

Supporting Information

***In Vitro* Screening for Chemical Inhibition of the Iodide Recycling Enzyme, Iodotyrosine Deiodinase**

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Supplementary Figures

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Example layouts for assay plates: [A] Single-concentration screening at a target concentration of 200 μM . Chemical source plates were received with column 1 empty for the concentration-response curve for the model inhibitor, 3-Nitro-L-tyrosine (MNT) from the high concentration of 200 μM . Twelve additional wells were left empty on the source plate to which dimethyl sulfoxide (DMSO) was added to 3 wells (white blocks), 0.05 M sodium hydroxide (NaOH) was added to 3 wells (medium grey blocks), and the model inhibitor MNT (red blocks) was added to the remaining 6 wells to establish the fully inhibited response level. Chemicals from the replicated test-set were repeated across multiple plates and example wells for these chemicals are indicated with an asterisk. These were randomly assigned to wells on each plate. [B] Concentration-response screening with seven concentrations in serial dilutions from maximum tested concentration. The concentration-response curve for the model inhibitor, MNT was in column 1. Row H had 3 DMSO wells (white blocks), 3 0.05 M NaOH wells (medium grey blocks), and 6 model inhibitor MNT wells (red blocks). Final MNT concentrations in column 1 were 200, 1.0, 0.16, 0.075, 0.025, 0.005, and 0.0005 μM from highest (row A) to lowest (row G). Column 1 row H contained 0.05 M NaOH.
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Single-concentration screening results for the 10 test chemicals replicated across multiple chemical source plates (represented by different colors) to evaluate the plate-to-plate variability. Deiodinase inhibition produced by test chemicals that were randomly replicated across the chemical source plates. The following chemicals were included: Tribromsalan (CASRN: 87-10-5), Bithionol (CASRN: 97-18-7), Triclosan (CASRN: 3380-34-5), Bromoxynil (CASRN: 1689-84-5), Bisphenol A (80-05-7), Dibutyl phthalate (84-74-2), Acetochlor (34256-82-1), Genistein (446-72-0), 4-nonylphenol (104-40-5), 2,2',4,4'-Tetrahydroxybenzophenone (131-55-5), based on availability for plating on the chemical source plates and previous testing for IYD inhibition in Shimizu et al. (2013) or Renko et al. (2016).
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Concentration-response curves for inhibition of IYD by model inhibitor MNT for all single-concentration and concentration-response assay plates, with multiple plates included on each of the following four pages. Each triplicate test of a plate has different symbols and fit line, solid circle with solid line = rep 1, open triangle with dashed line = rep 2, \times with dotted line = rep 3. DMSO = dimethyl sulfoxide; NaOH = sodium hydroxide.
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Concentration-response screening data. Inhibition of iodotyrosine deiodinase (IYD) produced by all chemicals tested in concentration-response (CR) screening at seven concentrations. Hill model curve, absolute IC_{50} , and Hill slope included for the chemicals where Hill model fit in ToxCast pipeline (tcp1 v2.0); the following 154 pages include CR results for one chemical per page. DMSO = dimethyl sulfoxide; NaOH = sodium hydroxide. NA = not applicable (Hill model did not fit data and/or 50% inhibition not produced in concentration-response testing).

Supplementary Table 1. Chemical samples that were identified as interfering with the assay and therefore were excluded from analyses.

Chemical	CASRN	Source ^a	Reason Excluded
3-Iodo-2-propynyl-N-butylcarbamate	55406-53-6	ph1v2	Interference with Sandell-Kolthoff (SK) reaction
Methylene bis(thiocyanate)	6317-18-6	ph1v2	Interference with Sandell-Kolthoff (SK) reaction
Amiodarone hydrochloride	19774-82-4	ph2	Contains free iodide or possibly being deiodinated by enzyme
1H,1H,2H,2H-Perfluorooctyl iodide	2043-57-4	ph2	Contains free iodide or possibly being deiodinated by enzyme
3,5,3'-Triiodothyronine	6893-02-3	ph2	Abnormal time course of absorbance at 420 nm ^b
FD&C Red 3	16423-68-0	e1k	Contains free iodide or possibly being deiodinated by enzyme
Thiocyanic acid, ammonium salt	1762-95-4	e1k	Interference with Sandell-Kolthoff (SK) reaction
C.I. Acid Blue 22	28631-66-5	e1k	Abnormal time course of absorbance at 420 nm
1,2-Ethanediamine dihydriodide	5700-49-2	e1k	Contains free iodide or possibly being deiodinated by enzyme
Sodium iodide	7681-82-5	e1k	Contains free iodide or possibly being deiodinated by enzyme
C.I. Acid Yellow 3 disodium salt	8004-92-0	e1k	Interference with Sandell-Kolthoff (SK) reaction
Iopanoic acid	96-83-3	e1k	Contains free iodide or possibly being deiodinated by enzyme

^a Source. ToxCast Chemical sets: ph1v2 indicates ToxCast phase1_v2 chemical library, ph2 indicates ToxCast phase2 chemical library, and e1k indicates ToxCast e1k chemical library obtained via Dr. Ann Richard, EPA/ORD, Research Triangle Park, NC, USA.

^b Abnormal time course of absorbance at 420 nm: Chemical flagged based on absorbance at time 0 or 10 minutes outside of expected range based on DMSO and MNT (model inhibitor).

Supplementary Table 2. Single-concentration screening results. List of all chemicals tested in the iodotyrosine deiodinase (IYD) inhibition assay, organized by source; maximum concentration tested and median % inhibition (n = 3 replicates) produced in single-concentration screening, with indication (Y = yes, N = no) of whether chemical was tested in concentration-response (CR).

^a Source. Test indicates set of chemicals selected based on previous testing for IYD inhibition and were replicated across multiple chemical source plates. ToxCast Chemical sets: ph1v2 indicates ToxCast phase 1_v2 chemical library, ph2 indicates ToxCast phase 2 chemical library, ph3 indicates ToxCast phase 3 chemical library, and e1k indicates ToxCast e1k chemical library, all obtained via Dr. Ann Richard, EPA/ORD, Research Triangle Park, NC, USA. ^b Concentrations in μM , except where indicated as in $\mu\text{g/ml}$ for the following compounds: adipic acid, polypropyleneglycol, laurate; clove leaf oil; C10-21 sulfonic acids phenyl esters; Grinstad Soft-N-Safe; cremophor EL; corrmint oil; peppermint oil; anise oil; polyoxyethylene monoleate; Igepal CO-890.

DSSTox_Substance_Id	Chemical	CASRN	Source ^a	Max conc., μM ^b	% Inhibition, median	Tested in CR?	Replicated across plates?
DTXSID9021342	Bithionol	97-18-7	test	200	98	Y	Y
DTXSID5033836	4-Nonylphenol	104-40-5	test	200	67	Y	Y
DTXSID5032498	Triclosan	3380-34-5	test	200	65	Y	Y
DTXSID4026181	Tribromsalan	87-10-5	test	200	80	Y	Y
DTXSID2021781	Dibutyl phthalate	84-74-2	test	200	19	Y	Y
DTXSID7020182	Bisphenol A	80-05-7	test	200	6	Y	Y
DTXSID5022308	Genistein	446-72-0	test	200	4	Y	Y
DTXSID3022162	Bromoxynil	1689-84-5	test	160	1	Y	Y
DTXSID8023848	Acetochlor	34256-82-1	test	200	2	Y	Y
DTXSID5041306	2,2',4,4'-Tetrahydroxybenzophenone	131-55-5	test	200	1	Y	Y
DTXSID1034973	Tralkoxydim	87820-88-0	ph1	200	6	N	N
DTXSID1032488	Thiazopyr	117718-60-2	ph1	200	18	N	N
DTXSID0034695	Mancozeb	8018-01-7	ph1	100	9	N	N
DTXSID0023951	Carboxin	5234-68-4	ph1	200	8	N	N
DTXSID1032640	Pyriproxyfen	95737-68-1	ph1	200	18	N	N
DTXSID0032572	Prallethrin	23031-36-9	ph1	200	28	N	N
DTXSID0020446	Diuron	330-54-1	ph1	200	15	N	N
DTXSID0023901	Bentazone	25057-89-0	ph1	200	5	N	N
DTXSID1032355	Clomazone	81777-89-1	ph1	200	7	N	N
DTXSID0034930	Fosthiazate	98886-44-3	ph1	200	7	N	N
DTXSID1021409	Triphenyltin hydroxide	76-87-9	ph1	200	10	N	N

DTXSID0032520	Azoxystrobin	131860-33-8	ph1	200	10	N	N
DTXSID0021389	Trichlorfon	52-68-6	ph1	200	1	N	N
DTXSID2020426	Dicloran	99-30-9	ph1	200	10	N	N
DTXSID1022267	Methomyl	16752-77-5	ph1	200	5	N	N
DTXSID0021337	Thiabendazole	148-79-8	ph1	200	6	N	N
DTXSID1032690	Indoxacarb	173584-44-6	ph1	160	-2	N	N
DTXSID1021160	Picloram	1918-02-1	ph1	200	0	N	N
DTXSID0024216	Nitrapyrin	1929-82-4	ph1	200	14	N	N
DTXSID0021385	Folpet	133-07-3	ph1	200	1	N	N
DTXSID0032601	Cyproconazole	94361-06-5	ph1	200	6	N	N
DTXSID0032493	Triadimenol	55219-65-3	ph1	200	6	N	N
DTXSID1034212	Spiroxamine	118134-30-8	ph1	200	13	N	N
DTXSID1024170	Mepiquat chloride	24307-26-4	ph1	200	8	N	N
DTXSID2021995	DEET	134-62-3	ph1	200	6	N	N
DTXSID1032359	Cyprodinil	121552-61-2	ph1	200	23	N	N
DTXSID1024091	EPTC	759-94-4	ph1	200	7	N	N
DTXSID1024259	Phosalone	2310-17-0	ph1	200	-1	N	N
DTXSID0034300	Acetamiprid	135410-20-7	ph1	200	8	N	N
DTXSID1024174	Tribufos	78-48-8	ph1	200	10	Y	N
DTXSID1038666	Chlorpyrifos oxon	5598-15-2	ph1	199	9	N	N
DTXSID0032655	Triticonazole	131983-72-7	ph1	199	10	N	N
DTXSID1020855	Methyl parathion	298-00-0	ph1	200	6	N	N
DTXSID0024266	Pirimiphos-methyl	29232-93-7	ph1	200	7	N	N
DTXSID1032519	Acibenzolar-S-methyl	135158-54-2	ph1	200	4	N	N
DTXSID0032497	Triclopyr	55335-06-3	ph1	204	3	N	N
DTXSID1024209	Naled	300-76-5	ph1	200	6	N	N
DTXSID2020686	Lindane	58-89-9	ph1	200	24	N	N
DTXSID0020319	Chlorothalonil	1897-45-6	ph1	200	13	N	N
DTXSID0020022	Acifluorfen	50594-66-6	ph1	200	10	N	N
DTXSID0037495	Deisopropylatrazine	1007-28-9	ph1	200	1	N	N
DTXSID0034227	Icaridin	119515-38-7	ph1	200	5	N	N

DTXSID1032569	Pirimicarb	23103-98-2	ph1	200	3	N	N
DTXSID0034803	Penoxsulam	219714-96-2	ph1	200	5	N	N
DTXSID0020442	2,4-Dichlorophenoxyacetic acid	94-75-7	ph1	200	-3	N	N
DTXSID1023998	Cypermethrin	52315-07-8	ph1	200	5	N	N
DTXSID0034223	Tebufenpyrad	119168-77-3	ph1	200	11	N	N
DTXSID1032482	Tebupirimfos	96182-53-5	ph1	200	11	N	N
DTXSID1022265	Alachlor	15972-60-8	ph1	200	6	N	N
DTXSID2021105	Pentachloronitrobenzene	82-68-8	ph1	200	-5	N	N
DTXSID0032651	Thidiazuron	51707-55-2	ph1	200	-1	N	N
DTXSID1024338	Thiophanate-methyl	23564-05-8	ph1	200	4	N	N
DTXSID1020560	Endosulfan	115-29-7	ph1	200	25	N	N
DTXSID0034566	Emamectin benzoate	155569-91-8	ph1	200	37	N	N
DTXSID0022018	Disulfoton	298-04-4	ph1	89	1	N	N
DTXSID0032605	Methyl (RS)-2-[4-(2,4-dichlorophenoxy)phenoxy]propionate	51338-27-3	ph1	200	11	N	N
DTXSID1034634	Forchlorfenuron	68157-60-8	ph1	200	2	N	N
DTXSID1023869	Ametryn	834-12-8	ph1	200	6	N	N
DTXSID1020194	Boric acid	10043-35-3	ph1	200	2	N	N
DTXSID0032578	Thiodicarb	59669-26-0	ph1	200	3	N	N
DTXSID1021166	Piperonyl butoxide	51-03-6	ph1	202	9	N	N
DTXSID2020420	Propyzamide	23950-58-5	ph1	200	1	N	N
DTXSID2021151	2-Phenylphenol	90-43-7	ph1	200	9	Y	N
DTXSID1034210	Prodiamine	29091-21-2	ph1	200	19	N	N
DTXSID0039223	Aldicarb	116-06-3	ph1	200	-2	N	N
DTXSID1023990	Cyanazine	21725-46-2	ph1	200	9	N	N
DTXSID2020347	Coumaphos	56-72-4	ph1	200	2	N	N
DTXSID0024002	Fenpropathrin	39515-41-8	ph1	200	10	N	N
DTXSID1034503	Cyhalofop-butyl	122008-85-9	ph1	199	15	N	N
DTXSID0034855	Fluazifop-P-butyl	79241-46-6	ph1	201	11	N	N
DTXSID2032500	Triflumizole	68694-11-1	ph1	200	33	Y	N
DTXSID2027204	Methyl isothiocyanate	556-61-6	ph1	200	16	N	N

DTXSID4032580	Trifloxystrobin	141517-21-7	ph1	200	11	N	N
DTXSID3021196	Propazine	139-40-2	ph1	200	13	N	N
DTXSID3024154	Iprodione	36734-19-7	ph1	200	19	Y	N
DTXSID3024287	Imazethapyr	81335-77-5	ph1	200	16	N	N
DTXSID4022020	Bromacil	314-40-9	ph1	200	19	Y	N
DTXSID4024018	Dicamba	1918-00-9	ph1	200	13	N	N
DTXSID4024195	MCPA	94-74-6	ph1	200	3	N	N
DTXSID2025680	MEHP	4376-20-9	ph1	203	12	N	N
DTXSID4024272	Prometryn	7287-19-6	ph1	200	11	N	N
DTXSID2024242	Pacllobutrazol	76738-62-0	ph1	200	6	N	N
DTXSID2032552	Flufenacet	142459-58-3	ph1	200	10	N	N
DTXSID2032550	Fenpyroximate (Z,E)	111812-58-9	ph1	200	3	N	N
DTXSID4022448	Metolachlor	51218-45-2	ph1	200	6	N	N
DTXSID3032547	Etridiazole	2593-15-9	ph1	200	10	N	N
DTXSID4020791	Malathion	121-75-5	ph1	200	8	N	N
DTXSID2034590	Fenamidone	161326-34-7	ph1	200	-8	N	N
DTXSID3034612	Fluazifop-butyl	69806-50-4	ph1	200	1	N	N
DTXSID3034872	Chloridazon	1698-60-8	ph1	200	10	N	N
DTXSID3032464	Profenofos	41198-08-7	ph1	100	12	N	N
DTXSID4032376	Dimethenamid	87674-68-8	ph1	200	3	N	N
DTXSID2039336	S-Bioallethrin	28434-00-6	ph1	200	16	N	N
DTXSID4032532	Carfentrazone-ethyl	128639-02-1	ph1	200	9	N	N
DTXSID4020242	Captafol	2425-06-1	ph1	200	11	N	N
DTXSID2034673	Iodosulfuron-methyl-sodium	144550-36-7	ph1	200	1	N	N
DTXSID2024163	Linuron	330-55-2	ph1	200	5	N	N
DTXSID4024270	Prochloraz	67747-09-5	ph1	200	12	Y	N
DTXSID3034664	Imazamox	114311-32-9	ph1	200	-2	N	N
DTXSID4023412	Oxytetracycline dihydrate	6153-64-6	ph1	200	17	N	N
DTXSID2026523	Symclosene	87-90-1	ph1	200	1	N	N
DTXSID3031864	Perfluorooctanesulfonic acid	1763-23-1	ph1	168	41	Y	N
DTXSID2032344	Chlorethoxyfos	54593-83-8	ph1	200	3	N	N

DTXSID2032683	Mevinphos	7786-34-7	ph1	200	-5	N	N
DTXSID3032337	Butralin	33629-47-9	ph1	200	9	N	N
DTXSID3020122	Azinphos-methyl	86-50-0	ph1	200	10	N	N
DTXSID2034625	Fluoxastrobin	361377-29-9	ph1	200	-2	N	N
DTXSID2032392	Fenoxaprop-ethyl	66441-23-4	ph1	200	-2	Y	N
DTXSID3024235	Flusilazole	85509-19-9	ph1	200	10	N	N
DTXSID4022361	Vinclozolin	50471-44-8	ph1	200	0	N	N
DTXSID3023897	Triadimefon	43121-43-3	ph1	200	2	N	N
DTXSID4021975	Diphenylamine	122-39-4	ph1	200	3	N	N
DTXSID3032628	Methoxyfenozide	161050-58-4	ph1	200	13	N	N
DTXSID4021268	Simazine	122-34-9	ph1	200	0	N	N
DTXSID3024316	Tebuthiuron	34014-18-1	ph1	200	-8	N	N
DTXSID4021395	Trifluralin	1582-09-8	ph1	200	-1	N	N
DTXSID4024276	Propargite	2312-35-8	ph1	200	24	N	N
DTXSID3024102	Fenamiphos	22224-92-6	ph1	200	4	N	N
DTXSID2034881	Quinoxifen	124495-18-7	ph1	200	9	N	N
DTXSID3024152	Imazaquin	81335-37-7	ph1	200	-6	N	N
DTXSID3032549	Fenhexamid	126833-17-8	ph1	200	10	N	N
DTXSID2034627	Fluroxypyr	69377-81-7	ph1	200	-7	N	N
DTXSID3022455	Dimethyl phthalate	131-11-3	ph1	200	-6	N	N
DTXSID3034618	Flufenpyr-ethyl	188489-07-8	ph1	200	-4	N	N
DTXSID4024145	Hexazinone	51235-04-2	ph1	200	-8	N	N
DTXSID2032637	Pymetrozine	123312-89-0	ph1	200	-8	N	N
DTXSID3034456	Cinmethylin	87818-31-3	ph1	200	10	N	N
DTXSID2032556	Fluthiacet-methyl	117337-19-6	ph1	200	11	N	N
DTXSID4020450	Dicofol	115-32-2	ph1	200	48	Y	N
DTXSID2032390	Fenarimol	60168-88-9	ph1	200	21	Y	N
DTXSID2040363	Diniconazole	83657-24-3	ph1	200	32	N	N
DTXSID3024239	Oxadiazon	19666-30-9	ph1	200	12	N	N
DTXSID2032398	Fludioxonil	131341-86-1	ph1	200	3	N	N
DTXSID3023899	Benfluralin	1861-40-1	ph1	200	8	N	N

DTXSID2040361	Metam-sodium hydrate	6734-80-1	ph1	200	-2	N	N
DTXSID2034962	Thiamethoxam	153719-23-4	ph1	200	0	N	N
DTXSID2034465	Clothianidin	210880-92-5	ph1	200	-2	N	N
DTXSID4032405	Formetanate hydrochloride	23422-53-9	ph1	201	4	N	N
DTXSID2024793	Chloroneb	2675-77-6	ph1	200	4	N	N
DTXSID4032372	Difenoconazole	119446-68-3	ph1	200	2	Y	N
DTXSID3034402	Butachlor	23184-66-9	ph1	200	16	N	N
DTXSID2032554	Flumiclorac-pentyl	87546-18-7	ph1	200	13	N	N
DTXSID9023881	Clofentezine	74115-24-5	ph1	200	1	N	N
DTXSID5020607	Di(2-ethylhexyl) phthalate	117-81-7	ph1	200	-2	N	N
DTXSID6032358	Cymoxanil	57966-95-7	ph1	200	8	N	N
DTXSID4032611	Ethoprop	13194-48-4	ph1	200	9	N	N
DTXSID6024048	Difenzoquat metilsulfate	43222-48-6	ph1	200	2	N	N
DTXSID5032365	Dichlobenil	1194-65-6	ph1	200	3	N	N
DTXSID5024211	Napropamide	15299-99-7	ph1	200	10	Y	N
DTXSID5020819	Methidathion	950-37-8	ph1	200	16	N	N
DTXSID6032356	Cycloate	1134-23-2	ph1	200	6	N	N
DTXSID7022253	Resmethrin	10453-86-8	ph1	200	20	N	N
DTXSID4032667	Esfenvalerate	66230-04-4	ph1	200	7	Y	N
DTXSID6024337	Thiobencarb	28249-77-6	ph1	200	4	N	N
DTXSID7031248	Diquat dibromide monohydrate	6385-62-2	ph1	100	90	Y	N
DTXSID6024204	Metribuzin	21087-64-9	ph1	200	-5	N	N
DTXSID7024245	Pendimethalin	40487-42-1	ph1	200	14	N	N
DTXSID5023900	Benomyl	17804-35-2	ph1	200	14	N	N
DTXSID5037523	Diazoxon	962-58-3	ph1	201	11	Y	N
DTXSID6021086	Oxamyl	23135-22-0	ph1	200	0	N	N
DTXSID5021332	Thiram	137-26-8	ph1	200	6	N	N
DTXSID6032647	2-(Thiocyanomethylthio)benzothiazole	21564-17-0	ph1	200	2	N	N
DTXSID5032525	Bifenazate	149877-41-8	ph1	200	6	N	N
DTXSID5020601	Ethylene thiourea	96-45-7	ph1	200	4	N	N
DTXSID4034948	Tebufenozide	112410-23-8	ph1	200	0	N	N

DTXSID6022341	Prometon	1610-18-0	ph1	200	5	N	N
DTXSID5020449	Dichlorvos	62-73-7	ph1	100	12	N	N
DTXSID5023871	Amitraz	33089-61-1	ph1	200	35	N	N
DTXSID6024175	Metalaxyl	57837-19-1	ph1	200	4	N	N
DTXSID4032613	Fenitrothion	122-14-5	ph1	200	4	N	N
DTXSID5024182	2-Methoxyethanol	109-86-4	ph1	200	2	N	N
DTXSID6034265	Clopyralid-olamine	57754-85-5	ph1	200	1	N	N
DTXSID7024035	2,4-Dichlorophenoxybutyric acid	94-82-6	ph1	203	8	N	N
DTXSID5034723	Isoxaflutole	141112-29-0	ph1	200	2	N	N
DTXSID6032645	Sulfentrazone	122836-35-5	ph1	200	10	N	N
DTXSID5034270	Imazapic	104098-48-8	ph1	200	9	N	N
DTXSID7024085	Ethephon	16672-87-0	ph1	200	5	N	N
DTXSID5032577	Tefluthrin	79538-32-2	ph1	200	8	N	N
DTXSID6034928	Spirodiclofen	148477-71-8	ph1	200	4	N	N
DTXSID5034303	Fluroxypyr-meptyl	81406-37-3	ph1	200	22	N	N
DTXSID6032562	Octylbicycloheptenedicarboximide	113-48-4	ph1	200	27	N	N
DTXSID7020764	Chlorpropham	101-21-3	ph1	200	11	N	N
DTXSID6032352	Chlorpyrifos-methyl	5598-13-0	ph1	200	11	N	N
DTXSID5020154	Chlorophene	120-32-1	ph1	202	36	N	N
DTXSID7024160	Lactofen	77501-63-4	ph1	200	7	N	N
DTXSID6032641	Quinclorac	84087-01-4	ph1	200	15	N	N
DTXSID5032600	Cyclanilide	113136-77-9	ph1	200	23	N	N
DTXSID6023999	Cyromazine	66215-27-8	ph1	200	5	N	N
DTXSID7024299	Hexythiazox	78587-05-0	ph1	200	3	N	N
DTXSID5034773	Novaluron	116714-46-6	ph1	100	-4	N	N
DTXSID4034609	Fipronil	120068-37-3	ph1	201	14	N	N
DTXSID4032615	Flumetsulam	98967-40-9	ph1	200	-3	N	N
DTXSID4034653	Hexaconazole	79983-71-4	ph1	200	16	N	N
DTXSID6024206	Molinate	2212-67-1	ph1	200	14	N	N
DTXSID7032393	Fenoxycarb	72490-01-8	ph1	200	14	N	N
DTXSID7021948	Propoxur	114-26-1	ph1	200	3	N	N

DTXSID7024902	Dazomet	533-74-4	ph1	200	7	N	N
DTXSID7020508	Dimethylarsinic acid	75-60-5	ph1	200	3	N	N
DTXSID6024177	Methamidophos	10265-92-6	ph1	200	-8	N	N
DTXSID5032573	Pyridaben	96489-71-3	ph1	200	1	N	N
DTXSID6032354	Clodinafop-propargyl	105512-06-9	ph1	200	9	N	N
DTXSID7023936	Butylate	2008-41-5	ph1	200	18	N	N
DTXSID5035957	Cyfluthrin	68359-37-5	ph1	200	22	N	N
DTXSID4034528	Diclosulam	145701-21-9	ph1	200	39	N	N
DTXSID6034392	Boscalid	188425-85-6	ph1	200	-9	N	N
DTXSID7020479	Dimethoate	60-51-5	ph1	200	3	N	N
DTXSID5024344	Tri-allate	2303-17-5	ph1	200	17	N	N
DTXSID7021100	Parathion	56-38-2	ph1	100	13	N	N
DTXSID7024241	Oxyfluorfen	42874-03-3	ph1	200	11	N	N
DTXSID6032649	Tetramethrin	7696-12-0	ph1	200	21	N	N
DTXSID6021248	Rotenone	83-79-4	ph1	200	3	N	N
DTXSID4040002	Monobutyl phthalate	131-70-4	ph1	200	12	N	N
DTXSID5032442	Imidacloprid	138261-41-3	ph1	200	7	N	N
DTXSID6034849	Propamocarb hydrochloride	25606-41-1	ph1	200	14	N	N
DTXSID8022292	Permethrin	52645-53-1	ph1	200	-9	N	N
DTXSID8034742	Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3)	NOCAS_34742	ph1	195	37	N	N
DTXSID8034956	Tetraconazole	112281-77-3	ph1	199	7	N	N
DTXSID8024238	Oryzalin	19044-88-3	ph1	200	31	N	N
DTXSID8024280	Propiconazole	60207-90-1	ph1	200	16	N	N
DTXSID8031865	Perfluorooctanoic acid	335-67-1	ph1	200	10	N	N
DTXSID9020247	Carbaryl	63-25-2	ph1	200	-1	N	N
DTXSID9020792	Maleic hydrazide	123-33-1	ph1	200	17	N	N
DTXSID9032329	Bensulide	741-58-2	ph1	200	14	N	N
DTXSID8024109	Flutolanil	66332-96-5	ph1	200	9	Y	N
DTXSID8020620	Fenthion	55-38-9	ph1	200	-2	N	N
DTXSID8032386	Ethalfuralin	55283-68-6	ph1	200	3	N	N

DTXSID8024159	Isoxaben	82558-50-7	ph1	200	1	N	N
DTXSID9032327	Bendiocarb	22781-23-3	ph1	200	11	N	N
DTXSID8024234	Norflurazon	27314-13-2	ph1	200	7	N	N
DTXSID7034545	Dimethomorph	110488-70-5	ph1	200	2	N	N
DTXSID8023892	Abamectin	71751-41-2	ph1	121	7	N	N
DTXSID8034401	Buprofezin	69327-76-0	ph1	200	17	N	N
DTXSID9024304	Sethoxydim	74051-80-2	ph1	201	3	N	N
DTXSID9032581	Zoxamide	156052-68-5	ph1	201	7	N	N
DTXSID7040362	Niclosamide	50-65-7	ph1	100	7	N	N
DTXSID8023846	Acephate	30560-19-1	ph1	200	-1	N	N
DTXSID8024315	Myclobutanil	88671-89-0	ph1	200	5	N	N
DTXSID9034818	Azamethiphos	35575-96-3	ph1	200	-2	N	N
DTXSID8035180	Allethrin	584-79-2	ph1	210	18	N	N
DTXSID8022111	Propanil	709-98-8	ph1	200	1	N	N
DTXSID9020243	Captan	133-06-2	ph1	197	7	N	N
DTXSID9020112	Atrazine	1912-24-9	ph1	200	-2	N	N
DTXSID9040001	Monomethyl phthalate	4376-18-5	ph1	200	-3	N	N
DTXSID9020370	Daminozide	1596-84-5	ph1	200	-3	N	N
DTXSID8034665	Imazapyr	81334-34-1	ph1	200	-9	N	N
DTXSID9034232	Cloprop	101-10-0	ph1	200	-5	N	N
DTXSID9020827	Methoxychlor	72-43-5	ph1	199	5	N	N
DTXSID7034961	Thiacloprid	111988-49-9	ph1	200	5	N	N
DTXSID9023889	Quizalofop-ethyl	76578-14-8	ph1	172	11	N	N
DTXSID8034588	Famoxadone	131807-57-3	ph1	201	8	N	N
DTXSID8024151	Imazalil	35554-44-0	ph1	200	5	N	N
DTXSID9020407	Diazinon	333-41-5	ph1	200	-8	N	N
DTXSID9034864	Propoxycarbazone-sodium	181274-15-7	ph1	200	-4	N	N
DTXSID8034586	Etoxazole	153233-91-1	ph1	132	0	N	N
DTXSID9034365	Butafenacil	134605-64-4	ph1	201	11	N	N
DTXSID8032548	Fenbuconazole	114369-43-6	ph1	200	4	N	N
DTXSID8034877	Pyrimethanil	53112-28-0	ph1	200	7	N	N

DTXSID8032673	Pyriithiobac-sodium	123343-16-8	ph1	200	1	N	N
DTXSID9029221	Clopyralid	1702-17-6	ph1	200	1	N	N
DTXSID8034580	Ethofumesate	26225-79-6	ph1	200	-5	N	N
DTXSID7032553	Flumetralin	62924-70-3	ph1	200	-2	N	N
DTXSID9034490	Cyanamide	420-04-2	ph1	200	-2	N	N
DTXSID9020790	Malaoxon	1634-78-2	ph1	200	1	N	N
DTXSID9034492	Cyazofamid	120116-88-3	ph1	200	19	N	N
DTXSID7032638	Pyraclostrobin	175013-18-0	ph1	200	4	N	N
DTXSID7032555	Flumioxazin	103361-09-7	ph1	200	7	N	N
DTXSID9034816	Monocrotophos	6923-22-4	ph1	200	8	N	N
DTXSID8024317	Terbacil	5902-51-2	ph1	200	1	N	N
DTXSID8034871	Pyraflufen-ethyl	129630-19-9	ph1	200	1	N	N
DTXSID8020628	Fluometuron	2164-17-2	ph1	200	0	N	N
DTXSID9020794	Maneb	12427-38-2	ph1	100	-2	N	N
DTXSID8040222	Trifloxysulfuron-sodium	199119-58-9	ph1	200	-6	N	N
DTXSID9021976	2-Phenoxyethanol	122-99-6	ph1	200	-7	N	N
DTXSID7034252	Tepraloxymid	149979-41-9	ph1	200	-2	N	N
DTXSID9023914	Dicrotophos	141-66-2	ph1	201	-6	N	N
DTXSID9032379	Dithiopyr	97886-45-8	ph1	199	3	N	N
DTXSID7032551	Fluazinam	79622-59-6	ph1	200	40	N	N
DTXSID8023890	Asulam	3337-71-1	ph1	200	6	N	N
DTXSID7032424	Mesotrione	104206-82-8	ph1	200	-3	N	N
DTXSID9020089	Anilazine	101-05-3	ph1	200	0	N	N
DTXSID7034676	Isazofos	42509-80-8	ph1	200	5	N	N
DTXSID8032544	Dipropyl 2,5-pyridinedicarboxylate	136-45-8	ph1	200	-2	N	N
DTXSID8022325	2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane	2971-36-0	ph1	200	24	N	N
DTXSID9020160	Bifenthrin	82657-04-3	ph1	200	16	N	N
DTXSID7032470	Propetamphos	31218-83-4	ph1	200	8	N	N
DTXSID4024066	1,2-Dinitrobenzene	528-29-0	ph2	200	61	Y	N
DTXSID8026773	1,3-Butanediol	107-88-0	ph2	200	-1	N	N

DTXSID8027034	2-(Hydroxymethyl)-2-nitro-1,3-propanediol	126-11-4	ph2	200	0	N	N
DTXSID9020877	1-Methylnaphthalene	90-12-0	ph2	200	0	N	N
DTXSID6020147	1,2,3-Benzotriazole	95-14-7	ph2	200	3	N	N
DTXSID4021137	1,3-Benzenediamine	108-45-2	ph2	200	-4	N	N
DTXSID0020440	Dichlorprop	120-36-5	ph1	200	-2	N	N
DTXSID6025010	1,3-Dichloro-2-propanol	96-23-1	ph2	200	1	N	N
DTXSID3035341	1,3-Dibromo-5,5-dimethylhydantoin	77-48-5	ph2	200	2	N	N
DTXSID4042206	1-Dodecyl-2-pyrrolidinone	2687-96-9	ph2	200	31	N	N
DTXSID8024284	1-Methoxy-2-propanol	107-98-2	ph2	200	1	N	N
DTXSID0021965	1,2,4-Trichlorobenzene	120-82-1	ph2	200	-3	N	N
DTXSID5020576	17alpha-Ethinylestradiol	57-63-6	ph2	0.2	-5	N	N
DTXSID3047261	(2S,3S)-3-Methyl-2-(3-oxo-1,2-benzothiazol-2(3H)-yl)pentanoic acid	177785-47-6	ph2	200	-1	N	N
DTXSID2021947	1-Tridecanol	112-70-9	ph2	206	19	N	N
DTXSID8021195	1,3-Propane sultone	1120-71-4	ph2	200	1	N	N
DTXSID6021402	1,2,4-Trimethylbenzene	95-63-6	ph2	208	7	N	N
DTXSID8027581	1,5,9-Cyclododecatriene	4904-61-4	ph2	200	2	N	N
DTXSID7025132	1,2-Dimethyl-3-nitrobenzene	83-41-0	ph2	200	2	N	N
DTXSID2022331	2-(Butan-2-yl)phenol	89-72-5	ph2	200	1	N	N
DTXSID3025881	1,2-Phenylenediamine	95-54-5	ph2	200	9	N	N
DTXSID7020710	1,2-Diphenylhydrazine	122-66-7	ph2	200	9	N	N
DTXSID1038298	1-Hydroxypyrene	5315-79-7	ph2	200	20	N	N
DTXSID4026684	2-(Phenylmethylene)octanal	101-86-0	ph2	200	22	N	N
DTXSID8026193	1,2,3-Trichlorobenzene	87-61-6	ph2	200	3	N	N
DTXSID9047257	Zamifenacin	127308-82-1	ph2	200	1	N	N
DTXSID8044593	1-Benzylquinolinium chloride	15619-48-4	ph2	200	-1	N	N
DTXSID9020087	(E)-Anethole	4180-23-8	ph2	200	2	N	N
DTXSID0026915	1-Undecanol	112-42-5	ph2	200	16	N	N
DTXSID7021946	1-Decanol	112-30-1	ph2	200	12	N	N
DTXSID8035001	10-Undecenoic acid	112-38-9	ph2	200	3	N	N

DTXSID5044493	1-[3-(Triethoxysilyl)propyl]urea	23779-32-0	ph2	200	-2	N	N
DTXSID7024320	1,2,4,5-Tetrachlorobenzene	95-94-3	ph2	200	0	N	N
DTXSID6027131	1H-1,2,4-Triazole	288-88-0	ph2	200	-5	N	N
DTXSID8022377	17alpha-Estradiol	57-91-0	ph2	200	-5	N	N
DTXSID8026640	1,3-Diisopropylbenzene	99-62-7	ph2	200	-2	N	N
DTXSID9026926	1-Tetradecanol	112-72-1	ph2	200	14	N	N
DTXSID9024065	1,3-Dinitrobenzene	99-65-0	ph2	207	16	N	N
DTXSID5026918	1-Dodecanol	112-53-8	ph2	200	9	N	N
DTXSID2025133	1,2-Dimethyl-4-nitrobenzene	99-51-4	ph2	200	-2	N	N
DTXSID0047296	Zenarestat	112733-06-9	ph2	100	4	N	N
DTXSID6022056	1,3-Dichlorobenzene	541-73-1	ph2	200	1	N	N
DTXSID1020431	1,4-Dichlorobenzene	106-46-7	ph2	200	1	N	N
DTXSID4027367	1-Tetradecene	1120-36-1	ph2	200	7	N	N
DTXSID0034192	17beta-Trenbolone	10161-33-8	ph2	0.2	-4	N	N
DTXSID5032523	1,2-Benzisothiazolin-3-one	2634-33-5	ph2	200	-4	N	N
DTXSID3026728	(2Z)-3,7-Dimethylocta-2,6-dien-1-ol	106-25-2	ph2	200	5	N	N
DTXSID8021519	2-(2-Butoxyethoxy)ethanol	112-34-5	ph2	200	-1	N	N
DTXSID6032514	1,2-Benzenedicarboxaldehyde	643-79-8	ph2	200	63	Y	N
DTXSID1048176	YM218	NOCAS_48176	ph2	125	-1	N	N
DTXSID4027991	1-Hexadecanol	36653-82-4	ph2	100	1	N	N
DTXSID4024985	1,3-Dichloro-5,5-dimethylhydantoin	118-52-5	ph2	200	-2	N	N
DTXSID6035152	1-(Hydroxymethyl)-5,5-dimethylhydantoin	116-25-6	ph2	200	-1	N	N
DTXSID6020430	1,2-Dichlorobenzene	95-50-1	ph2	200	3	N	N
DTXSID0021206	1,2-Propylene glycol	57-55-6	ph2	200	-4	N	N
DTXSID0028666	1,2-Benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich	68515-49-1	ph2	200	-3	N	N
DTXSID5020281	1-Chloro-4-nitrobenzene	100-00-5	ph2	200	1	N	N
DTXSID3020916	1,5-Naphthalenediamine	2243-62-1	ph2	200	20	N	N
DTXSID3025178	1,3-Diphenylguanidine	102-06-7	ph2	200	-1	N	N
DTXSID9021390	1,2,3-Trichloropropane	96-18-4	ph2	200	4	N	N

DTXSID3021485	1,3-Benzenedicarboxylic acid	121-91-5	ph2	200	8	N	N
DTXSID6040747	17alpha-Hydroxyprogesterone	68-96-2	ph2	200	2	N	N
DTXSID7021940	1-Octanol	111-87-5	ph2	207	0	N	N
DTXSID0020573	17beta-Estradiol	50-28-2	ph2	200	-3	N	N
DTXSID9047259	1,3-Dichloro-6,7,8,9,10,12-hexahydroazepino[2,1-b]quinazoline hydrochloride (1:1)	149062-75-9	ph2	100	10	Y	N
DTXSID0027270	1-Pentadecanol	629-76-5	ph2	200	1	N	N
DTXSID1033664	17-Methyltestosterone	58-18-4	ph2	0.2	10	N	N
DTXSID2021941	2-(2-Ethoxyethoxy)ethanol	111-90-0	ph2	200	-2	N	N
DTXSID8026307	2,6-Dimethylaniline	87-62-7	ph2	207	-7	N	N
DTXSID9025110	2,5-Dimethyl-2,5-di-(tert-butylperoxy)hexane	78-63-7	ph2	200	10	N	N
DTXSID6020068	2-Aminoanthraquinone	117-79-3	ph2	200	11	N	N
DTXSID4020959	2-Methyl-5-nitroaniline	99-55-8	ph2	200	15	N	N
DTXSID7024087	2-Ethoxyethanol	110-80-5	ph2	200	8	N	N
DTXSID5021386	2,4,6-Trichlorophenol	88-06-2	ph2	200	8	N	N
DTXSID1020807	2-Mercaptobenzothiazole	149-30-4	ph2	200	9	Y	N
DTXSID4024359	2,4,5-Trichlorophenol	95-95-4	ph2	200	18	Y	N
DTXSID2026525	2-tert-Butylphenol	88-18-6	ph2	200	6	N	N
DTXSID4027494	2,3-Diaminotoluene	2687-25-4	ph2	200	18	N	N
DTXSID6020141	2,3-Benzofuran	271-89-6	ph2	200	2	N	N
DTXSID3024657	3-Bromo-1-propanol	627-18-9	ph2	200	5	N	N
DTXSID5027061	2-Naphthalenol	135-19-3	ph2	200	11	N	N
DTXSID4024062	3,4-Dimethylphenol	95-65-8	ph2	205	15	N	N
DTXSID5020605	2-Ethyl-1-hexanol	104-76-7	ph2	200	8	N	N
DTXSID7027041	2,4,7,9-Tetramethyl-5-decyne-4,7-diol	126-86-3	ph2	200	3	N	N
DTXSID5021885	2-Methyl-2,4-pentanediol	107-41-5	ph2	209	1	N	N
DTXSID9021928	Ethylene glycol monoethyl ether acetate	111-15-9	ph2	200	3	N	N
DTXSID9024063	2,6-Dimethylphenol	576-26-1	ph2	200	9	N	N

DTXSID1027635	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	ph2	200	15	N	N
DTXSID5024059	3,3'-Dimethylbenzidine	119-93-7	ph2	200	1	N	N
DTXSID7029241	2,4-Bis(1-methyl-1-phenylethyl)phenol	2772-45-4	ph2	200	61	Y	N
DTXSID0020529	2,4-Dinitrotoluene	121-14-2	ph2	200	5	N	N
DTXSID3021277	2E,4E-Hexadienoic acid	110-44-1	ph2	200	-8	N	N
DTXSID4044581	2-tert-Butyl-4-ethylphenol	96-70-8	ph2	200	20	N	N
DTXSID6027052	2,6-Di-tert-butylphenol	128-39-2	ph2	200	21	Y	N
DTXSID6025145	2,5-Dimethylphenol	95-87-4	ph2	205	7	N	N
DTXSID2021864	2,4-Dimethylphenol	105-67-9	ph2	207	0	N	N
DTXSID8020127	3'-Azido-3'-deoxythymidine	30516-87-1	ph2	200	0	N	N
DTXSID2026602	2,4-Di-tert-butylphenol	96-76-4	ph2	200	56	Y	N
DTXSID1022053	2-Methyl-4,6-dinitrophenol	534-52-1	ph2	200	7	N	N
DTXSID5020528	2,6-Dinitrotoluene	606-20-2	ph2	200	-8	N	N
DTXSID8024999	3,4-Dichloronitrobenzene	99-54-7	ph2	200	-8	N	N
DTXSID9025293	2-Ethylhexanoic acid	149-57-5	ph2	200	5	N	N
DTXSID1020350	2-Methoxy-5-methylaniline	120-71-8	ph2	200	-2	N	N
DTXSID1020439	2,4-Dichlorophenol	120-83-2	ph2	200	7	N	N
DTXSID1021821	2-Butanone oxime	96-29-7	ph2	200	-3	N	N
DTXSID0020943	2-Methoxy-5-nitroaniline	99-59-2	ph2	200	-1	N	N
DTXSID1026164	2-Methylaniline	95-53-4	ph2	200	-2	N	N
DTXSID6024836	3,7-Dimethyl-2,6-octadienal	5392-40-5	ph2	200	3	N	N
DTXSID1021877	2-Chloroethanol	107-07-3	ph2	200	-4	N	N
DTXSID2026529	2-Tert-Butyl-5-methylphenol	88-60-8	ph2	200	23	N	N
DTXSID6022927	2',3'-Dideoxyinosine	69655-05-6	ph2	200	-2	N	N
DTXSID1024097	2-Butoxyethanol	111-76-2	ph2	200	3	N	N
DTXSID5032361	2,2-Dibromo-3-nitrilopropionamide	10222-01-2	ph2	200	6	N	N
DTXSID3024368	2-[2-(2-Ethoxyethoxy)ethoxy]ethanol	112-50-5	ph2	200	-2	N	N
DTXSID1026908	2-Hexyloxyethanol	112-25-4	ph2	200	0	N	N
DTXSID1026081	3,3',5,5'-Tetrabromobisphenol A	79-94-7	ph2	191	70	Y	N
DTXSID4027236	2,3-Dinitrotoluene	602-01-7	ph2	143	25	N	N

DTXSID9020293	2-Chloroacetophenone	532-27-4	ph2	200	-1	N	N
DTXSID9044742	2,2'-[Ethane-1,2-diylbis(oxy)]diethanamine	929-59-9	ph2	200	7	N	N
DTXSID8041248	2,5-Di-tert-butylbenzene-1,4-diol	88-58-4	ph2	200	6	N	N
DTXSID0020523	2,4-Dinitrophenol	51-28-5	ph2	200	6	N	N
DTXSID5023877	2-Anisidine	90-04-0	ph2	203	11	N	N
DTXSID9024930	3,4-Diaminotoluene	496-72-0	ph2	200	10	N	N
DTXSID7040788	2-tert-Butyl-4-methoxyphenol	121-00-6	ph2	200	17	N	N
DTXSID6022187	2,3,6-Trimethylphenol	2416-94-6	ph2	200	3	N	N
DTXSID9026974	2,4-Di-tert-pentylphenol	120-95-6	ph2	200	64	Y	N
DTXSID4020402	2,4-Diaminotoluene	95-80-7	ph2	200	-6	N	N
DTXSID2020921	2-Naphthylamine	91-59-8	ph2	200	13	N	N
DTXSID3025091	3,3'-Dimethoxybenzidine	119-90-4	ph2	200	4	N	N
DTXSID6027218	2,6-Diethylaniline	579-66-8	ph2	200	12	N	N
DTXSID0047456	2-Norbornene-5,6-dicarboxylic anhydride	826-62-0	ph2	200	7	N	N
DTXSID1020485	3,3'-Dimethoxybenzidine dihydrochloride	20325-40-0	ph2	200	3	N	N
DTXSID1020069	2-Amino-5-azotoluene	97-56-3	ph2	200	29	N	N
DTXSID7022049	2,4,6-Trimethylphenol	527-60-6	ph2	200	9	N	N
DTXSID1044564	2,6,10-Trimethyl-2,6,10-triazaundecane	3855-32-1	ph2	200	-8	N	N
DTXSID9047592	9-Phenanthrol	484-17-3	ph2	200	30	N	N
DTXSID3040722	4-Cyclohexylcyclohexanol	2433-14-9	ph2	200	15	N	N
DTXSID1026665	3-Pyridinecarbonitrile	100-54-9	ph2	200	0	N	N
DTXSID5024394	Acetic acid	64-19-7	ph2	200	3	N	N
DTXSID9022312	4-Octylphenol	1806-26-4	ph2	200	71	Y	N
DTXSID0020604	4-Vinyl-1-cyclohexene dioxide	106-87-6	ph2	200	1	N	N
DTXSID8040721	4-Cyclohexylcyclohexanone	92-68-2	ph2	200	5	N	N
DTXSID9033058	4-Amino-1,2,4-triazole	584-13-4	ph2	200	14	N	N
DTXSID1020699	4-Hexylresorcinol	136-77-6	ph2	200	25	N	N
DTXSID0021834	4-Nitrophenol	100-02-7	ph2	200	-1	N	N

DTXSID1026792	3-Methylaniline	108-44-1	ph2	200	6	N	N
DTXSID7020005	Acetamide	60-35-5	ph2	200	2	N	N
DTXSID5021831	3-Nitrotoluene	99-08-1	ph2	200	0	N	N
DTXSID1046970	5HPP-33	105624-86-0	ph2	200	18	N	N
DTXSID5029055	4-Nonylphenol, branched	84852-15-3	ph2	200	71	Y	N
DTXSID6023652	6-Thioguanine	154-42-7	ph2	200	3	N	N
DTXSID9047540	3-Hydroxyfluorene	6344-67-8	ph2	200	-1	N	N
DTXSID9025453	3-Methylbutyl acetate	123-92-2	ph2	200	2	N	N
DTXSID8020961	4-Nitroaniline	100-01-6	ph2	200	7	N	N
DTXSID9022360	4-(1,1,3,3-Tetramethylbutyl)phenol	140-66-9	ph2	200	61	Y	N
DTXSID9020295	4-Chloroaniline	106-47-8	ph2	203	2	N	N
DTXSID0040707	4-Pentylaniline	33228-44-3	ph2	200	6	N	N
DTXSID3037094	4-Hydroxytamoxifen	68392-35-8	ph2	50	3	Y	N
DTXSID9024489	5-Amino-2-methylphenol	2835-95-2	ph2	200	9	N	N
DTXSID1044697	4-Ethyl-1-yn-3-ol	5877-42-9	ph2	200	-3	N	N
DTXSID2027593	4-Chlorobenzotrichloride	5216-25-1	ph2	200	9	N	N
DTXSID1020510	7,12-Dimethylbenz(a)anthracene	57-97-6	ph2	200	1	N	N
DTXSID4034287	5-Heptyldihydro-2(3H)-furanone	104-67-6	ph2	200	2	N	N
DTXSID4021717	4-Chloro-3-methylphenol	59-50-7	ph2	200	0	N	N
DTXSID5020730	8-Hydroxyquinoline	148-24-3	ph2	200	-4	N	N
DTXSID3022588	4-Aminofolic acid	54-62-6	ph2	200	-4	N	N
DTXSID0021969	4-Hydroxy-3-methoxybenzaldehyde	121-33-5	ph2	200	0	N	N
DTXSID5020869	4,4'-Methylenebis(N,N-dimethylaniline)	101-61-1	ph2	200	1	N	N
DTXSID2037712	4,4',4''-Ethane-1,1,1-triyltriphenol	27955-94-8	ph2	200	6	N	N
DTXSID6022422	4,4'-Diaminobiphenyl methane	101-77-9	ph2	200	1	N	N
DTXSID6024460	4-Aminoazobenzene	60-09-3	ph2	200	3	N	N
DTXSID3020887	6-Methylquinoline	91-62-3	ph2	200	-7	N	N
DTXSID8024523	4-Androstene-3,17-dione	63-05-8	ph2	0.2	0	N	N
DTXSID3023845	Acenaphthylene	208-96-8	ph2	200	8	N	N
DTXSID1020221	4-tert-Butylphenol	98-54-4	ph2	200	0	N	N

DTXSID2020006	Acetaminophen	103-90-2	ph2	200	-4	N	N
DTXSID2020634	5-Fluorouracil	51-21-8	ph2	204	-4	N	N
DTXSID8020541	5,5-Diphenylhydantoin	57-41-0	ph2	200	2	N	N
DTXSID3047558	6:2 Fluorotelomer methacrylate	2144-53-8	ph2	200	-3	N	N
DTXSID5044572	6:2 Fluorotelomer alcohol	647-42-7	ph2	200	-7	N	N
DTXSID2037714	4-Heptylphenol	1987-50-4	ph2	200	55	Y	N
DTXSID9022364	5alpha-Dihydrotestosterone	521-18-6	ph2	200	-5	N	N
DTXSID5020867	4,4'-Diamino-3,3'-dimethyldiphenylmethane	838-88-0	ph2	200	3	N	N
DTXSID0021094	4,4'-Oxydianiline	101-80-4	ph2	200	3	N	N
DTXSID3020966	4-Nitrobenzoic acid	62-23-7	ph2	200	1	N	N
DTXSID5021209	6-Propyl-2-thiouracil	51-52-5	ph2	200	0	N	N
DTXSID3021774	Acenaphthene	83-32-9	ph2	200	7	N	N
DTXSID6024466	4-Aminobenzoic acid	150-13-0	ph2	200	-4	N	N
DTXSID7029904	8:2 Fluorotelomer alcohol	678-39-7	ph2	200	-2	N	N
DTXSID5023792	4-Nitrotoluene	99-99-0	ph2	200	4	N	N
DTXSID7022332	4-(Butan-2-yl)phenol	99-71-8	ph2	200	0	N	N
DTXSID9047598	4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol]	41481-66-7	ph2	200	11	N	N
DTXSID2020890	6-Methyl-2-thiouracil	56-04-2	ph2	200	4	N	N
DTXSID8021771	4-(2-Methylbutan-2-yl)phenol	80-46-6	ph2	200	14	N	N
DTXSID5020283	4-Chloro-1,2-diaminobenzene	95-83-0	ph2	200	4	N	N
DTXSID9040716	4-(2-Methylbutan-2-yl)cyclohexanol	5349-51-9	ph2	200	6	N	N
DTXSID2026781	4-Methyl-2-pentanol	108-11-2	ph2	200	-8	N	N
DTXSID9034286	5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	ph2	200	3	N	N
DTXSID1038321	3-Phenoxybenzoic acid	3739-38-6	ph2	200	8	N	N
DTXSID6020224	4-Butyrolactone	96-48-0	ph2	200	9	N	N
DTXSID3022536	4-Cumylphenol	599-64-4	ph2	0.2	1	N	N
DTXSID2027200	4,4'-Bipyridine	553-26-4	ph2	200	8	N	N
DTXSID5021754	5,5-Dimethylhydantoin	77-71-4	ph2	201	5	N	N

DTXSID1047526	C10-21 sulfonic acids phenyl esters	91082-17-6	ph2	200 µg/ml	2	N	N
DTXSID2026446	Acetyl tributyl citrate	77-90-7	ph2	200	0	N	N
DTXSID9020249	Carbofuran	1563-66-2	ph2	200	-2	N	N
DTXSID0047377	AVE6324	NOCAS_47377	ph2	189	38	Y	N
DTXSID7027047	alpha-Isomethylionone	127-51-5	ph2	200	10	N	N
DTXSID6022472	Butylbenzene	104-51-8	ph2	200	4	N	N
DTXSID4020240	Caprolactam	105-60-2	ph2	200	8	N	N
DTXSID9022817	Carminic acid	1260-17-9	ph2	200	5	N	N
DTXSID6021828	Acetophenone	98-86-2	ph2	200	17	N	N
DTXSID6047527	Adipic acid, polypropyleneglycol, laurate	66456-53-9	ph2	200 µg/ml	4	N	N
DTXSID7025055	Bis(2-ethylhexyl) decanedioate	122-62-3	ph2	200	8	N	N
DTXSID9027360	Ammonium carbamate	1111-78-0	ph2	200	-5	N	N
DTXSID6020143	Benzoic acid	65-85-0	ph2	205	7	N	N
DTXSID3020205	Benzyl butyl phthalate	85-68-7	ph2	200	5	N	N
DTXSID8020040	Aldrin	309-00-2	ph2	200	25	N	N
DTXSID7024538	Anthralin	1143-38-0	ph2	200	5	N	N
DTXSID4047381	AVE8923	NOCAS_47381	ph2	18	0	N	N
DTXSID4020161	Biphenyl	92-52-4	ph2	200	3	N	N
DTXSID6047319	Carabersat	184653-84-7	ph2	195	0	N	N
DTXSID0047375	AVE9423	862243-29-6	ph2	200	0	N	N
DTXSID4024436	Allura Red C.I.16035	25956-17-6	ph2	200	11	Y	N
DTXSID3026697	Bis(2-ethylhexyl) nonanedioate	103-24-2	ph2	200	-6	N	N
DTXSID3047344	Cariporide mesylate	159138-81-5	ph2	149	-1	N	N
DTXSID5023902	Benz(a)anthracene	56-55-3	ph2	200	10	N	N
DTXSID4022731	Carbamazepine	298-46-4	ph2	200	2	N	N
DTXSID4022442	Bisphenol B	77-40-7	ph2	200	13	N	N
DTXSID5023950	Carbosulfan	55285-14-8	ph2	200	9	N	N
DTXSID9020168	Bis(2-chloroethyl) ether	111-44-4	ph2	200	1	N	N
DTXSID8040694	Butyl benzoate	136-60-7	ph2	200	2	N	N

DTXSID8037708	Ammonium perfluorooctanoate	3825-26-1	ph2	200	-2	N	N
DTXSID1020148	Benzotrichloride	98-07-7	ph2	200	-3	N	N
DTXSID0047371	AVE5638	725228-45-5	ph2	200	18	N	N
DTXSID9024431	Aldicarb oxime	1646-75-9	ph2	200	8	N	N
DTXSID7041623	Benodanil	15310-01-7	ph2	200	-2	N	N
DTXSID0020606	Bis(2-ethylhexyl)hexanedioate	103-23-1	ph2	200	11	N	N
DTXSID5047376	AVE2865	648917-13-9	ph2	100	4	N	N
DTXSID4020119	Azathioprine	446-86-6	ph2	199	-1	N	N
DTXSID7030698	alpha-Cyclodextrin	10016-20-3	ph2	105	-4	N	N
DTXSID8020123	Azobenzene	103-33-3	ph2	200	7	N	N
DTXSID0023878	Anthracene	120-12-7	ph2	200	3	N	N
DTXSID0020232	Caffeine	58-08-2	ph2	200	1	N	N
DTXSID1047528	Benzylloctyl adipate	58394-64-2	ph2	200	9	N	N
DTXSID6025014	Benzal chloride	98-87-3	ph2	200	5	N	N
DTXSID5044576	Acetyltriethyl citrate	77-89-4	ph2	200	-5	N	N
DTXSID5020152	Benzyl alcohol	100-51-6	ph2	200	2	N	N
DTXSID4024729	Carbendazim	10605-21-7	ph2	200	-4	N	N
DTXSID8021515	Butanoic acid	107-92-6	ph2	200	4	N	N
DTXSID0023907	Benzo(b)fluoranthene	205-99-2	ph2	200	13	N	N
DTXSID7021239	all-trans-Retinoic acid	302-79-4	ph2	200	6	N	N
DTXSID7027625	Bis(2-ethylhexyl) terephthalate	6422-86-2	ph2	100	-8	N	N
DTXSID5020027	Acrylamide	79-06-1	ph2	200	0	N	N
DTXSID4021135	C.I. Solvent Yellow 14	842-07-9	ph2	200	2	N	N
DTXSID8024652	Bronopol	52-51-7	ph2	200	7	N	N
DTXSID3020257	Catechol	120-80-9	ph2	200	0	N	N
DTXSID5020108	Aspirin	50-78-2	ph2	200	-8	N	N
DTXSID0047535	Butyryl trihexyl citrate	82469-79-2	ph2	200	0	N	N
DTXSID5041691	Butam	35256-85-0	ph2	200	6	N	N
DTXSID7037717	Bisphenol AF	1478-61-1	ph2	200	26	N	N
DTXSID5047372	AVE3295	478263-98-8	ph2	200	-4	N	N
DTXSID6047286	Candoxatril	123122-55-4	ph2	200	-2	N	N

DTXSID7020685	beta-Hexachlorocyclohexane	319-85-7	ph2	200	5	N	N
DTXSID4047383	AVE3247	NOCAS_47383	ph2	48	8	N	N
DTXSID0021961	Benzophenone	119-61-9	ph2	200	1	N	N
DTXSID2047270	Besoprodil	253450-09-8	ph2	200	2	N	N
DTXSID3020209	Butylparaben	94-26-8	ph2	200	5	N	N
DTXSID2020137	Benzidine	92-87-5	ph2	200	2	N	N
DTXSID3020910	Busulfan	55-98-1	ph2	200	7	N	N
DTXSID2047303	CJ-013790	179465-71-5	ph2	100	-3	N	N
DTXSID4047254	CP-457920	220860-50-4	ph2	200	6	N	N
DTXSID4020371	Dapsone	80-08-0	ph2	200	4	N	N
DTXSID8020337	Clomiphene citrate (1:1)	50-41-9	ph2	200	22	Y	N
DTXSID9021554	Decanoic acid	334-48-5	ph2	209	10	N	N
DTXSID6024917	Diacetone alcohol	123-42-2	ph2	200	8	N	N
DTXSID5047297	CP-085958	134002-60-1	ph2	100	16	N	N
DTXSID0024000	Chlorthal-dimethyl	1861-32-1	ph2	200	12	N	N
DTXSID3047265	CP-471358	NOCAS_47265	ph2	200	6	N	N
DTXSID0047248	CI-1018	NOCAS_47248	ph2	200	14	N	N
DTXSID3047267	CP-642931	NOCAS_47267	ph2	100	0	N	N
DTXSID5048182	Cyclohexylphenylketone	712-50-5	ph2	200	6	N	N
DTXSID9047253	CP-401387	199171-88-5	ph2	100	5	N	N
DTXSID0047246	Darbufelone mesylate	139340-56-0	ph2	100	12	N	N
DTXSID7020348	Coumarin	91-64-5	ph2	200	1	N	N
DTXSID6024882	Cycloheximide	66-81-9	ph2	200	1	N	N
DTXSID9047251	CP-122721	145742-28-5	ph2	200	11	N	N
DTXSID3020332	Citric acid	77-92-9	ph2	200	-2	N	N
DTXSID7047306	CP-634384	290352-28-2	ph2	200	16	N	N
DTXSID0047294	CP-863187	668981-02-0	ph2	200	-1	N	N
DTXSID7047304	CP-100829	135080-03-4	ph2	100	19	N	N
DTXSID2047274	CP-114271	113734-18-2	ph2	200	0	N	N
DTXSID1023996	Cyclohexylamine	108-91-8	ph2	200	0	N	N
DTXSID8047262	CI-1029	207736-05-8	ph2	190	11	N	N

DTXSID1047283	CP-728663	368832-42-2	ph2	200	-1	N	N
DTXSID7024827	Chlorpromazine hydrochloride	69-09-0	ph2	200	8	N	N
DTXSID2047305	CP-608039	NOCAS_47305	ph2	200	3	N	N
DTXSID2021575	Dalapon	75-99-0	ph2	200	0	N	N
DTXSID6047280	CP-607366	289716-94-5	ph2	200	2	N	N
DTXSID7024873	Cyanuric acid	108-80-5	ph2	199	-1	N	N
DTXSID8022828	Cladribine	4291-63-8	ph2	200	2	N	N
DTXSID8047264	CP-283097	171866-31-2	ph2	100	9	N	N
DTXSID5024891	Cytarabine hydrochloride	69-74-9	ph2	200	0	N	N
DTXSID6043709	Cyclopamine	4449-51-8	ph2	200	1	N	N
DTXSID1047281	CP-612372	353280-07-6	ph2	200	-1	N	N
DTXSID7047279	CP-532623	261947-38-0	ph2	200	-4	N	N
DTXSID6024888	Cyclophosphamide monohydrate	6055-19-2	ph2	200	3	N	N
DTXSID4021894	Cyclohexanol	108-93-0	ph2	200	-6	N	N
DTXSID9047255	CP-465394	NOCAS_47255	ph2	100	-1	N	N
DTXSID2020262	Chloramben	133-90-4	ph2	200	-2	N	N
DTXSID3020336	Clofibrate	637-07-0	ph2	200	-4	N	N
DTXSID5020366	Cyproterone acetate	427-51-0	ph2	200	8	N	N
DTXSID2047278	CP-457677	214535-77-0	ph2	200	-3	N	N
DTXSID6047282	CP-671305	445295-04-5	ph2	200	-3	N	N
DTXSID5047291	CI-1044	NOCAS_47291	ph2	200	4	N	N
DTXSID8047266	CP-544439	230954-09-3	ph2	200	-4	N	N
DTXSID2047301	CP-456773	210826-40-7	ph2	200	-1	N	N
DTXSID7020267	Chlordane	57-74-9	ph2	200	24	N	N
DTXSID7047308	CP-105696	158081-99-3	ph2	100	19	N	N
DTXSID9020299	Chlorobenzilate	510-15-6	ph2	200	10	N	N
DTXSID1047576	Cotinine	486-56-6	ph2	200	-3	N	N
DTXSID8047268	CI-959	104795-68-8	ph2	200	1	N	N
DTXSID6027921	Di(propylene glycol) dibenzoate	27138-31-4	ph2	200	2	N	N
DTXSID4020458	Chlorpyrifos	2921-88-2	ph2	200	7	N	N
DTXSID0021464	Ziram	137-30-4	ph2	200	1	N	N

DTXSID2047272	CJ-013610	249296-43-3	ph2	200	-4	N	N
DTXSID7029871	Clotrimazole	23593-75-1	ph2	200	6	N	N
DTXSID6020359	Cyclohexanone	108-94-1	ph2	200	-1	N	N
DTXSID3047429	Dexamethasone sodium phosphate	2392-39-4	ph2	200	2	N	N
DTXSID8044175	Clove leaf oil	8000-34-8	ph2	200 µg/ml	9	N	N
DTXSID5024845	Colchicine	64-86-8	ph2	200	-3	N	N
DTXSID5047299	CP-422935	NOCAS_47299	ph2	200	0	N	N
DTXSID2047276	CP-409092	194098-25-4	ph2	200	2	N	N
DTXSID3024869	Cumene hydroperoxide	80-15-9	ph2	200	0	N	N
DTXSID0022777	Celecoxib	169590-42-5	ph2	200	21	N	N
DTXSID3026726	Citronellol	106-22-9	ph2	200	1	N	N
DTXSID6022474	Corticosterone	50-22-6	ph2	200	2	N	N
DTXSID2020268	Chlorendic acid	115-28-6	ph2	200	4	N	N
DTXSID9022310	Daidzein	486-66-8	ph2	200	7	N	N
DTXSID6040111	Ethyl butyrate	105-54-4	ph2	200	-11	N	N
DTXSID1025017	Dicumyl peroxide	80-43-3	ph2	200	29	N	N
DTXSID7020392	Diallyl phthalate	131-17-9	ph2	200	22	N	N
DTXSID8020462	Diethylene glycol	111-46-6	ph2	200	10	N	N
DTXSID7024081	Endothal	145-73-3	ph2	200	20	N	N
DTXSID9020582	Ethoxyquin	91-53-2	ph2	200	29	N	N
DTXSID4020537	Diphenhydramine hydrochloride	147-24-0	ph2	200	19	N	N
DTXSID5024051	Diisopropyl methylphosphonate	1445-75-6	ph2	200	3	N	N
DTXSID2020505	Dimethylaminoethanol	108-01-0	ph2	200	14	N	N
DTXSID7021780	Diethyl phthalate	84-66-2	ph2	200	14	N	N
DTXSID6022000	Ethanolamine	141-43-5	ph2	200	7	N	N
DTXSID5025152	Dimethyl succinate	106-65-0	ph2	200	10	N	N
DTXSID4047258	Enadoline	124378-77-4	ph2	200	3	N	N
DTXSID0027983	Dipropylene glycol monomethyl ether	34590-94-8	ph2	200	4	N	N
DTXSID6020561	Endrin	72-20-8	ph2	200	11	N	N
DTXSID8025096	Dimethyl adipate	627-93-0	ph2	200	19	N	N

DTXSID2021993	Dibenzofuran	132-64-9	ph2	200	10	N	N
DTXSID8022959	Docusate sodium	577-11-7	ph2	200	94	Y	N
DTXSID5024055	Dimethyl sulfate	77-78-1	ph2	200	11	N	N
DTXSID6020480	Dimethoxane	828-00-2	ph2	200	0	N	N
DTXSID9022528	Ethylparaben	120-47-8	ph2	200	14	N	N
DTXSID4020375	Dichlorodiphenyltrichloroethane	50-29-3	ph2	200	23	Y	N
DTXSID3021932	Diethanolamine	111-42-2	ph2	200	0	N	N
DTXSID4047628	Dicyclohexyl disulfide	2550-40-5	ph2	200	24	N	N
DTXSID5027932	Dodecylbenzene sulfonate triethanolamine(1:1)	27323-41-7	ph2	180	57	Y	N
DTXSID1041847	Dibutyl decanedioate	109-43-3	ph2	200	4	N	N
DTXSID3020207	Dinoseb	88-85-7	ph2	200	8	N	N
DTXSID1024621	Diethylene glycol dimethyl ether	111-96-6	ph2	200	-2	N	N
DTXSID1023235	D-Mannitol	69-65-8	ph2	200	5	N	N
DTXSID9020453	Dieldrin	60-57-1	ph2	200	20	N	N
DTXSID8020597	Ethylene glycol	107-21-1	ph2	201	5	N	N
DTXSID6025068	Dihexyl phthalate	84-75-3	ph2	200	19	N	N
DTXSID7047277	Elzasonan	361343-19-3	ph2	200	7	N	N
DTXSID6048175	Difpas-pyrazole	151506-44-4	ph2	200	0	N	N
DTXSID9022522	Diisobutyl phthalate	84-69-5	ph2	200	12	N	N
DTXSID3024940	Dibromoacetonitrile	3252-43-5	ph2	200	-4	N	N
DTXSID8047395	Diisononyl cyclohexane-1,2-dicarboxylate	166412-78-8	ph2	200	10	N	N
DTXSID1024045	Diethyl sulfate	64-67-5	ph2	200	3	N	N
DTXSID1021956	Di-n-octyl phthalate	117-84-0	ph2	200	1	N	N
DTXSID0027856	Dipropylene glycol	25265-71-8	ph2	200	-5	N	N
DTXSID1020512	Dimethylcarbamoyl chloride	79-44-7	ph2	200	-3	N	N
DTXSID1040112	Ethyl heptanoate	106-30-9	ph2	200	2	N	N
DTXSID9036690	Diisobutyl adipate	141-04-8	ph2	200	3	N	N
DTXSID0026967	Diethylene glycol dibenzoate	120-55-8	ph2	200	8	N	N
DTXSID4029145	Dimethyl malonate	108-59-8	ph2	200	8	N	N

DTXSID0024052	Dimethipin	55290-64-7	ph2	200	-4	N	N
DTXSID2024955	Di-tert-butyl peroxide	110-05-4	ph2	105	-1	N	N
DTXSID6027923	Dodecylbenzenesulfonic acid	27176-87-0	ph2	200	88	Y	N
DTXSID3025122	Dimethyl glutarate	1119-40-0	ph2	200	2	N	N
DTXSID2038732	Diethyl butanedioate	123-25-1	ph2	200	-1	N	N
DTXSID0047537	Diethyl sebacate	2432-87-3	ph2	200	10	N	N
DTXSID2021866	Dibutyl adipate	105-99-7	ph2	200	3	N	N
DTXSID8037752	Diphenyl isophthalate	744-45-6	ph2	100	7	N	N
DTXSID7022174	EPN	2104-64-5	ph2	200	0	N	N
DTXSID4022367	Estrone	53-16-7	ph2	0.2	0	N	N
DTXSID0020498	Dimethyl terephthalate	120-61-6	ph2	200	1	N	N
DTXSID9032537	Didecyldimethylammonium chloride	7173-51-5	ph2	200	56	Y	N
DTXSID1021322	Disulfiram	97-77-8	ph2	200	-2	N	N
DTXSID3037208	Diclofenac sodium	15307-79-6	ph2	200	12	N	N
DTXSID4022991	Erythromycin	114-07-8	ph2	50	5	N	N
DTXSID2020428	Dichloroacetic acid	79-43-6	ph2	200	-5	N	N
DTXSID1027924	Diisodecyl hexanedioate	27178-16-1	ph2	200	5	N	N
DTXSID7026994	Dodecylbenzene	123-01-3	ph2	200	-1	N	N
DTXSID3020465	Diethylstilbestrol	56-53-1	ph2	0.2	14	N	N
DTXSID1026900	Dodecyltrimethylammonium chloride	112-00-5	ph2	200	3	Y	N
DTXSID2024086	Ethion	563-12-2	ph2	200	8	N	N
DTXSID5031131	Dipentyl phthalate	131-18-0	ph2	200	19	N	N
DTXSID3025049	Diethylene glycol monomethyl ether	111-77-3	ph2	200	8	N	N
DTXSID3047394	Grinstad Soft-N-Safe	NOCAS_47394	ph2	200 µg/ml	13	N	N
DTXSID9020663	Glycerol	56-81-5	ph2	200	10	N	N
DTXSID6025486	Isoproterenol hydrochloride	51-30-9	ph2	200	14	N	N
DTXSID5020863	Methyl dopa sesquihydrate	41372-08-1	ph2	200	1	N	N
DTXSID7020716	Hydroquinone	123-31-9	ph2	200	16	N	N
DTXSID1048174	FR167356	174185-16-1	ph2	200	31	Y	N
DTXSID5020653	Gentian Violet	548-62-9	ph2	200	19	Y	N

DTXSID1024126	Heptachlor epoxide B	1024-57-3	ph2	200	24	N	N
DTXSID7022413	Isoeugenol	97-54-1	ph2	200	10	N	N
DTXSID8020759	Isophorone	78-59-1	ph2	200	4	N	N
DTXSID2020713	Hydrochlorothiazide	58-93-5	ph2	200	6	N	N
DTXSID0023826	Isophorone diisocyanate	4098-71-9	ph2	200	5	N	N
DTXSID2020688	Hexachlorocyclopentadiene	77-47-4	ph2	200	6	N	N
DTXSID5047249	Fandosentan potassium salt	221246-12-4	ph2	100	12	N	N
DTXSID5027982	Hexanedioic acid, diisononyl ester	33703-08-1	ph2	200	5	N	N
DTXSID7047356	Ilepatril	473289-62-2	ph2	200	13	N	N
DTXSID8027955	Isooctyl acrylate	29590-42-9	ph2	200	4	Y	N
DTXSID3024104	Fluoranthene	206-44-0	ph2	200	15	N	N
DTXSID3025469	Isopentyl alcohol	123-51-3	ph2	200	7	N	N
DTXSID9032610	Etofenprox	80844-07-1	ph2	200	4	N	N
DTXSID7044928	Isopropyl triethanolamine titanate	36673-16-2	ph2	200	23	N	N
DTXSID3020627	Fluconazole	86386-73-4	ph2	200	3	N	N
DTXSID8025337	Formamide	75-12-7	ph2	200	5	N	N
DTXSID1048170	FR150011	149413-74-1	ph2	200	63	Y	N
DTXSID1020770	Kepone	143-50-0	ph2	200	56	Y	N
DTXSID4022369	Fulvestrant	129453-61-8	ph2	200	6	N	N
DTXSID7021605	Hexanedioic acid	124-04-9	ph2	200	-10	N	N
DTXSID7024112	Fomesafen	72178-02-0	ph2	200	5	N	N
DTXSID3020679	Heptachlor	76-44-8	ph2	200	35	N	N
DTXSID3032620	Hexaflumuron	86479-06-3	ph2	200	5	N	N
DTXSID9020617	Eugenol	97-53-0	ph2	200	7	N	N
DTXSID6025355	Glutaraldehyde	111-30-8	ph2	200	48	N	N
DTXSID2048167	FR900409	138472-01-2	ph2	200	-1	N	N
DTXSID9047338	HMR1426	262376-75-0	ph2	200	13	N	N
DTXSID9020740	Indomethacin	53-86-1	ph2	200	9	N	N
DTXSID1044643	Glycidyl trimethylammonium chloride	3033-77-0	ph2	200	0	N	N
DTXSID6021456	FD&C Yellow 6	2783-94-0	ph2	200	6	N	N
DTXSID2021600	Heptanoic acid	111-14-8	ph2	200	-3	N	N

DTXSID0047539	Hexane-1,6-diyl dibenzoate	22915-73-7	ph2	200	0	N	N
DTXSID1047312	GSK232420A	864283-48-7	ph2	200	7	N	N
DTXSID3042059	Isopentyl butyrate	106-27-4	ph2	200	-9	N	N
DTXSID7032004	Flutamide	13311-84-7	ph2	200	7	N	N
DTXSID8020755	Isoniazid	54-85-3	ph2	200	-11	N	N
DTXSID0020654	Geranyl acetate	105-87-3	ph2	200	-5	N	N
DTXSID8033562	Hydroxyflutamide	52806-53-8	ph2	200	-4	N	N
DTXSID4020666	Glycidol	556-52-5	ph2	200	-5	N	N
DTXSID6047313	GW473178E methyl benzene sulphonic acid	263553-33-9	ph2	135	-13	N	N
DTXSID8024107	Fluridone	59756-60-4	ph2	200	14	N	N
DTXSID7021607	Hexanoic acid	142-62-1	ph2	200	1	N	N
DTXSID7048168	Fabesetron hydrochloride	129299-90-7	ph2	178	7	N	N
DTXSID0022519	Folic acid	59-30-3	ph2	200	-4	N	N
DTXSID1021455	FD&C Yellow 5	1934-21-0	ph2	200	-3	N	N
DTXSID1048178	FR130739	136042-19-8	ph2	200	13	N	N
DTXSID2029874	Fenofibrate	49562-28-9	ph2	200	0	N	N
DTXSID6025438	Hydroxyurea	127-07-1	ph2	200	5	N	N
DTXSID0027195	Hexadecane	544-76-3	ph2	200	-12	N	N
DTXSID7029879	Ketoconazole	65277-42-1	ph2	200	21	N	N
DTXSID3021936	Hexanedinitrile	111-69-3	ph2	200	-10	N	N
DTXSID6040371	Fenaminosulf	140-56-7	ph2	200	64	Y	N
DTXSID4034150	Haloperidol	52-86-8	ph2	200	6	N	N
DTXSID5023825	Indium arsenide	1303-11-3	ph2	200	-1	N	N
DTXSID8024105	Fluorene	86-73-7	ph2	200	7	N	N
DTXSID3048522	HMR1171 trifluoroacetate (1:1)	NOCAS_48522	ph2	76	7	N	N
DTXSID8026727	Geraniol	106-24-1	ph2	200	6	N	N
DTXSID8024157	Isopropalin	33820-53-0	ph2	200	7	N	N
DTXSID6048171	FR145237	146011-65-6	ph2	177	10	N	N
DTXSID2020189	FD&C Blue No. 1	3844-45-9	ph2	200	29	Y	N
DTXSID4047252	Ingliforib	186392-65-4	ph2	200	19	N	N

DTXSID2036299	N,N-Dimethyloctylamine	7378-99-6	ph2	200	8	N	N
DTXSID9027441	Octabenzene	1843-05-6	ph2	200	0	N	N
DTXSID9047334	MK-968	NOCAS_47334	ph2	200	9	N	N
DTXSID6020856	N-Methyl-2-pyrrolidone	872-50-4	ph2	200	2	N	N
DTXSID4047331	MK-547	331623-06-4	ph2	200	9	N	N
DTXSID5047328	MK-274	NOCAS_47328	ph2	200	40	N	N
DTXSID8021800	N,N-Diethylaniline	91-66-7	ph2	200	3	N	N
DTXSID7025895	N-Phenyl-1,4-benzenediamine	101-54-2	ph2	200	10	N	N
DTXSID4022529	Methylparaben	99-76-3	ph2	200	3	N	N
DTXSID6025567	Methyl 2-aminobenzoate	134-20-3	ph2	200	-3	N	N
DTXSID2021026	N-Nitrosodibutylamine	924-16-3	ph2	200	3	N	N
DTXSID5020944	Nitrofurazone	59-87-0	ph2	200	62	Y	N
DTXSID8020913	Naphthalene	91-20-3	ph2	200	-8	N	N
DTXSID0021832	N,N,4-Trimethylaniline	99-97-8	ph2	200	-6	N	N
DTXSID2021028	N-Nitrosodiethylamine	55-18-5	ph2	200	7	N	N
DTXSID3036496	Levonorgestrel	797-63-7	ph2	200	-1	N	N
DTXSID4020820	Methimazole	60-56-0	ph2	200	0	N	N
DTXSID3020964	Nitrobenzene	98-95-3	ph2	200	8	N	N
DTXSID7020895	Mirex	2385-85-5	ph2	200	0	N	N
DTXSID2020894	Michler's ketone	90-94-8	ph2	200	2	N	N
DTXSID7042190	N,N-Dimethyldecylamine oxide	2605-79-0	ph2	200	-8	N	N
DTXSID7020972	Nitrofurantoin	67-20-9	ph2	200	48	N	N
DTXSID8023632	L-Tartaric acid	87-69-4	ph2	200	3	N	N
DTXSID5020784	Lovastatin	75330-75-5	ph2	200	0	N	N
DTXSID0047327	MK-578	313994-79-5	ph2	200	-4	N	N
DTXSID6025692	Myrcene	123-35-3	ph2	200	2	N	N
DTXSID5025659	Methyl salicylate	119-36-8	ph2	200	-1	N	N
DTXSID4047335	MK-812	851916-42-2	ph2	150	0	N	N
DTXSID2022381	meso-Hexestrol	84-16-2	ph2	0.2	-1	N	N
DTXSID0020311	Monuron	150-68-5	ph2	200	10	N	N
DTXSID6021030	N-Nitrosodiphenylamine	86-30-6	ph2	200	-3	N	N

DTXSID9043938	Monobenzyl phthalate	2528-16-7	ph2	200	-2	N	N
DTXSID9023380	Norethindrone	68-22-4	ph2	200	-3	N	N
DTXSID6022345	o,p'-DDT	789-02-6	ph2	200	8	N	N
DTXSID1032646	N-Ethylperfluorooctanesulfonamide	4151-50-2	ph2	200	5	N	N
DTXSID1020930	Nicotine	54-11-5	ph2	200	2	N	N
DTXSID7021029	N-Nitrosodimethylamine	62-75-9	ph2	200	-4	N	N
DTXSID5020811	Mercuric chloride	7487-94-7	ph2	200	2	N	N
DTXSID6021032	N-Nitrosodipropylamine	621-64-7	ph2	200	1	N	N
DTXSID8029600	Methacrylamide	79-39-0	ph2	200	-8	N	N
DTXSID5021837	N,N-Diethylethanolamine	100-37-8	ph2	200	-1	N	N
DTXSID3034165	Nilutamide	63612-50-0	ph2	200	5	N	N
DTXSID0047167	N-Methylacetamide	79-16-3	ph2	200	5	N	N
DTXSID3021641	Nonanoic acid	112-05-0	ph2	200	-3	N	N
DTXSID2020507	N,N-Dimethylaniline	121-69-7	ph2	207	-4	N	N
DTXSID5025607	Methyleugenol	93-15-2	ph2	200	-9	N	N
DTXSID5026889	Methyl dodecanoate	111-82-0	ph2	200	3	N	N
DTXSID7020845	Methyl methanesulfonate	66-27-3	ph2	200	-10	N	N
DTXSID9042209	N-Methyldioctylamine	4455-26-9	ph2	100	2	N	N
DTXSID2021440	N-Vinyl-2-pyrrolidone	88-12-0	ph2	200	2	N	N
DTXSID1020932	Nicotinic acid	59-67-6	ph2	200	0	N	N
DTXSID1025271	N-Ethylaniline	103-69-5	ph2	200	0	N	N
DTXSID2026864	Methyl octanoate	111-11-5	ph2	200	2	N	N
DTXSID5023322	Mifepristone	84371-65-3	ph2	200	5	N	N
DTXSID4042121	Mepanipyrim	110235-47-7	ph2	200	-2	Y	N
DTXSID0027640	Malic acid	6915-15-7	ph2	200	-1	N	N
DTXSID4021848	N-Ethyl-3-methylaniline	102-27-2	ph2	200	3	N	N
DTXSID9026689	N,N,Nâ€²,Nâ€²-Tetrakis(2-hydroxypropyl)ethylenediamine	102-60-3	ph2	200	-2	N	N
DTXSID7020970	Nitrofen	1836-75-5	ph2	200	-2	N	N
DTXSID0025523	Maltol	118-71-8	ph2	208	-1	N	N
DTXSID8025595	N,N'-Methylenebisacrylamide	110-26-9	ph2	200	6	N	N

DTXSID7047358	Nelivaptan	439687-69-1	ph2	185	3	N	N
DTXSID8021808	o-Cresol	95-48-7	ph2	200	-1	N	N
DTXSID5021419	l-Tryptophan	73-22-3	ph2	200	5	N	N
DTXSID6020692	Methenamine	100-97-0	ph2	204	-3	N	N
DTXSID4020822	Methotrexate	59-05-2	ph2	200	4	N	N
DTXSID6020939	Nitrilotriacetic acid	139-13-9	ph2	183	4	N	N
DTXSID0021125	Phenolphthalein	77-09-8	ph2	200	8	N	N
DTXSID9048514	PharmaGSID_48514	NOCAS_48514	ph2	200	1	N	N
DTXSID4047333	PharmaGSID_47333	NOCAS_47333	ph2	200	0	N	N
DTXSID3037707	Potassium perfluorobutanesulfonate	29420-49-3	ph2	200	-1	N	N
DTXSID6024254	Phenanthrene	85-01-8	ph2	200	6	N	N
DTXSID7027205	Octamethylcyclotetrasiloxane	556-67-2	ph2	200	0	N	N
DTXSID2047307	PD-0333941	501027-49-2	ph2	200	4	N	N
DTXSID4032459	Phorate	298-02-2	ph2	200	1	N	N
DTXSID3029289	Oxazolidine-E	7747-35-5	ph2	200	1	N	N
DTXSID7041097	PK 11195	85532-75-8	ph2	50	0	N	N
DTXSID5047538	Pentane-1,5-diyl dibenzoate	6624-73-3	ph2	200	2	N	N
DTXSID7048166	3,9-Epoxy-3H-azirino[2,3-c][1]benzazocine-5-carboxaldehyde, 1-acetyl-9-(acetyloxy)-8-[[[(aminocarbonyl)oxy]methyl]-1,1a,2,8,9,9a-hexahydro-7-methoxy-, (1aS,8R,9S,9aS)-	NOCAS_48166	ph2	200	-3	N	N
DTXSID9047330	PharmaGSID_47330	NOCAS_47330	ph2	200	-1	N	N
DTXSID6027268	Pentadecane	629-62-9	ph2	200	1	N	N
DTXSID1025805	Octhilinone	26530-20-1	ph2	208	21	N	N
DTXSID0047292	PD 0200347	NOCAS_47292	ph2	200	-2	N	N
DTXSID7021653	Pentanal	110-62-3	ph2	200	1	N	N
DTXSID4048519	PharmaGSID_48519	686756-87-6	ph2	200	2	N	N
DTXSID7021150	Phenylmercuric acetate	62-38-4	ph2	200	1	N	N
DTXSID3026645	p-Cymene	99-87-6	ph2	200	0	N	N
DTXSID0048505	PharmaGSID_48505	NOCAS_48505	ph2	200	0	N	N

DTXSID5021097	Oxytetracycline hydrochloride	2058-46-0	ph2	200	-2	N	N
DTXSID8023927	p-Bromodiphenyl ether	101-55-3	ph2	200	4	N	N
DTXSID1027263	Pentyl acetate	628-63-7	ph2	200	-6	N	N
DTXSID7047271	PD 0343701	676116-04-4	ph2	200	5	N	N
DTXSID5048506	PharmaGSID_48506	588941-45-1	ph2	200	0	N	N
DTXSID9048516	PharmaGSID_48516	NOCAS_48516	ph2	200	2	N	N
DTXSID1021164	Piperazine	110-85-0	ph2	200	0	N	N
DTXSID4048511	PharmaGSID_48511	1062243-51-9	ph2	186	0	N	N
DTXSID3047263	PharmaGSID_47263	349495-42-7	ph2	200	-3	N	N
DTXSID8047553	Perfluoroundecanoic acid	2058-94-8	ph2	200	27	Y	N
DTXSID8031863	Perfluorononanoic acid	375-95-1	ph2	200	13	N	N
DTXSID4047337	PharmaGSID_47337	1061517-62-1	ph2	200	57	Y	N
DTXSID0048509	PharmaGSID_48509	NOCAS_48509	ph2	200	0	N	N
DTXSID1048172	PharmaGSID_48172	NOCAS_48172	ph2	159	0	N	N
DTXSID9048518	PharmaGSID_48518	NOCAS_48518	ph2	200	2	N	N
DTXSID7021106	Pentachlorophenol	87-86-5	ph2	102	8	N	N
DTXSID4020373	p,p'-DDD	72-54-8	ph2	200	5	N	N
DTXSID3031862	Perfluorohexanoic acid	307-24-4	ph2	200	3	N	N
DTXSID5021126	Phenothiazine	92-84-2	ph2	200	2	N	N
DTXSID4040713	Octyl gallate	1034-01-1	ph2	200	49	Y	N
DTXSID3037709	Potassium perfluorohexanesulfonate	3871-99-6	ph2	200	5	N	N
DTXSID3021643	Octanal	124-13-0	ph2	200	3	N	N
DTXSID5023796	Pentamidine isethionate	140-64-7	ph2	175	7	N	N
DTXSID3044203	Pioglitazone hydrochloride	112529-15-4	ph2	200	-1	N	N
DTXSID8021642	Octadecanoic acid	57-11-4	ph2	100	-1	N	N
DTXSID9027522	Octrizole	3147-75-9	ph2	200	9	N	N
DTXSID1047285	PHA-00568487	527680-56-4	ph2	200	-3	N	N
DTXSID9020374	p,p'-DDE	72-55-9	ph2	200	9	N	N
DTXSID3038939	Perfluorooctanesulfonamide	754-91-6	ph2	200	13	N	N
DTXSID0048507	PharmaGSID_48507	NOCAS_48507	ph2	200	1	N	N
DTXSID5024261	Phosmet	732-11-6	ph2	200	3	N	N

DTXSID2026943	Pentaerythritol	115-77-5	ph2	200	4	N	N
DTXSID4020290	Pirinixic acid	50892-23-4	ph2	200	6	N	N
DTXSID5022439	Phenolphthalin	81-90-3	ph2	200	2	N	N
DTXSID3031860	Perfluorodecanoic acid	335-76-2	ph2	200	45	Y	N
DTXSID5021124	Phenol	108-95-2	ph2	200	1	N	N
DTXSID1037303	Perfluoroheptanoic acid	375-85-9	ph2	200	8	N	N
DTXSID2022179	Pentachloropyridine	2176-62-7	ph2	200	1	N	N
DTXSID3021645	Octanoic acid	124-07-2	ph2	200	-1	N	N
DTXSID9048510	PharmaGSID_48510	460081-99-6	ph2	200	3	N	N
DTXSID3048520	Piragliatin	625114-41-2	ph2	50	4	N	N
DTXSID9047542	Picoxystrobin	117428-22-5	ph2	200	3	N	N
DTXSID8048521	PharmaGSID_48521	1191914-21-2	ph2	180	4	N	N
DTXSID9020164	Pentaerythritol dibromide	3296-90-0	ph2	200	1	N	N
DTXSID4048513	PharmaGSID_48513	825643-57-0	ph2	163	12	N	N
DTXSID6047284	PHA-00543613	478149-53-0	ph2	200	3	N	N
DTXSID7021869	p-Cresol	106-44-5	ph2	200	2	N	N
DTXSID8020121	Sodium azide	26628-22-8	ph2	200	4	N	N
DTXSID5021201	Propyl gallate	121-79-9	ph2	200	10	N	N
DTXSID7021992	Sodium saccharin hydrate	82385-42-0	ph2	200	5	N	N
DTXSID4047339	SR144190	181640-09-5	ph2	173	1	N	N
DTXSID5047324	SB281832	219790-72-4	ph2	200	13	N	N
DTXSID0021254	Safrole	94-59-7	ph2	200	5	N	N
DTXSID6047369	SR146131 trifluoroacetate (1:1)	221671-62-1	ph2	200	15	N	N
DTXSID6027050	Sodium dimethyldithiocarbamate	128-04-1	ph2	200	5	N	N
DTXSID4047387	SAR102779	NOCAS_47387	ph2	200	16	N	N
DTXSID0020941	Sodium nitrite	7632-00-0	ph2	200	3	N	N
DTXSID1023819	Stavudine	3056-17-5	ph2	200	-1	N	N
DTXSID3026302	Sodium xylenesulfonate	1300-72-7	ph2	200	1	N	N
DTXSID3042390	Sodium (2-pyridylthio)-N-oxide	3811-73-2	ph2	200	-1	N	N
DTXSID5047322	SB243213A	200940-23-4	ph2	184	5	N	N
DTXSID4021185	Prednisone	53-03-2	ph2	200	4	N	N

DTXSID0020105	Sodium L-ascorbate	134-03-2	ph2	200	1	N	N
DTXSID6034186	Spirolactone	52-01-7	ph2	200	5	N	N
DTXSID4021218	Quercetin	117-39-5	ph2	200	15	N	N
DTXSID2047353	SSR 241586 HCl	NOCAS_47353	ph2	80	8	N	N
DTXSID3047342	SR125047	NOCAS_47342	ph2	181	31	N	N
DTXSID1047366	SAR115740	NOCAS_47366	ph2	200	5	N	N
DTXSID6034924	Sodium trichloroacetate	650-51-1	ph2	200	-3	N	N
DTXSID3042219	Propylbenzene	103-65-1	ph2	200	-3	N	N
DTXSID4047389	SAR 150640	433212-21-6	ph2	200	11	N	N
DTXSID3027320	Sodium 4-nitrophenolate	824-78-2	ph2	200	-2	N	N
DTXSID8047341	SSR146977	264618-44-2	ph2	50	9	N	N
DTXSID3047348	SSR504734	742693-38-5	ph2	200	11	N	N
DTXSID1026031	Sodium dodecyl sulfate	151-21-3	ph2	200	58	Y	N
DTXSID2021238	Resorcinol	108-46-3	ph2	200	0	N	N
DTXSID8047391	SAR102608	1068967-96-3	ph2	200	1	N	N
DTXSID4042416	Sodium myristyl sulfate	1191-50-0	ph2	200	82	Y	N
DTXSID1034181	Raloxifene hydrochloride	82640-04-8	ph2	200	3	N	N
DTXSID8037706	Potassium perfluorooctanesulfonate	2795-39-3	ph2	200	36	N	N
DTXSID9033923	Procymidone	32809-16-8	ph2	200	6	N	N
DTXSID1029677	Silica	7631-86-9	ph2	200	-2	N	N
DTXSID1047360	SR58611	929601-09-2	ph2	183	6	N	N
DTXSID2047359	SSR180711	298198-52-4	ph2	200	-2	N	N
DTXSID0047325	SB413217A	NOCAS_47325	ph2	93	1	N	N
DTXSID2021286	Styrene oxide	96-09-3	ph2	200	-1	N	N
DTXSID0023581	Simvastatin	79902-63-9	ph2	200	4	N	N
DTXSID1047362	SSR150106	NOCAS_47362	ph2	200	9	N	N
DTXSID7025219	Sodium dodecylbenzenesulfonate	25155-30-0	ph2	200	90	Y	N
DTXSID0047379	SSR126768	NOCAS_47379	ph2	200	2	N	N
DTXSID1020140	Sodium benzoate	532-32-1	ph2	200	-1	N	N
DTXSID9048512	Ro 23-7637	107071-66-9	ph2	183	2	N	N
DTXSID2047351	SSR 240612	464930-42-5	ph2	133	6	N	N

DTXSID3023556	Retinol	68-26-8	ph2	209	3	N	N
DTXSID1021798	Quinoline	91-22-5	ph2	200	-3	N	N
DTXSID7021237	Reserpine	50-55-5	ph2	103	-4	N	N
DTXSID7026029	Sodium dehydroacetate	4418-26-2	ph2	200	-4	N	N
DTXSID8021272	Sodium chlorite	7758-19-2	ph2	200	-6	N	N
DTXSID8047347	SR271425	155990-20-8	ph2	200	10	N	N
DTXSID6047525	Pravastatin sodium	81131-70-6	ph2	100	2	N	N
DTXSID5020570	Sodium erythorbate (1:1)	6381-77-7	ph2	200	1	N	N
DTXSID1047318	SB202235	139149-55-6	ph2	200	3	N	N
DTXSID0042400	Sodium hexyldecyl sulfate	1120-01-0	ph2	100	58	Y	N
DTXSID5047374	SSR161421	NOCAS_47374	ph2	200	6	N	N
DTXSID6027397	Sorbitan, mono-(9Z)-9-octadecenoate	1338-43-8	ph2	200	10	N	N
DTXSID4022527	Propylparaben	94-13-3	ph2	200	4	N	N
DTXSID4023541	Pyridoxine	65-23-6	ph2	200	-6	N	N
DTXSID3047346	SSR162369	NOCAS_47346	ph2	200	7	N	N
DTXSID1047368	SSR69071	344930-95-6	ph2	50	-3	N	N
DTXSID4047385	SAR377142	NOCAS_47385	ph2	200	-1	N	N
DTXSID9021217	Pyrimethamine	58-14-0	ph2	200	1	N	N
DTXSID1047364	SSR 103800	1075752-90-7	ph2	185	9	N	N
DTXSID3024289	Pyrene	129-00-0	ph2	200	7	N	N
DTXSID3022370	Progesterone	57-83-0	ph2	200	1	N	N
DTXSID6021244	Rifampicin	13292-46-1	ph2	200	9	N	N
DTXSID1021952	Triphenyl phosphate	115-86-6	ph2	200	3	N	N
DTXSID3047138	tert-Butylbenzene	98-06-6	ph2	200	1	N	N
DTXSID0047533	Trioctyl trimellitate	89-04-3	ph2	202	-1	N	N
DTXSID4021393	Triethylene glycol	112-27-6	ph2	200	1	N	N
DTXSID8023719	Troglitazone	97322-87-7	ph2	200	53	Y	N
DTXSID5028033	Triisononyl trimellitate	53894-23-8	ph2	200	3	N	N
DTXSID9032113	Tebuconazole	107534-96-3	ph2	200	3	N	N
DTXSID3021358	Tolazamide	1156-19-0	ph2	200	-1	N	N
DTXSID2021288	Sucrose	57-50-1	ph2	200	1	N	N

DTXSID8026224	Triethylene glycol dimethyl ether	112-49-2	ph2	200	-2	N	N
DTXSID3026223	Triethylene glycol diacetate	111-21-7	ph2	200	-1	N	N
DTXSID1021378	Trichloroacetic acid	76-03-9	ph2	200	0	N	N
DTXSID1047287	UK-333747	197077-55-7	ph2	200	1	N	N
DTXSID3026564	Triethylene glycol bis(2-ethylhexanoate)	94-28-0	ph2	200	3	N	N
DTXSID5047295	UK-373911	291305-06-1	ph2	200	10	N	N
DTXSID2047355	Trelanserlin	189003-92-7	ph2	200	-1	N	N
DTXSID7023645	Tetracycline	60-54-8	ph2	200	4	N	N
DTXSID2045232	Tiratricol	51-24-1	ph2	200	26	N	N
DTXSID1040742	Triamcinolone	124-94-7	ph2	200	1	N	N
DTXSID4021426	Urea	57-13-6	ph2	200	-1	N	N
DTXSID0040701	Triethyl citrate	77-93-0	ph2	200	1	N	N
DTXSID9026261	Tris(1,3-dichloro-2-propyl) phosphate	13674-87-8	ph2	200	2	N	N
DTXSID9036515	Testosterone propionate	57-85-2	ph2	200	8	N	N
DTXSID4027608	Terbutylazine	5915-41-3	ph2	200	3	N	N
DTXSID2047357	Surinabant	288104-79-0	ph2	200	0	N	N
DTXSID3021986	Tributyl phosphate	126-73-8	ph2	200	0	N	N
DTXSID3027403	Tributyltin chloride	1461-22-9	ph2	200	4	N	N
DTXSID9021427	Urethane	51-79-6	ph2	200	4	N	N
DTXSID0026252	Triphenyl phosphite	101-02-0	ph2	200	0	N	N
DTXSID5021336	Theophylline	58-55-9	ph2	200	-1	N	N
DTXSID1034187	Tamoxifen	10540-29-1	ph2	100	25	Y	N
DTXSID2026076	Tannic acid	1401-55-4	ph2	70	92	Y	N
DTXSID9021689	Undecane	1120-21-4	ph2	200	-5	N	N
DTXSID4026262	Triglycidyl isocyanurate	2451-62-9	ph2	200	-1	N	N
DTXSID9021392	Triethanolamine	102-71-6	ph2	200	2	N	N
DTXSID9024699	tert-Butyl perbenzoate	614-45-9	ph2	200	4	N	N
DTXSID7024376	Vernolate	1929-77-7	ph2	200	0	N	N
DTXSID2047309	UK-156819	162706-14-1	ph2	200	3	N	N
DTXSID0021256	Sulfasalazine	599-79-1	ph2	200	0	N	N

