

NAME: DMSO (spid not in DB)

CHID: NA CASRN: NA

SPID(S): DMSO

M4ID: 30230014 BRK

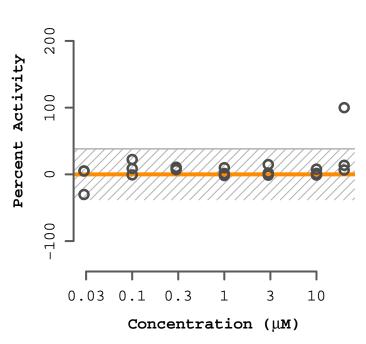
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: -17.4 MAX\_MED: -5.94e-15 BMAD: 12.8

COFF: 38.3 HIT-CALL: -1 FITC: 2 ACTP: NA



NAME: Chlorendic acid

CHID: 20268 CASRN: 115-28-6

SPID(S): TP0001649F01 M4ID: 30230025

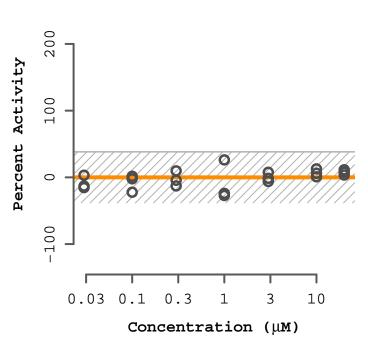
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 40 MAX\_MED: 13.6 BMAD: 12.8

COFF: 38.3 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Triphenyl phosphite

CHID: 26252 CASRN: 101-02-0

SPID(S): TP0001649E09 M4ID: 30230022

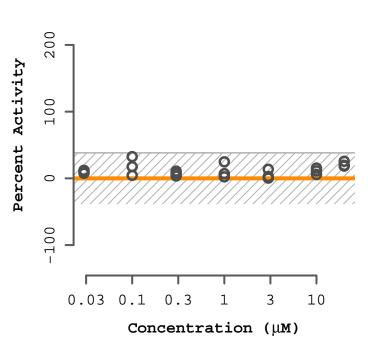
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 7.54 MAX\_MED: 7.67 BMAD: 12.8

COFF: 38.3 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Clothianidin

CHID: 34465 CASRN: 210880-92-5

SPID(S): TP0001649F07 M4ID: 30230026

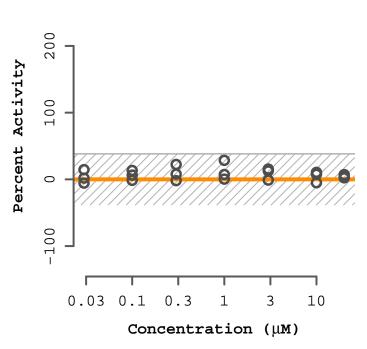
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 21.2 MAX\_MED: 19.5 BMAD: 12.8

COFF: 38.3 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Thiacloprid

CHID: 34961 CASRN: 111988-49-9

SPID(S): TP0001649E07 M4ID: 30230021

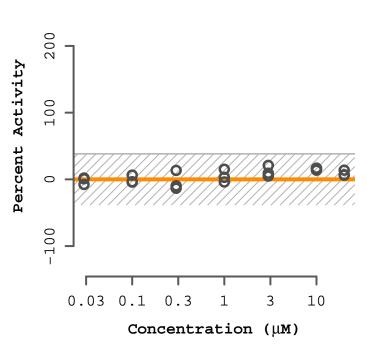
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 12.1 MAX\_MED: 12.6 BMAD: 12.8

COFF: 38.3 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Thiamethoxam

CHID: 34962 CASRN: 153719-23-4

SPID(S): TP0001649E10 M4ID: 30230023

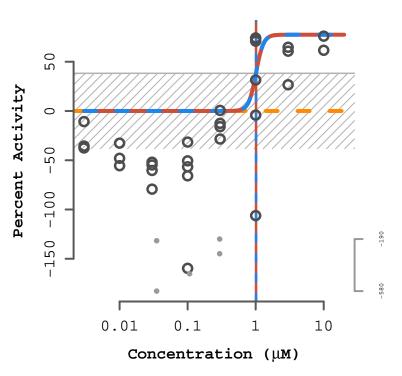
HILL MODEL: Not applicable.

