

Supporting Information

Screening the ToxCast Phase 1, Phase 2, and e1k Chemical Libraries for Inhibitors of Iodothyronine Deiodinases

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Supplemental Table 1. Description of the final assay conditions for iodotyrosine deiodinase enzyme inhibition assays. All incubations were three hours at 37 °C in a volume of 120 µl.

HEPES = 4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid; DTT = Dithiothreitol; EDTA = Ethylenediaminetetraacetic acid; DMSO = Dimethyl sulfoxide; rT3 = 3,3',5'-triiodo-L-thyronine (reverse T3); T4 = Thyroxine; T3 = Triiodothyronine; 3,3'-T2 = 3,3'-Diiodo-L-thyronine (T2).

Enzyme	Cell Lysate Protein^a	Substrate	Products	pH^b	Common Components
Deiodinase Type 1 (DIO1)	10 µg	10 µM rT3	3,3'-T2 and Iodide	7.0	0.1 M HEPES 40 mM DTT 1 mM EDTA 1% DMSO
Deiodinase Type 2 (DIO2)	20 µg	5 µM T4	T3 and Iodide	7.0	0.1 M HEPES 40 mM DTT 1 mM EDTA 1% DMSO
Deiodinase Type 3 (DIO3)	1 µg	5 µM T3	3,3'-T2 and Iodide	8.0	0.1 M HEPES 40 DTT mM 1 mM EDTA 1% DMSO

^a Based on optimum iodide release for Sandell-Kolthoff reaction; specific activity of enzymes approximated at 9, 5, and 90 pmoles iodide/h/µg of protein for DIO1, DIO2, and DIO3, respectively.

^b Selected based on optimum pH and reported assay conditions in previous studies (Hornung et al., 2018; Renko et al., 2015).

Supplemental Table 2. Model inhibitor (xanthohumol) concentration-response curve and assay performance metrics for the two test plates used in assay development for deiodinase type 2 (DIO2) and deiodinase type 3 (DIO3).

Enzyme	Plate	Xanthohumol			DMSO-MAD ^c median	Z' factor ^d	
		IC50 ^a , μM	Hill slope ^a	200 μM-MAD ^b median		mean	SD
DIO2	Test Plate 1	0.40	-0.82	3.40	1.83	0.821	0.085
DIO2	Test Plate 2	1.10	-0.98	6.88	1.89	0.727	0.052
DIO3	Test Plate 1	0.21	-0.78	3.36	2.01	0.757	0.060
DIO3	Test Plate 2	0.39	-0.91	2.04	1.03	0.886	0.019

^a IC50 and Hill slope from four-parameter logistic model was calculated from the three replicate runs of each test plate.

^b 200 μM-MAD is the platewise positive control median absolute deviation calculated from all the 200 μM wells of the model inhibitor in each of the replicated assay plates.

^c DMSO-MAD is the platewise median absolute deviation calculated from all the DMSO wells in each of the replicated assay plates.

^d Z' factor is a measure of assay quality, with value of >0.5 indicating good separation between the positive and negative controls.

Supplemental Table 3. Set of chemicals used in assay development and tested for inhibition of deiodinase type 2 (DIO2) in concentration-response mode with maximum concentration of 1 mM. Median percent inhibition (n=3 replicates) shown for 1 mM and 200 μ M, with absolute IC20, absolute IC50, and Hill slope for chemicals with Hill model as the best fit in ToxCast Pipeline (v1.0).

	Chemical	CASRN	Source ^a	Median % Inhibition		IC20 (μ M)	IC50 (μ M)	Hill slope
				1 mM	200 μ M			
Test Plate 1	Chlorophene	120-32-1	SA	101.4	77.8	86.7	134	-3.2
	Aurothioglucose hydrate ^b	12192-57-3	SA	-- ^c	77.5	2.8	28.9	-0.6
	2-Aminobenzothiazole	136-95-8	SA	-9.1	-4.7	NA ^d	NA	NA
	2-Mercaptobenzothiazole	149-30-4	FL	43.4	12.7	278	1,505	-1.4
	Oryzalin	19044-88-3	FL	-- ^e	82.5	103	142	-4.3
	Triclosan	3380-34-5	SA	96.8	93.6	25.1	47.0	-2.2
	5-Chloro-2-Mercaptobenzothiazole	5331-91-9	TCI	58.8	25.7	118	562	-1.1
	2-(Methylthio) Benzothiazole	615-22-5	TCI	14	-1.4	NA	NA	NA
	2-Hydroxybenzothiazole	934-34-9	SA	-0.5	-7.6	NA	NA	NA
Benzothiazole	95-16-9	SA	-9	-6.0	NA	NA	NA	
Test Plate 2	2-Aminobenzothiazole	136-95-8	SA	5.9	-0.7	NA	NA	NA
	Tert-Butylhydroquinone	1948-33-0	FL	30.3	7.1	426	NA	-1.3
	4-Pentylaniline	33228-44-3	SA	60.2	-0.7	714	901	-7.8
	2,2',4,4'-TBDPE	5436-43-1	CS	7.8	2.2	NA	NA	NA
	Methimazole	60-56-0	SA	1.1	-1.7	NA	NA	NA
	Bisphenol A	80-05-7	SA	60.3	7.1	324	751	-1.8
	Dibutylphthalate	84-74-2	SA	-2.4	-1.2	NA	NA	NA
	4-Bromobiphenyl	92-66-0	SA	0.4	9.5	NA	NA	NA
	2-Hydroxybenzothiazole	934-34-9	SA	2.6	-0.5	NA	NA	NA
	Benzotriazole	95-14-7	SA	4.9	4.7	NA	NA	NA
	Benzothiazole	95-16-9	SA	0.9	-4.9	NA	NA	NA

^a Chemicals used for development of the screening assay from stocks on hand at EPA/ORD/NHEERL/MED in Duluth, sources: SA = Sigma-Aldrich, FL=Honeywell Fluka, TCI=TCI America, CS=Chem Service Inc.

^b Previously reported to inhibit DIO1, DIO2, and DIO3 (Renko et al., 2015).

^c Not tested at 1 mM.

^d NA = not applicable. The chemical did not produce an inhibition curve or the curve did not reach 20% or 50% inhibition, and therefore an IC20 or IC50 could not be calculated.

^e Precipitate formation was observed and measured in 1 mM concentration.

Supplemental Table 4. Set of chemicals used in assay development and tested for inhibition of deiodinase type 3 (DIO3) in concentration-response mode with maximum concentration of 1 mM. Median percent inhibition (n=3 replicates) shown for 1 mM and 200 μ M, with absolute IC20, absolute IC50, and Hill slope for chemicals with Hill model as the best fit in ToxCast Pipeline (v1.0).

	Chemical	CASRN	Source ^a	Median % Inhibition		IC20 (μ M)	IC50 (μ M)	Hill slope
				1 mM	200 μ M			
Test Plate 1	Chlorophene	120-32-1	SA	99.9	79.2	126	159	-5.8
	Aurothioglucose hydrate ^b	12192-57-3	SA	-- ^c	107.8	1.1	6.8	-0.7
	2-Aminobenzothiazole	136-95-8	SA	0.5	0.8	NA ^d	NA	NA
	2-Mercaptobenzothiazole	149-30-4	FL	42.6	14.4	204	2,070	-1.0
	Oryzalin	19044-88-3	FL	-- ^e	25.0	181	NA	-5.8
	Triclosan	3380-34-5	SA	104.3	98.9	45.7	61.1	-4.7
	5-Chloro-2-Mercaptobenzothiazole	5331-91-9	TCI	74.1	29.8	131	375	-1.4
	2-(Methylthio) Benzothiazole	615-22-5	TCI	13.9	6.0	NA	NA	NA
	2-Hydroxybenzothiazole	934-34-9	SA	-1.6	0.6	NA	NA	NA
Benzothiazole	95-16-9	SA	1.7	-1.4	NA	NA	NA	
Test Plate 2	2-Aminobenzothiazole	136-95-8	SA	-2.3	-3.9	NA	NA	NA
	Tert-Butylhydroquinone	1948-33-0	FL	44.4	4.3	443	1,333	-2.5
	4-Pentylaniline	33228-44-3	SA	19.3	-3.0	1,008	NA	-8.0
	2,2',4,4'-TBDPE	5436-43-1	CS	5.0	1.2	NA	NA	NA
	Methimazole	60-56-0	SA	-7.6	-2.6	NA	NA	NA
	Bisphenol A	80-05-7	SA	32.9	-3.1	838	NA	-8.0
	Dibutylphthalate	84-74-2	SA	-0.2	-5.9	NA	NA	NA
	4-Bromobiphenyl	92-66-0	SA	-1.3	-5.7	NA	NA	NA
	2-Hydroxybenzothiazole	934-34-9	SA	-4.4	-3.8	NA	NA	NA
	Benzotriazole	95-14-7	SA	-7.1	-5.0	NA	NA	NA
	Benzothiazole	95-16-9	SA	-1.3	-3.2	NA	NA	NA

^a Chemicals used for development of the screening assay from stocks on hand at EPA/ORD/NHEERL/MED in Duluth, sources: SA = Sigma-Aldrich, FL=Honeywell Fluka, TCI=TCI America, CS=Chem Service Inc.

^b Previously reported to inhibit DIO1, DIO2, and DIO3 (Renko et al., 2015).

^c Not tested at 1 mM.

^d NA = not applicable. The chemical did not produce an inhibition curve or the curve did not reach 20% or 50% inhibition, and therefore an IC20 or IC50 could not be calculated.

^e Precipitate formation was observed and measured in 1 mM concentration.

Supplemental Table 5. 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
Diniconazole	83657-24-3	ph1v2	Abnormal time course of absorbance at 420 nm ^b
9-Phenanthrol	484-17-3	ph2	Interference, reaction without enzyme in DIO2 and DIO3
FD&C Blue No. 1	3844-45-9	ph2	Interference with Sandell-Kolthoff (SK) reaction
Isophorone diisocyanate	4098-71-9	ph2	Abnormal time course of absorbance at 420 nm ^b
Isopropyl triethanolamine titanate	36673-16-2	ph2	Abnormal time course of absorbance at 420 nm ^b
Reserpine	50-55-5	ph2	Abnormal time course of absorbance at 420 nm ^b
SSR150106	NOCAS_47362	ph2	Abnormal time course of absorbance at 420 nm ^b
3,5,3'-Triiodothyronine	6893-02-3	ph2	Contains free iodide or possibly being deiodinated by enzyme(s)
Amiodarone hydrochloride	19774-82-4	ph2	Contains free iodide or possibly being deiodinated by enzyme(s)
1H,1H,2H,2H-Perfluorooctyl iodide	2043-57-4	ph2	Contains free iodide or possibly being deiodinated by enzyme(s)
Tetrac	67-30-1	ph2	Contains free iodide or possibly being deiodinated by enzyme(s)
C.I. Acid Red 114	6459-94-5	e1k	Interference, supramaximal response ^c in DIO1
Thiocarbazide	2231-57-4	e1k	Interference with Sandell-Kolthoff (SK) reaction
Eosin	17372-87-1	e1k	Interference with Sandell-Kolthoff (SK) reaction
C.I. Acid Yellow 3 disodium salt	8004-92-0	e1k	Interference with Sandell-Kolthoff (SK) reaction
Thiocyanic acid, ammonium salt	1762-95-4	e1k	Interference with Sandell-Kolthoff (SK) reaction
Sodium decyl sulfate	142-87-0	e1k	Abnormal time course of absorbance at 420 nm ^b
Disiquonium chloride	68959-20-6	e1k	Abnormal time course of absorbance at 420 nm ^b
C.I. Acid Blue 22	28631-66-5	e1k	Abnormal time course of absorbance at 420 nm ^b
Silwet L77	27306-78-1	e1k	Abnormal time course of absorbance at 420 nm ^b
3-Trifluoromethyl-4-nitrophenol	88-30-2	e1k	Abnormal time course of absorbance at 420 nm ^b
Dodecanoic acid	143-07-7	e1k	Abnormal time course of absorbance at 420 nm ^b
Dodecyl sulfate triethanolamine	139-96-8	e1k	Abnormal time course of absorbance at 420 nm ^b
Sodium lauryl polyoxyethylene ether sulfate	9004-82-4	e1k	Abnormal time course of absorbance at 420 nm ^b
Sodium tridecyl sulfate	3026-63-9	e1k	Abnormal time course of absorbance at 420 nm ^b
Polyoxyethylene(10)nonylphenyl ether	26027-38-3	e1k	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(s)
Iopanoic acid	96-83-3	e1k	Contains free iodide or possibly being deiodinated by enzyme(s)
Sodium iodide	7681-82-5	e1k	Contains free iodide or possibly being deiodinated by enzyme(s)
1,2-Ethanediamine dihydriodide	5700-49-2	e1k	Contains free iodide or possibly being deiodinated by enzyme(s)

^a Source. ToxCast Chemical sets: ph1_v2 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/NCCT, Research Triangle Park, NC, USA.

^b Abnormal A420 time course: Chemical flagged based on absorbance at time 0 or 10 minutes outside of expected range based on DMSO and model inhibitor.

^c Interference, supramaximal response: Reaction appeared more inhibited than the fully inhibited response by positive control (PTU).

Supplemental Table 6. Single concentration results. List of all chemicals tested in the deiodinase (DIO) inhibition assays, ordered by ToxCast chemical library and CASRN; maximum concentration tested and median % inhibition (n = 3 replicates) produced in DIO1, DIO2, and DIO3 single-point screening assay, with indication (Y = yes, N = no) of whether chemical was tested in concentration-response (CR) for each enzyme.

^a Source. ToxCast Chemical sets: ph1v2 indicates ToxCast phase 1_v2 chemical library, ph2 indicates ToxCast phase 2 chemical library, and e1k indicates ToxCast e1k chemical library obtained via Dr. Ann Richard, EPA/ORD/NCCT, 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; cornmint oil; peppermint oil; anise oil; polyoxyethylene monooleate; Igepal CO-890.

Chemical	CASRN	Source ^a	DIO1			DIO2			DIO3		
			Max conc., μM ^b	% Inhibition, median	Tested in CR?	Max conc., μM ^b	% Inhibition, median	Tested in CR?	Max conc., μM ^b	% Inhibition, median	Tested in CR?
Boric acid	10043-35-3	ph1v2	200	-3.2	N	190	-2.6	N	190	-5.6	N
Deisopropylatrazine	1007-28-9	ph1v2	200	5.7	N	200	7.3	N	200	43.9	N
Anilazine	101-05-3	ph1v2	200	24.8	N	200	9.7	N	200	9.2	N
Cloprop	101-10-0	ph1v2	200	1.4	N	200	-5.3	N	200	4.6	N
Chlorpropham	101-21-3	ph1v2	200	-3.0	N	200	3.5	N	200	-5.3	N
Methamidophos	10265-92-6	ph1v2	200	0.1	N	200	1.0	N	200	-8.1	N
Flumioxazin	103361-09-7	ph1v2	200	9.2	N	200	19.0	N	200	3.8	N
Imazapic	104098-48-8	ph1v2	200	6.4	N	200	-5.9	N	200	-3.1	N
Mesotrione	104206-82-8	ph1v2	200	38.4	N	200	22.9	Y	200	56.1	Y
Resmethrin	10453-86-8	ph1v2	200	26.2	N	200	71.6	Y	200	70.4	Y
Clodinafop-propargyl	105512-06-9	ph1v2	200	44.7	N	200	8.1	N	200	8.4	N
2-Methoxyethanol	109-86-4	ph1v2	200	0.4	N	200	4.0	N	200	-16.9	N
Dimethomorph	110488-70-5	ph1v2	200	6.2	N	200	7.6	N	200	-8.5	N
Fenpyroximate (Z,E)	111812-58-9	ph1v2	200	-6.9	N	200	6.2	N	200	-22.6	N
Thiacloprid	111988-49-9	ph1v2	200	7.2	N	200	4.5	N	200	2.0	N
Tetraconazole	112281-77-3	ph1v2	200	4.5	N	190	11.8	N	190	-12.5	N
Tebufozide	112410-23-8	ph1v2	200	6.3	N	200	0.4	N	200	7.2	N
MGK-264	113-48-4	ph1v2	200	0.3	N	200	18.8	N	200	-13.2	N
Cyclanilide	113136-77-9	ph1v2	200	6.7	N	200	11.1	N	200	27.3	N
Cycloate	1134-23-2	ph1v2	200	3.5	N	200	-0.4	N	200	-16.7	N
Propoxur	114-26-1	ph1v2	200	-2.0	N	200	2.7	N	200	1.4	N
Imazamox	114311-32-9	ph1v2	200	9.3	N	200	-1.0	N	200	-19.8	N
Fenbuconazole	114369-43-6	ph1v2	200	-6.8	N	200	14.3	N	200	-9.1	N
Endosulfan	115-29-7	ph1v2	200	8.1	N	200	17.6	N	200	8.0	N
Dicofol	115-32-2	ph1v2	200	88.0	Y	190	74.8	Y	190	90.3	Y
Aldicarb	116-06-3	ph1v2	200	-0.8	N	200	-2.4	N	200	-6.8	N

Novaluron	116714-46-6	ph1v2	200	6.0	N	200	-1.7	N	200	2.4	N
Di(2-ethylhexyl) phthalate	117-81-7	ph1v2	200	-1.2	N	200	5.3	N	200	2.0	N
Fluthiacet-methyl	117337-19-6	ph1v2	200	-2.5	N	200	8.0	N	200	14.0	N
Thiazopyr	117718-60-2	ph1v2	200	-0.6	N	200	2.7	N	200	-8.3	N
Spiroxamine	118134-30-8	ph1v2	200	10.6	N	200	-3.3	N	200	-3.1	N
Tebufenpyrad	119168-77-3	ph1v2	200	-1.0	N	190	5.2	N	190	-38.2	N
Dichlobenil	1194-65-6	ph1v2	200	-1.6	N	200	2.0	N	200	-24.2	N
Difenoconazole	119446-68-3	ph1v2	200	-2.3	N	200	12.3	N	200	-12.5	N
Icaridin	119515-38-7	ph1v2	200	5.7	N	200	1.6	N	200	-3.6	N
Chlorophene	120-32-1	ph1v2	200	44.8	Y	200	71.9	Y	200	70.0	Y
Dichlorprop	120-36-5	ph1v2	200	4.5	N	200	1.6	N	200	-5.0	N
Fipronil	120068-37-3	ph1v2	200	57.8	Y	200	71.7	Y	200	96.6	Y
Cyazofamid	120116-88-3	ph1v2	200	71.5	Y	200	56.8	Y	200	18.5	Y
Malathion	121-75-5	ph1v2	200	47.8	N	200	9.0	N	200	8.4	N
Cyprodinil	121552-61-2	ph1v2	200	-1.9	N	200	13.1	N	200	-38.2	N
Fenitrothion	122-14-5	ph1v2	200	48.9	N	200	18.3	N	200	2.6	N
Simazine	122-34-9	ph1v2	200	-0.2	N	200	1.3	N	200	36.2	N
Diphenylamine	122-39-4	ph1v2	200	0.3	N	200	13.1	N	200	5.3	N
2-Phenoxyethanol	122-99-6	ph1v2	200	-1.6	N	200	-3.2	N	200	-4.9	N
Cyhalofop-butyl	122008-85-9	ph1v2	200	2.1	N	190	-4.2	N	190	9.6	N
Sulfentrazone	122836-35-5	ph1v2	200	-3.9	N	200	4.1	N	200	-0.8	N
Maleic hydrazide	123-33-1	ph1v2	200	1.2	N	190	-5.4	N	190	2.0	N
Pymetrozine	123312-89-0	ph1v2	200	0.9	N	200	10.6	N	200	-6.8	N
Pyriithiobac-sodium	123343-16-8	ph1v2	200	5.3	N	200	-0.5	N	200	1.3	N
Maneb	12427-38-2	ph1v2	200	67.9	Y	200	45.7	N	200	37.9	N
Quinoxifen	124495-18-7	ph1v2	200	43.4	N	200	59.6	Y	200	49.4	Y
Fenhexamid	126833-17-8	ph1v2	200	-13.6	Y	200	13.3	N	200	-15.5	N
Carfentrazone-ethyl	128639-02-1	ph1v2	200	0.4	N	200	28.0	N	200	46.9	N
Pyraflufen-ethyl	129630-19-9	ph1v2	200	-4.8	N	200	-1.5	N	200	7.1	N
Dimethyl phthalate	131-11-3	ph1v2	200	-1.0	N	200	2.5	N	200	4.7	N
Monobutyl phthalate	131-70-4	ph1v2	200	-3.6	N	200	-0.1	N	200	-6.2	N
Fludioxonil	131341-86-1	ph1v2	200	0.5	N	200	2.3	N	200	-44.8	N
Famoxadone	131807-57-3	ph1v2	200	5.2	N	200	8.2	N	200	18.2	N
Azoxystrobin	131860-33-8	ph1v2	200	-2.1	N	200	6.7	N	200	17.7	N
Ethoprop	13194-48-4	ph1v2	200	-5.3	N	200	-1.6	N	200	-10.5	N
Triticonazole	131983-72-7	ph1v2	200	-1.0	N	190	7.4	N	190	7.9	N
Captan	133-06-2	ph1v2	200	54.6	Y	190	28.7	N	190	28.1	N

Folpet	133-07-3	ph1v2	200	32.3	N	200	35.6	N	200	44.0	N
DEET	134-62-3	ph1v2	200	-0.8	N	200	0.2	N	200	-9.4	N
Butafenacil	134605-64-4	ph1v2	200	1.7	N	200	7.5	N	200	-7.9	N
Acibenzolar-S-methyl	135158-54-2	ph1v2	200	36.5	N	200	6.4	N	200	24.4	N
Acetamiprid	135410-20-7	ph1v2	200	-1.4	N	200	0.9	N	200	0.0	N
Dipropyl 2,5-pyridinedicarboxylate	136-45-8	ph1v2	200	-8.6	N	200	-4.2	N	200	-1.3	N
Thiram	137-26-8	ph1v2	200	3.0	N	200	37.2	Y	200	69.6	Y
Imidacloprid	138261-41-3	ph1v2	200	2.3	N	200	2.1	N	200	0.2	N
Propazine	139-40-2	ph1v2	200	4.2	N	200	2.2	N	200	44.4	N
Dicrotophos	141-66-2	ph1v2	200	0.7	N	200	5.4	N	200	-3.8	N
Isoxaflutole	141112-29-0	ph1v2	200	14.6	N	200	-1.6	N	200	2.1	N
Trifloxystrobin	141517-21-7	ph1v2	200	7.1	N	200	4.7	N	200	-21.5	N
Flufenacet	142459-58-3	ph1v2	200	5.4	N	200	16.2	N	200	31.0	N
Iodosulfuron-methyl-sodium	144550-36-7	ph1v2	200	6.7	N	190	-14.2	N	190	-26.9	N
Diclosulam	145701-21-9	ph1v2	200	58.9	Y	200	15.4	N	200	16.7	N
Thiabendazole	148-79-8	ph1v2	200	-0.2	N	200	-0.5	N	200	-11.8	N
Spirodiclofen	148477-71-8	ph1v2	200	-1.7	N	200	12.8	N	200	5.4	N
Bifenazate	149877-41-8	ph1v2	200	-9.6	N	200	4.0	N	200	5.6	N
Tepraloxydim	149979-41-9	ph1v2	200	7.6	N	200	9.9	N	200	4.6	N
Napropamide	15299-99-7	ph1v2	200	3.5	N	200	19.3	N	200	-11.1	N
Etoxazole	153233-91-1	ph1v2	200	8.9	N	200	-0.2	N	200	1.0	N
Thiamethoxam	153719-23-4	ph1v2	200	-8.4	N	200	-3.6	N	200	0.1	N
Emamectin benzoate	155569-91-8	ph1v2	200	100.4	Y	200	99.1	Y	200	92.3	Y
Zoxamide	156052-68-5	ph1v2	200	93.1	Y	200	91.5	Y	200	68.4	Y
Trifluralin	1582-09-8	ph1v2	200	-2.5	N	200	2.8	N	200	10.0	N
Daminozide	1596-84-5	ph1v2	200	-5.4	N	200	1.2	N	200	-1.0	N
Alachlor	15972-60-8	ph1v2	200	48.6	N	200	56.8	Y	200	39.7	Y
Prometon	1610-18-0	ph1v2	200	0.9	N	200	-2.5	N	200	-4.2	N
Methoxyfenozone	161050-58-4	ph1v2	200	2.2	N	190	12.8	N	190	33.3	N
Fenamidone	161326-34-7	ph1v2	200	4.7	N	200	3.3	N	200	-5.7	N
Malaoxon	1634-78-2	ph1v2	200	5.6	Y	200	11.6	N	200	7.3	N
Ethephon	16672-87-0	ph1v2	200	6.7	N	200	5.3	N	200	-13.6	N
Methomyl	16752-77-5	ph1v2	200	-1.9	N	200	5.2	N	200	1.1	N
Bromoxnil	1689-84-5	ph1v2	160	14.5	N	160	8.5	N	160	17.5	N
Chloridazon	1698-60-8	ph1v2	200	3.4	N	200	1.2	N	200	-0.1	N
Clopyralid	1702-17-6	ph1v2	200	11.4	N	200	10.0	N	200	3.1	N
Indoxacarb	173584-44-6	ph1v2	160	-1.8	N	160	0.1	N	160	8.9	N

Pyraclostrobin	175013-18-0	ph1v2	200	3.8	N	200	11.7	N	200	-12.2	N
PFOS	1763-23-1	ph1v2	170	42.7	N	160	66.5	Y	160	9.5	Y
Benomyl	17804-35-2	ph1v2	200	-0.1	N	200	-2.3	N	200	6.2	N
Propoxycarbazono-sodium	181274-15-7	ph1v2	200	-8.3	N	200	1.6	N	200	4.4	N
Benfluralin	1861-40-1	ph1v2	200	-0.5	N	200	-2.5	N	200	0.4	N
Boscalid	188425-85-6	ph1v2	200	1.7	N	200	7.6	N	200	-17.4	N
Flufenpyr-ethyl	188489-07-8	ph1v2	200	3.5	N	200	13.4	N	200	37.2	N
Chlorothalonil	1897-45-6	ph1v2	200	57.3	Y	200	70.8	Y	200	83.7	Y
Oryzalin	19044-88-3	ph1v2	200	81.9	Y	200	85.4	Y	200	52.5	Y
Atrazine	1912-24-9	ph1v2	200	5.8	N	200	15.3	Y	200	60.9	Y
Dicamba	1918-00-9	ph1v2	200	2.5	N	200	4.3	N	200	-15.9	N
Picloram	1918-02-1	ph1v2	200	-1.0	N	200	4.8	N	200	3.4	N
Nitrapyrin	1929-82-4	ph1v2	200	-4.0	N	200	2.7	N	200	7.9	N
Oxadiazon	19666-30-9	ph1v2	200	-5.4	N	200	13.0	N	200	-18.1	N
Trifloxysulfuron-sodium	199119-58-9	ph1v2	200	-0.6	N	200	20.2	N	200	11.5	N
Butylate	2008-41-5	ph1v2	200	2.2	N	200	2.8	N	200	-8.0	N
Metribuzin	21087-64-9	ph1v2	200	-0.7	N	200	13.5	N	200	9.7	N
Clothianidin	210880-92-5	ph1v2	200	0.8	N	200	-2.4	N	200	4.5	N
2-(Thiocyanomethylthio)benzothiazole	21564-17-0	ph1v2	200	4.4	N	200	43.5	N	200	22.8	N
Fluometuron	2164-17-2	ph1v2	200	1.2	N	200	-1.8	N	200	-2.3	N
Cyanazine	21725-46-2	ph1v2	200	1.2	N	200	21.3	Y	200	70.3	Y
Penoxsulam	219714-96-2	ph1v2	200	5.8	N	200	7.0	N	200	-3.3	N
Molinate	2212-67-1	ph1v2	200	-1.9	N	200	0.9	N	200	-2.9	N
Fenamiphos	22224-92-6	ph1v2	200	8.5	N	200	6.4	N	200	-21.1	N
Bendiocarb	22781-23-3	ph1v2	200	2.9	N	200	3.3	N	200	7.1	N
Tri-allate	2303-17-5	ph1v2	200	0.6	N	200	-0.9	N	200	-20.6	N
Prallethrin	23031-36-9	ph1v2	200	38.7	N	190	55.0	Y	190	77.7	Y
Phosalone	2310-17-0	ph1v2	200	2.4	N	200	0.5	N	200	-16.8	N
Pirimicarb	23103-98-2	ph1v2	200	33.9	N	200	52.0	Y	200	89.5	Y
Propargite	2312-35-8	ph1v2	200	29.2	N	200	19.6	N	200	-0.4	N
Oxamyl	23135-22-0	ph1v2	200	8.1	N	200	0.0	N	200	3.5	N
Butachlor	23184-66-9	ph1v2	200	57.5	Y	200	79.3	Y	200	66.9	Y
Formetanate hydrochloride	23422-53-9	ph1v2	200	0.8	N	200	2.3	N	200	-9.4	N
Thiophanate-methyl	23564-05-8	ph1v2	200	32.0	N	200	7.8	N	200	-20.1	N
Propyzamide	23950-58-5	ph1v2	200	-0.8	N	200	1.0	N	200	-8.3	N
Captafol	2425-06-1	ph1v2	200	89.0	Y	200	56.8	Y	200	55.8	Y
Mepiquat chloride	24307-26-4	ph1v2	200	-2.7	N	200	8.6	N	200	-12.7	N

Bentazone	25057-89-0	ph1v2	200	1.7	N	200	4.7	N	200	-0.4	N
Propamocarb hydrochloride	25606-41-1	ph1v2	200	-8.5	N	200	0.7	N	200	6.2	N
Etridiazole	2593-15-9	ph1v2	200	-5.4	N	200	11.7	N	200	1.5	N
Ethofumesate	26225-79-6	ph1v2	200	5.7	N	200	1.4	N	200	-21.0	N
Chloroneb	2675-77-6	ph1v2	200	0.9	N	200	3.1	N	200	-13.3	N
Norflurazon	27314-13-2	ph1v2	200	-1.8	N	200	6.2	N	200	-17.2	N
Thiobencarb	28249-77-6	ph1v2	200	-1.8	N	200	-5.0	N	200	-13.1	N
S-Bioallethrin	28434-00-6	ph1v2	200	5.7	N	200	42.0	N	200	47.0	N
Prodiamine	29091-21-2	ph1v2	200	10.6	N	190	30.6	Y	190	51.4	Y
Pirimiphos-methyl	29232-93-7	ph1v2	200	48.2	N	200	47.3	Y	200	54.4	Y
2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane	2971-36-0	ph1v2	200	38.4	N	200	64.2	Y	200	40.1	Y
Methyl parathion	298-00-0	ph1v2	200	20.8	N	200	13.2	N	200	2.9	N
Disulfoton	298-04-4	ph1v2	200	-0.9	N	200	4.4	N	200	11.1	N
Naled	300-76-5	ph1v2	200	3.5	N	200	23.1	N	200	4.6	N
Acephate	30560-19-1	ph1v2	200	1.9	N	200	1.0	N	200	-2.9	N
Propetamphos	31218-83-4	ph1v2	200	4.7	N	200	23.8	N	200	-0.4	N
Bromacil	314-40-9	ph1v2	200	-0.2	N	200	3.0	N	200	-10.0	N
Diuron	330-54-1	ph1v2	200	-1.9	N	200	-5.8	N	200	-4.5	N
Linuron	330-55-2	ph1v2	200	-1.6	N	200	0.2	N	200	-23.8	N
Amitraz	33089-61-1	ph1v2	200	24.4	N	200	47.5	N	200	19.7	N
Diazinon	333-41-5	ph1v2	200	12.1	N	200	8.6	N	200	11.2	N
Asulam	3337-71-1	ph1v2	200	1.4	N	200	-4.3	N	200	-2.7	N
PFOA	335-67-1	ph1v2	200	0.4	N	200	13.9	N	200	-34.1	N
Butralin	33629-47-9	ph1v2	200	-0.3	N	200	1.3	N	200	-6.8	N
Triclosan	3380-34-5	ph1v2	200	103.0	Y	200	98.1	Y	200	102.3	Y
Tebuthiuron	34014-18-1	ph1v2	200	0.1	N	200	3.8	N	200	-1.5	N
Acetochlor	34256-82-1	ph1v2	200	48.3	N	200	53.4	Y	200	41.6	Y
Imazalil	35554-44-0	ph1v2	200	0.6	N	200	7.5	N	200	-10.7	N
Azamethiphos	35575-96-3	ph1v2	200	37.7	N	200	28.7	N	200	22.6	N
Fluoxastrobin	361377-29-9	ph1v2	200	9.0	N	200	-1.5	Y	200	50.8	Y
Iprodione	36734-19-7	ph1v2	200	-0.1	N	200	11.8	N	200	-5.5	N
Fenpropathrin	39515-41-8	ph1v2	200	-2.8	N	200	9.1	N	200	8.2	N
Pendimethalin	40487-42-1	ph1v2	200	-1.8	N	200	7.3	N	200	-10.1	N
Profenofos	41198-08-7	ph1v2	100	-3.1	N	90	1.8	N	90	-29.6	N
Cyanamide	420-04-2	ph1v2	200	4.1	N	190	4.2	N	190	26.9	N
Isazofos	42509-80-8	ph1v2	200	6.3	N	200	-0.9	N	200	-1.4	N
Oxyfluorfen	42874-03-3	ph1v2	200	6.2	N	200	-0.6	N	200	7.7	N

Triadimefon	43121-43-3	ph1v2	200	2.4	N	200	6.4	N	200	-9.4	N
Difenzoquat metilsulfate	43222-48-6	ph1v2	200	-0.2	N	200	-3.6	N	200	-11.1	N
Monomethyl phthalate	4376-18-5	ph1v2	200	-4.8	N	200	0.0	N	200	1.8	N
MEHP	4376-20-9	ph1v2	200	-2.1	N	200	8.4	N	200	-7.3	N
Niclosamide	50-65-7	ph1v2	100	46.1	N	100	13.7	N	100	-16.4	N
Vinclozolin	50471-44-8	ph1v2	200	-0.3	N	200	0.7	N	200	7.7	N
Acifluorfen	50594-66-6	ph1v2	200	17.0	N	200	7.2	N	200	0.0	N
Piperonyl butoxide	51-03-6	ph1v2	200	-2.0	N	200	0.6	N	200	-5.3	N
Metolachlor	51218-45-2	ph1v2	200	56.9	Y	200	31.0	N	200	21.4	N
Hexazinone	51235-04-2	ph1v2	200	-5.4	N	200	5.4	N	200	-18.5	N
Diclofop-methyl	51338-27-3	ph1v2	200	-1.5	N	200	1.5	N	200	-2.9	N
Thidiazuron	51707-55-2	ph1v2	200	45.1	N	200	0.4	N	200	-5.9	N
Trichlorfon	52-68-6	ph1v2	200	1.1	N	200	1.9	N	200	-1.4	N
Cypermethrin	52315-07-8	ph1v2	200	4.3	N	200	5.9	N	200	16.8	N
Carboxin	5234-68-4	ph1v2	200	3.3	N	200	2.7	N	200	-7.9	N
Permethrin	52645-53-1	ph1v2	200	-1.6	N	200	7.0	N	200	3.6	N
Pyrimethanil	53112-28-0	ph1v2	200	-11.2	N	200	-0.4	N	200	1.9	N
Dazomet	533-74-4	ph1v2	200	1.3	N	200	2.7	N	200	13.8	N
Chlorethoxyfos	54593-83-8	ph1v2	200	16.7	N	200	15.0	N	200	17.8	N
Fenthion	55-38-9	ph1v2	200	74.3	Y	200	37.7	N	200	21.8	N
Triadimenol	55219-65-3	ph1v2	200	-0.7	N	200	11.3	N	200	-20.8	N
Ethalfuralin	55283-68-6	ph1v2	200	1.3	N	200	5.4	N	200	2.9	N
Triclopyr	55335-06-3	ph1v2	200	-9.7	N	200	9.0	N	200	-12.0	N
Methyl isothiocyanate	556-61-6	ph1v2	200	-1.0	N	200	0.1	N	200	3.2	N
Chlorpyrifos-methyl	5598-13-0	ph1v2	200	30.6	N	200	21.2	N	200	-9.2	N
Chlorpyrifos oxon	5598-15-2	ph1v2	200	9.8	N	190	5.7	N	190	47.1	N
Parathion	56-38-2	ph1v2	200	-0.7	N	200	1.9	N	200	-1.6	N
Coumaphos	56-72-4	ph1v2	200	-0.9	N	200	5.2	N	200	-10.8	N
Clopyralid-olamine	57754-85-5	ph1v2	200	1.3	N	200	3.0	N	200	6.2	N
Metalaxyl	57837-19-1	ph1v2	200	-3.2	N	200	7.0	N	200	3.7	N
Cymoxanil	57966-95-7	ph1v2	200	0.0	N	200	0.4	N	200	-12.7	N
Lindane	58-89-9	ph1v2	200	2.8	N	200	3.1	N	200	-10.6	N
Allethrin	584-79-2	ph1v2	200	-4.6	N	190	60.0	Y	190	72.3	Y
Terbacil	5902-51-2	ph1v2	200	2.5	N	200	-2.6	N	200	-20.6	N
Thiodicarb	59669-26-0	ph1v2	200	3.0	N	200	2.5	N	200	-20.4	N
Dimethoate	60-51-5	ph1v2	200	1.0	N	200	1.0	N	200	-1.0	N
Fenarimol	60168-88-9	ph1v2	200	1.3	N	200	13.0	N	200	-23.4	N

Propiconazole	60207-90-1	ph1v2	200	-2.7	N	200	6.5	N	200	-17.3	N
Oxytetracycline dihydrate	6153-64-6	ph1v2	200	90.8	Y	200	61.1	Y	200	87.5	Y
Dichlorvos	62-73-7	ph1v2	100	-4.3	N	90	25.4	N	90	7.7	N
Flumetralin	62924-70-3	ph1v2	200	-8.6	N	200	5.5	N	200	-12.0	N
Carbaryl	63-25-2	ph1v2	200	-0.4	N	200	13.4	N	200	-3.0	N
Diquat dibromide monohydrate	6385-62-2	ph1v2	100	0.1	N	100	-0.9	N	100	-9.9	N
Cyromazine	66215-27-8	ph1v2	200	2.1	N	200	2.9	N	200	-10.5	N
Esfenvalerate	66230-04-4	ph1v2	200	1.4	N	200	6.4	N	200	9.0	N
Flutolanil	66332-96-5	ph1v2	200	1.3	N	190	2.1	N	190	-15.2	N
Fenoxaprop-ethyl	66441-23-4	ph1v2	200	3.2	N	200	31.1	Y	200	70.3	Y
Metam-sodium hydrate	6734-80-1	ph1v2	200	-4.2	N	200	3.8	N	200	7.1	N
Prochloraz	67747-09-5	ph1v2	200	2.8	N	200	39.4	N	200	0.2	N
Forchlorfenuron	68157-60-8	ph1v2	200	14.5	N	190	20.6	N	190	-21.9	N
Cyfluthrin	68359-37-5	ph1v2	200	-1.0	N	200	7.9	N	200	7.0	N
Triflumizole	68694-11-1	ph1v2	200	88.8	Y	200	94.3	Y	200	99.1	Y
Monocrotophos	6923-22-4	ph1v2	200	0.5	N	200	8.4	N	200	7.3	N
Buprofezin	69327-76-0	ph1v2	200	2.7	N	200	1.2	N	200	0.1	N
Fluroxypyr	69377-81-7	ph1v2	200	5.1	N	200	-5.7	N	200	-3.1	N
Fluazifop-butyl	69806-50-4	ph1v2	200	5.0	N	200	2.2	N	200	0.1	N
Propanil	709-98-8	ph1v2	200	0.5	N	200	6.4	N	200	-12.2	N
Abamectin	71751-41-2	ph1v2	200	3.6	N	200	12.6	N	200	28.8	N
Methoxychlor	72-43-5	ph1v2	200	-2.6	N	190	2.5	N	190	1.5	N
Fenoxycarb	72490-01-8	ph1v2	200	0.4	N	200	-6.4	N	200	-21.3	N
Prometryn	7287-19-6	ph1v2	200	-0.5	N	200	8.4	N	200	27.8	N
Sethoxydim	74051-80-2	ph1v2	200	1.5	N	200	2.3	N	200	-1.5	N
Bensulide	741-58-2	ph1v2	200	3.0	N	200	20.8	N	200	-20.3	N
Clofentezine	74115-24-5	ph1v2	200	-2.5	N	200	2.9	N	200	6.1	N
Dimethylarsinic acid	75-60-5	ph1v2	200	-1.9	N	200	7.2	N	200	1.8	N
EPTC	759-94-4	ph1v2	200	-3.7	N	200	1.2	N	200	-18.0	N
Triphenyltin hydroxide	76-87-9	ph1v2	200	-1.0	N	200	20.4	N	200	33.7	N
Quizalofop-ethyl	76578-14-8	ph1v2	170	2.4	N	170	11.7	N	170	15.2	N
Paclobutrazol	76738-62-0	ph1v2	200	1.8	N	200	-0.3	N	200	-11.9	N
Tetramethrin	7696-12-0	ph1v2	200	19.3	N	200	62.8	Y	200	1.7	Y
Lactofen	77501-63-4	ph1v2	200	2.7	N	200	-2.6	N	200	-10.8	N
Mevinphos	7786-34-7	ph1v2	200	6.3	N	200	9.1	N	200	16.2	N
Tribufos	78-48-8	ph1v2	200	-1.0	N	200	9.6	N	200	-4.7	N
Hexythiazox	78587-05-0	ph1v2	200	-0.5	N	200	7.6	N	200	-17.2	N

Fluazifop-P-butyl	79241-46-6	ph1v2	200	-5.1	N	200	11.1	N	200	2.1	N
Tefluthrin	79538-32-2	ph1v2	200	-5.8	N	200	2.9	N	200	-13.4	N
Fluazinam	79622-59-6	ph1v2	180	76.3	Y	180	91.5	Y	180	98.2	Y
Hexaconazole	79983-71-4	ph1v2	200	3.8	N	200	6.1	N	200	-18.6	N
Bisphenol A	80-05-7	ph1v2	200	-0.5	N	200	4.8	N	200	-27.7	N
Mancozeb	8018-01-7	ph1v2	100	45.1	Y	100	46.3	Y	100	55.9	Y
Imazapyr	81334-34-1	ph1v2	200	1.8	N	200	5.5	N	200	-1.3	N
Imazaquin	81335-37-7	ph1v2	200	1.8	N	200	7.3	N	200	-2.4	N
Imazethapyr	81335-77-5	ph1v2	200	-1.3	N	200	0.1	N	200	-19.2	N
Fluroxypyr-meptyl	81406-37-3	ph1v2	200	5.7	N	200	10.9	N	200	-3.9	N
Clomazone	81777-89-1	ph1v2	200	1.2	N	200	1.7	N	200	-7.8	N
Pentachloronitrobenzene	82-68-8	ph1v2	200	-0.7	N	200	7.8	N	200	38.9	N
Isoxaben	82558-50-7	ph1v2	200	0.8	N	200	1.3	N	200	-0.9	N
Bifenthrin	82657-04-3	ph1v2	200	0.1	N	200	1.8	N	200	8.9	N
Rotenone	83-79-4	ph1v2	200	33.1	N	200	16.7	Y	200	55.2	Y
Ametryn	834-12-8	ph1v2	200	0.7	N	200	12.9	N	200	25.5	N
Dibutyl phthalate	84-74-2	ph1v2	200	0.8	N	200	1.8	N	200	-17.9	N
Quinclorac	84087-01-4	ph1v2	200	-0.5	N	200	7.6	N	200	-17.0	N
Flusilazole	85509-19-9	ph1v2	200	-1.1	N	200	11.1	N	200	-32.0	N
Azinphos-methyl	86-50-0	ph1v2	200	66.2	Y	200	28.9	N	200	11.5	N
Symclosene	87-90-1	ph1v2	200	10.7	N	200	7.5	N	200	-13.0	N
Flumiclorac-pentyl	87546-18-7	ph1v2	200	46.5	N	200	82.8	Y	200	47.7	Y
Dimethenamid	87674-68-8	ph1v2	200	12.7	N	200	40.1	N	200	13.8	N
Cinmethylin	87818-31-3	ph1v2	200	0.8	N	200	0.1	N	200	-5.9	N
Tralkoxydim	87820-88-0	ph1v2	200	-1.9	N	200	7.2	N	200	-1.8	N
Myclobutanil	88671-89-0	ph1v2	200	-0.1	N	200	2.2	N	200	-9.1	N
2-Phenylphenol	90-43-7	ph1v2	200	-6.8	N	200	11.3	N	200	-9.0	N
MCPA	94-74-6	ph1v2	200	-2.4	N	200	1.9	N	200	-0.5	N
2,4-Dichlorophenoxyacetic acid	94-75-7	ph1v2	200	-0.7	N	200	-4.1	N	200	-4.9	N
2,4-DB	94-82-6	ph1v2	200	6.5	N	200	3.8	N	200	-2.0	N
Cyproconazole	94361-06-5	ph1v2	200	-4.9	N	190	3.0	N	190	1.6	N
Methidathion	950-37-8	ph1v2	200	32.3	N	200	14.6	N	200	4.4	N
Pyriproxyfen	95737-68-1	ph1v2	200	-2.8	N	200	9.1	N	200	5.3	N
Ethylene thiourea	96-45-7	ph1v2	200	4.0	N	200	2.7	N	200	-0.6	N
Tebupirimfos	96182-53-5	ph1v2	200	3.7	N	200	9.9	N	200	-1.3	N
Diazoxon	962-58-3	ph1v2	200	-4.2	N	200	2.4	N	200	2.1	N
Pyridaben	96489-71-3	ph1v2	200	-9.1	N	200	11.4	N	200	7.7	N

Dithiopyr	97886-45-8	ph1v2	200	-0.2	N	190	2.6	N	190	-5.4	N
Fosthiazate	98886-44-3	ph1v2	200	-8.1	N	200	2.1	N	200	-1.7	N
Flumetsulam	98967-40-9	ph1v2	200	-1.5	N	200	1.1	N	200	-3.4	N
Dicloran	99-30-9	ph1v2	200	3.5	N	200	12.9	N	200	10.1	N
Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3)	NOCAS_34742	ph1v2	200	28.6	N	190	30.1	Y	190	67.7	Y
1-Chloro-4-nitrobenzene	100-00-5	ph2	200	-0.7	N	200	2.9	N	200	4.7	N
4-Nitroaniline	100-01-6	ph2	200	6.0	N	200	0.7	N	200	-2.4	N
4-Nitrophenol	100-02-7	ph2	200	-11.7	N	200	-4.1	N	200	-1.4	N
N,N-Diethylethanolamine	100-37-8	ph2	200	2.6	N	200	-1.0	N	200	-4.3	N
Benzyl alcohol	100-51-6	ph2	200	8.7	N	200	-16.4	N	200	-1.9	N
3-Pyridinecarbonitrile	100-54-9	ph2	200	-14.2	N	200	-1.1	N	200	3.5	N
Methenamine	100-97-0	ph2	200	-8.1	N	200	-6.8	N	200	4.1	N
alpha-Cyclodextrin	10016-20-3	ph2	100	3.3	N	100	-10.4	N	100	-4.8	N
Triphenyl phosphite	101-02-0	ph2	200	3.0	N	200	1.1	N	200	1.0	N
Triclocarban	101-20-2	ph2	200	1.2	N	200	-3.6	N	200	0.5	N
N-Phenyl-1,4-benzenediamine	101-54-2	ph2	200	0.8	N	200	30.8	N	200	23.3	N
p-Bromodiphenyl ether	101-55-3	ph2	200	-3.0	N	200	-0.5	N	200	3.0	N
4,4'-Methylenebis(N,N-dimethylaniline)	101-61-1	ph2	200	-0.6	N	200	15.4	N	200	2.0	N
4,4'-Methylenedianiline	101-77-9	ph2	200	15.1	N	200	2.5	N	200	4.8	N
4,4'-Oxydianiline	101-80-4	ph2	200	9.6	N	200	7.5	N	200	1.7	N
2-Benzylideneoctanal	101-86-0	ph2	200	12.5	N	200	52.1	Y	200	65.0	Y
17beta-Trenbolone	10161-33-8	ph2	200	42.1	N	200	35.8	Y	200	58.6	Y
1,3-Diphenylguanidine	102-06-7	ph2	200	1.7	N	200	-9.6	N	200	3.0	N
N-Ethyl-3-methylaniline	102-27-2	ph2	200	4.8	N	200	3.2	N	200	-4.3	N
N,N,N',N'-Tetrakis(2-Hydroxypropyl)ethylenediamine	102-60-3	ph2	200	-2.6	N	200	4.2	N	200	-1.1	N
Triethanolamine	102-71-6	ph2	200	10.4	N	200	0.9	N	200	-1.1	N
Triacetin	102-76-1	ph2	200	-1.1	N	200	-3.3	N	200	-1.5	N
Tributylamine	102-82-9	ph2	200	0.3	N	200	5.4	N	200	5.4	N
2,2-Dibromo-3-nitropropionamide	10222-01-2	ph2	200	0.0	N	200	8.2	N	200	6.6	N
Heptachlor epoxide	1024-57-3	ph2	200	-3.1	N	200	-1.0	N	200	3.5	N
Di(2-ethylhexyl) adipate	103-23-1	ph2	200	-0.5	N	200	6.2	N	200	-0.8	N
Bis(2-ethylhexyl) nonanedioate	103-24-2	ph2	200	-5.9	N	200	2.1	N	200	-9.1	N
Azobenzene	103-33-3	ph2	200	-2.4	N	200	-5.3	N	200	0.4	N
Propylbenzene	103-65-1	ph2	200	3.8	N	200	-1.8	N	200	-0.5	N
N-Ethylaniline	103-69-5	ph2	200	7.4	N	200	0.1	N	200	2.7	N

Acetaminophen	103-90-2	ph2	200	-6.0	N	200	8.5	N	200	1.6	N
Octyl gallate	1034-01-1	ph2	200	97.2	Y	200	99.4	Y	200	104.6	Y
4-Nonylphenol	104-40-5	ph2	200	87.9	Y	200	94.6	Y	200	99.1	Y
Butylbenzene	104-51-8	ph2	200	1.9	N	200	5.4	N	200	-2.2	N
5-Heptyldihydro-2(3H)-furanone	104-67-6	ph2	200	-2.1	N	200	6.0	N	200	-8.8	N
2-Ethyl-1-hexanol	104-76-7	ph2	200	7.4	N	200	-3.7	N	200	-5.0	N
CI-959	104795-68-8	ph2	200	-10.6	N	200	8.2	N	200	-8.0	N
Ethyl butyrate	105-54-4	ph2	200	0.3	N	200	0.5	N	200	0.6	N
Caprolactam	105-60-2	ph2	200	3.5	N	200	-2.3	N	200	3.2	N
2,4-Dimethylphenol	105-67-9	ph2	200	3.3	N	200	1.5	N	200	3.9	N
Geranyl acetate	105-87-3	ph2	200	7.9	N	200	4.3	N	200	14.7	N
Dibutyl hexanedioate	105-99-7	ph2	200	-0.1	N	200	-3.4	N	200	-4.7	N
Tamoxifen	10540-29-1	ph2	100	72.0	Y	100	95.1	Y	100	3.4	Y
5HPP-33	105624-86-0	ph2	200	3.7	N	200	29.9	N	200	-4.8	N
Citronellol	106-22-9	ph2	200	12.5	N	200	-0.4	N	200	4.3	N
Geraniol	106-24-1	ph2	200	6.1	N	200	4.3	N	200	8.5	N
(2Z)-3,7-Dimethylocta-2,6-dien-1-ol	106-25-2	ph2	200	3.2	N	200	30.5	N	200	49.8	N
Isopentyl butyrate	106-27-4	ph2	200	-10.1	N	200	5.3	N	200	5.7	N
Ethyl heptanoate	106-30-9	ph2	200	-1.4	N	200	1.1	N	200	-0.3	N
4-Chlorotoluene	106-43-4	ph2	200	3.3	N	200	0.5	N	200	6.8	N
p-Cresol	106-44-5	ph2	200	-2.7	N	200	-0.6	N	200	-2.0	N
1,4-Dichlorobenzene	106-46-7	ph2	200	-4.5	N	200	3.4	N	200	-4.8	N
4-Chloroaniline	106-47-8	ph2	200	-3.6	N	200	3.2	N	200	-1.4	N
4-Methylaniline	106-49-0	ph2	200	5.1	N	200	8.0	N	200	2.7	N
Dimethyl succinate	106-65-0	ph2	200	-1.3	N	200	1.2	N	200	-4.1	N
4-Vinyl-1-cyclohexene dioxide	106-87-6	ph2	200	5.4	N	200	25.0	N	200	17.7	N
Carbendazim	10605-21-7	ph2	200	-3.9	N	200	7.2	N	200	-0.9	N
PharmaGSID_47337	1061517-62-1	ph2	200	79.3	Y	200	56.7	Y	200	43.7	Y
PharmaGSID_48511	1062243-51-9	ph2	190	10.1	N	180	28.2	N	180	-11.2	N
SAR102608	1068967-96-3	ph2	200	-5.5	N	200	3.4	N	200	-10.2	N
2-Chloroethanol	107-07-3	ph2	200	-0.8	N	200	-0.6	N	200	2.7	N
Ethylene glycol	107-21-1	ph2	200	-5.3	N	200	4.0	N	200	-0.4	N
2-Methyl-2,4-pentanediol	107-41-5	ph2	210	-4.7	N	200	0.2	N	200	-4.6	N
1,3-Butanediol	107-88-0	ph2	200	-0.1	N	200	0.1	N	200	8.4	N
Butanoic acid	107-92-6	ph2	200	3.1	N	200	-1.0	N	200	-4.0	N
1-Methoxy-2-propanol	107-98-2	ph2	200	0.4	N	190	-4.5	N	190	4.9	N
Ro 23-7637	107071-66-9	ph2	200	-11.5	N	200	0.6	N	200	-5.1	N

Tebuconazole	107534-96-3	ph2	200	7.7	N	200	3.4	N	200	1.5	N
SSR103800	1075752-90-7	ph2	185	-2.2	N	180	26.0	N	180	-0.6	N
Dimethylaminoethanol	108-01-0	ph2	200	-3.8	N	200	1.2	N	200	3.4	N
4-Methyl-2-pentanol	108-11-2	ph2	200	-5.8	N	190	-1.5	N	190	3.6	N
3-Methylaniline	108-44-1	ph2	200	-2.9	N	200	0.9	N	200	-5.4	N
1,3-Benzenediamine	108-45-2	ph2	200	4.9	N	200	2.2	N	200	-4.8	N
Resorcinol	108-46-3	ph2	200	-2.9	N	200	-4.4	N	200	-3.2	N
Dimethyl malonate	108-59-8	ph2	200	4.9	N	200	2.9	N	200	5.7	N
1,3,5-Trimethylbenzene	108-67-8	ph2	200	-1.3	N	200	1.3	N	200	2.0	N
Cyanuric acid	108-80-5	ph2	200	2.3	N	190	-0.1	N	190	1.0	N
Cyclohexylamine	108-91-8	ph2	200	0.4	N	200	-9.2	N	200	-3.2	N
Cyclohexanol	108-93-0	ph2	200	0.1	N	200	-0.6	N	200	2.6	N
Cyclohexanone	108-94-1	ph2	200	-0.6	N	200	-16.7	N	200	-1.9	N
Phenol	108-95-2	ph2	200	-9.9	N	200	3.9	N	200	-1.9	N
Dibutyl decanedioate	109-43-3	ph2	200	0.9	N	200	2.7	N	200	0.2	N
Methadone hydrochloride	1095-90-5	ph2	140	7.2	N	140	-3.9	N	140	-0.7	N
Di-tert-butyl peroxide	110-05-4	ph2	200	0.0	N	200	0.4	N	200	-5.3	N
N,N'-Methylenebisacrylamide	110-26-9	ph2	200	8.6	N	200	-0.4	N	200	3.8	N
Sorbic acid	110-44-1	ph2	200	2.7	N	200	16.3	N	200	29.6	N
Pentanal	110-62-3	ph2	200	4.2	N	200	4.0	N	200	4.3	N
2-Ethoxyethanol	110-80-5	ph2	200	-5.1	N	200	5.3	N	200	0.3	N
Piperazine	110-85-0	ph2	200	-0.1	N	200	-4.3	N	200	-7.8	N
Mepanipirim	110235-47-7	ph2	200	68.1	Y	200	72.0	Y	200	78.9	Y
Methyl octanoate	111-11-5	ph2	200	1.3	N	200	0.9	N	200	-1.8	N
Heptanoic acid	111-14-8	ph2	200	4.2	N	200	-12.0	N	200	-8.9	N
2-Ethoxyethyl acetate	111-15-9	ph2	200	3.7	N	200	-0.8	N	200	6.8	N
Triethylene glycol diacetate	111-21-7	ph2	200	-5.5	N	200	-2.2	N	200	-2.0	N
Glutaraldehyde	111-30-8	ph2	200	-3.4	N	200	40.3	Y	200	76.3	Y
Diethanolamine	111-42-2	ph2	200	-6.2	N	200	9.1	N	200	5.2	N
Bis(2-chloroethyl) ether	111-44-4	ph2	200	21.6	N	200	-4.3	Y	200	9.4	Y
Diethylene glycol	111-46-6	ph2	200	-3.7	N	200	5.0	N	200	-2.7	N
Hexanedinitrile	111-69-3	ph2	200	-2.0	N	200	-10.8	N	200	-1.6	N
2-Butoxyethanol	111-76-2	ph2	200	-3.0	N	190	-1.2	N	190	-6.6	N
Diethylene glycol monomethyl ether	111-77-3	ph2	200	-7.3	N	200	8.6	N	200	-1.9	N
Methyl dodecanoate	111-82-0	ph2	200	-8.5	N	200	6.2	N	200	-4.9	N
1-Octanol	111-87-5	ph2	210	1.4	N	200	0.6	N	200	3.0	N
2-(2-Ethoxyethoxy)ethanol	111-90-0	ph2	200	3.7	N	200	-3.7	N	200	6.3	N

Bis(2-methoxyethyl) ether	111-96-6	ph2	200	-3.0	N	200	-3.9	N	200	-8.3	N
Ammonium carbamate	1111-78-0	ph2	200	-4.6	N	200	-5.3	N	200	2.2	N
Dimethyl glutarate	1119-40-0	ph2	200	2.5	N	200	2.1	N	200	-27.3	N
Dodecyltrimethylammonium chloride	112-00-5	ph2	200	67.0	Y	200	81.2	Y	200	83.6	Y
Nonanoic acid	112-05-0	ph2	200	-6.2	N	200	7.4	N	200	-3.4	N
2-(Hexyloxy)ethanol	112-25-4	ph2	200	-4.6	N	200	-15.2	N	200	1.1	N
Triethylene glycol	112-27-6	ph2	200	-4.4	N	200	0.2	N	200	0.6	N
1-Decanol	112-30-1	ph2	200	8.3	N	200	0.5	N	200	-2.2	N
2-(2-Butoxyethoxy)ethanol	112-34-5	ph2	200	-7.6	N	200	-2.2	N	200	-8.2	N
10-Undecenoic acid	112-38-9	ph2	200	-6.1	N	200	5.9	N	200	-1.5	N
1-Undecanol	112-42-5	ph2	200	12.3	N	200	16.1	Y	200	73.6	Y
Triethylene glycol dimethyl ether	112-49-2	ph2	200	5.2	N	200	-4.9	N	200	-8.8	N
2-[2-(2-Ethoxyethoxy)ethoxy]ethanol	112-50-5	ph2	200	3.9	N	200	-8.0	N	200	4.9	N
1-Dodecanol	112-53-8	ph2	200	7.4	N	200	35.2	Y	200	77.4	Y
1-Tridecanol	112-70-9	ph2	210	4.8	N	200	36.7	Y	200	61.7	Y
1-Tetradecanol	112-72-1	ph2	200	5.7	N	200	2.6	N	200	37.3	N
Sodium hexyldecyl sulfate	1120-01-0	ph2	100	100.4	Y	90	98.3	Y	90	98.6	Y
Undecane	1120-21-4	ph2	200	3.8	N	200	3.2	N	200	-1.8	N
1-Tetradecene	1120-36-1	ph2	200	-0.2	N	200	2.9	N	200	2.5	N
1,3-Propane sultone	1120-71-4	ph2	200	-2.5	N	190	-0.8	N	190	-2.4	N
Pioglitazone hydrochloride	112529-15-4	ph2	200	4.9	N	200	7.5	N	200	-3.1	N
Zenarestat	112733-06-9	ph2	100	1.0	N	100	3.7	N	100	4.0	N
CP-114271	113734-18-2	ph2	200	-6.1	N	200	-0.1	N	200	-2.9	N
Erythromycin	114-07-8	ph2	50	1.2	N	50	-12.4	N	50	8.9	N
Anthralin	1143-38-0	ph2	200	17.0	N	200	2.9	N	200	13.4	N
Chlorendic acid	115-28-6	ph2	200	-6.8	N	200	1.1	N	200	1.6	N
Pentaerythritol	115-77-5	ph2	200	-4.6	N	200	-3.9	N	200	-6.0	N
Triphenyl phosphate	115-86-6	ph2	200	8.3	N	200	11.3	N	200	-4.5	N
Tris(2-chloroethyl) phosphate	115-96-8	ph2	200	-0.5	N	200	1.0	N	200	8.4	N
Tolazamide	1156-19-0	ph2	200	-7.1	N	200	-5.0	N	200	5.1	N
1-(Hydroxymethyl)-5,5-dimethylhydantoin	116-25-6	ph2	200	-5.4	N	200	6.7	N	200	13.3	N
Quercetin	117-39-5	ph2	200	40.6	N	200	-2.8	N	200	-9.8	N
2-Aminoanthraquinone	117-79-3	ph2	200	0.4	N	200	-6.7	N	200	0.8	N
Diocetyl phthalate	117-84-0	ph2	200	0.5	N	200	4.7	N	200	9.4	N
Picoxystrobin	117428-22-5	ph2	200	2.3	N	200	5.1	N	200	6.5	N
1,3-Dichloro-5,5-dimethylhydantoin	118-52-5	ph2	200	-4.7	N	200	-2.5	N	200	-7.0	N
Maltol	118-71-8	ph2	210	-4.3	N	200	3.4	N	200	7.1	N

Methyl salicylate	119-36-8	ph2	200	-3.7	N	200	-2.9	N	200	-9.8	N
Benzophenone	119-61-9	ph2	200	6.1	N	200	-0.9	N	200	1.7	N
3,3'-Dimethoxybenzidine	119-90-4	ph2	200	-4.2	N	200	6.8	N	200	3.5	N
3,3'-Dimethylbenzidine	119-93-7	ph2	200	0.6	N	200	5.6	N	200	-6.1	N
Sodium myristyl sulfate	1191-50-0	ph2	200	108.1	Y	200	95.9	Y	200	67.7	Y
PharmaGSID_48521	1191914-21-2	ph2	180	-0.8	N	180	-12.0	N	180	3.5	N
Anthracene	120-12-7	ph2	200	2.8	N	200	5.8	N	200	-0.5	N
Ethylparaben	120-47-8	ph2	200	1.0	N	200	4.7	N	200	-11.4	N
Diethylene glycol dibenzoate	120-55-8	ph2	200	3.8	N	200	1.5	N	200	-11.3	N
Dimethyl terephthalate	120-61-6	ph2	200	-1.7	N	200	-1.8	N	200	1.1	N
2-Methoxy-5-methylaniline	120-71-8	ph2	200	6.4	N	200	4.0	N	200	6.5	N
Catechol	120-80-9	ph2	200	-5.2	N	200	7.6	N	200	6.8	N
1,2,4-Trichlorobenzene	120-82-1	ph2	200	-4.4	N	200	-2.7	N	200	1.0	N
2,4-Dichlorophenol	120-83-2	ph2	200	-9.1	N	200	2.5	N	200	-13.6	N
2,4-Bis(2-methylbutan-2-yl)phenol	120-95-6	ph2	200	101.1	Y	200	89.3	Y	200	96.1	Y
2-tert-Butyl-4-methoxyphenol	121-00-6	ph2	200	-4.4	N	200	0.9	N	200	-16.5	N
2,4-Dinitrotoluene	121-14-2	ph2	200	-6.9	N	200	-10.9	N	200	-1.5	N
4-Hydroxy-3-methoxybenzaldehyde	121-33-5	ph2	200	3.3	N	200	1.2	N	200	-0.6	N
N,N-Dimethylaniline	121-69-7	ph2	210	-5.1	N	200	2.2	N	200	3.6	N
Propyl gallate	121-79-9	ph2	200	-8.5	N	200	-2.3	N	200	-3.2	N
1,3-Benzenedicarboxylic acid	121-91-5	ph2	200	0.2	N	200	-1.2	N	200	-9.3	N
Bis(2-ethylhexyl) decanedioate	122-62-3	ph2	200	5.0	N	200	-1.0	N	200	-1.9	N
1,2-Diphenylhydrazine	122-66-7	ph2	200	-0.3	N	200	-0.1	N	200	-5.5	N
Dodecylbenzene	123-01-3	ph2	200	-5.3	N	200	-2.4	N	200	-6.4	N
Diethyl butanedioate	123-25-1	ph2	200	-3.3	N	200	4.0	N	200	-2.9	N
Hydroquinone	123-31-9	ph2	200	-3.1	N	190	3.3	N	190	-0.8	N
Myrcene	123-35-3	ph2	200	31.5	N	200	33.3	N	200	41.7	N
Diacetone alcohol	123-42-2	ph2	200	-1.4	N	200	-8.8	N	200	5.3	N
Isopentyl alcohol	123-51-3	ph2	200	-3.5	N	200	-1.3	N	200	0.4	N
3-Methylbutyl acetate	123-92-2	ph2	200	4.2	N	200	-1.0	N	200	1.3	N
Candoxatril	123122-55-4	ph2	120	-2.1	N	120	-7.9	N	120	-0.3	N
Hexanedioic acid	124-04-9	ph2	200	3.4	N	200	-3.7	N	200	3.3	N
Octanoic acid	124-07-2	ph2	200	1.6	N	200	1.7	N	200	5.2	N
Octanal	124-13-0	ph2	200	-0.9	N	200	8.8	N	200	3.6	N
Decane	124-18-5	ph2	200	3.5	N	200	5.2	N	200	3.4	N
Triamcinolone	124-94-7	ph2	200	-2.1	N	200	-0.9	N	200	7.9	N
Enadoline	124378-77-4	ph2	200	5.9	N	200	1.1	N	200	5.3	N

2-(Hydroxymethyl)-2-nitro-1,3-propanediol	126-11-4	ph2	200	-1.8	N	200	6.8	N	200	3.8	N
Sucrose octaacetate	126-14-7	ph2	150	9.9	N	150	5.0	N	150	-0.3	N
Tributyl phosphate	126-73-8	ph2	200	-5.1	N	200	6.6	N	200	-11.7	N
2,4,7,9-Tetramethyl-5-decyne-4,7-diol	126-86-3	ph2	200	1.0	N	200	2.5	N	200	-6.6	N
Carminic acid	1260-17-9	ph2	200	18.8	N	200	1.1	N	200	2.5	N
Hydroxyurea	127-07-1	ph2	200	4.0	N	200	2.4	N	200	5.1	N
alpha-Isomethylionone	127-51-5	ph2	200	3.3	N	200	10.8	N	200	23.9	N
Zamifenacin	127308-82-1	ph2	200	-21.5	N	200	3.1	N	200	4.3	N
Sodium dimethyldithiocarbamate	128-04-1	ph2	200	-2.6	N	200	9.2	N	200	18.8	N
2,6-Di-tert-butylphenol	128-39-2	ph2	200	-1.9	N	200	1.7	N	200	10.4	N
Pyrene	129-00-0	ph2	200	5.7	N	200	7.8	N	200	5.5	N
TNP-470	129298-91-5	ph2	60	71.4	Y	60	39.7	N	60	31.1	N
Fabesetron hydrochloride	129299-90-7	ph2	180	26.0	N	170	33.4	N	170	-5.7	N
Fulvestrant	129453-61-8	ph2	100	-4.6	N	100	3.9	N	100	5.6	N
Sodium xylenesulfonate	1300-72-7	ph2	200	-1.5	N	200	5.2	N	200	-5.5	N
Terbufos	13071-79-9	ph2	200	-11.3	N	200	9.4	N	200	0.3	N
Diallyl phthalate	131-17-9	ph2	200	2.5	N	200	2.6	N	200	-1.2	N
Dipentyl phthalate	131-18-0	ph2	200	6.8	N	200	1.9	N	200	-1.3	N
2,2',4,4'-Tetrahydroxybenzophenone	131-55-5	ph2	200	27.2	N	200	11.0	N	200	-0.4	N
Dibenzofuran	132-64-9	ph2	200	-7.6	N	200	11.1	N	200	-5.0	N
Rifampicin	13292-46-1	ph2	120	9.7	N	120	12.3	N	120	22.7	N
Chloramben	133-90-4	ph2	200	5.0	N	200	0.2	N	200	3.7	N
Flutamide	13311-84-7	ph2	200	33.3	N	200	8.0	N	200	-11.9	N
Sorbitan, mono-(9Z)-9-octadecenoate	1338-43-8	ph2	200	7.9	N	200	27.9	N	200	-4.5	N
Sodium L-ascorbate	134-03-2	ph2	200	3.7	N	200	2.2	N	200	10.9	N
Methyl 2-aminobenzoate	134-20-3	ph2	200	9.6	N	200	-4.1	N	200	-4.4	N
CP-085958	134002-60-1	ph2	100	2.8	N	100	14.4	N	100	9.5	N
2-Naphthalenol	135-19-3	ph2	200	3.6	N	200	-1.8	N	200	-3.3	N
CP-100829	135080-03-4	ph2	100	53.7	Y	100	11.1	N	100	-19.2	N
Butyl benzoate	136-60-7	ph2	200	1.0	N	200	-1.3	N	200	-1.0	N
4-Hexylresorcinol	136-77-6	ph2	200	65.5	Y	200	18.3	N	200	11.1	N
FR130739	136042-19-8	ph2	200	-4.7	N	200	19.5	N	200	-11.7	N
TDCPP	13674-87-8	ph2	200	14.8	N	200	8.6	N	200	-11.9	N
Ziram	137-30-4	ph2	200	-4.7	N	200	26.8	N	200	45.3	N
FR900409	138472-01-2	ph2	200	-2.6	N	200	7.2	N	200	19.7	N
Nitrilotriacetic acid	139-13-9	ph2	180	1.2	N	180	-12.4	N	180	5.9	N
SB202235	139149-55-6	ph2	200	-4.9	N	200	4.6	N	200	0.1	N

Volinanserin	139290-65-6	ph2	200	4.6	N	200	-0.7	N	200	-5.1	N
Darbufelone mesylate	139340-56-0	ph2	100	88.1	Y	100	58.0	Y	100	72.2	Y
Fenamino-sulf	140-56-7	ph2	200	28.1	N	200	22.9	N	200	41.7	N
Pentamidine isethionate	140-64-7	ph2	180	-6.0	N	170	8.8	N	170	-9.2	N
4-(1,1,3,3-Tetramethylbutyl)phenol	140-66-9	ph2	200	104.9	Y	200	87.5	Y	200	103.8	Y
Tannic acid	1401-55-4	ph2	60	98.5	Y	60	66.8	Y	60	64.4	Y
Diisobutyl adipate	141-04-8	ph2	200	-4.9	N	200	4.5	N	200	-15.6	N
Ethanolamine	141-43-5	ph2	200	-0.1	N	200	-3.3	N	200	-3.2	N
Hexanoic acid	142-62-1	ph2	200	0.6	N	200	-9.2	N	200	1.3	N
Kepone	143-50-0	ph2	200	97.0	Y	200	98.7	Y	200	88.1	Y
Diisopropyl methylphosphonate	1445-75-6	ph2	200	-7.3	N	200	-4.7	N	200	-2.5	N
Endothal	145-73-3	ph2	200	4.1	N	200	8.4	N	200	2.4	N
CP-122721	145742-28-5	ph2	200	12.7	N	200	33.8	N	200	-6.7	N
FR145237	146011-65-6	ph2	180	-3.6	N	150	-10.8	N	150	2.7	N
Tributyltin chloride	1461-22-9	ph2	200	1.9	N	200	26.2	N	200	6.3	N
Diphenhydramine hydrochloride	147-24-0	ph2	200	14.3	N	200	-19.2	N	200	-13.0	N
Bisphenol AF	1478-61-1	ph2	200	31.5	N	200	80.4	Y	200	50.0	Y
8-Hydroxyquinoline	148-24-3	ph2	200	-6.3	N	200	5.5	N	200	3.5	N
2-Mercaptobenzothiazole	149-30-4	ph2	200	88.2	Y	200	72.9	Y	200	45.8	Y
2-Ethylhexanoic acid	149-57-5	ph2	200	-2.1	N	200	-2.6	N	200	1.2	N
PharmaGSID_47259	149062-75-9	ph2	100	-0.3	N	100	-12.4	N	100	0.7	N
FR150011	149413-74-1	ph2	200	94.0	Y	200	85.6	Y	200	76.4	Y
4-Aminobenzoic acid	150-13-0	ph2	200	-3.9	N	200	2.2	N	200	-4.2	N
Monuron	150-68-5	ph2	200	7.0	N	200	-3.6	N	200	0.5	N
Sodium dodecyl sulfate	151-21-3	ph2	200	42.2	N	200	74.0	Y	200	81.1	Y
FR140423	151506-44-4	ph2	200	-3.8	N	200	-5.5	N	200	-8.3	N
Diclofenac sodium	15307-79-6	ph2	200	-9.3	N	200	2.9	N	200	3.2	N
Benodanil	15310-01-7	ph2	200	-8.1	N	200	-5.6	N	200	-8.8	N
6-Thioguanine	154-42-7	ph2	200	3.2	N	200	6.6	N	200	11.7	N
SR271425	155990-20-8	ph2	200	-11.4	N	200	2.0	N	200	3.8	N
1-Benzylquinolinium chloride	15619-48-4	ph2	200	-2.0	N	200	11.4	N	200	3.4	N
Carbofuran	1563-66-2	ph2	200	0.0	N	200	1.6	N	200	-1.5	N
CP-105696	158081-99-3	ph2	100	-10.4	N	100	48.8	N	100	6.0	N
Cariporide mesylate	159138-81-5	ph2	150	-5.2	N	140	8.9	N	140	9.8	N
UK-156819	162706-14-1	ph2	200	-6.8	N	200	3.9	N	200	-3.8	N
Aldicarb oxime	1646-75-9	ph2	200	-11.0	N	200	9.2	N	200	-8.4	N
Diisononyl cyclohexane-1,2-dicarboxylate	166412-78-8	ph2	200	2.7	N	200	2.9	N	200	9.4	N

Celecoxib	169590-42-5	ph2	200	75.1	Y	200	75.1	Y	200	88.9	Y
CP-283097	171866-31-2	ph2	100	-3.1	N	100	-0.6	N	100	9.0	N
FR167356	174185-16-1	ph2	200	2.2	N	200	10.5	N	200	-16.1	N
PharmaGSID_47261	177785-47-6	ph2	200	43.1	N	200	1.8	N	200	1.7	N
CJ-013790	179465-71-5	ph2	100	12.8	N	100	58.8	Y	100	50.4	Y
SB236057A	180084-01-9	ph2	170	-2.9	N	170	36.3	N	170	15.6	N
4-Octylphenol	1806-26-4	ph2	200	91.8	Y	200	93.8	Y	200	95.2	Y
SR144190	181640-09-5	ph2	200	-6.3	N	200	5.7	N	200	2.2	N
Nitrofen	1836-75-5	ph2	200	2.2	N	200	5.9	N	200	6.0	N
Octabenzene	1843-05-6	ph2	200	-15.1	N	200	0.3	N	200	0.8	N
Carabersat	184653-84-7	ph2	200	1.1	N	190	-0.1	N	190	-3.6	N
Chlorthal-dimethyl	1861-32-1	ph2	200	-3.8	N	190	-1.3	N	190	5.4	N
Ingliborib	186392-65-4	ph2	200	11.2	N	200	11.4	N	200	-7.5	N
Trelanserlin	189003-92-7	ph2	200	2.7	N	200	-7.8	N	200	-2.7	N
Vernolate	1929-77-7	ph2	200	-5.1	N	200	-0.2	N	200	-5.3	N
FD&C Yellow 5	1934-21-0	ph2	190	1.7	N	180	4.8	N	180	-3.2	N
CP-409092	194098-25-4	ph2	200	0.5	N	200	10.6	N	200	2.9	N
tert-Butylhydroquinone	1948-33-0	ph2	200	23.6	N	200	31.6	N	200	40.5	N
Farglitazar	196808-45-4	ph2	180	100.4	Y	170	100.1	Y	170	97.9	Y
UK-333747	197077-55-7	ph2	200	-0.4	N	200	-13.2	N	200	4.4	N
4-Heptylphenol	1987-50-4	ph2	200	99.5	Y	200	97.5	Y	200	103.0	Y
CP-401387	199171-88-5	ph2	100	-1.5	N	100	-0.4	N	100	-3.3	N
SB243213A	200940-23-4	ph2	180	-5.4	N	180	6.7	N	180	17.5	N
3,3'-Dimethoxybenzidine dihydrochloride	20325-40-0	ph2	200	-9.0	N	200	4.5	N	200	10.5	N
UK-337312	203942-49-8	ph2	200	103.4	Y	200	102.6	Y	200	99.7	Y
Benzo(b)fluoranthene	205-99-2	ph2	200	-5.8	N	100	1.6	N	100	-2.4	N
Oxytetracycline hydrochloride	2058-46-0	ph2	200	75.9	Y	200	29.1	Y	200	55.1	Y
Perfluoroundecanoic acid	2058-94-8	ph2	200	104.7	Y	100	96.1	Y	100	91.3	Y
Fluoranthene	206-44-0	ph2	200	-4.2	N	200	-1.0	N	200	3.9	N
CI-1029	207736-05-8	ph2	200	63.4	Y	200	12.5	N	200	39.8	N
Acenaphthylene	208-96-8	ph2	200	-5.0	N	200	-1.7	N	200	0.4	N
EPN	2104-64-5	ph2	200	-5.9	N	200	3.8	N	200	2.5	N
CP-456773	210826-40-7	ph2	200	-3.3	N	200	9.1	N	200	-0.5	N
Tridecafluorohexylethyl methacrylate	2144-53-8	ph2	200	-7.6	N	200	-3.6	N	200	-1.4	N
CP-457677	214535-77-0	ph2	200	9.6	N	200	4.3	N	200	-0.1	N
UK-343664	215297-27-1	ph2	100	-2.5	N	100	-0.5	N	100	-2.4	N
Tributyltin methacrylate	2155-70-6	ph2	200	-4.6	N	200	38.1	N	200	14.8	N

Pentachloropyridine	2176-62-7	ph2	200	27.9	N	200	55.7	Y	200	93.5	Y
SB281832	219790-72-4	ph2	200	4.3	N	200	-1.7	N	200	1.3	N
CP-457920	220860-50-4	ph2	200	-5.2	N	200	-0.5	N	200	5.9	N
Fandosentan potassium salt	221246-12-4	ph2	100	15.3	N	100	9.4	N	100	4.2	N
SR146131 trifluoroacetate (1:1)	221671-62-1	ph2	100	13.8	N	100	31.0	Y	100	97.1	Y
1,5-Naphthalenediamine	2243-62-1	ph2	200	8.9	N	200	23.6	N	200	48.1	N
Hexane-1,6-diyl dibenzoate	22915-73-7	ph2	200	-7.2	N	200	-0.8	N	200	-8.6	N
CP-544439	230954-09-3	ph2	200	4.5	N	200	0.5	N	200	1.7	N
Clotrimazole	23593-75-1	ph2	200	-9.0	N	200	41.9	N	200	12.1	N
1-[3-(Triethoxysilyl)propyl]urea	23779-32-0	ph2	200	1.6	N	200	1.3	N	200	0.9	N
Mirex	2385-85-5	ph2	200	2.3	N	200	-4.6	N	200	-3.1	N
Dexamethasone sodium phosphate	2392-39-4	ph2	200	8.0	N	200	2.4	N	200	5.5	N
2,3,6-Trimethylphenol	2416-94-6	ph2	200	2.6	N	200	-3.2	N	200	-5.3	N
Diocetyl succinate	2432-87-3	ph2	200	5.3	N	100	-3.5	N	100	2.0	N
4-Cyclohexylcyclohexanol	2433-14-9	ph2	200	8.2	N	200	0.6	N	200	-14.6	N
Triglycidyl isocyanurate	2451-62-9	ph2	200	2.2	N	200	2.8	N	200	9.2	N
Tridemorph	24602-86-6	ph2	200	-4.2	N	200	-7.2	N	200	1.8	N
CJ-013610	249296-43-3	ph2	200	2.5	N	200	3.3	N	200	-2.4	N
Sodium dodecylbenzenesulfonate	25155-30-0	ph2	200	103.9	Y	200	105.5	Y	200	95.8	Y
Dipropylene glycol	25265-71-8	ph2	200	0.6	N	200	-6.2	N	200	-2.1	N
Monobenzyl phthalate	2528-16-7	ph2	200	-6.1	N	200	1.0	N	200	7.8	N
Besonprodil	253450-09-8	ph2	200	-3.2	N	200	1.6	N	200	-3.3	N
Tripropylene glycol monomethyl ether	25498-49-1	ph2	200	-5.7	N	200	-3.1	N	200	-9.1	N
Dicyclohexyl disulfide	2550-40-5	ph2	200	7.0	N	200	-9.2	N	200	-2.4	N
Allura Red C.I.16035	25956-17-6	ph2	200	12.3	N	200	0.2	N	200	2.4	N
N,N-Dimethyldecylamine oxide	2605-79-0	ph2	200	-0.6	N	200	3.0	N	200	13.0	N
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	ph2	200	24.0	N	200	7.4	N	200	0.5	N
CP-532623	261947-38-0	ph2	200	-10.7	N	200	-0.1	N	200	-0.2	N
HMR1426	262376-75-0	ph2	200	65.4	Y	200	41.1	Y	200	64.4	Y
1,2-Benzisothiazolin-3-one	2634-33-5	ph2	200	11.8	N	200	-4.5	N	200	2.3	N
GW473178E methyl benzene sulphonic acid	263553-33-9	ph2	140	8.5	N	130	2.9	N	130	-5.6	N
SSR146977	264618-44-2	ph2	50	-14.1	N	50	16.3	N	50	-3.2	N
Octhilinone	26530-20-1	ph2	210	65.3	Y	200	84.1	Y	200	99.7	Y
Sodium azide	26628-22-8	ph2	200	3.0	N	200	1.7	N	200	-2.0	N
2,3-Diaminotoluene	2687-25-4	ph2	200	9.4	N	200	21.6	N	200	15.9	N
1-Dodecyl-2-pyrrolidinone	2687-96-9	ph2	200	92.5	Y	200	78.6	Y	200	88.2	Y
2,3-Benzofuran	271-89-6	ph2	200	-0.4	N	200	-0.3	N	200	-0.3	N

Di(propylene glycol) dibenzoate	27138-31-4	ph2	200	3.7	N	200	11.9	N	200	-2.5	N
Dodecylbenzenesulfonic acid	27176-87-0	ph2	200	106.2	Y	200	106.0	Y	200	102.5	Y
Diisodecyl hexanedioate	27178-16-1	ph2	200	-14.3	N	200	6.6	N	200	2.2	N
Dodecylbenzene sulfonate triethanolamine(1:1)	27323-41-7	ph2	180	102.0	Y	170	93.4	Y	170	94.7	Y
2,4-Bis(1-methyl-1-phenylethyl)phenol	2772-45-4	ph2	200	25.4	N	200	70.9	Y	200	68.6	Y
FD&C Yellow 6	2783-94-0	ph2	200	7.0	N	200	7.5	N	200	9.6	N
PFOS-K	2795-39-3	ph2	190	57.0	Y	190	63.5	Y	190	8.3	Y
4,4',4''-Ethane-1,1,1-triyltriphenol	27955-94-8	ph2	200	8.4	N	200	10.8	N	200	-1.7	N
5-Amino-2-methylphenol	2835-95-2	ph2	200	26.0	N	200	28.9	N	200	42.1	N
1H-1,2,4-Triazole	288-88-0	ph2	200	1.5	N	200	10.4	N	200	-2.4	N
Surinabant	288104-79-0	ph2	200	-10.2	N	200	1.6	N	200	16.5	N
CP-607366	289716-94-5	ph2	200	8.7	N	200	1.8	N	200	-6.6	N
CP-634384	290352-28-2	ph2	200	-0.9	N	200	8.3	N	200	-15.2	N
UK-373911	291305-06-1	ph2	200	45.9	N	200	85.1	Y	200	84.1	Y
Chlorpyrifos	2921-88-2	ph2	200	1.1	N	200	6.9	N	200	20.9	N
PFBS-K	29420-49-3	ph2	200	-11.2	N	200	8.0	N	200	-7.2	N
Triethoxyoctylsilane	2943-75-1	ph2	200	-4.6	N	200	-2.7	N	200	-1.2	N
Isooctyl acrylate	29590-42-9	ph2	200	71.1	Y	200	94.8	Y	200	77.0	Y
Phorate	298-02-2	ph2	200	3.4	N	200	3.0	N	200	1.3	N
Carbamazepine	298-46-4	ph2	200	0.1	N	200	-1.1	N	200	1.3	N
SSR180711	298198-52-4	ph2	200	1.9	N	200	-1.7	N	200	2.5	N
all-trans-Retinoic acid	302-79-4	ph2	200	21.0	N	200	57.3	Y	200	73.3	Y
N,N,N-Trimethyl(oxiran-2-yl)methanaminium chloride	3033-77-0	ph2	200	-1.3	N	200	2.4	N	200	-1.0	N
3'-Azido-3'-deoxythymidine	30516-87-1	ph2	200	-4.7	N	200	-2.1	N	200	2.6	N
Stavudine	3056-17-5	ph2	200	-0.7	N	200	3.3	N	200	4.9	N
PFHxA	307-24-4	ph2	200	-4.2	N	200	-2.6	N	200	1.7	N
Aldrin	309-00-2	ph2	200	-2.1	N	200	9.3	N	200	2.4	N
MK-578	313994-79-5	ph2	180	2.1	N	170	20.7	N	170	0.3	N
Octrizole	3147-75-9	ph2	200	6.3	N	200	-5.0	N	200	3.3	N
beta-Hexachlorocyclohexane	319-85-7	ph2	200	-0.1	N	200	5.1	N	200	5.5	N
Dibromoacetonitrile	3252-43-5	ph2	200	2.4	N	200	-1.2	N	200	3.7	N
Procymidone	32809-16-8	ph2	200	-2.5	N	200	0.3	Y	200	-5.6	Y
2,2-Bis(bromomethyl)-1,3-propanediol	3296-90-0	ph2	200	-12.1	N	200	2.9	N	200	-4.8	N
MK-547	331623-06-4	ph2	200	-4.6	N	200	12.1	N	200	2.8	N
Tris(2-ethylhexyl) trimellitate	3319-31-1	ph2	200	-7.5	N	200	2.1	N	200	3.0	N
4-Pentylaniline	33228-44-3	ph2	200	3.4	N	200	6.9	N	200	-8.4	N

Decanoic acid	334-48-5	ph2	210	-18.9	N	200	4.4	N	200	-5.7	N
PFDA	335-76-2	ph2	200	102.4	Y	200	103.1	Y	200	93.9	Y
Hexanedioic acid, diisononyl ester	33703-08-1	ph2	200	-6.1	N	200	-6.5	N	200	0.5	N
Isopropalin	33820-53-0	ph2	200	-1.2	N	200	3.9	N	200	6.4	N
SSR69071	344930-95-6	ph2	50	48.9	N	50	68.9	Y	50	88.2	Y
Dipropylene glycol monomethyl ether	34590-94-8	ph2	200	-1.4	N	200	3.2	N	200	2.6	N
PharmaGSID_47263	349495-42-7	ph2	200	-0.2	N	200	-0.3	N	200	-6.9	N
Butam	35256-85-0	ph2	200	-5.2	N	200	-8.0	N	200	-4.9	N
CP-612372	353280-07-6	ph2	200	-0.3	N	200	3.6	N	200	2.7	N
Elzasonan	361343-19-3	ph2	200	19.5	N	200	83.6	Y	200	-1.3	Y
1-Hexadecanol	36653-82-4	ph2	100	-0.5	N	100	-2.4	Y	100	0.3	Y
CP-728663	368832-42-2	ph2	200	-9.6	N	200	6.1	N	200	6.5	N
3-Phenoxybenzoic acid	3739-38-6	ph2	200	-10.8	N	200	-13.1	N	200	1.8	N
Perfluoroheptanoic acid	375-85-9	ph2	200	4.2	N	200	1.7	N	200	-19.2	N
PFNA	375-95-1	ph2	200	1.6	N	200	38.2	N	200	-8.0	N
Sodium (2-pyridylthio)-N-oxide	3811-73-2	ph2	200	0.3	N	200	10.6	N	200	4.0	N
PFOA, ammonium salt	3825-26-1	ph2	200	-3.7	N	200	0.0	Y	200	-15.2	Y
2,6,10-Trimethyl-2,6,10-triazaundecane	3855-32-1	ph2	200	-7.1	N	200	-9.2	N	200	3.8	N
PFHS-K	3871-99-6	ph2	200	-8.3	N	200	-9.8	N	200	-20.8	N
UK-416244	402910-27-4	ph2	200	8.5	N	200	17.5	N	200	-13.7	N
Methyl dopa sesquihydrate	41372-08-1	ph2	200	10.3	N	200	8.7	N	200	35.5	N
4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol]	41481-66-7	ph2	200	44.4	N	200	74.7	Y	200	58.3	Y
Sulfuramid	4151-50-2	ph2	190	-13.3	N	190	31.1	N	190	25.2	N
(E)-Anethole	4180-23-8	ph2	200	3.0	N	200	1.7	N	200	3.0	N
Cyproterone acetate	427-51-0	ph2	200	1.1	N	200	15.2	Y	200	87.2	Y
Cladribine	4291-63-8	ph2	200	1.5	N	100	1.6	N	100	2.5	N
SAR 150640	433212-21-6	ph2	190	51.6	Y	180	64.0	Y	180	35.8	Y
Nelivaptan	439687-69-1	ph2	200	13.2	N	200	10.1	N	200	6.1	N
Sodium dehydroacetate	4418-26-2	ph2	200	0.6	N	200	0.5	N	200	-0.3	N
Cycloamine	4449-51-8	ph2	200	-6.1	N	200	-13.3	N	200	-0.2	N
CP-671305	445295-04-5	ph2	200	-0.5	N	200	5.1	N	200	10.0	N
N-Methyldioctylamine	4455-26-9	ph2	200	-5.1	N	200	5.7	N	200	7.6	N
Genistein	446-72-0	ph2	200	90.1	Y	200	10.2	N	200	-2.5	N
Azathioprine	446-86-6	ph2	200	15.4	N	190	14.0	N	190	24.7	N
PharmaGSID_48510	460081-99-6	ph2	200	-11.0	N	200	3.1	N	200	-8.7	N
Aplaviroc hydrochloride	461023-63-2	ph2	200	-15.3	N	NA	NA	N	NA	NA	N
SSR 240612	464930-42-5	ph2	130	-21.4	N	90	-0.6	N	90	-4.5	N

Ilepatril	473289-62-2	ph2	200	13.5	N	200	-2.7	N	200	7.6	N
PHA-00543613	478149-53-0	ph2	200	5.0	N	200	-4.0	N	200	4.5	N
AVE3295	478263-98-8	ph2	170	13.0	N	170	11.0	N	170	15.7	N
Cotinine	486-56-6	ph2	200	-3.9	N	200	5.4	N	200	9.1	N
Daidzein	486-66-8	ph2	200	74.1	Y	200	-3.7	N	200	5.4	N
1,5,9-Cyclododecatriene	4904-61-4	ph2	200	0.4	N	200	-4.2	N	200	-1.7	N
Fenofibrate	49562-28-9	ph2	200	2.0	N	200	1.0	N	200	-4.6	N
3,4-Diaminotoluene	496-72-0	ph2	200	17.9	N	190	31.5	N	190	6.8	N
Corticosterone	50-22-6	ph2	200	-1.8	N	200	1.9	N	200	-5.0	N
17beta-Estradiol	50-28-2	ph2	200	-3.7	N	200	0.1	N	200	-2.5	N
p,p'-DDT	50-29-3	ph2	200	-4.6	N	200	2.7	N	200	-0.8	N
Thalidomide	50-35-1	ph2	200	1.7	N	200	-5.4	N	200	-3.7	N
Clomiphene citrate (1:1)	50-41-9	ph2	200	66.9	Y	200	94.6	Y	200	-2.5	Y
Aspirin	50-78-2	ph2	200	-5.0	N	200	1.7	N	200	3.9	N
PD-0333941	501027-49-2	ph2	200	-10.6	N	200	25.3	N	200	-3.0	N
Pirinixic acid	50892-23-4	ph2	200	-7.7	N	180	-3.8	N	180	5.4	N
5-Fluorouracil	51-21-8	ph2	200	-0.8	N	200	-3.2	N	200	0.3	N
Tiratricol	51-24-1	ph2	200	-23.1	N	2	0.5	N	2	-11.0	N
2,4-Dinitrophenol	51-28-5	ph2	200	-4.9	N	200	1.6	N	200	0.7	N
Isoproterenol hydrochloride	51-30-9	ph2	200	4.3	N	200	-1.9	N	200	5.5	N
6-Propyl-2-thiouracil	51-52-5	ph2	200	101.9	Y	200	1.7	N	200	4.0	N
Urethane	51-79-6	ph2	200	-0.5	N	200	-1.2	N	200	-3.8	N
Chlorobenzilate	510-15-6	ph2	200	3.4	N	200	9.8	N	200	10.5	N
Spiro lactone	52-01-7	ph2	200	8.0	N	200	84.4	Y	200	25.3	Y
Bronopol	52-51-7	ph2	200	4.3	N	200	0.8	N	200	6.1	N
Haloperidol	52-86-8	ph2	200	3.3	N	200	21.2	N	200	0.8	N
5alpha-Dihydrotestosterone	521-18-6	ph2	200	13.6	N	200	-5.7	N	200	-6.5	N
4-Chlorobenzotrithloride	5216-25-1	ph2	200	22.4	N	200	47.0	Y	200	55.6	Y
2,4,6-Trimethylphenol	527-60-6	ph2	200	-2.9	N	200	3.2	N	200	-5.9	N
PHA-00568487	527680-56-4	ph2	200	-5.3	N	200	-11.3	N	200	1.0	N
1,2-Dinitrobenzene	528-29-0	ph2	200	32.4	N	200	66.8	Y	200	78.0	Y
Hydroxyflutamide	52806-53-8	ph2	200	1.5	N	200	1.6	N	200	-6.7	N
Prednisone	53-03-2	ph2	200	-0.1	N	200	12.5	N	200	47.4	N
Estrone	53-16-7	ph2	200	-1.0	N	200	0.7	N	200	-7.5	N
Indomethacin	53-86-1	ph2	200	-18.2	N	200	4.6	N	200	-8.4	N
1-Hydroxypyrene	5315-79-7	ph2	200	60.1	Y	200	71.3	Y	200	91.0	Y
2-Chloroacetophenone	532-27-4	ph2	200	2.7	N	200	13.5	N	200	-2.6	N

Sodium benzoate	532-32-1	ph2	200	-3.8	N	200	1.5	N	200	1.3	N
2-Methyl-4,6-dinitrophenol	534-52-1	ph2	200	-9.1	N	200	6.2	N	200	6.9	N
4-(2-Methylbutan-2-yl)cyclohexanol	5349-51-9	ph2	200	3.6	N	200	-2.0	N	200	-11.0	N
Triisononyl trimellitate	53894-23-8	ph2	200	-1.9	N	200	3.2	N	200	0.7	N
3,7-Dimethyl-2,6-octadienal	5392-40-5	ph2	200	3.6	N	200	36.7	Y	200	67.2	Y
Nicotine	54-11-5	ph2	200	-2.7	N	190	0.3	N	190	1.4	N
4-Aminofolic acid	54-62-6	ph2	200	18.7	N	200	20.3	N	200	14.5	N
Isoniazid	54-85-3	ph2	90	8.1	N	80	1.2	N	80	-2.0	N
1,3-Dichlorobenzene	541-73-1	ph2	200	-13.9	N	200	-5.1	N	200	0.7	N
Hexadecane	544-76-3	ph2	200	-11.2	N	200	1.7	N	200	4.0	N
Gentian Violet	548-62-9	ph2	200	-4.2	N	200	31.9	Y	200	61.7	Y
Tamoxifen citrate	54965-24-1	ph2	180	95.1	Y	180	97.3	Y	180	33.0	Y
N-Nitrosodiethylamine	55-18-5	ph2	200	7.2	N	200	-6.5	N	200	-3.0	N
Busulfan	55-98-1	ph2	200	-9.1	N	200	0.4	N	200	2.2	N
Carbosulfan	55285-14-8	ph2	200	23.9	N	200	15.8	N	200	12.2	N
Dimethipin	55290-64-7	ph2	200	-0.4	N	200	3.7	N	200	9.9	N
4,4'-Bipyridine	553-26-4	ph2	200	-4.6	N	200	1.0	N	200	-1.9	N
Glycidol	556-52-5	ph2	200	-8.4	N	200	12.2	N	200	1.2	N
Octamethylcyclotetrasiloxane	556-67-2	ph2	200	-3.5	N	200	3.8	N	200	-3.0	N
6-Methyl-2-thiouracil	56-04-2	ph2	200	80.5	Y	200	8.3	N	200	3.2	N
Diethylstilbestrol	56-53-1	ph2	200	-5.7	N	200	45.6	N	200	28.4	N
Benz(a)anthracene	56-55-3	ph2	200	46.3	N	200	27.2	Y	200	57.7	Y
Glycerol	56-81-5	ph2	200	-0.6	N	200	2.0	N	200	2.5	N
Ethion	563-12-2	ph2	200	5.0	N	200	27.0	N	200	15.0	N
Octadecanoic acid	57-11-4	ph2	100	-3.5	N	100	15.0	N	100	18.6	N
Urea	57-13-6	ph2	200	-5.0	N	200	6.8	N	200	-4.2	N
Phenobarbital sodium	57-30-7	ph2	200	-3.8	N	200	0.4	N	200	-4.5	N
5,5-Diphenylhydantoin	57-41-0	ph2	200	-1.5	N	200	5.3	N	200	-5.5	N
Sucrose	57-50-1	ph2	200	-5.9	N	200	-1.6	N	200	-3.6	N
1,2-Propylene glycol	57-55-6	ph2	200	0.1	N	200	-3.3	N	200	-0.2	N
17alpha-Ethinylestradiol	57-63-6	ph2	200	7.2	N	200	5.5	N	200	-15.2	N
Chlordane	57-74-9	ph2	200	11.5	N	200	45.0	N	200	49.9	N
Progesterone	57-83-0	ph2	200	-6.3	N	200	2.2	N	200	-17.3	N
Testosterone propionate	57-85-2	ph2	200	0.9	N	0.2	-1.0	N	0.2	-0.9	N
17alpha-Estradiol	57-91-0	ph2	200	-8.7	N	200	0.5	N	200	-8.4	N
7,12-Dimethylbenz(a)anthracene	57-97-6	ph2	200	1.9	N	200	10.6	N	200	11.3	N
2,6-Dimethylphenol	576-26-1	ph2	200	-5.3	N	200	6.6	N	200	-3.1	N

Docusate sodium	577-11-7	ph2	200	106.2	Y	200	98.1	Y	200	90.4	Y
2,6-Diethylaniline	579-66-8	ph2	200	-4.4	N	200	2.0	N	200	-8.1	N
Caffeine	58-08-2	ph2	200	-4.4	N	200	-5.9	N	200	-1.3	N
Pyrimethamine	58-14-0	ph2	200	1.6	N	200	4.9	N	200	-7.6	N
17-Methyltestosterone	58-18-4	ph2	200	0.8	N	200	1.5	N	200	-3.8	N
Theophylline	58-55-9	ph2	200	-5.1	N	200	-14.7	N	200	2.7	N
Hydrochlorothiazide	58-93-5	ph2	200	0.1	N	200	-2.7	N	200	-1.2	N
Benzyloctyl adipate	58394-64-2	ph2	200	1.1	N	200	2.5	N	200	0.4	N
4-Amino-1,2,4-triazole	584-13-4	ph2	200	-4.5	N	200	0.1	N	200	-4.1	N
Toluene-2,4-diisocyanate	584-84-9	ph2	200	0.7	N	200	4.5	N	200	3.0	N
4-Ethyl-1-yn-3-ol	5877-42-9	ph2	200	0.6	N	200	49.9	N	200	34.6	N
PharmaGSID_48506	588941-45-1	ph2	200	-5.2	N	200	-4.3	N	200	4.2	N
Methotrexate	59-05-2	ph2	200	1.3	N	200	4.2	N	200	8.9	N
Folic acid	59-30-3	ph2	200	-4.4	N	200	7.0	N	200	-1.5	N
4-Chloro-3-methylphenol	59-50-7	ph2	200	-1.3	N	200	1.7	N	200	-15.0	N
Nicotinic acid	59-67-6	ph2	200	5.8	N	190	-0.9	N	190	6.0	N
Nitrofurazone	59-87-0	ph2	200	2.0	N	200	-2.0	N	200	19.7	N
Terbutylazine	5915-41-3	ph2	200	-2.3	N	200	14.1	Y	200	50.7	Y
Fluridone	59756-60-4	ph2	200	0.6	N	200	-5.7	N	200	-9.8	N
4-Cumylphenol	599-64-4	ph2	200	9.6	N	200	5.2	N	200	-7.5	N
Sulfasalazine	599-79-1	ph2	200	82.4	Y	200	3.8	N	200	-6.8	N
4-Aminoazobenzene	60-09-3	ph2	200	-5.0	N	200	4.2	N	200	-5.3	N
Acetamide	60-35-5	ph2	200	0.4	N	200	1.4	N	200	9.9	N
Tetracycline	60-54-8	ph2	200	64.4	Y	200	36.4	Y	200	50.1	Y
Methimazole	60-56-0	ph2	200	-13.4	N	200	1.3	N	200	0.6	N
Dieldrin	60-57-1	ph2	200	-4.4	N	190	13.8	N	190	22.8	N
2,3-Dinitrotoluene	602-01-7	ph2	140	28.1	N	140	53.7	Y	140	76.4	Y
2,6-Dinitrotoluene	606-20-2	ph2	200	-0.8	N	200	-0.8	N	200	-8.7	N
tert-Butyl perbenzoate	614-45-9	ph2	200	2.1	N	200	-4.9	N	200	8.9	N
4-Nitrobenzoic acid	62-23-7	ph2	200	1.0	N	200	1.3	N	200	4.2	N
Phenylmercuric acetate	62-38-4	ph2	200	23.5	N	200	26.4	N	200	5.1	N
N-Nitrosodimethylamine	62-75-9	ph2	200	1.9	N	200	0.3	N	200	-1.8	N
N-Nitrosodipropylamine	621-64-7	ph2	200	-6.3	N	190	-0.6	N	190	-0.6	N
Piragliatin	625114-41-2	ph2	50	-5.1	N	50	-9.3	N	50	0.1	N
3-Bromo-1-propanol	627-18-9	ph2	200	1.3	N	200	0.9	N	200	-2.0	N
Dimethyl adipate	627-93-0	ph2	200	-0.8	N	200	-12.3	N	200	3.2	N
Pentyl acetate	628-63-7	ph2	200	-1.1	N	200	-1.0	N	200	-0.1	N

Pentadecane	629-62-9	ph2	200	-1.0	N	200	3.8	N	200	2.7	N
1-Pentadecanol	629-76-5	ph2	200	-0.1	N	200	0.2	N	200	4.9	N
4-Androstene-3,17-dione	63-05-8	ph2	200	1.1	N	200	-2.5	N	200	-9.0	N
3-Hydroxyfluorene	6344-67-8	ph2	200	-13.4	N	200	14.8	N	200	-1.5	N
Nilutamide	63612-50-0	ph2	200	-3.9	N	200	2.6	N	200	-0.1	N
Clofibrate	637-07-0	ph2	200	3.5	N	200	-0.7	N	200	0.2	N
Sodium erythorbate (1:1)	6381-77-7	ph2	200	-5.8	N	200	1.8	N	200	6.7	N
Acetic acid	64-19-7	ph2	200	-15.8	N	200	3.4	N	200	0.2	N
Diethyl sulfate	64-67-5	ph2	200	0.3	N	200	0.2	N	200	-1.8	N
Colchicine	64-86-8	ph2	200	-3.1	N	200	-0.6	N	200	0.4	N
Bis(2-ethylhexyl) terephthalate	6422-86-2	ph2	200	-3.6	N	200	0.5	N	200	-5.2	N
1,2-Benzenedicarboxaldehyde	643-79-8	ph2	200	82.2	Y	200	87.6	Y	200	93.4	Y
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol	647-42-7	ph2	200	-11.8	N	200	-25.3	N	200	-42.7	N
AVE2865	648917-13-9	ph2	100	-15.0	N	100	1.7	N	100	-2.0	N
Pyridoxine	65-23-6	ph2	200	-15.6	N	200	5.8	N	200	3.1	N
Benzoic acid	65-85-0	ph2	200	-0.6	N	200	-1.6	N	200	3.2	N
Ketoconazole	65277-42-1	ph2	200	-2.8	N	200	24.3	N	200	17.6	N
Methyl methanesulfonate	66-27-3	ph2	200	-1.5	N	200	6.9	N	200	2.2	N
Cycloheximide	66-81-9	ph2	200	-4.6	N	200	-1.1	N	200	2.5	N
Pentane-1,5-diyl dibenzoate	6624-73-3	ph2	200	3.1	N	200	5.9	N	200	0.8	N
Adipic acid, polypropyleneglycol, laurate	66456-53-9	ph2	100 µg/ml	2.5	N	100 µg/ml	-9.1	N	100 µg/ml	-7.7	N
CP-863187	668981-02-0	ph2	200	-3.9	N	200	4.9	N	200	19.3	N
Nitrofurantoin	67-20-9	ph2	200	7.9	N	200	-0.1	N	200	11.1	N
PD 0343701	676116-04-4	ph2	200	-4.6	N	200	4.0	N	200	3.3	N
1,1,2,2-Tetrahydroperfluoro-1-decanol	678-39-7	ph2	200	-0.2	N	200	4.4	N	200	2.4	N
N,N-Dimethylformamide	68-12-2	ph2	200	-0.9	N	200	5.3	N	200	1.5	N
Norethindrone	68-22-4	ph2	200	4.9	N	200	11.3	N	200	33.0	N
Retinol	68-26-8	ph2	210	25.1	N	200	51.6	Y	200	72.1	Y
17alpha-Hydroxyprogesterone	68-96-2	ph2	200	-1.1	N	200	-2.1	N	200	-6.3	N
4-Hydroxytamoxifen	68392-35-8	ph2	130	103.7	Y	120	103.3	Y	120	28.3	Y
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	ph2	200	-1.2	N	200	2.9	N	200	1.4	N
1,2-Benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich	68515-49-1	ph2	200	-6.3	N	200	4.2	N	200	10.6	N
PharmaGSID_48519	686756-87-6	ph2	200	-10.4	N	200	23.5	Y	200	1.3	Y
Chlorpromazine hydrochloride	69-09-0	ph2	200	39.0	N	200	72.0	Y	200	45.1	Y
D-Mannitol	69-65-8	ph2	200	-3.4	N	200	2.4	N	200	7.5	N

Cytarabine hydrochloride	69-74-9	ph2	200	6.5	N	200	0.6	N	200	-1.9	N
Malic acid	6915-15-7	ph2	200	-5.8	N	200	5.6	N	200	1.3	N
2',3'-Dideoxyinosine	69655-05-6	ph2	200	-3.2	N	200	-9.6	N	200	-2.7	N
Cyclohexylphenylketone	712-50-5	ph2	200	3.3	N	200	4.7	N	200	2.1	N
Didecyldimethylammonium chloride	7173-51-5	ph2	200	106.0	Y	200	102.5	Y	200	98.0	Y
Endrin	72-20-8	ph2	200	-11.9	N	200	-0.4	N	200	8.1	N
p,p'-DDD	72-54-8	ph2	200	5.0	N	200	15.1	N	200	26.9	N
p,p'-DDE	72-55-9	ph2	200	6.9	N	200	-2.2	N	200	6.5	N
Fomesafen	72178-02-0	ph2	200	-7.6	N	200	0.5	N	200	9.7	N
AVE5638	725228-45-5	ph2	200	73.2	Y	200	94.5	Y	200	96.9	Y
Phosmet	732-11-6	ph2	200	76.3	Y	200	15.4	N	200	21.1	N
2,4,6-Tris(tert-butyl)phenol	732-26-3	ph2	200	-4.7	N	200	9.1	N	200	25.9	N
N,N-Dimethyloctylamine	7378-99-6	ph2	200	-1.0	N	200	-0.7	N	200	-3.5	N
SSR504734	742693-38-5	ph2	200	4.7	N	200	25.5	N	200	-1.6	N
Diphenyl isophthalate	744-45-6	ph2	200	37.6	N	200	38.6	Y	200	59.7	Y
Mercuric chloride	7487-94-7	ph2	200	43.0	N	200	27.7	N	200	36.6	N
Formamide	75-12-7	ph2	200	1.0	N	200	-13.3	N	200	1.6	N
Dalapon	75-99-0	ph2	200	-5.1	N	200	-19.9	N	200	-2.9	N
Lovastatin	75330-75-5	ph2	200	88.0	Y	200	31.9	Y	200	51.7	Y
PFOSA	754-91-6	ph2	200	16.7	N	200	17.6	N	200	-11.2	N
Trichloroacetic acid	76-03-9	ph2	200	0.4	N	200	3.0	N	200	0.3	N
Heptachlor	76-44-8	ph2	200	3.8	N	200	14.1	N	200	31.8	N
Silica	7631-86-9	ph2	200	0.5	N	200	-1.1	N	200	-1.8	N
Sodium nitrite	7632-00-0	ph2	200	6.6	N	200	1.7	N	200	3.3	N
Phenolphthalein	77-09-8	ph2	200	3.7	N	200	23.9	N	200	0.5	N
Bisphenol B	77-40-7	ph2	200	-1.4	N	200	20.0	N	200	-8.8	N
Hexachlorocyclopentadiene	77-47-4	ph2	200	69.2	Y	200	99.0	Y	200	95.6	Y
1,3-Dibromo-5,5-dimethylhydantoin	77-48-5	ph2	200	4.7	N	200	2.4	N	200	0.9	N
5,5-Dimethylhydantoin	77-71-4	ph2	200	0.6	N	200	6.4	N	200	-4.3	N
Dimethyl sulfate	77-78-1	ph2	200	6.0	N	200	4.9	N	200	-5.3	N
Acetyltriethyl citrate	77-89-4	ph2	200	-3.6	N	200	4.6	N	200	10.9	N
Acetyl tributyl citrate	77-90-7	ph2	200	-8.9	N	200	3.7	N	200	3.1	N
Citric acid	77-92-9	ph2	200	-5.5	N	200	2.6	N	200	4.9	N
Triethyl citrate	77-93-0	ph2	200	-1.8	N	200	6.6	N	200	2.2	N
5-Ethyl-1-aza-3,7-dioxabicyclo[3.3.0]octane	7747-35-5	ph2	200	-2.7	N	200	6.6	N	200	3.8	N
Sodium chlorite	7758-19-2	ph2	200	-6.8	N	200	2.2	N	200	-3.5	N
Tris(2-ethylhexyl) phosphate	78-42-2	ph2	200	1.7	N	200	-0.5	N	200	4.0	N

Isophorone	78-59-1	ph2	200	-7.3	N	200	-3.6	N	200	-7.4	N
2,5-Dimethyl-2,5-di-(tert-butylperoxy)hexane	78-63-7	ph2	200	7.4	N	200	6.0	N	200	-1.1	N
o,p'-DDT	789-02-6	ph2	200	-4.2	N	190	-3.9	N	190	5.1	N
Acrylamide	79-06-1	ph2	200	4.7	N	200	-10.0	N	200	2.2	N
N-Methylacetamide	79-16-3	ph2	200	3.1	N	200	2.6	N	200	-7.9	N
Methacrylamide	79-39-0	ph2	200	2.2	N	200	-13.8	N	200	2.1	N
Dichloroacetic acid	79-43-6	ph2	200	-0.4	N	200	3.3	N	200	2.3	N
Dimethylcarbamoyl chloride	79-44-7	ph2	200	-4.3	N	190	1.3	N	190	-2.7	N
3,3',5,5'-Tetrabromobisphenol A	79-94-7	ph2	190	106.0	Y	190	104.1	Y	190	87.4	Y
Norgestrel	797-63-7	ph2	200	-1.7	N	200	3.8	N	200	19.8	N
Simvastatin	79902-63-9	ph2	200	83.4	Y	200	34.7	Y	200	56.8	Y
Dapsone	80-08-0	ph2	200	-0.1	Y	200	2.3	N	200	-0.4	N
Cumene hydroperoxide	80-15-9	ph2	200	23.4	N	200	5.6	N	200	-6.1	N
Dicumyl peroxide	80-43-3	ph2	200	0.0	N	200	3.5	N	200	0.1	N
4-(2-Methylbutan-2-yl)phenol	80-46-6	ph2	200	-6.2	N	200	-2.4	N	200	-16.0	N
Clove leaf oil	8000-34-8	ph2	100 µg/ml	5.3	N	52 µg/ml	-6.0	N	52 µg/ml	-3.8	N
Etofenprox	80844-07-1	ph2	200	-0.3	N	200	2.1	N	200	-0.1	N
Warfarin	81-81-2	ph2	200	-2.9	N	200	1.0	N	200	-0.8	N
Phenolphthalin	81-90-3	ph2	200	2.9	N	200	22.5	N	200	5.7	N
Pravastatin sodium	81131-70-6	ph2	100	-15.9	N	100	-4.7	N	100	5.3	N
Sodium saccharin hydrate	82385-42-0	ph2	200	-3.6	N	200	8.7	N	200	6.3	N
Sodium 4-nitrophenolate	824-78-2	ph2	200	-9.6	N	200	-3.0	N	200	-3.0	N
Butyryl trihexyl citrate	82469-79-2	ph2	200	-10.3	Y	200	6.3	N	200	0.6	N
PharmaGSID_48513	825643-57-0	ph2	160	11.6	N	160	-8.1	N	160	27.0	N
2-Norbornene-5,6-dicarboxylic anhydride	826-62-0	ph2	200	-2.1	N	200	3.9	N	200	3.7	N
Raloxifene hydrochloride	82640-04-8	ph2	200	13.8	N	200	50.2	Y	200	-1.5	Y
Dimethoxane	828-00-2	ph2	200	-1.6	N	200	-9.0	N	200	1.0	N
Acenaphthene	83-32-9	ph2	200	0.6	N	200	0.1	N	200	2.0	N
1,2-Dimethyl-3-nitrobenzene	83-41-0	ph2	200	0.1	N	200	3.6	N	200	2.8	N
Theobromine	83-67-0	ph2	80	1.5	N	80	-1.9	N	80	-0.7	N
4,4'-Methylenebis(2-methylaniline)	838-88-0	ph2	200	0.3	N	200	10.7	N	200	-9.4	N
meso-Hexestrol	84-16-2	ph2	200	26.2	N	200	49.8	N	200	46.7	N
Diethyl phthalate	84-66-2	ph2	200	16.3	N	200	5.1	N	200	4.3	N
Diisobutyl phthalate	84-69-5	ph2	200	-6.1	N	200	-2.0	N	200	-10.4	N
Dihexyl phthalate	84-75-3	ph2	200	4.3	N	200	-16.6	N	200	-0.3	N
C.I. Solvent Yellow 14	842-07-9	ph2	200	11.1	N	200	0.1	N	200	24.2	N

Mifepristone	84371-65-3	ph2	200	-8.5	N	190	9.9	N	190	35.6	N
4-Nonylphenol, branched	84852-15-3	ph2	200	101.9	Y	200	92.1	Y	200	96.6	Y
Phenanthrene	85-01-8	ph2	200	-9.7	N	200	0.9	N	200	1.8	N
Benzyl butyl phthalate	85-68-7	ph2	200	-4.1	N	200	-6.8	N	200	-10.9	N
MK-812	851916-42-2	ph2	200	2.1	N	200	0.2	N	200	-1.9	N
PK 11195	85532-75-8	ph2	130	0.1	N	120	-1.7	N	120	-8.8	N
N-Nitrosodiphenylamine	86-30-6	ph2	200	3.4	N	200	7.7	N	200	1.2	N
Fluorene	86-73-7	ph2	200	-5.1	N	200	-4.0	N	200	2.0	N
AVE9423	862243-29-6	ph2	200	5.9	N	200	3.4	N	200	-0.3	N
Fluconazole	86386-73-4	ph2	200	-8.1	N	200	-7.1	N	200	-4.1	N
GSK232420A	864283-48-7	ph2	200	-5.4	N	200	5.3	N	200	1.2	N
Hexaflumuron	86479-06-3	ph2	200	-1.8	N	200	3.8	N	200	3.7	N
1,2,3-Trichlorobenzene	87-61-6	ph2	200	0.3	N	200	-6.0	N	200	11.3	N
2,6-Dimethylaniline	87-62-7	ph2	210	5.8	N	200	7.7	N	200	-0.9	N
L-Tartaric acid	87-69-4	ph2	200	1.9	N	200	1.3	N	200	0.4	N
Pentachlorophenol	87-86-5	ph2	100	46.9	N	100	15.4	N	100	4.3	N
N-Methyl-2-pyrrolidone	872-50-4	ph2	200	3.1	N	200	-0.4	N	200	4.9	N
2,4,6-Trichlorophenol	88-06-2	ph2	200	2.9	N	200	4.2	N	200	-3.1	N
N-Vinyl-2-pyrrolidone	88-12-0	ph2	200	-2.3	N	200	7.7	N	200	1.2	N
2-tert-Butylphenol	88-18-6	ph2	200	-0.3	N	200	-3.2	N	200	4.6	N
2,5-Di-tert-butylbenzene-1,4-diol	88-58-4	ph2	200	-1.5	N	200	0.8	N	200	0.0	N
2-tert-Butyl-5-methylphenol	88-60-8	ph2	200	5.1	N	200	-2.4	N	200	-3.4	N
2-Nitrotoluene	88-72-2	ph2	200	-4.4	N	200	-11.6	N	200	0.4	N
Dinoseb	88-85-7	ph2	200	-14.7	N	200	15.0	N	200	2.1	N
Trioctyl trimellitate	89-04-3	ph2	200	-0.6	N	200	-0.2	N	200	3.1	N
2-(Butan-2-yl)phenol	89-72-5	ph2	200	-5.0	N	200	5.0	N	200	-4.3	N
Thymol	89-83-8	ph2	200	-2.3	N	200	1.7	N	200	-7.5	N
2-Anisidine	90-04-0	ph2	200	-2.2	N	200	6.2	N	200	4.3	N
1-Methylnaphthalene	90-12-0	ph2	200	5.4	N	200	3.2	N	200	2.3	N
Michler's ketone	90-94-8	ph2	200	14.2	N	200	13.8	N	200	9.6	N
Naphthalene	91-20-3	ph2	200	-3.7	N	200	-6.5	N	200	-1.2	N
Quinoline	91-22-5	ph2	200	-3.7	N	200	-3.2	N	200	-3.3	N
Ethoxyquin	91-53-2	ph2	200	2.4	N	200	22.5	N	200	36.3	N
2-Naphthylamine	91-59-8	ph2	200	3.1	N	200	6.9	N	200	2.0	N
6-Methylquinoline	91-62-3	ph2	200	-1.2	N	200	4.3	N	200	3.6	N
Coumarin	91-64-5	ph2	200	-1.3	N	200	2.8	N	200	3.9	N
N,N-Diethylaniline	91-66-7	ph2	200	4.9	N	200	-9.1	N	200	2.1	N

C10-21 sulfonic acids phenyl esters	91082-17-6	ph2	100 µg/ml	3.5	N	100 µg/ml	-0.7	N	100 µg/ml	9.2	N
Biphenyl	92-52-4	ph2	200	-4.0	N	200	3.6	N	200	0.3	N
4-Cyclohexylcyclohexanone	92-68-2	ph2	200	0.4	N	200	10.0	N	200	34.2	N
Phenothiazine	92-84-2	ph2	200	0.3	N	200	7.3	N	200	-0.1	N
Benzidine	92-87-5	ph2	200	-5.7	N	200	-0.6	N	200	0.9	N
N-Nitrosodibutylamine	924-16-3	ph2	200	3.6	N	200	-1.4	N	200	-3.3	N
2,2'-[Ethane-1,2-diylbis(oxy)]diethanamine	929-59-9	ph2	200	1.4	N	200	2.1	N	200	6.3	N
SR58611	929601-09-2	ph2	180	4.0	N	180	35.5	N	180	-17.9	N
Methyleugenol	93-15-2	ph2	200	7.0	N	200	0.3	N	200	-2.9	N
Propylparaben	94-13-3	ph2	200	2.4	N	200	3.6	N	200	-4.0	N
Butylparaben	94-26-8	ph2	200	1.0	N	200	1.1	N	200	-10.7	N
Triethylene glycol bis(2-ethylhexanoate)	94-28-0	ph2	200	-5.1	N	200	2.9	N	200	-1.7	N
Safrole	94-59-7	ph2	200	-1.4	N	200	2.5	N	200	2.6	N
1,2,3-Benzotriazole	95-14-7	ph2	200	-3.4	N	200	-3.4	N	200	-1.3	N
o-Cresol	95-48-7	ph2	200	5.1	N	200	1.5	N	200	-0.7	N
2-Chlorotoluene	95-49-8	ph2	200	0.6	N	200	-0.2	N	200	0.5	N
1,2-Dichlorobenzene	95-50-1	ph2	200	-2.6	N	200	1.3	N	200	-1.2	N
2-Methylaniline	95-53-4	ph2	200	-0.1	N	200	5.7	N	200	-2.2	N
1,2-Phenylenediamine	95-54-5	ph2	200	-2.3	N	200	14.1	N	200	8.0	N
2-Chlorophenol	95-57-8	ph2	200	-5.1	N	200	2.4	N	200	-2.4	N
1,2,4-Trimethylbenzene	95-63-6	ph2	210	-5.1	N	200	2.4	N	200	3.2	N
3,4-Dimethylphenol	95-65-8	ph2	200	-1.1	N	200	-7.5	N	200	3.1	N
2,4-Diaminotoluene	95-80-7	ph2	200	14.3	N	200	-11.6	N	200	8.5	N
4-Chloro-1,2-diaminobenzene	95-83-0	ph2	200	4.7	N	200	7.3	N	200	-2.6	N
2,5-Dimethylphenol	95-87-4	ph2	200	-2.3	N	200	-0.7	N	200	2.9	N
1,2,4,5-Tetrachlorobenzene	95-94-3	ph2	200	1.7	N	200	2.0	N	200	-5.2	N
2,4,5-Trichlorophenol	95-95-4	ph2	200	-11.4	N	200	9.7	N	200	-3.5	N
Styrene oxide	96-09-3	ph2	200	7.0	N	200	-2.0	N	200	6.3	N
1,2,3-Trichloropropane	96-18-4	ph2	200	2.3	N	200	1.2	N	200	-6.3	N
1,3-Dichloro-2-propanol	96-23-1	ph2	200	-13.0	N	200	9.9	N	200	-6.7	N
2-Butanone oxime	96-29-7	ph2	200	4.3	N	200	-7.2	N	200	4.2	N
4-Butyrolactone	96-48-0	ph2	200	-2.5	N	200	1.6	N	200	-2.6	N
2-tert-Butyl-4-ethylphenol	96-70-8	ph2	200	4.7	N	200	0.5	N	200	-6.7	N
2,4-Di-tert-butylphenol	96-76-4	ph2	200	92.4	Y	200	61.6	Y	200	91.6	Y
Eugenol	97-53-0	ph2	200	4.8	N	200	15.8	N	200	11.0	N
Isoeugenol	97-54-1	ph2	200	9.9	N	200	51.3	Y	200	86.1	Y

