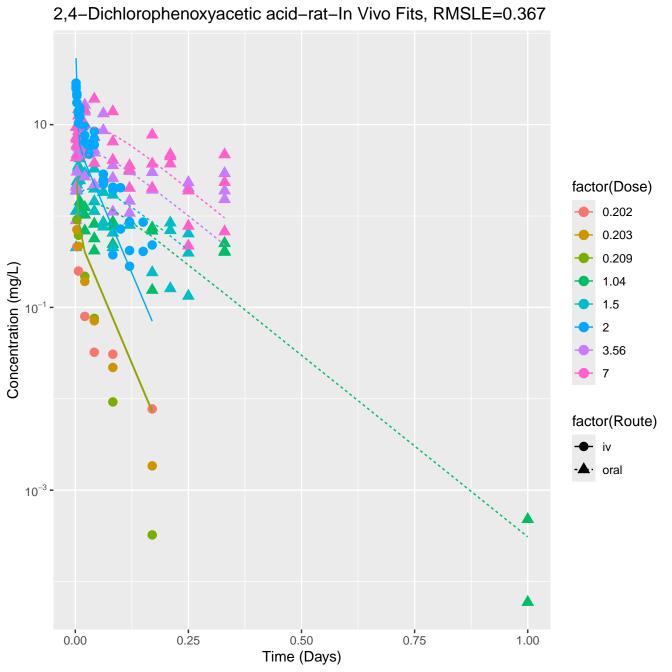
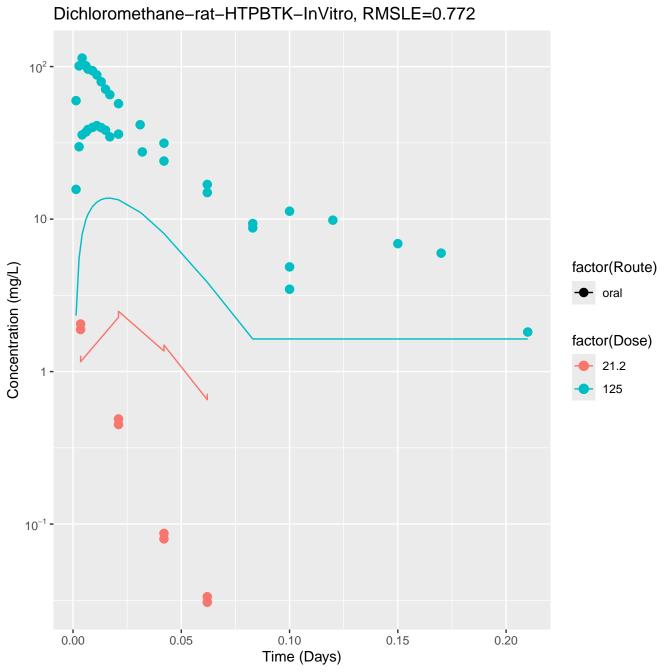
2,4-Dichlorophenoxyacetic acid-rat-HTPBTK-InVitro, RMSLE=0.76 10 factor(Dose) 0.202 0.203 0.209 Concentration (mg/L) 1.04 1.5 2 3.56 7 factor(Route) · oral 10<sup>-3</sup> -0.25 0.50 0.75 0.00 1.00 Time (Days)

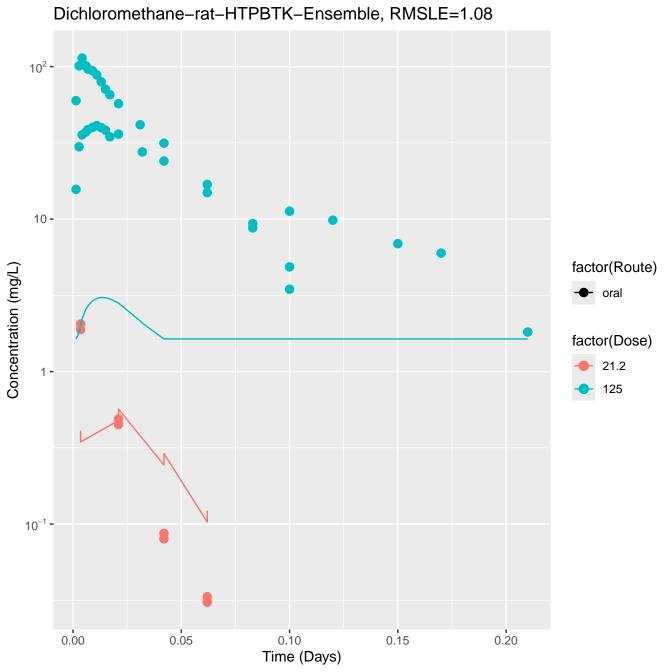
2,4-Dichlorophenoxyacetic acid-rat-HTPBTK-ADMET, RMSLE=1.99 10 factor(Dose) 0.202 0.203 0.209 Concentration (mg/L) 1.04 10<sup>-1</sup> 1.5 2 3.56 7 factor(Route) · oral 10<sup>-3</sup> -0.50 0.25 0.75 0.00 1.00 Time (Days)

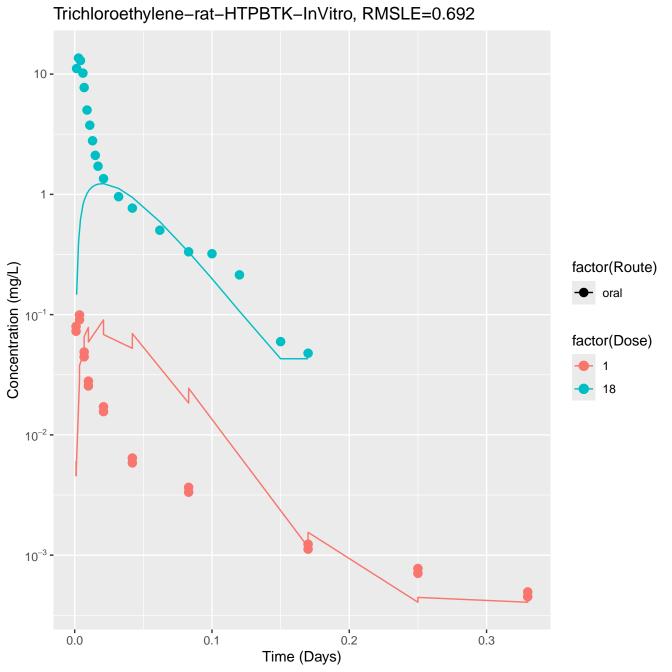
2,4-Dichlorophenoxyacetic acid-rat-HTPBTK-Pradeep, RMSLE=2.04 10 factor(Dose) 0.202 0.203 0.209 Concentration (mg/L) 1.04 10<sup>-1</sup> 1.5 2 3.56 7 factor(Route) · oral 10<sup>-3</sup> -0.50 0.25 0.75 0.00 1.00 Time (Days)

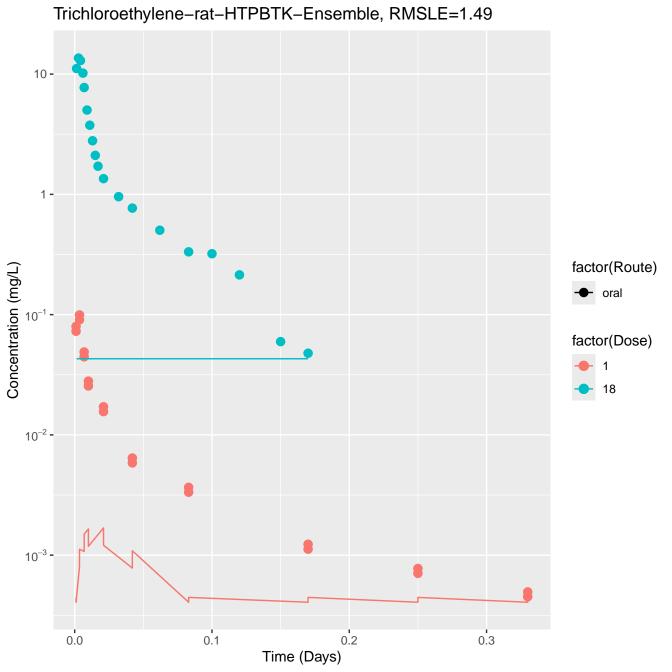
2,4-Dichlorophenoxyacetic acid-rat-HTPBTK-Ensemble, RMSLE=2.76 10 factor(Dose) 0.202 0.203 0.209 Concentration (mg/L) 1.04 10<sup>-1</sup> 1.5 2 3.56 7 factor(Route) · oral 10<sup>-3</sup> -0.25 0.50 0.75 0.00 1.00 Time (Days)





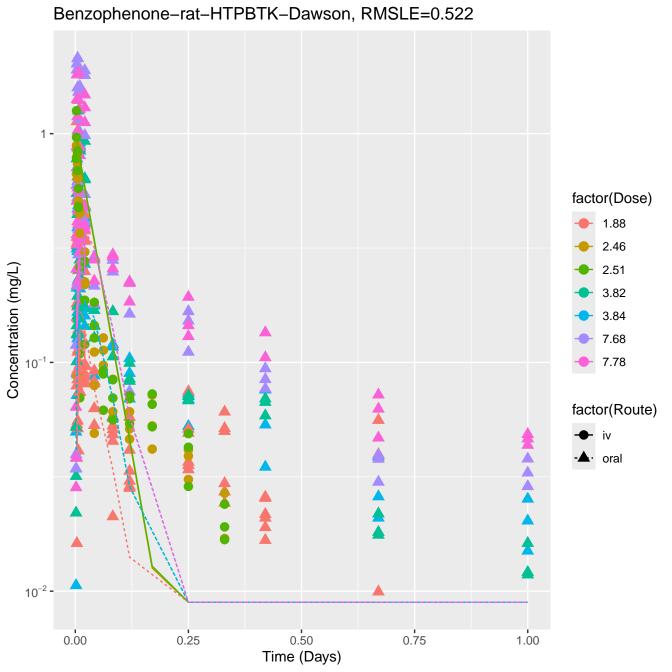


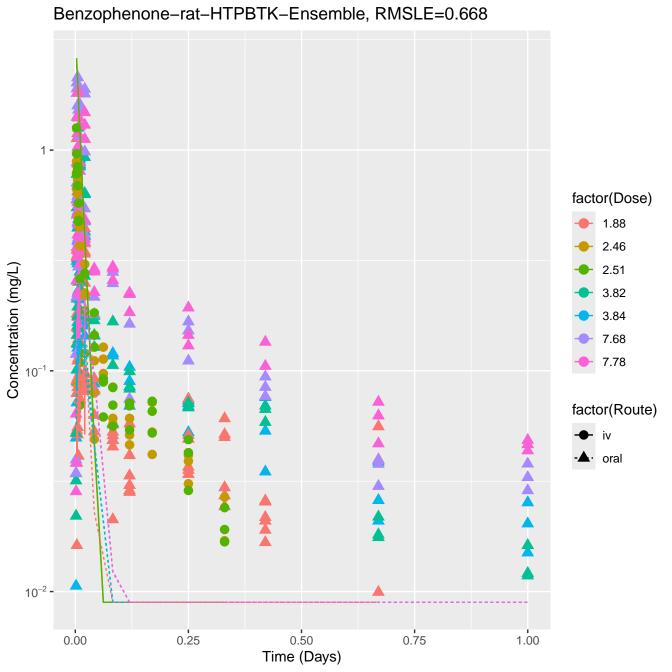




Benzophenone-rat-HTPBTK-InVitro, RMSLE=0.486 1 factor(Dose) 1.88 2.46 Concentration (mg/L) 2.51 3.82 3.84 7.68 10<sup>-1</sup> -7.78 factor(Route) iv · oral 10<sup>-2</sup> 0.25 0.50 0.75 0.00 1.00 Time (Days)

Benzophenone-rat-HTPBTK-ADMET, RMSLE=0.476 1 factor(Dose) 1.88 2.46 Concentration (mg/L) 2.51 3.82 3.84 7.68 10<sup>-1</sup> 7.78 factor(Route) iv · oral 10<sup>-2</sup> -0.25 0.50 0.75 0.00 1.00 Time (Days)





Benzophenone-rat-In Vivo Fits, RMSLE=0.321 1 factor(Dose) 1.88 2.46 Concentration (mg/L) 2.51 3.82 3.84 7.68 7.78 10<sup>-1</sup> factor(Route) ίV oral 10<sup>-2</sup> -0.25 0.50 0.75 0.00 1.00 Time (Days)

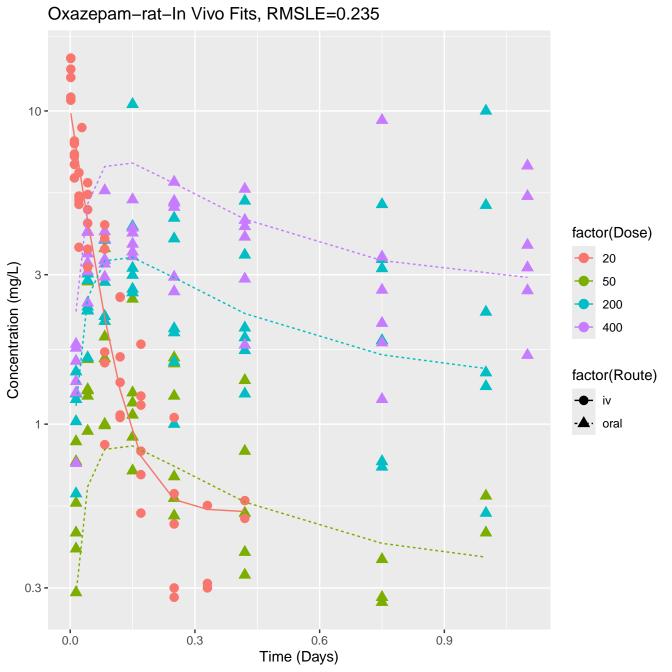
Oxazepam-rat-HTPBTK-InVitro, RMSLE=0.964 10<sup>2</sup> factor(Dose) 20 Concentration (mg/L) 50 200 400 factor(Route) · oral 1 -0.0 0.3 0.6 0.9 Time (Days)

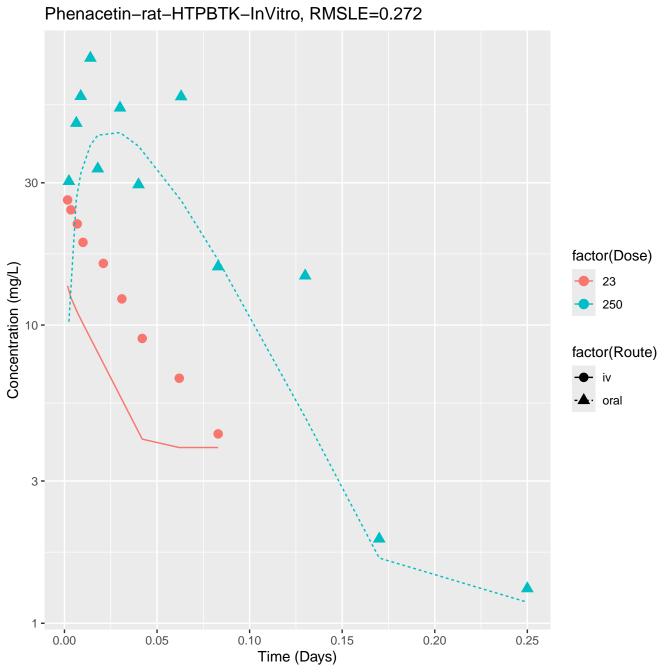
Oxazepam-rat-HTPBTK-ADMET, RMSLE=0.881 10<sup>2</sup> factor(Dose) 20 10 -Concentration (mg/L) 50 200 400 factor(Route) · oral 1 -0.0 0.3 0.6 0.9 Time (Days)

Oxazepam-rat-HTPBTK-Dawson, RMSLE=0.897 10<sup>2</sup> factor(Dose) 10 -20 Concentration (mg/L) 50 200 400 factor(Route) oral 1 -0.0 0.3 0.6 0.9 Time (Days)

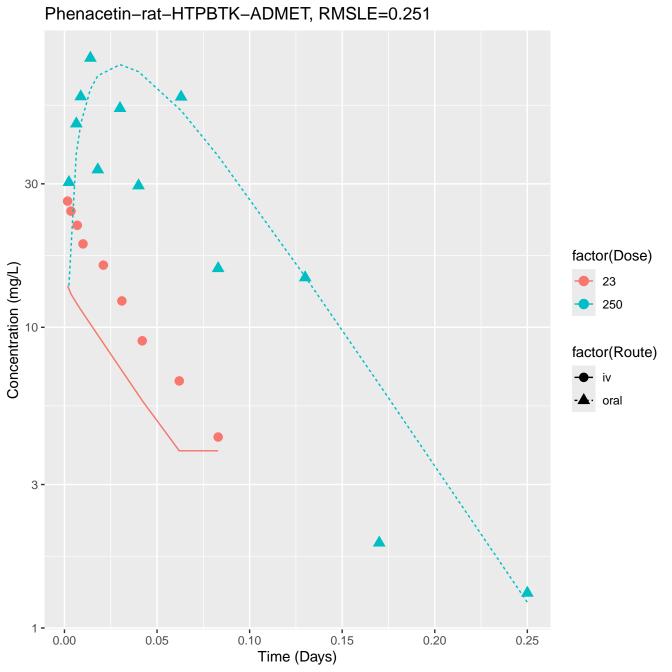
Oxazepam-rat-HTPBTK-Pradeep, RMSLE=0.914 10<sup>2</sup> factor(Dose) 20 Concentration (mg/L) 10 -50 200 400 factor(Route) · oral 1 -0.0 0.3 0.6 0.9 Time (Days)

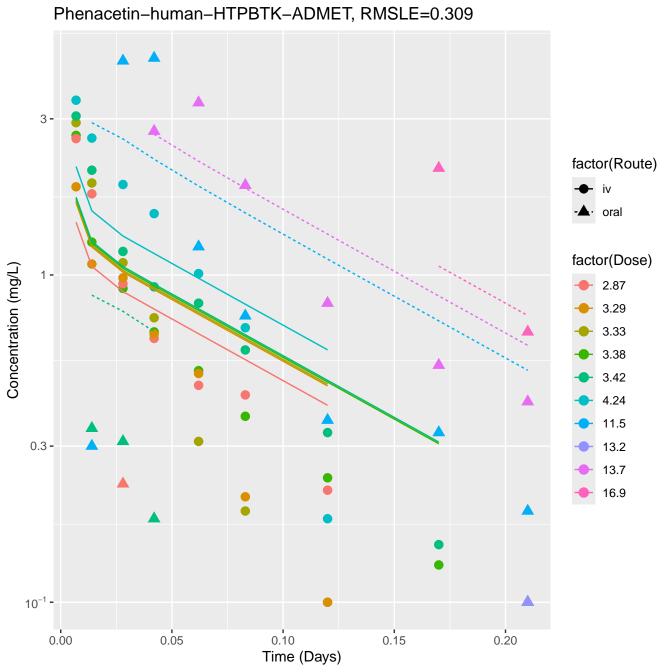
Oxazepam-rat-HTPBTK-Ensemble, RMSLE=0.849 30 -10factor(Dose) 20 Concentration (mg/L) 50 200 400 3 factor(Route) · oral 1 -0.3 -0.0 0.3 0.6 0.9 Time (Days)

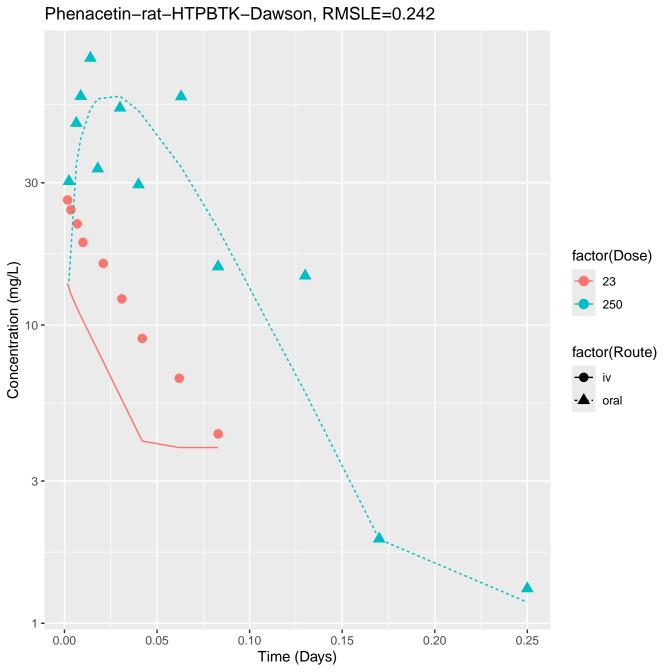


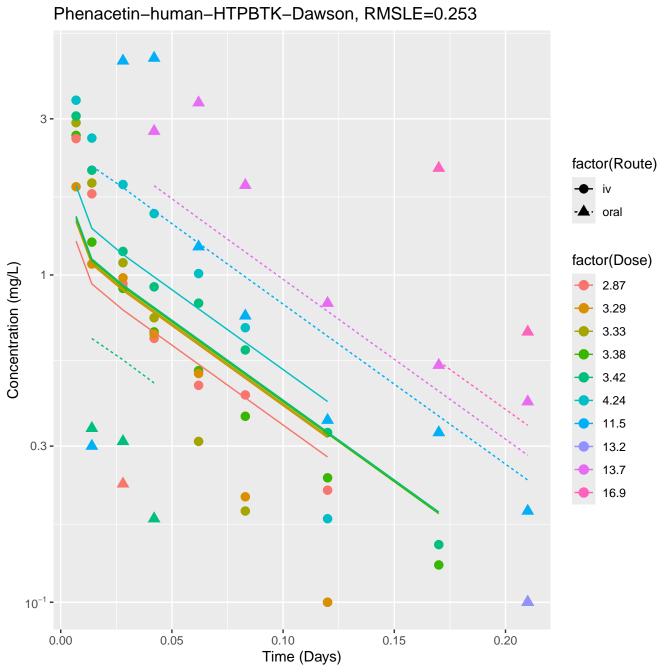


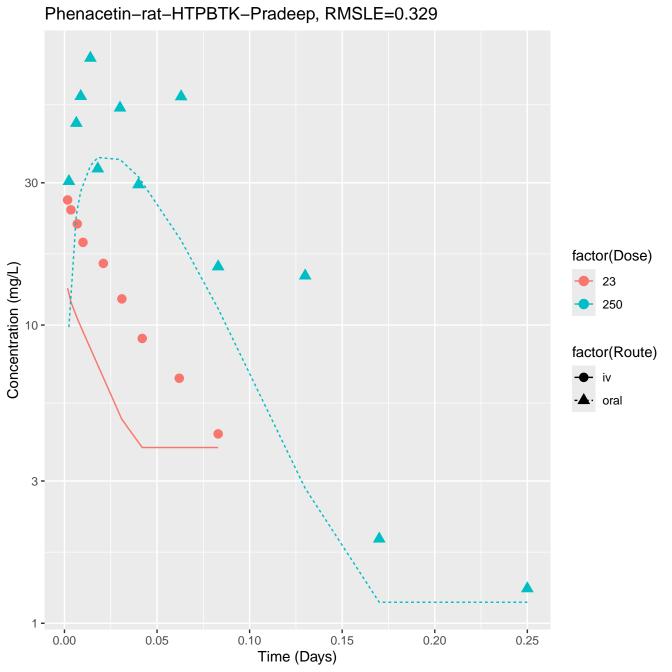
Phenacetin-human-HTPBTK-InVitro, RMSLE=0.26 3 factor(Route) oral factor(Dose) Concentration (mg/L) 2.87 3.29 3.33 3.38 3.42 4.24 11.5 0.3 -13.2 13.7 16.9 10<sup>-1</sup> -0.10 0.15 0.00 0.05 0.20 Time (Days)

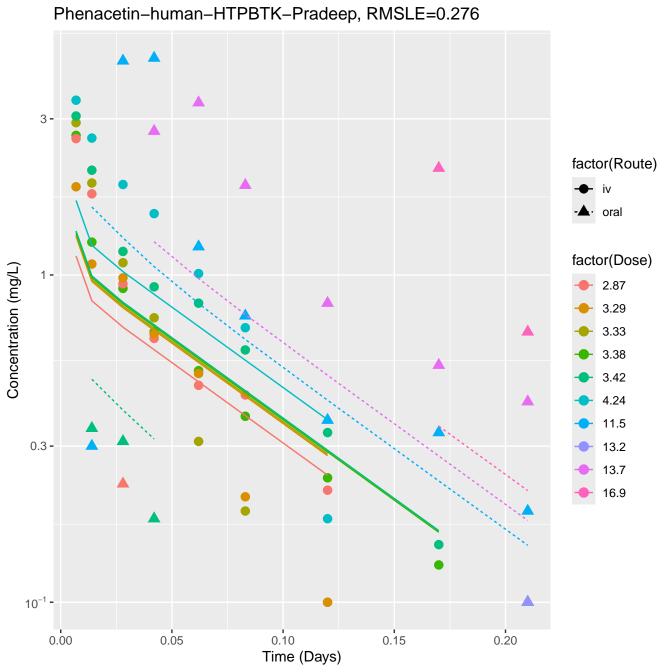


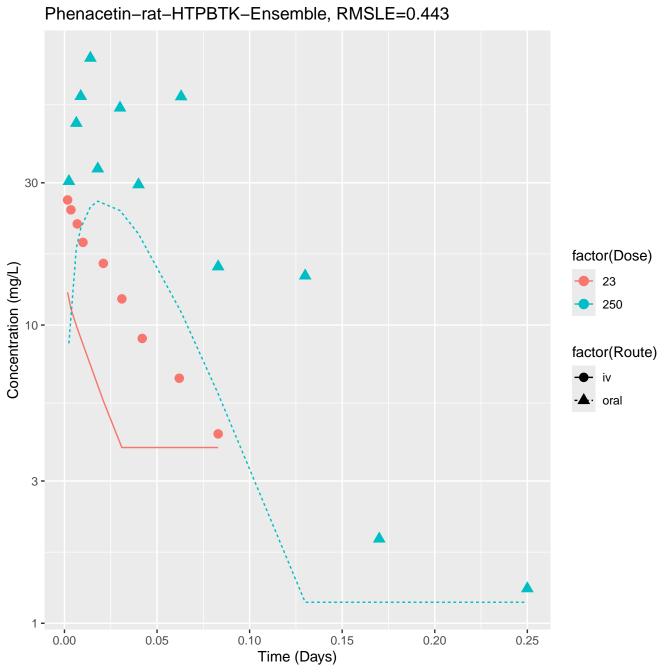




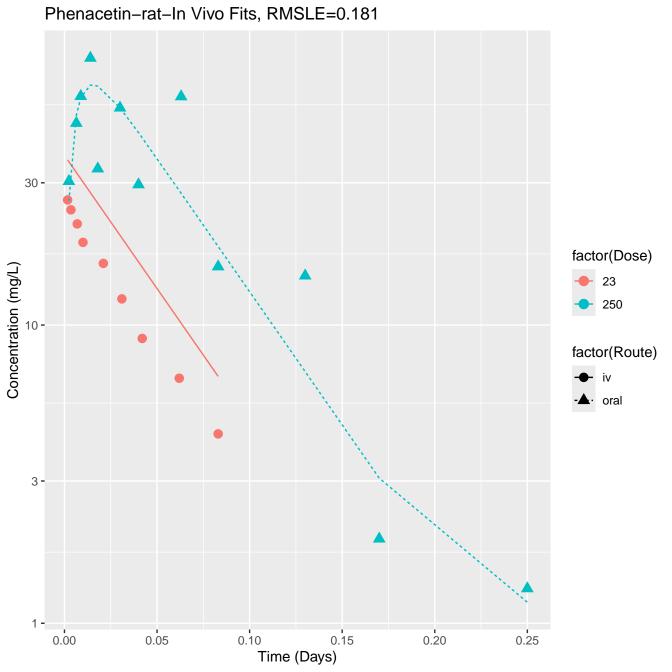




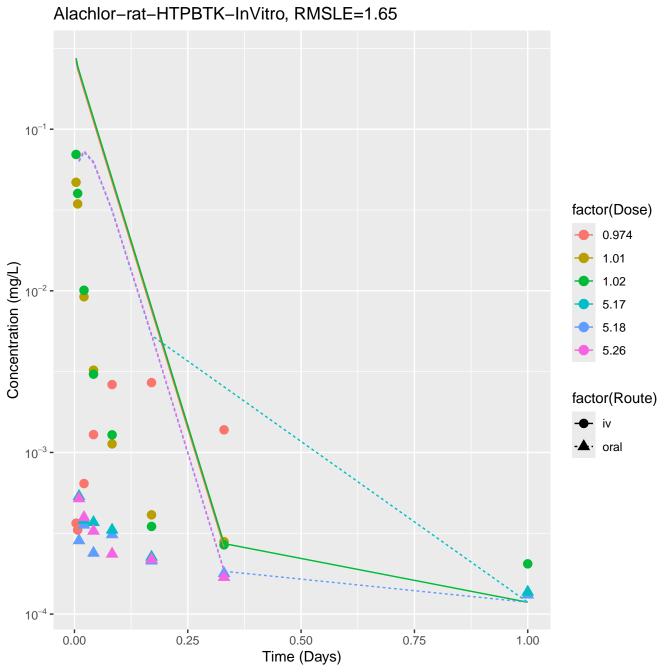


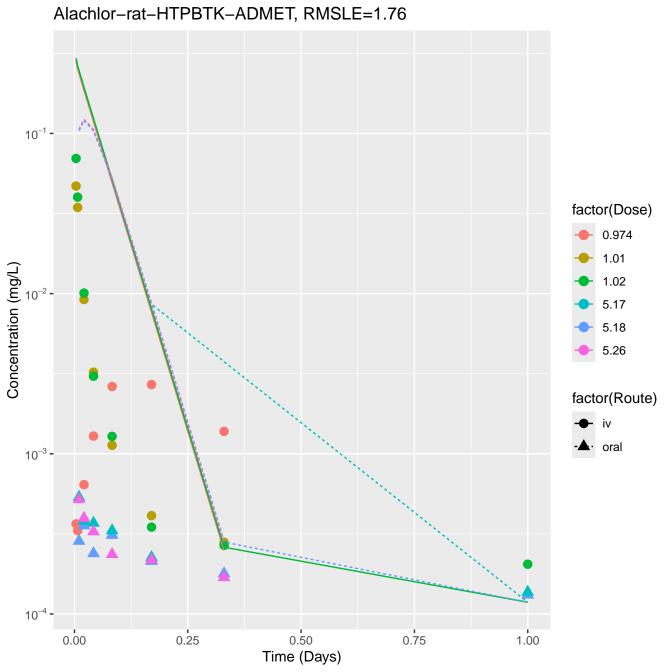


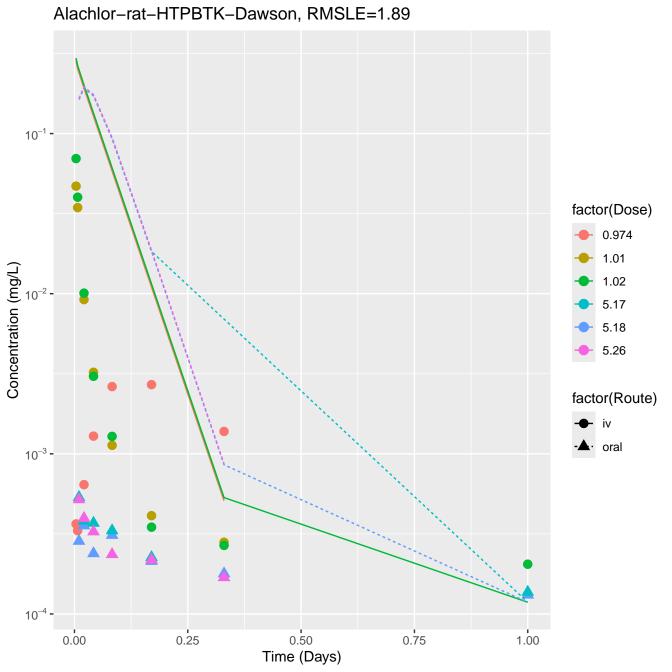
Phenacetin-human-HTPBTK-Ensemble, RMSLE=0.353 3 factor(Route) oral factor(Dose) Concentration (mg/L) 2.87 3.29 3.33 3.38 3.42 4.24 11.5 0.3 -13.2 13.7 16.9 10<sup>-1</sup> -0.10 0.15 0.00 0.05 0.20 Time (Days)

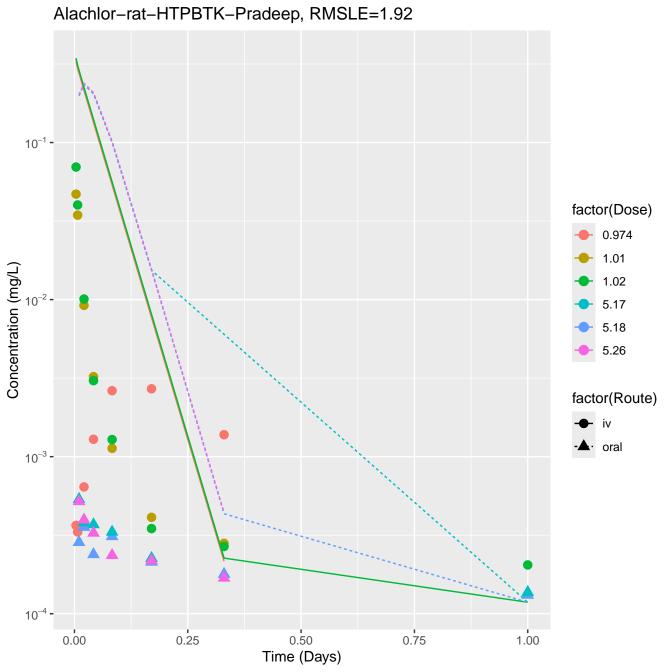


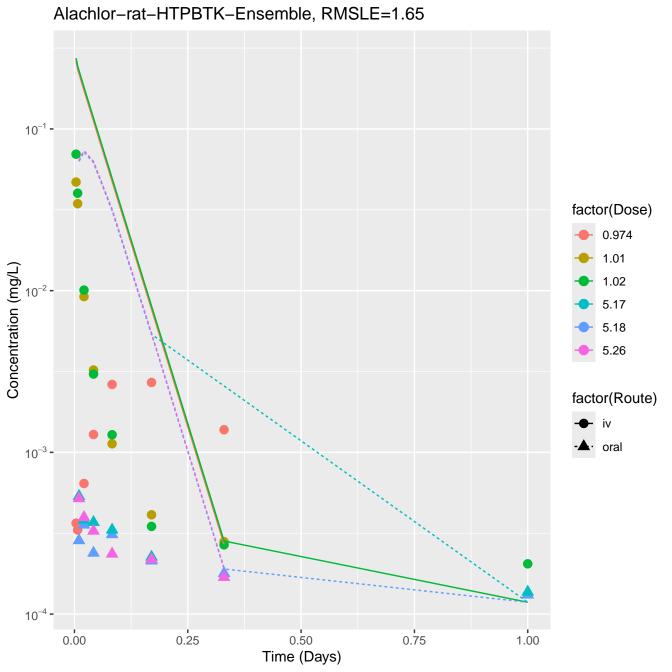
Phenacetin-human-In Vivo Fits, RMSLE=0.202 3 factor(Route) oral factor(Dose) Concentration (mg/L) 2.87 3.29 3.33 3.38 3.42 4.24 11.5 0.3 -13.2 13.7 16.9 10<sup>-1</sup> -0.10 0.15 0.00 0.05 0.20 Time (Days)