GAIN-LOSS MODEL: Not applicable.

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

MAX\_MEAN: 15.7 MAX\_MED: 16.5 BMAD: 12.8

COFF: 38.3 HIT-CALL: 0 FITC: 4 ACTP: 0



NAME: Lovastatin

CHID: 20784 CASRN: 75330-75-5

SPID(S): TP0001649D08 M4ID: 30230019 BRK

## HILL MODEL (in red):

tp ga gw val: 77.4 0.00554 8 sd: 15.6 0.0946 72.2

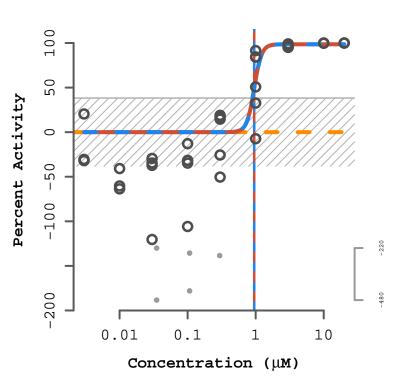
## GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 77.4 0.00557 8 1.83 15.6 15.6 0.095 72.4 34600 sd: 1180

CNST HILL GNLS
AIC: 521.63 511.5 515.5
PROB: 0.01 0.88 0.12
RMSE: 144.82 138.69 138.69

MAX\_MEAN: 89.8 MAX\_MED: 85.7 BMAD: 12.8

COFF: 38.3 HIT-CALL: 1 FITC: 41 ACTP: 0.99



NAME: Mercuric chloride

CHID: 20811 CASRN: 7487-94-7

SPID(S): TP0001649C11 M4ID: 30230017 BRK

HILL MODEL (in red):

tp ga gw val: 98.6 -0.0214 8 sd: 12 0.163 58.7

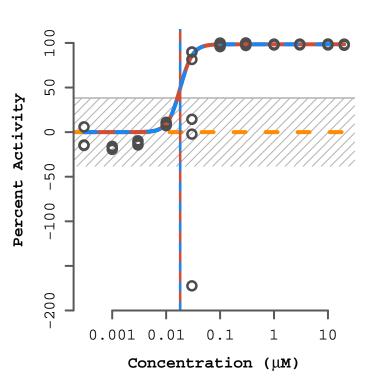
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 98.6 -0.0214 8 2.14 8.59 0.164 59.1 1250 12700 sd: 12

CNST HILL GNLS
AIC: 524.07 500.15 504.15
PROB: 0 0.88 0.12
RMSE: 136.93 124.62 124.62

MAX\_MEAN: 100 MAX\_MED: 100 BMAD: 12.8

COFF: 38.3 HIT-CALL: 1 FITC: 41 ACTP: 1



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

SPID(S): TP0001649D11 M4ID: 30230020

HILL MODEL (in red):

tp ga gw val: 98.5 -1.74 3.78 sd: 1.13 0.0302 0.464

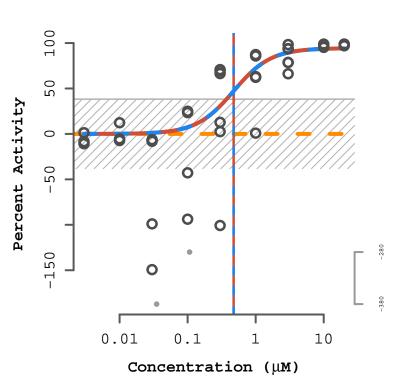
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 98.5 -1.74 3.78 3.19 12.4 sd: NA NA NA NA NA

