

NAME: DMSO (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO

M4ID: 30230155 BRK

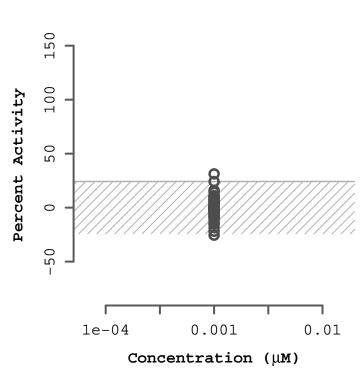
HILL MODEL: Not applicable.

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



NAME: Water (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Water

M4ID: 30230156

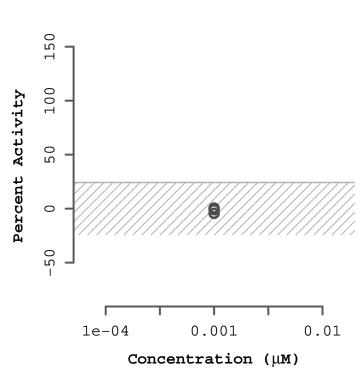
HILL MODEL: Not applicable.

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



NAME: DMSO/Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO/Ethanol M4ID: 30230157

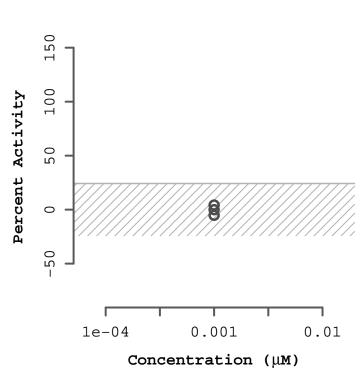
HILL MODEL: Not applicable.

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



NAME: Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Ethanol M4ID: 30230158

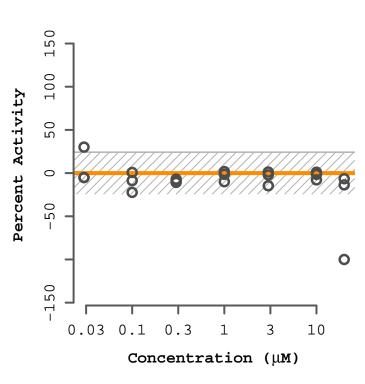
HILL MODEL: Not applicable.

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



NAME: Chlorendic acid

CHID: 20268 CASRN: 115-28-6

SPID(S): TP0001649F01 M4ID: 30230169

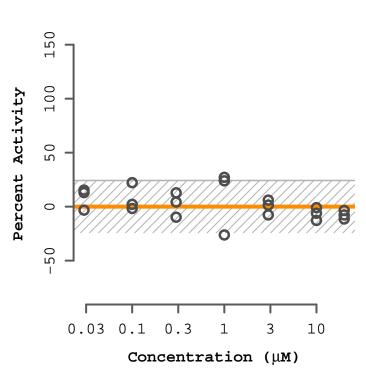
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 6.64 MAX_MED: -1.37 BMAD: 8.07

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



NAME: Triphenyl phosphite

CHID: 26252 CASRN: 101-02-0

SPID(S): TP0001649E09

M4ID: 30230166

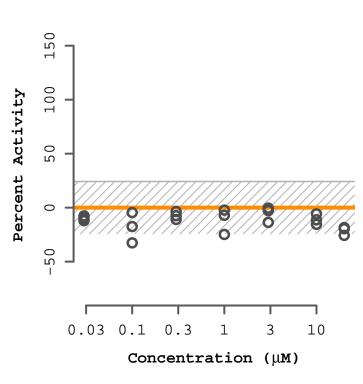
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 8.38 MAX_MED: 23.9 BMAD: 8.07

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



NAME: Clothianidin

CHID: 34465 CASRN: 210880-92-5

SPID(S): TP0001649F07 M4ID: 30230170

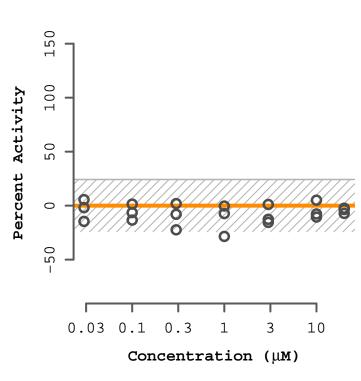
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: -5.61 MAX_MED: -2.76 BMAD: 8.07