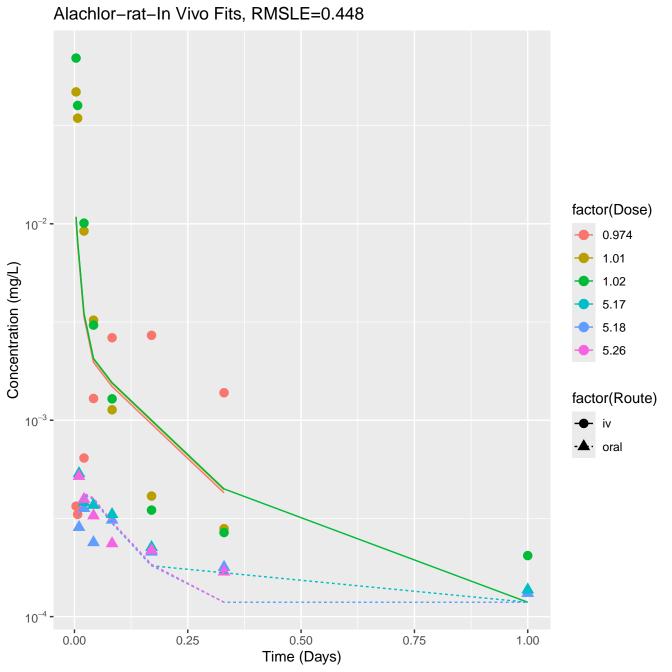


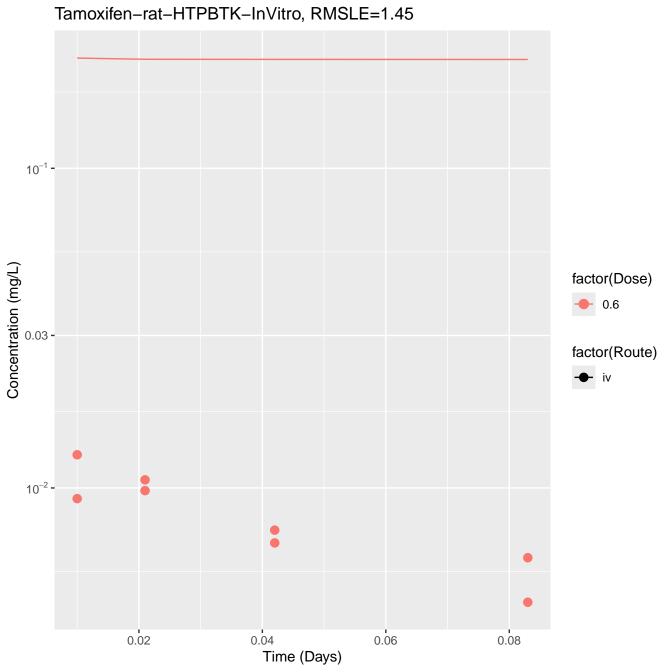


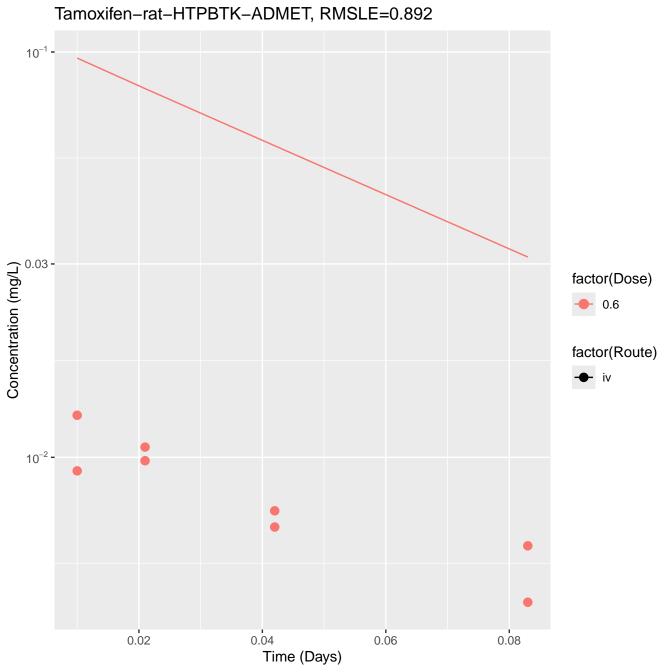


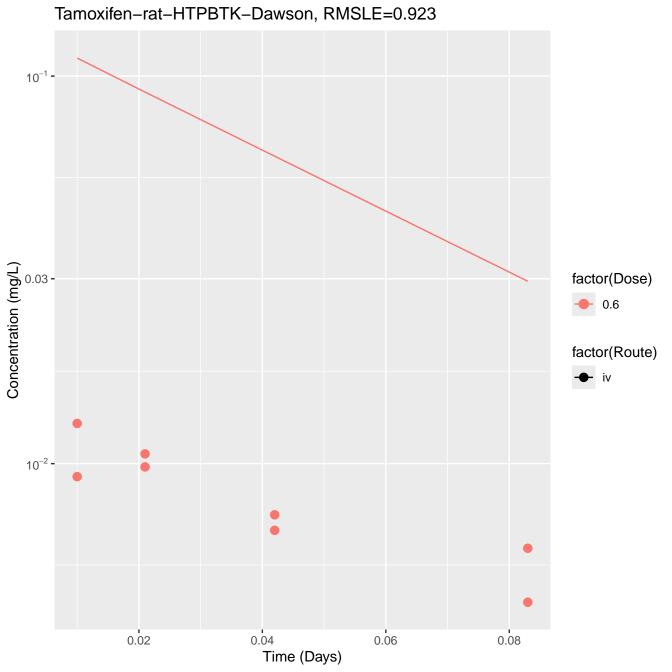


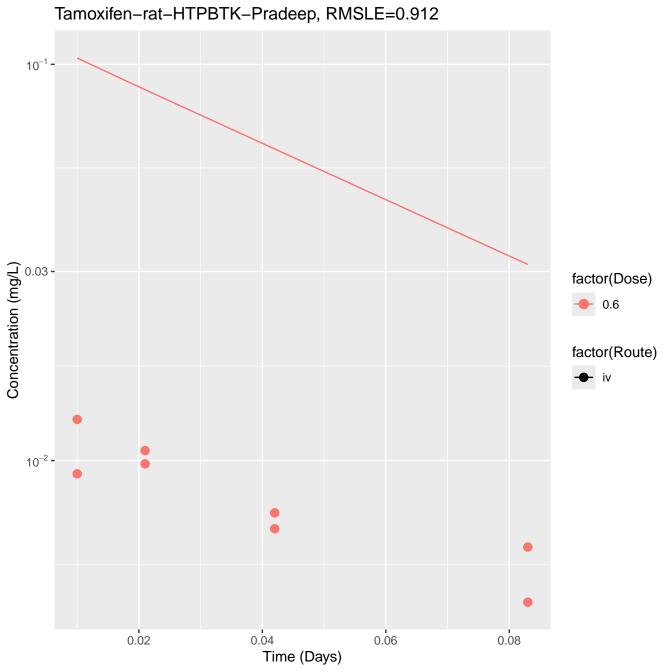


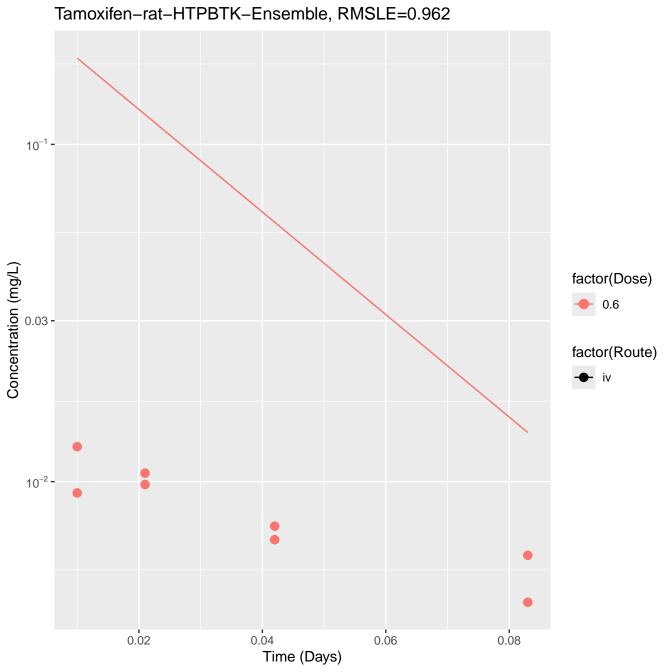


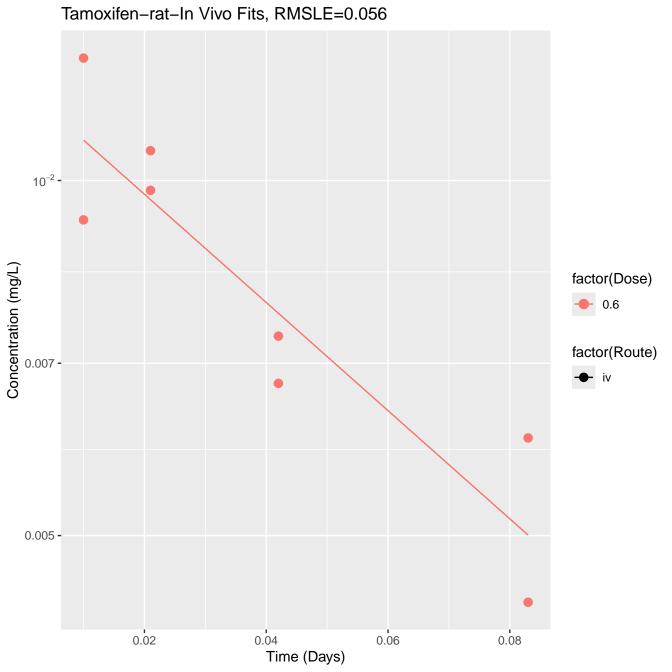


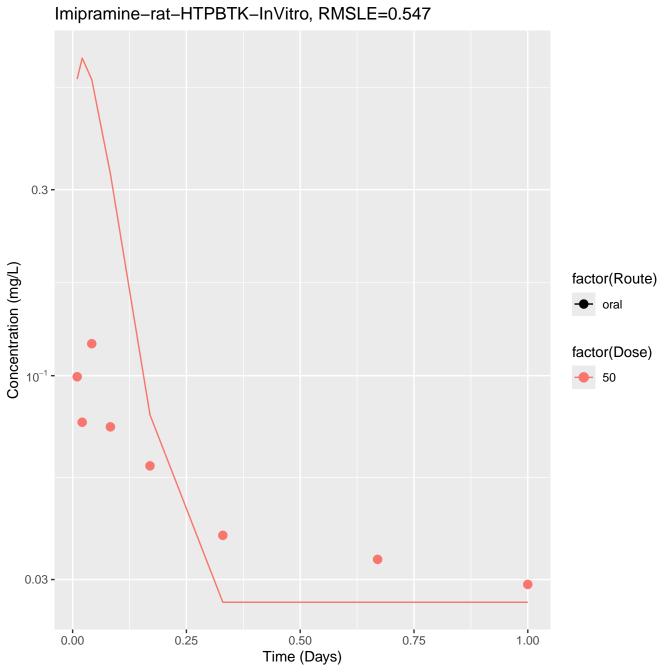


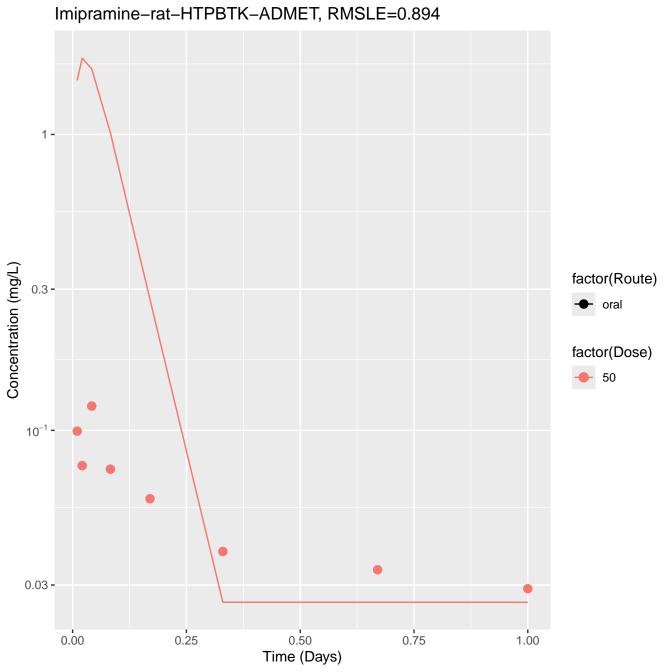


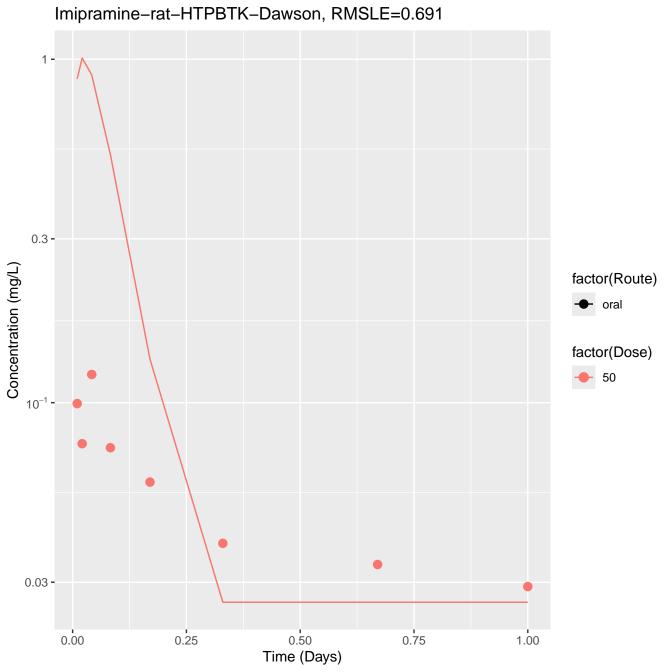


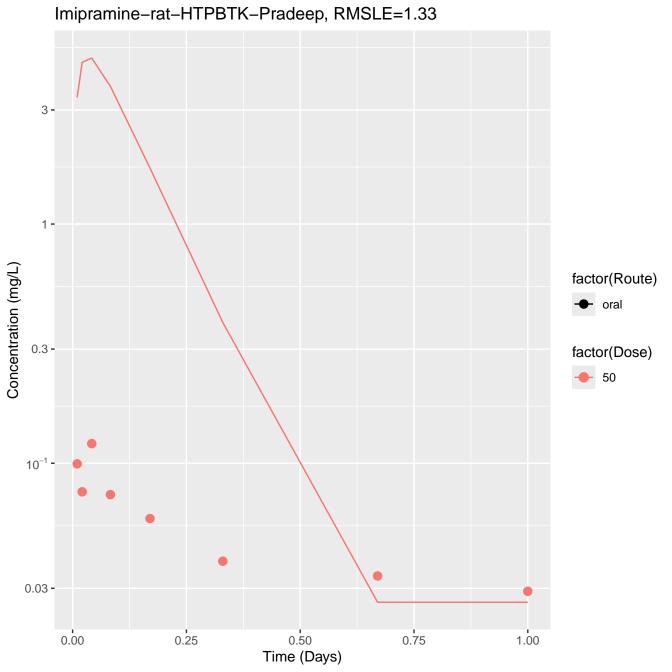


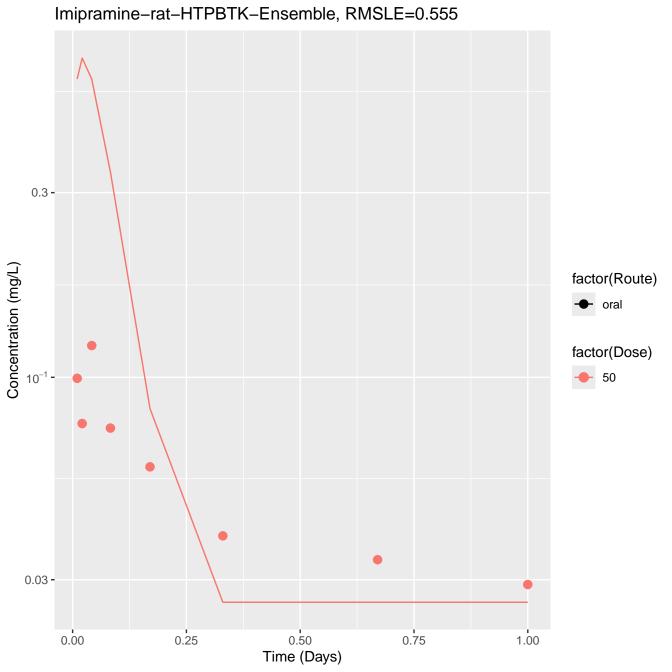


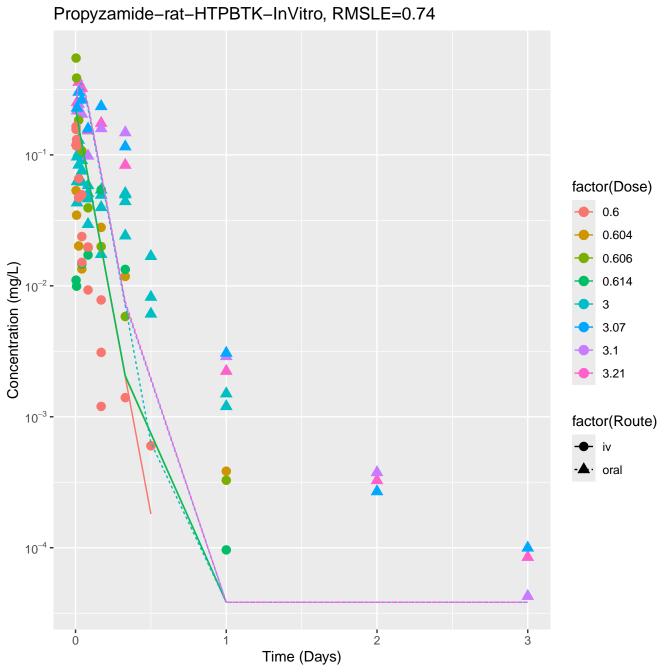


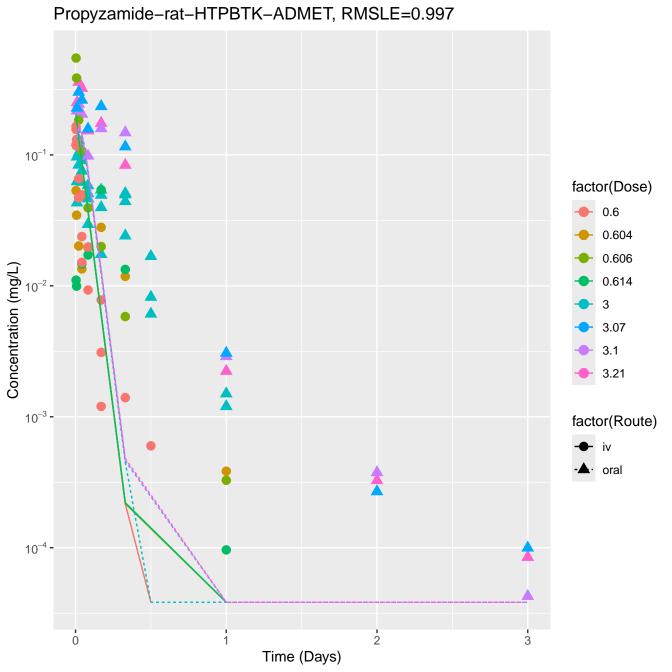


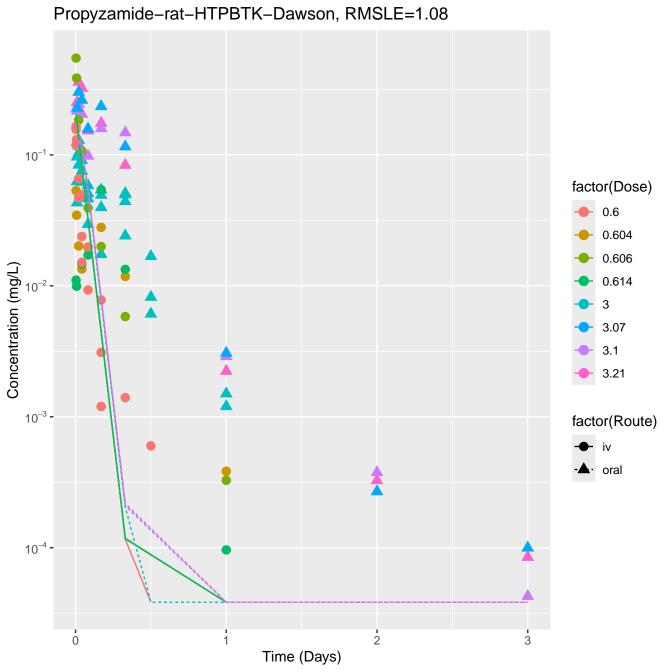


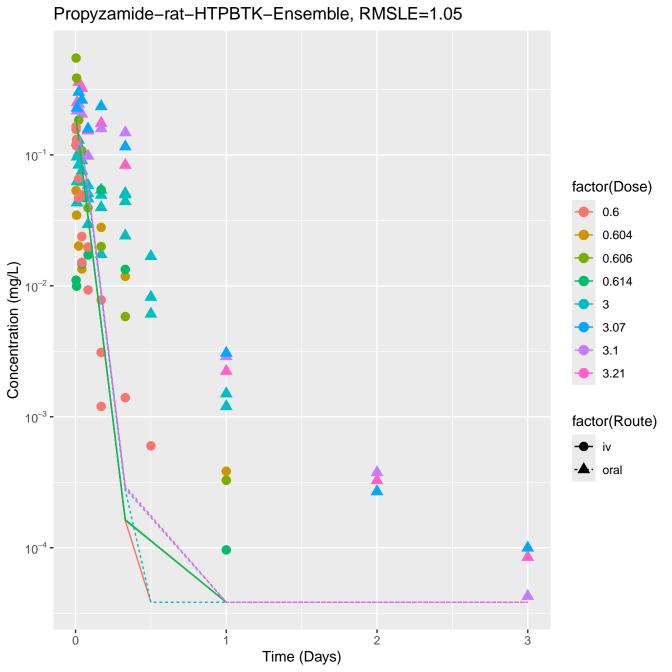


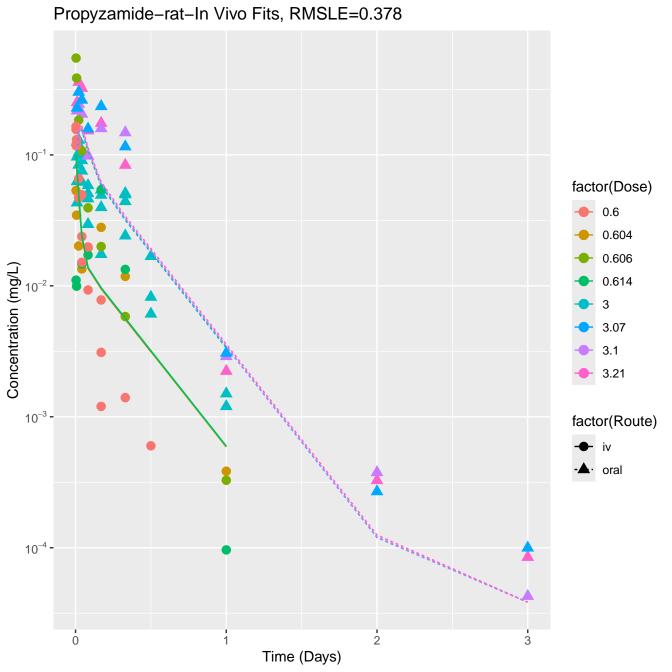




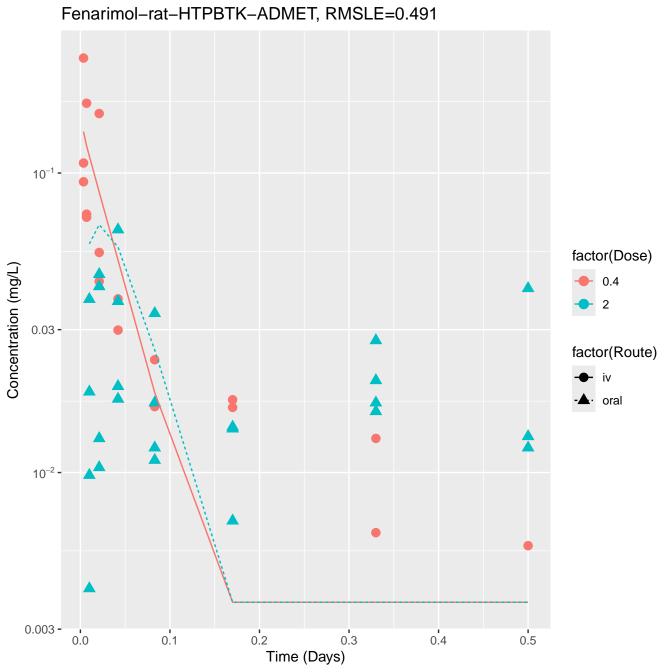


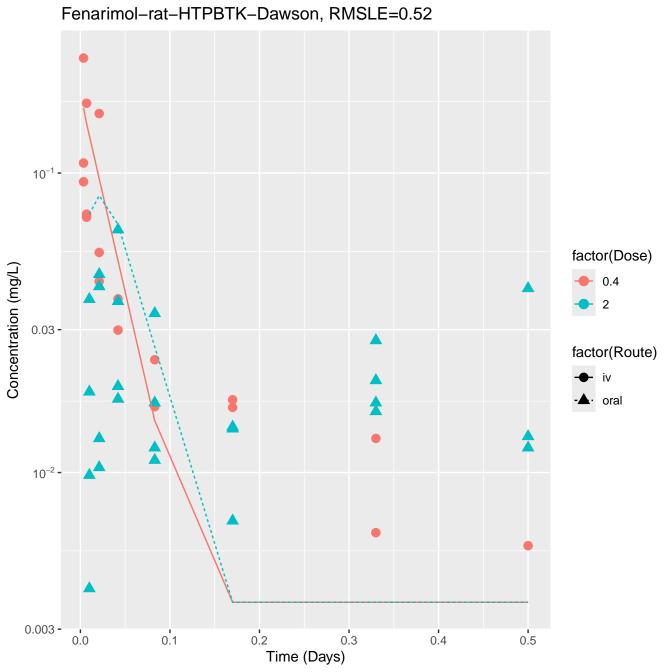






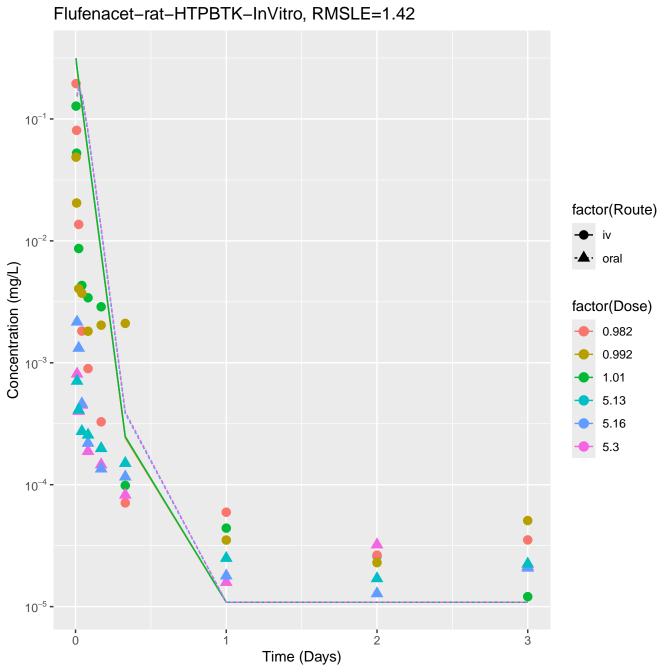
Fenarimol-rat-HTPBTK-InVitro, RMSLE=0.767 0.3 -10<sup>-1</sup> factor(Dose) Concentration (mg/L) 0.4 2 0.03 factor(Route) iv oral 10<sup>-2</sup> -0.003 -0.0 0.2 0.4 0.1 0.3 0.5 Time (Days)

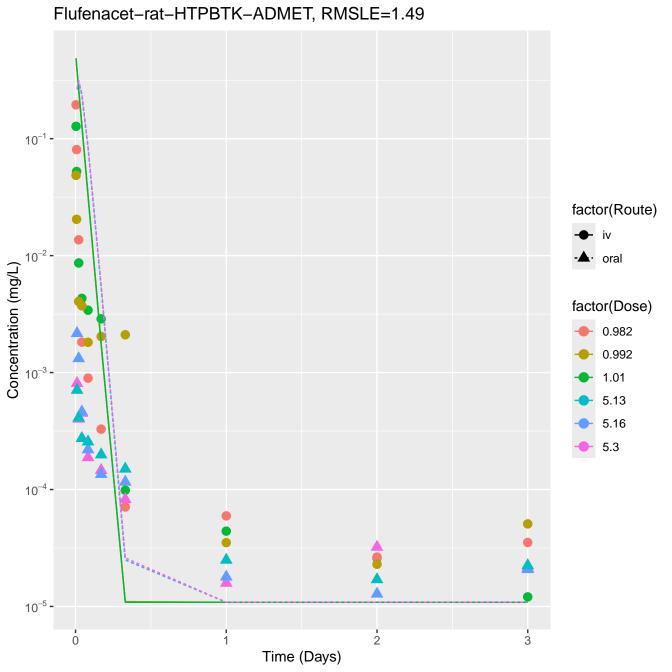


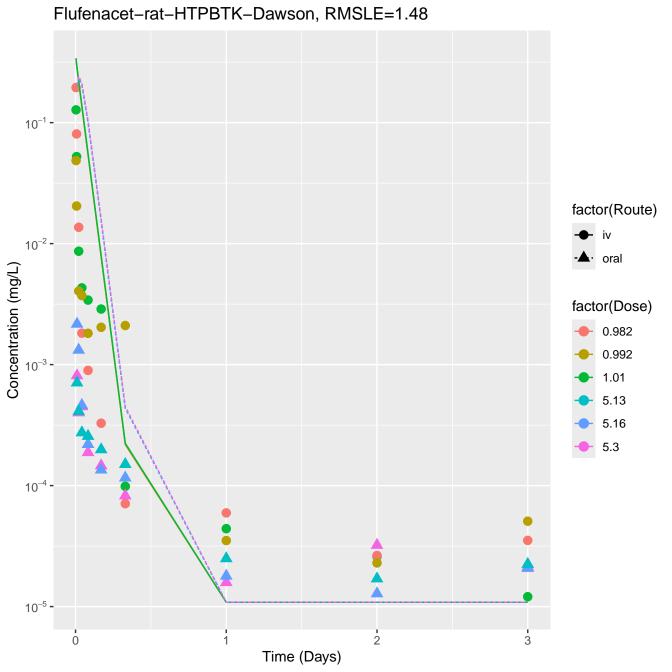


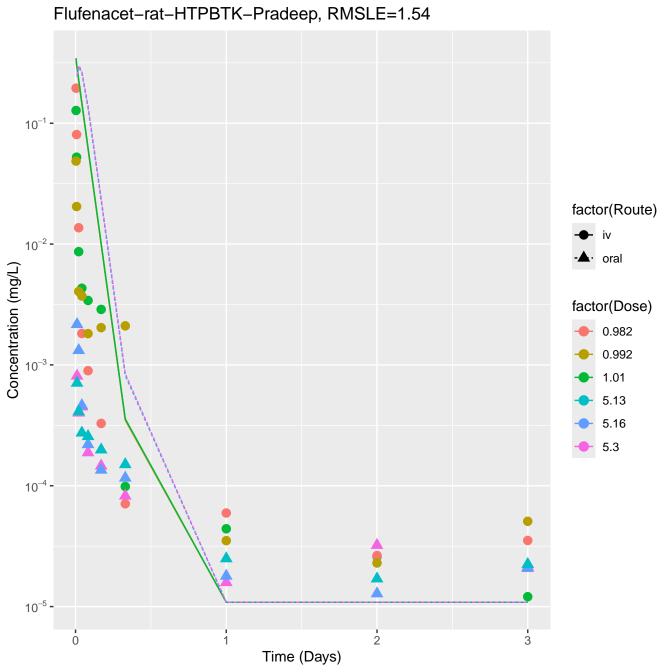
Fenarimol-rat-HTPBTK-Ensemble, RMSLE=0.492 10<sup>-1</sup> factor(Dose) Concentration (mg/L) 0.4 2 0.03 factor(Route) iv oral 10<sup>-2</sup> -0.003 -0.0 0.2 0.1 0.3 0.4 0.5 Time (Days)

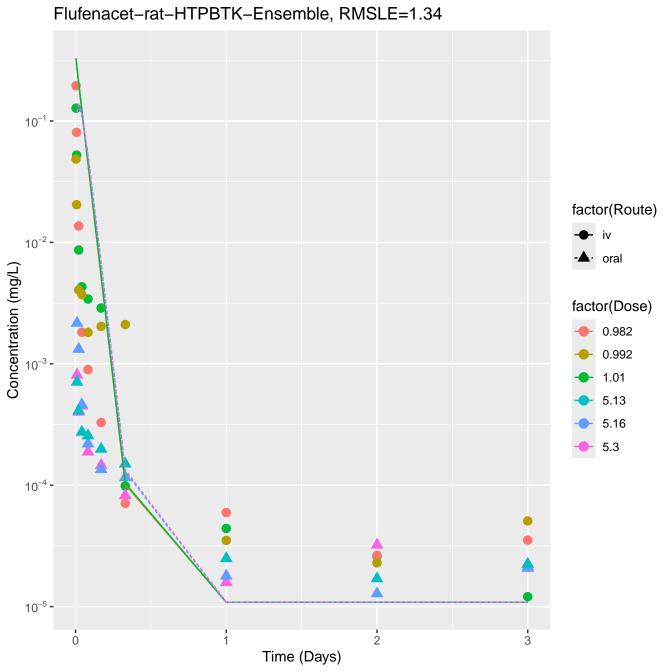
Fenarimol-rat-In Vivo Fits, RMSLE=0.24 10<sup>-1</sup> factor(Dose) Concentration (mg/L) 0.4 2 0.03 factor(Route) iv oral 10<sup>-2</sup> 0.2 0.4 0.1 0.3 0.0 0.5 Time (Days)

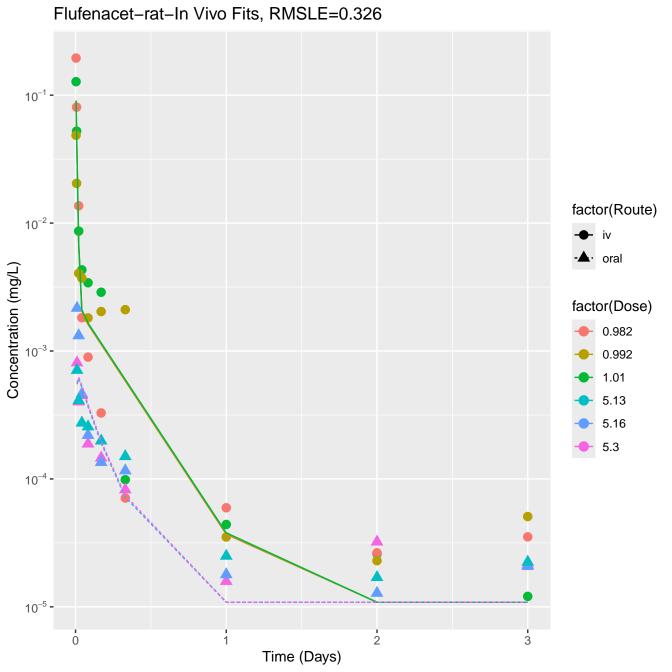


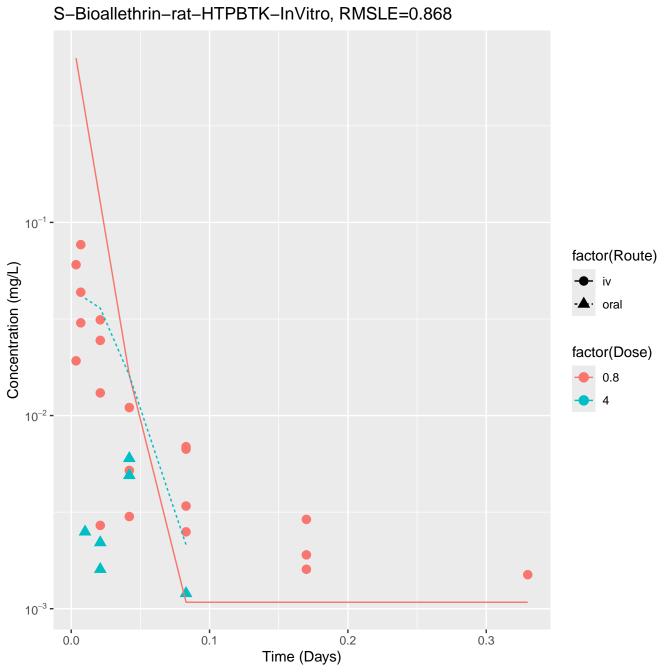


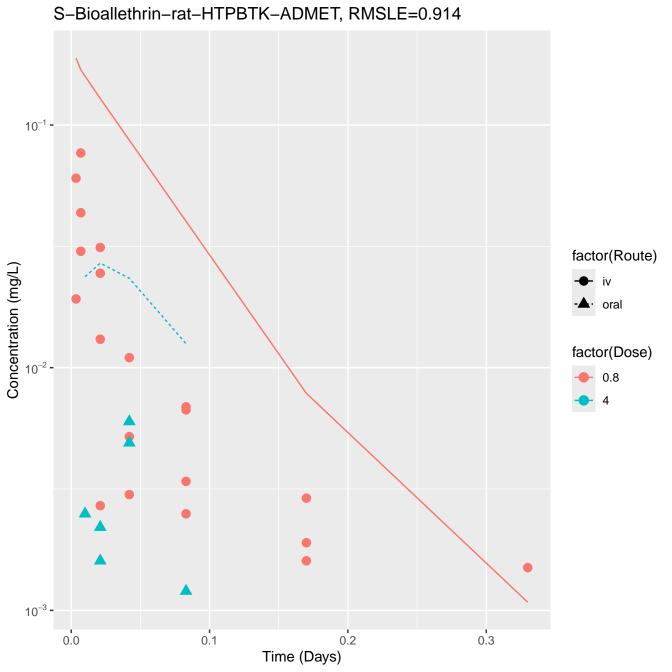


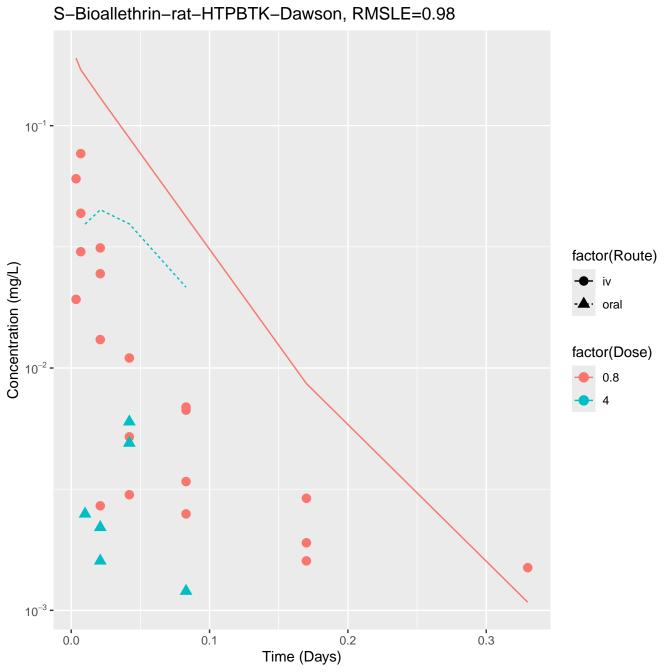


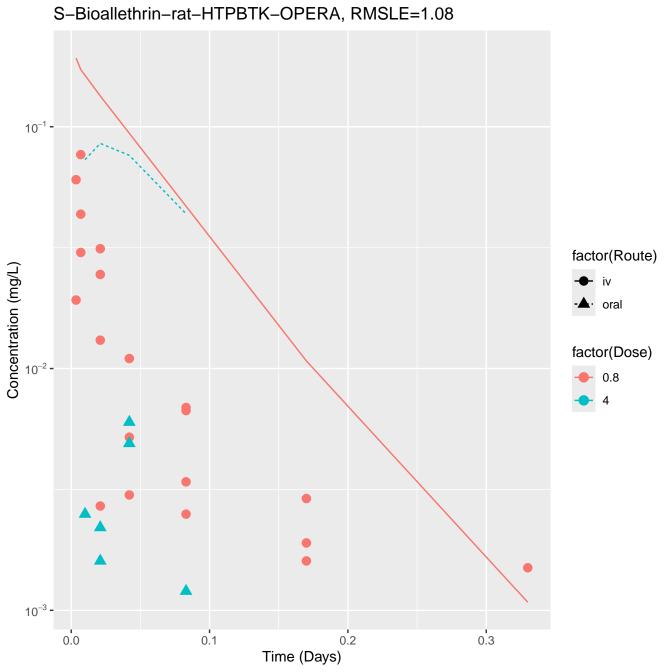


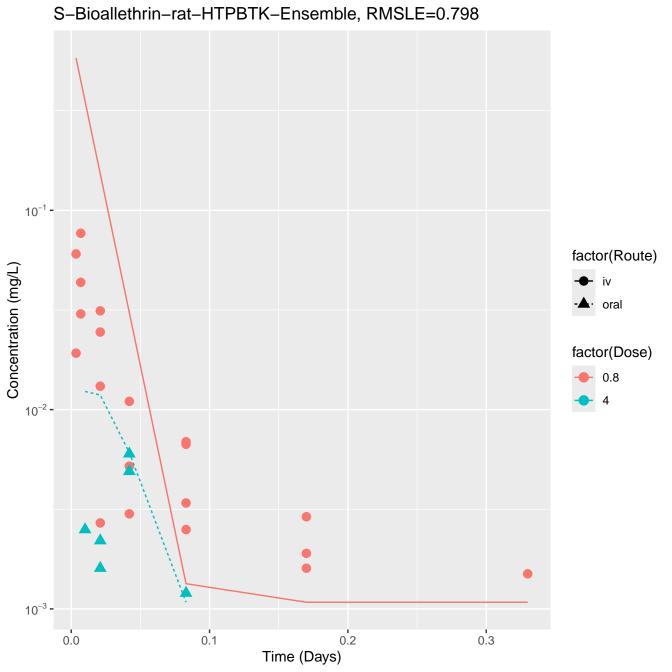




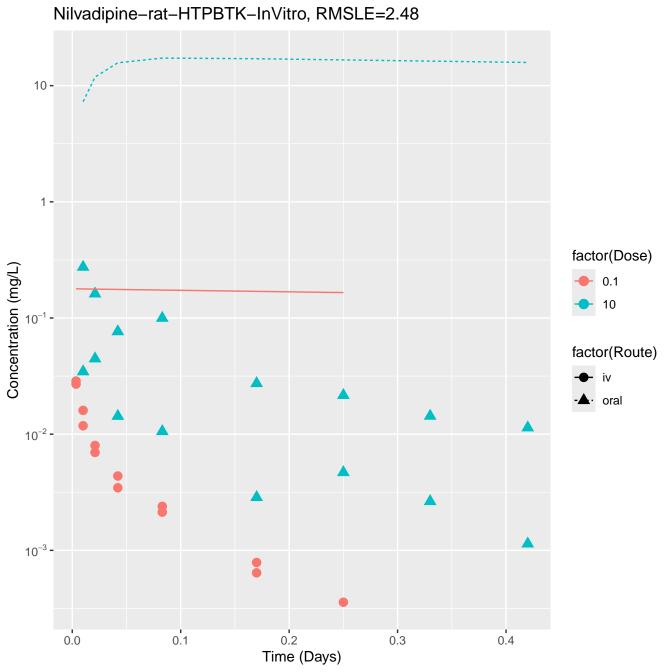


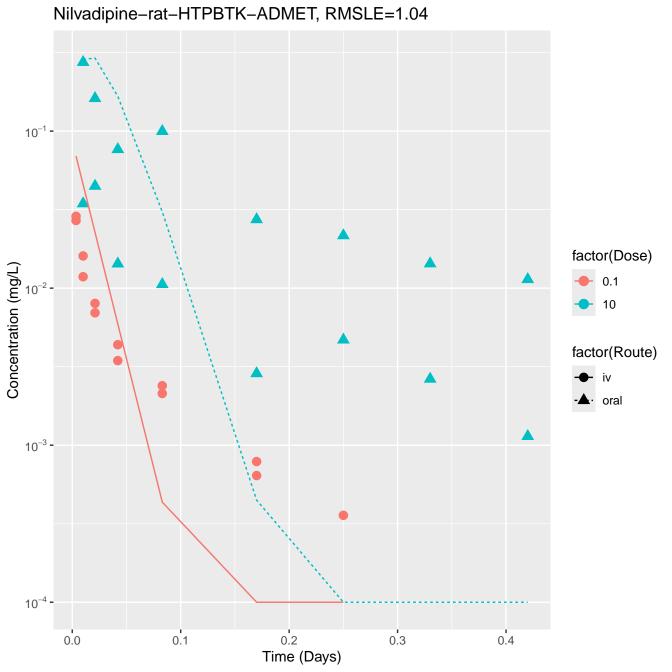


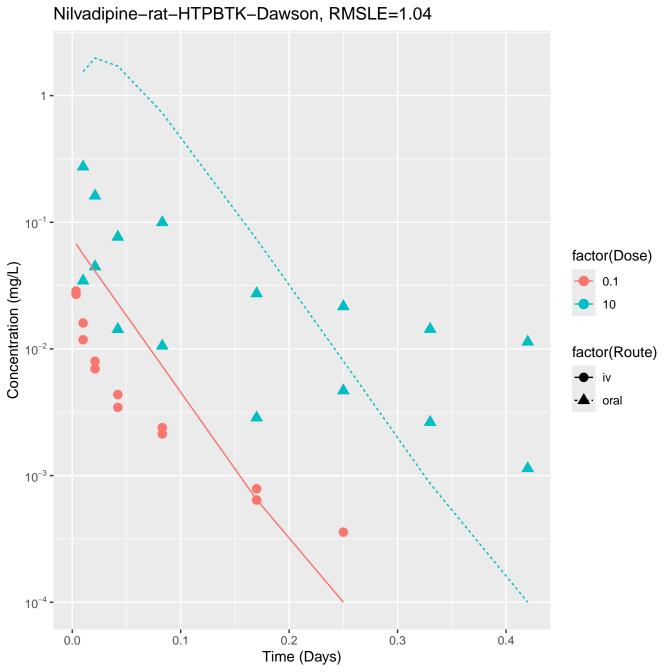


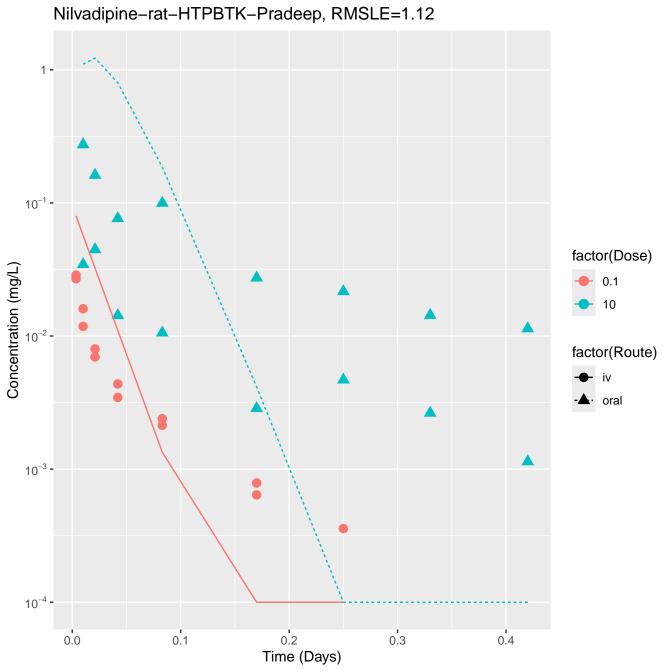


S-Bioallethrin-rat-In Vivo Fits, RMSLE=0.254 0.03 factor(Route) Concentration (mg/L) • oral 10<sup>-2</sup> factor(Dose) 0.8 0.003 -10<sup>-3</sup> -0.1 0.2 0.0 0.3 Time (Days)

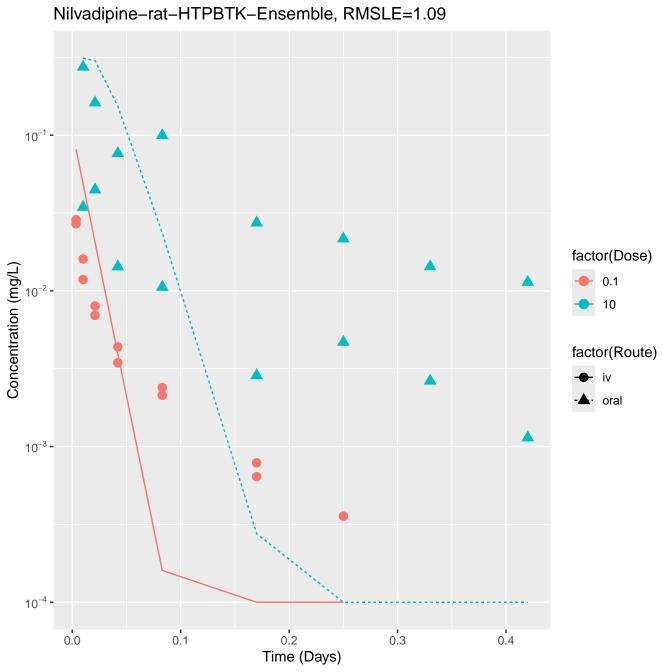


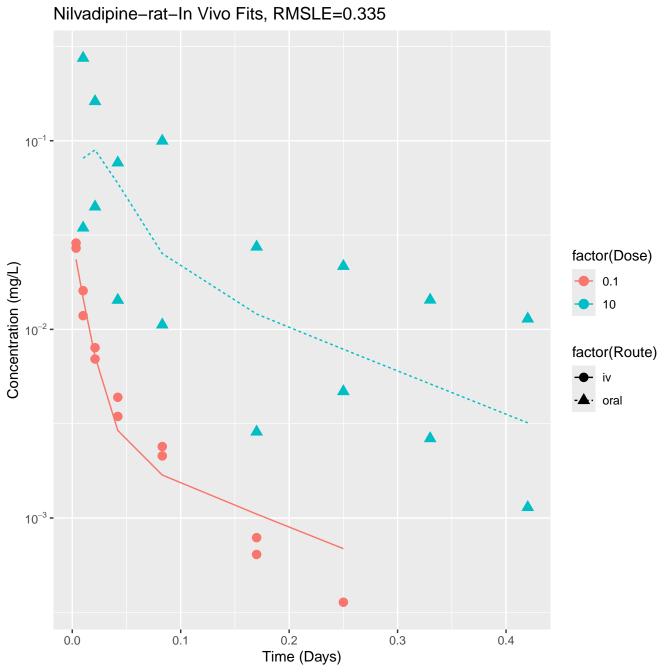




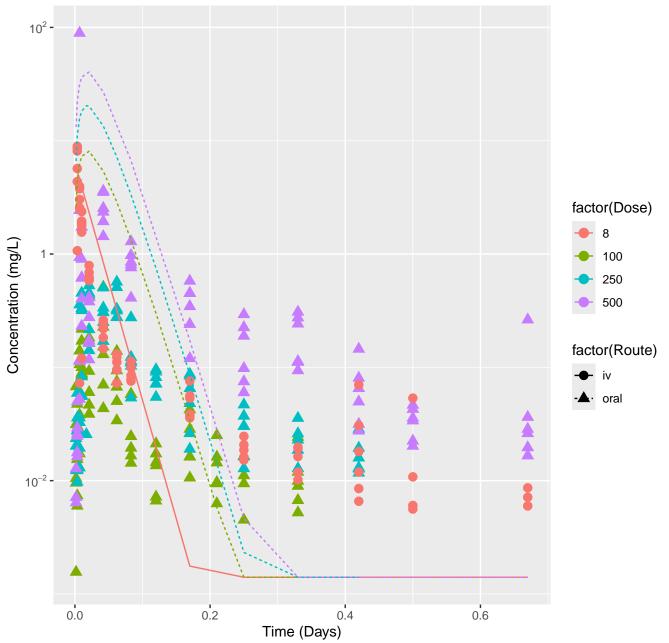


Nilvadipine-rat-HTPBTK-OPERA, RMSLE=1.15 10<sup>-1</sup> factor(Dose) Concentration (mg/L) 0.1 10 10<sup>-2</sup> factor(Route) iv · oral 10<sup>-3</sup> -10<sup>-4</sup> -0.0 0.1 0.2 0.3 0.4 Time (Days)

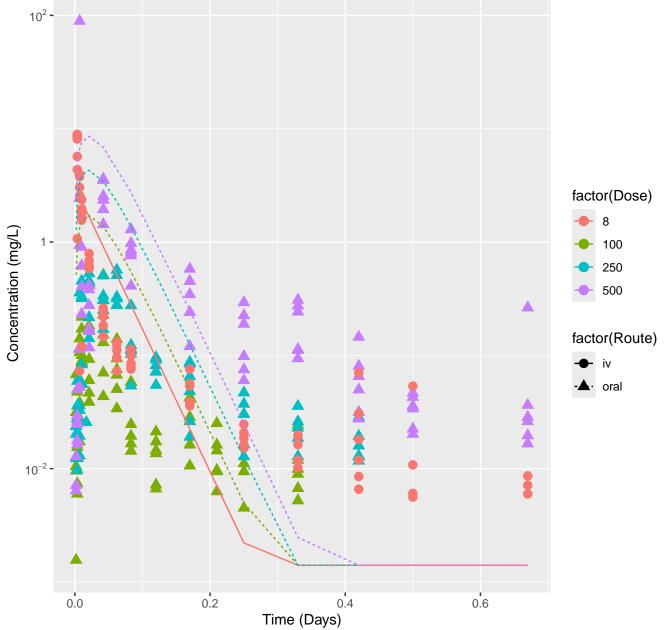




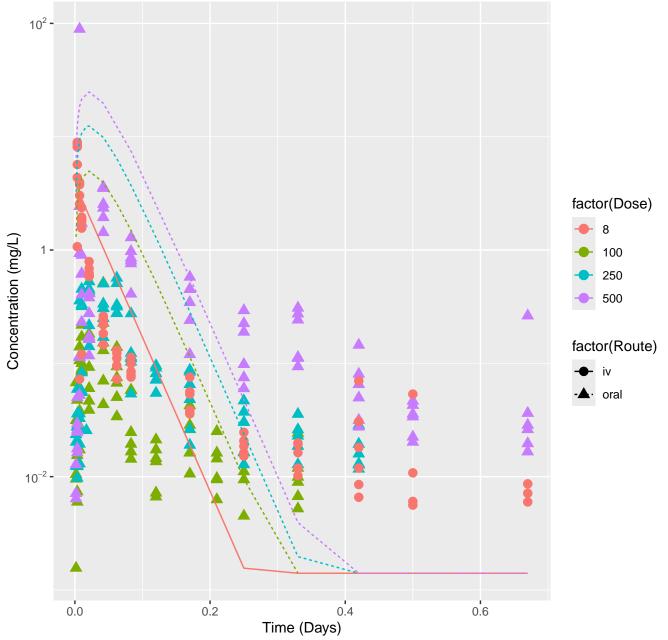
2-Hydroxy-4-methoxybenzophenone-rat-HTPBTK-InVitro, RMSLE=1.57



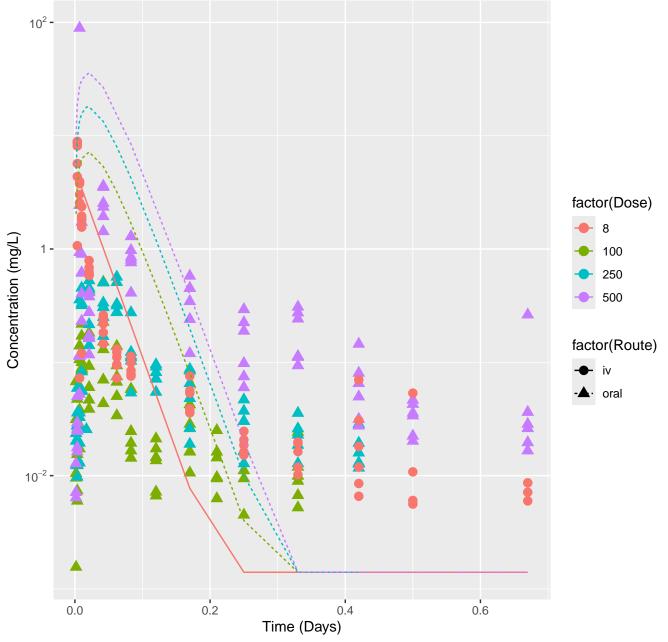
2-Hydroxy-4-methoxybenzophenone-rat-HTPBTK-ADMET, RMSLE=1.19



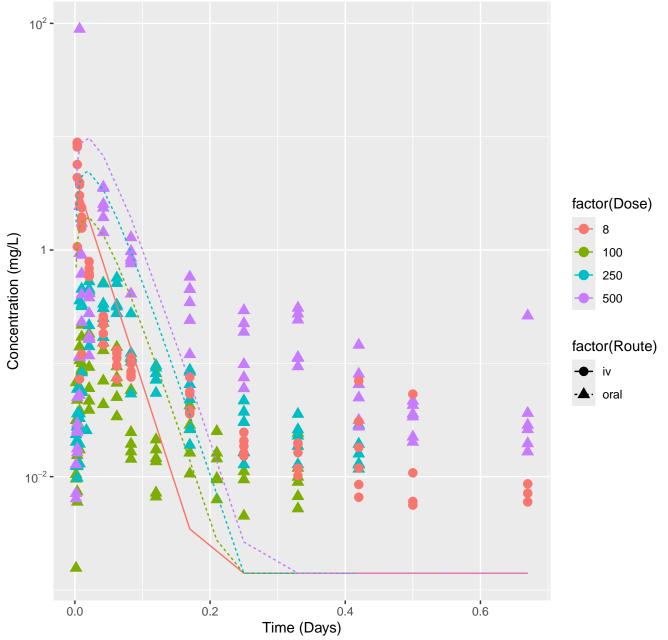
2-Hydroxy-4-methoxybenzophenone-rat-HTPBTK-Dawson, RMSLE=1.44



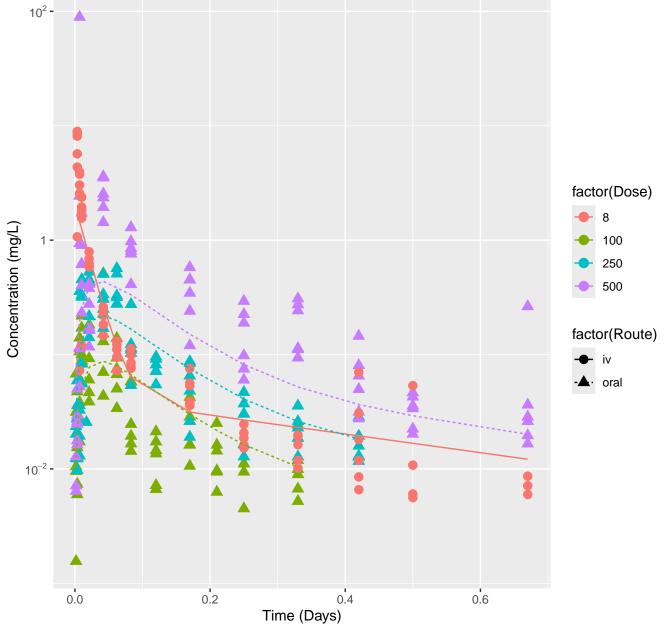
2-Hydroxy-4-methoxybenzophenone-rat-HTPBTK-Pradeep, RMSLE=1.54

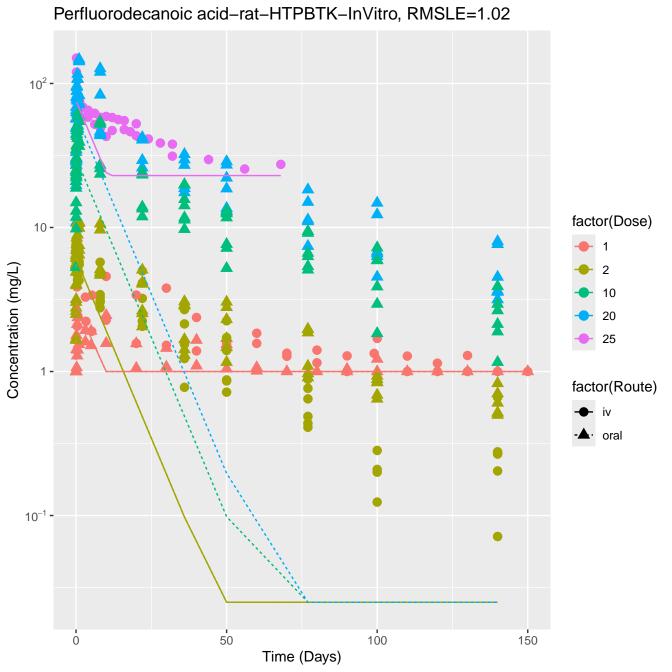


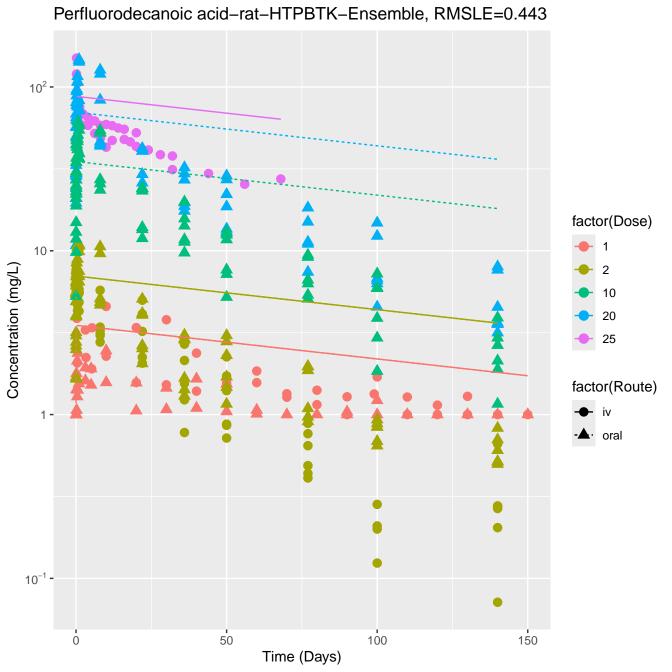
2-Hydroxy-4-methoxybenzophenone-rat-HTPBTK-Ensemble, RMSLE=1.26

