

NAME: DMSO (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO

M4ID: 30230059

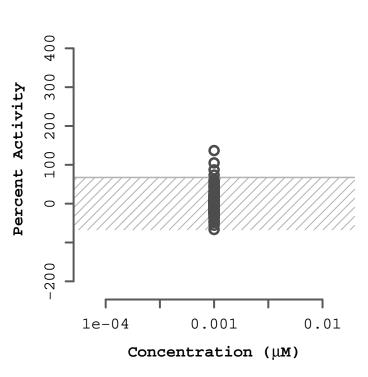
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 3.92 MAX\_MED: -0.0299 BMAD: 22.5

COFF: 67.5 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Water (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Water
M4ID: 30230060

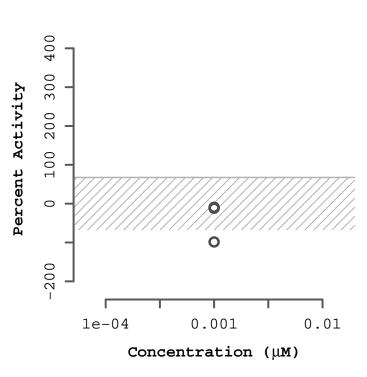
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 3.9 MAX\_MED: 0.461 BMAD: 22.5

COFF: 67.5 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: DMSO/Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO/Ethanol M4ID: 30230061

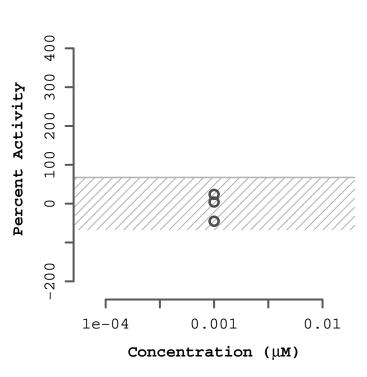
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: -39.9 MAX\_MED: -11.7 BMAD: 22.5

COFF: 67.5 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Ethanol M4ID: 30230062

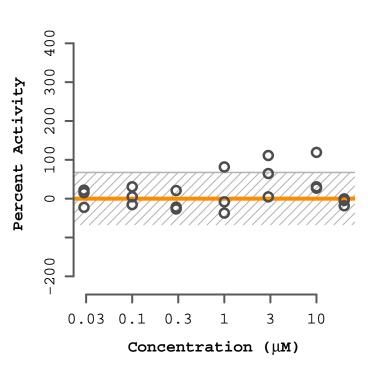
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: -5.72 MAX\_MED: 4.19 BMAD: 22.5

COFF: 67.5 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Triphenyl phosphite

CHID: 26252 CASRN: 101-02-0

SPID(S): TP0001649E09

M4ID: 30230070

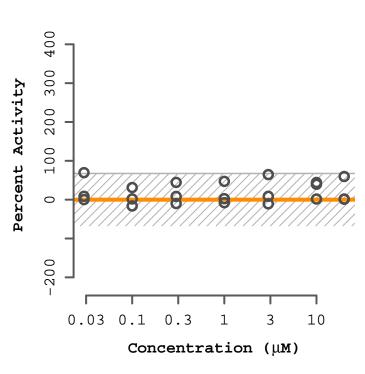
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 219.98 NA NA
PROB: 1 NA NA
RMSE: 46.27 NA NA

MAX\_MEAN: 60.2 MAX\_MED: 64.7 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Clothianidin

CHID: 34465 CASRN: 210880-92-5

SPID(S): TP0001649F07 M4ID: 30230074

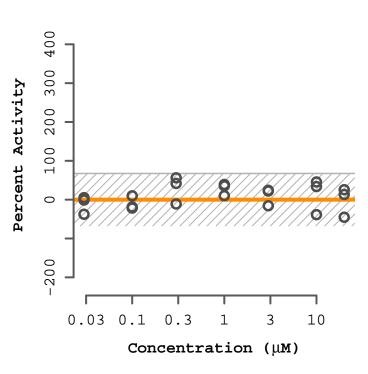
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 207.68 NA NA
PROB: 1 NA NA
RMSE: 32.4 NA NA

MAX\_MEAN: 28.5 MAX\_MED: 39.6 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Thiacloprid

CHID: 34961 CASRN: 111988-49-9

SPID(S): TP0001649E07 M4ID: 30230069

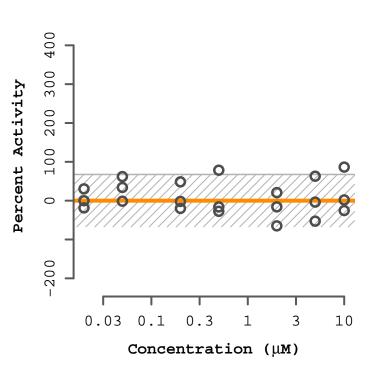
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 207.91 NA NA
PROB: 1 NA NA
RMSE: 30.25 NA NA