2-Amino-5-azotoluene	97-56-3	ph2	200	5.2	N	200	3.0	N	200	-2.6	N
Disulfiram	97-77-8	ph2	200	12.4	N	200	6.2	N	200	20.8	N
Troglitazone	97322-87-7	ph2	200	100.4	Y	200	86.3	Y	200	93.0	Y
Furfural	98-01-1	ph2	200	-1.0	N	200	0.0	N	200	4.2	N
tert-Butylbenzene	98-06-6	ph2	200	-5.6	N	200	4.7	N	200	2.9	N
Benzotrichloride	98-07-7	ph2	200	-2.5	N	200	10.3	N	200	2.4	N
4-tert-Butylphenol	98-54-4	ph2	200	-6.5	N	200	-2.1	N	200	-13.3	N
Acetophenone	98-86-2	ph2	200	-5.0	N	200	-1.9	N	200	-1.6	N
Benzal chloride	98-87-3	ph2	200	2.2	N	200	0.7	N	200	2.7	N
Nitrobenzene	98-95-3	ph2	200	-5.8	N	200	-1.9	N	200	-1.1	N
3-Nitrotoluene	99-08-1	ph2	200	-4.3	N	200	7.6	N	200	-9.1	N
1,2-Dimethyl-4-nitrobenzene	99-51-4	ph2	200	3.1	N	200	4.6	N	200	2.4	N
3,4-Dichloronitrobenzene	99-54-7	ph2	200	1.3	N	200	9.0	N	200	34.2	N
2-Methyl-5-nitroaniline	99-55-8	ph2	200	6.7	N	200	-1.4	N	200	-1.8	N
2-Methoxy-5-nitroaniline	99-59-2	ph2	200	-6.7	N	200	1.5	N	200	-20.6	N
1,3-Diisopropylbenzene	99-62-7	ph2	200	31.4	N	200	2.9	N	200	-0.5	N
1,3-Dinitrobenzene	99-65-0	ph2	210	-5.3	N	200	-18.1	N	200	5.3	N
Valproic acid	99-66-1	ph2	200	0.3	N	200	-1.7	N	200	5.0	N
4-(Butan-2-yl)phenol	99-71-8	ph2	200	-0.8	N	200	-4.1	N	200	-7.4	N
Methylparaben	99-76-3	ph2	200	-4.9	N	200	12.1	N	200	-1.3	N
p-Cymene	99-87-6	ph2	200	-3.9	N	200	3.0	N	200	2.2	N
N,N,4-Trimethylaniline	99-97-8	ph2	200	5.2	N	200	5.0	N	200	10.3	N
4-Nitrotoluene	99-99-0	ph2	200	-4.5	N	200	-0.2	N	200	0.9	N
CI-1018	NOCAS_47248	ph2	200	7.0	N	200	-4.7	N	200	-7.0	N
CP-465394	NOCAS_47255	ph2	100	-0.7	N	100	3.4	N	100	0.4	N
CP-471358	NOCAS_47265	ph2	200	-3.3	N	200	5.5	N	200	-1.6	N
CP-642931	NOCAS_47267	ph2	100	-2.4	N	100	-2.4	N	100	-5.8	N
CI-1044	NOCAS_47291	ph2	200	-1.5	N	200	-5.5	N	200	3.0	N
PD 0200347	NOCAS_47292	ph2	200	2.0	N	200	5.0	N	200	-3.8	N
CP-422935	NOCAS_47299	ph2	200	-4.8	N	200	0.8	N	200	-3.9	N
CP-608039	NOCAS_47305	ph2	190	-0.2	N	180	2.6	N	180	-2.0	N
SB413217A	NOCAS_47325	ph2	90	-3.3	N	90	-0.5	N	90	25.4	N
MK-274	NOCAS_47328	ph2	200	23.5	N	200	51.0	Y	200	35.2	Y
PharmaGSID_47330	NOCAS_47330	ph2	200	0.3	N	200	-5.0	N	200	12.0	N
PharmaGSID_47333	NOCAS_47333	ph2	200	-4.9	N	200	5.6	N	200	-0.9	N
MK-968	NOCAS_47334	ph2	200	-5.4	N	200	13.7	N	200	-4.1	N
SR125047	NOCAS_47342	ph2	180	-3.7	N	180	90.0	Y	180	73.7	Y

SSR162369	NOCAS_47346	ph2	200	1.5	N	200	9.1	N	200	26.1	N
SSR 241586 HCl	NOCAS_47353	ph2	120	12.3	N	120	77.6	Y	120	2.2	Y
SAR115740	NOCAS_47366	ph2	200	16.0	N	200	9.3	N	200	5.2	N
SSR161421	NOCAS_47374	ph2	200	-8.9	N	200	1.2	N	200	4.0	N
AVE6324	NOCAS_47377	ph2	200	88.4	Y	200	107.7	Y	200	96.9	Y
SSR126768	NOCAS_47379	ph2	200	-4.0	N	200	15.4	N	200	8.1	N
AVE8923	NOCAS_47381	ph2	20	9.5	N	10	14.4	N	10	-2.0	N
AVE3247	NOCAS_47383	ph2	50	-3.7	N	40	0.7	N	40	-3.1	N
SAR377142	NOCAS_47385	ph2	180	-4.9	N	170	2.5	N	170	12.9	N
SAR102779	NOCAS_47387	ph2	200	-3.7	N	150	61.2	Y	150	10.4	Y
Grinstad Soft-N-Safe	NOCAS_47394	ph2	100 µg/ml	-8.4	N	100 µg/ml	9.3	N	100 µg/ml	-16.5	N
3,9-Epoxy-3H-azirino[2,3-c][1]benzazocine-5-carboxaldehyde, 1-acetyl-9-(acetyloxy)-8-[[[(aminocarbonyloxy)methyl]-1,1a,2,8,9,9a-hexahydro-7-methoxy-, (1aS,8R,9S,9aS)-	NOCAS_48166	ph2	200	8.9	N	200	1.5	N	200	2.5	N
PharmaGSID_48172	NOCAS_48172	ph2	170	-21.0	N	160	0.7	N	160	4.4	N
YM218	NOCAS_48176	ph2	120	-11.0	N	120	2.9	N	120	-6.5	N
PharmaGSID_48505	NOCAS_48505	ph2	200	-2.8	N	200	5.7	N	200	-0.4	N
PharmaGSID_48507	NOCAS_48507	ph2	200	3.2	N	200	1.3	N	200	-7.5	N
PharmaGSID_48509	NOCAS_48509	ph2	200	-2.8	N	200	-5.7	N	200	4.9	N
PharmaGSID_48514	NOCAS_48514	ph2	200	-13.1	N	200	2.6	N	200	2.8	N
PharmaGSID_48516	NOCAS_48516	ph2	200	-7.3	N	200	1.7	N	200	-8.2	N
PharmaGSID_48518	NOCAS_48518	ph2	200	11.8	N	200	0.2	N	200	13.1	N
HMR1171 trifluoroacetate (1:1)	NOCAS_48522	ph2	80	65.8	Y	70	76.6	Y	70	39.8	Y
Terephthalic acid	100-21-0	e1k	200	-2.7	N	200	-1.3	N	200	4.6	N
Cyclohexanone oxime	100-64-1	e1k	200	-2.6	N	190	2.2	N	190	6.9	N
Dysprosium(III) chloride	10025-74-8	e1k	190	-4.9	N	180	7.9	N	180	7.8	N
2-Propyl-1-heptanol	10042-59-8	e1k	200	-1.7	N	200	7.9	N	200	0.0	N
Sodium 2-formylbenzenesulfonate	1008-72-6	e1k	200	-1.6	N	190	0.0	N	190	2.1	N
4-(2-Phenylpropan-2-yl)-N-[4-(2-phenylpropan-2-yl)phenyl]aniline	10081-67-1	e1k	200	-5.3	N	200	0.9	N	200	10.7	N
1,1-Dimethyl-2-phenylethyl butanoate	10094-34-5	e1k	200	-4.5	N	200	-13.8	N	200	3.2	N
2,4,6-Tris(allyloxy)-1,3,5-triazine	101-37-1	e1k	200	0.0	N	200	-9.4	N	200	-1.3	N
Fenuron	101-42-8	e1k	200	-0.3	N	200	-13.3	N	200	3.5	N
Diphenylmethane	101-81-5	e1k	200	1.0	N	200	4.2	N	200	4.7	N
Dicyclohexylamine	101-83-7	e1k	200	0.7	N	200	4.3	N	200	6.3	N
Diphenyl oxide	101-84-8	e1k	200	1.6	N	200	-4.3	N	200	6.0	N

Flufenoxuron	101463-69-8	e1k	200	0.8	N	200	1.5	N	200	2.4	N
Fadrozole hydrochloride	102676-31-3	e1k	100	-3.5	N	100	-2.4	N	100	3.7	N
2-Ethylhexyl acetate	103-09-3	e1k	200	-2.1	N	200	-1.4	N	200	6.5	N
2-Ethylhexyl acrylate	103-11-7	e1k	200	79.0	Y	200	87.9	Y	200	78.1	Y
4,4'-Dithiodimorpholine	103-34-4	e1k	200	12.6	N	200	1.2	N	200	-4.2	N
Benzyl cinnamate	103-41-3	e1k	200	10.6	N	200	62.0	Y	200	68.6	Y
1-Piperazineethanol	103-76-4	e1k	200	-0.9	N	200	4.8	N	200	7.0	N
Lufenuron	103055-07-8	e1k	200	-1.2	N	200	1.5	N	200	-0.4	N
Endosulfan sulfate	1031-07-8	e1k	200	1.5	N	200	-2.3	N	200	8.4	N
4-Butylaniline	104-13-2	e1k	200	4.0	N	200	0.2	N	200	4.9	N
4-Dodecylphenol	104-43-8	e1k	200	67.0	Y	200	79.2	Y	200	93.4	Y
4-Propylanisole	104-45-0	e1k	200	-3.4	N	200	-4.2	N	200	0.6	N
3-Phenyl-2-propen-1-ol	104-54-1	e1k	200	2.3	N	200	5.6	N	200	16.8	N
gamma-Nonanolactone	104-61-0	e1k	200	3.5	N	200	-8.6	N	200	-8.8	N
1,2-Diphenoxyethane	104-66-5	e1k	200	-5.1	N	200	-0.2	N	200	-3.3	N
1,4-Heptanolide	105-21-5	e1k	200	-6.6	N	200	-0.3	N	200	1.7	N
Ethyl propionate	105-37-3	e1k	200	-4.5	N	200	-12.3	N	200	8.3	N
Diethyl propanedioate	105-53-3	e1k	210	-2.6	N	200	2.1	N	200	6.4	N
N,N'-Diethylthiourea	105-55-5	e1k	200	4.4	N	200	0.3	N	200	-1.1	N
Citronellal	106-23-0	e1k	200	-2.9	N	200	12.3	N	200	4.4	N
4-Thiocresol	106-45-6	e1k	200	33.1	N	200	-8.1	N	200	4.8	N
4-Chlorophenol	106-48-9	e1k	200	-0.8	N	200	4.1	N	200	7.5	N
1,4-Benzenediamine	106-50-3	e1k	200	1.0	N	190	22.3	N	190	18.3	N
3-Octanone	106-68-3	e1k	200	-0.5	N	200	1.8	N	200	3.7	N
1,2-Dibromoethane	106-93-4	e1k	200	-2.9	N	200	-2.6	N	200	-3.8	N
Trimethoxypropylsilane	1067-25-0	e1k	200	5.3	N	200	1.5	N	200	7.9	N
Tris(2-methoxyethoxy)vinylsilane	1067-53-4	e1k	200	7.2	N	200	3.5	N	200	13.2	N
Acrylonitrile	107-13-1	e1k	200	-5.5	N	200	0.8	N	200	7.1	N
Allyl alcohol	107-18-6	e1k	200	-4.0	N	200	-3.3	N	200	13.3	N
Chloroacetaldehyde	107-20-0	e1k	200	-4.0	N	200	2.7	N	200	19.1	N
Chloromethyl methyl ether	107-30-2	e1k	70	-4.8	N	60	5.5	N	60	0.7	N
Hexamethyldisiloxane	107-46-0	e1k	200	0.7	N	200	-4.1	N	200	-6.3	N
Octamethyltrisiloxane	107-51-7	e1k	200	-0.9	N	200	-5.4	N	200	3.6	N
3,5-Dimethyl-1-hexyn-3-ol	107-54-0	e1k	200	-1.0	N	200	1.0	N	200	3.1	N
7-Hydroxy-3,7-dimethyloctanal	107-75-5	e1k	200	2.2	N	200	-0.4	N	200	1.3	N
2-Pentanone	107-87-9	e1k	200	-2.5	N	190	1.5	N	190	6.7	N
Sulfuric acid, monononyl ester, sodium salt	1072-15-7	e1k	200	7.1	N	200	5.0	N	200	-10.4	N

1,4-Cyclohexanedicarboxylic acid	1076-97-7	e1k	200	1.6	N	200	-9.7	N	200	3.3	N
Isopropyl acetate	108-21-4	e1k	200	-3.5	N	190	3.8	N	190	8.7	N
Propylene carbonate	108-32-7	e1k	200	1.7	N	200	-1.9	N	200	-0.5	N
m-Xylene	108-38-3	e1k	200	-1.4	N	200	-1.6	N	200	-4.7	N
m-Cresol	108-39-4	e1k	200	-4.0	N	200	3.0	N	200	1.5	N
3,5-Dimethylphenol	108-68-9	e1k	200	2.4	N	200	8.5	N	200	3.6	N
2,4,6-Trichloro-s-triazine	108-77-0	e1k	200	-5.3	N	200	0.1	N	200	-0.4	N
Diisobutyl ketone	108-83-8	e1k	200	-1.1	N	200	2.9	N	200	0.6	N
Benzenethiol	108-98-5	e1k	200	8.6	N	200	-2.9	N	200	18.1	N
3-Methylpyridine	108-99-6	e1k	200	-1.8	N	200	1.6	N	200	-0.4	N
Acetic acid, C8-10-branched alkyl esters, C9-rich	108419-33-6	e1k	200	-2.9	N	200	-1.3	N	200	1.1	N
Heptylparaben	1085-12-7	e1k	200	102.5	Y	200	96.5	Y	200	95.5	Y
4-Methylmorpholine	109-02-4	e1k	200	-3.8	N	200	-0.3	N	200	5.4	N
N,N'-Dibutylthiourea	109-46-6	e1k	200	1.9	N	200	0.2	N	200	0.4	N
Pentanoic acid	109-52-4	e1k	200	0.2	N	200	2.7	N	200	8.0	N
3-(Dimethylamino)propylamine	109-55-7	e1k	200	2.3	N	190	1.9	N	190	7.5	N
Propanedinitrile	109-77-3	e1k	200	5.1	N	190	51.0	Y	190	47.3	Y
5-Methyl-2-hexanone	110-12-3	e1k	200	3.2	N	200	1.1	N	200	3.6	N
Butanedioic acid	110-15-6	e1k	200	-1.7	N	200	-2.8	N	200	-1.2	N
Maleic acid	110-16-7	e1k	200	-6.2	N	190	-2.9	N	190	9.1	N
Fumaric acid	110-17-8	e1k	200	5.0	N	200	0.2	N	200	8.9	N
Oleyl sarcosine	110-25-8	e1k	200	102.5	Y	200	92.0	Y	200	100.2	Y
Isopropyl tetradecanoic acid	110-27-0	e1k	200	1.1	N	200	-4.3	N	200	-7.7	N
Dihexyl hexanedioate	110-33-8	e1k	200	-4.6	N	200	5.0	N	200	-9.9	N
Methyl decanoate	110-42-9	e1k	200	-1.0	N	200	-0.4	N	200	0.3	N
2-Heptanone	110-43-0	e1k	200	-4.4	N	200	2.9	N	200	6.8	N
1,4-Butanediol	110-63-4	e1k	200	-1.1	N	200	-0.5	N	200	-4.0	N
2-Butyne-1,4-diol	110-65-6	e1k	200	7.1	N	190	12.3	N	190	13.2	N
Butanal oxime	110-69-0	e1k	200	-1.6	N	200	-1.8	N	200	4.1	N
2-(Ethylamino)ethanol	110-73-6	e1k	200	-0.1	N	200	6.3	N	200	7.0	N
3,4-Dihydro-2H-pyran	110-87-2	e1k	200	-1.0	N	190	12.3	N	190	-5.7	N
Morpholine	110-91-8	e1k	200	-2.3	N	190	2.3	N	190	4.2	N
Diisopropanolamine	110-97-4	e1k	200	-2.6	N	200	7.8	N	200	7.3	N
Glyceryl stearates	11099-07-3	e1k	200	-5.0	N	200	2.8	N	200	3.5	N
Decanedioic acid	111-20-6	e1k	200	-1.7	N	200	1.4	N	200	10.4	N
1-Hexanol	111-27-3	e1k	200	-3.1	N	190	1.9	N	190	7.8	N
Diethylenetriamine	111-40-0	e1k	200	0.1	N	190	-0.5	N	190	1.6	N

Hexamethylenimine	111-49-9	e1k	200	0.8	N	190	-4.9	N	190	-0.7	N
1,2-Ethandiol diacetate	111-55-7	e1k	200	2.9	N	200	-2.6	N	200	-5.5	N
Ethyl oleate	111-62-6	e1k	200	13.7	N	200	10.9	N	200	20.9	N
1-Heptanol	111-70-6	e1k	200	-0.3	N	200	-2.3	N	200	9.4	N
Heptanal	111-71-7	e1k	200	-1.5	N	200	11.9	N	200	22.9	N
Nonane	111-84-2	e1k	200	-5.0	N	200	2.2	N	200	11.4	N
Dimethoxydimethylsilane	1112-39-6	e1k	200	-2.9	N	200	0.2	N	200	1.0	N
Pebulate	1114-71-2	e1k	200	4.0	N	200	1.4	N	200	-6.0	N
Butyltin trichloride	1118-46-3	e1k	200	-2.1	N	200	21.3	N	200	20.2	N
N,N-Dimethyloctanamide	1118-92-9	e1k	200	-2.2	N	200	-0.4	N	200	-3.2	N
Nicosulfuron	111991-09-4	e1k	200	-7.3	N	200	-0.7	N	200	2.0	N
2-Butoxyethyl acetate	112-07-2	e1k	200	-2.6	N	200	1.0	N	200	-7.6	N
2-Undecanone	112-12-9	e1k	200	3.8	N	200	2.2	N	200	6.7	N
Octyl acetate	112-14-1	e1k	200	1.6	N	200	2.5	N	200	-0.3	N
N,N-Dimethyldodecan-1-amine	112-18-5	e1k	200	18.3	N	200	-2.5	N	200	3.7	N
Decanal	112-31-2	e1k	200	-7.1	N	200	1.7	N	200	-2.9	N
2-[2-(2-Methoxyethoxy)ethoxy]ethanol	112-35-6	e1k	200	-5.3	N	200	-5.0	N	200	-6.3	N
1-Dodecanethiol	112-55-0	e1k	200	-2.6	N	200	4.4	N	200	30.2	N
Tetraethylene glycol	112-60-7	e1k	200	9.0	N	200	1.9	N	200	-1.6	N
Methyl linoleate	112-63-0	e1k	200	52.9	Y	200	77.9	Y	200	89.2	Y
Oleic acid	112-80-1	e1k	200	98.7	Y	200	94.4	Y	200	97.0	Y
Octadecyl sulfate sodium salt	1120-04-3	e1k	200	100.2	Y	200	104.8	Y	200	96.2	Y
Halofenozide	112226-61-6	e1k	200	5.4	N	200	-1.7	N	200	1.6	N
Letrozole	112809-51-5	e1k	140	-0.5	N	140	10.7	N	140	2.4	N
Bromophenol blue	115-39-9	e1k	190	73.3	Y	180	76.6	Y	180	88.5	Y
Linalyl acetate	115-95-7	e1k	200	12.9	N	200	-1.9	N	200	-5.7	N
3,3,5-Trimethylcyclohexanol	116-02-9	e1k	200	3.7	N	200	3.5	N	200	-1.4	N
Bromuconazole	116255-48-2	e1k	200	2.3	N	200	1.3	N	200	-11.8	N
Dodecyl gallate	1166-52-5	e1k	200	91.3	Y	200	85.3	Y	200	99.4	Y
Tetrachlorophthalic anhydride	117-08-8	e1k	200	1.7	N	200	4.2	N	200	11.2	N
Dichlone	117-80-6	e1k	200	79.8	Y	200	87.8	Y	200	89.5	Y
2-Hydroxybenzophenone	117-99-7	e1k	200	-1.8	N	200	-2.5	N	200	-4.7	N
Pyrazolone T	118-47-8	e1k	200	61.7	Y	200	6.0	N	200	2.6	N
Phenyl salicylate	118-55-8	e1k	200	-0.5	N	200	8.2	N	200	32.6	N
3,3,5-Trimethylcyclohexyl salicylate	118-56-9	e1k	200	1.8	N	200	2.0	N	200	1.7	N
Benzyl salicylate	118-58-1	e1k	200	-1.4	N	200	-0.4	N	200	7.3	N
2,4,6-Tribromophenol	118-79-6	e1k	200	8.3	N	200	24.9	N	200	14.8	N

4,4'-Methylenebis(2,6-di-t-butylphenol)	118-82-1	e1k	200	1.6	N	200	5.7	N	200	11.2	N
2-Hydroxyacetophenone	118-93-4	e1k	200	-0.9	N	200	-5.7	N	200	-1.2	N
1,3-Butyleneglycol dimethacrylate	1189-08-8	e1k	200	15.1	N	200	63.9	Y	200	57.0	Y
Octyl decyl phthalate	119-07-3	e1k	200	-0.9	N	200	0.1	N	200	0.1	N
2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	119-47-1	e1k	200	26.7	N	200	56.5	Y	200	83.4	Y
Benzoin	119-53-9	e1k	200	-1.7	N	200	8.2	N	200	0.5	N
Tetralin	119-64-2	e1k	200	4.1	N	200	0.4	N	200	-2.9	N
4,5-Dichloro-3H-1,2-dithiol-3-one	1192-52-5	e1k	200	103.8	Y	200	88.6	Y	200	94.8	Y
Veratraldehyde	120-14-9	e1k	200	2.6	N	200	-5.6	N	200	-6.7	N
Naphthalene-2-sulfonic acid	120-18-3	e1k	200	-1.4	N	200	0.5	N	200	2.7	N
1,3-Diphenyl-1,3-propanedione	120-46-7	e1k	200	-1.6	N	200	-1.2	N	200	3.8	N
Benzyl benzoate	120-51-4	e1k	200	2.7	N	200	-2.2	N	200	-4.2	N
Triethylene glycol dibenzoate	120-56-9	e1k	200	4.0	N	200	1.7	N	200	-3.3	N
2-((Dimethylamino)methyl)phenol	120-65-0	e1k	200	-0.8	N	200	-7.6	N	200	-0.6	N
Indole	120-72-9	e1k	200	-2.2	N	190	13.8	N	190	-4.3	N
Cyclopentanone	120-92-3	e1k	200	3.2	N	200	-2.4	N	200	4.3	N
Anastrozole	120511-73-1	e1k	70	-0.6	N	60	1.7	N	60	-9.6	N
3-Ethoxy-4-hydroxybenzaldehyde	121-32-4	e1k	200	3.7	N	200	2.2	N	200	3.3	N
Ethyl 3-phenylglycidate	121-39-1	e1k	200	-4.3	N	200	26.1	N	200	42.2	N
(Methylcyclopentadienyl)tricarbonylmanganese	12108-13-3	e1k	200	1.0	N	200	-4.1	N	200	5.6	N
N-Benzyladenine	1214-39-7	e1k	200	-7.1	N	200	-3.0	N	200	-4.6	N
Octylparaben	1219-38-1	e1k	200	105.8	Y	200	85.5	Y	200	97.5	Y
Triisopropanolamine	122-20-3	e1k	200	-9.1	N	200	-1.8	N	200	9.7	N
Pentylcinnamaldehyde	122-40-7	e1k	200	2.3	N	200	41.1	Y	200	76.1	Y
Propham	122-42-9	e1k	200	3.5	N	200	1.3	N	200	-3.4	N
Ethyl orthoformate	122-51-0	e1k	200	-3.5	N	200	1.9	N	200	-0.3	N
Methyl styryl ketone	122-57-6	e1k	200	4.1	N	200	40.8	N	200	41.6	N
Phenylacetaldehyde	122-78-1	e1k	200	2.8	N	200	23.2	Y	200	53.5	Y
4-Chlorophenoxyacetic acid	122-88-3	e1k	200	-1.3	N	200	2.5	N	200	-2.3	N
Chlorfenapyr	122453-73-0	e1k	200	22.6	N	200	29.1	N	200	41.1	N
4-Morpholinepropanamine	123-00-2	e1k	200	5.1	N	200	2.2	N	200	-4.1	N
2-Ethylhexanal	123-05-7	e1k	210	-1.3	N	200	0.6	N	200	-0.7	N
4-Ethylphenol	123-07-9	e1k	200	-0.9	N	200	2.4	N	200	4.1	N
4-Methoxybenzaldehyde	123-11-5	e1k	200	0.1	N	200	-3.5	N	200	-10.9	N
2,6,8-Trimethyl-4-nonanol	123-17-1	e1k	200	-0.8	N	200	-0.2	N	200	3.4	N
Ethyl hexanoate	123-66-0	e1k	200	1.1	N	200	5.0	N	200	1.1	N
Azodicarbonamide	123-77-3	e1k	200	3.1	N	200	2.4	N	200	-2.6	N

2-Octanol	123-96-6	e1k	200	4.4	N	200	-6.9	N	200	1.2	N
Nonanedioic acid	123-99-9	e1k	200	-1.5	N	200	2.7	N	200	7.7	N
1,6-Hexanediamine	124-09-4	e1k	200	-3.5	N	200	3.4	N	200	1.0	N
Nonanal	124-19-6	e1k	200	-1.6	N	200	13.8	N	200	11.3	N
1-Dodecanamine	124-22-1	e1k	180	21.8	N	180	58.0	Y	180	78.3	Y
Dimethylamine	124-40-3	e1k	200	2.1	N	190	-3.2	N	190	2.3	N
2-Amino-2-methylpropan-1-ol	124-68-5	e1k	200	3.3	N	200	0.0	N	200	-5.8	N
Isoborneol	124-76-5	e1k	200	-0.6	N	200	2.5	N	200	-1.0	N
2-Ethylhexyl diphenyl phosphate	1241-94-7	e1k	200	1.3	N	200	7.8	N	200	4.1	N
Isobornyl acetate	125-12-2	e1k	200	4.7	N	200	6.8	N	200	5.6	N
Aminoglutethimide	125-84-8	e1k	200	-1.9	N	200	7.2	N	200	-7.8	N
Metconazole	125116-23-6	e1k	200	-2.4	N	200	1.2	N	200	-11.0	N
Ipconazole	125225-28-7	e1k	200	-2.6	N	200	13.7	N	200	14.7	N
Bispyribac-sodium	125401-92-5	e1k	200	-0.9	N	200	-4.8	N	200	-2.1	N
Diphenolic acid	126-00-1	e1k	200	0.7	N	200	4.9	N	200	22.2	N
3-Bromo-1-chloro-5,5-dimethylhydantoin	126-06-7	e1k	200	1.1	N	200	2.3	N	200	4.8	N
2,2-Dimethylpropane-1,3-diol	126-30-7	e1k	200	-1.4	N	200	2.1	N	200	4.2	N
Tris(2,3-dibromopropyl) phosphate	126-72-7	e1k	170	-4.5	N	170	4.7	N	170	5.2	N
Sodium ethasulfate	126-92-1	e1k	200	4.3	N	200	7.5	N	200	3.5	N
Methacrylonitrile	126-98-7	e1k	200	1.8	N	190	-0.7	N	190	3.0	N
N,N-Dimethylacetamide	127-19-5	e1k	200	1.3	N	200	5.0	N	200	3.4	N
Methyl abietate	127-25-3	e1k	200	-1.9	N	200	26.1	Y	200	59.6	Y
Sodium 1,4-diisobutyl sulfosuccinate	127-39-9	e1k	200	-2.3	N	200	4.6	N	200	1.0	N
alpha-Ionone	127-41-3	e1k	200	-3.5	N	200	13.2	N	200	28.1	N
Retinol acetate	127-47-9	e1k	200	13.3	N	200	49.7	Y	200	72.3	Y
Butylated hydroxytoluene	128-37-0	e1k	200	-2.3	N	200	6.4	N	200	7.7	N
1,4-Diaminoanthraquinone	128-95-0	e1k	200	-6.7	N	200	3.9	N	200	4.5	N
Sodium warfarin	129-06-6	e1k	200	-0.8	N	200	-2.3	N	200	0.9	N
Sulfan blue	129-17-9	e1k	200	-1.4	N	200	10.3	N	200	14.5	N
Sodium 1-naphthalenesulfonate	130-14-3	e1k	200	-2.1	N	200	1.5	N	200	0.4	N
Dimethylaniline	1300-73-8	e1k	200	-6.3	N	200	-0.4	N	200	4.7	N
2,4-Dihydroxybenzophenone	131-56-6	e1k	200	-10.4	N	200	7.9	N	200	-8.2	N
2-Hydroxy-4-methoxybenzophenone	131-57-7	e1k	200	0.4	N	200	2.0	N	200	-12.2	N
1-(6-tert-Butyl-1,1-dimethyl-2,3-dihydro-1H-inden-4-yl)ethanone	13171-00-1	e1k	200	-0.9	N	200	3.8	N	200	-8.0	N
Dibenzothiophene	132-65-0	e1k	200	5.3	N	200	1.1	N	200	-4.2	N
C.I. Acid Orange 24, monosodium salt	1320-07-6	e1k	200	70.3	Y	200	31.7	Y	200	57.4	Y

Divinylbenzene	1321-74-0	e1k	200	-4.7	N	200	3.5	N	200	5.4	N
Sodium triisopropyl naphthalene sulfonate	1323-19-9	e1k	200	3.3	N	200	36.8	N	200	2.8	N
Glyceryl monoricinoleate	1323-38-2	e1k	200	-0.6	N	200	47.4	N	200	35.3	N
2,6-Dimethyl-2-heptanol	13254-34-7	e1k	200	1.3	N	200	-2.1	N	200	-4.4	N
Tricresyl phosphate	1330-78-5	e1k	200	-3.7	N	200	8.7	N	200	4.1	N
Diisooctyl adipate	1330-86-5	e1k	200	5.1	N	200	-1.7	N	200	8.2	N
C.I. Disperse Orange 37	13301-61-6	e1k	200	34.9	N	200	11.4	Y	200	77.6	Y
Phenolsulfonic acid	1333-39-7	e1k	200	-1.3	N	200	1.4	N	200	6.4	N
Methylionone	1335-46-2	e1k	200	8.7	N	200	43.0	Y	200	58.0	Y
Epoxiconazole	133855-98-8	e1k	200	10.9	N	200	-7.0	N	200	-3.5	N
8-Hydroxyquinoline sulfate	134-31-6	e1k	200	5.4	N	200	8.2	N	200	9.0	N
Atorvastatin calcium	134523-03-8	e1k	180	-12.0	N	170	10.1	N	170	1.3	N
Zinc pyrithione	13463-41-7	e1k	200	0.2	N	200	-2.9	N	200	6.4	N
Cupferron	135-20-6	e1k	200	-4.2	N	200	11.0	N	200	11.7	N
Tris(2-chloroisopropyl)phosphate	13674-84-5	e1k	190	-1.2	N	190	3.5	N	190	-8.6	N
4,4'-Methylenebis(2,6-diethylaniline)	13680-35-8	e1k	200	1.9	N	200	-3.1	N	200	-13.1	N
Desmedipham	13684-56-5	e1k	200	0.7	N	200	-1.0	N	200	4.6	N
Phenmedipham	13684-63-4	e1k	200	2.9	N	200	-4.0	N	200	3.6	N
Metam-sodium	137-42-8	e1k	200	-1.4	N	200	9.2	N	200	1.7	N
Ascorbyl palmitate	137-66-6	e1k	200	94.7	Y	200	99.1	Y	200	95.1	Y
Sodium tetrafluoroborate	13755-29-8	e1k	200	-2.6	N	200	8.7	N	200	5.3	N
Butyl lactate	138-22-7	e1k	200	4.1	N	190	-0.8	N	190	3.5	N
Limonene	138-86-3	e1k	210	-2.1	N	200	7.7	N	200	5.2	N
3-Phenoxybenzenemethanol	13826-35-2	e1k	200	-3.1	N	200	-2.5	N	200	-3.3	N
Sodium phenolate	139-02-6	e1k	200	30.1	N	190	16.1	N	190	-0.3	N
Ethyl diethanolamine	139-87-7	e1k	200	-4.1	N	200	1.5	N	200	10.6	N
7-Ethyl-2-methyl-4-undecanolsulfate, sodium salt	139-88-8	e1k	200	1.2	N	190	26.0	N	190	-6.6	N
Tris(2-chloroethyl) phosphite	140-08-9	e1k	200	-0.9	N	200	3.6	N	200	4.6	N
E-Cinnamic acid	140-10-3	e1k	200	-1.8	N	200	-2.4	N	200	4.6	N
Benzyl acetate	140-11-4	e1k	200	-3.9	N	200	-4.5	N	200	9.9	N
1-(2-Aminoethyl)piperazine	140-31-8	e1k	200	1.8	N	200	-0.9	N	200	4.7	N
4-Chlorophenylurea	140-38-5	e1k	200	-2.0	N	190	-34.7	N	190	0.6	N
Estragole	140-67-0	e1k	200	-2.0	N	200	3.6	N	200	0.4	N
Dimethylolurea	140-95-4	e1k	200	-0.3	N	190	4.7	N	190	4.7	N
(9Z,12R)-12-Hydroxyoctadec-9-enoic acid	141-22-0	e1k	200	5.4	N	200	41.0	N	200	19.3	N
Butyl acrylate	141-32-2	e1k	200	0.1	N	200	2.2	N	200	5.7	N
4-Methylpent-3-en-2-one	141-79-7	e1k	200	-3.1	N	200	3.0	N	200	1.6	N

Aniline hydrochloride	142-04-1	e1k	200	2.1	N	200	-0.7	N	200	10.1	N
Bis(2-ethylhexyl) maleate	142-16-5	e1k	200	5.3	N	200	14.0	N	200	21.9	N
1-Monolaurin	142-18-7	e1k	200	15.7	N	200	41.5	N	200	46.6	N
Sodium octyl sulfate	142-31-4	e1k	200	-0.4	N	200	2.3	N	200	1.2	N
1,4-Bis(N-isopropylamino)anthraquinone	14233-37-5	e1k	110	-0.5	N	100	-4.8	N	100	7.7	N
1-Nonanol	143-08-8	e1k	200	-0.2	N	200	-0.1	N	200	6.8	N
2-[2-(2-Butoxyethoxy)ethoxy]ethanol	143-22-6	e1k	200	-1.3	N	200	-4.1	N	200	7.8	N
Phenol red	143-74-8	e1k	200	10.6	N	200	41.0	Y	200	47.8	Y
Kresoxim-methyl	143390-89-0	e1k	200	-2.5	N	200	0.6	N	200	-2.2	N
Pregnenolone carbonitrile	1434-54-4	e1k	120	-2.0	N	110	-6.7	N	110	-2.3	N
Sodium abietate	14351-66-7	e1k	200	29.1	N	200	33.8	Y	200	61.4	Y
(2E)-3-Phenylprop-2-enal	14371-10-9	e1k	200	0.9	N	200	30.7	N	200	47.9	N
Fluoroacetic acid	144-49-0	e1k	200	-2.8	N	200	-3.2	N	200	0.4	N
Oxalic acid	144-62-7	e1k	200	-0.3	N	200	2.5	N	200	2.5	N
Dimethyl isophthalate	1459-93-4	e1k	200	2.9	N	200	-4.9	N	200	-2.3	N
Tetrabutyltin	1461-25-2	e1k	200	-4.1	N	200	11.7	N	200	0.5	N
Arabinose	147-81-9	e1k	200	-2.5	N	200	11.1	N	200	3.5	N
2-sec-Butylcyclohexanone	14765-30-1	e1k	200	-9.7	N	200	-0.7	N	200	-2.9	N
1,3-Benzenedimethanamine	1477-55-0	e1k	200	0.9	N	200	4.2	N	200	10.5	N
Phoxim	14816-18-3	e1k	200	-1.4	N	200	6.5	N	200	8.0	N
Menthol	1490-04-6	e1k	200	-0.4	N	200	-1.8	N	200	-0.9	N
4-(2,6,6-Trimethyl-cyclohex-1-enyl)-but-3-en-2-one	14901-07-6	e1k	200	-2.9	N	200	13.0	N	200	27.2	N
4-Methoxyphenol	150-76-5	e1k	200	2.2	N	200	2.1	N	200	0.7	N
Hydroquinone dimethyl ether	150-78-7	e1k	200	1.9	N	200	2.5	N	200	10.8	N
Sodium 2-methylbenzenesulfonate	15046-75-0	e1k	200	-2.7	N	200	2.0	N	200	2.5	N
Dimethylbenzylcarbonyl acetate	151-05-3	e1k	200	0.7	N	200	-1.1	N	200	0.0	N
2-Acrylamido-2-methyl-1-propanesulfonic acid	15214-89-8	e1k	200	-4.5	N	200	-1.4	N	200	3.7	N
4-Dodecylmorpholine	1541-81-7	e1k	200	0.5	N	200	1.6	N	200	-6.4	N
4-Butylchlorobenzene	15499-27-1	e1k	200	-1.5	N	200	4.7	N	200	-0.5	N
3,6,9,12-Tetraoxahexadecan-1-ol	1559-34-8	e1k	200	-0.7	N	200	-6.6	N	200	-1.1	N
2-(2-Ethylhexyloxy)ethanol	1559-35-9	e1k	200	2.4	N	200	1.9	N	200	0.2	N
4-Nitrosodiphenylamine	156-10-5	e1k	200	36.2	N	200	50.7	Y	200	28.5	Y
4-Ethoxyaniline	156-43-4	e1k	200	-0.3	N	200	3.5	N	200	6.0	N
(E)-1,2-Dichloroethylene	156-60-5	e1k	200	-1.6	N	190	2.2	N	190	-1.3	N
2,3-Dihydro-2,2-dimethyl-7-benzofuranol	1563-38-8	e1k	200	-4.3	N	200	-1.6	N	200	5.2	N
1-Propoxy-2-propanol	1569-01-3	e1k	200	0.5	N	200	-1.3	N	200	-0.2	N
1-Ethoxy-2-propanol	1569-02-4	e1k	200	2.0	N	200	-3.6	N	200	3.6	N

4-Chloro-2-methylphenol	1570-64-5	e1k	200	-8.9	N	200	-1.7	N	200	2.0	N
Ethylenediaminetetraacetic acid ferric sodium salt	15708-41-5	e1k	200	1.5	N	200	8.4	N	200	24.3	N
1-Bromo-3-chloro-5,5-dimethylhydantoin	16079-88-2	e1k	200	-2.3	N	200	-1.2	N	200	4.6	N
5-Ethylidene-2-norbornene	16219-75-3	e1k	200	11.2	N	200	46.3	Y	200	65.5	Y
4,4'-Di-tert-butylbiphenyl	1625-91-8	e1k	200	-2.7	N	200	0.3	N	200	-3.5	N
Fenchol	1632-73-1	e1k	200	0.9	N	200	8.8	N	200	2.8	N
Isoxadifen-ethyl	163520-33-0	e1k	200	0.1	N	200	-2.1	N	200	1.2	N
4-Butylphenol	1638-22-8	e1k	200	-1.3	N	200	6.1	N	200	-11.3	N
Aldicarb sulfoxide	1646-87-3	e1k	200	-4.2	N	200	-0.7	N	200	-2.5	N
Aldoxycarb	1646-88-4	e1k	200	0.1	N	200	-1.7	N	200	4.5	N
Dinotefuran	165252-70-0	e1k	190	-0.8	N	190	-1.9	N	190	0.6	N
4-(tert-Pentyl)-cyclohexanone	16587-71-6	e1k	200	-1.4	N	200	11.9	N	200	2.9	N
Heptanophenone	1671-75-6	e1k	200	-1.1	N	200	1.8	N	200	0.2	N
Bisphenol A diglycidyl ether	1675-54-3	e1k	200	102.7	Y	200	94.8	Y	200	88.6	Y
Sodium hexafluorosilicate	16893-85-9	e1k	200	-5.7	N	200	-3.3	N	200	2.7	N
Cyclododecanol	1724-39-6	e1k	200	-3.3	N	200	-1.0	N	200	-16.7	N
1,1-Bis(3,4-dimethylphenyl)ethane	1742-14-9	e1k	200	0.4	N	200	0.6	N	200	4.0	N
gamma-Cyclodextrin	17465-86-0	e1k	80	6.4	N	70	5.8	N	70	6.5	N
N-[3-(Trimethoxysilyl)propyl]ethane-1,2-diamine	1760-24-3	e1k	200	-14.5	N	200	-1.9	N	200	-1.9	N
Phenylparaben	17696-62-7	e1k	200	15.5	N	200	48.1	Y	200	61.4	Y
N-(Cyclohexylthio)phthalimide	17796-82-6	e1k	200	33.3	N	200	19.4	N	200	27.5	N
Zearalenone	17924-92-4	e1k	200	1.5	N	200	6.5	N	200	-32.6	N
Flucarbazono-sodium	181274-17-9	e1k	190	-4.1	N	180	-2.3	N	180	-3.9	N
(-)-beta-Pinene	18172-67-3	e1k	200	-5.5	N	200	-1.6	N	200	3.5	N
Pentachloroanisole	1825-21-4	e1k	200	-1.0	N	200	3.2	N	200	-3.4	N
1,1,1,3,5,5,5-Heptamethyltrisiloxane	1873-88-7	e1k	200	1.3	N	200	-7.9	N	200	2.6	N
2,2'-(Tetradecylimino)diethanol	18924-66-8	e1k	200	94.5	Y	200	92.6	Y	200	96.1	Y
4-(Hexyloxy)phenol	18979-55-0	e1k	200	-4.1	N	200	9.3	N	200	-7.7	N
N-Butyl-p-toluenesulfonamide	1907-65-9	e1k	200	0.2	N	200	-4.0	N	200	-2.2	N
Propachlor	1918-16-7	e1k	200	83.1	Y	200	46.1	N	200	35.1	N
2,4-D-Butotyl	1929-73-3	e1k	200	4.7	N	200	4.4	N	200	-2.6	N
C.I. Acid Orange 10	1936-15-8	e1k	200	2.4	N	200	-0.7	N	200	-2.8	N
(2-Dodeceny)succinic anhydride	19780-11-1	e1k	200	51.8	Y	200	52.3	Y	200	56.9	Y
1-Methoxy-4-tert-pentylcyclohexane	199584-38-8	e1k	200	-4.6	N	200	3.4	N	200	0.0	N
1-Decanamine	2016-57-1	e1k	200	4.5	N	200	5.7	N	200	-13.0	N
4-Methoxyaniline hydrochloride	20265-97-8	e1k	200	-2.8	N	200	5.1	N	200	17.7	N
Triethoxymethylsilane	2031-67-6	e1k	200	-0.3	N	200	2.7	N	200	5.6	N

N,N-Dimethylacetoacetamide	2044-64-6	e1k	200	2.4	N	200	-1.4	N	200	-6.3	N
Propofol	2078-54-8	e1k	200	4.3	N	200	2.0	N	200	2.5	N
3,7-Dimethyloctan-3-yl acetate	20780-48-7	e1k	200	0.0	N	200	-3.5	N	200	1.2	N
Digoxin	20830-75-5	e1k	140	0.9	N	130	-1.1	N	130	11.7	N
Topramezone	210631-68-8	e1k	90	-0.6	N	80	-3.7	N	80	11.8	N
2-(3-Phenylpropyl)pyridine	2110-18-1	e1k	200	-3.3	N	200	-0.4	N	200	-2.6	N
6-Acetyl-1,1,2,4,4,7-hexamethyltetralin	21145-77-7	e1k	200	1.4	N	200	10.6	N	200	-8.9	N
Ethyl 1-naphthaleneacetate	2122-70-5	e1k	200	4.0	N	200	0.5	N	200	-7.8	N
2-Ethylhexyl 4-(dimethylamino)benzoate	21245-02-3	e1k	200	-1.5	N	200	7.9	N	200	14.9	N
(4Z)-4-Decenal	21662-09-9	e1k	200	-2.3	N	200	36.1	N	200	16.0	N
2-Ethylhexyl octadecanoate	22047-49-0	e1k	200	-2.8	N	200	9.7	N	200	4.4	N
Z-Tetrachlorvinphos	22248-79-9	e1k	200	95.5	Y	200	31.9	N	200	41.6	N
Bromocriptine mesylate	22260-51-1	e1k	70	-2.3	N	60	5.5	N	60	18.8	N
Potassium dichloroisocyanurate	2244-21-5	e1k	200	0.6	N	200	2.0	N	200	0.6	N
Aspartame	22839-47-0	e1k	200	1.5	N	200	2.7	N	200	14.0	N
Levomenol	23089-26-1	e1k	200	-5.8	N	200	34.5	N	200	9.8	N
Fluorescein	2321-07-5	e1k	200	1.2	N	200	1.5	N	200	6.7	N
Dicyclohexyl sodium sulfosuccinate	23386-52-9	e1k	200	0.9	N	200	3.8	N	200	-9.7	N
FD&C Green No. 3	2353-45-9	e1k	130	58.9	Y	130	53.3	Y	130	74.2	Y
Thiophanate	23564-06-9	e1k	200	29.0	N	200	3.7	N	200	-4.1	N
UT-632	2386-87-0	e1k	200	-2.5	N	200	10.0	N	200	41.8	N
Basic Blue 7	2390-60-5	e1k	200	10.9	N	200	80.7	Y	200	95.5	Y
4-tert-Butylbenzenethiol	2396-68-1	e1k	200	62.3	Y	200	0.9	N	200	12.7	N
2-tert-Butyl-4-methylphenol	2409-55-4	e1k	200	0.7	N	200	14.1	N	200	-8.9	N
2,6-Diisopropyl-naphthalene	24157-81-1	e1k	200	4.3	N	200	0.8	N	200	1.9	N
Econazole nitrate	24169-02-6	e1k	200	-3.2	N	200	52.9	Y	200	10.5	Y
2-Hexyl-1-decanol	2425-77-6	e1k	200	1.1	N	200	1.1	N	200	-2.3	N
Butyl glycidyl ether	2426-08-6	e1k	200	-0.1	N	200	-0.2	N	200	-2.0	N
2-(2H-Benzotriazol-2-yl)-4-methylphenol	2440-22-4	e1k	200	-0.3	N	200	3.4	N	200	0.3	N
2-Methylbutyl isovalerate	2445-77-4	e1k	200	7.4	N	200	-2.6	N	200	-2.5	N
2-Ethyl-6-methylaniline	24549-06-2	e1k	200	-1.8	N	200	3.3	N	200	2.3	N
Barium bis(2-ethylhexanoate)	2457-01-4	e1k	200	1.0	N	200	3.3	N	200	4.0	N
Auramine hydrochloride	2465-27-2	e1k	200	9.0	N	200	6.4	N	200	4.3	N
2,2'-Bisphenol F	2467-02-9	e1k	200	1.8	N	200	13.4	N	200	-11.9	N
Tripropylene glycol	24800-44-0	e1k	200	1.2	N	200	-0.7	N	200	0.8	N
Methyl dihydrojasmonate	24851-98-7	e1k	200	3.6	N	200	3.4	N	200	-0.2	N
2-Bromo-4-hydroxyacetophenone	2491-38-5	e1k	200	0.9	N	200	14.5	N	200	44.4	N

Sodium 2-mercaptobenzothiolate	2492-26-4	e1k	200	23.6	N	200	26.6	Y	200	53.4	Y
Methylbenzethonium chloride	25155-18-4	e1k	200	103.1	Y	200	98.7	Y	200	103.8	Y
Chlorotoluene	25168-05-2	e1k	200	-2.7	N	200	0.6	N	200	8.8	N
Polypropylene glycol	25322-69-4	e1k	200	0.9	N	200	-3.1	N	200	8.0	N
tert-Nonanethiol	25360-10-5	e1k	200	10.6	N	200	-0.4	N	200	2.4	N
Glyceryl monooleate	25496-72-4	e1k	200	31.8	N	200	71.2	Y	200	78.0	Y
1,3,5,7-Tetramethyl-1,3,5,7-tetравinylcyclotetrasiloxane	2554-06-5	e1k	200	0.8	N	200	-0.1	N	200	-2.6	N
Diisodecylphenyl phosphite	25550-98-5	e1k	200	5.8	N	200	6.4	N	200	-12.9	N
Butylphthalenesulfonic acid sodium salt	25638-17-9	e1k	200	0.0	N	200	18.3	N	200	-14.0	N
Gemfibrozil	25812-30-0	e1k	200	3.2	N	200	5.0	N	200	-3.8	N
Phenothrin	26002-80-2	e1k	200	-2.8	N	200	3.7	N	200	0.3	N
Bis(2-ethylhexyl) tetrabromophthalate	26040-51-7	e1k	150	2.3	N	140	3.5	N	140	3.1	N
C.I. Direct Red 81 disodium salt	2610-11-9	e1k	200	41.2	N	200	21.2	N	200	34.4	N
Calcium dodecylbenzene sulfonate	26264-06-2	e1k	200	101.0	Y	200	98.8	Y	200	102.6	Y
1,3-Divinyl-1,1,3,3-tetramethyl disiloxane	2627-95-4	e1k	200	-2.6	N	200	-1.7	N	200	4.1	N
Glyceryl monooctanoate	26402-26-6	e1k	200	-2.8	N	200	-0.7	N	200	0.1	N
Ammonium xylene sulfonate	26447-10-9	e1k	200	-1.7	N	200	3.6	N	200	4.0	N
Triforine	26644-46-2	e1k	200	-1.5	N	200	14.4	N	200	20.3	N
N-Octyl-2-pyrrolidone	2687-94-7	e1k	200	-2.7	N	200	-7.8	N	200	0.8	N
Neodecanoic acid	26896-20-8	e1k	200	-2.5	N	200	6.3	N	200	3.7	N
Triallyl trimellitate	2694-54-4	e1k	200	1.0	N	200	5.1	N	200	4.5	N
4-Propylaniline	2696-84-6	e1k	200	0.8	N	200	0.5	N	200	-2.0	N
2,4-D sodium salt	2702-72-9	e1k	200	-0.6	N	200	0.5	N	200	0.3	N
N,N,N',N'-Tetrabutyl-1,6-hexanediamine	27090-63-7	e1k	200	-5.1	N	200	0.6	N	200	10.2	N
Dodecylphenol	27193-86-8	e1k	200	64.2	Y	200	85.3	Y	200	103.5	Y
Calcium neodecanoate	27253-33-4	e1k	200	-2.9	N	200	2.3	N	200	0.3	N
Disodium 4,4'-bis(2-sulfostyryl)biphenyl	27344-41-8	e1k	200	56.0	Y	200	45.3	Y	200	50.8	Y
Isobornyl propanoate	2756-56-1	e1k	200	-3.9	N	190	-6.4	N	190	-1.8	N
Triethoxypentylsilane	2761-24-2	e1k	200	0.6	N	200	2.6	N	200	0.7	N
Troclosene	2782-57-2	e1k	200	5.3	N	200	1.2	N	200	11.3	N
2-Propoxyethanol	2807-30-9	e1k	200	-2.4	N	200	-4.1	N	200	0.1	N
Cybutryne	28159-98-0	e1k	200	1.3	N	200	12.5	N	200	40.0	N
Spiromesifen	283594-90-1	e1k	200	-2.4	N	200	-2.6	N	200	-3.4	N
C.I. Direct Yellow 12	2870-32-8	e1k	200	94.9	Y	200	96.5	Y	200	87.1	Y
Imidazole	288-32-4	e1k	200	-5.2	N	200	-0.2	N	200	3.5	N
Dimethylnaphthalene	28804-88-8	e1k	200	1.2	N	200	13.3	N	200	8.7	N

Sodium dichloroisocyanurate	2893-78-9	e1k	200	-3.2	N	200	3.9	N	200	4.9	N
Atenolol	29122-68-7	e1k	200	-0.7	N	200	-0.4	N	200	1.1	N
Dibutyl nonanedioate	2917-73-9	e1k	200	-1.9	N	200	6.1	N	200	1.6	N
Melengestrol acetate	2919-66-6	e1k	130	-1.6	N	120	19.6	N	120	20.7	N
2,4-Diisopropylphenol	2934-05-6	e1k	200	-1.0	N	200	5.5	N	200	-7.3	N
Tolyltriazole	29385-43-1	e1k	200	-7.9	N	200	9.9	N	200	9.2	N
Propylene glycol monobutyl ether	29387-86-8	e1k	200	2.2	N	200	2.2	N	200	-1.1	N
Bis(2-ethylhexyl) phosphate	298-07-7	e1k	200	-3.2	N	200	39.3	N	200	-6.5	N
Octyl beta-D-glucopyranoside	29836-26-8	e1k	200	-3.8	N	200	4.0	N	200	-0.5	N
Trimethoxyphenylsilane	2996-92-1	e1k	200	-1.8	N	200	-5.5	N	200	3.8	N
Ethyl (2E,4Z)-deca-2,4-dienoate	3025-30-7	e1k	210	22.7	N	200	76.0	Y	200	63.5	Y
Isooctadecanoic acid	30399-84-9	e1k	200	77.8	Y	200	91.2	Y	200	98.6	Y
Paraoxon	311-45-5	e1k	200	-4.1	N	200	-1.5	N	200	4.3	N
1,4-Dihydroxy-2-naphthoic acid	31519-22-9	e1k	200	57.9	Y	200	51.4	Y	200	70.2	Y
Potassium 2-ethylhexanoate	3164-85-0	e1k	200	-1.1	N	200	-1.0	N	200	3.8	N
1,2,5,6,9,10-Hexabromocyclododecane	3194-55-6	e1k	170	4.3	Y	170	14.3	N	170	18.4	N
1-Cedr-8-en-9-ylethanone	32388-55-9	e1k	200	-2.8	N	200	9.2	N	200	2.8	N
3-(Methylthio)propanal	3268-49-3	e1k	200	-3.6	N	190	1.9	N	190	28.0	N
1,2-Dichloro-4-(trifluoromethyl)benzene	328-84-7	e1k	200	-3.2	N	200	-4.4	N	200	-4.7	N
4-Hexylaniline	33228-45-4	e1k	200	2.2	N	200	9.6	N	200	-3.7	N
Temephos	3383-96-8	e1k	200	95.8	Y	200	41.4	N	200	49.5	N
1-Octen-3-ol	3391-86-4	e1k	200	0.1	N	200	-0.9	N	200	6.7	N
Codlure	33956-49-9	e1k	200	21.5	N	200	61.9	Y	200	67.2	Y
Butyl (2S)-2-hydroxypropanoate	34451-19-9	e1k	200	-3.6	N	200	-2.4	N	200	4.1	N
3,5,5-Trimethyl-1-hexanol	3452-97-9	e1k	200	-3.5	N	200	-1.1	N	200	1.2	N
Diflubenzuron	35367-38-5	e1k	200	-2.3	N	200	1.7	N	200	3.4	N
Sulprofos	35400-43-2	e1k	200	14.6	N	200	8.0	N	200	6.7	N
2-Hydroxyethyl octyl sulfide	3547-33-9	e1k	200	3.3	N	200	1.6	N	200	-14.6	N
1,2-Dibromo-2,4-dicyanobutane	35691-65-7	e1k	200	2.9	N	200	14.7	N	200	36.2	N
N-Butylbenzenesulfonamide	3622-84-2	e1k	200	0.9	N	200	-7.2	N	200	1.0	N
MCPA-sodium	3653-48-3	e1k	200	-1.2	N	200	-0.4	N	200	-3.0	N
Triisodecyl trimellitate	36631-30-8	e1k	163	3.4	N	160	14.0	N	160	8.6	N
(3Z)-3-Hexenyl acetate	3681-71-8	e1k	200	0.8	N	200	-7.3	N	200	-8.1	N
Chlorophacinone	3691-35-8	e1k	200	64.9	Y	200	61.4	Y	200	64.1	Y
Denatonium benzoate	3734-33-6	e1k	200	-3.2	N	200	-3.9	N	200	-0.4	N
C.I. Acid Red 1	3734-67-6	e1k	200	3.5	N	200	7.1	N	200	21.8	N
Dichlormid	37764-25-3	e1k	200	-0.4	N	200	0.6	N	200	-0.5	N

Potassium chlorate	3811-04-9	e1k	200	4.5	N	190	-3.6	N	190	2.0	N
2-Butyloctan-1-ol	3913-02-8	e1k	200	-0.9	N	200	8.4	N	200	10.8	N
Imidazolidinyl urea	39236-46-9	e1k	200	0.4	N	200	-1.1	N	200	27.0	N
Sodium chloroacetate	3926-62-3	e1k	200	9.9	N	200	0.6	N	200	-1.7	N
Dinocap	39300-45-3	e1k	200	98.1	Y	200	50.9	Y	200	67.0	Y
4-Hexyloxyaniline	39905-57-2	e1k	200	4.5	N	200	2.7	N	200	-5.5	N
4-Propylcyclohexanone	40649-36-3	e1k	200	0.7	N	200	-1.4	N	200	-2.3	N
Sulisobenzone	4065-45-6	e1k	200	3.6	N	200	-1.3	N	200	0.3	N
N,N-Diisopropylaniline	4107-98-6	e1k	200	-8.3	N	200	1.4	N	200	7.2	N
2,6-Di-tert-butyl-4-ethylphenol	4130-42-1	e1k	200	-3.7	N	200	5.7	N	200	5.5	N
Apomorphine hydrochloride hydrate	41372-20-7	e1k	80	10.3	N	70	13.4	N	70	36.9	N
Tributyltin benzoate	4342-36-3	e1k	200	-3.8	N	200	20.2	N	200	9.8	N
4-Butyloxyaniline	4344-55-2	e1k	200	-5.8	N	200	-0.4	N	200	5.4	N
Butylene carbonate	4437-85-8	e1k	200	-2.7	N	190	-8.3	N	190	6.6	N
3-Phenylhexane	4468-42-2	e1k	200	0.8	N	200	-9.3	N	200	-0.5	N
1,2-Diphenylethanone	451-40-1	e1k	200	0.3	N	200	5.5	N	200	3.3	N
FD&C Red 4	4548-53-2	e1k	100	5.0	N	100	10.6	N	100	0.8	N
2-Methylpentanedinitrile	4553-62-2	e1k	200	-1.5	N	200	13.1	N	200	6.5	N
Myristyltrimethylammonium chlorideN,N,N-Trimethyltetradecan-1-aminium chloride	4574-04-3	e1k	180	91.9	Y	170	100.8	Y	170	95.9	Y
1-Bromo-4-fluorobenzene	460-00-4	e1k	200	1.8	N	200	-3.5	N	200	-8.3	N
Farnesol	4602-84-0	e1k	200	16.3	N	200	76.7	Y	200	86.2	Y
Cyanoguanidine	461-58-5	e1k	200	-0.8	N	190	5.5	N	190	11.5	N
Linolenic acid	463-40-1	e1k	200	92.2	Y	200	87.7	Y	200	90.4	Y
5-Chlorosalicylanilide	4638-48-6	e1k	200	2.6	N	200	-7.1	N	200	-5.5	N
D-Camphor	464-49-3	e1k	200	-3.8	N	200	4.1	N	200	3.5	N
1,8-Cineol	470-82-6	e1k	200	-1.7	N	200	0.9	N	200	2.3	N
Methyl 2,4-dihydroxy-3,6-dimethylbenzoate	4707-47-5	e1k	200	0.2	N	200	8.8	N	200	-13.7	N
Diphenyl phosphite	4712-55-4	e1k	200	-3.9	N	200	12.0	N	200	1.5	N
Equilin	474-86-2	e1k	200	1.8	N	200	11.6	N	200	-1.4	N
Chrysin	480-40-0	e1k	200	0.9	N	200	3.0	N	200	-4.3	N
2,4,6-Trimethylbenzoic acid	480-63-7	e1k	200	-1.1	N	200	4.4	N	200	5.1	N
5,7-Dimethoxy-2H-chromen-2-one	487-06-9	e1k	200	-5.8	N	200	8.2	N	200	0.9	N
2,6-Di-tert-butyl-4-methoxyphenol	489-01-0	e1k	200	3.8	N	190	-1.3	N	190	-2.5	N
Biochanin A	491-80-5	e1k	200	35.3	N	200	13.2	N	200	-6.8	N
Methyl red	493-52-7	e1k	200	-2.0	N	200	4.0	N	200	8.4	N
2-Ethyl-3-hydroxy-4H-pyran-4-one	4940-11-8	e1k	200	-3.8	N	200	1.5	N	200	2.5	N

Glycoluril	496-46-8	e1k	200	-2.1	N	200	-3.0	N	200	0.5	N
Isopropyl-o-cresol	499-75-2	e1k	200	-2.1	N	200	-3.2	N	200	0.3	N
2,6-Pyridinedicarboxylic acid	499-83-2	e1k	200	-1.2	N	200	0.4	N	200	4.2	N
Ergocalciferol	50-14-6	e1k	200	58.9	Y	200	77.4	Y	200	93.7	Y
Lactic acid	50-21-5	e1k	200	-2.0	N	190	-0.7	N	190	-2.6	N
Estriol	50-27-1	e1k	200	-8.2	N	200	7.5	N	200	3.5	N
D-Glucitol	50-70-4	e1k	190	-1.3	N	190	-2.0	N	190	4.5	N
L-Ascorbic acid	50-81-7	e1k	200	4.3	N	200	7.4	N	200	-7.5	N
Nordihydroguaiaretic acid	500-38-9	e1k	200	75.4	Y	200	77.0	Y	200	94.5	Y
Procaine hydrochloride	51-05-8	e1k	200	-0.3	N	200	16.9	N	200	6.8	N
Monotridecyl phosphate	5116-94-9	e1k	200	94.8	Y	200	81.6	Y	200	101.1	Y
Sodium methyl sulfate	512-42-5	e1k	200	-2.0	N	200	-2.6	N	200	3.6	N
Trimethyl phosphate	512-56-1	e1k	200	-2.7	N	200	0.9	N	200	3.9	N
Chloroallyl methenamine chloride	51229-78-8	e1k	200	-4.4	N	200	9.6	Y	200	51.6	Y
Methyltrioctylammonium chloride	5137-55-3	e1k	200	83.7	Y	200	95.9	Y	200	90.7	Y
Sulfosuccinic acid	5138-18-1	e1k	200	2.6	N	200	5.5	N	200	5.0	N
3,7-Dimethyl-2,6-octadienenitrile	5146-66-7	e1k	210	0.1	N	200	-9.7	N	200	6.8	N
2-Ethylhexylparaben	5153-25-3	e1k	200	97.8	Y	200	96.2	Y	200	96.5	Y
Sodium dichloro-s-triazinetriene dihydrate	51580-86-0	e1k	200	-0.4	N	200	1.7	N	200	3.3	N
Fenvalerate	51630-58-1	e1k	200	4.0	N	200	7.1	N	200	7.6	N
1-(Bromomethyl)-3-phenoxybenzene	51632-16-7	e1k	200	0.1	N	200	3.9	N	200	6.0	N
Kaempferol	520-18-3	e1k	200	22.8	N	190	6.1	N	190	0.2	N
Apigenin	520-36-5	e1k	200	0.3	N	200	-0.5	N	200	-10.5	N
Dehydroacetic acid	520-45-6	e1k	200	1.2	N	200	-2.2	N	200	11.8	N
dl-alpha-Tocopheryl acetate	52225-20-4	e1k	200	-1.0	N	200	-0.7	N	200	21.0	N
Kinetin	525-79-1	e1k	200	-1.7	N	200	-4.1	N	200	2.5	N
Flavone	525-82-6	e1k	200	-2.4	N	190	-1.2	N	190	-18.1	N
2,3-Dimethylphenol	526-75-0	e1k	200	0.0	N	200	7.6	N	200	6.9	N
Deltamethrin	52918-63-5	e1k	200	-6.5	N	200	5.7	N	200	15.4	N
o,p'-DDD	53-19-0	e1k	200	-6.0	N	200	13.3	N	200	17.0	N
Dehydroepiandrosterone	53-43-0	e1k	200	2.5	N	200	6.0	N	200	-22.2	N
Dibenz(a,h)anthracene	53-70-3	e1k	180	14.1	N	170	27.0	N	170	41.6	N
Sodium 2-naphthalenesulfonate	532-02-5	e1k	200	-6.3	N	200	-3.6	N	200	-2.1	N
Dihydromyrcenol	53219-21-9	e1k	200	7.1	N	200	4.2	N	200	2.1	N
Sulfamic acid	5329-14-6	e1k	200	-0.3	N	200	-3.3	N	200	-0.4	N
2,4-D-ethyl ester	533-23-3	e1k	200	2.8	N	200	0.1	N	200	-0.2	N
2-Octyl-1-dodecanol	5333-42-6	e1k	200	-2.0	N	200	-9.6	N	200	0.6	N

N,N'-Dimethylthiourea	534-13-4	e1k	200	0.1	N	200	2.6	N	200	2.8	N
(Z)-11-Hexadecenal	53939-28-9	e1k	200	1.7	N	200	33.1	N	200	25.8	N
5-Ethyl-5-methylhydantoin	5394-36-5	e1k	200	-4.9	N	200	6.2	N	200	2.9	N
Pentyl butyrate	540-18-1	e1k	200	-1.9	N	200	3.0	N	200	10.6	N
tert-Butyl acetate	540-88-5	e1k	200	0.1	N	200	0.4	N	200	-4.3	N
Cyclobutyl phenyl ketone	5407-98-7	e1k	200	-2.3	N	200	-0.4	N	200	-2.0	N
Decamethylcyclpentasiloxane	541-02-6	e1k	200	-3.1	N	200	-5.7	N	200	1.4	N
1,3-Cyclopentadiene	542-92-7	e1k	200	4.9	N	200	-4.1	N	200	0.1	N
Benzyl bromoacetate	5437-45-6	e1k	200	-3.4	N	200	-2.8	N	200	3.4	N
Tetradecanoic acid	544-63-8	e1k	200	63.0	Y	200	81.3	Y	200	76.6	Y
N-Methylphthalimide	550-44-7	e1k	200	2.4	N	200	-0.3	N	200	-3.9	N
Trimellitic anhydride	552-30-7	e1k	200	6.3	N	200	5.4	N	200	0.3	N
Magnesium dibenzoate	553-70-8	e1k	200	2.8	N	200	4.4	N	200	2.8	N
Sodium methacrylate	5536-61-8	e1k	200	0.3	N	200	7.9	N	200	6.8	N
Pyridate	55512-33-9	e1k	200	1.3	N	200	6.3	N	200	5.0	N
Acesulfame potassium	55589-62-3	e1k	200	-2.8	N	200	-0.5	N	200	-4.0	N
Mepronil	55814-41-0	e1k	200	3.6	N	200	-3.1	N	200	-1.6	N
Tripropylene glycol butyl ether	55934-93-5	e1k	200	-1.6	N	200	0.5	N	200	2.8	N
Chlorhexidine diacetate	56-95-1	e1k	200	89.8	Y	200	103.0	Y	200	105.1	Y
N,N-Dibutyl-N-methylbutan-1-aminium chloride	56375-79-2	e1k	200	1.2	N	200	-0.6	N	200	2.3	N
Allyl isothiocyanate	57-06-7	e1k	210	4.3	N	200	-4.5	N	200	6.0	N
Hexadecyltrimethylammonium bromide	57-09-0	e1k	200	98.3	Y	200	97.3	Y	200	104.8	Y
Hexadecanoic acid	57-10-3	e1k	200	-11.7	N	200	21.2	N	200	34.9	N
1,1-Dimethylhydrazine	57-14-7	e1k	200	-4.3	N	200	1.9	N	200	12.7	N
1,4-Dimethylnaphthalene	571-58-4	e1k	200	-1.0	N	200	-2.7	N	200	1.9	N
Pyridoxine hydrochloride	58-56-0	e1k	200	3.6	N	200	-0.5	N	200	3.9	N
Triphenylethylene	58-72-0	e1k	200	-3.2	N	200	0.8	N	200	16.2	N
Biotin	58-85-5	e1k	200	-0.6	N	200	-5.2	N	200	4.2	N
D-Xylose	58-86-6	e1k	200	-0.9	N	200	-3.9	N	200	6.1	N
2,5-Dichlorophenol	583-78-8	e1k	200	5.9	N	200	1.9	N	200	2.7	N
3,5,5-Trimethylhexyl acetate	58430-94-7	e1k	200	-2.6	N	200	5.5	N	200	-4.1	N
3-tert-Butylphenol	585-34-2	e1k	200	-1.0	N	200	8.8	N	200	-1.5	N
C.I. Acid Orange 8, monosodium salt	5850-86-2	e1k	200	1.9	N	200	24.3	Y	200	12.6	Y
Terpinolene	586-62-9	e1k	200	2.6	N	200	10.9	N	200	21.1	N
2-Chloro-N-phenylacetamide	587-65-5	e1k	200	103.2	Y	200	37.9	N	200	11.0	N
Diphenylmercury(II)	587-85-9	e1k	200	-5.5	N	200	-1.7	N	200	-1.2	N
Heptyl butanoate	5870-93-9	e1k	200	2.8	N	200	-1.3	N	200	-1.5	N

Decyl beta-D-glucopyranoside	58846-77-8	e1k	200	2.7	N	200	-3.8	N	200	-4.5	N
Tetradecanoic acid, 2,3-dihydroxypropyl ester	589-68-4	e1k	200	-0.2	N	200	25.8	Y	200	54.4	Y
Sulfaquinoxaline	59-40-5	e1k	200	3.6	N	200	4.0	N	200	8.3	N
Laurocapram	59227-89-3	e1k	200	0.1	N	200	74.0	Y	200	65.8	Y
2,2-Dichloropropane	594-20-7	e1k	200	1.3	N	200	-0.6	N	200	7.3	N
Methyl carbamate	598-55-0	e1k	200	-6.8	N	200	10.8	N	200	-10.1	N
2-Phenylethanol	60-12-8	e1k	200	-6.5	N	200	-7.8	N	200	-0.4	N
Linoleic acid	60-33-3	e1k	200	87.7	Y	200	89.1	Y	200	96.5	Y
Triphenylphosphine	603-35-0	e1k	200	3.1	N	200	-5.2	N	200	1.2	N
Oxazepam	604-75-1	e1k	170	-1.3	N	170	5.7	N	170	15.1	N
Diisopropyl phthalate	605-45-8	e1k	200	-0.1	N	200	4.4	N	200	-2.1	N
6-Hydroxy-2-naphthyl disulfide	6088-51-3	e1k	200	98.2	Y	200	87.5	Y	200	94.6	Y
2,5-Dimethylbenzenesulfonic acid	609-54-1	e1k	200	0.4	N	200	1.2	N	200	-6.0	N
Methylene blue	61-73-4	e1k	200	3.8	N	200	42.1	N	200	16.5	N
Amitrole	61-82-5	e1k	200	4.3	N	200	1.8	N	200	1.5	N
2-Hydroxybenzotrile	611-20-1	e1k	200	-1.7	N	190	-28.0	N	190	-9.0	N
Isopropyl phenyl ketone	611-70-1	e1k	200	3.2	N	200	-1.9	N	200	-8.7	N
3,3'-Dimethylbenzidine dihydrochloride	612-82-8	e1k	200	1.6	N	200	15.5	N	200	-3.6	N
Sodium 4-octylbenzenesulfonate	6149-03-7	e1k	200	1.8	N	200	39.9	N	200	-4.7	N
Sodium 2-phenylphenate tetrahydrate	6152-33-6	e1k	200	47.7	N	200	68.2	Y	200	70.6	Y
2-Pyrrolidinone	616-45-5	e1k	200	-3.7	N	190	-1.1	N	190	-9.6	N
Cremophor EL	61791-12-6	e1k	100 µg/ml	5.1	N	100 µg/ml	9.1	N	100 µg/ml	8.4	N
3-Isopropylphenol	618-45-1	e1k	200	-2.8	N	200	3.0	N	200	-1.4	N
Deethylatrazine	6190-65-4	e1k	200	-1.8	N	200	-4.3	N	200	28.5	N
Thiourea	62-56-6	e1k	200	5.4	N	200	-6.0	N	200	9.7	N
Sodium fluoroacetate	62-74-8	e1k	200	0.8	N	200	-3.9	N	200	-0.1	N
3-Ethylphenol	620-17-7	e1k	200	0.3	N	200	0.2	N	200	-4.0	N
4-Methylstyrene	622-97-9	e1k	200	-3.0	N	200	5.7	N	200	-1.7	N
Isopropyl formate	625-55-8	e1k	200	-0.8	N	200	2.9	N	200	1.4	N
Hexyl salicylate	6259-76-3	e1k	200	-4.7	N	200	-13.3	N	200	-1.1	N
3,5-Dichloroaniline	626-43-7	e1k	200	3.5	N	200	-3.0	N	200	-5.3	N
Ethyl 4-chlorophenyl ketone	6285-05-8	e1k	200	1.2	N	200	-2.0	N	200	-2.7	N
Lactose	63-42-3	e1k	200	2.7	N	200	-1.3	N	200	2.1	N
Hydroxyprogesterone caproate	630-56-8	e1k	200	2.2	N	200	6.3	N	200	0.9	N
C.I. Acid Orange 7	633-96-5	e1k	100	0.5	N	100	3.9	N	100	5.9	N
Benzyl-C8-18-alkyldimethylammonium chlorides	63449-41-2	e1k	200	94.9	Y	200	95.9	Y	200	101.9	Y

Acid Yellow 11	6359-82-6	e1k	200	0.8	N	200	0.7	N	200	1.5	N
C.I. Acid Yellow 34, monosodium salt	6359-90-6	e1k	200	0.1	N	200	32.7	N	200	0.7	N
C.I. Acid Yellow 17, disodium salt	6359-98-4	e1k	200	-0.3	N	200	20.2	N	200	8.8	N
2-Methylaniline hydrochloride	636-21-5	e1k	200	0.1	N	190	0.5	N	190	8.6	N
1-Phenylurea	64-10-8	e1k	190	-3.7	N	190	-0.2	N	190	4.6	N
4,5-Dichloro-2-octyl-3(2H)-isothiazolone	64359-81-5	e1k	200	105.9	Y	200	96.6	Y	200	96.4	Y
Phenyl phosphorus dichloride	644-97-3	e1k	200	3.9	N	190	-4.3	N	190	2.6	N
4-Propylphenol	645-56-7	e1k	200	1.0	N	200	2.5	N	200	-8.1	N
2-Ethyl-2-hexenal	645-62-5	e1k	200	1.5	N	190	3.8	N	190	11.0	N
Triclopyr-butotyl	64700-56-7	e1k	200	-1.8	N	200	4.0	N	200	1.1	N
R-(-)-Carvone	6485-40-1	e1k	200	-0.6	N	200	21.2	N	200	35.8	N
Salicylamide	65-45-2	e1k	200	-4.5	N	200	2.9	N	200	8.9	N
Morin hydrate	654055-01-3	e1k	200	96.1	Y	200	19.8	Y	200	91.7	Y
Sodium 4-methylbenzenesulfonate	657-84-1	e1k	200	-1.5	N	200	-3.5	N	200	2.3	N
1,10-Phenanthroline	66-71-7	e1k	200	-2.4	N	200	4.4	N	200	-4.0	N
N-Methylhydrazinecarbothioamide	6610-29-3	e1k	200	3.4	N	200	-0.4	N	200	5.6	N
C.I. Acid Violet 12, disodium salt	6625-46-3	e1k	190	6.2	N	180	-2.6	N	180	10.9	N
Ranitidine	66357-35-5	e1k	200	-10.4	N	200	0.7	N	200	4.7	N
Forskolin	66575-29-9	e1k	200	-2.4	N	200	-9.7	N	200	-4.2	N
Irganox 1010	6683-19-8	e1k	90	-1.5	N	80	-1.5	N	80	9.2	N
Dimethyl sulfoxide	67-68-5	e1k	200	-3.4	N	200	-0.6	N	200	6.7	N
L-Glucitol	6706-59-8	e1k	200	5.4	N	200	-3.3	N	200	-0.3	N
(2E)-2-Hexenal	6728-26-3	e1k	200	4.6	N	200	27.0	N	200	38.5	N
Hydramethylnon	67485-29-4	e1k	200	-0.2	N	200	86.6	Y	200	9.1	Y
(2R,6S)-Fenpropimorph	67564-91-4	e1k	200	-4.3	N	200	3.8	N	200	-2.8	N
Acid Red 337	67786-14-5	e1k	200	14.4	N	200	29.0	N	200	18.4	N
Hexyl benzoate	6789-88-4	e1k	200	-0.6	N	200	7.9	N	200	7.4	N
Thioglycolic acid	68-11-1	e1k	200	14.3	N	200	13.9	N	200	16.9	N
(Dicyclopentadienyloxy)ethyl methacrylate	68169-03-9	e1k	200	28.5	N	200	82.0	Y	200	83.3	Y
Tetrapropyl orthosilicate	682-01-9	e1k	200	8.1	N	200	-3.7	N	200	1.5	N
Dibutyltin dichloride	683-18-1	e1k	200	7.3	N	200	17.2	N	200	9.5	N
N-Nitroso-N-methylurea	684-93-5	e1k	200	3.1	N	200	8.1	N	200	1.0	N
DINP branched	68515-48-0	e1k	200	-6.7	N	200	2.0	N	200	-6.4	N
Hexanedioic acid, di-C7-9-branched and linear alkyl esters	68515-75-3	e1k	200	-2.2	N	200	8.2	N	200	-2.5	N
Acid Orange 156	68555-86-2	e1k	200	13.2	N	200	38.8	Y	200	66.7	Y
C12-14-Alkyl glycidyl ether	68609-97-2	e1k	119	75.3	Y	110	58.6	Y	110	47.2	Y

Cornmint oil	68917-18-0	e1k	100 µg/ml	5.1	N	100 µg/ml	8.5	N	100 µg/ml	6.3	N
Salicylic acid	69-72-7	e1k	200	-4.5	N	200	-1.9	N	200	-2.1	N
Ethyl undec-10-enoate	692-86-4	e1k	200	9.2	N	200	4.7	N	200	6.5	N
gamma-Caprolactone	695-06-7	e1k	200	2.2	N	190	-1.3	N	190	2.8	N
Haloxypop-methyl	69806-40-2	e1k	200	-0.3	N	200	0.9	N	200	5.7	N
4-Toluenesulfonamide	70-55-3	e1k	200	-4.0	N	190	-1.9	N	190	6.3	N
Dihydrojasmane lactone	7011-83-8	e1k	200	2.9	N	200	5.3	N	200	-0.9	N
(2-Nitro-1-propenyl)benzene	705-60-2	e1k	200	8.7	N	200	73.8	Y	200	55.2	Y
4-Butylcyclohexanol	70568-60-4	e1k	200	-2.1	N	200	2.9	N	200	-9.1	N
gamma-Decanolactone	706-14-9	e1k	200	3.2	N	200	8.3	N	200	-8.7	N
Chloramine-T trihydrate	7080-50-4	e1k	200	10.3	N	200	6.9	N	200	15.8	N
1-Propanol	71-23-8	e1k	200	1.3	N	200	-4.2	N	200	1.0	N
Fenoxaprop-P-ethyl	71283-80-2	e1k	200	11.2	N	200	25.3	Y	200	71.5	Y
MON-4660	71526-07-3	e1k	200	9.0	N	200	4.9	N	200	11.0	N
1,3,5-Triisopropylbenzene	717-74-8	e1k	200	3.1	N	200	-0.2	N	200	-1.8	N
Mestranol	72-33-3	e1k	200	2.1	N	200	8.0	N	200	-4.8	N
Nerolidol	7212-44-4	e1k	200	7.4	N	200	18.4	N	200	18.5	N
Melatonin	73-31-4	e1k	200	-2.1	N	200	0.5	N	200	8.2	N
Dimethyldiallylammonium chloride	7398-69-8	e1k	200	-0.8	N	200	-0.5	N	200	2.8	N
Trimethylamine	75-50-3	e1k	200	-5.7	N	200	-1.9	N	200	4.5	N
tert-Butylamine	75-64-9	e1k	200	-1.9	N	200	-1.5	N	200	-5.4	N
2-Hydroxy-2-methylpropanenitrile	75-86-5	e1k	200	0.4	N	200	6.8	N	200	6.3	N
Dimethyltin dichloride	753-73-1	e1k	200	-0.1	N	200	2.6	N	200	-5.7	N
(S)-(-)-beta-Citronellol	7540-51-4	e1k	200	-7.4	N	200	5.9	N	200	-2.2	N
Dimethyl methylphosphonate	756-79-6	e1k	200	-3.7	N	200	7.5	N	200	3.3	N
Bornyl acetate	76-49-3	e1k	200	2.1	N	200	12.5	N	200	8.0	N
3,4-Dichloro-1-butene	760-23-6	e1k	200	7.4	N	200	14.0	N	200	37.2	N
Diethyl phosphite	762-04-9	e1k	200	-0.6	N	200	0.9	N	200	1.8	N
2-Ethylhexyl sulfanylacetate	7659-86-1	e1k	200	4.0	N	200	5.3	N	200	-12.0	N
Phosphoric acid	7664-38-2	e1k	200	5.4	N	200	-1.0	N	200	1.5	N
Ronidazole	7681-76-7	e1k	200	-2.4	N	200	8.0	N	200	2.8	N
4-tert-Butylaniline	769-92-6	e1k	200	2.3	N	200	1.9	N	200	-2.1	N
Gibberellic acid	77-06-5	e1k	200	0.7	N	200	2.3	N	200	3.6	N
Dicyclopentadiene	77-73-6	e1k	200	3.9	N	190	1.6	N	190	7.9	N
Ethyl methylphenylglycidate	77-83-8	e1k	200	-4.5	N	200	6.8	N	200	10.0	N
Tromethamine	77-86-1	e1k	200	2.1	N	190	-1.2	N	190	6.5	N

1-Phenoxy-2-propanol	770-35-4	e1k	200	2.8	N	200	-4.6	N	200	0.0	N
Potassium nitrate	7757-79-1	e1k	200	-5.8	N	190	-1.9	N	190	3.6	N
Ammonium sulfamate	7773-06-0	e1k	200	0.4	N	190	0.8	N	190	-2.6	N
Sodium persulfate	7775-27-1	e1k	200	-3.1	N	200	0.6	N	200	3.9	N
1,3,5-Triethylhexahydro-s-triazine	7779-27-3	e1k	200	3.3	N	200	-3.3	N	200	4.7	N
(-)-alpha-Pinene	7785-26-4	e1k	200	-0.2	N	200	5.6	N	200	-2.8	N
Ethyltriethoxysilane	78-07-9	e1k	200	-1.7	N	200	18.0	N	200	-0.9	N
Pentaerythritol tetranitrate	78-11-5	e1k	200	-8.3	N	200	0.4	N	200	2.3	N
Triethyl phosphate	78-40-0	e1k	200	-2.3	N	200	-1.1	N	200	1.9	N
Tris(2-butoxyethyl) phosphate	78-51-3	e1k	200	4.4	N	200	5.2	N	200	-9.8	N
3,7-Dimethyl-3-octanol	78-69-3	e1k	200	-0.9	N	200	3.6	N	200	1.5	N
Linalool	78-70-6	e1k	200	2.7	N	200	4.4	N	200	4.8	N
2-Methylpropanenitrile	78-82-0	e1k	200	0.7	N	200	-2.5	N	200	-4.1	N
1-Amino-2-propanol	78-96-6	e1k	200	-9.2	N	200	-1.5	N	200	-0.3	N
Enterolactone	78473-71-9	e1k	70	10.5	N	60	-2.4	N	60	-11.3	N
Diazolidinyl urea	78491-02-8	e1k	200	-5.6	N	200	10.5	N	200	15.2	N
Glycolic acid	79-14-1	e1k	200	5.9	N	190	4.1	N	190	5.9	N
Nitroethane	79-24-3	e1k	200	-0.7	N	200	-0.1	N	200	-8.3	N
Oxytetracycline	79-57-2	e1k	200	80.8	Y	200	45.5	Y	200	83.7	Y
Camphene	79-92-5	e1k	200	-2.0	N	200	5.4	N	200	-2.5	N
2,2',6,6'-Tetrachlorobisphenol A	79-95-8	e1k	200	103.6	Y	200	90.3	Y	200	74.5	Y
4-Chloropentylbenzene	79098-20-7	e1k	200	-0.3	N	200	2.1	N	200	-2.2	N
Thifensulfuron-methyl	79277-27-3	e1k	200	-1.8	N	200	-5.0	N	200	-0.3	N
4,4'-Dichlorodiphenyl sulfone	80-07-9	e1k	200	-0.3	N	200	-1.9	N	200	11.5	N
4,4'-Sulfonyldiphenol	80-09-1	e1k	200	2.6	N	200	-4.6	N	200	2.0	N
alpha-Terpinyol acetate	80-26-2	e1k	200	9.3	N	200	0.3	N	200	11.2	N
Terpinyol propionate	80-27-3	e1k	200	13.9	N	200	2.0	N	200	3.6	N
3-(4-tert-Butylphenyl)-2-methylpropanal	80-54-6	e1k	200	12.2	N	200	17.7	N	200	10.8	N
alpha-Pinene	80-56-8	e1k	200	2.8	N	200	-2.6	N	200	-3.0	N
Terpineol	8000-41-7	e1k	200	0.4	N	200	-6.4	N	200	-0.4	N
Benzalkonium chloride	8001-54-5	e1k	200	104.2	Y	200	98.5	Y	200	102.1	Y
Peppermint oil	8006-90-4	e1k	100 µg/ml	19.8	N	100 µg/ml	21.9	N	100 µg/ml	10.2	N
Anise oil	8007-70-3	e1k	100 µg/ml	11.7	N	100 µg/ml	7.9	N	100 µg/ml	10.2	N
Saccharin	81-07-2	e1k	200	-1.7	N	200	4.0	N	200	2.8	N
Rhodamine B	81-88-9	e1k	200	2.1	N	200	14.8	N	200	12.2	N

Imazamethabenz	81405-85-8	e1k	200	0.7	N	200	-2.0	N	200	-5.7	N
Tributyltetradecylphosphonium chloride	81741-28-8	e1k	200	100.8	Y	200	98.8	Y	200	85.1	Y
2-Hydroxyethyl acrylate	818-61-1	e1k	200	0.5	N	200	14.7	N	200	13.1	N
Sodium 2-nitrophenolate	824-39-5	e1k	200	-4.7	N	200	1.2	N	200	-3.8	N
Sodium 2,5-dimethylbenzenesulfonate	827-19-0	e1k	200	2.1	N	200	3.5	N	200	4.1	N
Sodium m-xylene-4-sulfonate	827-21-4	e1k	200	-0.9	N	200	4.7	N	200	0.0	N
Riboflavin	83-88-5	e1k	190	6.6	N	180	17.1	N	180	28.2	N
Diphenyl phosphate	838-85-7	e1k	200	-0.1	N	200	-1.7	N	200	-6.6	N
2-Ethylhexyl trans-4-methoxycinnamate	83834-59-7	e1k	200	7.0	N	200	15.2	N	200	5.1	N
Dicyclohexyl phthalate	84-61-7	e1k	210	0.5	N	200	9.4	N	200	2.6	N
1,2,3,6-Tetrahydrophthalimide	85-40-5	e1k	200	-9.6	N	200	-4.7	N	200	-0.5	N
Phthalimide	85-41-6	e1k	200	1.0	N	200	2.3	N	200	-8.3	N
(3,5-Dimethyl-1H-pyrazol-1-yl)methanol	85264-33-1	e1k	200	-3.9	N	200	3.5	N	200	7.7	N
Phthalic acid, diundecyl ester, branched and linear	85507-79-5	e1k	200	-0.6	N	200	5.0	N	200	2.3	N
1-Naphthaleneacetic acid	86-87-3	e1k	200	0.3	N	200	7.0	N	200	-0.2	N
C.I. Acid Blue 74	860-22-0	e1k	200	15.9	N	200	-1.9	N	200	8.7	N
Dimethyl hydrogen phosphite	868-85-9	e1k	200	0.9	N	200	-1.6	N	200	0.4	N
7-(Dimethylamino)-4-methylcoumarin	87-01-4	e1k	200	3.3	N	200	7.1	N	200	-1.6	N
4-tert-Butylphenyl salicylate	87-18-3	e1k	200	-3.9	N	200	-1.2	N	200	10.9	N
Ethyl 2-methylbenzoate	87-24-1	e1k	200	-2.2	N	200	-9.3	N	200	1.9	N
Ethyl anthranilate	87-25-2	e1k	200	-3.8	N	200	1.5	N	200	0.1	N
Hexachloro-1,3-butadiene	87-68-3	e1k	200	-0.3	N	200	2.6	N	200	5.4	N
S-Metolachlor	87392-12-9	e1k	200	46.2	N	200	27.2	N	200	20.6	N
Monopotassium phthalate	877-24-7	e1k	200	-0.8	N	200	2.9	N	200	4.0	N
4-Chloro-3,5-dimethylphenol	88-04-0	e1k	200	1.1	N	200	2.6	N	200	-8.1	N
2,2'-Methylenebis(ethyl-6-tert-butylphenol)	88-24-4	e1k	200	9.1	N	200	48.9	Y	200	75.6	Y
2-tert-Butylcyclohexyl acetate	88-41-5	e1k	200	0.7	N	200	-1.4	N	200	2.4	N
2-Isopropylphenol	88-69-7	e1k	200	0.4	N	200	2.2	N	200	2.5	N
2-Nitroaniline	88-74-4	e1k	200	2.4	N	200	7.7	N	200	2.3	N
2-Nitrophenol	88-75-5	e1k	200	-4.6	N	200	-4.3	N	200	8.2	N
Methyl 2-methylbenzoate	89-71-4	e1k	200	0.2	N	200	1.8	N	200	0.9	N
dl-Menthol	89-78-1	e1k	200	-0.9	N	200	1.6	N	200	-2.8	N
1,3-Dimethyl-4-nitrobenzene	89-87-2	e1k	200	-4.2	N	200	1.5	N	200	3.8	N
2-Ethylphenol	90-00-6	e1k	200	0.4	N	190	3.1	N	190	5.8	N
Salicylaldehyde	90-02-8	e1k	200	-3.5	N	200	-0.6	N	200	12.2	N
2-Methoxyphenol	90-05-1	e1k	200	4.1	N	200	2.5	N	200	9.8	N
1-Naphthol	90-15-3	e1k	200	14.3	N	200	34.3	N	200	37.1	N

N-Phenyl-1-naphthylamine	90-30-2	e1k	200	1.3	N	200	19.0	N	200	12.8	N
2,4,6-Tris(dimethylaminomethyl)phenol	90-72-2	e1k	200	-0.6	N	200	0.2	N	200	-1.1	N
Pluronic F-127	9003-11-6	e1k	200	-2.5	N	200	1.1	N	200	-0.4	N
Polyoxyethylene monoleate	9004-96-0	e1k	100 µg/ml	46.8	N	100 µg/ml	59.5	Y	100 µg/ml	40.3	Y
Polysorbate 80	9005-65-6	e1k	179	4.6	N	170	10.2	N	170	3.8	N
Polydimethylsiloxane	9016-00-6	e1k	200	-4.7	N	200	-2.4	N	200	-1.0	N
Polymethylene polyphenyl isocyanate	9016-87-9	e1k	200	-4.8	N	200	1.7	N	200	2.1	N
Bicalutamide	90357-06-5	e1k	200	-0.3	N	200	0.7	N	200	-8.2	N
Denatonium saccharide	90823-38-4	e1k	200	-1.6	N	200	-0.5	N	200	-3.6	N
lambda-Cyhalothrin	91465-08-6	e1k	170	-8.1	N	170	6.2	N	170	6.3	N
3-Aminopropyltriethoxysilane	919-30-2	e1k	200	3.4	N	200	-5.9	N	200	12.3	N
2-Chloro-4-phenylphenol	92-04-6	e1k	200	-5.3	N	200	27.5	N	200	-3.6	N
4-Phenylphenol	92-69-3	e1k	200	-13.6	N	200	9.4	N	200	-17.0	N
(Z)-3-Hexen-1-ol	928-96-1	e1k	200	-2.4	N	200	0.7	N	200	3.9	N
2'-Acetonaphthone	93-08-3	e1k	200	2.9	N	200	-4.2	N	200	-8.1	N
Styrene glycol	93-56-1	e1k	200	-1.1	N	200	-2.4	N	200	1.1	N
Mecoprop	93-65-2	e1k	200	1.3	N	200	1.1	N	200	8.1	N
2,4,5-Trichlorophenoxyacetic acid	93-76-5	e1k	200	-6.3	N	200	0.0	N	200	7.8	N
Ethyl benzoate	93-89-0	e1k	200	-1.8	N	200	-9.0	N	200	8.0	N
(+/-)-alpha-Methylbenzyl acetate	93-92-5	e1k	200	0.7	N	200	1.5	N	200	-8.4	N
Phenyl benzoate	93-99-2	e1k	200	13.7	N	200	38.7	N	200	20.4	N
N-Nitrosopyrrolidine	930-55-2	e1k	200	1.2	N	190	10.5	N	190	-11.4	N
tert-Butyl phenyl ketone	938-16-9	e1k	200	4.9	N	200	1.4	N	200	-2.6	N
Ethyl 4-methylbenzoate	94-08-6	e1k	200	3.5	N	200	-1.8	N	200	-4.0	N
Benzocaine	94-09-7	e1k	200	1.9	N	200	0.7	N	200	5.8	N
Benzylparaben	94-18-8	e1k	200	-0.5	N	200	8.4	N	200	-19.6	N
Isopentyl benzoate	94-46-2	e1k	200	1.3	N	200	8.4	N	200	-3.5	N
2-Phenylethyl benzoate	94-47-3	e1k	200	0.4	N	200	4.3	N	200	-3.5	N
Dimethyl hexahydroterephthalate	94-60-0	e1k	200	-2.7	N	200	-1.6	N	200	0.7	N
2-Ethoxyphenol	94-71-3	e1k	200	-1.8	N	200	-3.3	N	200	2.7	N
2,4-D 1-butyl ester	94-80-4	e1k	200	-3.2	N	200	3.4	N	200	0.1	N
MCPB	94-81-5	e1k	200	-5.8	N	200	3.7	N	200	-6.6	N
N,N'-Disalicylidene-1,2-diaminopropane	94-91-7	e1k	200	-3.5	N	200	-9.5	N	200	6.4	N
2-Ethyl-1,3-hexanediol	94-96-2	e1k	200	4.7	N	190	4.7	N	190	-1.0	N
1-Phenyl-1H-pyrrole-2,5-dione	941-69-5	e1k	200	15.6	N	200	14.9	N	200	23.4	N
Indene	95-13-6	e1k	200	6.6	N	200	25.7	N	200	29.2	N

Benzothiazole	95-16-9	e1k	200	3.1	N	200	-0.8	N	200	-2.3	N
2-(8-Heptadecenyl)-2-imidazoline-1-ethanol	95-38-5	e1k	200	92.9	Y	200	97.2	Y	200	98.4	Y
3-Chloro-4-methylaniline	95-74-9	e1k	210	-0.5	N	200	5.5	N	200	-1.9	N
3,4-Dichloroaniline	95-76-1	e1k	200	2.9	N	200	-1.4	N	200	4.5	N
1,2,4,5-Tetramethylbenzene	95-93-2	e1k	200	0.1	N	200	-3.3	N	200	-7.5	N
Trinexapac-ethyl	95266-40-3	e1k	200	-2.8	N	200	0.0	N	200	-0.4	N
Diphenamid	957-51-7	e1k	200	-0.1	N	200	2.4	N	200	-3.8	N
Endosulfan I	959-98-8	e1k	200	-2.6	N	200	-3.5	N	200	0.9	N
3-Chloro-1,2-propanediol	96-24-2	e1k	200	-1.4	N	190	8.5	N	190	-12.2	N
Cyclopentanol	96-41-3	e1k	200	-0.6	N	190	-2.6	N	190	-2.4	N
Triphenylborane	960-71-4	e1k	200	-2.2	N	200	56.4	Y	200	44.9	Y
1-Chloro-2,4-dinitrobenzene	97-00-7	e1k	200	52.9	Y	200	86.1	Y	200	95.0	Y
Dichlorophen	97-23-4	e1k	200	93.6	Y	200	91.9	Y	200	98.4	Y
2-Methoxy-4-nitroaniline	97-52-9	e1k	200	0.2	N	200	-10.2	N	200	6.7	N
Allantoin	97-59-6	e1k	200	-1.7	N	200	-2.1	N	200	-1.4	N
N-Dodecanoyl-N-methylglycine	97-78-9	e1k	200	9.9	N	190	8.8	N	190	-0.8	N
Tetrahydrofurfuryl alcohol	97-99-4	e1k	200	-0.6	N	200	-2.7	N	200	1.6	N
Furfuryl alcohol	98-00-0	e1k	200	4.5	N	190	20.7	N	190	36.8	N
4-tert-Butyltoluene	98-51-1	e1k	200	-3.3	N	200	-4.2	N	200	4.0	N
4-tert-Butylcyclohexanol	98-52-2	e1k	200	-1.8	N	200	0.2	N	200	-9.0	N
4-tert-Butylcyclohexanone	98-53-3	e1k	200	-2.5	N	200	-0.7	N	200	4.8	N
1-Chloro-4-(trifluoromethyl)benzene	98-56-6	e1k	200	2.3	N	200	-3.1	N	200	8.2	N
Niacinamide	98-92-0	e1k	210	6.6	N	200	2.5	N	200	1.4	N
Finasteride	98319-26-7	e1k	200	0.9	N	200	6.6	N	200	-3.5	N
Benoxacor	98730-04-2	e1k	200	7.7	N	200	12.9	N	200	23.6	N
Rhodamine 6G	989-38-8	e1k	200	0.5	N	200	59.5	Y	200	55.6	Y
3-Dimethylaminophenol	99-07-0	e1k	200	10.6	N	200	14.7	N	200	10.3	N
1,3-Benzenedicarbonyl dichloride	99-63-8	e1k	200	-2.6	N	200	4.4	N	200	1.7	N
gamma-Terpinene	99-85-4	e1k	200	5.3	N	200	-3.5	N	200	-0.5	N
alpha-Terpinene	99-86-5	e1k	200	0.6	N	200	22.8	N	200	40.5	N
4-Isopropylphenol	99-89-8	e1k	200	-1.1	N	200	-6.4	N	200	3.2	N
4-Hydroxyacetophenone	99-93-4	e1k	200	-1.7	N	200	6.1	N	200	10.2	N
4-Hydroxybenzoic acid	99-96-7	e1k	200	2.4	N	200	-2.1	N	200	-6.2	N
Cloquintocet-mexyl	99607-70-2	e1k	200	2.1	N	200	7.1	N	200	-0.5	N
Hexamethyldisilazane	999-97-3	e1k	200	-2.8	N	200	7.6	N	200	18.2	N
Igepal CO-890	NOCAS_47708	e1k	100 µg/ml	4.0	N	100 µg/ml	-2.6	N	100 µg/ml	-3.1	N

Formalin	NOCAS_47796	e1k	208	-0.3	N	200	0.5	N	200	5.9	N
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Supplemental Table 7. Concentration-response results. Chemicals that produced greater than 50% median inhibition in the single-point screening in an assay as well as a subset that produced less than 50% median inhibition were further tested in concentration-response; the 240 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 (v1.0).

^a Maximum concentration in concentration-response testing, in μM except indicated as $\mu\text{g}/\text{ml}$ for polyoxyethylene monoleate. ^b Median % inhibition at maximum tested concentration for each chemical in concentration-response testing, $n = 3$ replicates. ^c --, not tested in concentration-response. ^d NA = not applicable. The 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. ^e IC50 estimated at greater 500 μM due to incomplete inhibition curve.

Source	Chemical	CASRN	DIO1					DIO2					DIO3				
			Max conc., μM ^a	% Inhibition at max conc. ^b , median	IC20	IC50	Hill slope	Max conc., μM ^a	% Inhibition at max conc. ^b , median	IC20	IC50	Hill slope	Max conc., μM ^a	% Inhibition at max conc. ^b , median	IC20	IC50	Hill slope
ToxCast phase 1_v2	Mesotrione	104206-82-8	-- ^c	--	--	--	--	200	30.1	56.14	NA ^d	-0.5	200	59.2	12.56	101.65	-0.8
	Resmethrin	10453-86-8	--	--	--	--	--	200	73.4	16.68	60.17	-1.2	200	76.4	15.79	58.51	-1.1
	Dicofol	115-32-2	200	69.4	35.75	91.95	-1.7	190	78.3	50.84	96.49	-2.3	190	95.4	9.96	16.22	-2.9
	Chlorophene	120-32-1	200	1.0	NA	NA	NA	200	46.7	111.90	231.75	-3.5	200	76.3	119.27	146.15	-8.0
	Fipronil	120068-37-3	200	47.9	30.78	NA	-1.8	200	74.4	11.75	43.74	-1.2	200	101.0	0.27	1.16	-0.9
	Cyazofamid	120116-88-3	200	62.7	21.09	94.51	-1.1	200	52.7	48.46	176.57	-1.9	200	22.6	165.90	NA	-1.7
	Maneb	12427-38-2	200	73.9	15.52	50.10	-1.3	--	--	--	--	--	--	--	--	--	--
	Quinoxifen	124495-18-7	--	--	--	--	--	200	63.3	4.91	18.72	-1.4	200	88.3	0.21	1.29	-0.8
	Fenhexamid	126833-17-8	200	-13.6	NA	NA	NA	--	--	--	--	--	--	--	--	--	--
	Captan	133-06-2	200	48.5	45.26	166.10	-2.8	--	--	--	--	--	--	--	--	--	--
	Thiram	137-26-8	--	--	--	--	--	200	36.7	50.62	>500 ^e	-0.9	200	71.2	18.62	69.60	-1.1
	Diclosulam	145701-21-9	200	51.8	23.84	161.27	-0.9	--	--	--	--	--	--	--	--	--	--
	Emamectin benzoate	155569-91-8	200	94.4	16.68	26.41	-3.1	200	101.9	20.34	30.88	-3.3	200	89.2	15.81	38.19	-1.7
	Zoxamide	156052-68-5	200	98.2	8.18	17.01	-1.9	200	94.6	3.09	12.86	-1.0	200	56.9	26.57	97.30	-1.7
	Alachlor	15972-60-8	--	--	--	--	--	200	57.5	28.05	158.69	-1.0	200	61.5	28.60	108.66	-1.4
	Malaoxon	1634-78-2	200	5.6	NA	NA	NA	--	--	--	--	--	--	--	--	--	--
	PFOS	1763-23-1	--	--	--	--	--	160	54.0	75.23	163.67	-3.1	160	23.8	186.84	NA	-8.0
	Chlorothalonil	1897-45-6	200	57.9	24.52	51.35	-3.2	200	62.7	2.45	30.60	-0.8	200	75.6	0.15	0.49	-1.3
	Oryzalin	19044-88-3	200	49.0	146.06	206.99	-7.0	200	53.4	114.26	187.28	-4.0	200	52.8	120.61	185.62	-5.9
	Atrazine	1912-24-9	--	--	--	--	--	200	5.0	NA	NA	NA	200	68.8	10.94	39.05	-1.4
	Cyanazine	21725-46-2	--	--	--	--	--	200	14.3	NA	NA	NA	200	77.6	4.91	28.02	-0.8
	Prallethrin	23031-36-9	--	--	--	--	--	190	48.7	29.25	184.25	-1.1	190	73.3	16.06	52.67	-1.3
	Pirimicarb	23103-98-2	--	--	--	--	--	200	59.6	21.88	109.31	-1.0	200	88.6	2.15	11.21	-0.9
	Butachlor	23184-66-9	200	66.9	18.63	40.57	-2.4	200	75.5	6.39	28.09	-1.0	200	64.8	13.62	71.02	-1.0
Captafol	2425-06-1	200	94.4	4.78	12.90	-1.5	200	52.7	28.95	171.90	-1.2	200	76.7	10.86	55.15	-0.9	
Prodiamine	29091-21-2	--	--	--	--	--	190	33.7	25.22	NA	-1.4	190	48.6	16.72	207.9	-1.2	
Pirimiphos-methyl	29232-93-7	--	--	--	--	--	200	49.7	10.79	216.65	-0.7	200	64.3	13.26	57.19	-1.3	
2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane	2971-36-0	--	--	--	--	--	200	45.6	79.21	233.81	-1.8	200	55.6	106.41	147.33	-8.0	
Triclosan	3380-34-5	200	106.4	39.56	49.19	-6.7	200	92.6	45.6	85.26	-2.1	200	107.6	62.06	73.31	-8.0	

	Acetochlor	34256-82-1	--	--	--	--	--	200	57.1	24.89	131.53	-1.0	200	64.9	25.89	115.7	-1.1	
	Fluoxastrobin	361377-29-9	--	--	--	--	--	200	-3.5	NA	NA	NA	200	56.7	9.96	59.76	-1.3	
	Metolachlor	51218-45-2	200	45.3	55.73	370.84	-1.8	--	--	--	--	--	--	--	--	--	--	
	Fenthion	55-38-9	200	67.8	3.79	26.38	-0.9	--	--	--	--	--	--	--	--	--	--	
	Allethrin	584-79-2	--	--	--	--	--	190	56.3	28.27	131.62	-1.5	190	71.5	19.64	67.57	-1.3	
	Oxytetracycline dihydrate	6153-64-6	200	83.1	7.00	20.24	-1.4	200	50.3	43.67	199.88	-1.4	200	93.3	8.94	26.51	-1.3	
	Fenoxaprop-ethyl	66441-23-4	--	--	--	--	--	200	29.0	51.51	NA	-2.0	200	64.7	7.76	31.93	-1.3	
	Triflumizole	68694-11-1	200	73.8	13.39	18.79	-5.1	200	98.1	0.71	2.87	-1.0	200	101.9	0.46	2.25	-0.9	
	Tetramethrin	7696-12-0	--	--	--	--	--	200	63.9	28.50	113.26	-1.1	200	-0.5	NA	NA	NA	
	Fluazinam	79622-59-6	180	62.4	15.26	37.03	-2.3	180	99.9	0.48	2.21	-0.9	180	100.6	0.41	2.03	-0.9	
	Mancozeb	8018-01-7	100	50.6	31.09	89.28	-4.1	100	41.6	35.70	250.79	-1.8	100	49.8	30.09	98.87	-1.9	
	Rotenone	83-79-4	--	--	--	--	--	200	17.1	NA	NA	-1.1	200	61.1	1.15	7.05	-1.1	
	Azinphos-methyl	86-50-0	200	64.4	24.09	85.76	-1.3	--	--	--	--	--	--	--	--	--	--	
	Flumiclorac-pentyl	87546-18-7	--	--	--	--	--	200	81.8	21.34	64.50	-1.2	200	32.6	107.69	NA	-2.6	
	Milbemectin (mixture of 70% Milbemecin A4, 30% Milbemycin A3)	NOCAS_34742	--	--	--	--	--	190	34.2	76.87	NA	-1.2	190	72.1	30.37	84.43	-1.5	
ToxCast phase 2	2-Benzylideneoctanal	101-86-0	--	--	--	--	--	200	67.4	5.05	45.01	-0.7	200	84.5	1.07	4.74	-1.0	
	17beta-Trenbolone	10161-33-8	--	--	--	--	--	200	48.7	68.51	237.52	-1.7	200	68.3	8.74	47.51	-1.0	
	Octyl gallate	1034-01-1	200	100.6	85.76	101.93	-8.0	200	89.5	94.04	133.46	-3.7	200	97.6	42.85	80.92	-2.0	
	4-Nonylphenol	104-40-5	200	85.7	72.90	88.15	-8.0	200	72.9	98.31	121.91	-8.0	200	100.0	13.11	15.57	-8.0	
	Tamoxifen	10540-29-1	100	71.3	52.29	65.54	-7.9	100	91.2	37.95	45.58	-8.0	100	12.4	NA	NA	NA	
	PharmaGSID_47337	1061517-62-1	200	75.2	106.24	148.74	-4.2	200	58.1	54.83	165.44	-1.5	200	73.0	100.59	125.35	-8.0	
	Mepanipyrim	110235-47-7	200	68.4	15.30	49.85	-1.6	200	68	7.54	49.13	-0.8	200	84.6	1.26	5.64	-1.1	
	Glutaraldehyde	111-30-8	--	--	--	--	--	200	39.8	75.42	>500 °	-1.8	200	87.3	2.61	11.27	-1.0	
	Bis(2-chloroethyl) ether	111-44-4	--	--	--	--	--	200	-7.3	NA	NA	NA	200	9.4	NA	NA	NA	
	Dodecyltrimethylammonium chloride	112-00-5	200	64.3	52.25	134.16	-1.6	200	77.4	83.08	102.17	-8.0	200	82.7	90.04	109.08	-8.0	
	1-Undecanol	112-42-5	--	--	--	--	--	200	2.5	NA	NA	NA	200	79.4	103.92	126.75	-8.0	
	1-Dodecanol	112-53-8	--	--	--	--	--	200	4.4	NA	NA	NA	200	78.3	58.94	72.23	-8.0	
	1-Tridecanol	112-70-9	--	--	--	--	--	200	-0.7	NA	NA	NA	200	71.3	39.32	65.68	-3.5	
	Sodium hexyldecyl sulfate	1120-01-0	100	103.3	34.25	40.57	-8.0	90	84.6	14.84	28.12	-2.3	90	96.8	3.35	5.76	-2.6	
	Sodium myristyl sulfate	1191-50-0	200	100.6	62.91	74.55	-8.0	200	100.6	20.88	36.27	-2.5	200	96.9	14.90	17.73	-8.0	
	2,4-Bis(2-methylbutan-2-yl)phenol	120-95-6	200	102.8	33.41	45.55	-4.4	200	81.6	48.08	86.60	-2.5	200	102.4	15.89	18.9	-8.0	
	TNP-470	129298-91-5	60	64.3	6.34	36.49	-0.9	--	--	--	--	--	--	--	--	--	--	--
	CP-100829	135080-03-4	100	62.1	19.49	58.31	-1.6	--	--	--	--	--	--	--	--	--	--	--
	4-Hexylresorcinol	136-77-6	200	61.3	97.72	162.27	-3.5	--	--	--	--	--	--	--	--	--	--	--
	Darbufelone mesylate	139340-56-0	100	73.8	1.35	4.7	-1.3	100	65.9	11.53	50.1	-1.1	100	85.4	3.49	17.16	-0.8	
	4-(1,1,3,3-Tetramethylbutyl)phenol	140-66-9	200	102.2	71.56	84.93	-8	200	85	92.42	111.79	-8	200	99.4	55.37	65.82	-8	
	Tannic acid	1401-55-4	60	95.7	9.73	17.39	-2.4	60	54.4	11.85	49.78	-1.2	60	88.3	4.66	15.05	-1.1	
	Kepon	143-50-0	200	95.9	10.11	27.93	-1.4	200	90.6	12.21	30.45	-1.6	200	100.4	2.23	4.37	-2	
	Bisphenol AF	1478-61-1	--	--	--	--	--	200	74.5	91.63	137.31	-3.8	200	69.2	99.24	125.06	-8	
	2-Mercaptobenzothiazole	149-30-4	200	88.2	6.82	25.62	-1.1	200	65.3	13.92	81	-0.9	200	67.4	44.76	117.27	-1.7	
	FR150011	149413-74-1	200	102.6	62.28	99.2	-2.7	200	67.3	87.96	143.39	-3.2	200	80.9	101.88	124.35	-8	

Sodium dodecyl sulfate	151-21-3	--	--	--	--	--	200	76.8	88.86	109.59	-8	200	81.6	86.66	105.83	-8
Celecoxib	169590-42-5	200	60.3	151.1	183.61	-8.0	200	53.5	122.19	177.99	-8.0	200	64.1	152.55	183.76	-8.0
CJ-013790	179465-71-5	--	--	--	--	--	100	55.3	24.54	78.80	-1.5	100	49.4	23.04	100.79	-1.6
4-Octylphenol	1806-26-4	200	102.3	29.79	49.78	-2.6	200	78.0	106.34	130.01	-8.0	200	100.7	16.65	19.78	-8.0
Farglitazar	196808-45-4	180	105.4	45.59	53.97	-8.0	170	102.2	19.89	40.78	-1.9	170	103.8	40.04	47.49	-8.0
4-Heptylphenol	1987-50-4	200	101.7	53.96	75.51	-4.0	200	77.2	97.25	119.04	-8.0	200	104.4	53.10	62.95	-8.0
UK-337312	203942-49-8	200	103.2	40.49	56.55	-4.1	200	99.3	24.37	38.04	-3.1	200	99.5	54.98	65.36	-8.0
Oxytetracycline hydrochloride	2058-46-0	200	76.8	14.42	40.24	-1.5	200	30.6	117.22	NA	-1.4	200	60.5	47.25	135.40	-1.6
Perfluoroundecanoic acid	2058-94-8	200	106.8	111.98	131.96	-8.0	100	39.1	37.98	219.01	-1.6	100	99.8	9.28	15.20	-2.8
CI-1029	207736-05-8	200	64.7	38.01	121.79	-1.4	--	--	--	--	--	--	--	--	--	--
Pentachloropyridine	2176-62-7	--	--	--	--	--	200	57.1	8.39	46.69	-1.2	200	98.0	0.15	0.97	-0.7
SR146131 trifluoroacetate (1:1)	221671-62-1	--	--	--	--	--	100	15.6	40.93	NA	-1.3	100	100.2	6.46	7.68	-8.0
Sodium dodecylbenzenesulfonate	25155-30-0	200	88.6	80.88	97.18	-8.0	200	93.1	39.21	70.08	-2.3	200	104.9	27.61	39.53	-3.8
HMR1426	262376-75-0	200	71.6	12.17	32.71	-1.8	200	38.0	73.30	NA	-1.5	200	67.9	70.35	132.72	-2.5
Octhilinone	26530-20-1	210	52.4	30.11	175.21	-1	200	78.7	3.40	12.18	-1.2	200	95.4	3.21	15.16	-0.9
1-Dodecyl-2-pyrrolidinone	2687-96-9	200	83.3	123.37	148.45	-8.0	200	38.4	112.40	NA	-8.0	200	91.2	68.09	81.71	-8.0
Dodecylbenzenesulfonic acid	27176-87-0	200	103.0	54.35	64.42	-8.0	200	96.7	21.31	42.74	-2.0	200	98.2	15.68	18.63	-8.0
Dodecylbenzene sulfonate triethanolamine(1:1)	27323-41-7	180	97.1	87.12	103.81	-8.0	170	87.7	41.90	83.61	-2.0	170	102.5	20.97	37.25	-2.4
2,4-Bis(1-methyl-1-phenylethyl)phenol	2772-45-4	--	--	--	--	--	200	57.2	69.20	147.64	-2.7	200	85.1	11.43	19.67	-2.8
PFOS-K	2795-39-3	190	46.0	158.57	206.11	-8.0	190	60.3	83.17	160.08	-2.6	190	26.3	129.64	NA	-8.0
UK-373911	291305-06-1	--	--	--	--	--	200	85.8	19.02	55.35	-1.3	200	89.4	8.19	35.09	-0.9
Isooctyl acrylate	29590-42-9	200	76.8	12.95	41.03	-1.4	200	95.8	4.62	18.67	-1.0	200	86.7	7.82	33.96	-0.9
all-trans-Retinoic acid	302-79-4	--	--	--	--	--	200	51.3	34.19	167.44	-1.3	200	78.5	8.00	38.64	-0.9
Procymidone	32809-16-8	--	--	--	--	--	200	1.3	NA	NA	NA	200	-5.6	NA	NA	NA
PFDA	335-76-2	200	97.8	87.91	104.88	-8.0	200	78.0	44.24	104.94	-1.6	200	103.6	69.30	82.08	-8.0
SSR69071	344930-95-6	--	--	--	--	--	50	76.8	4.48	13.76	-1.4	50	90.1	1.57	5.13	-1.2
Elzasonan	361343-19-3	--	--	--	--	--	200	72.3	94.09	117.40	-8.0	200	1.1	NA	NA	NA
1-Hexadecanol	36653-82-4	--	--	--	--	--	100	-6.0	NA	NA	NA	100	0.3	NA	NA	NA
PFOA, ammonium salt	3825-26-1	--	--	--	--	--	200	0.0	NA	NA	NA	200	-12.8	NA	NA	NA
4,4'-Sulfonylbis [2-(prop-2-en-1-yl)phenol]	41481-66-7	--	--	--	--	--	200	73.3	85.55	137.81	-3.1	200	74.9	21.34	78.30	-1.1
Cyproterone acetate	427-51-0	--	--	--	--	--	200	14.5	NA	NA	NA	200	90.0	1.14	6.08	-0.9
SAR 150640	433212-21-6	190	50.1	59.94	237.05	-1.5	180	58.0	81.66	163.60	-2.6	180	41.8	100.85	NA	-8.0
Genistein	446-72-0	200	95.5	0.84	2.62	-1.2	--	--	--	--	--	--	--	--	--	--
Daidzein	486-66-8	200	84.4	6.57	22.16	-1.2	--	--	--	--	--	--	--	--	--	--
Clomiphene citrate (1:1)	50-41-9	200	80.3	44.33	76.34	-2.9	200	99.4	27.62	45.89	-2.7	200	1.4	NA	NA	NA
6-Propyl-2-thiouracil	51-52-5	200	101.1	1.08	3.81	-1.1	--	--	--	--	--	--	--	--	--	--
Spironolactone	52-01-7	--	--	--	--	--	200	78.1	6.51	33.13	-0.9	200	26.3	91.65	NA	-1.8
4-Chlorobenzotrichloride	5216-25-1	--	--	--	--	--	200	51.3	34.04	229.76	-0.9	200	73.3	36.76	89.31	-1.7
1,2-Dinitrobenzene	528-29-0	--	--	--	--	--	200	66.2	18.87	96.53	-0.9	200	83.3	8.84	40.51	-0.9
1-Hydroxypyrene	5315-79-7	200	42.6	82.07	>500 ^a	-1.9	200	35.8	103.14	NA	-1.7	200	87.2	19.10	63.86	-1.1
3,7-Dimethyl-2,6-octadienal	5392-40-5	--	--	--	--	--	200	41.2	82.08	364.78	-2.1	200	71.2	13.98	51.52	-1.2
Gentian Violet	548-62-9	--	--	--	--	--	200	28.4	119.09	NA	-8.0	200	75.9	14.94	30.59	-2.4

	Tamoxifen citrate	54965-24-1	180	95.8	34.70	51.60	-3.6	180	95.2	34.97	49.49	-4.1	180	35.6	84.82	NA	-8.0
	6-Methyl-2-thiouracil	56-04-2	200	87.9	3.93	18.38	-0.9	--	--	--	--	--	--	--	--	--	--
	Benz(a)anthracene	56-55-3	--	--	--	--	--	200	27.2	113.34	NA	-2.1	200	50.4	47.77	215.33	-1.4
	Docusate sodium	577-11-7	200	103	79.18	93.91	-8.0	200	86.0	59.96	90.38	-3.6	200	94.7	74.88	89.64	-8.0
	Terbutylazine	5915-41-3	--	--	--	--	--	200	9.6	NA	NA	NA	200	68.0	5.51	27.32	-1.2
	Sulfasalazine	599-79-1	200	87.5	4.42	23.66	-0.8	--	--	--	--	--	--	--	--	--	--
	Tetracycline	60-54-8	200	71.9	24.40	75.81	-1.4	200	23.0	178.44	NA	-3.6	200	60.7	34.88	125.19	-1.3
	2,3-Dinitrotoluene	602-01-7	--	--	--	--	--	140	63.5	11.88	52.81	-1.1	140	78.5	4.35	22.51	-0.9
	1,2-Benzenedicarboxaldehyde	643-79-8	200	79.3	18.82	61.88	-1.2	200	86.8	8.64	37.83	-0.9	200	93.5	0.73	3.50	-0.9
	Retinol	68-26-8	--	--	--	--	--	200	54.6	29.32	129.51	-1.7	200	80.8	5.25	30.54	-0.8
	4-Hydroxytamoxifen	68392-35-8	130	95.5	29.22	49.57	-2.4	120	107.7	16.88	31.06	-2.1	120	56.6	53.18	71.5	-8.0
	PharmaGSID_48519	686756-87-6	--	--	--	--	--	200	16.6	NA	NA	-8.0	200	1.3	NA	NA	NA
	Chlorpromazine hydrochloride	69-09-0	--	--	--	--	--	200	67.4	91.08	115.13	-8.0	200	50.6	125.14	186.49	-8.0
	Didecylmethylammonium chloride	7173-51-5	200	105.9	4.89	17.06	-1.0	200	99.7	46.06	62.47	-4.5	200	100.5	2.78	3.31	-8.0
	AVE5638	725228-45-5	200	70.9	63.53	108.25	-3.1	200	95.6	4.96	22.77	-0.9	200	99.7	2.43	14.56	-0.7
	Phosmet	732-11-6	200	76.8	10.96	54.32	-0.9	--	--	--	--	--	--	--	--	--	--
	Diphenyl isophthalate	744-45-6	--	--	--	--	--	200	40.1	31.25	NA	-1.7	200	68.9	17.59	80.09	-1.0
	Lovastatin	75330-75-5	200	78.5	18.62	63.93	-1.2	200	25.0	80.12	NA	-8.0	200	67.8	68.73	127.32	-2.8
	Hexachlorocyclopentadiene	77-47-4	200	62.5	48.16	133.91	-1.5	200	86.8	5.95	25.53	-1.0	200	98.9	0.70	3.30	-0.9
	3,3',5,5'-Tetrabromobisphenol A	79-94-7	190	107.0	22.82	37.41	-2.7	190	92.7	20.85	49.47	-1.6	190	90.7	12.16	38.35	-1.2
	Simvastatin	79902-63-9	200	78.3	20.23	58.48	-1.4	200	38.6	61.49	NA	-1.1	200	74.4	59.97	110.86	-2.5
	Dapsone	80-08-0	200	-0.1	NA	NA	NA	--	--	--	--	--	--	--	--	--	--
	Butyryl trihexyl citrate	82469-79-2	200	-10.3	NA	NA	NA	--	--	--	--	--	--	--	--	--	--
	Raloxifene hydrochloride	82640-04-8	--	--	--	--	--	200	39.9	98.28	NA	-8.0	200	0.2	NA	NA	NA
	4-Nonylphenol, branched	84852-15-3	200	99.3	27.72	32.95	-8.0	200	90.5	76.67	92.21	-8.0	200	104.0	15.28	18.17	-8.0
	2,4-Di-tert-butylphenol	96-76-4	200	95.3	94.00	112.23	-8.0	200	44.9	139.88	NA	-7.6	200	96.4	80.34	95.91	-8.0
	Isoeugenol	97-54-1	--	--	--	--	--	200	40.2	63.11	NA	-1.4	200	89.7	4.21	16.70	-1.0
	Troglitazone	97322-87-7	200	99.2	63.64	75.64	-8.0	200	89.3	25.33	63.50	-1.5	200	97.8	78.40	93.42	-8.0
	MK-274	NOCAS_47328	--	--	--	--	--	200	27.1	114.00	NA	-8.0	200	36.8	169.93	216.97	-8.0
	SR125047	NOCAS_47342	--	--	--	--	--	180	75.6	42.86	106.16	-1.5	180	74.1	11.77	51.48	-1.0
	SSR 241586 HCl	NOCAS_47353	--	--	--	--	--	120	76.3	55.97	68.64	-8.0	120	20.6	94.05	NA	-7.3
	AVE6324	NOCAS_47377	200	80.0	84.07	102.72	-8.0	200	98.3	18.62	41.74	-1.7	200	86.0	0.37	1.76	-1.0
	SARI02779	NOCAS_47387	--	--	--	--	--	150	59.7	66.34	133.8	-2.7	150	17.8	NA	NA	-8.0
	HMR1171 trifluoroacetate (1:1)	NOCAS_48522	80	47.3	48.67	84.67	-2.8	70	74.3	38.05	47.05	-8.0	70	44.7	46.24	NA	-8.0
ToxCast e1k	2-Ethylhexyl acrylate	103-11-7	200	88.3	3.93	19.37	-0.9	200	88.1	2.97	20.15	-0.7	200	75.1	14.09	55.69	-1.1
	Benzyl cinnamate	103-41-3	--	--	--	--	--	200	51.7	8.09	185.69	-0.9	200	74.8	2.24	11.29	-1.1
	4-Dodecylphenol	104-43-8	200	95	9.23	37.24	-0.9	200	86.2	40.92	74.18	-2.5	200	101.0	8.37	11.22	-4.7
	Heptylparaben	1085-12-7	200	98.4	44.24	70.67	-2.9	200	90.0	90.74	110.37	-7.5	200	100.3	52.42	62.37	-8.0
	Propanedinitrile	109-77-3	--	--	--	--	--	190	51.6	26.84	363.88	-0.8	190	59.9	27.06	129.26	-1.1
	Oleyl sarcosine	110-25-8	200	102.1	78.29	92.98	-8.0	200	97.1	17.51	48.72	-1.3	200	97.3	11.33	22.29	-2.1
	Methyl linoleate	112-63-0	200	56.4	7.39	99.89	-0.7	200	78.4	11.39	47.13	-1.0	200	91.9	4.56	17.67	-1.0
	Oleic acid	112-80-1	200	95.5	45.66	68.46	-3.4	200	79.3	32.86	93.48	-1.3	200	97.7	16.91	29.78	-2.5
	Octadecyl sulfate sodium salt	1120-04-3	200	94.4	71.65	85.79	-8.0	200	98.0	18.65	39.42	-1.8	200	93.4	1.69	3.26	-2.2
	Bromophenol blue	115-39-9	190	69.5	31.75	89.54	-1.5	180	67.0	19.05	62.82	-1.5	180	93.7	4.85	16.56	-1.1

