

ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: DMSO (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO

M4ID: 30230171 BRK

HILL MODEL: Not applicable.

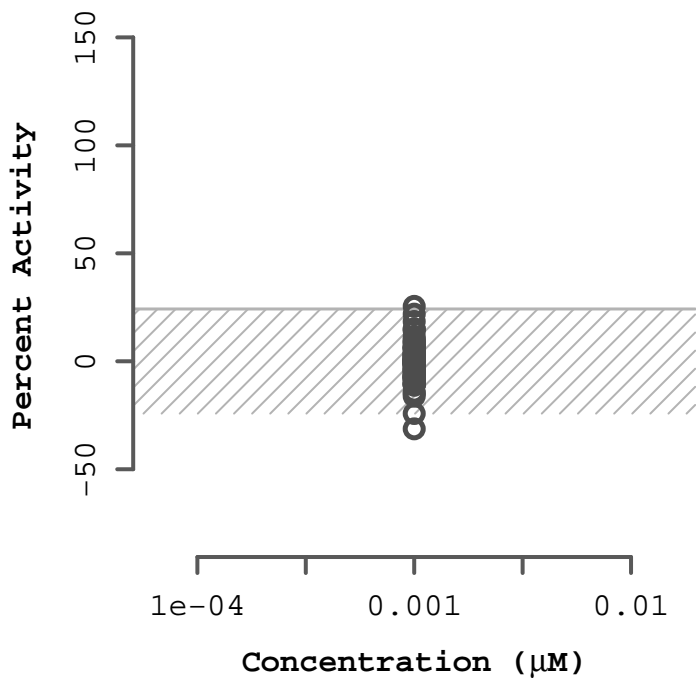
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	NA	NA	NA
PROB:	NA	NA	NA
RMSE:	NA	NA	NA

MAX\_MEAN: -0.289 MAX\_MED: 0.0393 BMAD: 8.07

COFF: 24.2 HIT-CALL: -1 FITC: 2 ACTP: NA

FLAGS:



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Water (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Water

M4ID: 30230172

HILL MODEL: Not applicable.

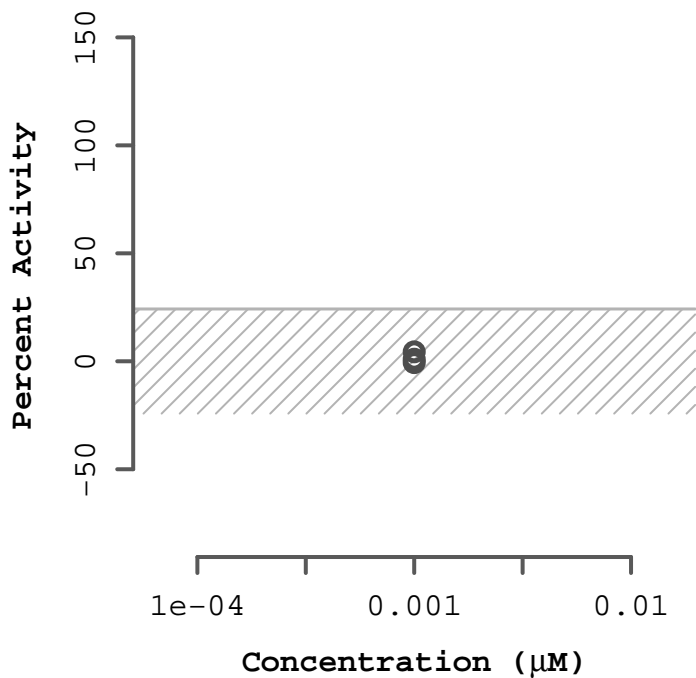
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	NA	NA	NA
PROB:	NA	NA	NA
RMSE:	NA	NA	NA

MAX\_MEAN: -0.717 MAX\_MED: -0.26 BMAD: 8.07

COFF: 24.2 HIT-CALL: -1 FITC: 2 ACTP: NA

FLAGS:



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: DMSO/Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO/Ethanol

M4ID: 30230173

HILL MODEL: Not applicable.

