ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: SB-431542
CHID: 42693   CASRN: 301836-41-9
SPID(S): ES211_56_56
M4ID: 42676087

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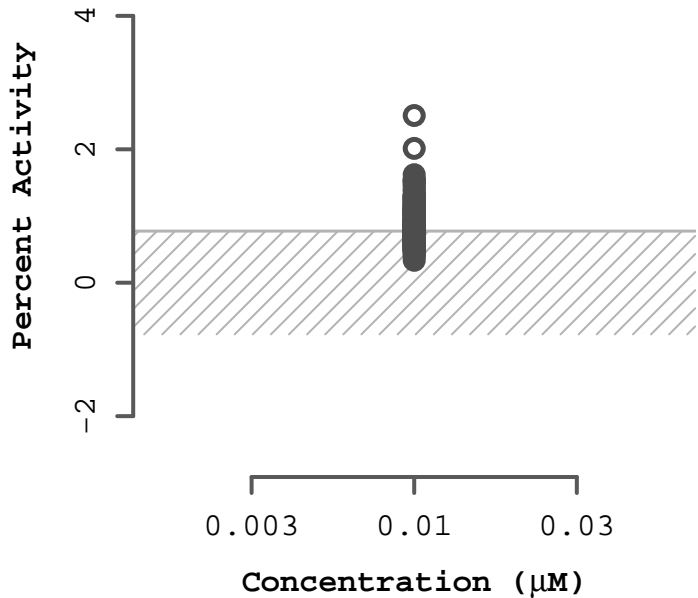
GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 0.765   MAX_MED: 0.731   BMAD: 0.258

COFF: 0.774 HIT-CALL: -1 FITC: 2   ACTP: NA

FLAGS:

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: DMSO (spid not in DB)
CHID: NA   CASRN: NA
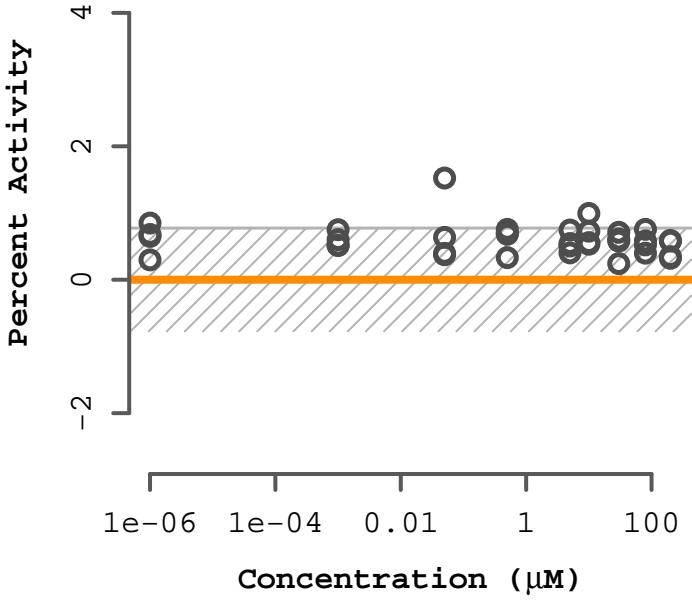SPID(S): DMSO
M4ID: 42676049

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: 0.884   MAX_MED: 0.828   BMAD: 0.258

COFF: 0.774   HIT-CALL: -1   FITC: 2   ACTP: NA

FLAGS:

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Hydroxyurea
CHID: 25438   CASRN: 127-07-1
SPID(S): ES211_35_35
M4ID: 42676097

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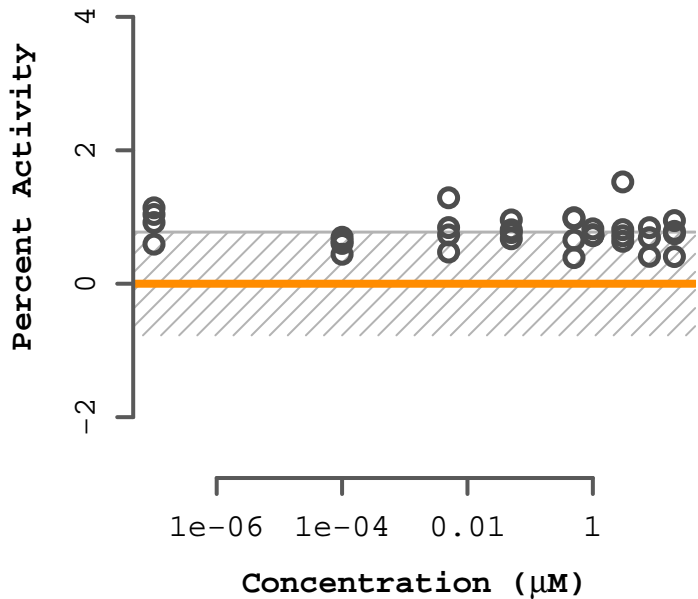
GAIN-LOSS MODEL: Not applicable.

	CNST	HILL	GNLS
AIC:	78.1	NA	NA
PROB:	1	NA	NA
RMSE:	0.64	NA	NA

MAX_MEAN: 0.733   MAX_MED: 0.69   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 4   ACTP: 0

FLAGS:

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Dexamethasone sodium phosphate
CHID: 47429   CASRN: 2392-39-4
SPID(S): ES211_28_28
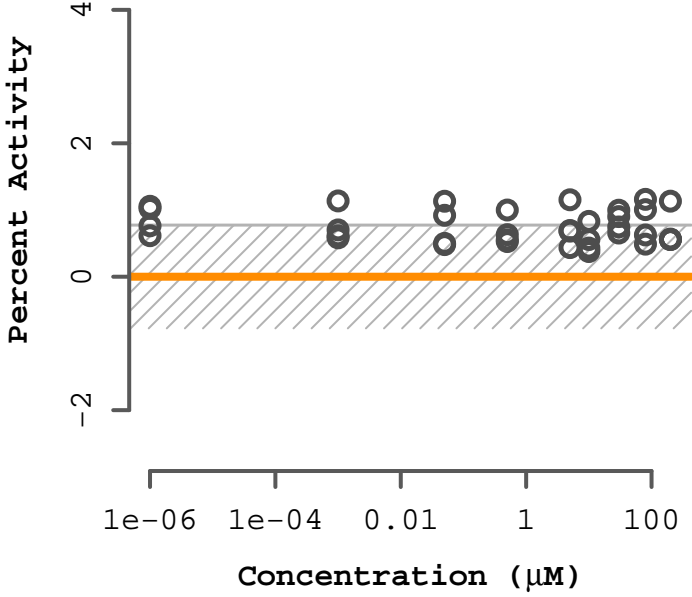M4ID: 42676103

HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

	CNST	HILL	GNLS
AIC:	93.73	NA	NA
PROB:	1	NA	NA
RMSE:	0.81	NA	NA

MAX_MEAN: 0.923   MAX_MED: 0.979   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 7   ACTP: 0

FLAGS: 8; 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Pomalidomide
CHID: 893458   CASRN: 19171-19-8
SPID(S): ES211_50_50
M4ID: 42676070

HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

	CNST	HILL	GNLS
AIC:	93.67	NA	NA
PROB:	1	NA	NA
RMSE:	0.78	NA	NA

MAX_MEAN: 0.865   MAX_MED: 0.894   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 7   ACTP: 0

FLAGS: 8; 10
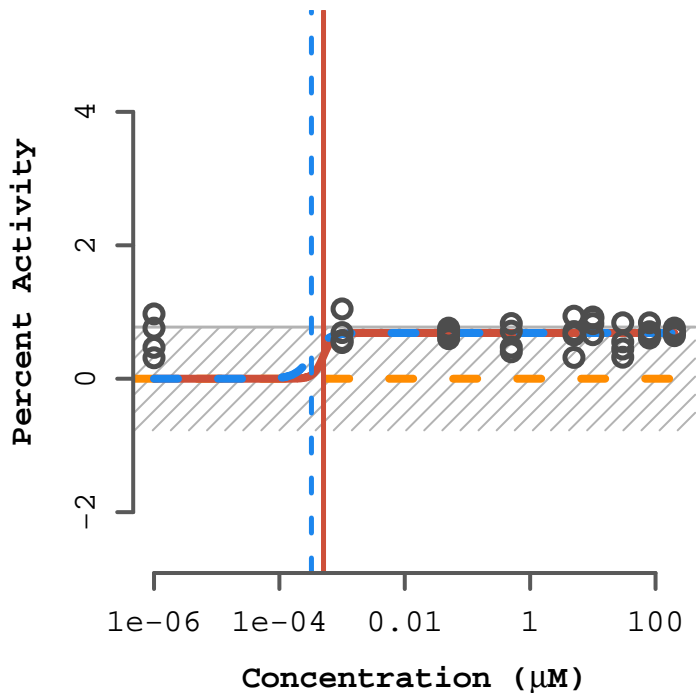
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Acetaminophen
CHID: 20006   CASRN: 103-90-2
SPID(S): ES211_9_9
M4ID: 42676089

HILL MODEL (in red):
        tp   ga   gw
val: 0.686   -3.3   5.49
sd: 0.0371   4.62   85.8

GAIN-LOSS MODEL (in blue):
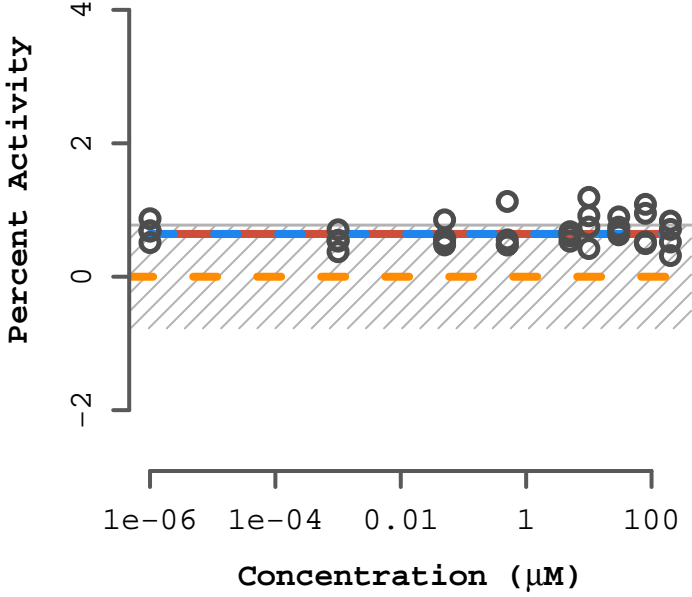   tp   ga   gw   la   lw
val: 0.686   -3.49   3.33   3.92   4.88
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 85.96   9.71   13.71
PROB: 0   0.88   0.12
RMSE: 0.7   0.28   0.28

MAX_MEAN: 0.829   MAX_MED: 0.865   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Boric acid (H3BO3)
CHID: 20194   CASRN: 10043-35-3
SPID(S): ES211_17_17
M4ID: 42676065

HILL MODEL (in red):
       tp   ga   gw
val: 0.641   -7   7.02
sd: 0.0335   186   1200

GAIN-LOSS MODEL (in blue):
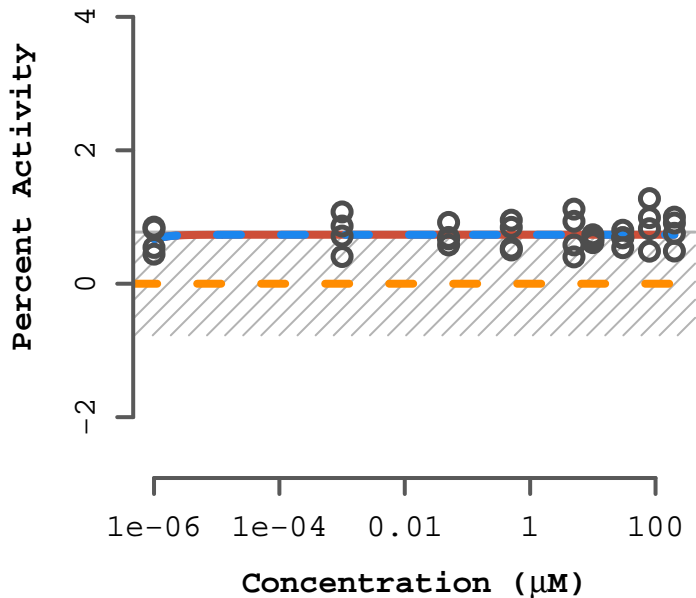   tp   ga   gw   la   lw
val: 0.641   -7   7.1   4.3   18
sd: NA   NA   NA   NA   NA

       CNST   HILL   GNLS
AIC: 85.79   -2.29   1.71
PROB: 0   0.88   0.12
RMSE: 0.7   0.21   0.21

MAX_MEAN: 0.818   MAX_MED: 0.83   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Ethylene glycol
CHID: 20597   CASRN: 107-21-1
SPID(S): ES211_32_32
M4ID: 42676050

HILL MODEL (in red):
       tp   ga   gw
val: 0.734   -6.47   2.14
sd: 0.0387   8.22   37.5

GAIN-LOSS MODEL (in blue):
       tp   ga   gw   la   lw
val: 0.734   -6.48   2.09   2.92   17.6
sd: 0.0387   8.77   38.2   5270   131000

           CNST   HILL   GNLS
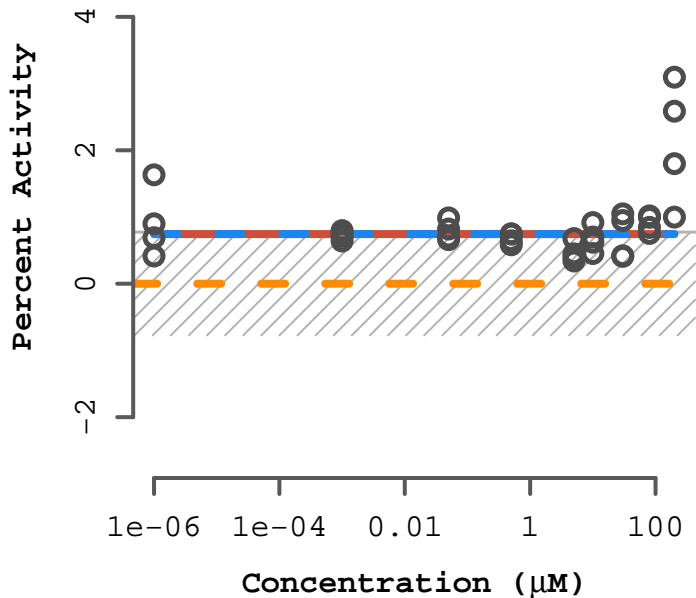AIC: 92.68   0.29   4.29
PROB: 0   0.88   0.12
RMSE: 0.77   0.21   0.21

MAX_MEAN: 0.895   MAX_MED: 0.908   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Busulfan
CHID: 20910   CASRN: 55-98-1
SPID(S): ES211_18_18
M4ID: 42676080

HILL MODEL (in red):
        tp   ga   gw
val: 0.745   -7   6.59
sd: 0.0493   262   1650

GAIN-LOSS MODEL (in blue):
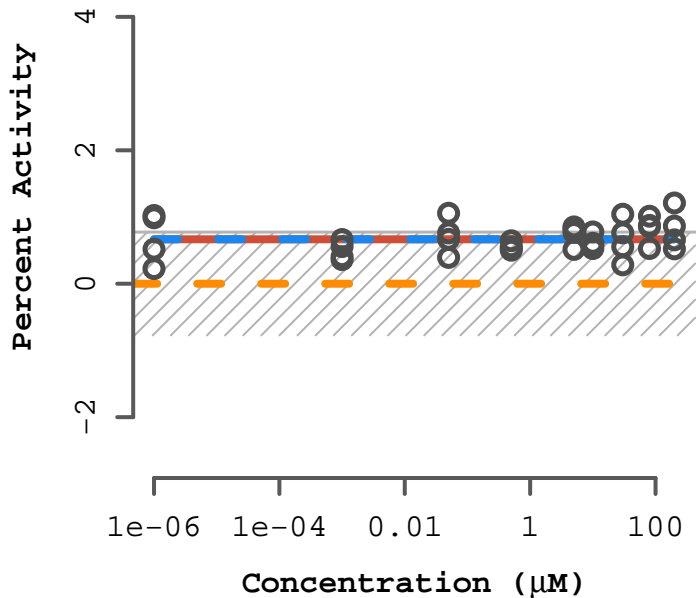   tp   ga   gw   la   lw
val: 0.745   -7   6.5   2.9   18
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 108.43   46.22   50.22
PROB: 0   0.88   0.12
RMSE: 1.05   0.58   0.58

MAX_MEAN: 2.12   MAX_MED: 2.19   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Nicotinic acid
CHID: 20932   CASRN: 59-67-6
SPID(S): ES211_48_48
M4ID: 42676105

HILL MODEL (in red):
        tp   ga   gw
val: 0.666   -7   7.14
sd: 0.0401   341   2200

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
val: 0.666   -7   6.91   4   4.97
sd: 0.0401   299   1930   2130   6200

