

SUPPORTING INFORMATION

Cardiotoxicity hazard and risk characterization of ToxCast chemicals using human induced pluripotent stem cell (iPSC)-derived cardiomyocytes from multiple donors

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Supplemental Figure 1. Plate maps. (A) Representative map for Plates 1-15. (B) Plate map for Plate 16, which includes 11 chemicals. *TAB = Tetraoctylammonium bromide, ISO = Isoproterenol, PRO = Propranolol, CIS = Cisapride, QT1 = N-acetylprocainamide, QT2 = Sematilide, QT3 = Sotalol, QT-1 = Mifepristone, QT-2 = Cabazitaxel, QT-3 = Lamotrigine, VEH = Vehicle-only wells, MEDIA = Media-only wells.

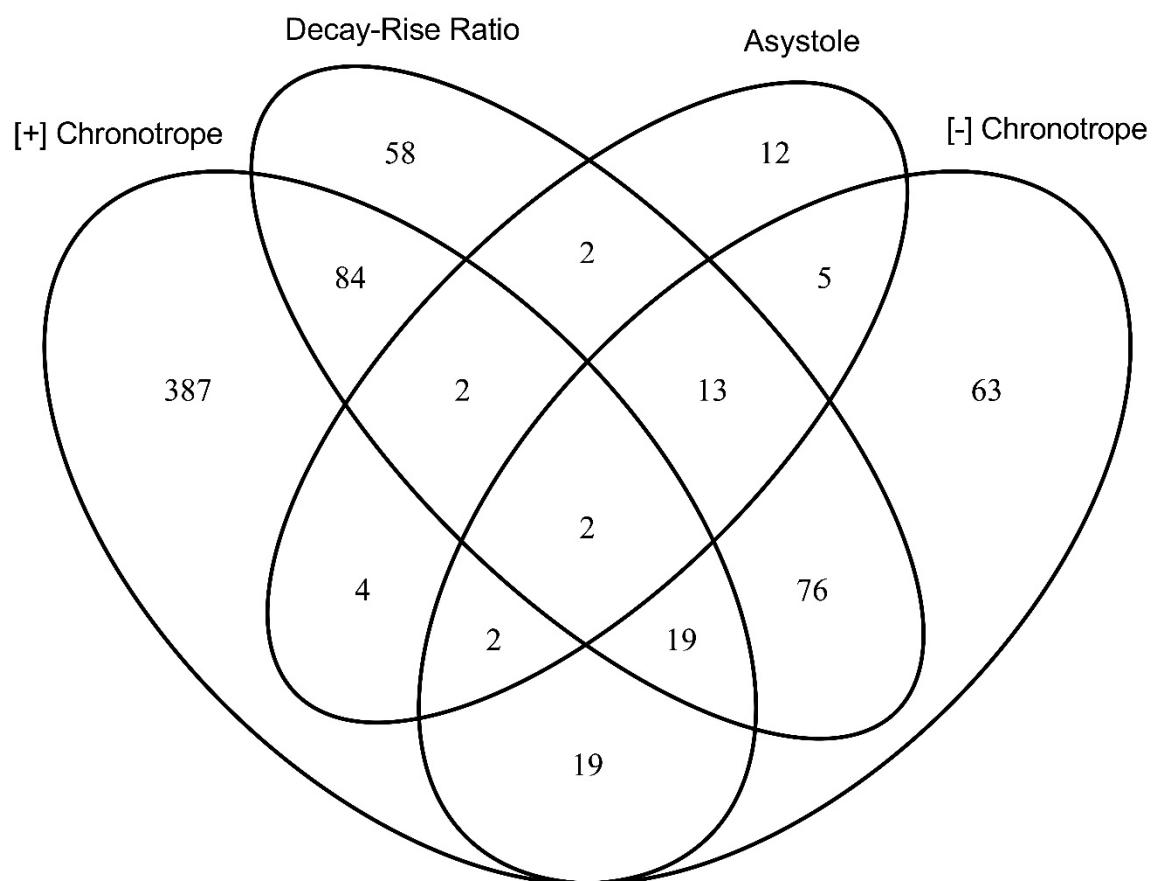
(A)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	μM																							
B	100																							
C	10	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
D	1																							
E	0.2																							
F		TAB	ISO	VEH	VEH	ISO	QT1	QT2	QT3	MEDIA	MEDIA	QT1	QT2	QT3	MEDIA	PRO	QT-1	QT-2	QT-3	VEH	VEH	ISO	TAB	
G	100																							
H	10																							
I	1																							
J	0.2																							
K		TAB	CIS	VEH	VEH	CIS	QT1	QT2	QT3	MEDIA	MEDIA	QT-1	QT-2	QT-3	MEDIA	PRO	QT-1	QT-2	QT-3	VEH	VEH	CIS	PRO	
L	100																							
M	10																							
N	1																							
O	0.2																							
P		45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	VEH	

(B)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	μM																							
B	100																							
C	10	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	
D	1																							
E	0.2																							
F		TAB	ISO	VEH	VEH	ISO	QT1	QT2	QT3	MEDIA	MEDIA	QT1	QT2	QT3	MEDIA	PRO	QT-1	QT-2	QT-3	VEH	VEH	ISO	TAB	
G	100																							
H	10	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	
I	1																							
J	0.2																							
K		TAB	CIS	VEH	VEH	CIS	QT1	QT2	QT3	MEDIA	MEDIA	QT-1	QT-2	QT-3	MEDIA	PRO	QT-1	QT-2	QT-3	VEH	VEH	CIS	PRO	
L	100																							
M	10	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	66	126	162	217	291	403	462	574	613	689	720	VEH	
N	1																							
O	0.2																							
P																								

Supplemental Figure 2. Venn diagram of the number of chemicals active for each phenotype.



Supplemental Table 1. Test chemicals with their CASRN, DTXSID, classification, and source.

*Starred chemicals were included as inter-plate replicates in each screening experiment. NCCTE = National Center for Computational Toxicology and Exposure (US EPA).

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#	Chemical Name	CASRN	DTXSID	Chemical Classification	Use Details for Chemicals Classified as "Other"	Chemical Source	Chemical Concentration in Master Plate from NCCTE (mM)	Chemical Quality Control Flags
1	N-Nitrosopyrrolidine	930-55-2	DTXSID8021062	Other	Research chemical	NCCTE	19.989	
2	Isoniazid	54-85-3	DTXSID8020755	Pharmaceutical		NCCTE	19.9992	
3	Methotrexate	59-05-2	DTXSID4020822	Pharmaceutical		NCCTE	19.9979	
4	2-Chloroethanol	107-07-3	DTXSID1021877	Solvent		NCCTE	19.9996	
5	Dicrotophos	141-66-2	DTXSID9023914	Pesticide (non-herbicide)		NCCTE	20.076	
6	Safrole	94-59-7	DTXSID0021254	FoodFlavorFragrance		NCCTE	19.9963	
7	Triethylene glycol bis(2-ethylhexanoate)	94-28-0	DTXSID3026564	Solvent		NCCTE	20	
8	2-Chloro-4-phenylphenol	92-04-6	DTXSID0022353	Microbiocide		NCCTE	20	
9	4-Androstene-3,17-dione	63-05-8	DTXSID8024523	Pharmaceutical		NCCTE	19.9995	
10	Prednisone	53-03-2	DTXSID4021185	Pharmaceutical		NCCTE	19.9993	
11	3-Phenoxybenzoic acid	3739-38-6	DTXSID1038321	Pesticide (non-herbicide)		NCCTE	20	
12	2-[4-(Diethylamino)-2-hydroxybenzoyl]benzoic	5809-23-4	DTXSID4027604	Chemical intermediate		NCCTE	20.0006	
13	Formetanate	23422-53-9	DTXSID4032405	Pesticide (non-herbicide)		NCCTE	20.1492	
14	3-Methylbutyl acetate	123-92-2	DTXSID9025453	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
15	Pyraclostrobin	175013-18-0	DTXSID7032638	Microbiocide		NCCTE	19.9993	
16	Toluene-2,4-diisocyanate	584-84-9	DTXSID7026156	Chemical intermediate		NCCTE	19.9997	
17	Methyl (RS)-2-[4-(2,4-dichlorophenoxy)phenoxy]propionate	51338-27-3	DTXSID0032605	Herbicide		NCCTE	19.9993	
18	Citronellol	106-22-9	DTXSID3026726	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
19	Dihexyl phthalate	84-75-3	DTXSID6025068	Plasticizer		NCCTE	20	
20	N-Ethylperfluorooctanesulfonamide	4151-50-2	DTXSID1032646	Pesticide (non-herbicide)		NCCTE	19.2528	
21	Valproic acid	99-66-1	DTXSID6023733	Pharmaceutical		NCCTE	20.0003	
22	Clorophene	120-32-1	DTXSID5020154	Microbiocide		NCCTE	20.222	
23	Flutamide	13311-84-7	DTXSID7032004	Pharmaceutical		NCCTE	20	
24	Cyclohexylphenylketone	712-50-5	DTXSID5048182	FoodFlavorFragrance		NCCTE	19.9997	
25	Fenvalerate	51630-58-1	DTXSID3020621	Pesticide (non-herbicide)		NCCTE	19.9995	
26	Dicyclohexyl disulfide	2550-40-5	DTXSID4047628	FoodFlavorFragrance		NCCTE	20.0004	
27	Aminoglutethimide	125-84-8	DTXSID8022589	Pharmaceutical		NCCTE	19.9997	
28	Cyclopamine	4449-51-8	DTXSID6043709	Pharmaceutical		NCCTE	20	
29	Endothal	145-73-3	DTXSID7024081	Herbicide		NCCTE	20	
30	4,4'-Methylenebis(N,N-dimethylaniline)	101-61-1	DTXSID5020869	Chemical intermediate		NCCTE	19.9997	
31	4,4'-(9H-Fluorene-9,9-diyil)diphenol	3236-71-3	DTXSID5037731	Chemical intermediate		NCCTE	20	
32	Trifloxysulfuron-sodium	199119-58-9	DTXSID8040222	Herbicide		NCCTE	19.999	
33	Chlorimuron-ethyl	90982-32-4	DTXSID0023955	Herbicide		NCCTE	20.0003	
34	Molinate	2212-67-1	DTXSID6024206	Herbicide		NCCTE	20.0002	
35	1,2-Dichlorobenzene	95-50-1	DTXSID6020430	Solvent		NCCTE	20	MASSPEC: VocBinBase volatile compounds database
36	17beta-Estradiol	50-28-2	DTXSID0020573	Pharmaceutical		NCCTE	20.0002	
37	1,2,3-Trichlorobenzene	87-61-6	DTXSID8026193	Solvent		NCCTE	20	
38	2,4-Diaminotoluene	95-80-7	DTXSID4020402	Chemical intermediate		NCCTE	19.9998	
39	Chlorpyrifos oxon	5598-15-2	DTXSID1038666	Pesticide (non-herbicide)		NCCTE	19.9288	
40	Imazamox	114311-32-9	DTXSID3034664	Herbicide		NCCTE	20.0006	
41	Hexythiazox	78587-05-0	DTXSID7024299	Pesticide (non-herbicide)		NCCTE	20.0015	
42	Tetrahydrocurcumin	36062-04-1	DTXSID30865801	FoodFlavorFragrance		NCCTE	19.9981	

43	1-Tetradecene	1120-36-1	DTXSID4027367	Solvent		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
44	Indeno(1,2,3-cd)pyrene	193-39-5	DTXSID8024153	PAH		NCCTE	10	
45	Dalapon	75-99-0	DTXSID2021575	Herbicide		NCCTE	20	
46	3-Iodo-2-propynyl-N-butylcarbamate	55406-53-6	DTXSID0028038	Microbiocide		NCCTE	20.0004	
47	Pyridaben	96489-71-3	DTXSID5032573	Pesticide (non-herbicide)		NCCTE	19.9997	
48	Dimethylarsinic acid	75-60-5	DTXSID7020508	Herbicide		NCCTE	20	
49	EPN	2104-64-5	DTXSID7022174	Pesticide (non-herbicide)		NCCTE	19.9995	
50	Chloridazon	1698-60-8	DTXSID3034872	Herbicide		NCCTE	20	
51	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	DTXSID1027635	Chemical intermediate		NCCTE	20	
52	Norethindrone	68-22-4	DTXSID9023380	Pharmaceutical		NCCTE	19.9966	
53	Butralin	33629-47-9	DTXSID3032337	Herbicide		NCCTE	19.9993	
54	Pacllobutrazol	76738-62-0	DTXSID2024242	Herbicide		NCCTE	20	
55	Diclofenac sodium	15307-79-6	DTXSID3037208	Pharmaceutical		NCCTE	19.9997	
56	Flumioxazin	103361-09-7	DTXSID7032555	Herbicide		NCCTE	20.0153	
57	4-Heptylphenol	1987-50-4	DTXSID2037714	Chemical intermediate		NCCTE	20	
58	4-Chlorophenyl methyl sulfide	123-09-1	DTXSID8023973	Other		NCCTE	19.9997	
59	Dimethipin	55290-64-7	DTXSID0024052	Herbicide		NCCTE	20	
60	Tripropylene glycol monomethyl ether	25498-49-1	DTXSID2029329	Solvent		NCCTE	20	
61	Cyfluthrin	68359-37-5	DTXSID5035957	Pesticide (non-herbicide)		NCCTE	20.0002	
62	Sethoxydim	74051-80-2	DTXSID9024304	Herbicide		NCCTE	20.0894	
63	Oxazepam	604-75-1	DTXSID1021087	Pharmaceutical		NCCTE	17.4387	
64	Sodium dehydroacetate	4418-26-2	DTXSID7026029	Plasticizer		NCCTE	20.0002	
65	alpha-Cyclodextrin	10016-20-3	DTXSID7030698	FoodFlavorFragrance		NCCTE	10.4743	
*66	1-Tridecanol	112-70-9	DTXSID2021947	FoodFlavorFragrance		NCCTE	20.5623	
67	Bifenthrin	82657-04-3	DTXSID9020160	Pesticide (non-herbicide)		NCCTE	20	
68	6:2 Fluorotelomer alcohol	647-42-7	DTXSID5044572	Chemical intermediate		NCCTE	20	
69	Methylene	6317-18-6	DTXSID8025599	Microbiocide		NCCTE	20	
70	Etephon	16672-87-0	DTXSID7024085	Herbicide		NCCTE	20	
71	2-(Butan-2-yl)phenol	89-72-5	DTXSID2022331	Chemical intermediate		NCCTE	20	
72	Nitrapyrin	1929-82-4	DTXSID0024216	Microbiocide		NCCTE	20	
73	2-(2-	111-90-0	DTXSID2021941	Solvent		NCCTE	20	
74	Pyriproxyfen	95737-68-1	DTXSID1032640	Pesticide (non-herbicide)		NCCTE	20.0002	
75	Forchlorfenuron	68157-60-8	DTXSID1034634	Herbicide		NCCTE	19.9871	
76	4,4'-Sulfonyldiphenol	80-09-1	DTXSID3022409	Chemical intermediate		NCCTE	20	
77	Pendimethalin	40487-42-1	DTXSID7024245	Herbicide		NCCTE	19.9995	
78	Clodinafop-propargyl	105512-06-9	DTXSID6032354	Herbicide		NCCTE	20	
79	1,2,4-Tribromobenzene	615-54-3	DTXSID5024346	Chemical intermediate		NCCTE	20	
80	Benzoylctyl adipate	58394-64-2	DTXSID1047528	Plasticizer		NCCTE	20	
81	2,4,4'-Trihydroxybenzophenone	1470-79-7	DTXSID8044836	PAH		NCCTE	20	
82	Di-n-octyl phthalate	117-84-0	DTXSID1021956	Plasticizer		NCCTE	20	
83	Propylbenzene	103-65-1	DTXSID3042219	Solvent		NCCTE	20.0081	
84	3,4-Diaminotoluene	496-72-0	DTXSID9024930	Chemical intermediate		NCCTE	19.9915	
85	tert-Butylhydroquinone	1948-33-0	DTXSID6020220	Chemical intermediate		NCCTE	20	
86	Perfluorooctanesulfonam	754-91-6	DTXSID3038939	Surfactant		NCCTE	20	
87	Hexanedinitrile	111-69-3	DTXSID3021936	Chemical intermediate		NCCTE	19.9966	
88	Oxamyl	23135-22-0	DTXSID6021086	Pesticide (non-herbicide)		NCCTE	20	
89	N-Nitrosodimethylamine	62-75-9	DTXSID7021029	Chemical intermediate		NCCTE	20.0007	
90	6-Thioguanine	154-42-7	DTXSID6023652	Pharmaceutical		NCCTE	19.9997	
91	Isopropyl triethanolamine titanate	36673-16-2	DTXSID7044928	Other	Coupling agent; fracking	NCCTE	20.0004	
92	Busulfan	55-98-1	DTXSID3020910	Pharmaceutical		NCCTE	19.9997	
93	Monobenzyl phthalate	2528-16-7	DTXSID9043938	Plasticizer		NCCTE	19.9995	
94	4-Hydroxytamoxifen	68392-35-8	DTXSID3037094	Pharmaceutical		NCCTE	5.99902	
95	5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	DTXSID9034286	Microbiocide		NCCTE	19.9997	
96	2-Hexyloxyethanol	112-25-4	DTXSID1026908	Solvent		NCCTE	20	
97	Cypermethrin	52315-07-8	DTXSID1023998	Pesticide (non-herbicide)		NCCTE	20.0007	
98	3,3',5,5'-Tetrabromobisphenol A	79-94-7	DTXSID1026081	Flame retardant		NCCTE	19.0852	
99	Thymol	89-83-8	DTXSID6034972	FoodFlavorFragrance		NCCTE	20	
100	Triethanolamine	102-71-6	DTXSID9021392	Surfactant		NCCTE	19.9983	
101	1,2-Propylene glycol	57-55-6	DTXSID0021206	Solvent		NCCTE	19.9996	
102	Trichloroacetic acid	76-03-9	DTXSID1021378	Pharmaceutical		NCCTE	20	
103	Carminic acid	1260-17-9	DTXSID9022817	Dye		NCCTE	19.9917	
104	Triflumizole	68694-11-1	DTXSID2032500	Microbiocide		NCCTE	20.002	
105	SHPP-33	105624-86-0	DTXSID1046970	Pharmaceutical		NCCTE	19.9994	