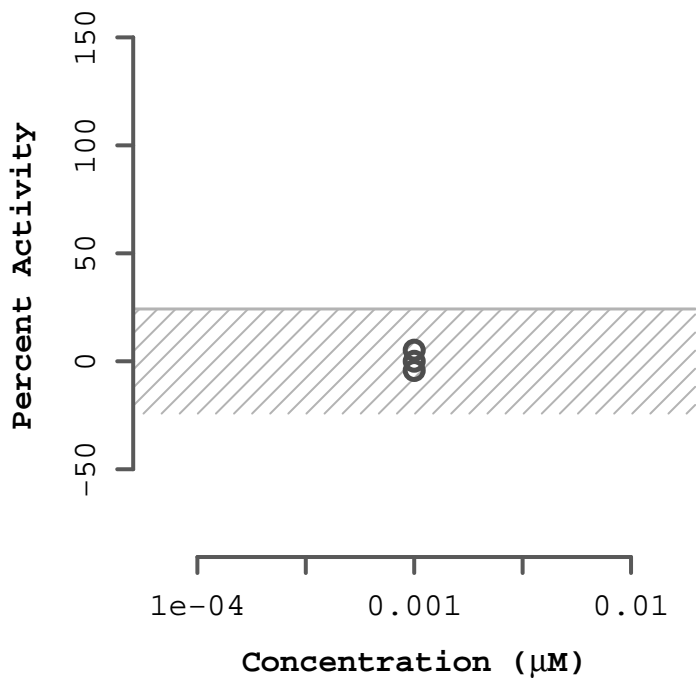
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	NA	NA	NA
PROB:	NA	NA	NA
RMSE:	NA	NA	NA

MAX\_MEAN: 1.59 MAX\_MED: 0.974 BMAD: 8.07

COFF: 24.2 HIT-CALL: -1 FITC: 2 ACTP: NA

FLAGS:



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Ethanol

M4ID: 30230174

HILL MODEL: Not applicable.

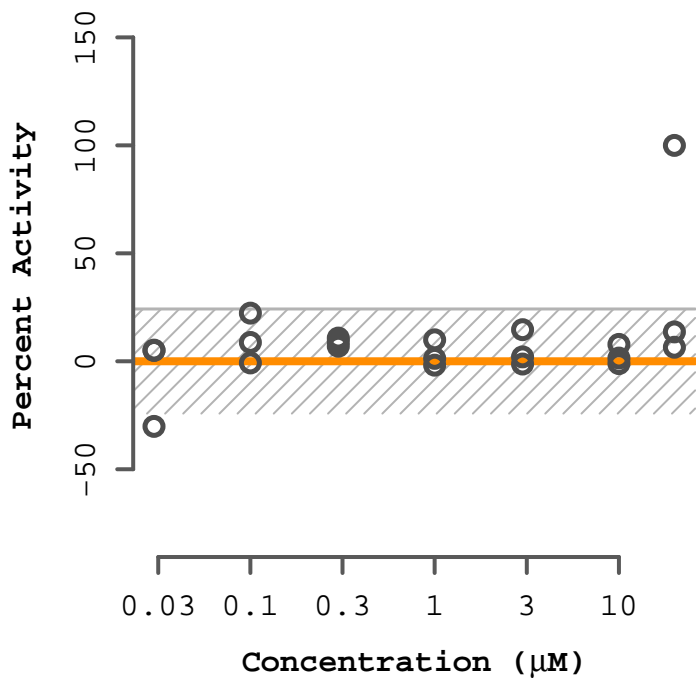
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	NA	NA	NA
PROB:	NA	NA	NA
RMSE:	NA	NA	NA

MAX\_MEAN: 0.316 MAX\_MED: 0.0305 BMAD: 8.07

COFF: 24.2 HIT-CALL: -1 FITC: 2 ACTP: NA

FLAGS:



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Chlorendic acid

CHID: 20268 CASRN: 115-28-6

SPID(S): TP0001649F01

M4ID: 30230185

HILL MODEL: Not applicable.