	CNST	HILL	GNLS
AIC:	87.47	7.87	11.87
PROB:	0	0.88	0.12
RMSE:	0.72	0.23	0.23

MAX_MEAN: 0.818   MAX_MED: 0.865   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12
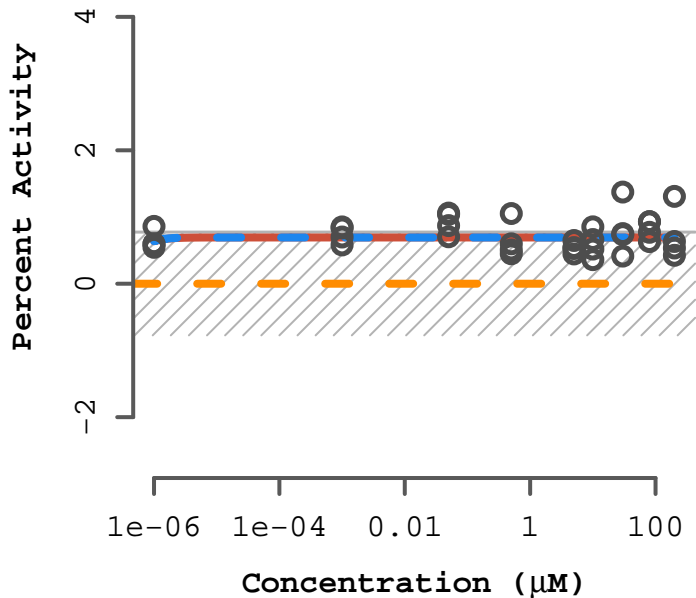
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: 1,2-Propylene glycol
CHID: 21206   CASRN: 57-55-6
SPID(S): ES211_1_1
M4ID: 42676067

HILL MODEL (in red):
        tp   ga   gw
val: 0.693   -6.44   2.37
sd: 0.0415   7.99   42.6

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
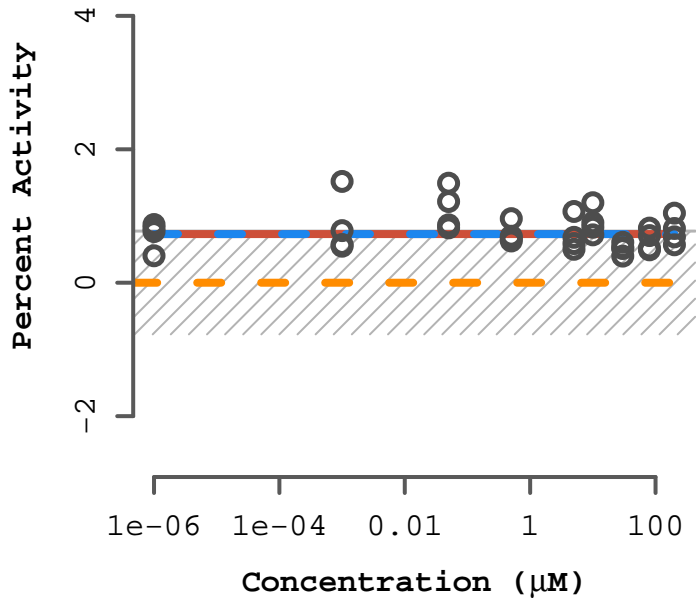val: 0.693   -6.39   2.73   3.11   17.8
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 91.07   6.96   10.96
PROB: 0   0.88   0.12
RMSE: 0.76   0.24   0.24

MAX_MEAN: 0.919   MAX_MED: 0.955   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Saccharin
CHID: 21251   CASRN: 81-07-2
SPID(S): ES211_54_54
M4ID: 42676094

HILL MODEL (in red):
        tp   ga   gw
val: 0.729   -6.97   7.42
sd: 0.0396   305   1930

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
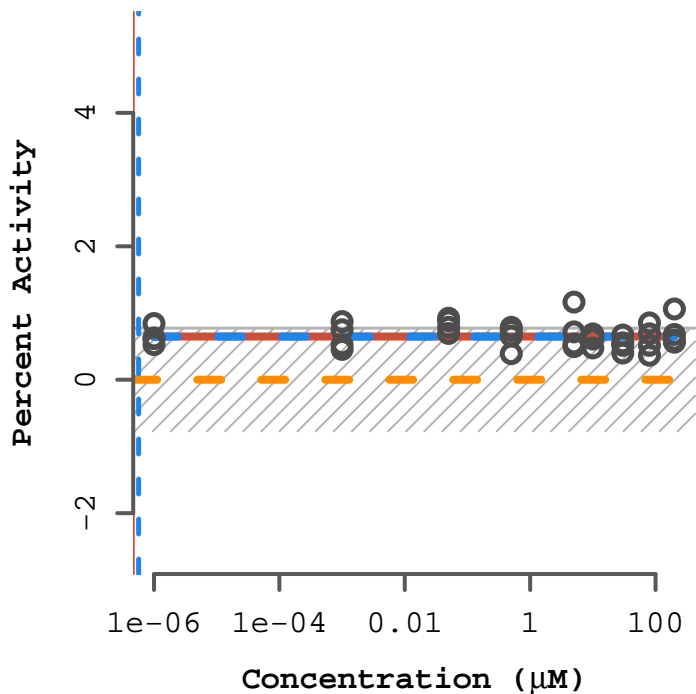val: 0.729   -7   6.62   3.59   7.12
sd: 0.0396   234   1470   5020   27900

        CNST   HILL   GNLS
AIC: 96.42   12.96   16.96
PROB: 0   0.88   0.12
RMSE: 0.82   0.27   0.27

MAX_MEAN: 1.1   MAX_MED: 1.04   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Dimethyl phthalate
CHID: 22455   CASRN: 131-11-3
SPID(S): ES211_30_30
M4ID: 42676098

HILL MODEL (in red):
          tp   ga   gw
val: 0.648   -6.35   5.65
sd: 0.0324   0.873   15.1

GAIN-LOSS MODEL (in blue):
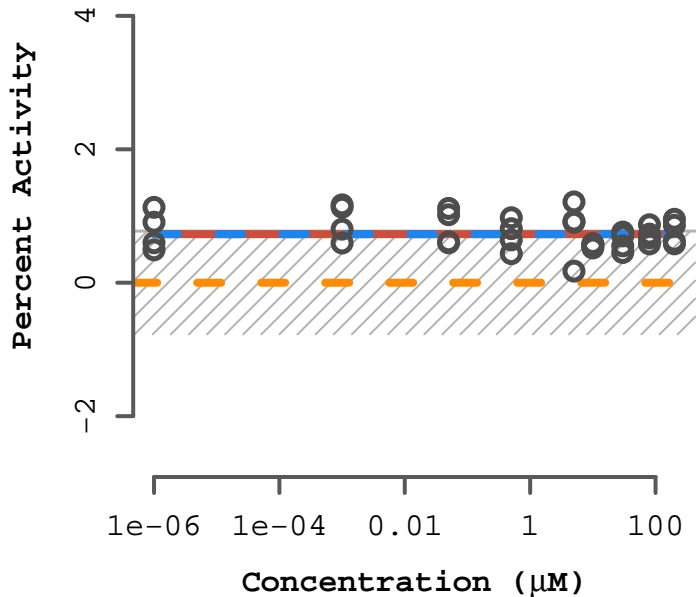   tp   ga   gw   la   lw
val: 0.648   -6.25   8   4.3   17
sd: NA   NA   NA   NA   NA

          CNST   HILL   GNLS
AIC: 84.67   -13.08   -9.08
PROB: 0   0.88   0.12
RMSE: 0.69   0.18   0.18

MAX_MEAN: 0.821   MAX_MED: 0.835   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 12

```
ASSAY:    AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME:     Thalidomide
CHID:     22524    CASRN: 50-35-1
SPID(S): ES211_62_62
M4ID:     42676106

HILL MODEL (in red):
        tp          ga          gw
val:    0.728       -7          6.92
sd:     0.0416      289         1860

GAIN-LOSS MODEL (in blue):
        tp          ga          gw          la          lw
val:    0.728       -6.94       7.78        4           18
sd:     NA          NA          NA          NA          NA

        CNST        HILL        GNLS
AIC:    93.79       9.97        13.97
PROB:   0           0.88        0.12
RMSE:   0.78        0.24        0.24

MAX_MEAN: 0.925      MAX_MED: 0.968      BMAD: 0.258

COFF: 0.774   HIT-CALL: 0      FITC: 20    ACTP: 1

FLAGS: 8; 12
```
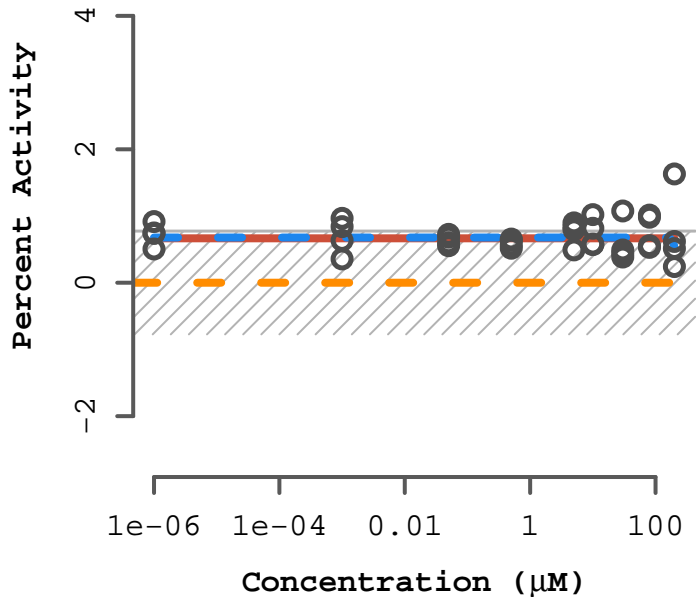
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Valproic acid
CHID: 23733   CASRN: 99-66-1
SPID(S): ES211_63_63
M4ID: 42676056

HILL MODEL (in red):
        tp   ga   gw
val: 0.666   -7   7.4
sd: 0.0382   225   1420

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
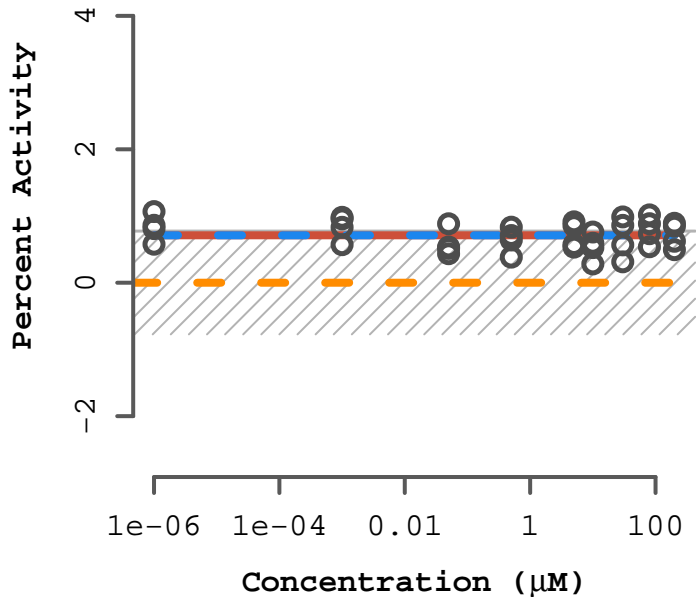val: 0.678   -6.99   8   2.34   15.9
sd: 0.0392   465   2120   0.0417   19.6

        CNST   HILL   GNLS
AIC: 89.32   8.3   11.01
PROB: 0   0.8   0.2
RMSE: 0.74   0.26   0.27

MAX_MEAN: 0.771   MAX_MED: 0.815   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Salicylic acid
CHID: 26368   CASRN: 69-72-7
SPID(S): ES211_55_55
M4ID: 42676043

HILL MODEL (in red):
        tp   ga   gw
val: 0.711   -7   7.39
sd: 0.0386   173   1090

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
val: 0.711   -7   7.23   3.96   4.33
sd: 0.0386   156   1010   1440   3590

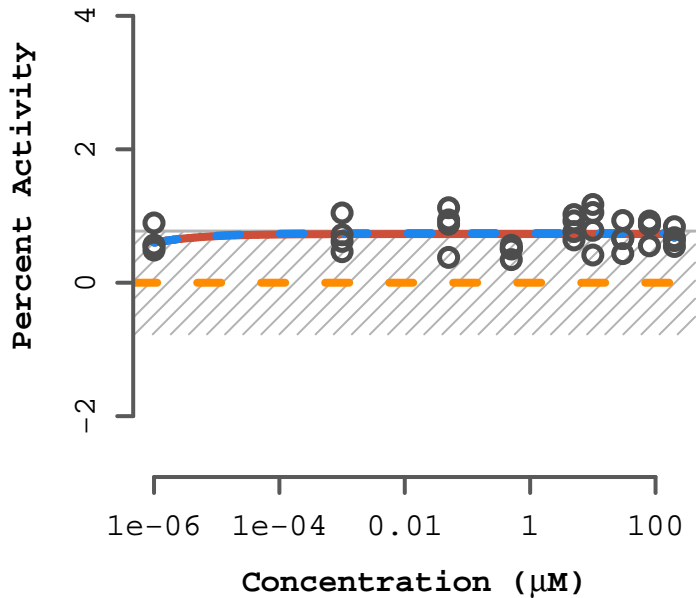   CNST   HILL   GNLS
AIC: 89.56   1.52   5.52
PROB: 0   0.88   0.12
RMSE: 0.73   0.21   0.21

MAX_MEAN: 0.835   MAX_MED: 0.894   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Penicillin G potassium
CHID: 45106   CASRN: 113-98-4
SPID(S): ES211_49_49
M4ID: 42676074

HILL MODEL (in red):
        tp   ga   gw
val: 0.73   -7   0.674
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
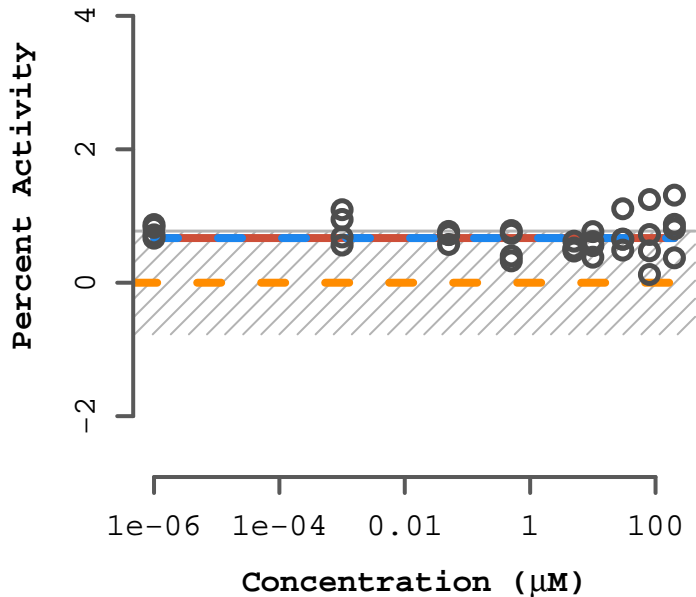   tp   ga   gw   la   lw
val: 0.745   -6.99   0.627   2.35   18
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 91.42   5.9   9.42
PROB: 0   0.85   0.15
RMSE: 0.76   0.22   0.22

MAX_MEAN: 0.857   MAX_MED: 0.92   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Lenalidomide
CHID: 46664   CASRN: 191732-72-6
SPID(S): ES211_41_41
M4ID: 42676064

HILL MODEL (in red):
          tp   ga   gw
val: 0.67   -7   7.49
sd: 0.0378   181   1120

GAIN-LOSS MODEL (in blue):
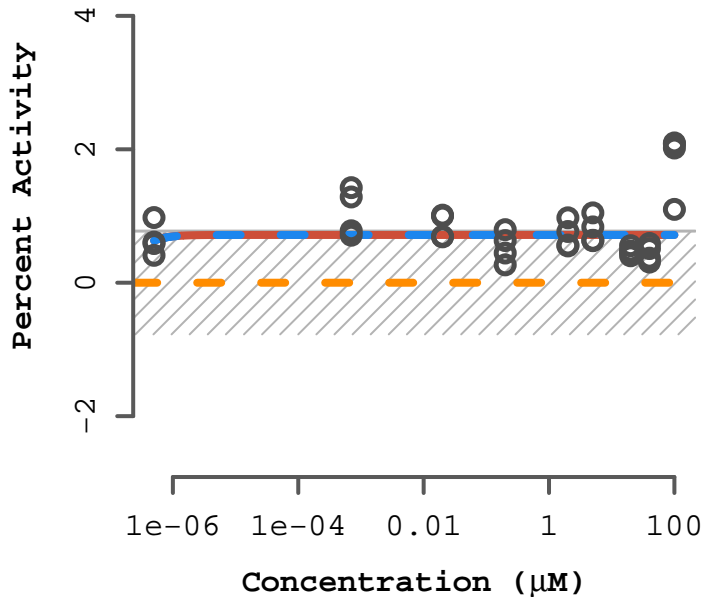   tp   ga   gw   la   lw
val: 0.67   -7   7.53   2.94   18
sd: NaN   NaN   NaN   NaN   NaN

          CNST   HILL   GNLS
AIC: 88.38   9.24   13.24
PROB: 0   0.88   0.12
RMSE: 0.73   0.25   0.25

MAX_MEAN: 0.843   MAX_MED: 0.842   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Ketanserin tartrate
CHID: 1003945 CASRN: 83846-83-7
SPID(S): ES211_40_40
M4ID: 42676085