DTXSID5023742	Warfarin	81-81-2	ph2	200	2	N	N
DTXSID6047288	UK-337312	203942-49-8	ph2	200	57	Y	N
DTXSID7026156	Toluene-2,4-diisocyanate	584-84-9	ph2	200	-2	N	N
DTXSID3041376	Tridemorph	24602-86-6	ph2	200	4	N	N
DTXSID5047320	SB236057A	180084-01-9	ph2	200	6	N	N
DTXSID4026183	Tributylamine	102-82-9	ph2	200	1	N	N
DTXSID2029246	Triethoxyoctylsilane	2943-75-1	ph2	200	-3	N	N
DTXSID5048186	Tetrac	67-30-1	ph2	22	-1	N	N
DTXSID8021301	Tamoxifen citrate	54965-24-1	ph2	183	46	Y	N
DTXSID0041141	o-(Chloroacetylcarbamoyl)fumagillol	129298-91-5	ph2	64	1	N	N
DTXSID3042423	Sucrose octaacetate	126-14-7	ph2	151	-1	N	N
DTXSID6034972	Thymol	89-83-8	ph2	200	-1	N	N
DTXSID9026265	Tris(2-ethylhexyl) trimellitate	3319-31-1	ph2	200	-1	N	N
DTXSID6047311	GSK163929B	NOCAS_47311	ph2	200	4	N	N
DTXSID4026214	Triclocarban	101-20-2	ph2	200	-1	N	N
DTXSID0047290	UK-416244	402910-27-4	ph2	200	2	N	N
DTXSID2022254	Terbufos	13071-79-9	ph2	200	3	N	N
DTXSID3026691	Triacetin	102-76-1	ph2	200	1	N	N
DTXSID9022524	Thalidomide	50-35-1	ph2	200	-1	N	N
DTXSID6020220	tert-Butylhydroquinone	1948-33-0	ph2	200	5	N	N
DTXSID6047363	Volinanserin	139290-65-6	ph2	200	2	N	N
DTXSID5021411	Tris(2-chloroethyl) phosphate	115-96-8	ph2	200	1	N	N
DTXSID1047289	UK-343664	215297-27-1	ph2	100	1	N	N
DTXSID2029329	Tripropylene glycol monomethyl ether	25498-49-1	ph2	200	3	N	N
DTXSID9026132	Theobromine	83-67-0	ph2	84	3	N	N
DTXSID9035204	Tributyltin methacrylate	2155-70-6	ph2	200	7	N	N
DTXSID6023733	Valproic acid	99-66-1	ph2	200	1	N	N
DTXSID0021414	Tris(2-ethylhexyl) phosphate	78-42-2	ph2	200	3	N	N
DTXSID2031089	D&C Red 27	13473-26-2	ph3	132	78	Y	N
DTXSID9034737	Metiram	9006-42-2	ph3	60	11	N	N
DTXSID9023209	L-Dopa	59-92-7	ph3	50	-1	N	N

DTXSID8047896	Enzacamene	36861-47-9	ph3	200	10	N	N
DTXSID7021784	Salicylanilide	87-17-2	ph3	200	0	Y	N
DTXSID5052832	2,2',3,4',5,5',6-Heptachloro-1,1'-biphenyl	52663-68-0	ph3	125	15	N	N
DTXSID6021290	Sulfamethazine	57-68-1	ph3	200	0	N	N
DTXSID5044811	Chlordimeform hydrochloride	19750-95-9	ph3	200	-2	N	N
DTXSID4031980	Resveratrol	501-36-0	ph3	200	5	N	N
DTXSID4040767	3,5-Dichlorosalicyl-3,4-dichloroanilide	1154-59-2	ph3	200	78	Y	N
DTXSID3047003	Potassium perchlorate	7778-74-7	ph3	208	12	N	N
DTXSID4024515	Ammonium perchlorate	7790-98-9	ph3	200	-5	N	N
DTXSID3041403	2-Chloro-1,4-dimethoxybenzene	2100-42-7	ph3	200	2	N	N
DTXSID3040300	4-Chlorobiphenyl	2051-62-9	ph3	200	7	N	N
DTXSID3034903	Sodium bromide	7647-15-6	ph3	200	2	N	N
DTXSID0041985	Fluorosalan	4776-06-1	ph3	200	54	Y	N
DTXSID0027014	2-Octanol	123-96-6	e1k	200	5	N	N
DTXSID0034229	gamma-Nonanolactone	104-61-0	e1k	200	2	N	N
DTXSID0020151	Benzyl acetate	140-11-4	e1k	200	-3	N	N
DTXSID0029133	4-Hydroxyacetophenone	99-93-4	e1k	200	1	N	N
DTXSID0029761	Sodium dichloro-s-triazinetriene dihydrate	51580-86-0	e1k	200	6	N	N
DTXSID0024553	Azodicarbonamide	123-77-3	e1k	200	-2	N	N
DTXSID0023296	Methylene blue	61-73-4	e1k	200	54	Y	N
DTXSID0021175	Polysorbate 80	9005-65-6	e1k	179	10	N	N
DTXSID0034518	Desmedipham	13684-56-5	e1k	200	5	N	N
DTXSID0021888	2-Pentanone	107-87-9	e1k	200	2	N	N
DTXSID0025234	Eosin	17372-87-1	e1k	193	96	Y	N
DTXSID0020737	Indole	120-72-9	e1k	200	6	N	N
DTXSID0032316	4-Chloro-3,5-dimethylphenol	88-04-0	e1k	200	7	N	N
DTXSID0026171	Tolyltriazole	29385-43-1	e1k	200	-2	N	N
DTXSID0029210	Butyltin trichloride	1118-46-3	e1k	200	6	N	N
DTXSID0029214	Methylionone	1335-46-2	e1k	200	5	N	N

DTXSID0029848	Acetic acid, C8-10-branched alkyl esters, C9-rich	108419-33-6	e1k	200	4	N	N
DTXSID0020076	Amitrole	61-82-5	e1k	200	-2	N	N
DTXSID0027721	4-(2-Phenylpropan-2-yl)-N-[4-(2-phenylpropan-2-yl)phenyl]aniline	10081-67-1	e1k	200	11	N	N
DTXSID0038700	2-Methoxy-4-nitroaniline	97-52-9	e1k	200	10	N	N
DTXSID0023113	2-Methoxyphenol	90-05-1	e1k	201	6	N	N
DTXSID0035160	alpha-Ionone	127-41-3	e1k	200	1	N	N
DTXSID0020107	Aspartame	22839-47-0	e1k	200	2	N	N
DTXSID0041357	Ethyl (2E,4Z)-deca-2,4-dienoate	3025-30-7	e1k	207	6	N	N
DTXSID0022480	3-Ethylphenol	620-17-7	e1k	205	-1	N	N
DTXSID0038887	Fluorescein	2321-07-5	e1k	200	3	Y	N
DTXSID0025101	3-Dimethylaminophenol	99-07-0	e1k	200	7	N	N
DTXSID0026258	Tris(2-chloroethyl) phosphite	140-08-9	e1k	200	10	N	N
DTXSID0042406	Sodium methyl sulfate	512-42-5	e1k	200	1	N	N
DTXSID0027222	Terpinolene	586-62-9	e1k	200	0	N	N
DTXSID0041567	(9Z,12R)-12-Hydroxyoctadec-9-enoic acid	141-22-0	e1k	200	11	N	N
DTXSID0037730	1,4-Dihydroxy-2-naphthoic acid	31519-22-9	e1k	200	37	N	N
DTXSID0042167	Monopotassium phthalate	877-24-7	e1k	205	-2	N	N
DTXSID0021460	Zearalenone	17924-92-4	e1k	200	8	N	N
DTXSID0020656	Gibberellic acid	77-06-5	e1k	200	0	N	N
DTXSID0023745	D-Xylose	58-86-6	e1k	200	-1	N	N
DTXSID0027191	1,3-Cyclopentadiene	542-92-7	e1k	200	4	N	N
DTXSID0034722	Topramezone	210631-68-8	e1k	86	0	N	N
DTXSID0038881	C.I. Acid Orange 7	633-96-5	e1k	100	8	N	N
DTXSID0025864	4-Ethoxyaniline	156-43-4	e1k	200	2	N	N
DTXSID0025816	Oxalic acid	144-62-7	e1k	200	5	N	N
DTXSID0042454	Tetradecanoic acid, 2,3-dihydroxypropyl ester	589-68-4	e1k	200	13	Y	N
DTXSID0035748	Chloroallyl methenamine chloride	51229-78-8	e1k	200	3	N	N
DTXSID0022353	2-Chloro-4-phenylphenol	92-04-6	e1k	200	24	N	N

DTXSID0020575	Estragole	140-67-0	e1k	200	1	N	N
DTXSID0042379	Dimethoxydimethylsilane	1112-39-6	e1k	200	-1	N	N
DTXSID0021597	Heptanal	111-71-7	e1k	200	37	N	N
DTXSID0047957	Octylparaben	1219-38-1	e1k	200	82	Y	N
DTXSID0020286	3-Chloro-4-methylaniline	95-74-9	e1k	207	0	N	N
DTXSID0041981	Fluoroacetic acid	144-49-0	e1k	200	-2	N	N
DTXSID0042086	Laurocapram	59227-89-3	e1k	200	23	N	N
DTXSID0042169	Monotridecyl phosphate	5116-94-9	e1k	200	76	Y	N
DTXSID0029559	Diazolidinyl urea	78491-02-8	e1k	200	-7	N	N
DTXSID0026838	Isopropyl tetradecanoate	110-27-0	e1k	200	-1	N	N
DTXSID0022436	Diphenolic acid	126-00-1	e1k	200	5	N	N
DTXSID0041646	C.I. Acid Yellow 34, monosodium salt	6359-90-6	e1k	200	6	N	N
DTXSID0020494	Dimethyl methylphosphonate	756-79-6	e1k	200	1	N	N
DTXSID0044575	MON-4660	71526-07-3	e1k	200	4	N	N
DTXSID0025363	Glycolic acid	79-14-1	e1k	200	1	N	N
DTXSID0047741	Dibenzothiophene	132-65-0	e1k	200	7	N	N
DTXSID0020814	Mestranol	72-33-3	e1k	200	2	N	N
DTXSID0041270	3,5,5-Trimethylhexyl acetate	58430-94-7	e1k	200	-2	N	N
DTXSID0026880	1,2-Ethanediol diacetate	111-55-7	e1k	200	-4	N	N
DTXSID0042325	4-Propylanisole	104-45-0	e1k	201	-3	N	N
DTXSID0020652	Gemfibrozil	25812-30-0	e1k	200	-1	N	N
DTXSID0027852	Chlorotoluene	25168-05-2	e1k	200	1	N	N
DTXSID0041484	(3Z)-3-Hexenyl acetate	3681-71-8	e1k	200	3	N	N
DTXSID0044571	3-Isopropylphenol	618-45-1	e1k	200	11	N	N
DTXSID0044818	2-Butyloctan-1-ol	3913-02-8	e1k	200	16	N	N
DTXSID0022014	Hydroquinone dimethyl ether	150-78-7	e1k	200	3	N	N
DTXSID0041274	1-Phenyl-1H-pyrrole-2,5-dione	941-69-5	e1k	200	-2	N	N
DTXSID0042038	Heptyl butanoate	5870-93-9	e1k	200	5	N	N
DTXSID1021792	Salicylaldehyde	90-02-8	e1k	200	9	N	N
DTXSID1025300	2-Ethylhexyl diphenyl phosphate	1241-94-7	e1k	200	11	N	N

DTXSID1027479	2-(2H-Benzotriazol-2-yl)-4-methylphenol	2440-22-4	e1k	200	15	N	N
DTXSID1020354	Cyanoguanidine	461-58-5	e1k	200	10	N	N
DTXSID1025857	1,10-Phenanthroline	66-71-7	e1k	200	-3	N	N
DTXSID0048185	Apomorphine hydrochloride hydrate	41372-20-7	e1k	80	8	N	N
DTXSID1027891	Calcium dodecylbenzene sulfonate	26264-06-2	e1k	200	102	Y	N
DTXSID1020805	dl-Menthol	89-78-1	e1k	200	-2	N	N
DTXSID1022396	Chrysin	480-40-0	e1k	200	-1	N	N
DTXSID1027633	Irganox 1010	6683-19-8	e1k	89	1	N	N
DTXSID1025148	3,5-Dimethylphenol	108-68-9	e1k	205	4	N	N
DTXSID1029170	4-Methylpent-3-en-2-one	141-79-7	e1k	200	6	N	N
DTXSID1026033	Sodium ethasulfate	126-92-1	e1k	200	9	N	N
DTXSID1026904	2-Butoxyethyl acetate	112-07-2	e1k	200	4	N	N
DTXSID1027926	Dodecylphenol	27193-86-8	e1k	200	97	Y	N
DTXSID1026118	Tetralin	119-64-2	e1k	200	-2	N	N
DTXSID1022421	Melatonin	73-31-4	e1k	200	3	N	N
DTXSID1027429	Cyclododecanol	1724-39-6	e1k	200	6	N	N
DTXSID1032513	(3,5-Dimethyl-1H-pyrazol-1-yl)methanol	85264-33-1	e1k	200	1	N	N
DTXSID0048189	Lauryl gallate	1166-52-5	e1k	200	87	Y	N
DTXSID1021790	2-Nitrophenol	88-75-5	e1k	200	-2	N	N
DTXSID1027390	Phenolsulfonic acid	1333-39-7	e1k	200	4	N	N
DTXSID1040792	Pyridoxine hydrochloride	58-56-0	e1k	200	-3	N	N
DTXSID1024049	Diflubenzuron	35367-38-5	e1k	200	-5	N	N
DTXSID1020190	C.I. Acid Blue 74	860-22-0	e1k	200	0	N	N
DTXSID1026879	Hexamethyleneimine	111-49-9	e1k	200	-5	N	N
DTXSID1029128	Tetrahydrofurfuryl alcohol	97-99-4	e1k	200	2	N	N
DTXSID1032309	2,4-D-Butotyl	1929-73-3	e1k	200	1	N	N
DTXSID1025726	2-Nitroaniline	88-74-4	e1k	200	2	N	N
DTXSID1021871	4-Chlorophenol	106-48-9	e1k	200	1	N	N
DTXSID1022394	Biochanin A	491-80-5	e1k	200	8	N	N

DTXSID1024704	4-tert-Butyltoluene	98-51-1	e1k	200	-1	N	N
DTXSID1034260	Oxytetracycline	79-57-2	e1k	200	40	N	N
DTXSID1038795	1,1,1,3,5,5,5-Heptamethyltrisiloxane	1873-88-7	e1k	200	-6	N	N
DTXSID1022479	2-Ethylphenol	90-00-6	e1k	200	-3	N	N
DTXSID1034929	Spiromesifen	283594-90-1	e1k	200	-1	N	N
DTXSID1024598	Benzyl salicylate	118-58-1	e1k	200	8	N	N
DTXSID0048187	1-Methoxy-4-tert-pentylcyclohexane	199584-38-8	e1k	200	2	N	N
DTXSID1022055	tert-Butyl acetate	540-88-5	e1k	200	-3	N	N
DTXSID1026906	N,N-Dimethyldodecan-1-amine	112-18-5	e1k	200	5	N	N
DTXSID1020516	1,1-Dimethylhydrazine	57-14-7	e1k	200	-2	N	N
DTXSID1025306	5-Ethylidene-2-norbornene	16219-75-3	e1k	200	5	N	N
DTXSID1032511	1,3,5-Triethylhexahydro-s-triazine	7779-27-3	e1k	200	-4	N	N
DTXSID1022508	4-Dodecylphenol	104-43-8	e1k	200	90	Y	N
DTXSID1040611	Silwet L 77	27306-78-1	e1k	200	15	N	N
DTXSID1021031	4-Nitrosodiphenylamine	156-10-5	e1k	200	-3	N	N
DTXSID1029124	1,2,4,5-Tetramethylbenzene	95-93-2	e1k	200	-2	N	N
DTXSID1021403	Trimethyl phosphate	512-56-1	e1k	200	-3	N	N
DTXSID1027550	Sodium chloroacetate	3926-62-3	e1k	200	-2	N	N
DTXSID1026035	Sodium 2-mercaptobenzothiolate	2492-26-4	e1k	200	-2	N	N
DTXSID1035288	Codlure	33956-49-9	e1k	200	0	N	N
DTXSID1032484	Temephos	3383-96-8	e1k	200	6	N	N
DTXSID1037565	Mepronil	55814-41-0	e1k	200	1	N	N
DTXSID1027134	Bis(2-ethylhexyl) phosphate	298-07-7	e1k	200	50	Y	N
DTXSID1033371	Cyclopentanol	96-41-3	e1k	200	-5	N	N
DTXSID1030606	Acesulfame potassium	55589-62-3	e1k	200	0	N	N
DTXSID1025809	Oleic acid	112-80-1	e1k	200	87	Y	N
DTXSID1026241	3,3,5-Trimethylcyclohexyl salicylate	118-56-9	e1k	200	27	N	N
DTXSID1027899	Ammonium xylene sulfonate	26447-10-9	e1k	200	-2	N	N
DTXSID0048210	Phenyl benzoate	93-99-2	e1k	200	0	N	N
DTXSID1020144	Benzoin	119-53-9	e1k	200	-1	N	N
DTXSID1024255	Phenmedipham	13684-63-4	e1k	200	0	N	N

DTXSID1040110	Ethyl propionate	105-37-3	e1k	200	0	N	N
DTXSID1032648	Z-Tetrachlorvinphos	22248-79-9	e1k	200	-4	Y	N
DTXSID1021243	Rhodamine 6G	989-38-8	e1k	200	23	N	N
DTXSID1024176	Methacrylonitrile	126-98-7	e1k	200	-2	N	N
DTXSID1033161	Aldicarb sulfoxide	1646-87-3	e1k	200	0	N	N
DTXSID0048181	4-tert-Butylaniline	769-92-6	e1k	200	-1	N	N
DTXSID0048183	Enterolactone	78473-71-9	e1k	67	0	N	N
DTXSID1040372	Epoxiconazole	133855-98-8	e1k	200	-1	N	N
DTXSID1020352	Cupferron	135-20-6	e1k	200	-1	N	N
DTXSID1024124	hifensulfuron methyl	79277-27-3	e1k	200	1	N	N
DTXSID1027500	2-Propoxyethanol	2807-30-9	e1k	200	-1	N	N
DTXSID1042154	Methyl red	493-52-7	e1k	200	19	N	N
DTXSID2027412	3,6,9,12-Tetraoxahexadecan-1-ol	1559-34-8	e1k	200	5	N	N
DTXSID1044693	Magnesium dibenzoate	553-70-8	e1k	200	5	N	N
DTXSID2025478	Isopropyl acetate	108-21-4	e1k	200	2	N	N
DTXSID2022048	Flavone	525-82-6	e1k	198	11	N	N
DTXSID1040794	Sodium 2-phenylphenate tetrahydrate	6152-33-6	e1k	204	11	N	N
DTXSID1048122	Benzyl-C8-18-alkyldimethylammonium chlorides	63449-41-2	e1k	200	89	Y	N
DTXSID2032558	Kresoxim-methyl	143390-89-0	e1k	200	3	N	N
DTXSID2025347	Furfuryl alcohol	98-00-0	e1k	198	-1	N	N
DTXSID2027333	3-Aminopropyltriethoxysilane	919-30-2	e1k	200	-4	N	N
DTXSID1041267	1-Ethoxy-2-propanol	1569-02-4	e1k	200	11	N	N
DTXSID1047497	Octyl decyl phthalate	119-07-3	e1k	200	8	N	N
DTXSID1041421	5,7-Dimethoxy-2H-chromen-2-one	487-06-9	e1k	200	-1	N	N
DTXSID2034700	MCPA-sodium	3653-48-3	e1k	200	0	N	N
DTXSID1041425	(2E)-2-Hexenal	6728-26-3	e1k	200	0	N	N
DTXSID1041346	2,4-D-ethyl ester	533-23-3	e1k	200	1	N	N
DTXSID2027094	Bis(2-ethylhexyl) maleate	142-16-5	e1k	200	11	N	N
DTXSID1048203	Ethyl 4-chlorophenyl ketone	6285-05-8	e1k	200	5	N	N
DTXSID2025688	Morpholine	110-91-8	e1k	200	-3	N	N

DTXSID2021739	1-Propanol	71-23-8	e1k	200	4	N	N
DTXSID1041978	Flufenoxuron	101463-69-8	e1k	200	5	N	N
DTXSID2029298	Sodium lauryl polyoxyethylene ether sulfate	9004-82-4	e1k	200	82	Y	N
DTXSID2025395	Hexamethyldisilazane	999-97-3	e1k	200	-5	N	N
DTXSID1041550	(S)-(-)-beta-Citronellol	7540-51-4	e1k	200	7	N	N
DTXSID2020212	2-tert-Butyl-4-methylphenol	2409-55-4	e1k	200	15	N	N
DTXSID2027414	2,3-Dihydro-2,2-dimethyl-7-benzofuranol	1563-38-8	e1k	200	-2	N	N
DTXSID2022678	Bicalutamide	90357-06-5	e1k	116	-1	N	N
DTXSID2022123	2-Hydroxyethyl acrylate	818-61-1	e1k	200	-3	N	N
DTXSID2026238	Trimethylamine	75-50-3	e1k	200	-5	N	N
DTXSID1041265	2-Hexyl-1-decanol	2425-77-6	e1k	200	15	N	N
DTXSID2029167	Metam-sodium	137-42-8	e1k	200	19	N	N
DTXSID2021602	Hexadecanoic acid	57-10-3	e1k	200	57	Y	N
DTXSID2022628	Atenolol	29122-68-7	e1k	200	4	N	N
DTXSID1048201	Cyclobutyl phenyl ketone	5407-98-7	e1k	200	8	N	N
DTXSID2027963	Isooctadecanoic acid	30399-84-9	e1k	200	94	Y	N
DTXSID2024664	Butanal oxime	110-69-0	e1k	200	-6	N	N
DTXSID1041184	(-)-beta-Pinene	18172-67-3	e1k	200	-1	N	N
DTXSID1041970	Fenchol	1632-73-1	e1k	200	-1	N	N
DTXSID2029290	(1S,5S) 2,6,6-Trimethyl-Bicyclo(3.1.1)hept-2-ene	7785-26-4	e1k	200	0	N	N
DTXSID2029616	Imidazole	288-32-4	e1k	200	-7	N	N
DTXSID1041188	(2-Nitro-1-propenyl)benzene	705-60-2	e1k	200	2	N	N
DTXSID2023193	Lactose	63-42-3	e1k	200	-1	N	N
DTXSID2032348	Chlorophacinone	3691-35-8	e1k	200	25	N	N
DTXSID2021997	1-(2-Aminoethyl)piperazine	140-31-8	e1k	200	-8	N	N
DTXSID1048207	Diphenyl phosphate	838-85-7	e1k	200	-1	N	N
DTXSID1041920	2-(2-Ethylhexyloxy)ethanol	1559-35-9	e1k	200	21	N	N
DTXSID2025050	Diethylenetriamine	111-40-0	e1k	200	2	N	N

DTXSID2029325	Methyl dihydrojasmonate	24851-98-7	e1k	200	4	N	N
DTXSID2024666	1,4-Butanediol	110-63-4	e1k	200	3	N	N
DTXSID2023723	Tromethamine	77-86-1	e1k	200	-1	N	N
DTXSID2020929	Niacinamide	98-92-0	e1k	210	-4	N	N
DTXSID2022171	1-Decanamine	2016-57-1	e1k	200	-3	N	N
DTXSID2025892	N-Phenyl-1-naphthylamine	90-30-2	e1k	200	14	N	N
DTXSID2026496	alpha-Terpinyl acetate	80-26-2	e1k	200	-8	N	N
DTXSID1041639	Sodium m-xylene-4-sulfonate	827-21-4	e1k	200	0	N	N
DTXSID2025505	Linoleic acid	60-33-3	e1k	200	29	Y	N
DTXSID2034598	Fenoxaprop-P-ethyl	71283-80-2	e1k	200	4	N	N
DTXSID2025216	Divinylbenzene	1321-74-0	e1k	200	-6	N	N
DTXSID2026789	Propylene carbonate	108-32-7	e1k	200	1	N	N
DTXSID1044487	Methyltrioctylammonium chloride	5137-55-3	e1k	200	96	Y	N
DTXSID2027466	ECC	2386-87-0	e1k	200	-3	N	N
DTXSID2027258	Isopropyl formate	625-55-8	e1k	200	2	N	N
DTXSID2021943	2-Undecanone	112-12-9	e1k	203	4	N	N
DTXSID2023430	Pentaerythritol tetranitrate	78-11-5	e1k	200	-5	N	N
DTXSID2026997	4-Methoxybenzaldehyde	123-11-5	e1k	200	4	N	N
DTXSID2025135	1,3-Dimethyl-4-nitrobenzene	89-87-2	e1k	200	5	N	N
DTXSID1044435	Procaine hydrochloride	51-05-8	e1k	200	5	N	N
DTXSID2032639	Pyridate	55512-33-9	e1k	200	10	N	N
DTXSID1048209	tert-Butyl phenyl ketone	938-16-9	e1k	200	5	N	N
DTXSID1041891	Diphenylmethane	101-81-5	e1k	200	4	N	N
DTXSID2021735	Dimethyl sulfoxide	67-68-5	e1k	200	-4	N	N
DTXSID2029612	Limonene	138-86-3	e1k	206	-1	N	N
DTXSID1042491	Triethoxypentylsilane	2761-24-2	e1k	200	12	N	N
DTXSID2042060	Isoborneol	124-76-5	e1k	200	12	N	N
DTXSID3032412	Imazamethabenz	81405-85-8	e1k	200	7	N	N
DTXSID2041252	1,4-Diaminoanthraquinone	128-95-0	e1k	200	20	Y	N
DTXSID2040151	Imidazolidinyl urea	39236-46-9	e1k	200	9	N	N
DTXSID3021483	Phenylacetaldehyde	122-78-1	e1k	200	29	N	N

DTXSID2036588	Polyoxyethylene(10)nonylphenyl ether	26027-38-3	e1k	200	21	N	N
DTXSID2041200	N,N'-Disalicylidene-1,2-diaminopropane	94-91-7	e1k	200	40	N	N
DTXSID2041389	2'-Acetonaphthone	93-08-3	e1k	200	-5	N	N
DTXSID2042191	N,N'-Dimethylthiourea	534-13-4	e1k	200	4	N	N
DTXSID3038696	Ethyl benzoate	93-89-0	e1k	200	16	N	N
DTXSID3024528	Anise oil	8007-70-3	e1k	200 µg/ml	17	N	N
DTXSID3034583	Ethyl 1-naphthaleneacetate	2122-70-5	e1k	200	9	N	N
DTXSID2044553	Sodium 2-methylbenzenesulfonate	15046-75-0	e1k	200	1	N	N
DTXSID3021356	dl-alpha-Tocopheryl acetate	52225-20-4	e1k	200	8	N	N
DTXSID2041703	Butylnaphthalenesulfonic acid sodium salt	25638-17-9	e1k	200	12	N	N
DTXSID3021770	2,2',6,6'-Tetrachlorobisphenol A	79-95-8	e1k	200	62	Y	N
DTXSID3038808	1,3,5,7-Tetramethyl-1,3,5,7-tetravinylcyclotetrasiloxane	2554-06-5	e1k	200	19	N	N
DTXSID2042276	o-Ethoxyphenol	94-71-3	e1k	200	17	N	N
DTXSID3027877	Diisodecylphenyl phosphite	25550-98-5	e1k	200	21	N	N
DTXSID3037541	Endosulfan sulfate	1031-07-8	e1k	200	27	N	N
DTXSID2041208	Decyl beta-D-glucopyranoside	58846-77-8	e1k	200	6	N	N
DTXSID3026641	1,3-Benzenedicarbonyl dichloride	99-63-8	e1k	200	6	N	N
DTXSID2047517	Hexanedioic acid, di-C7-9-branched and linear alkyl esters	68515-75-3	e1k	200	4	N	N
DTXSID3020093	4-Methoxyaniline hydrochloride	20265-97-8	e1k	200	11	N	N
DTXSID3020889	4-Methylstyrene	622-97-9	e1k	200	-4	N	N
DTXSID3020091	Aniline hydrochloride	142-04-1	e1k	200	4	N	N
DTXSID3034531	Thiophanate	23564-06-9	e1k	200	-8	N	N
DTXSID3020625	Finasteride	98319-26-7	e1k	200	10	N	N
DTXSID2044713	Acid Red 337	67786-14-5	e1k	200	51	Y	N
DTXSID3027875	Glyceryl monooleate	25496-72-4	e1k	200	62	Y	N
DTXSID2036112	2-(8-Heptadecenyl)-2-imidazoline-1-ethanol	95-38-5	e1k	200	91	Y	N

DTXSID3020043	Allantoin	97-59-6	e1k	200	-2	N	N
DTXSID3026647	4-Hydroxybenzoic acid	99-96-7	e1k	200	-1	N	N
DTXSID2044391	2-Isopropylphenol	88-69-7	e1k	200	2	N	N
DTXSID3020415	1,2-Dibromoethane	106-93-4	e1k	202	-13	N	N
DTXSID3026566	Dimethyl hexahydroterephthalate	94-60-0	e1k	200	-3	N	N
DTXSID3036105	2-tert-Butylcyclohexyl acetate	88-41-5	e1k	200	7	N	N
DTXSID2041250	1,4-Bis(N-isopropylamino)anthraquinone	14233-37-5	e1k	106	4	N	N
DTXSID3036286	Citralva	5146-66-7	e1k	206	15	N	N
DTXSID3021726	Salicylamide	65-45-2	e1k	200	-7	N	N
DTXSID3021853	1-Piperazineethanol	103-76-4	e1k	203	3	N	N
DTXSID3022409	4,4'-Sulfonyldiphenol	80-09-1	e1k	200	0	N	N
DTXSID3021518	Fumaric acid	110-17-8	e1k	200	-8	N	N
DTXSID2047696	Cremophor EL	61791-12-6	e1k	200 µg/ml	4	N	N
DTXSID3029154	Cyclopentanone	120-92-3	e1k	200	7	N	N
DTXSID2038788	1,4-Cyclohexanedicarboxylic acid	1076-97-7	e1k	200	-8	N	N
DTXSID3036288	2-Octyl-1-dodecanol	5333-42-6	e1k	200	6	N	N
DTXSID3022405	2-Hydroxy-4-methoxybenzophenone	131-57-7	e1k	200	14	N	N
DTXSID3020047	Allyl isothiocyanate	57-06-7	e1k	206	-5	N	N
DTXSID3020673	FD&C Green No. 3	2353-45-9	e1k	132	83	Y	N
DTXSID2042062	Isobornyl propanoate	2756-56-1	e1k	197	2	N	N
DTXSID3021980	Ethyl hexanoate	123-66-0	e1k	200	-16	N	N
DTXSID3034614	Flucarbazono-sodium	181274-17-9	e1k	187	1	N	N
DTXSID3035214	1-Octen-3-ol	3391-86-4	e1k	200	-3	N	N
DTXSID3026514	Phthalimide	85-41-6	e1k	200	-12	N	N
DTXSID3024994	Sodium dichloroisocyanurate	2893-78-9	e1k	200	1	N	N
DTXSID3029572	Benoxacor	98730-04-2	e1k	200	-1	N	N
DTXSID2041709	C.I. Acid Orange 8, monosodium salt	5850-86-2	e1k	200	44	N	N
DTXSID3040776	Morin hydrate	654055-01-3	e1k	200	29	Y	N
DTXSID2040731	Diisopropyl phthalate	605-45-8	e1k	200	2	N	N

DTXSID3022247	Nerolidol	7212-44-4	e1k	200	18	N	N
DTXSID3032389	Farnesol	4602-84-0	e1k	200	27	N	N
DTXSID3020621	Fenvalerate	51630-58-1	e1k	200	-9	N	N
DTXSID3026065	Sulfan blue	129-17-9	e1k	200	15	N	N
DTXSID3022320	Triphenylethylene	58-72-0	e1k	200	5	N	N
DTXSID3032591	1-Bromo-3-chloro-5,5-dimethylhydantoin	16079-88-2	e1k	200	0	N	N
DTXSID3040352	Dinocap	39300-45-3	e1k	200	88	Y	N
DTXSID2042436	Sulisobenzone	4065-45-6	e1k	200	-3	N	N
DTXSID3032416	Cybutryne	28159-98-0	e1k	200	13	N	N
DTXSID3024944	1,2-Dibromo-2,4-dicyanobutane	35691-65-7	e1k	200	7	N	N
DTXSID4025080	Diisobutyl ketone	108-83-8	e1k	200	6	N	N
DTXSID3047180	Triisodecyl trimellitate	36631-30-8	e1k	163	7	N	N
DTXSID4027282	Phenyl phosphorus dichloride	644-97-3	e1k	200	3	N	N
DTXSID4027527	1,2,5,6,9,10-Hexabromocyclododecane	3194-55-6	e1k	174	9	N	N
DTXSID3041877	Dimethylbenzylcarbinyl acetate	151-05-3	e1k	200	-6	N	N
DTXSID4020292	Chloroacetaldehyde	107-20-0	e1k	200	5	N	N
DTXSID4020618	Fadrozole hydrochloride	102676-31-3	e1k	100	3	N	N
DTXSID4036435	1-Octyl-2-pyrrolidone	2687-94-7	e1k	200	12	N	N
DTXSID4022523	Heptylparaben	1085-12-7	e1k	200	82	Y	N
DTXSID4025296	2-Ethyl-2-hexenal	645-62-5	e1k	200	3	N	N
DTXSID4027153	1-Bromo-4-fluorobenzene	460-00-4	e1k	200	3	N	N
DTXSID3041794	Cloquintocet-mexyl	99607-70-2	e1k	200	7	N	N
DTXSID3042130	Diphenylmercury(II)	587-85-9	e1k	200	9	N	N
DTXSID4029692	Potassium nitrate	7757-79-1	e1k	200	7	N	N
DTXSID3041247	1,3-Diphenyl-1,3-propanedione	120-46-7	e1k	200	16	N	N
DTXSID4020664	3-Chloro-1,2-propanediol	96-24-2	e1k	200	7	N	N
DTXSID4026769	Hexamethyldisiloxane	107-46-0	e1k	200	0	N	N
DTXSID4027997	Dichlormid	37764-25-3	e1k	200	1	N	N
DTXSID4021391	Tris(methylphenyl) phosphate	1330-78-5	e1k	200	3	N	N
DTXSID4023202	Letrozole	112809-51-5	e1k	142	6	N	N

DTXSID4022109	gamma-Decanolactone	706-14-9	e1k	204	1	N	N
DTXSID3044833	Terpinyl propionate	80-27-3	e1k	200	4	N	N
DTXSID3041530	7-Ethyl-2-methyl-4-undecanolsulfate, sodium salt	139-88-8	e1k	200	4	N	N
DTXSID3041663	Benzyl cinnamate	103-41-3	e1k	200	10	N	N
DTXSID4036229	Sodium decyl sulfate	142-87-0	e1k	200	6	N	N
DTXSID4035708	Methylbenzethonium chloride	25155-18-4	e1k	1000	103	Y	N
DTXSID3041954	3-Octanone	106-68-3	e1k	202	-1	N	N
DTXSID4020870	2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	119-47-1	e1k	200	72	Y	N
DTXSID4025612	2-Methylpentanedinitrile	4553-62-2	e1k	200	3	N	N
DTXSID4027076	Dodecyl sulfate triethanolamine	139-96-8	e1k	200	61	Y	N
DTXSID4025292	2-Ethyl-1,3-hexanediol	94-96-2	e1k	200	1	N	N
DTXSID4022525	2-Ethylhexylparaben	5153-25-3	e1k	200	85	Y	N
DTXSID4034576	2-Bromo-4-hydroxyacetophenone	2491-38-5	e1k	200	3	N	N
DTXSID3047473	Polymethylene polyphenyl isocyanate	9016-87-9	e1k	200	-2	N	N
DTXSID3041611	Ascorbyl palmitate	137-66-6	e1k	200	63	Y	N
DTXSID3041299	Dihydrojasmane lactone	7011-83-8	e1k	200	4	N	N
DTXSID4021977	4-Ethylphenol	123-07-9	e1k	202	-1	N	N
DTXSID3042394	Sodium 1-naphthalenesulfonate	130-14-3	e1k	200	-3	N	N
DTXSID3041409	2-Chloro-N-phenylacetamide	587-65-5	e1k	200	5	Y	N
DTXSID4024193	MCPB	94-81-5	e1k	200	-2	N	N
DTXSID4020828	4-Methoxyphenol	150-76-5	e1k	200	3	N	N
DTXSID3042007	Glyceryl monoricinoleate	1323-38-2	e1k	200	23	N	N
DTXSID4032619	Halofenozide	112226-61-6	e1k	200	0	N	N
DTXSID4021921	2-Butyne-1,4-diol	110-65-6	e1k	200	-4	N	N
DTXSID3047425	4-Butylphenol	1638-22-8	e1k	200	11	Y	N
DTXSID3047633	Ethyl oleate	111-62-6	e1k	200	-1	N	N
DTXSID4029698	Sodium persulfate	7775-27-1	e1k	200	-2	N	N
DTXSID4029565	Phthalic acid, diundecyl ester, branched and linear	85507-79-5	e1k	200	0	N	N

DTXSID4020616	1,8-Cineol	470-82-6	e1k	200	1	N	N
DTXSID4024721	D-Camphor	464-49-3	e1k	200	1	N	N
DTXSID4034497	Metconazole	125116-23-6	e1k	200	2	N	N
DTXSID4025662	Methyl styryl ketone	122-57-6	e1k	200	5	N	N
DTXSID4022446	2,2'-Bisphenol F	2467-02-9	e1k	1000	25	N	N
DTXSID4026501	alpha-Pinene	80-56-8	e1k	200	-1	N	N
DTXSID4027072	Sodium phenolate	139-02-6	e1k	200	1	N	N
DTXSID3041293	2-((Dimethylamino)methyl)phenol	120-65-0	e1k	200	-5	N	N
DTXSID4020379	Dehydroepiandrosterone	53-43-0	e1k	200	3	N	N
DTXSID4021553	Decanal	112-31-2	e1k	200	-1	N	N
DTXSID3041661	2-Hydroxybenzoxitrile	611-20-1	e1k	200	1	N	N
DTXSID3041790	Citronellal	106-23-0	e1k	200	1	N	N
DTXSID4029353	Acetyl cedrene	32388-55-9	e1k	200	26	N	N
DTXSID4027868	tert-Nonanethiol	25360-10-5	e1k	200	2	N	N
DTXSID4027656	2-Ethylhexyl thioglycolate	7659-86-1	e1k	200	1	N	N
DTXSID4024274	Propachlor	1918-16-7	e1k	200	-2	N	N
DTXSID4026842	Methyl decanoate	110-42-9	e1k	200	1	N	N
DTXSID3047712	Cornmint oil	68917-18-0	e1k	200 µg/ml	3	N	N
DTXSID4021006	N-Nitroso-N-methylurea	684-93-5	e1k	200	2	N	N
DTXSID4027496	2,4-D sodium salt	2702-72-9	e1k	200	1	N	N
DTXSID4022288	4-Hexyloxyaniline	39905-57-2	e1k	200	6	N	N
DTXSID4027525	Potassium 2-ethylhexanoate	3164-85-0	e1k	200	3	N	N
DTXSID4021842	Cyclohexanone oxime	100-64-1	e1k	200	1	N	N
DTXSID4034601	(2R,6S)-Fenpropimorph	67564-91-4	e1k	200	29	N	N
DTXSID5022510	4-Chloro-2-methylphenol	1570-64-5	e1k	200	5	N	N
DTXSID4048199	4-Butyloxyaniline	4344-55-2	e1k	200	-1	N	N
DTXSID5032579	Triclopyr butotyl	64700-56-7	e1k	200	10	N	N
DTXSID5020029	Acrylonitrile	107-13-1	e1k	200	5	Y	N
DTXSID5023875	Ammonium sulfamate	7773-06-0	e1k	200	-8	N	N
DTXSID5021758	Tris(2-butoxyethyl) phosphate	78-51-3	e1k	200	4	N	N

DTXSID4044828	Ethyl undec-10-enoate	692-86-4	e1k	200	16	N	N
DTXSID4041442	Sodium 2-naphthalenesulfonate	532-02-5	e1k	200	10	N	N
DTXSID4047127	4-(tert-Pentyl)-cyclohexanone	16587-71-6	e1k	200	2	N	N
DTXSID5032654	Triforine	26644-46-2	e1k	200	0	N	N
DTXSID4048193	4,4'-Di-tert-butylbiphenyl	1625-91-8	e1k	200	6	Y	N
DTXSID5029217	1-Propoxy-2-propanol	1569-01-3	e1k	200	0	N	N
DTXSID4038924	Hexyl salicylate	6259-76-3	e1k	200	29	N	N
DTXSID5027142	1,2-Dichloro-4-(trifluoromethyl)benzene	328-84-7	e1k	200	4	N	N
DTXSID5025021	Dicyclohexyl phthalate	84-61-7	e1k	209	4	N	N
DTXSID5024263	Phosphoric acid	7664-38-2	e1k	200	-12	N	N
DTXSID5024681	tert-Butylamine	75-64-9	e1k	200	3	N	N
DTXSID5020106	L-Ascorbic acid	50-81-7	e1k	200	-6	N	N
DTXSID4042096	L-Glucitol	6706-59-8	e1k	200	-1	N	N
DTXSID5020233	Ergocalciferol	50-14-6	e1k	200	34	N	N
DTXSID5027356	Tris(2-methoxyethoxy)vinylsilane	1067-53-4	e1k	200	9	N	N
DTXSID4040343	Benzyl bromoacetate	5437-45-6	e1k	200	1	N	N
DTXSID5022489	E-Cinnamic acid	140-10-3	e1k	200	4	N	N
DTXSID5026461	2-Methylpropanenitrile	78-82-0	e1k	200	-12	N	N
DTXSID4040711	Ethyl 2-methylbenzoate	87-24-1	e1k	200	-5	N	N
DTXSID5020443	2,4-D Butyl ester	94-80-4	e1k	200	-2	N	N
DTXSID5024922	1,6-Hexanediamine	124-09-4	e1k	200	-4	N	N
DTXSID4042094	Levomenol	23089-26-1	e1k	200	28	N	N
DTXSID4041818	2-sec-Butylcyclohexanone	14765-30-1	e1k	200	0	N	N
DTXSID5026251	Triphenylphosphine	603-35-0	e1k	200	-3	N	N
DTXSID5021415	Triisopropanolamine	122-20-3	e1k	200	1	N	N
DTXSID5034981	Tributyltin benzoate	4342-36-3	e1k	200	13	Y	N
DTXSID5024057	Dimethylamine	124-40-3	e1k	200	-7	N	N
DTXSID5027304	Dimethyltin dichloride	753-73-1	e1k	200	-5	N	N
DTXSID5025023	Dicyclopentadiene	77-73-6	e1k	197	-12	N	N
DTXSID5021968	3-Ethoxy-4-hydroxybenzaldehyde	121-32-4	e1k	200	1	N	N

DTXSID5026623	4-tert-Butylcyclohexanol	98-52-2	e1k	200	-3	N	N
DTXSID5026548	2,4,6-Tris(dimethylaminomethyl)phenol	90-72-2	e1k	200	0	N	N
DTXSID4041440	2-Methylbutyl isovalerate	2445-77-4	e1k	200	3	N	N
DTXSID4041232	1,3,5-Triisopropylbenzene	717-74-8	e1k	200	12	N	N
DTXSID4047597	Poloxalene	9003-11-6	e1k	200	-3	N	N
DTXSID5027774	Ethylenediaminetetraacetic acid ferric sodium salt	15708-41-5	e1k	200	24	N	N
DTXSID5021413	Tris(2,3-dibromopropyl) phosphate	126-72-7	e1k	174	13	N	N
DTXSID4047882	Phenylparaben	17696-62-7	e1k	200	5	N	N
DTXSID4041604	Pentyl butyrate	540-18-1	e1k	200	-7	N	N
DTXSID5020499	N,N-Dimethylacetamide	127-19-5	e1k	200	-8	N	N
DTXSID5023588	D-Glucitol	50-70-4	e1k	193	14	N	N
DTXSID5021251	Saccharin	81-07-2	e1k	200	1	N	N
DTXSID5021916	2-Heptanone	110-43-0	e1k	200	-8	N	N
DTXSID5027770	2-Acrylamido-2-methyl-1-propanesulfonic acid	15214-89-8	e1k	200	3	N	N
DTXSID5026259	Tris(2-chloroisopropyl)phosphate	13674-84-5	e1k	190	-3	N	N
DTXSID5022934	Digoxin	20830-75-5	e1k	135	-8	N	N
DTXSID4044537	Sodium triisopropyl naphthalene sulfonate	1323-19-9	e1k	200	49	N	N
DTXSID4042418	Sodium tridecyl sulfate	3026-63-9	e1k	200	95	Y	N
DTXSID5026912	2-[2-(2-Methoxyethoxy)ethoxy]ethanol	112-35-6	e1k	200	-8	N	N
DTXSID5034357	Lufenuron	103055-07-8	e1k	200	11	N	N
DTXSID5022437	Nordihydroguaiaretic acid	500-38-9	e1k	200	13	Y	N
DTXSID5021388	2,4,5-Trichlorophenoxyacetic acid	93-76-5	e1k	200	-3	N	N
DTXSID4041492	3-Phenylhexane	4468-42-2	e1k	200	3	N	N
DTXSID4048191	4,4'-Methylenebis(2,6-diethylaniline)	13680-35-8	e1k	200	3	N	N
DTXSID5028665	DINP branched	68515-48-0	e1k	200	-11	N	N
DTXSID5021590	Dodecanoic acid	143-07-7	e1k	200	0	N	N
DTXSID5026706	1,2-Diphenoxyethane	104-66-5	e1k	200	-2	N	N

DTXSID5032315	4,5-Dichloro-2-octyl-3(2H)-isothiazolone	64359-81-5	e1k	200	2	Y	N
DTXSID5025102	3-(Dimethylamino)propylamine	109-55-7	e1k	200	2	N	N
DTXSID4048195	4-(Hexyloxy)phenol	18979-55-0	e1k	200	35	N	N
DTXSID4044901	Triallyl trimellitate	2694-54-4	e1k	200	5	N	N
DTXSID5020493	Dimethyl hydrogen phosphite	868-85-9	e1k	200	-6	N	N
DTXSID5021914	5-Methyl-2-hexanone	110-12-3	e1k	200	-4	N	N
DTXSID4042335	Butyl (2S)-2-hydroxypropanoate	34451-19-9	e1k	200	5	N	N
DTXSID4041521	4-Morpholinepropanamine	123-00-2	e1k	200	5	N	N
DTXSID4042171	4-Dodecylmorpholine	1541-81-7	e1k	200	19	Y	N
DTXSID5027198	N-Methylphthalimide	550-44-7	e1k	200	-2	N	N
DTXSID5040700	Trimethoxyphenylsilane	2996-92-1	e1k	200	0	N	N
DTXSID6024834	(2E)-3-Phenylprop-2-enal	14371-10-9	e1k	200	8	N	N
DTXSID6025141	1,3-Dimethylolurea	140-95-4	e1k	200	5	N	N
DTXSID6023523	Propofol	2078-54-8	e1k	200	13	N	N
DTXSID6021793	1-Naphthol	90-15-3	e1k	200	12	N	N
DTXSID5044815	Dibutyl nonanedioate	2917-73-9	e1k	200	5	N	N
DTXSID5048180	4-Propylaniline	2696-84-6	e1k	200	15	N	N
DTXSID5041726	C.I. Direct Red 81 disodium salt	2610-11-9	e1k	200	97	Y	N
DTXSID6024123	Haloxypop-methyl	69806-40-2	e1k	200	11	N	N
DTXSID5042243	Oleyl sarcosine	110-25-8	e1k	200	96	Y	N
DTXSID6025018	Dicyclohexylamine	101-83-7	e1k	200	8	N	N
DTXSID6021240	Retinol acetate	127-47-9	e1k	200	7	N	N
DTXSID6025226	Econazole nitrate	24169-02-6	e1k	200	16	N	N
DTXSID5044784	1,3-Butyleneglycol dimethacrylate	1189-08-8	e1k	200	1	N	N
DTXSID5041641	2,5-Dimethylbenzenesulfonic acid	609-54-1	e1k	200	4	N	N
DTXSID6021082	C.I. Acid Orange 10	1936-15-8	e1k	200	7	N	N
DTXSID5044865	2,2'-(Tetradecylimino)diethanol	18924-66-8	e1k	200	71	Y	N
DTXSID5048188	4-Thiocresol	106-45-6	e1k	200	15	N	N
DTXSID6023602	Butanedioic acid	110-15-6	e1k	200	9	N	N

DTXSID6021113	Peppermint oil	8006-90-4	e1k	200 µg/ml	3	N	N
DTXSID5040708	4-Hexylaniline	33228-45-4	e1k	200	28	N	N
DTXSID6021959	2,4,6-Tribromophenol	118-79-6	e1k	200	4	N	N
DTXSID5041512	4-Chlorophenylurea	140-38-5	e1k	199	0	N	N
DTXSID5047033	gamma-Cyclodextrin	17465-86-0	e1k	79	-2	N	N
DTXSID5041302	(Dicyclopentadienyloxy)ethyl methacrylate	68169-03-9	e1k	200	6	N	N
DTXSID6024676	Butyl acrylate	141-32-2	e1k	205	4	N	N
DTXSID5035589	Disiquonium chloride	68959-20-6	e1k	200	64	Y	N
DTXSID6023868	Hydramethylnon	67485-29-4	e1k	200	15	N	N
DTXSID5047611	1,4-Heptanolide	105-21-5	e1k	200	0	N	N
DTXSID5048184	Melengestrol acetate	2919-66-6	e1k	126	11	N	N
DTXSID5047879	2-Hydroxybenzophenone	117-99-7	e1k	200	2	N	N
DTXSID5035616	Sodium 2-nitrophenolate	824-39-5	e1k	200	-1	N	N
DTXSID5042299	4-Isopropylphenol	99-89-8	e1k	200	-1	N	N
DTXSID5044788	Naphthalene-2-sulfonic acid	120-18-3	e1k	200	-2	N	N
DTXSID6024624	Bisphenol A diglycidyl ether	1675-54-3	e1k	200	12	Y	N
DTXSID6021907	Propanedinitrile	109-77-3	e1k	200	9	N	N
DTXSID6020511	3,3'-Dimethylbenzidine dihydrochloride	612-82-8	e1k	200	1	N	N
DTXSID6025220	1-Dodecanethiol	112-55-0	e1k	200	18	N	N
DTXSID5041643	Sodium 2-formylbenzenesulfonate	1008-72-6	e1k	200	13	N	N
DTXSID6026298	m-Xylene	108-38-3	e1k	200	0	N	N
DTXSID5038830	1,1-Dimethyl-2-phenylethyl butanoate	10094-34-5	e1k	200	5	N	N
DTXSID6024046	Paraoxon	311-45-5	e1k	200	-1	N	N
DTXSID6025436	8-Hydroxyquinoline sulfate	134-31-6	e1k	200	6	N	N
DTXSID5048211	Ethyl 4-methylbenzoate	94-08-6	e1k	200	5	N	N
DTXSID6025143	2,3-Dimethylphenol	526-75-0	e1k	205	7	N	N
DTXSID5041516	2-Ethyl-3-hydroxy-4H-pyran-4-one	4940-11-8	e1k	200	-2	N	N
DTXSID6025272	Ethyl anthranilate	87-25-2	e1k	200	4	N	N

DTXSID5047451	Acid Yellow 11	6359-82-6	e1k	200	2	N	N
DTXSID5038888	Basic Blue 7	2390-60-5	e1k	200	38	N	N
DTXSID6020197	Bromocriptine mesylate	22260-51-1	e1k	67	2	N	N
DTXSID5037494	Deethylatrazine	6190-65-4	e1k	200	4	N	N
DTXSID5041275	1-Monolaurin	142-18-7	e1k	200	8	N	N
DTXSID6022137	(Z)-3-Hexen-1-ol	928-96-1	e1k	200	0	N	N
DTXSID5044578	Sodium 2,5-dimethylbenzenesulfonate	827-19-0	e1k	200	5	N	N
DTXSID5041514	(4Z)-4-Decenal	21662-09-9	e1k	200	9	N	N
DTXSID6024200	m-Cresol	108-39-4	e1k	200	-1	N	N
DTXSID6020307	Chloromethyl methyl ether	107-30-2	e1k	70	5	N	N
DTXSID6022008	1-Nonanol	143-08-8	e1k	200	9	N	N
DTXSID5044443	N,N-Dibutyl-N-methylbutan-1-aminium chloride	56375-79-2	e1k	200	3	N	N
DTXSID6020278	1-Chloro-2,4-dinitrobenzene	97-00-7	e1k	200	23	N	N
DTXSID5041273	Pyrazolone T	118-47-8	e1k	200	0	N	N
DTXSID5037028	Hexadecyltrimethylammonium bromide	57-09-0	e1k	200	97	Y	N
DTXSID6021957	Phenyl salicylate	118-55-8	e1k	200	3	N	N
DTXSID6021666	Tetradecanoic acid	544-63-8	e1k	200	77	Y	N
DTXSID5047796	Formalin	NOCAS_47796	e1k	208	9	N	N
DTXSID6023862	Aldoxycarb	1646-88-4	e1k	200	4	N	N
DTXSID6021824	Dichlorophen	97-23-4	e1k	200	51	Y	N
DTXSID5041487	3,7-Dimethyloctan-3-yl acetate	20780-48-7	e1k	200	0	N	N
DTXSID6022391	Apigenin	520-36-5	e1k	200	6	N	N
DTXSID6026080	Terephthalic acid	100-21-0	e1k	200	0	N	N
DTXSID6020014	Dehydroacetic acid	520-45-6	e1k	200	8	N	N
DTXSID6032516	2-Hydroxyethyl octyl sulfide	3547-33-9	e1k	200	21	N	N
DTXSID6041682	Bromophenol blue	115-39-9	e1k	186	61	Y	N
DTXSID7024586	Benzothiazole	95-16-9	e1k	200	4	N	N
DTXSID7021863	Diethyl propanedioate	105-53-3	e1k	206	0	N	N
DTXSID7021520	2-[2-(2-Butoxyethoxy)ethoxy]ethanol	143-22-6	e1k	200	2	N	N
DTXSID6048208	Methyl 2-methylbenzoate	89-71-4	e1k	200	2	N	N

DTXSID7022679	Biotin	58-85-5	e1k	200	-2	N	N
DTXSID6047103	Octadecyl sulfate sodium salt	1120-04-3	e1k	200	72	Y	N
DTXSID7020425	Dichlone	117-80-6	e1k	200	41	Y	N
DTXSID6034005	Sulfamic acid	5329-14-6	e1k	200	1	N	N
DTXSID6042490	Triethoxymethylsilane	2031-67-6	e1k	200	3	N	N
DTXSID7026867	Decanedioic acid	111-20-6	e1k	200	1	N	N
DTXSID6048204	4-Butylcyclohexanol	70568-60-4	e1k	200	5	N	N
DTXSID6042232	Hydroxycitronellal	107-75-5	e1k	200	5	N	N
DTXSID7025502	Linalool	78-70-6	e1k	200	-2	N	N
DTXSID7024821	1-Chloro-4-(trifluoromethyl)benzene	98-56-6	e1k	200	-3	N	N
DTXSID7025429	6-Hydroxy-2-naphthyl disulfide	6088-51-3	e1k	200	58	Y	N
DTXSID6042234	Octyl beta-D-glucopyranoside	29836-26-8	e1k	200	-2	N	N
DTXSID6041210	gamma-Terpinene	99-85-4	e1k	200	12	N	N
DTXSID6041719	C.I. Acid Yellow 17, disodium salt	6359-98-4	e1k	200	7	N	N
DTXSID7026314	Zinc pyrithione	13463-41-7	e1k	200	3	N	N
DTXSID6044430	1,2-Diphenylethanone	451-40-1	e1k	200	-7	N	N
DTXSID7021655	Pentanoic acid	109-52-4	e1k	200	1	N	N
DTXSID6043915	Hydroxyprogesterone caproate	630-56-8	e1k	200	3	N	N
DTXSID7020766	Propham	122-42-9	e1k	200	2	N	N
DTXSID6045400	Ronidazole	7681-76-7	e1k	200	-3	N	N
DTXSID6042369	Rhodamine B	81-88-9	e1k	200	16	N	N
DTXSID6048202	Isopropyl phenyl ketone	611-70-1	e1k	200	3	N	N
DTXSID6031380	Glycoluril	496-46-8	e1k	200	3	N	N
DTXSID7021815	3,4-Dichloroaniline	95-76-1	e1k	200	5	N	N
DTXSID6029755	Propylene glycol monobutyl ether	29387-86-8	e1k	200	3	N	N
DTXSID7022043	2,6-Pyridinedicarboxylic acid	499-83-2	e1k	200	-1	N	N
DTXSID7025506	Linolenic acid	463-40-1	e1k	200	43	Y	N
DTXSID6032518	4,5-Dichloro-3H-1,2-dithiol-3-one	1192-52-5	e1k	200	3	Y	N
DTXSID7026235	Trimellitic anhydride	552-30-7	e1k	200	-4	N	N
DTXSID6041422	7-(Dimethylamino)-4-methylcoumarin	87-01-4	e1k	200	3	N	N
DTXSID7025130	Dimethylnaphthalene	28804-88-8	e1k	200	9	N	N

DTXSID6048206	4-Chloropentylbenzene	79098-20-7	e1k	200	12	N	N
DTXSID7026811	Benzenethiol	108-98-5	e1k	200	10	N	N
DTXSID6041557	Dihydromyrcenol	53219-21-9	e1k	200	-2	N	N
DTXSID6032431	S-Metolachlor	87392-12-9	e1k	200	5	N	N
DTXSID6044303	Atorvastatin calcium	134523-03-8	e1k	180	5	N	N
DTXSID6034764	Nicosulfuron	111991-09-4	e1k	200	4	N	N
DTXSID6048200	2,4,6-Trimethylbenzoic acid	480-63-7	e1k	200	1	Y	N
DTXSID6042074	Isopropyl-o-cresol	499-75-2	e1k	200	3	N	N
DTXSID6040795	Chloramine-T trihydrate	7080-50-4	e1k	200	2	N	N
DTXSID7024031	(E)-1,2-Dichloroethylene	156-60-5	e1k	200	-5	N	N
DTXSID7025217	(2-Dodeceny)succinic anhydride	19780-11-1	e1k	200	15	N	N
DTXSID6042494	Trimethoxypropylsilane	1067-25-0	e1k	200	4	N	N
DTXSID7023192	Lactic acid	50-21-5	e1k	200	-3	N	N
DTXSID6041424	2,6-Dimethyl-2-heptanol	13254-34-7	e1k	200	-5	N	N
DTXSID7025427	2-Hydroxy-2-methylpropanenitrile	75-86-5	e1k	200	9	N	N
DTXSID7020843	Methyl linoleate	112-63-0	e1k	200	16	Y	N
DTXSID6047448	Potassium chlorate	3811-04-9	e1k	200	10	N	N
DTXSID7026285	Veratraldehyde	120-14-9	e1k	200	-6	N	N
DTXSID7020768	Kaempferol	520-18-3	e1k	143	11	N	N
DTXSID6041426	3,4-Dihydro-2H-pyran	110-87-2	e1k	200	0	N	N
DTXSID7026102	Tetrachlorophthalic anhydride	117-08-8	e1k	200	3	N	N
DTXSID6041472	3,5-Dimethyl-1-hexyn-3-ol	107-54-0	e1k	200	-1	N	N
DTXSID7021152	4-Phenylphenol	92-69-3	e1k	200	14	N	N
DTXSID7025003	2,5-Dichlorophenol	583-78-8	e1k	200	3	N	N
DTXSID6036467	Disodium 4,4'-bis(2-sulfostyryl)biphenyl	27344-41-8	e1k	200	94	Y	N
DTXSID6041715	C.I. Acid Violet 12, disodium salt	6625-46-3	e1k	190	11	Y	N
DTXSID7021788	3-Trifluoromethyl-4-nitrophenol	88-30-2	e1k	200	7	N	N
DTXSID7026368	Salicylic acid	69-72-7	e1k	200	3	N	N
DTXSID6028022	1-(Bromomethyl)-3-phenoxybenzene	51632-16-7	e1k	200	14	N	N
DTXSID7021364	2-Methylaniline hydrochloride	636-21-5	e1k	200	1	N	N

DTXSID7020683	Hexachloro-1,3-butadiene	87-68-3	e1k	200	5	N	N
DTXSID6027345	Triphenylborane	960-71-4	e1k	200	10	N	N
DTXSID6027713	Polyoxyethylene monooleate	9004-96-0	e1k	200 µg/ml	56	Y	N
DTXSID7022411	4,4'-Methylenebis(2,6-di- butylphenol)	118-82-1	e1k	200	10	N	N
DTXSID6041636	(+/-)-alpha-Methylbenzyl acetate	93-92-5	e1k	200	-1	N	N
DTXSID7038864	2,2'-Methylenebis(ethyl-6-tert- butylphenol)	88-24-4	e1k	1000	87	Y	N
DTXSID7027916	Neodecanoic acid	26896-20-8	e1k	200	1	N	N
DTXSID7041889	Diphenyl phosphite	4712-55-4	e1k	200	5	N	N
DTXSID7034549	Dinotofuran	165252-70-0	e1k	191	5	N	N
DTXSID7037262	Pregnenolone carbonitrile	1434-54-4	e1k	120	3	N	N
DTXSID8021224	C.I. Acid Red 114	6459-94-5	e1k	140	99	Y	N
DTXSID7034674	Ipconazole	125225-28-7	e1k	200	33	N	N
DTXSID7047433	Equilin	474-86-2	e1k	200	4	N	N
DTXSID7029611	Triethylene glycol dibenzoate	120-56-9	e1k	200	13	N	N
DTXSID7042196	Butyl lactate	138-22-7	e1k	200	6	N	N
DTXSID7027540	N-Butylbenzenesulfonamide	3622-84-2	e1k	200	1	N	N
DTXSID8021937	1-Heptanol	111-70-6	e1k	200	5	N	N
DTXSID7027388	Diisooctyl adipate	1330-86-5	e1k	200	8	N	N
DTXSID7029320	2-Ethylhexyl 4- (dimethylamino)benzoate	21245-02-3	e1k	200	15	N	N
DTXSID7029110	3,7-Dimethyl-3-octanol	78-69-3	e1k	200	4	N	N
DTXSID8024311	Sodium fluoroacetate	62-74-8	e1k	200	4	N	N
DTXSID7042011	N-Dodecanoyl-N-methylglycine	97-78-9	e1k	195	13	N	N
DTXSID8021062	N-Nitrosopyrrolidine	930-55-2	e1k	200	-6	N	N
DTXSID8021199	Pebulate	1114-71-2	e1k	200	9	N	N
DTXSID7030307	3,5-Dichloroaniline	626-43-7	e1k	200	4	N	N
DTXSID8022406	2,4-Dihydroxybenzophenone	131-56-6	e1k	200	-4	N	N
DTXSID8021804	Benzocaine	94-09-7	e1k	200	9	N	N
DTXSID7035010	Sodium warfarin	129-06-6	e1k	200	5	N	N

DTXSID7026946	Linalyl acetate	115-95-7	e1k	200	-6	N	N
DTXSID8024072	Diphenamid	957-51-7	e1k	200	-9	N	N
DTXSID7027887	Bis(2-ethylhexyl) tetrabromophthalate	26040-51-7	e1k	147	-1	N	N
DTXSID7047487	Sulfuric acid, monononyl ester, sodium salt	1072-15-7	e1k	200	8	N	N
DTXSID8020381	Deltamethrin	52918-63-5	e1k	200	5	N	N
DTXSID7041413	R-(-)-Carvone	6485-40-1	e1k	200	14	N	N
DTXSID7030060	2,2-Dichloropropane	594-20-7	e1k	200	-5	N	N
DTXSID7044394	4-tert-Butylcyclohexanone	98-53-3	e1k	200	-9	N	N
DTXSID8022408	Phenol red	143-74-8	e1k	200	0	N	N
DTXSID7032688	Phenothrin	26002-80-2	e1k	200	4	N	N
DTXSID7027756	3-Phenoxybenzenemethanol	13826-35-2	e1k	200	-5	N	N
DTXSID7044390	N-Methylhydrazinecarbothioamide	6610-29-3	e1k	200	-12	N	N
DTXSID8021856	4-Butylaniline	104-13-2	e1k	200	6	N	N
DTXSID7032559	ÃŹÃŹ»-Cyhalothrin	91465-08-6	e1k	171	2	N	N
DTXSID7038810	Divinyltetramethyldisiloxane	2627-95-4	e1k	200	-2	N	N
DTXSID8020591	Ethyl methylphenylglycidate	77-83-8	e1k	200	0	N	N
DTXSID7032345	Chlorhexidine diacetate	56-95-1	e1k	200	84	Y	N
DTXSID7044718	Acid Orange 156	68555-86-2	e1k	200	51	Y	N
DTXSID8022113	3,4-Dichloro-1-butene	760-23-6	e1k	204	-2	N	N
DTXSID8020044	Allyl alcohol	107-18-6	e1k	200	2	N	N
DTXSID7041544	6-Acetyl-1,1,2,4,4,7-hexamethyltetralin	21145-77-7	e1k	200	35	N	N
DTXSID7027461	Thiocarbazide	2231-57-4	e1k	200	10	N	N
DTXSID7027833	2-Ethyl-6-methylaniline	24549-06-2	e1k	200	5	N	N
DTXSID8021777	Riboflavin	83-88-5	e1k	188	52	Y	N
DTXSID7041962	Ethyltriethoxysilane	78-07-9	e1k	200	9	N	N
DTXSID7028774	C12-14-Alkyl glycidyl ether	68609-97-2	e1k	119	34	N	N
DTXSID8021931	1-Hexanol	111-27-3	e1k	200	-4	N	N
DTXSID7042198	N-Butyl-p-toluenesulfonamide	1907-65-9	e1k	200	2	N	N
DTXSID7037551	Fenuron	101-42-8	e1k	200	1	N	N

DTXSID7029162	3-Bromo-1-chloro-5,5-dimethylhydantoin	126-06-7	e1k	200	0	N	N
DTXSID7035272	2,6-Diisopropyl-naphthalene	24157-81-1	e1k	200	31	N	N
DTXSID8020834	Methyl carbamate	598-55-0	e1k	200	-3	N	N
DTXSID8020179	Diisopropanolamine	110-97-4	e1k	200	1	N	N
DTXSID7040360	Isoxadifen-ethyl	163520-33-0	e1k	200	4	N	N
DTXSID7032630	N-Benzyladenine	1214-39-7	e1k	200	-1	N	N
DTXSID7029164	Sodium 1,4-diisobutyl sulfosuccinate	127-39-9	e1k	200	0	N	N
DTXSID8020969	Nitroethane	79-24-3	e1k	200	-4	N	N
DTXSID8022589	Aminogluthethimide	125-84-8	e1k	200	-3	N	N
DTXSID8020915	1-Naphthaleneacetic acid	86-87-3	e1k	200	-6	N	N
DTXSID7042356	2-(3-Phenylpropyl)pyridine	2110-18-1	e1k	200	2	N	N
DTXSID7029661	3,5,5-Trimethyl-1-hexanol	3452-97-9	e1k	200	2	N	N
DTXSID8021517	Maleic acid	110-16-7	e1k	200	0	N	N
DTXSID7041675	Bornyl acetate	76-49-3	e1k	200	7	N	N
DTXSID8020466	N,N'-Diethylthiourea	105-55-5	e1k	200	-2	N	N
DTXSID7042061	Isobornyl acetate	125-12-2	e1k	200	-2	N	N
DTXSID7040285	2-Hydroxyacetophenone	118-93-4	e1k	200	1	N	N
DTXSID7027837	Tripropylene glycol	24800-44-0	e1k	200	-3	N	N
DTXSID7034383	Bispyribac-sodium	125401-92-5	e1k	200	13	N	N
DTXSID8021640	Nonanedioic acid	123-99-9	e1k	200	2	N	N
DTXSID8026694	2-Ethylhexyl acetate	103-09-3	e1k	200	-3	N	N
DTXSID9021639	Nonanal	124-19-6	e1k	200	19	Y	N
DTXSID9021348	Thiourea	62-56-6	e1k	200	10	N	N
DTXSID9025297	2-Ethylhexyl acrylate	103-11-7	e1k	200	9	N	N
DTXSID9020114	Auramine hydrochloride	2465-27-2	e1k	200	6	N	N
DTXSID8042189	N,N-Diisopropylaniline	4107-98-6	e1k	200	11	N	N
DTXSID8029157	2-(Phenylmethylene)-heptanal	122-40-7	e1k	200	30	N	N
DTXSID8041957	Ethyl orthoformate	122-51-0	e1k	200	6	N	N
DTXSID9021764	1-Amino-2-propanol	78-96-6	e1k	200	12	N	N
DTXSID9022100	4-Propylphenol	645-56-7	e1k	200	4	Y	N

DTXSID8042422	Styrene glycol	93-56-1	e1k	200	5	N	N
DTXSID8037754	2,4,6-Tris(allyloxy)-1,3,5-triazine	101-37-1	e1k	200	5	N	N
DTXSID8026698	4,4'-Dithiodimorpholine	103-34-4	e1k	200	1	N	N
DTXSID8041298	gamma-Caprolactone	695-06-7	e1k	200	1	Y	N
DTXSID8029153	Benzyl benzoate	120-51-4	e1k	200	10	N	N
DTXSID9022526	Benzylparaben	94-18-8	e1k	200	16	N	N
DTXSID8034324	Phoxim	14816-18-3	e1k	200	10	N	N
DTXSID8026141	Thioglycolic acid	68-11-1	e1k	200	5	N	N
DTXSID8035423	1,4-Dimethylnaphthalene	571-58-4	e1k	200	1	N	N
DTXSID8041610	Arabinose	147-81-9	e1k	200	-2	N	N
DTXSID9026342	2-Phenylethanol	60-12-8	e1k	200	-4	N	N
DTXSID9020409	Dibenz(a,h)anthracene	53-70-3	e1k	180	8	N	N
DTXSID9024691	Butyl glycidyl ether	2426-08-6	e1k	200	2	N	N
DTXSID9024194	Mecoprop	93-65-2	e1k	200	3	N	N
DTXSID8027292	Dibutyltin dichloride	683-18-1	e1k	200	3	N	N
DTXSID8042052	Indene	95-13-6	e1k	200	13	N	N
DTXSID8026228	Triethyl phosphate	78-40-0	e1k	200	-8	N	N
DTXSID8029159	2,6,8-Trimethyl-4-nonanol	123-17-1	e1k	200	20	N	N
DTXSID8044202	Octyl acetate	112-14-1	e1k	200	1	N	N
DTXSID8032675	Sulprofos	35400-43-2	e1k	200	1	N	N
DTXSID8027377	Dimethylaniline	1300-73-8	e1k	200	-3	Y	N
DTXSID8040484	Forskolin	66575-29-9	e1k	200	-6	N	N
DTXSID9025291	2-Ethylhexanal	123-05-7	e1k	209	-6	N	N
DTXSID8027793	N-(Cyclohexylthio)phthalimide	17796-82-6	e1k	200	13	N	N
DTXSID9021477	Sodium tetrafluoroborate	13755-29-8	e1k	200	2	N	N
DTXSID8042424	Sulfaquinoxaline	59-40-5	e1k	200	-3	N	N
DTXSID8027036	2,2-Dimethylpropane-1,3-diol	126-30-7	e1k	200	2	N	N
DTXSID8027402	Dimethyl isophthalate	1459-93-4	e1k	200	-2	N	N
DTXSID8029650	Menthol	1490-04-6	e1k	200	1	N	N
DTXSID8029105	4-Toluenesulfonamide	70-55-3	e1k	199	10	N	N
DTXSID9024986	4,4'-Dichlorodiphenyl sulfone	80-07-9	e1k	200	-4	N	N

DTXSID9022366	Estriol	50-27-1	e1k	200	-14	N	N
DTXSID8042399	Sodium abietate	14351-66-7	e1k	200	31	N	N
DTXSID9023833	Polydimethylsiloxane	9016-00-6	e1k	200	3	N	N
DTXSID8040775	Terpineol	8000-41-7	e1k	200	7	N	N
DTXSID9021922	2-(Ethylamino)ethanol	110-73-6	e1k	200	8	N	N
DTXSID8027032	2-Amino-2-methylpropan-1-ol	124-68-5	e1k	200	5	N	N
DTXSID8045191	Ranitidine	66357-35-5	e1k	200	10	N	N
DTXSID9025451	4-(2,6,6-Trimethyl-cyclohex-1-enyl)-but-3-en-2-one	14901-07-6	e1k	200	4	N	N
DTXSID8042426	Sulfosuccinic acid	5138-18-1	e1k	200	-3	N	N
DTXSID8042503	Tripropylene glycol butyl ether	55934-93-5	e1k	200	-4	N	N
DTXSID9025403	Hexyl benzoate	6789-88-4	e1k	200	14	N	N
DTXSID8041955	Ethyl diethanolamine	139-87-7	e1k	200	0	N	N
DTXSID8042187	N,N'-Dibutylthiourea	109-46-6	e1k	200	6	N	N
DTXSID8024993	Troclosene	2782-57-2	e1k	200	7	N	N
DTXSID9021847	Diphenyl oxide	101-84-8	e1k	200	6	N	N
DTXSID8042507	1-Phenylurea	64-10-8	e1k	191	3	N	N
DTXSID8026513	1,2,3,6-Tetrahydrophthalimide	85-40-5	e1k	200	-1	N	N
DTXSID8025886	Ethyl 3-phenylglycidate	121-39-1	e1k	200	10	N	N
DTXSID8042006	Glyceryl monoctanoate	26402-26-6	e1k	200	1	N	N
DTXSID8027826	Dicyclohexyl sodium sulfosuccinate	23386-52-9	e1k	200	1	N	N
DTXSID8026488	Camphene	79-92-5	e1k	200	11	N	N
DTXSID9025796	Nonane	111-84-2	e1k	200	-1	N	N
DTXSID8027454	N,N-Dimethylacetoacetamide	2044-64-6	e1k	200	-2	N	N
DTXSID8027246	2-Pyrrolidinone	616-45-5	e1k	200	5	N	N
DTXSID8047185	Isopentyl benzoate	94-46-2	e1k	200	13	N	N
DTXSID8034376	Denatonium benzoate	3734-33-6	e1k	200	6	N	N
DTXSID9021138	1,4-Benzenediamine	106-50-3	e1k	200	16	Y	N
DTXSID9020372	o,p'-DDD	53-19-0	e1k	200	30	N	N
DTXSID9022607	Anastrozole	120511-73-1	e1k	68	4	N	N
DTXSID9021897	3-Methylpyridine	108-99-6	e1k	200	3	N	N

DTXSID8041909	Dysprosium(III) chloride	10025-74-8	e1k	188	19	N	N
DTXSID9040710	Octamethyltrisiloxane	107-51-7	e1k	200	2	N	N
DTXSID9035175	Kinetin	525-79-1	e1k	200	0	N	N
DTXSID9041861	Diethyl phosphite	762-04-9	e1k	200	-7	N	N
DTXSID9042382	Tetrapropyl orthosilicate	682-01-9	e1k	200	-2	N	N
DTXSID9048190	Methyl abietate	127-25-3	e1k	200	30	N	N
DTXSID9029223	1,1-Bis(3,4-dimethylphenyl)ethane	1742-14-9	e1k	200	28	N	N
DTXSID9041815	3,3,5-Trimethylcyclohexanol	116-02-9	e1k	200	5	N	N
DTXSID9032531	Bromuconazole	116255-48-2	e1k	200	16	N	N
DTXSID9029302	2-Propyl-1-heptanol	10042-59-8	e1k	200	5	N	N
DTXSID9026841	Dihexyl hexanedioate	110-33-8	e1k	200	8	N	N
DTXSID9041289	Myristyltrimethylammonium chloride N,N,N-Trimethyltetradecan-1-aminium chloride	4574-04-3	e1k	177	78	Y	N
DTXSID9034282	4-Chlorophenoxyacetic acid	122-88-3	e1k	200	0	N	N
DTXSID9041237	alpha-Terpinene	99-86-5	e1k	200	13	N	N
DTXSID9029649	1,3-Benzenedimethanamine	1477-55-0	e1k	200	2	N	N
DTXSID9036226	Sodium octyl sulfate	142-31-4	e1k	200	4	N	N
DTXSID9040342	Butylene carbonate	4437-85-8	e1k	200	-7	N	N
DTXSID9044538	C.I. Disperse Orange 37	13301-61-6	e1k	200	72	Y	N
DTXSID9042415	Sodium 4-methylbenzenesulfonate	657-84-1	e1k	200	3	N	N
DTXSID9034361	Denatonium saccharide	90823-38-4	e1k	200	4	N	N
DTXSID9047590	2-Phenylethyl benzoate	94-47-3	e1k	200	1	N	N
DTXSID9037749	5-Chlorosalicylanilide	4638-48-6	e1k	200	11	Y	N
DTXSID9027528	3-(Methylthio)propanal	3268-49-3	e1k	200	0	N	N
DTXSID9027312	1-Phenoxy-2-propanol	770-35-4	e1k	200	-3	N	N
DTXSID9041653	Methyl 2,4-dihydroxy-3,6-dimethylbenzoate	4707-47-5	e1k	200	2	N	N
DTXSID9032535	Trinexapac-ethyl	95266-40-3	e1k	200	2	N	N
DTXSID9026500	2-(4-Tert-Butylbenzyl)propionaldehyde	80-54-6	e1k	200	49	N	N
DTXSID9026922	Tetraethylene glycol	112-60-7	e1k	200	0	N	N

DTXSID9034997	Tributyltetradecylphosphonium chloride	81741-28-8	e1k	200	102	Y	N
DTXSID9041368	5-Ethyl-5-methylhydantoin	5394-36-5	e1k	200	0	N	N
DTXSID9029146	4-Methylmorpholine	109-02-4	e1k	200	2	N	N
DTXSID9029304	Glyceryl stearates	11099-07-3	e1k	200	-1	N	N
DTXSID9047594	Sodium 4-octylbenzenesulfonate	6149-03-7	e1k	200	62	Y	N
DTXSID9048192	4-Butylchlorobenzene	15499-27-1	e1k	200	-1	N	N
DTXSID9048194	Heptanophenone	1671-75-6	e1k	200	24	N	N
DTXSID9032533	Chlorfenapyr	122453-73-0	e1k	200	17	N	N
DTXSID9027364	N,N-Dimethyloctanamide	1118-92-9	e1k	200	4	N	N
DTXSID9041491	3-Phenyl-2-propen-1-ol	104-54-1	e1k	200	-4	N	N
DTXSID9044823	Sodium methacrylate	5536-61-8	e1k	200	-1	N	N
DTXSID9048198	4-Propylcyclohexanone	40649-36-3	e1k	200	-1	N	N
DTXSID9027863	Polypropylene glycol	25322-69-4	e1k	200	-2	N	N
DTXSID9044825	3-tert-Butylphenol	585-34-2	e1k	200	6	N	N
DTXSID9047205	2-Ethylhexyl trans-4-methoxycinnamate	83834-59-7	e1k	200	17	Y	N
DTXSID9048196	4-tert-Butylbenzenethiol	2396-68-1	e1k	200	-3	N	N
DTXSID9047708	Igepal CO-890	NOCAS_47708	e1k	200 µg/ml	1	N	N
DTXSID9044536	1-(6-tert-Butyl-1,1-dimethyl-2,3-dihydro-1H-inden-4-yl)ethanone	13171-00-1	e1k	200	33	N	N
DTXSID9037745	4-tert-Butylphenyl salicylate	87-18-3	e1k	200	19	N	N
DTXSID9044902	Calcium neodecanoate	27253-33-4	e1k	200	-1	N	N
DTXSID9034317	Benzalkonium chloride	8001-54-5	e1k	200	93	Y	N
DTXSID9037539	Endosulfan I	959-98-8	e1k	200	28	N	N

Supplementary Table 3. Concentration-response results. All chemicals tested in concentration-response screening, including the 10 replicated test chemicals, 80 ToxCast chemicals that produced greater than 50% median inhibition in single-concentration screening, and 64 additional ToxCast chemicals that produced no or low to moderate inhibition in single-concentration screening; the 154 chemicals are organized by source, with name, CASRN, maximum concentration tested, median % inhibition at maximum concentration, and, absolute IC₂₀, absolute IC₅₀, and Hill slope for chemicals with Hill model as the best fit in ToxCast Pipeline (v2.0).

^a Source. Test indicates set of chemicals selected based on previous testing for IYD inhibition and were replicated across multiple chemical source plates. ToxCast Chemical sets: ph1v2 indicates ToxCast phase 1_v2 chemical library, ph2 indicates ToxCast phase 2 chemical library, ph3 indicates ToxCast phase 3 chemical library, and e1k indicates ToxCast e1k chemical library, all obtained via Dr. Ann Richard, EPA/ORD, Research Triangle Park, NC, USA. ^b Maximum concentration in concentration-response screening, in μM except indicated as $\mu\text{g/ml}$ for polyoxyethylene monoleate. ^c Median % inhibition at maximum tested concentration for each chemical in concentration-response testing, n = 3 replicates. ^d --, chemical did not produce an inhibition curve or the IC₂₀ or IC₅₀ could not be calculated because the curve did not reach 20% or 50% inhibition.

DSSTox_Substance_Id	Chemical	CASRN	Source ^a	Max conc., μM ^b	% Inhibition at max conc. ^c , median	IC ₂₀	IC ₅₀	Hillslope
DTXSID9021342	Bithionol	97-18-7	test	200	97	26.64	53.79	-1.9
DTXSID5033836	4-Nonylphenol	104-40-5	test	200	98	8.94	23.62	-1.4
DTXSID5032498	Triclosan	3380-34-5	test	200	112	10.41	28.71	-1.2
DTXSID4026181	Tribromsalan	87-10-5	test	200	98	87.80	105.00	-7.9
DTXSID2021781	Dibutyl phthalate	84-74-2	test	200	29	22.51	-- ^d	-8.0
DTXSID7020182	Bisphenol A	80-05-7	test	200	14	--	--	--
DTXSID5022308	Genistein	446-72-0	test	200	4	--	--	--
DTXSID3022162	Bromoxynil	1689-84-5	test	160	9	--	--	--
DTXSID8023848	Acetochlor	34256-82-1	test	200	8	--	--	--
DTXSID5041306	2,2',4,4'-Tetrahydroxybenzophenone	131-55-5	test	200	7	--	--	--
DTXSID1024174	Tribufos	78-48-8	ph1	200	13	--	--	--
DTXSID2021151	2-Phenylphenol	90-43-7	ph1	200	13	--	--	--
DTXSID2032500	Triflumizole	68694-11-1	ph1	200	21	--	--	--
DTXSID3024154	Iprodione	36734-19-7	ph1	200	6	--	--	--
DTXSID4022020	Bromacil	314-40-9	ph1	200	10	--	--	--
DTXSID4024270	Prochloraz	67747-09-5	ph1	200	5	--	--	--
DTXSID3031864	Perfluorooctanesulfonic acid	1763-23-1	ph1	168	25	91.95	--	-8.0
DTXSID2032392	Fenoxaprop-ethyl	66441-23-4	ph1	200	13	--	--	--
DTXSID4020450	Dicofol	115-32-2	ph1	200	46	72.02	220.73	-1.4
DTXSID2032390	Fenarimol	60168-88-9	ph1	200	0	--	--	--

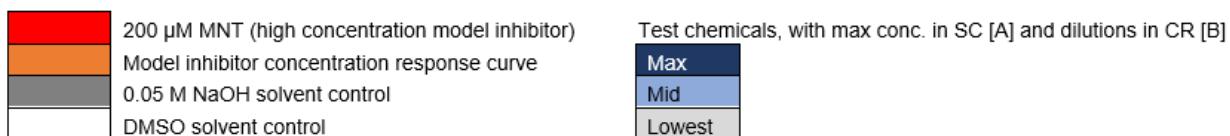
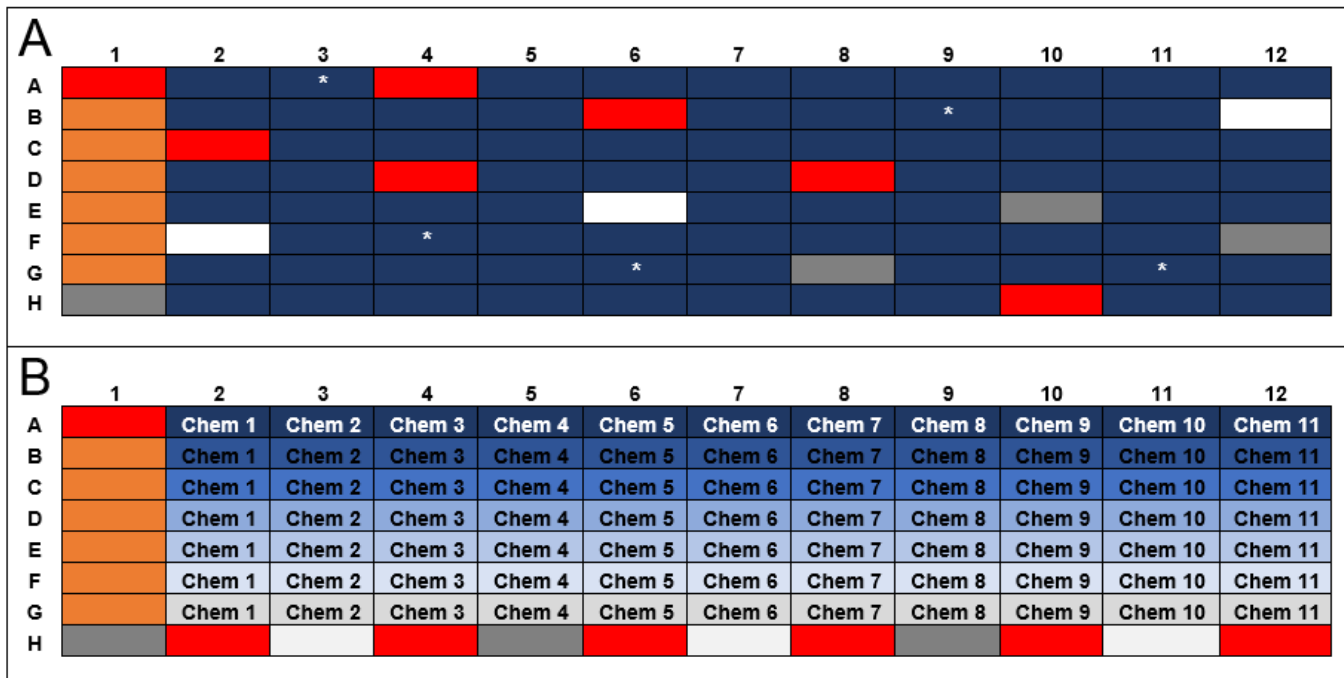
DTXSID4032372	Difenoconazole	119446-68-3	ph1	200	19	--	--	--
DTXSID5024211	Napropamide	15299-99-7	ph1	200	7	--	--	--
DTXSID4032667	Esfenvalerate	66230-04-4	ph1	200	10	--	--	--
DTXSID7031248	Diquat dibromide monohydrate	6385-62-2	ph1	100	98	5.77	11.67	-2.0
DTXSID5037523	Diazoxon	962-58-3	ph1	201	8	--	--	--
DTXSID8024109	Flutolanil	66332-96-5	ph1	200	9	--	--	--
DTXSID4024066	1,2-Dinitrobenzene	528-29-0	ph2	200	60	26.91	124.47	-1.0
DTXSID6032514	1,2-Benzenedicarboxaldehyde	643-79-8	ph2	200	76	26.71	77.13	-1.3
DTXSID9047259	1,3-Dichloro-6,7,8,9,10,12-hexahydroazepino[2,1-b]quinazoline hydrochloride (1:1)	149062-75-9	ph2	100	8	--	--	--
DTXSID1020807	2-Mercaptobenzothiazole	149-30-4	ph2	200	-5	--	--	--
DTXSID4024359	2,4,5-Trichlorophenol	95-95-4	ph2	200	22	247.71	--	-8.0
DTXSID7029241	2,4-Bis(1-methyl-1-phenylethyl)phenol	2772-45-4	ph2	200	80	12.29	42.67	-1.2
DTXSID6027052	2,6-Di-tert-butylphenol	128-39-2	ph2	200	39	102.92	--	-8.0
DTXSID2026602	2,4-Di-tert-butylphenol	96-76-4	ph2	200	82	41.25	92.21	-1.7
DTXSID1026081	3,3',5,5'-Tetrabromobisphenol A	79-94-7	ph2	191	105	24.12	59.82	-1.3
DTXSID9026974	2,4-Di-tert-pentylphenol	120-95-6	ph2	200	89	13.63	38.99	-1.3
DTXSID9022312	4-Octylphenol	1806-26-4	ph2	200	88	23.27	39.12	-2.9
DTXSID5029055	4-Nonylphenol, branched	84852-15-3	ph2	200	105	17.39	39.52	-1.6
DTXSID9022360	4-(1,1,3,3-Tetramethylbutyl)phenol	140-66-9	ph2	200	101	24.65	61.3	-1.3
DTXSID3037094	4-Hydroxytamoxifen	68392-35-8	ph2	50	16	--	--	--
DTXSID2037714	4-Heptylphenol	1987-50-4	ph2	200	98	22.85	50.71	-1.7
DTXSID0047377	AVE6324	NOCAS_47377	ph2	189	61	41.39	90.63	-2.8
DTXSID4024436	Allura Red C.I.16035	25956-17-6	ph2	200	46	130.82	220.85	-4.1
DTXSID8020337	Clomiphene citrate (1:1)	50-41-9	ph2	200	32	23.81	--	-1.4
DTXSID8022959	Docusate sodium	577-11-7	ph2	200	100	16.21	33.02	-1.9
DTXSID4020375	Dichlorodiphenyltrichloroethane	50-29-3	ph2	200	25	22.00	--	-8.0
DTXSID5027932	Dodecylbenzene sulfonate triethanolamine(1:1)	27323-41-7	ph2	180	92	48.75	86.66	-2.3
DTXSID6027923	Dodecylbenzenesulfonic acid	27176-87-0	ph2	200	102	20.11	34.55	-2.5

DTXSID9032537	Didecyldimethylammonium chloride	7173-51-5	ph2	200	98	25.18	60.08	-1.5
DTXSID1026900	Dodecyltrimethylammonium chloride	112-00-5	ph2	200	19	--	--	--
DTXSID1048174	FR167356	174185-16-1	ph2	200	0	--	--	--
DTXSID5020653	Gentian Violet	548-62-9	ph2	200	12	--	--	--
DTXSID8027955	Isooctyl acrylate	29590-42-9	ph2	200	4	--	--	--
DTXSID1048170	FR150011	149413-74-1	ph2	200	102	29.99	65.62	-1.6
DTXSID1020770	Kepone	143-50-0	ph2	200	95	7.58	33.41	-0.9
DTXSID6040371	Fenaminosulf	140-56-7	ph2	200	70	18.12	74.92	-1.1
DTXSID2020189	FD&C Blue No. 1	3844-45-9	ph2	200	42	60.60	777.39	-1.3
DTXSID5020944	Nitrofurazone	59-87-0	ph2	200	66	27.58	118.62	-1.0
DTXSID4042121	Mepanipirim	110235-47-7	ph2	200	10	--	--	--
DTXSID8047553	Perfluoroundecanoic acid	2058-94-8	ph2	200	73	23.50	55.35	-1.9
DTXSID4047337	PharmaGSID_47337	1061517-62-1	ph2	200	100	71.97	108.49	-3.1
DTXSID7021784	Salicylanilide	87-17-2	ph2	200	1	--	--	--
DTXSID4040713	Octyl gallate	1034-01-1	ph2	200	97	32.83	71.42	-1.7
DTXSID3031860	Perfluorodecanoic acid	335-76-2	ph2	200	91	21.70	48.02	-1.7
DTXSID1026031	Sodium dodecyl sulfate	151-21-3	ph2	200	96	27.01	65.24	-1.5
DTXSID4042416	Sodium myristyl sulfate	1191-50-0	ph2	200	104	11.25	25.73	-1.6
DTXSID7025219	Sodium dodecylbenzenesulfonate	25155-30-0	ph2	200	107	17.80	32.05	-2.3
DTXSID0042400	Sodium hexyldecyl sulfate	1120-01-0	ph2	100	102	14.49	29.5	-1.9
DTXSID8023719	Troglitazone	97322-87-7	ph2	200	114	51.32	80.53	-2.8
DTXSID1034187	Tamoxifen	10540-29-1	ph2	100	60	15.50	61.7	-1.2
DTXSID2026076	Tannic acid	1401-55-4	ph2	70	101	6.60	7.85	-8.0
DTXSID6047288	UK-337312	203942-49-8	ph2	200	91	13.86	47.1	-1.1
DTXSID8021301	Tamoxifen citrate	54965-24-1	ph2	183	46	44.20	404.17	-1.5
DTXSID4040767	3,5-Dichlorosalicyl-3,4-dichloroanilide	1154-59-2	ph3	200	95	33.46	75.99	-1.6
DTXSID2031089	D&C Red 27	13473-26-2	ph3	132	78	4.14	13.41	-1.2
DTXSID0041985	Fluorosalan	4776-06-1	ph3	200	85	49.75	101.06	-1.8
DTXSID0023296	Methylene blue	61-73-4	e1k	200	53	1.86	3.36	-3.1

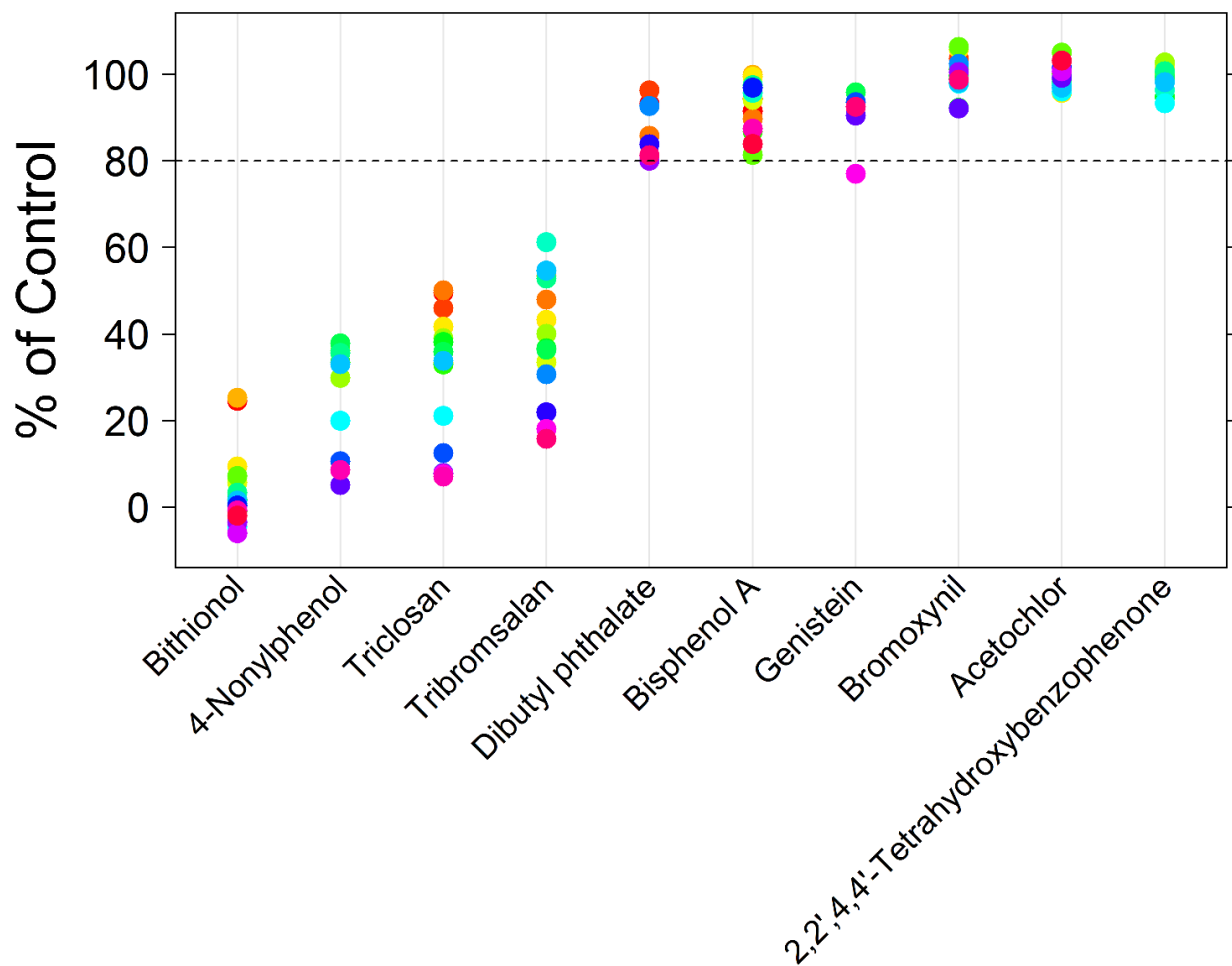
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DTXSID0042454	Tetradecanoic acid, 2,3-dihydroxypropyl ester	589-68-4	e1k	200	38	75.81	--	-2.2
DTXSID0047957	Octylparaben	1219-38-1	e1k	200	107	16.84	35.24	-1.8
DTXSID0042169	Monotridecyl phosphate	5116-94-9	e1k	200	107	20.88	37.6	-2.3
DTXSID1027891	Calcium dodecylbenzene sulfonate	26264-06-2	e1k	200	105	17.08	26.00	-3.2
DTXSID1027926	Dodecylphenol	27193-86-8	e1k	200	100	11.60	20.08	-2.5
DTXSID0048189	Lauryl gallate	1166-52-5	e1k	200	107	11.87	22.31	-2.2
DTXSID1022508	4-Dodecylphenol	104-43-8	e1k	200	99	6.92	23.09	-1.1
DTXSID1027134	Bis(2-ethylhexyl) phosphate	298-07-7	e1k	200	57	97.27	135.34	-8.0
DTXSID1025809	Oleic acid	112-80-1	e1k	200	89	21.29	34.10	-3.1
DTXSID1032648	Z-Tetrachlorvinphos	22248-79-9	e1k	200	10	--	--	--
DTXSID1048122	Benzyl-C8-18-alkyldimethylammonium chlorides	63449-41-2	e1k	200	101	33.69	71.72	-1.7
DTXSID2029298	Sodium lauryl polyoxyethylene ether sulfate	9004-82-4	e1k	200	97	42.62	74.57	-2.4
DTXSID2021602	Hexadecanoic acid	57-10-3	e1k	200	60	55.20	132.7	-2.2
DTXSID2027963	Isooctadecanoic acid	30399-84-9	e1k	200	104	20.82	39.24	-2.1
DTXSID2025505	Linoleic acid	60-33-3	e1k	200	77	97.31	119.22	-8.0
DTXSID1044487	Methyltrioctylammonium chloride	5137-55-3	e1k	200	101	7.68	26.09	-1.0
DTXSID2041252	1,4-Diaminoanthraquinone	128-95-0	e1k	200	20	--	--	--
DTXSID3021770	2,2',6,6'-Tetrachlorobisphenol A	79-95-8	e1k	200	75	86.37	138.68	-3.0
DTXSID2044713	Acid Red 337	67786-14-5	e1k	200	60	91.28	157.83	-3.0
DTXSID3027875	Glyceryl monooleate	25496-72-4	e1k	200	62	43.71	99.16	-2.1
DTXSID2036112	2-(8-Heptadecenyl)-2-imidazoline-1-ethanol	95-38-5	e1k	200	108	23.93	56.88	-1.4
DTXSID3020673	FD&C Green No. 3	2353-45-9	e1k	132	83	54.32	74.41	-4.1
DTXSID3040776	Morin hydrate	654055-01-3	e1k	200	70	101.68	127.56	-8
DTXSID3040352	Dinocap	39300-45-3	e1k	200	98	19.76	23.76	-8
DTXSID4022523	Heptylparaben	1085-12-7	e1k	200	97	16.14	45.84	-1.2
DTXSID4035708	Methylbenzethonium chloride	25155-18-4	e1k	1000	105	13.55	32.22	-1.6

