACT:111045	9.34e-27	2.75e-24	52	408/34680 genes: 1.18%
21.	Wnt signaling pathway	KEGG:04310	2.33e-26	6.88e-24	35	161/34680 genes: 0.46%
22.	Drug metabolism - cytochrome P450	KEGG:00982	1.07e-25	3.15e-23	26	75/34680 genes: 0.22%
23.	Hemostasis	REACT:604	6.01e-24	1.77e-21	53	487/34680 genes: 1.40%
24.	Metabolism of xenobiotics by cytochrome P450	KEGG:00980	1.62e-23	4.77e-21	24	71/34680 genes: 0.20%
25.	Regulation of actin cytoskeleton	KEGG:04810	1.76e-23	5.19e-21	37	222/34680 genes: 0.64%
26.	Basal cell carcinoma	KEGG:05217	3.39e-20	9.99e-18	20	57/34680 genes: 0.16%
27.	Transmembrane transport of small molecules	REACT:15518	5.94e-19	1.75e-16	44	432/34680 genes: 1.25%
28.	Thyroid cancer	KEGG:05216	6.57e-17	1.94e-14	14	29/34680 genes: 0.08%
29.	Long-term potentiation	KEGG:04720	7.21e-17	2.13e-14	19	70/34680 genes: 0.20%
30.	Melanoma	KEGG:05218	9.66e-17	2.85e-14	19	71/34680 genes: 0.20%

Chlorpyrifos

Basics | Gene Interactions | Genes | Diseases | Comps | Pathways | GO | References

These GO terms are enriched significantly among genes that interact with *Chlorpyrifos* or its descendants. We show only terms with a corrected p-value less than 0.01.

Filter by — Ontology: Biological Process — Highest GO level: 4 — Filter

1–100 of 778 results.

First | Previous | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | Next | Last

	Ontology	Highest GO Level	GO Term	P-value	Corrected P-value	Annotated Genes	Genome Frequency
1.	BP	4	nervous system development	1.80e-129	1.51e-125	266	1686/34817 genes: 4.84%
2.	BP	4	neurological system process	4.14e-105	3.46e-101	208	1231/34817 genes: 3.54%
3.	BP	4	synaptic transmission	1.35e-101	1.13e-97	156	649/34817 genes: 1.86%
4.	BP	4	cell surface receptor signaling pathway	1.91e-94	1.60e-90	263	2293/34817 genes: 6.59%
5.	BP	4	neurogenesis	3.13e-78	2.61e-74	170	1108/34817 genes: 3.18%
6.	BP	4	phosphate-containing compound metabolic process	2.62e-77	2.19e-73	193	1472/34817 genes: 4.23%
7.	BP	5	phosphorylation	1.81e-76	1.51e-72	178	1255/34817 genes: 3.60%
8.	BP	5	generation of neurons	3.21e-76	2.68e-72	163	1041/34817 genes: 2.99%
9.	BP	4	neuron differentiation	1.78e-72	1.48e-68	153	960/34817 genes: 2.76%
10.	BP	4	cellular response to organic substance	1.64e-65	1.37e-61	156	1120/34817 genes: 3.22%
11.	BP	4	cellular protein metabolic process	2.44e-64	2.04e-60	267	3234/34817 genes: 9.29%
12.	BP	4	apoptotic process	3.17e-	2.65e-58	177	1527/34817 genes: 4.39%

ctd™ *Illuminating how chemicals affect humar*

Comparative Toxicogenomics Database

Home | Search | Analyze | Downl

Analysis Tools

Batch Query
Download custom data associat
or references.

Set Analyzer
Perform analyses such as set-b
for collections of genes.

MyGeneVenn
Compare your gene list to gene

MyVenn
View relationships among your
data.

VennViewer
Compare associated data sets f

Set Analyzer

Perform analyses such as set-based enrichment for collections of chemicals or genes, and pathway generation for collections of genes.

