SUPPORTING INFORMATION

High-Throughput Screening and Quantitative Chemical Ranking for Sodium Iodide Symporter (NIS) Inhibitors in ToxCast Phase I Chemical Library

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Part I. Supplemental Materials and Methods

Identification of Iodide Interference using Sandell-Kolthoff Reaction

Sandell-Kolthoff (SK) reaction is a colorimetric method to quantify iodide concentration through measurement of the iodide-catalyzed conversion of Ce^{4+} (yellow) to Ce^{3+} (colorless) [1, 2]. SK reaction assay was used to detect the presence of iodide contamination or structural iodide in chemical samples that could possibly interfere with the RAIU assay and cause a false positive response. All 310 samples were tested by SK reaction following a previously developed protocol [3]. Briefly, 0.35µL of 100µM chemical samples were transferred to assay plate wells containing 69.7µL uptake buffer. Then standards (NaI, 100, 200, 300, 400, 500 nM) were added to specified duplicate wells at 70µL each. To initiate the reaction, 70µL of 24mM sodium arsenite solution and 70µL of 9.9mM ammonium cerium sulfate solution was added to all wells. The reaction was incubated for 20 minutes at room temperature and subsequently measured for absorbance at 420nm on a SpectraMax Plus Microplate Reader (Molecular Devices, Sunnyvale, CA). Raw A_{420} readings were log10-transformed and NaI standards readings were fitted with linear regression to interpolate iodide concentration for each chemical. All testing was performed in triplicates.

Only two chemicals (iodosulfuron-methyl-sodium and 3-iodo-2-propynyl-N-butylcarbamate) produced positive SK reactions, suggesting that overall iodide contamination was not introducing false positive results in the RAIU assay. Iodosulfuron-methyl-sodium had <20% RAIU inhibition in the single-concentration screening and therefore was not tested in the multi-concentration assay. 3-iodo-2-propynyl-N-butylcarbamate produced A_{420} readings beyond the upper range of the standard curve (> 35pmol/well). However, since 3-iodo-2-propynyl-N-butylcarbamate structurally contains iodide, it is unclear whether the strong S-K reaction was triggered by the chemical itself or the iodide contamination in the sample. This uncertainty about iodide contamination confounds any intrepetation of 3-iodo-2-propynyl-N-butylcarbamate results as an efficacious NIS inhibitor in the RAIU assay.

Dose-response curve fitting and plotting

Dose-response curves were fitted using the Hill model provided in U.S. EPA's ToxCast Pipeline (tcpl v1.2.2) R package.[4] The Hill model contains three parameters with bottom asymptote constrained to 0 and is given by the formula:

$$f(x,(tp,ga,gw)) = \frac{tp}{1+10^{(ga-x)gw}} \quad (1)$$

Where x is the log concentration, tp is the top asymptote for the given chemical, ga is the AC_{50} (the log concentration where the modeled activity equals 50% of the top asymptote), and gw is the Hill coefficient. The Hill model provided in the tcpl R package constrains the three parameters as following:

(1) $0 \leq tp \leq 1.2$ times the maximum response value

(2) (minimum log concentration minus 2) $\leq ga \leq$ (maximum log concentration plus 0.5)

(3) $0.3 \leq gw \leq 8$

Prior to curve fitting, the modeling function in the tcpl R package first checked for significant response by comparing the median of normalized chemical responses at each concentration to the 3bMAD value of each assay. The 3bMAD of the multi-concentration RAIU and cell viability assay (23.8% and 17.7% respectively) were calculated separately for each assay using the normalized response values collected from the two lowest concentrations of all test chemical samples. Curve fitting was only performed when a significant response was present.

Prior to curve fitting, the normalized multi-concentration response data were also inverted by subtracting normalized value from 100. This was done because the modeling function in the tcpl R package requires multi-concentration assay data to be conformed in the positive direction, whereas the RAIU and cell viability assay results were in the negative direction (inhibition from maximal response). Predicted response values (yhat) were calculated using the fitted Hill model parameters for each chemical. To visualize assay data and fitted dose-response curve together in the original negative direction, yhat values were subtracted from 100 and used to plot the dose-response curve. The normalized RAIU and cell viability responses, along with their fitted dose-response curve were plotted together in one graph for each chemical using the R package ggplot2 v2.2.[5]

Abbreviations

U.S.EPA (United States Environmental Protection Agency), AOP (adverse outcome pathway), EDSP (Endocrine Disruptor Screening Program), ToxCast (Toxicity Forecaster), HTS (high-throughput screening), NIS (sodium iodide symporter), T_3 (triiodothyronine), T_4 (thyroxine), TH (thyroid hormone), RAIU (radioactive iodide uptake), RLU (relative light unit), SD (standard deviation), CV (coefficient of variation), 3bMAD (three times the baseline median absolute deviation), DMSO (dimethylsulfoxide), 2,4-D (2,4-dichlorophenoxyacetic acid), DCNQ (2,3-dichloro-1,4-napthoquinone), HEK (human embryonic kidney), DMEM (Dulbecco’s Modified Eagle Medium), CPM (counts per minute), TAA (toxicity-adjusted area), PFOS (perfluorooctanesulfonic acid), PFOA (perfluorooctanoic acid), BDE-47 (2,2',4,4'-Tetrabromodiphenyl ether)

References

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Part II. Supplemental Figures and Tables

Single Concentration Screen: 96-well Plate Format												
	1	2	3	4	5	6	7	8	9	10	11	12
A	Sample 1	100uM NaNO3	100uM NaClO4	100uM NaClO4	100uM NaClO4	10uM NaClO4	1uM NaClO4	0.1uM NaClO4	0.01uM NaClO4	0.001uM NaClO4	100uM 2,4-D	100uM NaSCN
B	Sample 2	Sample 3	Sample 4	Sample 5	Sample 6	0.5% DMSO	Sample 7	Sample 8	Sample 9	Sample 10	Sample 11	0.5% DMSO
C	Sample 12	Sample 13	Sample 14	Sample 15	Sample 16	0.5% DMSO	Sample 17	Sample 18	Sample 19	Sample 20	Sample 21	0.5% DMSO
D	Sample 22	Sample 23	Sample 24	Sample 25	Sample 26	0.5% DMSO	Sample 27	Sample 28	Sample 29	Sample 30	Sample 31	0.5% DMSO
E	Sample 32	Sample 33	Sample 34	Sample 35	Sample 36	0.5% DMSO	Sample 37	Sample 38	Sample 39	Sample 40	Sample 41	0.5% DMSO
F	Sample 42	Sample 43	Sample 44	Sample 45	Sample 46	0.5% DMSO	Sample 47	Sample 48	Sample 49	Sample 50	Sample 51	0.5% DMSO
G	Sample 52	Sample 53	Sample 54	Sample 55	Sample 56	0.5% DMSO	Sample 57	Sample 58	Sample 59	Sample 60	Sample 61	0.5% DMSO
H	100uM NaSCN	100uM 2,4-D	0.001uM NaClO4	0.01uM NaClO4	0.1uM NaClO4	1uM NaClO4	10uM NaClO4	100uM NaClO4	100uM NaClO4	100uM NaClO4	100uM NaNO3	Sample 62

Concentration Resposne: 96-well Plate Format												
	1	2	3	4	5	6	7	8	9	10	11	12
A	0.5% DMSO	100uM NaNO3	100uM NaClO4	100uM NaClO4	100uM NaClO4	10uM NaClO4	1uM NaClO4	0.1uM NaClO4	0.01uM NaClO4	0.001uM NaClO4	100uM 2,4-D	100uM NaSCN
B	0.001uM DCNQ	0.001μM TC1	0.001μM TC2	0.001μM TC3	0.001μM TC4	0.001μM TC5	0.001μM TC6	0.001μM TC7	0.001μM TC8	0.001μM TC9	0.001μM TC10	0.5% DMSO
C	0.01uM DCNQ	0.01μM TC1	0.01μM TC2	0.01μM TC3	0.01μM TC4	0.01μM TC5	0.01μM TC6	0.01μM TC7	0.01μM TC8	0.01μM TC9	0.01μM TC10	0.5% DMSO
D	0.1uM DCNQ	0.1μM TC1	0.1μM TC2	0.1μM TC3	0.1μM TC4	0.1μM TC5	0.1μM TC6	0.1μM TC7	0.1μM TC8	0.1μM TC9	0.1μM TC10	0.5% DMSO
E	1uM DCNQ	1μM TC1	1μM TC2	1μM TC3	1μM TC4	1μM TC5	1μM TC6	1μM TC7	1μM TC8	1μM TC9	1μM TC10	0.5% DMSO
F	10uM DCNQ	10μM TC1	10μM TC2	10μM TC3	10μM TC4	10μM TC5	10μM TC6	10μM TC7	10μM TC8	10μM TC9	10μM TC10	0.5% DMSO
G	100uM DCNQ	100μM TC1	100μM TC2	100μM TC3	100μM TC4	100μM TC5	100μM TC6	100μM TC7	100μM TC8	100μM TC9	100μM TC10	0.5% DMSO
H	100uM NaSCN	100uM 2,4-D	0.001uM NaClO4	0.01uM NaClO4	0.1uM NaClO4	1uM NaClO4	10uM NaClO4	100uM NaClO4	100uM NaClO4	100uM NaClO4	100uM NaNO3	0.5% DMSO

Figure S1. Chemical assay plate map for single-concentration and multi-concentration screening. For single-concentration screening, each plate can test 62 samples. For multiple-concentration screening, ten test chemicals (TC), each in six dilutions, can be tested on each assay plate.

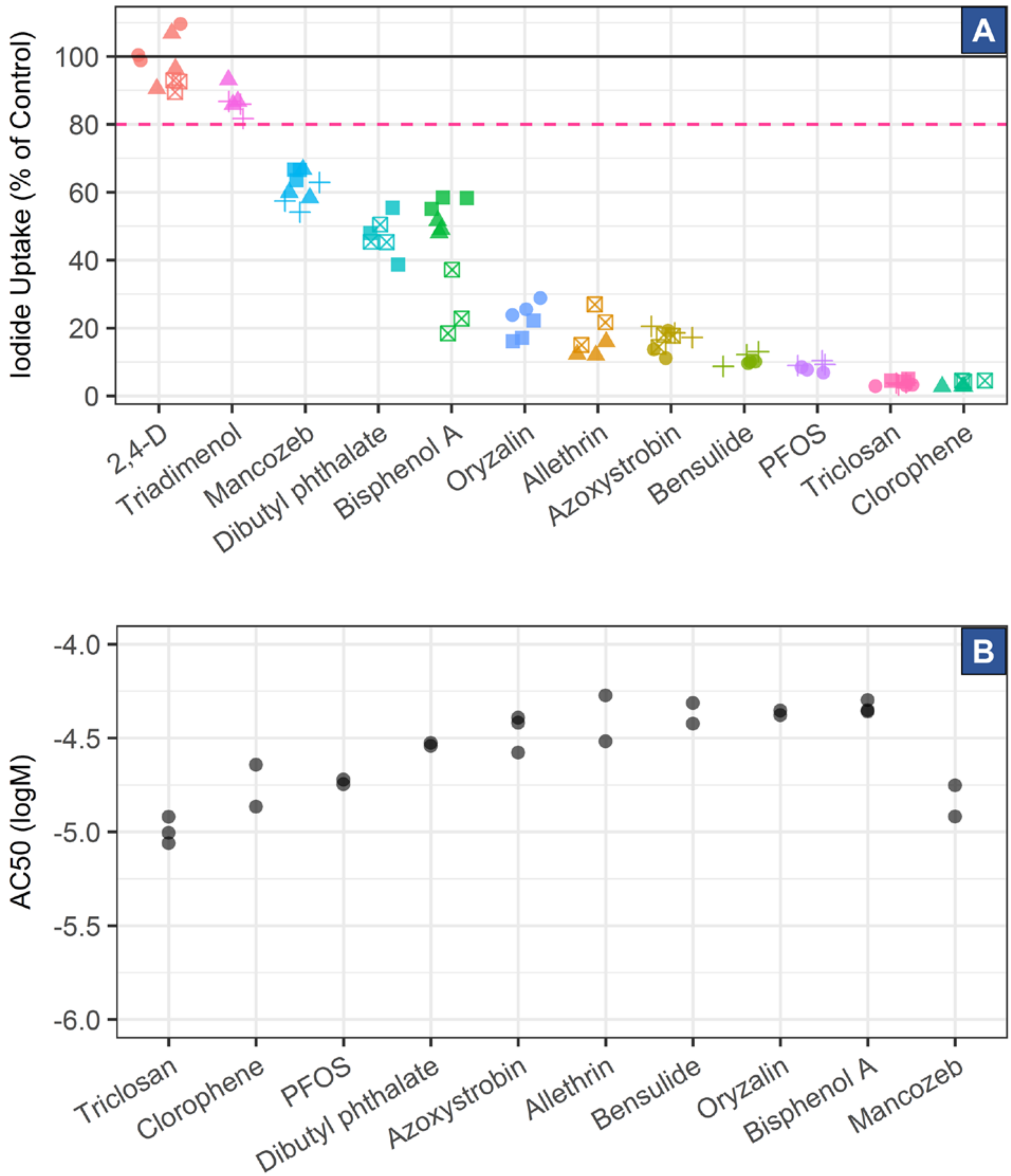


Figure S2. (A) Responses of internal replicates in single-concentration screening. 12 chemicals in the ToxCast phase1_v2 library were replicated 2 or 3 times (supplied in 2 or 3 blinded chemical samples). Colors represent different chemicals, while shapes indicate different internally replicated samples for a given chemical. Since each sample was tested in three bioreplicates, each shape for a given chemical has three data points. Ten of the 12 replicated chemicals that gave >20% inhibition (pink horizontal line) in this single-concentration test were subsequently tested in multi-concentration format (Fig. S3B). **(B) AC_{50} of internal replicates in multi-concentration screening.** Each symbol represents one AC50 value obtained from one sample of the chemical tested in three bioreplicates in multi-concentration**.**

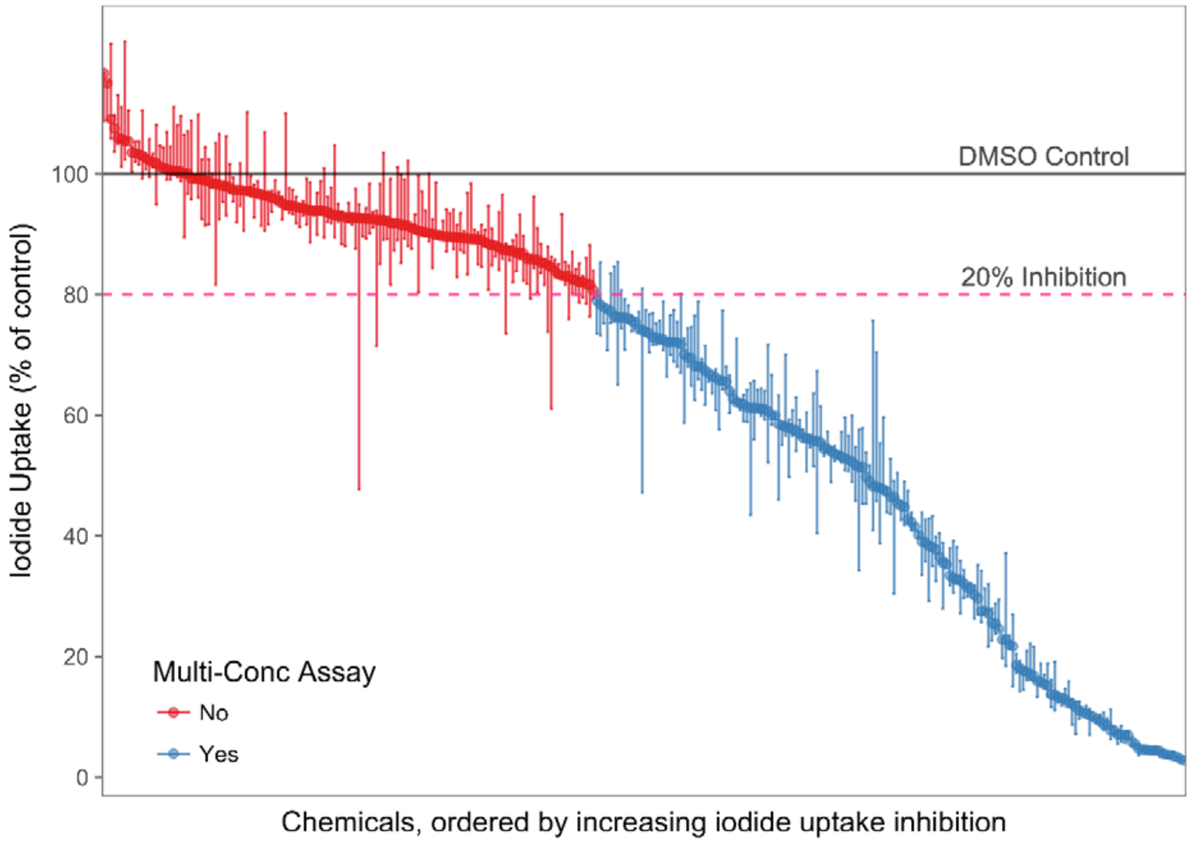


Figure S3. Median and range of test chemical responses in single-concentration RAIU screening. Median response of each chemical is represented by the dot and vertical bar shows the maximal iodide uptake (top of the bar) and the minimum iodide uptake (bottom of the bar). The pink horizontal line represents the 20% inhibition threshold. 310 blinded samples were tested at maximum permissible concentrations (typically 100 μM). 169 chemicals (54.5%) were selected for further testing in multi-concentration format based on a 20% inhibition activity threshold.

Table S1. List of test chemicals and screening results

Max Conc: the maximum permissible concentration tested in single-concentration screening. The Max Conc was obtained by 200X dilution of the supplied stock chemicals (concentrations ≤ 20mM). Serial dilution of samples for multi-concentration assay started with the Max Conc. *: precipitate visually observed in the well of stock chemical plate.

Multi-Conc Test: indicates whether a chemical was further tested in multi-concentration format. +: yes, -: no.

AC50: the AC50 value derived from multi-concentration dose-response curve.

absEC50: the absEC50 value derived from multi-concentration dose-response curve if the maximum inhibition achieved by the chemical was over 50%.

Cytotox-point: the log concentration where the chemical started to show significant toxicity (absEC82.3). NA: indicates no significant cytotoxicity.

Non-cytotoxic RAIU inhibition at 1 or 2 concentrations: show chemicals that have significant RAIU inhibition without significant cytotoxicity at one or two concentrations tested in multi-concentration screening. +: yes, -: no.

	Sample ID	Chemical	CAS NO.	Max Conc (M)	Multi-Conc Test	TAA	Median Difference	AC50 Cytotox	AC50 RAIU	absEC50 Cytotox	absEC50 RAIU	Cytotox-point	Non-cytotoxic RAIU inhibition at 1 or 2 concentrations	Ranking Score
1	TP0001500G04	Etoxazole	153233-91-1	1.00E-04	+	117.08	69.73	-4.39	-5.92	NA	-5.88	-4.32	+	150.41
2	TP0001502E10	Triphenyltin hydroxide	76-87-9	1.00E-04	+	78.91	59.75	-4.83	-5.39	NA	-5.39	-5.17	-	114.70
3	TP0001501D03	Niclosamide	50-65-7	5.00E-05	+	111.12	34.25	-6.03	-6.95	NA	-6.79	-6.91	-	109.38
4	TP0001502G01	3-Iodo-2-propynyl-N-butylcarbamate	55406-53-6	1.00E-04	+	70.75	58.13	-4.43	-5.09	NA	-5.30	-4.80	+	107.61
5	TP0001501E07	PFOS	1763-23-1	8.00E-05	+	36.81	67.33	-4.44	-4.75	NA	-4.78	-4.09	+	94.75
6	TP0001498G01	PFOS	1763-23-1	8.00E-05	+	34.34	67.82	NA	-4.72	NA	-4.74	NA	+	93.63
7	TP0001498B02	Cyprodinil	121552-61-2	1.00E-04	+	22.88	70.76	NA	-4.43	NA	-4.43	NA	+	89.12
8	TP0001501G03	Rotenone	83-79-4	1.00E-04	+	81.11	31.04	-6.66	-7.15	NA	-6.22	-7.30	+	86.15
9	TP0001501C09	Pyridaben	96489-71-3	1.00E-04	+	97.26	13.18	-6.85	-8.64	NA	-7.49	-7.60	-	78.17
10	TP0001500E11	Methoxyfenozide	161050-58-4	1.00E-04	+	37.63	49.80	-4.78	-4.78	NA	-4.72	-4.68	+	76.97
11	TP0001500E05	2-(Thiocyanomethylthio)benzothiazole	21564-17-0	1.00E-04	+	18.69	56.54	-4.50	-4.33	NA	-4.37	-4.91	-	71.48
12	TP0001500D09	Oxyfluorfen	42874-03-3	1.00E-04	+	21.34	51.79	NA	-4.55	NA	-4.39	NA	+	68.27
13	TP0001499D08	Captan	133-06-2	9.50E-05	+	22.48	48.69	-4.39	-4.49	NA	-4.50	-4.81	-	65.79
14	TP0001502F03	Fipronil	120068-37-3	1.00E-04	+	26.79	44.56	-4.52	-4.57	NA	-4.63	-4.92	+	64.32
15	TP0001502E07	Fluroxypyr-meptyl	81406-37-3	1.00E-04	+	34.57	39.42	-4.24	-4.77	NA	-4.74	-4.74	+	64.10
16	TP0001500D03	Cyhalofop-butyl	122008-85-9	9.50E-05	+	37.45	32.21	-5.13	-5.47	NA	-4.75	-5.07	-	58.47
17	TP0001499A01	Fenpyroximate (Z,E)	111812-58-9	1.00E-04	+	72.42	8.99	-5.76	-6.79	NA	-6.07	-7.09	-	57.34
18	TP0001498C01	Thiobencarb	28249-77-6	1.00E-04	+	17.29	41.85	-4.17	-4.38	NA	-4.34	-4.70	-	55.20
19	TP0001500E07	Emamectin benzoate	155569-91-8	1.00E-04	+	36.73	29.18	-4.56	-4.88	-4.40	-4.99	-5.18	-	54.82
20	TP0001499C08	Diphenylamine	122-39-4	1.00E-04	+	20.68	38.57	-6.53	-4.74	NA	-4.28	-5.59	-	54.01
21	TP0001499G03	Folpet	133-07-3	1.00E-04	+	28.94	29.96	-4.76	-4.93	-4.17	-4.92	-5.65	-	50.48
22	TP0001499B03	Endosulfan	115-29-7	1.00E-04	+	6.95	43.17	-4.90	-4.35	NA	-4.39	-4.92	-	49.72
23	TP0001498C04	Prometryn	7287-19-6	1.00E-04	+	8.56	41.19	NA	-4.44	NA	NA	NA	+	48.73
24	TP0001502F02	Zoxamide	156052-68-5	1.00E-04	+	17.68	35.40	-4.51	-4.48	NA	-4.37	-4.66	-	48.72
25	TP0001499E01	Cyazofamid	120116-88-3	1.00E-04	+	23.13	31.74	-6.50	-5.59	NA	NA	NA	+	48.49
26	TP0001501E01	Parathion	56-38-2	1.00E-04	+	18.21	32.70	-4.74	-4.72	NA	-4.49	-4.01	-	46.24
27	TP0001498F01	Fenthion	55-38-9	1.00E-04	+	10.98	36.93	-4.29	-4.40	NA	-4.18	-3.72	-	45.87
28	TP0001499G11	Mancozeb	2234562	5.00E-05	+	11.69	33.73	-8.21	-4.92	NA	NA	-4.80	-	43.00
29	TP0001502F04	Bifenazate	149877-41-8	1.00E-04	+	12.05	32.60	-4.29	-4.42	NA	-4.39	-4.87	-	42.05
30	TP0001502F09	Clorophene	120-32-1	1.00E-04	+	41.67	13.77	-4.34	-4.87	-4.34	-5.07	-4.68	+	41.98
31	TP0001499F10	Trifloxystrobin	141517-21-7	1.00E-04	+	32.63	18.86	-5.14	-5.67	NA	-5.05	-5.99	-	41.32
32	TP0001500D07	Triclosan	3380-34-5	1.00E-04	+	42.32	12.63	-4.47	-5.01	-4.48	-5.00	-4.98	+	41.22
33	TP0001502B03	Methoxychlor	72-43-5	9.50E-05	+	8.19	33.80	NA	-4.58	NA	NA	NA	+	40.75
34	TP0001499F01	Quinoxyfen	124495-18-7	1.00E-04	+	15.11	29.11	-4.52	-4.47	NA	-4.44	-4.85	-	40.43
35	TP0001499G01	Triflumizole	68694-11-1	1.00E-04	+	20.48	25.56	-4.41	-4.53	-4.26	-4.61	-4.82	-	40.28
36	TP0001501E11	Prallethrin	23031-36-9	9.50E-05	+	10.01	29.52	-4.40	-4.38	NA	-4.33	-4.66	-	37.48
37	TP0001499C01	S-Bioallethrin	28434-00-6	1.00E-04	+	12.54	27.83	-4.37	-4.42	NA	-4.37	-4.62	-	37.39
38	TP0001502B10	Coumaphos	56-72-4	1.00E-04	+	29.15	17.16	-4.52	-5.00	-4.20	-4.79	-4.95	-	37.24
39	TP0001502F07	Chlorpyrifos-methyl	5598-13-0	1.00E-04	+	22.77	20.26	-4.58	-5.01	NA	NA	-5.16	+	36.26
40	TP0001498D10	Fluoxastrobin	361377-29-9	1.00E-04	+	24.45	18.81	-4.86	-4.95	-4.16	-4.84	-5.63	-	35.85
41	TP0001501C11	Triclosan	3380-34-5	1.00E-04	+	34.50	12.45	-4.58	-5.06	-4.57	-5.11	-5.13	-	35.85

42	TP0001498H12	Pyraclostrobin	175013-18-0	1.00E-04	+	40.06	8.29	-4.93	-6.02	-4.05	-5.91	-6.27	-	35.19
43	TP0001502G11	Fenoxaprop-ethyl	66441-23-4	1.00E-04	+	12.00	25.91	-5.04	-4.53	NA	-4.09	-5.05	-	35.03
44	TP0001501D10	Fenoxycarb	72490-01-8	1.00E-04	+	12.39	25.23	-4.51	-4.47	-4.30	-4.51	-4.91	-	34.58
45	TP0001500G01	Hexaconazole	79983-71-4	1.00E-04	+	10.02	26.66	-4.39	-4.45	NA	-4.13	-4.55	-	34.50
46	TP0001499E10	Diclosulam	145701-21-9	1.00E-04	+	11.50	25.61	-6.14	-4.82	NA	NA	-4.92	-	34.38
47	TP0001499D01	Clorophene	120-32-1	1.00E-04	+	26.21	16.05	-4.34	-4.64	-4.32	-4.75	-4.69	+	34.14
48	TP0001498D08	Tebupirimfos	96182-53-5	1.00E-04	+	15.29	22.18	-4.42	-4.61	NA	-4.42	-4.54	-	33.31
49	TP0001501C02	Abamectin	71751-41-2	1.00E-04*	+	5.35	27.70	NA	-4.33	NA	NA	NA	+	32.50
50	TP0001500E08	Pyriproxyfen	95737-68-1	1.00E-04	+	17.91	19.65	-4.67	-4.70	NA	-4.11	-4.90	-	32.40
51	TP0001498B11	Triclosan	3380-34-5	1.00E-04	+	27.09	13.76	-4.48	-4.92	-4.46	-4.90	-5.01	+	32.32
52	TP0001502C11	Carfentrazone-ethyl	128639-02-1	1.00E-04	+	7.37	25.91	-4.36	-4.35	NA	-4.03	-4.40	-	31.97
53	TP0001498A01	Pirimiphos-methyl	29232-93-7	1.00E-04	+	6.69	26.10	-4.80	-4.43	NA	NA	-4.18	-	31.71
54	TP0001502G02	Dibutyl phthalate	84-74-2	1.00E-04	+	6.83	25.96	-5.04	-4.54	NA	NA	-3.98	-	31.65
55	TP0001498C09	Methylene bis(thiocyanate)	6317-18-6	1.00E-04	+	23.33	14.57	-4.41	-4.66	-4.40	-4.79	-4.86	+	30.68
56	TP0001502D03	Bisphenol A	80-05-7	1.00E-04	+	3.01	26.66	NA	-4.36	NA	NA	NA	+	29.86
57	TP0001498B08	Dithiopyr	97886-45-8	9.50E-05	+	4.55	24.62	NA	-4.65	NA	NA	NA	+	28.75
58	TP0001500D05	Tebufenpyrad	119168-77-3	1.00E-04	+	44.54	-0.88	-4.94	-5.60	-5.01	-5.82	-6.21	+	28.57
59	TP0001502D04	Diclofop-methyl	51338-27-3	1.00E-04	+	9.36	21.20	-4.33	-4.49	NA	-4.12	-4.51	-	28.35
60	TP0001500G11	Dibutyl phthalate	84-74-2	1.00E-04	+	8.88	21.21	-5.81	-4.53	NA	NA	-4.29	-	28.05
61	TP0001498G03	Lactofen	77501-63-4	1.00E-04	+	3.22	24.45	NA	-4.79	NA	NA	NA	+	27.70
62	TP0001500C09	Piperonyl butoxide	51-03-6	1.00E-04	+	6.04	21.84	-6.26	-4.22	NA	NA	-4.87	-	26.83
63	TP0001500B08	Buprofezin	69327-76-0	1.00E-04	+	1.80	24.15	-4.89	-4.55	-4.80	-4.61	-4.95	+	26.43
64	TP0001502G03	Cloprop	101-10-0	1.00E-04	+	5.86	21.41	-5.57	-4.49	NA	NA	-3.45	-	26.25
65	TP0001498C10	Flutolanil	66332-96-5	1.00E-04	+	3.56	22.53	NA	-4.50	NA	NA	NA	+	25.91
66	TP0001500G03	Cinmethylin	87818-31-3	1.00E-04	+	6.94	18.92	-4.52	-4.23	NA	NA	-4.43	-	24.38
67	TP0001502D09	Chlorpropham	101-21-3	1.00E-04	+	2.02	21.99	NA	-4.42	NA	NA	NA	+	24.33
68	TP0001499C09	Clodinafop-propargyl	105512-06-9	1.00E-04	+	4.96	20.06	NA	-5.70	NA	NA	NA	+	24.25
69	TP0001501G11	Phosalone	2310-17-0	1.00E-04	+	11.28	15.74	-4.35	-4.46	-4.04	-4.35	-4.59	-	23.91
70	TP0001502F05	Allethrin	584-79-2	1.00E-04	+	11.84	14.16	-4.40	-4.52	-4.25	-4.49	-4.82	-	22.64
71	TP0001501G10	Disulfoton	298-04-4	1.00E-04	+	7.02	16.53	-4.41	-4.27	NA	NA	-4.44	-	21.93
72	TP0001502B05	Flumiclorac-pentyl	87546-18-7	1.00E-04	+	7.21	16.35	-4.79	-4.50	NA	-4.16	-5.26	-	21.87
73	TP0001502D11	Forchlorfenuron	68157-60-8	1.00E-04	+	7.16	16.17	-4.46	-4.44	-4.40	-4.50	-4.94	-	21.64
74	TP0001500F07	Flumetralin	62924-70-3	1.00E-04	+	3.23	18.36	NA	-4.33	NA	NA	NA	+	21.33
75	TP0001501E03	Ethalfluralin	55283-68-6	1.00E-04	+	20.37	6.86	-4.93	-5.16	-4.44	-4.93	-5.93	-	20.66
76	TP0001500B09	Lindane	58-89-9	1.00E-04	+	0.09	19.55	NA	-4.32	NA	NA	NA	+	20.50
77	TP0001500G08	Fluazinam	79622-59-6	9.00E-05	+	23.08	4.58	-4.72	-5.16	-4.75	-5.13	-5.40	-	20.06
78	TP0001501D02	Cyfluthrin	68359-37-5	1.00E-04	+	1.04	18.35	NA	-4.57	NA	NA	NA	+	19.87
79	TP0001499D02	Tri-allate	2303-17-5	1.00E-04	+	12.78	10.27	-4.42	-4.61	-4.32	-4.57	-4.84	+	19.20
80	TP0001502G07	Imazalil	35554-44-0	1.00E-04	+	6.53	14.20	-4.56	-4.50	NA	NA	-4.94	-	19.16
81	TP0001502E08	Cypermethrin	52315-07-8	1.00E-04	+	0.76	17.20	NA	-4.96	NA	NA	NA	+	18.48
82	TP0001500F09	Amitraz	33089-61-1	1.00E-04	+	6.97	12.95	-4.18	-4.22	NA	NA	-4.94	-	18.15
83	TP0001499E11	Tetraconazole	112281-77-3	9.50E-05	+	13.62	8.60	-4.41	-4.65	-4.17	-4.33	-4.86	-	18.01
84	TP0001502C07	Thiazopyr	117718-60-2	1.00E-04	+	0.05	17.07	NA	-4.62	NA	NA	NA	+	17.88
85	TP0001502E02	Trifluralin	1582-09-8	1.00E-04	+	16.64	6.45	-4.26	-4.95	NA	NA	-5.61	+	17.76
86	TP0001500F11	Tebufenozide	112410-23-8	1.00E-04	+	4.74	13.98	NA	-4.68	NA	NA	NA	+	17.75
87	TP0001502B07	Azoxystrobin	131860-33-8	1.00E-04	+	9.69	10.74	-4.52	-4.58	-4.42	-4.59	-5.04	+	17.64
88	TP0001501B01	Mancozeb	2234562	5.00E-05	+	0.01	16.75	NA	-4.75	NA	NA	NA	+	17.52
89	TP0001500F01	Fluazifop-butyl	69806-50-4	1.00E-04	+	3.60	14.37	-4.45	-4.36	NA	NA	-4.26	-	17.41
90	TP0001502F10	Fenarimol	60168-88-9	1.00E-04	+	2.31	14.65	-6.18	-5.11	NA	NA	-1.70	-	16.84
91	TP0001499B11	Allethrin	584-79-2	1.00E-04	+	1.36	14.88	-4.37	-4.27	-4.18	-4.24	-4.69	-	16.46
92	TP0001498E08	Maneb	12427-38-2	1.00E-04	+	1.46	14.75	NA	-4.37	NA	NA	NA	+	16.39
93	TP0001498D07	Flusilazole	85509-19-9	1.00E-04	+	1.30	14.68	-4.33	-4.25	-4.04	-4.16	-4.66	-	16.20
94	TP0001499B01	Bisphenol A	80-05-7	1.00E-04	+	0.54	14.20	NA	-4.35	NA	NA	NA	+	15.20
95	TP0001498G05	Ametryn	834-12-8	1.00E-04	+	0.18	14.02	NA	-4.26	NA	NA	NA	+	14.78
96	TP0001499G10	Fluazifop-P-butyl	79241-46-6	1.00E-04	+	2.17	12.47	-5.72	-4.41	NA	NA	-4.84	-	14.47
97	TP0001500E10	Diniconazole	83657-24-3	1.00E-04	+	10.00	7.26	-4.38	-4.50	-4.40	-4.56	-4.79	-	14.21
98	TP0001501G09	Pendimethalin	40487-42-1	1.00E-04	+	3.21	11.06	-4.46	-4.32	NA	NA	-4.36	-	13.68
99	TP0001501F07	Fenitrothion	122-14-5	1.00E-04	+	0.11	12.82	NA	-4.49	NA	NA	NA	+	13.48
100	TP0001502B04	Isazofos	42509-80-8	1.00E-04	+	0.02	12.85	NA	-4.26	NA	NA	NA	+	13.45
101	TP0001502B01	Oxadiazon	19666-30-9	1.00E-04	+	3.82	9.10	-4.36	-4.30	NA	NA	-4.43	-	12.04
102	TP0001498D11	Hexythiazox	78587-05-0	1.00E-04	+	0.28	10.69	NA	-4.46	NA	NA	NA	+	11.36
103	TP0001500E09	Fenamidone	161326-34-7	1.00E-04	+	1.21	9.99	-4.83	-4.29	NA	NA	-4.09	-	11.25
104	TP0001498F05	Difenoconazole	119446-68-3	1.00E-04	+	17.47	-0.50	-4.52	-4.75	-4.57	-4.90	-5.09	-	11.04
105	TP0001502C04	Fluthiacet-methyl	117337-19-6	1.00E-04	+	1.26	9.42	-4.52	-4.72	NA	NA	-3.59	-	10.68
106	TP0001501F01	Azoxystrobin	131860-33-8	1.00E-04	+	-0.60	10.18	-4.54	-4.42	-4.51	-4.47	-5.06	-	10.24
107	TP0001498E01	Oryzalin	19044-88-3	1.00E-04	+	3.52	6.81	-4.35	-4.38	-4.03	-4.17	-4.63	-	9.45
108	TP0001501E05	Thidiazuron	51707-55-2	1.00E-04	+	1.43	8.12	-5.12	-4.44	NA	NA	-4.23	-	9.43

109	TP0001500B05	Famoxadone	131807-57-3	1.00E-04	+	12.44	0.72	-5.16	-5.69	-4.49	-4.81	-6.04	-	8.99
110	TP0001502E04	Dicofol	115-32-2	1.00E-04	+	11.70	1.10	-4.35	-4.54	-4.39	-4.61	-4.72	+	8.89
111	TP0001500F02	Propargite	2312-35-8	1.00E-04	+	3.84	5.99	-4.41	-4.40	NA	NA	-4.64	-	8.80
112	TP0001501E02	2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane	2971-36-0	1.00E-04	+	2.22	6.91	-4.44	-4.39	-4.44	-4.46	-4.90	-	8.69
113	TP0001502G09	Propiconazole	60207-90-1	1.00E-04	+	2.04	6.27	-4.89	-4.39	NA	NA	-4.75	-	7.91
114	TP0001498E11	Chlorethoxyfos	54593-83-8	1.00E-04	+	0.06	7.17	NA	-4.41	NA	NA	NA	+	7.53
115	TP0001502G04	Thiodicarb	59669-26-0	1.00E-04	+	1.93	4.68	-4.24	-4.91	NA	NA	-4.83	-	6.17
116	TP0001500D04	Ethofumesate	26225-79-6	1.00E-04	+	2.29	4.30	-4.42	-4.52	NA	NA	-4.56	-	6.01
117	TP0001498F07	Bensulide	741-58-2	1.00E-04	+	2.19	3.96	-4.41	-4.42	-4.40	-4.43	-4.83	-	5.59
118	TP0001500G09	Prodiamine	29091-21-2	1.00E-04	+	7.18	0.65	-4.38	-4.49	-4.39	-4.52	-4.80	-	5.44
119	TP0001501D04	Bensulide	741-58-2	1.00E-04	+	-0.55	5.55	-4.36	-4.31	-4.36	-4.34	-4.72	-	5.44
120	TP0001500C04	Bisphenol A	80-05-7	1.00E-04	+	0.26	4.15	-4.62	-4.30	NA	NA	-3.77	-	4.51
121	TP0001500G05	Flumioxazin	103361-09-7	1.00E-04	+	0.71	2.45	-4.41	-4.38	-4.40	-4.40	-4.84	-	3.04
122	TP0001502A01	Methidathion	950-37-8	1.00E-04	+	0.10	2.62	-4.38	-4.42	NA	NA	-4.22	-	2.81
123	TP0001498B05	Azoxystrobin	131860-33-8	1.00E-04	+	-2.89	3.89	-4.52	-4.39	-4.46	-4.39	-5.02	-	2.15
124	TP0001498B09	Butralin	33629-47-9	1.00E-04	+	-0.12	1.08	-4.40	-4.35	NA	NA	-4.67	-	1.05
125	TP0001498D01	Dicloran	99-30-9	1.00E-04	+	-4.51	3.13	-5.02	-4.63	NA	NA	-5.03	-	0.28
126	TP0001500D11	Oryzalin	19044-88-3	1.00E-04	+	0.33	-0.83	-4.36	-4.35	NA	NA	-4.60	-	-0.65
127	TP0001501B10	Fenbuconazole	114369-43-6	1.00E-04	+	-4.70	1.61	-4.36	-4.27	-4.39	-4.30	-4.72	-	-1.43
128	TP0001499E09	Thiram	137-26-8	1.00E-04	+	-6.47	2.16	-4.38	-4.18	-4.05	-4.04	-4.88	-	-2.03
129	TP0001500B02	Tetramethrin	7696-12-0	1.00E-04	+	0.15	-2.88	-4.42	-4.41	-4.32	-4.32	-4.88	-	-2.91
130	TP0001498D05	Profenofos	41198-08-7	5.00E-05	+	-2.71	-2.74	-4.60	-4.55	NA	NA	-4.90	-	-4.66
131	TP0001501D01	Quizalofop-ethyl	76578-14-8	8.50E-05	+	-1.00	-6.27	-4.46	-4.42	NA	NA	-4.65	-	-7.22
132	TP0001498D03	Prochloraz	67747-09-5	1.00E-04	+	-7.11	-3.20	-4.36	-4.18	-4.24	-4.12	-4.69	-	-8.05
133	TP0001501C04	Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3)	NOCAS_34742	9.50E-05	+	0.01	-8.55	-4.86	-4.22	NA	NA	-5.04	-	-8.94
134	TP0001498B07	Captafol	191906	1.00E-04	+	-5.19	-7.60	-4.49	-4.45	-4.56	-4.49	-5.06	-	-11.37
135	TP0001499G02	Tribufos	78-48-8	1.00E-04	+	-2.26	-9.57	-4.63	-4.94	NA	NA	-5.22	-	-11.50
136	TP0001499C07	Benfluralin	1861-40-1	1.00E-04	+	-3.73	-10.75	-4.49	-4.62	NA	NA	-4.78	-	-13.71
137	TP0001500E01	MGK-264	113-48-4	1.00E-04	+	-8.36	-22.95	-4.37	-4.28	-4.13	NA	-4.73	-	-29.52
138	TP0001498D02	Chlorothalonil	1897-45-6	1.00E-04	+	NA	-6.23	-4.56	NA	NA	NA	-4.03		NA
139	TP0001498G02	Propanil	709-98-8	1.00E-04	+	NA	-4.01	-4.75	NA	NA	NA	-3.88		NA
140	TP0001498C03	Bromoxynil	1689-84-5	8.00E-05	+	NA	-14.76	-4.62	NA	NA	NA	-5.22		NA
141	TP0001498F03	Napropamide	15299-99-7	1.00E-04	+	NA	0.69	-8.71	NA	NA	NA	NA		NA
142	TP0001498E04	Nitrapyrin	1929-82-4	1.00E-04	+	NA	6.98	NA	NA	NA	NA	NA		NA
143	TP0001498G08	Propetamphos	31218-83-4	1.00E-04	+	NA	7.17	NA	NA	NA	NA	NA		NA
144	TP0001498G09	Myclobutanil	88671-89-0	1.00E-04	+	NA	-1.80	NA	NA	NA	NA	NA		NA
145	TP0001498C11	Malathion	121-75-5	1.00E-04	+	NA	-1.12	-4.36	NA	NA	NA	-4.32		NA
146	TP0001499E02	Resmethrin	10453-86-8	1.00E-04	+	NA	-1.96	-4.65	NA	NA	NA	-4.41		NA
147	TP0001499E03	Fenpropathrin	39515-41-8	1.00E-04	+	NA	3.23	NA	NA	NA	NA	NA		NA
148	TP0001499B05	Picloram	6607	1.00E-04	+	NA	-13.00	NA	NA	NA	NA	NA		NA
149	TP0001499B07	Fludioxonil	131341-86-1	1.00E-04	+	NA	2.36	-4.31	NA	NA	NA	-4.17		NA
150	TP0001500A01	Acibenzolar-S-methyl	135158-54-2	1.00E-04	+	NA	9.07	NA	NA	NA	NA	NA		NA
151	TP0001500G02	Azinphos-methyl	86-50-0	1.00E-04	+	NA	-2.63	-4.50	NA	NA	NA	-3.99		NA
152	TP0001500F03	Mancozeb	2234562	5.00E-05	+	NA	11.54	NA	NA	NA	NA	NA		NA
153	TP0001500F04	Boscalid	188425-85-6	1.00E-04	+	NA	-3.30	-4.81	NA	NA	NA	-3.30		NA
154	TP0001500C05	Butachlor	23184-66-9	1.00E-04	+	NA	-8.98	-5.46	NA	NA	NA	-4.37		NA
155	TP0001500B07	Tefluthrin	79538-32-2	1.00E-04	+	NA	6.59	NA	NA	NA	NA	NA		NA
156	TP0001500G07	Butafenacil	134605-64-4	1.00E-04	+	NA	-3.64	-4.58	NA	NA	NA	-4.04		NA
157	TP0001501A01	Tralkoxydim	87820-88-0	1.00E-04	+	NA	10.76	NA	NA	NA	NA	NA		NA
158	TP0001501C01	Pyraflufen-ethyl	129630-19-9	1.00E-04	+	NA	-20.38	-3.50	NA	NA	NA	-4.33		NA
159	TP0001501G02	Prometon	1610-18-0	1.00E-04	+	NA	-3.53	NA	NA	NA	NA	NA		NA
160	TP0001501C03	Vinclozolin	50471-44-8	1.00E-04	+	NA	-2.76	NA	NA	NA	NA	NA		NA
161	TP0001501F04	2-Phenylphenol	90-43-7	1.00E-04	+	NA	0.77	NA	NA	NA	NA	NA		NA
162	TP0001501G04	Clomazone	81777-89-1	1.00E-04	+	NA	-4.36	NA	NA	NA	NA	NA		NA
163	TP0001501B05	Flufenpyr-ethyl	188489-07-8	1.00E-04	+	NA	-8.15	NA	NA	NA	NA	NA		NA
164	TP0001501D05	Chlorpyrifos oxon	5598-15-2	9.50E-05	+	NA	-7.40	-4.57	NA	NA	NA	-4.01		NA
165	TP0001501B08	Fenhexamid	126833-17-8	1.00E-04	+	NA	-2.35	-4.39	NA	NA	NA	-4.15		NA
166	TP0001501B11	Cycloate	1134-23-2	1.00E-04	+	NA	7.20	NA	NA	NA	NA	NA		NA
167	TP0001502E01	Naled	300-76-5	1.00E-04	+	NA	-10.21	-8.70	NA	NA	NA	NA		NA
168	TP0001502E03	Linuron	330-55-2	1.00E-04	+	NA	-3.50	-8.92	NA	NA	NA	NA		NA
169	TP0001502C09	EPTC	759-94-4	1.00E-04	+	NA	-6.40	NA	NA	NA	NA	NA		NA
170	TP0001498B01	Bifenthrin	82657-04-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
171	TP0001498C02	Bentazone	25057-89-0	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
172	TP0001498E02	Mesotrione	104206-82-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
173	TP0001498F02	Esfenvalerate	66230-04-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA

174	TP0001498B03	Thiophanate-methyl	23564-05-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
175	TP0001498E03	Trichlorfon	52-68-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
176	TP0001498B04	Carbaryl	63-25-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
177	TP0001498D04	2,4-Dichlorophenoxyacetic acid	94-75-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
178	TP0001498F04	Boric acid	10043-35-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
179	TP0001498G04	Dichlorprop	120-36-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
180	TP0001498C05	Dicrotophos	141-66-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
181	TP0001498E05	Butylate	2008-41-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
182	TP0001498C07	Dimethylarsinic acid	75-60-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
183	TP0001498E07	Dichlorvos	62-73-7	5.00E-05	-	NA	NA	NA	NA	NA	NA	NA	NA
184	TP0001498G07	Malaoxon	1634-78-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
185	TP0001498C08	Cyanazine	21725-46-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
186	TP0001498F08	Methomyl	16752-77-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
187	TP0001498D09	PFOA	335-67-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
188	TP0001498E09	Propoxur	114-26-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
189	TP0001498F09	Imazethapyr	81335-77-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
190	TP0001498B10	Imidacloprid	138261-41-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
191	TP0001498E10	Fenamiphos	22224-92-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
192	TP0001498F10	Clopyralid	1702-17-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
193	TP0001498G10	Metalaxyl	57837-19-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
194	TP0001498F11	Monocrotophos	6923-22-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
195	TP0001498G11	Indoxacarb	173584-44-6	8.00E-05	-	NA	NA	NA	NA	NA	NA	NA	NA
196	TP0001499B02	Acephate	30560-19-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
197	TP0001499C02	Anilazine	101-05-3	1.00E-04*	-	NA	NA	NA	NA	NA	NA	NA	NA
198	TP0001499F02	Diuron	330-54-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
199	TP0001499C03	Clofentezine	74115-24-5	1.00E-04*	-	NA	NA	NA	NA	NA	NA	NA	NA
200	TP0001499D03	Methamidophos	10265-92-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
201	TP0001499F03	Thiamethoxam	153719-23-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
202	TP0001499B04	Formetanate hydrochloride	23422-53-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
203	TP0001499C04	Fluometuron	2164-17-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
204	TP0001499D04	Difenzoquat metilsulfate	43222-48-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
205	TP0001499E04	Bendiocarb	22781-23-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
206	TP0001499F04	Alachlor	15972-60-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
207	TP0001499G04	Dimethenamid	87674-68-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
208	TP0001499C05	2,4-Dichlorophenoxyacetic acid	94-75-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
209	TP0001499D05	Ethylene thiourea	96-45-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
210	TP0001499E05	Azamethiphos	35575-96-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
211	TP0001499F05	Dazomet	533-74-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
212	TP0001499G05	Pyrimethanil	53112-28-0	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
213	TP0001499D07	Propyzamide	23950-58-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
214	TP0001499E07	Triadimenol	55219-65-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
215	TP0001499F07	Pirimicarb	23103-98-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
216	TP0001499G07	Isoxaben	82558-50-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
217	TP0001499B08	Acetochlor	34256-82-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
218	TP0001499E08	Acifluorfen	50594-66-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
219	TP0001499F08	Tepraloxydim	149979-41-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
220	TP0001499G08	Clopyralid-olamine	57754-85-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
221	TP0001499B09	2,4-DB	94-82-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
222	TP0001499D09	Hexazinone	51235-04-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
223	TP0001499F09	Tebuthiuron	34014-18-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
224	TP0001499G09	Iprodione	36734-19-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
225	TP0001499B10	Dicamba	1918-00-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
226	TP0001499C10	Methyl parathion	298-00-0	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
227	TP0001499D10	Fluroxypyr	69377-81-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
228	TP0001499C11	Dimethomorph	110488-70-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
229	TP0001499D11	Benomyl	17804-35-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
230	TP0001499F11	Monomethyl phthalate	4376-18-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
231	TP0001499H12	Diazinon	333-41-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
232	TP0001500B01	Cyclanilide	113136-77-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
233	TP0001500C01	Cyanamide	420-04-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
234	TP0001500D01	Ethoprop	13194-48-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
235	TP0001500C02	Penoxsulam	219714-96-2	1.00E-04*	-	NA	NA	NA	NA	NA	NA	NA	NA
236	TP0001500D02	Clothianidin	210880-92-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
237	TP0001500E02	Di(2-ethylhexyl) phthalate	117-81-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
238	TP0001500B03	Acetamiprid	135410-20-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
239	TP0001500C03	Novaluron	116714-46-6	1.00E-04*	-	NA	NA	NA	NA	NA	NA	NA	NA
240	TP0001500E03	Isoxaflutole	141112-29-0	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA

241	TP0001500B04	Imazamox	114311-32-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
242	TP0001500E04	Sulfentrazone	122836-35-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
243	TP0001500F05	Cyproconazole	94361-06-5	9.50E-05	-	NA	NA	NA	NA	NA	NA	NA		NA
244	TP0001500C07	Pymetrozine	123312-89-0	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
245	TP0001500C08	Spiroxamine	118134-30-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
246	TP0001500D08	Quinclorac	84087-01-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
247	TP0001500F08	Triclopyr	55335-06-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
248	TP0001500B10	Propamocarb hydrochloride	25606-41-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
249	TP0001500C10	Monobutyl phthalate	131-70-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
250	TP0001500D10	Pentachloronitrobenzene	82-68-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
251	TP0001500F10	Flufenacet	142459-58-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
252	TP0001500G10	Imazapyr	81334-34-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
253	TP0001500B11	Trifloxysulfuron-sodium	199119-58-9	1.00E-04*	-	NA	NA	NA	NA	NA	NA	NA		NA
254	TP0001500C11	Propazine	139-40-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
255	TP0001500H12	Thiacloprid	111988-49-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
256	TP0001501G01	2-Methoxyethanol	109-86-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
257	TP0001501B02	Chloridazon	1698-60-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
258	TP0001501F02	Asulam	3337-71-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
259	TP0001501B03	Pyrithiobac-sodium	123343-16-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
260	TP0001501F03	Deisopropylatrazine	1007-28-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
261	TP0001501B04	Molinate	2212-67-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
262	TP0001501E04	Oxytetracycline dihydrate	6153-64-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
263	TP0001501C05	Spirodiclofen	148477-71-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
264	TP0001501F05	Carboxin	5234-68-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
265	TP0001501G05	Oxamyl	23135-22-0	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
266	TP0001501B07	Symclosene	87-90-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
267	TP0001501C07	Fosthiazate	98886-44-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
268	TP0001501D07	Sethoxydim	74051-80-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
269	TP0001501G07	Dimethoate	60-51-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
270	TP0001501C08	MCPA	94-74-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
271	TP0001501D08	Paclobutrazol	76738-62-0	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
272	TP0001501E08	Dipropyl 2,5-pyridinedicarboxylate	136-45-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
273	TP0001501F08	Methyl isothiocyanate	556-61-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
274	TP0001501G08	DEET	134-62-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
275	TP0001501B09	Cyromazine	66215-27-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
276	TP0001501D09	Imazaquin	81335-37-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
277	TP0001501E09	Metribuzin	21087-64-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
278	TP0001501F09	Flumetsulam	98967-40-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
279	TP0001501C10	Triadimefon	43121-43-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
280	TP0001501E10	Metolachlor	51218-45-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
281	TP0001501F10	Permethrin	52645-53-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
282	TP0001501D11	Terbacil	5902-51-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
283	TP0001501F11	Triadimenol	55219-65-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
284	TP0001501H12	Etridiazole	2593-15-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
285	TP0001502C01	Propoxycarbazone-sodium	181274-15-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
286	TP0001502D01	Mevinphos	7786-34-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
287	TP0001502F01	Bromacil	314-40-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
288	TP0001502B02	Metam-sodium hydrate	6734-80-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
289	TP0001502C02	2,4-Dichlorophenoxyacetic acid	94-75-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
290	TP0001502D02	Thiabendazole	148-79-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
291	TP0001502C03	Atrazine	1912-24-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
292	TP0001502C05	2-Phenoxyethanol	122-99-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
293	TP0001502D05	Icaridin	119515-38-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
294	TP0001502E05	Imazapic	104098-48-8	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
295	TP0001502G05	Aldicarb	116-06-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
296	TP0001502D07	Triticonazole	131983-72-7	9.50E-05	-	NA	NA	NA	NA	NA	NA	NA		NA
297	TP0001502B08	Diazoxon	962-58-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
298	TP0001502C08	Maleic hydrazide	123-33-1	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
299	TP0001502D08	Daminozide	1596-84-5	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
300	TP0001502F08	Mepiquat chloride	24307-26-4	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
301	TP0001502G08	Norflurazon	27314-13-2	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
302	TP0001502B09	Chloroneb	2675-77-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
303	TP0001502E09	Ethephon	16672-87-0	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
304	TP0001502C10	Iodosulfuron-methyl-sodium	144550-36-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
305	TP0001502D10	Simazine	122-34-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
306	TP0001502G10	MEHP	4376-20-9	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA
307	TP0001502B11	Cymoxanil	57966-95-7	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA		NA

308	TP0001502E11	Diquat dibromide monohydrate	6385-62-2	5.00E-05	-	NA	NA	NA	NA	NA	NA	NA	NA
309	TP0001502F11	Dimethyl phthalate	131-11-3	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA
310	TP0001502H12	Dichlobenil	1194-65-6	1.00E-04	-	NA	NA	NA	NA	NA	NA	NA	NA

Table S2. Control chemicals included on each assay plate

Control Chemical	DMSO	2,4-D	DCNQ	NaClO4	$NaNO_3$	NaSCN
CAS No.	67-68-5	94-75-7	117-80-6	7601-89-0	7631-99-4	540-72-7
Purity (%)	99.9	98	98	98	99	98
Purpose	Vehicle control	Negative control	Cell viability assay, positive control	RAIU assay, positive control	RAIU assay, positive control (20% inhibition)	RAIU assay, positive control (80% inhibition)
Concentration (% or M)	0.5%	1E-4	1E-9, 1E-8, 1E-7, 1E-6, 1E-5, 1E-4	1E-9, 1E-8, 1E-7, 1E-6, 1E-5, 1E-4	1E-4	1E-4
Reps*/plate in Single-Con Screening	12	2	3 for 1E-4M, 1 for the rest	6 for 1E-4M, 2 for the rest	2	2
Reps*/plate in Multi-Con Screening	8	2	3 for 1E-4M, 1 for the rest	6 for 1E-4M, 2 for the rest	2	2

*Number of wells

Table S3. Summary of assay performance metrics for single-concentration and multi-concentration screening

Assay[1]	CV of DMSO		Z' Score		AC50 of positive control[2]	
	mean±SD	range	mean±SD	range	mean±SD	range
Single-con RAIU	7.14% ± 1.56%	4.91% - 11.04%	0.77 ± 0.05	0.65 - 0.84	-6.44 ± 0.11	-6.56 - -6.06
Multi-con RAIU	8.61% ± 1.01%	6.70% - 11.50%	0.72 ± 0.03	0.64 - 0.78	-6.38 ± 0.13	-6.57 - -6.04
Multi-con Cell Viability	5.42% ± 1.47%	2.80% - 9.53%	n.a.	n.a.	-4.83 ± 0.12	-4.92 - -4.47

1: All metrics were calculated per assay plate (single-con: n=15, multi-con: n=54) and summarized separately for single-concentration and multi-concentration screenings.

2: AC50 of positive controls were calculated from the dose-responses of $NaClO_4$ and DCNQ for RAIU and cell viability assay respectively. Unit: logM.

n.a.: unable to calculate.

Table S4. Summary of normalized responses of control chemicals across all plates

Assay[1]	DMSO	2,4-D	DCNQ[2] (1E-4M)	$NaClO_4$[2] (1E-4M)	$NaNO_3$	NaSCN
single-con RAIU	100.63 ± 7.11	92.41 ± 4.24	n.a.	2.85 ± 0.36	81.25 ± 7.56	20.64 ± 1.12
multi-con RAIU	99.5 ± 8.28	90.86 ± 4.49	3.92 ± 3.37	3.28 ± 0.38	83.08 ± 7.17	24.69 ± 2.71
multi-con Cell Viability	100.92 ± 5.41	99.34 ± 3.21	3.72 ± 0.38	99.19 ± 4.69	98.95 ± 5.43	104.3 ± 3.98

Mean ± S.D.

n.a.: not available as DCNQ was not included in the single-concentration screening.

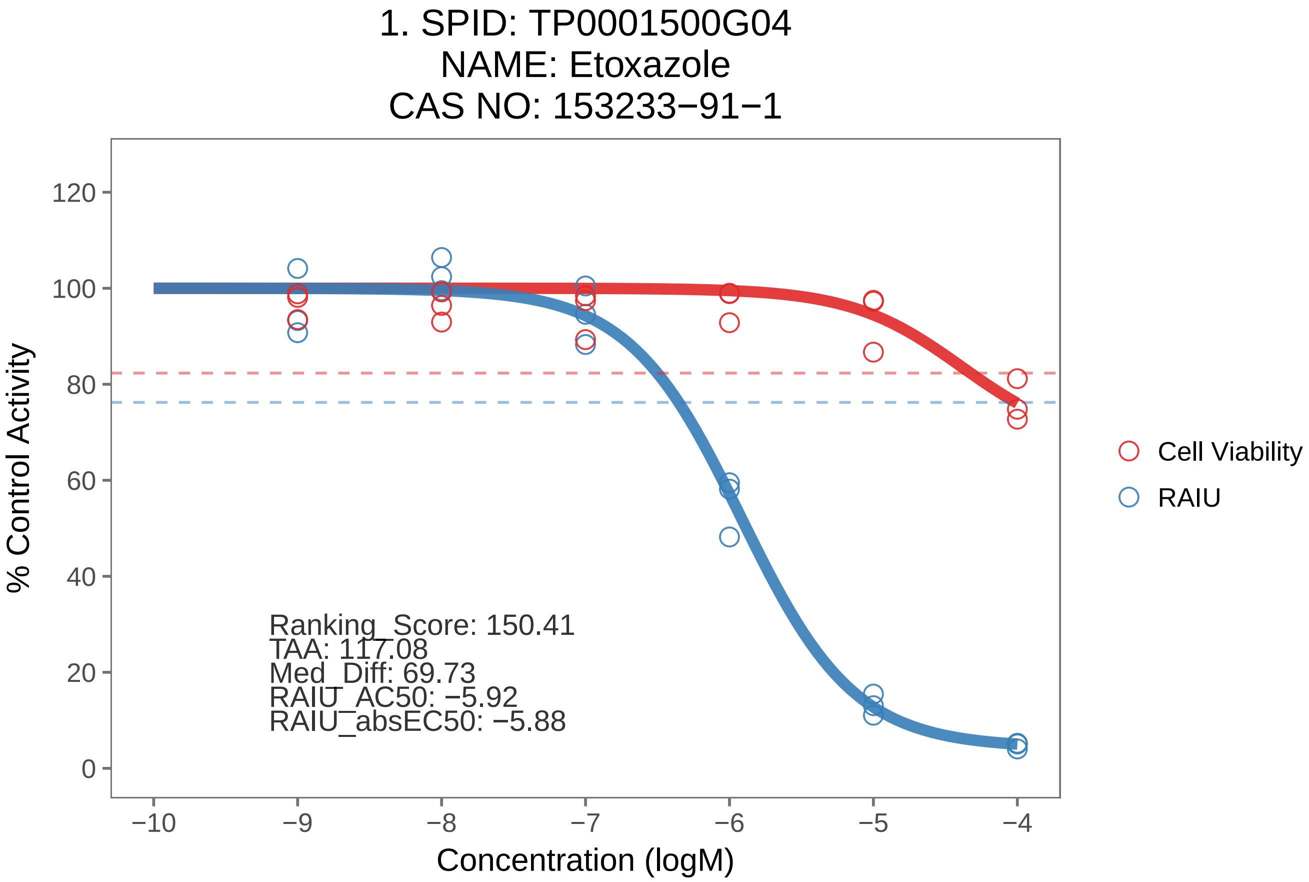
1. Data were calculated by collecting normalized response for each chemical from all assay plates. Values represent the percent of control activity. 2,4-D, $NaNO_3$, and NaSCN were at a concentration of 100 µM.

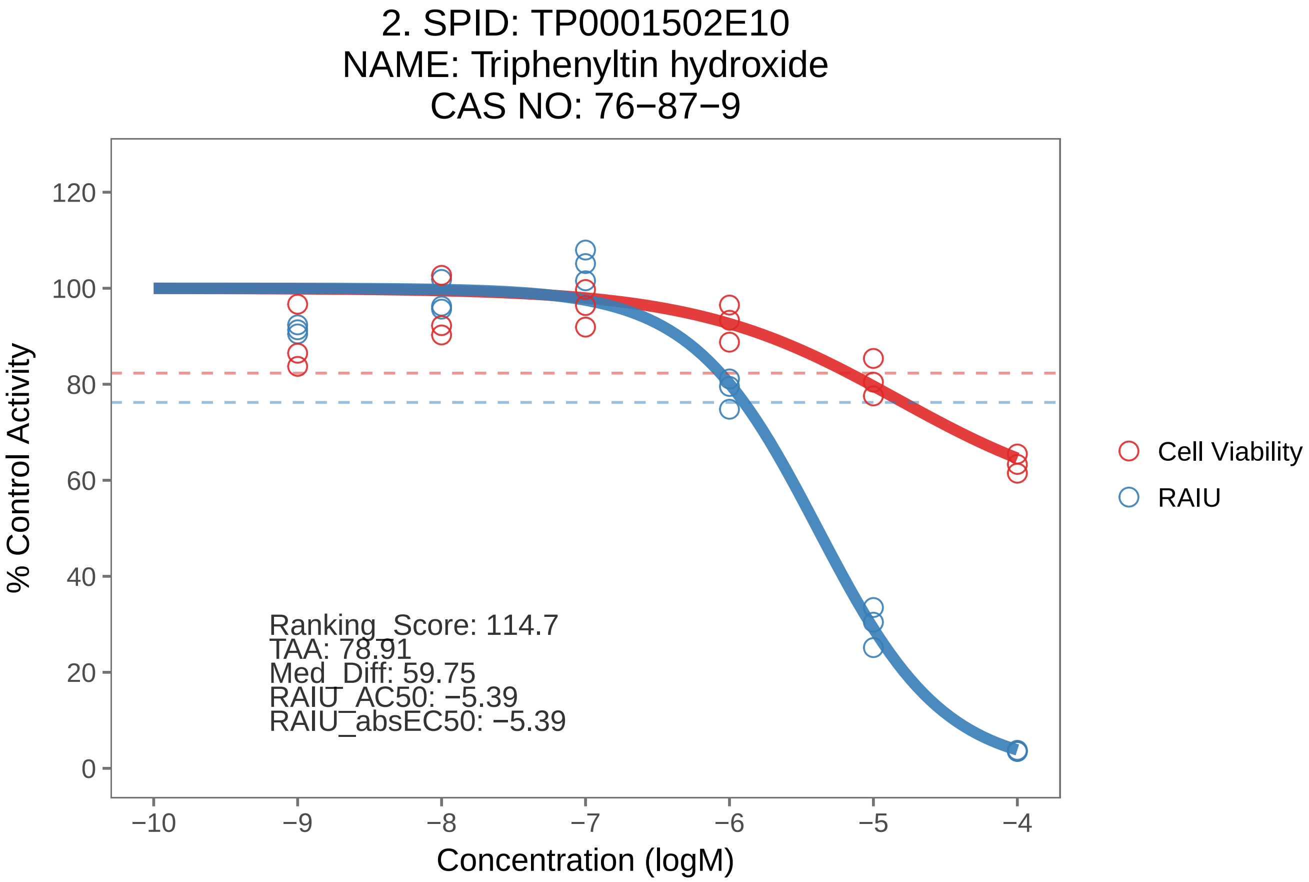
2. For DCNQ and $NaClO_4$, though they were included on each assay plate in six concentrations, only the responses from 100 µM concentration are summarized in this table.

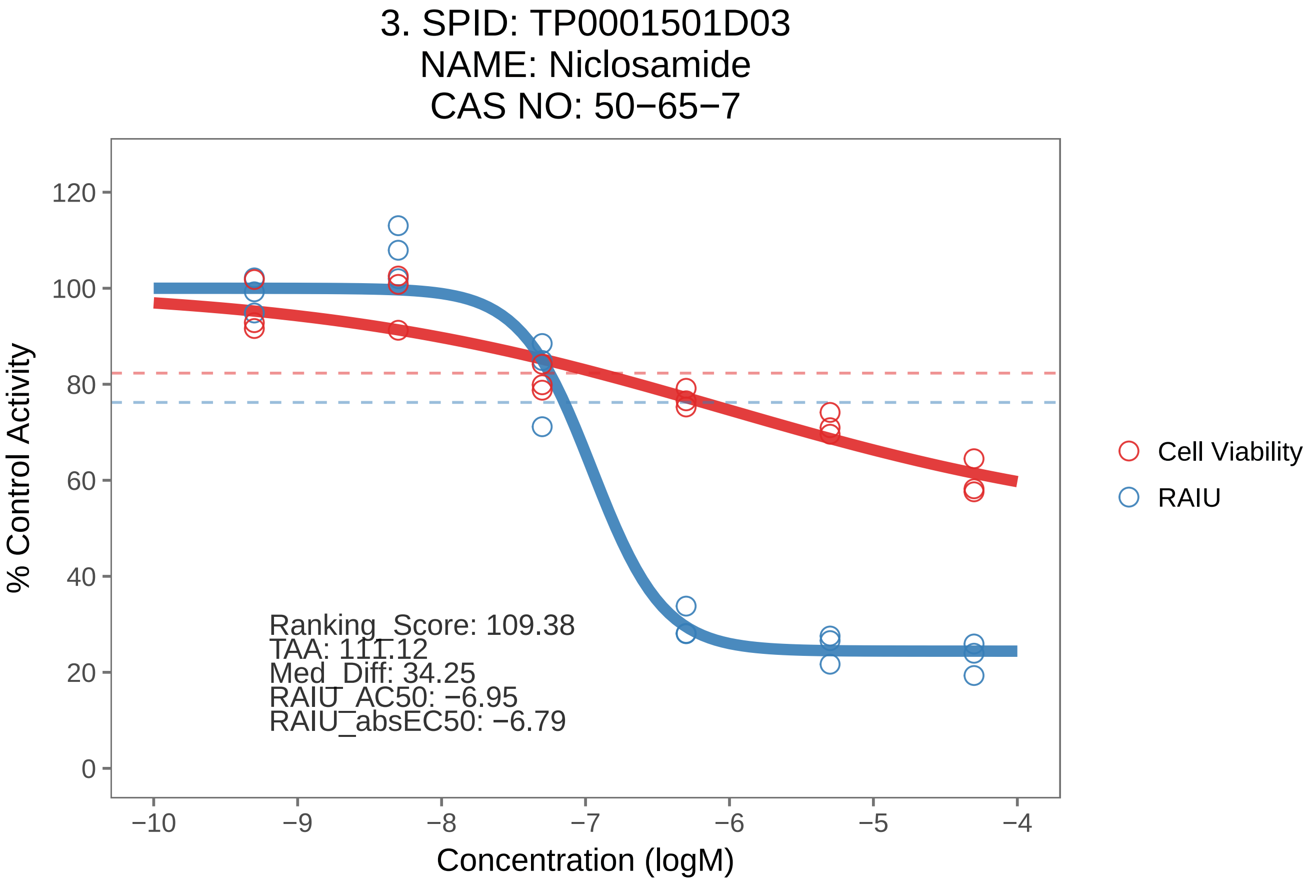
Table S5. Range of AC50 for 10 internal replicated chemicals in ToxCast phase I_v2 library

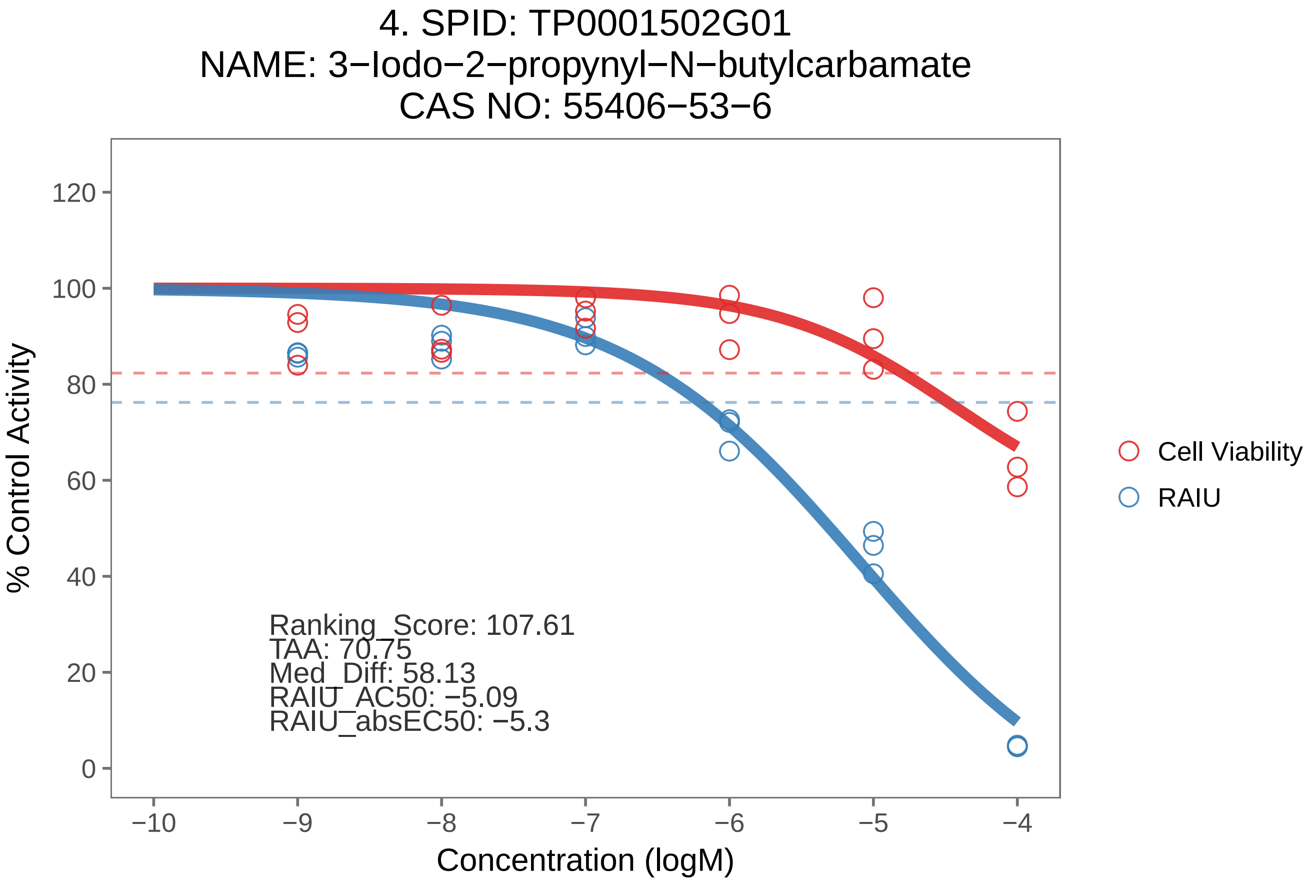
Name	**Min**	**Max**	**Range**
Dibutyl phthalate	-4.54	-4.53	-0.02
PFOS	-4.75	-4.72	-0.02
Oryzalin	-4.38	-4.35	-0.03
Bisphenol A	-4.36	-4.30	-0.06
Bensulide	-4.42	-4.31	-0.11
Triclosan	-5.06	-4.92	-0.14
Mancozeb	-4.92	-4.75	-0.17
Azoxystrobin	-4.58	-4.39	-0.19
Clorophene	-4.87	-4.64	-0.22
Allethrin	-4.52	-4.27	-0.24

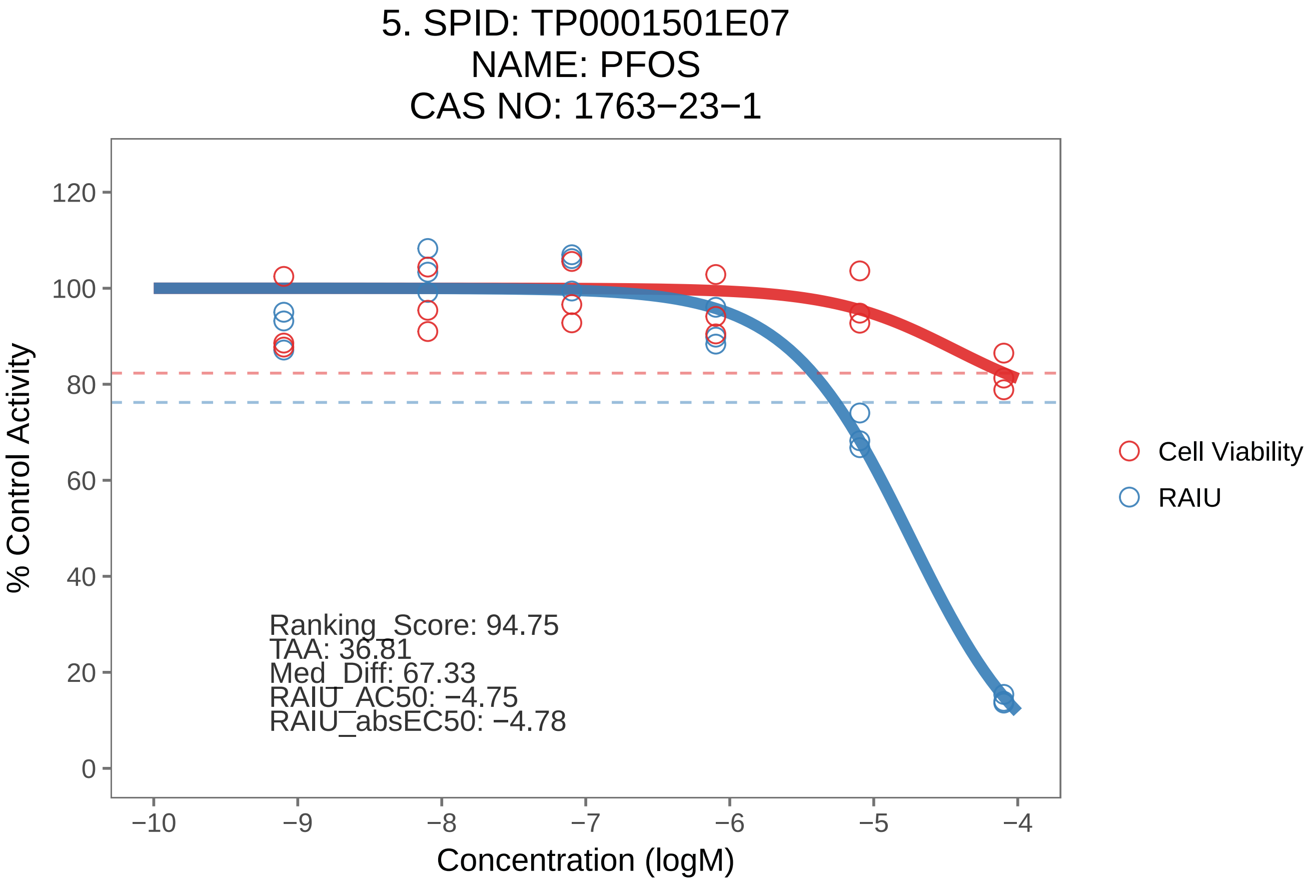
Part III. Dose-response of all chemicals tested in multi-concentration with plots ordered by ranking scores

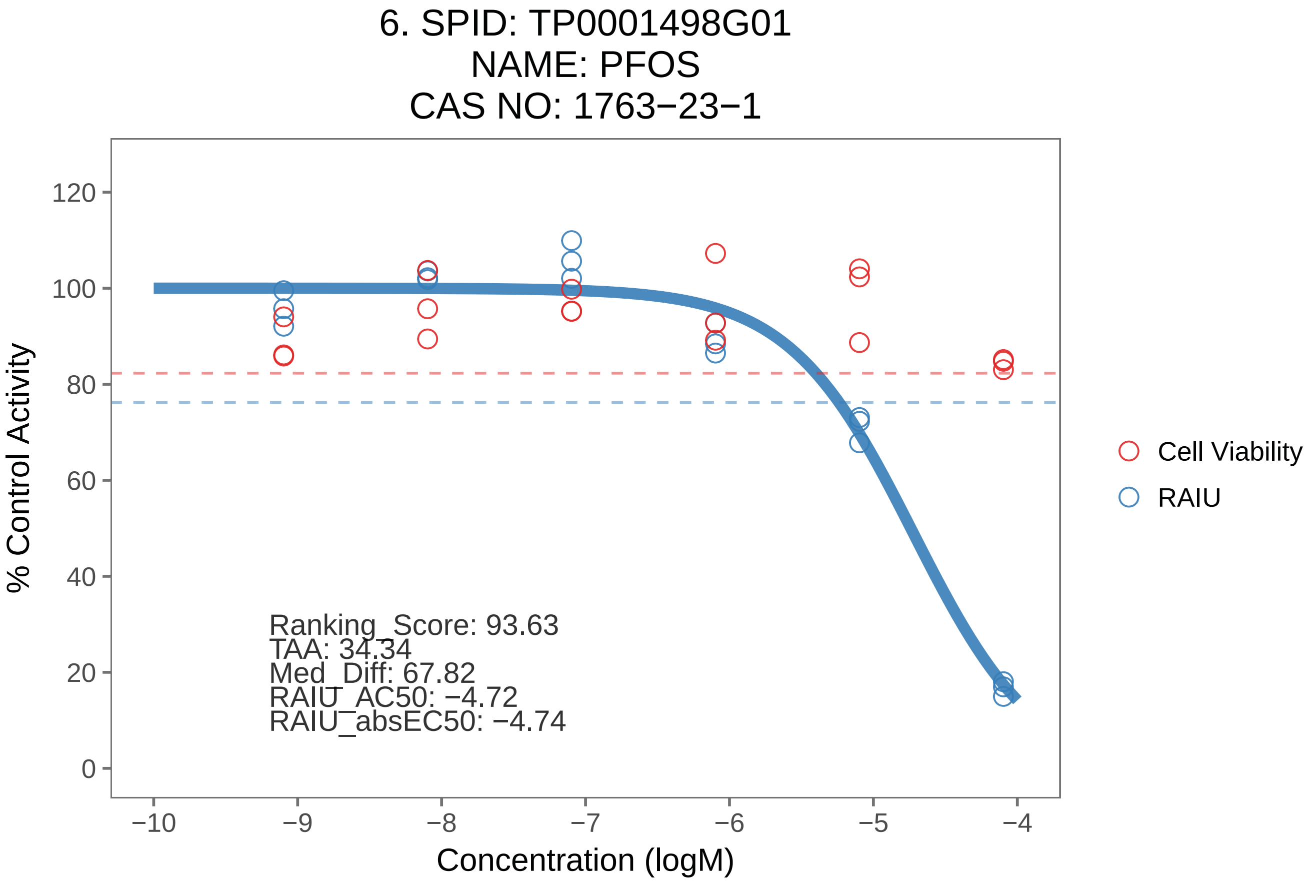

1. SPID: TP0001500G04
NAME: Etoxazole
CAS NO: 153233−91−1
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 150.41
TAA: 117.08
Med_Diff: 69.73
RAIU_AC50: −5.92
RAIU_absEC50: −5.88
Cell Viability
RAIU