106	Equilin	474-86-2	DTXSID7047433	Pharmaceutical		NCCTE	19.9995	
107	Acenaphthylene	208-96-8	DTXSID3023845	PAH		NCCTE	20	
108	Ethoxyquin	91-53-2	DTXSID9020582	FoodFlavorFragrance		NCCTE	20.0004	
109	Propoxycarbazone-	181274-15-7	DTXSID9034864	Herbicide		NCCTE	19.9975	
110	Triacetin	102-76-1	DTXSID3026691	FoodFlavorFragrance		NCCTE	20	
111	Sodium trichloroacetate	650-51-1	DTXSID6034924	Herbicide		NCCTE	20	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
112	Bendiocarb	22781-23-3	DTXSID9032327	Pesticide (non-herbicide)		NCCTE	20.0341	
113	Maneb	12427-38-2	DTXSID9020794	Microbiocide		NCCTE	19.9985	
114	Phenolphthalin	81-90-3	DTXSID5022439	Dye		NCCTE	20	
115	Pioglitazone	112529-15-4	DTXSID3044203	Pharmaceutical		NCCTE	19.9997	
116	Simazine	122-34-9	DTXSID4021268	Herbicide		NCCTE	19.9997	
117	Hexazinone	51235-04-2	DTXSID4024145	Herbicide		NCCTE	20.0004	
118	1,3-Benzenediamine	108-45-2	DTXSID4021137	Chemical intermediate		NCCTE	20.0003	
119	2-Methyl-4,6-	534-52-1	DTXSID1022053	Pesticide (non-herbicide)		NCCTE	20	
120	Fluazifop-butyl	69806-50-4	DTXSID3034612	Herbicide		NCCTE	20	
121	1-Butanol	71-36-3	DTXSID1021740	Solvent		NCCTE	20.0003	
122	4-(2-Methylbutan-2-yl)phenol	80-46-6	DTXSID8021771	Chemical intermediate		NCCTE	20	
123	Cyprodinil	121552-61-2	DTXSID1032359	Microbiocide		NCCTE	19.9997	MASSSPEC: VocBinBase volatile compounds database
124	Diphenolic acid	126-00-1	DTXSID0022436	Plasticizer		NCCTE	20	
125	Acetamide	60-35-5	DTXSID7020005	Solvent		NCCTE	20	
*126	Pyrimethanil	53112-28-0	DTXSID8034877	Microbiocide		NCCTE	19.9998	
127	1,3,5-Tribromobenzene	626-39-1	DTXSID3052307	Chemical intermediate		NCCTE	20.0017	
128	Mercuric chloride	7487-94-7	DTXSID5020811	Microbiocide		NCCTE	19.9998	
129	Hexanedioic acid, diisonyl ester	33703-08-1	DTXSID5027982	Plasticizer		NCCTE	20	
130	Ammonium perchlorate	7790-98-9	DTXSID4024515	Other	Explosives	NCCTE	19.9899	
131	1,2,3-Benzotriazole	95-14-7	DTXSID6020147	Solvent		NCCTE	20.0023	
132	Octamethylcyclotetrasiloxane	556-67-2	DTXSID7027205	Chemical intermediate		NCCTE	20.0007	
133	D-Mannitol	69-65-8	DTXSID1023235	FoodFlavorFragrance		NCCTE	20	
134	5,5-Diphenylhydantoin	57-41-0	DTXSID8020541	Pharmaceutical		NCCTE	20	
135	1,3-Dichloro-2-propanol	96-23-1	DTXSID6025010	Solvent		NCCTE	20	
136	Clofentezine	74115-24-5	DTXSID9023881	Pesticide (non-herbicide)		NCCTE	20	
137	2-Tert-Butyl-5-	88-60-8	DTXSID2026529	Chemical intermediate		NCCTE	20.0003	
138	Pirimicarb	23103-98-2	DTXSID1032569	Pesticide (non-herbicide)		NCCTE	19.9997	
139	4-Hydroxy-3-methoxybenzaldehyde	121-33-5	DTXSID0021969	FoodFlavorFragrance		NCCTE	19.9997	
140	Carbamazepine	298-46-4	DTXSID4022731	Pharmaceutical		NCCTE	20.0003	
141	Isopentyl alcohol	123-51-3	DTXSID3025469	Solvent		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
142	2,6-Diethylaniline	579-66-8	DTXSID6027218	Chemical intermediate		NCCTE	20	
143	Folpet	133-07-3	DTXSID0021385	Microbiocide		NCCTE	19.9997	MASSSPEC: VocBinBase volatile compounds database
144	Oxyfluorfen	42874-03-3	DTXSID7024241	Herbicide		NCCTE	20.0007	
145	Heptachlor	76-44-8	DTXSID3020679	Pesticide (non-herbicide)		NCCTE	20	
146	Terbutryn	886-50-0	DTXSID3024318	Herbicide		NCCTE	20	
147	Flufenpyr-ethyl	188489-07-8	DTXSID3034618	Herbicide		NCCTE	20.0008	
148	Fludioxonil	131341-86-1	DTXSID2032398	Microbiocide		NCCTE	20.0457	
149	Isoxaben	82558-50-7	DTXSID8024159	Herbicide		NCCTE	20	
150	Mepanipyrim	110235-47-7	DTXSID4042121	Microbiocide		NCCTE	20	
151	2,3,4,6-	58-90-2	DTXSID9021716	Microbiocide		NCCTE	20	
152	Methenamine	100-97-0	DTXSID6020692	Chemical intermediate		NCCTE	20.4189	
153	p-Bromodiphenyl ether	101-55-3	DTXSID8023927	Chemical intermediate		NCCTE	19.9992	
154	Boscalid	188425-85-6	DTXSID6034392	Microbiocide		NCCTE	19.9997	
155	Dodecytrimethylammonium chloride	112-00-5	DTXSID1026900	Microbiocide		NCCTE	20.0004	
156	Dibutyl decanedioate	109-43-3	DTXSID1041847	Plasticizer		NCCTE	20.0015	
157	Reserpine	50-55-5	DTXSID7021237	Pharmaceutical		NCCTE	16.9216	
158	Quinclorac	84087-01-4	DTXSID6032641	Herbicide		NCCTE	19.9996	
159	Tebuconazole	107534-96-3	DTXSID9032113	Microbiocide		NCCTE	19.9995	
160	Methyl methanesulfonate	66-27-3	DTXSID7020845	Pesticide (non-herbicide)		NCCTE	19.9994	

161	3,4-Dichloronitrobenzene	99-54-7	DTXSID8024999	Chemical intermediate		NCCTE	20	
*162	Coumarin	91-64-5	DTXSID7020348	FoodFlavorFragrance		NCCTE	20	
163	4-Nitrobenzoic acid	62-23-7	DTXSID3020966	Chemical intermediate		NCCTE	20	
164	Bispyribac-sodium	125401-92-5	DTXSID7034383	Herbicide		NCCTE	20.0004	
165	2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane	2971-36-0	DTXSID8022325	Pesticide (non-herbicide)		NCCTE	20.0009	
166	Nilutamide	63612-50-0	DTXSID3034165	Pharmaceutical		NCCTE	20	
167	Chlorethoxyfos	54593-83-8	DTXSID2032344	Pesticide (non-herbicide)		NCCTE	20	
168	Dibutyl phthalate	84-74-2	DTXSID2021781	Plasticizer		NCCTE	19.9996	
169	Diphenylamine	122-39-4	DTXSID4021975	Dye		NCCTE	20.0002	
170	Pentachloropyridine	2176-62-7	DTXSID2022179	Chemical intermediate		NCCTE	20.0004	
171	Dexamethasone sodium phosphate	2392-39-4	DTXSID3047429	Pharmaceutical		NCCTE	20.0055	CHEMINV: EPA ToxCast Cheminventory chemicals with stability problems
172	1,2,3,4-	634-66-2	DTXSID6026088	Chemical intermediate		NCCTE	20.0002	
173	Sodium dodecylbenzenesulfonate	25155-30-0	DTXSID7025219	Surfactant		NCCTE	20	
174	Trichlorfon	52-68-6	DTXSID0021389	Pesticide (non-herbicide)		NCCTE	20	
175	1,3-Diphenylguanidine	102-06-7	DTXSID3025178	Chemical intermediate		NCCTE	20.0074	
176	1,2-Diphenylhydrazine	122-66-7	DTXSID7020710	Chemical intermediate		NCCTE	20	
177	Codeine	76-57-3	DTXSID2020341	Pharmaceutical		NCCTE	19.9988	
178	N-Nitrosodiethylamine	55-18-5	DTXSID2021028	Plasticizer		NCCTE	19.9995	
179	Testosterone propionate	57-85-2	DTXSID9036515	Pharmaceutical		NCCTE	19.9996	
180	Triethoxycyclotilsilane	2943-75-1	DTXSID2029246	Chemical intermediate		NCCTE	19.9995	
181	Glutaraldehyde	111-30-8	DTXSID6025355	Chemical intermediate		NCCTE	20.0005	
182	Acetophenone	98-86-2	DTXSID6021828	FoodFlavorFragrance		NCCTE	19.9954	MASSSPEC: VocBinBase volatile compounds database
183	Triphenyltin hydroxide	76-87-9	DTXSID1021409	Microbiocide		NCCTE	20.0007	
184	Methyl 2-aminobenzoate	134-20-3	DTXSID6025567	FoodFlavorFragrance		NCCTE	20.0003	
185	Triglycidyl isocyanurate	2451-62-9	DTXSID4026262	Chemical intermediate		NCCTE	19.9998	
186	Spironolactone	52-01-7	DTXSID6034186	Pharmaceutical		NCCTE	19.9978	
187	Sulfasalazine	599-79-1	DTXSID0021256	Pharmaceutical		NCCTE	20.0004	
188	Cyclohexylamine	108-91-8	DTXSID1023996	Chemical intermediate		NCCTE	19.9993	
189	Methidathion	950-37-8	DTXSID5020819	Pesticide (non-herbicide)		NCCTE	20.0031	
190	2-Amino-5-azotoluene	97-56-3	DTXSID1020069	Chemical intermediate		NCCTE	20.0003	
191	Di(2-ethylhexyl)	117-81-7	DTXSID5020607	Plasticizer		NCCTE	19.996	
192	2E,4E-Hexadienoic acid	110-44-1	DTXSID3021277	Microbiocide		NCCTE	19.997	
193	4-Nitroaniline	100-01-6	DTXSID8020961	Chemical intermediate		NCCTE	20.0004	
194	Diethylene glycol monomethyl ether	111-77-3	DTXSID3025049	Solvent		NCCTE	20	
195	Simvastatin	79902-63-9	DTXSID0023581	Pharmaceutical		NCCTE	19.9996	
196	Kaempferol	520-18-3	DTXSID7020768	FoodFlavorFragrance		NCCTE	14.2502	
197	4-Aminoazobenzene	60-09-3	DTXSID6024460	Chemical intermediate		NCCTE	20.0007	
198	Warfarin	81-81-2	DTXSID5023742	Pharmaceutical		NCCTE	20	
199	Tebufenozide	112410-23-8	DTXSID4034948	Pesticide (non-herbicide)		NCCTE	19.9995	
200	Fulvestrant	129453-61-8	DTXSID4022369	Pharmaceutical		NCCTE	20	
201	Quercetin	117-39-5	DTXSID4021218	FoodFlavorFragrance		NCCTE	19.9996	
202	Alachlor	15972-60-8	DTXSID1022265	Herbicide		NCCTE	20.0004	
203	Bronopol	52-51-7	DTXSID8024652	Microbiocide		NCCTE	20.0003	
204	N,N,N',N'-Tetrakis(2-hydroxypropyl)ethylenediamine	102-60-3	DTXSID9026689	Plasticizer		NCCTE	20	
205	17alpha-Ethinylestradiol	57-63-6	DTXSID5020576	Pharmaceutical		NCCTE	20.0015	
206	Fluconazole	86386-73-4	DTXSID3020627	Microbiocide		NCCTE	20.0004	
207	Hydramethylnon	67485-29-4	DTXSID6023868	Pesticide (non-herbicide)		NCCTE	19.9998	
208	Acetamiprid	135410-20-7	DTXSID0034300	Pesticide (non-herbicide)		NCCTE	19.9997	
209	Cymoxanil	57966-95-7	DTXSID6032358	Microbiocide		NCCTE	20.0235	
210	Diethyl butanedioate	123-25-1	DTXSID2038732	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
211	2,4-Dichlorophenoxyacetic	94-75-7	DTXSID0020442	Herbicide		NCCTE	20	
212	Piperonyl butoxide	51-03-6	DTXSID1021166	Pesticide (non-herbicide)		NCCTE	19.9981	
213	Gentian Violet	548-62-9	DTXSID5020653	Microbiocide		NCCTE	20.0006	

214	Diacetone alcohol	123-42-2	DTXSID6024917	Solvent		NCCTE	20.0003	MASSSPEC: VocBinBase volatile compounds database
215	Mirex	2385-85-5	DTXSID7020895	Pesticide (non-herbicide)		NCCTE	20.0005	
216	Flumiclorac-pentyl	87546-18-7	DTXSID2032554	Herbicide		NCCTE	19.9996	
*217	Fenthion	55-38-9	DTXSID8020620	Pesticide (non-herbicide)		NCCTE	20.0003	
218	Daidzein	486-66-8	DTXSID9022310	FoodFlavorFragrance		NCCTE	20	
219	N,N-Diethylethanolamine	100-37-8	DTXSID5021837	Chemical intermediate		NCCTE	20.0099	
220	Propanil	709-98-8	DTXSID8022111	Herbicide		NCCTE	19.9997	
221	Sulpiride	15676-16-1	DTXSID1042574	Pharmaceutical		NCCTE	20	
222	S-Bioallethrin	28434-00-6	DTXSID2039336	Pesticide (non-herbicide)		NCCTE	19.9997	
223	Cyclohexanone	108-94-1	DTXSID6020359	Solvent		NCCTE	20	
224	4-Octylphenol	1806-26-4	DTXSID9022312	Plasticizer		NCCTE	20	
225	Diuron	330-54-1	DTXSID0020446	Herbicide		NCCTE	20.0003	
226	Perfluorohexanoic acid	307-24-4	DTXSID3031862	Surfactant		NCCTE	20.0077	
227	Methyleugenol	93-15-2	DTXSID5025607	FoodFlavorFragrance		NCCTE	19.9997	
228	Diisodecyl hexanedioate	27178-16-1	DTXSID1027924	Plasticizer		NCCTE	20.0006	
229	4-Methyl-2-pentanol	108-11-2	DTXSID2026781	Solvent		NCCTE	19.9944	
230	PHA-00568487	527680-56-4	DTXSID1047285	Pharmaceutical		NCCTE	20	
231	Imazapyr	81334-34-1	DTXSID8034665	Herbicide		NCCTE	19.9997	
232	Ethyl butyrate	105-54-4	DTXSID6040111	FoodFlavorFragrance		NCCTE	20.0032	MASSSPEC: VocBinBase volatile compounds database
233	1-(Hydroxymethyl)-5,5-dimethylhydantoin	116-25-6	DTXSID6035152	Microbiocide		NCCTE	19.9997	
234	5-Heptyldihydro-2(3H)-furanone	104-67-6	DTXSID4034287	FoodFlavorFragrance		NCCTE	20	
235	Acetyltriethyl citrate	77-89-4	DTXSID5044576	Chemical intermediate		NCCTE	20	
236	o-Cresol	95-48-7	DTXSID8021808	Solvent		NCCTE	19.9972	MASSSPEC: VocBinBase volatile compounds database
237	Chlorothalonil	1897-45-6	DTXSID0020319	Microbiocide		NCCTE	20.0004	
238	Sodium erythorbate (1:1)	6381-77-7	DTXSID5020570	FoodFlavorFragrance		NCCTE	20	
239	Maltool	118-71-8	DTXSID0025523	FoodFlavorFragrance		NCCTE	20.795	
240	Metalaxyl	57837-19-1	DTXSID6024175	Microbiocide		NCCTE	19.9994	MASSSPEC: VocBinBase volatile compounds database
241	Ethalfuralin	55283-68-6	DTXSID8032386	Herbicide		NCCTE	20	
242	Methomyl	16752-77-5	DTXSID1022267	Pesticide (non-herbicide)		NCCTE	20	
243	Methylparaben	99-76-3	DTXSID4022529	Microbiocide		NCCTE	20	
244	Fenitrothion	122-14-5	DTXSID4032613	Pesticide (non-herbicide)		NCCTE	20	
245	Cyclanilide	113136-77-9	DTXSID5032600	Herbicide		NCCTE	20.0453	
246	3,7-Dimethyl-2,6-	5392-40-5	DTXSID6024836	FoodFlavorFragrance		NCCTE	20	
247	Carfentrazone-ethyl	128639-02-1	DTXSID4032532	Herbicide		NCCTE	20.0498	
248	4-Nonylphenol	104-40-5	DTXSID5033836	Surfactant		NCCTE	20	
249	Formamide	75-12-7	DTXSID8025337	Chemical intermediate		NCCTE	20	
250	Butylbenzene	104-51-8	DTXSID6022472	Solvent		NCCTE	20.0007	
251	2,6-Dinitrotoluene	606-20-2	DTXSID5020528	Chemical intermediate		NCCTE	20.0002	
252	Chloramben	133-90-4	DTXSID2020262	Herbicide		NCCTE	20	
253	Pyraflufen-ethyl	129630-19-9	DTXSID8034871	Herbicide		NCCTE	20.0007	
254	6:2 Fluorotelomer methacrylate	2144-53-8	DTXSID3047558	Chemical intermediate		NCCTE	20.0004	
255	Penoxsulam	219714-96-2	DTXSID0034803	Herbicide		NCCTE	19.9992	
256	Dipropylene glycol monomethyl ether	34590-94-8	DTXSID0027983	Pharmaceutical		NCCTE	20.0006	
257	Spiroxamine	118134-30-8	DTXSID1034212	Microbiocide		NCCTE	20	
258	Spirodiclofen	148477-71-8	DTXSID6034928	Pesticide (non-herbicide)		NCCTE	20	
259	Sodium 4-nitrophenoate	824-78-2	DTXSID3027320	Herbicide		NCCTE	20	
260	Cyclohexanol	108-93-0	DTXSID4021894	Chemical intermediate		NCCTE	19.9994	
261	Ammonium perfluoroctanoate	3825-26-1	DTXSID8037708	Chemical intermediate		NCCTE	20.0006	
262	Dimethyl adipate	627-93-0	DTXSID8025096	Solvent		NCCTE	20	
263	2,4-Bis(1-methyl-1-phenylethyl)phenol	2772-45-4	DTXSID7029241	Chemical intermediate		NCCTE	19.9995	
264	Clotrimazole	23593-75-1	DTXSID7029871	Microbiocide		NCCTE	20	
265	Tetrabromophenolphthal ein ethyl ester	1176-74-5	DTXSID5044520	Chemical intermediate		NCCTE	15.6503	
266	Sulisobenzene	4065-45-6	DTXSID2042436	FoodFlavorFragrance		NCCTE	20	