DTXSID4020870	2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	119-47-1	e1k	200	92	7.75	28.94	-1.0
DTXSID4027076	Dodecyl sulfate triethanolamine	139-96-8	e1k	200	81	28.52	70.62	-1.6
DTXSID4022525	2-Ethylhexylparaben	5153-25-3	e1k	200	103	27.13	44.07	-2.8
DTXSID3041611	Ascorbyl palmitate	137-66-6	e1k	200	48	18.27	159.56	-1.8
DTXSID3041409	2-Chloro-N-phenylacetamide	587-65-5	e1k	200	6	--	--	--
DTXSID3047425	4-Butylphenol	1638-22-8	e1k	200	25	167.44	--	-6.5
DTXSID5020029	Acrylonitrile	107-13-1	e1k	200	5	--	--	--
DTXSID4048193	4,4'-Di-tert-butylbiphenyl	1625-91-8	e1k	200	6	--	--	--
DTXSID5034981	Tributyltin benzoate	4342-36-3	e1k	200	14	--	--	--
DTXSID4042418	Sodium tridecyl sulfate	3026-63-9	e1k	200	107	16.06	31.66	-2.0
DTXSID5022437	Nordihydroguaiaietic acid	500-38-9	e1k	200	26	129.69	--	-7.9
DTXSID5032315	4,5-Dichloro-2-octyl-3(2H)-isothiazolone	64359-81-5	e1k	200	33	132.86	647.73	-2.8
DTXSID4042171	4-Dodecylmorpholine	1541-81-7	e1k	200	45	49.09	442.07	-1.0
DTXSID5041726	C.I. Direct Red 81 disodium salt	2610-11-9	e1k	200	98	73.18	87.40	-8.0
DTXSID5042243	Oleyl sarcosine	110-25-8	e1k	200	99	21.00	54.51	-1.3
DTXSID5044865	2,2'-(Tetradecylimino)diethanol	18924-66-8	e1k	200	62	11.93	103.99	-0.7
DTXSID5035589	Disiquonium chloride	68959-20-6	e1k	200	69	32.99	100.59	-1.3
DTXSID6024624	Bisphenol A diglycidyl ether	1675-54-3	e1k	200	9	--	--	--
DTXSID5037028	Hexadecyltrimethylammonium bromide	57-09-0	e1k	200	104	20.72	24.73	-7.7
DTXSID6021666	Tetradecanoic acid	544-63-8	e1k	200	66	53.89	124.40	-1.9
DTXSID6021824	Dichlorophen	97-23-4	e1k	200	47	94.60	594.89	-2.4
DTXSID6041682	Bromophenol blue	115-39-9	e1k	186	74	85.05	105.84	-8.0
DTXSID6047103	Octadecyl sulfate sodium salt	1120-04-3	e1k	200	69	6.61	41.02	-0.8
DTXSID7020425	Dichlone	117-80-6	e1k	200	33	72.55	--	-1.1
DTXSID7025429	6-Hydroxy-2-naphthyl disulfide	6088-51-3	e1k	200	52	29.89	187.96	-0.8
DTXSID7025506	Linolenic acid	463-40-1	e1k	200	8	--	--	--
DTXSID6032518	4,5-Dichloro-3H-1,2-dithiol-3-one	1192-52-5	e1k	200	7	--	--	--
DTXSID6048200	2,4,6-Trimethylbenzoic acid	480-63-7	e1k	200	1	--	--	--

DTXSID7020843	Methyl linoleate	112-63-0	e1k	200	27	130.42	--	-2.2
DTXSID6036467	Disodium 4,4'-bis(2-sulfoxyethyl)phenyl	27344-41-8	e1k	200	102	50.75	88.84	-2.3
DTXSID6041715	C.I. Acid Violet 12, disodium salt	6625-46-3	e1k	190	29	102.80	--	-0.8
DTXSID6027713	Polyoxyethylene monoleate	9004-96-0	e1k	200 µg/ml	39	107.26	--	-8
DTXSID7038864	2,2'-Methylenebis(ethyl-6-tert-butylphenol)	88-24-4	e1k	1000	87	42.50	113.84	-1.5
DTXSID8021224	C.I. Acid Red 114	6459-94-5	e1k	140	103	18.01	36.87	-1.7
DTXSID7032345	Chlorhexidine diacetate	56-95-1	e1k	200	69	32.02	77.69	-1.9
DTXSID7044718	Acid Orange 156	68555-86-2	e1k	200	10	--	--	--
DTXSID8021777	Riboflavin	83-88-5	e1k	188	35	97.7	--	-1.9
DTXSID9021639	Nonanal	124-19-6	e1k	200	-1	--	--	--
DTXSID9022100	4-Propylphenol	645-56-7	e1k	200	-4	--	--	--
DTXSID8041298	gamma-Caprolactone	695-06-7	e1k	200	1	--	--	--
DTXSID8027377	Dimethylaniline	1300-73-8	e1k	200	-3	--	--	--
DTXSID9021138	1,4-Benzenediamine	106-50-3	e1k	200	9	--	--	--
DTXSID9041289	Myristyltrimethylammonium chloride N,N,N-Trimethyltetradecan-1-aminium chloride	4574-04-3	e1k	177	56	75.17	164.09	-2.3
DTXSID9044538	C.I. Disperse Orange 37	13301-61-6	e1k	200	45	123.08	--	-7.8
DTXSID9037749	5-Chlorosalicylanilide	4638-48-6	e1k	200	2	--	--	--
DTXSID9034997	Tributyltetradecylphosphonium chloride	81741-28-8	e1k	200	96	55.23	94.40	-2.4
DTXSID9047594	Sodium 4-octylbenzenesulfonate	6149-03-7	e1k	200	44	101.18	--	-7.9
DTXSID9047205	2-Ethylhexyl trans-4-methoxycinnamate	83834-59-7	e1k	200	5	--	--	--
DTXSID9034317	Benzalkonium chloride	8001-54-5	e1k	200	72	41.35	98.48	-1.8



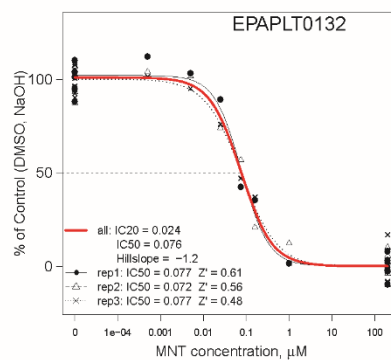
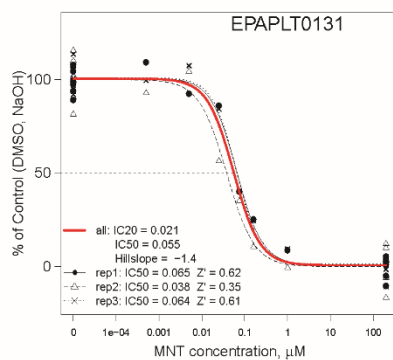
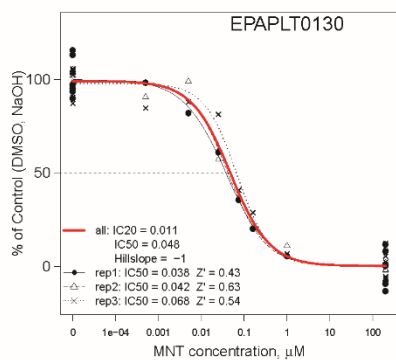
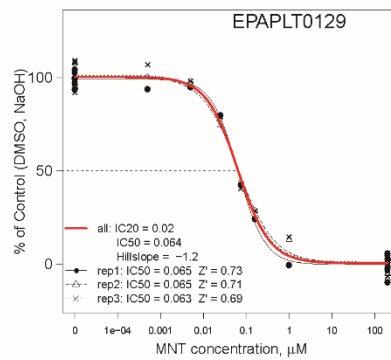
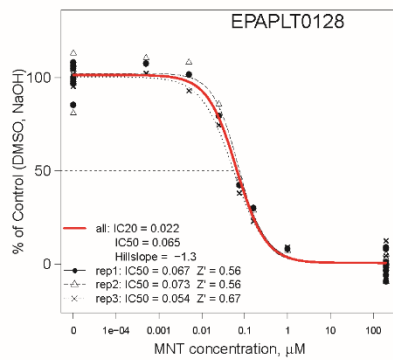
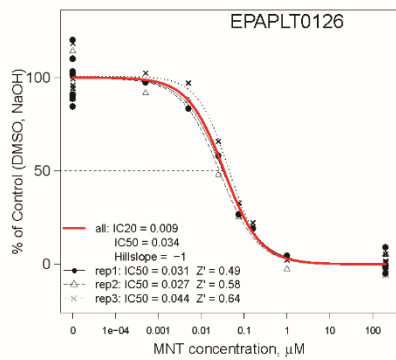
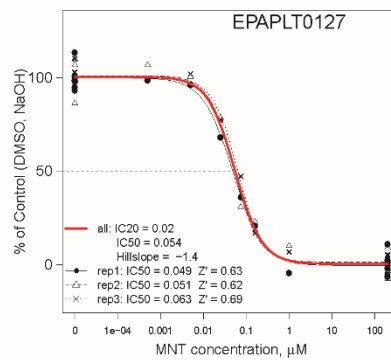
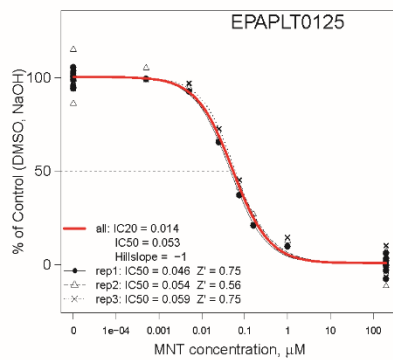
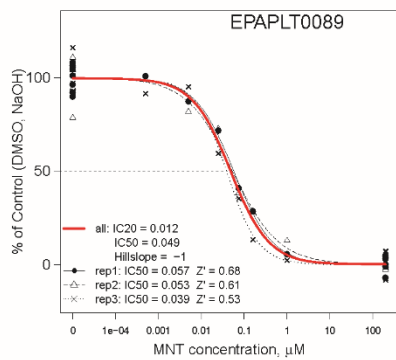
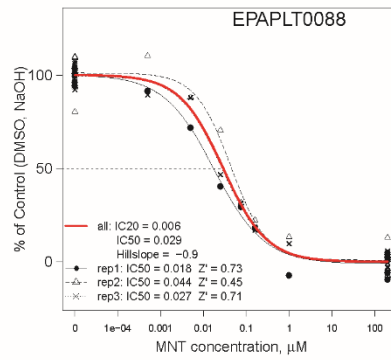
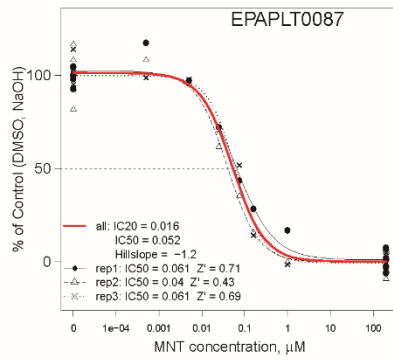
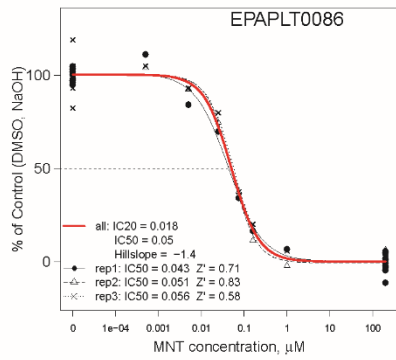
Supplementary Figure 1. Example layouts for assay plates: [A] Single-concentration screening at a target concentration of 200 μ M. Chemical source plates were received with column 1 empty for the concentration-response curve for the model inhibitor, 3-Nitro-L-tyrosine (MNT) from the high concentration of 200 μ M. Twelve additional wells were left empty on the source plate to which dimethyl sulfoxide (DMSO) was added to 3 wells (white blocks), 0.05 M sodium hydroxide (NaOH) was added to 3 wells (medium grey blocks), and the model inhibitor MNT (red blocks) was added to the remaining 6 wells to establish the fully inhibited response level. Chemicals from the replicated test-set were repeated across multiple plates and example wells for these chemicals are indicated with an asterisk. These were randomly assigned to wells on each plate. [B] Concentration-response screening with seven concentrations in serial dilutions from maximum tested concentration. The concentration-response curve for the model inhibitor, MNT was in column 1. Row H had 3 DMSO wells (white blocks), 3 0.05 M NaOH wells (medium grey blocks), and 6 model inhibitor MNT wells (red blocks). Final MNT concentrations in column 1 were 200, 1.0, 0.16, 0.075, 0.025, 0.005, and 0.0005 μ M from highest (row A) to lowest (row G). Column 1 row H contained 0.05 M NaOH.

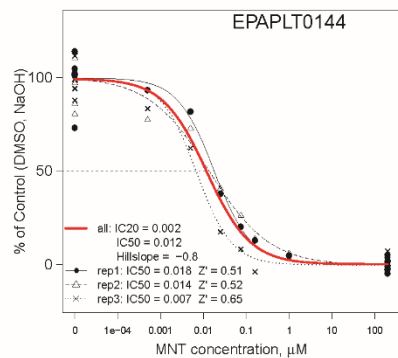
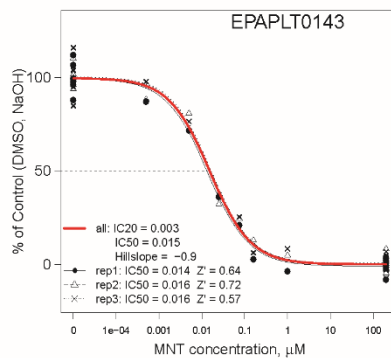
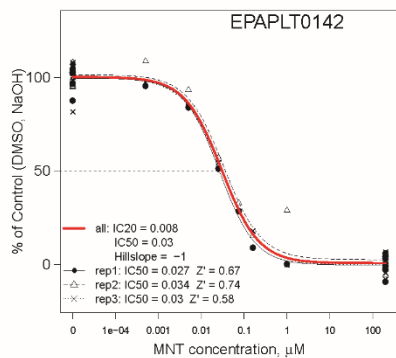
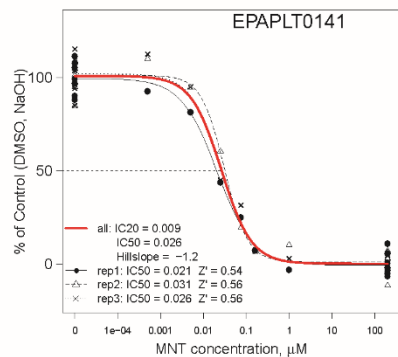
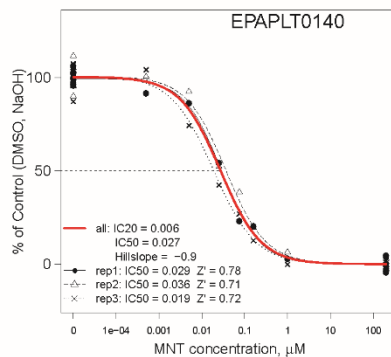
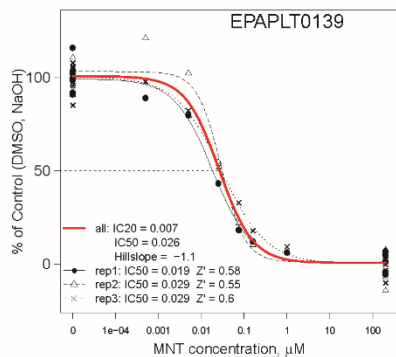
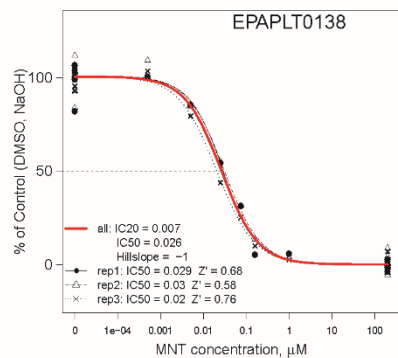
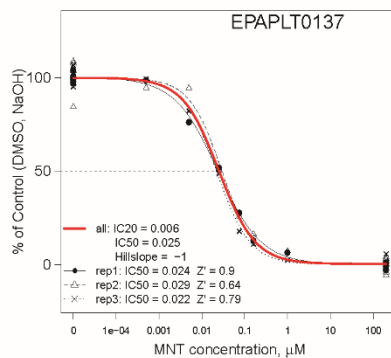
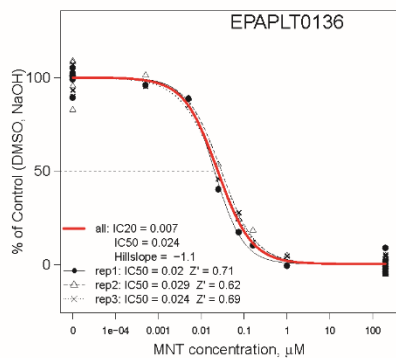
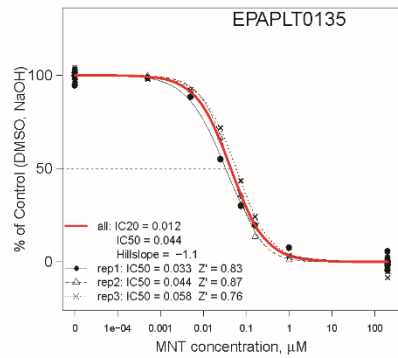
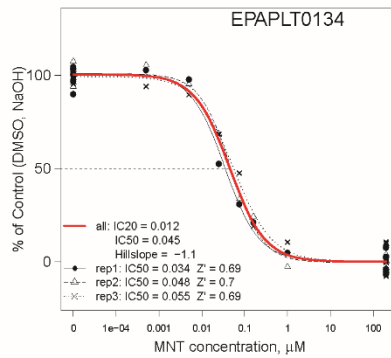
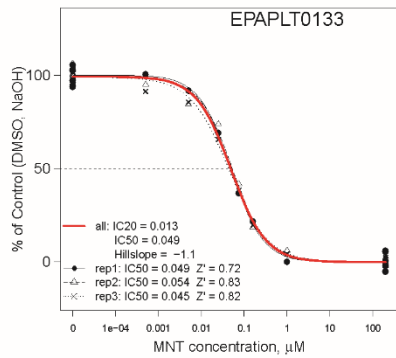


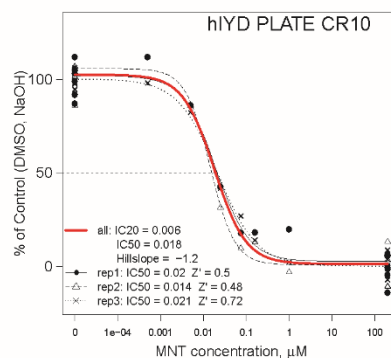
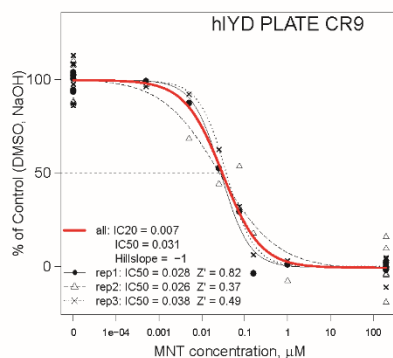
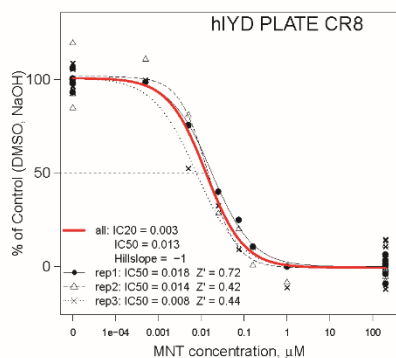
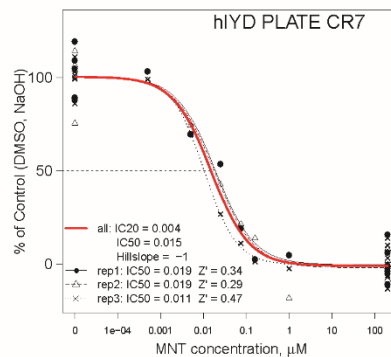
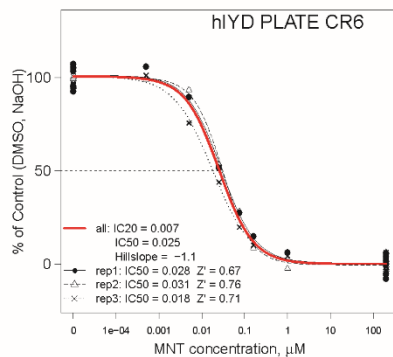
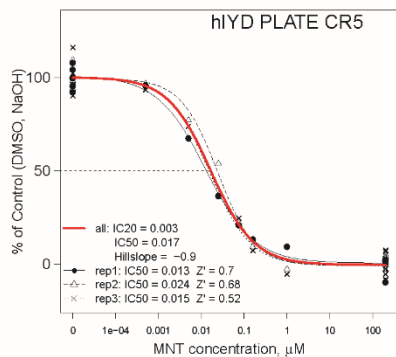
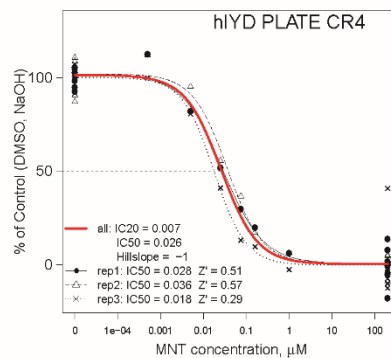
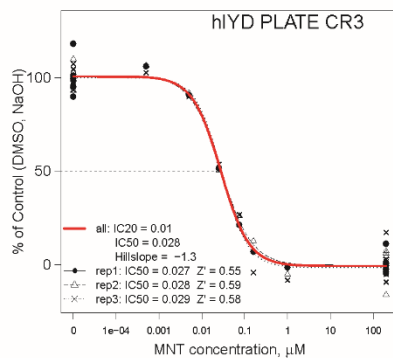
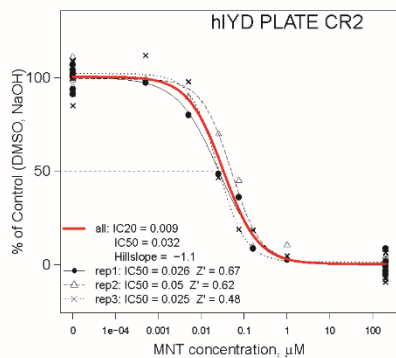
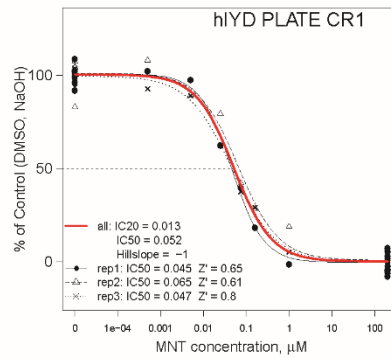
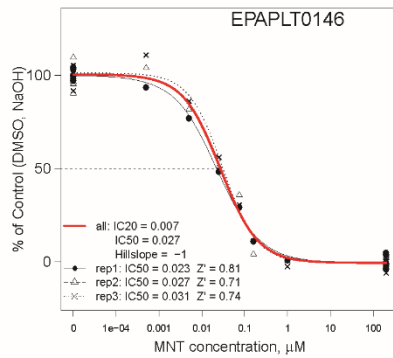
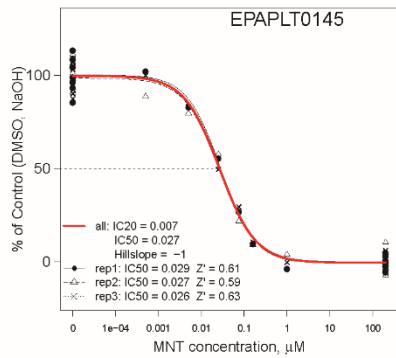
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| EPAPLT0087 | ● | EPAPLT0129 | ● | EPAPLT0136 | ● | EPAPLT0143 | ● |
| EPAPLT0088 | ● | EPAPLT0130 | ● | EPAPLT0137 | ● | EPAPLT0144 | ● |
| EPAPLT0089 | ● | EPAPLT0131 | ● | EPAPLT0138 | ● | EPAPLT0145 | ● |
| EPAPLT0125 | ● | EPAPLT0132 | ● | EPAPLT0139 | ● | EPAPLT0146 | ● |
| EPAPLT0126 | ● | EPAPLT0133 | ● | EPAPLT0140 | ● | | |
| EPAPLT0127 | ● | EPAPLT0134 | ● | EPAPLT0141 | ● | | |

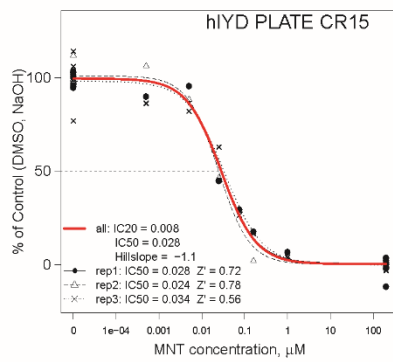
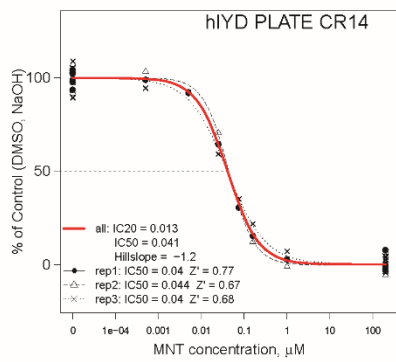
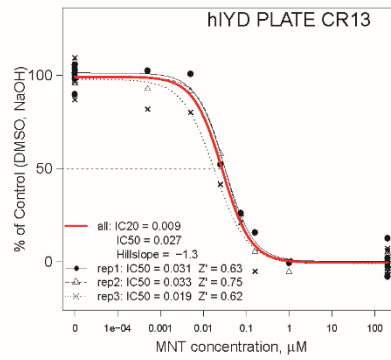
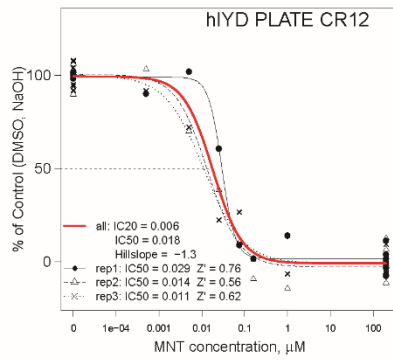
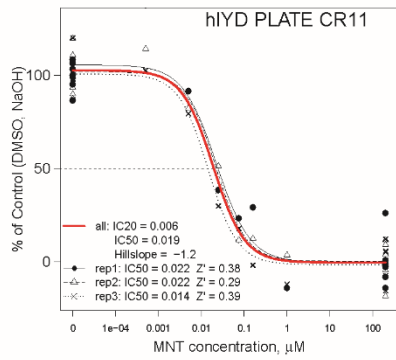
Supplementary Figure 2. Single-concentration screening results for the 10 test chemicals replicated across multiple chemical source plates (represented by different colors) to evaluate the plate-to-plate variability. Deiodinase inhibition produced by test chemicals that were randomly replicated across the chemical source plates. The following chemicals were included: Tribromsalan (CASRN: 87-10-5), Bithionol (CASRN: 97-18-7), Triclosan (CASRN: 3380-34-5), Bromoxynil (CASRN: 1689-84-5), Bisphenol A (80-05-7), Dibutyl phthalate (84-74-2), Acetochlor (34256-82-1), Genistein (446-72-0), 4-nonylphenol (104-40-5), 2,2',4,4'-Tetrahydroxybenzophenone (131-55-5), based on availability for plating on the chemical source plates and previous testing for IYD inhibition in Shimizu et al. (2013) or Renko et al. (2016).

Supplementary Figure 3. Concentration-response curves for inhibition of IYD by model inhibitor MNT for all single-concentration and concentration-response assay plates, with multiple plates included on each of the following four pages. Each triplicate test of a plate has different symbols and fit line, solid circle with solid line = rep 1, open triangle with dashed line = rep 2, × with dotted line = rep 3. DMSO = dimethyl sulfoxide; NaOH = sodium hydroxide.





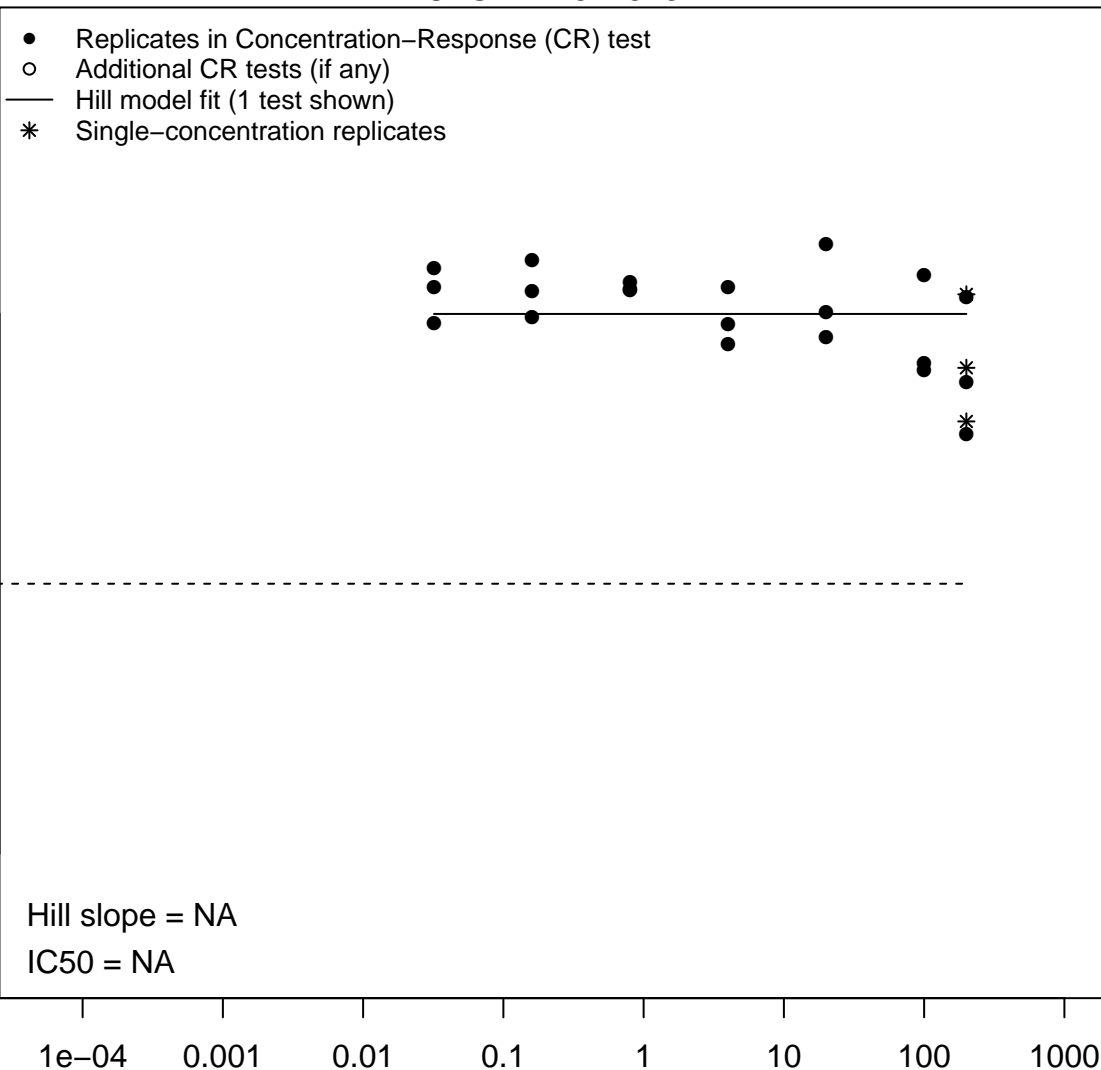




Supplementary Figure 4. Concentration-response screening data. Inhibition of iodotyrosine deiodinase (IYD) produced by all chemicals tested in concentration-response (CR) screening at seven concentrations. Hill model curve, absolute IC_{50} , and Hill slope included for the chemicals where Hill model fit in ToxCast pipeline (tpl v2.0); the following 154 pages include CR results for one chemical per page. DMSO = dimethyl sulfoxide; NaOH = sodium hydroxide. NA = not applicable (Hill model did not fit data and/or 50% inhibition not produced in concentration-response testing).

Tribufos

CASRN: 78-48-8



Bithionol

CASRN: 97-18-7

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100

50

0

Hill slope = -1.9

IC50 = 53.8

1e-04

0.001

0.01

0.1

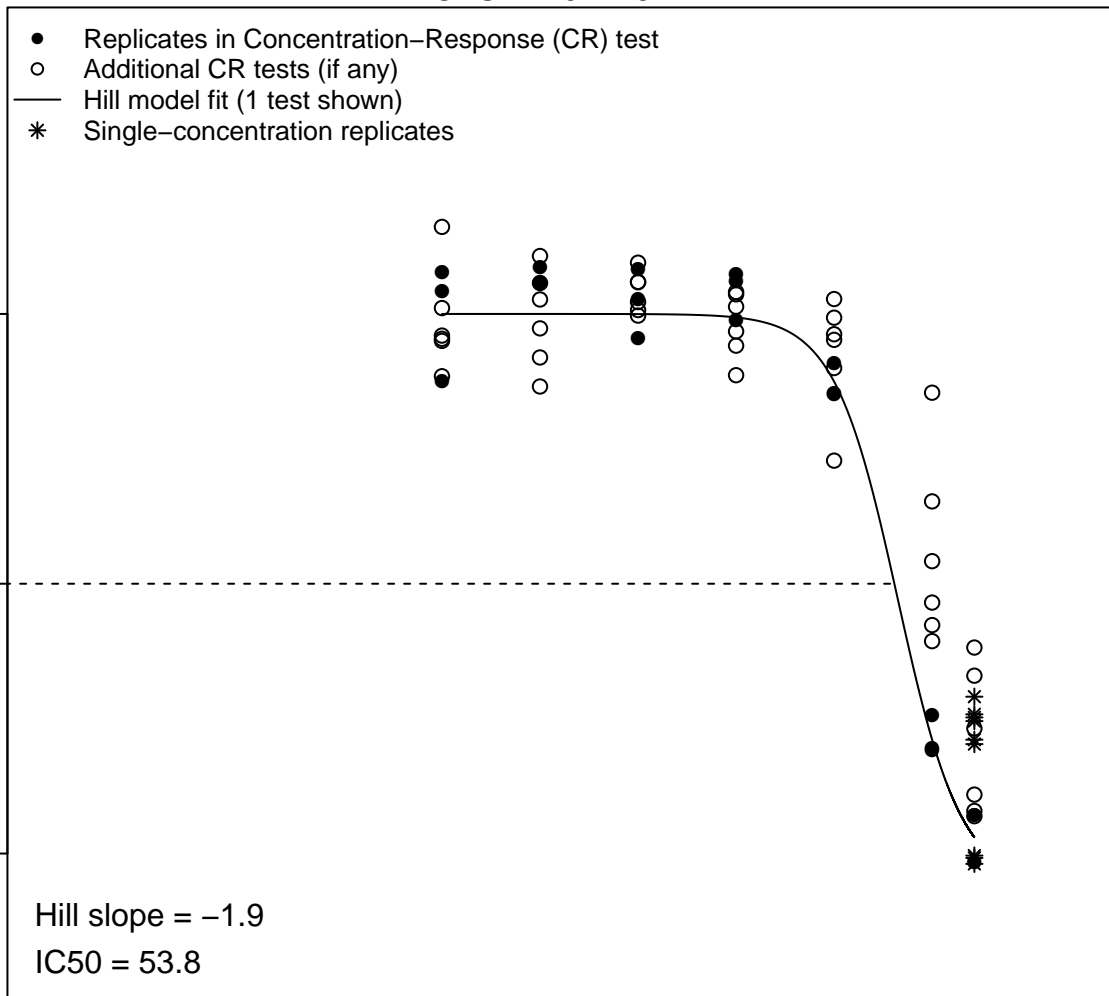
1

10

100

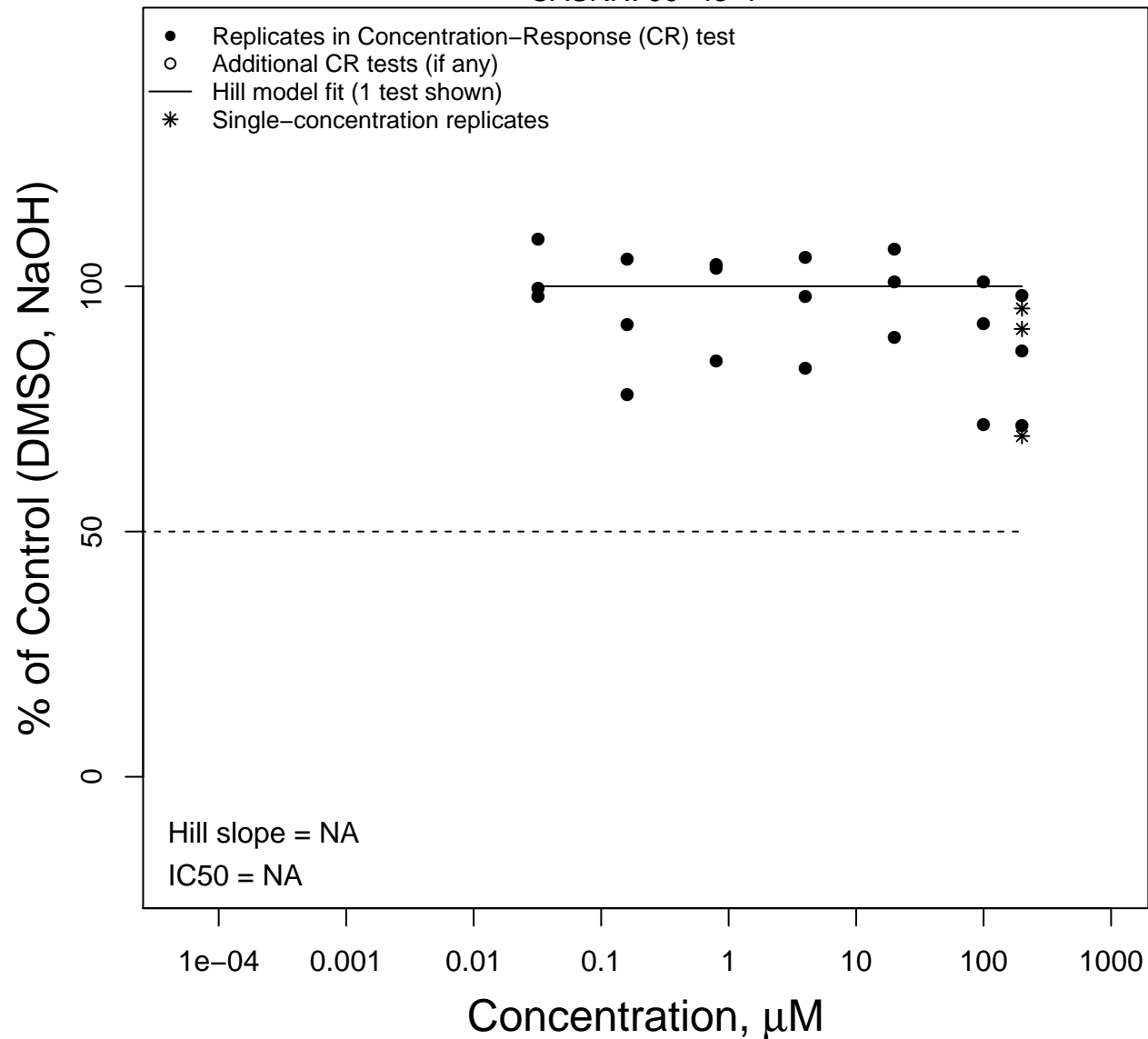
1000

Concentration, μM



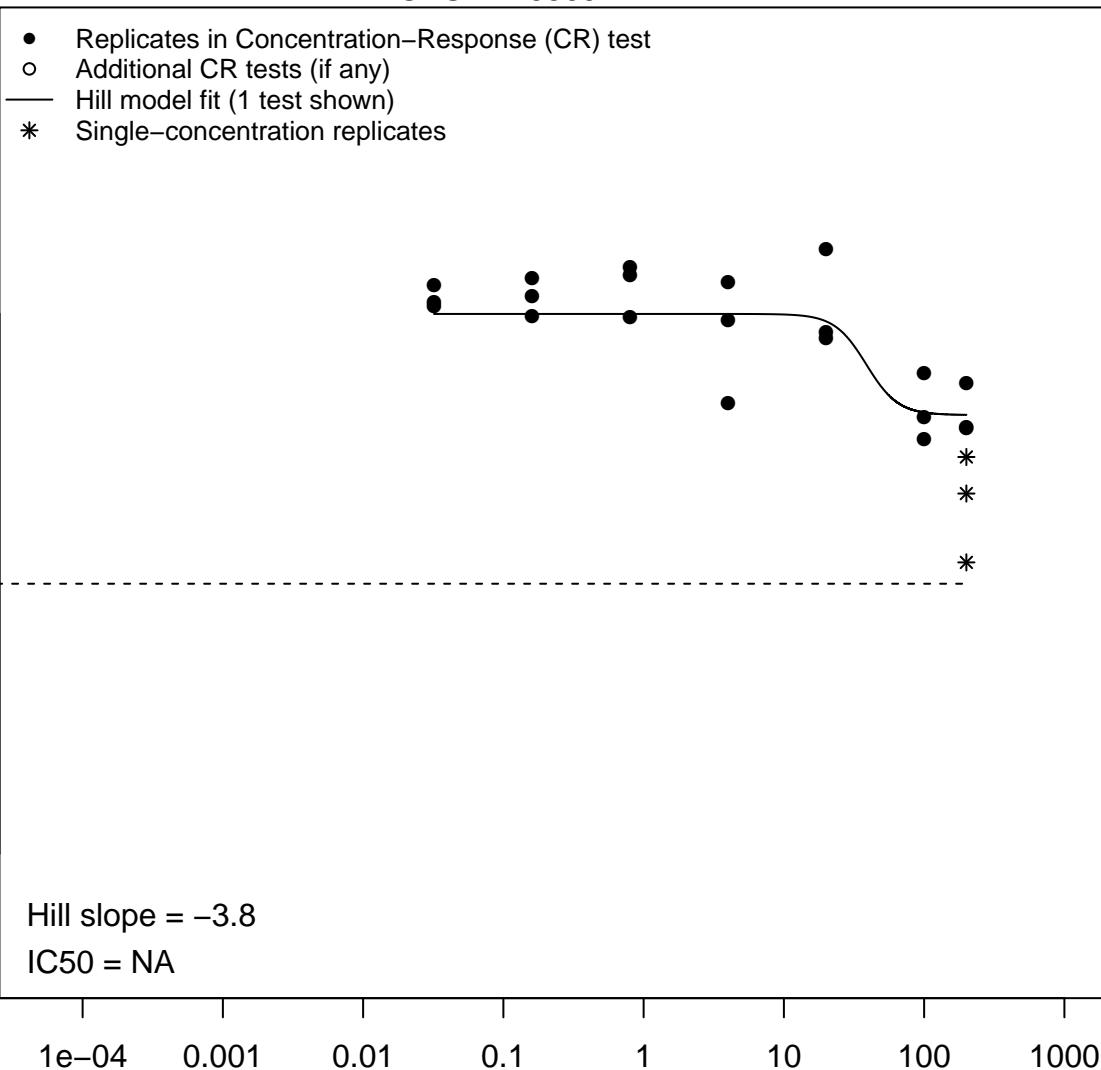
2-Phenylphenol

CASRN: 90-43-7



Triflumizole

CASRN: 68694-11-1

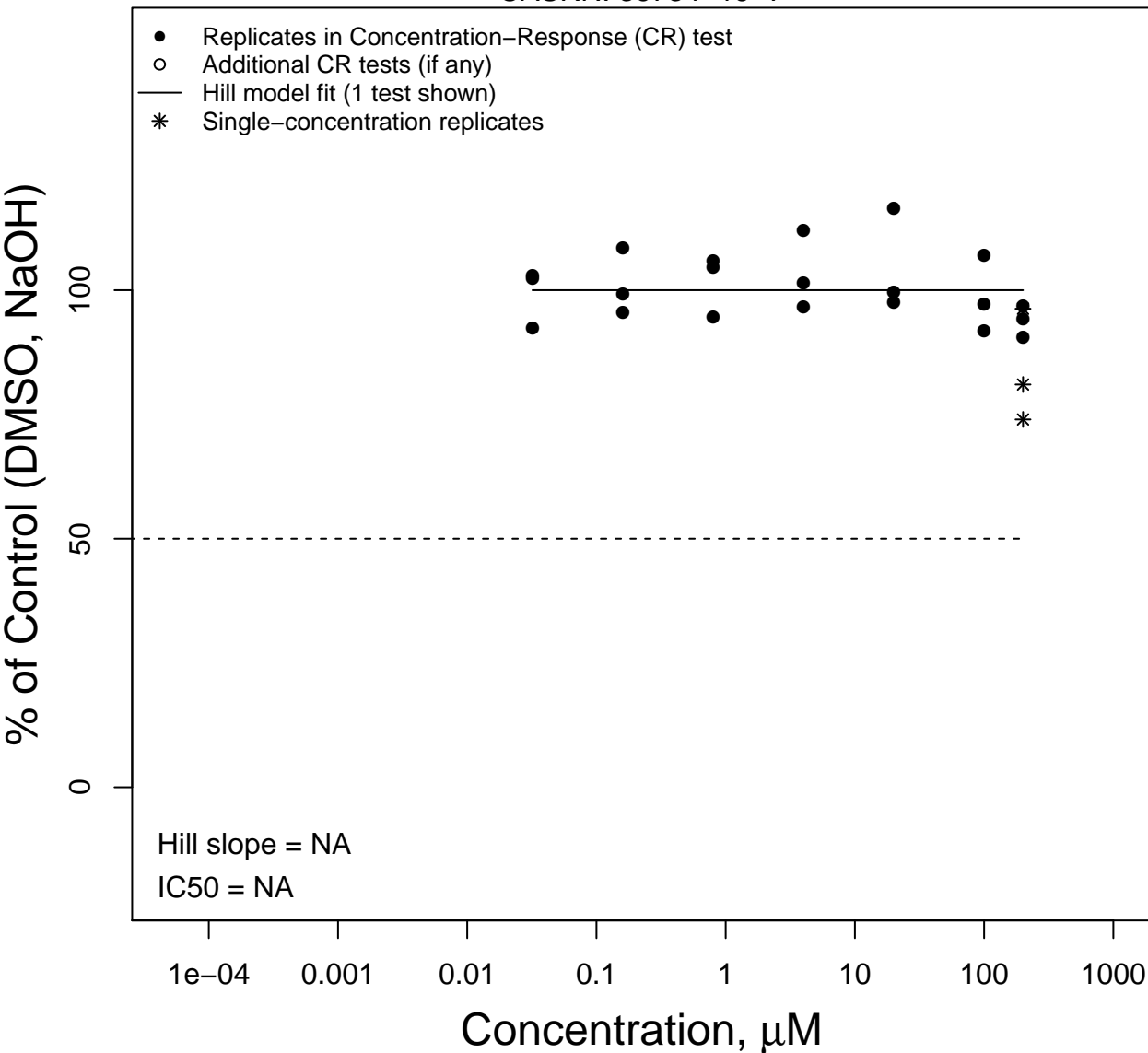


Concentration, µM

% of Control (DMSO, NaOH)

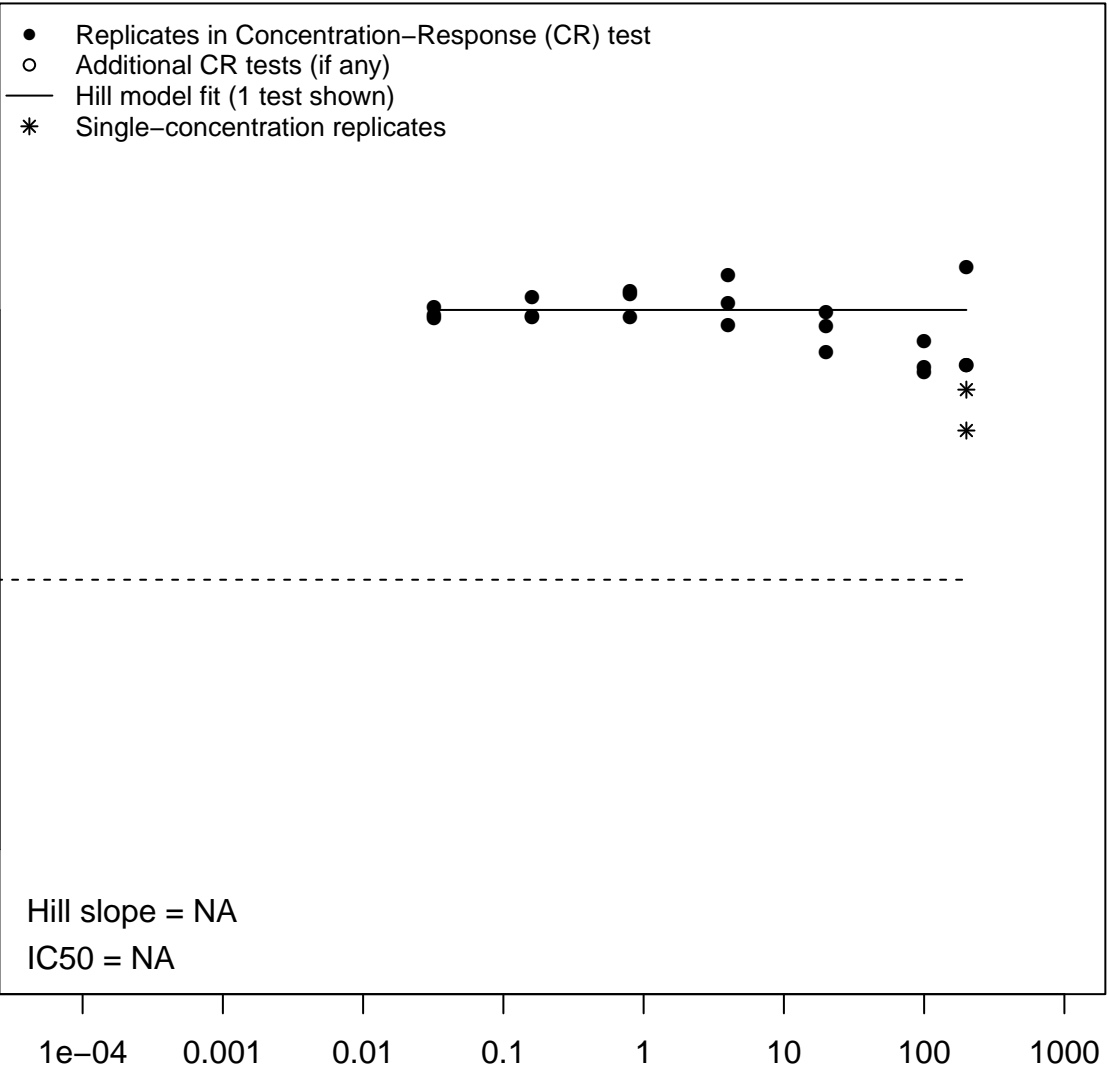
Iprodione

CASRN: 36734-19-7



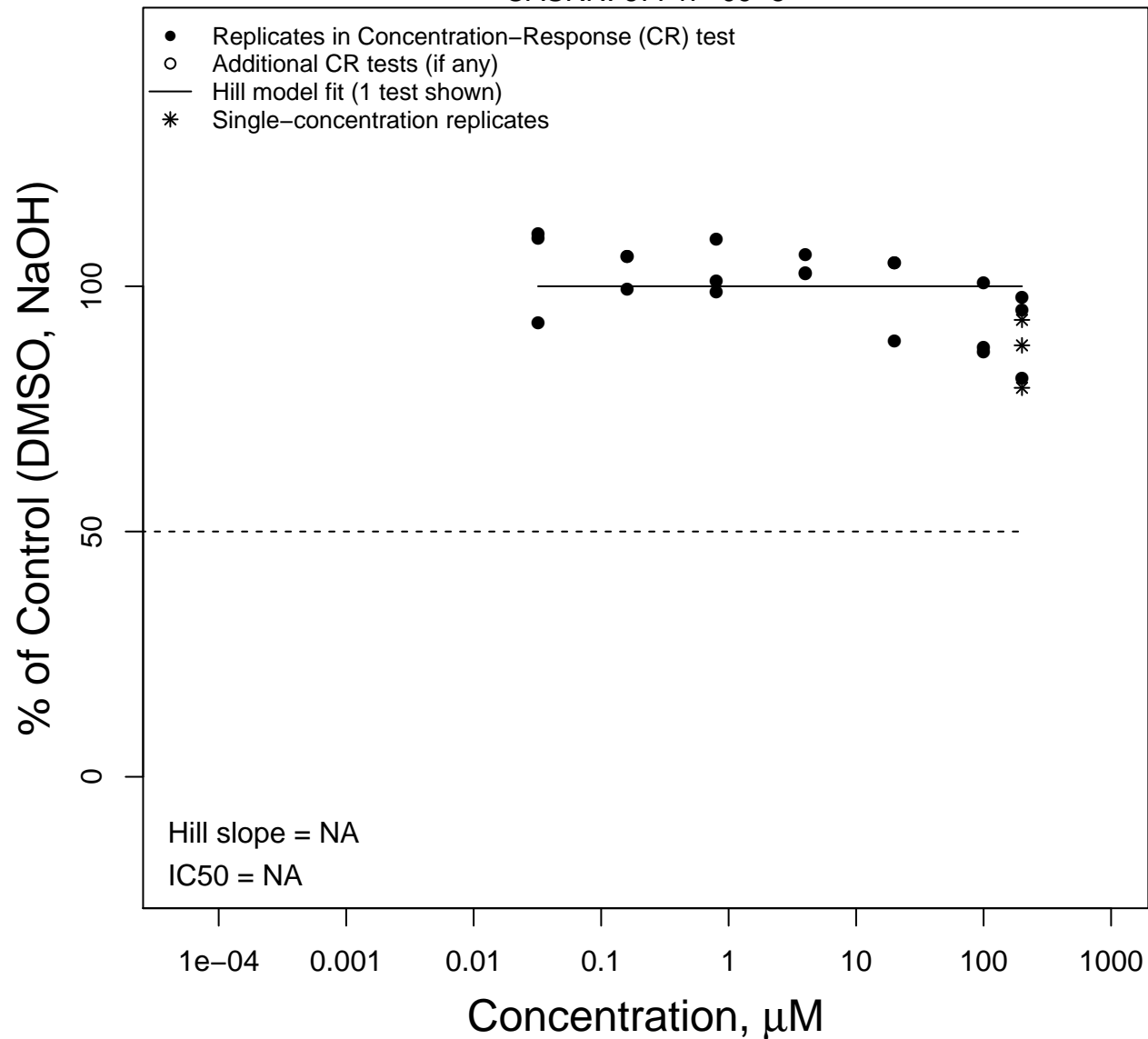
Bromacil

CASRN: 314-40-9



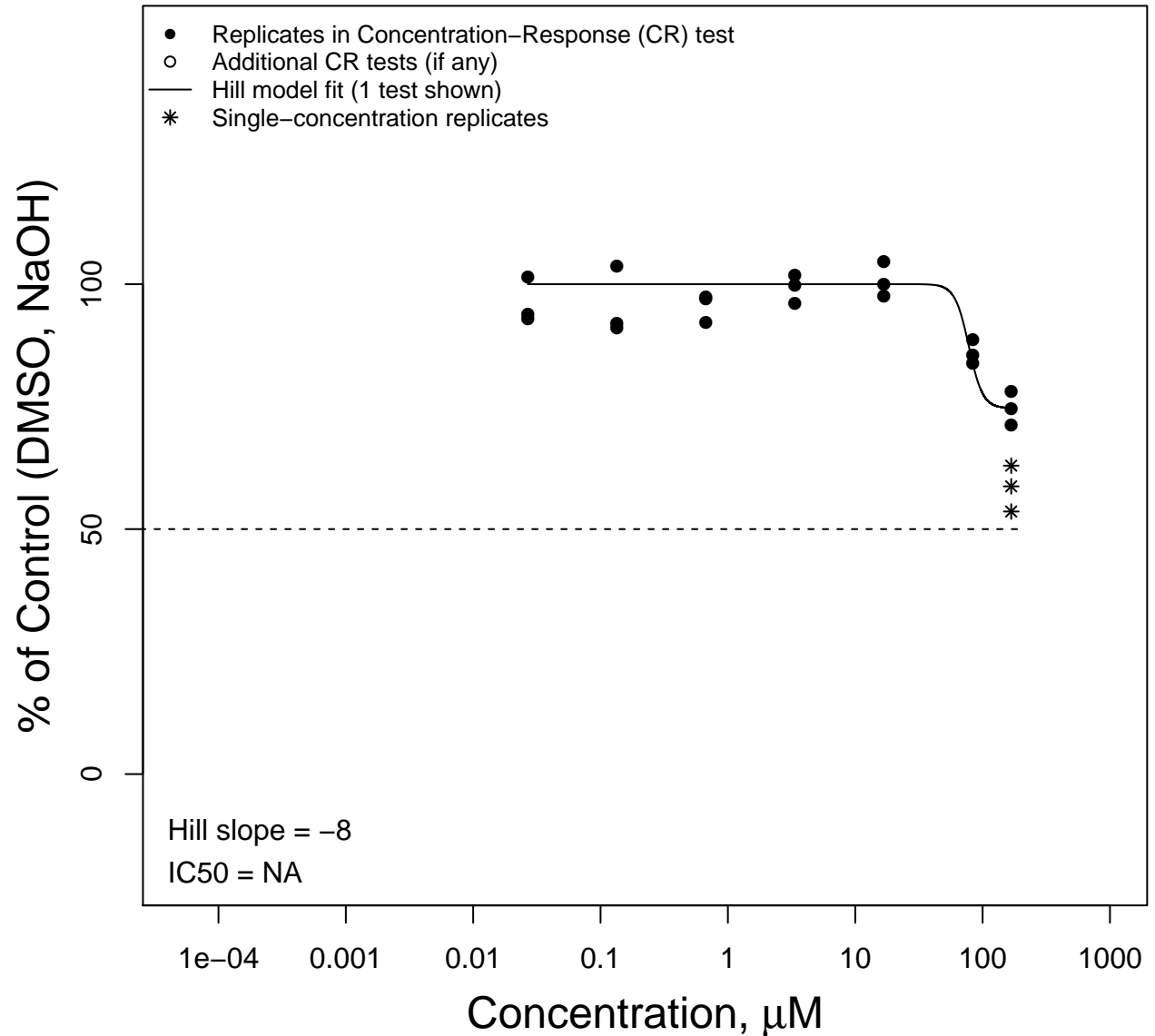
Prochloraz

CASRN: 67747-09-5



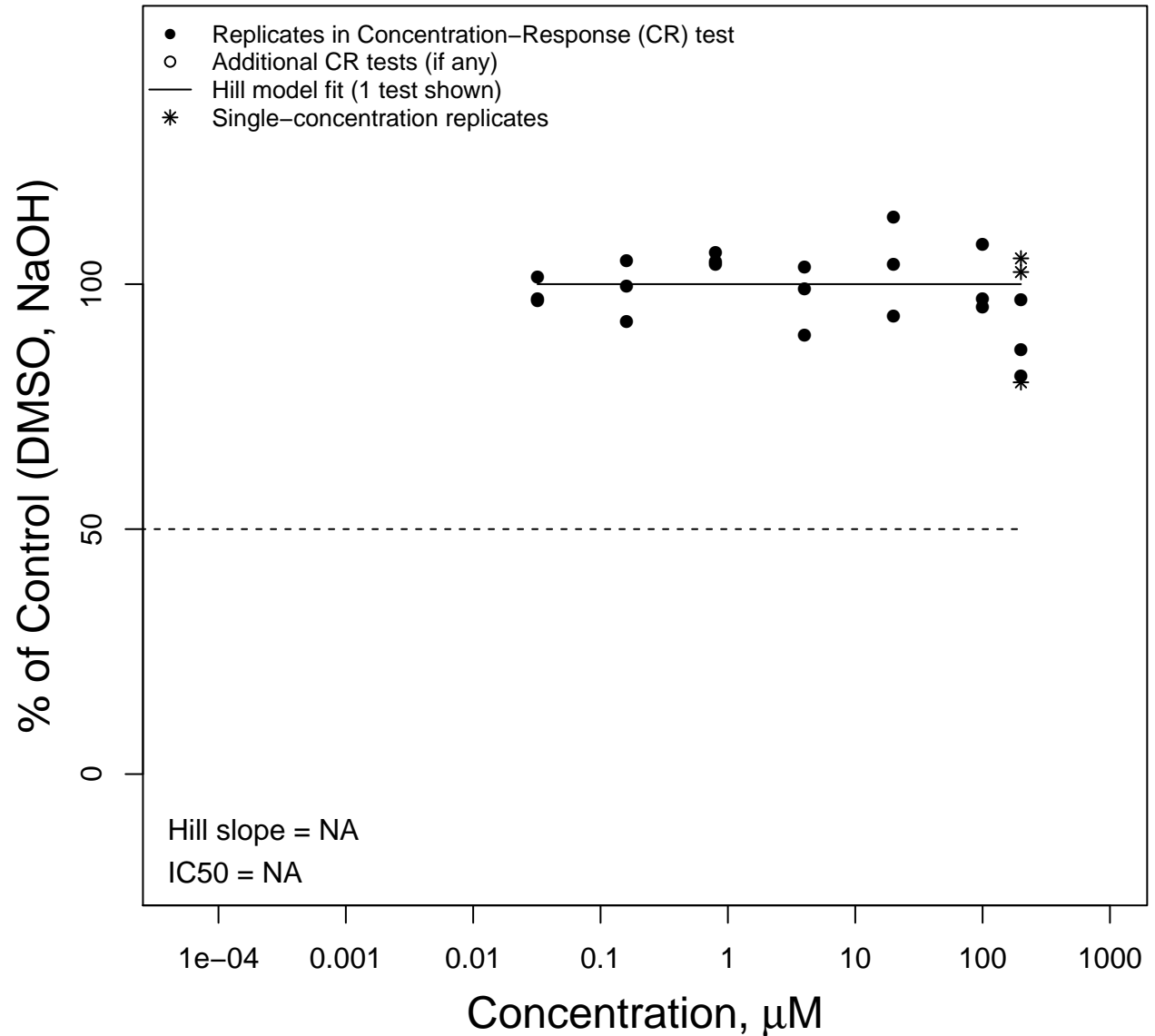
Perfluorooctanesulfonic acid

CASRN: 1763-23-1



Fenoxaprop-ethyl

CASRN: 66441-23-4



Dicofol

CASRN: 115-32-2

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100

50

0

Hill slope = -1.4

IC50 = 220.7

1e-04

0.001

0.01

0.1

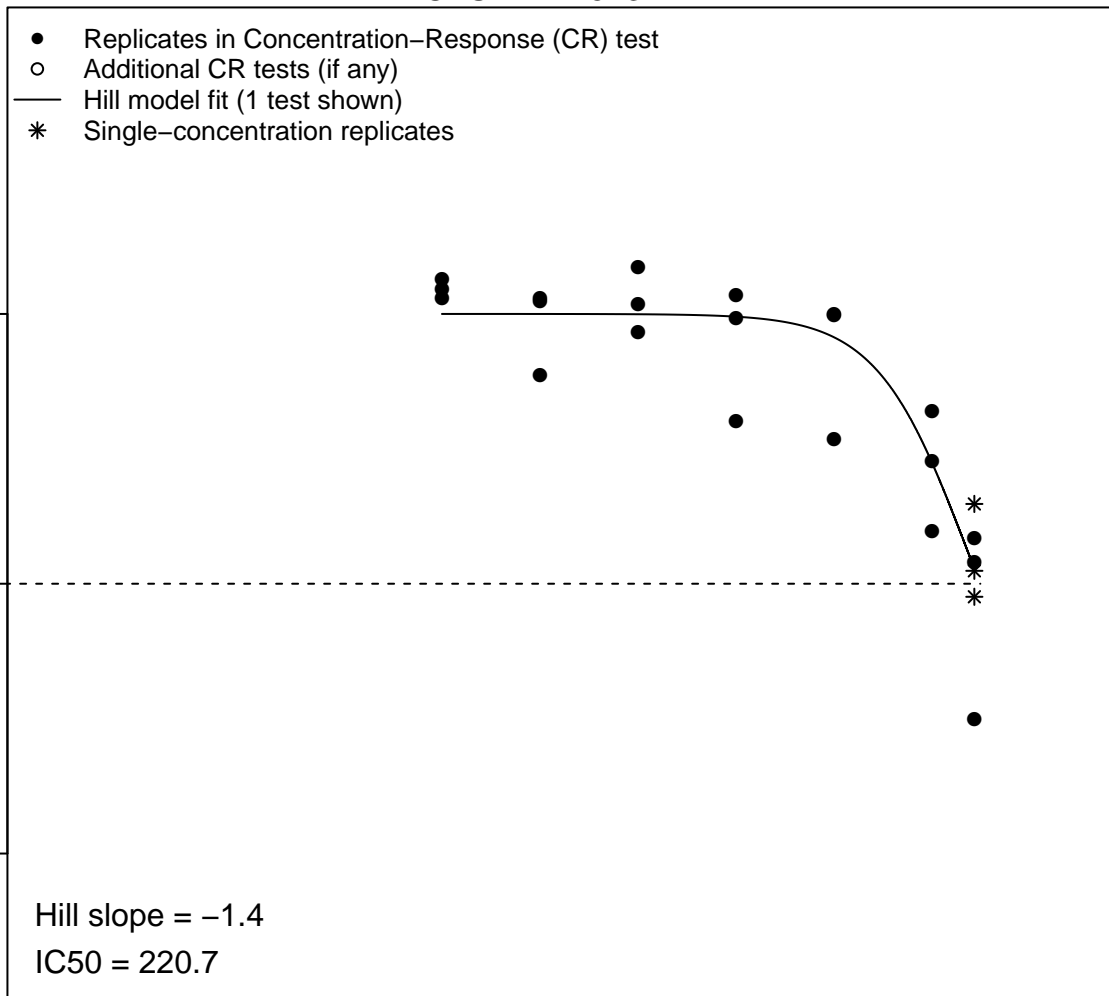
1

10

100

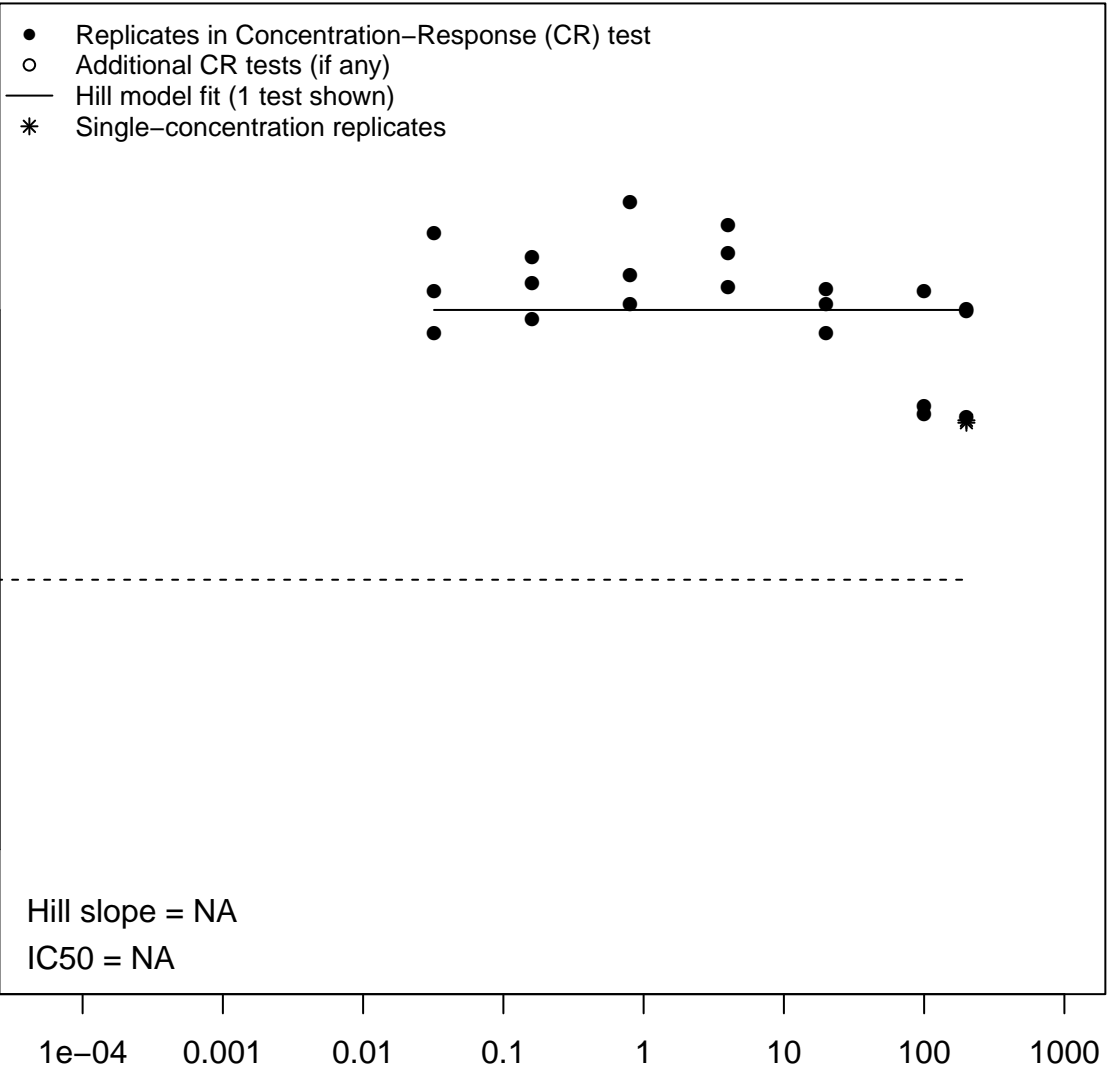
1000

Concentration, μM



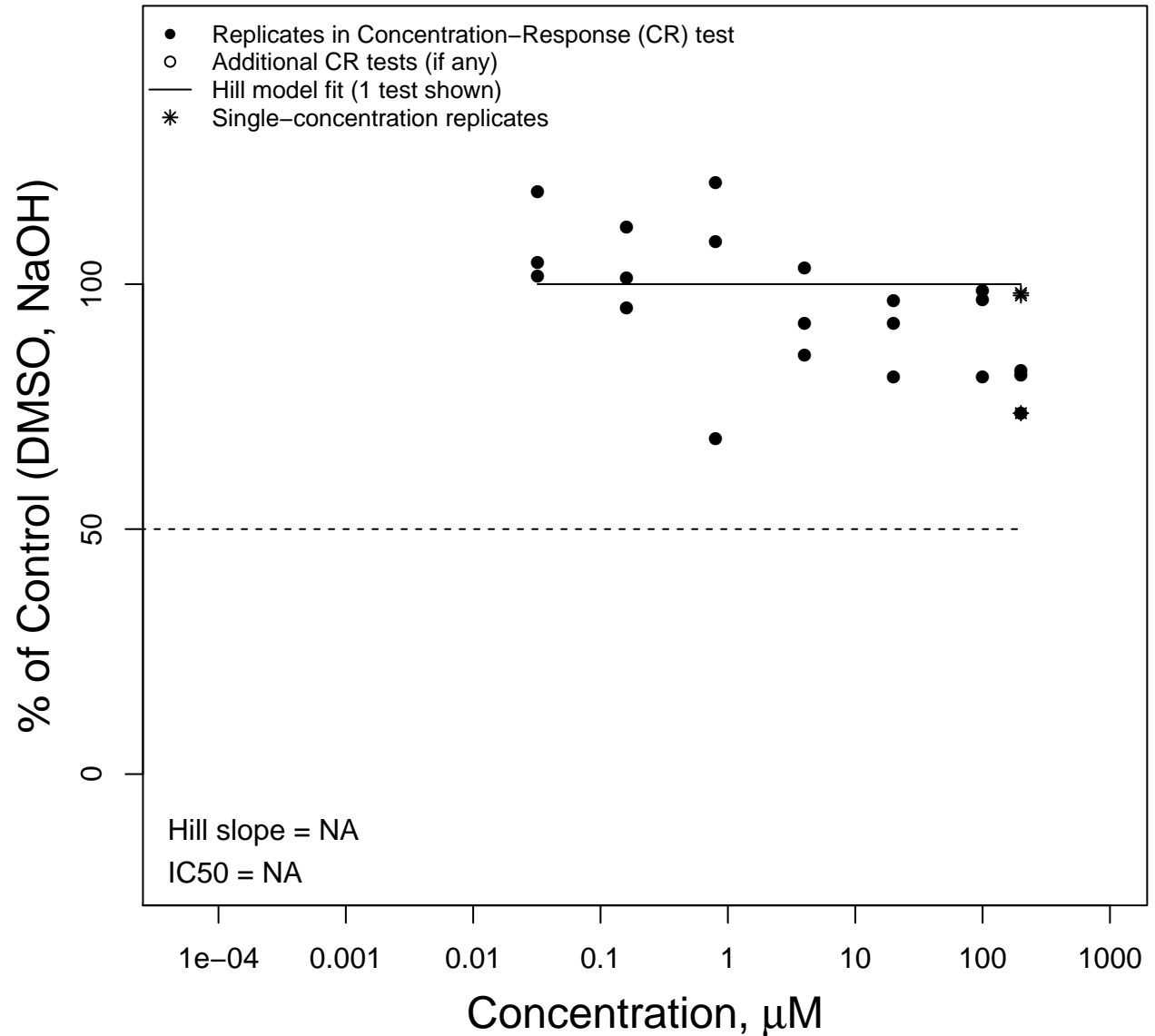
Fenarimol

CASRN: 60168-88-9



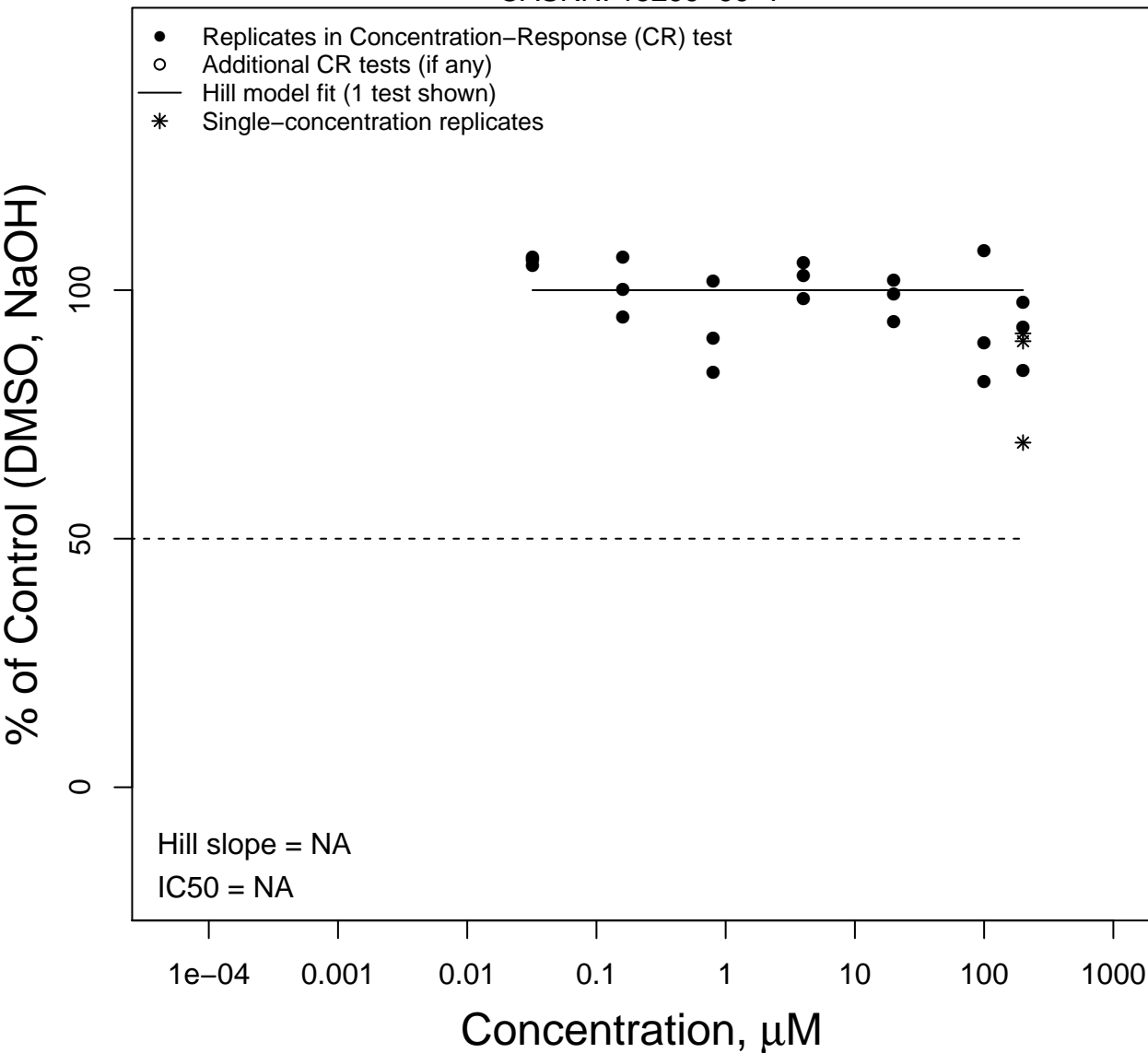
Difenoconazole

CASRN: 119446-68-3



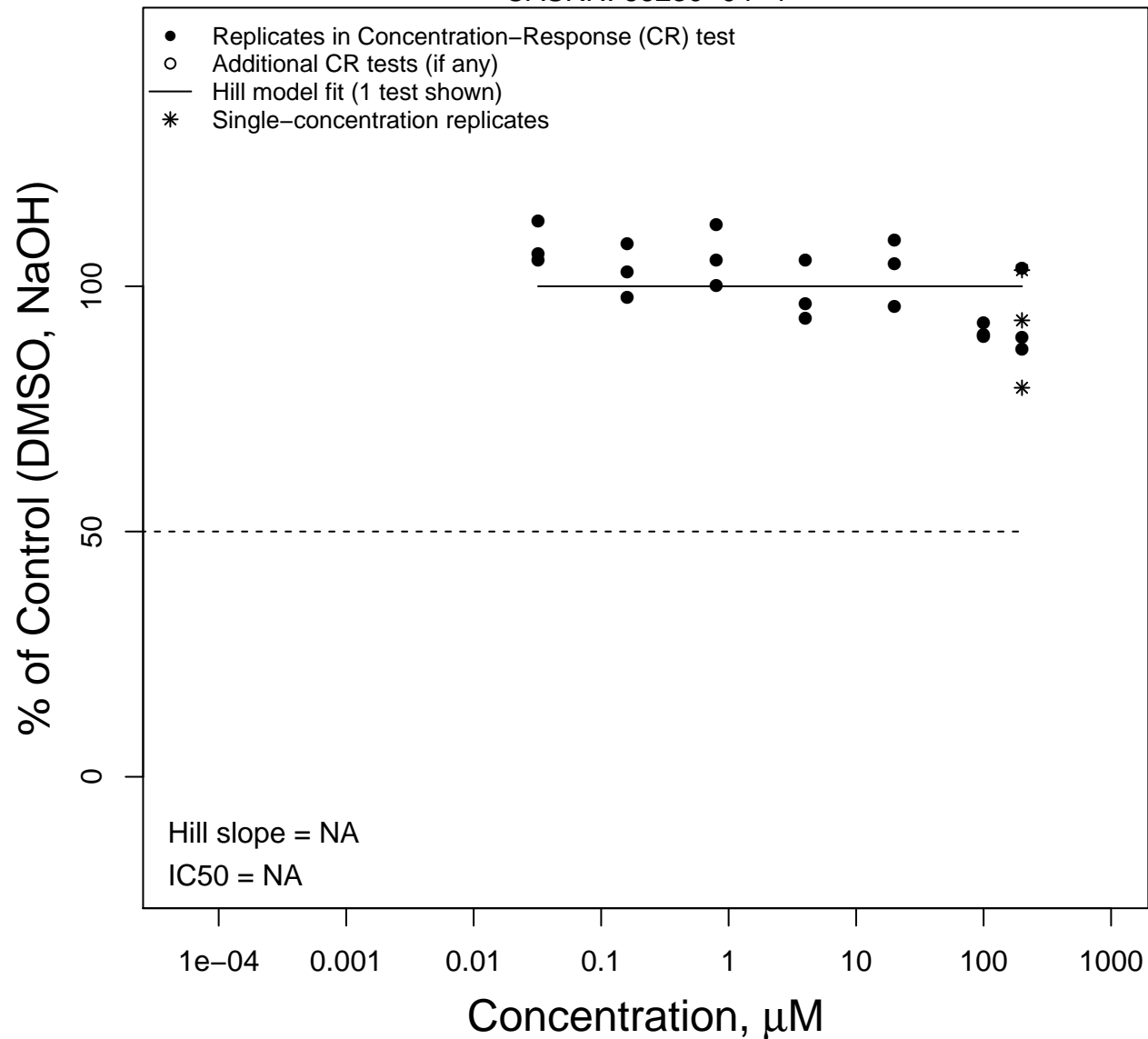
Napropamide

CASRN: 15299-99-7



Esfenvalerate

CASRN: 66230-04-4

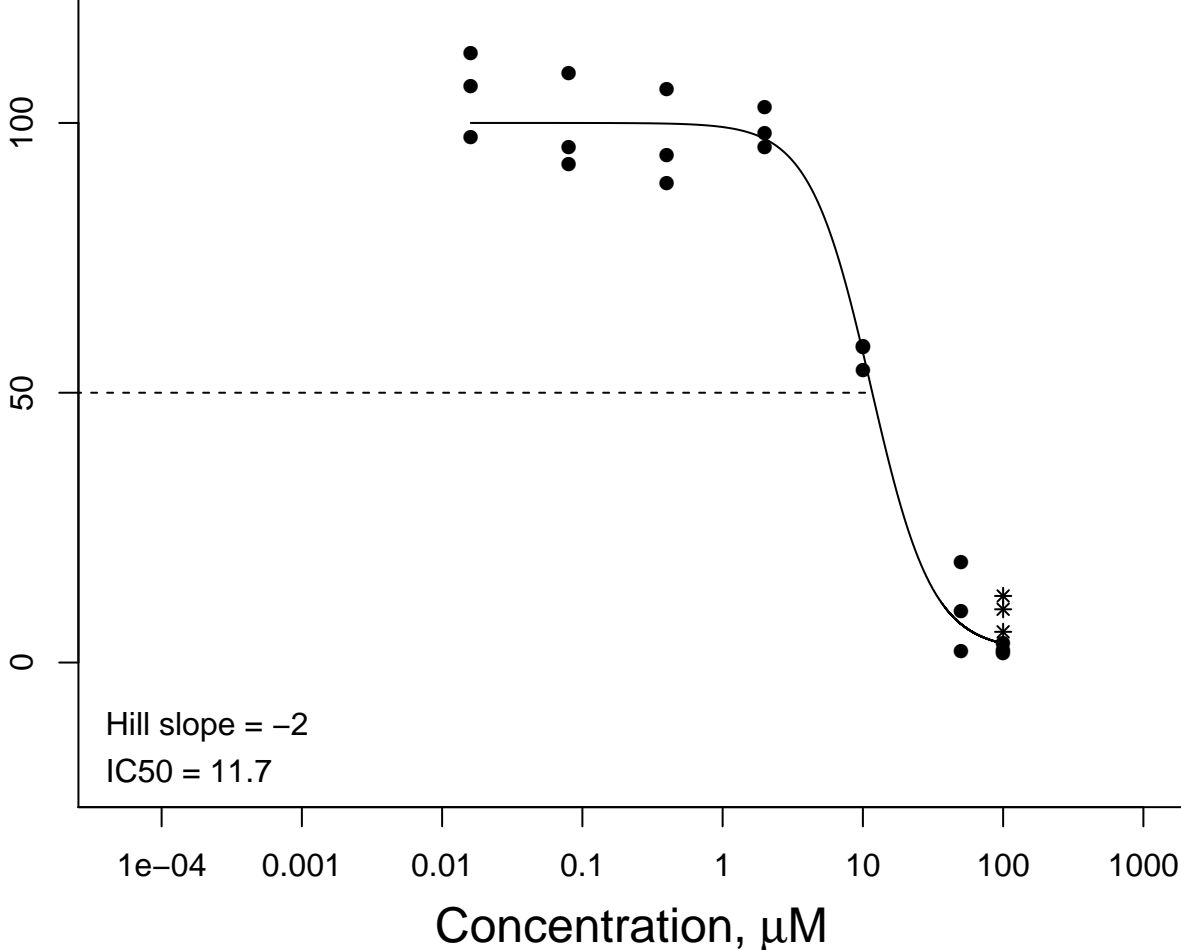


Diquat dibromide monohydrate

CASRN: 6385-62-2

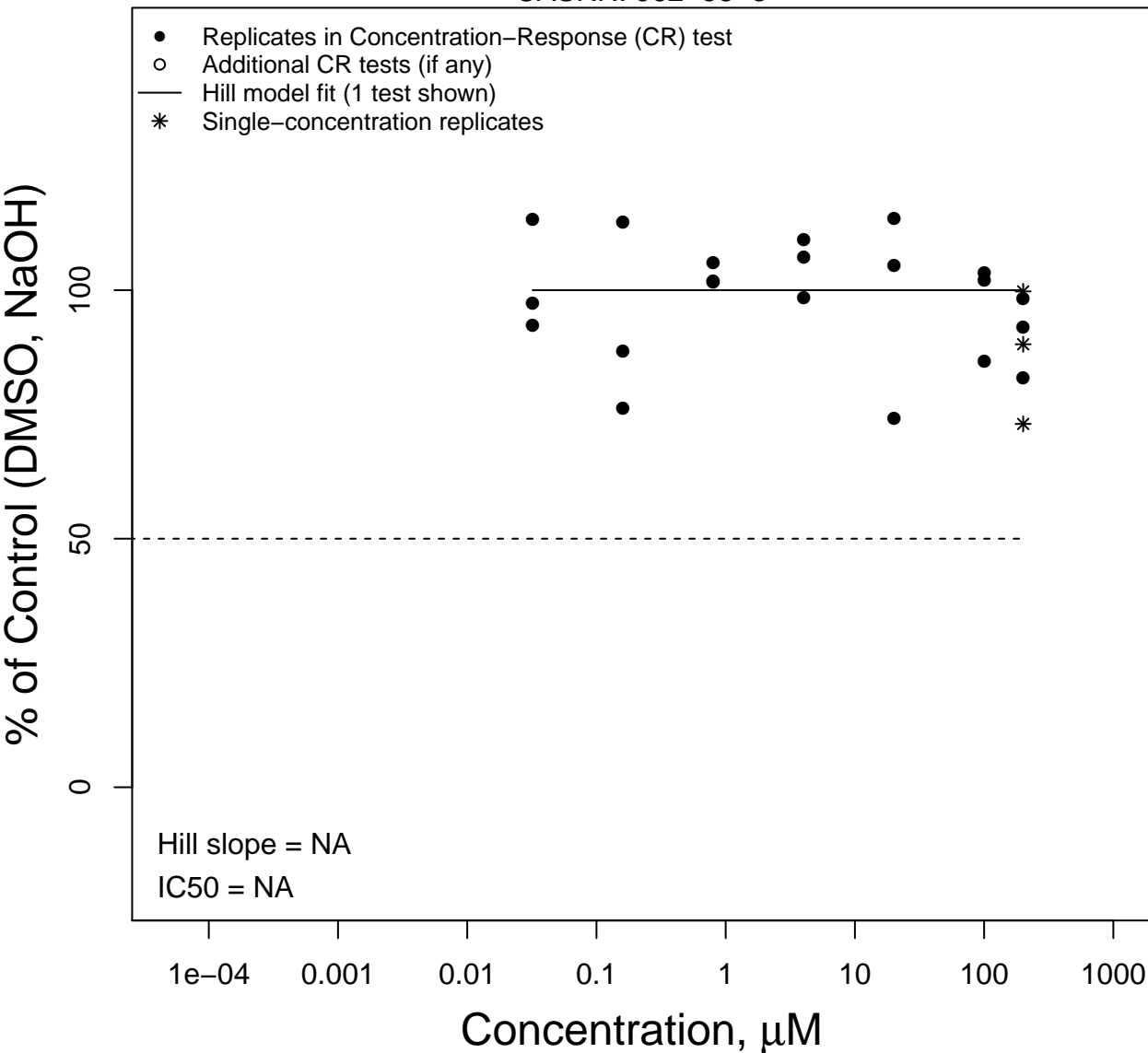
- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)