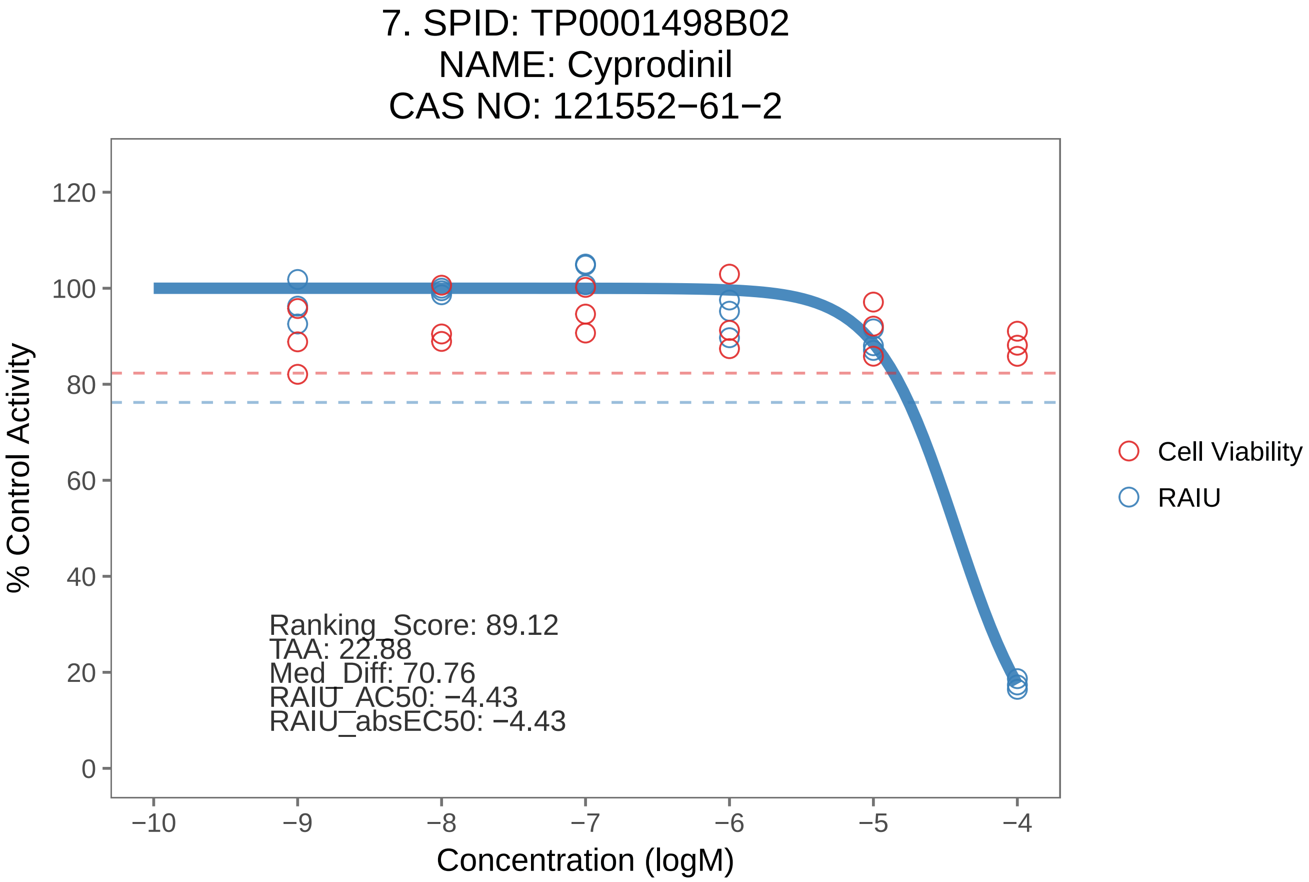

2. SPID: TP0001502E10
NAME: Triphenyltin hydroxide
CAS NO: 76−87−9
% Control Activity
120
100
80
60
40
20
0
Ranking_Score: 114.7
TAA: 78.91
Med_Diff: 59.75
RAIU_AC50: −5.39
RAIU_absEC50: −5.39
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU

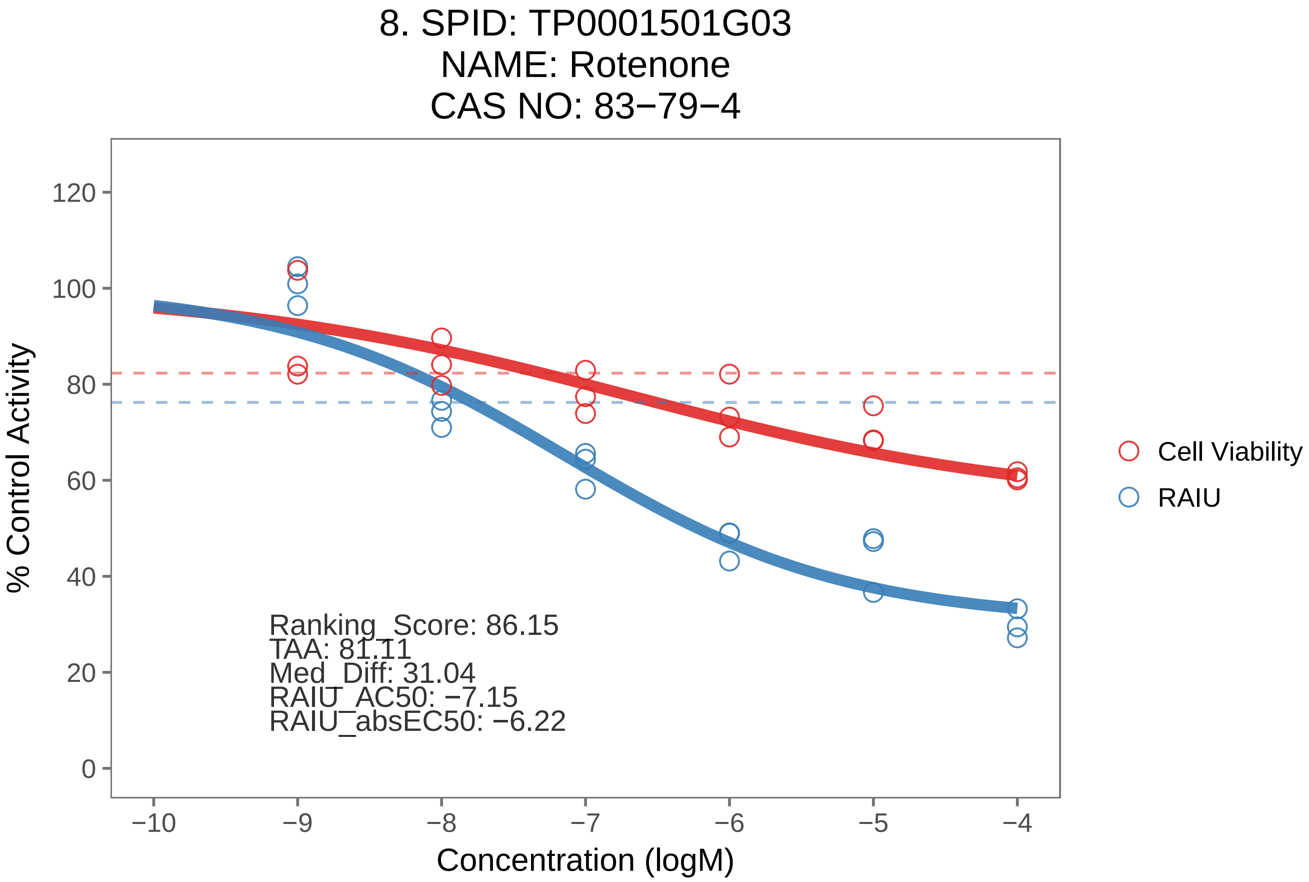

3. SPID: TP0001501D03
NAME: Niclosamide
CAS NO: 50−65−7
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 109.38
TAA: 111.12
Med_Diff: 34.25
RAIU_AC50: −6.95
RAIU_absEC50: −6.79
Cell Viability
RAIU


4. SPID: TP0001502G01
NAME: 3−Iodo−2−propynyl−N−butylcarbamate
CAS NO: 55406−53−6
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 107.61
TAA: 70.75
Med_Diff: 58.13
RAIU_AC50: −5.09
RAIU_absEC50: −5.3

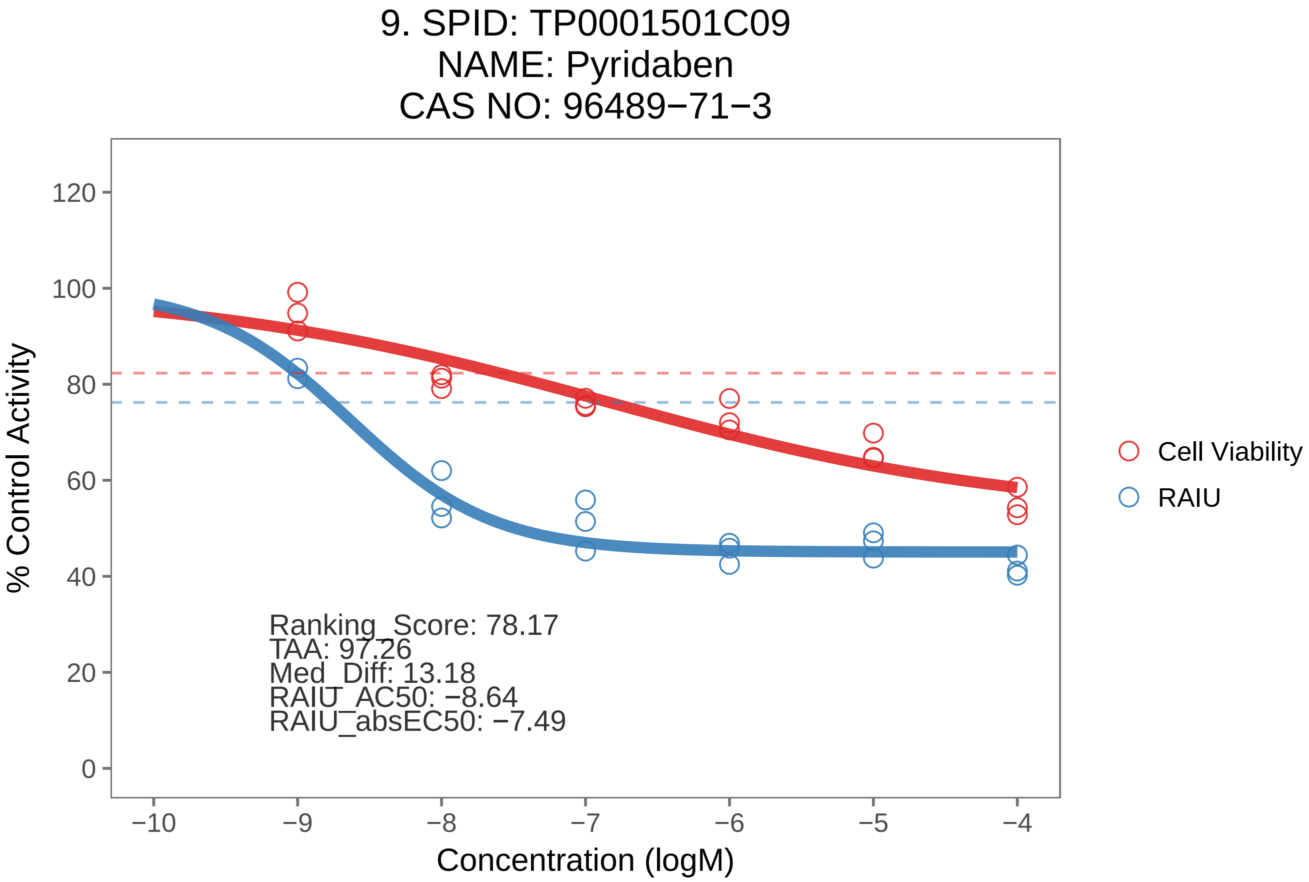

5. SPID: TP0001501E07
NAME: PFOS
CAS NO: 1763−23−1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 94.75
TAA: 36.81
Med_Diff: 67.33
RAIU_AC50: −4.75
RAIU_absEC50: −4.78
Cell Viability
RAIU

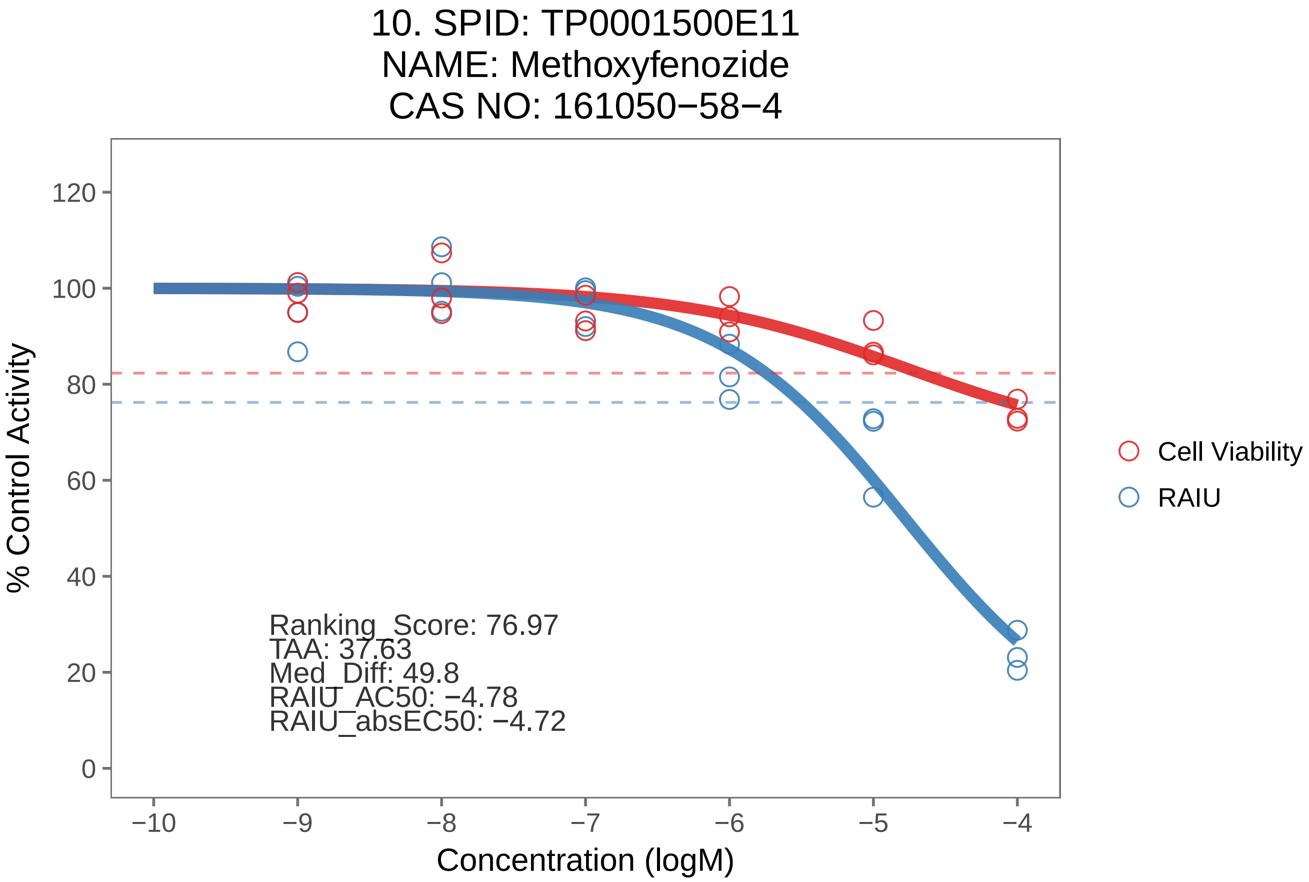

6. SPID: TP0001498G01
NAME: PFOS
CAS NO: 1763−23−1
% Control Activity
Concentration (logM)
Ranking_Score: 93.63
TAA: 34.34
Med_Diff: 67.82
RAIU_AC50: −4.72
RAIU_absEC50: −4.74
Cell Viability
RAIU
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

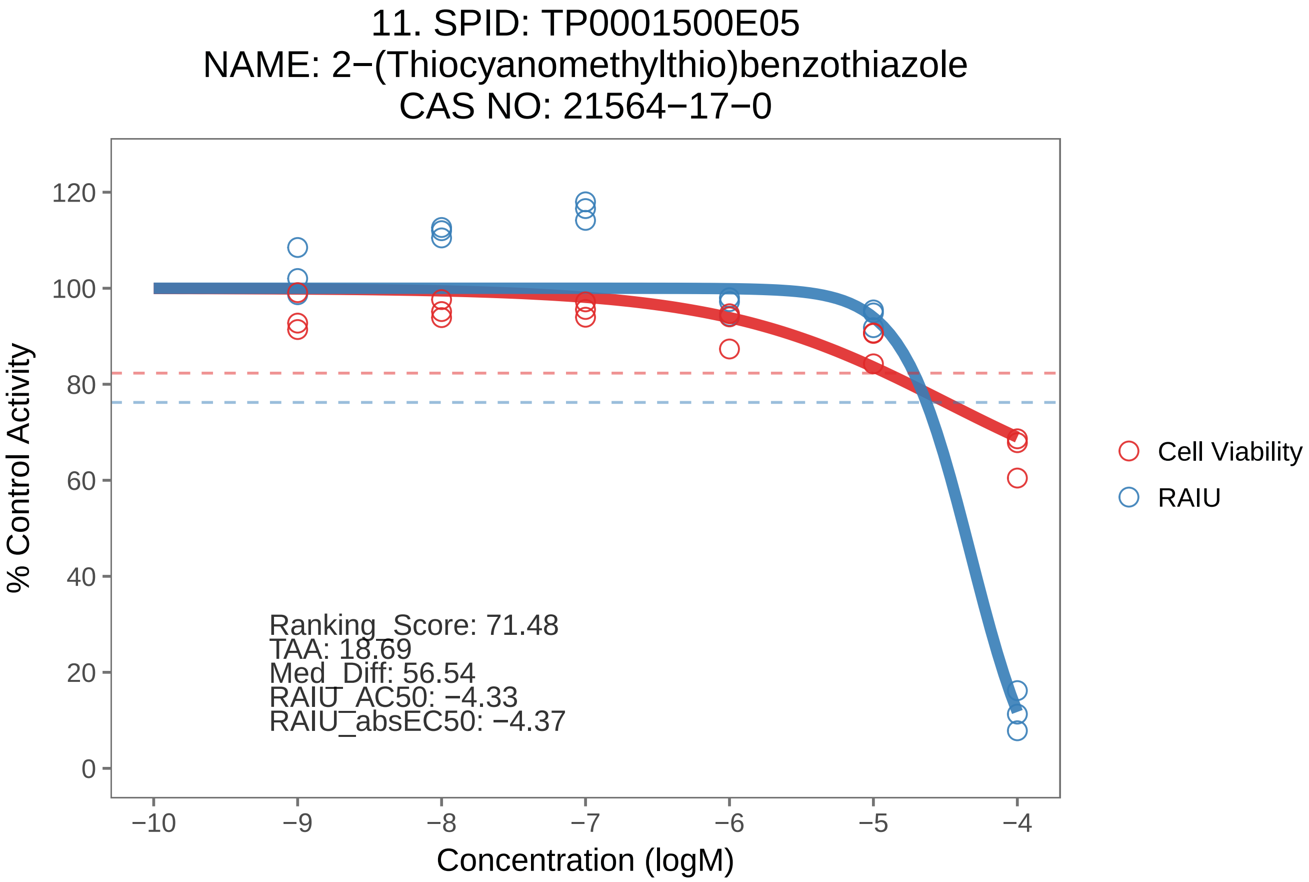

7. SPID: TP0001498B02
NAME: Cyprodinil
CAS NO: 121552−61−2
% Control Activity
0
20
40
60
80
100
120
Concentration (logM)
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 89.12
TAA: 22.88
Med_Diff: 70.76
RAIU_AC50: −4.43
RAIU_absEC50: −4.43
Cell Viability
RAIU

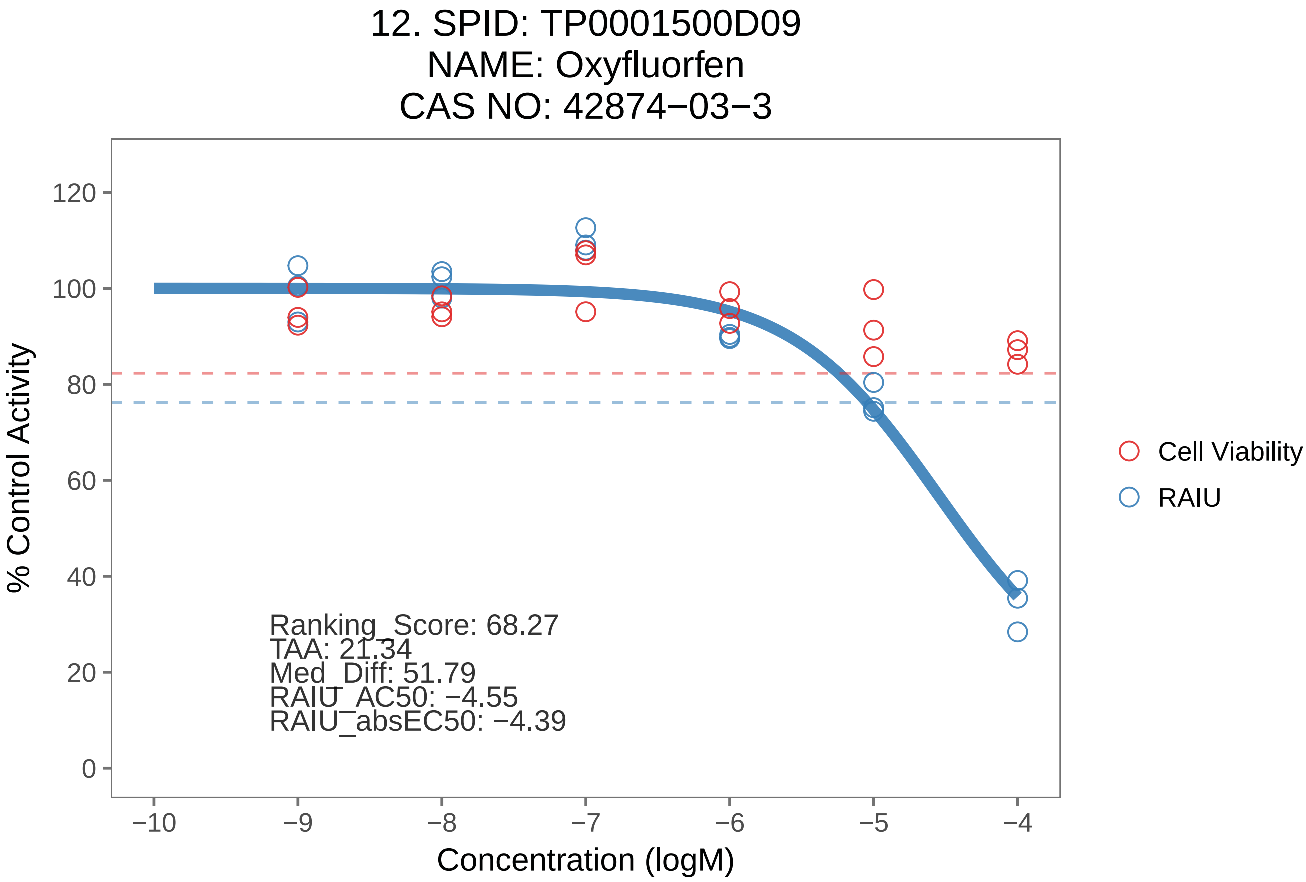


8. SPID: TP0001501G03
NAME: Rotenone
CAS NO: 83−79−4
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 86.15
TAA: 81.11
Med_Diff: 31.04
RAIU_AC50: −7.15
RAIU_absEC50: −6.22

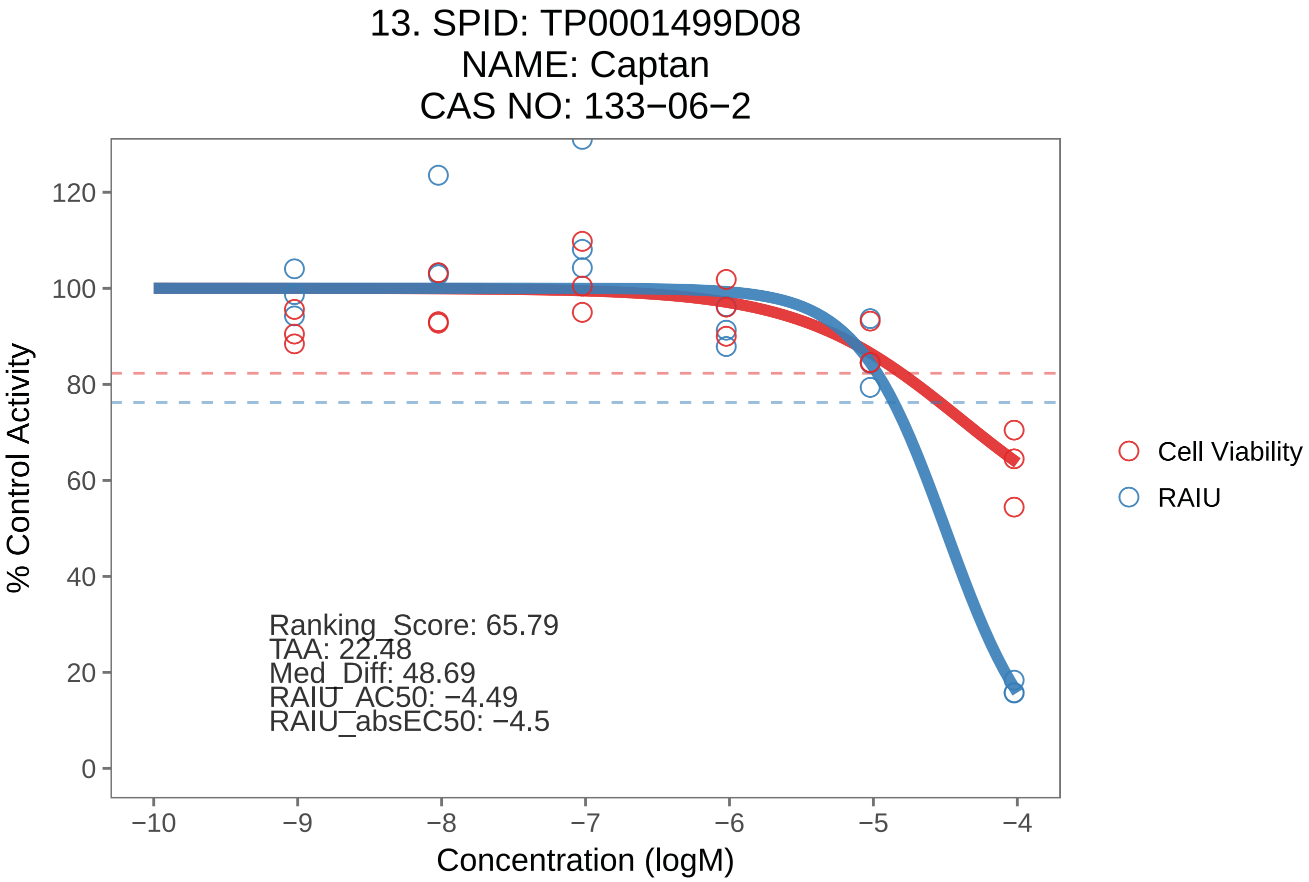

9. SPID: TP0001501C09
NAME: Pyridaben
CAS NO: 96489−71−3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 78.17
TAA: 97.26
Med_Diff: 13.18
RAIU_AC50: −8.64
RAIU_absEC50: −7.49

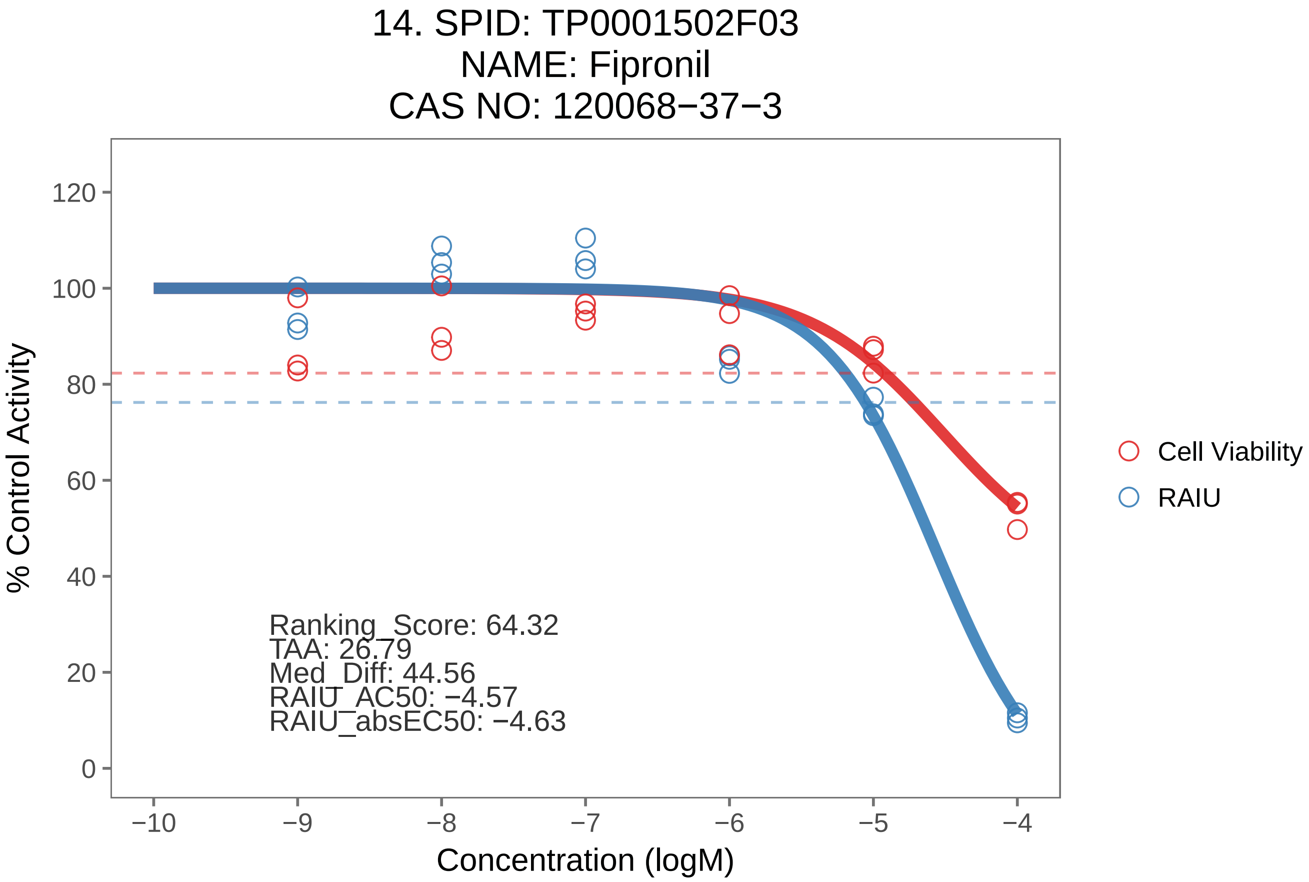

10. SPID: TP0001500E11
NAME: Methoxyfenozide
CAS NO: 161050−58−4
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 76.97
TAA: 37.63
Med_Diff: 49.8
RAIU_AC50: −4.78
RAIU_absEC50: −4.72
Cell Viability
RAIU

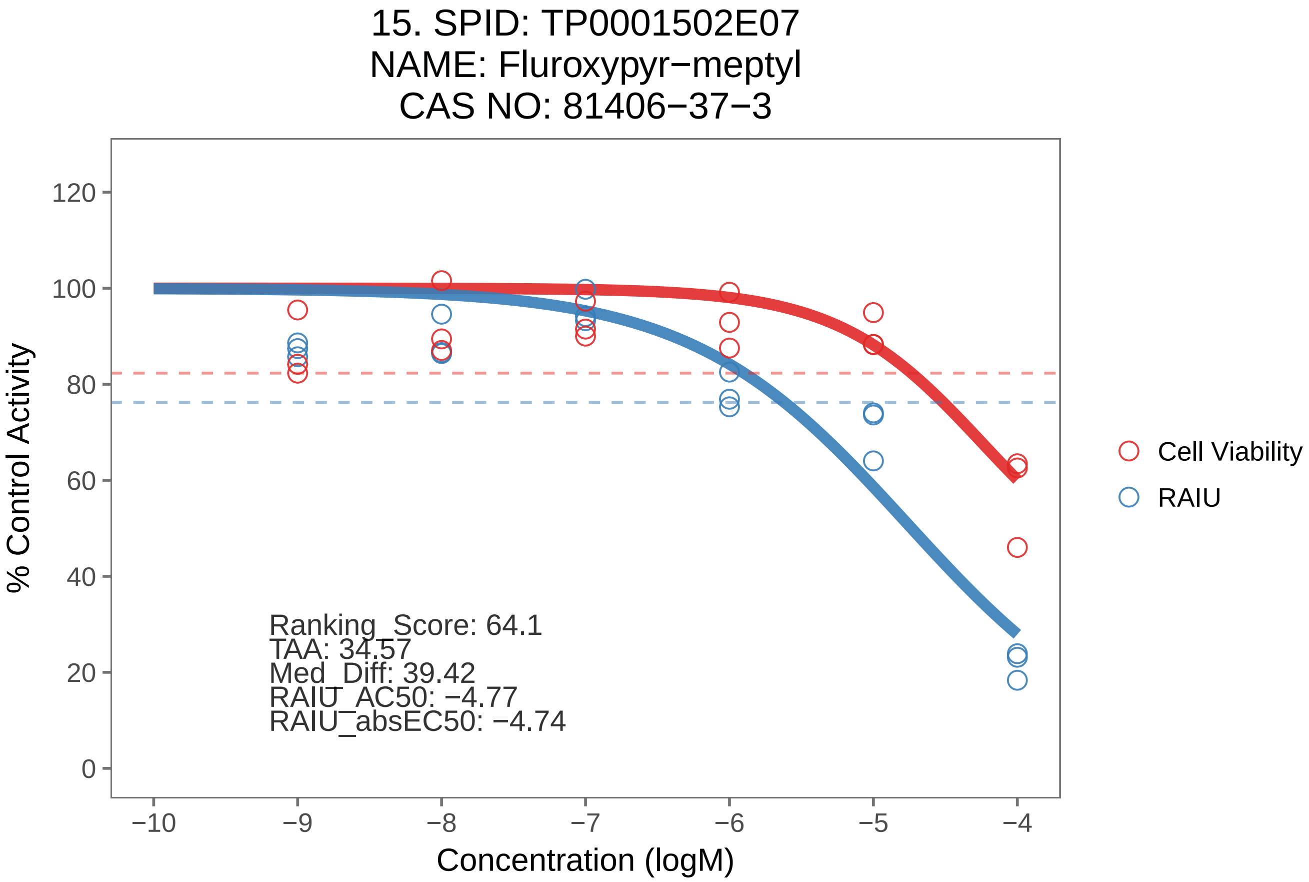

11. SPID: TP0001500E05
NAME: 2−(Thiocyanomethylthio)benzothiazole
CAS NO: 21564−17−0
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 71.48
TAA: 18.69
Med_Diff: 56.54
RAIU_AC50: −4.33
RAIU_absEC50: −4.37
Cell Viability
RAIU

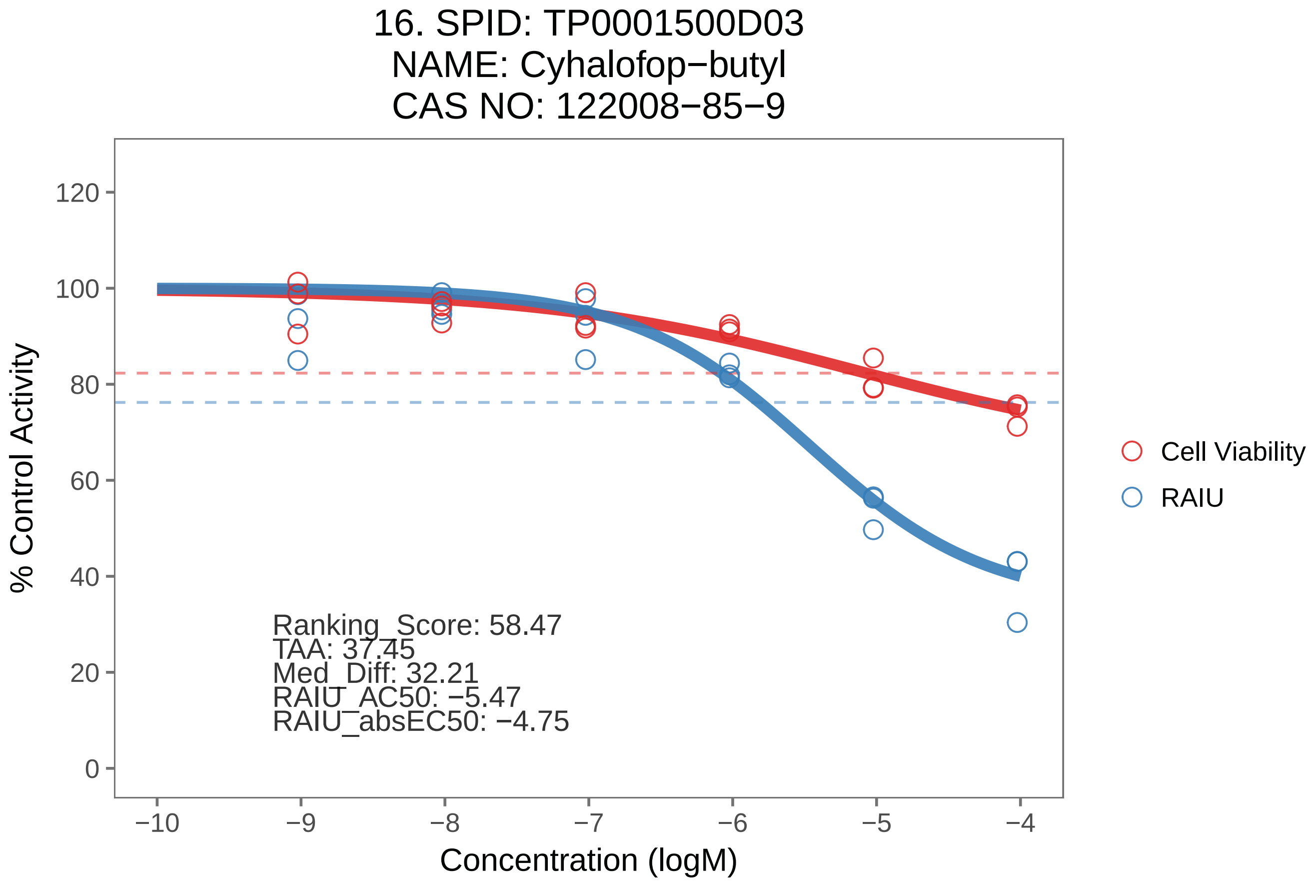


12. SPID: TP0001500D09
NAME: Oxyfluorfen
CAS NO: 42874−03−3
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 68.27
TAA: 21.34
Med_Diff: 51.79
RAIU_AC50: −4.55
RAIU_absEC50: −4.39
Cell Viability
RAIU

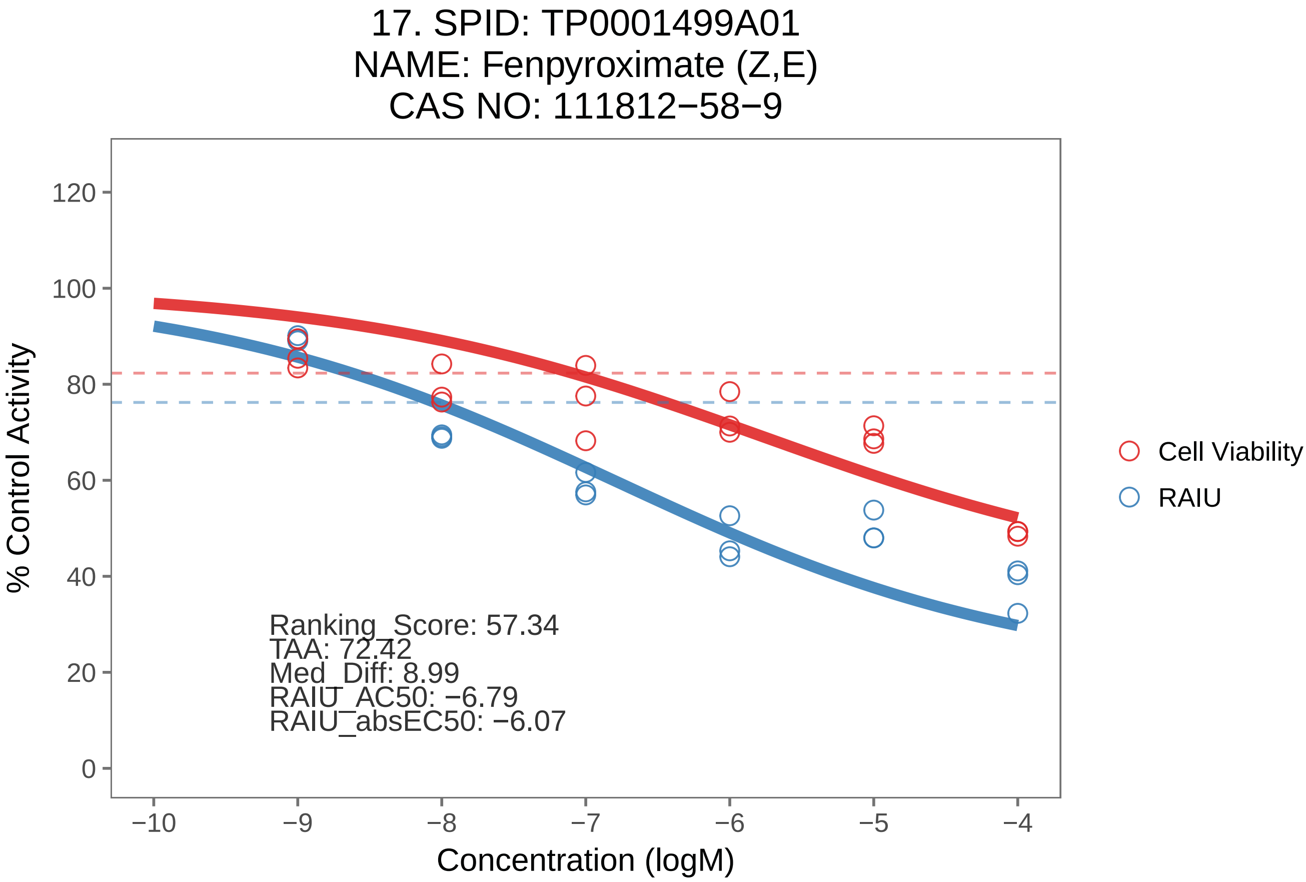

13. SPID: TP0001499D08
NAME: Captan
CAS NO: 133−06−2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 65.79
TAA: 22.48
Med_Diff: 48.69
RAIU_AC50: −4.49
RAIU_absEC50: −4.5
Cell Viability
RAIU

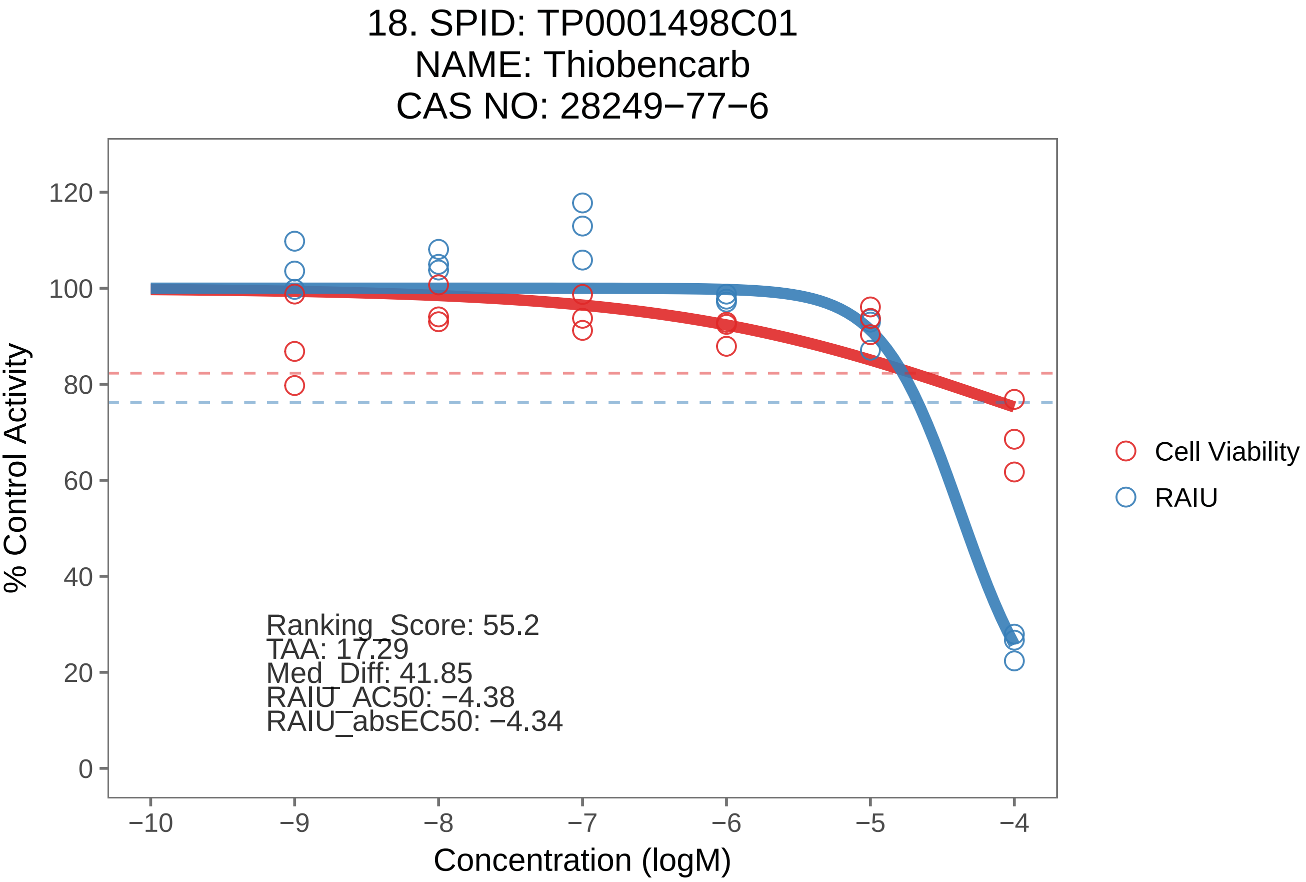

14. SPID: TP0001502F03
NAME: Fipronil
CAS NO: 120068−37−3
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 64.32
TAA: 26.79
Med_Diff: 44.56
RAIU_AC50: −4.57
RAIU_absEC50: −4.63
Cell Viability
RAIU


15. SPID: TP0001502E07
NAME: Fluroxypyr−meptyl
CAS NO: 81406−37−3
% Control Activity
0
20
40
60
80
100
120
Concentration (logM)
−10
−9
−8
−7
−6
−5
−4
Cell Viability
RAIU
Ranking_Score: 64.1
TAA: 34.57
Med_Diff: 39.42
RAIU_AC50: −4.77
RAIU_absEC50: −4.74

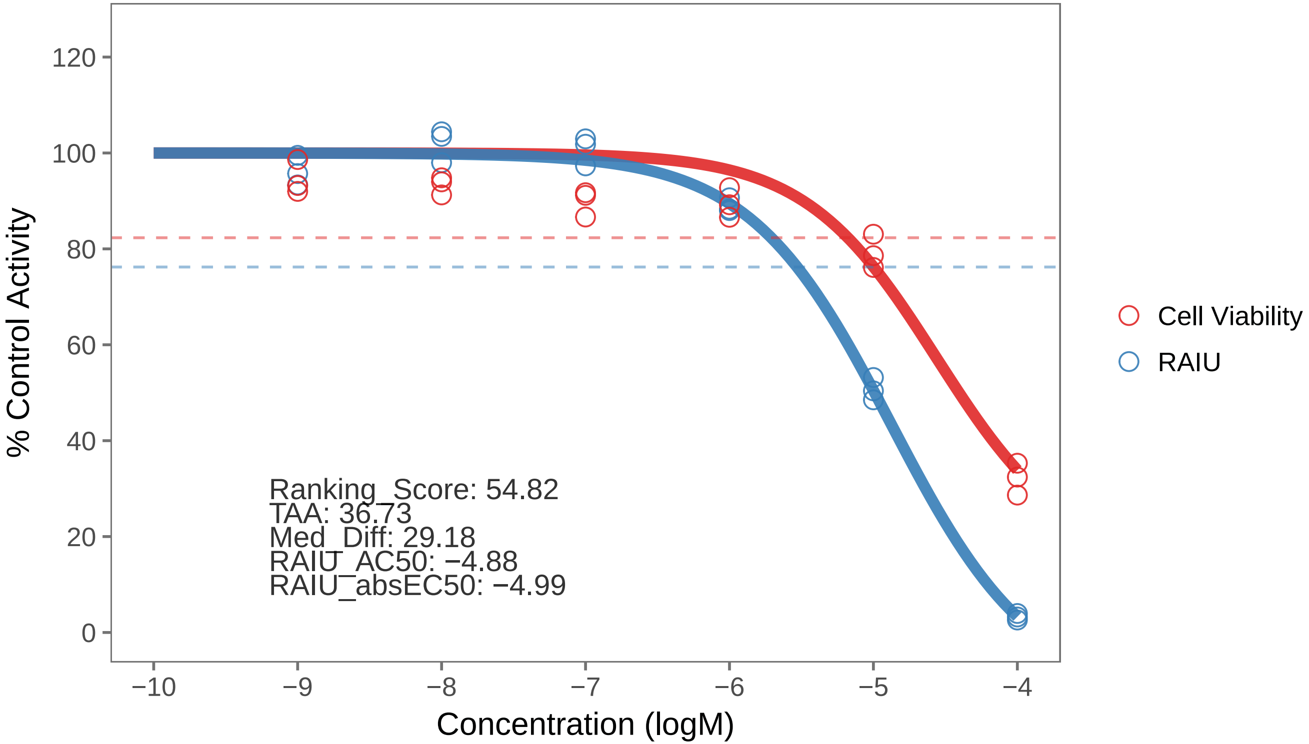


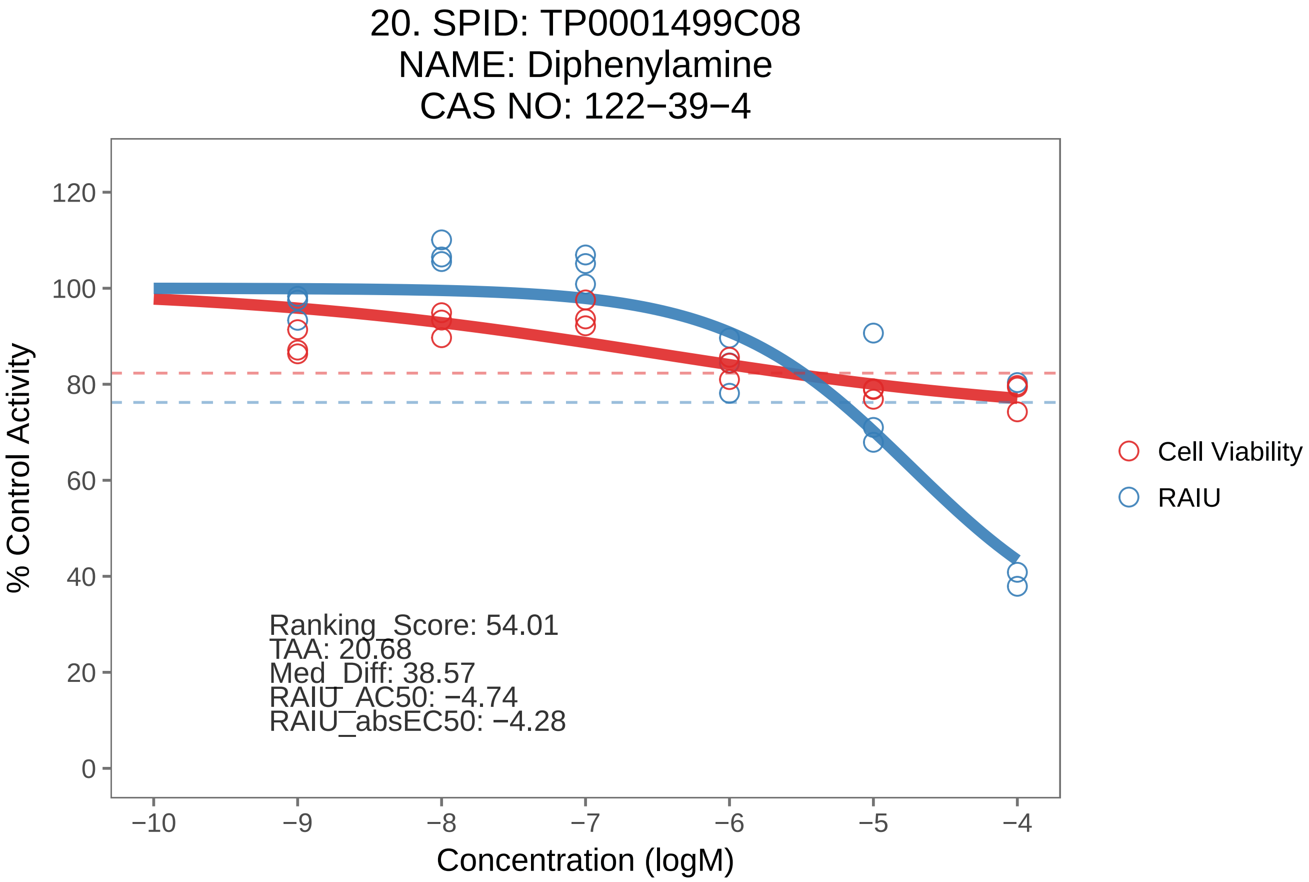
16. SPID: TP0001500D03
NAME: Cyhalofop−butyl
CAS NO: 122008−85−9
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 58.47
TAA: 37.45
Med_Diff: 32.21
RAIU_AC50: −5.47
RAIU_absEC50: −4.75
Cell Viability
RAIU

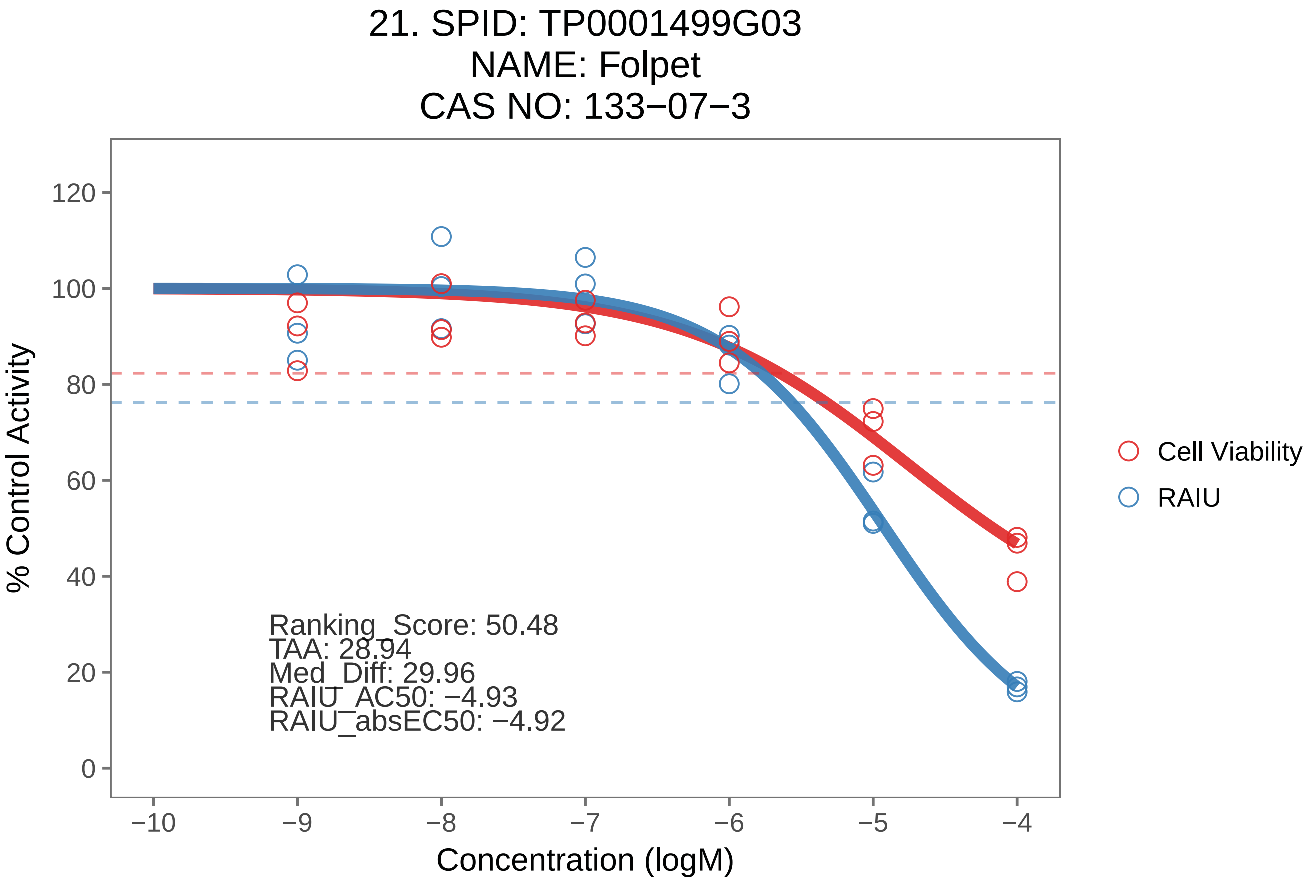

17. SPID: TP0001499A01
NAME: Fenpyroximate (Z,E)
CAS NO: 111812−58−9
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 57.34
TAA: 72.42
Med_Diff: 8.99
RAIU_AC50: −6.79
RAIU_absEC50: −6.07

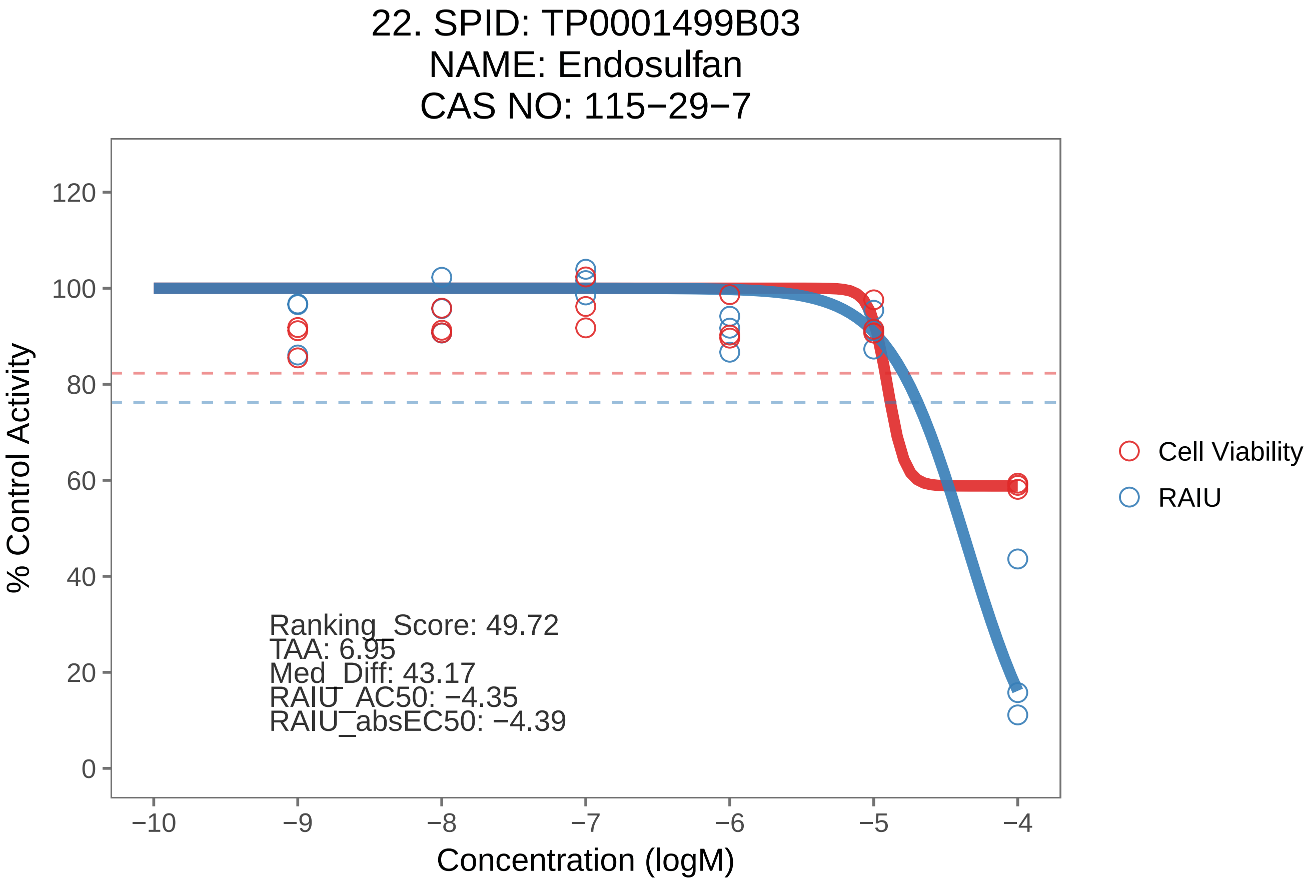

18. SPID: TP0001498C01
NAME: Thiobencarb
CAS NO: 28249−77−6
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 55.2
TAA: 17.29
Med_Diff: 41.85
RAIU_AC50: −4.38
RAIU_absEC50: −4.34

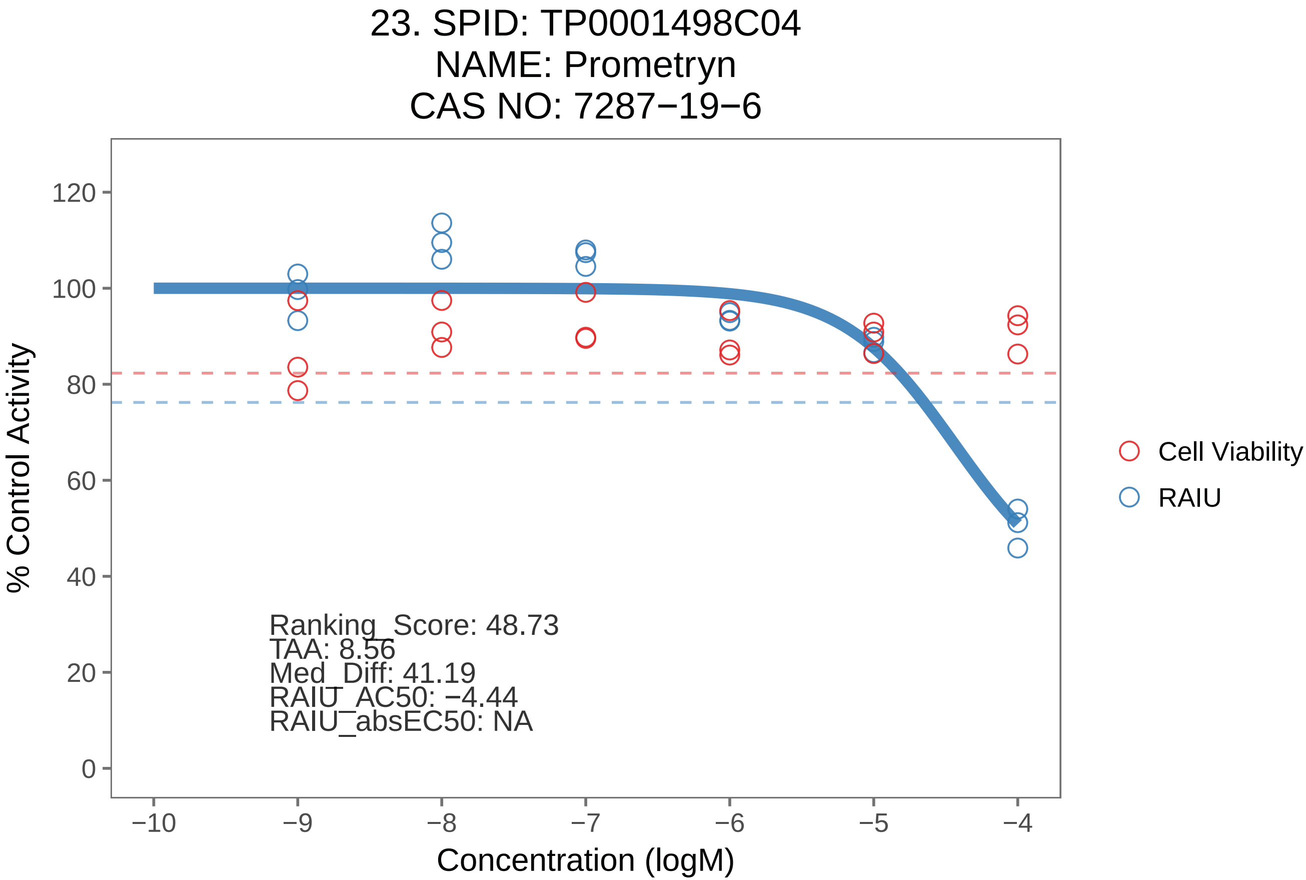
19. SPID: TP0001500E07
NAME: Emamectin benzoate
CAS NO: 155569−91−8

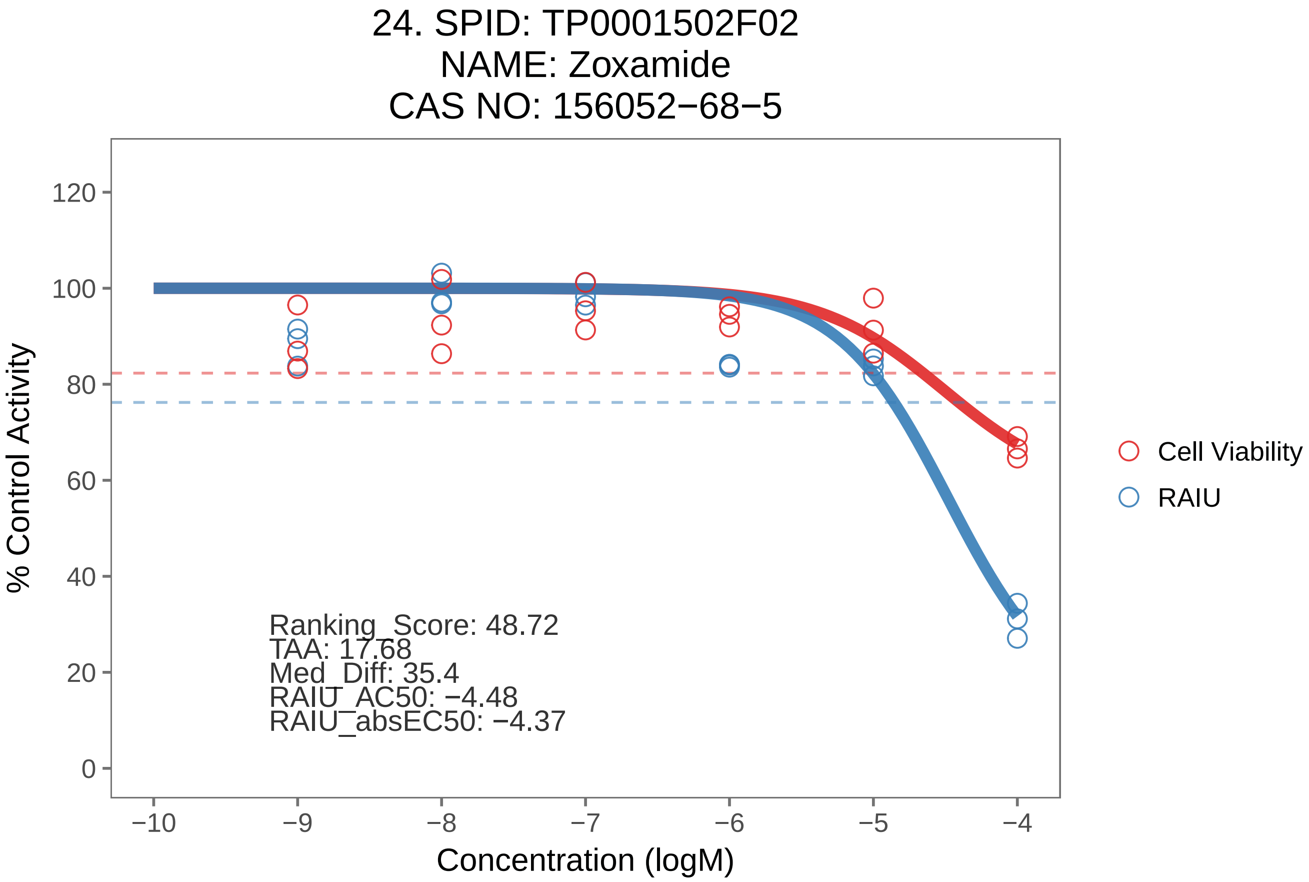


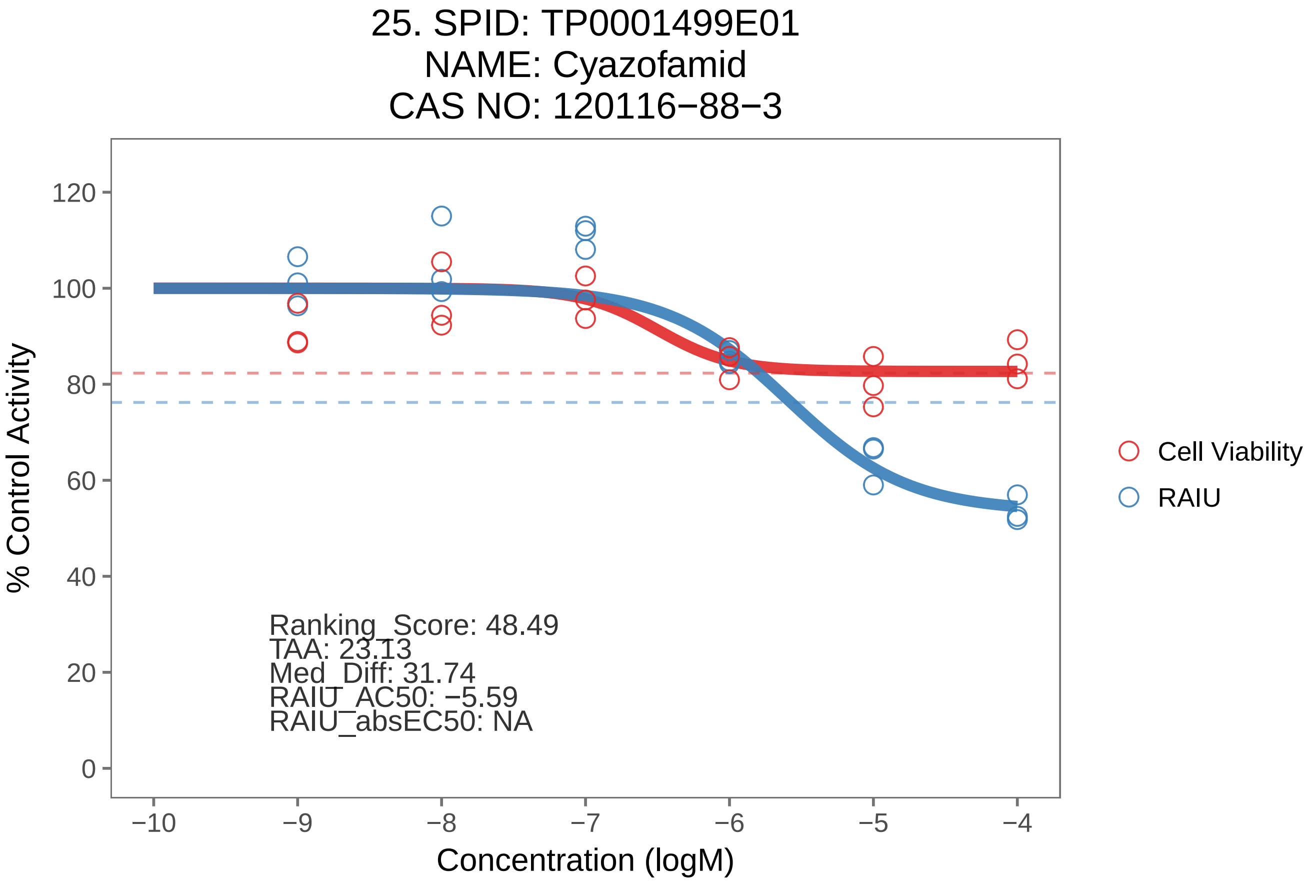

20. SPID: TP0001499C08
NAME: Diphenylamine
CAS NO: 122−39−4
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Cell Viability
RAIU
Ranking_Score: 54.01
TAA: 20.68
Med_Diff: 38.57
RAIU_AC50: −4.74
RAIU_absEC50: −4.28

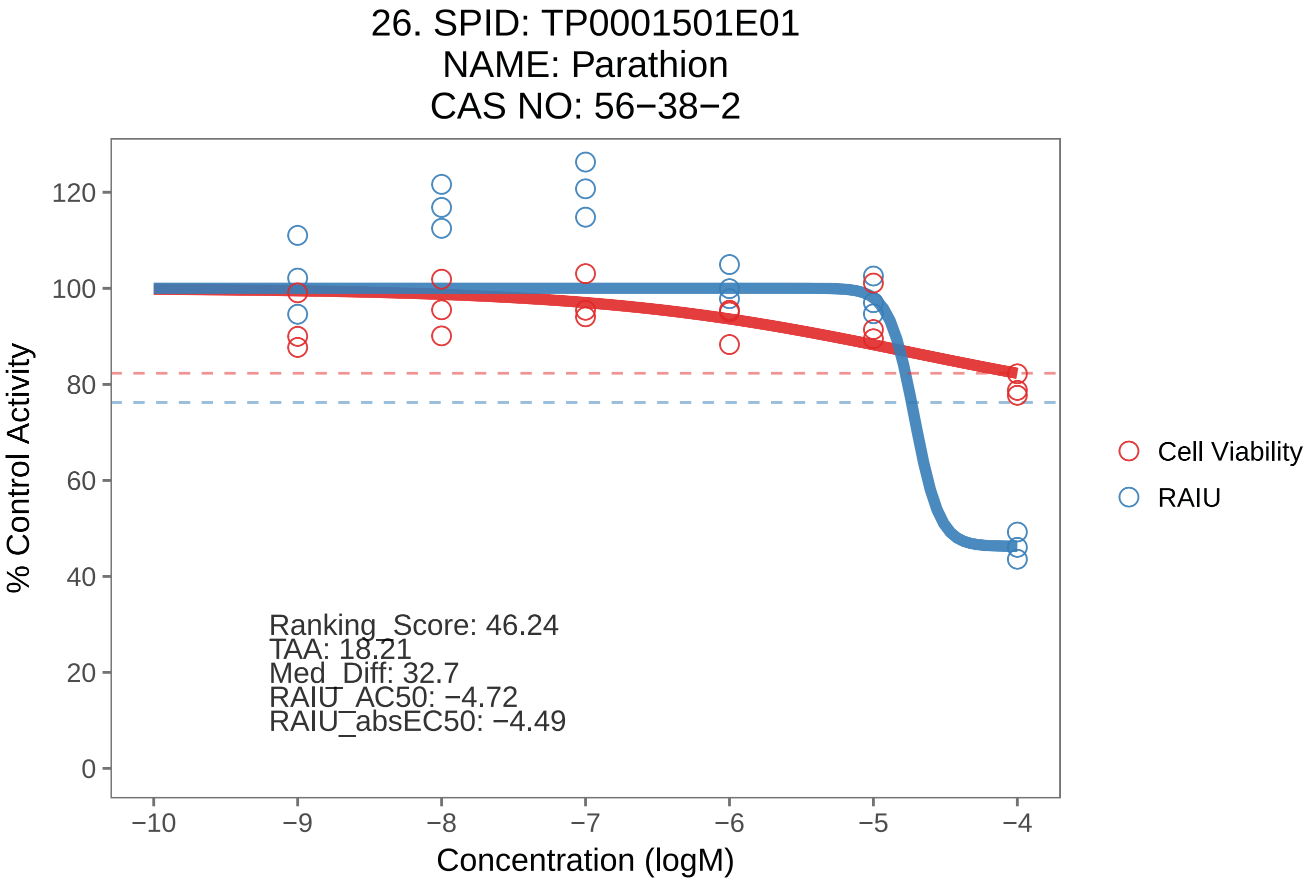

21. SPID: TP0001499G03
NAME: Folpet
CAS NO: 133−07−3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 50.48
TAA: 28.94
Med_Diff: 29.96
RAIU_AC50: −4.93
RAIU_absEC50: −4.92
Cell Viability
RAIU

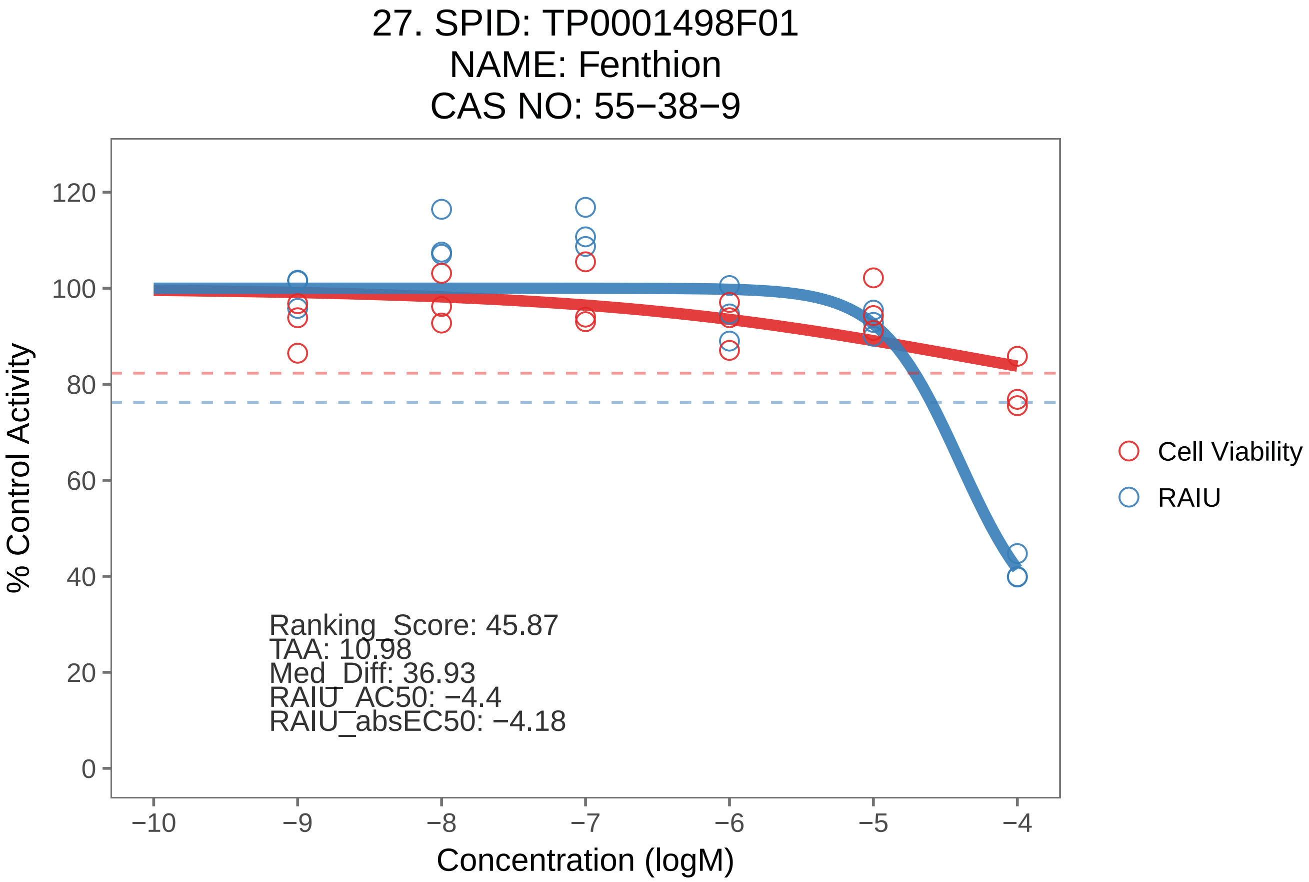

22. SPID: TP0001499B03
NAME: Endosulfan
CAS NO: 115−29−7
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 49.72
TAA: 6.95
Med_Diff: 43.17
RAIU_AC50: −4.35
RAIU_absEC50: −4.39
Cell Viability
RAIU

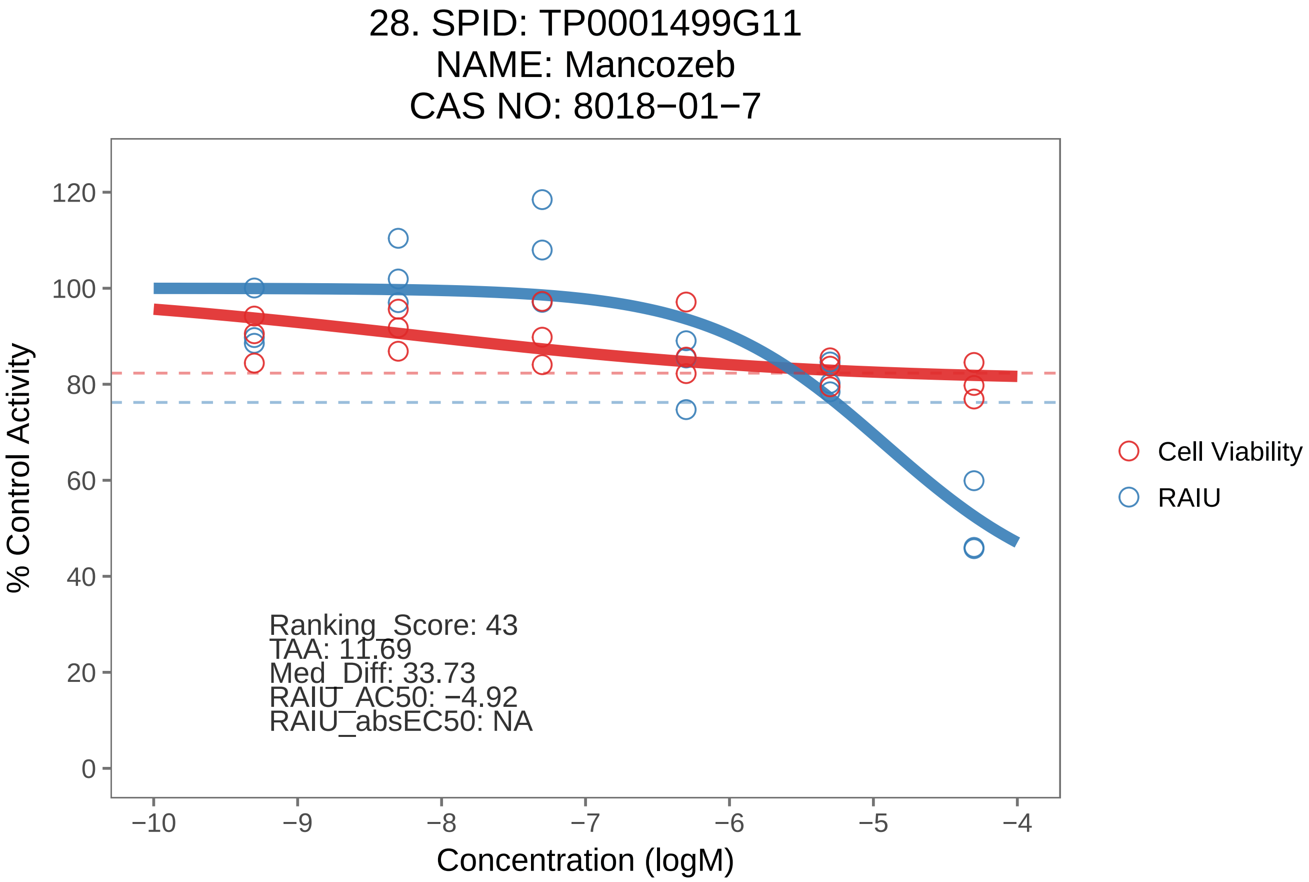

23. SPID: TP0001498C04
NAME: Prometryn
CAS NO: 7287−19−6
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 48.73
TAA: 8.56
Med_Diff: 41.19
RAIU_AC50: −4.44
RAIU_absEC50: NA
Cell Viability
RAIU