267	Kepone	143-50-0	DTXSID1020770	Pesticide (non-herbicide)		NCCTE	19.9996	
268	8-Hydroxyquinoline	148-24-3	DTXSID5020730	Microbiocide		NCCTE	20	
269	Acephate	30560-19-1	DTXSID8023846	Pesticide (non-herbicide)		NCCTE	20	
270	Prometon	1610-18-0	DTXSID6022341	Herbicide		NCCTE	20.0003	
271	N,N-Dimethyldecylamine oxide	2605-79-0	DTXSID7042190	Surfactant		NCCTE	20	
272	N,N,4-Trimethylaniline	99-97-8	DTXSID0021832	Dye		NCCTE	20.0003	
273	3,3'-Dimethoxybenzidine dihydrochloride	20325-40-0	DTXSID1020485	Chemical intermediate		NCCTE	20	
274	Fenarimol	60168-88-9	DTXSID2032390	Microbiocide		NCCTE	20.0168	
275	2-Naphthylamine	91-59-8	DTXSID2020921	Chemical intermediate		NCCTE	20	
276	Pyridoxine	65-23-6	DTXSID4023541	FoodFlavorFragrance		NCCTE	20.0002	
277	Tributylamine	102-82-9	DTXSID4026183	Chemical intermediate		NCCTE	20.0002	
278	L-Tartaric acid	87-69-4	DTXSID8023632	FoodFlavorFragrance		NCCTE	20	
279	Isopentyl butyrate	106-27-4	DTXSID3042059	FoodFlavorFragrance		NCCTE	20	
280	Carbosulfan	55285-14-8	DTXSID5023950	Pesticide (non-herbicide)		NCCTE	19.9996	
281	Undecane	1120-21-4	DTXSID9021689	Chemical intermediate		NCCTE	20.0045	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles; MASSSPEC: VocBinBase volatile compounds database
282	1,1'-Oxybis[2,3,4,5,6-pentabromobenzene]	1163-19-5	DTXSID9020376	Flame retardant		NCCTE	5.00011	
283	Chloromethyl methyl	107-30-2	DTXSID6020307	Solvent		NCCTE	6.95539	
284	Thidiazuron	51707-55-2	DTXSID0032651	Herbicide		NCCTE	20	
285	Octanoic acid	124-07-2	DTXSID3021645	Chemical intermediate		NCCTE	19.9998	MASSSPEC: VocBinBase volatile compounds database
286	4,4'-Diamino-3,3'-dimethyldiphenylmethan	838-88-0	DTXSID5020867	Chemical intermediate		NCCTE	19.9996	
287	1,2-Benzisothiazolin-3-	2634-33-5	DTXSID5032523	Microbiocide		NCCTE	20	
288	Benzal chloride	98-87-3	DTXSID6025014	Chemical intermediate		NCCTE	20	
289	2-Butoxyethanol	111-76-2	DTXSID1024097	Solvent		NCCTE	19.9912	
290	Propyzamide	23950-58-5	DTXSID2020420	Herbicide		NCCTE	20	
*291	Chlorendic acid	115-28-6	DTXSID2020268	Herbicide		NCCTE	20.0007	
292	Dimethomorph	110488-70-5	DTXSID7034545	Microbiocide		NCCTE	20	
293	Dimethenamid	87674-68-8	DTXSID4032376	Herbicide		NCCTE	19.9996	
294	4,4',4"-Ethane-1,1,1-triyltriphenol	27955-94-8	DTXSID2037712	Plasticizer		NCCTE	19.9996	
295	Dipropyl 2,5-pyridinedicarboxylate	136-45-8	DTXSID8032544	Pesticide (non-herbicide)		NCCTE	19.9996	
296	Perfluoroundecanoic acid	2058-94-8	DTXSID8047553	Surfactant		NCCTE	20.0076	
297	Resorcinol	108-46-3	DTXSID2021238	Chemical intermediate		NCCTE	20.0014	
298	Nitrofuranoin	67-20-9	DTXSID7020972	Pharmaceutical		NCCTE	20	
299	Benzyl-C8-18-alkyldimethylammonium chlorides	63449-41-2	DTXSID1048122	Microbiocide		NCCTE	20.0007	
300	Pentadecane	629-62-9	DTXSID6027268	Solvent		NCCTE	19.9997	MASSSPEC: VocBinBase volatile compounds database
301	N,N-Dimethylaniline	121-69-7	DTXSID2020507	Chemical intermediate		NCCTE	20.6506	
302	2-Methoxy-5-	120-71-8	DTXSID1020350	Chemical intermediate		NCCTE	20	
303	Propofol	2078-54-8	DTXSID6023523	Pharmaceutical		NCCTE	20.0004	
304	2,5-Dimethyl-2,5-di-(tert-butylperoxy)hexane	78-63-7	DTXSID9025110	Plasticizer		NCCTE	19.9995	
305	Imazaquin	81335-37-7	DTXSID3024152	Herbicide		NCCTE	20.0003	
306	(6)-Gingerol	23513-14-6	DTXSID3041035	FoodFlavorFragrance		NCCTE	20.0014	
307	2,4-	131-56-6	DTXSID8022406	Plasticizer		NCCTE	20	
308	2,4-Dimethylphenol	105-67-9	DTXSID2021864	FoodFlavorFragrance		NCCTE	19.9976	
309	Benzyl alcohol	100-51-6	DTXSID5020152	FoodFlavorFragrance		NCCTE	19.9972	MASSPEC: VocBinBase volatile compounds database
310	CJ-013610	249296-43-3	DTXSID2047272	Pharmaceutical		NCCTE	20	
311	2-Ethoxyethanol	110-80-5	DTXSID7024087	Solvent		NCCTE	19.9994	
312	Sodium saccharin hydrate	82385-42-0	DTXSID7021992	FoodFlavorFragrance		NCCTE	20.0002	

313	Nitrilotriacetic acid	139-13-9	DTXSID6020939	Chemical intermediate		NCCTE	18.3285	
314	1,4-Dibromobenzene	106-37-6	DTXSID4024012	Chemical intermediate		NCCTE	19.9996	
315	Propylparaben	94-13-3	DTXSID4022527	Microbiocide		NCCTE	20.0006	
316	Sucrose octaacetate	126-14-7	DTXSID3042423	FoodFlavorFragrance		NCCTE	15.0754	
317	Bis(2-ethylhexyl) nonanedioate	103-24-2	DTXSID3026697	Plasticizer		NCCTE	20.0004	
318	1,5-Naphthalenediamine	2243-62-1	DTXSID3020916	Chemical intermediate		NCCTE	19.9998	
319	2-Methoxyethanol	109-86-4	DTXSID5024182	Solvent		NCCTE	20.0405	
320	Phenothiazine	92-84-2	DTXSID5021126	Chemical intermediate		NCCTE	19.9997	
321	Aspirin	50-78-2	DTXSID5020108	Pharmaceutical		NCCTE	20.0003	
322	Styrene oxide	96-09-3	DTXSID2021286	Chemical intermediate		NCCTE	19.9986	
323	Diisopropyl methylphosphonate	1445-75-6	DTXSID5024051	Chemical intermediate		NCCTE	20	
324	Octadecanoic acid	57-11-4	DTXSID8021642	FoodFlavorFragrance		NCCTE	10.0002	MASSSPEC: VocBinBase volatile compounds database
325	2-Methylaniline	95-53-4	DTXSID1026164	Chemical intermediate		NCCTE	20.0109	
326	Dapsone	80-08-0	DTXSID4020371	Pharmaceutical		NCCTE	20	
327	Azamethiphos	35575-96-3	DTXSID9034818	Pesticide (non-herbicide)		NCCTE	20	
328	Imazapic	104098-48-8	DTXSID5034270	Herbicide		NCCTE	20.0005	
329	Ammonium carbamate	1111-78-0	DTXSID9027360	Chemical intermediate		NCCTE	20	
330	Diphenyl isophthalate	744-45-6	DTXSID8037752	Plasticizer		NCCTE	20.0013	
331	Cyproconazole	94361-06-5	DTXSID0032601	Microbiocide		NCCTE	19.9257	
332	Methyl isothiocyanate	556-61-6	DTXSID2027204	Pesticide (non-herbicide)		NCCTE	20.0034	
333	4-tert-Butylphenol	98-54-4	DTXSID1020221	Plasticizer		NCCTE	19.9998	
334	Isoproterenol	51-30-9	DTXSID6025486	Pharmaceutical		NCCTE	20.0003	
335	Monobutyl phthalate	131-70-4	DTXSID4040002	Plasticizer		NCCTE	20.0004	
336	p-Cymene	99-87-6	DTXSID3026645	FoodFlavorFragrance		NCCTE	20	
337	Dazomet	533-74-4	DTXSID7024902	Herbicide		NCCTE	20	
338	FD&C Blue No. 1	3844-45-9	DTXSID2020189	Dye		NCCTE	19.9995	
339	Diethanolamine	111-42-2	DTXSID3021932	Surfactant		NCCTE	19.9998	
340	Triethyl citrate	77-93-0	DTXSID0040701	Plasticizer		NCCTE	19.9996	
341	Butanoic acid	107-92-6	DTXSID8021515	FoodFlavorFragrance		NCCTE	20	
342	Phenylmercuric acetate	62-38-4	DTXSID7021150	Microbiocide		NCCTE	20.0004	
343	Phenol red	143-74-8	DTXSID8022408	Dye		NCCTE	19.9997	
344	Ziram	137-30-4	DTXSID0021464	Microbiocide		NCCTE	20	
345	Z-Tetrachlorvinphos	22248-79-9	DTXSID1032648	Pesticide (non-herbicide)		NCCTE	19.9995	
346	2-Butanone oxime	96-29-7	DTXSID1021821	Chemical intermediate		NCCTE	19.9996	
347	Azathioprine	446-86-6	DTXSID4020119	Pharmaceutical		NCCTE	19.8812	
348	Benzophenone	119-61-9	DTXSID0021961	FoodFlavorFragrance		NCCTE	20.0003	MASSSPEC: VocBinBase volatile compounds database
349	2-Mercaptobenzothiazole	149-30-4	DTXSID1020807	Microbiocide		NCCTE	19.9976	
350	PK 11195	85532-75-8	DTXSID7041097	Pharmaceutical		NCCTE	12.7244	
351	Triphenyl phosphite	101-02-0	DTXSID0026252	Chemical intermediate		NCCTE	20.0004	
352	(2Z)-3,7-Dimethylocta-2,6-dien-1-ol	106-25-2	DTXSID3026728	FoodFlavorFragrance		NCCTE	20	
353	Ethylene thiourea	96-45-7	DTXSID5020601	Chemical intermediate		NCCTE	20.0102	
354	Cycloheximide	66-81-9	DTXSID6024882	Microbiocide		NCCTE	20.0005	
355	4-Aminofolic acid	54-62-6	DTXSID3022588	Pesticide (non-herbicide)		NCCTE	19.9997	
356	Hexachlorophene	70-30-4	DTXSID6020690	Microbiocide		NCCTE	20.0004	
357	2-tert-Butylphenol	88-18-6	DTXSID2026525	Chemical intermediate		NCCTE	19.9998	
358	Chlorpropham	101-21-3	DTXSID7020764	Herbicide		NCCTE	19.9997	
359	delta-Hexachlorocyclohexane	319-86-8	DTXSID5024134	Pesticide (non-herbicide)		NCCTE	20.0026	
360	Diflubenzuron	35367-38-5	DTXSID1024049	Pesticide (non-herbicide)		NCCTE	20	
361	Rifampicin	13292-46-1	DTXSID6021244	Pharmaceutical		NCCTE	19.9969	
362	Fluometuron	2164-17-2	DTXSID8020628	Herbicide		NCCTE	20	
363	Tepraloxymid	149979-41-9	DTXSID7034252	Herbicide		NCCTE	20.0006	
364	Phenazone	60-80-0	DTXSID6021117	Pharmaceutical		NCCTE	20.0003	
365	1,2-Phenylenediamine	95-54-5	DTXSID3025881	Chemical intermediate		NCCTE	20.0117	
366	4-(1,1,3,3-Tetramethylbutyl)phenol	140-66-9	DTXSID9022360	Chemical intermediate		NCCTE	20.0005	
367	Butyl benzoate	136-60-7	DTXSID8040694	FoodFlavorFragrance		NCCTE	19.9997	
368	2-tert-Butyl-4-methoxyphenol	121-00-6	DTXSID7040788	Microbiocide		NCCTE	19.9998	
369	Butylparaben	94-26-8	DTXSID3020209	Microbiocide		NCCTE	20.0004	
370	Famotidine	76824-35-6	DTXSID5023039	Pharmaceutical		NCCTE	19.9997	
371	Quinalphos	13593-03-8	DTXSID7024291	Pesticide (non-herbicide)		NCCTE	20.0004	
372	Triisononyl trimellitate	53894-23-8	DTXSID5028033	Plasticizer		NCCTE	20	
373	Di(propylene glycol) dibenzoate	27138-31-4	DTXSID6027921	Plasticizer		NCCTE	19.9998	

374	Diazoxon	962-58-3	DTXSID5037523	Pesticide (non-herbicide)		NCCTE	20.0508	
375	Ethylene glycol	107-21-1	DTXSID8020597	Chemical intermediate		NCCTE	20.1389	
376	2-Ethyl-1-hexanol	104-76-7	DTXSID5020605	Chemical intermediate		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
377	2,4-Dinitrotoluene	121-14-2	DTXSID0020529	Chemical intermediate		NCCTE	20.0002	
378	Didecyldimethylammonium chloride	7173-51-5	DTXSID9032537	Microbiocide		NCCTE	19.9995	
379	3-Hydroxyfluorene	6344-67-8	DTXSID9047540	PAH		NCCTE	20	
380	Dexamethasone	50-02-2	DTXSID3020384	Pharmaceutical		NCCTE	19.9992	
381	Potassium perfluorobutanesulfonate	29420-49-3	DTXSID3037707	Flame retardant		NCCTE	19.9998	
382	Deisopropylatrazine	1007-28-9	DTXSID0037495	Herbicide		NCCTE	20	
383	Zamifenacin	127308-82-1	DTXSID9047257	Pharmaceutical		NCCTE	20	
384	Tebufenpyrad	119168-77-3	DTXSID0034223	Pesticide (non-herbicide)		NCCTE	19.9683	
385	Strychnine	57-24-9	DTXSID6023600	Pesticide (non-herbicide)		NCCTE	20	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
386	Tribufos	78-48-8	DTXSID1024174	Pesticide (non-herbicide)		NCCTE	20.0006	
387	Aldicarb	116-06-3	DTXSID0039223	Pesticide (non-herbicide)		NCCTE	19.9998	
388	Trifloxystrobin	141517-21-7	DTXSID4032580	Microbiocide		NCCTE	19.9994	
389	Oxytetracycline hydrochloride	2058-46-0	DTXSID5021097	Pharmaceutical		NCCTE	20	
390	Dibenzofuran	132-64-9	DTXSID2021993	FoodFlavorFragrance		NCCTE	19.9997	
391	Clopyralid	1702-17-6	DTXSID9029221	Herbicide		NCCTE	19.9996	
392	Isophorone	78-59-1	DTXSID8020759	Solvent		NCCTE	20	
393	Metoprolol	51384-51-1	DTXSID2023309	CiPA pharmaceutical		NCCTE	20	
394	Zileuton	111406-87-2	DTXSID9023752	Pharmaceutical		NCCTE	20	
395	Diltiazem hydrochloride	33286-22-5	DTXSID8040147	CiPA pharmaceutical		NCCTE	20	
396	Glycidyl trimethylammonium chloride	3033-77-0	DTXSID1044643	Surfactant		NCCTE	20.0002	
397	Sulfotepp	3689-24-5	DTXSID7024328	Pesticide (non-herbicide)		NCCTE	19.9997	
398	Diethyl phthalate	84-66-2	DTXSID7021780	Plasticizer		NCCTE	19.9996	MASSPEC: VocBinBase volatile compounds database
399	Isophorone diisocyanate	4098-71-9	DTXSID0023826	Chemical intermediate		NCCTE	20.0003	
400	3,3'-Dimethylbenzidine	119-93-7	DTXSID5024059	Chemical intermediate		NCCTE	20.0003	
401	Terbacil	5902-51-2	DTXSID8024317	Herbicide		NCCTE	20.0004	
402	Dimethoate	60-51-5	DTXSID7020479	Pesticide (non-herbicide)		NCCTE	20.0094	
*403	Bifenazate	149877-41-8	DTXSID5032525	Pesticide (non-herbicide)		NCCTE	20.0044	
404	Monocrotophos	6923-22-4	DTXSID9034816	Pesticide (non-herbicide)		NCCTE	19.9997	
405	Quinoxifen	124495-18-7	DTXSID2034881	Herbicide		NCCTE	20	
406	Tridemorph	24602-86-6	DTXSID3041376	Microbiocide		NCCTE	19.9995	
407	2-Methyl-2,4-pentanediol	107-41-5	DTXSID5021885	Solvent		NCCTE	20.922	
408	Allyl alcohol	107-18-6	DTXSID8020044	Chemical intermediate		NCCTE	19.9997	
409	Adipic acid, polypropyleneglycol,	66456-53-9	DTXSID6047527	Surfactant		NCCTE	20	
410	Triadimenol	55219-65-3	DTXSID0032493	Microbiocide		NCCTE	19.9985	
411	Myclobutanil	88671-89-0	DTXSID8024315	Microbiocide		NCCTE	19.9997	MASSPEC: VocBinBase volatile compounds database
412	Thiobencarb	28249-77-6	DTXSID6024337	Herbicide		NCCTE	20.0003	
413	DEET	134-62-3	DTXSID2021995	Pesticide (non-herbicide)		NCCTE	20	
414	EPTC	759-94-4	DTXSID1024091	Herbicide		NCCTE	20	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
415	Thiram	137-26-8	DTXSID5021332	Microbiocide		NCCTE	20.0015	
416	2,6-Dimethylaniline	87-62-7	DTXSID8026307	Chemical intermediate		NCCTE	20.6919	
417	Methyl ethyl ketone	78-93-3	DTXSID3021516	FoodFlavorFragrance		NCCTE	19.9988	
418	all-trans-Retinoic acid	302-79-4	DTXSID7021239	Pharmaceutical		NCCTE	19.9995	
419	Genistein	446-72-0	DTXSID5022308	FoodFlavorFragrance		NCCTE	19.9996	
420	Triphenyl phosphate	115-86-6	DTXSID1021952	Flame retardant		NCCTE	20.0004	
421	N,N-Dimethyloctylamine	7378-99-6	DTXSID2036299	Chemical intermediate		NCCTE	19.9997	
422	Tri-allate	2303-17-5	DTXSID5024344	Herbicide		NCCTE	20	