HILL MODEL (in red):
        tp   ga   gw
val: 0.716   -6.71   2.15
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
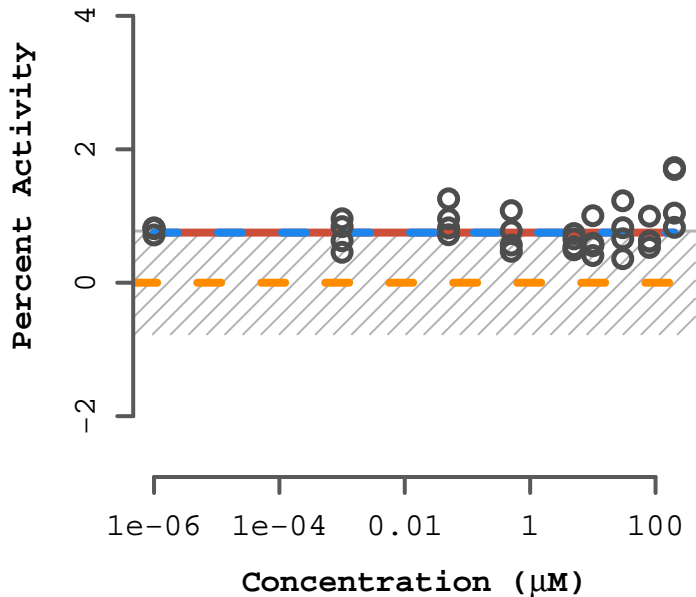   tp   ga   gw   la   lw
val: 0.716   -6.74   1.99   2.98   11
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 102.66   46.32   50.32
PROB: 0   0.88   0.12
RMSE: 0.93   0.47   0.47

MAX_MEAN: 1.82   MAX_MED: 2.05   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: (2R,3S)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-
CHID: 1017388 CASRN: 225937-10-0
SPID(S):   ES211_22_22
M4ID: 42676068

HILL MODEL (in red):
         tp   ga   gw
val: 0.751   -7   6.94
sd: 0.0442   197   1270

GAIN-LOSS MODEL (in blue):
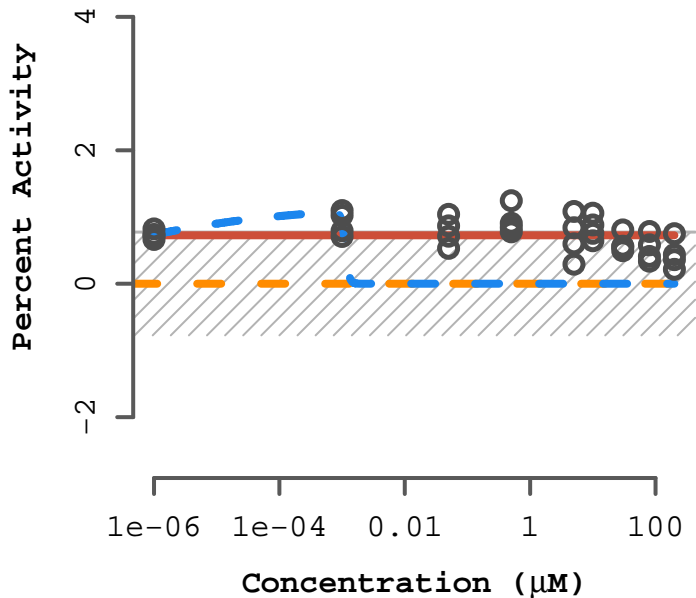   tp   ga   gw   la   lw
val: 0.751   -6.96   7.95   4.29   16.6
sd: NA   NA   NA   NA   NA

         CNST   HILL   GNLS
AIC: 99.44   21.58   25.58
PROB: 0   0.88   0.12
RMSE: 0.86   0.31   0.31

MAX_MEAN: 1.32   MAX_MED: 1.37   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 20   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: 5,5-Diphenylhydantoin
CHID: 20541   CASRN: 57-41-0
SPID(S): ES211_3_3
M4ID: 42676082

HILL MODEL (in red):
        tp   ga   gw
val: 0.726   -7   6.73
sd: 0.0402   279   1740

GAIN-LOSS MODEL (in blue):
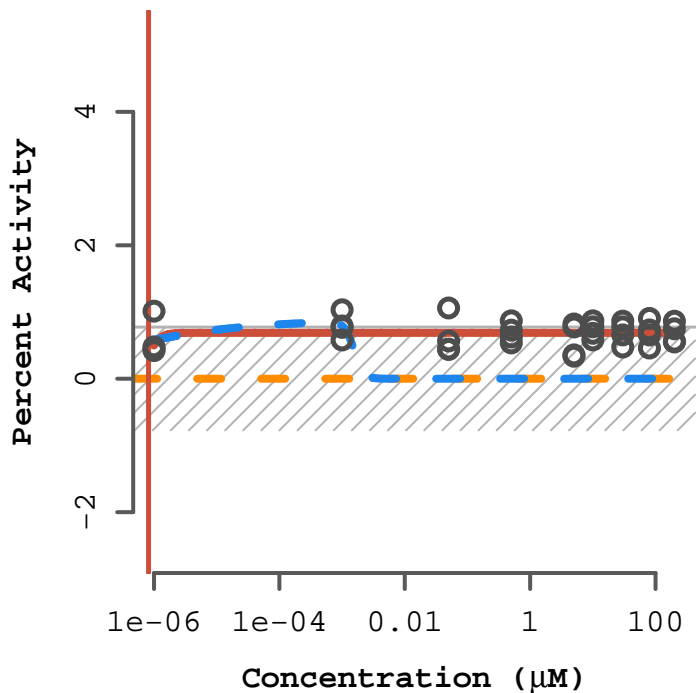   tp   ga   gw   la   lw
val: 1.16   -6.8   0.301   -2.95   14.2
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 91.66   9.99   88.82
PROB: 0   1   0
RMSE: 0.76   0.24   0.65

MAX_MEAN: 0.943   MAX_MED: 0.909   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 21   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Isoniazid
CHID: 20755   CASRN: 54-85-3
SPID(S): ES211_39_39
M4ID: 42676055

HILL MODEL (in red):
          tp   ga   gw
val: 0.687   -6.09   4.82
sd: 0.034   0.0838   4.77

GAIN-LOSS MODEL (in blue):
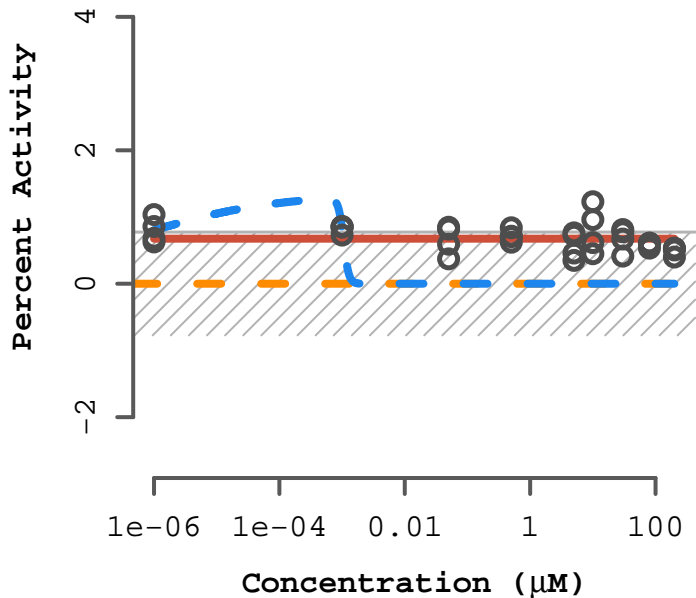   tp   ga   gw   la   lw
val: 0.876   -6.69   0.42   -2.81   5.98
sd: NaN   NaN   NaN   NaN   NaN

          CNST   HILL   GNLS
AIC: 86.11   -7.4   86.08
PROB: 0   1   0
RMSE: 0.7   0.19   0.62

MAX_MEAN: 0.794   MAX_MED: 0.781   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 21   ACTP: 1

FLAGS: 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Methyldopa sesquihydrate
CHID: 20863   CASRN: 41372-08-1
SPID(S): ES211_46_46
M4ID: 42676079

HILL MODEL (in red):
         tp   ga   gw
val: 0.675   -6.98   7.4
sd: 0.032   142   919

GAIN-LOSS MODEL (in blue):
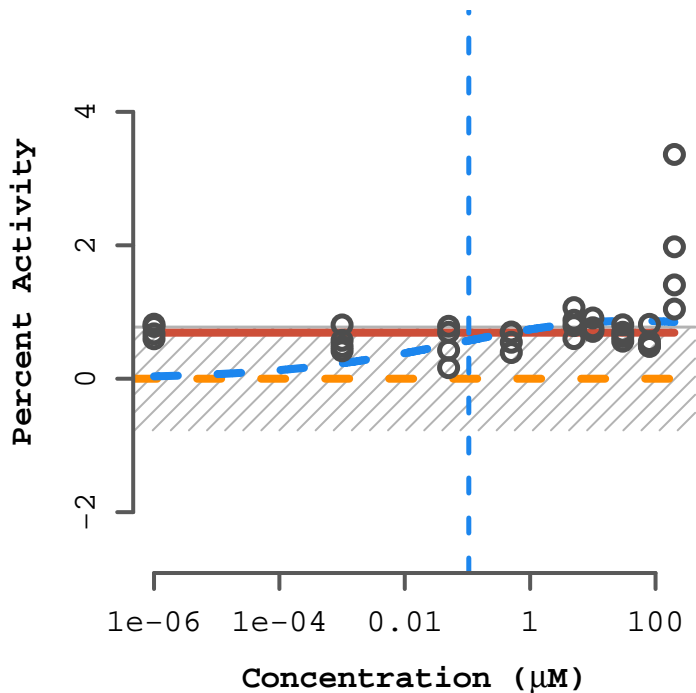   tp   ga   gw   la   lw
val: 1.36   -6.42   0.38   -2.98   10.5
sd: NaN   NaN   NaN   NaN   NaN

         CNST   HILL   GNLS
AIC: 86.93   -7.1   82.87
PROB: 0   1   0
RMSE: 0.71   0.19   0.6

MAX_MEAN: 0.823   MAX_MED: 0.851   BMAD: 0.258

COFF: 0.774   HIT-CALL: 0   FITC: 21   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: MEHP
CHID: 25680   CASRN: 4376-20-9
SPID(S): ES211_44_44
M4ID: 42676069

HILL MODEL (in red):
         tp   ga   gw
val: 0.69   -7   6.72
sd: 0.0386   200   1270

GAIN-LOSS MODEL (in blue):
         tp   ga   gw   la   lw
val: 1.17   -0.979   0.3   4.3   0.3
sd: NaN   NaN   NaN   NaN   NaN
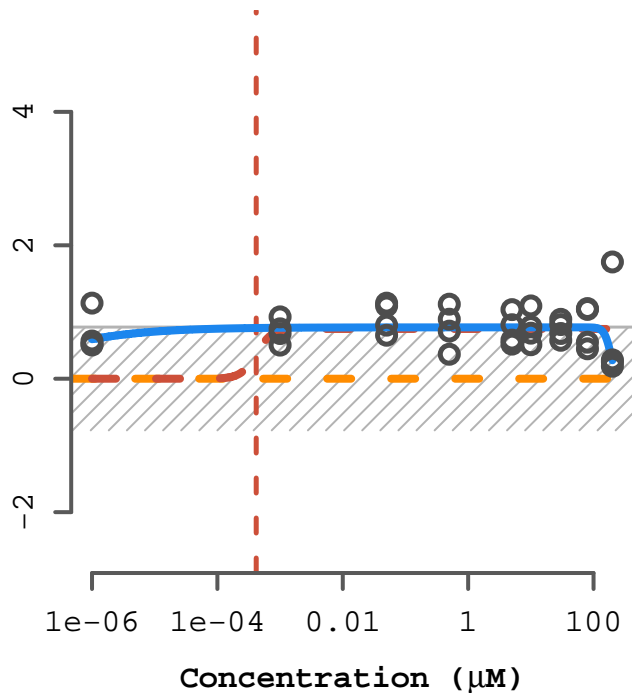
         CNST   HILL   GNLS
AIC: 100.53   29.4   57.24
PROB: 0   1   0
RMSE: 0.96   0.54   0.56

MAX_MEAN: 1.95   MAX_MED: 1.69   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 21   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Sulfasalazine
CHID: 21256   CASRN: 599-79-1
SPID(S): ES211_59_59
M4ID: 42676092

HILL MODEL (in red):
        tp   ga   gw
val: 0.746   -3.38   3.55
sd: 0.0651   17.4   162

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
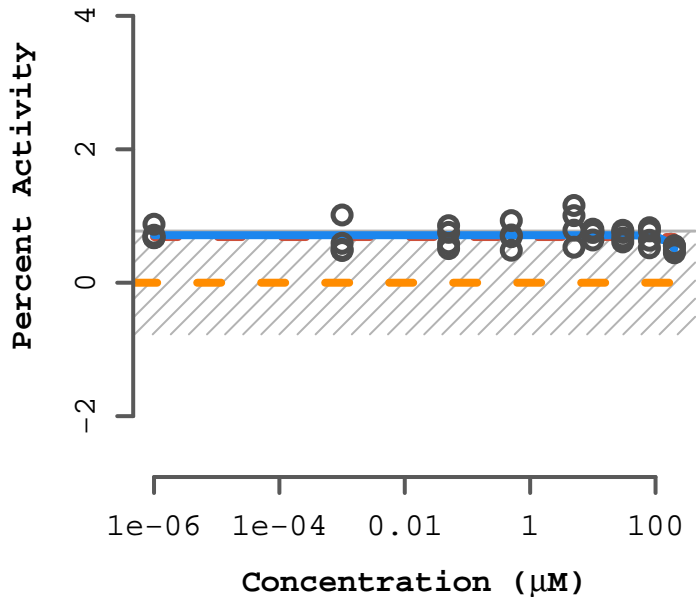val: 0.77   -7   0.522   2.27   8.42
sd: 0.0571   4.75   2.66   0.0847   23.6

        CNST   HILL   GNLS
AIC: 95.11   40.09   20.18
PROB: 0   0   1
RMSE: 0.81   0.38   0.33

MAX_MEAN: 0.92   MAX_MED: 0.948   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 31   ACTP: 1

FLAGS: 8; 12

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Cyclophosphamide monohydrate
CHID: 24888   CASRN: 6055-19-2
SPID(S): ES211_24_24
M4ID: 42676086

HILL MODEL (in red):
	tp	ga	gw
val:	0.685	-7	7.93
sd:	0.0278	327	1600

GAIN-LOSS MODEL (in blue):
	tp	ga	gw	la	lw
val:	0.712	-7	7.02	2.43	3.18
sd:	0.0288	197	1250	0.233	5.76

	CNST	HILL	GNLS
AIC:	88.09	-17.34	-21.37
PROB:	0	0.12	0.88
RMSE:	0.72	0.17	0.15

MAX_MEAN: 0.871   MAX_MED: 0.897   BMAD: 0.258

COFF: 0.774 HIT-CALL: 0   FITC: 31   ACTP: 1

FLAGS: 12
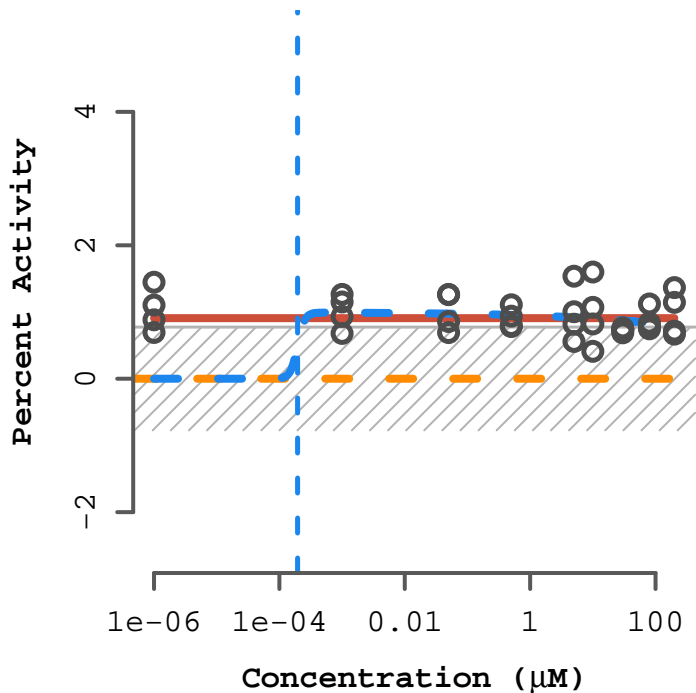
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Acrylamide
CHID: 20027   CASRN: 79-06-1
SPID(S): ES211_10_10
M4ID: 42676052

HILL MODEL (in red):
	tp	ga	gw
val:	0.908	-6.98	7.28
sd:	0.0478	188	1230

GAIN-LOSS MODEL (in blue):
	tp	ga	gw	la	lw
val:	0.996	-3.71	7.71	4.3	0.3
sd:	0.236	76.3	829	2.88	0.634