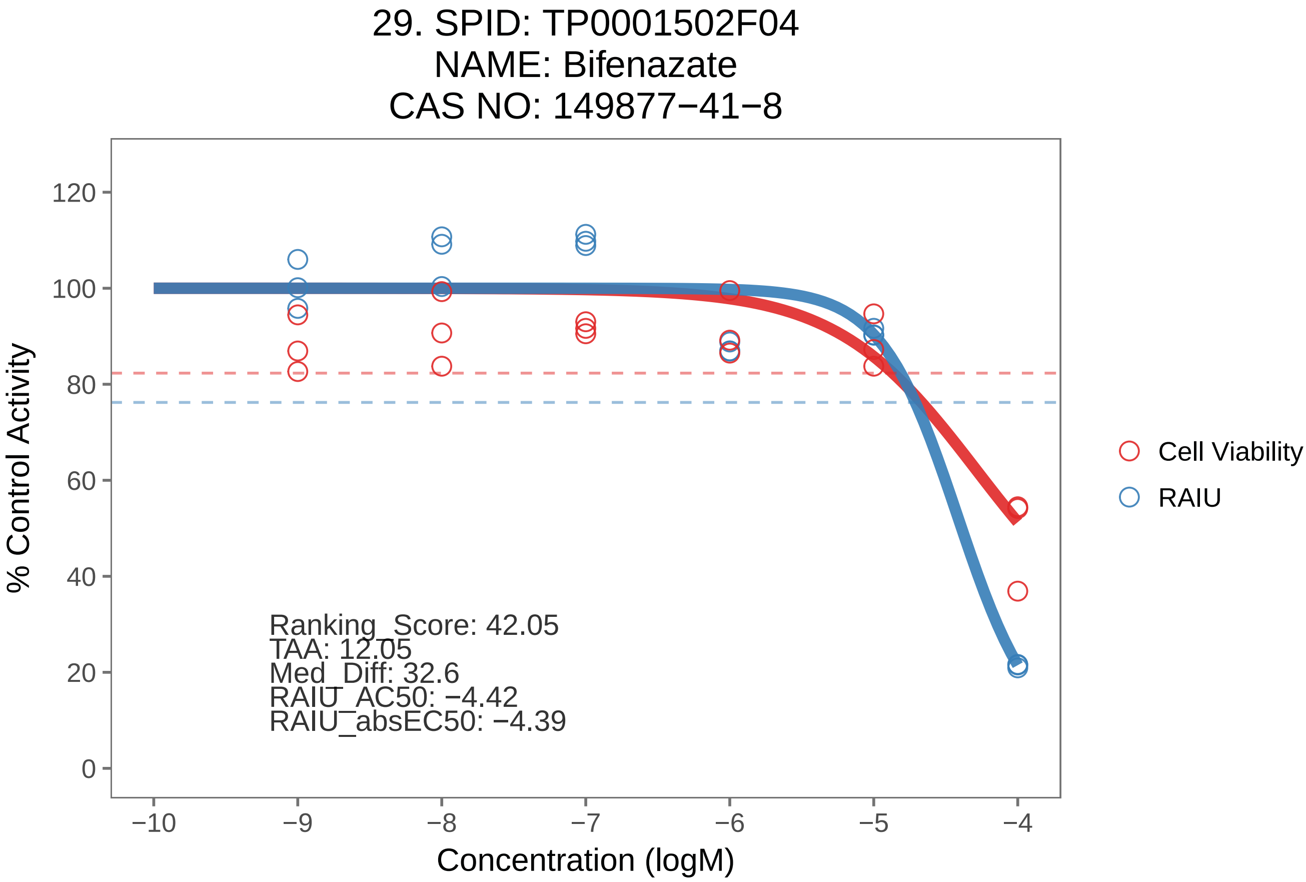

24. SPID: TP0001502F02
NAME: Zoxamide
CAS NO: 156052−68−5
% Control Activity
0
20
40
60
80
100
120
Ranking_Score: 48.72
TAA: 17.68
Med_Diff: 35.4
RAIU_AC50: −4.48
RAIU_absEC50: −4.37
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU

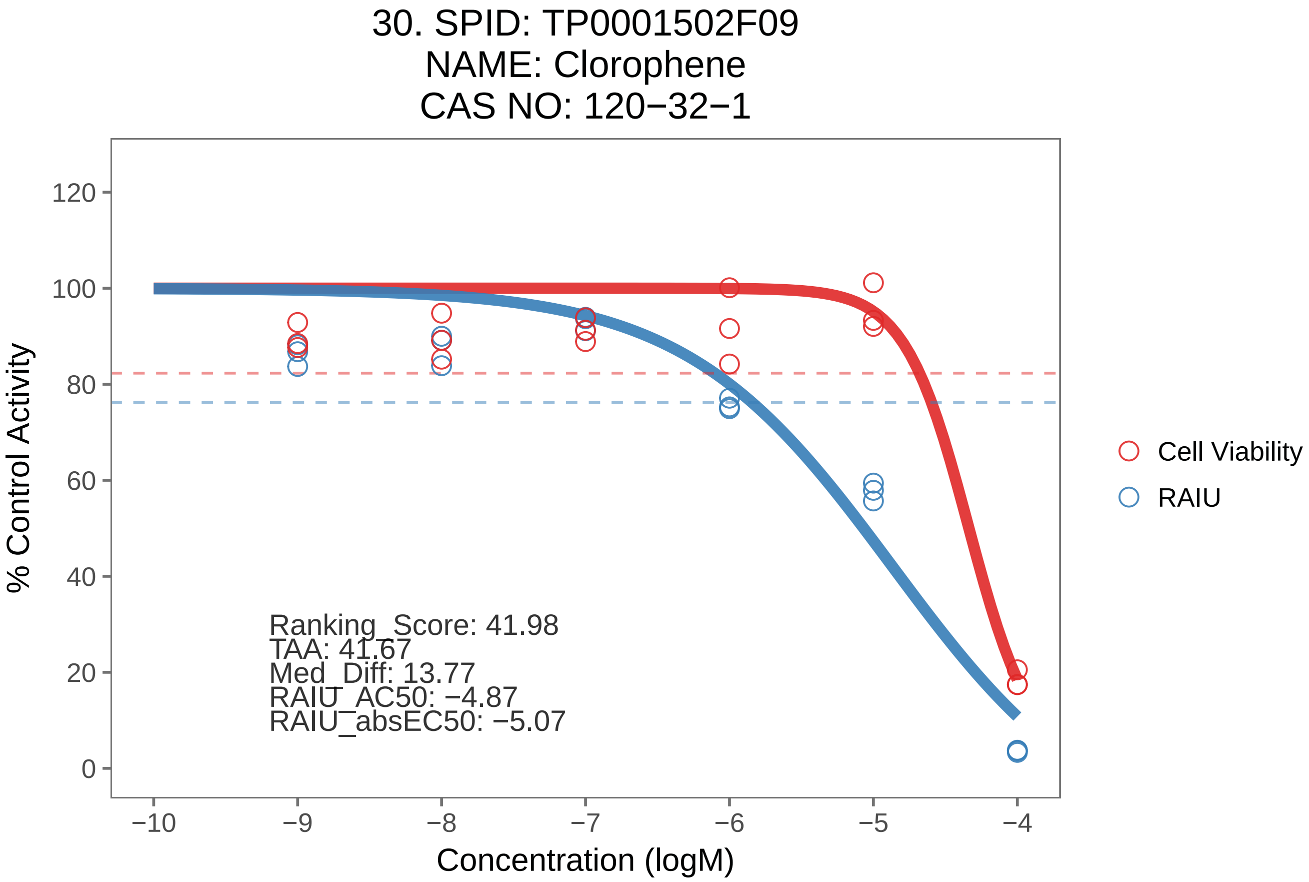

25. SPID: TP0001499E01
NAME: Cyazofamid
CAS NO: 120116−88−3
120
100
80
60
40
20
0
% Control Activity
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 48.49
TAA: 23.13
Med_Diff: 31.74
RAIU_AC50: −5.59
RAIU_absEC50: NA
Cell Viability
RAIU

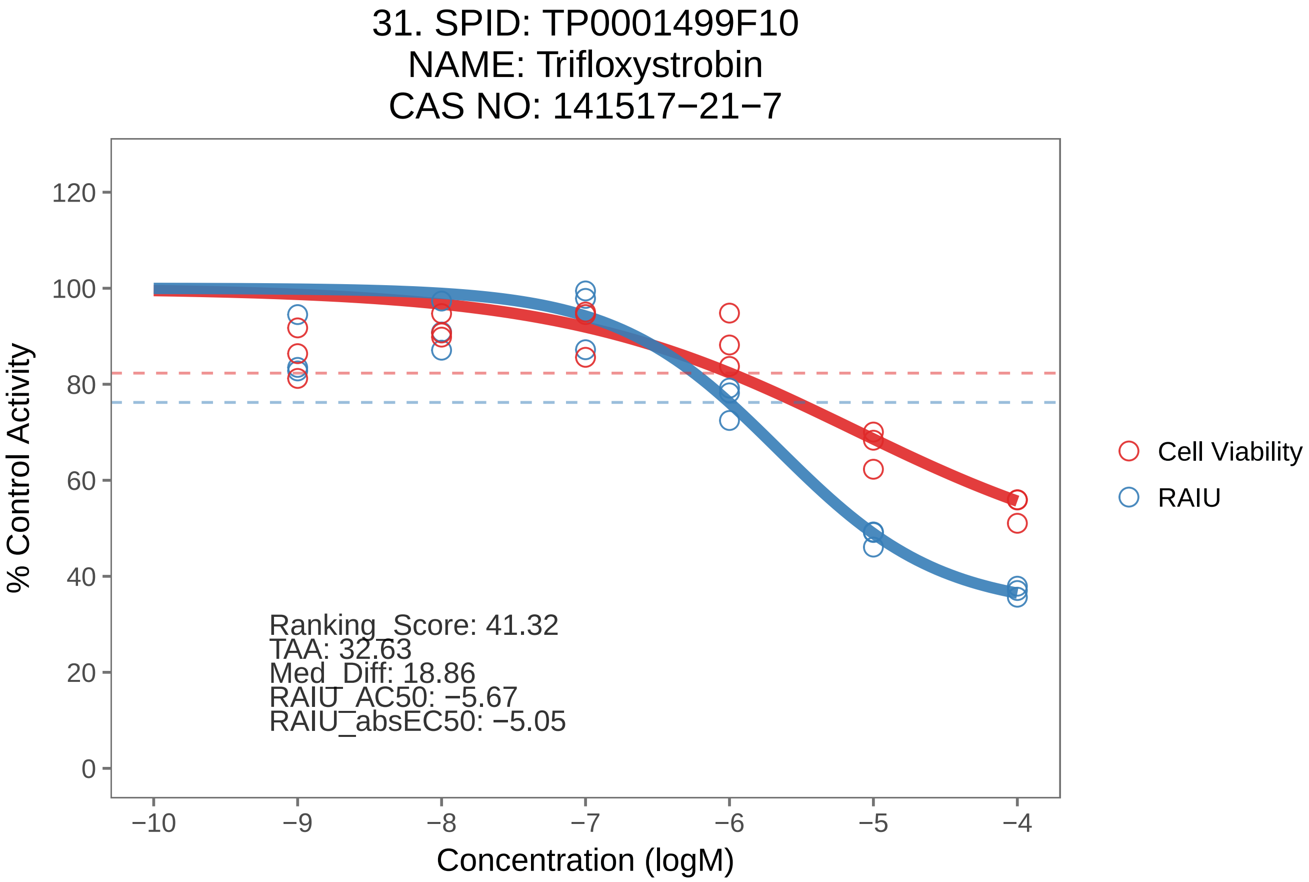

26. SPID: TP0001501E01
NAME: Parathion
CAS NO: 56−38−2
% Control Activity
0
20
40
60
80
100
120
Concentration (logM)
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 46.24
TAA: 18.21
Med_Diff: 32.7
RAIU_AC50: −4.72
RAIU_absEC50: −4.49
Cell Viability
RAIU


27. SPID: TP0001498F01
NAME: Fenthion
CAS NO: 55−38−9
% Control Activity
0
20
40
60
80
100
120
Concentration (logM)
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 45.87
TAA: 10.98
Med_Diff: 36.93
RAIU_AC50: −4.4
RAIU_absEC50: −4.18
Cell Viability
RAIU

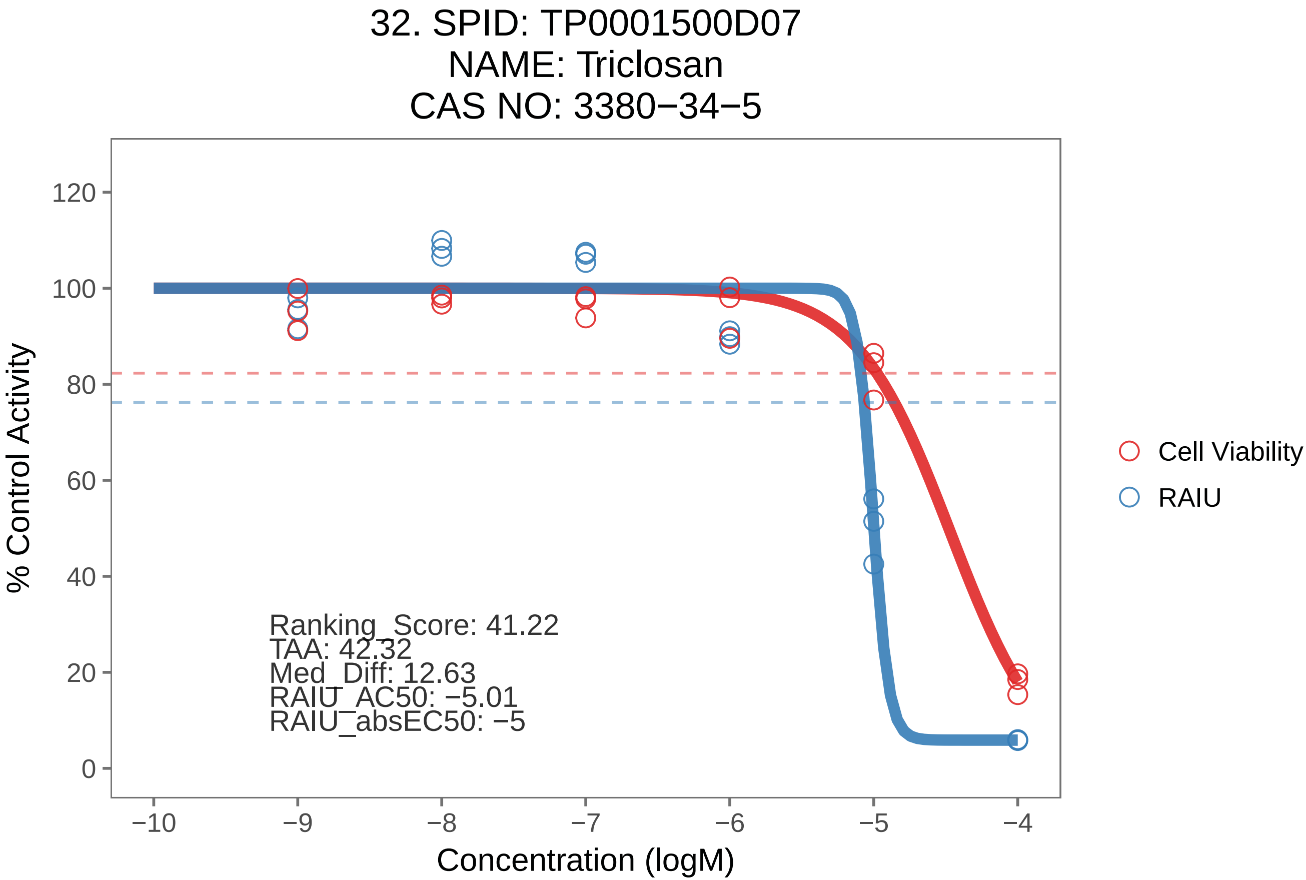

28. SPID: TP0001499G11
NAME: Mancozeb
CAS NO: 8018−01−7
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 43
TAA: 11.69
Med_Diff: 33.73
RAIU_AC50: −4.92
RAIU_absEC50: NA
Cell Viability
RAIU

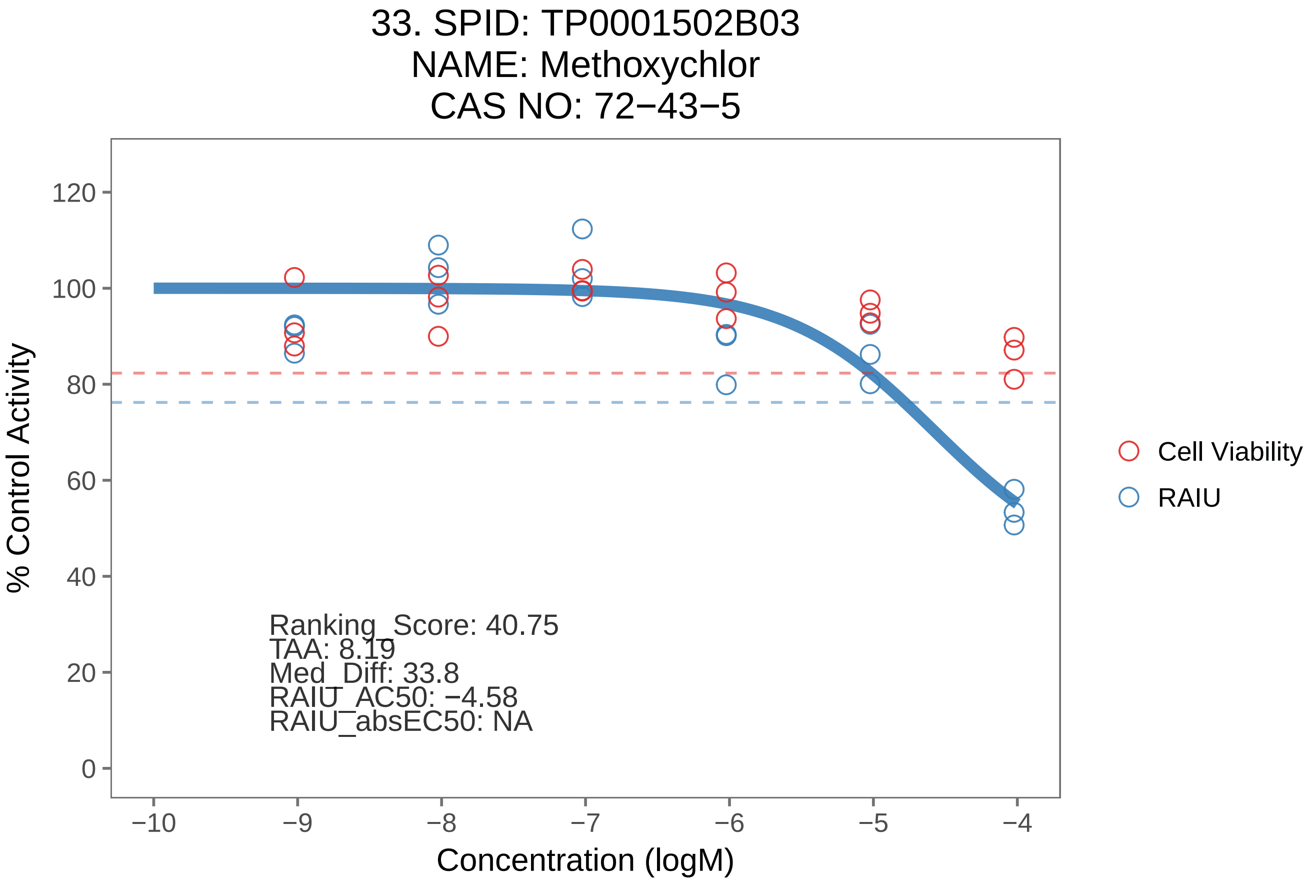

29. SPID: TP0001502F04
NAME: Bifenazate
CAS NO: 149877−41−8
Ranking_Score: 42.05
TAA: 12.05
Med_Diff: 32.6
RAIU_AC50: −4.42
RAIU_absEC50: −4.39
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU

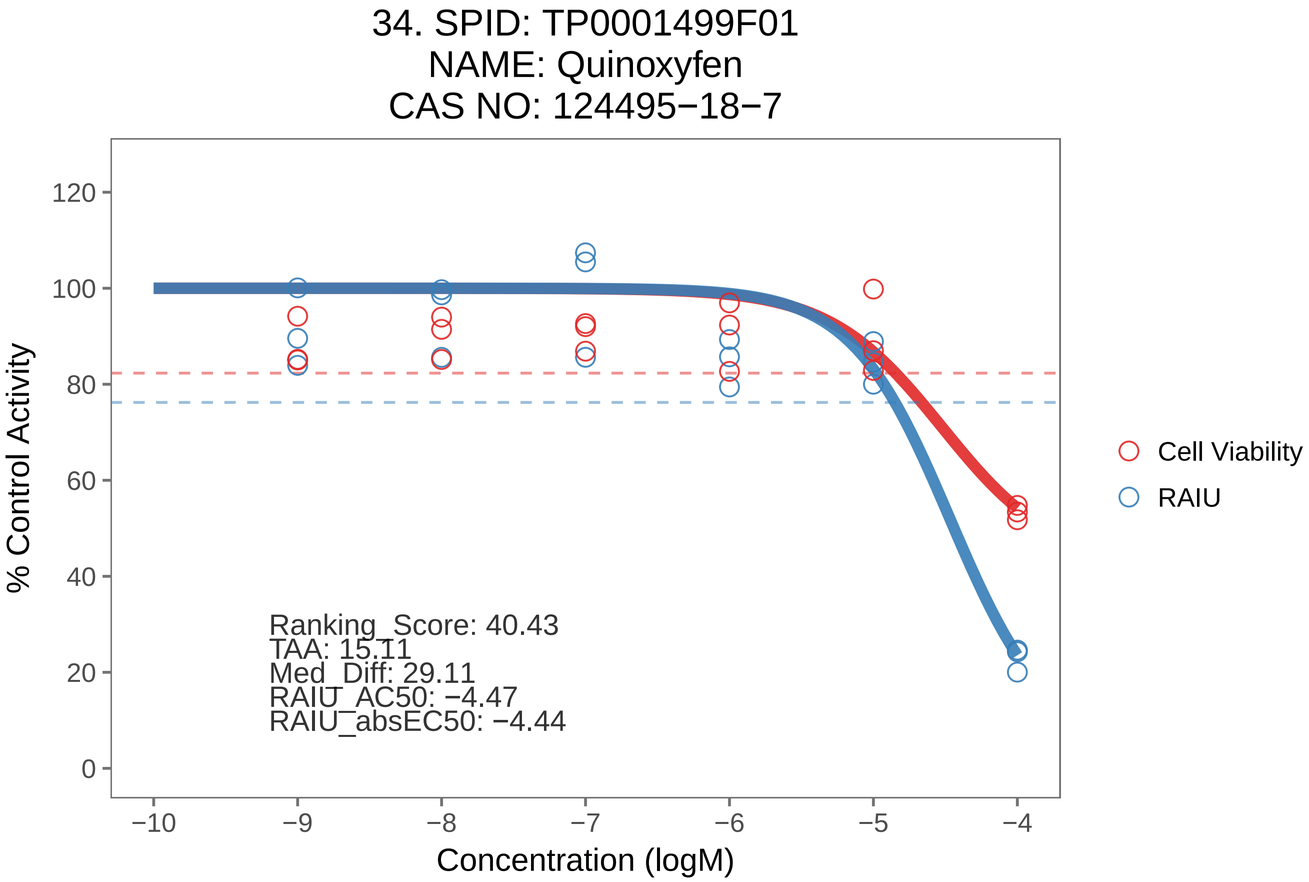

30. SPID: TP0001502F09
NAME: Clorophene
CAS NO: 120−32−1
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Cell Viability
RAIU
Ranking_Score: 41.98
TAA: 41.67
Med_Diff: 13.77
RAIU_AC50: −4.87
RAIU_absEC50: −5.07

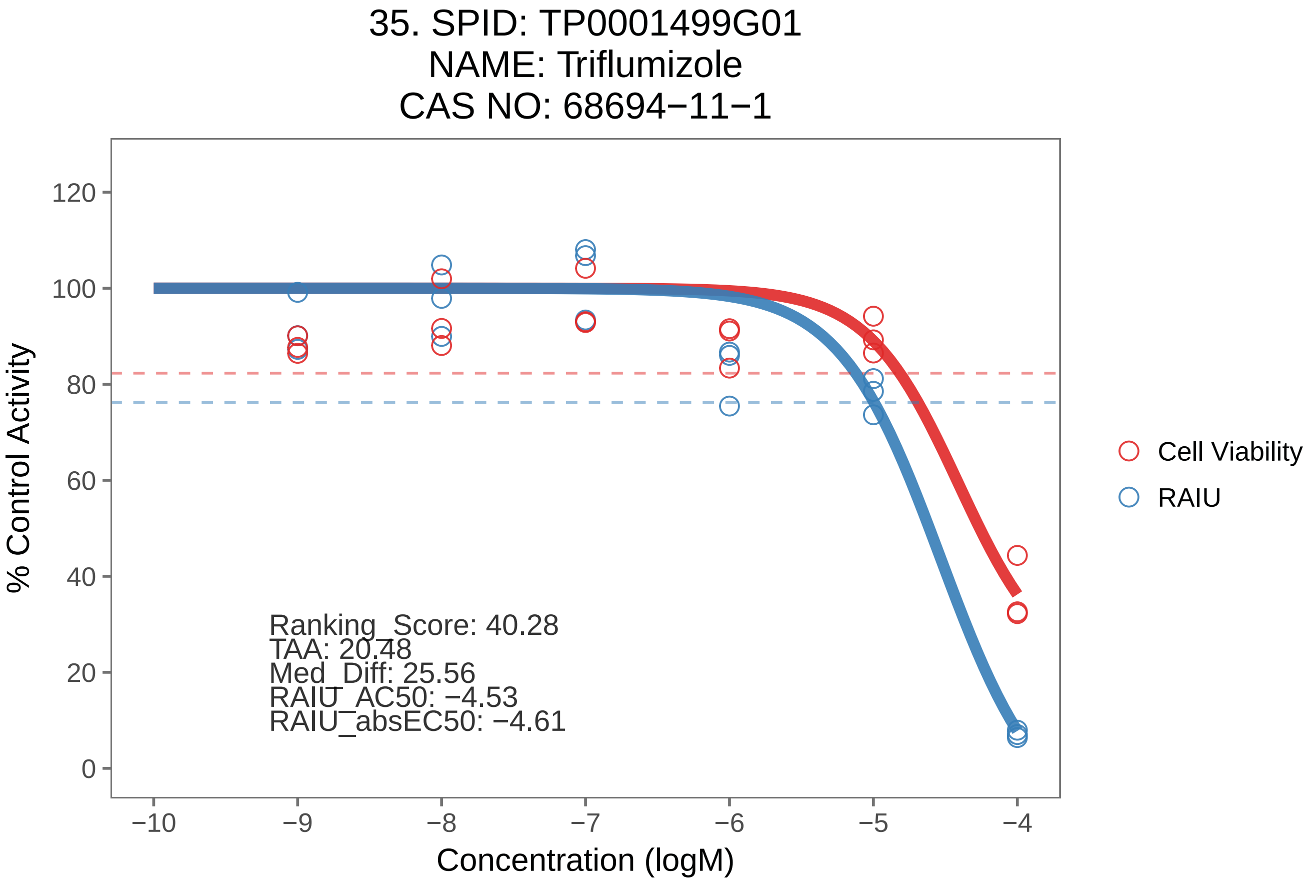


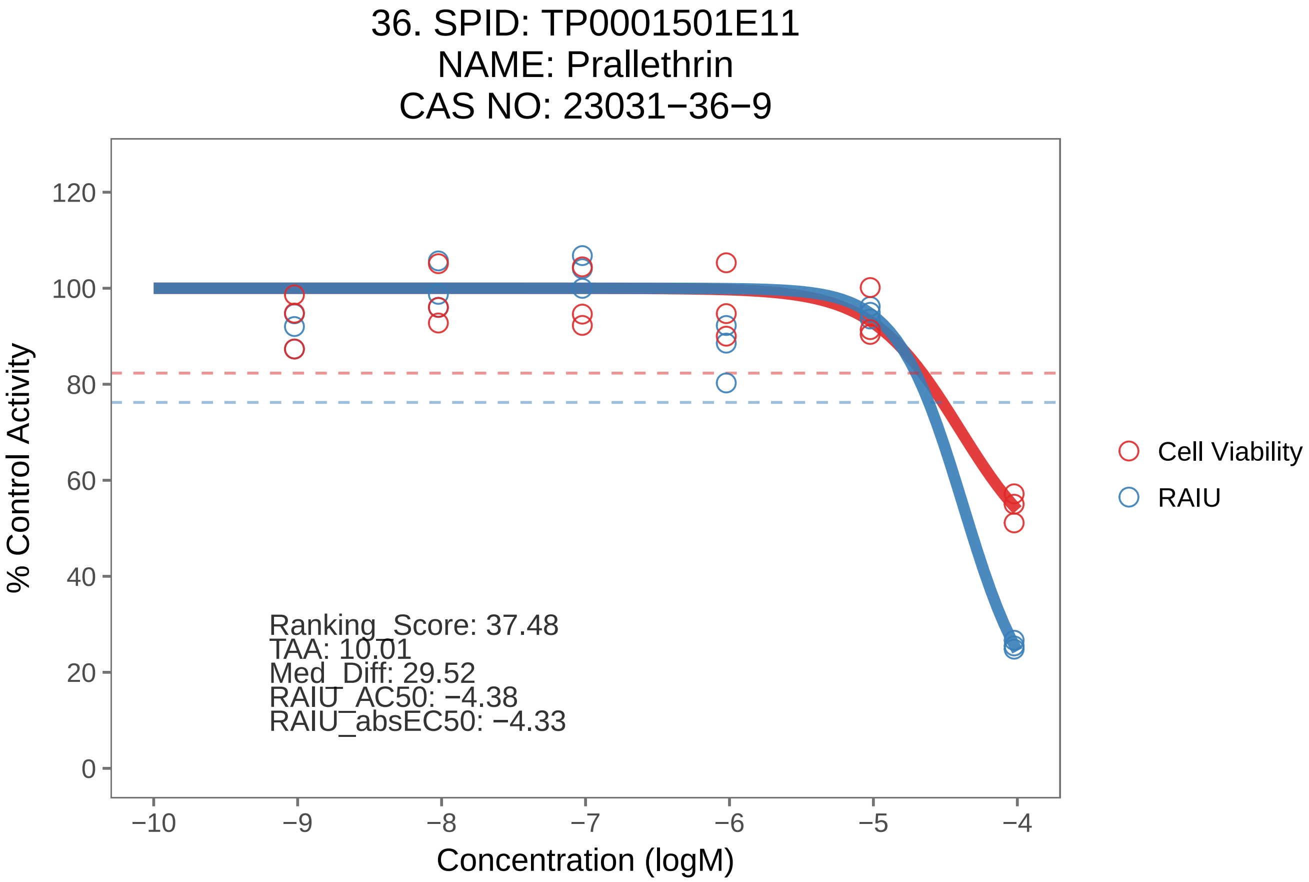
31. SPID: TP0001499F10
NAME: Trifloxystrobin
CAS NO: 141517−21−7
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 41.32
TAA: 32.63
Med_Diff: 18.86
RAIU_AC50: −5.67
RAIU_absEC50: −5.05

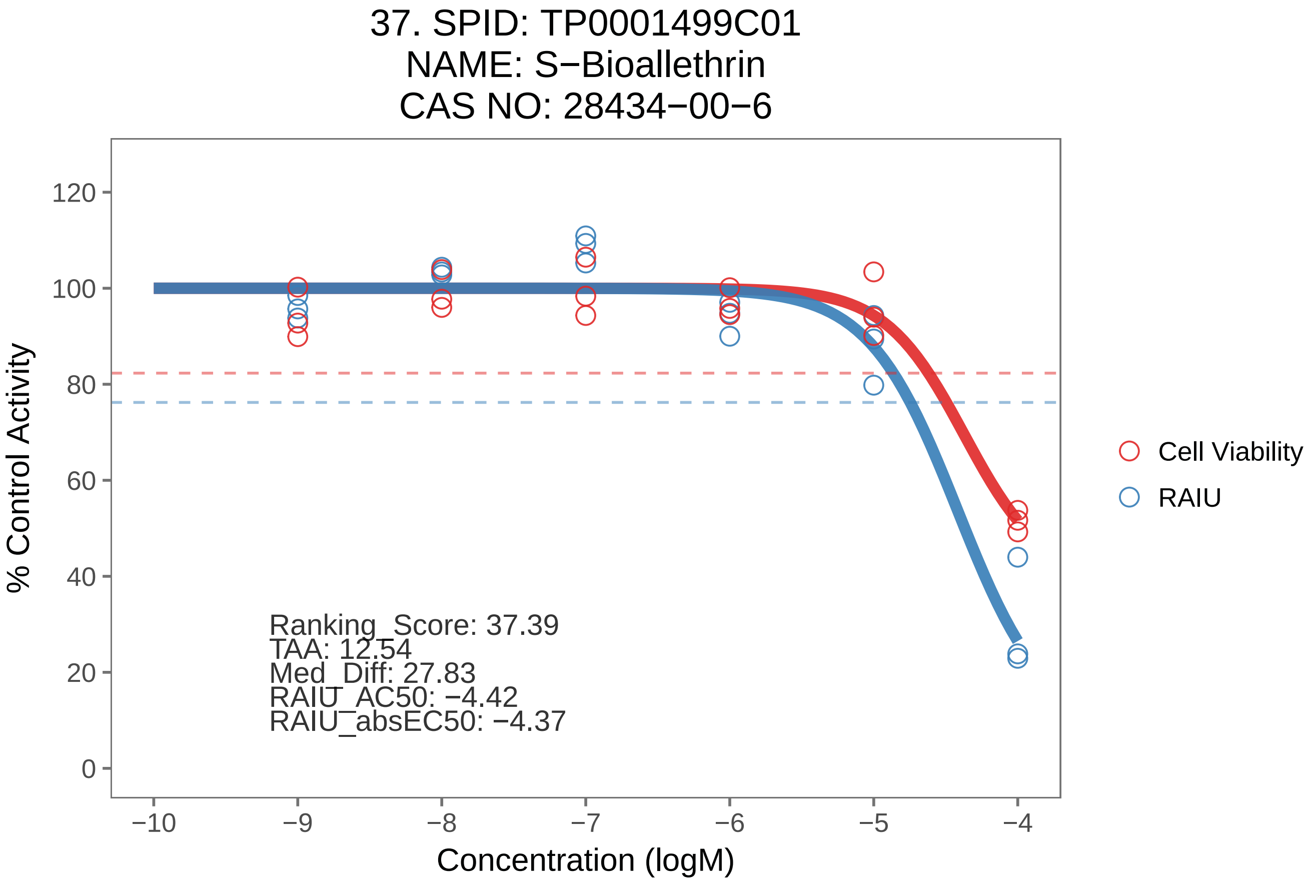

32. SPID: TP0001500D07
NAME: Triclosan
CAS NO: 3380−34−5
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 41.22
TAA: 42.32
Med_Diff: 12.63
RAIU_AC50: −5.01
RAIU_absEC50: −5
Cell Viability
RAIU

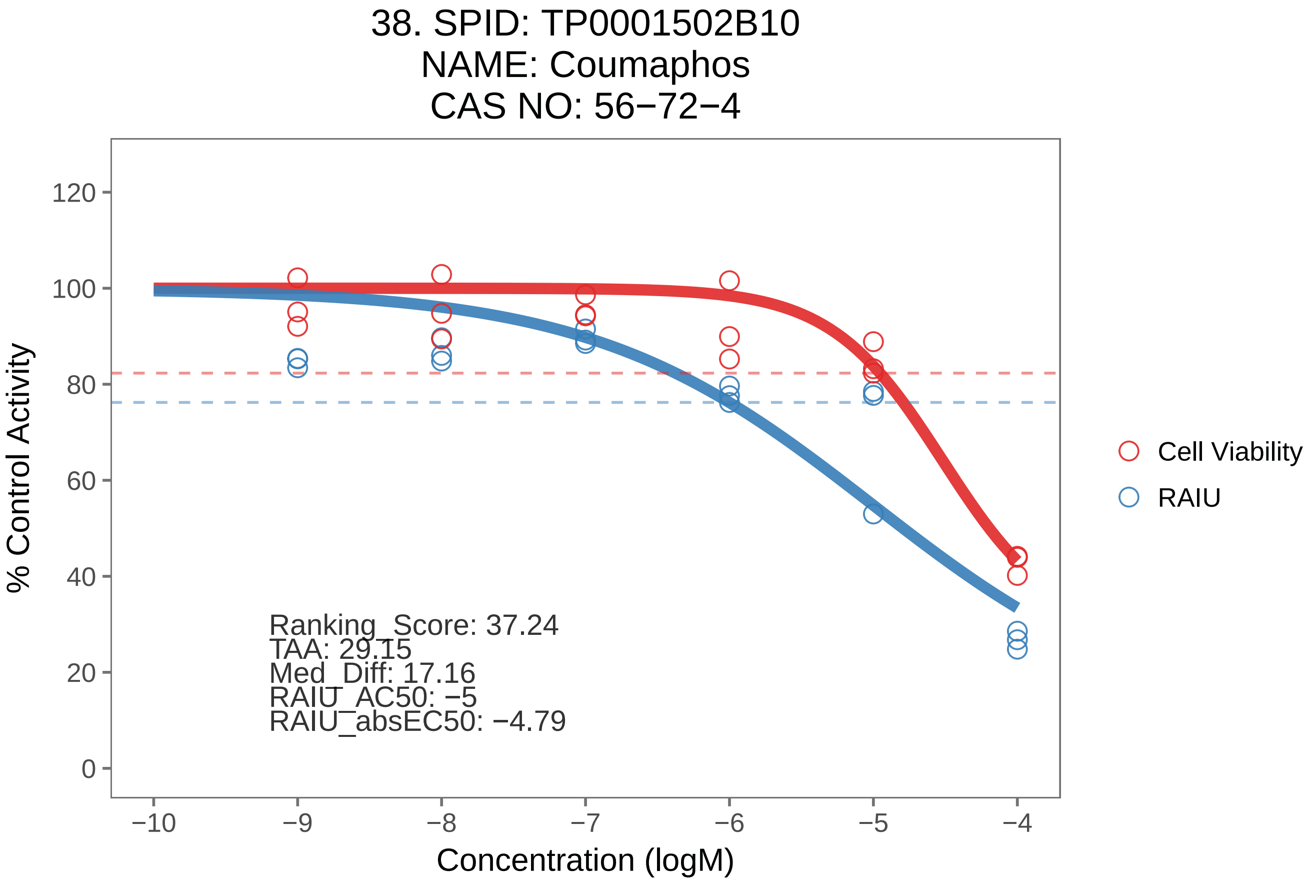

33. SPID: TP0001502B03
NAME: Methoxychlor
CAS NO: 72−43−5
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 40.75
TAA: 8.19
Med_Diff: 33.8
RAIU_AC50: −4.58
RAIU_absEC50: NA
Cell Viability
RAIU

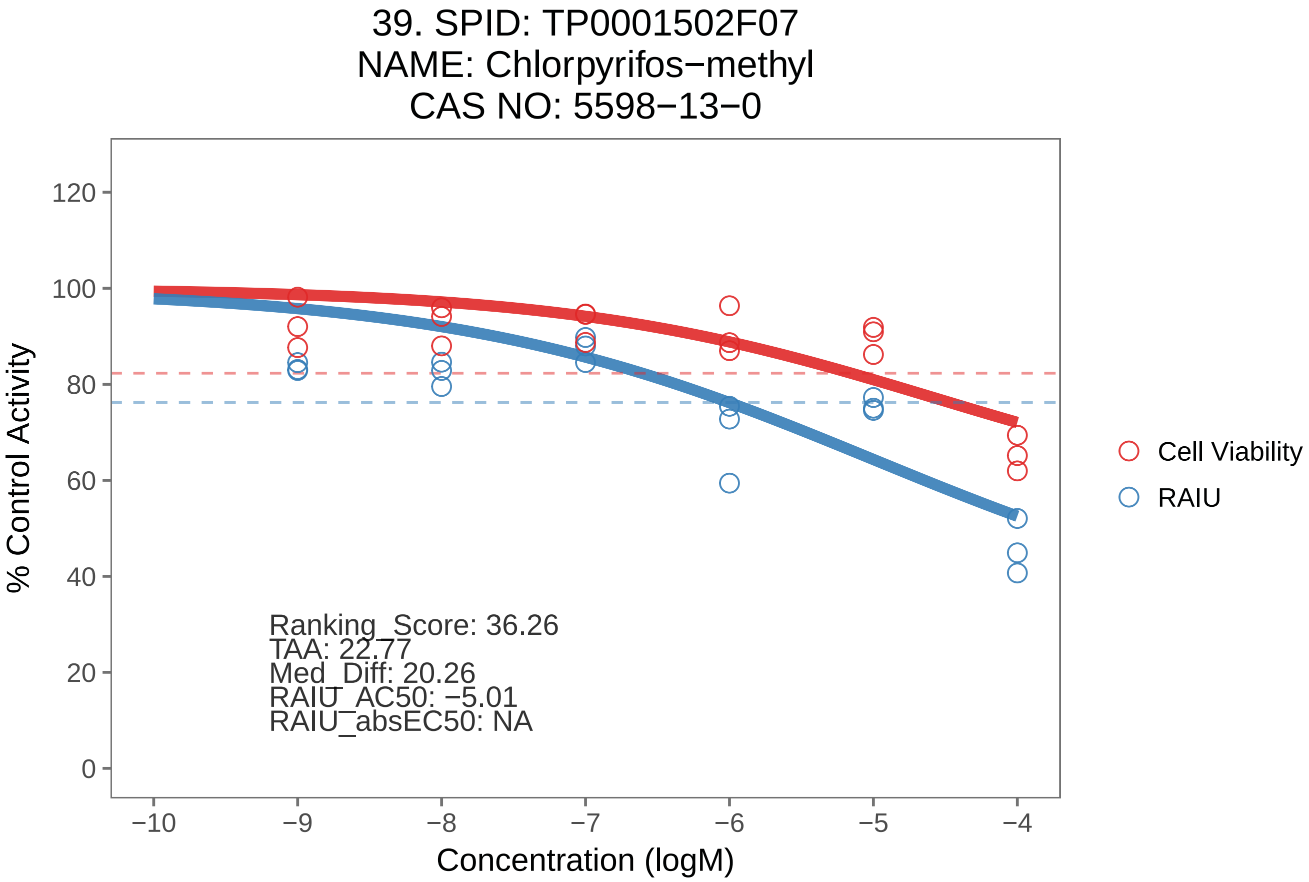

34. SPID: TP0001499F01
NAME: Quinoxyfen
CAS NO: 124495−18−7
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 40.43
TAA: 15.11
Med_Diff: 29.11
RAIU_AC50: −4.47
RAIU_absEC50: −4.44
Cell Viability
RAIU

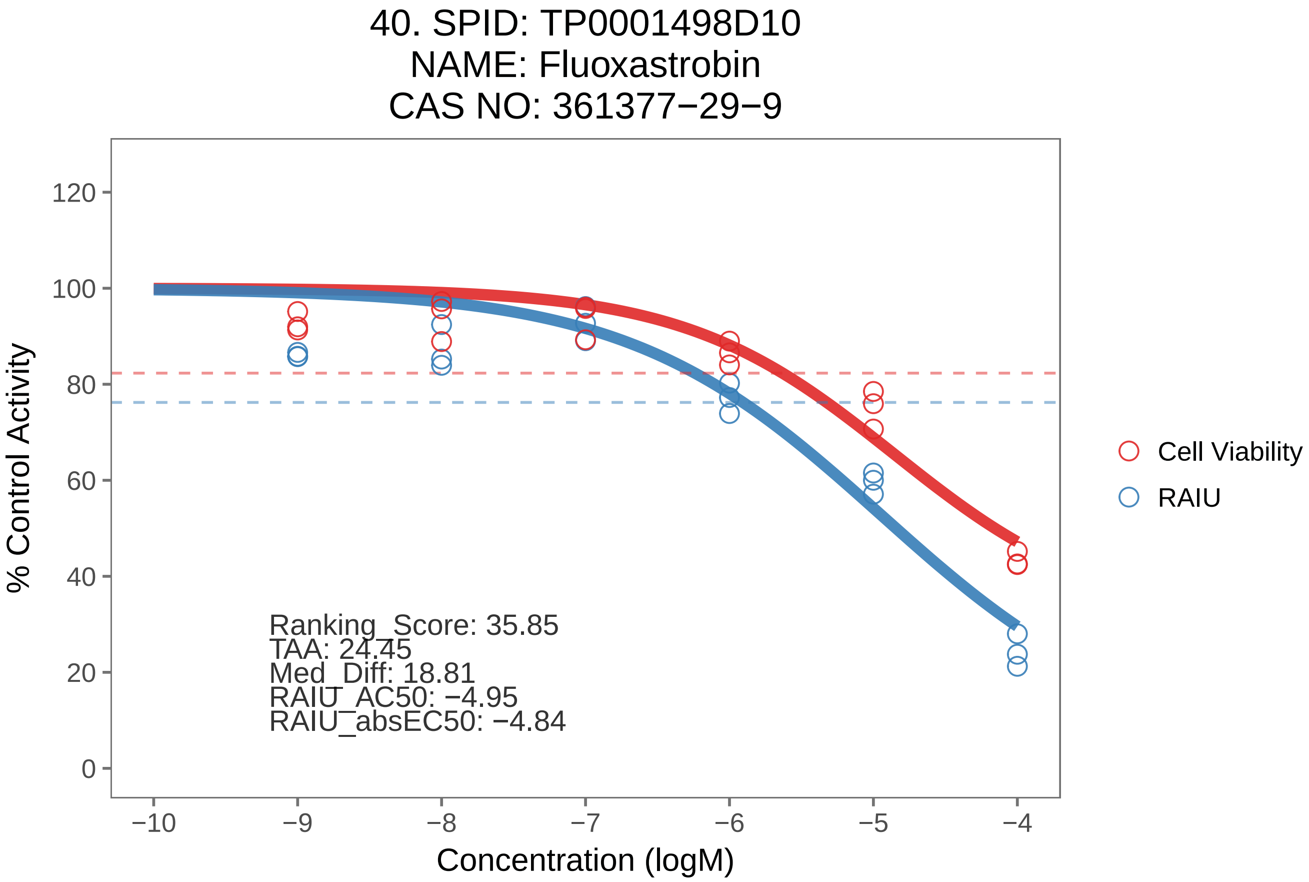

35. SPID: TP0001499G01
NAME: Triflumizole
CAS NO: 68694−11−1
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 40.28
TAA: 20.48
Med_Diff: 25.56
RAIU_AC50: −4.53
RAIU_absEC50: −4.61
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4

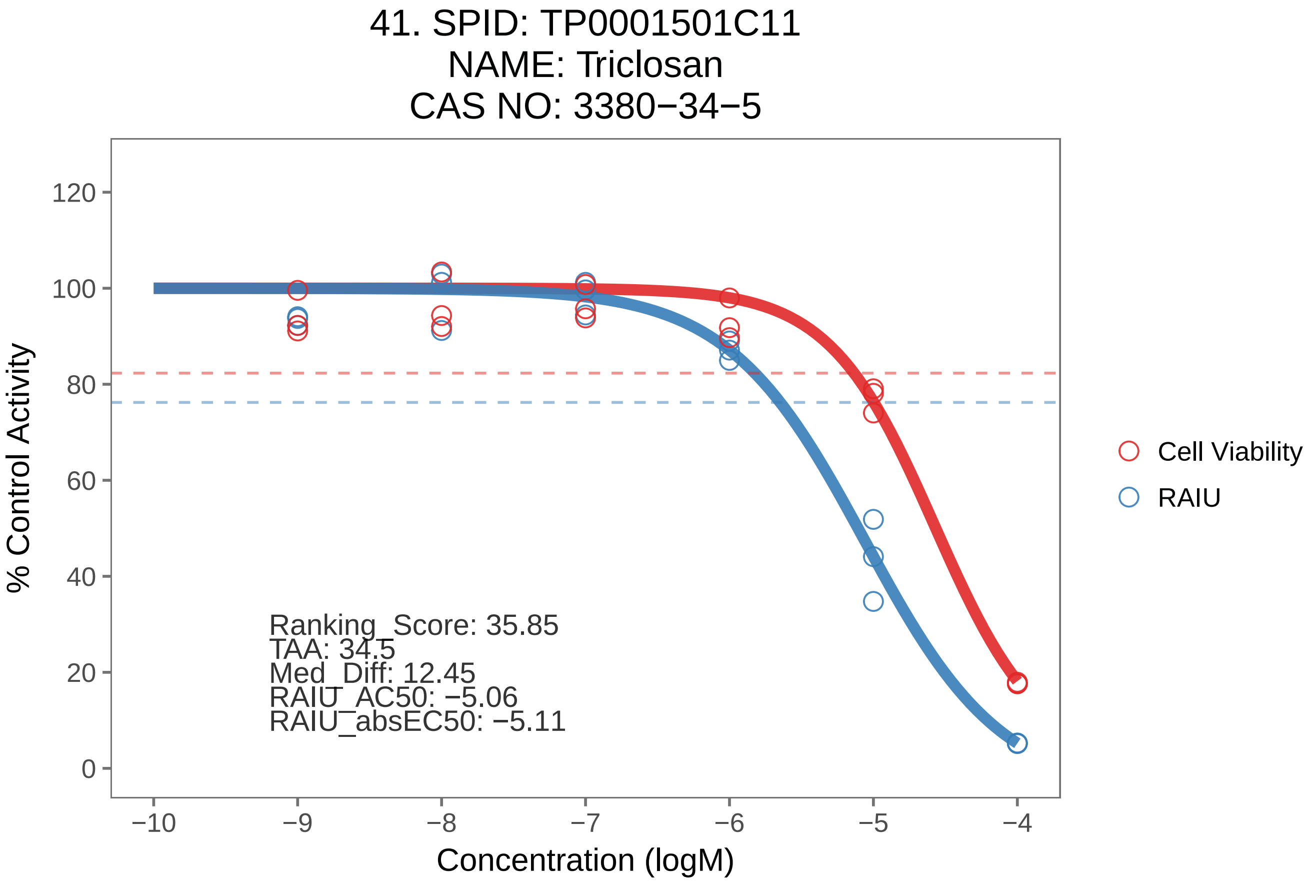

36. SPID: TP0001501E11
NAME: Prallethrin
CAS NO: 23031−36−9
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 37.48
TAA: 10.01
Med_Diff: 29.52
RAIU_AC50: −4.38
RAIU_absEC50: −4.33
Cell Viability
RAIU

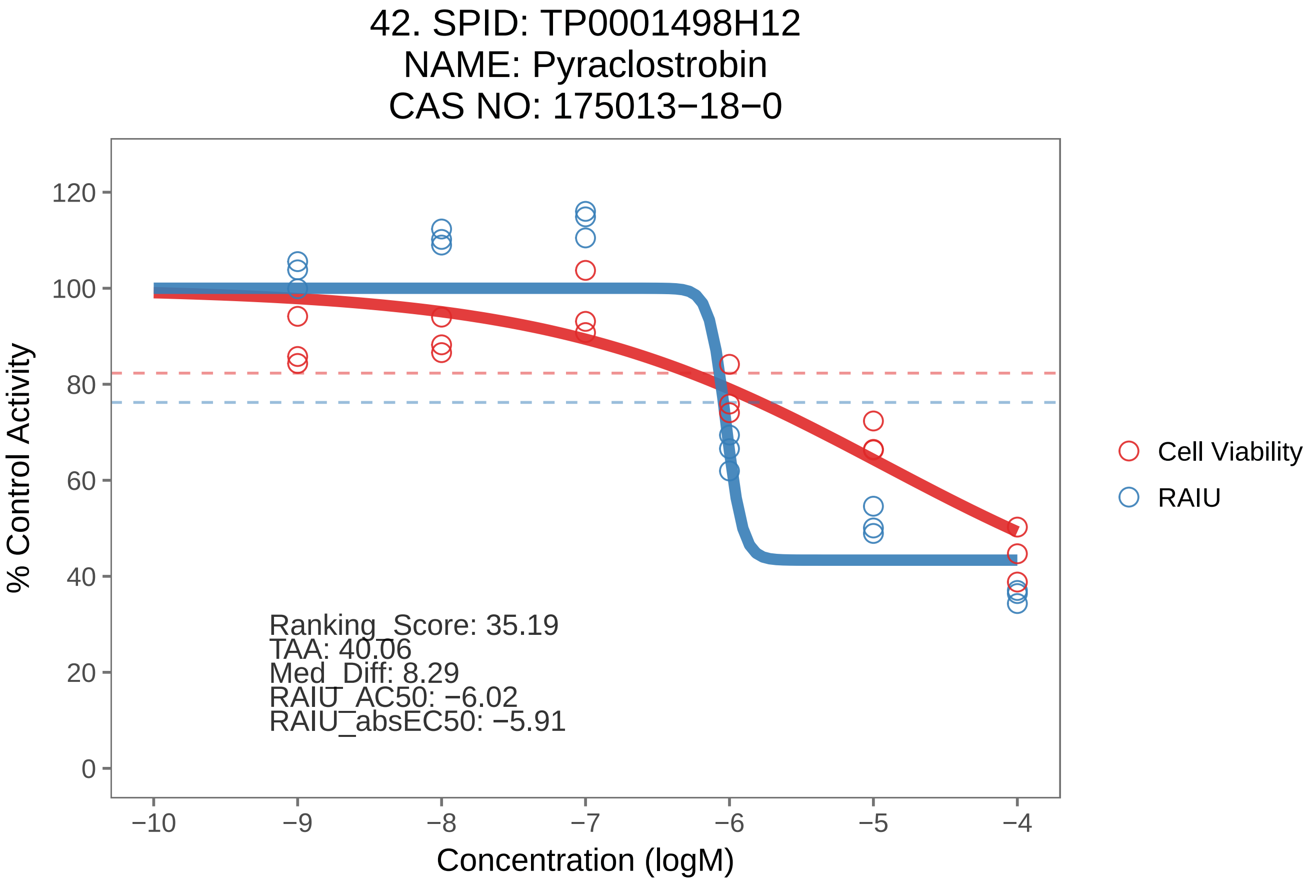

37. SPID: TP0001499C01
NAME: S−Bioallethrin
CAS NO: 28434−00−6
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 37.39
TAA: 12.54
Med_Diff: 27.83
RAIU_AC50: −4.42
RAIU_absEC50: −4.37

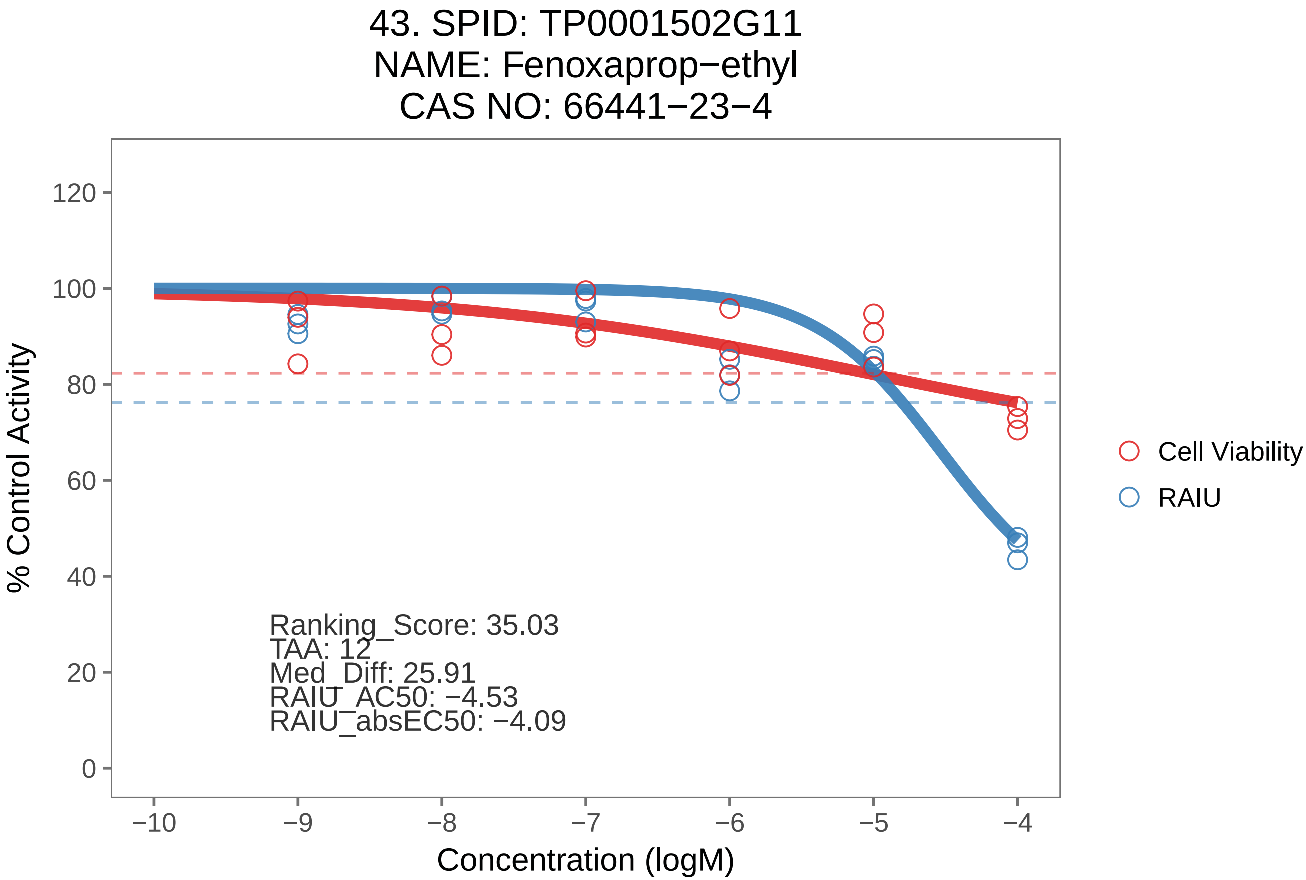

38. SPID: TP0001502B10
NAME: Coumaphos
CAS NO: 56−72−4
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 37.24
TAA: 29.15
Med_Diff: 17.16
RAIU_AC50: −5
RAIU_absEC50: −4.79
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4


39. SPID: TP0001502F07
NAME: Chlorpyrifos−methyl
CAS NO: 5598−13−0
% Control Activity
0
20
40
60
80
100
120
Concentration (logM)
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 36.26
TAA: 22.77
Med_Diff: 20.26
RAIU_AC50: −5.01
RAIU_absEC50: NA
Cell Viability
RAIU

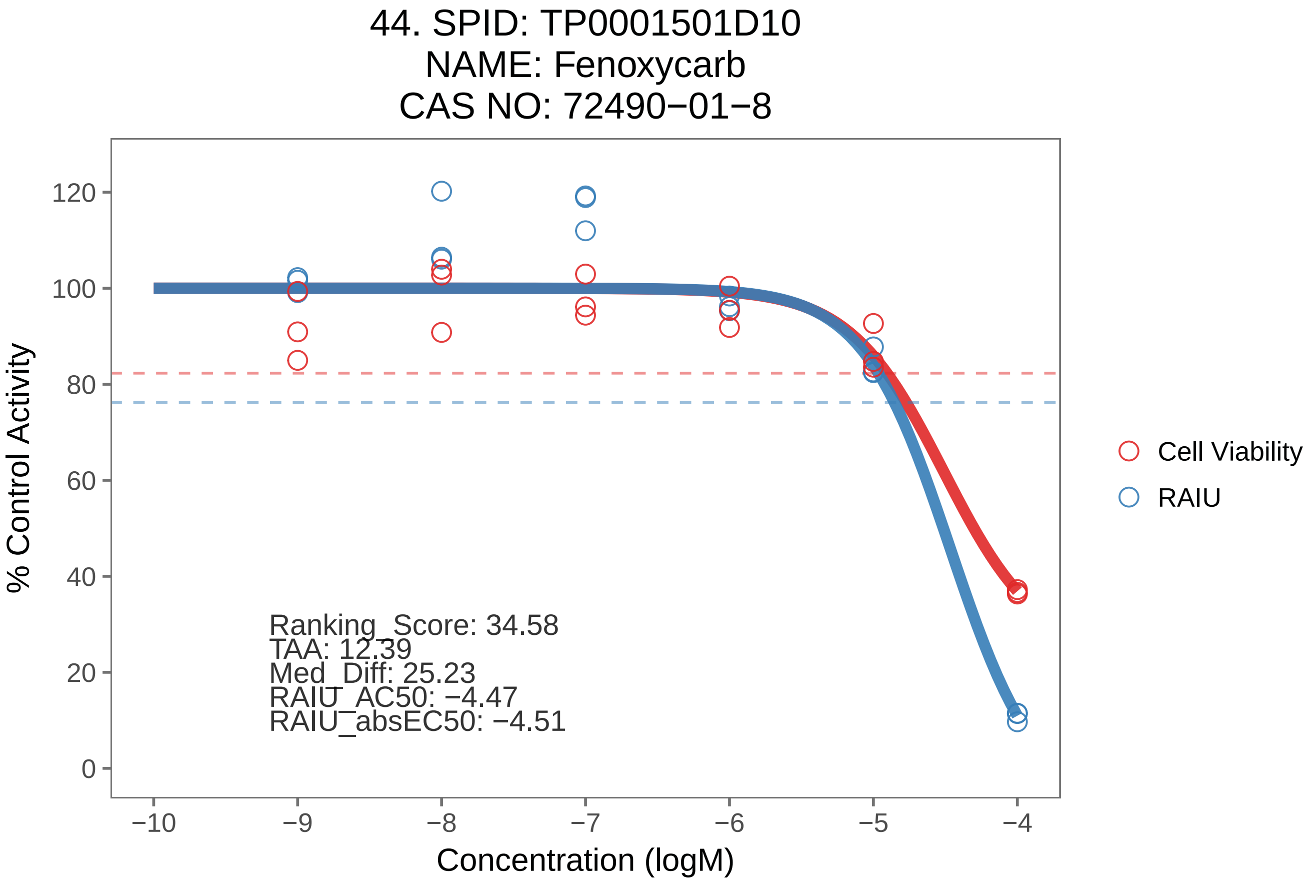

40. SPID: TP0001498D10
NAME: Fluoxastrobin
CAS NO: 361377−29−9
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 35.85
TAA: 24.45
Med_Diff: 18.81
RAIU_AC50: −4.95
RAIU_absEC50: −4.84
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

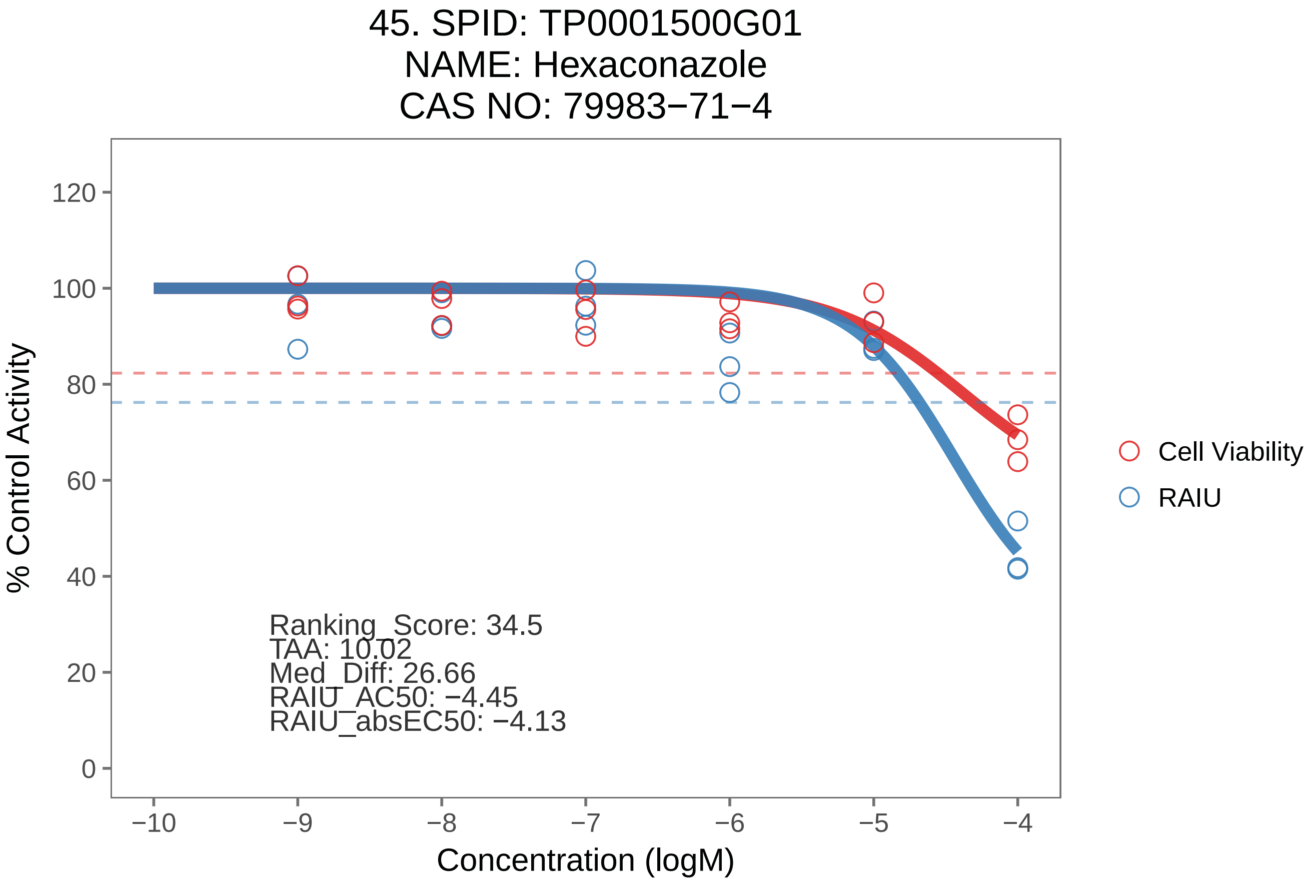

41. SPID: TP0001501C11
NAME: Triclosan
CAS NO: 3380−34−5
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 35.85
TAA: 34.5
Med_Diff: 12.45
RAIU_AC50: −5.06
RAIU_absEC50: −5.11
Cell Viability
RAIU

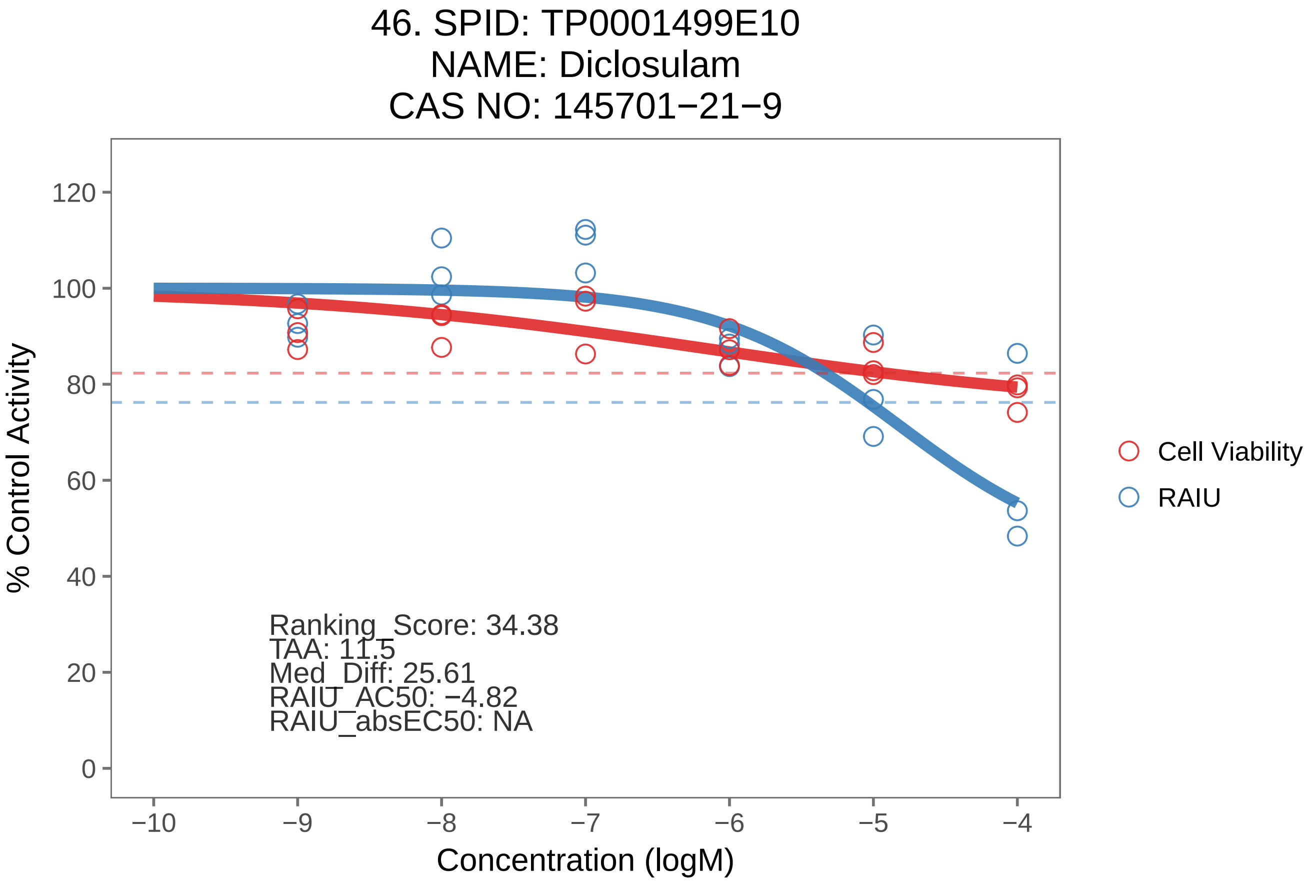

42. SPID: TP0001498H12
NAME: Pyraclostrobin
CAS NO: 175013−18−0
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Cell Viability
RAIU
Ranking_Score: 35.19
TAA: 40.06
Med_Diff: 8.29
RAIU_AC50: −6.02
RAIU_absEC50: −5.91

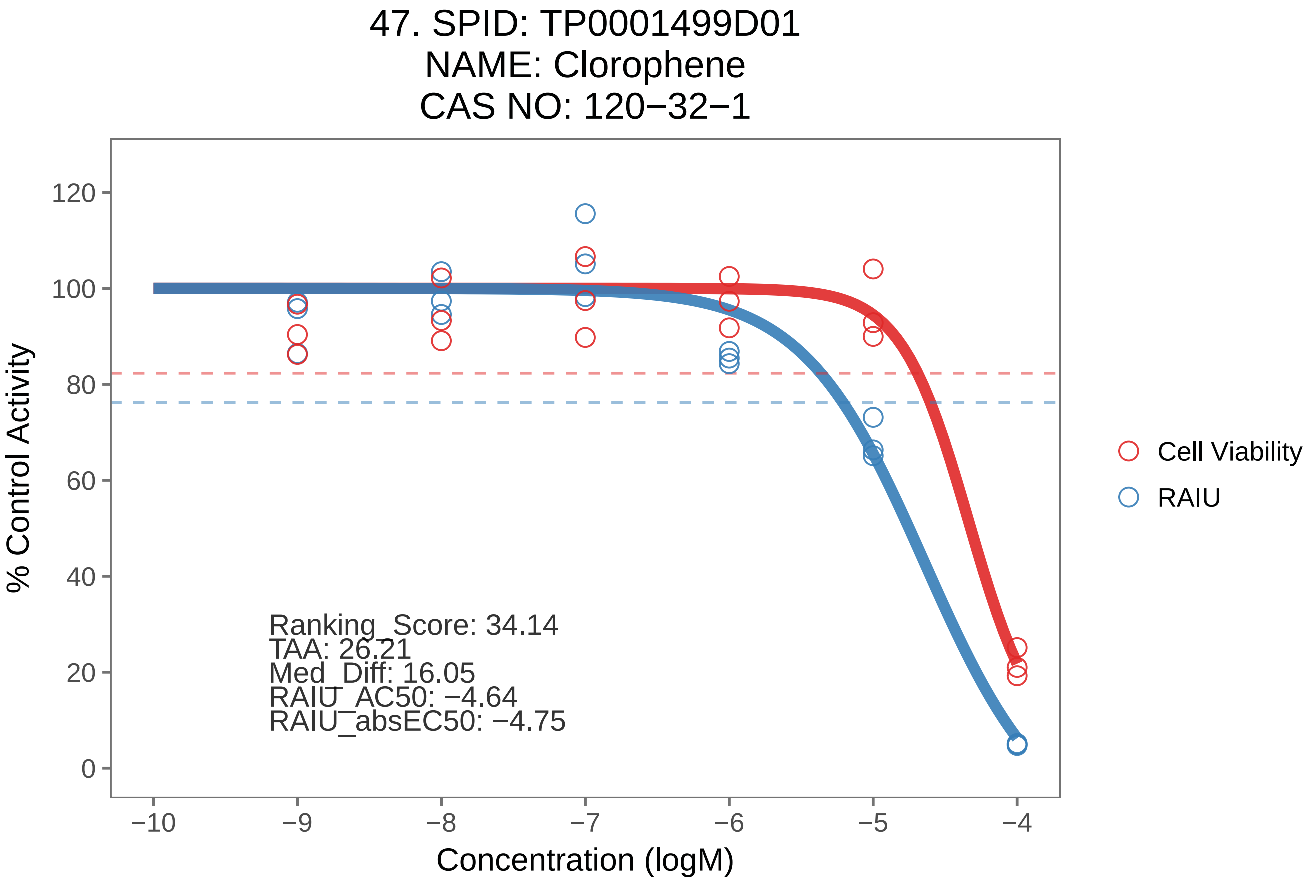


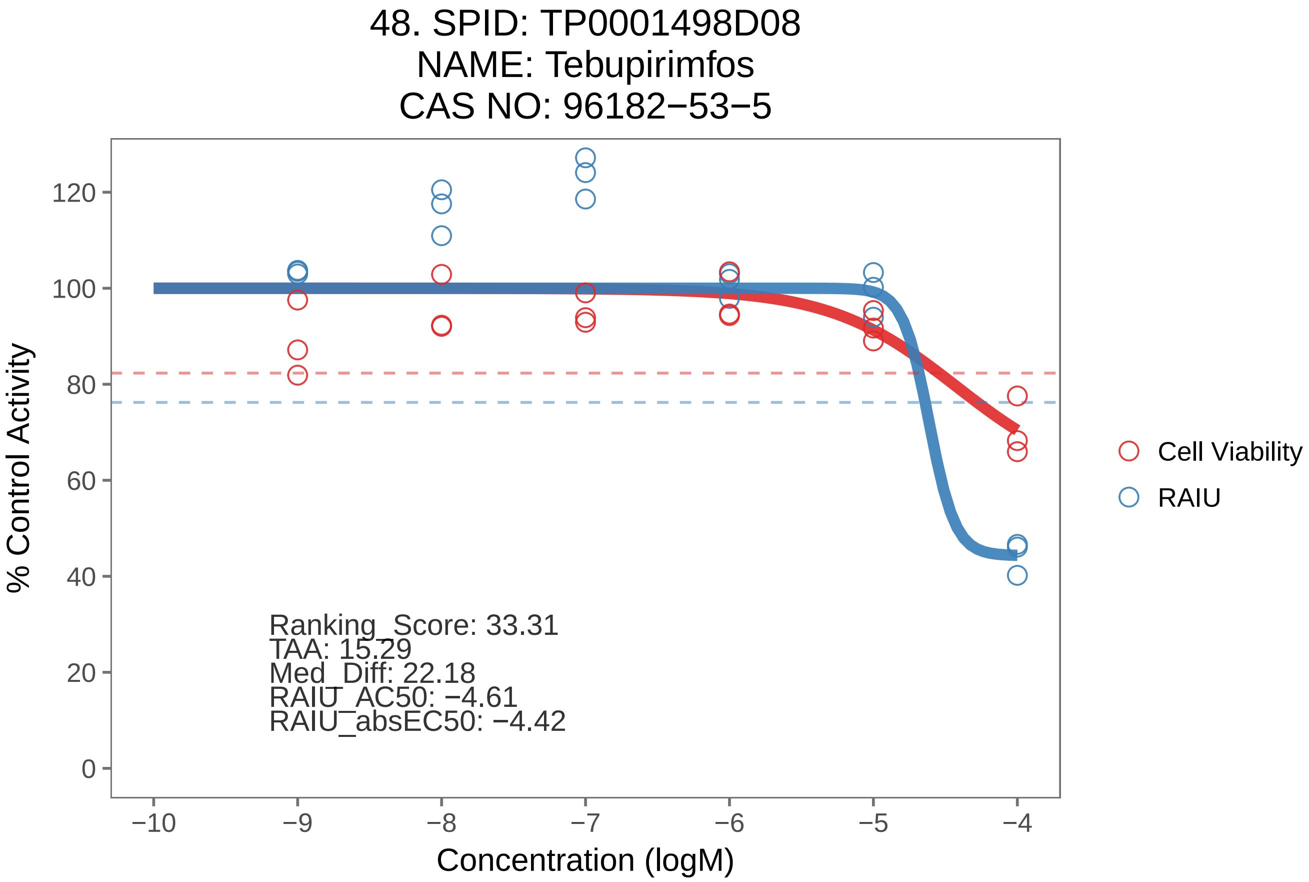
43. SPID: TP0001502G11
NAME: Fenoxaprop−ethyl
CAS NO: 66441−23−4
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 35.03
TAA: 12
Med_Diff: 25.91
RAIU_AC50: −4.53
RAIU_absEC50: −4.09
Cell Viability
RAIU

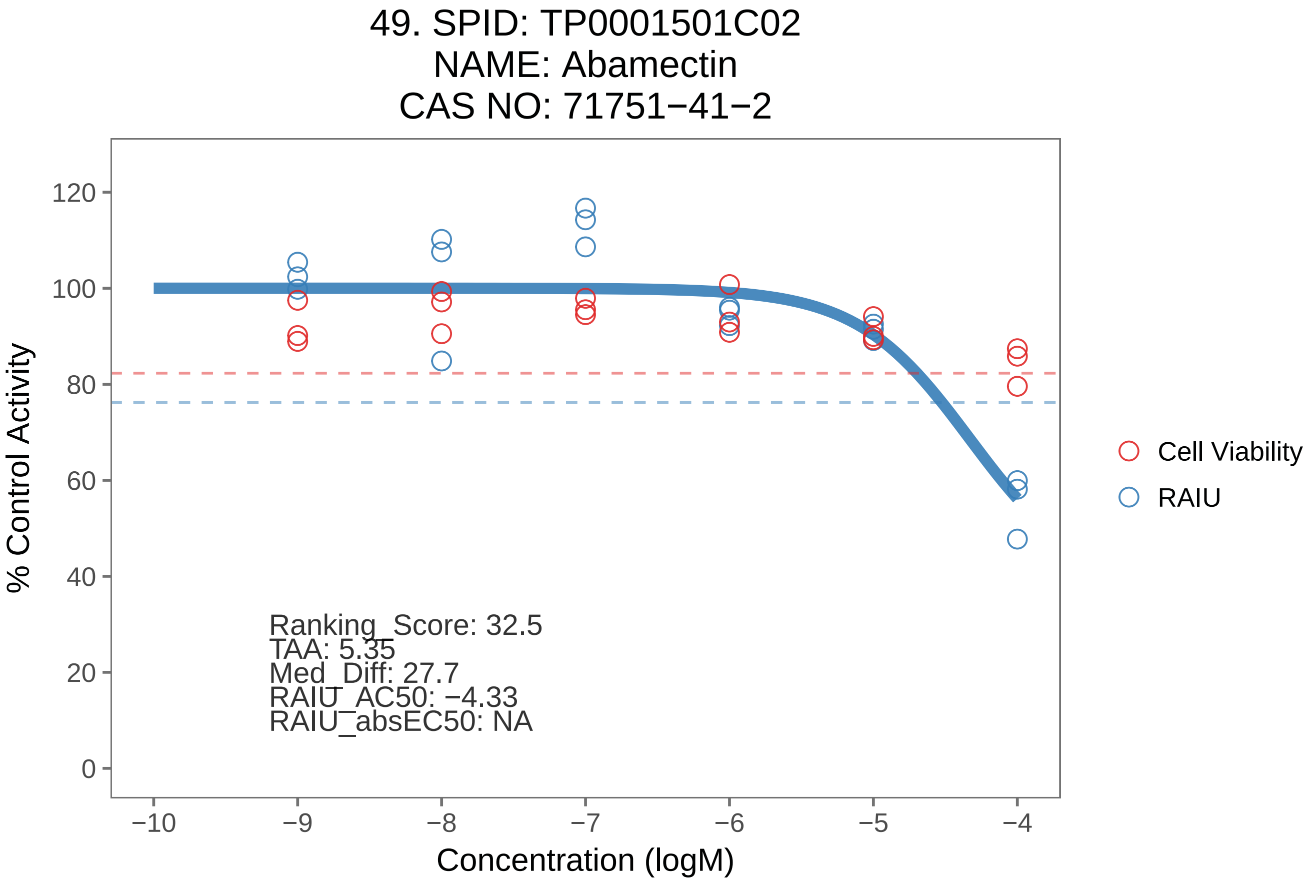

44. SPID: TP0001501D10
NAME: Fenoxycarb
CAS NO: 72490−01−8
120
100
80
60
40
20
0
% Control Activity
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 34.58
TAA: 12.39
Med_Diff: 25.23
RAIU_AC50: −4.47
RAIU_absEC50: −4.51
Cell Viability
RAIU