MAX\_MEAN: 29 MAX\_MED: 41.7 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Pravastatin sodium

CHID: 47525 CASRN: 81131-70-6

SPID(S): TP0001649E12 M4ID: 30230072

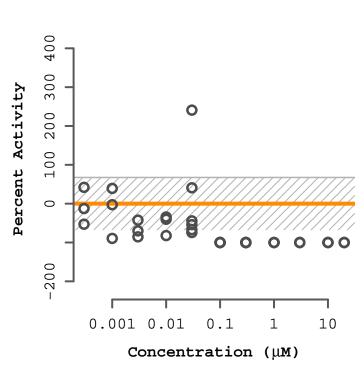
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

CNST HILL GNLS
AIC: 219.33 NA NA
PROB: 1 NA NA
RMSE: 41.39 NA NA

MAX\_MEAN: 31.6 MAX\_MED: 34 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Tributyltin chloride

CHID: 27403 CASRN: 1461-22-9

SPID(S): TP0001649C09

M4ID: 30230064

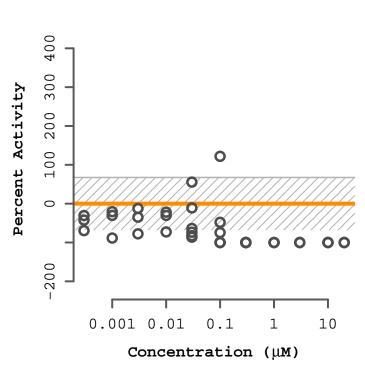
HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

CNST HILL GNLS
AIC: 25673.55 NA NA
PROB: 1 NA NA
RMSE: 91.6 NA NA

MAX\_MEAN: 7.04 MAX\_MED: -2.69 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 7 ACTP: 0



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

SPID(S): TP0001649D04 M4ID: 30230066

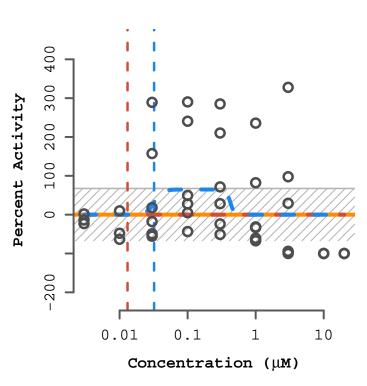
HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

CNST HILL GNLS
AIC: 504.96 NA NA
PROB: 1 NA NA
RMSE: 83.16 NA NA

MAX\_MEAN: -41.6 MAX\_MED: -30.2 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 7 ACTP: 0



NAME: Lovastatin

CHID: 20784 CASRN: 75330-75-5

SPID(S): TP0001649D08 M4ID: 30230067

HILL MODEL (in red):

tp ga gw val: 6.46e-07 -1.88 4.94 sd: NaN NaN NaN

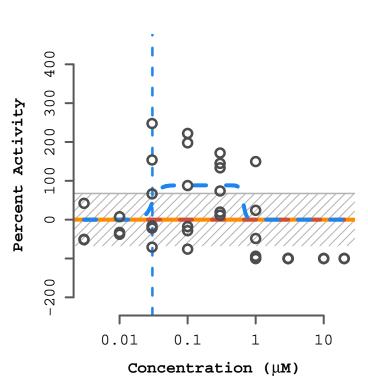
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 64.7 -1.49 7.53 -0.374 14.9 48.7 0.381 80.2 12.6 1230 sd:

CNST HILL GNLS
AIC: 525.73 531.73 531.76
PROB: 0.91 0.05 0.04
RMSE: 127.44 127.44 117.34

MAX\_MEAN: 95 MAX\_MED: 49.9 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 9 ACTP: 0.09



NAME: Mercuric chloride

CHID: 20811 CASRN: 7487-94-7

SPID(S): TP0001649C11 M4ID: 30230065

HILL MODEL (in red):

tp ga gw val: 92.8 1.8 8 sd: NaN NaN NaN

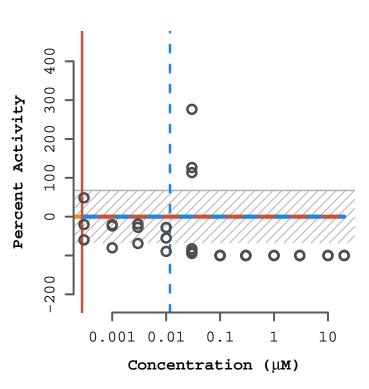
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 88.4 -1.52 -0.184 18 30.8 0.188 142 sd: 211 1.45