CNST HILL GNLS
AIC: 586.6 350.72 354.72
PROB: 0 0.88 0.12
RMSE: 82.74 43.98 43.98

MAX\_MEAN: 98.9 MAX\_MED: 99.2 BMAD: 12.8

COFF: 38.3 HIT-CALL: 1 FITC: 41 ACTP: 1



NAME: Simvastatin

CHID: 23581 CASRN: 79902-63-9

SPID(S): TP0001649C08 M4ID: 30230015 BRK

HILL MODEL (in red):

tp ga gw val: 94.3 -0.324 1.59 sd: 10.4 0.194 0.682

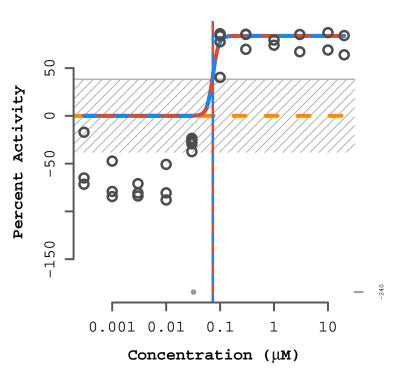
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 94.3 -0.324 1.59 1.9 18 10.4 0.194 0.682 12700 381000 sd:

CNST HILL GNLS
AIC: 502.19 460.79 464.79
PROB: 0 0.88 0.12
RMSE: 100.92 85.66 85.66

MAX MEAN: 98.2 MAX MED: 98.6 BMAD: 12.8

COFF: 38.3 HIT-CALL: 1 FITC: 41 ACTP: 1



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

SPID(S): TP0001649C09 M4ID: 30230016 BRK

HILL MODEL (in red):

tp ga gw val: 83.7 -1.13 8 sd: 7.22 0.169 8.48

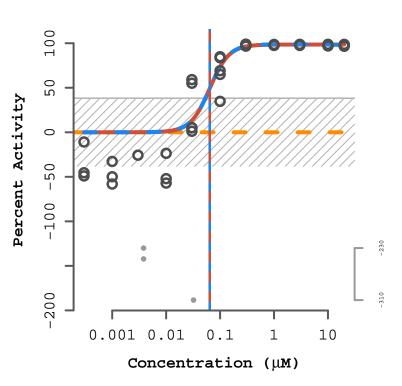
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 83.7 -1.13 8 2.34 14.9 sd: NA NA NA NA NA

CNST HILL GNLS
AIC: 497.92 449.88 453.88
PROB: 0 0.88 0.12
RMSE: 82.78 55.1 55.1

MAX\_MEAN: 89.1 MAX\_MED: 91.4 BMAD: 12.8

COFF: 38.3 HIT-CALL: 1 FITC: 41 ACTP: 1



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

SPID(S): TP0001649D04 M4ID: 30230018 BRK

HILL MODEL (in red):

tp ga gw val: 98.5 -1.19 2.44 sd: 5.53 0.101 0.84

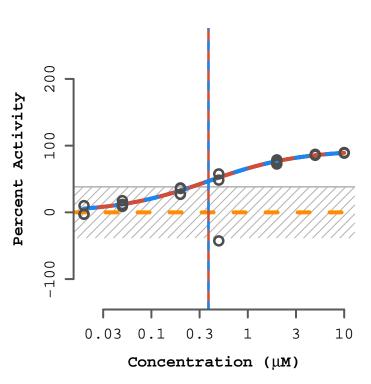
GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 98.8 -1.19 2.43 2.21 2.12 22.6 0.167 1.18 86.2 222 sd:

CNST HILL GNLS
AIC: 510.8 447.35 451.34
PROB: 0 0.88 0.12
RMSE: 102.48 76.4 76.41

MAX\_MEAN: 98.3 MAX\_MED: 98.6 BMAD: 12.8

COFF: 38.3 HIT-CALL: 1 FITC: 41 ACTP: 1



NAME: Pravastatin sodium

CHID: 47525 CASRN: 81131-70-6

SPID(S): TP0001649E12 M4ID: 30230024

HILL MODEL (in red):

tp ga gw val: 93.7 -0.408 0.924 sd: 3.35 0.0697 0.101

GAIN-LOSS MODEL (in blue):

tр ga gw la lw val: 93.7 -0.408 0.925 1.76 11.3 3.35 0.0697 0.101 1770 26200 sd:

CNST HILL GNLS
AIC: 236.44 152.23 156.23
PROB: 0 0.88 0.12
RMSE: 59.68 21.07 21.07

MAX\_MEAN: 89.3 MAX\_MED: 89.5 BMAD: 12.8

COFF: 38.3 HIT-CALL: 1 FITC: 41 ACTP: 1