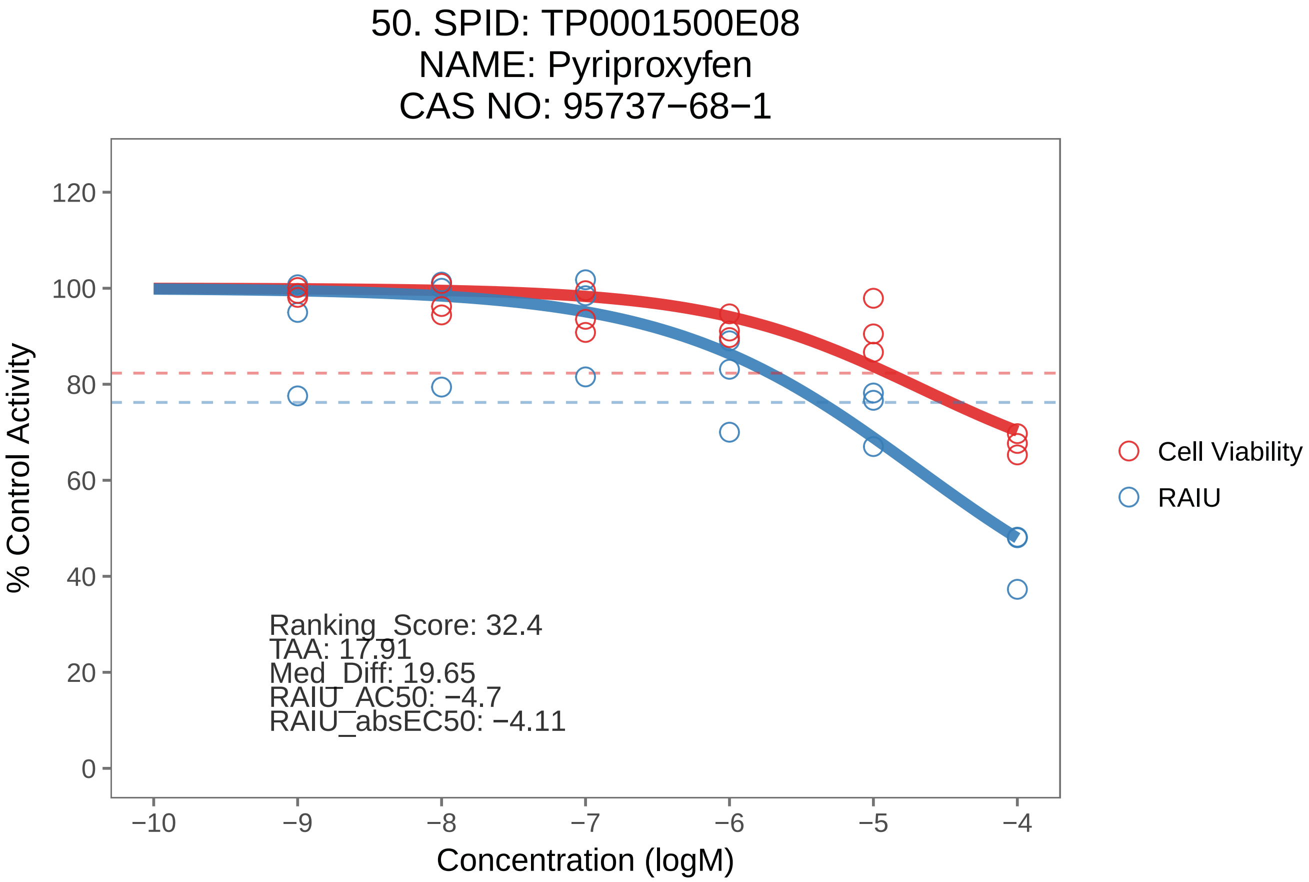

45. SPID: TP0001500G01
NAME: Hexaconazole
CAS NO: 79983−71−4
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 34.5
TAA: 10.02
Med_Diff: 26.66
RAIU_AC50: −4.45
RAIU_absEC50: −4.13
Cell Viability
RAIU


46. SPID: TP0001499E10
NAME: Diclosulam
CAS NO: 145701−21−9
Ranking_Score: 34.38
TAA: 11.5
Med_Diff: 25.61
RAIU_AC50: −4.82
RAIU_absEC50: NA
% Control Activity
Concentration (logM)
Cell Viability
RAIU
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

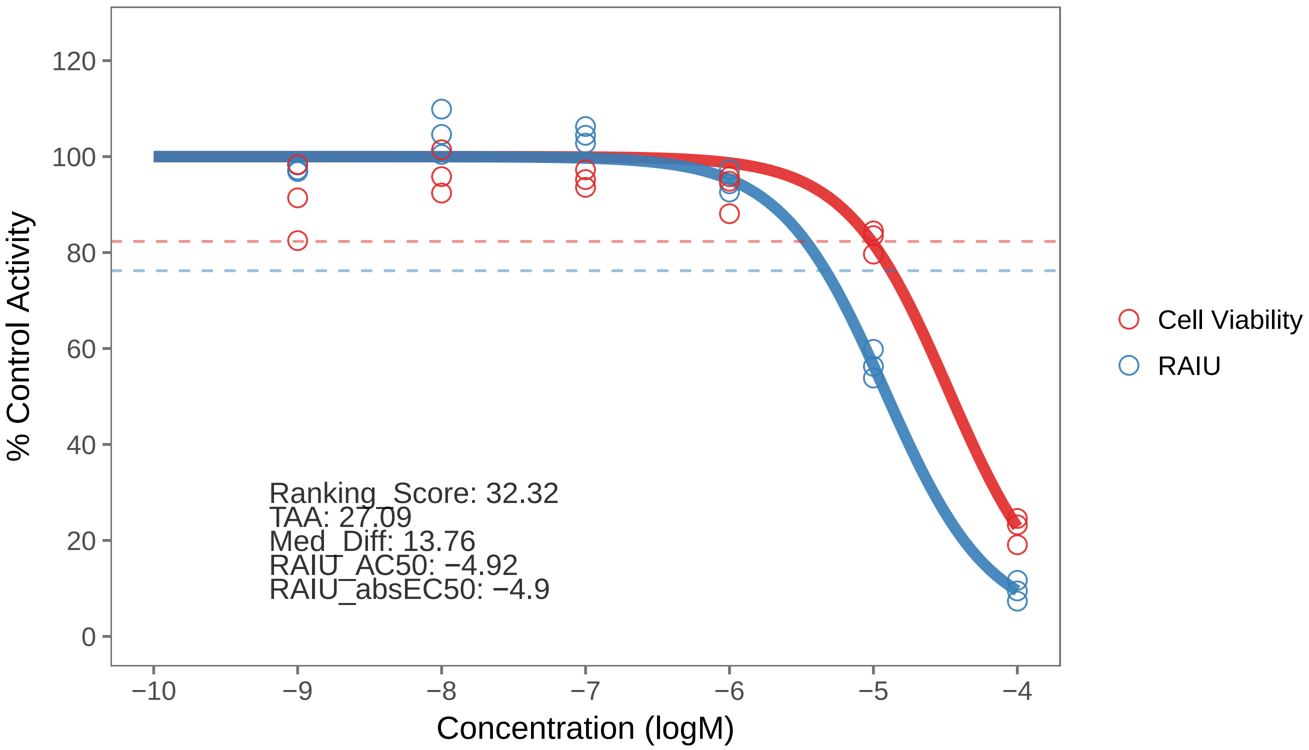

47. SPID: TP0001499D01
NAME: Clorophene
CAS NO: 120−32−1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 34.14
TAA: 26.21
Med_Diff: 16.05
RAIU_AC50: −4.64
RAIU_absEC50: −4.75
Cell Viability
RAIU

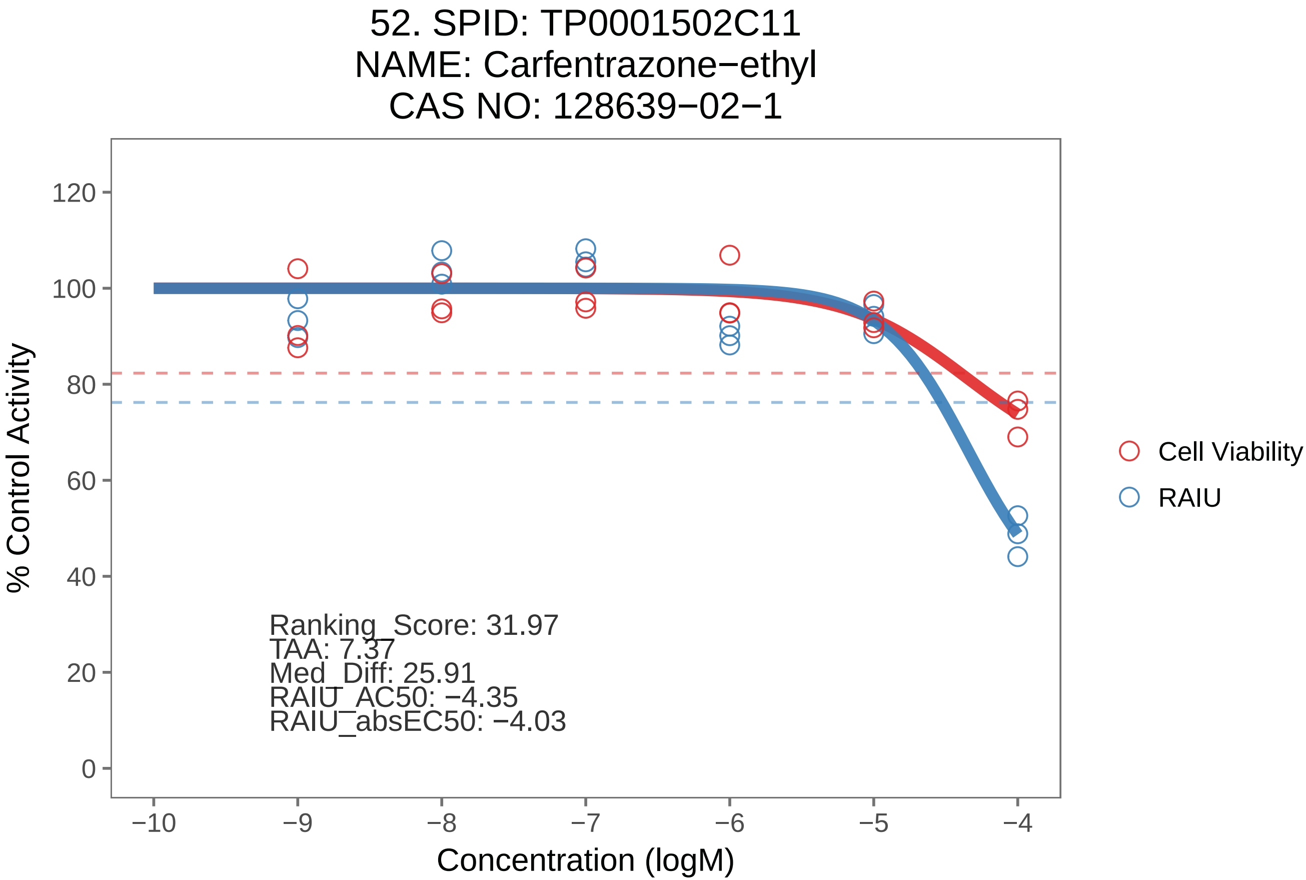

48. SPID: TP0001498D08
NAME: Tebupirimfos
CAS NO: 96182−53−5
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 33.31
TAA: 15.29
Med_Diff: 22.18
RAIU_AC50: −4.61
RAIU_absEC50: −4.42
Cell Viability
RAIU

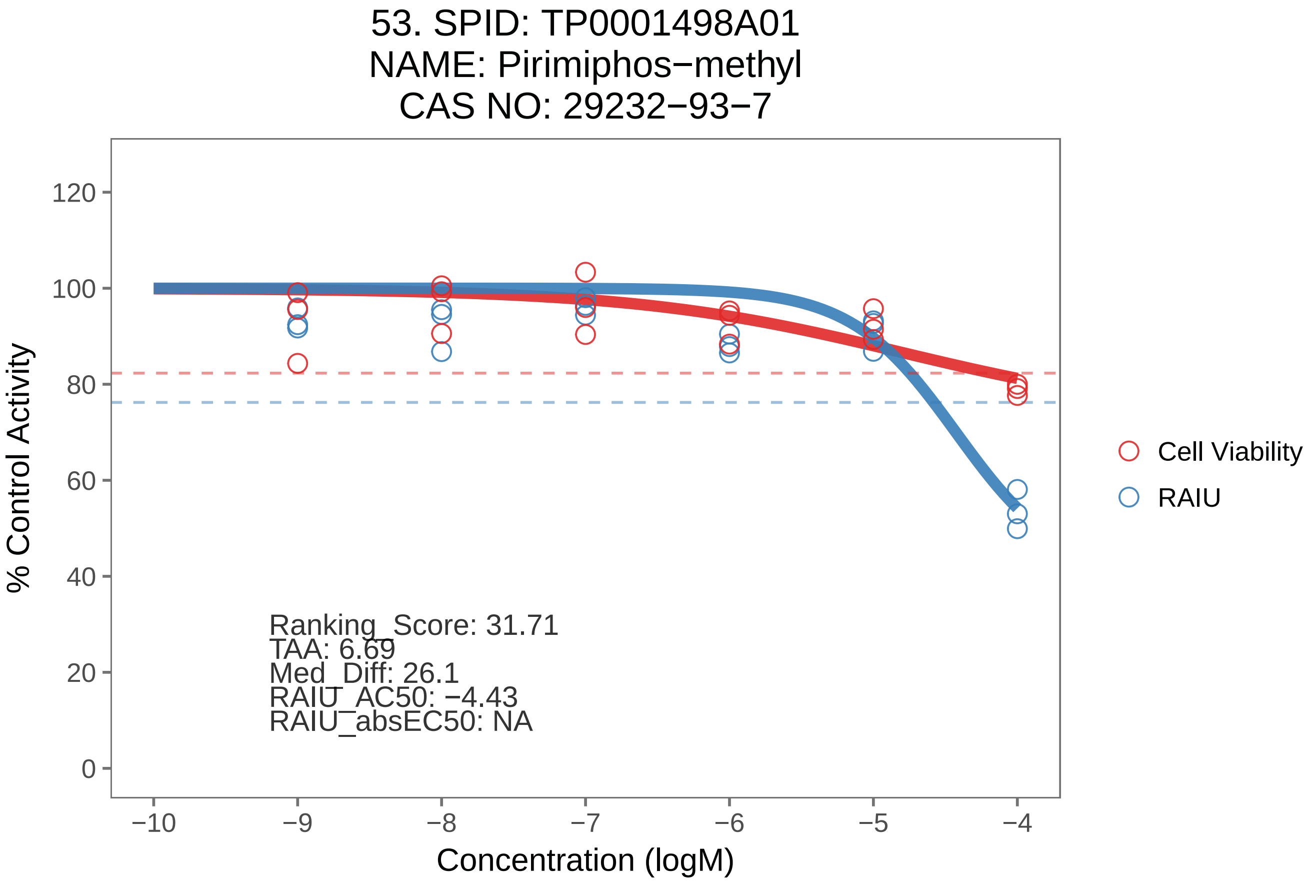

49. SPID: TP0001501C02
NAME: Abamectin
CAS NO: 71751−41−2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 32.5
TAA: 5.35
Med_Diff: 27.7
RAIU_AC50: −4.33
RAIU_absEC50: NA
Cell Viability
RAIU

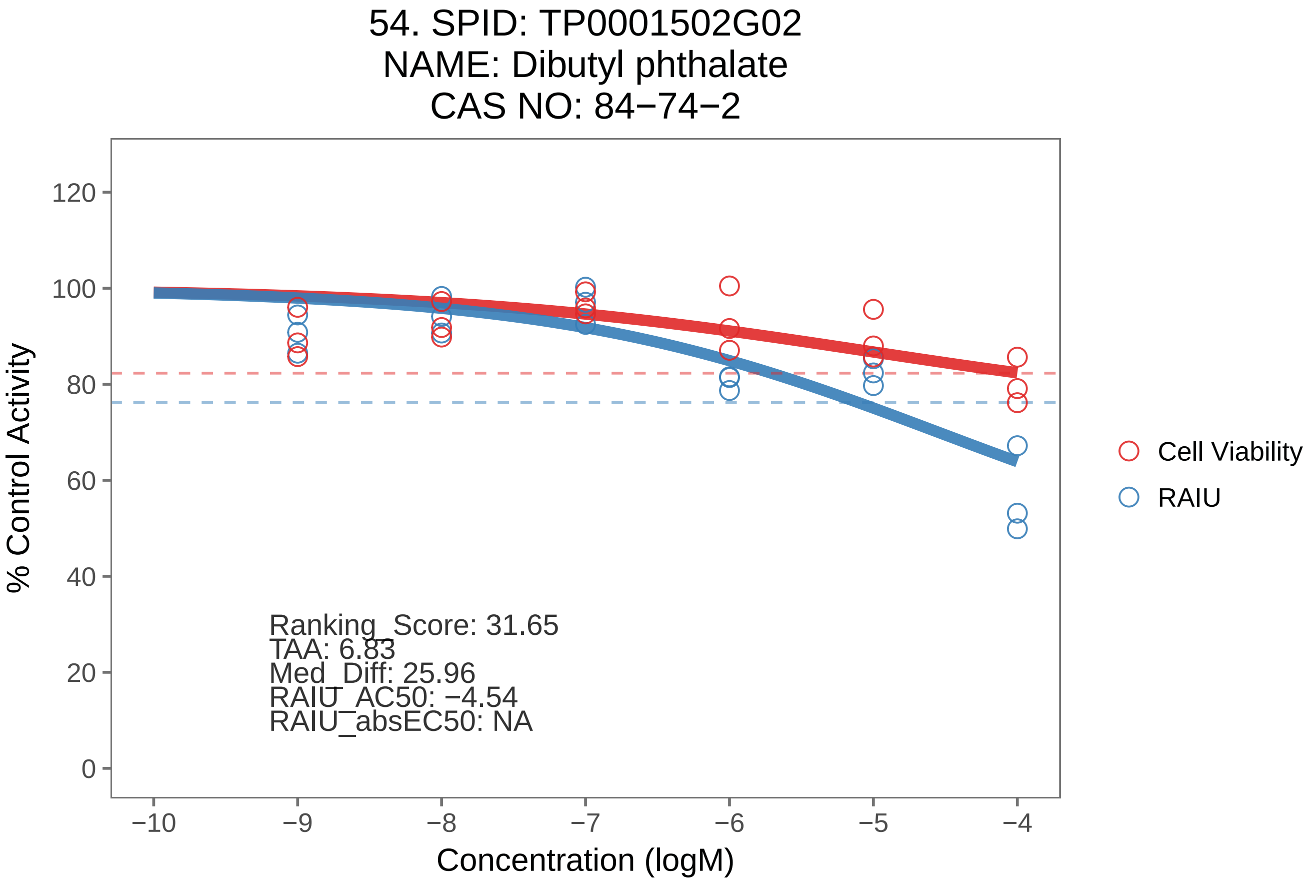

50. SPID: TP0001500E08
NAME: Pyriproxyfen
CAS NO: 95737−68−1
120
100
80
60
40
20
0
% Control Activity
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 32.4
TAA: 17.91
Med_Diff: 19.65
RAIU_AC50: −4.7
RAIU_absEC50: −4.11
Cell Viability
RAIU

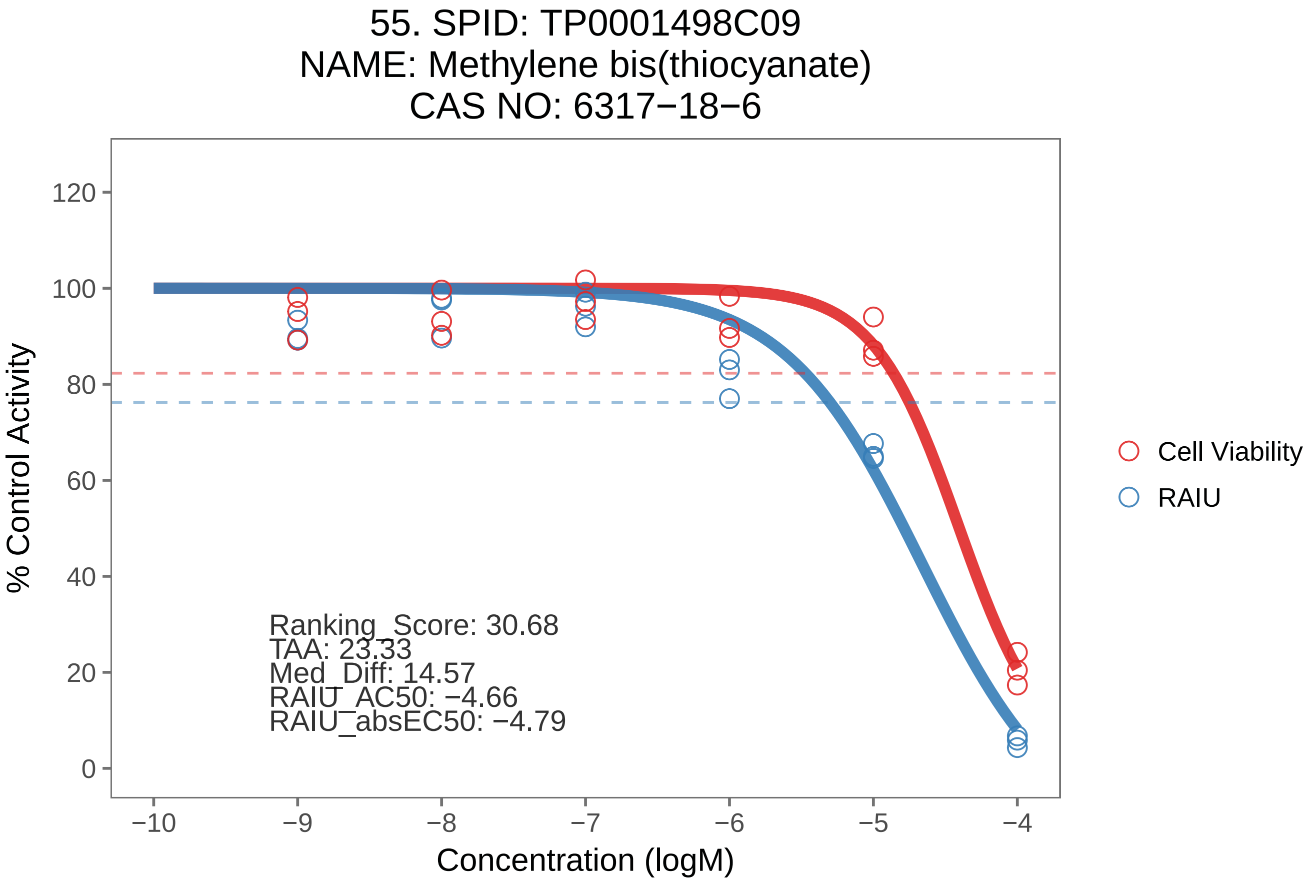
51. SPID: TP0001498B11
NAME: Triclosan
CAS NO: 3380−34−5

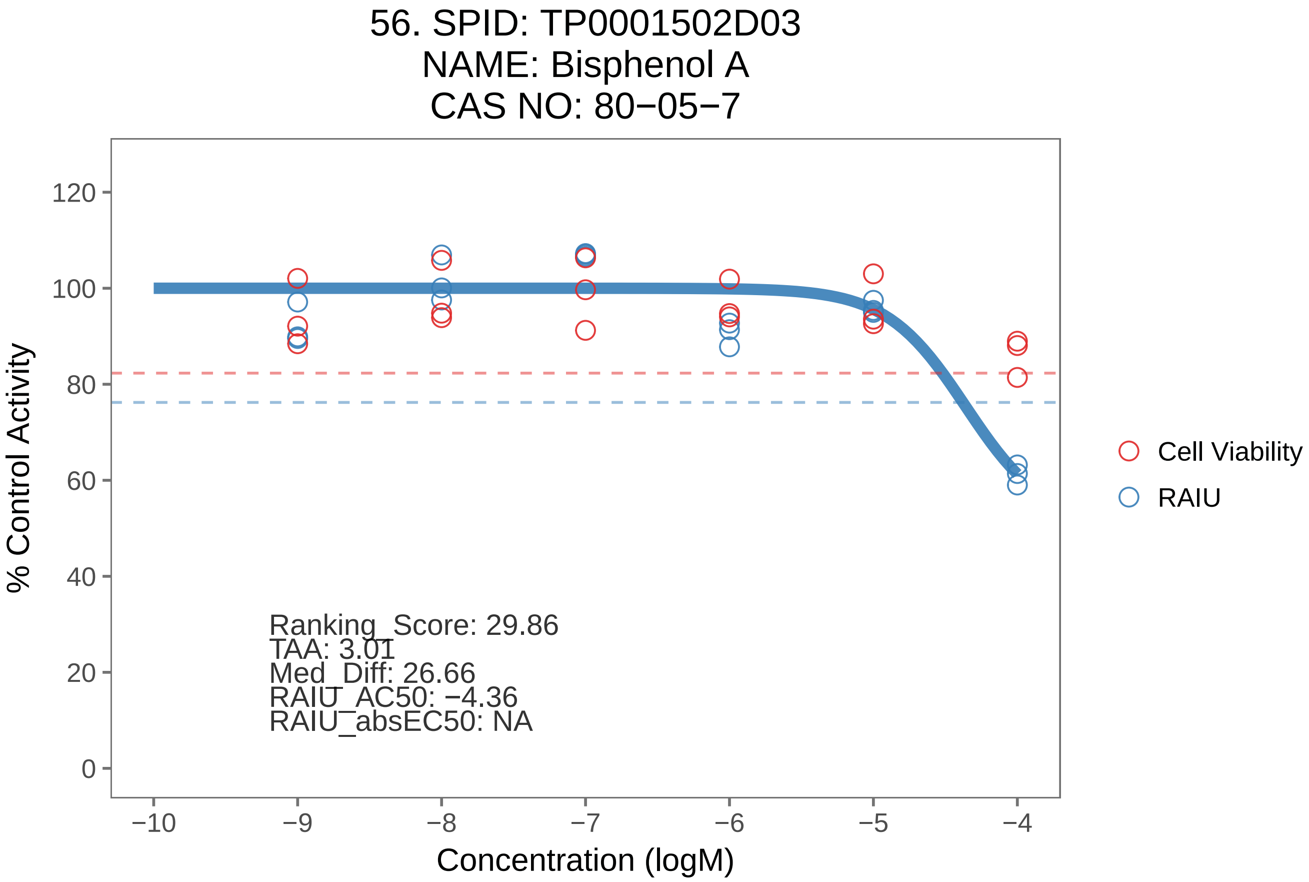



52. SPID: TP0001502C11
NAME: Carfentrazone−ethyl
CAS NO: 128639−02−1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 31.97
TAA: 7.37
Med_Diff: 25.91
RAIU_AC50: −4.35
RAIU_absEC50: −4.03
Cell Viability
RAIU

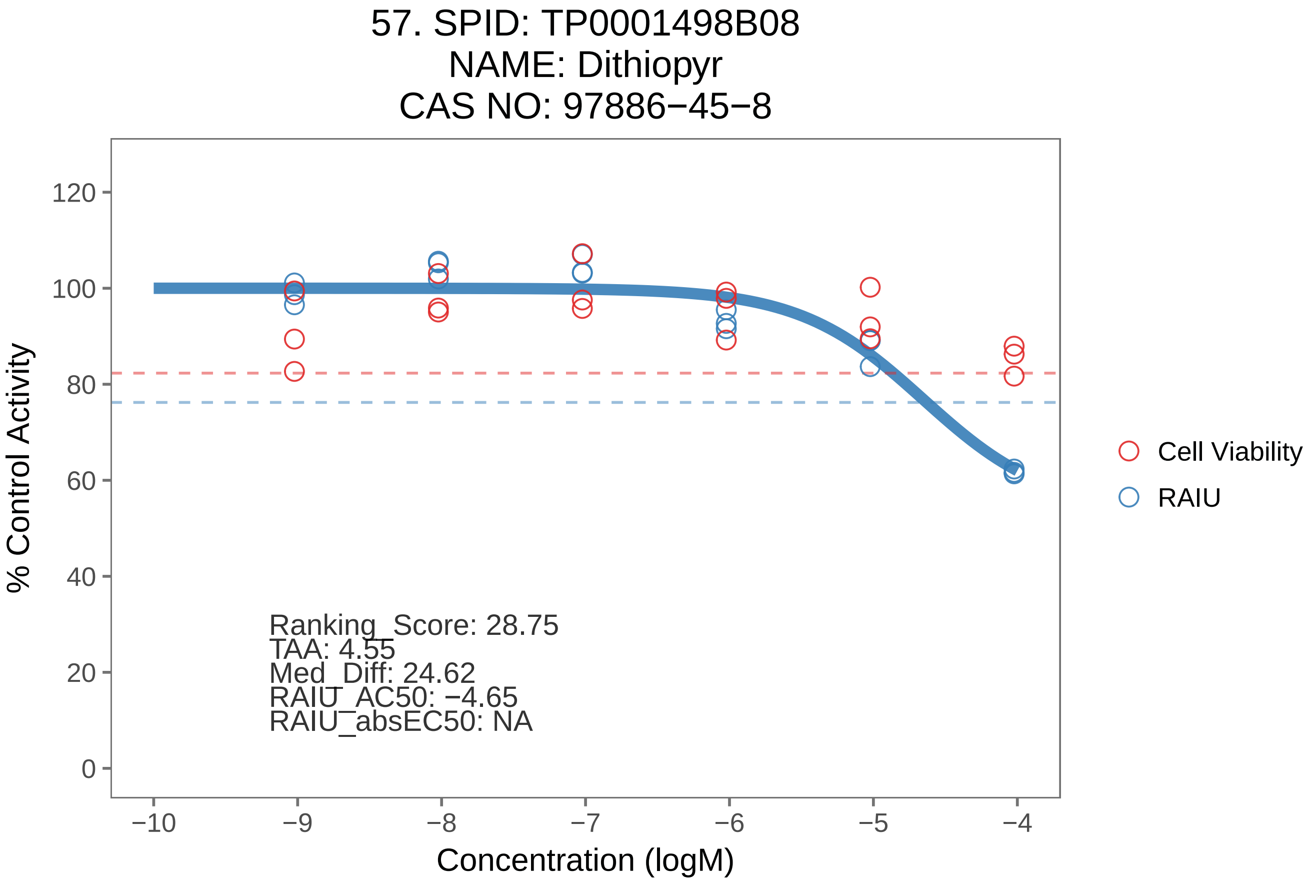

53. SPID: TP0001498A01
NAME: Pirimiphos−methyl
CAS NO: 29232−93−7
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 31.71
TAA: 6.69
Med_Diff: 26.1
RAIU_AC50: −4.43
RAIU_absEC50: NA

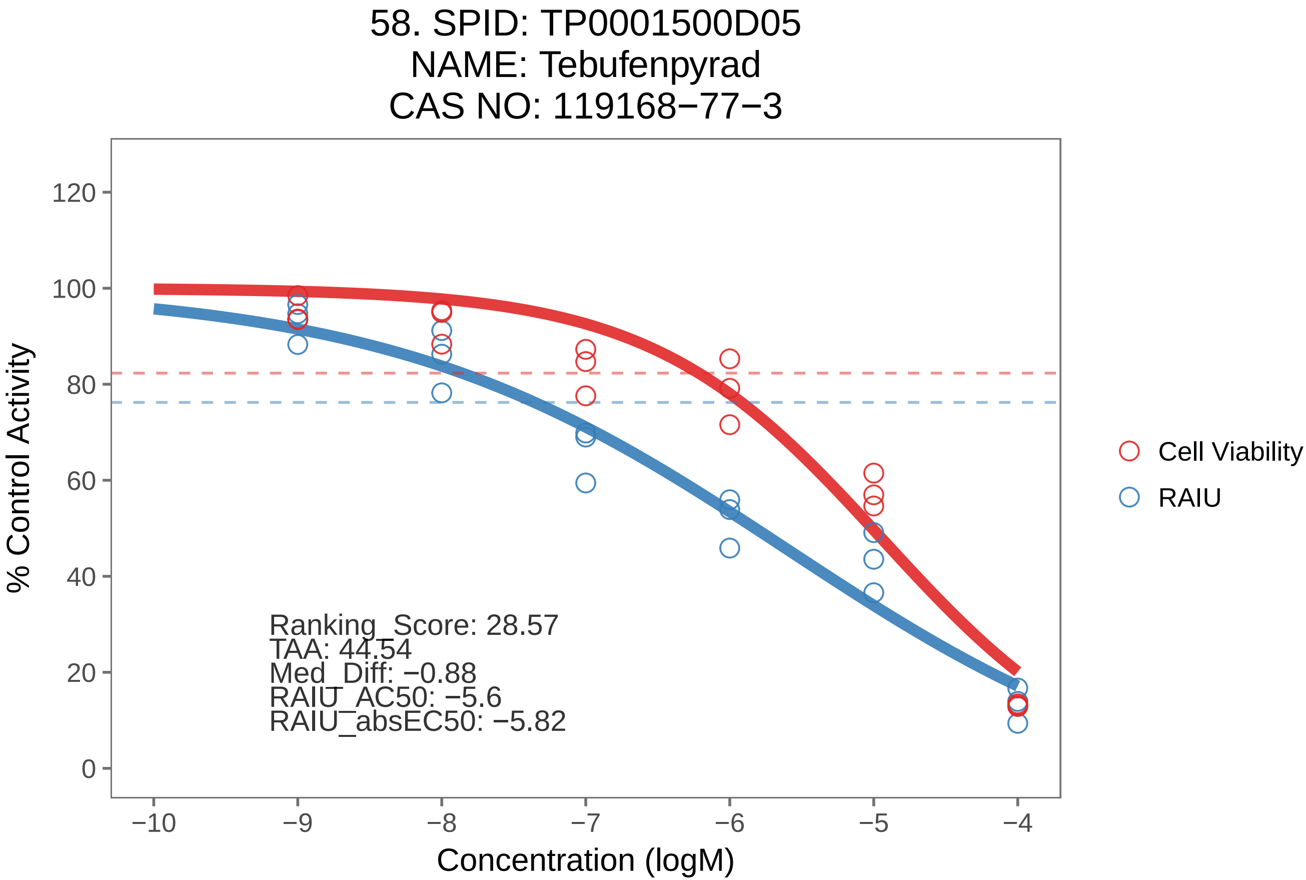

54. SPID: TP0001502G02
NAME: Dibutyl phthalate
CAS NO: 84−74−2
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 31.65
TAA: 6.83
Med_Diff: 25.96
RAIU_AC50: −4.54
RAIU_absEC50: NA
Cell Viability
RAIU

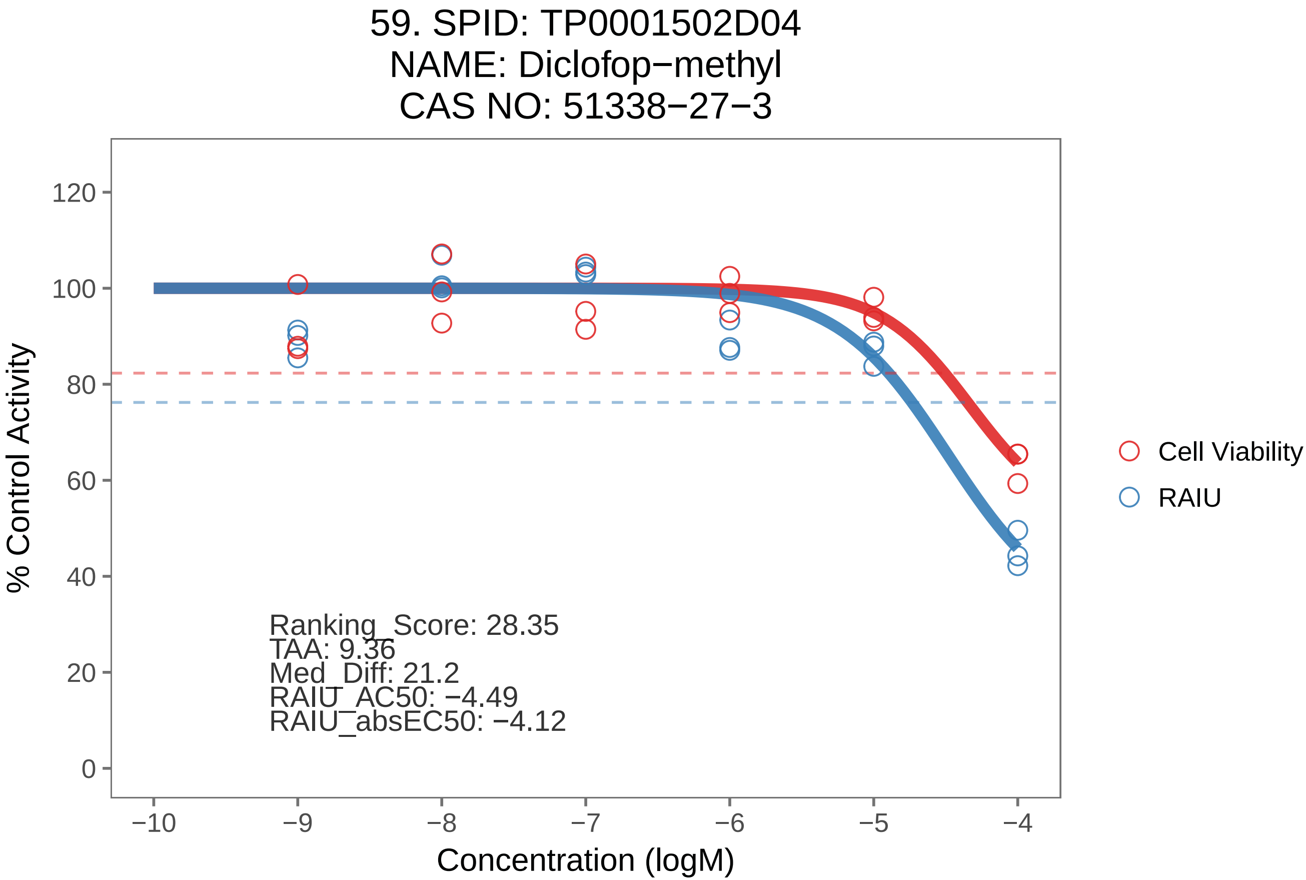

55. SPID: TP0001498C09
NAME: Methylene bis(thiocyanate)
CAS NO: 6317−18−6
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 30.68
TAA: 23.33
Med_Diff: 14.57
RAIU_AC50: −4.66
RAIU_absEC50: −4.79
Cell Viability
RAIU

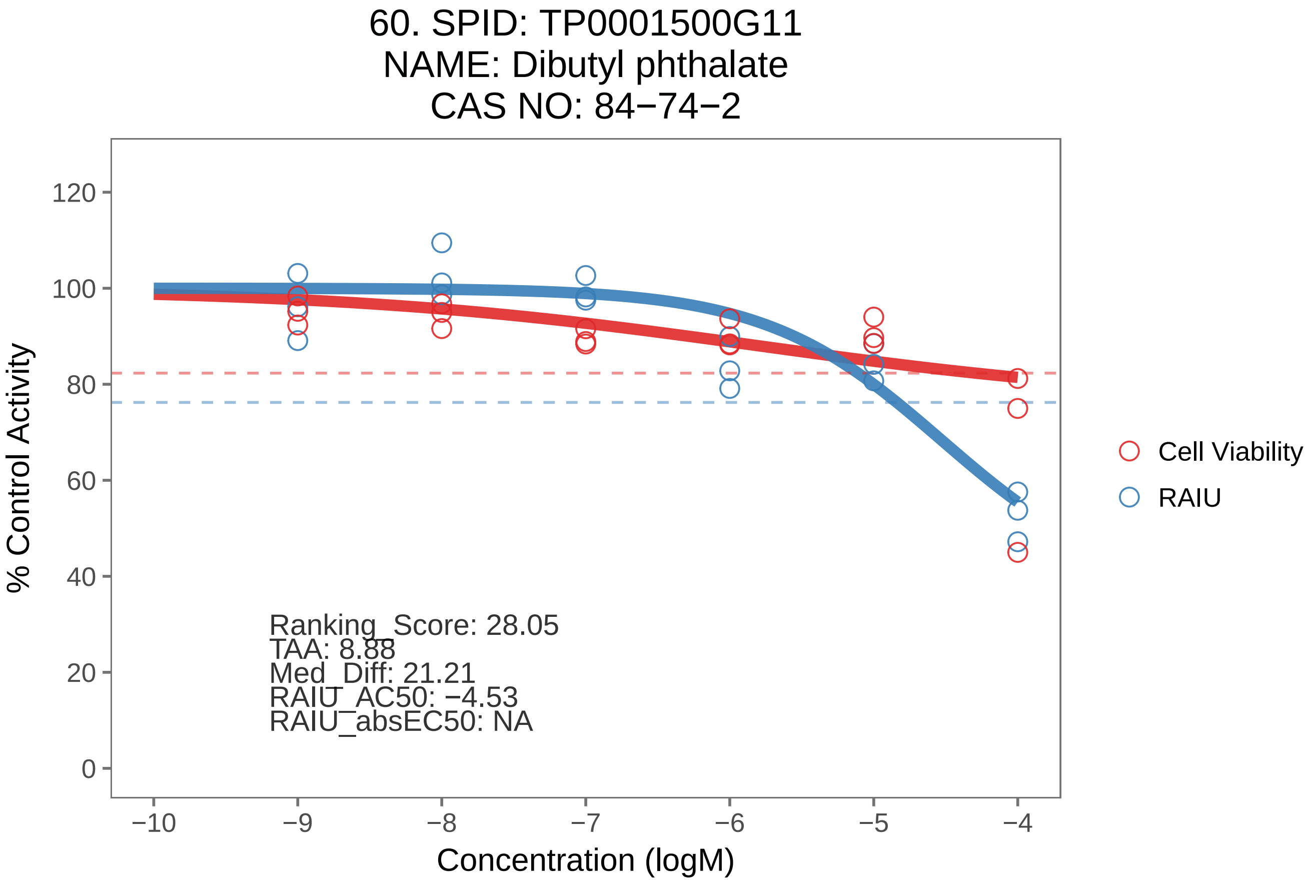


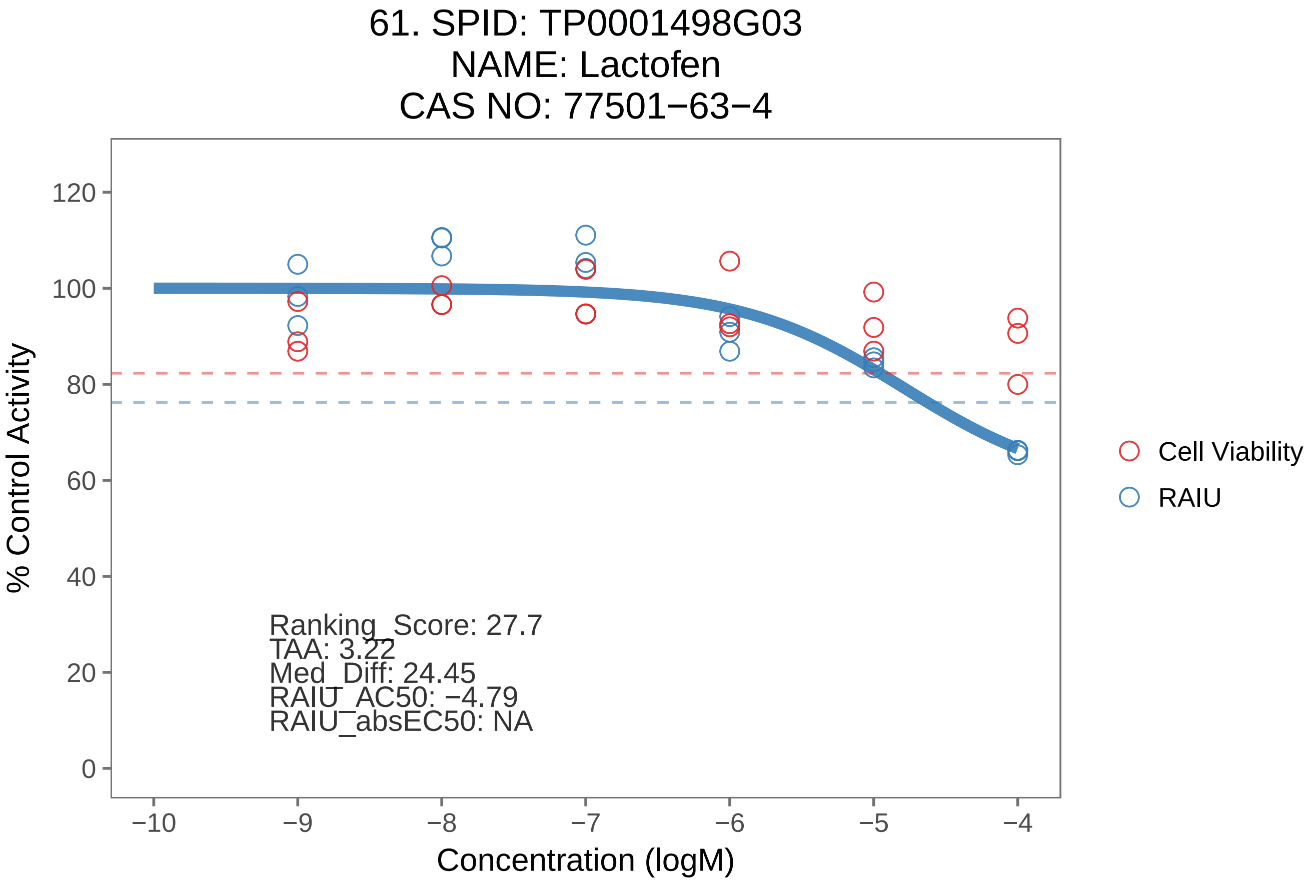
56. SPID: TP0001502D03
NAME: Bisphenol A
CAS NO: 80−05−7
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 29.86
TAA: 3.01
Med_Diff: 26.66
RAIU_AC50: −4.36
RAIU_absEC50: NA
Cell Viability
RAIU

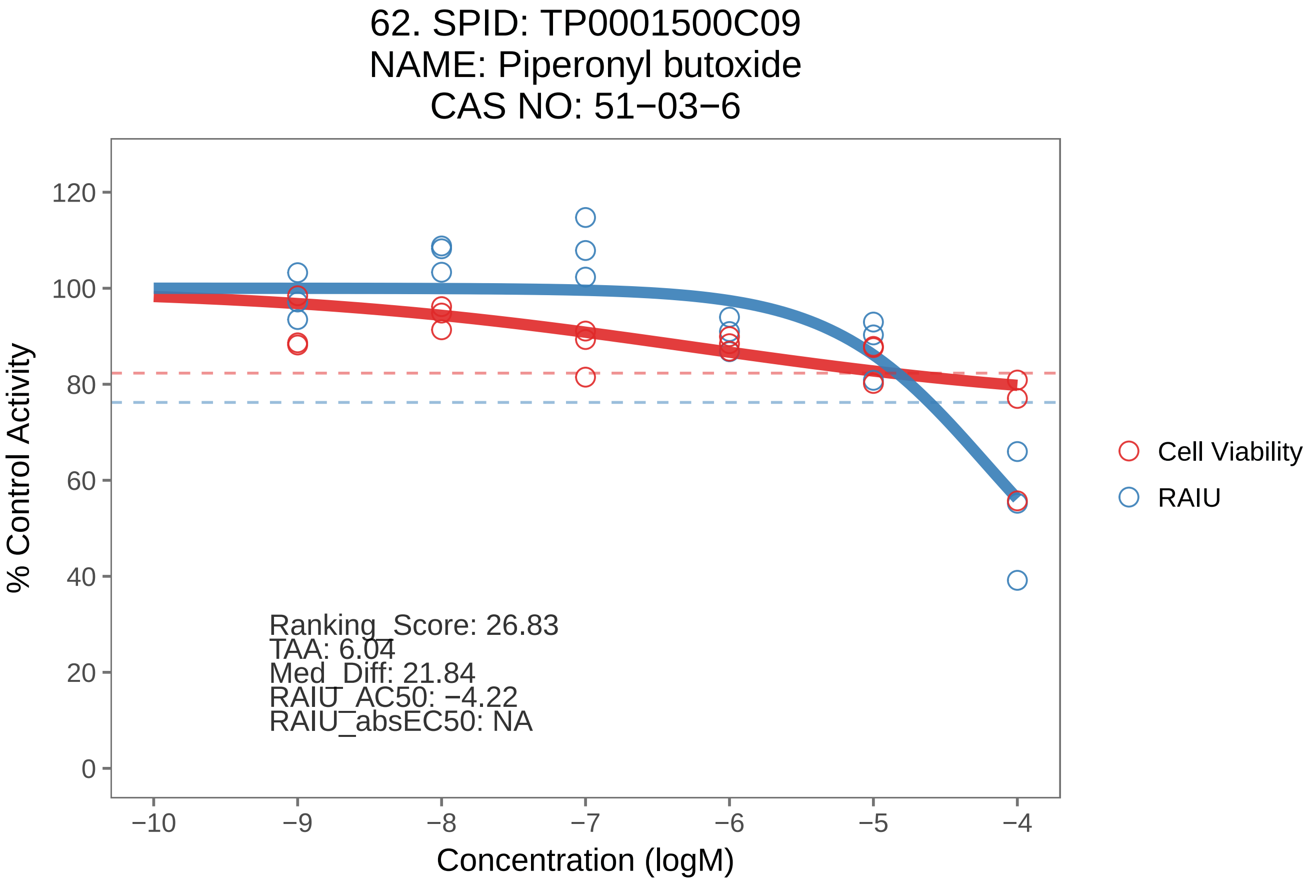

57. SPID: TP0001498B08
NAME: Dithiopyr
CAS NO: 97886−45−8
% Control Activity
0
20
40
60
80
100
120
Concentration (logM)
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 28.75
TAA: 4.55
Med_Diff: 24.62
RAIU_AC50: −4.65
RAIU_absEC50: NA
Cell Viability
RAIU

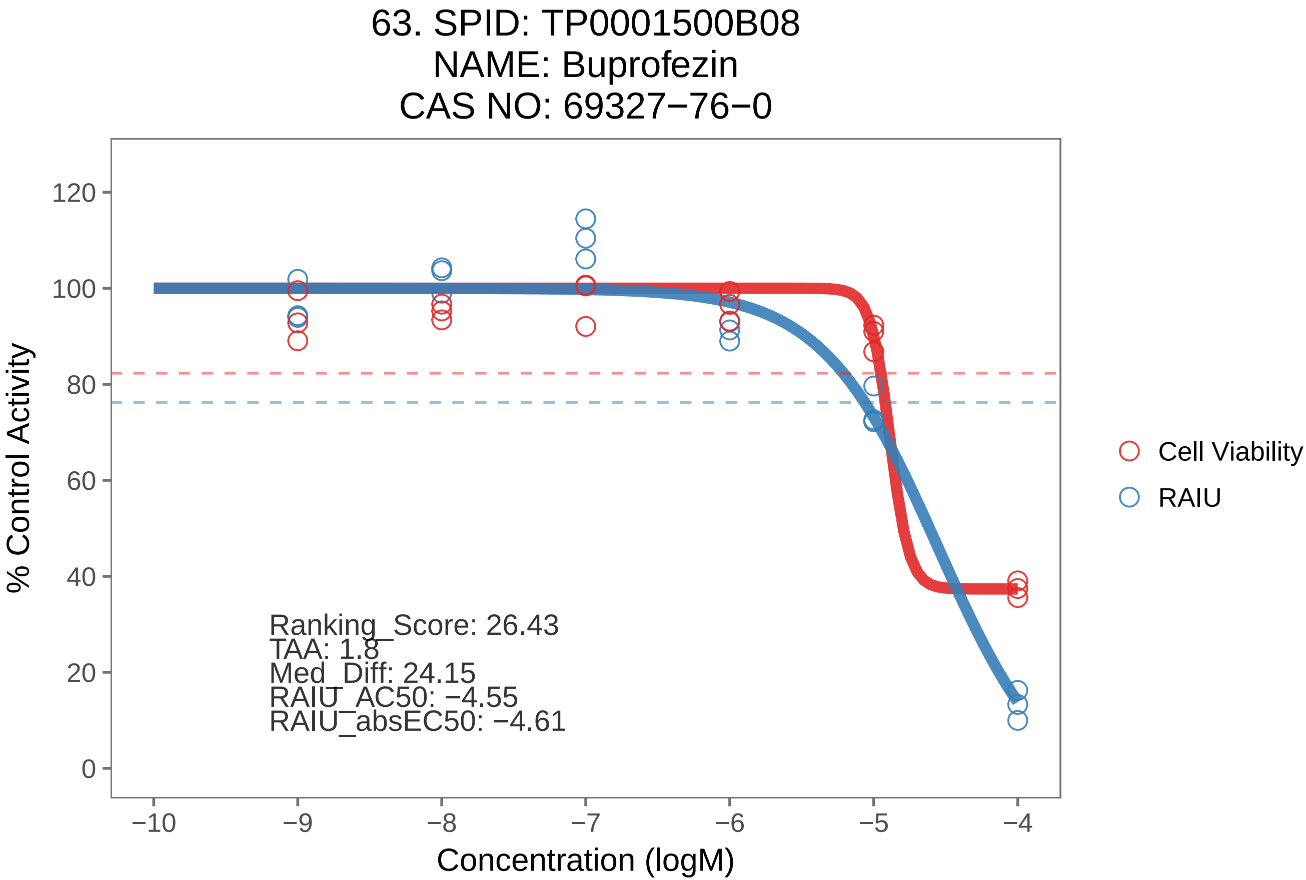

58. SPID: TP0001500D05
NAME: Tebufenpyrad
CAS NO: 119168−77−3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 28.57
TAA: 44.54
Med_Diff: −0.88
RAIU_AC50: −5.6
RAIU_absEC50: −5.82
Cell Viability
RAIU

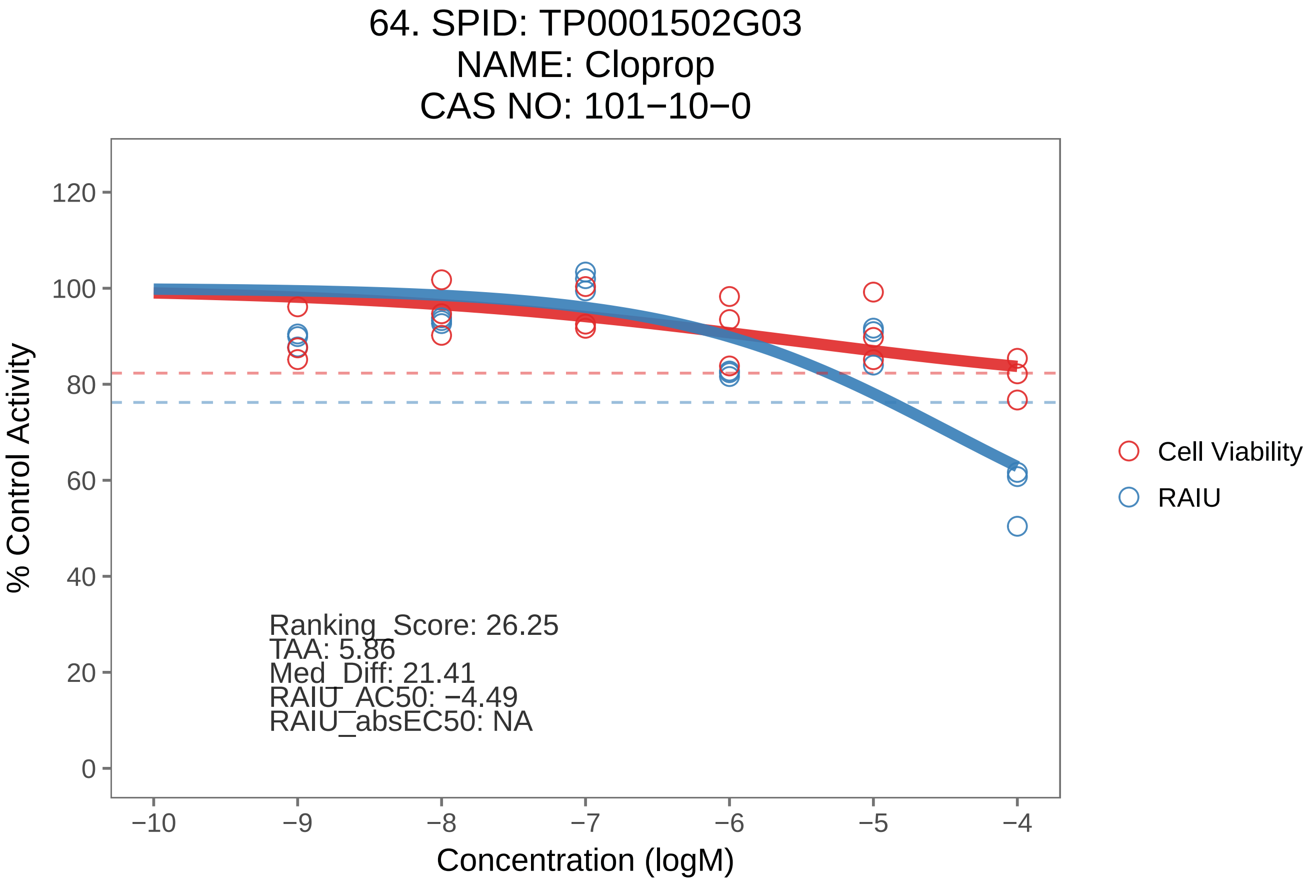

59. SPID: TP0001502D04
NAME: Diclofop−methyl
CAS NO: 51338−27−3
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 28.35
TAA: 9.36
Med_Diff: 21.2
RAIU_AC50: −4.49
RAIU_absEC50: −4.12
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4

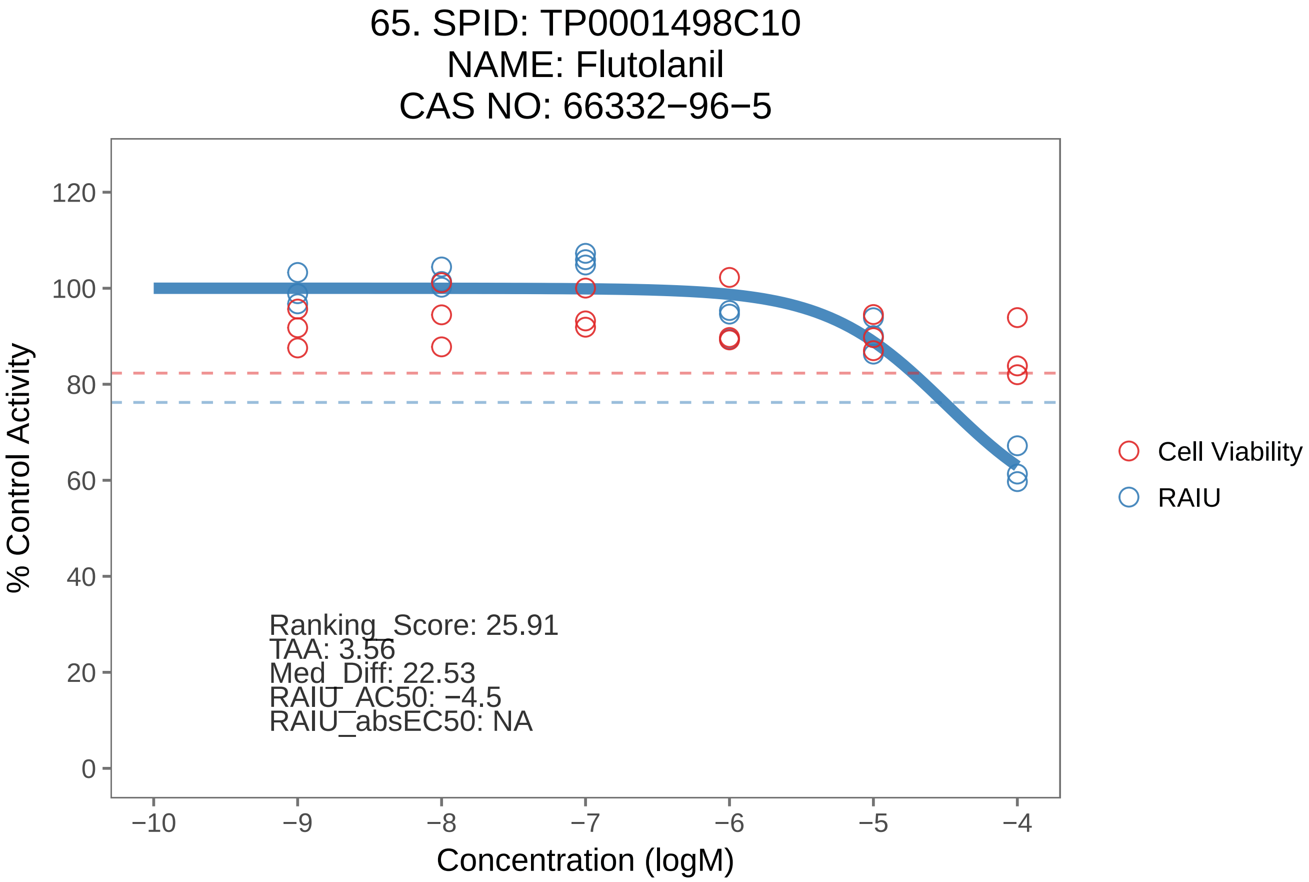

60. SPID: TP0001500G11
NAME: Dibutyl phthalate
CAS NO: 84−74−2
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 28.05
TAA: 8.88
Med_Diff: 21.21
RAIU_AC50: −4.53
RAIU_absEC50: NA
Cell Viability
RAIU


61. SPID: TP0001498G03
NAME: Lactofen
CAS NO: 77501−63−4
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 27.7
TAA: 3.22
Med_Diff: 24.45
RAIU_AC50: −4.79
RAIU_absEC50: NA
Cell Viability
RAIU

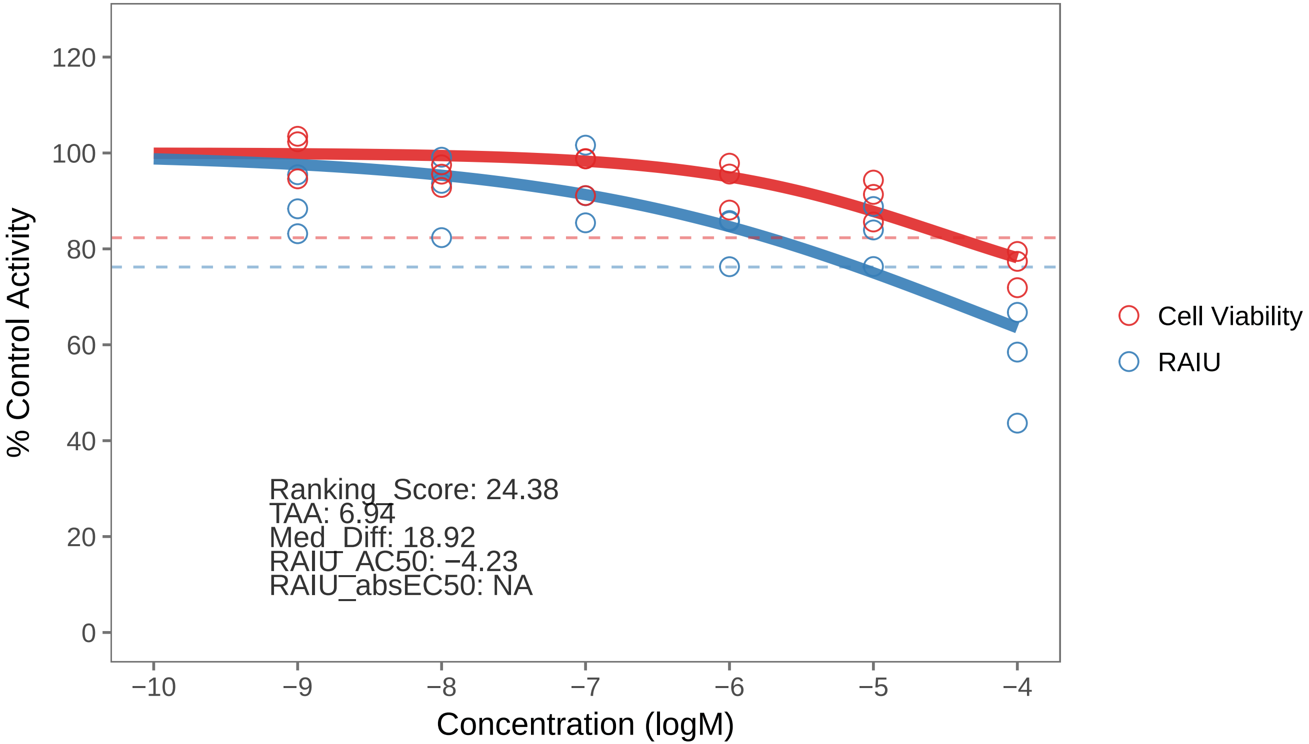

62. SPID: TP0001500C09
NAME: Piperonyl butoxide
CAS NO: 51−03−6
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 26.83
TAA: 6.04
Med_Diff: 21.84
RAIU_AC50: −4.22
RAIU_absEC50: NA
Cell Viability
RAIU

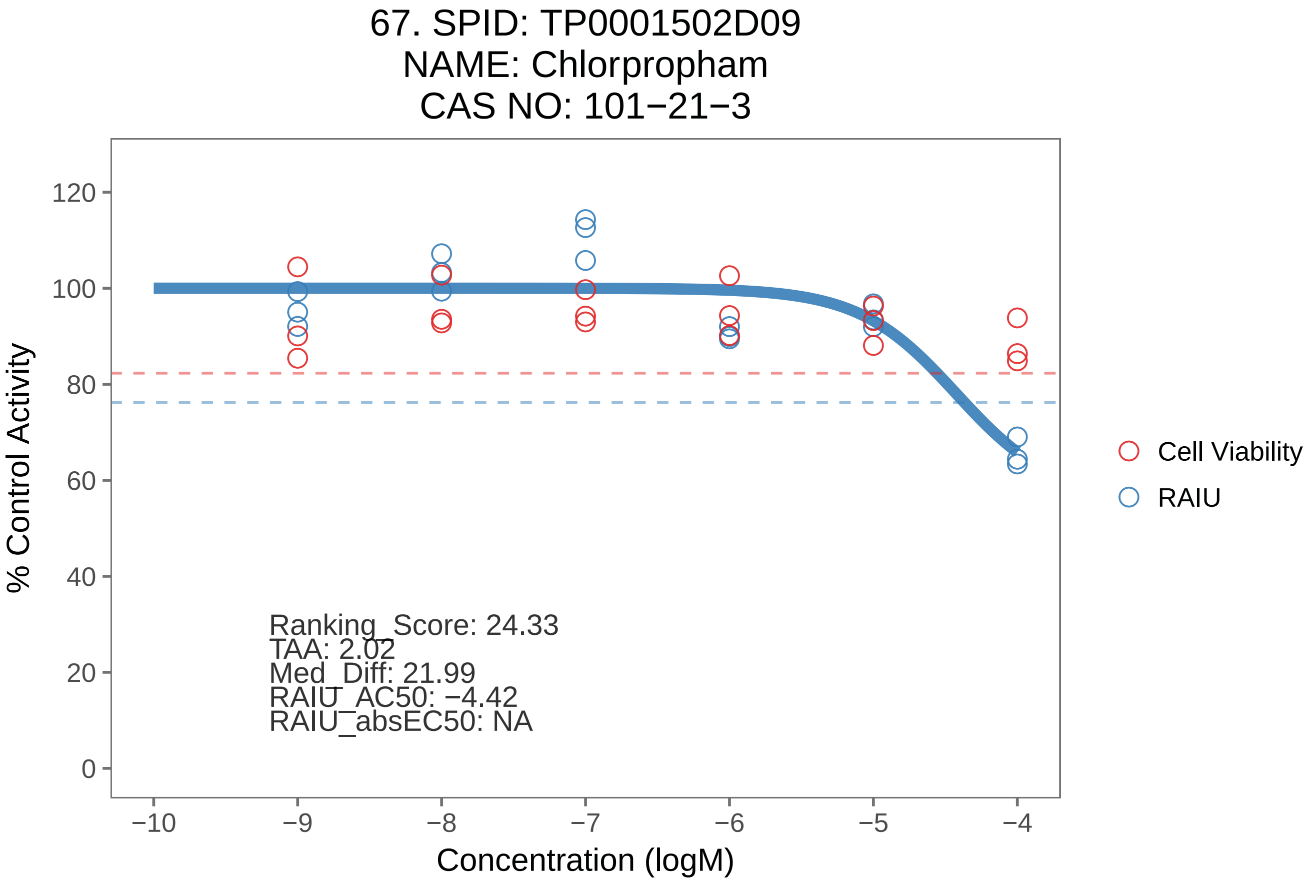

63. SPID: TP0001500B08
NAME: Buprofezin
CAS NO: 69327−76−0
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 26.43
TAA: 1.8
Med_Diff: 24.15
RAIU_AC50: −4.55
RAIU_absEC50: −4.61
Cell Viability
RAIU

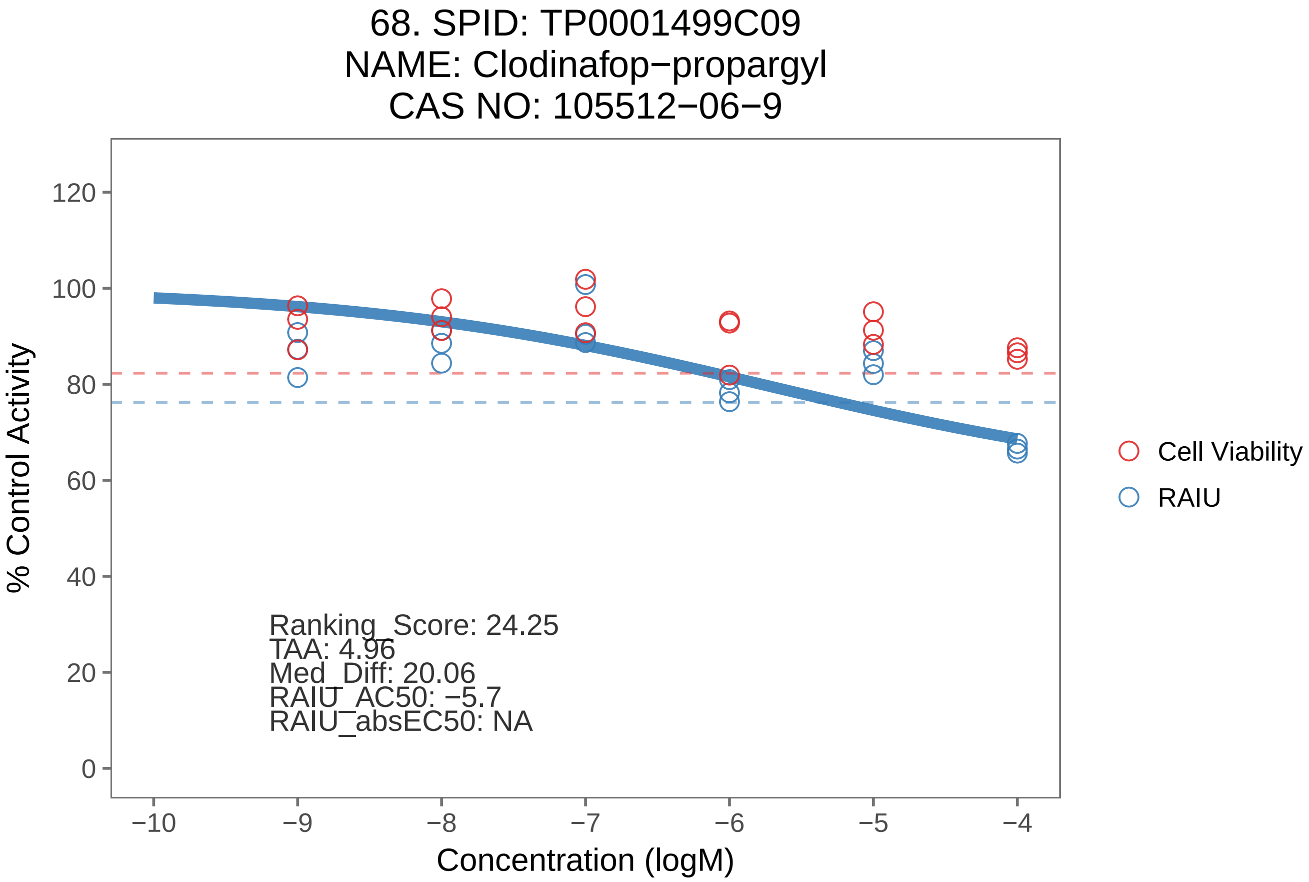

64. SPID: TP0001502G03
NAME: Cloprop
CAS NO: 101−10−0
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Cell Viability
RAIU
Ranking_Score: 26.25
TAA: 5.86
Med_Diff: 21.41
RAIU_AC50: −4.49
RAIU_absEC50: NA

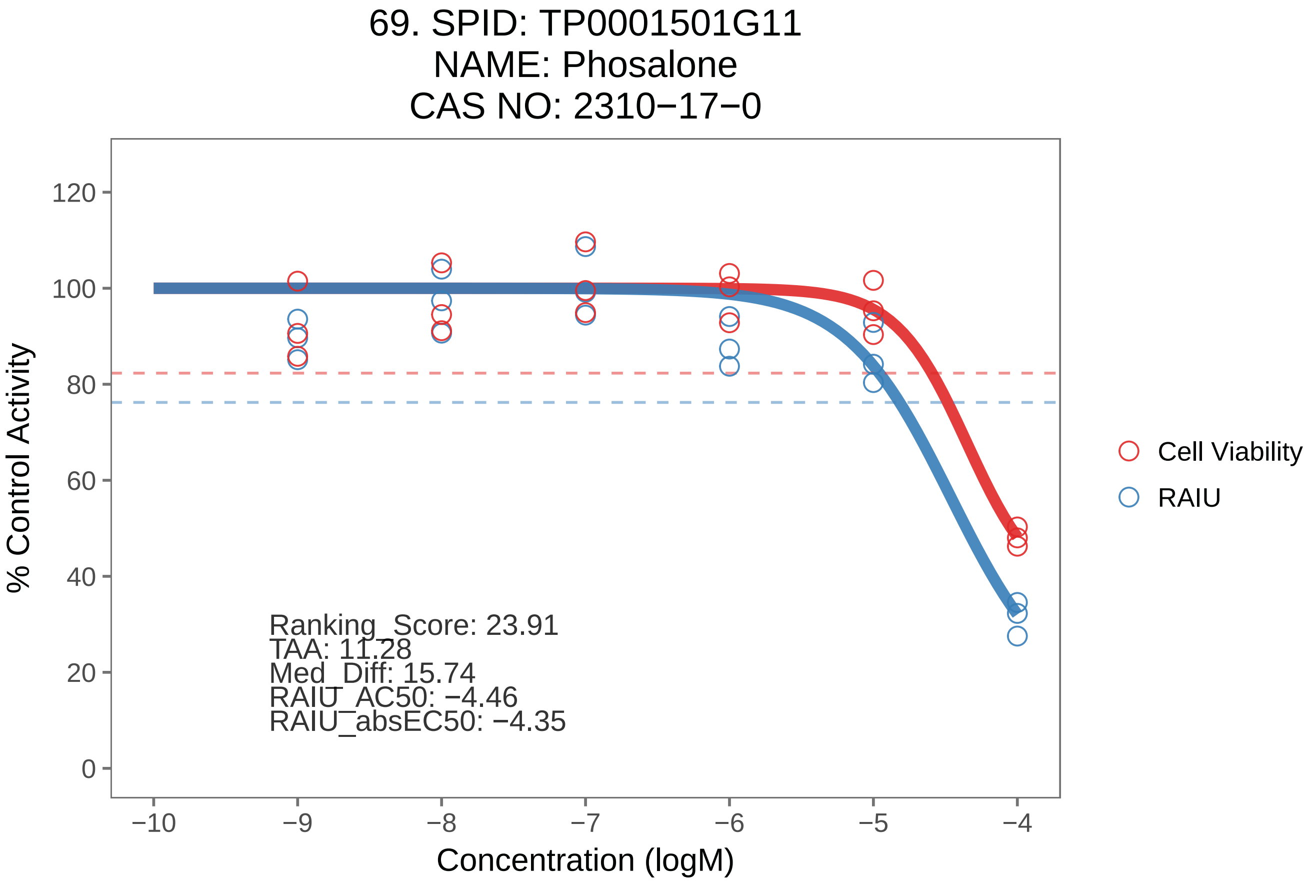

65. SPID: TP0001498C10
NAME: Flutolanil
CAS NO: 66332−96−5
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 25.91
TAA: 3.56
Med_Diff: 22.53
RAIU_AC50: −4.5
RAIU_absEC50: NA
Cell Viability
RAIU

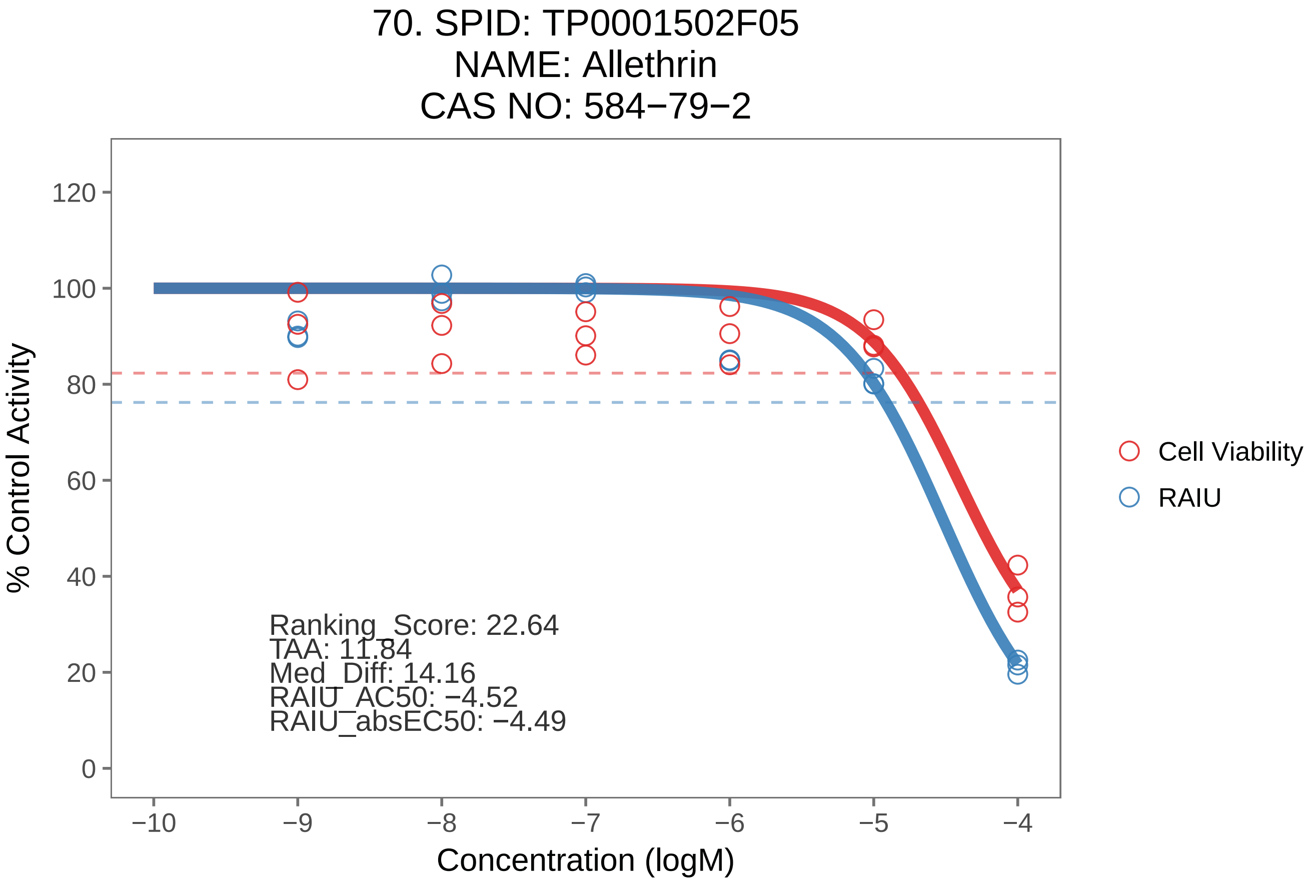
66. SPID: TP0001500G03
NAME: Cinmethylin
CAS NO: 87818−31−3