1 Select your input type

- ○ Chemicals (MeSH® names, synonyms, or IDs, or CAS RNs)
- ◉ Genes (NCBI symbols or IDs)

2 Enter your data set

Return-, tab- or |-delimited

3 Choose the analysis

- ◉ Enriched diseases
- ○ Enriched GO functional annotations
  - Ontology
    - ○ All
    - ○ Biological Process
    - ○ Molecular Function
    - ○ Cellular Component
- ○ Enriched pathways
- ○ Common gene–gene interactions

4 Configure the analysis

P-value

Threshold: 0.01 (0–1.0)

- ◉ Corrected *(recommended)*
- ○ Raw

Submit | Clear

CTD Data (June 2013)	Status
Curated Chemicals	12,985
Curated Genes	32,464
Curated Diseases	6,354
Chemical-Gene Interactions	869,902
Unique Chemicals	10,150
Unique Genes	31,344
Unique Organisms	492
Curated Gene-Disease Relationship	27,397
Curated Chemical-Disease Relationships	186,986

>300 manuscripts using CTD data
>30 public databases incorporating CTD data

Exposure data

- Grounding CTD data in “real-world” exposure data
- Centralizing exposure data
- Integrating exposure information with other biological data

ExO

Exposure Stressor

Interacts with

Exposure Receptor

Exposure Event

Exposure Outcome

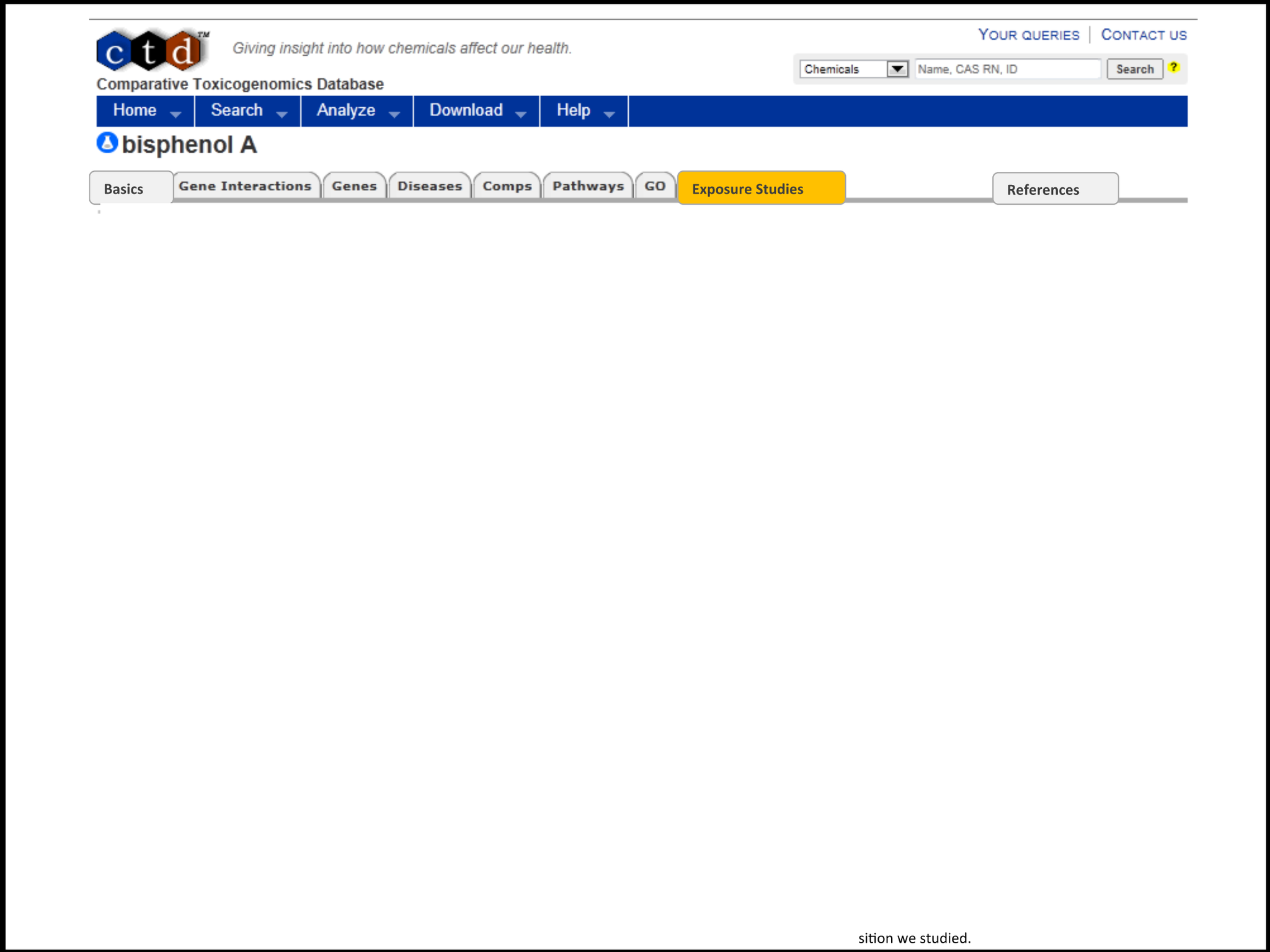
Exposure data

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	CURATION IDENTIFIERS		STUDY IDENTIFIERS		EXPOSURE STRESSOR			EXPOSURE RECEPTOR			EXPOSURE EVENT				EXPOSURE OUTCOME		SUMMARY
2	4 fields		4 fields		6 fields			15 fields			17 fields				6 fields		2 fields
3	Curator	PMID	Study Title	Collection Years	Stressor Agent	Source	Number Samples	Age	Gender	Race	Methods	Limits of Detection	Assay Value	Event Location	Disease	Phenotype	Comments
4	cmurphy	22264316		1969-1990	Tetrachloroethylene	Dietary	1512	29.3 years	M/F	98.5% White				Cape Cod, MA	Bipolar Disorder		Results provide support for an in
5	cmurphy	22264316		1969-1990	Tetrachloroethylene	Dietary	1512	29.3 years	M/F	98.5% White				Cape Cod, MA	Stress Disorders, Post-Traumatic		Results provide support for an in
6	cmurphy	22264316		1969-1990	Tetrachloroethylene	Dietary	1512	29.3 years	M/F	98.5% White				Cape Cod, MA	Schizophrenia		Results provide support for an in
7																	
8	cmurphy	22239864		2001-2006	Particulate Matter	Environmental			M/F		distance-weighting estimation	13 u/m3		United States			This study generated estimates c
9	cmurphy	22239864		2001-2006	Ozone	Environmental			M/F		distance-weighting estimation	44 ppb		United States			This study generated estimates c
10																	