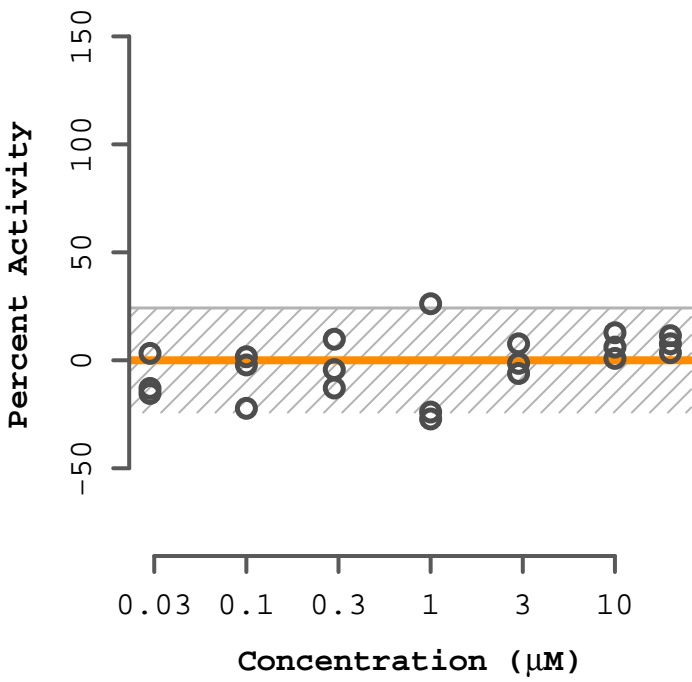
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	177.01	NA	NA
PROB:	1	NA	NA
RMSE:	24.3	NA	NA

MAX\_MEAN: 40 MAX\_MED: 13.6 BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS: 10



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Triphenyl phosphite  
CHID: 26252 CASRN: 101-02-0  
SPID(S): TP0001649E09  
M4ID: 30230182

HILL MODEL: Not applicable.

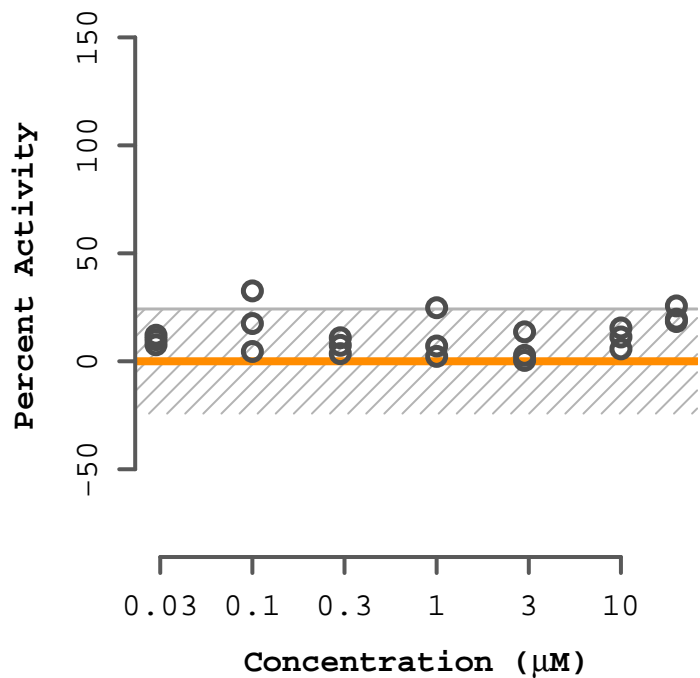
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	171.27	NA	NA
PROB:	1	NA	NA
RMSE:	13.26	NA	NA

MAX\_MEAN: 7.54      MAX\_MED: 7.67      BMAD: 8.07

COFF: 24.2      HIT-CALL: 0      FITC: 4      ACTP: 0

FLAGS:



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

CHID: 34465 CASRN: 210880-92-5

**M4ID: 30230186**

HILL MODEL: Not applicable.