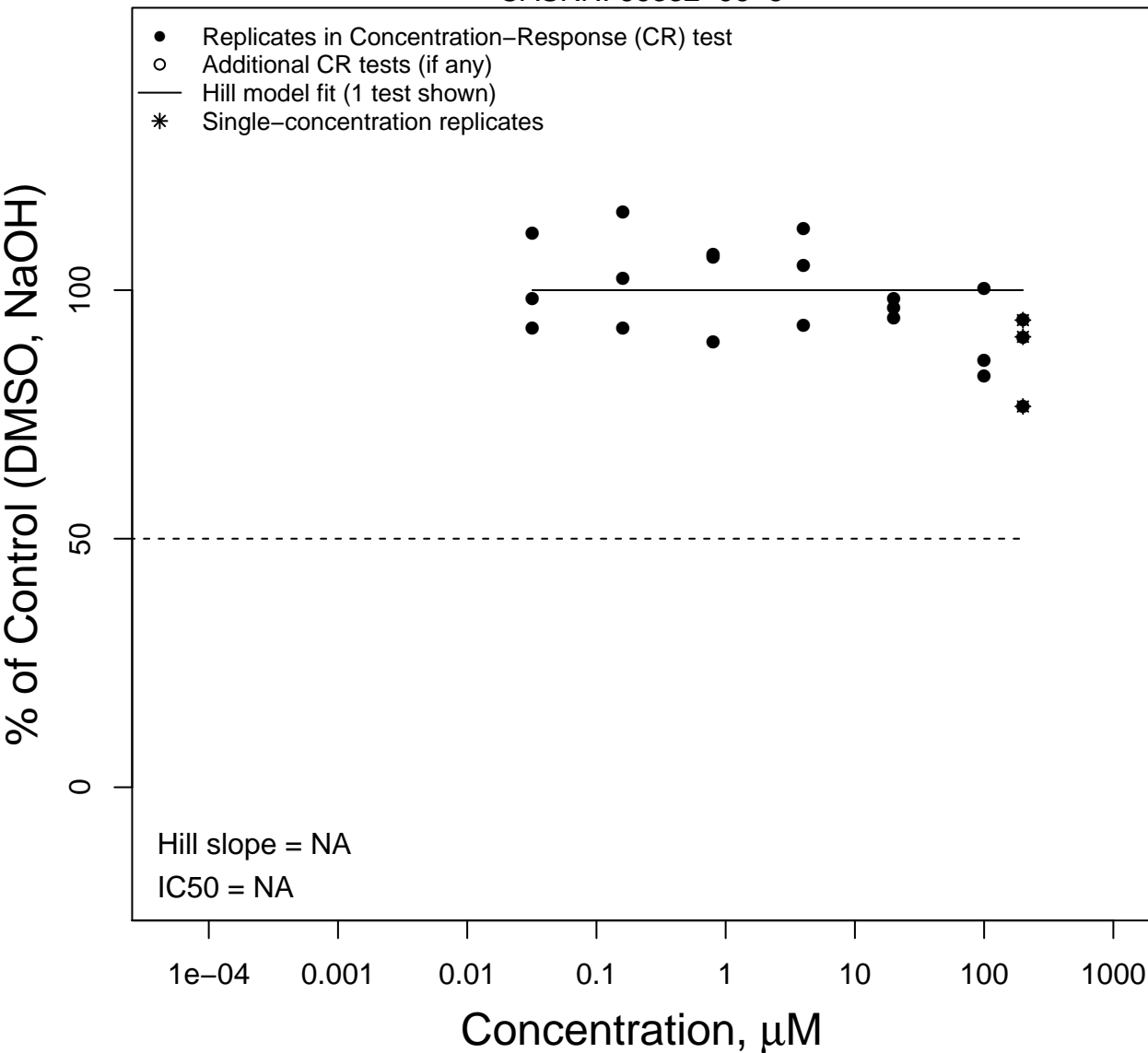
Diazoxon

CASRN: 962-58-3



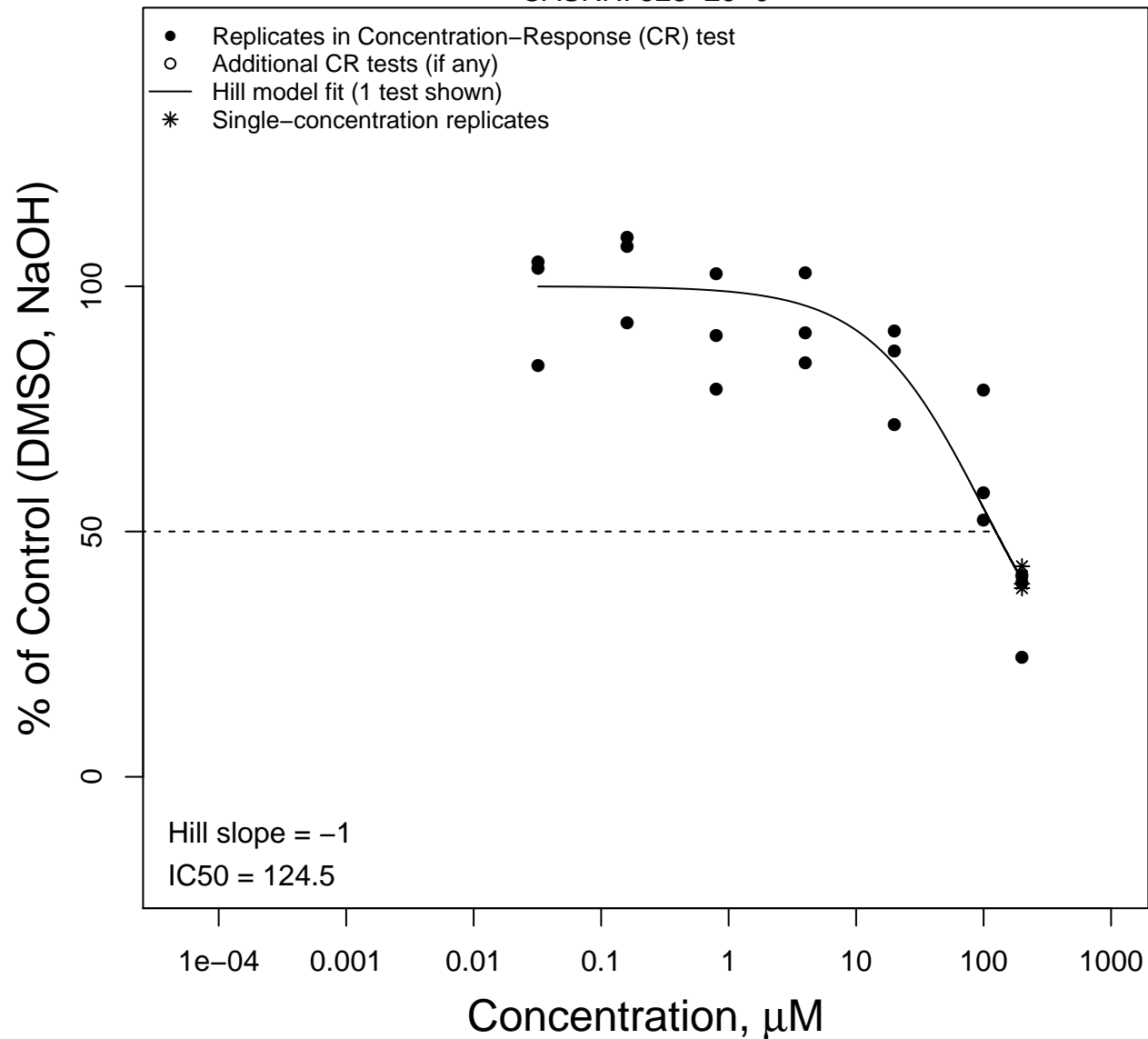
Flutolanil

CASRN: 66332-96-5



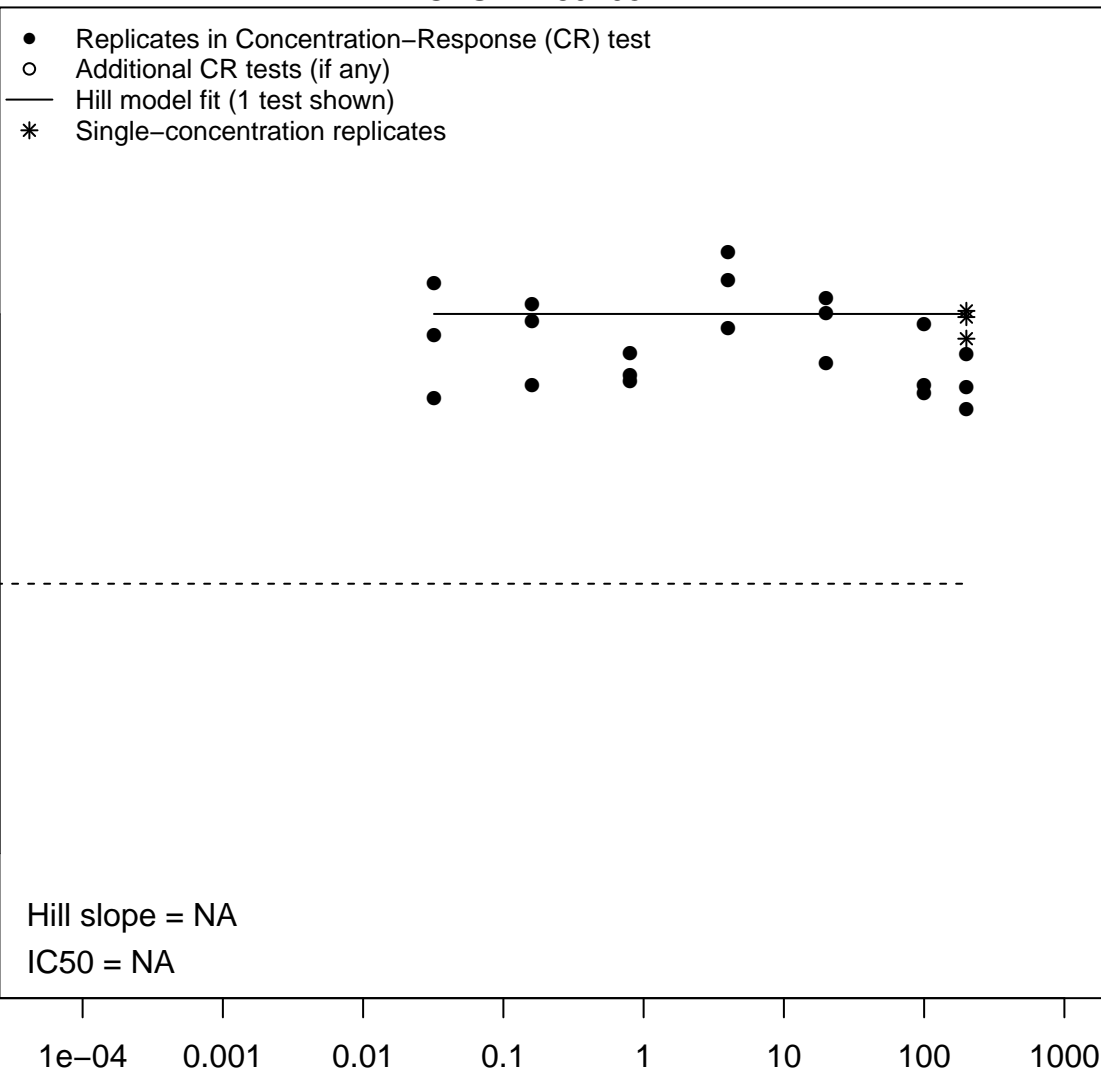
1,2-Dinitrobenzene

CASRN: 528-29-0



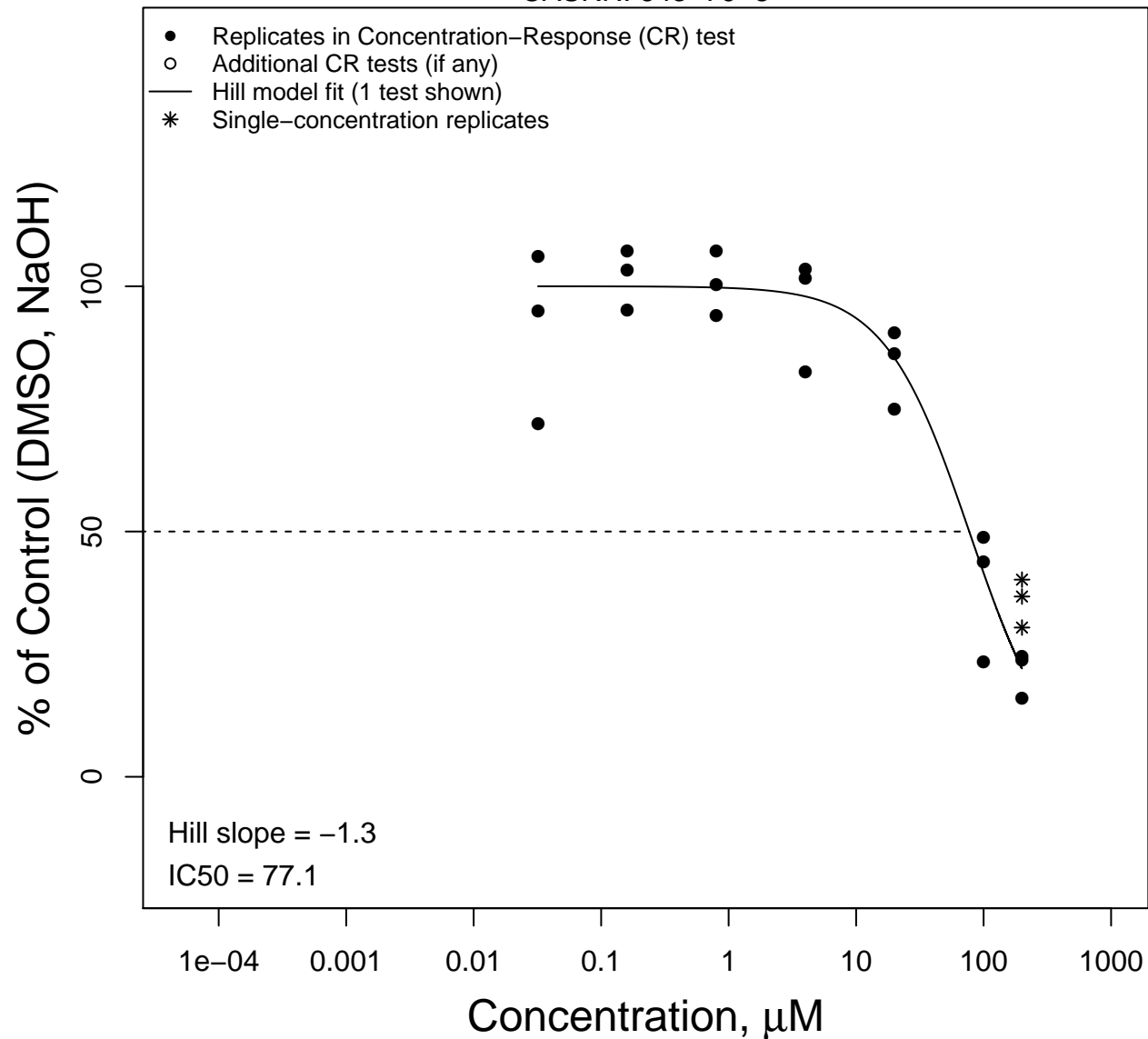
Bisphenol A

CASRN: 80-05-7



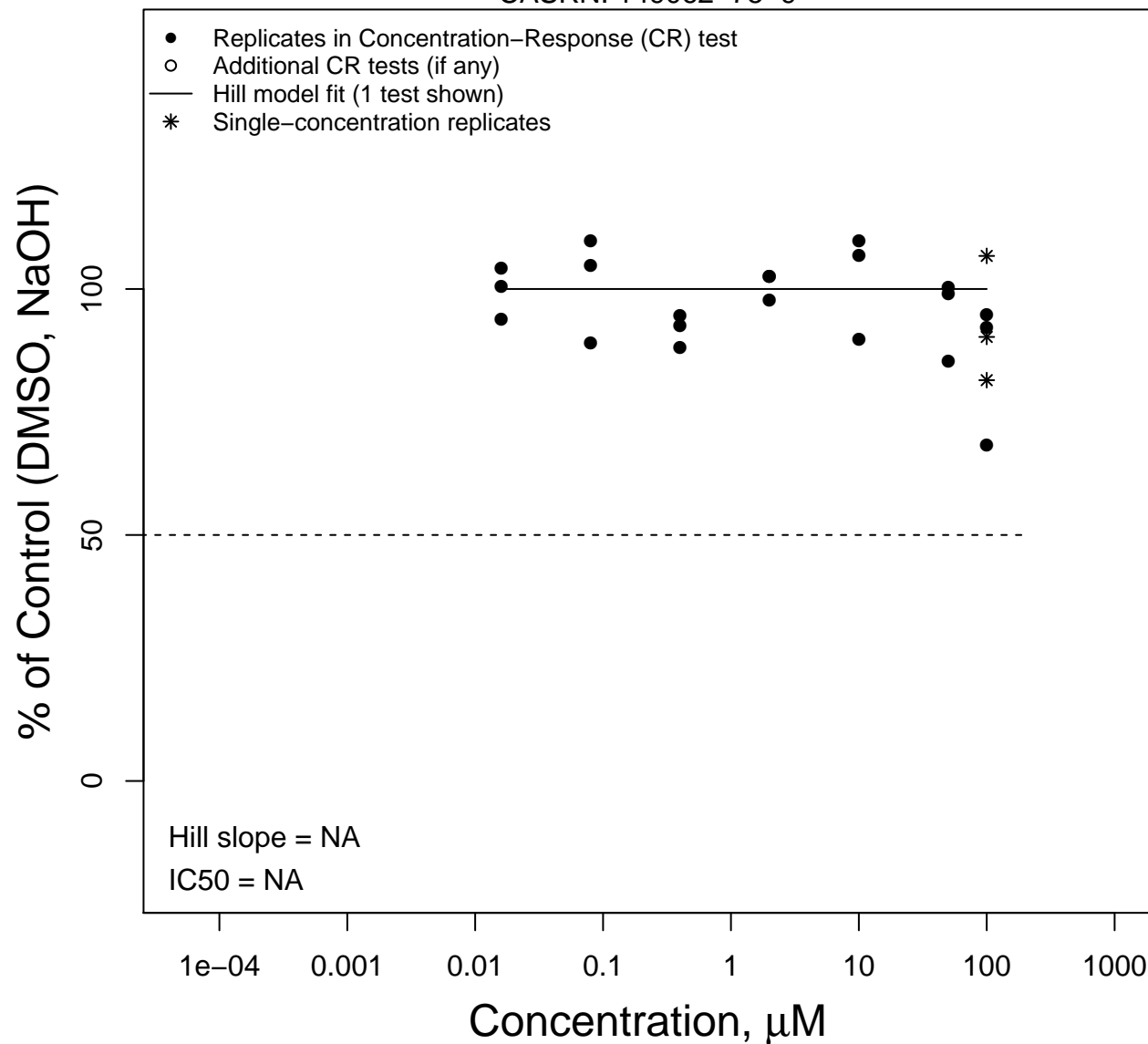
1,2-Benzenedicarboxaldehyde

CASRN: 643-79-8



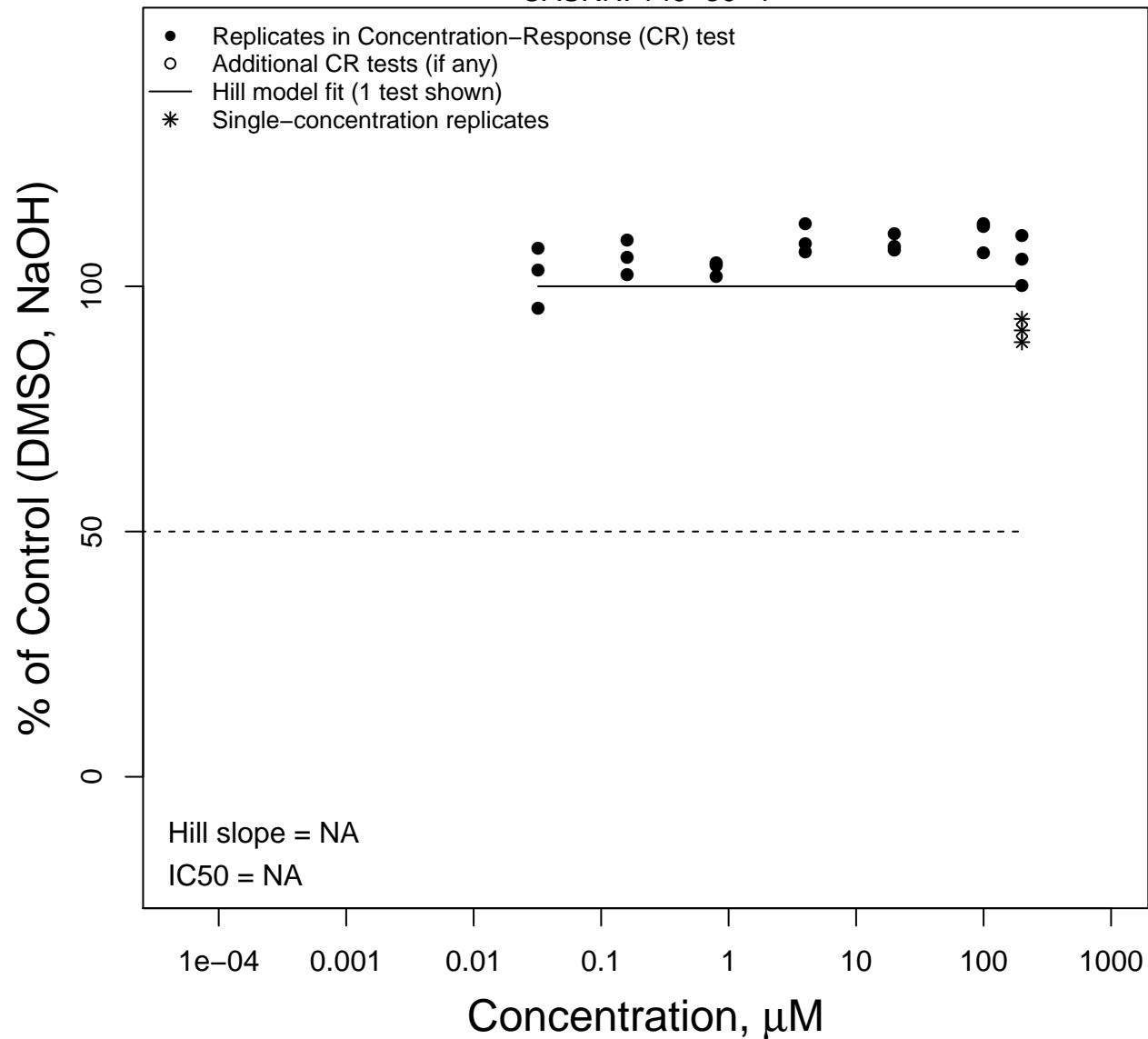
1,3-Dichloro-6,7,8,9,10,12-hexahydroazepino[2,1-b]quinazoline hydrochloride (1:1)

CASRN: 149062-75-9



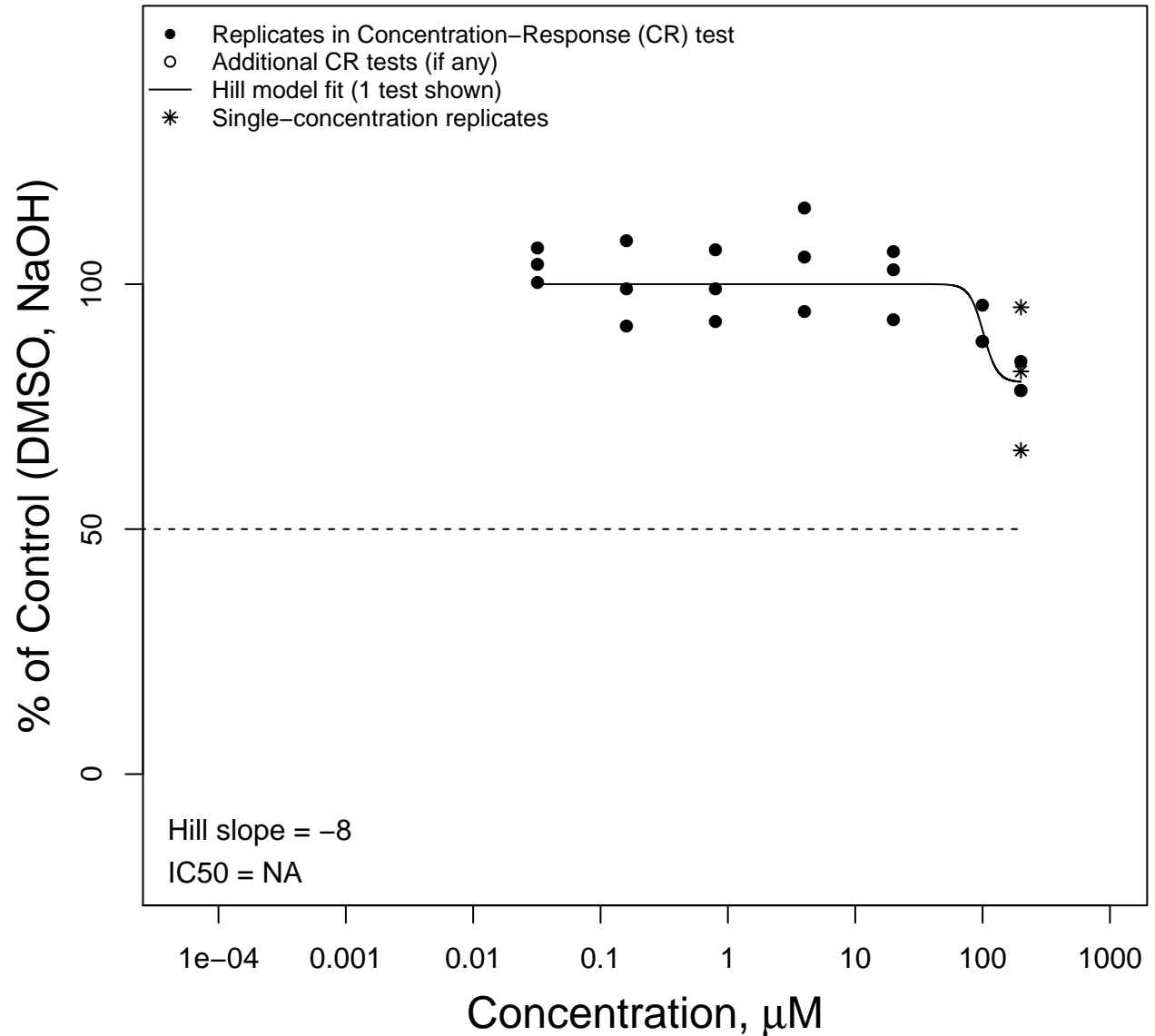
2-Mercaptobenzothiazole

CASRN: 149-30-4



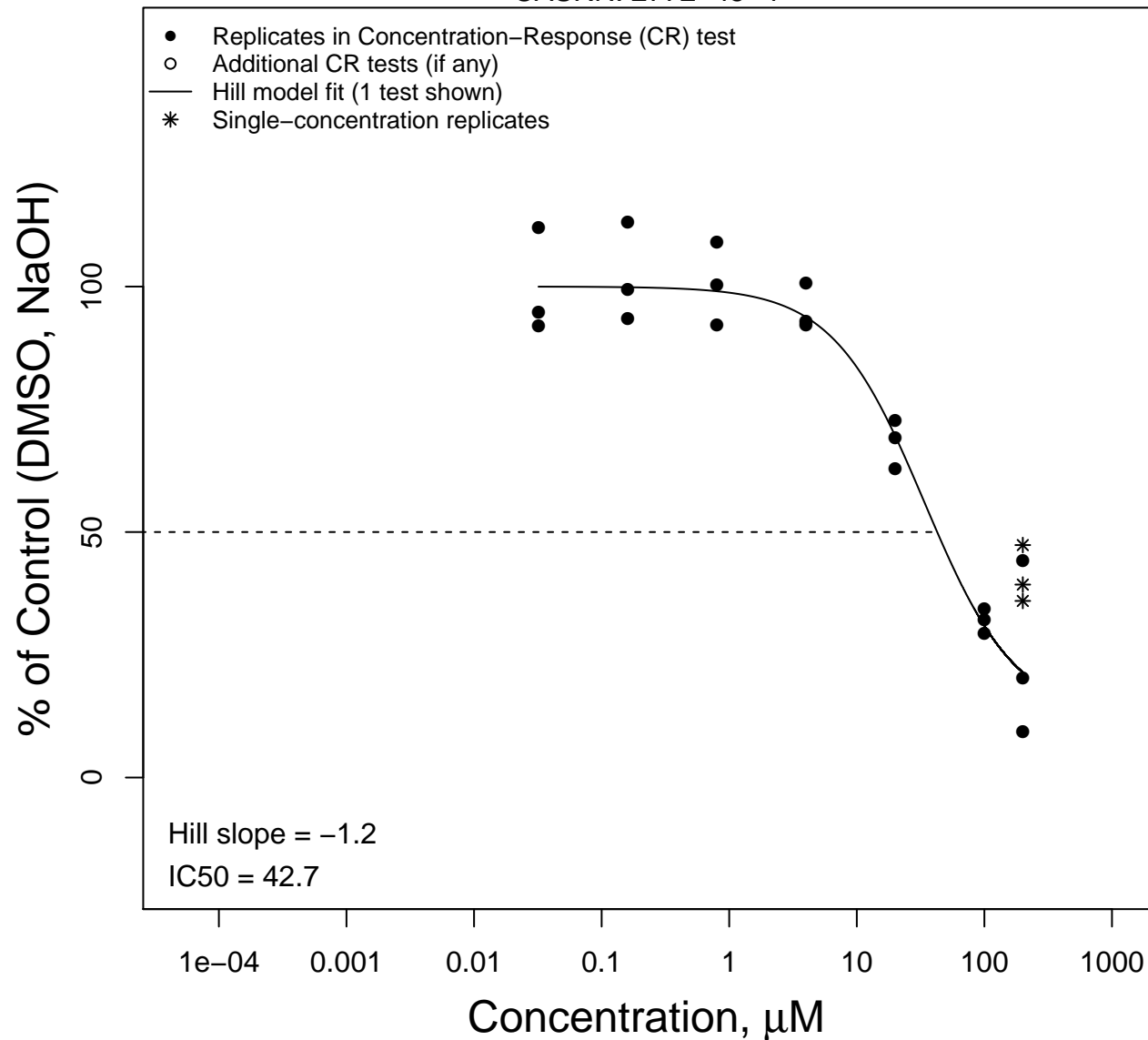
2,4,5-Trichlorophenol

CASRN: 95-95-4



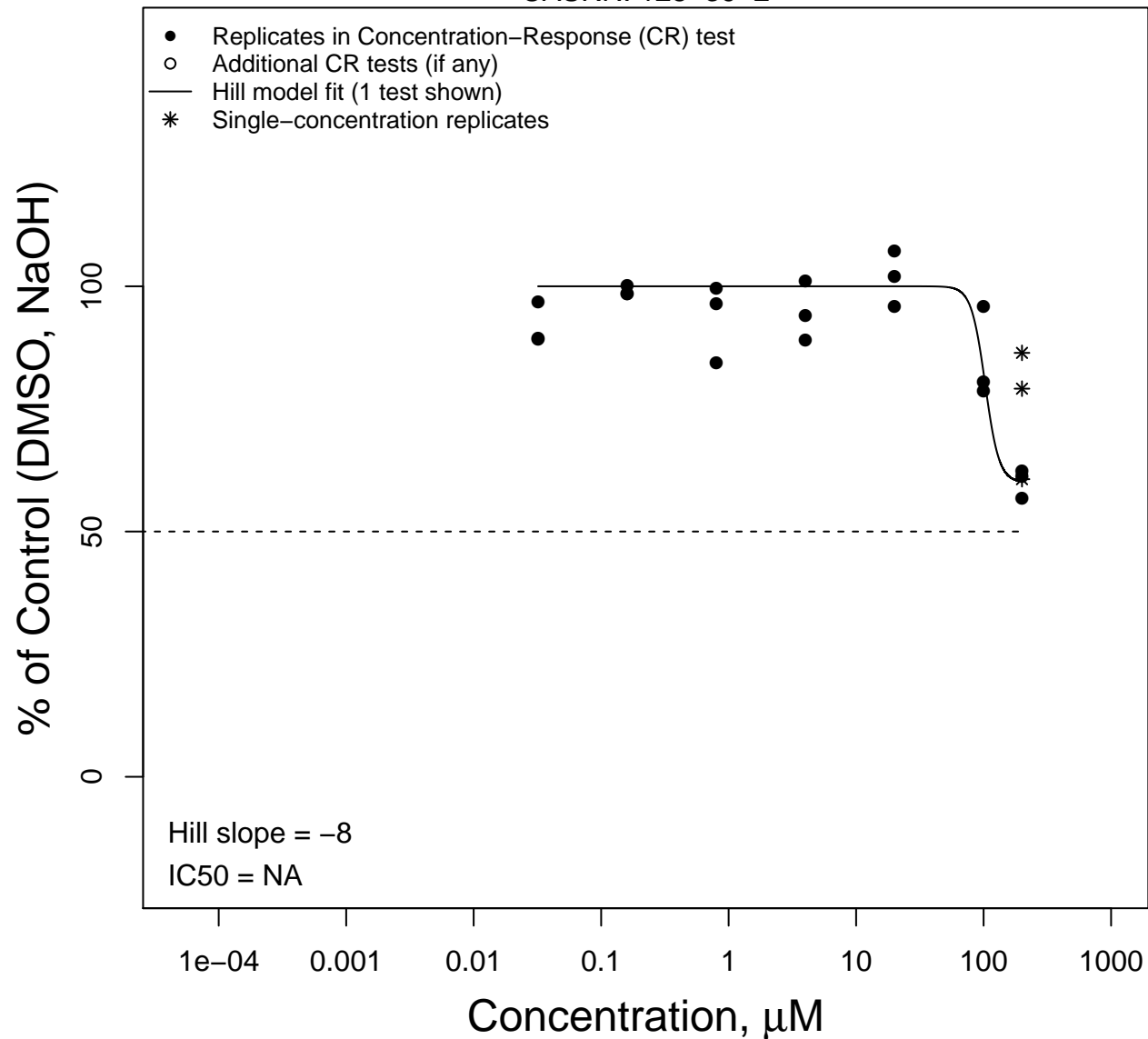
2,4-Bis(1-methyl-1-phenylethyl)phenol

CASRN: 2772-45-4



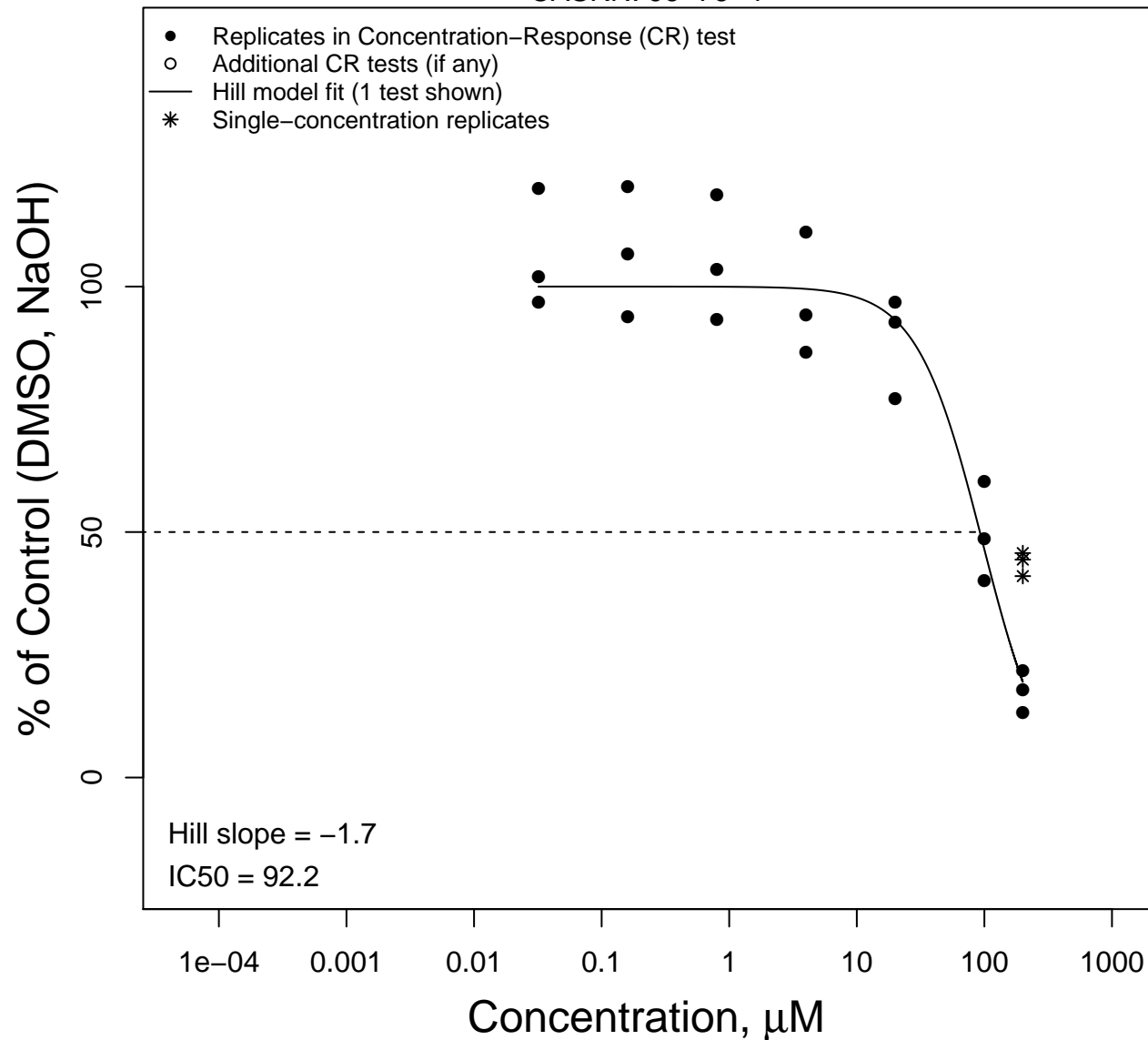
2,6-Di-tert-butylphenol

CASRN: 128-39-2



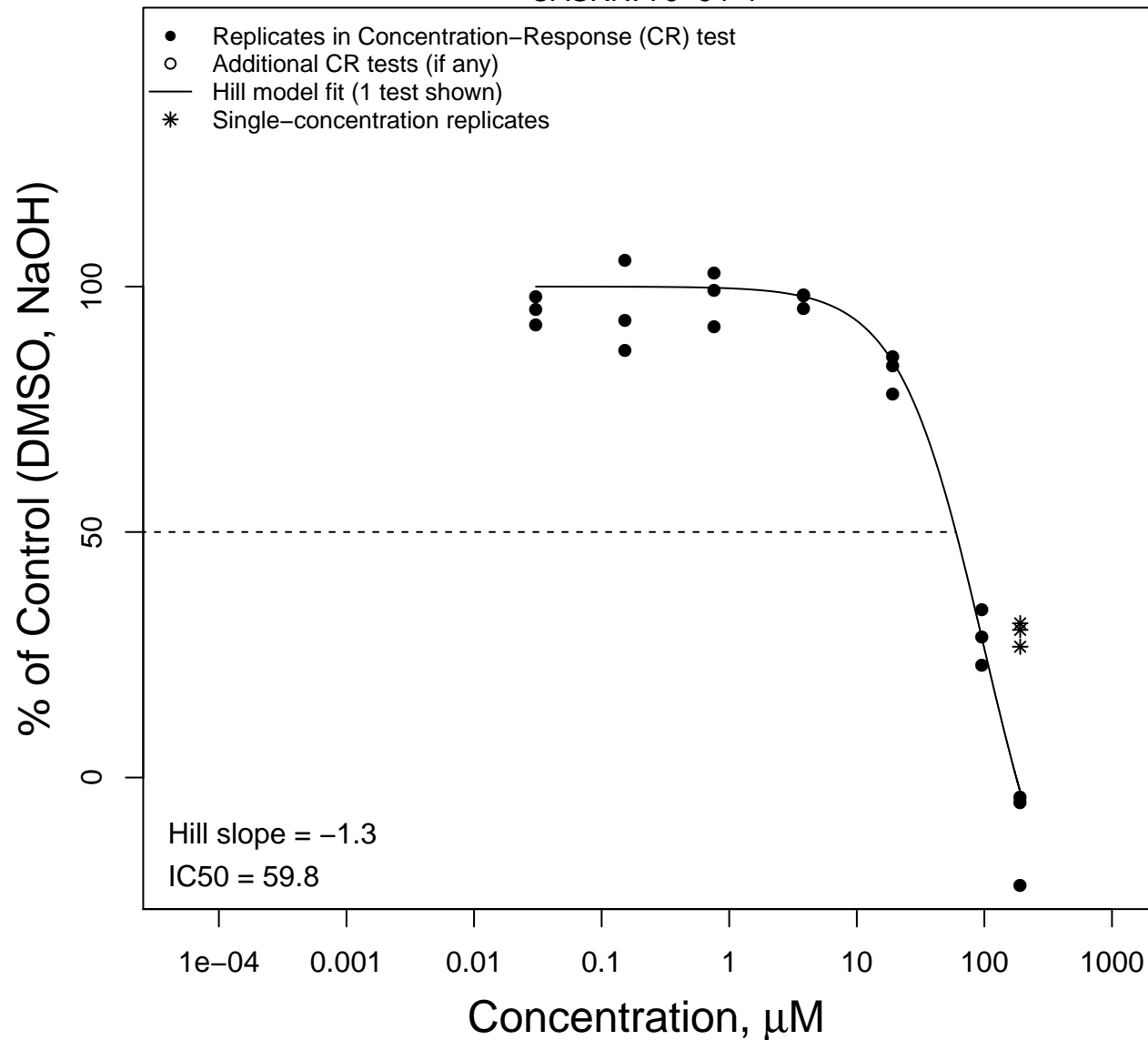
2,4-Di-tert-butylphenol

CASRN: 96-76-4



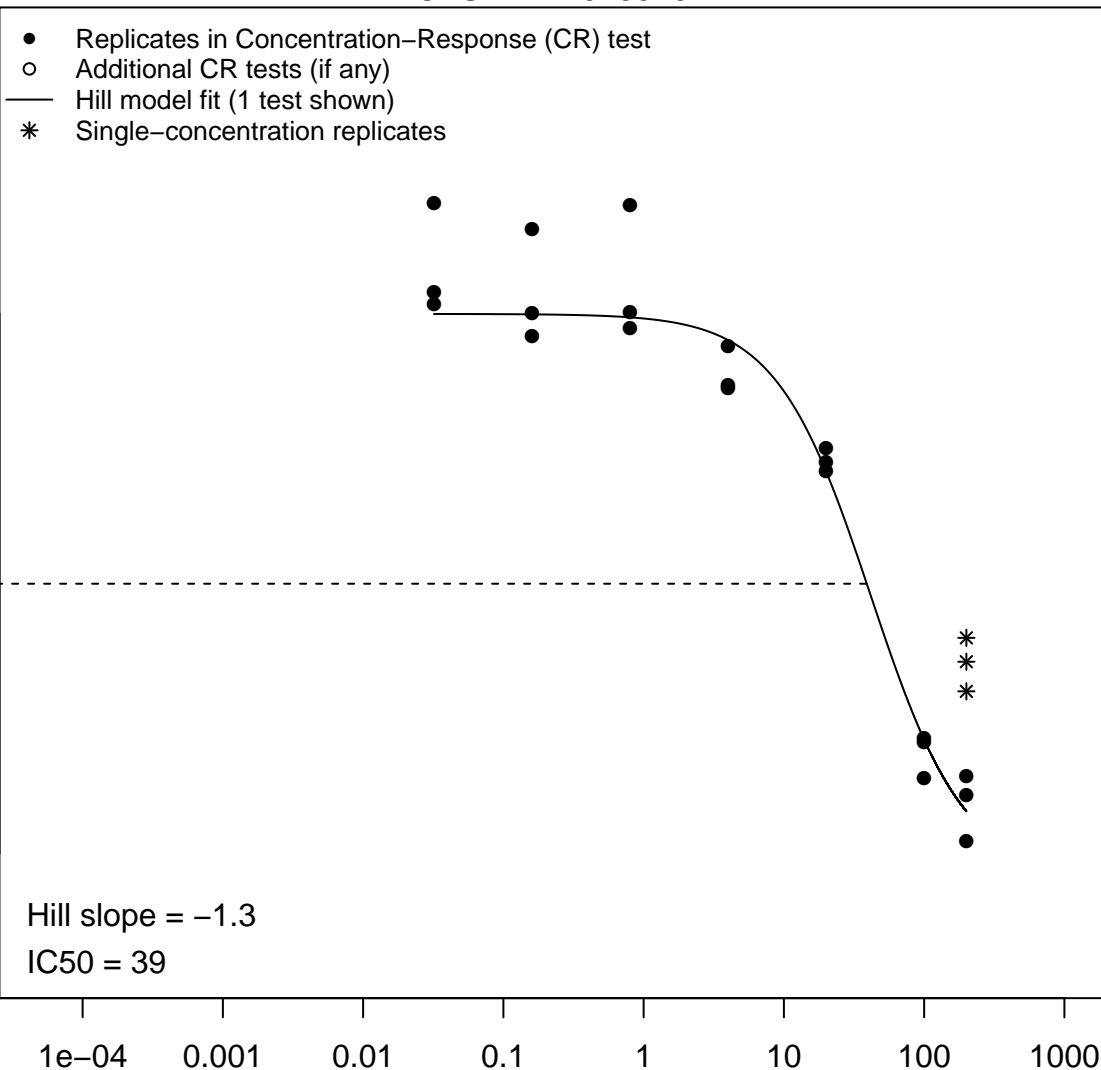
3,3',5,5'-Tetrabromobisphenol A

CASRN: 79-94-7



2,4-Di-tert-pentylphenol

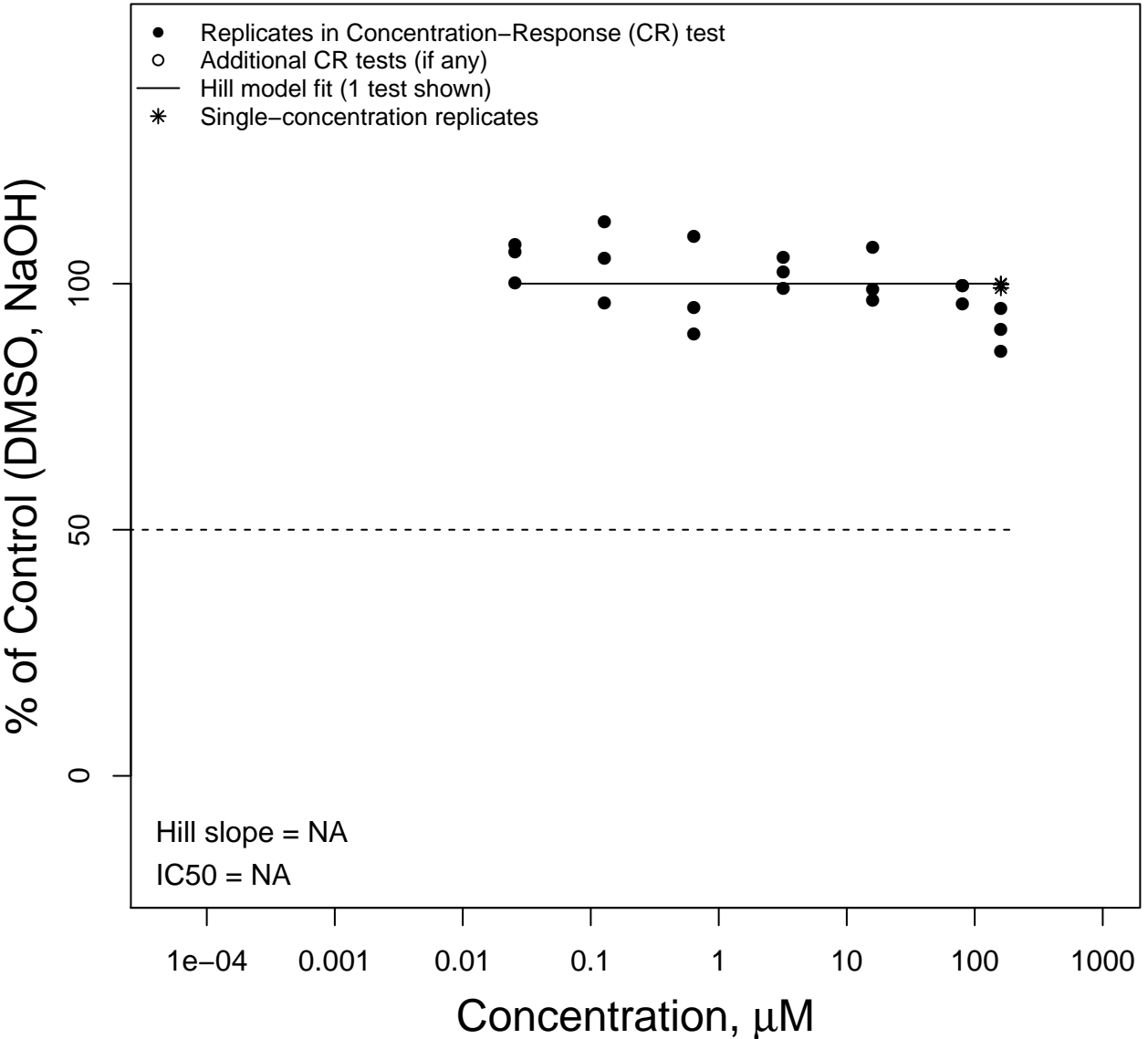
CASRN: 120-95-6



Concentration, µM

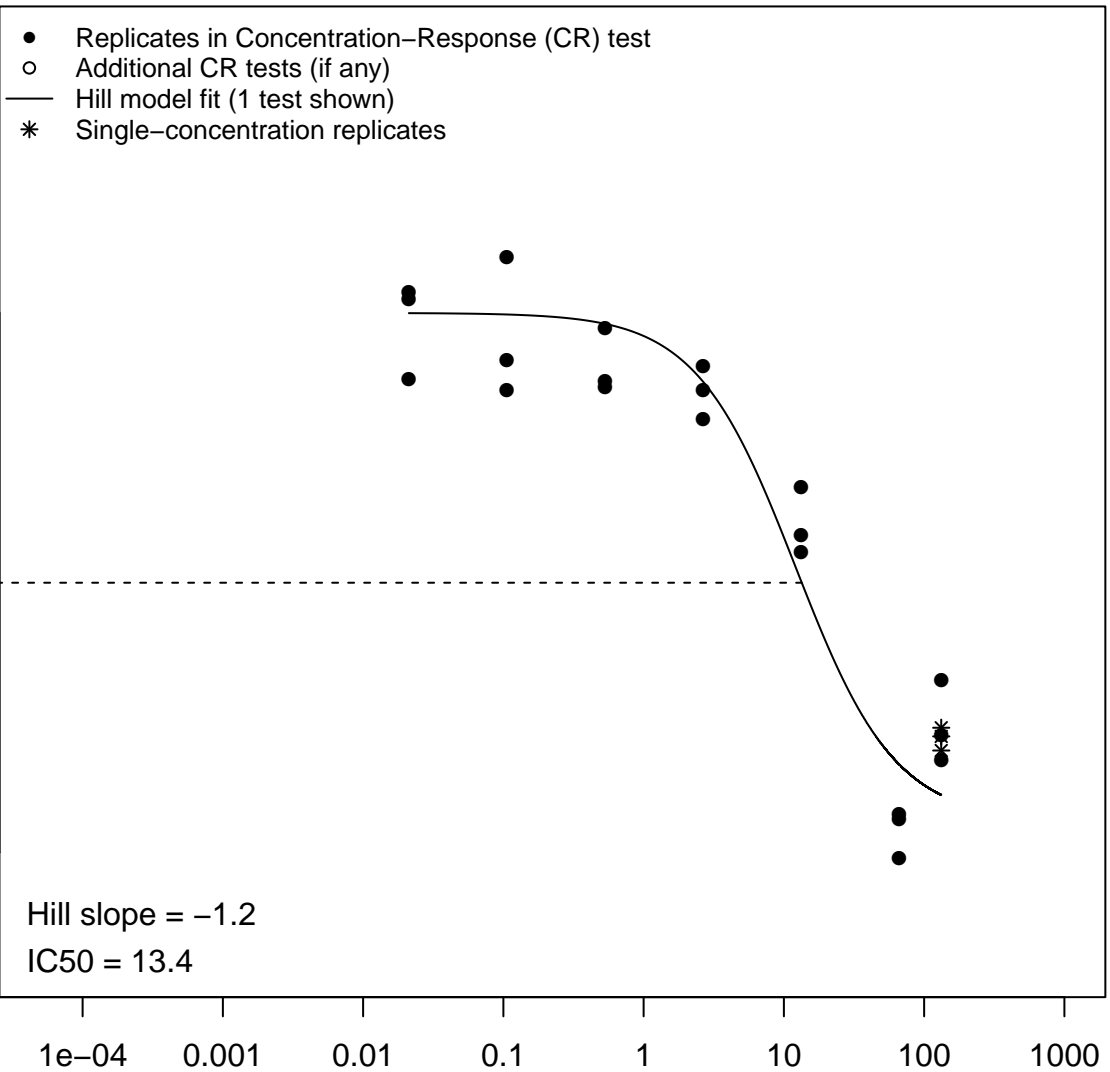
Bromoxynil

CASRN: 1689-84-5



D&C Red 27

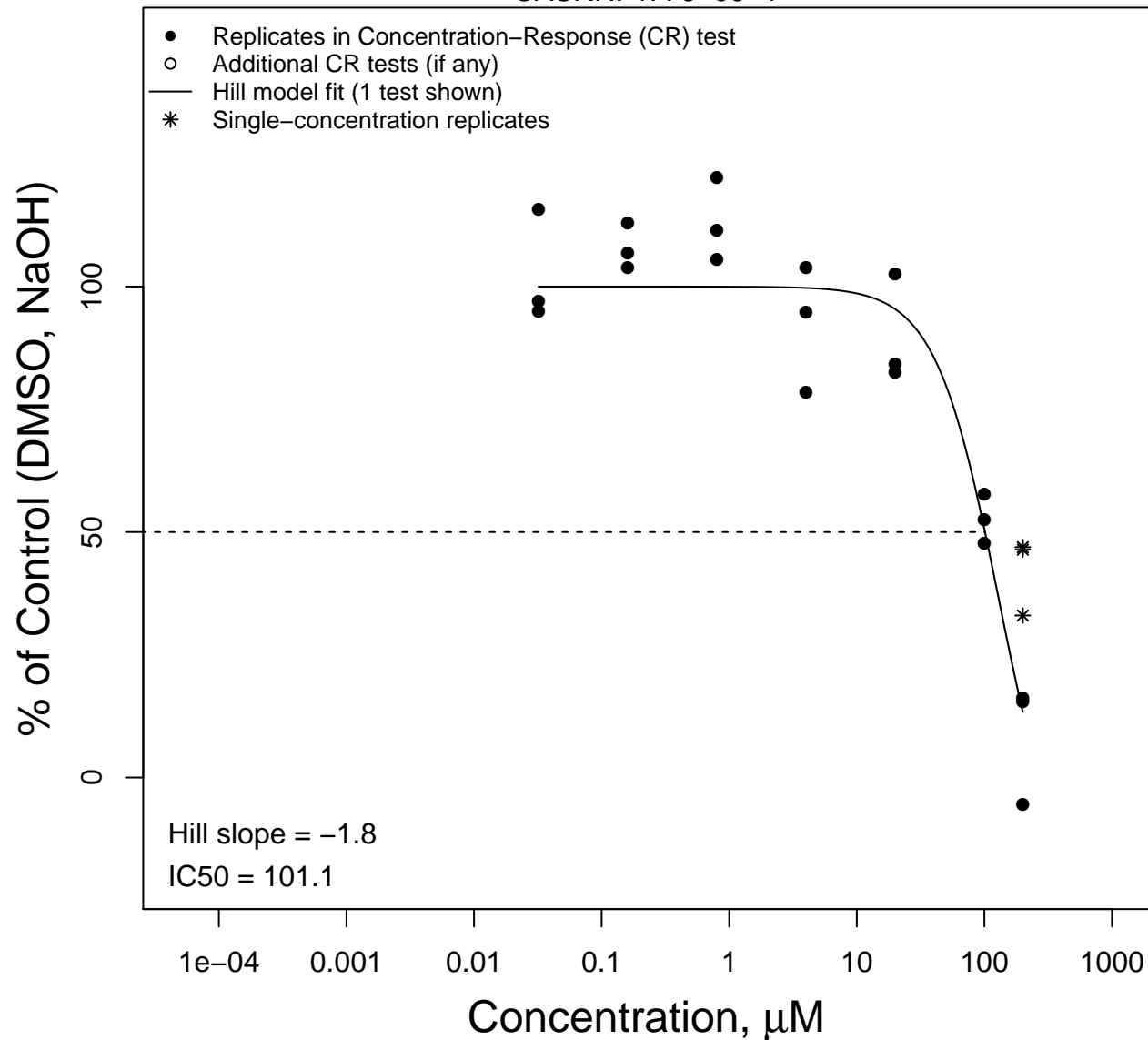
CASRN: 13473-26-2



Concentration, μM

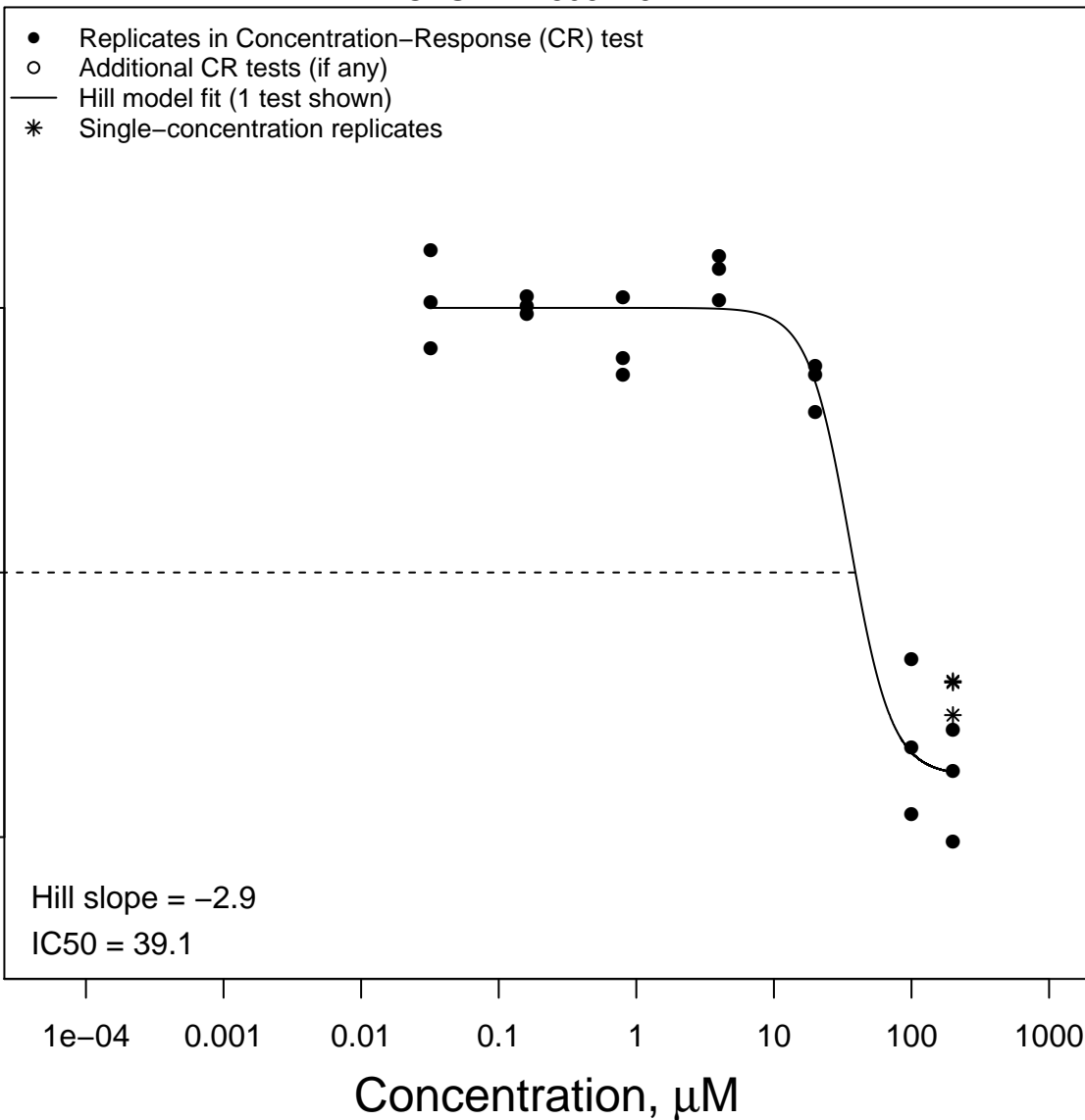
Fluorosalan

CASRN: 4776-06-1



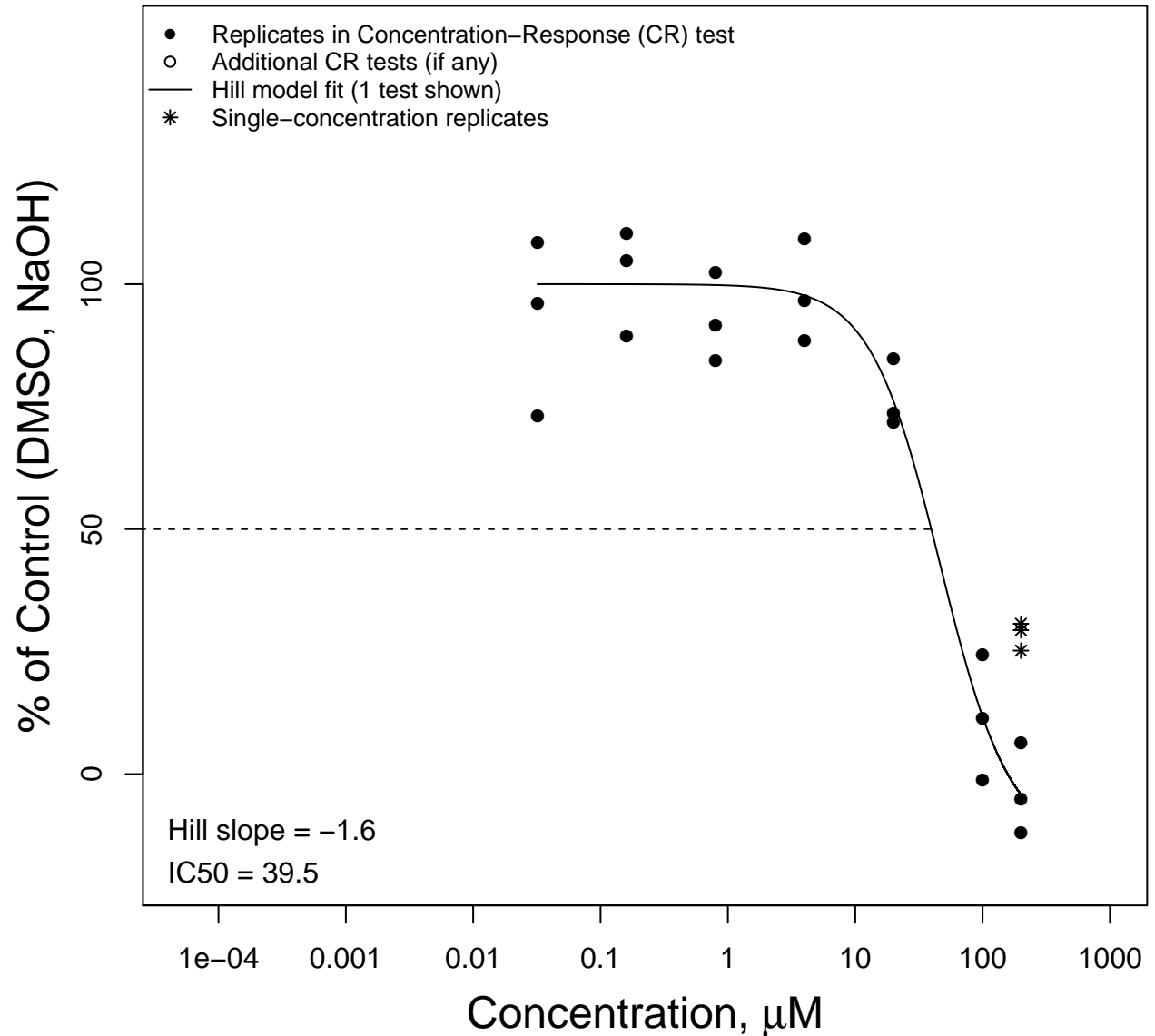
4-Octylphenol

CASRN: 1806-26-4



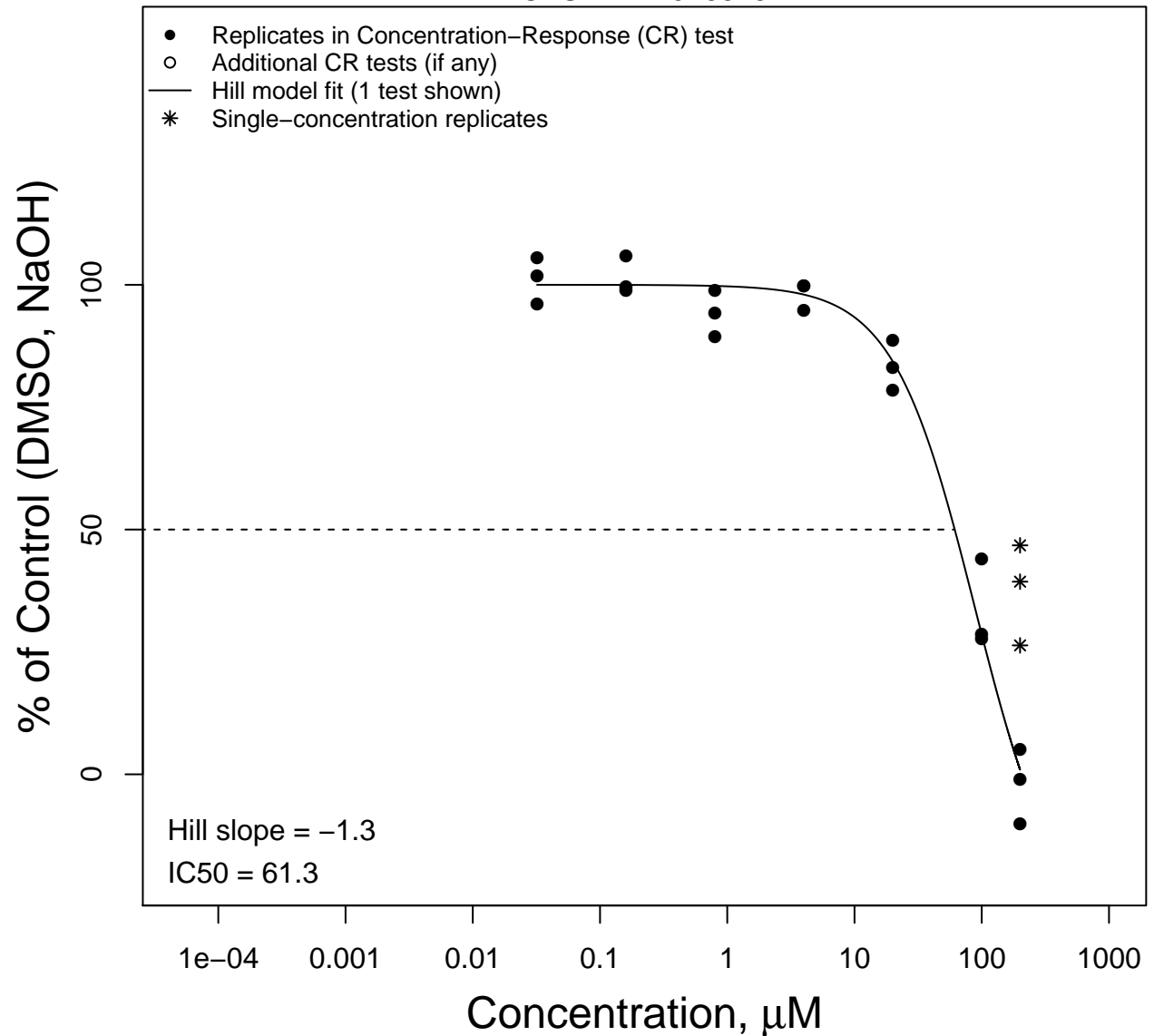
4-Nonylphenol, branched

CASRN: 84852-15-3



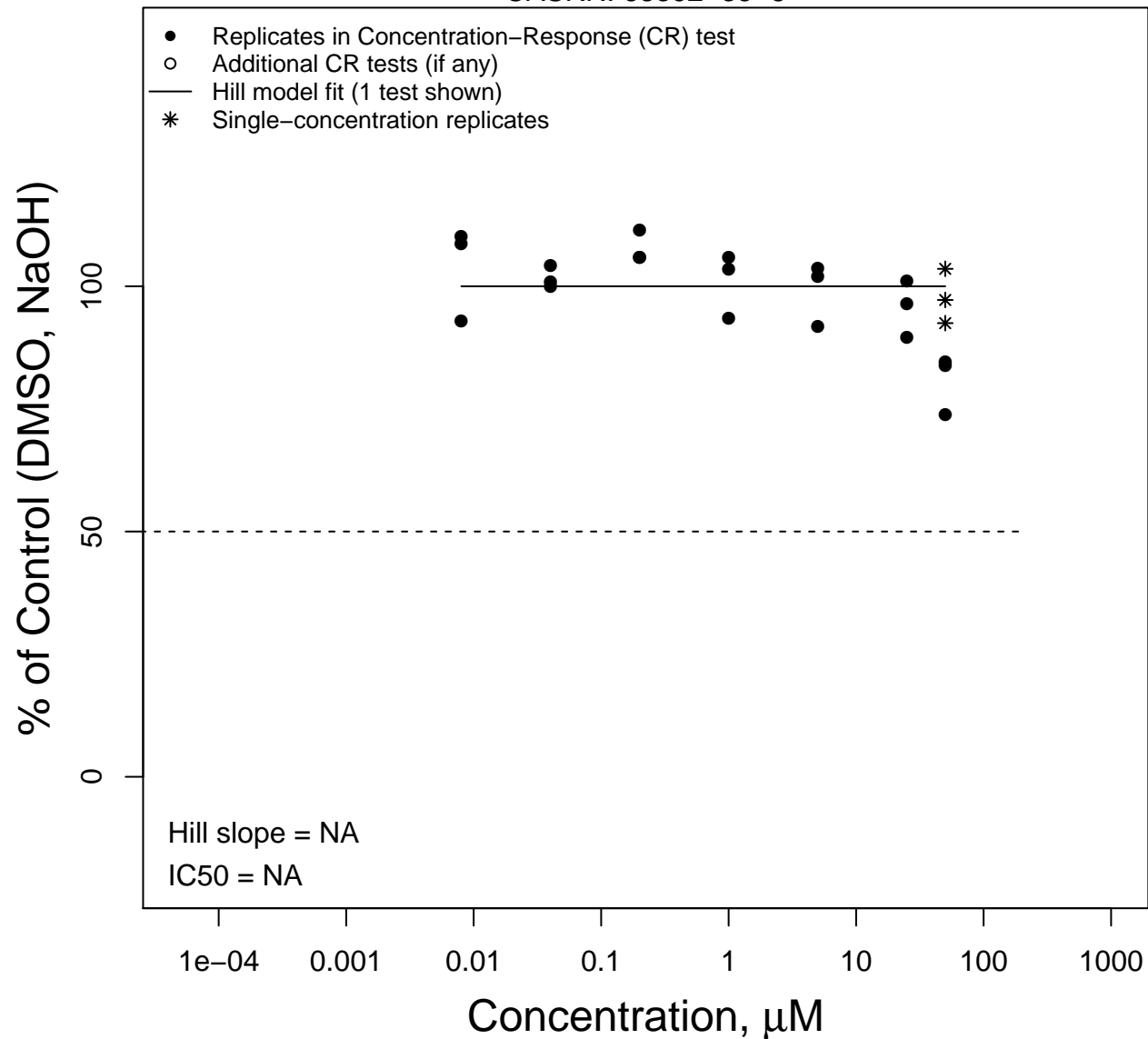
4-(1,1,3,3-Tetramethylbutyl)phenol

CASRN: 140-66-9



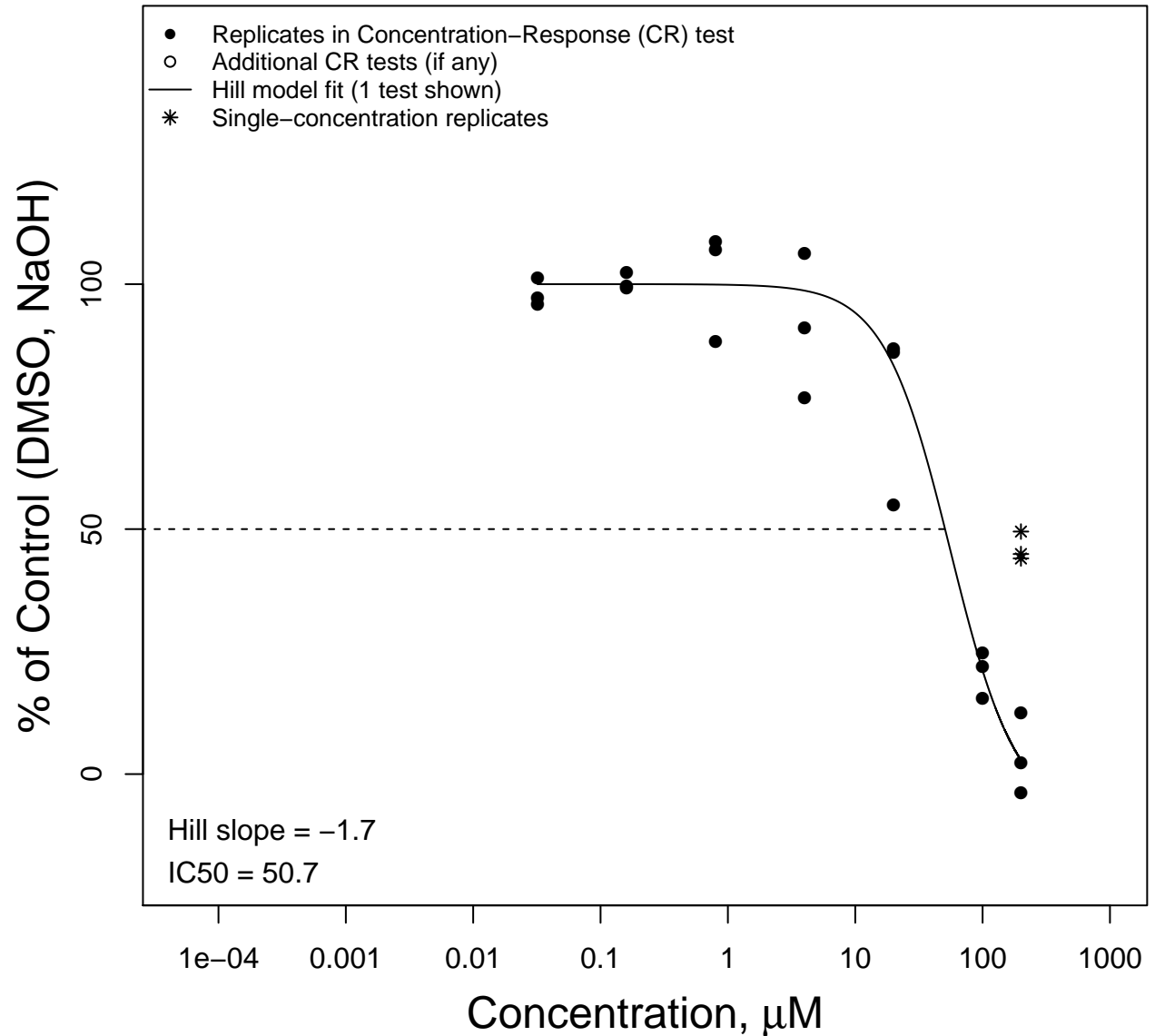
4-Hydroxytamoxifen

CASRN: 68392-35-8



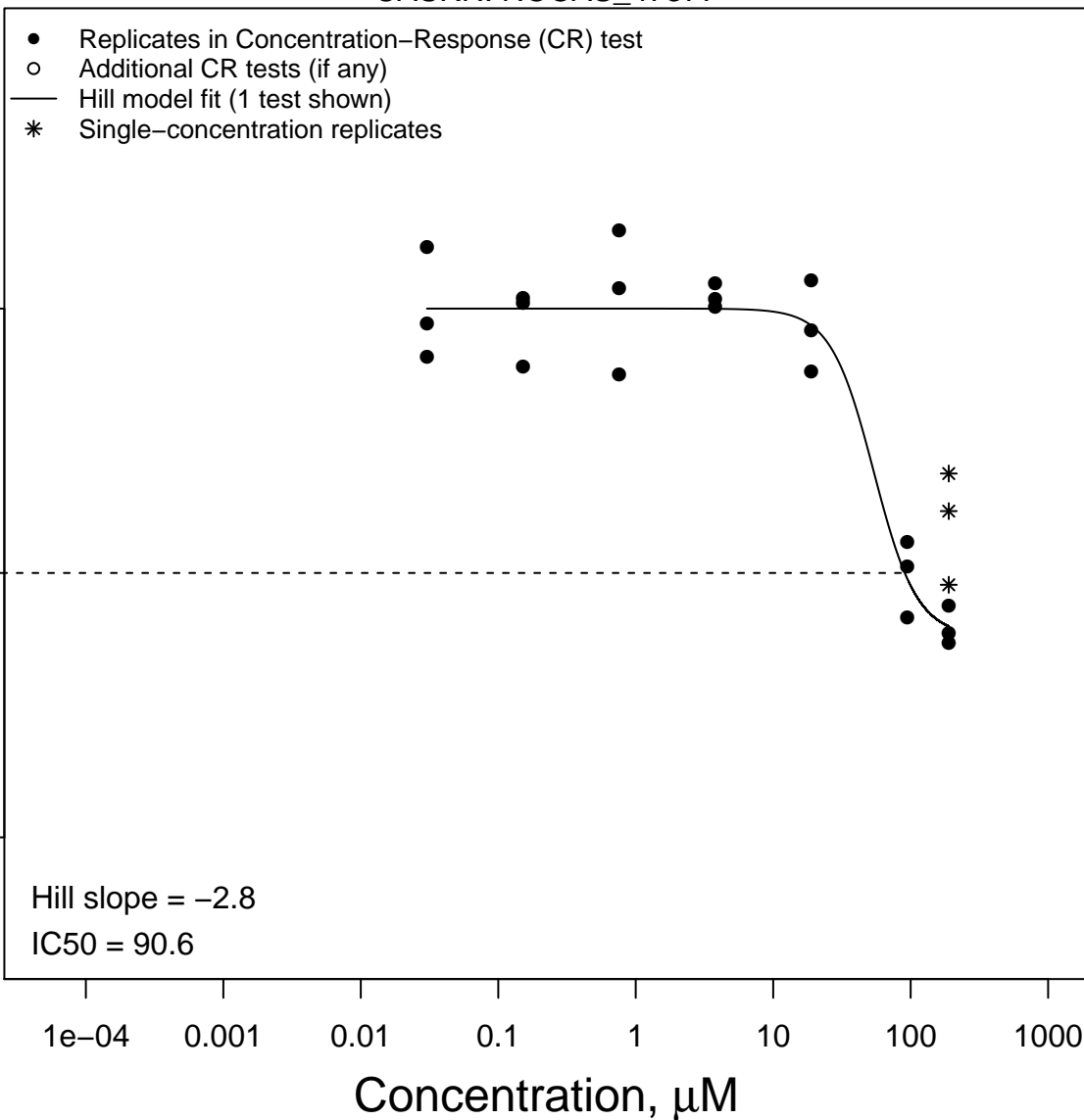
4-Heptylphenol

CASRN: 1987-50-4



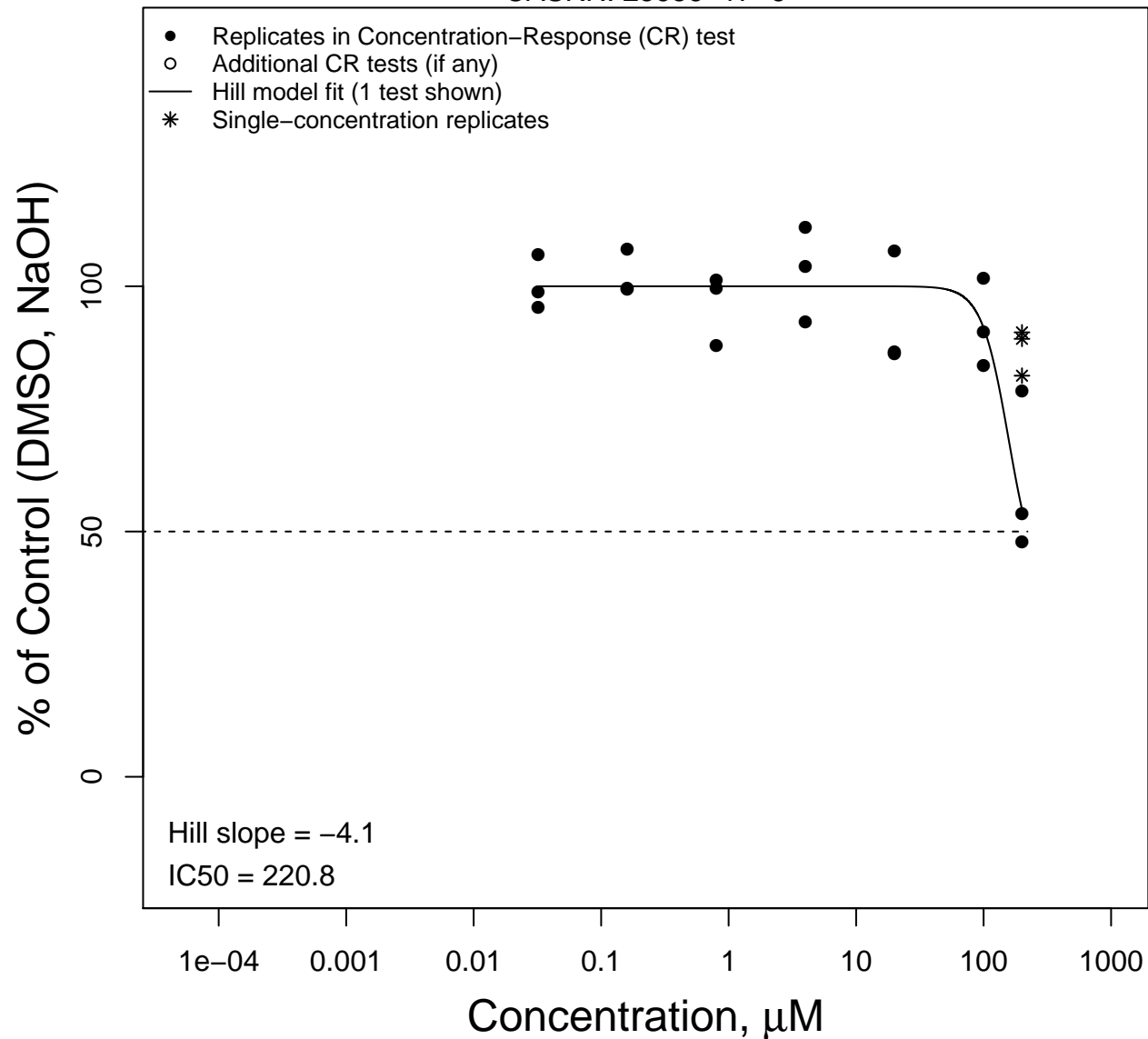
AVE6324

CASRN: NOCAS_47377



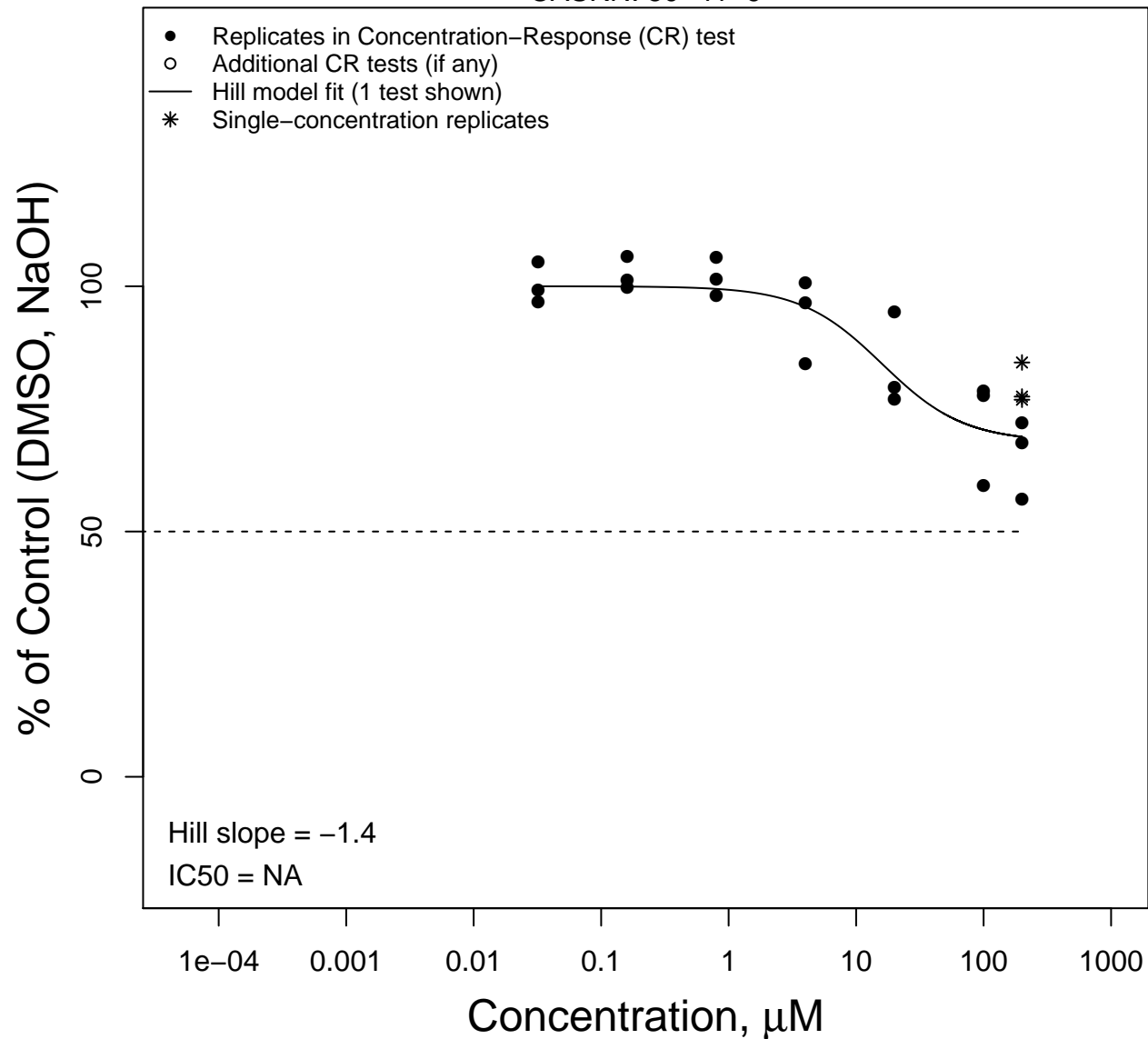
Allura Red C.I.16035

CASRN: 25956-17-6



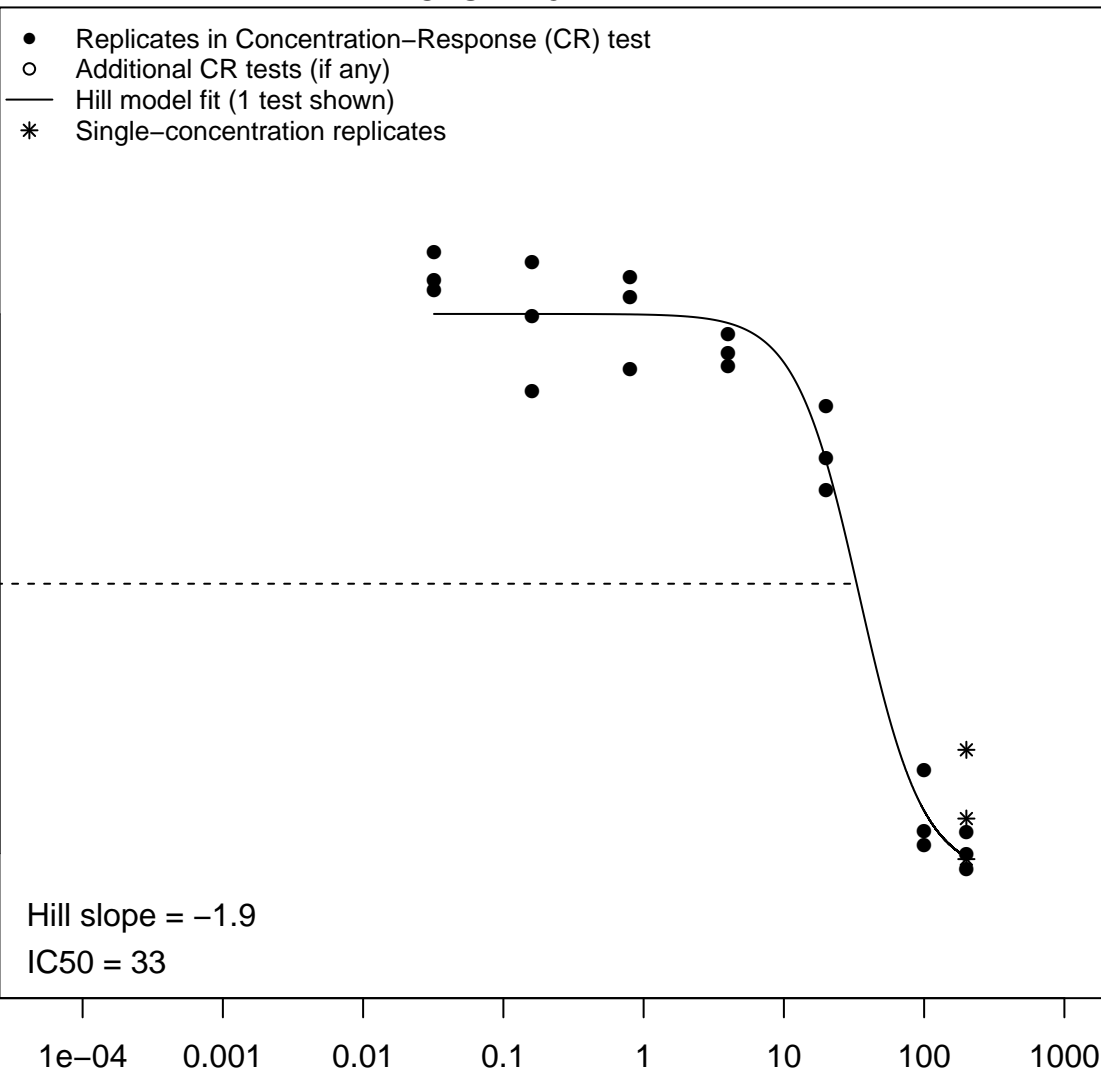
Clomiphene citrate (1:1)

CASRN: 50-41-9



Docusate sodium

CASRN: 577-11-7

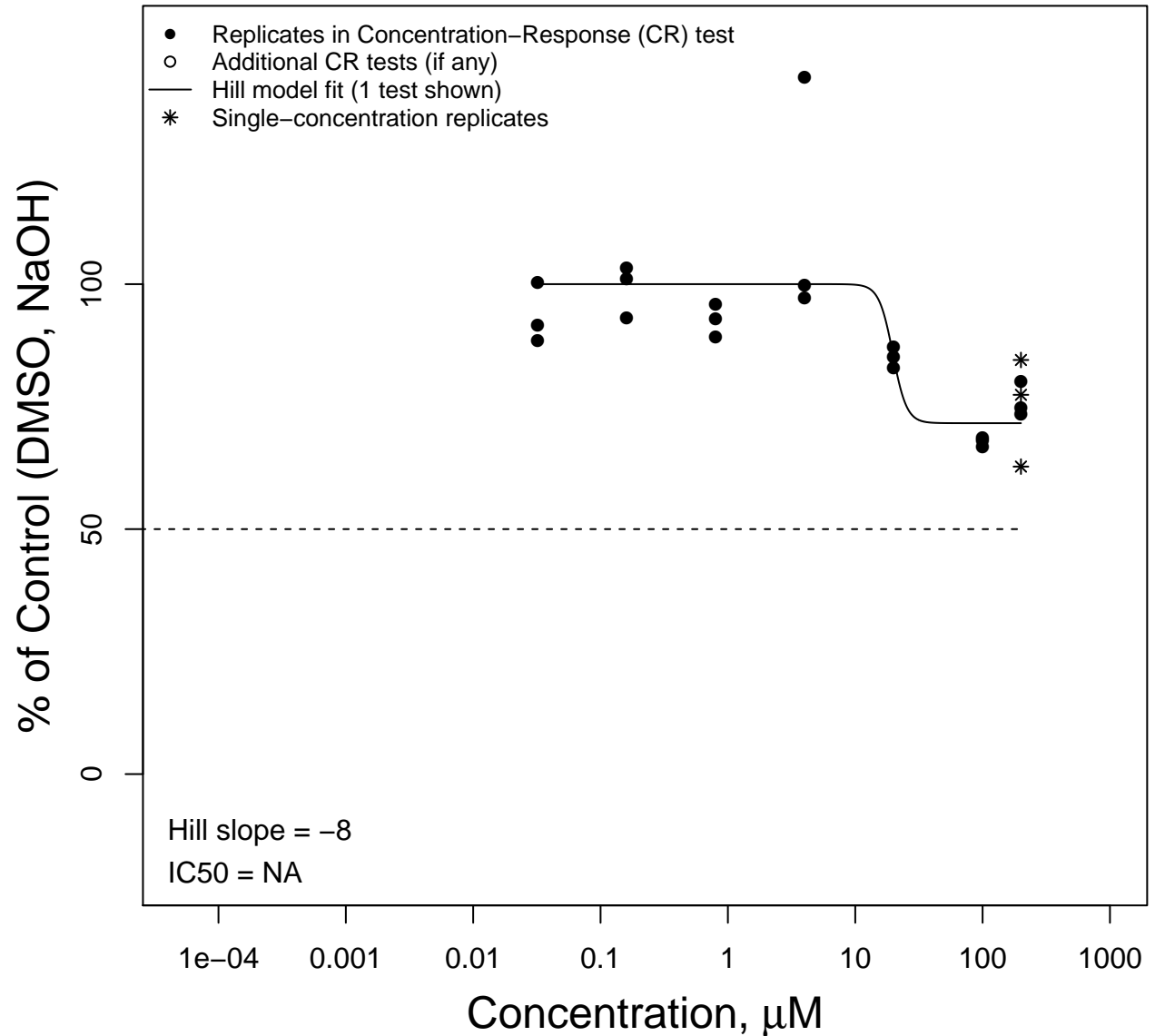


Concentration, µM

% of Control (DMSO, NaOH)

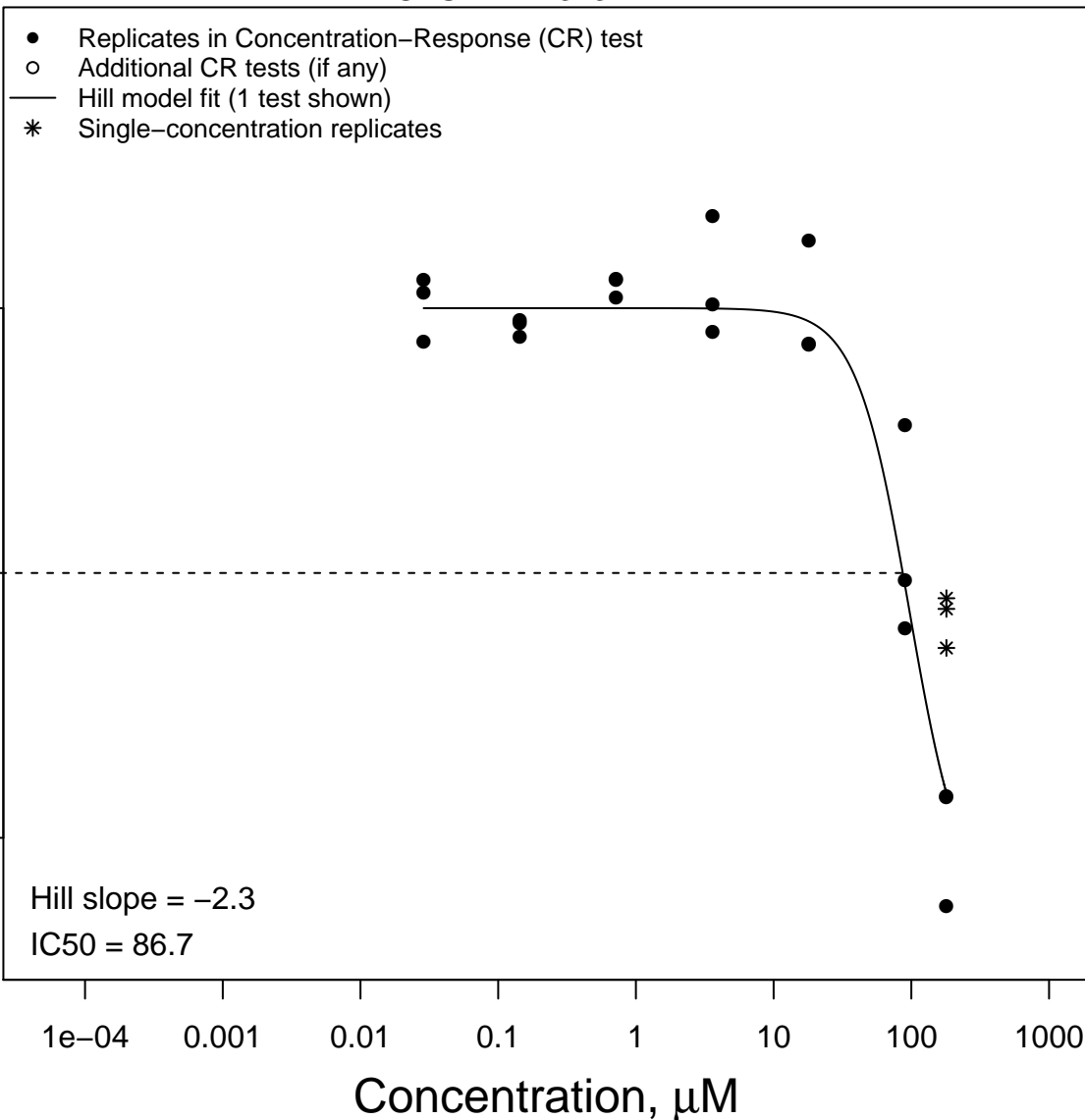
Dichlorodiphenyltrichloroethane

CASRN: 50-29-3



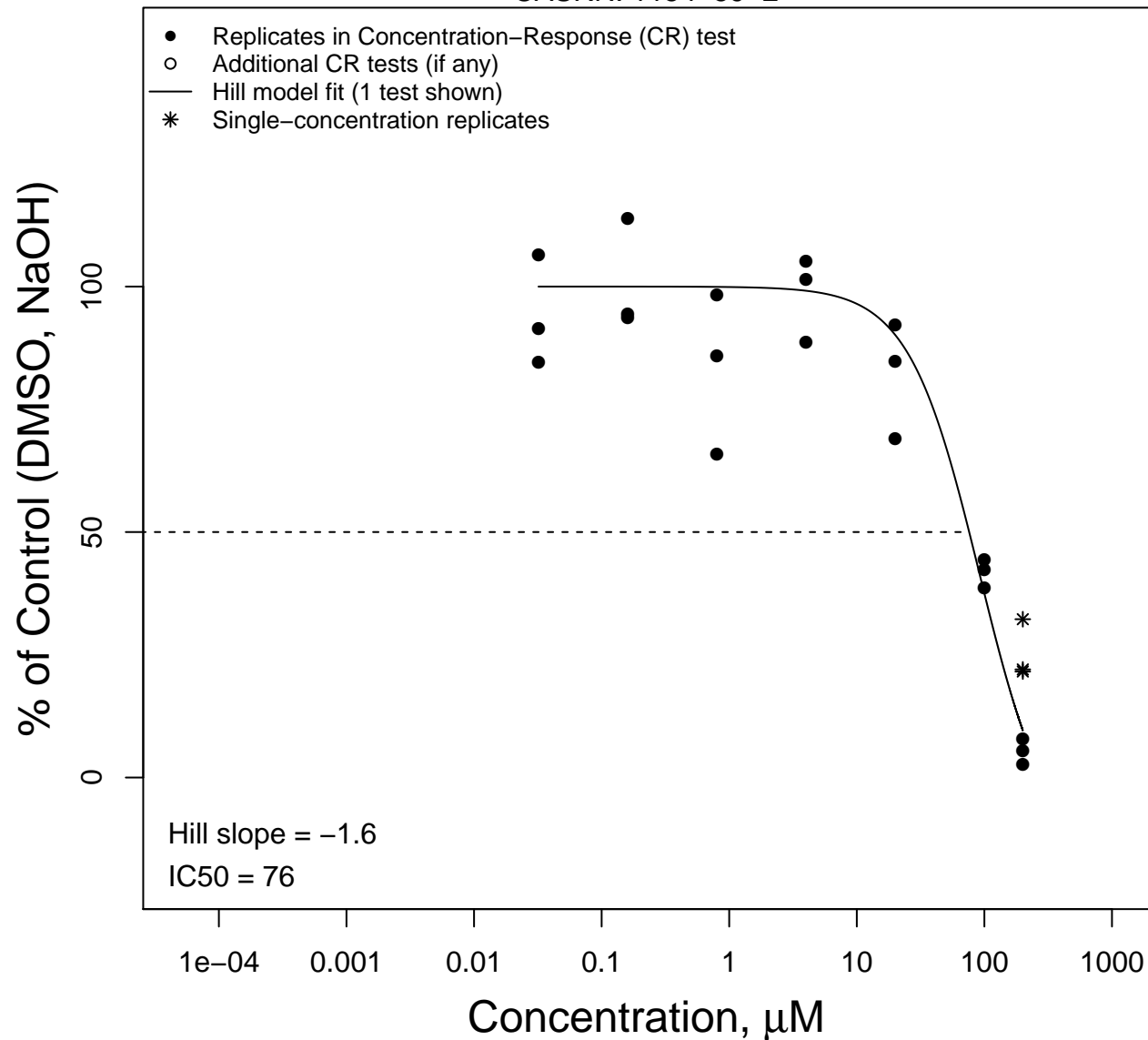
Dodecylbenzene sulfonate triethanolamine(1:1)