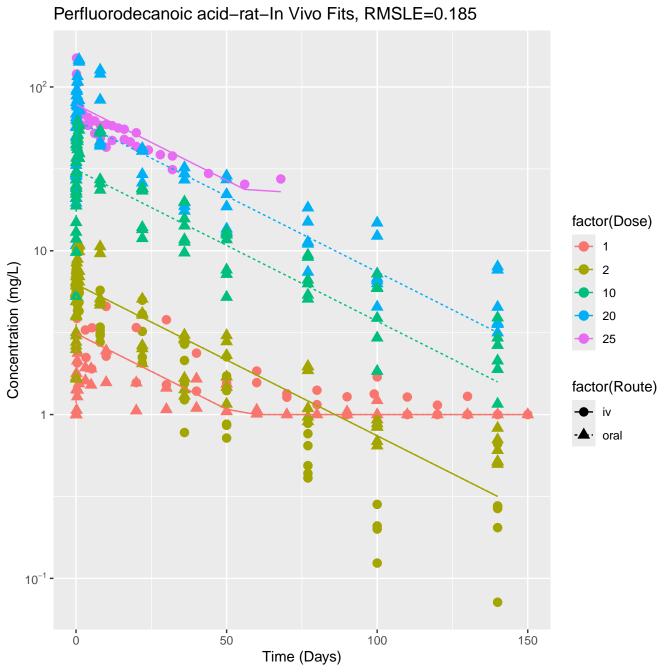


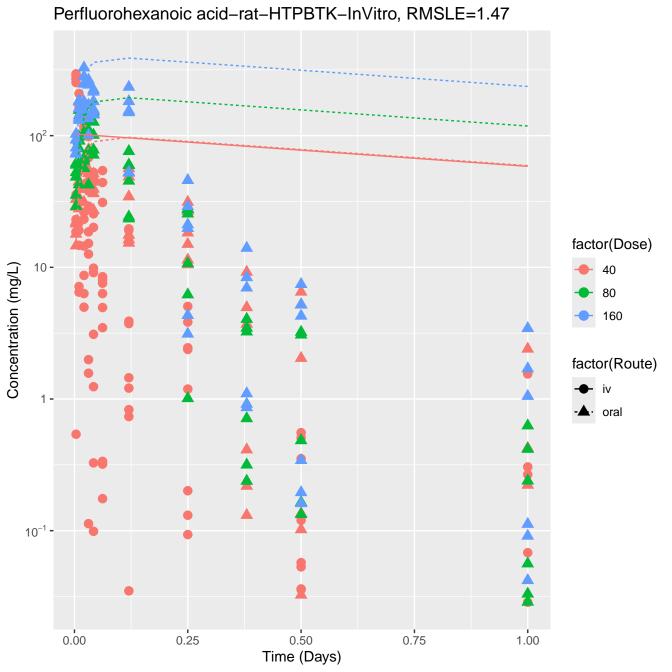
2-Hydroxy-4-methoxybenzophenone-rat-In Vivo Fits, RMSLE=0.426 10<sup>2</sup> -



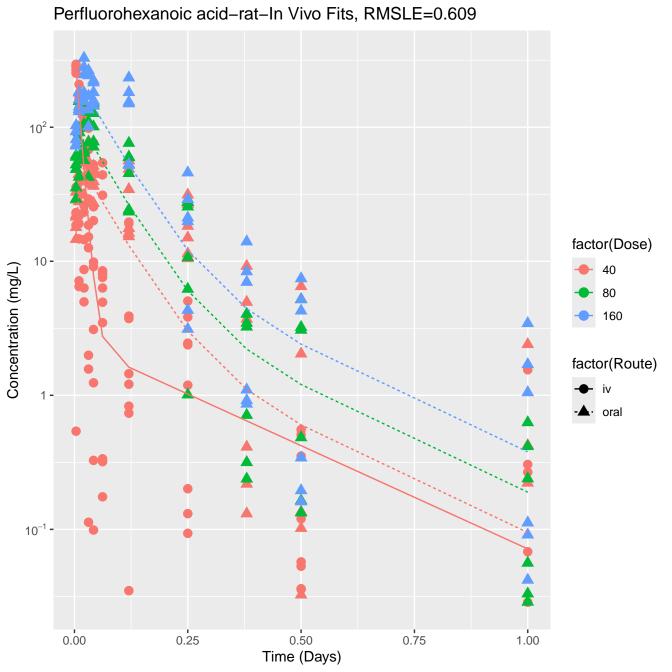


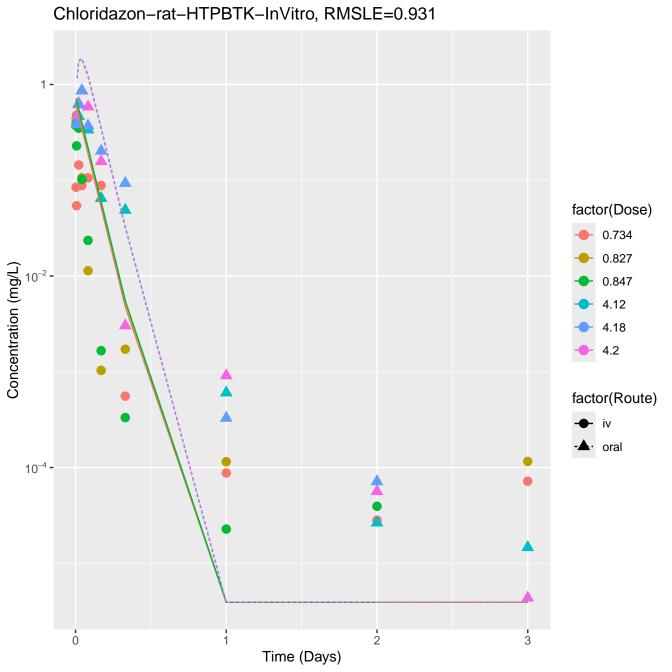


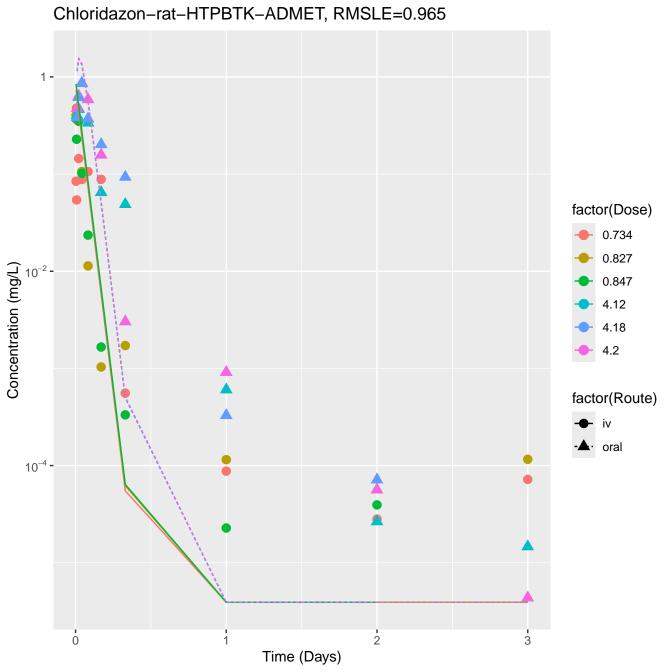


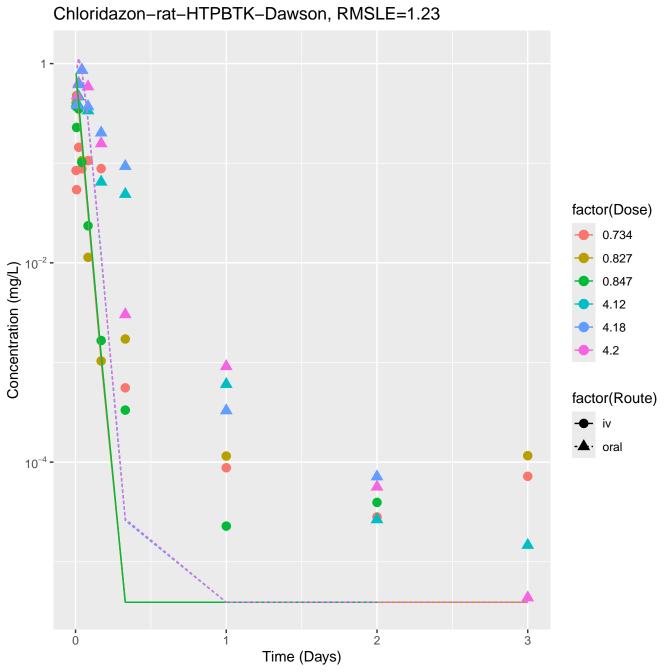


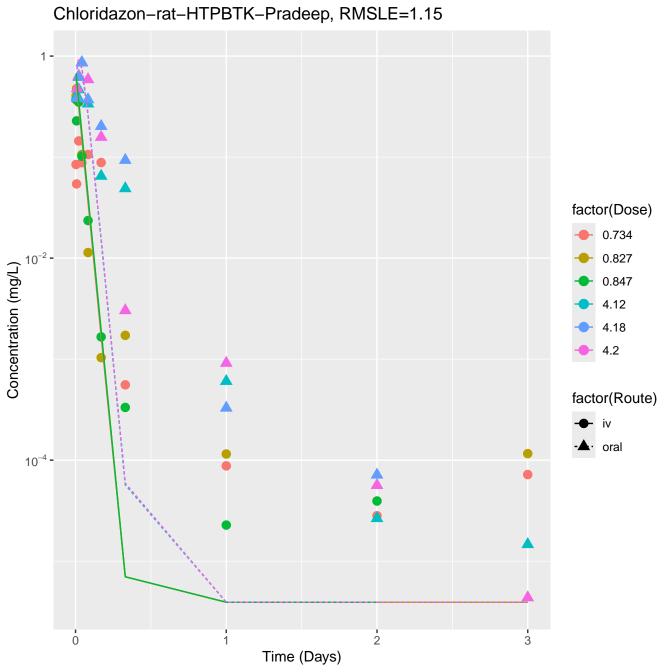
Perfluorohexanoic acid-rat-HTPBTK-Ensemble, RMSLE=1.46 10<sup>2</sup> factor(Dose) 10 -Concentration (mg/L) 40 80 160 factor(Route) · oral 10<sup>-1</sup> -0.50 0.00 0.25 0.75 1.00 Time (Days)

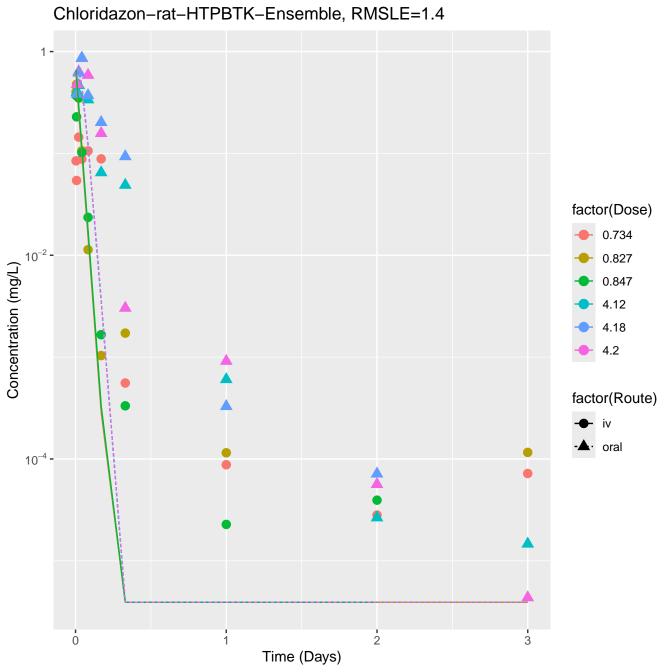


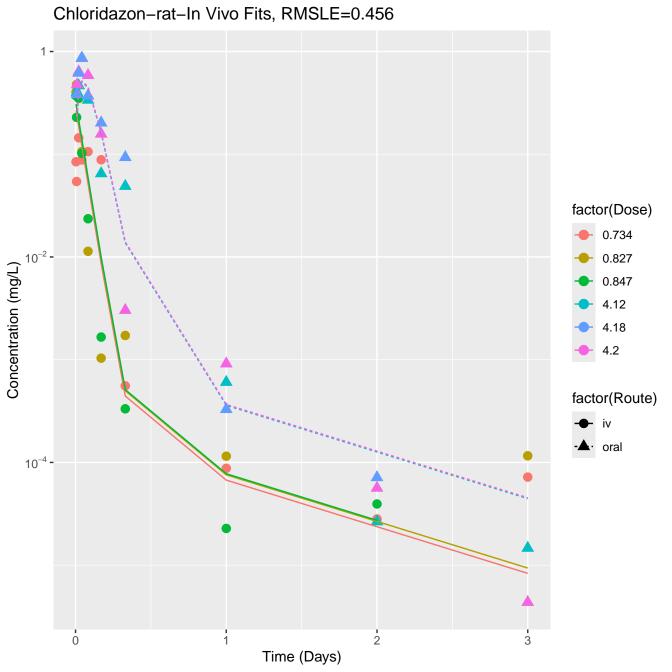






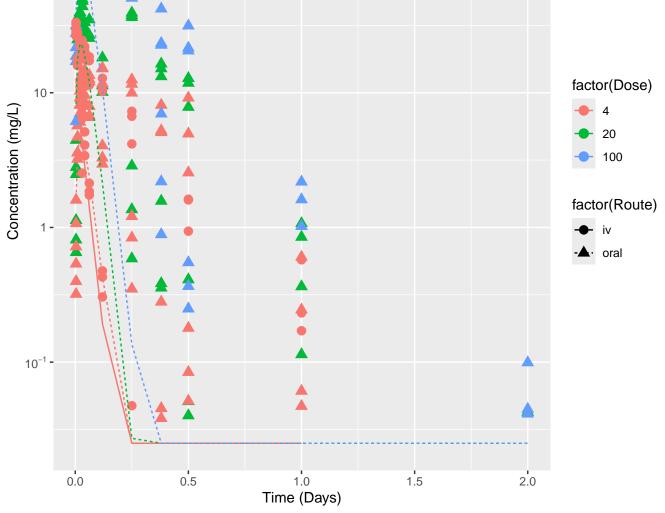






Potassium perfluorobutanesulfonate-rat-HTPBTK-InVitro, RMSLE=1.24 10<sup>2</sup> factor(Dose) 10 -Concentration (mg/L) 20 100 factor(Route) 1 -· oral 10<sup>-1</sup> -0.5 1.0 1.5 0.0 2.0 Time (Days)

Potassium perfluorobutanesulfonate-rat-HTPBTK-OPERA, RMSLE=1.24 10<sup>2</sup> factor(Dose) 10 -Concentration (mg/L) 20 100 factor(Route) 1 -



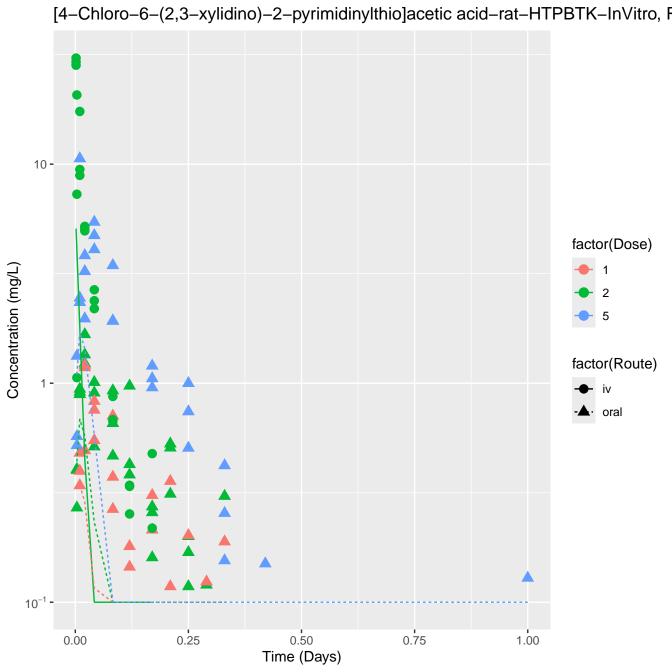
Potassium perfluorobutanesulfonate-rat-HTPBTK-Ensemble, RMSLE=1.24 10<sup>2</sup> factor(Dose) 10 -Concentration (mg/L) 20 100 factor(Route) 1 -· oral 10<sup>-1</sup> -0.5 1.0 1.5 0.0 2.0 Time (Days)

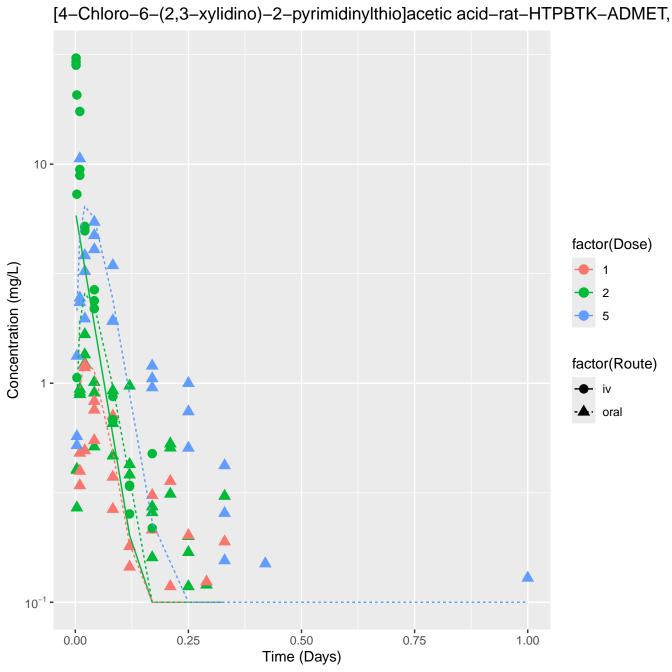
Potassium perfluorobutanesulfonate-rat-In Vivo Fits, RMSLE=0.496 10<sup>2</sup> factor(Dose) 10 -Concentration (mg/L) 20 100 factor(Route) · oral 10<sup>-1</sup> -0.5 1.0 2.0 0.0 1.5 Time (Days)

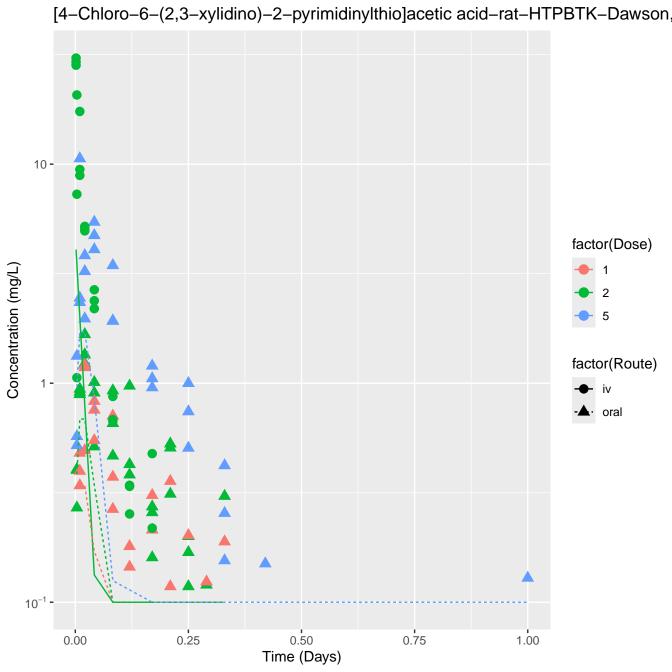
Potassium perfluorohexanesulfonate-rat-HTPBTK-InVitro, RMSLE=0.705 10<sup>2</sup> factor(Dose) 10 -Concentration (mg/L) 16 32 factor(Route) oral 10<sup>-1</sup> -0 10 20 40 30 50 Time (Days)

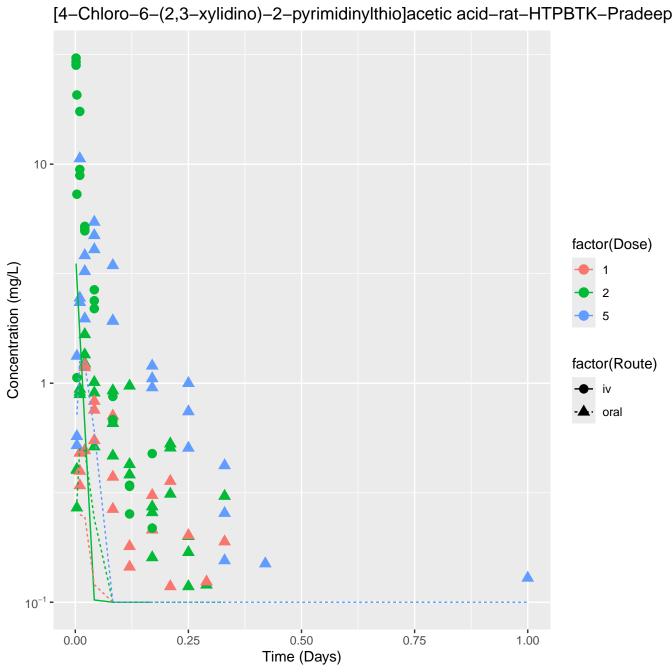
Potassium perfluorohexanesulfonate-rat-HTPBTK-Ensemble, RMSLE=0.8 10<sup>2</sup> factor(Dose) 10 -Concentration (mg/L) 16 32 factor(Route) 1 -· oral 10<sup>-1</sup> -0 10 20 40 30 50 Time (Days)

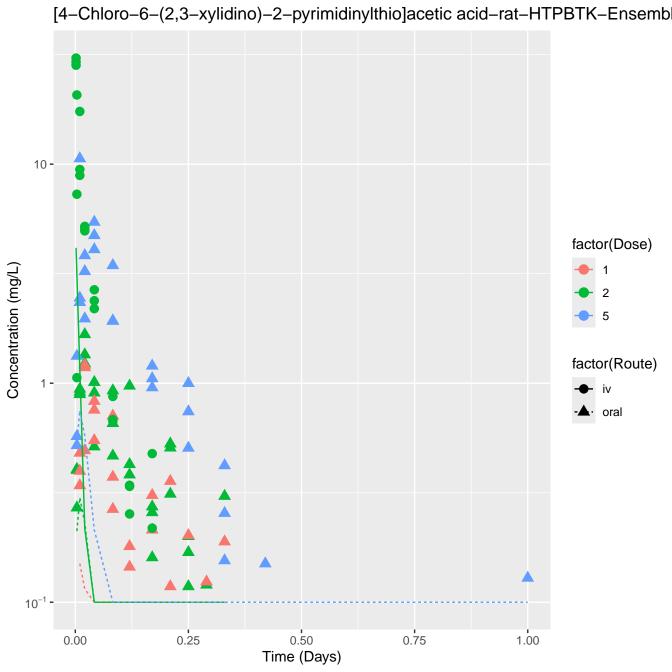
Potassium perfluorohexanesulfonate-rat-In Vivo Fits, RMSLE=0.611 10<sup>2</sup> factor(Dose) 10 -Concentration (mg/L) 16 32 factor(Route) 1 -· oral 10<sup>-1</sup> -0 10 20 40 30 50 Time (Days)

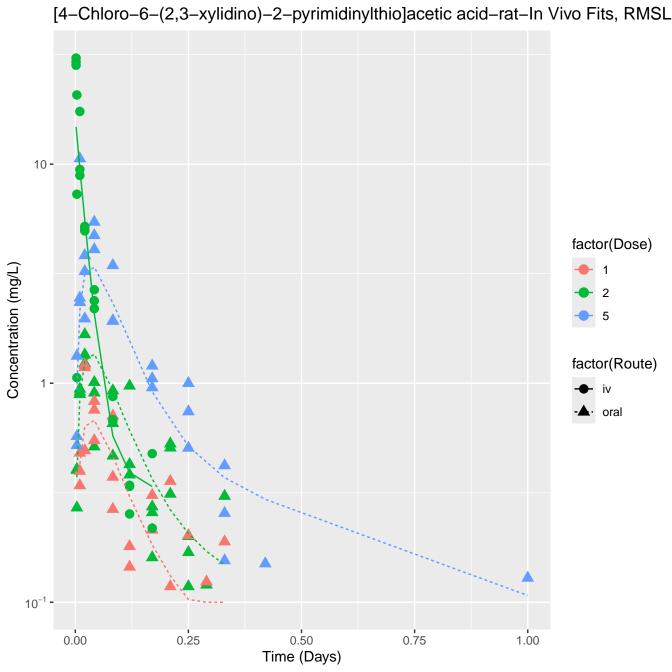


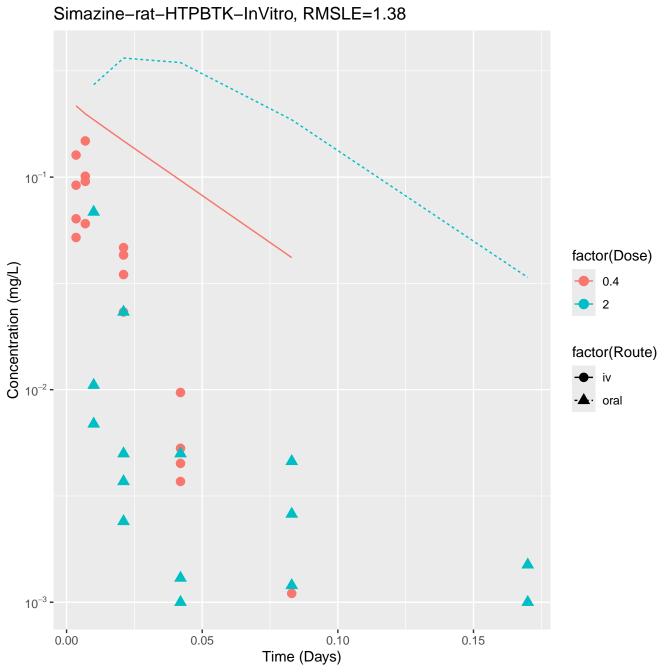


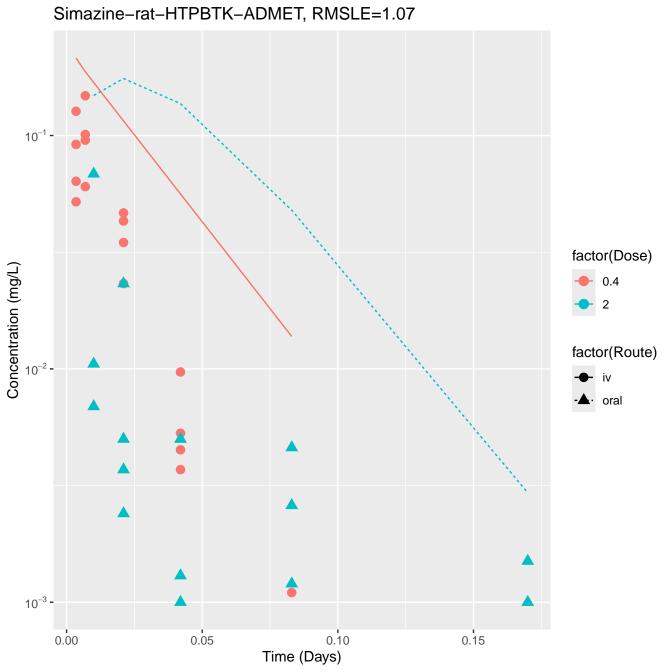


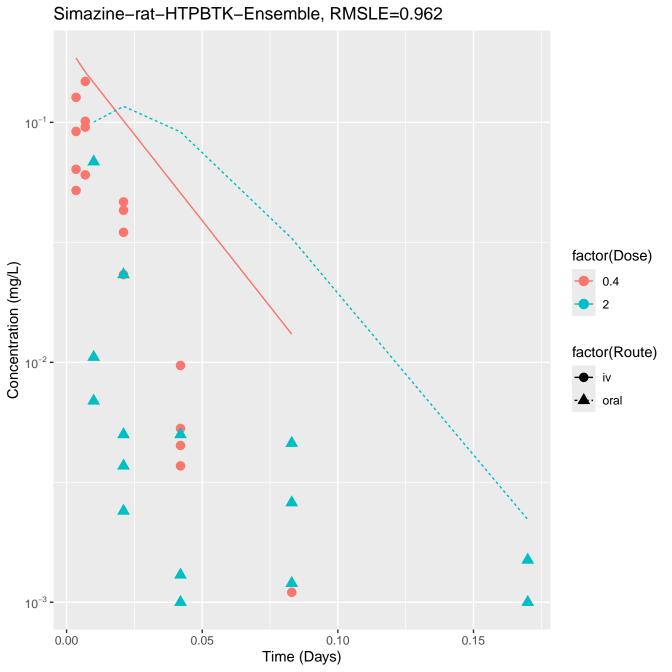




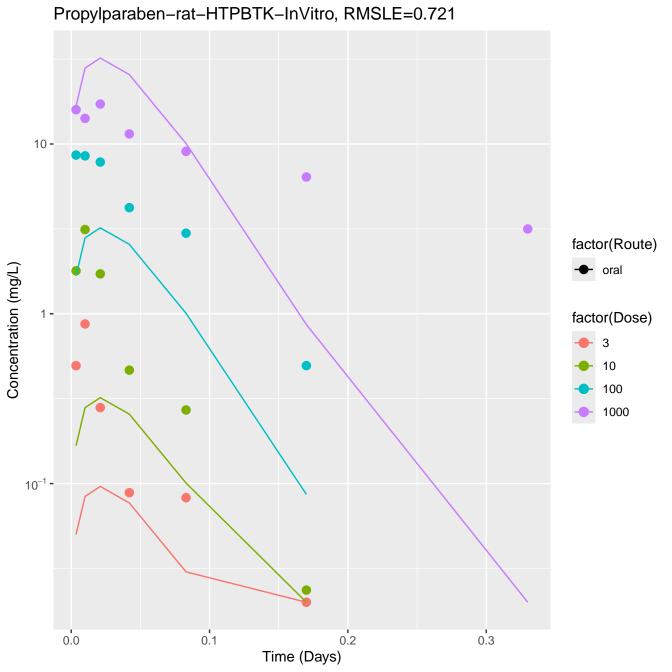


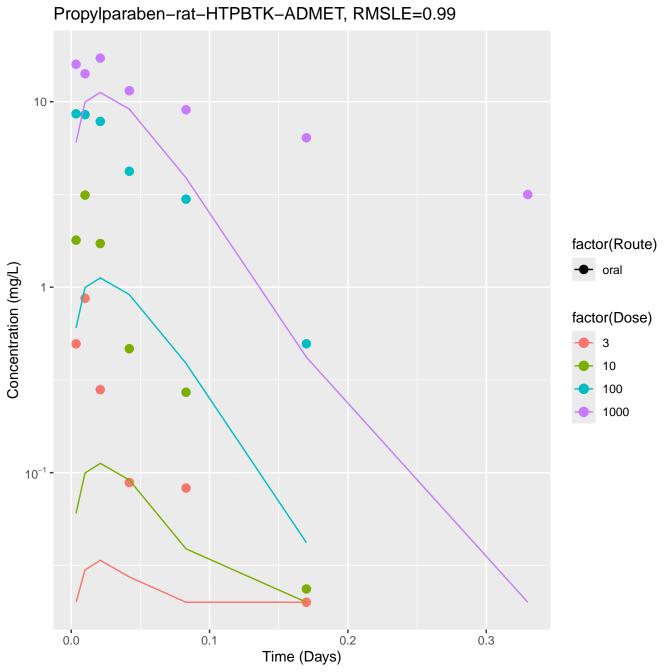


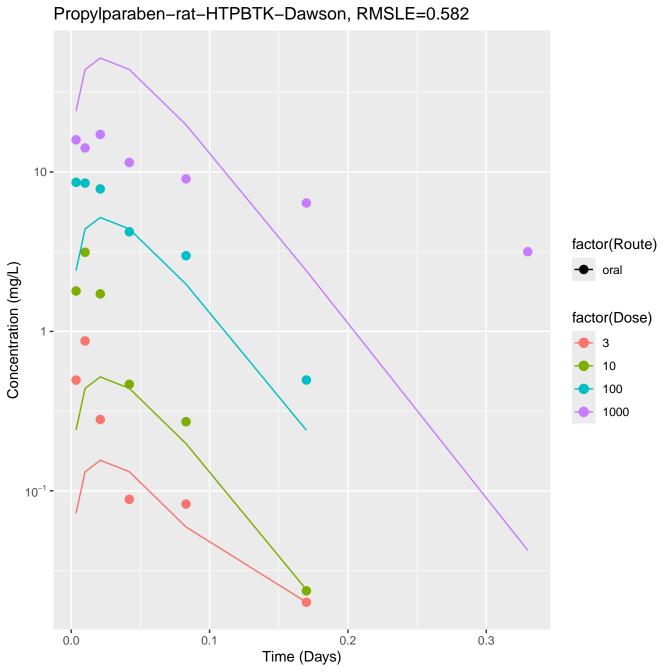


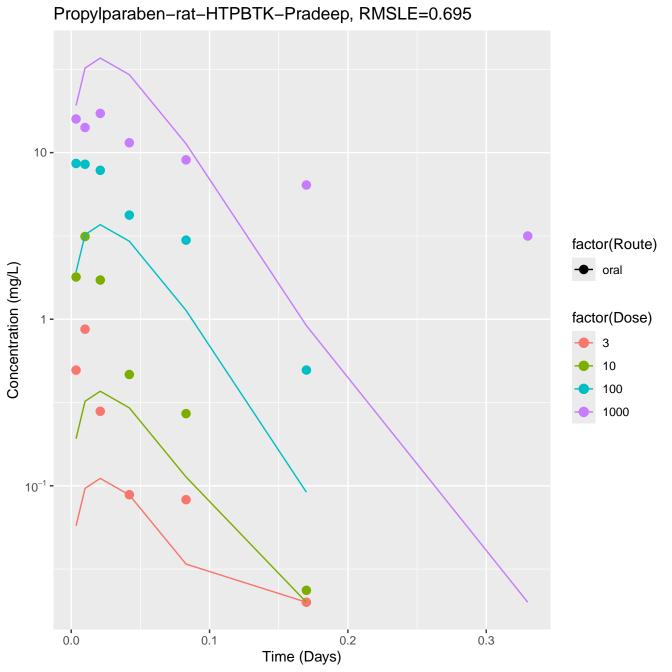


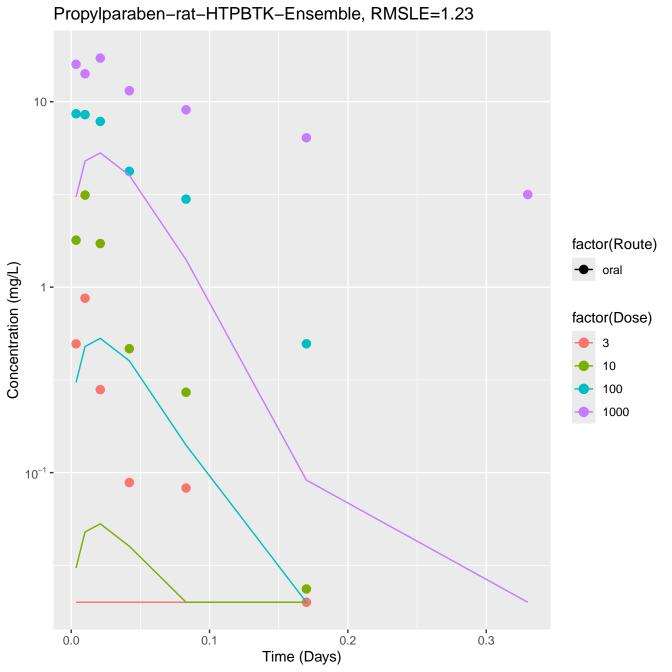
Simazine-rat-In Vivo Fits, RMSLE=0.326 10<sup>-1</sup> factor(Dose) Concentration (mg/L) 0.4 2 10<sup>-2</sup> factor(Route) iv · oral 10<sup>-3</sup> -0.05 0.10 0.15 0.00 Time (Days)

