Supplemental Material

Respirometric Screening and Characterization of Mitochondrial Toxicants Within the ToxCast Phase I and II Chemical Libraries

Daniel R. Hallinger¹, Hayley B. Lindsay², Katie Paul Friedman¹, Danielle A. Suarez³, and Steven O. Simmons¹

¹National Center for Computational Toxicology; ²Oak Ridge Associated Universities, Contractor; ³Environmental and Public Health Division, National Health and Environmental Effects Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency

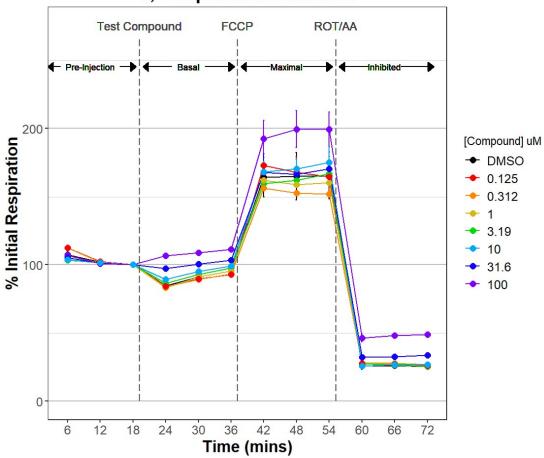
Authors DRH and HBL contributed equally to this work.

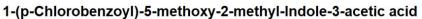
Corresponding Author:

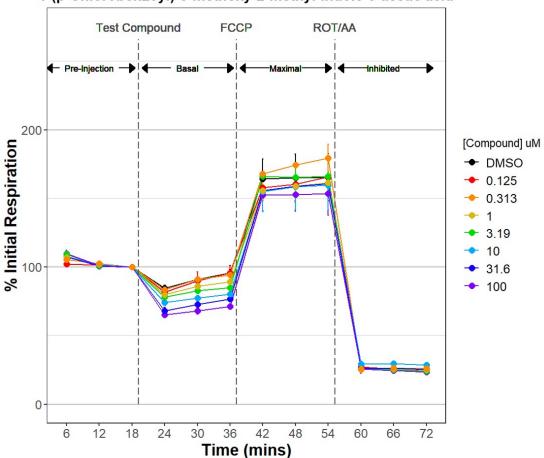
Steven O. Simmons, Ph.D. 109 TW Alexander Drive MD B205-01 Research Triangle Park, North Carolina 27711 USA

Supplemental Figure 2 shows the temporal dose-response plots (median % initial respiration \pm mad) for all 243 chemicals tested in Tier 2 RSA screening.

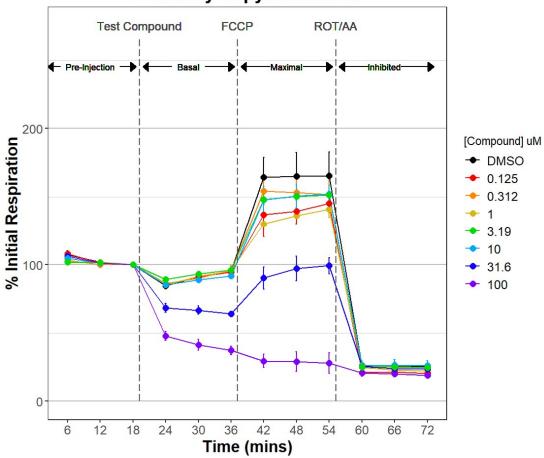
1,5-Naphthalenediamine



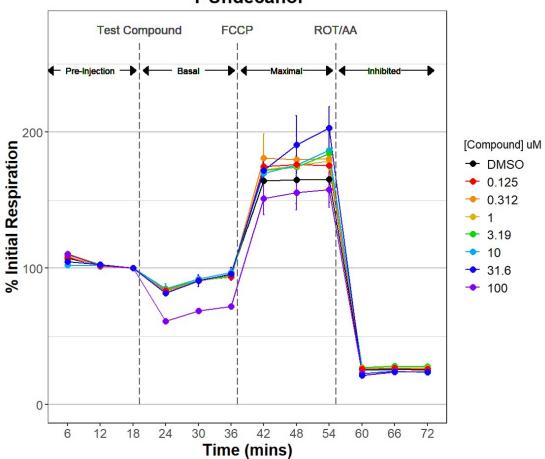




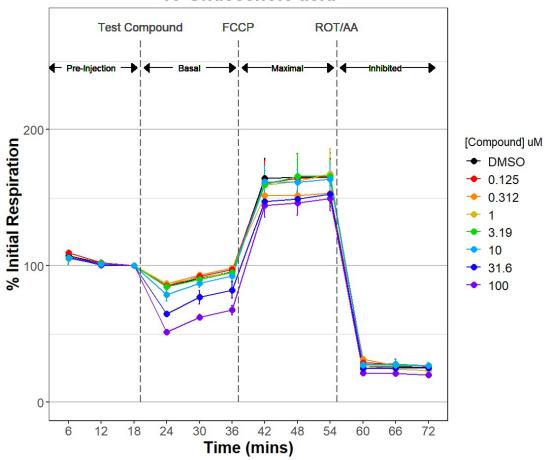
1-Dodecyl-2-pyrrolidinone



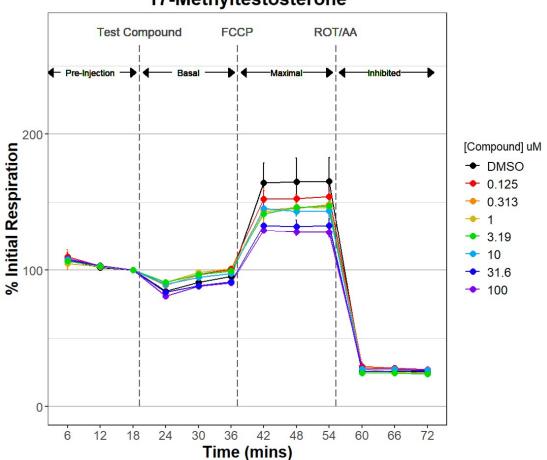
1-Undecanol



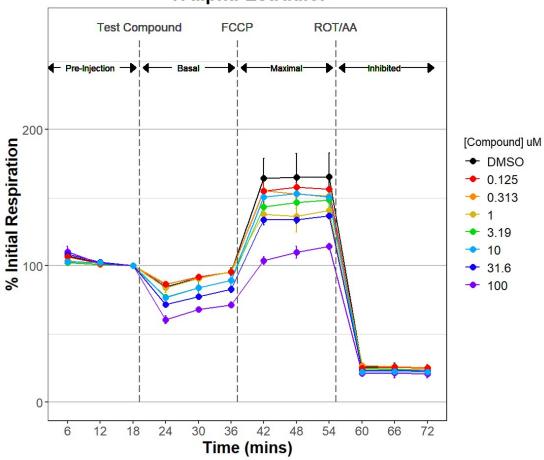
10-Undecenoic acid



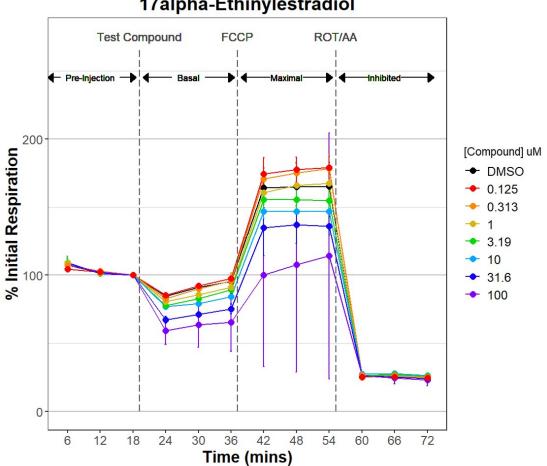
17-Methyltestosterone



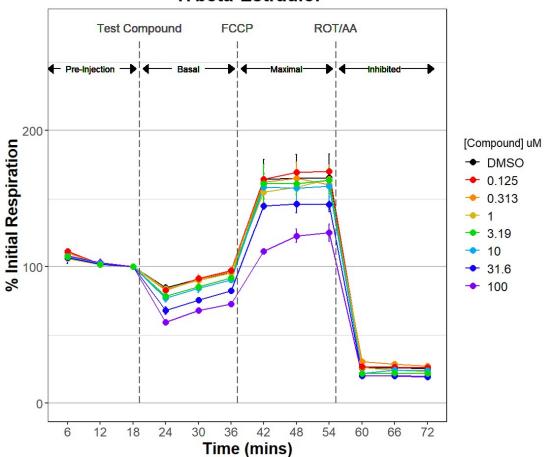
17alpha-Estradiol



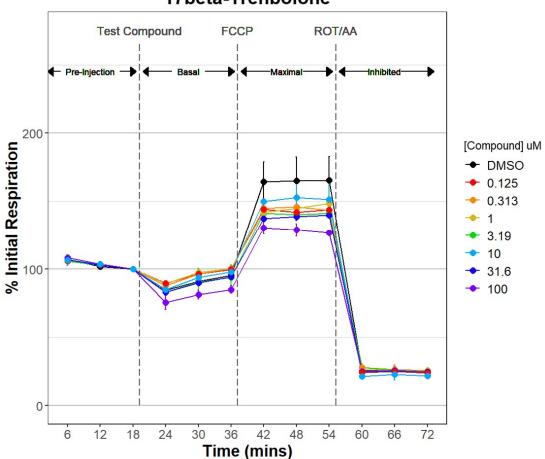
17alpha-Ethinylestradiol



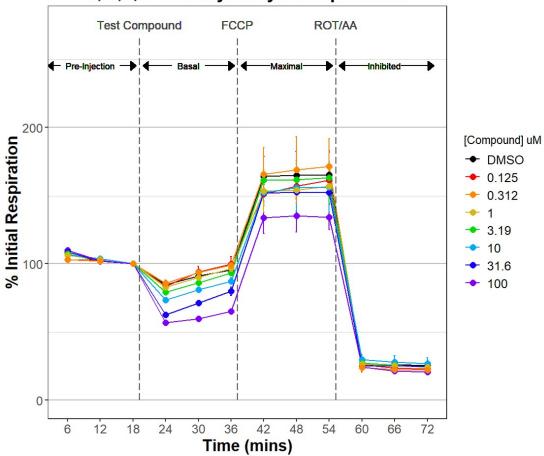
17beta-Estradiol



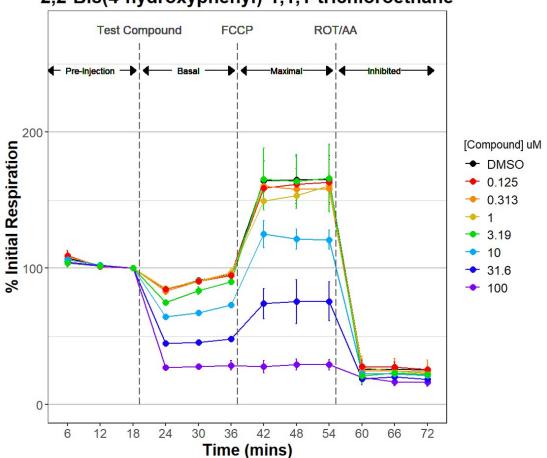
17beta-Trenbolone



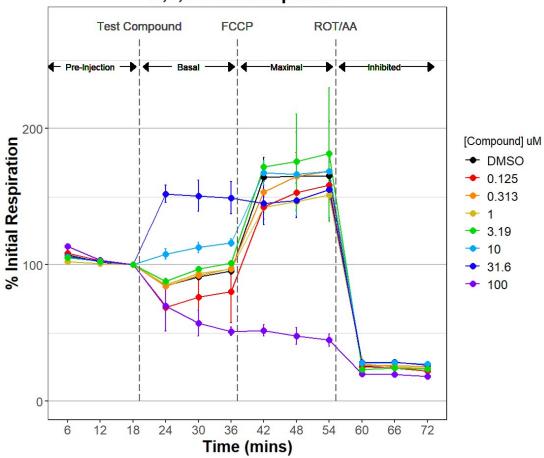
2,2',4,4'-Tetrahydroxybenzophenone



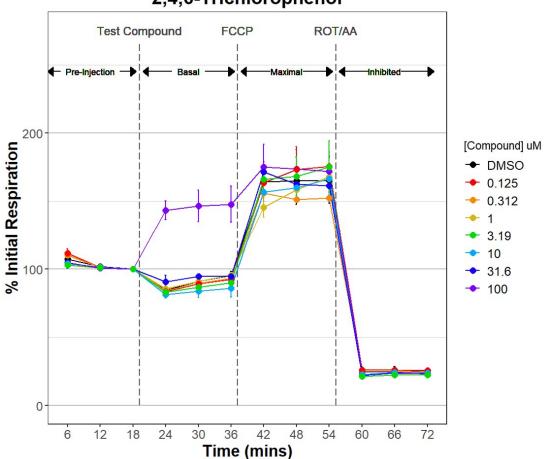
2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane



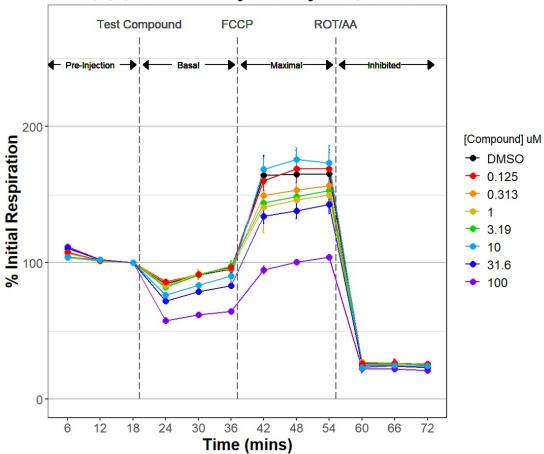
2,4,5-Trichlorophenol



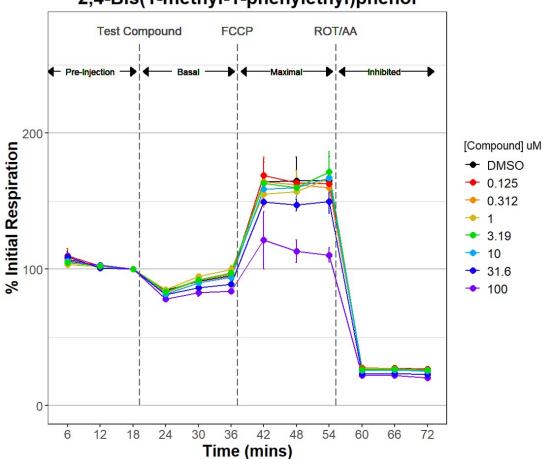
2,4,6-Trichlorophenol



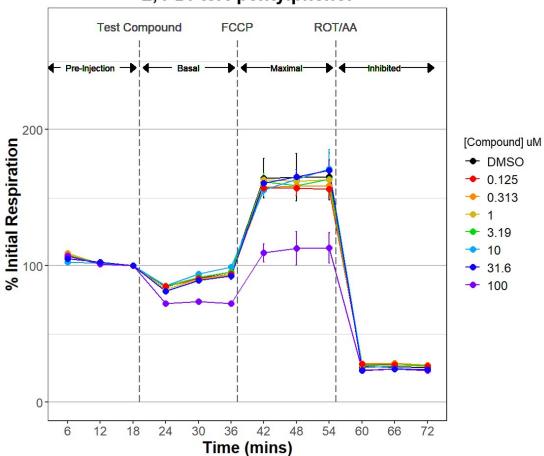
2,4,7,9-Tetramethyl-5-decyne-4,7-diol



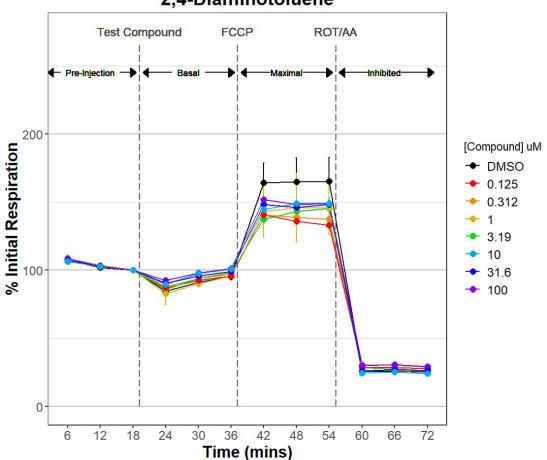
2,4-Bis(1-methyl-1-phenylethyl)phenol



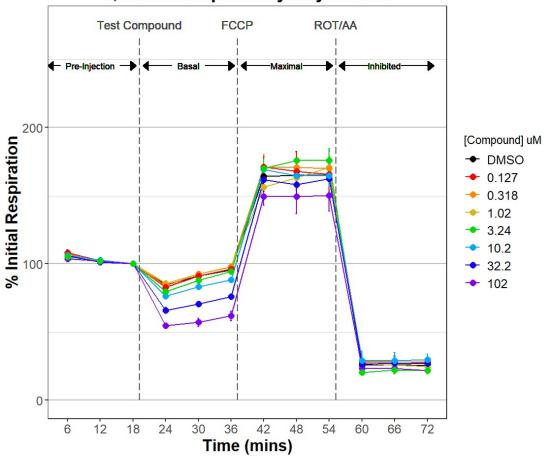
2,4-Di-tert-pentylphenol



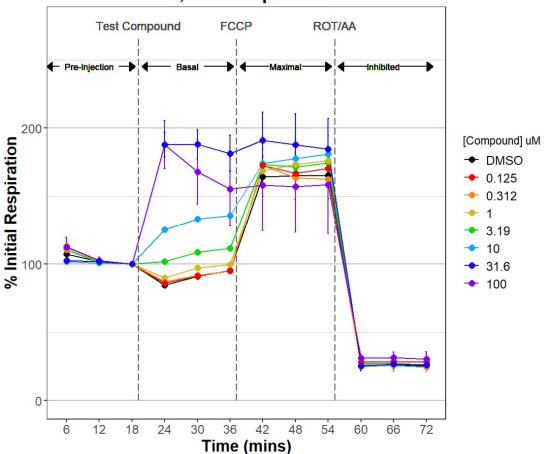
2,4-Diaminotoluene



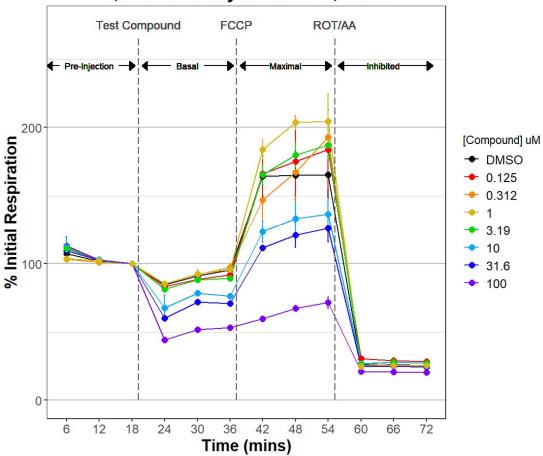
2,4-Dichlorophenoxybutyric acid

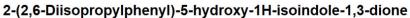


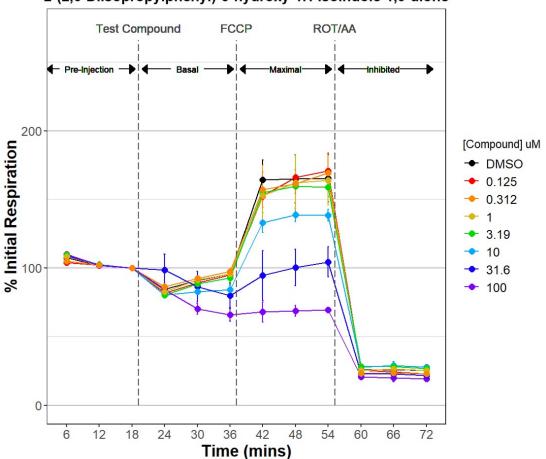
2,4-Dinitrophenol



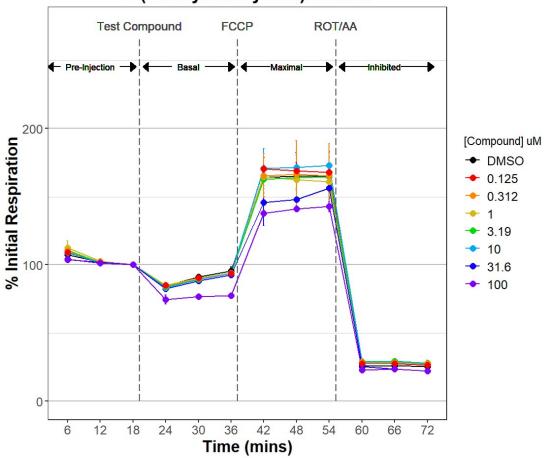
2,5-Di-tert-butylbenzene-1,4-diol



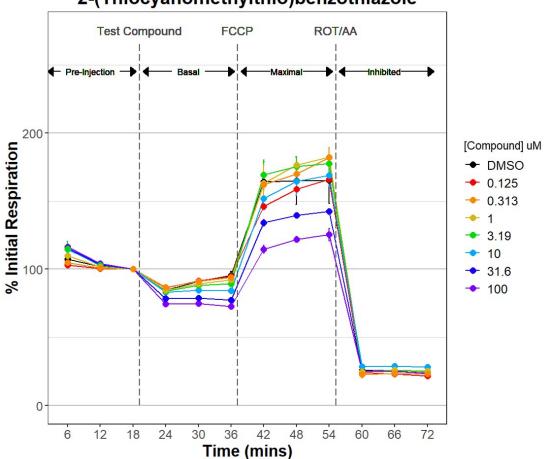




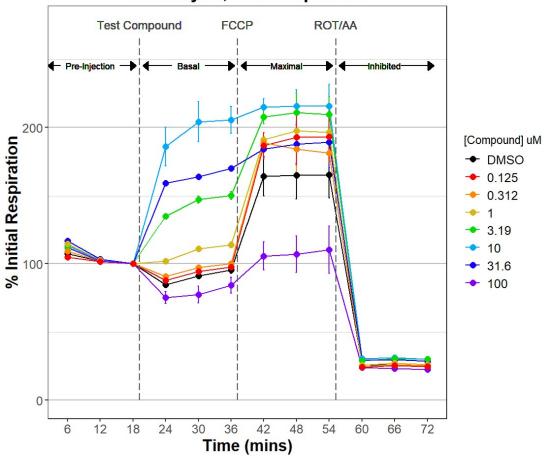
2-(Phenylmethylene)octanal



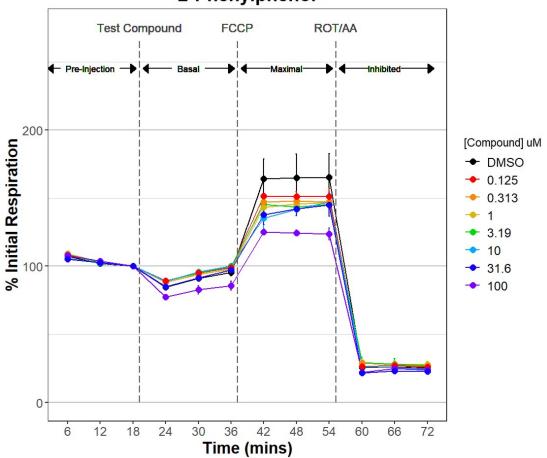




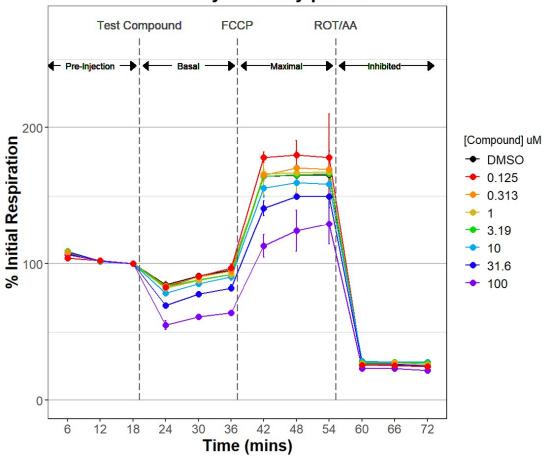
2-Methyl-4,6-dinitrophenol



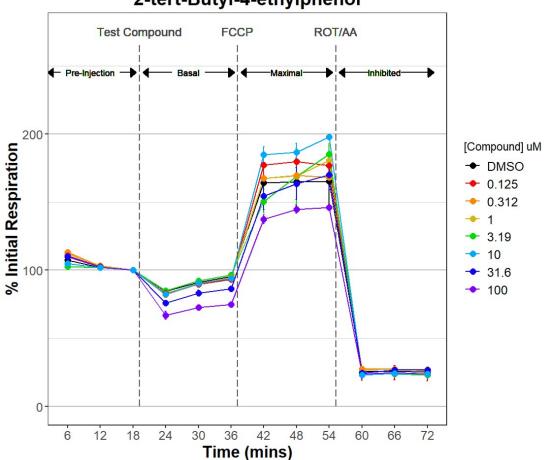
2-Phenylphenol



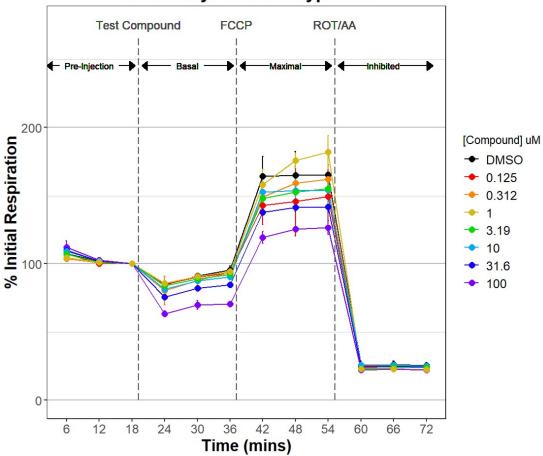
2-Tert-Butyl-5-methylphenol



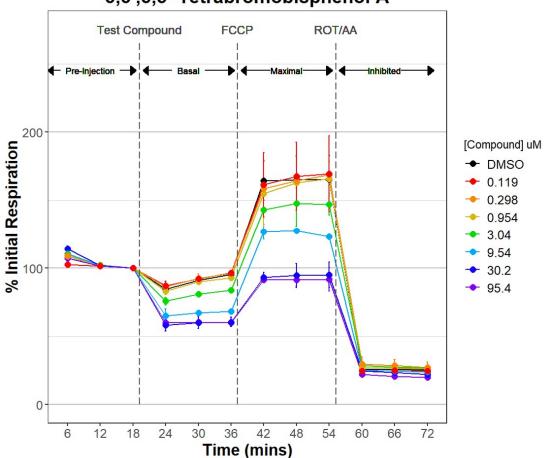
2-tert-Butyl-4-ethylphenol



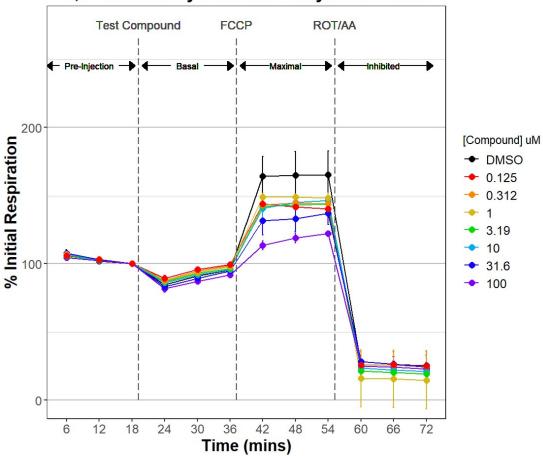
2-tert-Butyl-4-methoxyphenol



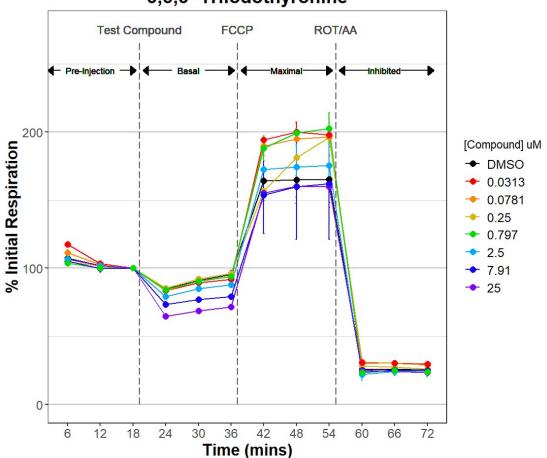




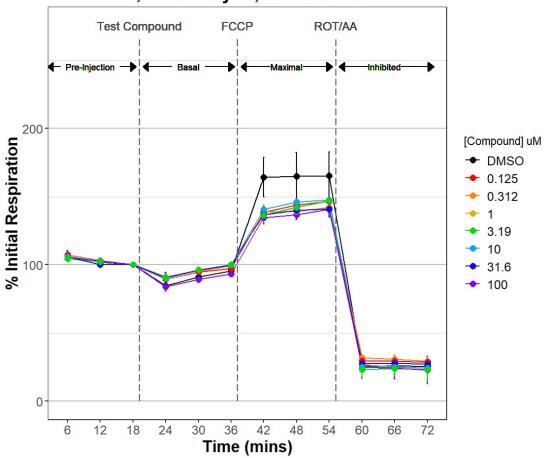
3,3'-Dimethoxybenzidine dihydrochloride



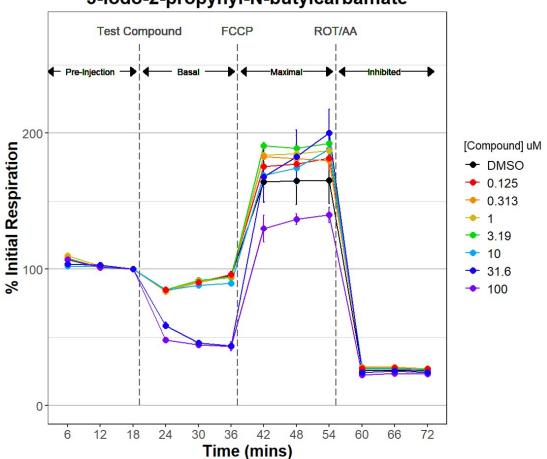




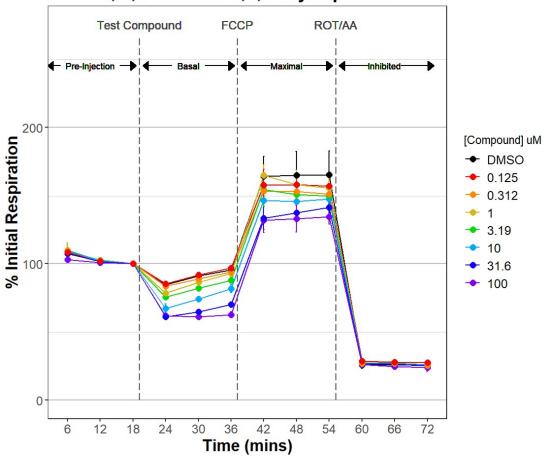
3,7-Dimethyl-2,6-octadienal



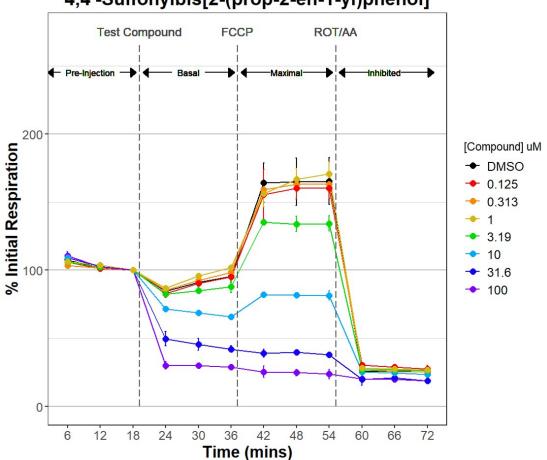
3-lodo-2-propynyl-N-butylcarbamate



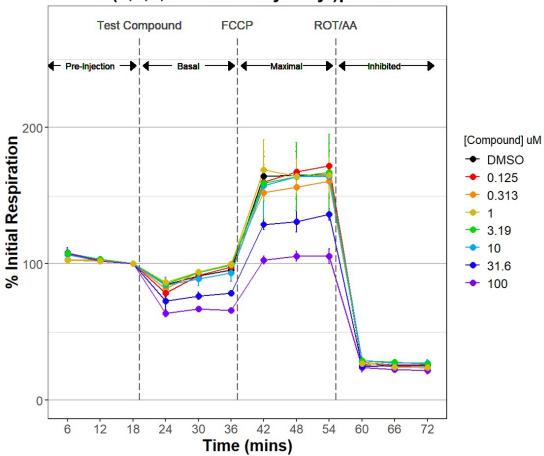
4,4',4"-Ethane-1,1,1-triyltriphenol



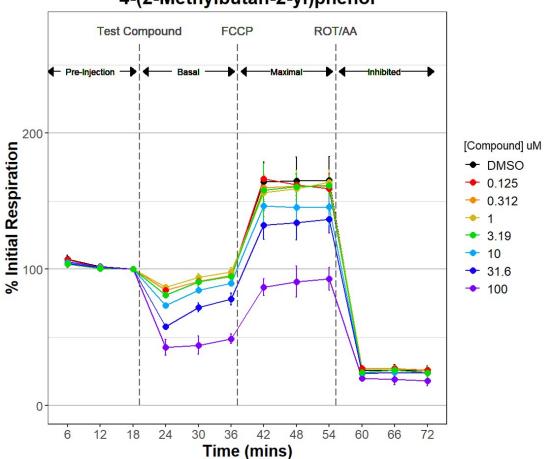
4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol]



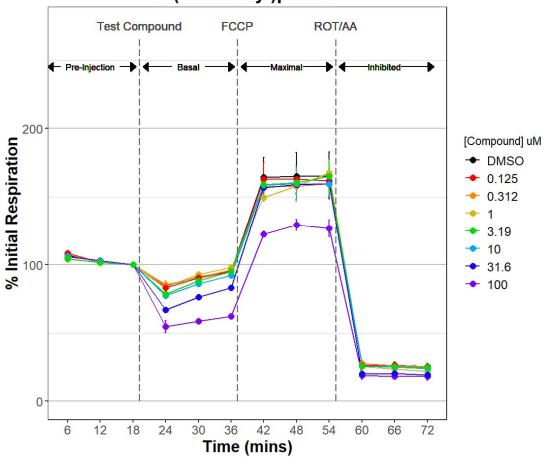
4-(1,1,3,3-Tetramethylbutyl)phenol



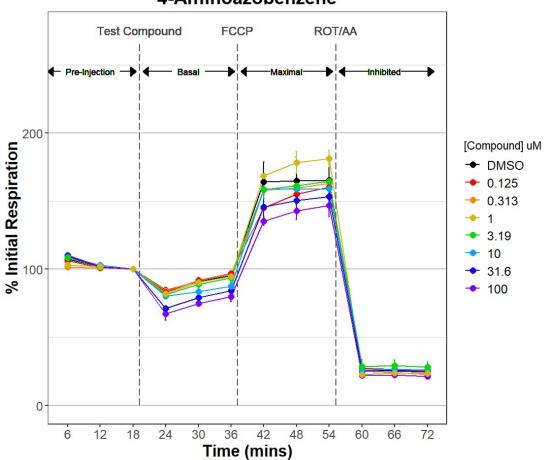
4-(2-Methylbutan-2-yl)phenol



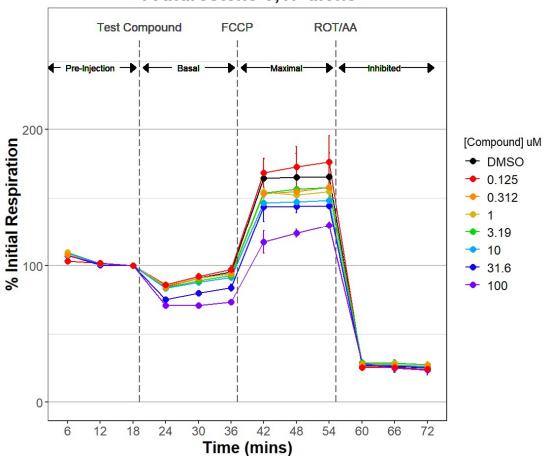
4-(Butan-2-yl)phenol



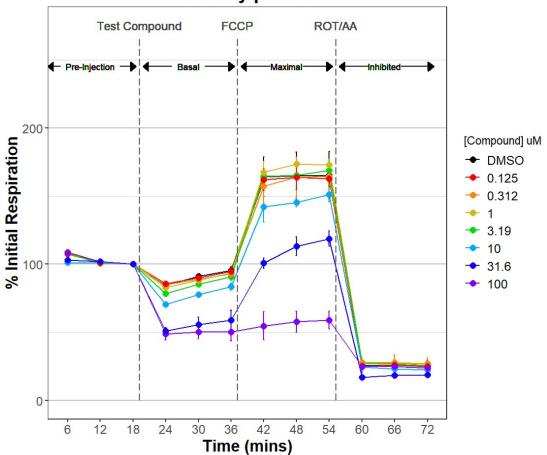
4-Aminoazobenzene



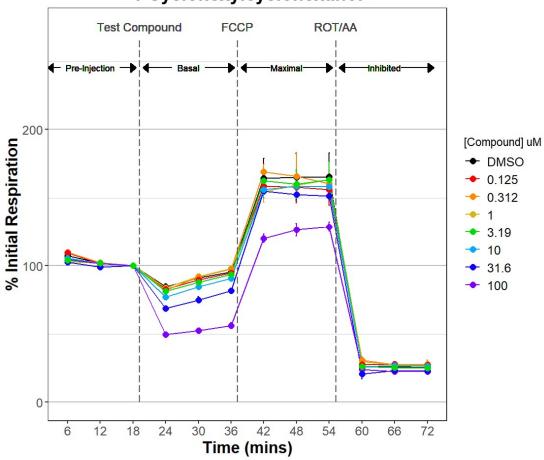
4-Androstene-3,17-dione



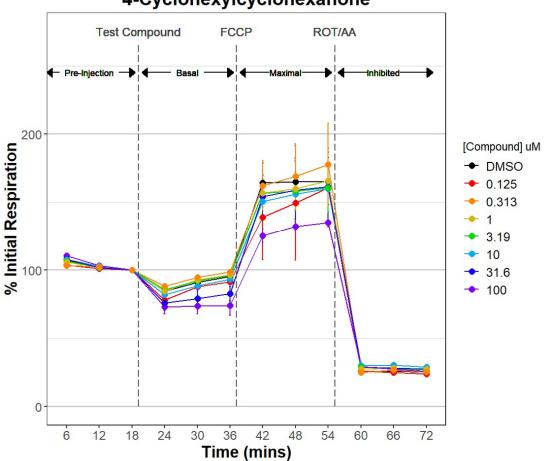




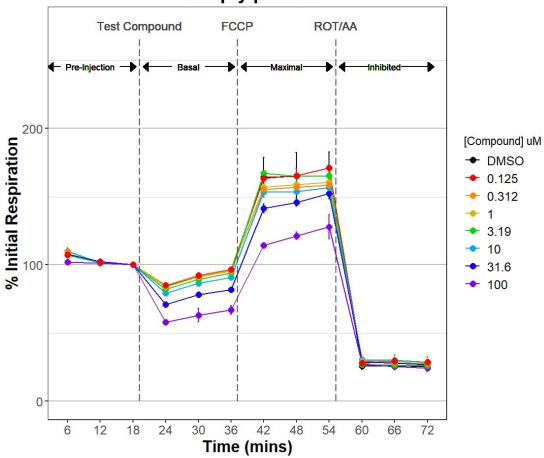
4-Cyclohexylcyclohexanol



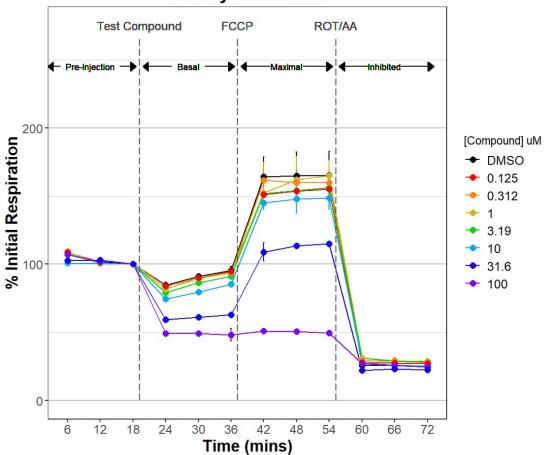
4-Cyclohexylcyclohexanone



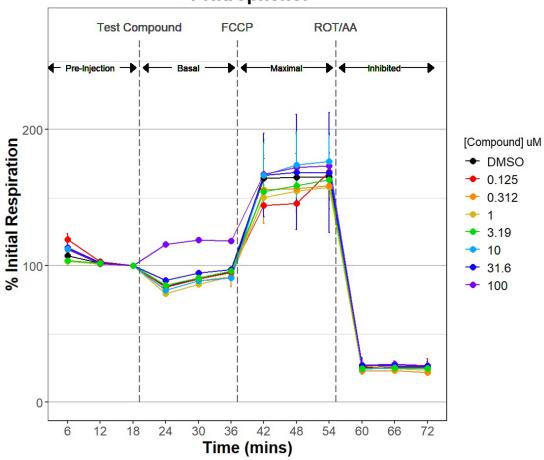
4-Heptylphenol



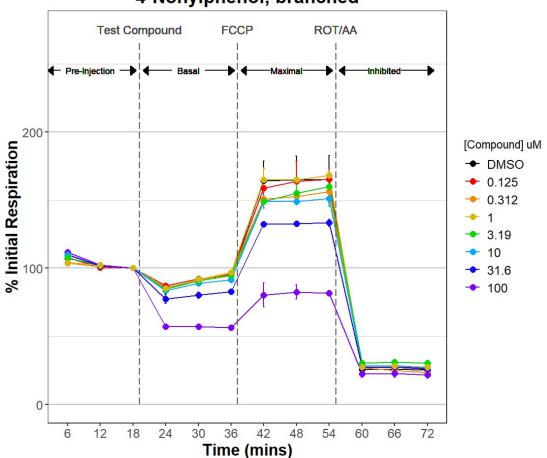
4-Hexylresorcinol



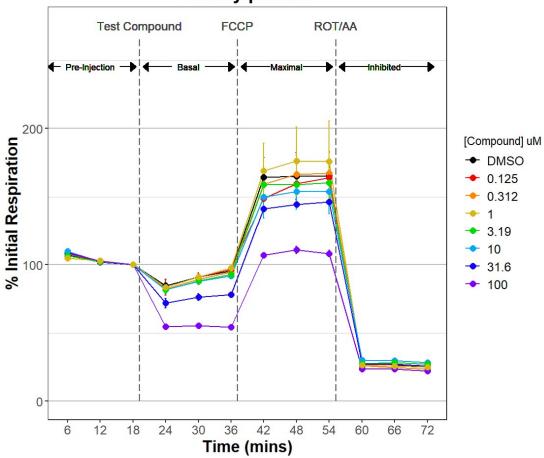
4-Nitrophenol



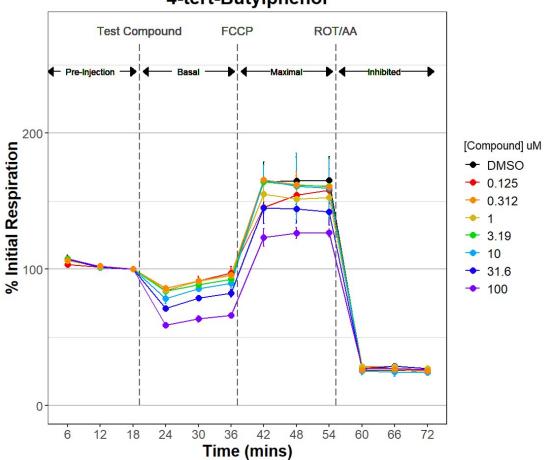
4-Nonylphenol, branched



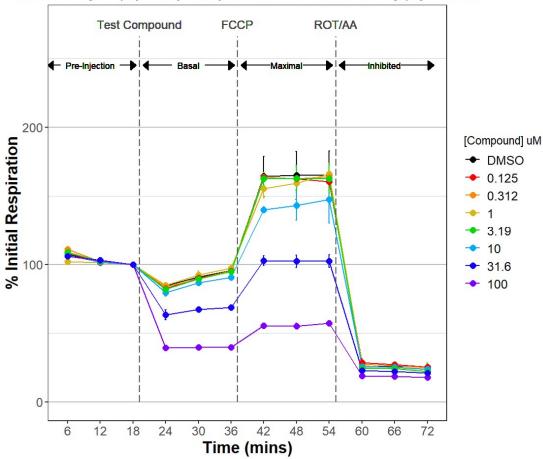
4-Octylphenol

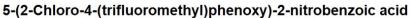


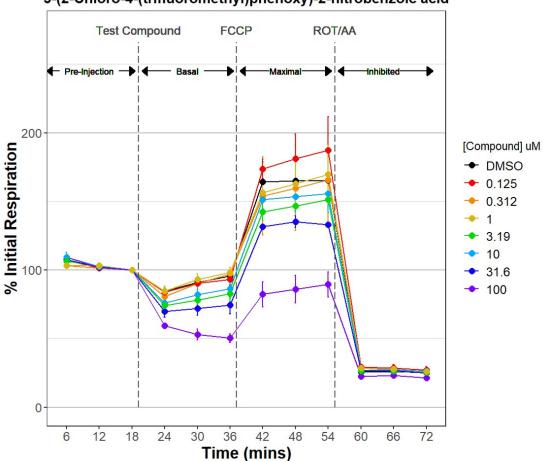
4-tert-Butylphenol



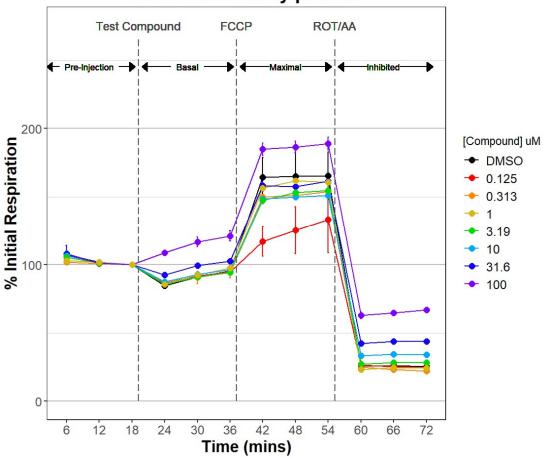
5,5-Dimethyl-3-(alpha,alpha,alpha-trifluoro-4-nitro-m-tolyl)hydantoin