CASRN: 27323-41-7



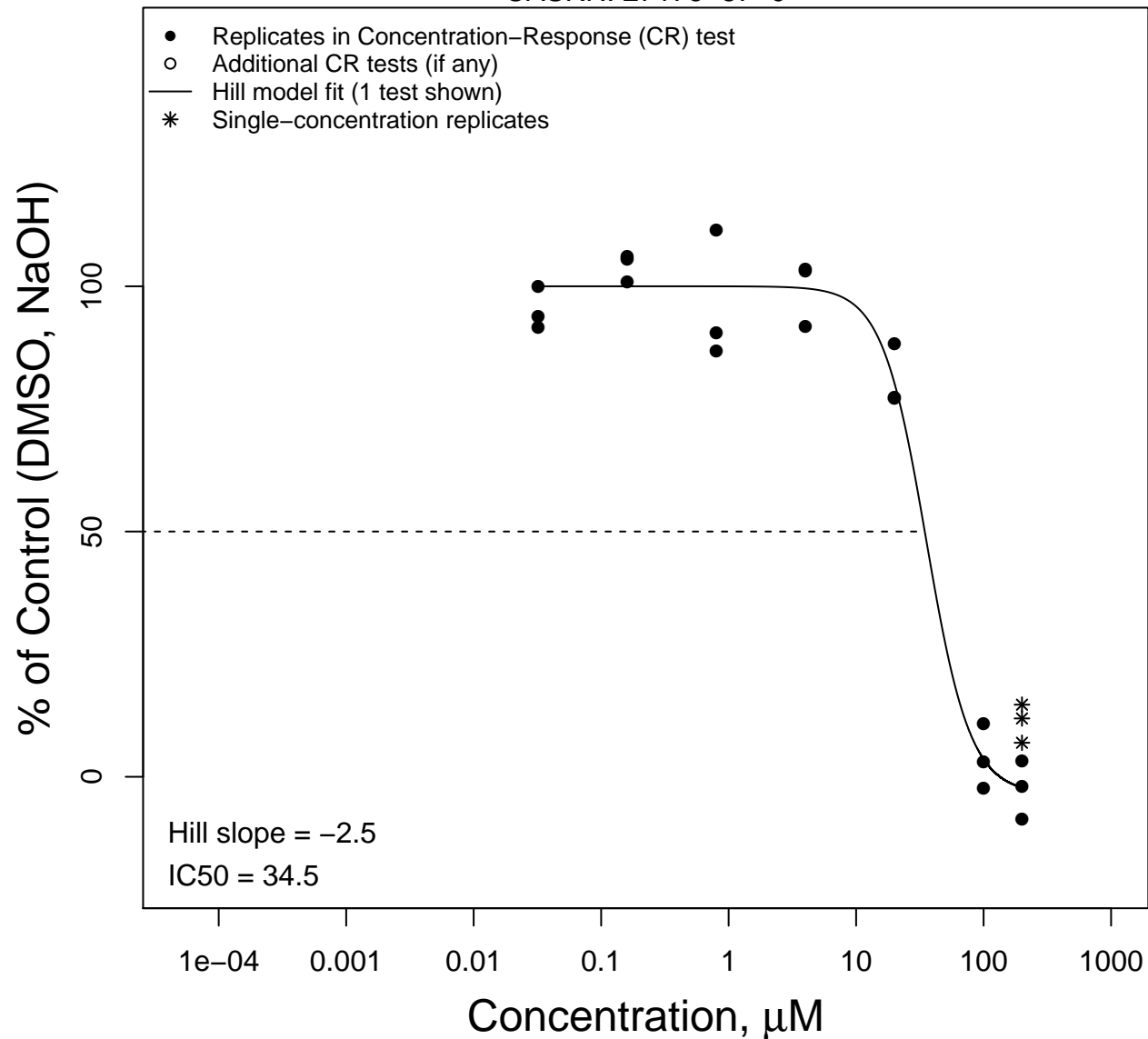
3,5-Dichlorosalicyl-3,4-dichloroanilide

CASRN: 1154-59-2



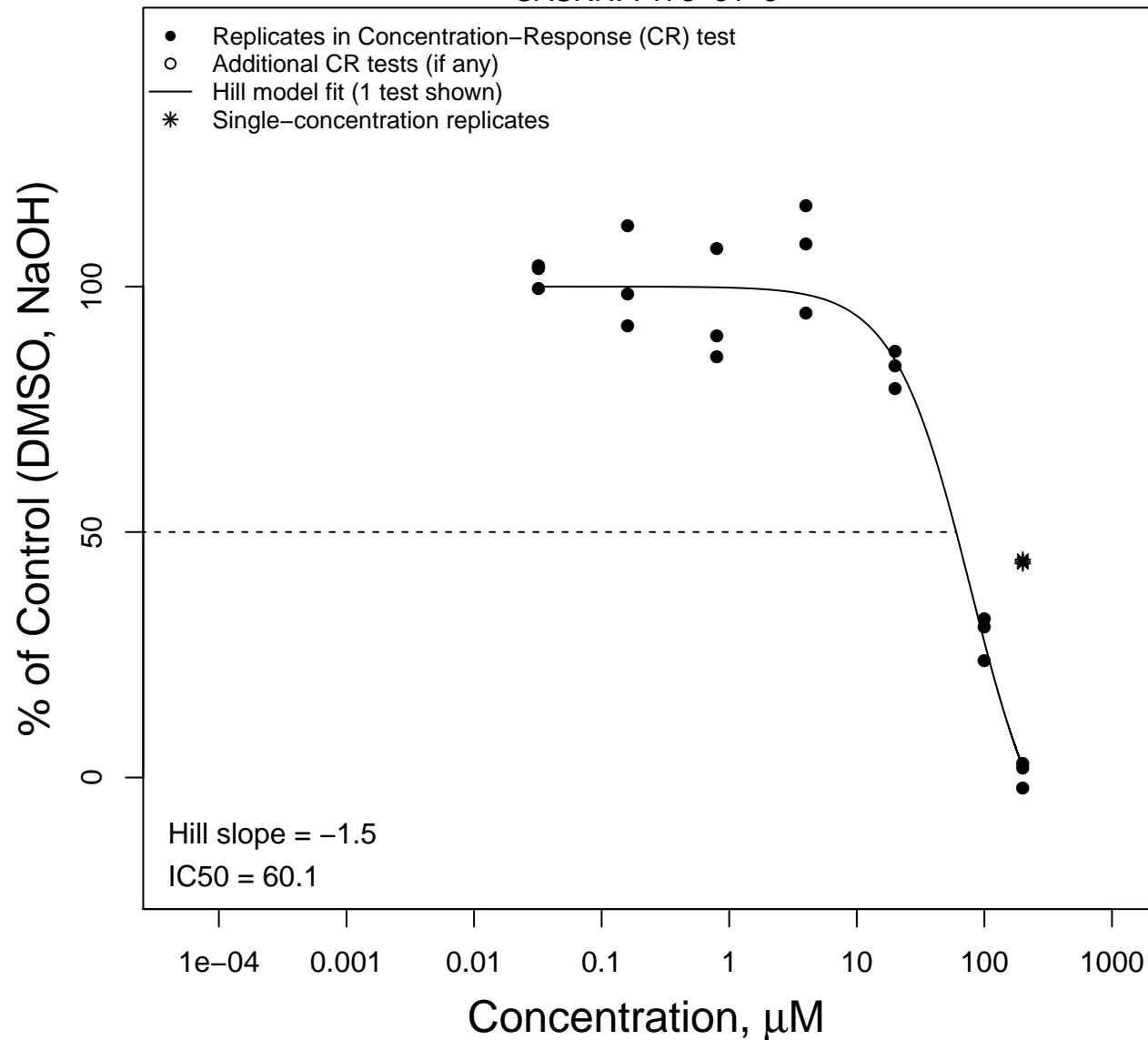
Dodecylbenzenesulfonic acid

CASRN: 27176-87-0



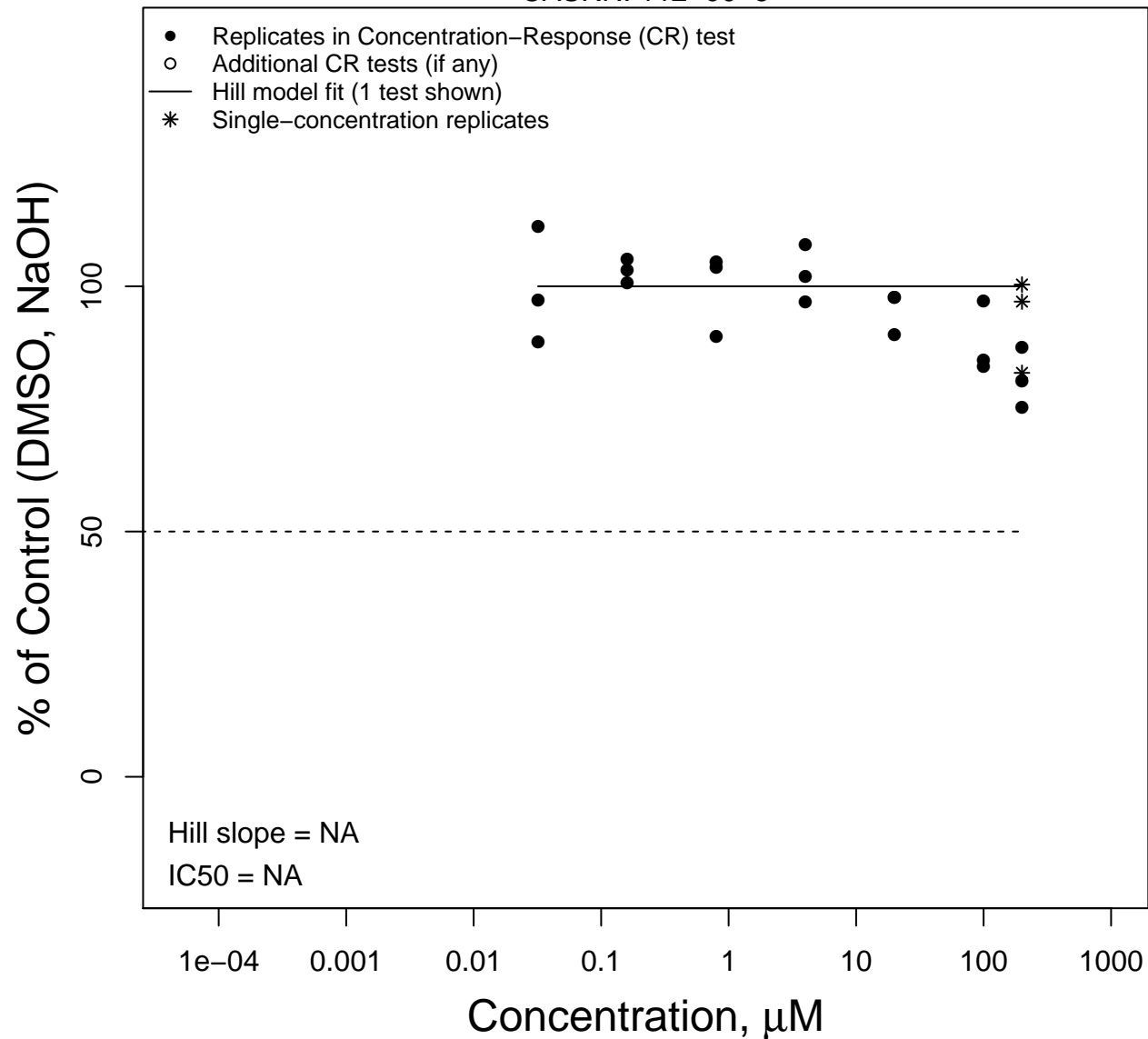
Didecyldimethylammonium chloride

CASRN: 7173-51-5



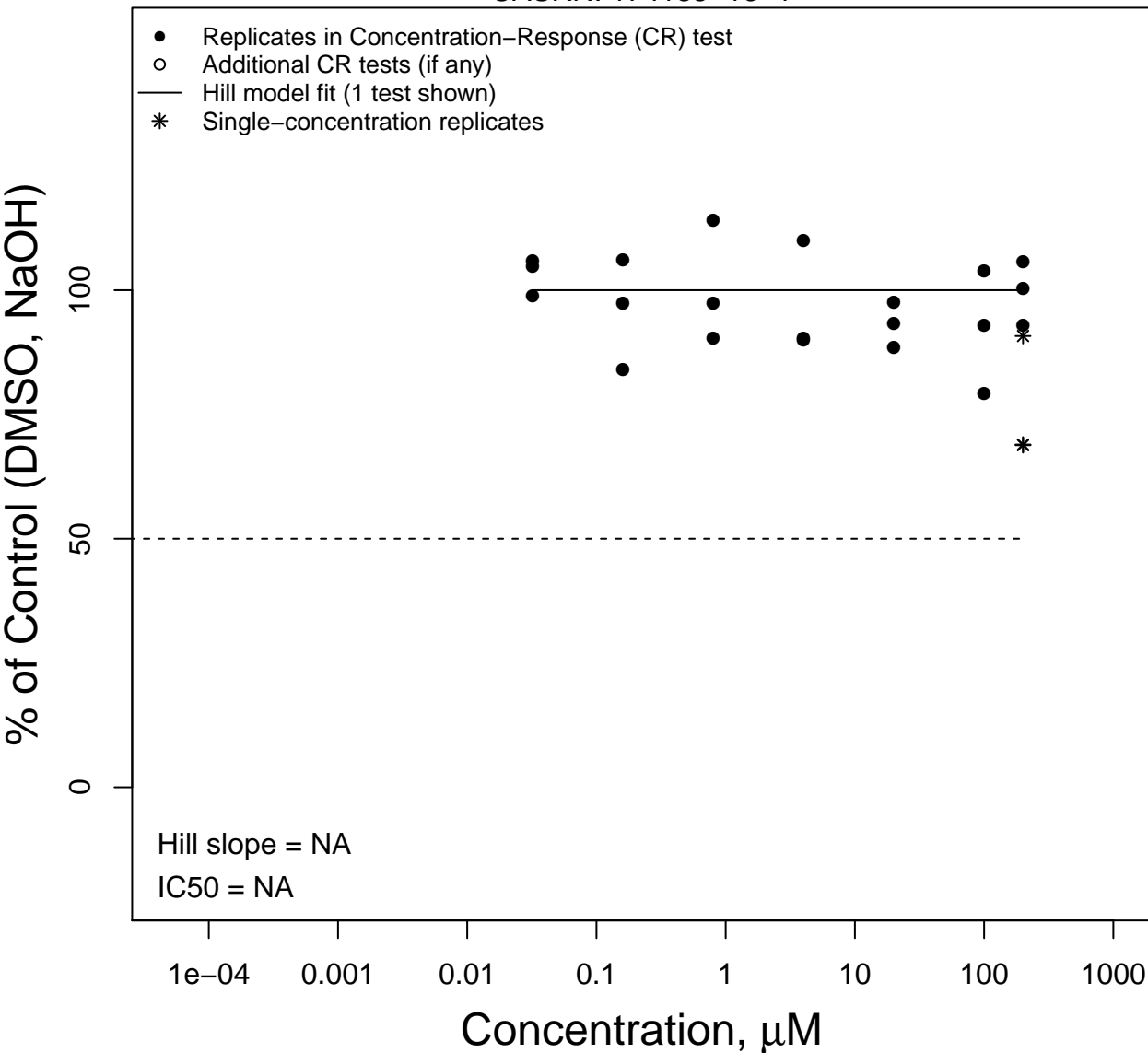
Dodecyltrimethylammonium chloride

CASRN: 112-00-5



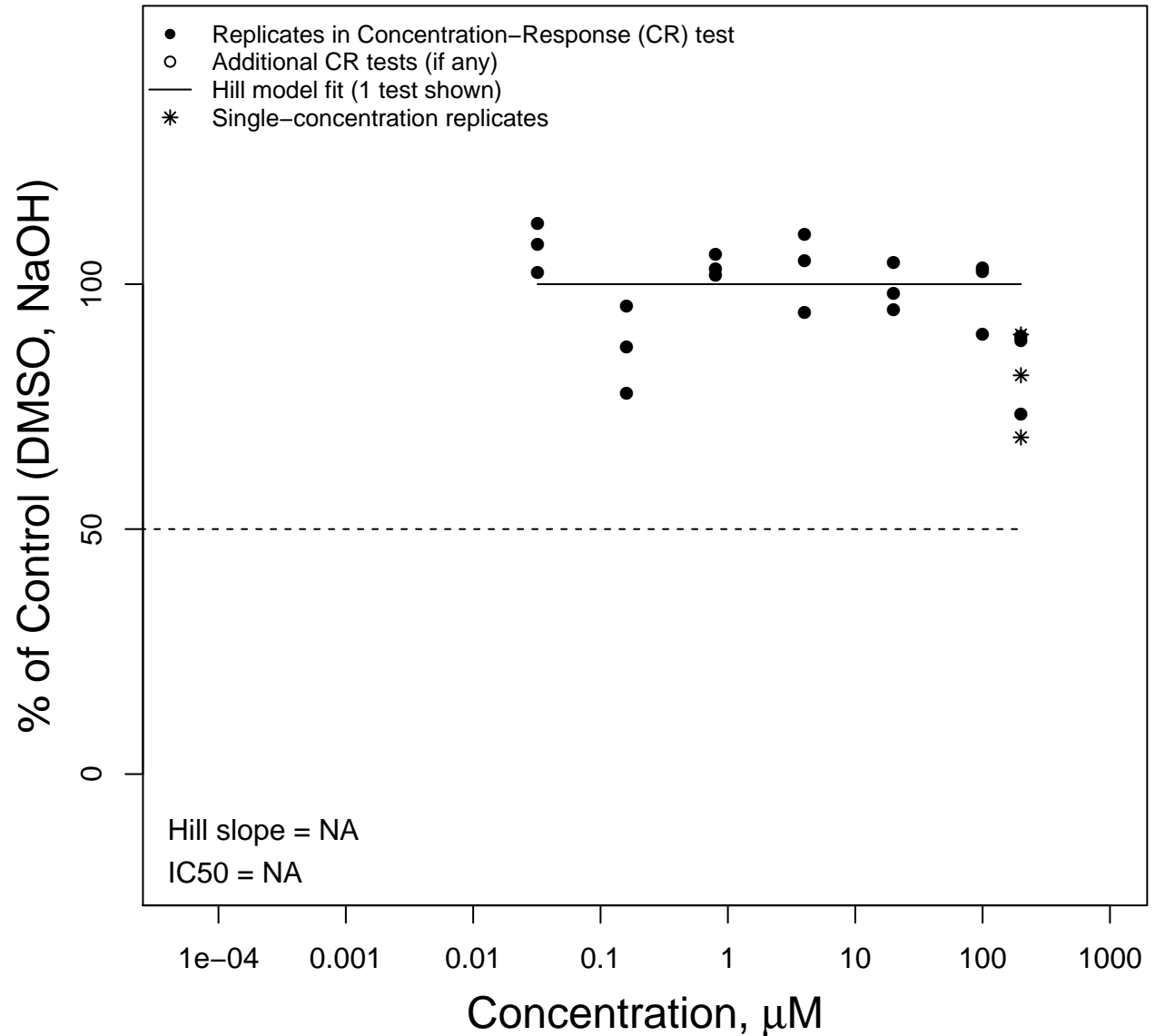
FR167356

CASRN: 174185-16-1



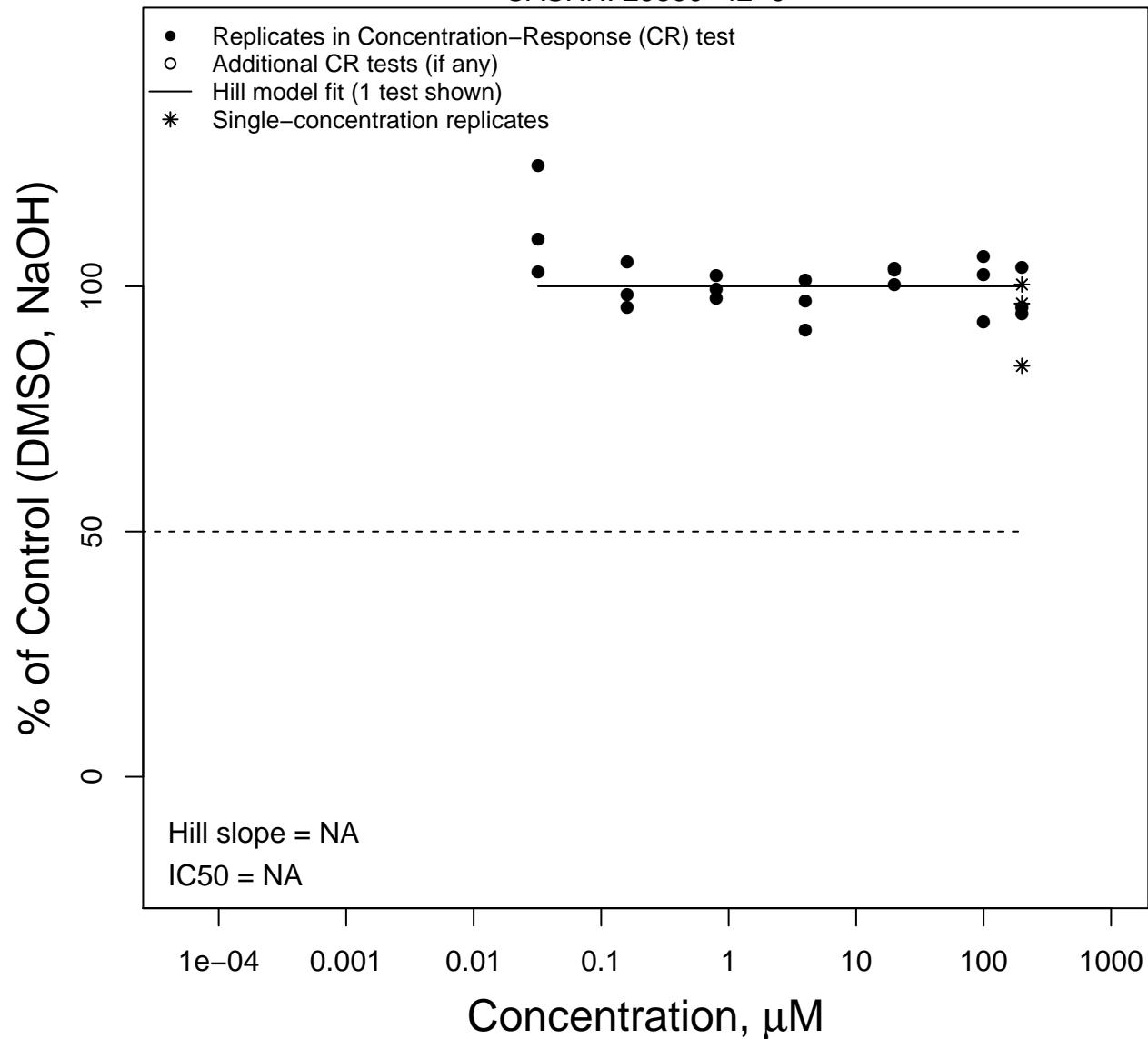
Gentian Violet

CASRN: 548-62-9



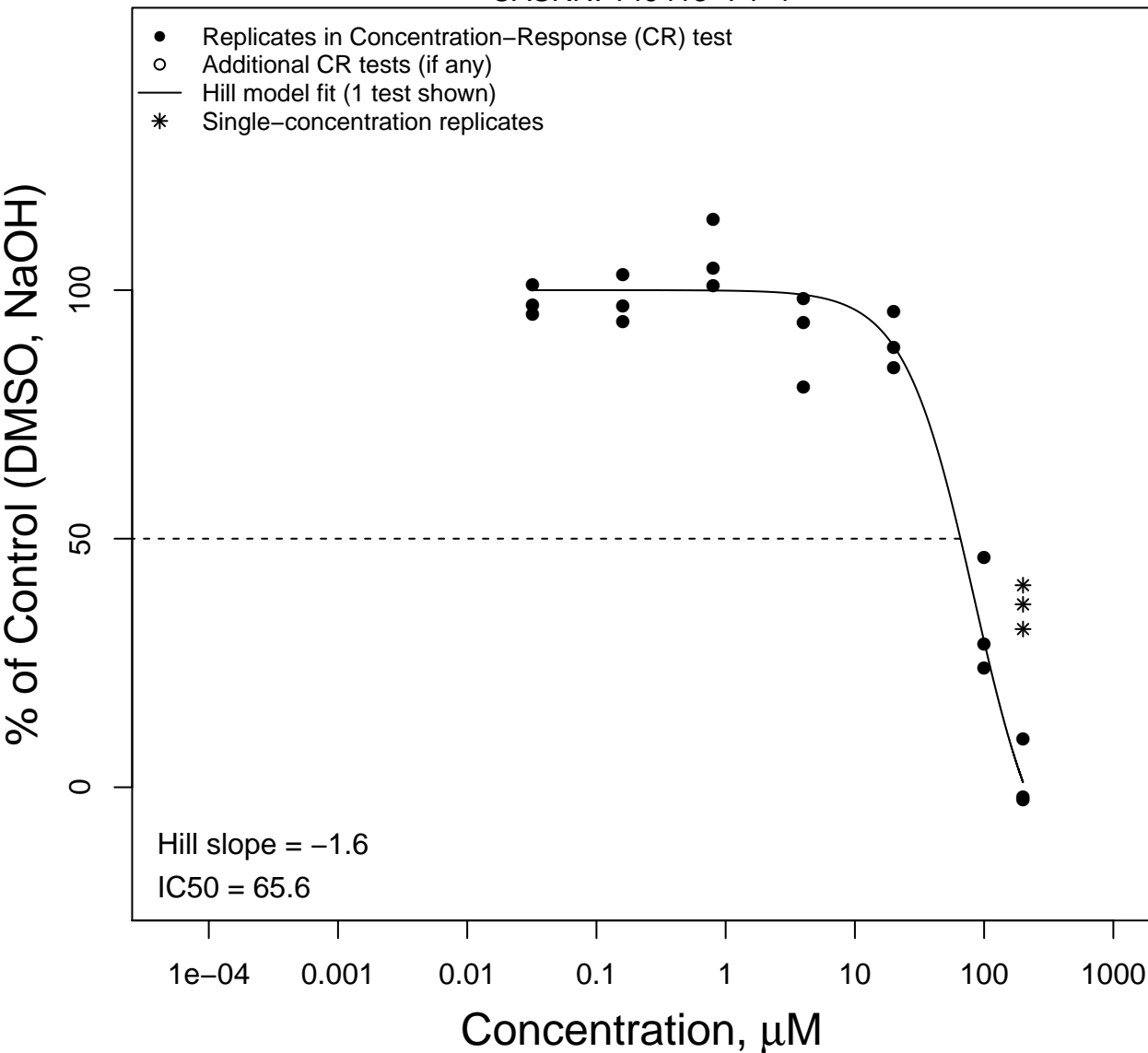
Isooctyl acrylate

CASRN: 29590-42-9



FR150011

CASRN: 149413-74-1

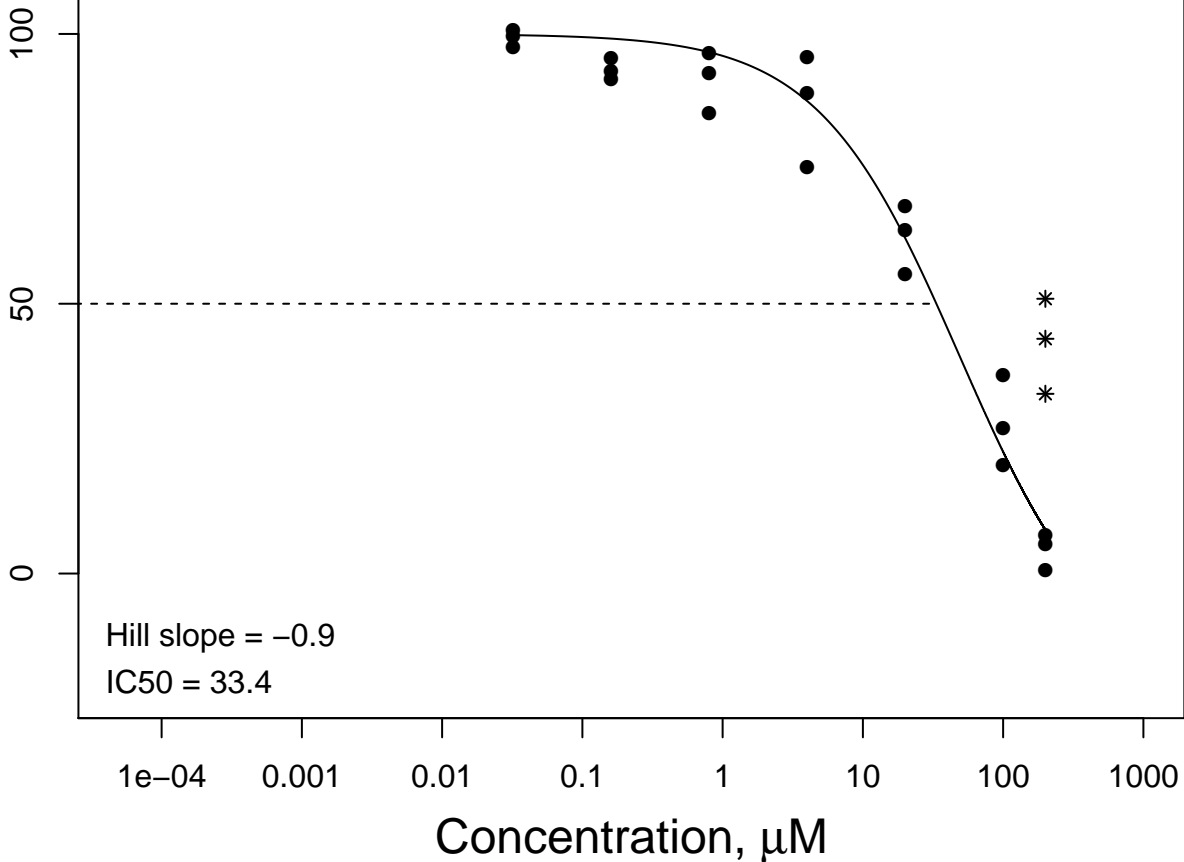


Kepone

CASRN: 143-50-0

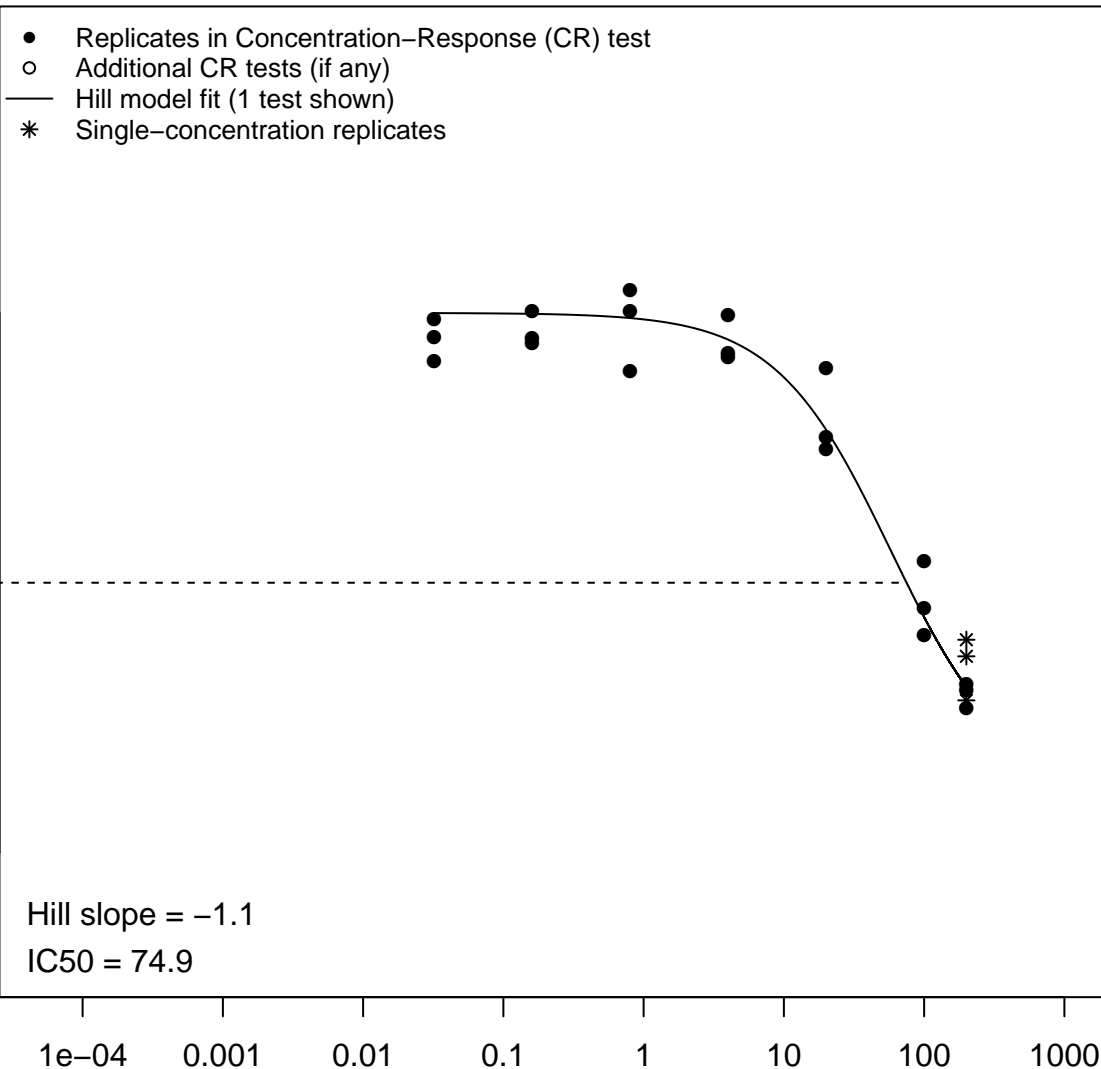
- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)



Fenaminosulf

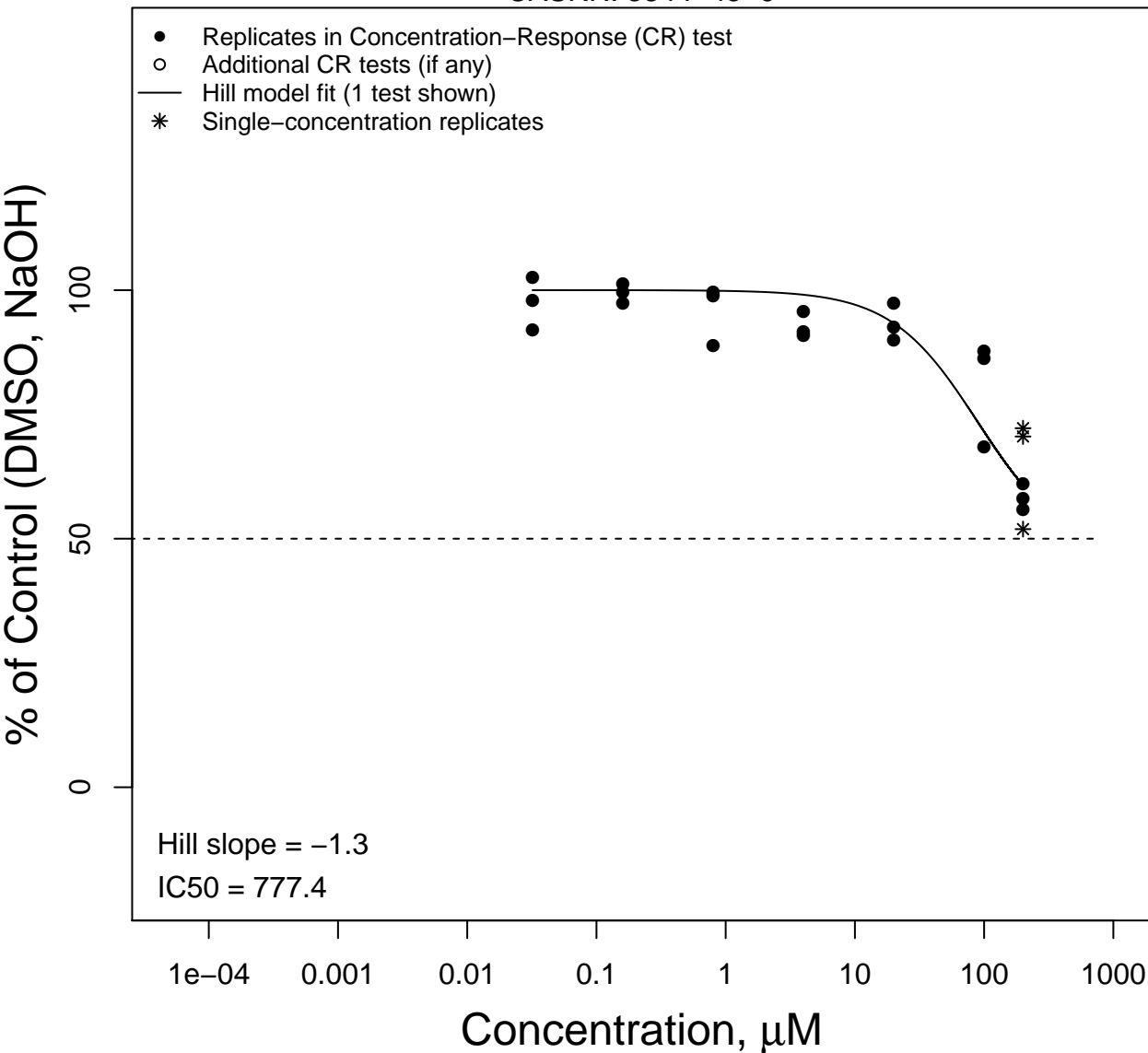
CASRN: 140-56-7



Concentration, μM

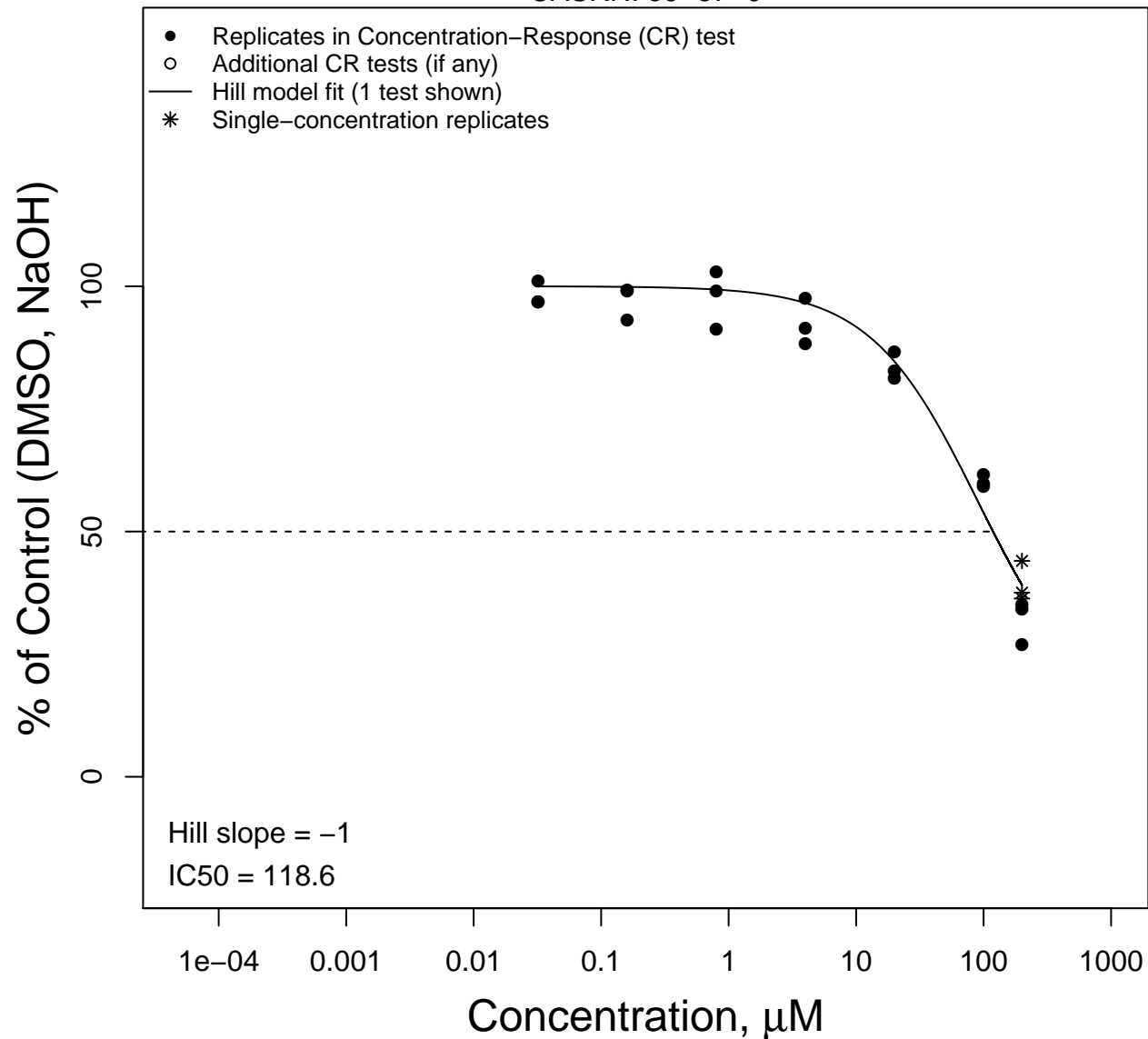
FD&C Blue No. 1

CASRN: 3844-45-9



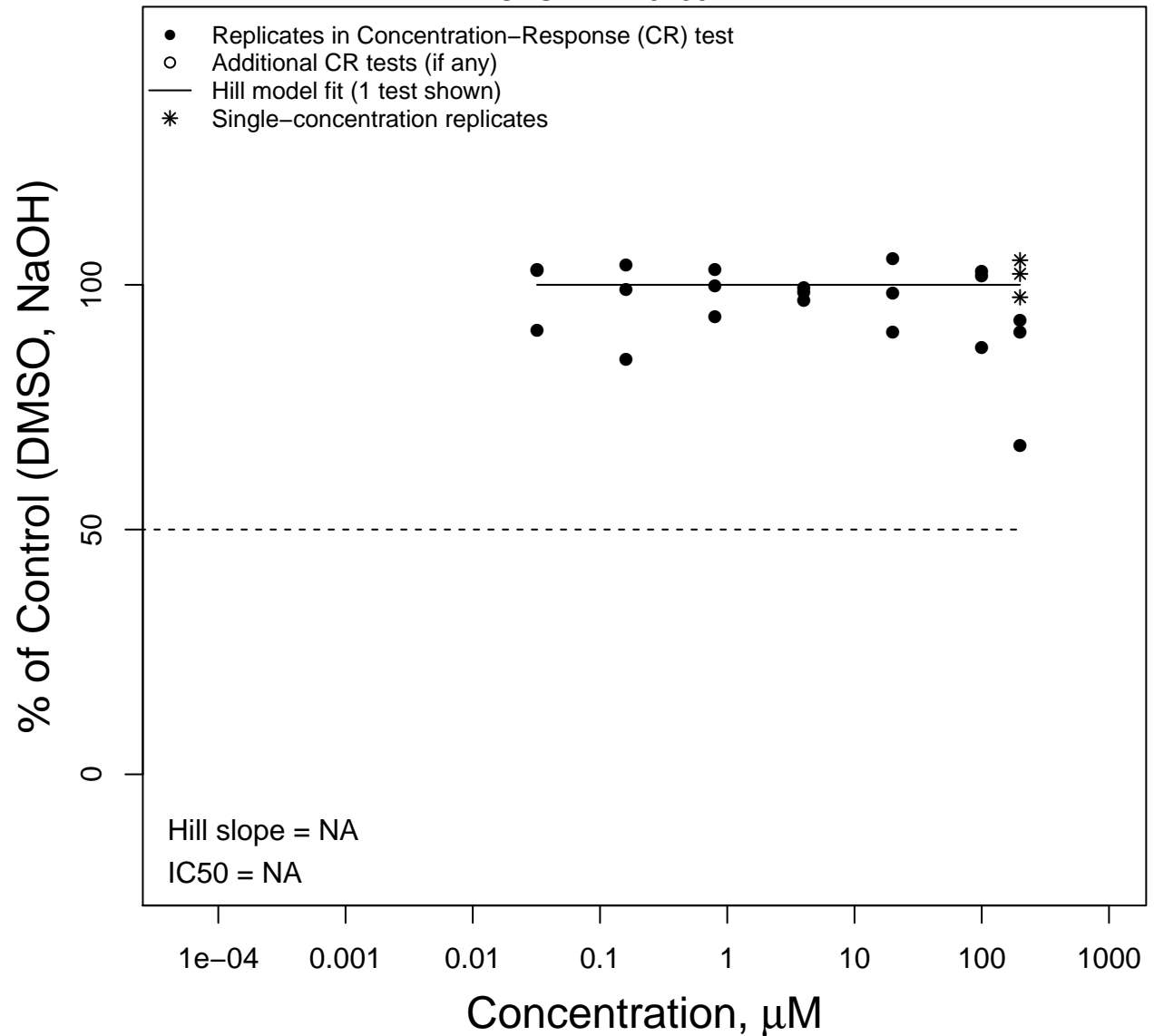
Nitrofurazone

CASRN: 59-87-0



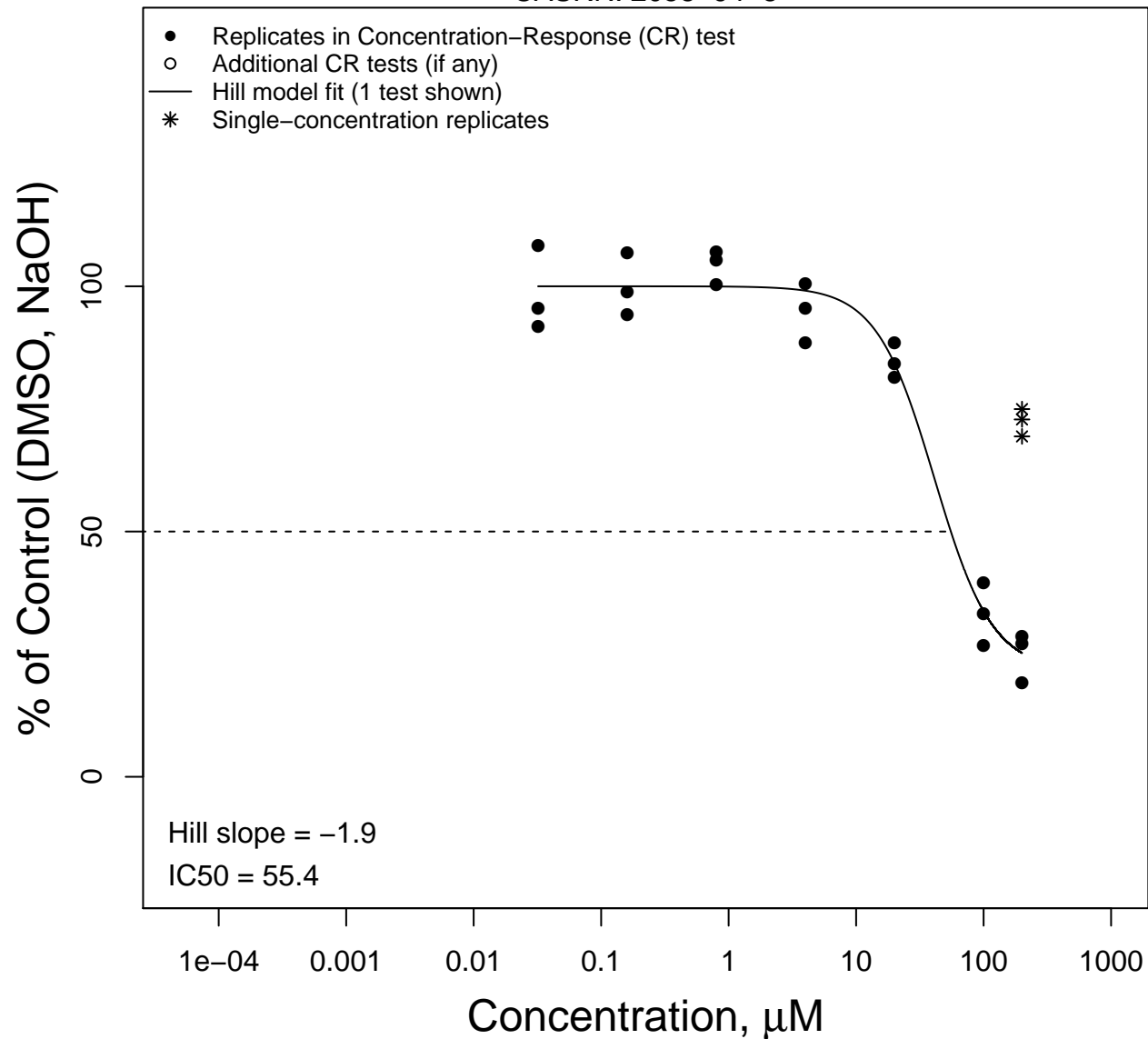
Mepaniprym

CASRN: 110235-47-7



Perfluoroundecanoic acid

CASRN: 2058-94-8



PharmaGSID_47337

CASRN: 1061517-62-1

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100

50

0

Hill slope = -3.1

IC50 = 108.5

1e-04

0.001

0.01

0.1

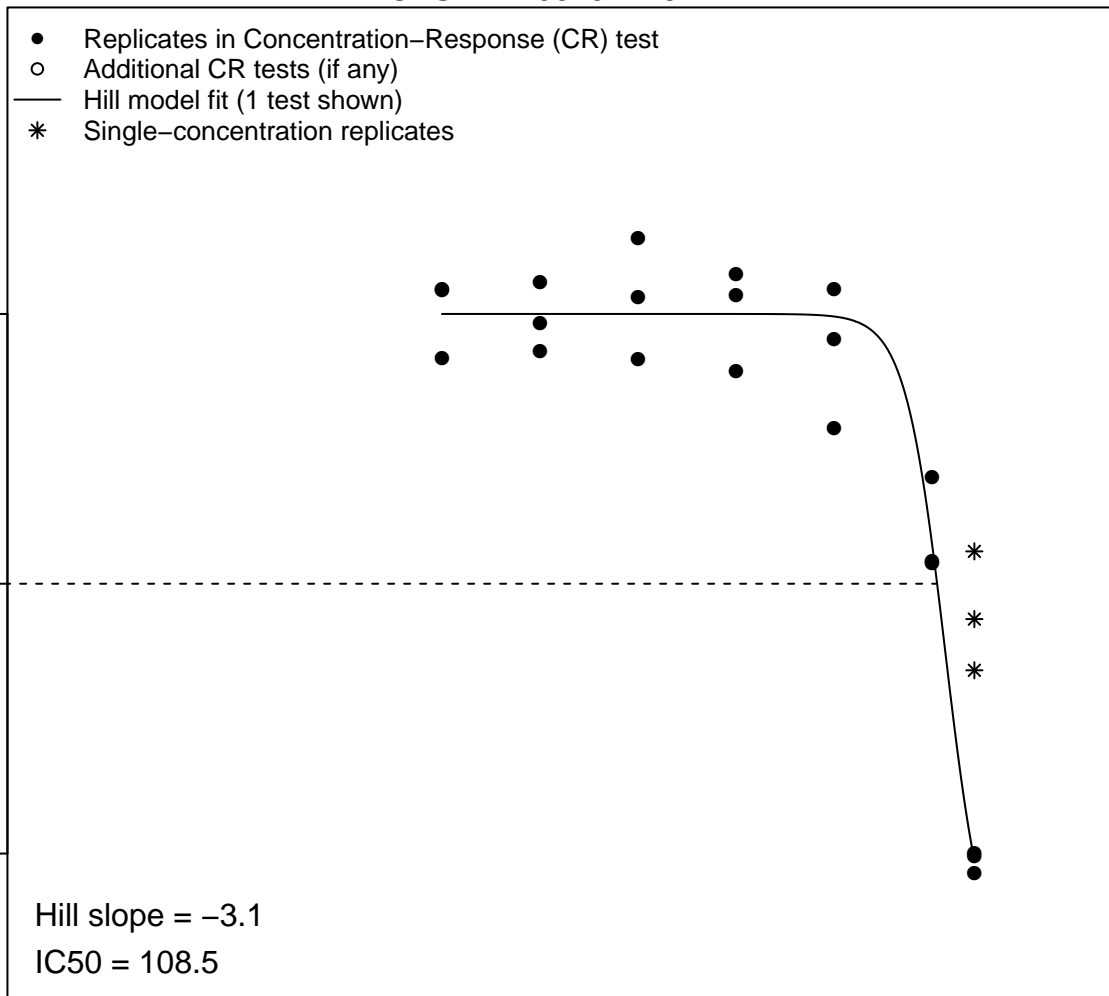
1

10

100

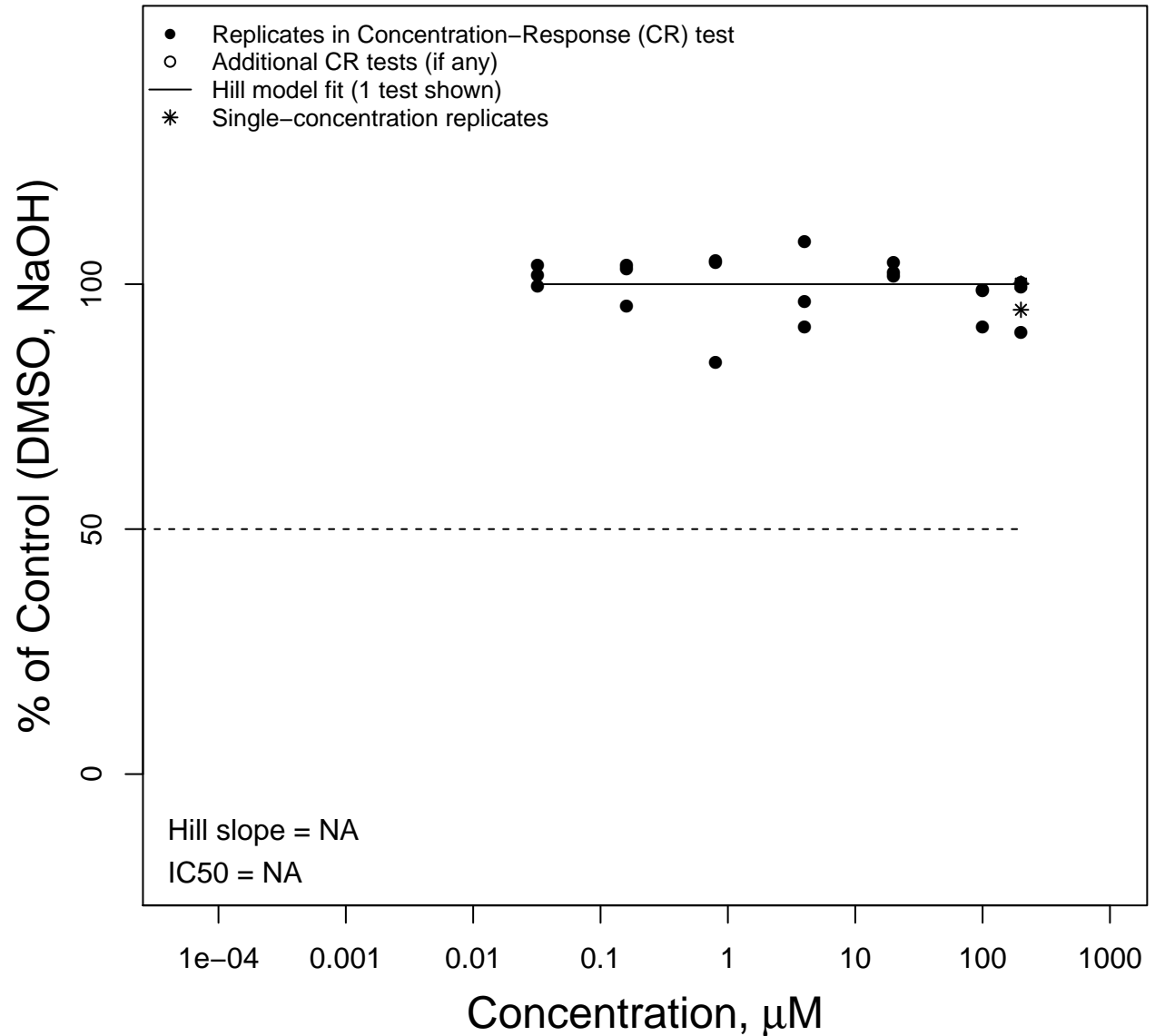
1000

Concentration, μM



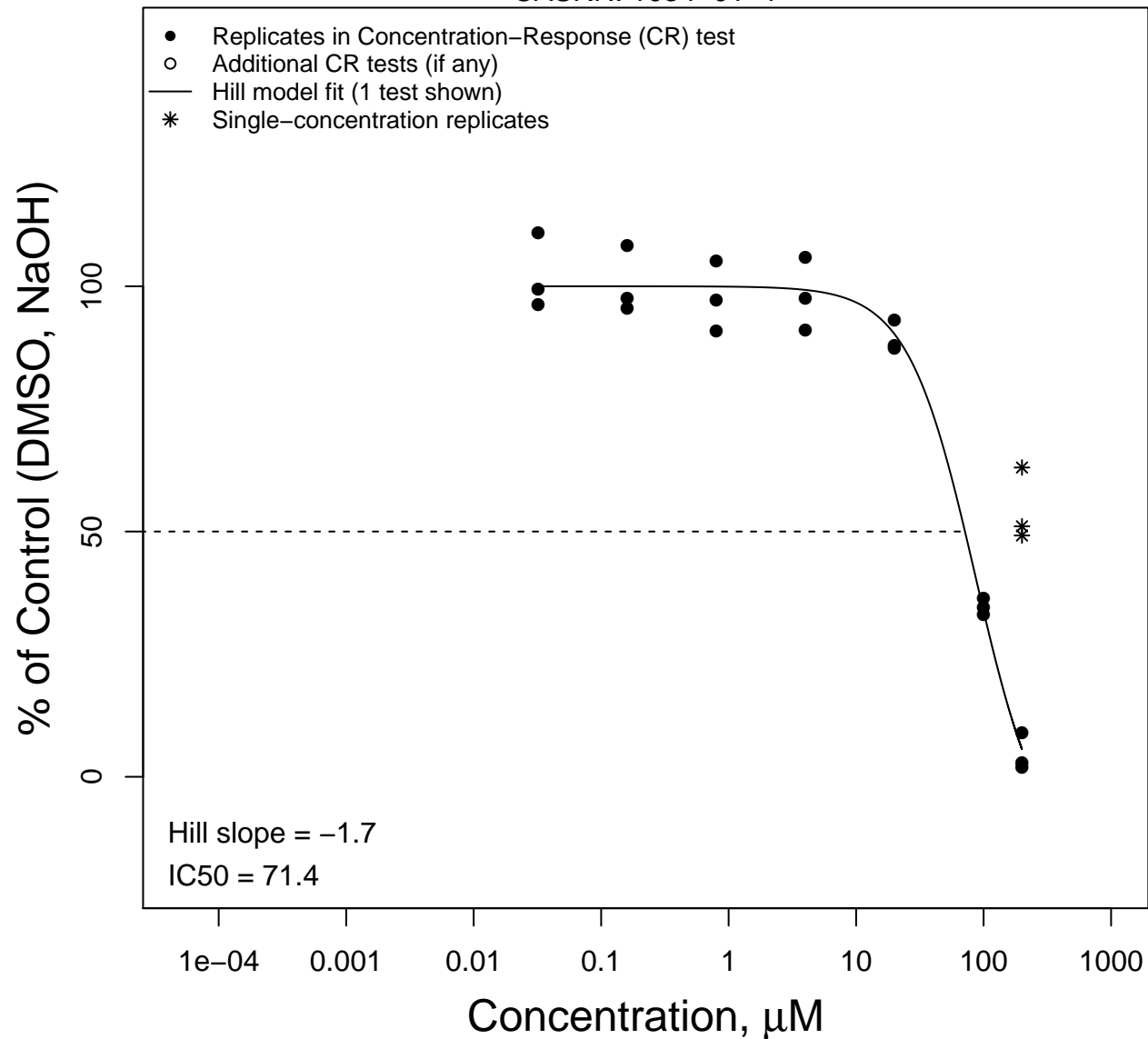
Salicylanilide

CASRN: 87-17-2



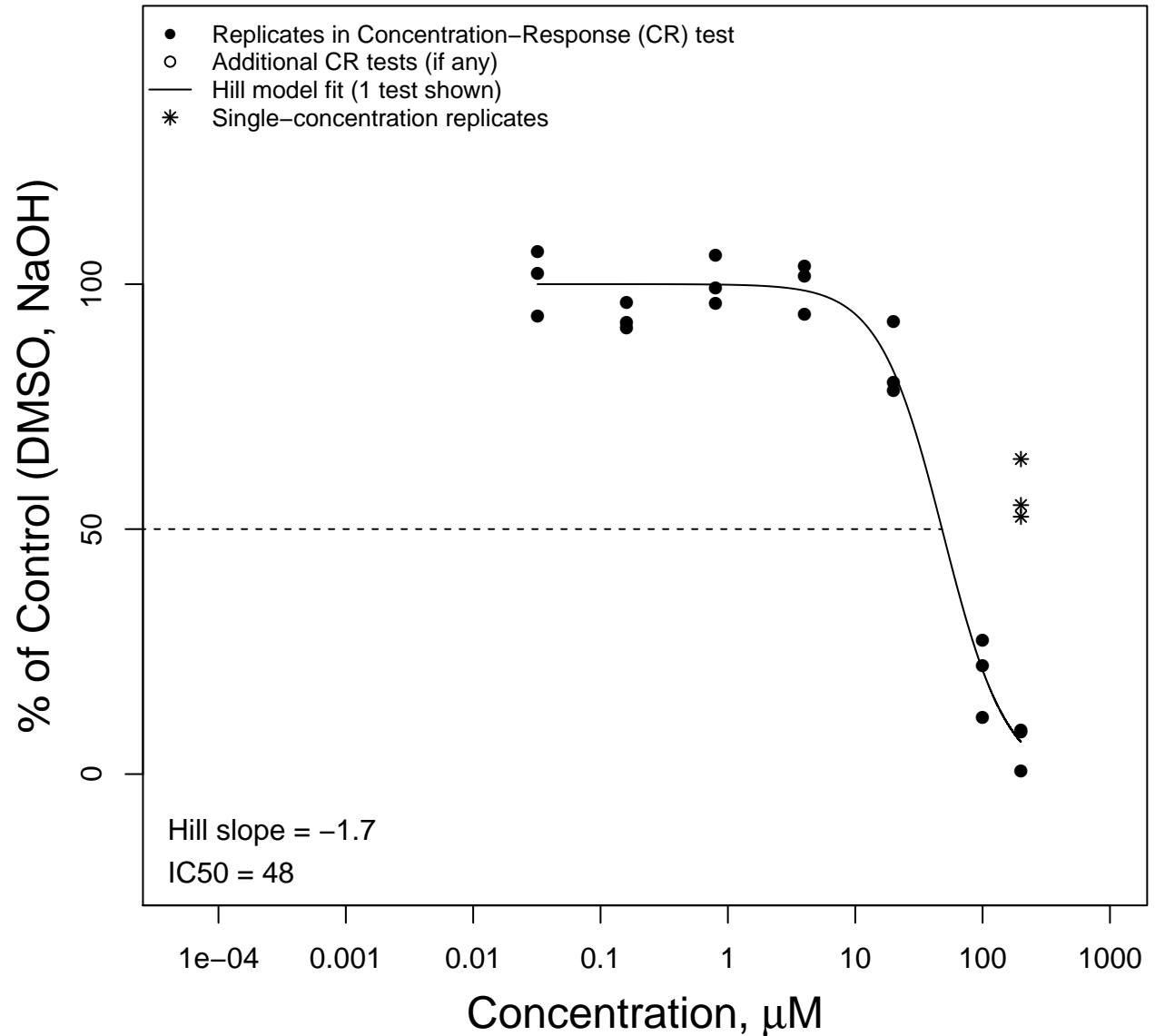
Octyl gallate

CASRN: 1034-01-1



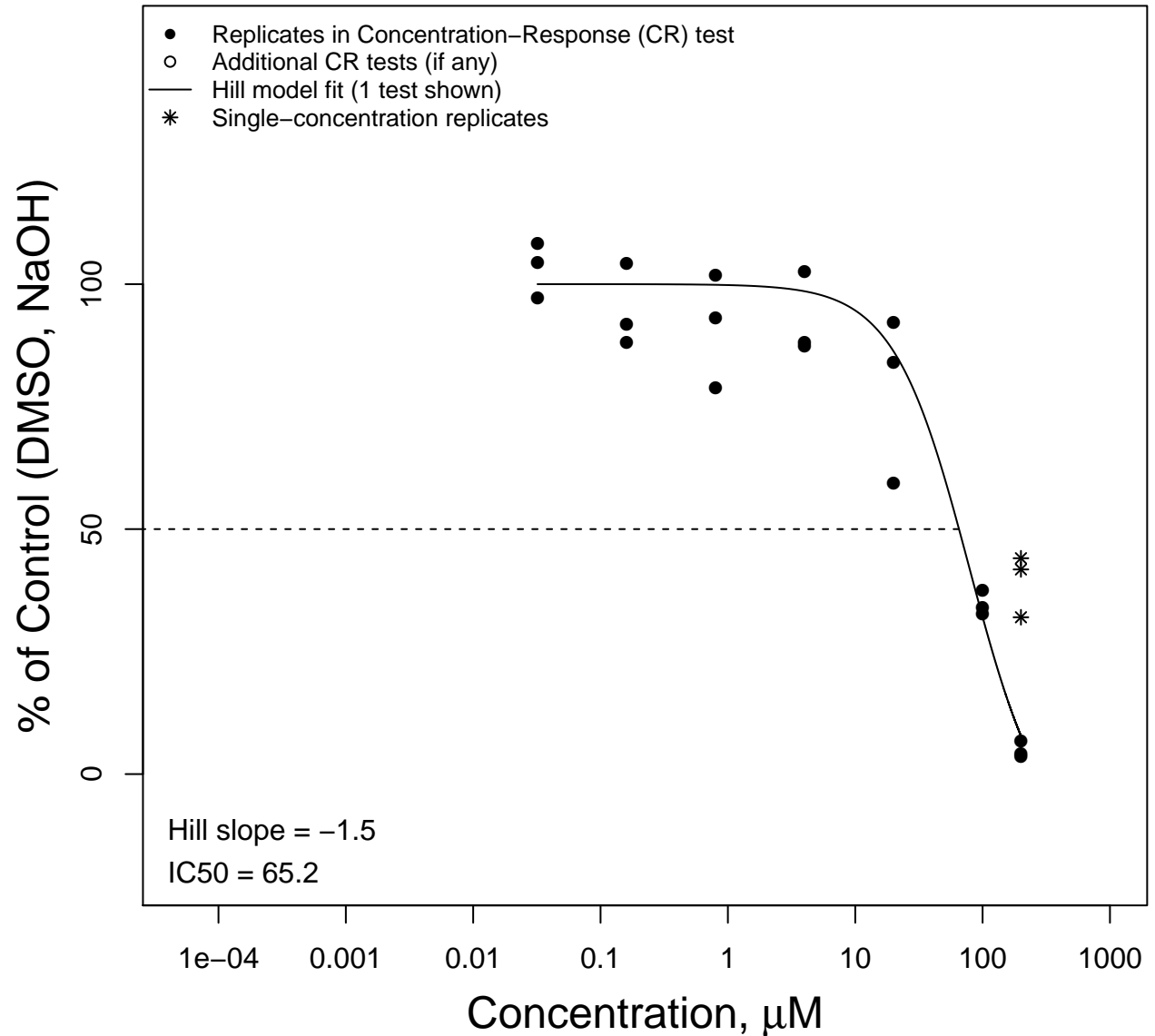
Perfluorodecanoic acid

CASRN: 335-76-2



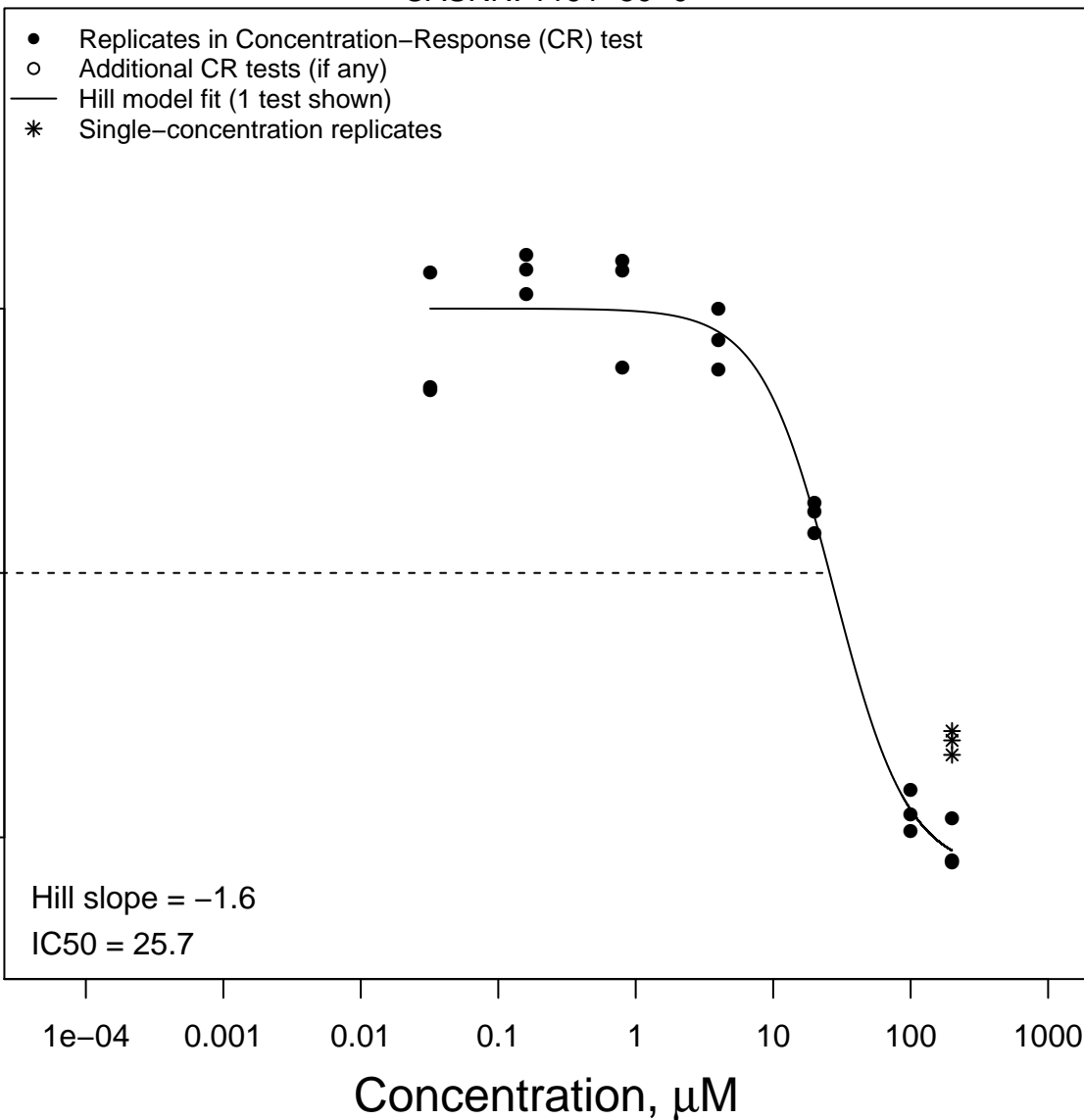
Sodium dodecyl sulfate

CASRN: 151-21-3



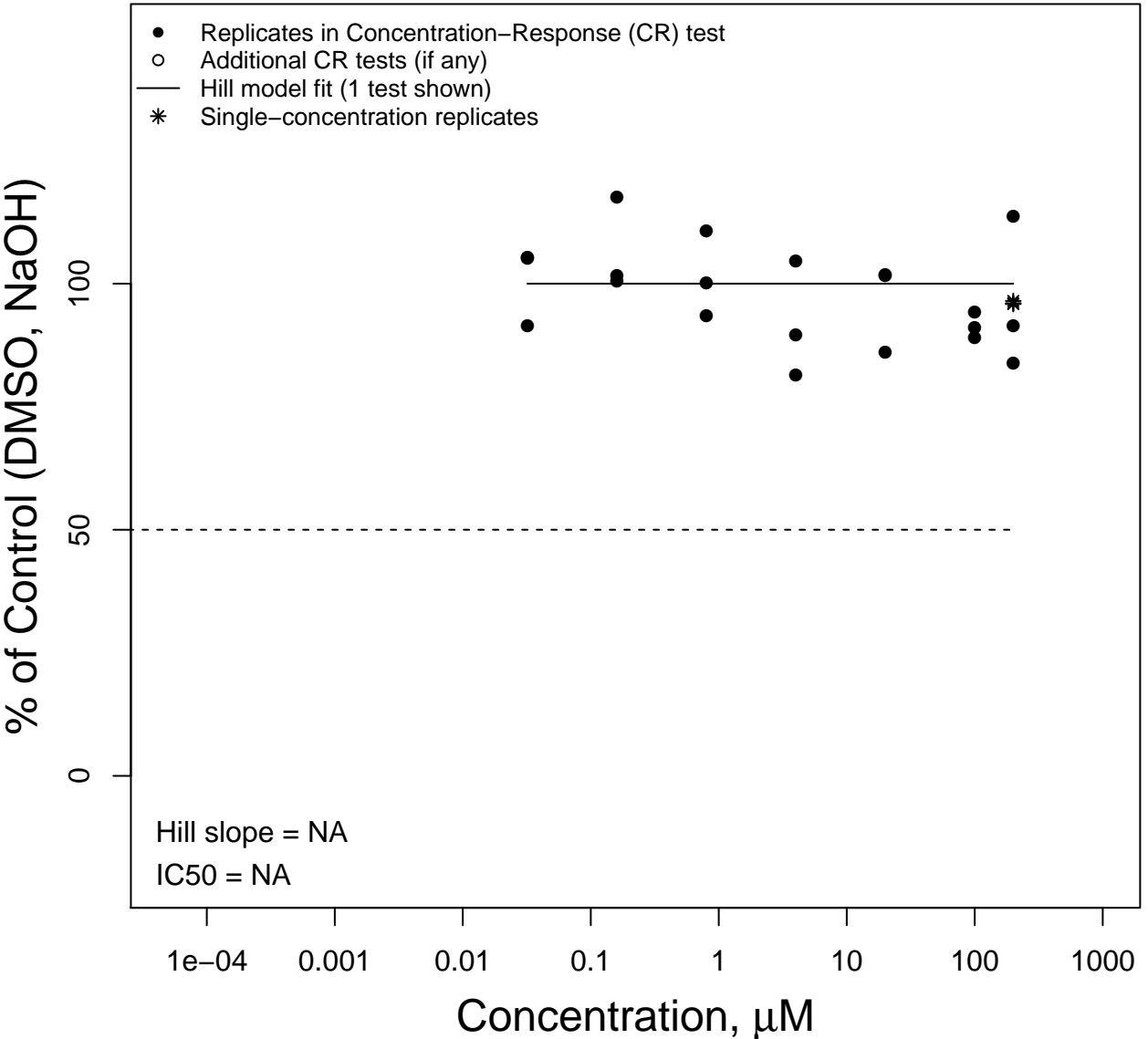
Sodium myristyl sulfate

CASRN: 1191-50-0



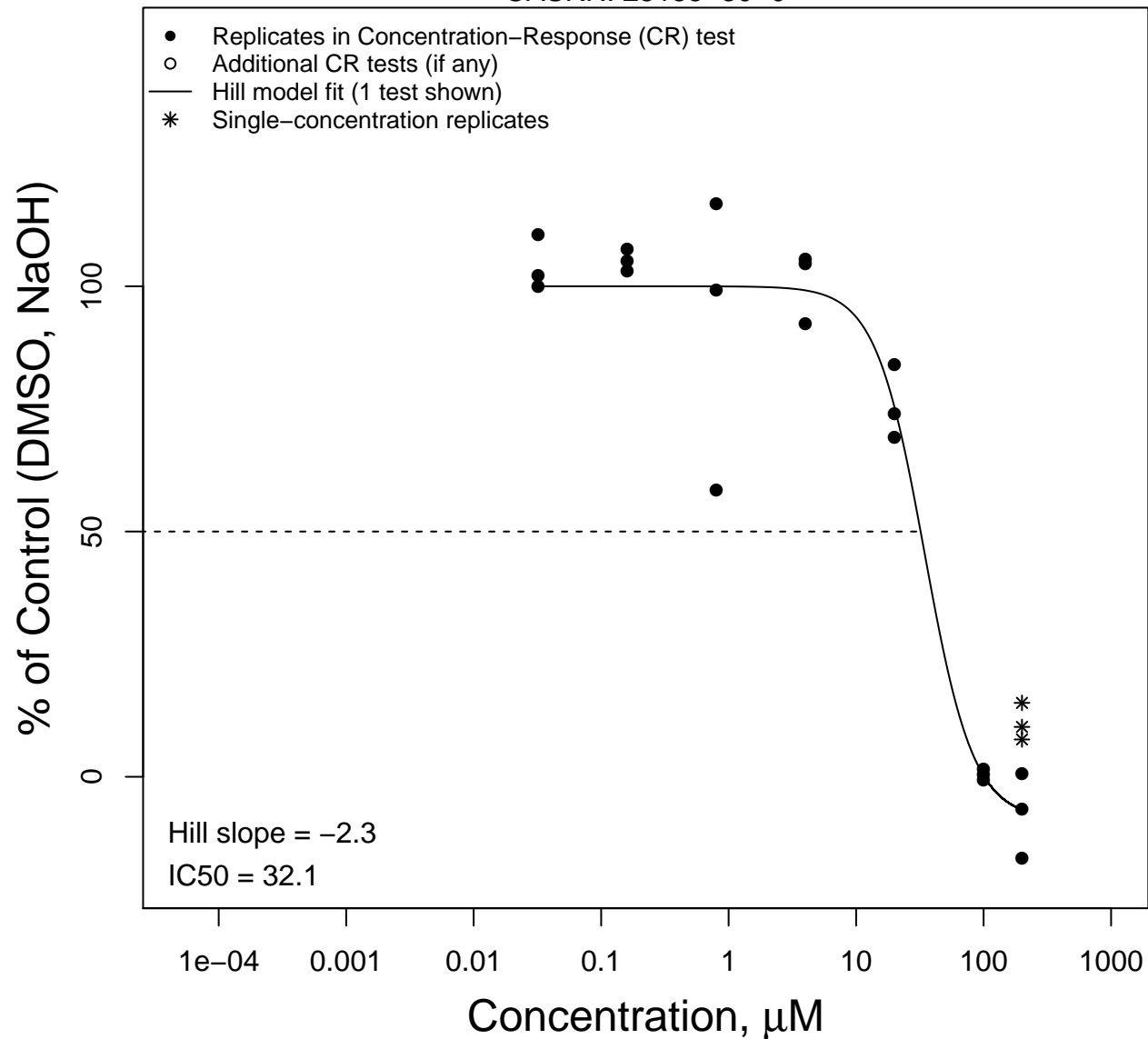
Acetochlor

CASRN: 34256-82-1



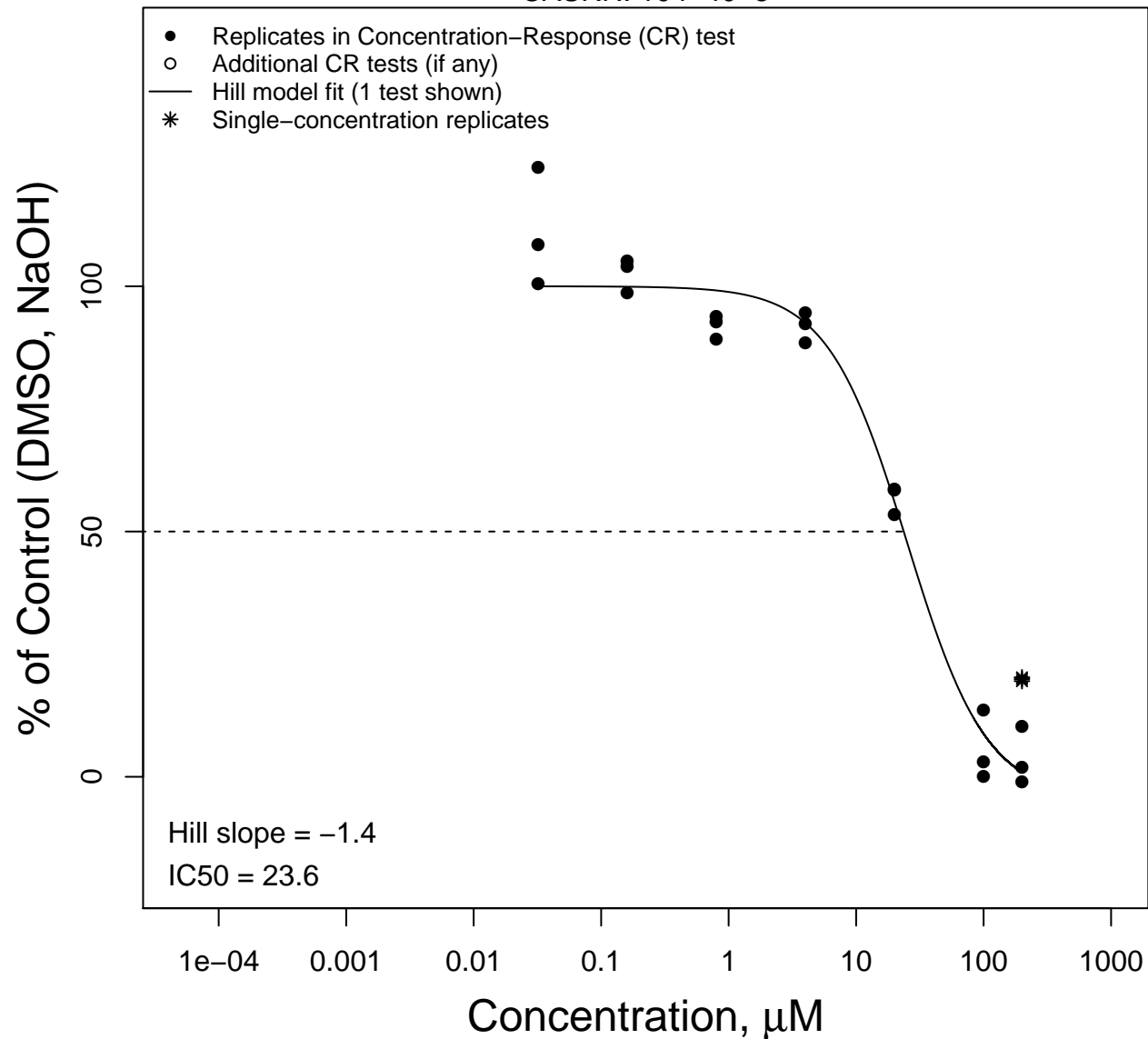
Sodium dodecylbenzenesulfonate

CASRN: 25155-30-0



4-Nonylphenol

CASRN: 104-40-5



Sodium hexyldecyl sulfate

CASRN: 1120-01-0

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100

50

0

Hill slope = -1.9

IC50 = 29.5

1e-04

0.001

0.01

0.1

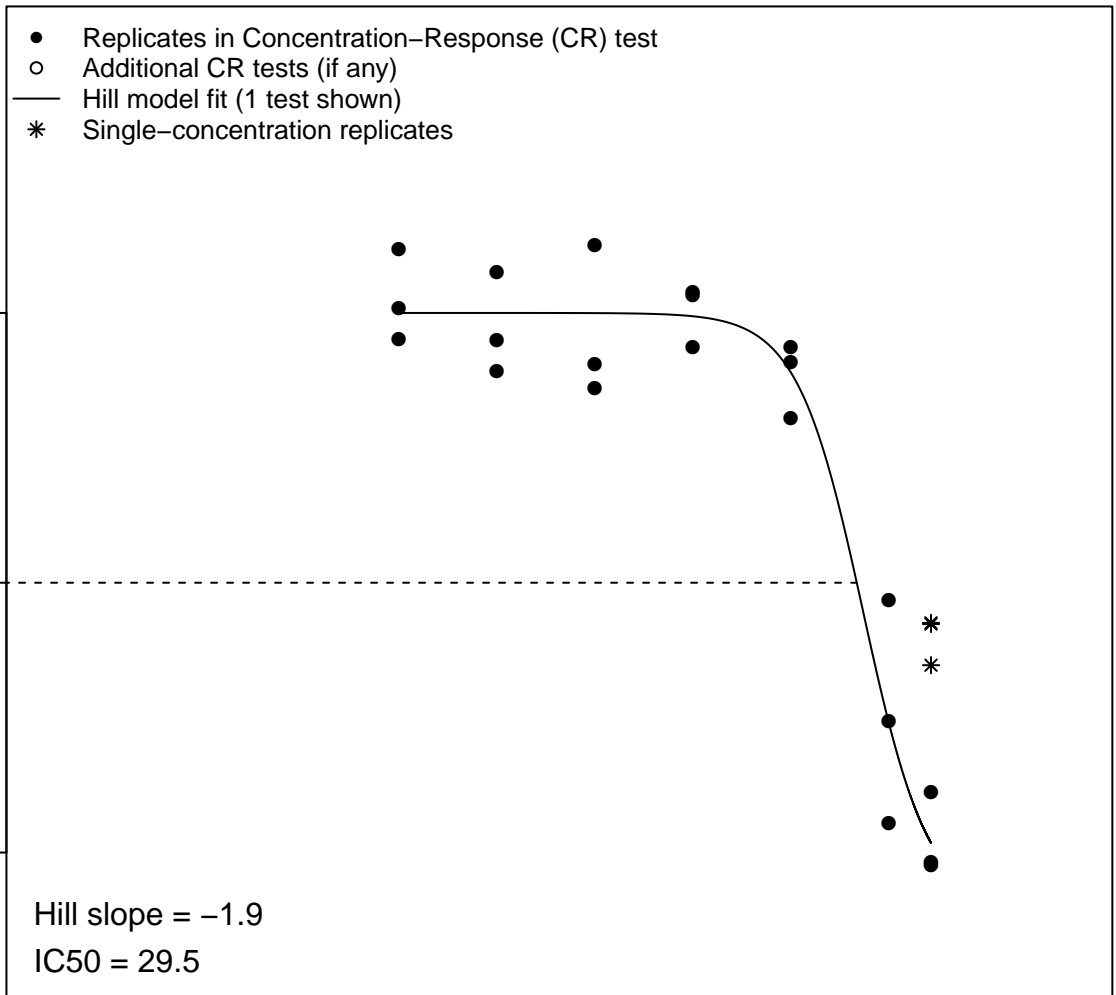
1

10

100

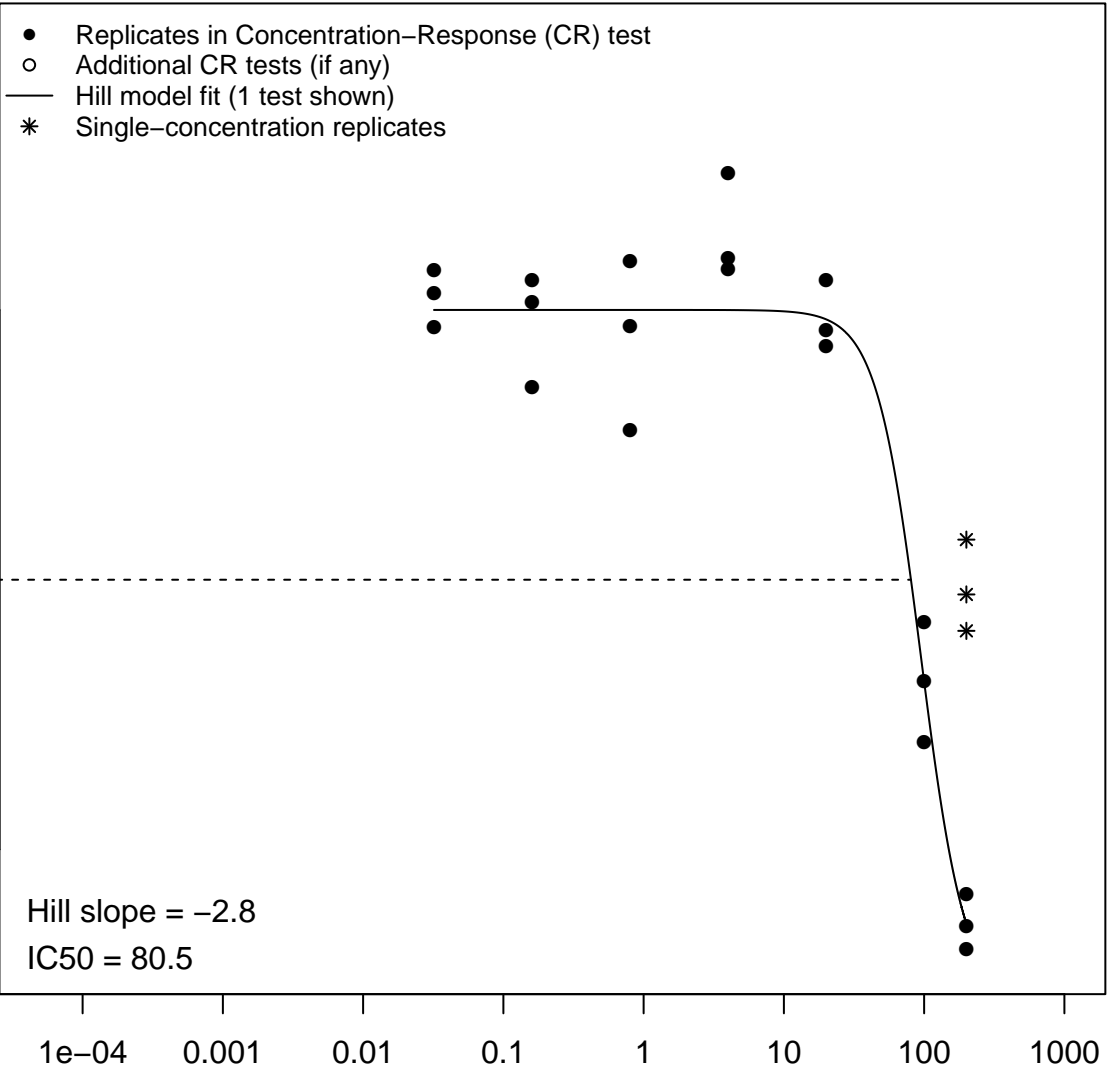
1000

Concentration, μM



Troglitazone

CASRN: 97322-87-7

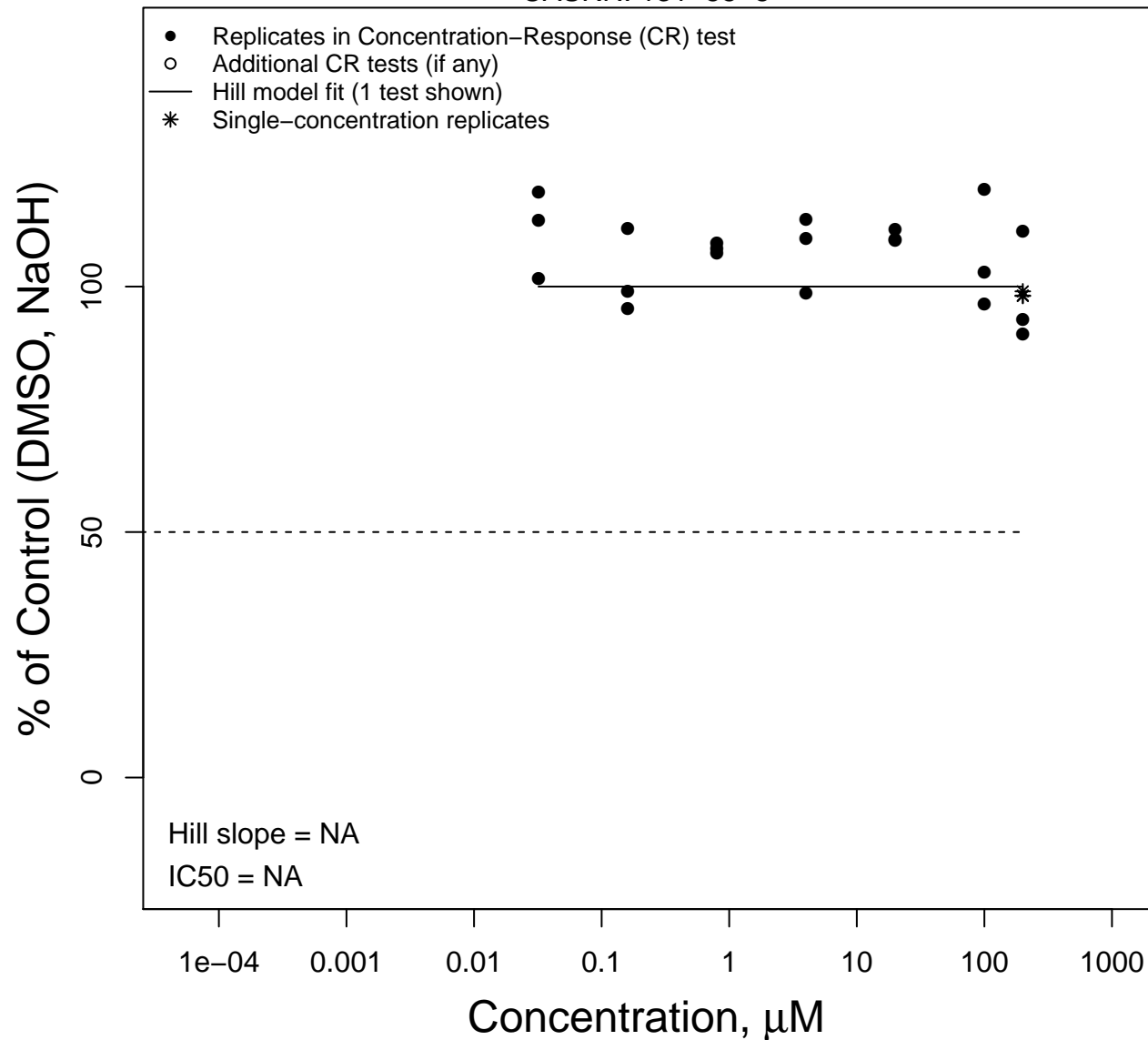


% of Control (DMSO, NaOH)

Concentration, µM

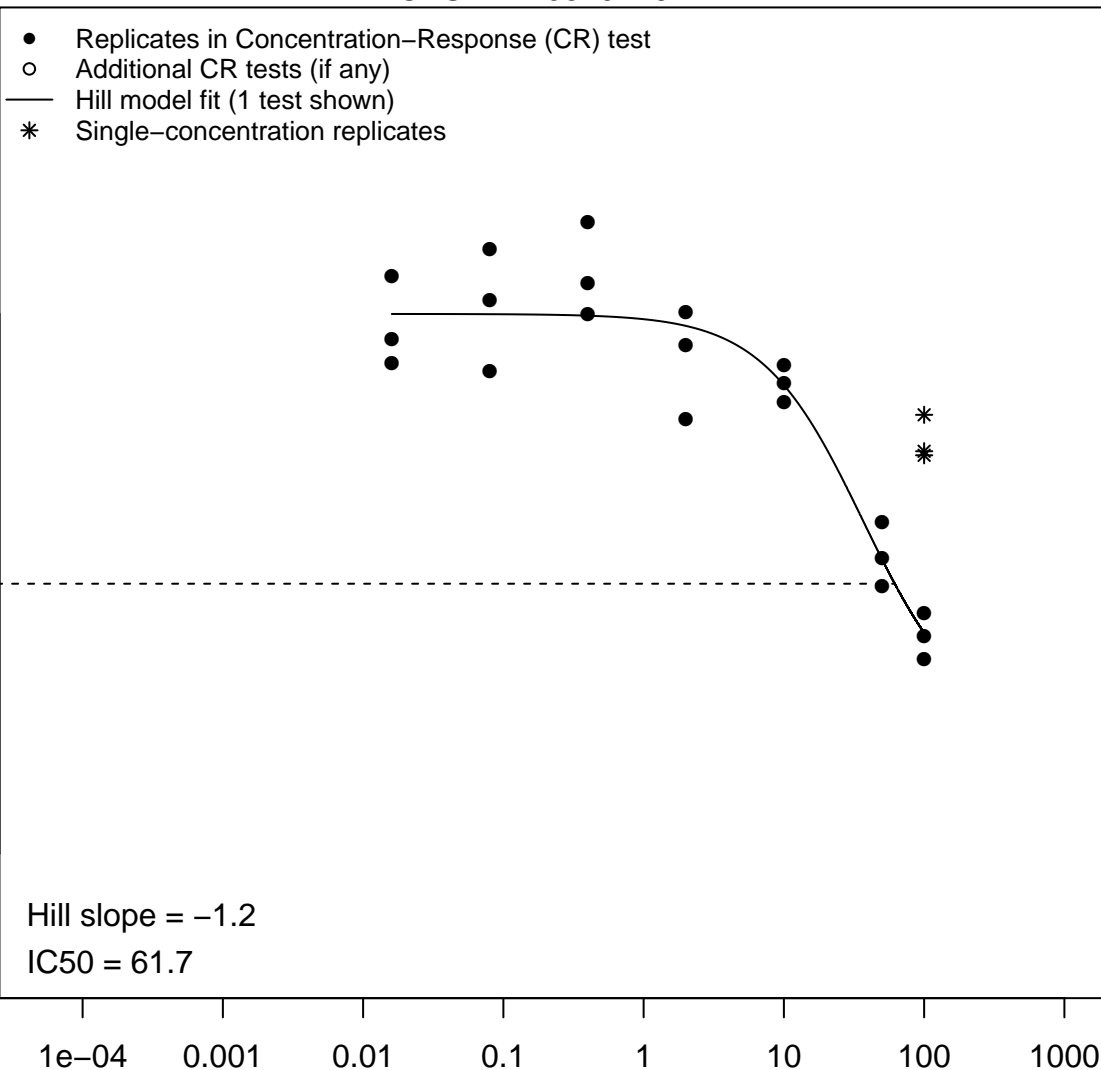
2,2',4,4'-Tetrahydroxybenzophenone

CASRN: 131-55-5



Tamoxifen

CASRN: 10540-29-1

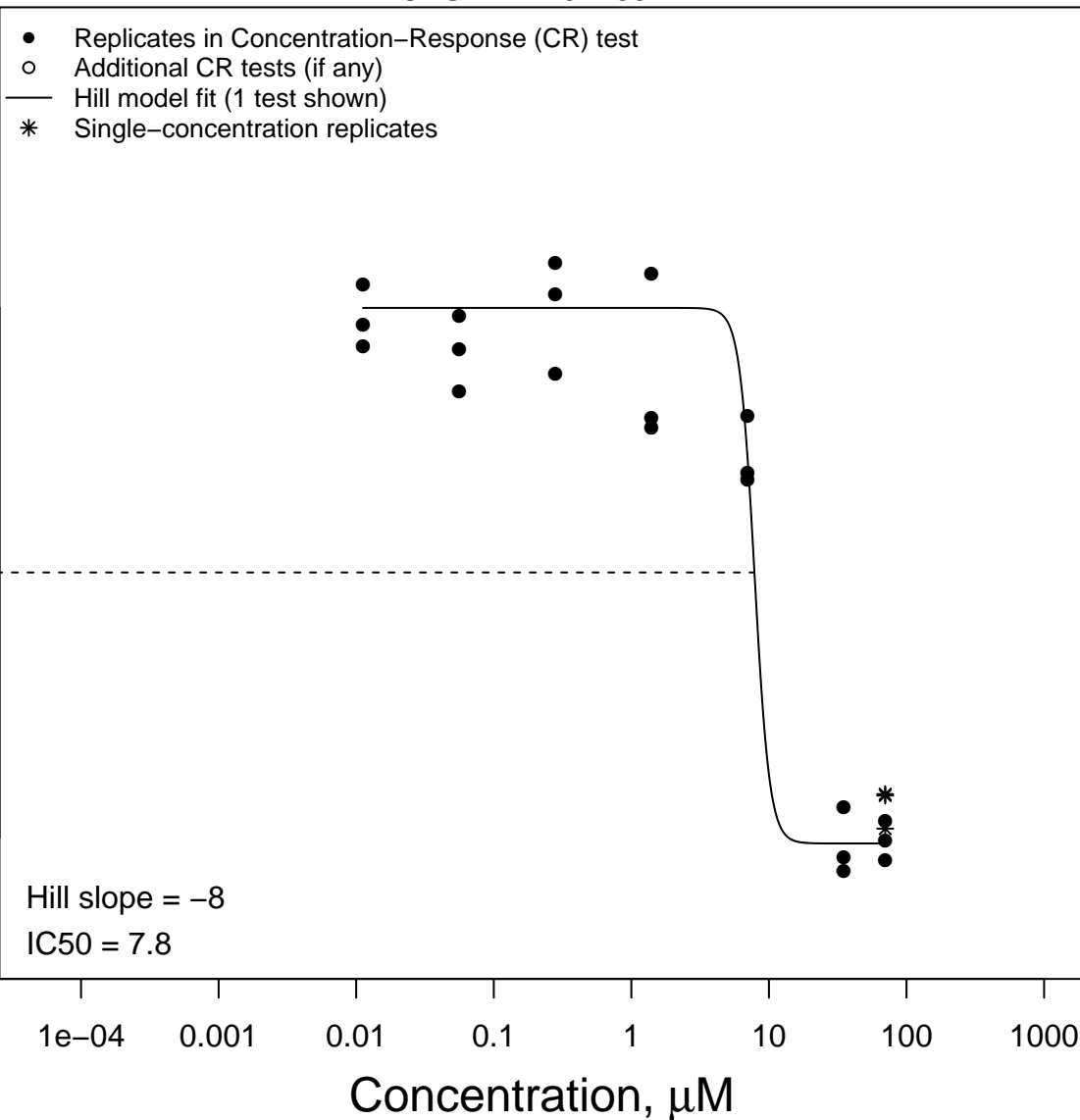


Concentration, μM

% of Control (DMSO, NaOH)