423	2,2',4,4'-Tetrahydroxybenzopheno	131-55-5	DTXSID5041306	FoodFlavorFragrance		NCCTE	20	
424	Triethylene glycol dimethyl ether	112-49-2	DTXSID8026224	Solvent		NCCTE	20	
425	Cladribine	4291-63-8	DTXSID8022828	Pharmaceutical		NCCTE	20	
426	Fluroxypyrr-methyl	81406-37-3	DTXSID5034303	Herbicide		NCCTE	19.9995	
427	Tetraconazole	112281-77-3	DTXSID8034956	Microbiocide		NCCTE	19.9043	
428	Aldicarb oxime	1646-75-9	DTXSID9024431	Pesticide (non-herbicide)		NCCTE	20	
429	N-Ethyl-3-methylaniline	102-27-2	DTXSID4021848	Chemical intermediate		NCCTE	20	
430	Methacrylonitrile	126-98-7	DTXSID1024176	Chemical intermediate		NCCTE	19.9929	
431	Butam	35256-85-0	DTXSID5041691	Herbicide		NCCTE	19.9996	
432	Chlorpromazine hydrochloride	69-09-0	DTXSID7024827	CiPA pharmaceutical		NCCTE	20	
433	Clove leaf oil	8000-34-8	DTXSID8044175	FoodFlavorFragrance		NCCTE	20	
434	Symclosene	87-90-1	DTXSID2026523	Herbicide		NCCTE	20.0003	
435	Diethylstilbestrol	56-53-1	DTXSID3020465	Pharmaceutical		NCCTE	20	
436	Fenpyroximate (Z,E)	111812-58-9	DTXSID2032550	Pesticide (non-herbicide)		NCCTE	20	
437	Bensulide	741-58-2	DTXSID9032329	Herbicide		NCCTE	20.0007	
438	Iodosulfuron-methyl-	144550-36-7	DTXSID2034673	Herbicide		NCCTE	19.972	
439	Fenoxyprop-P-ethyl	71283-80-2	DTXSID2034598	Herbicide		NCCTE	20.0006	
440	3'-Azido-3'	30516-87-1	DTXSID8020127	Pharmaceutical		NCCTE	20	
441	1,2,3,4,5,6-Hexachlorocyclohexane	608-73-1	DTXSID7020687	Pesticide (non-herbicide)		NCCTE	20	
442	Butylphthalyl	85-70-1	DTXSID7023938	Plasticizer		NCCTE	20	
443	p-Cresol	106-44-5	DTXSID7021869	Chemical intermediate		NCCTE	20.0108	
444	Diethylene glycol dimethyl ether	111-96-6	DTXSID1024621	Solvent		NCCTE	19.9998	
445	Efpronil	120068-37-3	DTXSID4034609	Pesticide (non-herbicide)		NCCTE	20.0663	
446	Ibuprofen	15687-27-1	DTXSID5020732	Pharmaceutical		NCCTE	20	
447	Potassium perfluorohexanesulfonate	3871-99-6	DTXSID3037709	Flame retardant		NCCTE	20	
448	N-Methyl-2-pyrrolidone	872-50-4	DTXSID6020856	Solvent		NCCTE	20.0002	
449	Diethyl sulfate	64-67-5	DTXSID1024045	Chemical intermediate		NCCTE	20.0004	
450	Dichlorprop	120-36-5	DTXSID0020440	Herbicide		NCCTE	19.9997	
451	Ethyl heptanoate	106-30-9	DTXSID1040112	FoodFlavorFragrance		NCCTE	20.0038	
452	beta-	319-85-7	DTXSID7020685	Pesticide (non-herbicide)		NCCTE	20	
453	2,4,6-Trichlorophenol	88-06-2	DTXSID5021386	Herbicide		NCCTE	20	
454	Fomesafen	72178-02-0	DTXSID7024112	Herbicide		NCCTE	20.0008	
455	Triethylene glycol	111-21-7	DTXSID3026223	Plasticizer		NCCTE	20	
456	1,2-Dibromoethane	106-93-4	DTXSID3020415	Chemical intermediate		NCCTE	20.1877	
457	Tacrine	321-64-2	DTXSID1037272	Pharmaceutical		NCCTE	20.0003	
458	Chlorpyrifos-methyl	5598-13-0	DTXSID6032352	Pesticide (non-herbicide)		NCCTE	20.0006	
459	FD&C Green No. 3	2353-45-9	DTXSID3020673	Dye		NCCTE	13.2163	
460	p,p'-DDD	72-54-8	DTXSID4020373	Pesticide (non-herbicide)		NCCTE	20.0005	
461	2,4-Di-tert-butylphenol	96-76-4	DTXSID2026602	Chemical intermediate		NCCTE	20.0003	
*462	2,2'-Methylenebis(4-methyl-6-tert-	119-47-1	DTXSID4020870	Chemical intermediate		NCCTE	20	
463	Quizalofop-ethyl	76578-14-8	DTXSID9023889	Herbicide		NCCTE	17.1798	
464	3,3'-Dimethoxybenzidine	119-90-4	DTXSID3025091	Chemical intermediate		NCCTE	20	
465	Glybendiamide	10238-21-8	DTXSID0037237	Pharmaceutical		NCCTE	20	
466	4,4'-Dibromodiphenyl	2050-47-7	DTXSID9024015	Flame retardant		NCCTE	19.9997	
467	Cyclosporin A	59865-13-3	DTXSID0020365	Pharmaceutical		NCCTE	8.70604	
468	Nicotine	54-11-5	DTXSID1020930	FoodFlavorFragrance		NCCTE	19.9899	
469	1H,1H,2H,2H-Perfluoroctyl iodide	2043-57-4	DTXSID2047565	Surfactant		NCCTE	5.00026	
470	MEHP	4376-20-9	DTXSID2025680	Plasticizer		NCCTE	20.3107	
471	Fluoranthene	206-44-0	DTXSID3024104	PAH		NCCTE	20	
472	Ethanolamine	141-43-5	DTXSID6022000	Chemical intermediate		NCCTE	19.9998	
473	Urethane	51-79-6	DTXSID9021427	Chemical intermediate		NCCTE	19.9994	
474	Methoxyfenozone	161050-58-4	DTXSID3032628	Pesticide (non-herbicide)		NCCTE	19.9549	
475	10-Undecenoic acid	112-38-9	DTXSID8035001	Microbiocide		NCCTE	19.9996	
476	Denatonium saccharide	90823-38-4	DTXSID9034361	Pesticide (non-herbicide)		NCCTE	20.0004	
477	1,2-Dimethyl-4-nitrobenzene	99-51-4	DTXSID2025133	Chemical intermediate		NCCTE	20	
478	Perfluoroheptanoic acid	375-85-9	DTXSID1037303	Surfactant		NCCTE	20.0002	
479	Resveratrol	501-36-0	DTXSID4031980	FoodFlavorFragrance		NCCTE	20	
480	1,3-Diisopropylbenzene	99-62-7	DTXSID8026640	Solvent		NCCTE	20.0002	
481	Perfluorononanoic acid	375-95-1	DTXSID8031863	Surfactant		NCCTE	19.9994	
482	Bromophenol blue	115-39-9	DTXSID6041682	Dye		NCCTE	18.6428	
483	Tamoxifen citrate	54965-24-1	DTXSID8021301	CiPA pharmaceutical		NCCTE	18.2916	
484	4-Nonylphenol, branched	84852-15-3	DTXSID5029055	Surfactant		NCCTE	20	
485	Fluroxypyrr	69377-81-7	DTXSID2034627	Herbicide		NCCTE	20.0003	
486	Zoxamide	156052-68-5	DTXSID9032581	Microbiocide		NCCTE	20.0708	
487	Oxadiazon	19666-30-9	DTXSID3024239	Herbicide		NCCTE	19.9997	
488	Bis(2-ethylhexyl)decanoate	122-62-3	DTXSID7025055	Plasticizer		NCCTE	20	

489	Mecoprop	93-65-2	DTXSID9024194	Herbicide		NCCTE	20	
490	p-Xylenol blue	125-31-5	DTXSID8026303	Dye		NCCTE	20.0007	
491	Fenamiphos	22224-92-6	DTXSID3024102	Pesticide (non-herbicide)		NCCTE	20.0028	
492	Norflurazon	27314-13-2	DTXSID8024234	Herbicide		NCCTE	20.0003	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
493	Furosemide	54-31-9	DTXSID6020648	Pharmaceutical		NCCTE	20.0004	
494	Sodium dodecyl sulfate	151-21-3	DTXSID1026031	Surfactant		NCCTE	19.9997	
495	Phenolphthalein	77-09-8	DTXSID0021125	Dye		NCCTE	20.0003	
496	Procymidone	32809-16-8	DTXSID9033923	Microbiocide		NCCTE	20	
497	Terbutylazine	5915-41-3	DTXSID4027608	Herbicide		NCCTE	20.0004	
498	N-Methyldioctylamine	4455-26-9	DTXSID9042209	Chemical intermediate		NCCTE	20.0012	
499	Aldrin	309-00-2	DTXSID8020040	Pesticide (non-herbicide)		NCCTE	20.0007	
500	2-Ethoxyethyl acetate	111-15-9	DTXSID9021928	Solvent		NCCTE	20	
501	Nitrofurazone	59-87-0	DTXSID5020944	Microbiocide		NCCTE	20	
502	1-Hexadecanol	36653-82-4	DTXSID4027991	FoodFlavorFragrance		NCCTE	10.0001	MASSSPEC: VocBinBase volatile compounds database
503	Cyazofamid	120116-88-3	DTXSID9034492	Microbiocide		NCCTE	20.0002	
504	CP-122721	145742-28-5	DTXSID9047251	Pharmaceutical		NCCTE	20	
505	Potassium perfluoroctanesulfonate	2795-39-3	DTXSID8037706	Surfactant		NCCTE	19.2487	
506	Benzotrichloride	98-07-7	DTXSID1020148	Chemical intermediate		NCCTE	19.9997	
507	Iprodione	36734-19-7	DTXSID3024154	Microbiocide		NCCTE	20	
508	Oryzalin	19044-88-3	DTXSID8024238	Herbicide		NCCTE	19.9994	
509	Icaridin	119515-38-7	DTXSID0034227	Pesticide (non-herbicide)		NCCTE	20.0004	
510	Phosmet	732-11-6	DTXSID5024261	Pesticide (non-herbicide)		NCCTE	20	
511	Octylbicycloheptenedicarboximide	113-48-4	DTXSID6032562	Chemical intermediate		NCCTE	20.0006	
512	Dicumyl peroxide	80-43-3	DTXSID1025017	Chemical intermediate		NCCTE	20.0004	
513	1,4-Benzquinone	106-51-4	DTXSID6020145	Chemical intermediate		NCCTE	19.9821	
514	Tamoxifen	10540-29-1	DTXSID1034187	Pharmaceutical		NCCTE	9.99969	
515	Carboxin	5234-68-4	DTXSID0023951	Microbiocide		NCCTE	20	
516	Diniconazole	83657-24-3	DTXSID2040363	Microbiocide		NCCTE	19.9996	
517	Ethoprop	13194-48-4	DTXSID4032611	Pesticide (non-herbicide)		NCCTE	20.0318	
518	Theophylline	58-55-9	DTXSID5021336	Pharmaceutical		NCCTE	20	
519	Biphenyl	92-52-4	DTXSID4020161	Chemical intermediate		NCCTE	20.0033	
520	Phenol	108-95-2	DTXSID5021124	Chemical intermediate		NCCTE	20.0006	
521	2-Ethylhexanoic acid	149-57-5	DTXSID9025293	Chemical intermediate		NCCTE	19.9998	MASSPEC: VocBinBase volatile compounds database
522	Novaluron	116714-46-6	DTXSID5034773	Pesticide (non-herbicide)		NCCTE	19.9983	
523	Methimazole	60-56-0	DTXSID4020820	Pharmaceutical		NCCTE	19.9998	
524	Paraoxon	311-45-5	DTXSID6024046	Pesticide (non-herbicide)		NCCTE	19.9997	
525	Hydroxyflutamide	52806-53-8	DTXSID8033562	Pharmaceutical		NCCTE	20.0011	
526	(E)-Anethole	4180-23-8	DTXSID9020087	FoodFlavorFragrance		NCCTE	20	
527	Nitrobenzene	98-95-3	DTXSID3020964	Chemical intermediate		NCCTE	19.9995	
528	Nalidixic acid	389-08-2	DTXSID3020912	Pharmaceutical		NCCTE	19.9997	
529	Imazalil	35554-44-0	DTXSID8024151	Microbiocide		NCCTE	19.9998	
530	Perfluoroctanoic acid	335-67-1	DTXSID8031865	Surfactant		NCCTE	20.0006	
531	Hexaconazole	79983-71-4	DTXSID4034653	Microbiocide		NCCTE	19.9996	
532	Mifepristone	84371-65-3	DTXSID5023322	Pharmaceutical		NCCTE	19.9919	
533	Ametryn	834-12-8	DTXSID1023869	Herbicide		NCCTE	19.9997	
534	Levonorgestrel	797-63-7	DTXSID3036496	Pharmaceutical		NCCTE	19.9996	
535	Tefluthrin	79538-32-2	DTXSID5032577	Pesticide (non-herbicide)		NCCTE	20	
536	Tris(1,3-dichloro-2-propyl) phosphate	13674-87-8	DTXSID9026261	Flame retardant		NCCTE	20	
537	(-)-Epigallocatechin	989-51-5	DTXSID1029889	FoodFlavorFragrance		NCCTE	19.3511	
538	Ethyl phthalyl ethyl	84-72-0	DTXSID3024100	Plasticizer		NCCTE	19.9997	
539	Esfenvalerate	66230-04-4	DTXSID4032667	Pesticide (non-herbicide)		NCCTE	20.0007	
540	Buprofezin	69327-76-0	DTXSID8034401	Pesticide (non-herbicide)		NCCTE	20	
541	4-Chloroaniline	106-47-8	DTXSID9020295	Chemical intermediate		NCCTE	20.3412	
542	Cresol	1319-77-3	DTXSID3024364	FoodFlavorFragrance		NCCTE	19.9996	
543	Dibutyl adipate	105-99-7	DTXSID2021866	Plasticizer		NCCTE	19.9996	

544	N-Nitrosodibutylamine	924-16-3	DTXSID2021026	Other	Research chemical; not commercial, but a byproduct of manufacturing	NCCTE	20	
545	Acrylamide	79-06-1	DTXSID5020027	Chemical intermediate		NCCTE	20	
546	Indoxacarb	173584-44-6	DTXSID1032690	Pesticide (non-herbicide)		NCCTE	16.0465	
547	Tributyl phosphate	126-73-8	DTXSID3021986	Solvent		NCCTE	20	
548	2-Chloro-N-phenylacetamide	587-65-5	DTXSID3041409	Other	Inert (pesticides)	NCCTE	20	
549	2,3,6-Trimethylphenol	2416-94-6	DTXSID6022187	FoodFlavorFragrance		NCCTE	19.9997	
550	N,N-Diethylaniline	91-66-7	DTXSID8021800	Chemical intermediate		NCCTE	20.0006	
551	1,5,9-Cyclododecatriene	4904-61-4	DTXSID8027581	Chemical intermediate		NCCTE	19.9996	
552	2-Methyl-1-propanol	78-83-1	DTXSID0021759	FoodFlavorFragrance		NCCTE	19.999	
553	Fluthiacet-methyl	117337-19-6	DTXSID2032556	Herbicide		NCCTE	20	
554	Vinclozolin	50471-44-8	DTXSID4022361	Microbiocide		NCCTE	20.0005	
555	Permethrin	52645-53-1	DTXSID8022292	Pesticide (non-herbicide)		NCCTE	19.9998	
556	Maleic hydrazide	123-33-1	DTXSID9020792	Herbicide		NCCTE	19.9912	
557	Ocithilinone	26530-20-1	DTXSID1025805	Microbiocide		NCCTE	20.8237	
558	Dodecylbenzene sulfonate	27323-41-7	DTXSID5027932	Surfactant		NCCTE	17.9737	
559	Bisphenol A	80-05-7	DTXSID7020182	Plasticizer		NCCTE	20.2592	
560	Diclosulam	145701-21-9	DTXSID4034528	Herbicide		NCCTE	20	
561	4-	58-15-1	DTXSID7020504	Pharmaceutical		NCCTE	20	
562	Diisobutyl phthalate	84-69-5	DTXSID9022522	Plasticizer		NCCTE	20.0004	
563	Phenacetin	62-44-2	DTXSID1021116	Pharmaceutical		NCCTE	20.0002	
564	Chlorotriakisene	569-57-3	DTXSID1021299	Pharmaceutical		NCCTE	20	
565	Bis(2-chloroethyl) ether	111-44-4	DTXSID9020168	Solvent		NCCTE	20	
566	3-Nitrotoluene	99-08-1	DTXSID5021831	Chemical intermediate		NCCTE	20.0002	
567	17-Methyltestosterone	58-18-4	DTXSID1033664	Pharmaceutical		NCCTE	20.0089	
568	Bisphenol AF	1478-61-1	DTXSID7037717	Plasticizer		NCCTE	20.0002	
569	Dimethyl succinate	106-65-0	DTXSID5025152	Chemical intermediate		NCCTE	20	
570	Fenamidone	161326-34-7	DTXSID2034590	Microbiocide		NCCTE	19.9996	
571	Sodium (2-pyridylthio)-N-oxide	3811-73-2	DTXSID3042390	Microbiocide		NCCTE	20	
572	Corticosterone	50-22-6	DTXSID6022474	Pharmaceutical		NCCTE	20.0004	
573	1,4-Dichlorobenzene	106-46-7	DTXSID1020431	Chemical intermediate		NCCTE	20	
*574	Dichlorophen	97-23-4	DTXSID6021824	Microbiocide		NCCTE	20	
575	Piperazine	110-85-0	DTXSID1021164	Pesticide (non-herbicide)		NCCTE	19.9995	
576	Gibberellic acid	77-06-5	DTXSID0020656	Herbicide		NCCTE	20.0005	
577	2,3-Dinitrotoluene	602-01-7	DTXSID4027236	Chemical intermediate		NCCTE	14.3162	
578	Cinmethilin	87818-31-3	DTXSID3034456	Herbicide		NCCTE	20.0014	
579	Isoxaflutole	141112-29-0	DTXSID5034723	Herbicide		NCCTE	19.9998	
580	Propiconazole	60207-90-1	DTXSID8024280	Microbiocide		NCCTE	20.0005	
581	Butachlor	23184-66-9	DTXSID3034402	Herbicide		NCCTE	20.0002	
582	1-Chloro-4-nitrobenzene	100-00-5	DTXSID5020281	Chemical intermediate		NCCTE	20	
583	Pirimiphos-methyl	29232-93-7	DTXSID0024266	Pesticide (non-herbicide)		NCCTE	19.9994	
584	Cyromazine	66215-27-8	DTXSID6023999	Pesticide (non-herbicide)		NCCTE	19.9997	
585	1-Chloro-2-nitrobenzene	88-73-3	DTXSID0020280	Chemical intermediate		NCCTE	5	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
586	Bisphenol E	2081-08-5	DTXSID3047891	Plasticizer		NCCTE	20	
587	Dichlobenil	1194-65-6	DTXSID5032365	Herbicide		NCCTE	19.9998	
588	Sulfentrazone	122836-35-5	DTXSID6032645	Herbicide		NCCTE	20	
589	7,12-Dimethylbenz(a)anthracene	57-97-6	DTXSID1020510	PAH		NCCTE	20.0003	
590	1-Methoxy-2-propanol	107-98-2	DTXSID8024284	Solvent		NCCTE	19.9949	
591	Hydrochlorothiazide	58-93-5	DTXSID2020713	Pharmaceutical		NCCTE	19.9995	
592	FR900409	138472-01-2	DTXSID2048167	Pharmaceutical		NCCTE	19.9998	
593	2-Methoxy-5-nitroaniline	99-59-2	DTXSID0020943	Chemical intermediate		NCCTE	20.0003	
594	Dipropylene glycol	25265-71-8	DTXSID0027856	Solvent		NCCTE	20	
595	Asulam	3337-71-1	DTXSID8023890	Herbicide		NCCTE	20.003	
596	Oxyphenisatin	125-13-3	DTXSID5044528	Pharmaceutical		NCCTE	20.0005	
597	Lactofen	77501-63-4	DTXSID7024160	Herbicide		NCCTE	20.0008	
598	Octanal	124-13-0	DTXSID3021643	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
599	Dichloroacetic acid	79-43-6	DTXSID2020428	Microbiocide		NCCTE	20	
600	Acrylonitrile	107-13-1	DTXSID5020029	Chemical intermediate		NCCTE	19.9995	
601	Docusate sodium	577-11-7	DTXSID8022959	Pharmaceutical		NCCTE	19.9995	