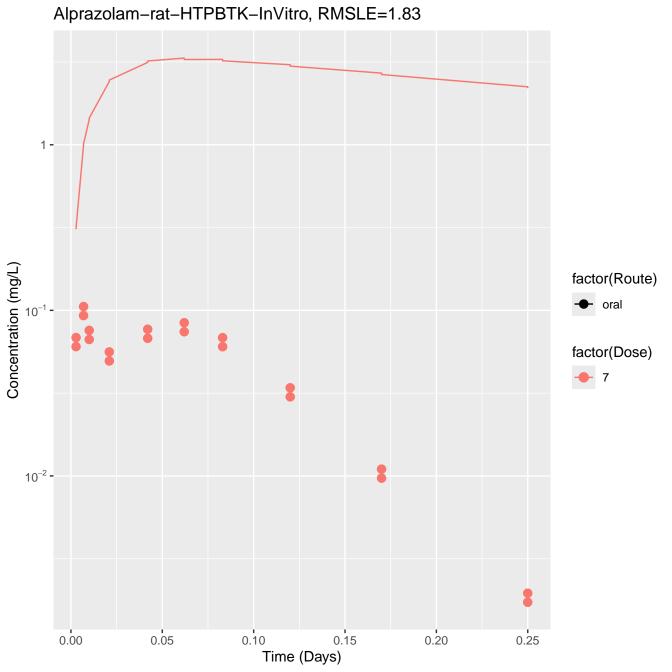


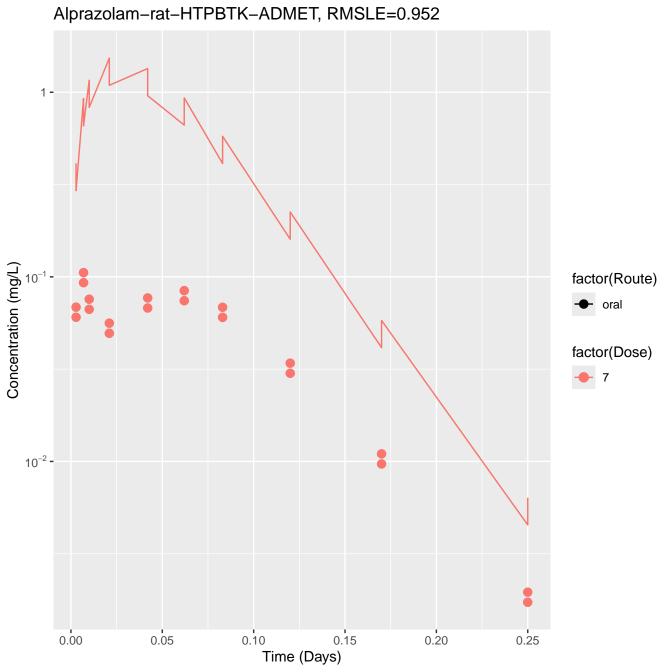


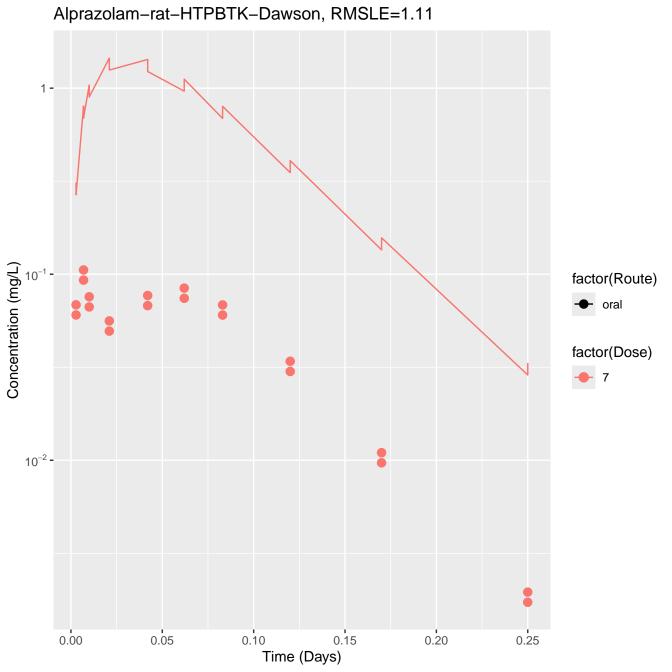


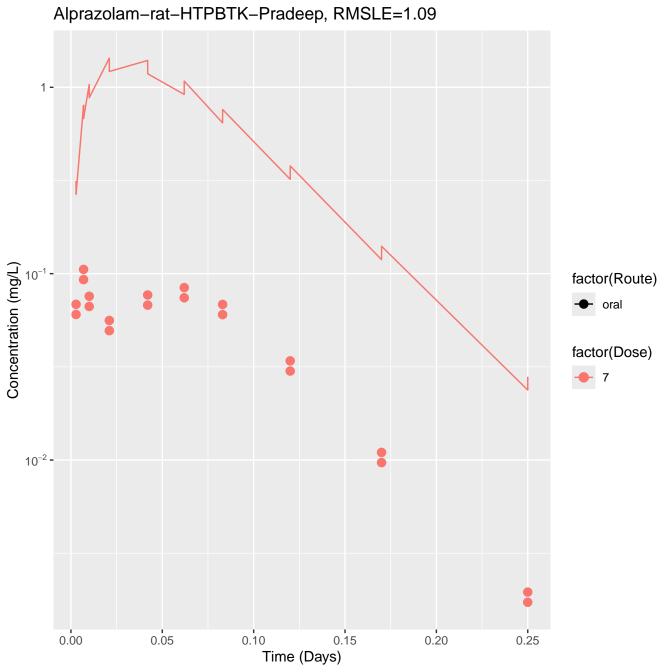


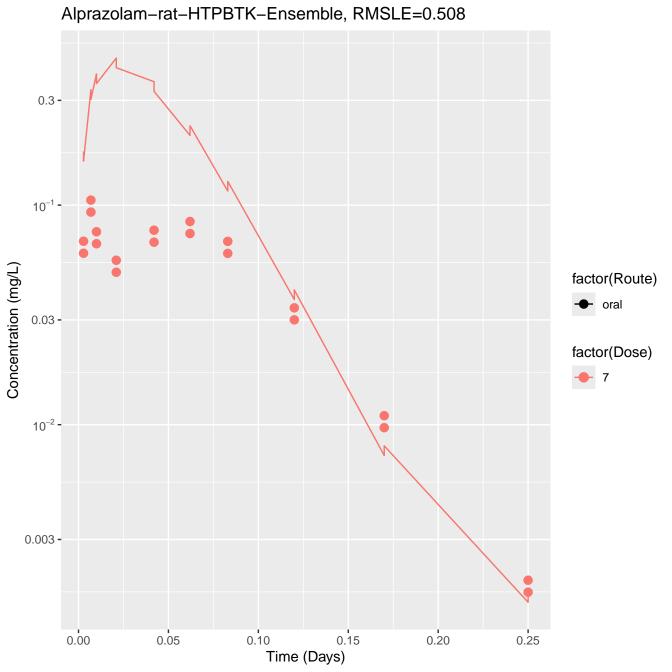


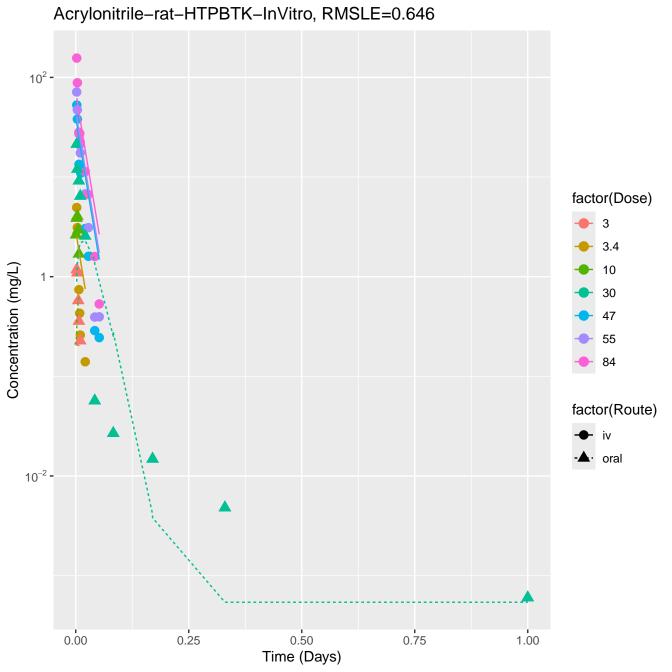


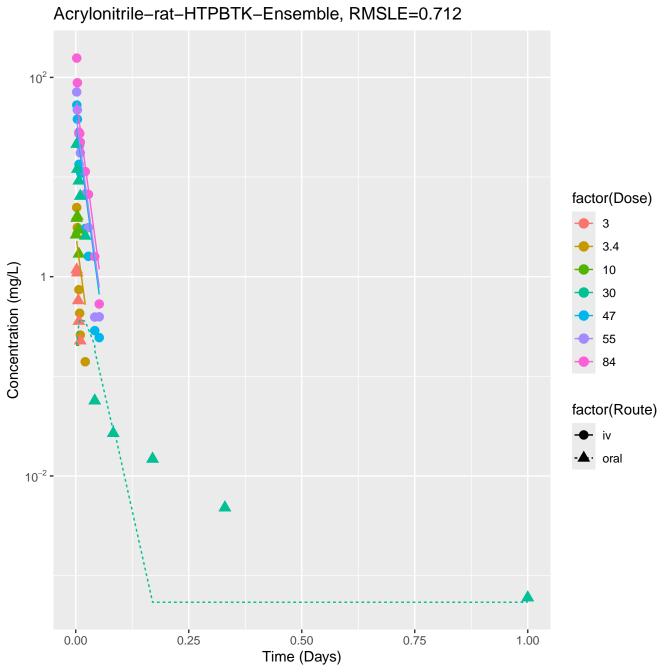


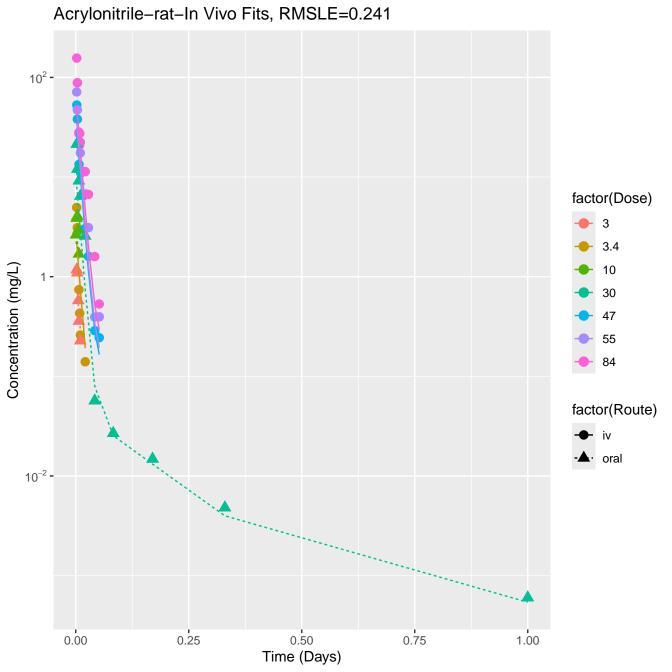


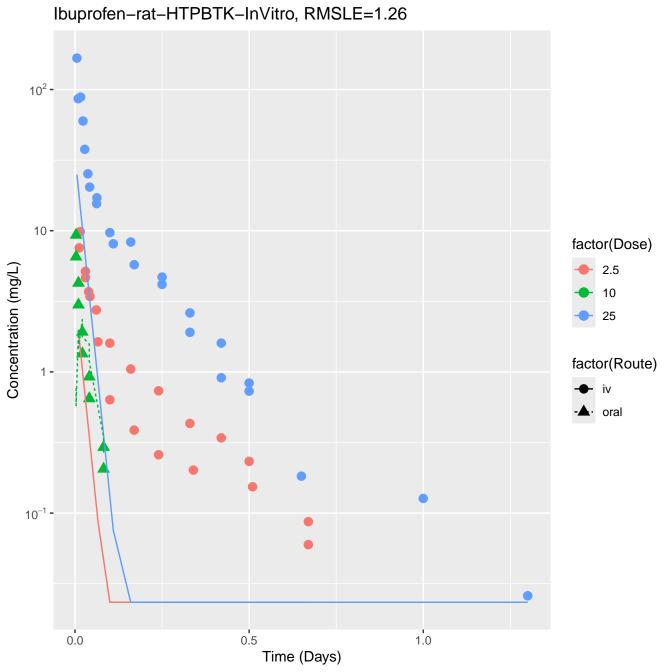


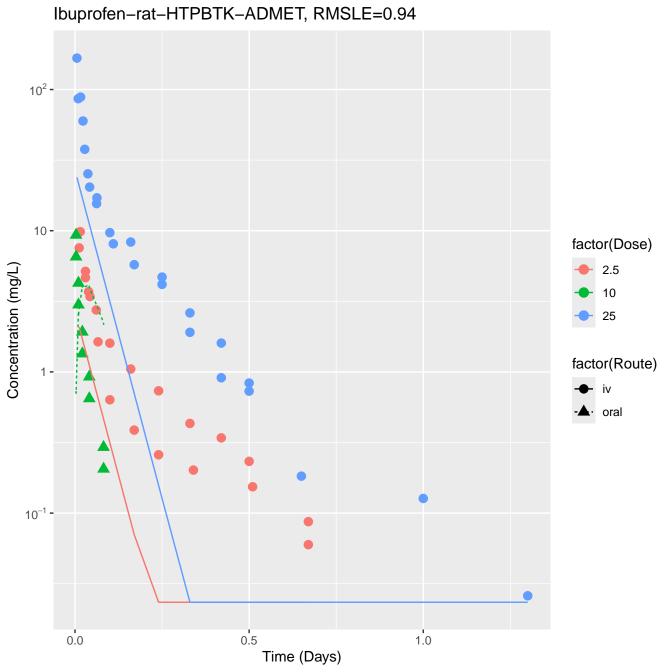


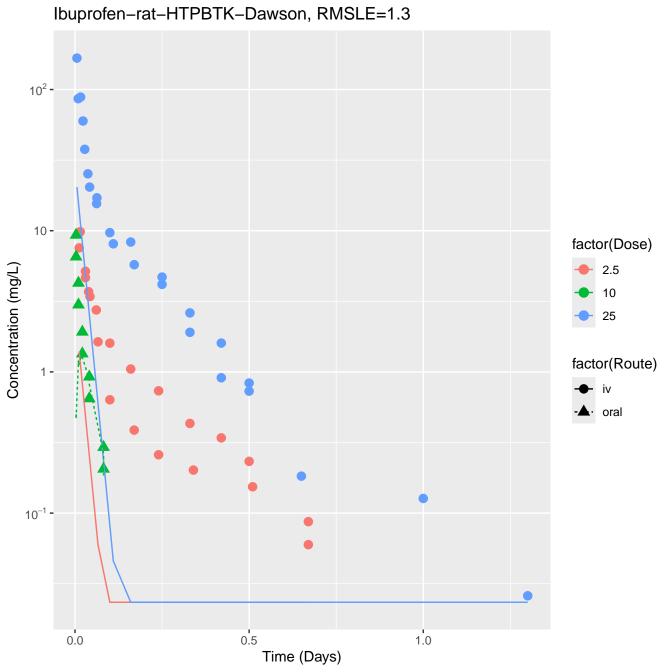


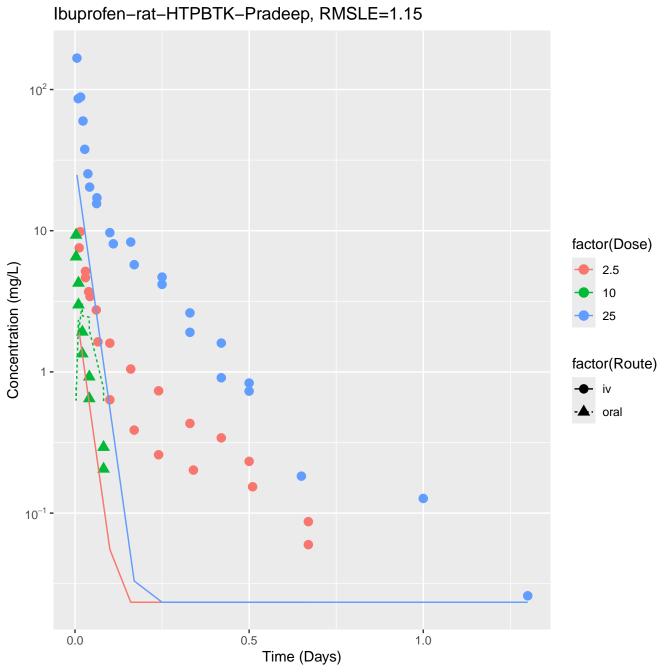


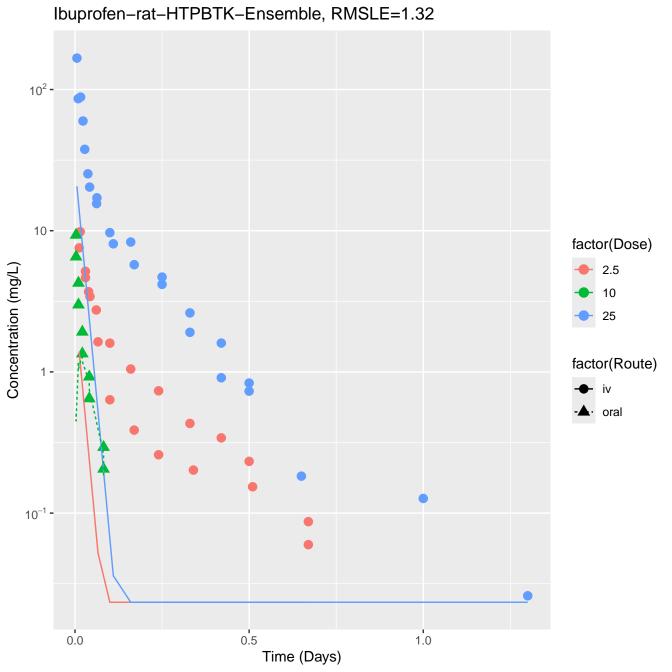


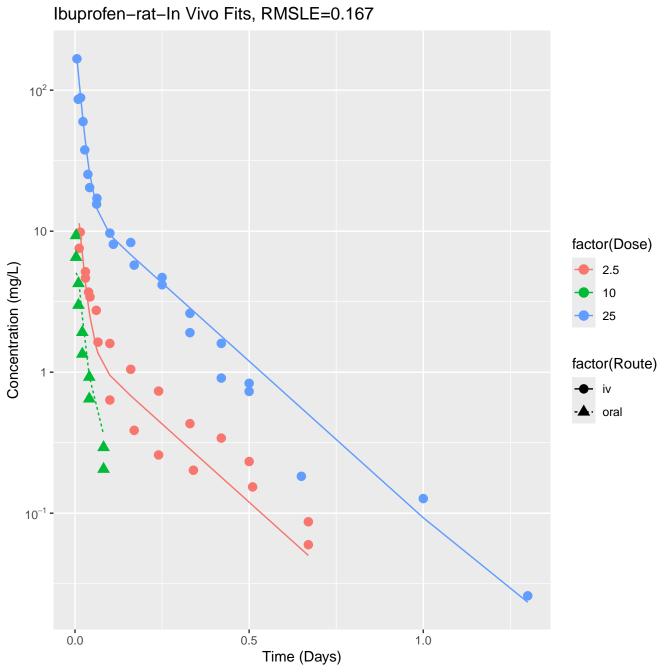


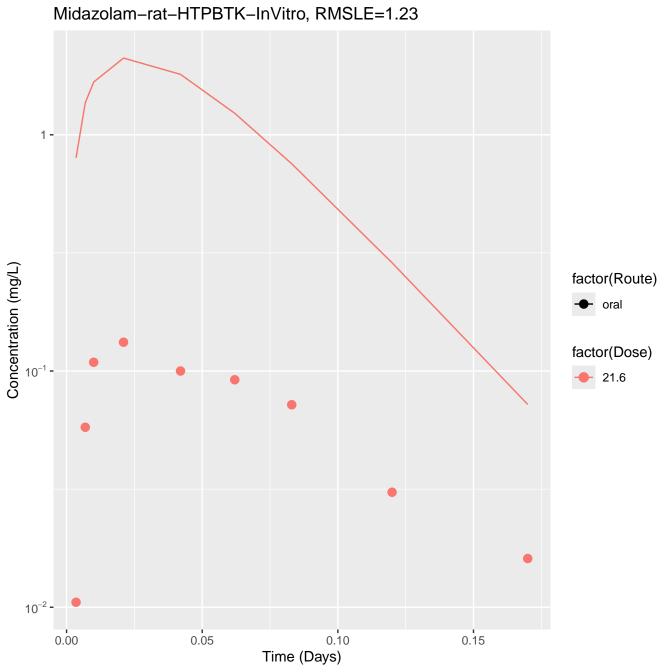


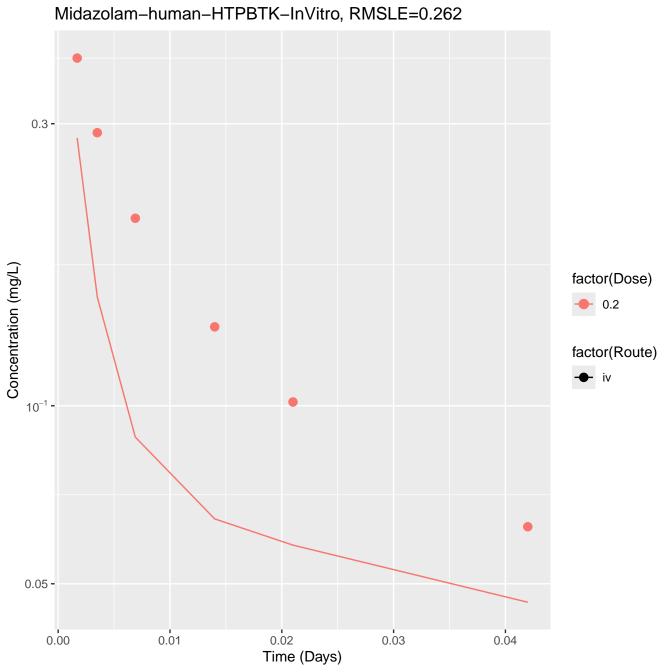


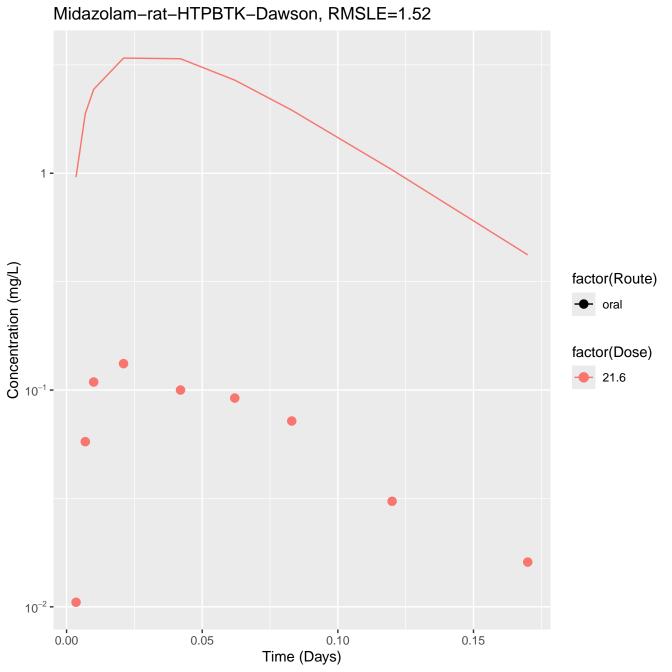






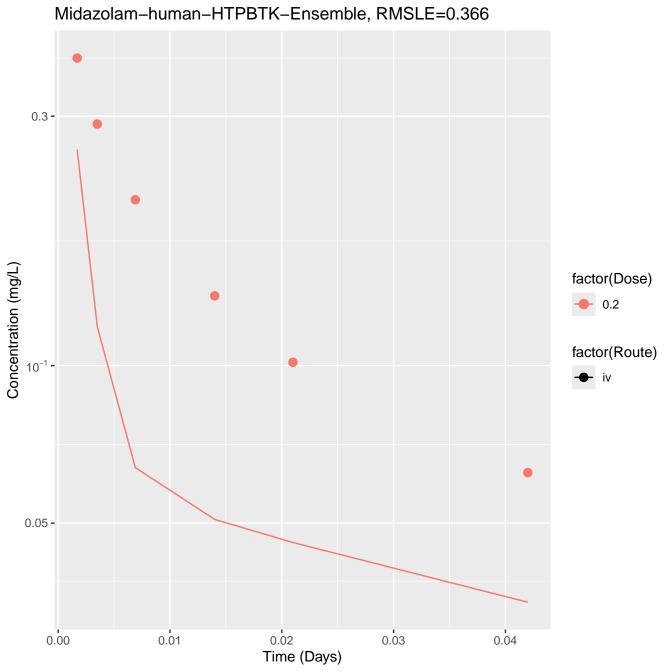


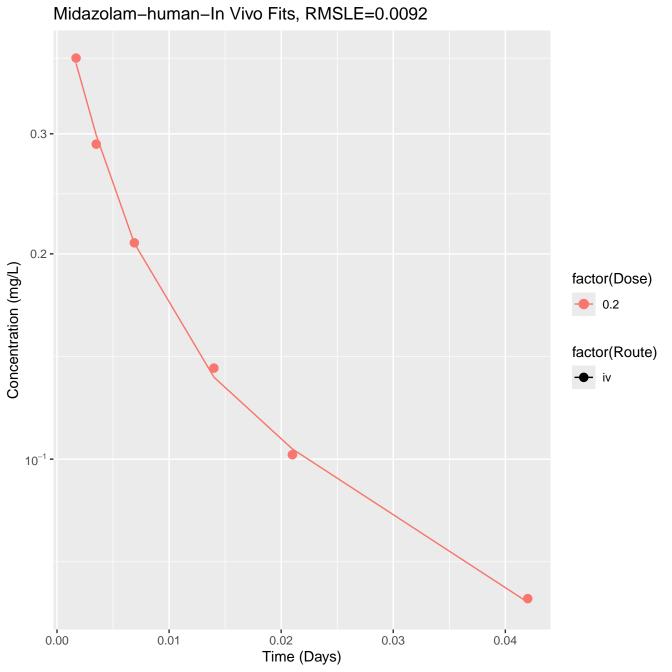


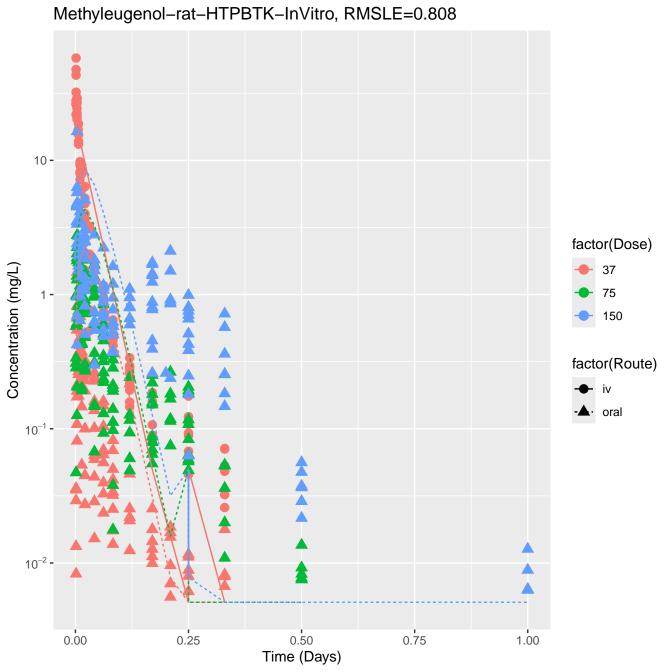


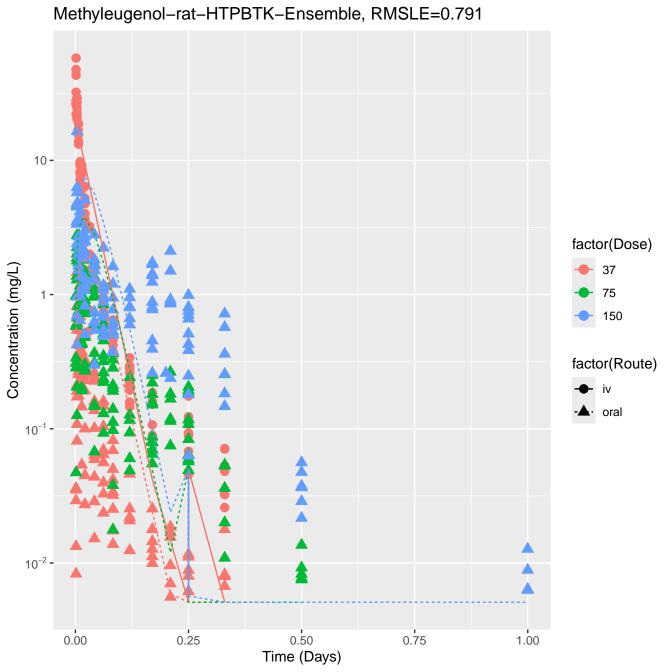
Midazolam-human-HTPBTK-Dawson, RMSLE=0.222 0.3 -Concentration (mg/L) factor(Dose) 0.2 factor(Route) ⊢ iv 10<sup>-1</sup> -0.05 -0.01 0.02 0.03 0.04 0.00 Time (Days)

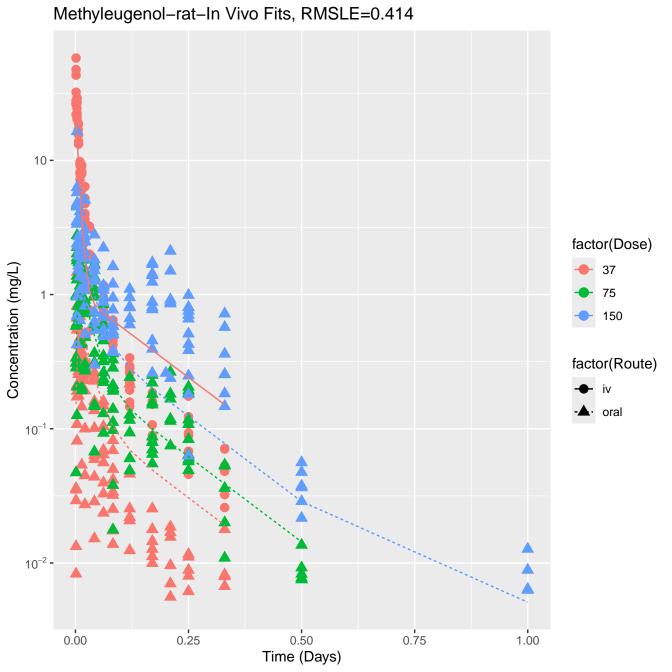
Midazolam-rat-HTPBTK-Ensemble, RMSLE=0.554 0.3 -10<sup>-1</sup> Concentration (mg/L) factor(Route) ⊢ oral factor(Dose) 21.6 0.03 -10<sup>-2</sup> 0.10 0.00 0.05 0.15 Time (Days)