	CNST	HILL	GNLS
AIC:	110.38	20.93	49.77
PROB:	0	1	0
RMSE:	0.98	0.28	0.44

MAX_MEAN: 1.03   MAX_MED: 1.06   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18
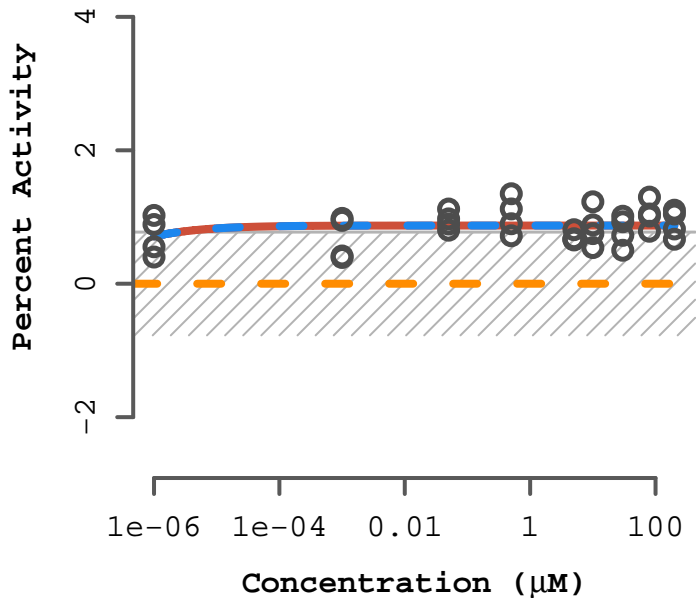
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Aspirin
CHID: 20108   CASRN: 50-78-2
SPID(S): ES211_15_15
M4ID: 42676063

HILL MODEL (in red):

	tp	ga	gw
val:	0.872	-7	0.644
sd:	NaN	NaN	NaN

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	0.872	-7	0.644	4.16	6.4
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	102.99	10.1	14.1
PROB:	0	0.88	0.12
RMSE:	0.89	0.24	0.24

MAX_MEAN: 1.04   MAX_MED: 1.03   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Caffeine
CHID: 20232   CASRN: 58-08-2
SPID(S): ES211_20_20
M4ID: 42676076

HILL MODEL (in red):
        tp   ga   gw
val: 0.854   -7   0.738
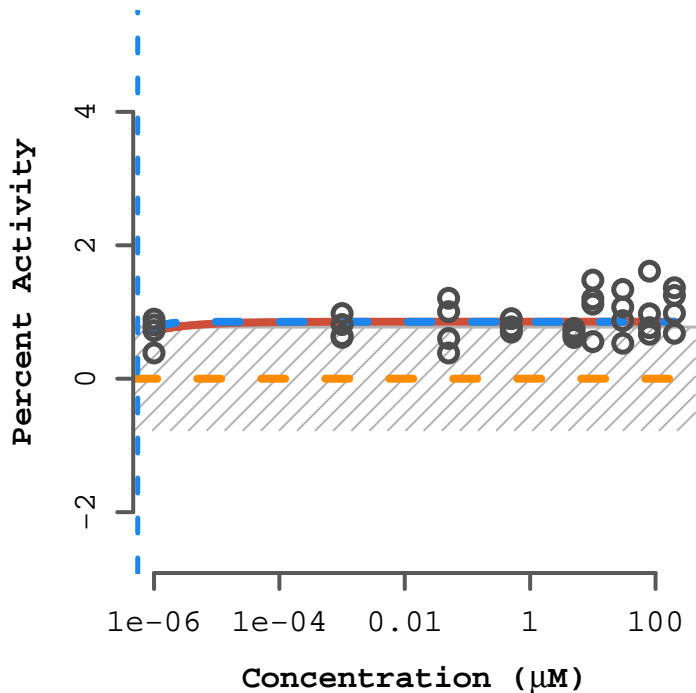sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
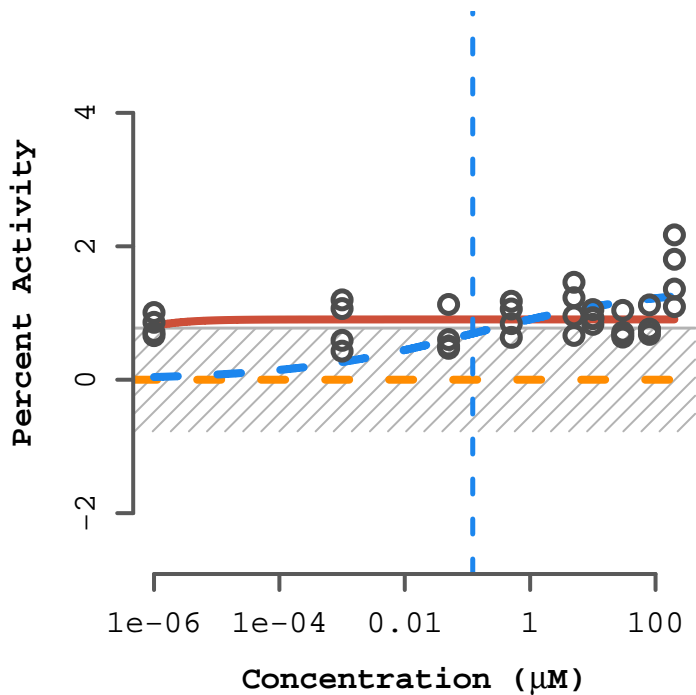val: 0.853   -6.26   2.9   3.94   9.69
sd: NA   NA   NA   NA   NA

        CNST   HILL   GNLS
AIC: 105.2   22.44   26.45
PROB: 0   0.88   0.12
RMSE: 0.92   0.29   0.29

MAX_MEAN: 1.09   MAX_MED: 1.16   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Diphenhydramine hydrochloride
CHID: 20537   CASRN: 147-24-0
SPID(S): ES211_31_31
M4ID: 42676100

HILL MODEL (in red):
        tp   ga   gw
val: 0.904   -7   0.918
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
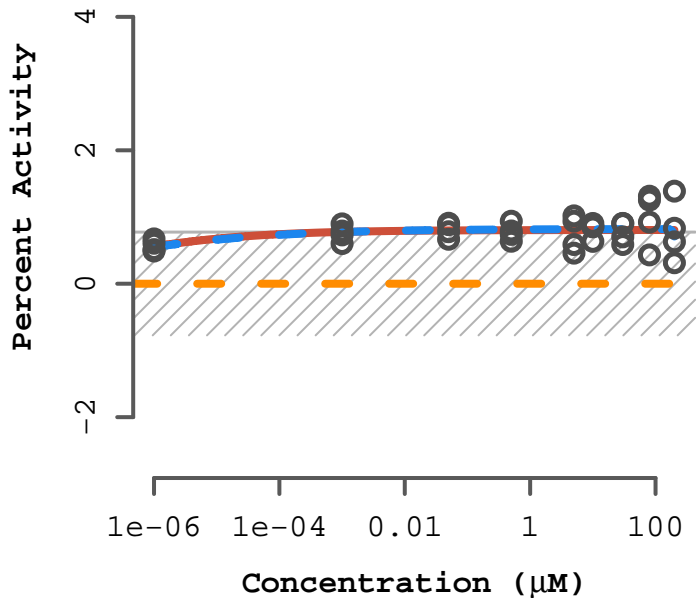   tp   ga   gw   la   lw
val: 1.39   -0.916   0.3   3.19   9.75
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 110.79   32.07   61.58
PROB: 0   1   0
RMSE: 1.01   0.36   0.46

MAX_MEAN: 1.61   MAX_MED: 1.58   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Acyclovir
CHID: 22556   CASRN: 59277-89-3
SPID(S): ES211_12_12
M4ID: 42676054

HILL MODEL (in red):
         tp   ga   gw
val: 0.806   -7   0.356
sd: 0.055   1.53   0.602

GAIN-LOSS MODEL (in blue):
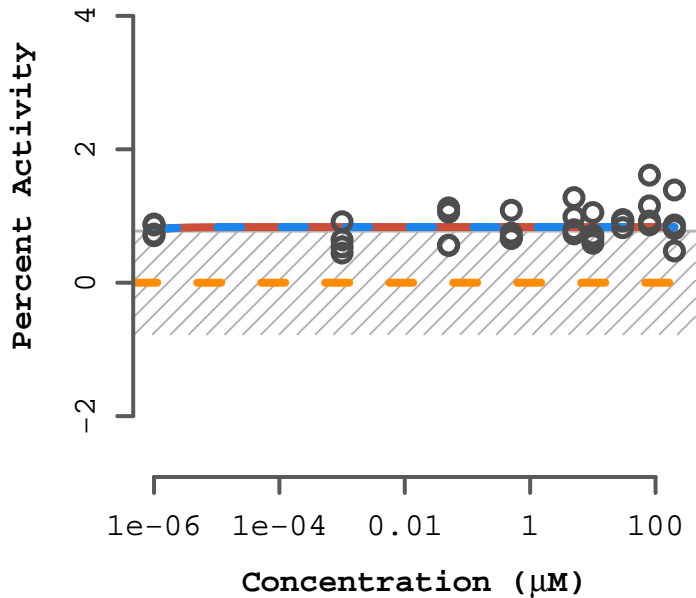   tp   ga   gw   la   lw
val: 0.82   -7   0.307   2.35   17.9
sd: NaN   NaN   NaN   NaN   NaN

         CNST   HILL   GNLS
AIC: 96.69   -1.33   2.02
PROB: 0   0.84   0.16
RMSE: 0.81   0.22   0.22

MAX_MEAN: 0.981   MAX_MED: 1.09   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Carbamazepine
CHID: 22731   CASRN: 298-46-4
SPID(S): ES211_21_21
M4ID: 42676095

HILL MODEL (in red):
        tp   ga   gw
val: 0.835   -7   1.31
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
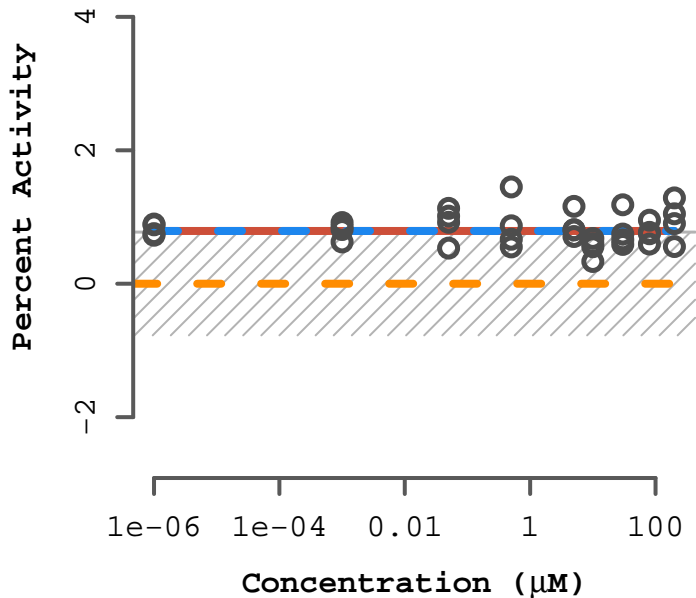   tp   ga   gw   la   lw
val: 0.835   -7   1.3   2.5   13
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 103.09   10.08   14.08
PROB: 0   0.88   0.12
RMSE: 0.89   0.25   0.25

MAX_MEAN: 1.14   MAX_MED: 1.04   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Warfarin
CHID: 23742   CASRN: 81-81-2
SPID(S): ES211_65_65
M4ID: 42676078

HILL MODEL (in red):
          tp   ga   gw
val: 0.791   -7   6.87
sd: 0.0368   201   1280

GAIN-LOSS MODEL (in blue):
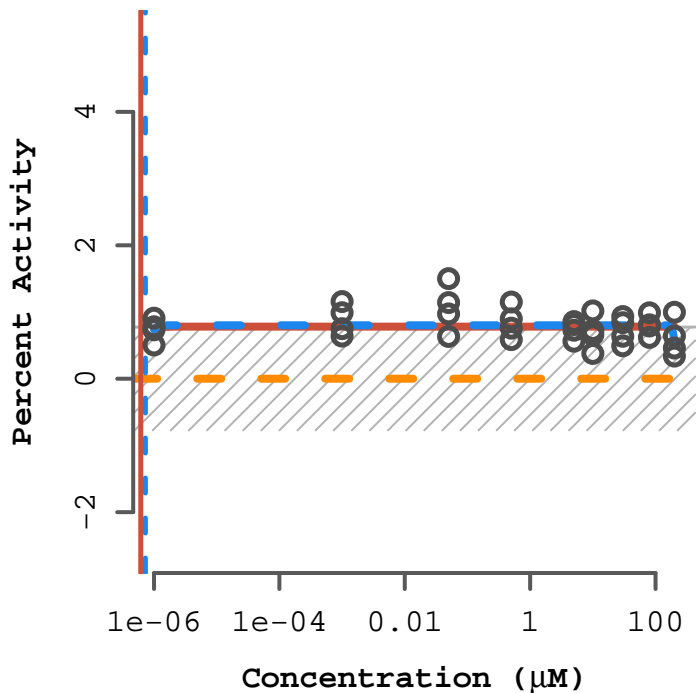   tp   ga   gw   la   lw
val: 0.791   -7   7.05   4.29   4.08
sd: 0.0368   227   1450   1320   2710

          CNST   HILL   GNLS
AIC: 99.59   5.22   9.22
PROB: 0   0.88   0.12
RMSE: 0.85   0.23   0.23

MAX_MEAN: 0.949   MAX_MED: 0.975   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Stavudine
CHID: 23819   CASRN: 3056-17-5
SPID(S): ES211_58_58
M4ID: 42676047

HILL MODEL (in red):
        tp   ga   gw
val: 0.781   -6.21   6.01
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
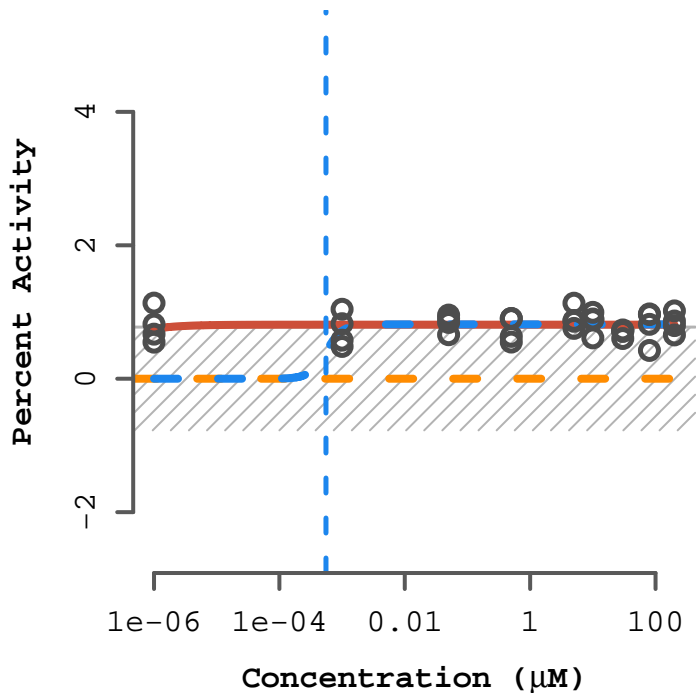   tp   ga   gw   la   lw
val: 0.801   -6.14   8   2.32   18
sd: NaN   NaN   NaN   NaN   NaN

         CNST   HILL   GNLS
AIC: 97.56   7.33   8.28
PROB: 0   0.62   0.38
RMSE: 0.82   0.24   0.23

MAX_MEAN: 1.06   MAX_MED: 1.06   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: D-Camphor
CHID: 24721   CASRN: 464-49-3
SPID(S):   ES211_27_27
M4ID: 42676088

HILL MODEL (in red):
        tp   ga   gw
val: 0.81   -7   1.08
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
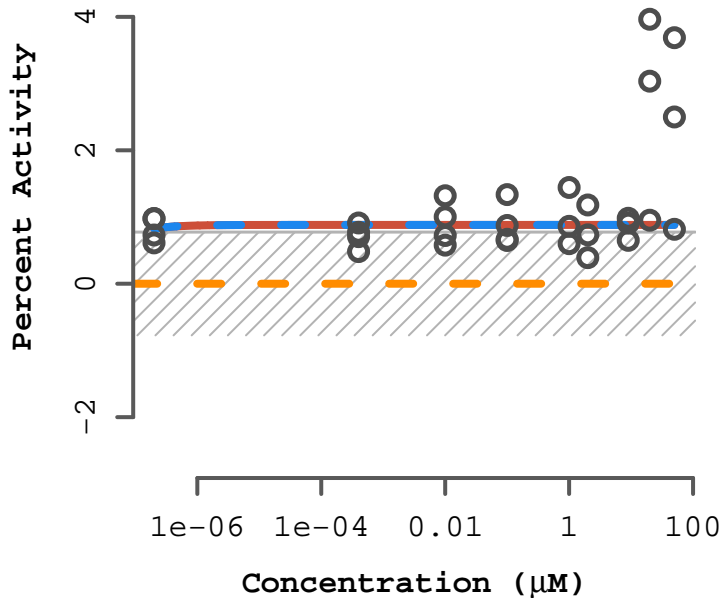   tp   ga   gw   la   lw
val: 0.815   -3.26   3.35   3.7   5.41
sd: 0.0399   8.09   105   1170   4540

        CNST   HILL   GNLS
AIC: 97.63   -11.84   21.48
PROB: 0   1   0
RMSE: 0.82   0.18   0.32

MAX_MEAN: 0.906   MAX_MED: 0.891   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Ritanserin
CHID: 42594   CASRN: 87051-43-2
SPID(S): ES211_53_53
M4ID: 42676107