**GAIN-LOSS MODEL:** Not applicable.

	CNST	HILL	GNLS
AIC:	176.22	NA	NA
PROB:	1	NA	NA
RMSE:	14.68	NA	NA

PROB: 1

RMSE: 14.68

HILL

NA

NA

NA

**G-NLS**

NA

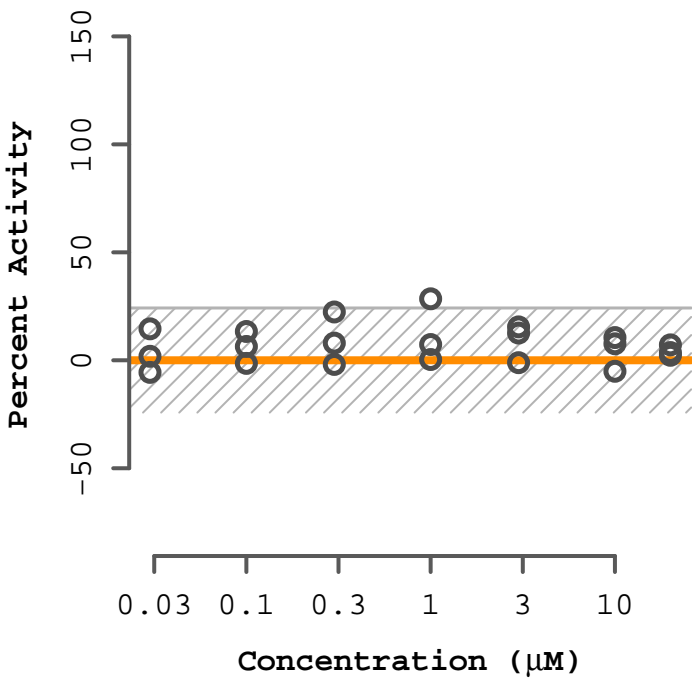
NA

NA

MAX\_MEAN: 21.2      MAX\_MED: 19.5      BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 4 ACTP: 0

**FLAGS :**



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Thiocloprid

CHID: 34961 CASRN: 111988-49-9

SPID(S): TP0001649E07

M4ID: 30230181

HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

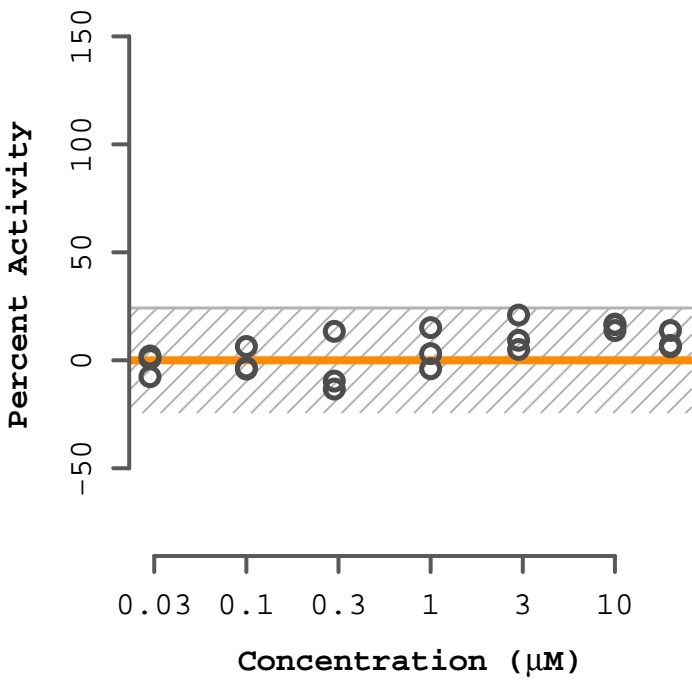
	CNST	HILL	GNLS
AIC:	162.48	NA	NA
PROB:	1	NA	NA
RMSE:	11.06	NA	NA

MAX\_MEAN: 12.1 MAX\_MED: 12.6 BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:





ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Thiamethoxam

CHID: 34962 CASRN: 153719-23-4

SPID(S): TP0001649E10

M4ID: 30230183

HILL MODEL: Not applicable.