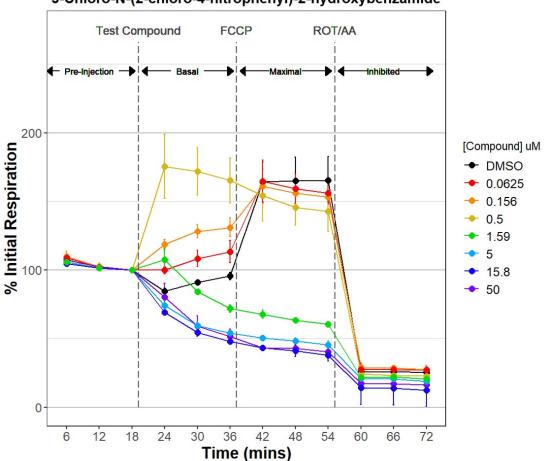




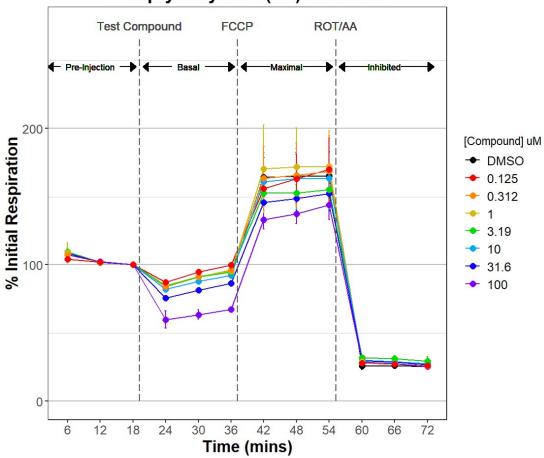
5-Amino-2-methylphenol



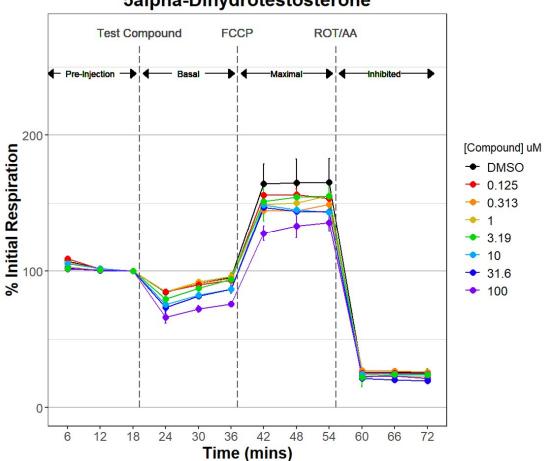




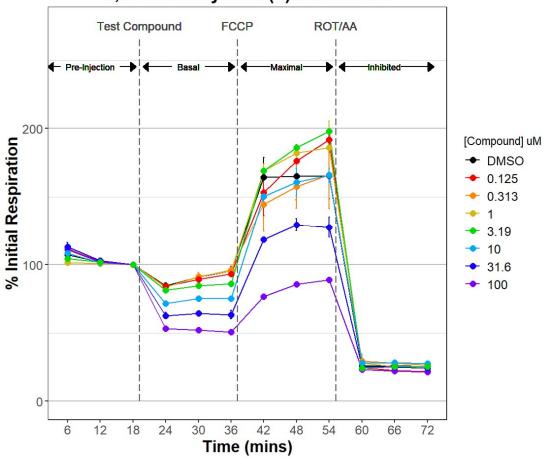
5-Heptyldihydro-2(3H)-furanone



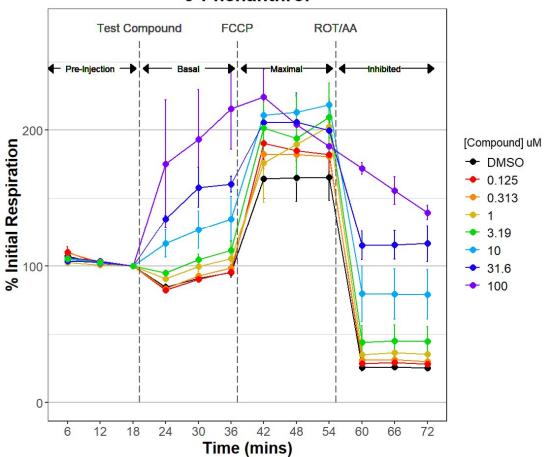
5alpha-Dihydrotestosterone

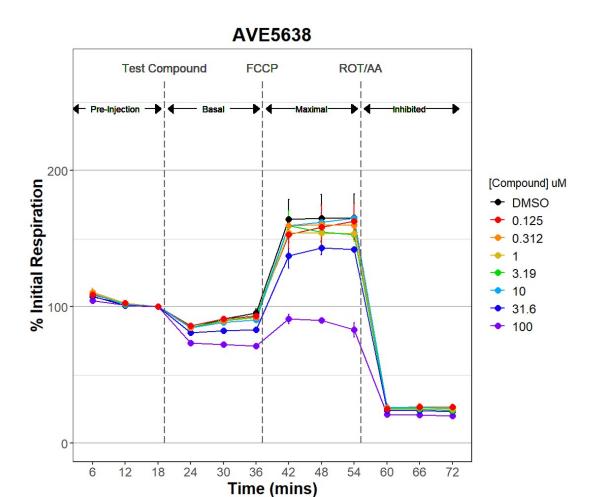


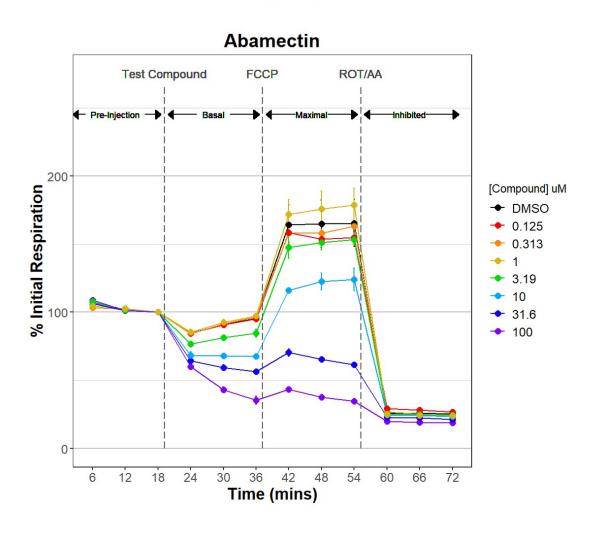
7,12-Dimethylbenz(a)anthracene

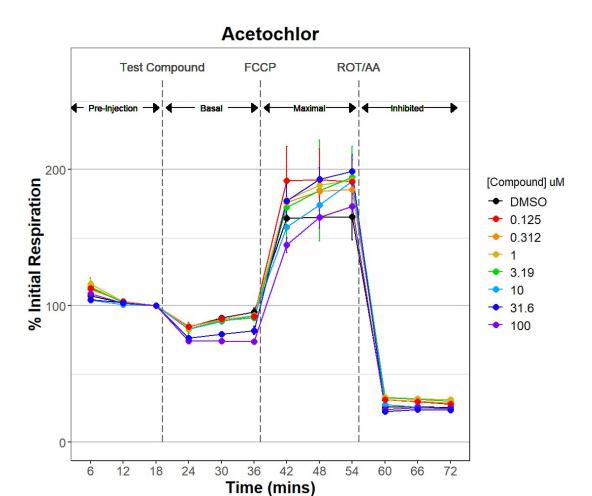


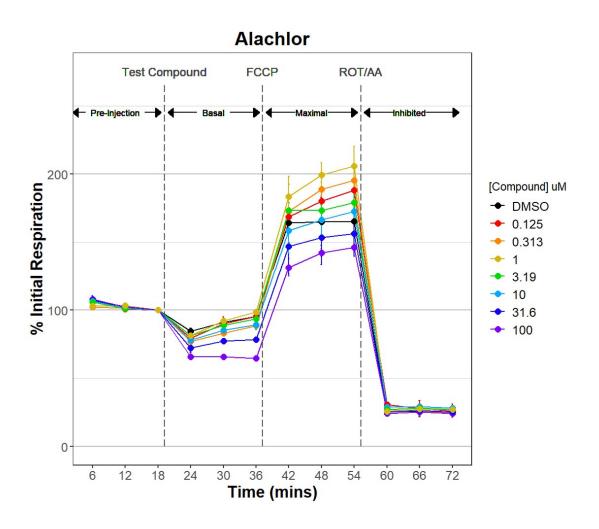
9-Phenanthrol

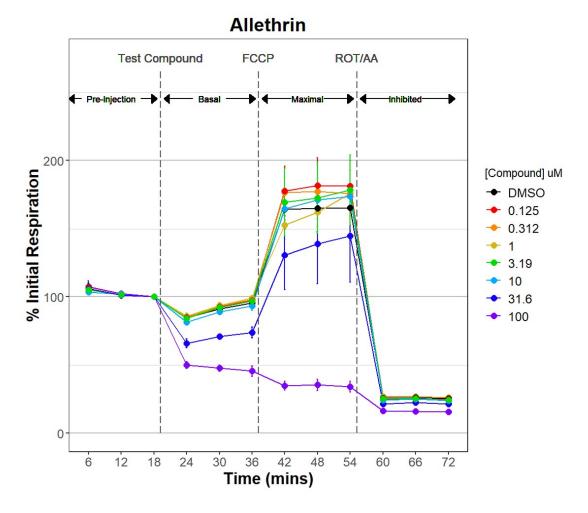


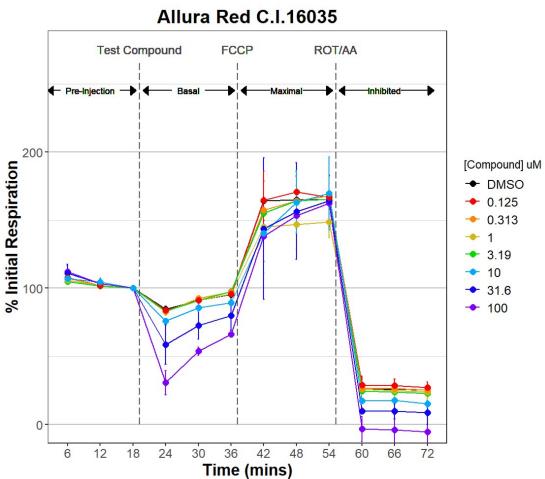


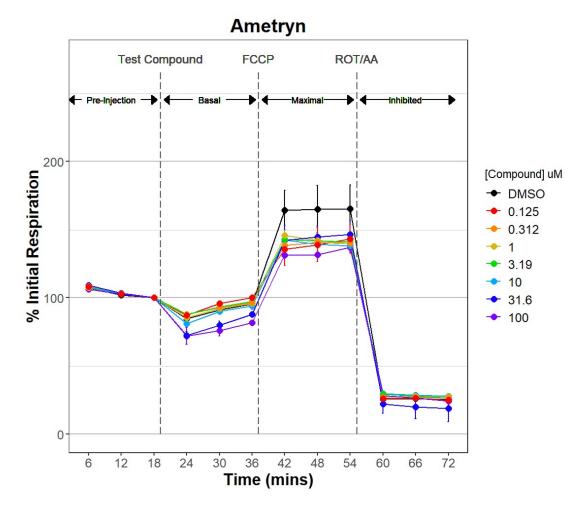


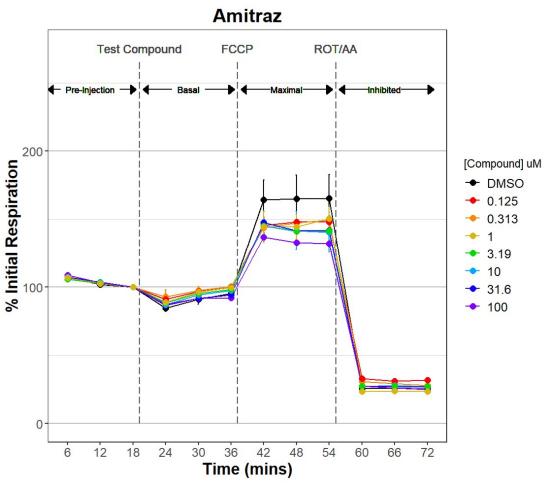


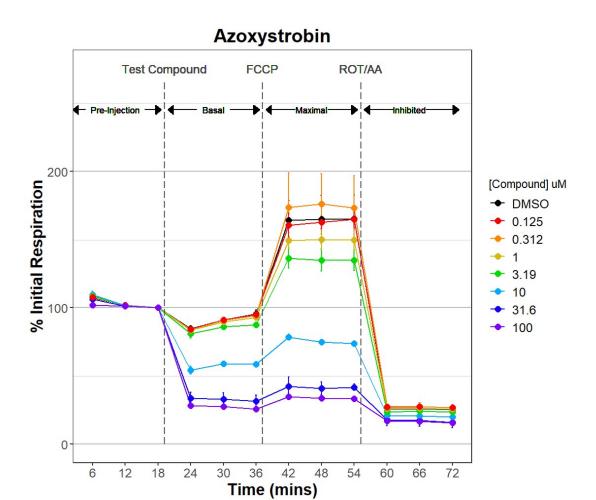


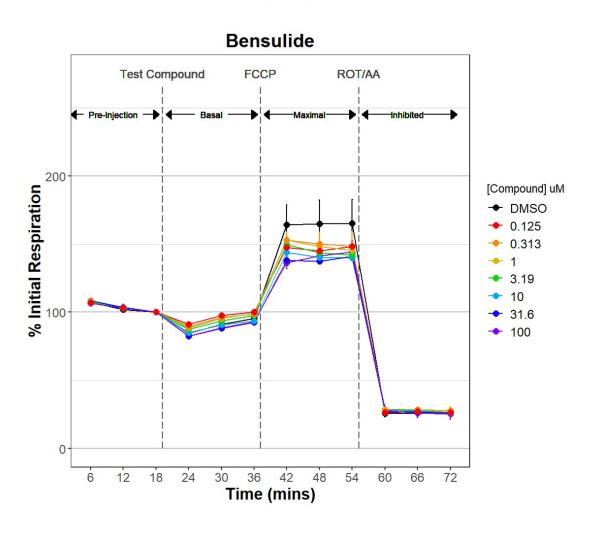


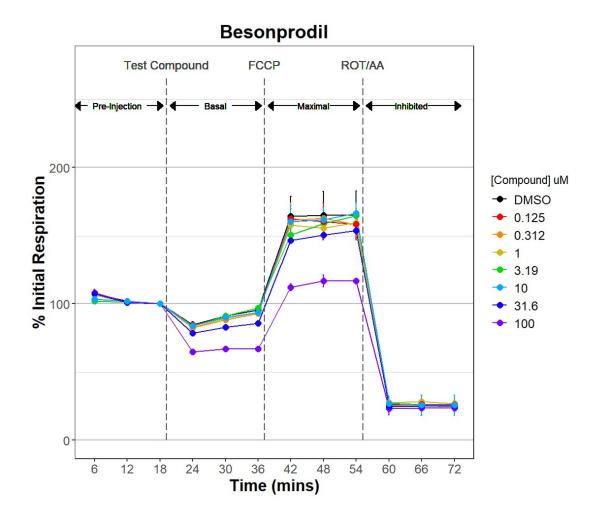


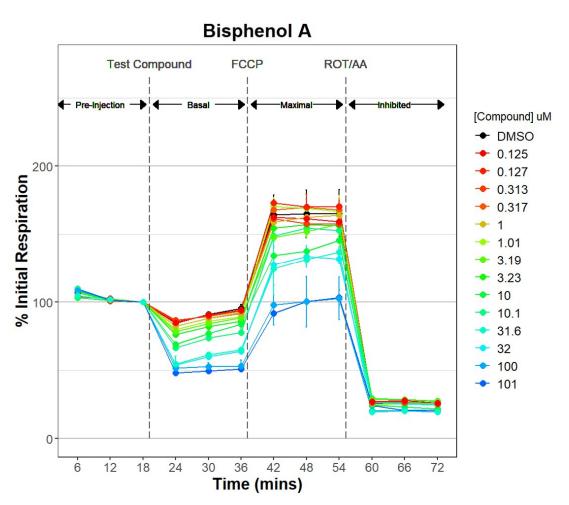




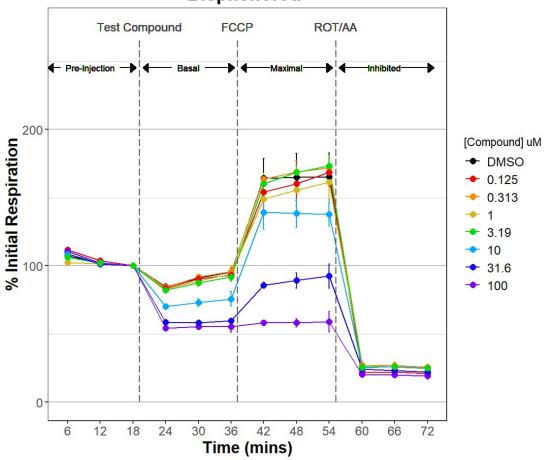




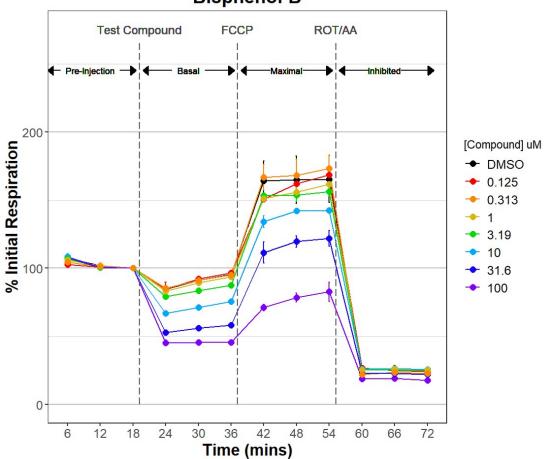


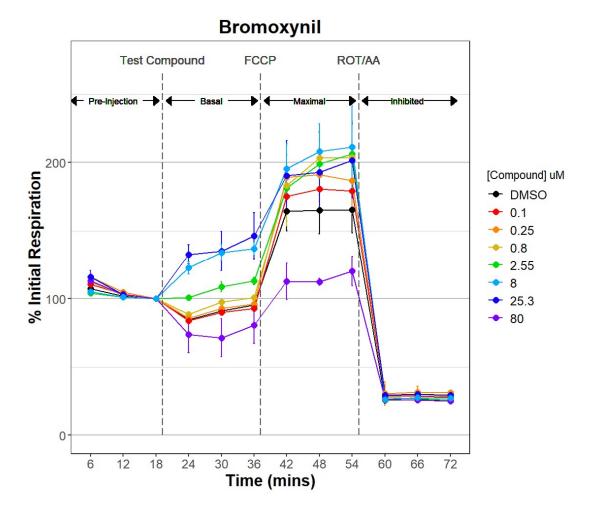


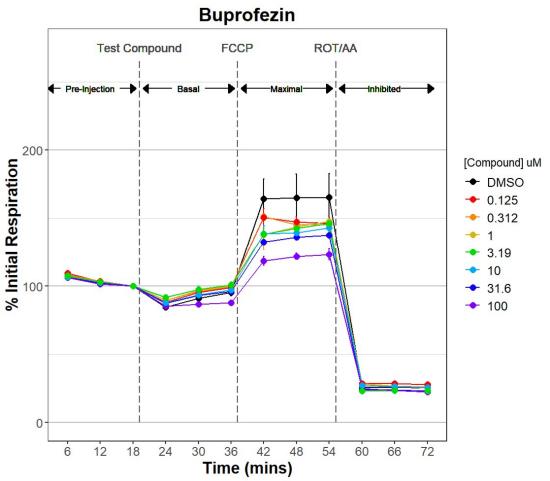


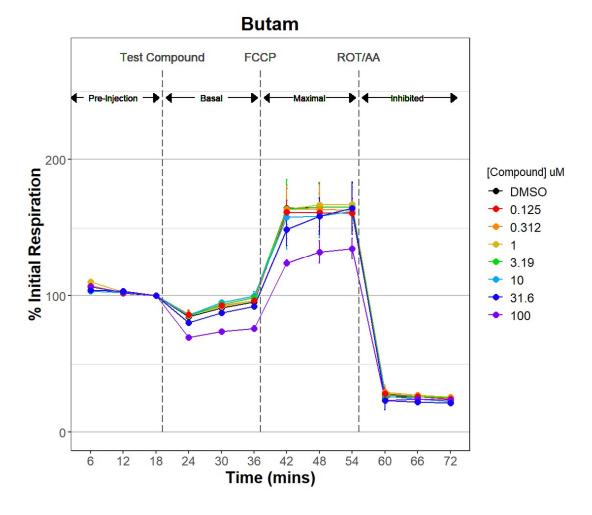


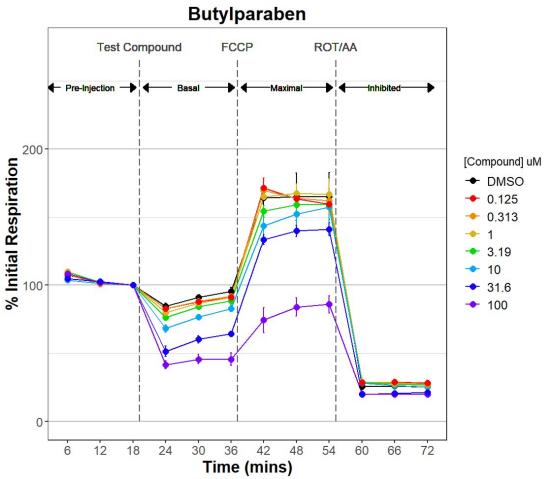




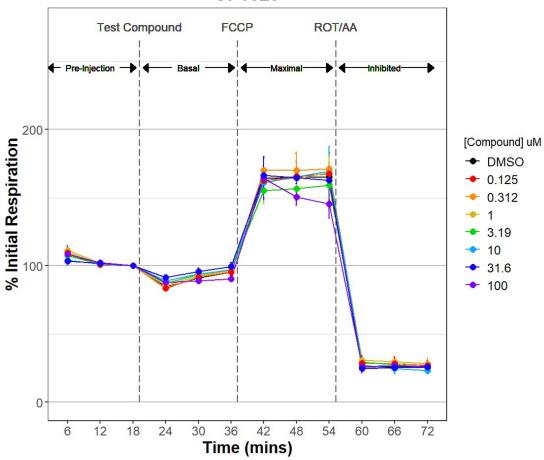


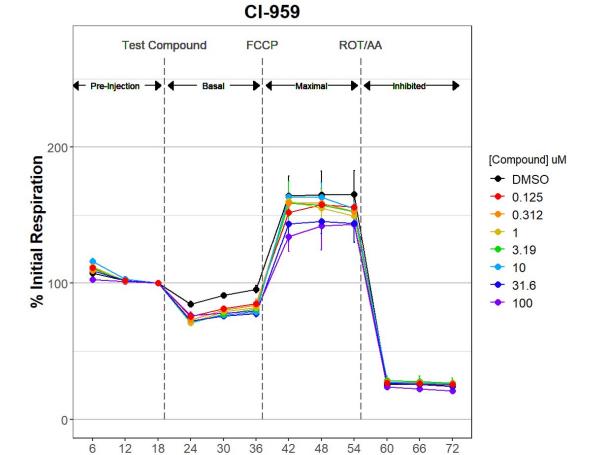






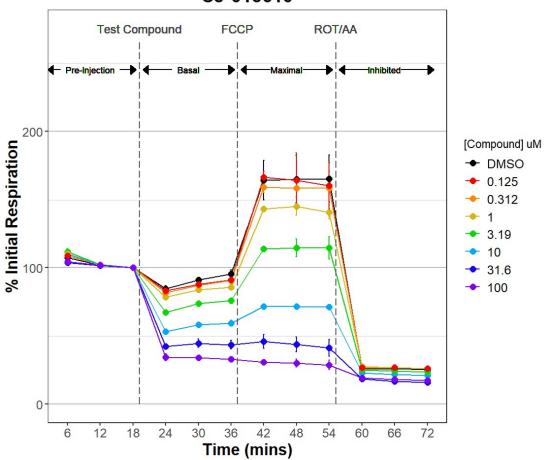




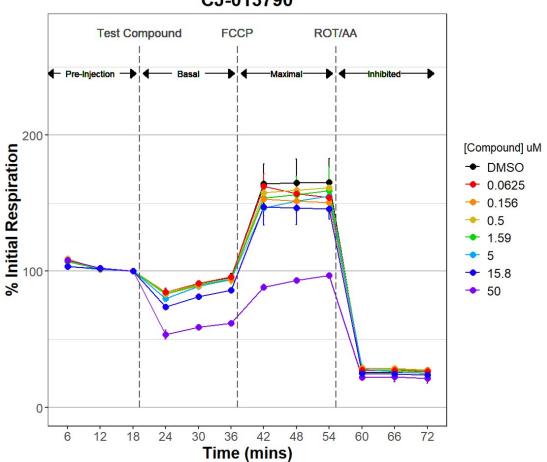


Time (mins)