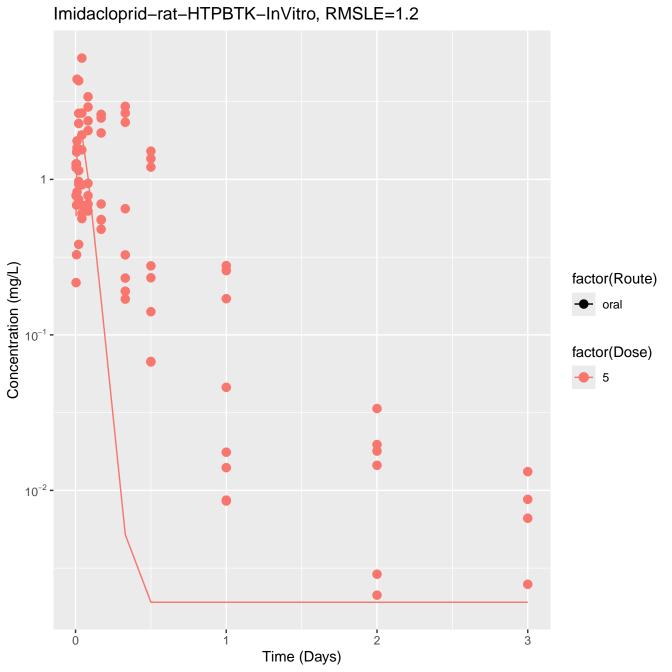


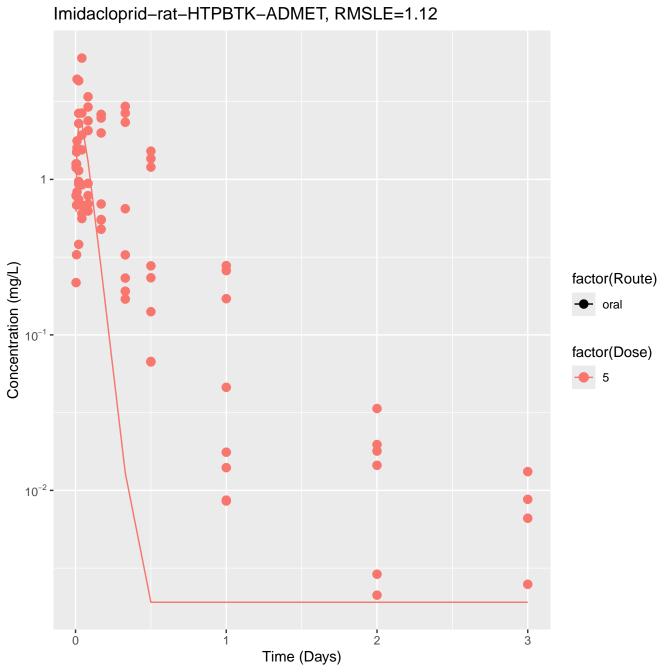


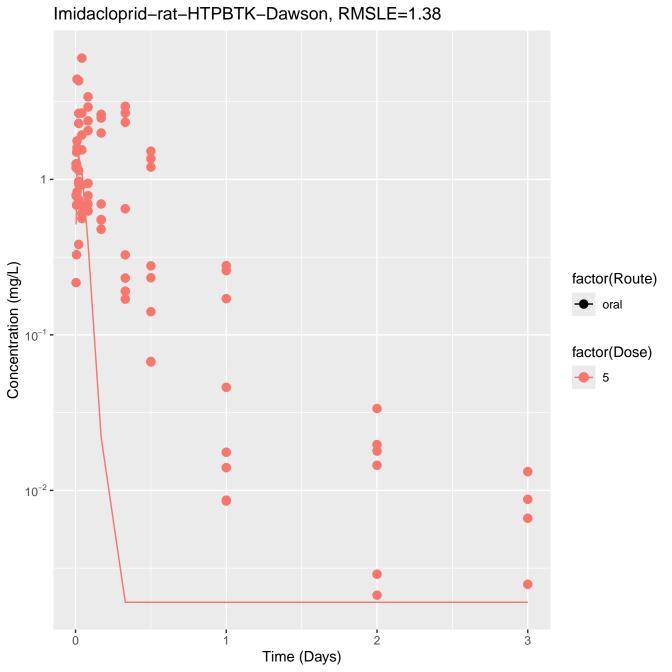


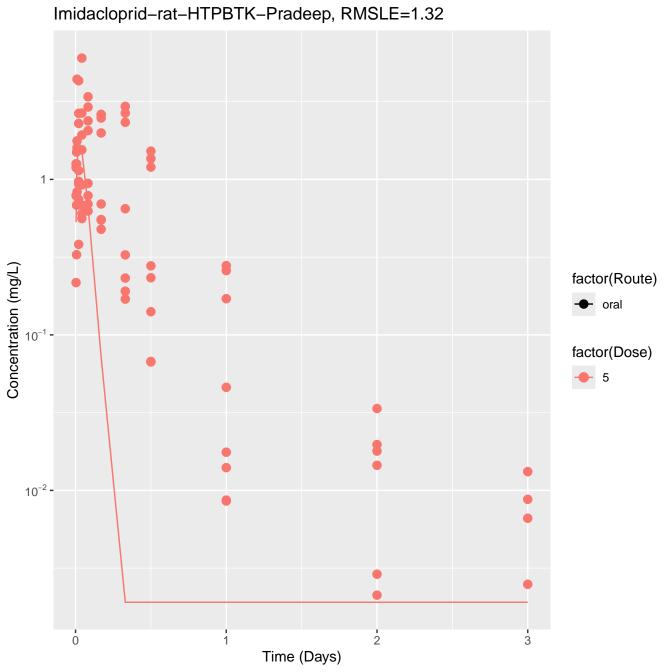


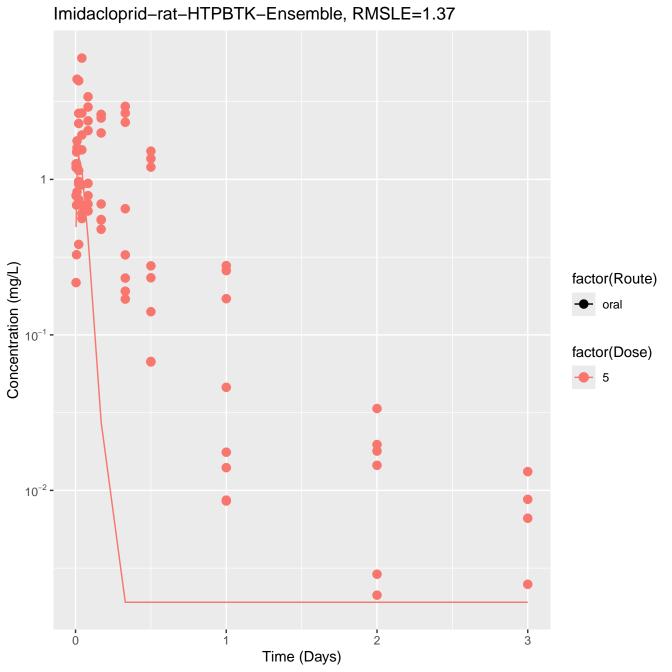


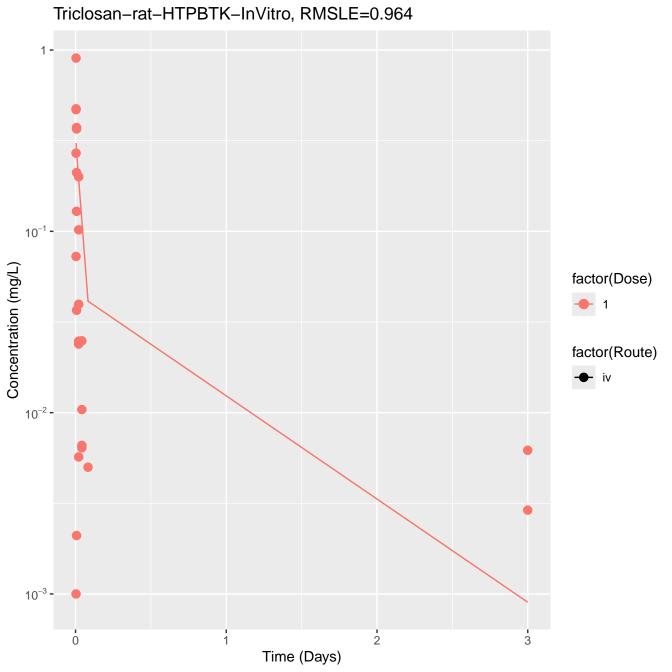


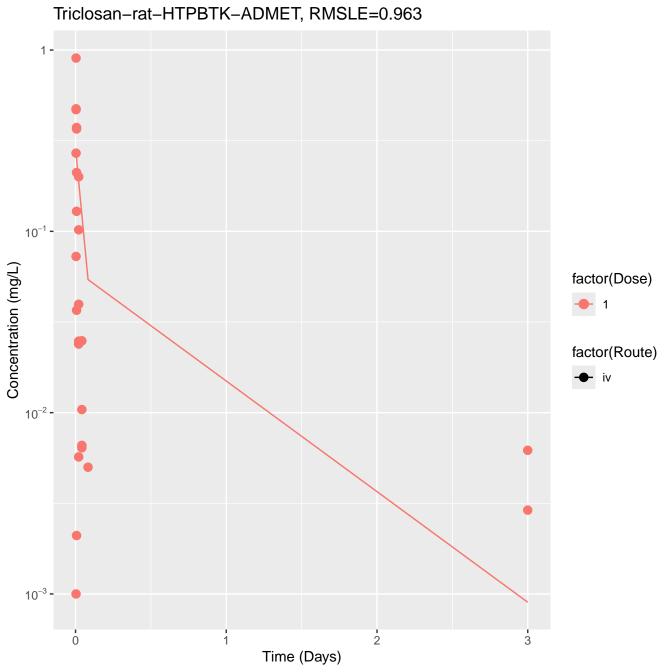


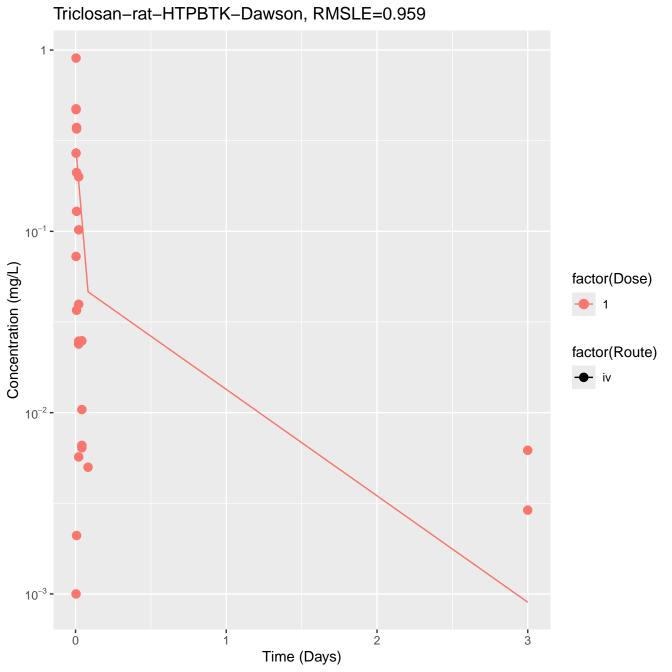


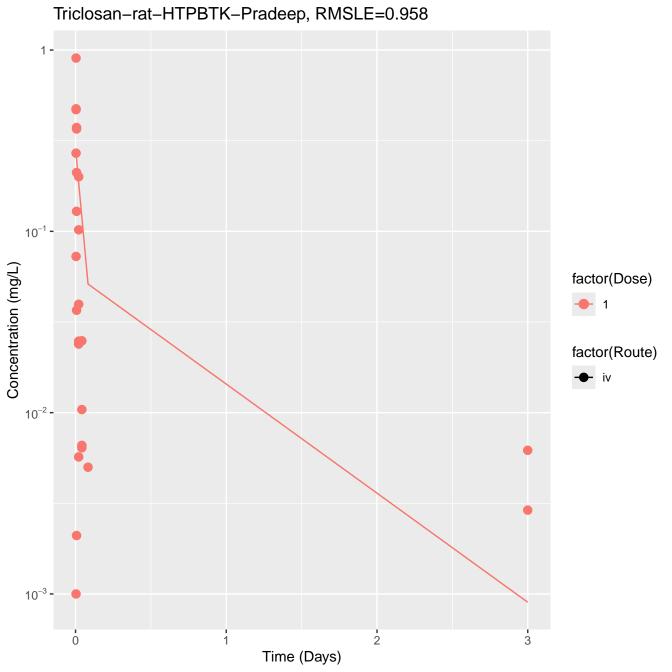


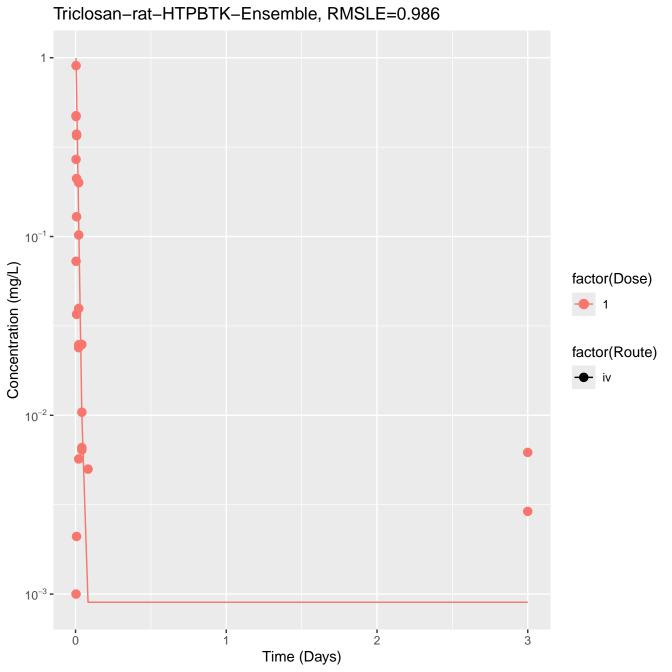


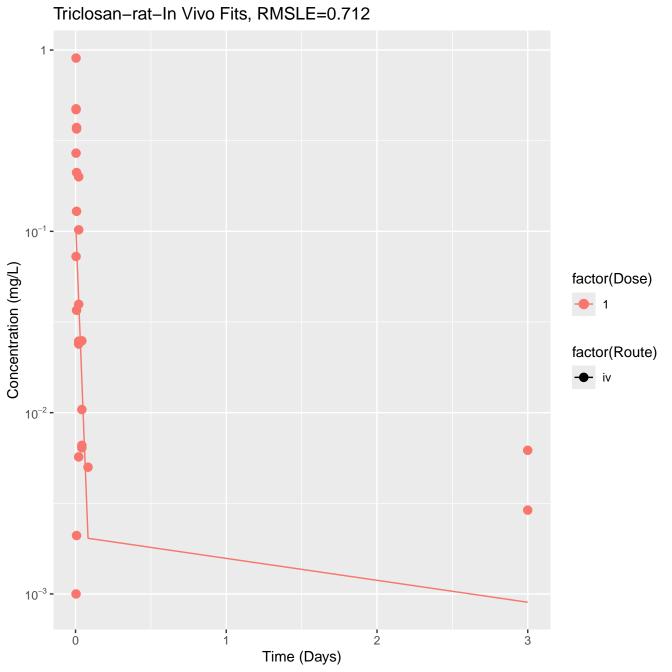


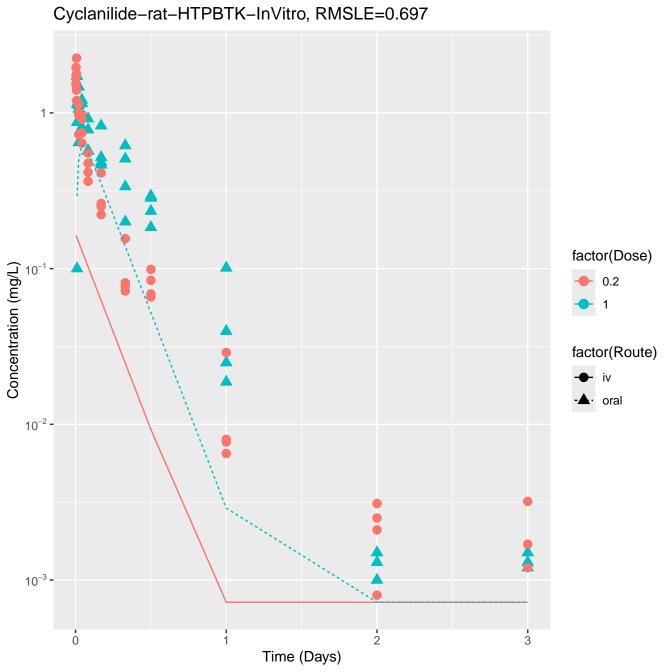


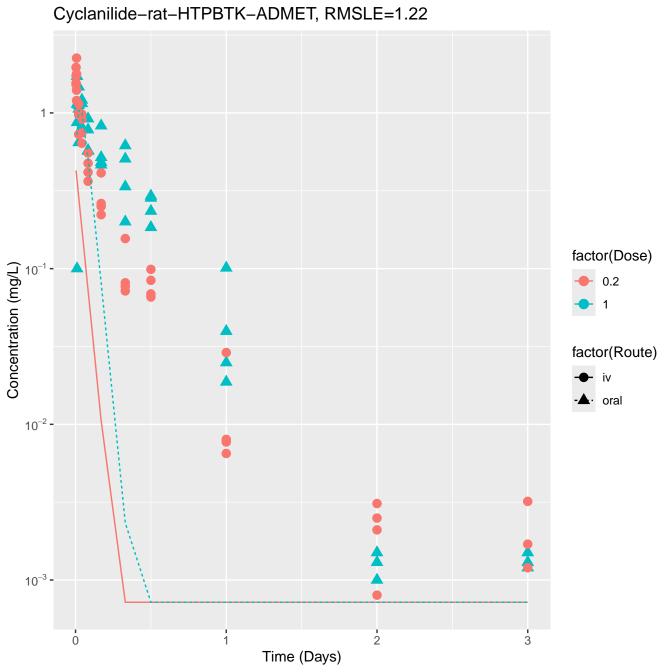


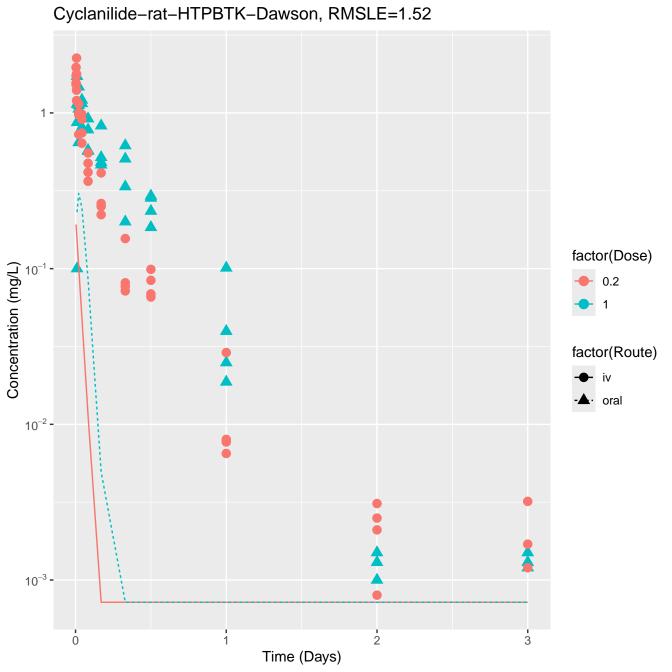


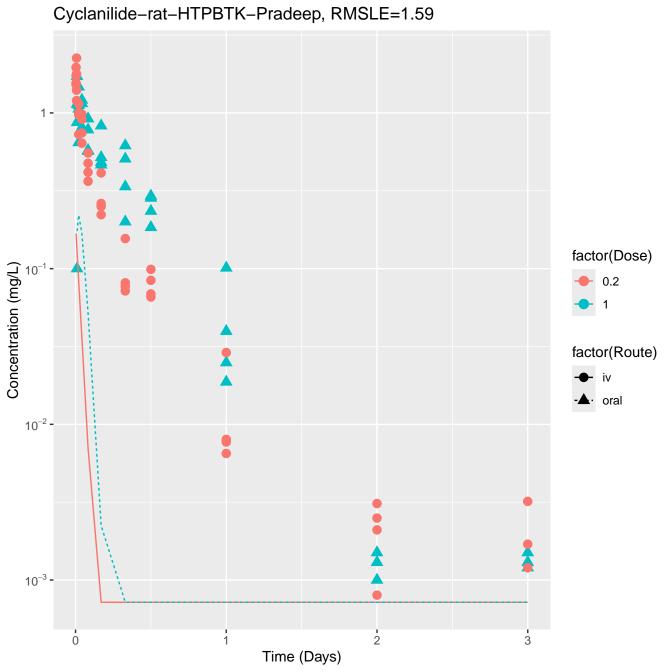


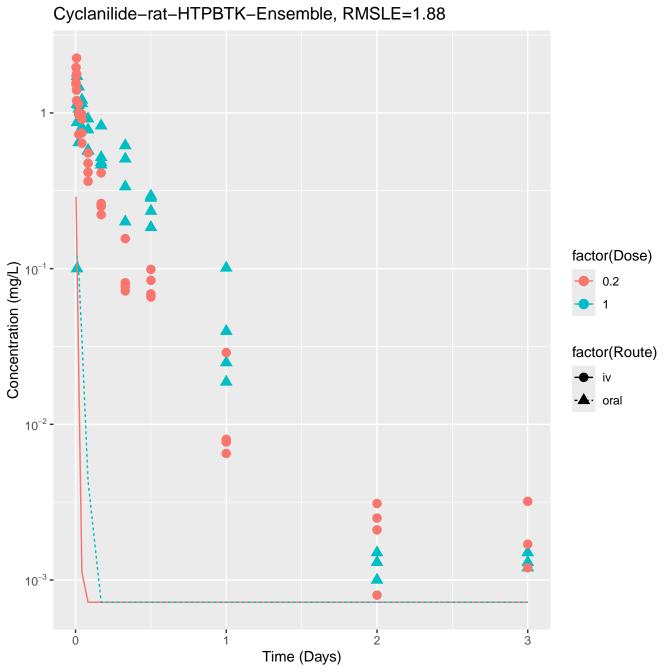


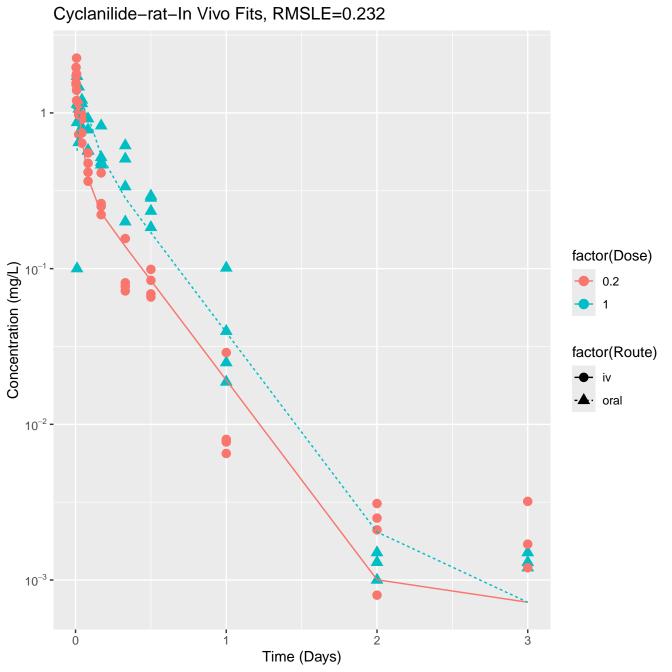


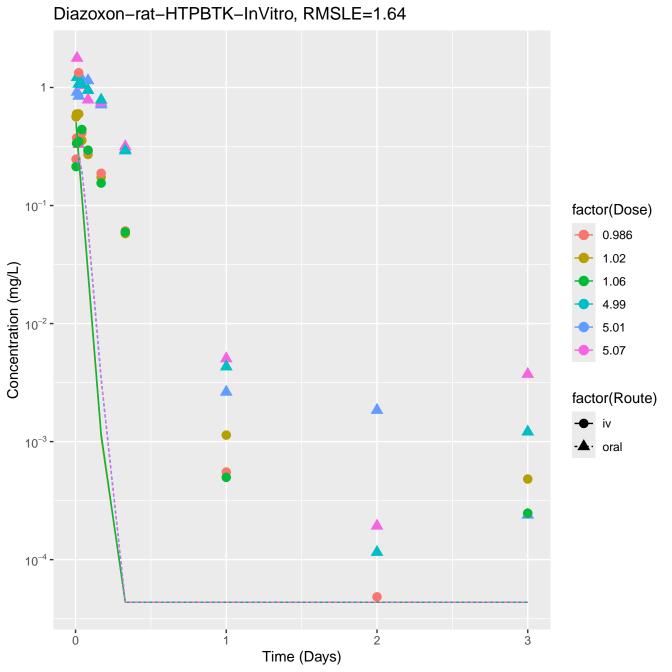


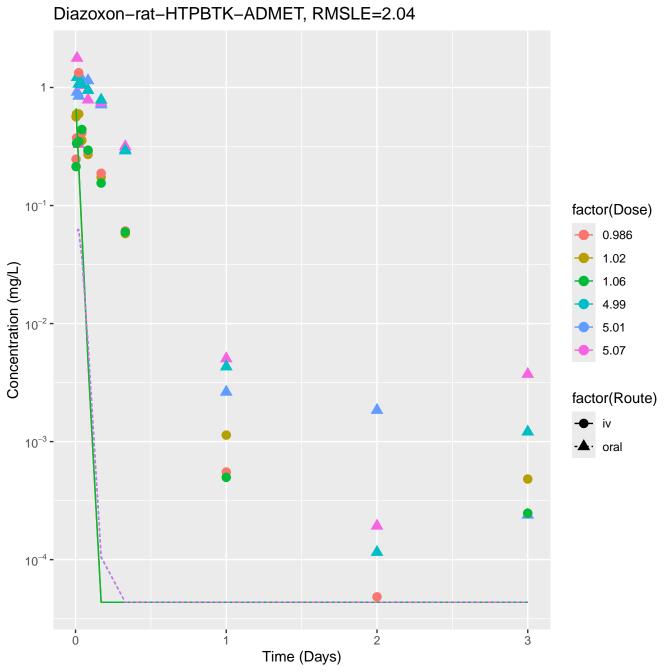


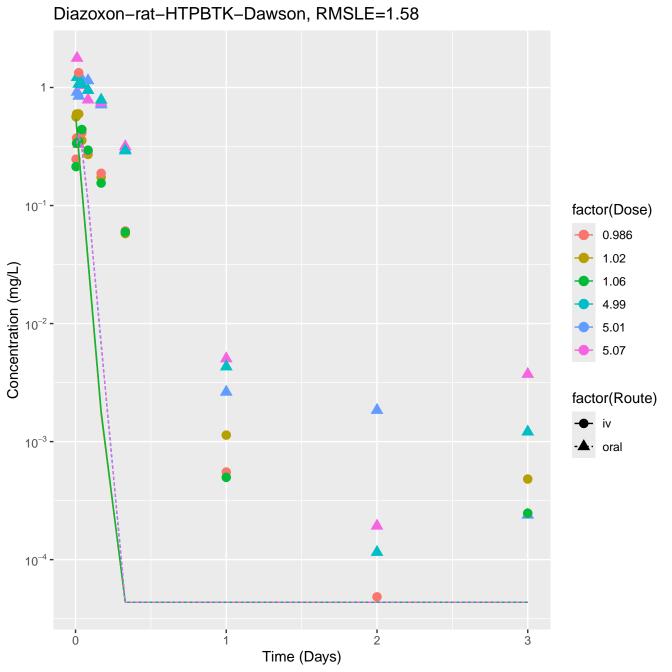


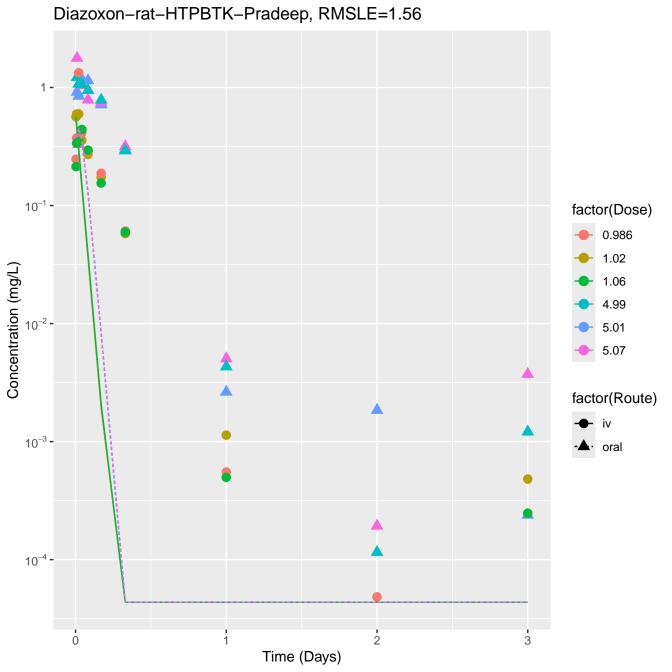


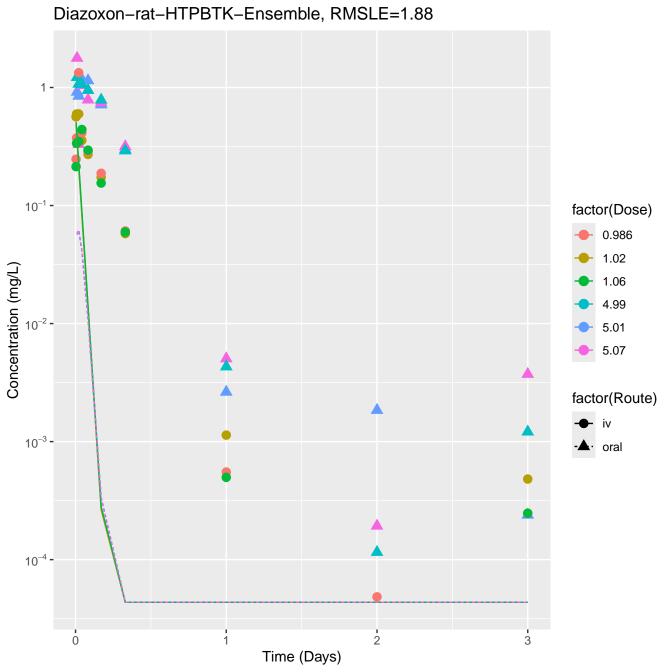


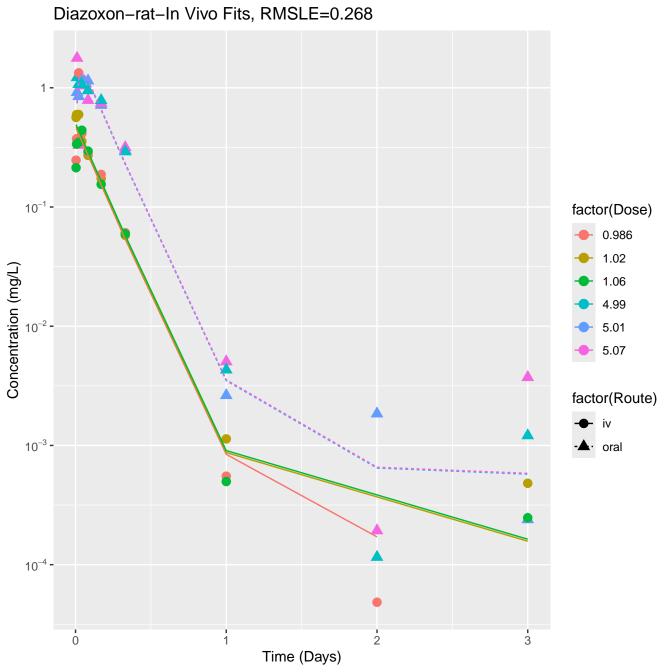


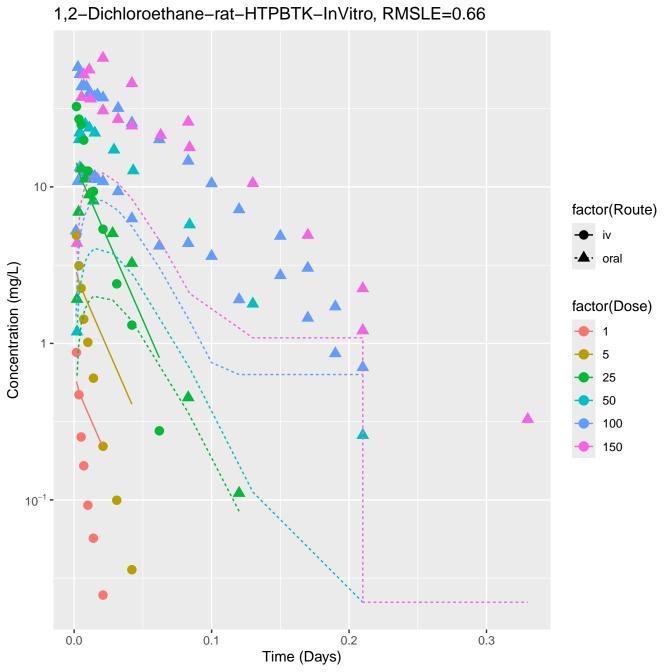


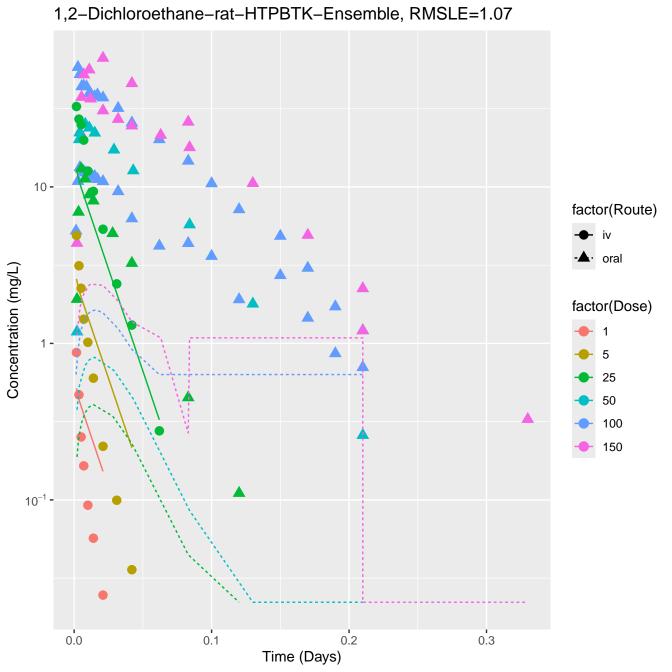


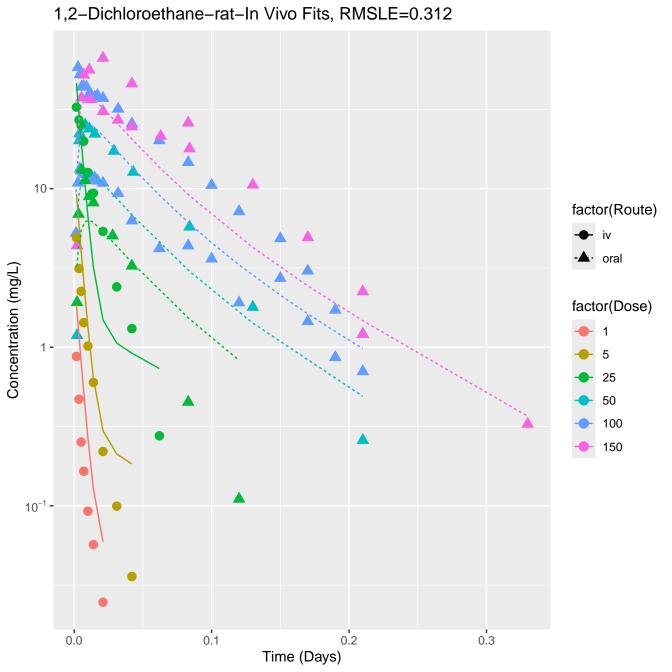


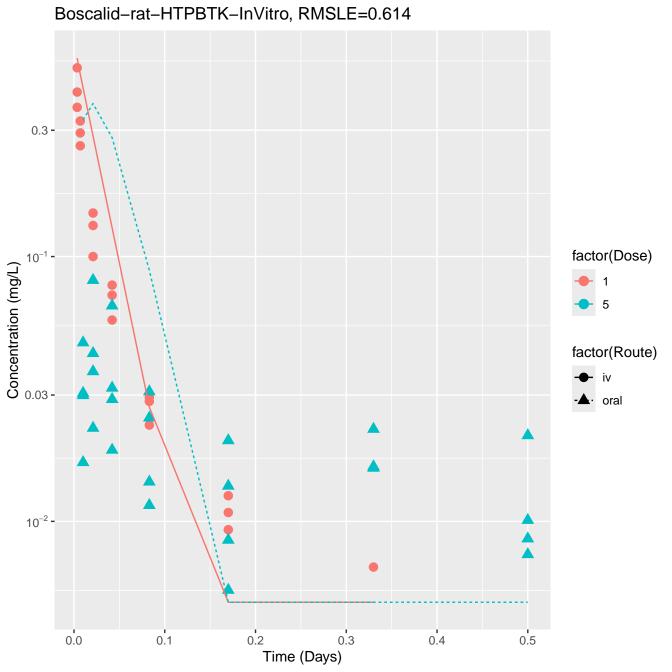


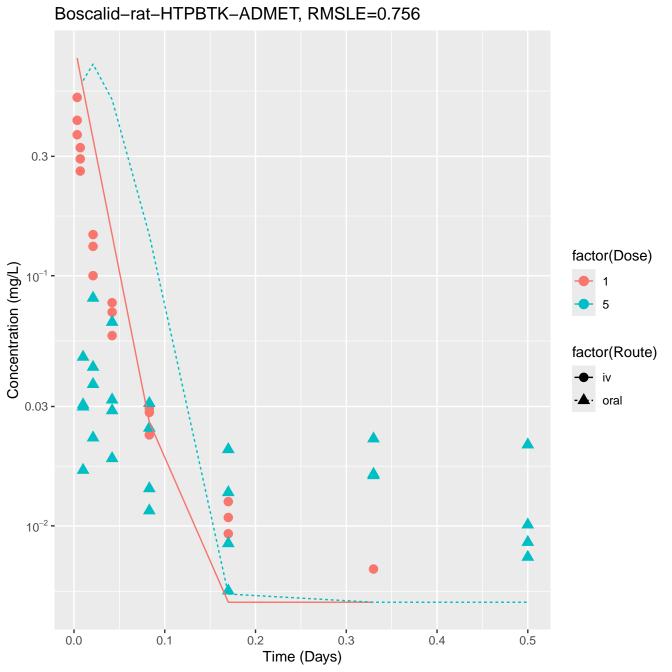


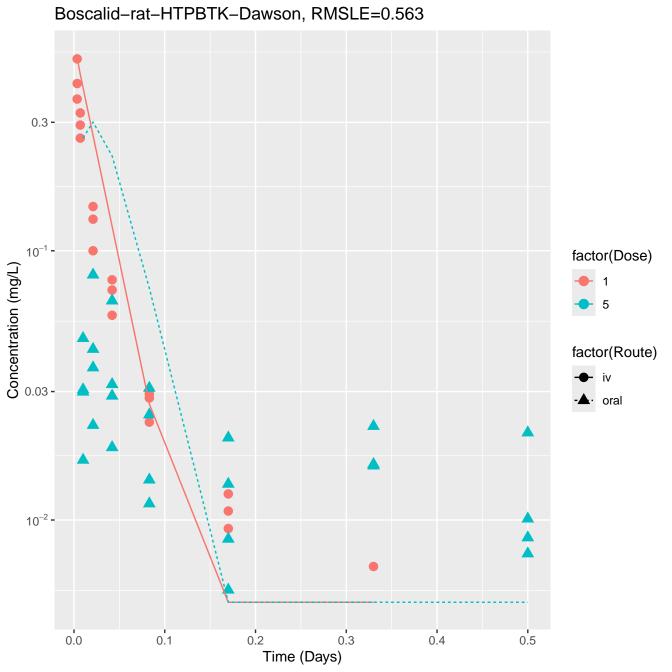


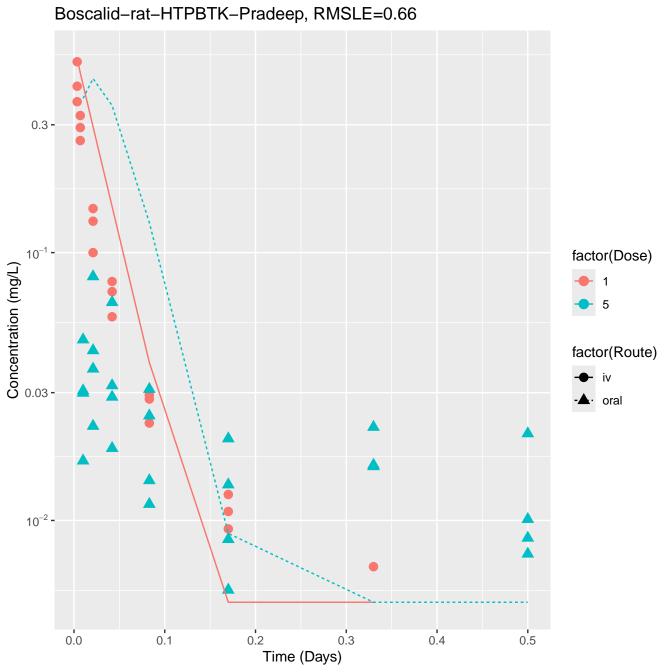


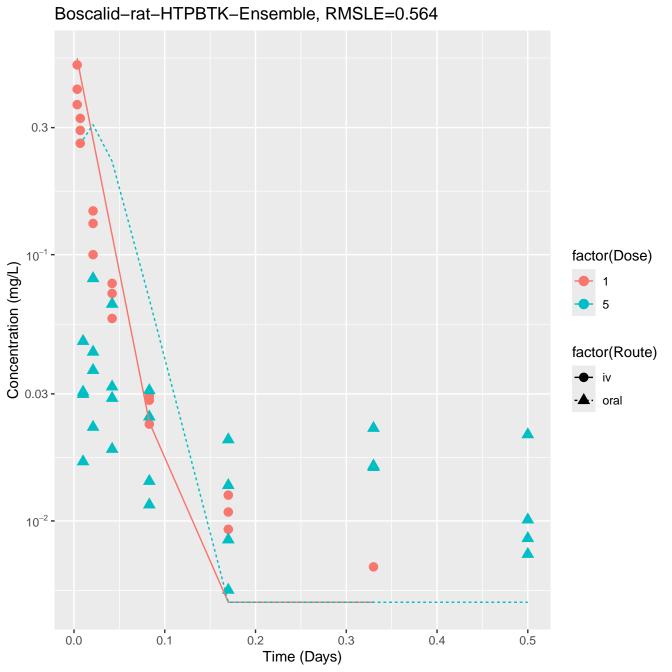


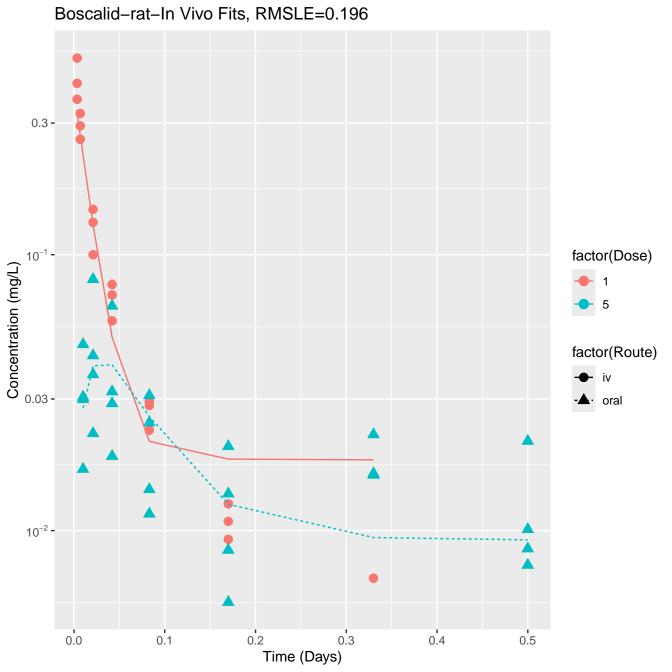










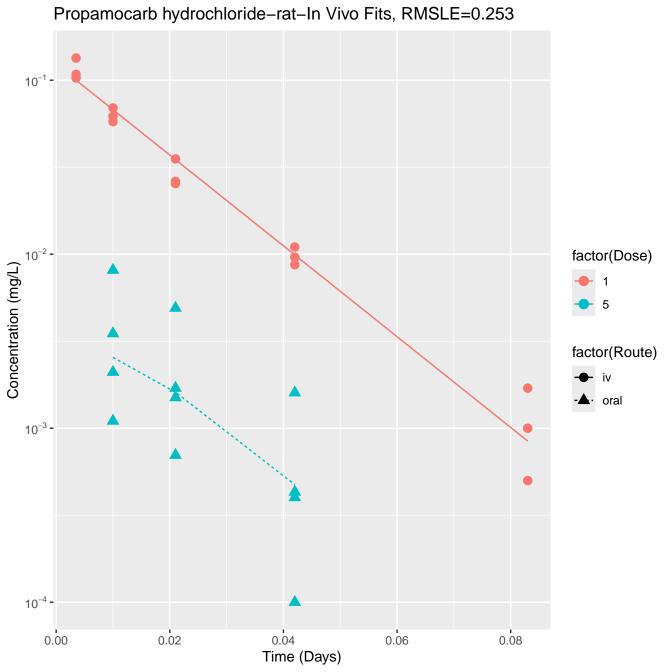


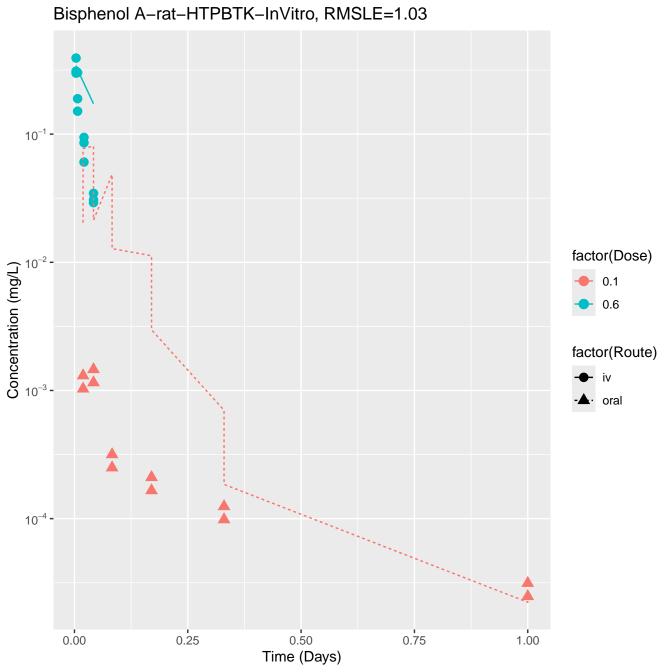
Propamocarb hydrochloride-rat-HTPBTK-InVitro, RMSLE=2.2 1 -10<sup>-1</sup> factor(Dose) Concentration (mg/L) 10<sup>-2</sup> factor(Route) iv · oral 10<sup>-3</sup> -10<sup>-4</sup> -0.02 0.04 0.00 0.06 0.08 Time (Days)

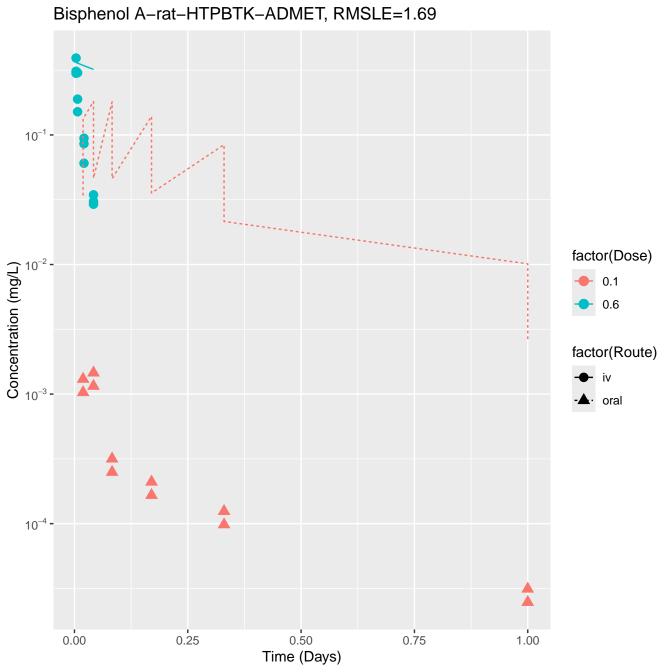
Propamocarb hydrochloride-rat-HTPBTK-ADMET, RMSLE=1.93 10<sup>-1</sup> factor(Dose) Concentration (mg/L) 10<sup>-2</sup> factor(Route) iv · oral 10<sup>-3</sup> -10<sup>-4</sup> -0.02 0.04 0.00 0.06 0.08 Time (Days)

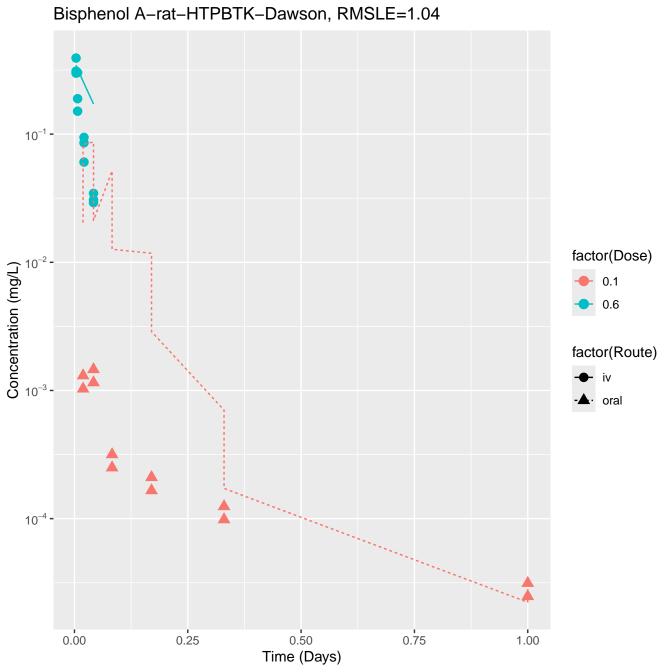
Propamocarb hydrochloride-rat-HTPBTK-Dawson, RMSLE=2.43 1 -10<sup>-1</sup> factor(Dose) Concentration (mg/L) 10<sup>-2</sup> factor(Route) iv · oral 10<sup>-3</sup> -10<sup>-4</sup> -0.02 0.00 0.04 0.06 0.08 Time (Days)

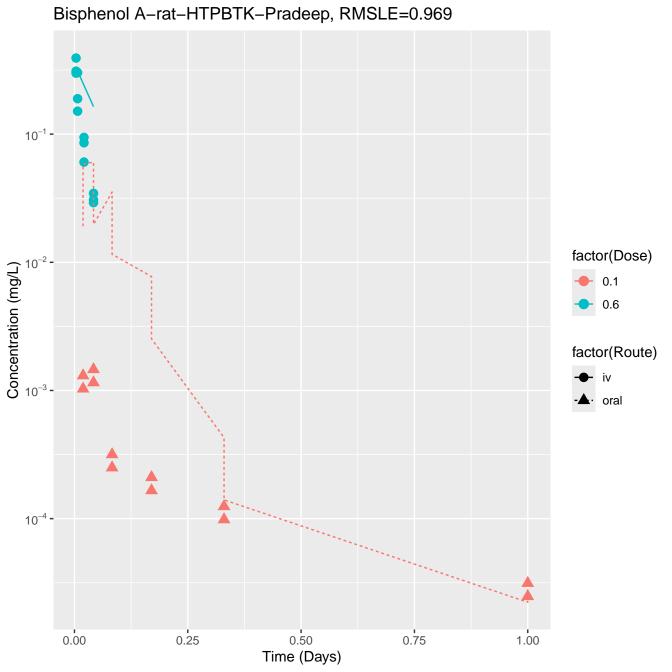
Propamocarb hydrochloride-rat-HTPBTK-Ensemble, RMSLE=1.94 10<sup>-1</sup> factor(Dose) Concentration (mg/L) 10<sup>-2</sup> factor(Route) iv · oral 10<sup>-3</sup> -10<sup>-4</sup> -0.02 0.04 0.00 0.06 0.08 Time (Days)

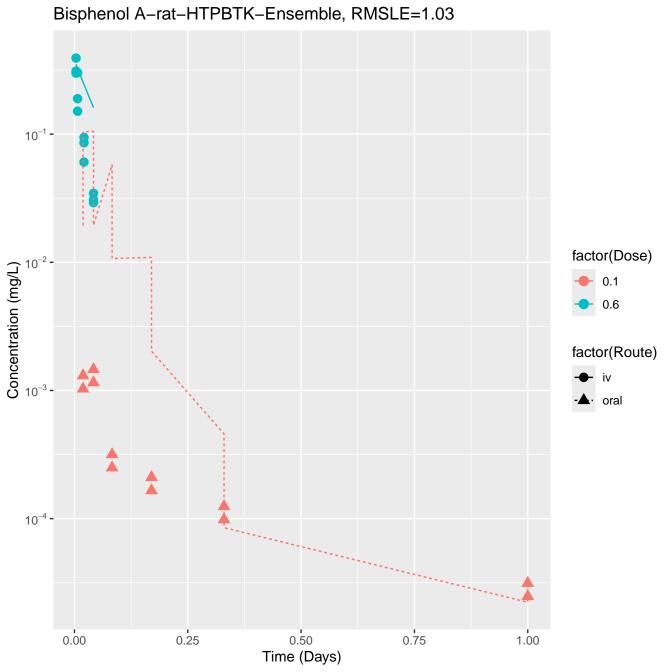


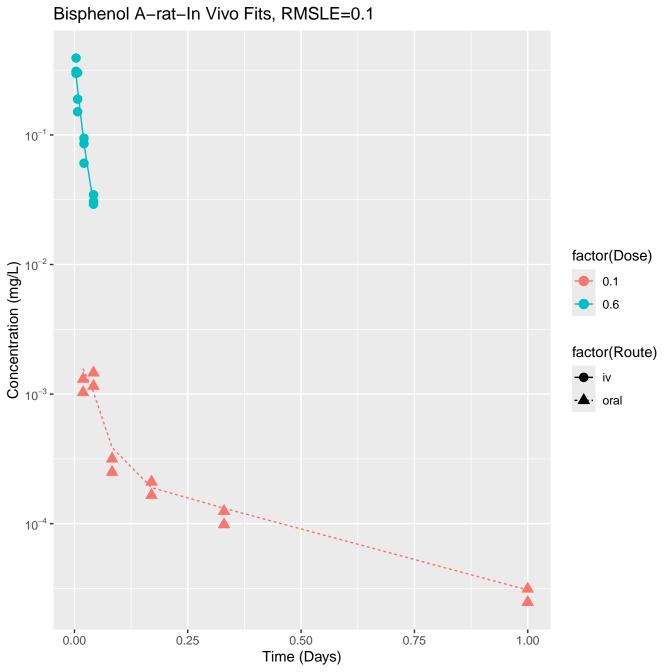




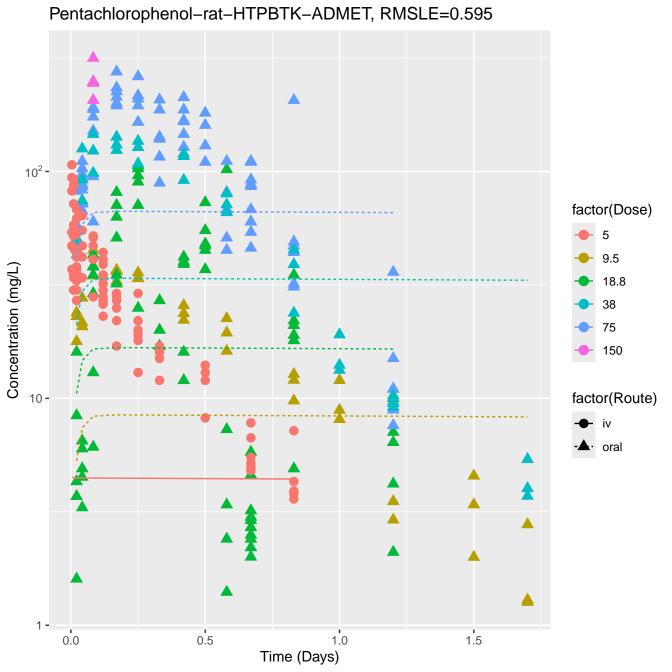


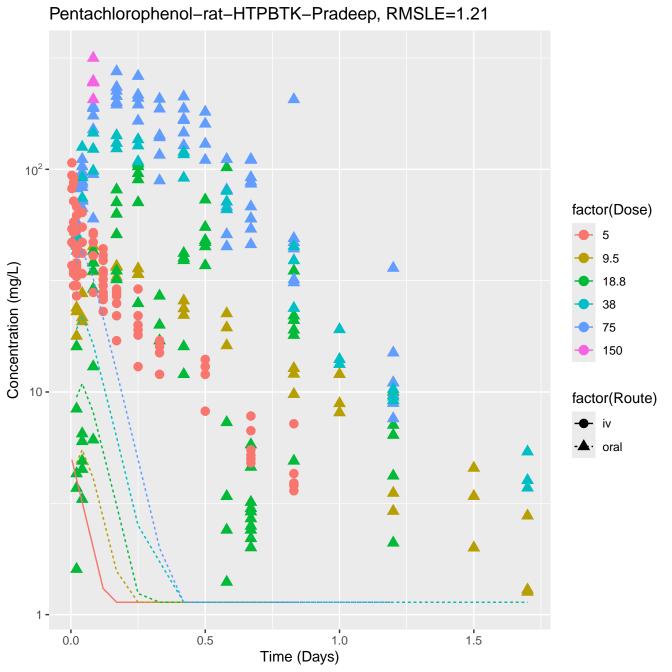


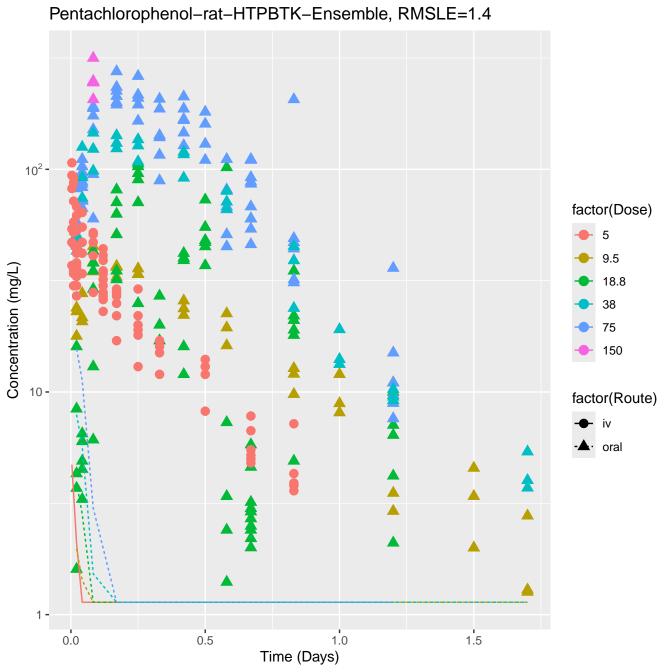




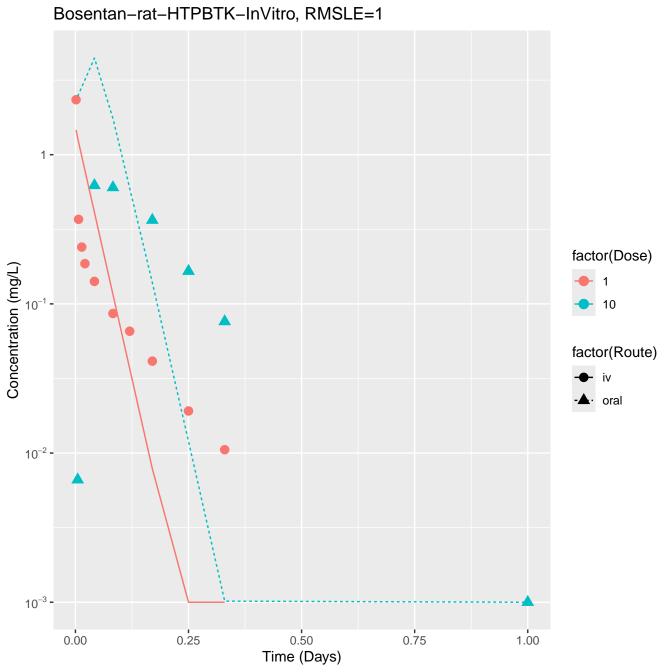
Pentachlorophenol-rat-HTPBTK-InVitro, RMSLE=0.872 10<sup>2</sup> factor(Dose) 5 9.5 Concentration (mg/L) 18.8 38 75 150 10 factor(Route) oral 1 -0.5 0.0 1.0 1.5 Time (Days)

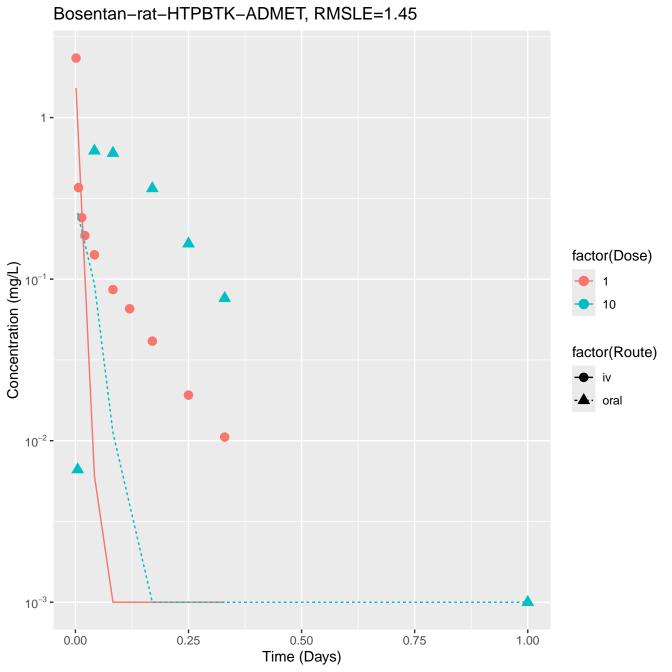


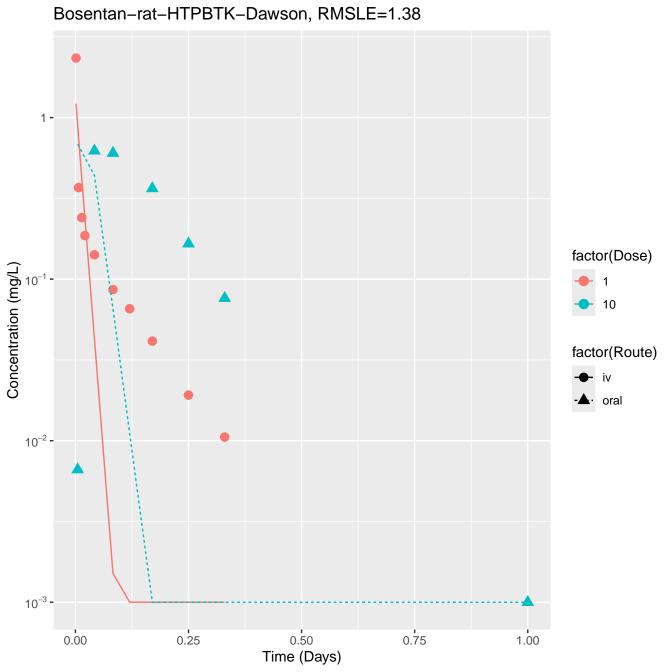


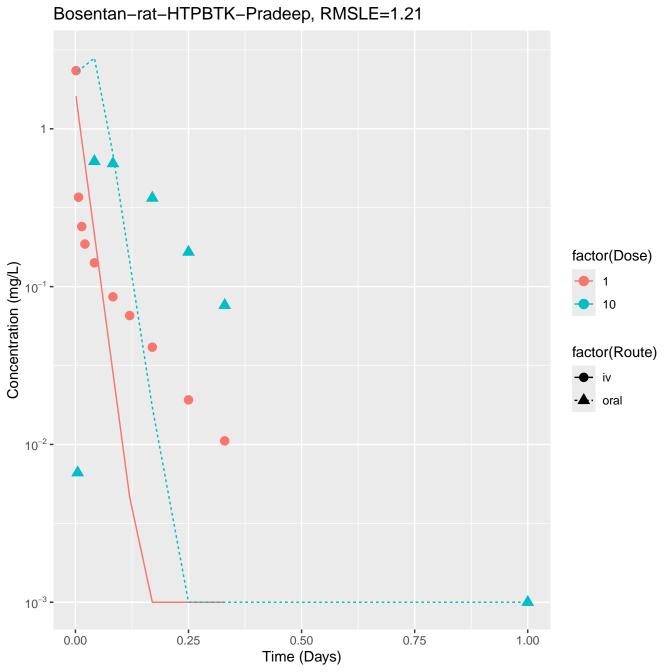


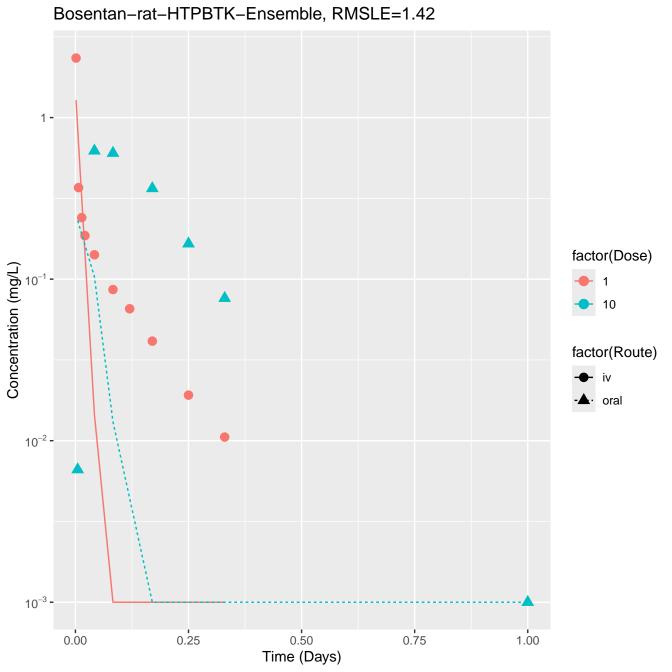
Pentachlorophenol-rat-In Vivo Fits, RMSLE=0.293 10<sup>2</sup> factor(Dose) 5 9.5 Concentration (mg/L) 18.8 38 75 150 10 factor(Route) oral 1 -0.0 0.5 1.0 1.5 Time (Days)



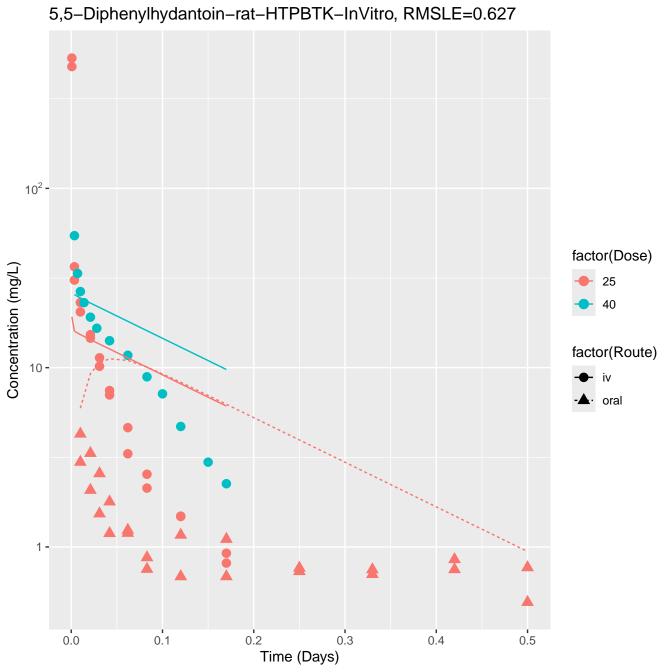


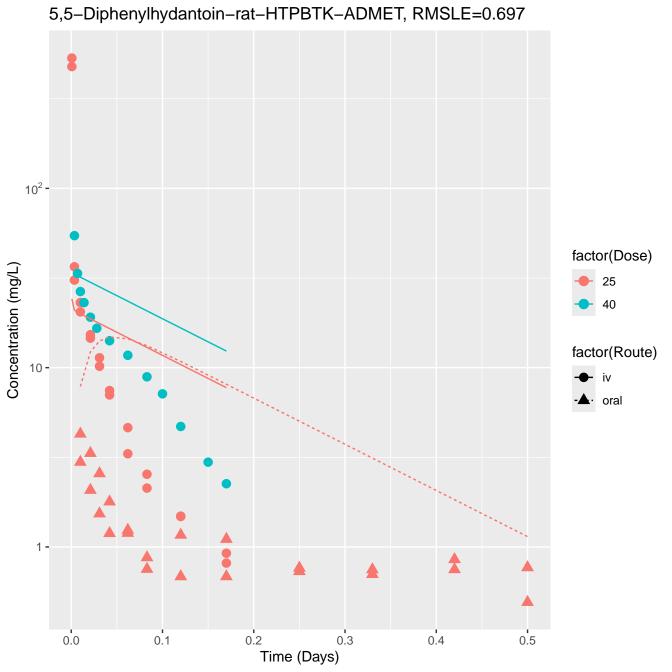


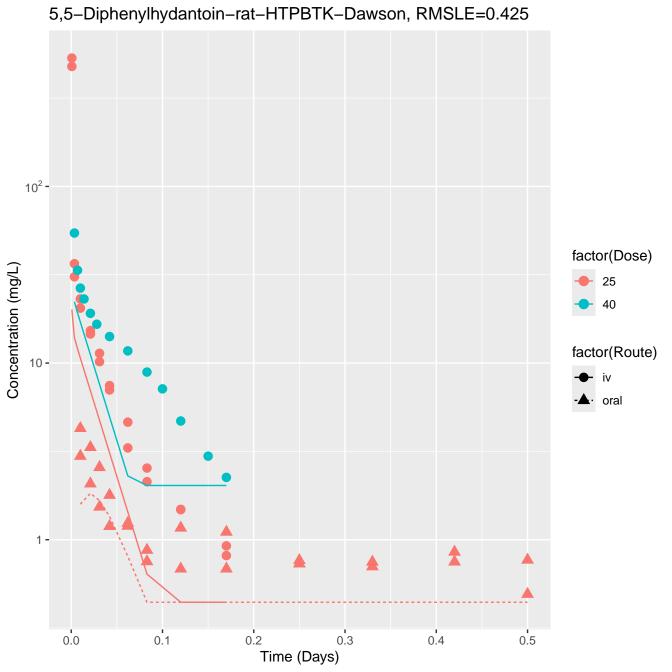


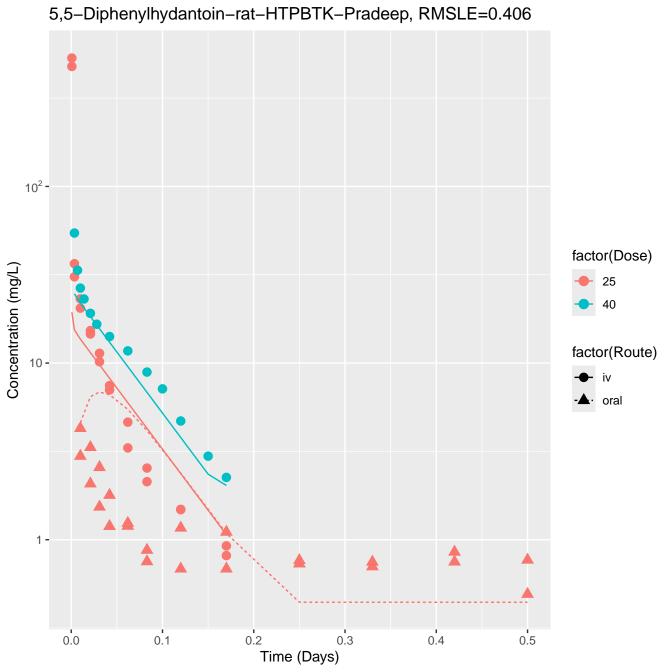


Bosentan-rat-In Vivo Fits, RMSLE=0.321 1 factor(Dose) Concentration (mg/L) 10 factor(Route) iv · oral 10<sup>-2</sup> -10<sup>-3</sup> -0.25 0.50 0.75 0.00 1.00 Time (Days)

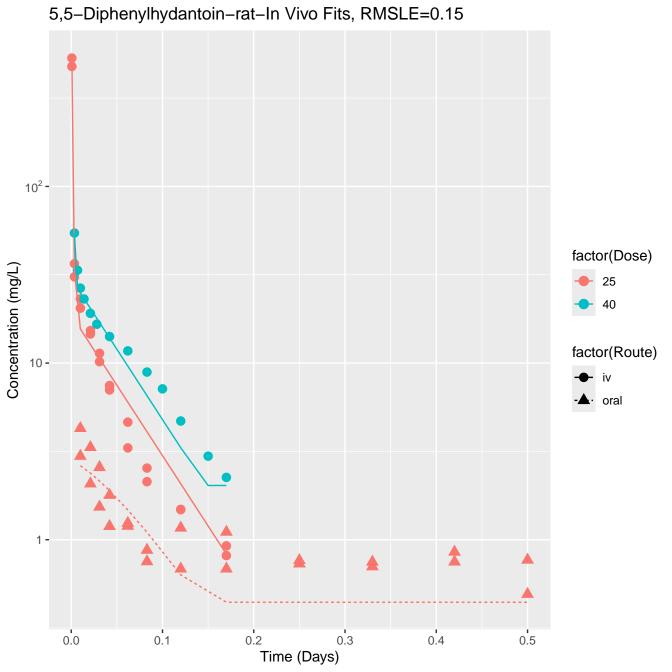


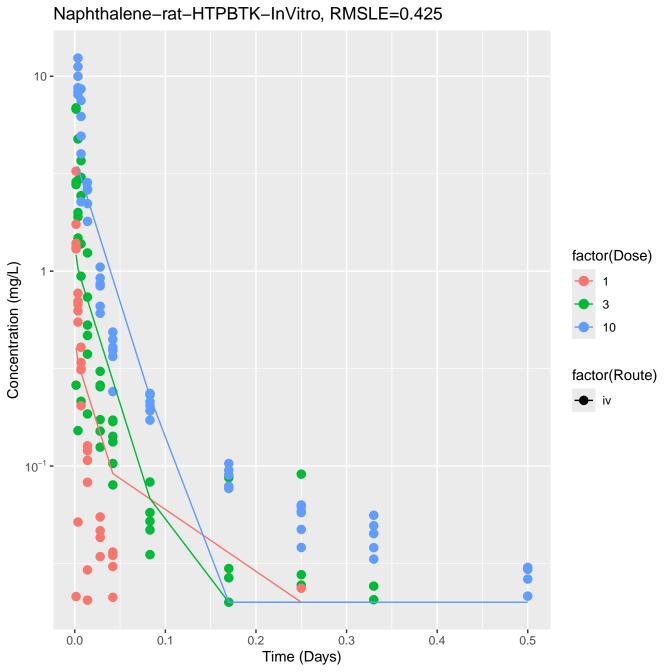


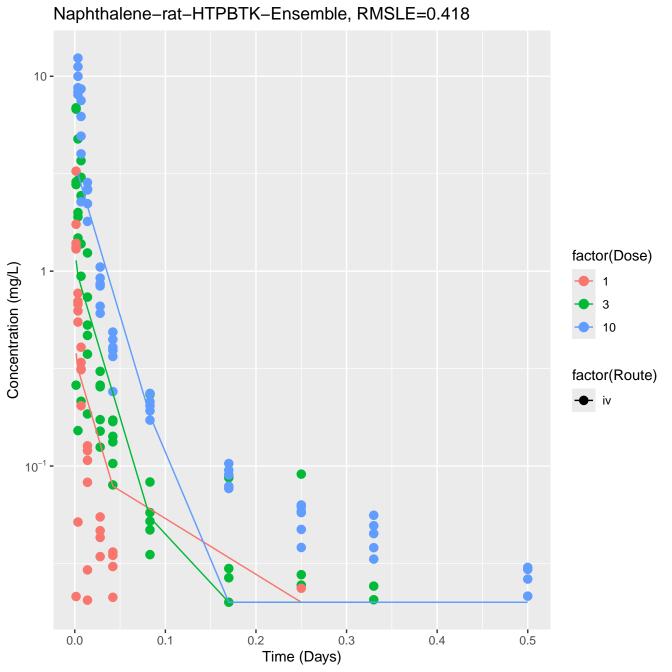


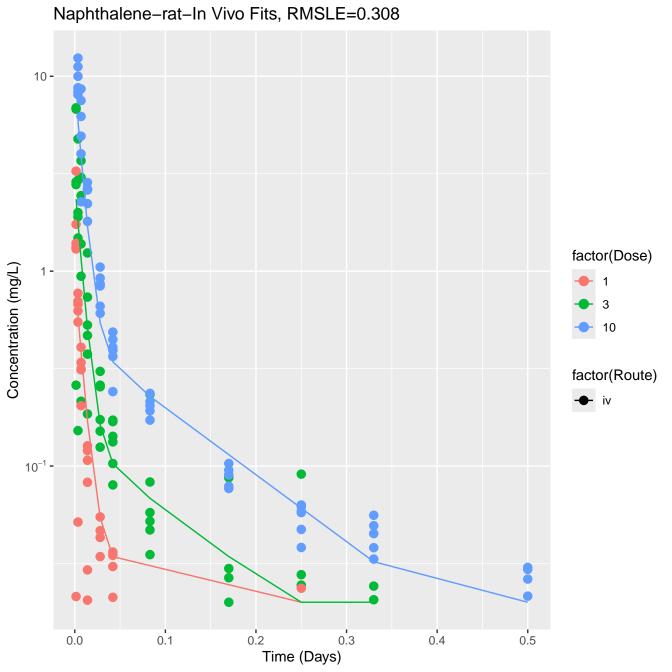


5,5-Diphenylhydantoin-rat-HTPBTK-Ensemble, RMSLE=0.425 10<sup>2</sup> factor(Dose) Concentration (mg/L) 25 40 factor(Route) 10 iv · oral 1 -0.0 0.1 0.2 0.3 0.4 0.5 Time (Days)









Tolbutamide-rat-HTPBTK-InVitro, RMSLE=0.521 10<sup>2</sup> factor(Dose) Concentration (mg/L) 10 factor(Route) iv · oral 1 -0.25 0.50 0.75 0.00 1.00 Time (Days)

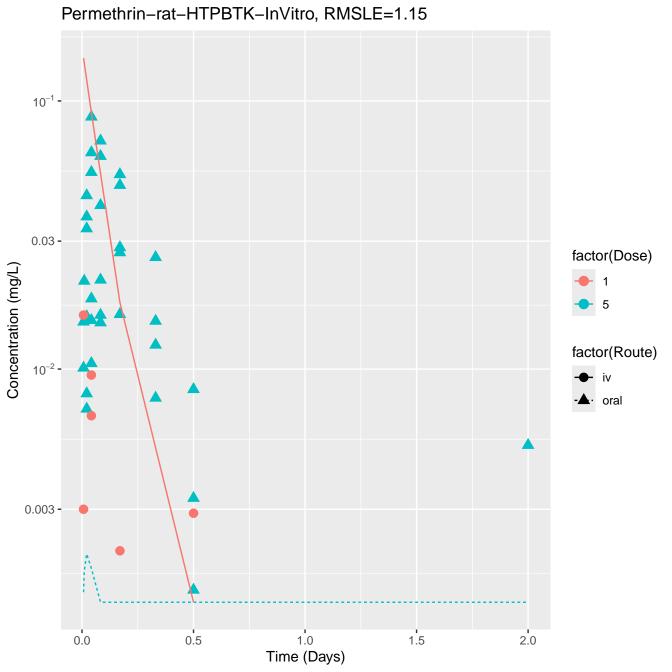
Tolbutamide-rat-HTPBTK-ADMET, RMSLE=0.536 10<sup>2</sup> factor(Dose) Concentration (mg/L) 10 factor(Route) iv · oral 1 -0.50 0.75 0.00 0.25 1.00 Time (Days)

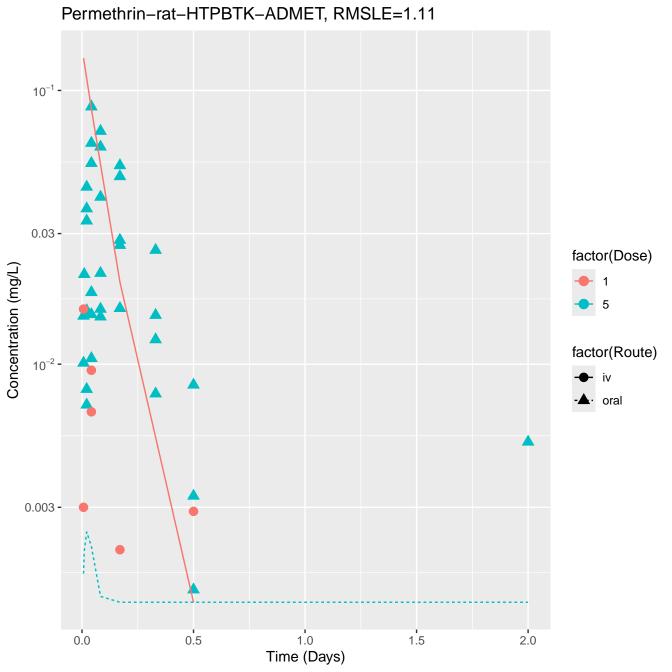
Tolbutamide-rat-HTPBTK-Dawson, RMSLE=0.536 10<sup>2</sup> factor(Dose) Concentration (mg/L) 10 factor(Route) iv · oral 1 -0.50 0.75 0.00 0.25 1.00 Time (Days)

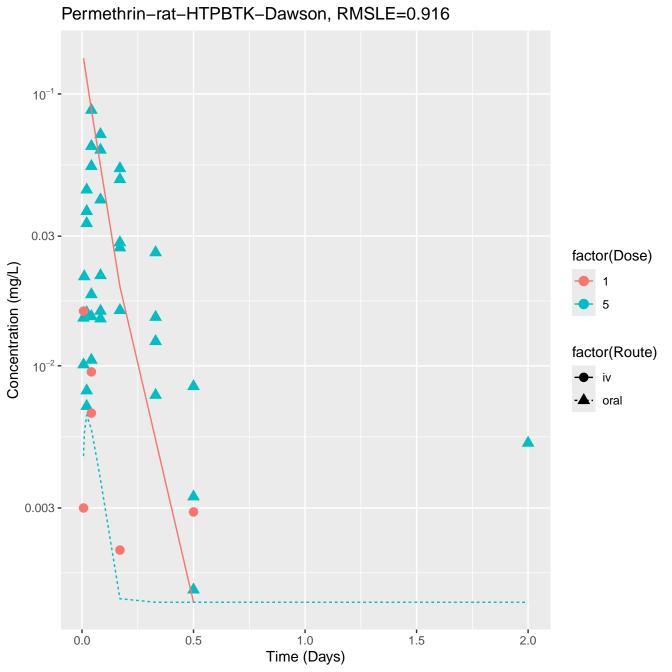
Tolbutamide-rat-HTPBTK-Pradeep, RMSLE=0.536 10<sup>2</sup> factor(Dose) Concentration (mg/L) 10 factor(Route) iv · oral 1 -0.50 0.75 0.00 0.25 1.00 Time (Days)

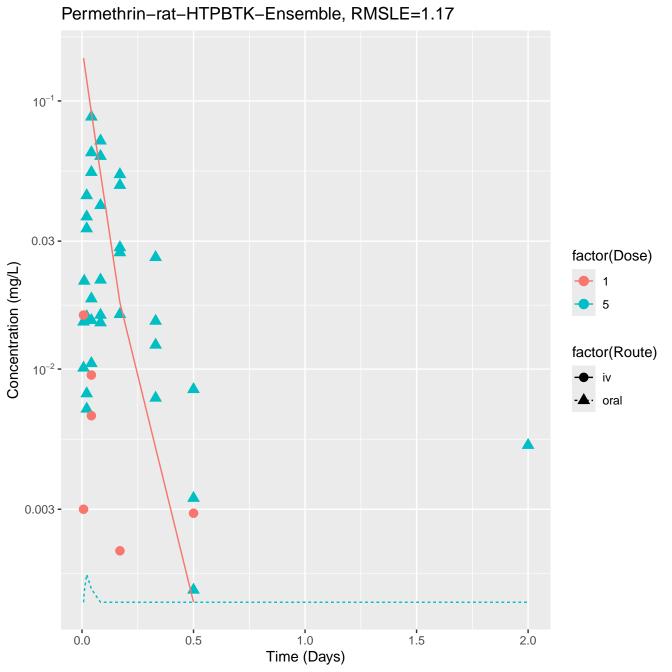
Tolbutamide-rat-HTPBTK-Ensemble, RMSLE=0.536 10<sup>2</sup> factor(Dose) Concentration (mg/L) 10 factor(Route) iv · oral 1 -0.50 0.75 0.00 0.25 1.00 Time (Days)

Tolbutamide-rat-In Vivo Fits, RMSLE=0.0942 10<sup>2</sup> factor(Dose) Concentration (mg/L) 10 factor(Route) iv oral 1 -0.50 0.75 0.00 0.25 1.00 Time (Days)





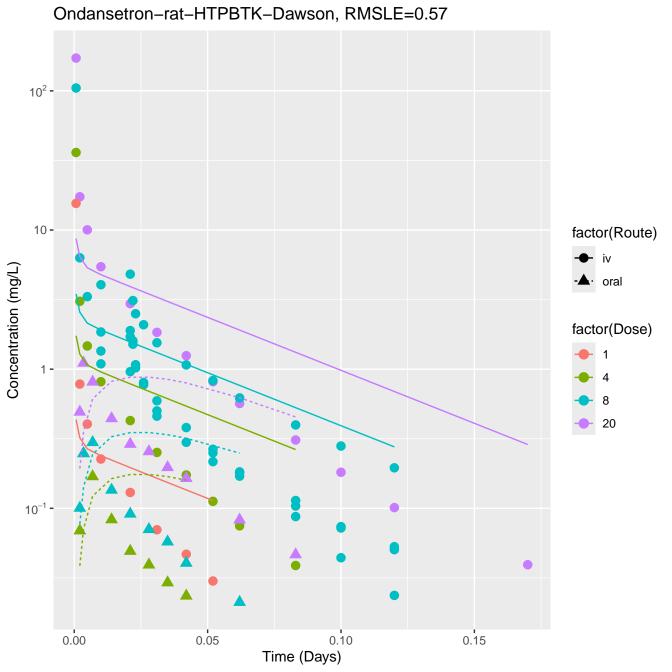


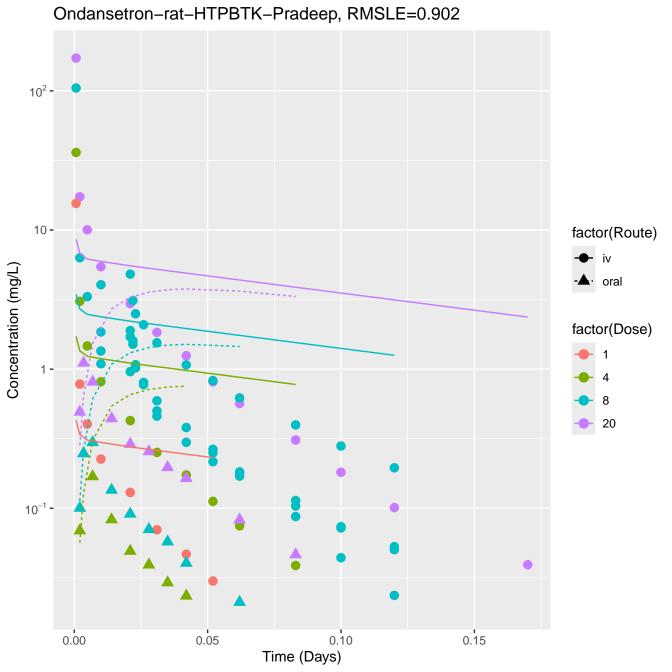


Permethrin-rat-In Vivo Fits, RMSLE=0.296 10<sup>-1</sup> -0.03 factor(Dose) Concentration (mg/L) 10<sup>-2</sup> factor(Route) iv · oral 0.003 -0.5 0.0 1.0 2.0 1.5 Time (Days)

Ondansetron-rat-HTPBTK-InVitro, RMSLE=0.932 10<sup>2</sup> -10 factor(Route) Concentration (mg/L) · oral factor(Dose) 20 10<sup>-1</sup> -0.05 0.10 0.00 0.15 Time (Days)

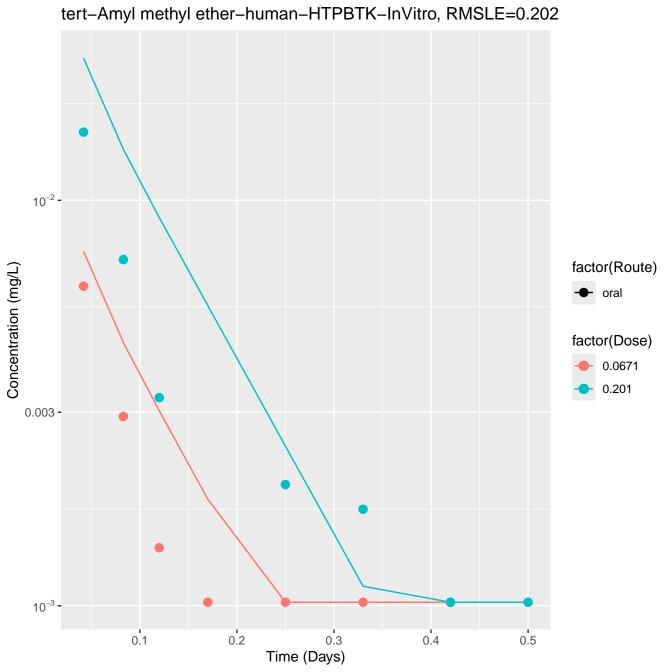
Ondansetron-rat-HTPBTK-ADMET, RMSLE=0.65 10<sup>2</sup> -10 factor(Route) Concentration (mg/L) · oral factor(Dose) 20 10<sup>-1</sup> -0.05 0.10 0.00 0.15 Time (Days)



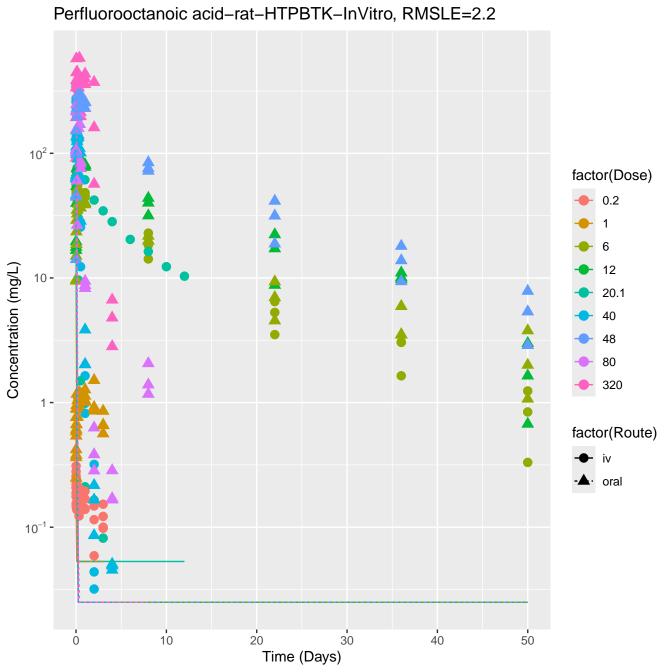


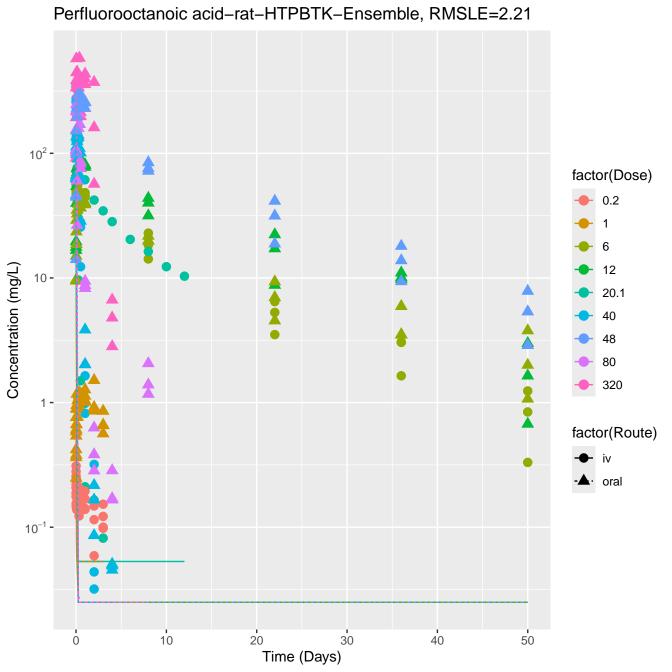
Ondansetron-rat-HTPBTK-Ensemble, RMSLE=0.577 10<sup>2</sup> -10 factor(Route) Concentration (mg/L) · oral factor(Dose) 20 10<sup>-1</sup> -0.05 0.10 0.00 0.15 Time (Days)

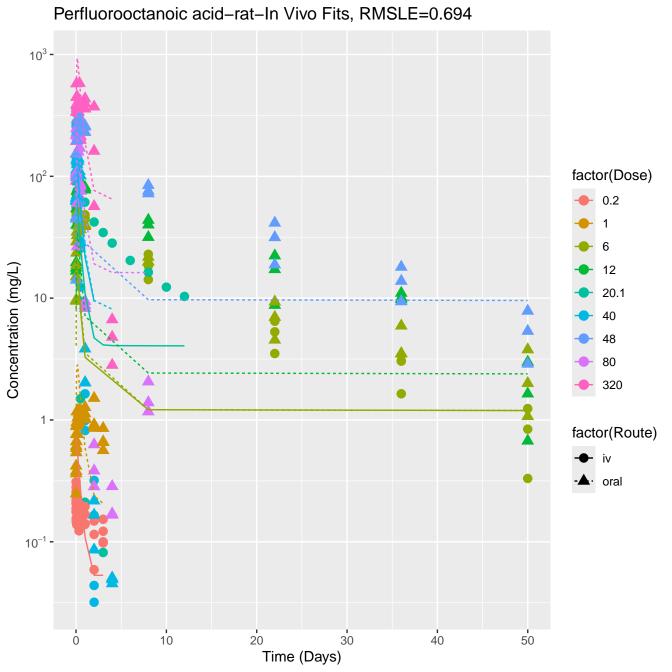
Ondansetron-rat-In Vivo Fits, RMSLE=0.212 10<sup>2</sup> factor(Route) 10-Concentration (mg/L) · oral factor(Dose) 20 10<sup>-1</sup> -0.10 0.05 0.00 0.15 Time (Days)

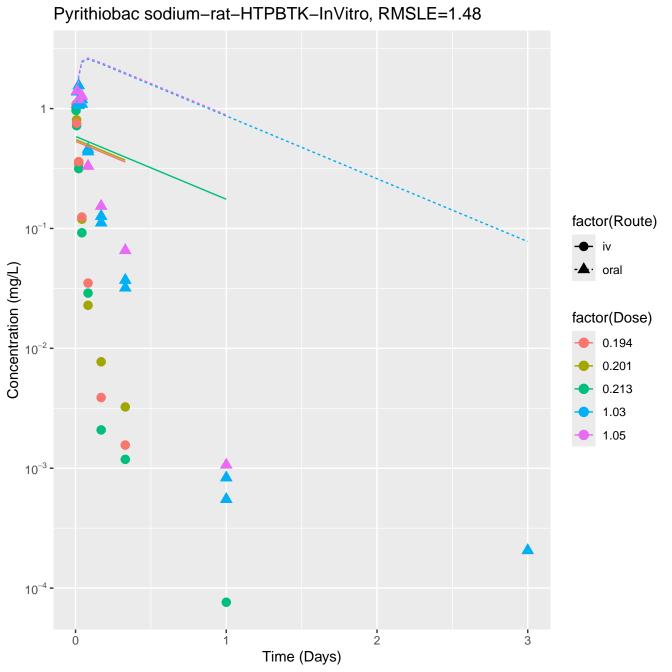


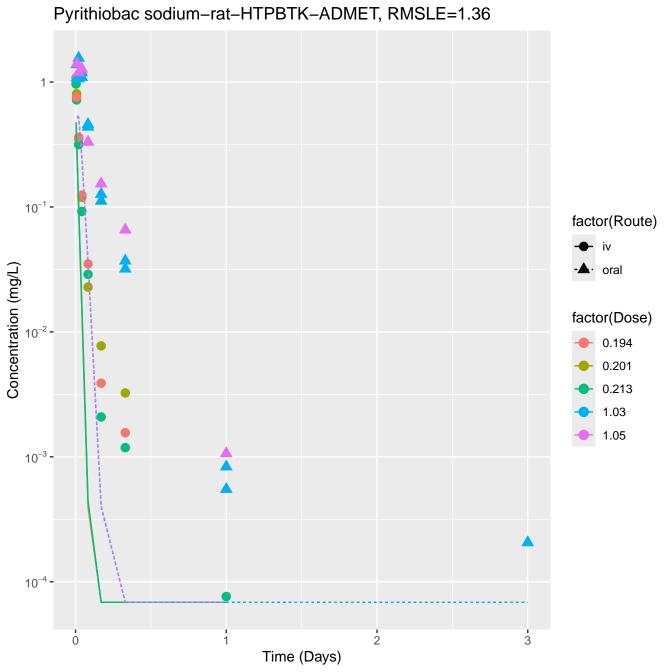
tert-Amyl methyl ether-human-HTPBTK-Ensemble, RMSLE=0.306 10<sup>-2</sup> -Concentration (mg/L) factor(Route) oral factor(Dose) 0.0671 0.201 10<sup>-3</sup> -0.1 0.2 0.4 0.3 0.5 Time (Days)

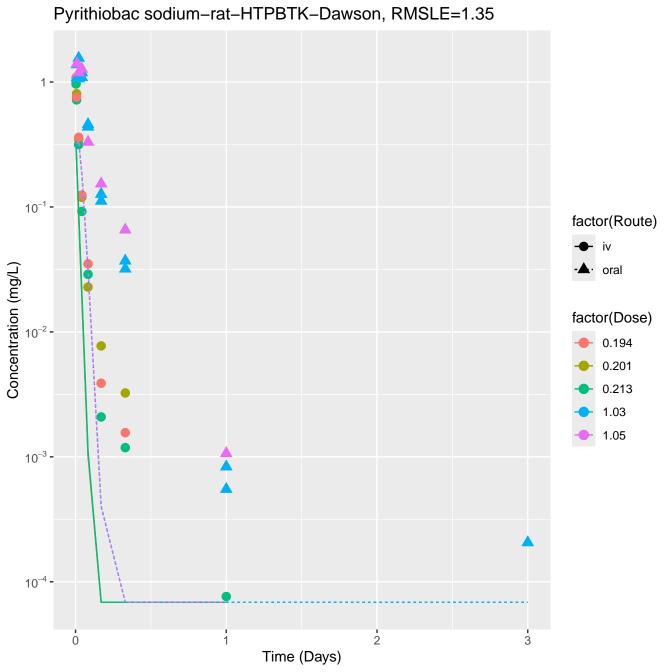


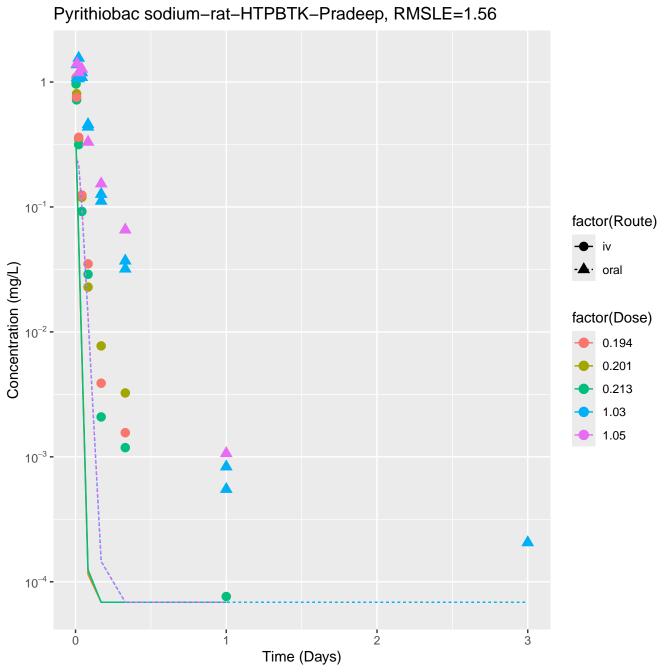


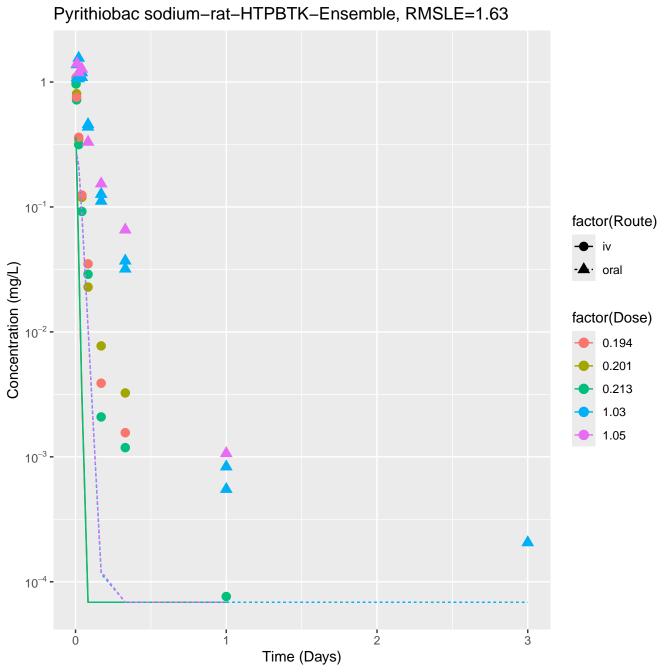


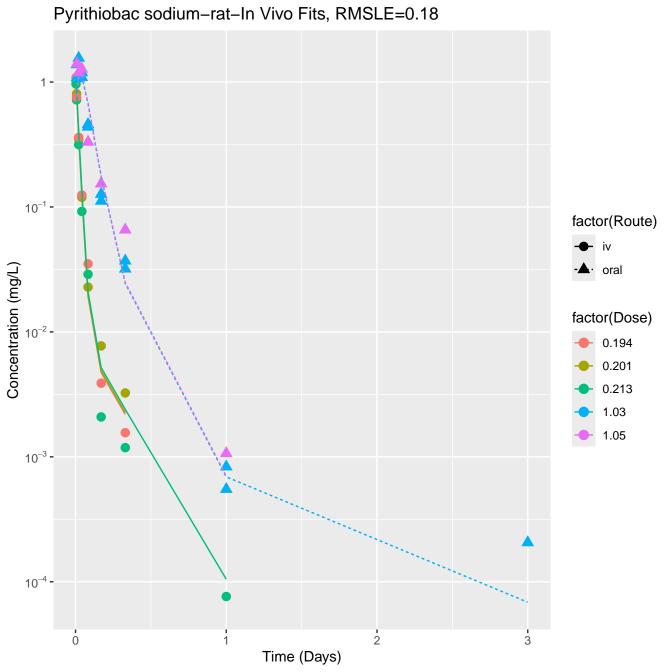


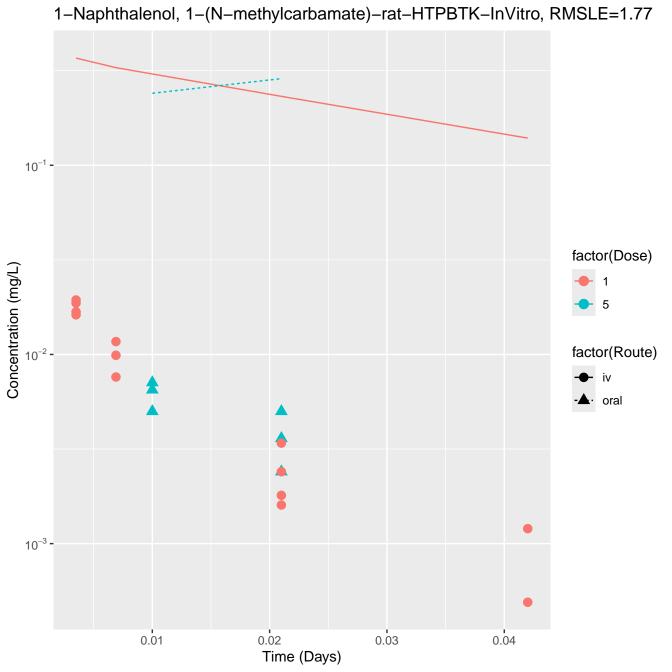






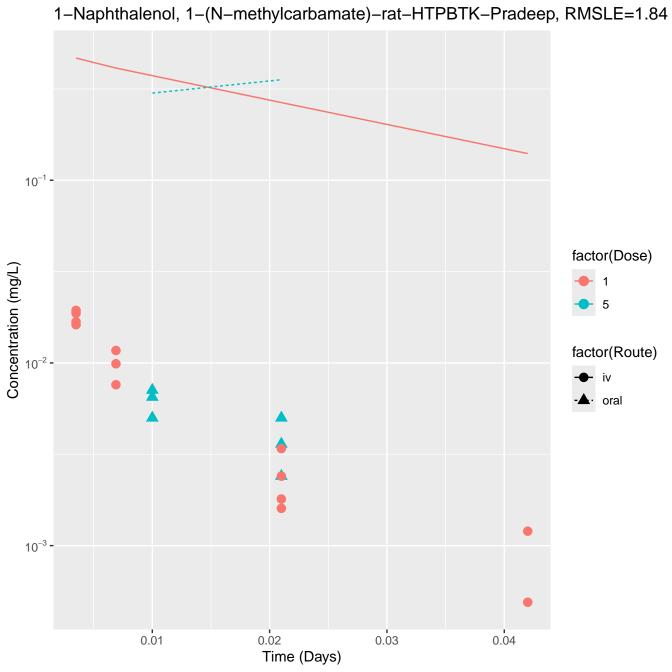


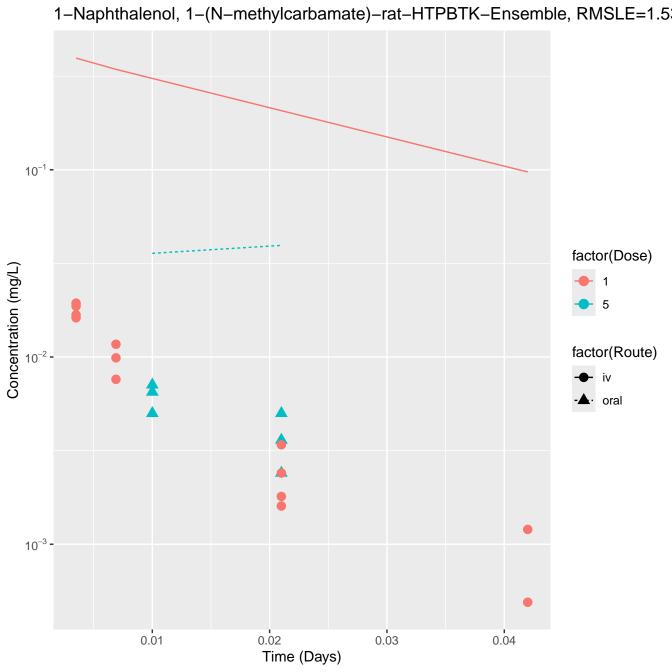




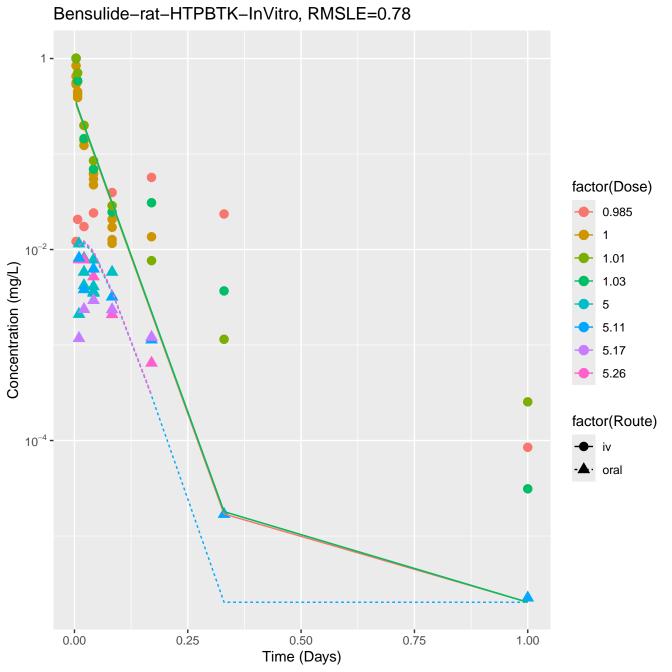
1-Naphthalenol, 1-(N-methylcarbamate)-rat-HTPBTK-ADMET, RMSLE=1.56 10<sup>-1</sup> factor(Dose) Concentration (mg/L) factor(Route) 10<sup>-2</sup> iv · oral 10<sup>-3</sup> -0.02 0.01 0.03 0.04 Time (Days)

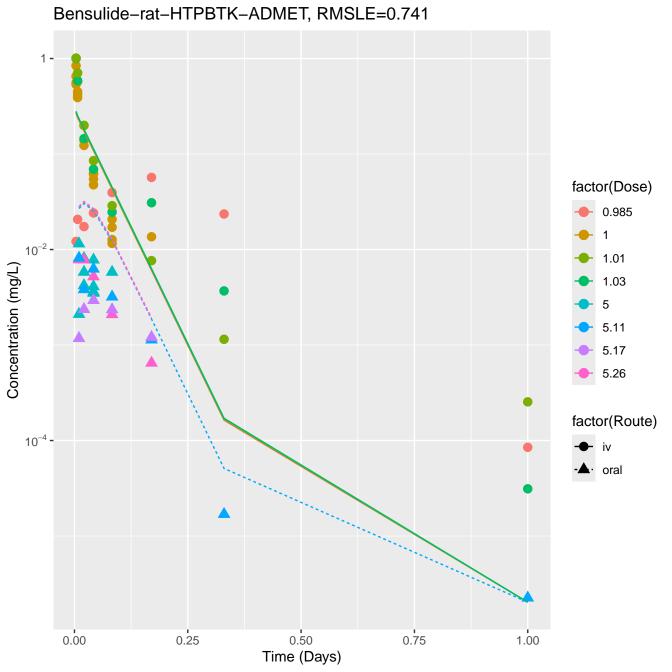
1-Naphthalenol, 1-(N-methylcarbamate)-rat-HTPBTK-Dawson, RMSLE=1.84 10<sup>-1</sup> factor(Dose) Concentration (mg/L) factor(Route) 10<sup>-2</sup> iv · oral 10<sup>-3</sup> -0.02 0.01 0.03 0.04 Time (Days)

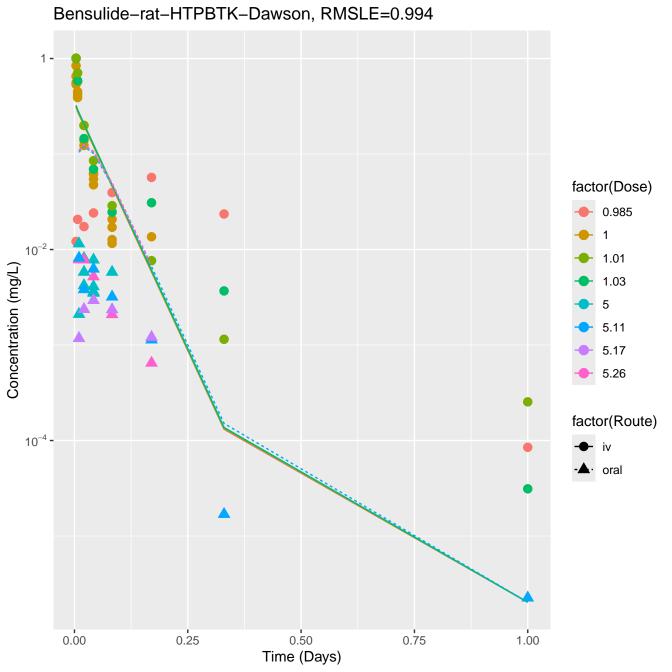


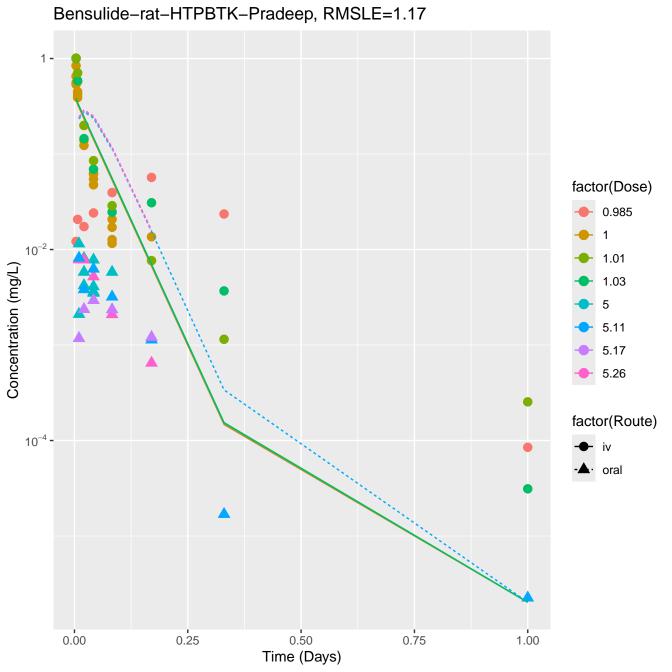


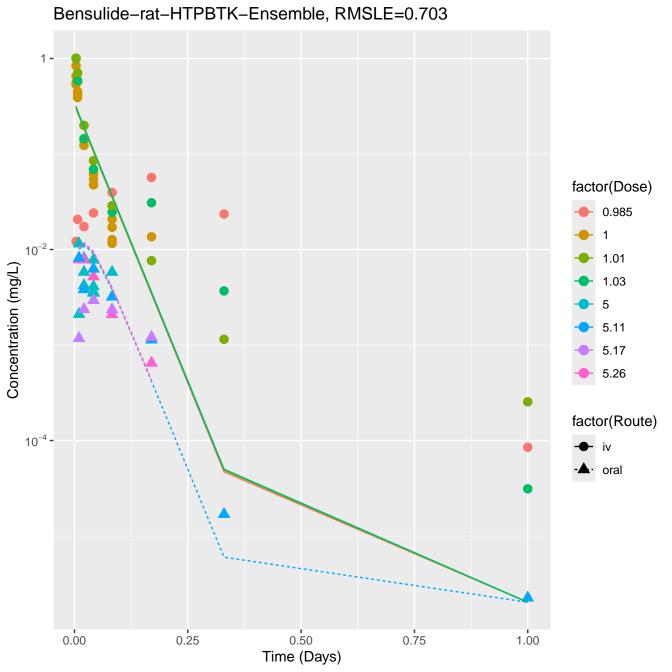
1-Naphthalenol, 1-(N-methylcarbamate)-rat-In Vivo Fits, RMSLE=0.109 10<sup>-2</sup> factor(Dose) Concentration (mg/L) factor(Route) iv oral 10<sup>-3</sup> -0.02 0.01 0.03 0.04 Time (Days)



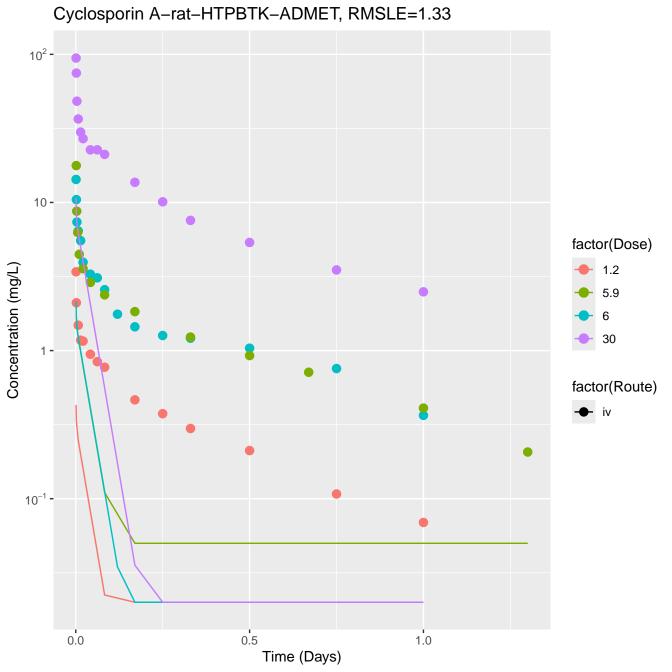


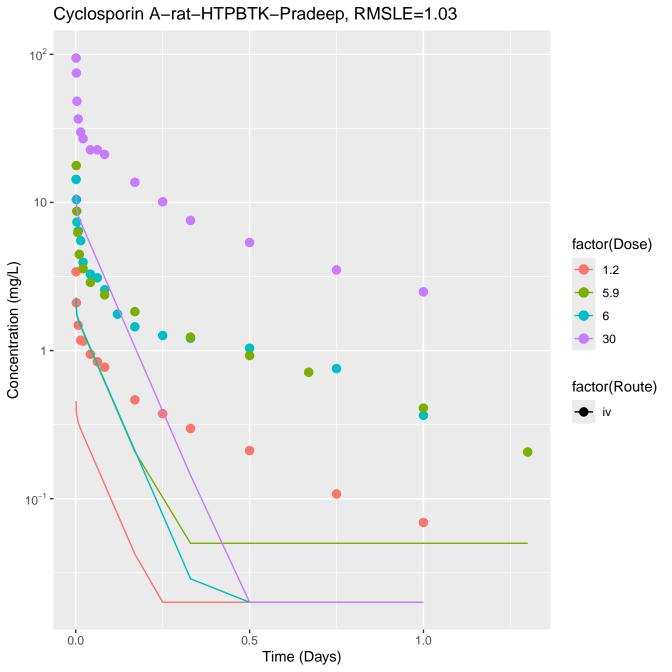


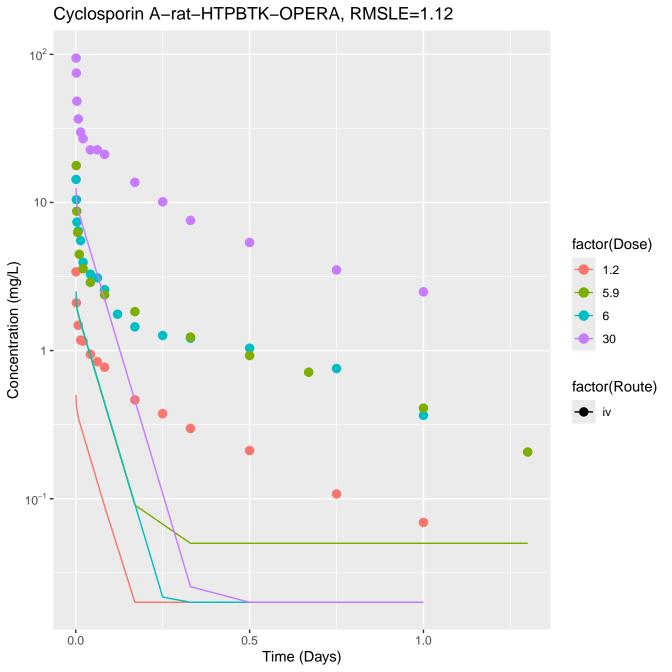


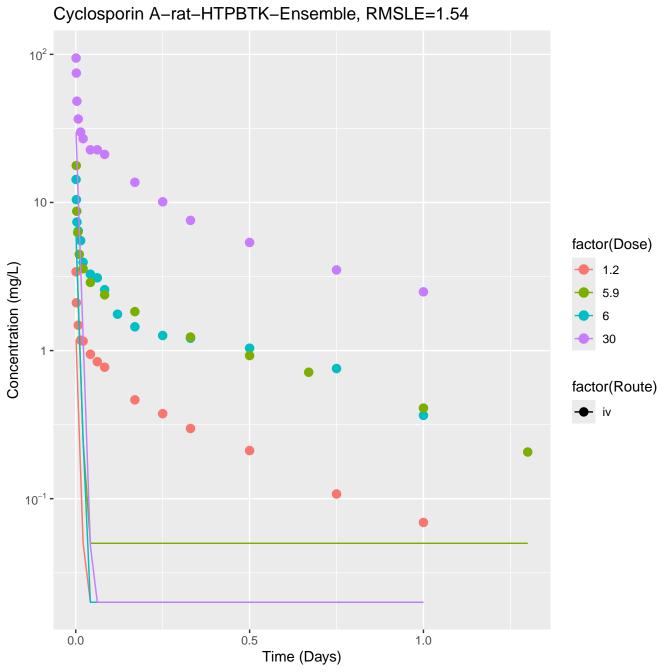


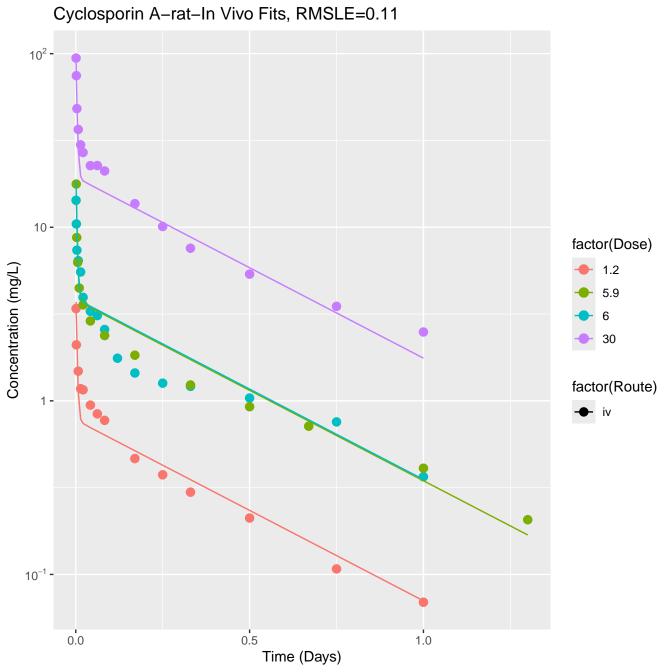
Bensulide-rat-In Vivo Fits, RMSLE=0.385 1 factor(Dose) 0.985 Concentration (mg/L) 1.01 1.03 5 5.11 5.17 5.26 factor(Route) 10<sup>-4</sup> -· oral 0.50 0.00 0.25 0.75 1.00 Time (Days)











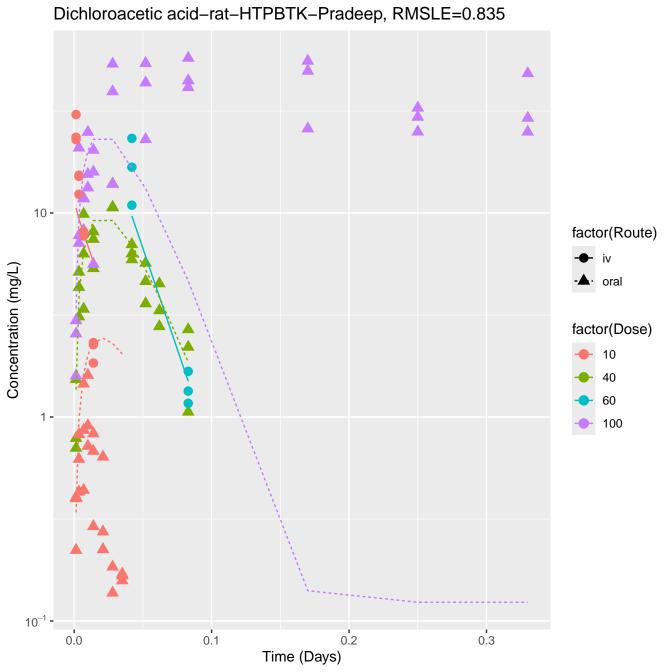
Dibromoacetic acid-rat-HTPBTK-ADMET, RMSLE=0.803 10<sup>2</sup> factor(Dose) 10 10 -25 Concentration (mg/L) 40 50 100 110 125 factor(Route) 1 oral 10<sup>-1</sup> -0.0 0.1 0.2 0.3 Time (Days)

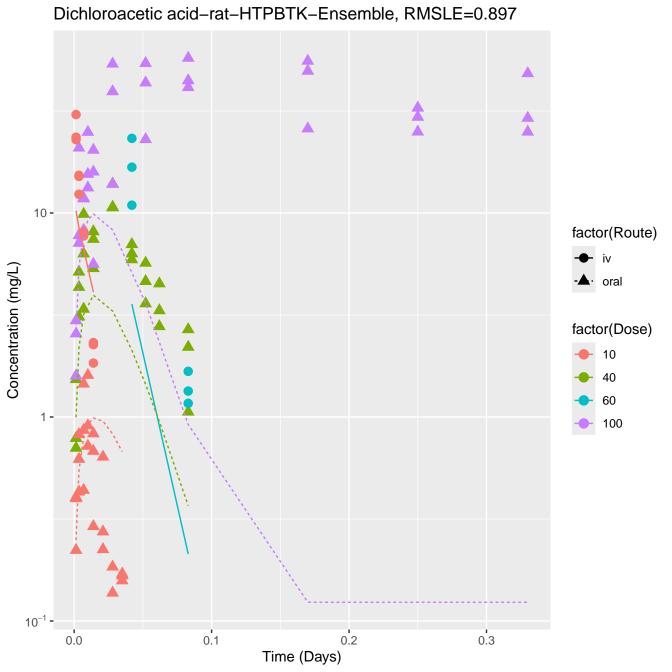
Dibromoacetic acid-rat-HTPBTK-Pradeep, RMSLE=0.587 10<sup>2</sup> factor(Dose) 10 10-25 Concentration (mg/L) 40 50 100 110 125 factor(Route) 1 oral 10<sup>-1</sup> -0.1 0.2 0.0 0.3 Time (Days)

Dibromoacetic acid-rat-HTPBTK-Ensemble, RMSLE=0.733 10<sup>2</sup> factor(Dose) 10 10-25 Concentration (mg/L) 40 50 100 110 125 factor(Route) 1 oral 10<sup>-1</sup> -0.1 0.2 0.0 0.3 Time (Days)

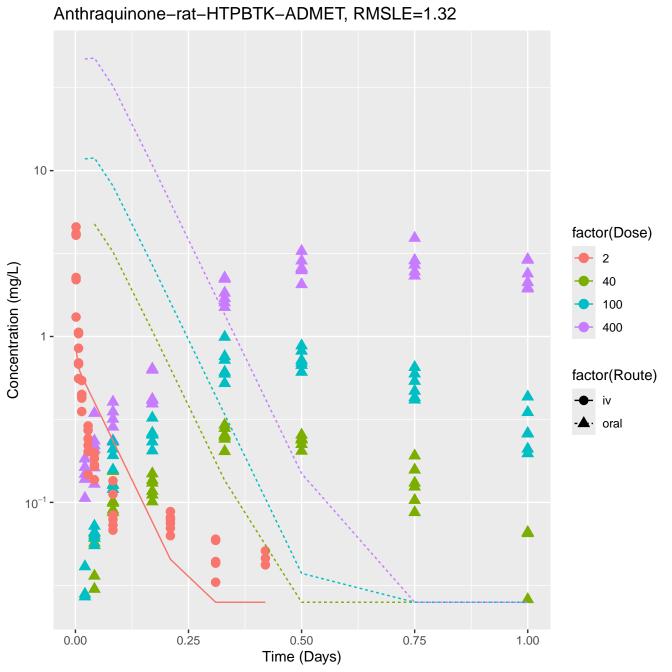
Dibromoacetic acid-rat-In Vivo Fits, RMSLE=0.336 10<sup>2</sup> factor(Dose) 10 10-25 Concentration (mg/L) 40 50 100 110 125 factor(Route) 1 oral 10<sup>-1</sup> -0.0 0.1 0.2 0.3 Time (Days)

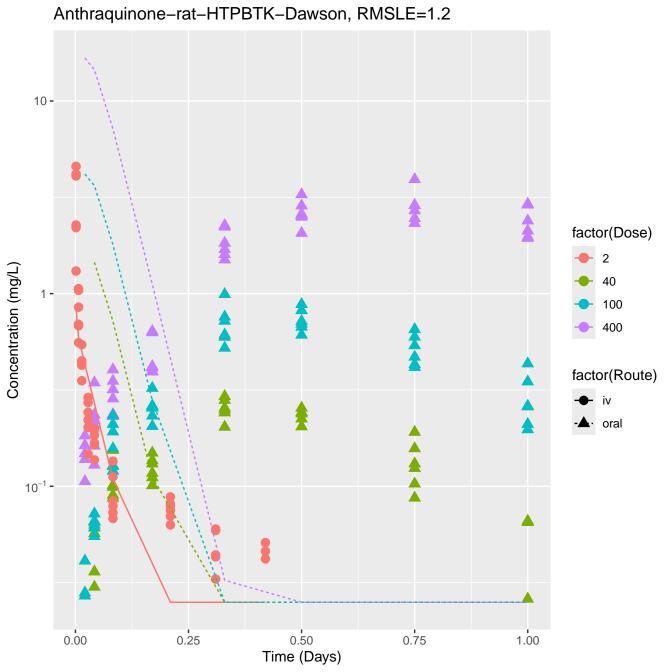
Dichloroacetic acid-rat-HTPBTK-ADMET, RMSLE=0.742 10<sup>2</sup> factor(Route) 10 -Concentration (mg/L) · oral factor(Dose) 10 40 60 100 1 -10<sup>-1</sup> 0.0 0.1 0.2 0.3 Time (Days)

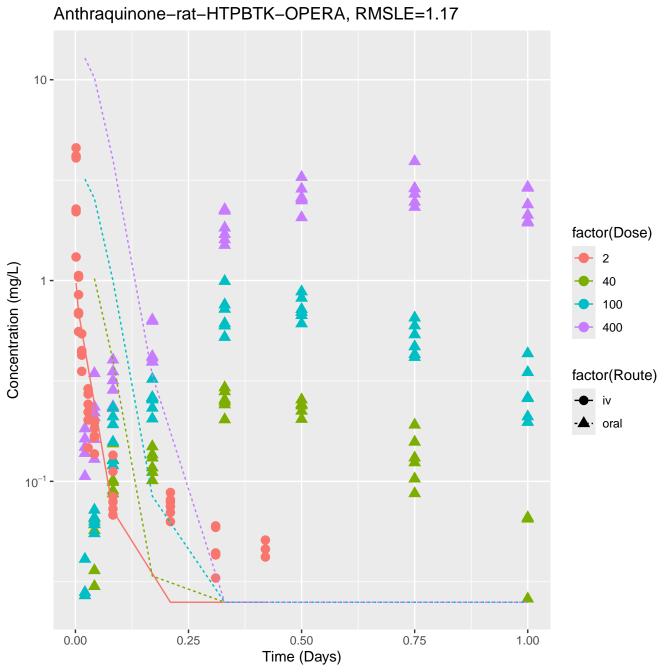




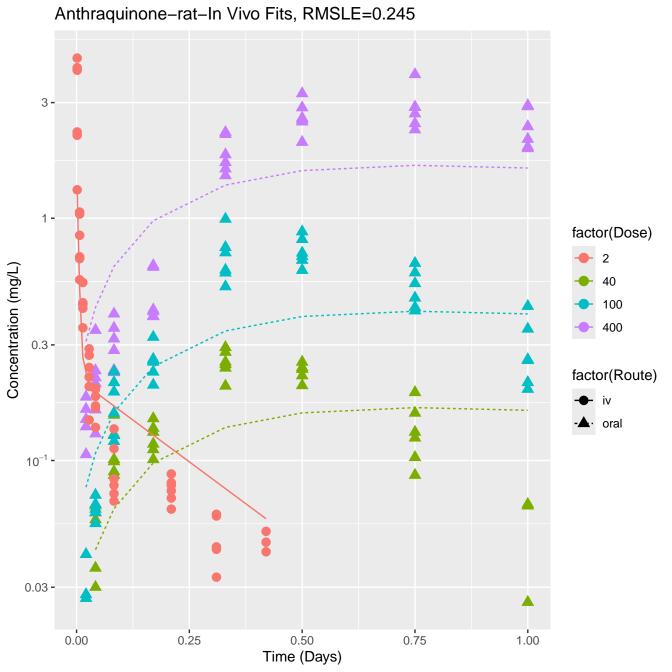
Dichloroacetic acid-rat-In Vivo Fits, RMSLE=0.375 30 -10factor(Route) Concentration (mg/L) · oral 3 factor(Dose) 10 40 60 1 -100 0.3 -0.1 0.2 0.0 0.3 Time (Days)

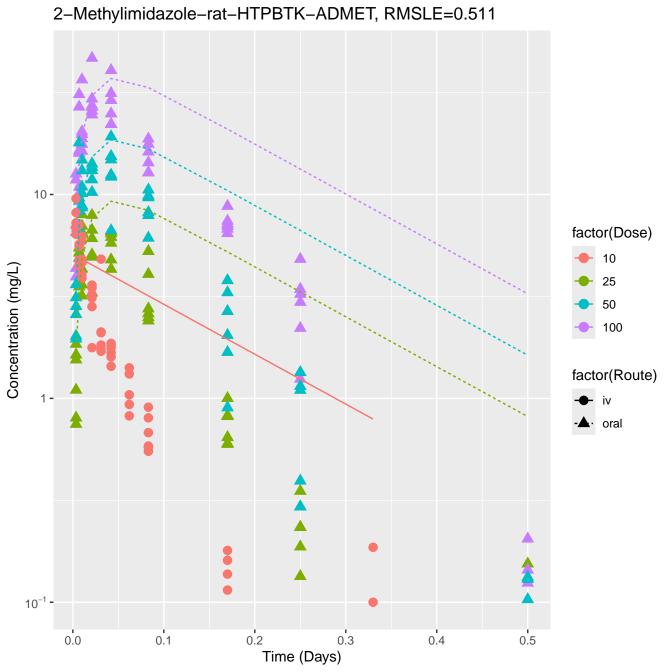


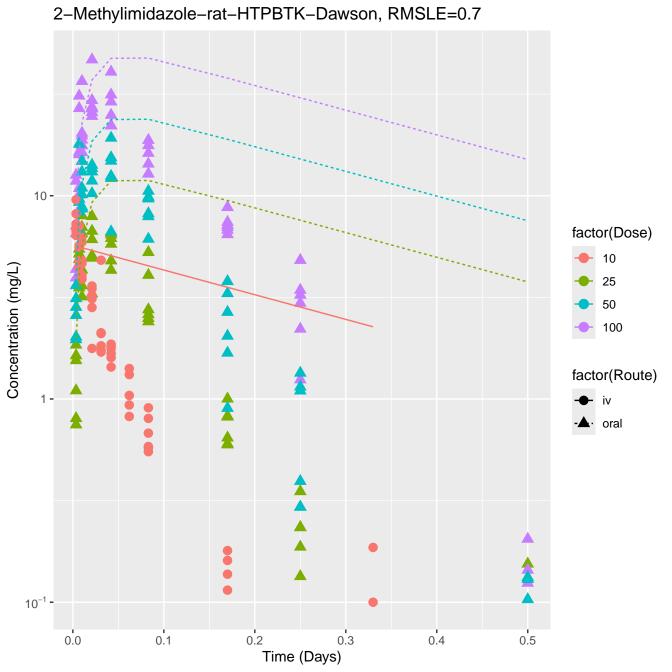


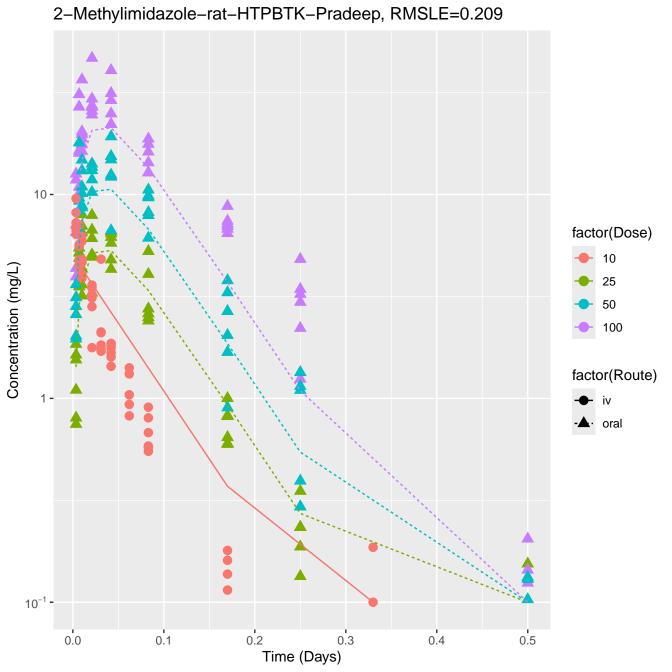


Anthraquinone-rat-HTPBTK-Ensemble, RMSLE=1.16 10 factor(Dose) 2 Concentration (mg/L) 40 100 400 factor(Route) · oral 10<sup>-1</sup> -0.25 0.50 0.75 1.00 0.00 Time (Days)

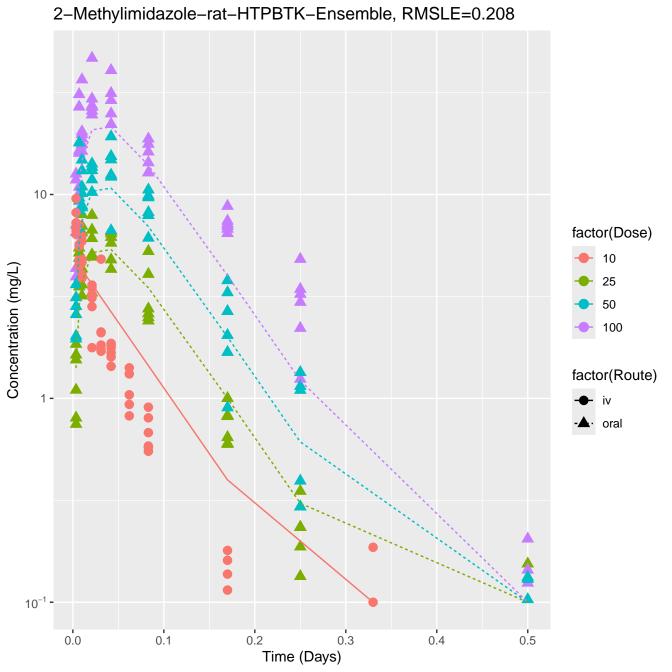


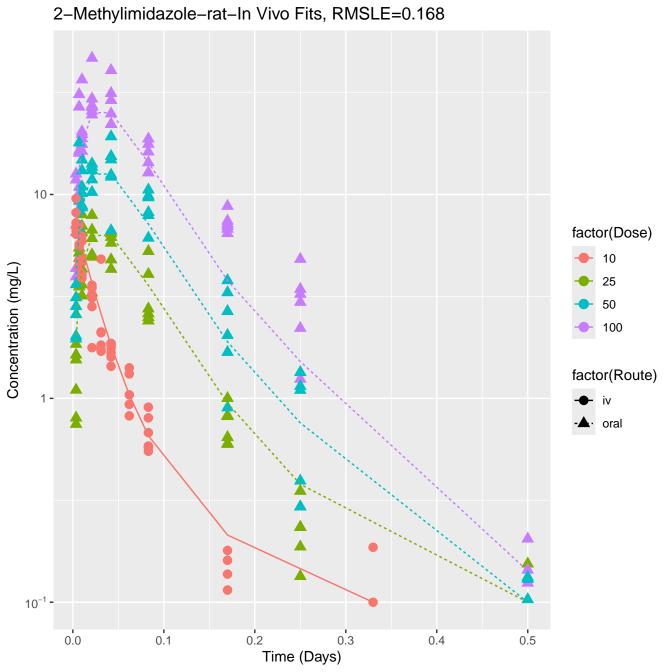






 $2-Methylimidazole-rat-HTPBTK-OPERA,\,RMSLE=0.65$ 10factor(Dose) 10 Concentration (mg/L) 25 50 100 factor(Route) · oral 10<sup>-1</sup> -0.1 0.2 0.3 0.4 0.5 0.0 Time (Days)



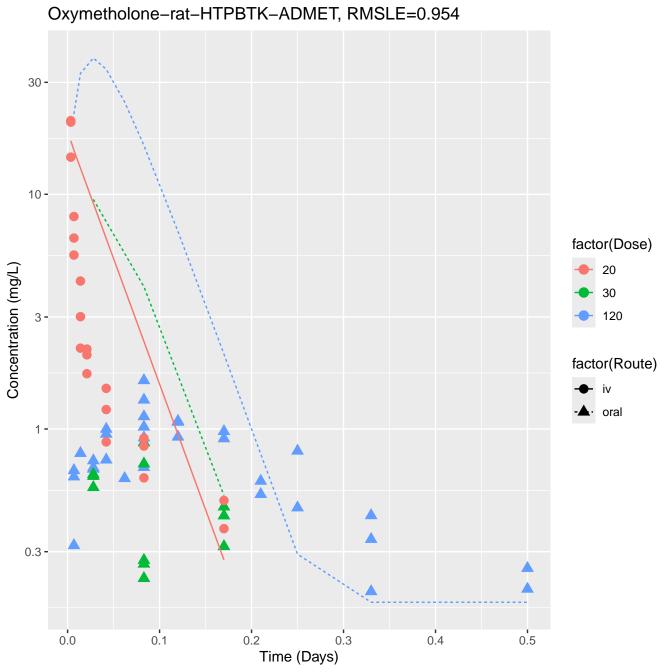


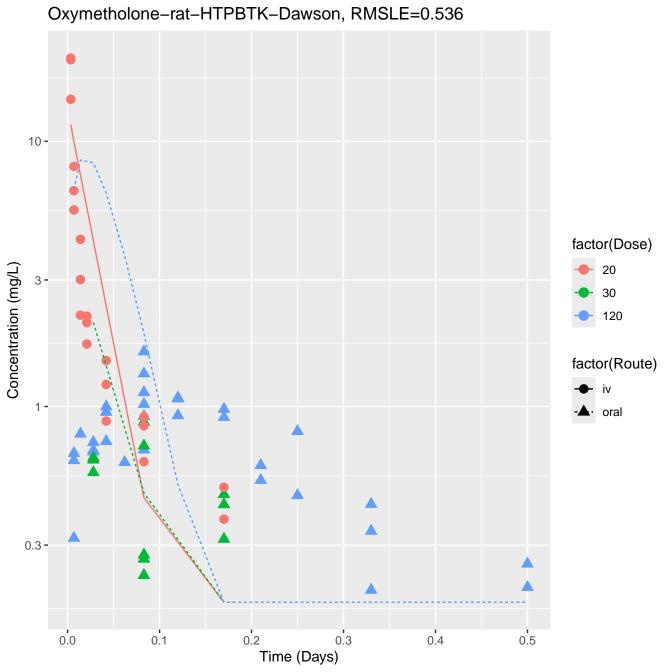
Bromochloroacetic acid-rat-HTPBTK-ADMET, RMSLE=1.01 10<sup>2</sup> -10 factor(Dose) 10 Concentration (mg/L) 40 80 100 factor(Route) oral 10<sup>-1</sup> -0.1 0.0 0.2 0.3 Time (Days)

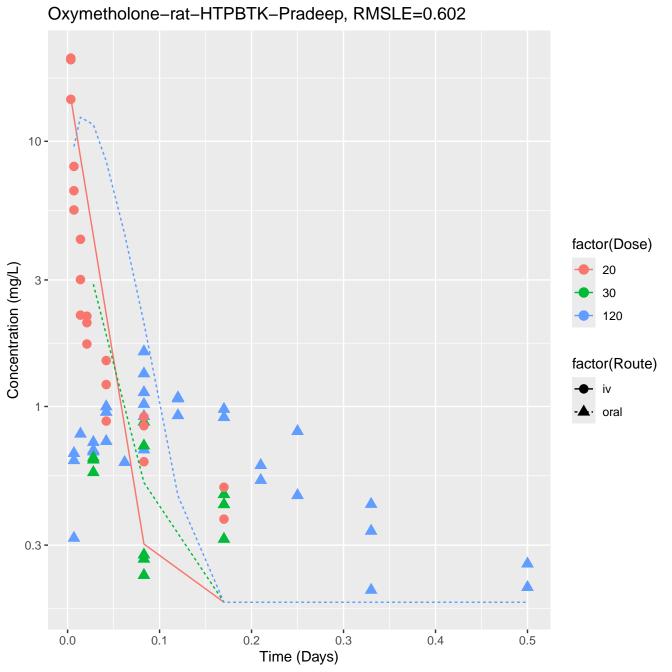
Bromochloroacetic acid-rat-HTPBTK-Pradeep, RMSLE=0.662 10 factor(Dose) 10 Concentration (mg/L) 40 80 100 factor(Route) oral 10<sup>-1</sup> -0.1 0.0 0.2 0.3 Time (Days)

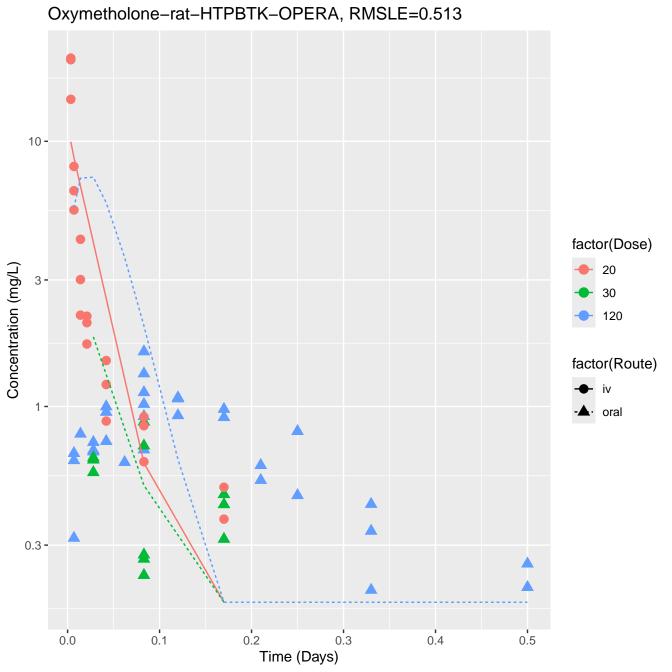
Bromochloroacetic acid-rat-HTPBTK-Ensemble, RMSLE=0.729 10 factor(Dose) 10 Concentration (mg/L) 40 80 100 factor(Route) oral 10<sup>-1</sup> -0.1 0.0 0.2 0.3 Time (Days)

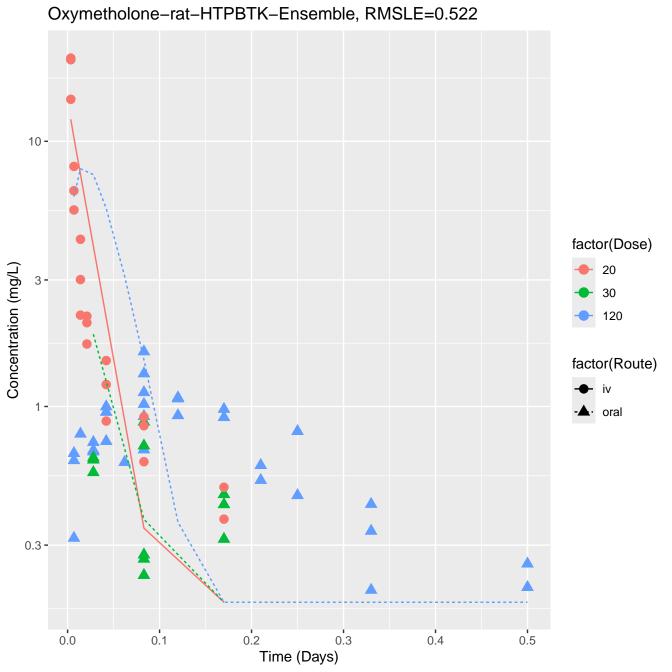
Bromochloroacetic acid-rat-In Vivo Fits, RMSLE=0.386 10 factor(Dose) 10 Concentration (mg/L) 40 80 100 factor(Route) · oral 10<sup>-1</sup> -0.1 0.0 0.2 0.3 Time (Days)

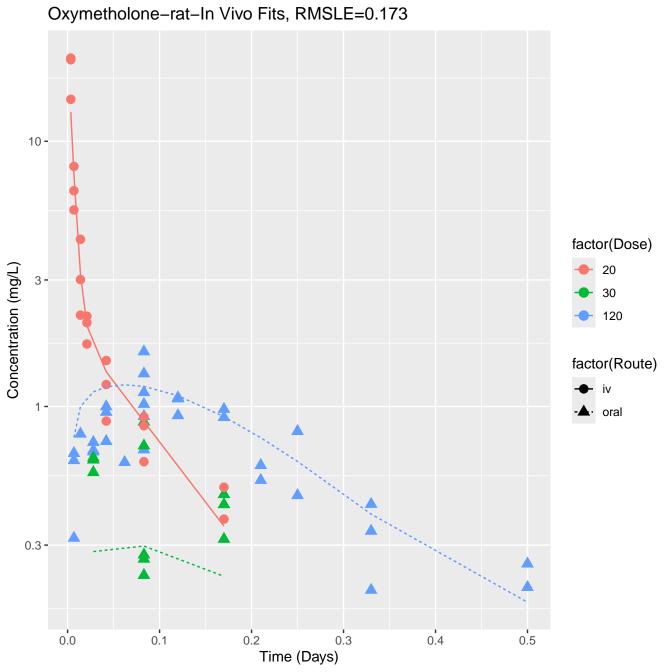




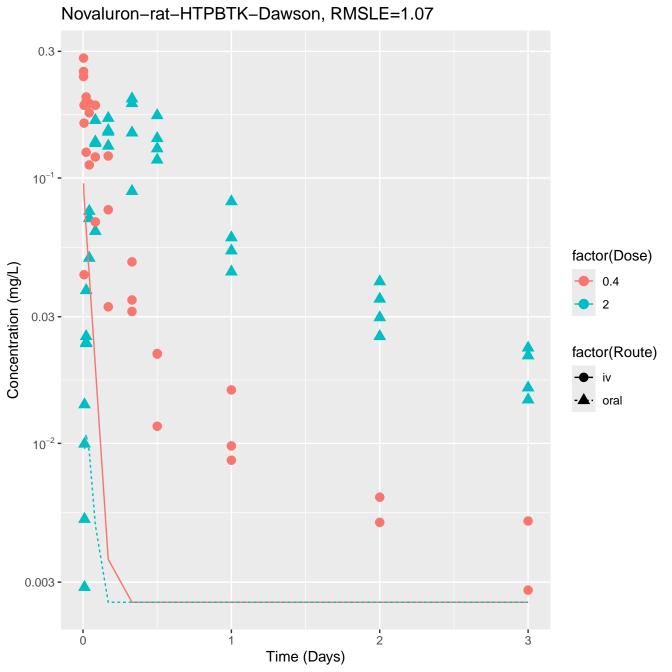




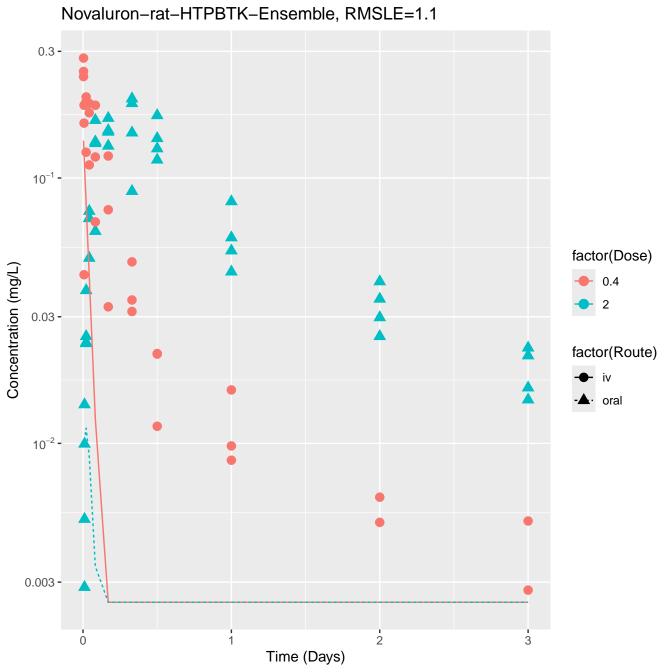




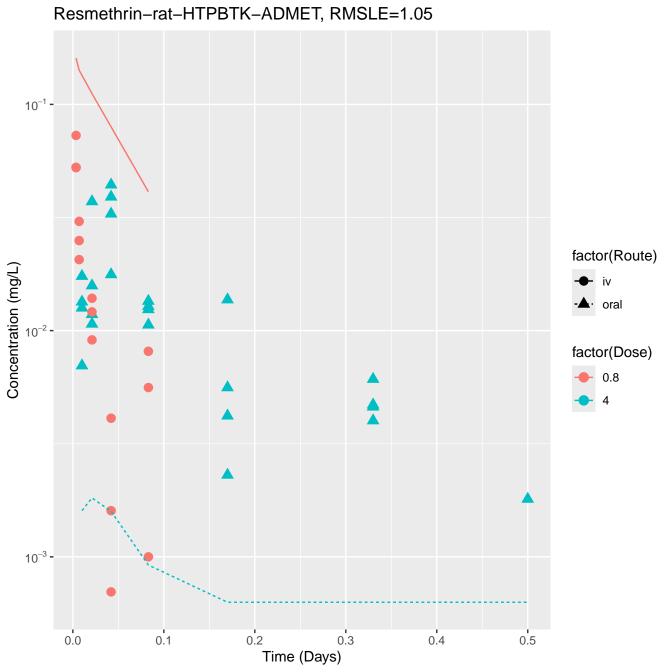
Novaluron-rat-HTPBTK-ADMET, RMSLE=1.08 0.3 -10<sup>-1</sup> factor(Dose) Concentration (mg/L) 0.4 2 0.03 factor(Route) iv · oral 10<sup>-2</sup> -0.003 -2 Ö 3 Time (Days)

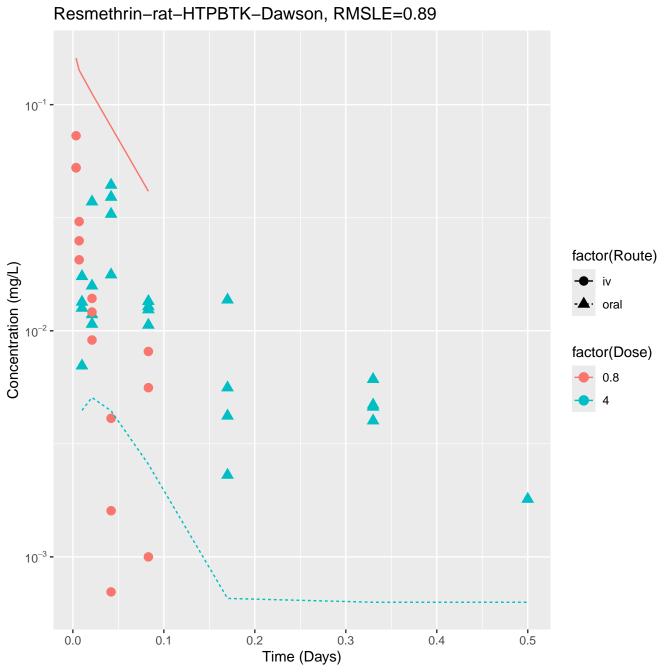


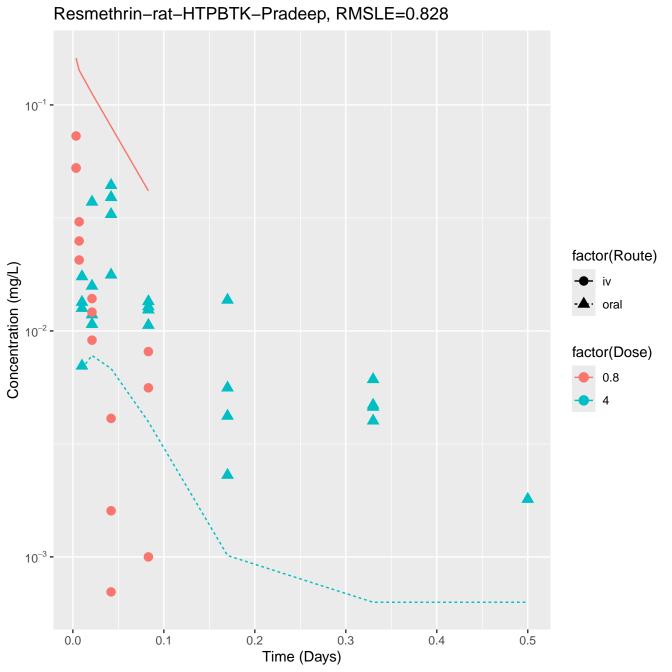
Novaluron-rat-HTPBTK-Pradeep, RMSLE=0.984 0.3 -10<sup>-1</sup> factor(Dose) Concentration (mg/L) 0.4 2 0.03 factor(Route) iv · oral 10<sup>-2</sup> -0.003 -2 Ö 3 Time (Days)

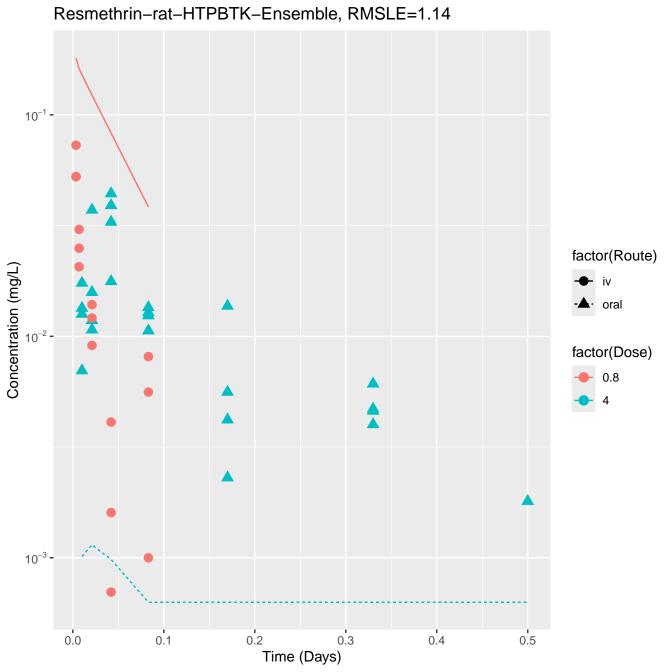


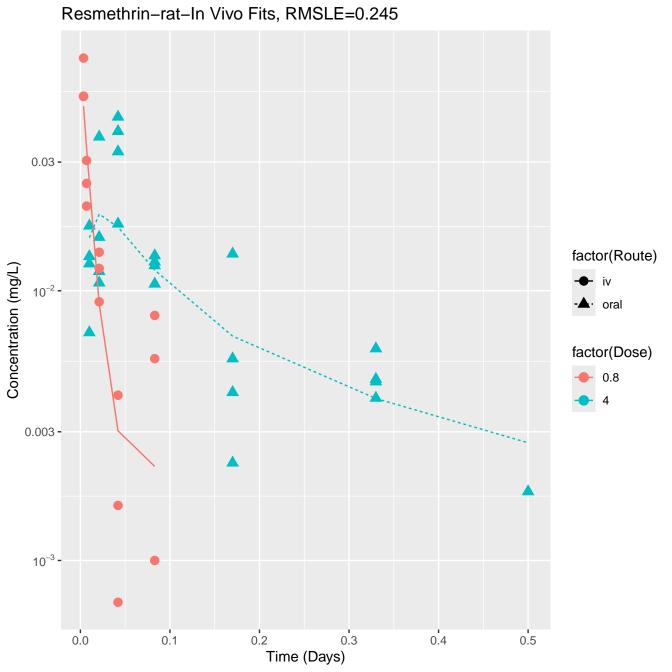
Novaluron-rat-In Vivo Fits, RMSLE=0.173 0.3 -10<sup>-1</sup> factor(Dose) Concentration (mg/L) 0.4 2 0.03 factor(Route) iv oral 10<sup>-2</sup> -0.003 -2 Ó 3 Time (Days)

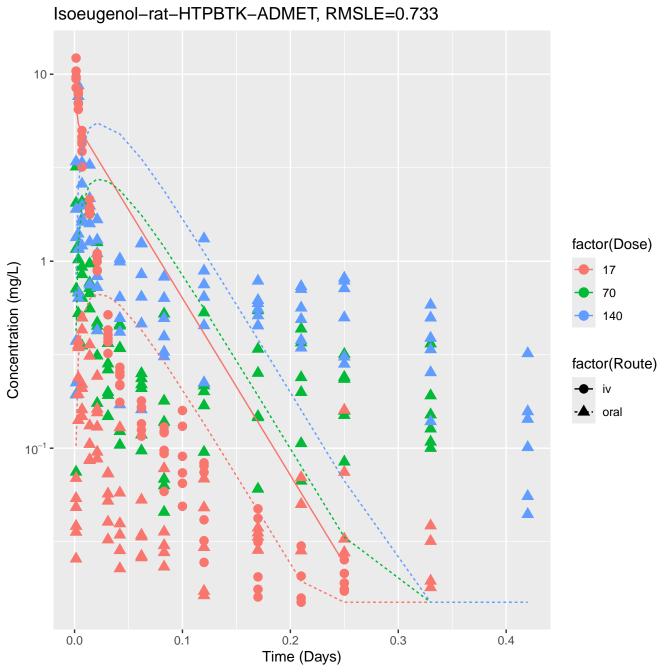


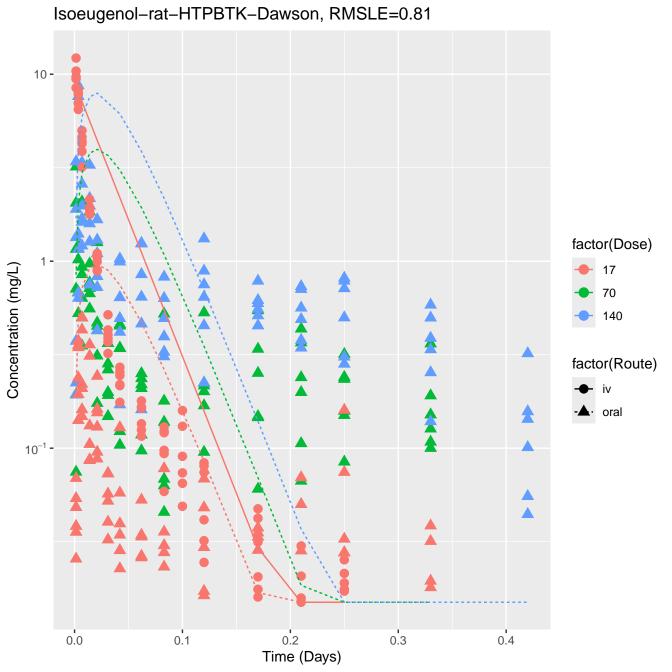


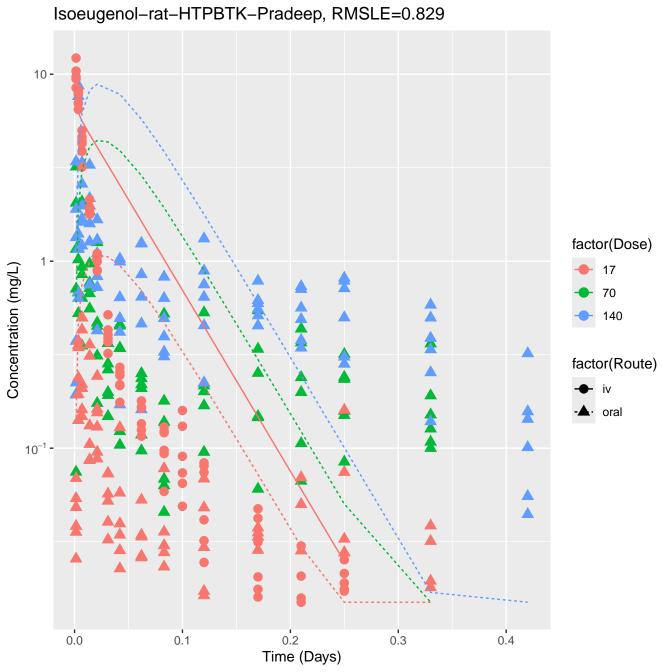






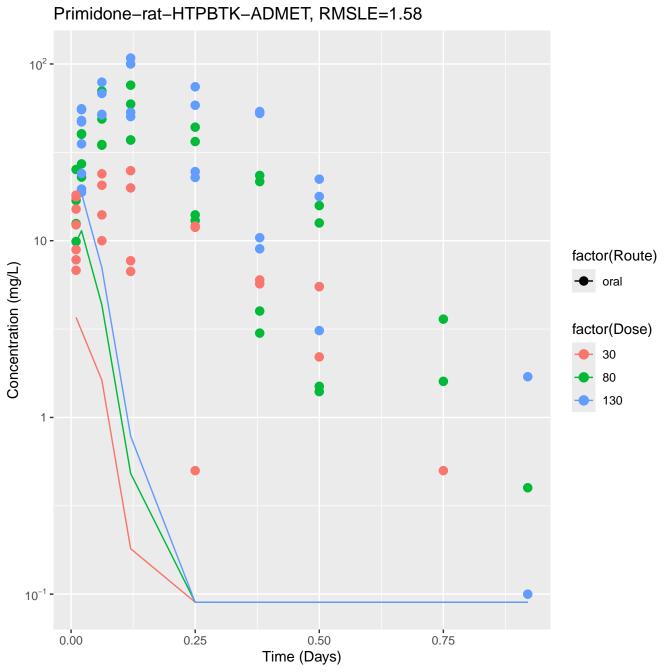


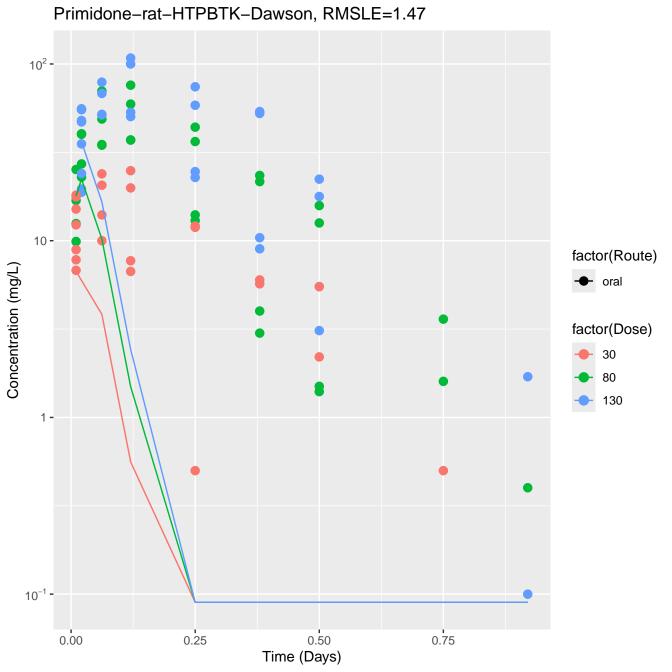


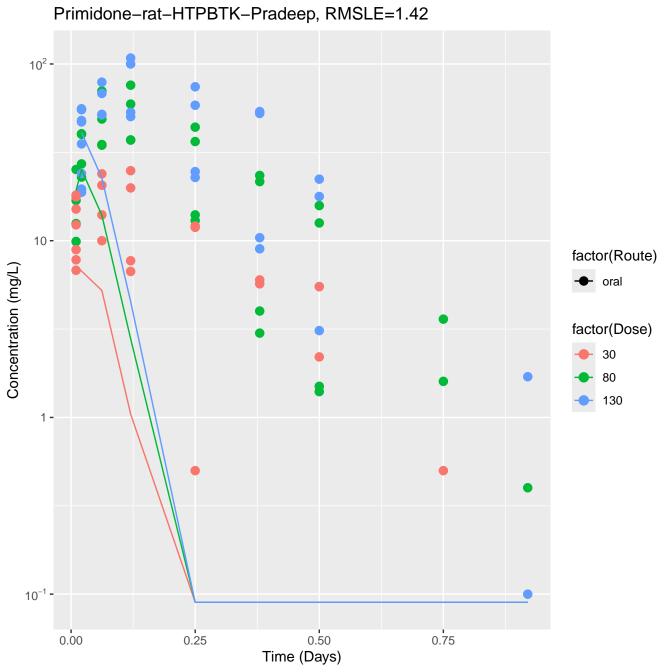


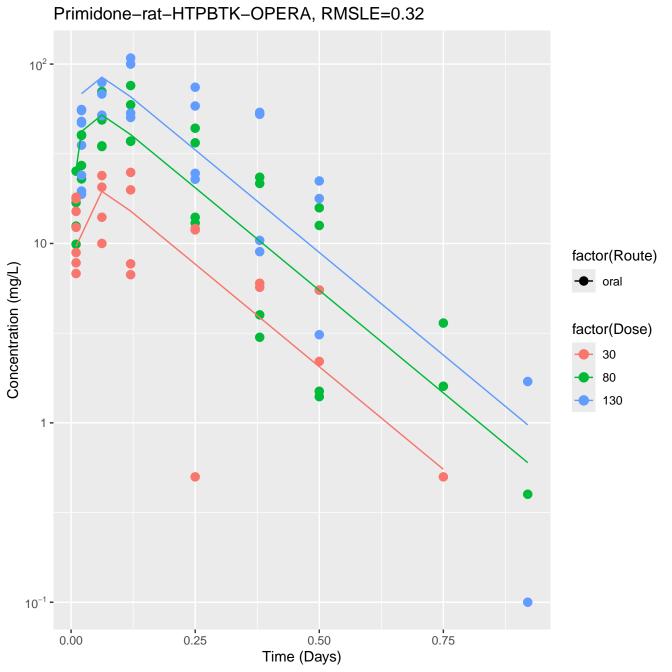
Isoeugenol-rat-HTPBTK-Ensemble, RMSLE=0.658 10 factor(Dose) Concentration (mg/L) 17 70 140 factor(Route) · oral 10<sup>-1</sup> -0.3 0.0 0.1 0.2 0.4 Time (Days)

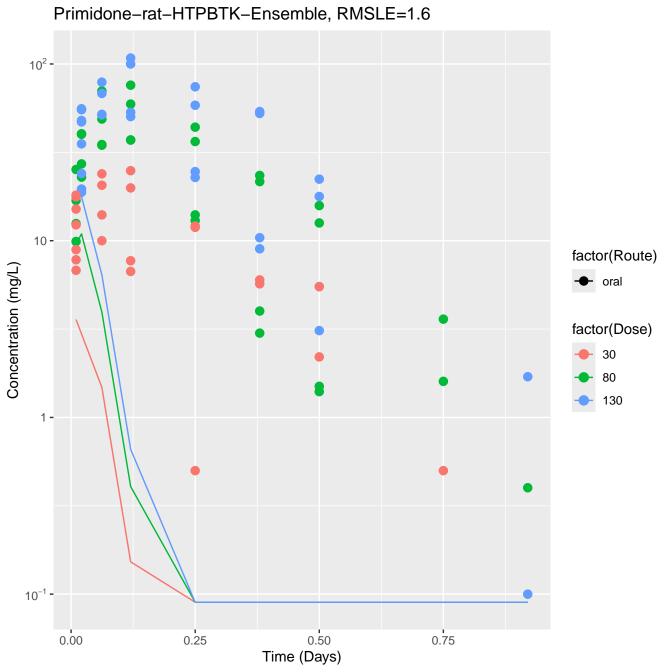
Isoeugenol-rat-In Vivo Fits, RMSLE=0.36 10 factor(Dose) Concentration (mg/L) 17 70 140 factor(Route) · oral 10<sup>-1</sup> -0.0 0.1 0.2 0.3 0.4 Time (Days)

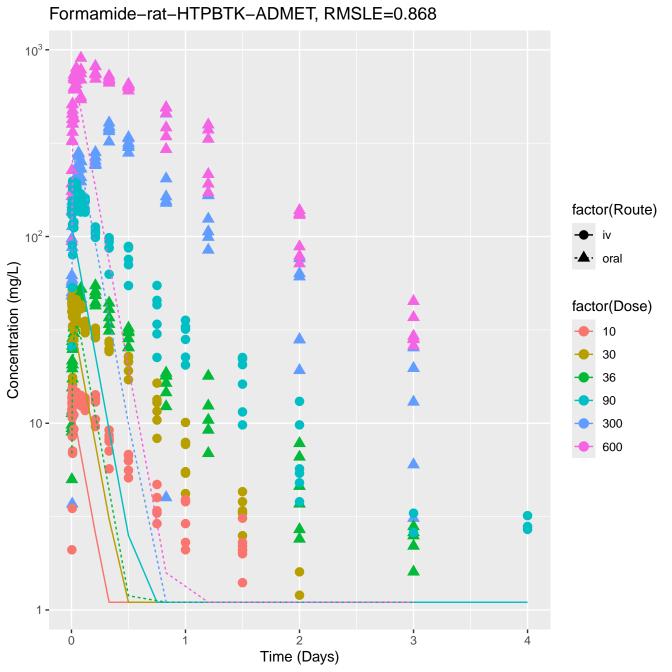


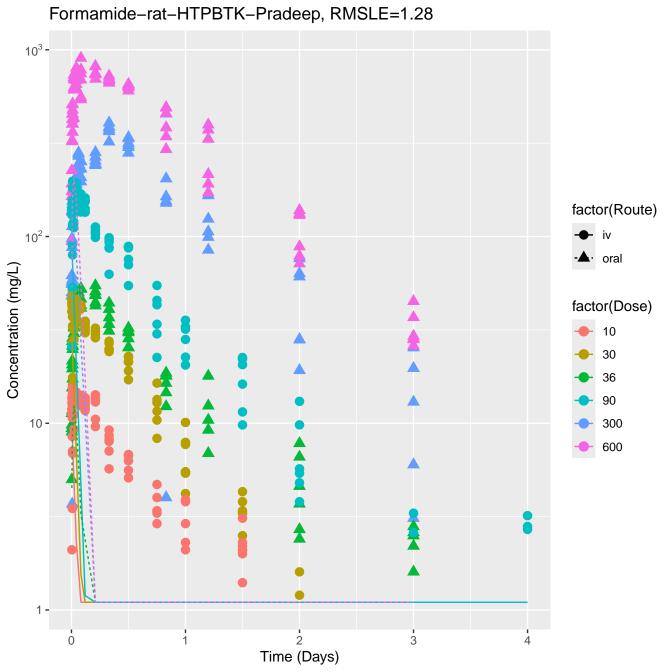


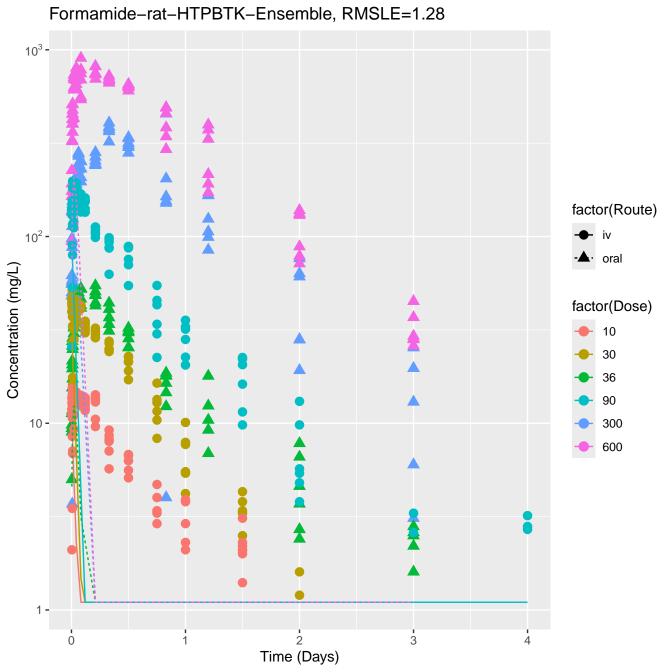


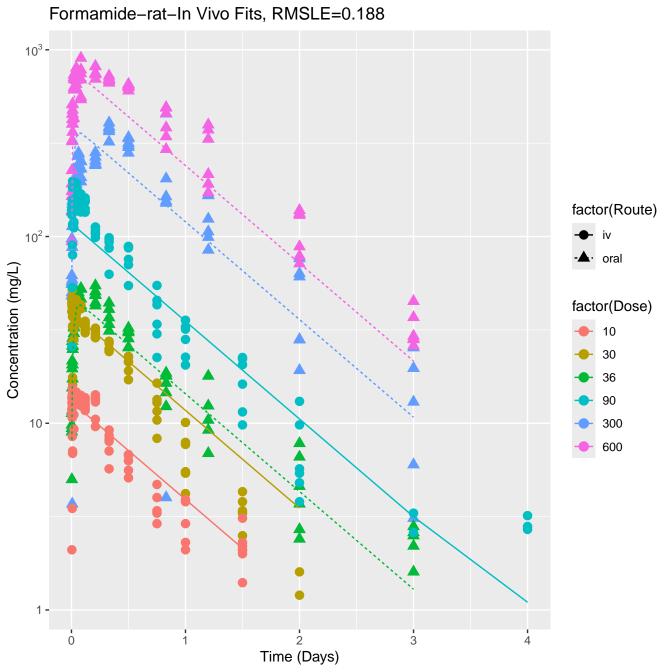


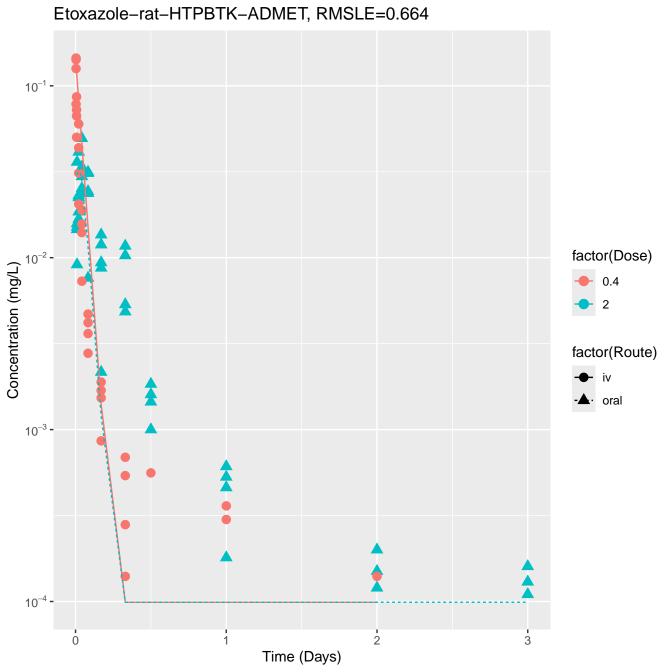


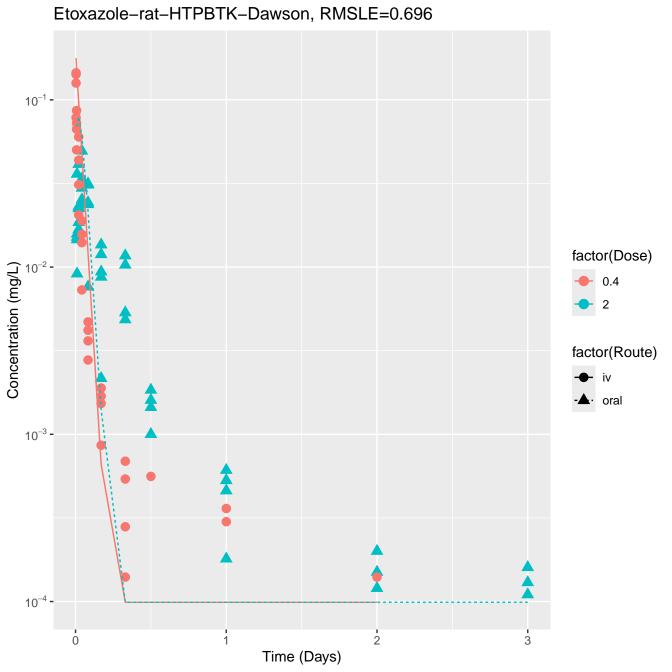


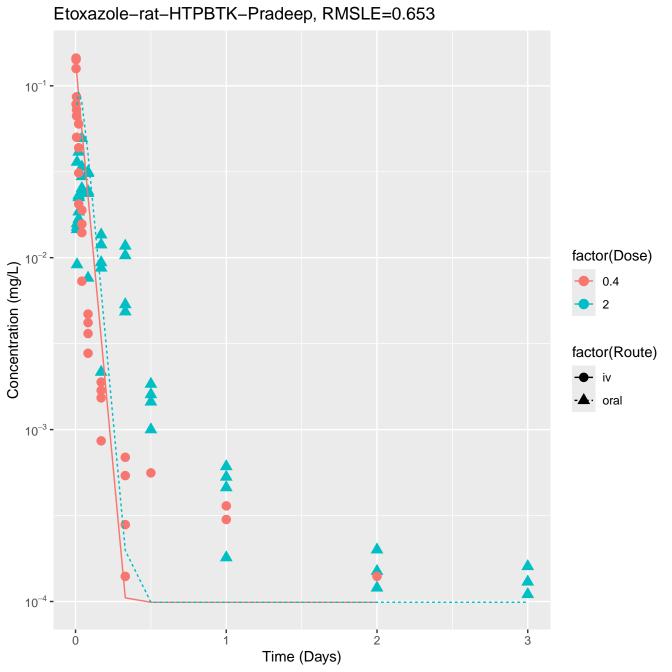


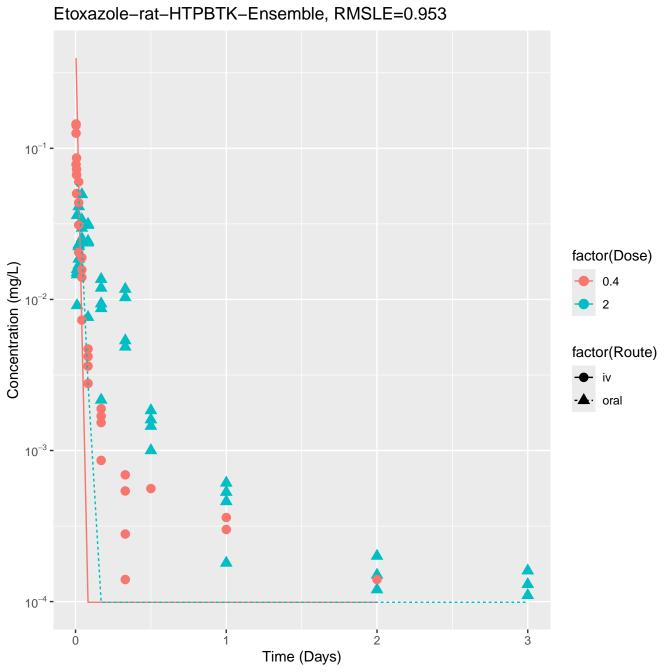


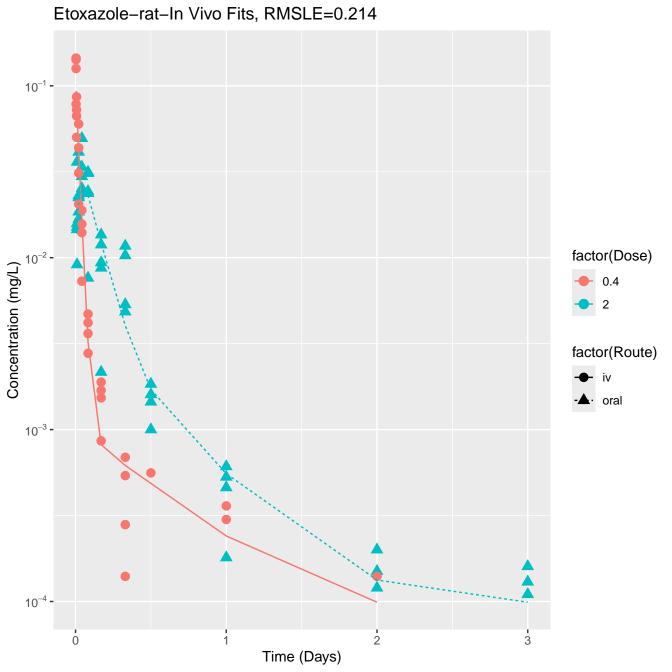


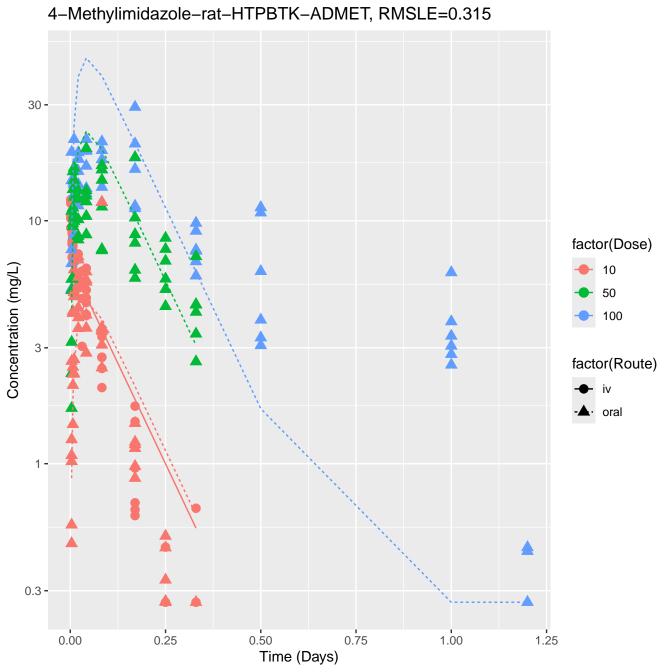


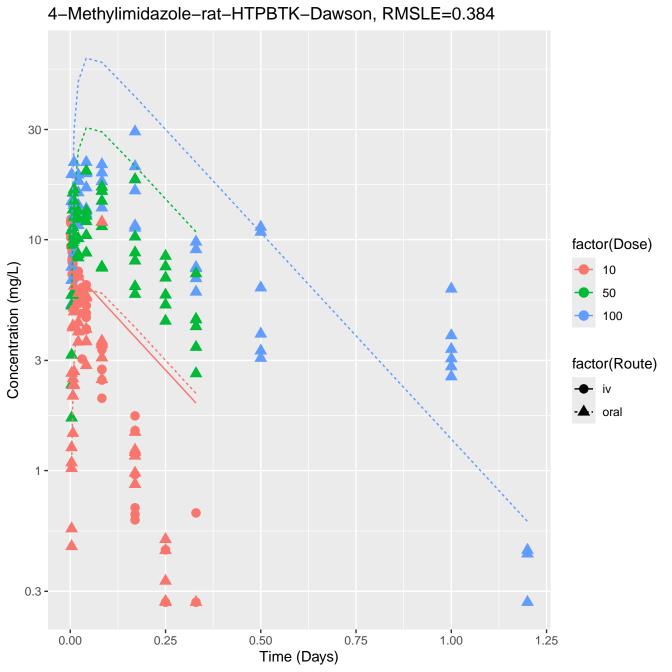




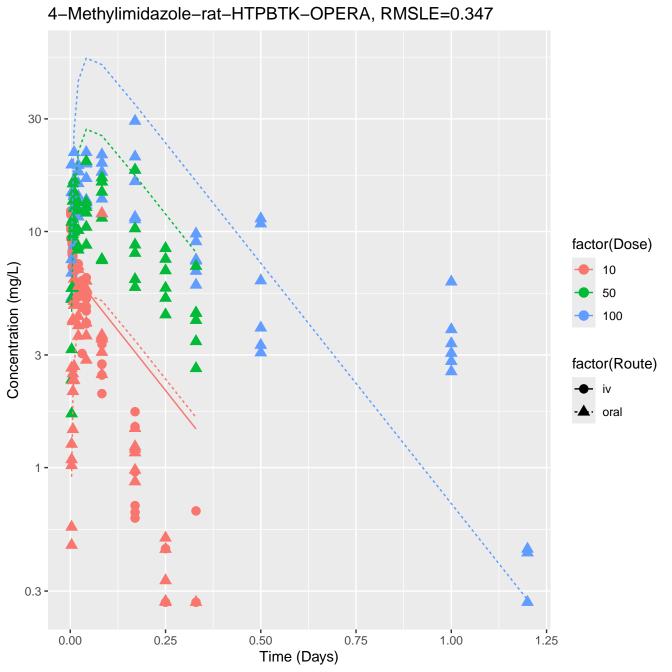




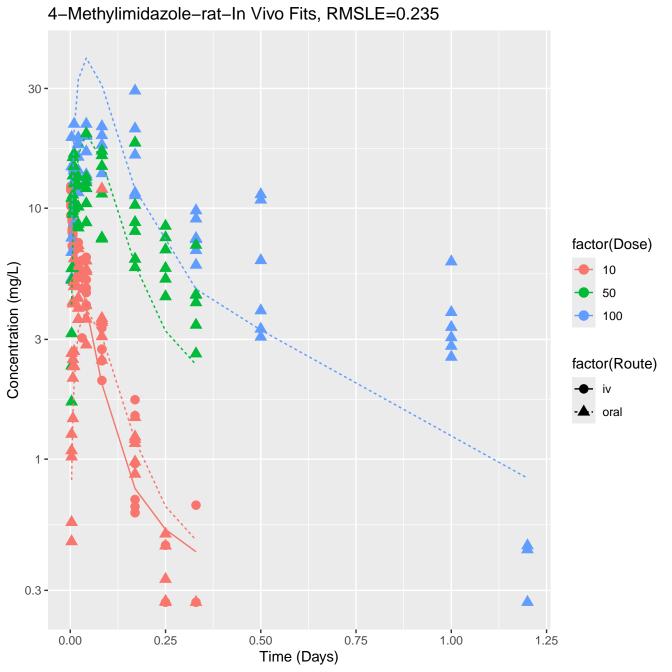


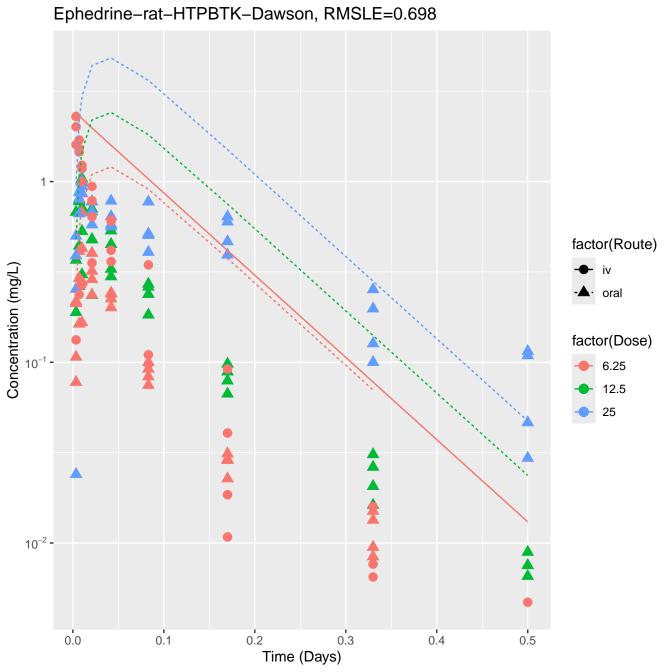


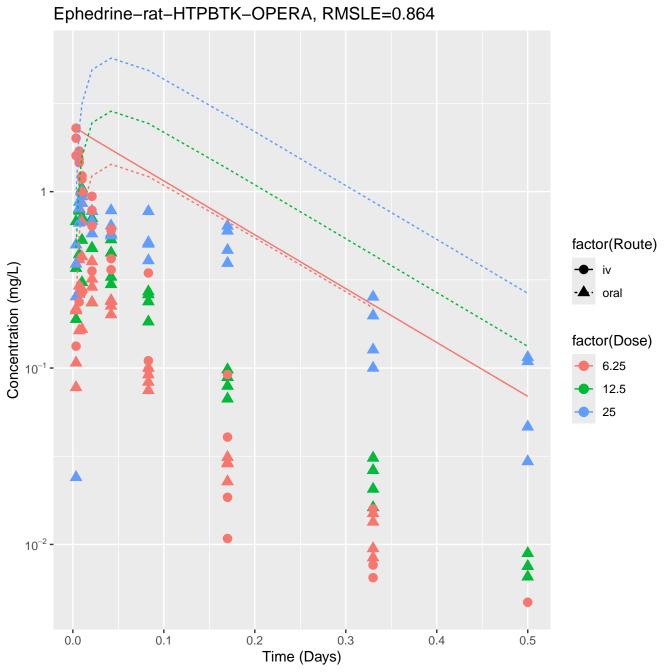
 $4-Methylimidazole-rat-HTPBTK-Pradeep,\ RMSLE=0.6$ 30 -10 factor(Dose) Concentration (mg/L) 10 50 100 3 factor(Route) · oral 1 -0.3 -0.50 0.75 0.00 0.25 1.00 1.25 Time (Days)

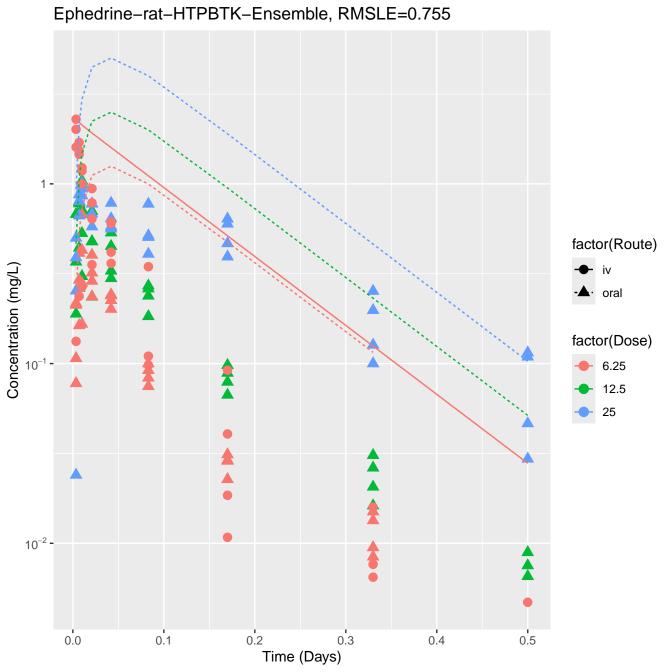


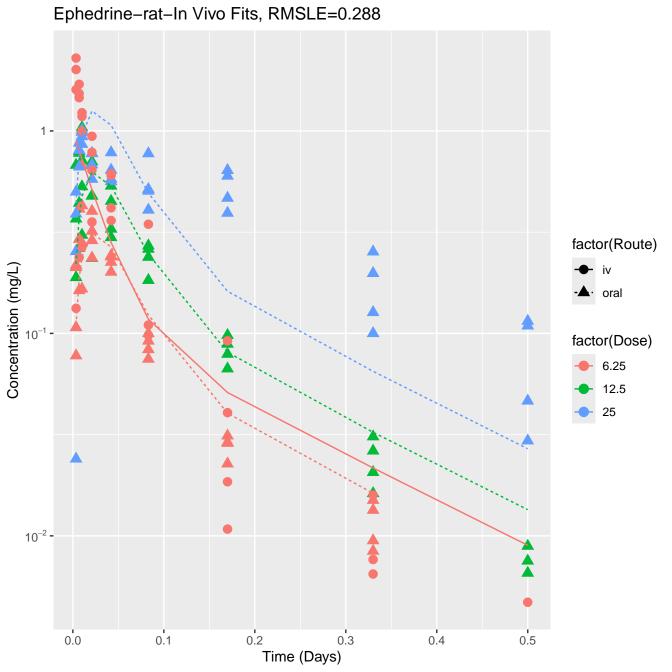
 $4-Methylimidazole-rat-HTPBTK-Ensemble,\ RMSLE=0.596$ 30 -10 factor(Dose) Concentration (mg/L) 10 50 100 3 factor(Route) · oral 1 -0.3 -0.50 0.75 0.00 0.25 1.00 1.25 Time (Days)

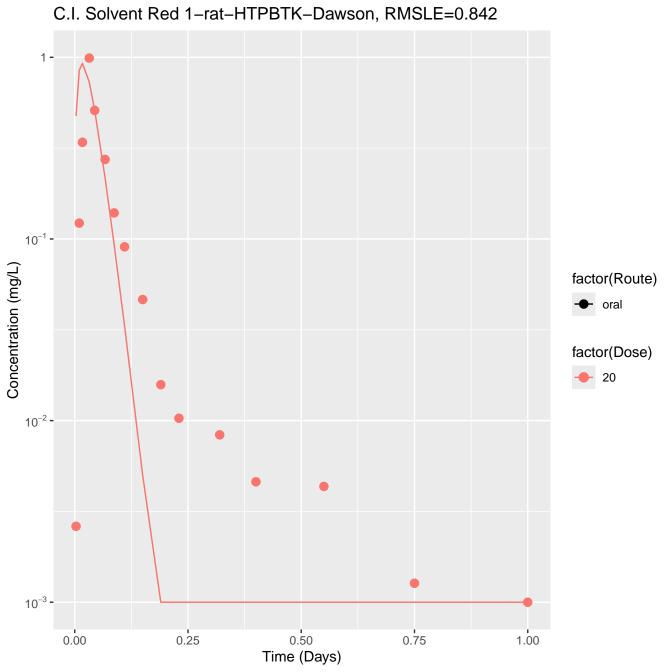


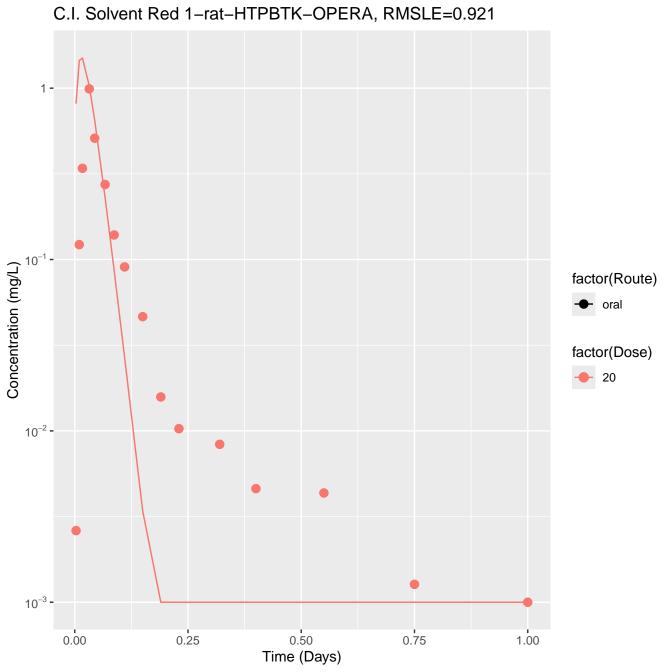


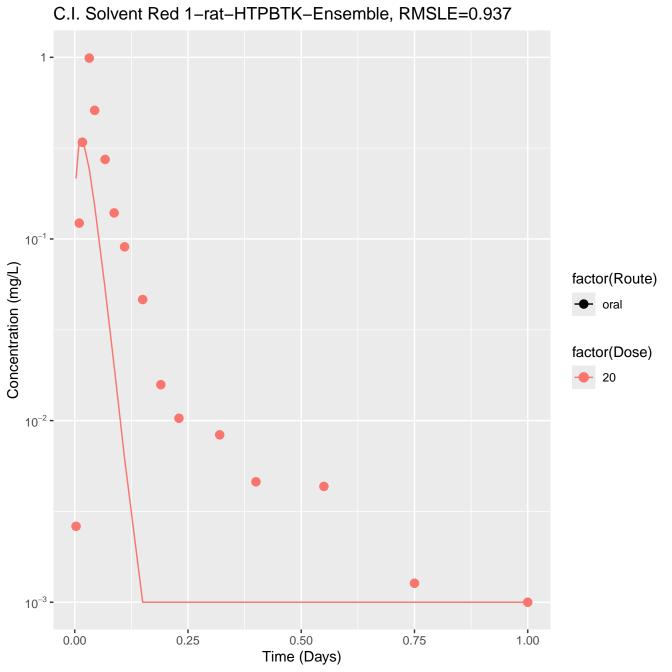


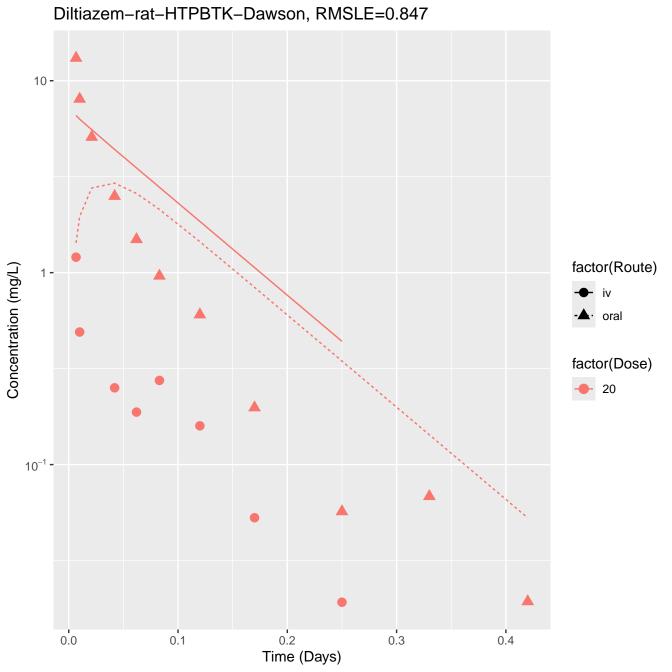


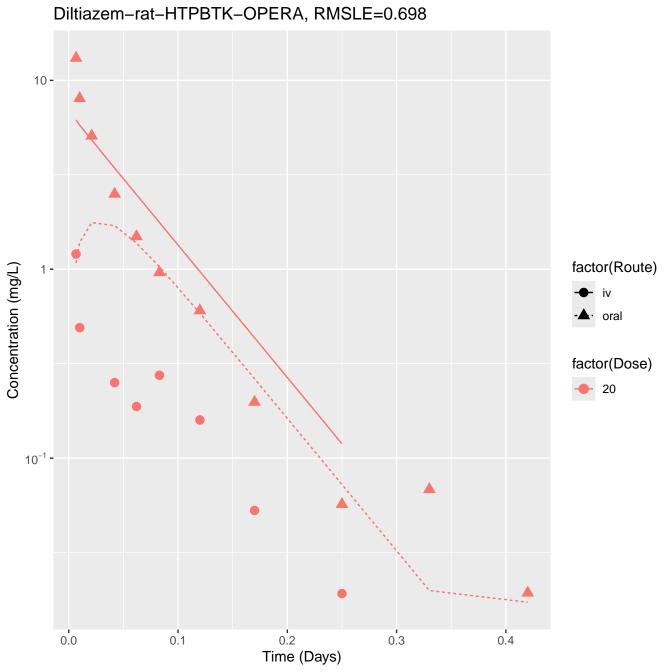


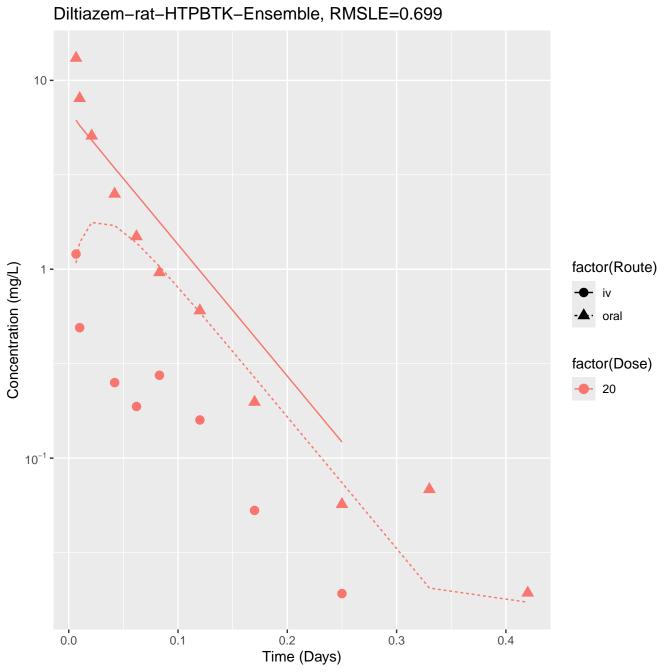




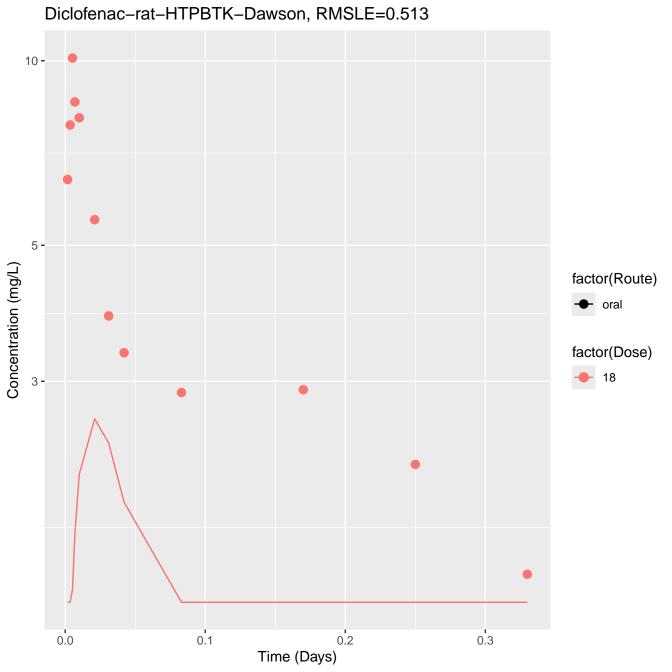


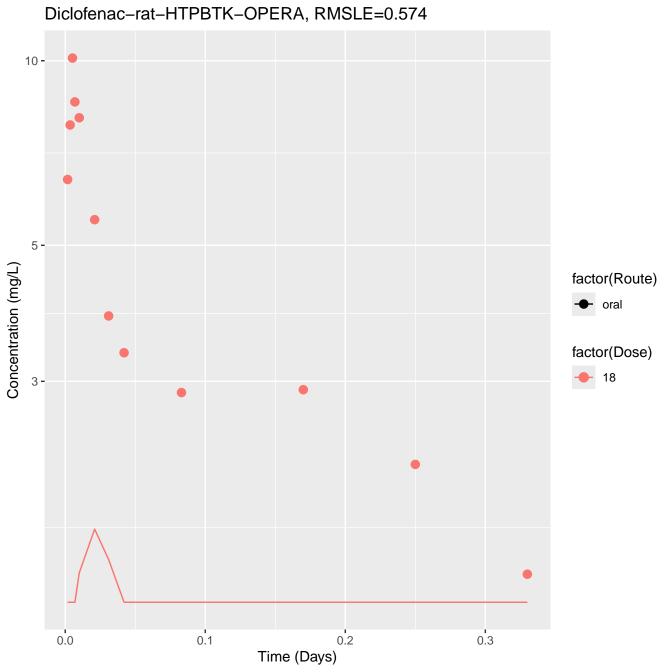


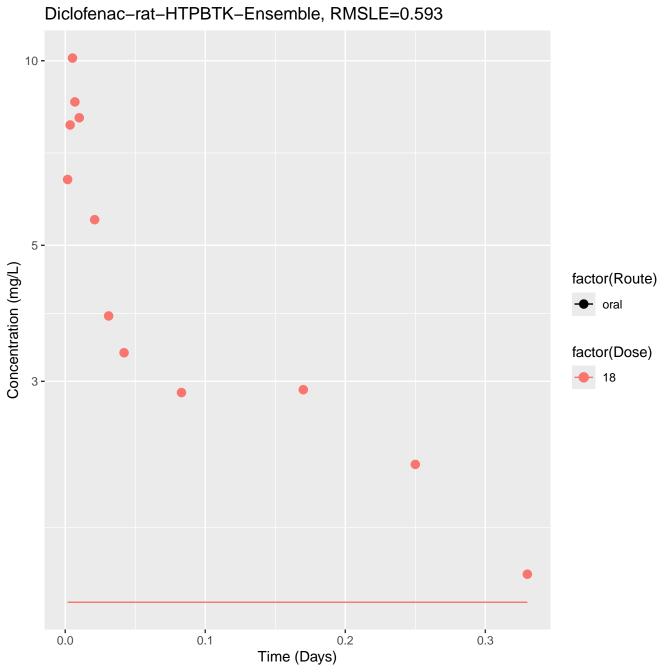




Diltiazem-rat-In Vivo Fits, RMSLE=0.439 10factor(Route) Concentration (mg/L) · oral factor(Dose) 20 10<sup>-1</sup> -0.2 0.0 0.1 0.3 0.4 Time (Days)

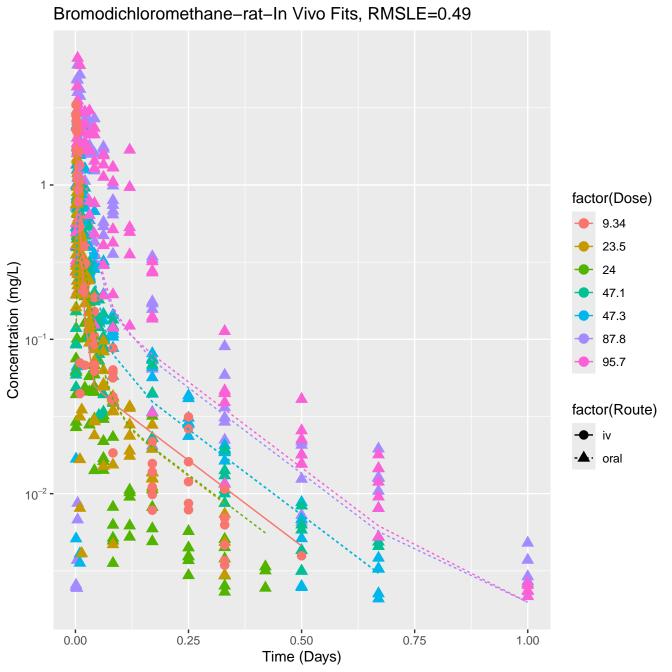


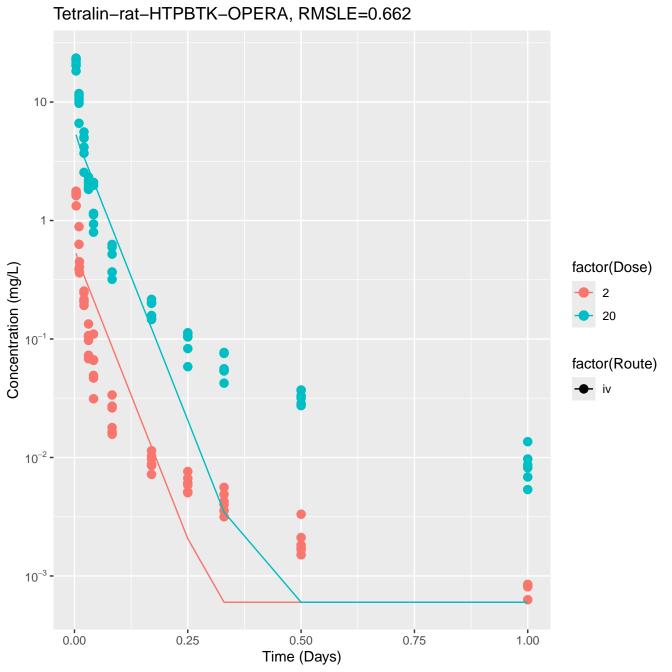


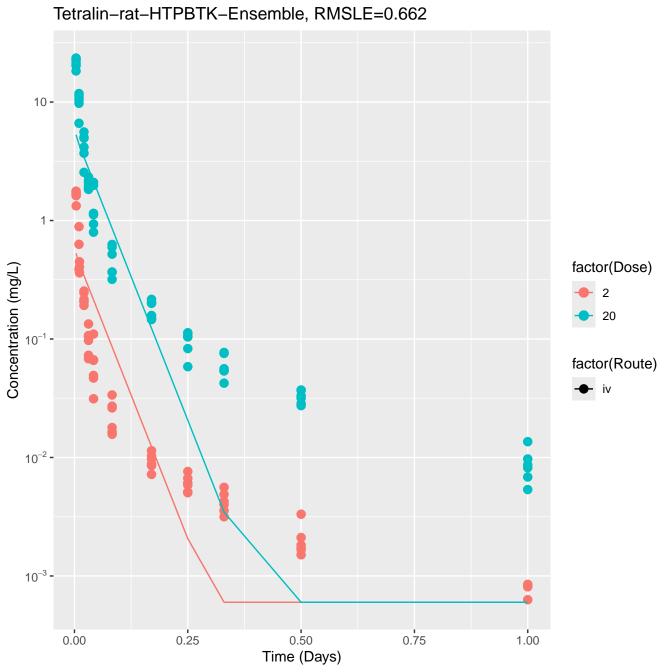


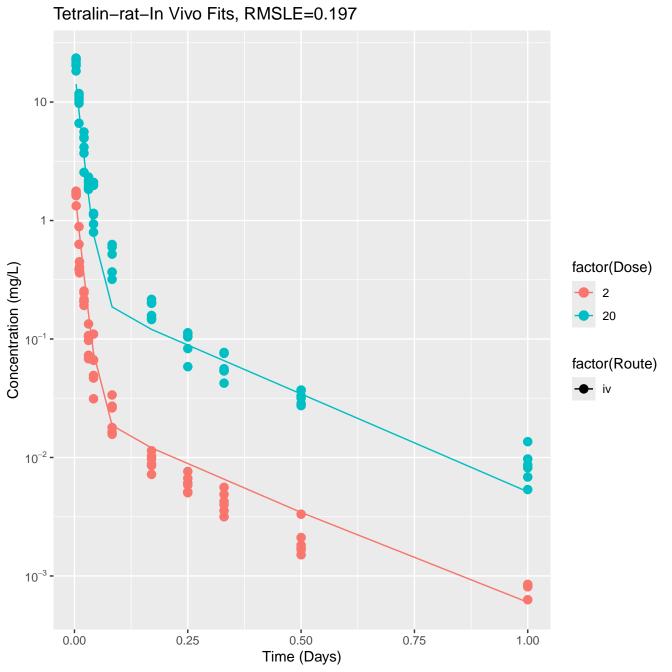
Bromodichloromethane-rat-HTPBTK-OPERA, RMSLE=1.17 10 factor(Dose) 9.34 1 -23.5 Concentration (mg/L) 24 47.1 47.3 87.8 95.7 factor(Route) · oral 10<sup>-2</sup> -0.25 0.50 0.75 0.00 1.00 Time (Days)

Bromodichloromethane-rat-HTPBTK-Ensemble, RMSLE=1.17 10 factor(Dose) 9.34 1 -23.5 Concentration (mg/L) 24 47.1 47.3 87.8 95.7 factor(Route) · oral 10<sup>-2</sup> -0.25 0.50 0.75 0.00 1.00 Time (Days)

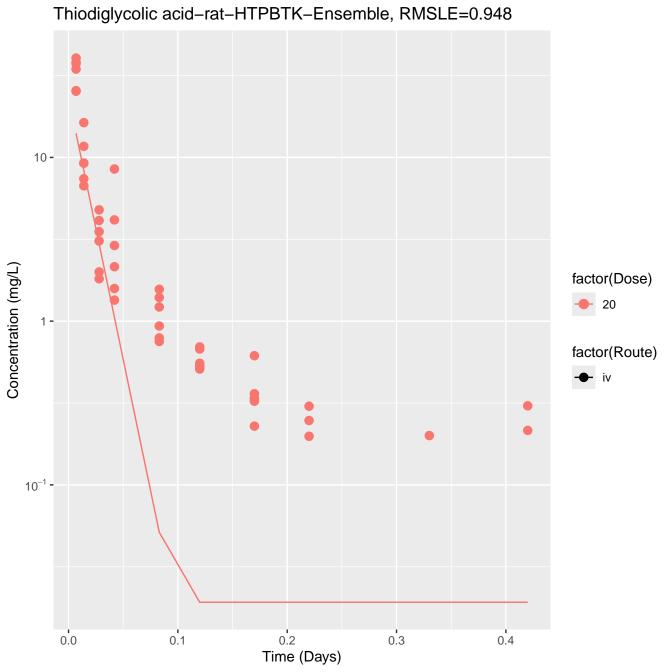


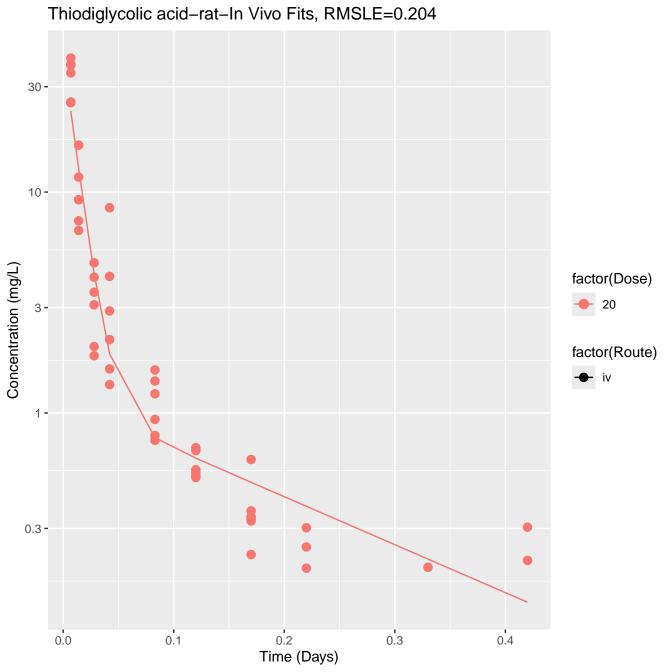


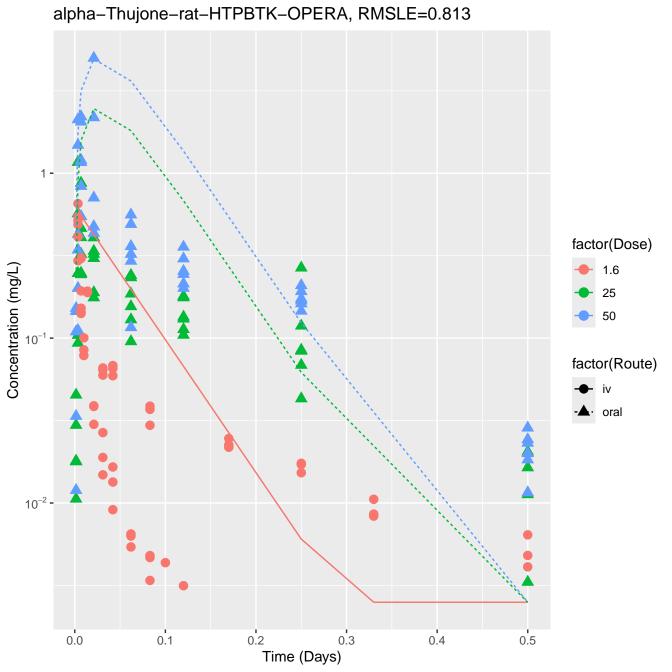


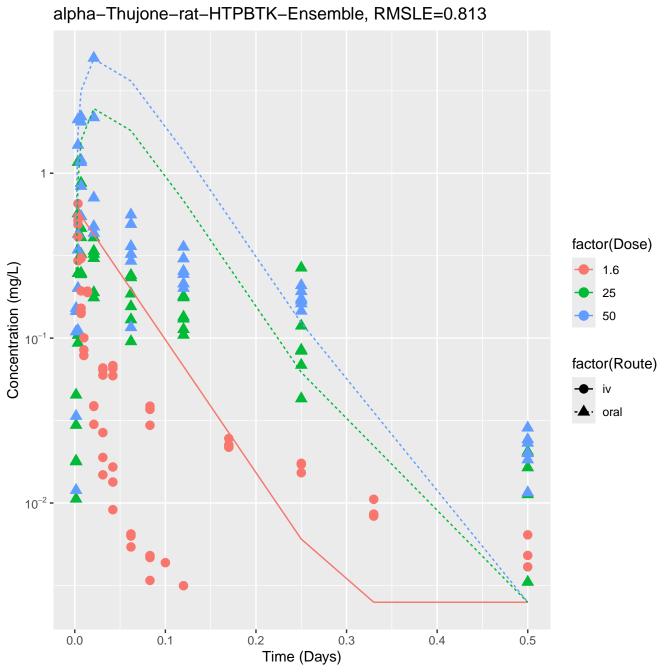


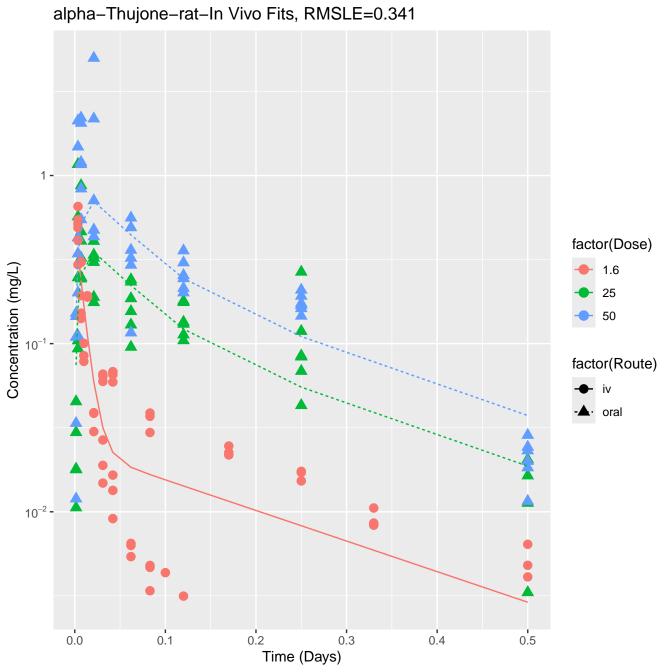
Thiodiglycolic acid-rat-HTPBTK-OPERA, RMSLE=1.03 30 -10-Concentration (mg/L) factor(Dose) 20 3 factor(Route) iv iv 1 -0.3 -0.0 0.1 0.2 0.3 0.4 Time (Days)





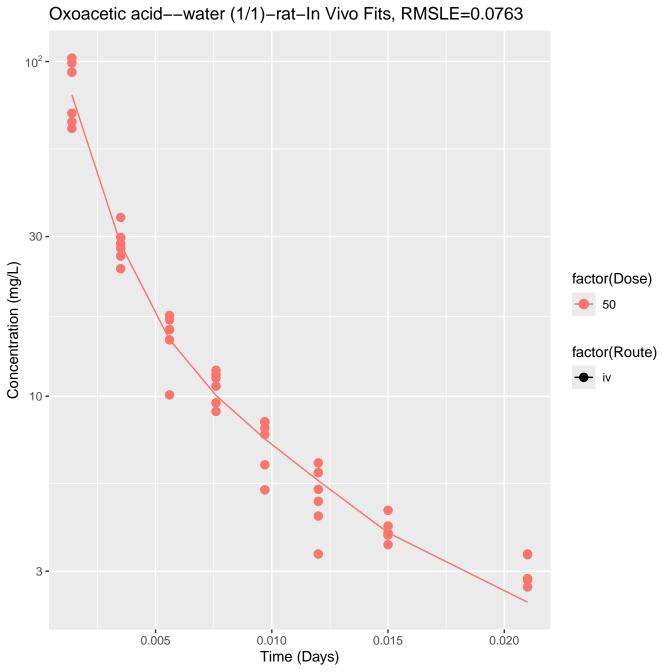


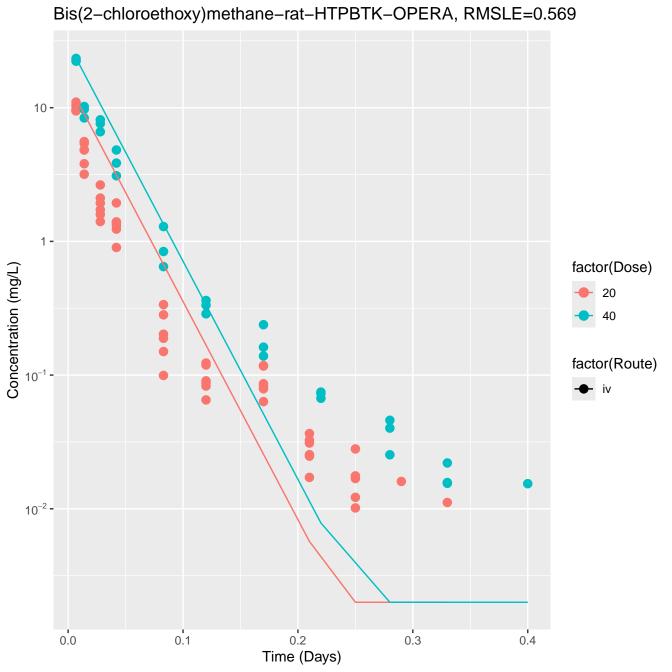




Oxoacetic acid--water (1/1)-rat-HTPBTK-OPERA, RMSLE=0.706 10<sup>2</sup> -30 -Concentration (mg/L) factor(Dose) 50 factor(Route) iv 10 -3 -0.005 0.010 0.015 0.020 Time (Days)

Oxoacetic acid--water (1/1)-rat-HTPBTK-Ensemble, RMSLE=0.706 10<sup>2</sup> -30 -Concentration (mg/L) factor(Dose) 50 factor(Route) iv 10 -3 -0.005 0.010 0.015 0.020 Time (Days)





Bis(2-chloroethoxy)methane-rat-HTPBTK-Ensemble, RMSLE=0.569 10 -1 -Concentration (mg/L) factor(Dose) 20 40 factor(Route) 10<sup>-2</sup> -0.2 0.3 0.0 0.1 0.4 Time (Days)