Dodecyl gallate	1166-52-5	200	70.9	32.43	39.97	-8.0	200	91.0	47.99	82.09	-2.6	200	101.3	1.81	5.52	-1.2
Dichlone	117-80-6	200	86.7	5.22	25.58	-0.9	200	94.0	4.02	22.59	-0.7	200	92.5	2.84	12.37	-1.0
Pyrazolone T	118-47-8	200	70.5	21.94	81.34	-1.1	--	--	--	--	--	--	--	--	--	--
1,3-Butyleneglycol dimethacrylate	1189-08-8	--	--	--	--	--	200	66.7	22.84	89.18	-1.1	200	71	17.46	54.66	-1.5
2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	119-47-1	--	--	--	--	--	200	59.3	88.98	119.84	-8.0	200	96.2	11.41	14.57	-5.9
4,5-Dichloro-3H-1,2-dithiol-3-one	1192-52-5	200	99.7	0.06	0.17	-1.3	200	91.8	2.98	15.62	-0.8	200	102.8	0.74	3.33	-0.9
Octylparaben	1219-38-1	200	101.2	64.42	76.55	-8.0	200	89.6	58.67	93.38	-3.0	200	102.0	18.20	30.19	-2.7
Pentylcinnamaldehyde	122-40-7	--	--	--	--	--	200	42.9	45.35	444.76	-1.0	200	88.1	3.10	17.17	-0.8
Phenylacetaldehyde	122-78-1	--	--	--	--	--	200	19.8	228.88	NA	-1.5	200	57.9	33.75	138.44	-1.3
1-Dodecanamine	124-22-1	--	--	--	--	--	180	6.9	NA	NA	NA	180	57.6	113.44	154.92	-7.7
Methyl abietate	127-25-3	--	--	--	--	--	200	37.6	48.88	>500 °	-0.8	200	68.0	12.81	64.10	-0.9
Retinol acetate	127-47-9	--	--	--	--	--	200	49.1	36.12	226.84	-1.5	200	78.1	8.91	41.95	-0.9
C.I. Acid Orange 24, monosodium salt	1320-07-6	200	76.8	20.14	63.99	-1.3	200	18.2	NA	NA	-8.0	200	73.2	68.27	121.5	-2.5
C.I. Disperse Orange 37	13301-61-6	--	--	--	--	--	200	20.4	255.89	NA	-1.0	200	92.5	25.29	63.19	-1.4
Methylionone	1335-46-2	--	--	--	--	--	200	47.1	87.46	NA	-8.0	200	71.5	24.76	81.36	-1.2
Ascorbyl palmitate	137-66-6	200	51.7	78.94	136.62	-8.0	200	97.2	6.91	26.40	-1.0	200	97.9	1.19	4.21	-1.1
Phenol red	143-74-8	--	--	--	--	--	200	26.5	118.76	NA	-2.1	200	47.8	70.27	222.16	-1.5
Sodium abietate	14351-66-7	--	--	--	--	--	200	40.4	62.30	410.77	-1.2	200	66.3	30.25	104.2	-1.3
4-Nitrosodiphenylamine	156-10-5	--	--	--	--	--	200	52.2	44.51	181.61	-1.2	200	54.7	23.89	156.37	-1.0
5-Ethylidene-2-norbornene	16219-75-3	--	--	--	--	--	200	44.1	62.77	>500 °	-1.5	200	71.8	18.15	67.78	-1.2
Bisphenol A diglycidyl ether	1675-54-3	200	103.6	0.36	1.32	-1.0	200	101.4	1.20	3.73	-1.2	200	94.1	0.86	4.09	-0.9
Phenylparaben	17696-62-7	--	--	--	--	--	200	42.3	60.38	388.77	-1.5	200	69.2	16.07	70.79	-1.0
2,2'-(Tetraethylimino)diethanol	18924-66-8	200	94.1	5.08	28.78	-0.7	200	94.6	21.72	41.27	-2.2	200	93.0	4.49	7.78	-2.6
Propachlor	1918-16-7	200	94.7	6.32	29.73	-0.8	--	--	--	--	--	--	--	--	--	--
(2-Dodeceny)succinic anhydride	19780-11-1	200	50.0	19.71	NA	-1.5	200	45.3	48.67	252.21	-1.2	200	65.5	12.72	70.20	-0.9
Z-Tetrachlorvinphos	22248-79-9	200	91.1	16.98	48.17	-1.3	--	--	--	--	--	--	--	--	--	--
FD&C Green No. 3	2353-45-9	130	49.5	51.05	100.48	-3.2	130	35.8	58.53	NA	-2.8	130	86.3	38.16	60.83	-2.9
Basic Blue 7	2390-60-5	--	--	--	--	--	200	87.0	21.14	39.03	-2.5	200	82.4	4.80	9.89	-2.1
4-tert-Butylbenzenethiol	2396-68-1	200	80.3	4.89	21.23	-1.0	--	--	--	--	--	--	--	--	--	--
Econazole nitrate	24169-02-6	--	--	--	--	--	200	49.2	89.17	NA	-8.0	200	12.0	NA	NA	NA
Sodium 2-mercaptobenzothiolate	2492-26-4	--	--	--	--	--	200	19.9	161.45	NA	-0.7	200	52.0	33.81	178.77	-1.1
Methylbenzethonium chloride	25155-18-4	200	100.9	20.44	39.10	-2.1	200	99.9	17.05	31.30	-2.3	200	100.9	5.32	8.04	-3.3
Glyceryl monooleate	25496-72-4	--	--	--	--	--	200	75.1	17.69	56.55	-1.5	200	85.2	6.94	24.97	-1.1
Calcium dodecylbenzene sulfonate	26264-06-2	200	99.8	60.78	72.41	-8.0	200	94.1	16.46	25.59	-3.3	200	101.2	13.43	22.42	-2.7
Dodecylphenol	27193-86-8	200	78.3	20.96	61.36	-1.4	200	86.8	45.39	84.2	-2.3	200	100.4	12.6	14.99	-8.0
Disodium 4,4'-bis(2-sulfostyryl)biphenyl	27344-41-8	200	47.6	98.30	NA	-8.0	200	26.3	139.89	NA	-2.2	200	62.0	84.18	150.43	-2.8
C.I. Direct Yellow 12	2870-32-8	200	102.7	0.22	0.76	-1.1	200	86.5	14.90	50.22	-1.1	200	86.4	4.84	30.05	-0.7
Ethyl (2E,4Z)-deca-2,4-dienoate	3025-30-7	--	--	--	--	--	200	70.6	14.61	62.99	-1.1	200	71.8	14.16	46.10	-1.5
Isocostadecanoic acid	30399-84-9	200	87.0	47.36	57.49	-8.0	200	82.4	78.31	122.38	-3.1	200	101.7	16.35	19.46	-8.0

1,4-Dihydroxy-2-naphthoic acid	31519-22-9	200	61.0	15.60	92.48	-0.9	200	54.8	29.43	149.21	-1.5	200	69.5	17.29	74.70	-1.0
1,2,5,6,9,10-Hexabromocyclododecane	3194-55-6	170	-9.9	NA	NA	NA	--	--	--	--	--	--	--	--	--	--
Temephos	3383-96-8	200	92.9	0.10	1.34	-0.5	--	--	--	--	--	--	--	--	--	--
Codlure	33956-49-9	--	--	--	--	--	200	65.2	15.15	31.11	-2.9	200	72.5	7.62	28.48	-1.3
Chlorophacinone	3691-35-8	200	68.2	2.94	65.86	-0.4	200	48.5	68.65	233.46	-2.0	200	79.3	21.77	70.86	-1.1
Dinocap	39300-45-3	200	103.5	32.22	50.57	-3.0	200	92.9	3.20	18.22	-0.7	200	97.8	1.36	6.38	-0.9
Myristyltrimethylammonium chlorideN,N-Trimethyltetradecan-1-aminium chloride	4574-04-3	170	95.2	18.13	28.84	-3.0	170	100.1	16.26	27.32	-2.7	170	102.2	3.93	7.92	-2.0
Farnesol	4602-84-0	--	--	--	--	--	200	75.2	11.48	47.63	-1.1	200	95.0	2.49	13.96	-0.8
Linolenic acid	463-40-1	200	93.6	5.54	19.98	-1.1	200	77.6	8.89	31.02	-1.2	200	93.8	3.79	13.19	-1.1
Ergocalciferol	50-14-6	200	60.0	3.54	57.52	-0.5	200	79.2	6.02	28.31	-1.0	200	95.0	0.53	2.58	-0.9
Nordihydroguaiaretic acid	500-38-9	200	79.9	1.56	11.00	-0.8	200	72.5	8.59	34.61	-1.2	200	97.1	0.01	0.12	-0.6
Monotridecyl phosphate	5116-94-9	200	85.3	74.22	89.89	-8.0	200	90.9	30.41	69.54	-1.6	200	96.0	6.28	10.57	-2.7
Chloroallyl methenamine chloride	51229-78-8	--	--	--	--	--	200	13.1	NA	NA	NA	200	53.9	61.88	173.62	-1.8
Methyltriocetylammmonium chloride	5137-55-3	200	95.2	41.59	49.63	-8.0	200	99.3	12.41	20.85	-2.7	200	88.8	3.21	3.84	-8.0
2-Ethylhexylparaben	5153-25-3	200	100.1	62.80	74.79	-8.0	200	87.3	50.12	87.99	-2.5	200	100.0	48.44	57.64	-8.0
Tetradecanoic acid	544-63-8	200	52.3	160.30	196.69	-8.0	200	47.3	82.97	214.31	-2.0	200	69.7	111.03	138.11	-8.0
Chlorhexidine diacetate	56-95-1	200	87.4	1.24	13.05	-0.6	200	99.2	5.70	13.09	-1.7	200	103.0	1.31	2.58	-2.0
Hexadecyltrimethylammonium bromide	57-09-0	200	96.2	5.87	12.90	-1.8	200	101.0	16.65	19.87	-8.0	200	97.4	0.96	1.59	-2.8
C.I. Acid Orange 8, monosodium salt	5850-86-2	--	--	--	--	--	200	15.5	NA	NA	NA	200	12.6	NA	NA	NA
2-Chloro-N-phenylacetamide	587-65-5	200	104.8	7.04	18.82	-1.4	--	--	--	--	--	--	--	--	--	--
Tetradecanoic acid, 2,3-dihydroxypropyl ester	589-68-4	--	--	--	--	--	200	32.8	102.17	NA	-1.7	200	42.0	43.96	NA	-2.2
Laurocapram	59227-89-3	--	--	--	--	--	200	56.2	92.32	171.80	-2.9	200	60.6	75.56	100.11	-8.0
Linoleic acid	60-33-3	200	96.1	0.69	10.44	-0.5	200	77.5	16.31	49.77	-1.4	200	101.0	3.73	14.17	-1.0
6-Hydroxy-2-naphthyl disulfide	6088-51-3	200	92.8	0.48	2.74	-0.8	200	84.5	2.69	21.10	-0.7	200	102.1	0.57	3.08	-0.8
Sodium 2-phenylphenate tetrahydrate	6152-33-6	--	--	--	--	--	200	71.5	9.66	50.25	-0.9	200	83.1	48.89	97.54	-2.0
Benzyl-C8-18-alkyldimethylammonium chlorides	63449-41-2	200	99.8	20.62	32.04	-3.1	200	100.6	15.01	30.27	-2.0	200	102.5	4.57	7.80	-2.6
4,5-Dichloro-2-octyl-3(2H)-isothiazolone	64359-81-5	200	99.3	0.18	0.44	-1.5	200	95.0	2.35	16.95	-0.6	200	92.5	2.43	8.45	-1.1
Morin hydrate	654055-01-3	200	94.2	0.58	7.37	-0.5	200	27.6	85.66	NA	-1.4	200	96.8	10.92	31.56	-1.2
Hydramethylnon	67485-29-4	--	--	--	--	--	200	85.7	16.28	19.77	-8.0	200	18.4	NA	NA	-8.0
(Dicyclopentadienyloxy)ethyl methacrylate	68169-03-9	--	--	--	--	--	200	83.1	4.39	18.37	-1.0	200	86.9	1.69	8.12	-0.9
Acid Orange 156	68555-86-2	--	--	--	--	--	200	44.2	90.69	295.15	-2.2	200	66.0	79.80	146.16	-2.5
C12-14-Alkyl glycidyl ether	68609-97-2	119	64.9	0.76	4.15	-0.9	110	47.3	25.57	108.11	-1.3	110	58.0	1.41	16.78	-1.0
(2-Nitro-1-propenyl)benzene	705-60-2	--	--	--	--	--	200	76.2	12.46	54.28	-1.0	200	55.2	44.29	162.25	-1.5
Fenoxaprop-P-ethyl	71283-80-2	--	--	--	--	--	200	39.9	22.04	>500 °	-0.5	200	78.4	2.01	11.59	-0.9
Oxytetracycline	79-57-2	200	87.3	11.61	30.63	-1.5	200	46.8	58.59	252.95	-1.1	200	92.6	9.93	25.71	-1.5

2,2',6,6'-Tetrachlorobisphenol A	79-95-8	200	109.9	42.02	66.89	-2.8	200	84.1	59.34	104.87	-2.4	200	73.1	14.21	55.81	-1.1
Benzalkonium chloride	8001-54-5	200	104.2	4.70	20.10	-0.9	200	99.7	16.67	22.46	-4.7	200	105.9	12.30	14.58	-8.0
Tributyltetradecylphosphonium chloride	81741-28-8	200	93.9	5.45	12.45	-1.7	200	97.1	9.00	17.83	-2.1	200	80.9	2.80	3.35	-8.0
2,2'-Methylenebis(ethyl-6-tert-butylphenol)	88-24-4	--	--	--	--	--	200	48.3	73.11	206.58	-3.6	200	80.6	5.77	11.51	-2.3
Polyoxyethylene monoleate	9004-96-0	--	--	--	--	--	100 µg/ml	59.8	10.42	47.40	-1.2	100 µg/ml	50.6	8.64	80.21	-0.9
2-(8-Heptadecenyl)-2-imidazoline-1-ethanol	95-38-5	200	92.9	6.77	32.61	-0.8	200	98.6	34.84	58.85	-2.6	200	101.0	3.26	3.88	-8.0
Triphenylborane	960-71-4	--	--	--	--	--	200	59.6	36.36	128.70	-1.4	200	44.1	91.36	256.95	-1.8
1-Chloro-2,4-dinitrobenzene	97-00-7	200	42.0	70.39	445.59	-1.5	200	92.1	7.10	28.31	-1.0	200	93.7	2.06	8.39	-1.0
Dichlorophen	97-23-4	200	97.9	84.13	100.16	-8.0	200	77.4	58.98	115.12	-2.1	200	101.3	39.69	56.71	-3.8
Rhodamine 6G	989-38-8	--	--	--	--	--	200	40.0	123.13	NA	-7.9	200	33.8	131.18	NA	-8.0

	1	2	3	4	5	6	7	8	9	10	11	12
A												
B					*							
C												
D												
E												
F					*							
G												
H												

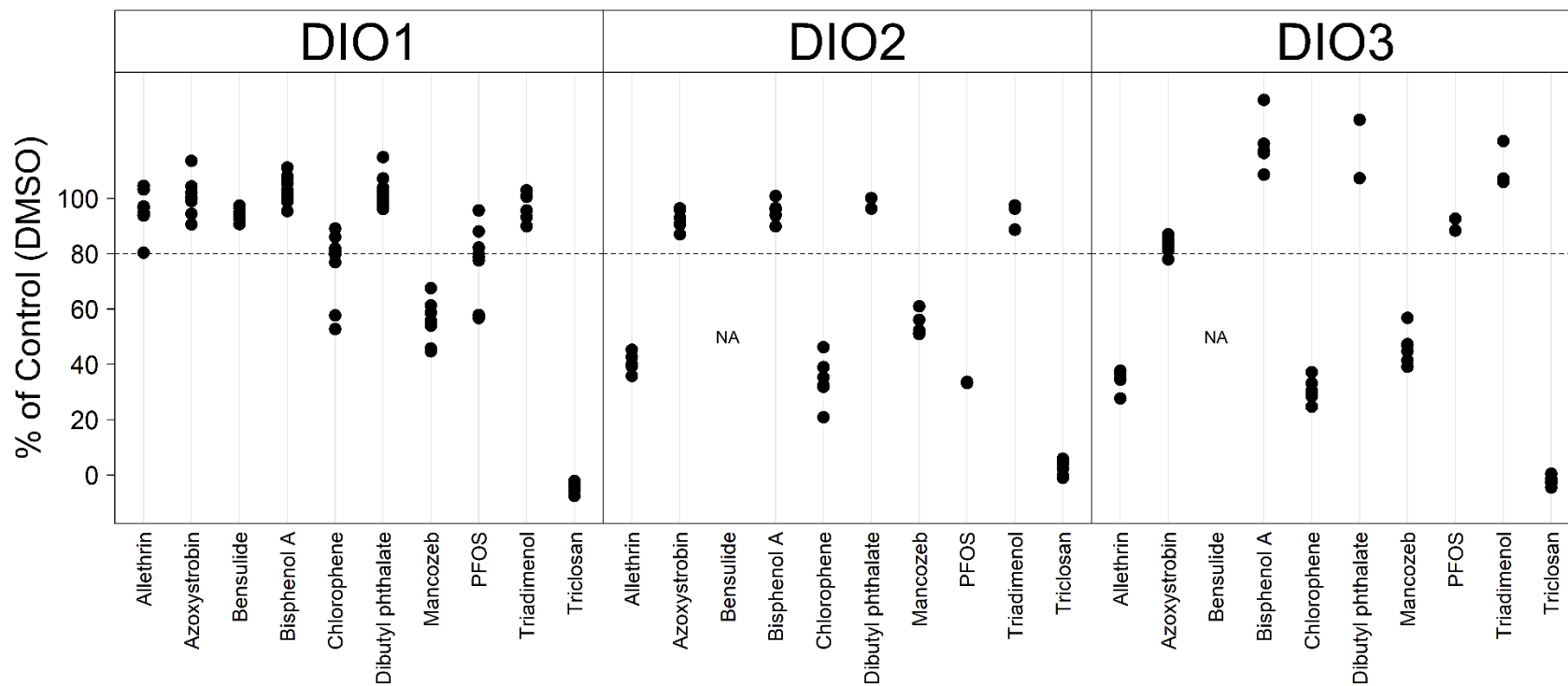
		Model Inhibitor Concentration Response Curve: PTU from 1000 to 0.03 μ M for DIO1, XTH from 200 to 0.0002 μ M for DIO2 and DIO3
		DMSO
		200 μ M Model Inhibitor (PTU or XTH)
		Sample
	*	Sample that is repeated on two or more chemical plates

Supplemental Figure 1. An example layout for the assay plate for the single-point screening with single target concentration of 200 μ M. Plates were received with column 1 empty for the concentration-response curve for the model inhibitor, 6-propylthiouracil (PTU) or xanthohumol (XTH) to be added. Twelve additional wells were left empty on the source plate to which dimethyl sulfoxide (DMSO) was added to 6 of these wells (white blocks) and the model inhibitor (orange blocks) was added to the remaining 6 wells to establish the fully inhibited response level. Sample chemicals repeated across multiple plates are indicated with an asterisk. These were randomly assigned to wells on each plate. DIO1 = Deiodinase Type 1; DIO2 = Deiodinase Type 2; DIO3 = Deiodinase Type 3.

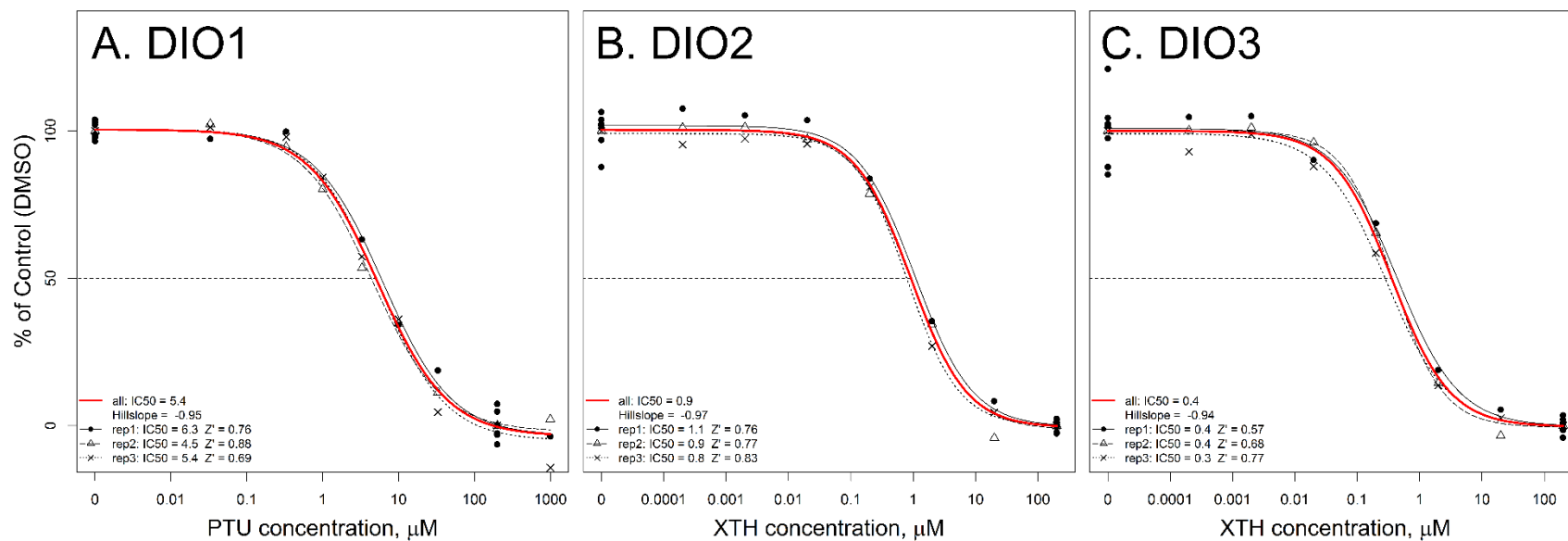
	1	2	3	4	5	6	7	8	9	10	11	12
A		Chem 1	Chem 2	Chem 3	Chem 4	Chem 5	Chem 6	Chem 7	Chem 8	Chem 9	Chem 10	Chem 11
B		Chem 1	Chem 2	Chem 3	Chem 4	Chem 5	Chem 6	Chem 7	Chem 8	Chem 9	Chem 10	Chem 11
C		Chem 1	Chem 2	Chem 3	Chem 4	Chem 5	Chem 6	Chem 7	Chem 8	Chem 9	Chem 10	Chem 11
D		Chem 1	Chem 2	Chem 3	Chem 4	Chem 5	Chem 6	Chem 7	Chem 8	Chem 9	Chem 10	Chem 11
E		Chem 1	Chem 2	Chem 3	Chem 4	Chem 5	Chem 6	Chem 7	Chem 8	Chem 9	Chem 10	Chem 11
F		Chem 1	Chem 2	Chem 3	Chem 4	Chem 5	Chem 6	Chem 7	Chem 8	Chem 9	Chem 10	Chem 11
G		Chem 1	Chem 2	Chem 3	Chem 4	Chem 5	Chem 6	Chem 7	Chem 8	Chem 9	Chem 10	Chem 11
H												

		Model Inhibitor Concentration Response Curve: PTU from 1000 to 0.03 μ M for DIO1, XTH from 200 to 0.0002 μ M for DIO2 and DIO3
		DMSO
		200 μ M Model Inhibitor (PTU or XTH)
		Sample

Supplemental Figure 2. Assay plate layout for concentration-response screening. The concentration-response curve for the model inhibitor, 6-propylthiouracil (PTU) or xanthohumol (XTH) was in column 1. Row H had 5 additional dimethyl sulfoxide (DMSO) wells (white blocks) and 6 additional wells with the model inhibitor (orange blocks) to establish the fully inhibited response level. DIO1 = Deiodinase Type 1; DIO2 = Deiodinase Type 2; DIO3 = Deiodinase Type 3.



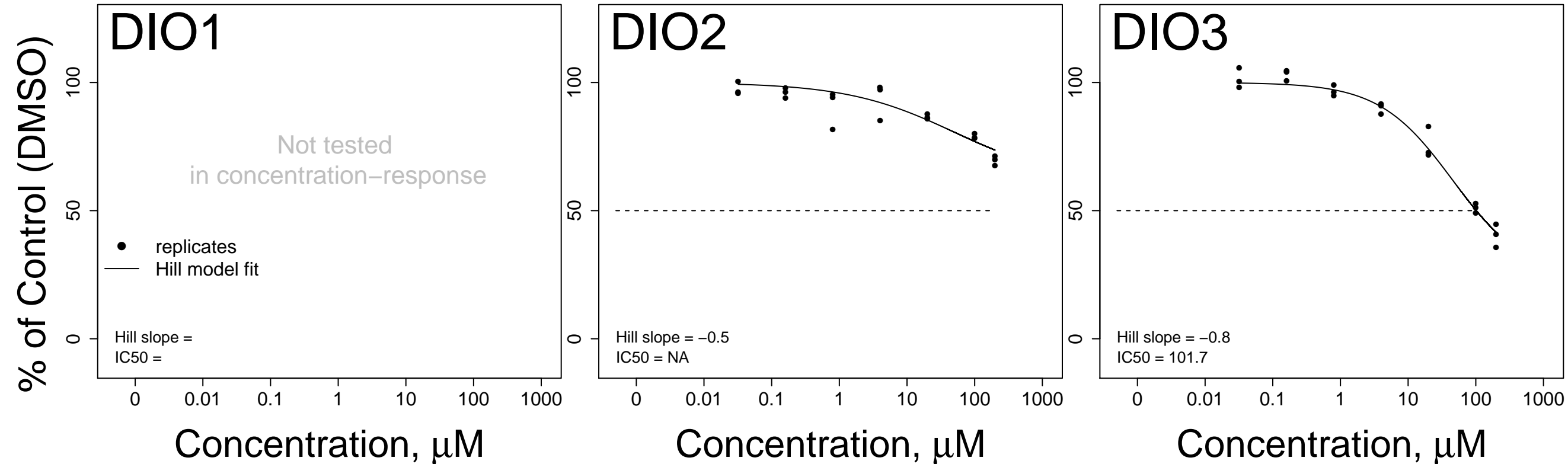
Supplemental Figure 3. Deiodinase inhibition produced by test chemicals that were randomly replicated across the chemical source plates to evaluate the plate-to-plate variability. These included allethrin, azoxystrobin, bensulide (DIO1 only), bisphenol A, chlorophene, dibutyl phthalate, mancozeb, perfluorooctane sulfonic acid (PFOS), triadimenol, and triclosan. NA = not replicated across plates in this assay. DMSO = dimethyl sulfoxide; DIO1 = Deiodinase Type 1; DIO2 = Deiodinase Type 2; DIO3 = Deiodinase Type 3.



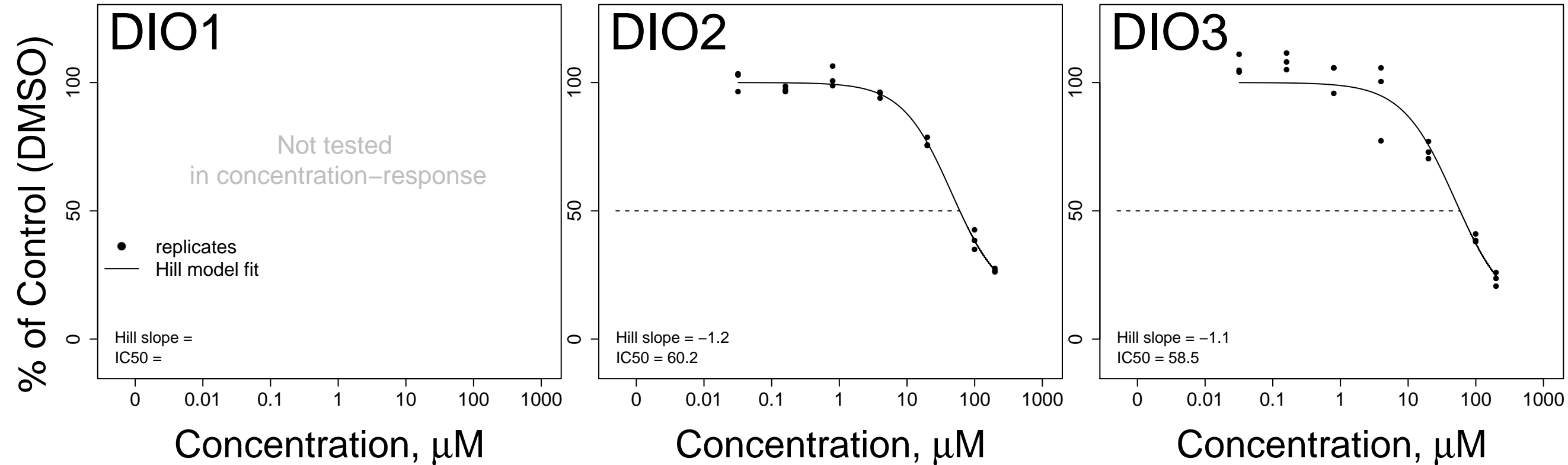
Supplemental Figure 4. Concentration-response curves for deiodinase inhibition by model inhibitors with 6-propylthiouracil (PTU) for DIO1 and xanthohumol (XTH) for DIO2 and DIO3 from three example assay plates. Each triplicate test of a plate has different symbols and fit line, solid circle with solid line = rep 1, open triangle with dashed line = rep 2, × with dotted line = rep 3. DMSO = dimethyl sulfoxide; DIO1 = Deiodinase Type 1; DIO2 = Deiodinase Type 2; DIO3 = Deiodinase Type 3.

Supplemental Figure 5. Concentration-response data. Deiodinase inhibition produced by all chemicals tested in concentration-response mode at seven concentrations. Hill model curve, absolute IC50, and Hill slope included for the chemicals where Hill model fit in ToxCast pipeline (tcpl v1.0). Results from all three assays are provided side-by-side for each chemical on the following 240 pages, with chemicals ordered by ToxCast library, matching Supplemental Table 7. DMSO = dimethyl sulfoxide; DIO1 = Deiodinase Type 1; DIO2 = Deiodinase Type 2; DIO3 = Deiodinase Type 3. NA = not applicable (Hill model did not fit data and/or 50% inhibition not produced in concentration-response testing).

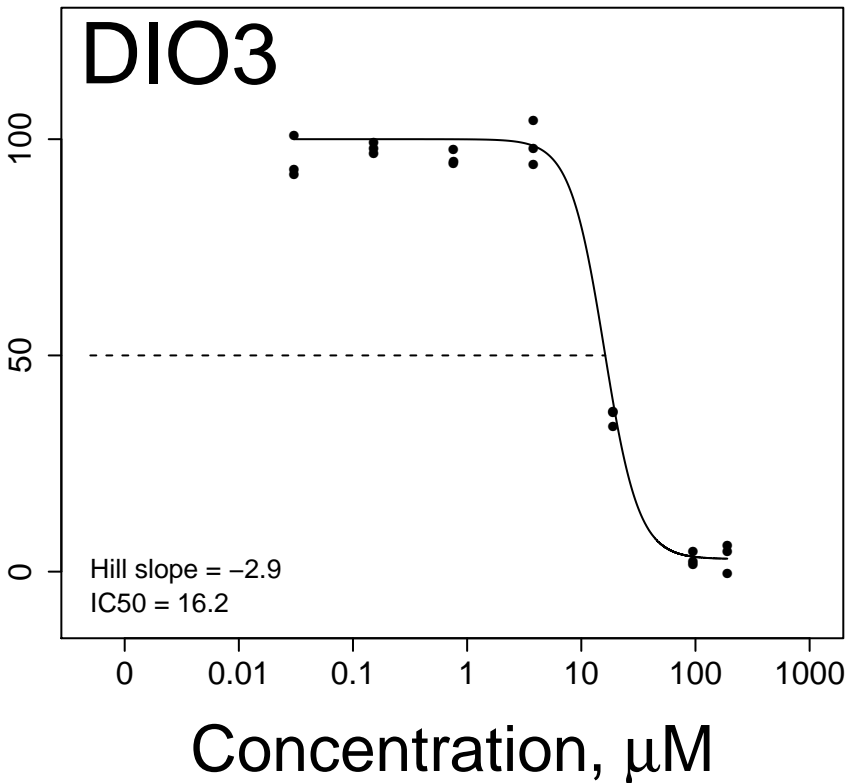
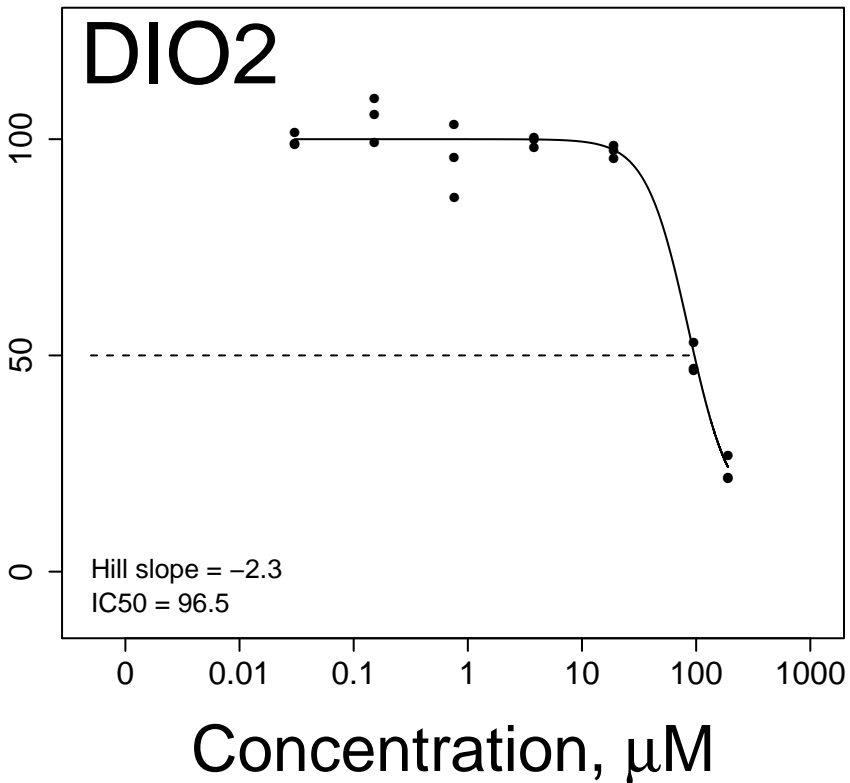
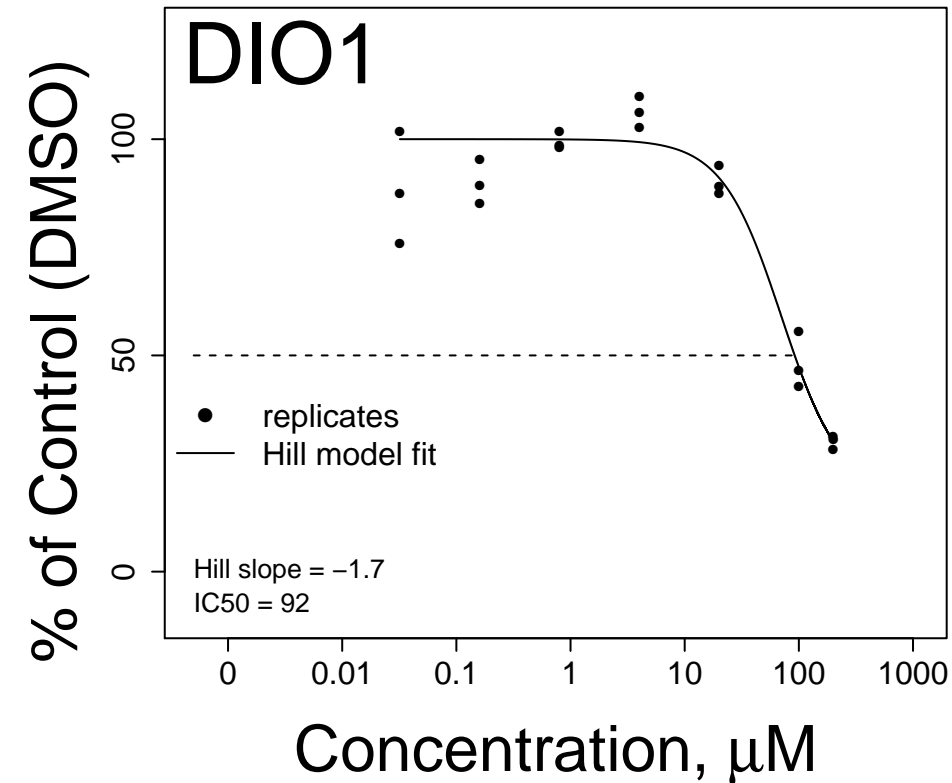
Mesotrione CASRN: 104206-82-8



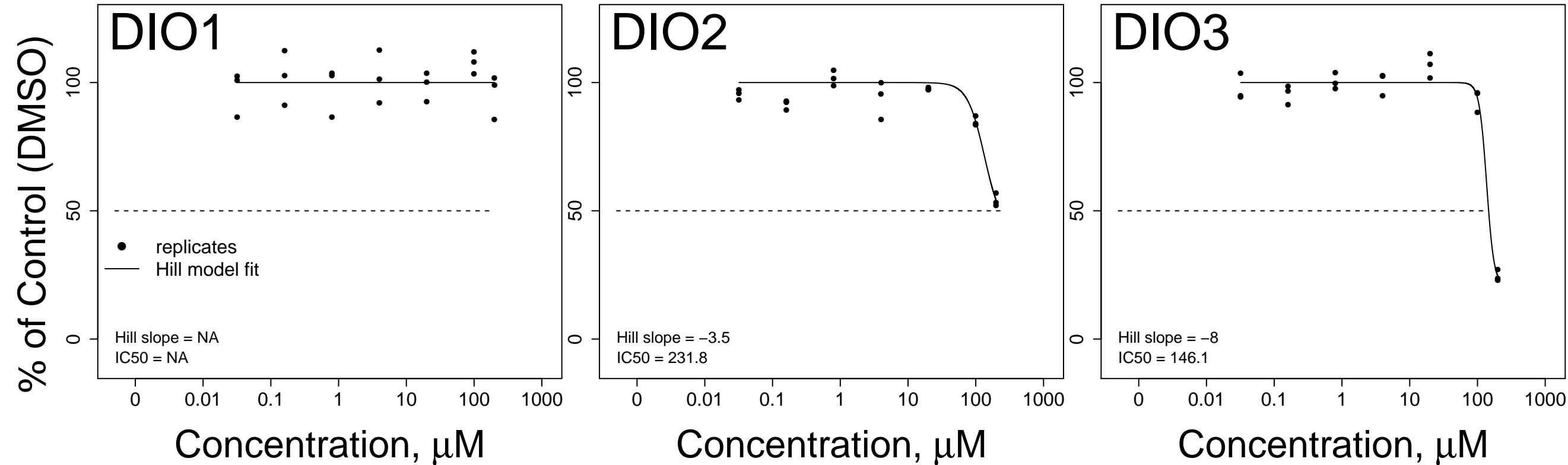
Resmethrin CASRN: 10453-86-8



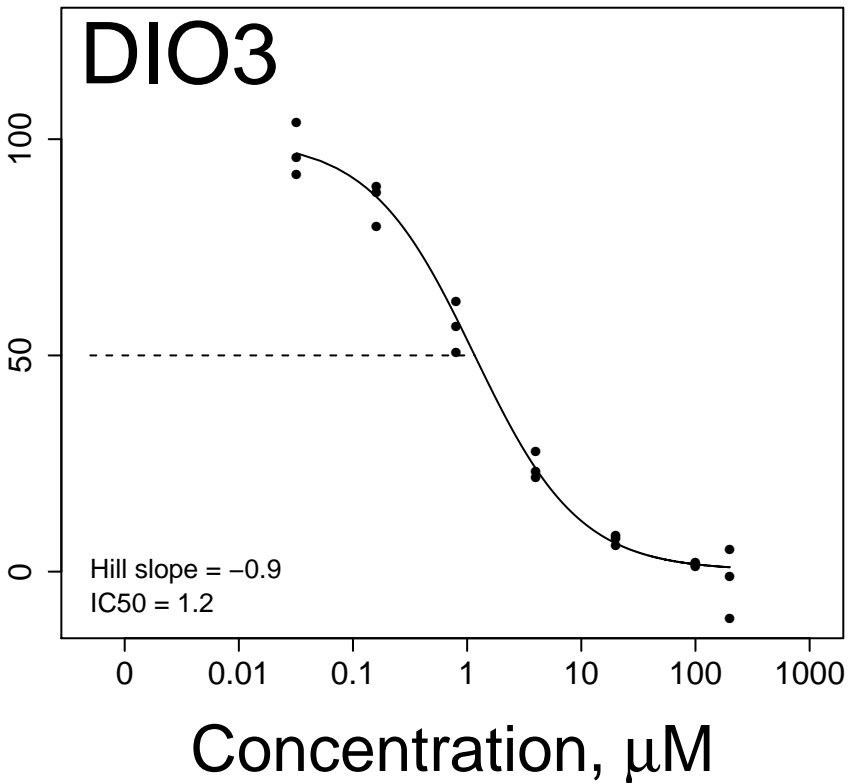
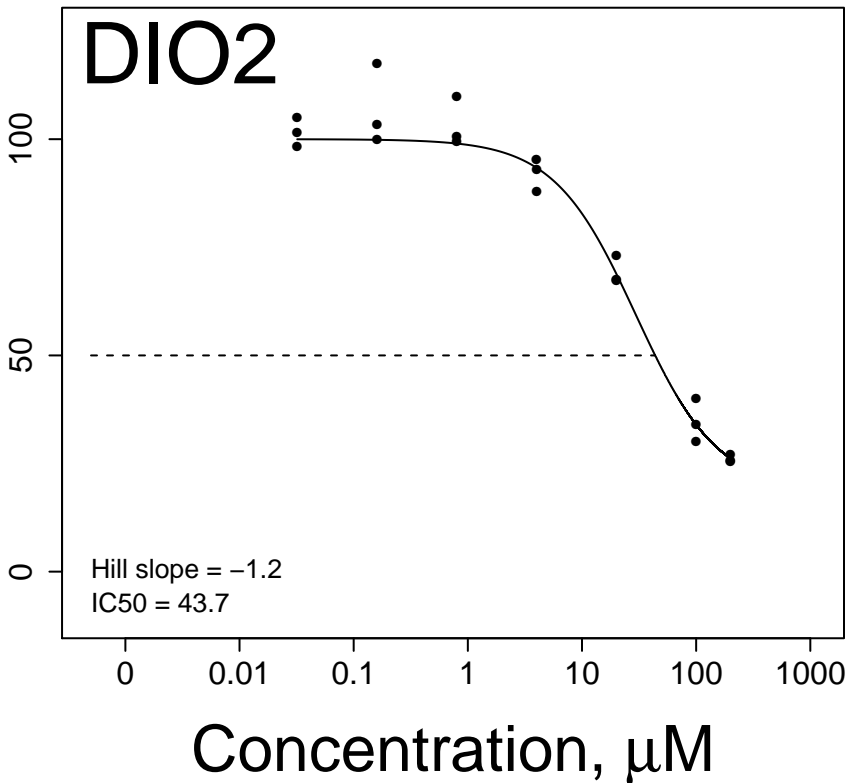
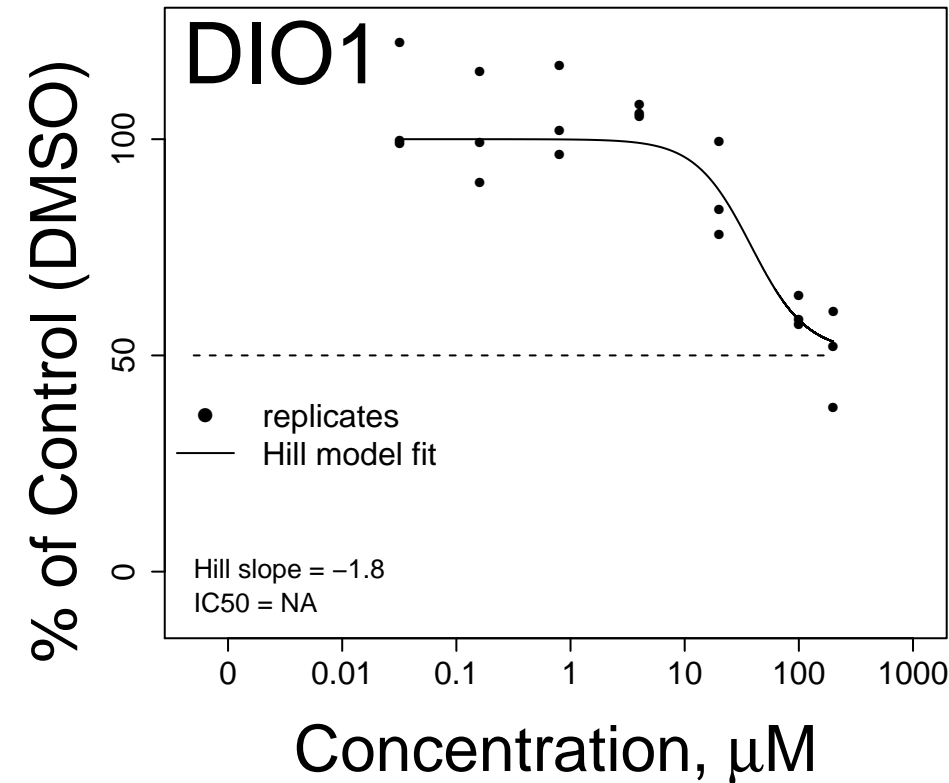
Dicofol CASRN: 115-32-2



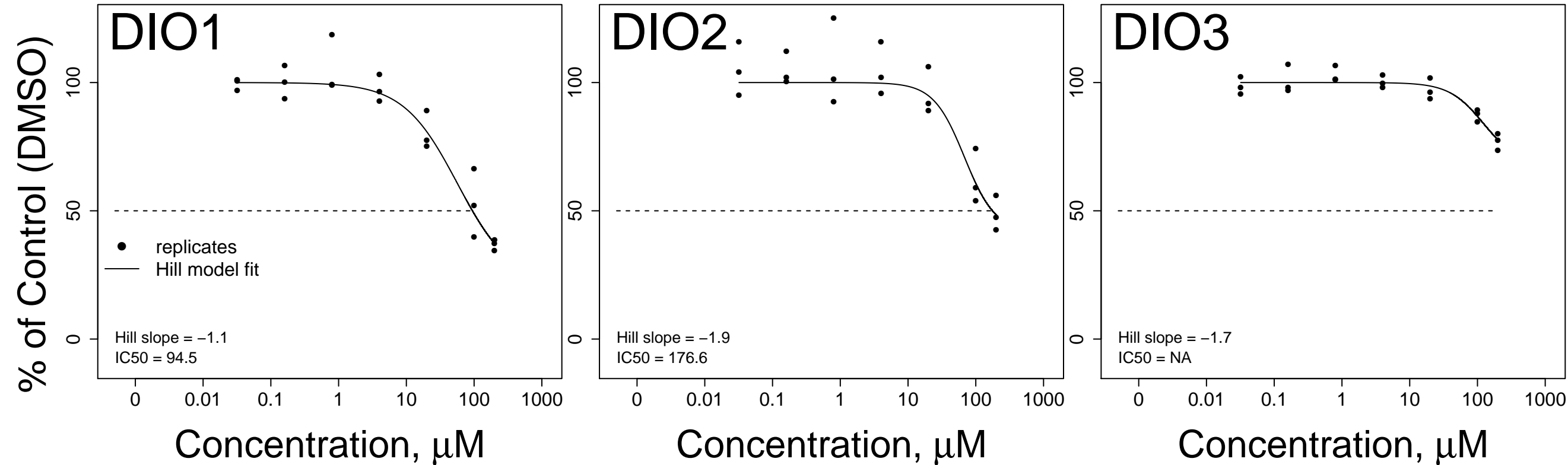
Chlorophene CASRN: 120-32-1

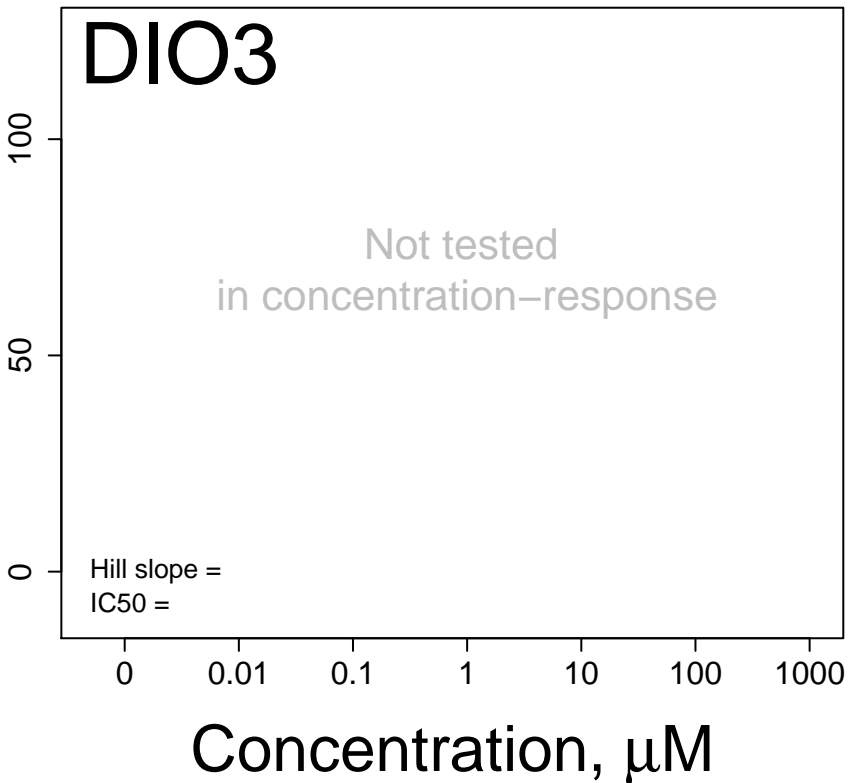
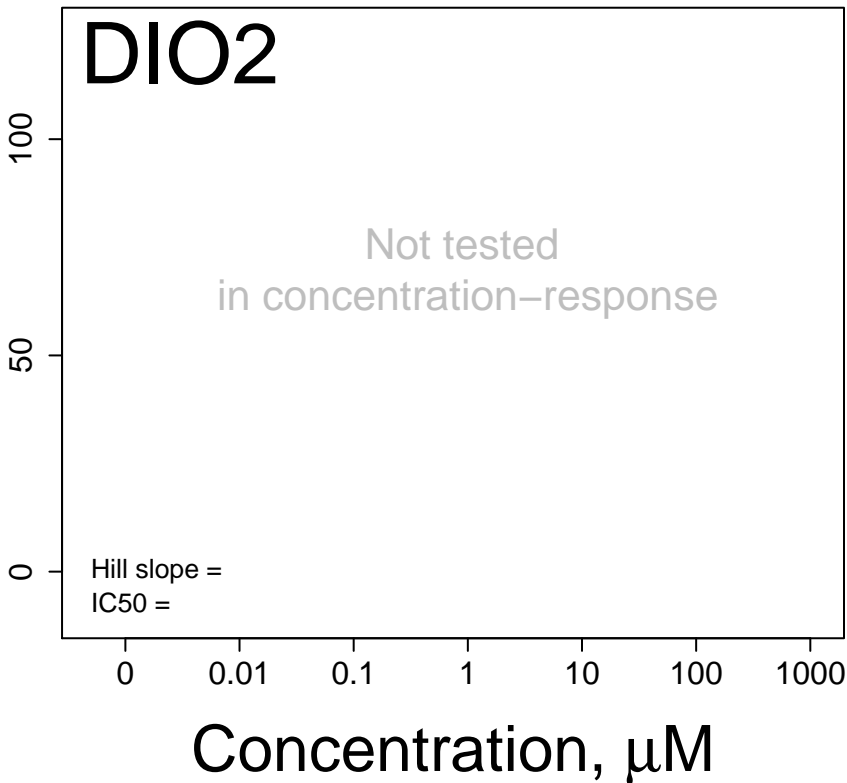
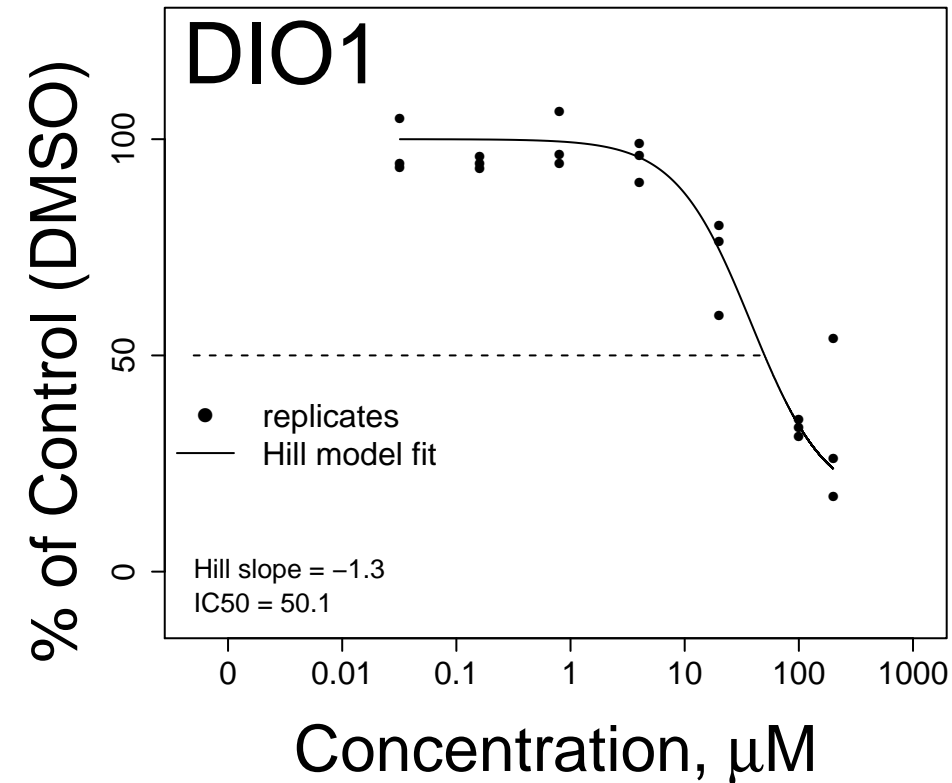


Fipronil CASRN: 120068-37-3

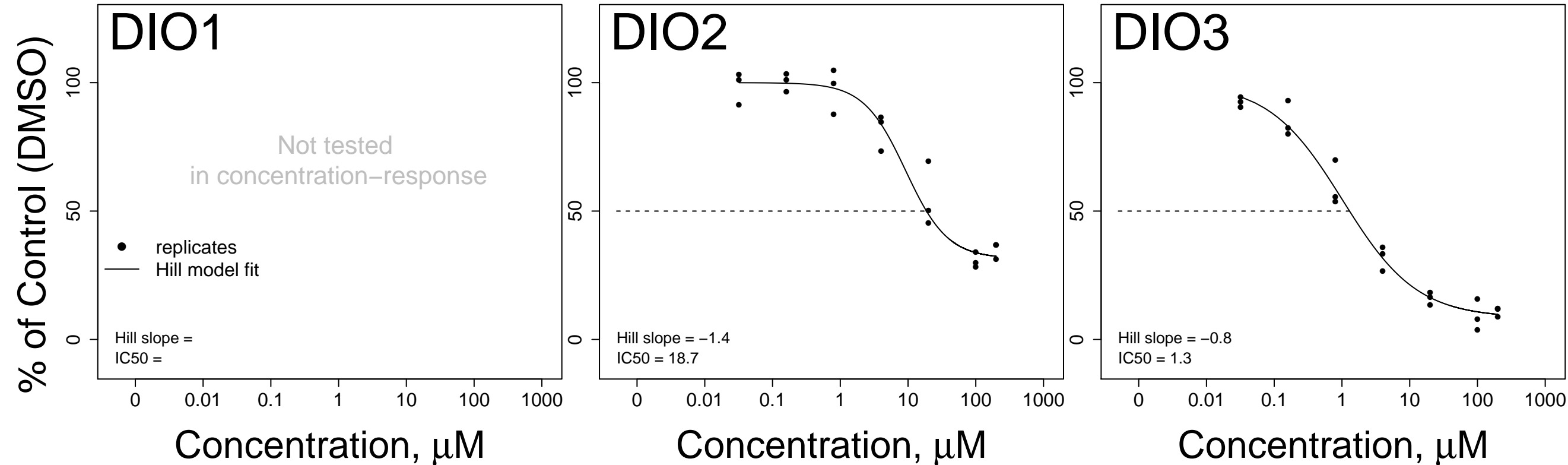


Cyazofamid CASRN: 120116-88-3

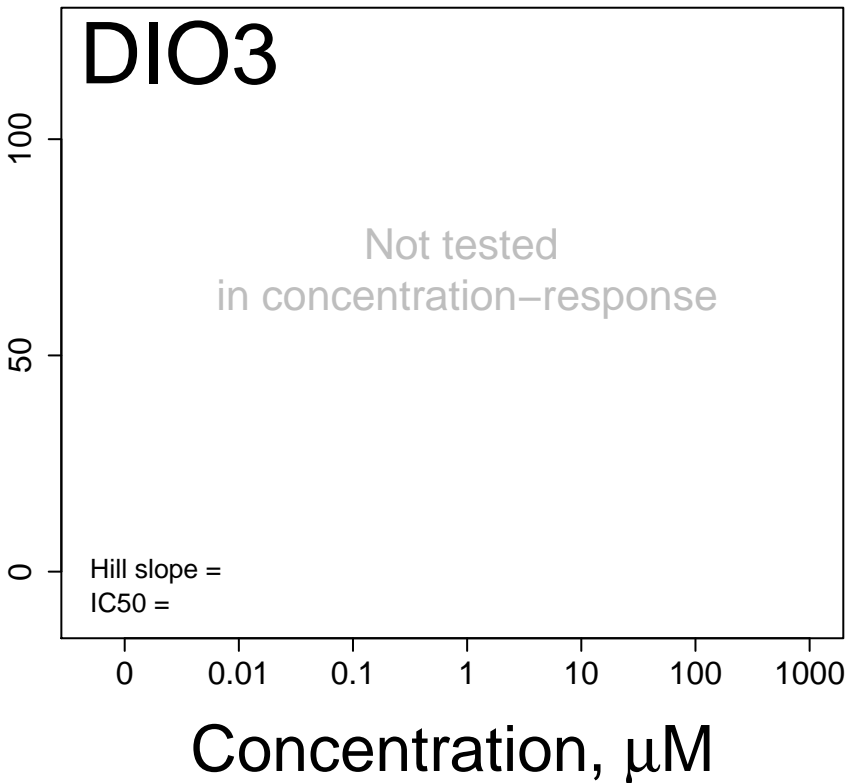
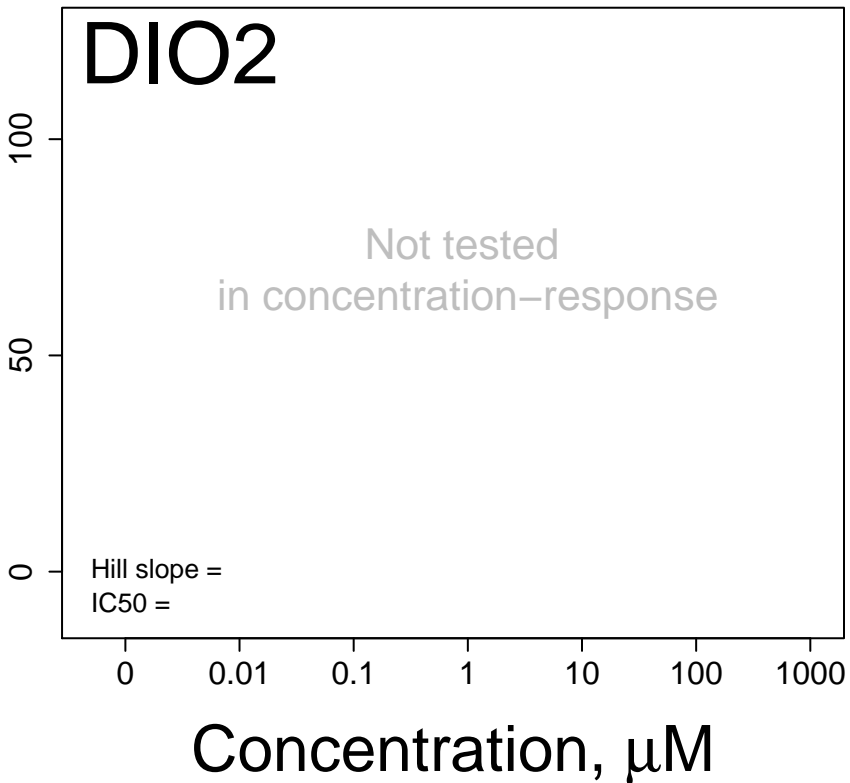
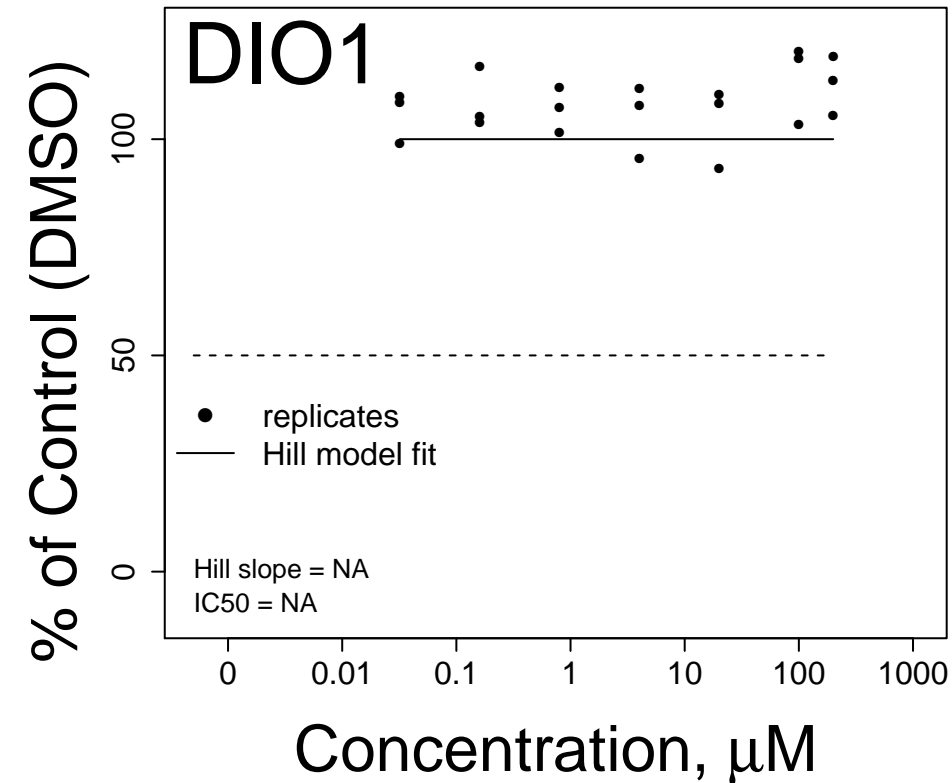




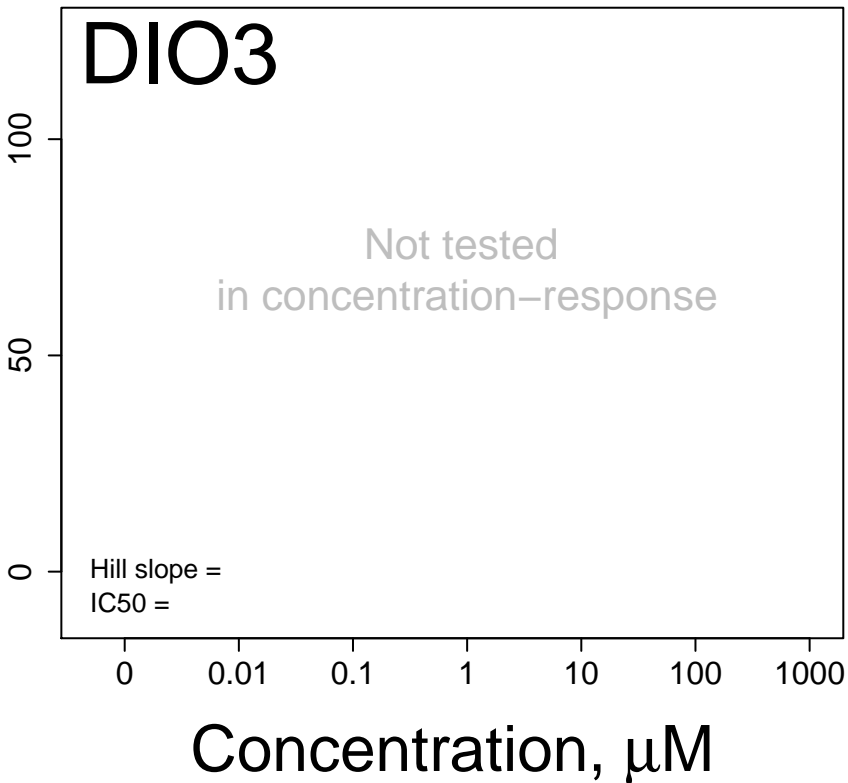
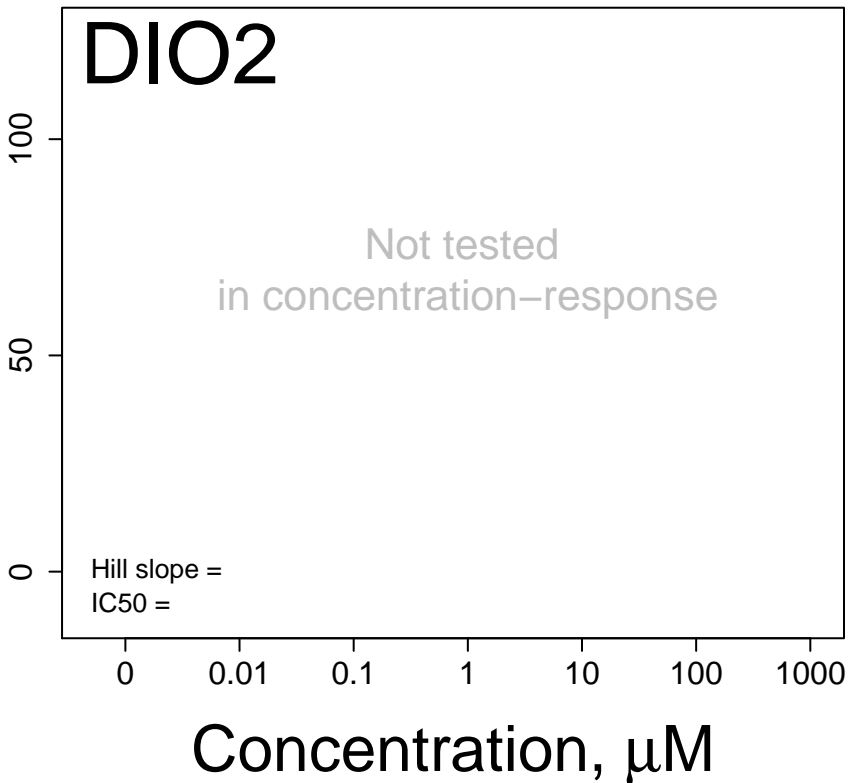
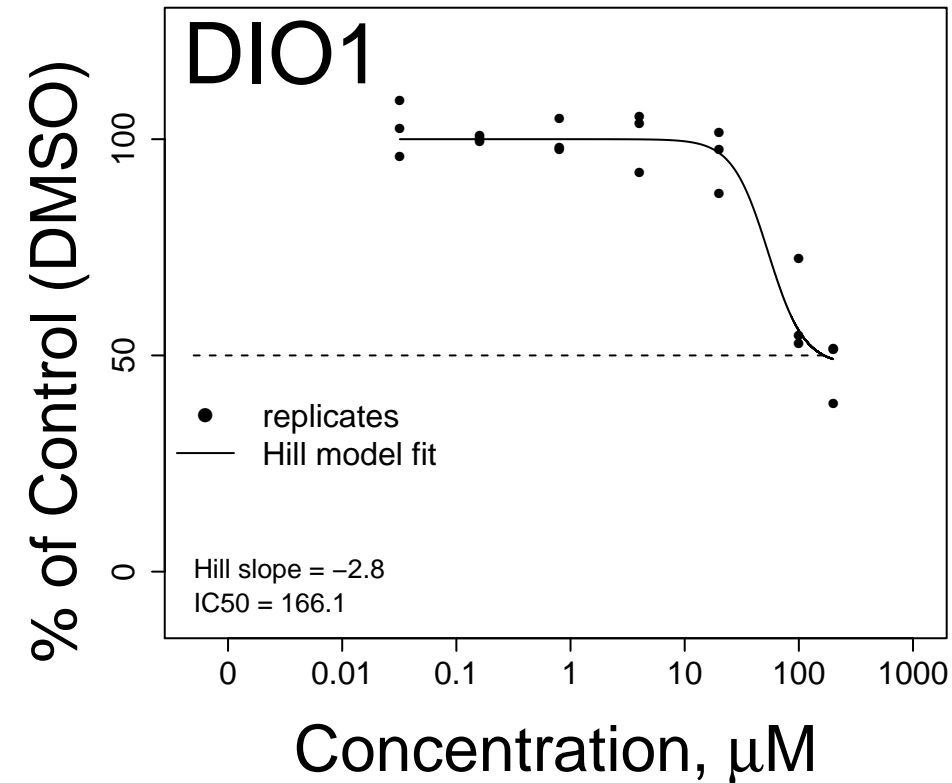
Quinoxifen CASRN: 124495-18-7



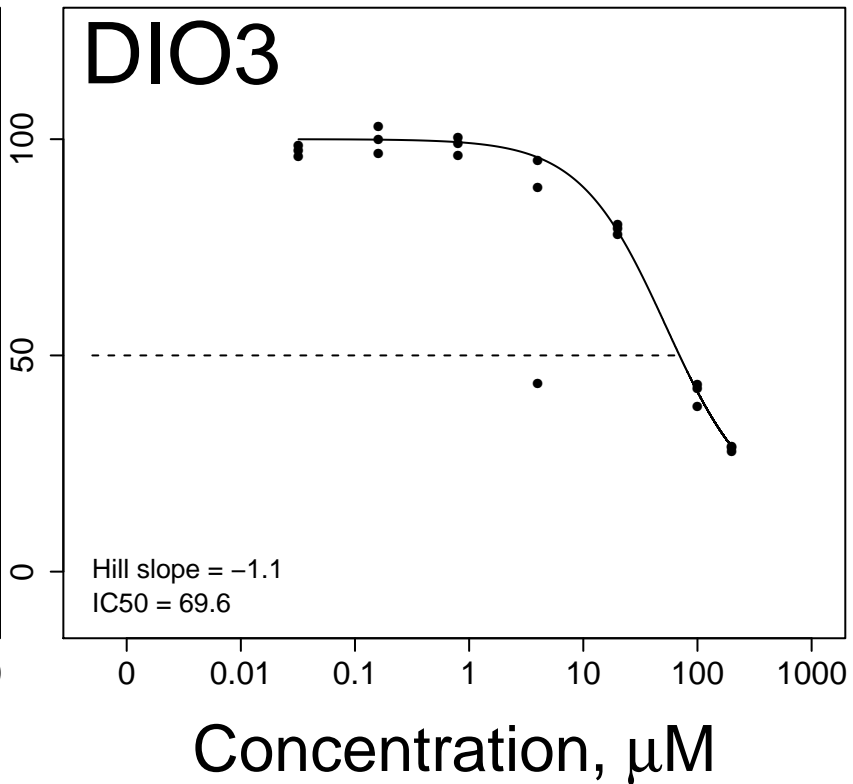
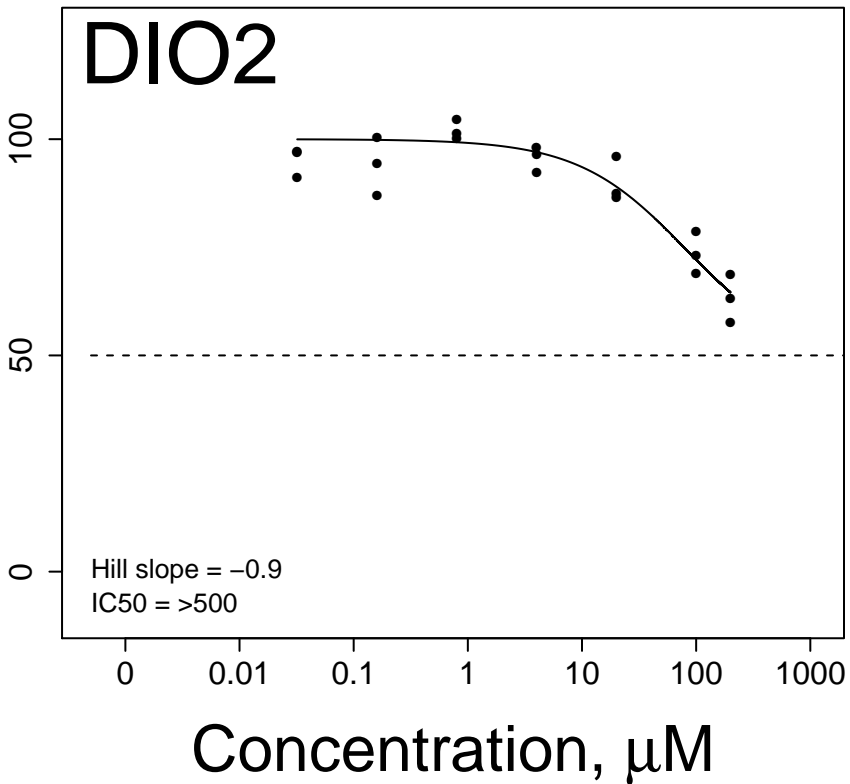
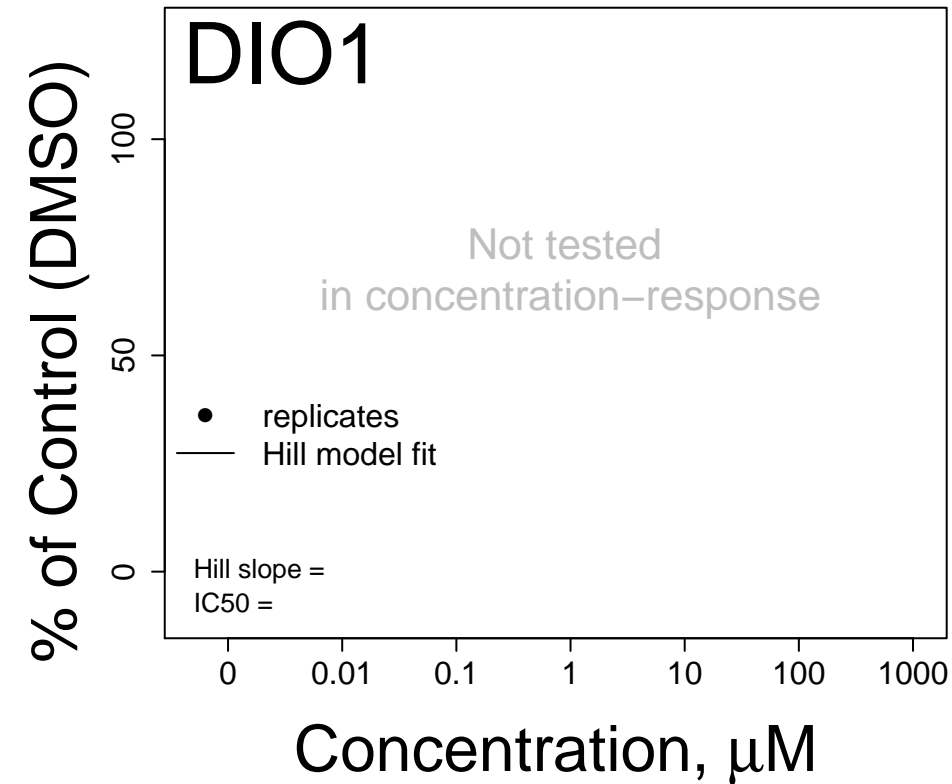
Fenhexamid CASRN: 126833-17-8



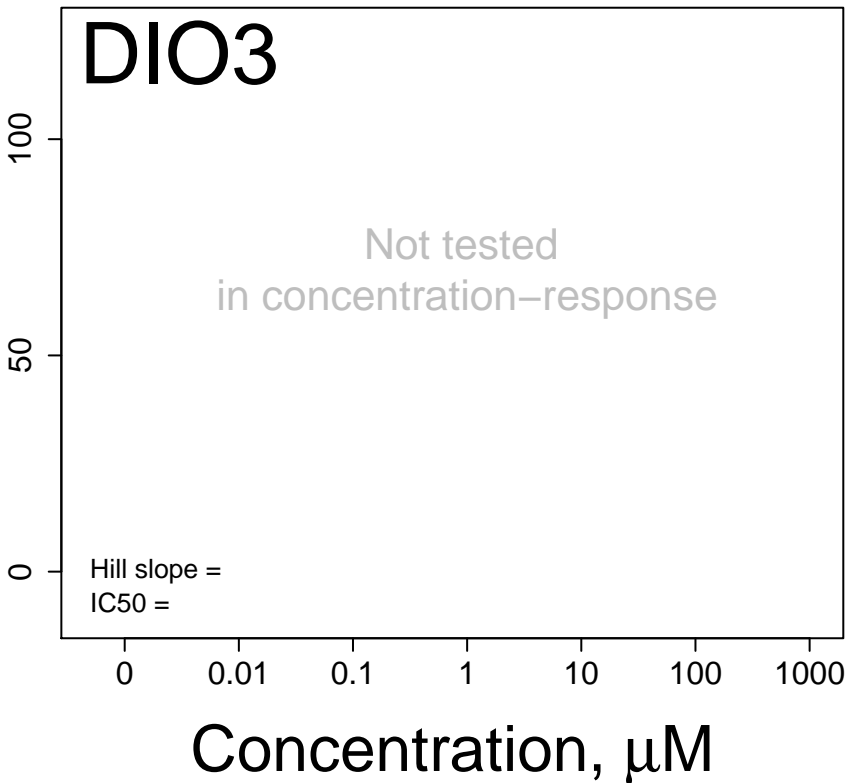
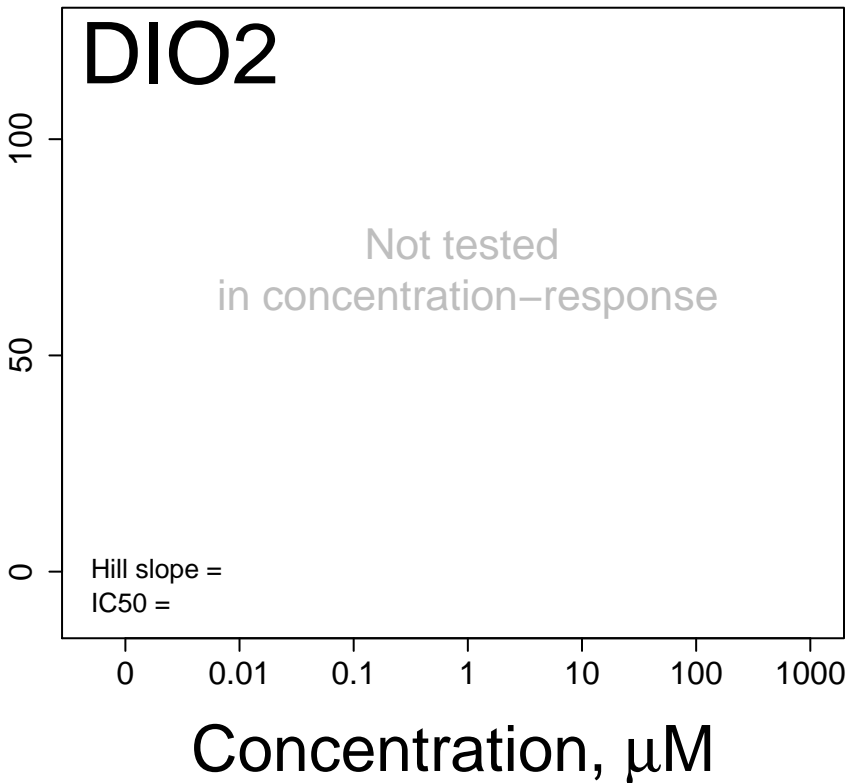
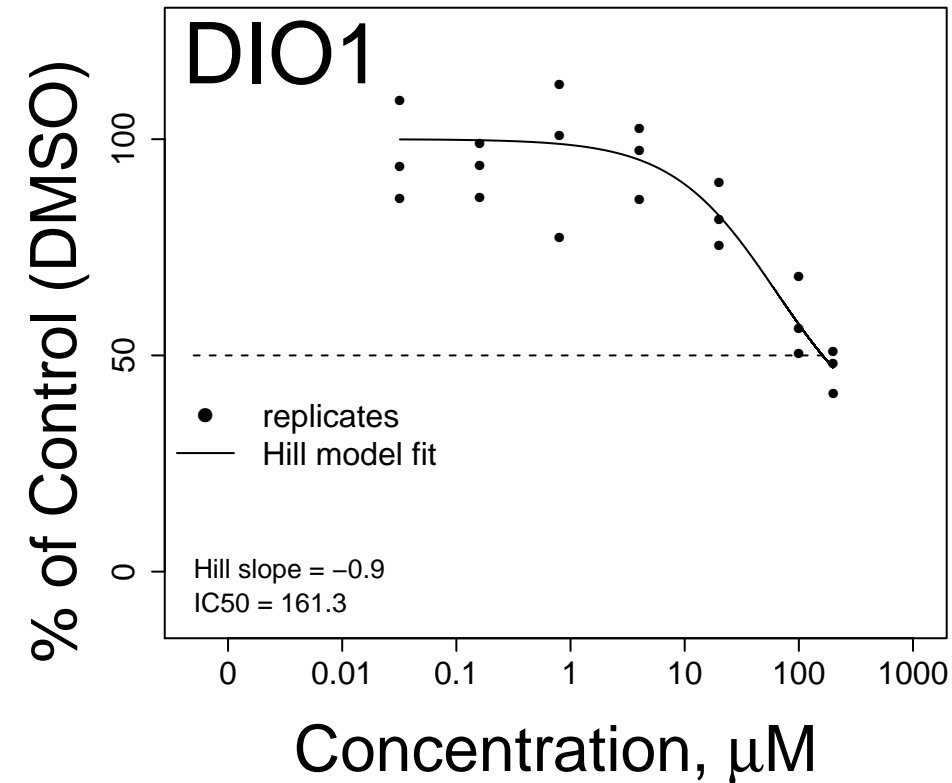
Captan CASRN: 133-06-2



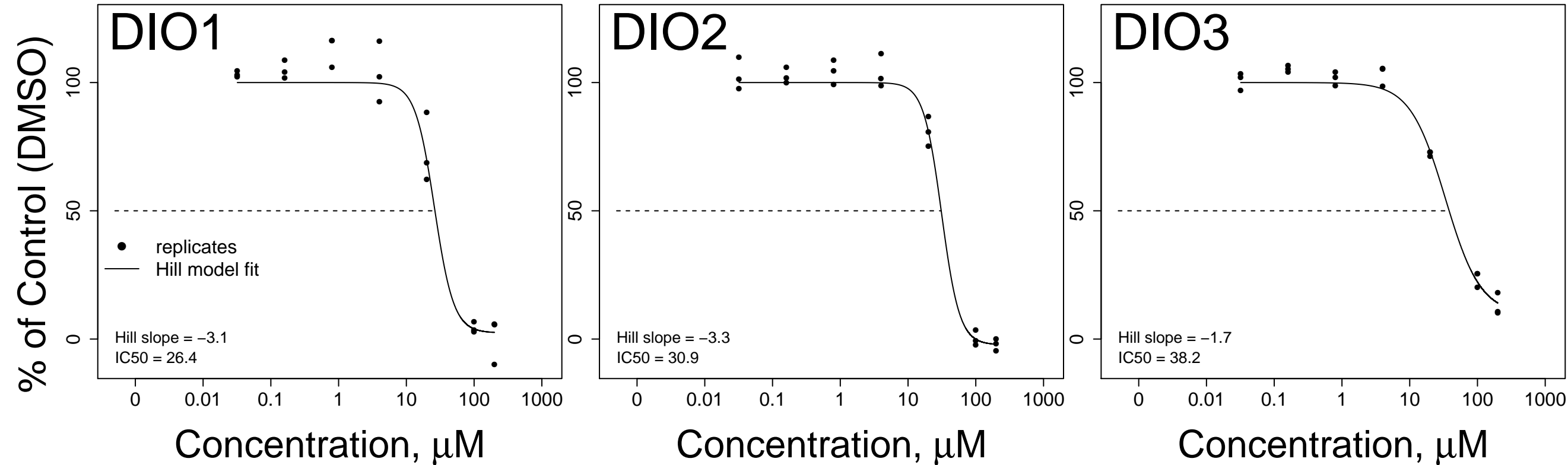
Thiram CASRN: 137-26-8



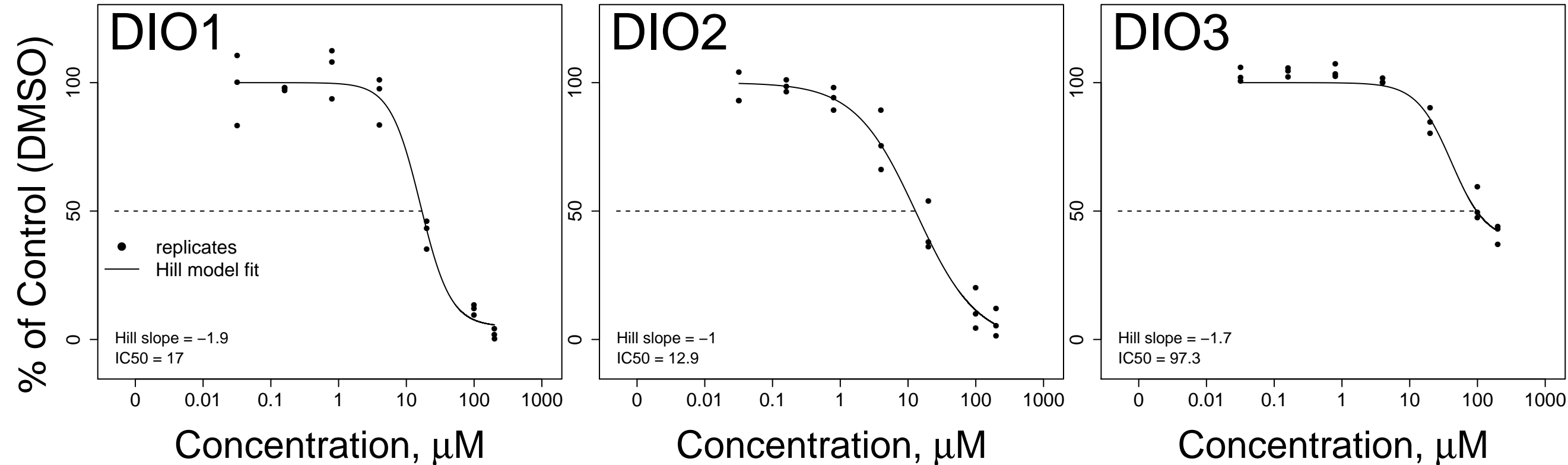
Diclofulam CASRN: 145701-21-9



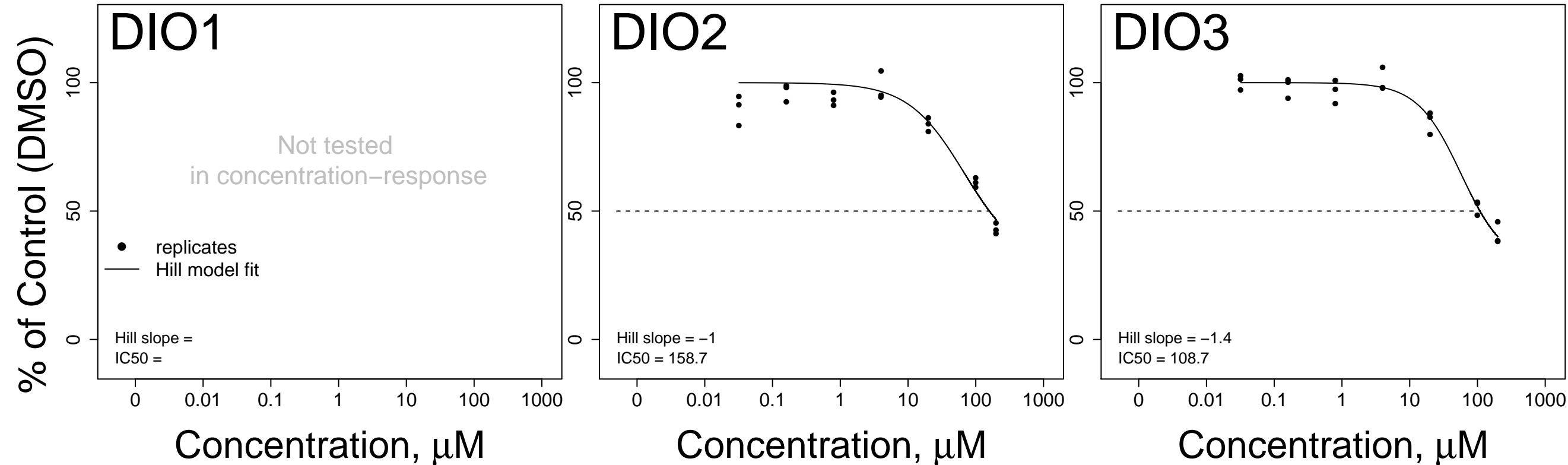
Emamectin benzoate CASRN: 155569-91-8



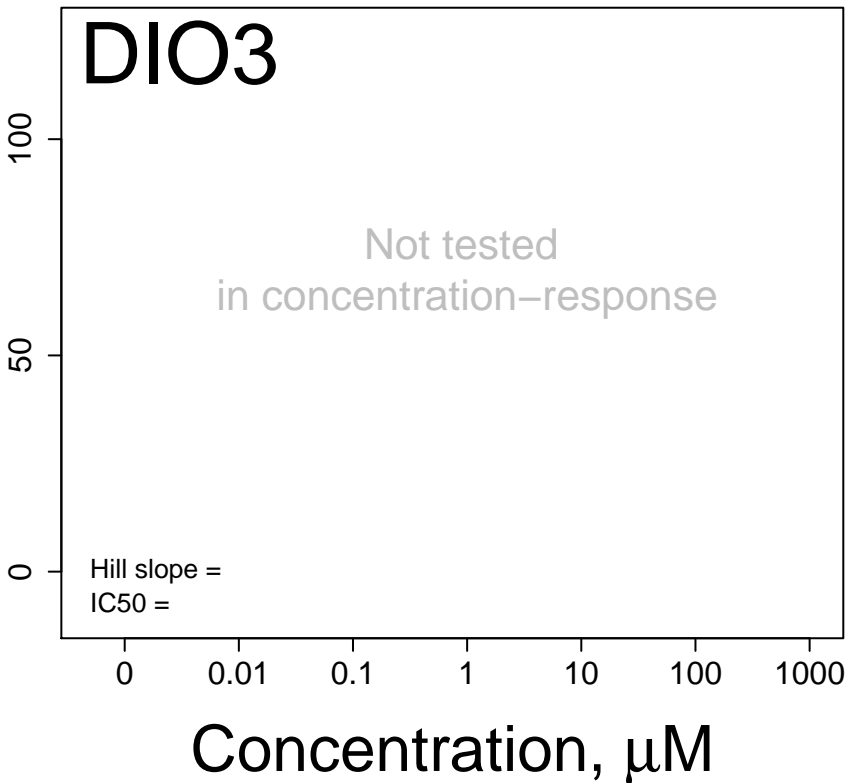
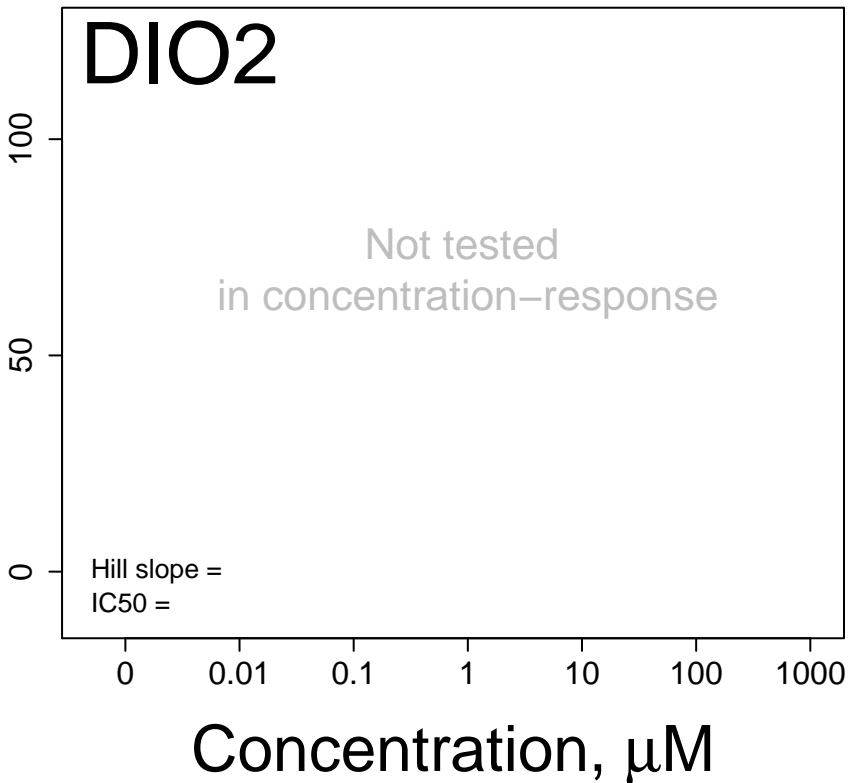
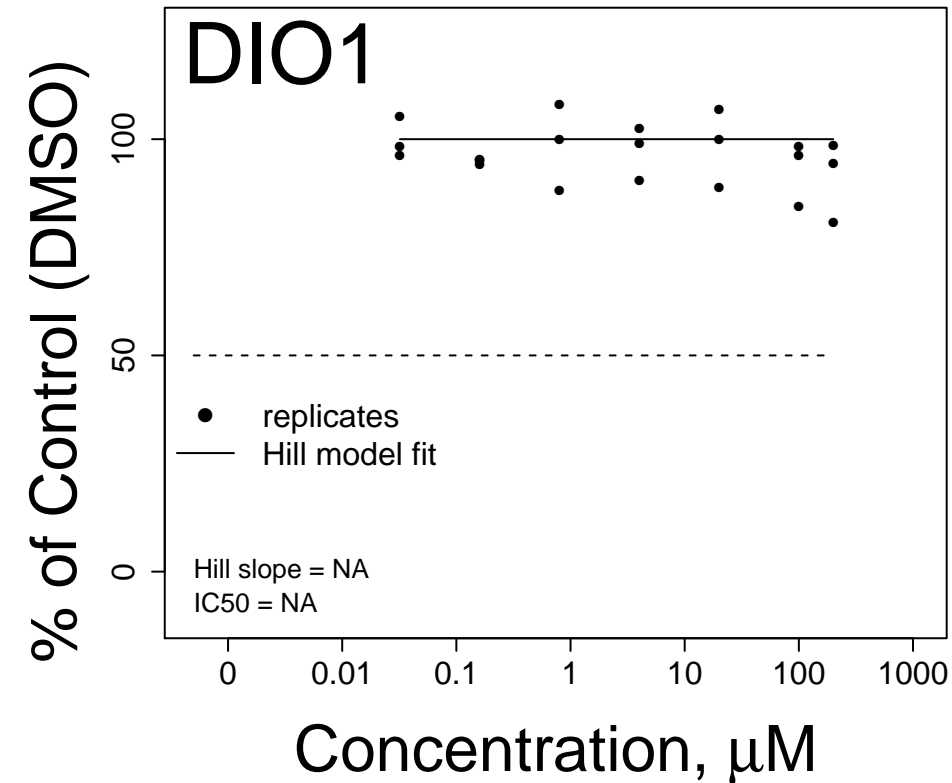
Zoxamide CASRN: 156052-68-5



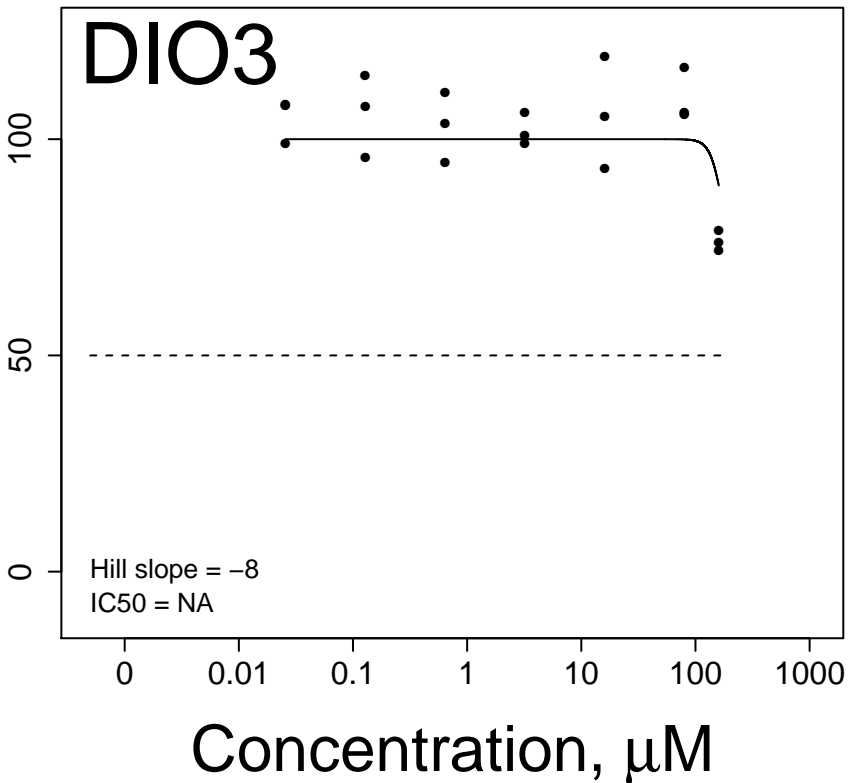
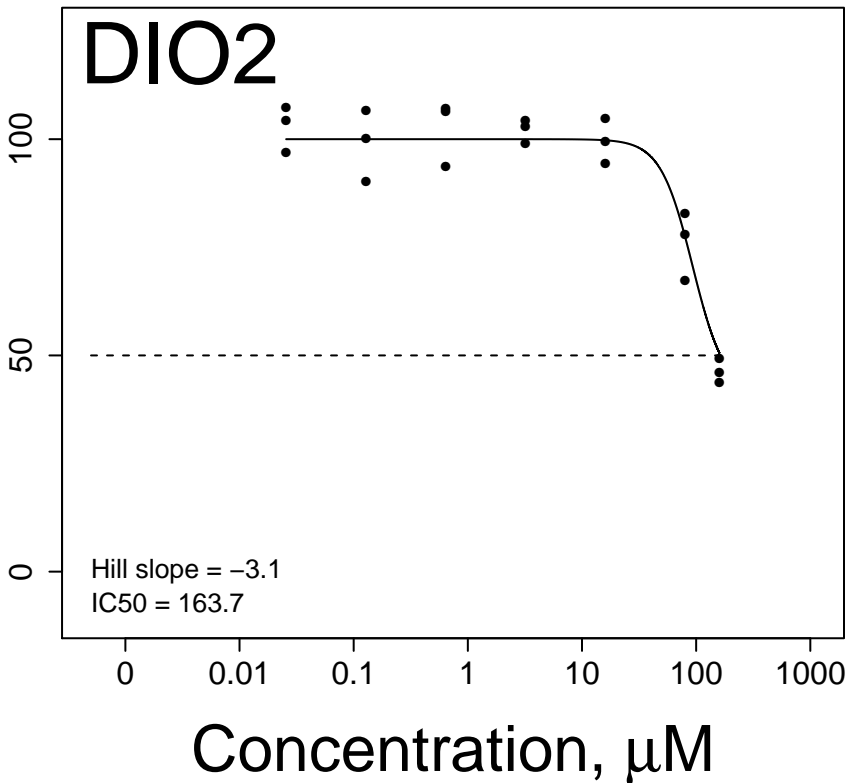
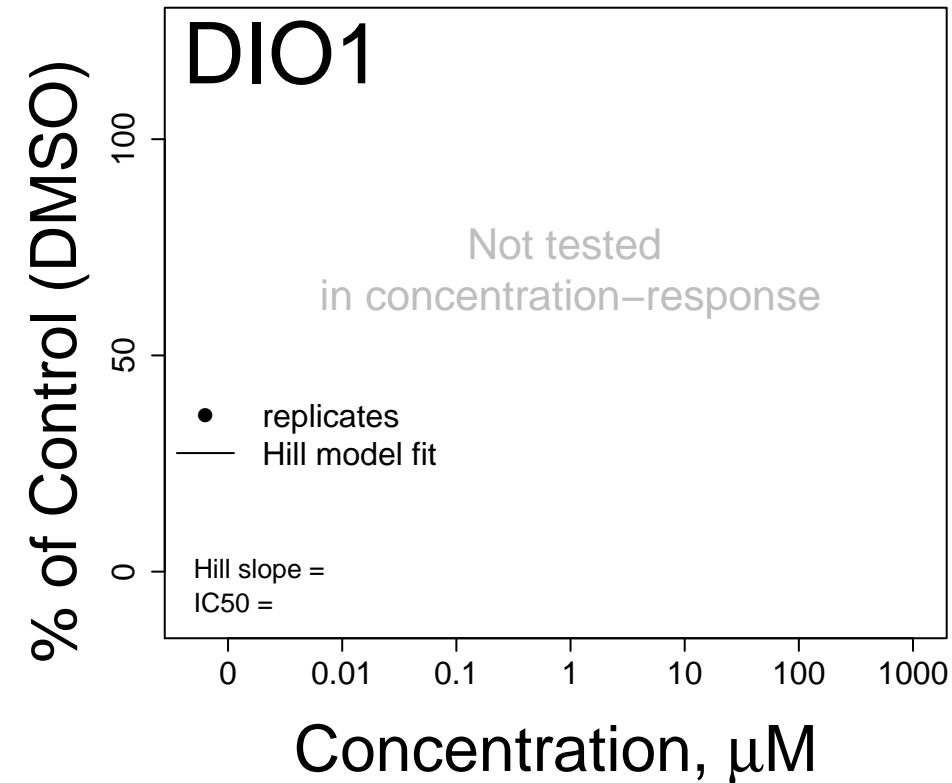
Alachlor CASRN: 15972-60-8



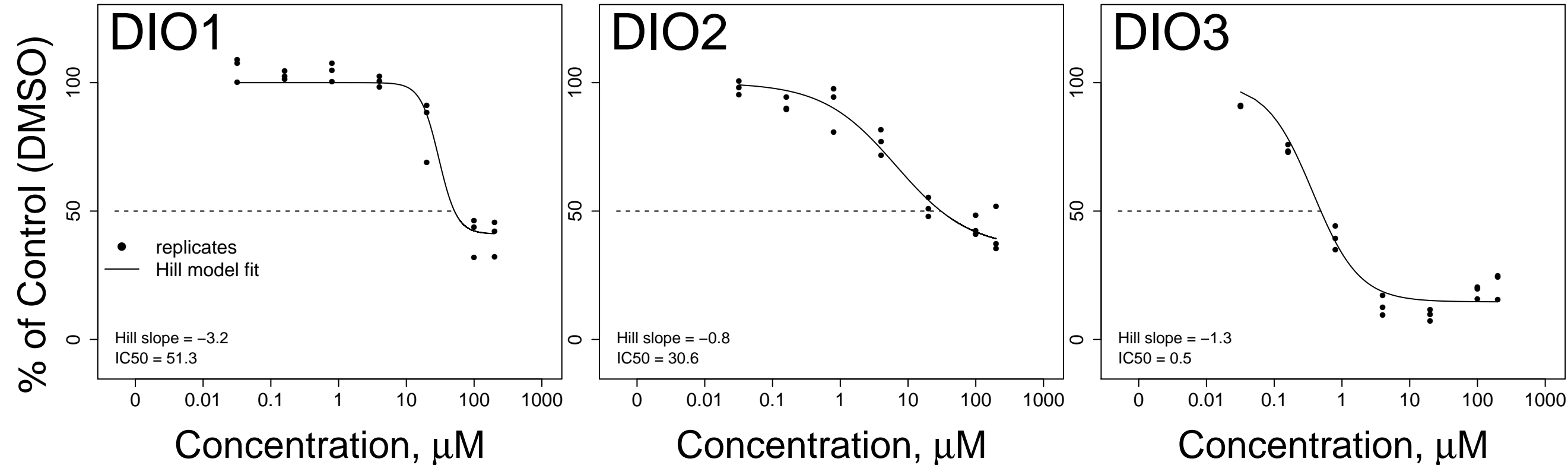
Malaoxon CASRN: 1634-78-2



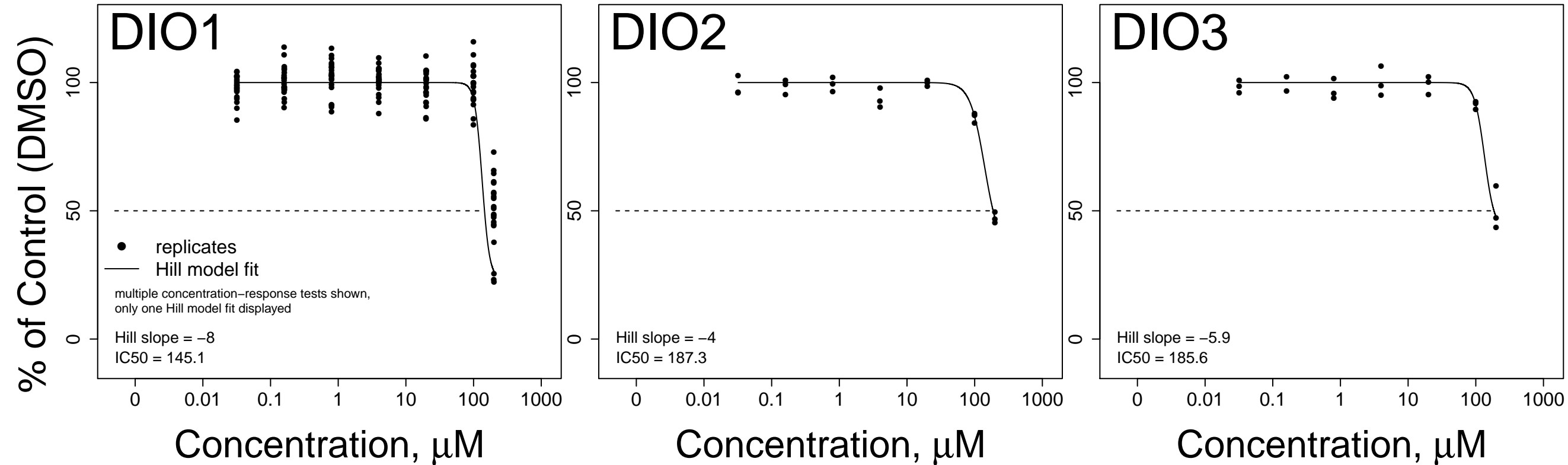
PFOS CASRN: 1763-23-1



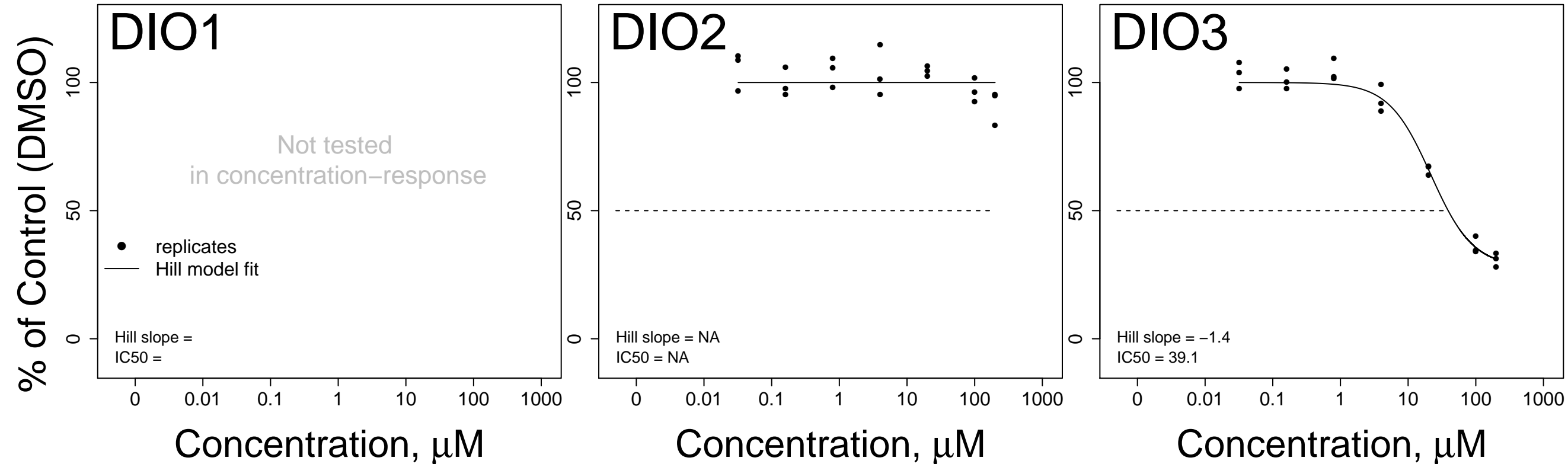
Chlorothalonil CASRN: 1897-45-6



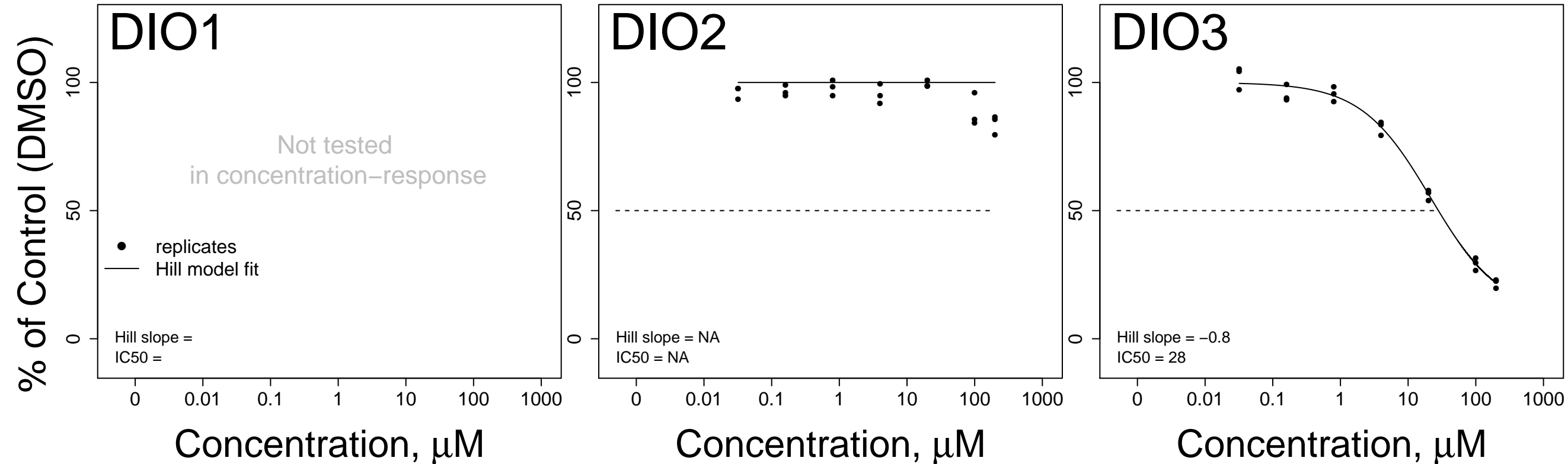
Oryzalin CASRN: 19044-88-3



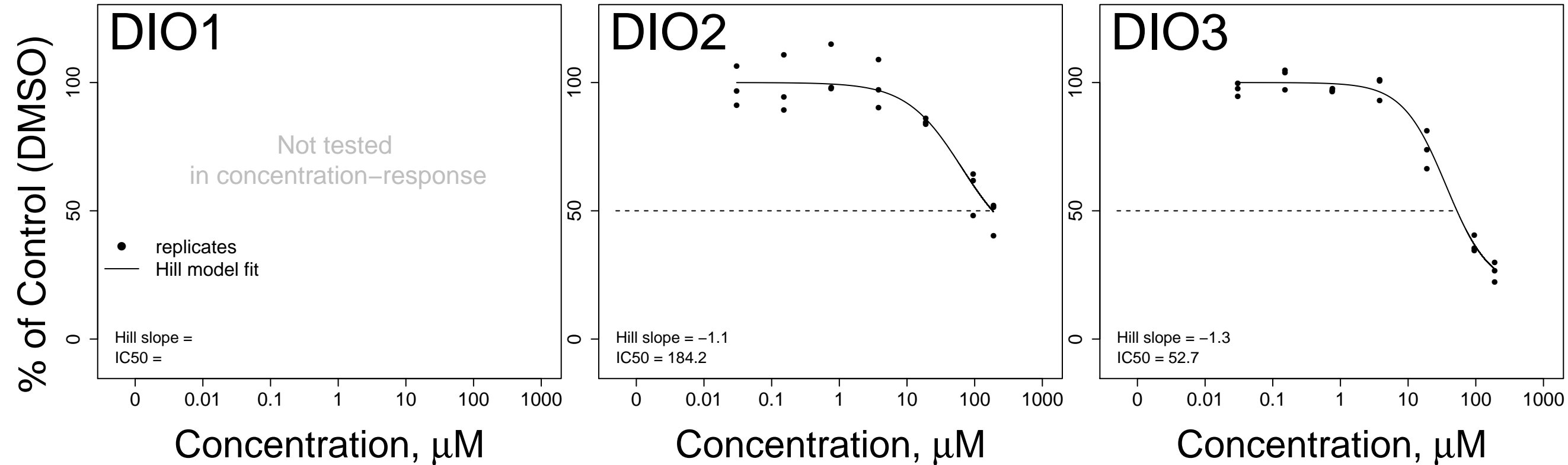
Atrazine CASRN: 1912-24-9



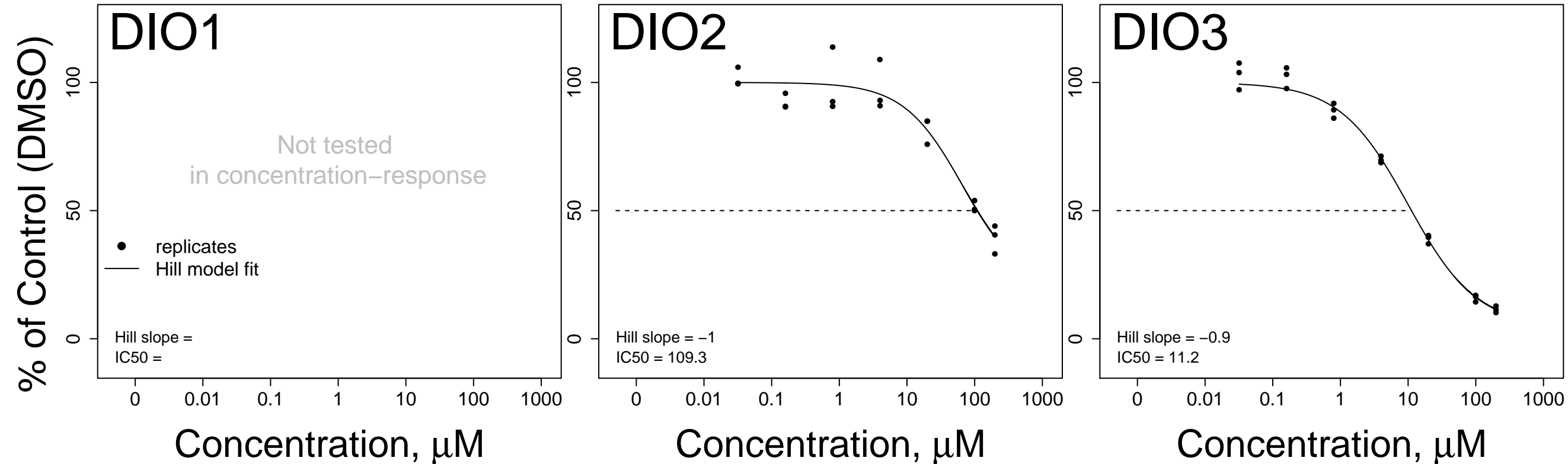
Cyanazine CASRN: 21725-46-2



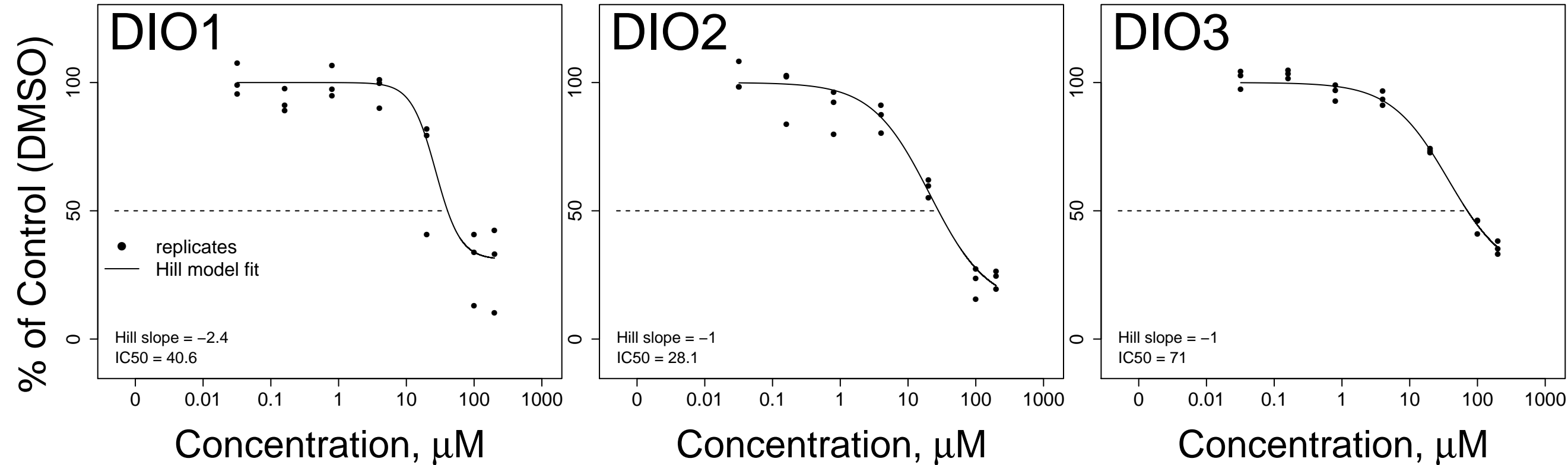
Prallethrin CASRN: 23031-36-9



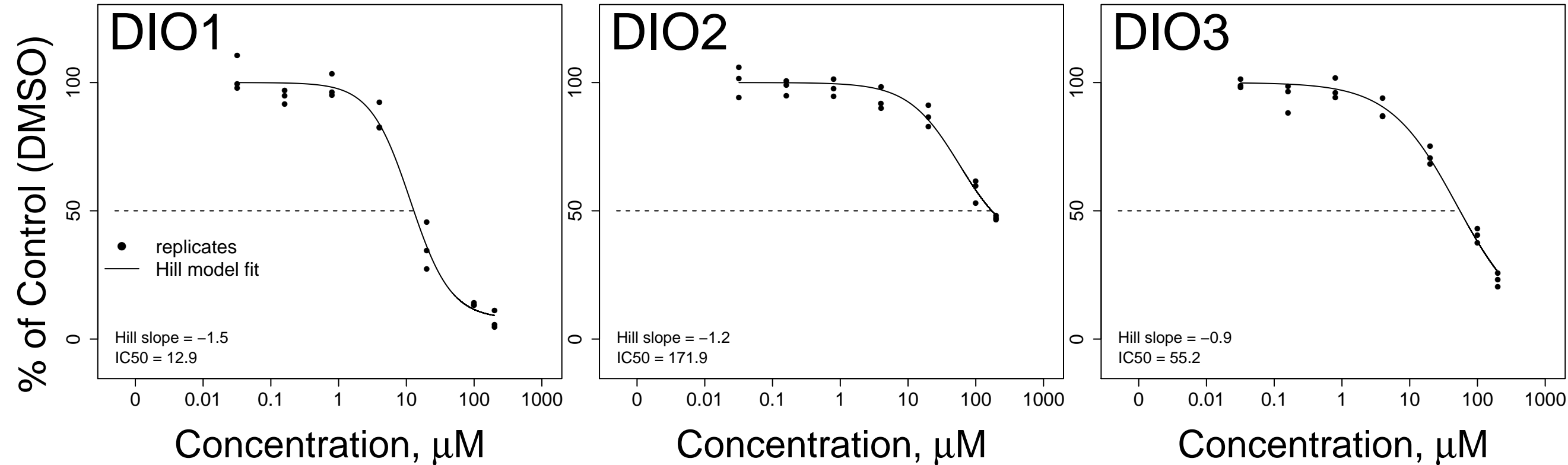
Pirimicarb CASRN: 23103-98-2



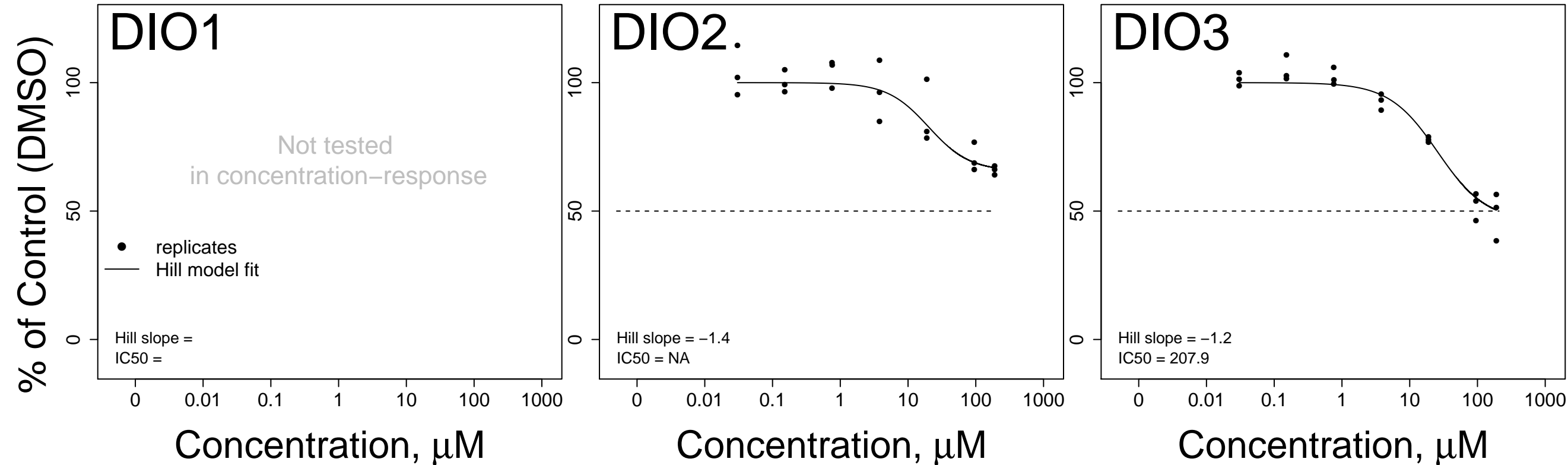
Butachlor CASRN: 23184-66-9



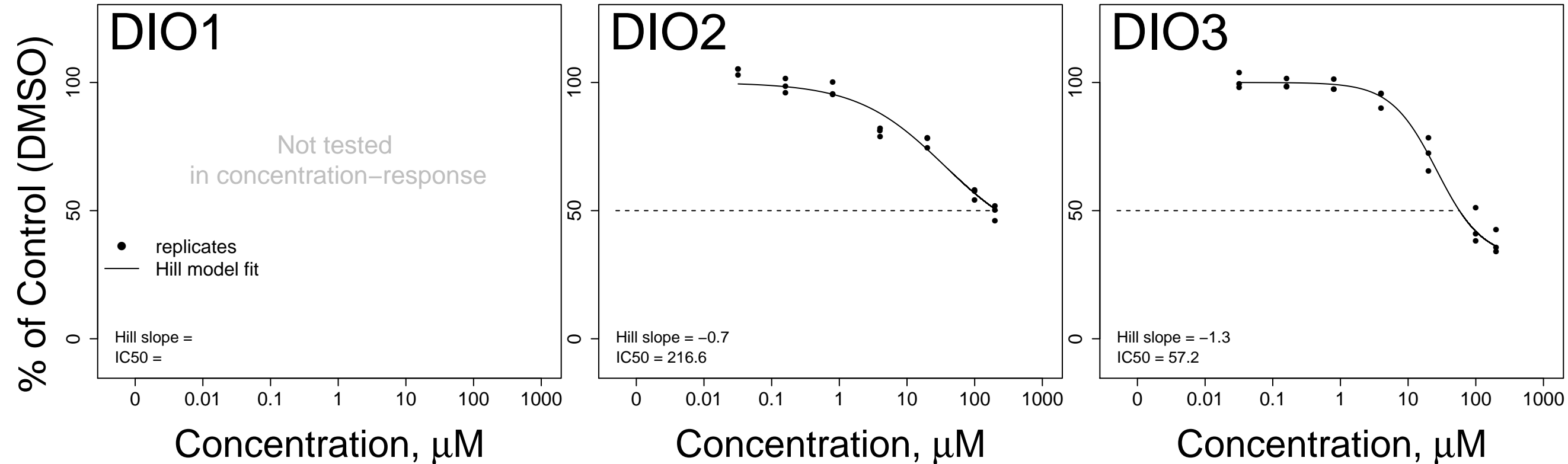
Captafol CASRN: 2425-06-1



Prodiamine CASRN: 29091-21-2

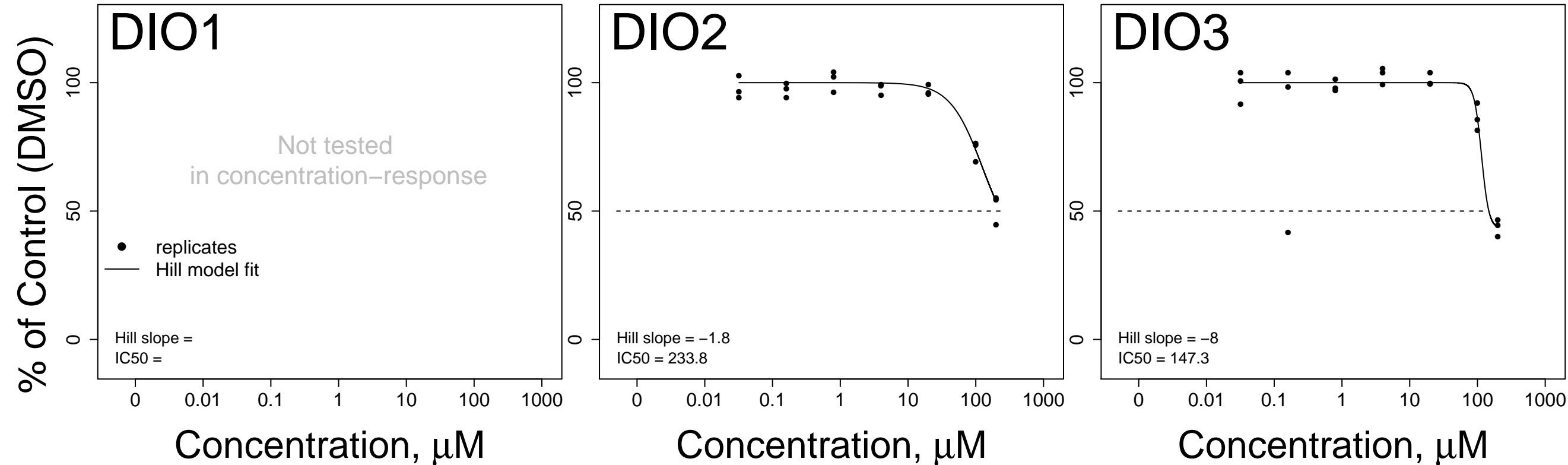


Pirimiphos-methyl CASRN: 29232-93-7

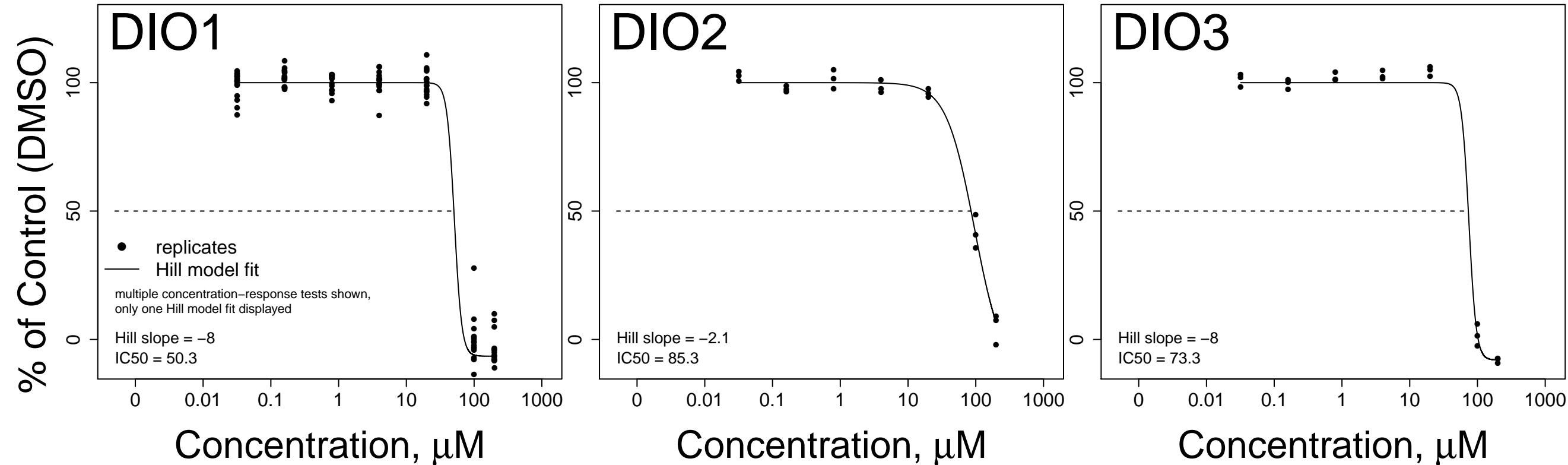


2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane

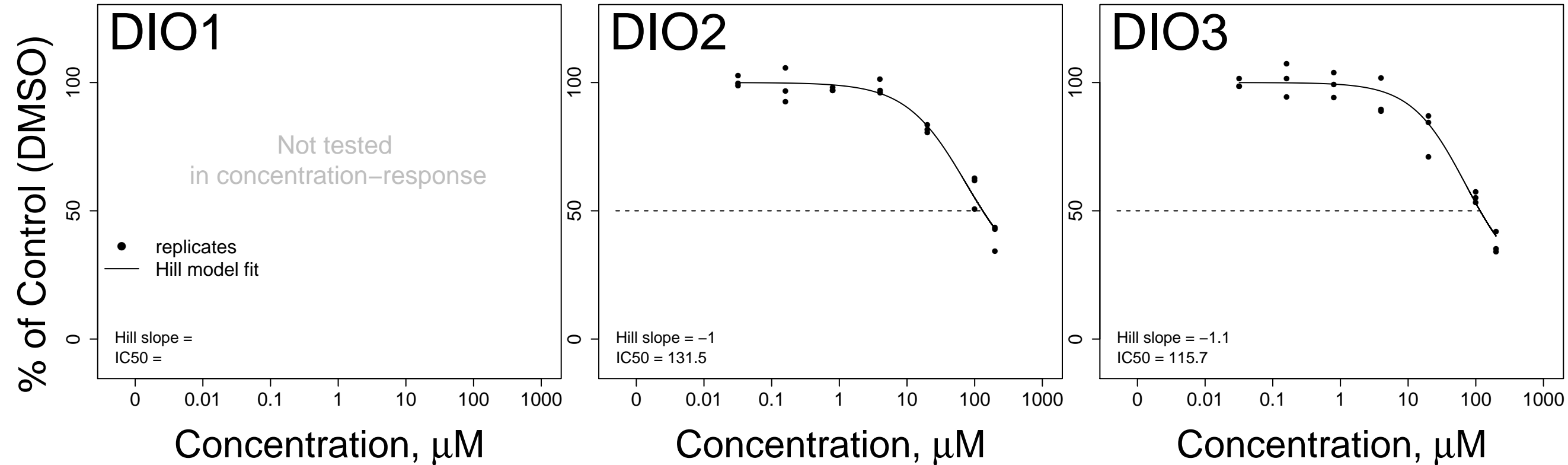
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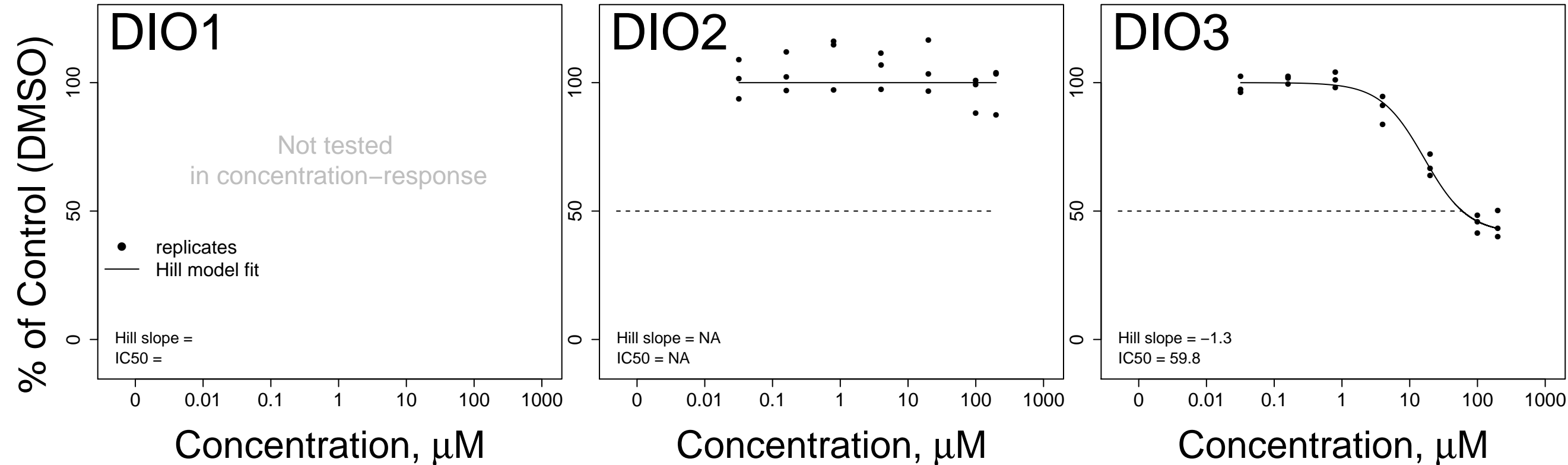
Triclosan CASRN: 3380-34-5