602	Sodium dimethylthiocarbamate	128-04-1	DTXSID6027050	Microbiocide		NCCTE	20	
603	Bisphenol B	77-40-7	DTXSID4022442	Plasticizer		NCCTE	20.0004	
604	Rotenone	83-79-4	DTXSID6021248	Pesticide (non-herbicide)		NCCTE	19.9997	
605	Acetochlor	34256-82-1	DTXSID8023848	Herbicide		NCCTE	19.9996	
606	Dichlorodiphenyltrichloroethane	50-29-3	DTXSID4020375	Pesticide (non-herbicide)		NCCTE	20.0002	
607	Chlorpyrifos	2921-88-2	DTXSID4020458	Pesticide (non-herbicide)		NCCTE	19.9997	
608	Phorate	298-02-2	DTXSID4032459	Pesticide (non-herbicide)		NCCTE	20	
609	Pentachloronitrobenzene	82-68-8	DTXSID2021105	Microbiocide		NCCTE	20	
610	Boric acid	10043-35-3	DTXSID1020194	Pesticide (non-herbicide)		NCCTE	19.9911	
611	1,3-Dibromo-5,5-dimethylhydantoin	77-48-5	DTXSID3035341	Microbiocide		NCCTE	20	
612	Gemfibrozil	25812-30-0	DTXSID0020652	Pharmaceutical		NCCTE	20	
*613	Fenpropothrin	39515-41-8	DTXSID0024002	Pesticide (non-herbicide)		NCCTE	20	
614	4,4'-Diaminobiphenyl methane	101-77-9	DTXSID6022422	Chemical intermediate		NCCTE	20	
615	Ethion	563-12-2	DTXSID2024086	Pesticide (non-herbicide)		NCCTE	19.9997	
616	4-Cumylphenol	599-64-4	DTXSID3022536	Chemical intermediate		NCCTE	19.9996	
617	tert-Butyl perbenzoate	614-45-9	DTXSID9024699	Chemical intermediate		NCCTE	20	
618	Mepiquat chloride	24307-26-4	DTXSID1024170	Herbicide		NCCTE	19.9997	
619	D-Limonene	5989-27-5	DTXSID1020778	FoodFlavorFragrance		NCCTE	20	
620	Estrone	53-16-7	DTXSID4022367	Pharmaceutical		NCCTE	20.0003	
621	I-Tryptophan	73-22-3	DTXSID5021419	FoodFlavorFragrance		NCCTE	20	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
622	Diisobutyl adipate	141-04-8	DTXSID9036690	Plasticizer		NCCTE	20	
623	MCPA	94-74-6	DTXSID4024195	Herbicide		NCCTE	19.9997	
624	Methylprednisolone	83-43-2	DTXSID7023300	Pharmaceutical		NCCTE	20	
625	Pymetrozine	123312-89-0	DTXSID2032637	Pesticide (non-herbicide)		NCCTE	20	
626	4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol]	41481-66-7	DTXSID9047598	Other	Thermal recording material/paper manufacturing	NCCTE	20.0003	
627	Dichlorvos	62-73-7	DTXSID5020449	Pesticide (non-herbicide)		NCCTE	9.95147	
628	Methoxychlor	72-43-5	DTXSID9020827	Pesticide (non-herbicide)		NCCTE	19.8979	
629	Troglitazone	97322-87-7	DTXSID8023719	Pharmaceutical		NCCTE	20.0009	
630	Flumetralin	62924-70-3	DTXSID7032553	Herbicide		NCCTE	20.0005	
631	Benz(a)anthracene	56-55-3	DTXSID5023902	PAH		NCCTE	19.9996	
632	Geranyl acetate	105-87-3	DTXSID0020654	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
633	Tolcapone	134308-13-7	DTXSID3023685	Pharmaceutical		NCCTE	20.0003	
634	Bis(2-ethylhexyl)hexanedioate	103-23-1	DTXSID0020606	Pharmaceutical		NCCTE	19.9997	
635	Pyrithiobac-sodium	123343-16-8	DTXSID8032673	Herbicide		NCCTE	20	
636	hifensulfuron methyl	79277-27-3	DTXSID1024124	Herbicide		NCCTE	19.9993	
637	C.I. Solvent Yellow 14	842-07-9	DTXSID4021135	Dye		NCCTE	20	
638	Chlorhexidine diacetate	56-95-1	DTXSID7032345	Microbiocide		NCCTE	20	
639	1-Dodecyl-2-	2687-96-9	DTXSID4042206	Surfactant		NCCTE	19.9997	
640	Pentyl acetate	628-63-7	DTXSID1027263	FoodFlavorFragrance		NCCTE	20	
641	Pentaerythritol	3296-90-0	DTXSID9020164	Flame retardant		NCCTE	20	
642	Dicamba	1918-00-9	DTXSID4024018	Herbicide		NCCTE	20	
643	Methyl salicylate	119-36-8	DTXSID5025659	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
644	5,5-Dimethylhydantoin	77-71-4	DTXSID5021754	Chemical intermediate		NCCTE	20.1161	
645	1-Benzylquinolinium chloride	15619-48-4	DTXSID8044593	Other	Fracking; oilfield inhibitor	NCCTE	20	
646	2,4-Dichlorophenol	120-83-2	DTXSID1020439	Chemical intermediate		NCCTE	19.9997	CHEMINV: EPA ToxCast CHEMINV list of volatiles
647	Triticonazole	131983-72-7	DTXSID0032655	Microbiocide		NCCTE	19.9278	
648	Nicotinic acid	59-67-6	DTXSID1020932	FoodFlavorFragrance		NCCTE	19.9935	
649	Azoxystrobin	131860-33-8	DTXSID0032520	Microbiocide		NCCTE	19.9993	
650	Coumaphos	56-72-4	DTXSID2020347	Pesticide (non-herbicide)		NCCTE	20	

651	4-Ethylcyclo-1-yn-3-ol	5877-42-9	DTXSID1044697	Chemical intermediate		NCCTE	19.995	
652	Tannic acid	1401-55-4	DTXSID2026076	FoodFlavorFragrance		NCCTE	6.08385	
653	Captan	133-06-2	DTXSID9020243	Microbiocide		NCCTE	19.732	
654	Fluoxastrobin	361377-29-9	DTXSID2034625	Microbiocide		NCCTE	20	
655	Fenoxaprop-ethyl	66441-23-4	DTXSID2032392	Herbicide		NCCTE	20.0003	
656	tert-Butylbenzene	98-06-6	DTXSID3047138	Solvent		NCCTE	20	
657	Fenbuconazole	114369-43-6	DTXSID8032548	Microbiocide		NCCTE	19.9993	
658	Phenmedipham	13684-63-4	DTXSID1024255	Herbicide		NCCTE	19.9997	
659	Hexanoic acid	142-62-1	DTXSID7021607	Chemical intermediate		NCCTE	20.0106	MASSSPEC: VocBinBase volatile compounds database
660	1,2,3-Trichloropropane	96-18-4	DTXSID9021390	Chemical intermediate		NCCTE	20	
661	N-Nitrosodipropylamine	621-64-7	DTXSID6021032	Other	Research chemical; not commercial, but a byproduct of manufacturing	NCCTE	19.9941	
662	Captafol	2425-06-1	DTXSID4020242	Microbiocide		NCCTE	20	
663	Ethylparaben	120-47-8	DTXSID9022528	Microbiocide		NCCTE	20	
664	4-(Butan-2-yl)phenol	99-71-8	DTXSID7022332	Chemical intermediate		NCCTE	19.9998	
665	Sodium chlorite	7758-19-2	DTXSID8021272	Microbiocide		NCCTE	19.9997	
666	Cyanamide	420-04-2	DTXSID9034490	Chemical intermediate		NCCTE	19.9808	
667	Cloprop	101-10-0	DTXSID9034232	Herbicide		NCCTE	20	
668	4,4'-Oxydianiline	101-80-4	DTXSID0021094	Chemical intermediate		NCCTE	19.9997	
669	Heptanoic acid	111-14-8	DTXSID2021600	FoodFlavorFragrance		NCCTE	20	
670	Malaoxon	1634-78-2	DTXSID9020790	Pesticide (non-herbicide)		NCCTE	19.9997	
671	Imidacloprid	138261-41-3	DTXSID5032442	Pesticide (non-herbicide)		NCCTE	20	
672	Pentaerythritol	115-77-5	DTXSID2026943	Flame retardant		NCCTE	19.9998	
673	1-Tetradecanol	112-72-1	DTXSID9026926	Chemical intermediate		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
674	Retinol	68-26-8	DTXSID3023556	Pharmaceutical		NCCTE	20.86	
675	Phenanthrene	85-01-8	DTXSID6024254	PAH		NCCTE	20.0002	
676	Prochloraz	67747-09-5	DTXSID4024270	Microbiocide		NCCTE	20.0006	
677	Thiacloprid	111988-49-9	DTXSID7034961	Pesticide (non-herbicide)		NCCTE	20	
678	alpha-Isomethylionone	127-51-5	DTXSID7027047	FoodFlavorFragrance		NCCTE	20.0003	
679	Flusilazole	85509-19-9	DTXSID3024235	Microbiocide		NCCTE	20	
680	Rhodamine 6G	989-38-8	DTXSID1021243	Dye		NCCTE	19.9994	
681	Hexanedioic acid	124-04-9	DTXSID7021605	FoodFlavorFragrance		NCCTE	20	
682	Dicofol	115-32-2	DTXSID4020450	Pesticide (non-herbicide)		NCCTE	19.9935	
683	Myrcene	123-35-3	DTXSID6025692	FoodFlavorFragrance		NCCTE	20	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles; MASSPEC: VocBinBase volatile compounds database
684	Bromocresol green sodium salt	62625-32-5	DTXSID3044704	Dye		NCCTE	14.4723	
685	Imazethapyr	81335-77-5	DTXSID3024287	Herbicide		NCCTE	20	
686	Propham	122-42-9	DTXSID7020766	Herbicide		NCCTE	19.9997	
687	2,5-Furandione	108-31-6	DTXSID7024166	Chemical intermediate		NCCTE	20.0006	
688	1,2,4-Trimethylbenzene	95-63-6	DTXSID6021402	Solvent		NCCTE	20.7995	
*689	Iooctyl acrylate	29590-42-9	DTXSID8027955	Plasticizer		NCCTE	20	
690	Cycloate	1134-23-2	DTXSID6032356	Herbicide		NCCTE	20	
691	17alpha-Estradiol	57-91-0	DTXSID8022377	Pharmaceutical		NCCTE	20.0004	
692	4-Nitrophenol	100-02-7	DTXSID0021834	Chemical intermediate		NCCTE	20	
693	Dimethoxane	828-00-2	DTXSID6020480	Microbiocide		NCCTE	20	
694	Diphenhydramine hydrochloride	147-24-0	DTXSID4020537	Pharmaceutical		NCCTE	20.0002	
695	2-Phenoxyethanol	122-99-6	DTXSID9021976	FoodFlavorFragrance		NCCTE	20	
696	Carbendazim	10605-21-7	DTXSID4024729	Microbiocide		NCCTE	20	
697	Fenhexamid	126833-17-8	DTXSID3032549	Microbiocide		NCCTE	20	
698	Fluazinam	79622-59-6	DTXSID7032551	Microbiocide		NCCTE	20	
699	Tetramethrin	7696-12-0	DTXSID6032649	Pesticide (non-herbicide)		NCCTE	20.0005	
700	2-Phenylphenol	90-43-7	DTXSID2021151	Microbiocide		NCCTE	20.0003	
701	Linuron	330-55-2	DTXSID2024163	Herbicide		NCCTE	19.9997	

702	Atrazine	1912-24-9	DTXSID9020112	Herbicide		NCCTE	19.9997	
703	Tebuthiuron	34014-18-1	DTXSID3024316	Herbicide		NCCTE	19.9998	
704	2,2'-[Ethane-1,2-diylibis(oxy)]diethanamine	929-59-9	DTXSID9044742	Chemical intermediate		NCCTE	19.9997	
705	Pimozide	2062-78-4	DTXSID8023474	CiPA pharmaceutical		NCCTE	20.0007	
706	Diclofenac	15307-86-5	DTXSID6022923	Pharmaceutical		NCCTE	20	
707	3,4-Dimethylphenol	95-65-8	DTXSID4024062	FoodFlavorFragrance		NCCTE	20.5047	
708	Caffeine	58-08-2	DTXSID0020232	FoodFlavorFragrance		NCCTE	20.0003	
709	Thiabendazole	148-79-8	DTXSID0021337	Microbiocide		NCCTE	19.9997	
710	1,3-Dichlorobenzene	541-73-1	DTXSID6022056	Pesticide (non-herbicide)		NCCTE	20	
711	Tris(2-ethylhexyl) trimellitate	3319-31-1	DTXSID9026265	Plasticizer		NCCTE	19.9996	
712	Salph-a-	521-18-6	DTXSID9022364	Pharmaceutical		NCCTE	20.0004	
713	Triamcinolone	124-94-7	DTXSID1040742	Pharmaceutical		NCCTE	20.0003	
714	Prometryn	7287-19-6	DTXSID4024272	Herbicide		NCCTE	20.0004	
715	4,4'-(Isopropylidenebis(4,1-	13080-86-9	DTXSID5051650	Other		NCCTE	19.9997	
716	Propyl gallate	121-79-9	DTXSID5021201	FoodFlavorFragrance		NCCTE	19.9996	
717	1,2-Dimethyl-3-nitrobenzene	83-41-0	DTXSID7025132	Chemical intermediate		NCCTE	20	
718	Ammonium sulfamate	7773-06-0	DTXSID5023875	Herbicide		NCCTE	19.9939	
719	Dicloran	99-30-9	DTXSID2020426	Microbiocide		NCCTE	20	
*720	Glycidol	556-52-5	DTXSID4020666	Chemical intermediate		NCCTE	20	
721	Lovastatin	75330-75-5	DTXSID5020784	Pharmaceutical		NCCTE	19.9976	
722	Diquat dibromide monohydrate	6385-62-2	DTXSID7031248	Herbicide		NCCTE	9.99988	
723	Diazinon	333-41-5	DTXSID9020407	Pesticide (non-herbicide)		NCCTE	20	
724	Clothianidin	210880-92-5	DTXSID2034465	Pesticide (non-herbicide)		NCCTE	19.9995	
725	meso-Hexestrol	84-16-2	DTXSID2022381	Pharmaceutical		NCCTE	20.0005	
726	Oxytetracycline dihydrate	6153-64-6	DTXSID4023412	Pharmaceutical		NCCTE	19.9994	
727	Propachlor	1918-16-7	DTXSID4024274	Herbicide		NCCTE	19.9998	
728	Tris(2-chloroethyl) phosphate	115-96-8	DTXSID5021411	Flame retardant		NCCTE	20	
729	Resmethrin	10453-86-8	DTXSID7022253	Pesticide (non-herbicide)		NCCTE	20	
730	Silica	7631-86-9	DTXSID1029677	Chemical intermediate		NCCTE	20	
731	Fenoxycarb	72490-01-8	DTXSID7032393	Pesticide (non-herbicide)		NCCTE	20.0003	
732	1,2-Dinitrobenzene	528-29-0	DTXSID4024066	Chemical intermediate		NCCTE	20	
733	Cyanazine	21725-46-2	DTXSID1023990	Herbicide		NCCTE	20	
734	Difenoquat metilsulfate	43222-48-6	DTXSID6024048	Herbicide		NCCTE	19.9998	
735	Michler's ketone	90-94-8	DTXSID2020894	Chemical intermediate		NCCTE	19.9996	
736	N,N'-Methylenebisacrylamide	110-26-9	DTXSID8025595	Chemical intermediate		NCCTE	19.9997	
737	2-Norbornene-5,6-dicarboxylic anhydride	826-62-0	DTXSID0047456	FoodFlavorFragrance		NCCTE	20.0066	
738	Monuron	150-68-5	DTXSID0020311	Herbicide		NCCTE	20	
739	Diethylene glycol	111-46-6	DTXSID8020462	Solvent		NCCTE	19.9996	
740	Prodiamine	29091-21-2	DTXSID1034210	Herbicide		NCCTE	19.963	
741	Quinoline	91-22-5	DTXSID1021798	Solvent		NCCTE	20	
742	Hexachlorocyclopentadiene	77-47-4	DTXSID2020688	Chemical intermediate		NCCTE	20	
743	Tralkoxydim	87820-88-0	DTXSID1034973	Herbicide		NCCTE	20.0005	
744	Diallyl phthalate	131-17-9	DTXSID7020392	Plasticizer		NCCTE	20	
745	Carbaryl	63-25-2	DTXSID9020247	Pesticide (non-herbicide)		NCCTE	20	
746	N-Phenyl-1,4-benzenediamine	101-54-2	DTXSID7025895	Chemical intermediate		NCCTE	20	
747	Difenoconazole	119446-68-3	DTXSID4032372	Microbiocide		NCCTE	20.0008	
748	Perfluoroctanesulfonic acid	1763-23-1	DTXSID3031864	Surfactant		NCCTE	16.7757	
749	Azinphos-methyl	86-50-0	DTXSID3020122	Pesticide (non-herbicide)		NCCTE	20.0004	
750	Famoxadone	131807-57-3	DTXSID8034588	Microbiocide		NCCTE	20.0824	
751	Colchicine	64-86-8	DTXSID5024845	Pharmaceutical		NCCTE	20	
752	Ethofumesate	26225-79-6	DTXSID8034580	Herbicide		NCCTE	20.0005	
753	Clomazone	81777-89-1	DTXSID1032355	Herbicide		NCCTE	19.9996	
754	Levothyroxine	51-48-9	DTXSID8023214	Pharmaceutical		NCCTE	13.7861	
755	Folic acid	59-30-3	DTXSID0022519	FoodFlavorFragrance		NCCTE	20	
756	Propamocarb	25606-41-1	DTXSID6034849	Pesticide (non-herbicide)		NCCTE	19.9997	
757	2,6-Di-tert-butylphenol	128-39-2	DTXSID6027052	Chemical intermediate		NCCTE	20	
758	Vernolate	1929-77-7	DTXSID7024376	Herbicide		NCCTE	20	
759	o,p'-DDT	789-02-6	DTXSID6022345	Pesticide (non-herbicide)		NCCTE	19.9996	
760	Perfluorodecanoic acid	335-76-2	DTXSID3031860	Solvent		NCCTE	20.0008	
761	Pyrene	129-00-0	DTXSID3024289	PAH		NCCTE	19.9997	
762	Fosthiazate	98886-44-3	DTXSID0034930	Pesticide (non-herbicide)		NCCTE	19.9998	
763	Isoeugenol	97-54-1	DTXSID7022413	FoodFlavorFragrance		NCCTE	20	
764	Bentazone	25057-89-0	DTXSID0023901	Herbicide		NCCTE	19.9998	
765	Metolachlor	51218-45-2	DTXSID4022448	Herbicide		NCCTE	20.0003	
766	Acifluorfen	50594-66-6	DTXSID0020022	Herbicide		NCCTE	19.9994	
767	Dithiopyr	97886-45-8	DTXSID9032379	Herbicide		NCCTE	19.9297	
768	Aldoxycarb	1646-88-4	DTXSID6023862	Pesticide (non-herbicide)		NCCTE	20	