11	cmurphy	20978189	Agricultural H	1993-2004	Fonofos	occupationa	2,220		M	100% Caucasian	questionnaires			IA, NC, United States	Prostatic Neoplasms		In conclusion, we observed an int
12	cmurphy	20978189	Agricultural H	1993-2004	Coumaphos	occupationa	2,220		M	100% Caucasian	questionnaires			IA, NC, United States	Prostatic Neoplasms		In conclusion, we observed an int
13	cmurphy	20978189	Agricultural H	1993-2004	terbufos	occupationa	2,220		M	100% Caucasian	questionnaires			IA, NC, United States	Prostatic Neoplasms		In conclusion, we observed an int
14	cmurphy	20978189	Agricultural H	1993-2004	Phorate	occupationa	2,220		M	100% Caucasian	questionnaires			IA, NC, United States	Prostatic Neoplasms		In conclusion, we observed an int
15	cmurphy	20978189	Agricultural H	1993-2004	Permethrin	occupationa	2,220		M	100% Caucasian	questionnaires			IA, NC, United States	Prostatic Neoplasms		In conclusion, we observed an int
16																	
17	cmurphy	22251442	NHANES III	1988-1994	dimethyl phosphate	Dietary	192		M/F		GC-MS	0.5 u/L	2.07 u/L	United States			Human exposure to organophos
18	cmurphy	22251442	NHANES III	1988-1994	dimethyl phosphate	Dietary	192		M/F		GC-MS	0.5 u/L	13.4 u/L	United States			Human exposure to organophos
19	cmurphy	22251442	NHANES III	1988-1994	dimethyl phosphate	Dietary	192		M/F		GC-MS	0.5 u/L	2.14 u/g creatinine	United States			Human exposure to organophos
20	cmurphy	22251442	NHANES III	1988-1994	dimethyl phosphate	Dietary	192		M/F		GC-MS	0.5 u/L	25.2 u/g creatinin	United States			Human exposure to organophos
21	cmurphy	22251442	NHANES 199	1999-2000	dimethyl phosphate	Dietary	814		M/F		GC-MS	0.58 u/L	0.68 u/L	United States			Human exposure to organophos
22	cmurphy	22251442	NHANES 199	1999-2000	dimethyl phosphate	Dietary	814		M/F		GC-MS	0.58 u/L	9.7 u/L	United States			Human exposure to organophos
23	cmurphy	22251442	NHANES 199	1999-2000	dimethyl phosphate	Dietary	814		M/F		GC-MS	0.58 u/L	0.76 u/g creatinin	United States			Human exposure to organophos
24	cmurphy	22251442	NHANES 199	1999-2000	dimethyl phosphate	Dietary	814		M/F		GC-MS	0.58 u/L	14.6 u/g creatinine	United States			Human exposure to organophos
25	cmurphy	22251442	NHANES 199	2001-2002	dimethyl phosphate	Dietary	1,121		M/F		GC-MS	0.5 u/L	11.5 u/L	United States			Human exposure to organophos

- Status
  - ~50 data points captured
  - ~3,000 priority articles: 600 curated, 16,000 exposure statements, 300 unique chemicals, 100 diseases

Mattingly CJ, McKone TE, Callahan MA, Blake JA, Hubal EA. Environ Sci Technol.