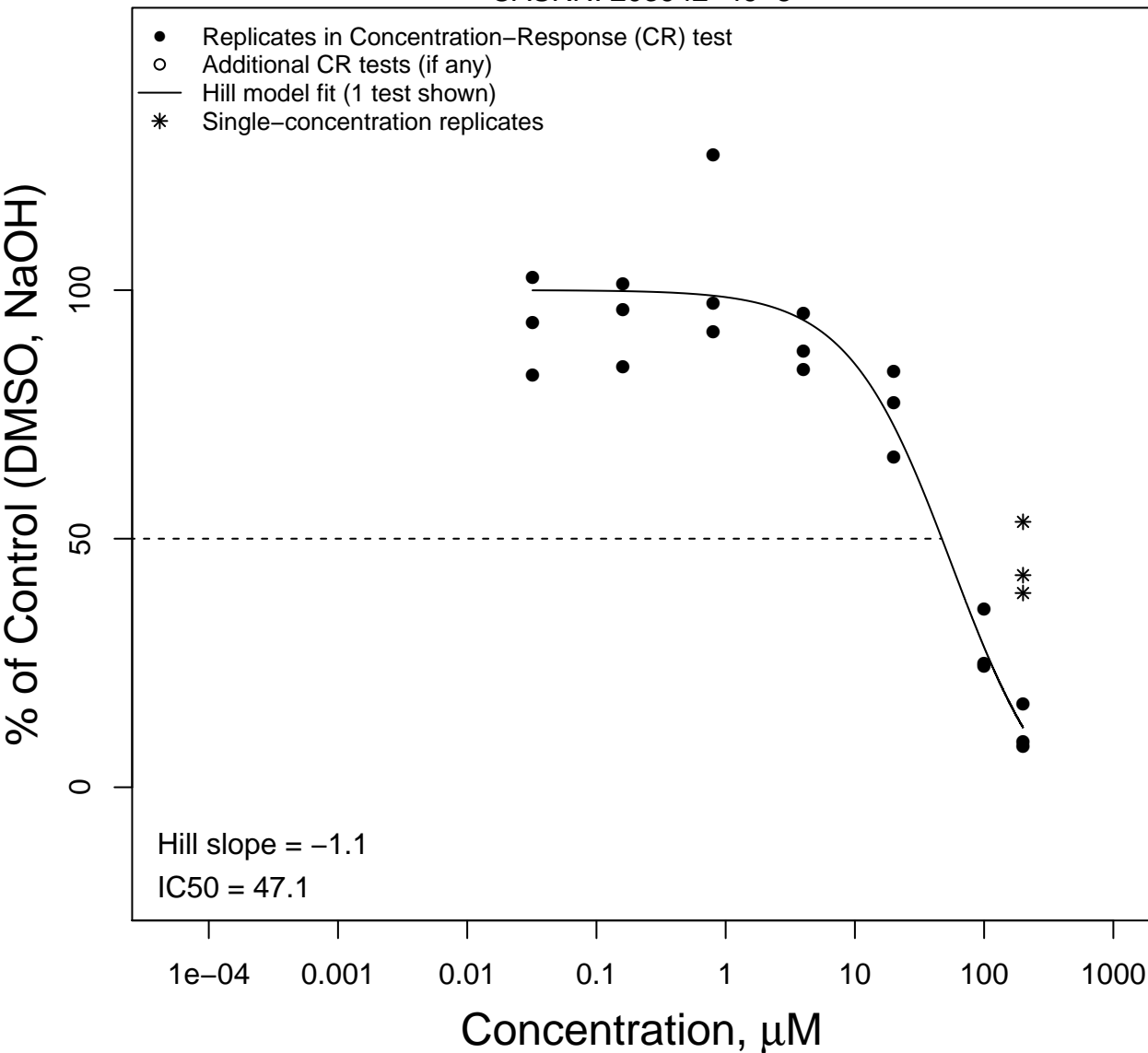
Tannic acid

CASRN: 1401-55-4



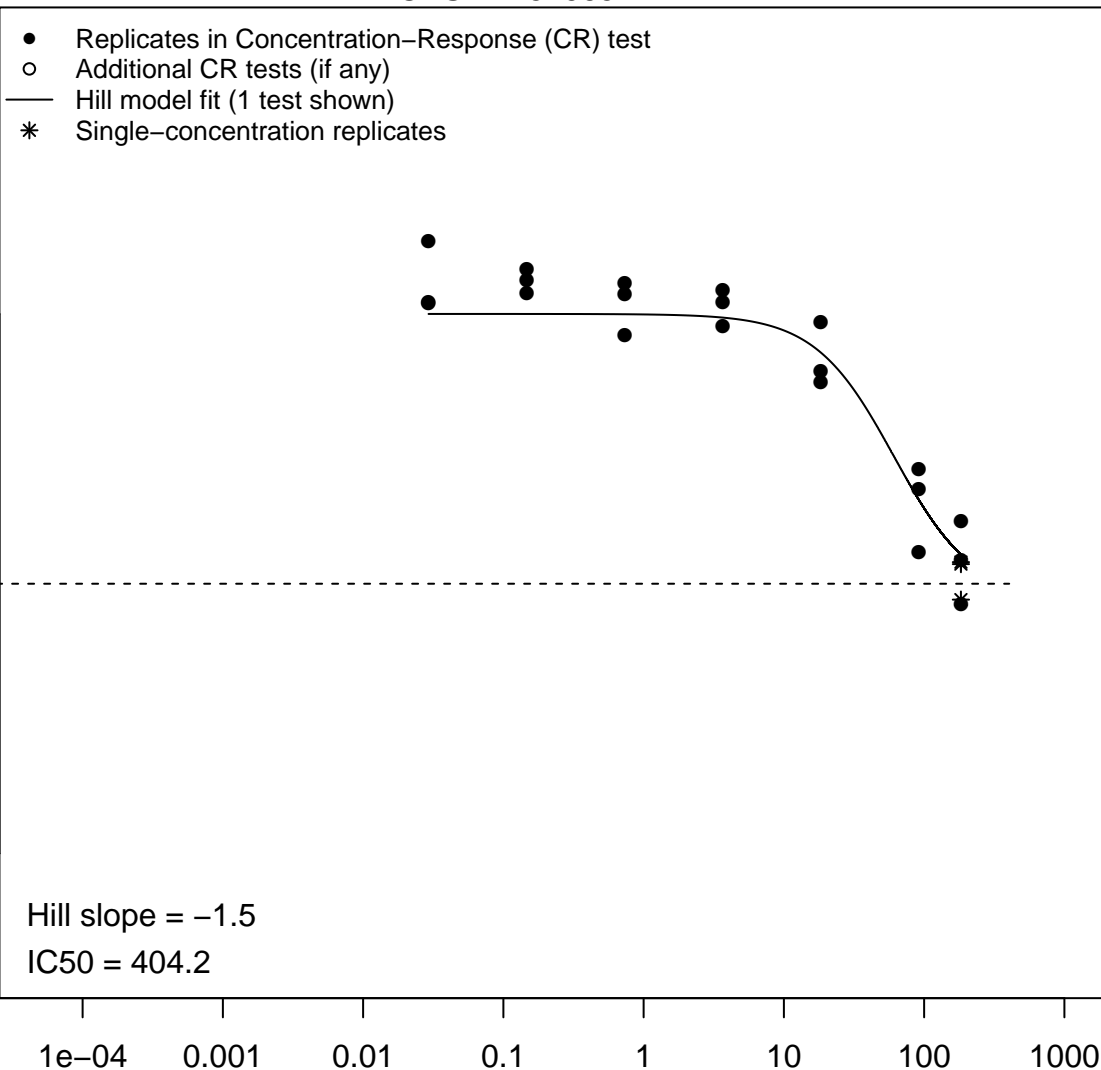
UK-337312

CASRN: 203942-49-8



Tamoxifen citrate

CASRN: 54965-24-1

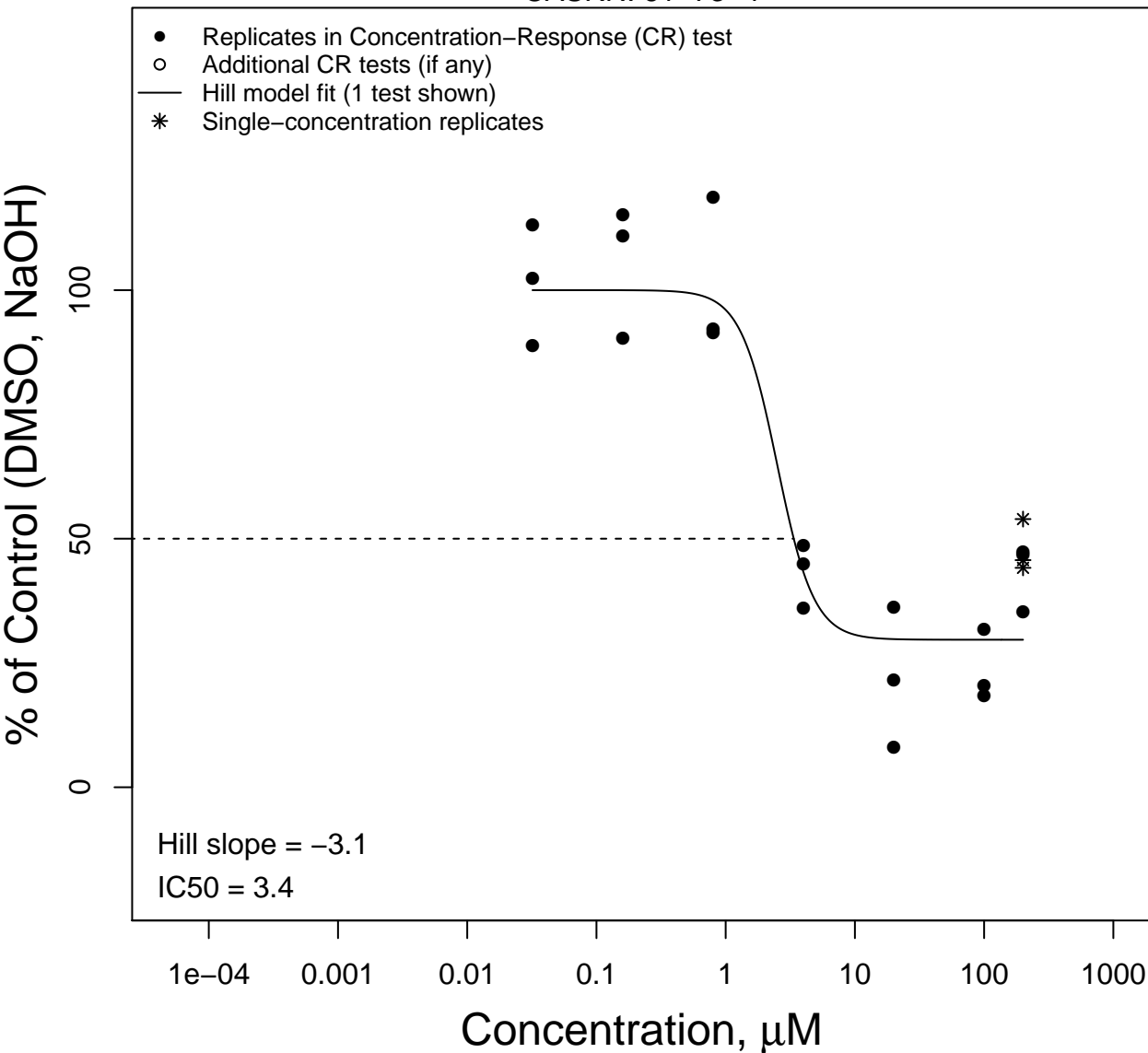


Concentration, µM

% of Control (DMSO, NaOH)

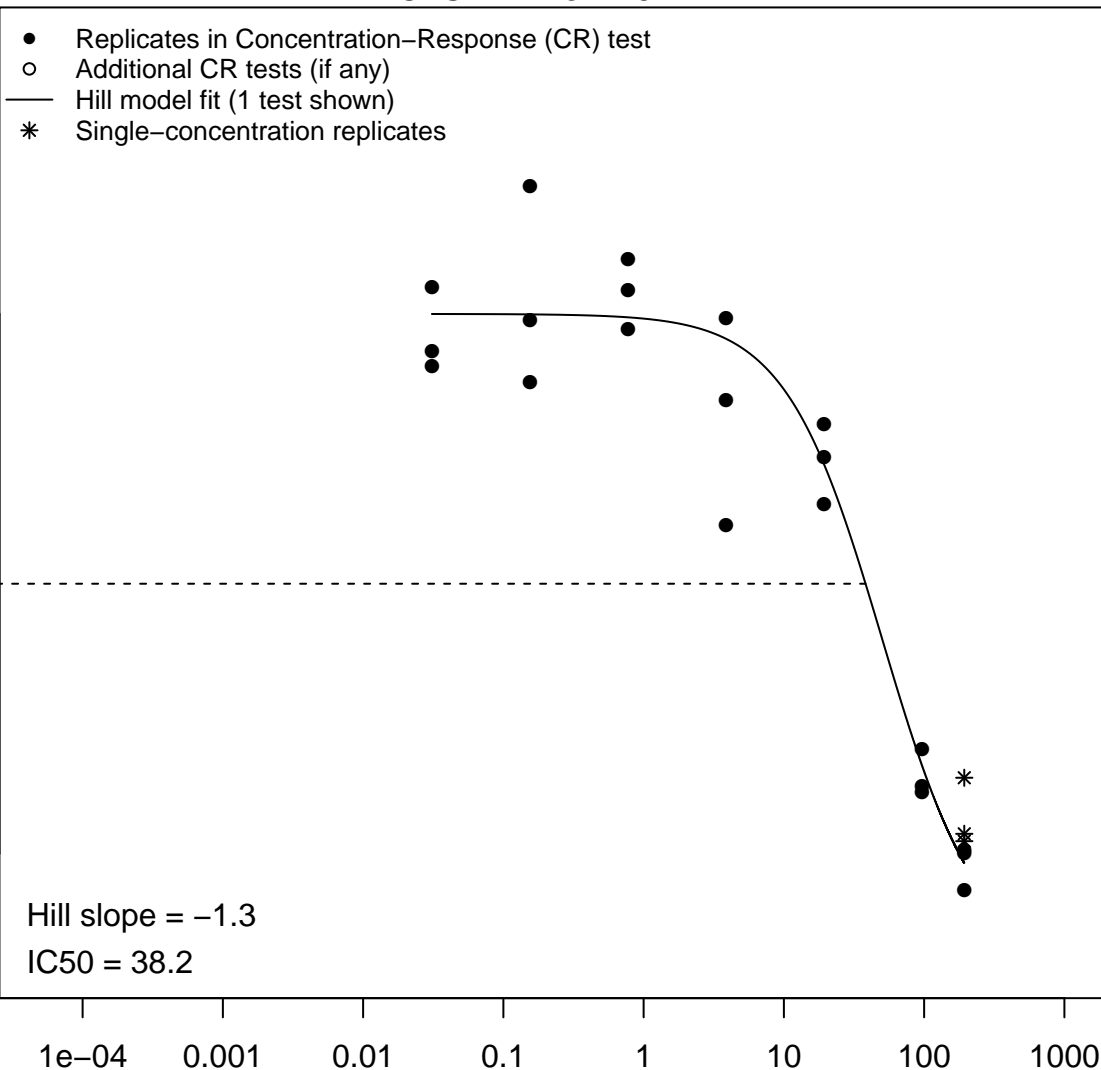
Methylene blue

CASRN: 61-73-4



Eosin

CASRN: 17372-87-1

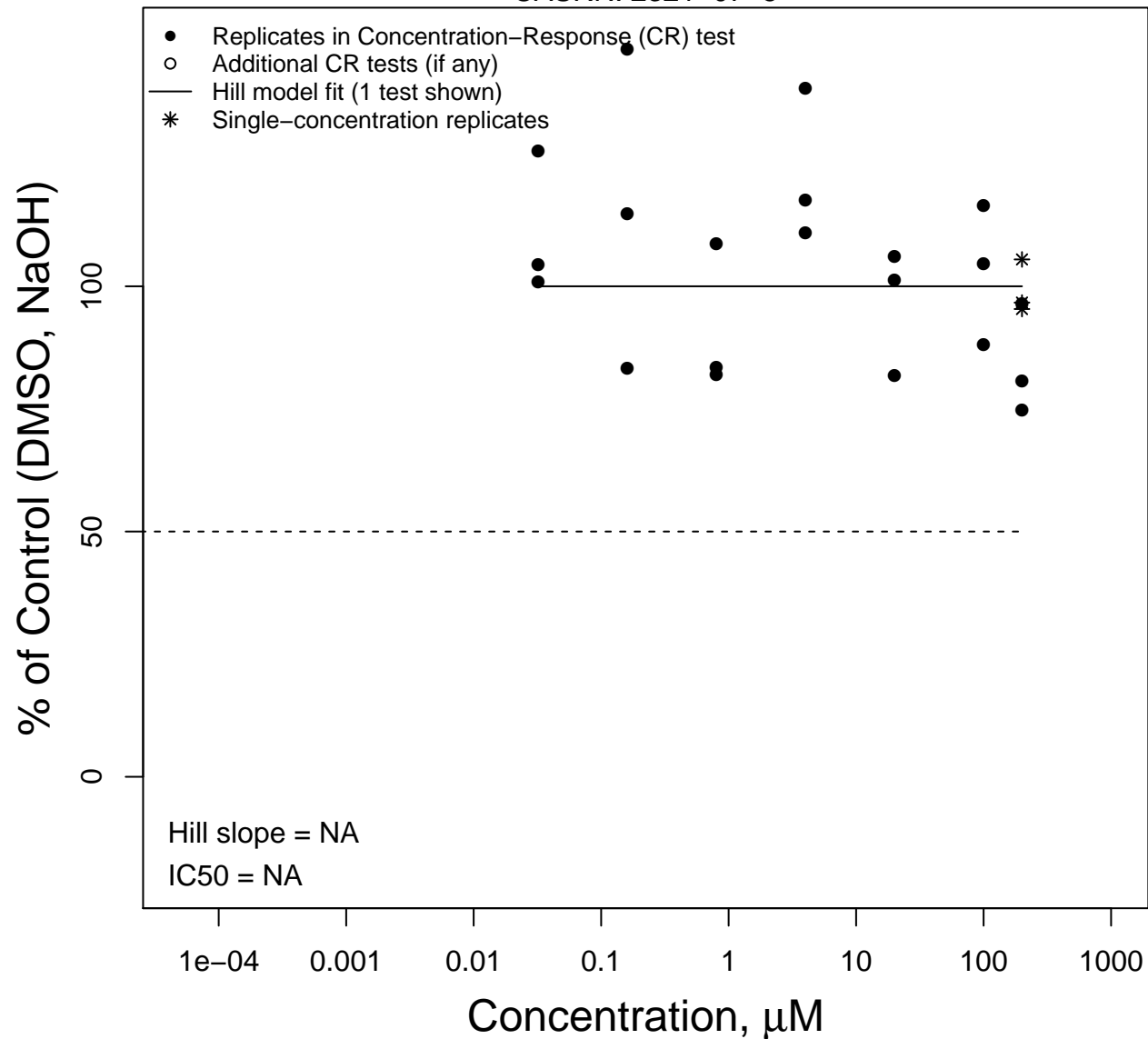


Concentration, µM

% of Control (DMSO, NaOH)

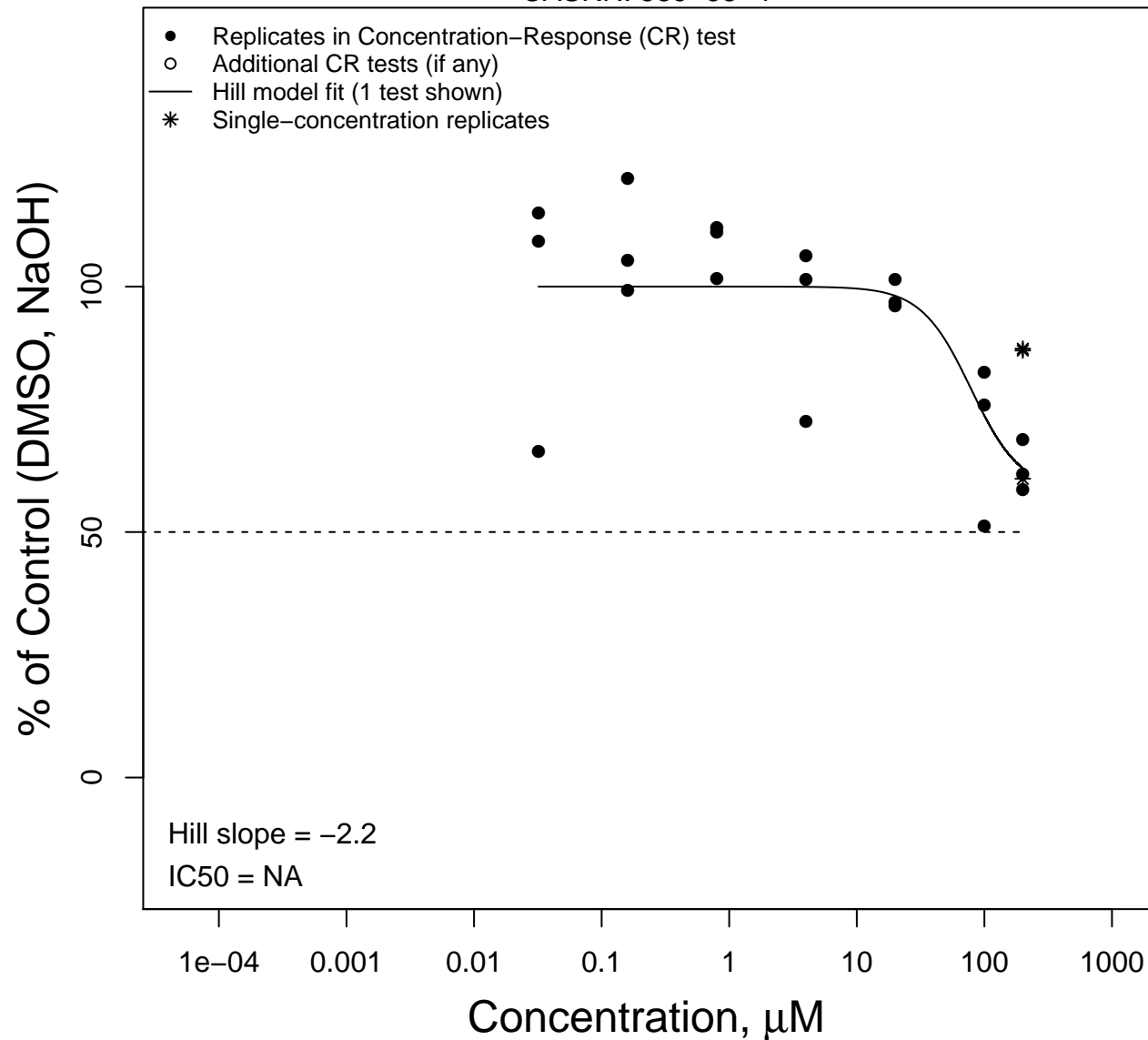
Fluorescein

CASRN: 2321-07-5



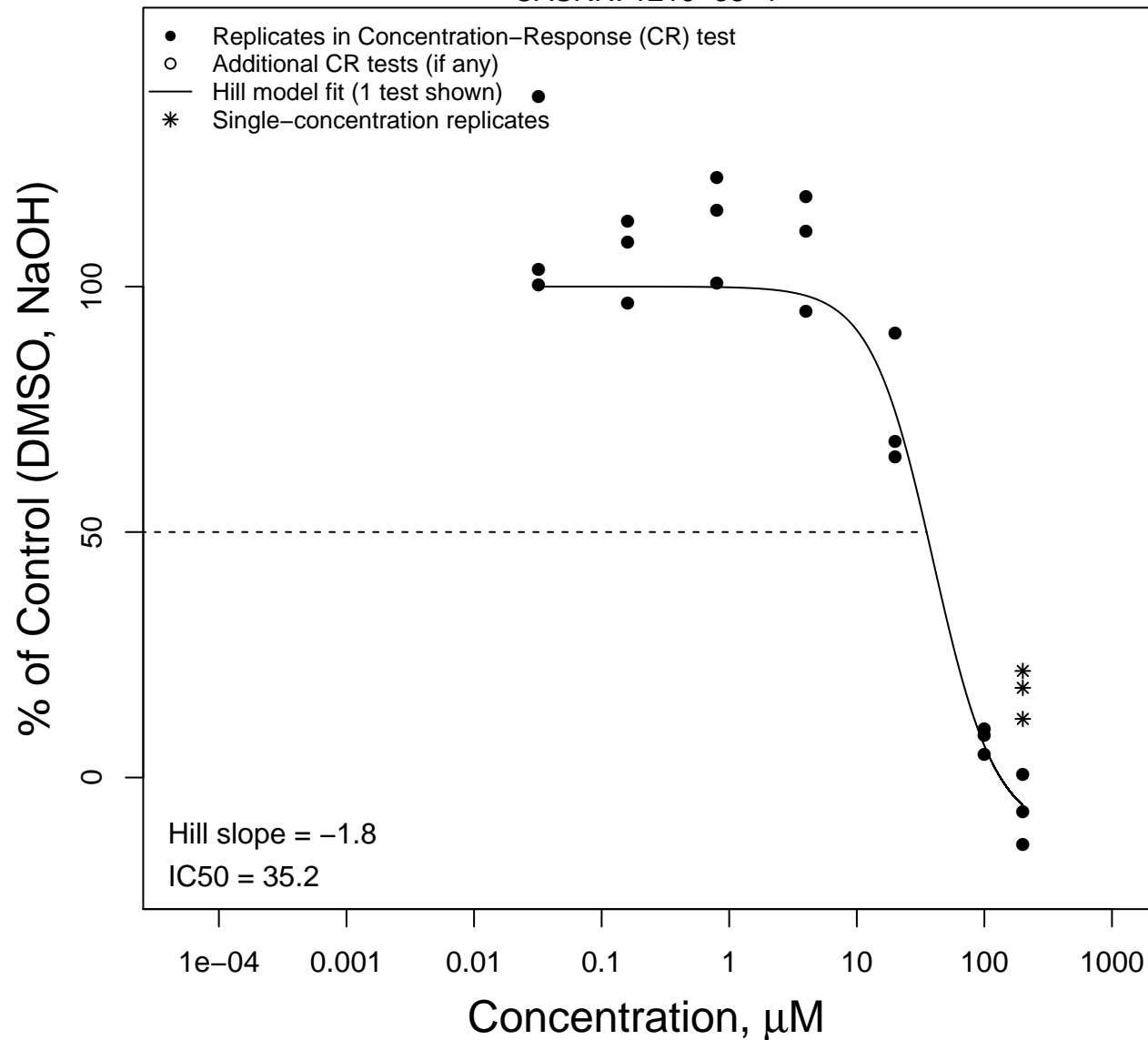
Tetradecanoic acid, 2,3-dihydroxypropyl ester

CASRN: 589-68-4



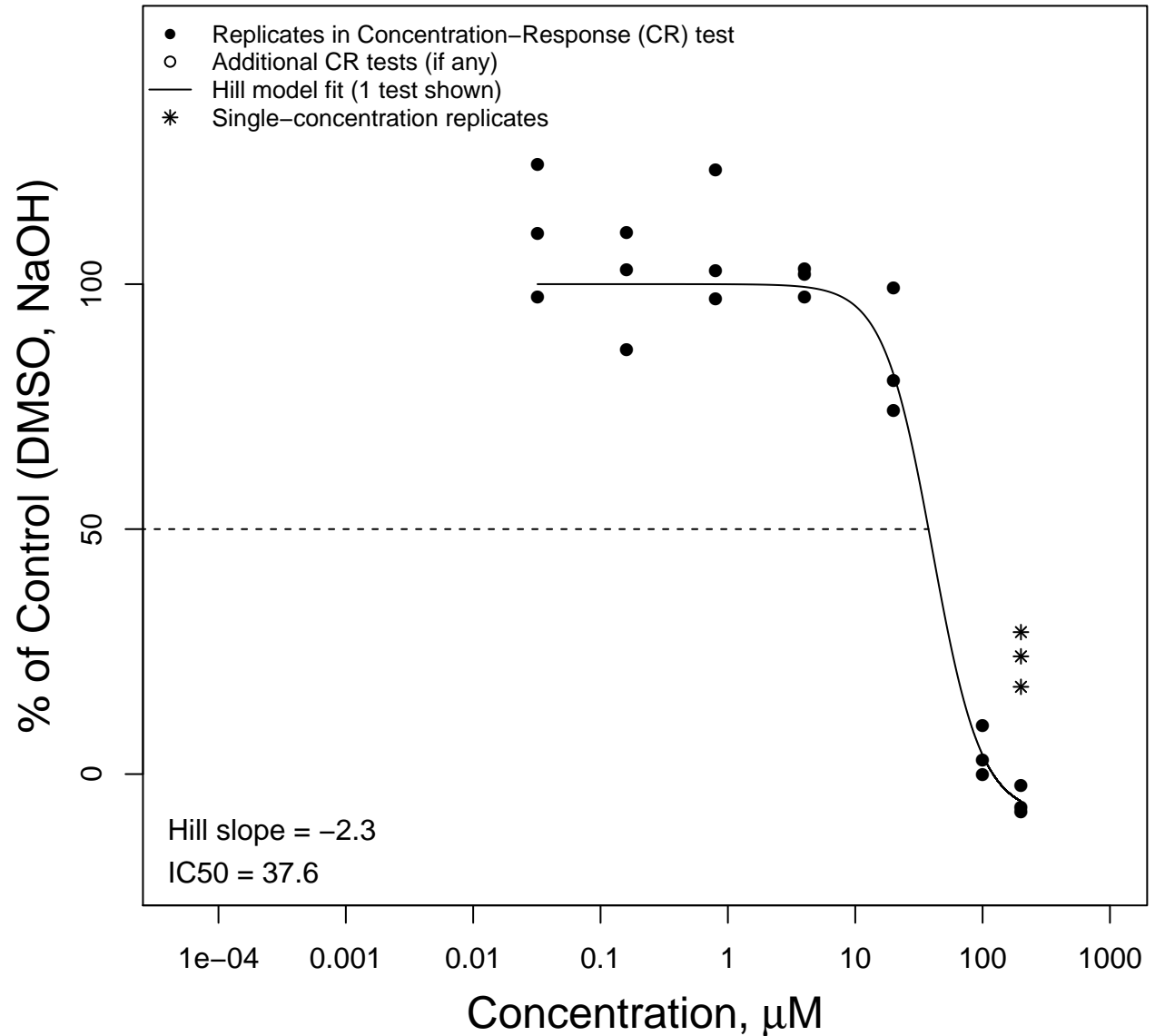
Octylparaben

CASRN: 1219-38-1



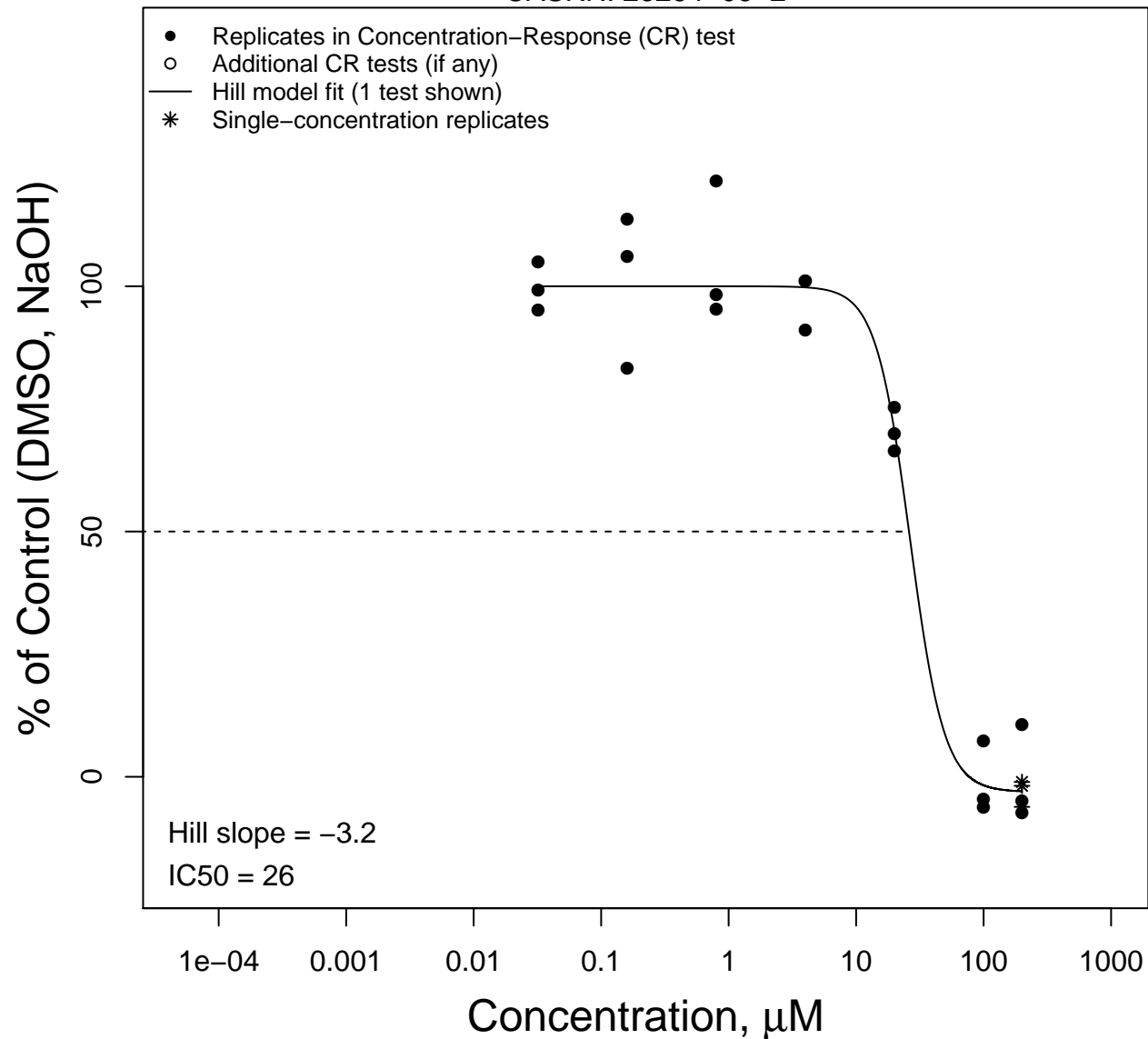
Monotridecyl phosphate

CASRN: 5116-94-9



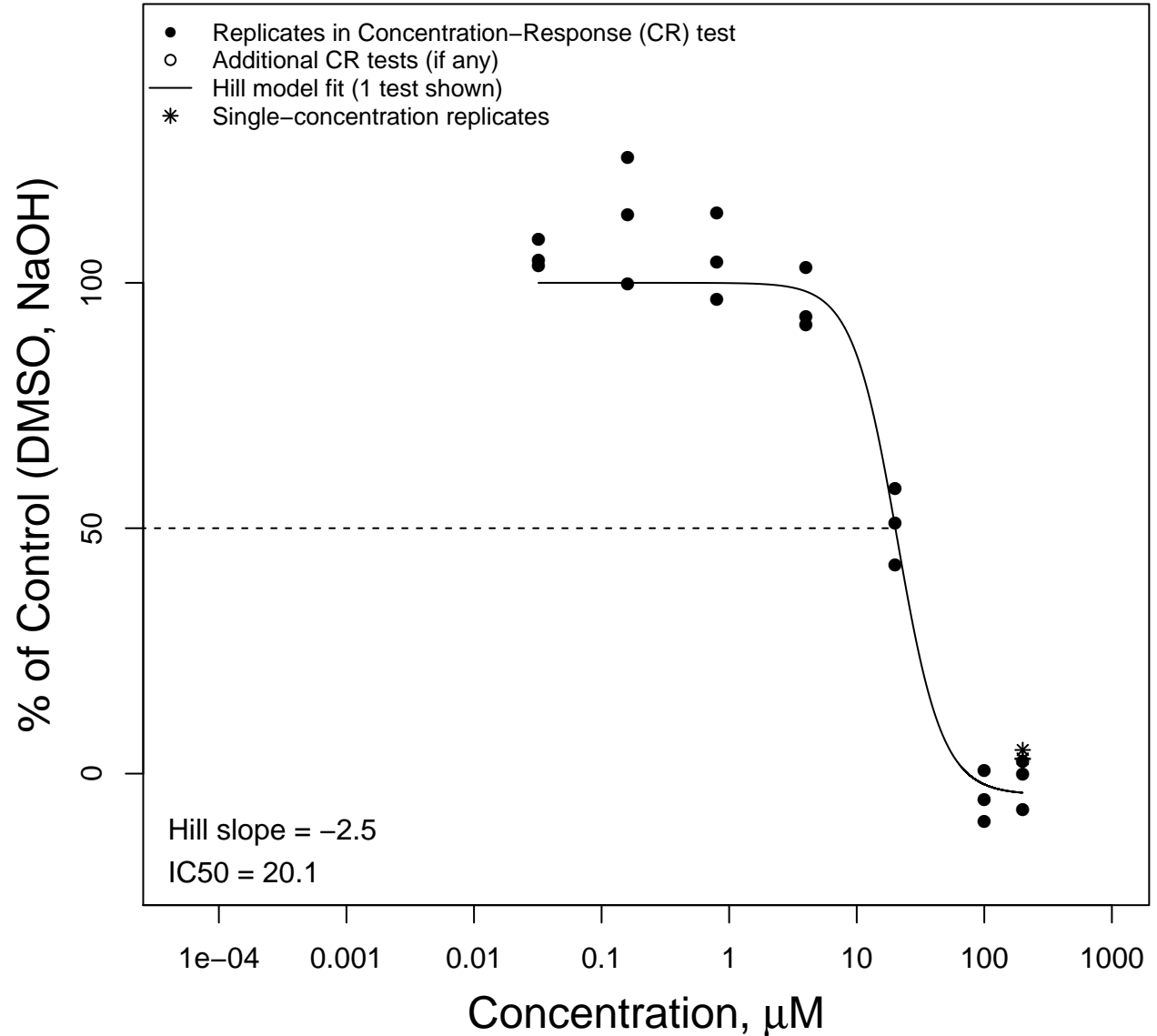
Calcium dodecylbenzene sulfonate

CASRN: 26264-06-2



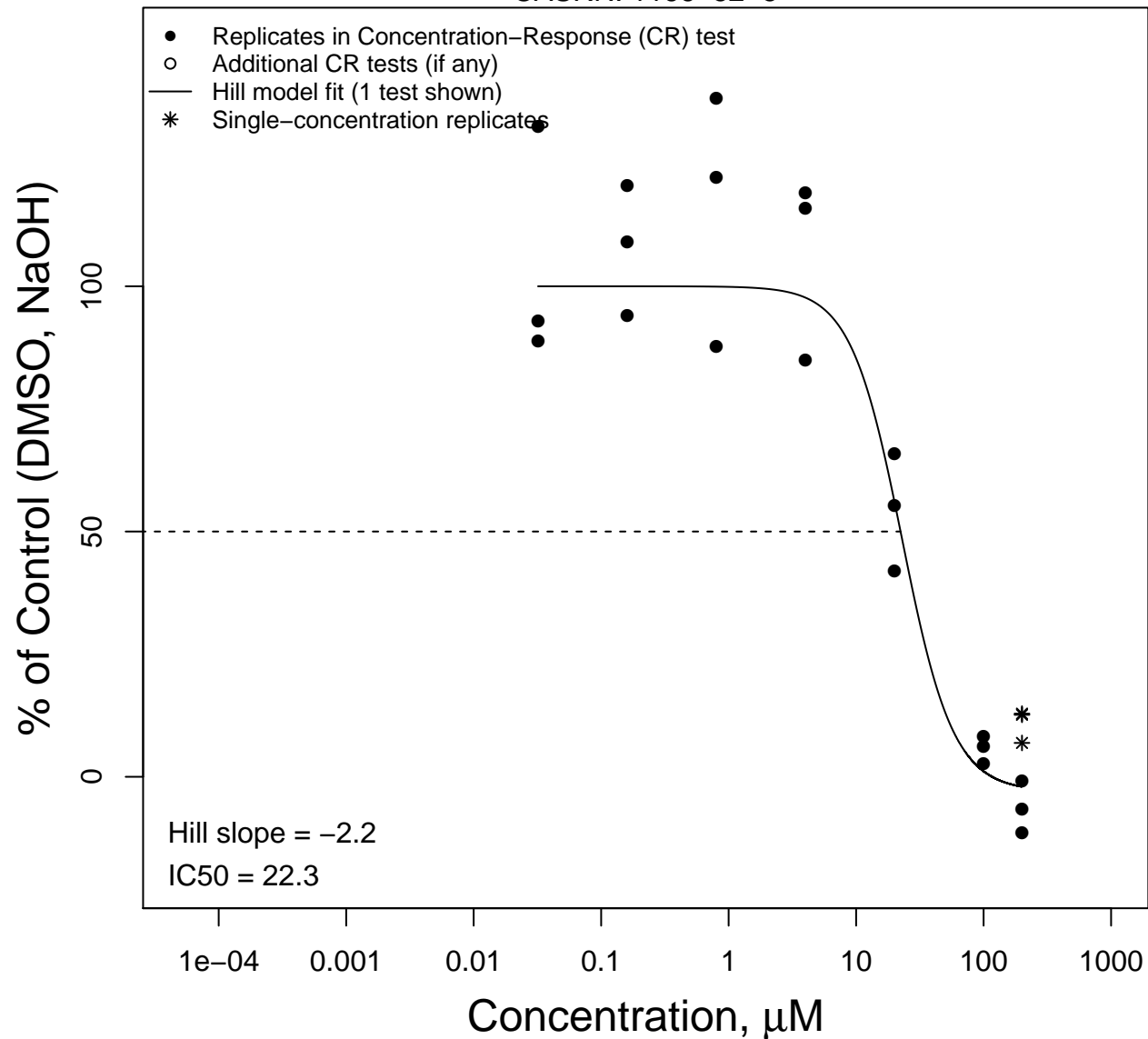
Dodecylphenol

CASRN: 27193-86-8



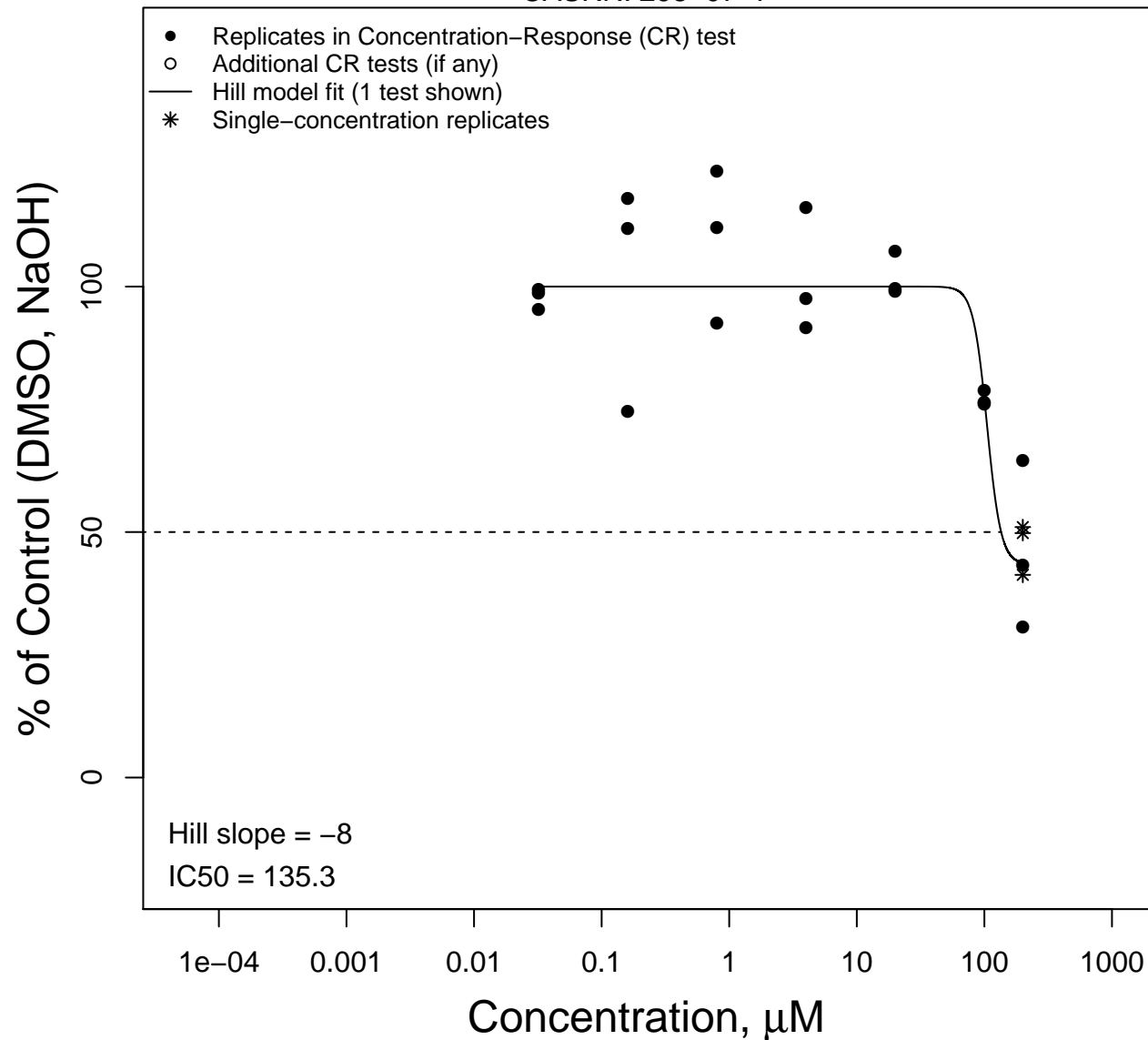
Lauryl gallate

CASRN: 1166-52-5



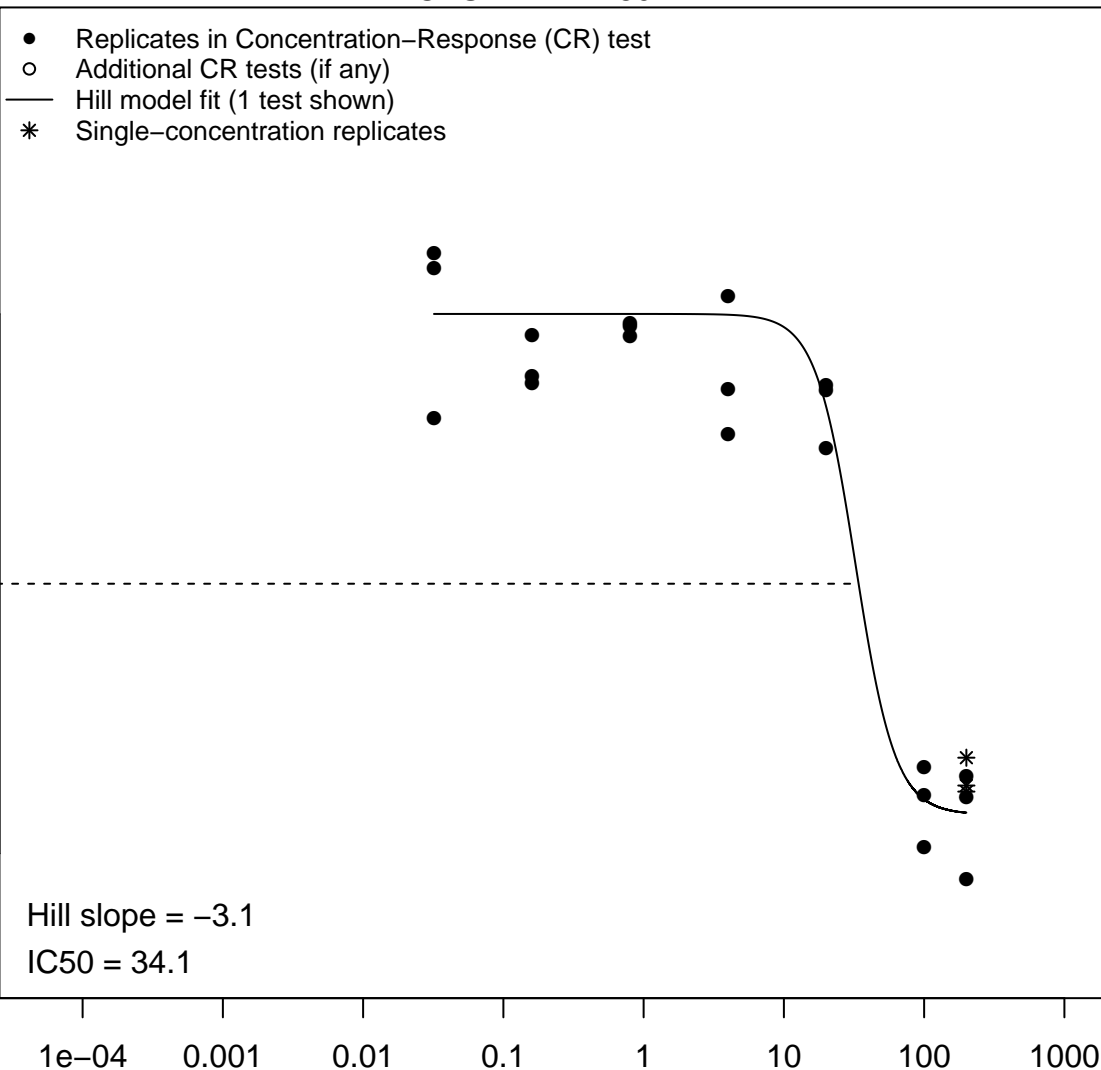
Bis(2-ethylhexyl) phosphate

CASRN: 298-07-7



Oleic acid

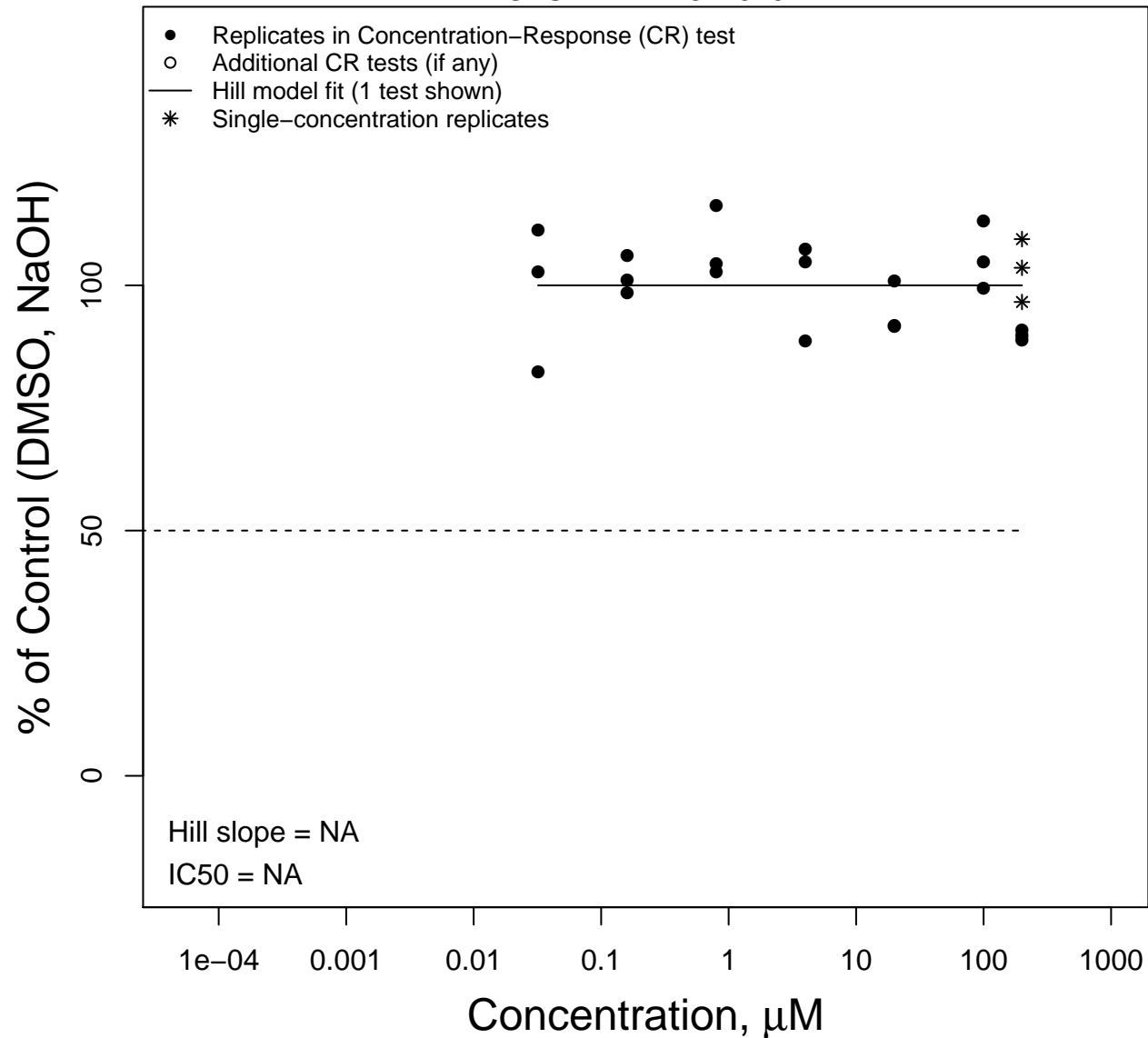
CASRN: 112-80-1



Concentration, µM

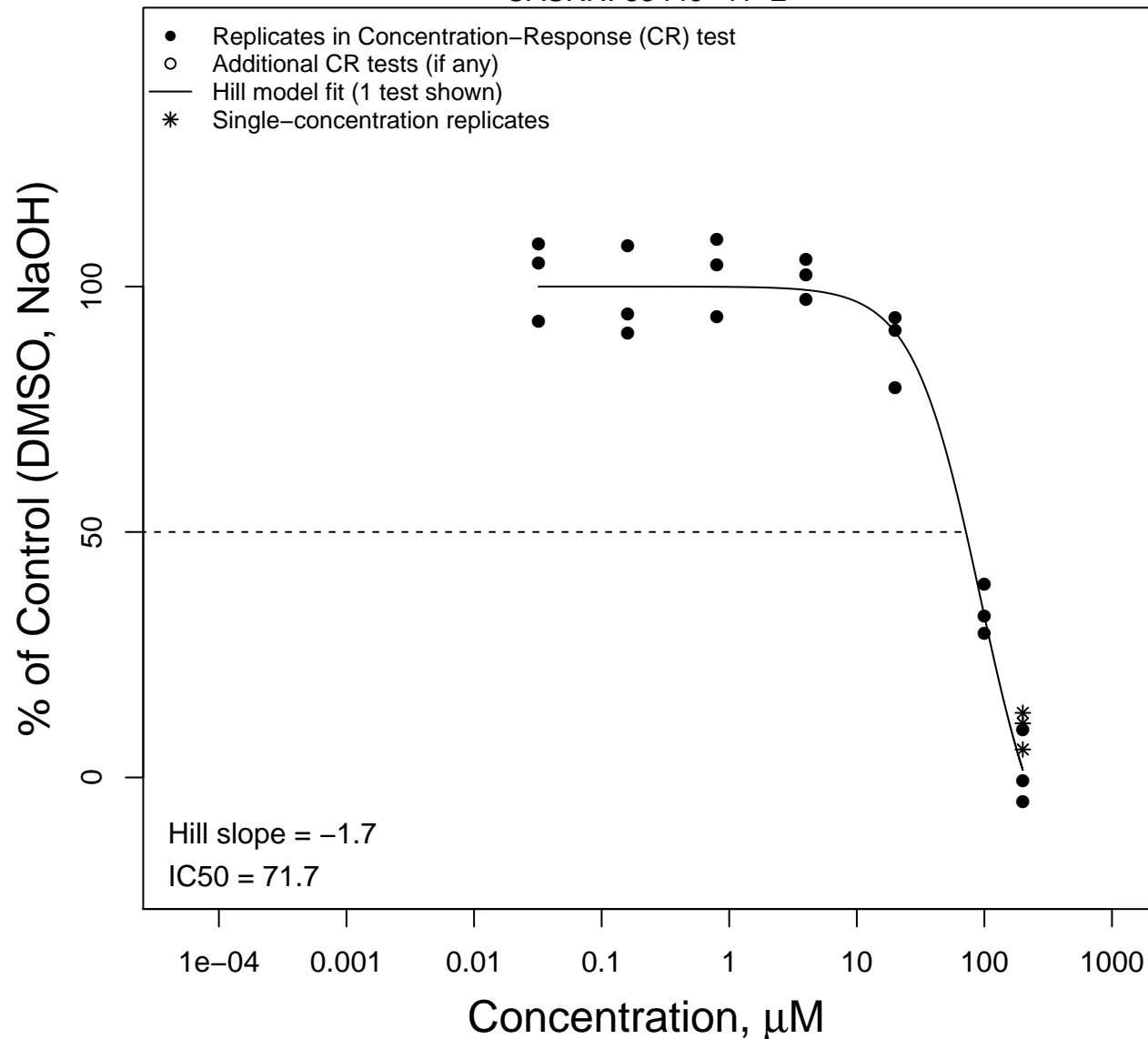
Z-Tetrachlorvinphos

CASRN: 22248-79-9



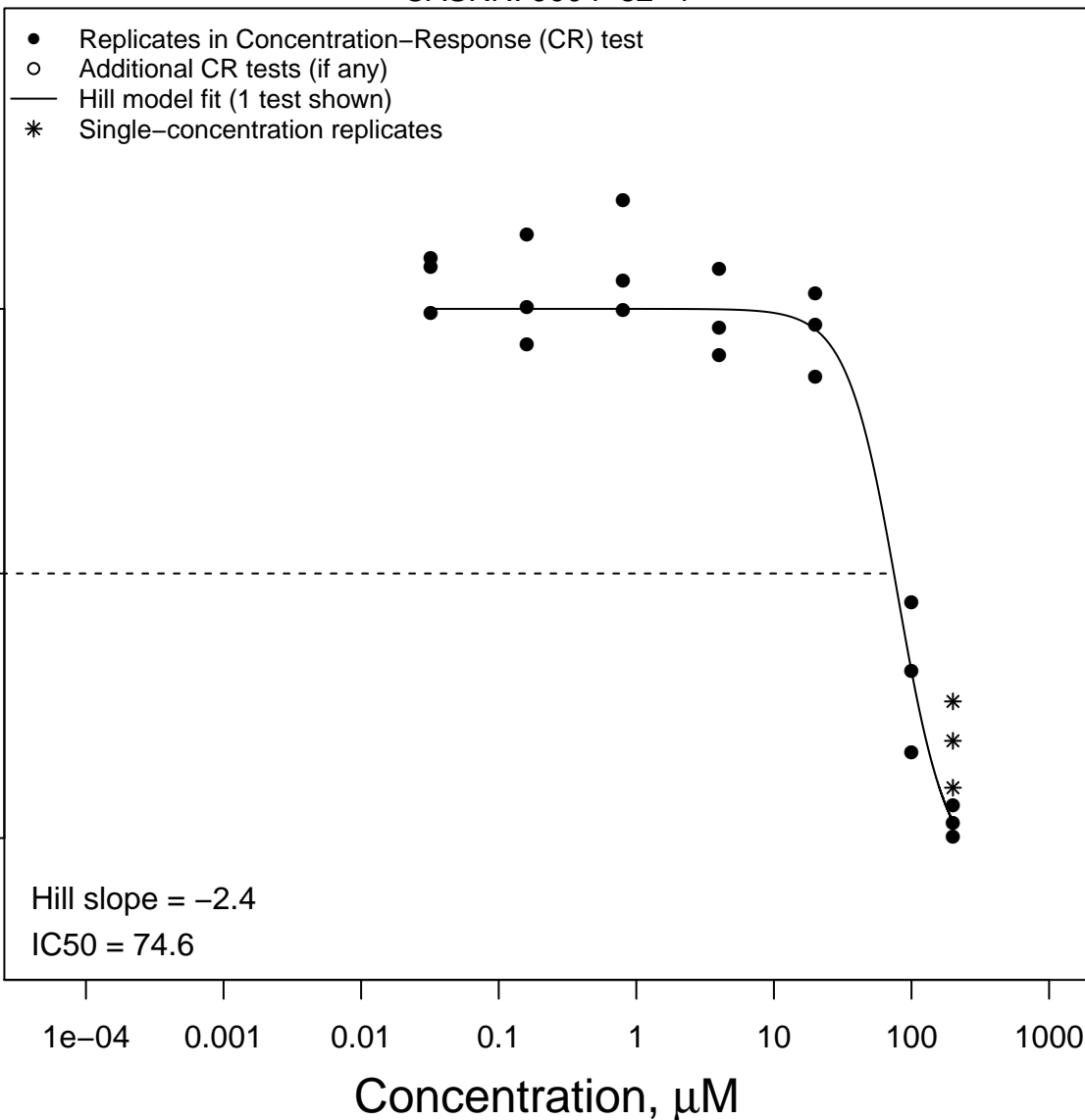
Benzyl-C8-18-alkyldimethylammonium chlorides

CASRN: 63449-41-2



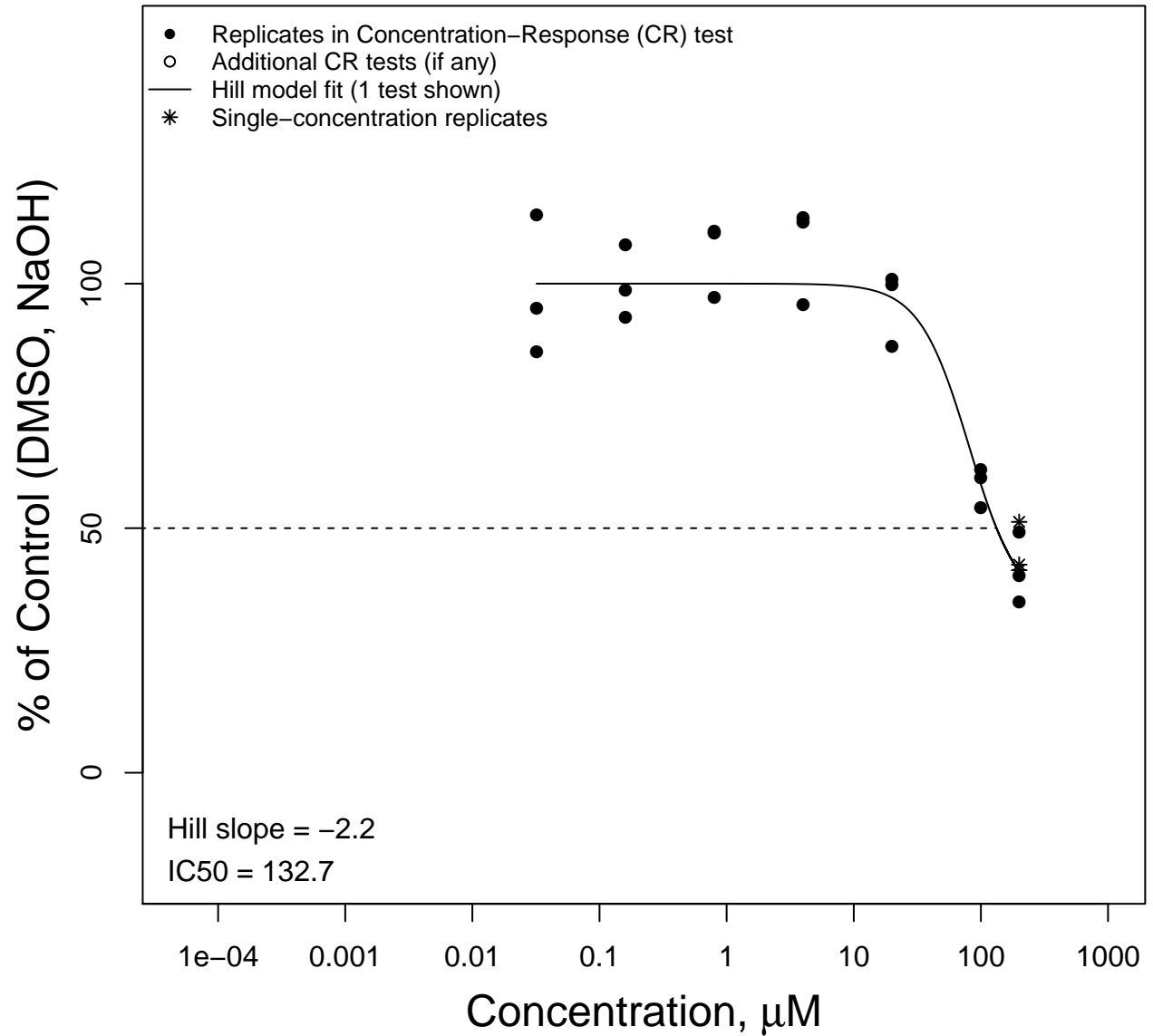
Sodium lauryl polyoxyethylene ether sulfate

CASRN: 9004-82-4



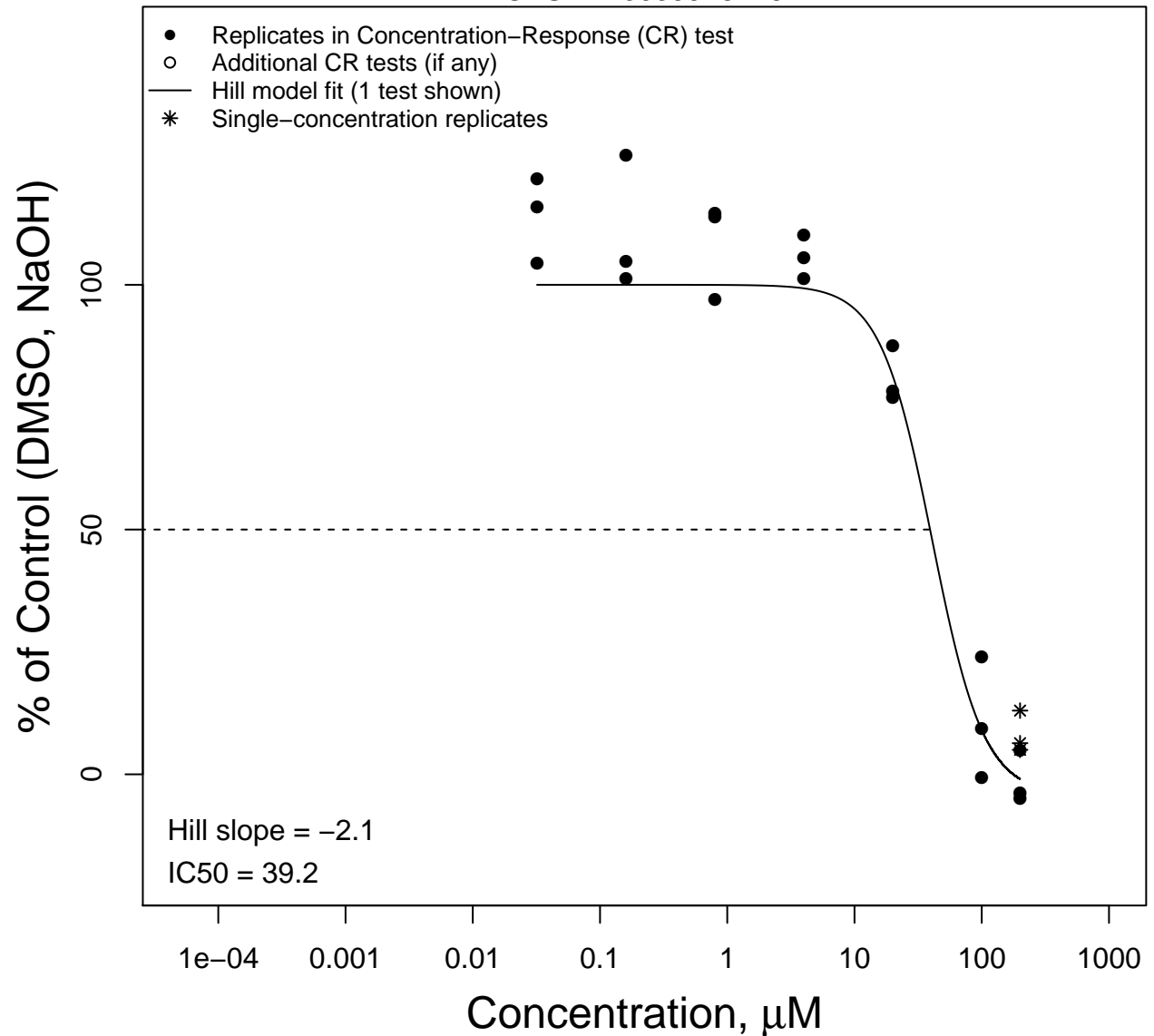
Hexadecanoic acid

CASRN: 57-10-3



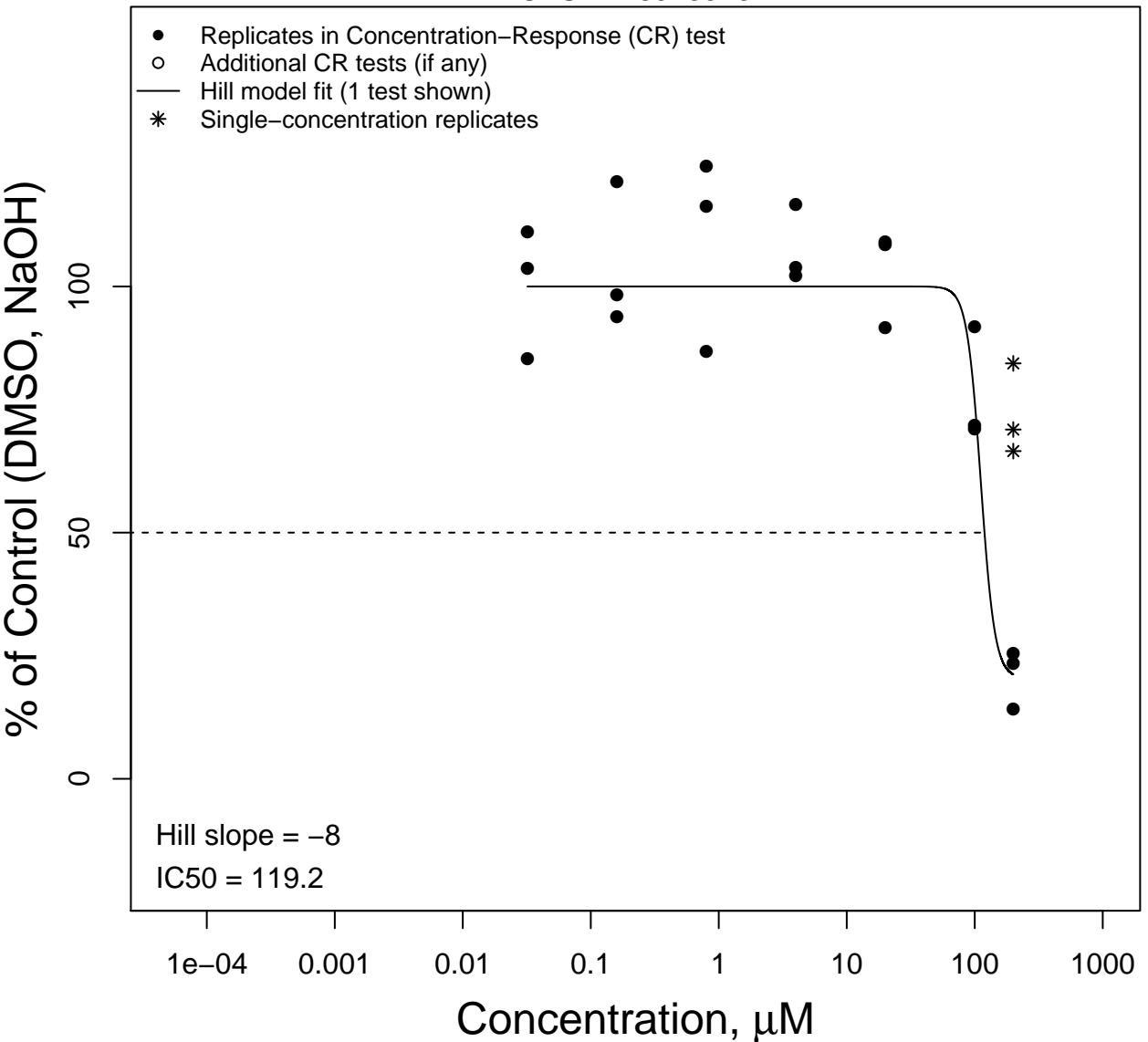
Isooctadecanoic acid

CASRN: 30399-84-9



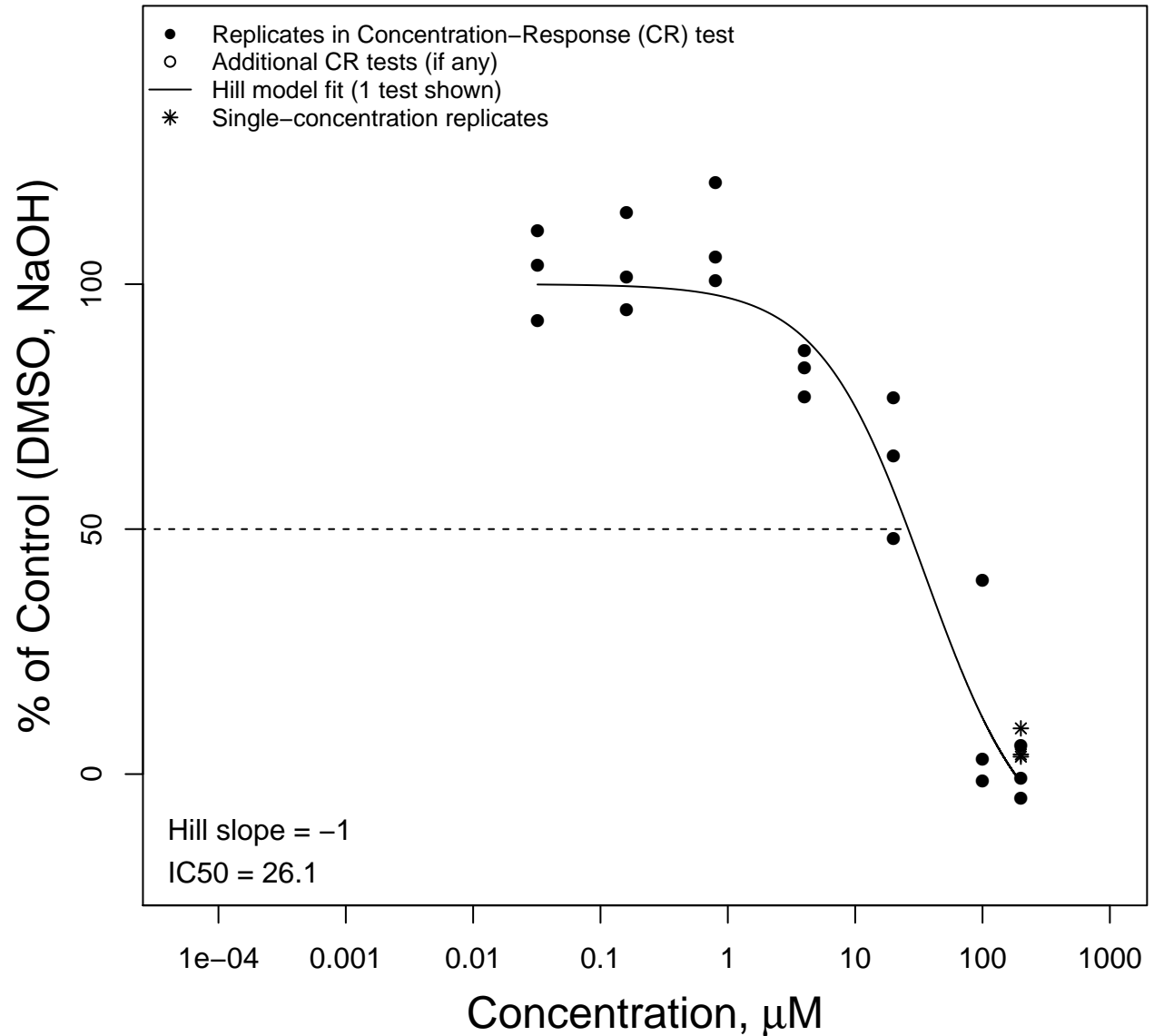
Linoleic acid

CASRN: 60-33-3



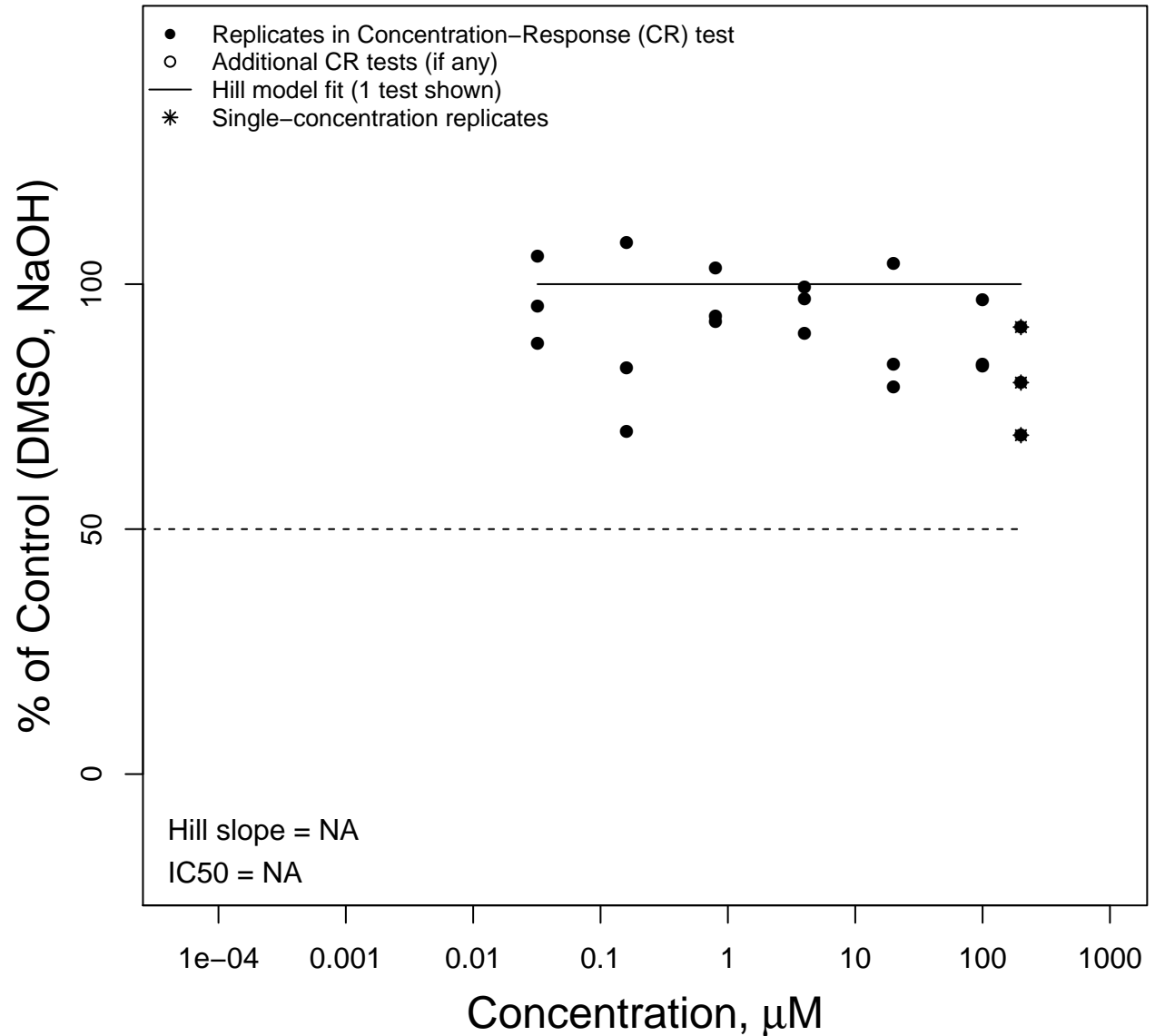
Methyltrioctylammonium chloride

CASRN: 5137-55-3



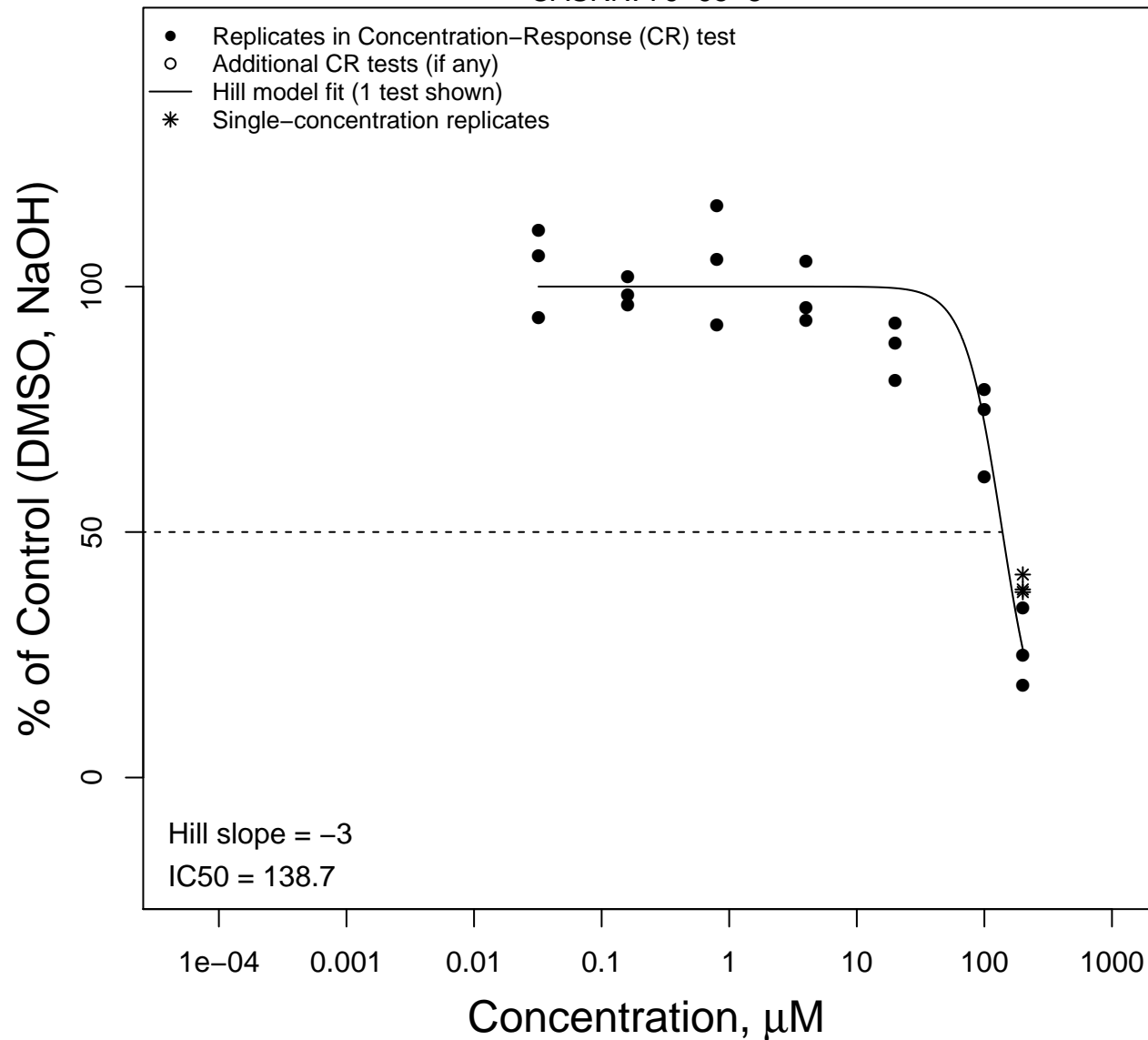
1,4-Diaminoanthraquinone

CASRN: 128-95-0



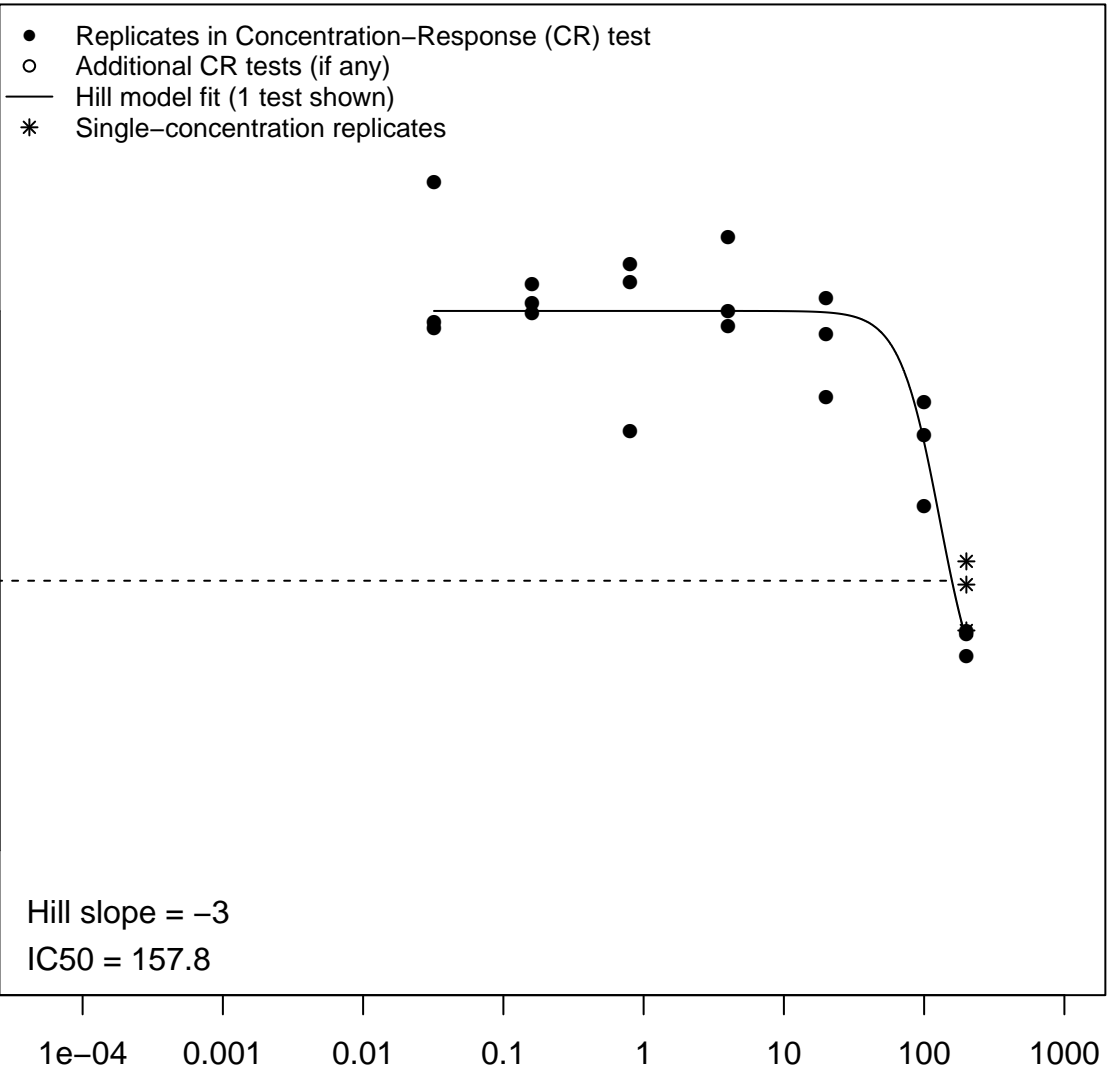
2,2',6,6'-Tetrachlorobisphenol A

CASRN: 79-95-8



Acid Red 337

CASRN: 67786-14-5

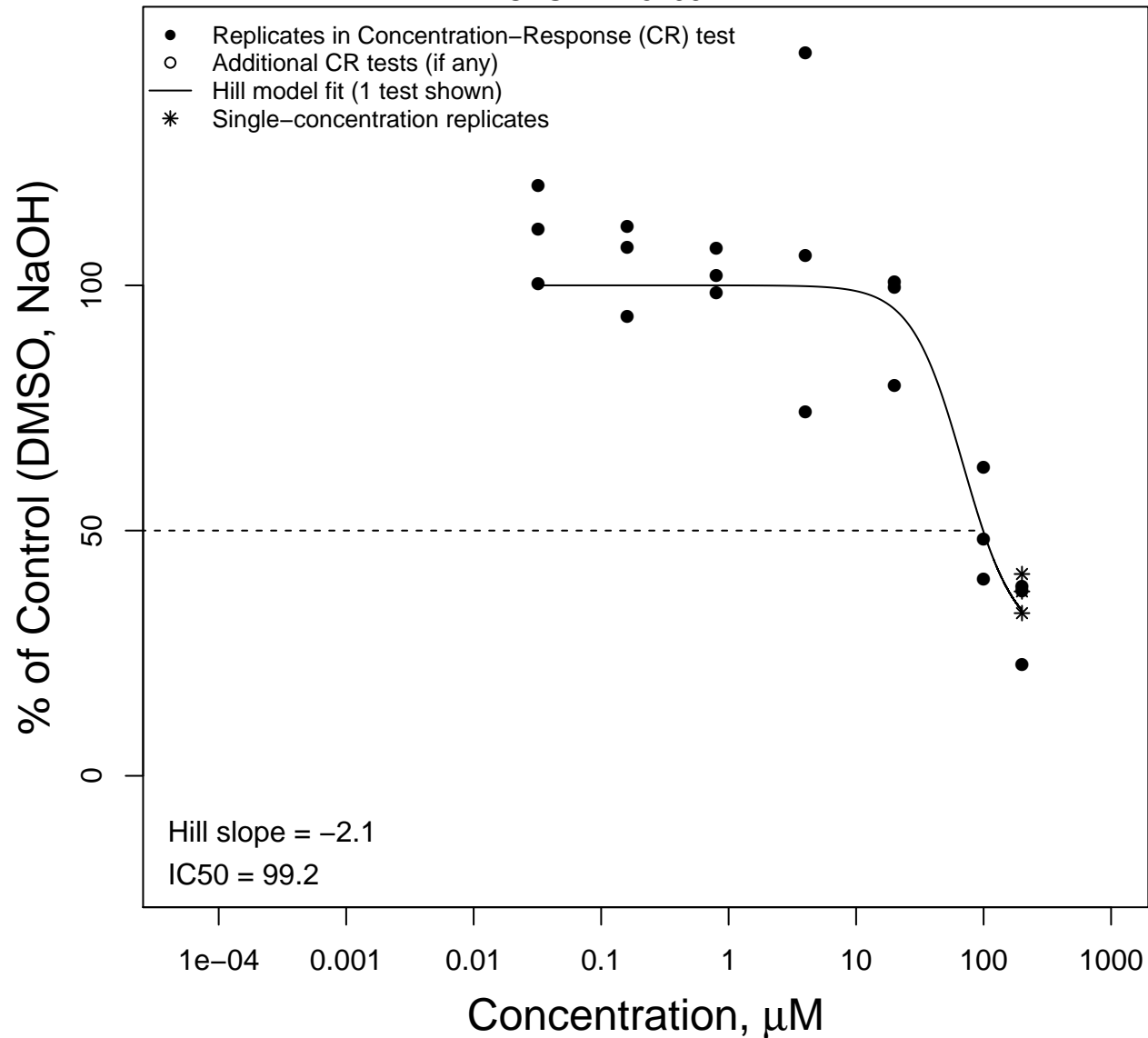


% of Control (DMSO, NaOH)

Concentration, µM

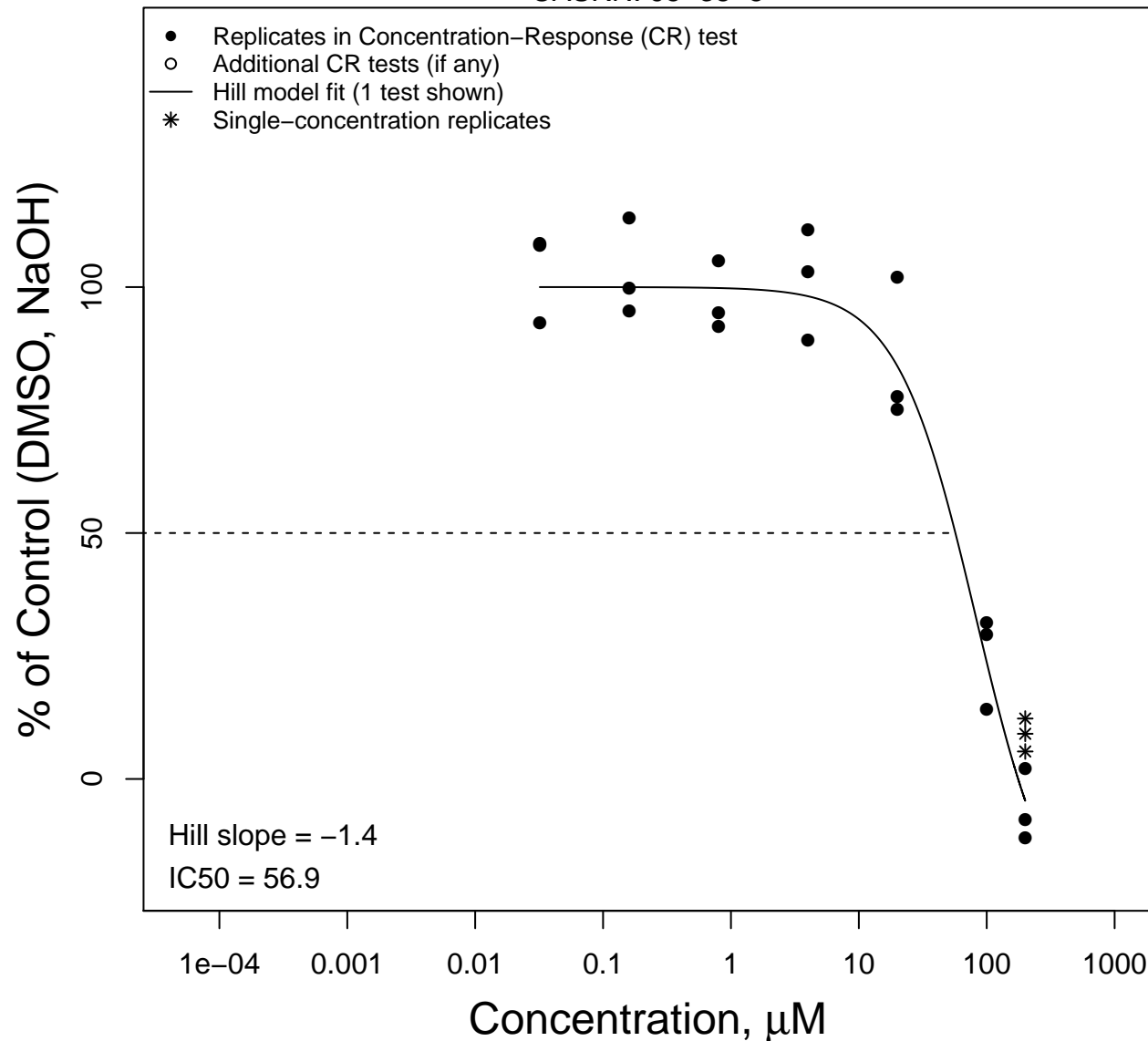
Glyceryl monooleate

CASRN: 25496-72-4



2-(8-Heptadecenyl)-2-imidazoline-1-ethanol

CASRN: 95-38-5



FD&C Green No. 3

CASRN: 2353-45-9

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100
50
0

1e-04

0.001

0.01

0.1

1

10

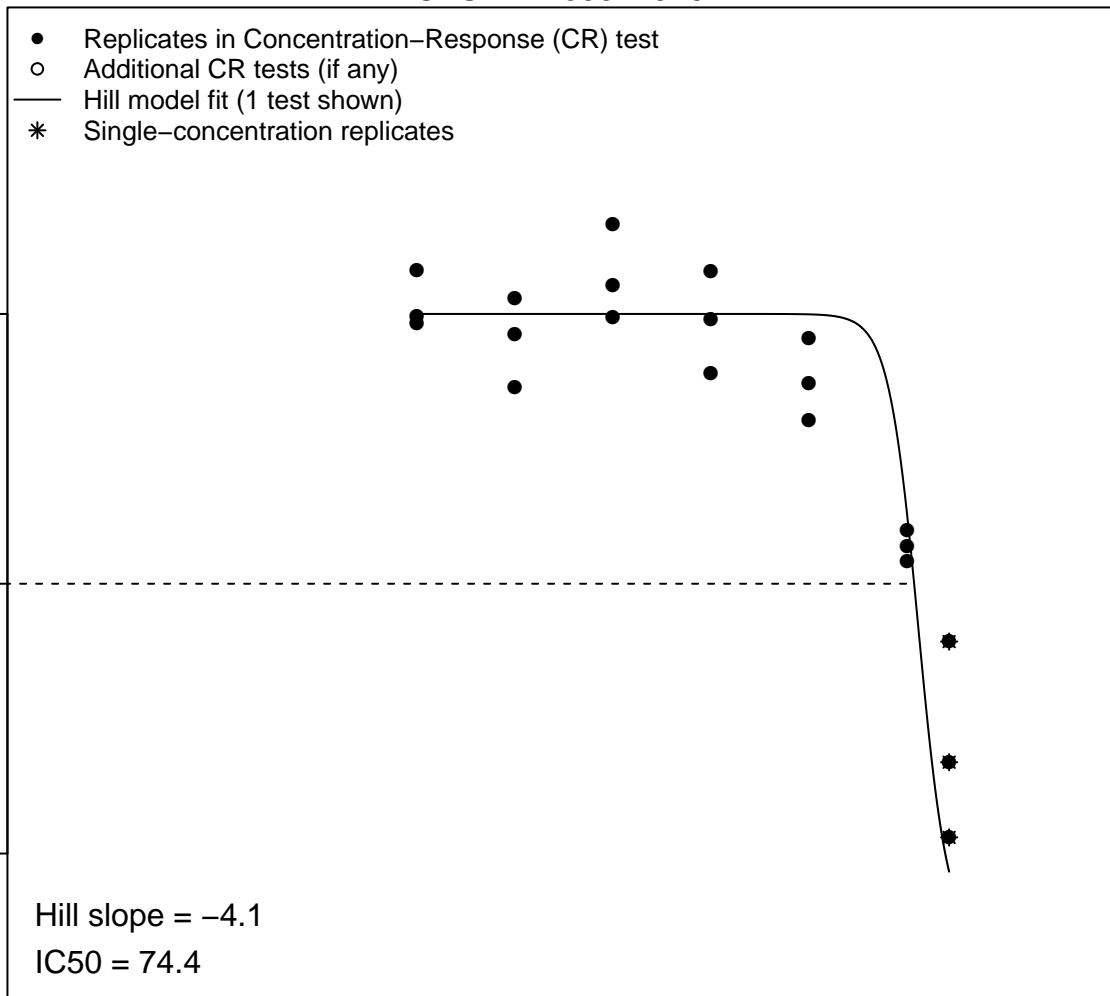
100

1000

Concentration, μM

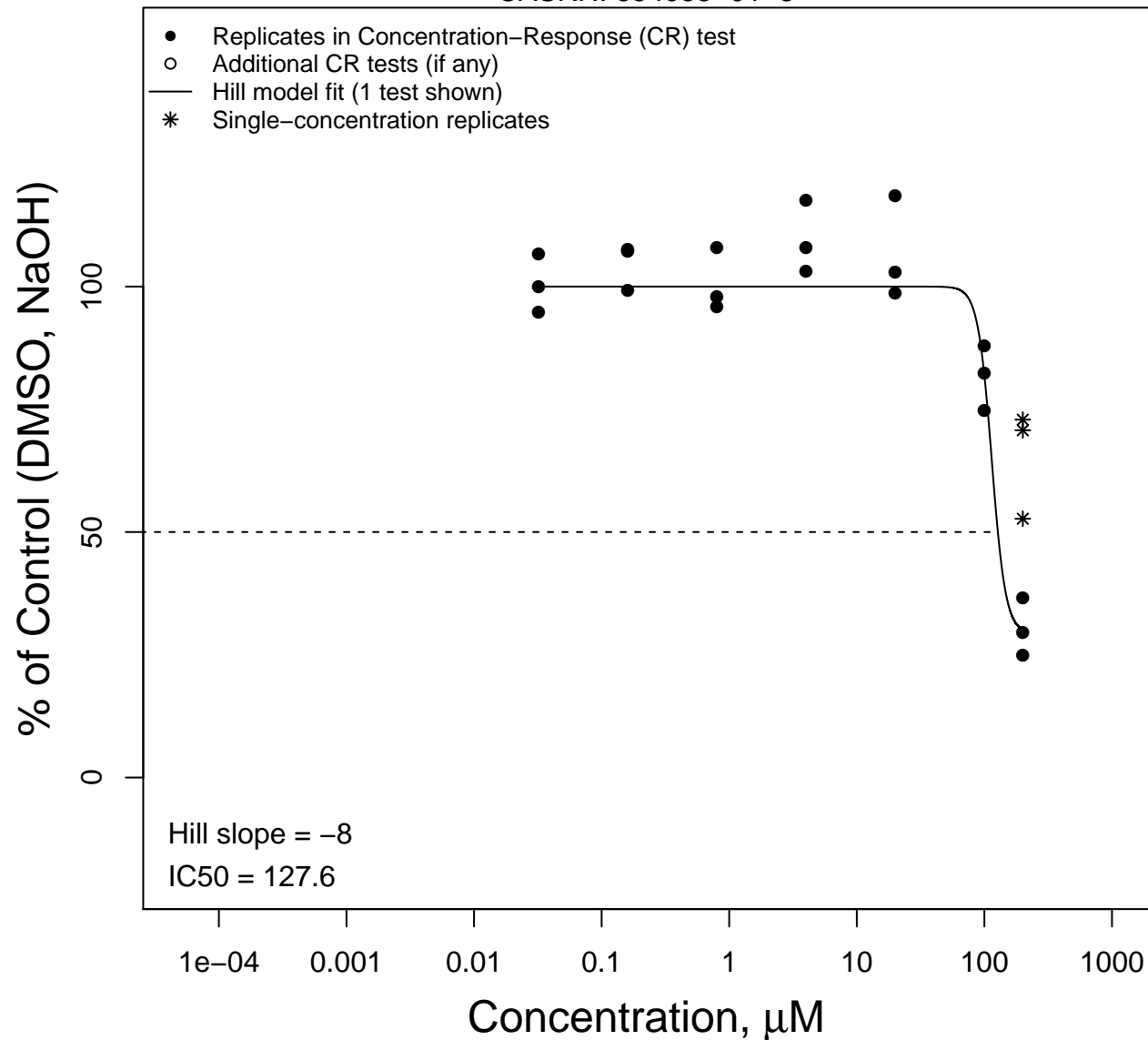
Hill slope = -4.1

IC50 = 74.4



Morin hydrate

CASRN: 654055-01-3



Dinocap

CASRN: 39300-45-3

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100

50

0

Hill slope = -8

IC50 = 23.8

1e-04

0.001

0.01

0.1

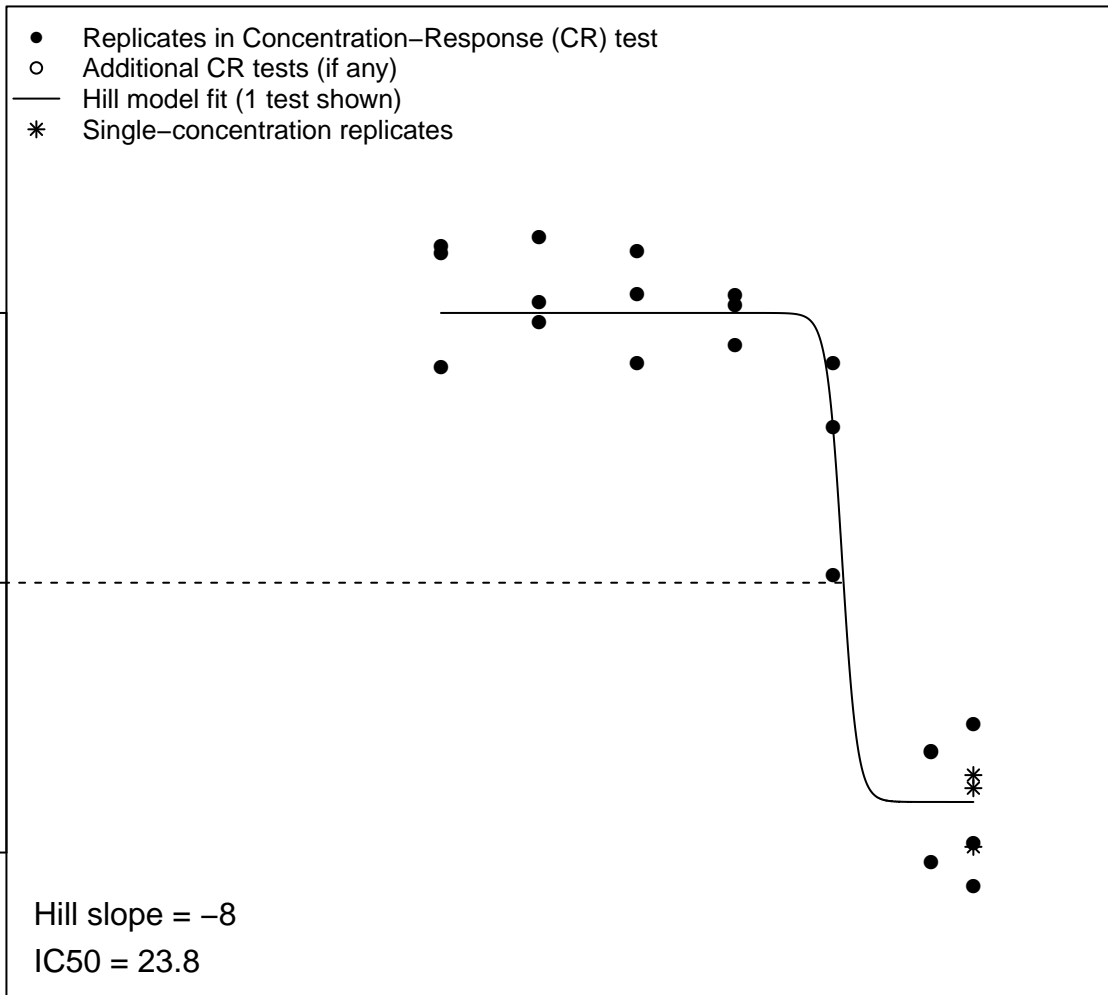
1

10

100

1000

Concentration, μM



Heptylparaben

CASRN: 1085-12-7

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100

50

0

Hill slope = -1.2

IC50 = 45.8

1e-04

0.001

0.01

0.1

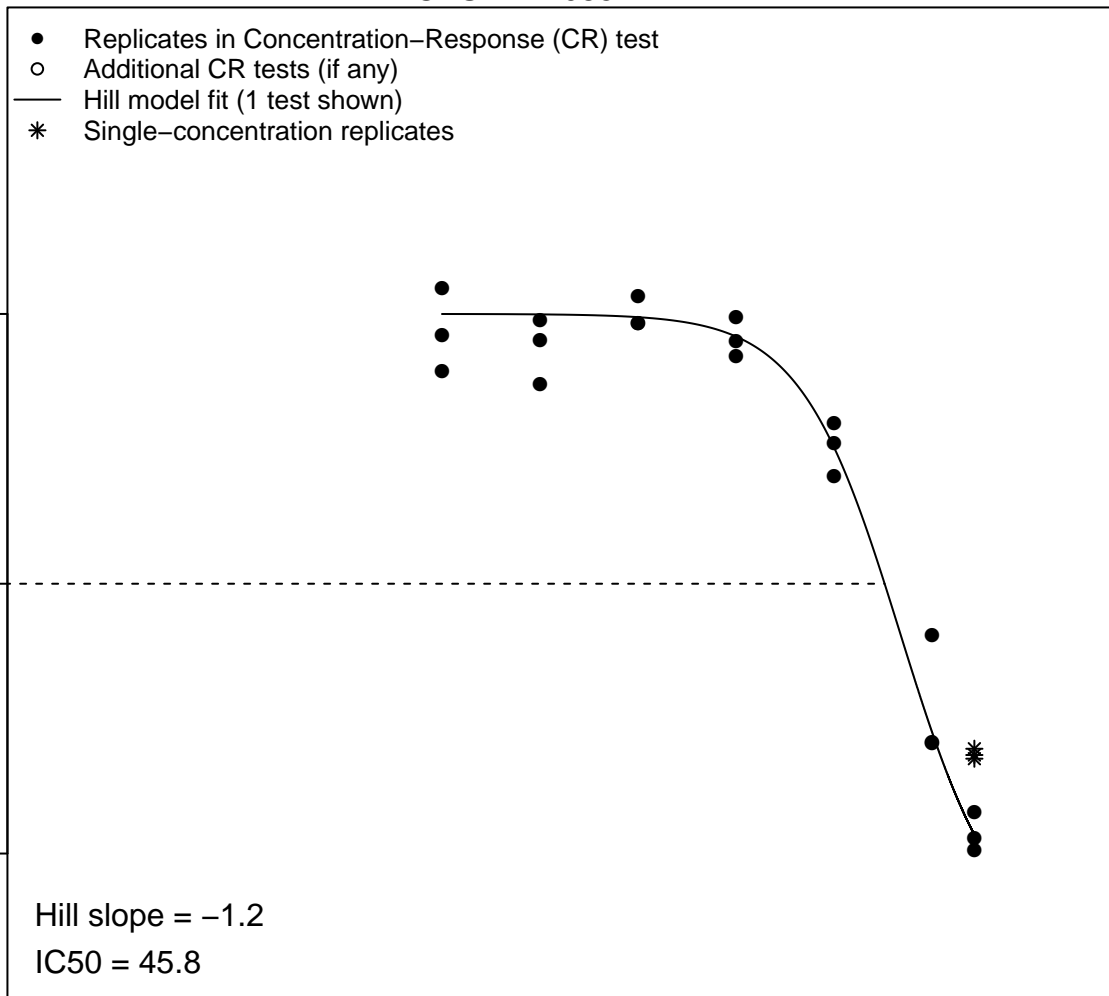
1

10

100

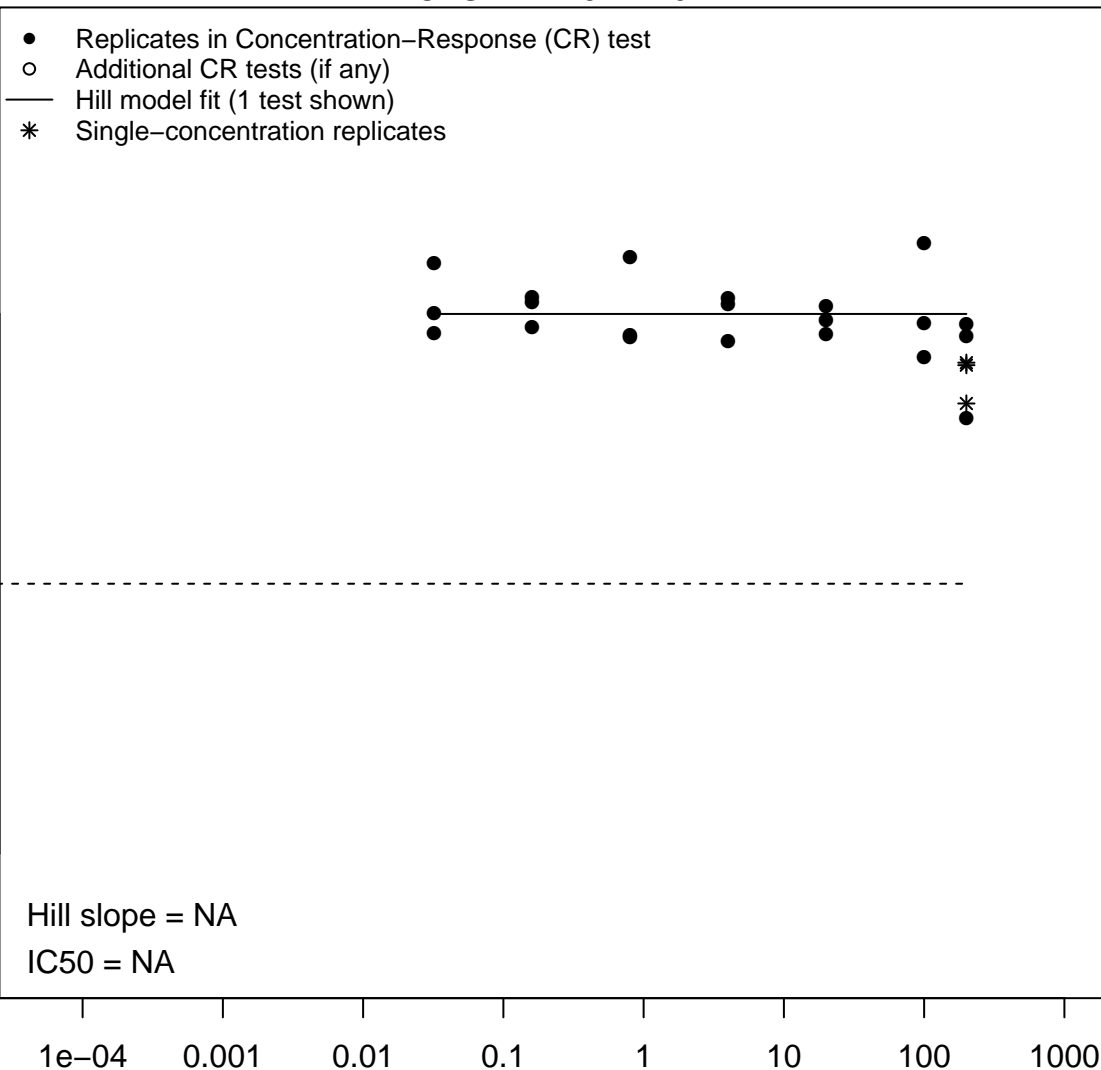
1000

Concentration, μM



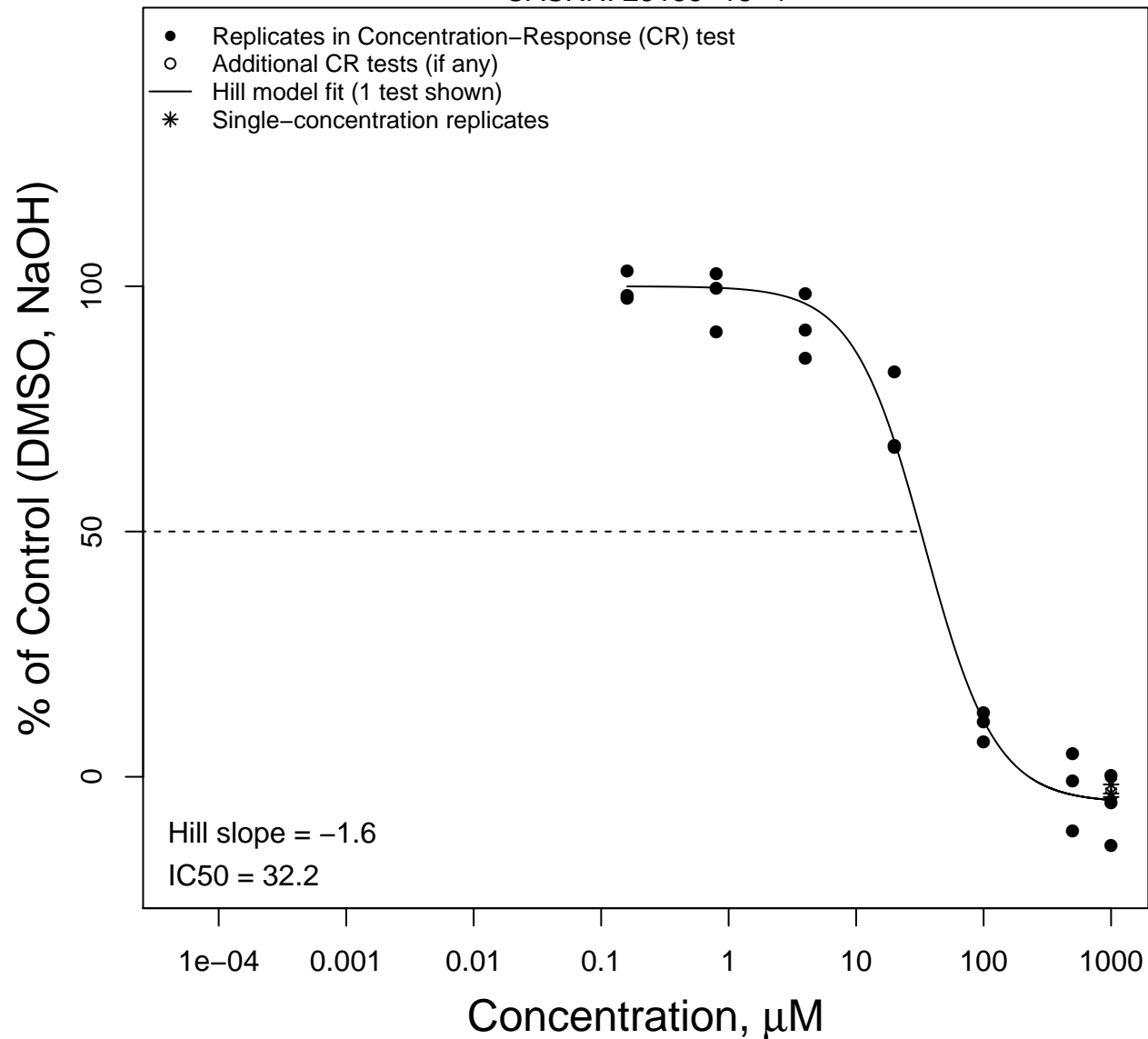
Genistein

CASRN: 446-72-0



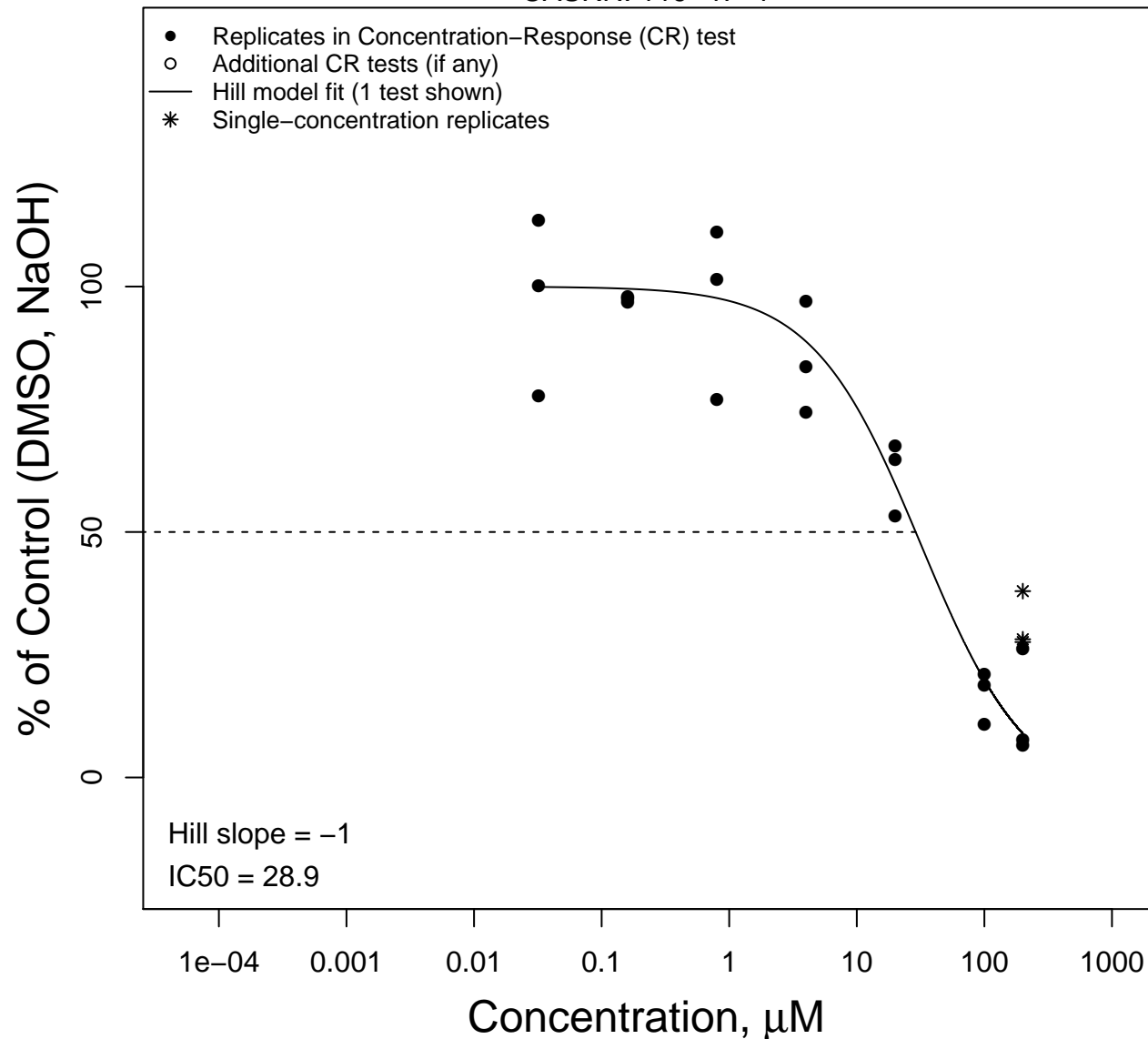
Methylbenzethonium chloride

CASRN: 25155-18-4



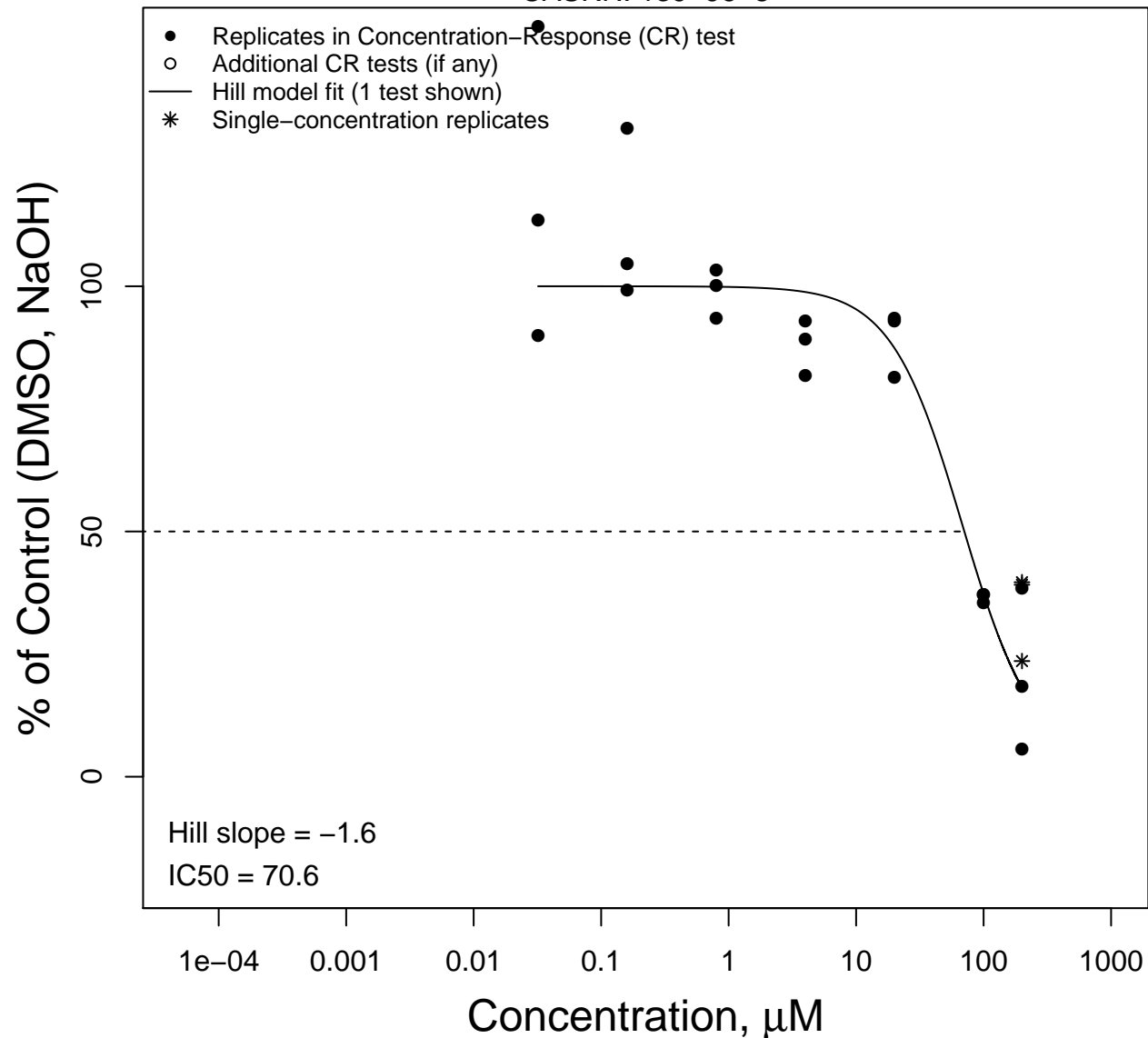
2,2'-Methylenebis(4-methyl-6-tert-butylphenol)

CASRN: 119-47-1



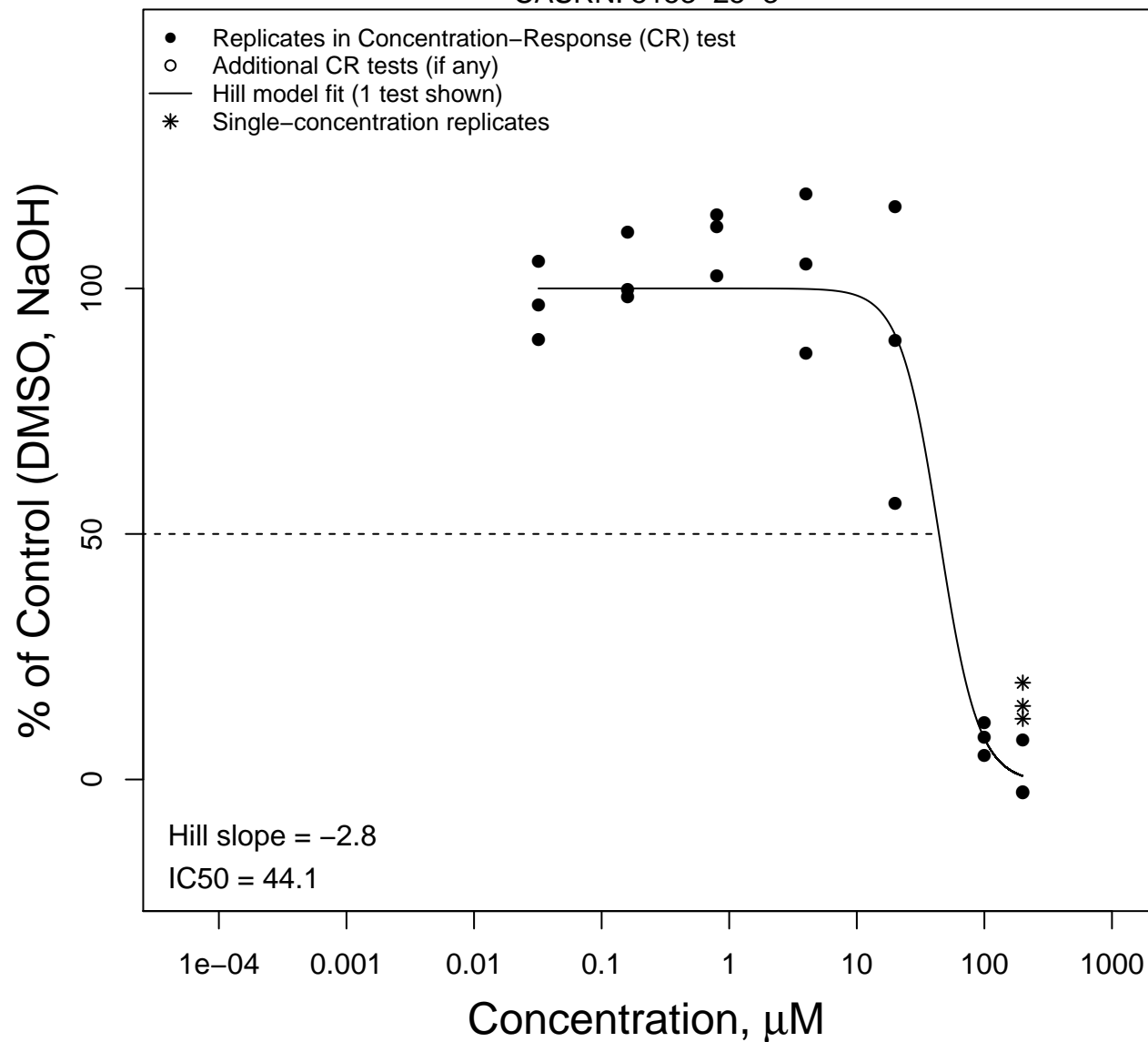
Dodecyl sulfate triethanolamine

CASRN: 139-96-8



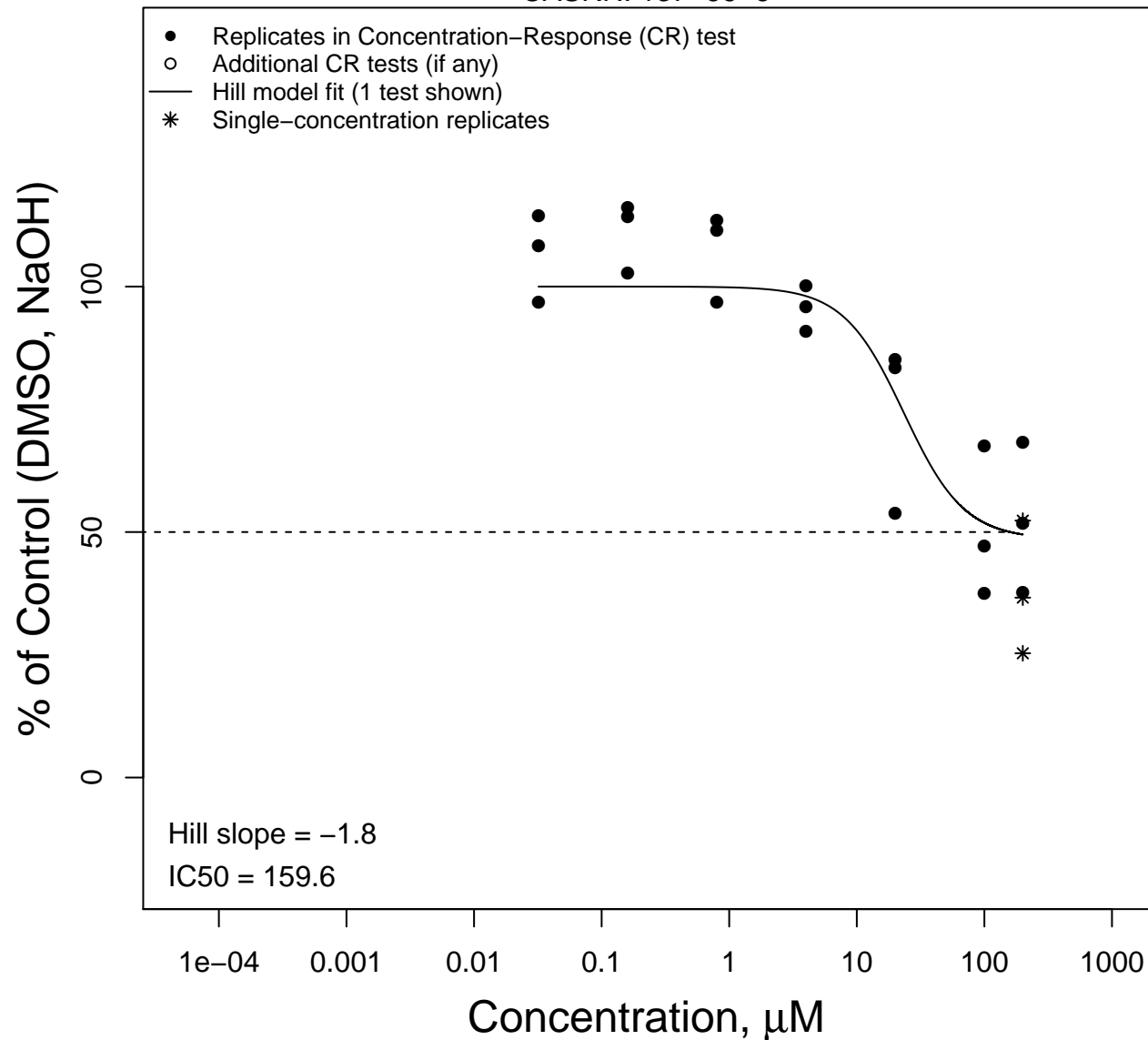
2-Ethylhexylparaben

CASRN: 5153-25-3



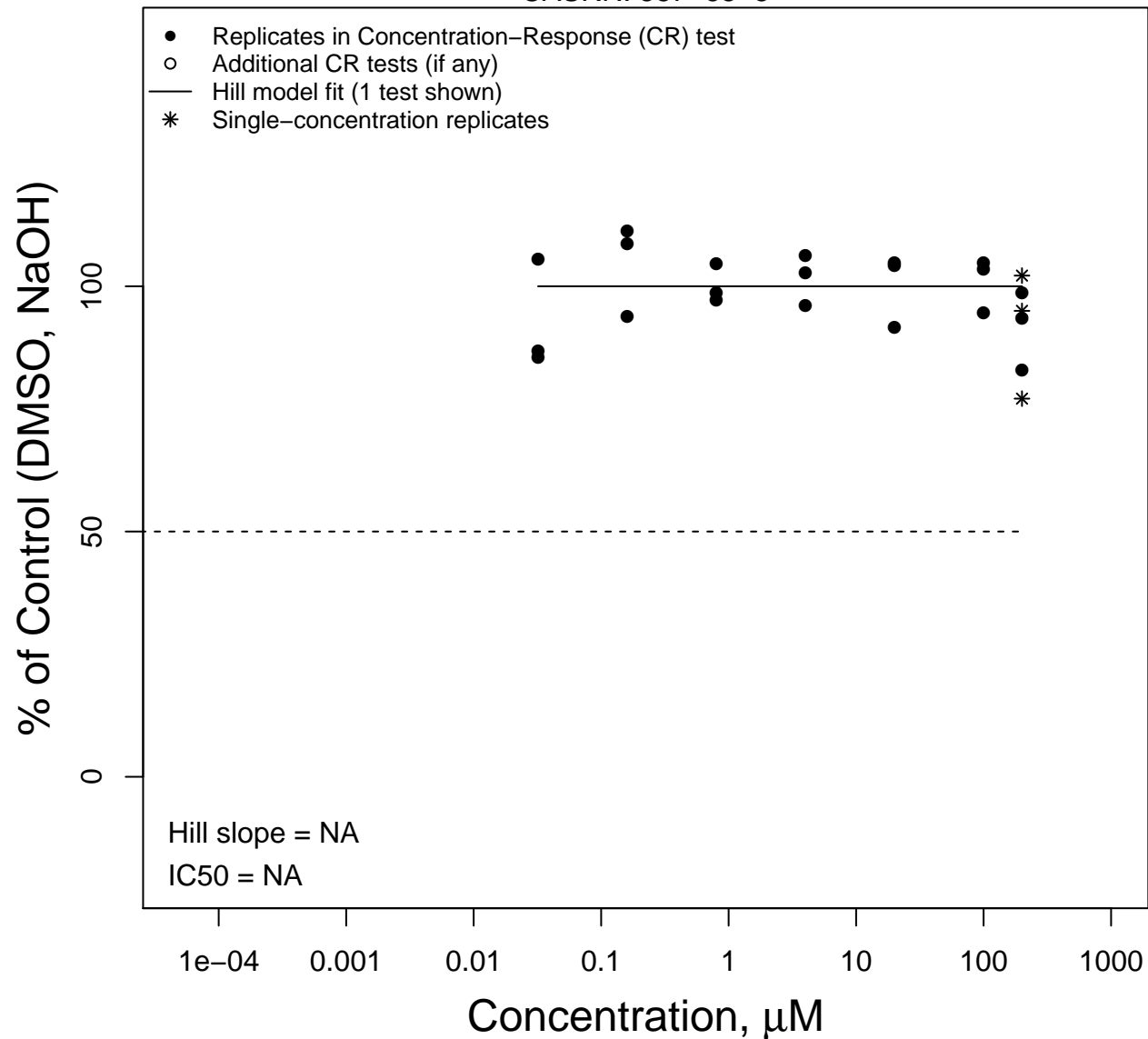
Ascorbyl palmitate

CASRN: 137-66-6



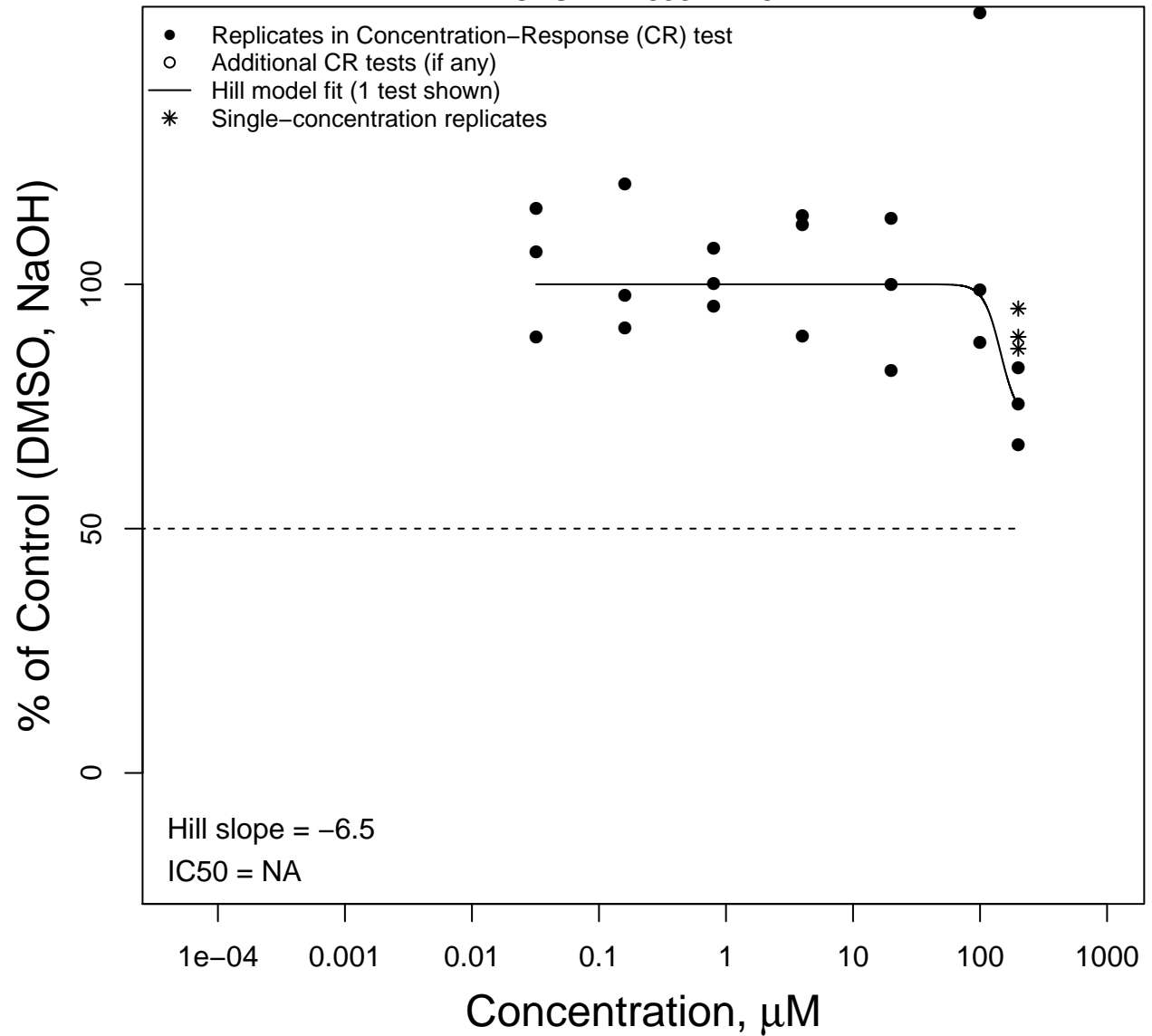
2-Chloro-N-phenylacetamide

CASRN: 587-65-5



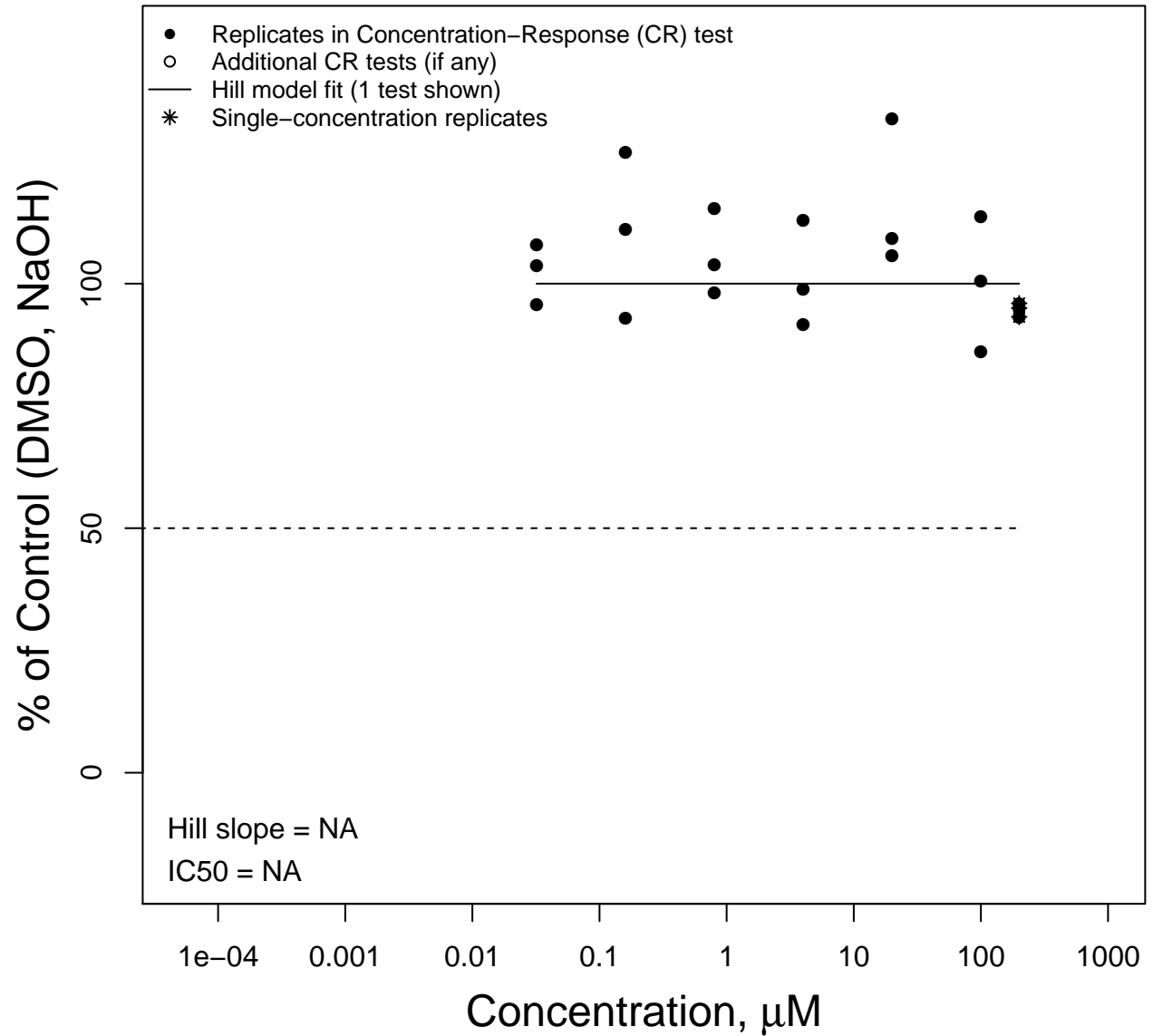
4-Butylphenol

CASRN: 1638-22-8



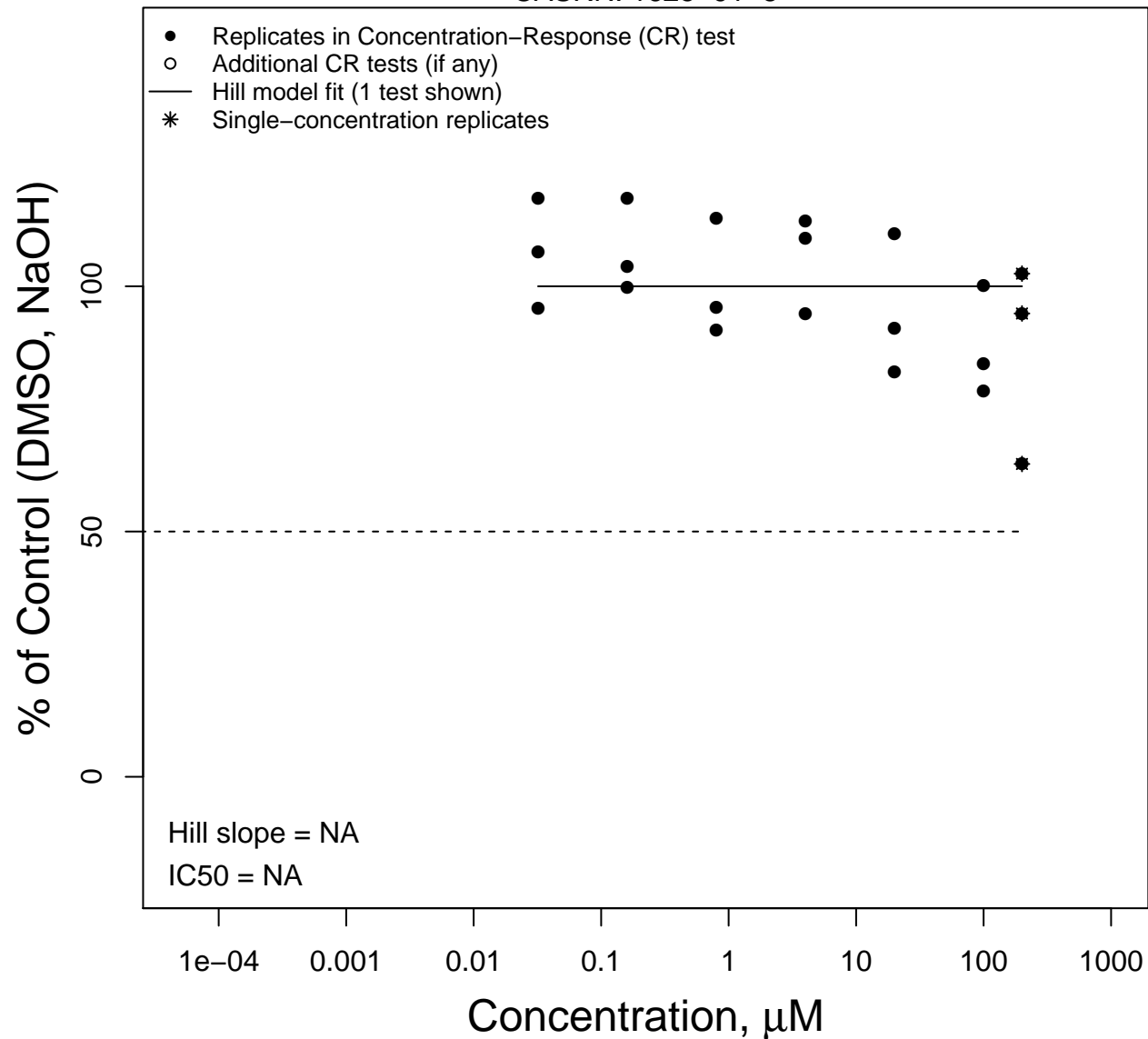
Acrylonitrile

CASRN: 107-13-1



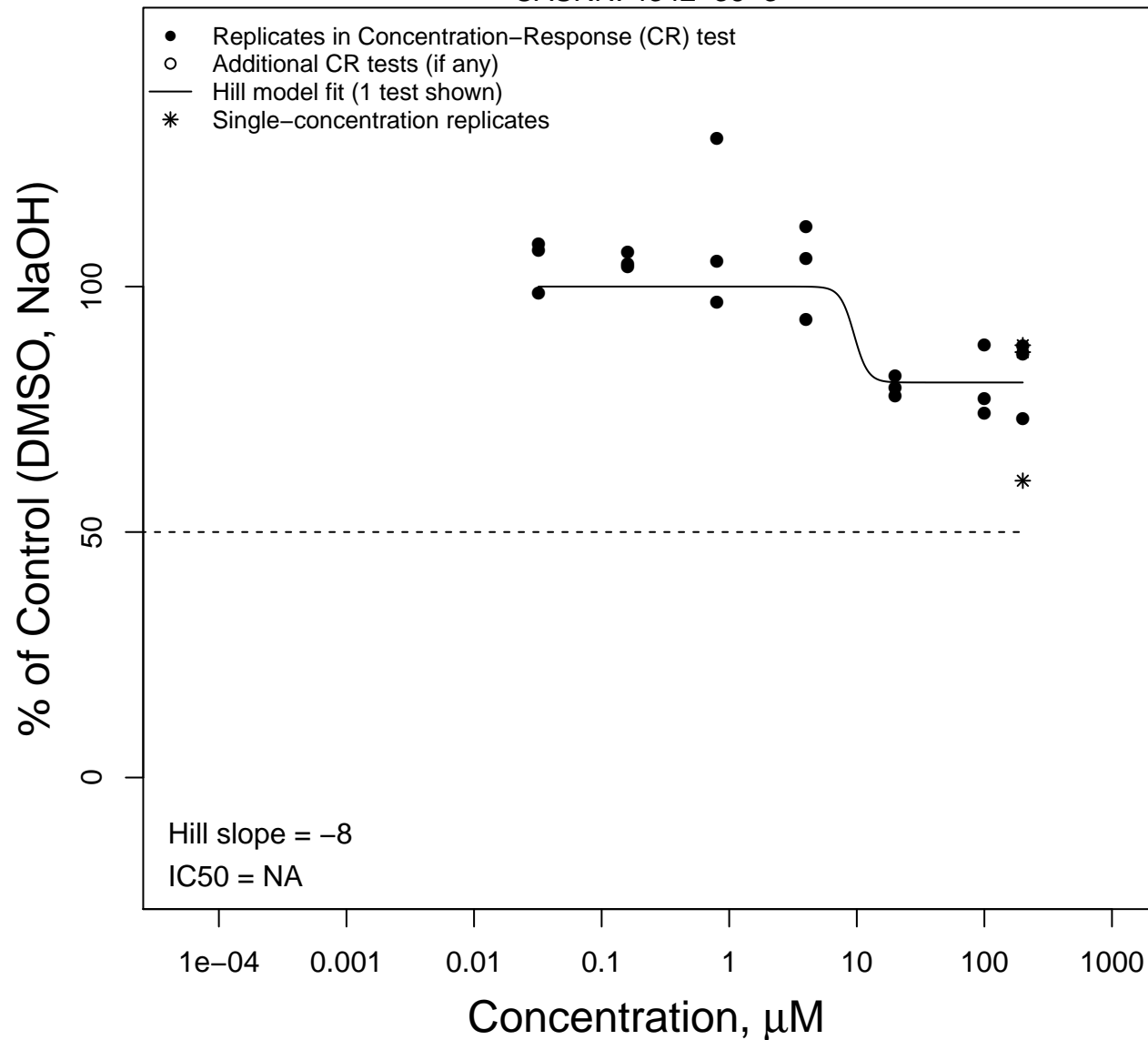
4,4'-Di-tert-butylbiphenyl

CASRN: 1625-91-8



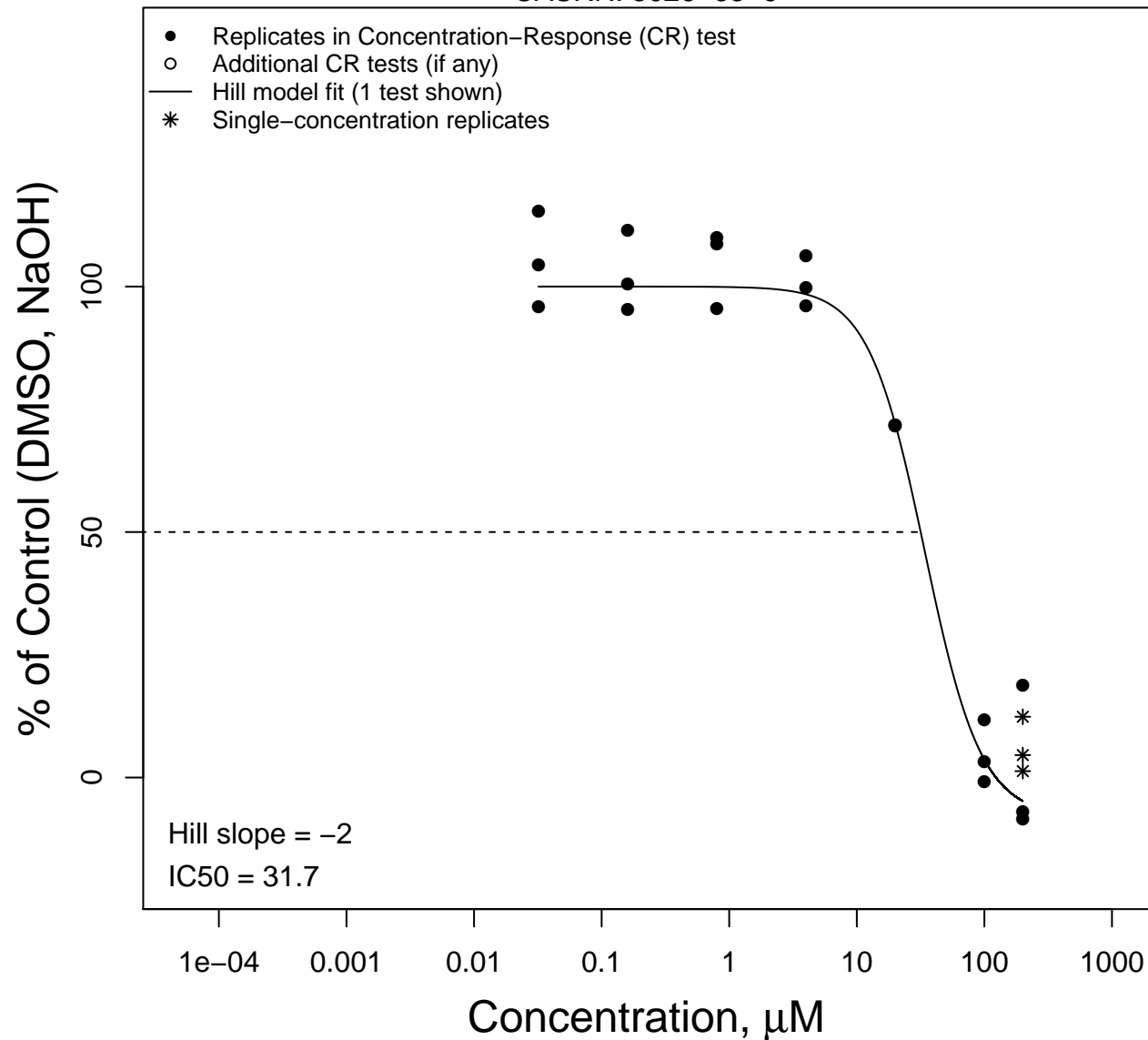
Tributyltin benzoate

CASRN: 4342-36-3



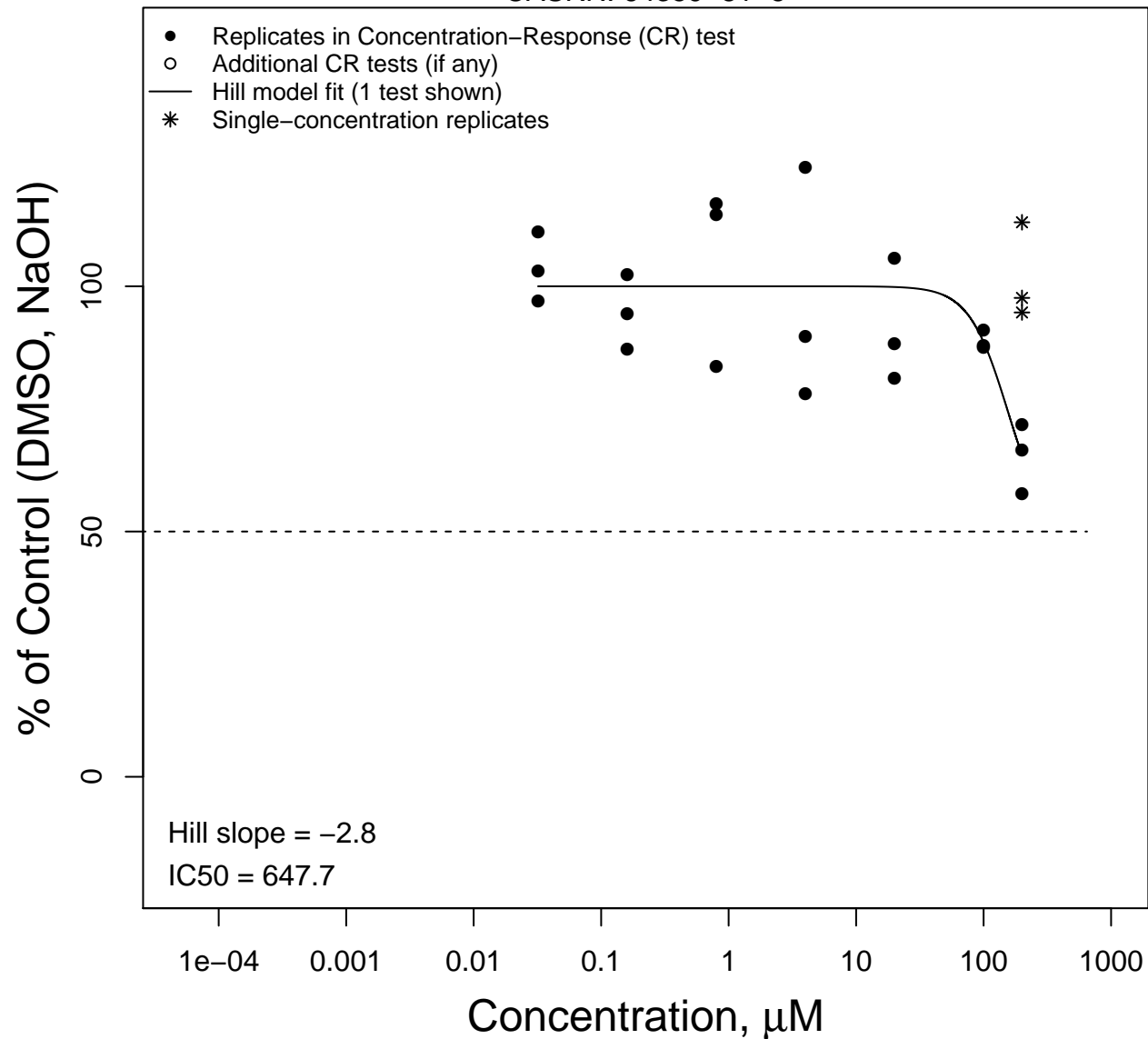
Sodium tridecyl sulfate

CASRN: 3026-63-9



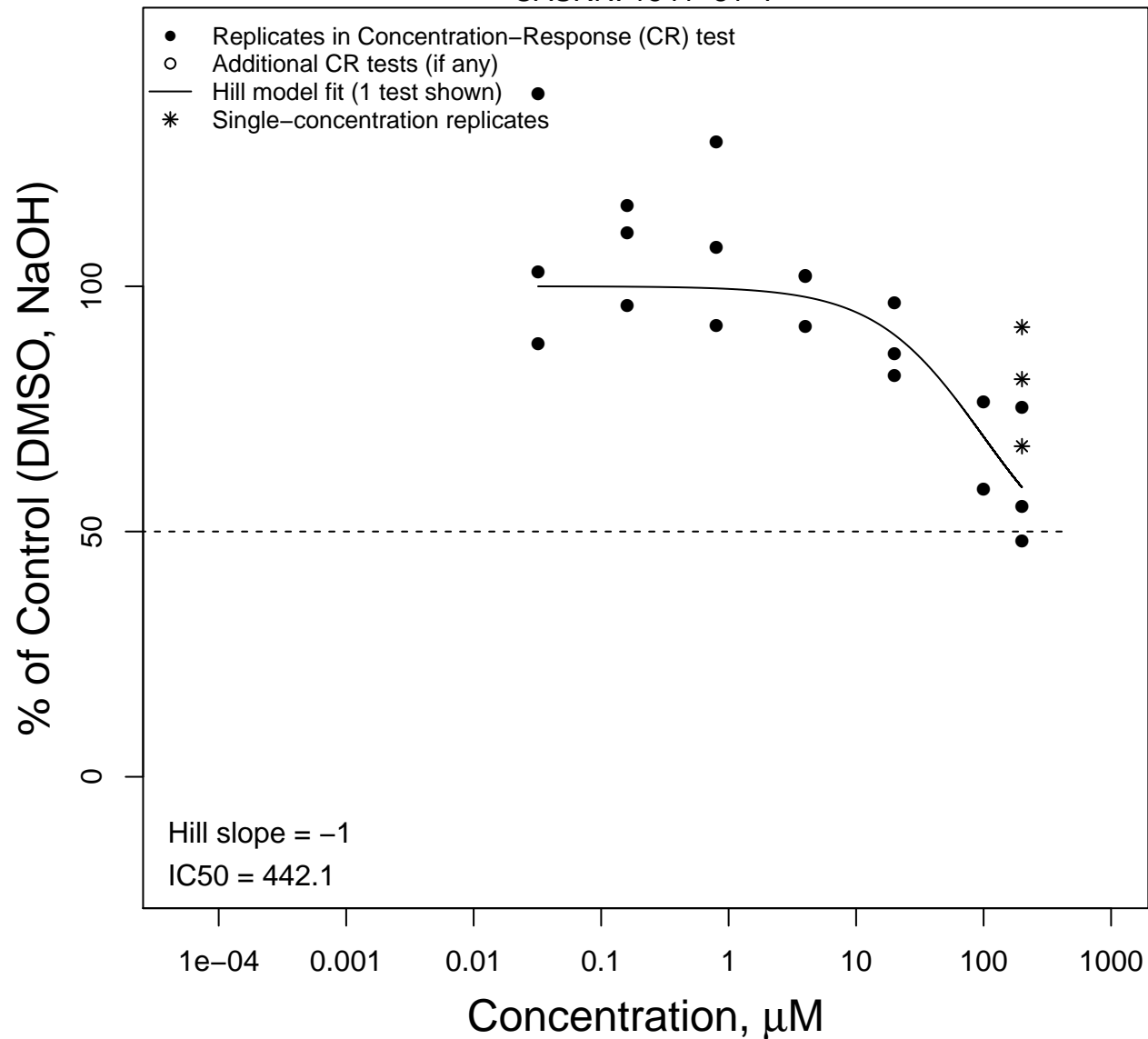
4,5-Dichloro-2-octyl-3(2H)-isothiazolone