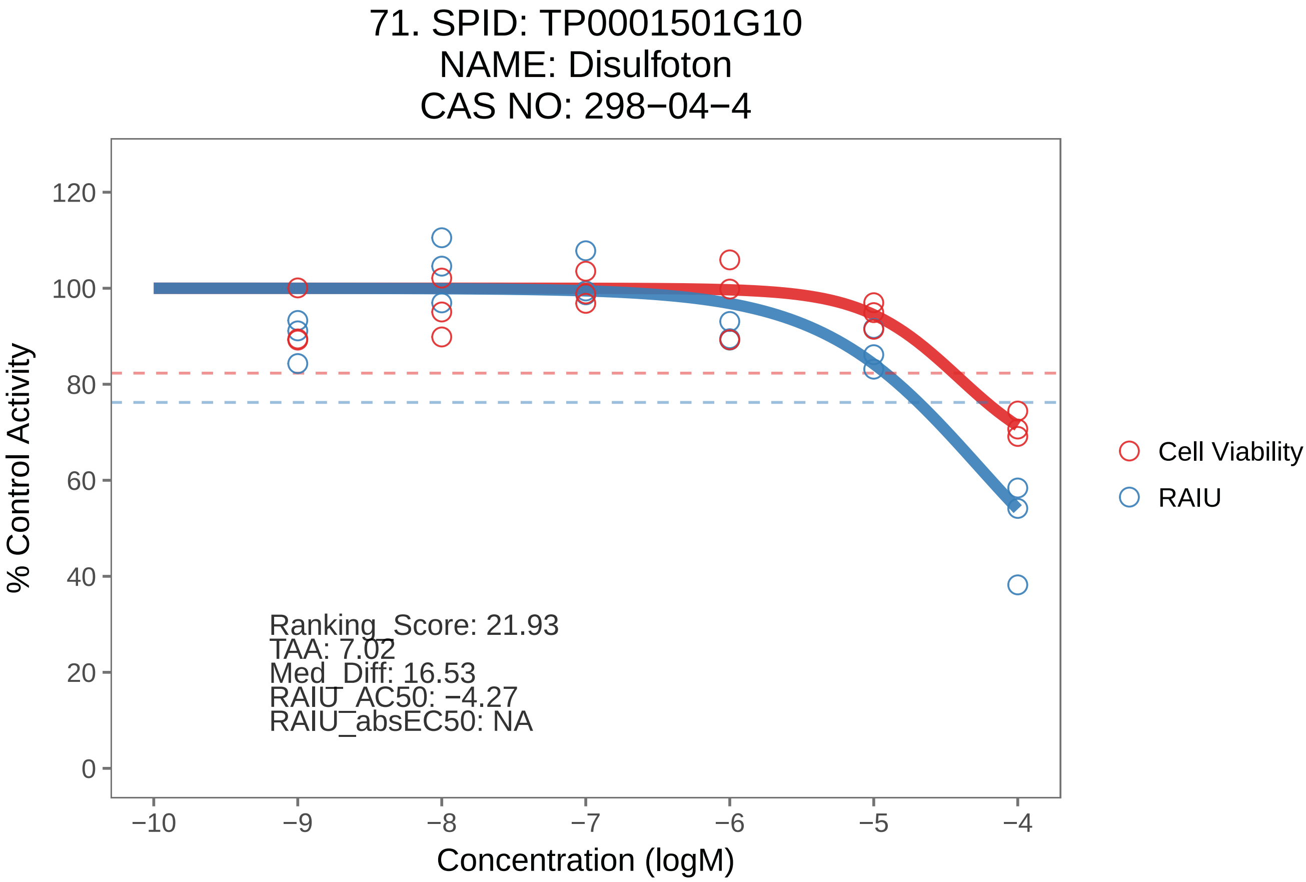


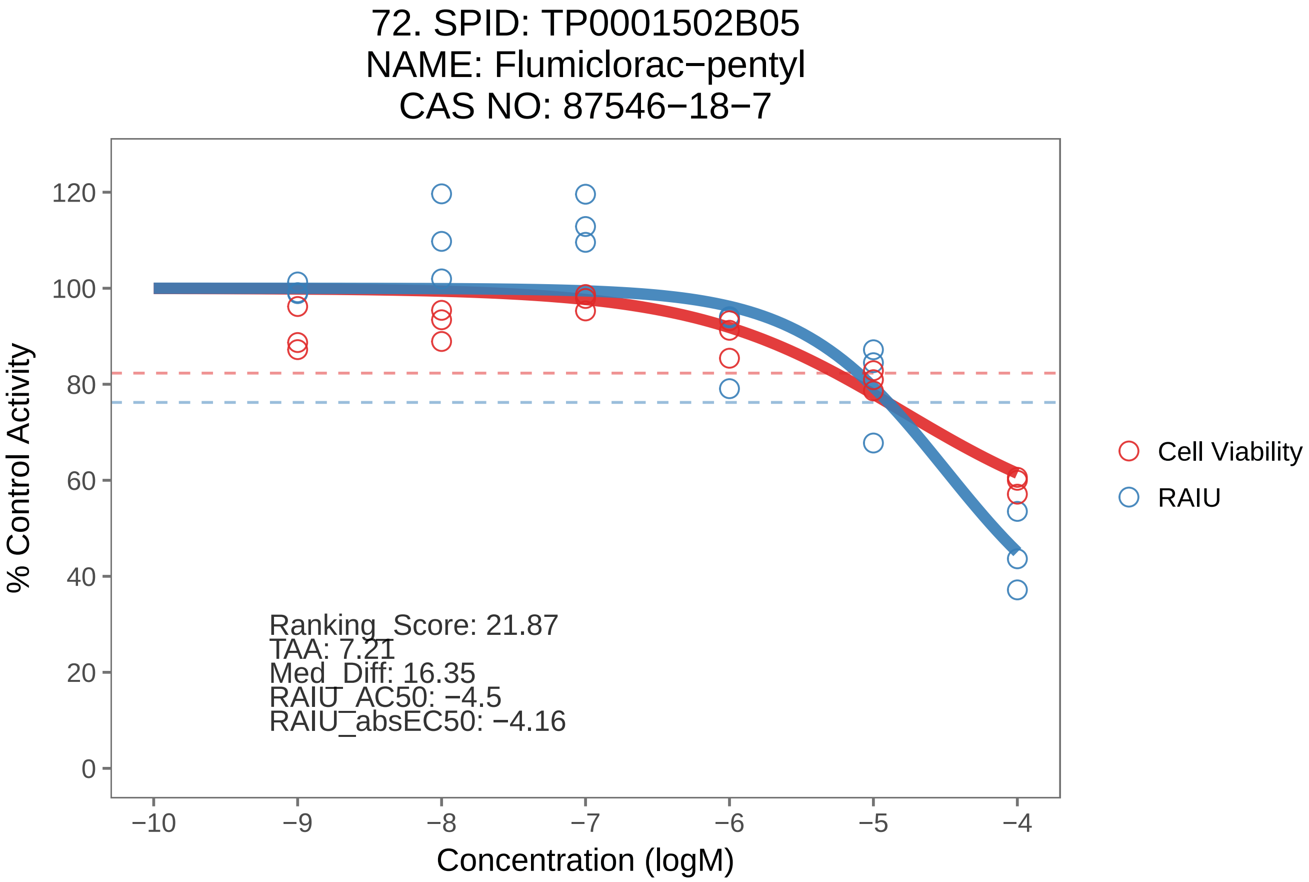

67. SPID: TP0001502D09
NAME: Chlorpropham
CAS NO: 101−21−3
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 24.33
TAA: 2.02
Med_Diff: 21.99
RAIU_AC50: −4.42
RAIU_absEC50: NA
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

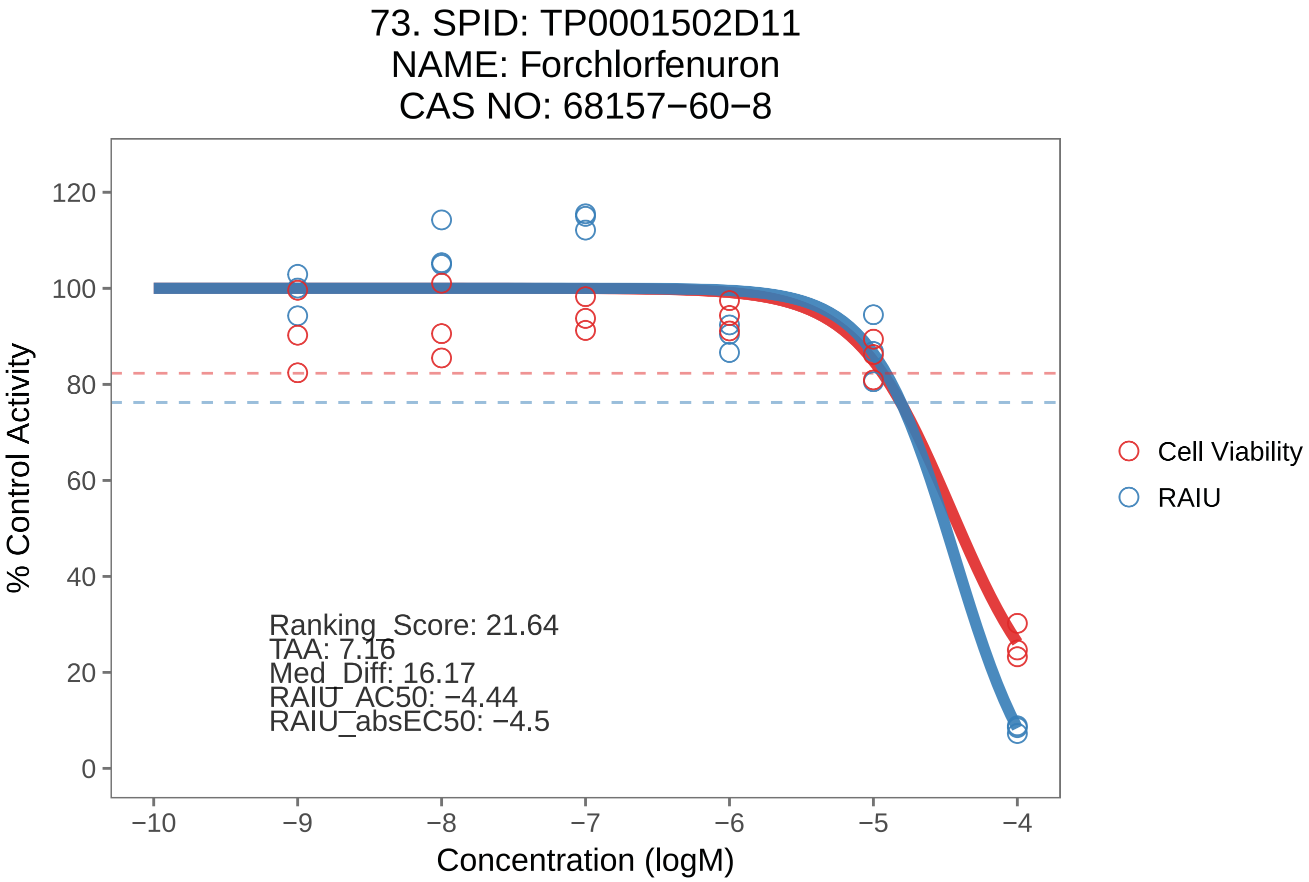

68. SPID: TP0001499C09
NAME: Clodinafop−propargyl
CAS NO: 105512−06−9
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 24.25
TAA: 4.96
Med_Diff: 20.06
RAIU_AC50: −5.7
RAIU_absEC50: NA

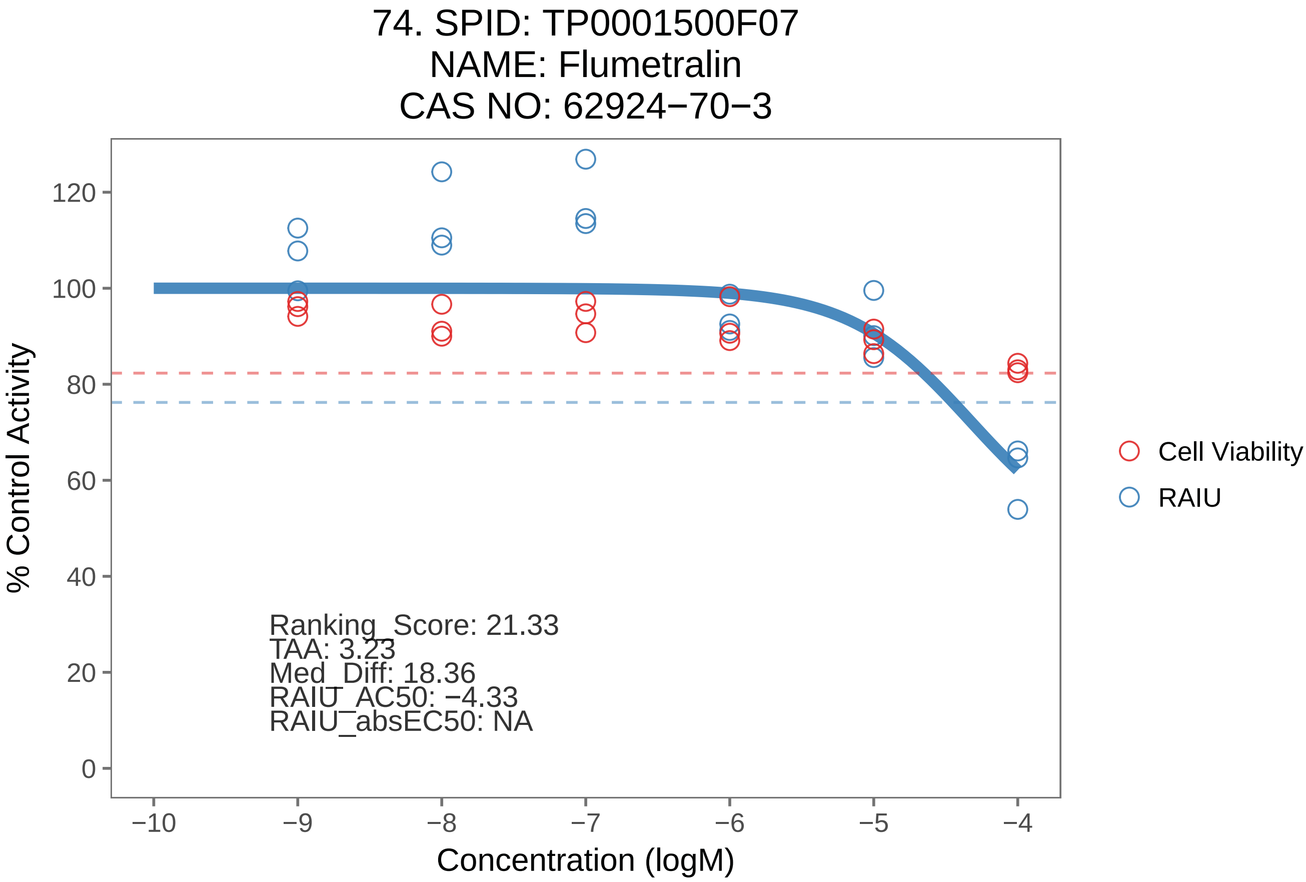

69. SPID: TP0001501G11
NAME: Phosalone
CAS NO: 2310−17−0
120
100
80
60
40
20
0
% Control Activity
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 23.91
TAA: 11.28
Med_Diff: 15.74
RAIU_AC50: −4.46
RAIU_absEC50: −4.35

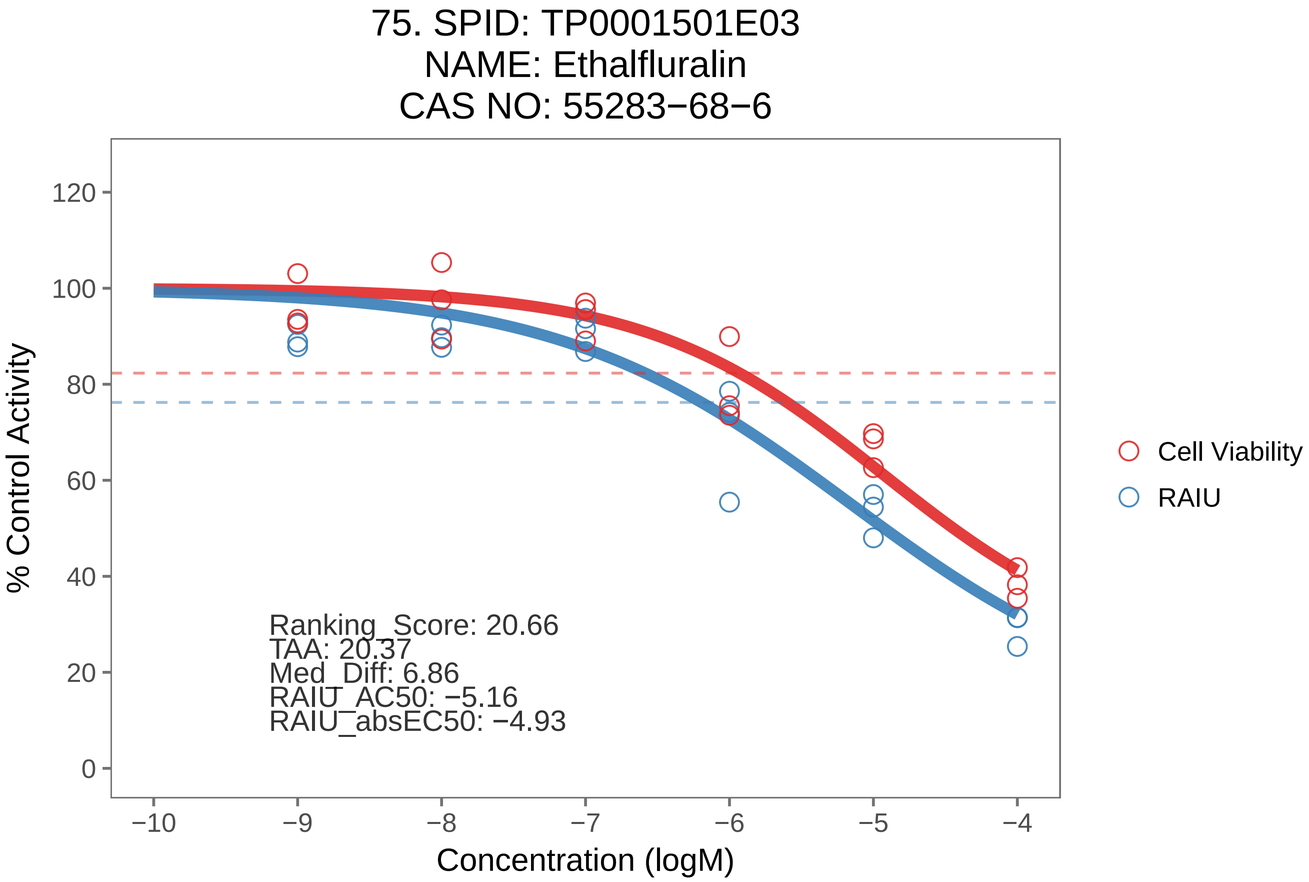

70. SPID: TP0001502F05
NAME: Allethrin
CAS NO: 584−79−2
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 22.64
TAA: 11.84
Med_Diff: 14.16
RAIU_AC50: −4.52
RAIU_absEC50: −4.49
Cell Viability
RAIU

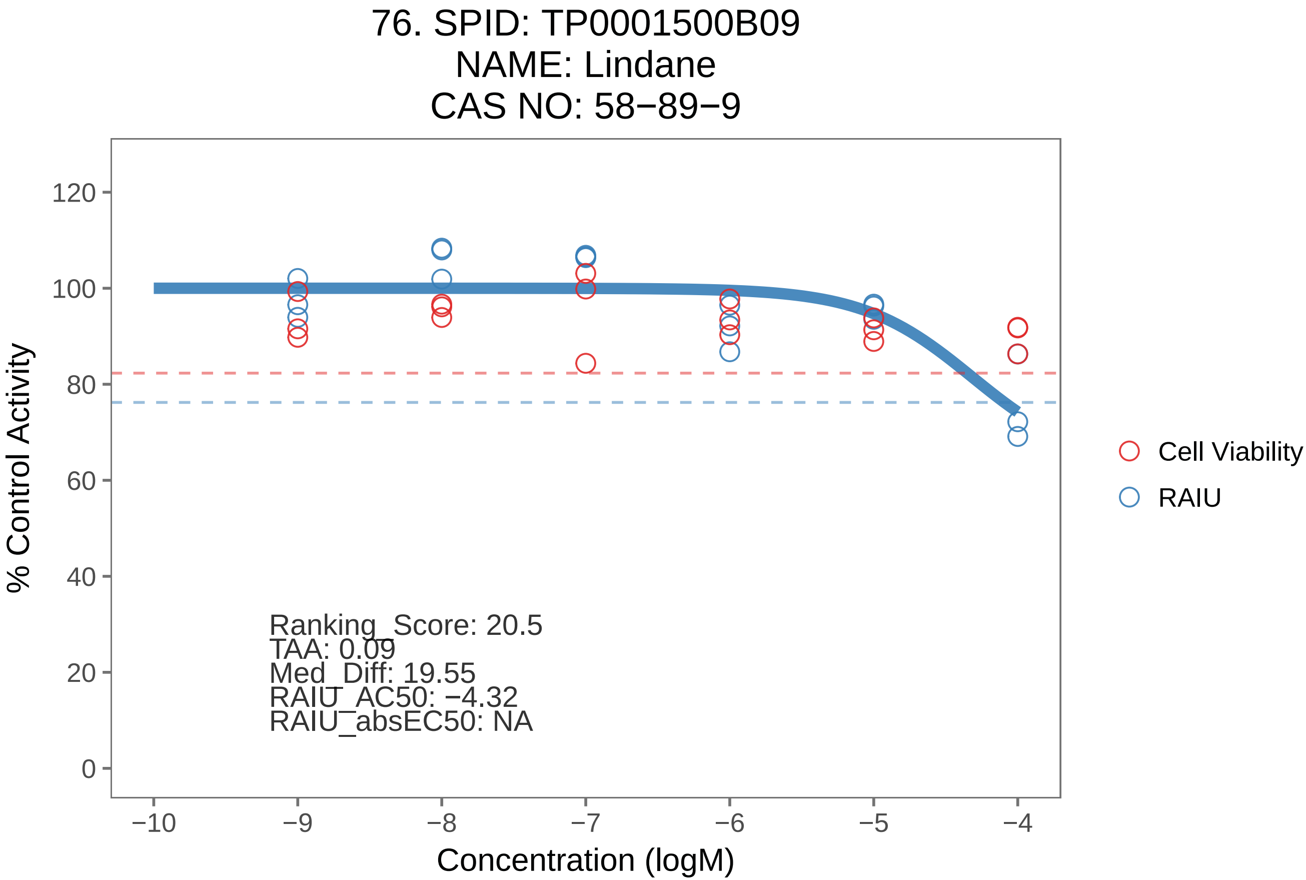

71. SPID: TP0001501G10
NAME: Disulfoton
CAS NO: 298−04−4
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 21.93
TAA: 7.02
Med_Diff: 16.53
RAIU_AC50: −4.27
RAIU_absEC50: NA
Cell Viability
RAIU

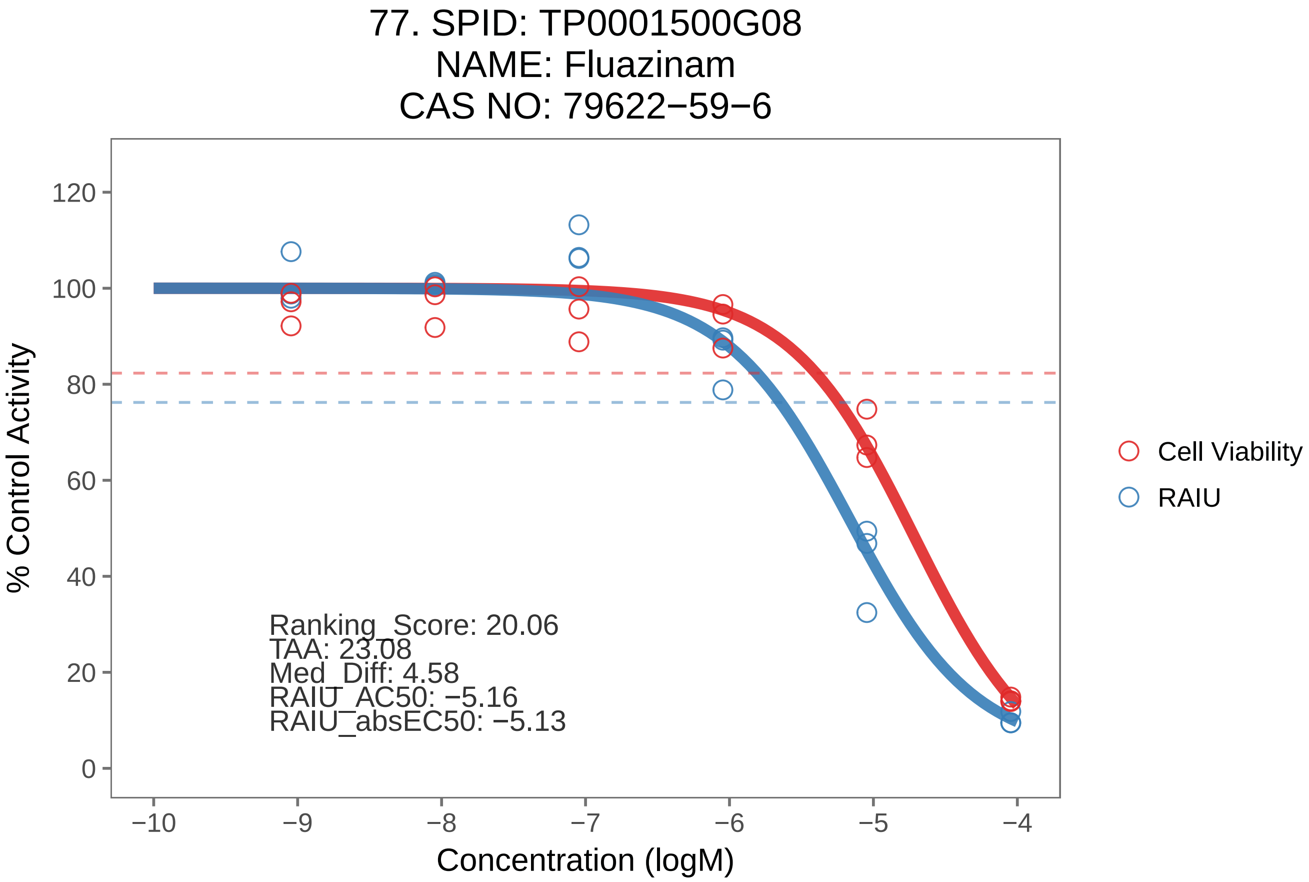

72. SPID: TP0001502B05
NAME: Flumiclorac−pentyl
CAS NO: 87546−18−7
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Cell Viability
RAIU
Ranking_Score: 21.87
TAA: 7.21
Med_Diff: 16.35
RAIU_AC50: −4.5
RAIU_absEC50: −4.16

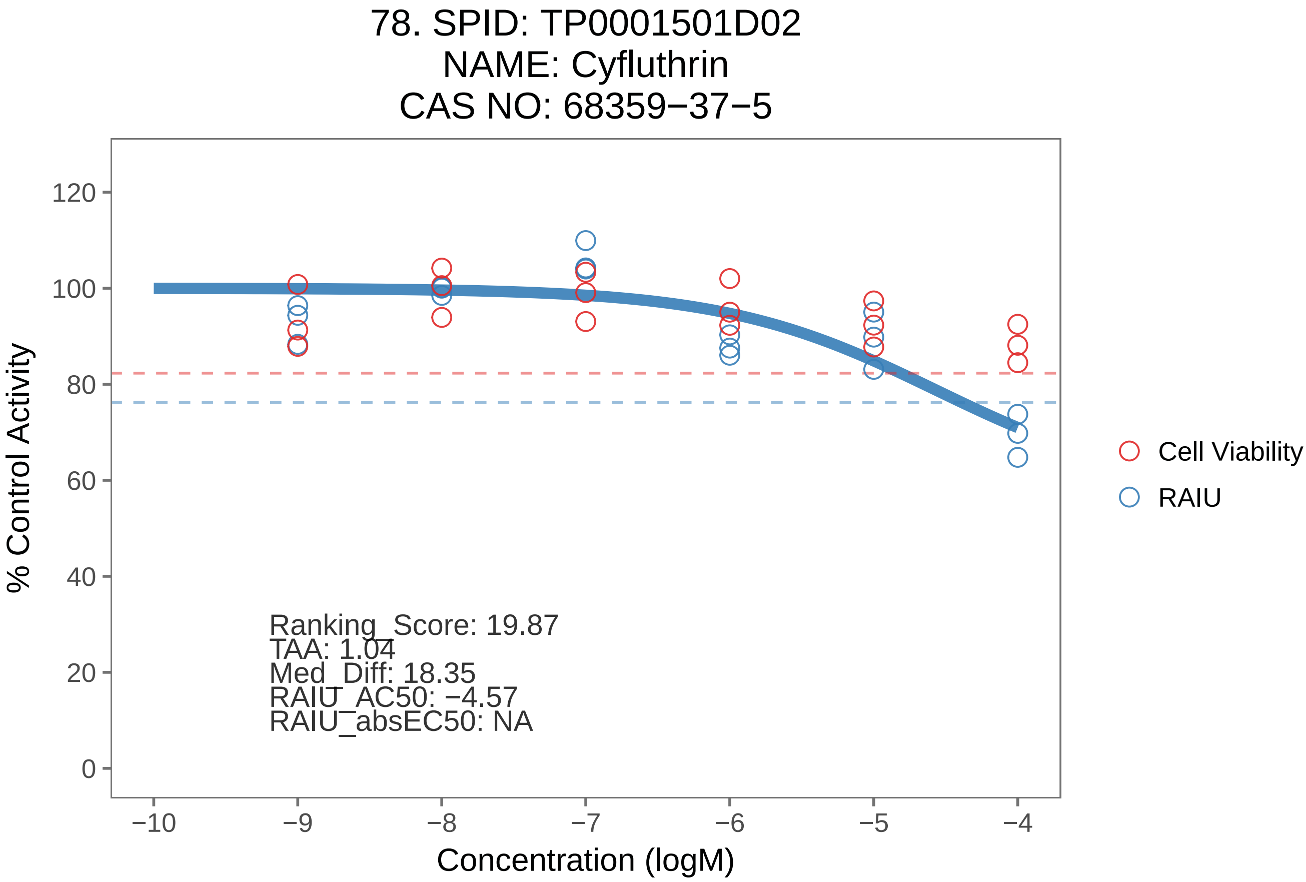

73. SPID: TP0001502D11
NAME: Forchlorfenuron
CAS NO: 68157−60−8
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 21.64
TAA: 7.16
Med_Diff: 16.17
RAIU_AC50: −4.44
RAIU_absEC50: −4.5
Cell Viability
RAIU

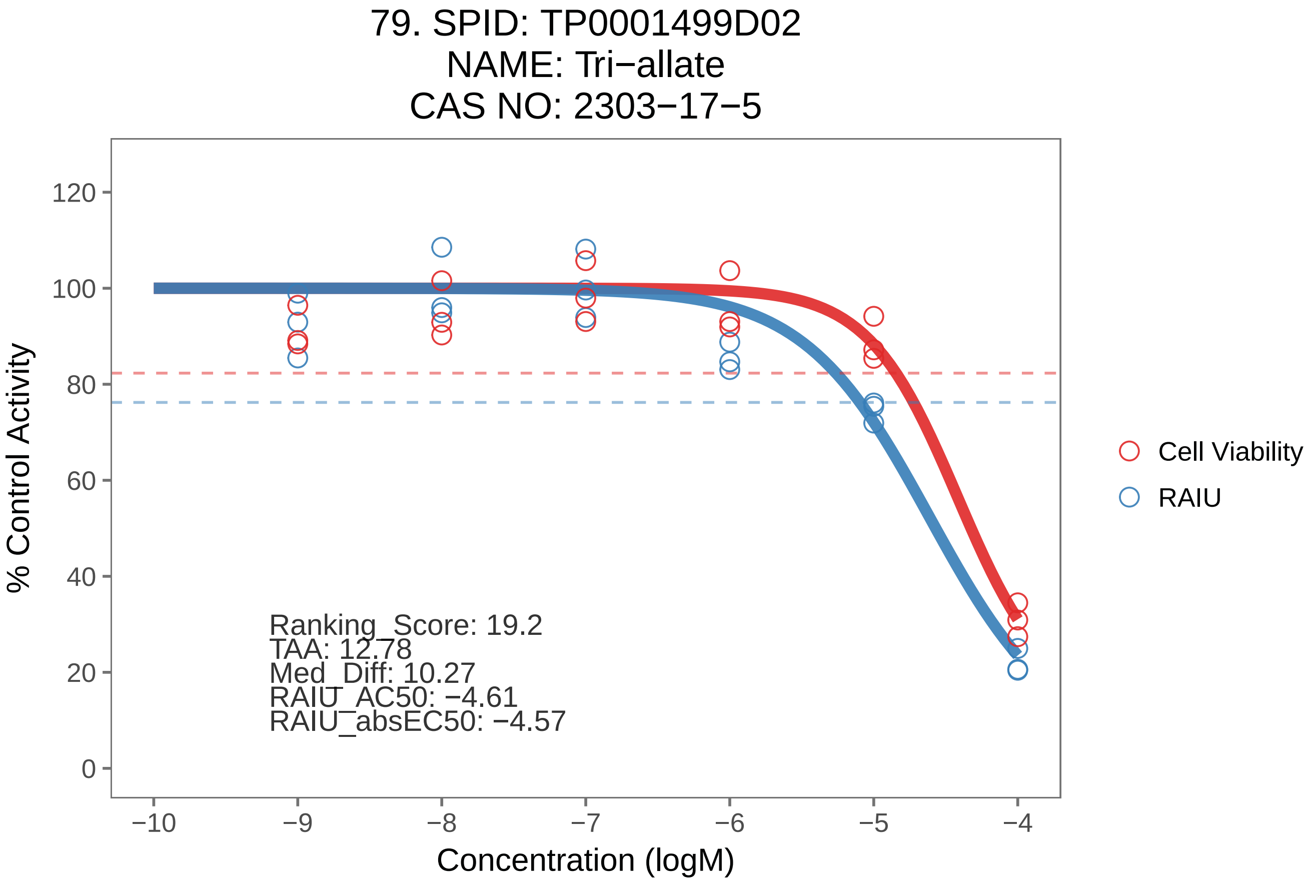

74. SPID: TP0001500F07
NAME: Flumetralin
CAS NO: 62924−70−3
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 21.33
TAA: 3.23
Med_Diff: 18.36
RAIU_AC50: −4.33
RAIU_absEC50: NA
Cell Viability
RAIU

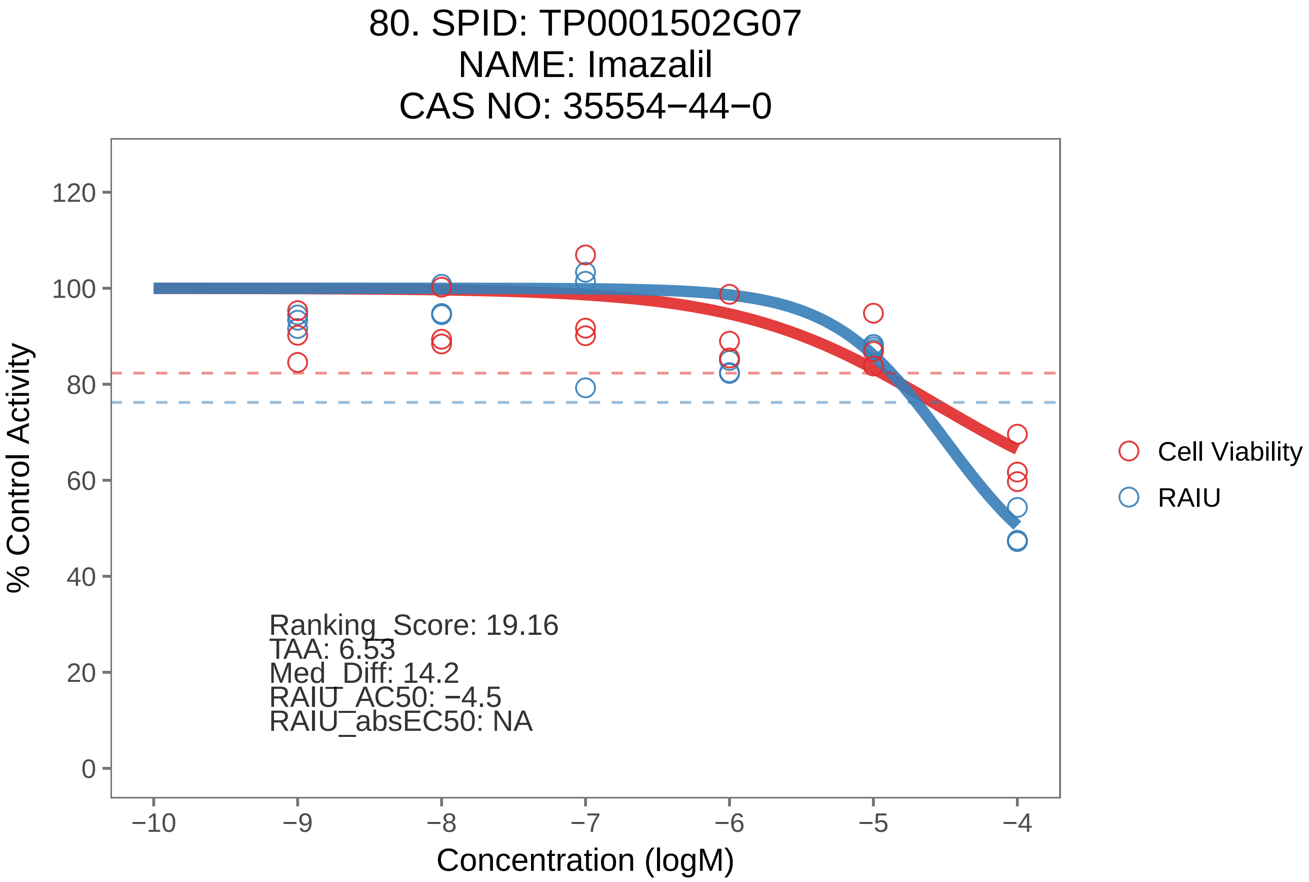

75. SPID: TP0001501E03
NAME: Ethalfluralin
CAS NO: 55283−68−6
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 20.66
TAA: 20.37
Med_Diff: 6.86
RAIU_AC50: −5.16
RAIU_absEC50: −4.93
Cell Viability
RAIU

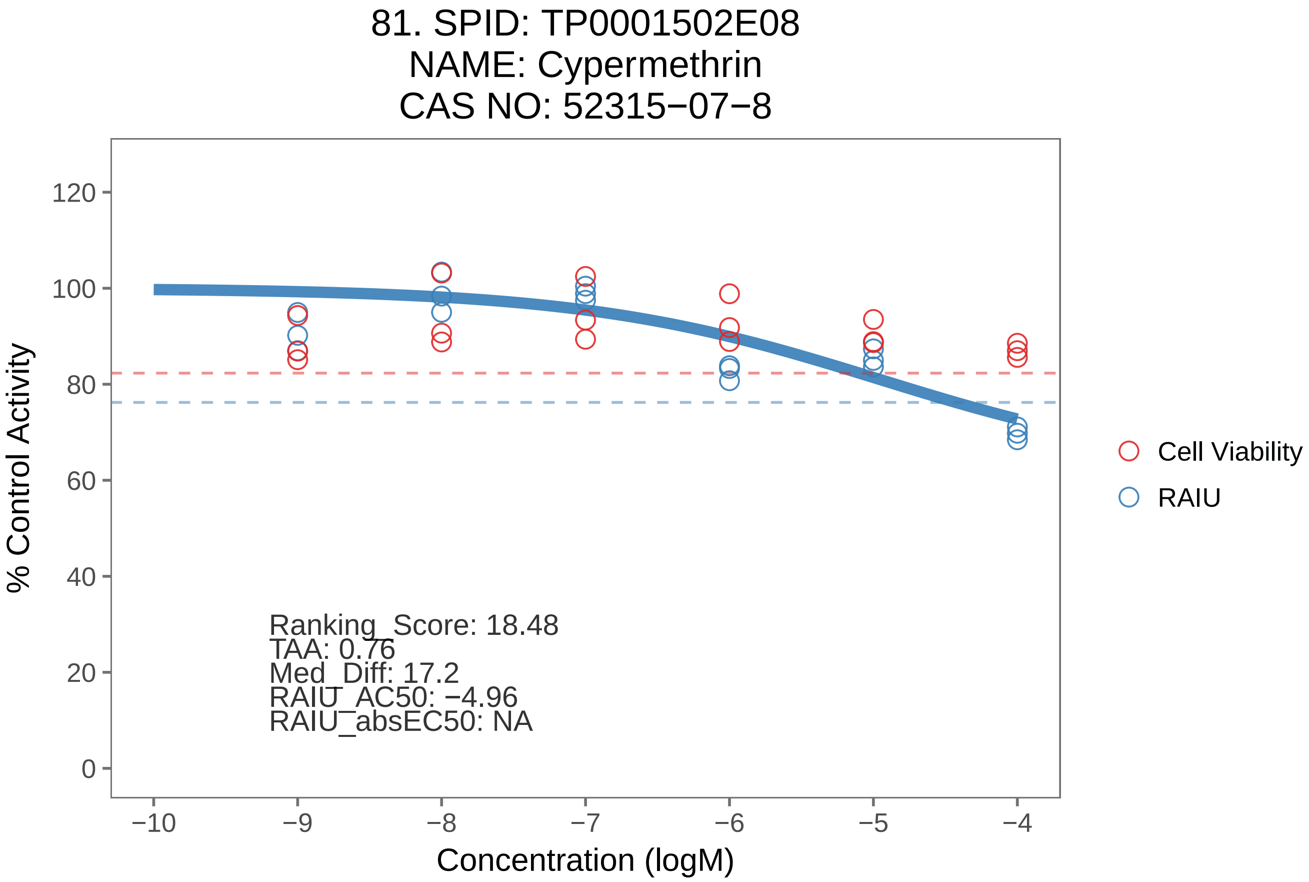

76. SPID: TP0001500B09
NAME: Lindane
CAS NO: 58−89−9
120
100
80
60
40
20
0
% Control Activity
Ranking_Score: 20.5
TAA: 0.09
Med_Diff: 19.55
RAIU_AC50: −4.32
RAIU_absEC50: NA
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU

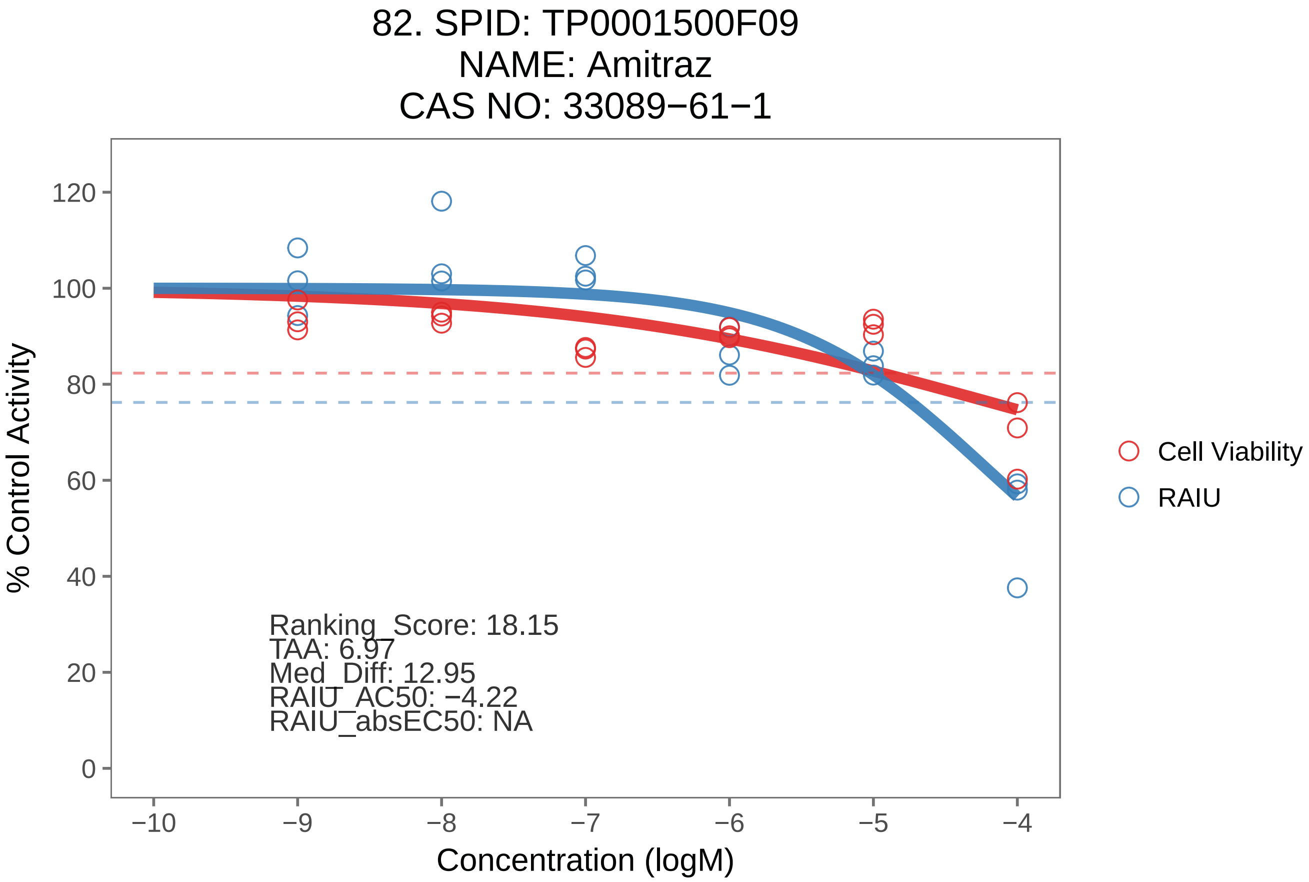

77. SPID: TP0001500G08
NAME: Fluazinam
CAS NO: 79622−59−6
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 20.06
TAA: 23.08
Med_Diff: 4.58
RAIU_AC50: −5.16
RAIU_absEC50: −5.13
Cell Viability
RAIU

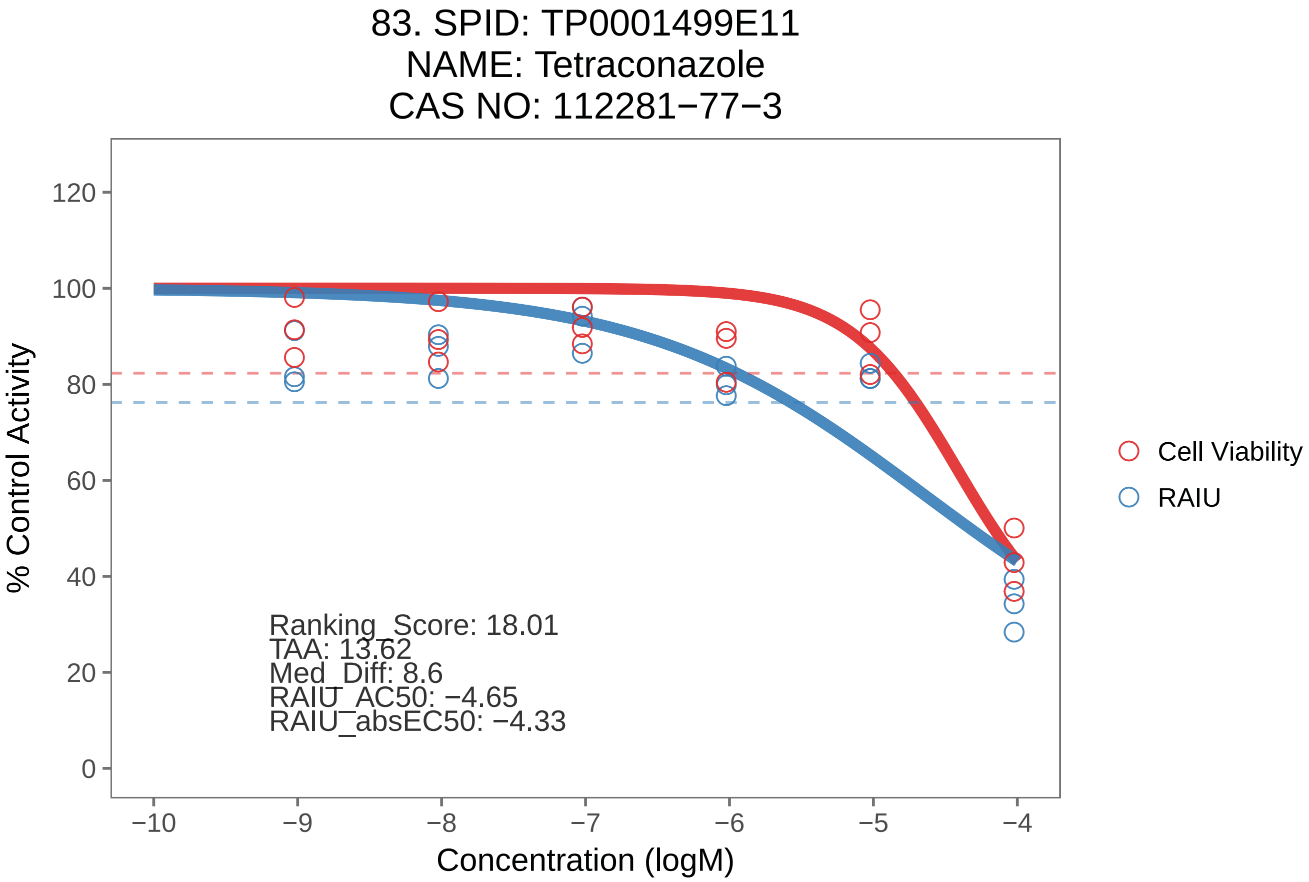

78. SPID: TP0001501D02
NAME: Cyfluthrin
CAS NO: 68359−37−5
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 19.87
TAA: 1.04
Med_Diff: 18.35
RAIU_AC50: −4.57
RAIU_absEC50: NA
Cell Viability
RAIU

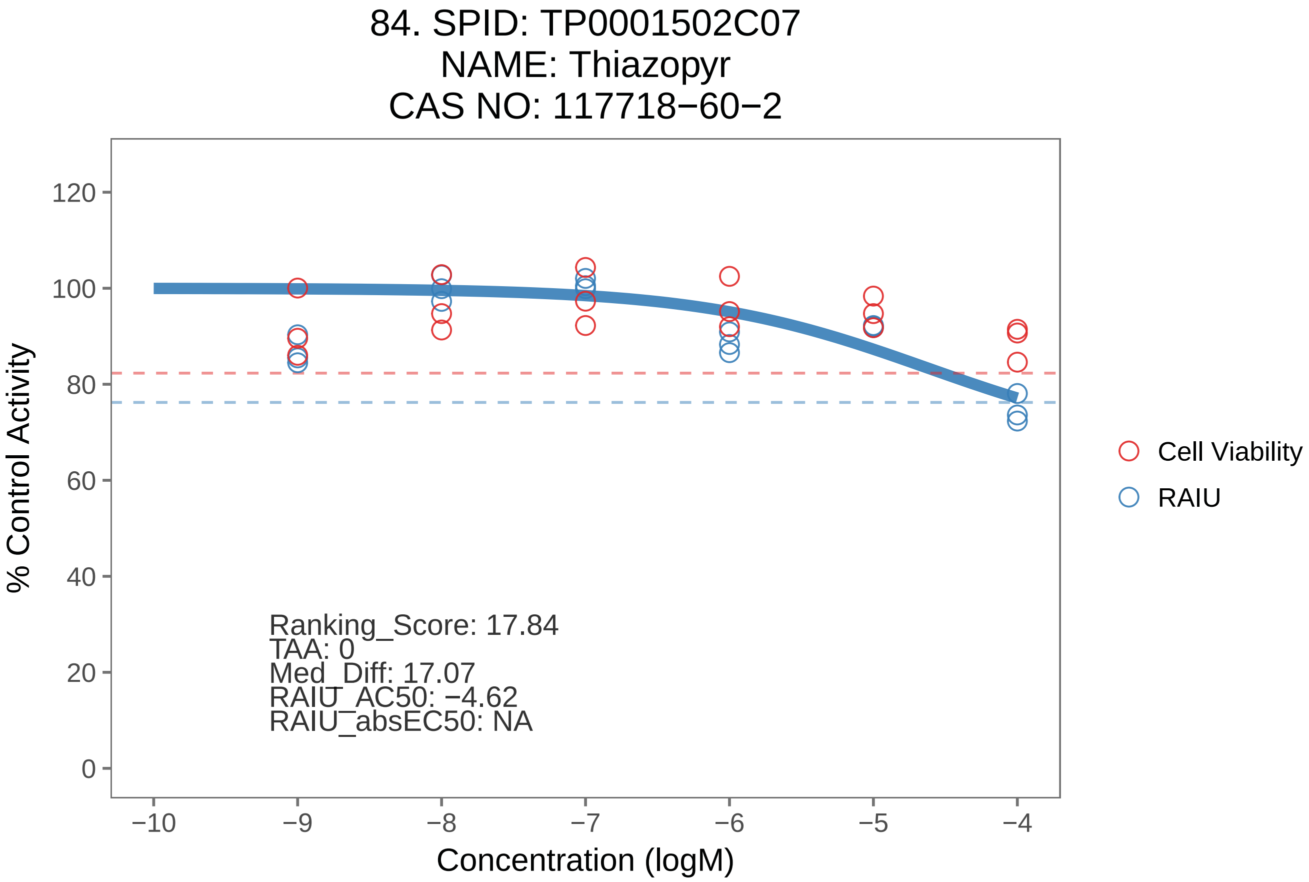

79. SPID: TP0001499D02
NAME: Tri−allate
CAS NO: 2303−17−5
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 19.2
TAA: 12.78
Med_Diff: 10.27
RAIU_AC50: −4.61
RAIU_absEC50: −4.57
Cell Viability
RAIU

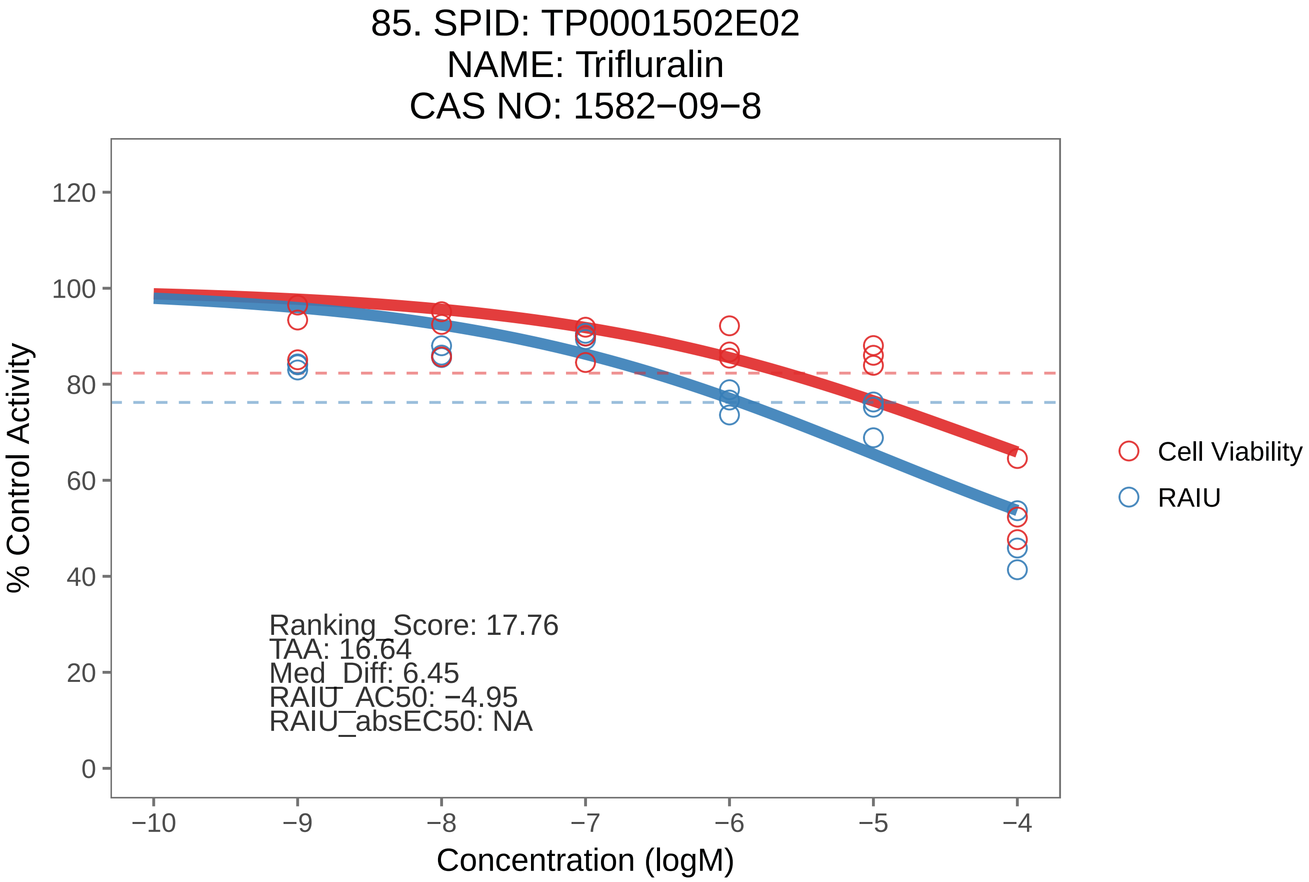

80. SPID: TP0001502G07
NAME: Imazalil
CAS NO: 35554−44−0
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 19.16
TAA: 6.53
Med_Diff: 14.2
RAIU_AC50: −4.5
RAIU_absEC50: NA
Cell Viability
RAIU

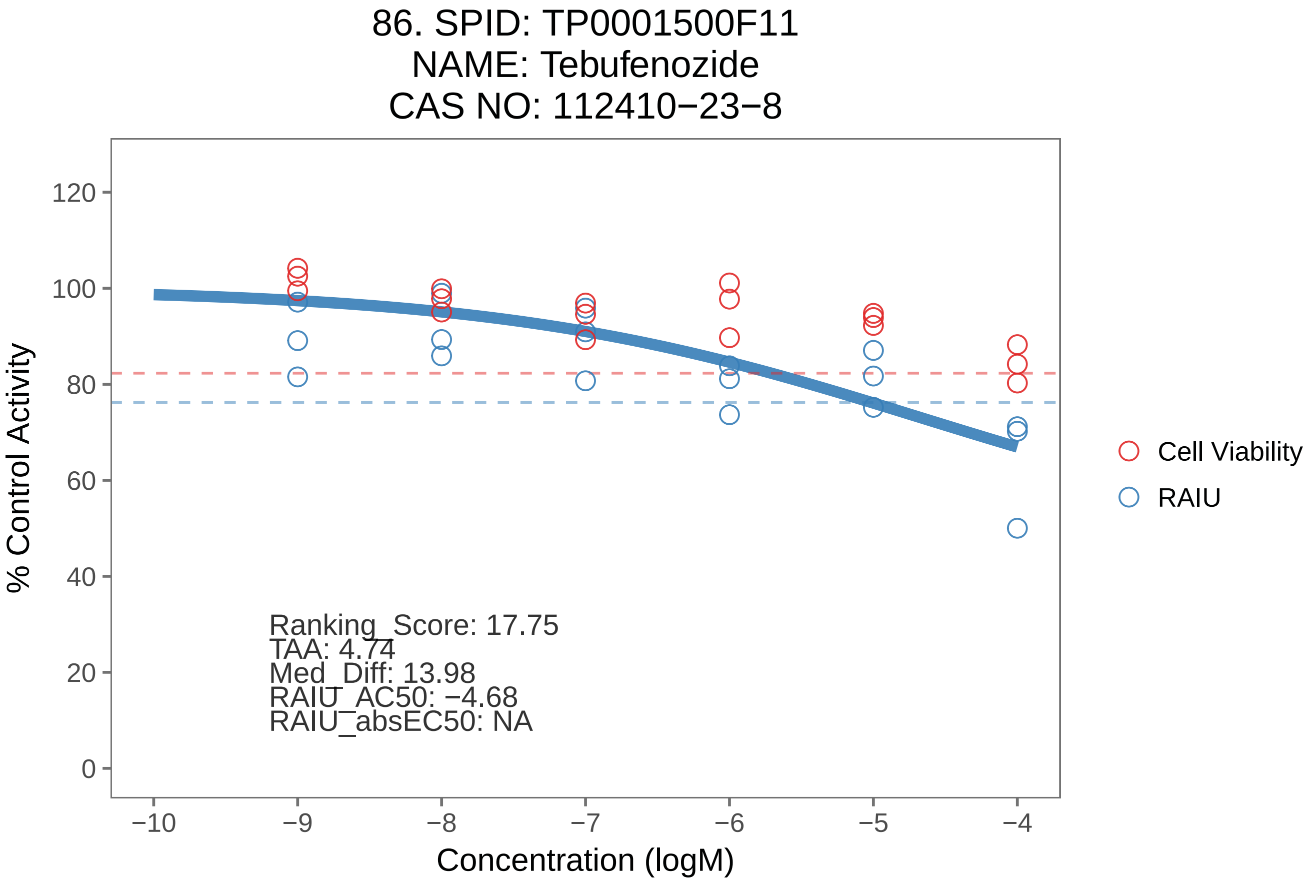

81. SPID: TP0001502E08
NAME: Cypermethrin
CAS NO: 52315−07−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 18.48
TAA: 0.76
Med_Diff: 17.2
RAIU_AC50: −4.96
RAIU_absEC50: NA
Cell Viability
RAIU

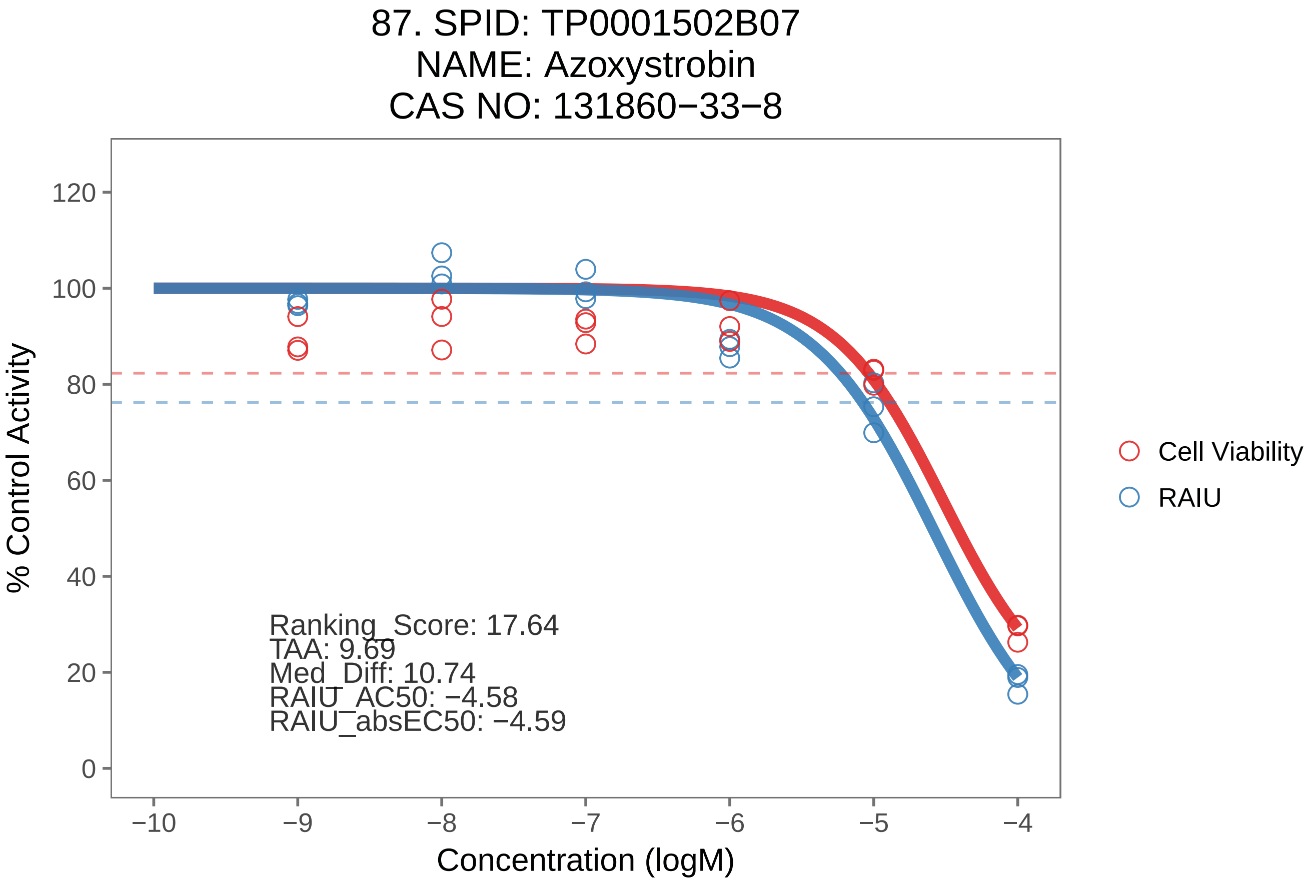

82. SPID: TP0001500F09
NAME: Amitraz
CAS NO: 33089−61−1
% Control Activity
Concentration (logM)
Ranking_Score: 18.15
TAA: 6.97
Med_Diff: 12.95
RAIU_AC50: −4.22
RAIU_absEC50: NA
Cell Viability
RAIU
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

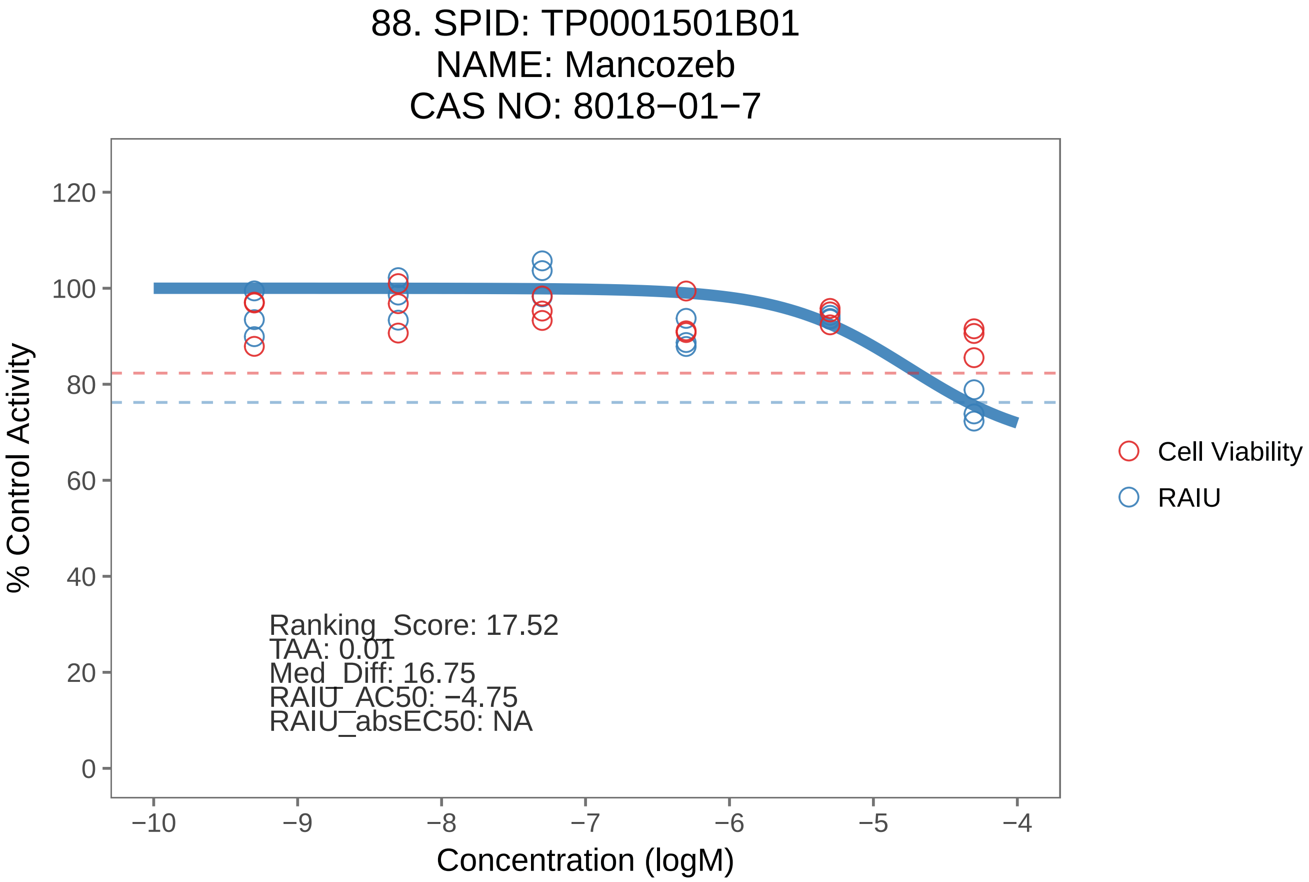

83. SPID: TP0001499E11
NAME: Tetraconazole
CAS NO: 112281−77−3
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 18.01
TAA: 13.62
Med_Diff: 8.6
RAIU_AC50: −4.65
RAIU_absEC50: −4.33
Cell Viability
RAIU

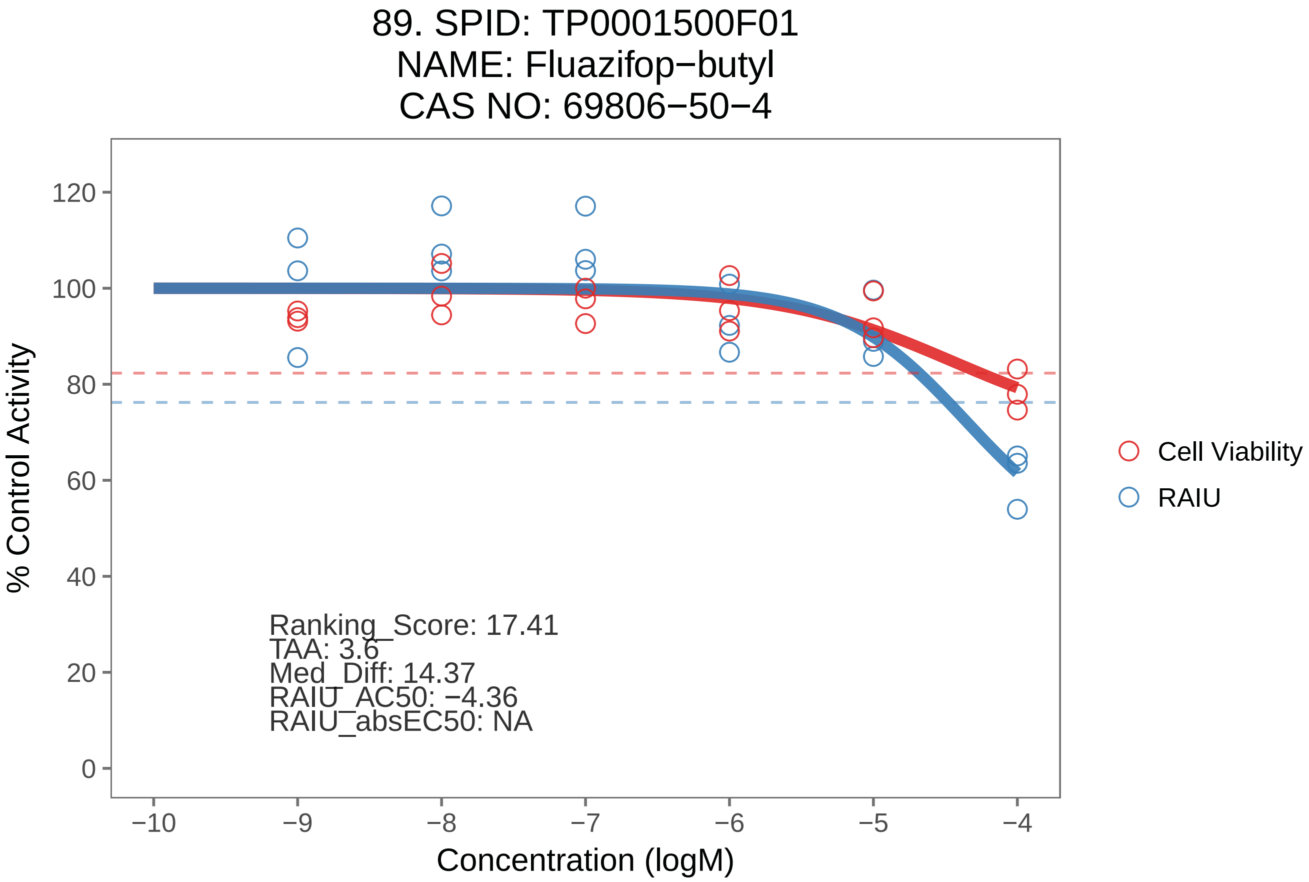

84. SPID: TP0001502C07
NAME: Thiazopyr
CAS NO: 117718−60−2
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 17.84
TAA: 0
Med_Diff: 17.07
RAIU_AC50: −4.62
RAIU_absEC50: NA
Cell Viability
RAIU

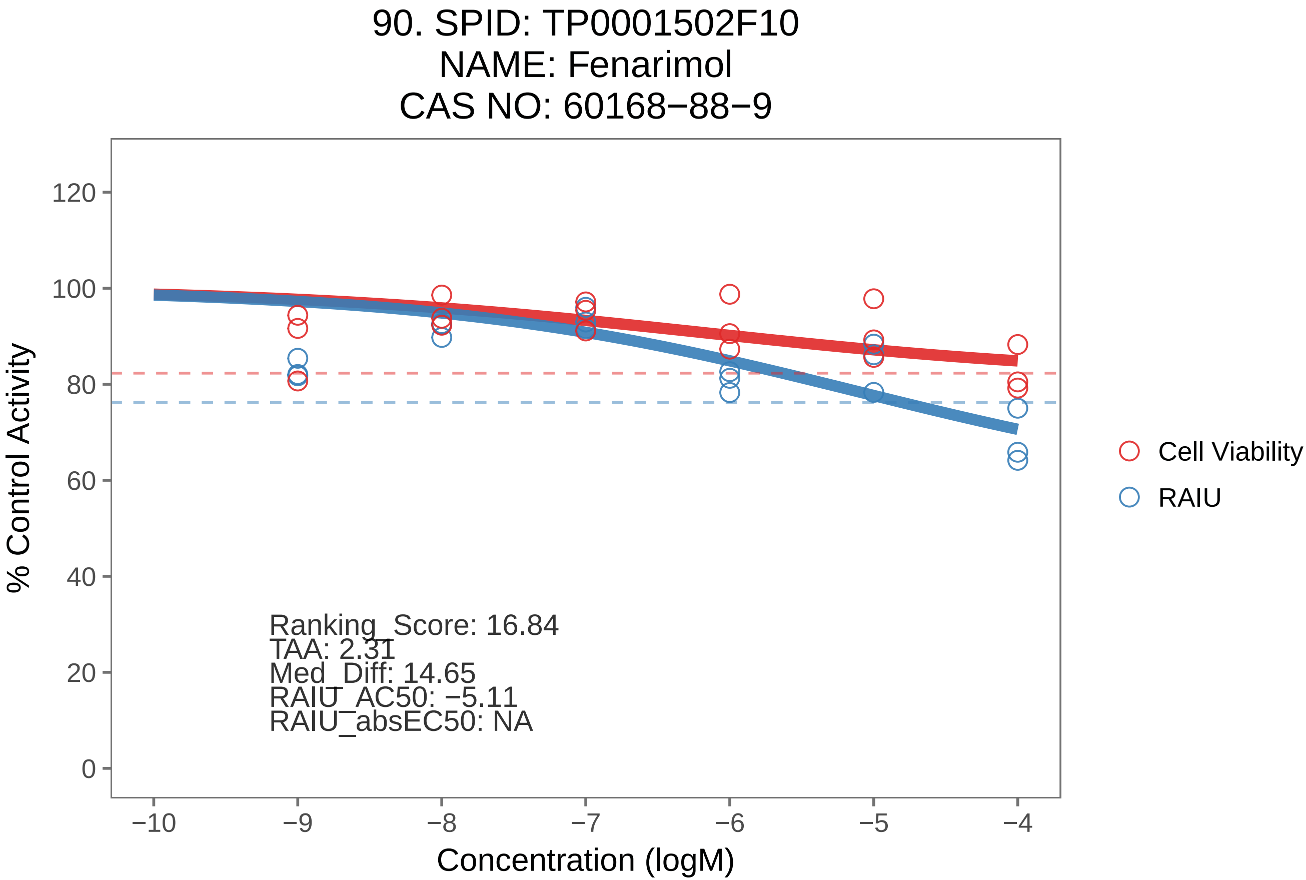

85. SPID: TP0001502E02
NAME: Trifluralin
CAS NO: 1582−09−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 17.76
TAA: 16.64
Med_Diff: 6.45
RAIU_AC50: −4.95
RAIU_absEC50: NA
Cell Viability
RAIU


86. SPID: TP0001500F11
NAME: Tebufenozide
CAS NO: 112410−23−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 17.75
TAA: 4.74
Med_Diff: 13.98
RAIU_AC50: −4.68
RAIU_absEC50: NA
Cell Viability
RAIU

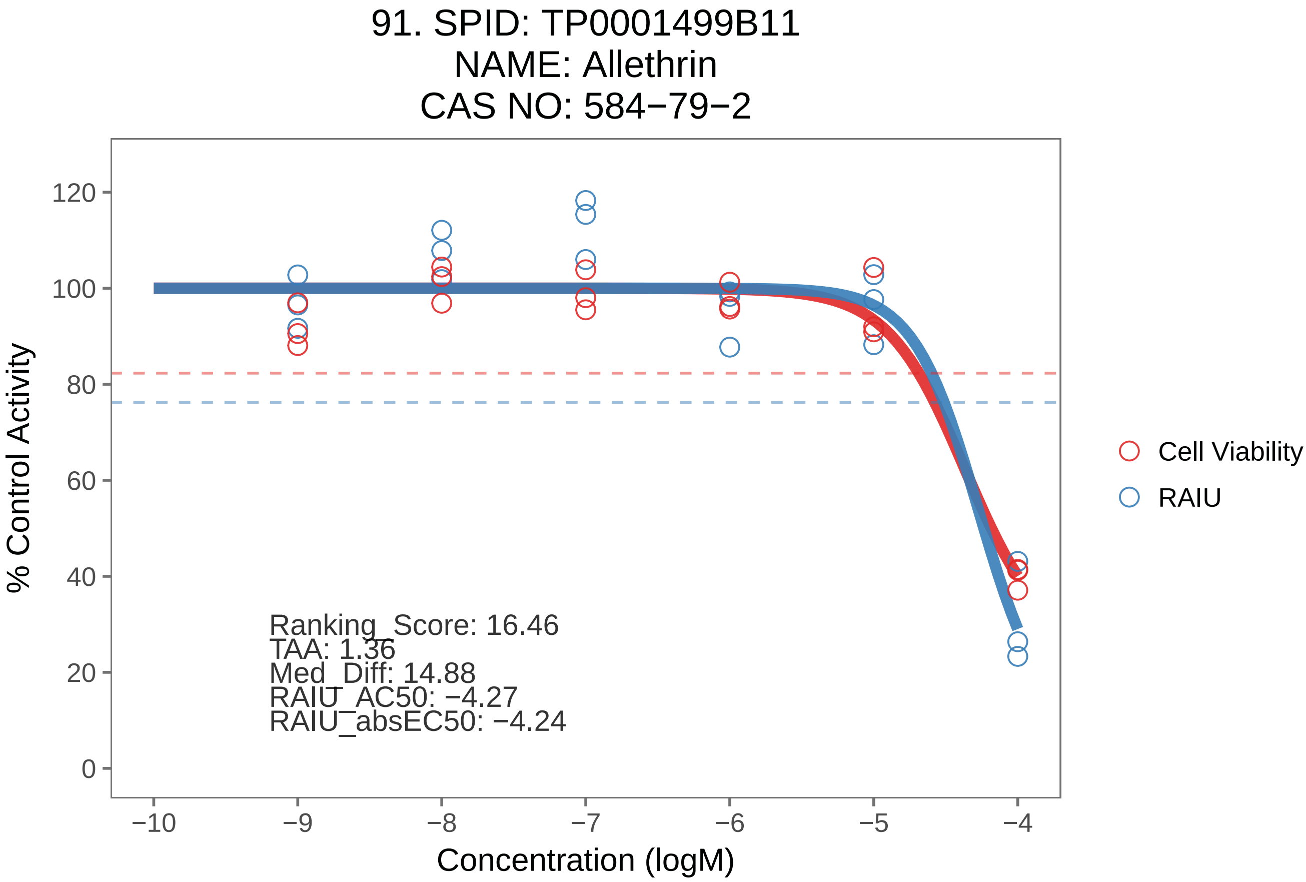

87. SPID: TP0001502B07
NAME: Azoxystrobin
CAS NO: 131860−33−8
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 17.64
TAA: 9.69
Med_Diff: 10.74
RAIU_AC50: −4.58
RAIU_absEC50: −4.59
Cell Viability
RAIU

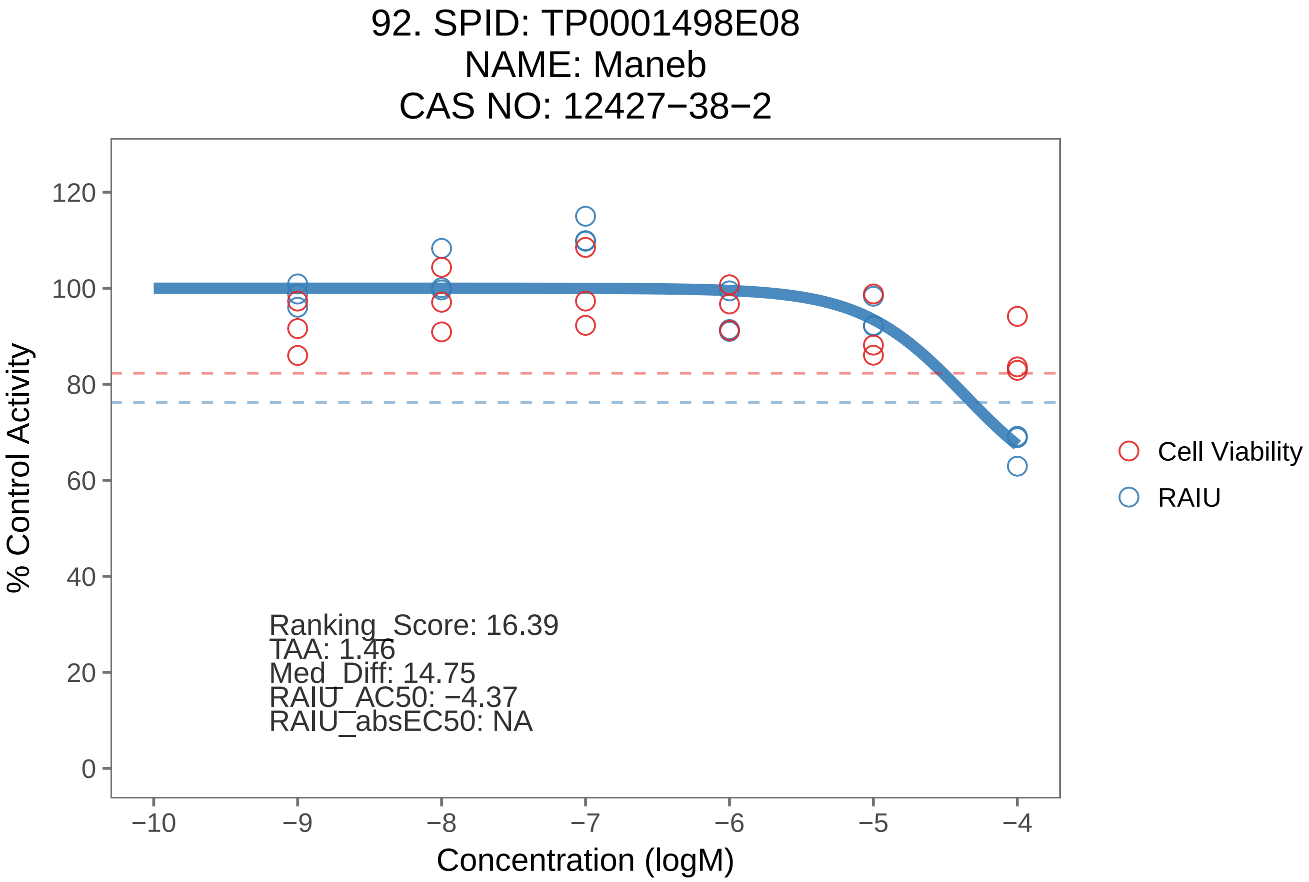

88. SPID: TP0001501B01
NAME: Mancozeb
CAS NO: 8018−01−7
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 17.52
TAA: 0.01
Med_Diff: 16.75
RAIU_AC50: −4.75
RAIU_absEC50: NA
Cell Viability
RAIU