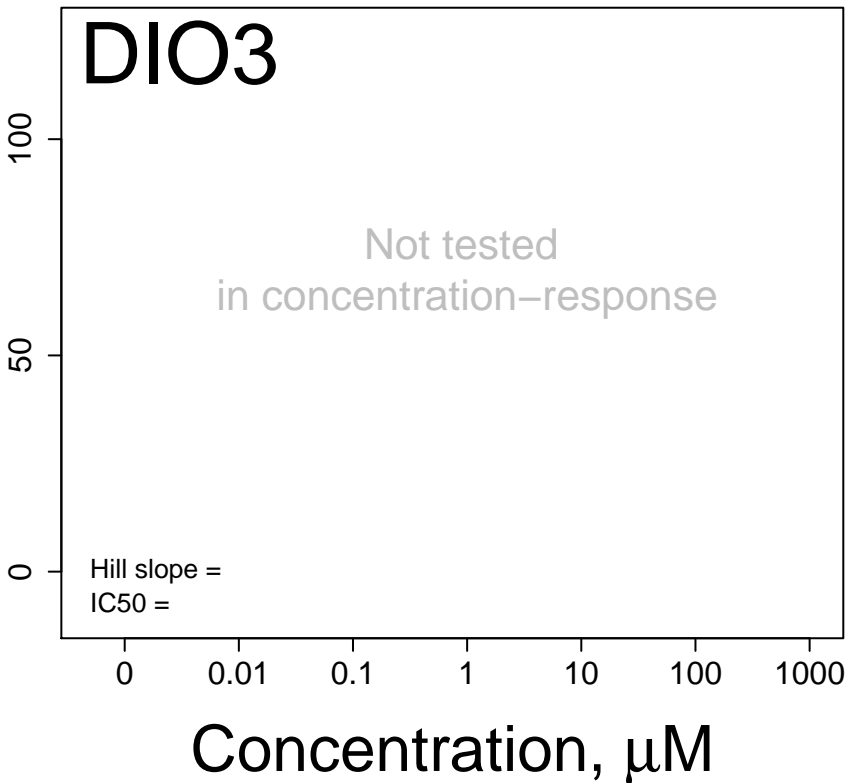
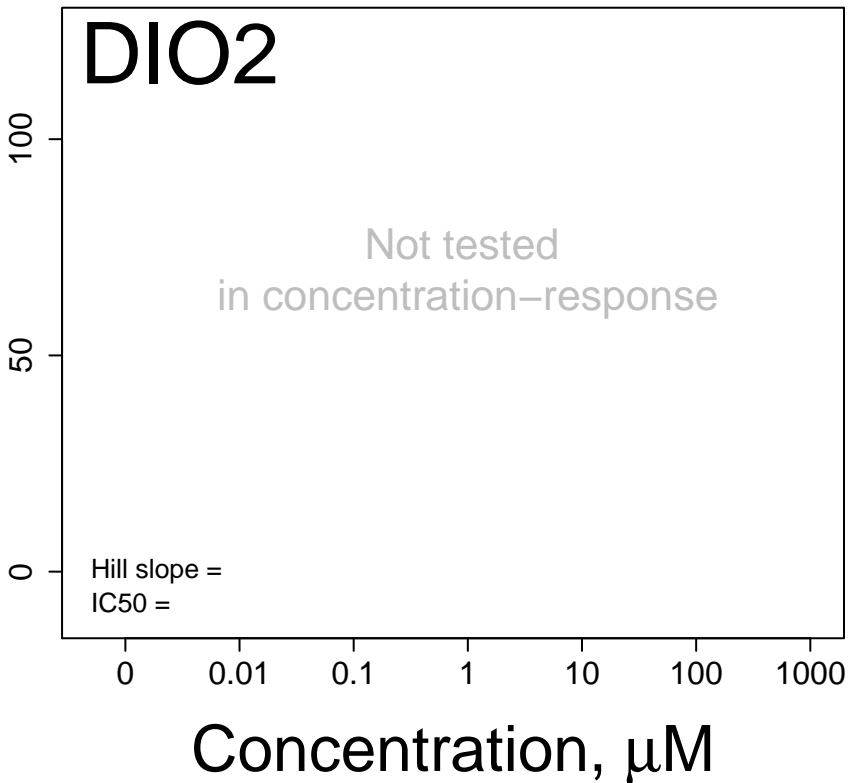
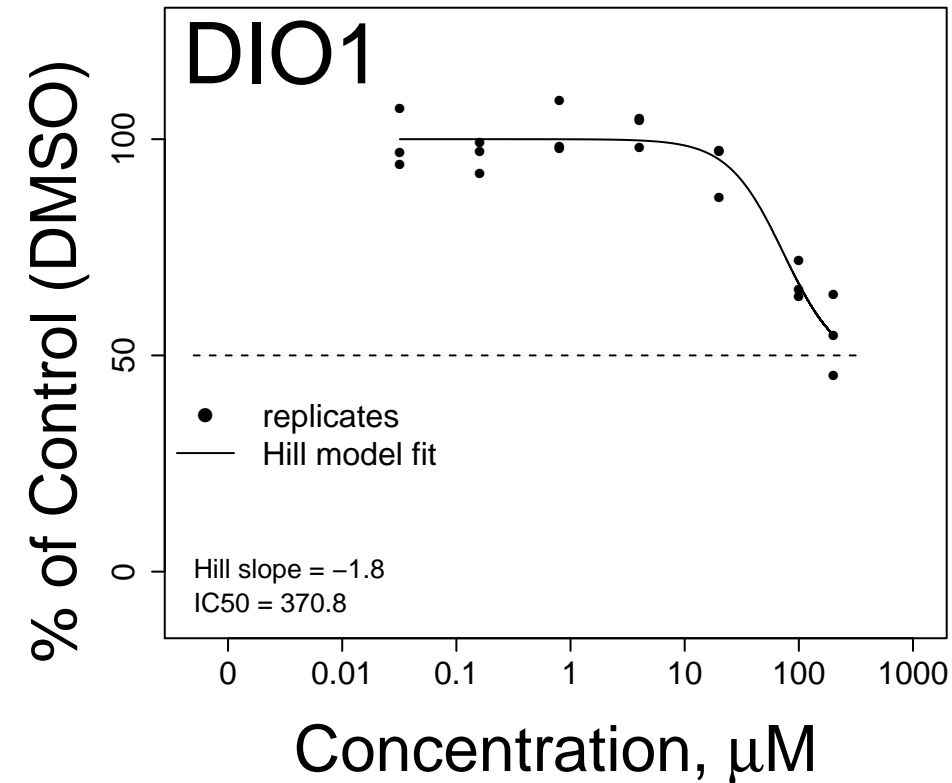
Acetochlor CASRN: 34256-82-1



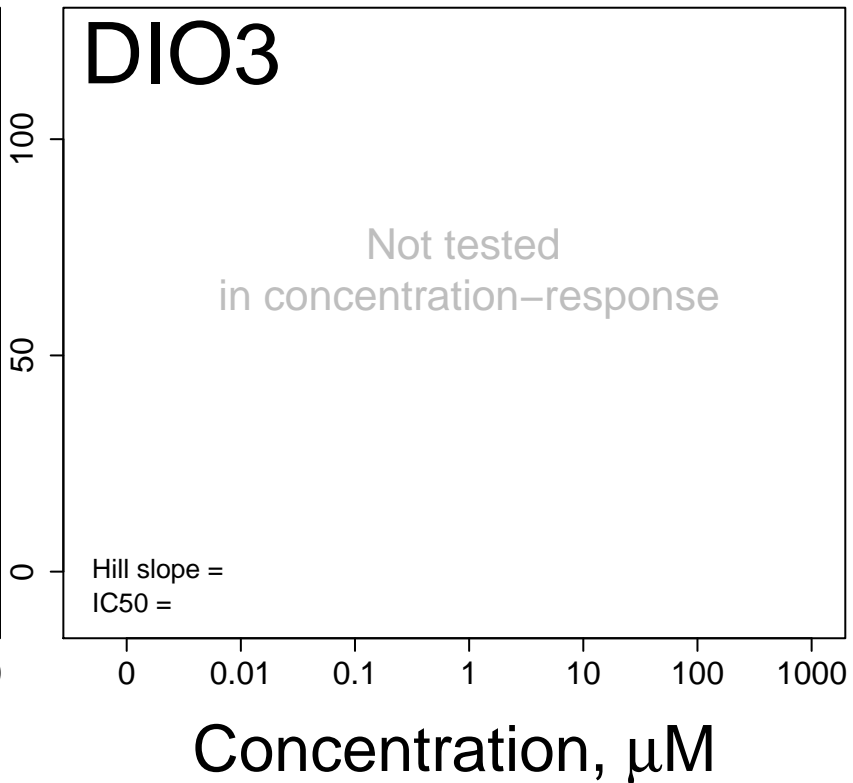
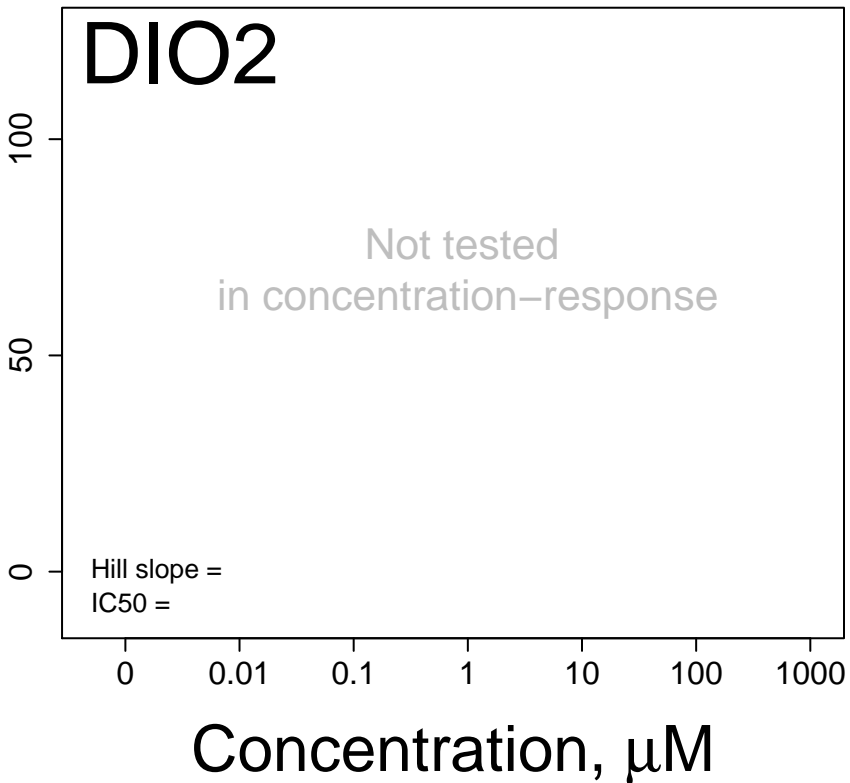
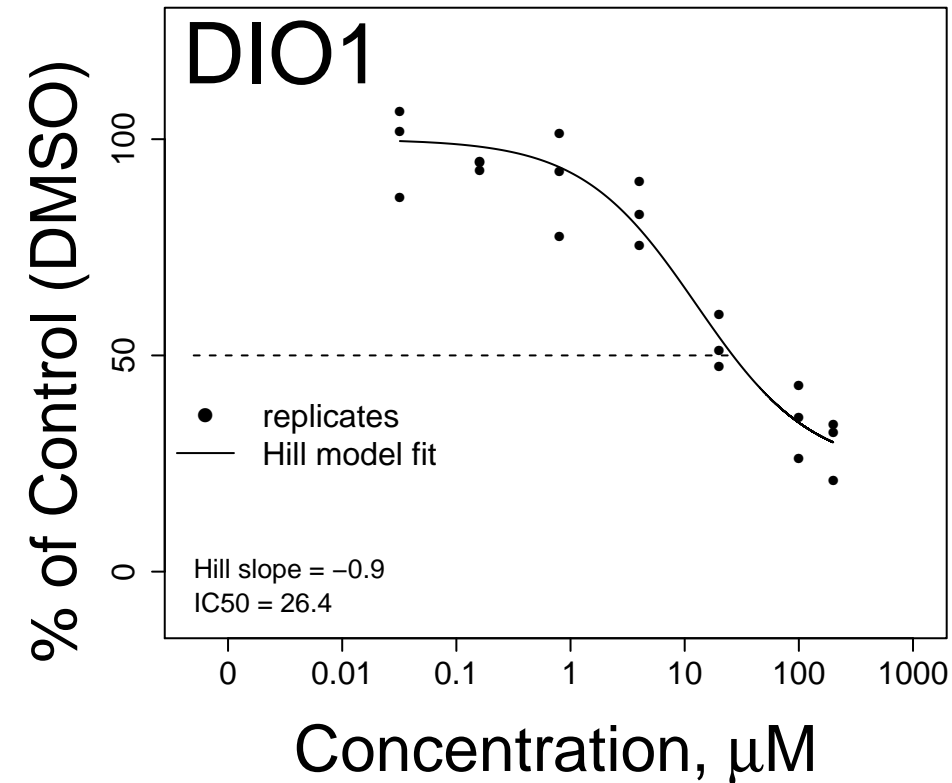
Fluoxastrobin CASRN: 361377-29-9



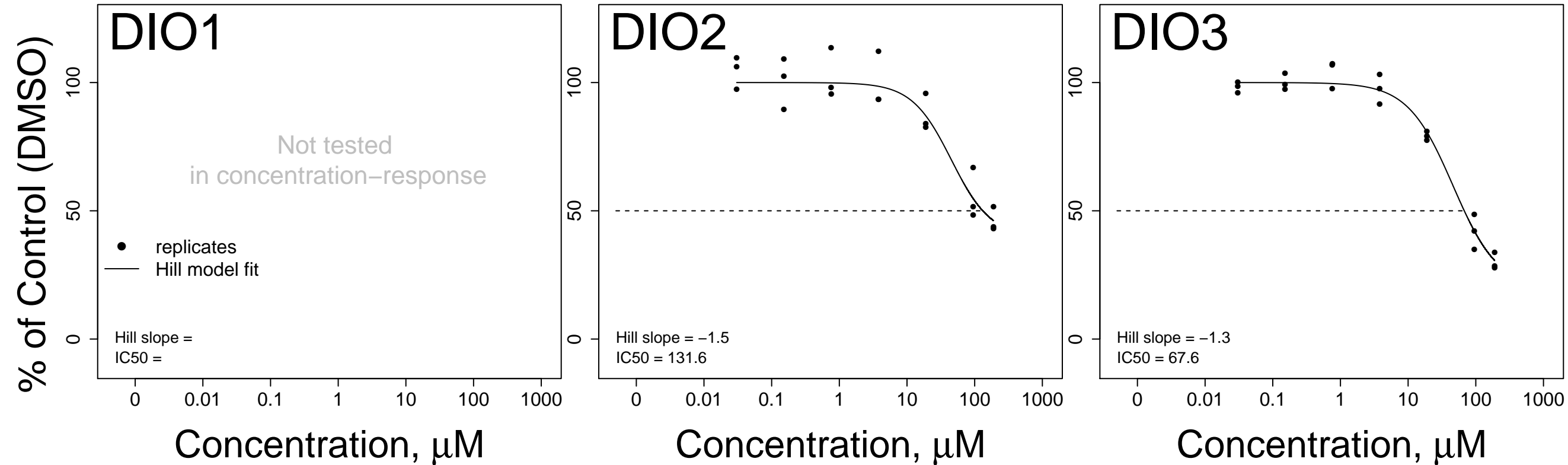
Metolachlor CASRN: 51218-45-2



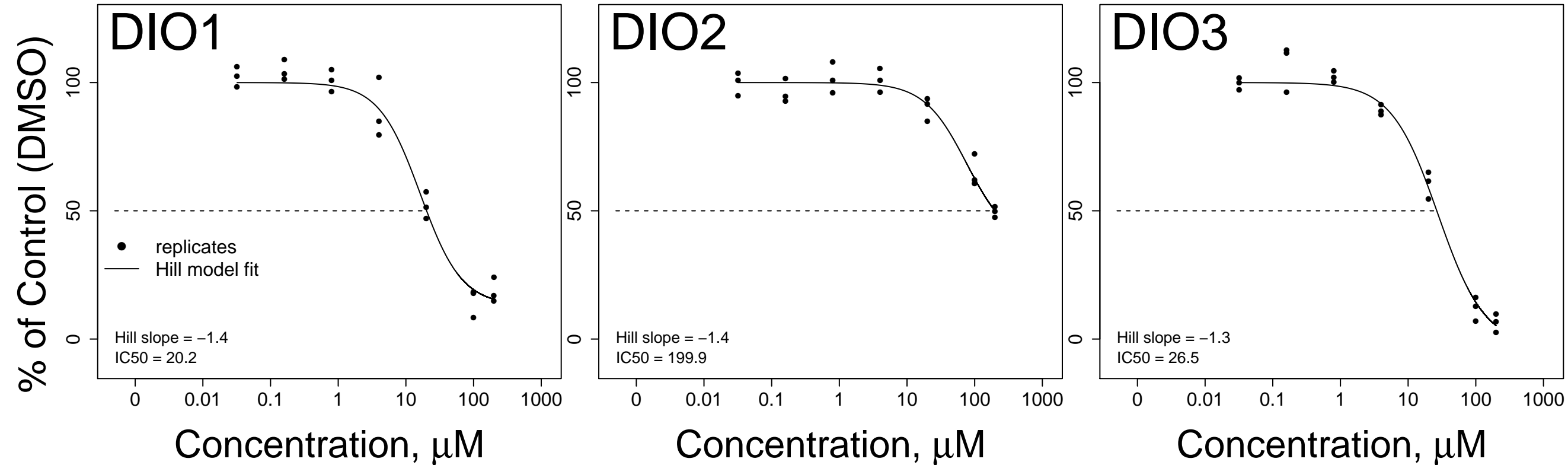
Fenthion CASRN: 55-38-9



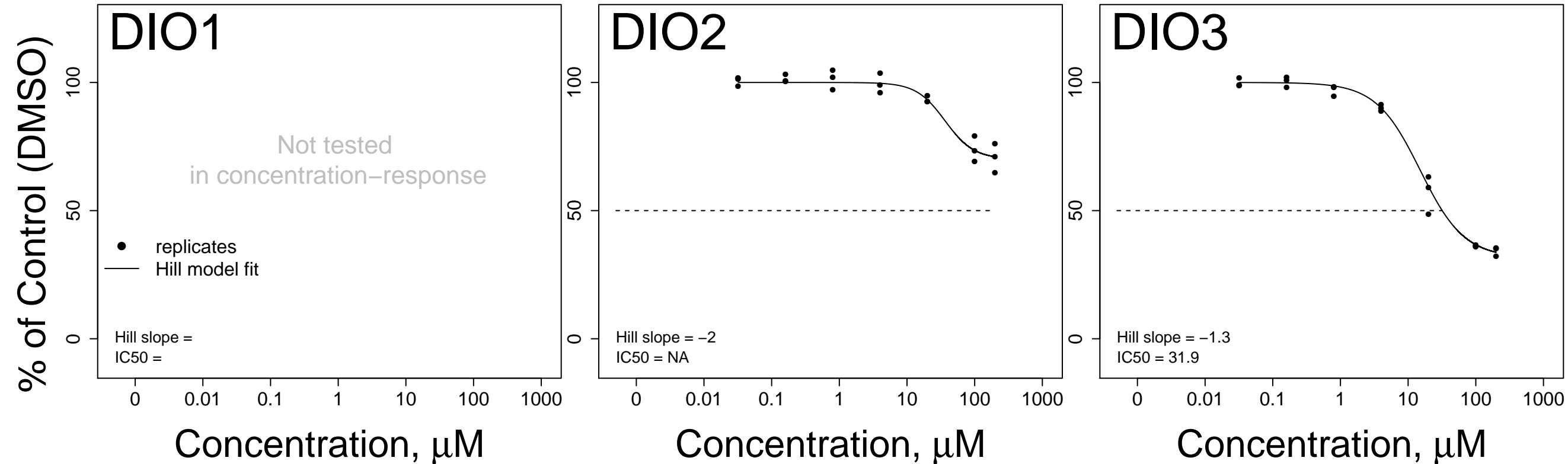
Allethrin CASRN: 584-79-2



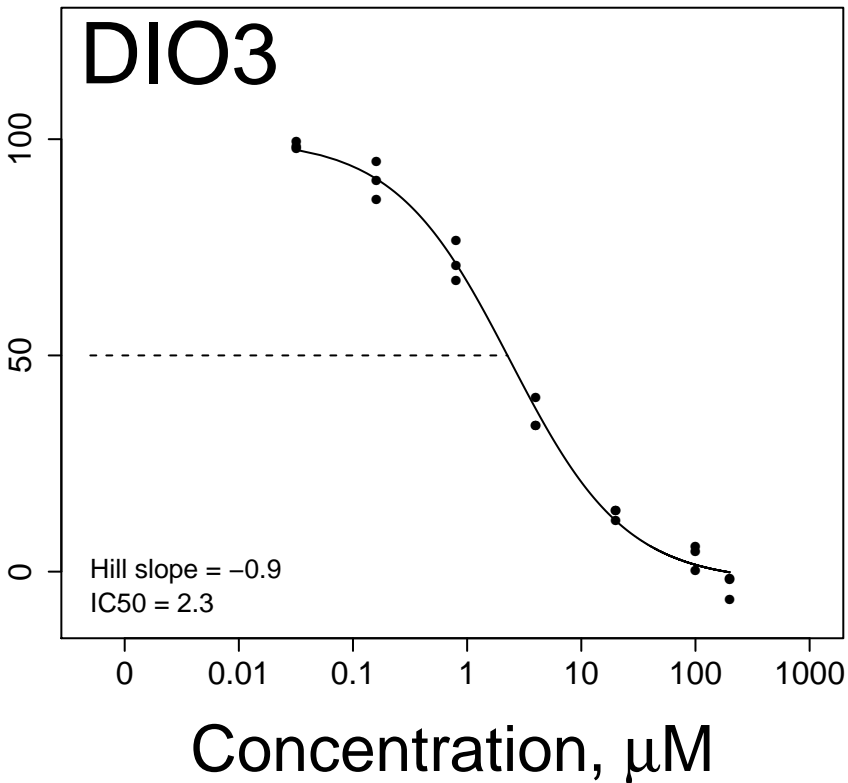
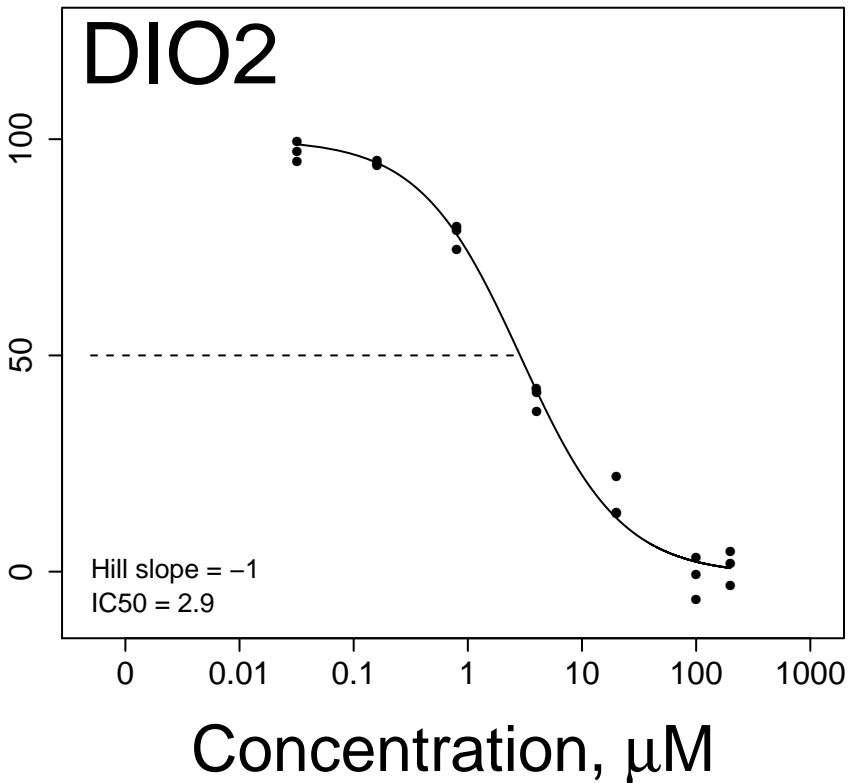
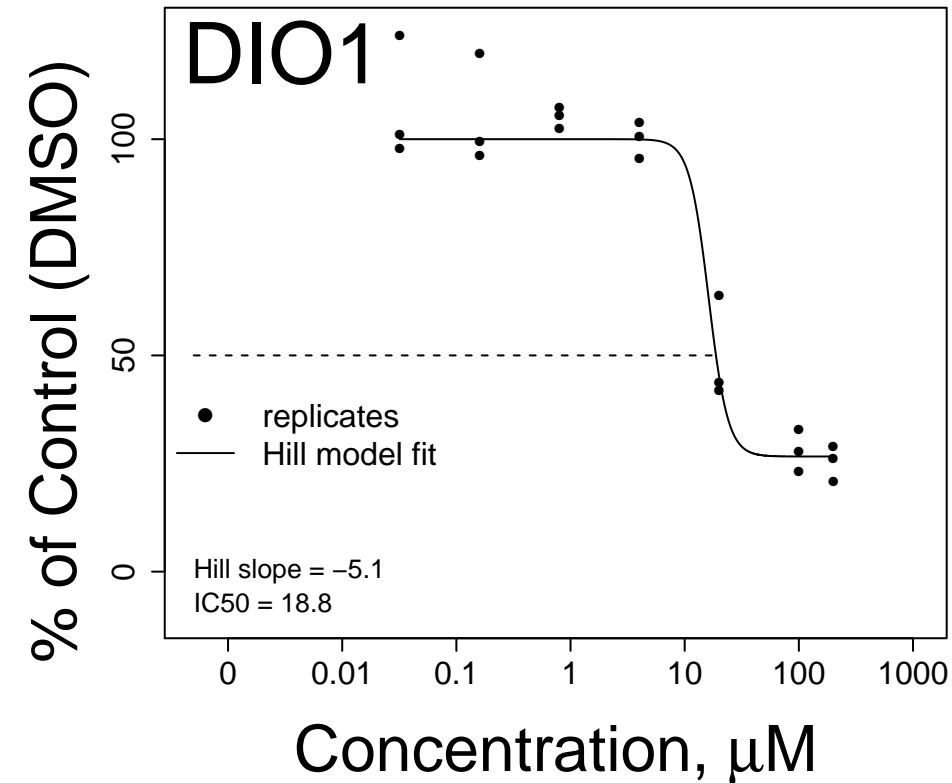
Oxytetracycline dihydrate CASRN: 6153-64-6



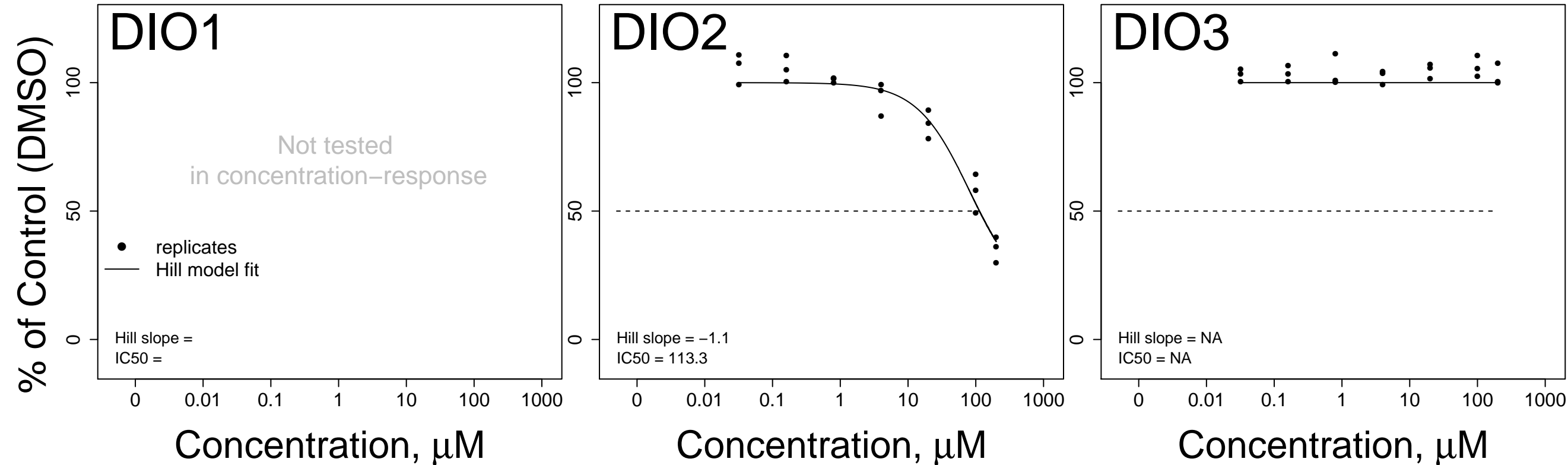
Fenoxaprop-ethyl CASRN: 66441-23-4



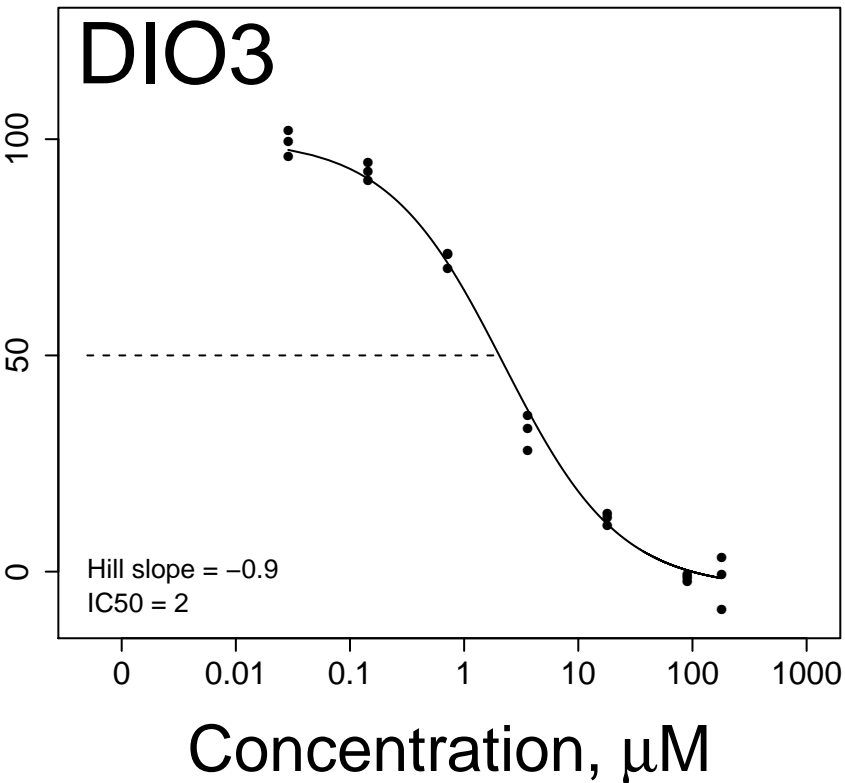
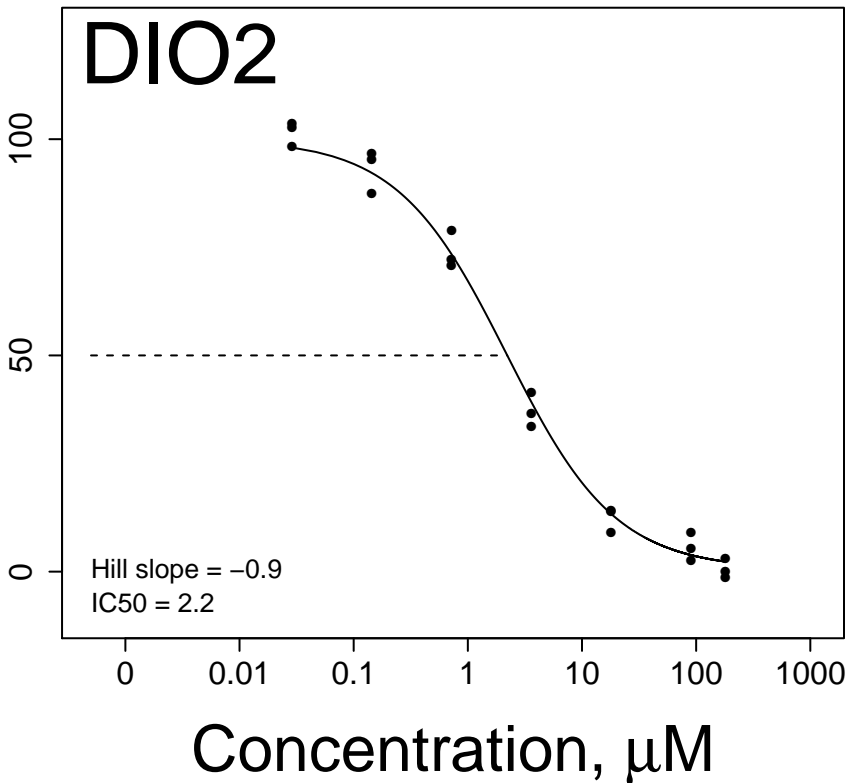
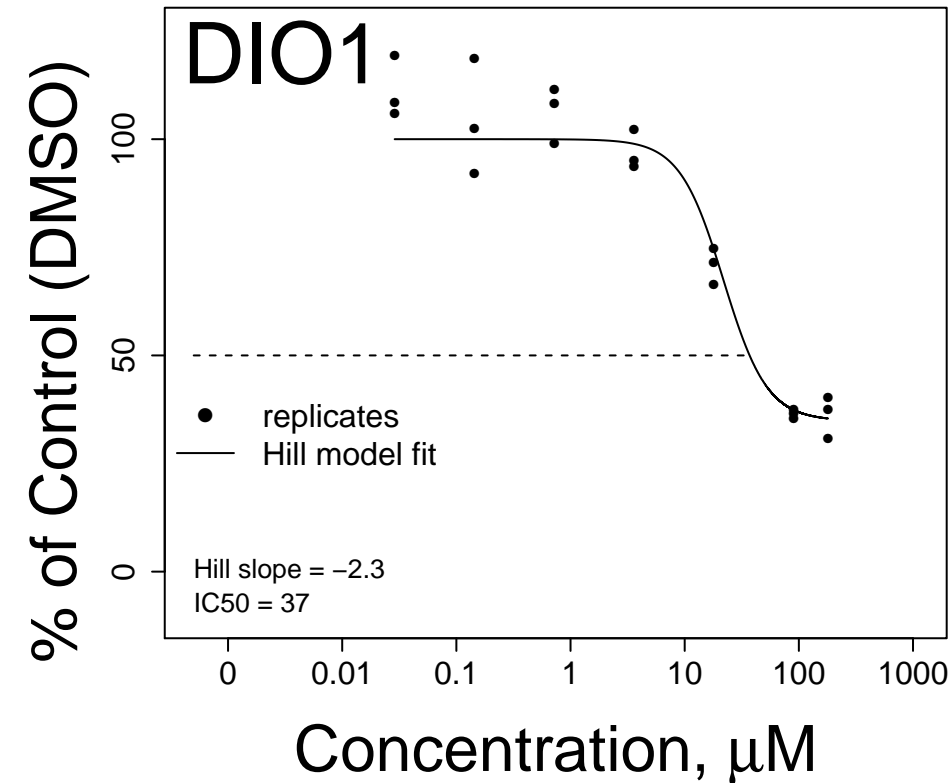
Triflumizole CASRN: 68694-11-1

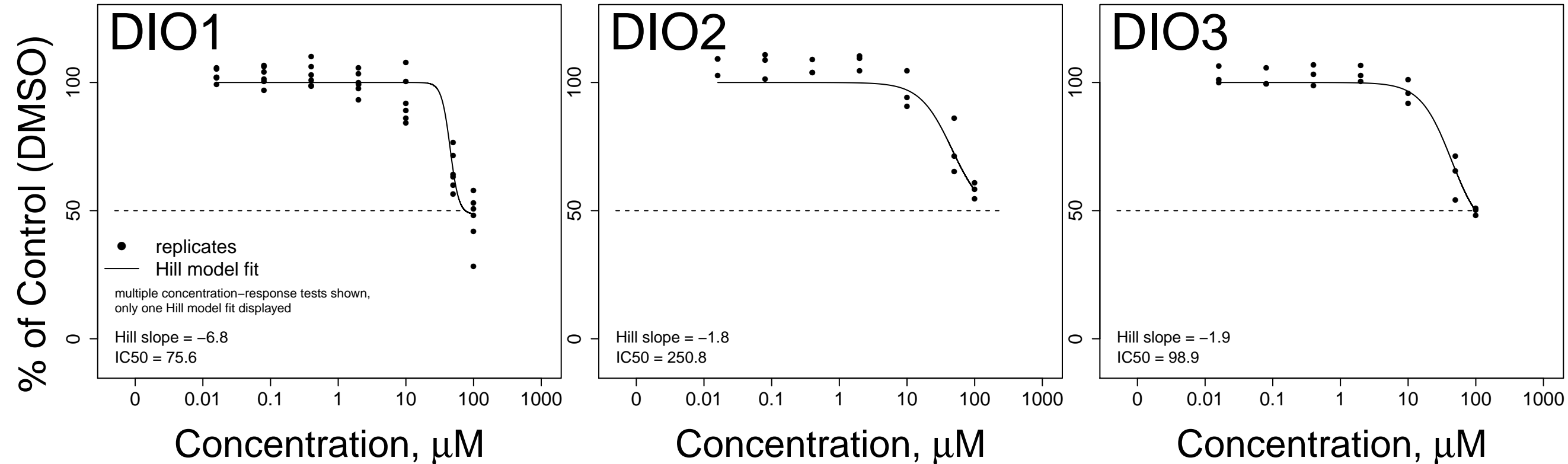


Tetramethrin CASRN: 7696-12-0

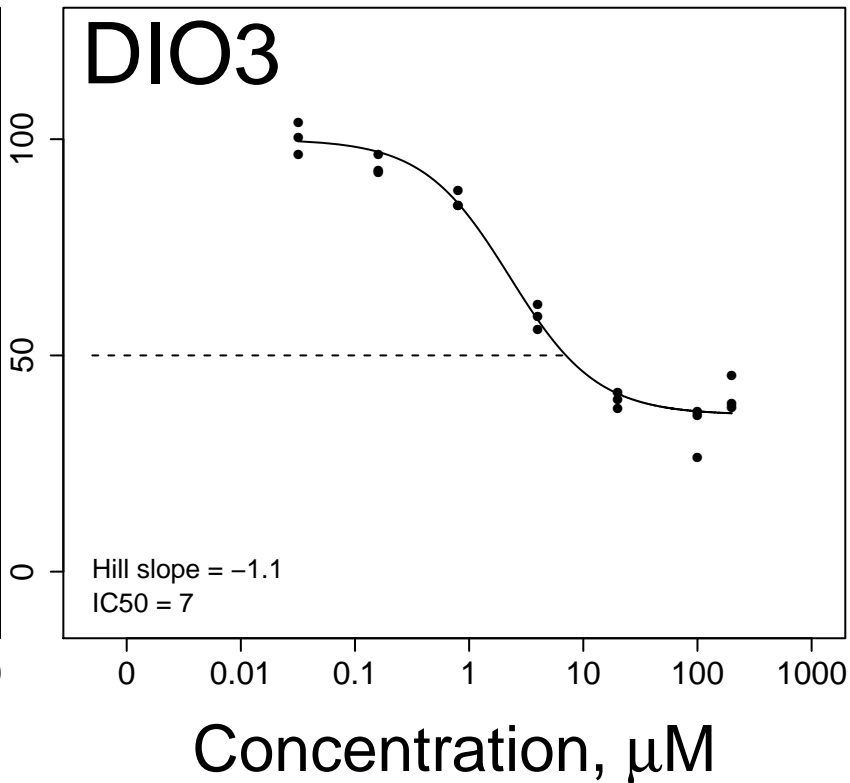
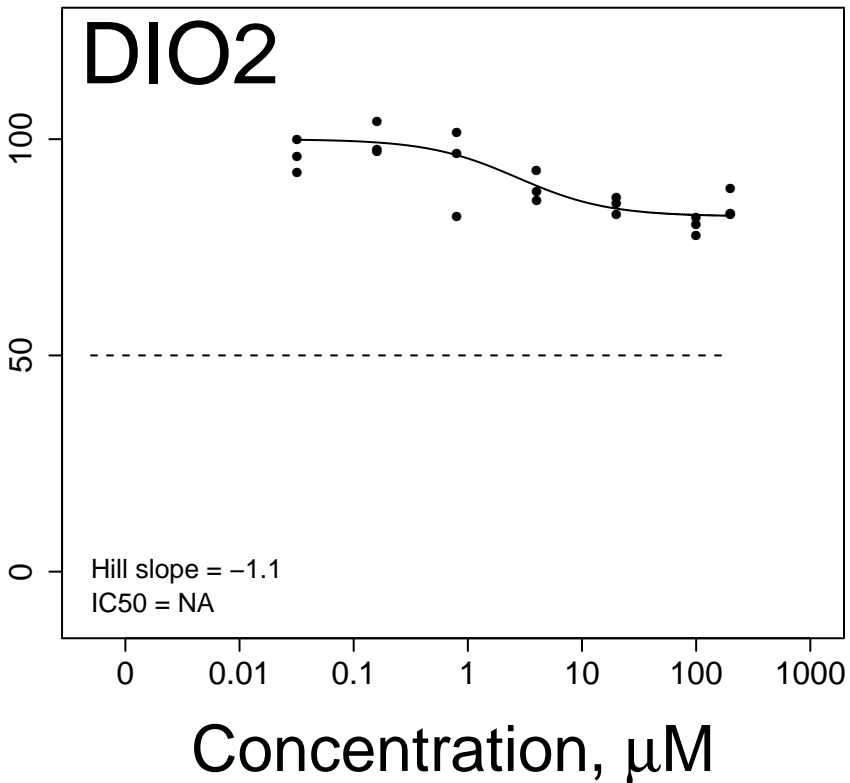
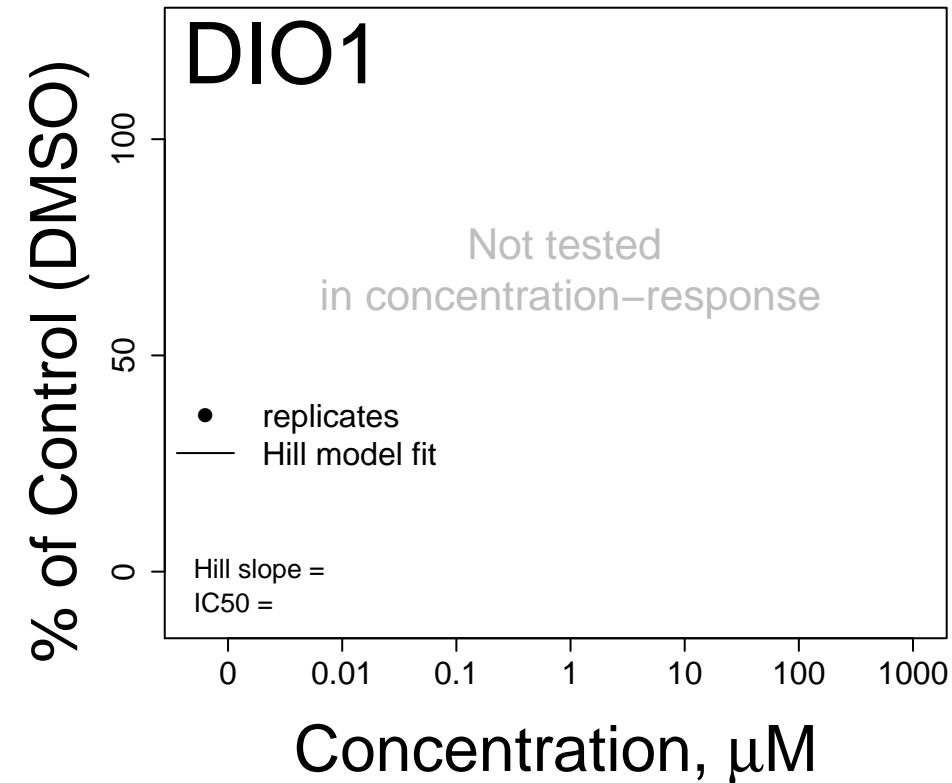


Fluazinam CASRN: 79622-59-6

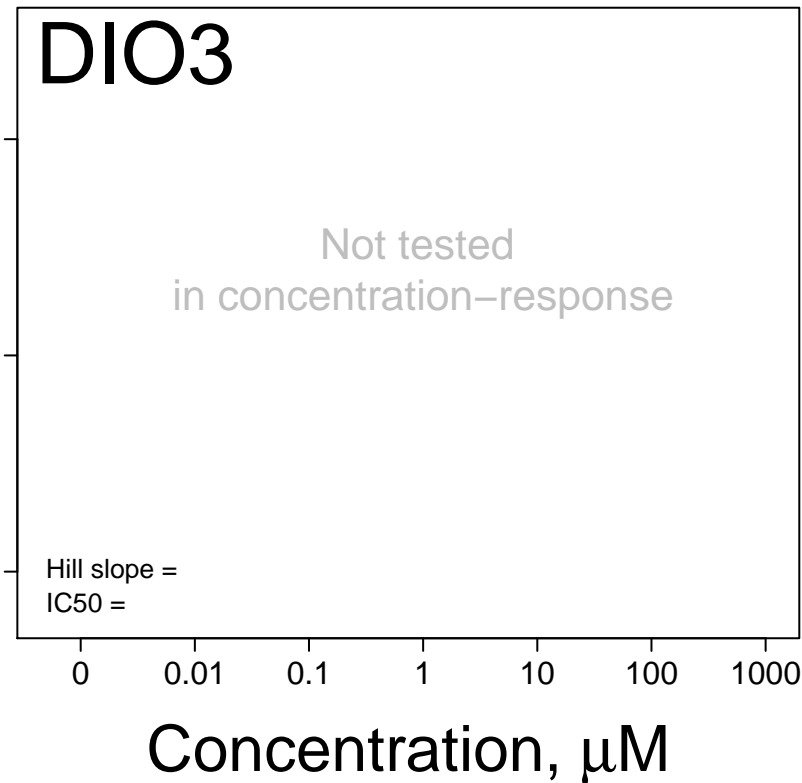
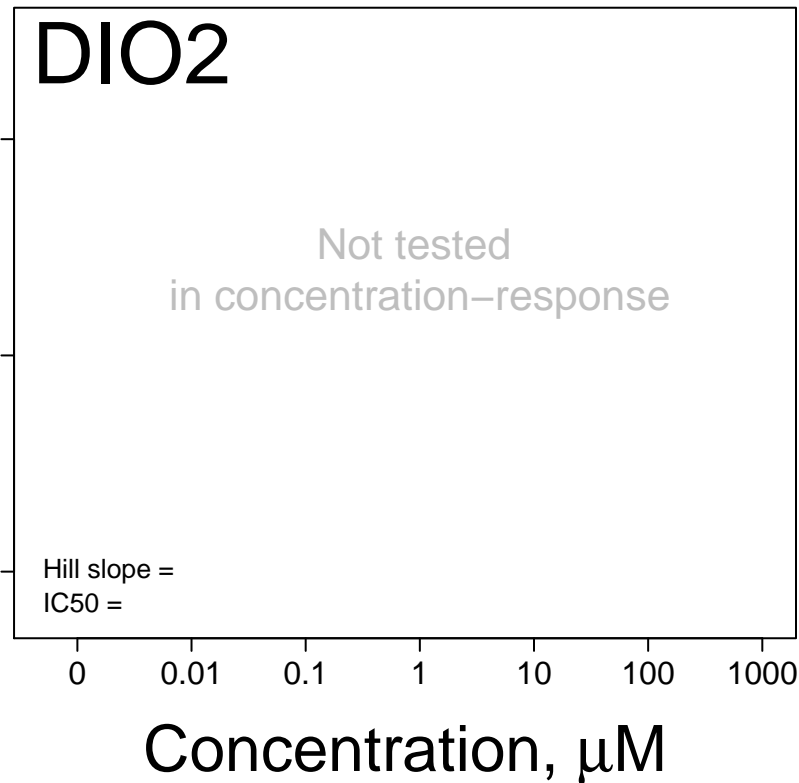
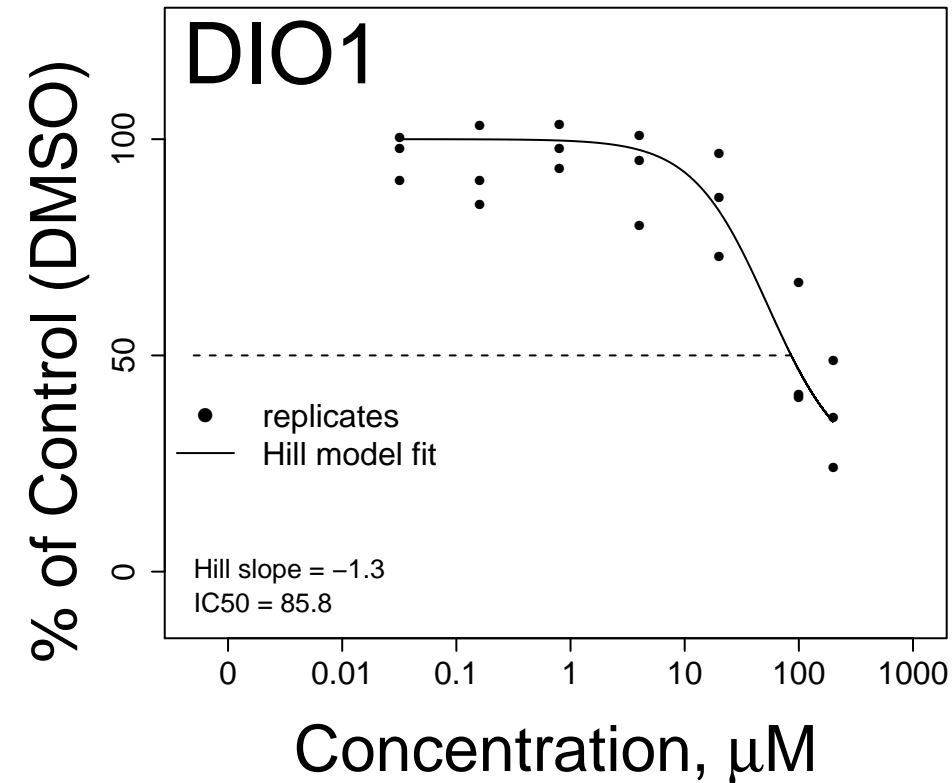




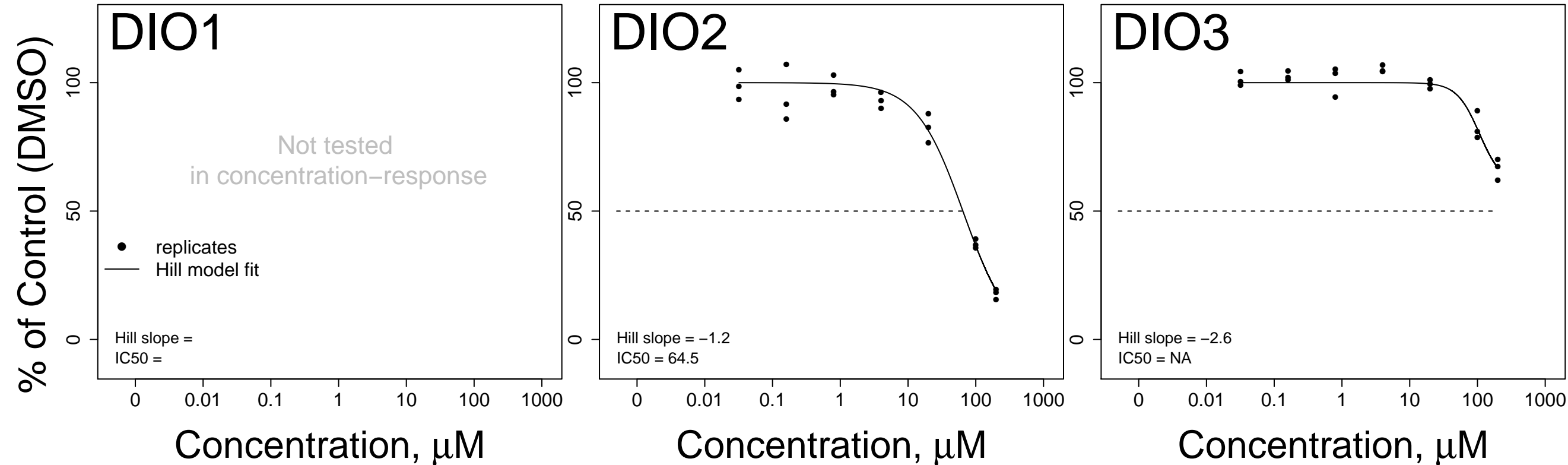
Rotenone CASRN: 83-79-4



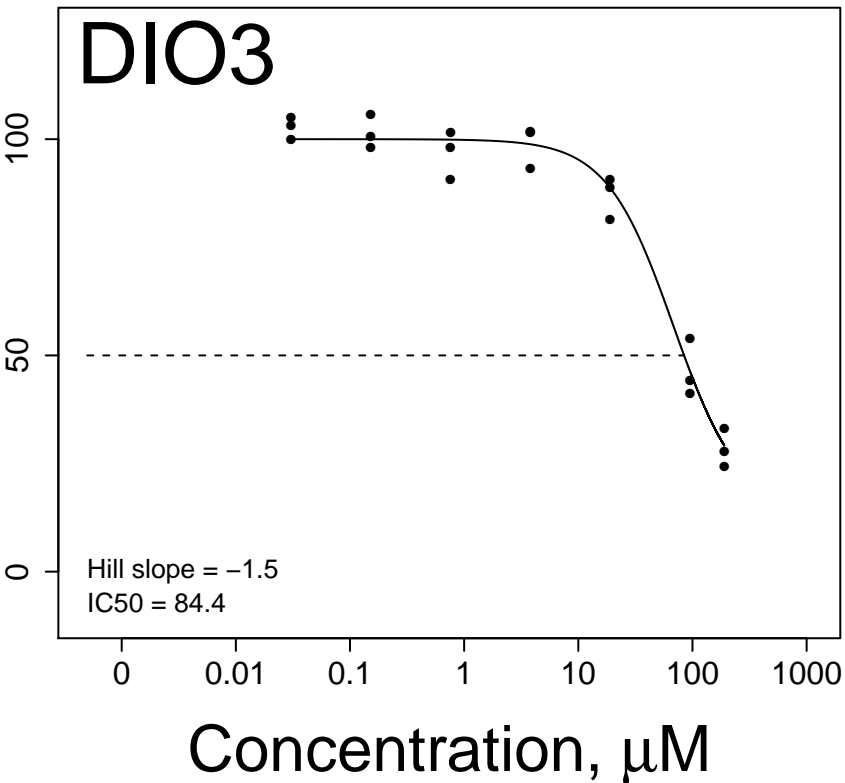
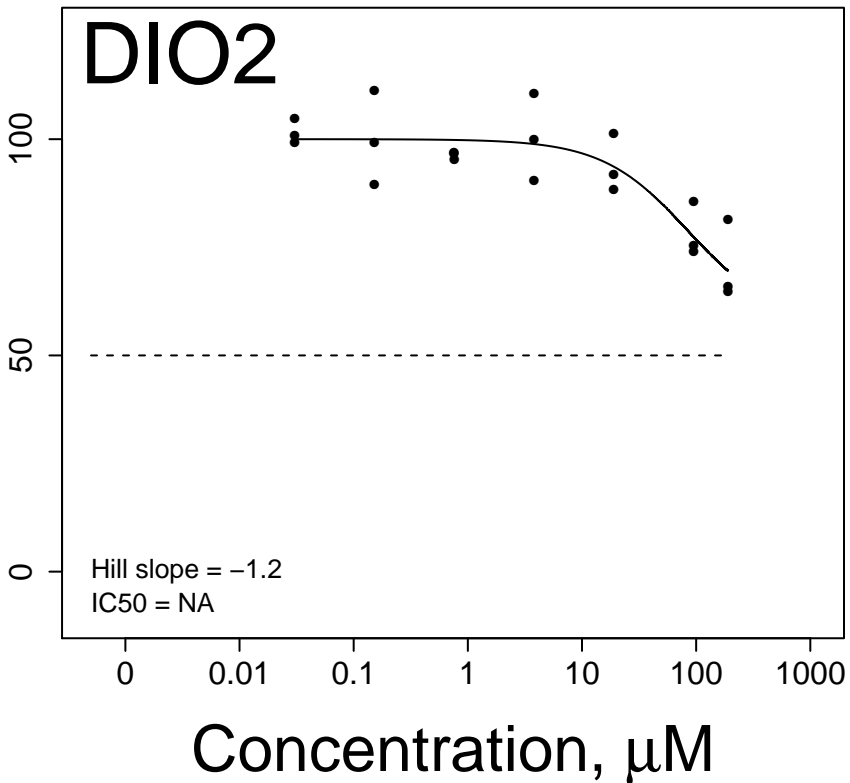
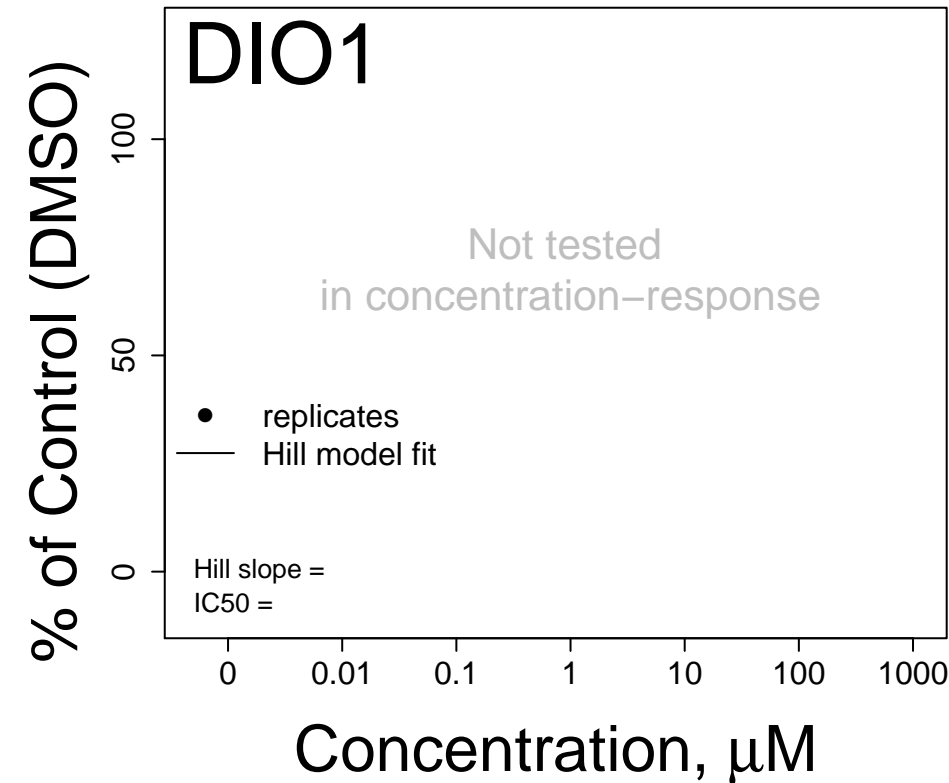
Azinphos-methyl CASRN: 86-50-0



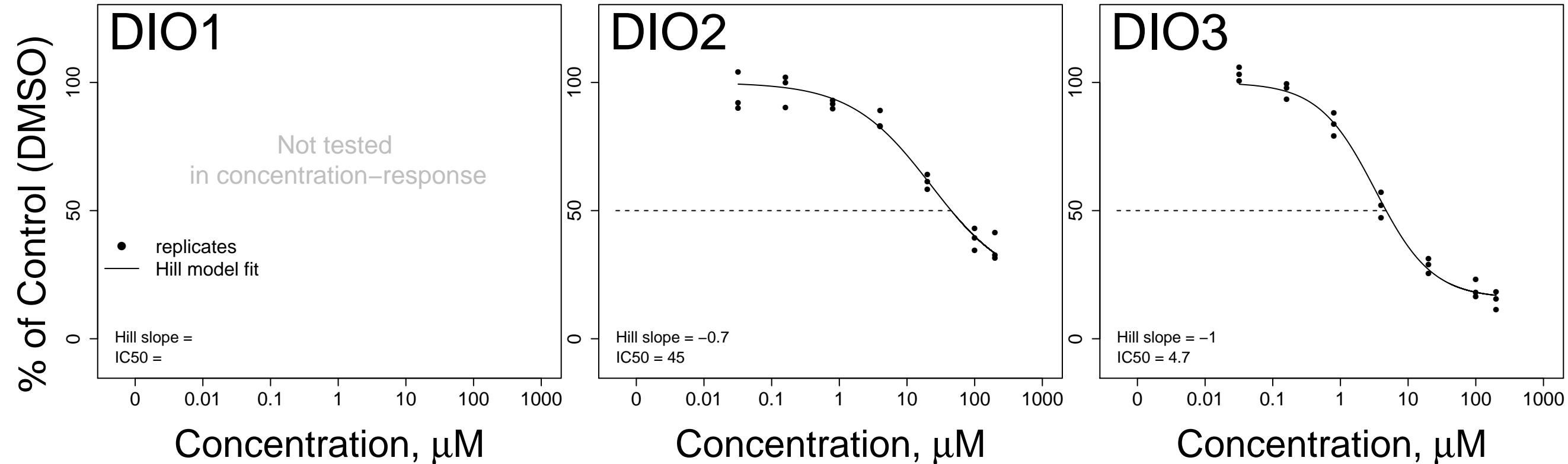
Flumiclorac-pentyl CASRN: 87546-18-7



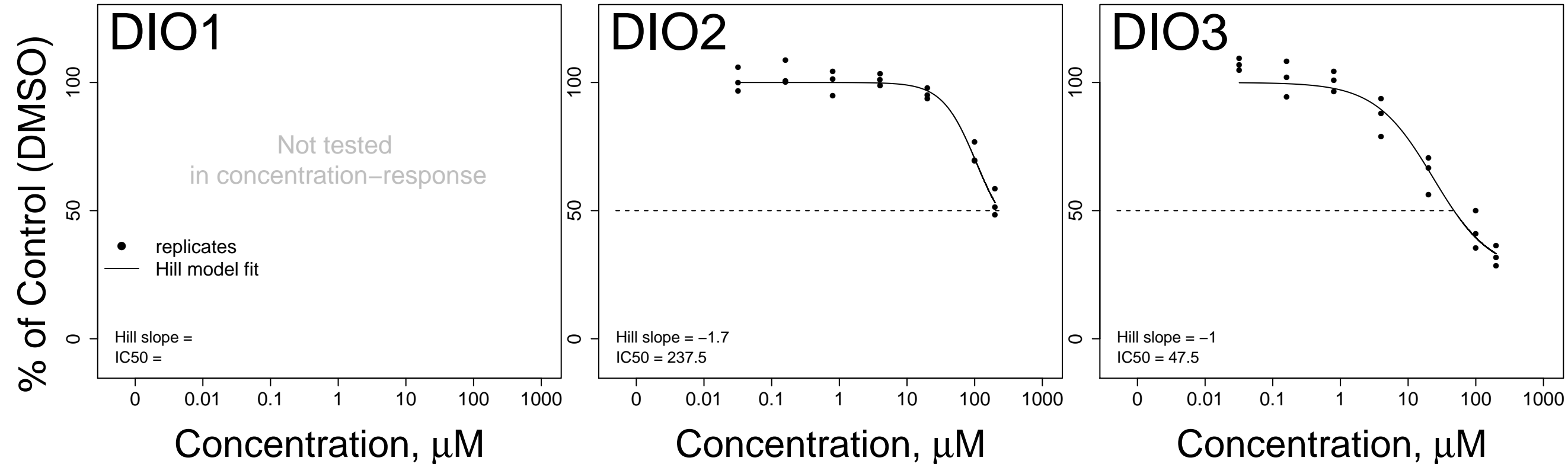
Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3) CASRN: NOCAS_34742



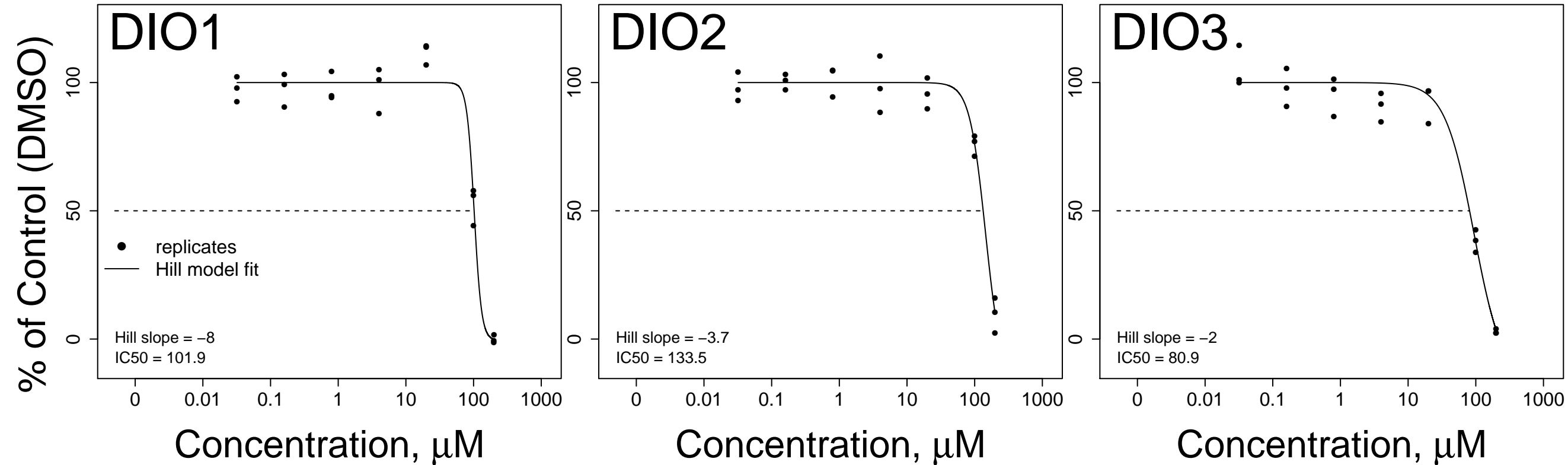
2-Benzylideneoctanal CASRN: 101-86-0



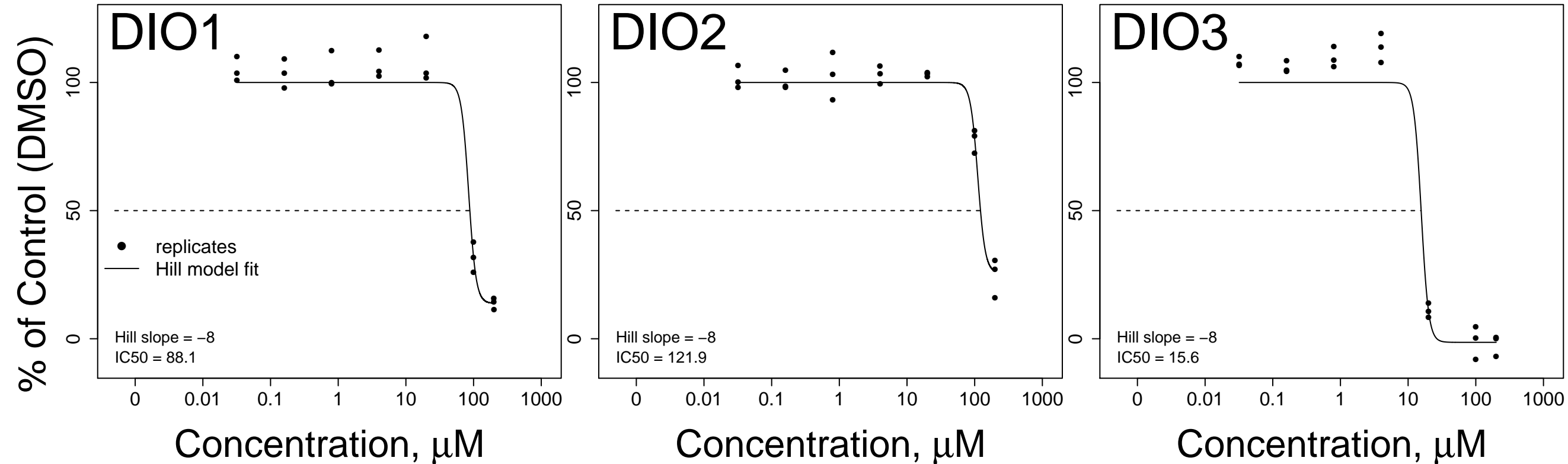
17beta-Trenbolone CASRN: 10161-33-8



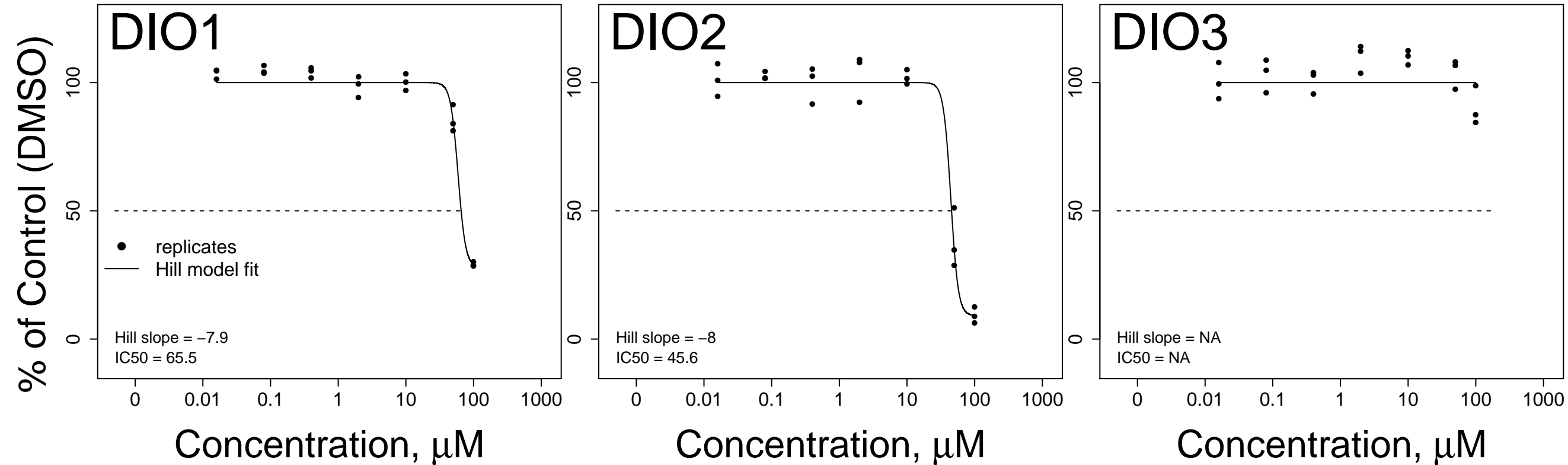
Octyl gallate CASRN: 1034-01-1



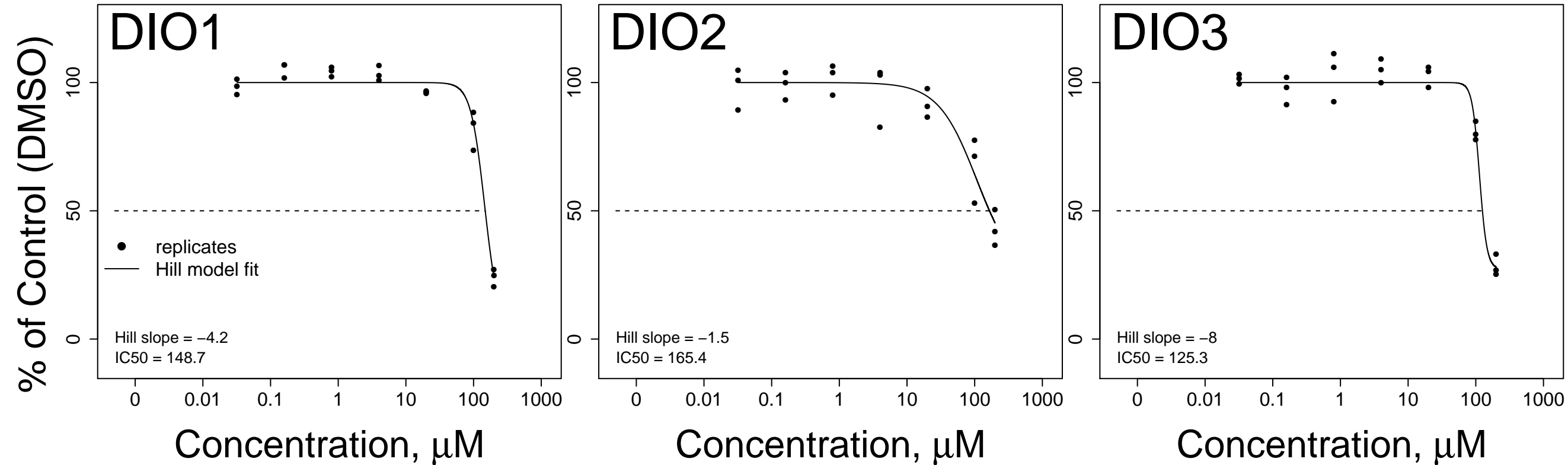
4-Nonylphenol CASRN: 104-40-5



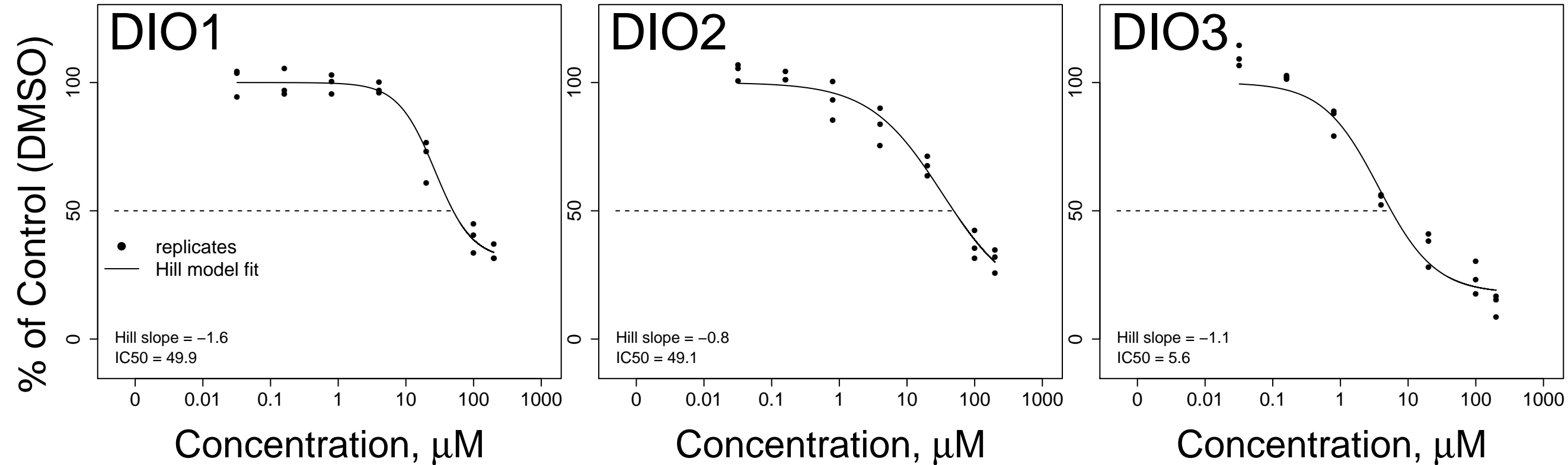
Tamoxifen CASRN: 10540-29-1



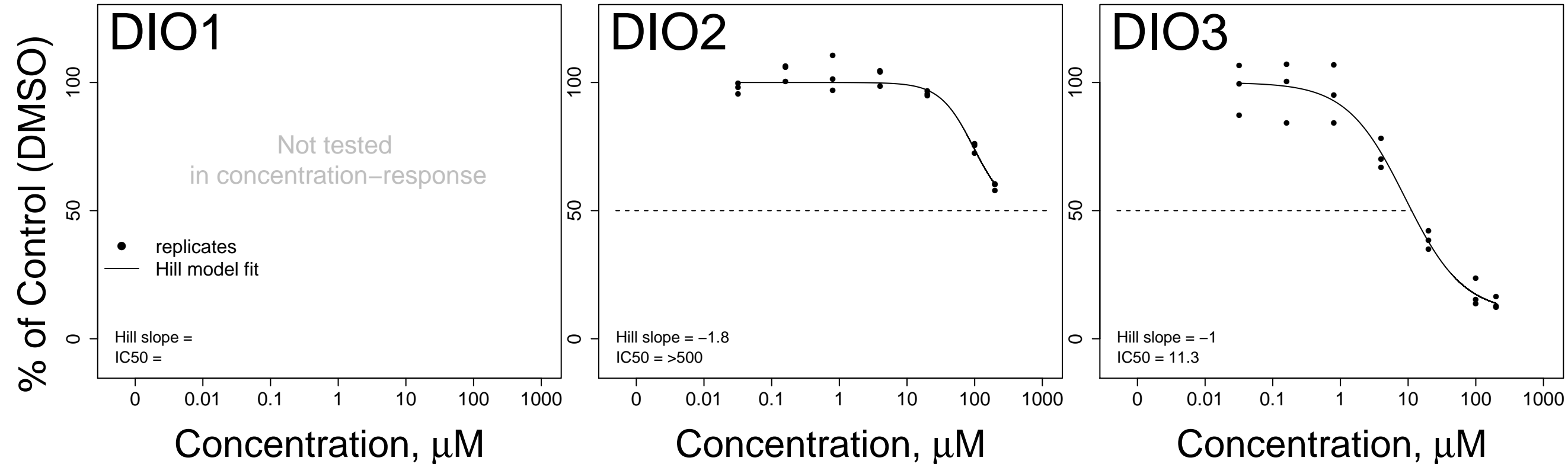
PharmaGSID_47337 CASRN: 1061517-62-1



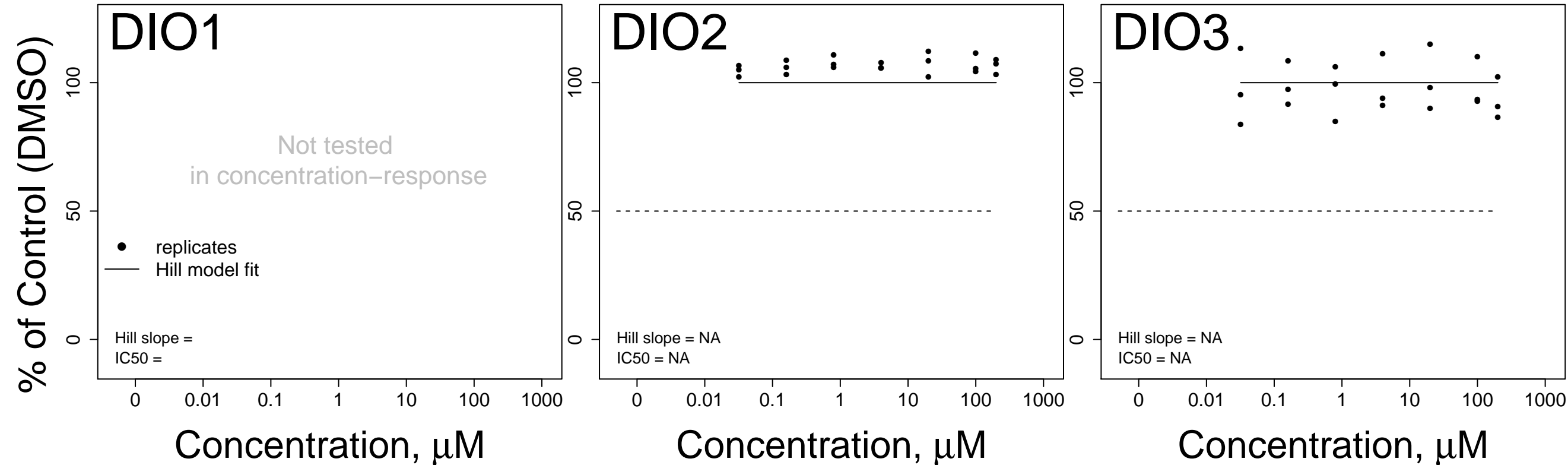
Mepanipyrim CASRN: 110235-47-7



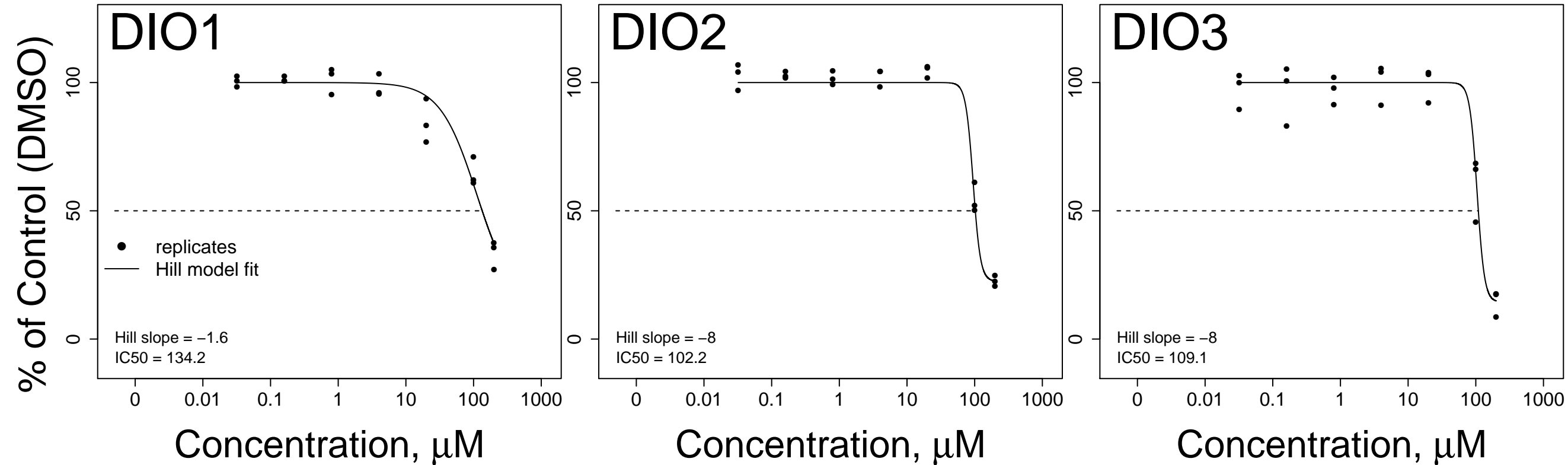
Glutaraldehyde CASRN: 111-30-8



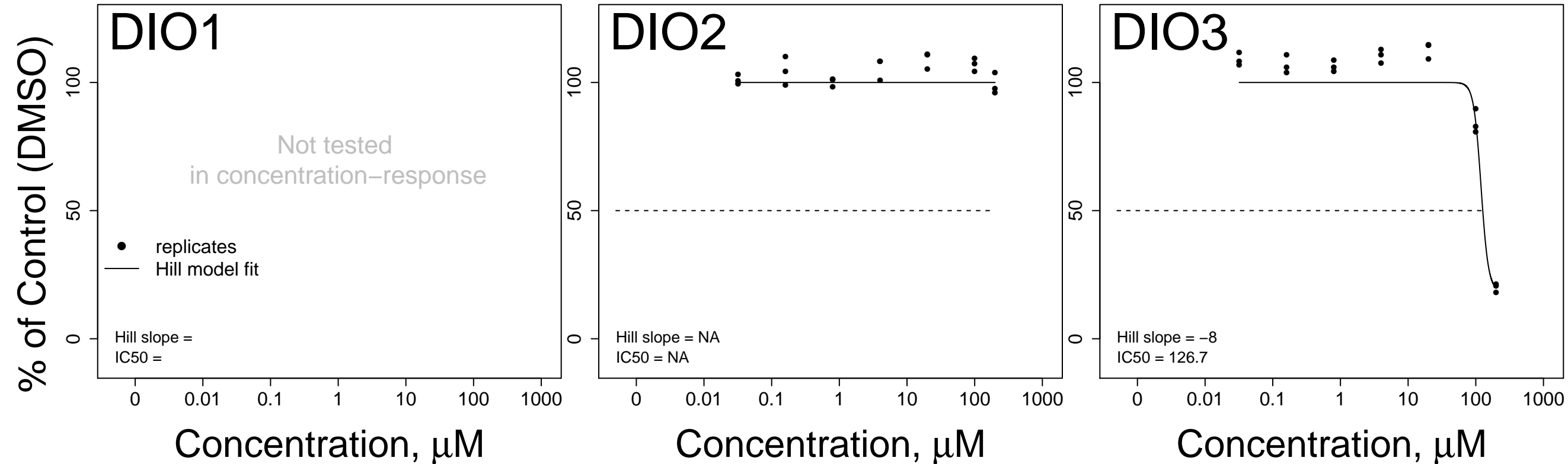
Bis(2-chloroethyl) ether CASRN: 111-44-4



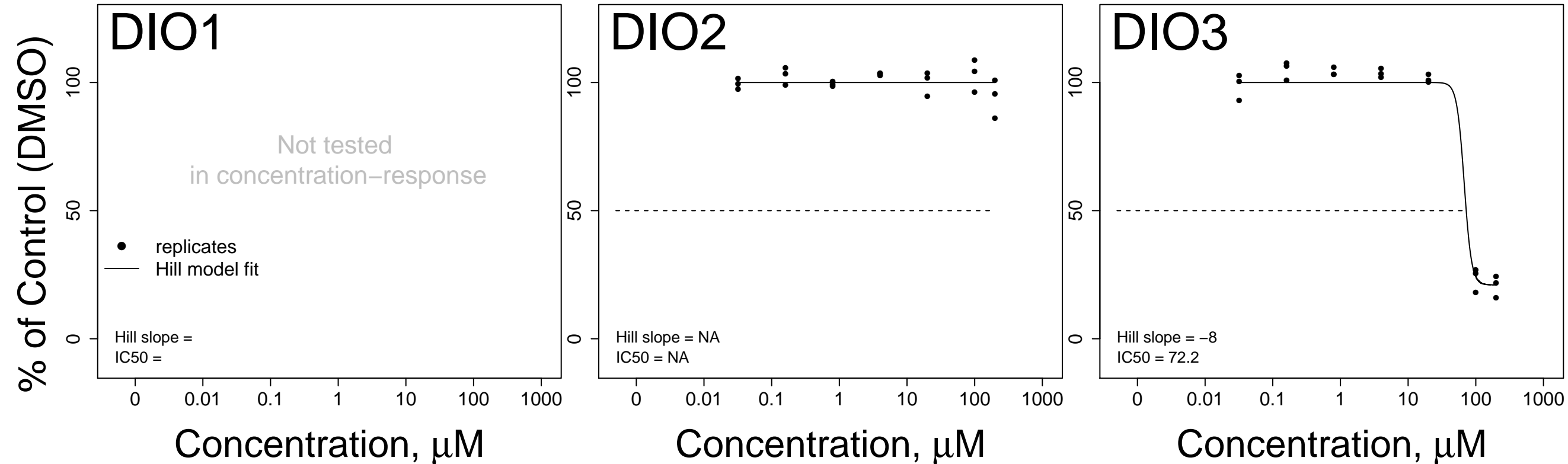
Dodecyltrimethylammonium chloride CASRN: 112-00-5



1-Undecanol CASRN: 112-42-5



1-Dodecanol CASRN: 112-53-8



DIO1

DIO2

DIO3

Not tested
in concentration-response

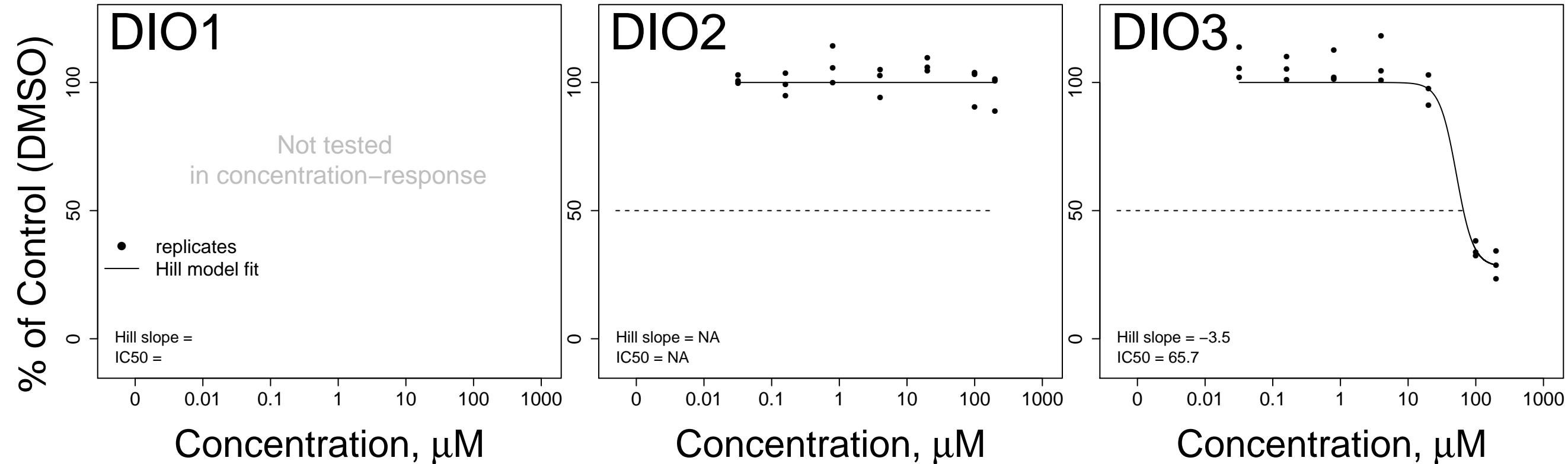
● replicates
— Hill model fit

Hill slope =
IC50 =

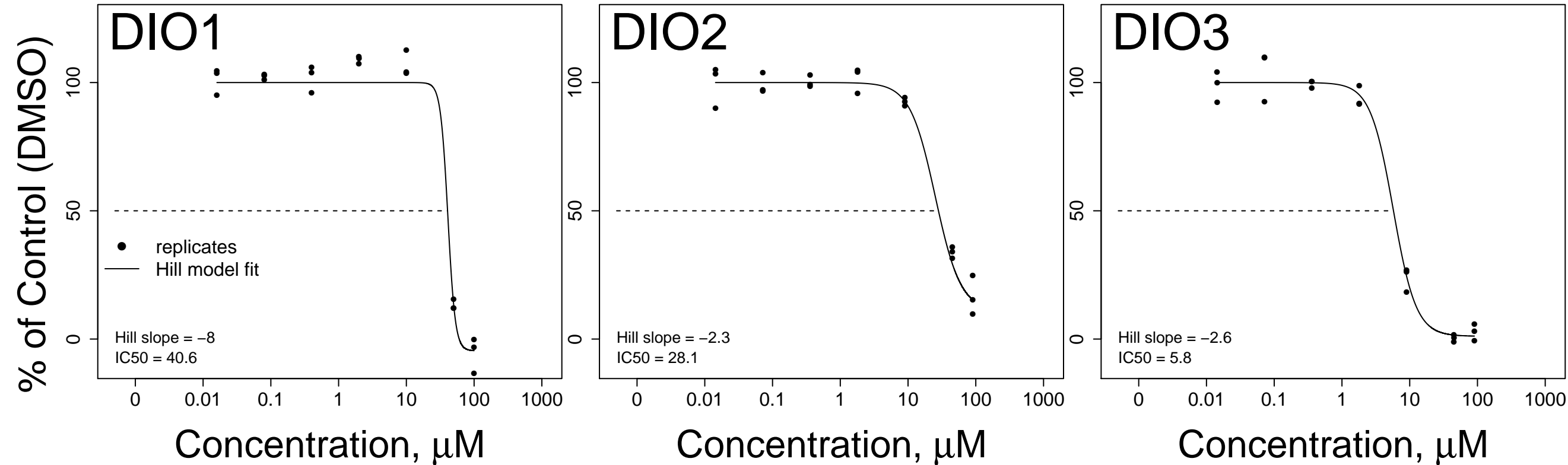
Hill slope = NA
IC50 = NA

Hill slope = -8
IC50 = 72.2

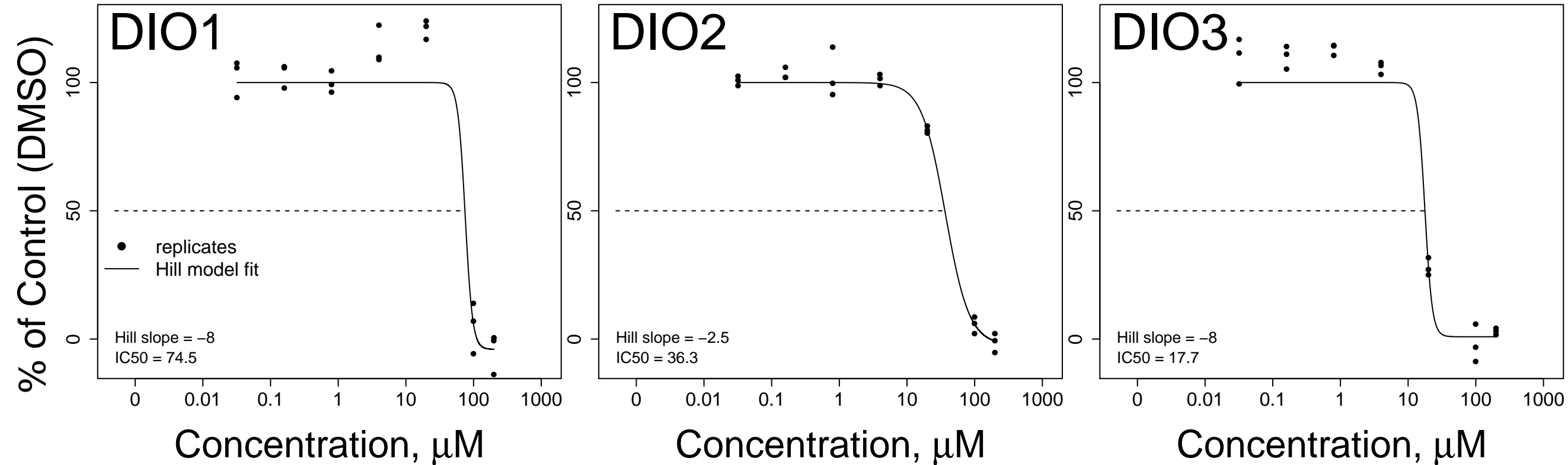
1-Tridecanol CASRN: 112-70-9



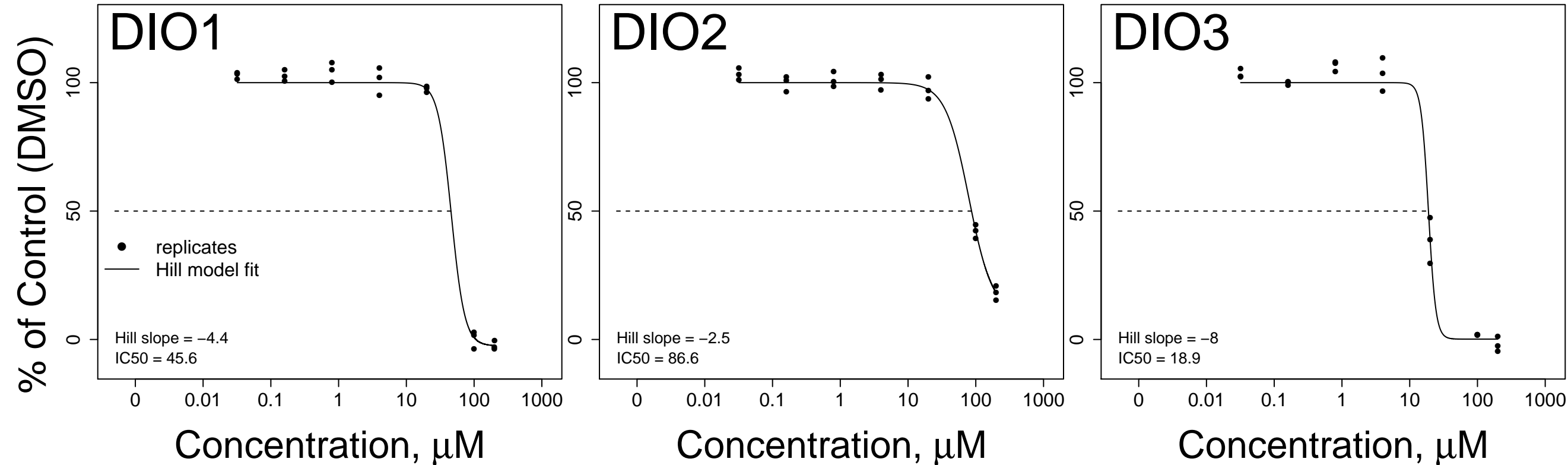
Sodium hexyldecyl sulfate CASRN: 1120-01-0



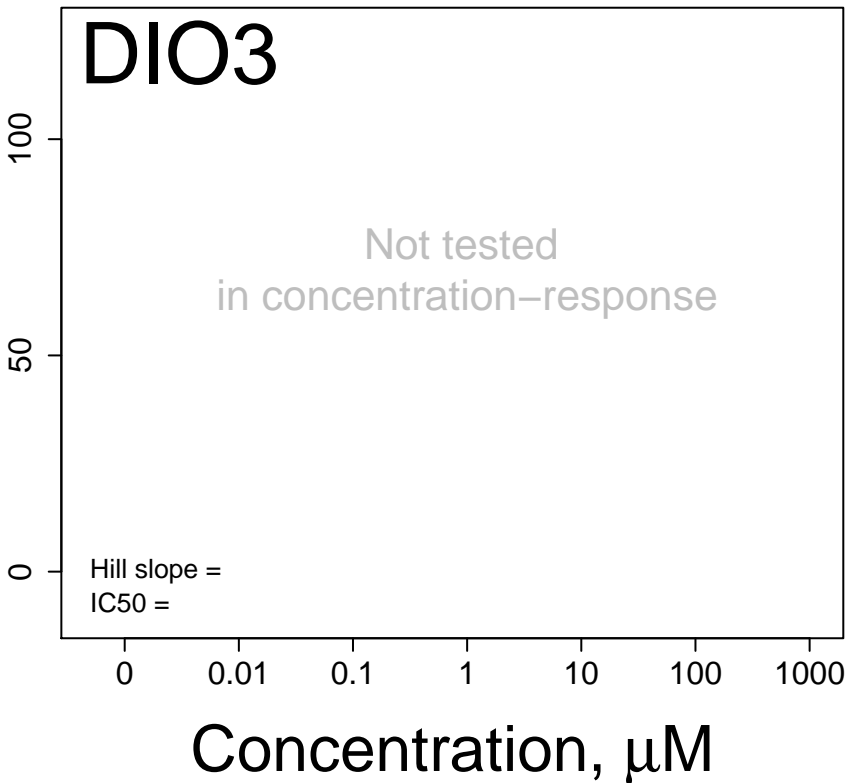
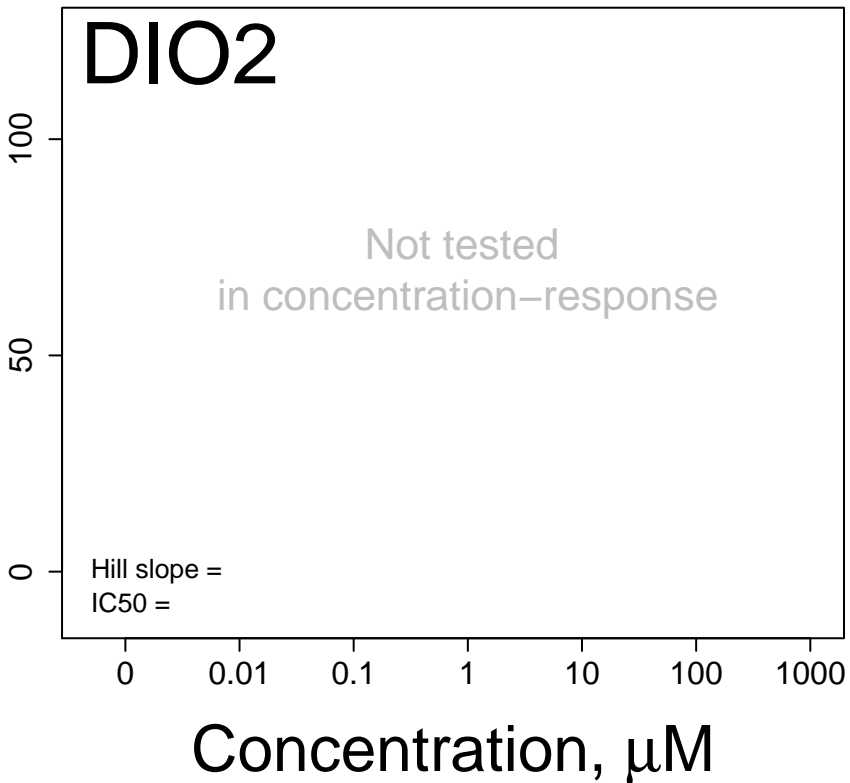
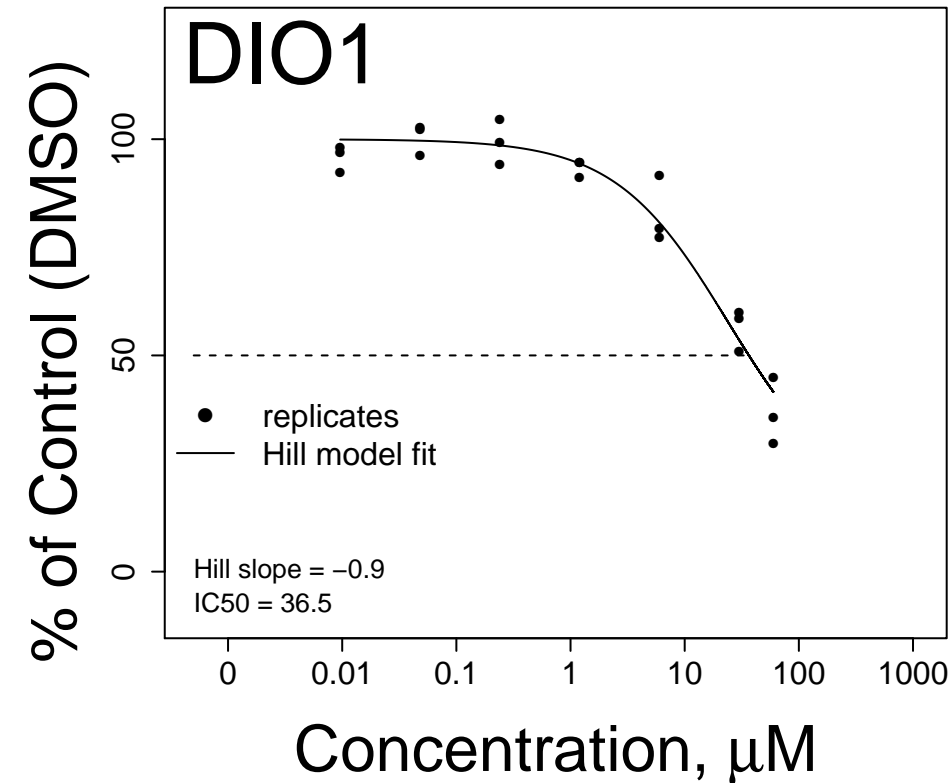
Sodium myristyl sulfate CASRN: 1191-50-0

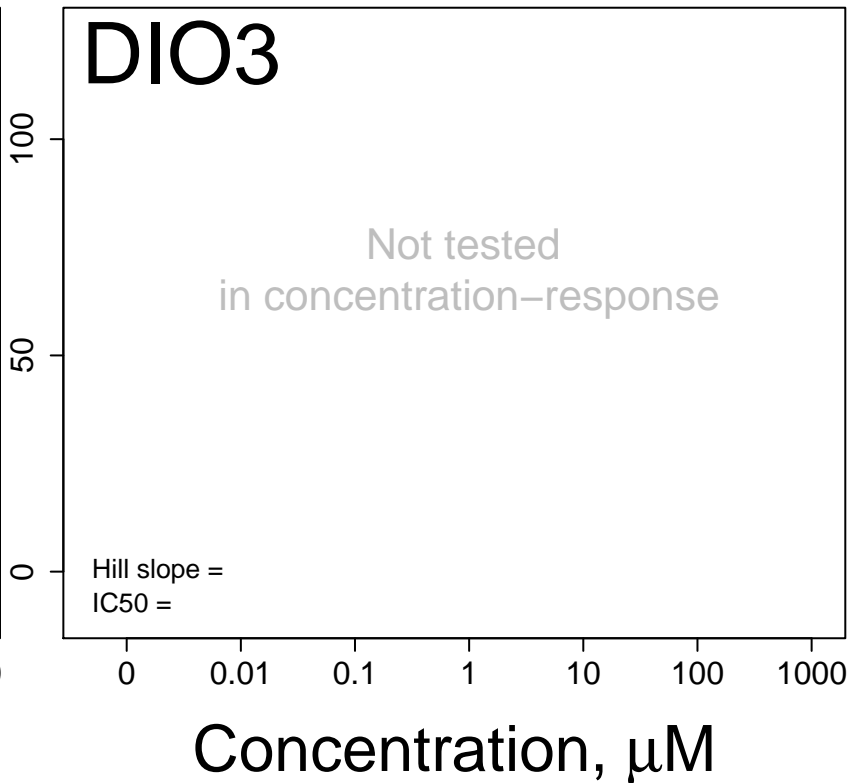
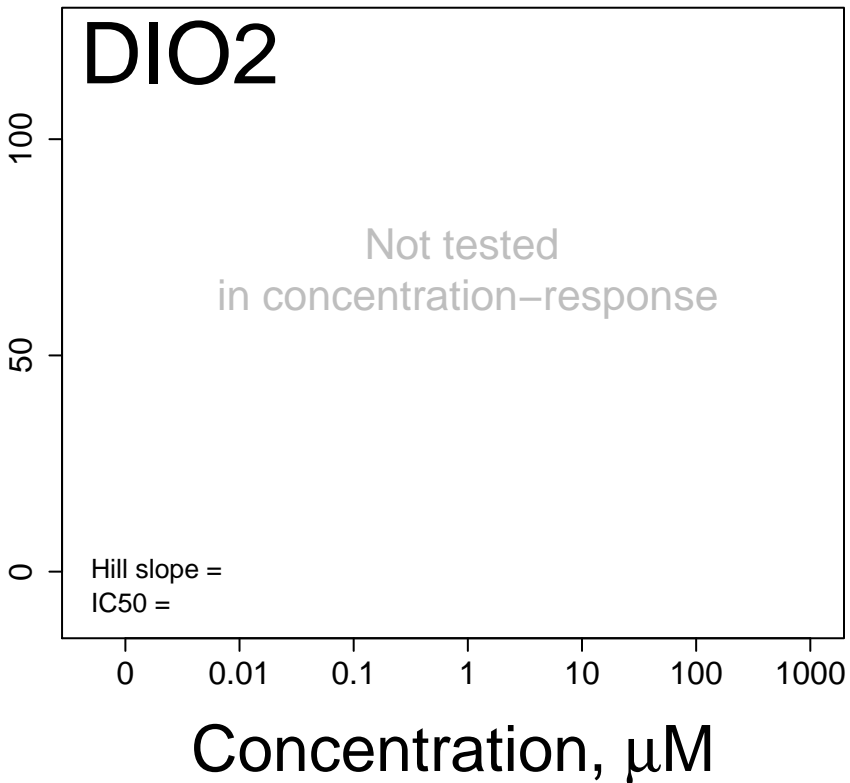
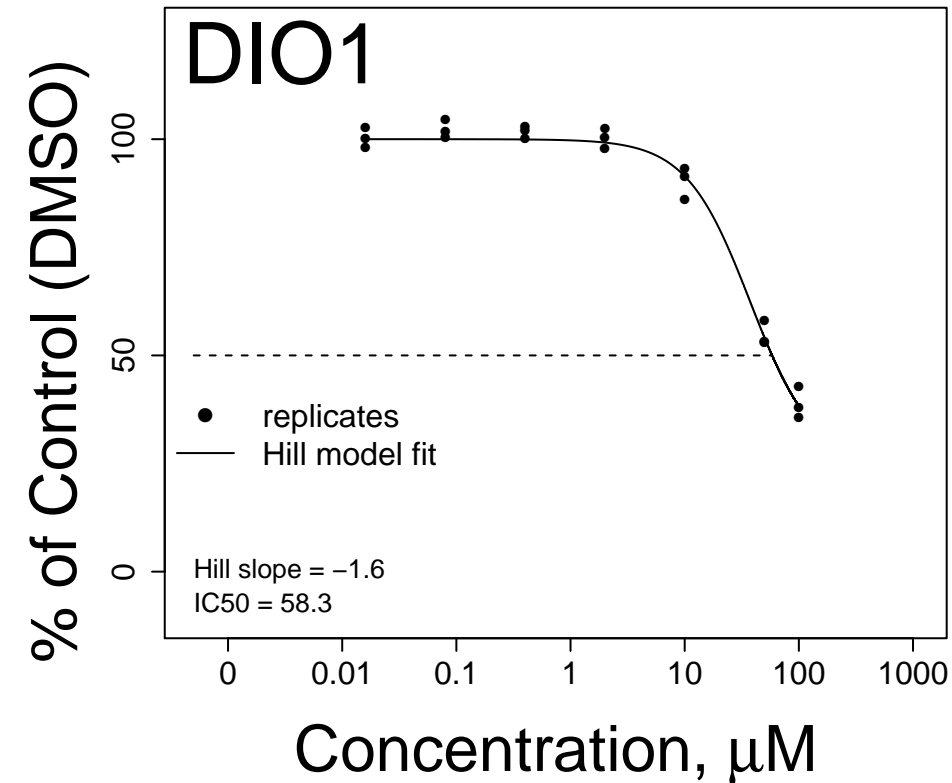


2,4-Bis(2-methylbutan-2-yl)phenol CASRN: 120-95-6

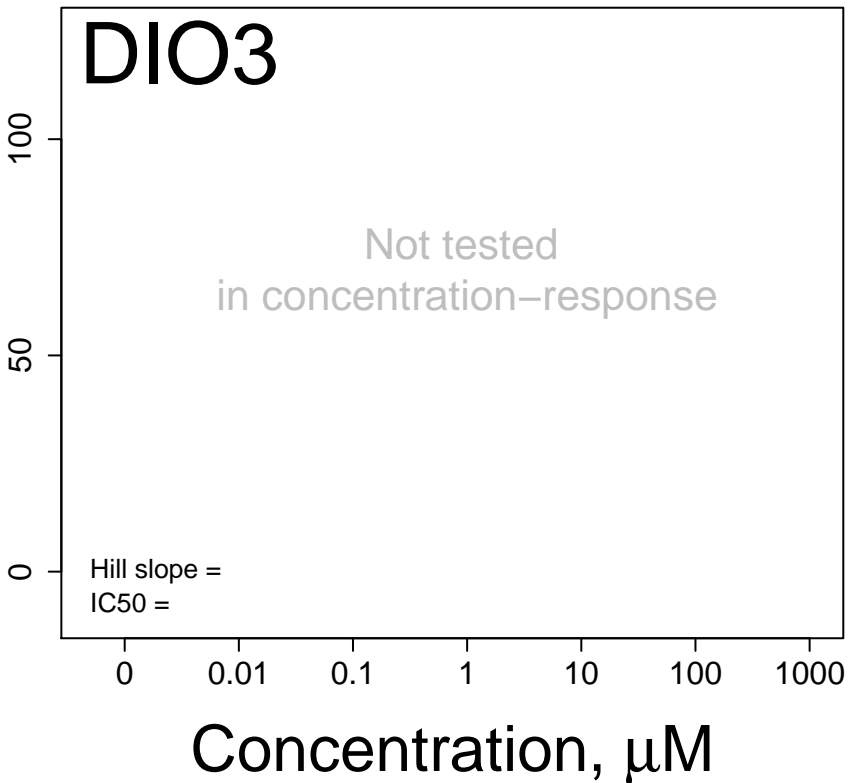
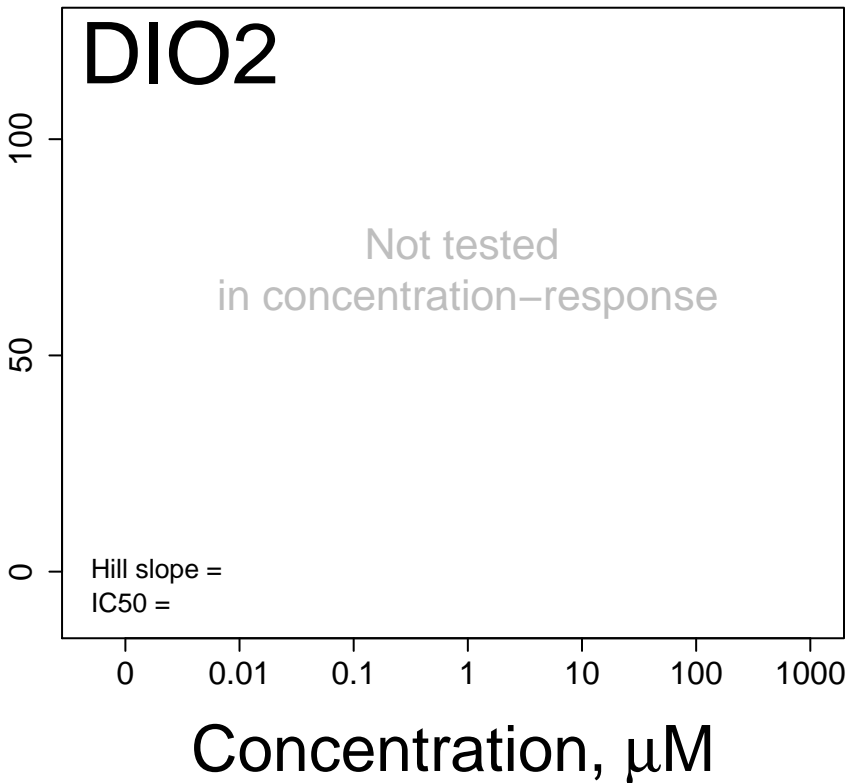
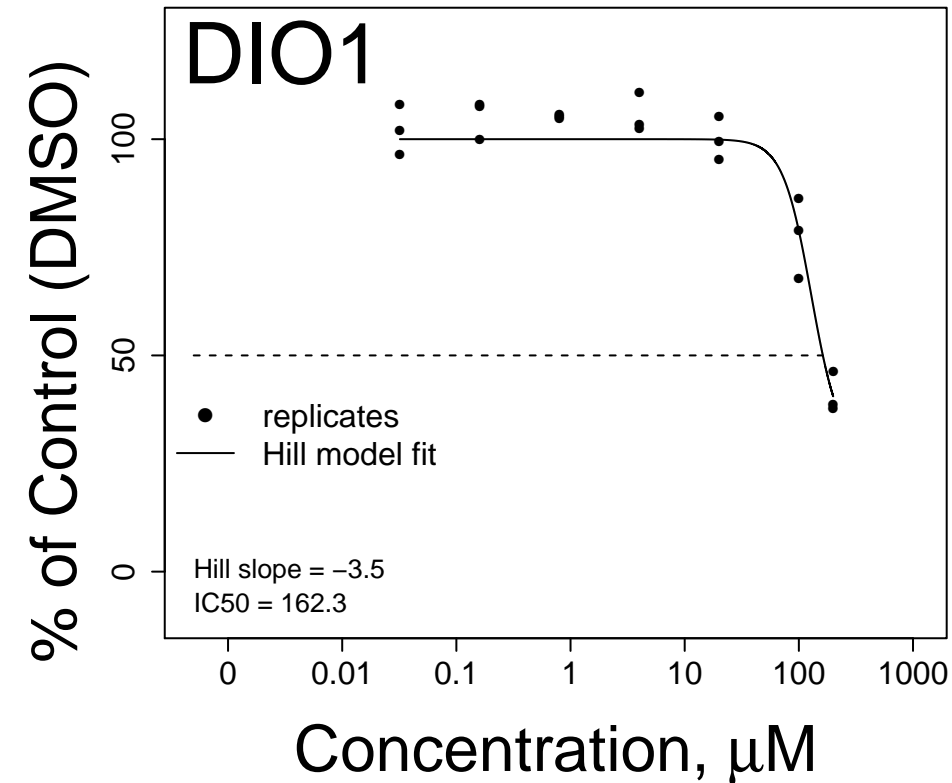