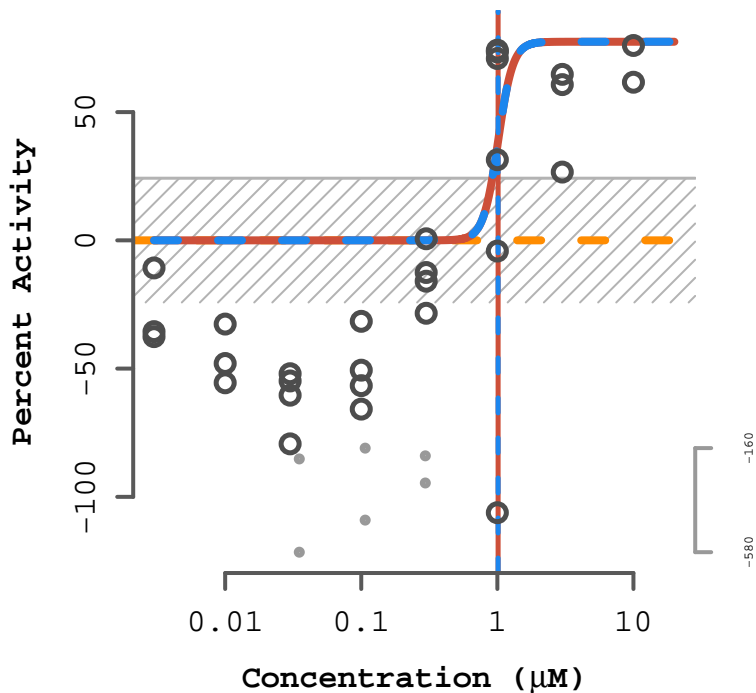
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	163.89	NA	NA
PROB:	1	NA	NA
RMSE:	10.71	NA	NA

MAX\_MEAN: 15.7 MAX\_MED: 16.5 BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 4 ACTP: 0

FLAGS:



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Lovastatin

CHID: 20784 CASRN: 75330-75-5

SPID(S): TP0001649D08

M4ID: 30230179 BRK

HILL MODEL (in red):

	tp	ga	gw
val:	77.4	0.00554	8
sd:	15.6	0.0946	72.2

GAIN-LOSS MODEL (in blue):

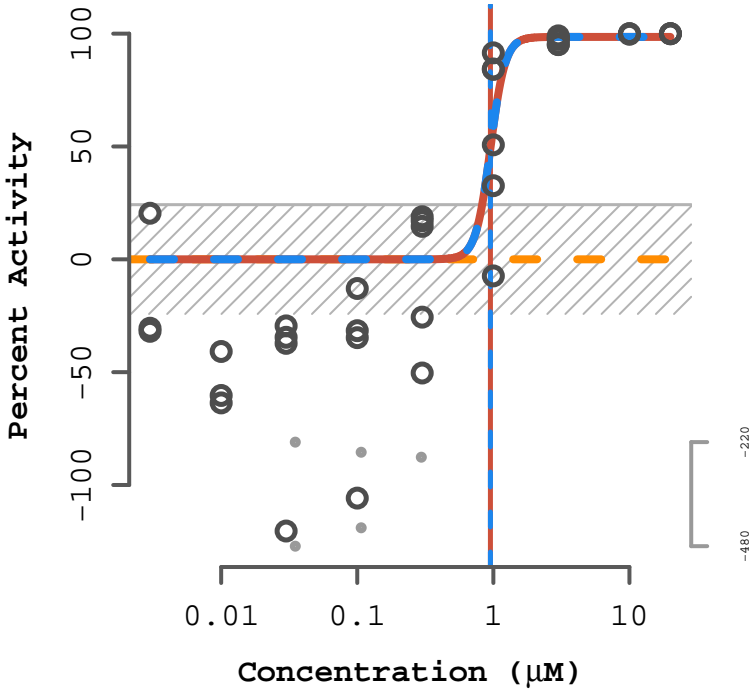
	tp	ga	gw	la	lw
val:	77.4	0.00557	8	1.83	15.6
sd:	15.6	0.095	72.4	1180	34600

	CNST	HILL	GNLS
AIC:	521.63	511.5	515.5
PROB:	0.01	0.88	0.12
RMSE:	144.82	138.69	138.69

MAX\_MEAN: 89.8 MAX\_MED: 85.7 BMAD: 8.07

COFF: 24.2 HIT-CALL: 1 FITC: 41 ACTP: 0.99

FLAGS: 10



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Mercuric chloride  
CHID: 20811 CASRN: 7487-94-7  
SPID(S): TP0001649C11  
M4ID: 30230177 BRK

HILL MODEL (in red):

	tp	ga	gw
val:	98.6	-0.0214	8
sd:	12	0.163	58.7

GAIN-LOSS MODEL (in blue):