Exposure data



sition we studied.

bisphenol A

Basics | Gene Interactions | Genes | Diseases | Comps | Pathways | GO | References | Exposure Studies | Exposure Levels

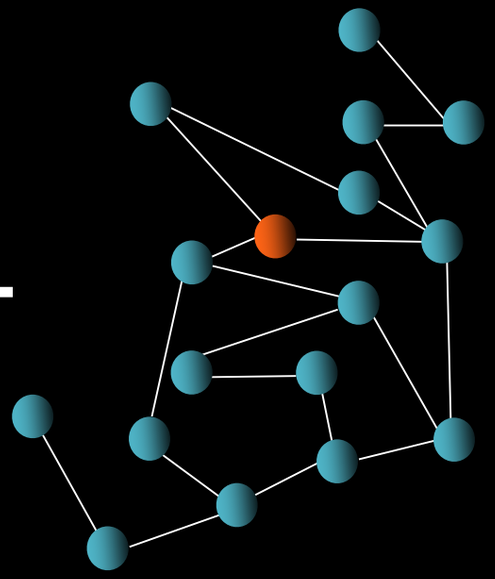
DETAILS

Stressor	Medium	Biomarker	Level	Units	Measurement description	Details
bisphenol A	urine	bisphenol A	1.340	nanograms per milliliter	mean	Nahar, et al. (2012)
Air Pollution	serum	bisphenol A	> 0.700	nanograms per milliliter	median	Nahar, et al. (2012)
Vehicle Emissions	plasma	bisphenol A	< 12.000	nanograms per milliliter	maximum	Nahar, et al. (2012)
bisphenol A	urine	bisphenol A	3.300	micrograms per gram creatinine	median	Madeup et al., (2010)
bisphenol A	urine	bisphenol A, disodium salt A	2.000	micrograms per gram creatinine	median	Madeup et al., (2010)
Estradiol	urine	bisphenol A, disodium salt A	2.600	micrograms per gram creatinine	median	Madeup et al., (2010)
bisphenol A	urine	bisphenol A	0.840	nanograms per milliliter	geometric mean	Madeup et al., (2010)
bisphenol A	urine	TPEN	1.240	parts per million	mean	Sgabjar et al. (2009)
bisphenol A	urine	TPEN	1.000	parts per million	median	Sgabjar et al. (2009)
bisphenol A	urine	TPEN	< 6.200	parts per million	maximum	Sgabjar et al. (2009)
bisphenol A	urine	TPEN	0.790	parts per million	geometric mean	Sgabjar et al. (2009)
bisphenol A	urine	bisphenol A	0.600	nanograms per milliliter	median	Woodruff, et al (2001)
bisphenol A	urine	bisphenol A	12.000	nanograms per milliliter	maximum	Woodruff, et al (2001)
bisphenol A	urine	aluminum-bisphenol A	0.890	nanograms per milliliter	geometric mean	Woodruff, et al (2001)
bisphenol A	urine	bisphenol A	2.830	nanograms per milliliter	mean	Woodruff, et al (2001)
bisphenol A	urine	bisphenol A	2.600	nanograms per milliliter	median	Woodruff, et al (2001)
bisphenol A	urine	bisphenol A	16.100	nanograms per milliliter	maximum	Woodruff, et al (2001)
bisphenol A	urine	bisphenol A	1.960	nanograms per milliliter	geometric mean	You, et al (2007)
bisphenol A	urine	bisphenol A	1.750	nanograms per milliliter	mean	You, et al (2007)
bisphenol A	urine	bisphenol A	1.020	nanograms per milliliter	median	You, et al (2007)
bisphenol A	urine	bisphenol A	10.800	nanograms per milliliter	maximum	You, et al (2007)
bisphenol A	urine	bisphenol A	1.000	nanograms per milliliter	geometric mean	You, et al (2007)
bisphen		A	2.130	nanograms per milliliter	mean	You, et al (2007)
bispher		A	1.020	nanograms per milliliter	median	Cantonwine, et al (2010)
bispher		A	10.800	nanograms per milliliter	maximum	Cantonwine, et al (2010)
bispher		A			mean	Galloway, et al (2009)
bispher		A				Galloway, et al (2009)
bispher		A				Galloway, et al (2009)

displays the actual measurements curated from multiple papers, providing a view of the different ranges

data displayed if chemical or its descendant is in the “Stressor” **or** “Biomarker” column