769	Naled	300-76-5	DTXSID1024209	Pesticide (non-herbicide)		NCCTE	19.9994	
770	Candoxatril	123122-55-4	DTXSID6047286	Pharmaceutical		NCCTE	20	
771	Acetyl tributyl citrate	77-90-7	DTXSID2026446	FoodFlavorFragrance		NCCTE	19.9992	
772	Malic acid	6915-15-7	DTXSID0027640	FoodFlavorFragrance		NCCTE	20	
773	Diethylene glycol dibenzoate	120-55-8	DTXSID0026967	Plasticizer		NCCTE	20	
774	Etoxazole	153233-91-1	DTXSID8034586	Pesticide (non-herbicide)		NCCTE	20.0002	
775	2,3-Diaminotoluene	2687-25-4	DTXSID4027494	Chemical intermediate		NCCTE	19.9952	
776	Benodanil	15310-01-7	DTXSID7041623	Microbiocide		NCCTE	19.9998	
777	Ranitidine	66357-35-5	DTXSID8045191	Pharmaceutical		NCCTE	20	
778	Thiamethoxam	153719-23-4	DTXSID2034962	Pesticide (non-herbicide)		NCCTE	20.0003	
779	Methyl parathion	298-00-0	DTXSID1020855	Pesticide (non-herbicide)		NCCTE	19.9964	
780	Anthracene	120-12-7	DTXSID0023878	Chemical intermediate		NCCTE	20	
781	Lindane	58-89-9	DTXSID2020686	Pesticide (non-herbicide)		NCCTE	20	
782	Acetaminophen	103-90-2	DTXSID2020006	Pharmaceutical		NCCTE	20	
783	Naproxen	22204-53-1	DTXSID4040686	Pharmaceutical		NCCTE	20	
784	Butylate	2008-41-5	DTXSID7023936	Herbicide		NCCTE	19.9997	
785	Dimethyl sulfate	77-78-1	DTXSID5024055	Chemical intermediate		NCCTE	20	
786	N-Vinyl-2-pyrrolidone	88-12-0	DTXSID2021440	Chemical intermediate		NCCTE	20.0016	
787	Darbufelone mesylate	139340-56-0	DTXSID0047246	Pharmaceutical		NCCTE	10	
788	Triclopyr	55335-06-3	DTXSID0032497	Herbicide		NCCTE	20.4005	
789	1-Undecanol	112-42-5	DTXSID0026915	FoodFlavorFragrance		NCCTE	20	MASSPEC: VocBinBase volatile compounds database
790	Bicalutamide	90357-06-5	DTXSID2022678	Pharmaceutical		NCCTE	19.9966	
791	Flumetsulam	98967-40-9	DTXSID4032615	Herbicide		NCCTE	20	
792	m-Cresol	108-39-4	DTXSID6024200	Chemical intermediate		NCCTE	19.9984	MASSPEC: VocBinBase volatile compounds database
793	Tolbutamide	64-77-7	DTXSID8021359	Pharmaceutical		NCCTE	20.0003	
794	Benomyl	17804-35-2	DTXSID5023900	Microbiocide		NCCTE	19.9996	
795	2,4,5-Trichlorophenol	95-95-4	DTXSID4024359	Microbiocide		NCCTE	20.0003	
796	1,3-Dinitrobenzene	99-65-0	DTXSID9024065	Chemical intermediate		NCCTE	20.7022	
797	Triclosan	3380-34-5	DTXSID5032498	Microbiocide		NCCTE	19.9998	
798	Physostigmine	57-47-6	DTXSID3023471	Pharmaceutical		NCCTE	20.0005	
799	Acetic acid	64-19-7	DTXSID5024394	Chemical intermediate		NCCTE	20	
800	3-Pyridinecarbonitrile	100-54-9	DTXSID1026665	Chemical intermediate		NCCTE	20.0026	
801	Dimethylcarbamoyl	79-44-7	DTXSID1020512	Chemical intermediate		NCCTE	19.9893	
802	Urea	57-13-6	DTXSID4021426	FoodFlavorFragrance		NCCTE	20	
803	Hydroquinone	123-31-9	DTXSID7020716	Chemical intermediate		NCCTE	19.9939	
804	2,4,7,9-Tetramethyl-5-decyne-4,7-diol	126-86-3	DTXSID7027041	Chemical intermediate		NCCTE	20.0004	
805	Trilocarban	101-20-2	DTXSID4026214	Microbiocide		NCCTE	19.9994	
806	2-Naphthalenol	135-19-3	DTXSID5027061	Chemical intermediate		NCCTE	20	
807	Allura Red C.I.16035	25956-17-6	DTXSID4024436	Dye		NCCTE	20.0007	
808	Iopanoic acid	96-83-3	DTXSID6023159	Pharmaceutical		NCCTE	17.664	
809	Raloxifene hydrochloride	82640-04-8	DTXSID1034181	Pharmaceutical		NCCTE	19.9988	
810	Haloxyfop-methyl	69806-40-2	DTXSID6024123	Herbicide		NCCTE	19.9996	
811	Cyproterone acetate	427-51-0	DTXSID5020366	Pharmaceutical		NCCTE	20.0071	
812	2,5-Di-tert-butylbenzene-1,4-diol	88-58-4	DTXSID8041248	Chemical intermediate		NCCTE	22.8041	
813	1,3-Dichloro-5,5-dimethylhydantoin	118-52-5	DTXSID4024985	Microbiocide		NCCTE	20	
814	Methacrylamide	79-39-0	DTXSID8029600	Chemical intermediate		NCCTE	20.0005	
815	Acenaphthene	83-32-9	DTXSID3021774	PAH		NCCTE	20	
816	Disulfiram	97-77-8	DTXSID1021322	Microbiocide		NCCTE	19.9997	
817	Tebupirimfos	96182-53-5	DTXSID1032482	Pesticide (non-herbicide)		NCCTE	20	
818	Dibromoacetonitrile	3252-43-5	DTXSID3024940	Microbiocide		NCCTE	20.0003	
819	2-Chloroacetophenone	532-27-4	DTXSID9020293	Other	Irritant (tear gas, mace); used in explosives and pesticide	NCCTE	20	
820	Apigenin	520-36-5	DTXSID6022391	FoodFlavorFragrance		NCCTE	20.0005	
821	Octrizole	3147-75-9	DTXSID9027522	Flame retardant		NCCTE	20.0004	
822	N-Methylacetamide	79-16-3	DTXSID0047167	Solvent		NCCTE	20.0005	
823	Medroxyprogesterone acetate	71-58-9	DTXSID0025527	Pharmaceutical		NCCTE	10.0001	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
824	Methamidophos	10265-92-6	DTXSID6024177	Pesticide (non-herbicide)		NCCTE	20	

825	FD&C Yellow 5	1934-21-0	DTXSID1021455	Dye		NCCTE	18.9383	
826	8:2 Fluorotelomer alcohol	678-39-7	DTXSID7029904	Chemical intermediate		NCCTE	19.9991	
827	Pyrimethamine	58-14-0	DTXSID9021217	Pharmaceutical		NCCTE	20.0002	
828	Cyanogen bromide	506-68-3	DTXSID9021550	Chemical intermediate		NCCTE	19.9998	
829	Flufenacet	142459-58-3	DTXSID2032552	Herbicide		NCCTE	19.9996	
830	Sorbitan, mono-(9Z)-9-octadecenoate	1338-43-8	DTXSID6027397	Surfactant		NCCTE	19.9994	
831	Mevinphos	7786-34-7	DTXSID2032683	Pesticide (non-herbicide)		NCCTE	20	
832	Indomethacin	53-86-1	DTXSID9020740	Pharmaceutical		NCCTE	20.0003	
833	2,4-Di-tert-pentylphenol	120-95-6	DTXSID9026974	Chemical intermediate		NCCTE	20.0003	
834	Sodium myristyl sulfate	1191-50-0	DTXSID4042416	Surfactant		NCCTE	20	
835	Octabenzone	1843-05-6	DTXSID9027441	Plasticizer		NCCTE	20.0004	
836	Propazine	139-40-2	DTXSID3021196	Herbicide		NCCTE	19.9997	
837	Glipizide	29094-61-9	DTXSID0040676	Pharmaceutical		NCCTE	20	
838	Citric acid	77-92-9	DTXSID3020332	FoodFlavorFragrance		NCCTE	20	
839	1,2-Benzenedicarboxaldehyd	643-79-8	DTXSID6032514	Chemical intermediate		NCCTE	20	
840	Trifluralin	1582-09-8	DTXSID4021395	Herbicide		NCCTE	20.0005	
841	2-tert-Butyl-4-	96-70-8	DTXSID4044581	Solvent		NCCTE	20	
842	Volinanserin	139290-65-6	DTXSID6047363	Pharmaceutical		NCCTE	20	
843	17beta-Trenbolone	10161-33-8	DTXSID0034192	Pharmaceutical		NCCTE	20.0005	
844	Deltamethrin	52918-63-5	DTXSID8020381	Pesticide (non-herbicide)		NCCTE	19.9997	
845	1,3-Benzenedicarboxylic	121-91-5	DTXSID3021485	Chemical intermediate		NCCTE	20	
846	Progesterone	57-83-0	DTXSID3022370	Pharmaceutical		NCCTE	20.0006	
847	1,2-Benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich	68515-49-1	DTXSID0028666	Plasticizer		NCCTE	19.9998	
848	2-Aminoanthraquinone	117-79-3	DTXSID6020068	Chemical intermediate		NCCTE	20.0037	
849	2,5-Dimethylphenol	95-87-4	DTXSID6025145	Chemical intermediate		NCCTE	20.5251	
850	Heptachlor epoxide	1024-57-3	DTXSID1024126	Pesticide (non-herbicide)		NCCTE	19.9994	
851	2-	101-86-0	DTXSID4026684	FoodFlavorFragrance		NCCTE	19.9996	
852	Phosphoric acid	7664-38-2	DTXSID5024263	FoodFlavorFragrance		NCCTE	20.0009	
853	Dimethylamine	124-40-3	DTXSID5024057	Surfactant		NCCTE	19.9902	
854	Sucrose	57-50-1	DTXSID2021288	FoodFlavorFragrance		NCCTE	20.0002	
855	Hexadecane	544-76-3	DTXSID0027195	Solvent		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
856	1H-1,2,4-Triazole	288-88-0	DTXSID6027131	Chemical intermediate		NCCTE	20.0004	
857	Dodecylbenzene	123-01-3	DTXSID7026994	Solvent		NCCTE	19.9997	
858	2,3,4-Trihydroxybenzophenone	1143-72-2	DTXSID6037728	Other	UV filter	NCCTE	20.0004	
859	2,4-Dichlorophenoxybutyric	94-82-6	DTXSID7024035	Herbicide		NCCTE	20.3474	
860	Eugenol	97-53-0	DTXSID9020617	FoodFlavorFragrance		NCCTE	20	
861	2,4,6-Trimethylphenol	527-60-6	DTXSID7022049	Chemical intermediate		NCCTE	20.0003	
862	Benfluralin	1861-40-1	DTXSID3023899	Herbicide		NCCTE	19.9994	
863	Dipentyl phthalate	131-18-0	DTXSID5031131	Plasticizer		NCCTE	20	
864	Chloroneb	2675-77-6	DTXSID2024793	Microbiocide		NCCTE	19.9997	
865	Triethylene glycol	112-27-6	DTXSID4021393	FoodFlavorFragrance		NCCTE	20	
866	Fluazifop-P-butyl	79241-46-6	DTXSID0034855	Herbicide		NCCTE	20.065	
867	Sodium nitrite	7632-00-0	DTXSID0020941	Chemical intermediate		NCCTE	20	
868	Umbelliferone	93-35-6	DTXSID5052626	Other	UV filter; in sunscreen; pH indicator; brightener for textiles	NCCTE	19.9992	
869	Thiophanate-methyl	23564-05-8	DTXSID1024338	Microbiocide		NCCTE	19.9997	
870	1-Dodecanol	112-53-8	DTXSID5026918	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
871	Endosulfan	115-29-7	DTXSID1020560	Pesticide (non-herbicide)		NCCTE	20.0004	
872	6-Propyl-2-thiouracil	51-52-5	DTXSID5021209	Pharmaceutical		NCCTE	20	
873	Basic Blue 7	2390-60-5	DTXSID5038888	Dye		NCCTE	19.999	
874	1-[3-(Triethoxysilyl)propyl]ure	23779-32-0	DTXSID5044493	Chemical intermediate		NCCTE	20.0003	
875	Tributyltin chloride	1461-22-9	DTXSID3027403	Microbiocide		NCCTE	20.0006	
876	Sodium benzoate	532-32-1	DTXSID1020140	Microbiocide		NCCTE	20	
877	Bis(2-ethylhexyl)terephthalate	6422-86-2	DTXSID7027625	Plasticizer		NCCTE	19.9952	
878	2-(Hydroxymethyl)-2-nitro-1,3-propanediol	126-11-4	DTXSID8027034	Microbiocide		NCCTE	20	
879	Sodium xylenesulfonate	1300-72-7	DTXSID3026302	Solvent		NCCTE	20.001	

880	3-Methylaniline	108-44-1	DTXSID1026792	Chemical intermediate		NCCTE	20	
881	2,4-Dinitrophenol	51-28-5	DTXSID0020523	Dye		NCCTE	20	
882	Hexachloro-1,3-butadiene	87-68-3	DTXSID7020683	Solvent		NCCTE	20	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
883	2-[2-(2-Butoxyethoxy)ethoxy]ethanol	143-22-6	DTXSID7021520	Plasticizer		NCCTE	20.0082	
884	Chlorthal-dimethyl	1861-32-1	DTXSID0024000	Herbicide		NCCTE	19.9731	
885	Dinoseb	88-85-7	DTXSID3020207	Herbicide		NCCTE	20	
886	Exifone	52479-85-3	DTXSID9044950	Pharmaceutical		NCCTE	20.0004	
887	1-Decanol	112-30-1	DTXSID7021946	Chemical intermediate		NCCTE	20	
888	(E)-1,2-Dichloroethylene	156-60-5	DTXSID7024031	Solvent		NCCTE	19.9907	
889	9-Phenanthrol	484-17-3	DTXSID9047592	Pharmaceutical		NCCTE	20.0004	
890	Dimethyl terephthalate	120-61-6	DTXSID0020498	Chemical intermediate		NCCTE	20.0003	
891	2-Anisidine	90-04-0	DTXSID5023877	Chemical intermediate		NCCTE	20.2996	
892	Daminozide	1596-84-5	DTXSID9020370	Herbicide		NCCTE	20.0002	
893	Nonanoic acid	112-05-0	DTXSID3021641	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
894	Methyl octanoate	111-11-5	DTXSID2026864	FoodFlavorFragrance		NCCTE	19.9993	MASSSPEC: VocBinBase volatile compounds database
895	SSR 241586 HCl	NOCAS_47353	DTXSID2047353	Pharmaceutical		NCCTE	12.2995	
896	Acibenzolar-S-methyl	135158-54-2	DTXSID1032519	Microbiocide		NCCTE	20.0004	
897	1,2,4-Trichlorobenzene	120-82-1	DTXSID0021965	Solvent		NCCTE	20	
898	Diphenamid	957-51-7	DTXSID8024072	Herbicide		NCCTE	20	
899	Parathion	56-38-2	DTXSID7021100	Pesticide (non-herbicide)		NCCTE	20.0013	
900	Propetamphos	31218-83-4	DTXSID7032470	Pesticide (non-herbicide)		NCCTE	20	
901	Benzyl butyl phthalate	85-68-7	DTXSID3020205	Plasticizer		NCCTE	19.9994	
902	Phosalone	2310-17-0	DTXSID1024259	Pesticide (non-herbicide)		NCCTE	20.0007	
903	4-Nitrosodiphenylamine	156-10-5	DTXSID1021031	Chemical intermediate		NCCTE	20	
904	Sodium hexyldecyl sulfate	1120-01-0	DTXSID0042400	Surfactant		NCCTE	9.97618	
905	Azobenzene	103-33-3	DTXSID8020123	Chemical intermediate		NCCTE	20	
906	Pirinixic acid	50892-23-4	DTXSID4020290	Pharmaceutical		NCCTE	19.9976	
907	Theobromine	83-67-0	DTXSID9026132	FoodFlavorFragrance		NCCTE	8.37419	CHEMINV: EPA ToxCast Cheminventory DMSO Insolubles
908	1-Methylnaphthalene	90-12-0	DTXSID9020877	Solvent		NCCTE	20	CHEMINV: EPA ToxCast CHEMINV list of volatiles
909	Benzo(b)fluoranthene	205-99-2	DTXSID0023907	PAH		NCCTE	19.9997	
910	1-Octanol	111-87-5	DTXSID7021940	FoodFlavorFragrance		NCCTE	20.6884	MASSSPEC: VocBinBase volatile compounds database
911	Ketoconazole	65277-42-1	DTXSID7029879	Microbiocide		NCCTE	20	
912	Sodium fluoroacetate	62-74-8	DTXSID8024311	Pesticide (non-herbicide)		NCCTE	20	
913	MCPB	94-81-5	DTXSID4024193	Herbicide		NCCTE	20	
914	Benzidine	92-87-5	DTXSID2020137	Chemical intermediate		NCCTE	20.0002	
915	2,2'-Bisphenol F	2467-02-9	DTXSID4022446	Plasticizer		NCCTE	19.9994	
916	Abamectin	71751-41-2	DTXSID8023892	Pesticide (non-herbicide)		NCCTE	20.0037	
917	Benzoic acid	65-85-0	DTXSID6020143	Microbiocide		NCCTE	20.512	
918	Methyl dodecanoate	111-82-0	DTXSID5026889	FoodFlavorFragrance		NCCTE	20	MASSPEC: VocBinBase volatile compounds database
919	4-Vinyl-1-cyclohexene dioxide	106-87-6	DTXSID0020604	Chemical intermediate		NCCTE	20	
920	Erythromycin	114-07-8	DTXSID4022991	Pharmaceutical		NCCTE	5.00012	
921	Amitraz	33089-61-1	DTXSID5023871	Pesticide (non-herbicide)		NCCTE	20.0005	
922	Dieldrin	60-57-1	DTXSID9020453	Pesticide (non-herbicide)		NCCTE	19.9941	
923	Pentachlorophenol	87-86-5	DTXSID7021106	Microbiocide		NCCTE	10.2103	

924	Geraniol	106-24-1	DTXSID8026727	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
925	4-Chloro-3-methylphenol	59-50-7	DTXSID4021717	Microbiocide		NCCTE	20	
926	Profenofos	41198-08-7	DTXSID3032464	Pesticide (non-herbicide)		NCCTE	9.95464	
927	2,2',6,6'-Tetrachlorobisphenol A	79-95-8	DTXSID3021770	Flame retardant		NCCTE	19.9997	
928	Digoxin	20830-75-5	DTXSID5022934	Pharmaceutical		NCCTE	13.4835	
929	Pravastatin sodium	81131-70-6	DTXSID6047525	Pharmaceutical		NCCTE	10	
930	Diphenyl phthalate	84-62-8	DTXSID3021778	Plasticizer		NCCTE	20	
931	Anilazine	101-05-3	DTXSID9020089	Microbiocide		NCCTE	20.0004	
932	Chloramphenicol	56-75-7	DTXSID7020265	Pharmaceutical		NCCTE	19.9998	
933	1,2,4,5-	95-94-3	DTXSID7024320	Chemical intermediate		NCCTE	20	
934	Malathion	121-75-5	DTXSID4020791	Pesticide (non-herbicide)		NCCTE	20.0009	
935	Sodium L-ascorbate	134-03-2	DTXSID0020105	FoodFlavorFragrance		NCCTE	20	
936	Niclosamide	50-65-7	DTXSID7040362	Pesticide (non-herbicide)		NCCTE	10.0003	CHEMIVIN: EPA ToxCast Cheminventory DMSO Insolubles
937	4-Aminobenzoic acid	150-13-0	DTXSID6024466	FoodFlavorFragrance		NCCTE	20	
938	Butyryl trihexyl citrate	82469-79-2	DTXSID0047535	Plasticizer		NCCTE	19.9995	
939	Carbofuran	1563-66-2	DTXSID9020249	Pesticide (non-herbicide)		NCCTE	20	
940	Tris(2-ethylhexyl)	78-42-2	DTXSID0021414	Flame retardant		NCCTE	19.9992	
941	Monomethyl phthalate	4376-18-5	DTXSID9040001	Plasticizer		NCCTE	20	
942	Napropamide	15299-99-7	DTXSID5024211	Herbicide		NCCTE	20.0002	
943	Trinexapac-ethyl	95266-40-3	DTXSID9032535	Herbicide		NCCTE	20	
944	Caprolactam	105-60-2	DTXSID4020240	Chemical intermediate		NCCTE	20	
945	Endrin	72-20-8	DTXSID6020561	Pesticide (non-herbicide)		NCCTE	20.0002	
946	Allethrin	584-79-2	DTXSID8035180	Pesticide (non-herbicide)		NCCTE	21.0268	
947	Flutolanil	66332-96-5	DTXSID8024109	Microbiocide		NCCTE	19.9635	
948	Glycerol	56-81-5	DTXSID9020663	FoodFlavorFragrance		NCCTE	19.9997	
949	2-(2-Butoxyethoxy)ethanol	112-34-5	DTXSID8021519	Solvent		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
950	Fluorene	86-73-7	DTXSID8024105	PAH		NCCTE	20.0041	
951	1-Pentadecanol	629-76-5	DTXSID0027270	FoodFlavorFragrance		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
952	Dimethyl glutarate	1119-40-0	DTXSID3025122	Chemical intermediate		NCCTE	19.9997	
953	2,6,10-Trimethyl-2,6,10-triazaundecane	3855-32-1	DTXSID1044564	Plasticizer		NCCTE	20	
954	Cyanuric acid	108-80-5	DTXSID7024873	Chemical intermediate		NCCTE	19.8721	
955	Propoxur	114-26-1	DTXSID7021948	Pesticide (non-herbicide)		NCCTE	19.9996	
956	Zearalenone	17924-92-4	DTXSID0021460	Other	Mycotoxin	NCCTE	19.9987	
957	Chrysin	480-40-0	DTXSID1022396	FoodFlavorFragrance		NCCTE	20	
958	Dibenz(a,h)anthracene	53-70-3	DTXSID9020409	PAH		NCCTE	17.9915	
959	Bis(4-hydroxyphenyl)methane	620-92-8	DTXSID9022445	Plasticizer		NCCTE	20.0002	
960	Haloperidol	52-86-8	DTXSID4034150	Pharmaceutical		NCCTE	19.9993	
961	p,p'-DDE	72-55-9	DTXSID9020374	Pesticide (non-herbicide)		NCCTE	20.0005	
962	2-[(4-Hydroxyphenyl)methyl]phenol	2467-03-0	DTXSID2044890	Chemical intermediate		NCCTE	20	
963	Prednisolone	50-24-8	DTXSID9021184	Pharmaceutical		NCCTE	19.9996	
964	Thiodicarb	59669-26-0	DTXSID0032578	Pesticide (non-herbicide)		NCCTE	20	
965	Mesotrione	104206-82-8	DTXSID7032424	Herbicide		NCCTE	20.2562	
966	Decanoic acid	334-48-5	DTXSID9021554	FoodFlavorFragrance		NCCTE	20.8782	MASSSPEC: VocBinBase volatile compounds database
967	6-Methylquinoline	91-62-3	DTXSID3020887	FoodFlavorFragrance		NCCTE	19.9998	
968	4-Butyrolactone	96-48-0	DTXSID6020224	Solvent		NCCTE	20	MASSSPEC: VocBinBase volatile compounds database
969	Naphthalene	91-20-3	DTXSID8020913	PAH		NCCTE	20.0314	
970	Trioctyl trimellitate	89-04-3	DTXSID0047533	Plasticizer		NCCTE	20.1727	

971	Propargite	2312-35-8	DTXSID4024276	Pesticide (non-herbicide)		NCCTE	20	
972	Bromacil	314-40-9	DTXSID4022020	Herbicide		NCCTE	20.0003	
973	Fluridone	59756-60-4	DTXSID8024107	Herbicide		NCCTE	20.0004	
974	2,6-Dimethylphenol	576-26-1	DTXSID9024063	Chemical intermediate		NCCTE	20.0003	
975	Isopropalin	33820-53-0	DTXSID8024157	Herbicide		NCCTE	19.9997	
976	Disulfoton	298-04-4	DTXSID0022018	Pesticide (non-herbicide)		NCCTE	20.0015	
977	N-Nitrosodiphenylamine	86-30-6	DTXSID6021030	Chemical intermediate		NCCTE	20	
978	Pentachlorobenzene	608-93-5	DTXSID7024247	Pesticide (non-herbicide)		NCCTE	20.0002	
979	FD&C Yellow 6	2783-94-0	DTXSID6021456	Dye		NCCTE	20.0006	
980	Cumene hydroperoxide	80-15-9	DTXSID3024869	Chemical intermediate		NCCTE	19.9996	
981	Bromoxynil	1689-84-5	DTXSID3022162	Herbicide		NCCTE	16.0078	
982	Dimethylaminoethanol	108-01-0	DTXSID2020505	Chemical intermediate		NCCTE	20.0003	
983	Di-tert-butyl peroxide	110-05-4	DTXSID2024955	Chemical intermediate		NCCTE	20.0012	
984	Dimethyl phthalate	131-11-3	DTXSID3022455	Plasticizer		NCCTE	19.9996	MASSSPEC: VocBinBase volatile compounds database
985	Dodecylbenzenesulfonic acid	27176-87-0	DTXSID6027923	Surfactant		NCCTE	19.9997	
986	Clopyralid-olamine	57754-85-5	DTXSID6034265	Herbicide		NCCTE	20	
987	2,4,5-Trichlorophenoxyacetic	93-76-5	DTXSID5021388	Herbicide		NCCTE	20.0004	
988	Finasteride	98319-26-7	DTXSID3020625	Pharmaceutical		NCCTE	20.0003	
989	4-Nitrotoluene	99-99-0	DTXSID5023792	Chemical intermediate		NCCTE	20	
990	Atenolol	29122-68-7	DTXSID2022628	Pharmaceutical		NCCTE	20.0004	
991	1,3-Butanediol	107-88-0	DTXSID8026773	Solvent		NCCTE	20	
992	Buspirone	36505-84-7	DTXSID2022707	Pharmaceutical		NCCTE	19.9995	
993	Catechol	120-80-9	DTXSID3020257	Chemical intermediate		NCCTE	19.9973	
994	Etridiazole	2593-15-9	DTXSID3032547	Microbiocide		NCCTE	19.9996	
995	Isazofos	42509-80-8	DTXSID7034676	Pesticide (non-herbicide)		NCCTE	20	
996	Pentalan	110-62-3	DTXSID7021653	FoodFlavorFragrance		NCCTE	19.9995	
997	Thiazopyr	117718-60-2	DTXSID1032488	Herbicide		NCCTE	20	
998	2,2-Dibromo-3-nitrilopropionamide	10222-01-2	DTXSID5032361	Microbiocide		NCCTE	19.9997	
999	2-Methyl-5-nitroaniline	99-55-8	DTXSID4020959	Chemical intermediate		NCCTE	20	
1000	Triadimefon	43121-43-3	DTXSID3023897	Microbiocide		NCCTE	19.9997	
1001	Phenol Red sodium salt	34487-61-1	DTXSID2044420	Dye		NCCTE	20	
1002	Sodium azide	26628-22-8	DTXSID8020121	Herbicide		NCCTE	20	
1003	Chlorobenzilate	510-15-6	DTXSID9020299	Pesticide (non-herbicide)		NCCTE	20	
1004	2-[2-(2-Ethoxyethoxy)ethoxy]ethanol	112-50-5	DTXSID3024368	Solvent		NCCTE	20.0003	
1005	Picloram	1918-02-1	DTXSID1021160	Herbicide		NCCTE	19.9998	
1006	4-Chlorophenyl methyl sulfone	98-57-7	DTXSID3023974	Pesticide (non-herbicide)		NCCTE	20	
1007	Bepridil hydrochloride	68099-86-5	DTXSID3022663	CiPA pharmaceutical		Fisher Scientific (Tocris Bioscience product)		
1008	Dofetilide	115256-11-6	DTXSID5046433	CiPA pharmaceutical		Fisher Scientific (ApexBio product)		
1009	Quinidine	56-54-2	DTXSID4023549	CiPA pharmaceutical		Fisher Scientific (Alfa Aesar product)		
1010	Sotalol hydrochloride	959-24-0	DTXSID0023589	CiPA pharmaceutical		Molecular Devices		
1011	Azimilide dihydrochloride	149888-94-8	DTXSID10869988	CiPA pharmaceutical		Fisher Scientific (Tocris Bioscience product)		
1012	Ibutilide hemifumarate	122647-32-9	DTXSID8048652	CiPA pharmaceutical		Fisher Scientific (TCI America product)		
1013	Vandetanib	443913-73-3	DTXSID1046681	CiPA pharmaceutical		Fisher Scientific (Biotang Inc. product)		

1014	Disopyramide	3737-09-5	DTXSID1045536	CiPA pharmaceutical		Fisher Scientific (TCl America product)		
1015	Cisapride monohydrate	260779-88-2	DTXSID3022825	CiPA pharmaceutical		MilliporeSigma		
1016	Terfenadine	50679-08-8	DTXSID2023642	CiPA pharmaceutical		MilliporeSigma		
1017	Ondansetron hydrochloride dihydrate	103639-04-9	DTXSID8023393	CiPA pharmaceutical		Fisher Scientific (ACROS Organics product)		
1018	Astemizole	68844-77-9	DTXSID9020110	CiPA pharmaceutical		Fisher Scientific (Tocris Bioscience product)		
1019	Clarithromycin	81103-11-9	DTXSID3022829	CiPA pharmaceutical		Fisher Scientific (TCl America product)		
1020	Clozapine	5786-21-0	DTXSID5022855	CiPA pharmaceutical		MilliporeSigma		
1021	Domperidone	57808-66-9	DTXSID1045116	CiPA pharmaceutical		Fisher Scientific (Alfa Aesar product)		
1022	Droperidol	548-73-2	DTXSID6022973	CiPA pharmaceutical		Fisher Scientific (ApexBio product)		
1023	Risperidone	106266-06-2	DTXSID8045193	CiPA pharmaceutical		Fisher Scientific (ACROS Organics product)		
1024	Mexiletine hydrochloride	5370-01-4	DTXSID8048446	CiPA pharmaceutical		Fisher Scientific (ACROS Organics product)		
1025	Ranolazine dihydrochloride	95635-56-6	DTXSID3045196	CiPA pharmaceutical		Fisher Scientific (TCl America product)		
1026	Verapamil hydrochloride	152-11-4	DTXSID9041152	CiPA pharmaceutical		Fisher Scientific (TCl America product)		
1027	Loratadine	79794-75-5	DTXSID2023224	CiPA pharmaceutical		Fisher Scientific (TCl America product)		
1028	Nifedipine	21829-25-4	DTXSID2025715	CiPA pharmaceutical		Fisher Scientific (ACROS Organics product)		
1029	Nitrendipine	39562-70-4	DTXSID0023373	CiPA pharmaceutical		MilliporeSigma		

Supplemental Table 2. Donor characteristics.

ID	Source*	Sex#	Ancestral Background#	Catalog Number
1434	CDI	Female	Mixed African American/European	CMC-100-010-001
1083	NHLBI	Female	African American	DDP-CMC-0.5X 01083.758
1118	NHLBI	Male	African American	DDP-CMC-0.5X 01118.704
1368	NHLBI	Female	European	DDP-CMC-0.5X 01368.716
1392	NHLBI	Male	European	DDP-CMC-0.5X 01392.734

*NHLBI = National Heart, Lung, and Blood Institute, CDI = Cellular Dynamics International (Fujifilm).

#Inferred from genotyping.

Supplemental Table 3. Efficacy (E_{max} as fractional increase or decrease) values for active compounds as compared to positive controls ([+] and [-] chronotropy, and decay-rise ratio).

Endpoint	Active Chemicals Median (IQR) [Range]	Positive Controls
[+] Chronotropy	0.84 (0.19-3.0) [0.073-58]	Isoproterenol: 0.73
[-] Chronotropy	0.70 (0.35-0.87) [0.070-0.99]	Propranolol: 0.86
Decay-Rise Ratio	1.77 (0.20-4.4) [0.07-71]	Sotalol: 15.5 Cisapride: 0.79 N-acetylprocainamide: 0.40 Sematilide: 1.14

Note: Posterior medians for E_{max} are used for each chemical.

Supplemental File 1. Model file for “upward” random-effects Hill model.

```

data {
    real scale_factor; // overall scaling factor
    int<lower=0> Ni; // Number of cell lines
    int<lower=0> Nj; // Number of data points
    vector[Nj] x; // concentrations
    vector[Nj] ys; // responses
    int<lower=0,upper=Ni> cell[Nj]; // cell line for each data point
    int<lower=1> Nquants; // Number of quantiles of EC10 to calculate
    vector[Nquants] quants; // Quantiles (e.g.,
    c(0.01,0.025,0.5,0.975,0.99))
}
parameters {
    // Population mean
    real m_y0; // background
    real m_x0; // numerator scale
    real<lower=-3> m_Emax; // max effect size
    real<lower =-2,upper =2> m_n; // Hill exponent
    // Population standard deviation
    real<lower=0> sd_y0;
    real<lower=0> sd_x0;
    real<lower=0> sd_Emax;
    real<lower=0> sd_n;
    // Inter-individual variability
    real z_y0[Ni];
    real z_x0[Ni];
    real z_Emax[Ni];
    real z_n[Ni];
    // Residual error variance
    real<lower=0> sigma_y;
}
transformed parameters {
    real y0[Ni]; // untransformed background
    real x0[Ni]; // untransformed numerator scale
    real Emax[Ni]; // untransformed max effect size
    real n[Ni]; // untransformed Hill exponent
    for (i in 1:Ni) { // un-log transform
        y0[i] = exp(m_y0 + sd_y0 * z_y0[i]);
        x0[i] = exp(m_x0 + sd_x0 * z_x0[i]);
        Emax[i] = exp(m_Emax + sd_Emax * z_Emax[i]); // Emax positive
        n[i] = exp(m_n + sd_n * z_n[i]);
    }
}
model {
    vector[Nj] yp;
    // prior distributions
    m_y0 ~ normal(0,5);
    m_x0 ~ normal(0,5);
    m_Emax ~ normal(0,5);
}

```

```

m_n ~ normal(0,1);
sd_y0 ~ normal(0,1);
sd_x0 ~ normal(0,1);
sd_Emax ~ normal(0,1);
sd_n ~ normal(0,0.2);
z_y0 ~ normal(0,1);
z_x0 ~ normal(0,1);
z_Emax ~ normal(0,1);
z_n ~ normal(0,1);
sigma_y ~ normal(0,0.2);
for (j in 1:Nj) {
    yp[j] = y0[cell[j]]*(1 + (x[j] / x0[cell[j]])^n[cell[j]] / (1 +
((x[j] / x0[cell[j]])^n[cell[j]])/Emax[cell[j]]));
}
ys ~ student_t(5,yp,sigma_y);
}
generated quantities {
    vector[Ni] ec99;           // Concentration at which the relative response
is 100%
    vector[Ni] ec95;           // Concentration at which the relative response
is 95%
    vector[Ni] ec50;           // Concentration at which the relative response
is 50%
    vector[Ni] ec10;           // Concentration at which the relative response
is 10%
    vector[Ni] ec05;           // Concentration at which the relative response
is 5%
    vector[Ni] ec025;          // Concentration at which the relative response
is 2.5%
    vector[Ni] ec01;           // Concentration at which the relative response
is 1%
    real ec10_GM;              // Geometric mean
    real ec10_GSD;              // Geometric standard deviation
//    real ec10_GSD_approx;      // Approximate GSD derived from
m_0,m_1,sd_0, and sd_1
    real ec99_median;          // Median ec99
    real ec95_median;          // Median ec95
    real ec50_median;          // Median ec50
    real ec10_median;          // Median
    real ec05_median;          // Median ec05
    real ec025_median;         // Median ec025
    real ec01_median;          // Median ec01
vector[Nquants] ec99_quants; // Quantiles ec99
vector[Nquants] ec99_quant_ratios; // Ratios of median to quantiles
ec99
vector[Nquants] ec95_quants; // Quantiles ec95
vector[Nquants] ec95_quant_ratios; // Ratios of median to quantiles
ec95
vector[Nquants] ec50_quants; // Quantiles ec50

```

```

vector[Nquants] ec50_quant_ratios; // Ratios of median to quantiles
ec50
vector[Nquants] ec10_quants; // Quantiles
vector[Nquants] ec10_quant_ratios; // Ratios of median to quantiles
vector[Nquants] ec05_quants; // Quantiles ec05
vector[Nquants] ec05_quant_ratios; // Ratios of median to quantiles
ec05
vector[Nquants] ec025_quants; // Quantiles ec02.5
vector[Nquants] ec025_quant_ratios; // Ratios of median to quantiles
ec02.5
vector[Nquants] ec01_quants; // Quantiles ec01
vector[Nquants] ec01_quant_ratios; // Ratios of median to quantiles
ec01

for (i in 1:Ni) {
    if (Emax[i] > 1)
        ec99[i] = x0[i]*(0.99 * Emax[i] / (Emax[i] -
0.99))^(1/n[i]);
    else
        ec99[i] = 1000;
}
for (i in 1:Ni) {
    if(Emax[i] > 0.95)
        ec95[i] = x0[i]*(0.95 * Emax[i] / (Emax[i] -
0.95))^(1/n[i]);
    else
        ec95[i] = 1000;
}
for (i in 1:Ni) {
    if (Emax[i] > 0.5)
        ec50[i] = x0[i]*(0.5 * Emax[i] / (Emax[i] - 0.5))^(1/n[i]);
    else
        ec50[i] = 1000;
}
for (i in 1:Ni) {
    if (Emax[i] > 0.1)
        ec10[i] = x0[i]*(0.1 * Emax[i] / (Emax[i] - 0.1))^(1/n[i]);
    else
        ec10[i] = 1000;
}
for (i in 1:Ni) {
    if (Emax[i] > 0.05)
        ec05[i] = x0[i]*(0.05 * Emax[i] / (Emax[i] -
0.05))^(1/n[i]);
    else
        ec05[i] = 1000;
}
for (i in 1:Ni) {
    if (Emax[i] > 0.025)

```

```

        ec025[i] = x0[i]*(0.025 * Emax[i] / (Emax[i] -
0.025))^(1/n[i]);
        else
            ec025[i] = 1000;
    }
    for (i in 1:Ni) {
        if (Emax[i] > 0.01)
            ec01[i] = x0[i]*(0.01 * Emax[i] / (Emax[i] -
0.01))^(1/n[i]);
        else
            ec01[i] = 1000;
    }
    ec10_GM = exp(mean(log(ec10)));
    ec10_GSD = exp(sd(log(ec10)));
//    ec10_GSD_approx = exp(sqrt((sd_0 / m_1)^2 + (sd_1 / m_1)^2 *
((log(0.1/(1-0.1)) - m_0)/m_1)^2));
{
    int ec99_idx[Ni];
    int ec95_idx[Ni];
    int ec50_idx[Ni];
    int ec10_idx[Ni];
    int ec05_idx[Ni];
    int ec025_idx[Ni];
    int ec01_idx[Ni];
    real p;
    real m;
    real g;
    int i;
    int itmp;
    ec99_idx= sort_indices_asc(ec99);
    ec95_idx= sort_indices_asc(ec95);
    ec50_idx= sort_indices_asc(ec50);
    ec10_idx= sort_indices_asc(ec10);
    ec05_idx= sort_indices_asc(ec05);
    ec025_idx= sort_indices_asc(ec025);
    ec01_idx= sort_indices_asc(ec01);
    p= 0.5;
    m=1-p;
    itmp=1;
    while (itmp <(Ni*p + m))
        itmp=itmp+1;
    i = itmp-1;
    g = Ni*p + m - i;
    ec99_median = (1-g)*ec99[ec99_idx[i]]+g*ec99[ec99_idx[i+1]];
    ec95_median = (1-g)*ec95[ec95_idx[i]]+g*ec95[ec95_idx[i+1]];
    ec50_median = (1-g)*ec50[ec50_idx[i]]+g*ec50[ec50_idx[i+1]];
    ec10_median = (1-g)*ec10[ec10_idx[i]]+g*ec10[ec10_idx[i+1]];
    ec05_median = (1-g)*ec05[ec05_idx[i]]+g*ec05[ec05_idx[i+1]];
    ec025_median = (1-g)*ec025[ec025_idx[i]]+g*ec025[ec025_idx[i+1]];
    ec01_median = (1-g)*ec01[ec01_idx[i]]+g*ec01[ec01_idx[i+1]];
}