TNP-470 CASRN: 129298-91-5

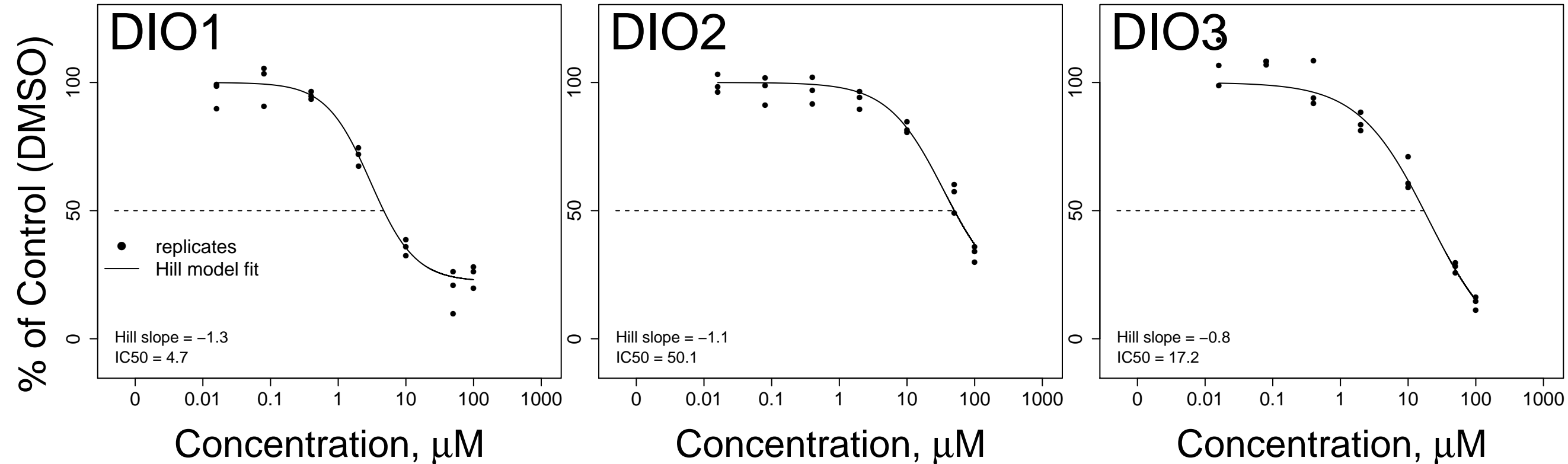




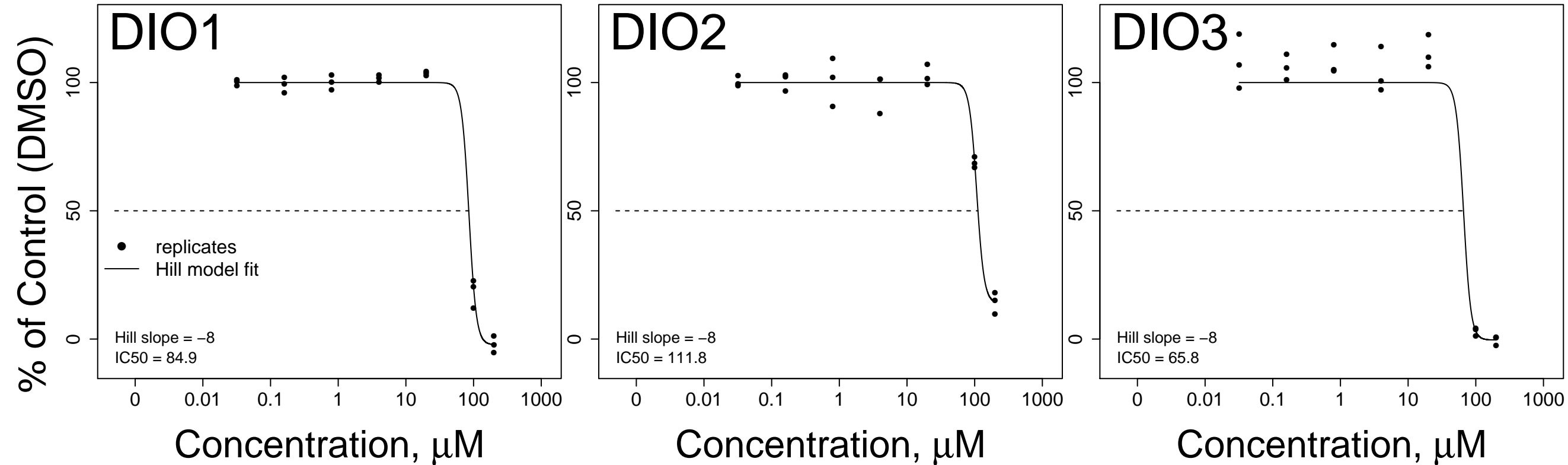
4-Hexylresorcinol CASRN: 136-77-6



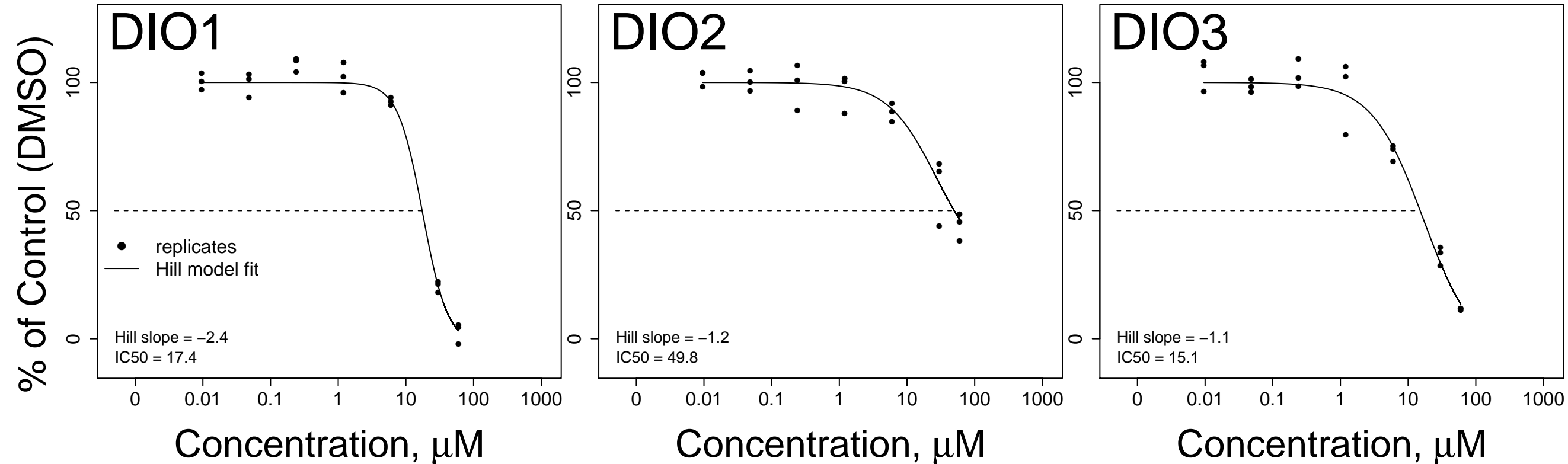
Darbufelone mesylate CASRN: 139340-56-0



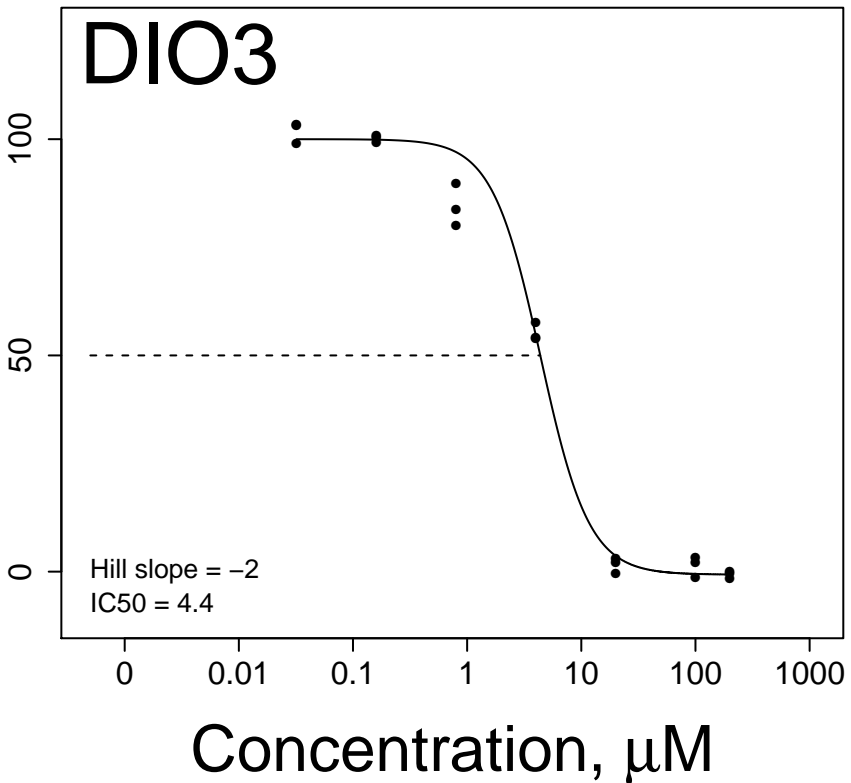
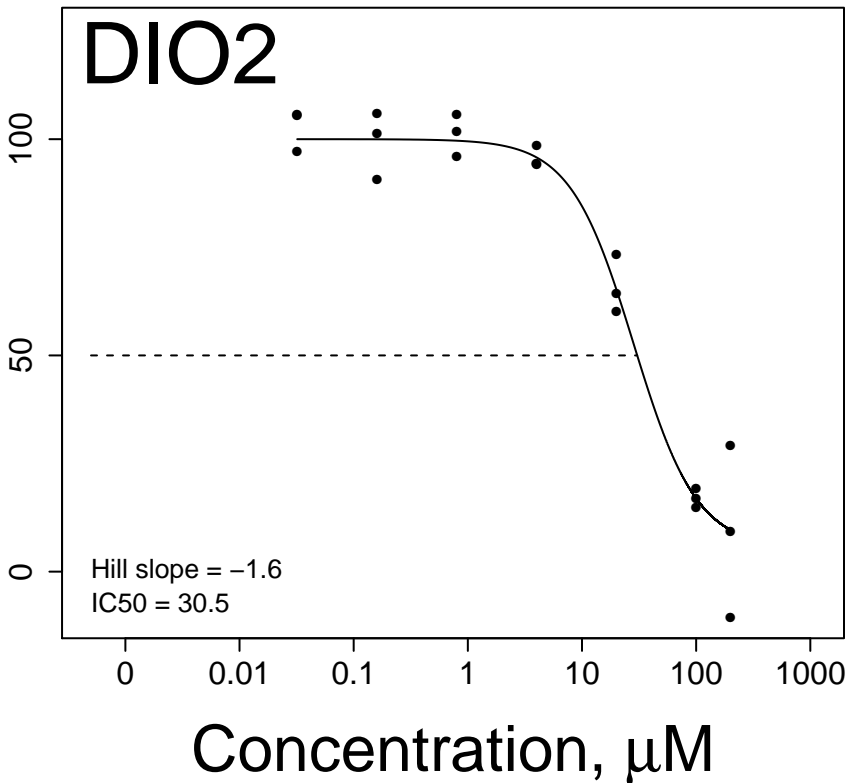
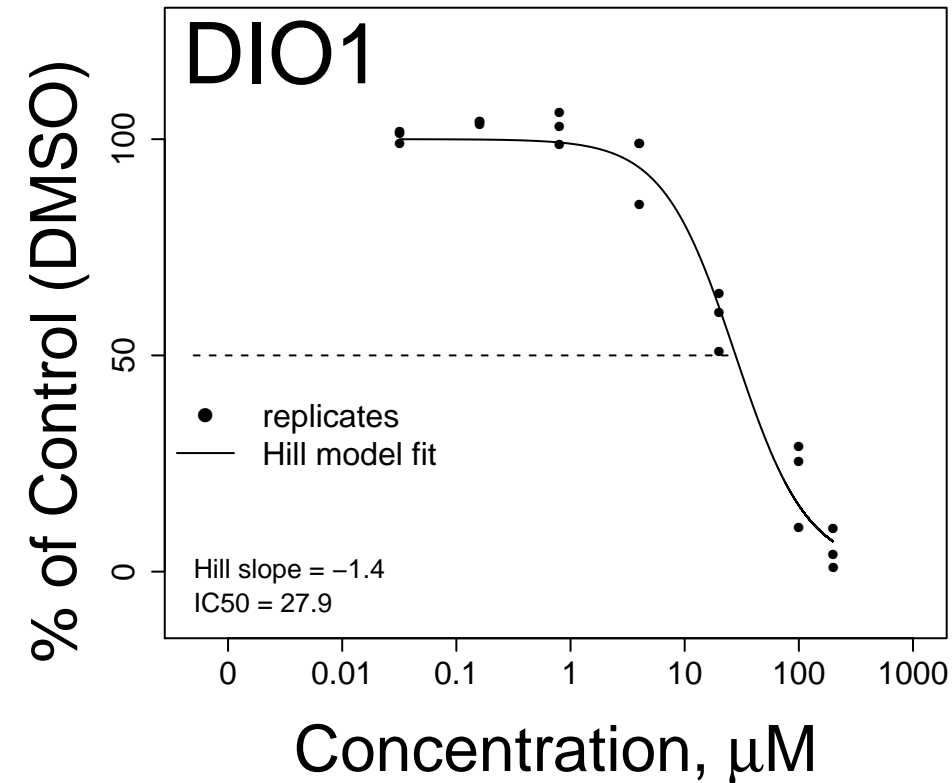
4-(1,1,3,3-Tetramethylbutyl)phenol CASRN: 140-66-9



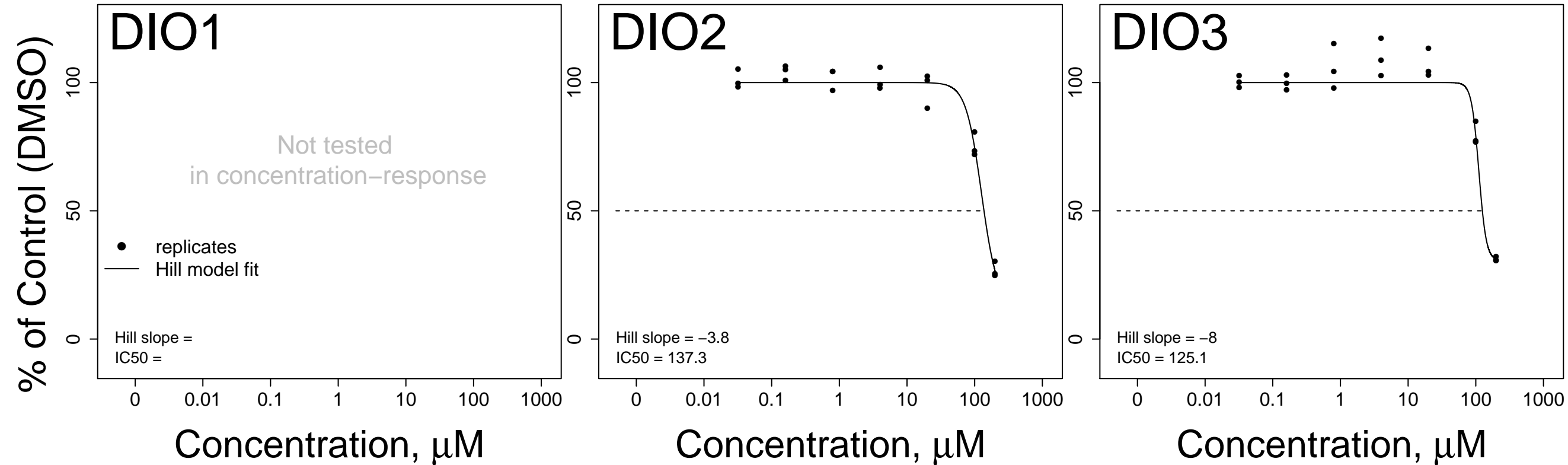
Tannic acid CASRN: 1401-55-4



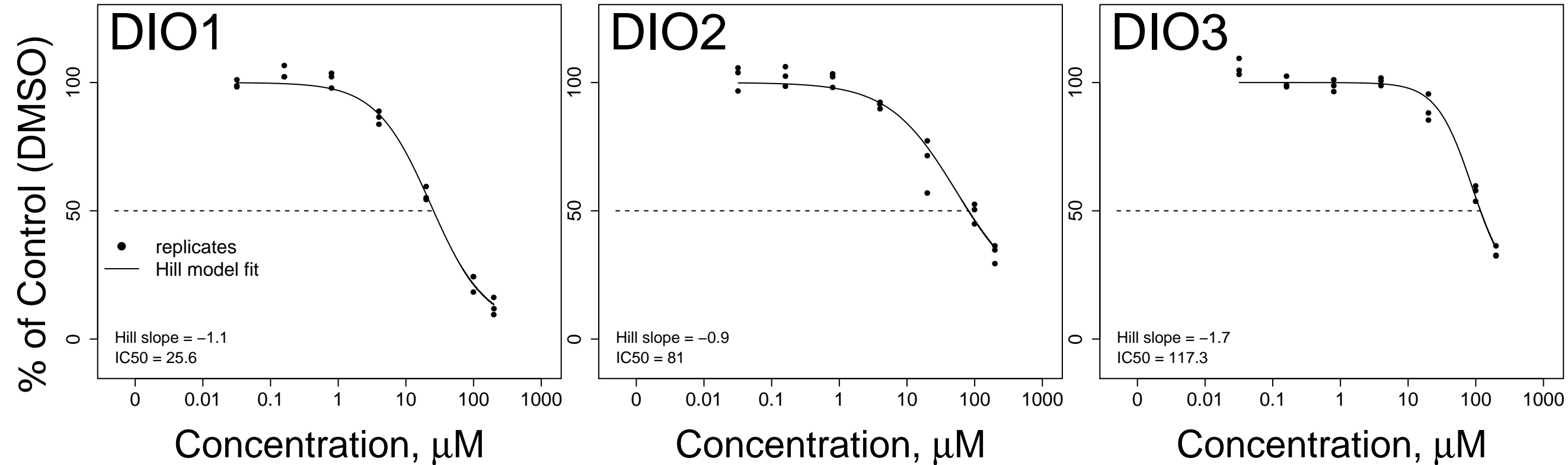
Kepone CASRN: 143-50-0



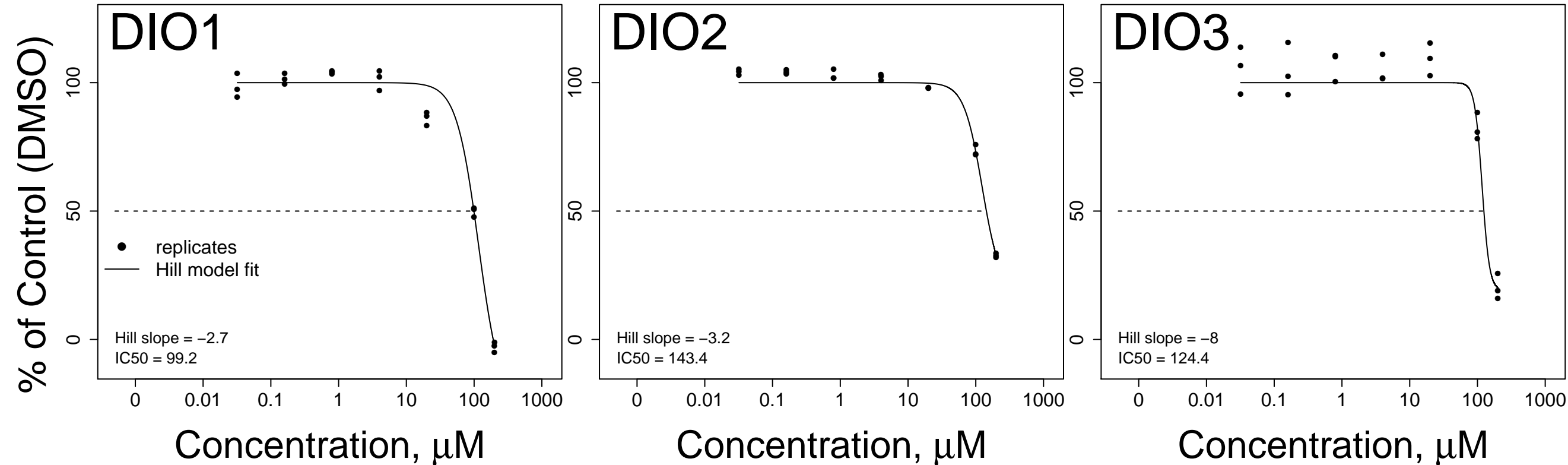
Bisphenol AF CASRN: 1478-61-1



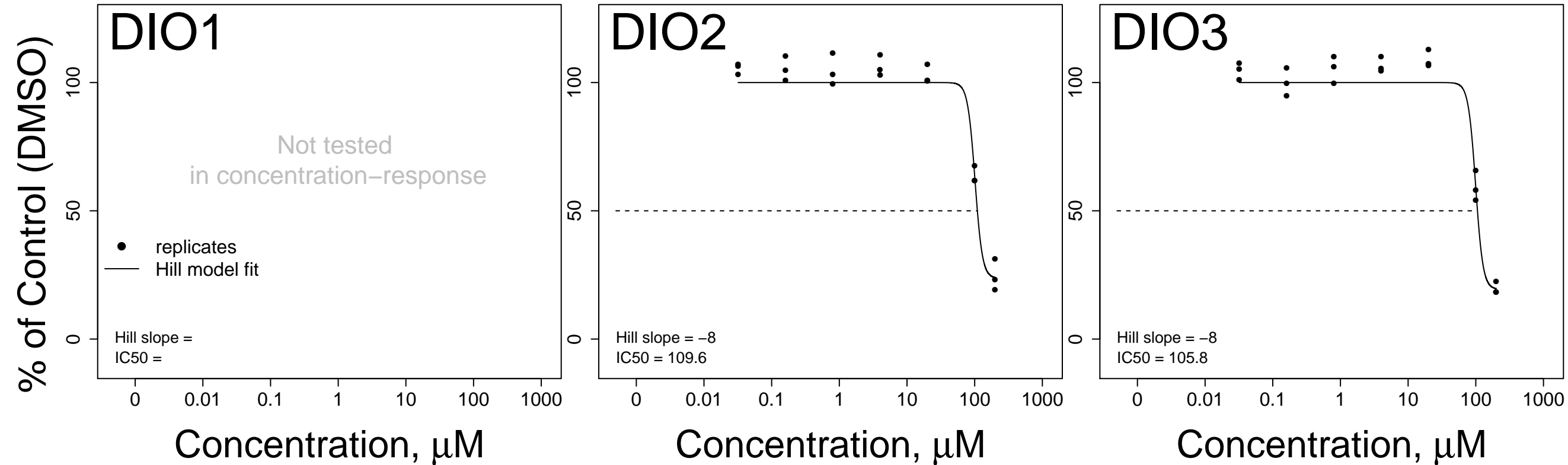
2-Mercaptobenzothiazole CASRN: 149-30-4



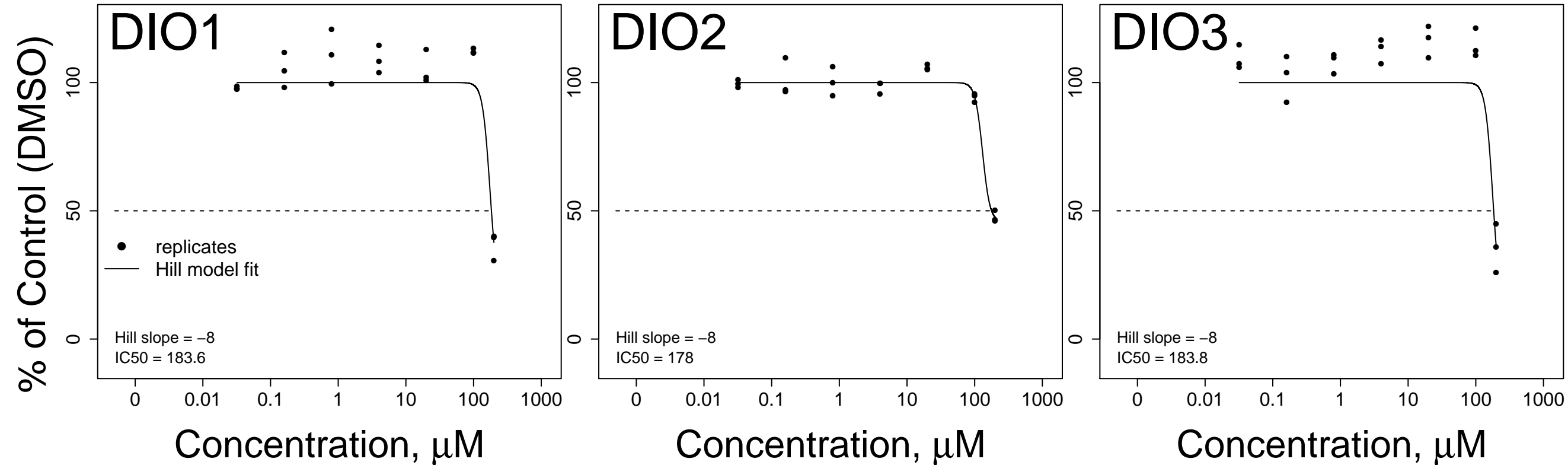
FR150011 CASRN: 149413-74-1



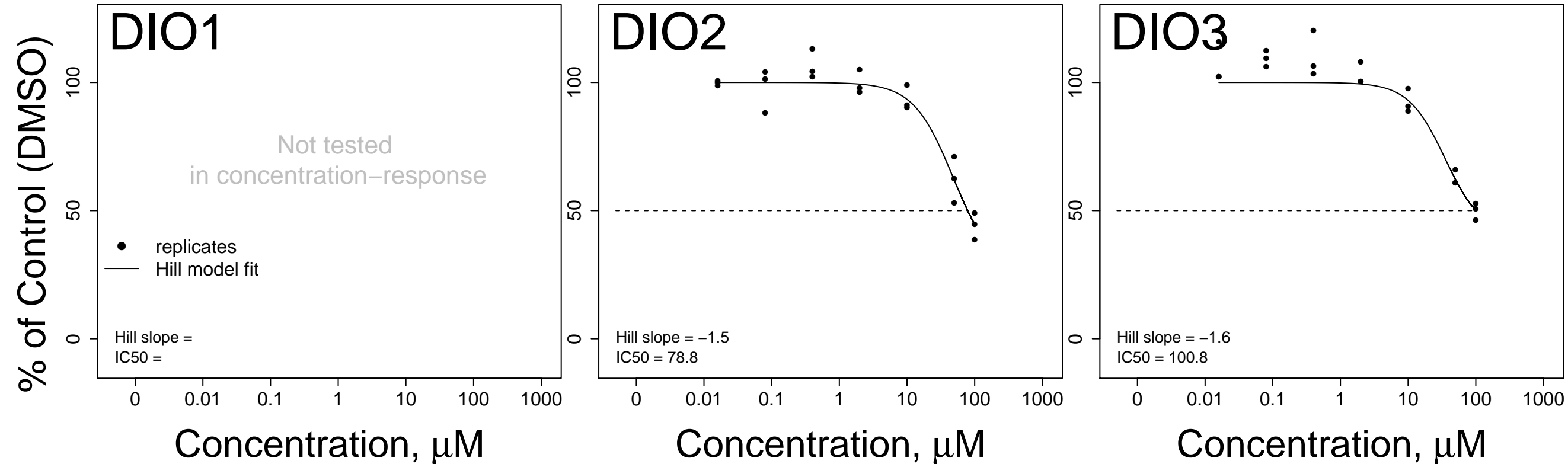
Sodium dodecyl sulfate CASRN: 151-21-3



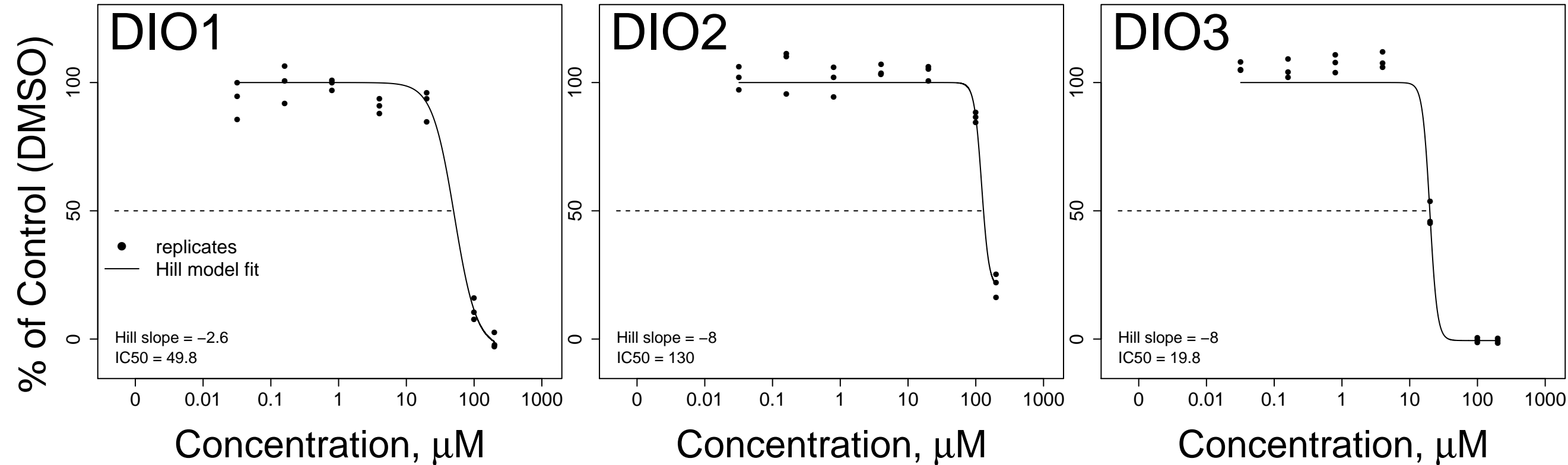
Celecoxib CASRN: 169590-42-5



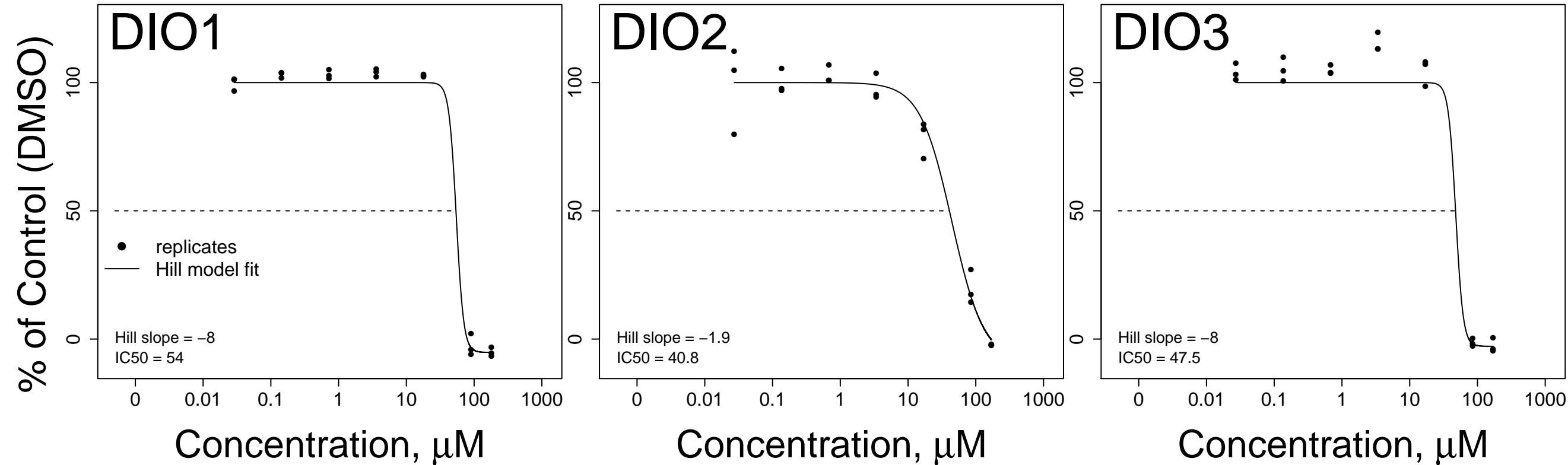
CJ-013790 CASRN: 179465-71-5



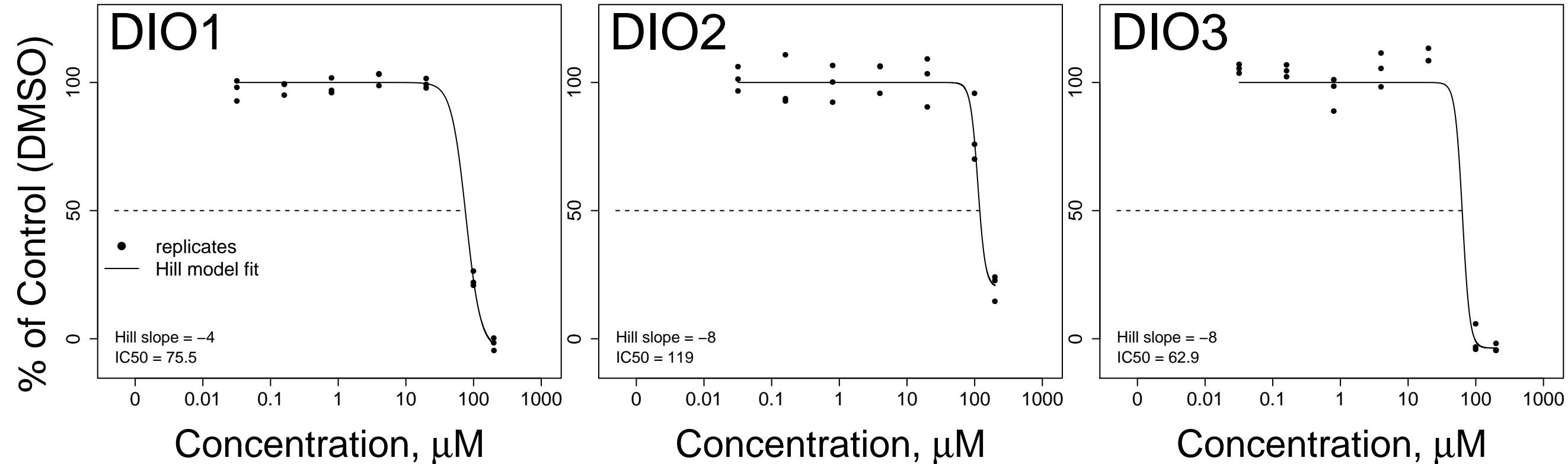
4-Octylphenol CASRN: 1806-26-4



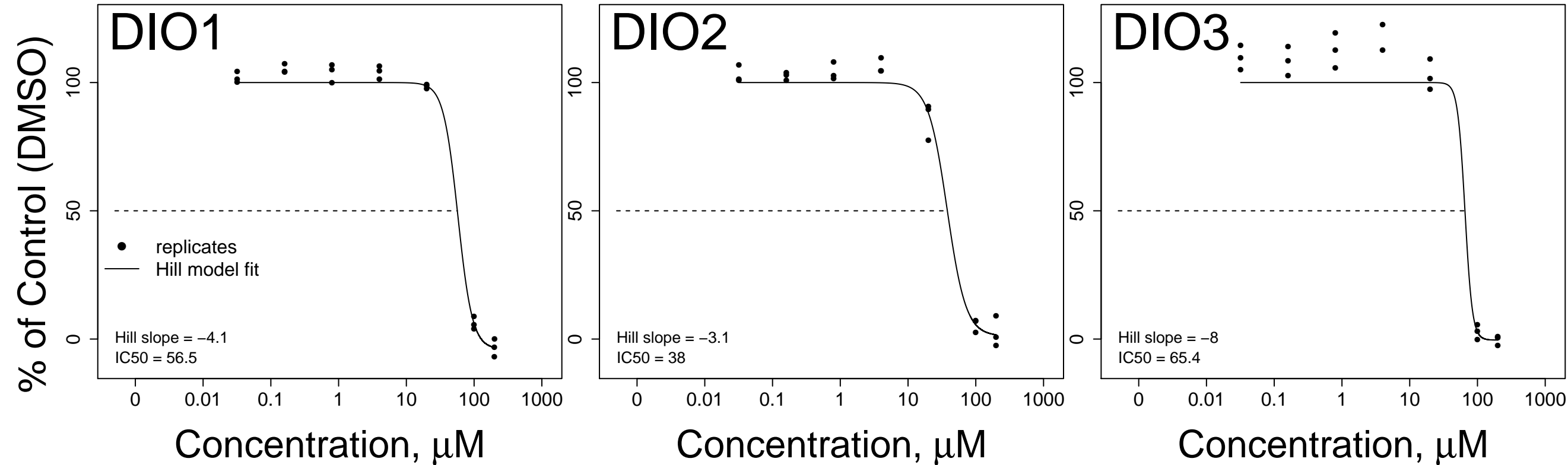
Farglitazar CASRN: 196808-45-4



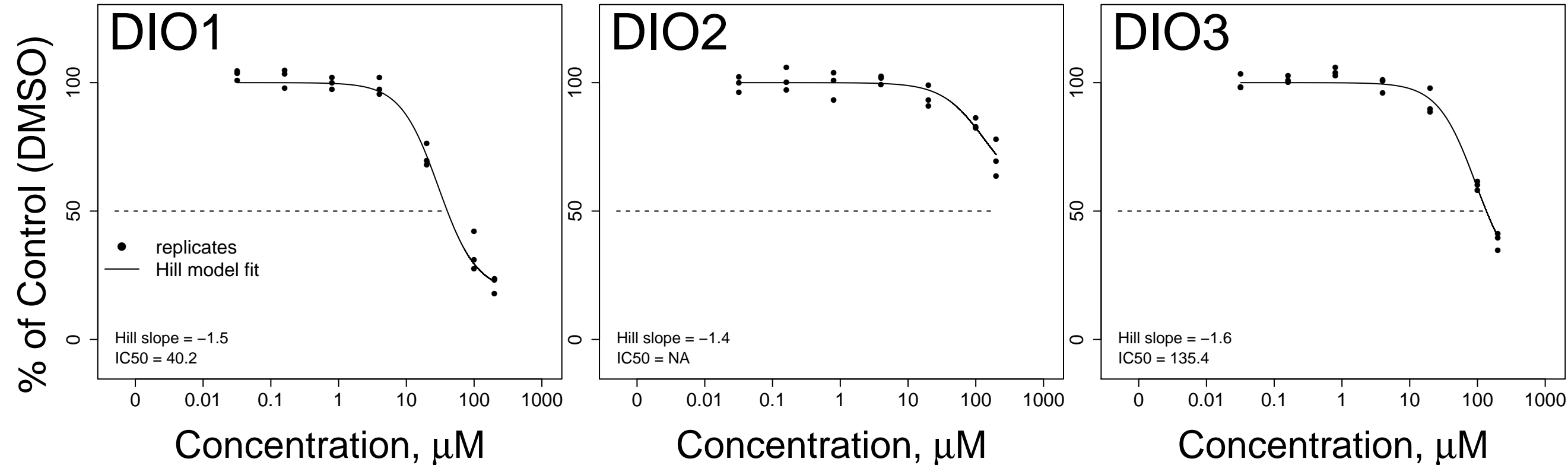
4-Heptylphenol CASRN: 1987-50-4



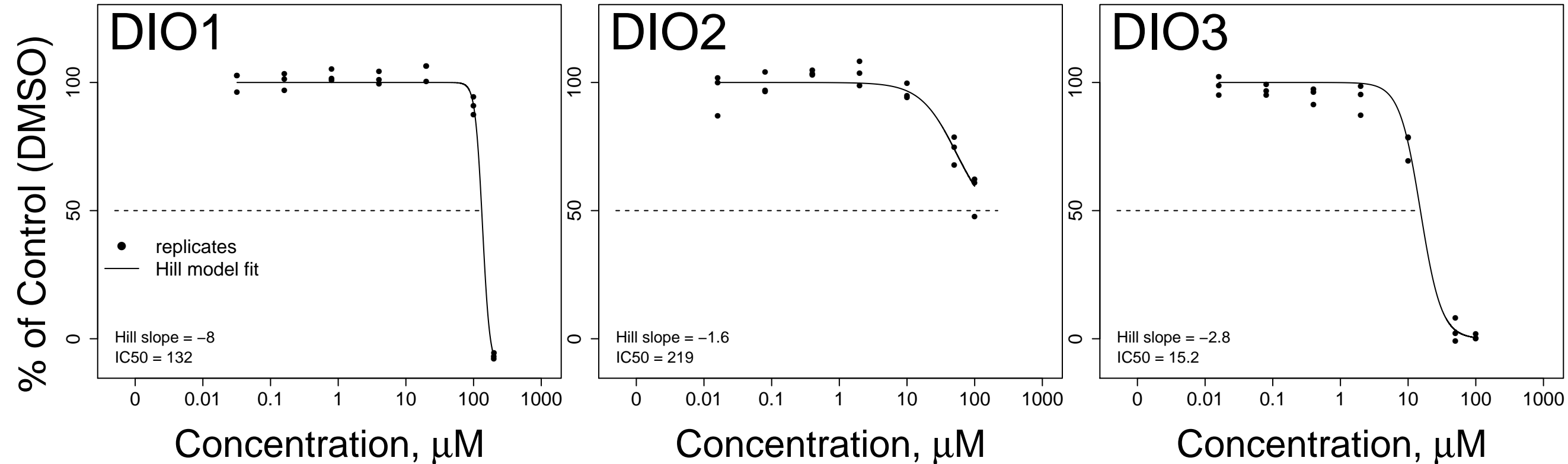
UK-337312 CASRN: 203942-49-8



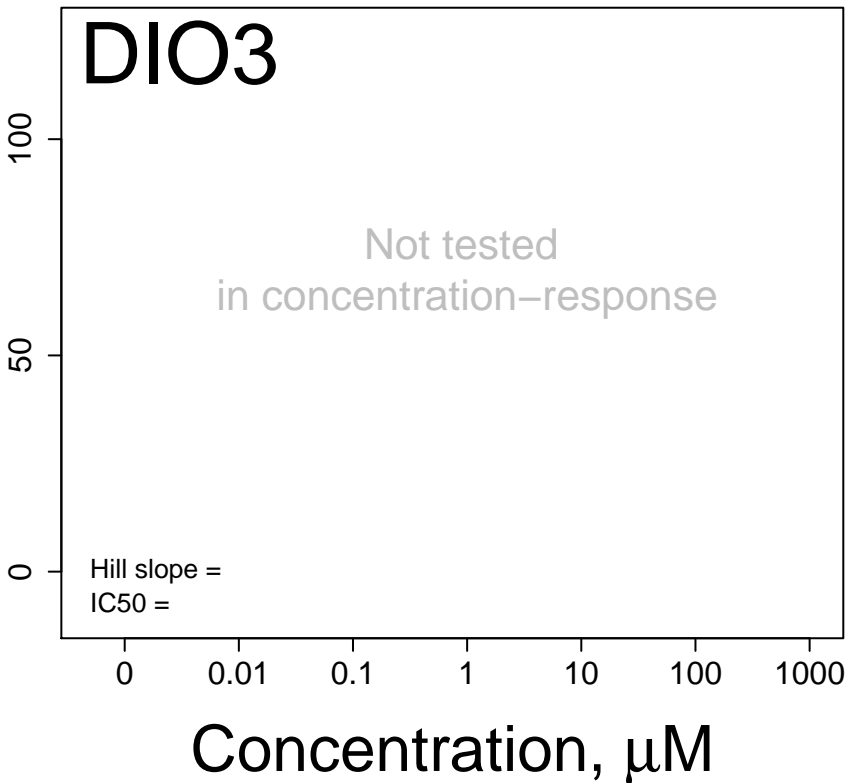
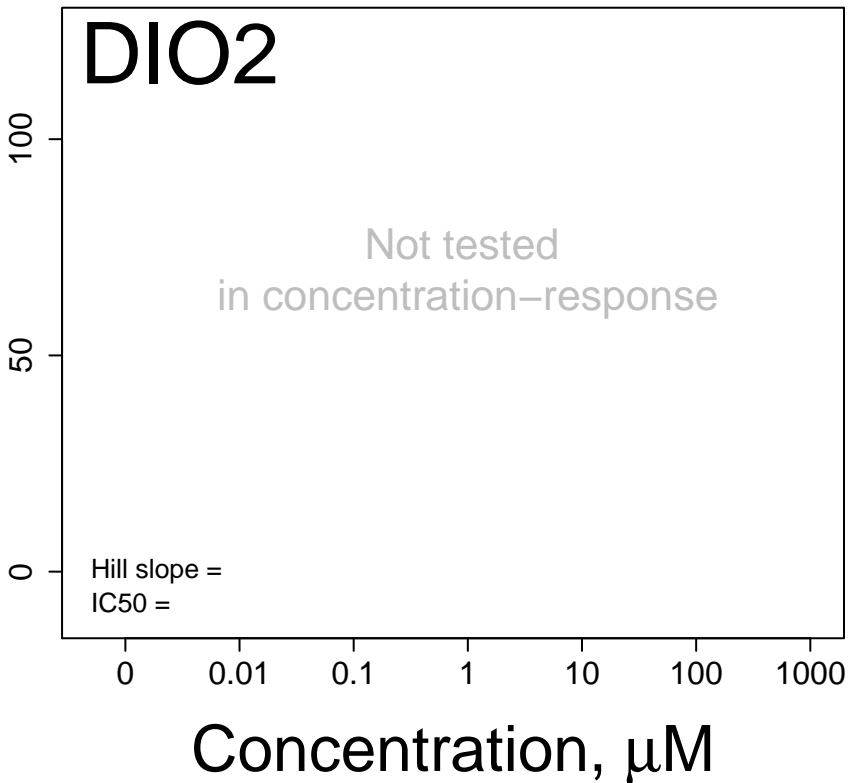
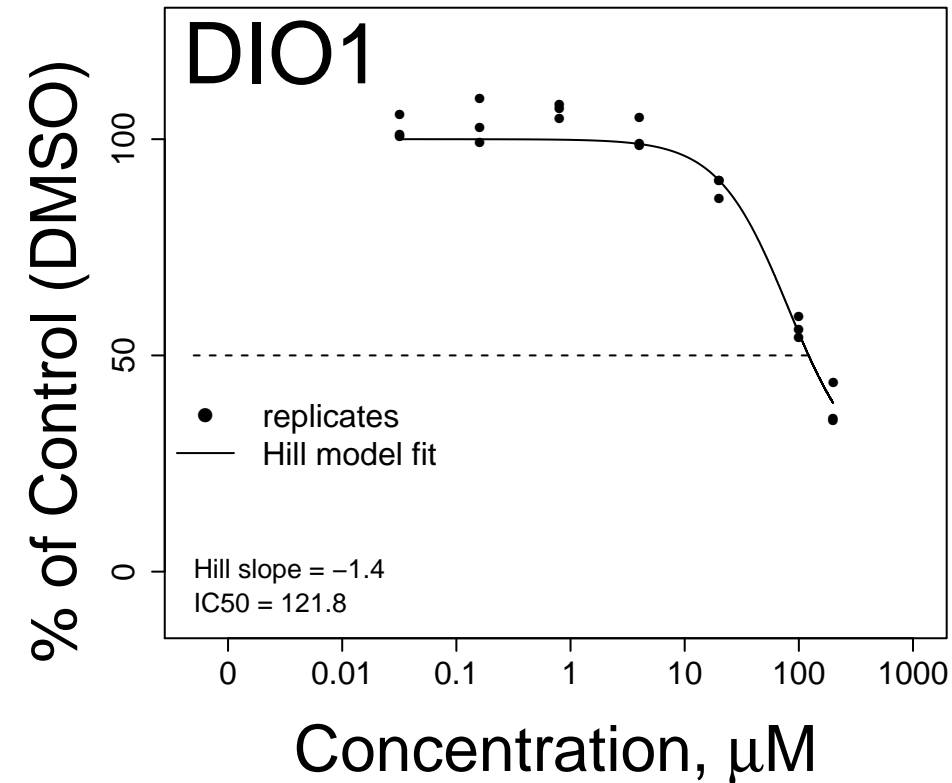
Oxytetracycline hydrochloride CASRN: 2058-46-0



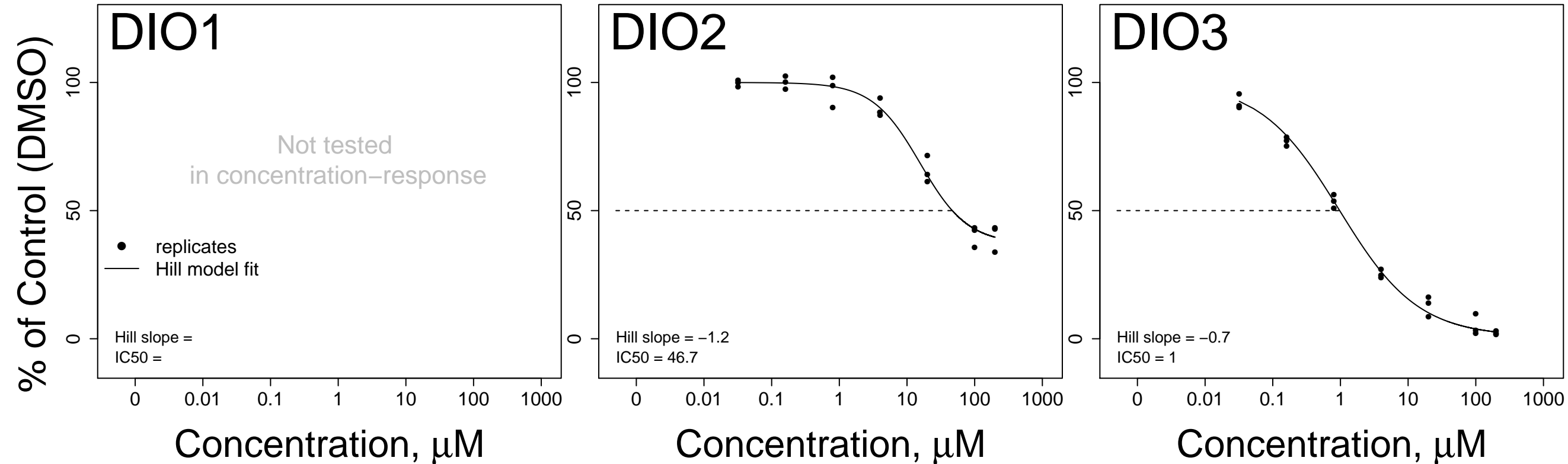
Perfluoroundecanoic acid CASRN: 2058-94-8



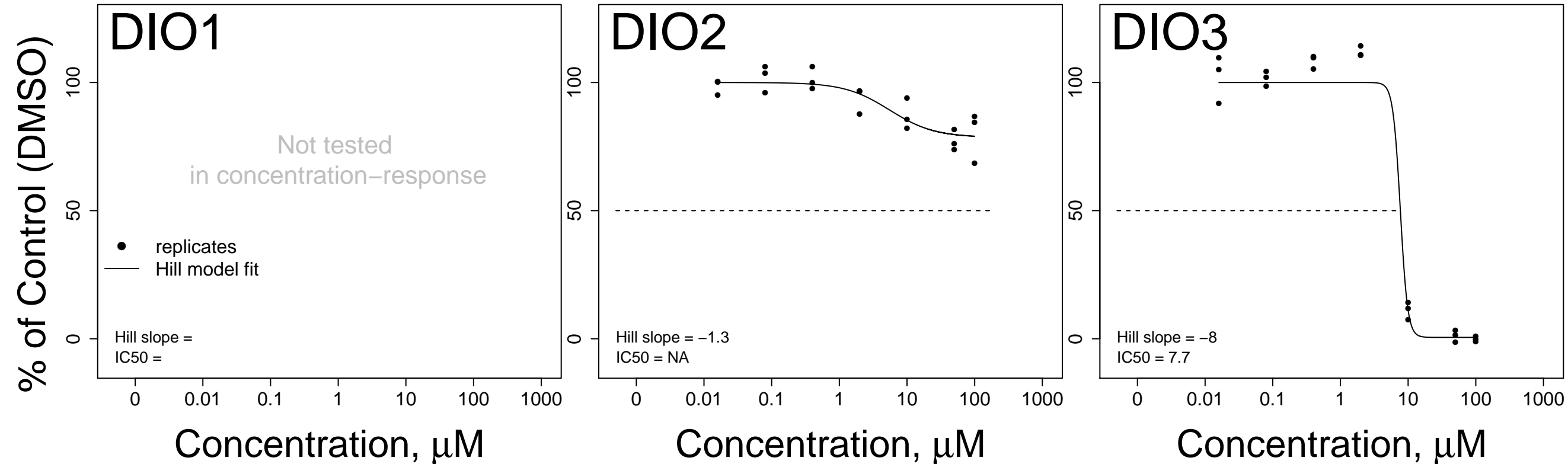
CI-1029 CASRN: 207736-05-8



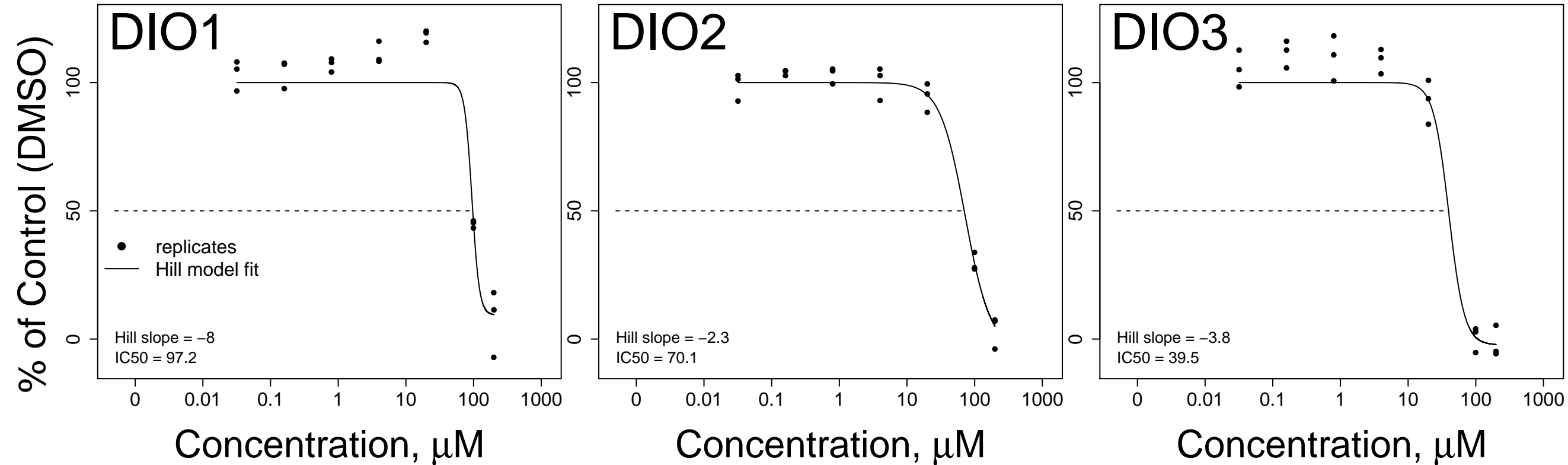
Pentachloropyridine CASRN: 2176-62-7



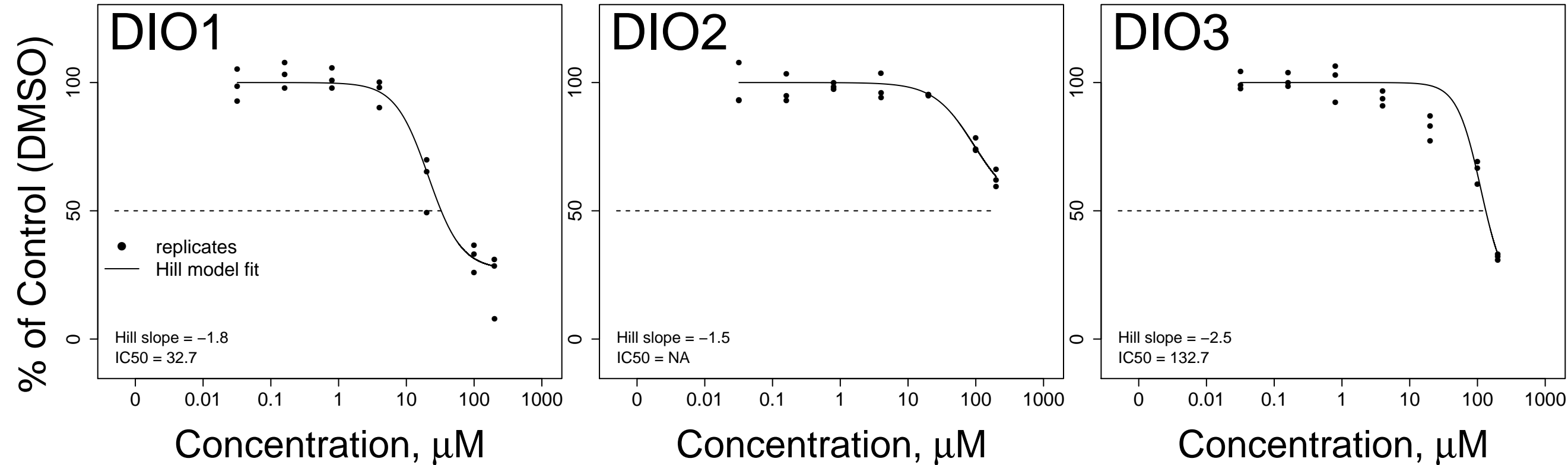
SR146131 trifluoroacetate (1:1) CASRN: 221671-62-1



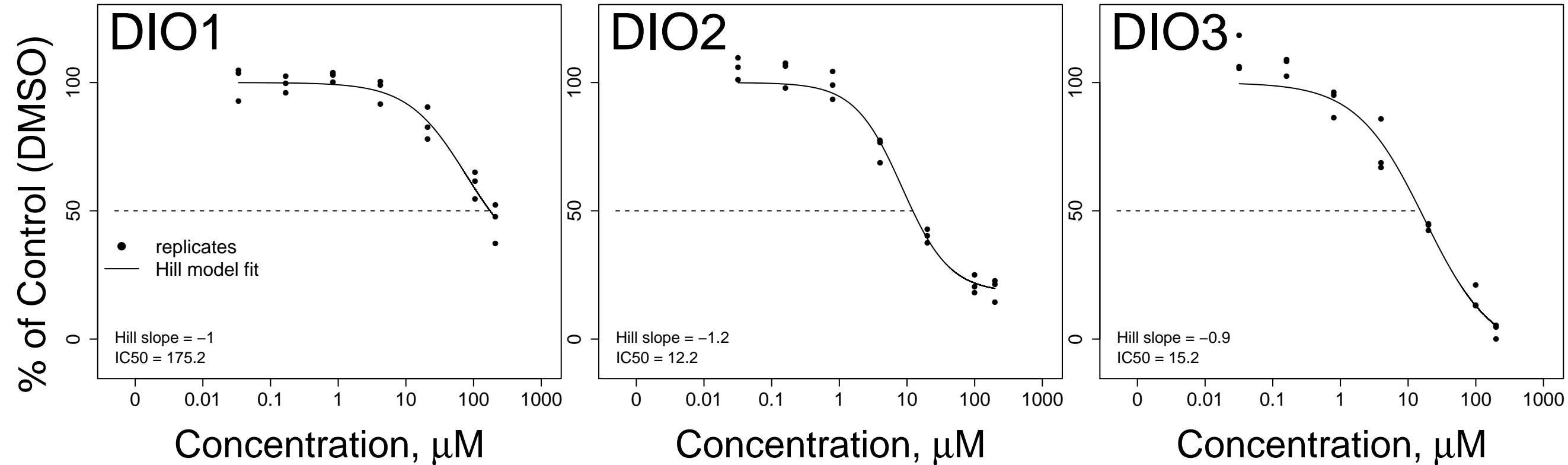
Sodium dodecylbenzenesulfonate CASRN: 25155-30-0



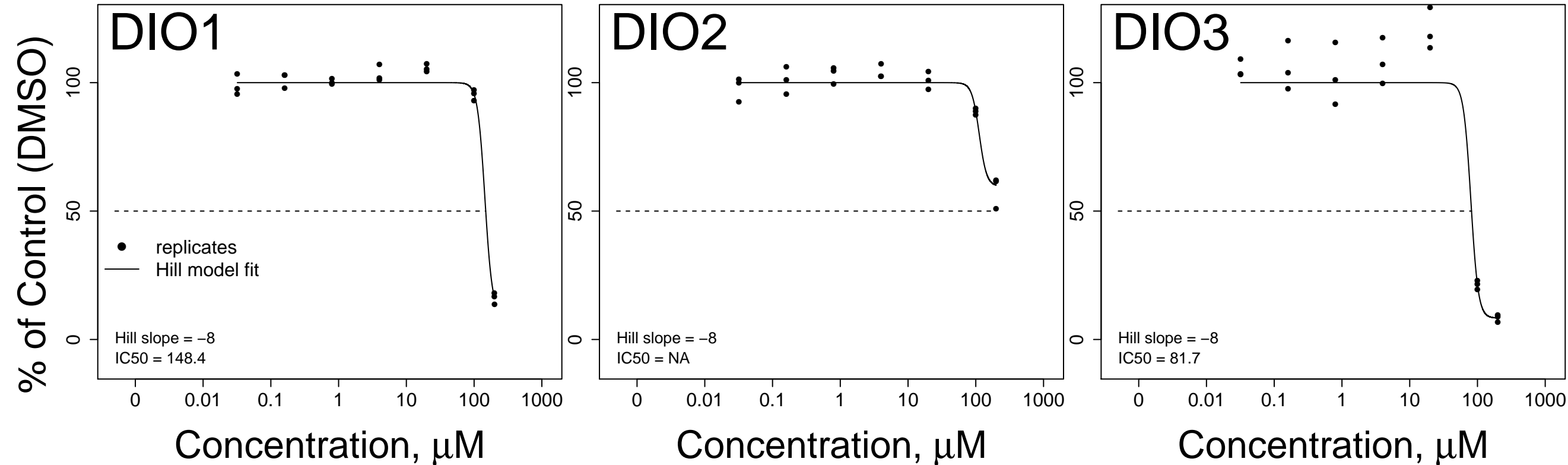
HMR1426 CASRN: 262376-75-0



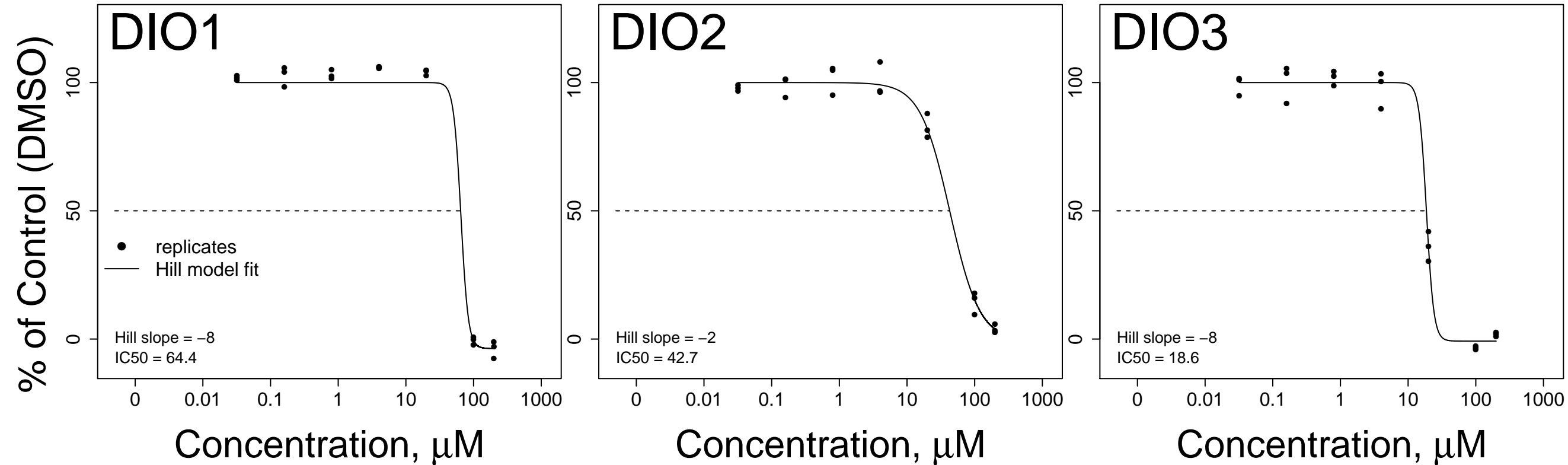
Octhilinone CASRN: 26530-20-1



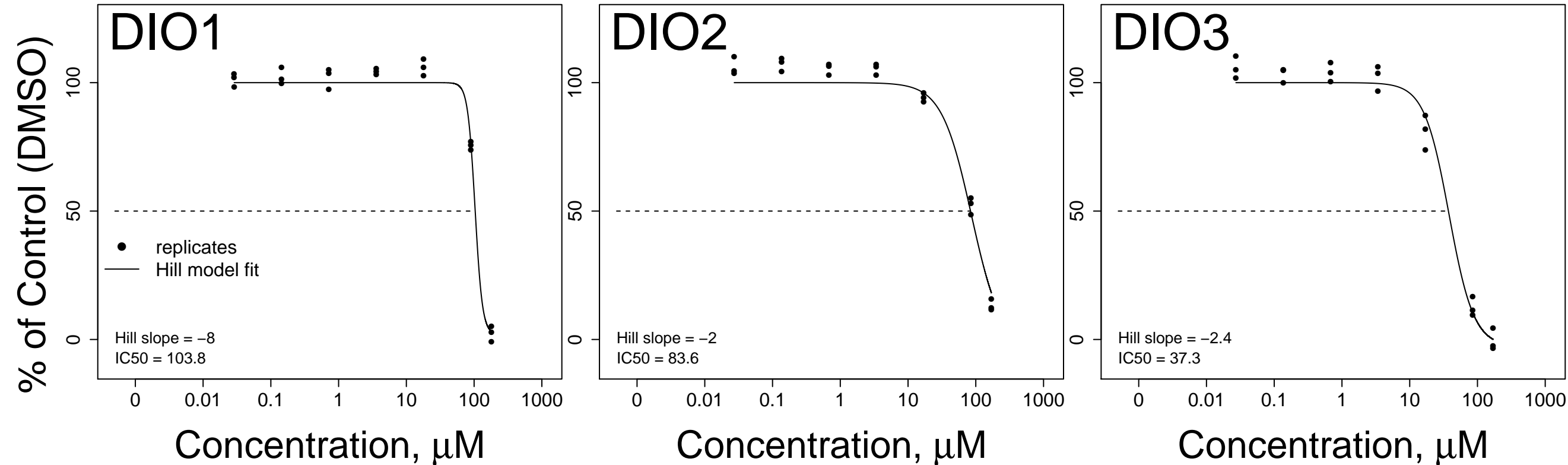
1-Dodecyl-2-pyrrolidinone CASRN: 2687-96-9



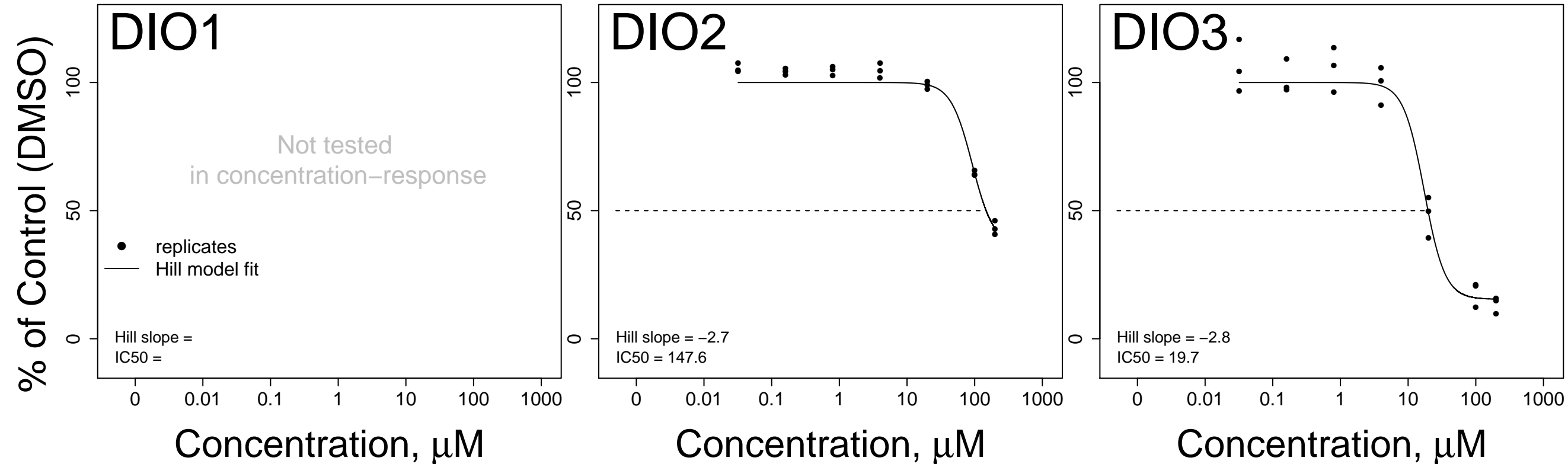
Dodecylbenzenesulfonic acid CASRN: 27176-87-0



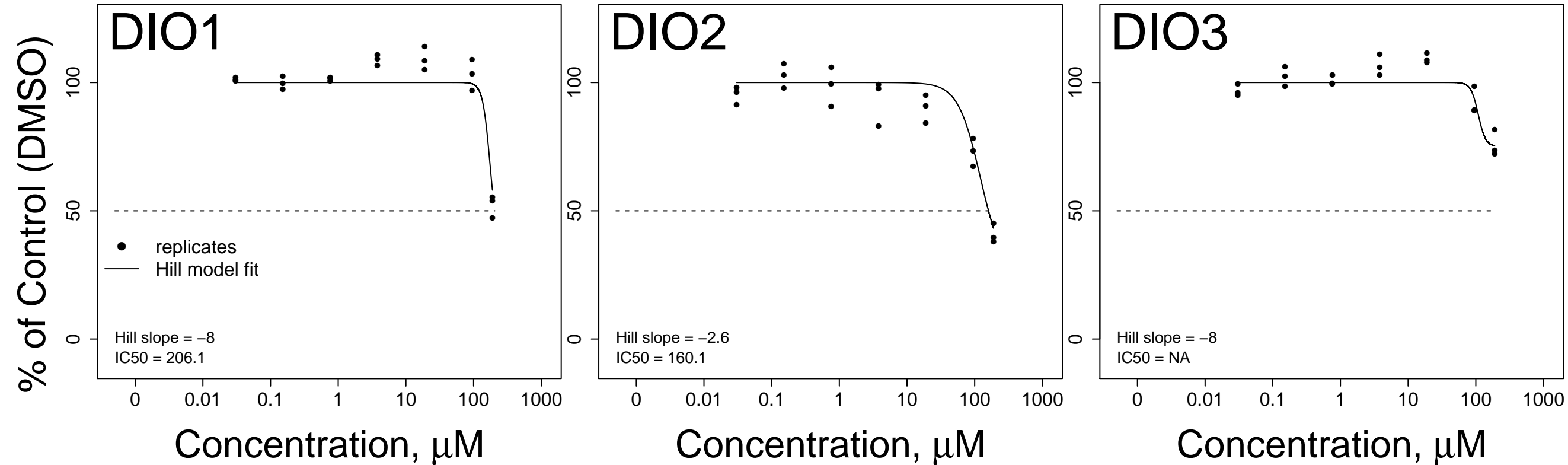
Dodecylbenzene sulfonate triethanolamine(1:1) CASRN: 27323-41-7



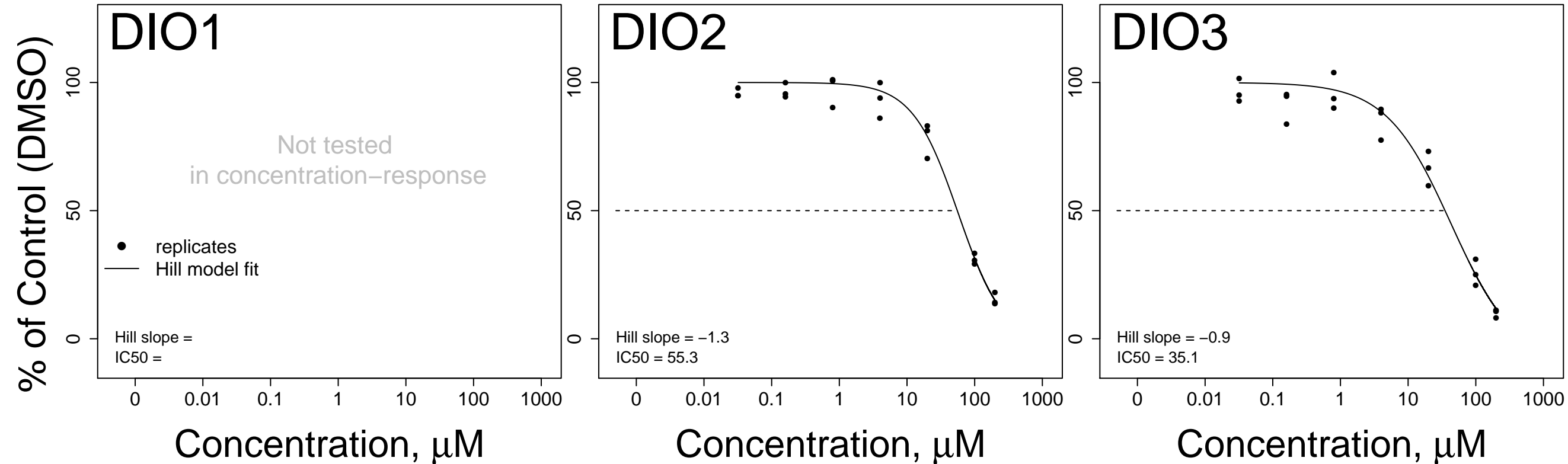
2,4-Bis(1-methyl-1-phenylethyl)phenol CASRN: 2772-45-4



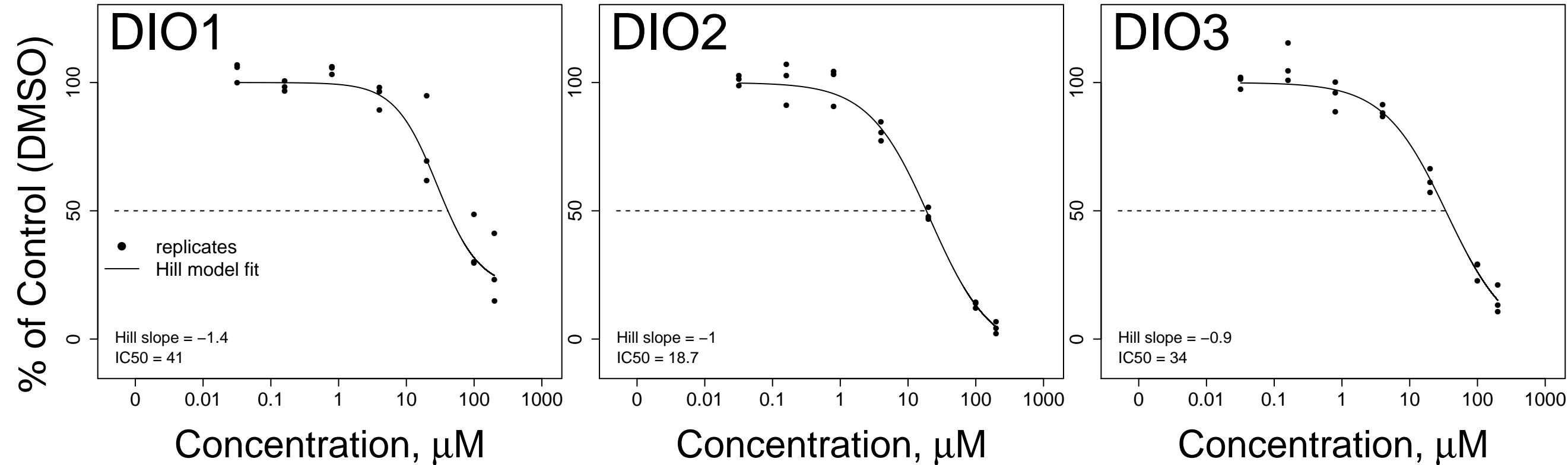
PFOS-K CASRN: 2795-39-3



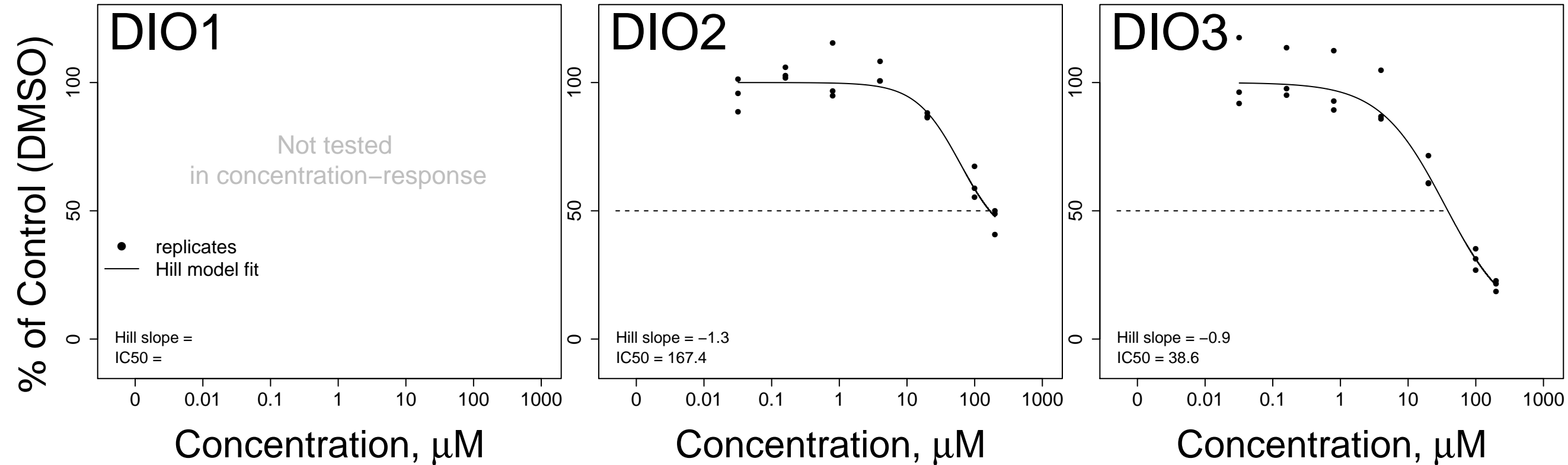
UK-373911 CASRN: 291305-06-1



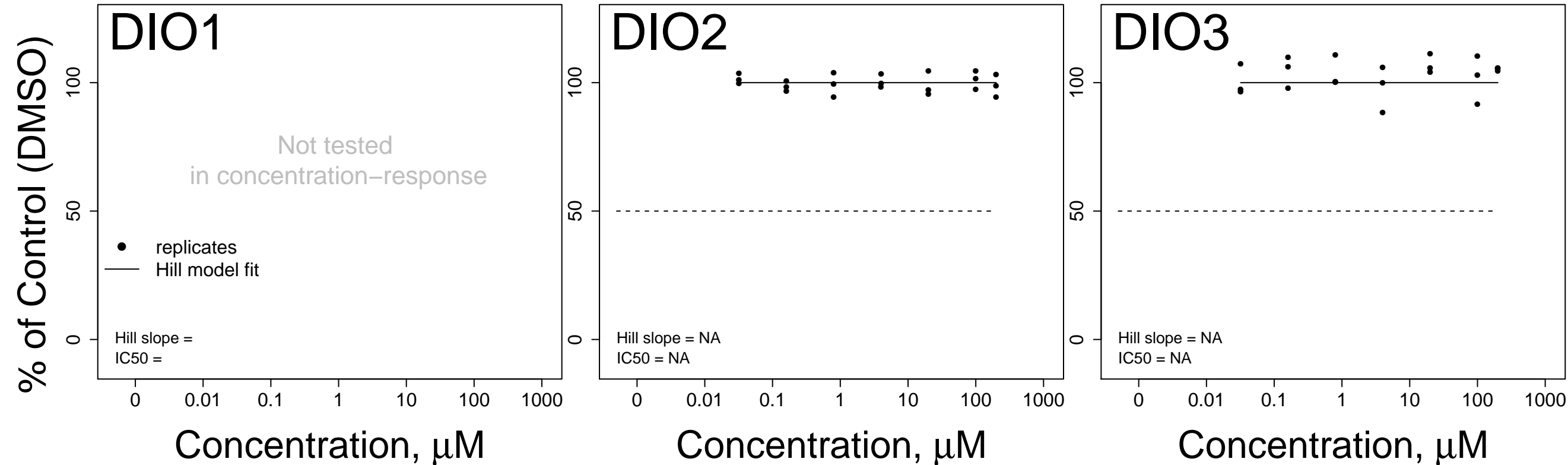
Isooctyl acrylate CASRN: 29590-42-9



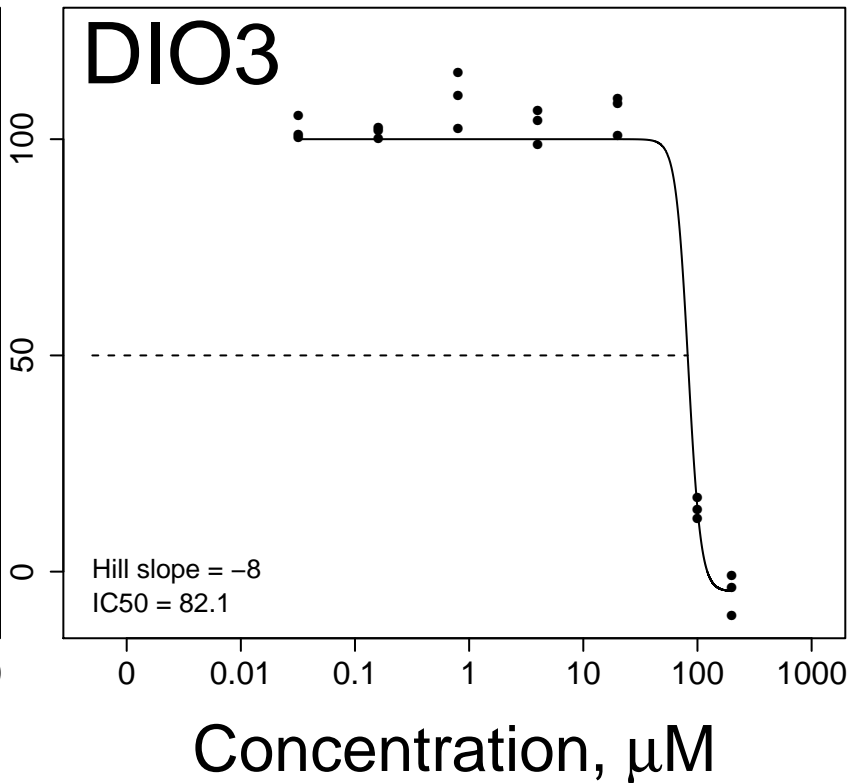
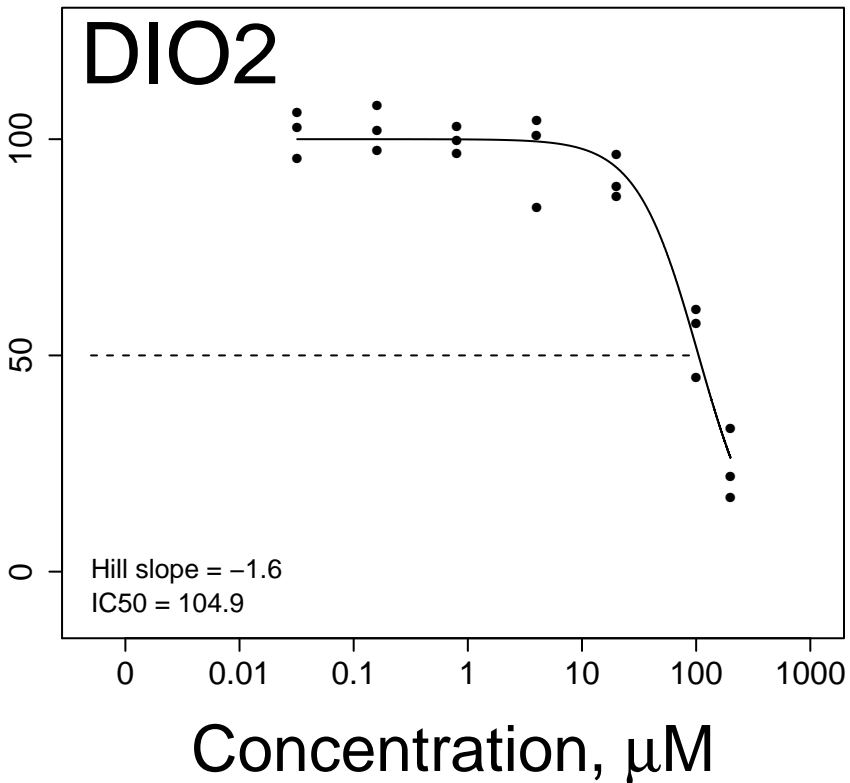
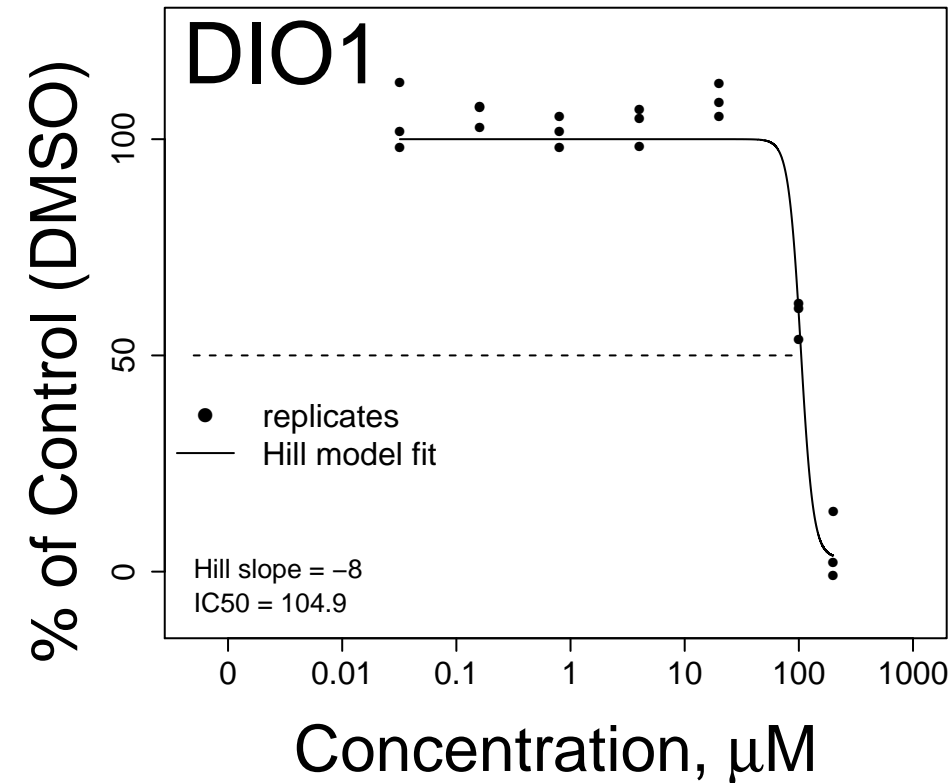
all-trans-Retinoic acid CASRN: 302-79-4



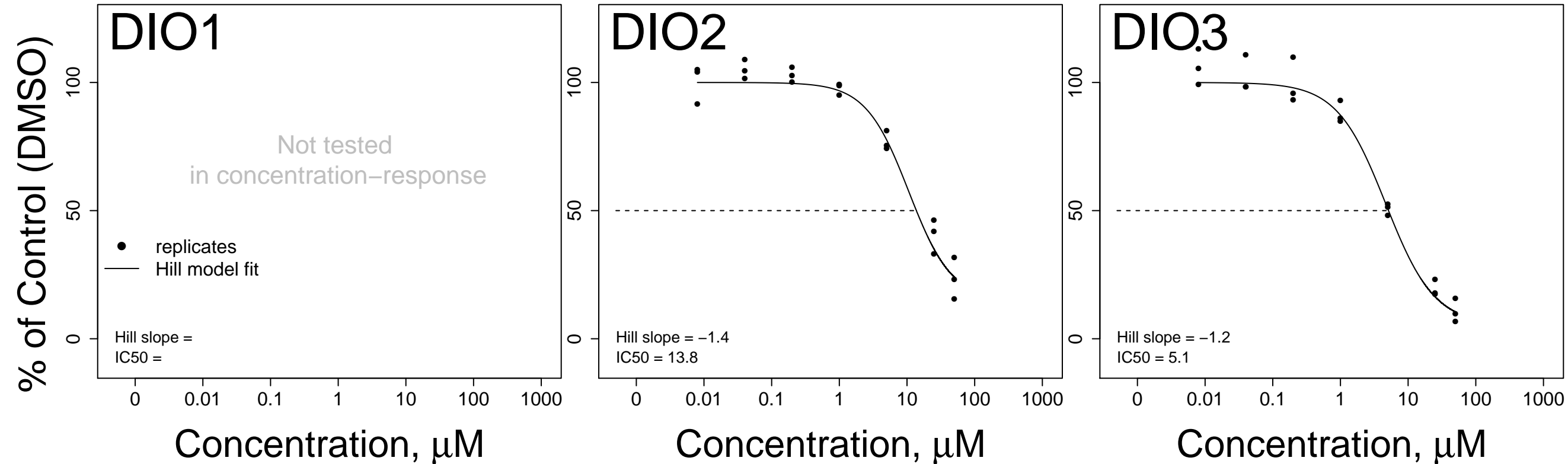
Procymidone CASRN: 32809-16-8



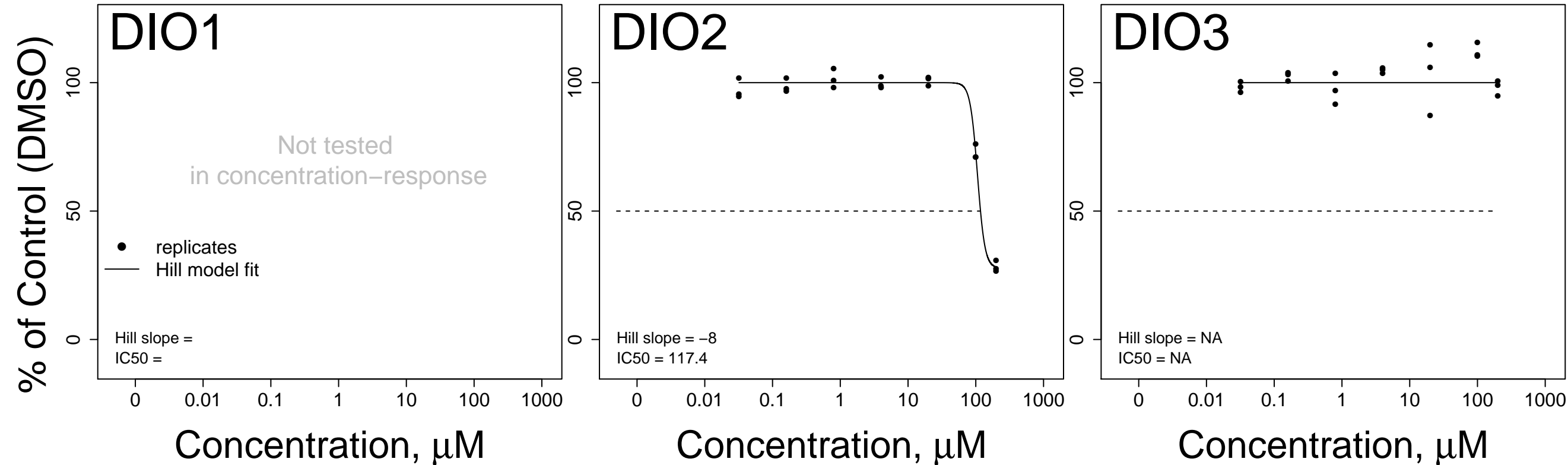
PFDA CASRN: 335-76-2



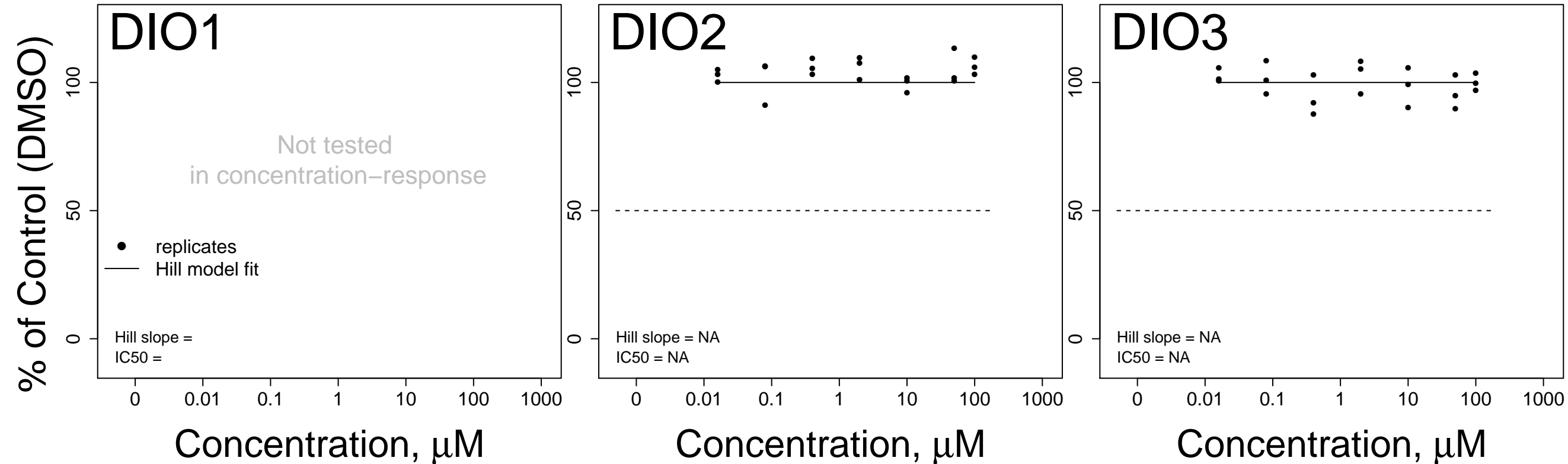
SSR69071 CASRN: 344930-95-6



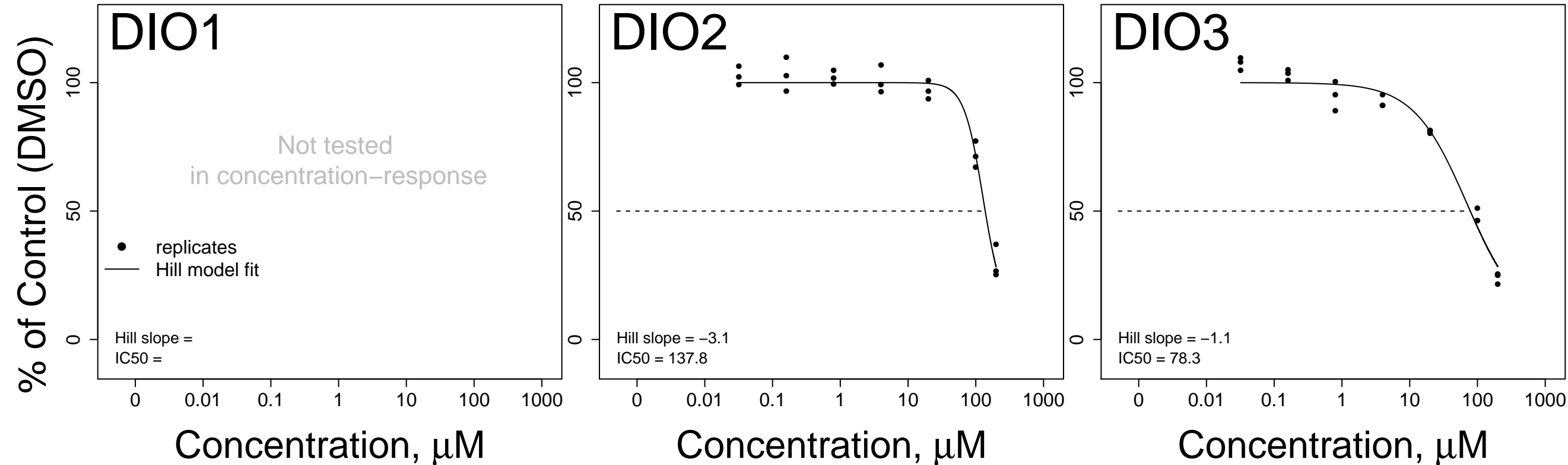
Elzasonan CASRN: 361343-19-3



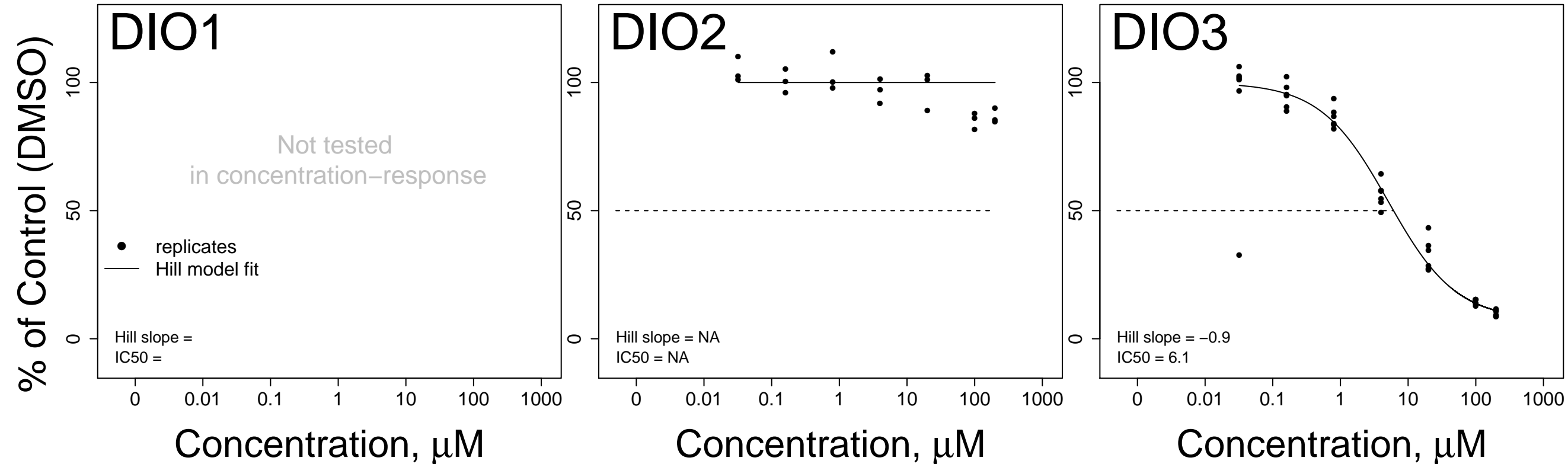
1-Hexadecanol CASRN: 36653-82-4



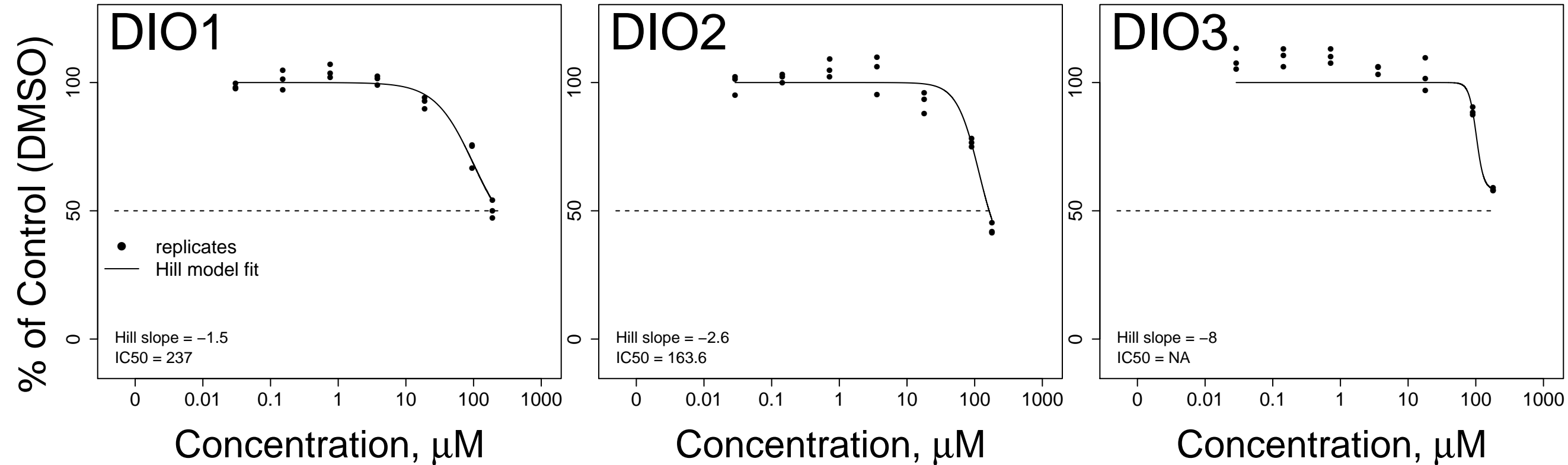
4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol] CASRN: 41481-66-7



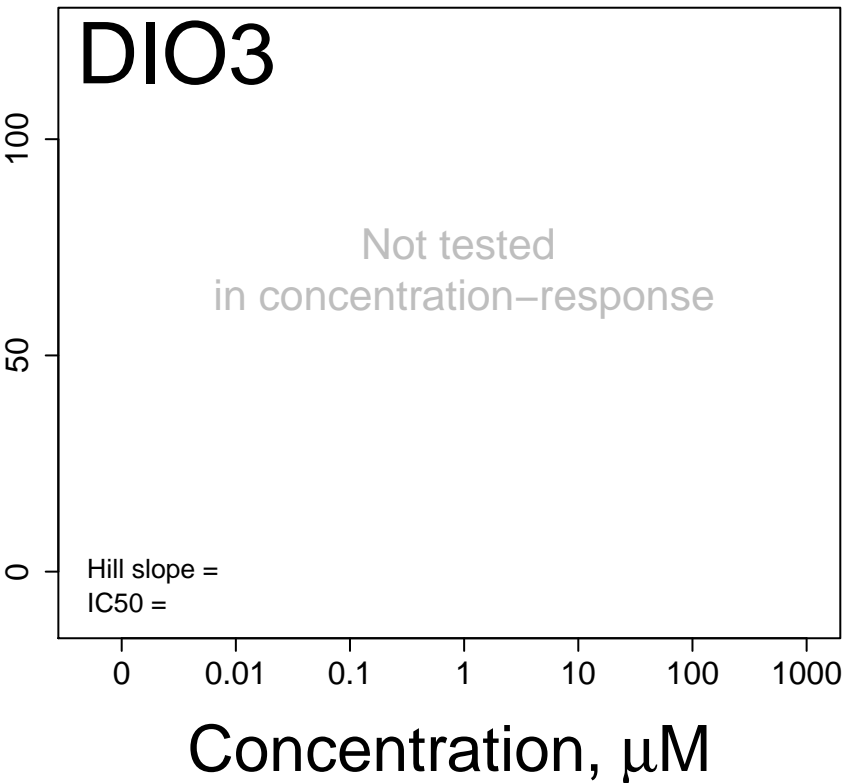
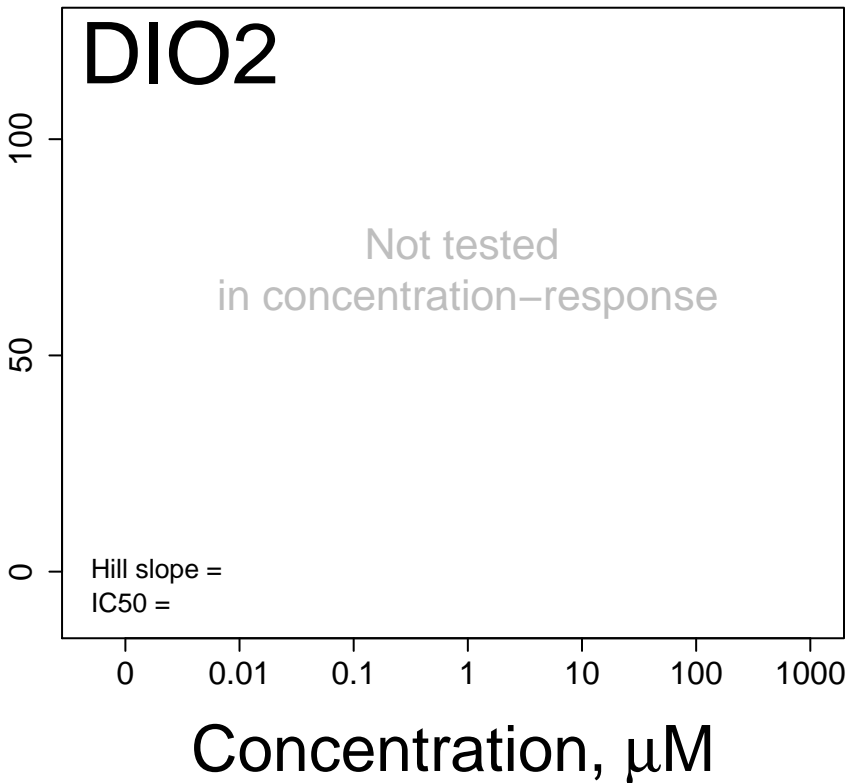
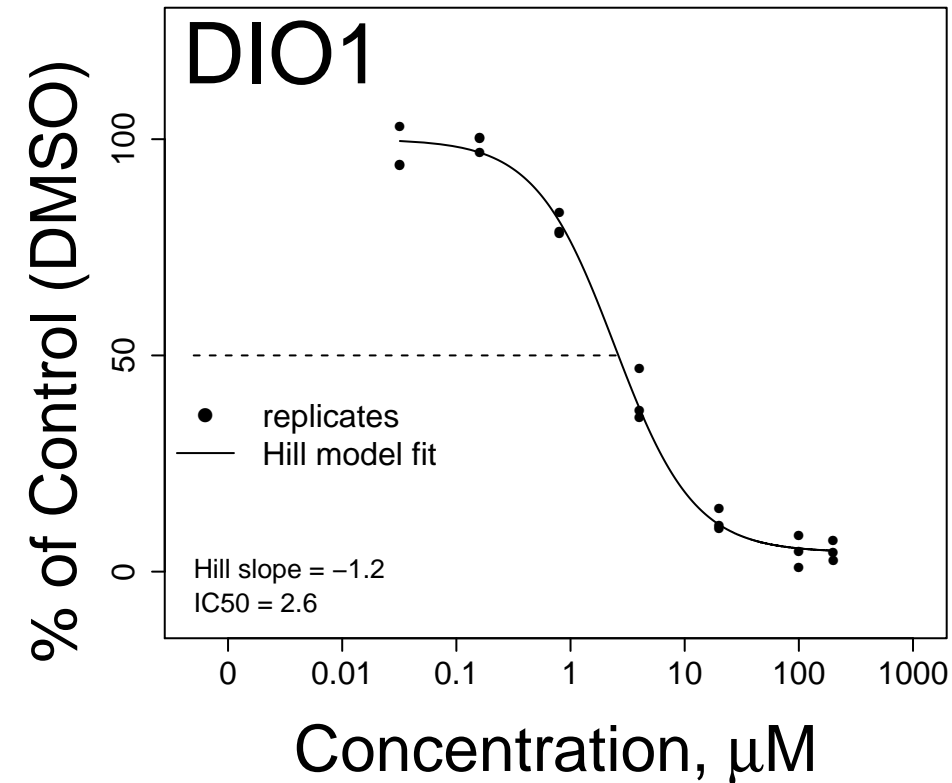
Cyproterone acetate CASRN: 427-51-0



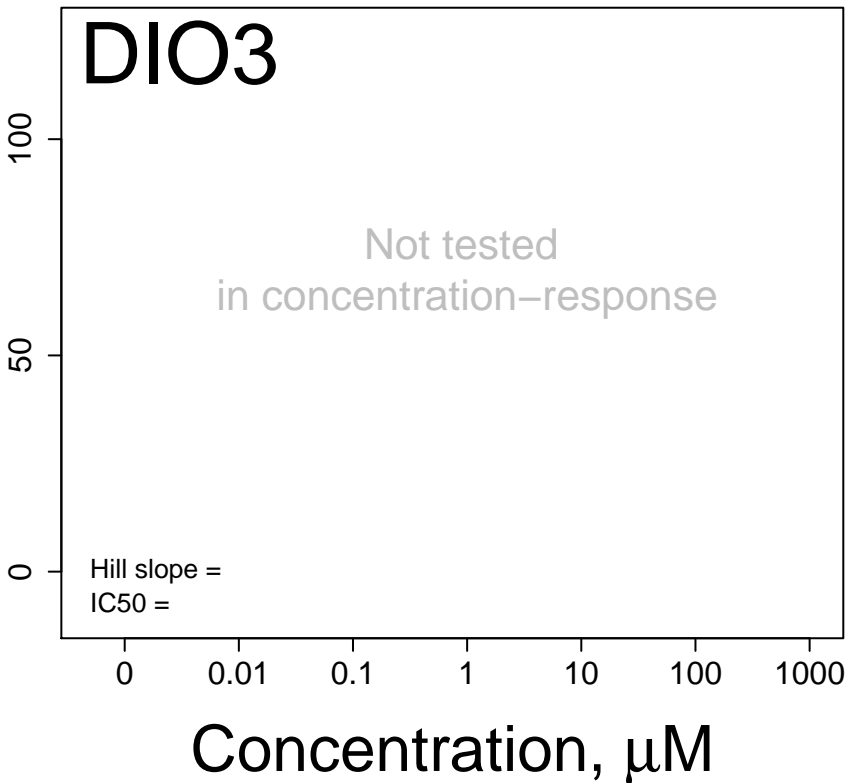
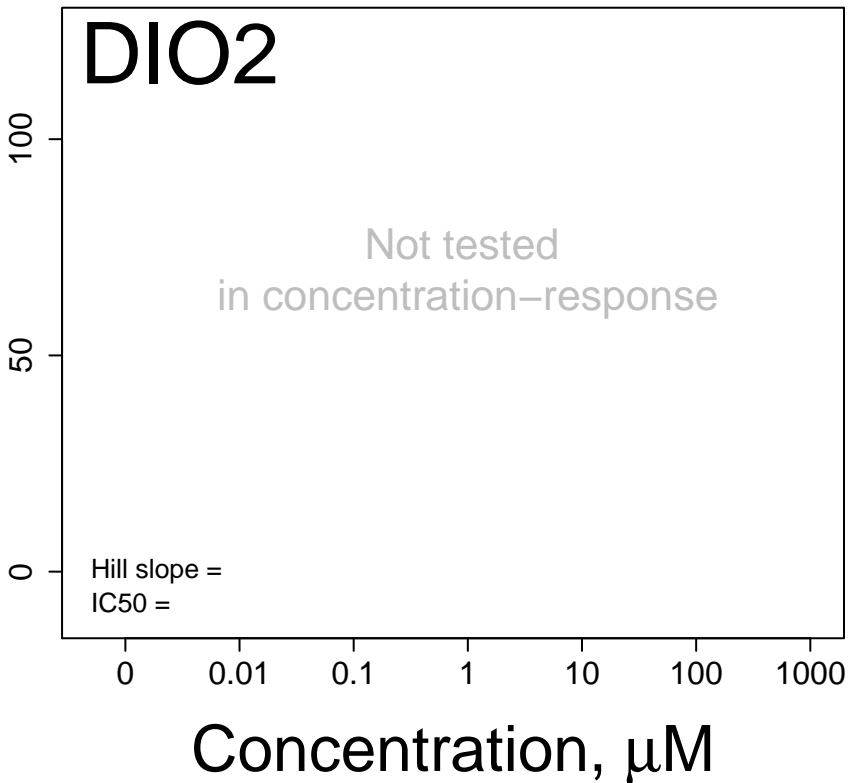
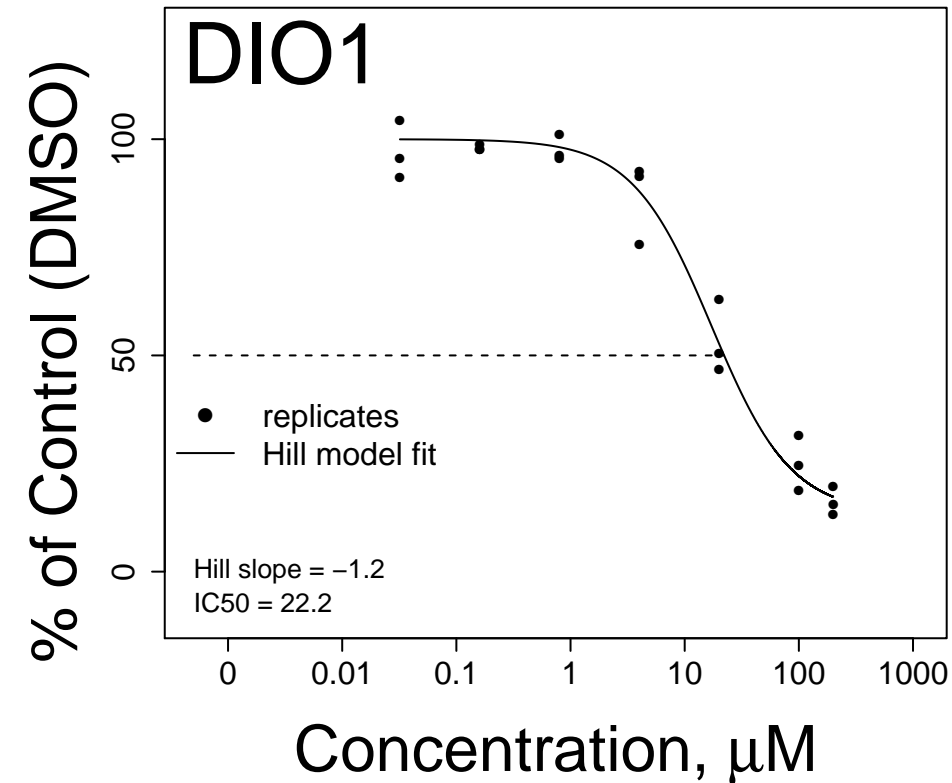
SAR 150640 CASRN: 433212-21-6



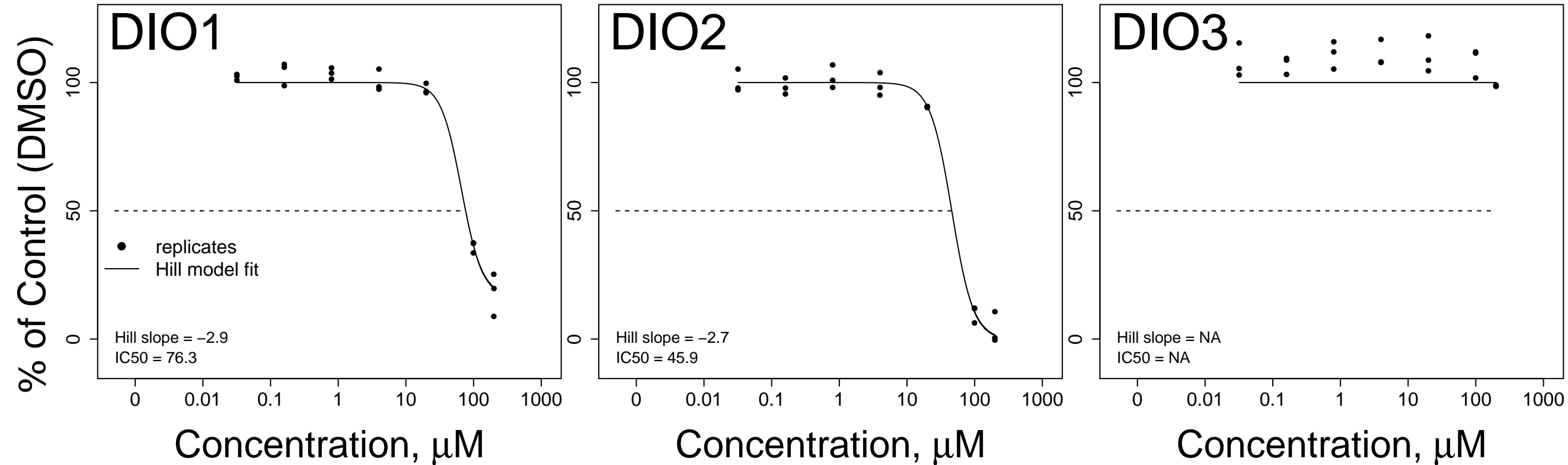
Genistein CASRN: 446-72-0



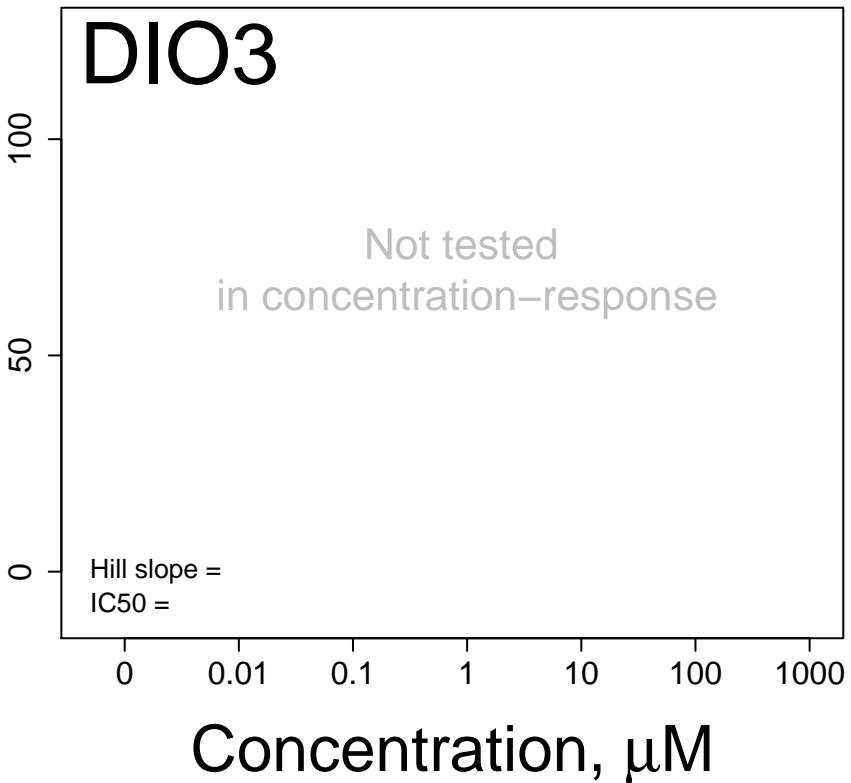
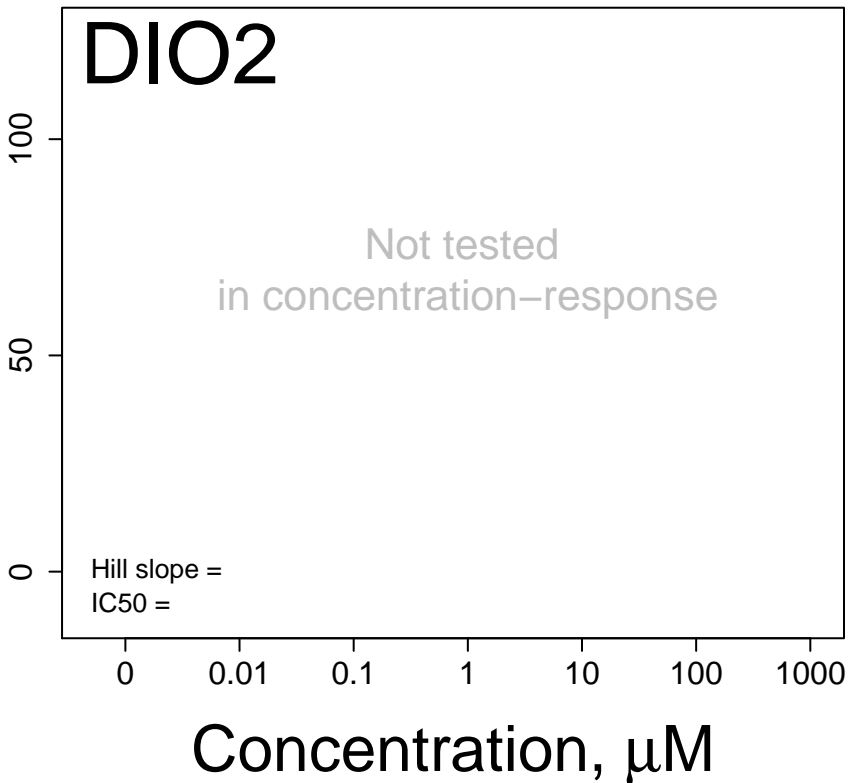
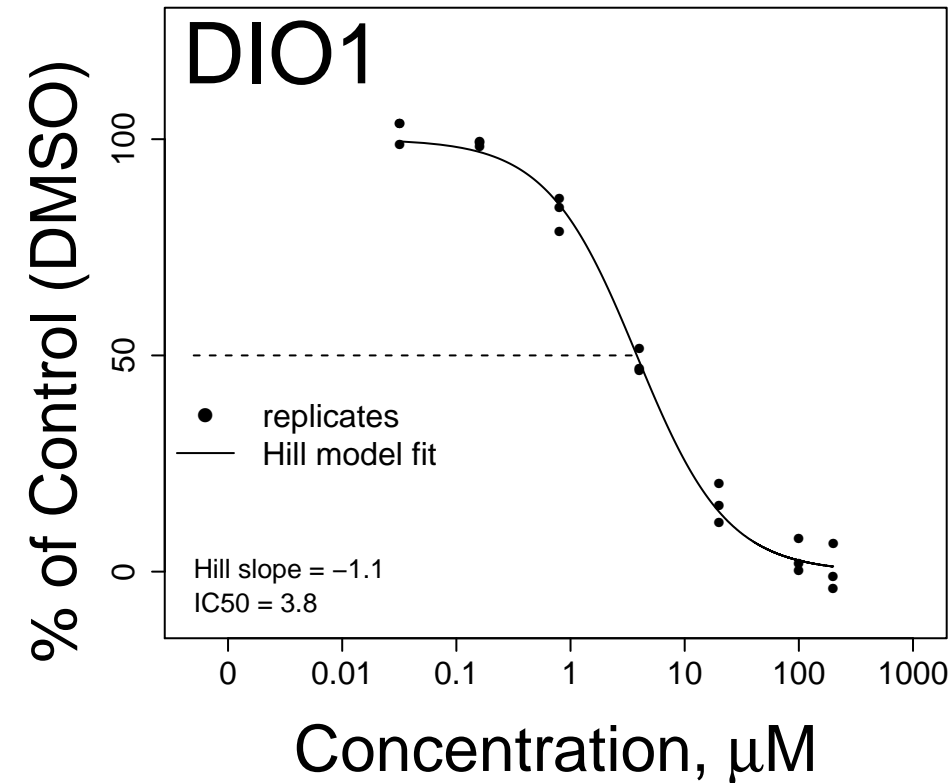
Daidzein CASRN: 486-66-8