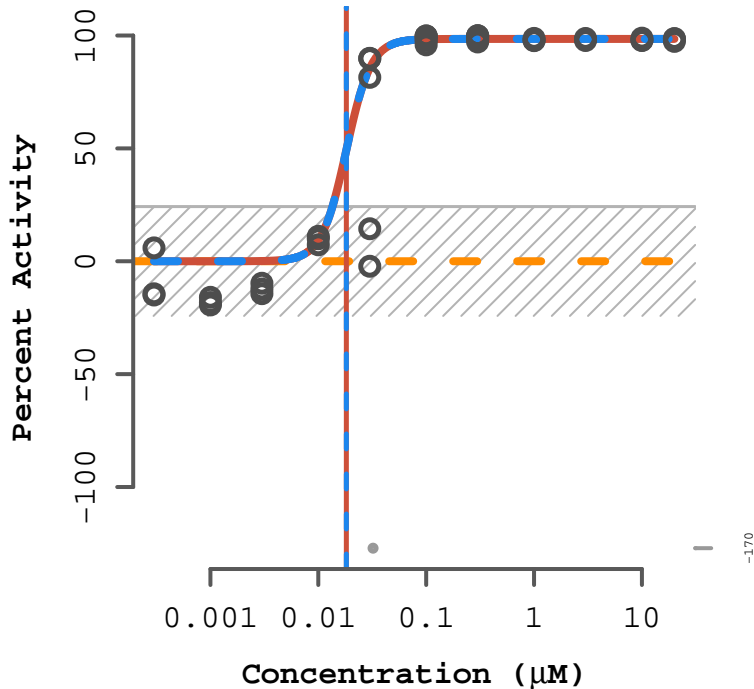
	tp	ga	gw	la	lw
val:	98.6	-0.0214	8	2.14	8.59
sd:	12	0.164	59.1	1250	12700

	CNST	HILL	GNLS
AIC:	524.07	500.15	504.15
PROB:	0	0.88	0.12
RMSE:	136.93	124.62	124.62

MAX\_MEAN: 100      MAX\_MED: 100      BMAD: 8.07

COFF: 24.2      HIT-CALL: 1      FITC: 41      ACTP: 1

FLAGS: 10



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Phenylmercuric acetate

CHID: 21150 CASRN: 62-38-4

SPID(S): TP0001649D11

M4ID: 30230180 BRK

HILL MODEL (in red):

	tp	ga	gw
val:	98.5	-1.74	3.78
sd:	1.13	0.0302	0.464

GAIN-LOSS MODEL (in blue):

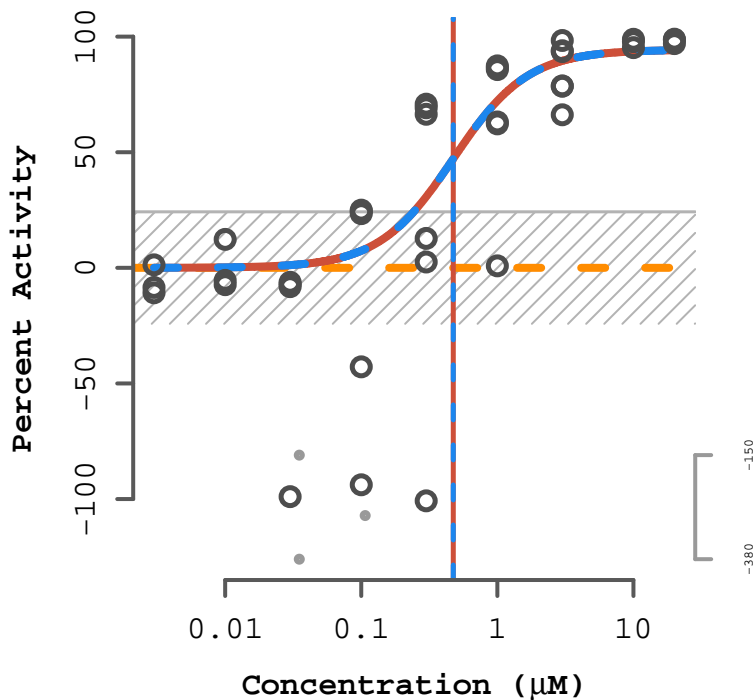
	tp	ga	gw	la	lw
val:	98.5	-1.74	3.78	3.19	12.4
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	586.6	350.72	354.72
PROB:	0	0.88	0.12
RMSE:	82.74	43.98	43.98