HILL MODEL (in red):
        tp   ga   gw
val: 0.881   -7.7   1.17
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
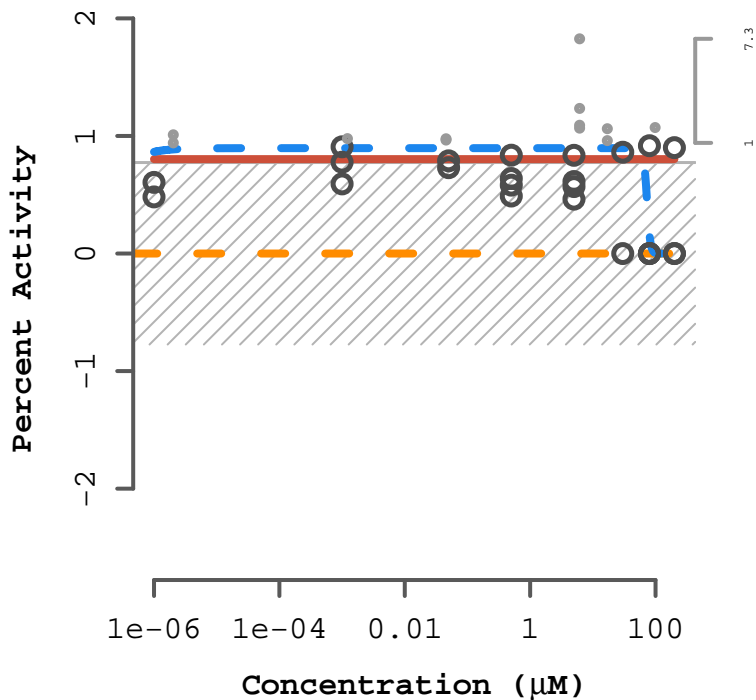   tp   ga   gw   la   lw
val: 0.881   -7.7   1.17   3.31   4.98
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 111.82   69.44   73.44
PROB: 0   0.88   0.12
RMSE: 1.46   0.92   0.92

MAX_MEAN: 2.65   MAX_MED: 3.04   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 10; 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Tegaserod maleate
CHID: 904761   CASRN: 189188-57-6
SPID(S): ES211_61_61
M4ID: 42676045   BRK

HILL MODEL (in red):
        tp   ga   gw
val: 0.803   -7   6.11
sd: 0.106   238   1420

GAIN-LOSS MODEL (in blue):
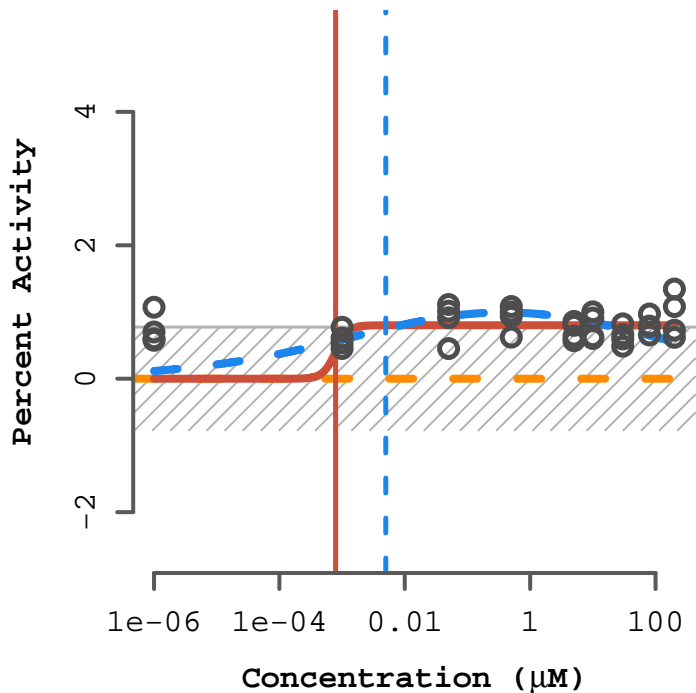   tp   ga   gw   la   lw
val: 0.896   -6.89   1.61   1.86   16.7
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 125.37   95.67   95.96
PROB: 0   0.54   0.46
RMSE: 1.63   1.27   1.25

MAX_MEAN: 3.57   MAX_MED: 2.57   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 36   ACTP: 1

FLAGS: 10; 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: 6-Propyl-2-thiouracil
CHID: 21209   CASRN: 51-52-5
SPID(S): ES211_8_8
M4ID: 42676073

HILL MODEL (in red):
        tp   ga   gw
val: 0.801   -3.1   4.3
sd: 0.0489   1.81   75.3

GAIN-LOSS MODEL (in blue):
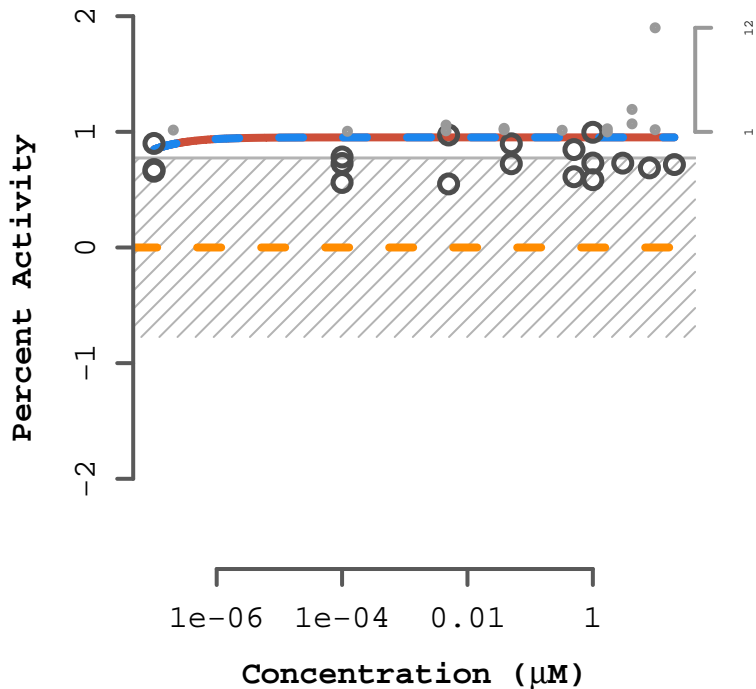   tp   ga   gw   la   lw
val: 1.61   -2.3   0.3   1.47   0.3
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 96.29   23.62   29.15
PROB: 0   0.94   0.06
RMSE: 0.81   0.32   0.32

MAX_MEAN: 0.944   MAX_MED: 0.969   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 37   ACTP: 1

FLAGS: 11

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Cyclopamine
CHID: 43709   CASRN: 4449-51-8
SPID(S): ES211_23_23
M4ID: 42676072 BRK

HILL MODEL (in red):
        tp   ga   gw
val: 0.952   -8   0.91
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
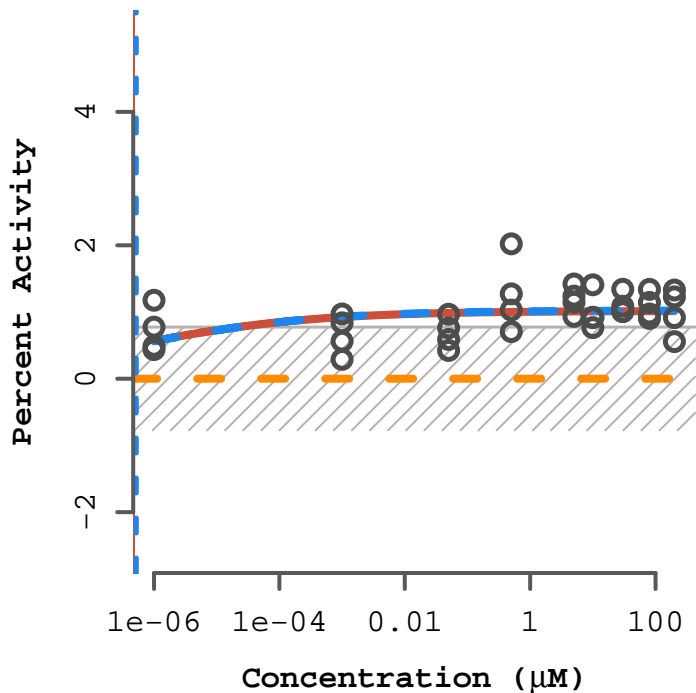   tp   ga   gw   la   lw
val: 0.952   -8   0.91   3.22   17.9
sd: NA   NA   NA   NA   NA

        CNST   HILL   GNLS
AIC: 119.61   71.14   75.14
PROB: 0   0.88   0.12
RMSE: 2.5   2.11   2.11

MAX_MEAN: 4.76   MAX_MED: 1.9   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 40   ACTP: 1

FLAGS: 10; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Methotrexate hydrate(1:x)
CHID: 1017640 CASRN: 133073-73-1
SPID(S): ES211_45_45
M4ID: 42676066

HILL MODEL (in red):
       tp   ga   gw
val: 1.02   -6.34   0.3
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
       tp   ga   gw   la   lw
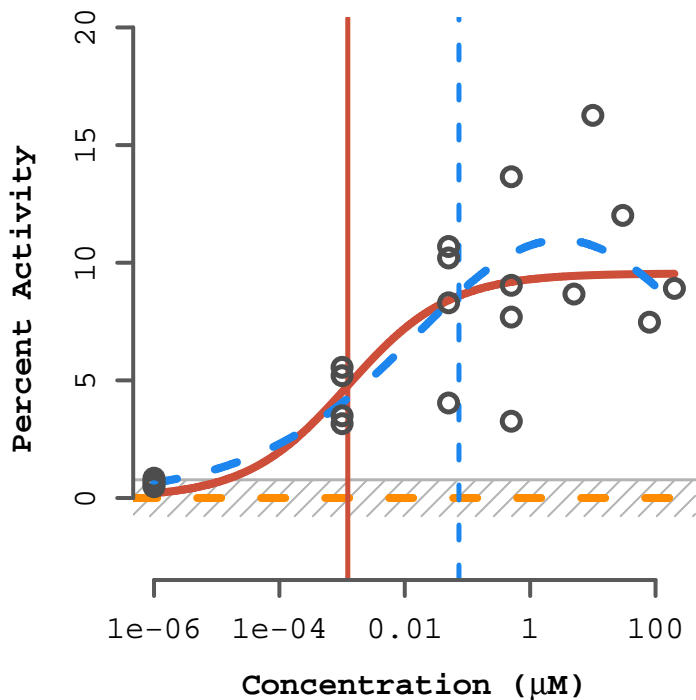val: 1.02   -6.28   0.3   4.16   5.05
sd: NaN   NaN   NaN   NaN   NaN

       CNST   HILL   GNLS
AIC: 113.13   28.07   32.05
PROB: 0   0.88   0.12
RMSE: 1.03   0.33   0.32

MAX_MEAN: 1.26   MAX_MED: 1.19   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 40   ACTP: 1

FLAGS: 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Actinomycin D
CHID: 20031   CASRN: 50-76-0
SPID(S): ES211_11_11
M4ID: 42676101

HILL MODEL (in red):

	tp	ga	gw
val:	9.55	-2.91	0.538
sd:	1.21	0.36	0.504

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	19.2	-1.14	0.3	2.12	0.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	151.5	106.5	110.95
PROB:	0	0.9	0.1
RMSE:	8	2.65	2.63

MAX_MEAN: 16.3   MAX_MED: 16.3   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10
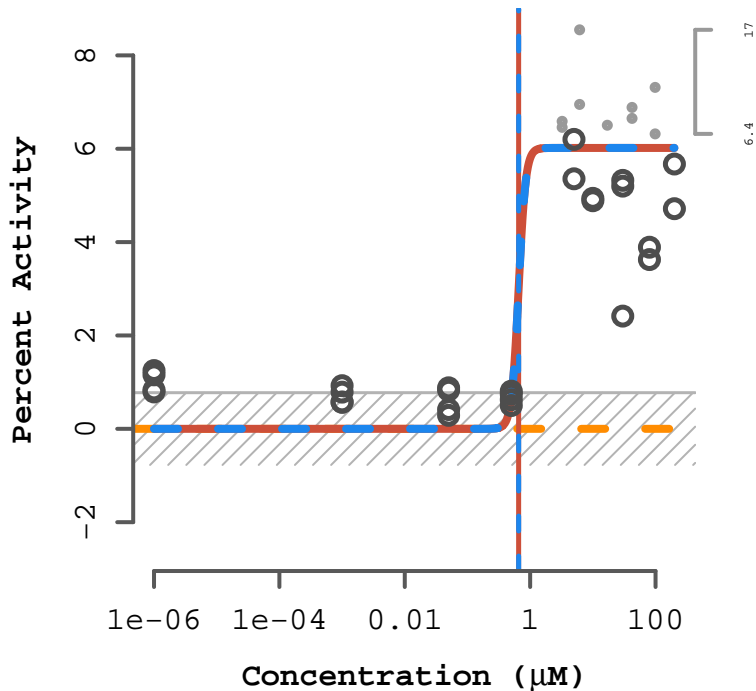
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Diethylstilbestrol
CHID: 20465   CASRN: 56-53-1
SPID(S): ES211_29_29
M4ID: 42676042   BRK

HILL MODEL (in red):
        tp   ga   gw
val: 6.02   -0.184   7.69
sd: 0.414   4.17   273

GAIN-LOSS MODEL (in blue):
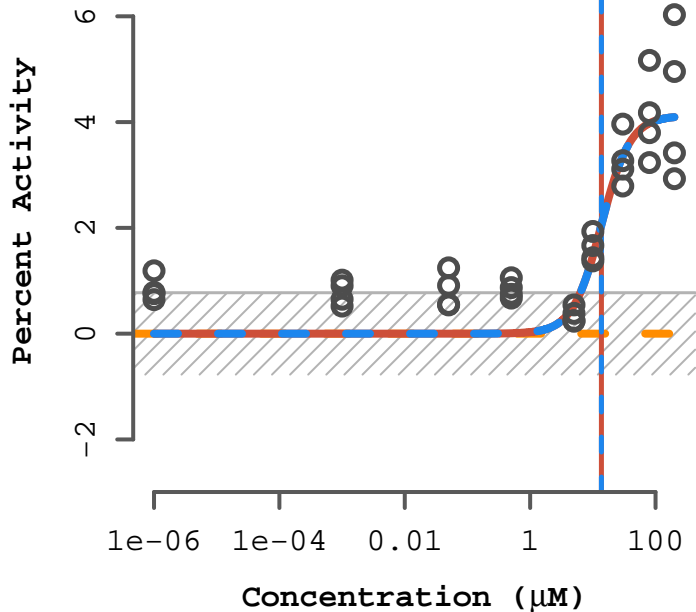   tp   ga   gw   la   lw
val: 6.02   -0.183   7.65   4.1   5.56
sd: 0.414   4.56   296   74700   230000

        CNST   HILL   GNLS
AIC: 227.65   156.68   160.68
PROB: 0   0.88   0.12
RMSE: 5.62   2.49   2.49

MAX_MEAN: 9.15   MAX_MED: 7.2   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: 5-Fluorouracil
CHID: 20634   CASRN: 51-21-8
SPID(S): ES211_5_5
M4ID: 42676057

HILL MODEL (in red):
        tp   ga   gw
val: 4.12   1.14   1.89
sd: 0.497   0.114   0.677

GAIN-LOSS MODEL (in blue):
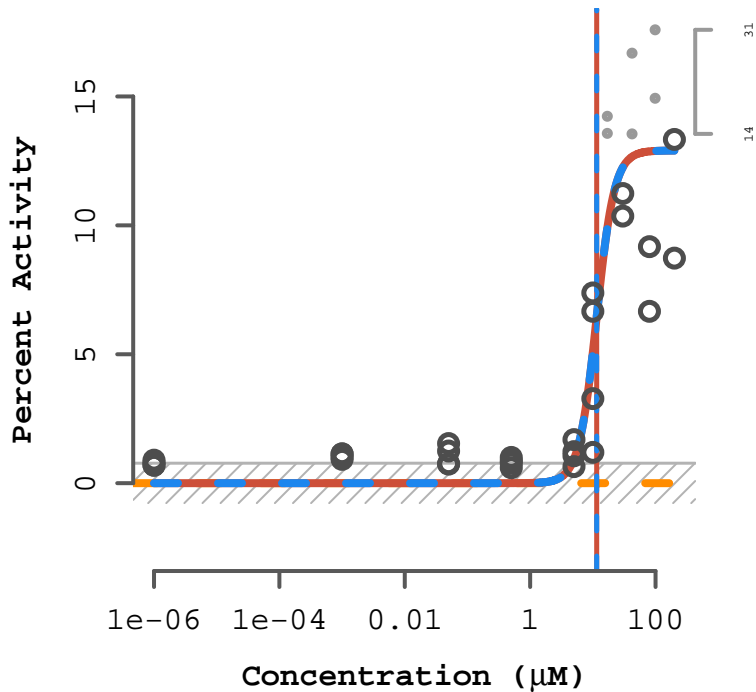   tp   ga   gw   la   lw
val: 4.12   1.14   1.89   3.47   6.49
sd: 0.497   0.114   0.677   1930   10700

         CNST   HILL   GNLS
AIC: 169.28   94.53   98.53
PROB: 0   0.88   0.12
RMSE: 2.45   0.76   0.76

MAX_MEAN: 4.33   MAX_MED: 4.19   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS:

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: all-trans-Retinoic acid
CHID: 21239   CASRN: 302-79-4
SPID(S): ES211_13_13
M4ID: 42676058   BRK

HILL MODEL (in red):

	tp	ga	gw
val:	12.9	1.06	3.05
sd:	1.19	0.078	1.32

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	12.9	1.06	3.05	4.21	7.71
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	260.82	193.55	197.55
PROB:	0	0.88	0.12
RMSE:	9.79	4.38	4.38

MAX_MEAN: 18.1   MAX_MED: 16.4   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10
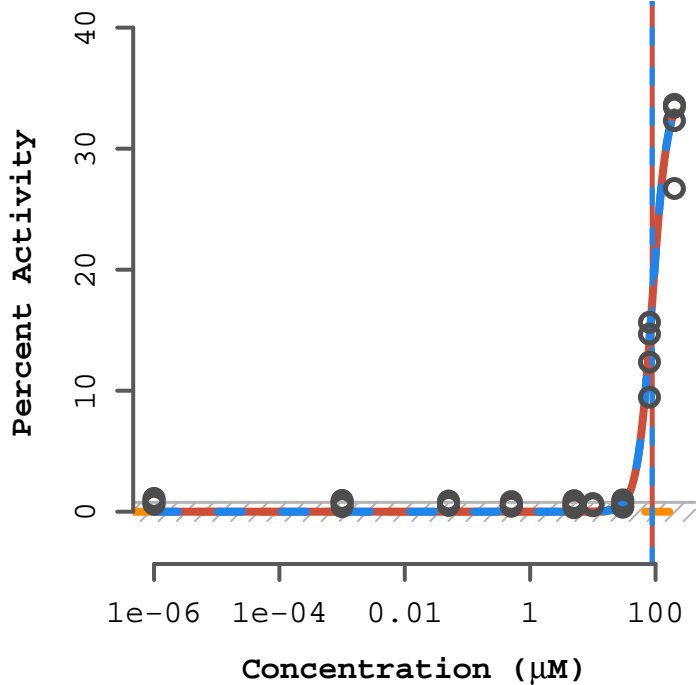
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Rifampicin
CHID: 21244   CASRN: 13292-46-1
SPID(S): ES211_52_52
M4ID: 42676041

HILL MODEL (in red):
        tp   ga   gw
val: 34.7   1.95   3.67
sd: 1.89   0.0294   0.91

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
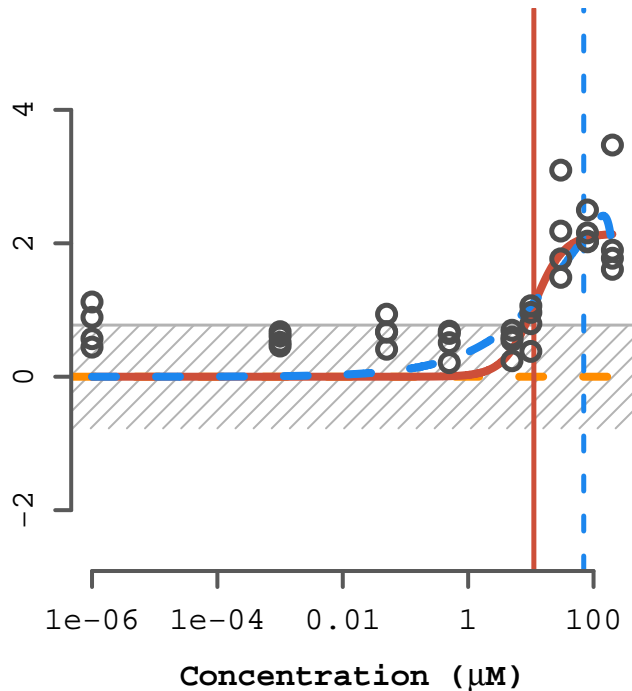val: 34.7   1.95   3.67   2.89   18
sd: 1.89   0.0294   0.91   21800   589000

        CNST   HILL   GNLS
AIC: 256.11   118.41   122.41
PROB: 0   0.88   0.12
RMSE: 11.46   1.49   1.49

MAX_MEAN: 31.5   MAX_MED: 32.9   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: 5-Bromo-2'-deoxyuridine
CHID: 33105   CASRN: 59-14-3
SPID(S): ES211_4_4
M4ID: 42676104

HILL MODEL (in red):
        tp   ga   gw
val: 2.15   1.05   1.81
sd: 0.214   0.106   0.824

GAIN-LOSS MODEL (in blue):
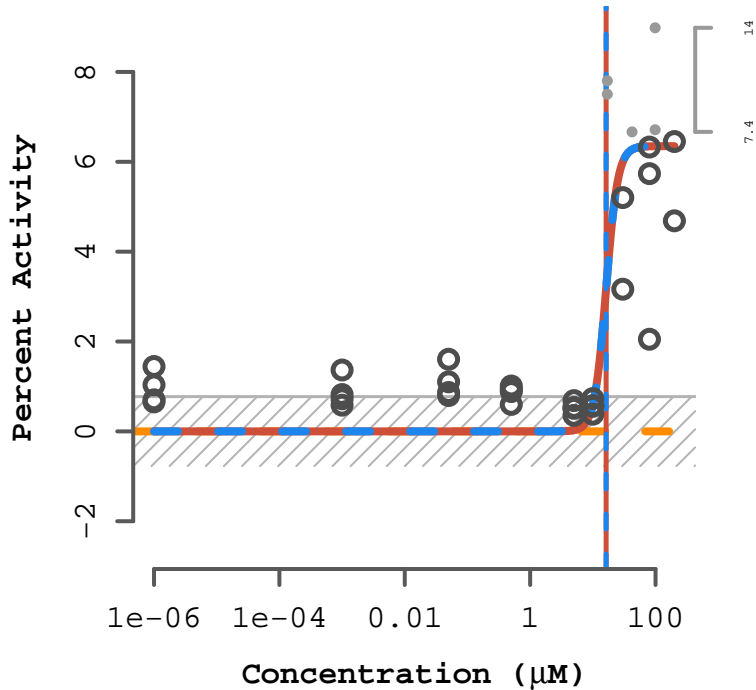   tp   ga   gw   la   lw
val: 4.17   1.84   0.549   2.35   7.59
sd: 2.83   1.15   0.379   0.0768   11.7

        CNST   HILL   GNLS
AIC: 130.66   72.65   74.37
PROB: 0   0.7   0.3
RMSE: 1.41   0.57   0.58

MAX_MEAN: 2.19   MAX_MED: 2.09   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS:

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Imatinib mesylate
CHID: 40502   CASRN: 220127-57-1
SPID(S): ES211_37_37
M4ID: 42676053 BRK

HILL MODEL (in red):

	tp	ga	gw
val:	6.35	1.21	4.63
sd:	0.536	0.222	5.27

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	6.35	1.21	4.63	3.73	5.76
sd:	0.536	0.222	5.27	1660	6700

	CNST	HILL	GNLS
AIC:	204.32	147.88	151.88
PROB:	0	0.88	0.12
RMSE:	4.48	2.03	2.03

MAX_MEAN: 8.22   MAX_MED: 7.53   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10
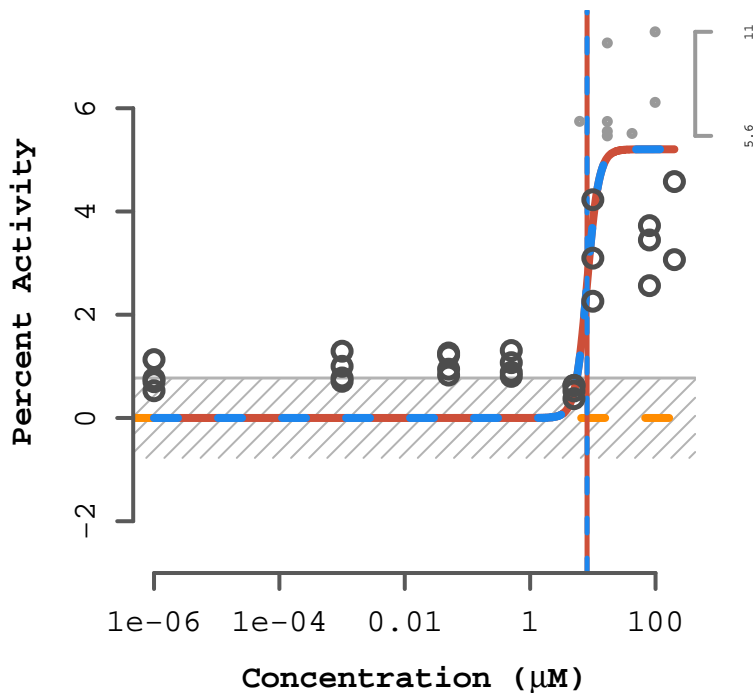
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Gefitinib
CHID: 41034   CASRN: 184475-35-2
SPID(S): ES211_34_34
M4ID: 42676093 BRK

HILL MODEL (in red):
	tp	ga	gw
val:	5.2	0.908	4.61
sd:	0.523	0.0665	1.92

GAIN-LOSS MODEL (in blue):
	tp	ga	gw	la	lw
val:	5.2	0.908	4.61	4.27	17.3
sd:	NA	NA	NA	NA	NA

	CNST	HILL	GNLS
AIC:	201.81	145.25	149.25
PROB:	0	0.88	0.12
RMSE:	4.05	1.81	1.81

MAX_MEAN: 7.12   MAX_MED: 6.09   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10
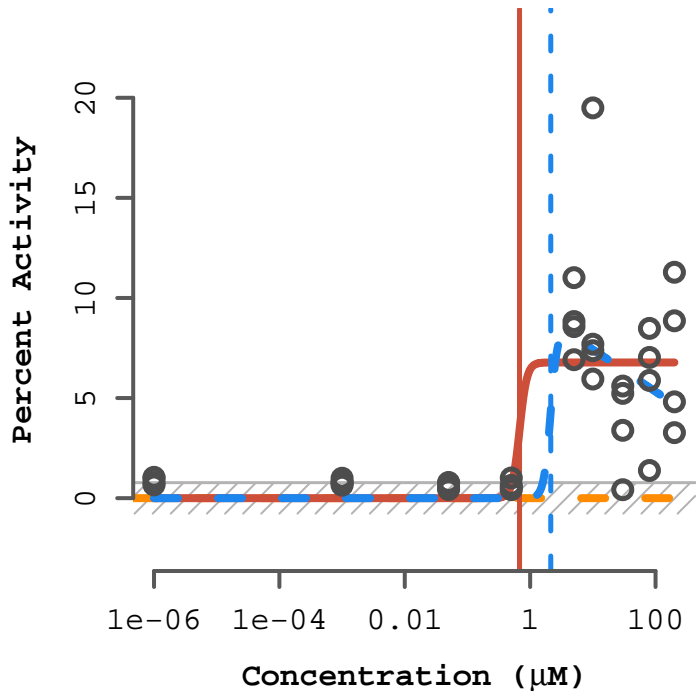
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Sorafenib
CHID: 41128   CASRN: 284461-73-0
SPID(S): ES211_57_57
M4ID: 42676051

HILL MODEL (in red):
        tp   ga   gw
val: 6.78   -0.17   7.43
sd: 0.528   3.29   186

GAIN-LOSS MODEL (in blue):
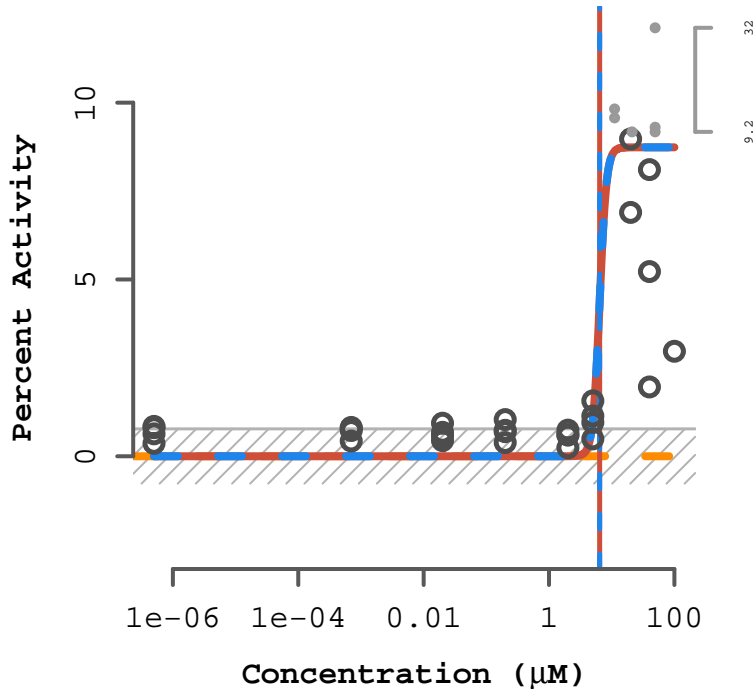   tp   ga   gw   la   lw
val: 12.3   0.329   8   1.6   0.3
sd: 25.2   1.34   29.3   6.28   0.6

        CNST   HILL   GNLS
AIC: 232.01   173.73   174.5
PROB: 0   0.6   0.4
RMSE: 6.07   3.01   2.92

MAX_MEAN: 10.1   MAX_MED: 8.7   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Vandetanib
CHID: 46681   CASRN: 443913-73-3
SPID(S): ES211_64_64
M4ID: 42676081 BRK

HILL MODEL (in red):
       tp   ga   gw
val: 8.74   0.808   8
sd: 0.588   0.569   42

GAIN-LOSS MODEL (in blue):
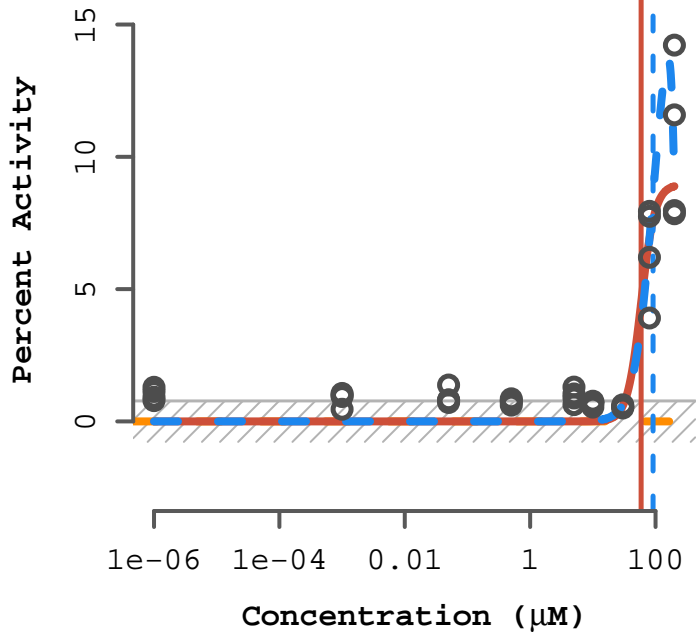   tp   ga   gw   la   lw
val: 8.74   0.808   8   2.78   10.6
sd: 0.588   0.579   42.7   662   8950

       CNST   HILL   GNLS
AIC: 226.71   168.97   172.97
PROB: 0   0.88   0.12
RMSE: 7.29   4.41   4.41

MAX_MEAN: 13.7   MAX_MED: 10.6   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Esomeprazole magnesium hydrate
CHID: 746660   CASRN: 668985-31-7
SPID(S):   ES211_43_43
M4ID: 42676083

HILL MODEL (in red):
        tp   ga   gw
val: 8.96   1.77   3.95
sd: 1.14   0.0644   1.1

GAIN-LOSS MODEL (in blue):
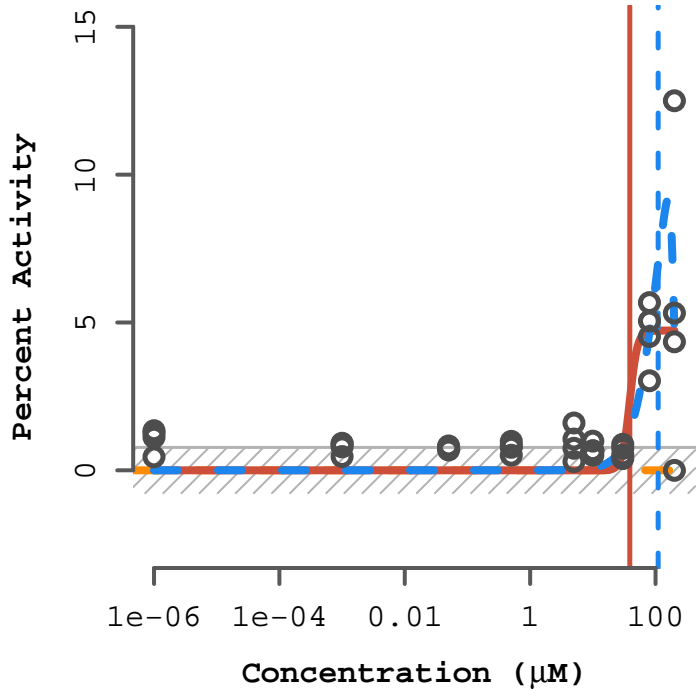   tp   ga   gw   la   lw
val: 17.1   1.96   2.94   2.31   12.9
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 194.2   126.47   130.35
PROB: 0   0.87   0.13
RMSE: 4.28   1.38   1.38

MAX_MEAN: 10.4   MAX_MED: 9.78   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Mianserin hydrochloride
CHID: 944145   CASRN: 21535-47-7
SPID(S): ES211_47_47
M4ID: 42676075

HILL MODEL (in red):
         tp   ga   gw
val: 4.73   1.59   7.17
sd: 1.27   1.2   75.6