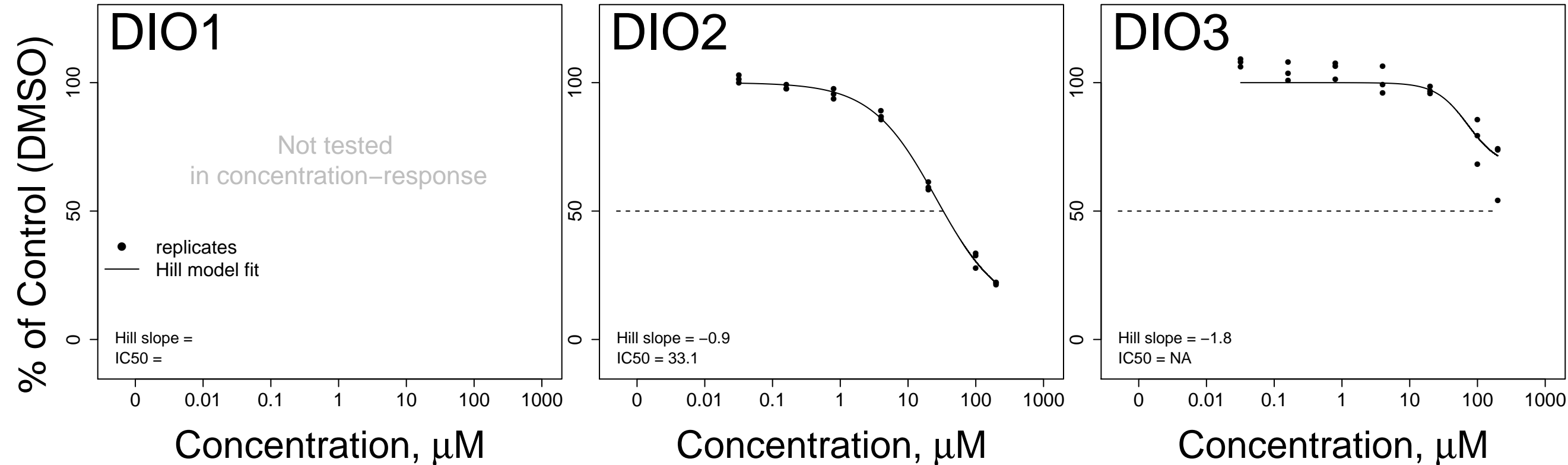
Clomiphene citrate (1:1) CASRN: 50-41-9



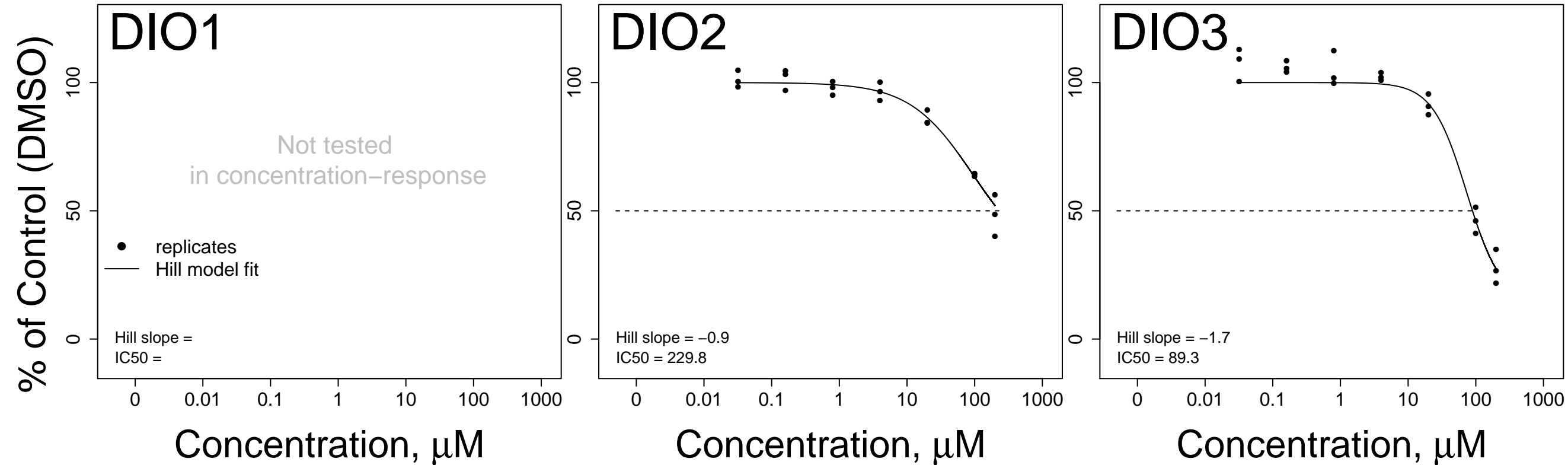
6-Propyl-2-thiouracil CASRN: 51-52-5



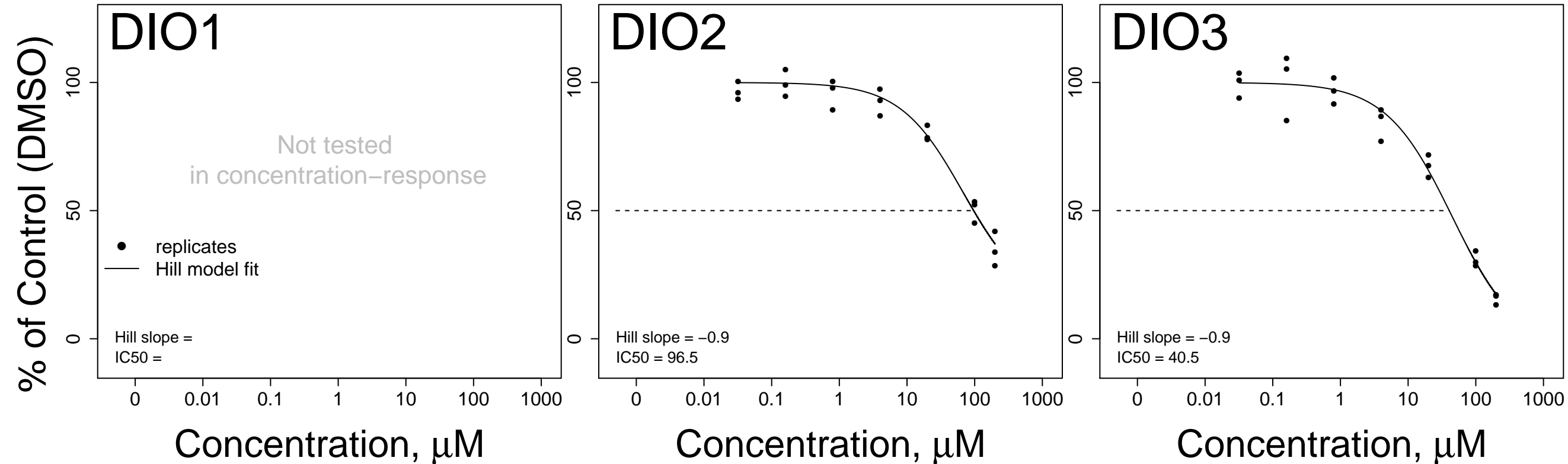
Spironolactone CASRN: 52-01-7



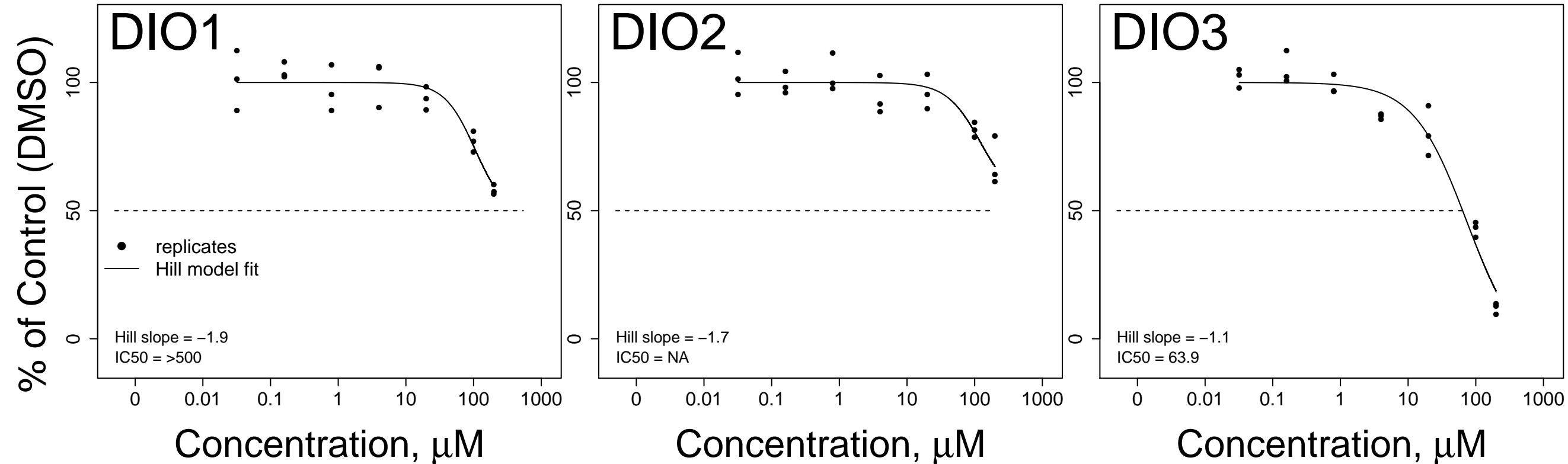
4-Chlorobenzotrichloride CASRN: 5216-25-1



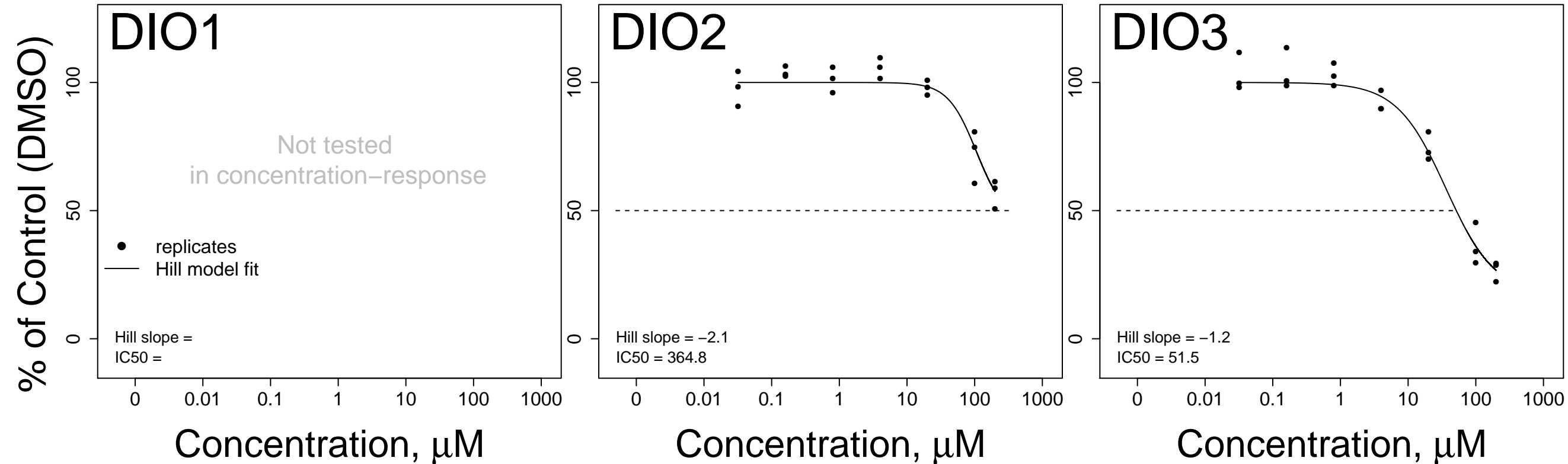
1,2-Dinitrobenzene CASRN: 528-29-0



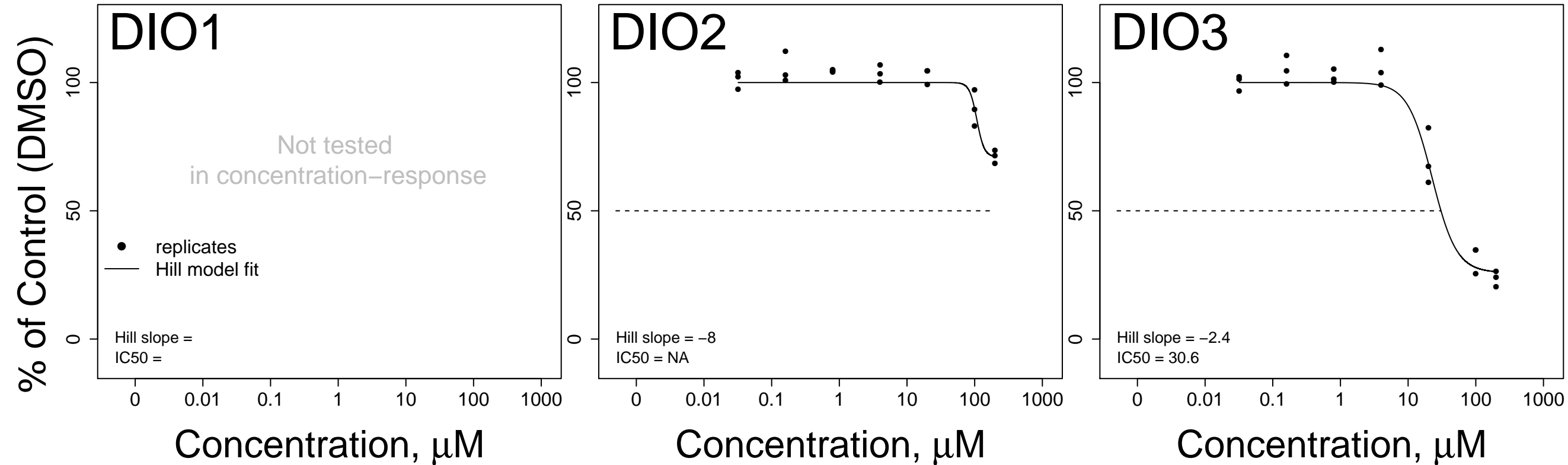
1-Hydroxypyrene CASRN: 5315-79-7



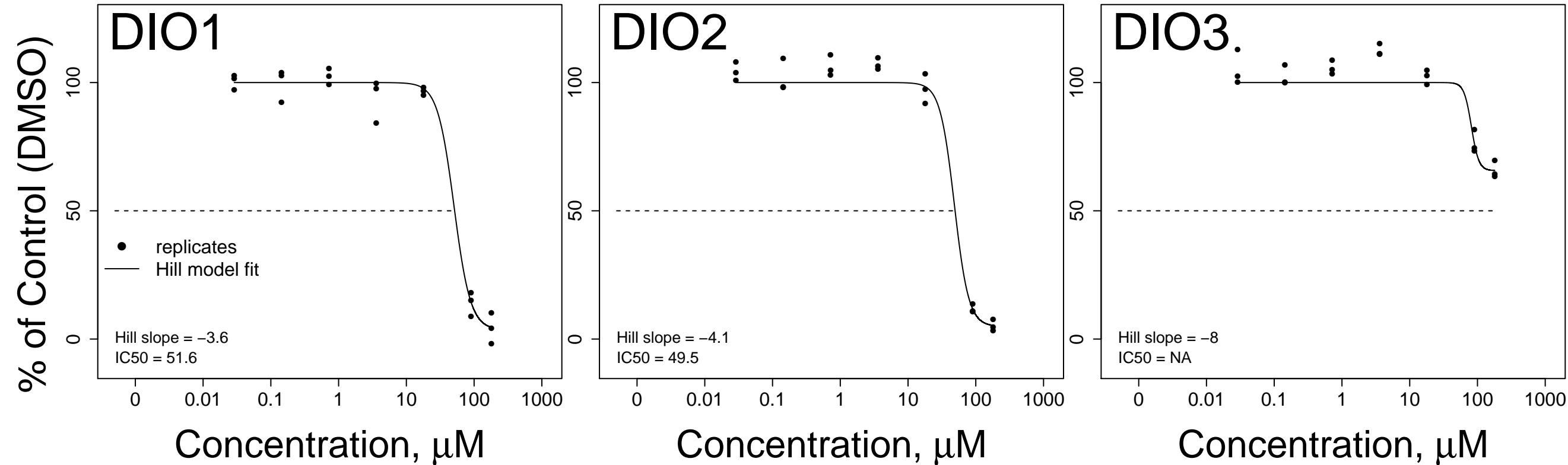
3,7-Dimethyl-2,6-octadienal CASRN: 5392-40-5



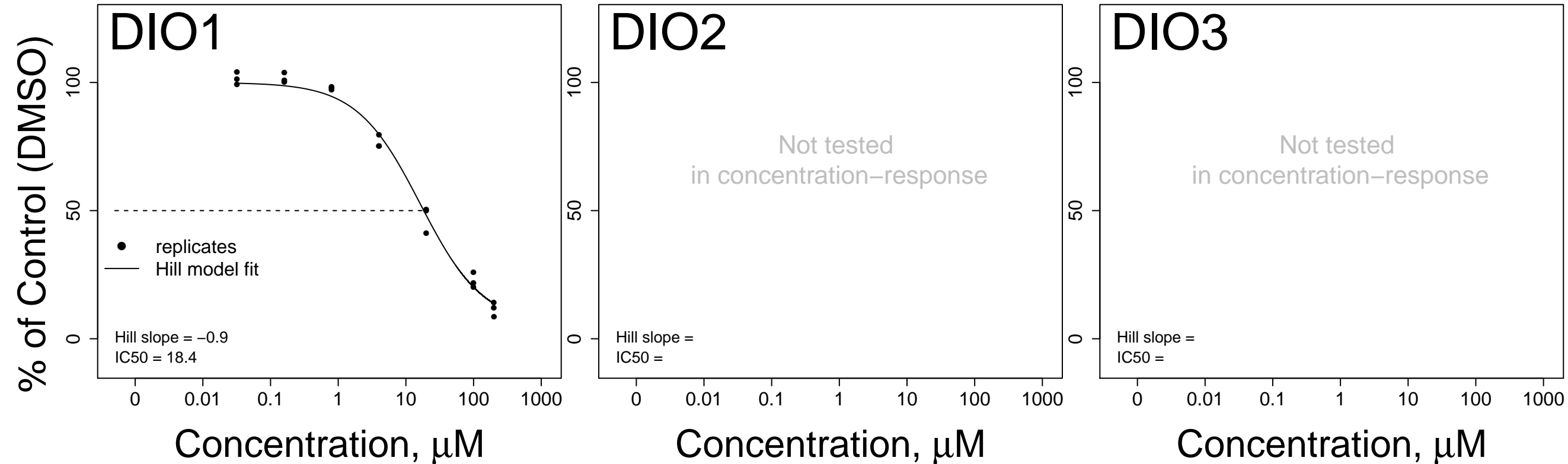
Gentian Violet CASRN: 548-62-9



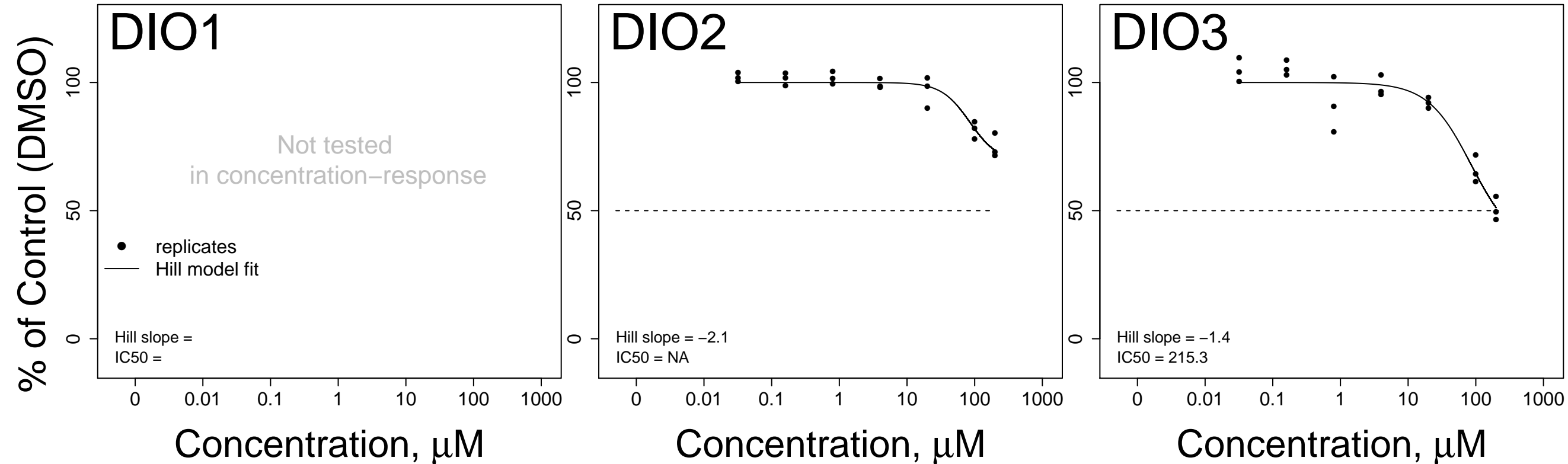
Tamoxifen citrate CASRN: 54965-24-1



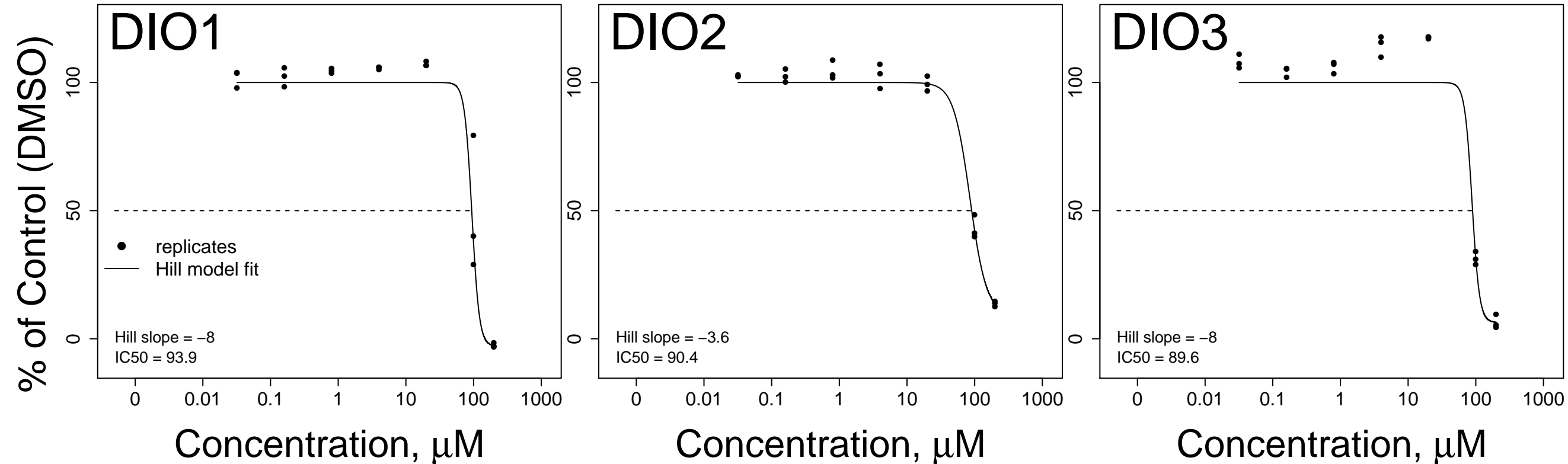
6-Methyl-2-thiouracil CASRN: 56-04-2



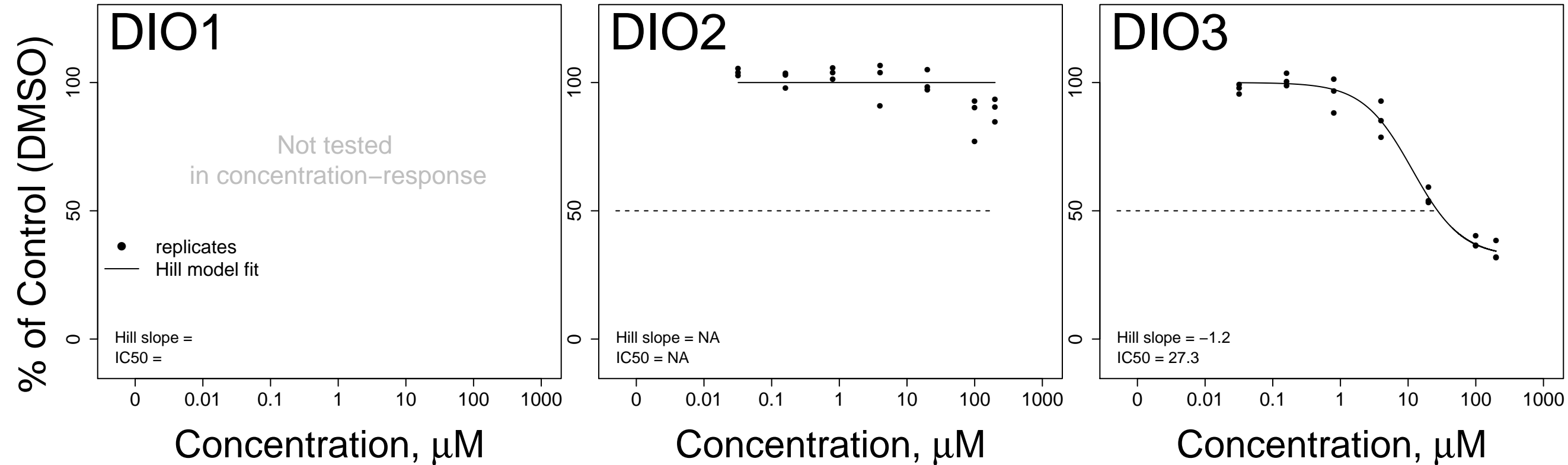
Benz(a)anthracene CASRN: 56-55-3



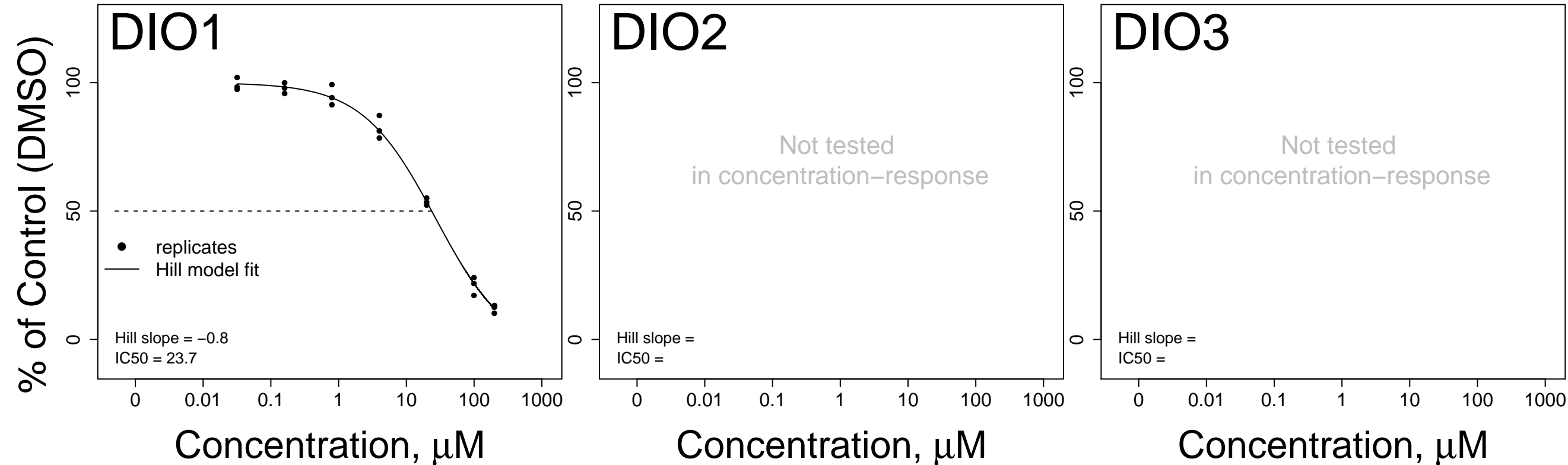
Docusate sodium CASRN: 577-11-7



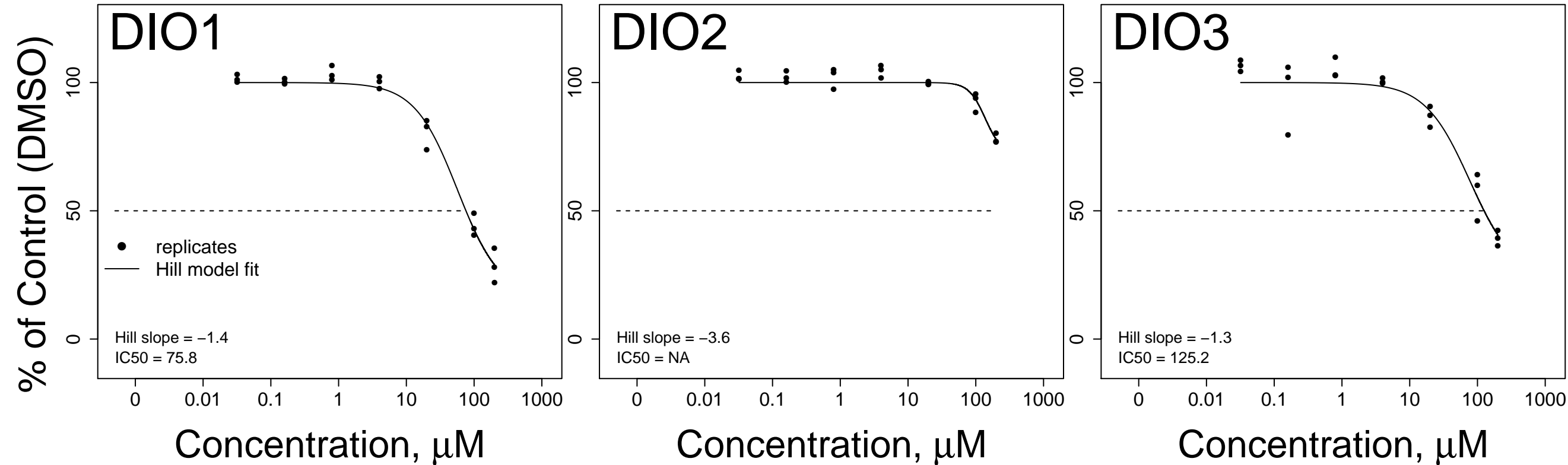
Terbutylazine CASRN: 5915-41-3



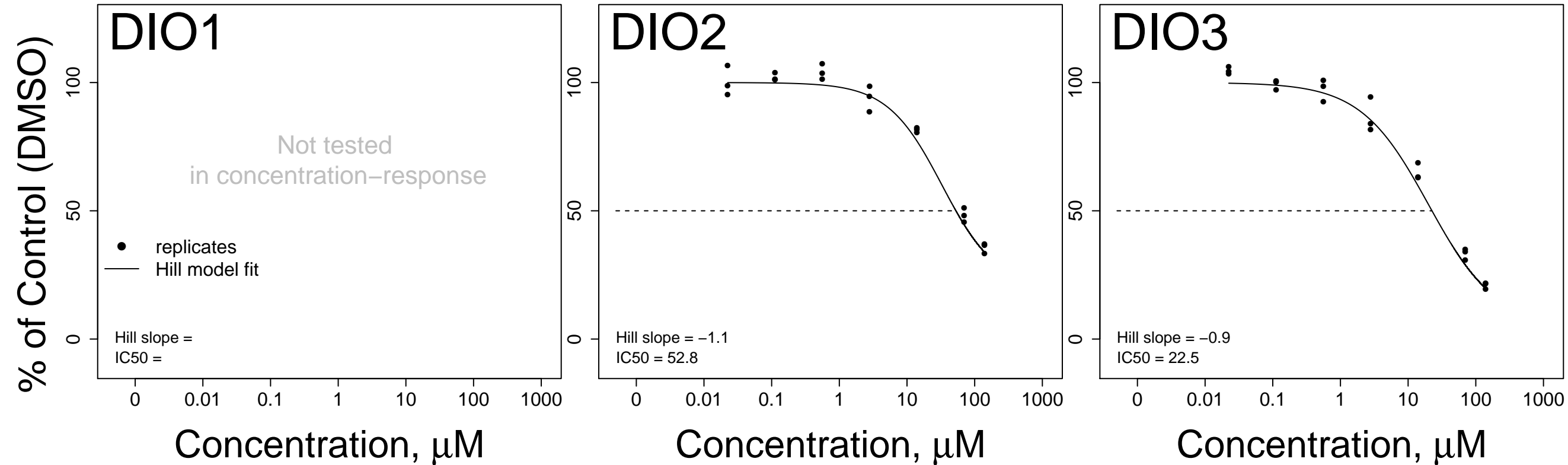
Sulfasalazine CASRN: 599-79-1



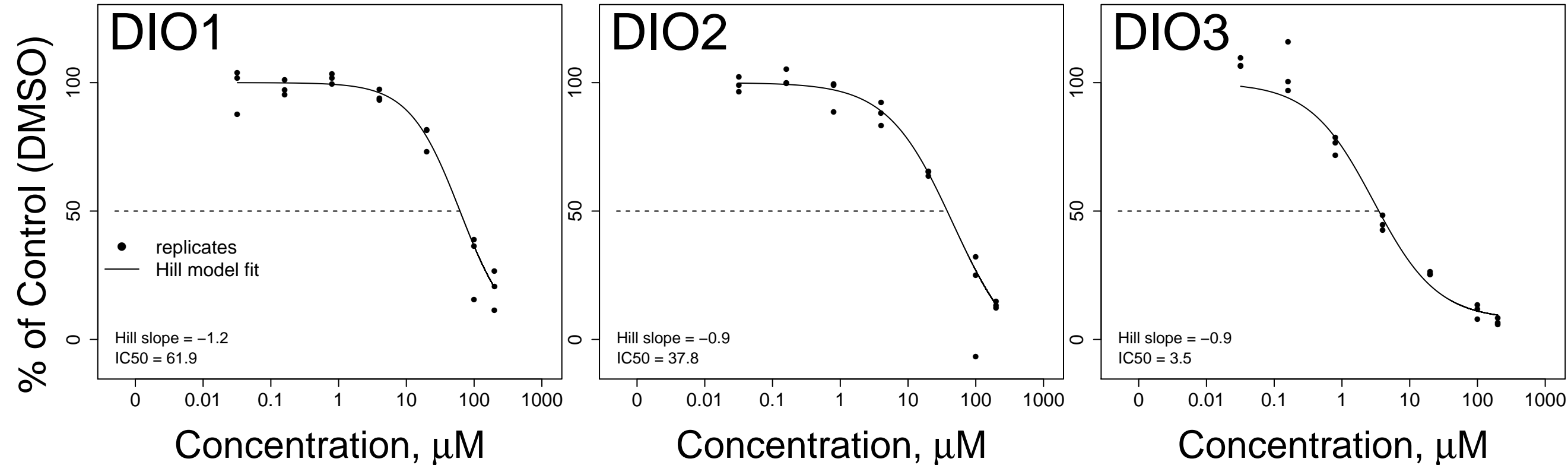
Tetracycline CASRN: 60-54-8



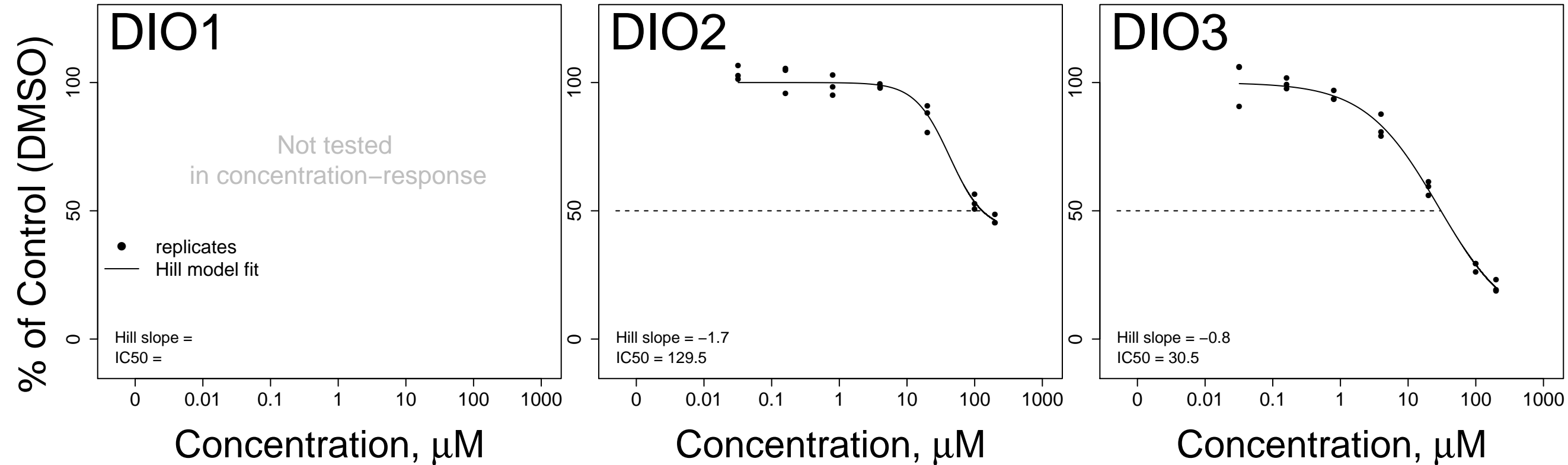
2,3-Dinitrotoluene CASRN: 602-01-7



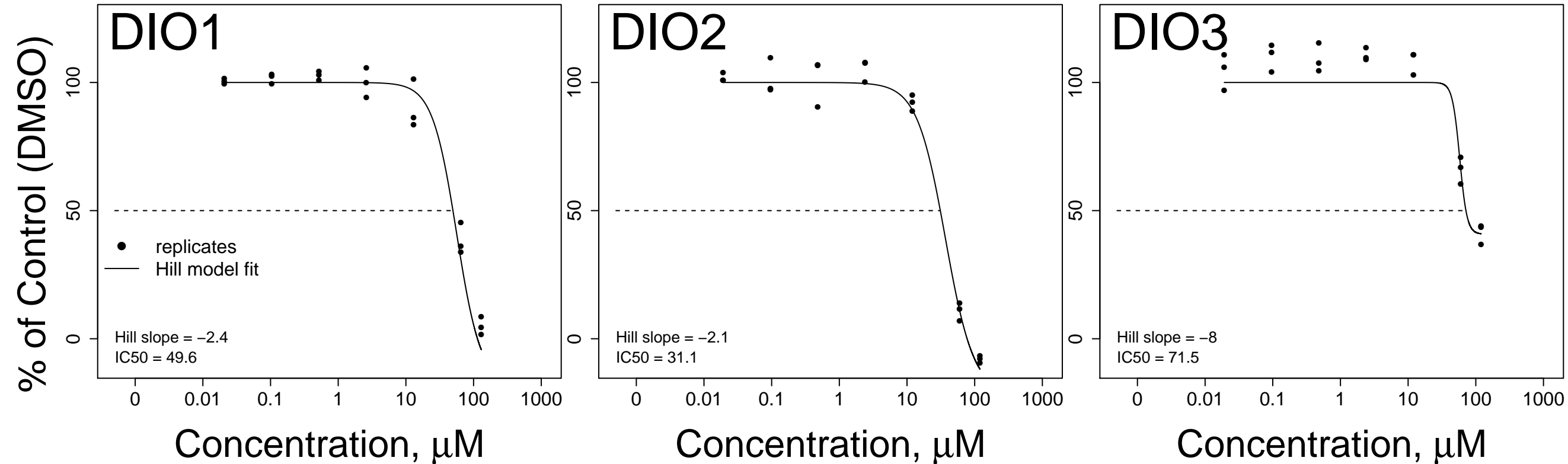
1,2-Benzenedicarboxaldehyde CASRN: 643-79-8



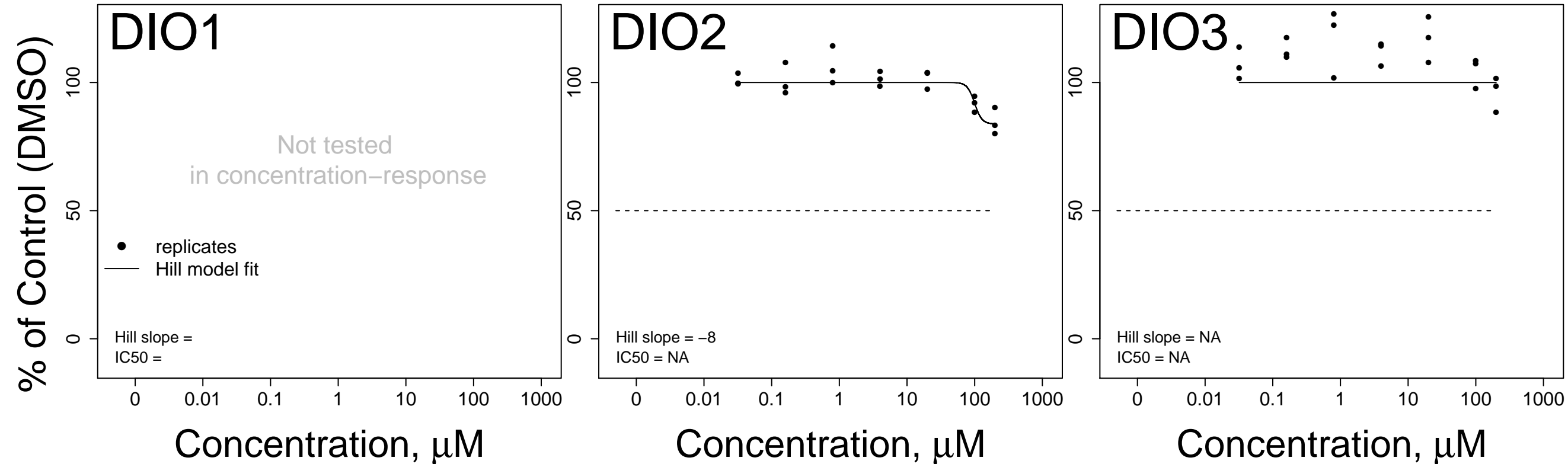
Retinol CASRN: 68-26-8



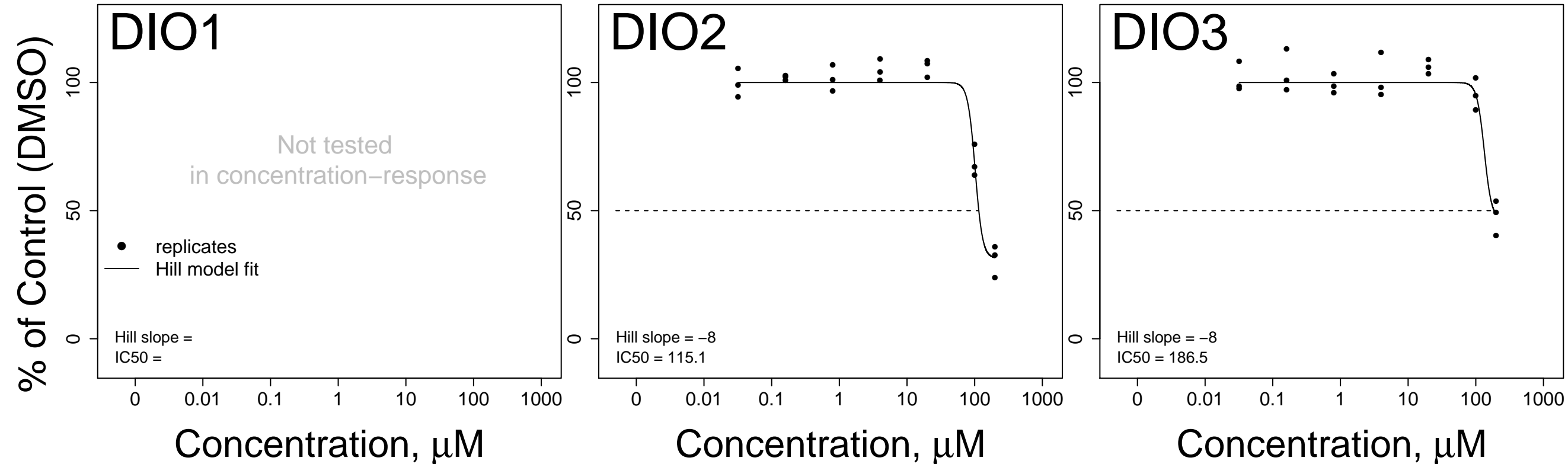
4-Hydroxytamoxifen CASRN: 68392-35-8



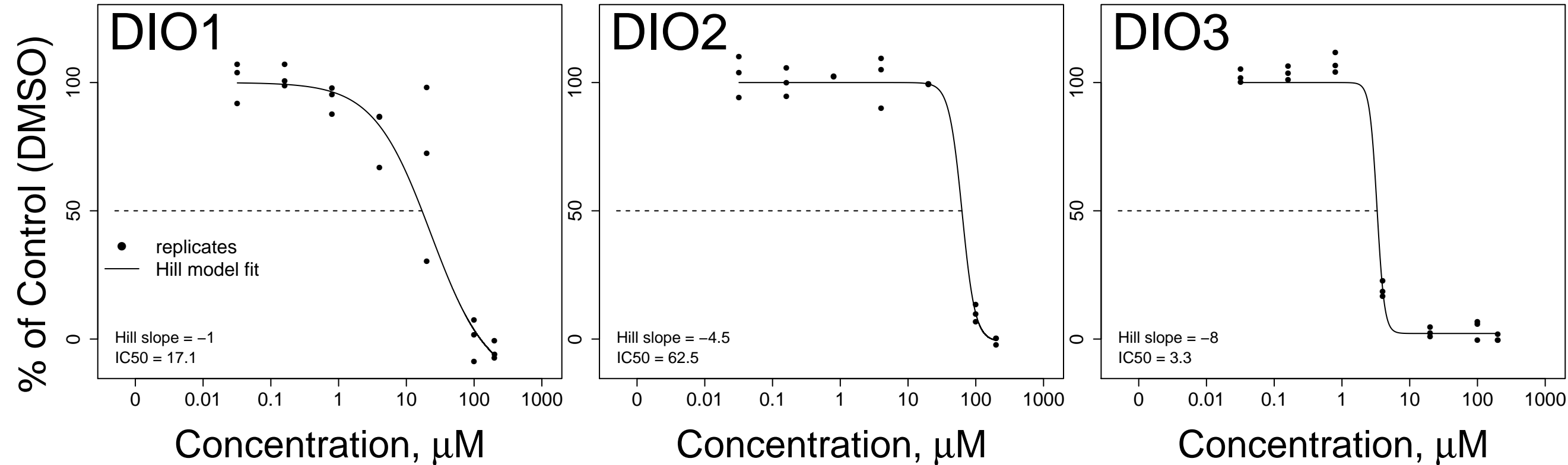
PharmaGSID_48519 CASRN: 686756-87-6



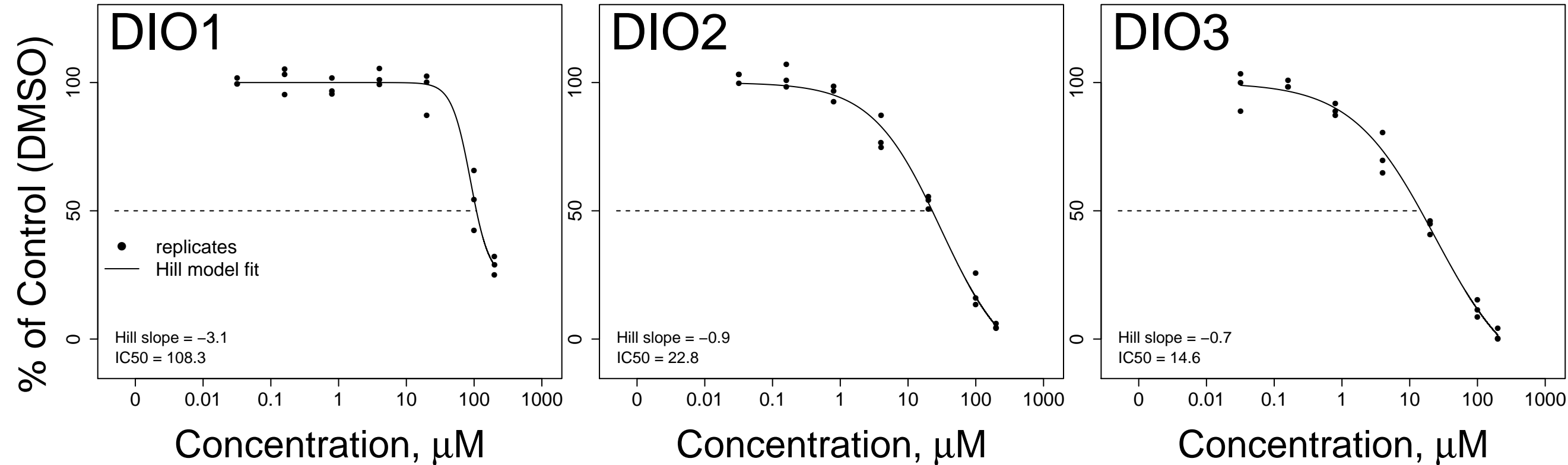
Chlorpromazine hydrochloride CASRN: 69-09-0



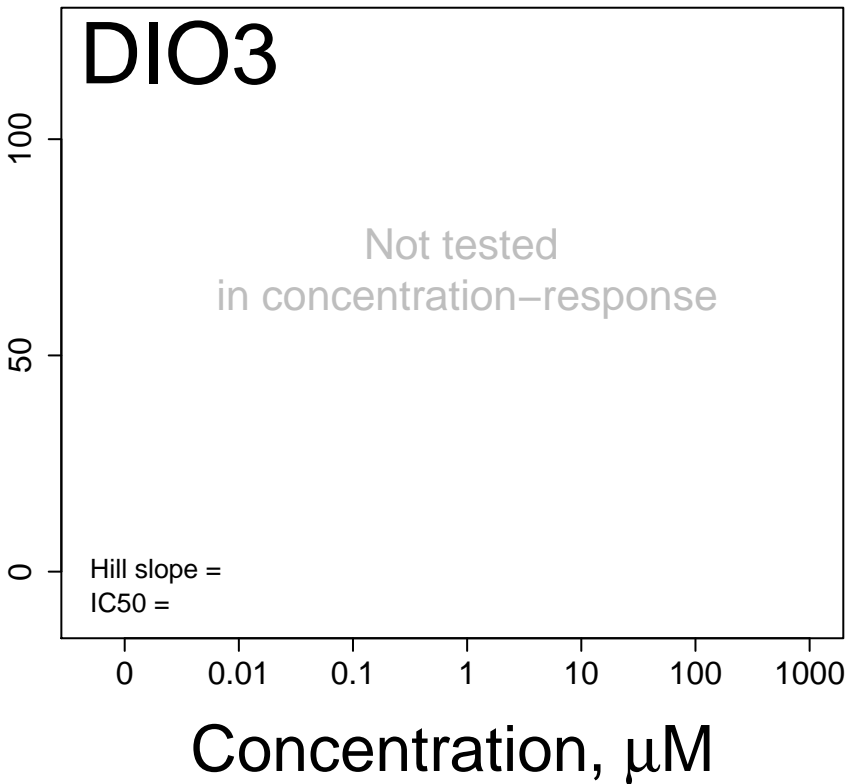
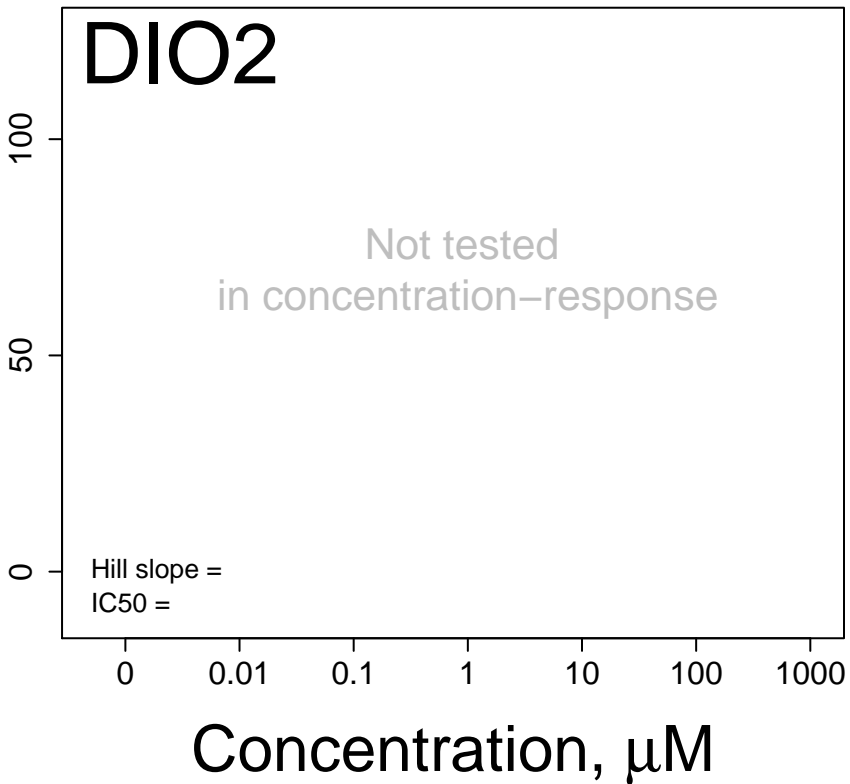
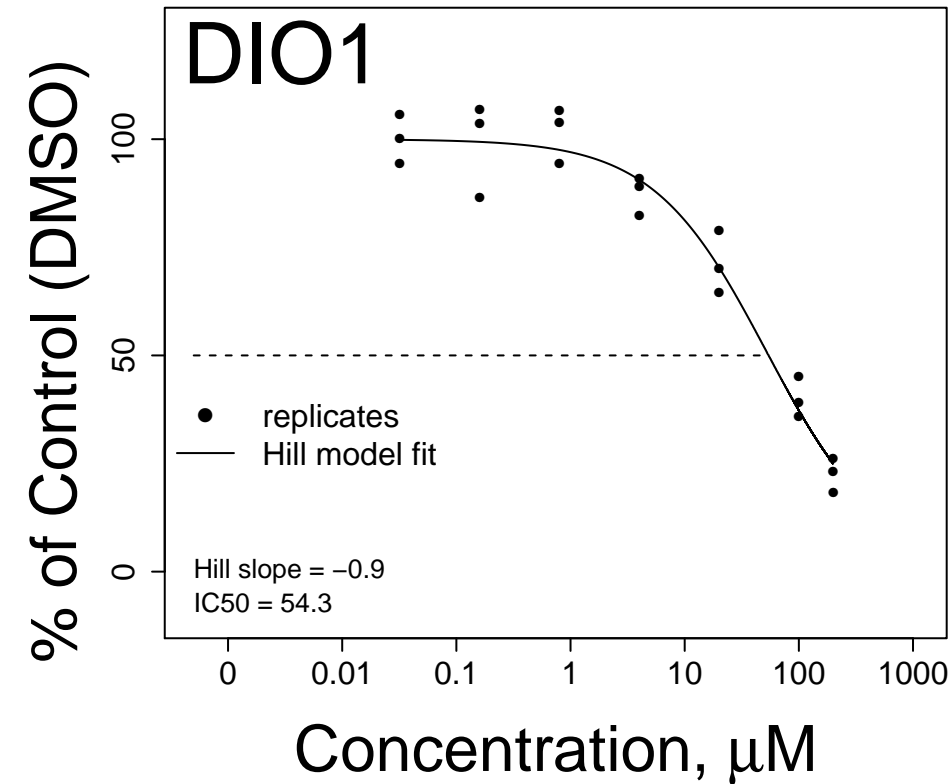
Didecyldimethylammonium chloride CASRN: 7173-51-5



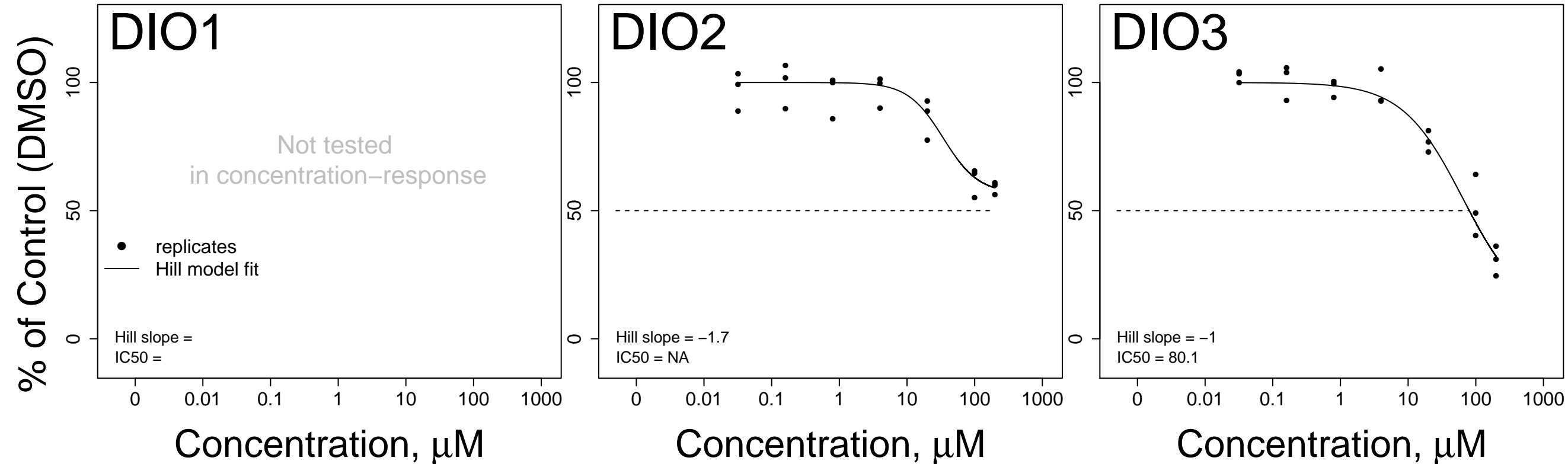
AVE5638 CASRN: 725228-45-5



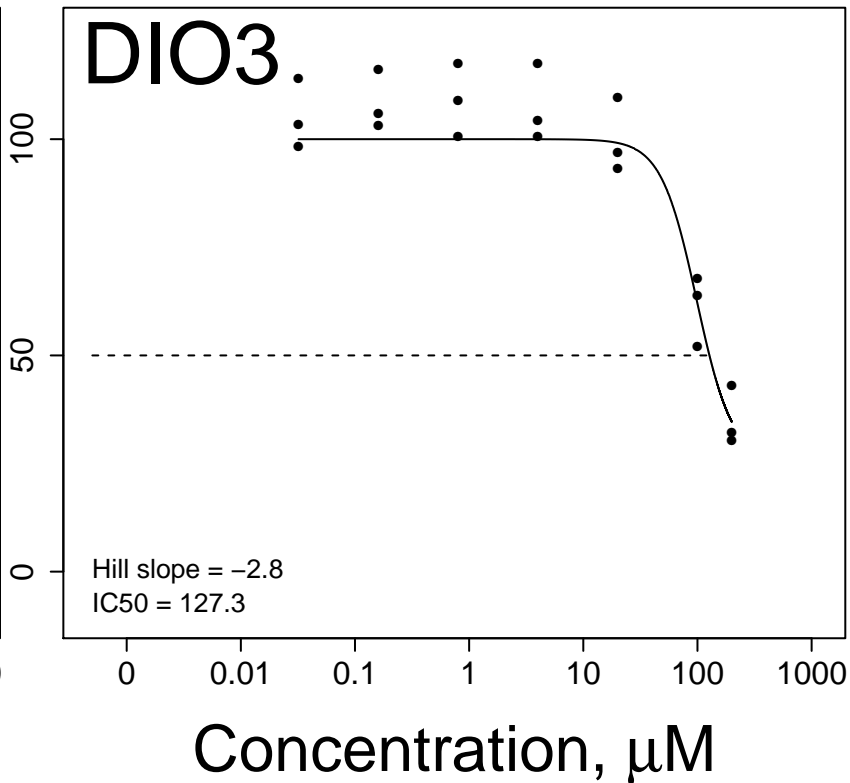
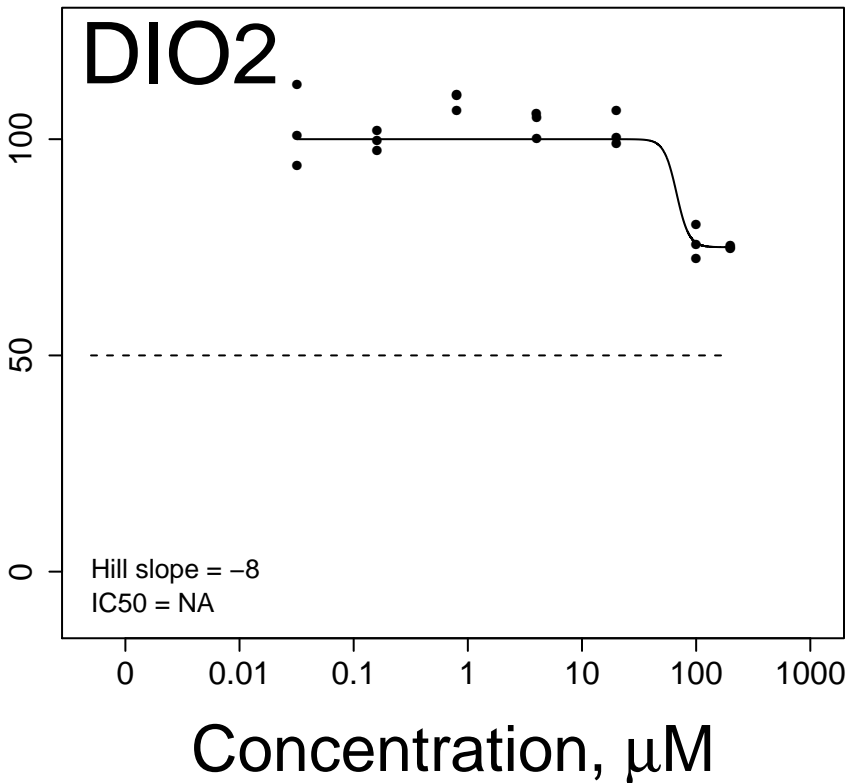
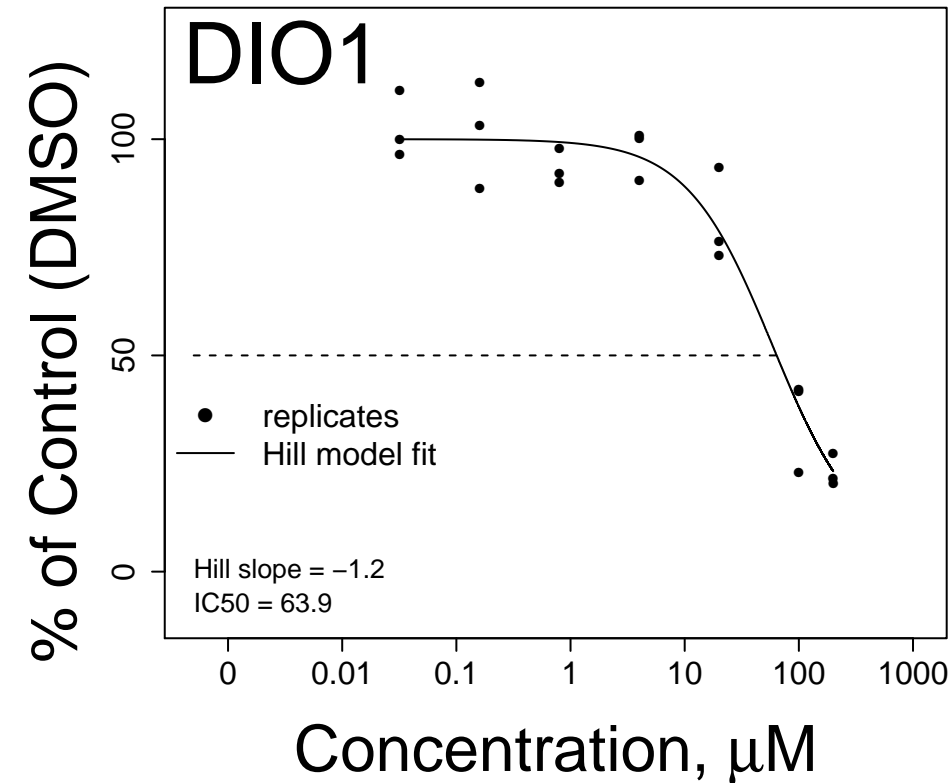
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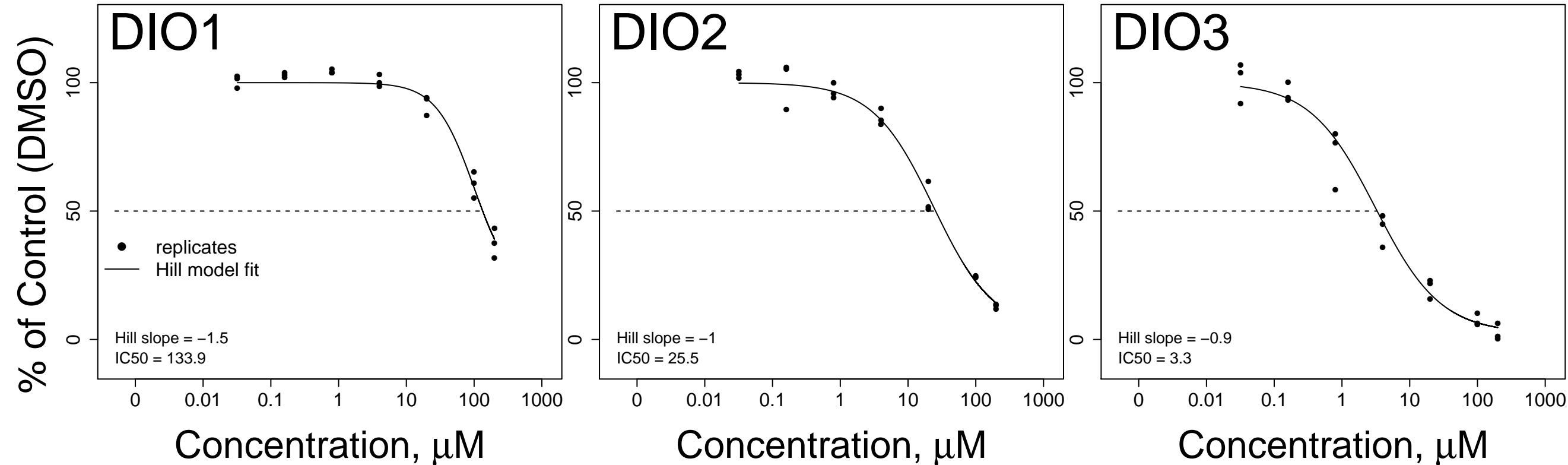
Diphenyl isophthalate CASRN: 744-45-6



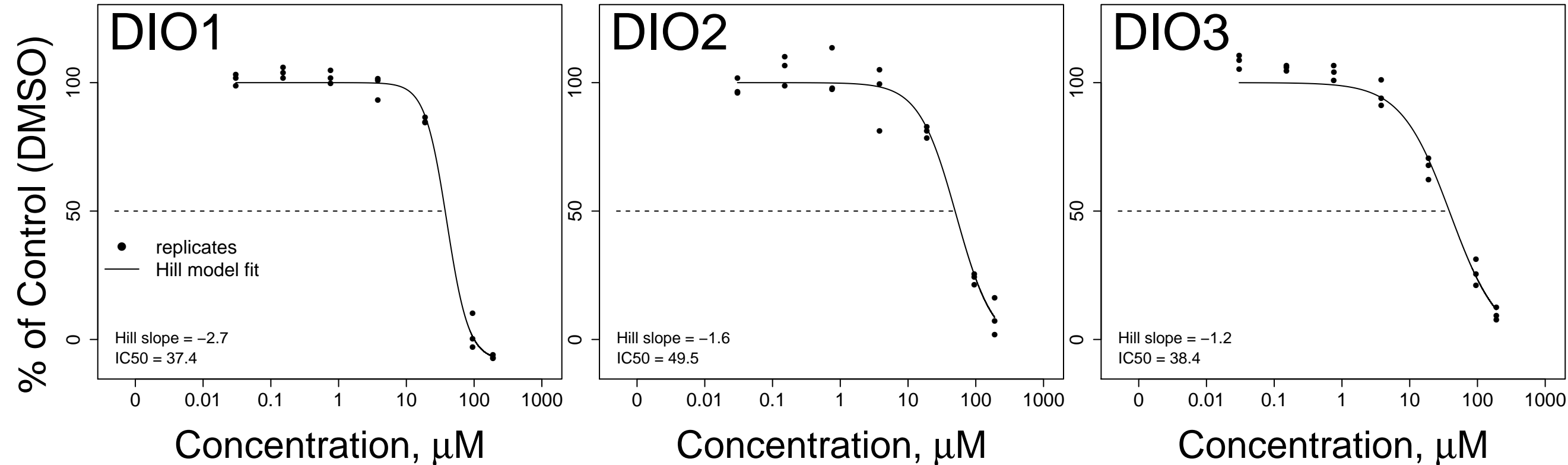
Lovastatin CASRN: 75330-75-5



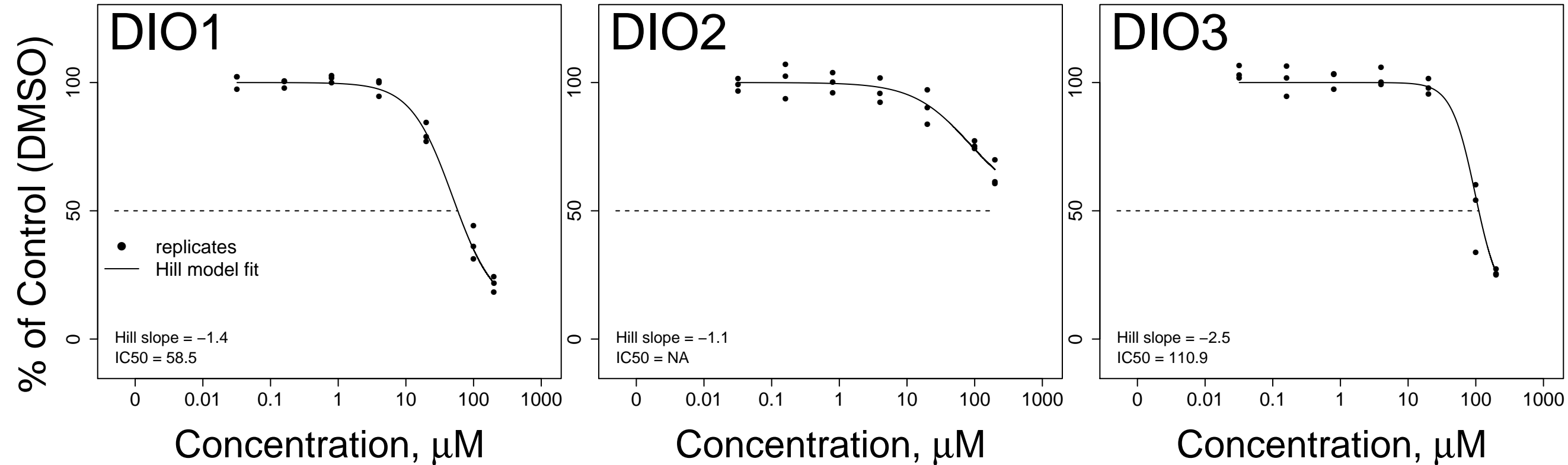
Hexachlorocyclopentadiene CASRN: 77-47-4



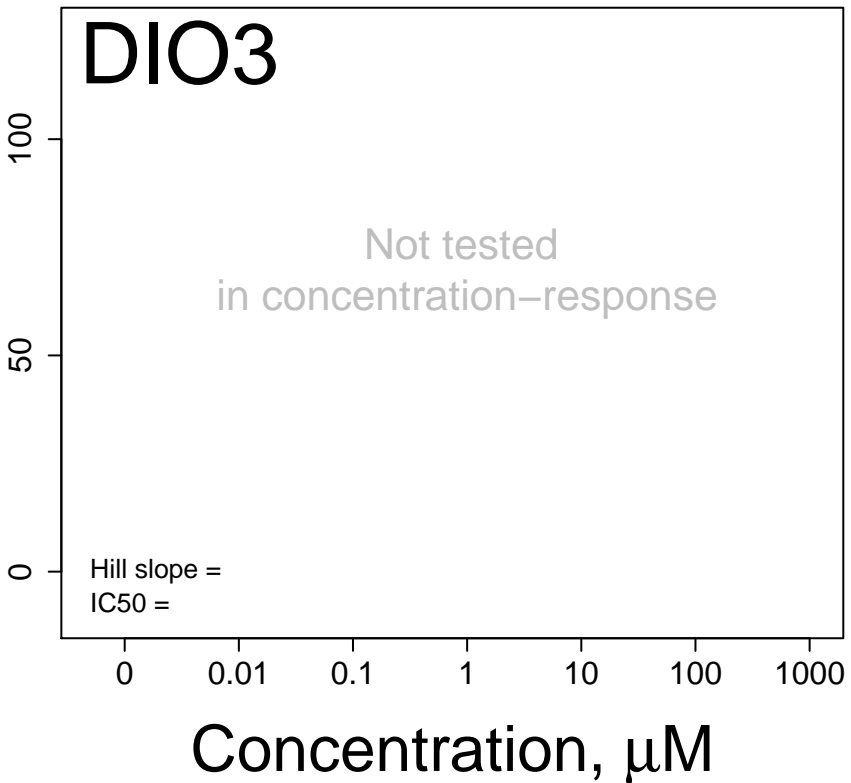
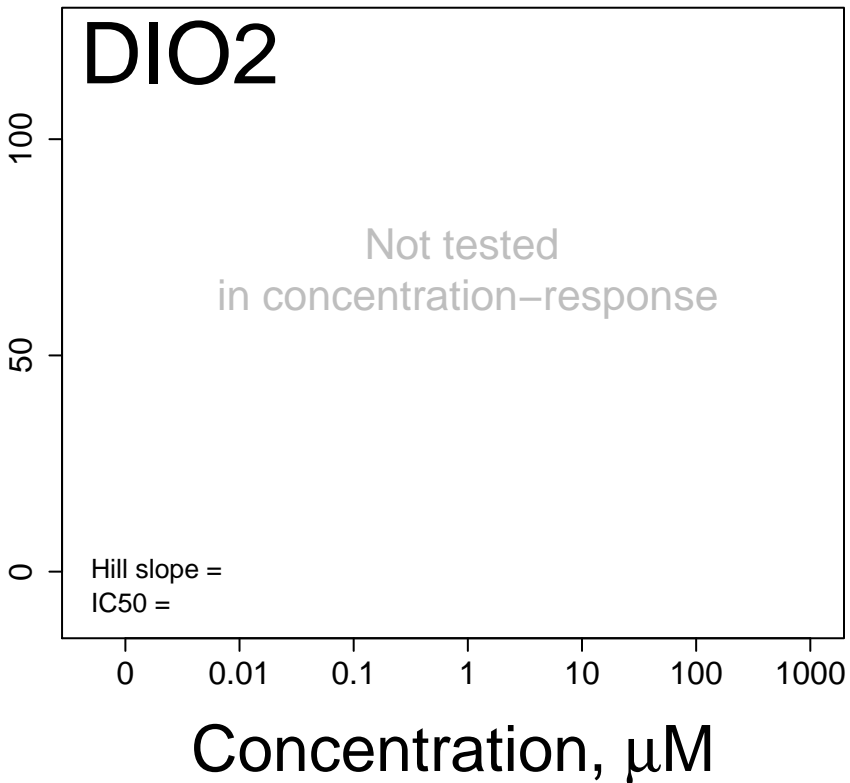
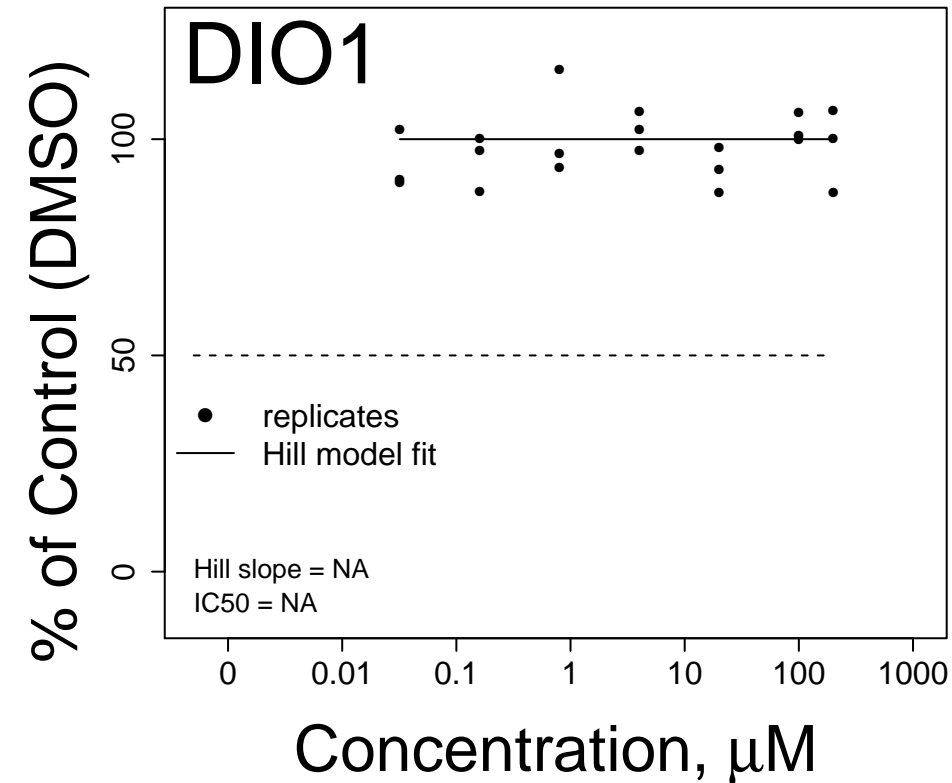
3,3',5,5'-Tetrabromobisphenol A CASRN: 79-94-7



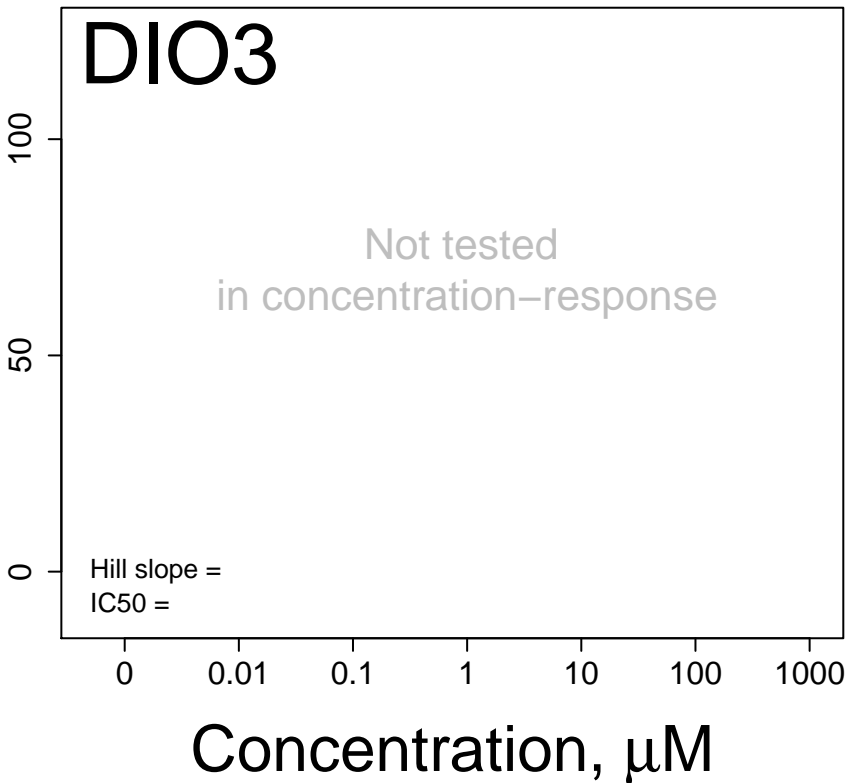
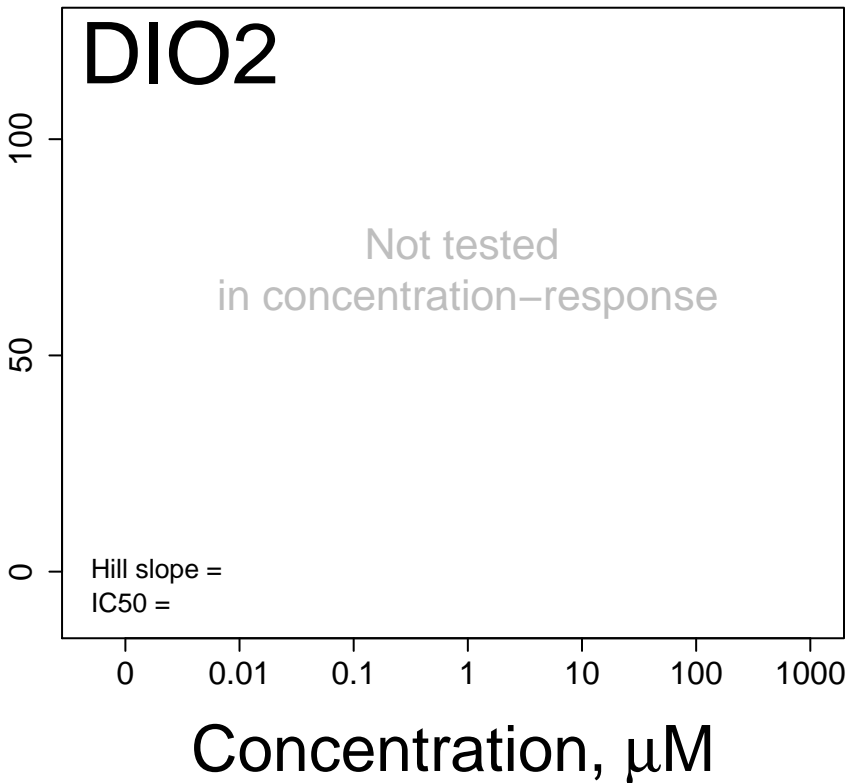
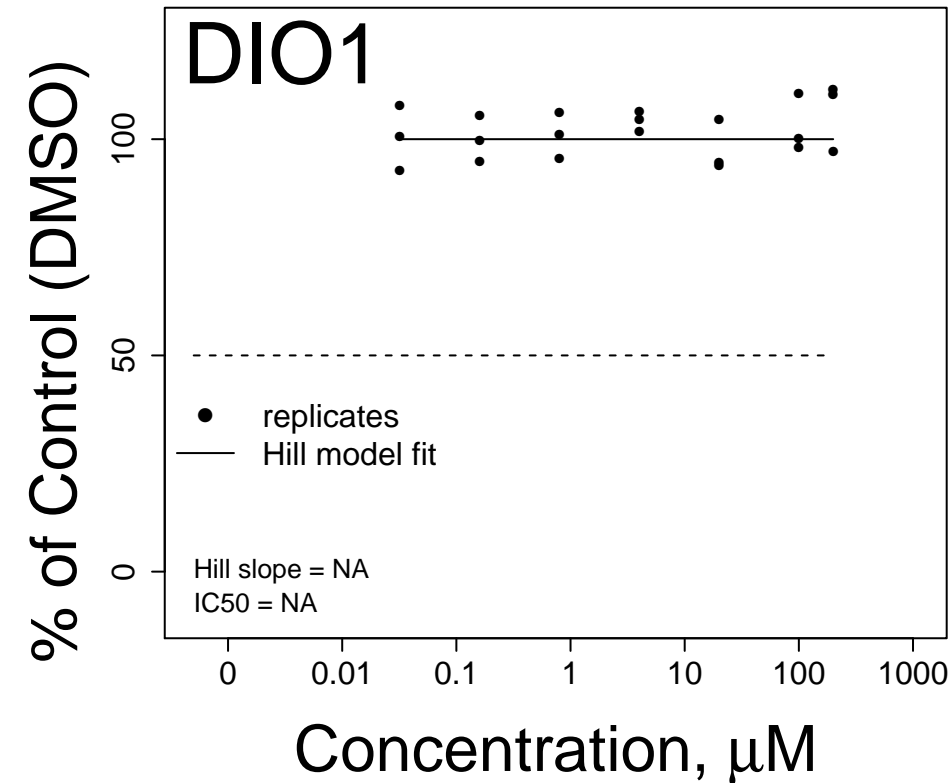
Simvastatin CASRN: 79902-63-9



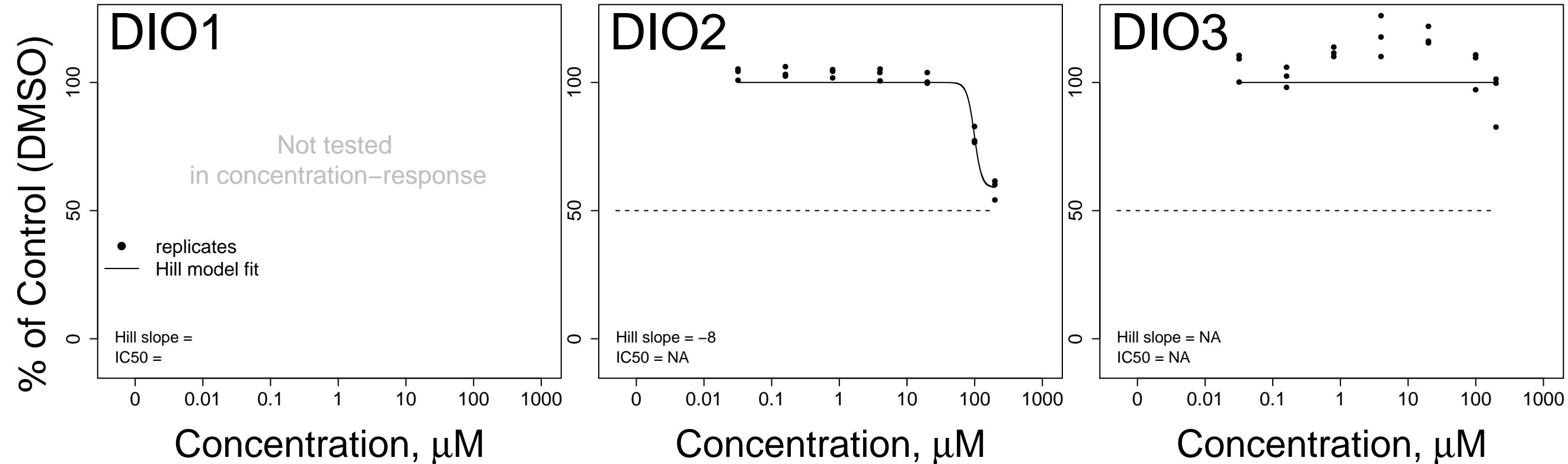
Dapsone CASRN: 80-08-0



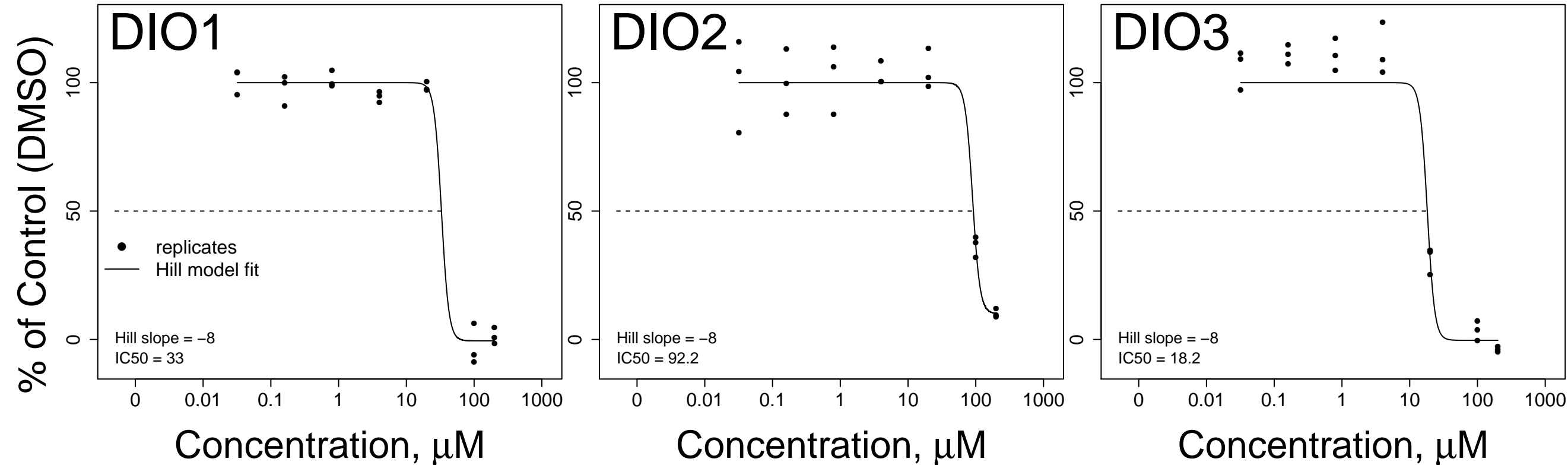
Butyryl trihexyl citrate CASRN: 82469-79-2



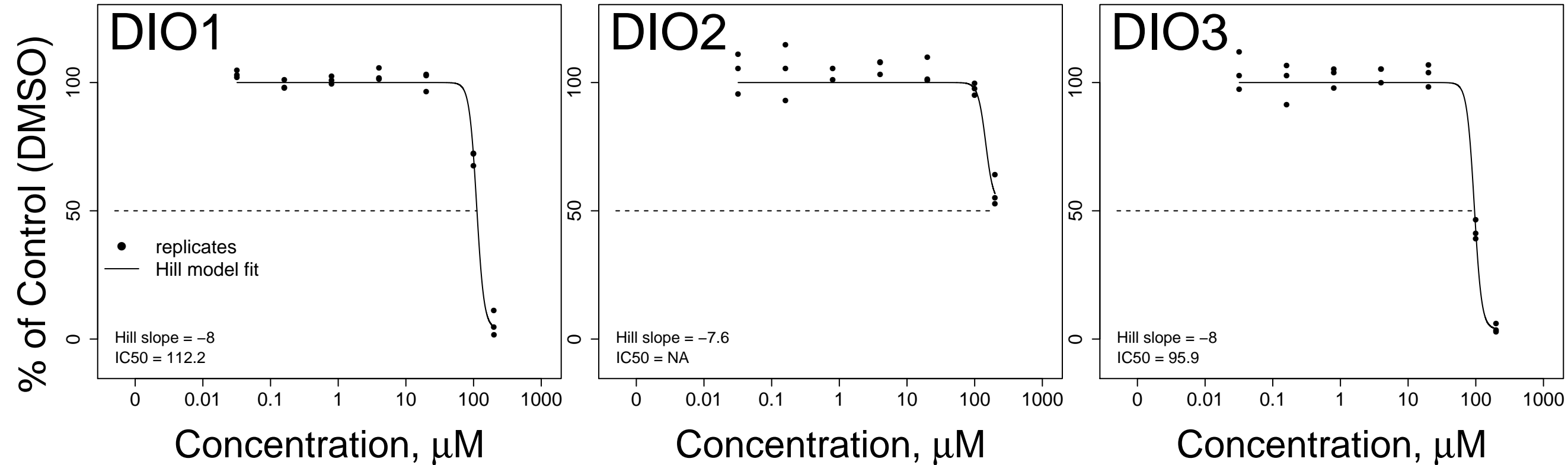
Raloxifene hydrochloride CASRN: 82640-04-8



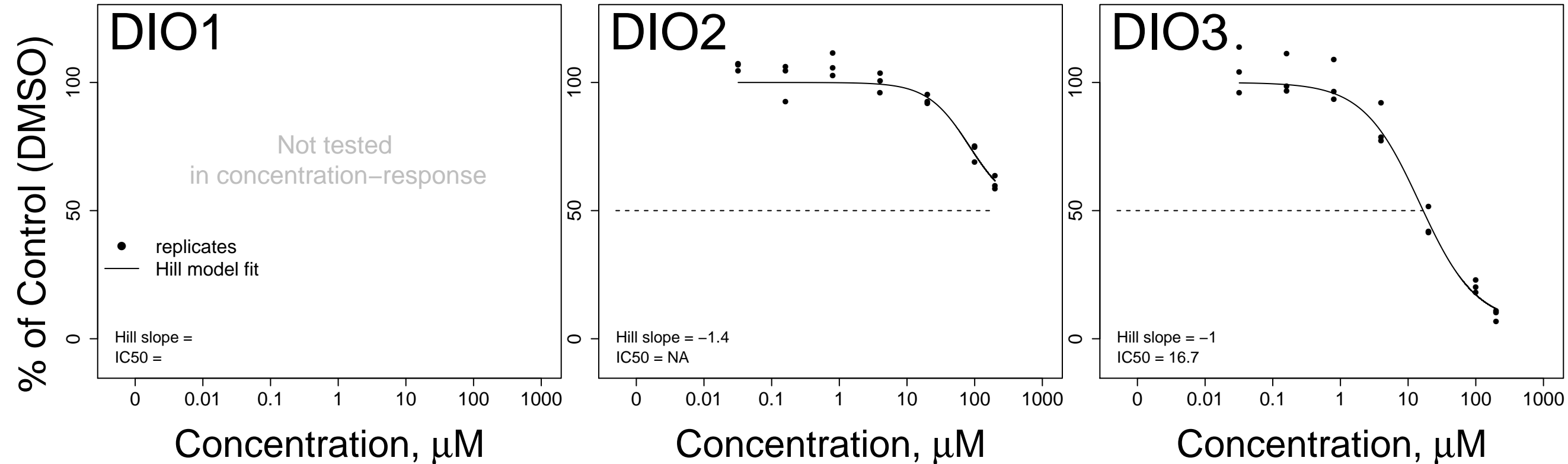
4-Nonylphenol, branched CASRN: 84852-15-3



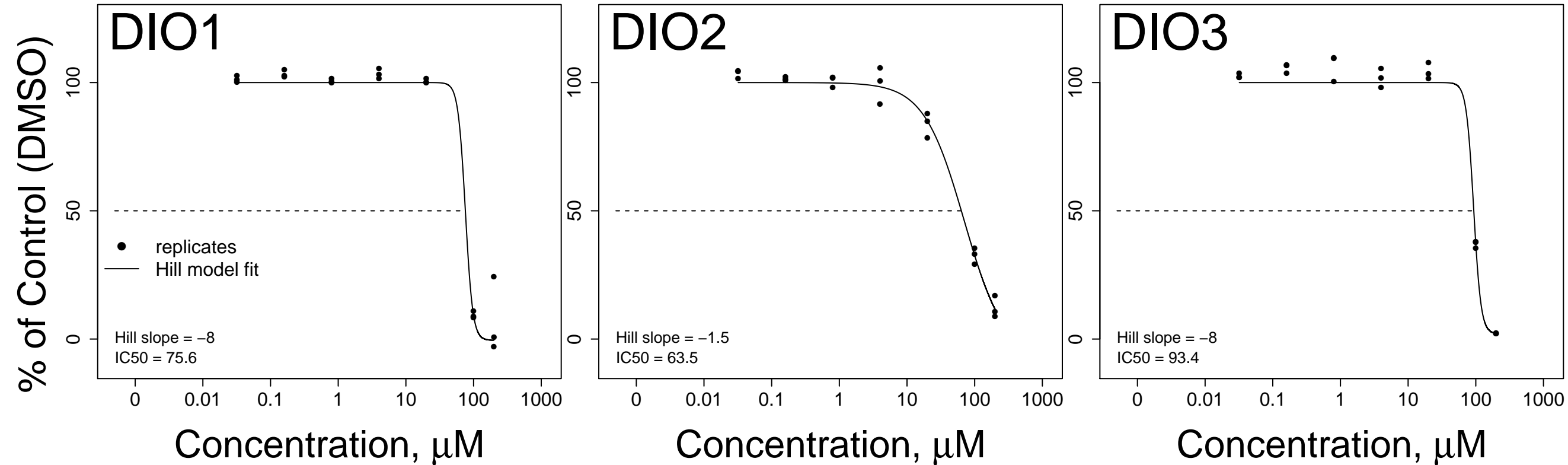
2,4-Di-tert-butylphenol CASRN: 96-76-4



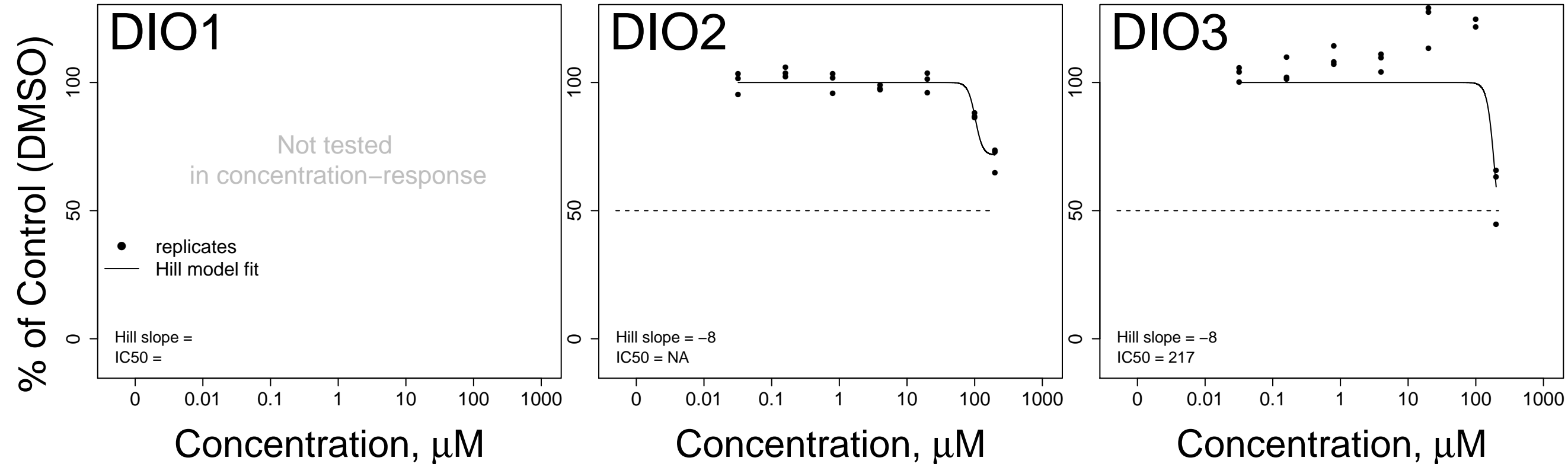
Isoeugenol CASRN: 97-54-1



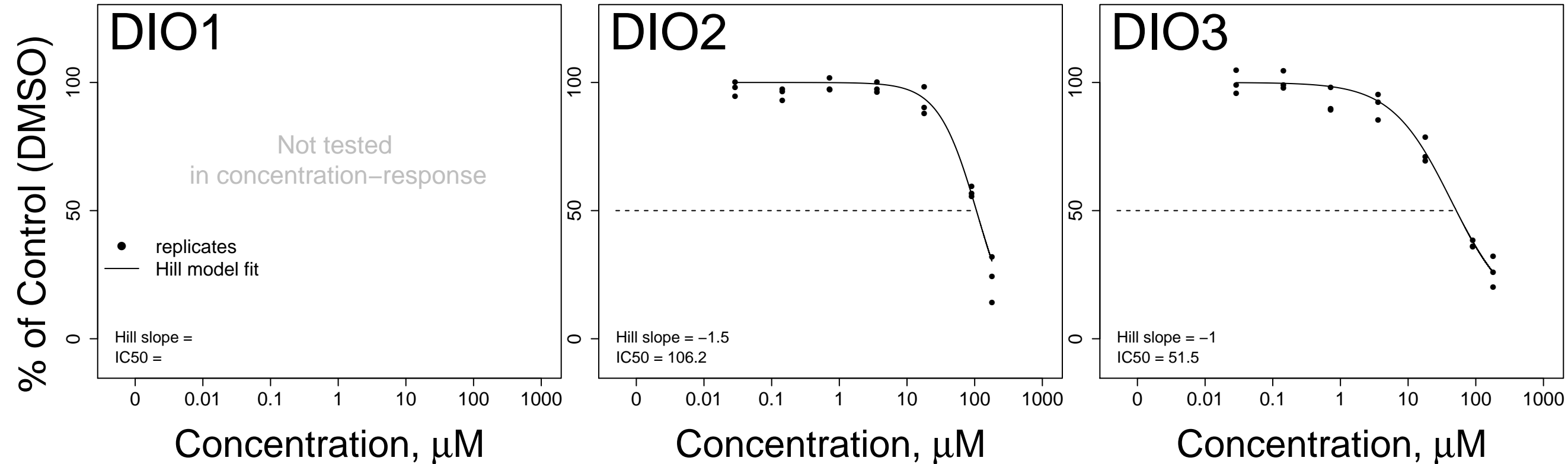
Troglitazone CASRN: 97322-87-7



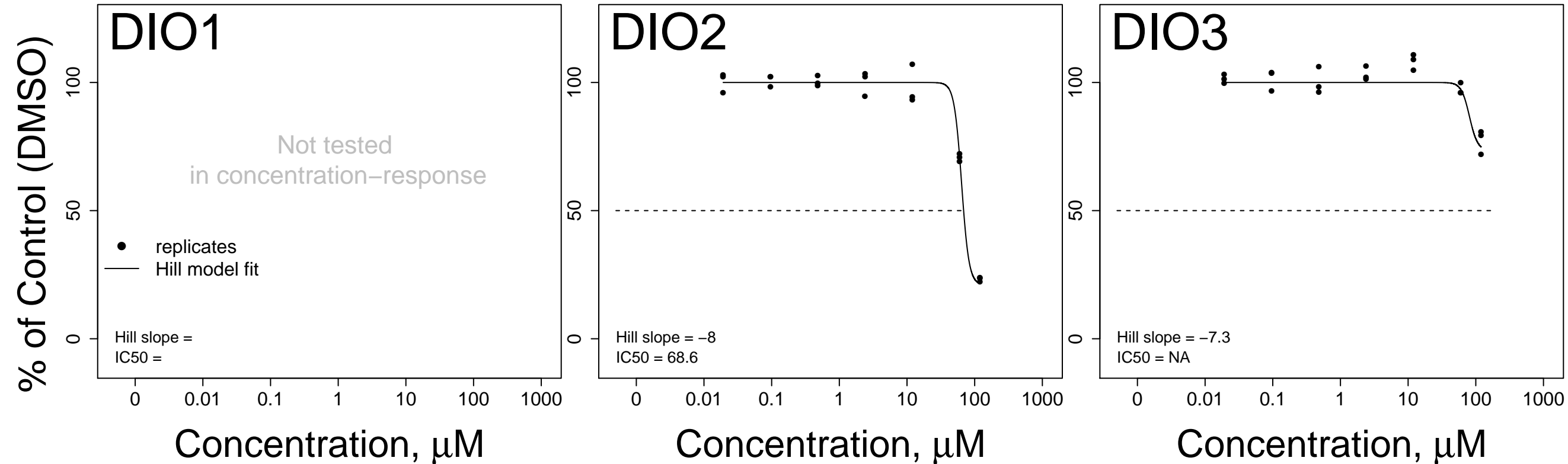
MK-274 CASRN: NOCAS_47328



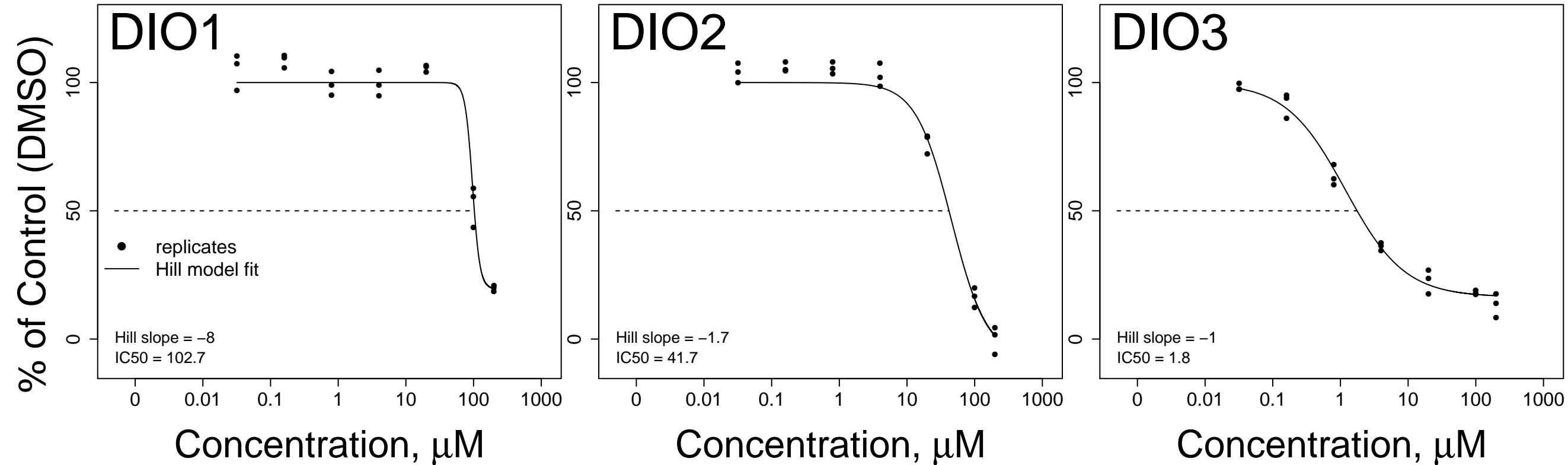
SR125047 CASRN: NOCAS_47342



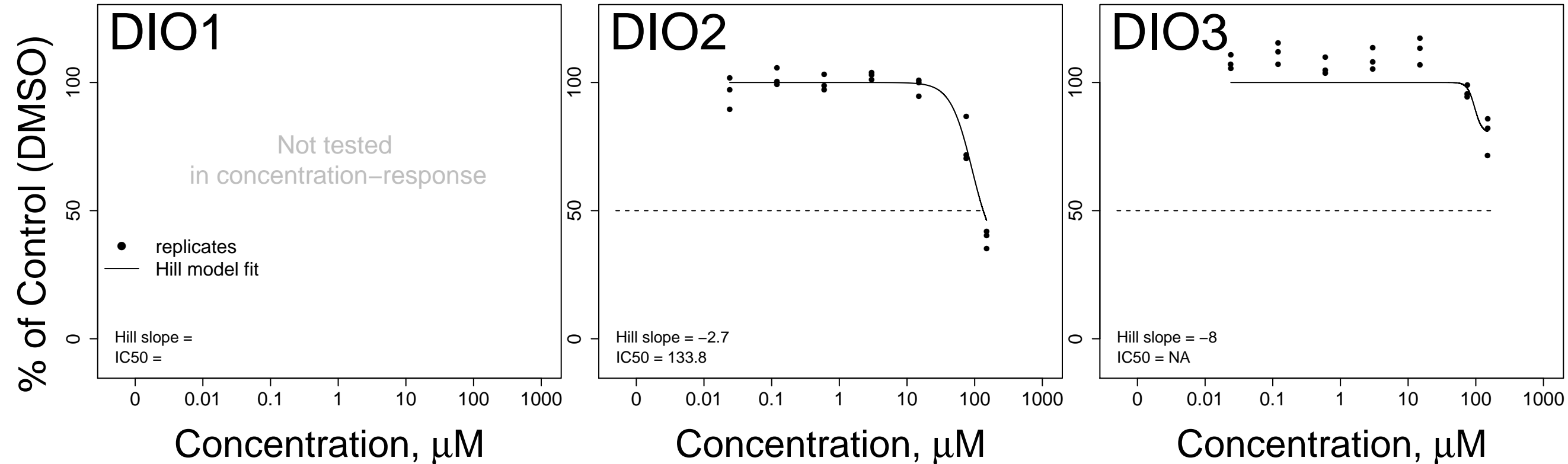
SSR 241586 HCI CASRN: NOCAS_47353



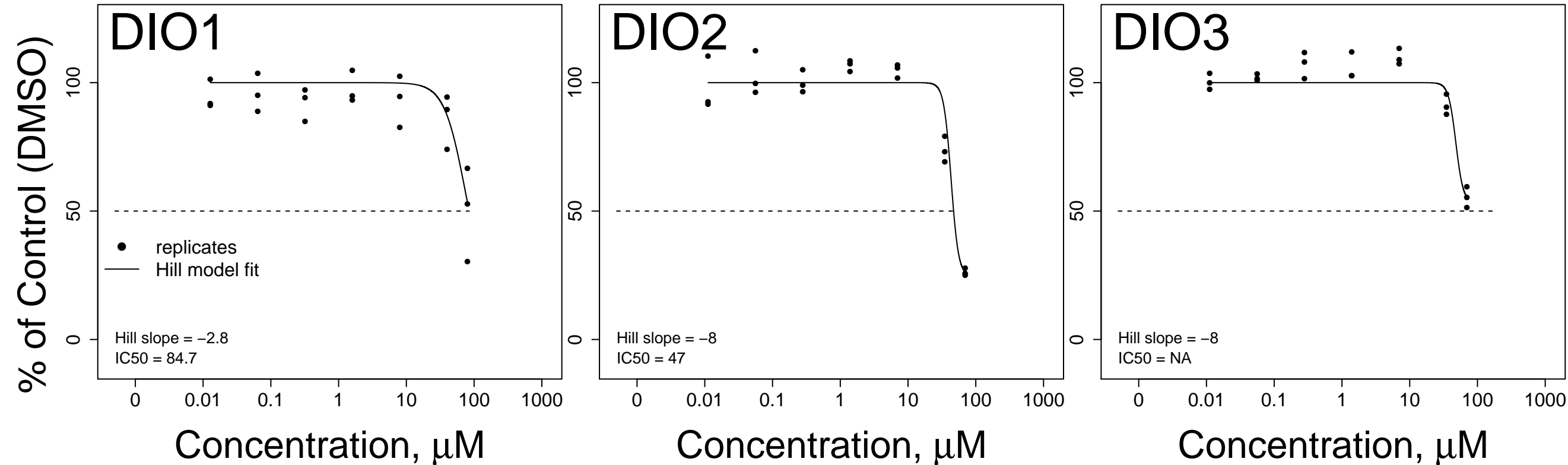
AVE6324 CASRN: NOCAS_47377



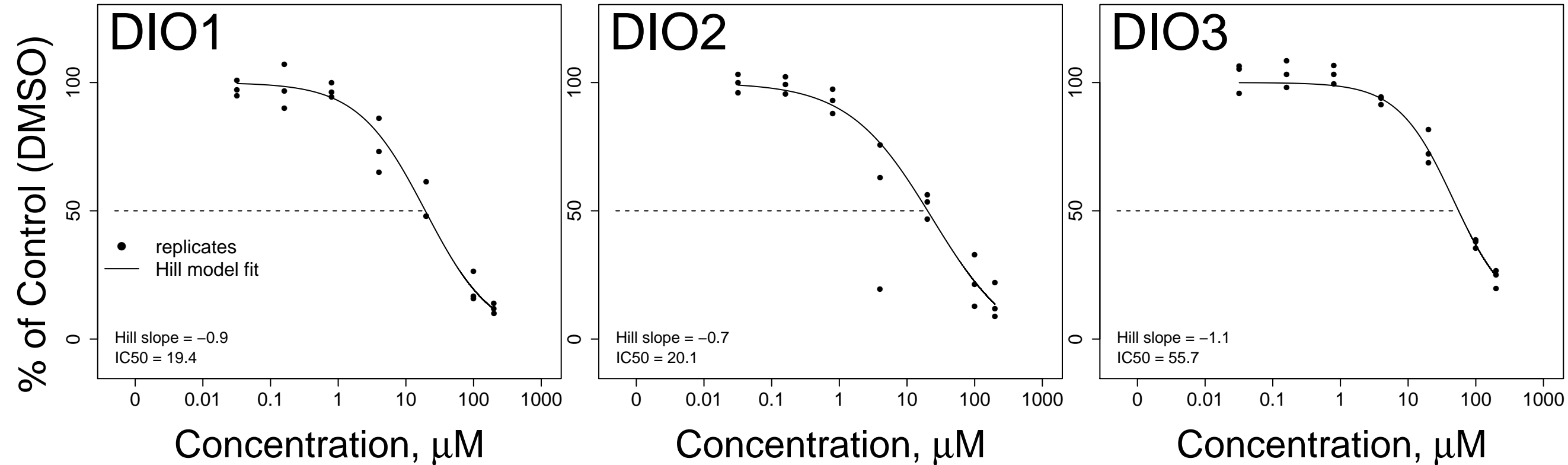
SAR102779 CASRN: NOCAS_47387



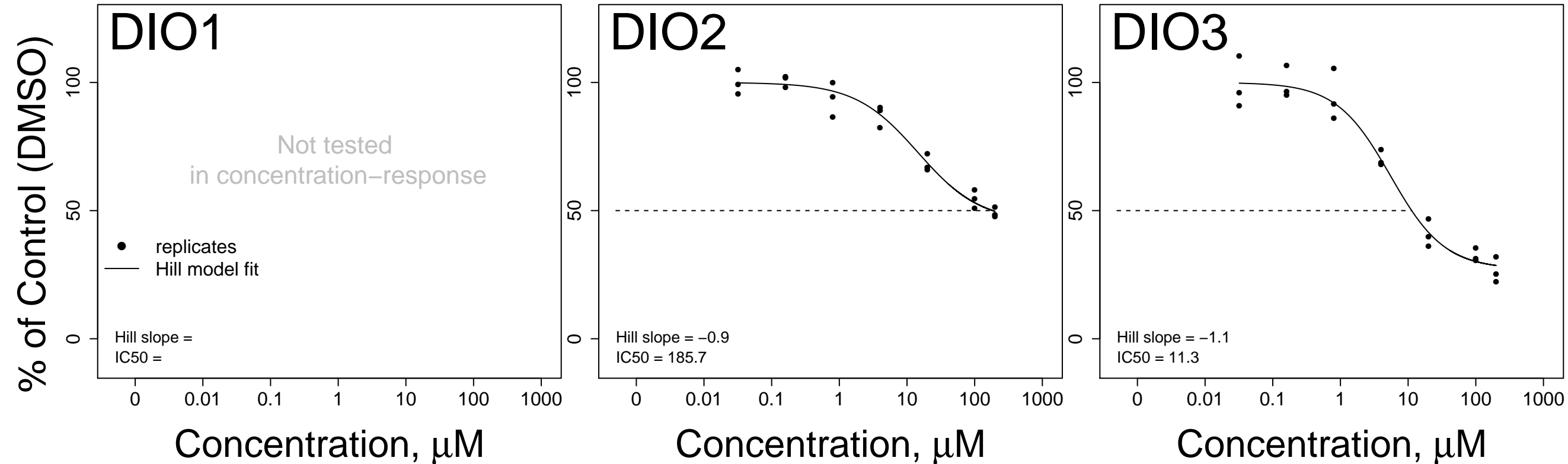
HMR1171 trifluoroacetate (1:1) CASRN: NOCAS_48522