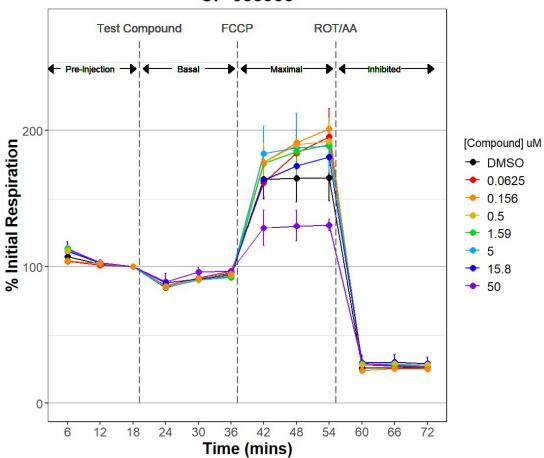
CJ-013610



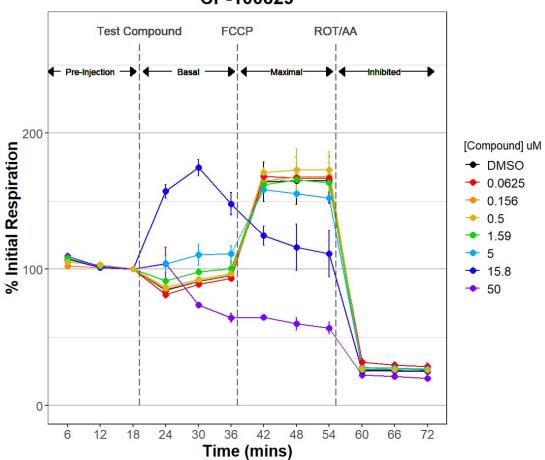




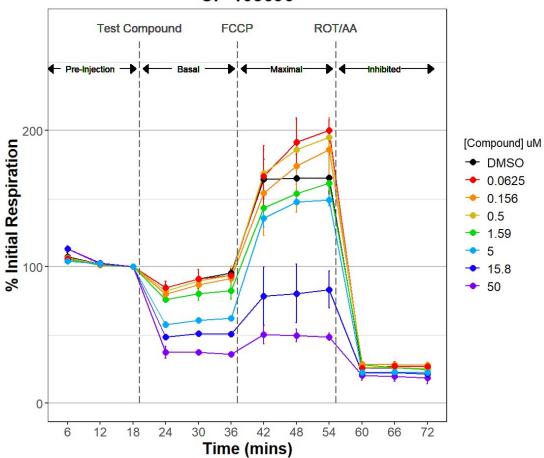
CP-085958



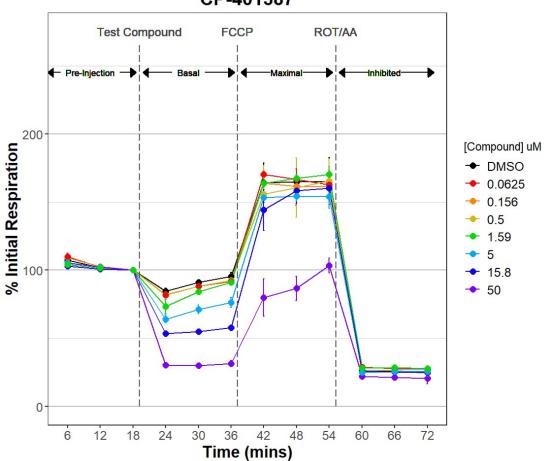




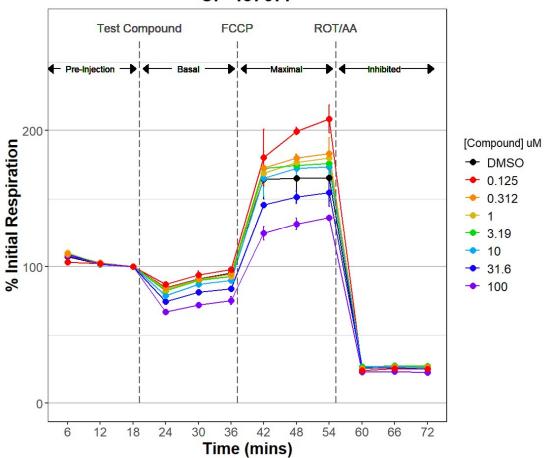
CP-105696



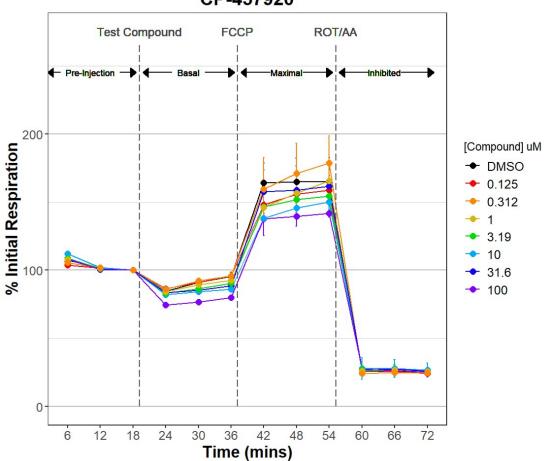




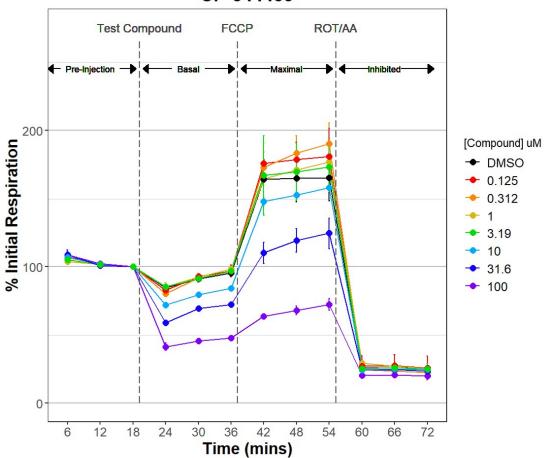
CP-457677



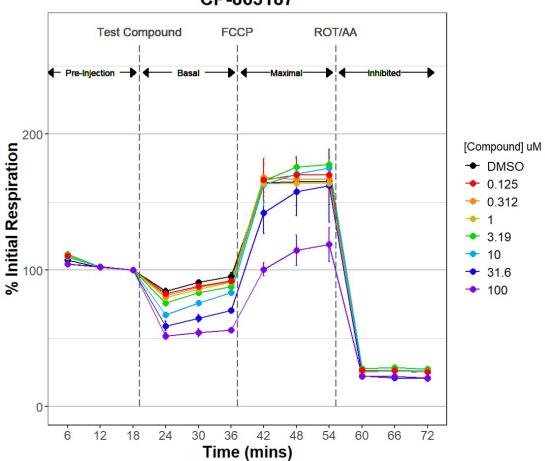


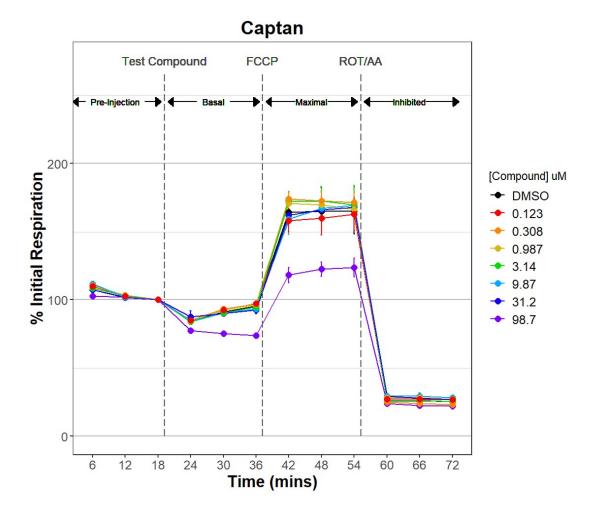


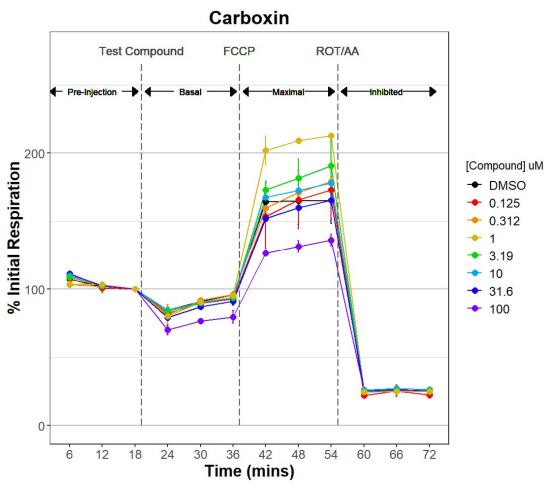
CP-544439



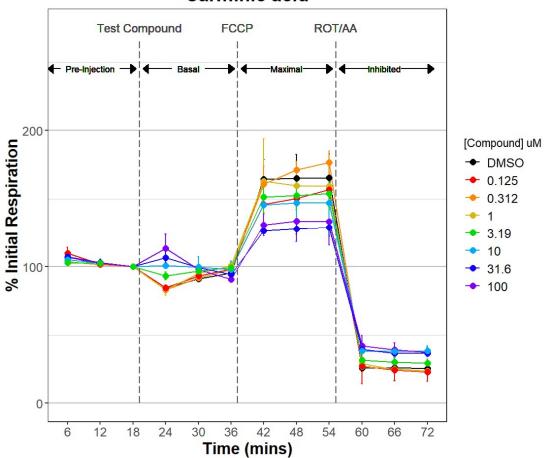




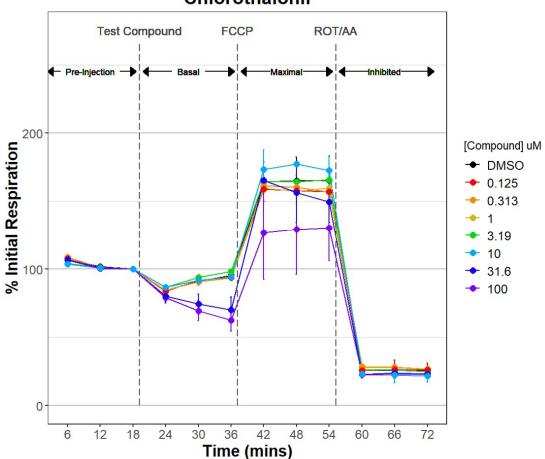




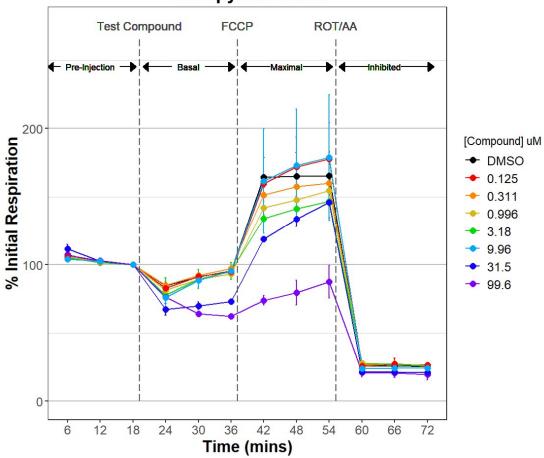
Carminic acid



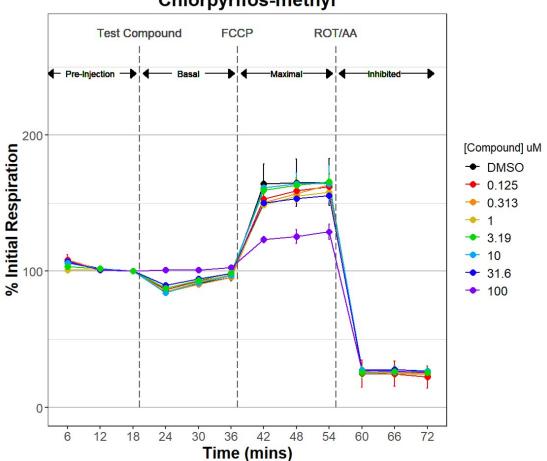




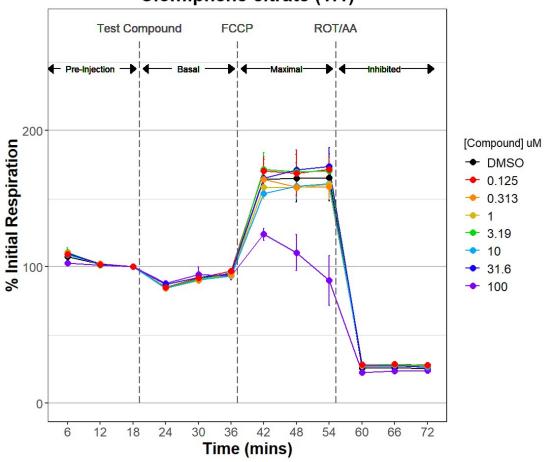
Chlorpyrifos oxon



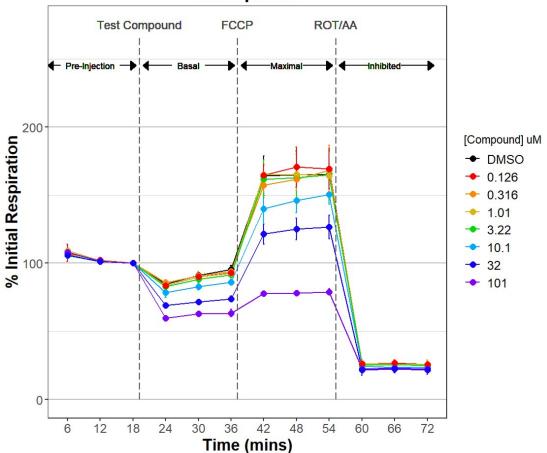
Chlorpyrifos-methyl



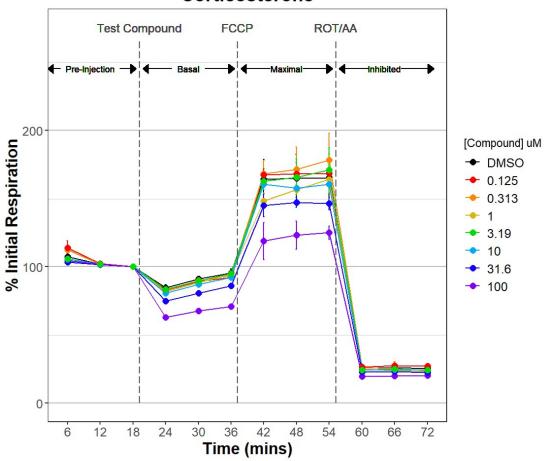
Clomiphene citrate (1:1)