MAX\_MEAN: 98.9 MAX\_MED: 99.2 BMAD: 8.07

COFF: 24.2 HIT-CALL: 1 FITC: 41 ACTP: 1

FLAGS: 10



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Simvastatin

CHID: 23581 CASRN: 79902-63-9

SPID(S): TP0001649C08

M4ID: 30230175 BRK

HILL MODEL (in red):

	tp	ga	gw
val:	94.3	-0.324	1.59
sd:	10.4	0.194	0.682

GAIN-LOSS MODEL (in blue):

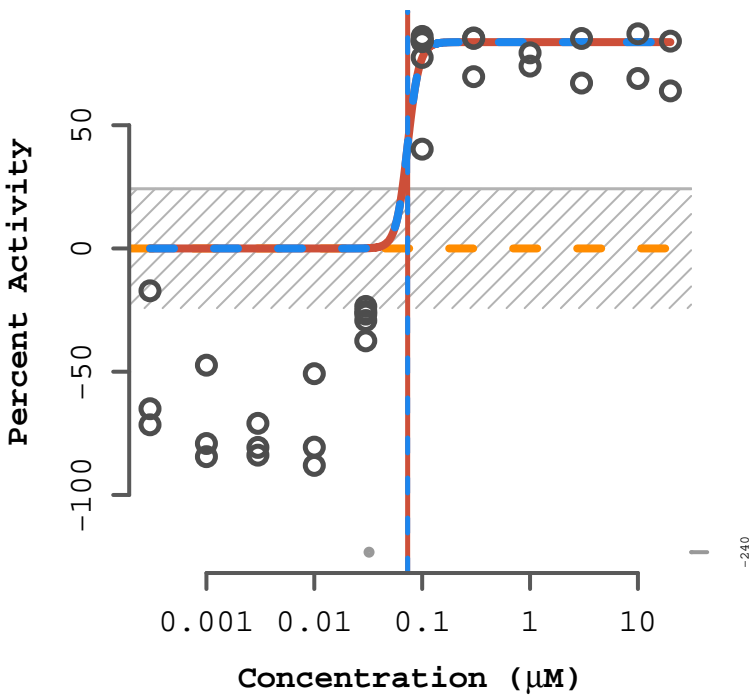
	tp	ga	gw	la	lw
val:	94.3	-0.324	1.59	1.9	18
sd:	10.4	0.194	0.682	12700	381000

	CNST	HILL	GNLS
AIC:	502.19	460.79	464.79
PROB:	0	0.88	0.12
RMSE:	100.92	85.66	85.66

MAX\_MEAN: 98.2 MAX\_MED: 98.6 BMAD: 8.07

COFF: 24.2 HIT-CALL: 1 FITC: 41 ACTP: 1

FLAGS: 10



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Tributyltin chloride  
CHID: 27403 CASRN: 1461-22-9  
SPID(S): TP0001649C09  
M4ID: 30230176 BRK

HILL MODEL (in red):

	tp	ga	gw
val:	83.7	-1.13	8
sd:	7.22	0.169	8.48

GAIN-LOSS MODEL (in blue):

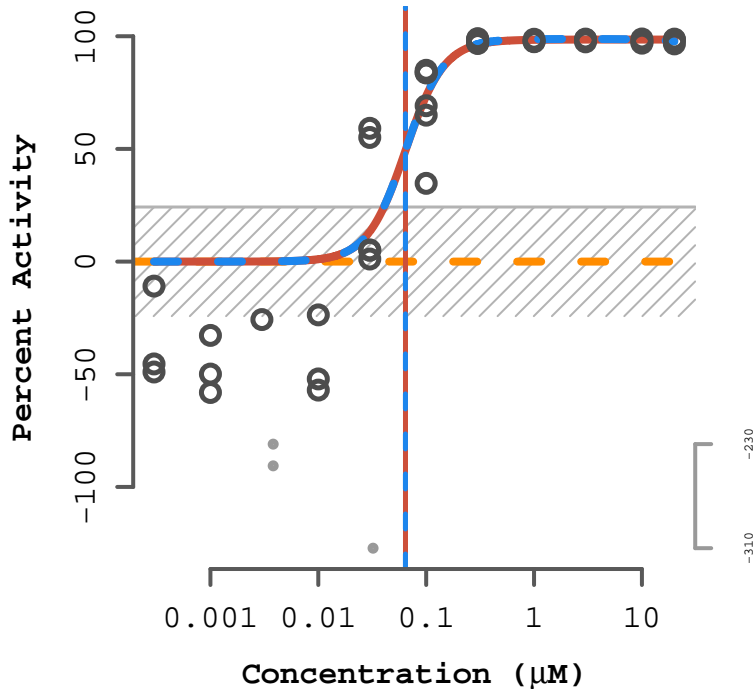
	tp	ga	gw	la	lw
val:	83.7	-1.13	8	2.34	14.9
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	497.92	449.88	453.88
PROB:	0	0.88	0.12
RMSE:	82.78	55.1	55.1