CNST HILL GNLS
AIC: 515.84 521.84 518.77
PROB: 0.78 0.04 0.18
RMSE: 104.21 104.21 93.09

MAX\_MEAN: 92.5 MAX\_MED: 104 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 10 ACTP: 0.22



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

SPID(S): TP0001649D11 M4ID: 30230068

HILL MODEL (in red):

tp ga gw val: 5.36e-09 -3.56 7.4 sd: NaN NaN NaN

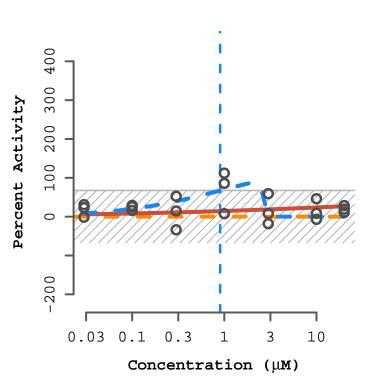
GAIN-LOSS MODEL (in blue):

tp ga gw la lw val: 6.81e-09 -1.93 6.63 1.51 17.1 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 25709.08 518.19 522.19
PROB: 0 0.88 0.12
RMSE: 97.66 97.66

MAX\_MEAN: 41.6 MAX\_MED: 15.4 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 13 ACTP: 1



NAME: Thiamethoxam

CHID: 34962 CASRN: 153719-23-4

SPID(S): TP0001649E10 M4ID: 30230071

HILL MODEL (in red):

tp ga gw val: 65 1.8 0.3 sd: NaN NaN NaN

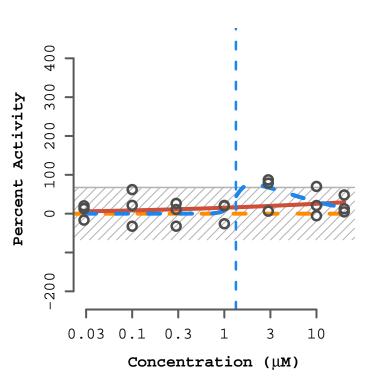
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 135 -0.0452 0.792 0.426 17.8 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 215.9 215.18 215.61
PROB: 0.28 0.4 0.32
RMSE: 40.71 34.67 30.7

MAX\_MEAN: 68.5 MAX\_MED: 85.8 BMAD: 22.5

COFF: 67.5 HIT-CALL: 0 FITC: 21 ACTP: 0.72



NAME: Chlorendic acid

CHID: 20268 CASRN: 115-28-6

SPID(S): TP0001649F01 M4ID: 30230073

HILL MODEL (in red):

tp ga gw val: 70.8 1.8 0.311 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

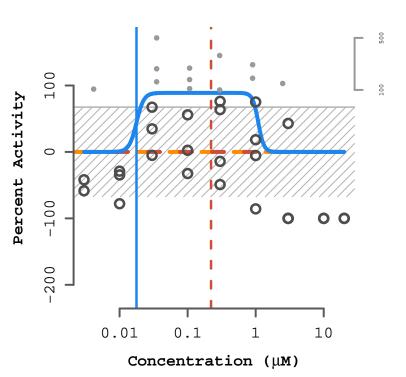
tр ga gw la lw val: 105 0.126 0.69 1.23 133 0.606 37.9 1.31 sd: 1.01

CNST HILL GNLS
AIC: 215.35 215.03 215.19
PROB: 0.31 0.36 0.33
RMSE: 38.6 32.17 29.2

MAX\_MEAN: 57.4 MAX\_MED: 78.6 BMAD: 22.5

COFF: 67.5 HIT-CALL: 1 FITC: 38 ACTP: 0.69

FLAGS: 16; 11; 7



NAME: Simvastatin

CHID: 23581 CASRN: 79902-63-9

SPID(S): TP0001649C08 M4ID: 30230063 BRK

HILL MODEL (in red):

tp ga gw val: 2.84e-05 -0.656 0.31 sd: NaN NaN NaN

GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 88.9 -1.75 0.0383 10.5 28.8 0.308 10.3 0.538 sd: 144

CNST HILL GNLS
AIC: 536.49 542.49 535.25
PROB: 0.34 0.02 0.64
RMSE: 147.83 147.83 123.37

MAX\_MEAN: 171 MAX\_MED: 117 BMAD: 22.5

COFF: 67.5 HIT-CALL: 1 FITC: 50 ACTP: 0.66

FLAGS: 16; 11; 10