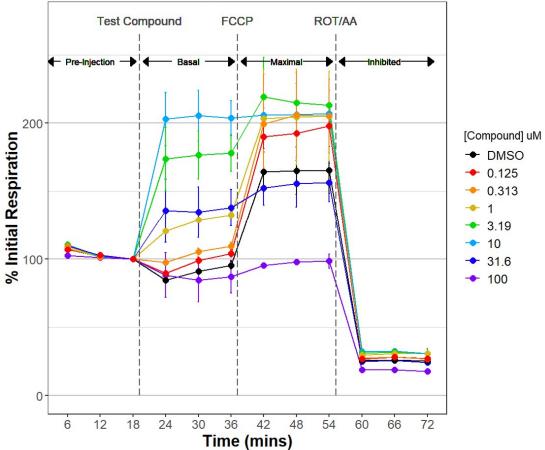


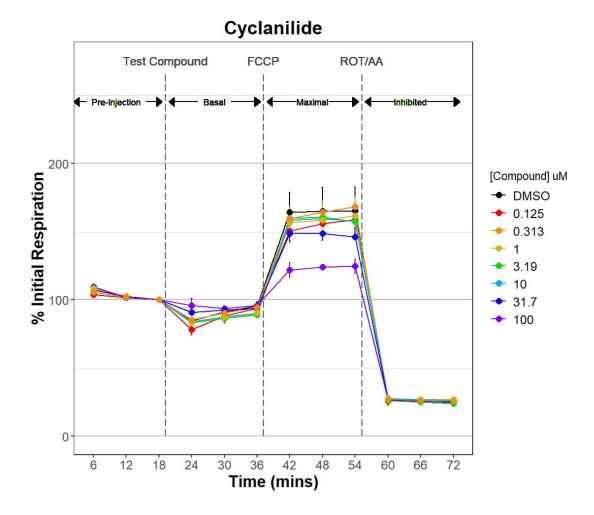


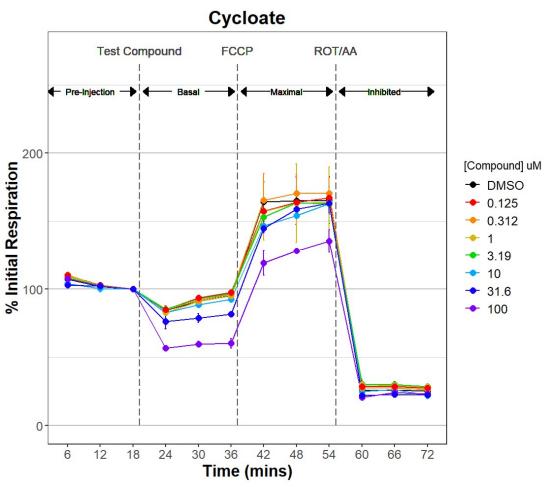
Corticosterone

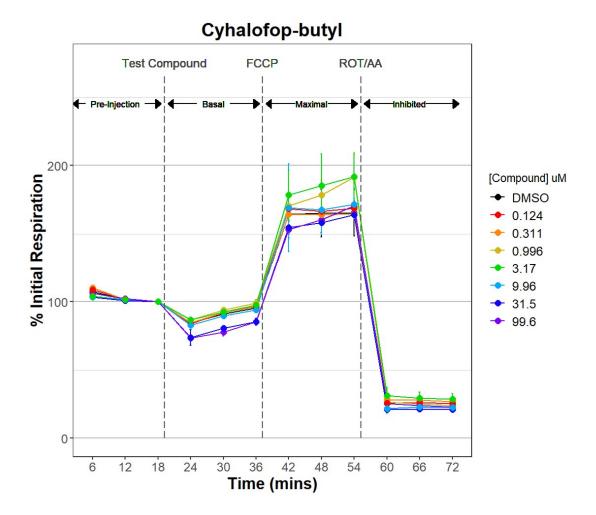


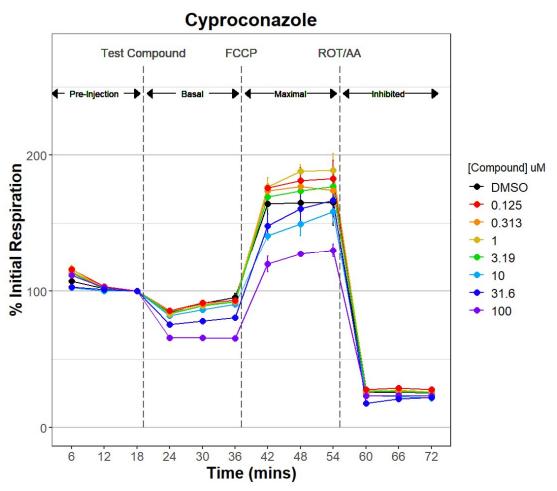




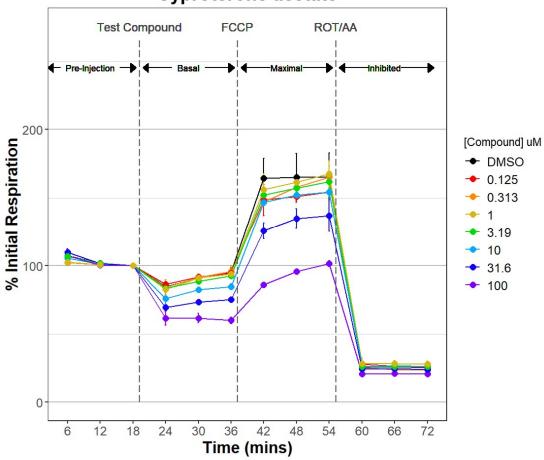




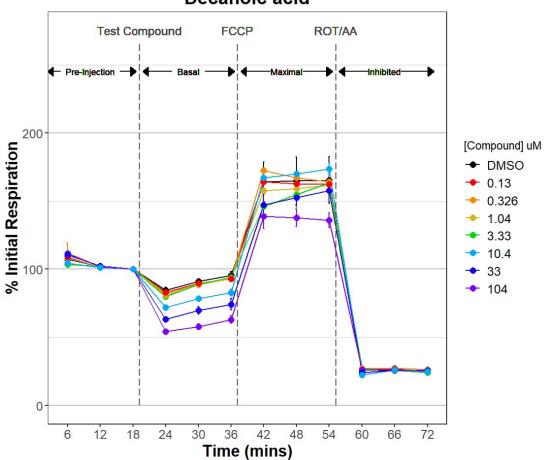


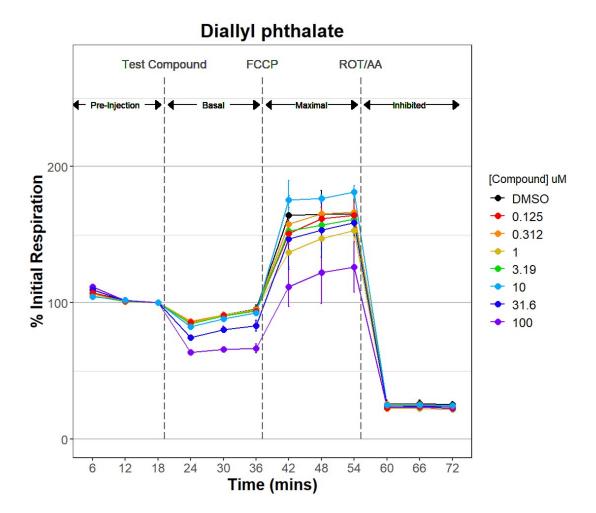


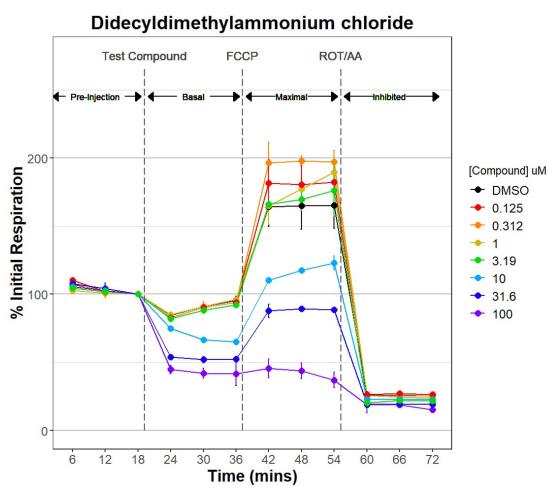
Cyproterone acetate



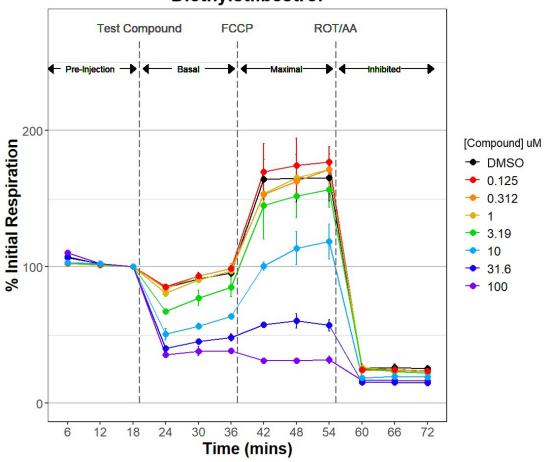
Decanoic acid



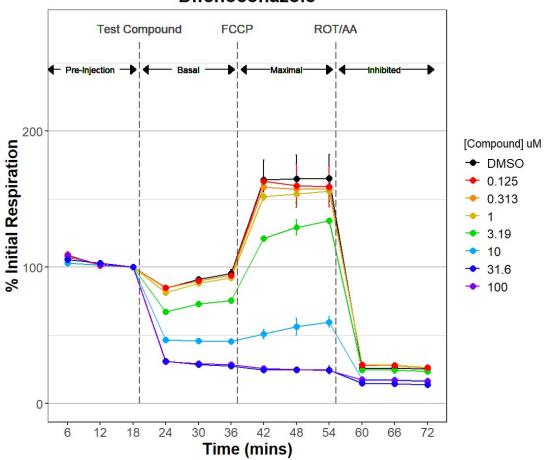




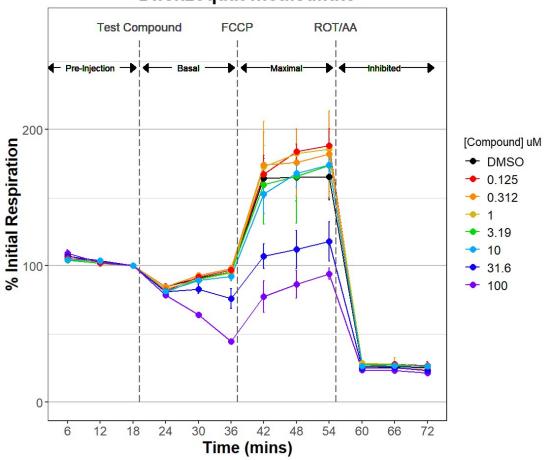
Diethylstilbestrol



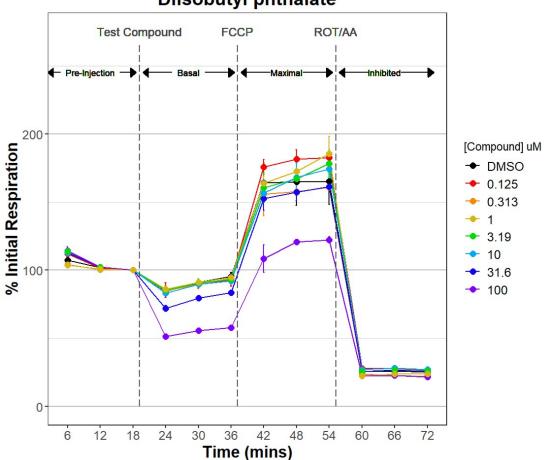
Difenoconazole



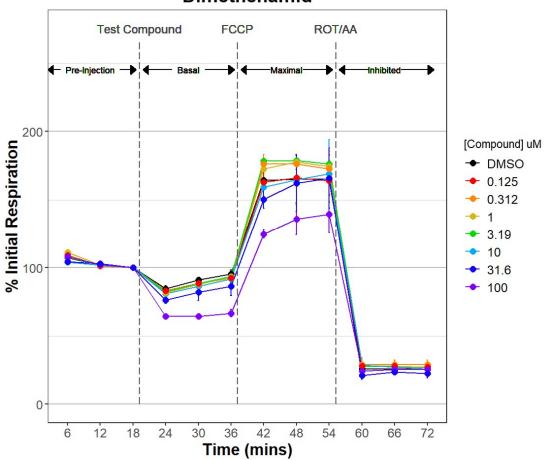
Difenzoquat metilsulfate



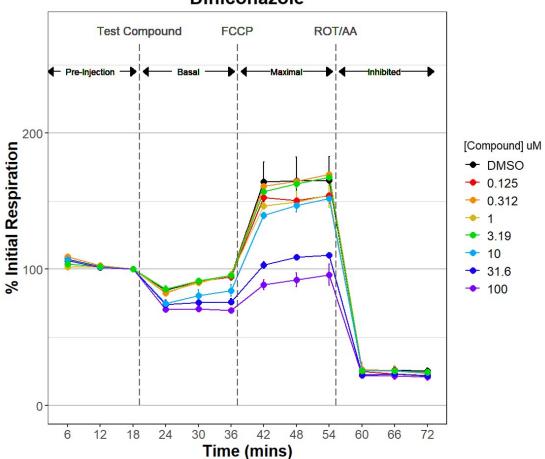
Diisobutyl phthalate

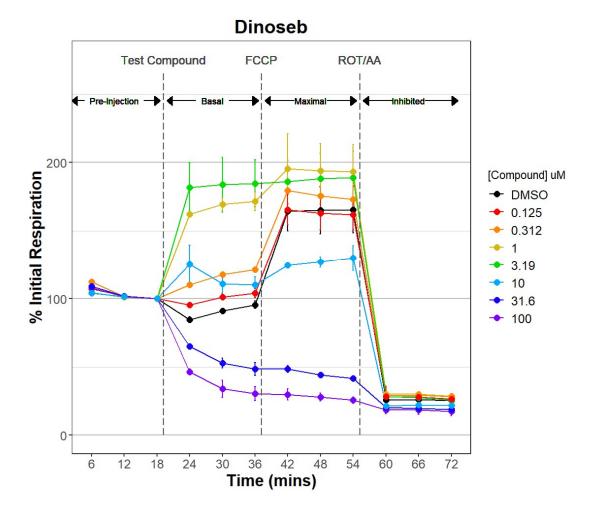


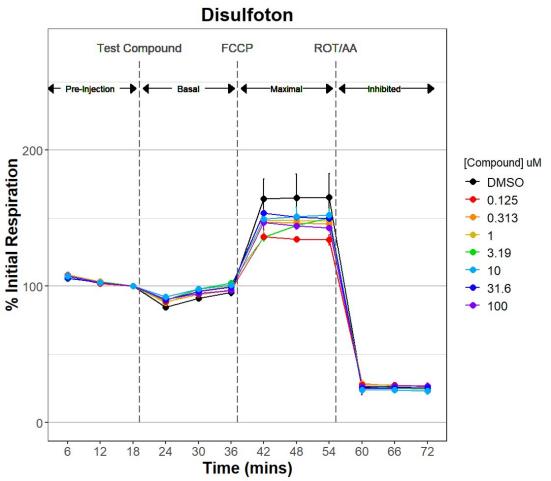
Dimethenamid



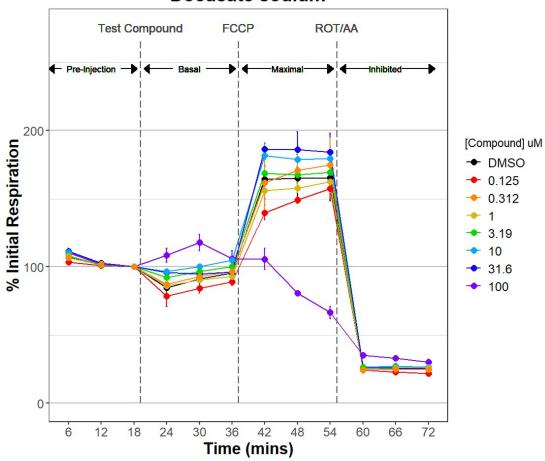
Diniconazole



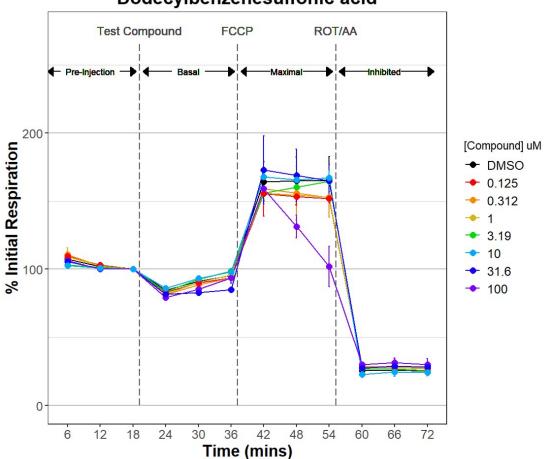




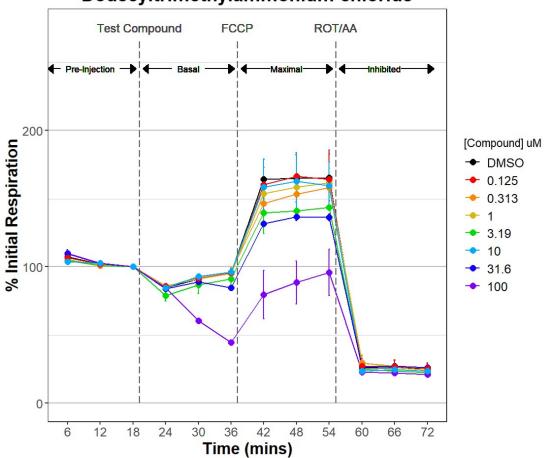
Docusate sodium



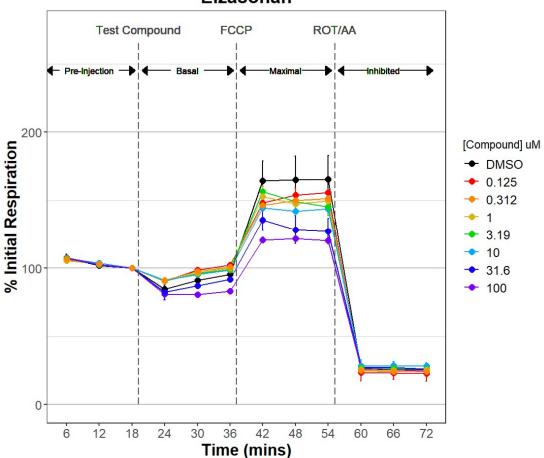
Dodecylbenzenesulfonic acid



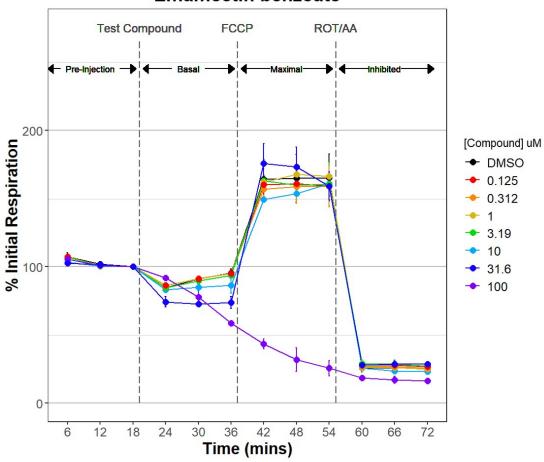
Dodecyltrimethylammonium chloride



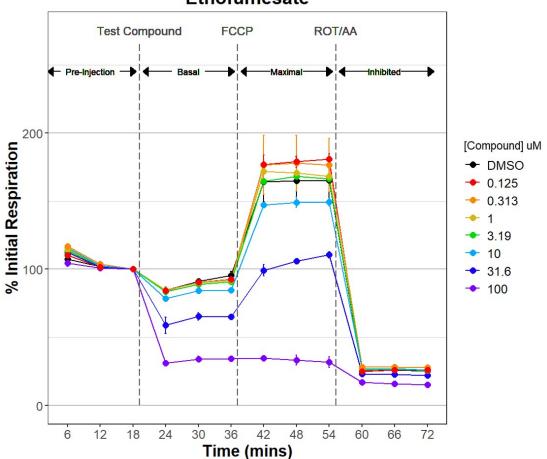


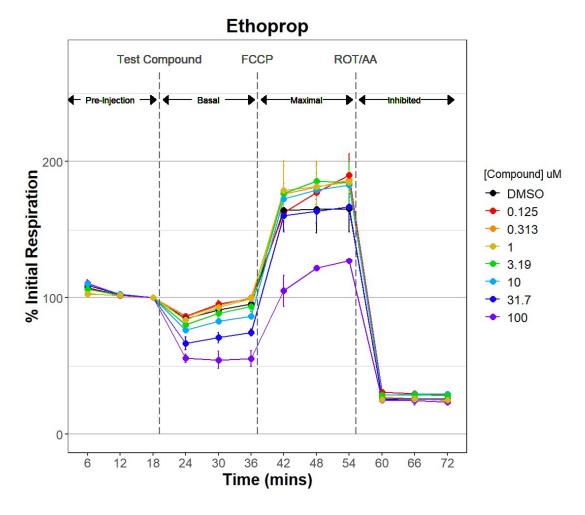


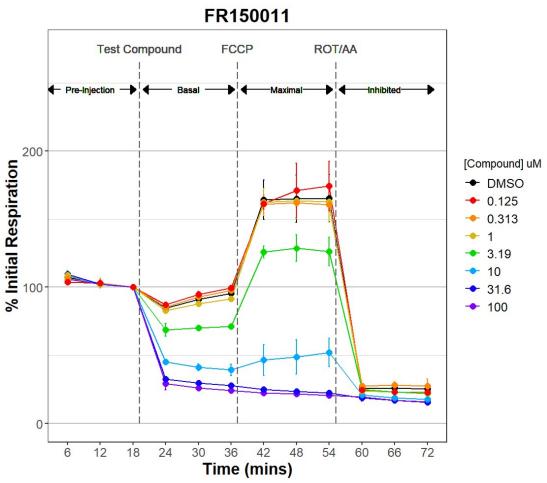
Emamectin benzoate



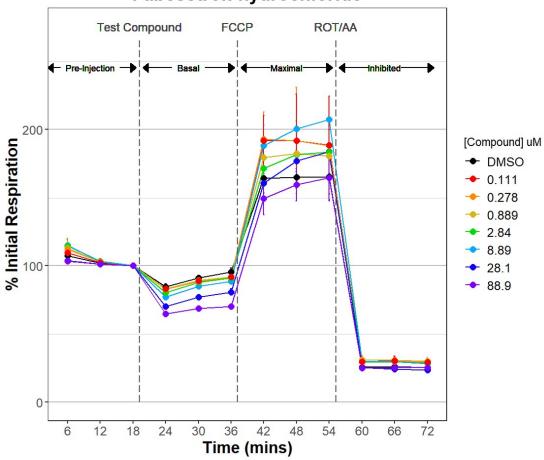




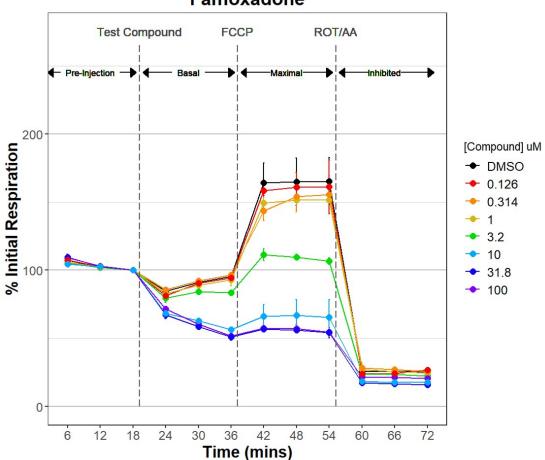




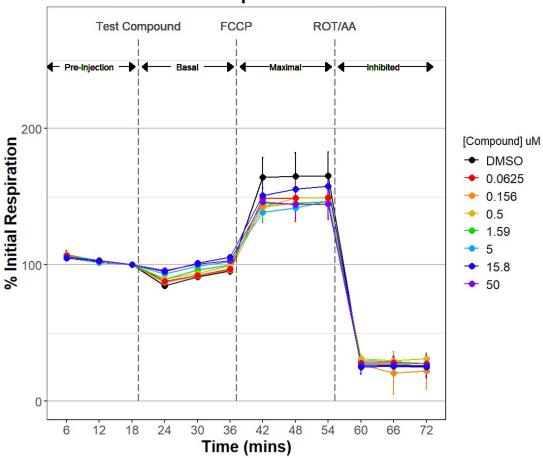
Fabesetron hydrochloride



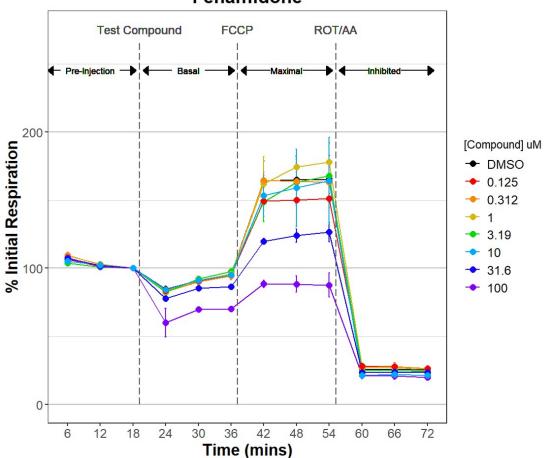
Famoxadone

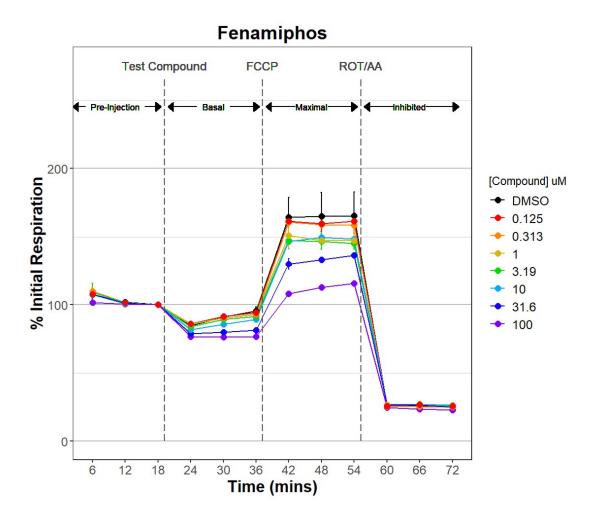


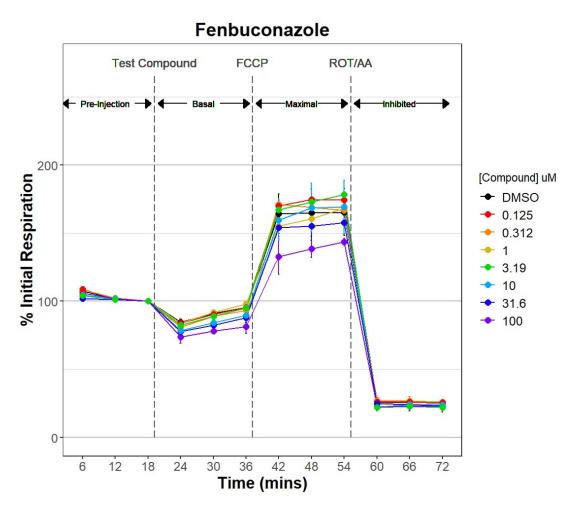
Fandosentan potassium salt

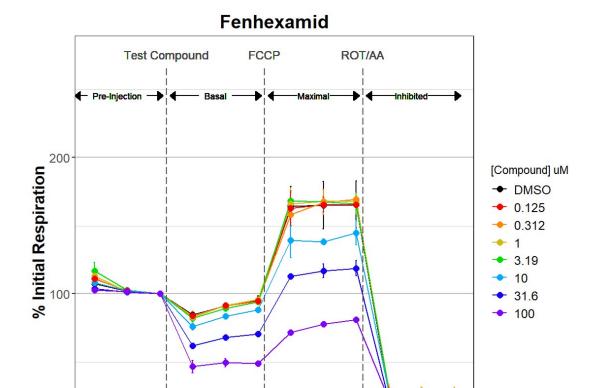




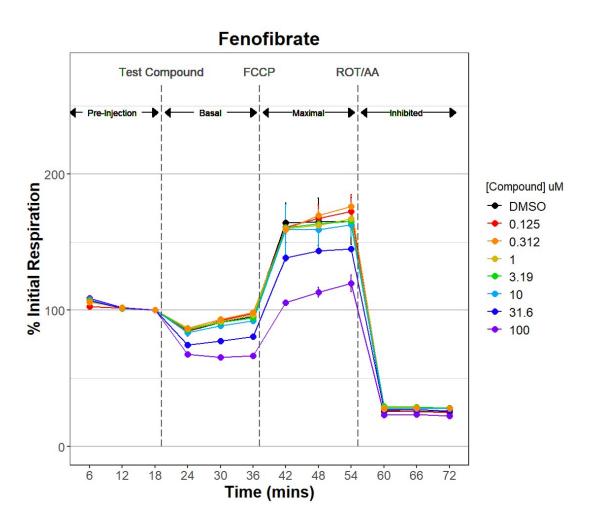


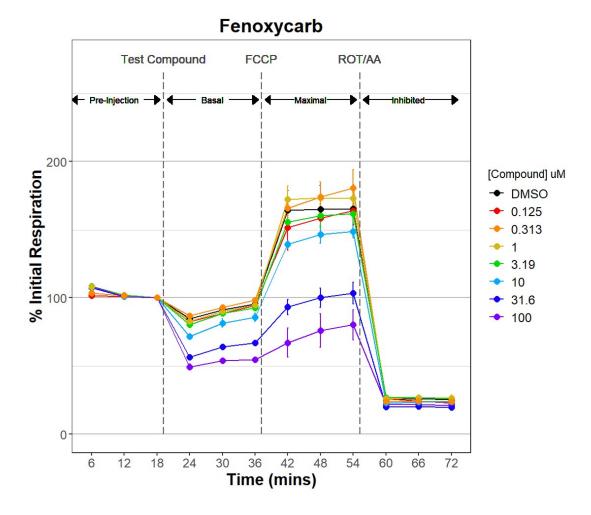


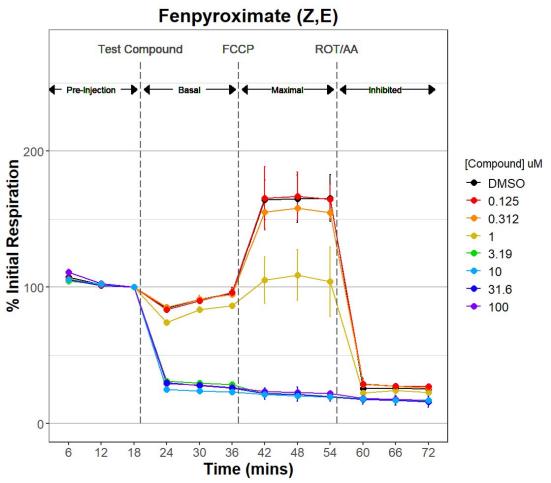


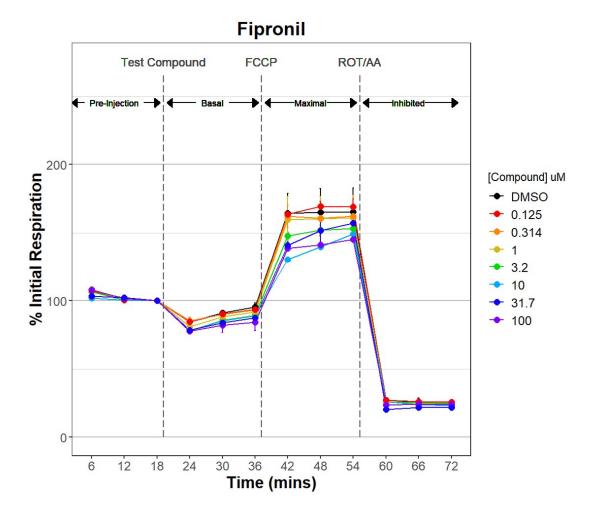


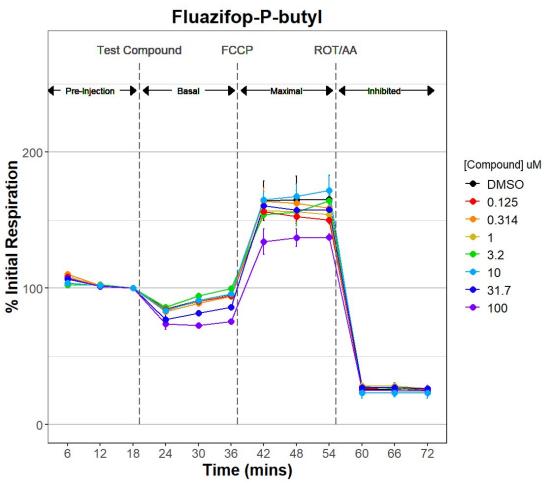
Time (mins)



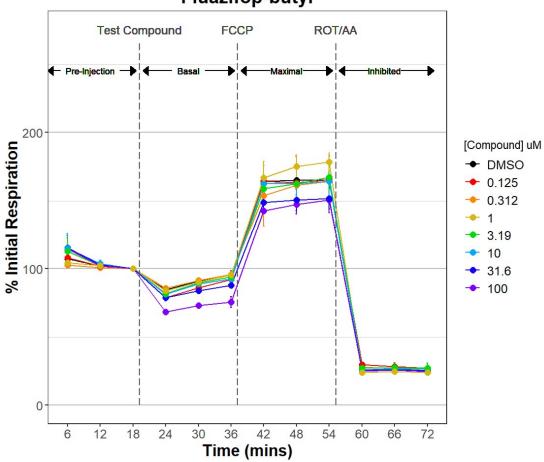




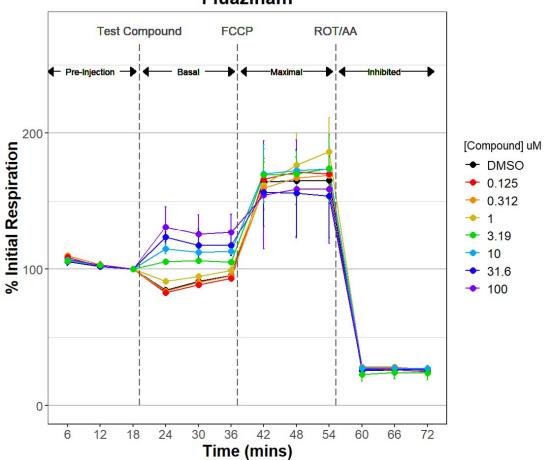




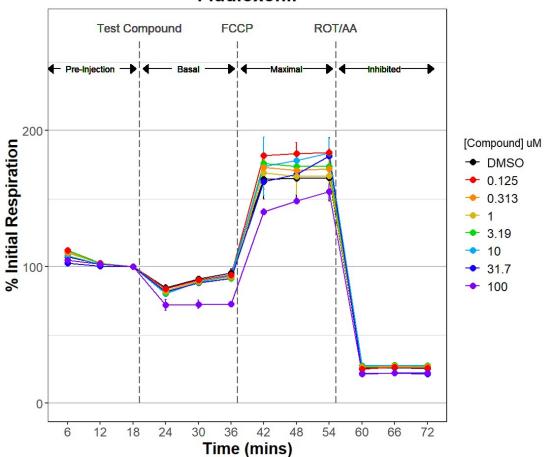
Fluazifop-butyl



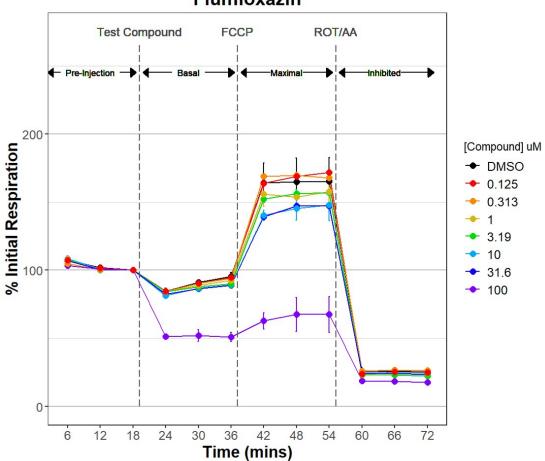




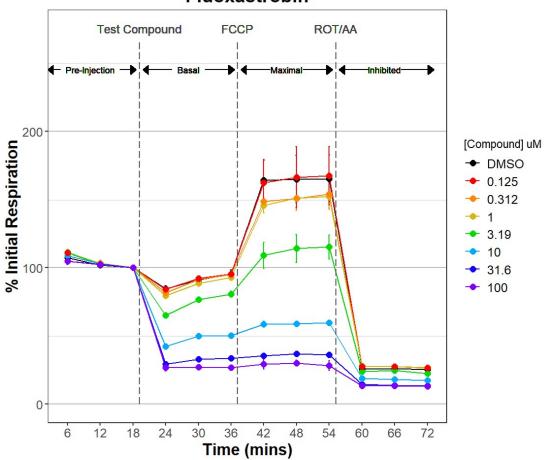
Fludioxonil



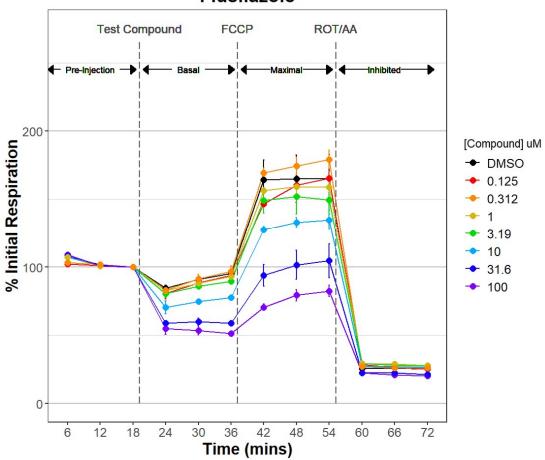




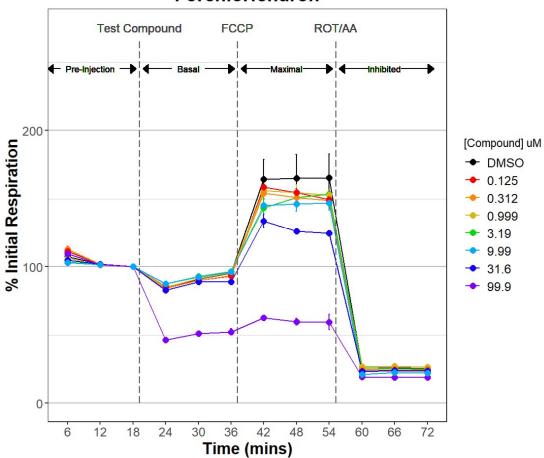
Fluoxastrobin



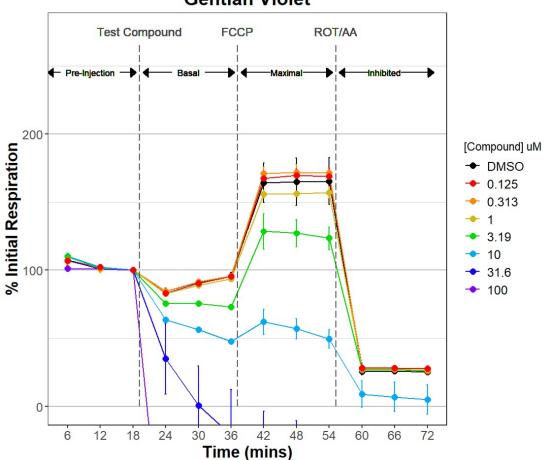


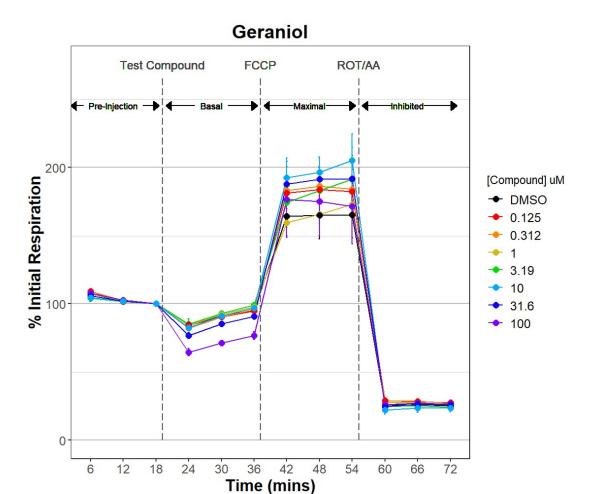


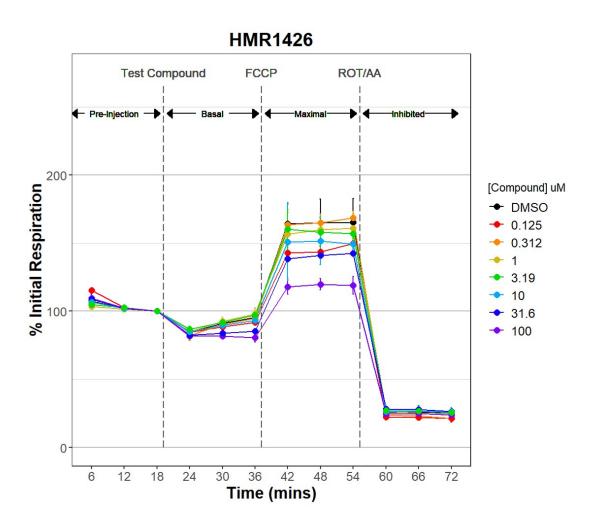
Forchlorfenuron



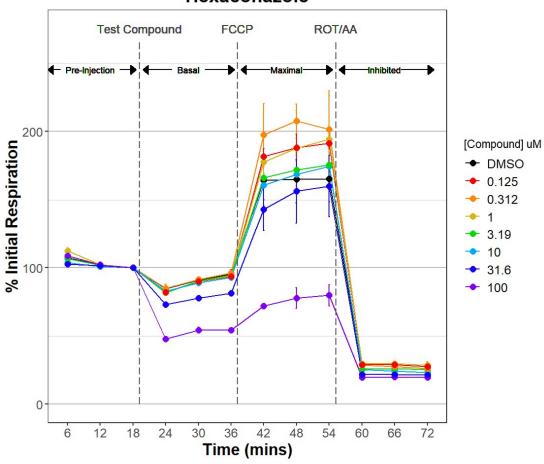
Gentian Violet



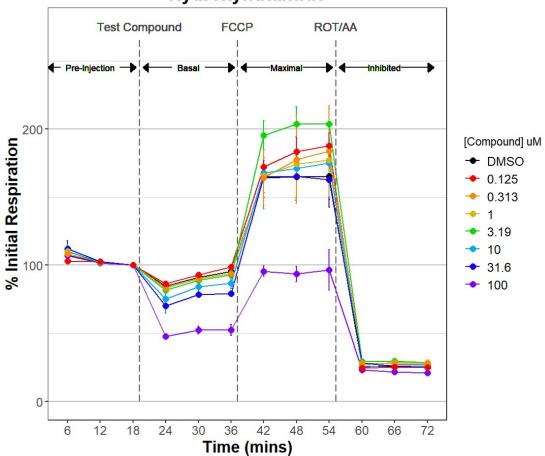


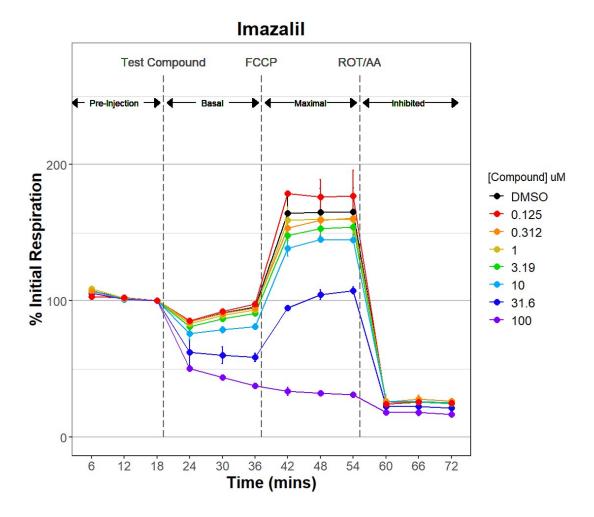


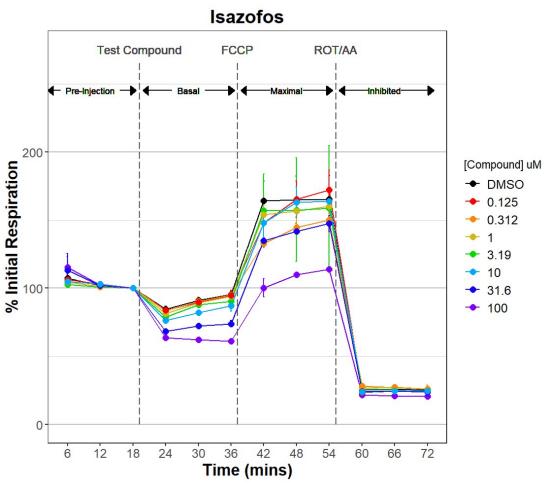
Hexaconazole

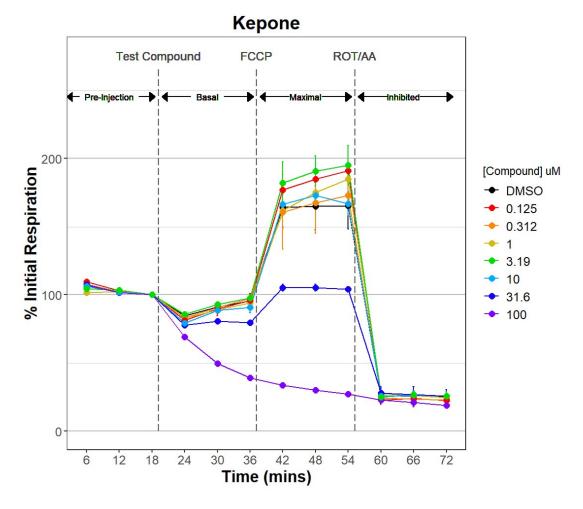


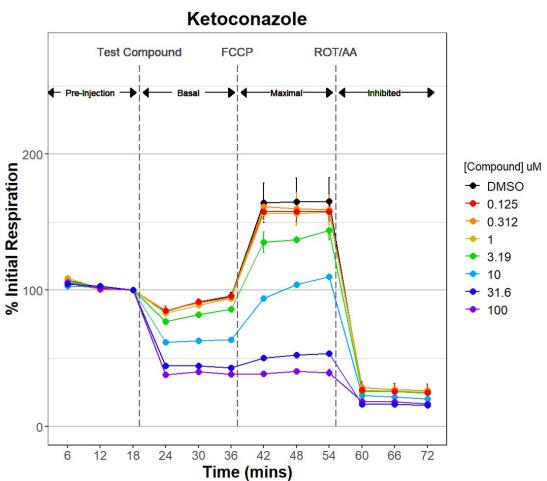


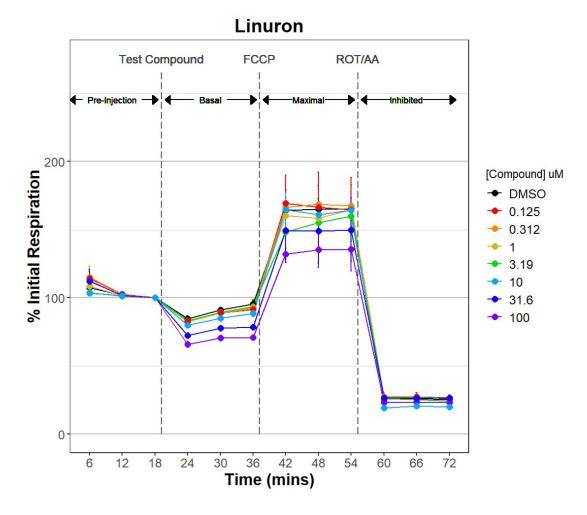


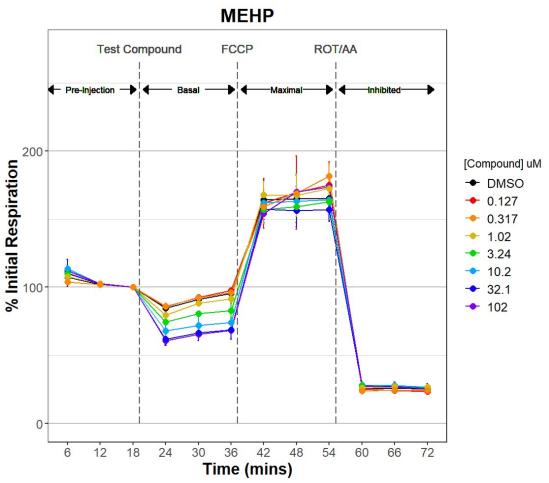




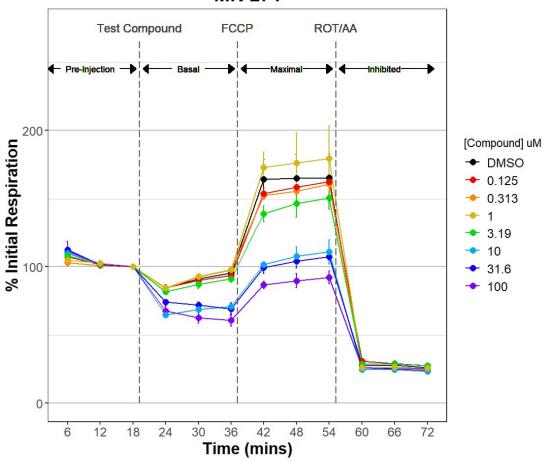




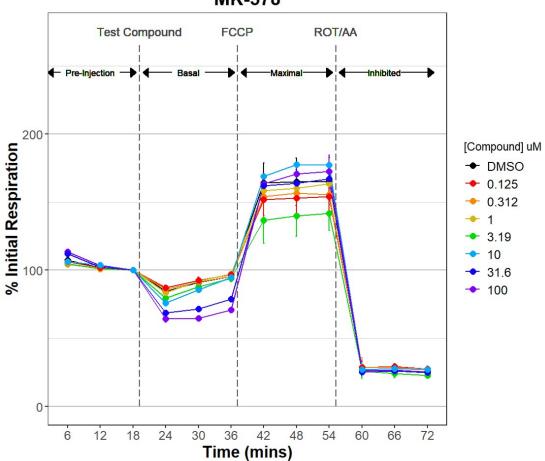




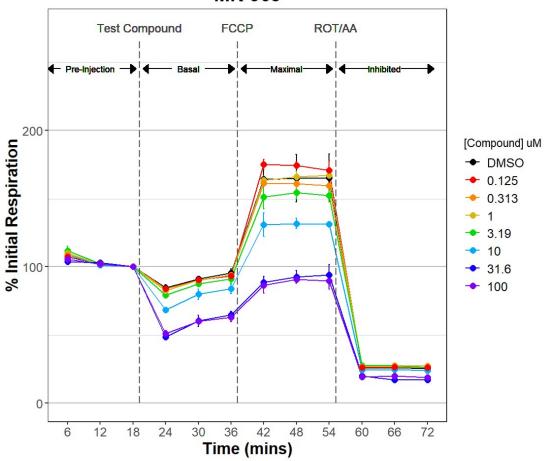




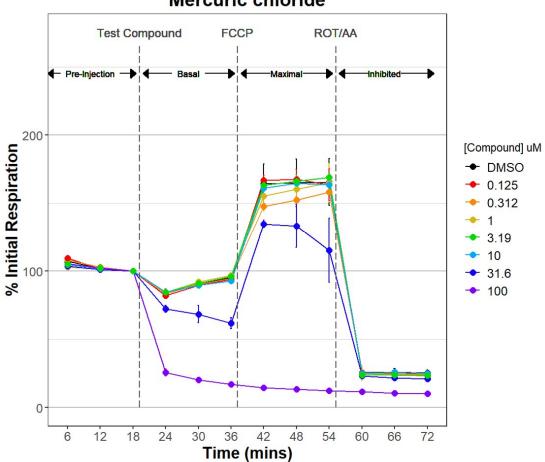


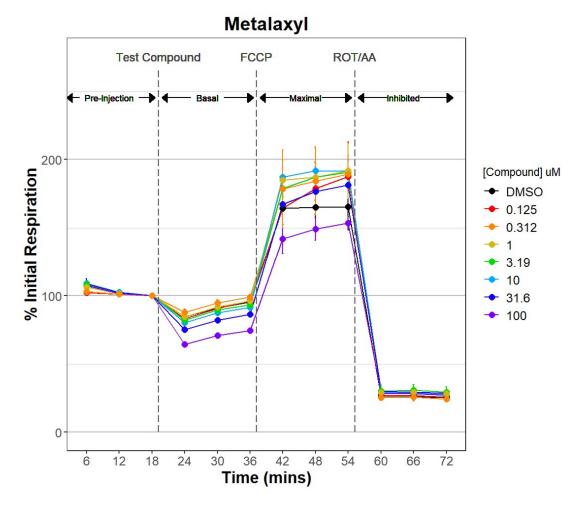


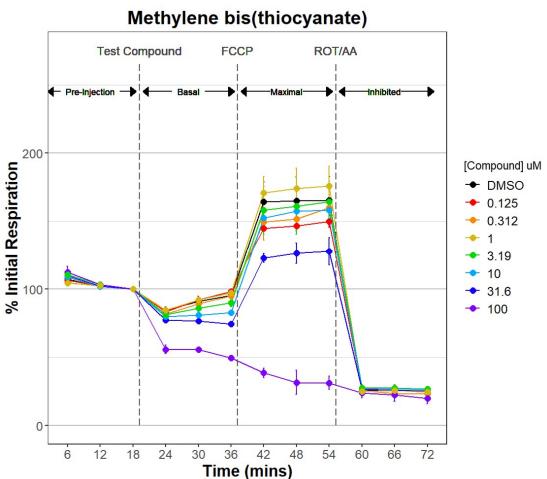
MK-968



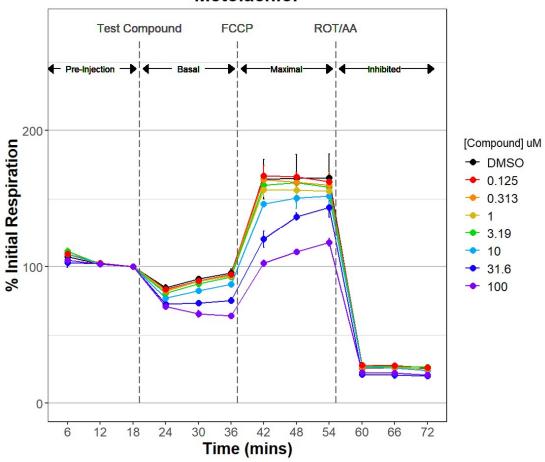
Mercuric chloride



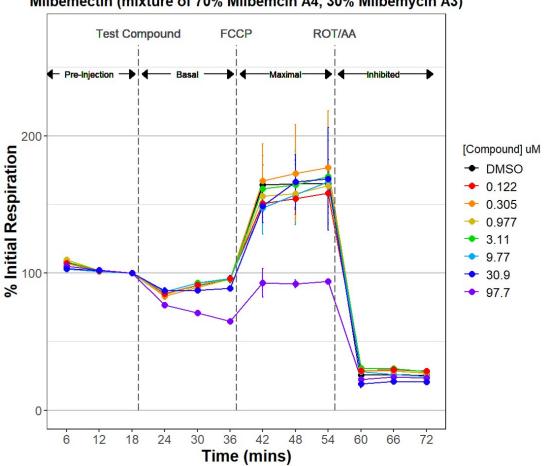


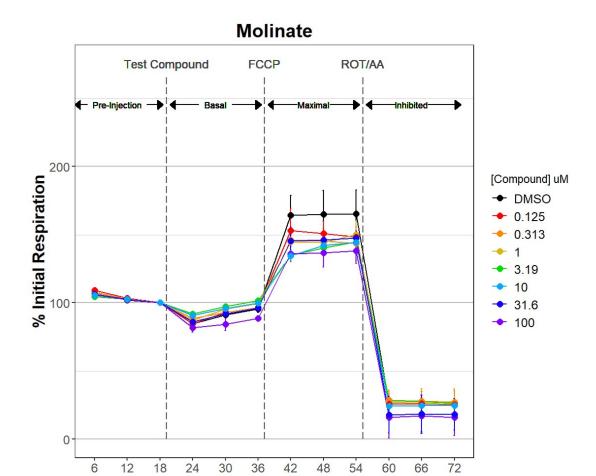


Metolachlor

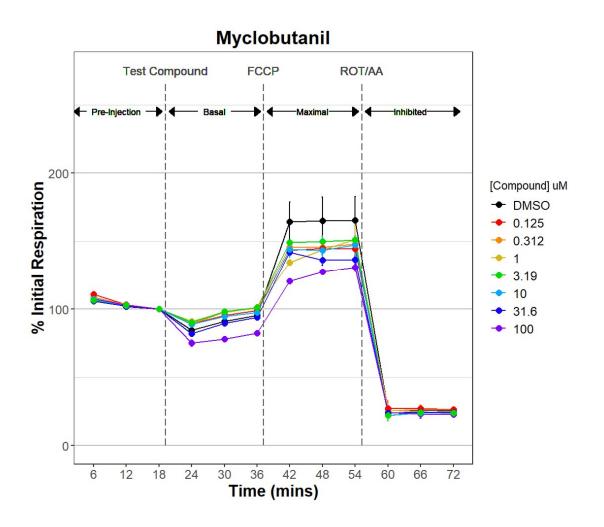


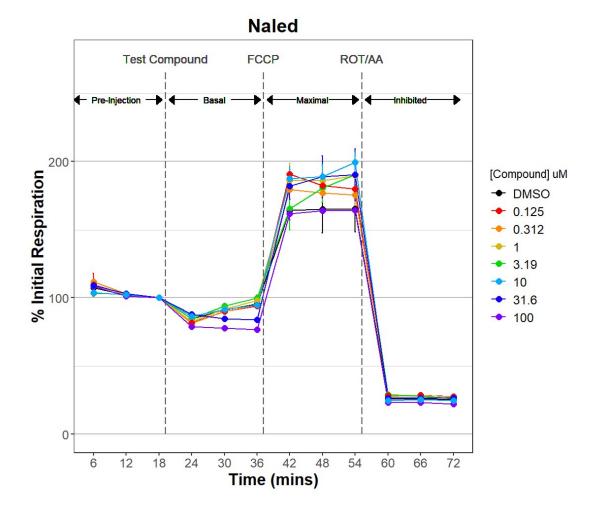
Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3)

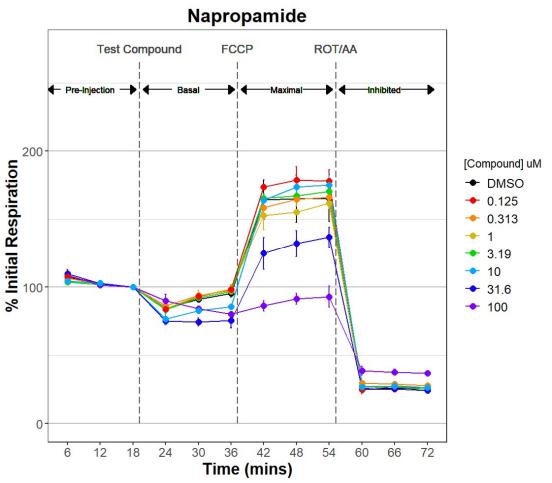


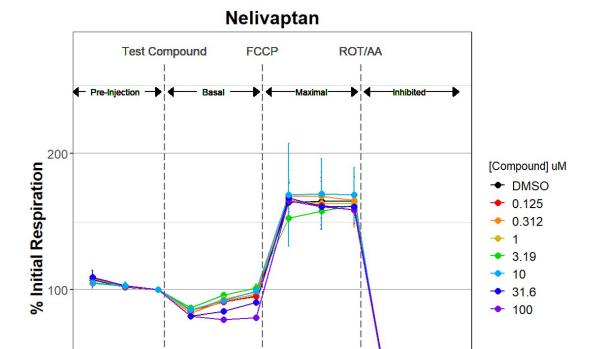


Time (mins)



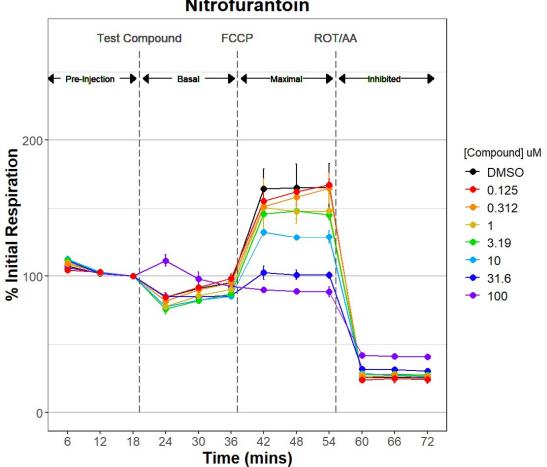




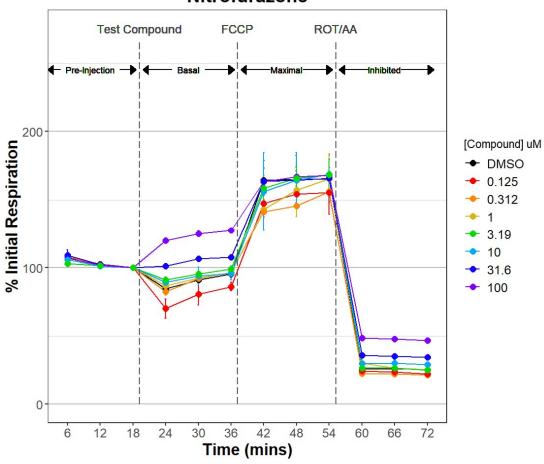




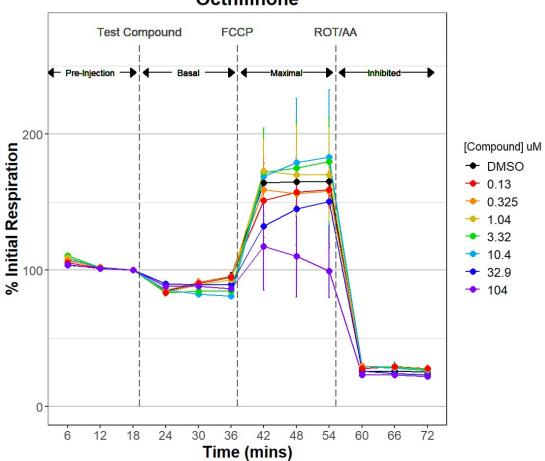
Time (mins)