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



NAME: Thiacloprid

CHID: 34961 CASRN: 111988-49-9

SPID(S): TP0001649E07 M4ID: 30230165

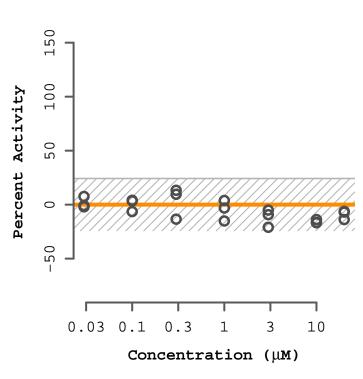
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: -3.62 MAX_MED: -1.87 BMAD: 8.07

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



NAME: Thiamethoxam

CHID: 34962 CASRN: 153719-23-4

SPID(S): TP0001649E10 M4ID: 30230167

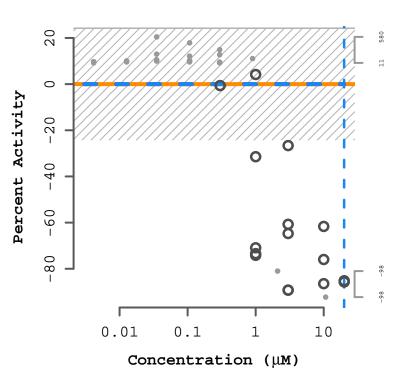
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 3.17 MAX_MED: 9.62 BMAD: 8.07

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



NAME: Lovastatin

CHID: 20784 CASRN: 75330-75-5

SPID(S): TP0001649D08 M4ID: 30230163 BRK

HILL MODEL (in red):

tp ga gw val: 8.75 1.8 7.94 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

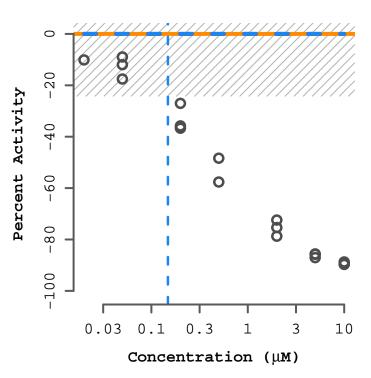
tр ga gw la lw val: 3.62e-08 1.3 8 1.57 0.609 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 521.63 527.63 531.63
PROB: 0.95 0.05 0.01
RMSE: 144.82 144.82 144.82

MAX_MEAN: 172 MAX_MED: 69.8 BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 7 ACTP: 0.05

FLAGS: 8; 10



NAME: Pravastatin sodium

CHID: 47525 CASRN: 81131-70-6

SPID(S): TP0001649E12 M4ID: 30230168

HILL MODEL (in red):

tp ga gw val: 0.00799 1.49 7.27 sd: NaN NaN NaN

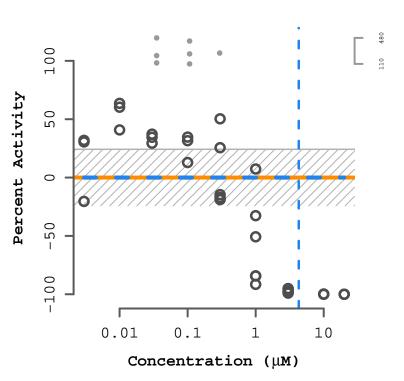
GAIN-LOSS MODEL (in blue):

tp ga gw la lw val: 8.07e-08 -0.829 2.27 -0.351 6.14 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 236.44 242.44 246.44
PROB: 0.95 0.05 0.01
RMSE: 59.68 59.68 59.68

MAX_MEAN: -1.55 MAX_MED: 2.71 BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 7 ACTP: 0.05



NAME: Mercuric chloride

CHID: 20811 CASRN: 7487-94-7

SPID(S): TP0001649C11 M4ID: 30230161 BRK

HILL MODEL (in red):

tp ga gw val: 92.7 1.8 7.98 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

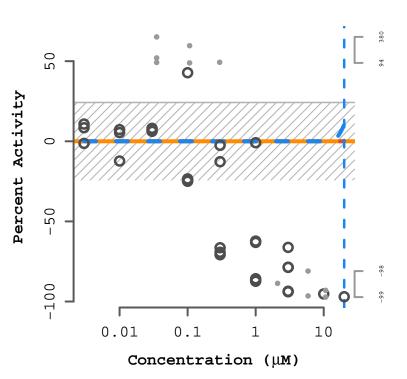
tp ga gw la lw val: 3.97e-06 0.633 8 0.895 15.4 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 524.07 530.07 534.07
PROB: 0.95 0.05 0.01
RMSE: 136.93 136.93 136.93