```

```

for (q in 1:Nquants) {
  p= quants[q];
  m= 1-p;
  itmp=1;
  while (itmp <(Ni*p + m))
    itmp=itmp+1;
  i = itmp-1;
  g = Ni*p + m - i;
  ec99_quants[q] = (1-g)*ec99[ec99_indx[i]]+g*ec99[ec99_indx[i+1]];
  ec95_quants[q] = (1-g)*ec95[ec95_indx[i]]+g*ec95[ec95_indx[i+1]];
  ec50_quants[q] = (1-g)*ec50[ec50_indx[i]]+g*ec50[ec50_indx[i+1]];
  ec10_quants[q] = (1-g)*ec10[ec10_indx[i]]+g*ec10[ec10_indx[i+1]];
  ec05_quants[q] = (1-g)*ec05[ec05_indx[i]]+g*ec05[ec05_indx[i+1]];
  ec025_quants[q] = (1-
g)*ec025[ec025_indx[i]]+g*ec025[ec025_indx[i+1]];
  ec01_quants[q] = (1-g)*ec01[ec01_indx[i]]+g*ec01[ec01_indx[i+1]];
}
for (q in 1:Nquants) {
  ec99_quant_ratios[q] = ec99_median/ec99_quants[q];
  ec95_quant_ratios[q] = ec95_median/ec95_quants[q];
  ec50_quant_ratios[q] = ec50_median/ec50_quants[q];
  ec10_quant_ratios[q] = ec10_median/ec10_quants[q];
  ec05_quant_ratios[q] = ec05_median/ec05_quants[q];
  ec025_quant_ratios[q] = ec025_median/ec025_quants[q];
  ec01_quant_ratios[q] = ec01_median/ec01_quants[q];
}
}
}

```

Supplemental File 2. Model file for “downward” random-effects Hill model.

```

data {
    real scale_factor; // overall scaling factor
    int<lower=0> Ni; // Number of cell lines
    int<lower=0> Nj; // Number of data points
    vector[Nj] x; // concentrations
    vector[Nj] ys; // responses
    int<lower=0,upper=Ni> cell[Nj]; // cell line for each data point
    int<lower=1> Nquants; // Number of quantiles of EC10 to calculate
    vector[Nquants] quants; // Quantiles (e.g.,
    c(0.01,0.025,0.5,0.975,0.99))
}
parameters {
    // Population mean
    real m_y0; // background
    real m_x0; // numerator scale
    real<lower =-3> m_Emax; // max effect size
    real<lower =-2,upper =2> m_n; // Hill exponent
    // Population standard deviation
    real<lower=0> sd_y0;
    real<lower=0> sd_x0;
    real<lower=0> sd_Emax;
    real<lower=0> sd_n;
    // Inter-individual variability
    real z_y0[Ni];
    real z_x0[Ni];
    real z_Emax[Ni];
    real z_n[Ni];
    // Residual error variance
    real<lower=0> sigma_y;
}
transformed parameters {
    real y0[Ni]; // untransformed background
    real x0[Ni]; // untransformed numerator scale
    real Emax[Ni]; // untransformed max effect size
    real n[Ni]; // untransformed Hill exponent
    for (i in 1:Ni) { // un-log transform
        y0[i] = exp(m_y0 + sd_y0 * z_y0[i]);
        x0[i] = exp(m_x0 + sd_x0 * z_x0[i]);
        Emax[i] = inv_logit(m_Emax + sd_Emax * z_Emax[i]); // Emax
    }
    between 0 and 1
    n[i] = exp(m_n + sd_n * z_n[i]);
}
model {
    vector[Nj] yp;
    // prior distributions
    m_y0 ~ normal(0,5);
    m_x0 ~ normal(0,5);
}

```

```

m_Emax ~ normal(0,5);
m_n ~ normal(0,1);
sd_y0 ~ normal(0,1);
sd_x0 ~ normal(0,1);
sd_Emax ~ normal(0,1);
sd_n ~ normal(0,0.2);
z_y0 ~ normal(0,1);
z_x0 ~ normal(0,1);
z_Emax ~ normal(0,1);
z_n ~ normal(0,1);
sigma_y ~ normal(0,0.2);
for (j in 1:Nj) {
    yp[j] = y0[cell[j]]*(1 - (x[j] / x0[cell[j]])^n[cell[j]] / (1 +
((x[j] / x0[cell[j]])^n[cell[j]])/Emax[cell[j]]));
}
ys ~ student_t(5,yp,sigma_y);
}
generated quantities {
    vector[Ni] ec99;           // Concentration at which the relative response
is 100%
    vector[Ni] ec95;           // Concentration at which the relative response
is 95%
    vector[Ni] ec50;           // Concentration at which the relative response
is 50%
    vector[Ni] ec10;           // Concentration at which the relative response
is 10%
    vector[Ni] ec05;           // Concentration at which the relative response
is 5%
    vector[Ni] ec025;          // Concentration at which the relative response
is 2.5%
    vector[Ni] ec01;           // Concentration at which the relative response
is 1%
    real ec10_GM;              // Geometric mean
    real ec10_GSD;             // Geometric standard deviation
//    real ec10_GSD_approx;     // Approximate GSD derived from
m_0,m_1,sd_0, and sd_1
    real ec99_median;          // Median ec99
    real ec95_median;          // Median ec95
    real ec50_median;          // Median ec50
    real ec10_median;          // Median
    real ec05_median;          // Median ec05
    real ec025_median;         // Median ec025
    real ec01_median;          // Median ec01

    vector[Nquants] ec99_quants; // Quantiles ec99
    vector[Nquants] ec99_quant_ratios; // Ratios of median to quantiles
ec99
    vector[Nquants] ec95_quants; // Quantiles ec95
    vector[Nquants] ec95_quant_ratios; // Ratios of median to quantiles
ec95

```

```

vector[Nquants] ec50_quants; // Quantiles ec50
vector[Nquants] ec50_quant_ratios; // Ratios of median to quantiles
ec50
vector[Nquants] ec10_quants; // Quantiles
vector[Nquants] ec10_quant_ratios; // Ratios of median to quantiles
vector[Nquants] ec05_quants; // Quantiles ec05
vector[Nquants] ec05_quant_ratios; // Ratios of median to quantiles
ec05
vector[Nquants] ec025_quants; // Quantiles ec02.5
vector[Nquants] ec025_quant_ratios; // Ratios of median to quantiles
ec02.5
vector[Nquants] ec01_quants; // Quantiles ec01
vector[Nquants] ec01_quant_ratios; // Ratios of median to quantiles
ec01

for (i in 1:Ni) {
    if (Emax[i] > 1)
        ec99[i] = x0[i]*(0.99 * Emax[i] / (Emax[i] -
0.99))^(1/n[i]);
    else
        ec99[i] = 1000;
}
for (i in 1:Ni) {
    if (Emax[i] > 0.95)
        ec95[i] = x0[i]*(0.95 * Emax[i] / (Emax[i] -
0.95))^(1/n[i]);
    else
        ec95[i] = 1000;
}
for (i in 1:Ni) {
    if (Emax[i] > 0.5)
        ec50[i] = x0[i]*(0.5 * Emax[i] / (Emax[i] - 0.5))^(1/n[i]);
    else
        ec50[i] = 1000;
}
for (i in 1:Ni) {
    if (Emax[i] > 0.1)
        ec10[i] = x0[i]*(0.1 * Emax[i] / (Emax[i] - 0.1))^(1/n[i]);
    else
        ec10[i] = 1000;
}
for (i in 1:Ni) {
    if (Emax[i] > 0.05)
        ec05[i] = x0[i]*(0.05 * Emax[i] / (Emax[i] -
0.05))^(1/n[i]);
    else
        ec05[i] = 1000;
}
for (i in 1:Ni) {

```

```

        if (Emax[i] > 0.025)
            ec025[i] = x0[i]*(0.025 * Emax[i] / (Emax[i] -
0.025))^(1/n[i]);
        else
            ec025[i] = 1000;
    }
    for (i in 1:Ni) {
        if (Emax[i] > 0.01)
            ec01[i] = x0[i]*(0.01 * Emax[i] / (Emax[i] -
0.01))^(1/n[i]);
        else
            ec01[i] = 1000;
    }
    ec10_GM = exp(mean(log(ec10)));
    ec10_GSD = exp(sd(log(ec10)));
//    ec10_GSD_approx = exp(sqrt((sd_0 / m_1)^2 + (sd_1 / m_1)^2 *
((log(0.1/(1-0.1)) - m_0)/m_1)^2));
{
    int ec99_indx[Ni];
    int ec95_indx[Ni];
    int ec50_indx[Ni];
    int ec10_indx[Ni];
    int ec05_indx[Ni];
    int ec025_indx[Ni];
    int ec01_indx[Ni];
    real p;
    real m;
    real g;
    int i;
    int itmp;
    ec99_indx= sort_indices_asc(ec99);
    ec95_indx= sort_indices_asc(ec95);
    ec50_indx= sort_indices_asc(ec50);
    ec10_indx= sort_indices_asc(ec10);
    ec05_indx= sort_indices_asc(ec05);
    ec025_indx= sort_indices_asc(ec025);
    ec01_indx= sort_indices_asc(ec01);
    p= 0.5;
    m=1-p;
    itmp=1;
    while (itmp <(Ni*p + m))
        itmp=itmp+1;
    i = itmp-1;
    g = Ni*p + m - i;
    ec99_median = (1-g)*ec99[ec99_indx[i]]+g*ec99[ec99_indx[i+1]];
    ec95_median = (1-g)*ec95[ec95_indx[i]]+g*ec95[ec95_indx[i+1]];
    ec50_median = (1-g)*ec50[ec50_indx[i]]+g*ec50[ec50_indx[i+1]];
    ec10_median = (1-g)*ec10[ec10_indx[i]]+g*ec10[ec10_indx[i+1]];
    ec05_median = (1-g)*ec05[ec05_indx[i]]+g*ec05[ec05_indx[i+1]];
    ec025_median = (1-g)*ec025[ec025_indx[i]]+g*ec025[ec025_indx[i+1]];
}

```

```

ec01_median = (1-g)*ec01[ec01_indx[i]]+g*ec01[ec01_indx[i+1]];
for (q in 1:Nquants) {
    p= quants[q];
    m= 1-p;
    itmp=1;
    while (itmp <(Ni*p + m))
        itmp=itmp+1;
    i = itmp-1;
    g = Ni*p + m - i;
    ec99_quants[q] = (1-g)*ec99[ec99_indx[i]]+g*ec99[ec99_indx[i+1]];
    ec95_quants[q] = (1-g)*ec95[ec95_indx[i]]+g*ec95[ec95_indx[i+1]];
    ec50_quants[q] = (1-g)*ec50[ec50_indx[i]]+g*ec50[ec50_indx[i+1]];
    ec10_quants[q] = (1-g)*ec10[ec10_indx[i]]+g*ec10[ec10_indx[i+1]];
    ec05_quants[q] = (1-g)*ec05[ec05_indx[i]]+g*ec05[ec05_indx[i+1]];
    ec025_quants[q] = (1-
g)*ec025[ec025_indx[i]]+g*ec025[ec025_indx[i+1]];
    ec01_quants[q] = (1-g)*ec01[ec01_indx[i]]+g*ec01[ec01_indx[i+1]];
}
for (q in 1:Nquants) {
    ec99_quant_ratios[q] = ec99_median/ec99_quants[q];
    ec95_quant_ratios[q] = ec95_median/ec95_quants[q];
    ec50_quant_ratios[q] = ec50_median/ec50_quants[q];
    ec10_quant_ratios[q] = ec10_median/ec10_quants[q];
    ec05_quant_ratios[q] = ec05_median/ec05_quants[q];
    ec025_quant_ratios[q] = ec025_median/ec025_quants[q];
    ec01_quant_ratios[q] = ec01_median/ec01_quants[q];
}
}
}
}

```

Supplemental File 3. Model file for “zero” random-effects Hill model.

```

// Concentration-response downward to 0 (three parameter Hill model)
data {
    real scale_factor; // overall scaling factor
    int<lower=0> Ni; // Number of cell lines
    int<lower=0> Nj; // Number of data points
    vector[Nj] x; // concentrations
    vector[Nj] ys; // responses
    int<lower=0,upper=Ni> cell[Nj]; // cell line for each data point
    int<lower=1> Nquants; // Number of quantiles of EC10 to calculate
    vector[Nquants] quants; // Quantiles (e.g.,
    c(0.01,0.025,0.5,0.975,0.99))
}
parameters { // all natural log-transformed
    // Population mean
    real m_y0; // background
    real m_x0; // numerator scale
    real<lower=-2,upper=2> m_n; // Hill exponent
    // Population standard deviation
    real<lower=0> sd_y0;
    real<lower=0> sd_x0;
    real<lower=0> sd_n;
    // Inter-individual variability
    real z_y0[Ni];
    real z_x0[Ni];
    real z_n[Ni];
    // Residual error variance
    real<lower=0> sigma_y;
}
transformed parameters {
    real y0[Ni]; // untransformed background
    real x0[Ni]; // untransformed numerator scale
    real n[Ni]; // untransformed Hill exponent
    for (i in 1:Ni) { // un-log transform
        y0[i] = exp(m_y0 + sd_y0 * z_y0[i]);
        x0[i] = exp(m_x0 + sd_x0 * z_x0[i]);
        n[i] = exp(m_n + sd_n * z_n[i]);
    }
}
model {
    vector[Nj] yp;
    // prior distributions
    m_y0 ~ normal(0,5);
    m_x0 ~ normal(0,5);
    m_n ~ normal(0,1);
    sd_y0 ~ normal(0,1);
    sd_x0 ~ normal(0,1);
    sd_n ~ normal(0,0.2);
}

```

```

z_y0 ~ normal(0,1);
z_x0 ~ normal(0,1);
z_n ~ normal(0,1);
sigma_y ~ normal(0,0.2);
for (j in 1:Nj) {
    yp[j] = y0[cell[j]]/ (1 + (x[j] / x0[cell[j]])^n[cell[j]]);
}
ys ~ student_t(5,yp,sigma_y);
}
generated quantities {
    vector[Ni] ec99;           // Concentration at which the relative response
is 100%
    vector[Ni] ec95;           // Concentration at which the relative response
is 95%
    vector[Ni] ec50;           // Concentration at which the relative response
is 50%
    vector[Ni] ec10;           // Concentration at which the relative response
is 10%
    vector[Ni] ec05;           // Concentration at which the relative response
is 5%
    vector[Ni] ec025;          // Concentration at which the relative response
is 2.5%
    vector[Ni] ec01;           // Concentration at which the relative response
is 1%
    real ec10_GM;              // Geometric mean
    real ec10_GSD;             // Geometric standard deviation
//    real ec10_GSD_approx;     // Approximate GSD derived from
m_0,m_1,sd_0, and sd_1
    real ec99_median;          // Median ec99
    real ec95_median;          // Median ec95
    real ec50_median;          // Median ec50
    real ec10_median;          // Median
    real ec05_median;          // Median ec05
    real ec025_median;         // Median ec025
    real ec01_median;          // Median ec01
    vector[Nquants] ec99_quants; // Quantiles ec99
    vector[Nquants] ec99_quant_ratios; // Ratios of median to quantiles
ec99
    vector[Nquants] ec95_quants; // Quantiles ec95
    vector[Nquants] ec95_quant_ratios; // Ratios of median to quantiles
ec95
    vector[Nquants] ec50_quants; // Quantiles ec50
    vector[Nquants] ec50_quant_ratios; // Ratios of median to quantiles
ec50
    vector[Nquants] ec10_quants; // Quantiles
    vector[Nquants] ec10_quant_ratios; // Ratios of median to quantiles
    vector[Nquants] ec05_quants; // Quantiles ec05
    vector[Nquants] ec05_quant_ratios; // Ratios of median to quantiles
ec05
    vector[Nquants] ec025_quants; // Quantiles ec02.5

```

```

vector[Nquants] ec025_quant_ratios; // Ratios of median to quantiles
ec02.5
vector[Nquants] ec01_quants; // Quantiles ec01
vector[Nquants] ec01_quant_ratios; // Ratios of median to quantiles
ec01

for (i in 1:Ni) {
  ec99[i] = x0[i]*(0.99 / (1 - 0.99))^(1/n[i]);
  ec95[i] = x0[i]*(0.95 / (1 - 0.95))^(1/n[i]);
  ec50[i] = x0[i]*(0.5 / (1 - 0.5))^(1/n[i]);
  ec10[i] = x0[i]*(0.1 / (1 - 0.1))^(1/n[i]);
  ec05[i] = x0[i]*(0.05 / (1 - 0.05))^(1/n[i]);
  ec025[i] = x0[i]*(0.025 / (1 - 0.025))^(1/n[i]);
  ec01[i] = x0[i]*(0.01 / (1 - 0.01))^(1/n[i]);
}
ec10_GM = exp(mean(log(ec10)));
ec10_GSD = exp(sd(log(ec10)));
{
int ec99_indx[Ni];
int ec95_indx[Ni];
int ec50_indx[Ni];
int ec10_indx[Ni];
int ec05_indx[Ni];
int ec025_indx[Ni];
int ec01_indx[Ni];
real p;
real m;
real g;
int i;
int itmp;
ec99_indx= sort_indices_asc(ec99);
ec95_indx= sort_indices_asc(ec95);
ec50_indx= sort_indices_asc(ec50);
ec10_indx= sort_indices_asc(ec10);
ec05_indx= sort_indices_asc(ec05);
ec025_indx= sort_indices_asc(ec025);
ec01_indx= sort_indices_asc(ec01);
p= 0.5;
m=1-p;
itmp=1;
while (itmp <(Ni*p + m))
  itmp=itmp+1;
i = itmp-1;
g = Ni*p + m - i;
ec99_median = (1-g)*ec99[ec99_indx[i]]+g*ec99[ec99_indx[i+1]];
ec95_median = (1-g)*ec95[ec95_indx[i]]+g*ec95[ec95_indx[i+1]];
ec50_median = (1-g)*ec50[ec50_indx[i]]+g*ec50[ec50_indx[i+1]];
ec10_median = (1-g)*ec10[ec10_indx[i]]+g*ec10[ec10_indx[i+1]];
ec05_median = (1-g)*ec05[ec05_indx[i]]+g*ec05[ec05_indx[i+1]];
ec025_median = (1-g)*ec025[ec025_indx[i]]+g*ec025[ec025_indx[i+1]];

```

```

ec01_median = (1-g)*ec01[ec01_indx[i]]+g*ec01[ec01_indx[i+1]];
for (q in 1:Nquants) {
    p= quants[q];
    m= 1-p;
    itmp=1;
    while (itmp <(Ni*p + m))
        itmp=itmp+1;
    i = itmp-1;
    g = Ni*p + m - i;
    ec99_quants[q] = (1-g)*ec99[ec99_indx[i]]+g*ec99[ec99_indx[i+1]];
    ec95_quants[q] = (1-g)*ec95[ec95_indx[i]]+g*ec95[ec95_indx[i+1]];
    ec50_quants[q] = (1-g)*ec50[ec50_indx[i]]+g*ec50[ec50_indx[i+1]];
    ec10_quants[q] = (1-g)*ec10[ec10_indx[i]]+g*ec10[ec10_indx[i+1]];
    ec05_quants[q] = (1-g)*ec05[ec05_indx[i]]+g*ec05[ec05_indx[i+1]];
    ec025_quants[q] = (1-
g)*ec025[ec025_indx[i]]+g*ec025[ec025_indx[i+1]];
    ec01_quants[q] = (1-g)*ec01[ec01_indx[i]]+g*ec01[ec01_indx[i+1]];
}
for (q in 1:Nquants) {
    ec99_quant_ratios[q] = ec99_median/ec99_quants[q];
    ec95_quant_ratios[q] = ec95_median/ec95_quants[q];
    ec50_quant_ratios[q] = ec50_median/ec50_quants[q];
    ec10_quant_ratios[q] = ec10_median/ec10_quants[q];
    ec05_quant_ratios[q] = ec05_median/ec05_quants[q];
    ec025_quant_ratios[q] = ec025_median/ec025_quants[q];
    ec01_quant_ratios[q] = ec01_median/ec01_quants[q];
}
}
}
}

```