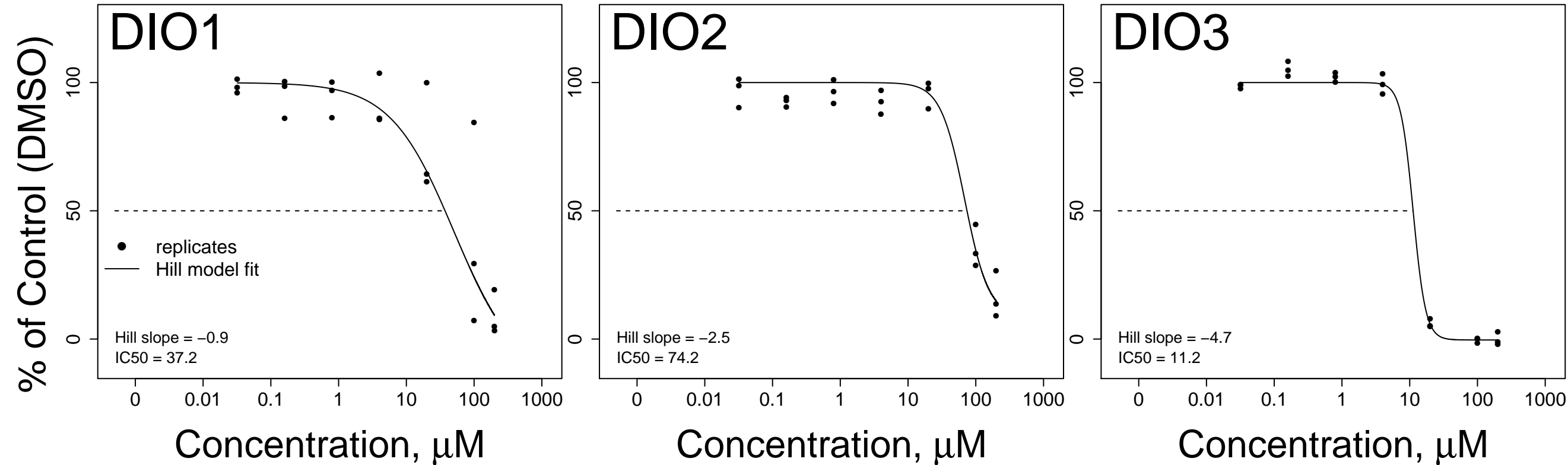
2-Ethylhexyl acrylate CASRN: 103-11-7



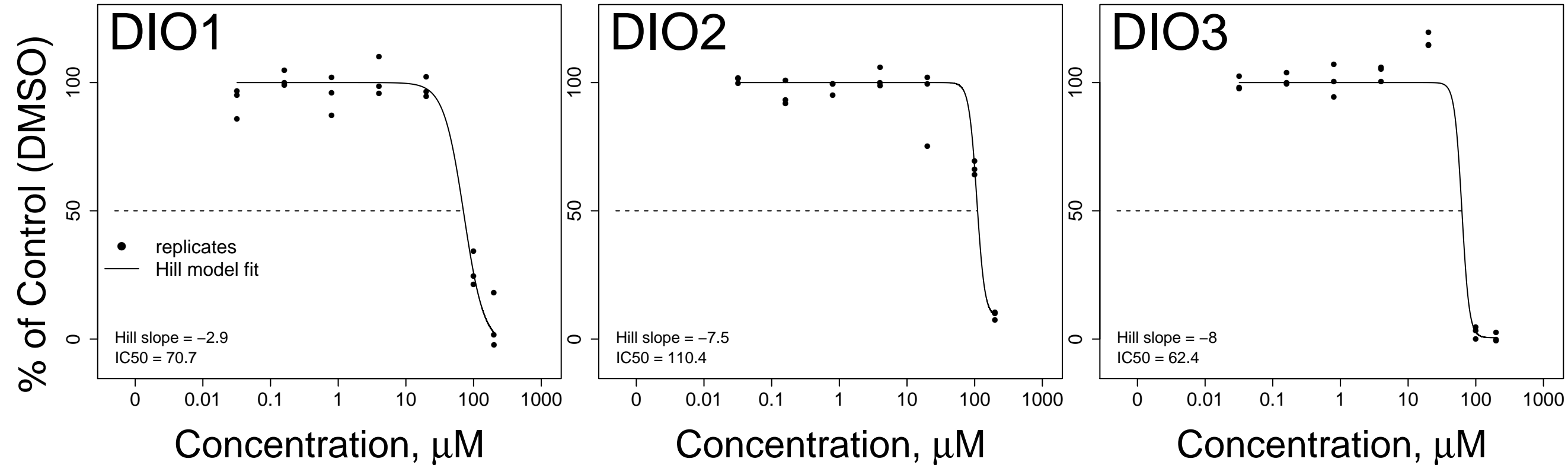
Benzyl cinnamate CASRN: 103-41-3



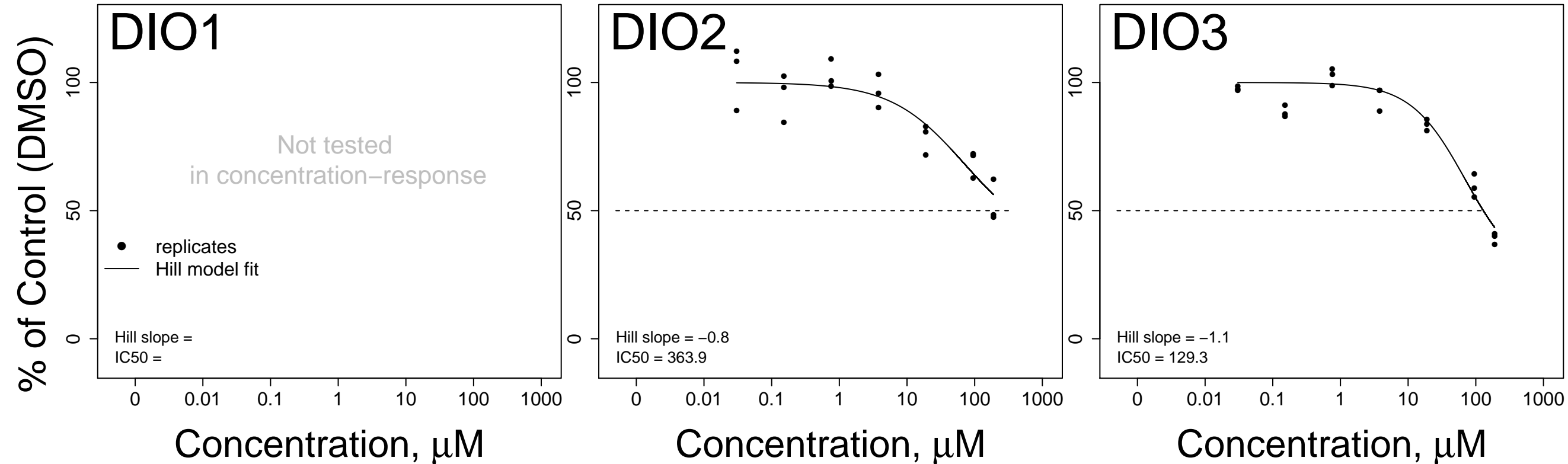
4-Dodecylphenol CASRN: 104-43-8



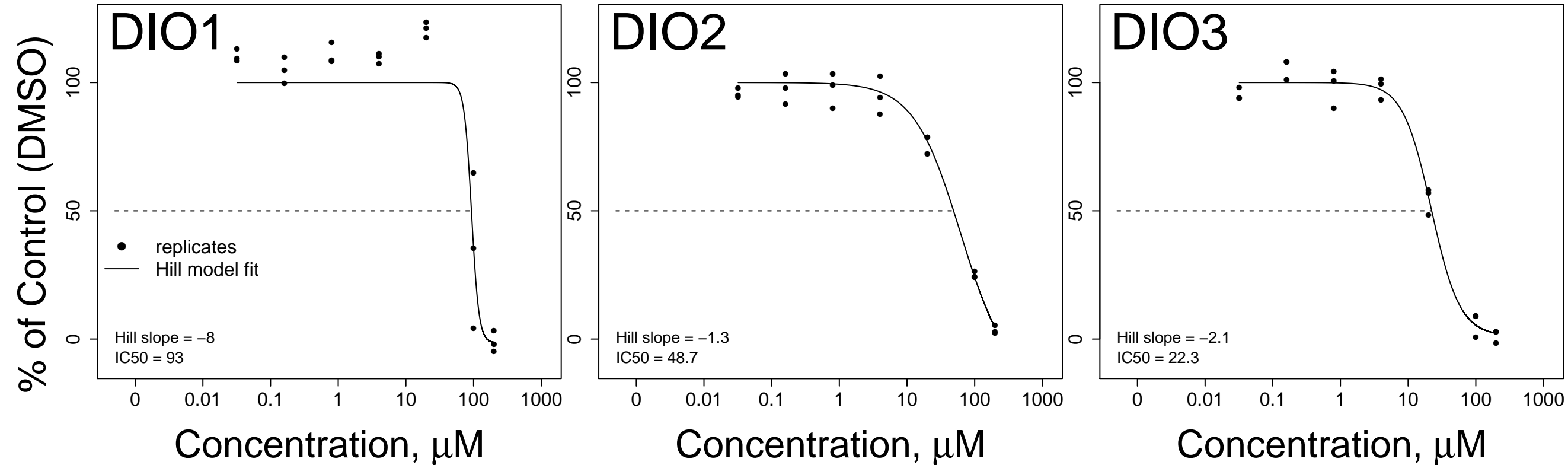
Heptylparaben CASRN: 1085-12-7



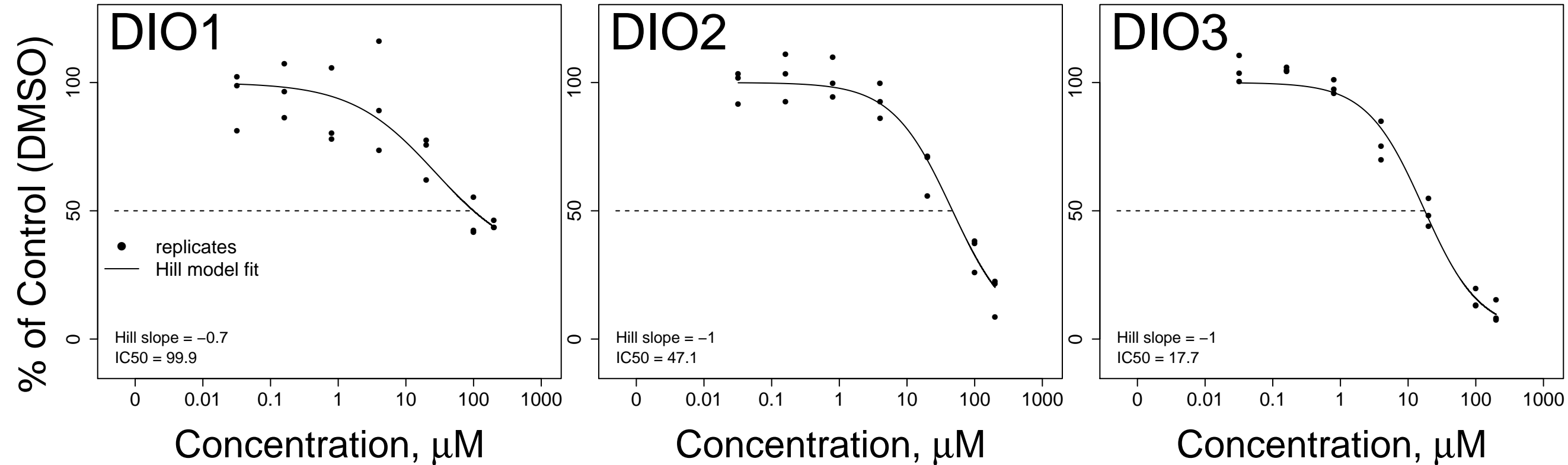
Propanedinitrile CASRN: 109-77-3



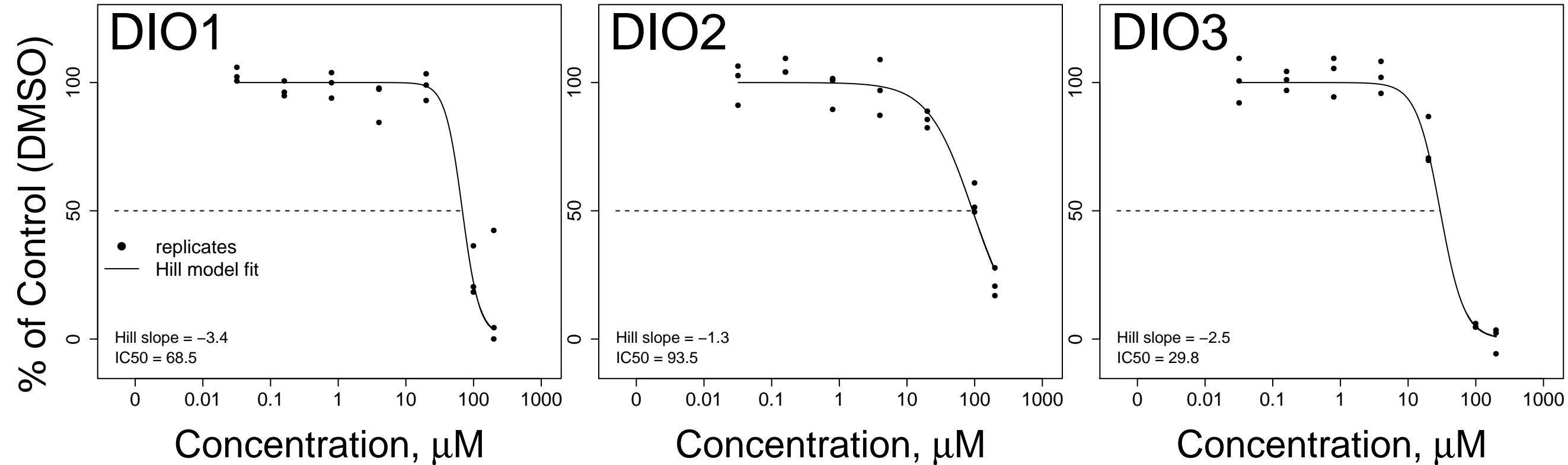
Oleyl sarcosine CASRN: 110-25-8



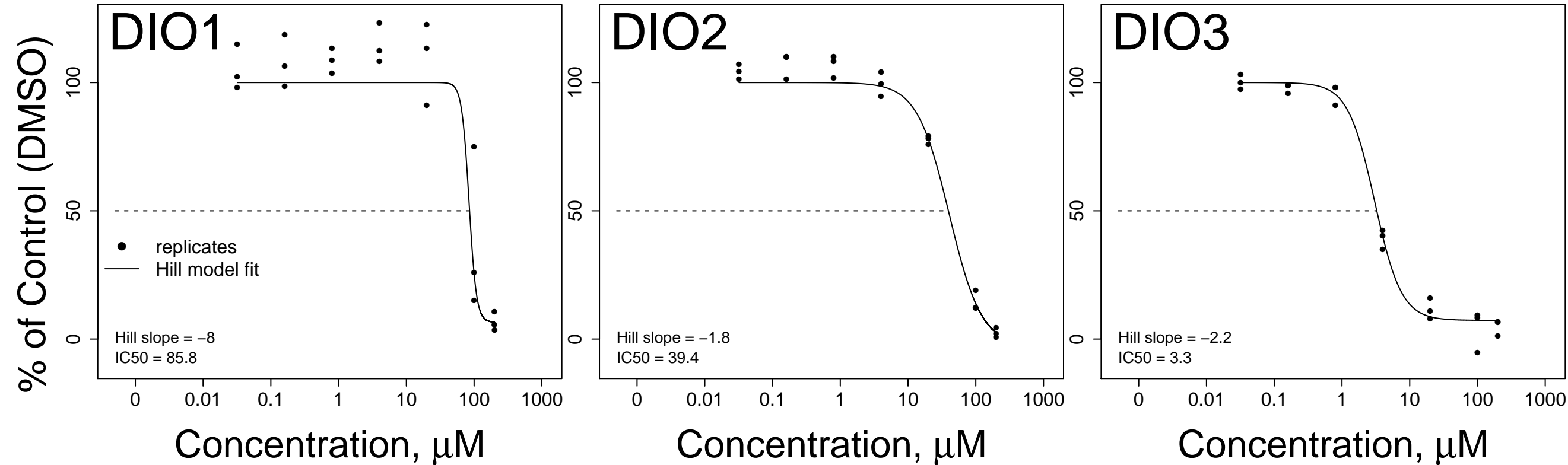
Methyl linoleate CASRN: 112-63-0



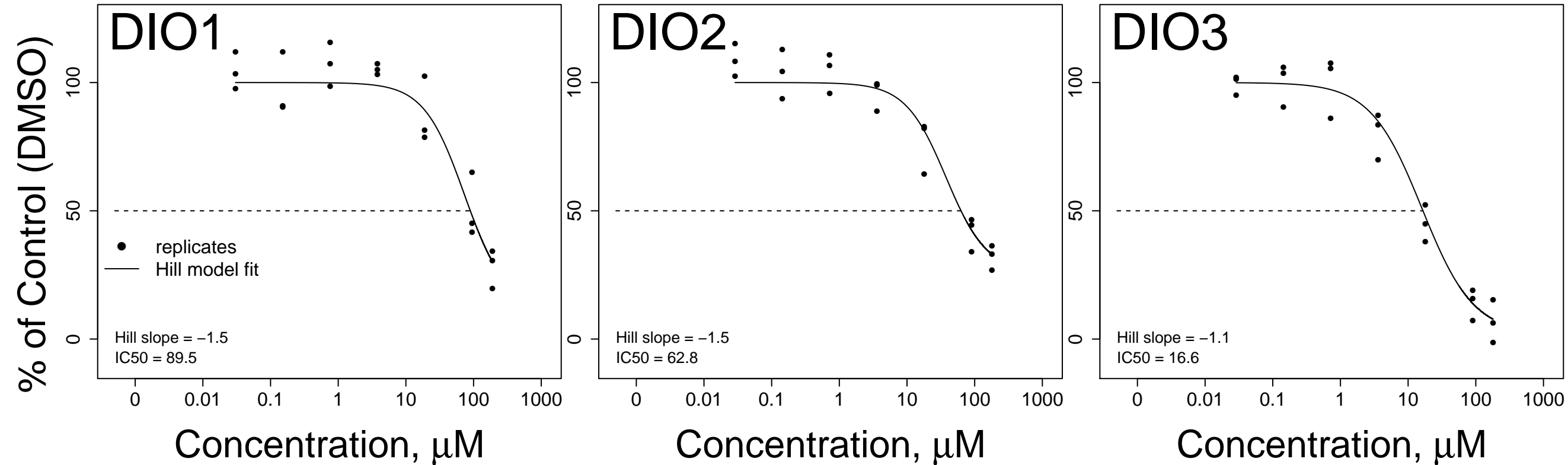
Oleic acid CASRN: 112-80-1



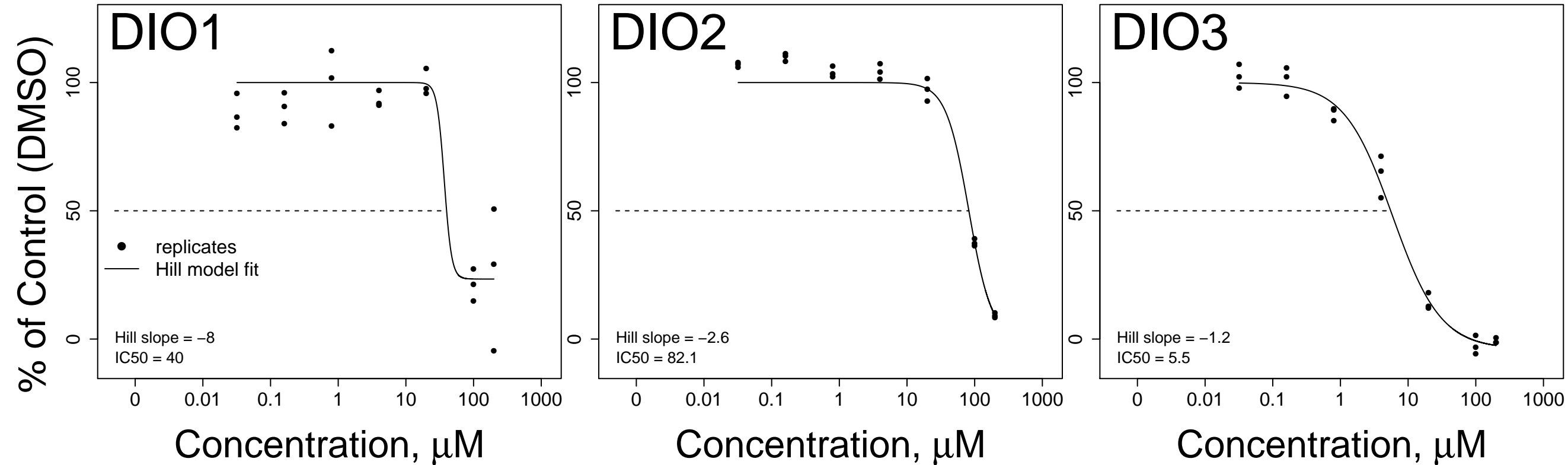
Octadecyl sulfate sodium salt CASRN: 1120-04-3



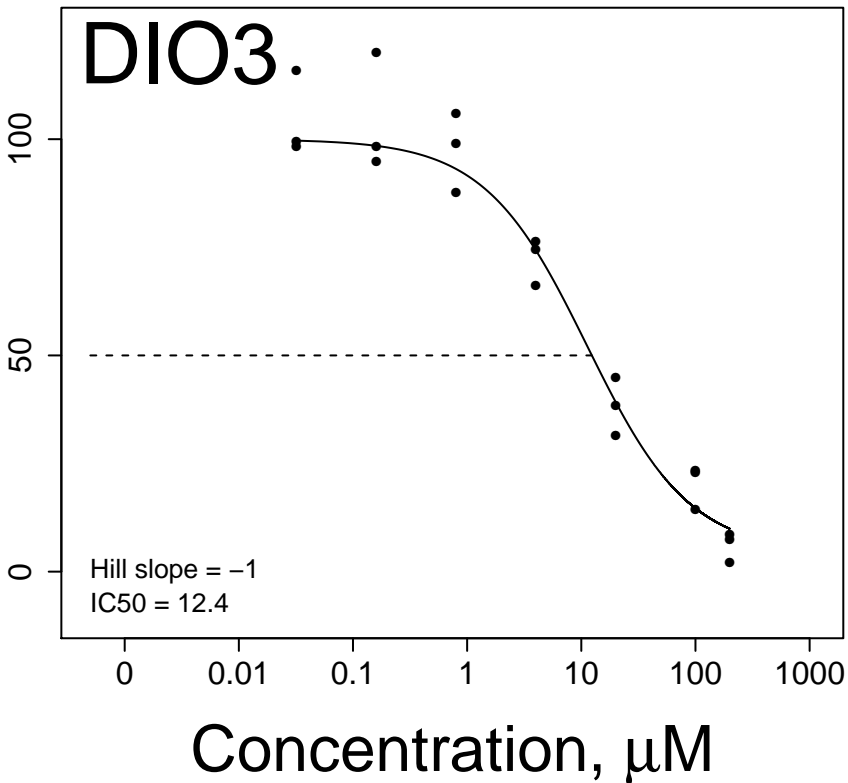
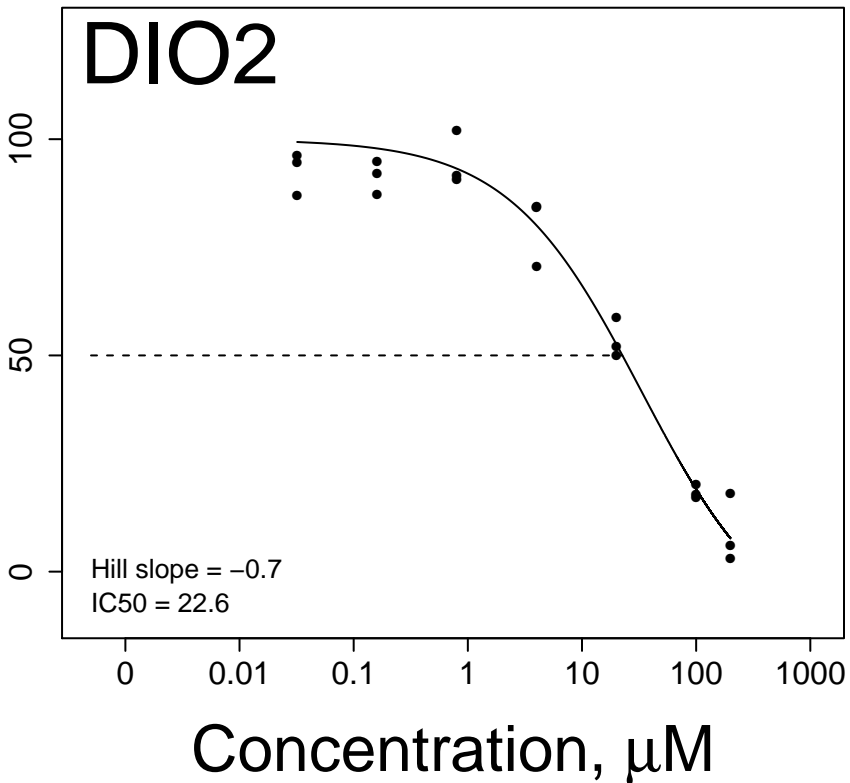
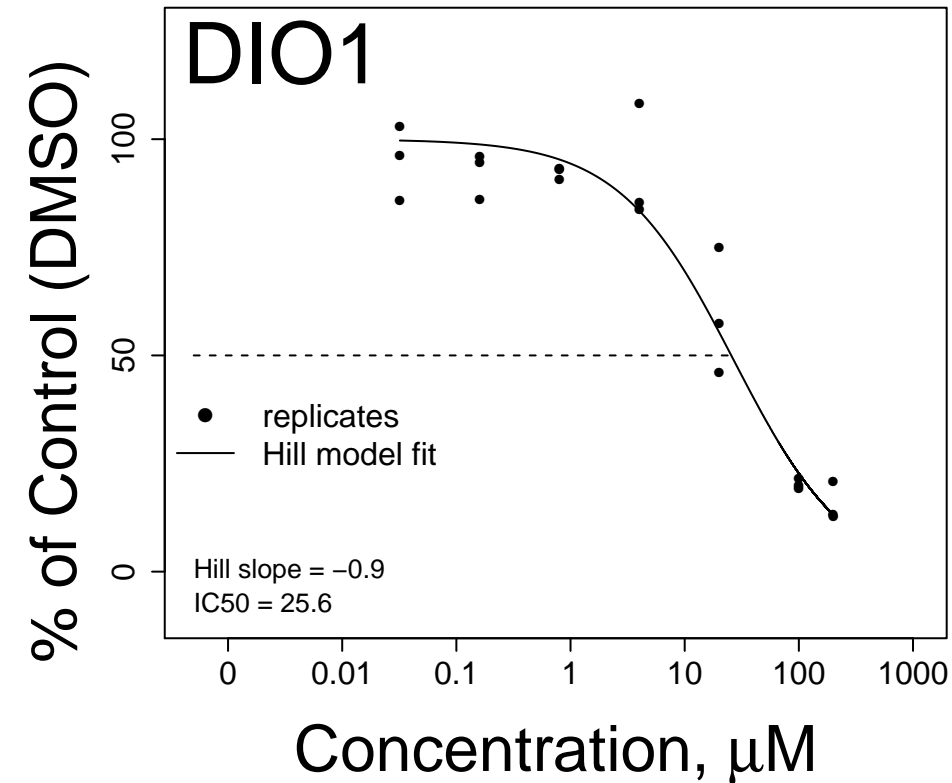
Bromophenol blue CASRN: 115-39-9



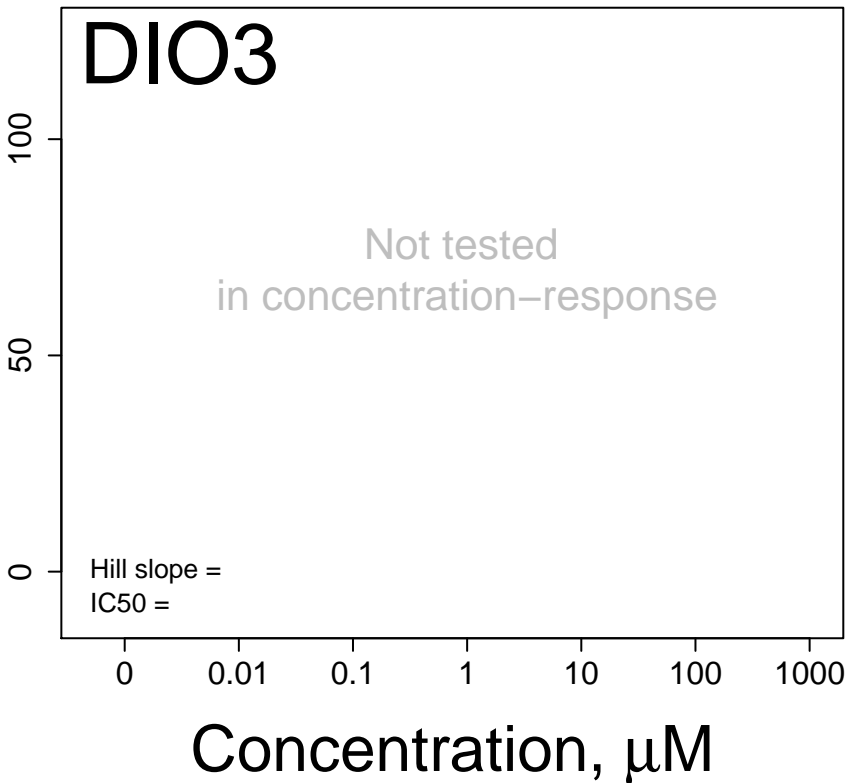
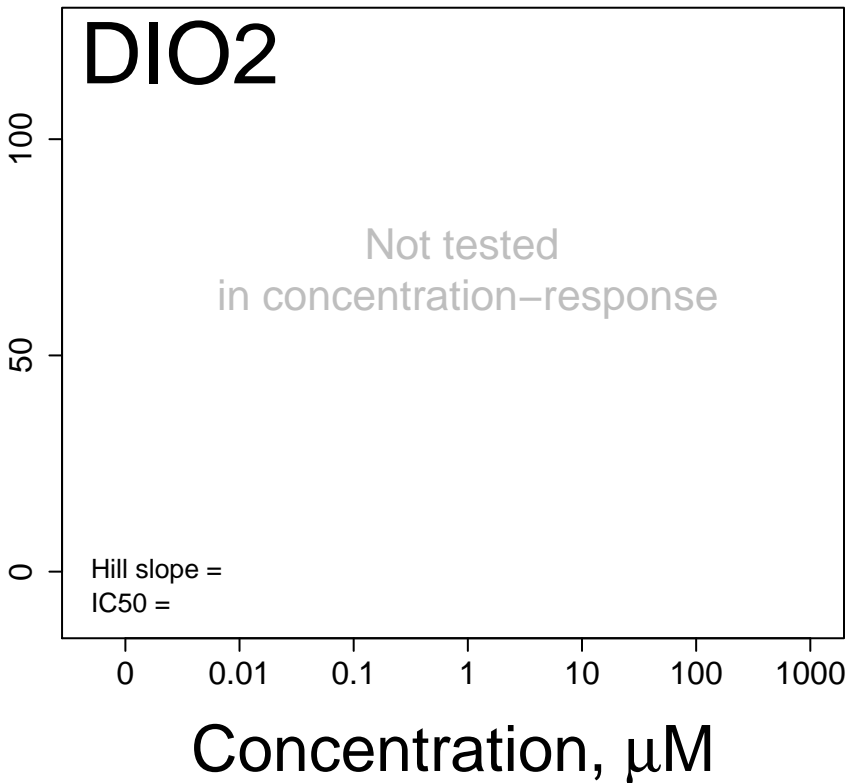
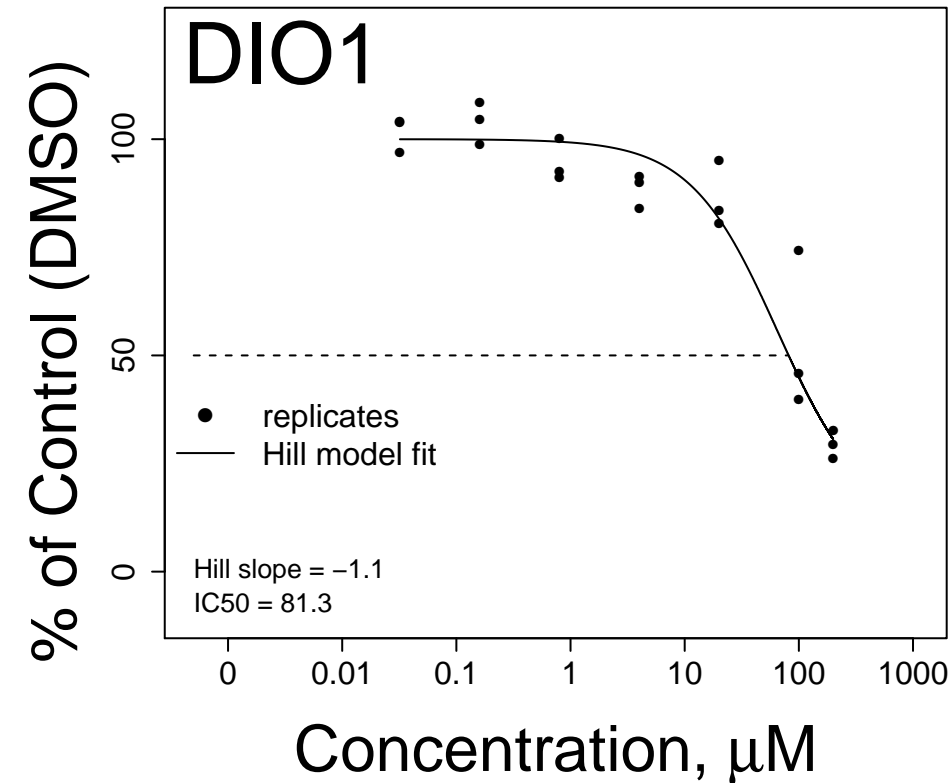
Dodecyl gallate CASRN: 1166-52-5



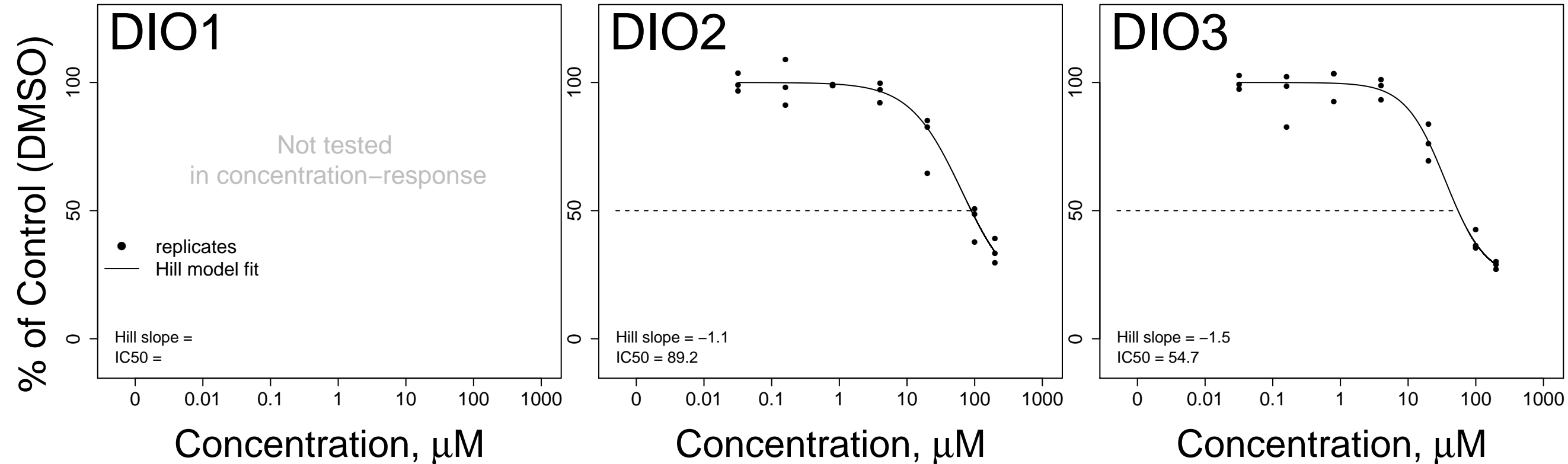
Dichlone CASRN: 117-80-6



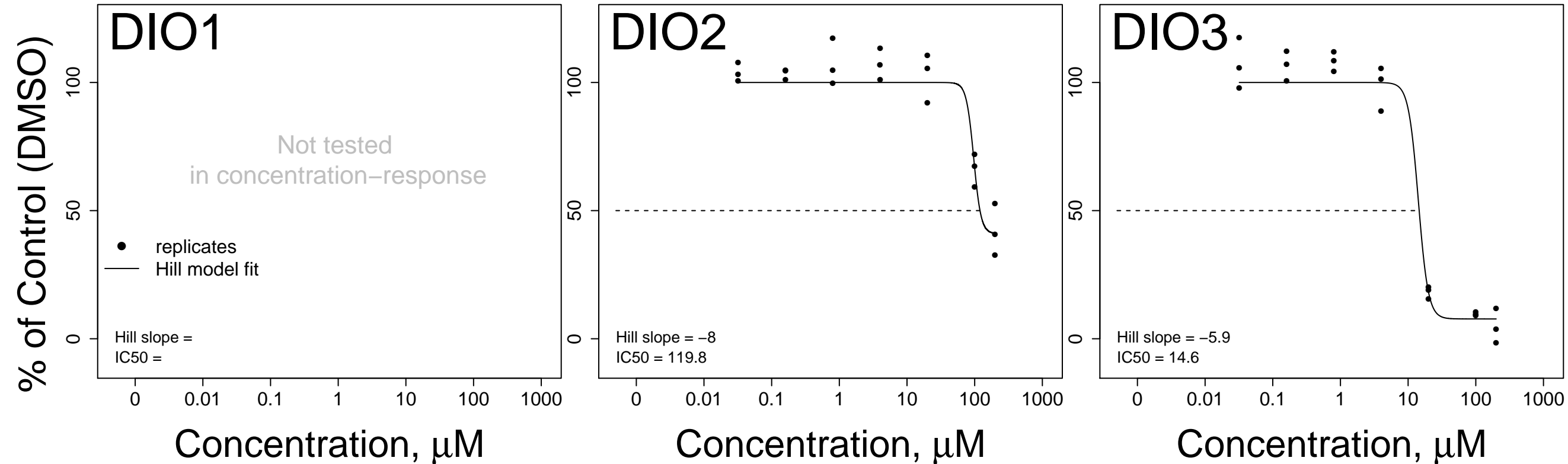
Pyrazolone T CASRN: 118-47-8



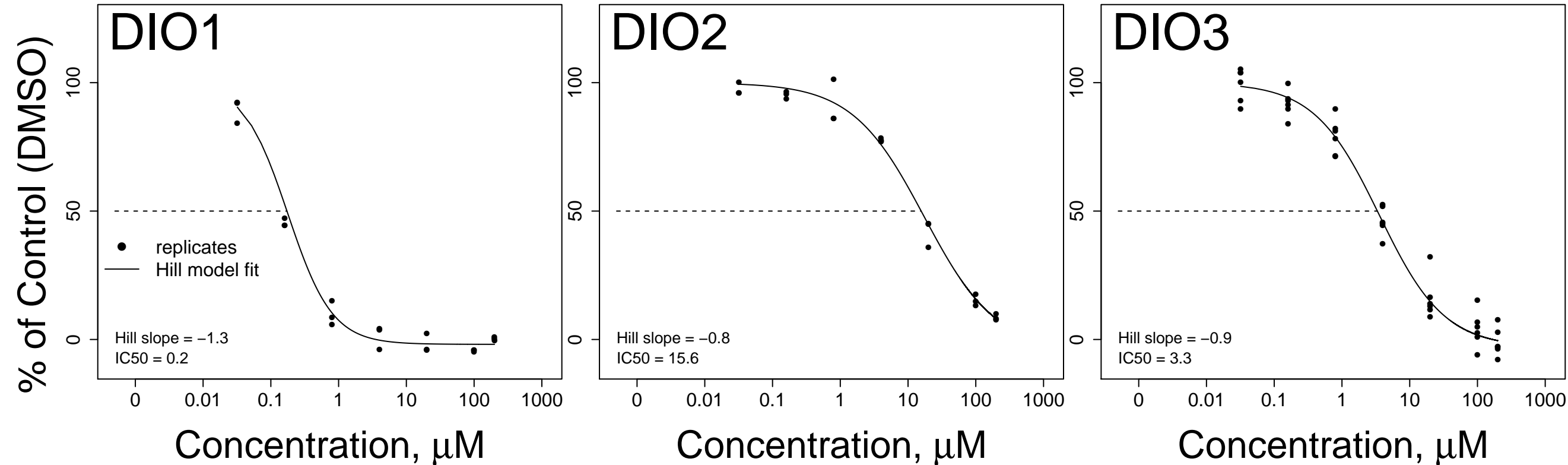
1,3-Butyleneglycol dimethacrylate CASRN: 1189-08-8



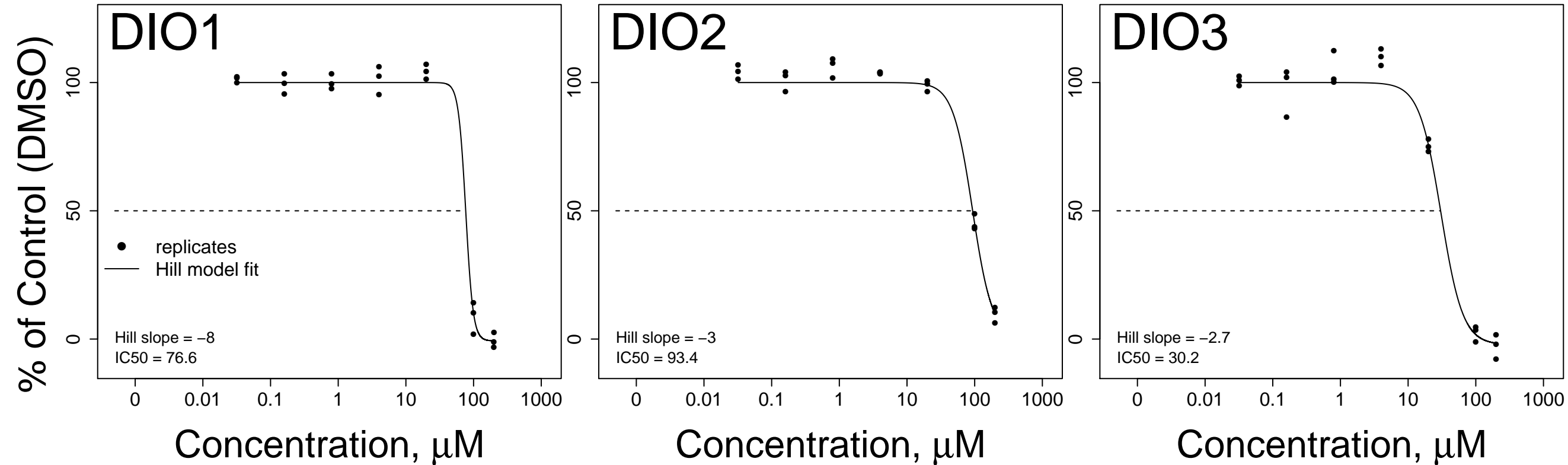
2,2'-Methylenebis(4-methyl-6-tert-butylphenol) CASRN: 119-47-1



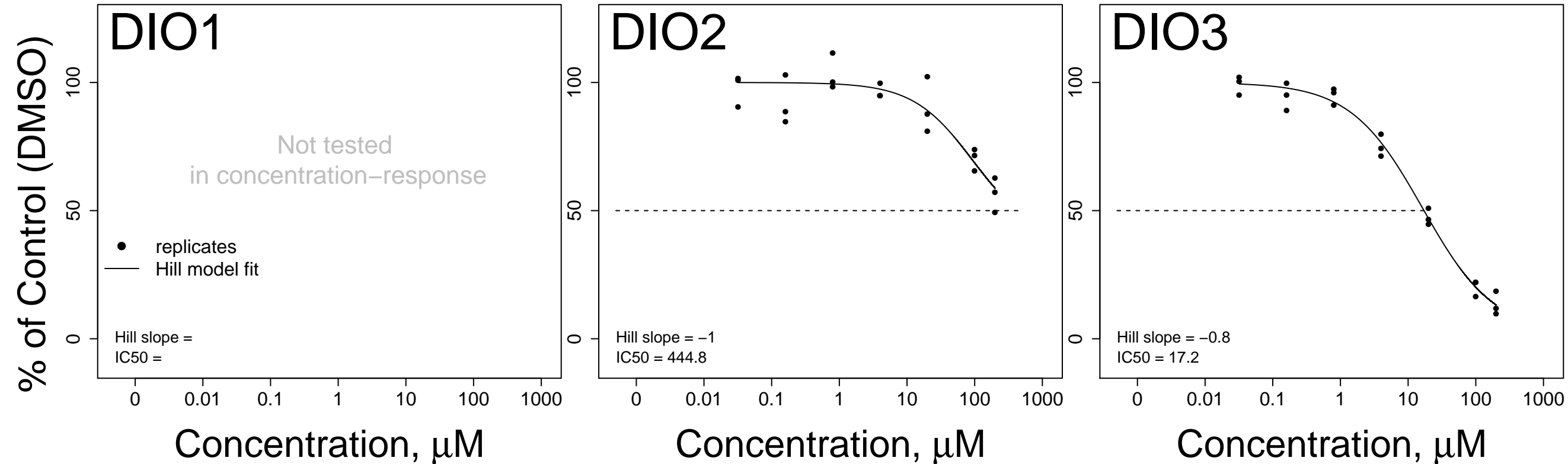
4,5-Dichloro-3H-1,2-dithiol-3-one CASRN: 1192-52-5



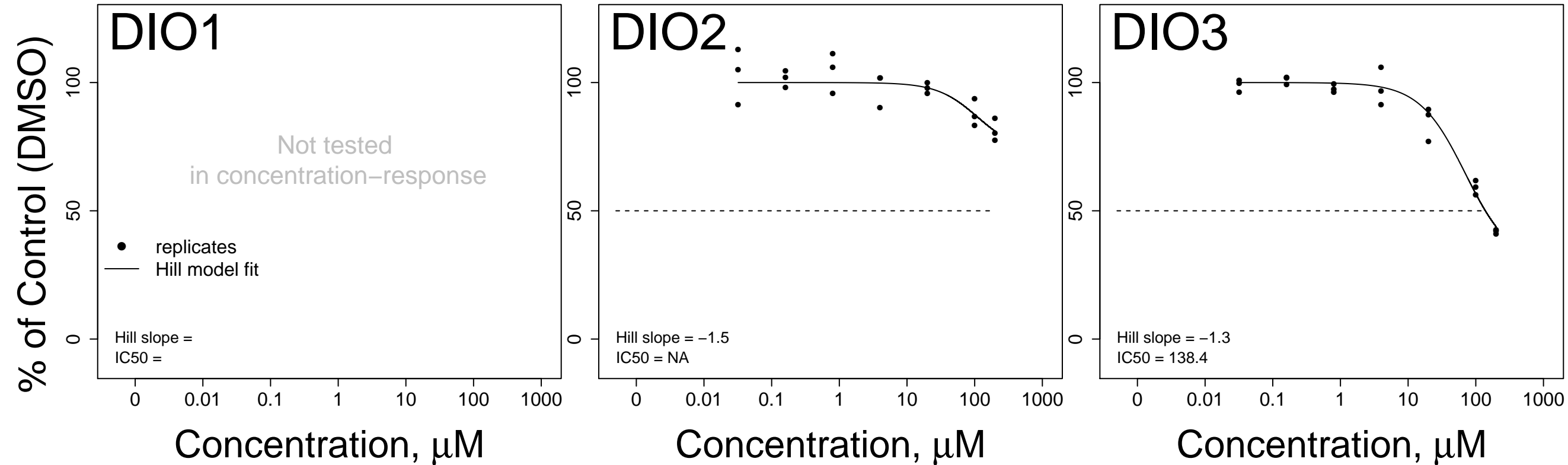
Octylparaben CASRN: 1219-38-1



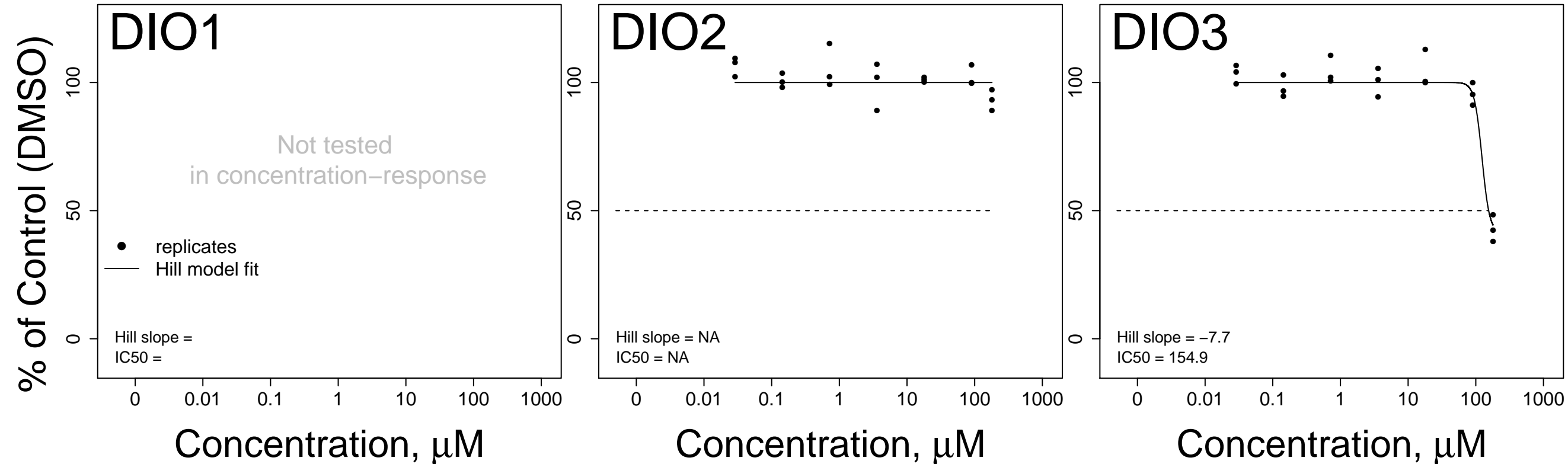
Pentylcinnamaldehyde CASRN: 122-40-7



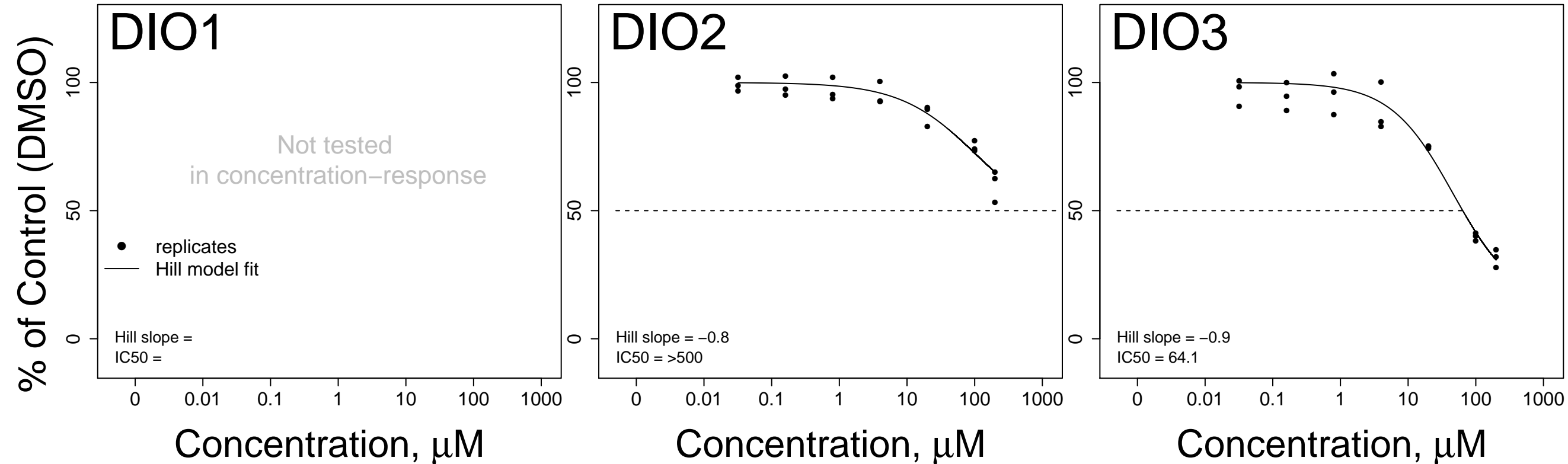
Phenylacetaldehyde CASRN: 122-78-1



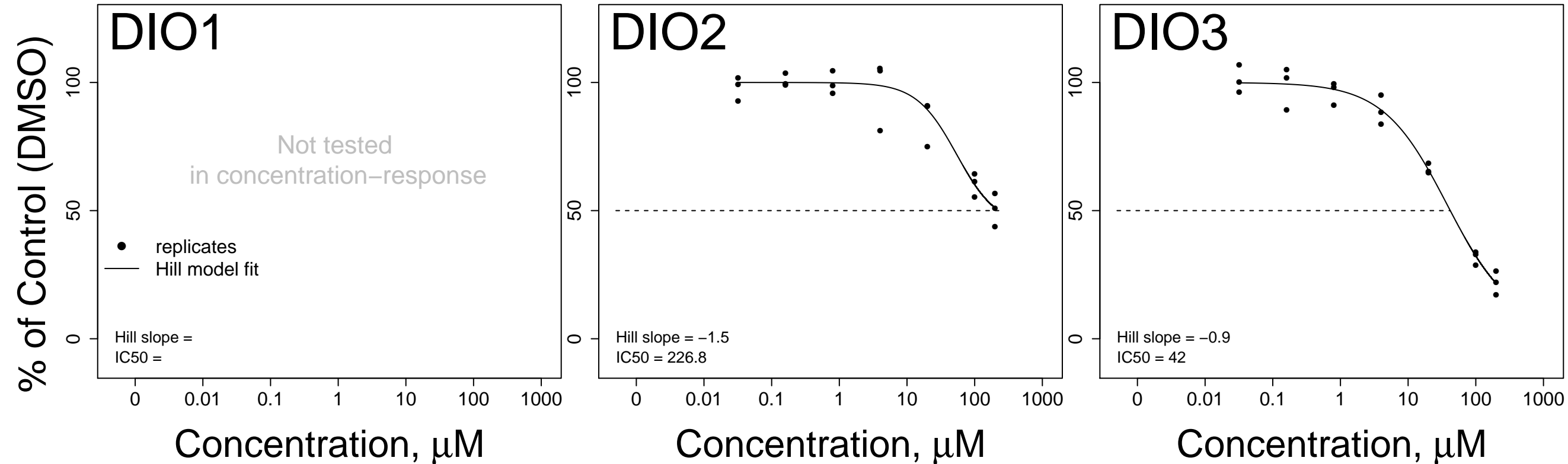
1-Dodecanamine CASRN: 124-22-1



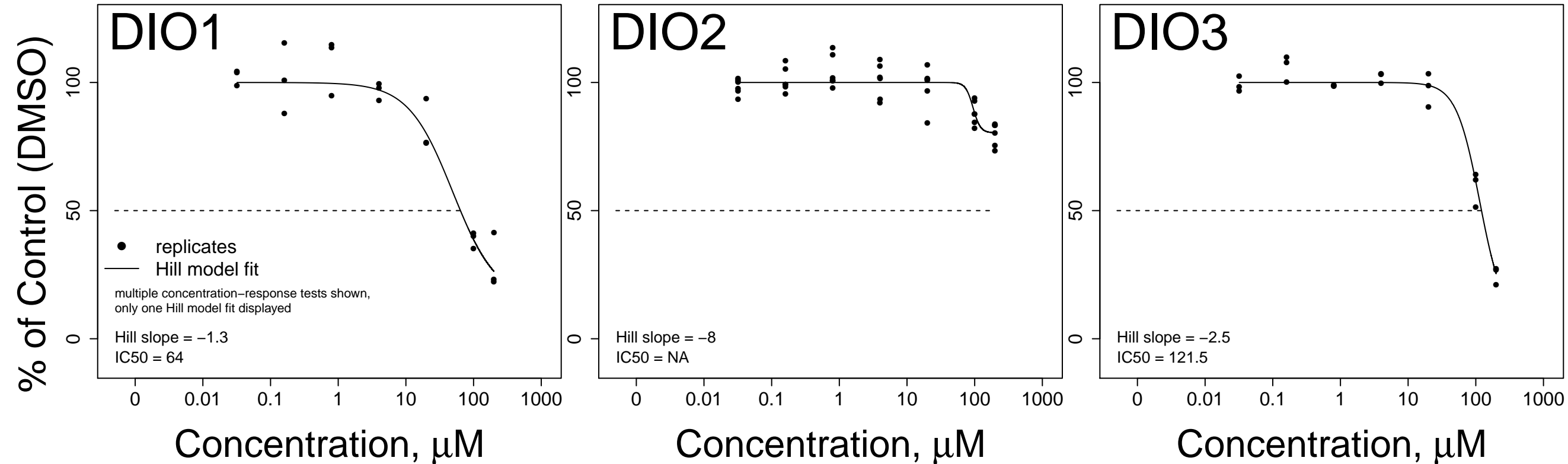
Methyl abietate CASRN: 127-25-3



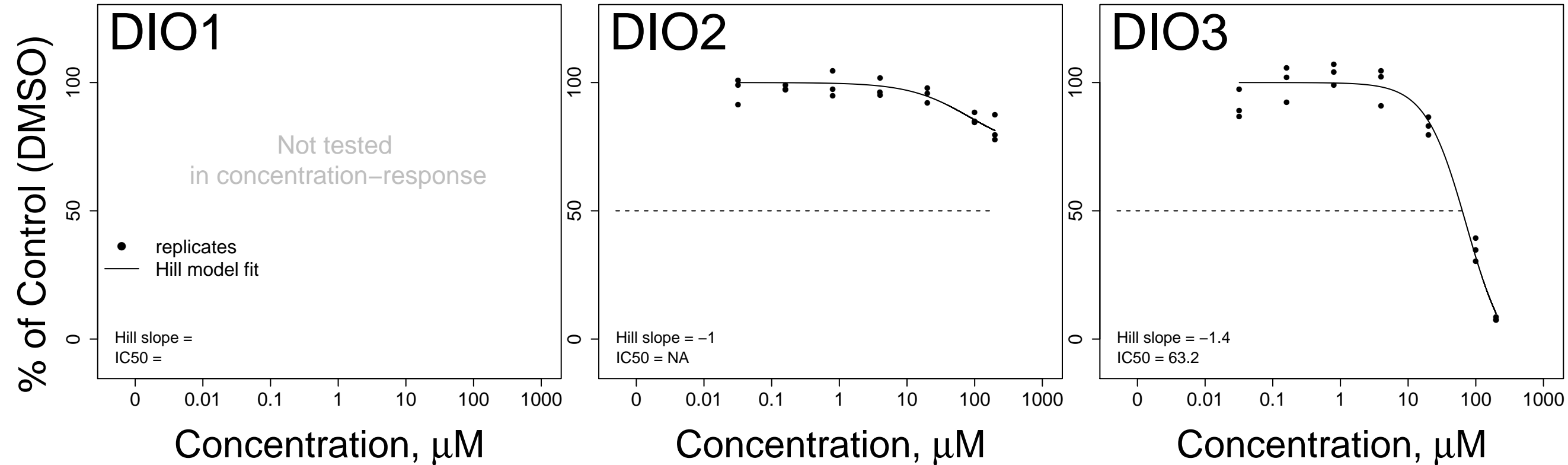
Retinol acetate CASRN: 127-47-9



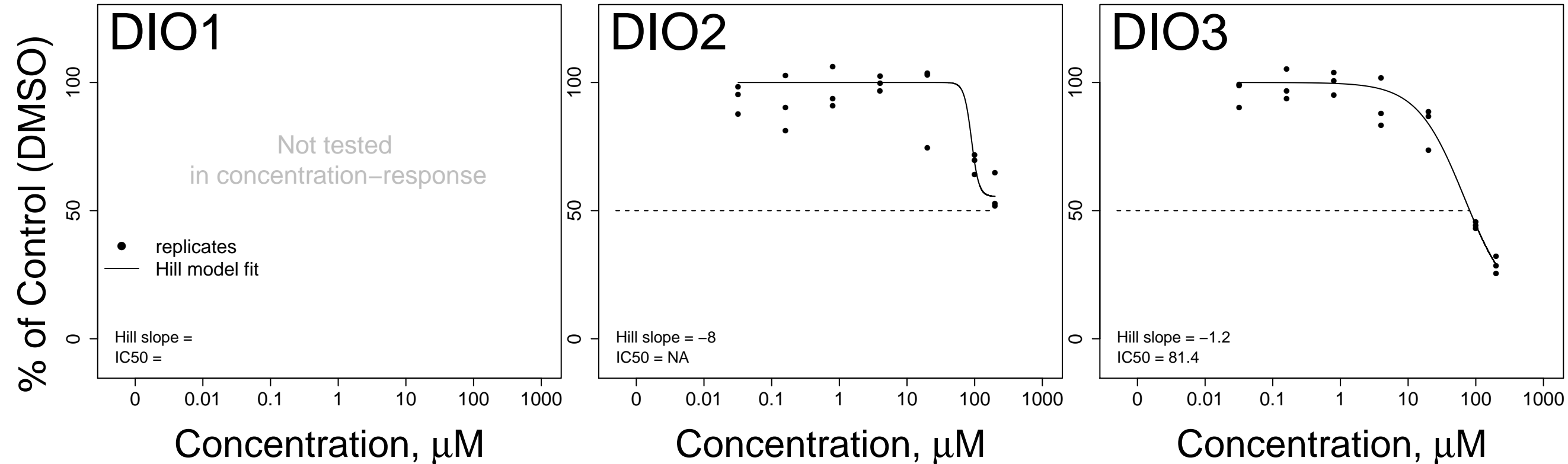
C.I. Acid Orange 24, monosodium salt CASRN: 1320-07-6



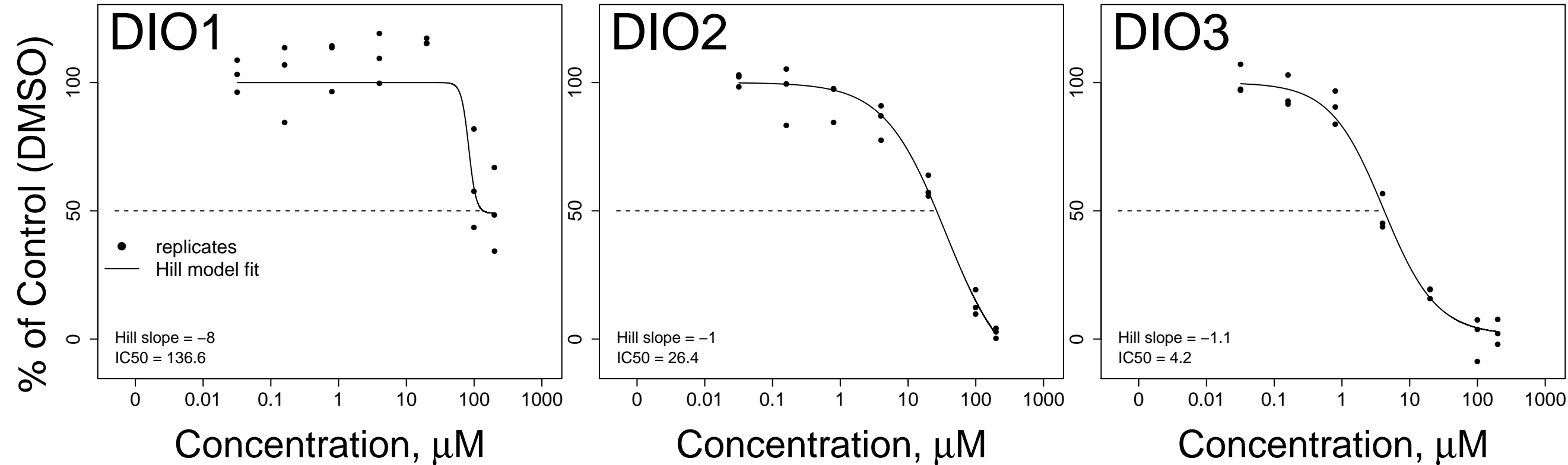
C.I. Disperse Orange 37 CASRN: 13301-61-6



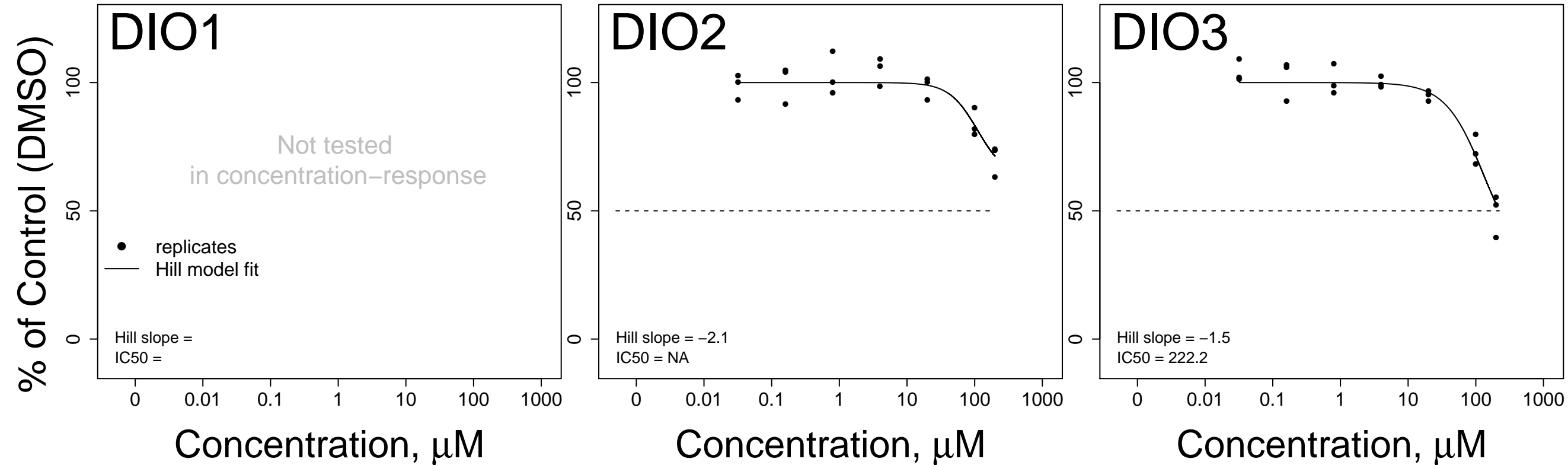
Methylionone CASRN: 1335-46-2



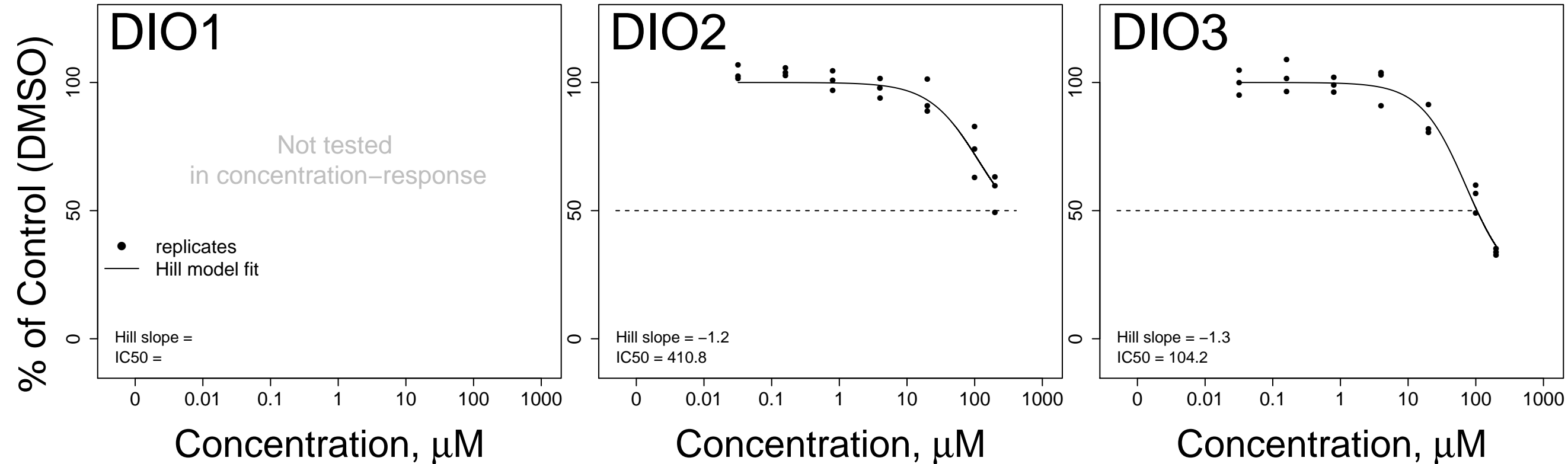
Ascorbyl palmitate CASRN: 137-66-6



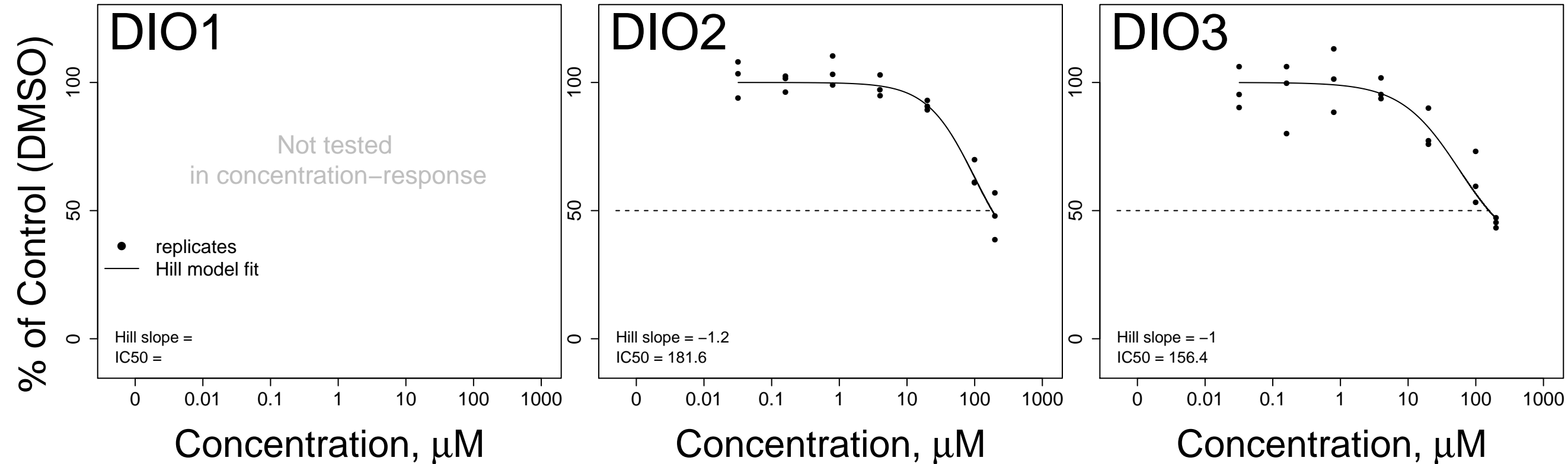
Phenol red CASRN: 143-74-8



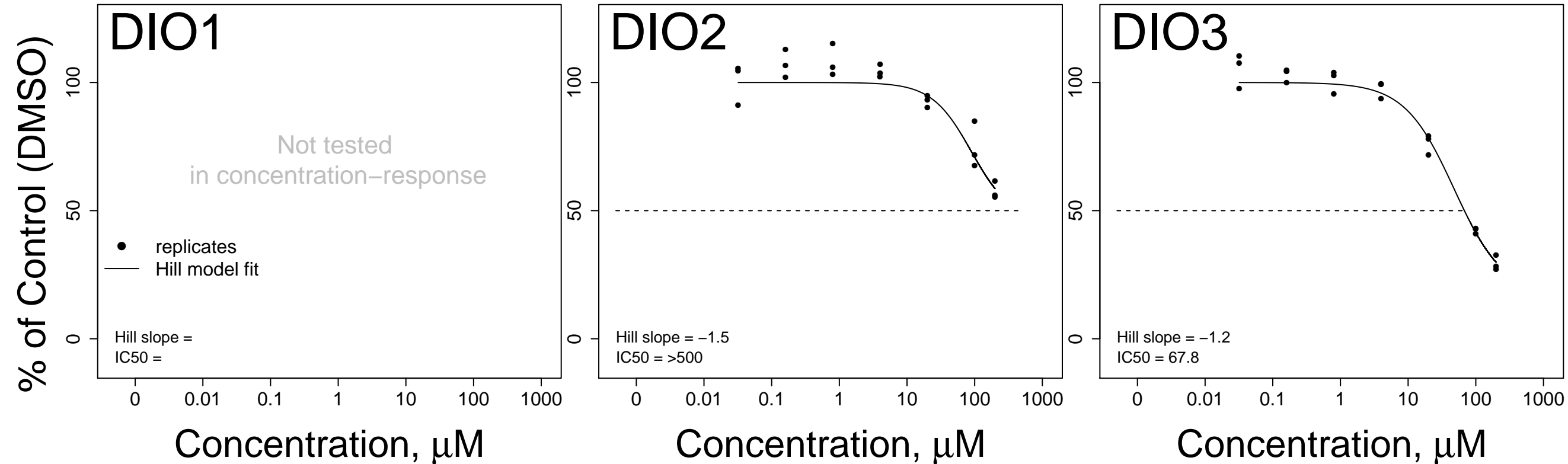
Sodium abietate CASRN: 14351-66-7



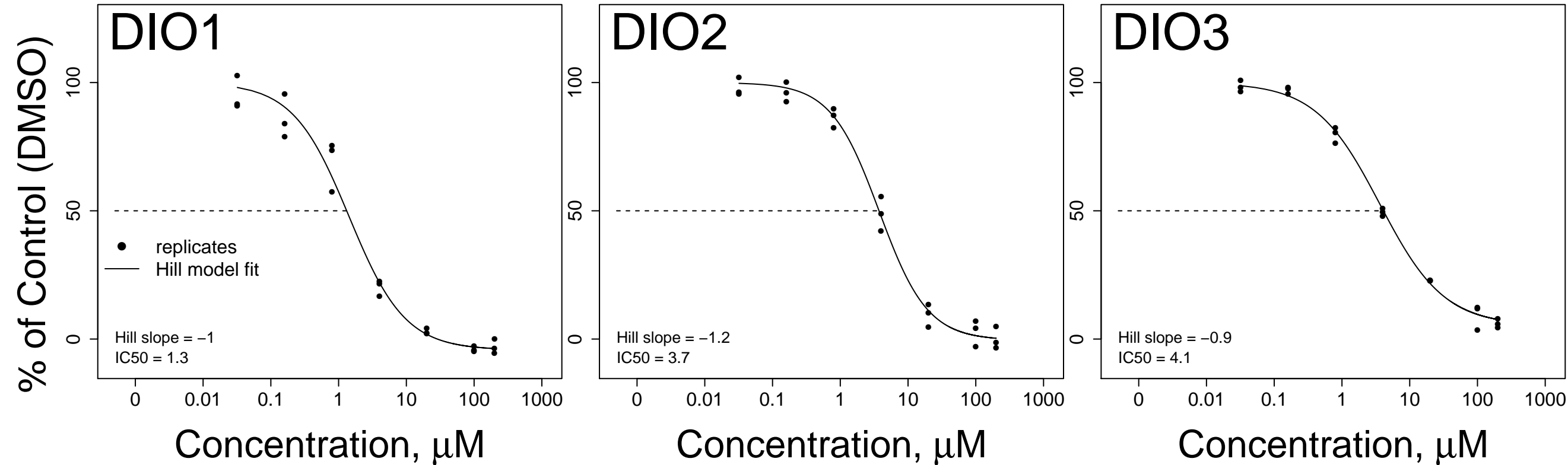
4-Nitrosodiphenylamine CASRN: 156-10-5



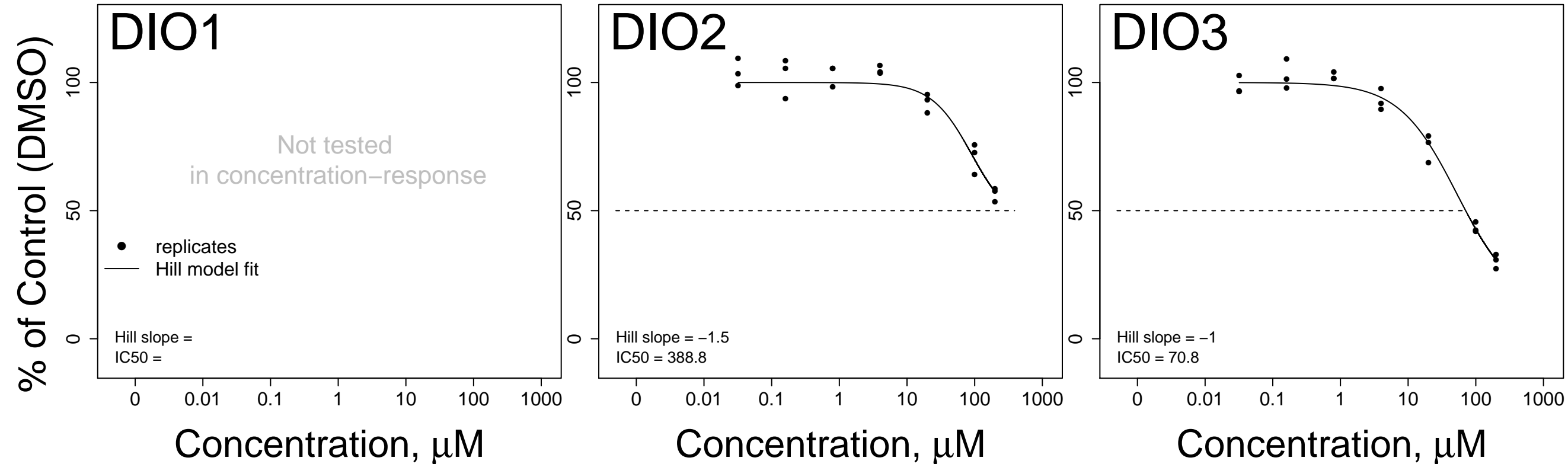
5-Ethylidene-2-norbornene CASRN: 16219-75-3



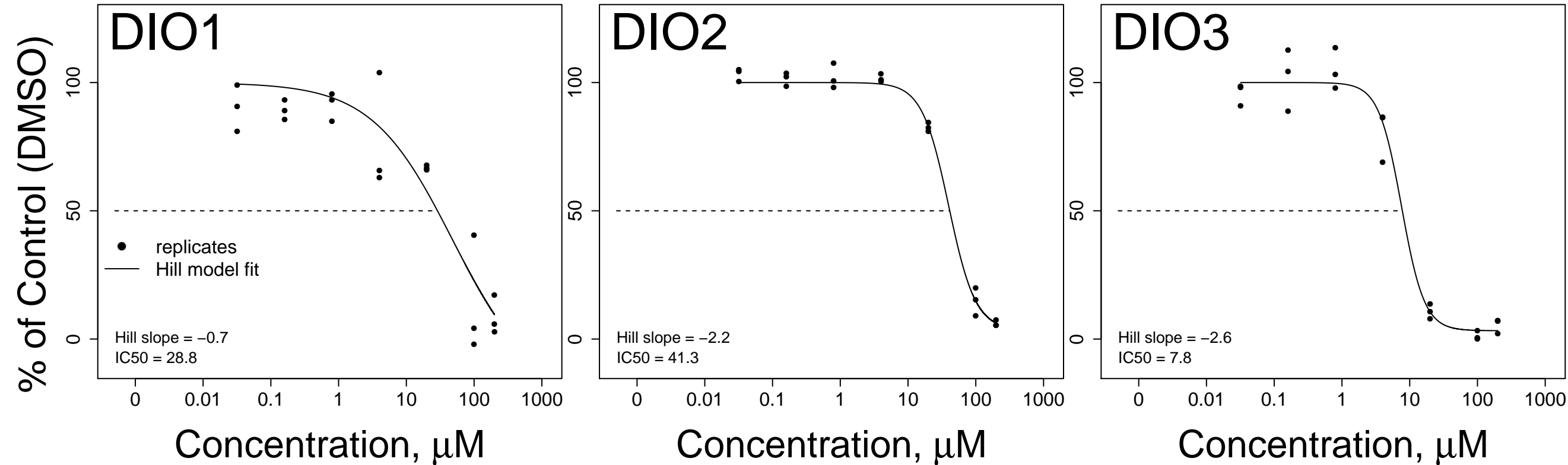
Bisphenol A diglycidyl ether CASRN: 1675-54-3



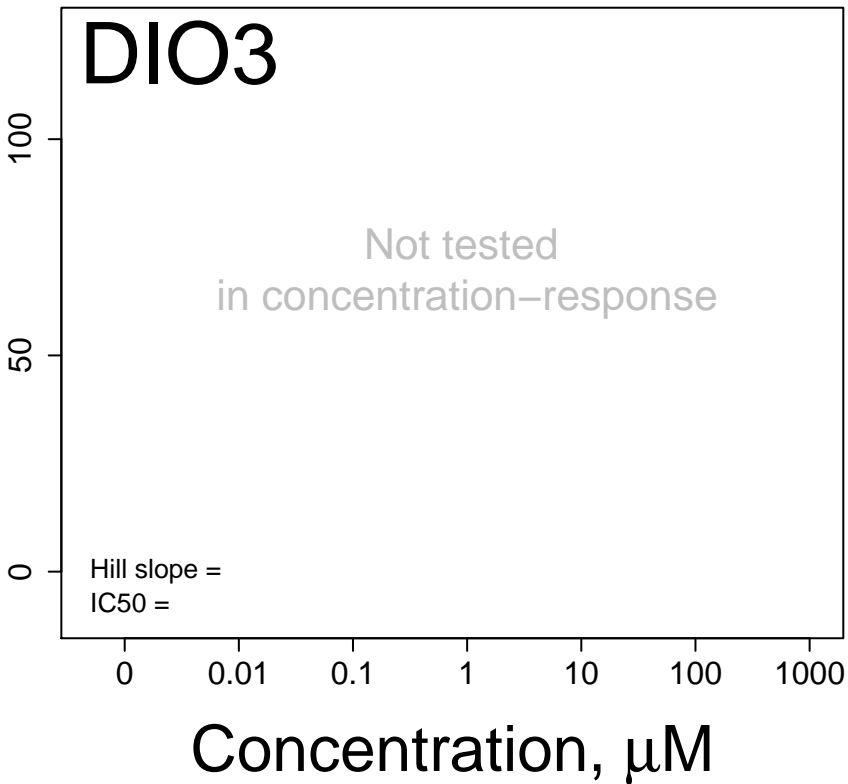
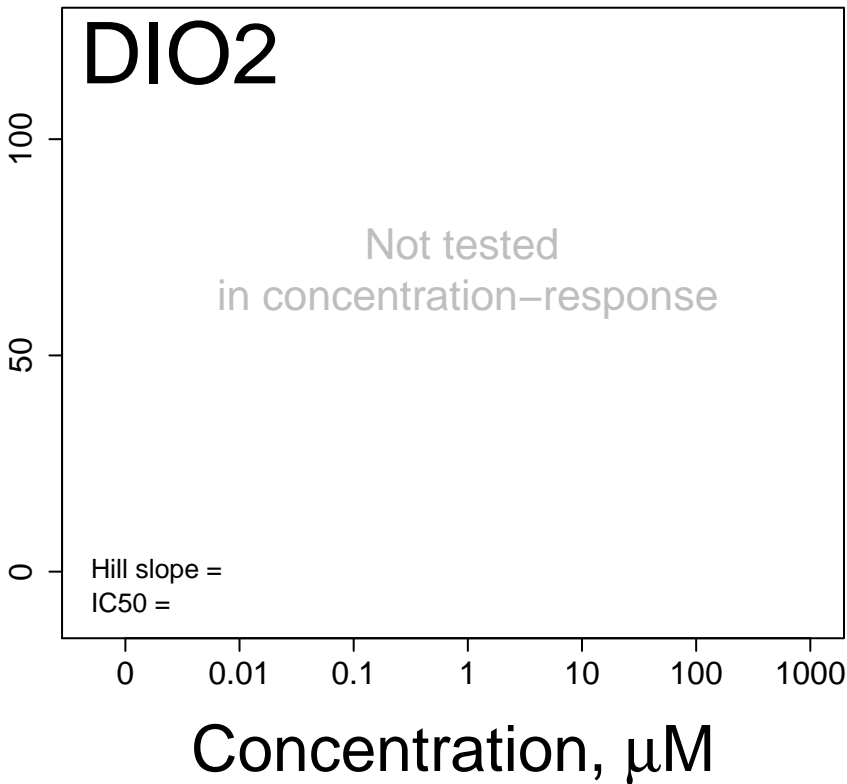
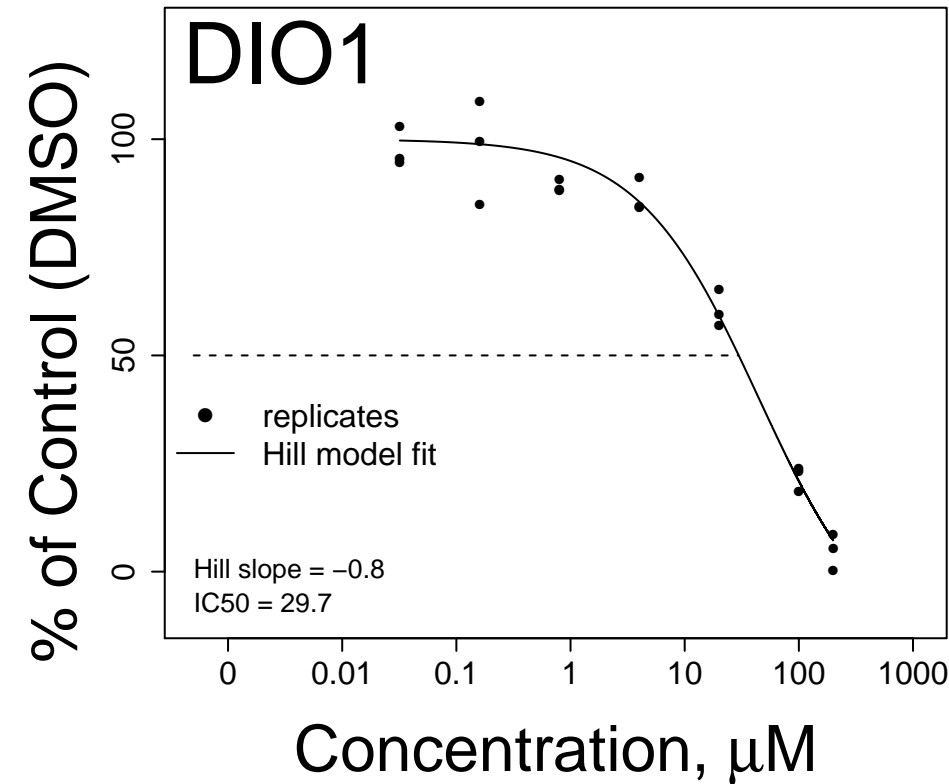
Phenylparaben CASRN: 17696-62-7



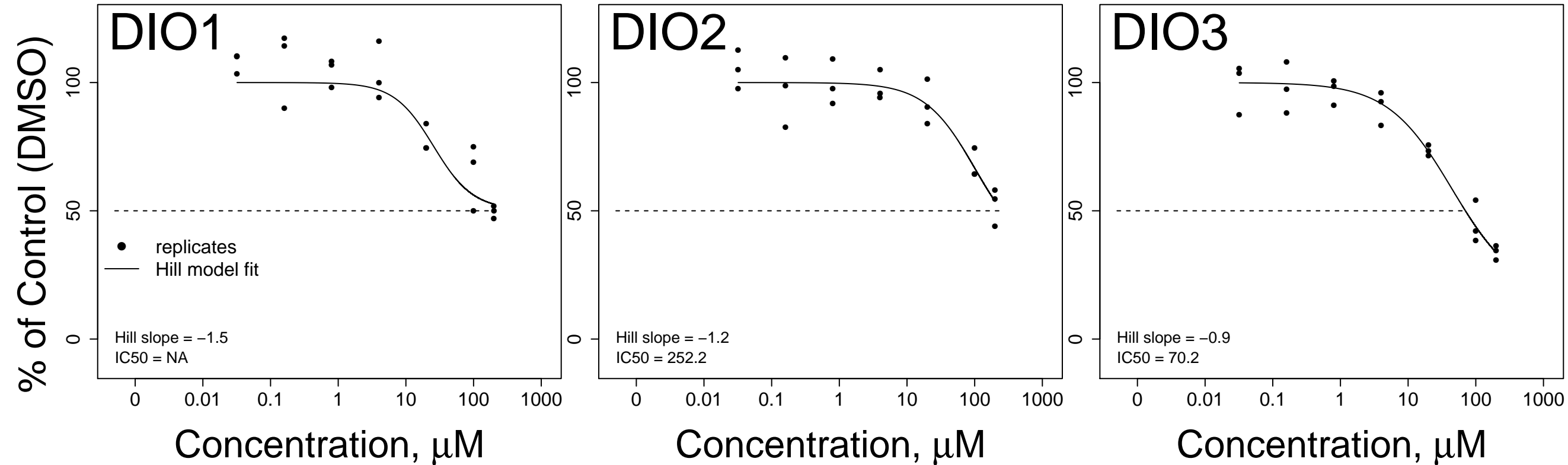
2,2'-(Tetradecylimino)diethanol CASRN: 18924-66-8



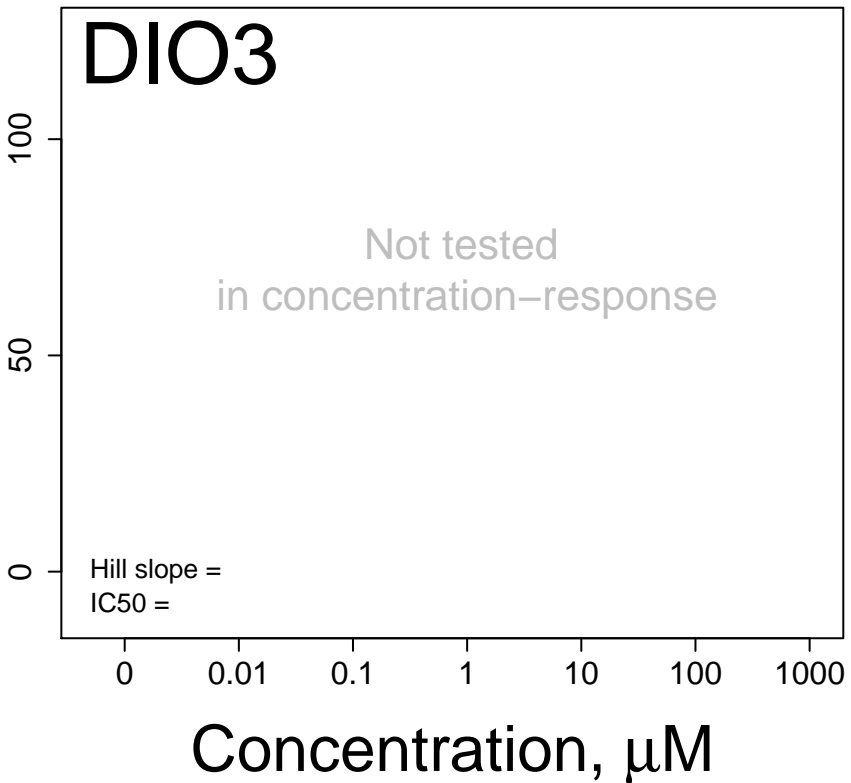
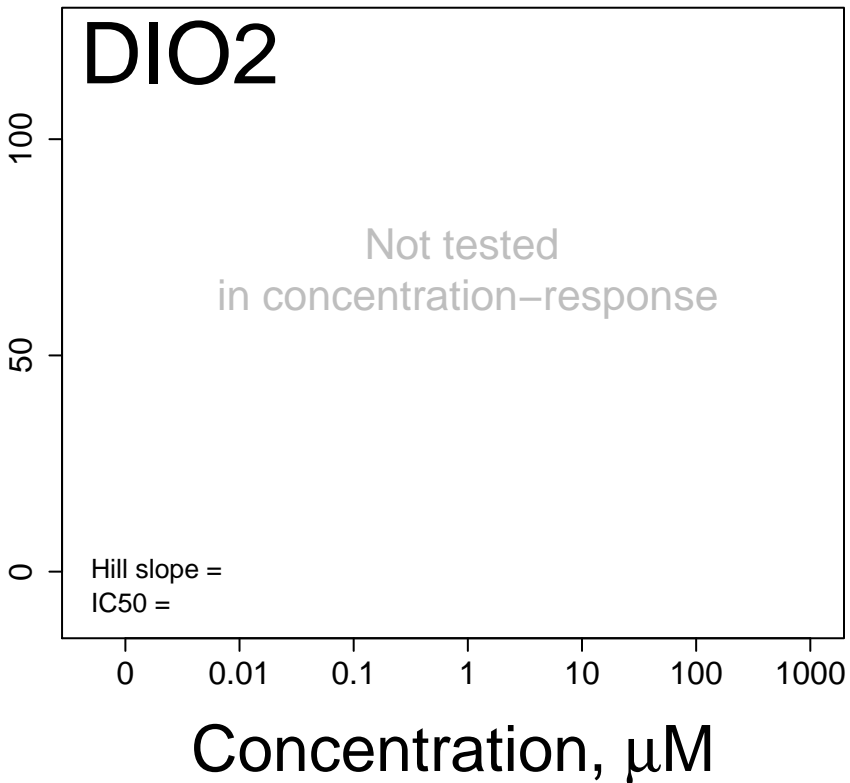
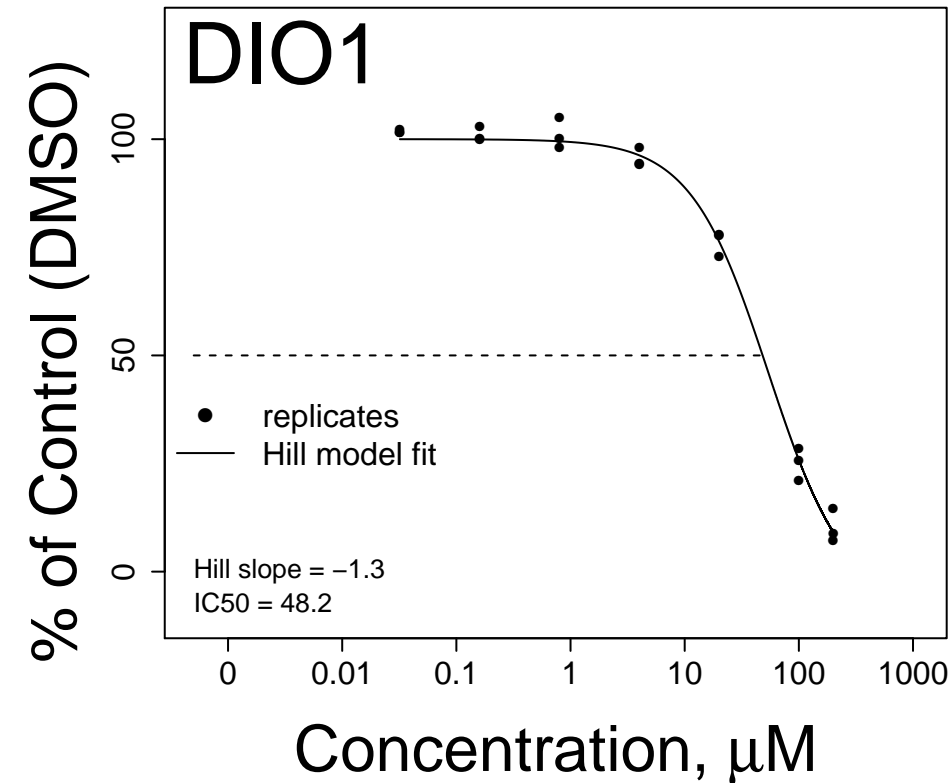
Propachlor CASRN: 1918-16-7



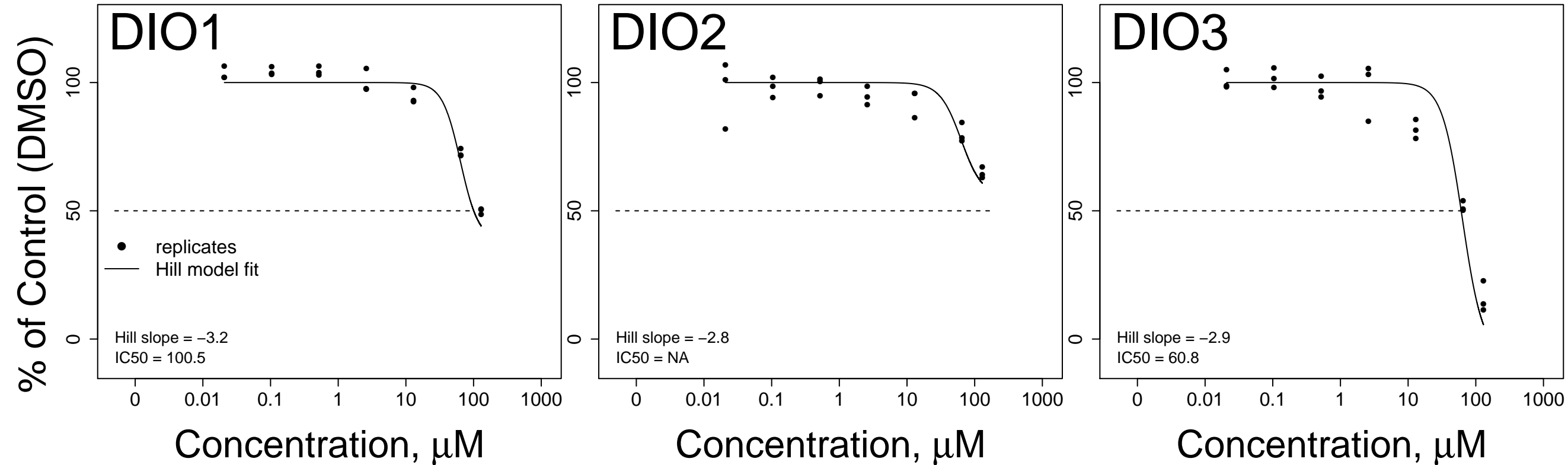
(2-Dodecenyl)succinic anhydride CASRN: 19780-11-1



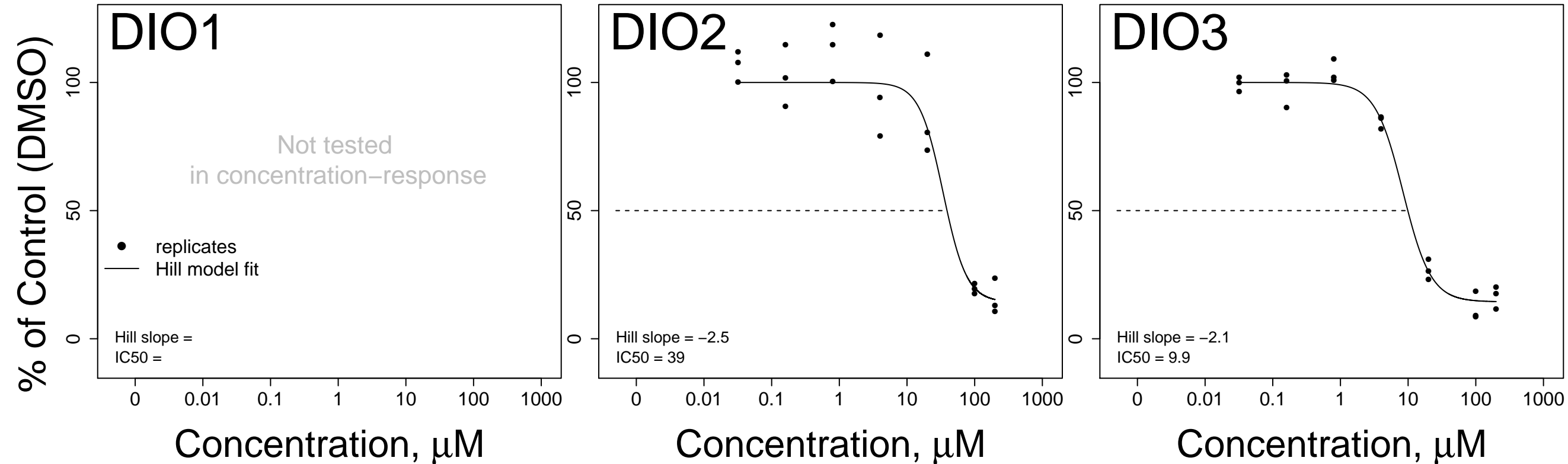
Z-Tetrachlorvinphos CASRN: 22248-79-9



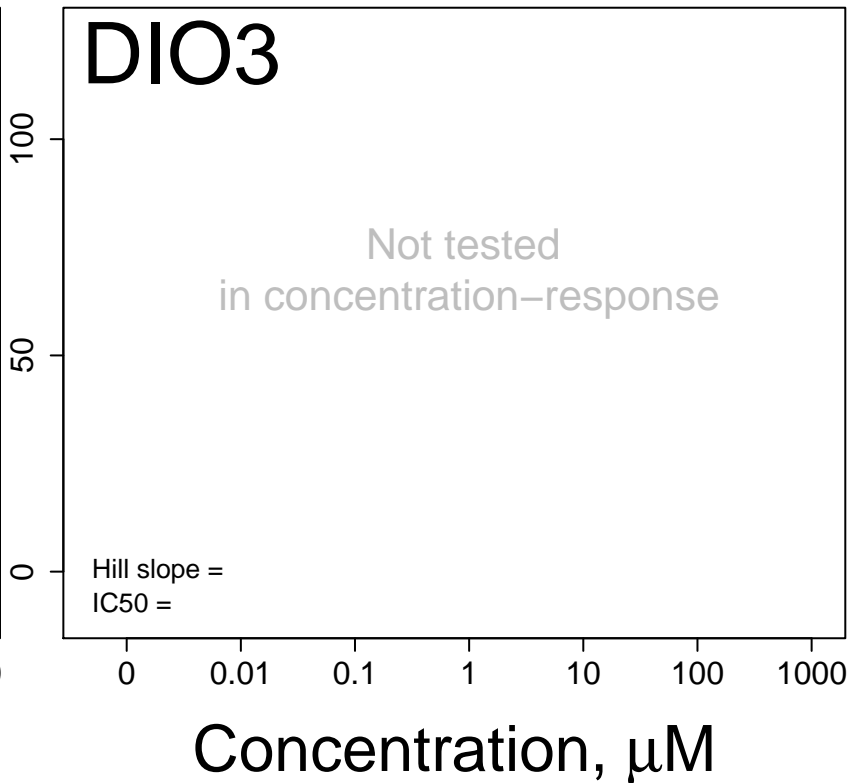
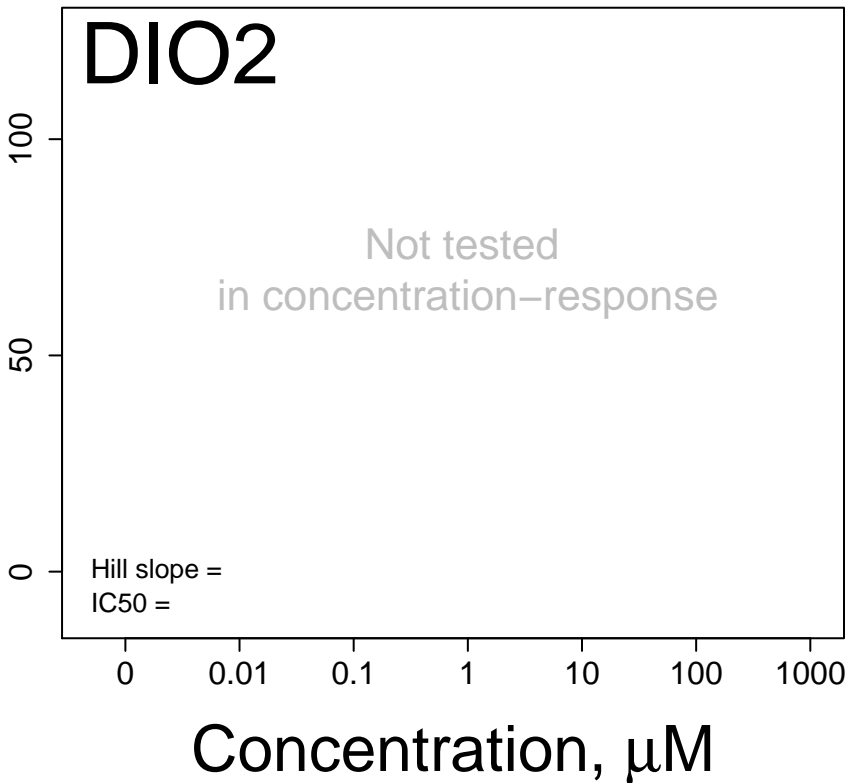
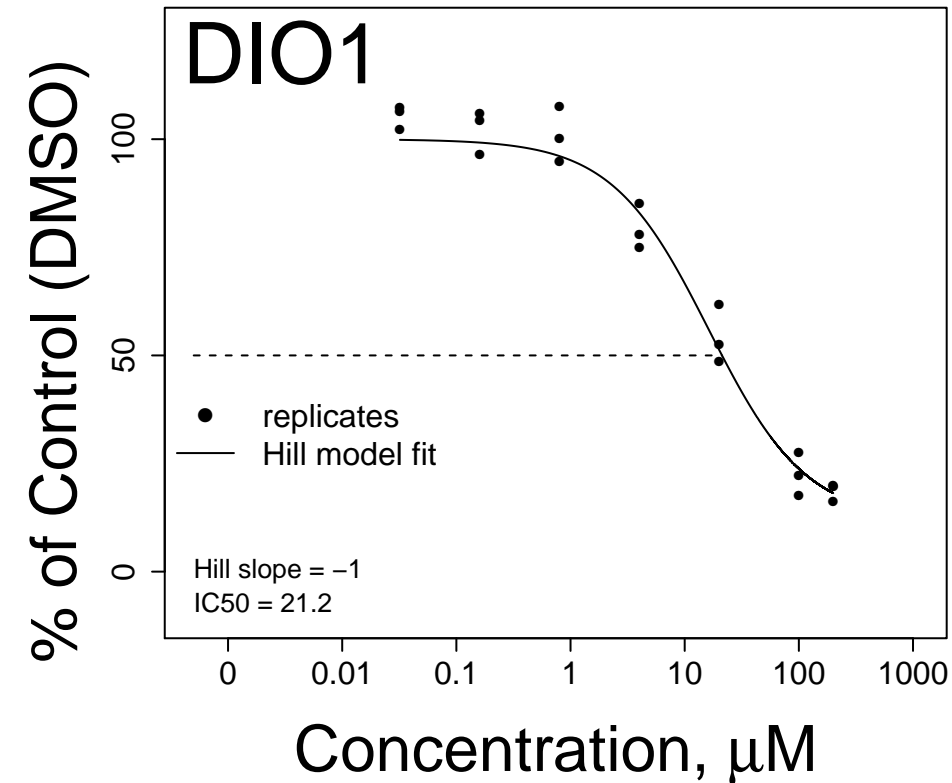
FD&C Green No. 3 CASRN: 2353-45-9



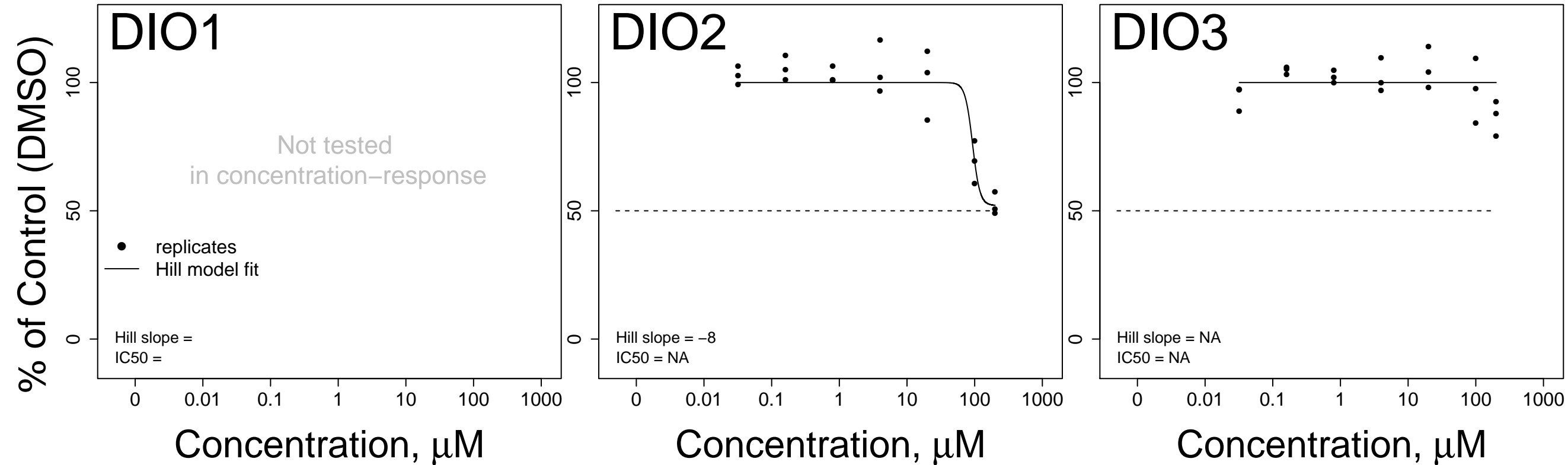
Basic Blue 7 CASRN: 2390-60-5



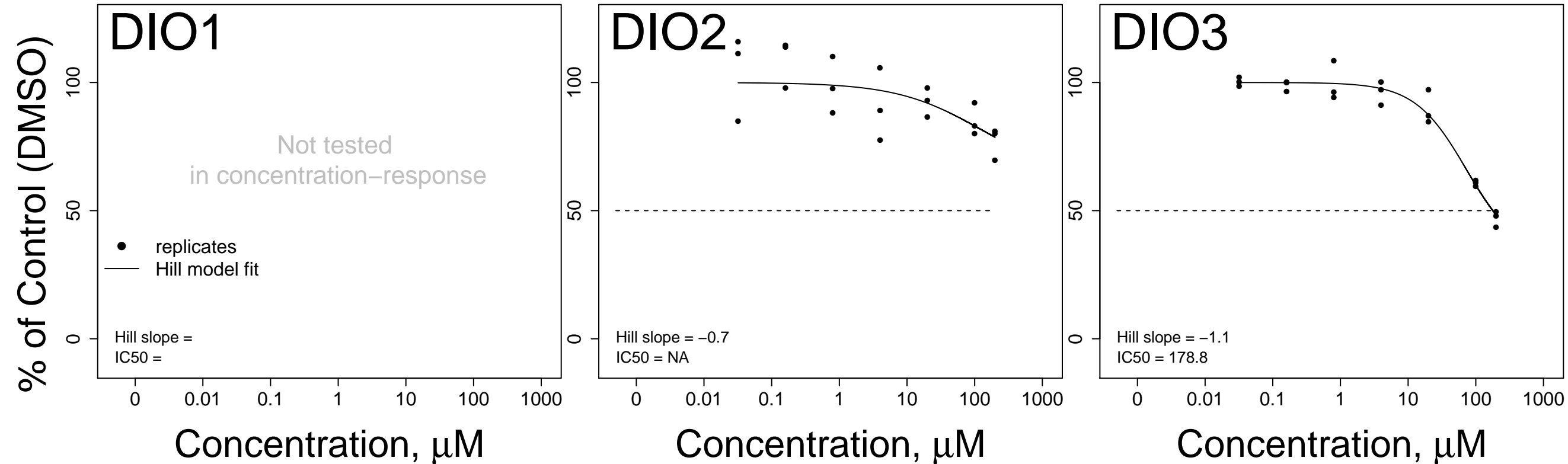
4-tert-Butylbenzenethiol CASRN: 2396-68-1



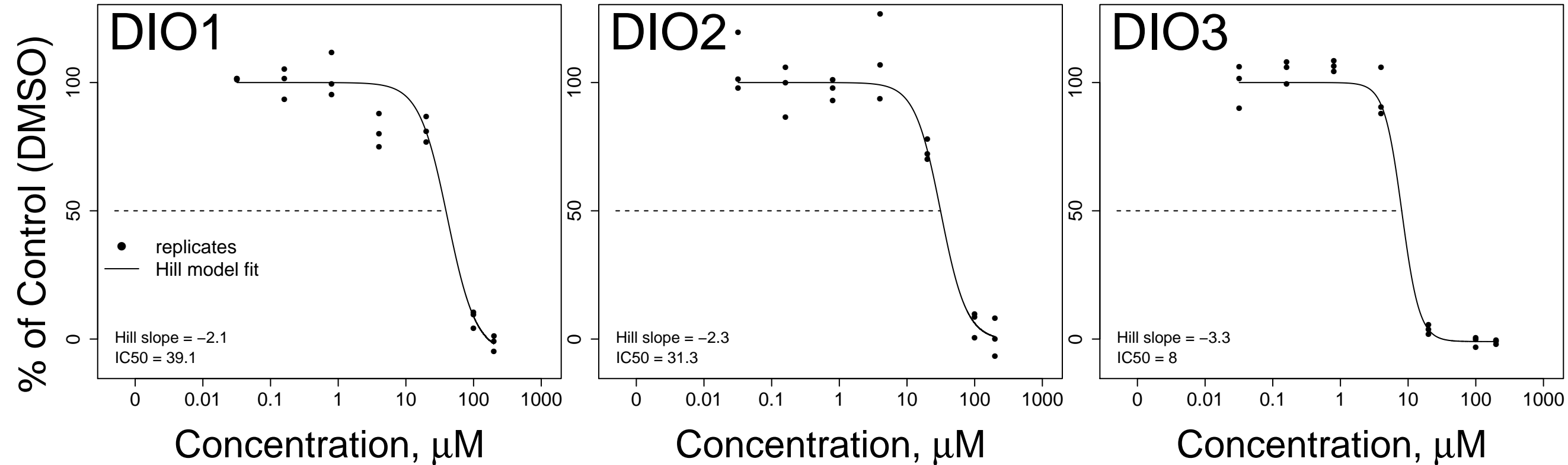
Econazole nitrate CASRN: 24169-02-6



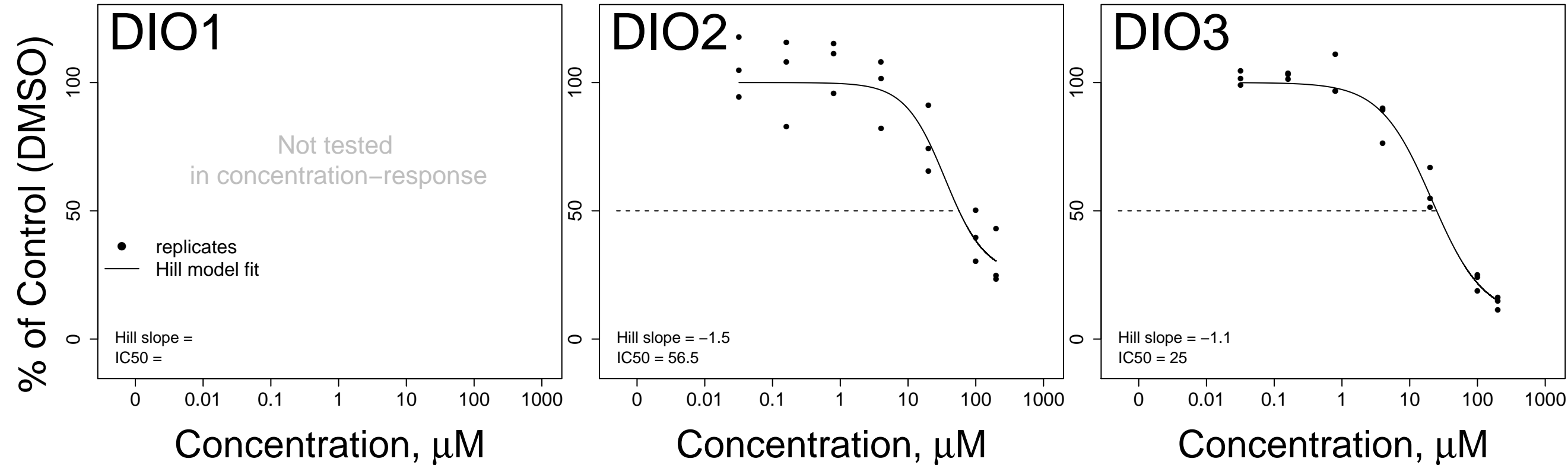
Sodium 2-mercaptobenzothiolate CASRN: 2492-26-4



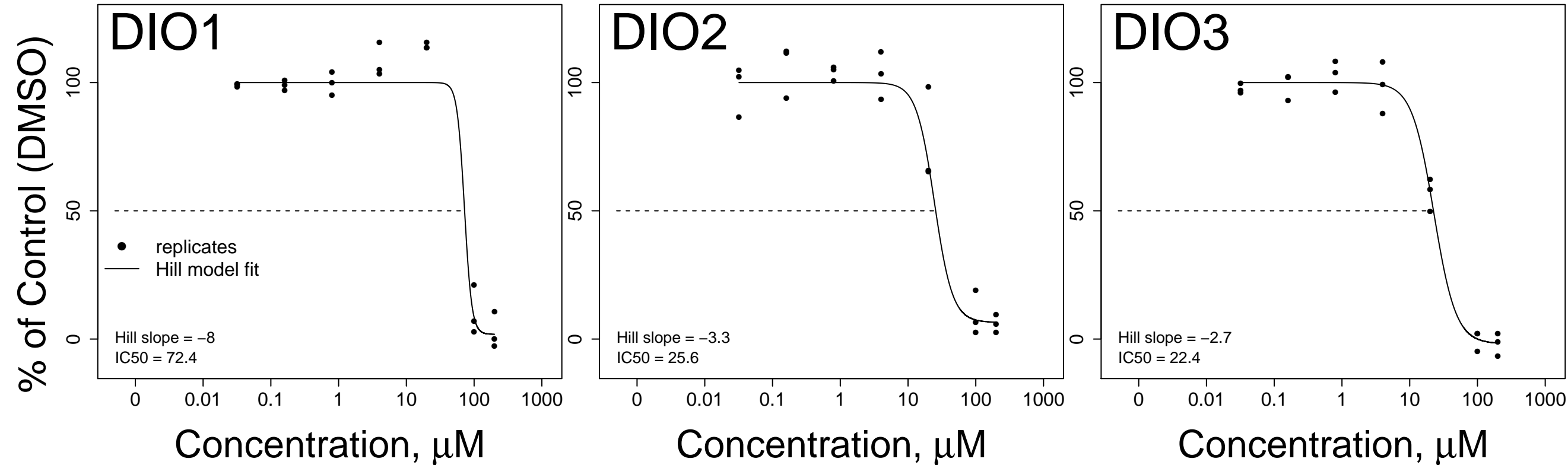
Methylbenzethonium chloride CASRN: 25155-18-4



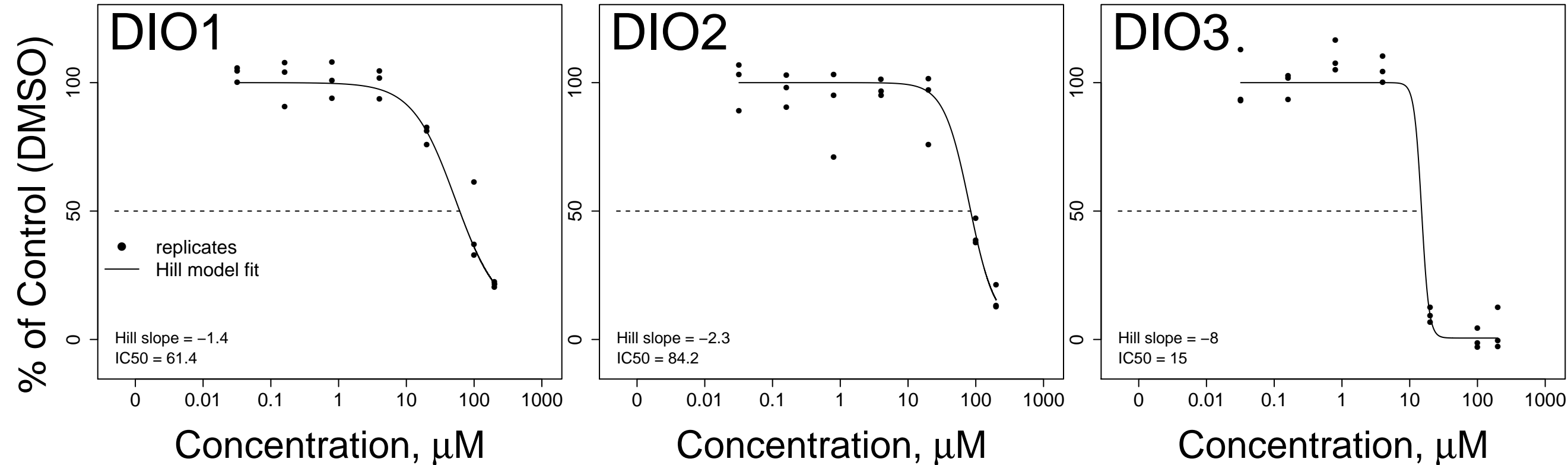
Glycerol monooleate CASRN: 25496-72-4



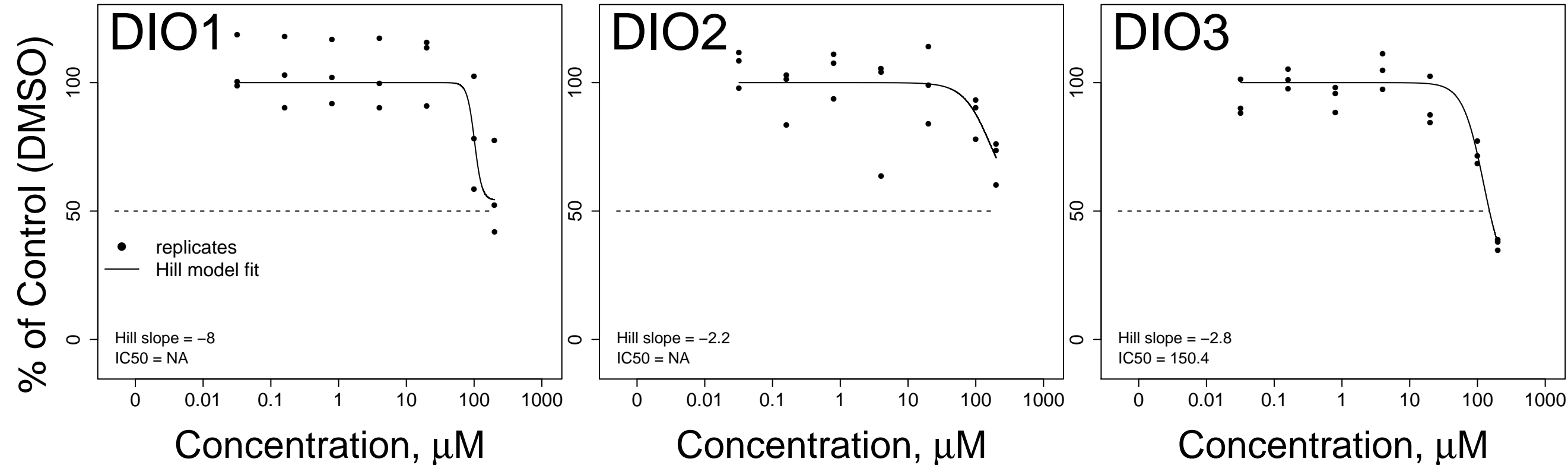
Calcium dodecylbenzene sulfonate CASRN: 26264-06-2



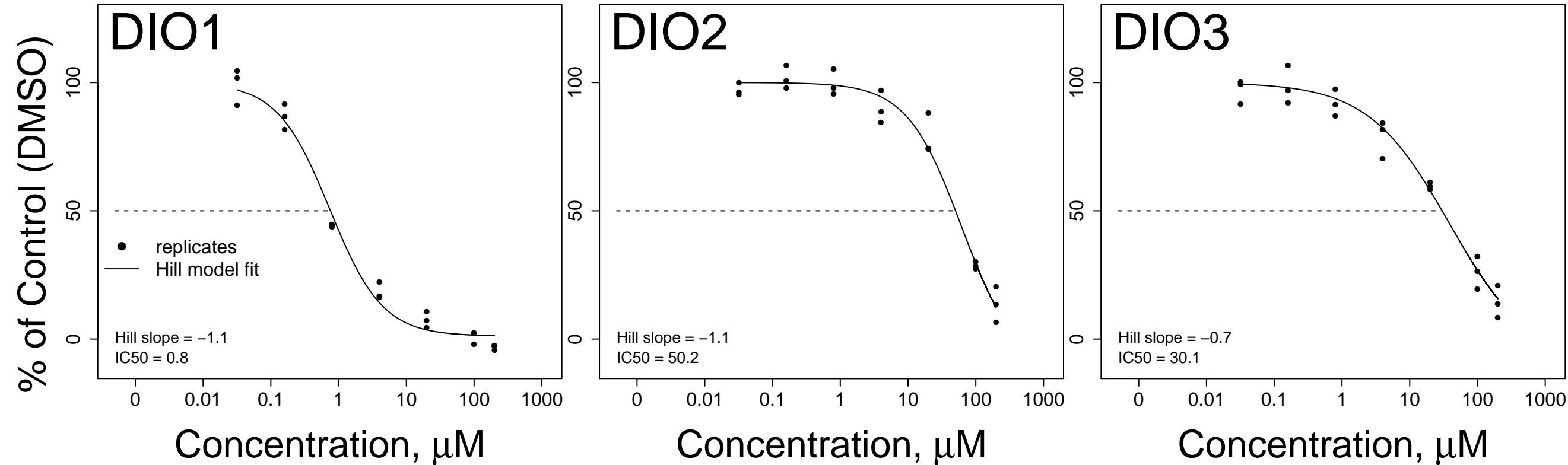
Dodecylphenol CASRN: 27193-86-8



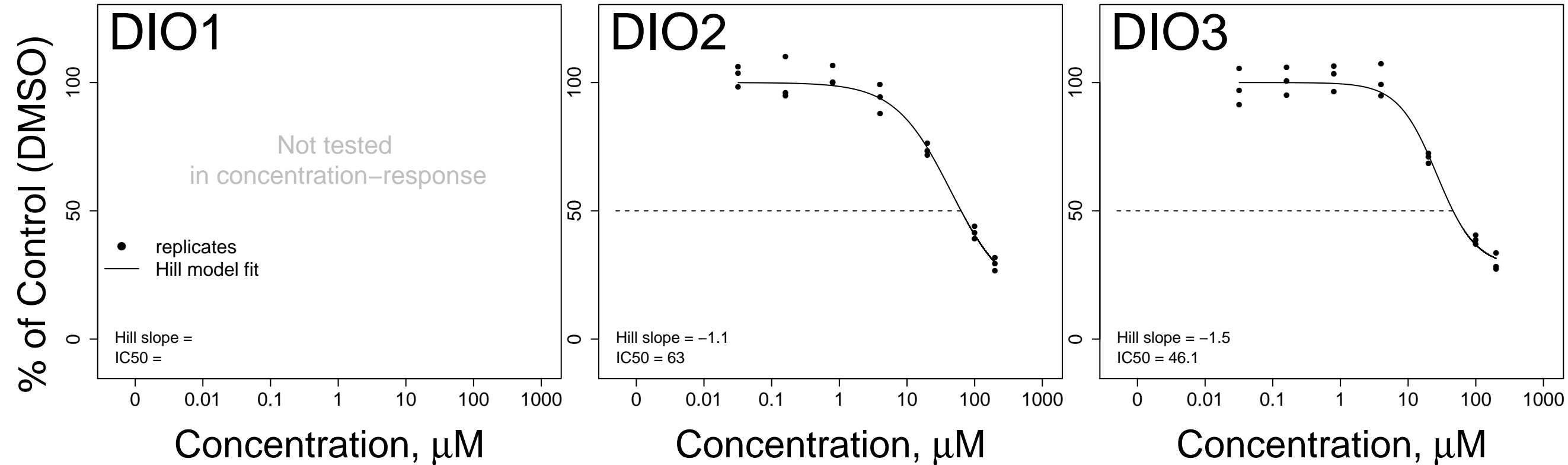
Disodium 4,4'-bis(2-sulfostyryl)biphenyl CASRN: 27344-41-8



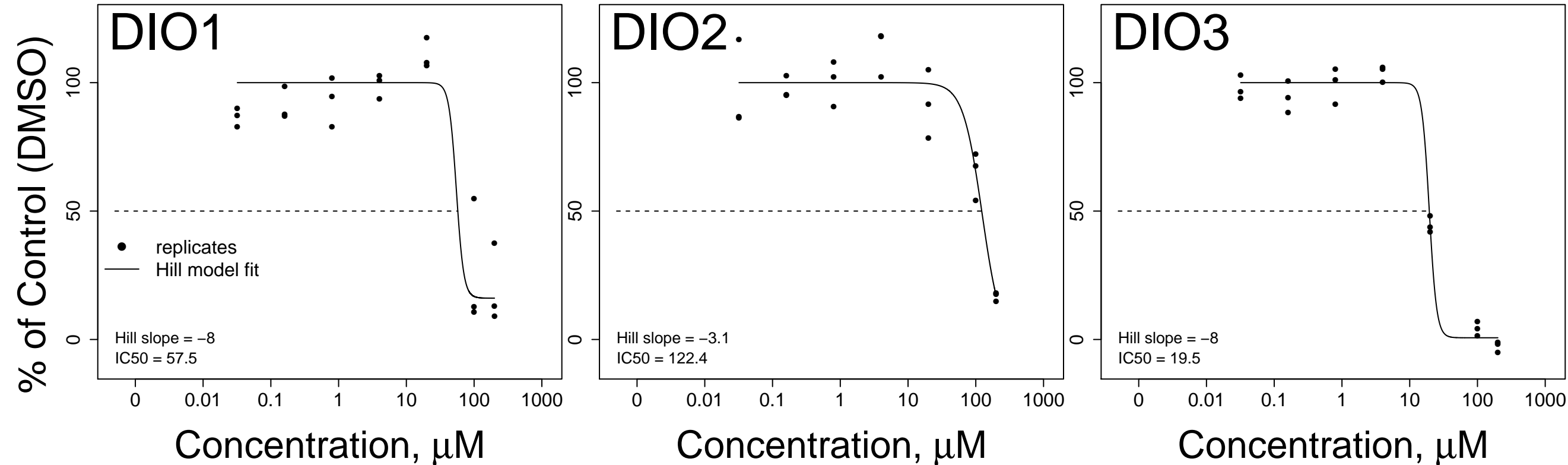
C.I. Direct Yellow 12 CASRN: 2870-32-8



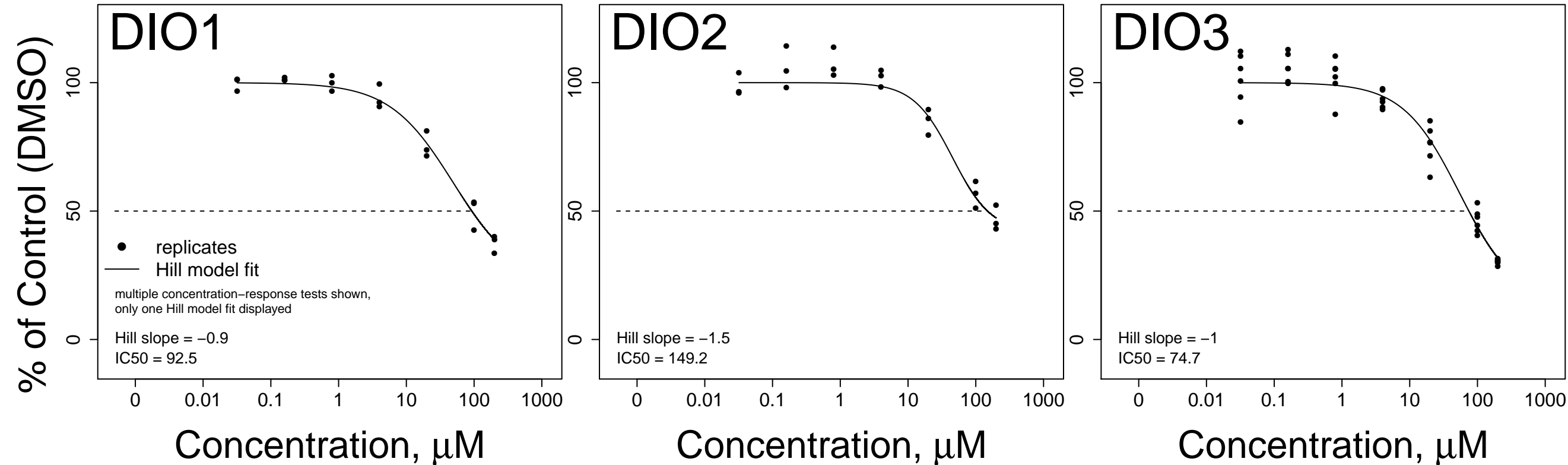
Ethyl (2E,4Z)-deca-2,4-dienoate CASRN: 3025-30-7