MAX\_MEAN: 89.1      MAX\_MED: 91.4      BMAD: 8.07

COFF: 24.2      HIT-CALL: 1      FITC: 41      ACTP: 1

FLAGS: 10



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Tributyltin methacrylate

CHID: 35204 CASRN: 2155-70-6

SPID(S): TP0001649D04

M4ID: 30230178 BRK

HILL MODEL (in red):

	tp	ga	gw
val:	98.5	-1.19	2.44
sd:	5.53	0.101	0.84

GAIN-LOSS MODEL (in blue):

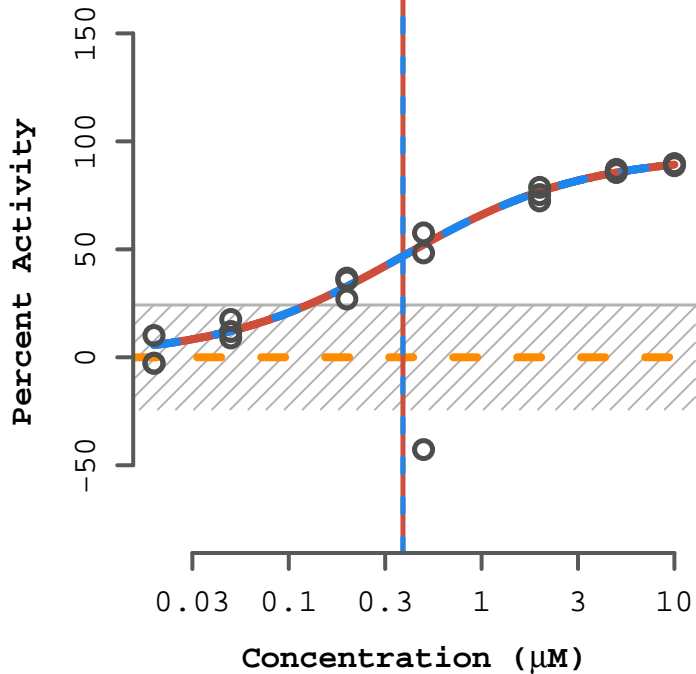
	tp	ga	gw	la	lw
val:	98.8	-1.19	2.43	2.21	2.12
sd:	22.6	0.167	1.18	86.2	222

	CNST	HILL	GNLS
AIC:	510.8	447.35	451.34
PROB:	0	0.88	0.12
RMSE:	102.48	76.4	76.41

MAX\_MEAN: 98.3 MAX\_MED: 98.6 BMAD: 8.07

COFF: 24.2 HIT-CALL: 1 FITC: 41 ACTP: 1

FLAGS: 10



ASSAY: AEID3271 (CCTE\_Shafer\_MEA\_dev\_LDH\_dn)

NAME: Pravastatin sodium

CHID: 47525 CASRN: 81131-70-6

SPID(S): TP0001649E12

M4ID: 30230184

HILL MODEL (in red):

	tp	ga	gw
val:	93.7	-0.408	0.924
sd:	3.35	0.0697	0.101

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	93.7	-0.408	0.925	1.76	11.3
sd:	3.35	0.0697	0.101	1770	26200

	CNST	HILL	GNLS
AIC:	236.44	152.23	156.23
PROB:	0	0.88	0.12
RMSE:	59.68	21.07	21.07

MAX\_MEAN: 89.3 MAX\_MED: 89.5 BMAD: 8.07

COFF: 24.2 HIT-CALL: 1 FITC: 41 ACTP: 1

FLAGS: