

NAME: DMSO (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO

M4ID: 30230027 BRK

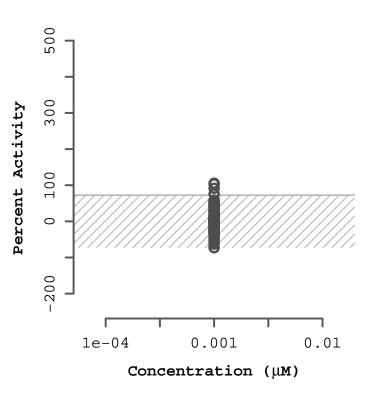
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 4.97 MAX_MED: 0 BMAD: 24.2

COFF: 72.5 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Water (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Water
M4ID: 30230028

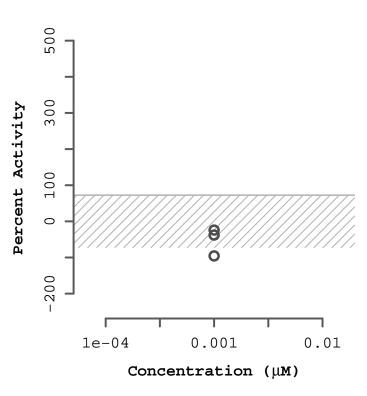
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 5.22 MAX_MED: 1.34 BMAD: 24.2

COFF: 72.5 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: DMSO/Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO/Ethanol M4ID: 30230029

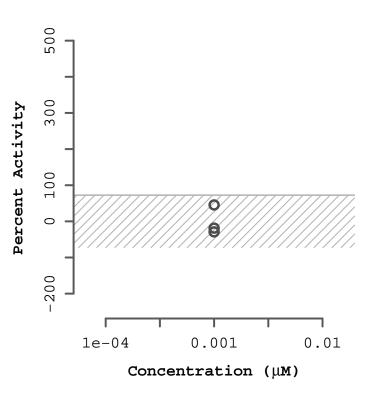
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: -52.5 MAX_MED: -37.8 BMAD: 24.2

COFF: 72.5 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Ethanol M4ID: 30230030

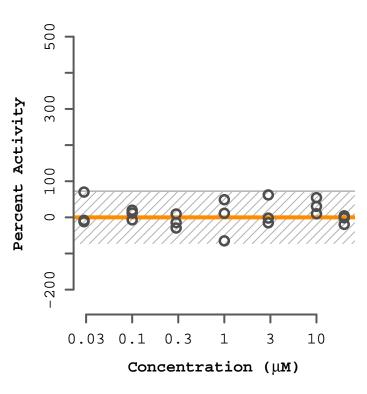
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: -0.772 MAX_MED: -18.7 BMAD: 24.2

COFF: 72.5 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Triphenyl phosphite

CHID: 26252 CASRN: 101-02-0

SPID(S): TP0001649E09 M4ID: 30230038

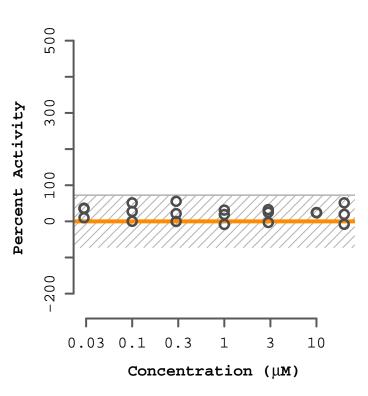
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 207.51 NA NA
PROB: 1 NA NA
RMSE: 32.45 NA NA

MAX_MEAN: 31.6 MAX_MED: 30.3 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Clothianidin

CHID: 34465 CASRN: 210880-92-5

SPID(S): TP0001649F07 M4ID: 30230042

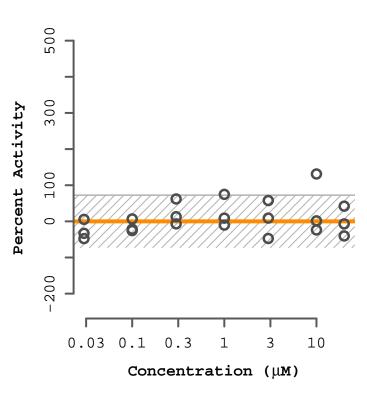
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 205.41 NA NA
PROB: 1 NA NA
RMSE: 28.88 NA NA

MAX_MEAN: 27.2 MAX_MED: 35.1 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Thiacloprid

CHID: 34961 CASRN: 111988-49-9

SPID(S): TP0001649E07 M4ID: 30230037

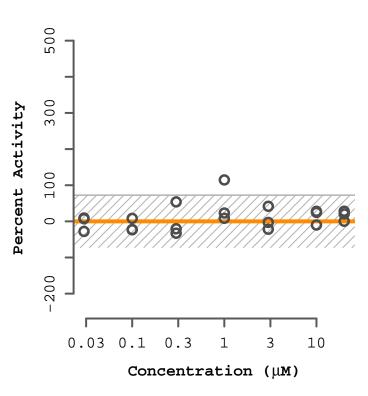
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 219.27 NA NA
PROB: 1 NA NA
RMSE: 44.33 NA NA

MAX_MEAN: 36.3 MAX_MED: 12.9 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Thiamethoxam

CHID: 34962 CASRN: 153719-23-4

SPID(S): TP0001649E10 M4ID: 30230039

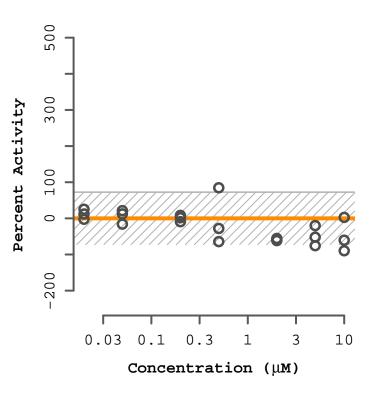
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 207.11 NA NA
PROB: 1 NA NA
RMSE: 34.6 NA NA

MAX_MEAN: 48.8 MAX_MED: 24.9 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Pravastatin sodium

CHID: 47525 CASRN: 81131-70-6

SPID(S): TP0001649E12 M4ID: 30230040

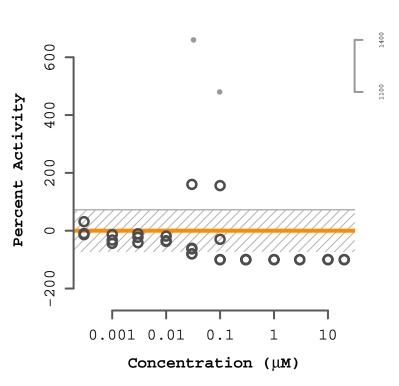
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 224.37 NA NA
PROB: 1 NA NA
RMSE: 46.18 NA NA

MAX_MEAN: 11.7 MAX_MED: 12.3 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Tributyltin methacrylate CHID: 35204 CASRN: 2155-70-6

SPID(S): TP0001649D04 M4ID: 30230034 BRK

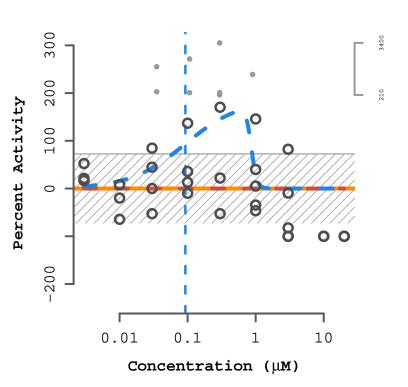
HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

CNST HILL GNLS
AIC: 539.47 NA NA
PROB: 1 NA NA
RMSE: 283.4 NA NA

MAX_MEAN: 206 MAX_MED: -9.82 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 7 ACTP: 0



NAME: Lovastatin

CHID: 20784 CASRN: 75330-75-5

SPID(S): TP0001649D08 M4ID: 30230035 BRK

HILL MODEL (in red):

tp ga gw val: 175 1.8 7.98 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

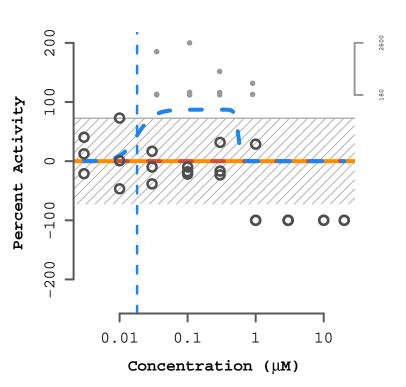
tр ga gw la lw val: 187 -1.03 1.07 -0.0633 11 392 2.18 2.41 292 sd: 1.68

CNST HILL GNLS
AIC: 611.28 617.28 614.39
PROB: 0.79 0.04 0.17
RMSE: 750 750 720.05

MAX_MEAN: 679 MAX_MED: 191 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 10 ACTP: 0.21

FLAGS: 10; 8



NAME: Mercuric chloride

CHID: 20811 CASRN: 7487-94-7

SPID(S): TP0001649C11 M4ID: 30230033 BRK

HILL MODEL (in red):

tp ga gw val: 107 1.8 8 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

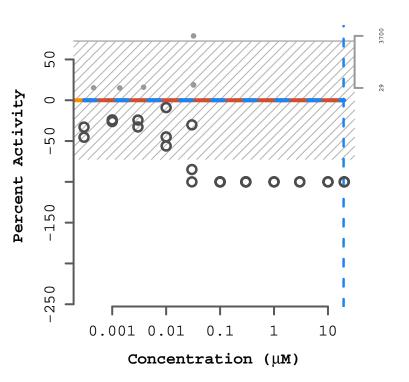
tр ga gw la lw val: 87.1 -1.74 3.6 -0.255 17.7 51.7 0.697 11.5 9.1 614 sd:

CNST HILL GNLS
AIC: 594.62 600.62 600.09
PROB: 0.9 0.04 0.06
RMSE: 583.37 583.37 560.75

MAX_MEAN: 505 MAX_MED: 107 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 10 ACTP: 0.1

FLAGS: 10; 8



NAME: Phenylmercuric acetate CHID: 21150 CASRN: 62-38-4

SPID(S): TP0001649D11 M4ID: 30230036 BRK

HILL MODEL (in red):

tp ga gw val: 14.4 1.8 7.97 sd: NaN NaN NaN

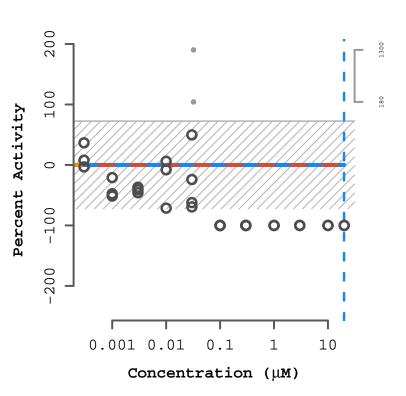
GAIN-LOSS MODEL (in blue):

tp ga gw la lw val: 3.47e-07 1.29 6.82 1.62 17.9 sd: NA NA NA NA NA

CNST HILL GNLS
AIC: 25718.4 546.39 550.39
PROB: 0 0.88 0.12
RMSE: 574.26 574.26 574.26

MAX_MEAN: 656 MAX_MED: 102 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 13 ACTP: 1



NAME: Tributyltin chloride

CHID: 27403 CASRN: 1461-22-9

SPID(S): TP0001649C09 M4ID: 30230032 BRK

HILL MODEL (in red):

tp ga gw val: 99.3 1.8 8 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

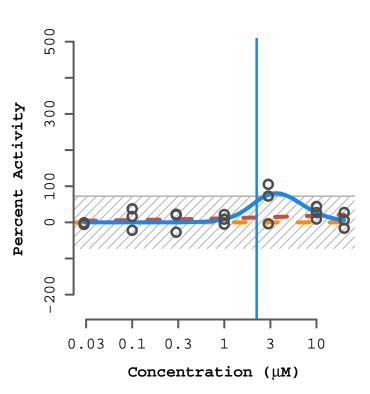
tp ga gw la lw val: 5.53e-07 1.3 4.35 2.95 0.463 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 25631.41 528.04 532.04
PROB: 0 0.88 0.12
RMSE: 216.92 216.92 216.92

MAX_MEAN: 228 MAX_MED: 12.9 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 18 ACTP: 1

FLAGS: 10; 12



NAME: Chlorendic acid

CHID: 20268 CASRN: 115-28-6

SPID(S): TP0001649F01 M4ID: 30230041

HILL MODEL (in red):

tp ga gw val: 50.6 1.8 0.3 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

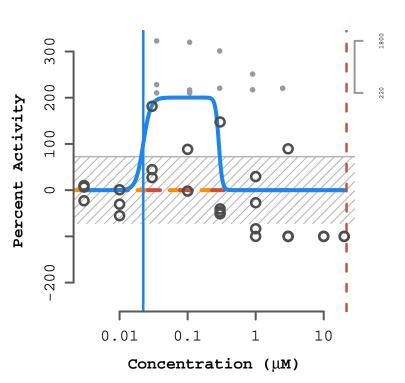
tр ga gw la lw val: 126 0.351 3.17 0.777 2.5 553 1.4 7.58 1.04 3.44 sd:

CNST HILL GNLS
AIC: 206.49 207.21 204.24
PROB: 0.21 0.15 0.64
RMSE: 34.26 29.65 24.97

MAX_MEAN: 58 MAX_MED: 72.7 BMAD: 24.2

COFF: 72.5 HIT-CALL: 1 FITC: 50 ACTP: 0.79

FLAGS: 11; 16; 7



NAME: Simvastatin

CHID: 23581 CASRN: 79902-63-9

SPID(S): TP0001649C08 M4ID: 30230031 BRK

HILL MODEL (in red):

tp ga gw val: 0.000246 1.34 0.302 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

tр ga gw la lw -1.65 val: 200 -0.541 17.3 73.7 0.47 24.7 sd: 1.11 1040

CNST HILL GNLS
AIC: 607.78 613.78 606.16
PROB: 0.3 0.02 0.68
RMSE: 505.86 505.86 459.38

MAX_MEAN: 466 MAX_MED: 244 BMAD: 24.2

COFF: 72.5 HIT-CALL: 1 FITC: 50 ACTP: 0.7

FLAGS: 11; 16; 10