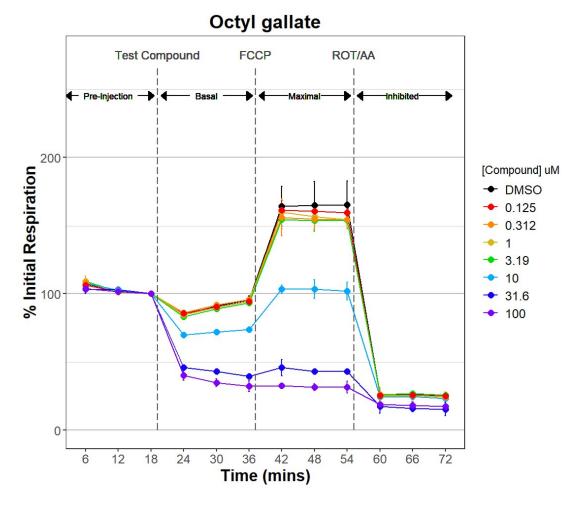


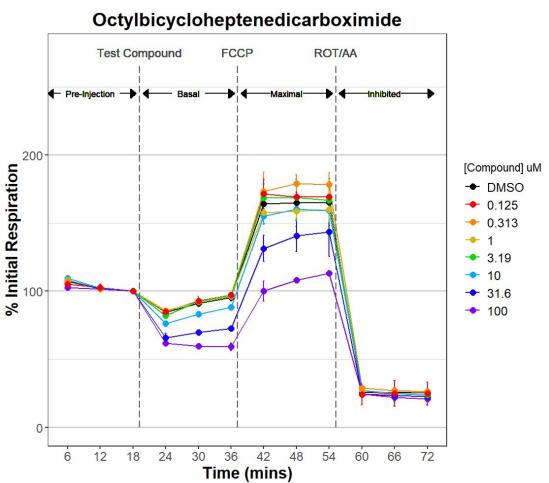
Nitrofurazone

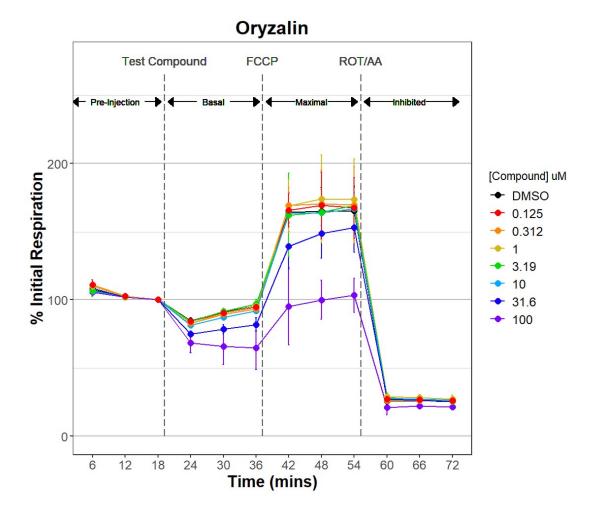


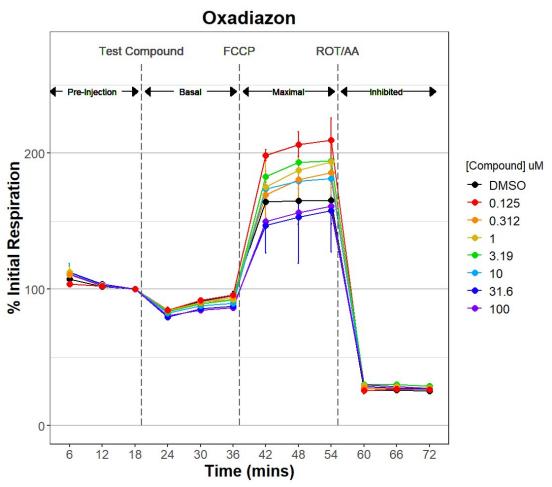
Octhilinone



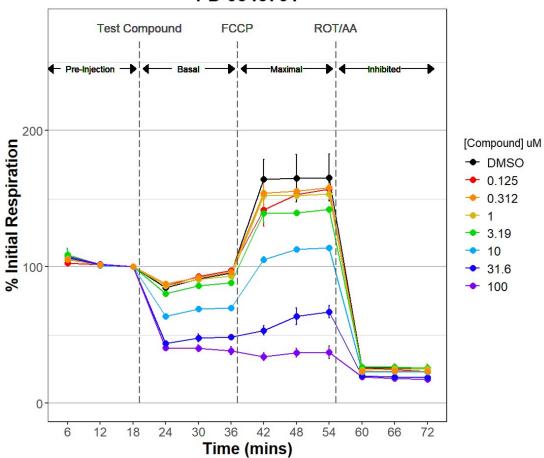




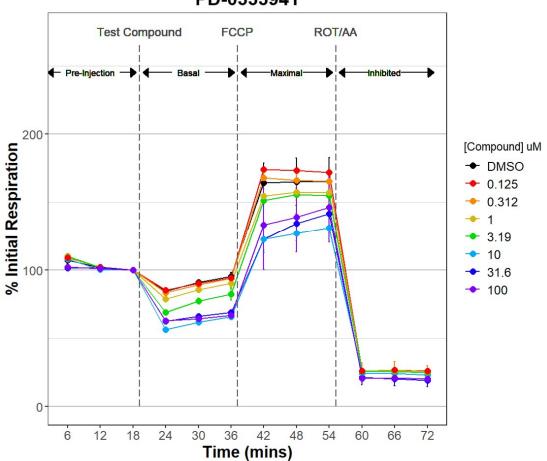




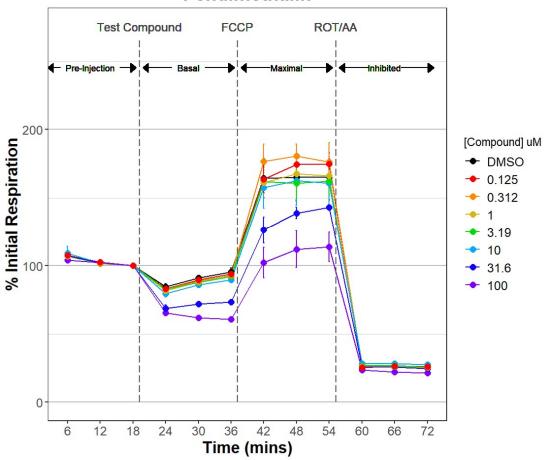
PD 0343701



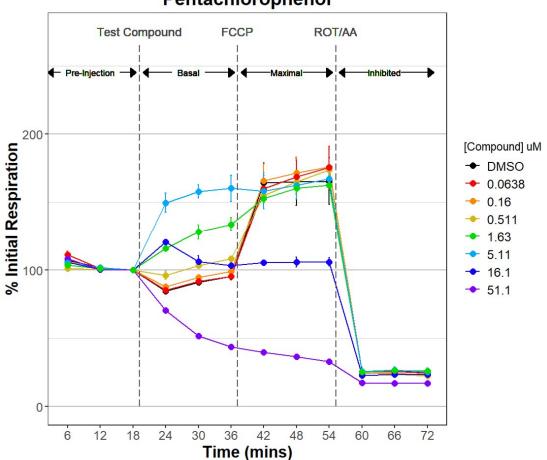




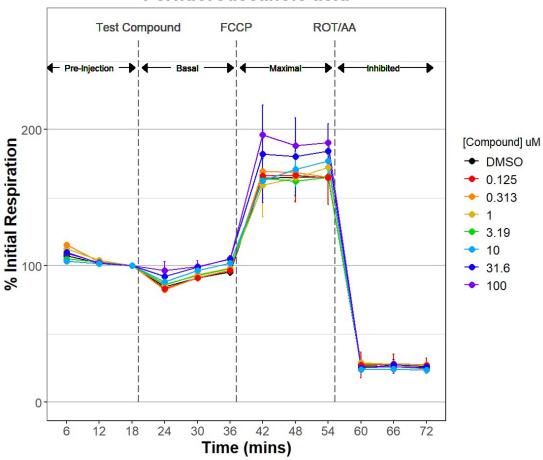
Pendimethalin



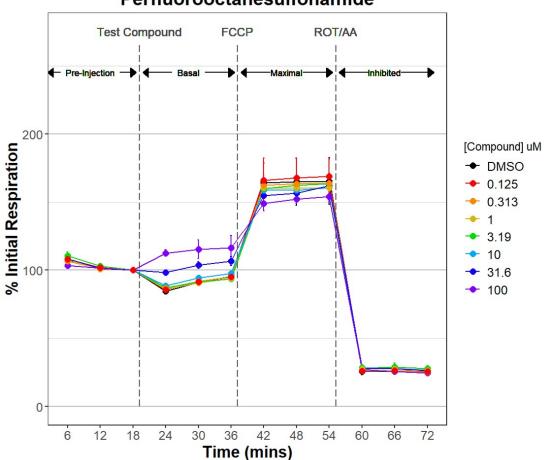
Pentachlorophenol



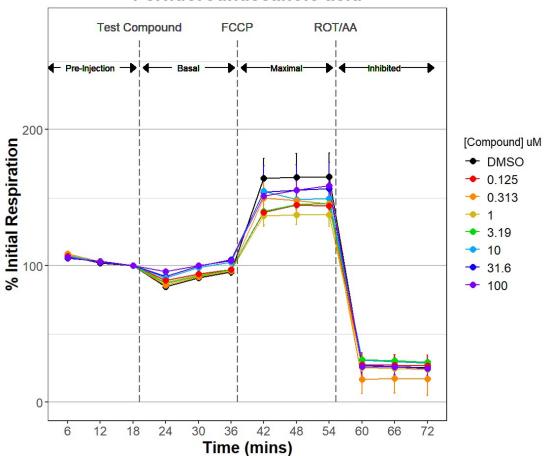
Perfluorodecanoic acid



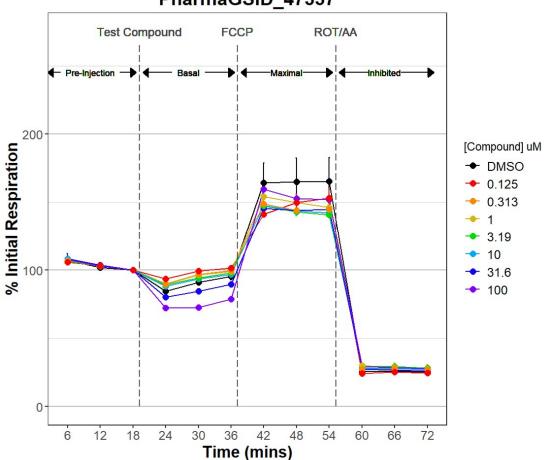
Perfluorooctanesulfonamide



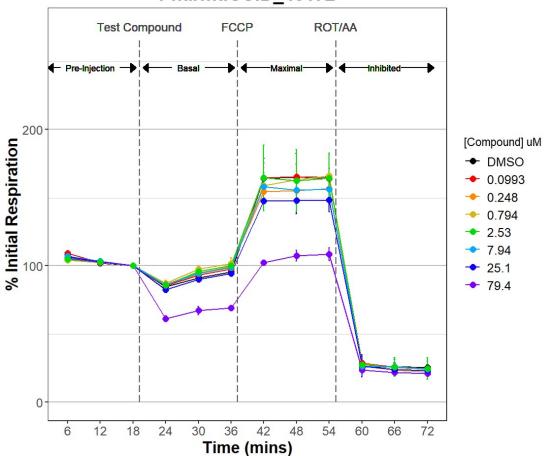
Perfluoroundecanoic acid



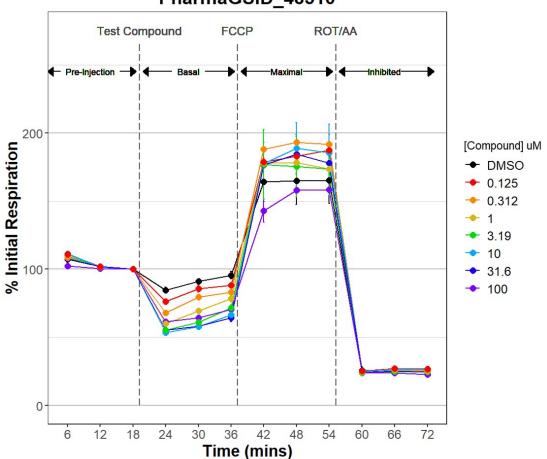




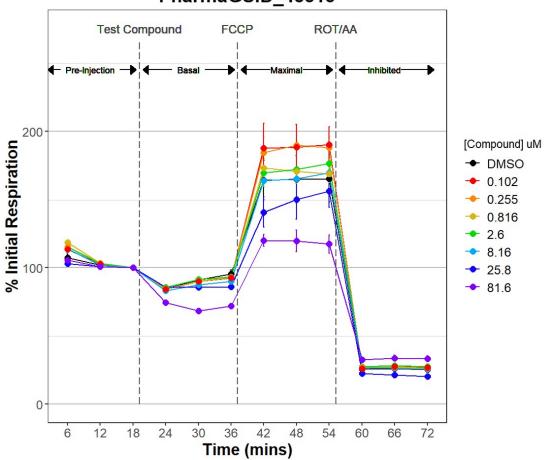
PharmaGSID_48172



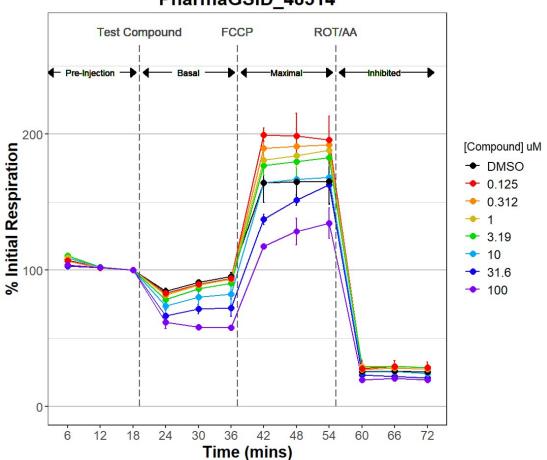




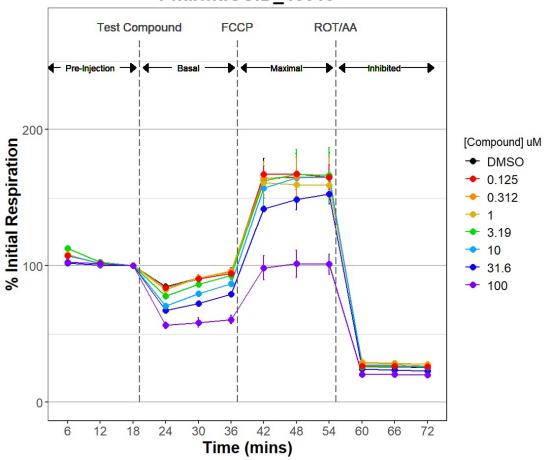
PharmaGSID_48513



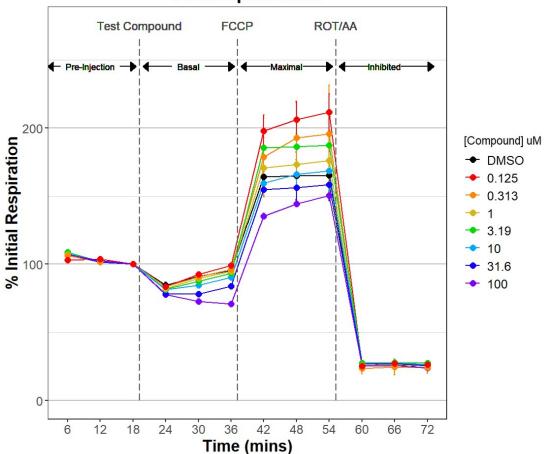
PharmaGSID_48514



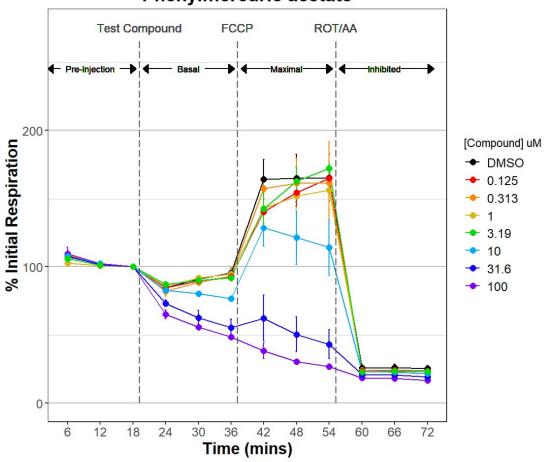
PharmaGSID_48519



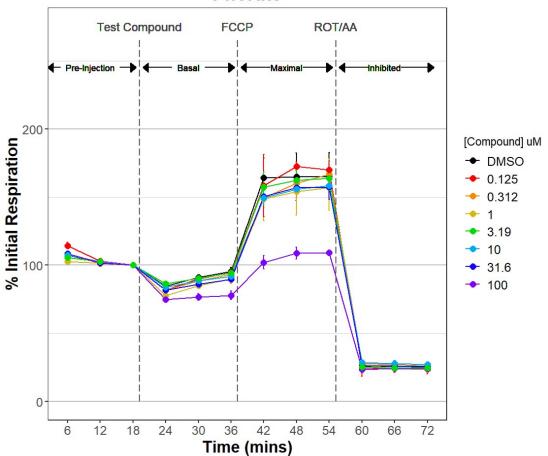
Phenolphthalein



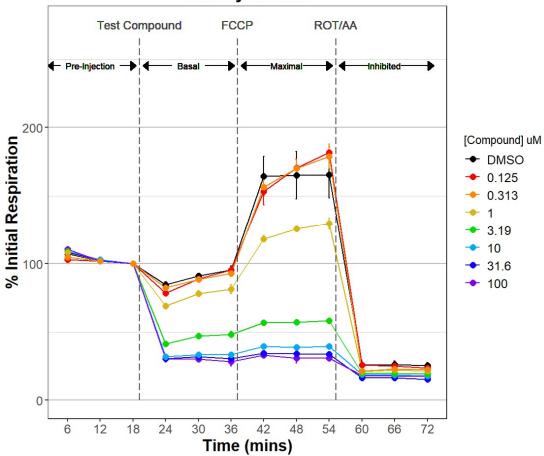
Phenylmercuric acetate



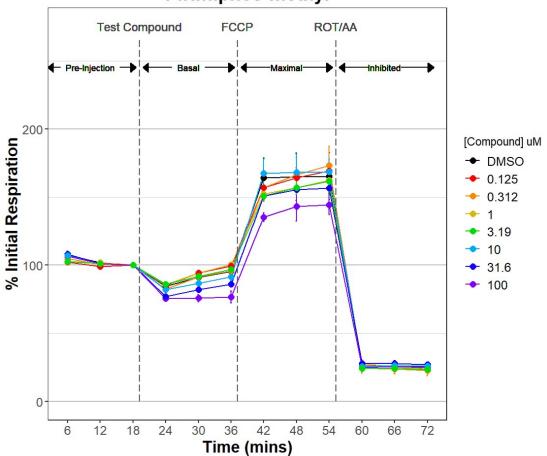




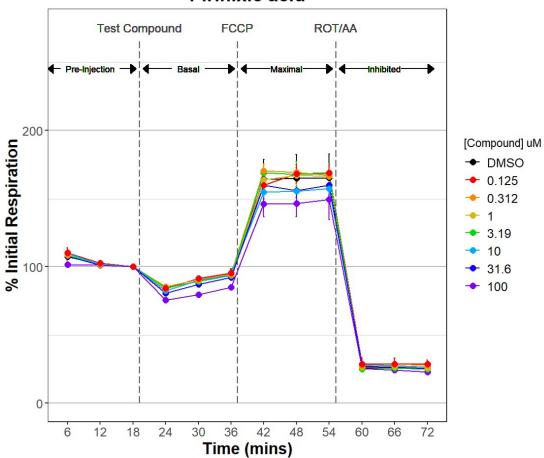
Picoxystrobin



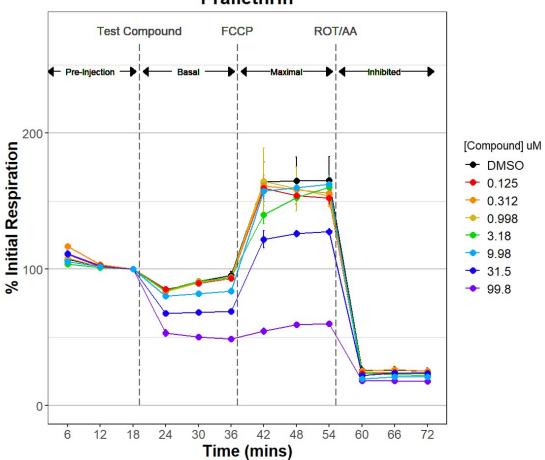
Pirimiphos-methyl



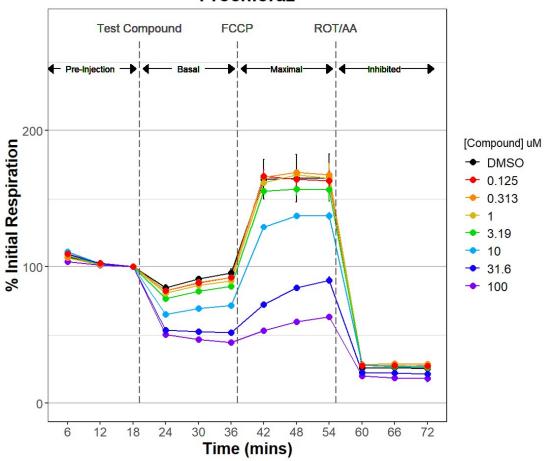
Pirinixic acid



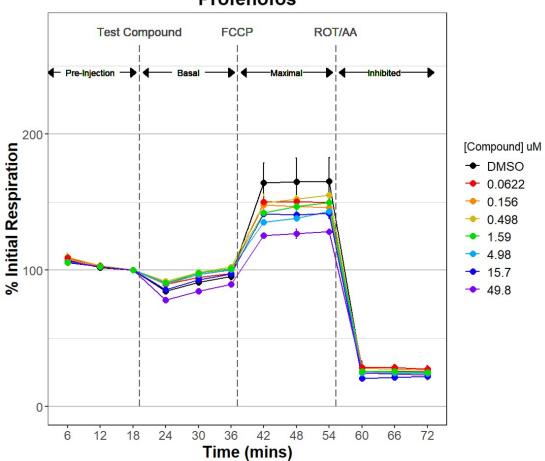




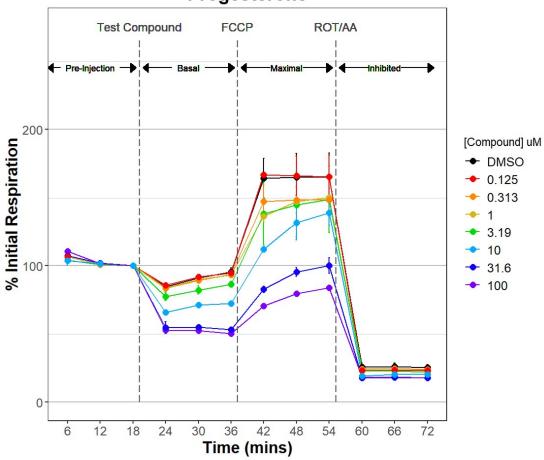
Prochloraz



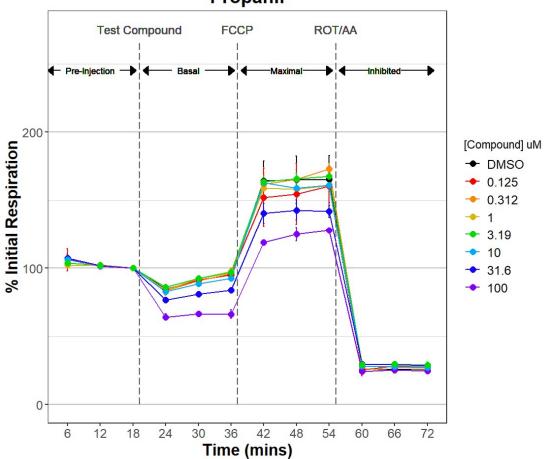
Profenofos

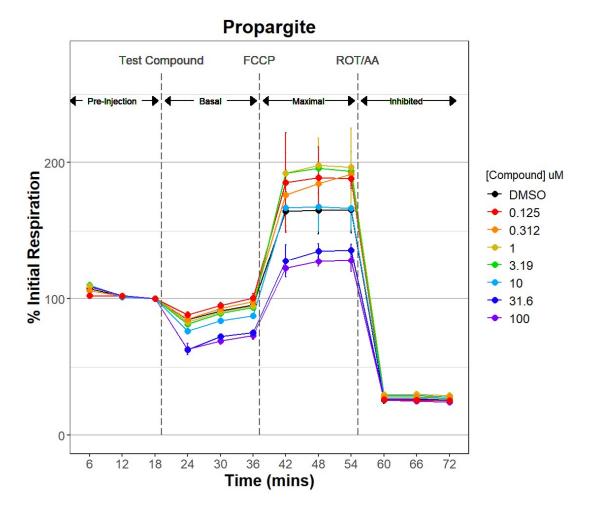


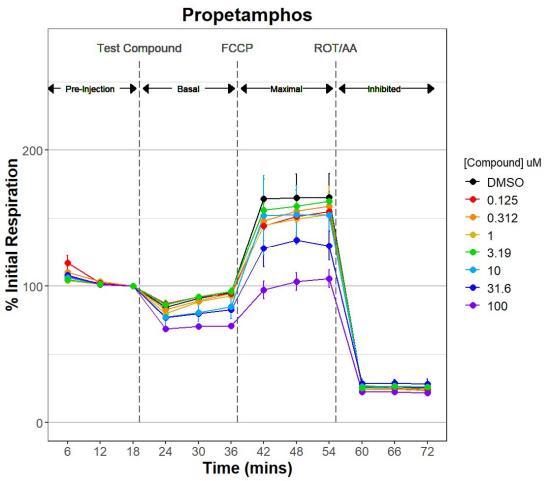
Progesterone



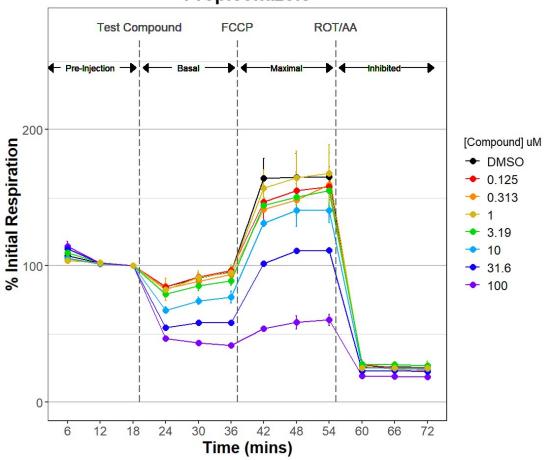




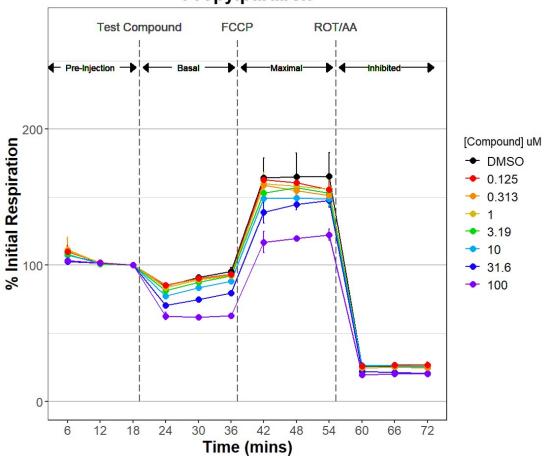




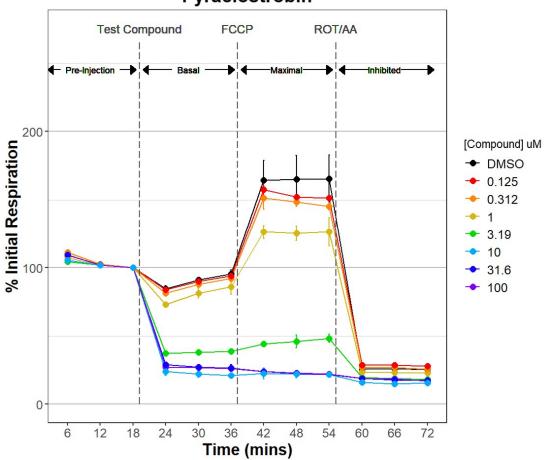
Propiconazole



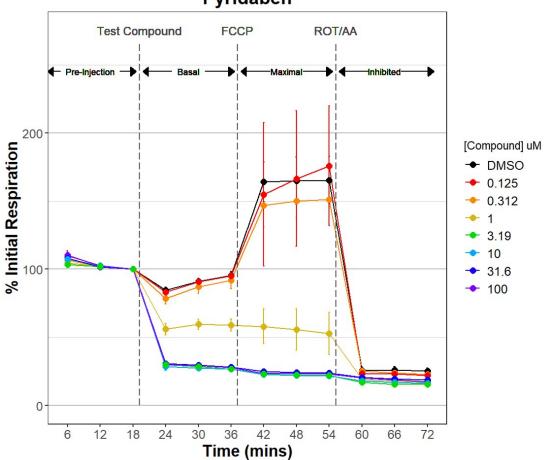
Propylparaben

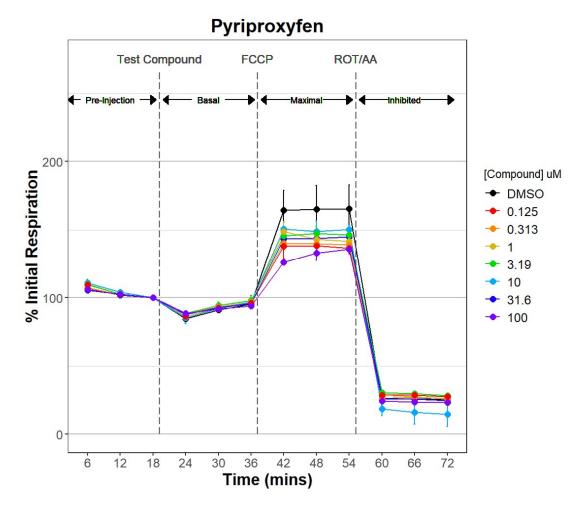


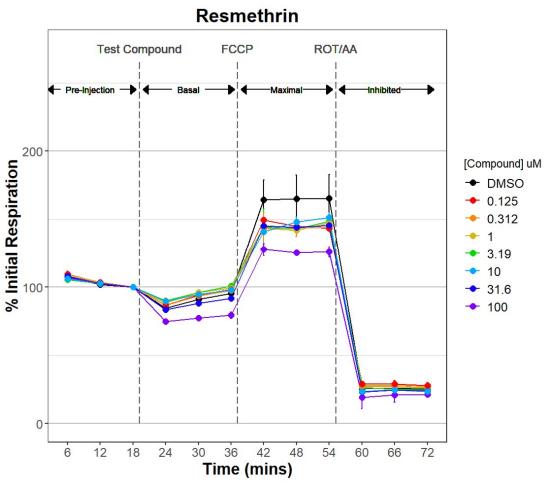
Pyraclostrobin



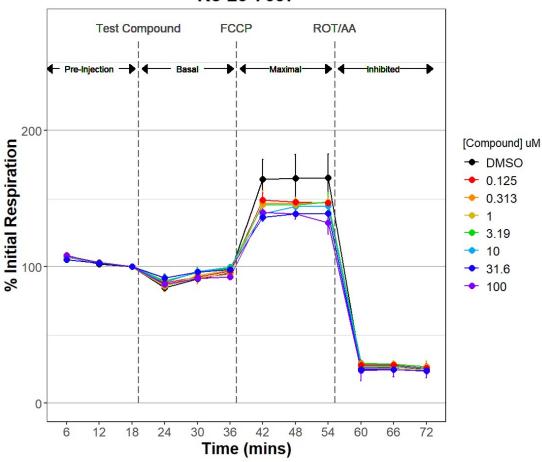
Pyridaben