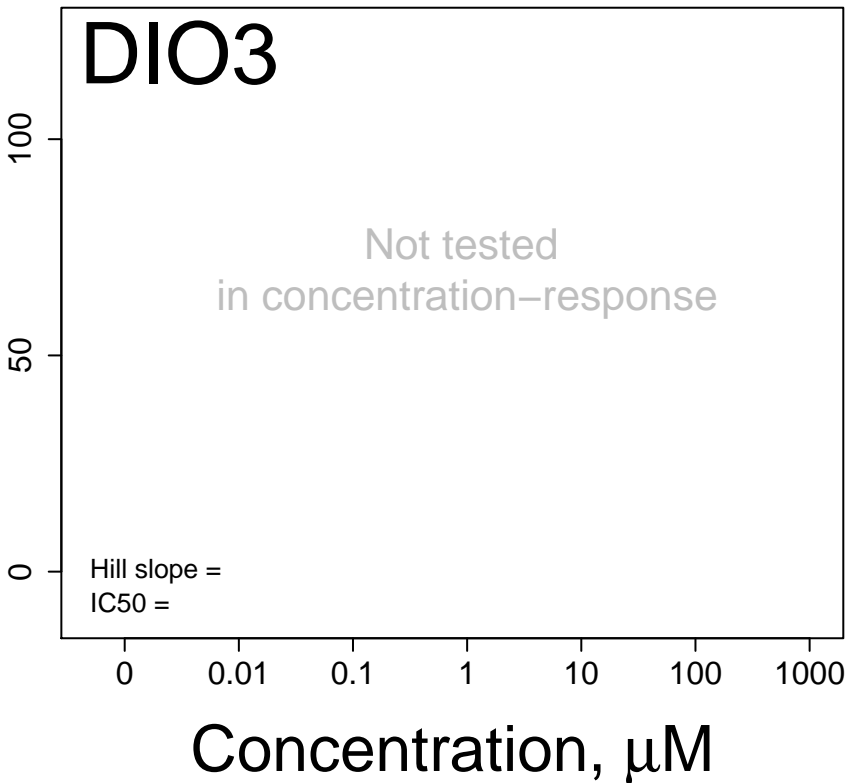
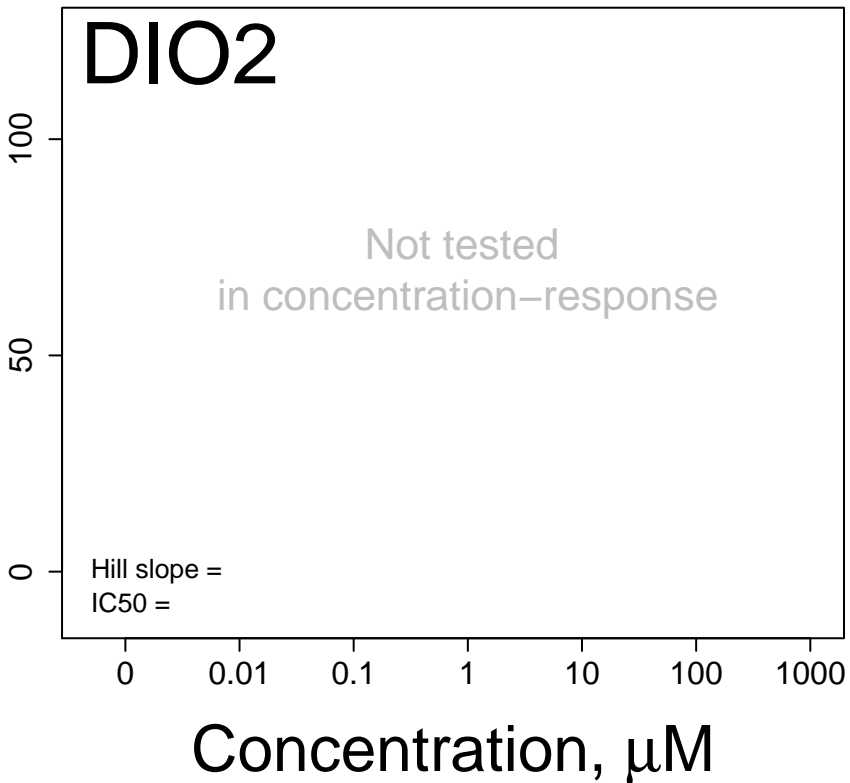
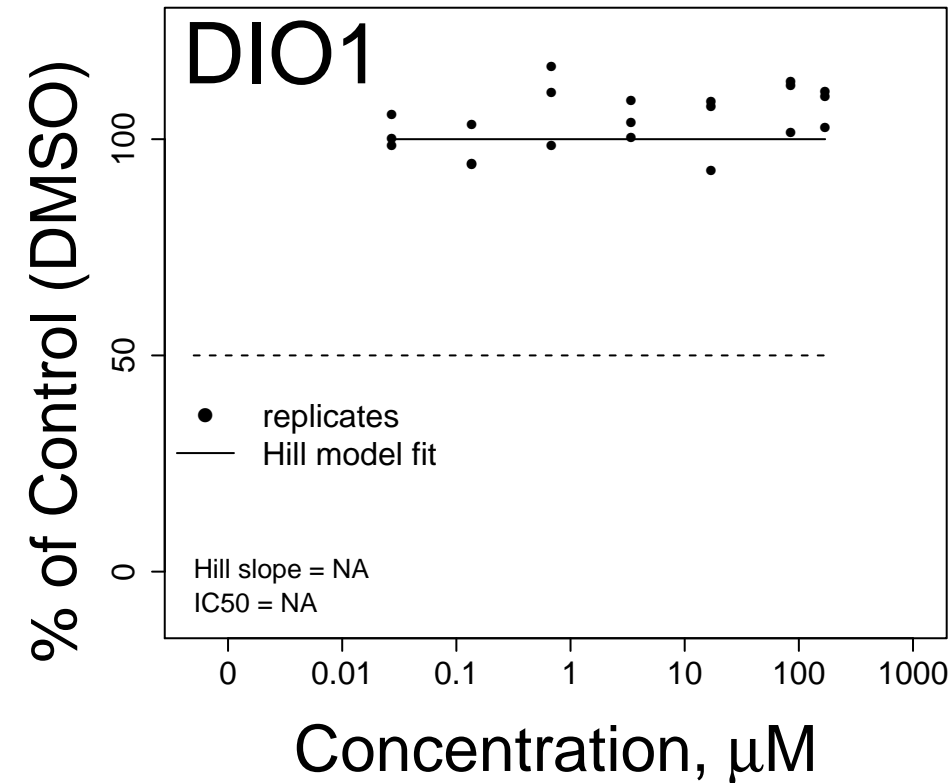
Isooctadecanoic acid CASRN: 30399-84-9



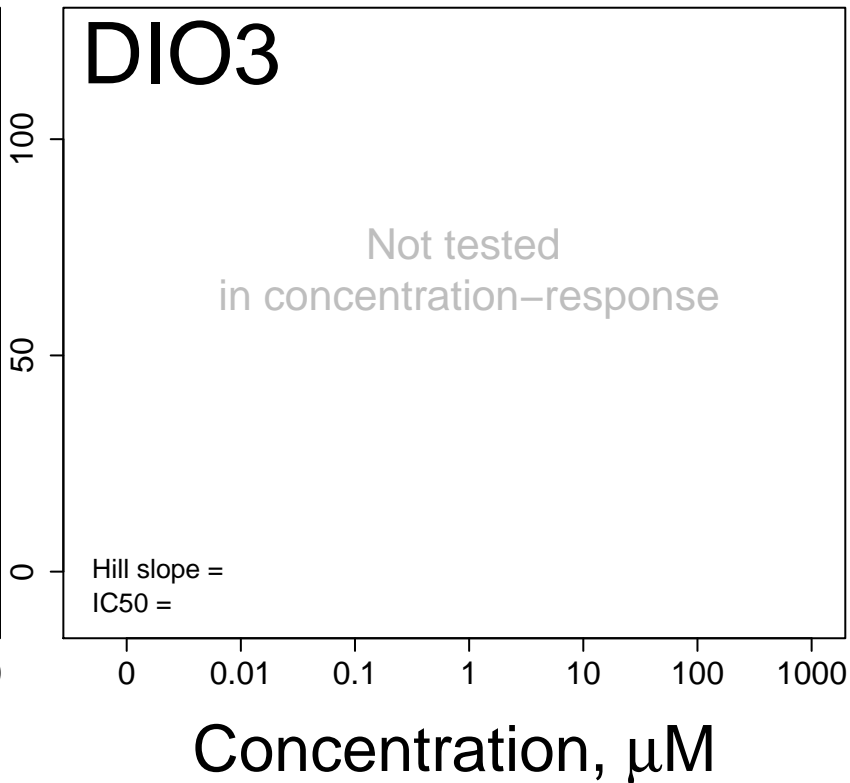
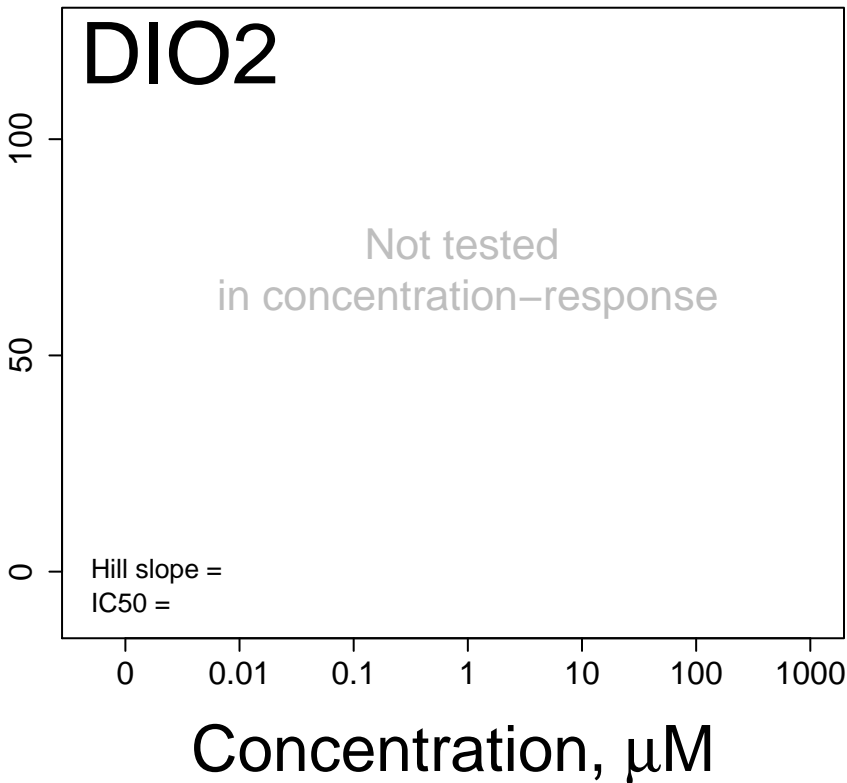
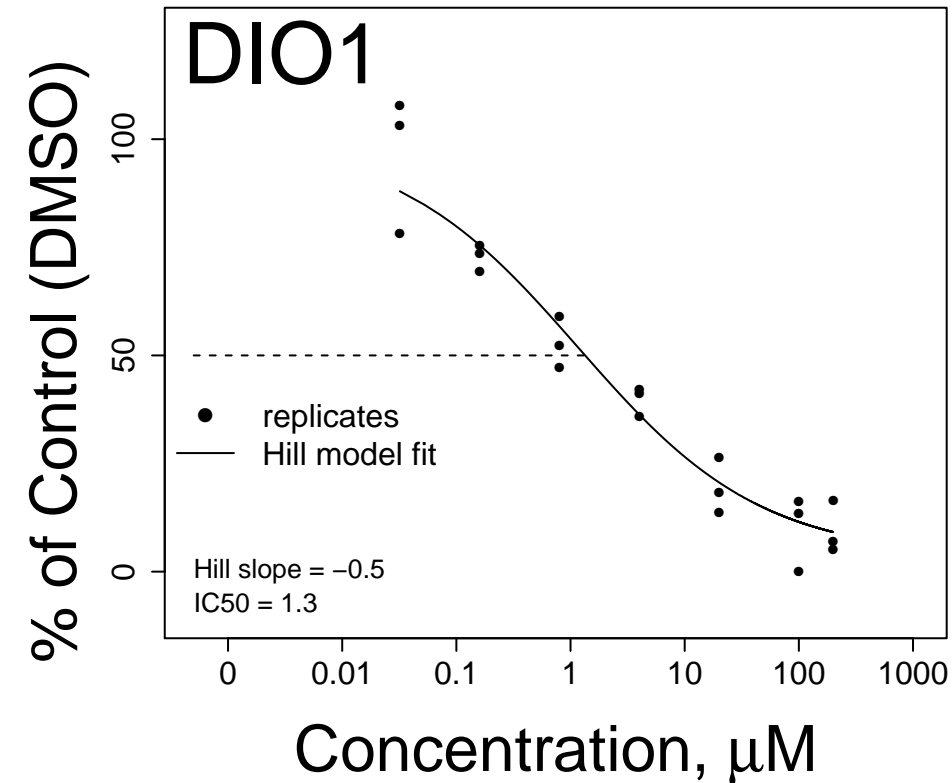
1,4-Dihydroxy-2-naphthoic acid CASRN: 31519-22-9



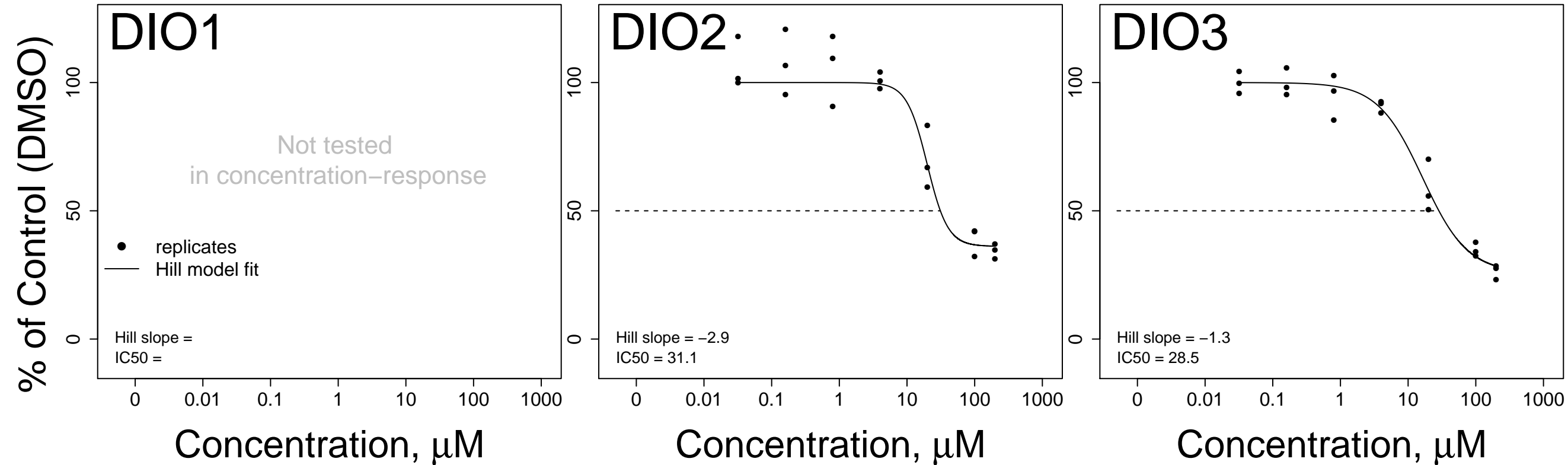
1,2,5,6,9,10–Hexabromocyclododecane CASRN: 3194–55–6



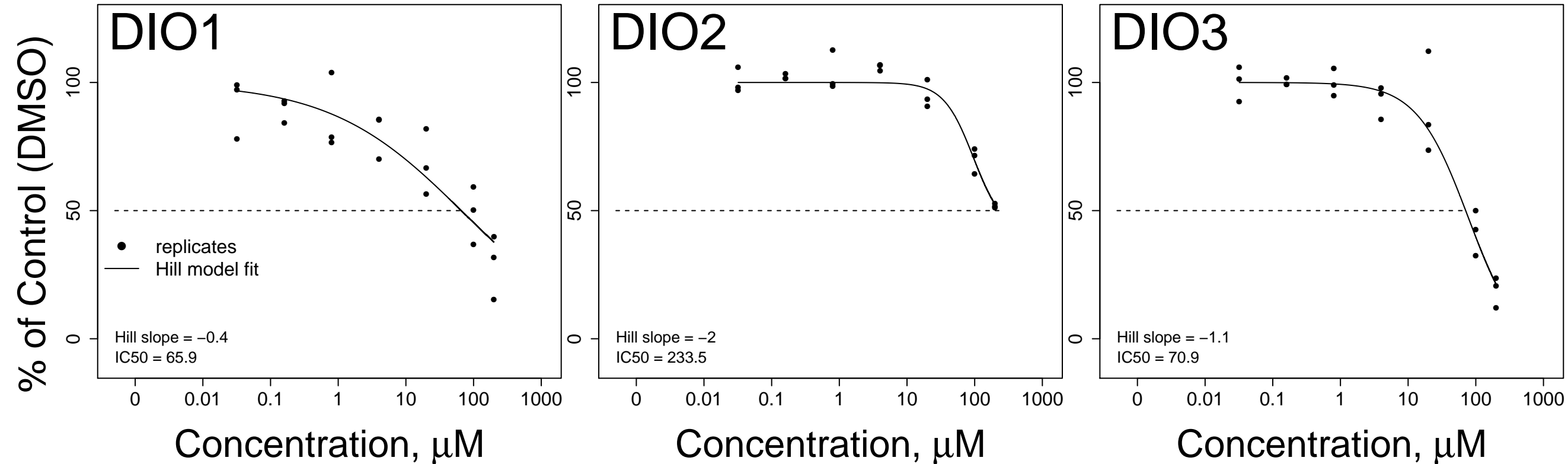
Temephos CASRN: 3383-96-8



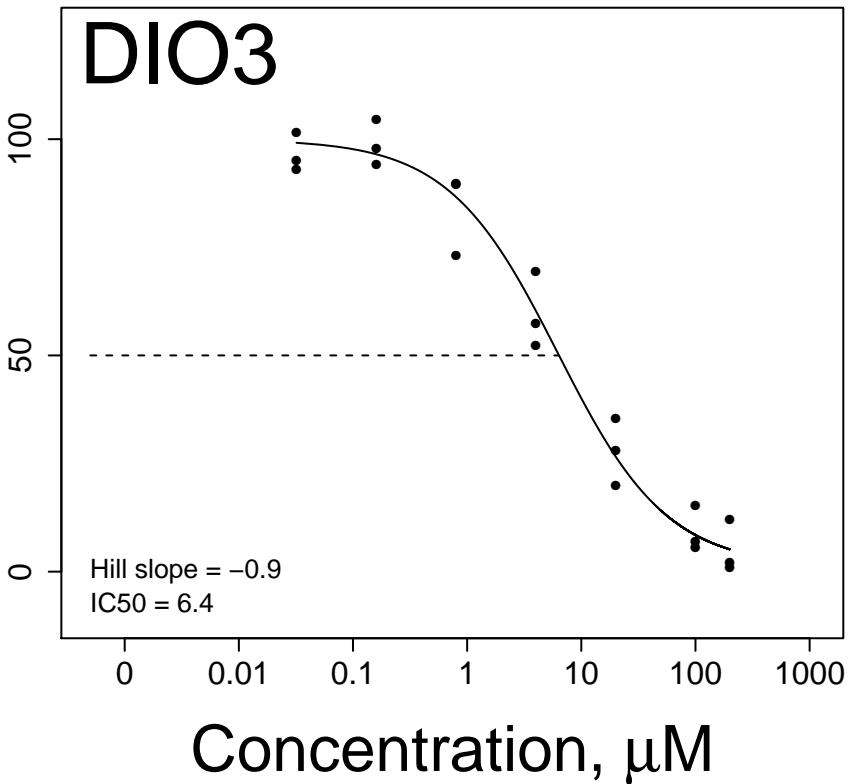
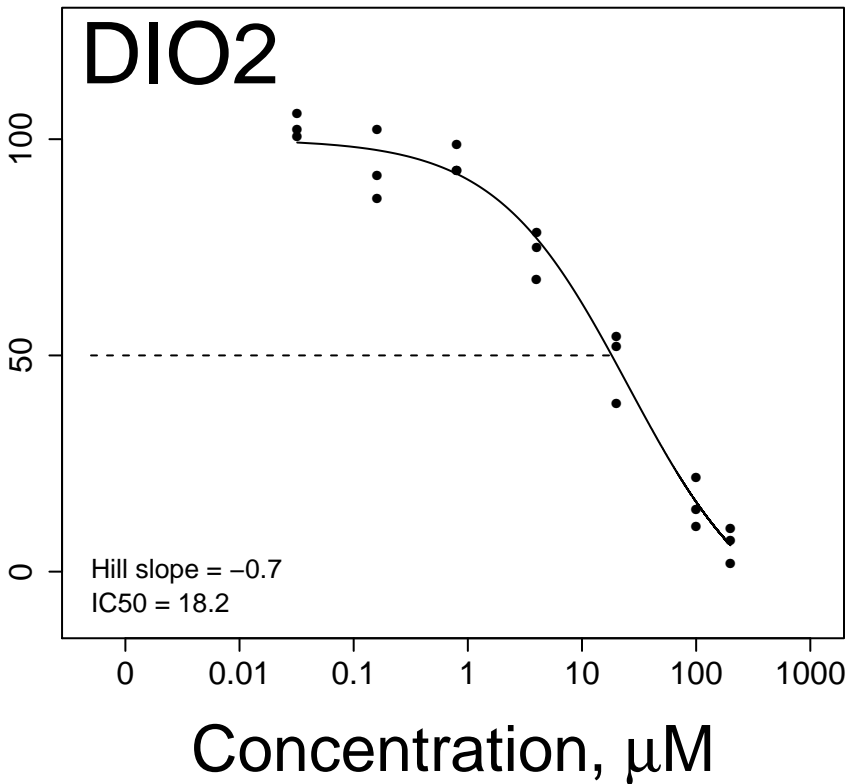
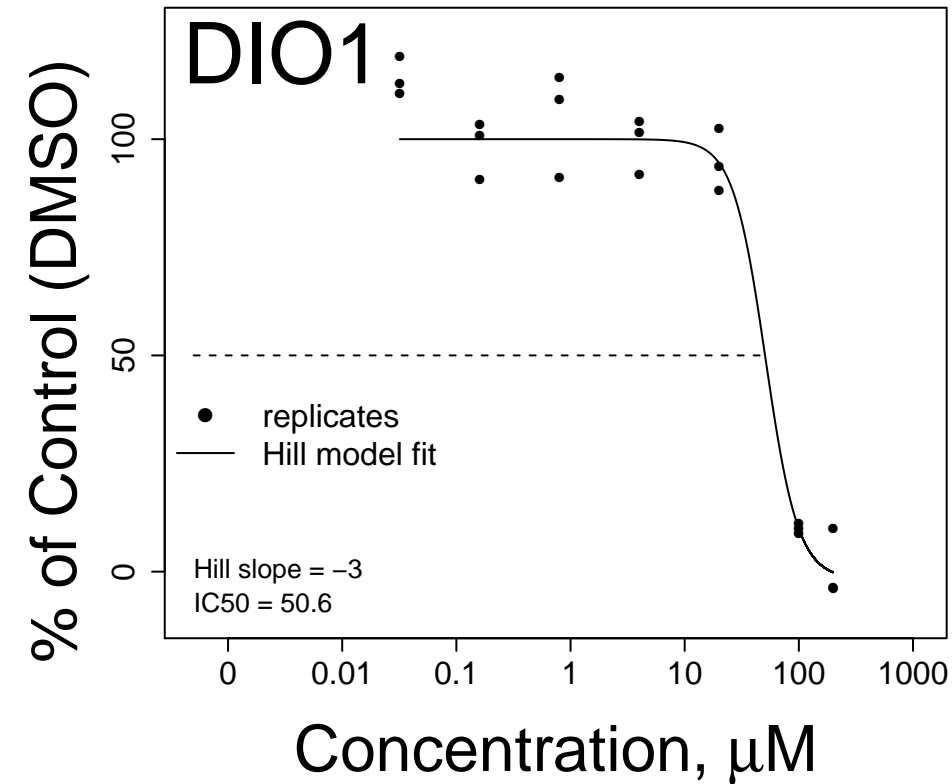
Codlure CASRN: 33956-49-9

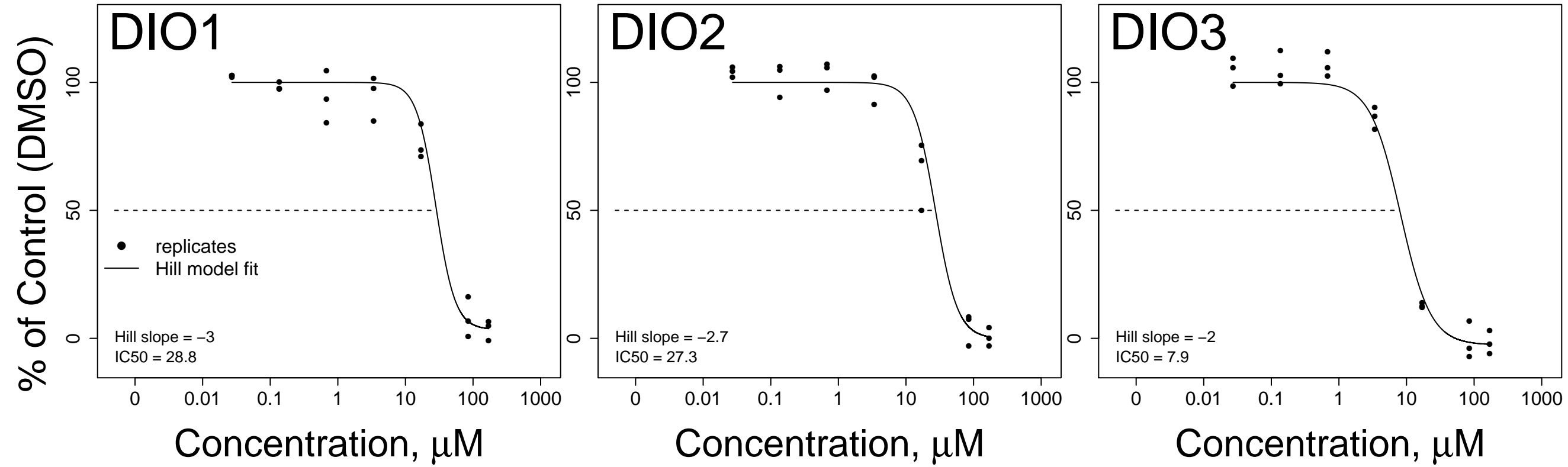


Chlorophacinone CASRN: 3691-35-8

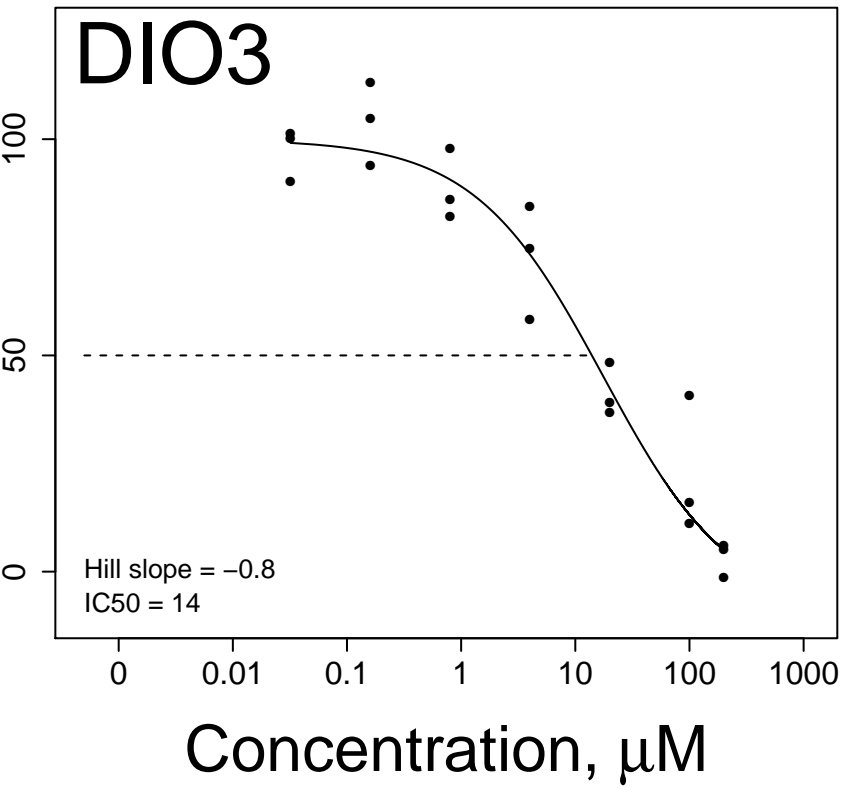
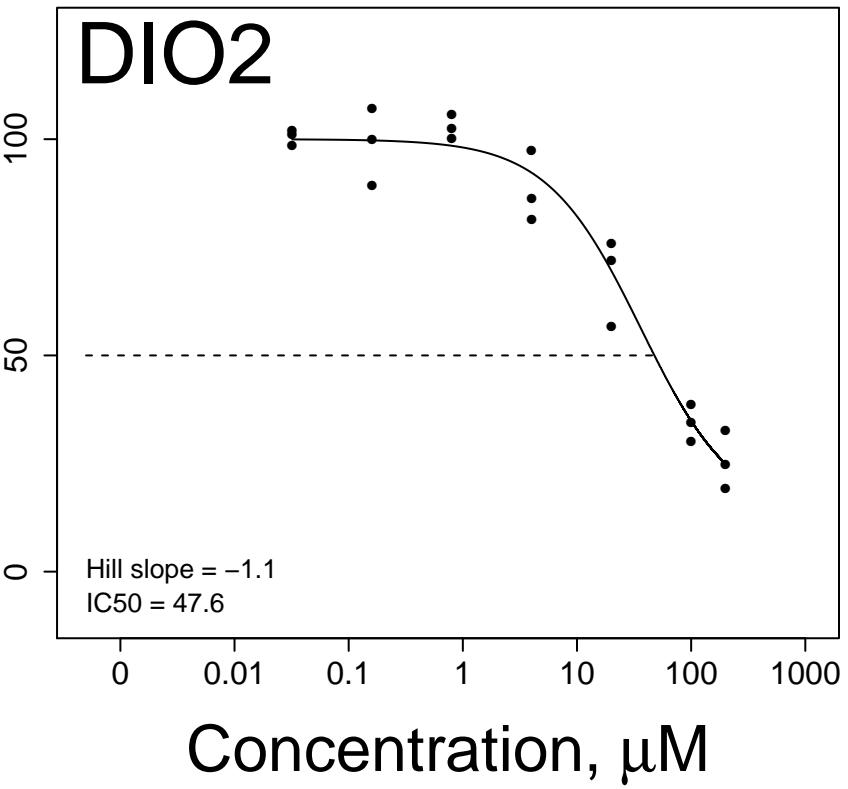
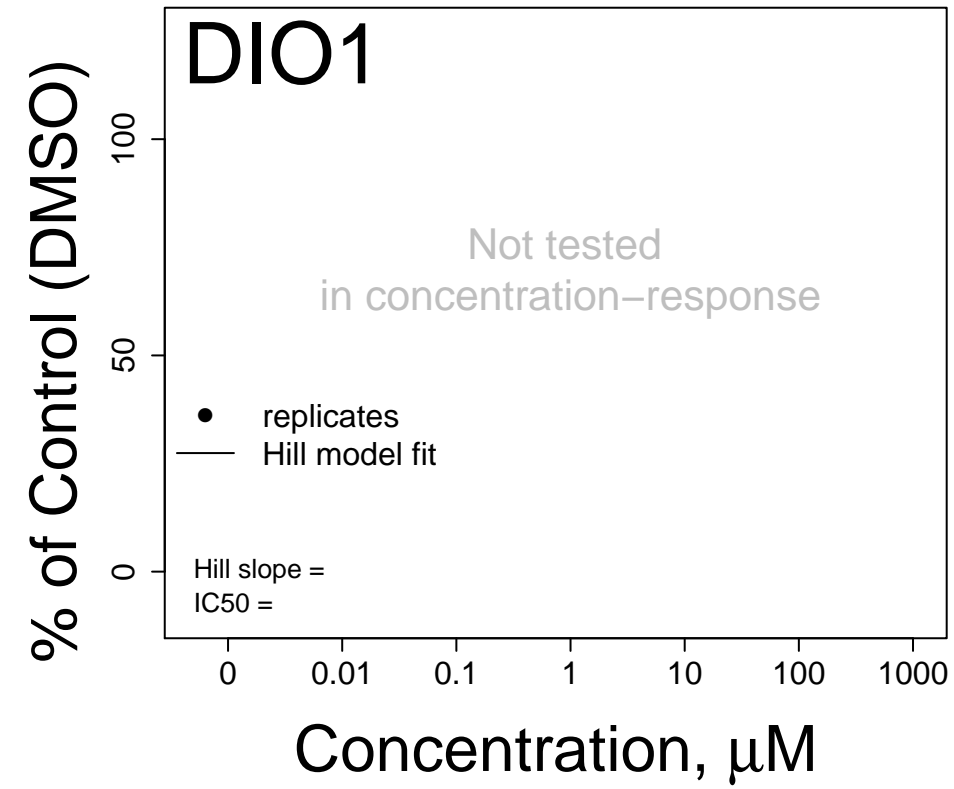


Dinocap CASRN: 39300-45-3

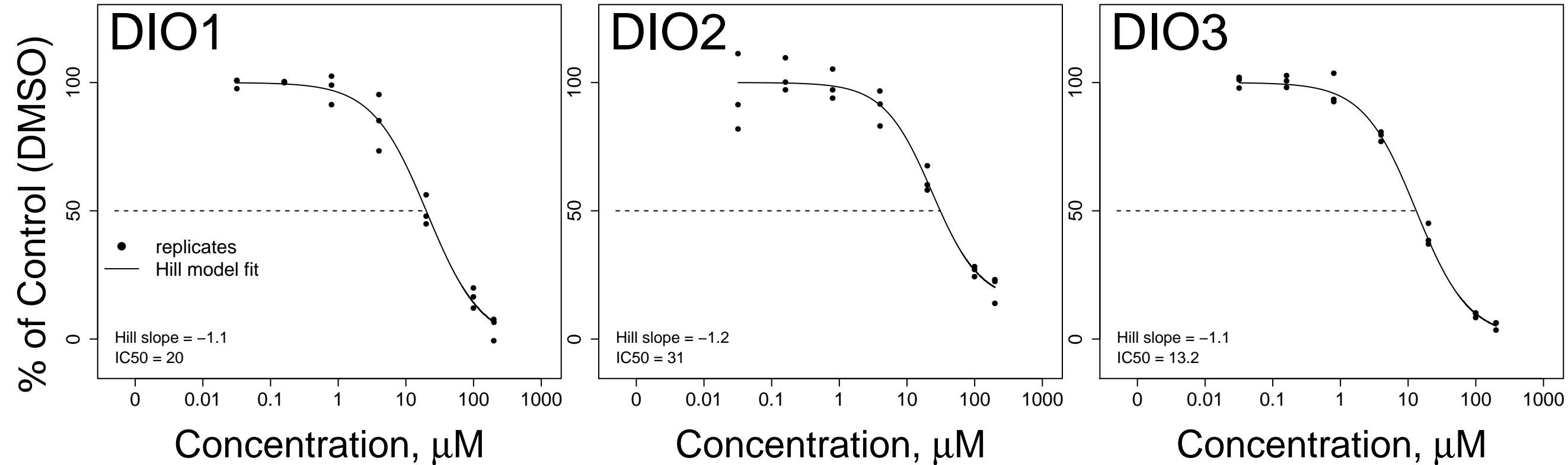




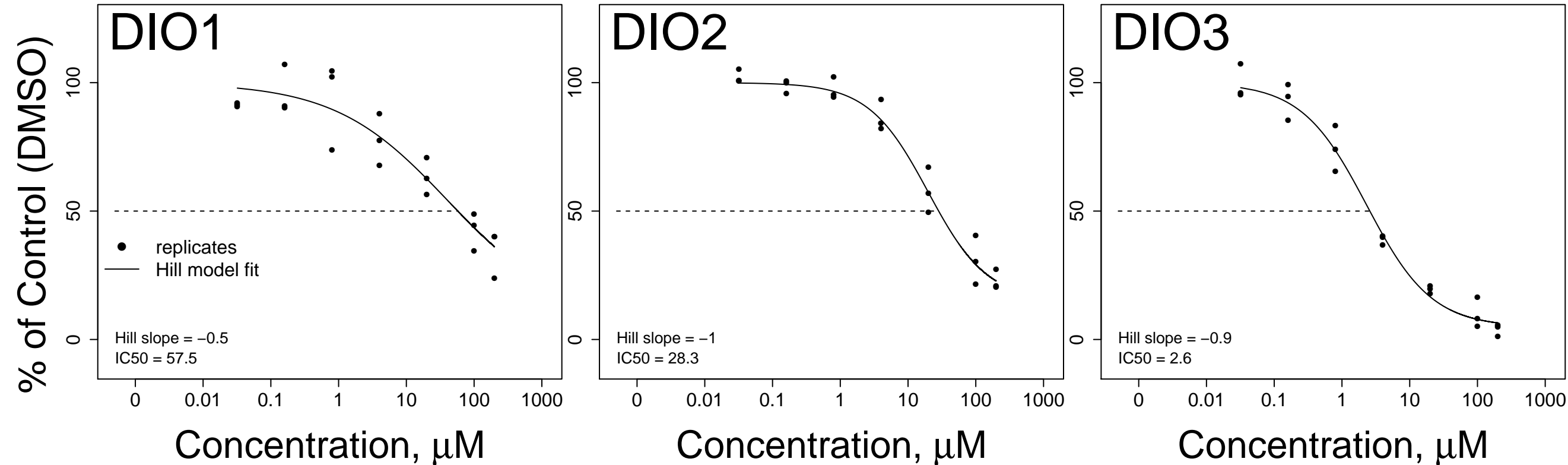
Farnesol CASRN: 4602-84-0



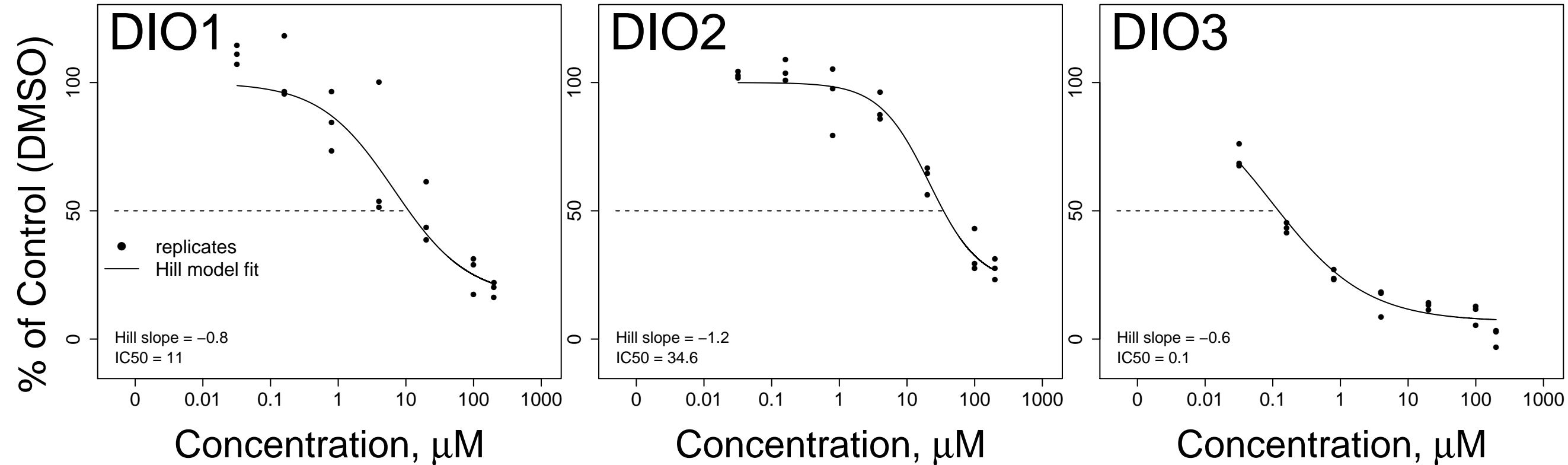
Linolenic acid CASRN: 463-40-1



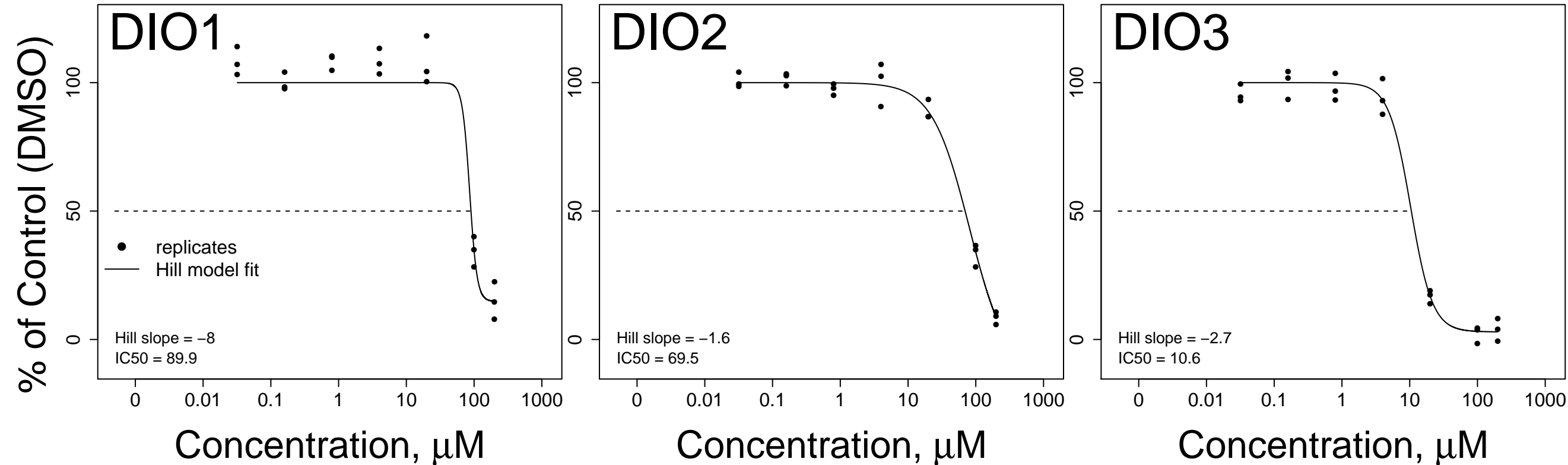
Ergocalciferol CASRN: 50-14-6



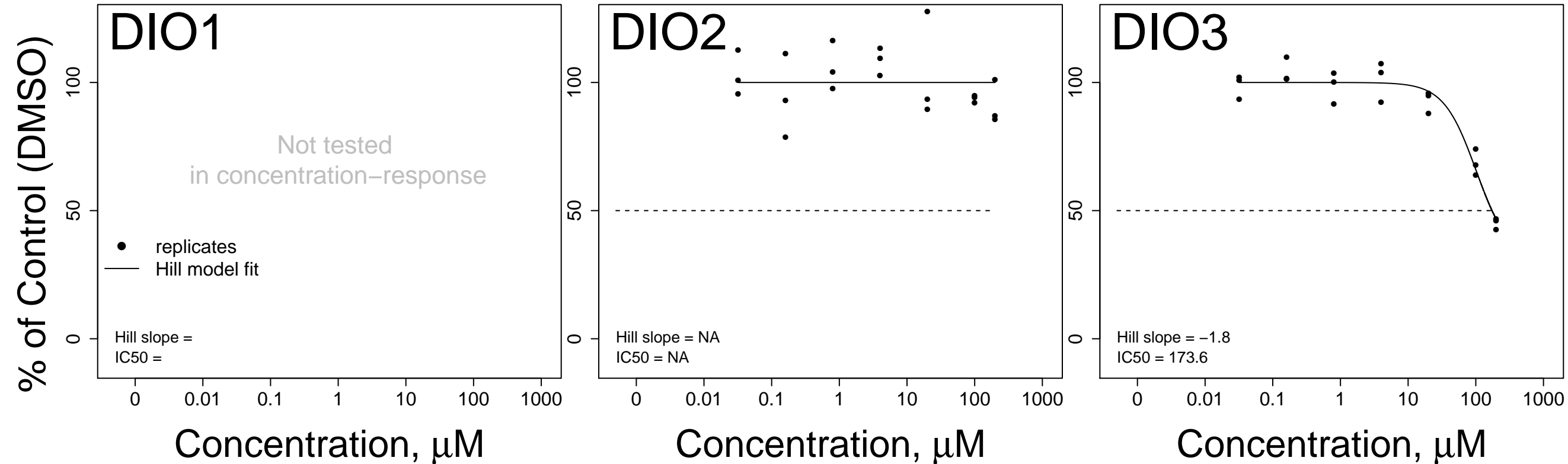
Nordihydroguaiaretic acid CASRN: 500-38-9



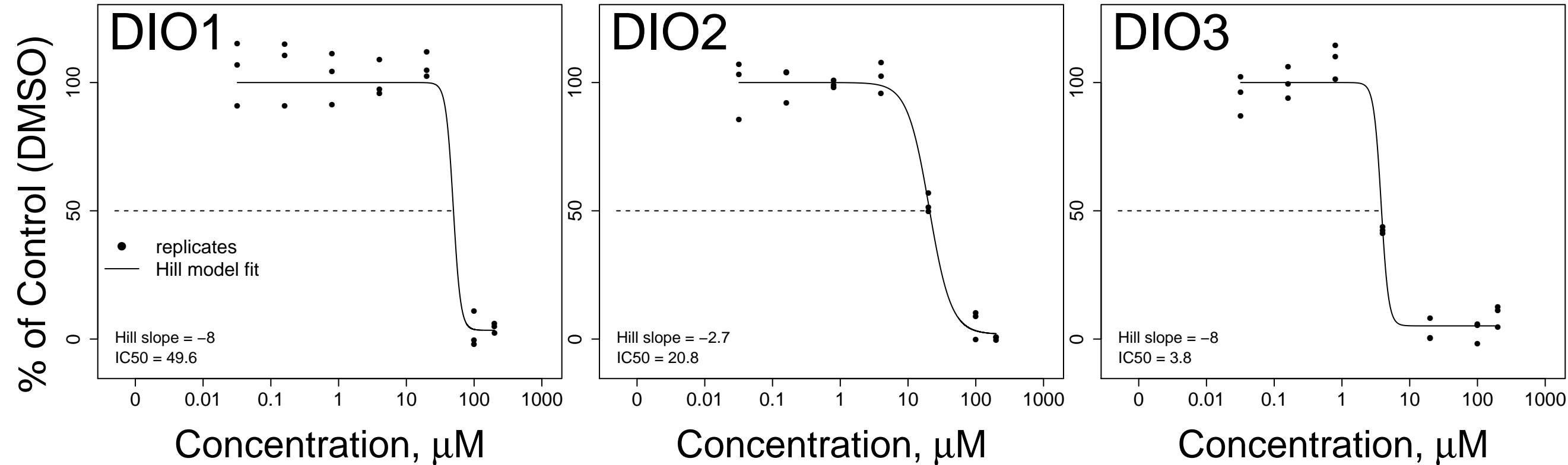
Monotridecyl phosphate CASRN: 5116-94-9



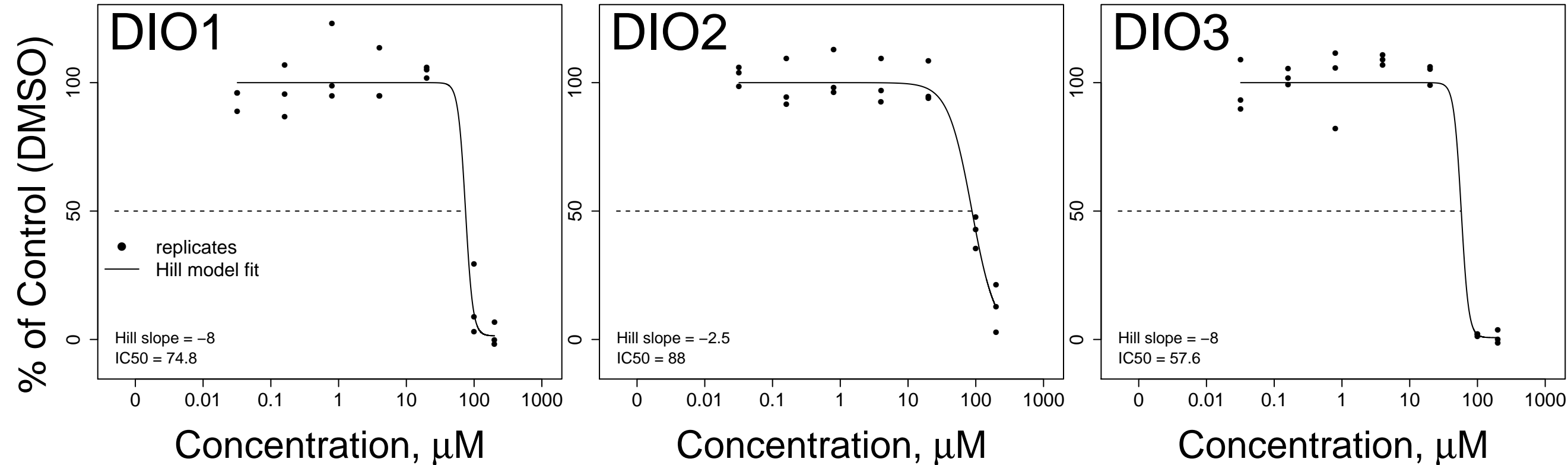
Chloroallyl methenamine chloride CASRN: 51229-78-8



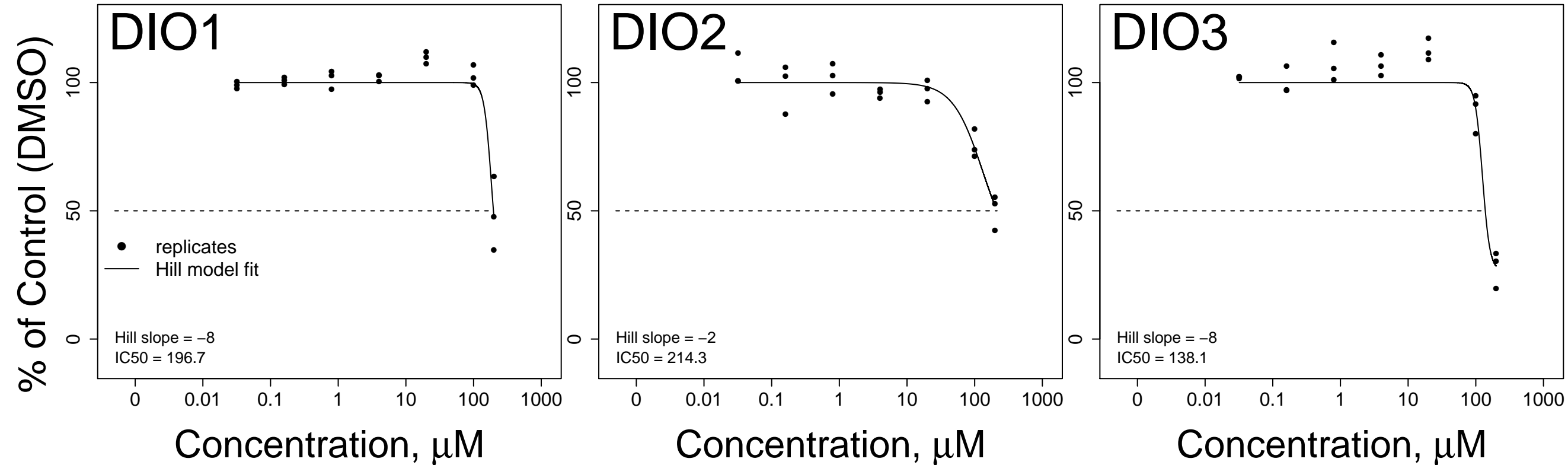
Methyltrioctylammonium chloride CASRN: 5137-55-3



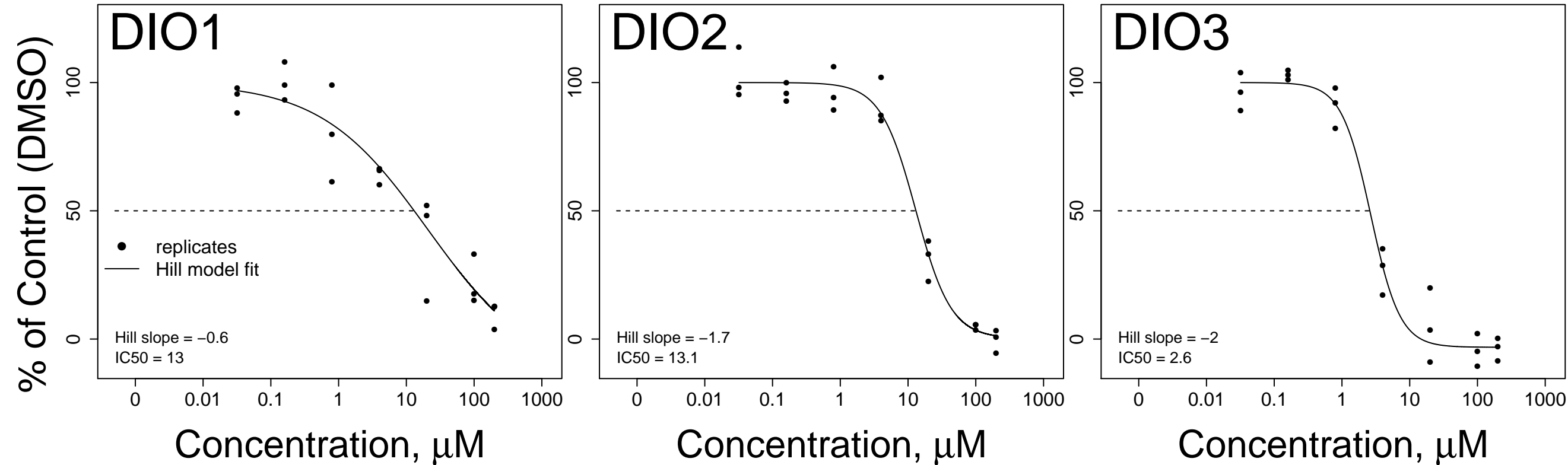
2-Ethylhexylparaben CASRN: 5153-25-3



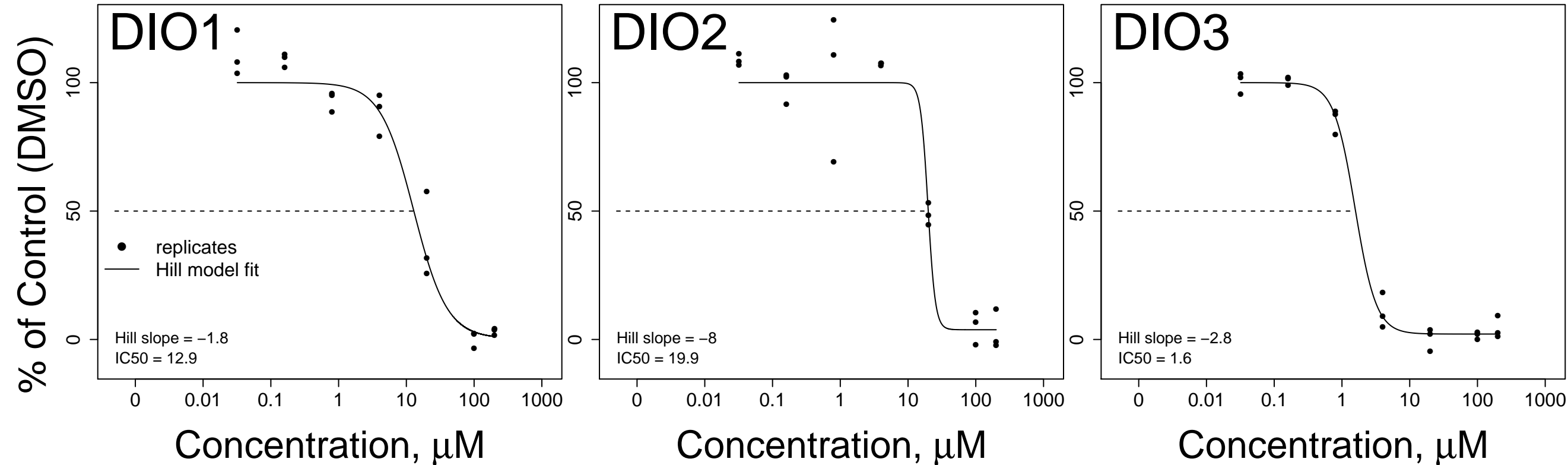
Tetradecanoic acid CASRN: 544-63-8



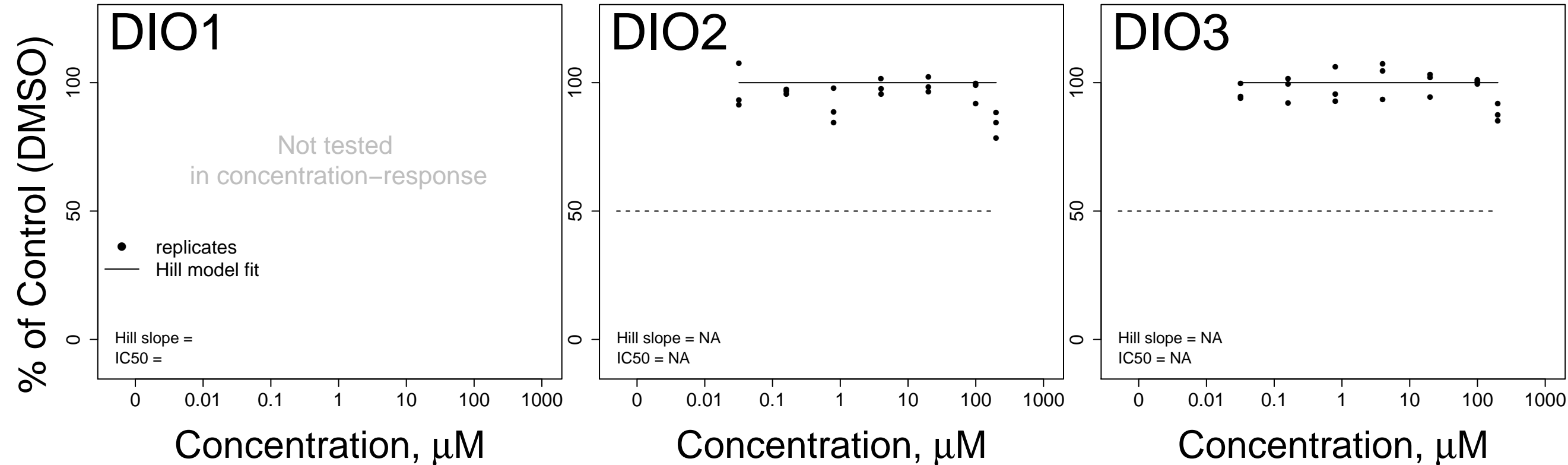
Chlorhexidine diacetate CASRN: 56-95-1



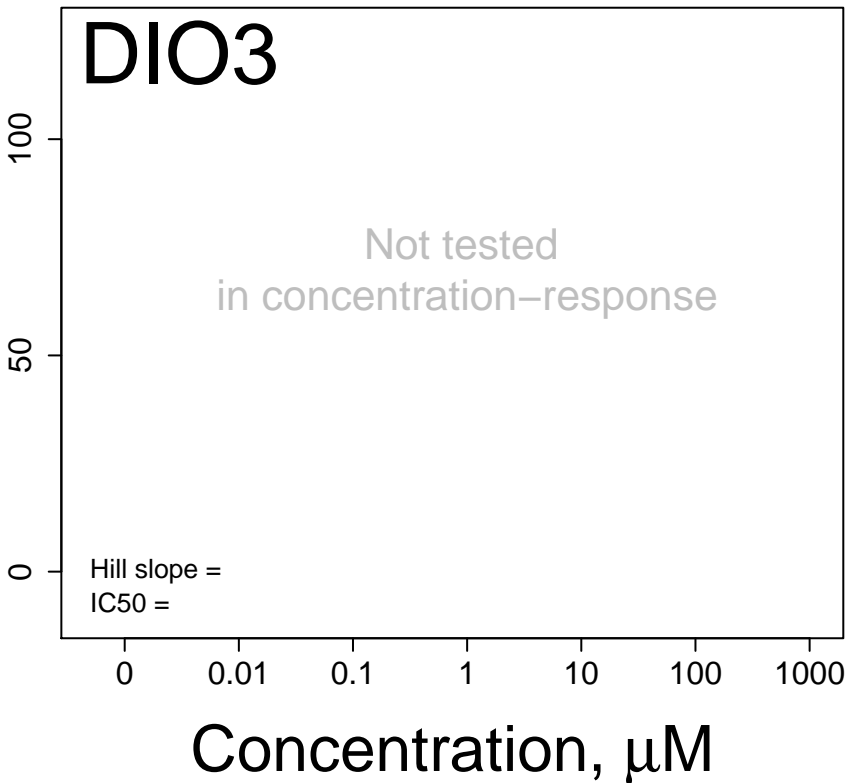
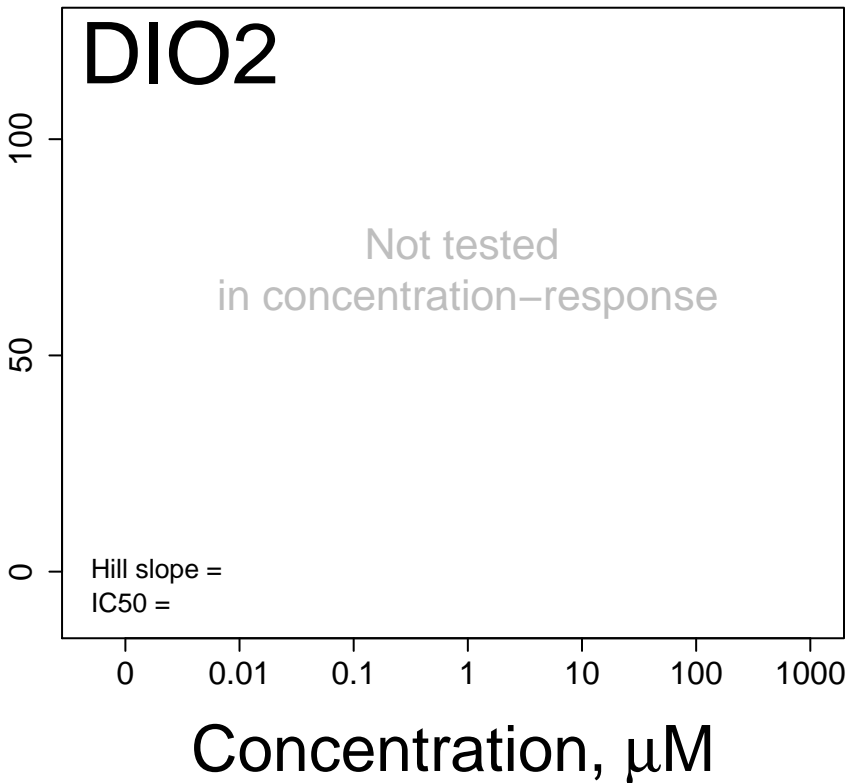
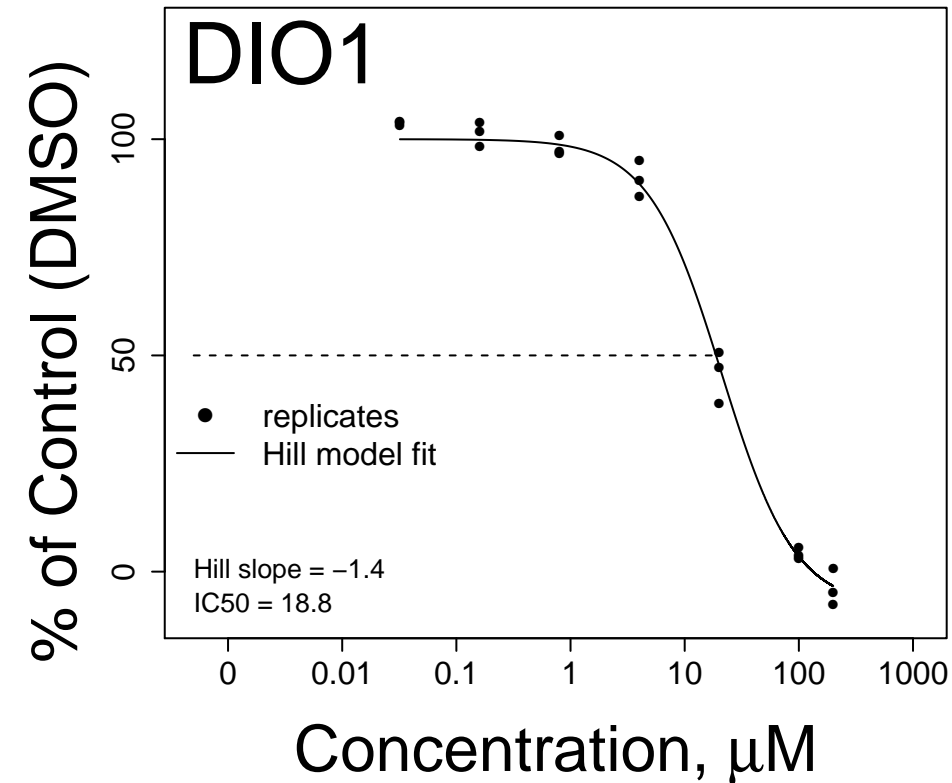
Hexadecyltrimethylammonium bromide CASRN: 57-09-0



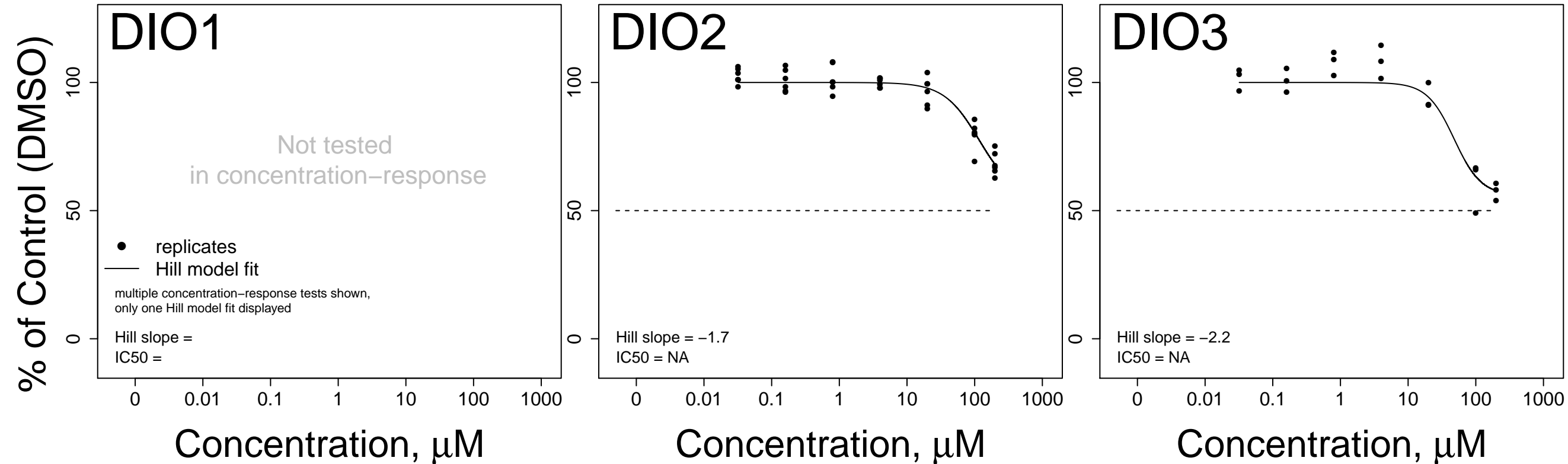
C.I. Acid Orange 8, monosodium salt CASRN: 5850-86-2



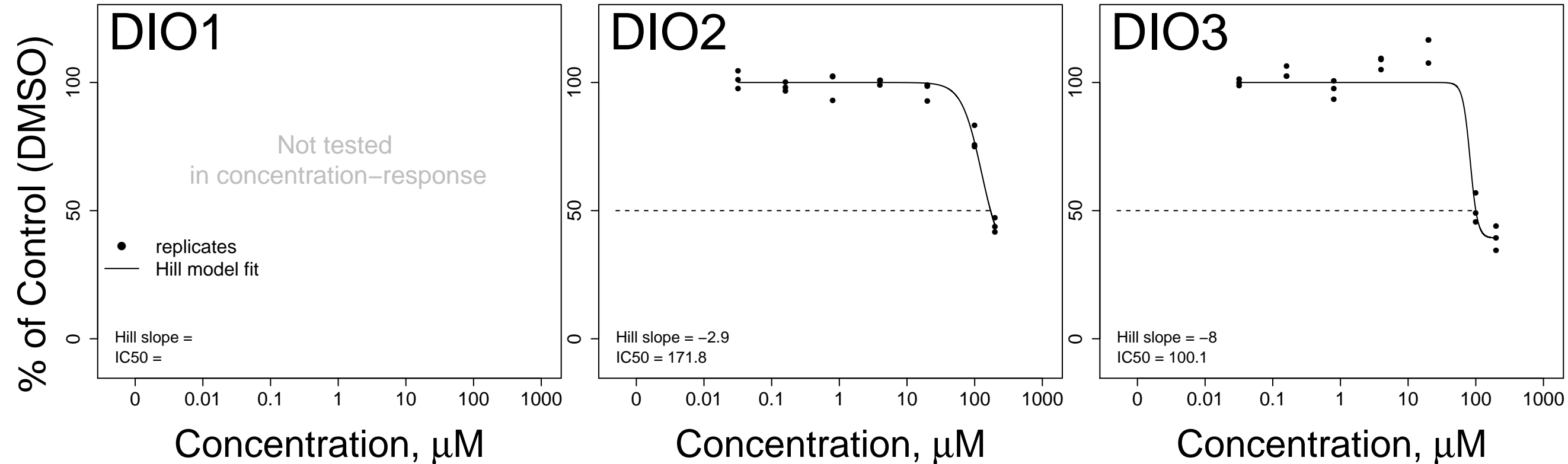
2-Chloro-N-phenylacetamide CASRN: 587-65-5



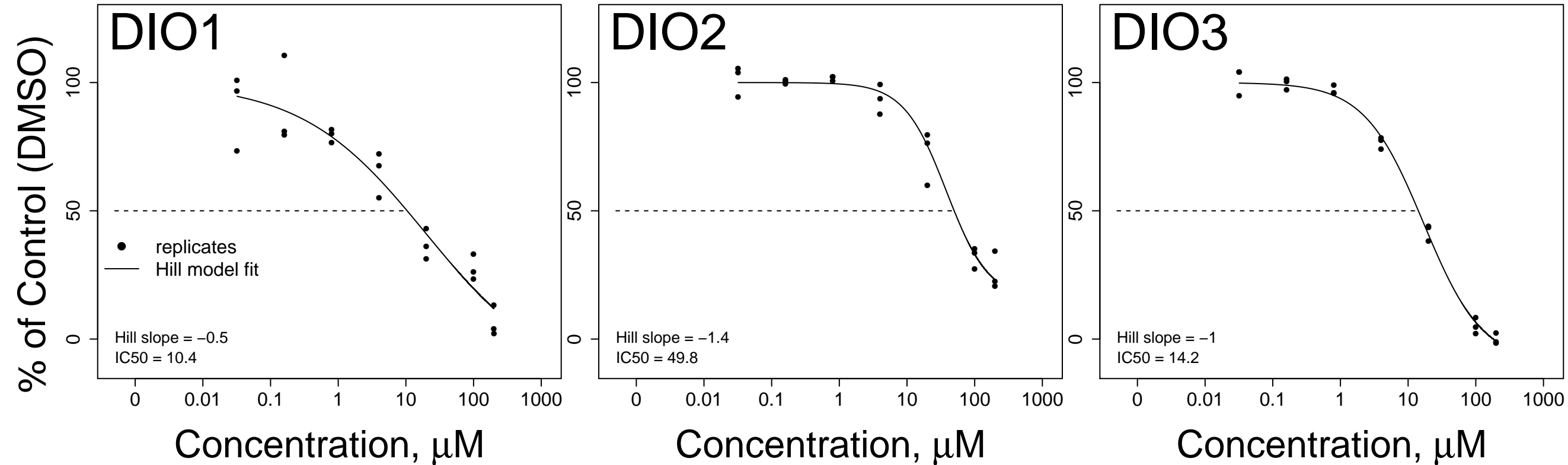
Tetradecanoic acid, 2,3-dihydroxypropyl ester CASRN: 589-68-4



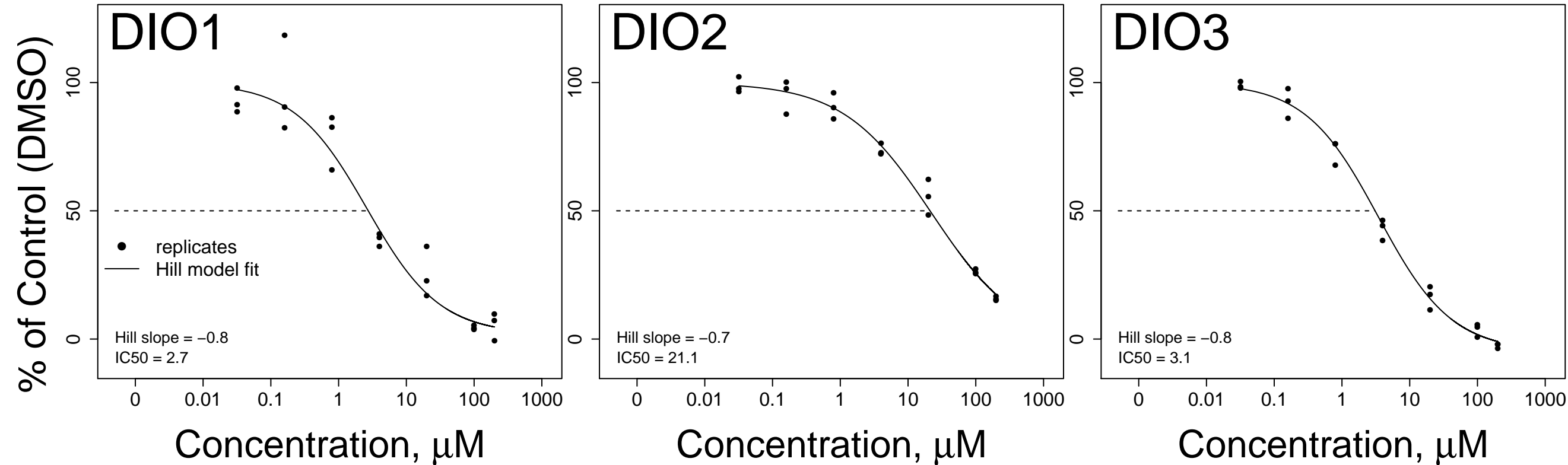
Laurocapram CASRN: 59227-89-3



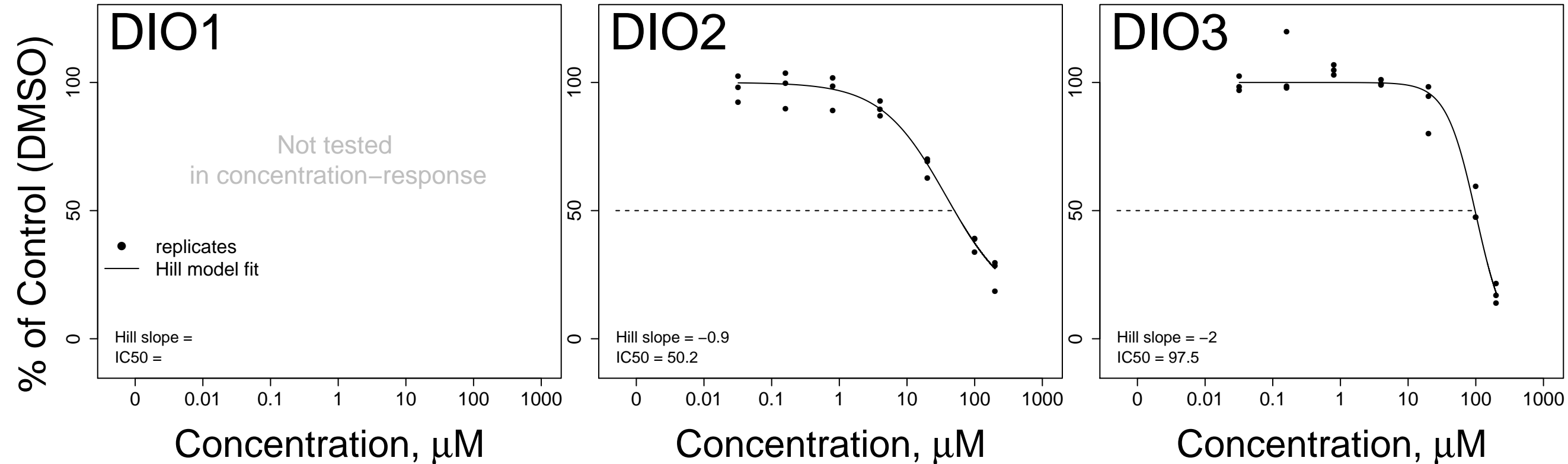
Linoleic acid CASRN: 60-33-3



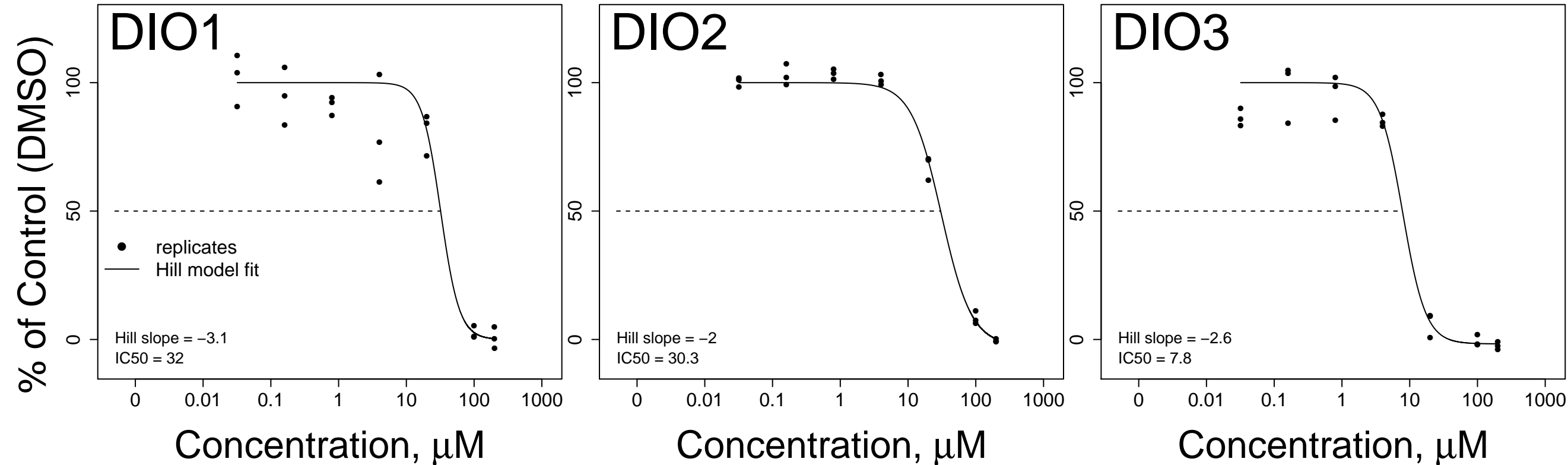
6-Hydroxy-2-naphthyl disulfide CASRN: 6088-51-3



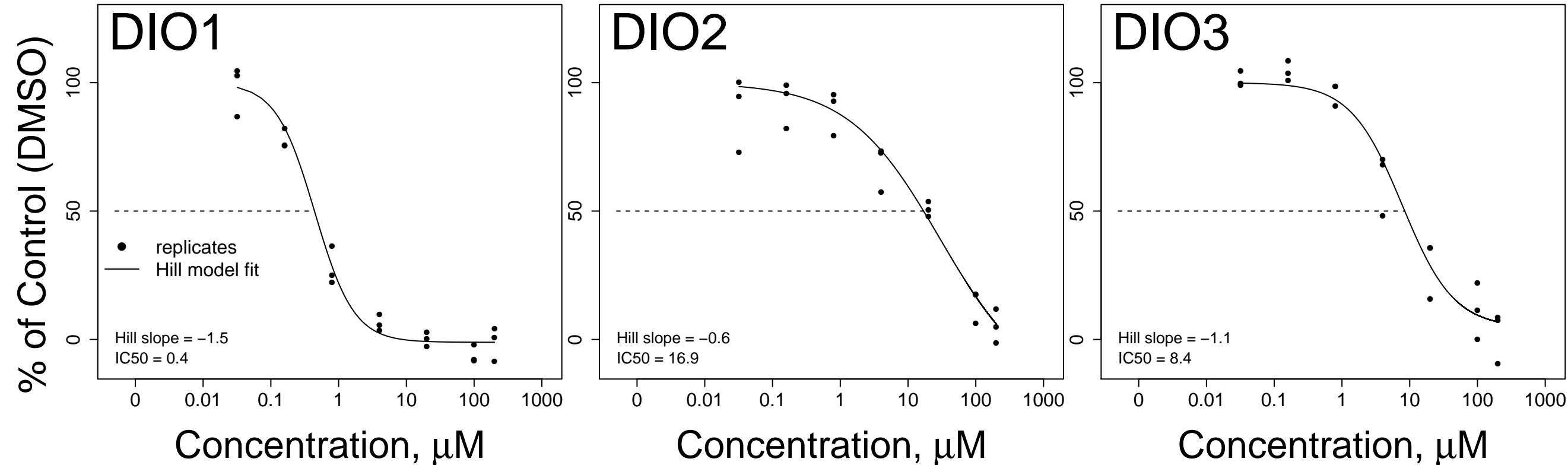
Sodium 2-phenylphenate tetrahydrate CASRN: 6152-33-6



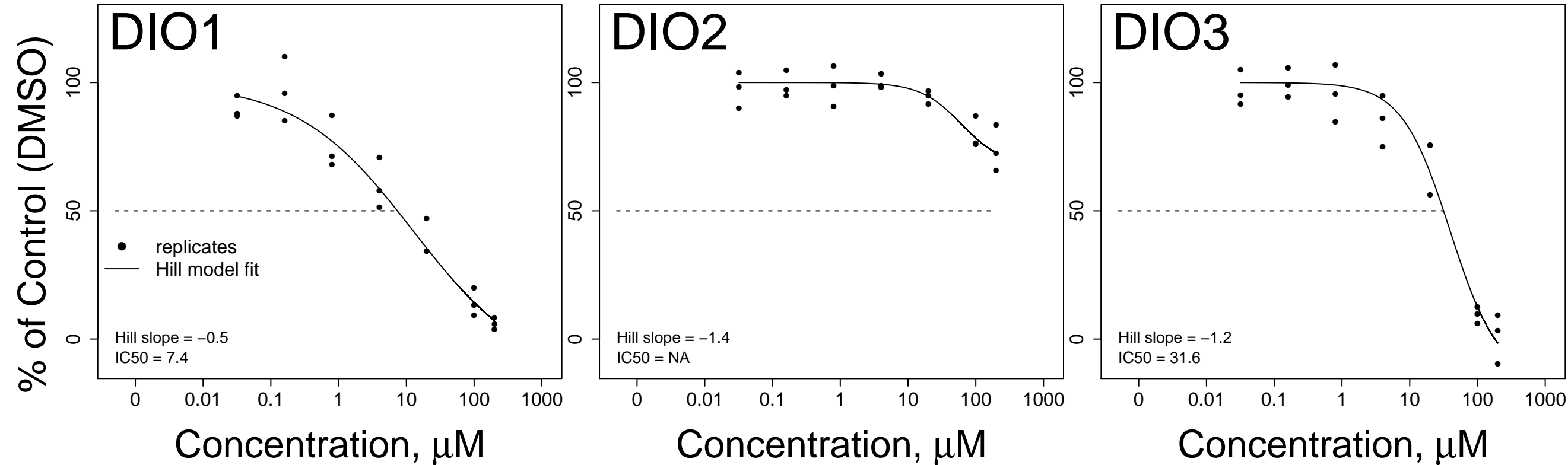
Benzyl-C8-18-alkyldimethylammonium chlorides CASRN: 63449-41-2



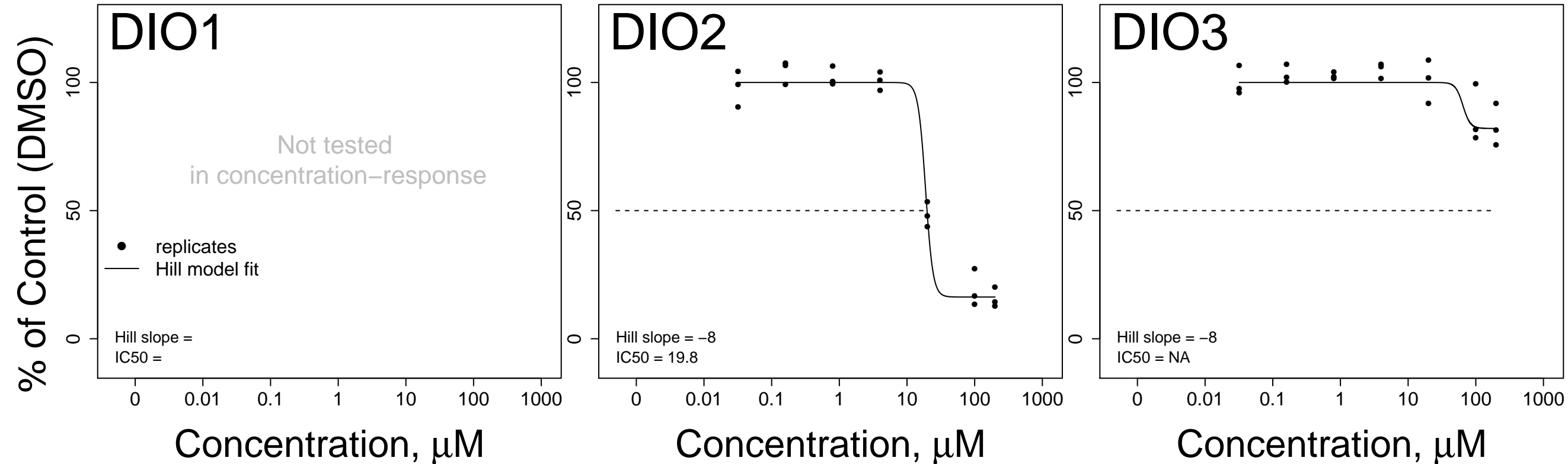
4,5-Dichloro-2-octyl-3(2H)-isothiazolone CASRN: 64359-81-5



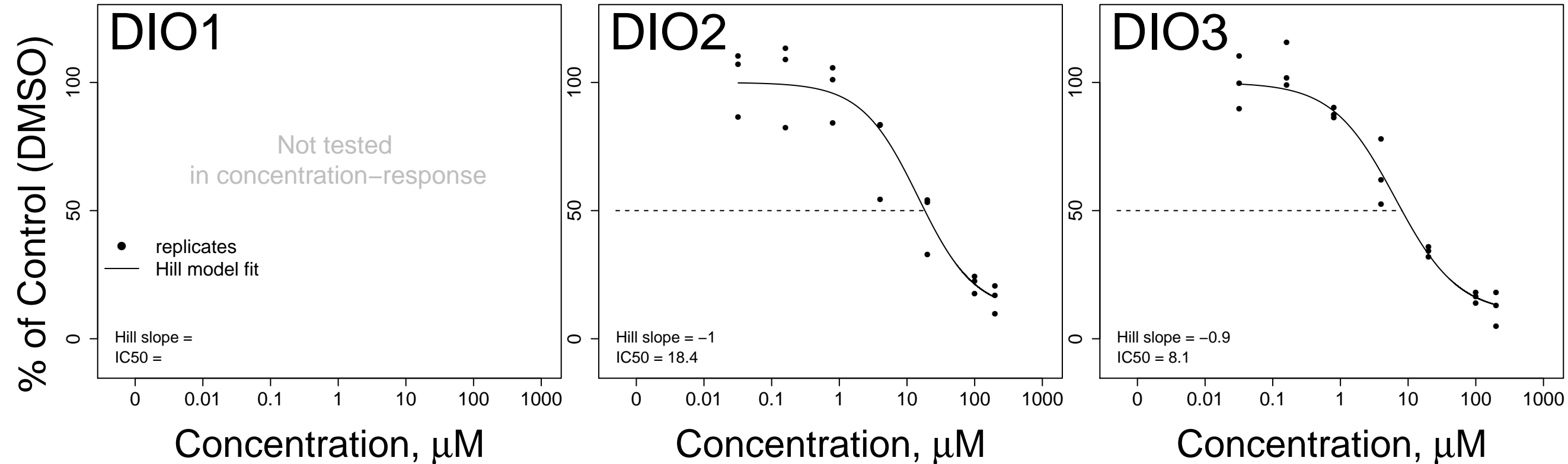
Morin hydrate CASRN: 654055-01-3



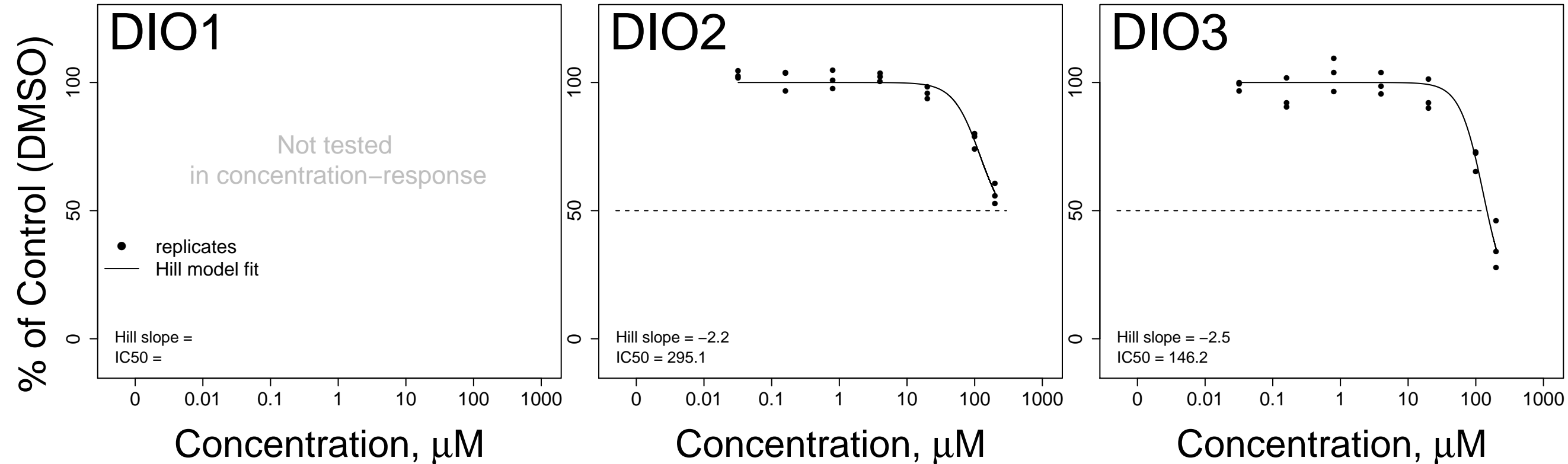
Hydramethylnon CASRN: 67485-29-4



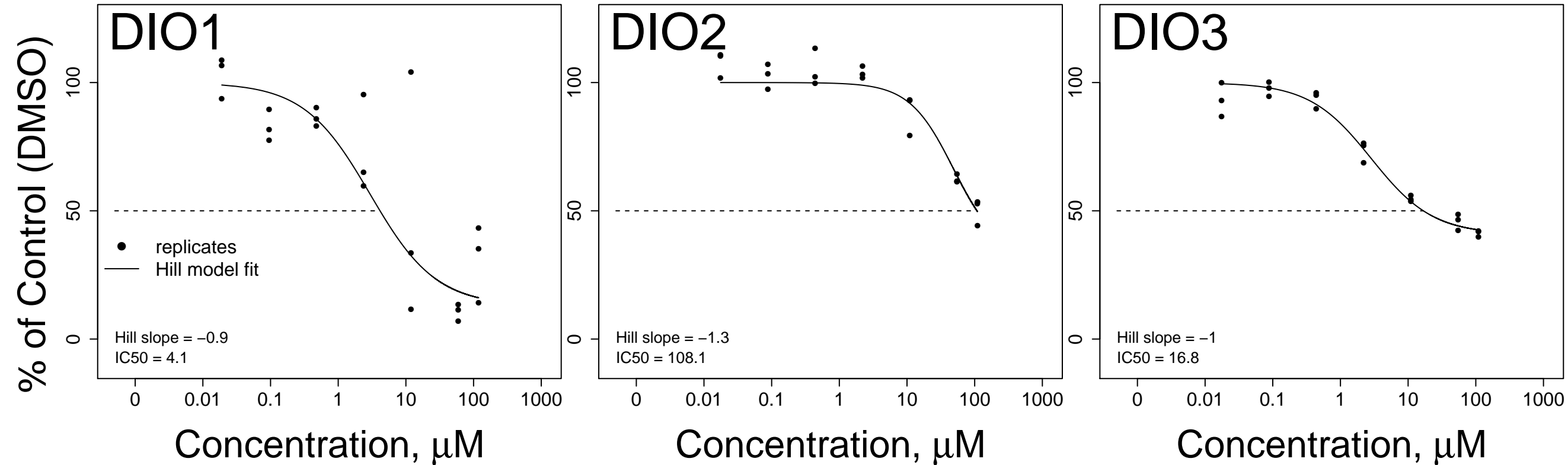
(Dicyclopentadienyloxy)ethyl methacrylate CASRN: 68169-03-9



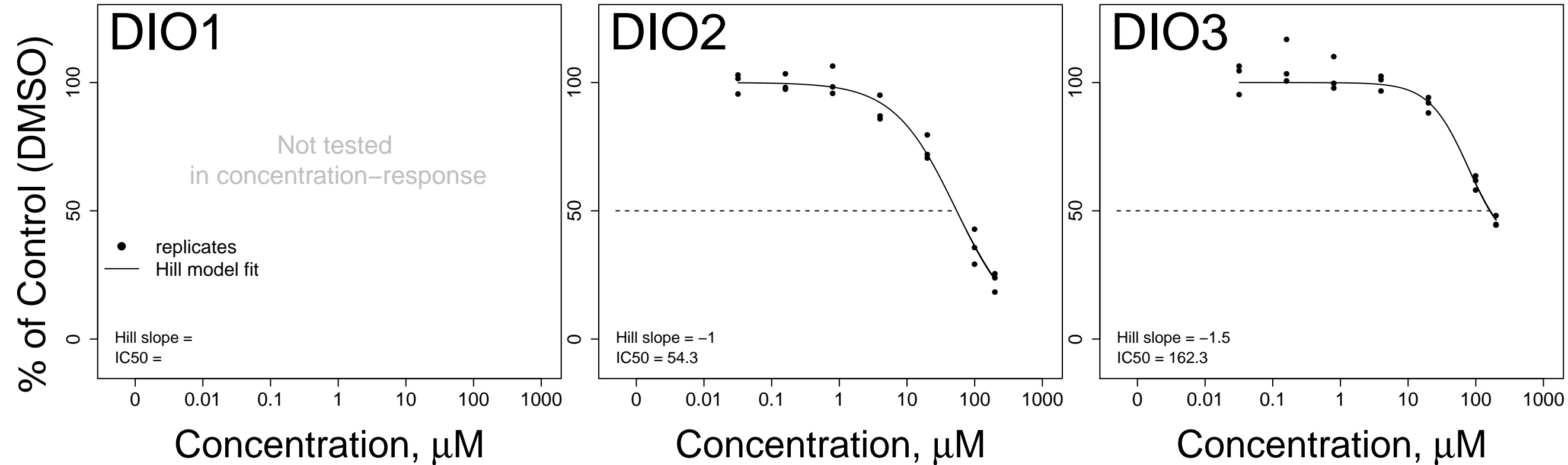
Acid Orange 156 CASRN: 68555-86-2



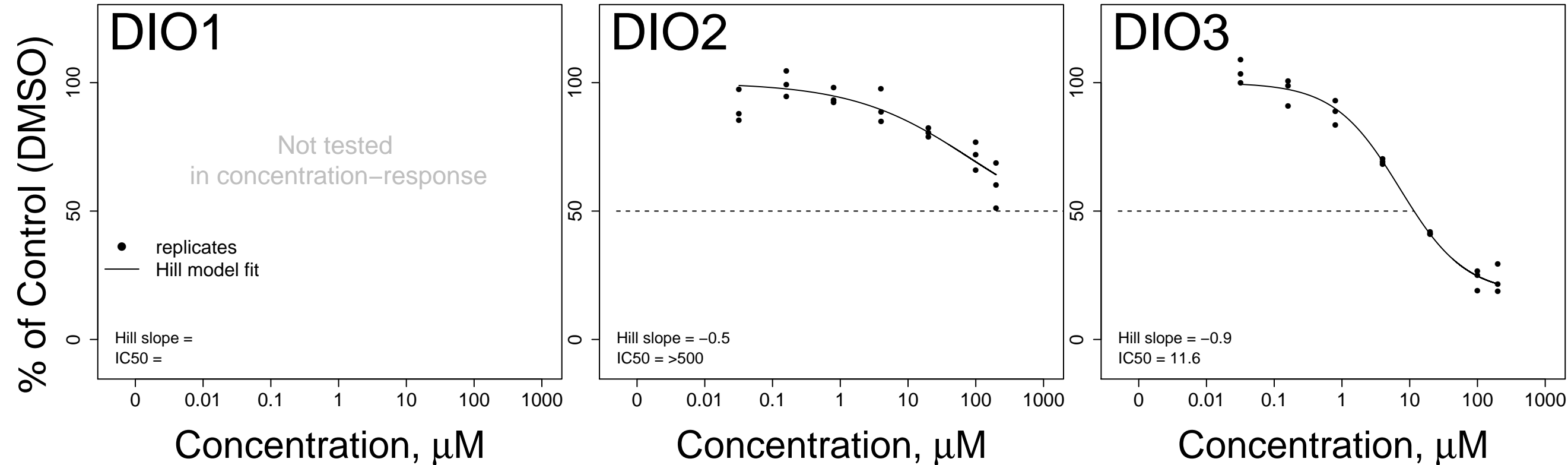
C12-14-Alkyl glycidyl ether CASRN: 68609-97-2



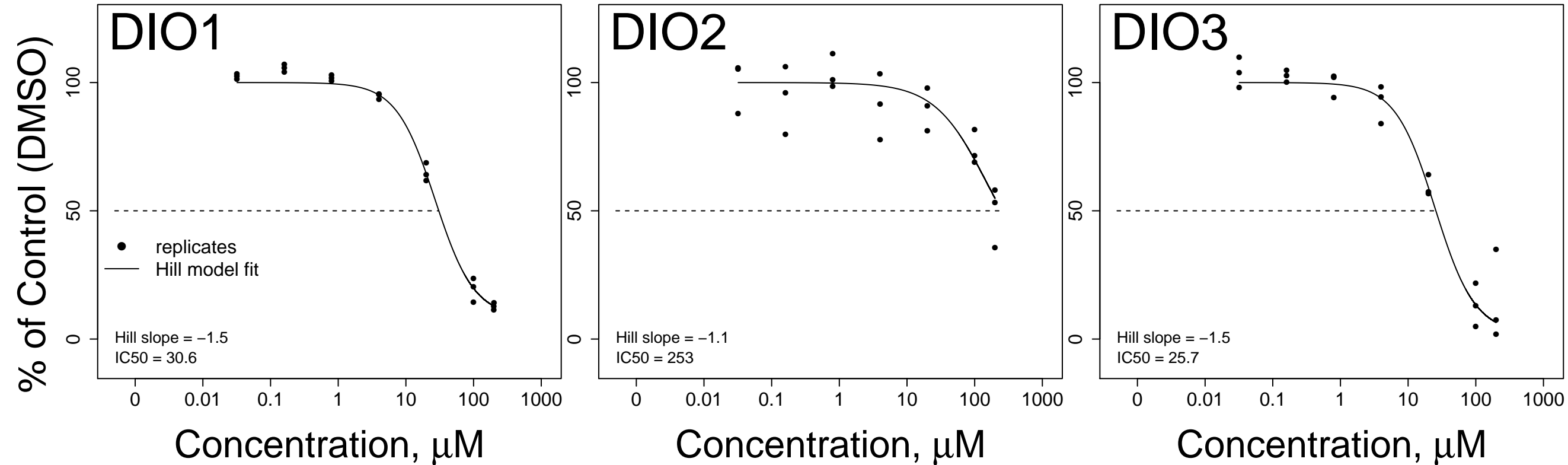
(2-Nitro-1-propenyl)benzene CASRN: 705-60-2



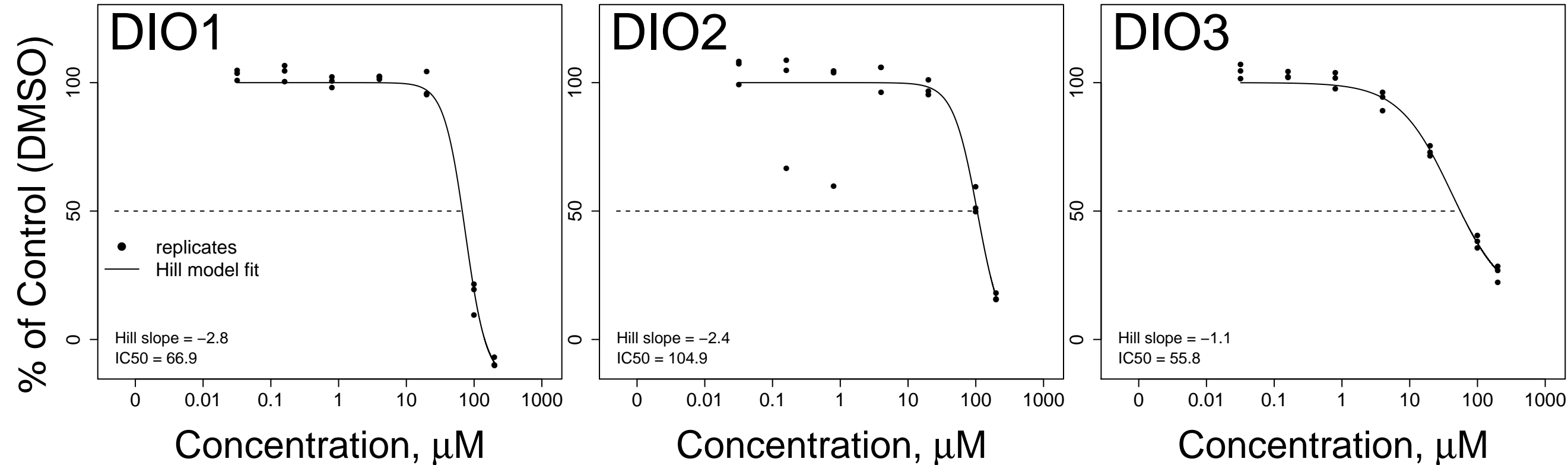
Fenoxaprop-P-ethyl CASRN: 71283-80-2



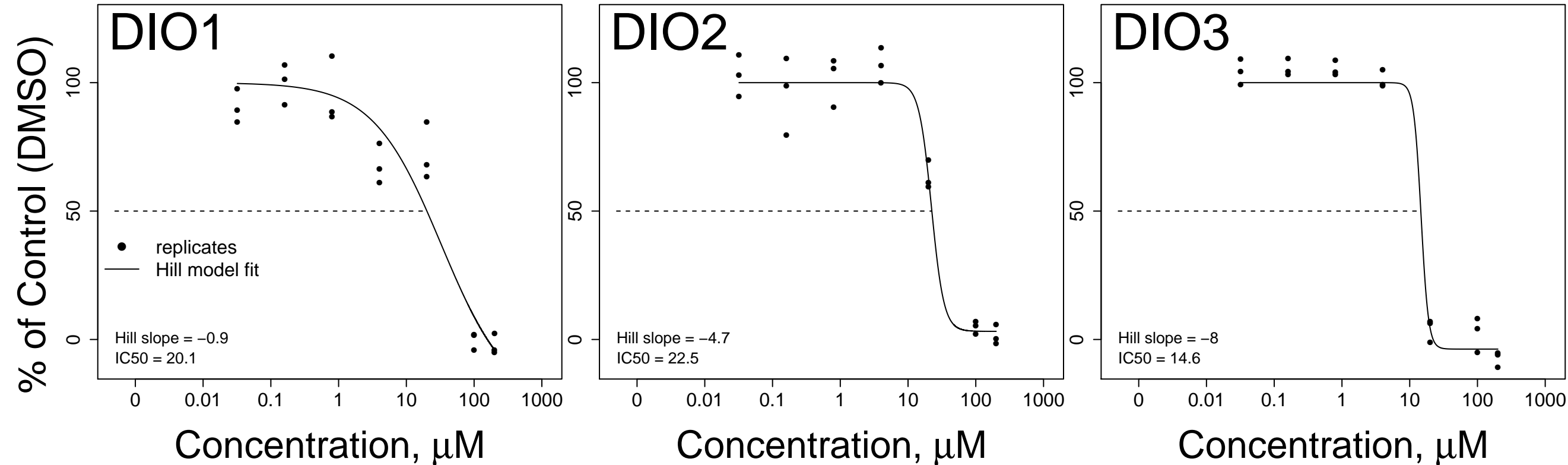
Oxytetracycline CASRN: 79-57-2



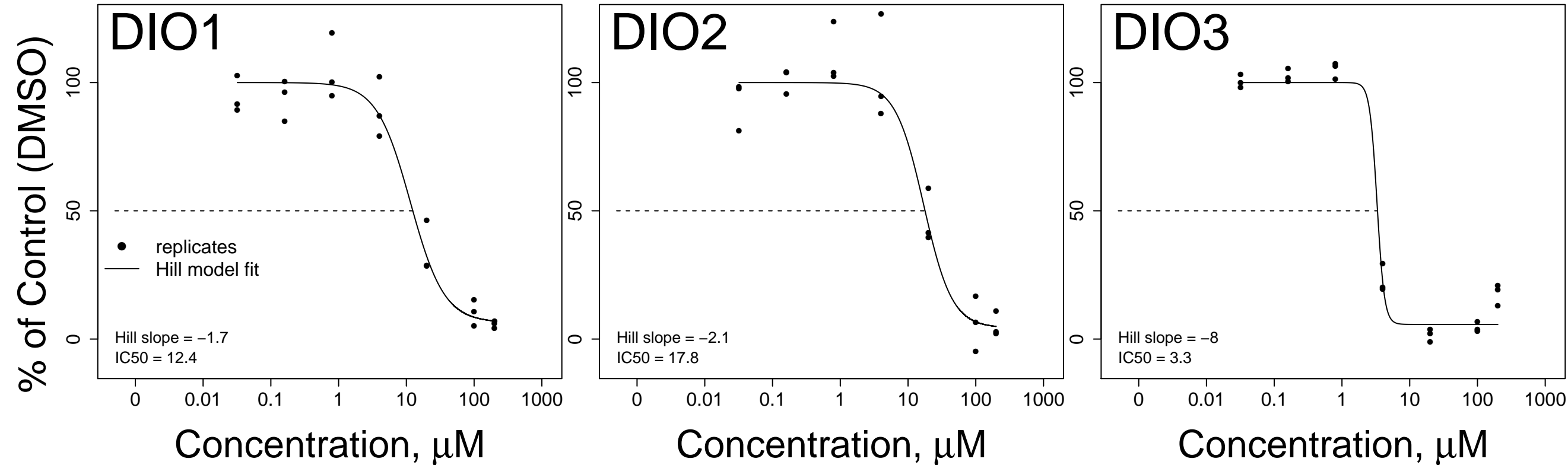
2,2',6,6'-Tetrachlorobisphenol A CASRN: 79-95-8



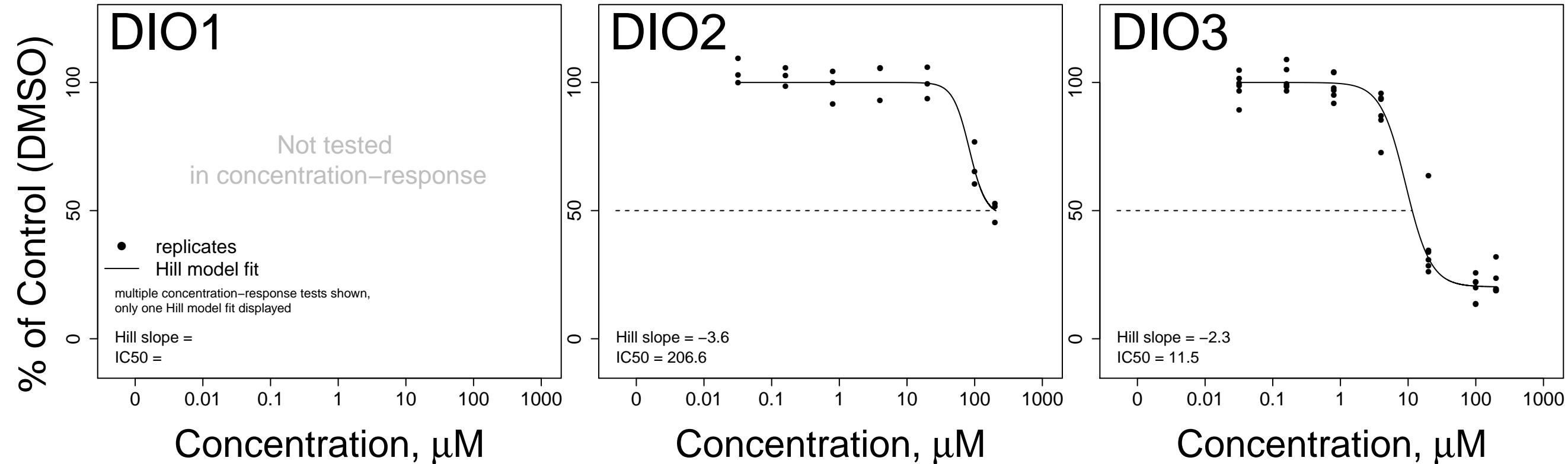
Benzalkonium chloride CASRN: 8001-54-5



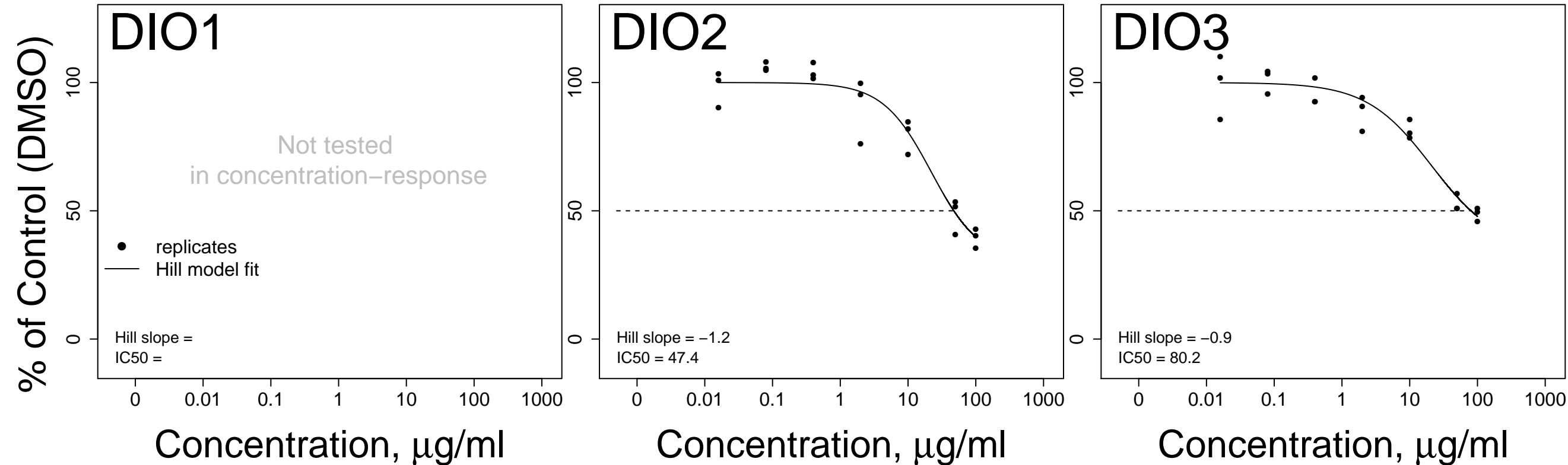
Tributyltetradecylphosphonium chloride CASRN: 81741-28-8



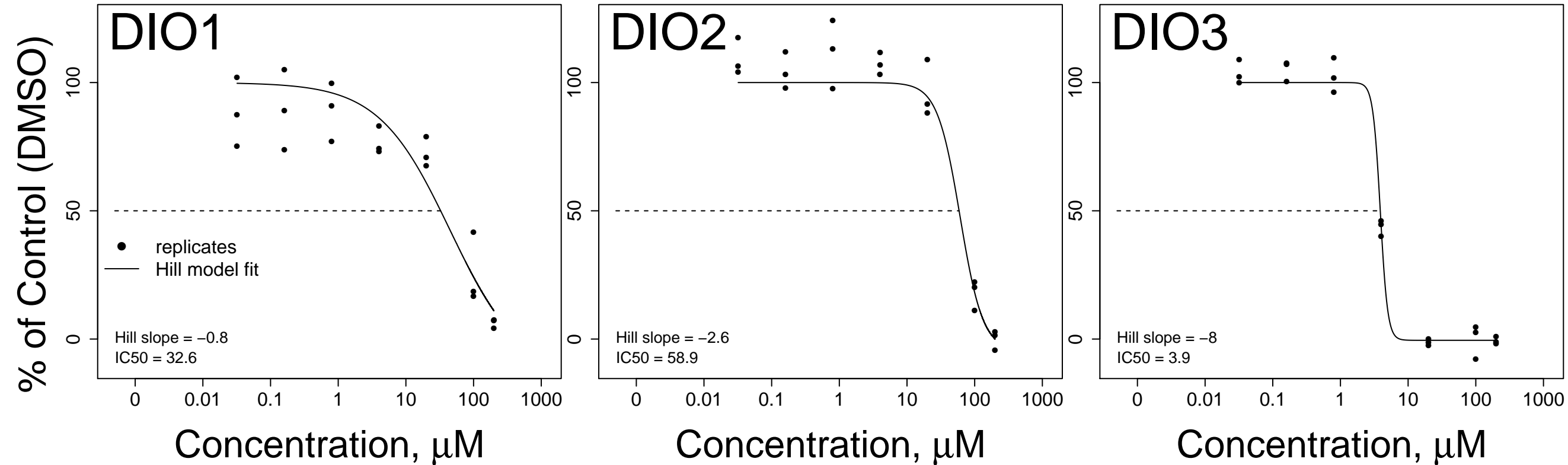
2,2'-Methylenebis(ethyl-6-tert-butylphenol) CASRN: 88-24-4



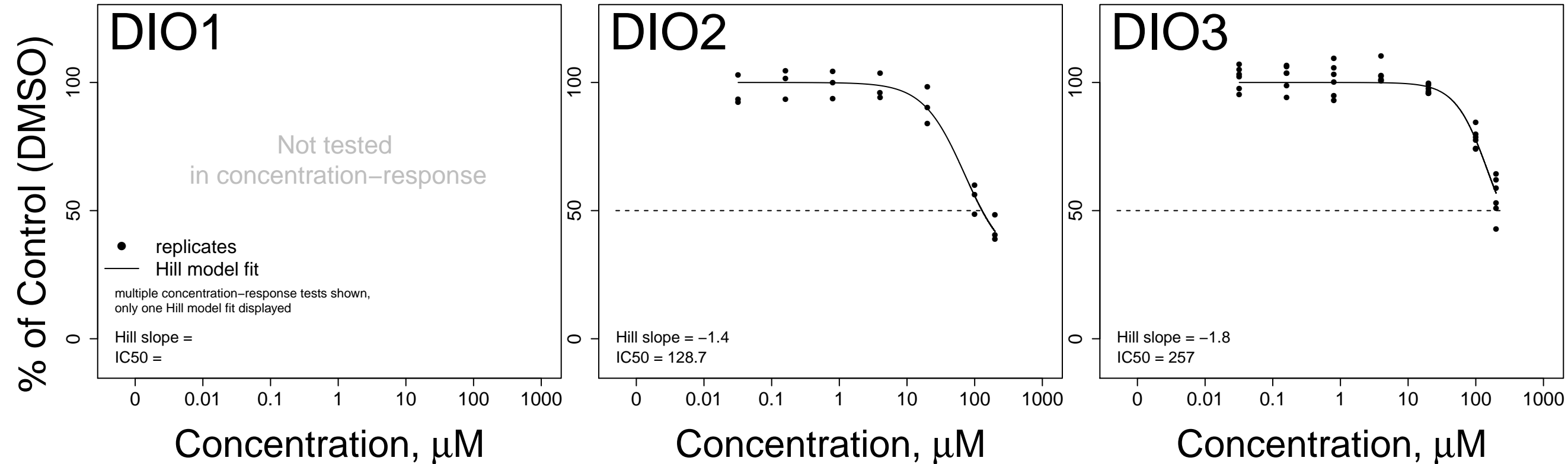
Polyoxyethylene monoleate CASRN: 9004-96-0



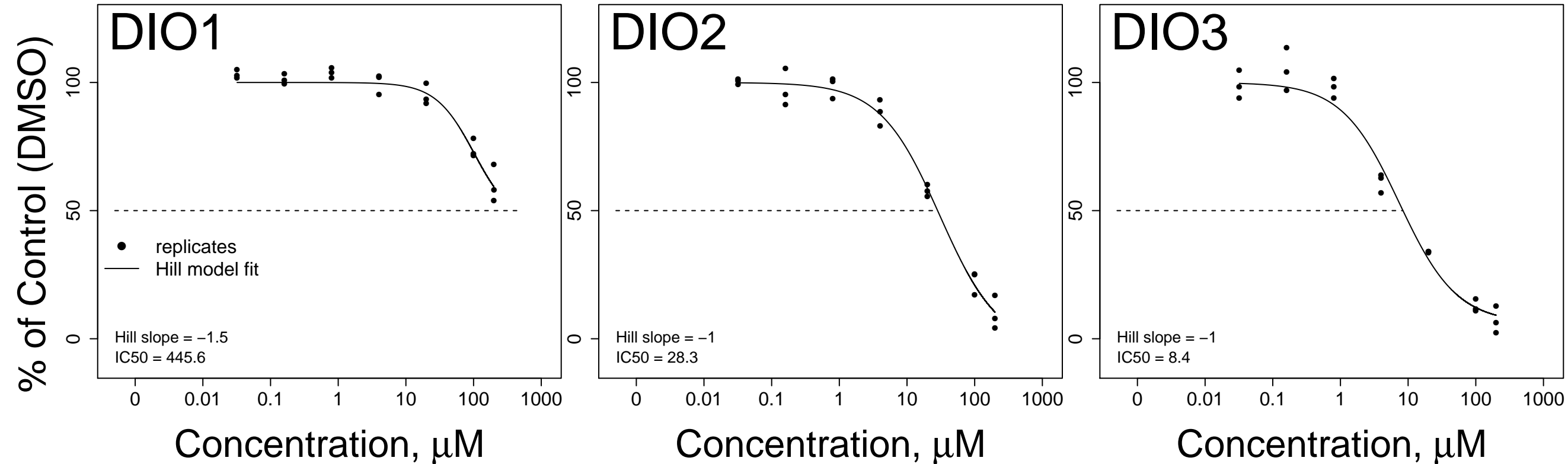
2-(8-Heptadecenyl)-2-imidazoline-1-ethanol CASRN: 95-38-5



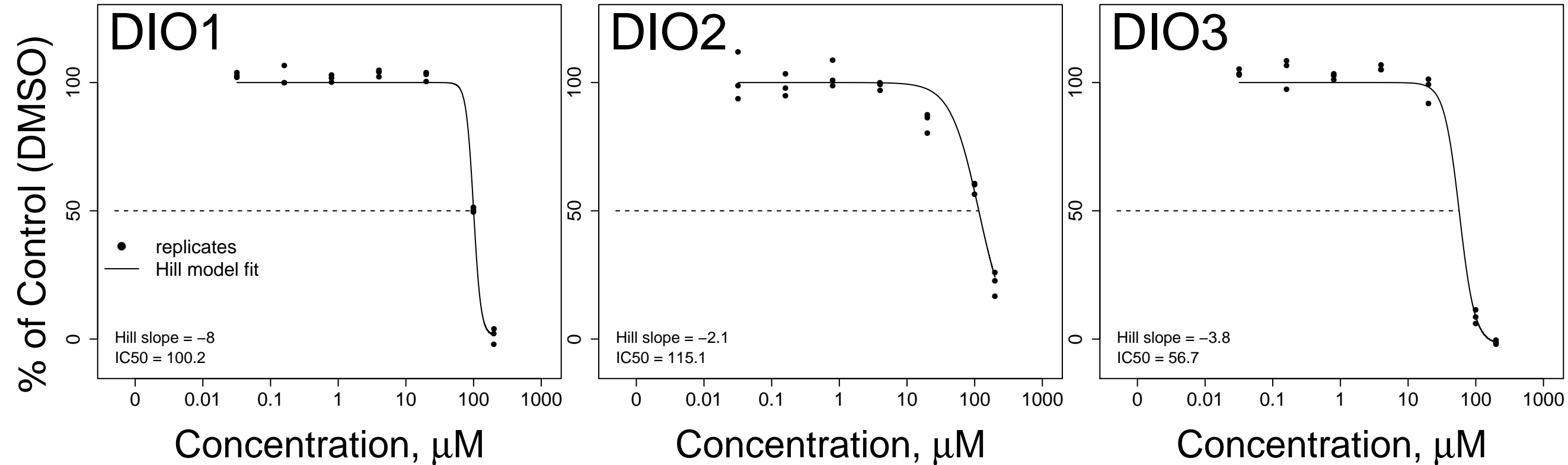
Triphenylborane CASRN: 960-71-4



1-Chloro-2,4-dinitrobenzene CASRN: 97-00-7



Dichlorophen CASRN: 97-23-4



Rhodamine 6G CASRN: 989-38-8