89. SPID: TP0001500F01
NAME: Fluazifop−butyl
CAS NO: 69806−50−4
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 17.41
TAA: 3.6
Med_Diff: 14.37
RAIU_AC50: −4.36
RAIU_absEC50: NA



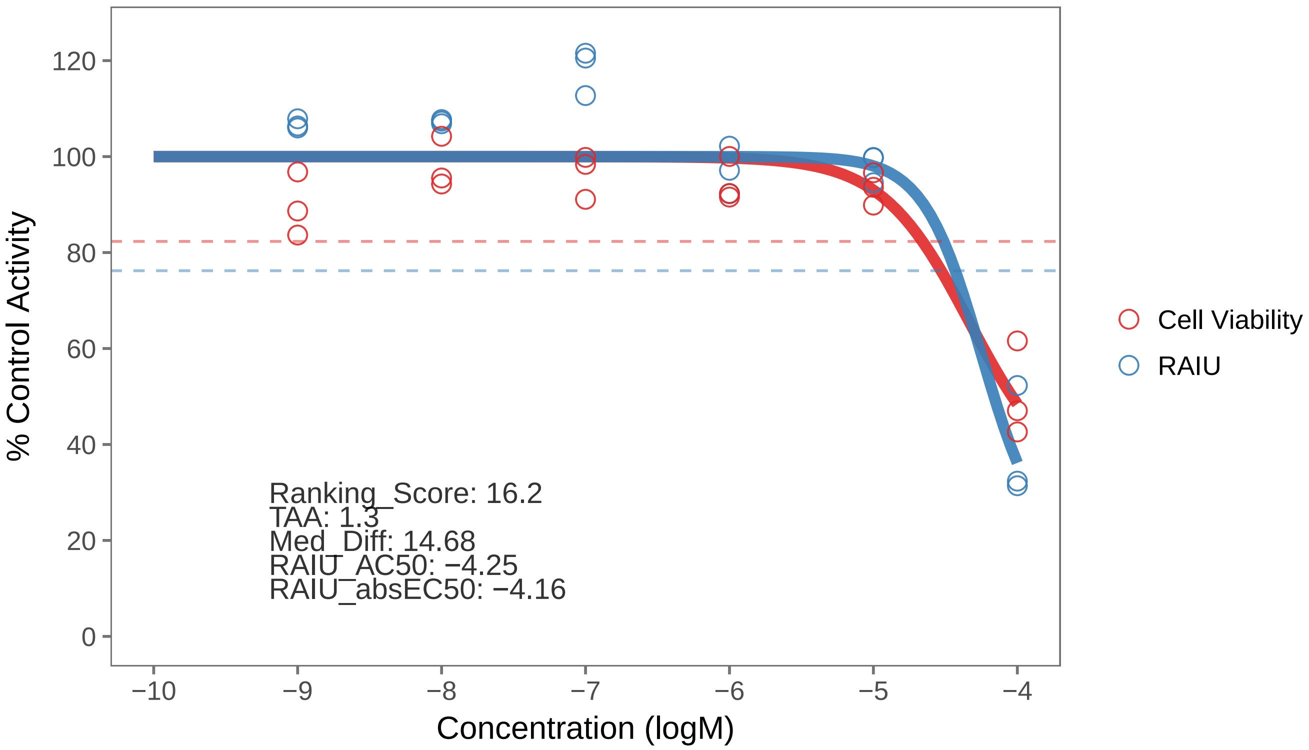
90. SPID: TP0001502F10
NAME: Fenarimol
CAS NO: 60168−88−9
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 16.84
TAA: 2.31
Med_Diff: 14.65
RAIU_AC50: −5.11
RAIU_absEC50: NA
Cell Viability
RAIU

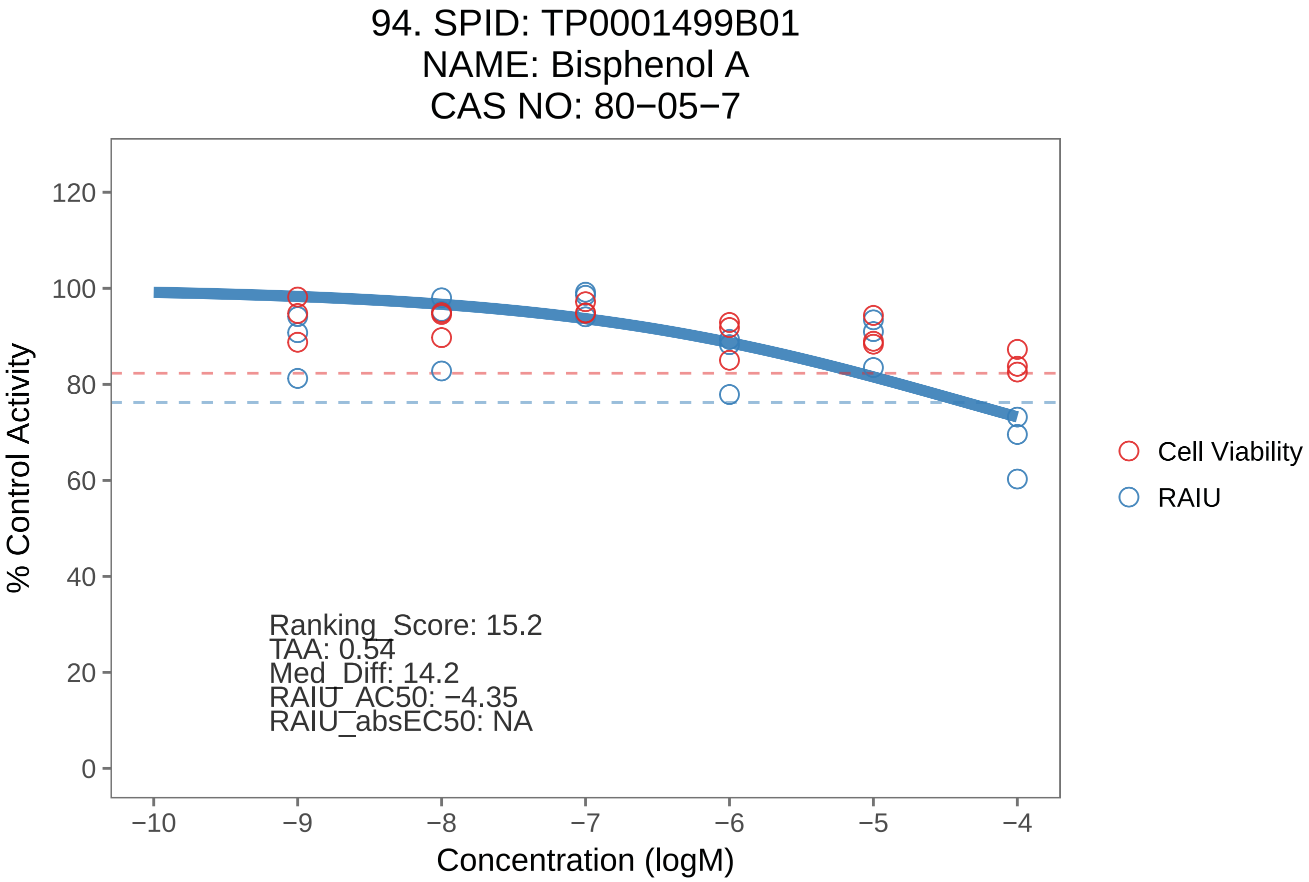

91. SPID: TP0001499B11
NAME: Allethrin
CAS NO: 584−79−2
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 16.46
TAA: 1.36
Med_Diff: 14.88
RAIU_AC50: −4.27
RAIU_absEC50: −4.24
Cell Viability
RAIU



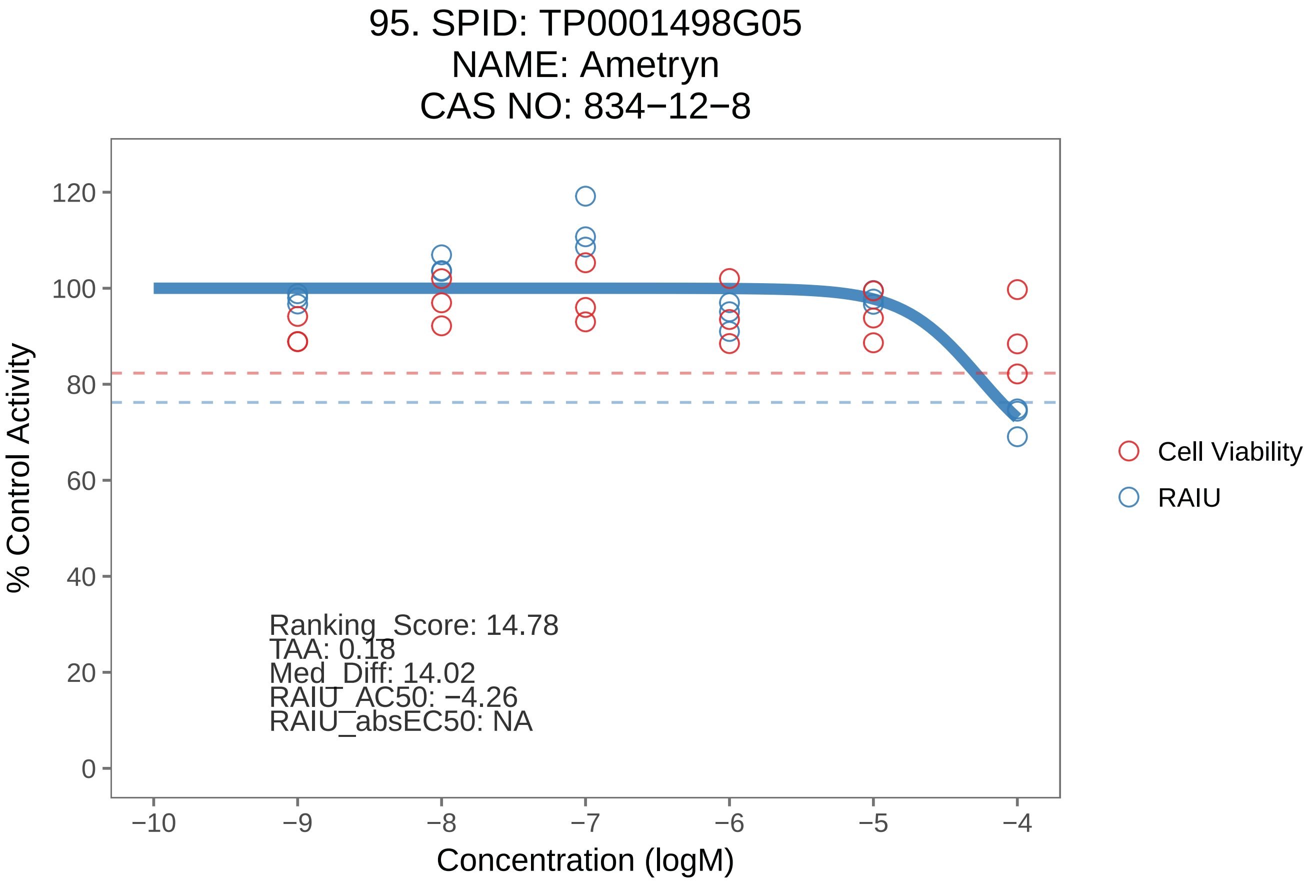
92. SPID: TP0001498E08
NAME: Maneb
CAS NO: 12427−38−2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 16.39
TAA: 1.46
Med_Diff: 14.75
RAIU_AC50: −4.37
RAIU_absEC50: NA
Cell Viability
RAIU

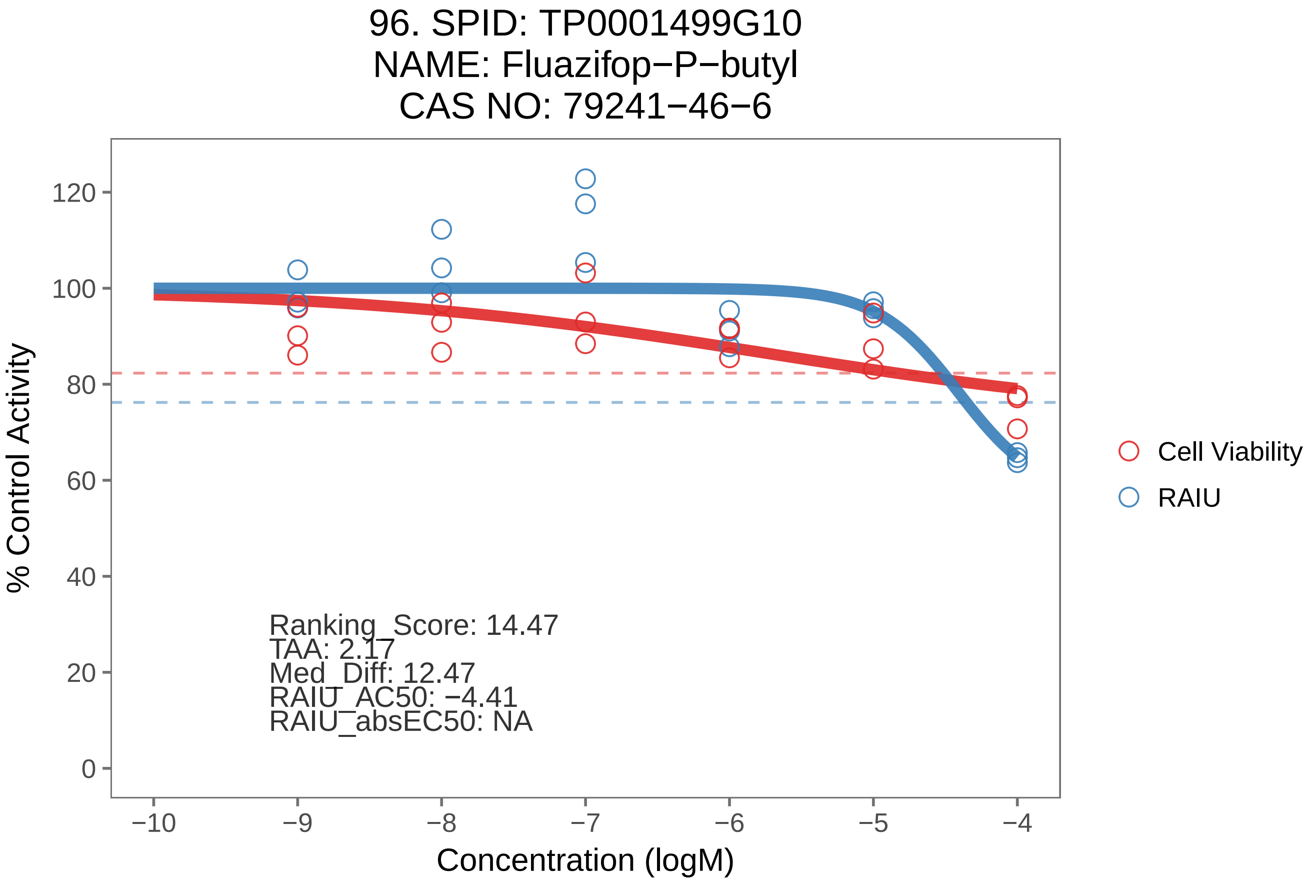
93. SPID: TP0001498D07
NAME: Flusilazole
CAS NO: 85509−19−9

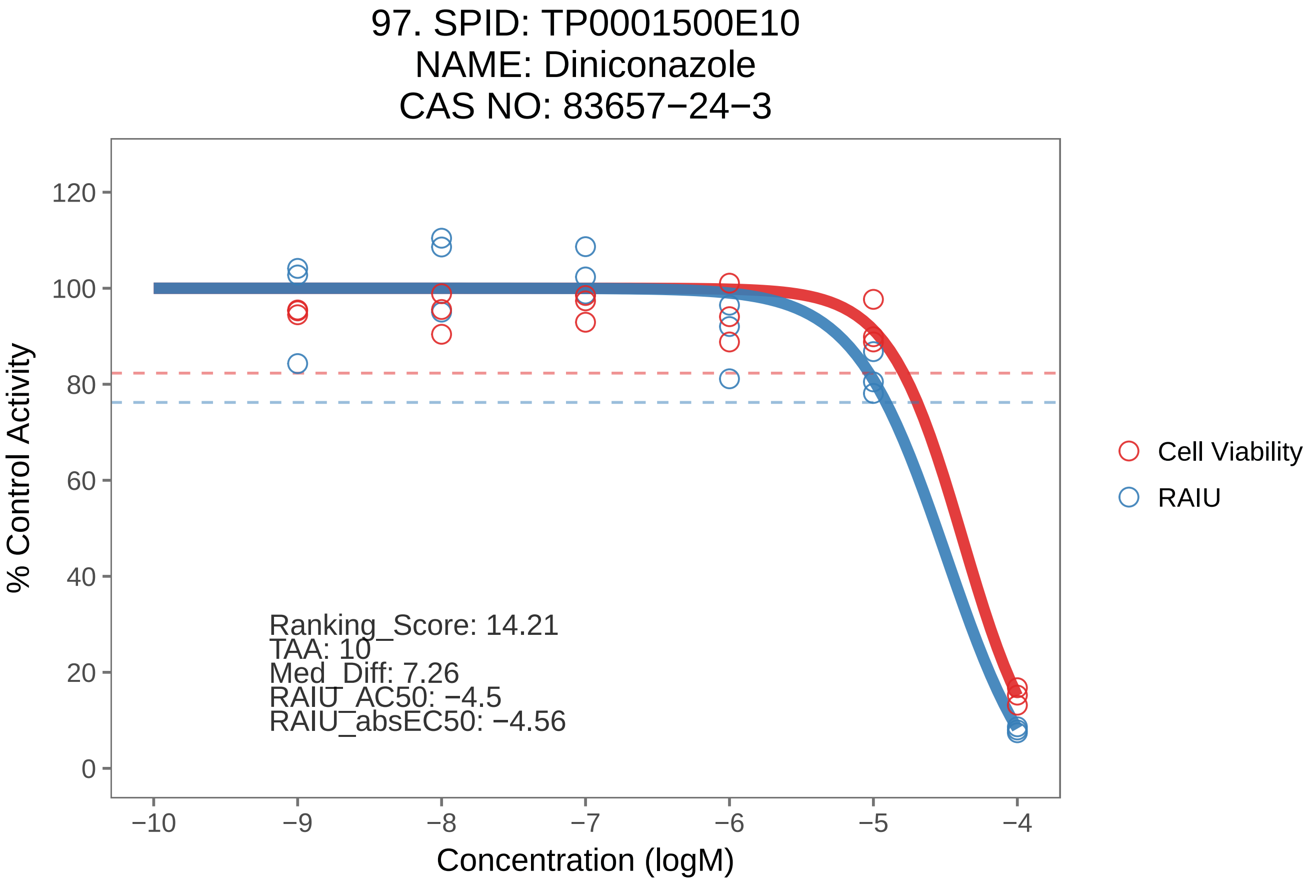


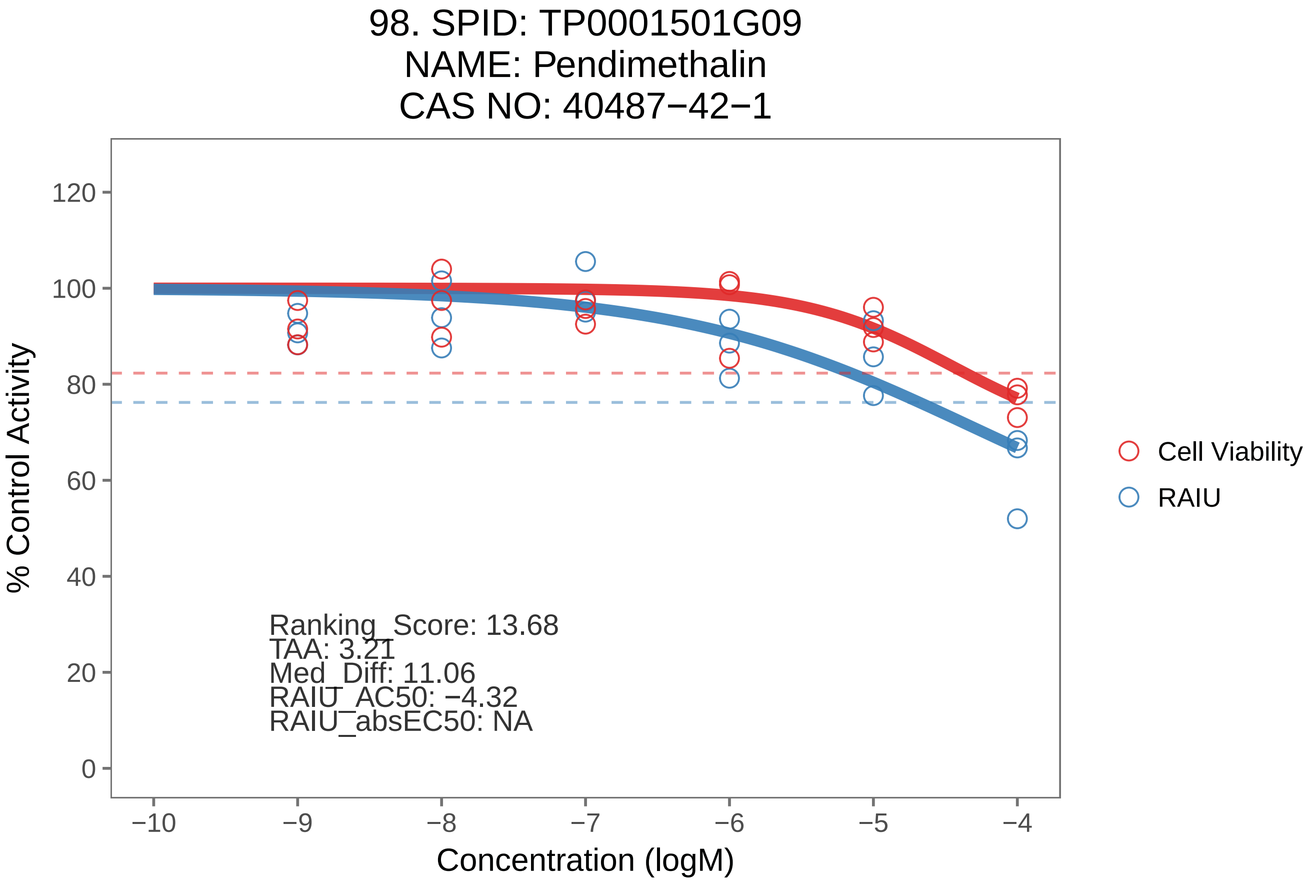


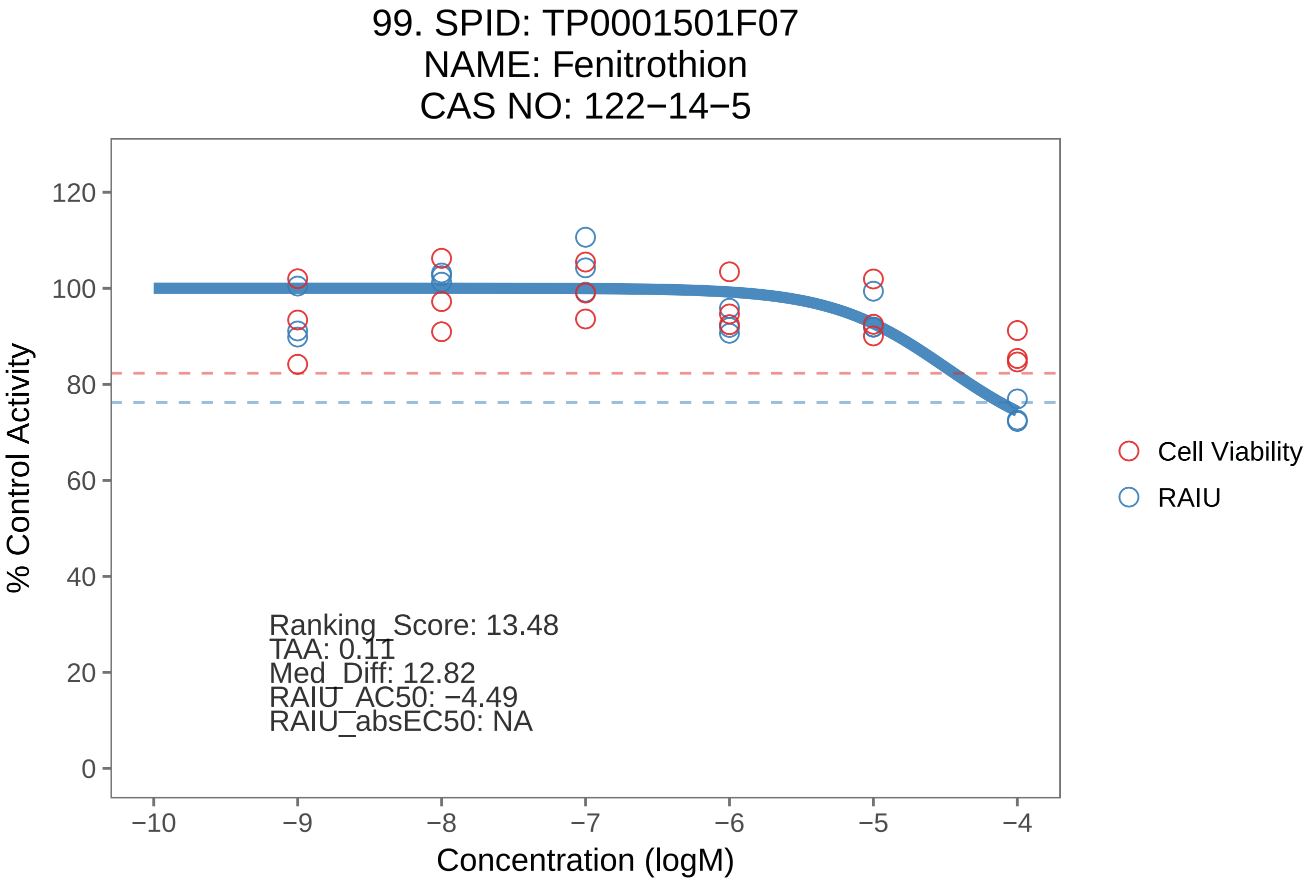
94. SPID: TP0001499B01
NAME: Bisphenol A
CAS NO: 80−05−7
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 15.2
TAA: 0.54
Med_Diff: 14.2
RAIU_AC50: −4.35
RAIU_absEC50: NA
Cell Viability
RAIU

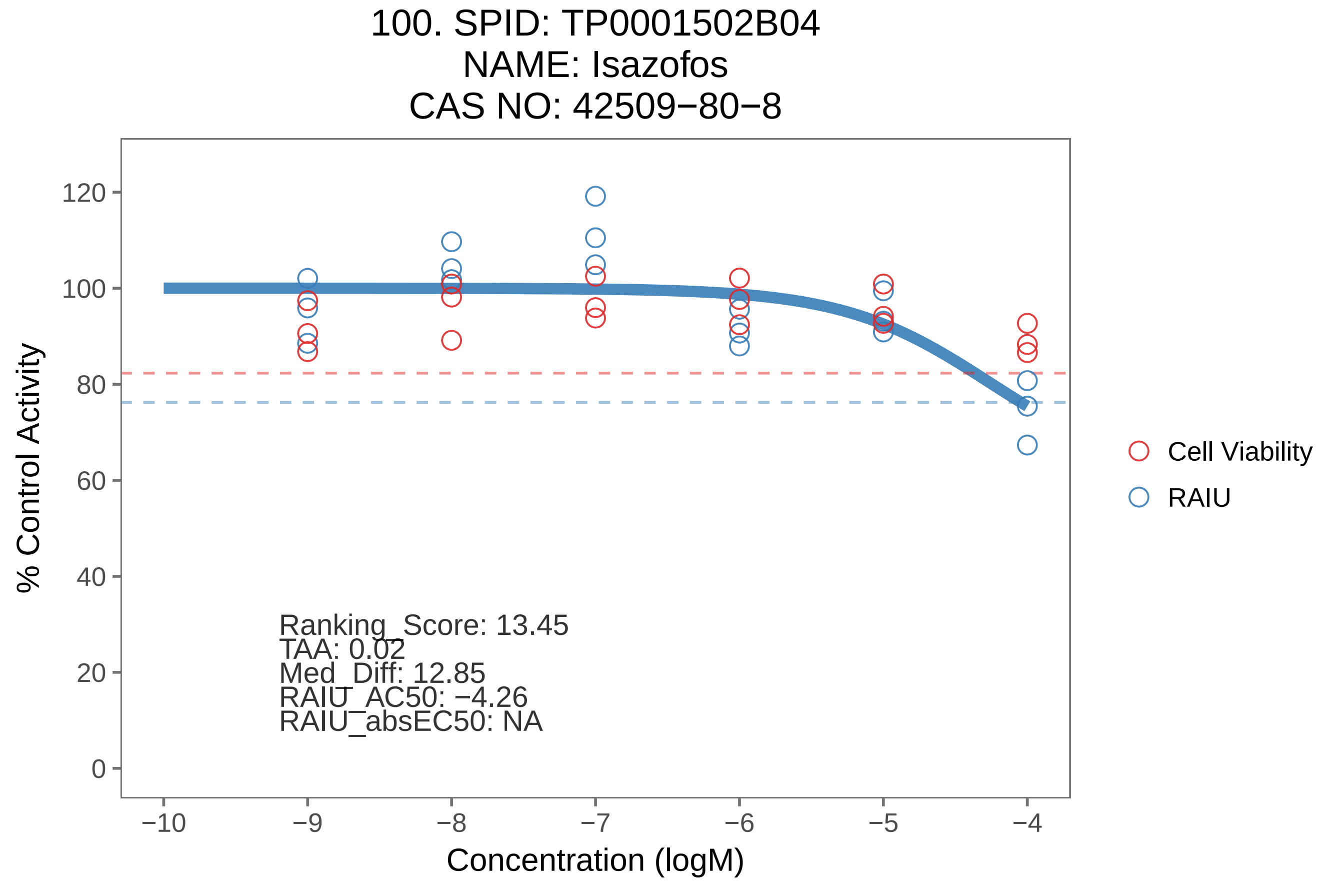

95. SPID: TP0001498G05
NAME: Ametryn
CAS NO: 834−12−8
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 14.78
TAA: 0.18
Med_Diff: 14.02
RAIU_AC50: −4.26
RAIU_absEC50: NA
Cell Viability
RAIU

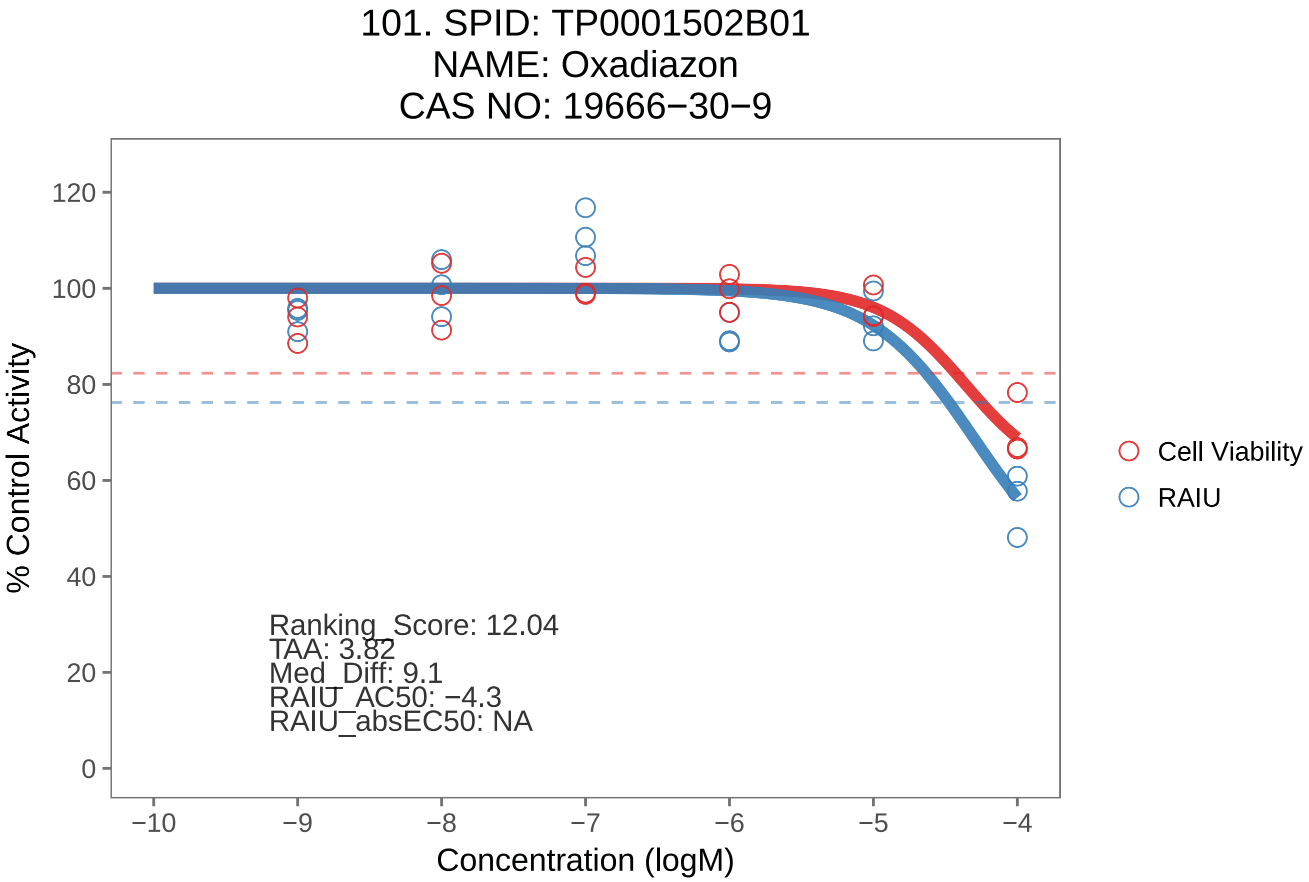

96. SPID: TP0001499G10
NAME: Fluazifop−P−butyl
CAS NO: 79241−46−6
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 14.47
TAA: 2.17
Med_Diff: 12.47
RAIU_AC50: −4.41
RAIU_absEC50: NA
Cell Viability
RAIU

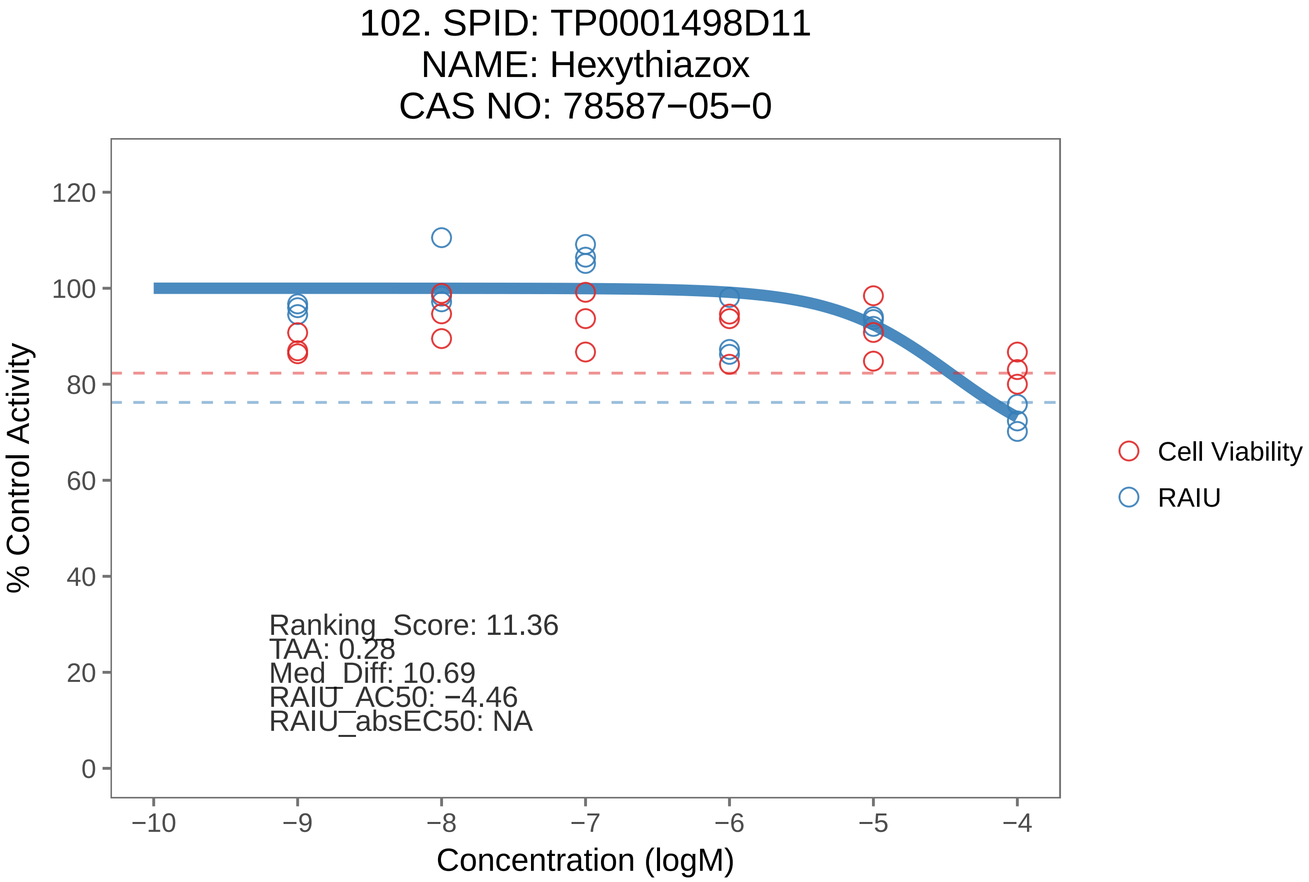

97. SPID: TP0001500E10
NAME: Diniconazole
CAS NO: 83657−24−3
% Control Activity
0
20
40
60
80
100
120
Concentration (logM)
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 14.21
TAA: 10
Med_Diff: 7.26
RAIU_AC50: −4.5
RAIU_absEC50: −4.56
Cell Viability
RAIU


98. SPID: TP0001501G09
NAME: Pendimethalin
CAS NO: 40487−42−1
% Control Activity
Concentration (logM)
Ranking_Score: 13.68
TAA: 3.21
Med_Diff: 11.06
RAIU_AC50: −4.32
RAIU_absEC50: NA
Cell Viability
RAIU

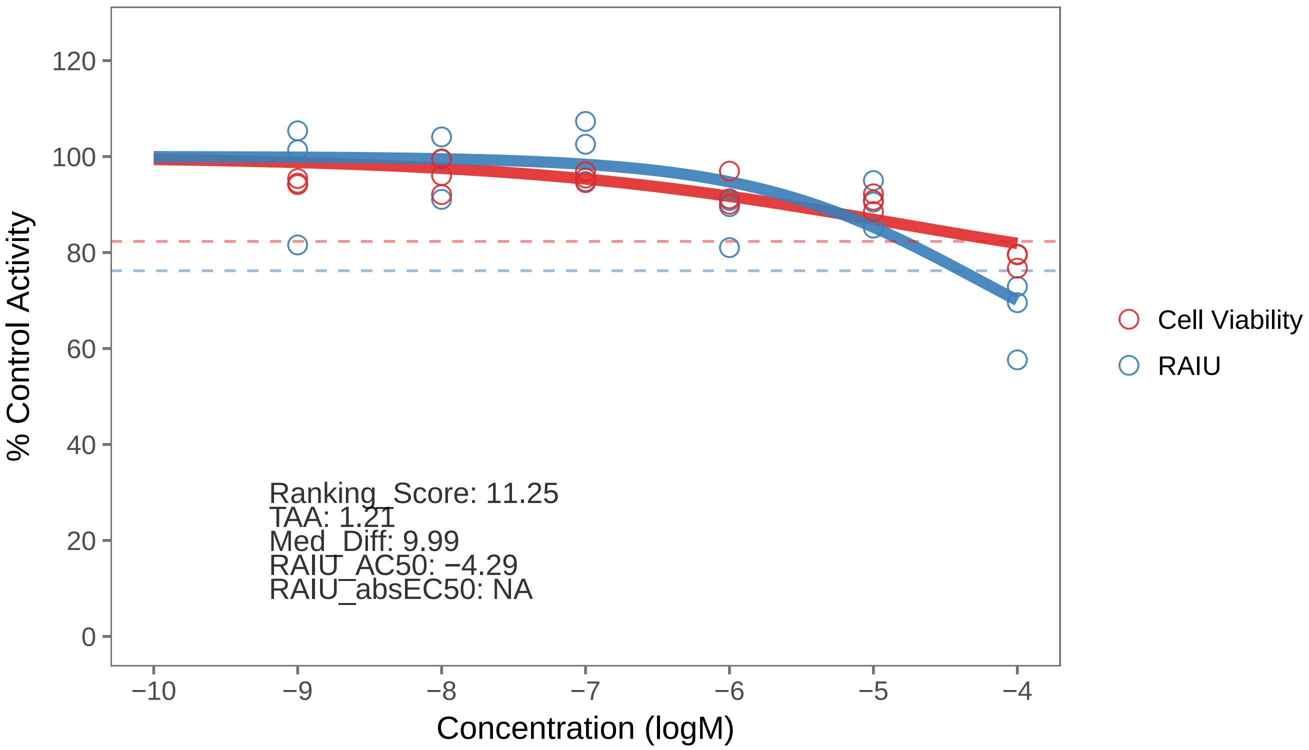

99. SPID: TP0001501F07
NAME: Fenitrothion
CAS NO: 122−14−5
% Control Activity
120
100
80
60
40
20
0
Ranking_Score: 13.48
TAA: 0.11
Med_Diff: 12.82
RAIU_AC50: −4.49
RAIU_absEC50: NA
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU

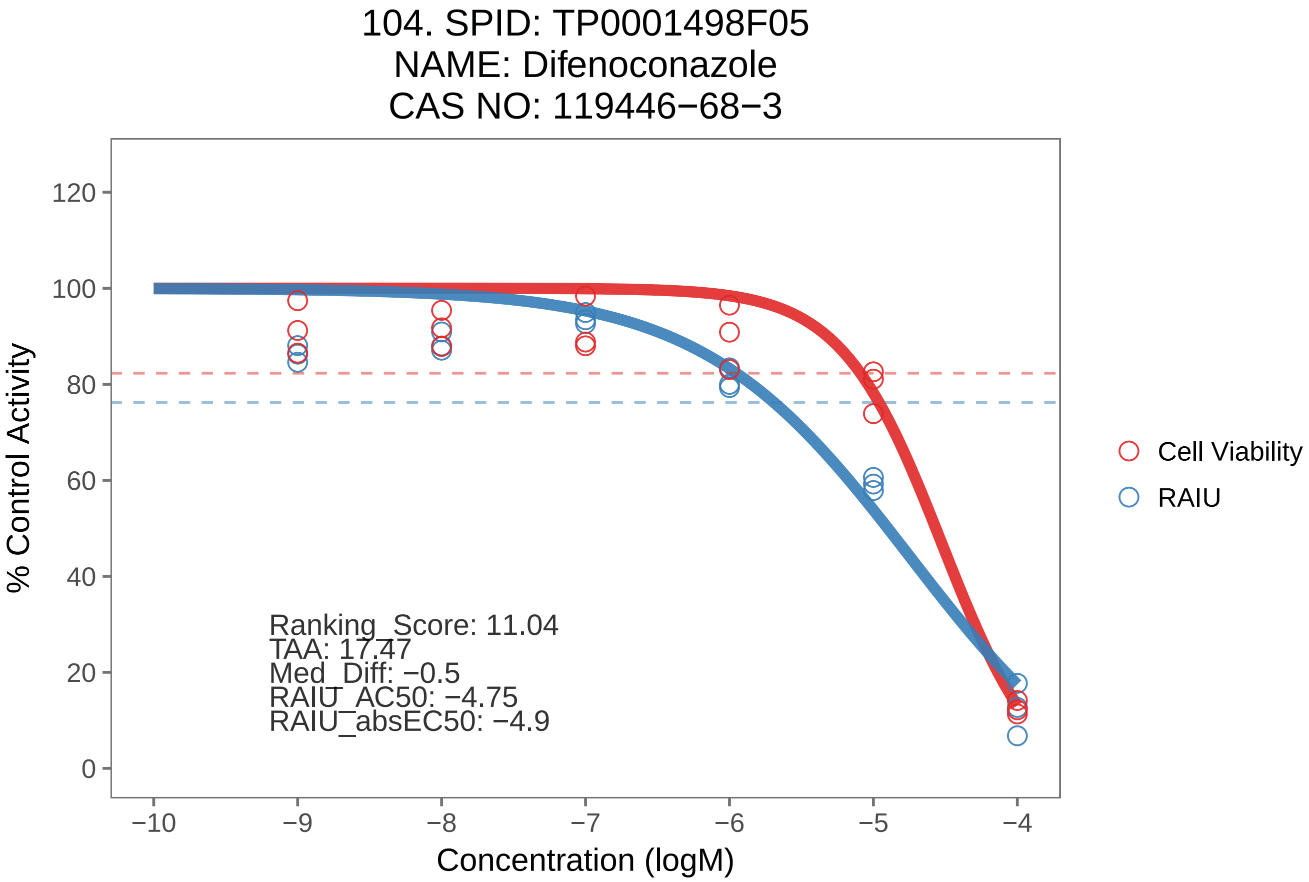

100. SPID: TP0001502B04
NAME: Isazofos
CAS NO: 42509−80−8
Ranking_Score: 13.45
TAA: 0.02
Med_Diff: 12.85
RAIU_AC50: −4.26
RAIU_absEC50: NA
% Control Activity
Concentration (logM)
Cell Viability
RAIU
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

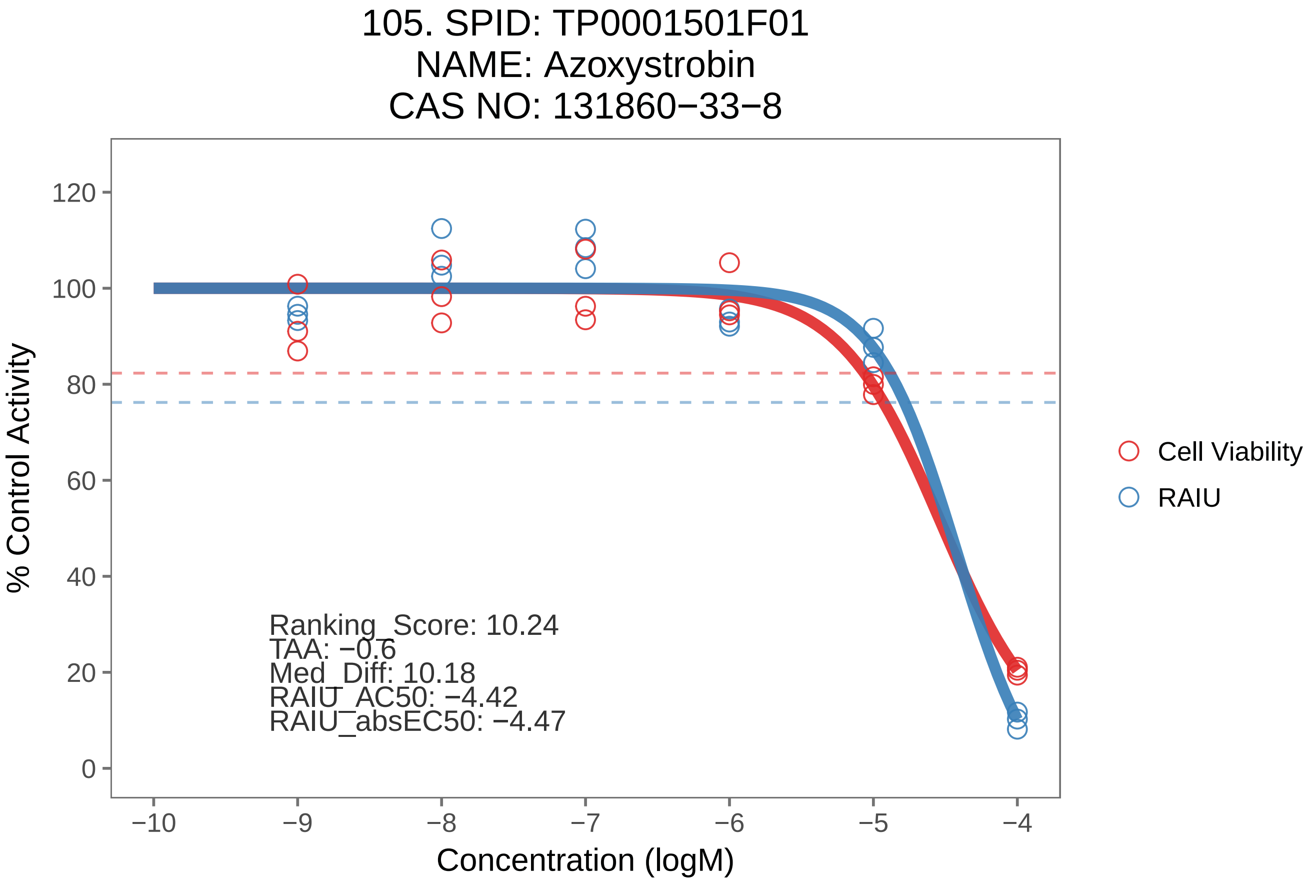

101. SPID: TP0001502B01
NAME: Oxadiazon
CAS NO: 19666−30−9
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 12.04
TAA: 3.82
Med_Diff: 9.1
RAIU_AC50: −4.3
RAIU_absEC50: NA
Cell Viability
RAIU

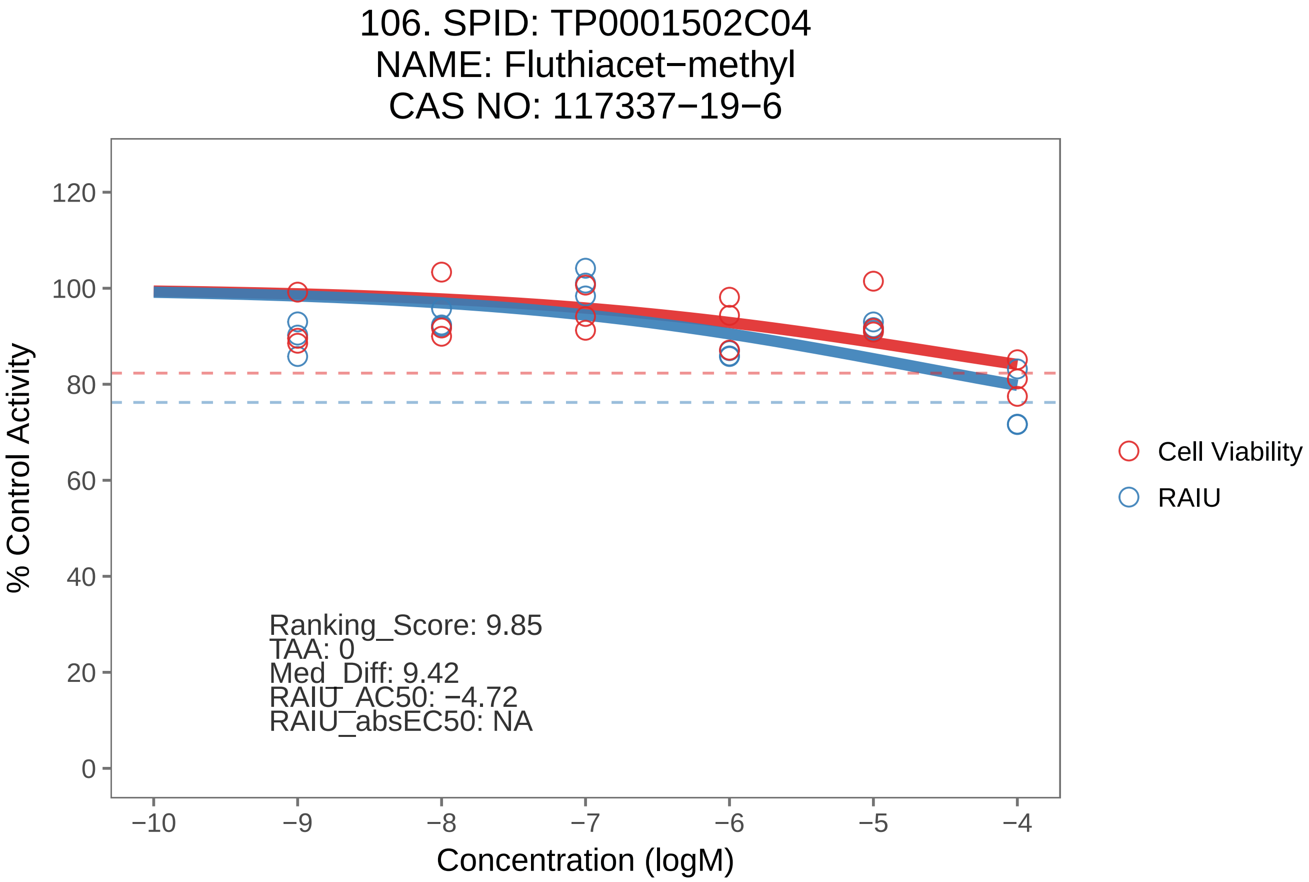

102. SPID: TP0001498D11
NAME: Hexythiazox
CAS NO: 78587−05−0
% Control Activity
Concentration (logM)
Ranking_Score: 11.36
TAA: 0.28
Med_Diff: 10.69
RAIU_AC50: −4.46
RAIU_absEC50: NA
Cell Viability
RAIU
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

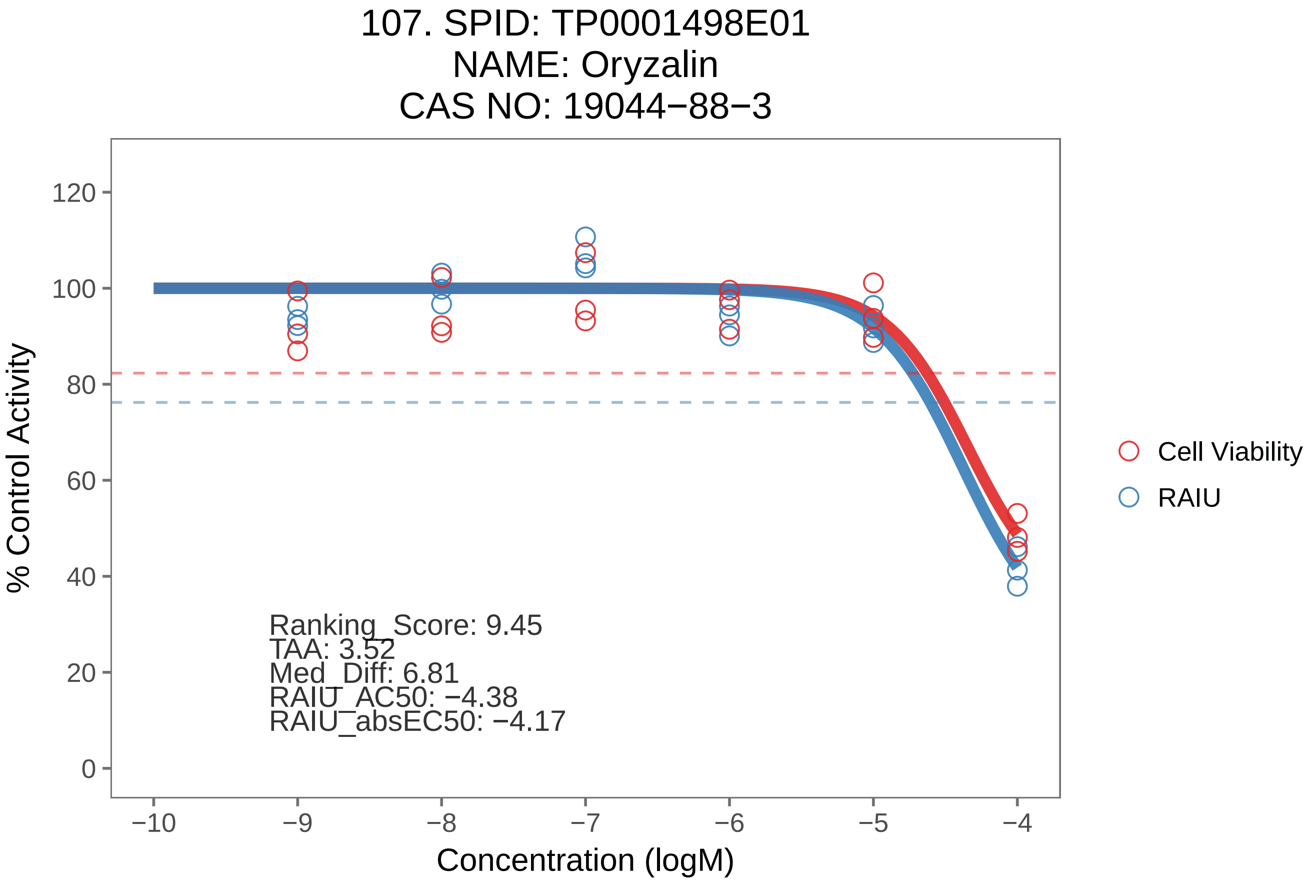
103. SPID: TP0001500E09
NAME: Fenamidone
CAS NO: 161326−34−7



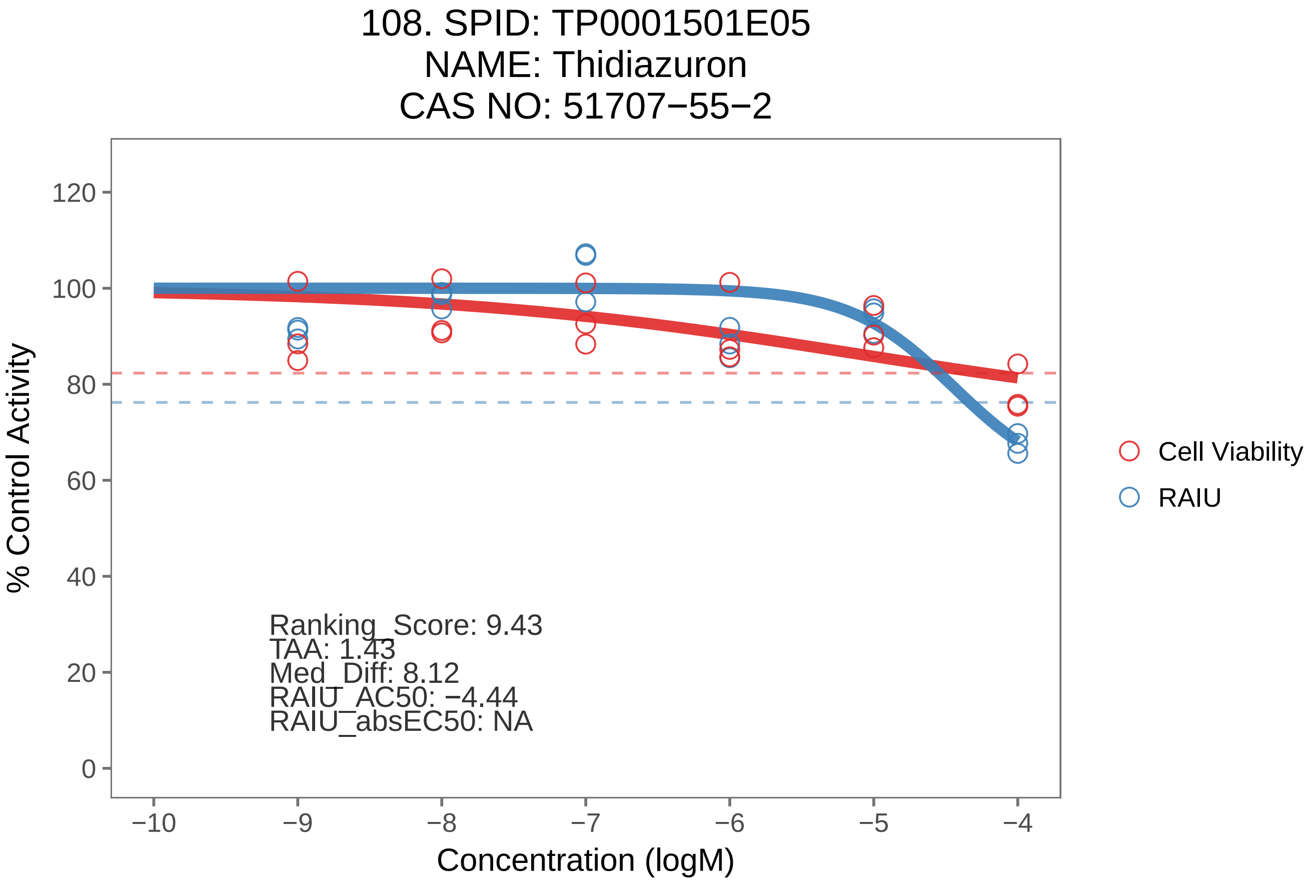

104. SPID: TP0001498F05
NAME: Difenoconazole
CAS NO: 119446−68−3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 11.04
TAA: 17.47
Med_Diff: −0.5
RAIU_AC50: −4.75
RAIU_absEC50: −4.9
Cell Viability
RAIU

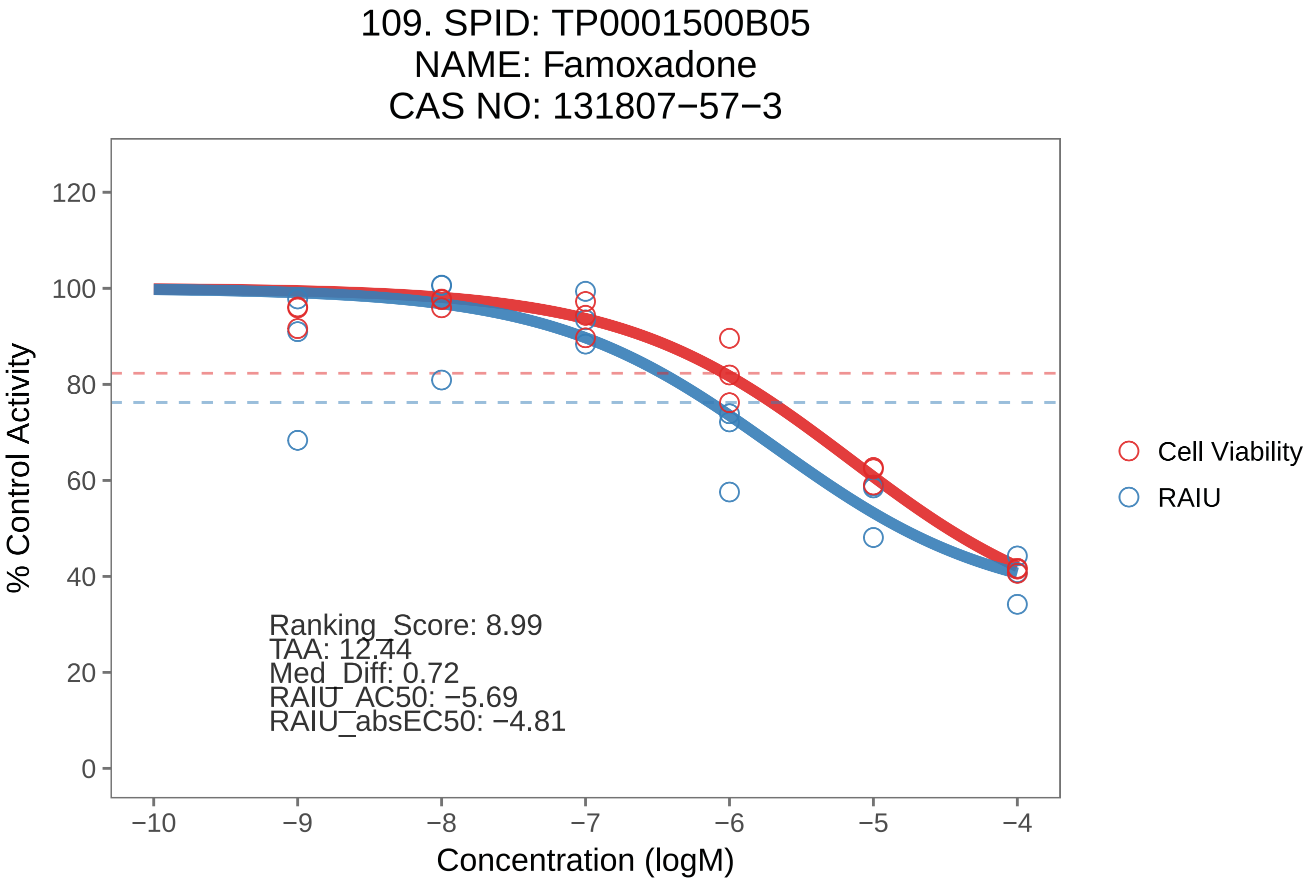

105. SPID: TP0001501F01
NAME: Azoxystrobin
CAS NO: 131860−33−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 10.24
TAA: −0.6
Med_Diff: 10.18
RAIU_AC50: −4.42
RAIU_absEC50: −4.47
Cell Viability
RAIU

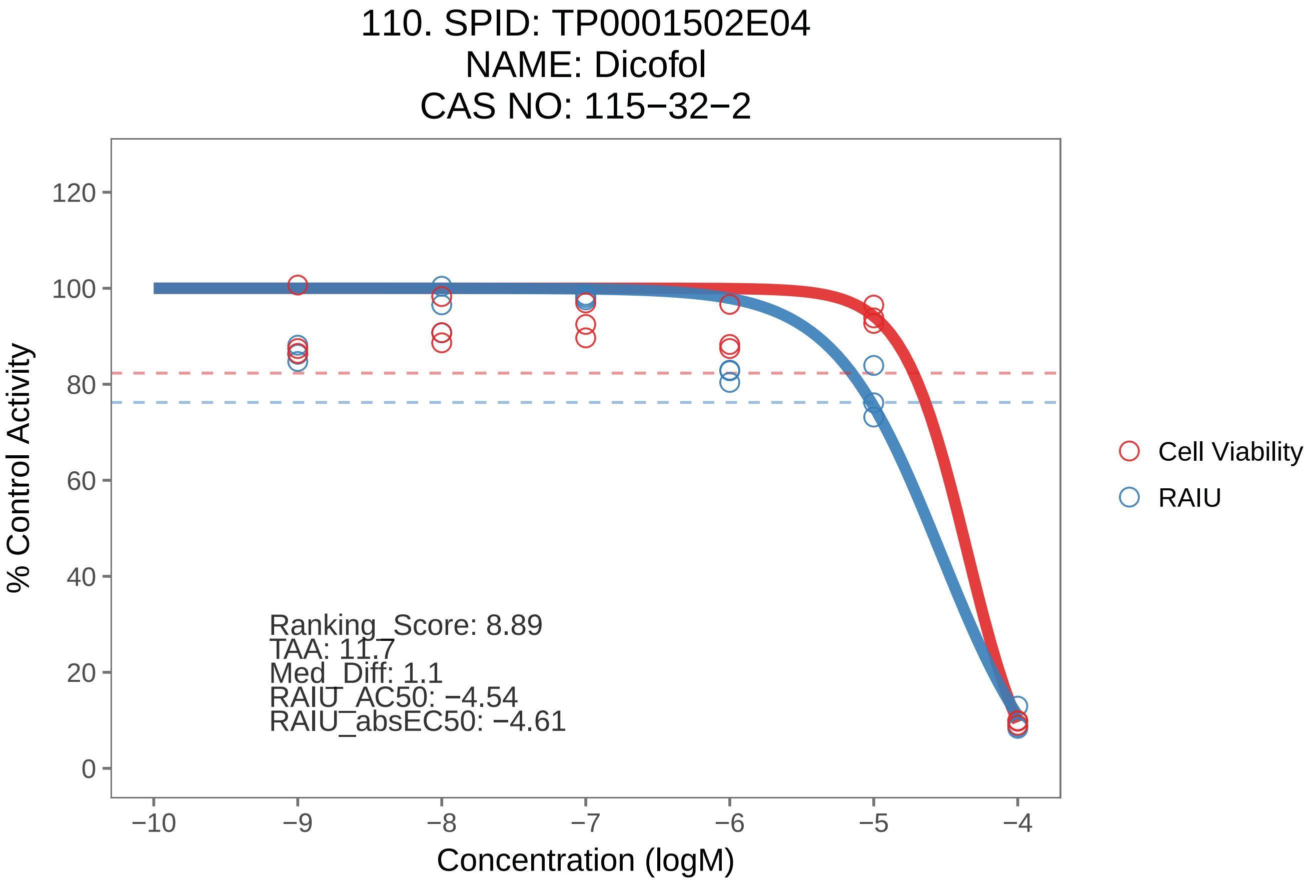

106. SPID: TP0001502C04
NAME: Fluthiacet−methyl
CAS NO: 117337−19−6
% Control Activity
Concentration (logM)
Ranking_Score: 9.85
TAA: 0
Med_Diff: 9.42
RAIU_AC50: −4.72
RAIU_absEC50: NA
Cell Viability
RAIU

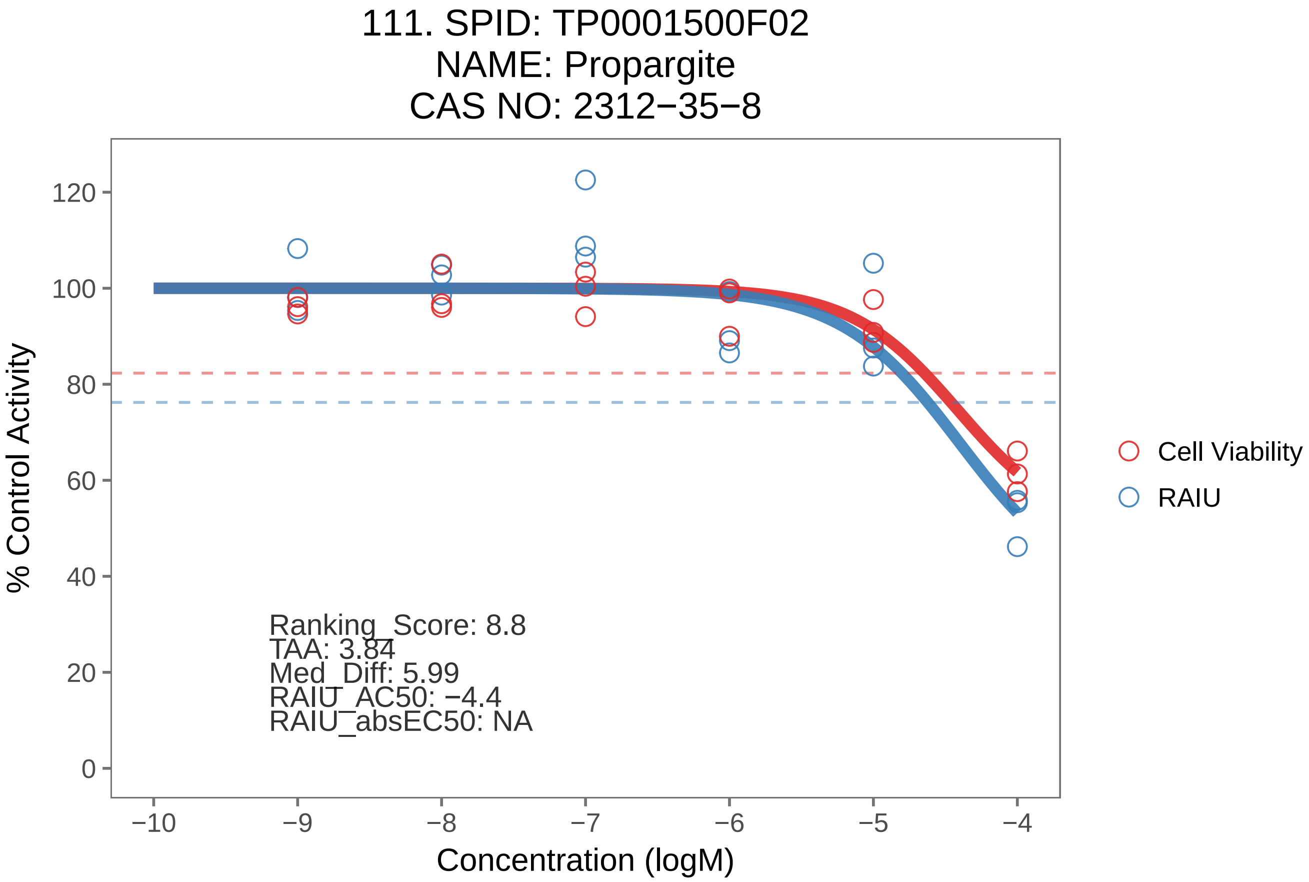


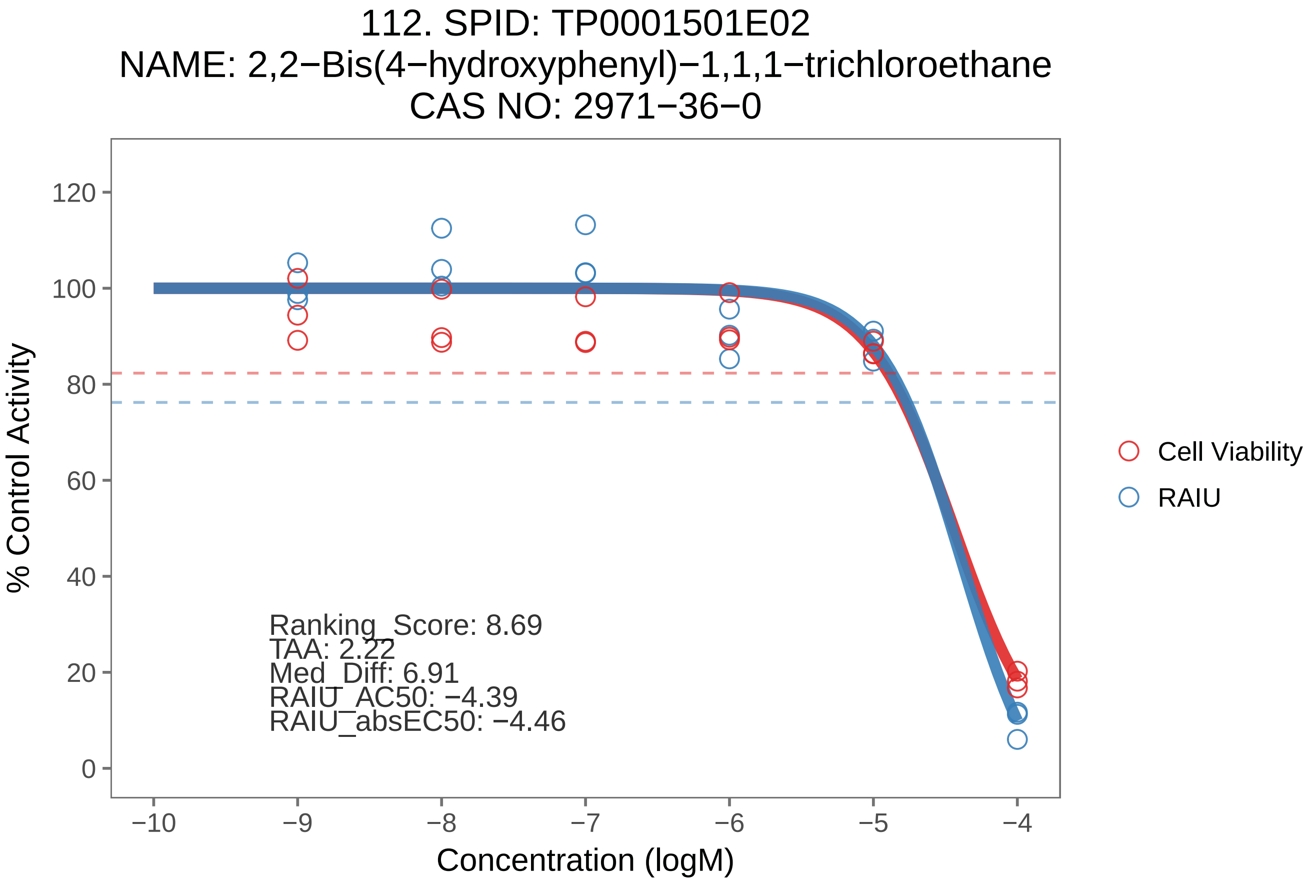
107. SPID: TP0001498E01
NAME: Oryzalin
CAS NO: 19044−88−3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 9.45
TAA: 3.52
Med_Diff: 6.81
RAIU_AC50: −4.38
RAIU_absEC50: −4.17
Cell Viability
RAIU

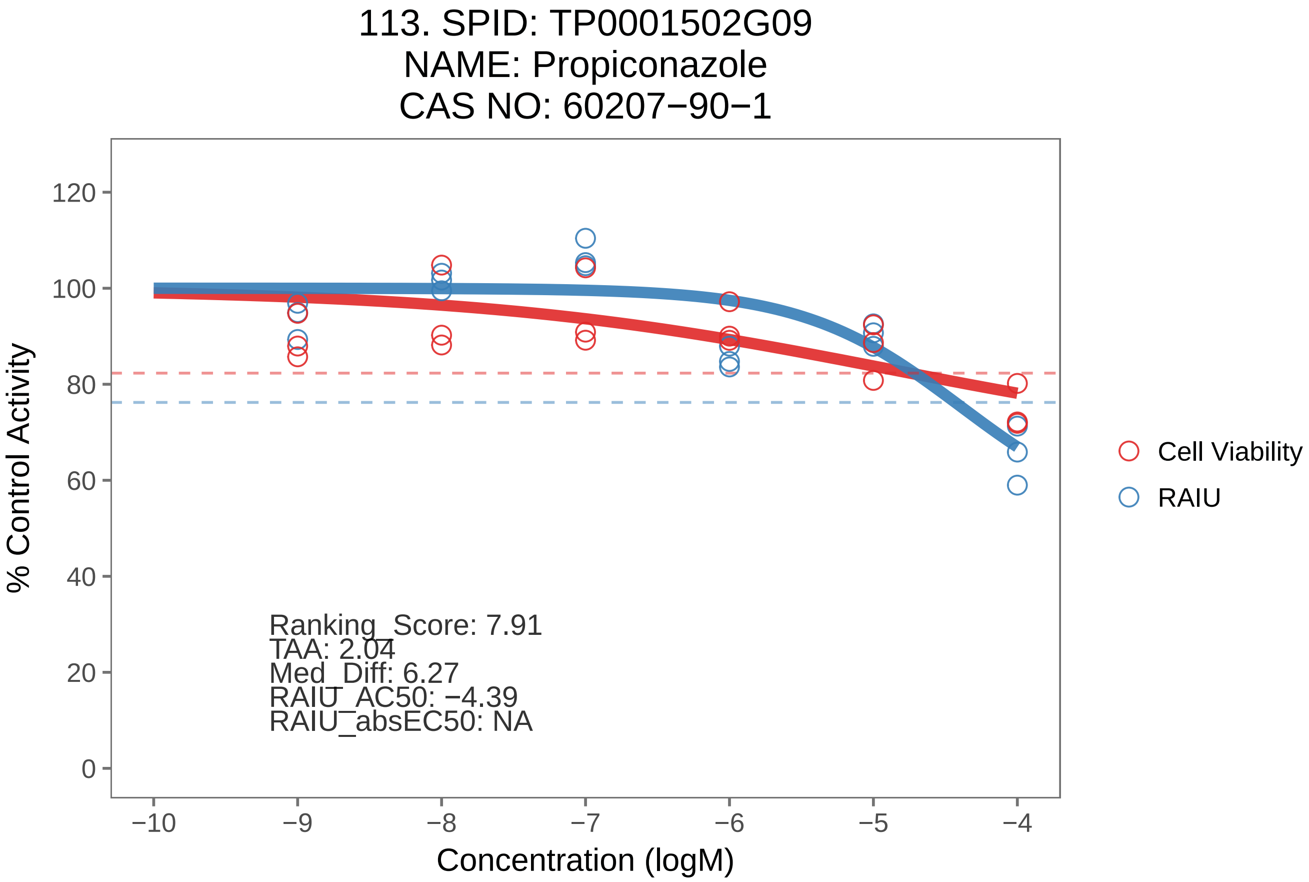

108. SPID: TP0001501E05
NAME: Thidiazuron
CAS NO: 51707−55−2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 9.43
TAA: 1.43
Med_Diff: 8.12
RAIU_AC50: −4.44
RAIU_absEC50: NA
Cell Viability
RAIU

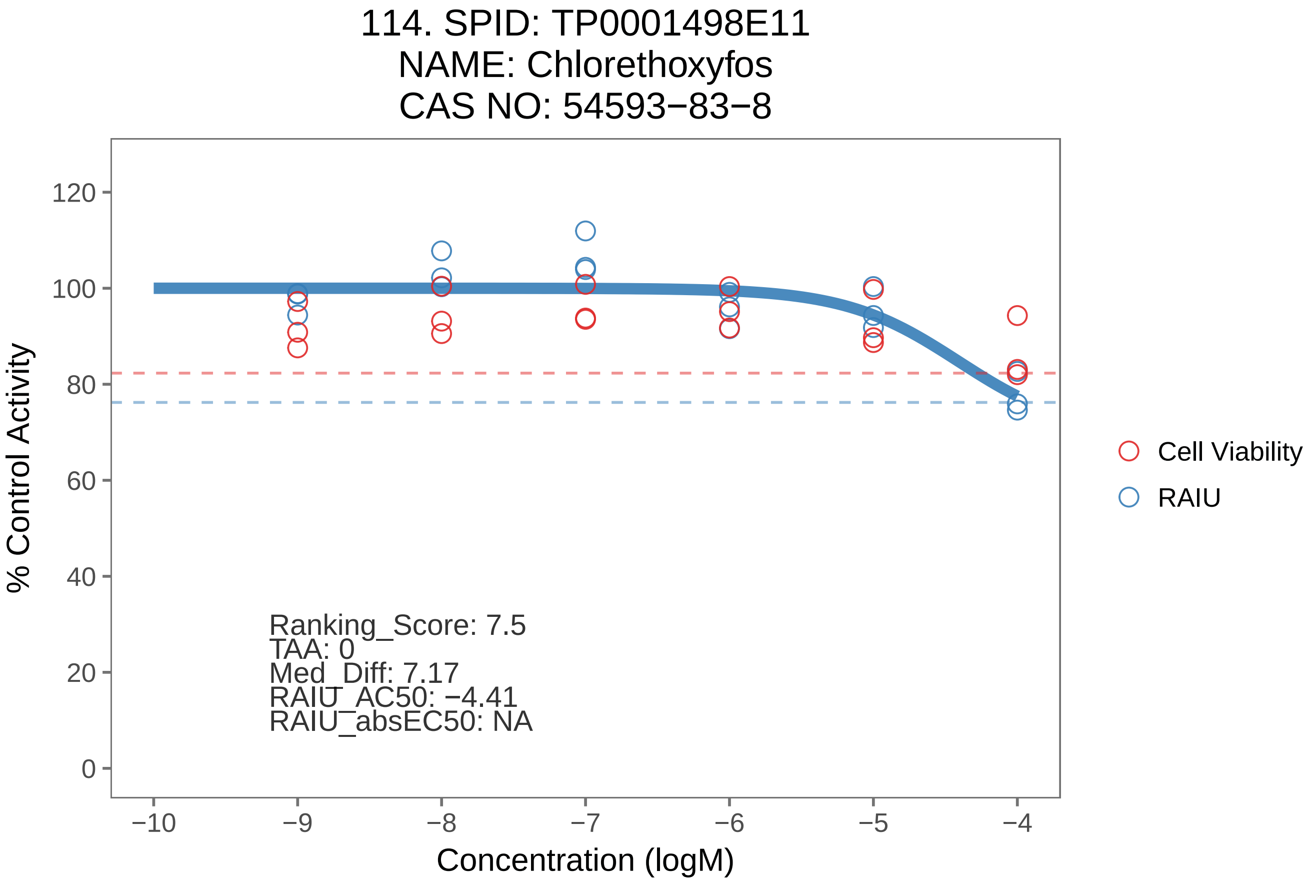

109. SPID: TP0001500B05
NAME: Famoxadone
CAS NO: 131807−57−3
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 8.99
TAA: 12.44
Med_Diff: 0.72
RAIU_AC50: −5.69
RAIU_absEC50: −4.81