CASRN: 64359-81-5



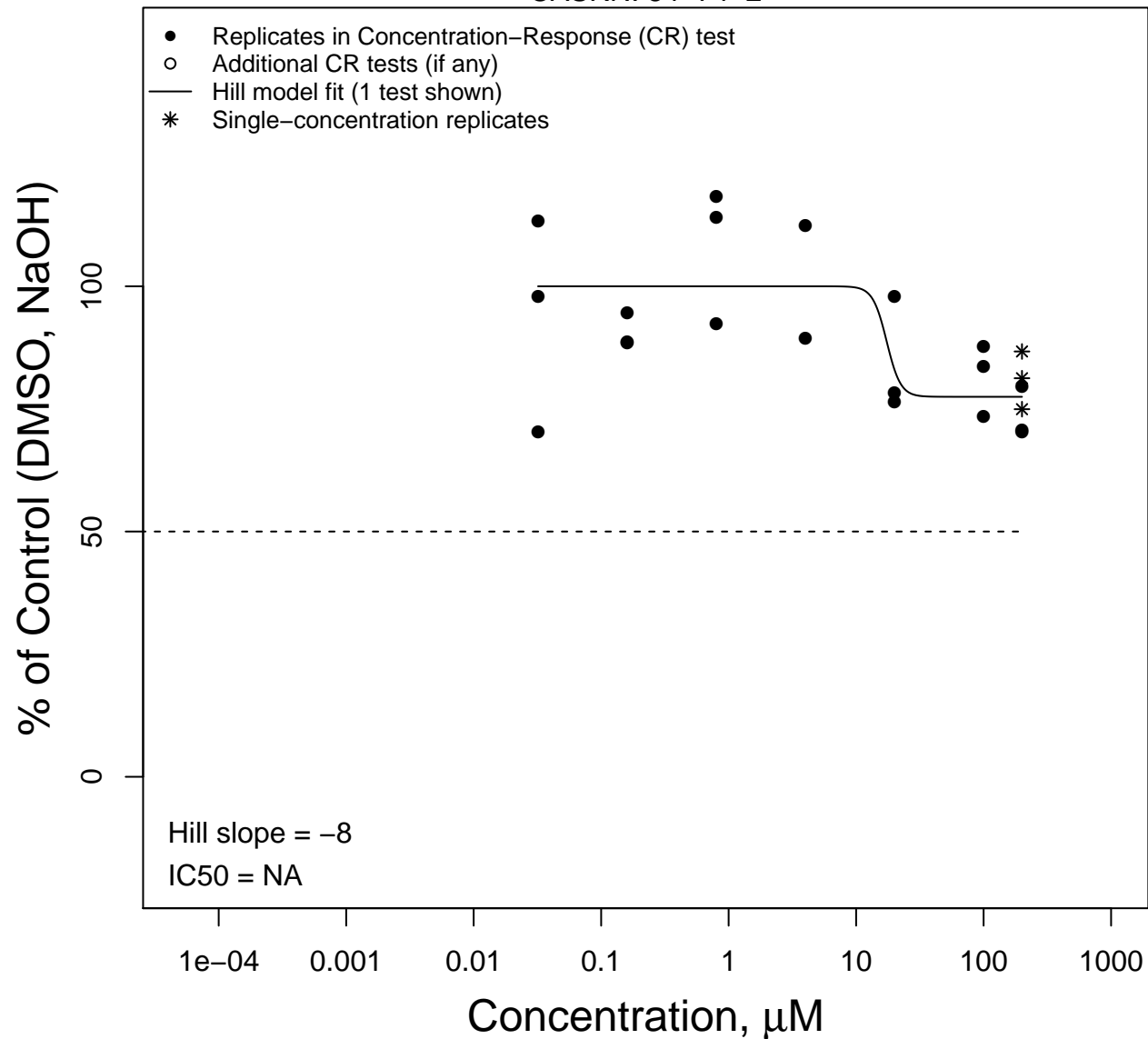
4-Dodecylmorpholine

CASRN: 1541-81-7



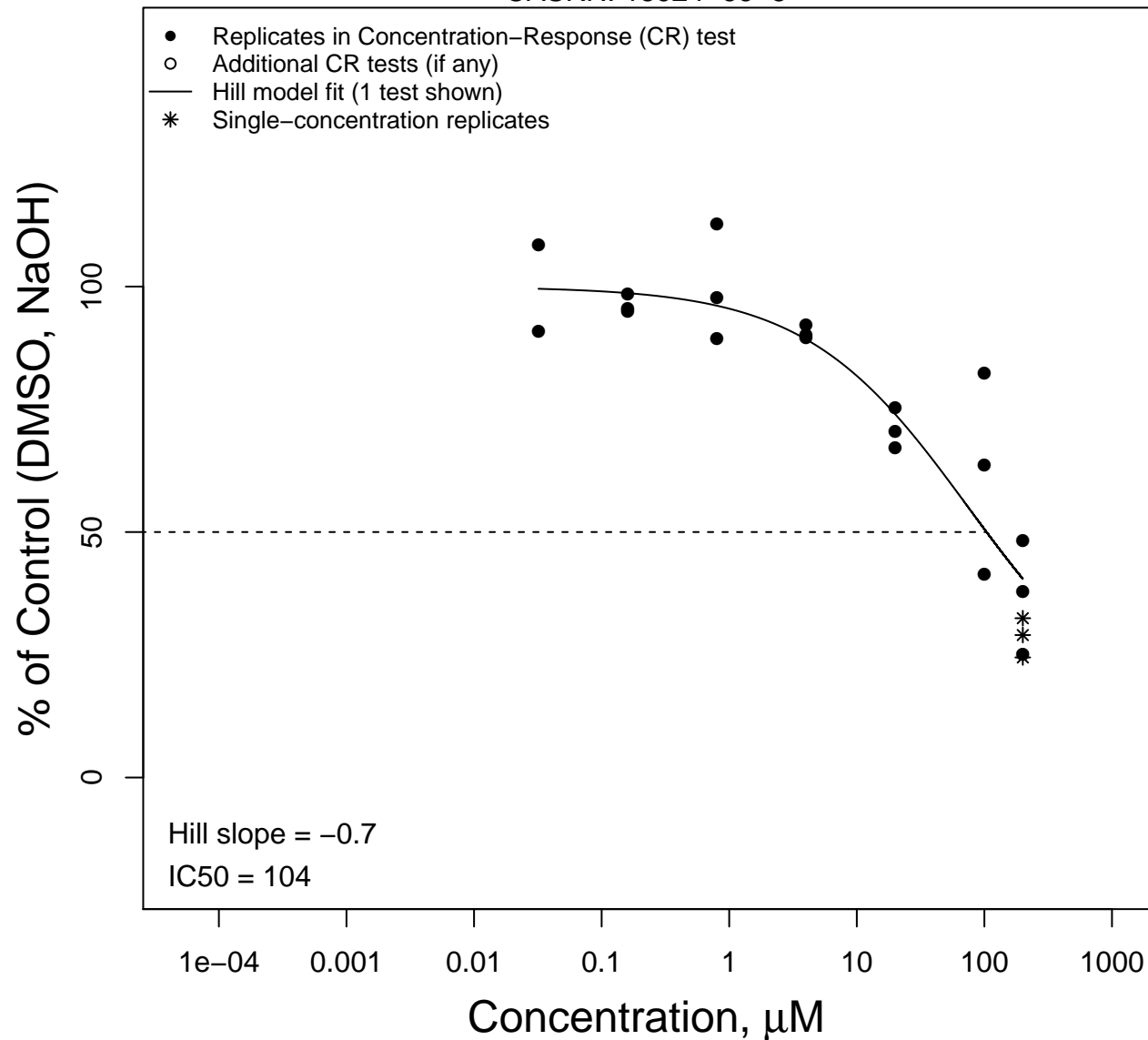
Dibutyl phthalate

CASRN: 84-74-2



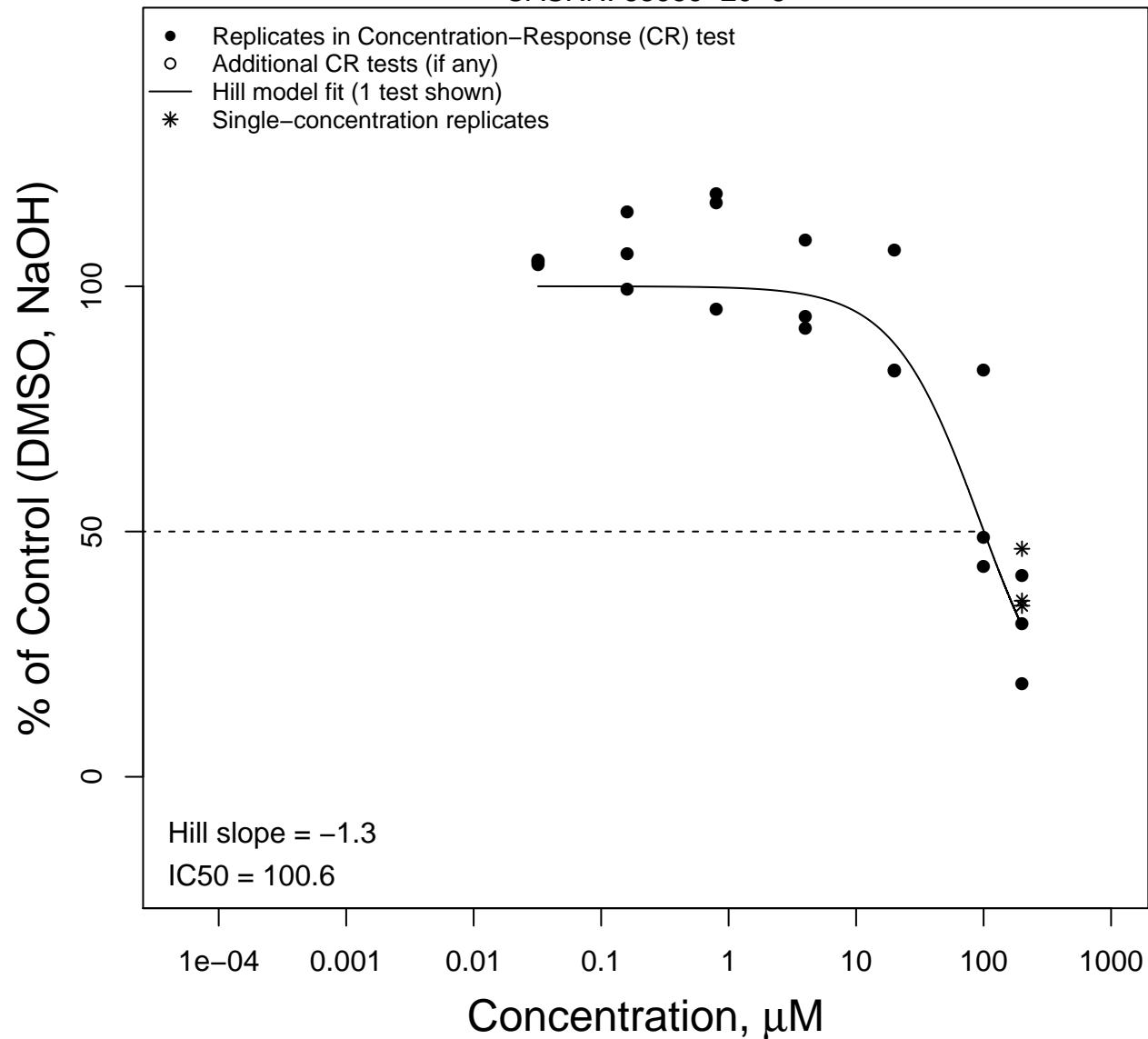
2,2'-(Tetradecylimino)diethanol

CASRN: 18924-66-8



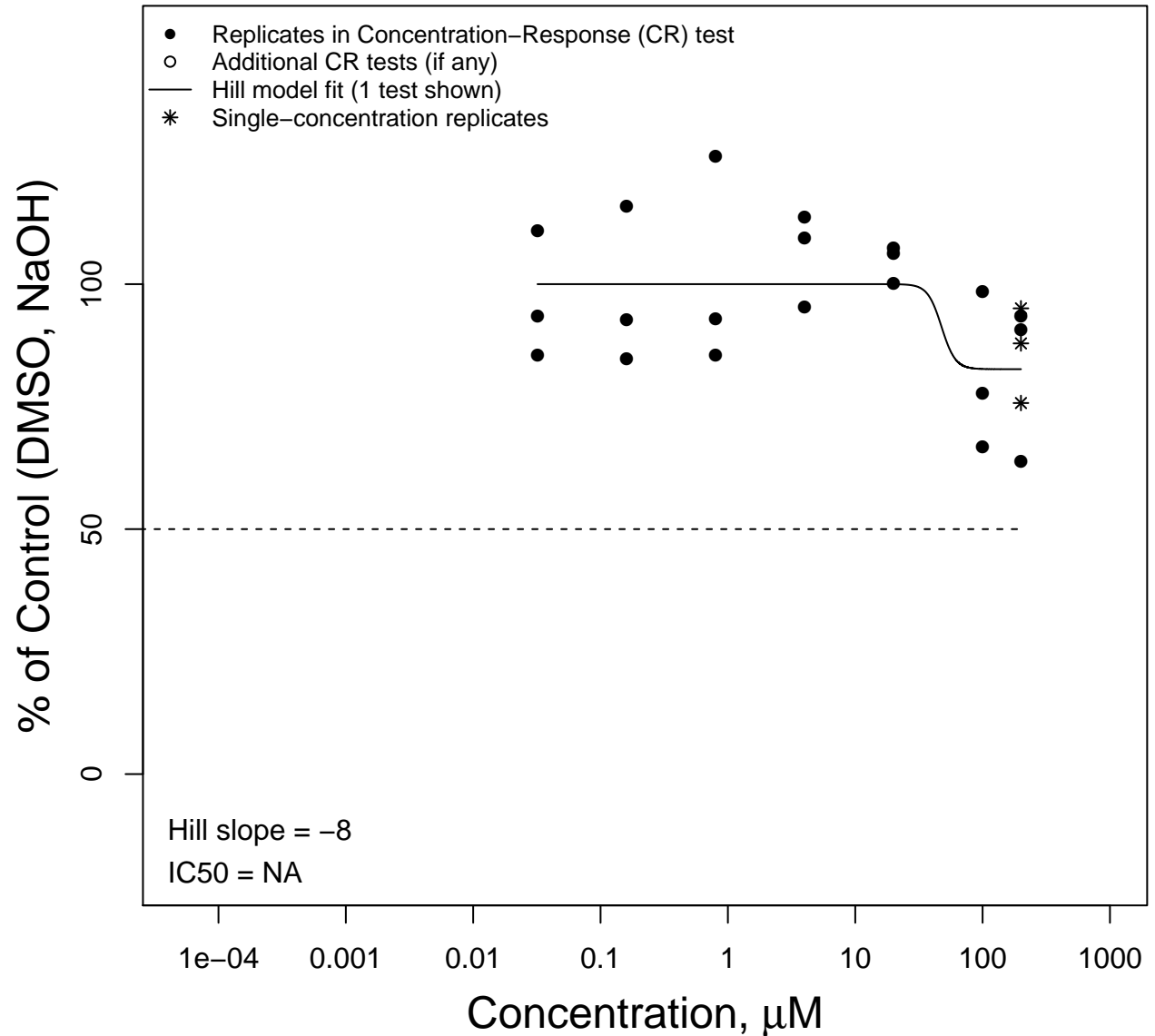
Disiquonium chloride

CASRN: 68959-20-6



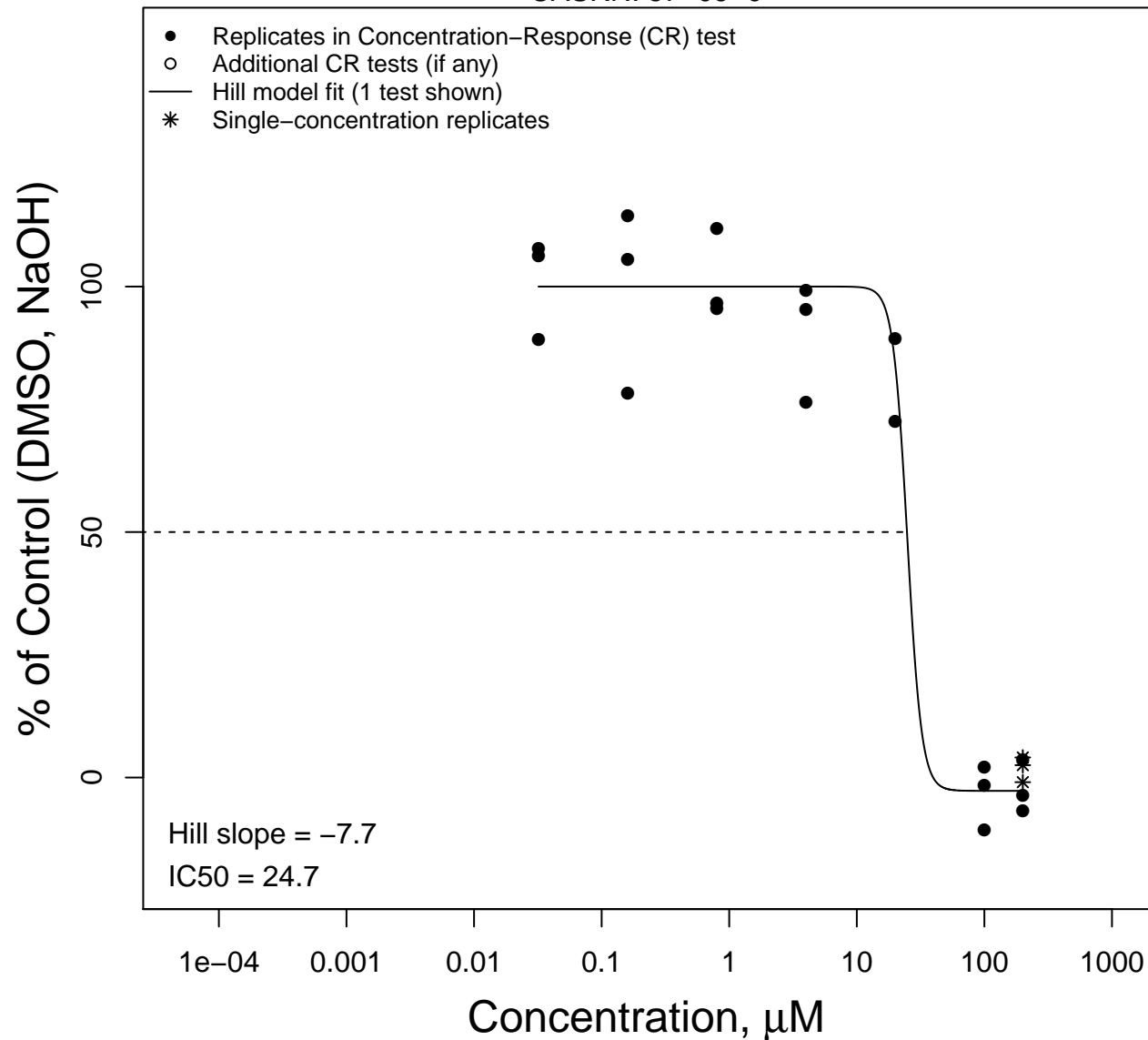
Bisphenol A diglycidyl ether

CASRN: 1675-54-3



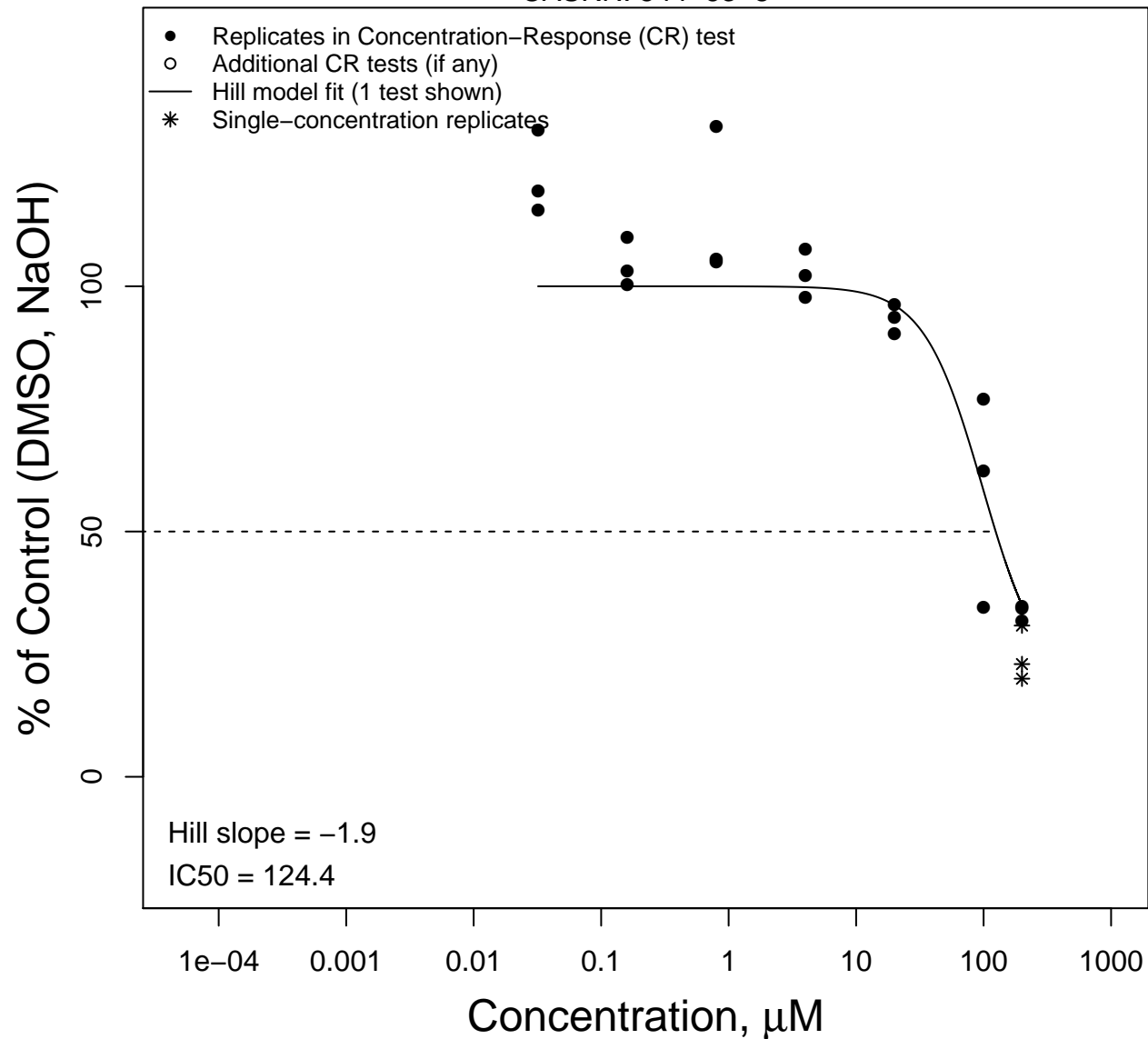
Hexadecyltrimethylammonium bromide

CASRN: 57-09-0



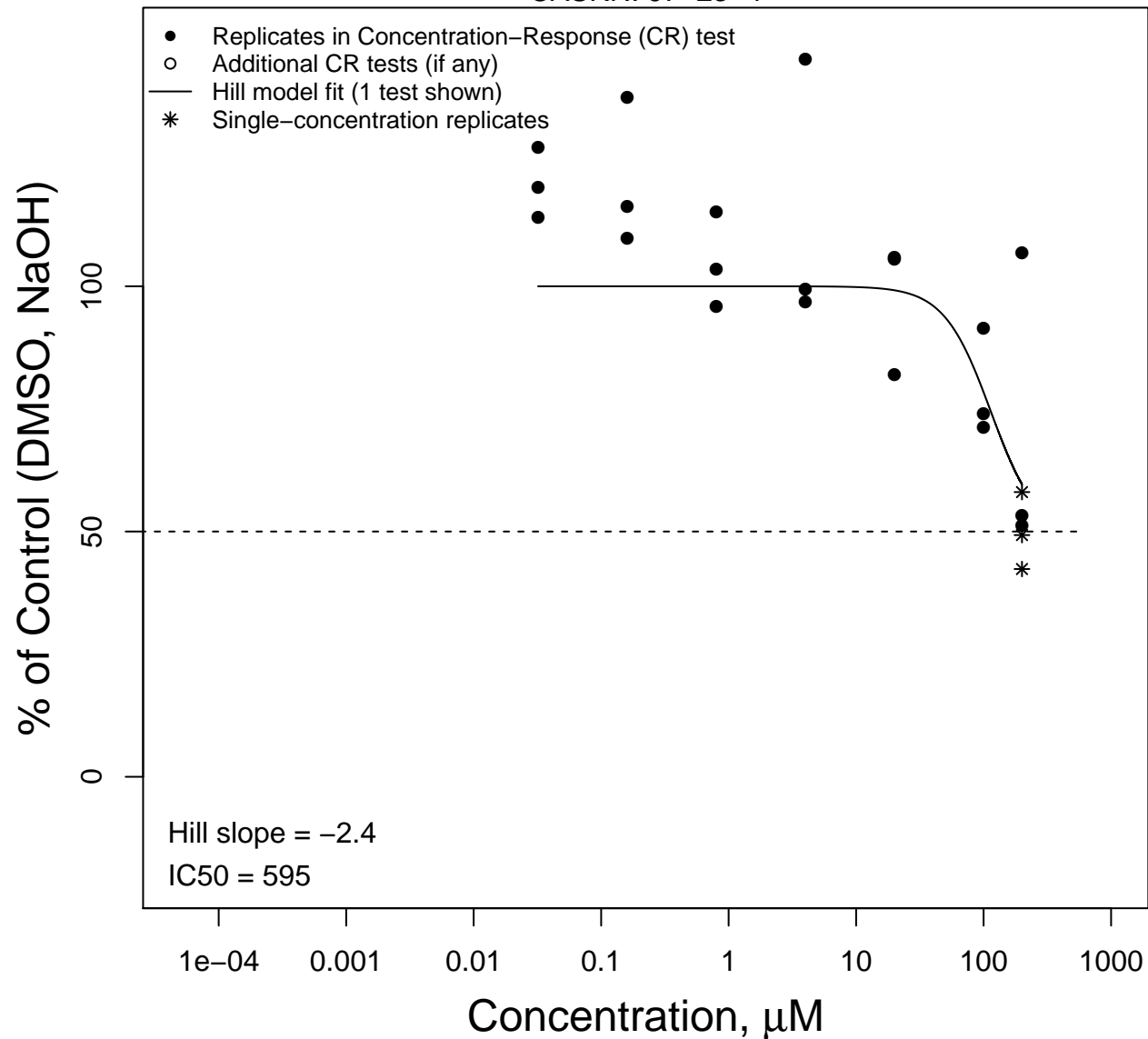
Tetradecanoic acid

CASRN: 544-63-8



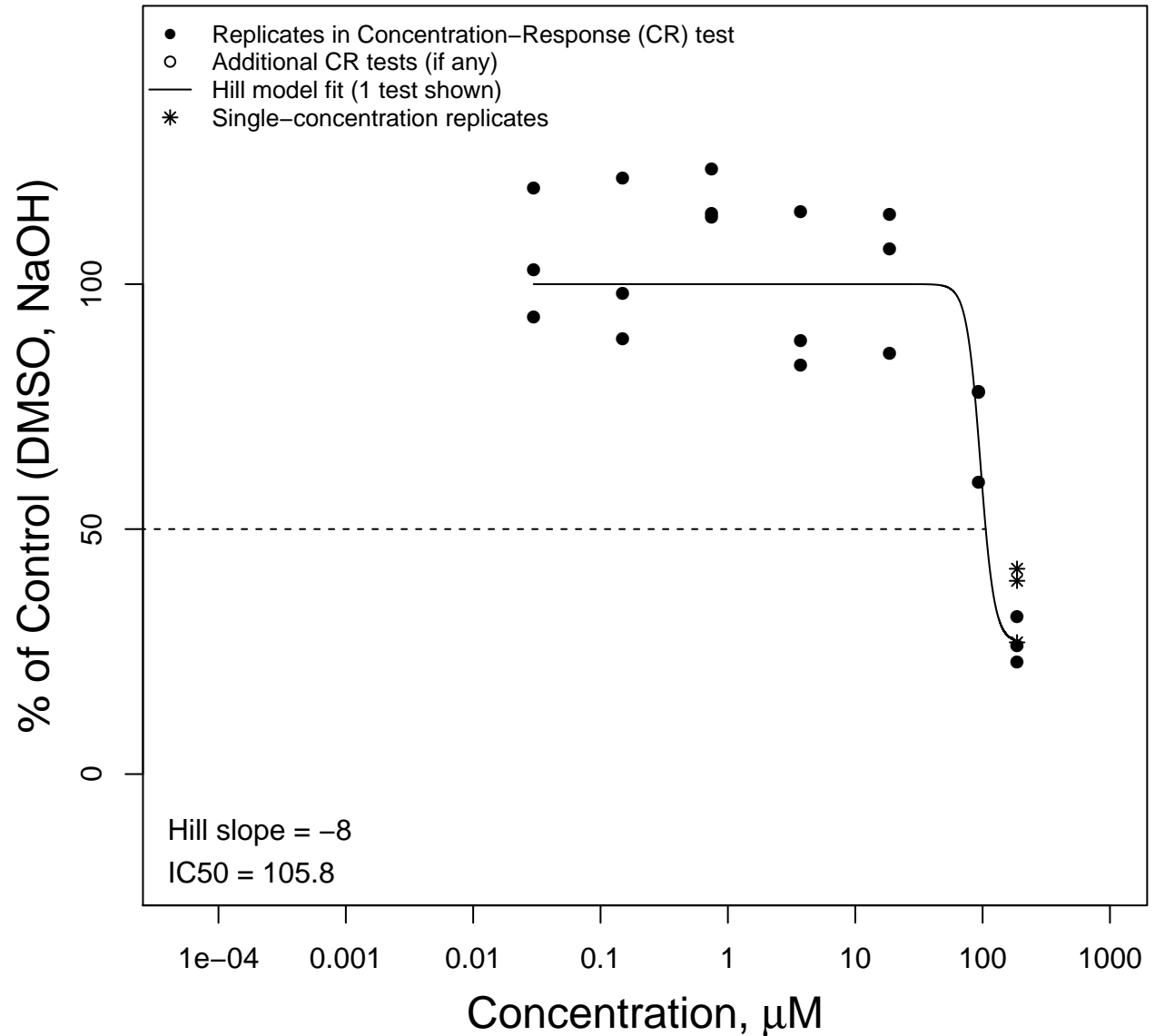
Dichlorophen

CASRN: 97-23-4



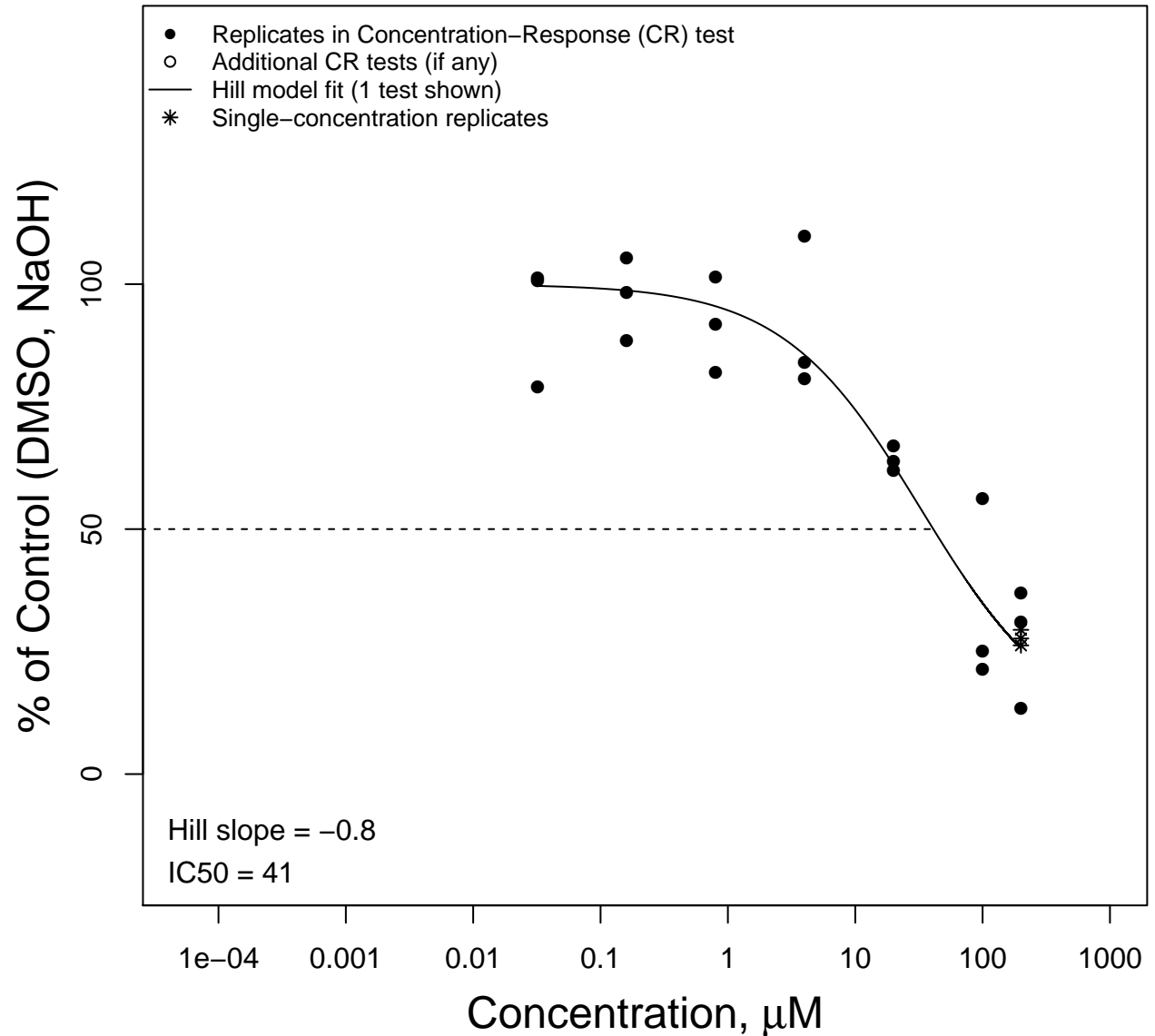
Bromophenol blue

CASRN: 115-39-9



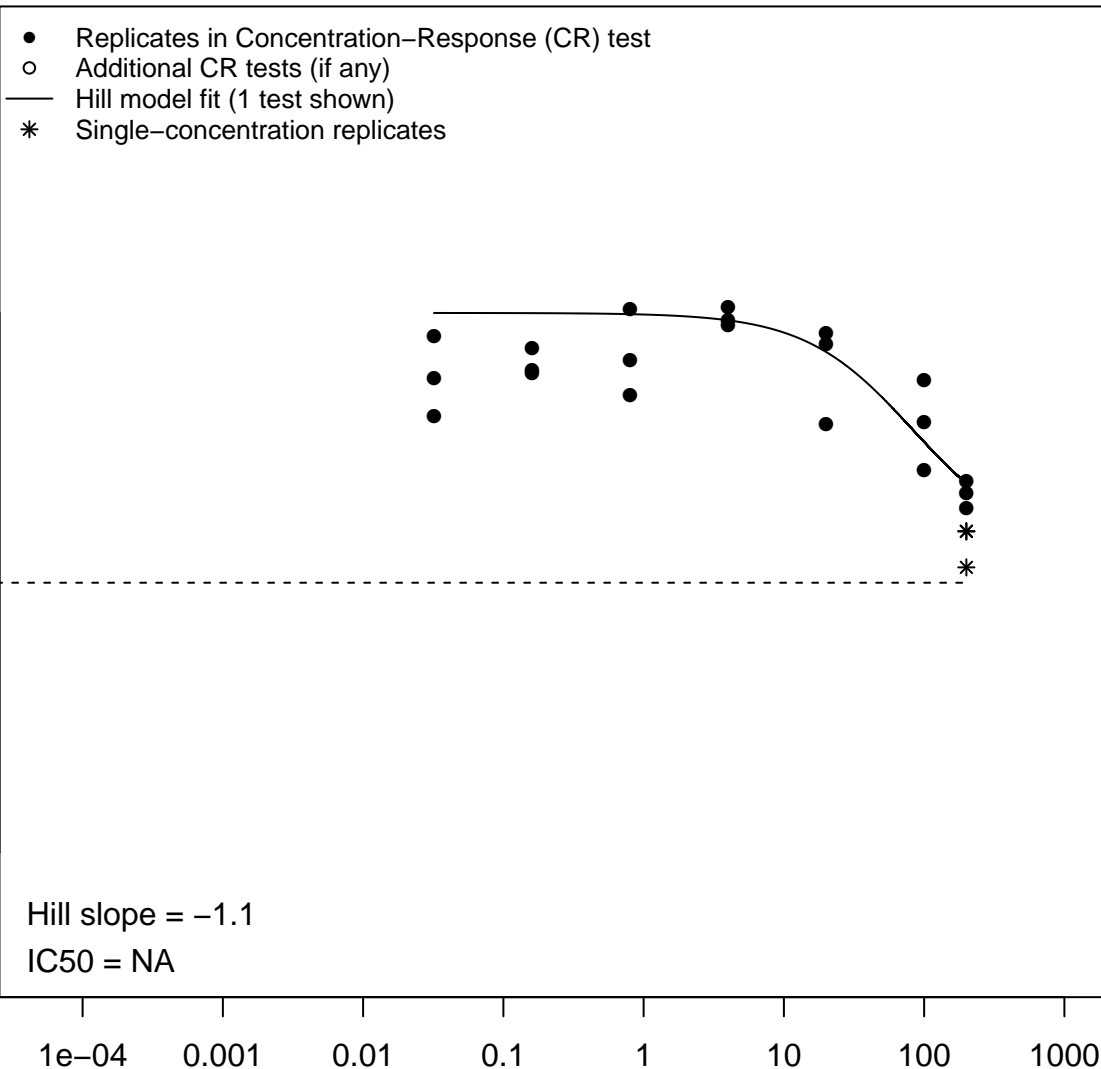
Octadecyl sulfate sodium salt

CASRN: 1120-04-3



Dichlone

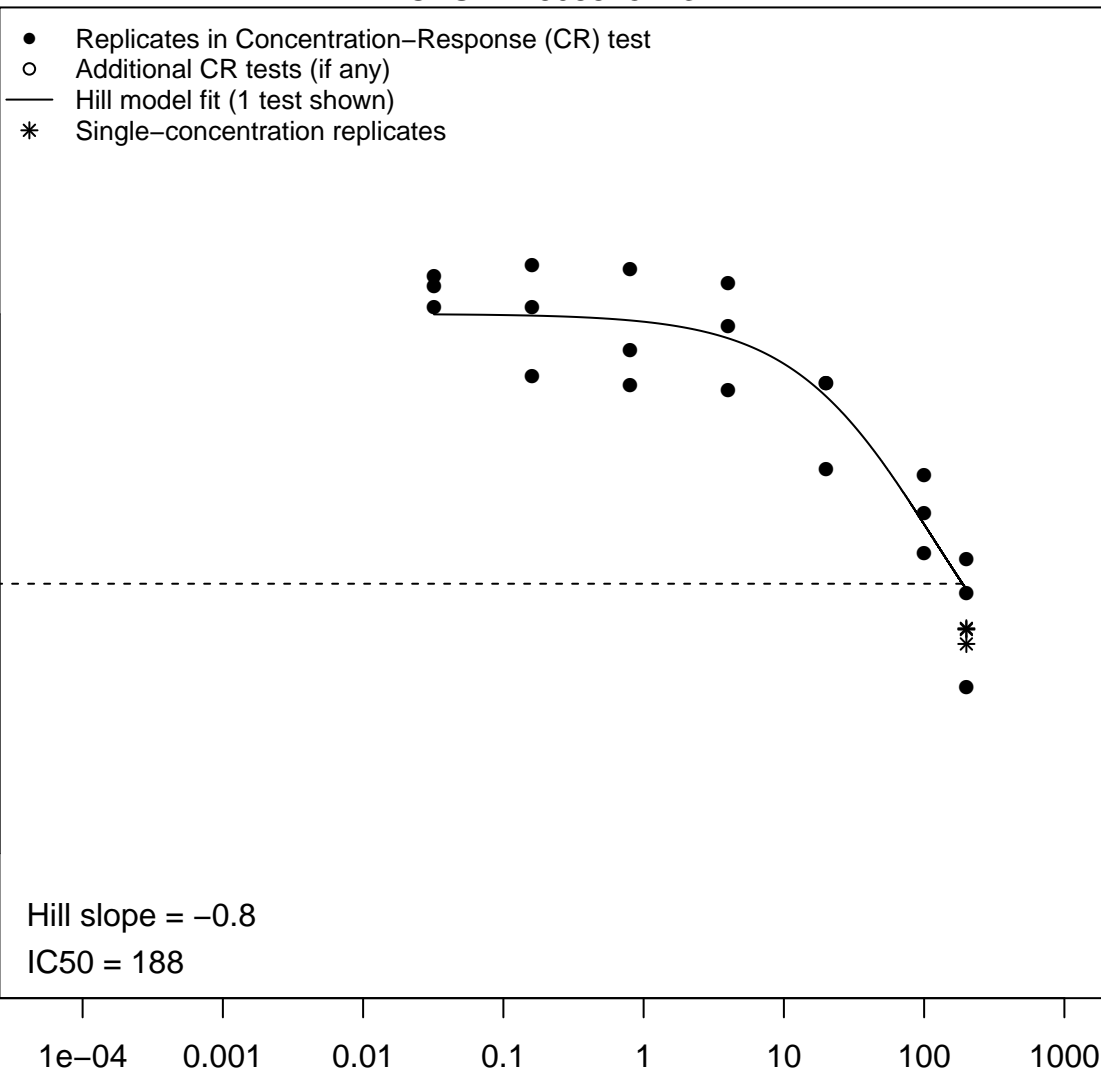
CASRN: 117-80-6



Concentration, µM

6-Hydroxy-2-naphthyl disulfide

CASRN: 6088-51-3



Concentration, µM

Linolenic acid

CASRN: 463-40-1

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100

50

0

Hill slope = NA

IC50 = NA

1e-04

0.001

0.01

0.1

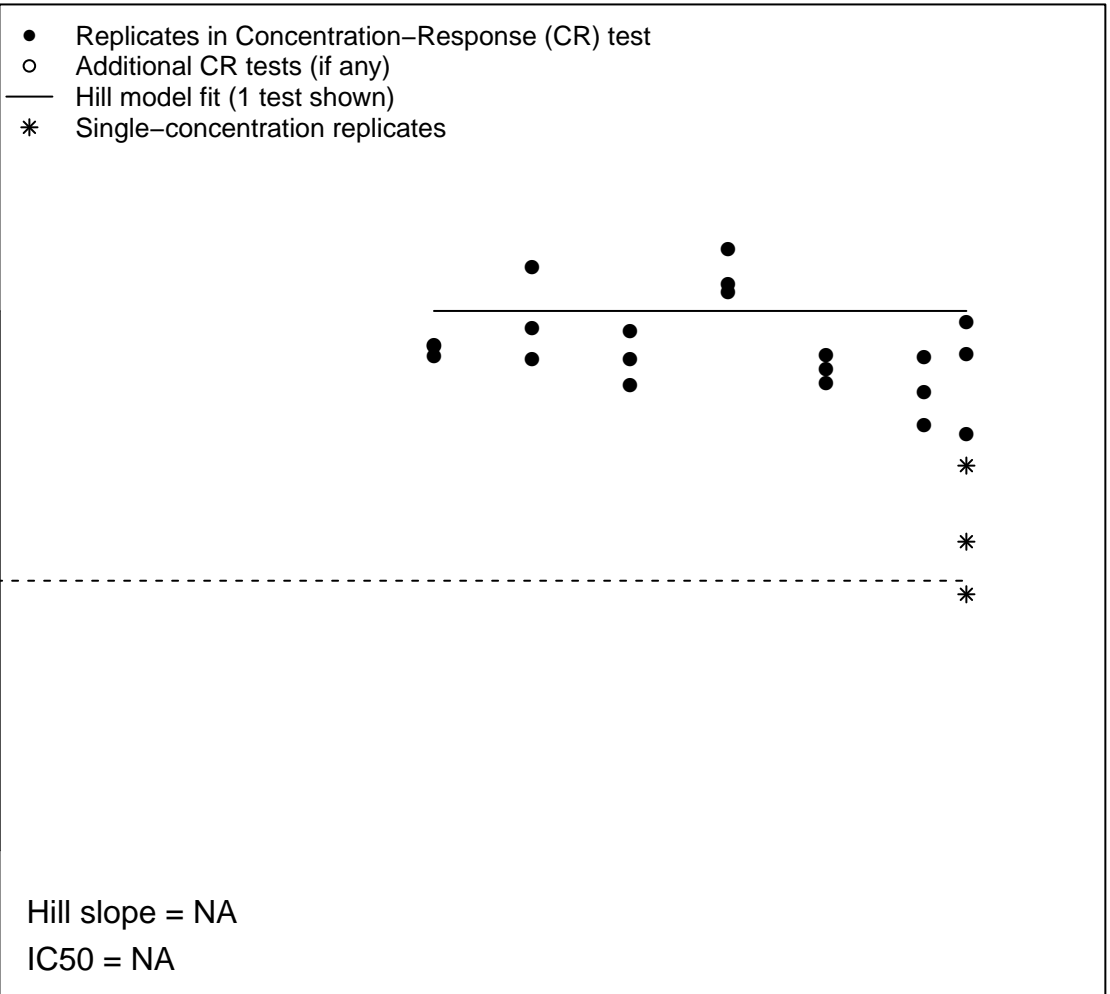
1

10

100

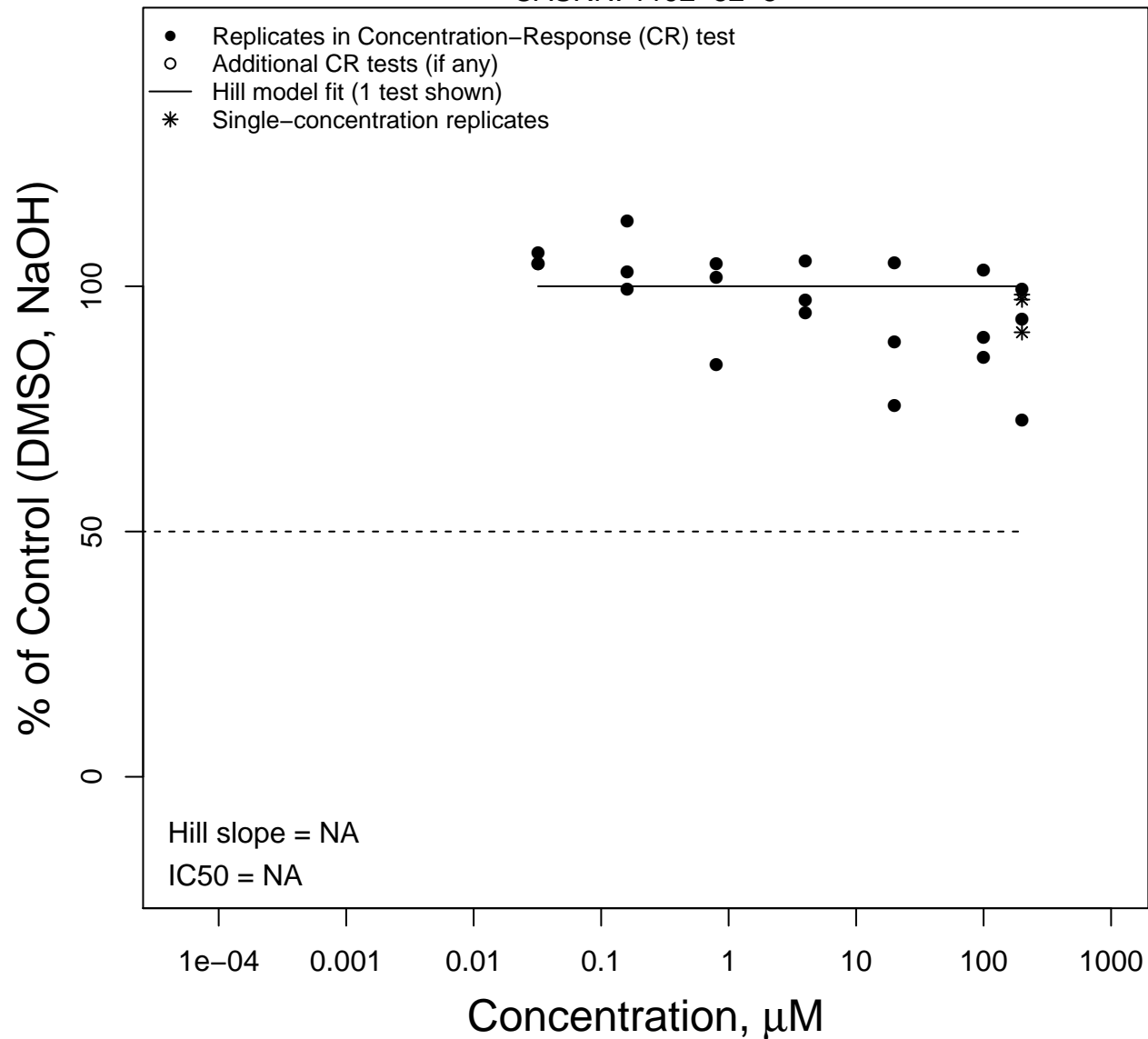
1000

Concentration, μM



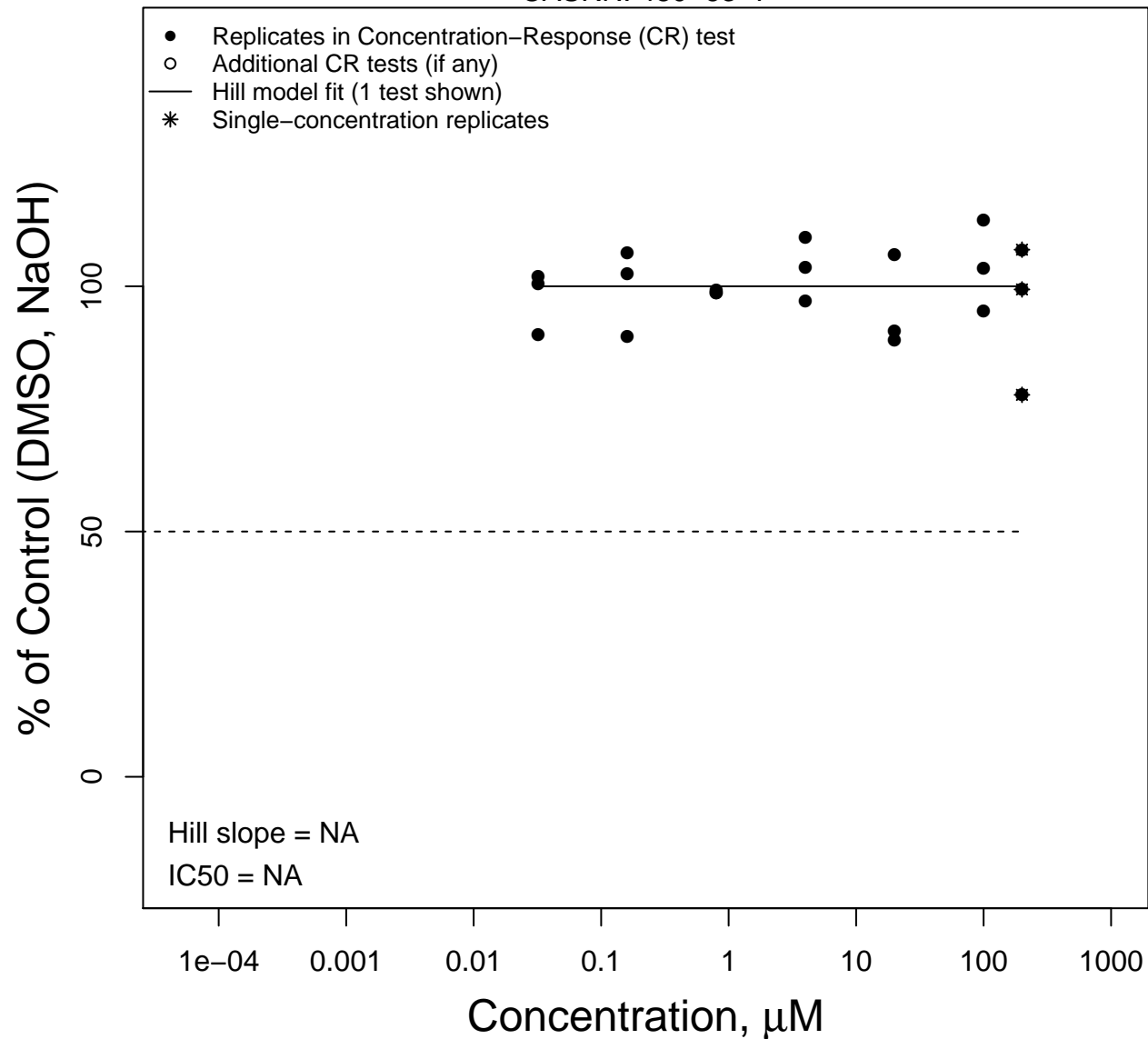
4,5-Dichloro-3H-1,2-dithiol-3-one

CASRN: 1192-52-5



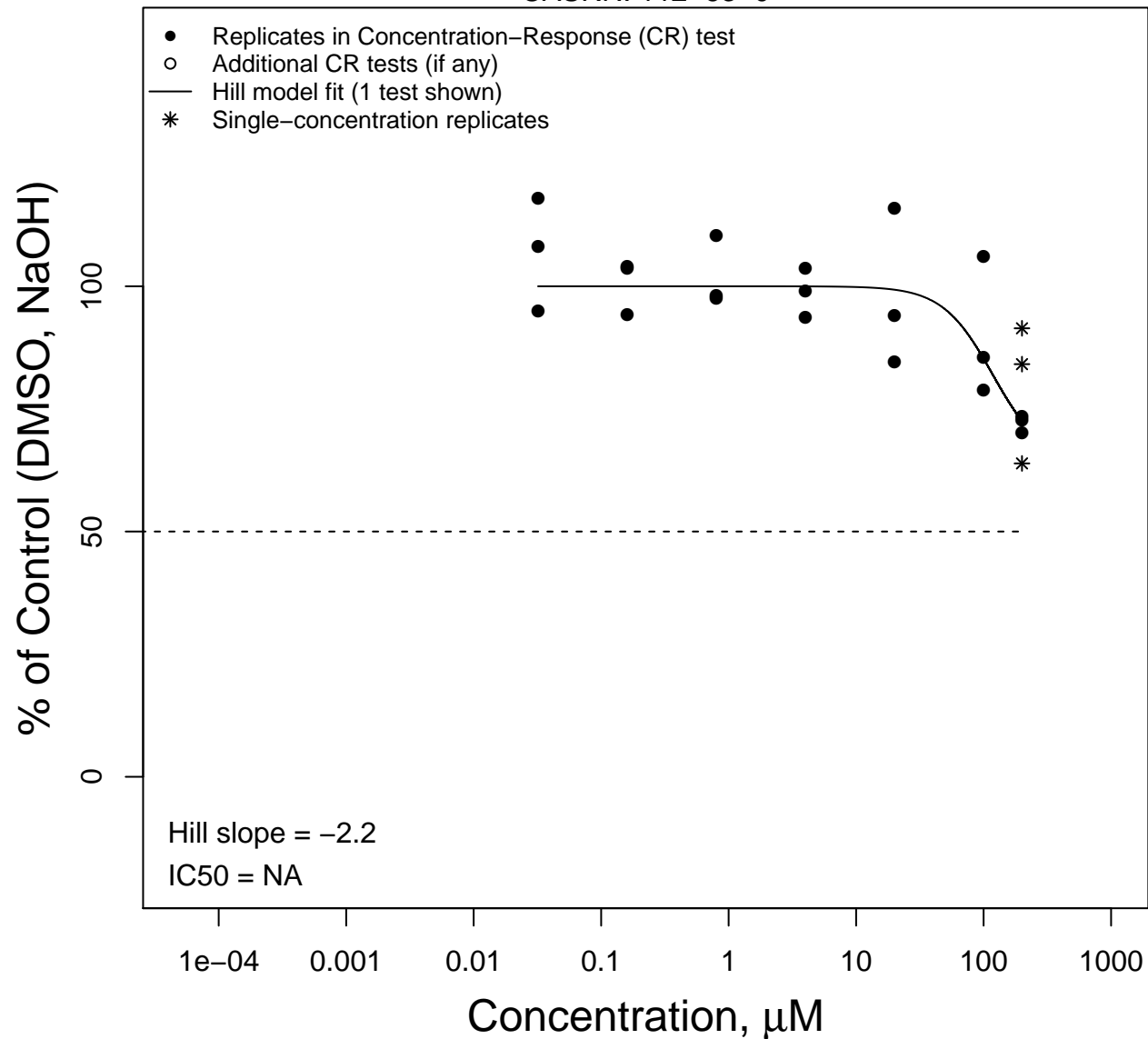
2,4,6-Trimethylbenzoic acid

CASRN: 480-63-7



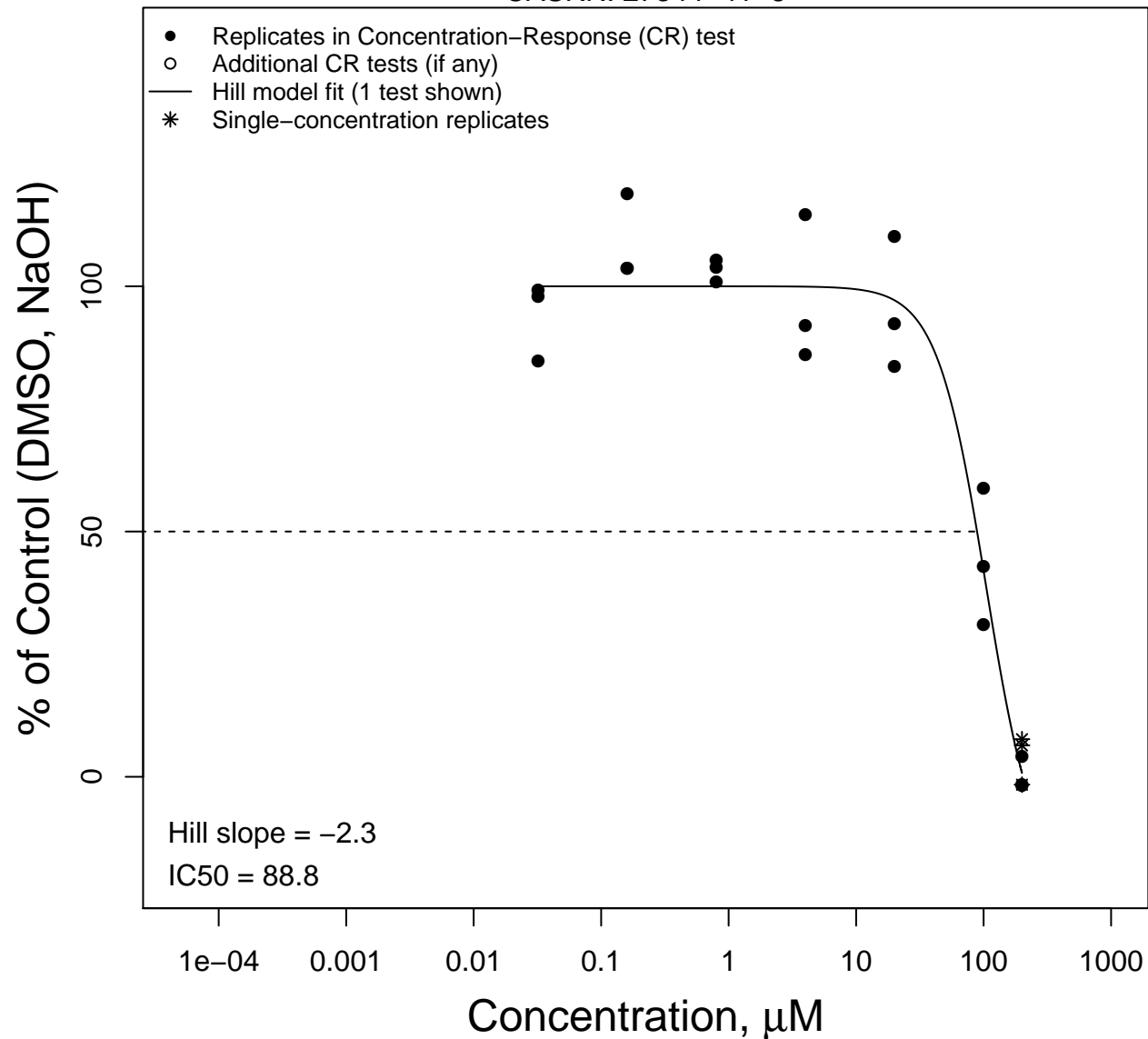
Methyl linoleate

CASRN: 112-63-0



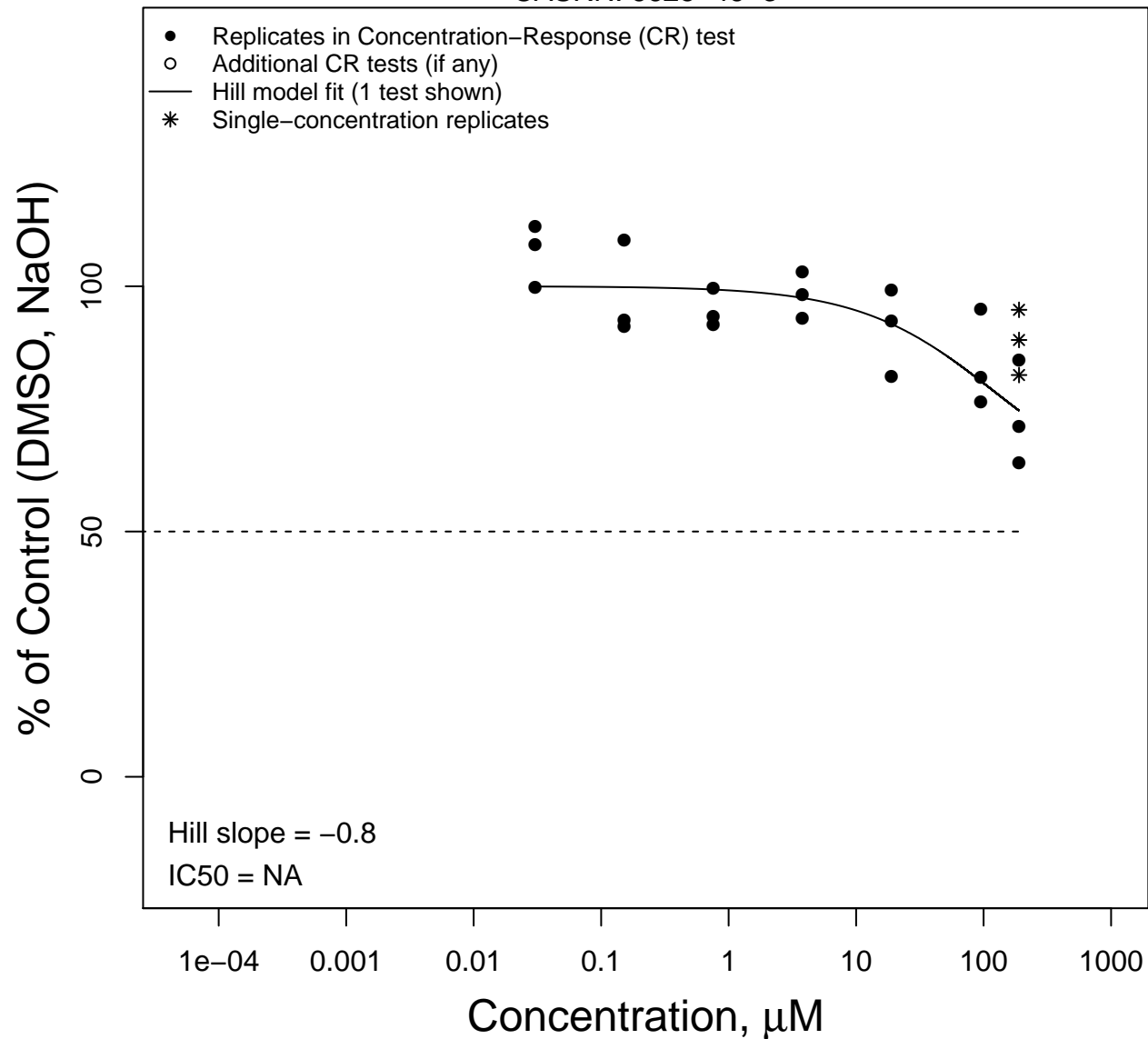
Disodium 4,4'-bis(2-sulfostyryl)biphenyl

CASRN: 27344-41-8



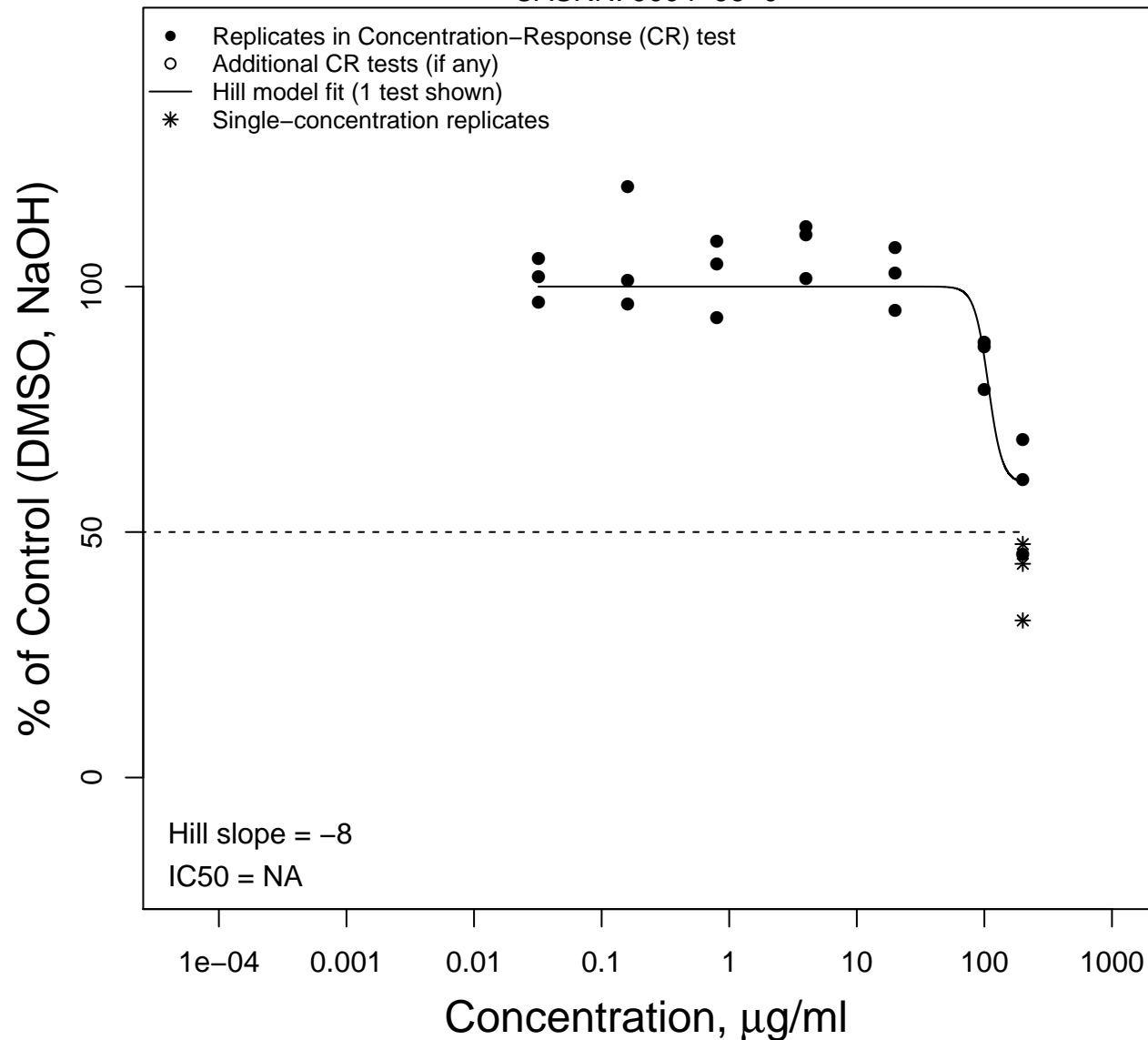
C.I. Acid Violet 12, disodium salt

CASRN: 6625-46-3



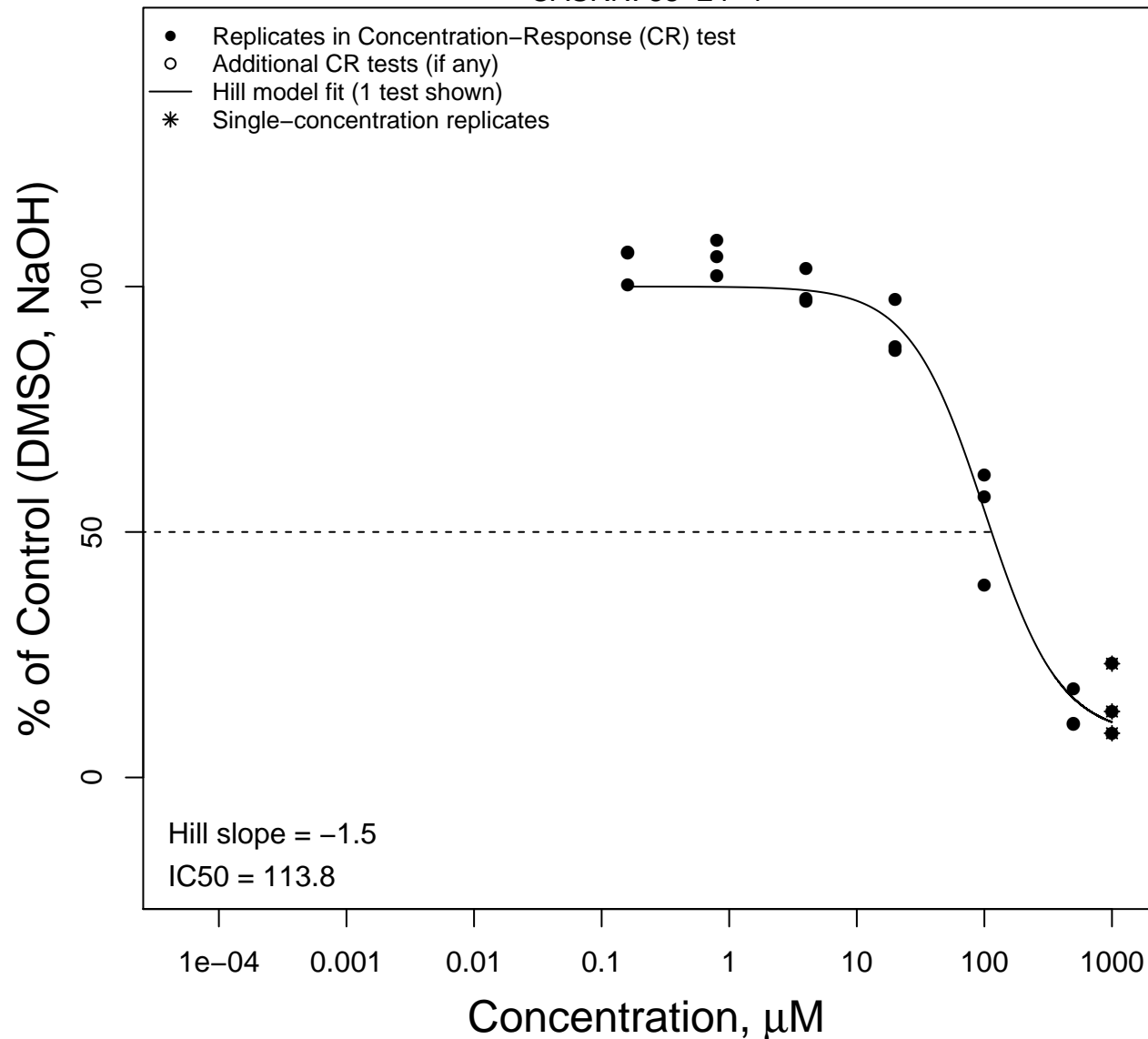
Polyoxyethylene monooleate

CASRN: 9004-96-0



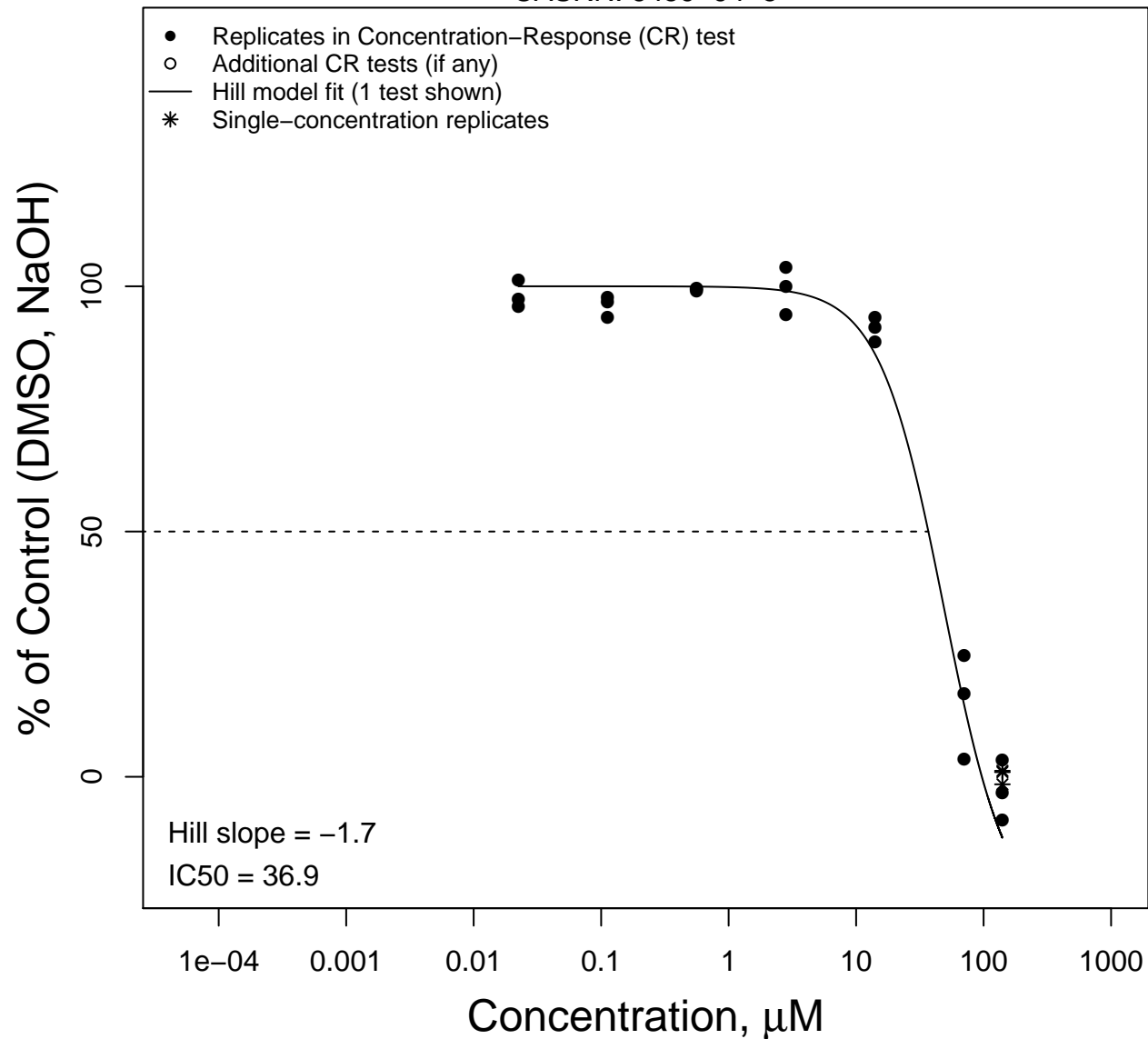
2,2'-Methylenebis(ethyl-6-tert-butylphenol)

CASRN: 88-24-4



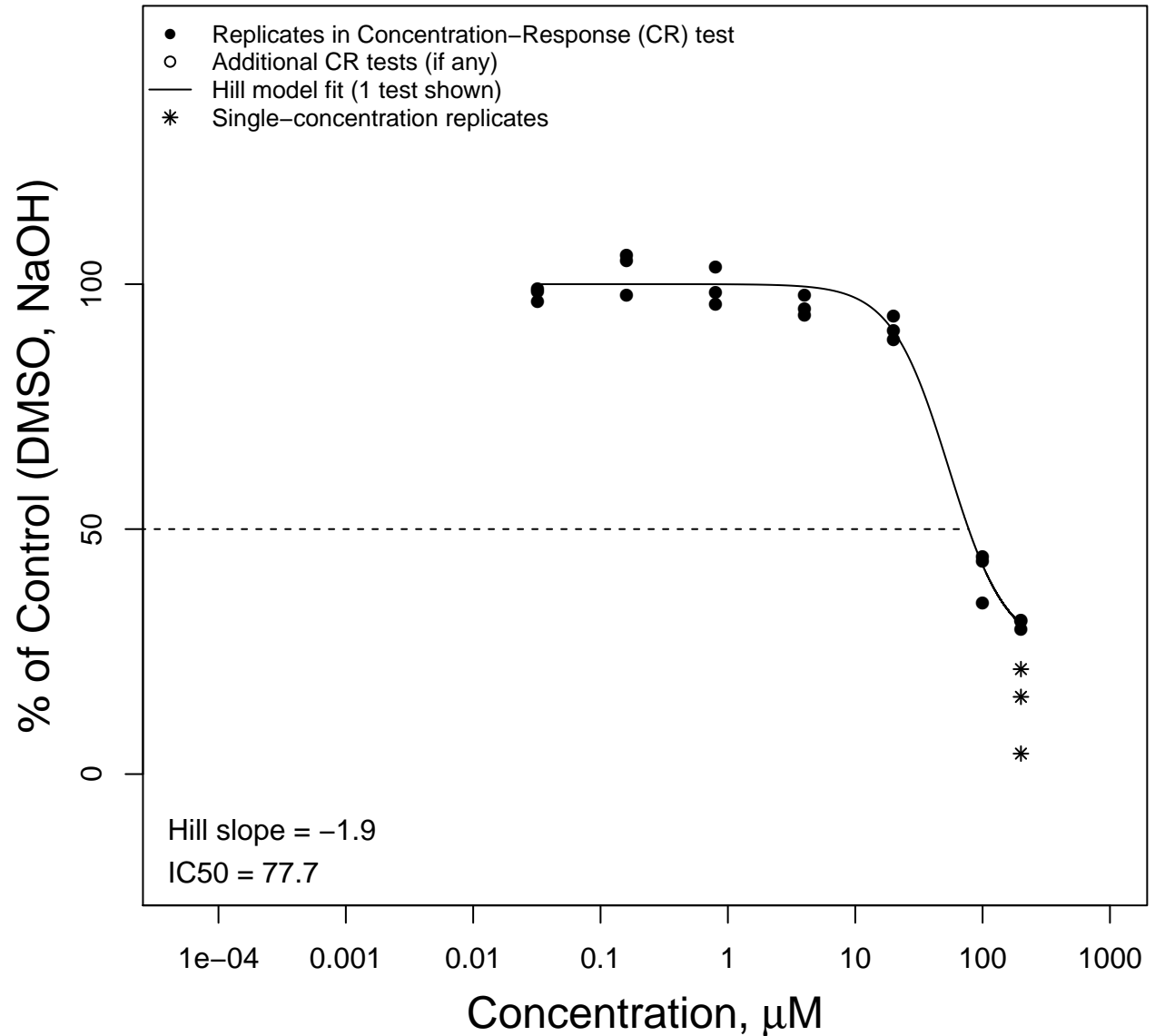
C.I. Acid Red 114

CASRN: 6459-94-5



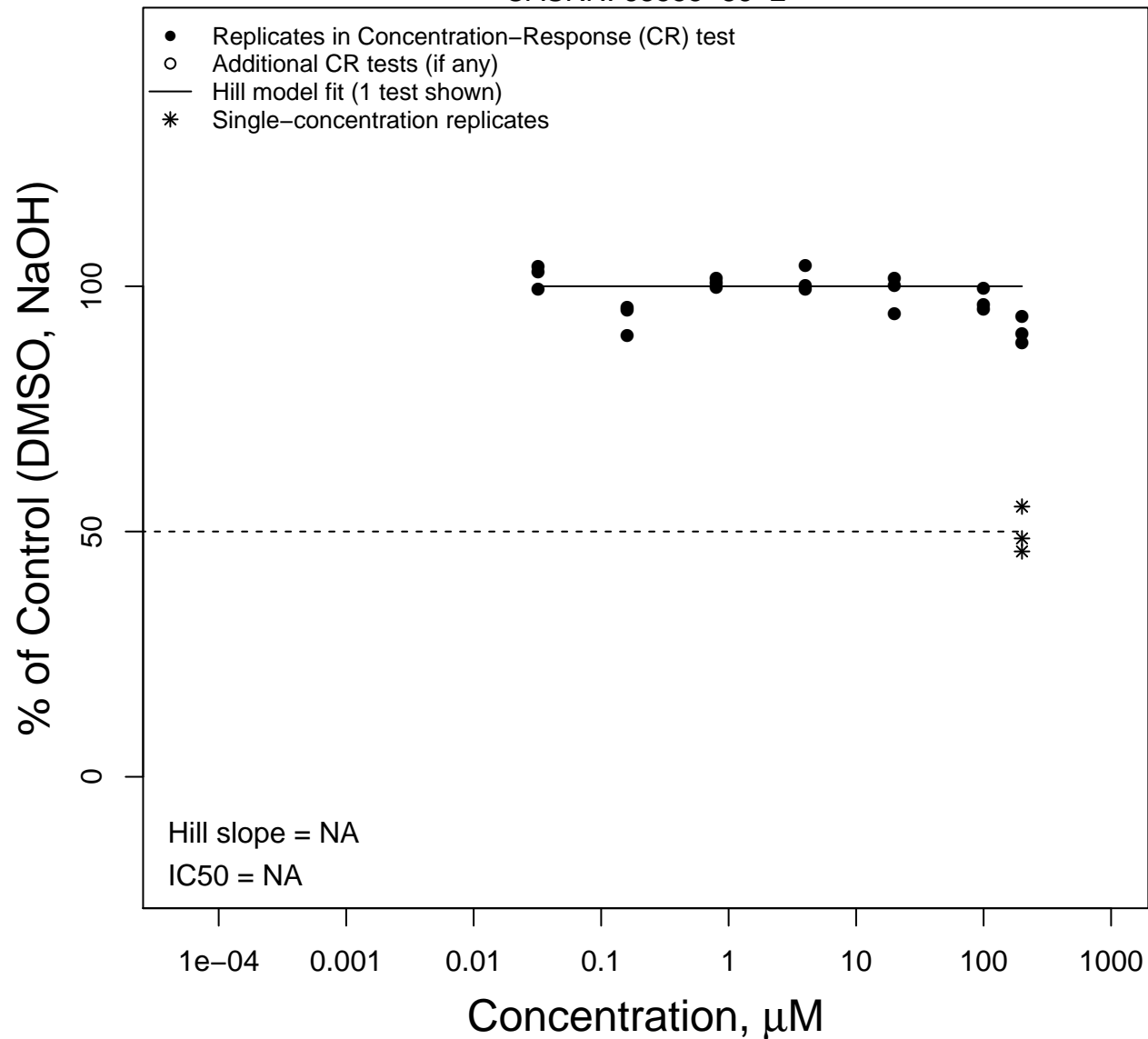
Chlorhexidine diacetate

CASRN: 56-95-1



Acid Orange 156

CASRN: 68555-86-2



Riboflavin

CASRN: 83-88-5

- Replicates in Concentration-Response (CR) test
- Additional CR tests (if any)
- Hill model fit (1 test shown)
- * Single-concentration replicates

% of Control (DMSO, NaOH)

100

50

0

Hill slope = -1.9

IC50 = NA

1e-04

0.001

0.01

0.1

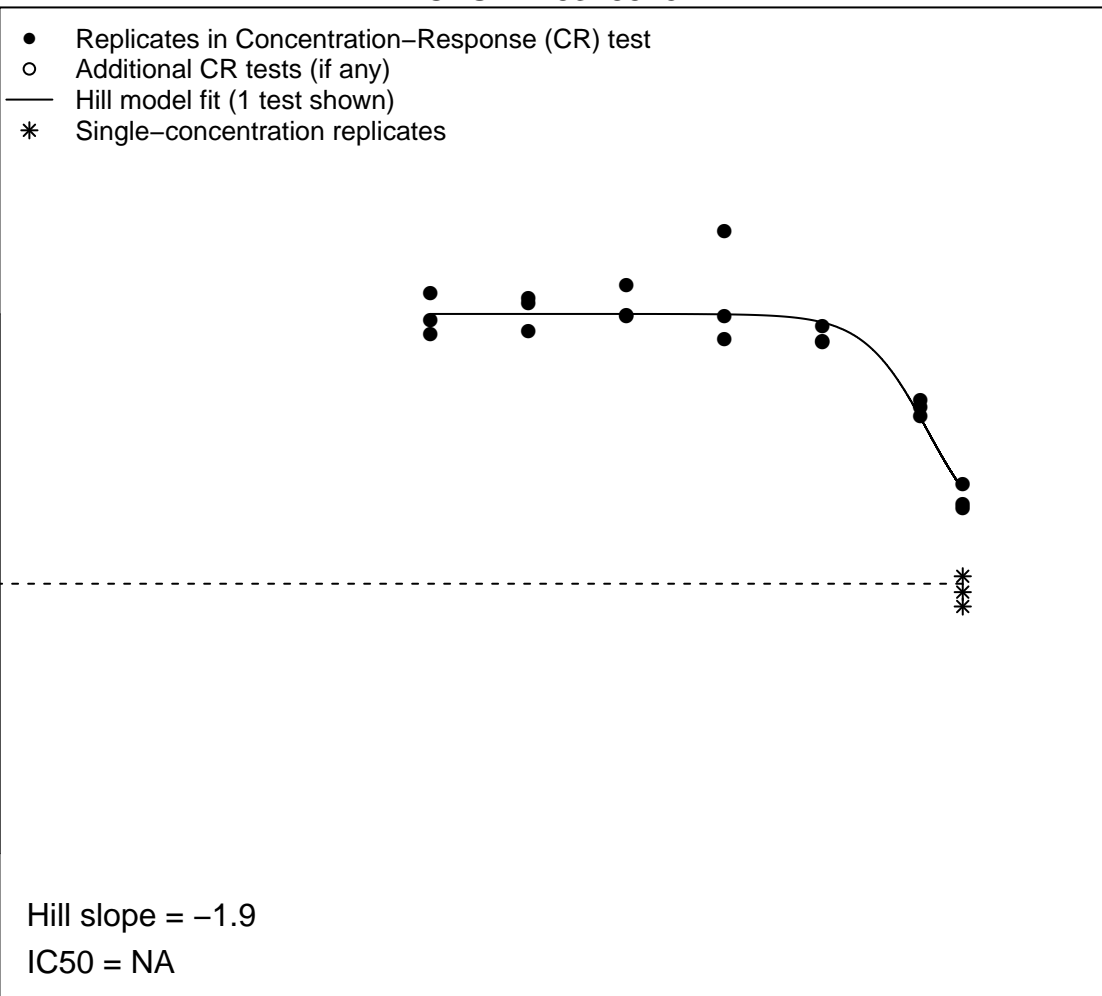
1

10

100

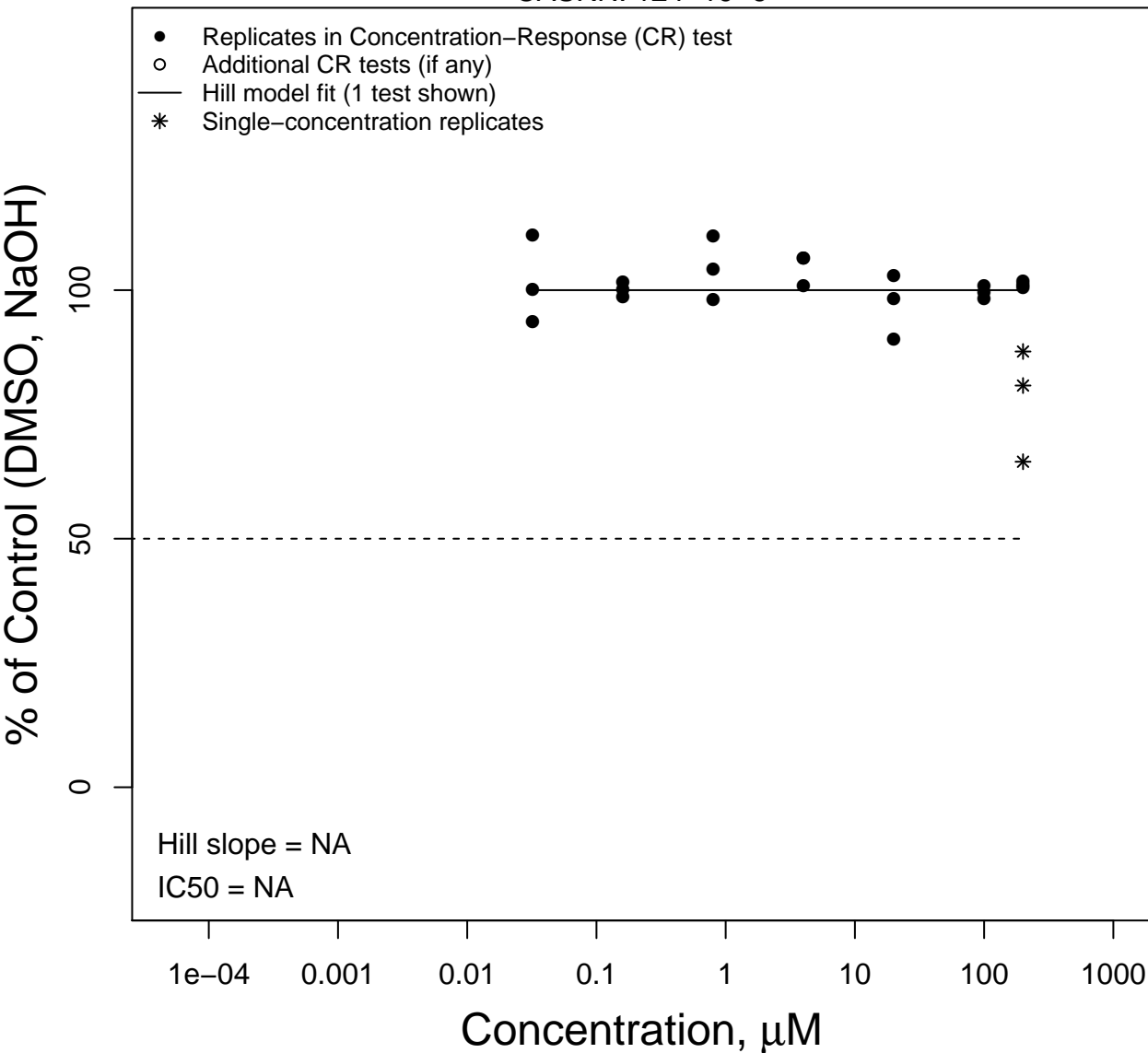
1000

Concentration, μM



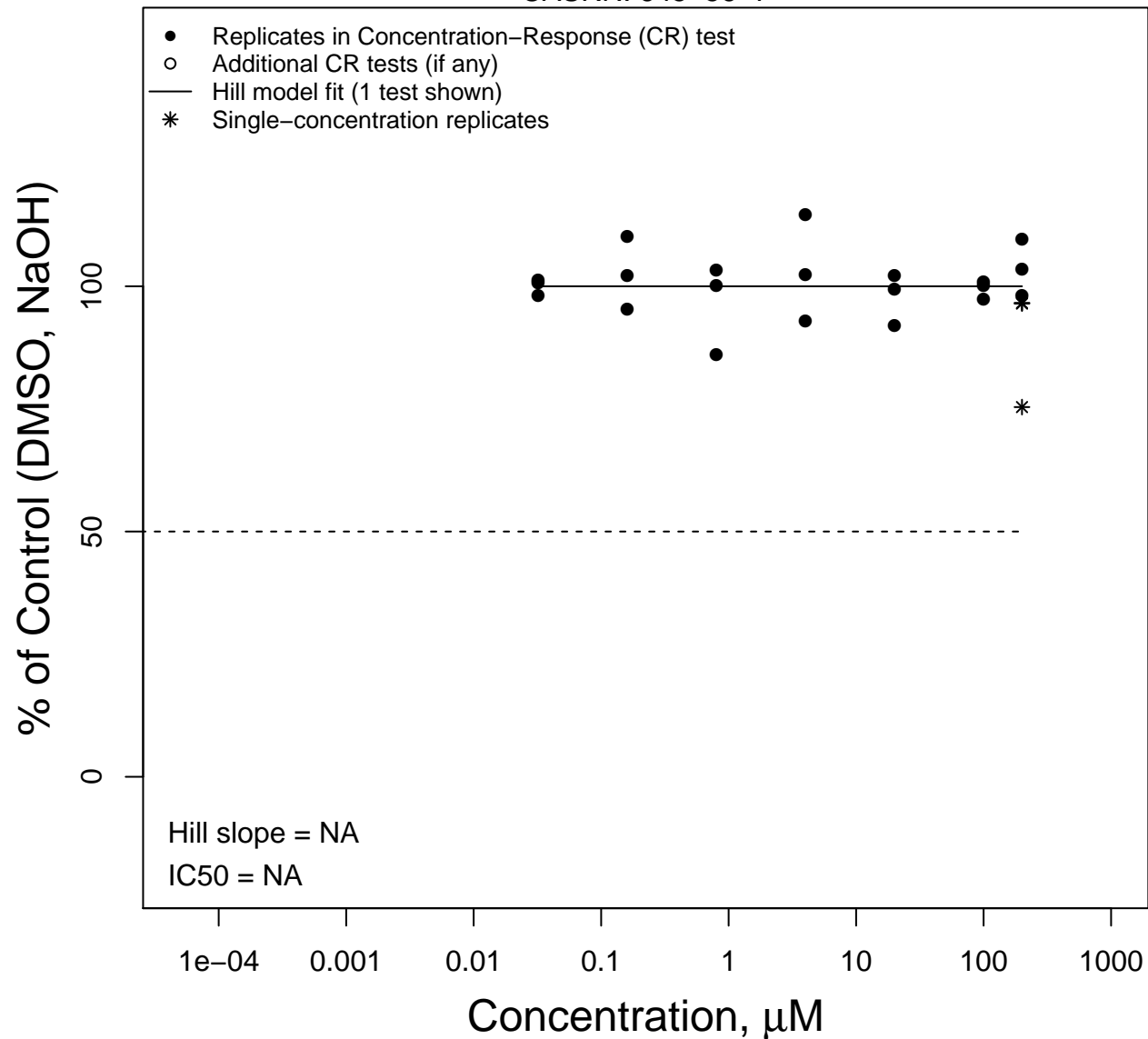
Nonanal

CASRN: 124-19-6



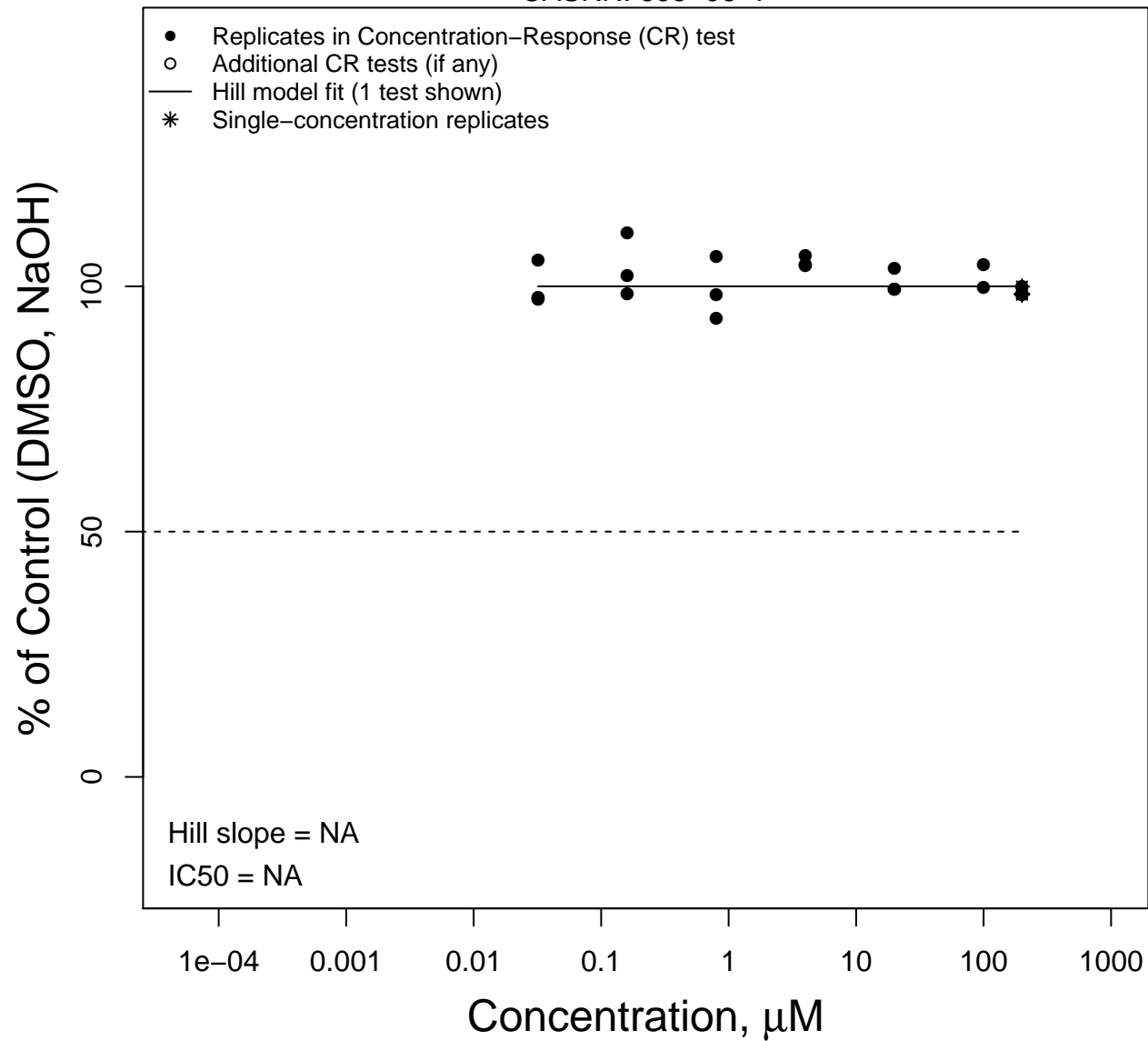
4-Propylphenol

CASRN: 645-56-7



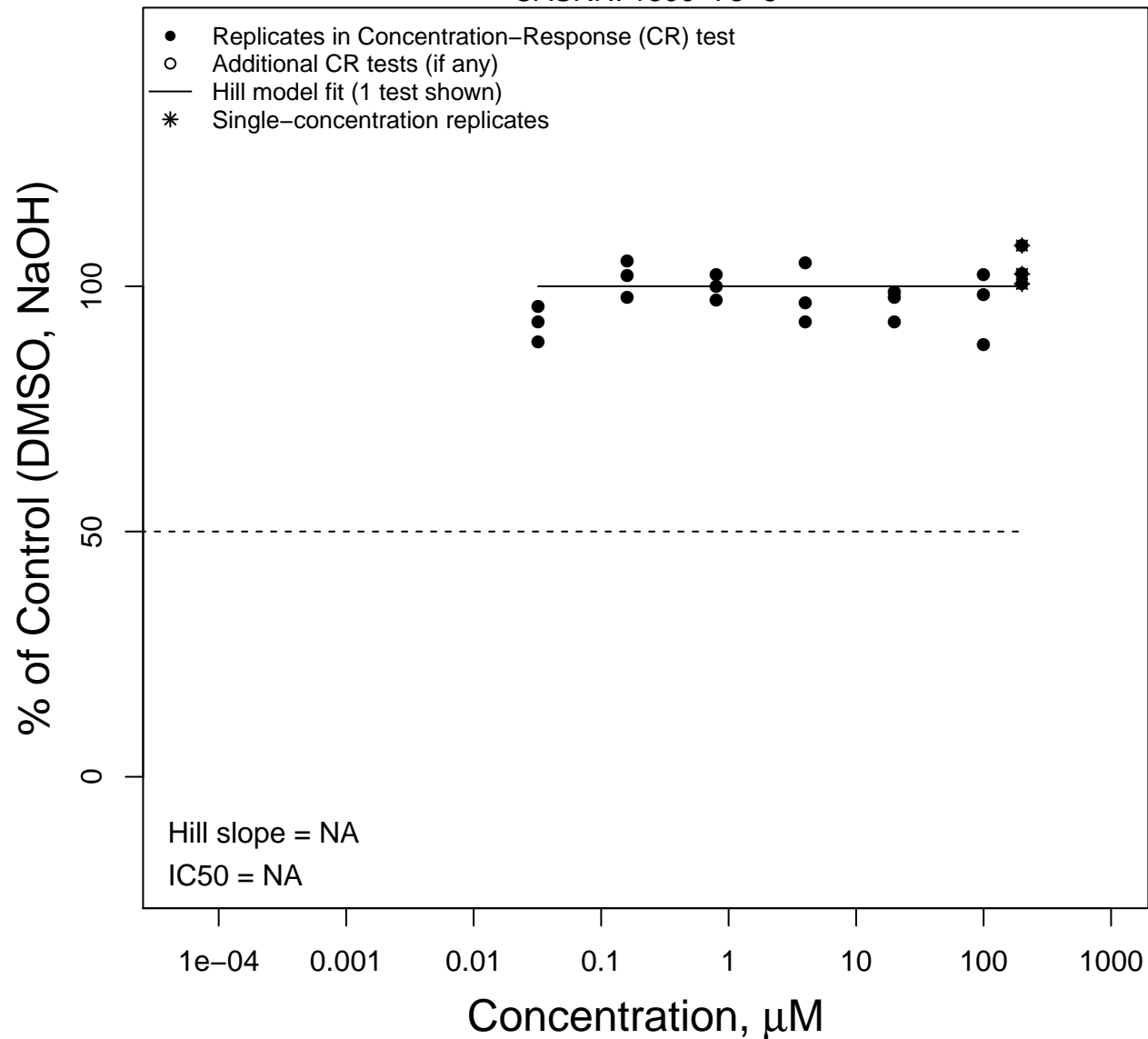
gamma-Caprolactone

CASRN: 695-06-7



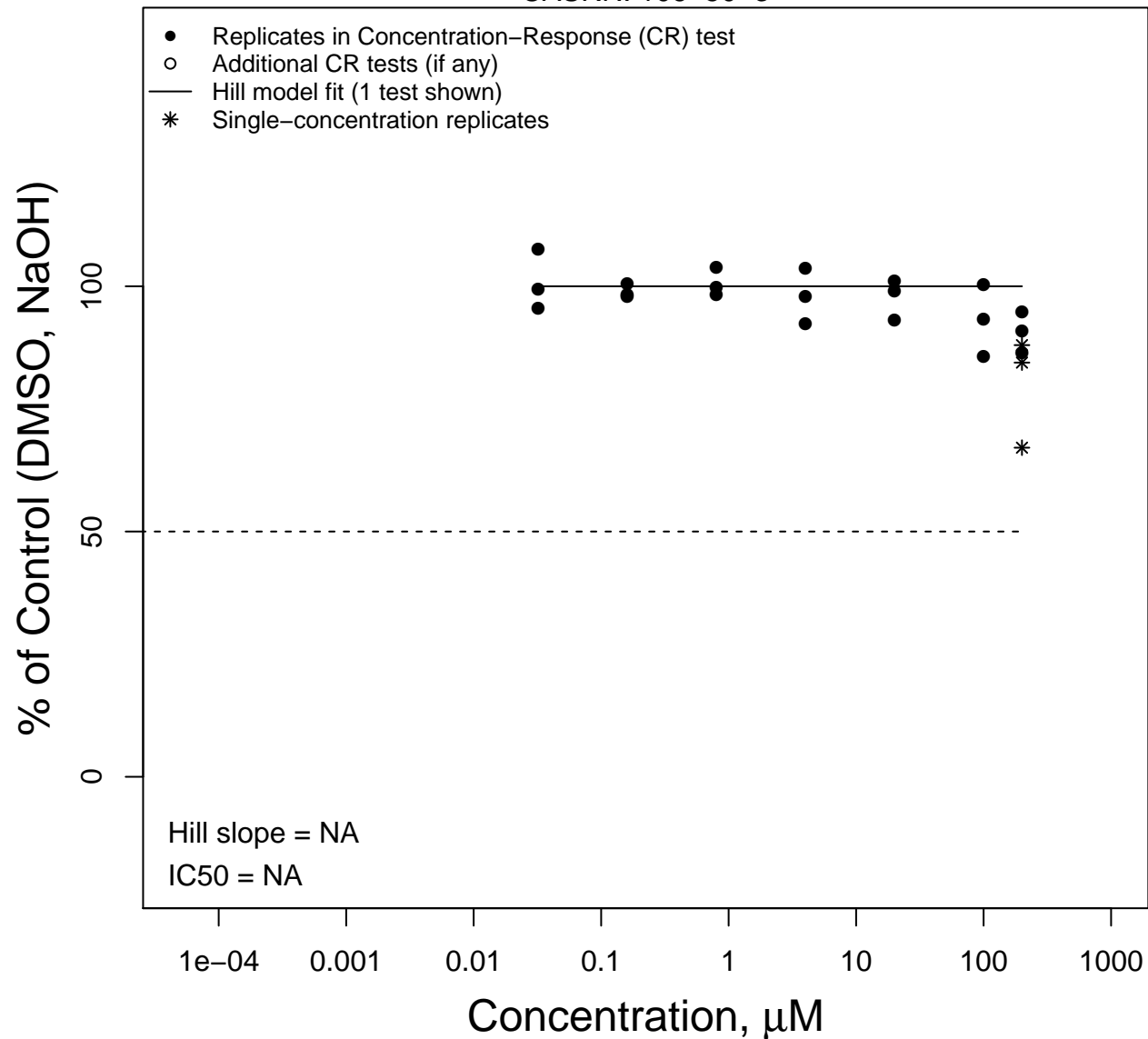
Dimethylaniline

CASRN: 1300-73-8



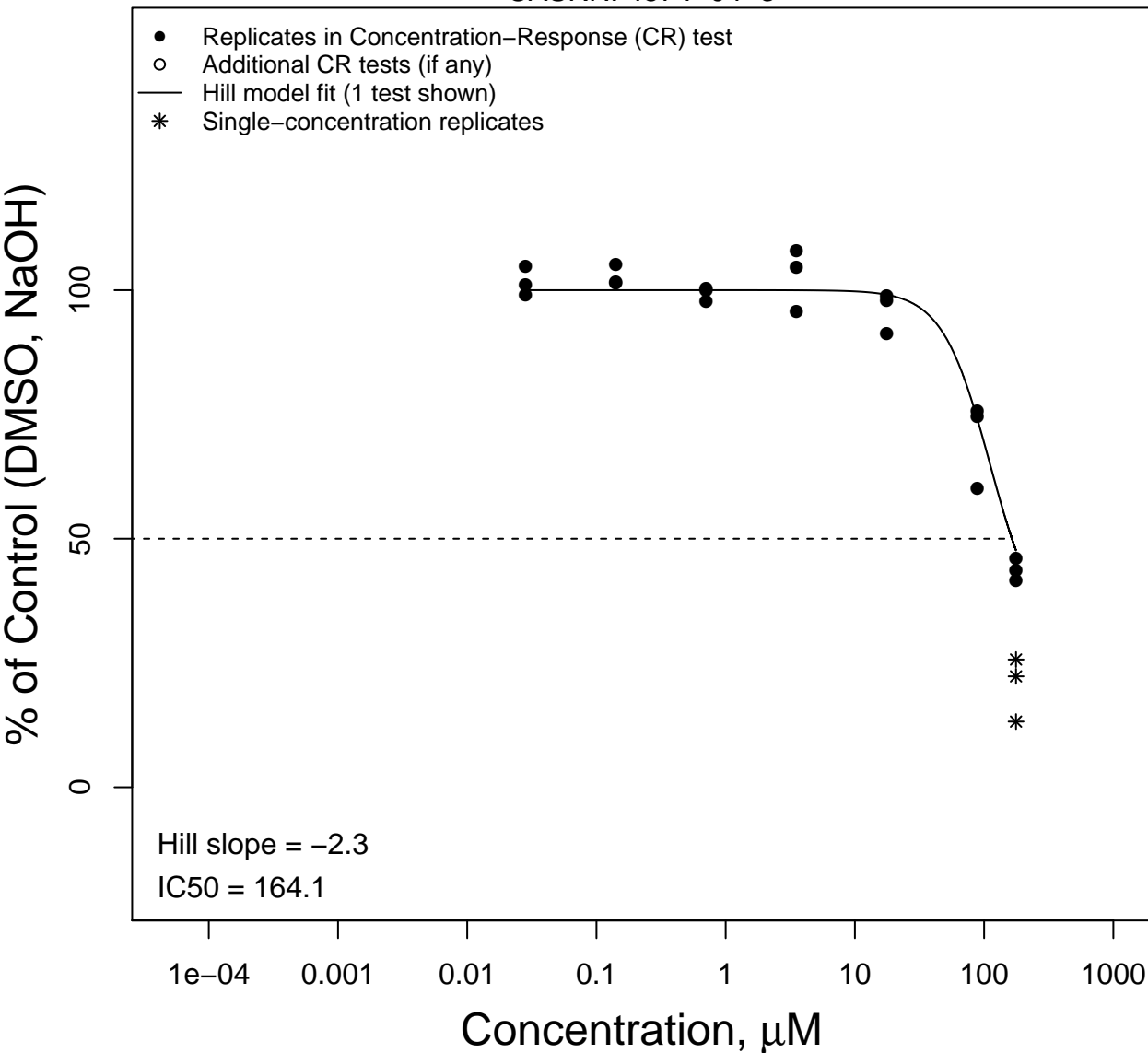
1,4-Benzenediamine

CASRN: 106-50-3



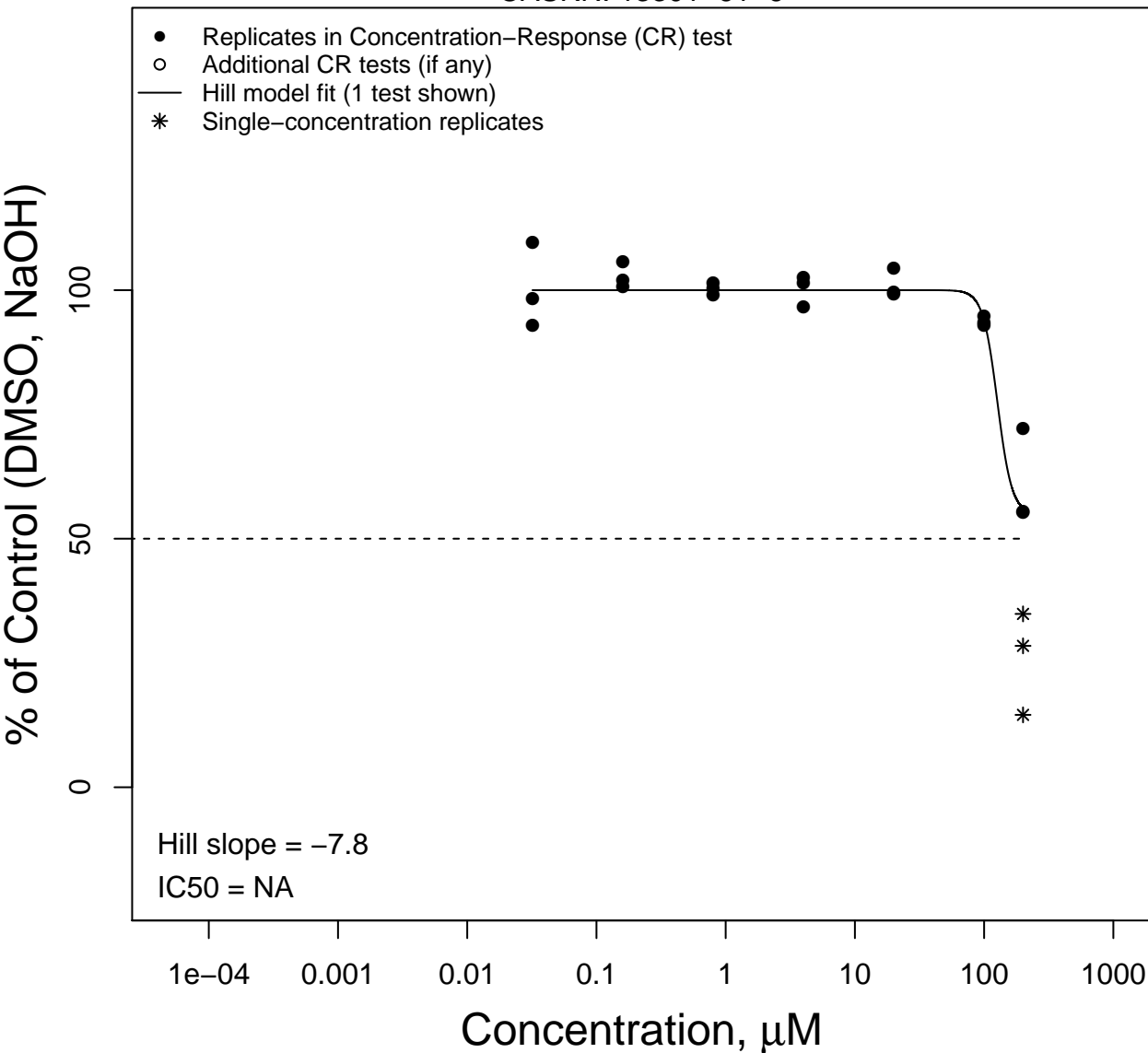
Myristyltrimethylammonium chloride N,N,N-Trimethyltetradecan-1-aminium chloride

CASRN: 4574-04-3



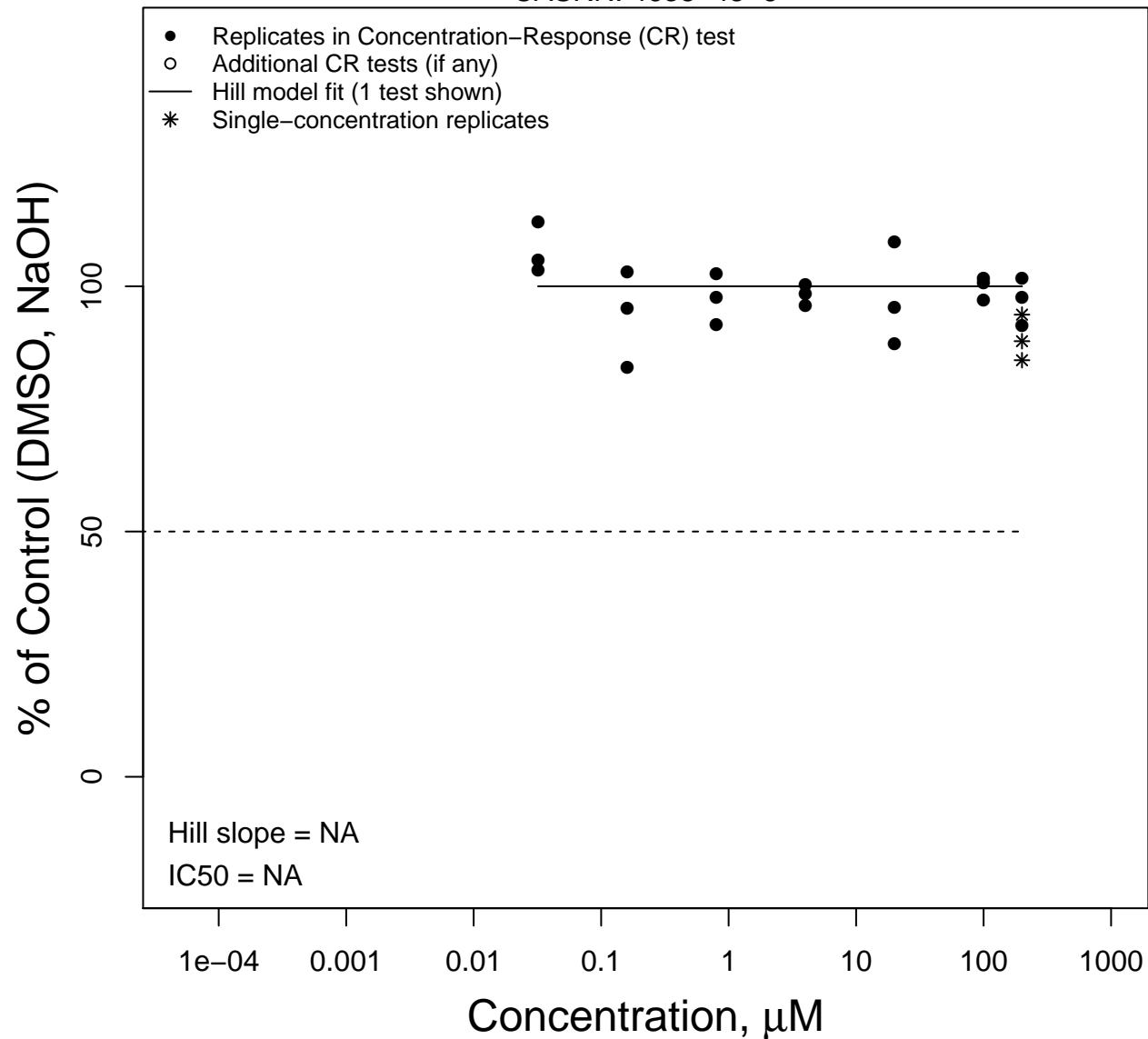
C.I. Disperse Orange 37

CASRN: 13301-61-6



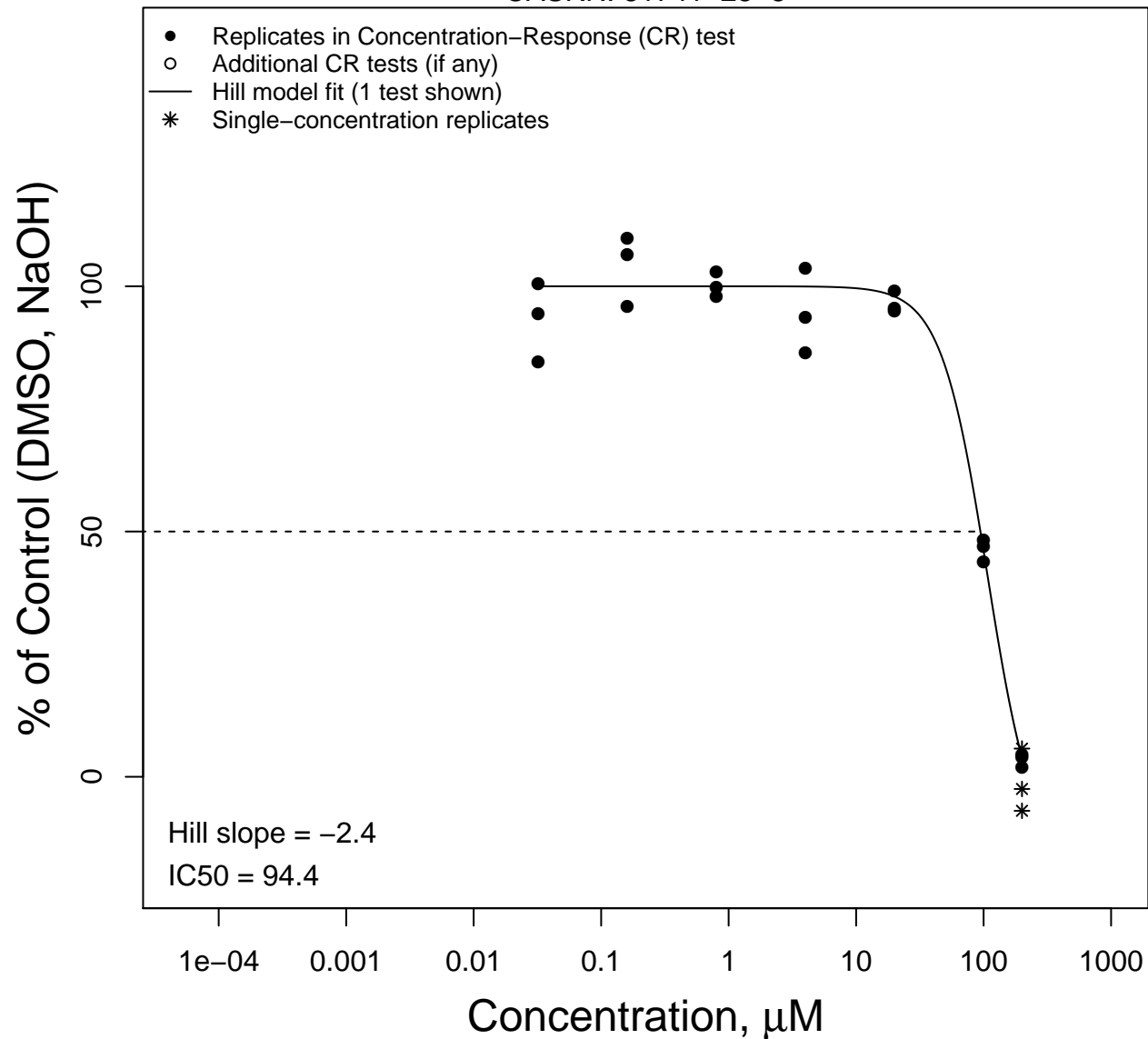
5-Chlorosalicylanilide

CASRN: 4638-48-6



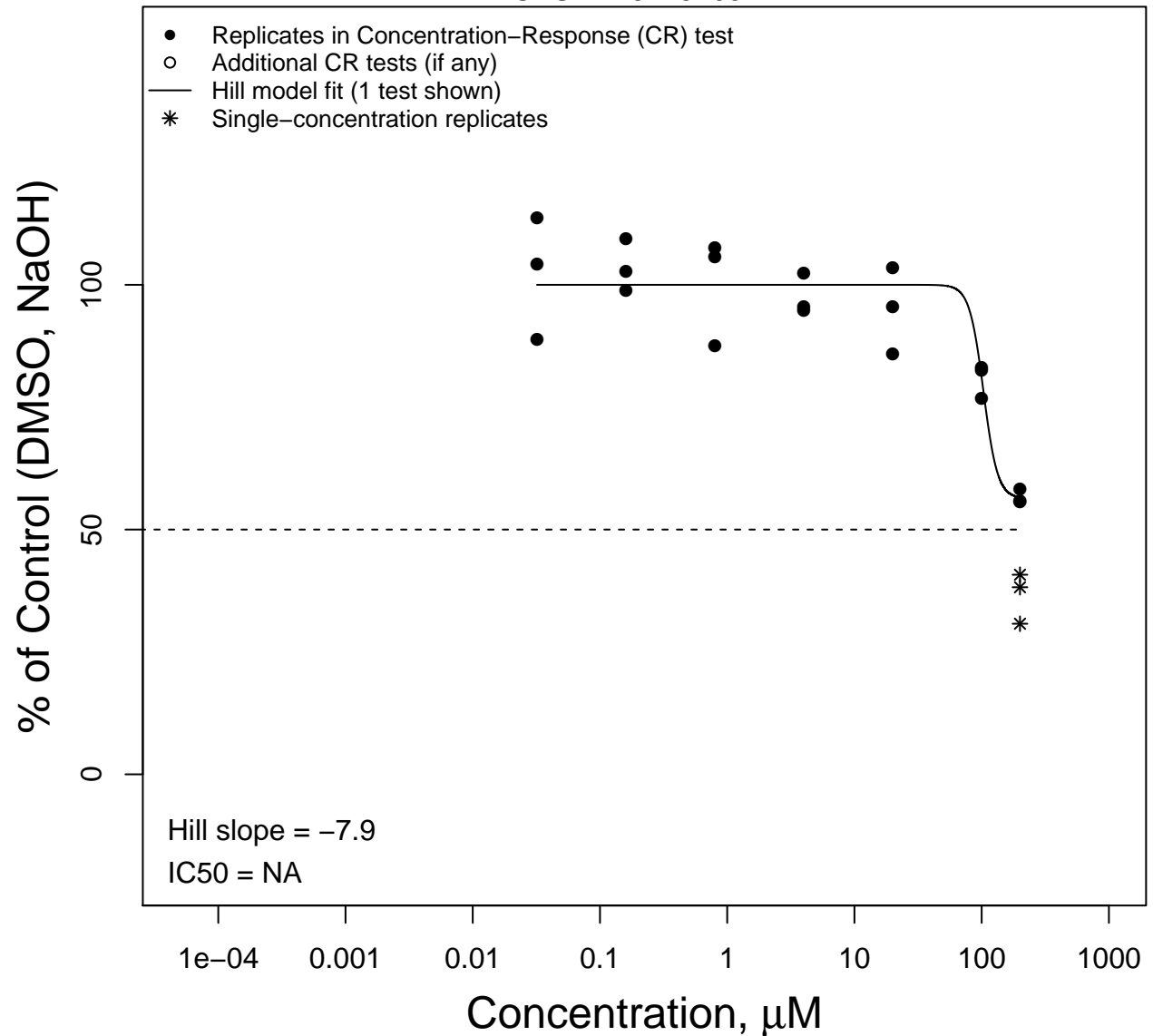
Tributyltetradecylphosphonium chloride

CASRN: 81741-28-8



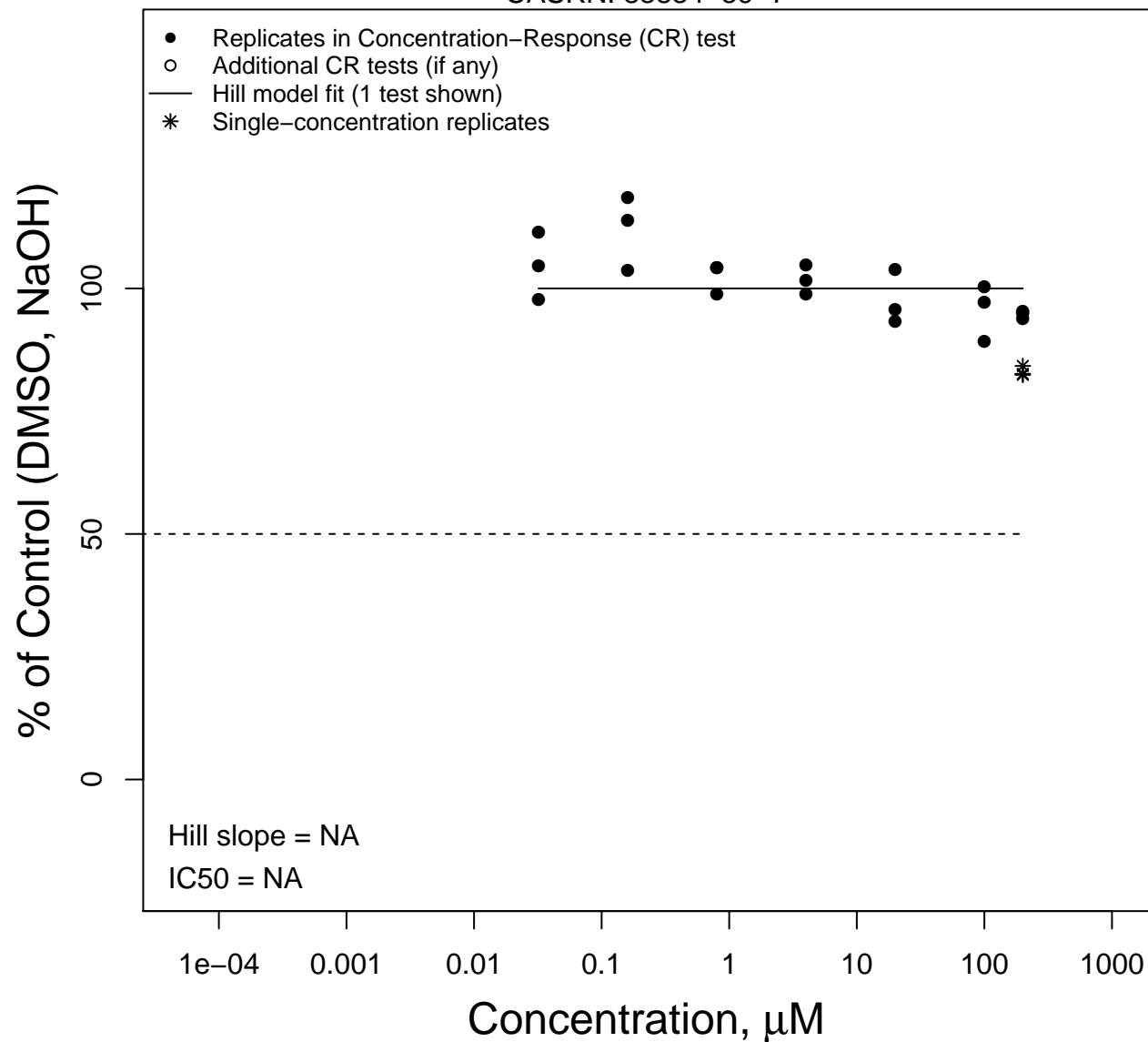
Sodium 4-octylbenzenesulfonate

CASRN: 6149-03-7



2-Ethylhexyl trans-4-methoxycinnamate

CASRN: 83834-59-7



Benzalkonium chloride

CASRN: 8001-54-5

