

NAME: DMSO (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO

M4ID: 30230043 BRK

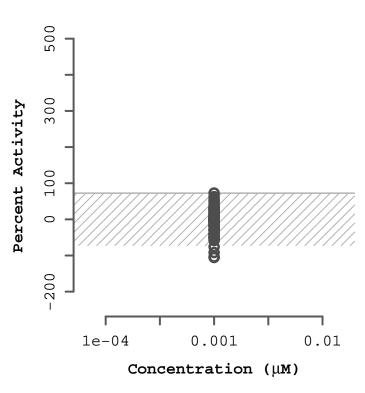
HILL MODEL: Not applicable.

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: 30230044

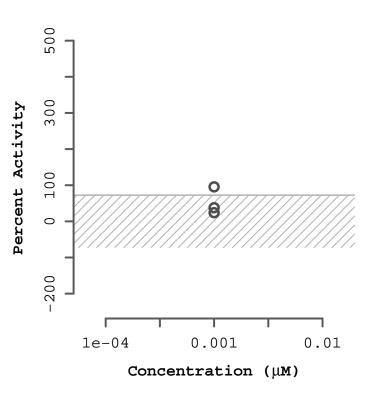
HILL MODEL: Not applicable.

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: 30230045

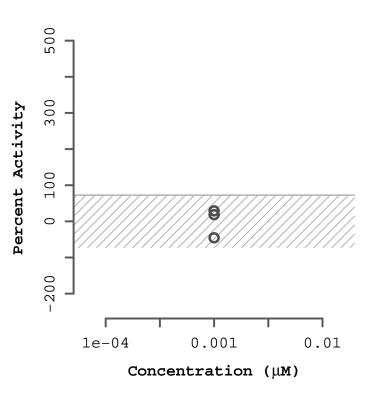
HILL MODEL: Not applicable.

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: 30230046

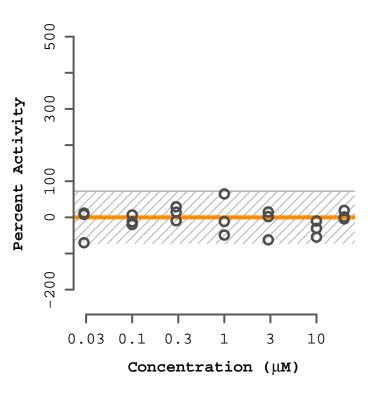
HILL MODEL: Not applicable.

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: 30230054

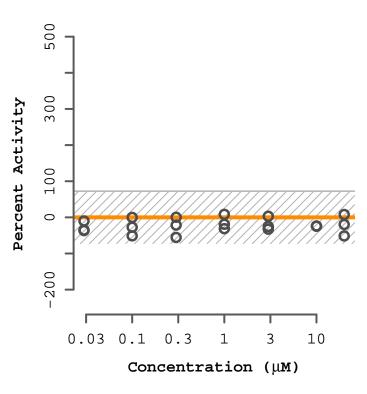
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 11.5 MAX_MED: 14.5 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: 30230058

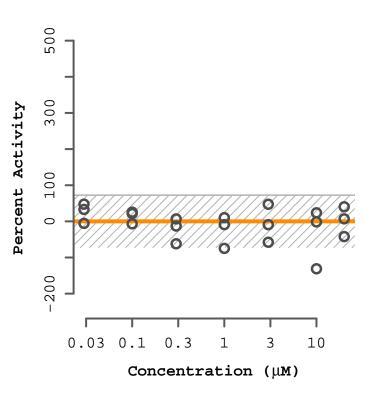
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: -13.9 MAX_MED: -19 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: 30230053

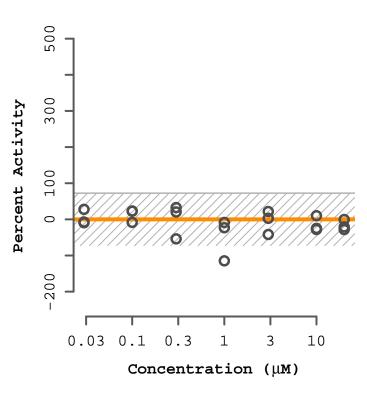
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 25.1 MAX_MED: 33.1 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: 30230055