MAX_MEAN: 154 MAX_MED: 78.8 BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 10 ACTP: 0.05

FLAGS: 8; 10



NAME: Simvastatin

CHID: 23581 CASRN: 79902-63-9

SPID(S): TP0001649C08 M4ID: 30230159 BRK

HILL MODEL (in red):

tp ga gw val: 46.6 1.8 7.98 sd: NaN NaN NaN

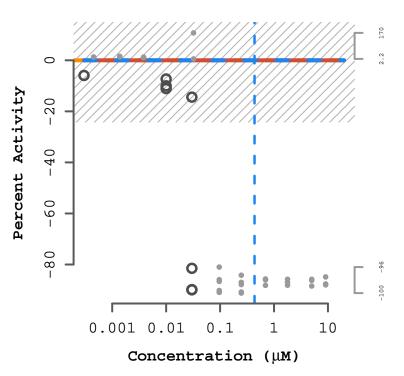
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 21 1.3 8 3.3 18 sd: NA NA NA NA NA

CNST HILL GNLS
AIC: 502.19 508.19 513.22
PROB: 0.95 0.05 0
RMSE: 100.92 100.92 101.69

MAX_MEAN: 109 MAX_MED: 53.5 BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 10 ACTP: 0.05



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

SPID(S): TP0001649D11 M4ID: 30230164 BRK

HILL MODEL (in red):

tp ga gw val: 0.513 1.8 7.78 sd: NaN NaN NaN

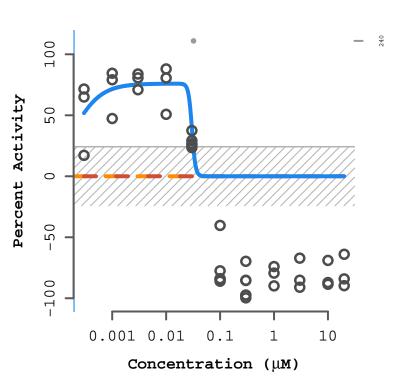
GAIN-LOSS MODEL (in blue):

tp ga gw la lw val: 4.96e-07 -0.361 7.6 -0.103 17.9 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 586.6 505.11 509.11
PROB: 0 0.88 0.12
RMSE: 82.74 82.74

MAX_MEAN: 17.9 MAX_MED: 18.3 BMAD: 8.07

COFF: 24.2 HIT-CALL: 0 FITC: 13 ACTP: 1



NAME: Tributyltin chloride

CHID: 27403 CASRN: 1461-22-9

SPID(S): TP0001649C09 M4ID: 30230160 BRK

HILL MODEL (in red):

tp ga gw val: 85.4 1.8 7.98 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

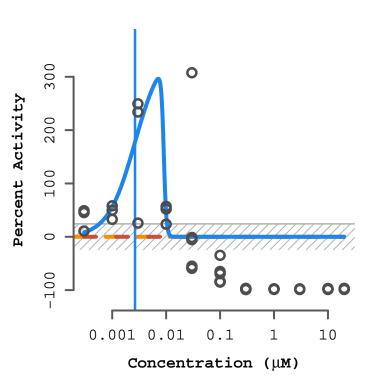
tр ga gw la lw val: 76 -3.72 1.67 -1.52 13.5 26.7 0.993 7.41 0.0924 sd: 493

CNST HILL GNLS
AIC: 497.92 503.92 492.6
PROB: 0.07 0 0.93
RMSE: 82.78 82.78 70.64

MAX MEAN: 78.5 MAX MED: 80.7 BMAD: 8.07

COFF: 24.2 HIT-CALL: 1 FITC: 49 ACTP: 0.93

FLAGS: 10; 15; 18



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

SPID(S): TP0001649D04 M4ID: 30230162

HILL MODEL (in red):

tp ga gw val: 267 1.8 8 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

tр ga gw la lw -2.04 val: 355 -2.58 1.72 18 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 510.8 516.81 510.8
PROB: 0.49 0.02 0.49
RMSE: 102.48 102.48 90.38

MAX_MEAN: 170 MAX_MED: 234 BMAD: 8.07

COFF: 24.2 HIT-CALL: 1 FITC: 50 ACTP: 0.51

FLAGS: 10; 11; 16