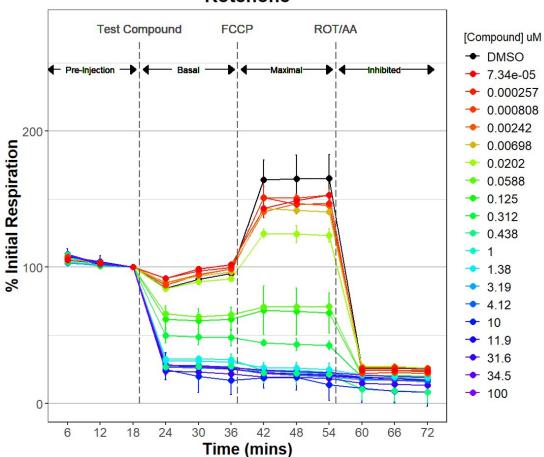




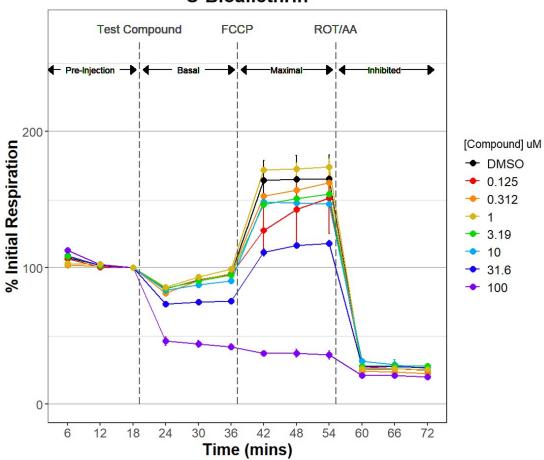
Ro 23-7637



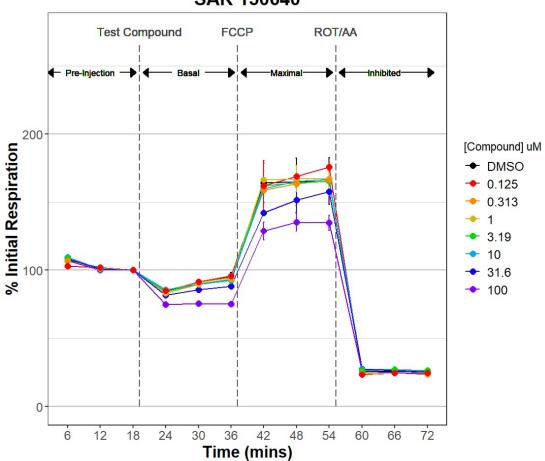




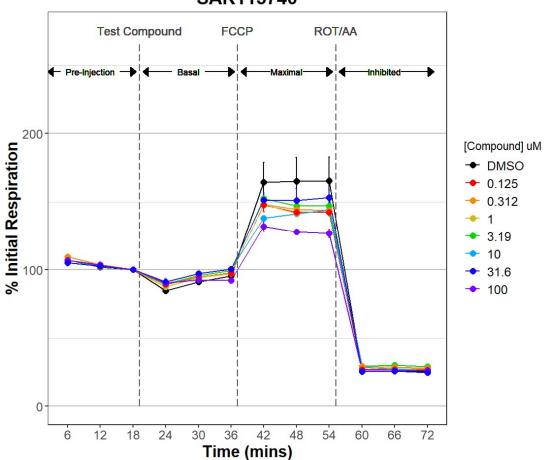
S-Bioallethrin



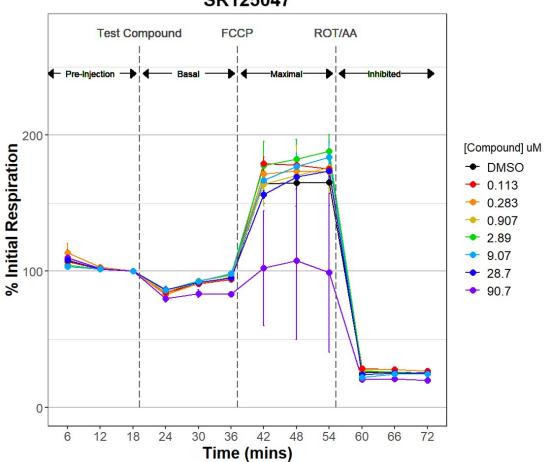
SAR 150640



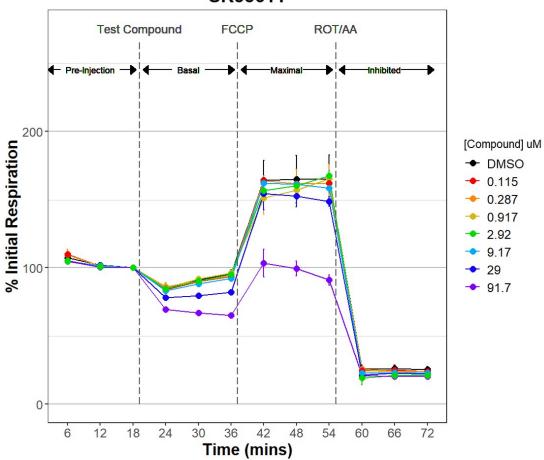
SAR115740



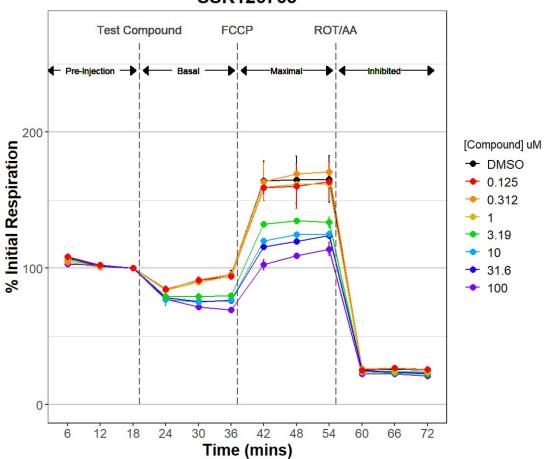




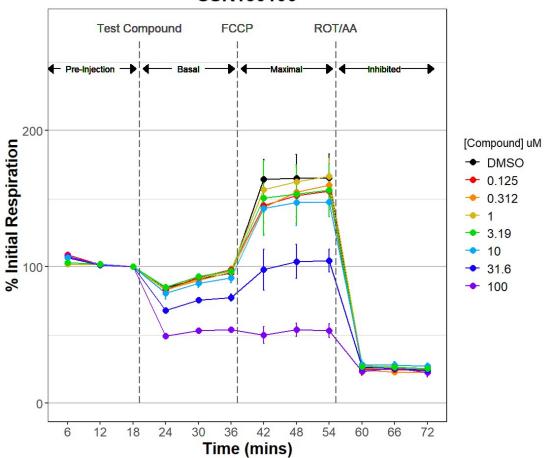
SR58611



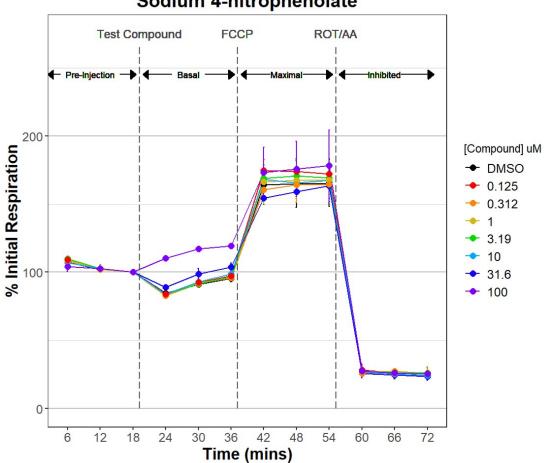




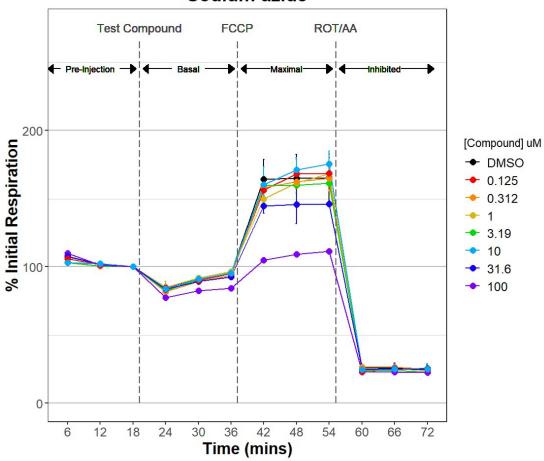
SSR150106



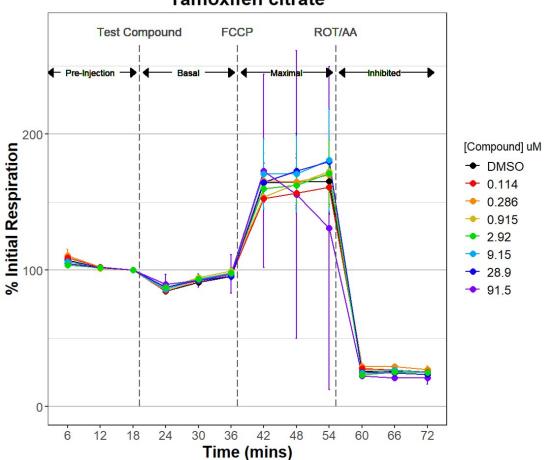
Sodium 4-nitrophenolate



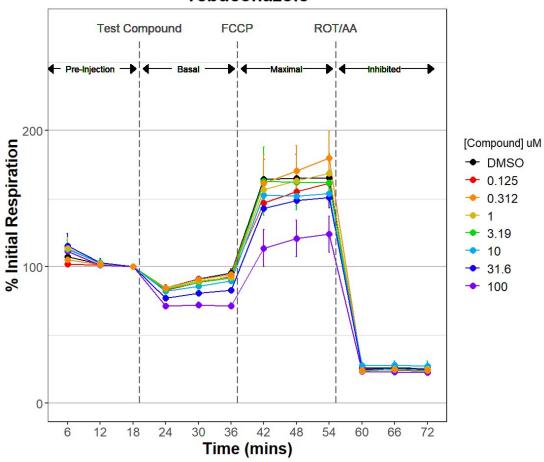
Sodium azide



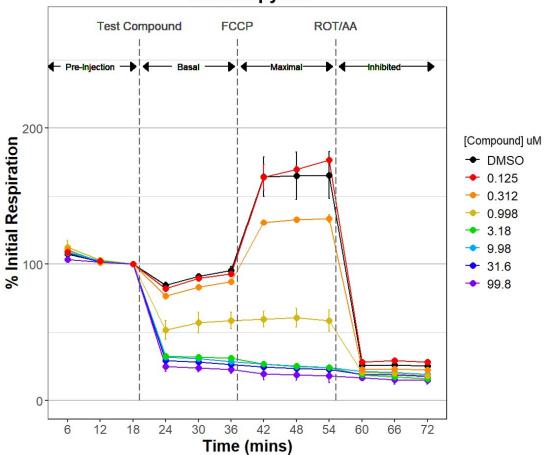
Tamoxifen citrate



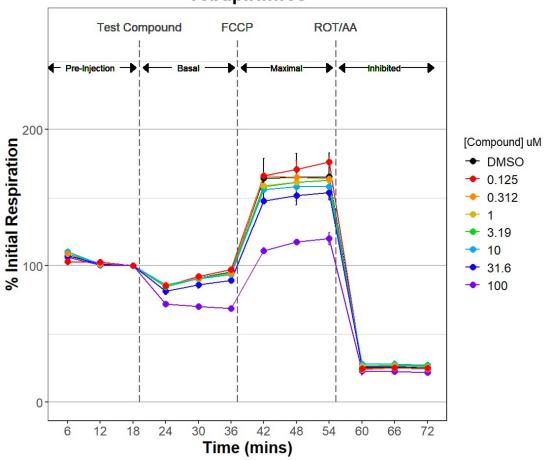
Tebuconazole



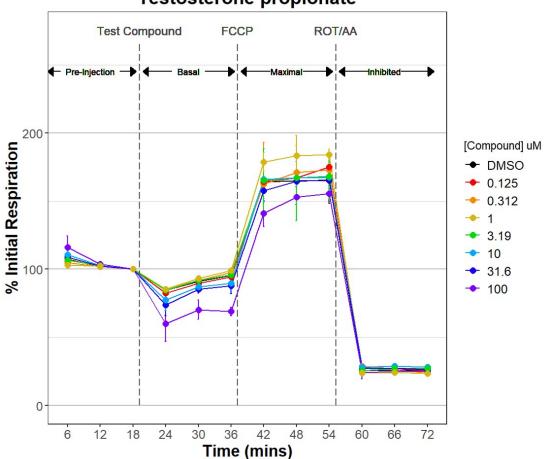


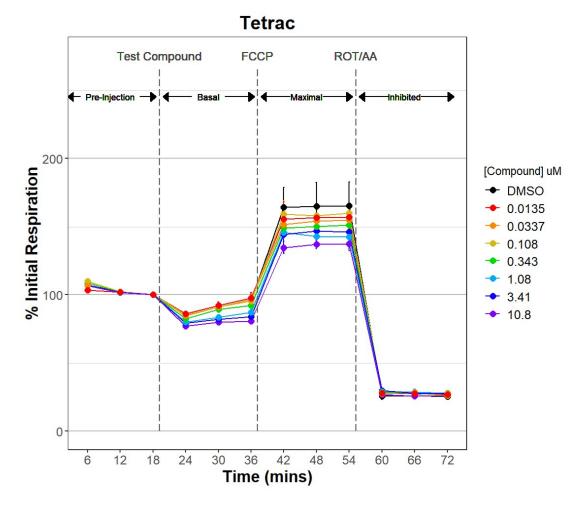


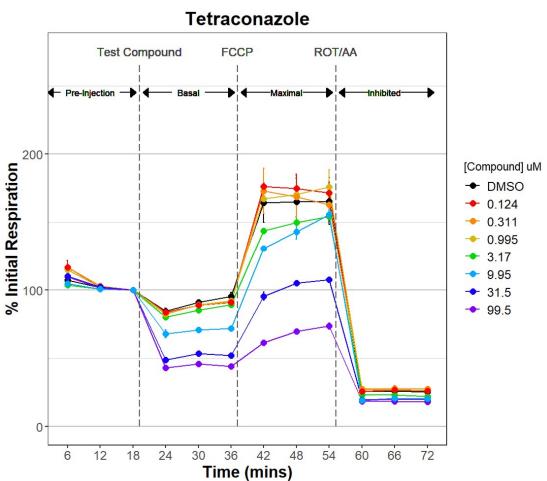
Tebupirimfos



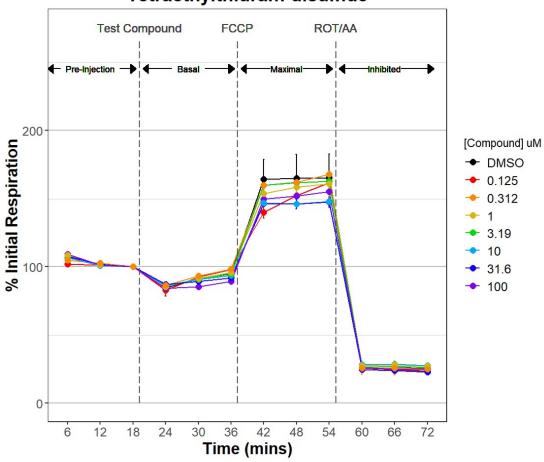
Testosterone propionate



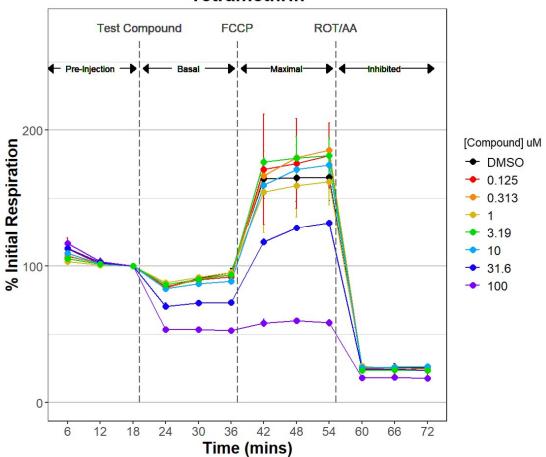


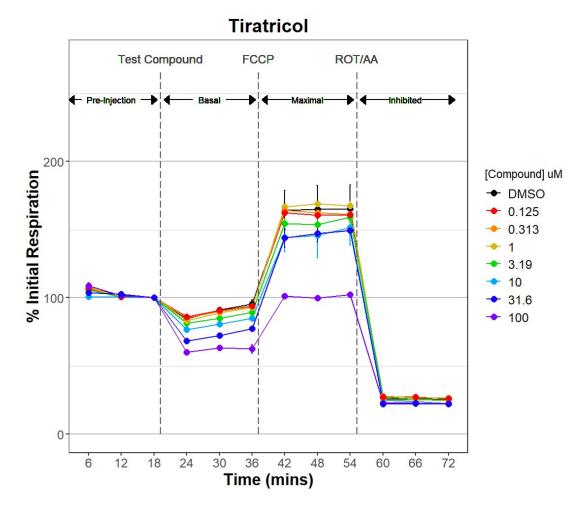


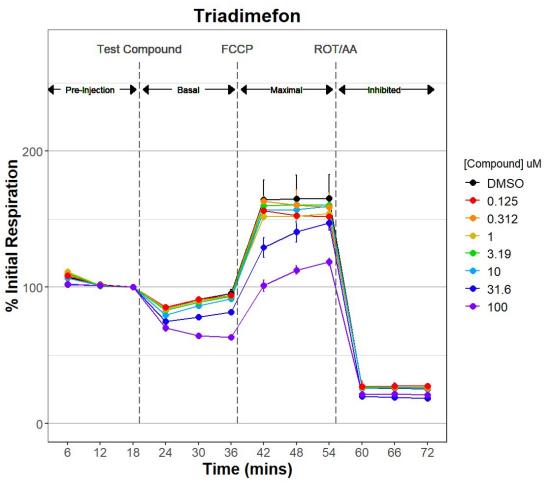
Tetraethylthiuram disulfide



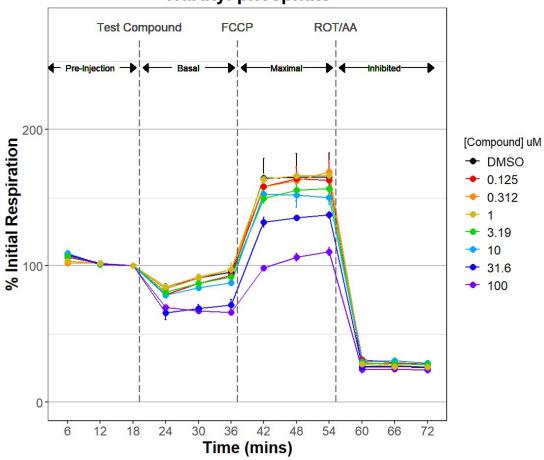
Tetramethrin



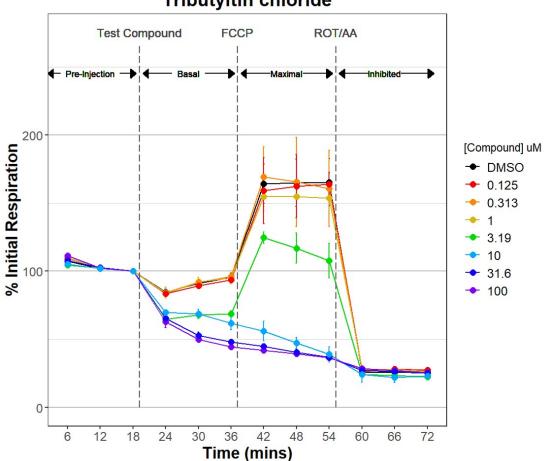




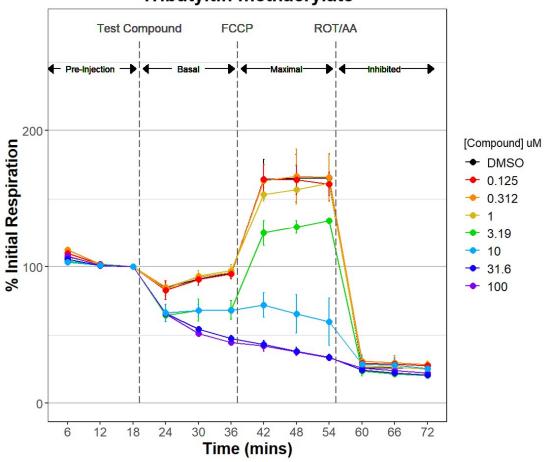
Tributyl phosphate



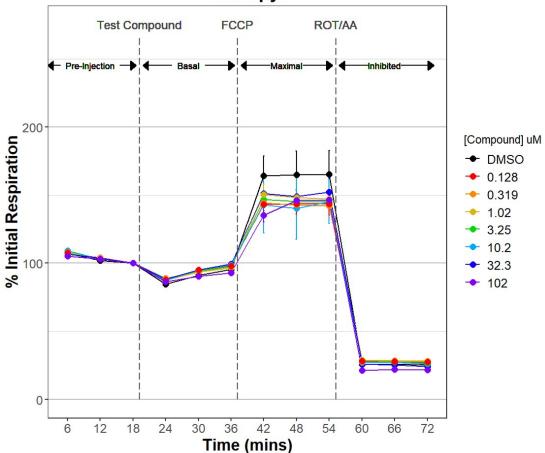
Tributyltin chloride

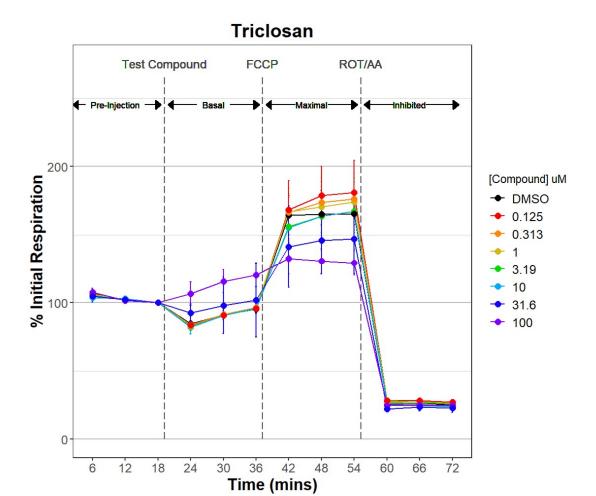


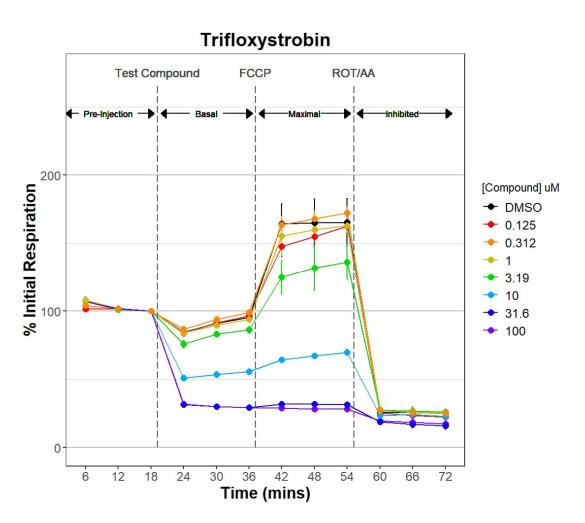
Tributyltin methacrylate

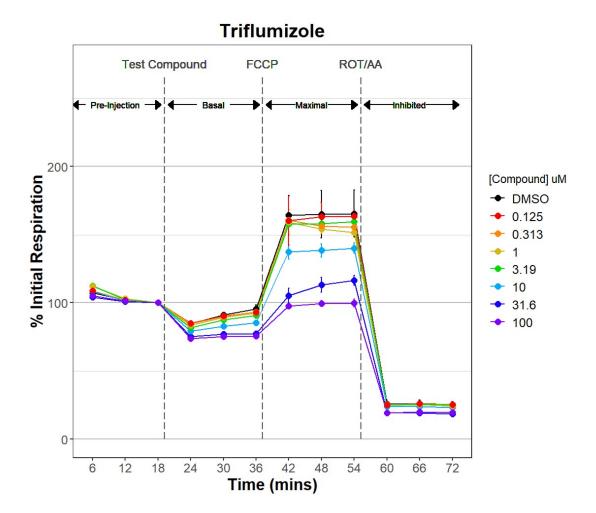


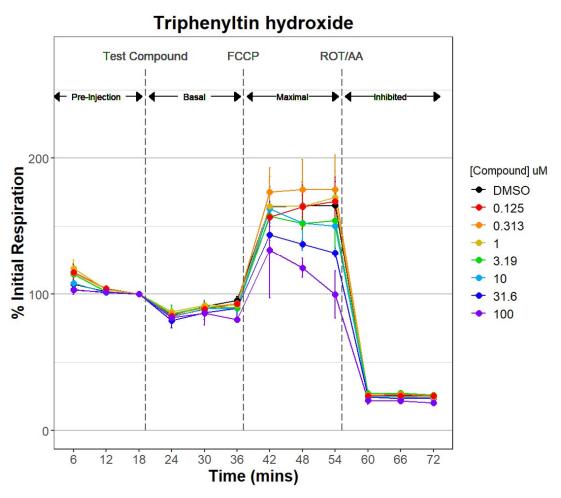




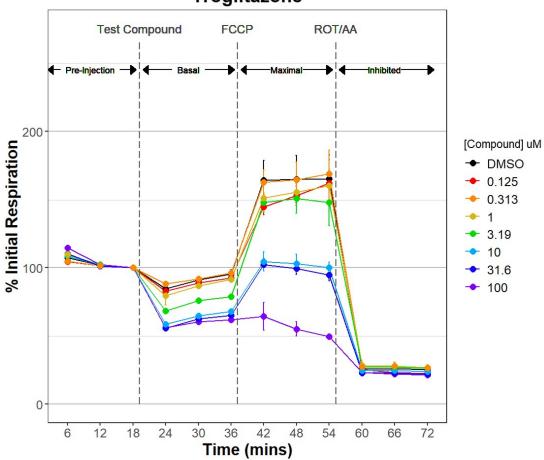




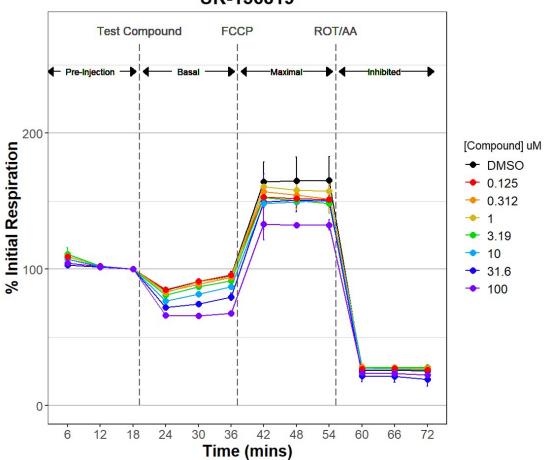




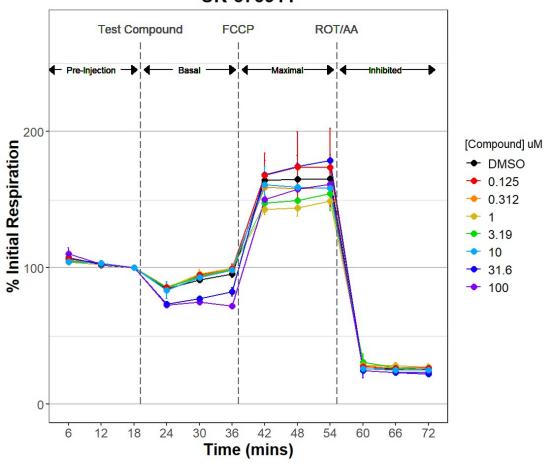
Troglitazone

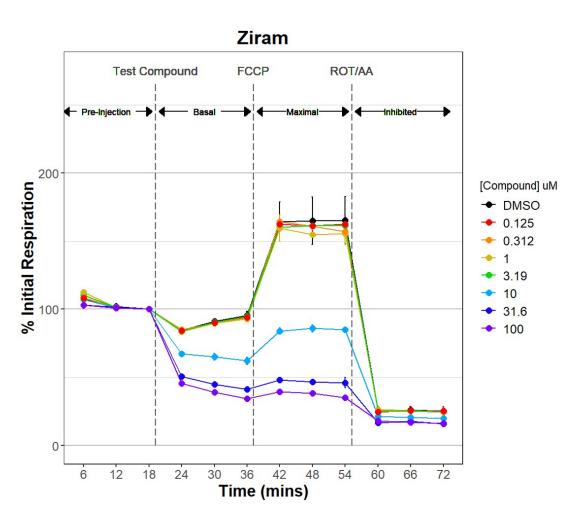


UK-156819

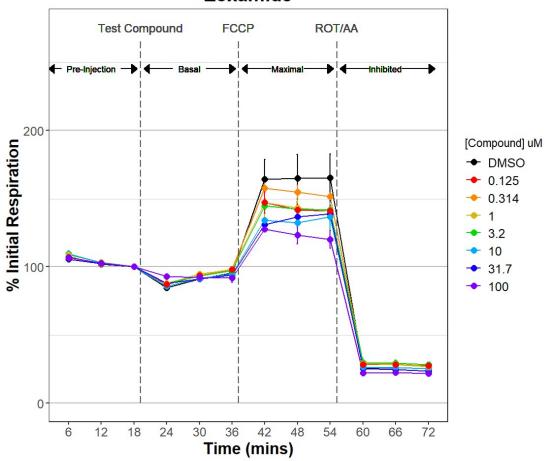


UK-373911

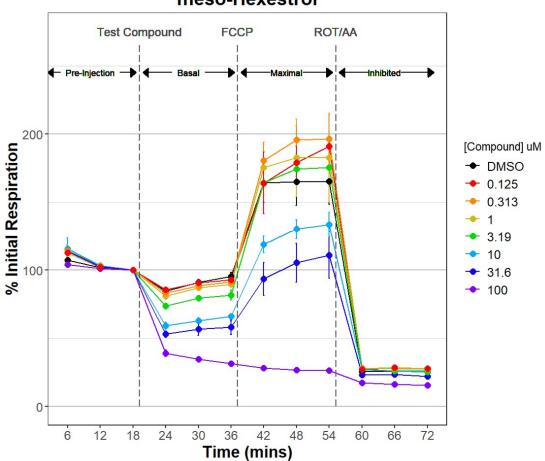




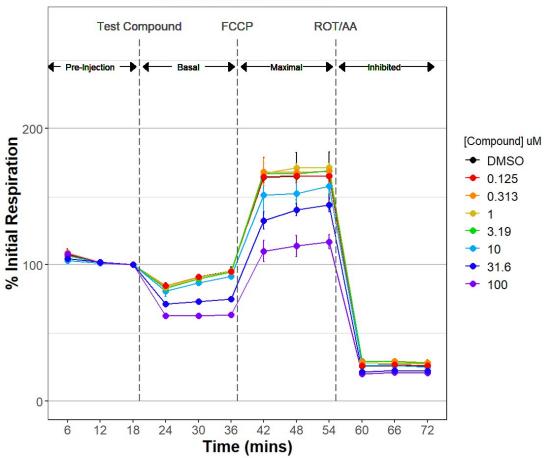
Zoxamide



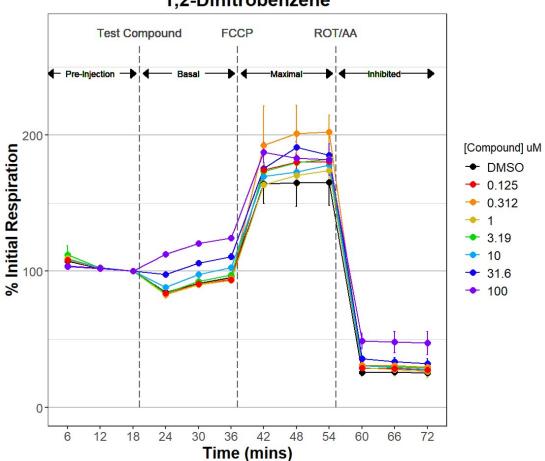
meso-Hexestrol



o-Aminoazotoluene



1,2-Dinitrobenzene



1,3-Benzenediamine