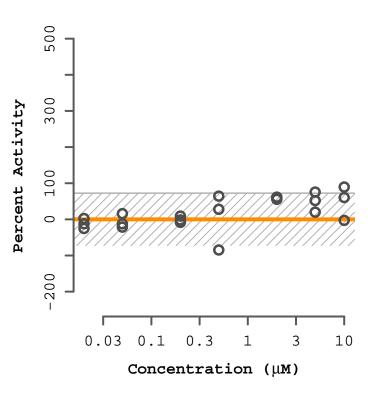
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 12.5 MAX_MED: 22.5 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: 30230056

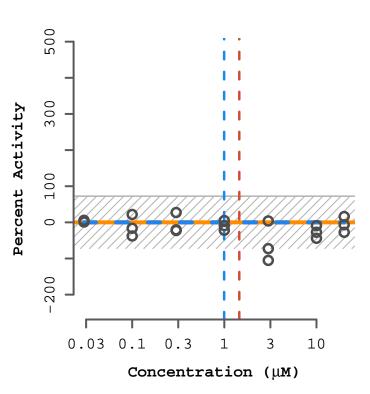
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX_MEAN: 58.7 MAX_MED: 60.4 BMAD: 24.2

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



NAME: Chlorendic acid

CHID: 20268 CASRN: 115-28-6

SPID(S): TP0001649F01 M4ID: 30230057

HILL MODEL (in red):

tp ga gw val: 3.6e-10 0.162 1.78 sd: 0.00069 25000 331000

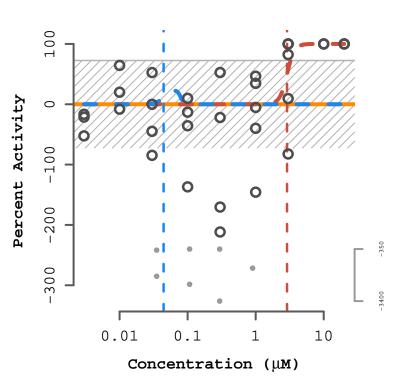
GAIN-LOSS MODEL (in blue):

tр ga gw la lw 5.5e-08 -0.002 2.09 0.258 5.31 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 206.49 212.49 216.49
PROB: 0.95 0.05 0.01
RMSE: 34.26 34.26 34.26

MAX_MEAN: 2.73 MAX_MED: 1.24 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 7 ACTP: 0.05



NAME: Lovastatin

CHID: 20784 CASRN: 75330-75-5

SPID(S): TP0001649D08 M4ID: 30230051 BRK

HILL MODEL (in red):

tp ga gw val: 100 0.461 8 sd: 42.1 0.171 63.8

GAIN-LOSS MODEL (in blue):

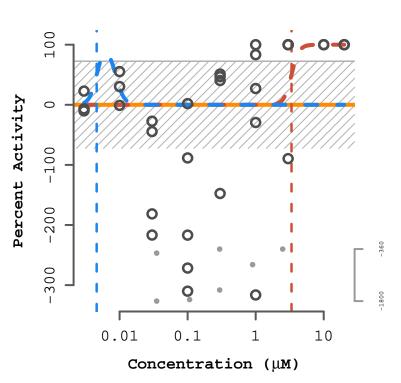
tр ga gw la lw val: 24.1 -1.35 -1.1 18 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 611.28 611.82 621.33
PROB: 0.56 0.43 0
RMSE: 750 748.8 750.11

MAX_MEAN: 100 MAX_MED: 100 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 10 ACTP: 0.44

FLAGS: 8; 10



NAME: Simvastatin

CHID: 23581 CASRN: 79902-63-9

SPID(S): TP0001649C08 M4ID: 30230047 BRK

HILL MODEL (in red):

tp ga gw val: 100 0.527 7.94 sd: 61.9 0.986 153

GAIN-LOSS MODEL (in blue):

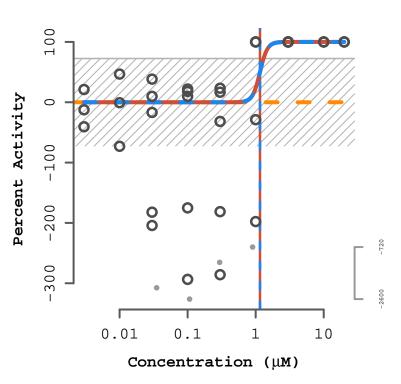
tр ga gw la lw val: 101 -2.34 8 -2.06 7.04 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 607.78 611.35 617.69
PROB: 0.85 0.14 0.01
RMSE: 505.86 504.64 505.81

MAX_MEAN: 100 MAX_MED: 100 BMAD: 24.2

COFF: 72.5 HIT-CALL: 0 FITC: 10 ACTP: 0.15

FLAGS: 10; 8



NAME: Mercuric chloride

CHID: 20811 CASRN: 7487-94-7

SPID(S): TP0001649C11 M4ID: 30230049 BRK

HILL MODEL (in red):

tp ga gw val: 100 0.0633 8 sd: 26.1 0.843 104

GAIN-LOSS MODEL (in blue):

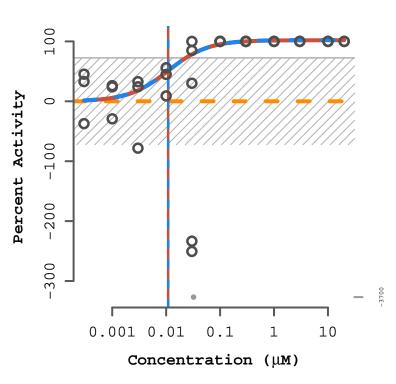
tр ga gw la lw val: 100 0.0635 2.96 3.17 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 594.62 590.91 594.91
PROB: 0.12 0.77 0.1
RMSE: 583.37 581.61 581.61

MAX_MEAN: 100 MAX_MED: 100 BMAD: 24.2

COFF: 72.5 HIT-CALL: 1 FITC: 41 ACTP: 0.88

FLAGS: 10; 11



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

SPID(S): TP0001649D11 M4ID: 30230052 BRK

HILL MODEL (in red):

tp ga gw val: 102 -1.96 1.19 sd: 3.88 0.151 0.404

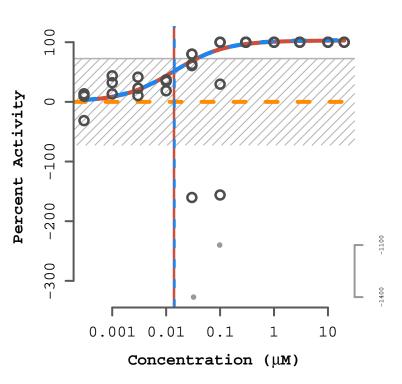
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 102 -1.96 1.17 1.39 17.8 4.38 0.151 0.403 0.24 sd: 46

CNST HILL GNLS
AIC: 25718.4 463.68 467.62
PROB: 0 0.88 0.12
RMSE: 574.26 582.74 582.71

MAX_MEAN: 100 MAX_MED: 100 BMAD: 24.2

COFF: 72.5 HIT-CALL: 1 FITC: 41 ACTP: 1



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

SPID(S): TP0001649D04 M4ID: 30230050 BRK

HILL MODEL (in red):

tp ga gw val: 103 -1.85 0.911 sd: 3.88 0.123 0.247

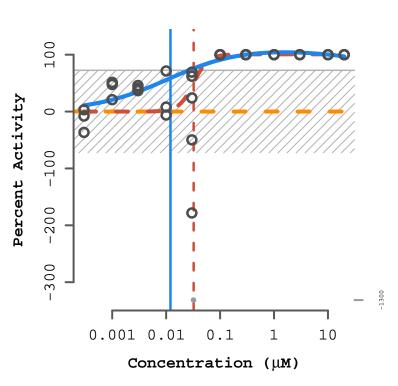
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 104 -1.85 0.888 1.44 10.6 4.58 0.124 0.245 0.742 57.8 sd:

CNST HILL GNLS
AIC: 539.47 465.13 468.97
PROB: 0 0.87 0.13
RMSE: 283.4 292.68 292.64

MAX_MEAN: 100 MAX_MED: 100 BMAD: 24.2

COFF: 72.5 HIT-CALL: 1 FITC: 41 ACTP: 1



NAME: Tributyltin chloride

CHID: 27403 CASRN: 1461-22-9

SPID(S): TP0001649C09 M4ID: 30230048 BRK

HILL MODEL (in red):

tp ga gw val: 101 -1.49 3.22 sd: 3.74 0.0921 2.75

GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 120 -1.92 0.624 3.3 0.324 55.1 0.544 0.176 2.08 0.752 sd:

CNST HILL GNLS
AIC: 25631.41 439.05 438.14
PROB: 0 0.39 0.61
RMSE: 216.92 210.93 216.46

MAX_MEAN: 100 MAX_MED: 100 BMAD: 24.2

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