

NAME: DMSO (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO

M4ID: 30230107 BRK

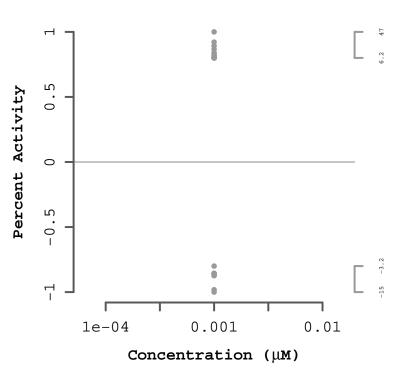
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: -2.45 MAX\_MED: 0 BMAD: 0

COFF: 0 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Water (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Water

M4ID: 30230108 BRK

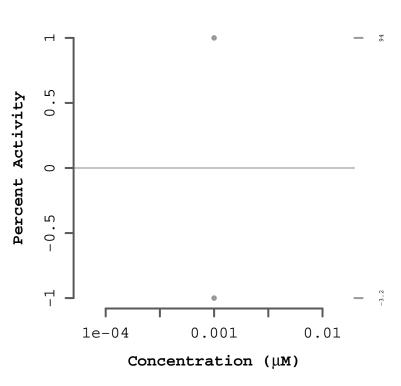
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 1.29 MAX\_MED: 0 BMAD: 0

COFF: 0 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: DMSO/Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO/Ethanol M4ID: 30230109 BRK

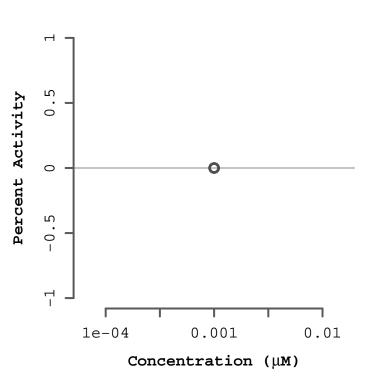
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 30.2 MAX\_MED: 0 BMAD: 0

COFF: 0 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Ethanol (spid not in DB)

CHID: NA CASRN: NA

SPID(S): Ethanol M4ID: 30230110

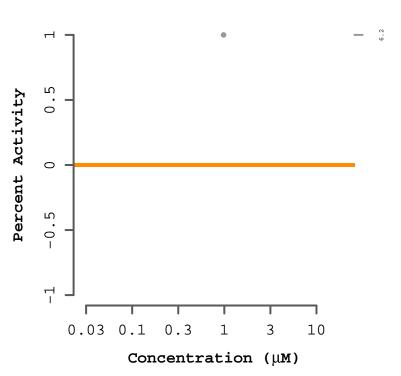
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 0 MAX\_MED: 0 BMAD: 0

COFF: 0 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Chlorendic acid

CHID: 20268 CASRN: 115-28-6

SPID(S): TP0001649F01 M4ID: 30230121 BRK

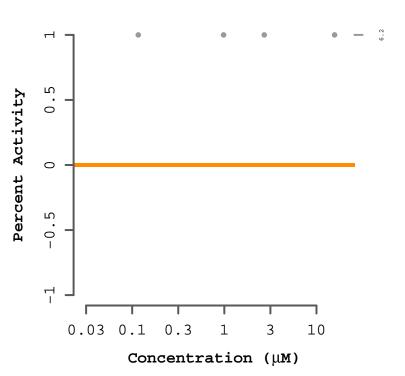
HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

CNST HILL GNLS
AIC: -2367.26 NA NA
PROB: 1 NA NA
RMSE: 1.36 NA NA

MAX\_MEAN: 2.08 MAX\_MED: 0 BMAD: 0

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



NAME: Triphenyl phosphite

CHID: 26252 CASRN: 101-02-0

SPID(S): TP0001649E09 M4ID: 30230118 BRK

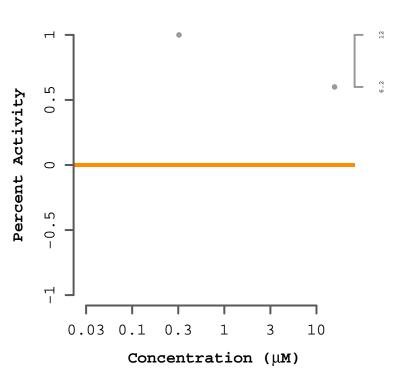
HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

CNST HILL GNLS
AIC: -62.59 NA NA
PROB: 1 NA NA
RMSE: 2.73 NA NA

MAX\_MEAN: 2.08 MAX\_MED: 0 BMAD: 0

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



NAME: Clothianidin

CHID: 34465 CASRN: 210880-92-5

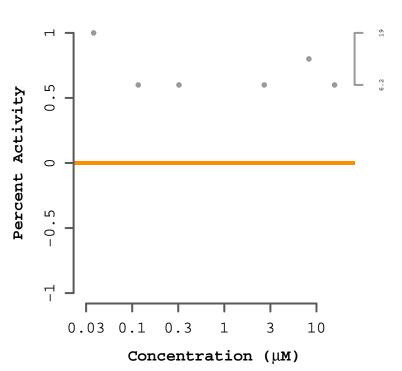
SPID(S): TP0001649F07 M4ID: 30230122 BRK

HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

CNST HILL GNLS
AIC: -1592.1 NA NA
PROB: 1 NA NA
RMSE: 3.05 NA NA

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



NAME: Thiacloprid

CHID: 34961 CASRN: 111988-49-9

SPID(S): TP0001649E07 M4ID: 30230117 BRK

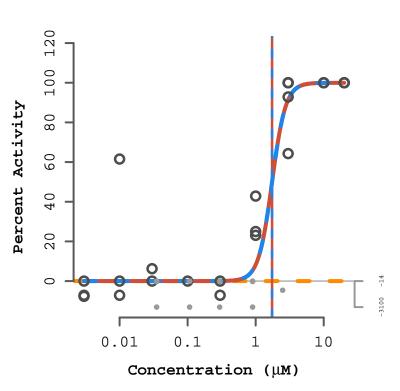
HILL MODEL: Failed to converge.

GAIN-LOSS MODEL: Failed to converge.

CNST HILL GNLS
AIC: 1419.77 NA NA
PROB: 1 NA NA
RMSE: 5.62 NA NA

MAX\_MEAN: 6.25 MAX\_MED: 0 BMAD: 0

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



NAME: Lovastatin

CHID: 20784 CASRN: 75330-75-5

SPID(S): TP0001649D08 M4ID: 30230115 BRK

HILL MODEL (in red):

tp ga gw val: 100 0.241 4.34 sd: 12.8 0.176 2.94

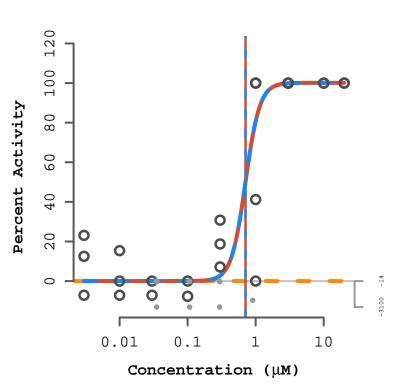
GAIN-LOSS MODEL (in blue):

tр ga gw la lw 0.241 val: 100 4.34 2.47 5.01 12.8 0.176 2.94 1510 6400 sd:

CNST HILL GNLS
AIC: 612.53 591.13 595.13
PROB: 0 0.88 0.12
RMSE: 973.23 975.18 975.18

MAX\_MEAN: 100 MAX\_MED: 100 BMAD: 0

COFF: 0 HIT-CALL: 1 FITC: 41 ACTP: 1



NAME: Mercuric chloride

CHID: 20811 CASRN: 7487-94-7

SPID(S): TP0001649C11 M4ID: 30230113 BRK

HILL MODEL (in red):

tp ga gw val: 100 -0.149 4.15 sd: 7 0.176 4.21

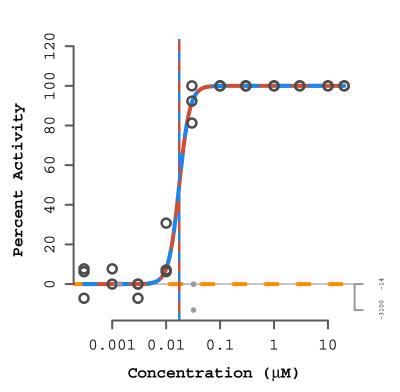
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 100 -0.1494.15 2.32 12.5 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 596.81 558.41 562.41
PROB: 0 0.88 0.12
RMSE: 903.61 906.93 906.93

MAX\_MEAN: 100 MAX\_MED: 100 BMAD: 0

COFF: 0 HIT-CALL: 1 FITC: 41 ACTP: 1



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

SPID(S): TP0001649D11 M4ID: 30230116 BRK

HILL MODEL (in red):

tp ga gw val: 100 -1.76 4.42 sd: 0.677 0.0296 0.557

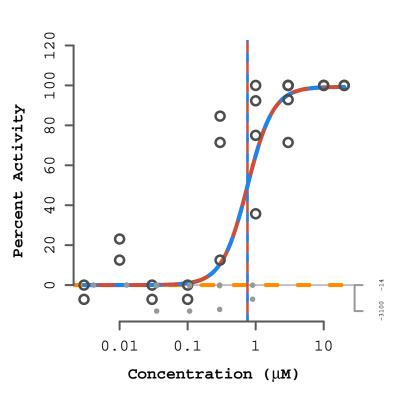
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 100 -1.76 4.42 1.52 17.9 0.837 0.0298 0.559 14.4 716 sd:

CNST HILL GNLS
AIC: 23330.97 362.55 366.55
PROB: 0 0.88 0.12
RMSE: 484.98 493.19 493.19

MAX\_MEAN: 100 MAX\_MED: 100 BMAD: 0

COFF: 0 HIT-CALL: 1 FITC: 41 ACTP: 1



NAME: Simvastatin

CHID: 23581 CASRN: 79902-63-9

SPID(S): TP0001649C08 M4ID: 30230111 BRK

HILL MODEL (in red):

tp ga gw val: 99.3 -0.12 2.29 sd: 11.7 0.183 1.48

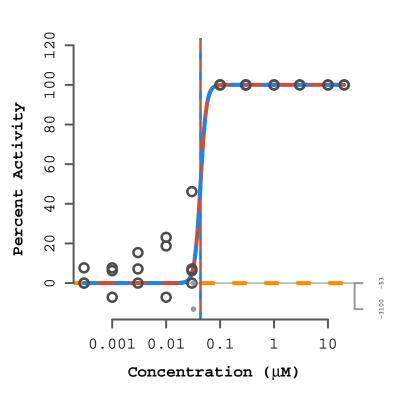
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 99.3 -0.12 2.29 3.15 12.8 sd: NA NA NA NA NA

CNST HILL GNLS
AIC: 594.04 567.62 571.62
PROB: 0 0.88 0.12
RMSE: 854.94 857.23 857.23

MAX\_MEAN: 100 MAX\_MED: 100 BMAD: 0

COFF: 0 HIT-CALL: 1 FITC: 41 ACTP: 1



NAME: Tributyltin chloride CHID: 27403 CASRN: 1461-22-9

SPID(S): TP0001649C09 M4ID: 30230112 BRK

HILL MODEL (in red):

tp ga gw val: 100 -1.36 8 sd: 0.926 0.293 14.5

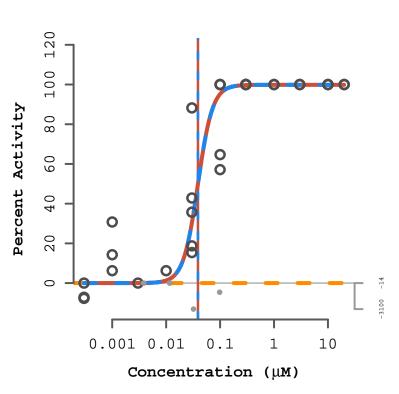
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 100 -1.36 3.17 1.76 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 22546.88 350.99 354.99
PROB: 0 0.88 0.12
RMSE: 484.44 479.27 479.27

MAX\_MEAN: 100 MAX\_MED: 100 BMAD: 0

COFF: 0 HIT-CALL: 1 FITC: 41 ACTP: 1



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

SPID(S): TP0001649D04 M4ID: 30230114 BRK

HILL MODEL (in red):

tp ga gw val: 99.8 -1.41 3.2 sd: 2.18 0.0623 1.2

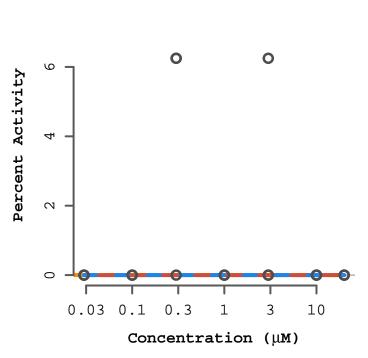
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 99.8 -1.41 3.2 2.52 11.3 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 542.79 426.21 430.21
PROB: 0 0.88 0.12
RMSE: 512.95 517.23 517.23

MAX\_MEAN: 100 MAX\_MED: 100 BMAD: 0

COFF: 0 HIT-CALL: 1 FITC: 41 ACTP: 1



NAME: Thiamethoxam

CHID: 34962 CASRN: 153719-23-4

SPID(S): TP0001649E10 M4ID: 30230119

HILL MODEL (in red):

tp ga gw val: 0 1.66 7.75 sd: NA NA NA

GAIN-LOSS MODEL (in blue):

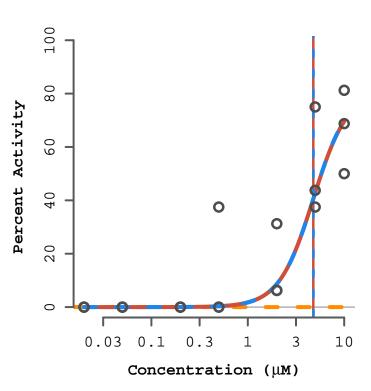
tр ga gw la lw val: 5.9 -2.52 0.3 -2.27 18 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: -830.81 -4095.4 -267.44
PROB: 0 1 0
RMSE: 2.36 2.36 2.36

MAX\_MEAN: 4.17 MAX\_MED: 6.25 BMAD: 0

COFF: 0 HIT-CALL: 1 FITC: 42 ACTP: 1

FLAGS: 17; 10



NAME: Pravastatin sodium

CHID: 47525 CASRN: 81131-70-6

SPID(S): TP0001649E12 M4ID: 30230120

HILL MODEL (in red):

tp ga gw val: 81.1 0.68 2.43 sd: 14.9 0.0889 0.768

GAIN-LOSS MODEL (in blue):

tр ga gw la lw 0.682 val: 81.6 2.43 1.13 17.5 sd: NaN NaN NaN NaN NaN

CNST HILL GNLS
AIC: 4481.4 165.44 169.44
PROB: 0 0.88 0.12
RMSE: 34.66 12.89 12.89

MAX\_MEAN: 66.7 MAX\_MED: 68.8 BMAD: 0

COFF: 0 HIT-CALL: 1 FITC: 42 ACTP: 1