Phenotype-disease curation



Phenotype → Disease

Blood Pressure
Heart Rate
Vasoconstriction → Hypertension
Hypotension
Arrhythmias, Cardiac

Pfizer

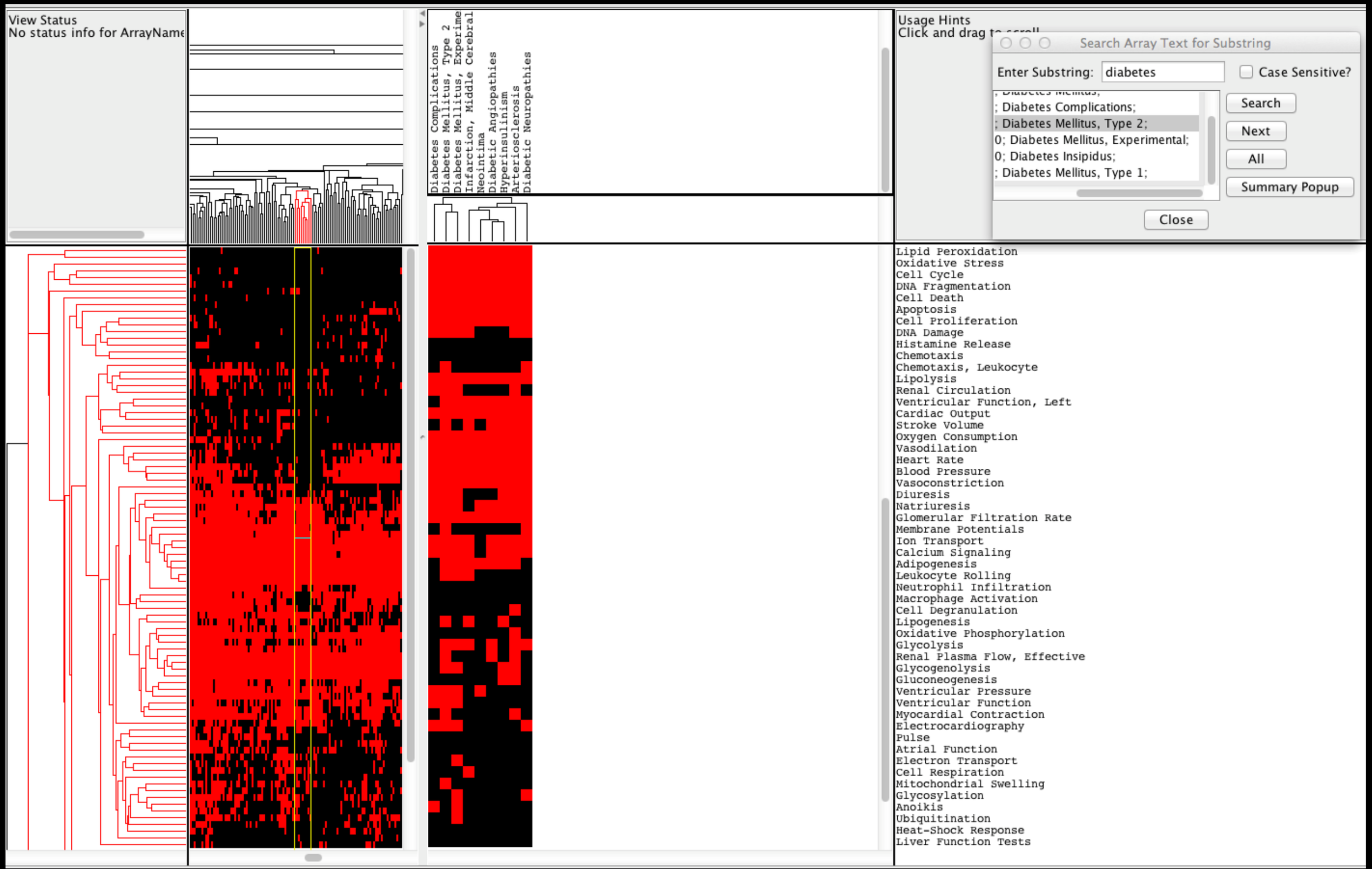
NTP
National Toxicology Program

Free public database

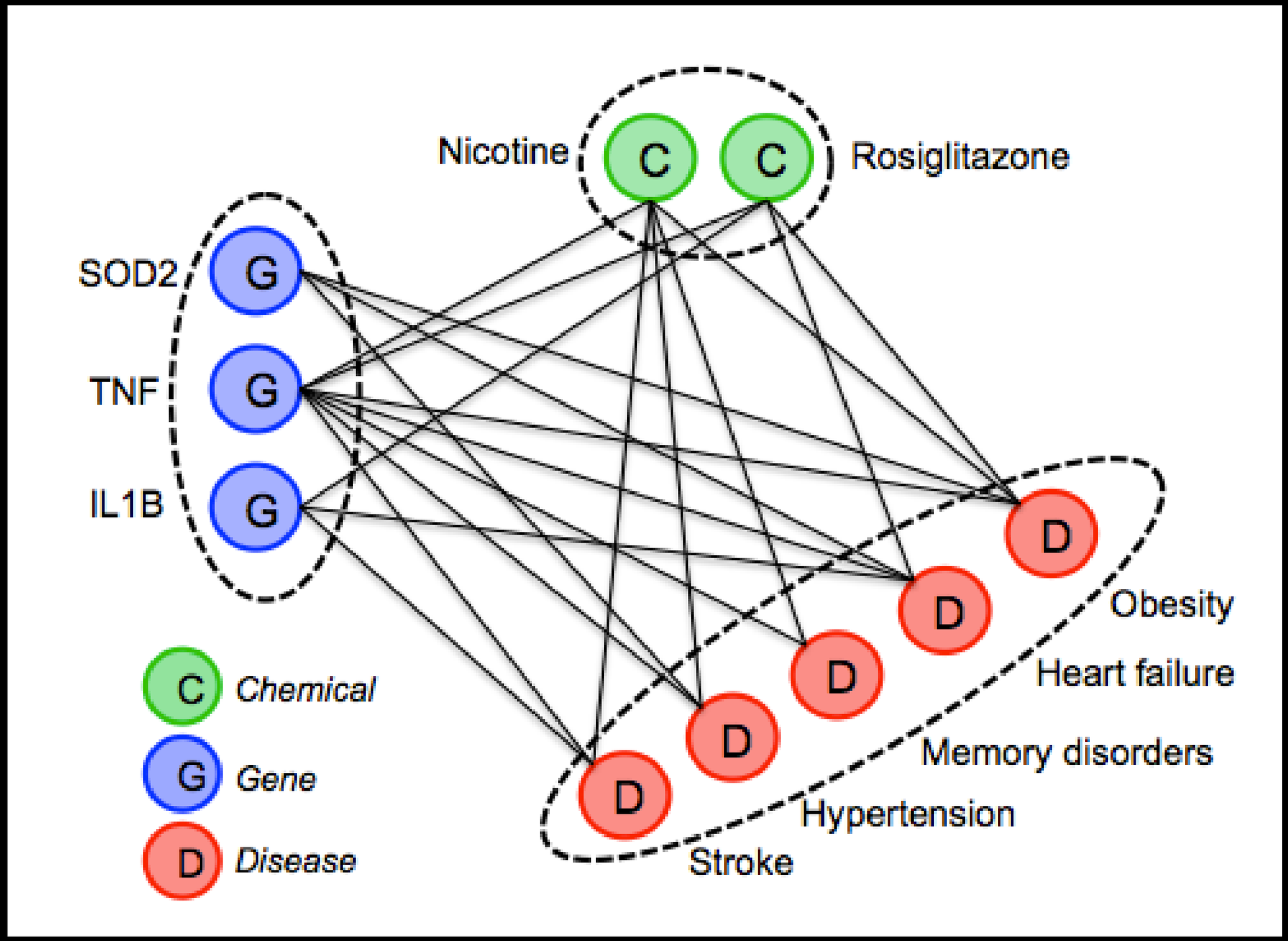
DrugMatrix® and ToxFX®

https://ntp.niehs.nih.gov/drugmatrix
https://ntp.niehs.nih.gov/toxfx

Phenotype-disease analysis



Phenotype-disease analysis



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Acknowledgements

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