GAIN-LOSS MODEL (in blue):
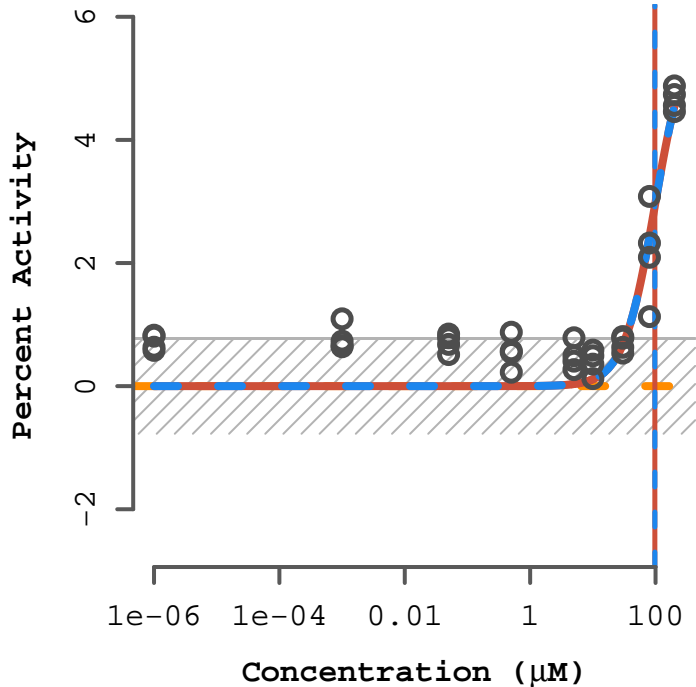   tp   ga   gw   la   lw
val: 14   2.04   2.16   2.29   14
sd: NaN   NaN   NaN   NaN   NaN

         CNST   HILL   GNLS
AIC: 163.6   126.57   130.01
PROB: 0   0.85   0.15
RMSE: 2.94   1.72   1.71

MAX_MEAN: 5.54   MAX_MED: 4.83   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 41   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: 4-Hydroxybenzoic acid butyl ester
CHID: 20209   CASRN: 94-26-8
SPID(S): ES211_19_19
M4ID: 42676062

HILL MODEL (in red):
	tp	ga	gw
val:	5.85	1.99	1.73
sd:	1.08	0.123	0.457

GAIN-LOSS MODEL (in blue):
	tp	ga	gw	la	lw
val:	5.85	1.99	1.73	4.06	4.76
sd:	1.08	0.123	0.457	1440	3910

	CNST	HILL	GNLS
AIC:	138.74	75	79
PROB:	0	0.88	0.12
RMSE:	1.82	0.58	0.58

MAX_MEAN: 4.66   MAX_MED: 4.65   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 42   ACTP: 1

FLAGS:
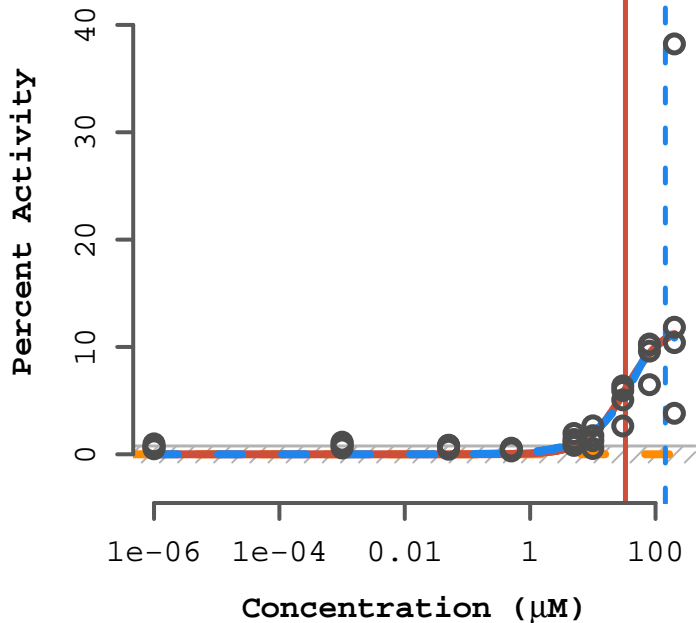
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Lovastatin
CHID: 20784   CASRN: 75330-75-5
SPID(S): ES211_42_42
M4ID: 42676060

HILL MODEL (in red):
        tp   ga   gw
val: 12.1   1.52   1.41
sd: 1.22   0.093   0.285

GAIN-LOSS MODEL (in blue):
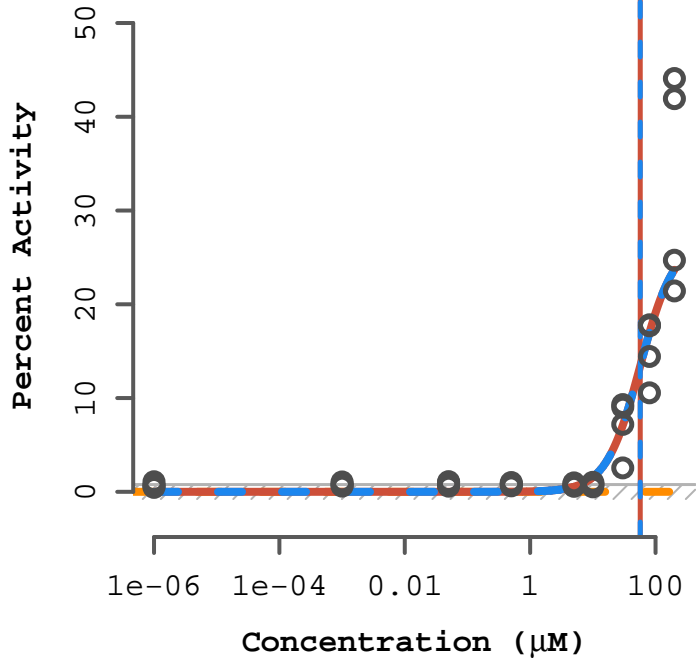   tp   ga   gw   la   lw
val: 31   2.16   0.995   2.41   1.72
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 224.93   148.19   150.62
PROB: 0   0.77   0.23
RMSE: 7.83   4.77   4.81

MAX_MEAN: 16.1   MAX_MED: 11.1   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 42   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: 13-cis Retinoic acid
CHID: 23177   CASRN: 4759-48-2
SPID(S): ES211_2_2
M4ID: 42676048

HILL MODEL (in red):
        tp   ga   gw
val: 26.9   1.76   1.6
sd: 3.3   0.0969   0.249

GAIN-LOSS MODEL (in blue):
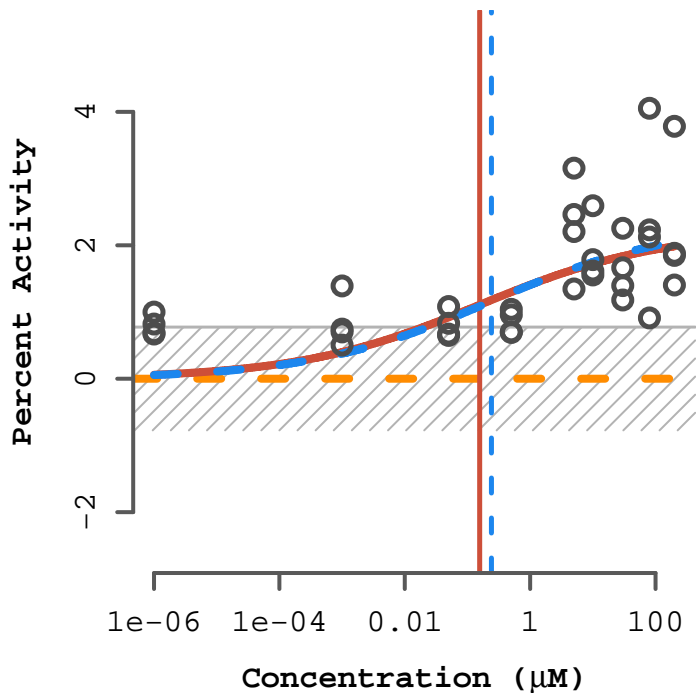   tp   ga   gw   la   lw
val: 26.9   1.76   1.6   4.14   4.14
sd: 3.3   0.0969   0.249   949   2160

        CNST   HILL   GNLS
AIC: 273.14   176.76   180.76
PROB: 0   0.88   0.12
RMSE: 12.87   4.85   4.85

MAX_MEAN: 33   MAX_MED: 33.3   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 42   ACTP: 1

FLAGS: 10

HILL MODEL (in red):

	tp	ga	gw		
val:	2.22	-0.805	0.3		
sd:	NaN	NaN	NaN		

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	2.32	-0.618	0.3	2.38	13.3
sd:	NaN	NaN	NaN	NaN	NaN

	CNST	HILL	GNLS
AIC:	148.22	84.96	88.83
PROB:	0	0.87	0.13
RMSE:	1.75	0.72	0.72

MAX_MEAN: 2.33   MAX_MED: 2.33   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 42   ACTP: 1

FLAGS:
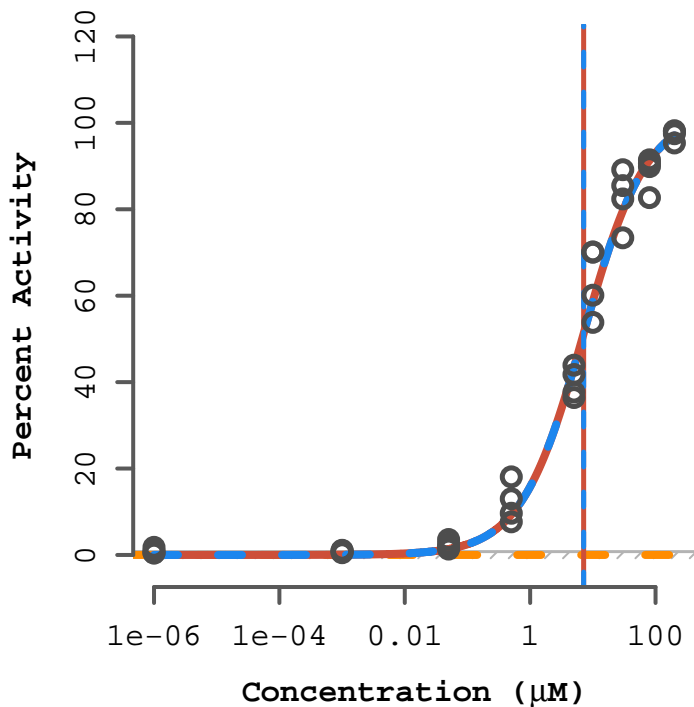
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Adriamycin hydrochloride
CHID: 30636   CASRN: 25316-40-9
SPID(S): ES211_67_67
M4ID: 42676061

HILL MODEL (in red):
         tp   ga   gw
val: 102   0.853   0.867
sd: 2.75   0.0488   0.0841

GAIN-LOSS MODEL (in blue):
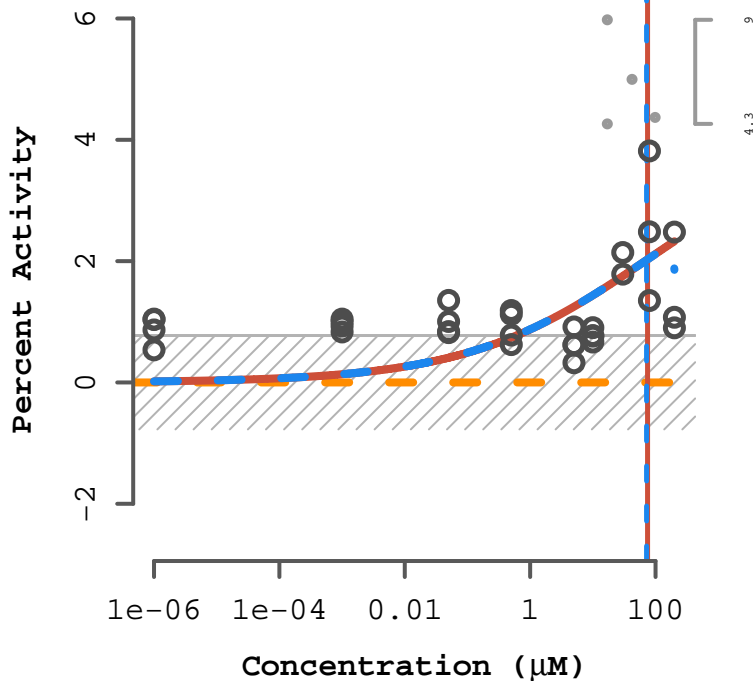   tp   ga   gw   la   lw
val: 102   0.853   0.867   3.52   11.4
sd: 2.75   0.0488   0.0841   106000   653000

         CNST   HILL   GNLS
AIC: 399.74   214.15   218.15
PROB: 0   0.88   0.12
RMSE: 57.79   4.51   4.51

MAX_MEAN: 97.3   MAX_MED: 97.8   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 42   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Amiodarone hydrochloride
CHID: 37185   CASRN: 19774-82-4
SPID(S): ES211_14_14
M4ID: 42676096   BRK

HILL MODEL (in red):
        tp   ga   gw
val: 4.06   1.87   0.3
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
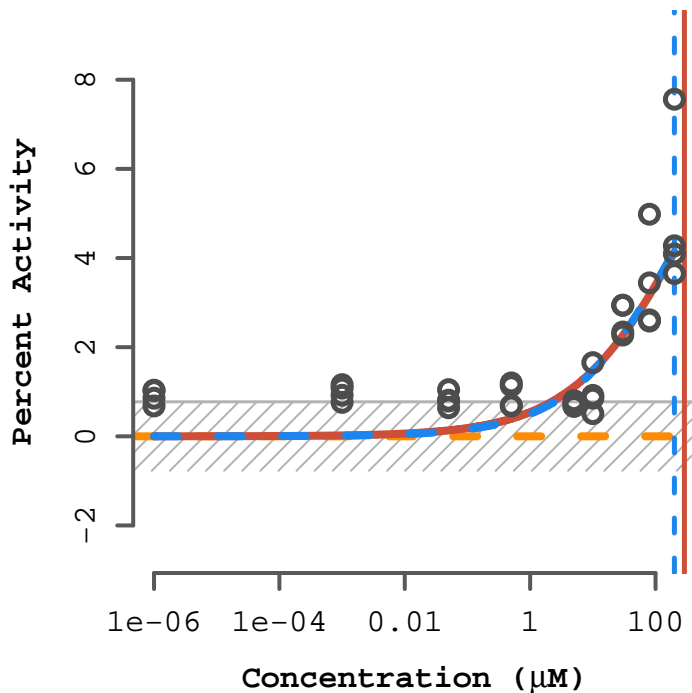   tp   ga   gw   la   lw
val: 4.04   1.86   0.3   2.34   16.1
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 158.84   129.65   133.16
PROB: 0   0.85   0.15
RMSE: 2.45   1.67   1.67

MAX_MEAN: 4.3   MAX_MED: 3.22   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 42   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: 6-aminopyridine-3-carboxamide
CHID: 51446   CASRN: 329-89-5
SPID(S): ES211_7_7
M4ID: 42676090

HILL MODEL (in red):
         tp   ga   gw
val: 9.08   2.46   0.486
sd: 6.51   1.25   0.21

GAIN-LOSS MODEL (in blue):
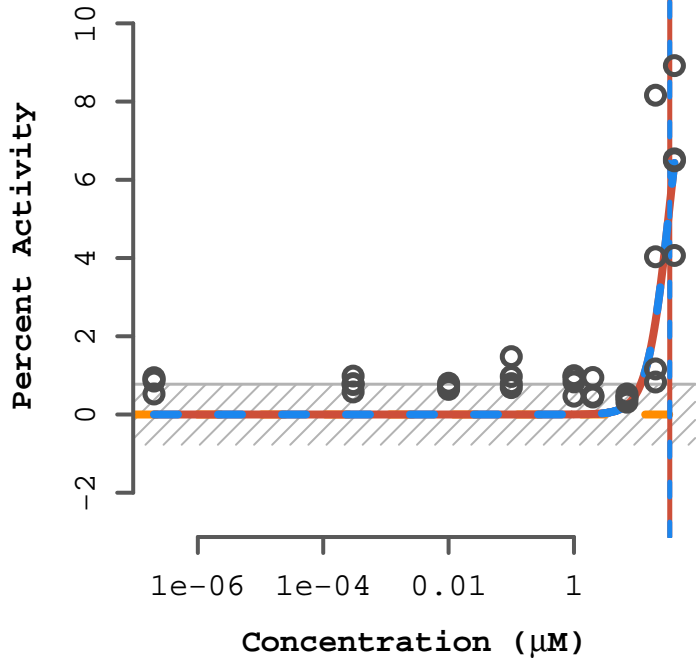   tp   ga   gw   la   lw
val: 8.34   2.3   0.518   3.61   14
sd: NA   NA   NA   NA   NA

         CNST   HILL   GNLS
AIC: 164.36   99.53   103.72
PROB: 0   0.89   0.11
RMSE: 2.38   0.91   0.91

MAX_MEAN: 4.9   MAX_MED: 4.18   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 42   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Dorsomorphin
CHID: 1006988 CASRN: 866405-64-3
SPID(S): ES211_6_6
M4ID: 42676084

HILL MODEL (in red):
        tp   ga   gw
val: 10.7   1.53   2.39
sd: 8.1   0.299   1.9