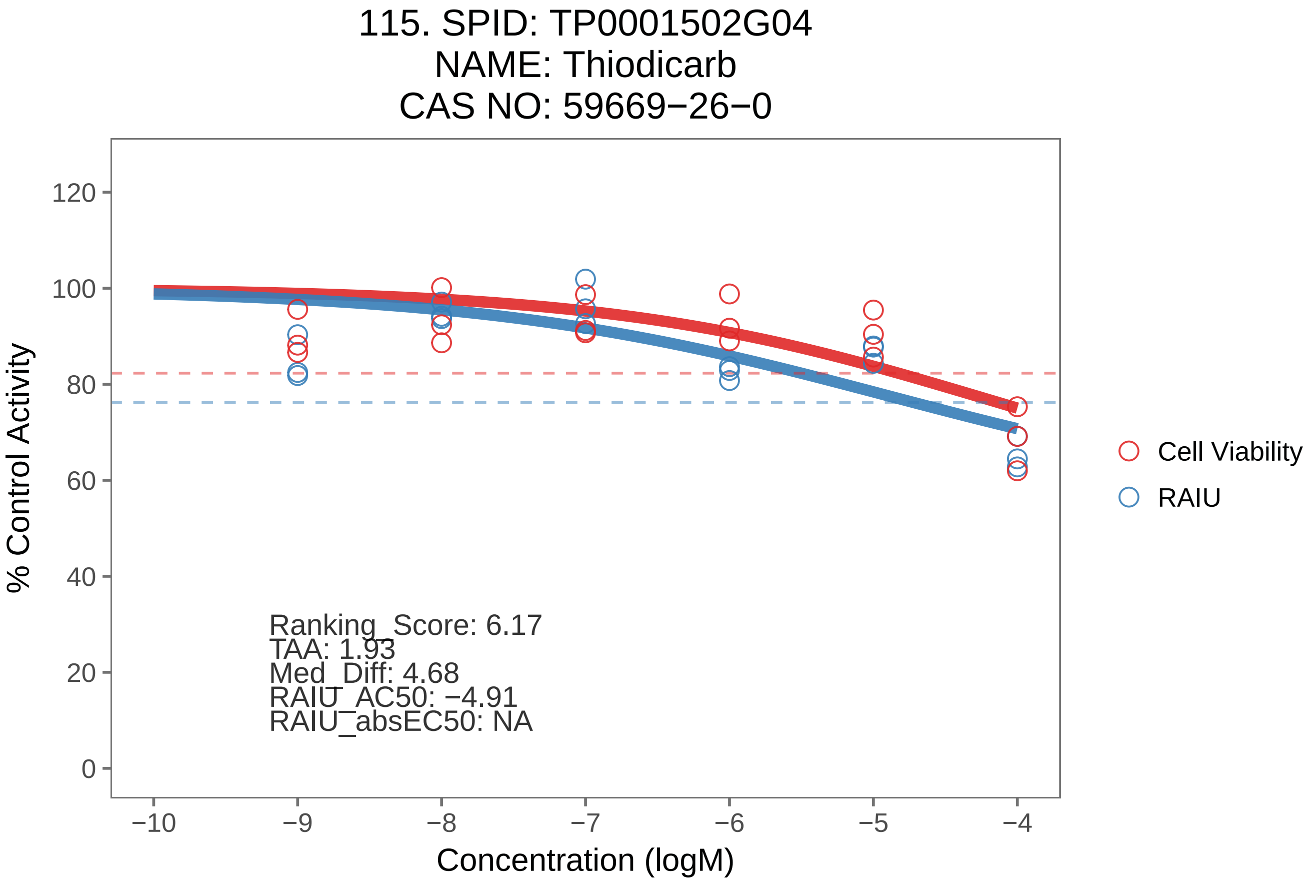

110. SPID: TP0001502E04
NAME: Dicofol
CAS NO: 115−32−2
% Control Activity
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: 8.89
TAA: 11.7
Med_Diff: 1.1
RAIU_AC50: −4.54
RAIU_absEC50: −4.61
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

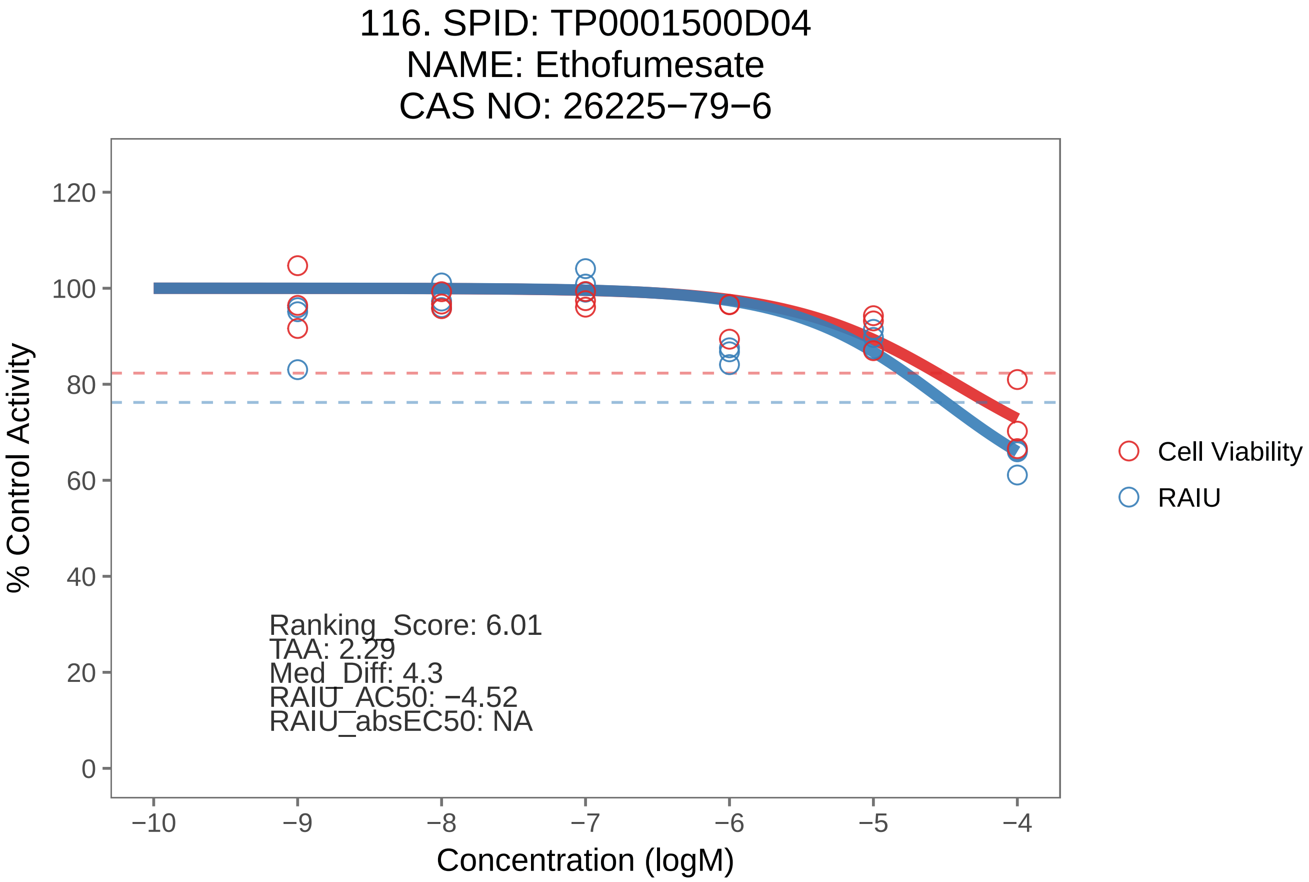

111. SPID: TP0001500F02
NAME: Propargite
CAS NO: 2312−35−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 8.8
TAA: 3.84
Med_Diff: 5.99
RAIU_AC50: −4.4
RAIU_absEC50: NA
Cell Viability
RAIU


112. SPID: TP0001501E02
NAME: 2,2−Bis(4−hydroxyphenyl)−1,1,1−trichloroethane
CAS NO: 2971−36−0
% Control Activity
Concentration (logM)
Ranking_Score: 8.69
TAA: 2.22
Med_Diff: 6.91
RAIU_AC50: −4.39
RAIU_absEC50: −4.46
Cell Viability
RAIU

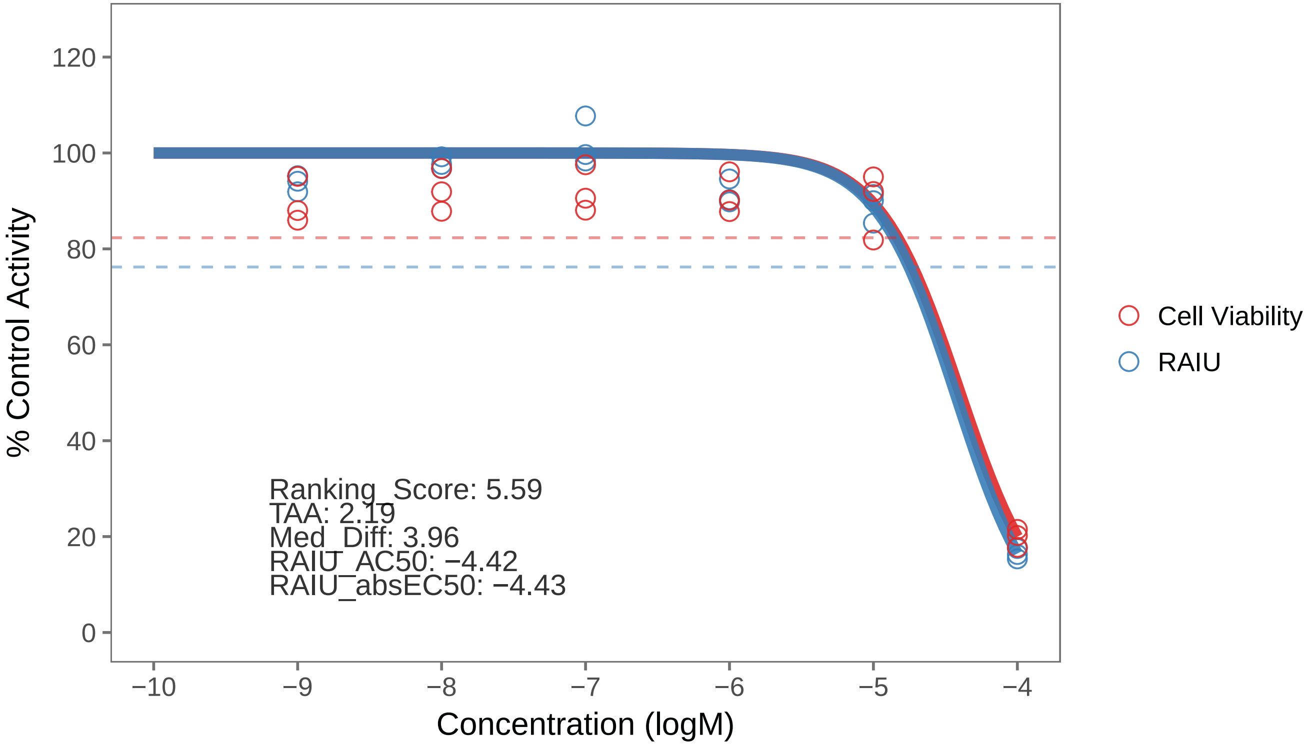

113. SPID: TP0001502G09
NAME: Propiconazole
CAS NO: 60207−90−1
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 7.91
TAA: 2.04
Med_Diff: 6.27
RAIU_AC50: −4.39
RAIU_absEC50: NA
Cell Viability
RAIU

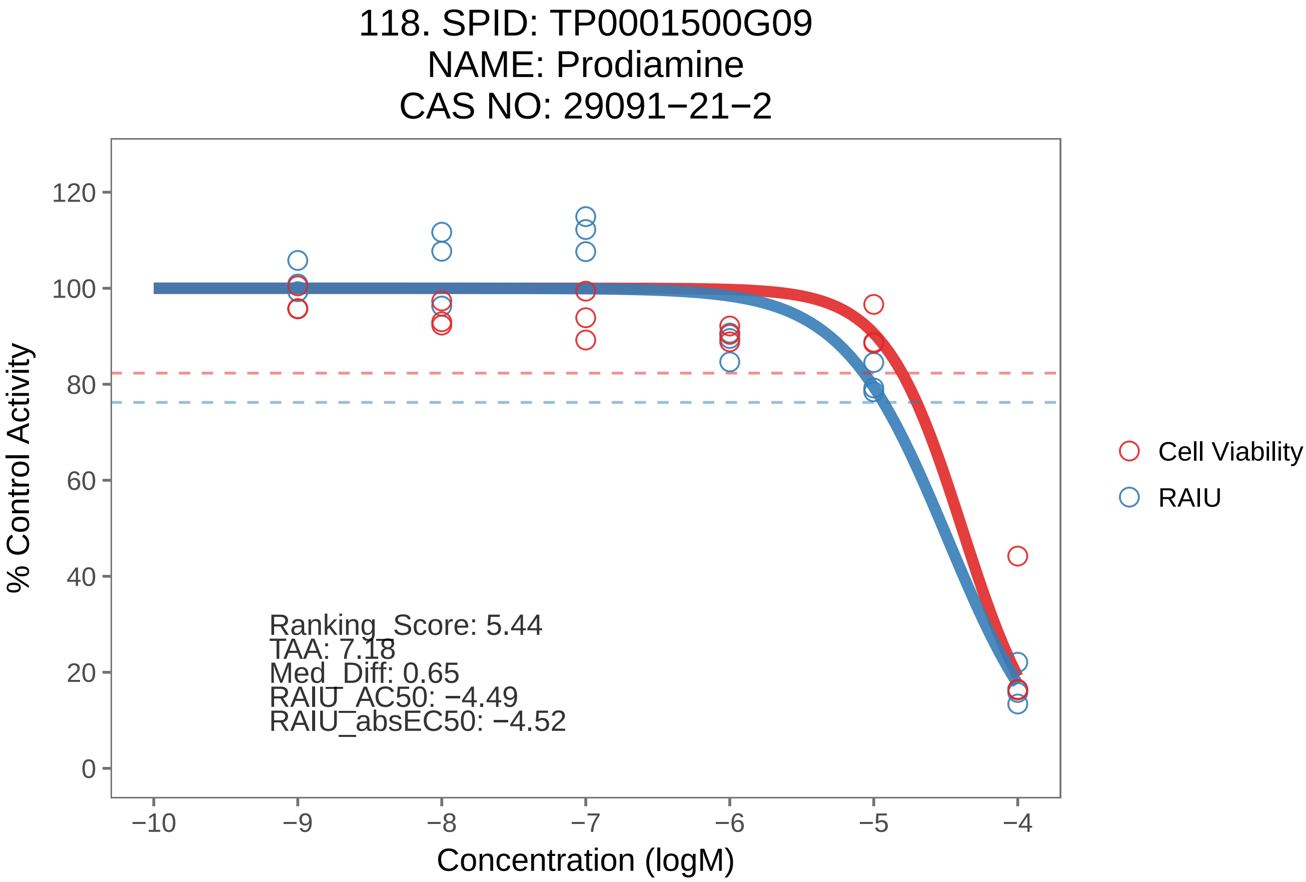

114. SPID: TP0001498E11
NAME: Chlorethoxyfos
CAS NO: 54593−83−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 7.5
TAA: 0
Med_Diff: 7.17
RAIU_AC50: −4.41
RAIU_absEC50: NA
Cell Viability
RAIU

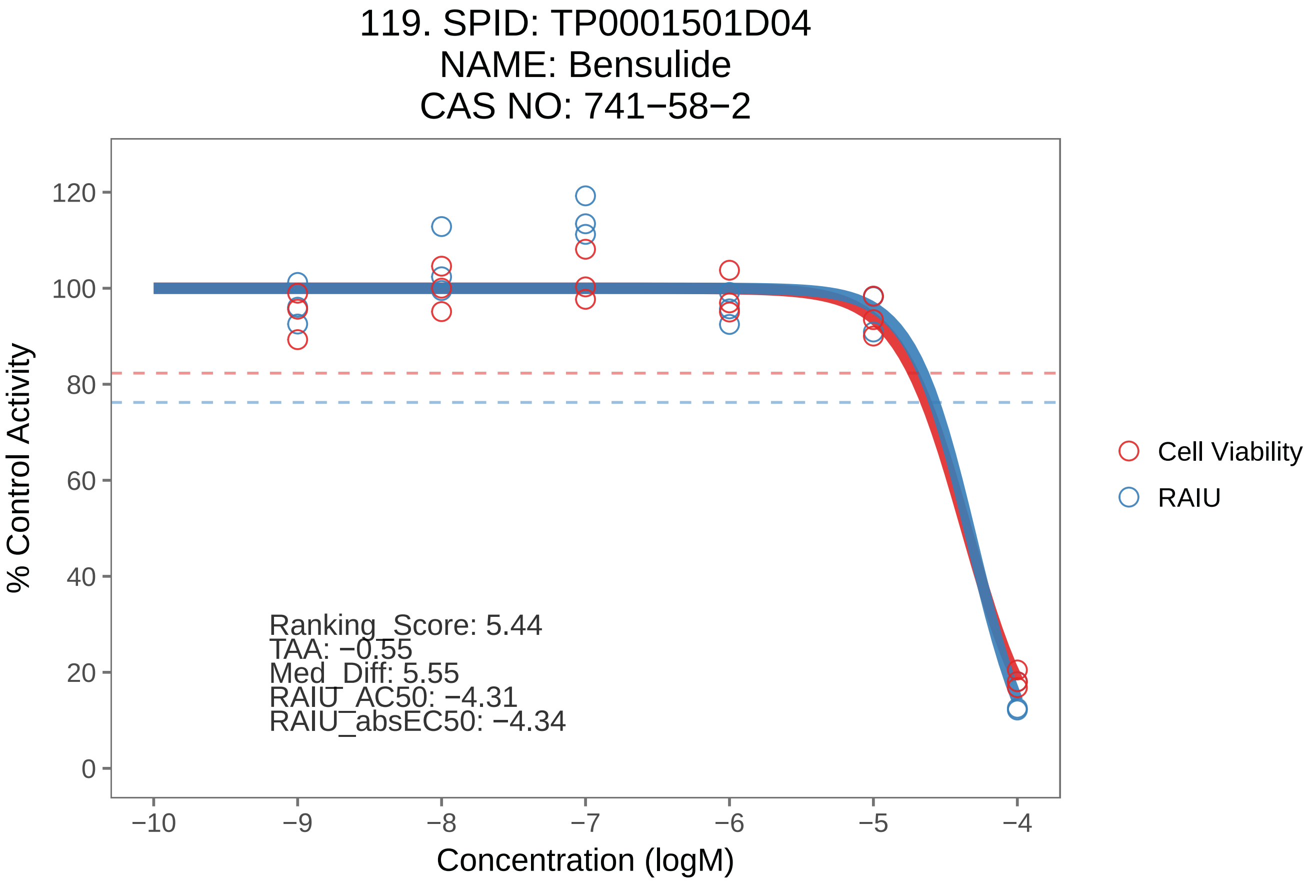

115. SPID: TP0001502G04
NAME: Thiodicarb
CAS NO: 59669−26−0
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 6.17
TAA: 1.93
Med_Diff: 4.68
RAIU_AC50: −4.91
RAIU_absEC50: NA
Cell Viability
RAIU

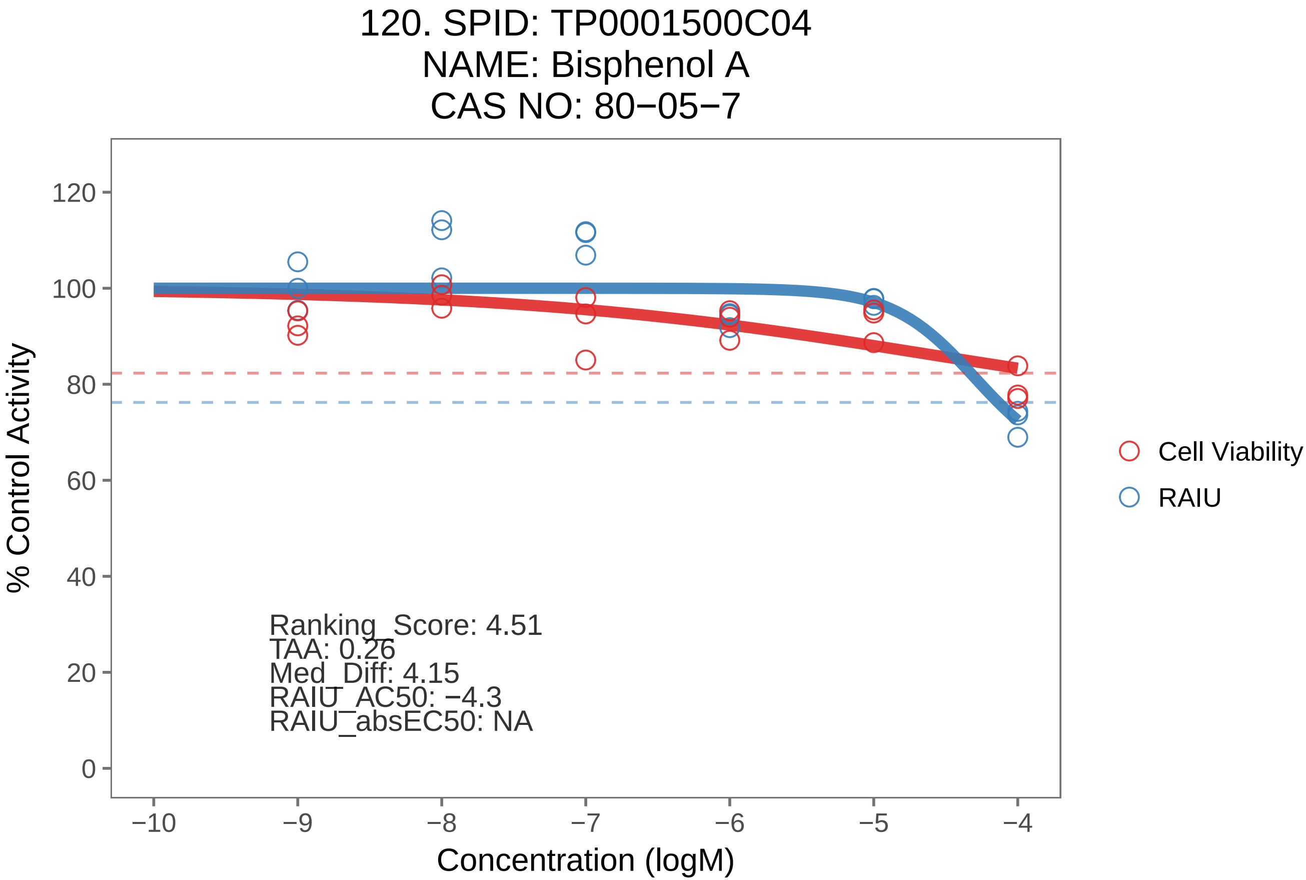

116. SPID: TP0001500D04
NAME: Ethofumesate
CAS NO: 26225−79−6
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 6.01
TAA: 2.29
Med_Diff: 4.3
RAIU_AC50: −4.52
RAIU_absEC50: NA
Cell Viability
RAIU

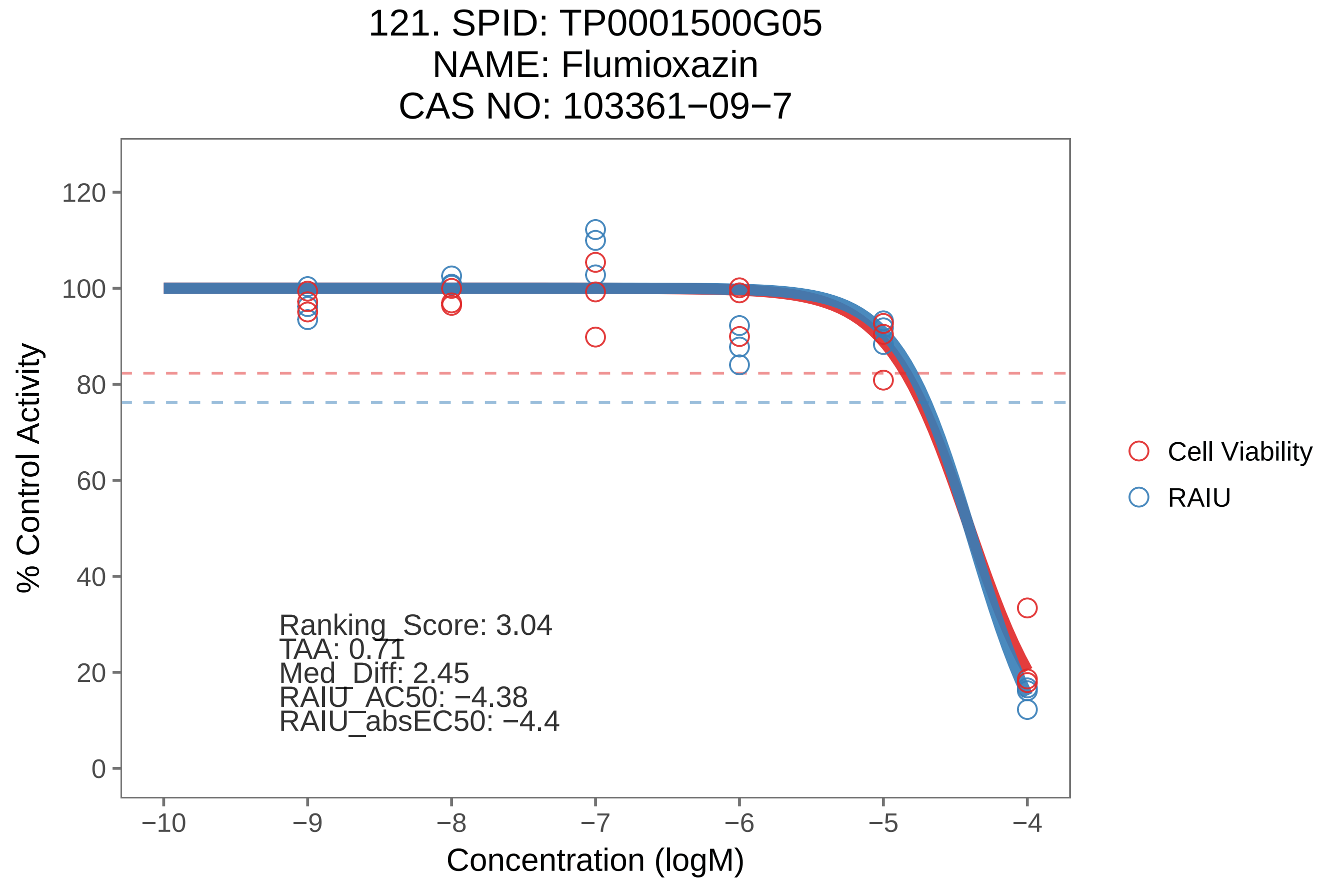
117. SPID: TP0001498F07
NAME: Bensulide
CAS NO: 741−58−2

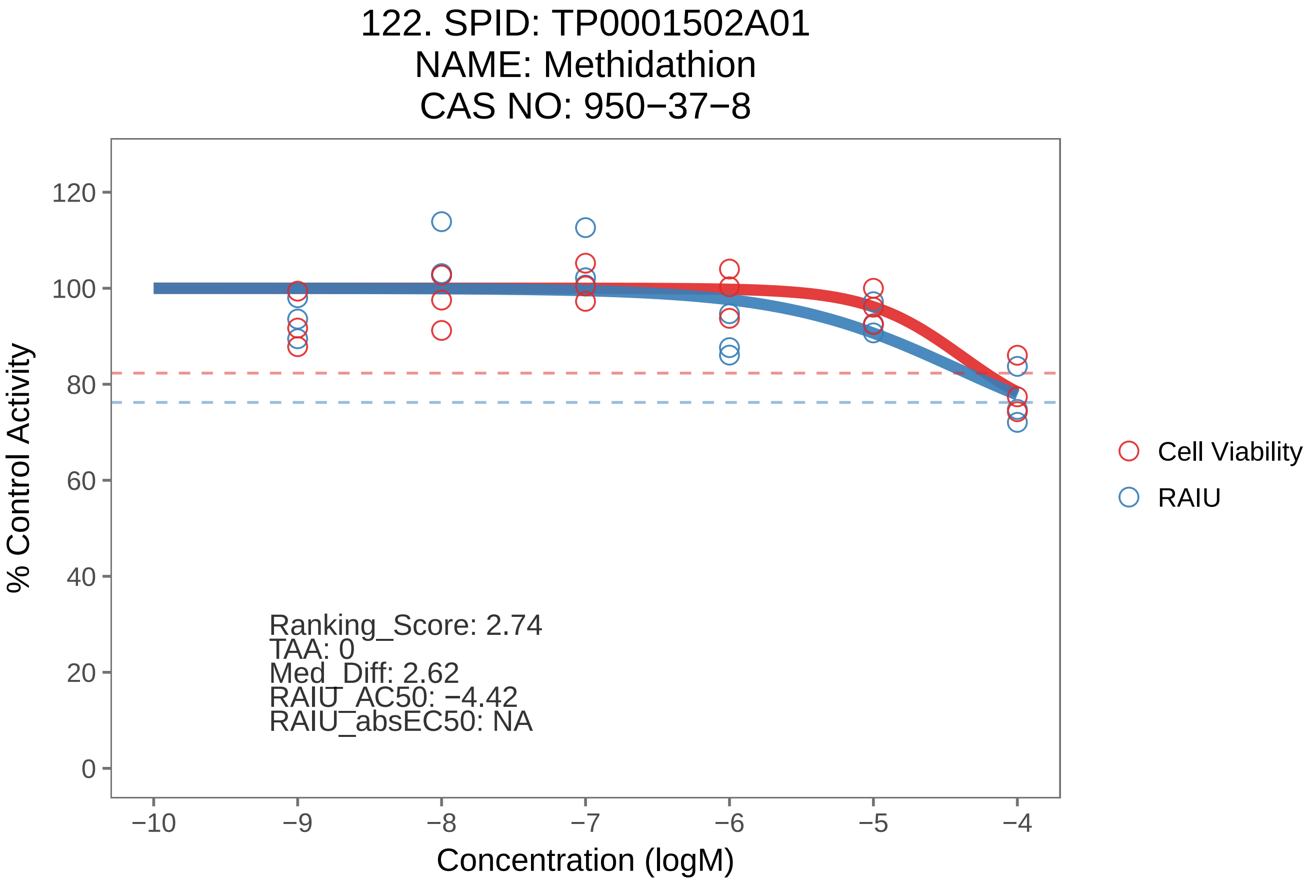


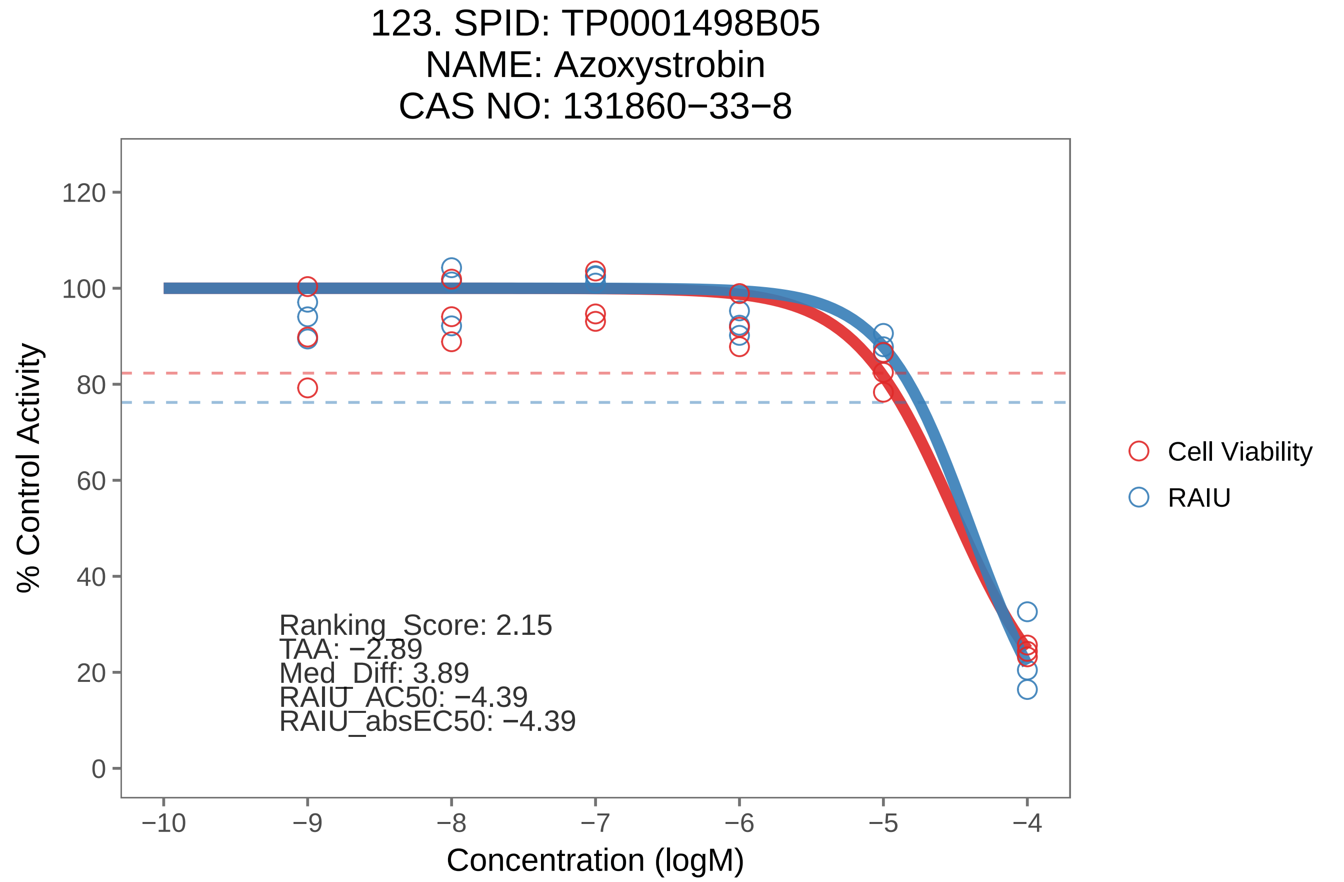

118. SPID: TP0001500G09
NAME: Prodiamine
CAS NO: 29091−21−2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 5.44
TAA: 7.18
Med_Diff: 0.65
RAIU_AC50: −4.49
RAIU_absEC50: −4.52
Cell Viability
RAIU

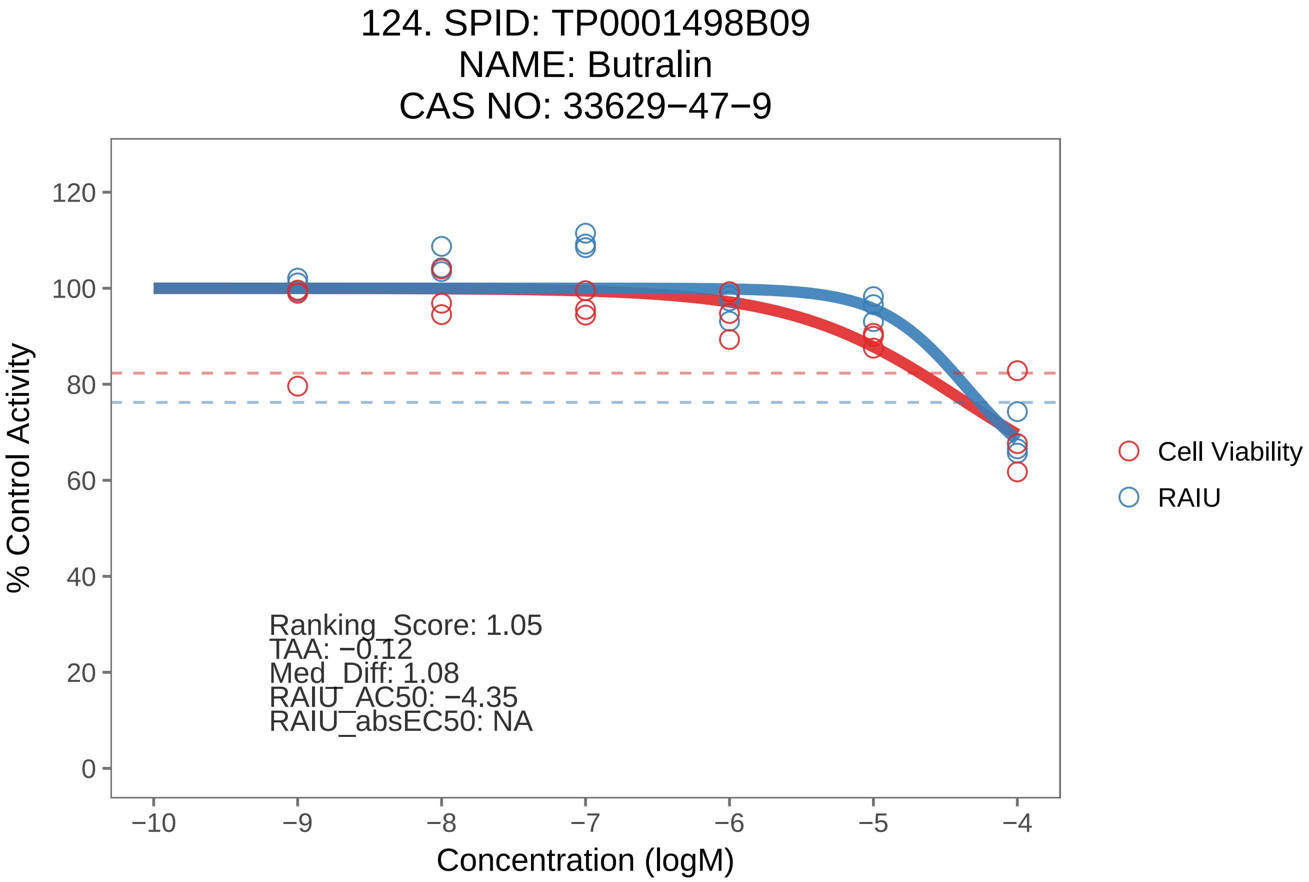

119. SPID: TP0001501D04
NAME: Bensulide
CAS NO: 741−58−2
% Control Activity
0
20
40
60
80
100
120
Concentration (logM)
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 5.44
TAA: −0.55
Med_Diff: 5.55
RAIU_AC50: −4.31
RAIU_absEC50: −4.34
Cell Viability
RAIU


120. SPID: TP0001500C04
NAME: Bisphenol A
CAS NO: 80−05−7
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: 4.51
TAA: 0.26
Med_Diff: 4.15
RAIU_AC50: −4.3
RAIU_absEC50: NA
Cell Viability
RAIU

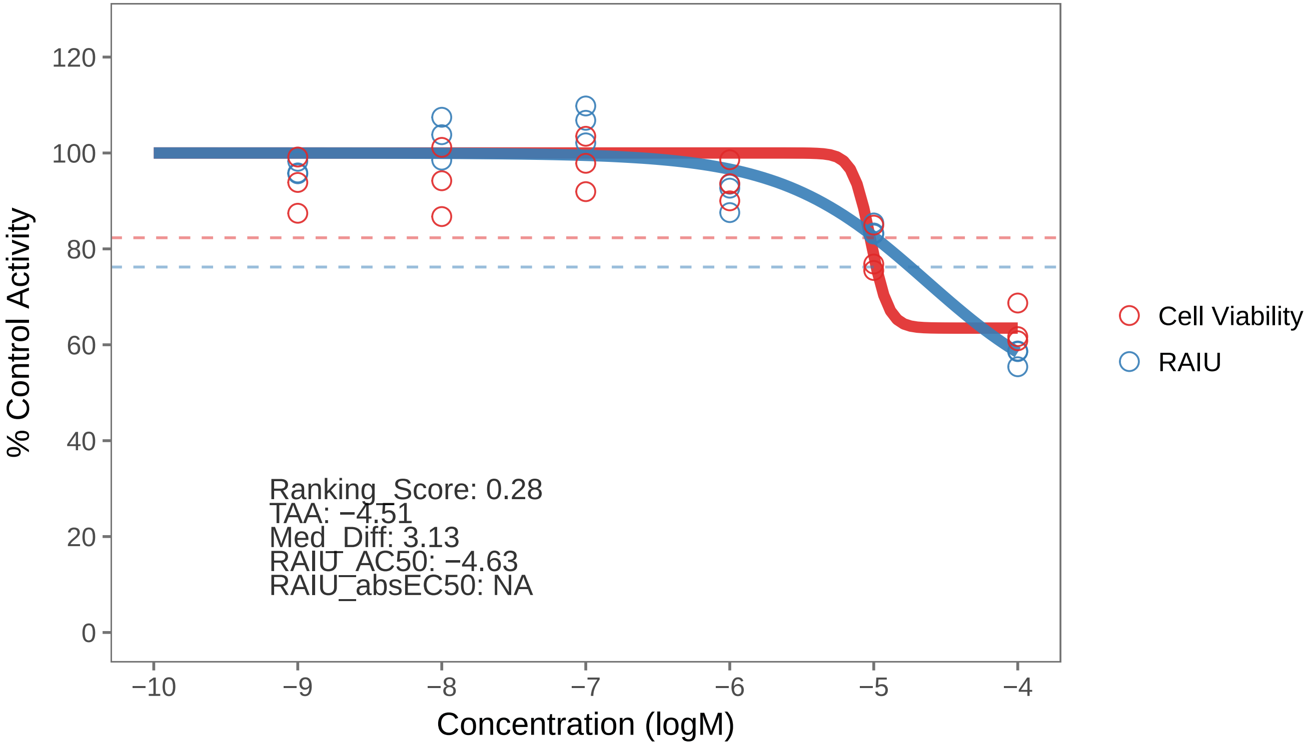

121. SPID: TP0001500G05
NAME: Flumioxazin
CAS NO: 103361−09−7
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 3.04
TAA: 0.71
Med_Diff: 2.45
RAIU_AC50: −4.38
RAIU_absEC50: −4.4
Cell Viability
RAIU

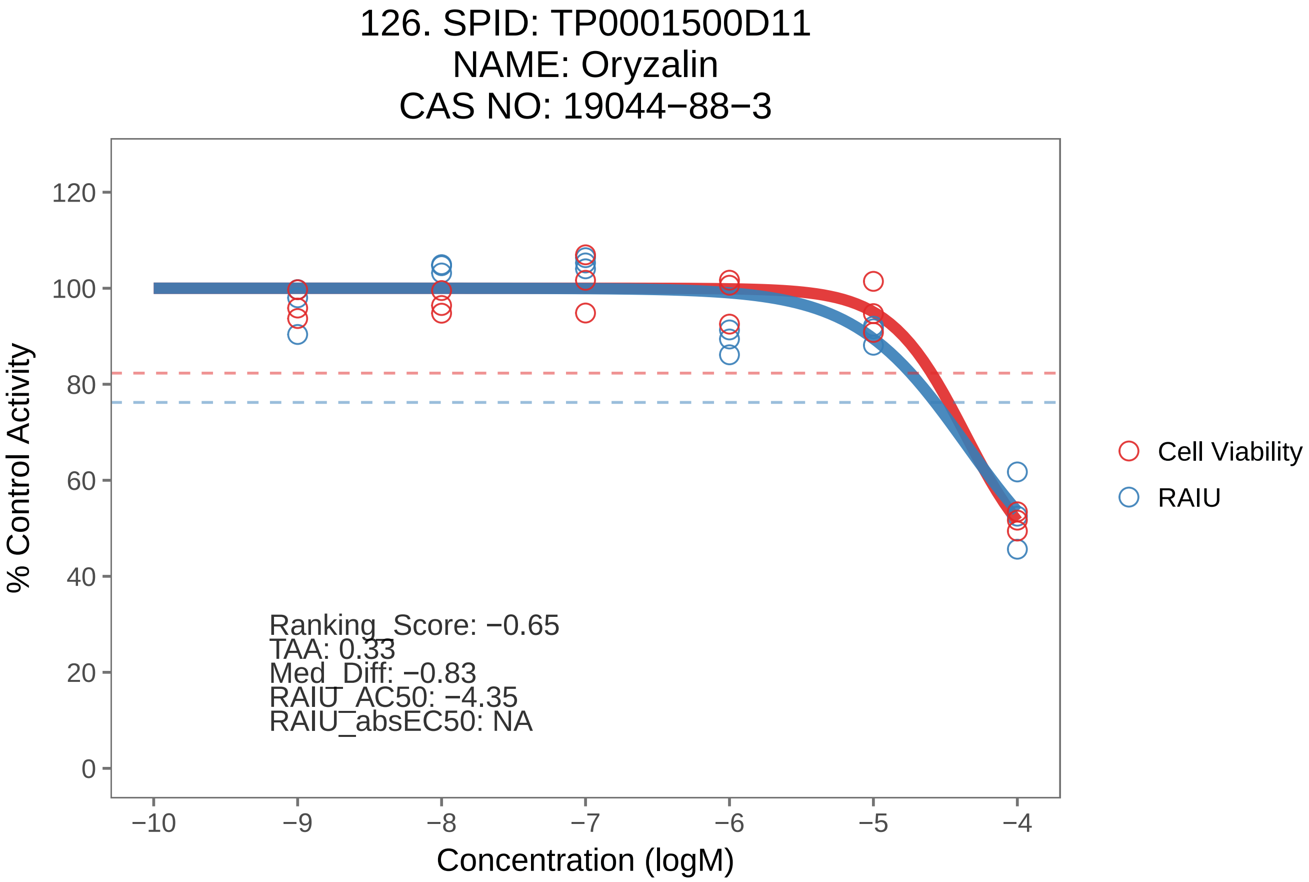

122. SPID: TP0001502A01
NAME: Methidathion
CAS NO: 950−37−8
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 2.74
TAA: 0
Med_Diff: 2.62
RAIU_AC50: −4.42
RAIU_absEC50: NA
Cell Viability
RAIU

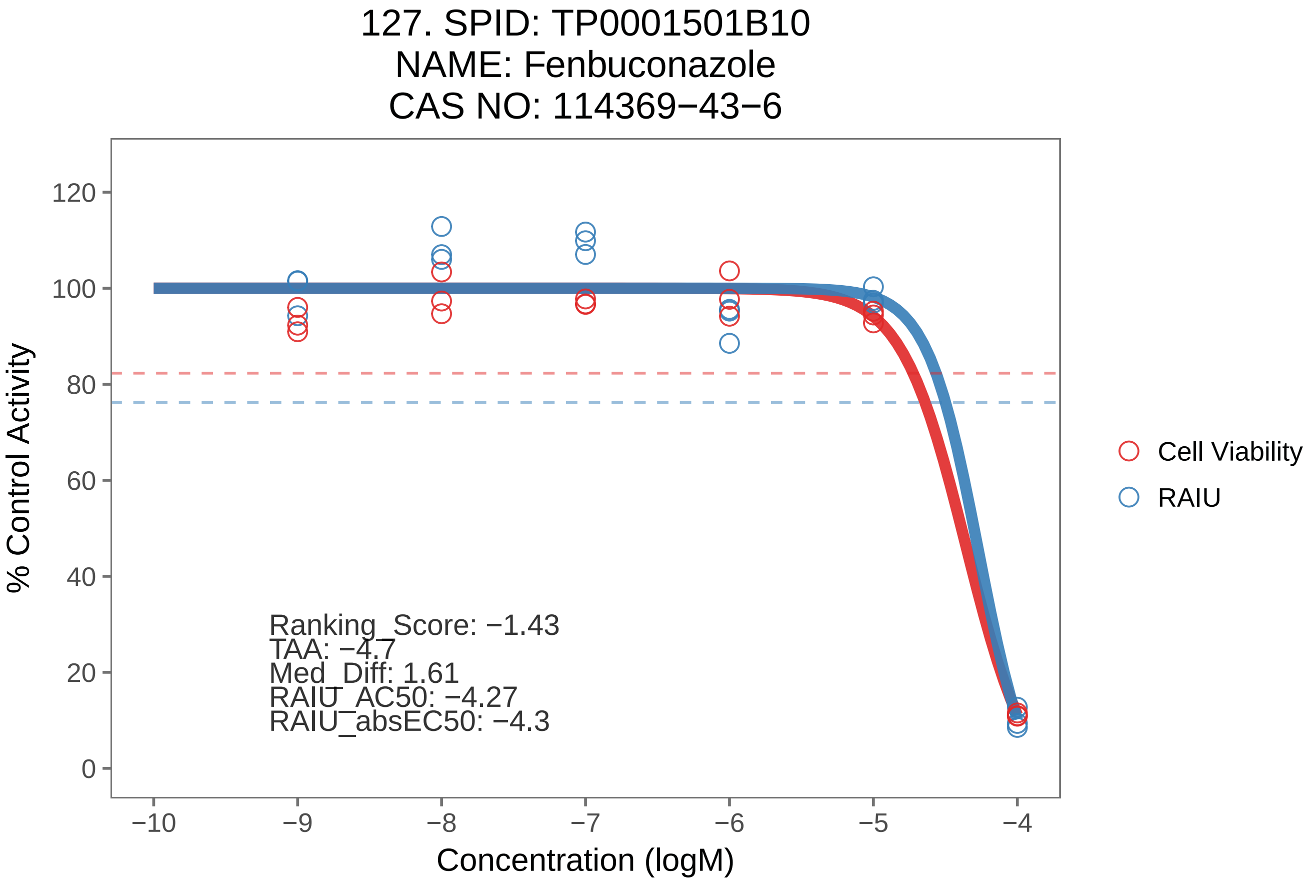

123. SPID: TP0001498B05
NAME: Azoxystrobin
CAS NO: 131860−33−8
Ranking_Score: 2.15
TAA: −2.89
Med_Diff: 3.89
RAIU_AC50: −4.39
RAIU_absEC50: −4.39
% Control Activity
Concentration (logM)
Cell Viability
RAIU
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4


124. SPID: TP0001498B09
NAME: Butralin
CAS NO: 33629−47−9
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: 1.05
TAA: −0.12
Med_Diff: 1.08
RAIU_AC50: −4.35
RAIU_absEC50: NA
Cell Viability
RAIU

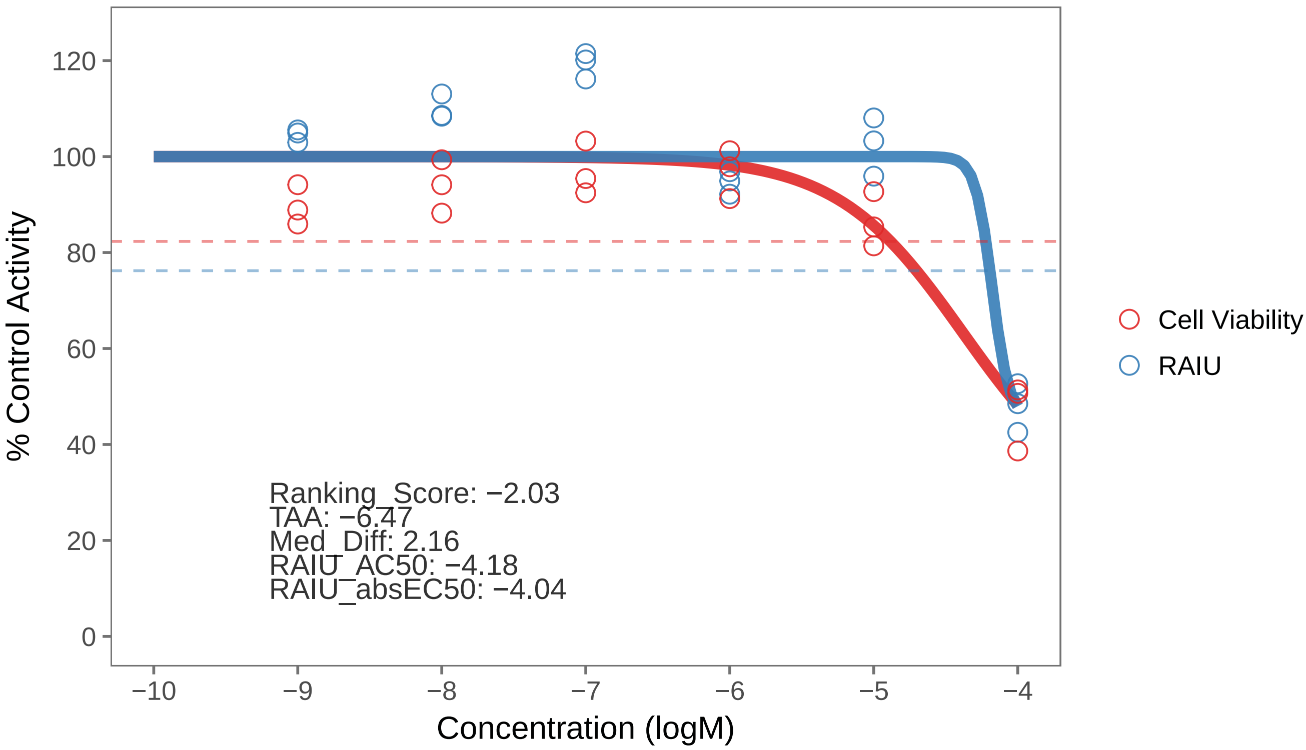
125. SPID: TP0001498D01
NAME: Dicloran
CAS NO: 99−30−9

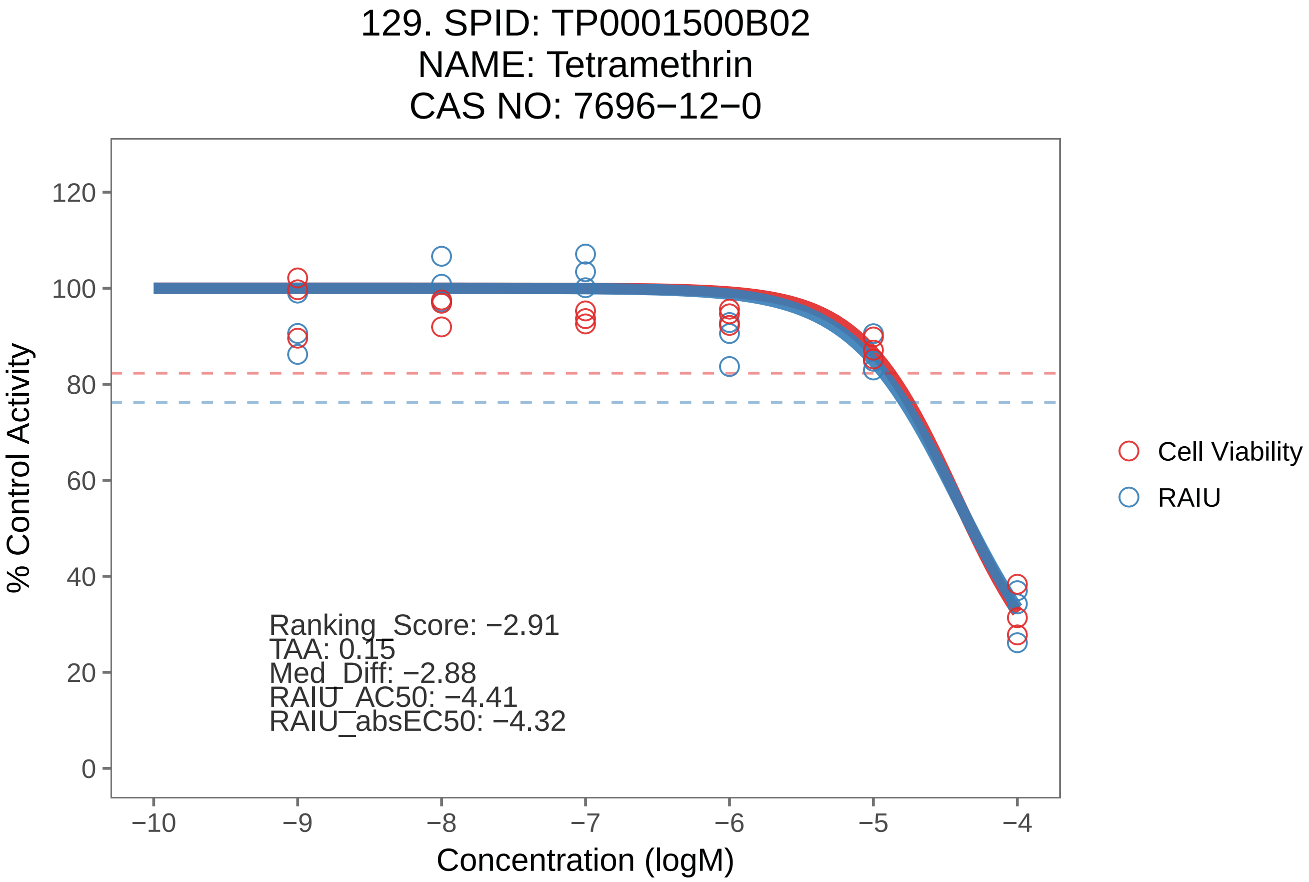


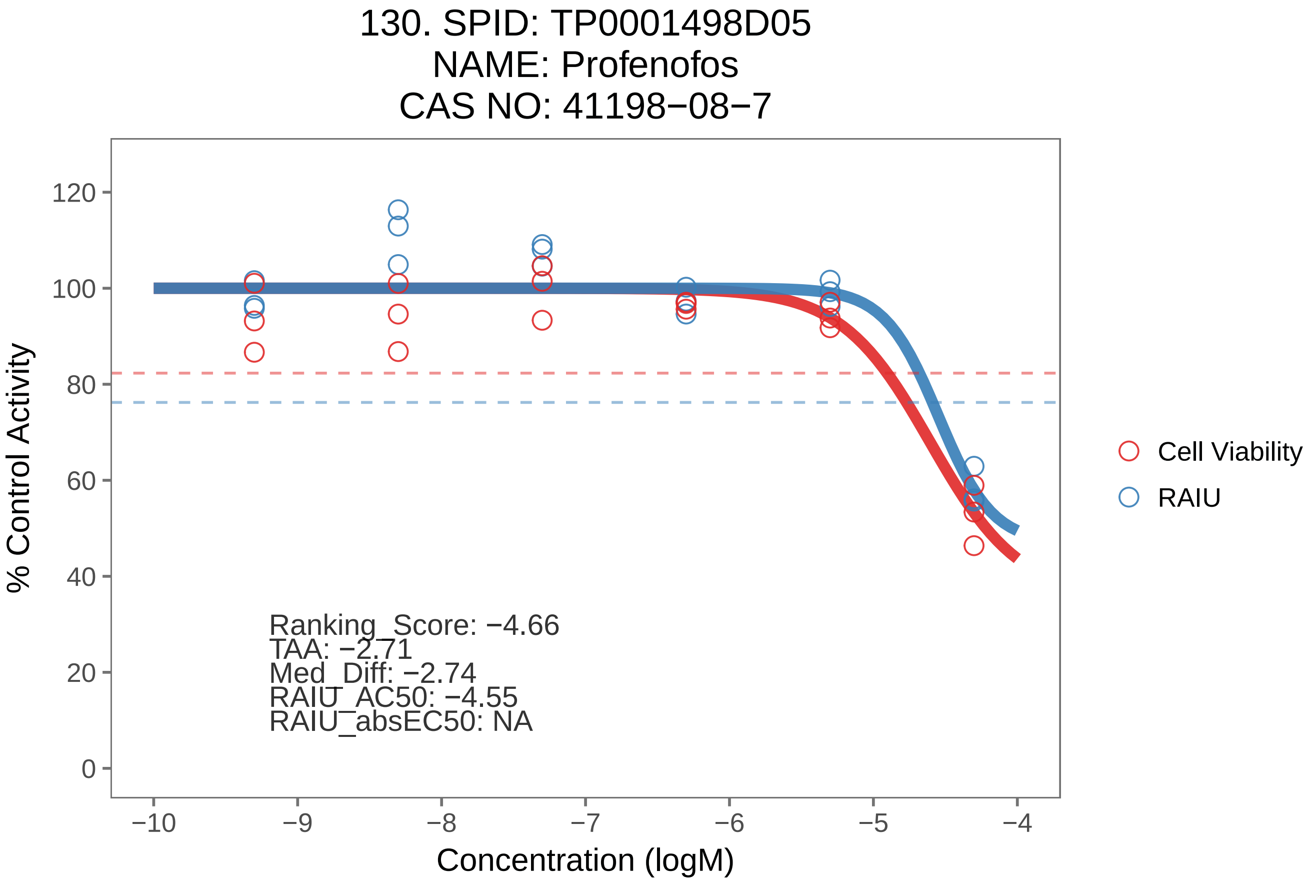

126. SPID: TP0001500D11
NAME: Oryzalin
CAS NO: 19044−88−3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: −0.65
TAA: 0.33
Med_Diff: −0.83
RAIU_AC50: −4.35
RAIU_absEC50: NA
Cell Viability
RAIU

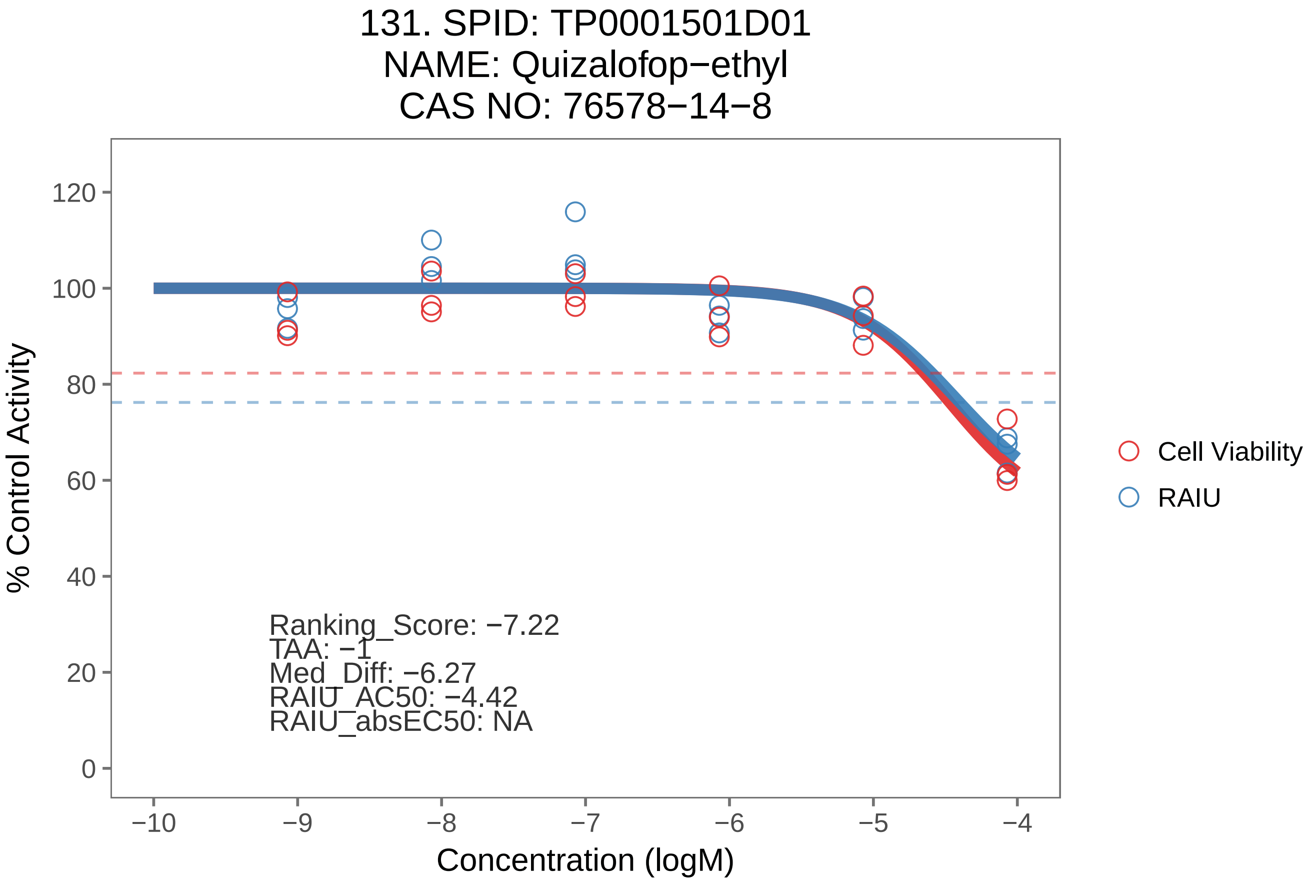

127. SPID: TP0001501B10
NAME: Fenbuconazole
CAS NO: 114369−43−6
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: −1.43
TAA: −4.7
Med_Diff: 1.61
RAIU_AC50: −4.27
RAIU_absEC50: −4.3
Cell Viability
RAIU

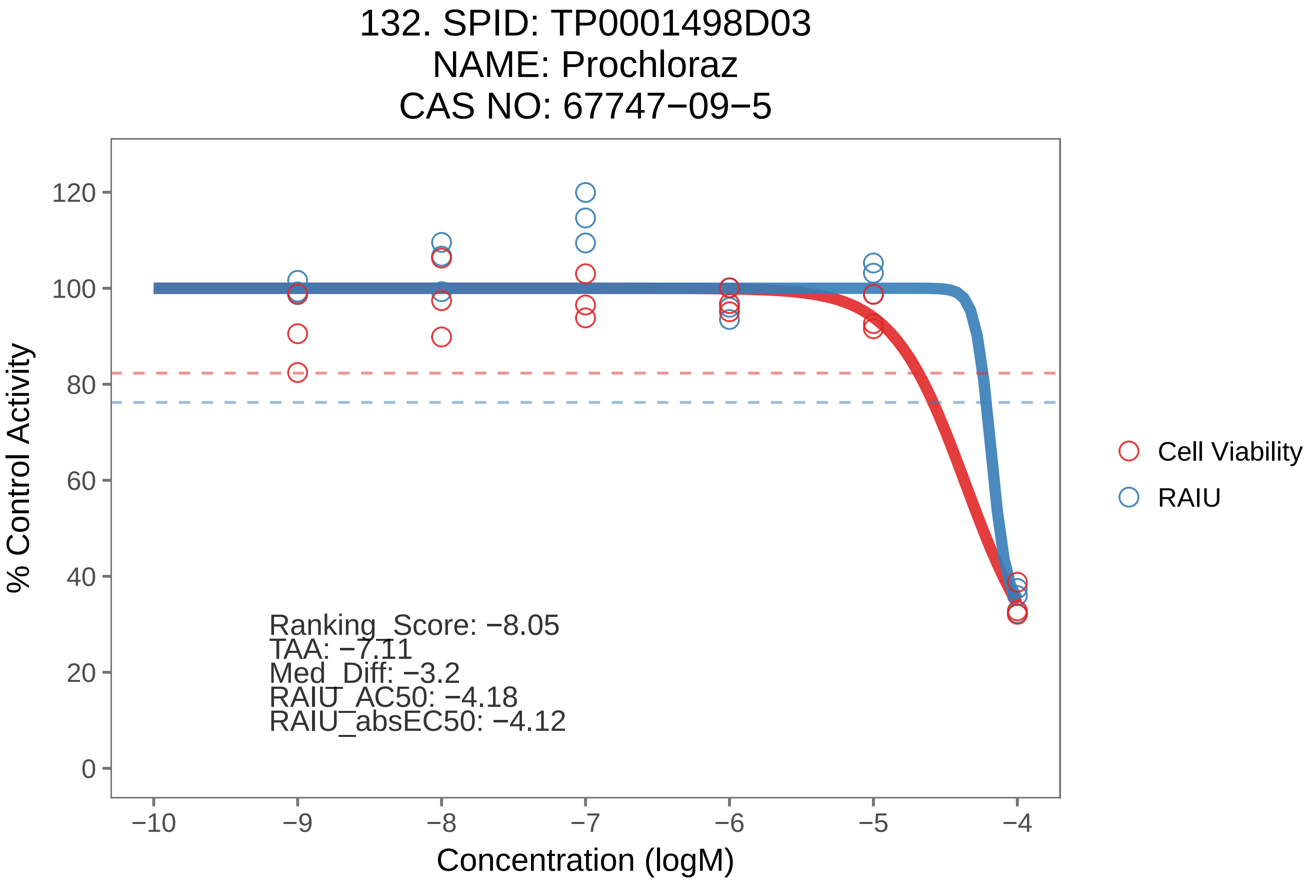
128. SPID: TP0001499E09
NAME: Thiram
CAS NO: 137−26−8

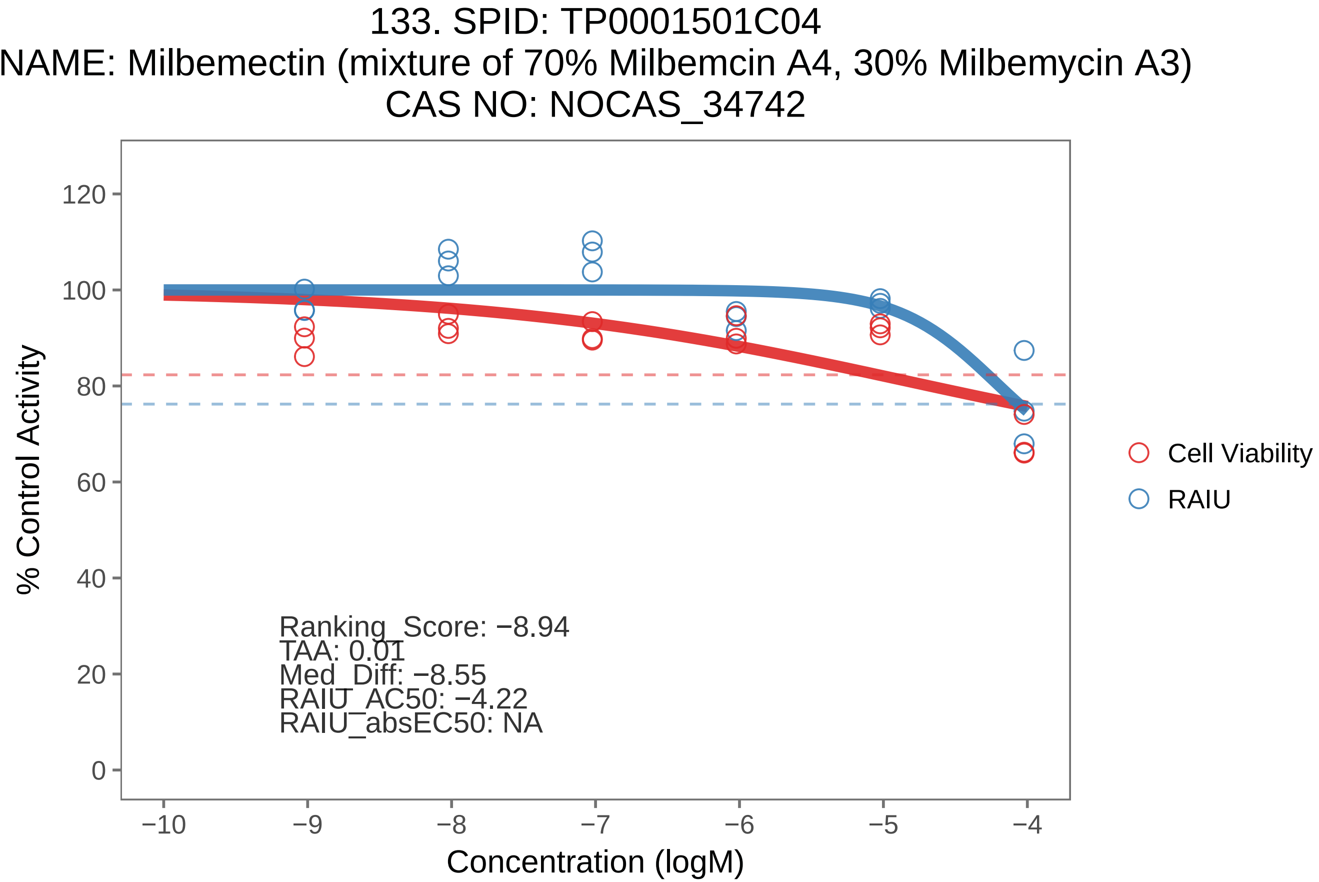


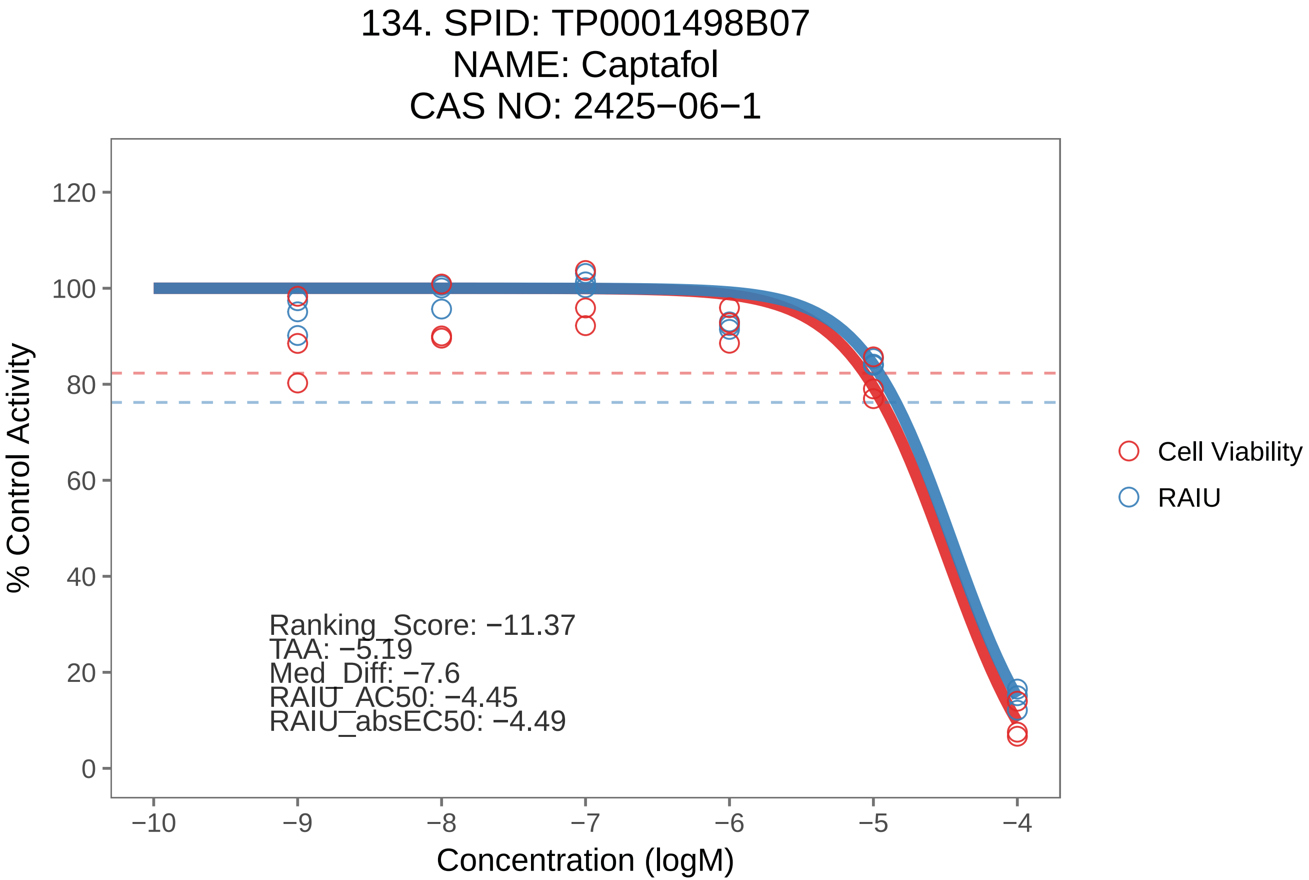

129. SPID: TP0001500B02
NAME: Tetramethrin
CAS NO: 7696−12−0
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: −2.91
TAA: 0.15
Med_Diff: −2.88
RAIU_AC50: −4.41
RAIU_absEC50: −4.32

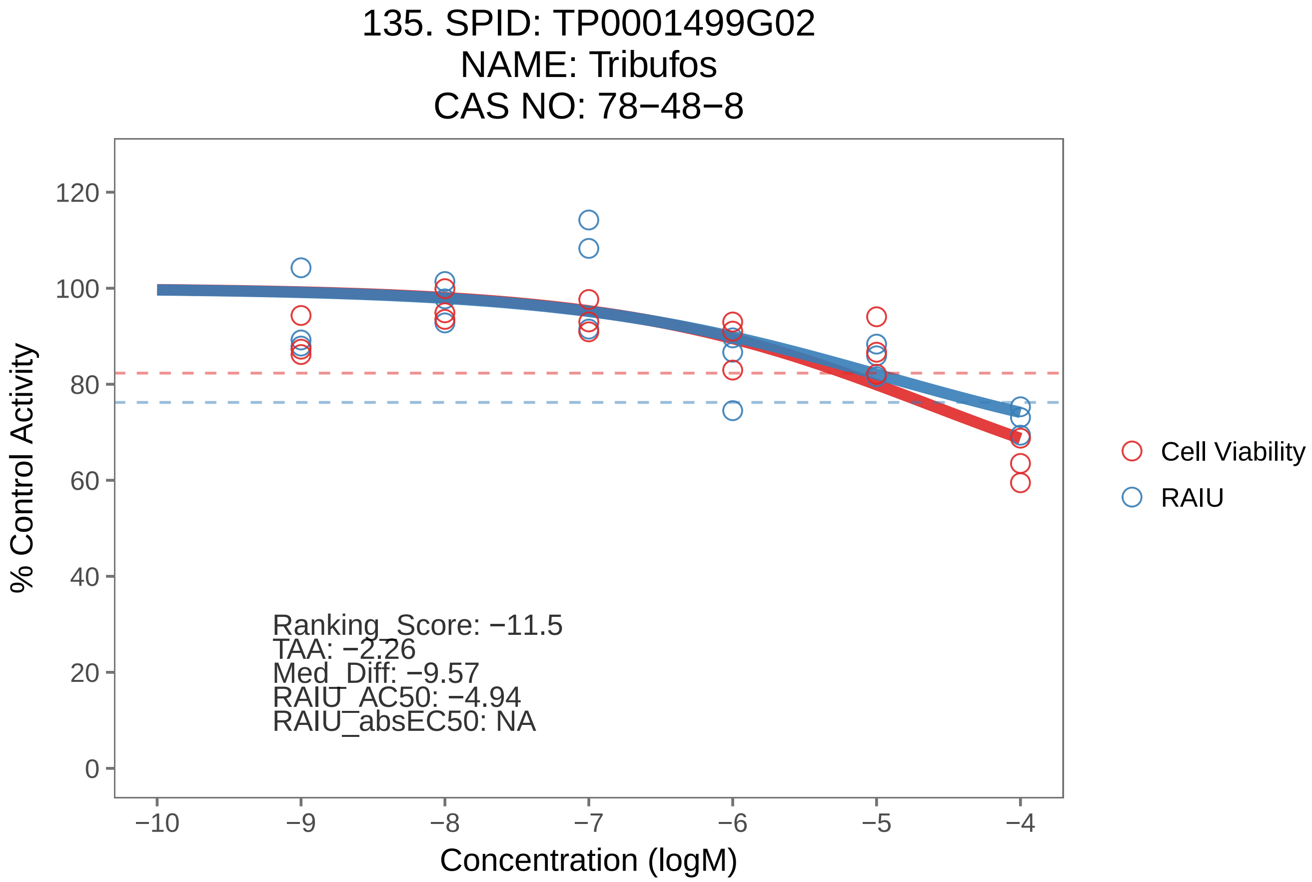

130. SPID: TP0001498D05
NAME: Profenofos
CAS NO: 41198−08−7
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
Ranking_Score: −4.66
TAA: −2.71
Med_Diff: −2.74
RAIU_AC50: −4.55
RAIU_absEC50: NA