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
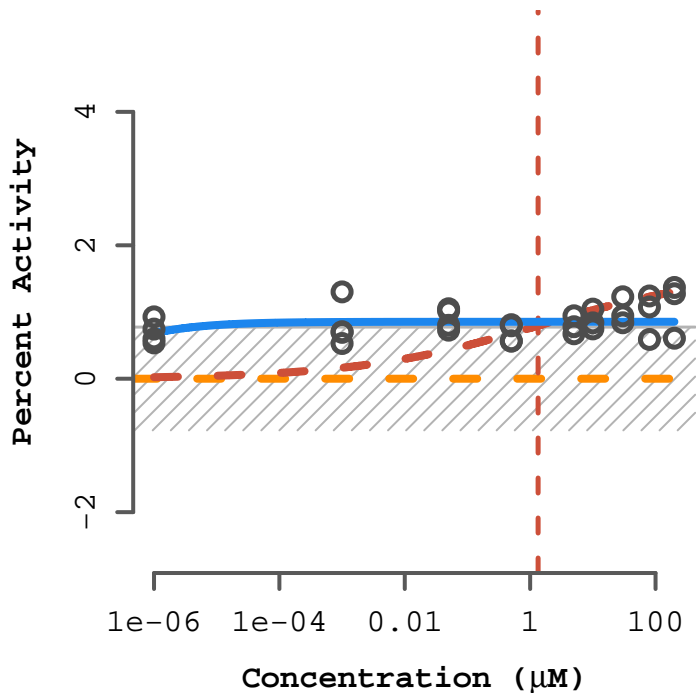val: 10.7   1.53   2.39   3.6   3.51
sd: 8.1   0.299   1.9   989   1760

        CNST   HILL   GNLS
AIC: 161.29   123.14   127.14
PROB: 0   0.88   0.12
RMSE: 2.8   1.37   1.37

MAX_MEAN: 6.5   MAX_MED: 6.51   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 42   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Folic acid
CHID: 22519   CASRN: 59-30-3
SPID(S): ES211_33_33
M4ID: 42676044

HILL MODEL (in red):
        tp   ga   gw
val: 1.59   0.127   0.3
sd: NaN   NaN   NaN

GAIN-LOSS MODEL (in blue):
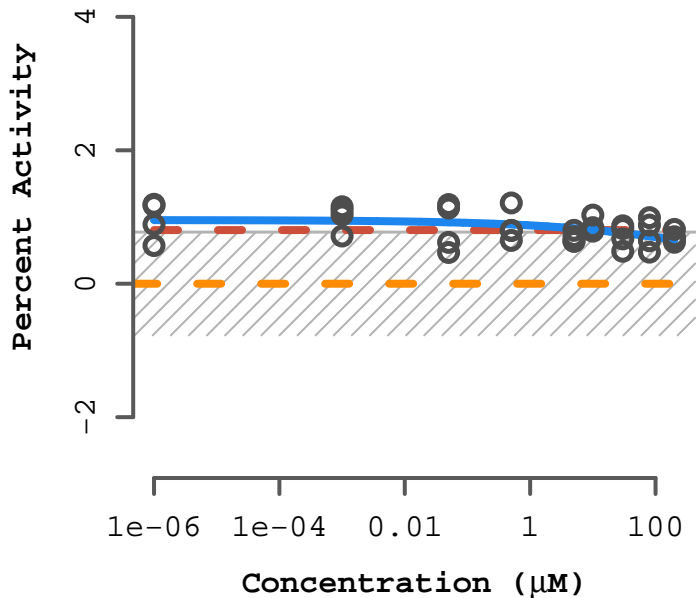   tp   ga   gw   la   lw
val: 0.853   -7   0.608   4.27   17.8
sd: NA   NA   NA   NA   NA

        CNST   HILL   GNLS
AIC: 89.21   47.51   13.03
PROB: 0   0   1
RMSE: 0.89   0.45   0.24

MAX_MEAN: 1.08   MAX_MED: 1.27   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 45   ACTP: 1

FLAGS: 11; 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Ibuprofen
CHID: 20732   CASRN: 15687-27-1
SPID(S): ES211_36_36
M4ID: 42676091

HILL MODEL (in red):
        tp   ga   gw
val: 0.804   -7   7.35
sd: 0.0381   161   1030

GAIN-LOSS MODEL (in blue):
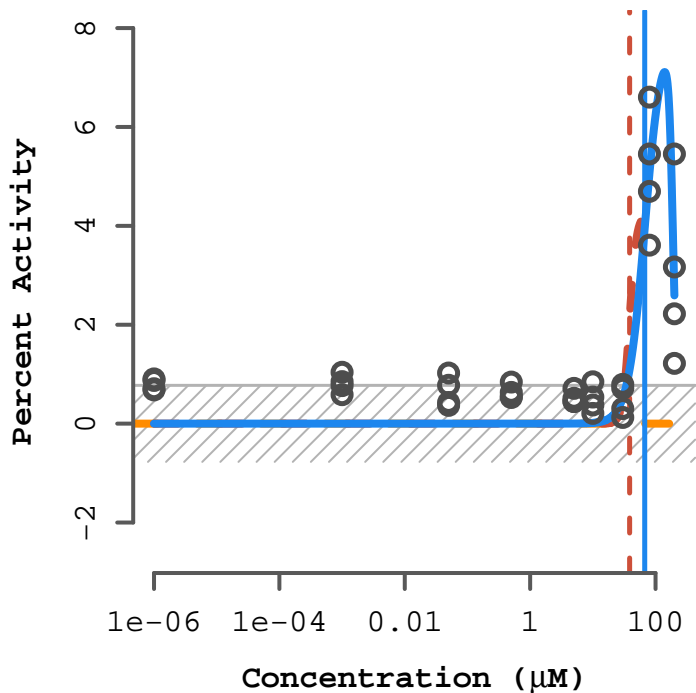   tp   ga   gw   la   lw
val: 0.955   -6.7   7.4   3.46   0.3
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 100.17   3.72   1.47
PROB: 0   0.24   0.76
RMSE: 0.85   0.22   0.2

MAX_MEAN: 1   MAX_MED: 1.07   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 49   ACTP: 1

FLAGS: 18

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Bisphenol A
CHID: 20182   CASRN: 80-05-7
SPID(S): ES211_16_16
M4ID: 42676059

HILL MODEL (in red):

	tp	ga	gw
val:	4.24	1.59	8
sd:	0.556	0.0838	5.61

GAIN-LOSS MODEL (in blue):

	tp	ga	gw	la	lw
val:	7.92	1.83	3.29	2.28	12.5
sd:	23.2	0.947	5.58	0.0231	66.3

	CNST	HILL	GNLS
AIC:	148.11	108.64	103.71
PROB:	0	0.08	0.92
RMSE:	2.16	0.99	0.86

MAX_MEAN: 5.09   MAX_MED: 5.08   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 50   ACTP: 1

FLAGS: 10
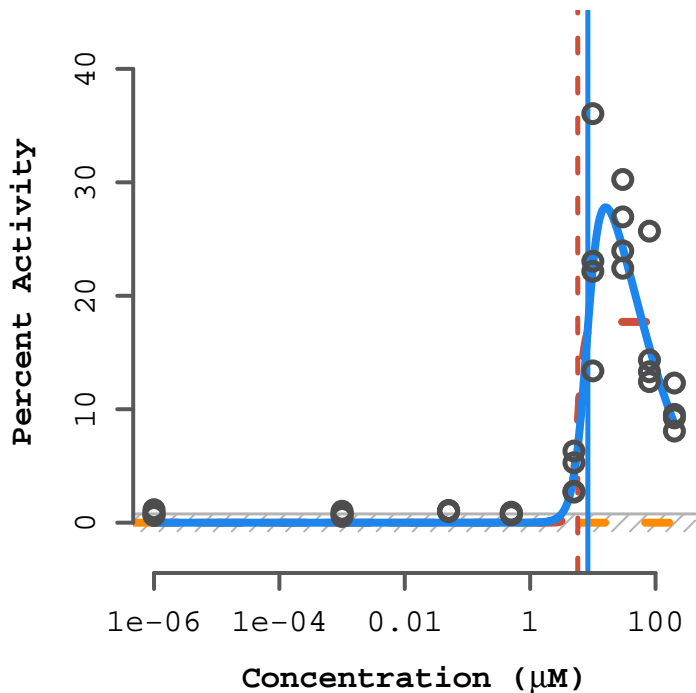
ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: 1-(p-Chlorobenzoyl)-5-methoxy-2-methyl-Indole-
CHID: 20740   CASRN: 53-86-1
SPID(S): ES211_38_38
M4ID: 42676077

HILL MODEL (in red):
        tp   ga   gw
val: 17.7   0.759   8
sd: 2.26   0.0415   4.36

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
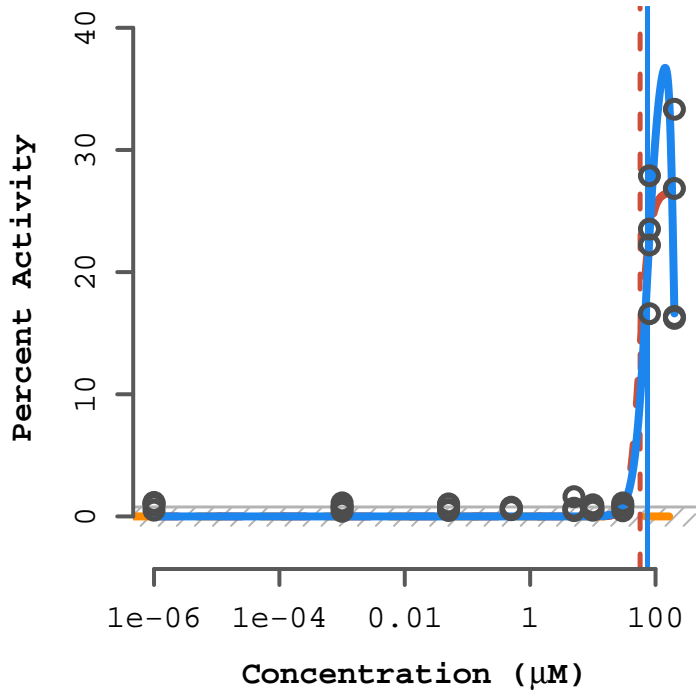val: 43.3   0.921   4.04   1.61   0.858
sd: 14   0.0404   0.542   0.335   0.187

        CNST   HILL   GNLS
AIC: 291.3   229.42   186.49
PROB: 0   0   1
RMSE: 13.85   5.59   3.62

MAX_MEAN: 25.9   MAX_MED: 25.5   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 50   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Retinol
CHID: 23556   CASRN: 68-26-8
SPID(S): ES211_51_51
M4ID: 42676071

HILL MODEL (in red):
        tp   ga   gw
val: 26.6   1.75   5.38
sd: 1.21   0.0304   0.794

GAIN-LOSS MODEL (in blue):
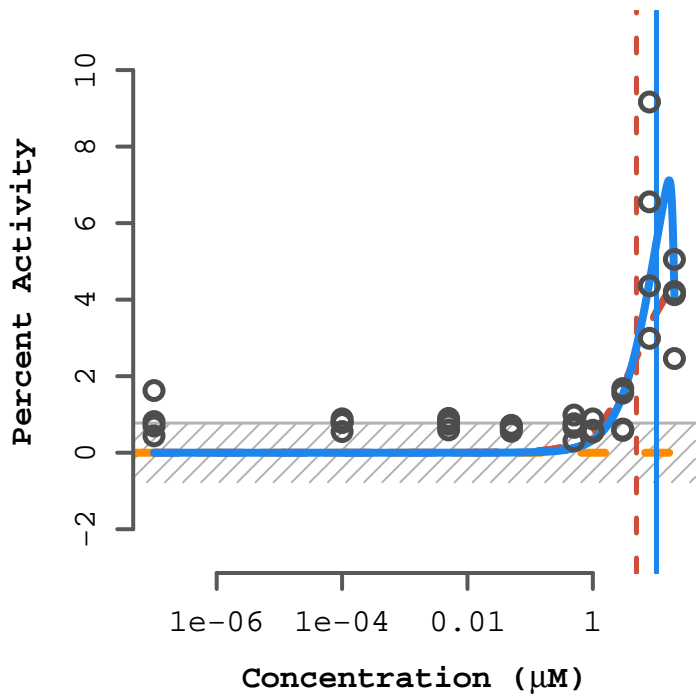   tp   ga   gw   la   lw
val: 40   1.87   4.21   2.29   12.2
sd: 9.43   0.0457   0.998   0.0239   21

        CNST   HILL   GNLS
AIC: 261.81   164.91   161.86
PROB: 0   0.18   0.82
RMSE: 11.16   3.07   3.6

MAX_MEAN: 23.2   MAX_MED: 22.9   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 50   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Ziprasidone
CHID: 23753   CASRN: 146939-27-7
SPID(S): ES211_66_66
M4ID: 42676046

HILL MODEL (in red):
        tp   ga   gw
val: 5.04   0.696   1.34
sd: 1.96   0.363   1.25

GAIN-LOSS MODEL (in blue):
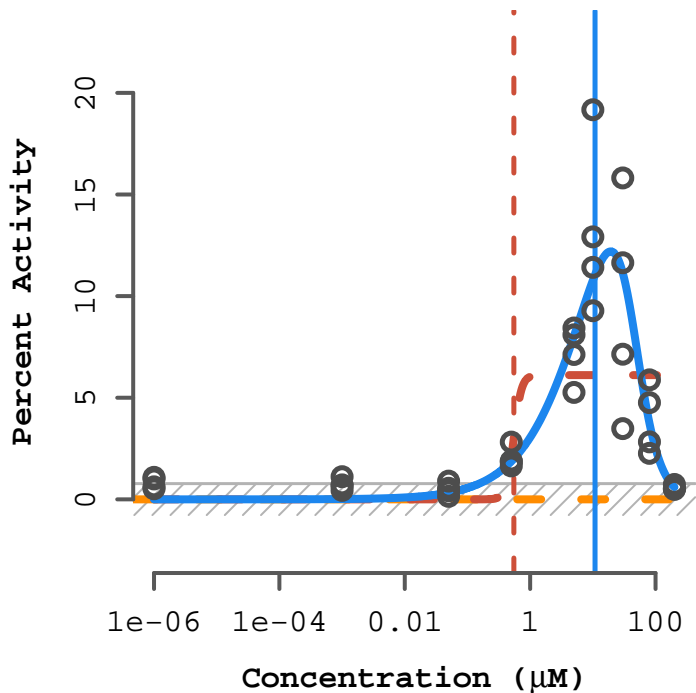   tp   ga   gw   la   lw
val: 11   1.02   1.48   1.3   17.9
sd: NaN   NaN   NaN   NaN   NaN

        CNST   HILL   GNLS
AIC: 161.94   114.79   114.7
PROB: 0   0.49   0.51
RMSE: 2.59   1.34   1.14

MAX_MEAN: 5.77   MAX_MED: 5.46   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 51   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra

NAME: Dasatinib
CHID: 40979   CASRN: 302962-49-8
SPID(S): ES211_26_26
M4ID: 42676040

HILL MODEL (in red):
       tp   ga   gw
val: 6.11   -0.26   7.22
sd: 0.915   2.82   493

GAIN-LOSS MODEL (in blue):
       tp   ga   gw   la   lw
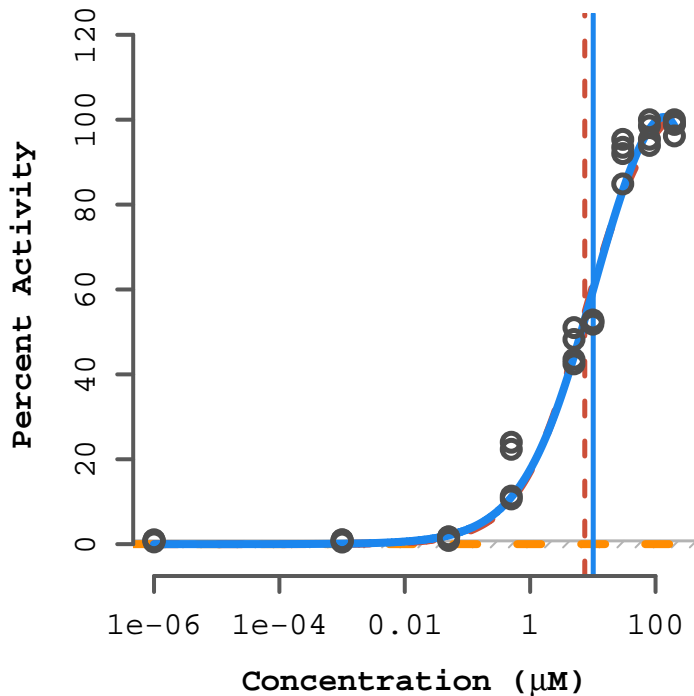val: 23   1.04   0.789   1.64   2.31
sd: 12   0.505   0.174   0.126   0.484

       CNST   HILL   GNLS
AIC: 233.91   202.71   156.69
PROB: 0   0   1
RMSE: 6.48   3.93   2.35

MAX_MEAN: 13.2   MAX_MED: 12.2   BMAD: 0.258

COFF: 0.774 HIT-CALL: 1   FITC: 51   ACTP: 1

FLAGS: 10

ASSAY: AEID3096 (CCTE_Deisenroth_DEVTOX_RUES2-GLR_Bra_

NAME: Sunitinib malate
CHID: 46492   CASRN: 341031-54-7
SPID(S): ES211_60_60
M4ID: 42676102

HILL MODEL (in red):
        tp   ga   gw
val: 108   0.871   0.829
sd: 3.88   0.0659   0.0944

GAIN-LOSS MODEL (in blue):
        tp   ga   gw   la   lw
val: 120   1.01   0.761   2.78   2.04
sd: 12.8   0.137   0.0805   0.461   2.5

        CNST   HILL   GNLS
AIC: 402.64   232.51   228.05
PROB: 0   0.1   0.9
RMSE: 60.31   5.65   5.13

MAX_MEAN: 98.5   MAX_MED: 99   BMAD: 0.258

COFF: 0.774   HIT-CALL: 1   FITC: 51   ACTP: 1

FLAGS: 10