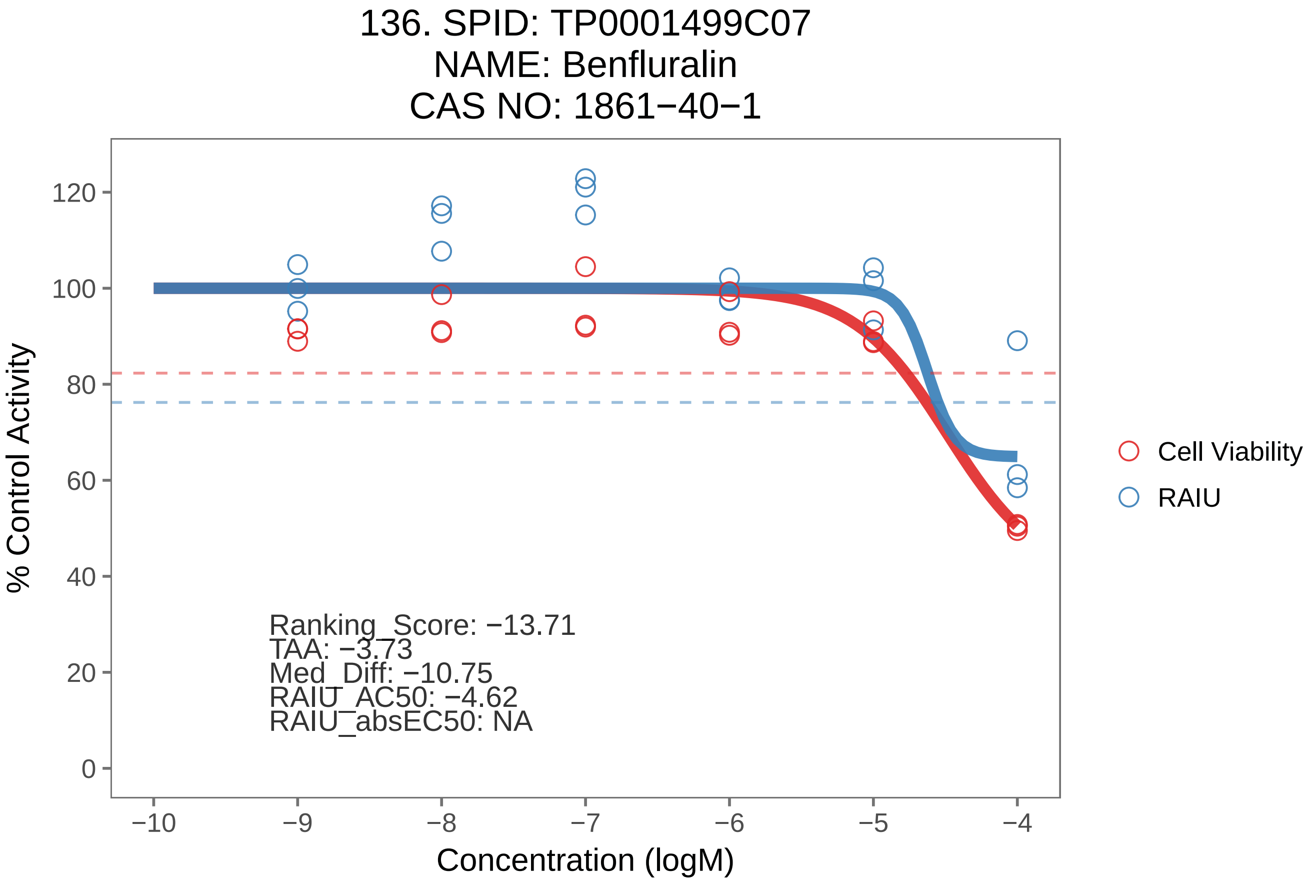

131. SPID: TP0001501D01
NAME: Quizalofop−ethyl
CAS NO: 76578−14−8
% Control Activity
Concentration (logM)
Ranking_Score: −7.22
TAA: −1
Med_Diff: −6.27
RAIU_AC50: −4.42
RAIU_absEC50: NA
Cell Viability
RAIU
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4

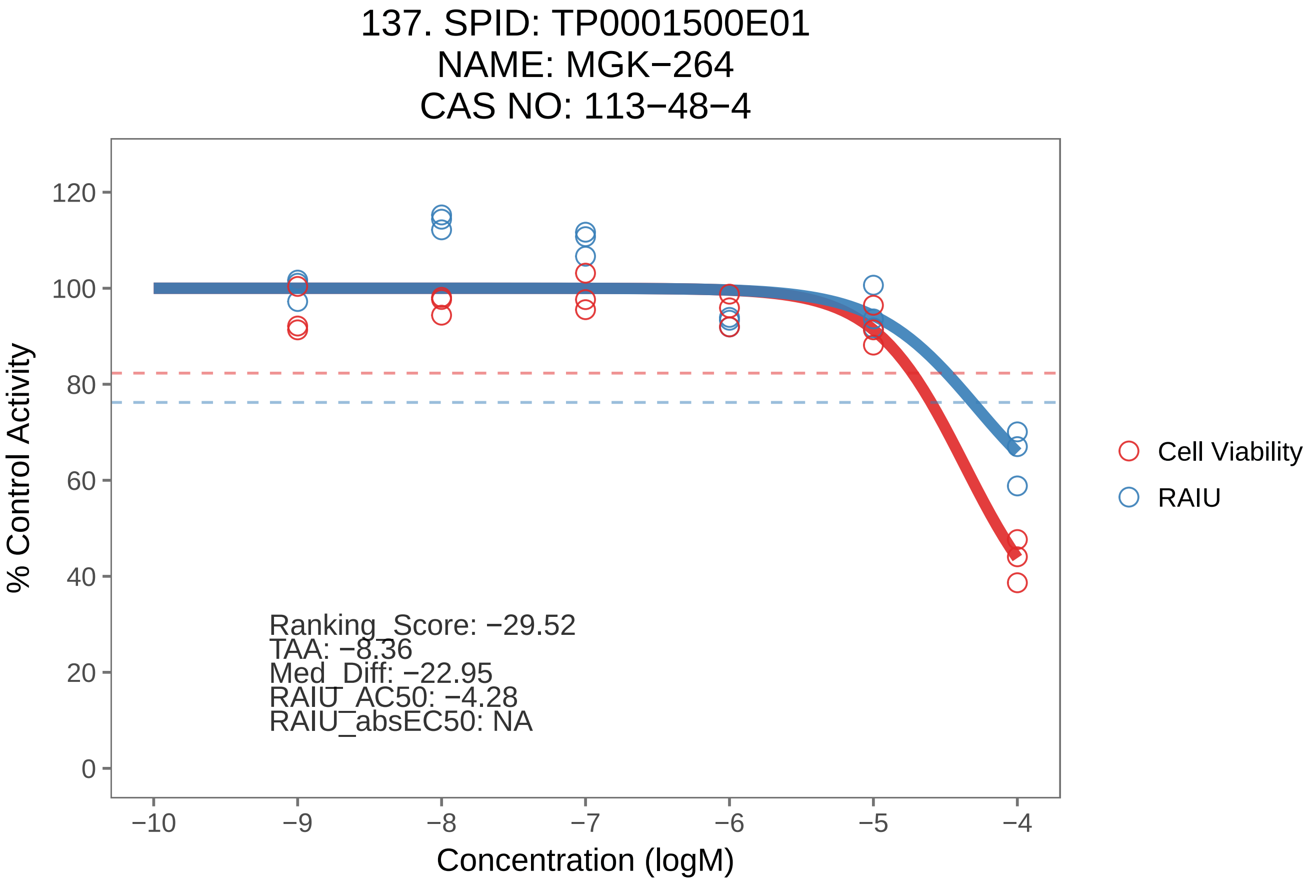

132. SPID: TP0001498D03
NAME: Prochloraz
CAS NO: 67747−09−5
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Ranking_Score: −8.05
TAA: −7.11
Med_Diff: −3.2
RAIU_AC50: −4.18
RAIU_absEC50: −4.12
Cell Viability
RAIU

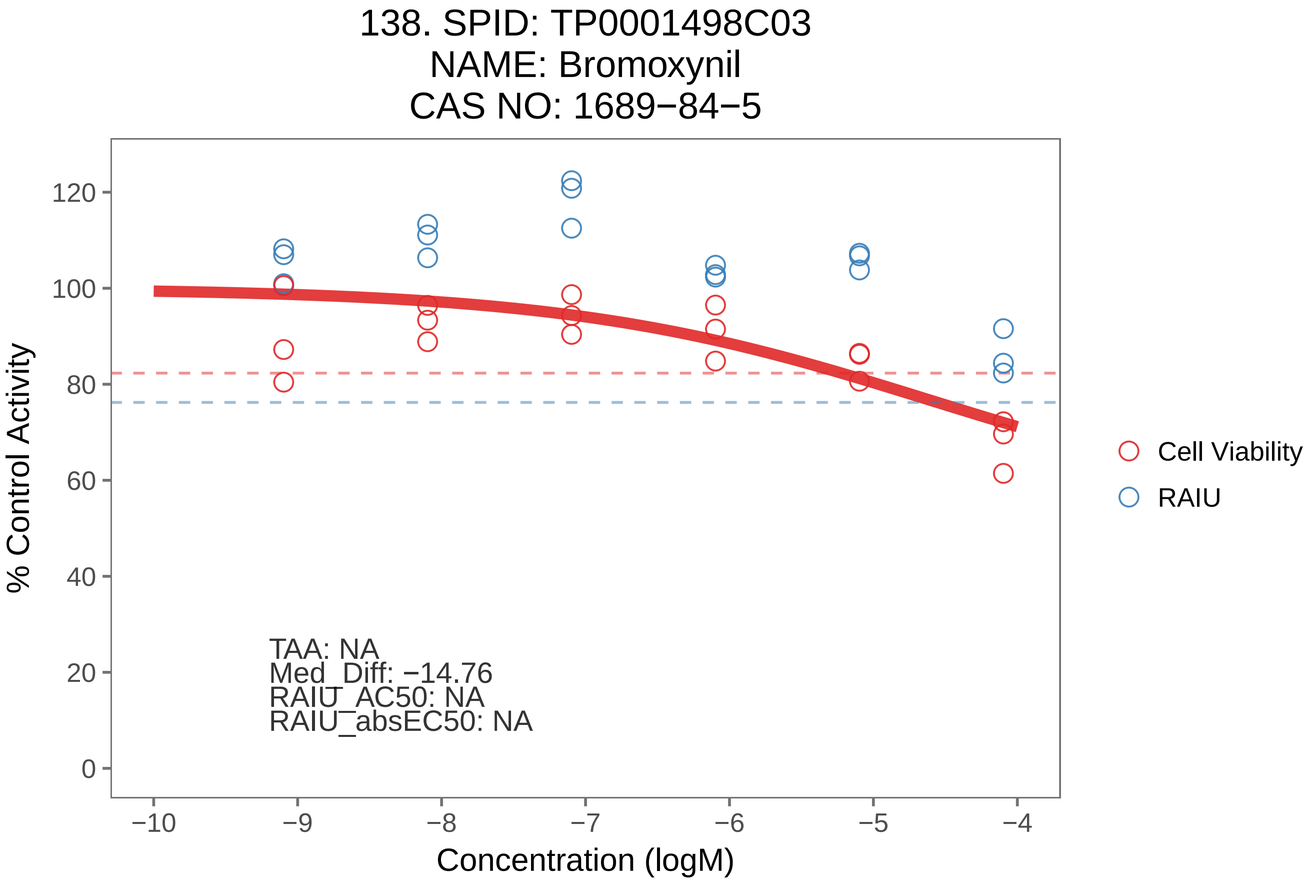

133. SPID: TP0001501C04
NAME: Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3)
CAS NO: NOCAS_34742
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: −8.94
TAA: 0.01
Med_Diff: −8.55
RAIU_AC50: −4.22
RAIU_absEC50: NA
Cell Viability
RAIU

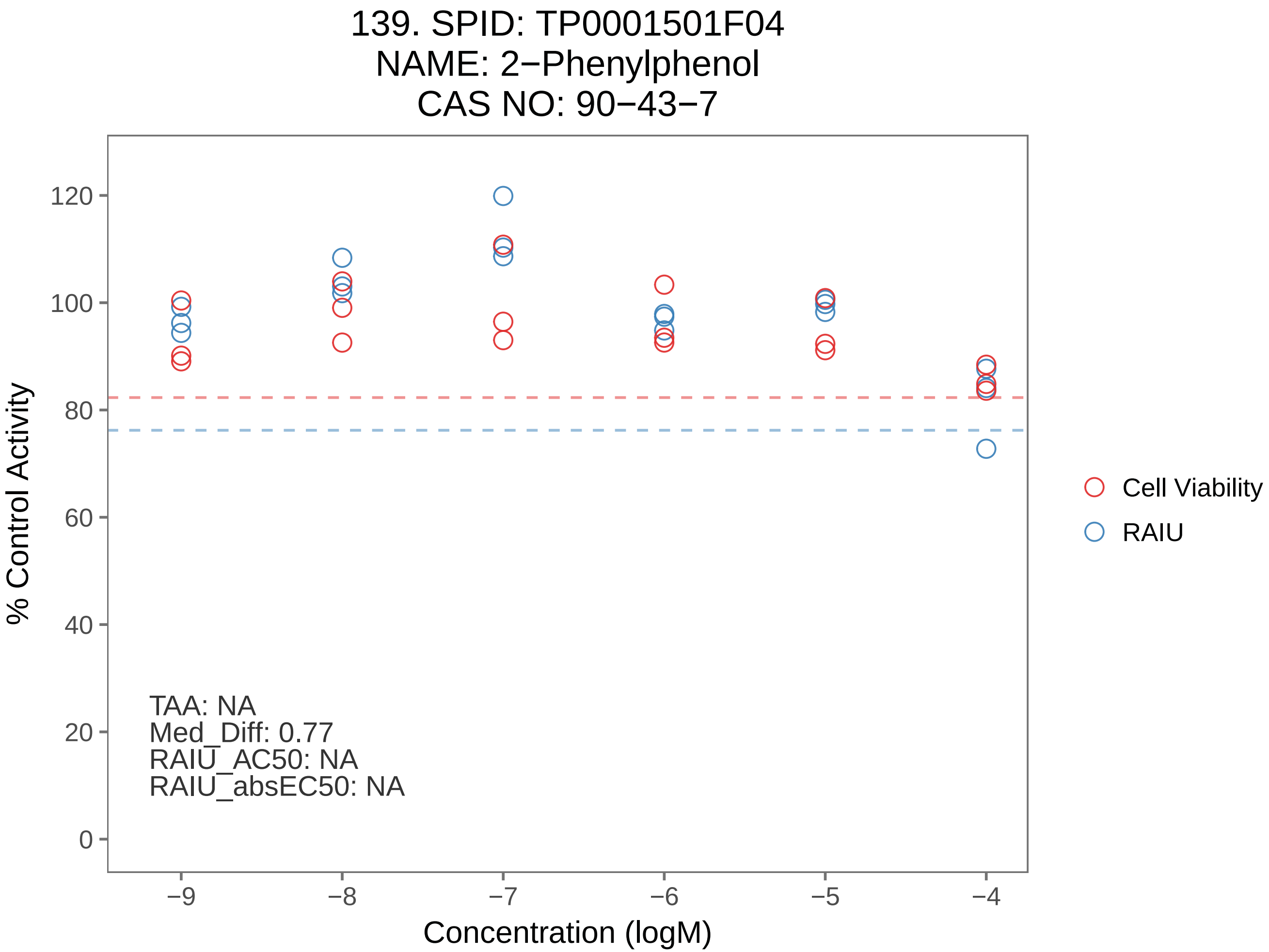

134. SPID: TP0001498B07
NAME: Captafol
CAS NO: 2425−06−1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: −11.37
TAA: −5.19
Med_Diff: −7.6
RAIU_AC50: −4.45
RAIU_absEC50: −4.49
Cell Viability
RAIU

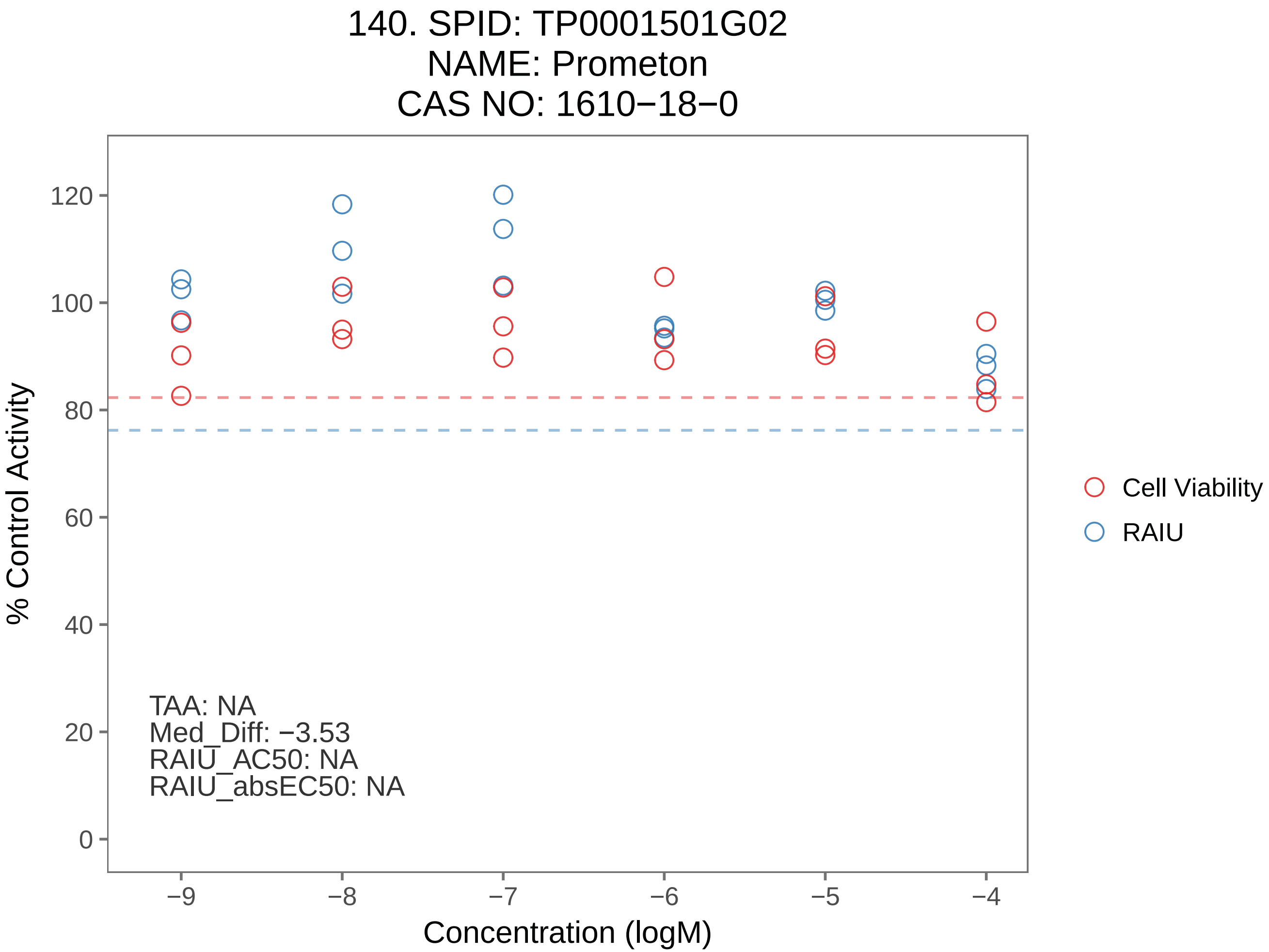

135. SPID: TP0001499G02
NAME: Tribufos
CAS NO: 78−48−8
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: −11.5
TAA: −2.26
Med_Diff: −9.57
RAIU_AC50: −4.94
RAIU_absEC50: NA
Cell Viability
RAIU

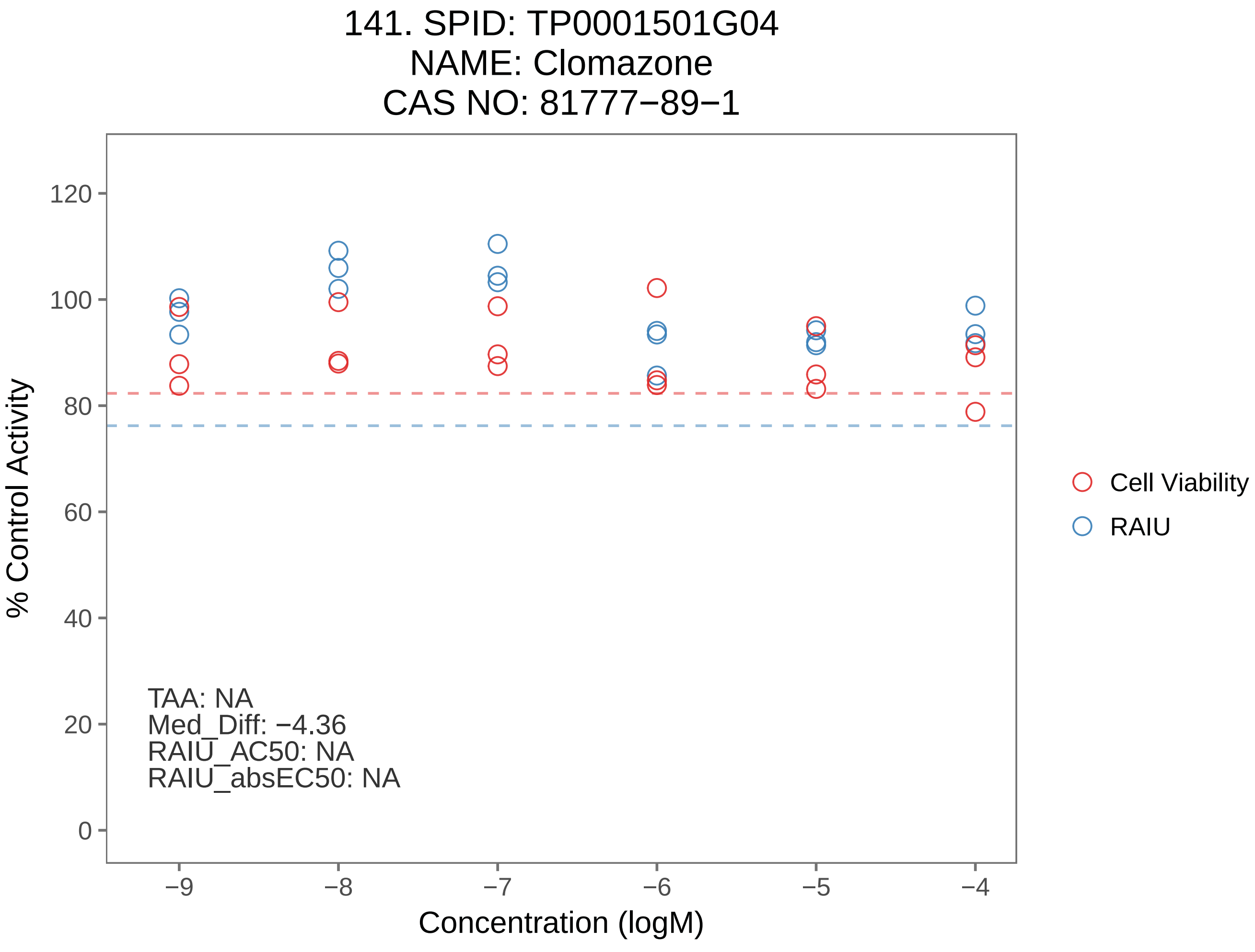

136. SPID: TP0001499C07
NAME: Benfluralin
CAS NO: 1861−40−1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: −13.71
TAA: −3.73
Med_Diff: −10.75
RAIU_AC50: −4.62
RAIU_absEC50: NA
Cell Viability
RAIU

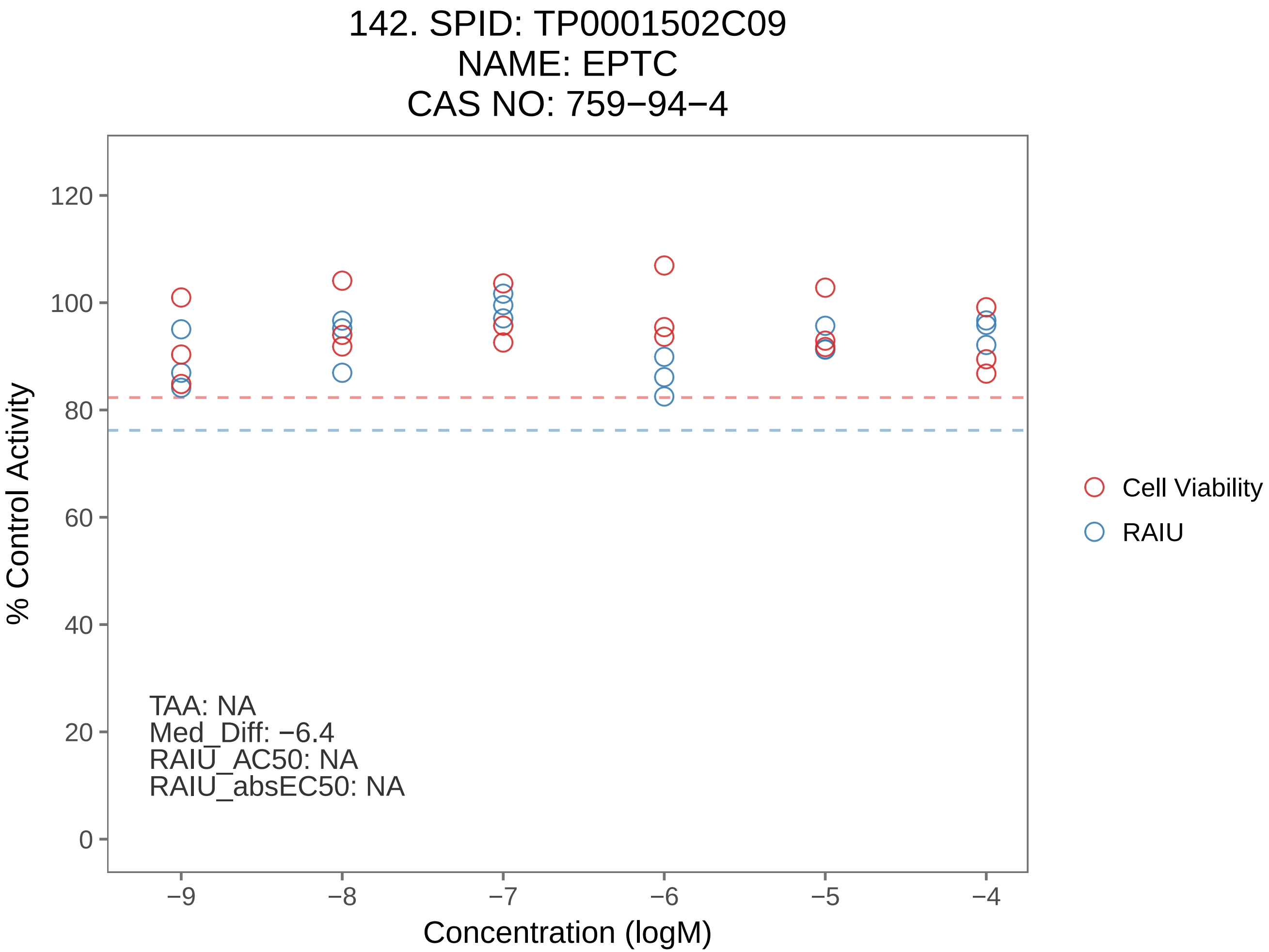

137. SPID: TP0001500E01
NAME: MGK−264
CAS NO: 113−48−4
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Ranking_Score: −29.52
TAA: −8.36
Med_Diff: −22.95
RAIU_AC50: −4.28
RAIU_absEC50: NA
Cell Viability
RAIU

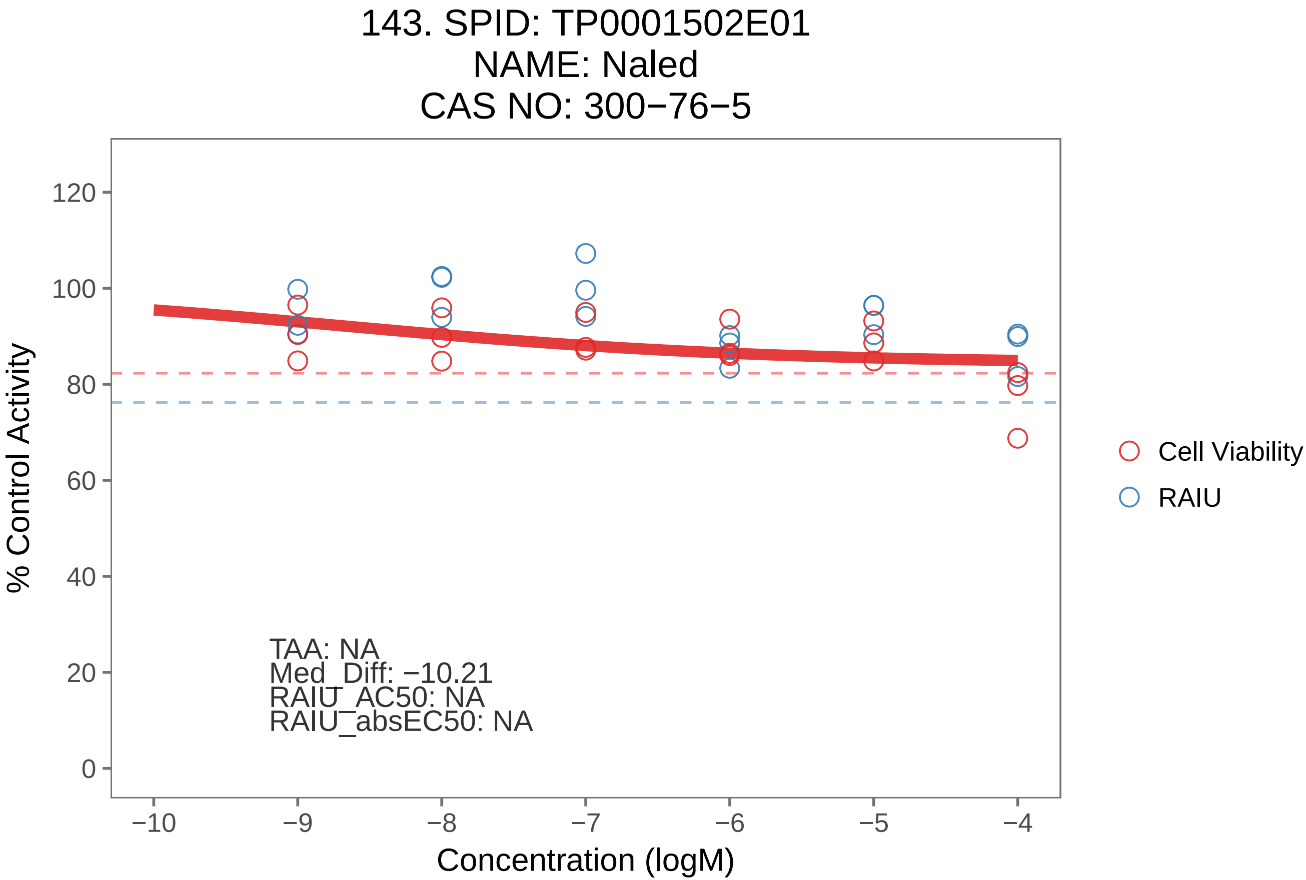

138. SPID: TP0001498C03
NAME: Bromoxynil
CAS NO: 1689−84−5
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −14.76
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

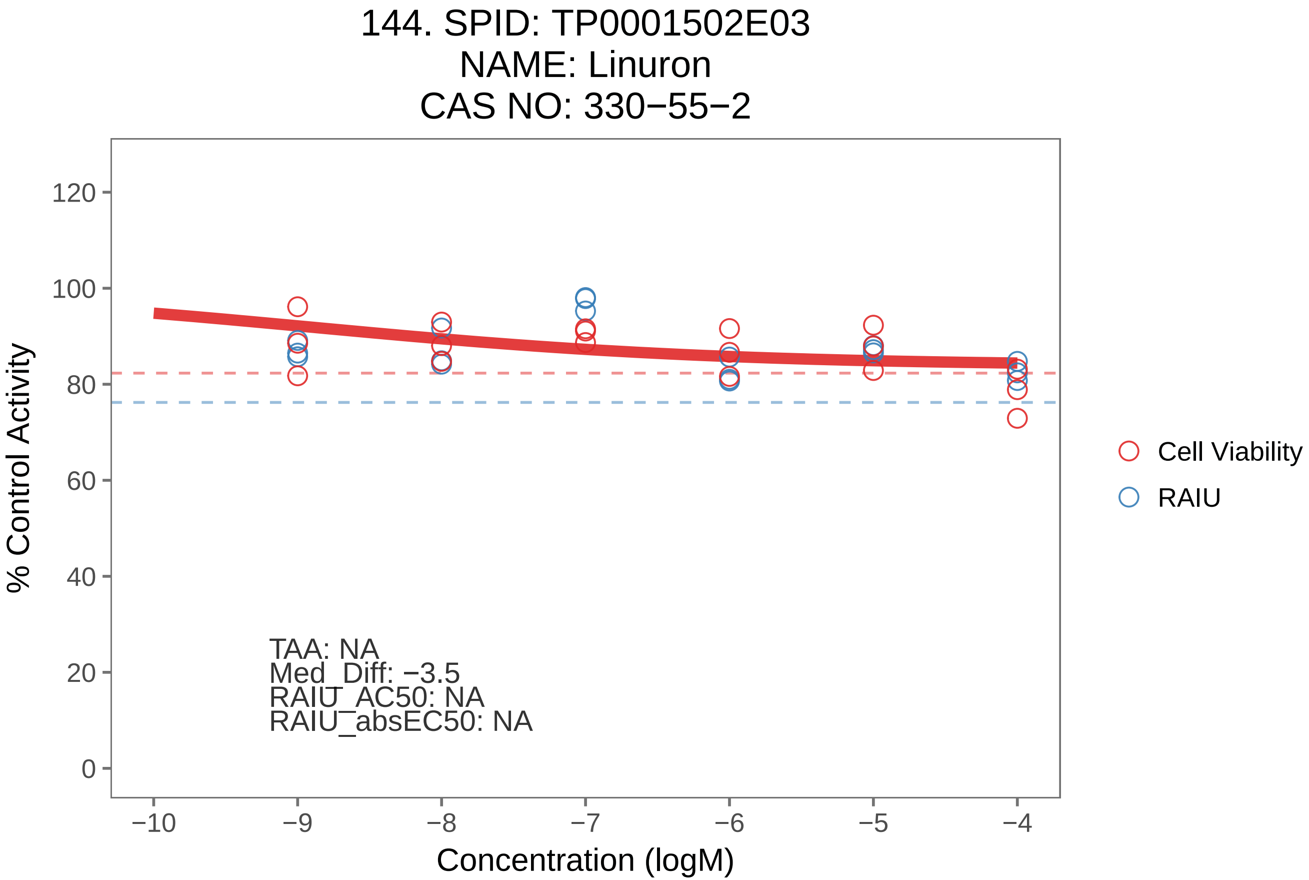

139. SPID: TP0001501F04
NAME: 2−Phenylphenol
CAS NO: 90−43−7
% Control Activity
Concentration (logM)
Cell Viability
RAIU
TAA: NA
Med_Diff: 0.77
RAIU_AC50: NA
RAIU_absEC50: NA

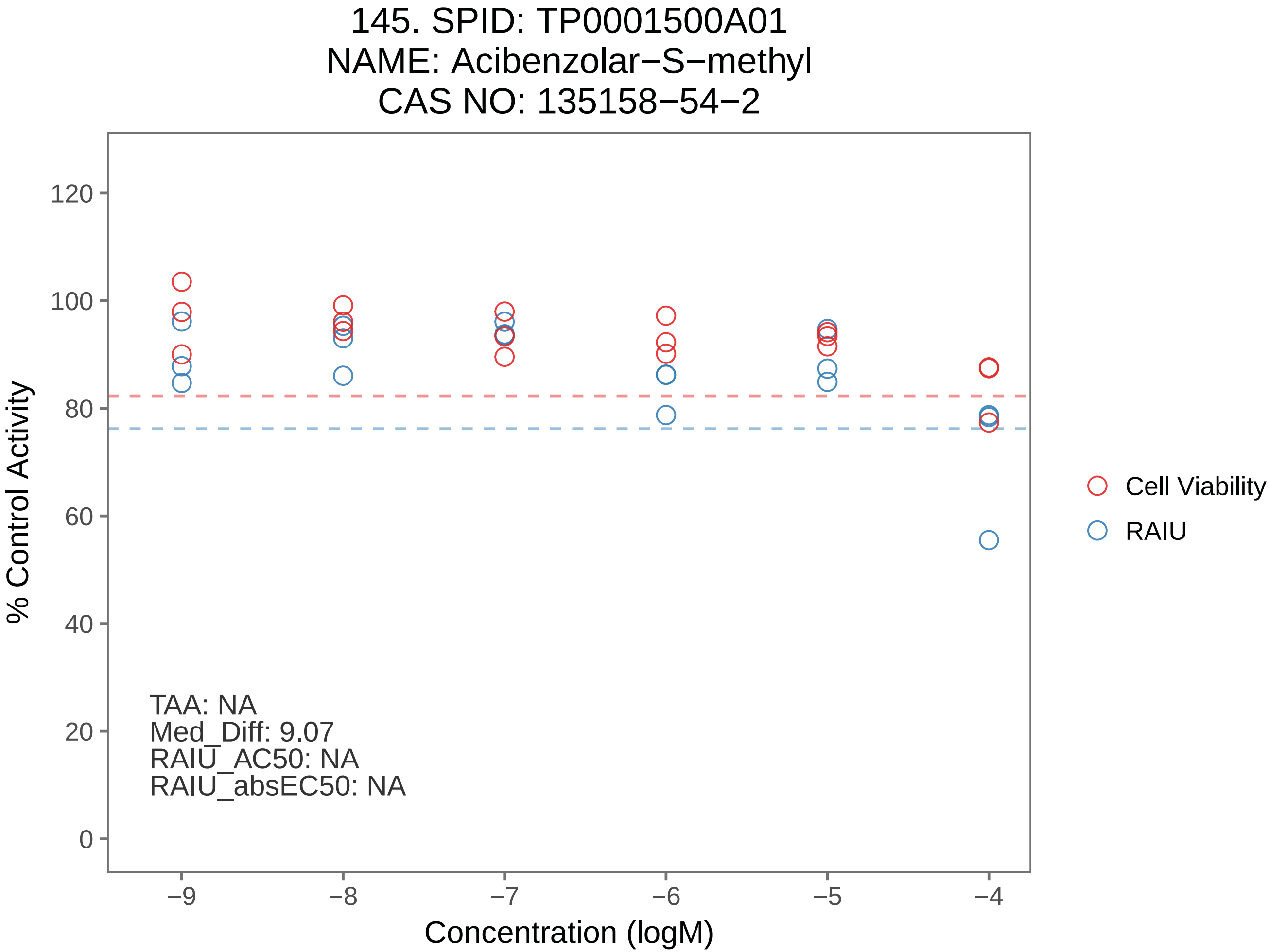

140. SPID: TP0001501G02
NAME: Prometon
CAS NO: 1610−18−0
% Control Activity
0
20
40
60
80
100
120
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −3.53
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

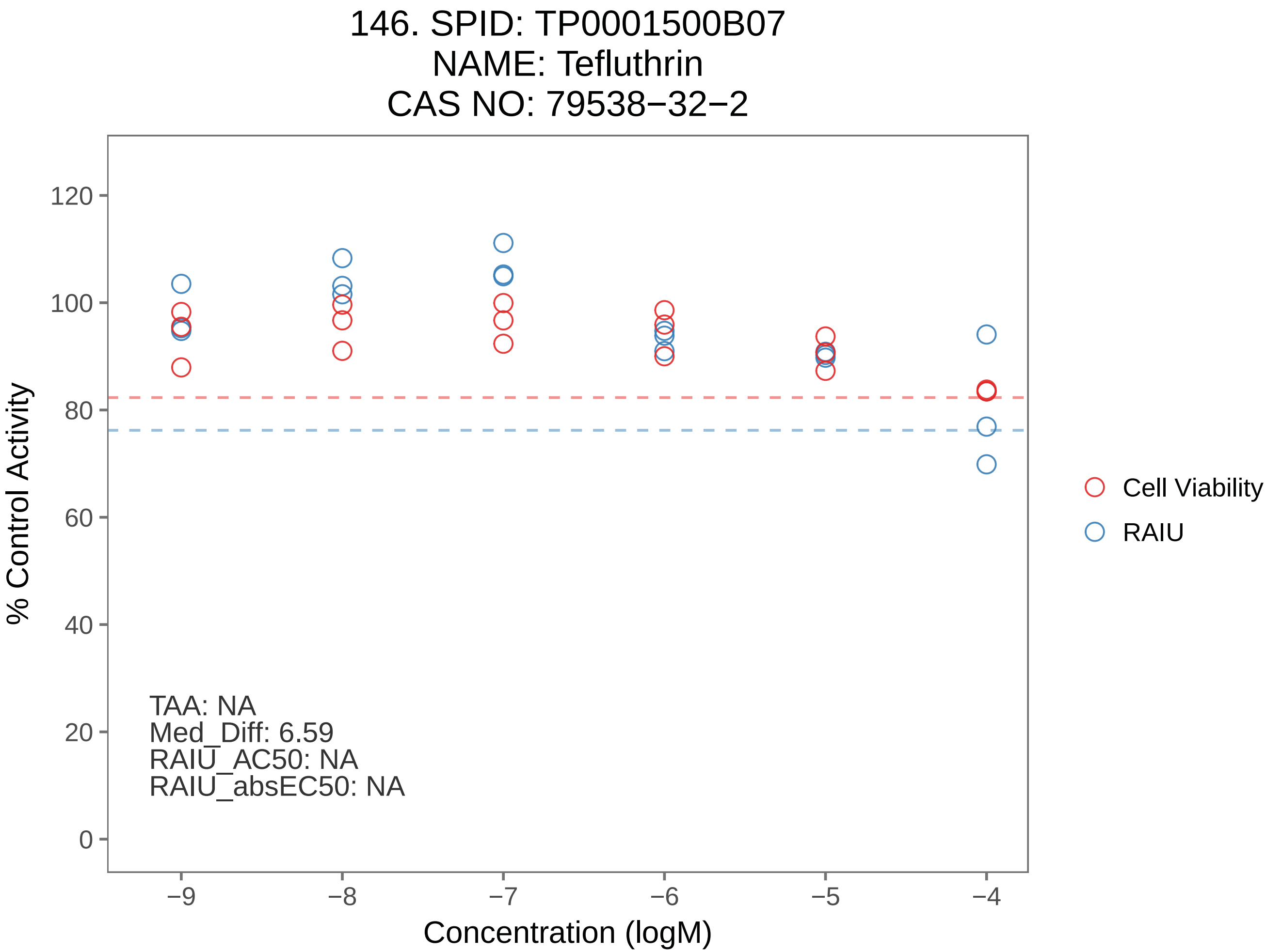

141. SPID: TP0001501G04
NAME: Clomazone
CAS NO: 81777−89−1
% Control Activity
120
100
80
60
40
20
0
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −4.36
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU


142. SPID: TP0001502C09
NAME: EPTC
CAS NO: 759−94−4
% Control Activity
0
20
40
60
80
100
120
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −6.4
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

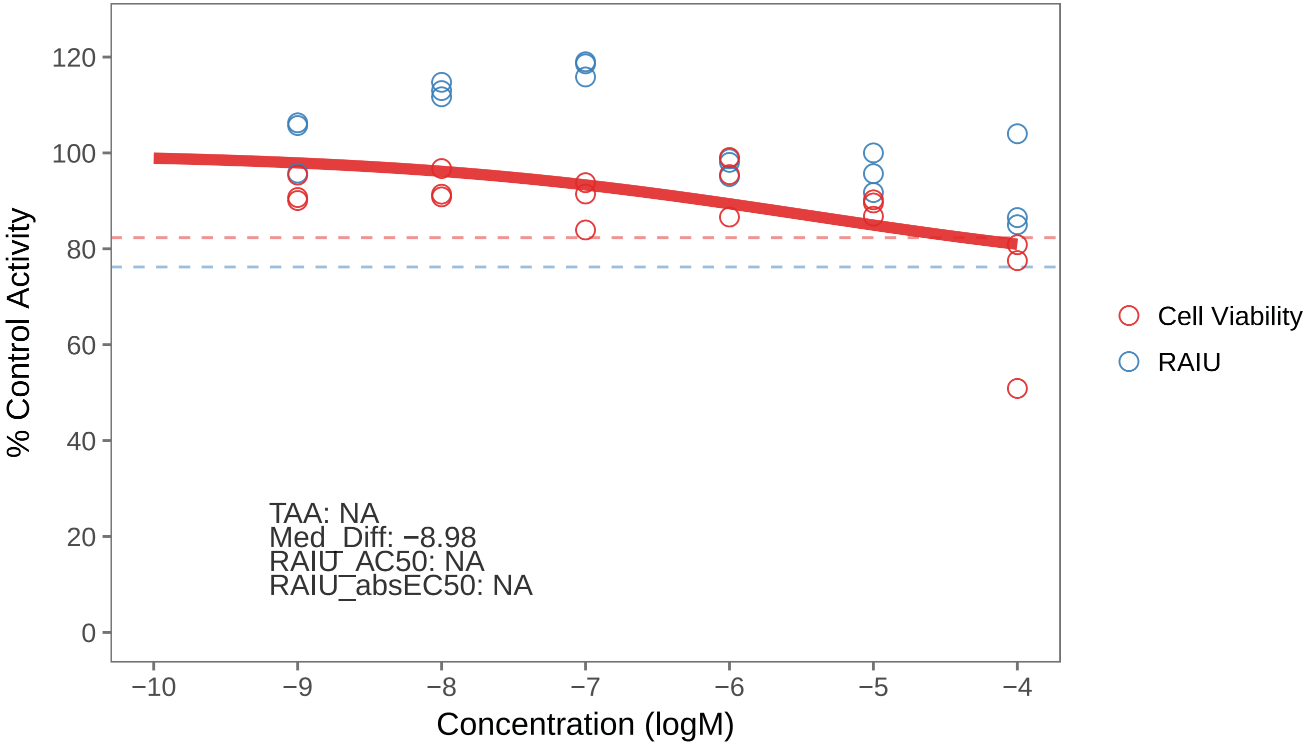

143. SPID: TP0001502E01
NAME: Naled
CAS NO: 300−76−5
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −10.21
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

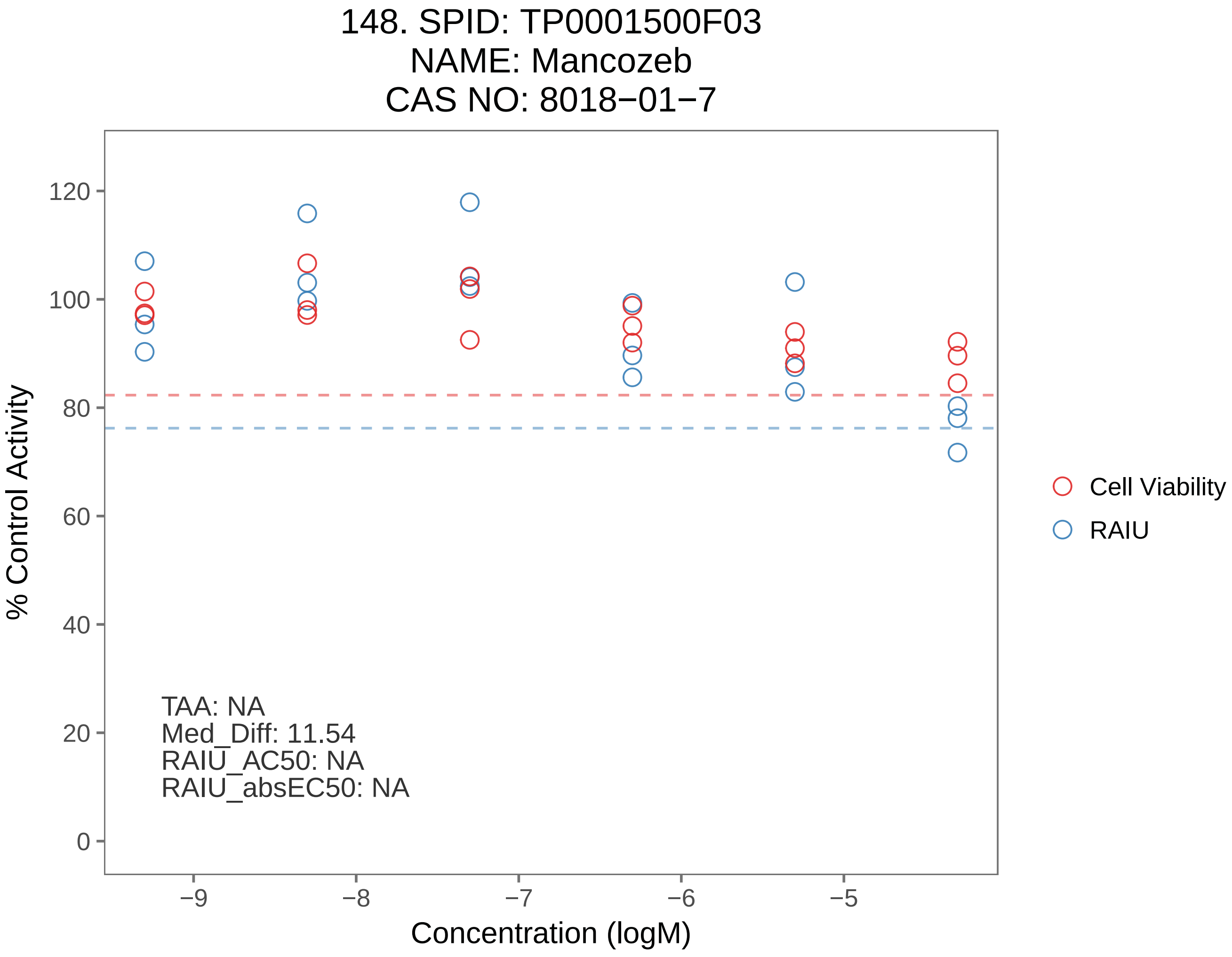

144. SPID: TP0001502E03
NAME: Linuron
CAS NO: 330−55−2
% Control Activity
120
100
80
60
40
20
0
TAA: NA
Med_Diff: −3.5
RAIU_AC50: NA
RAIU_absEC50: NA
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU

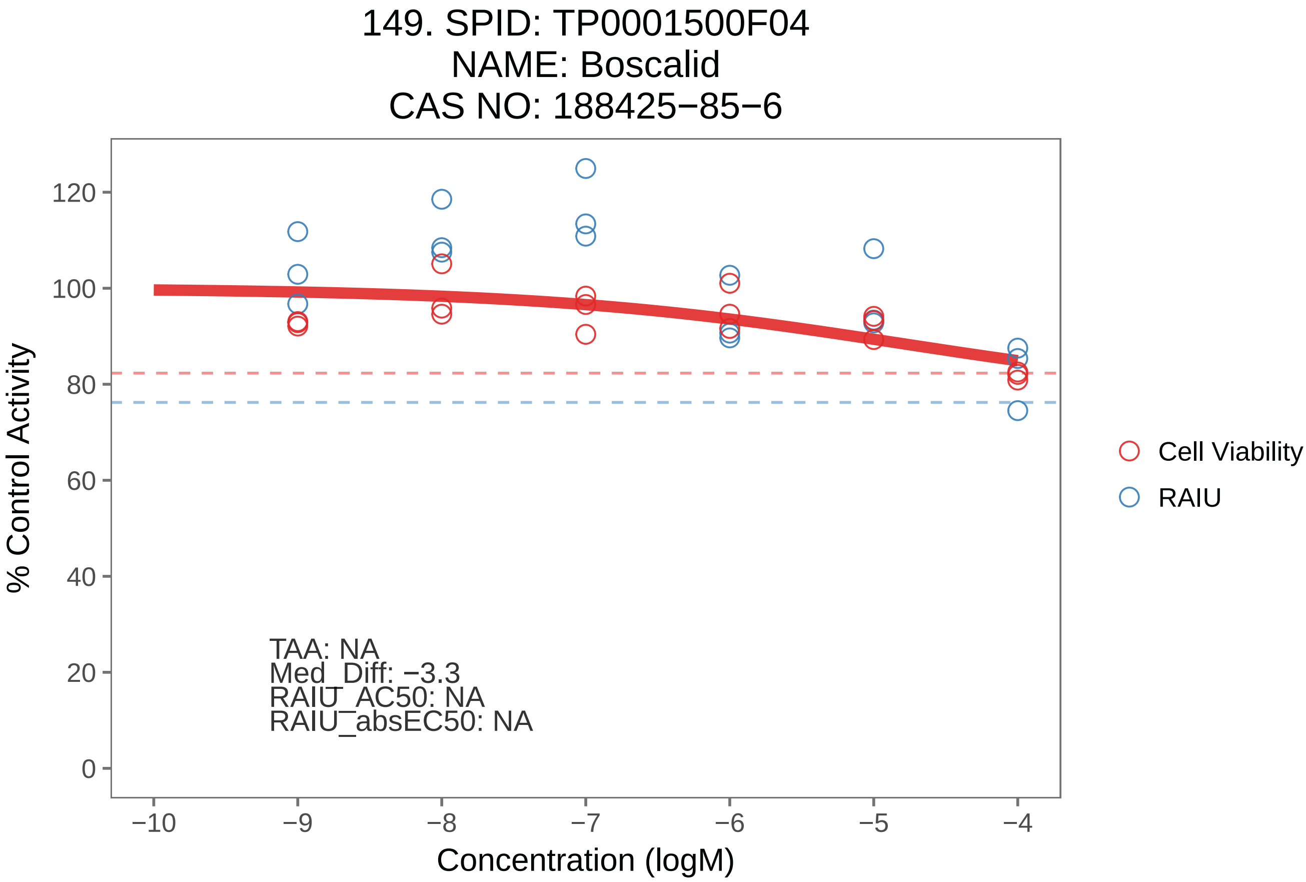

145. SPID: TP0001500A01
NAME: Acibenzolar−S−methyl
CAS NO: 135158−54−2
% Control Activity
0
20
40
60
80
100
120
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: 9.07
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

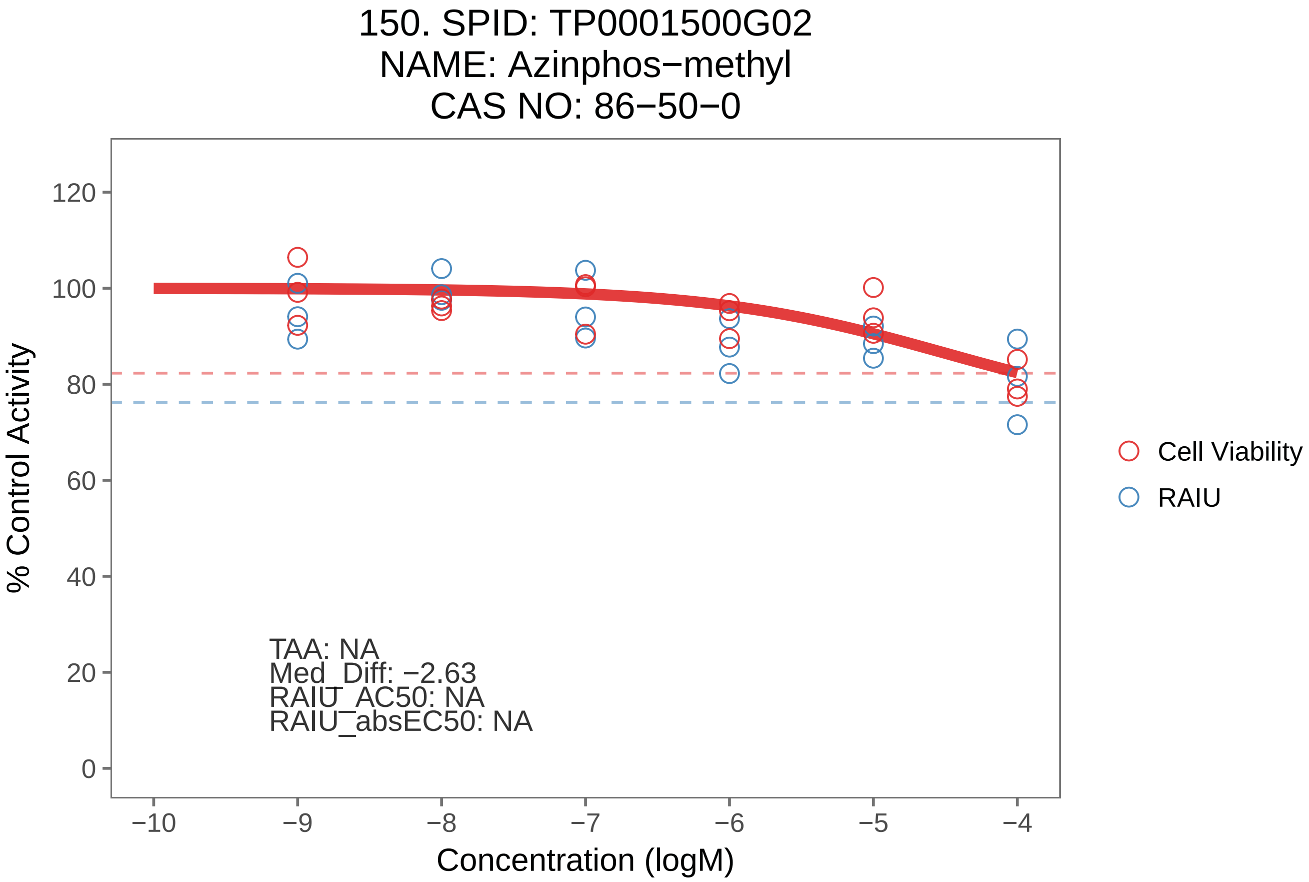

146. SPID: TP0001500B07
NAME: Tefluthrin
CAS NO: 79538−32−2
% Control Activity
0
20
40
60
80
100
120
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: 6.59
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

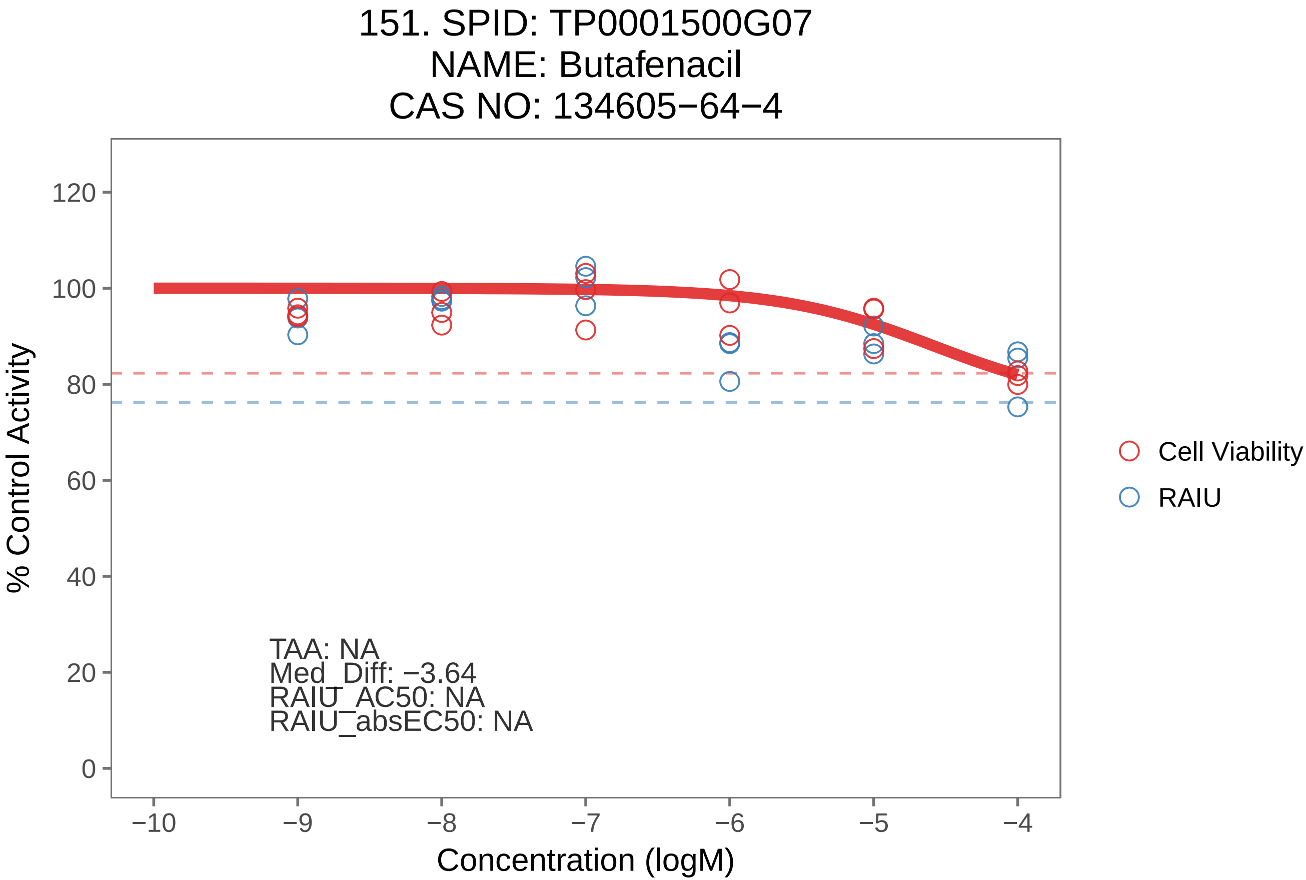
147. SPID: TP0001500C05
NAME: Butachlor
CAS NO: 23184−66−9

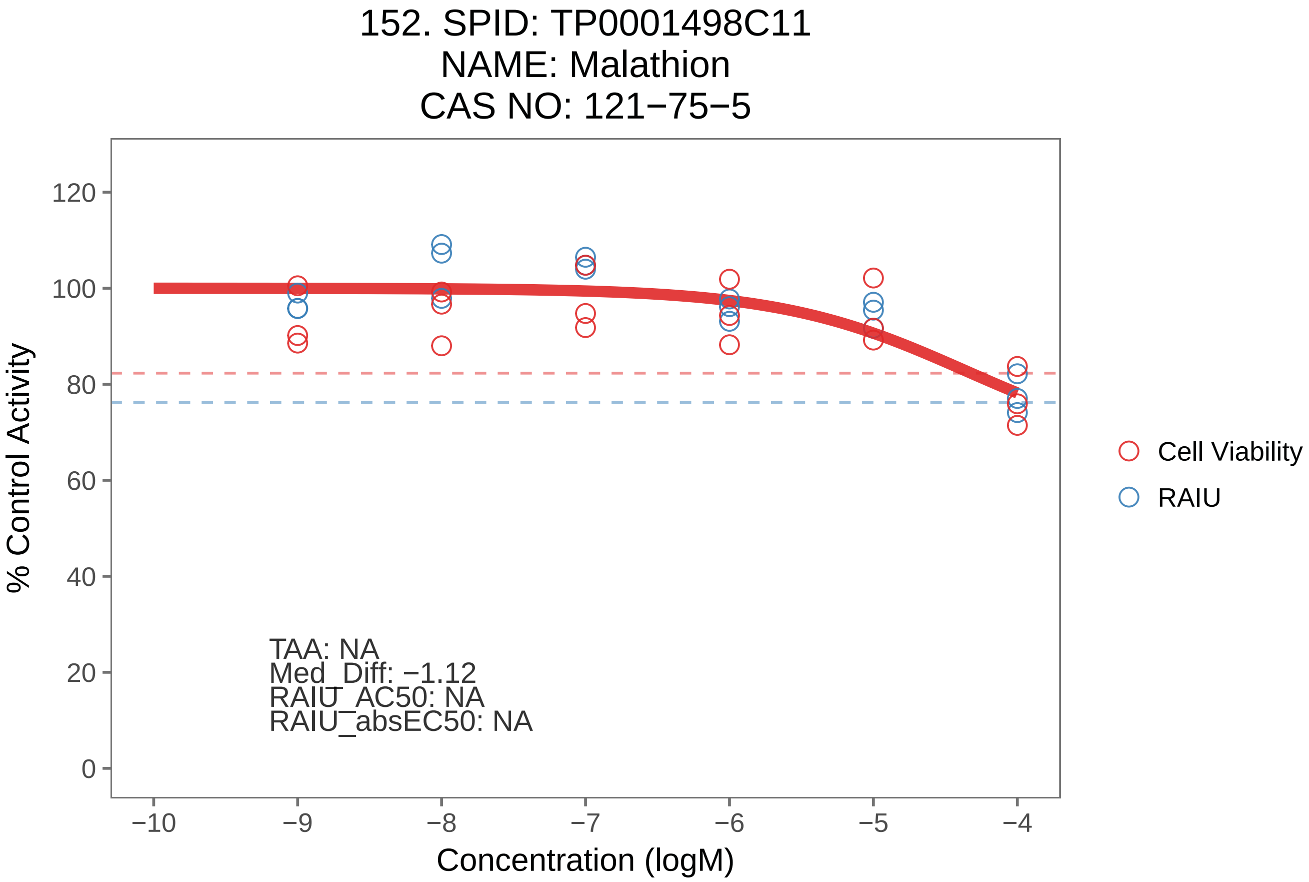


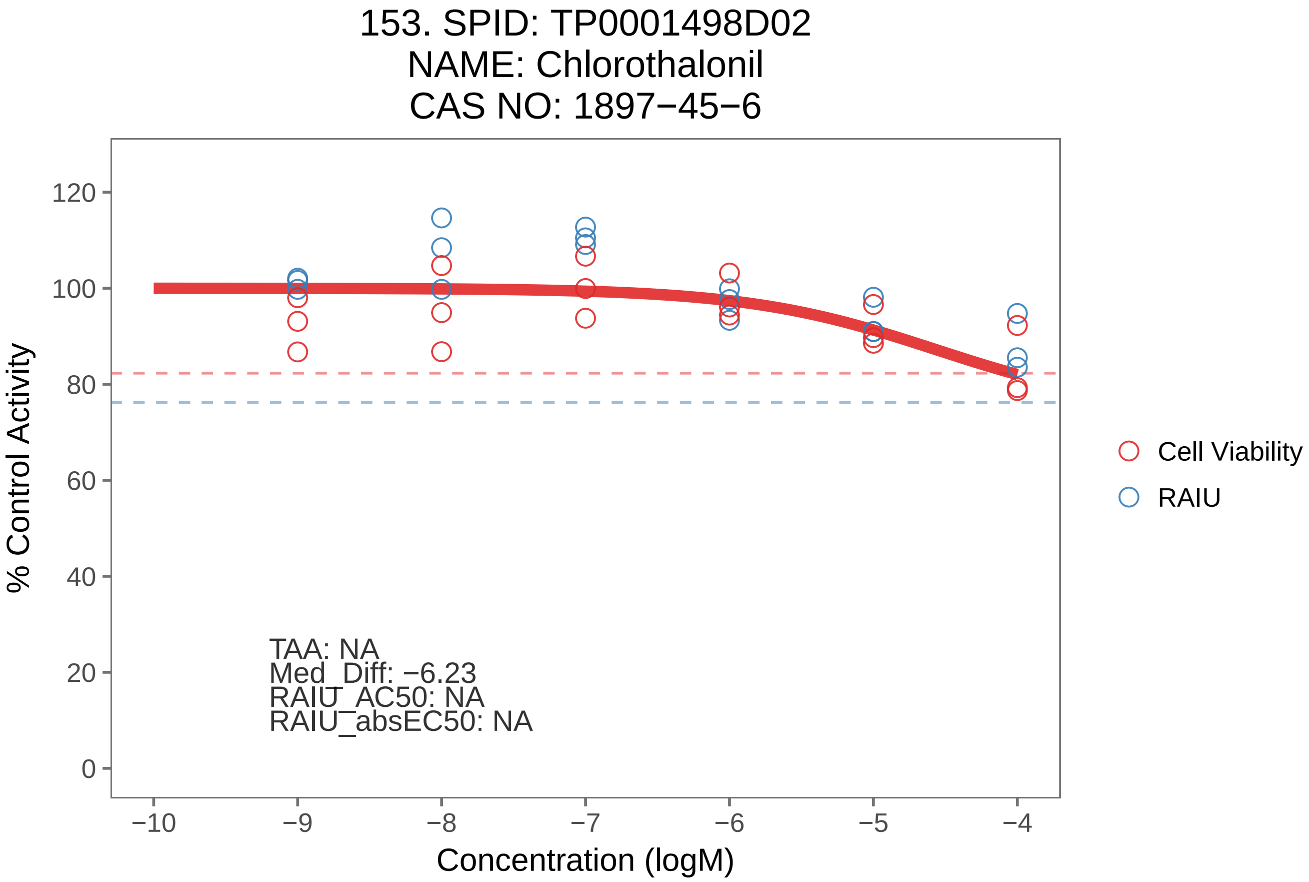

148. SPID: TP0001500F03
NAME: Mancozeb
CAS NO: 8018−01−7
% Control Activity
Concentration (logM)
Cell Viability
RAIU
TAA: NA
Med_Diff: 11.54
RAIU_AC50: NA
RAIU_absEC50: NA

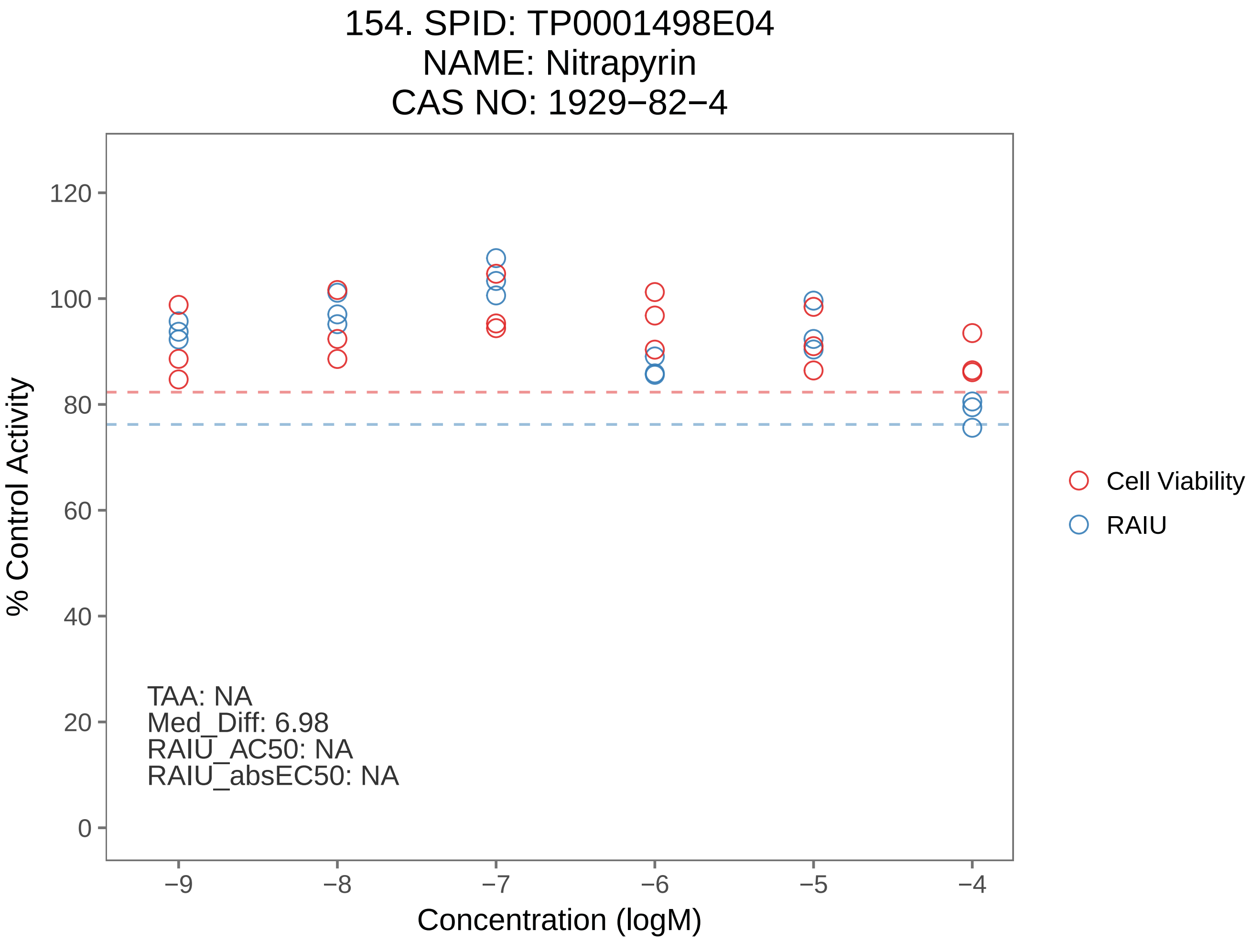

149. SPID: TP0001500F04
NAME: Boscalid
CAS NO: 188425−85−6
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −3.3
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

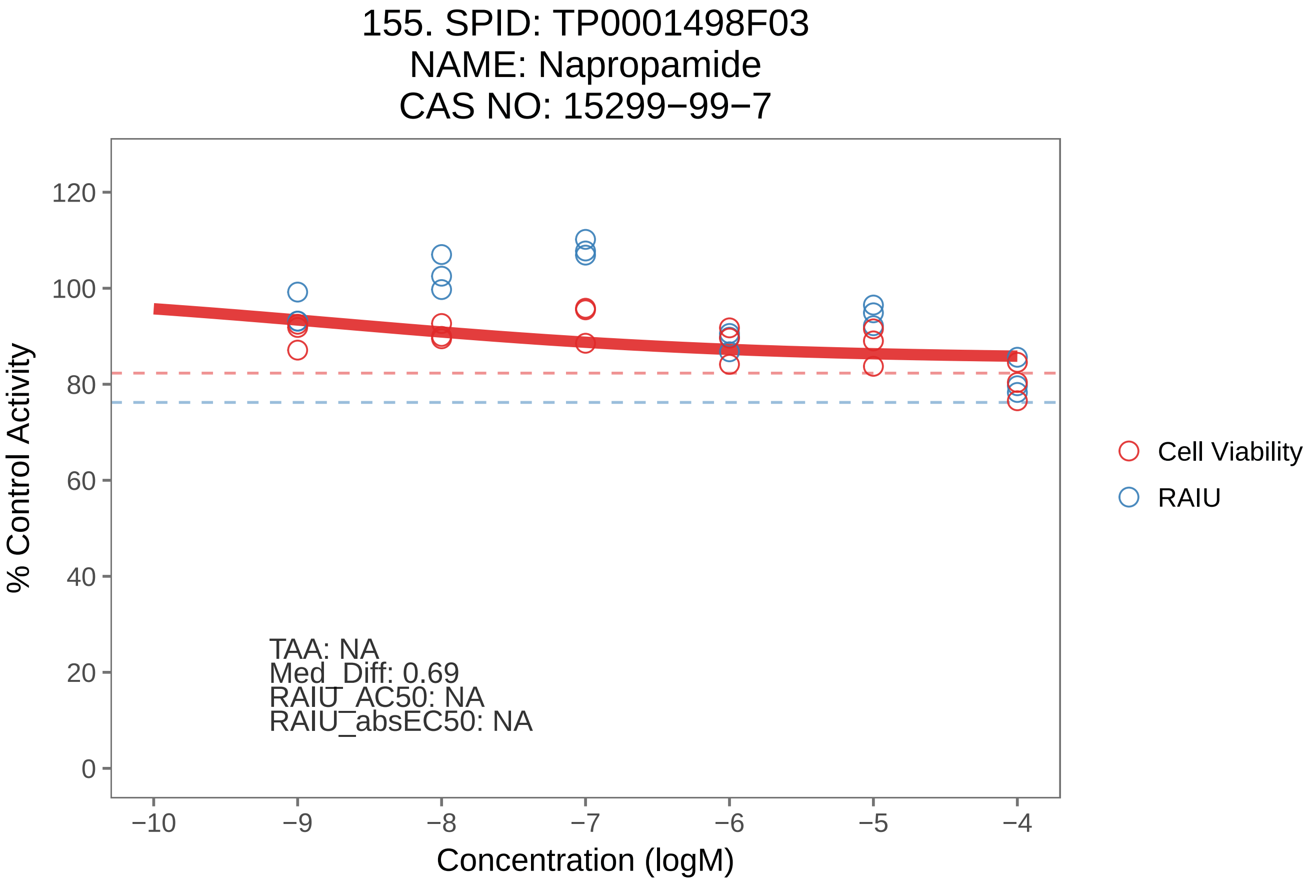

150. SPID: TP0001500G02
NAME: Azinphos−methyl
CAS NO: 86−50−0
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
TAA: NA
Med_Diff: −2.63
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

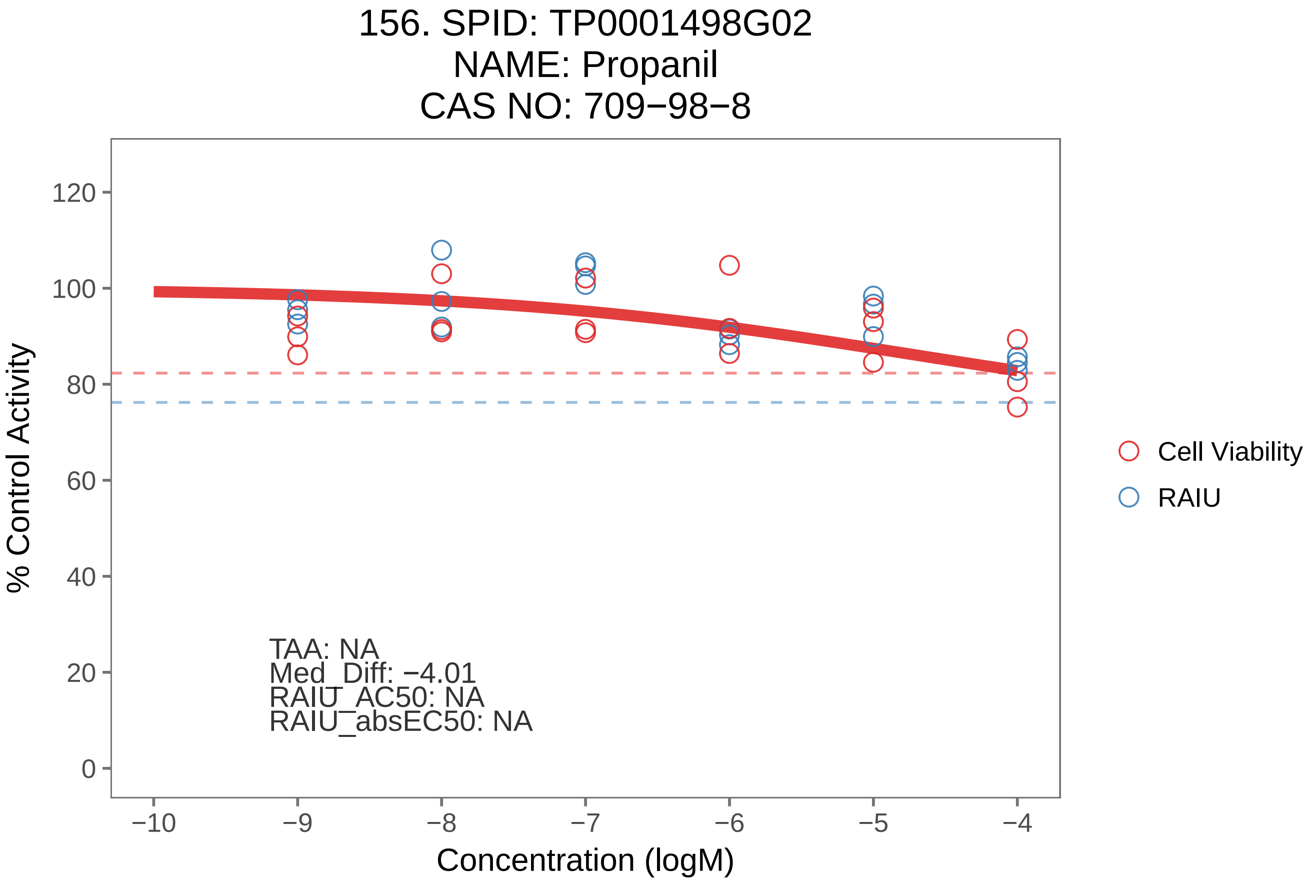

151. SPID: TP0001500G07
NAME: Butafenacil
CAS NO: 134605−64−4
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −3.64
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

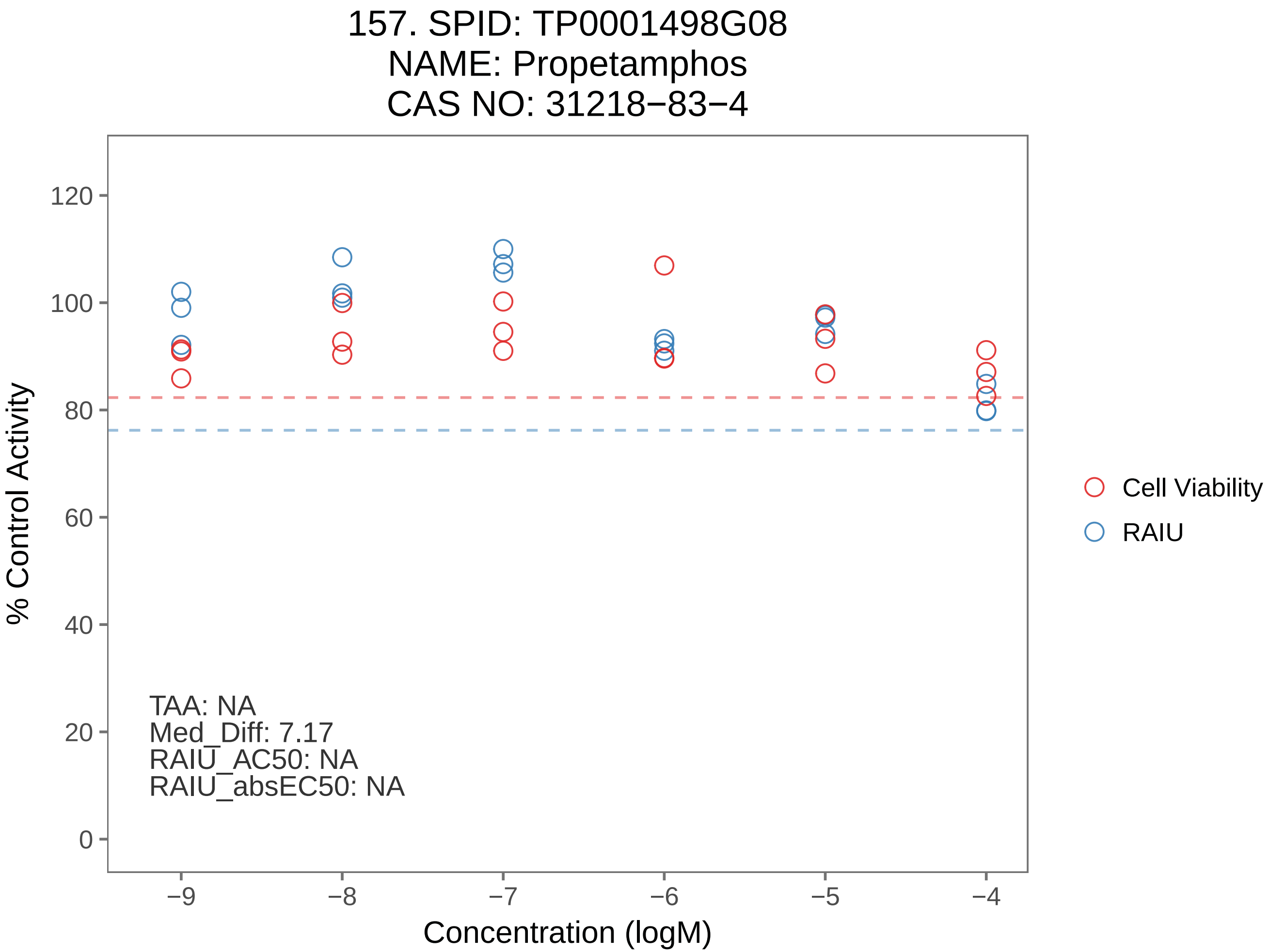

152. SPID: TP0001498C11
NAME: Malathion
CAS NO: 121−75−5
% Control Activity
120
100
80
60
40
20
0
TAA: NA
Med_Diff: −1.12
RAIU_AC50: NA
RAIU_absEC50: NA
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU

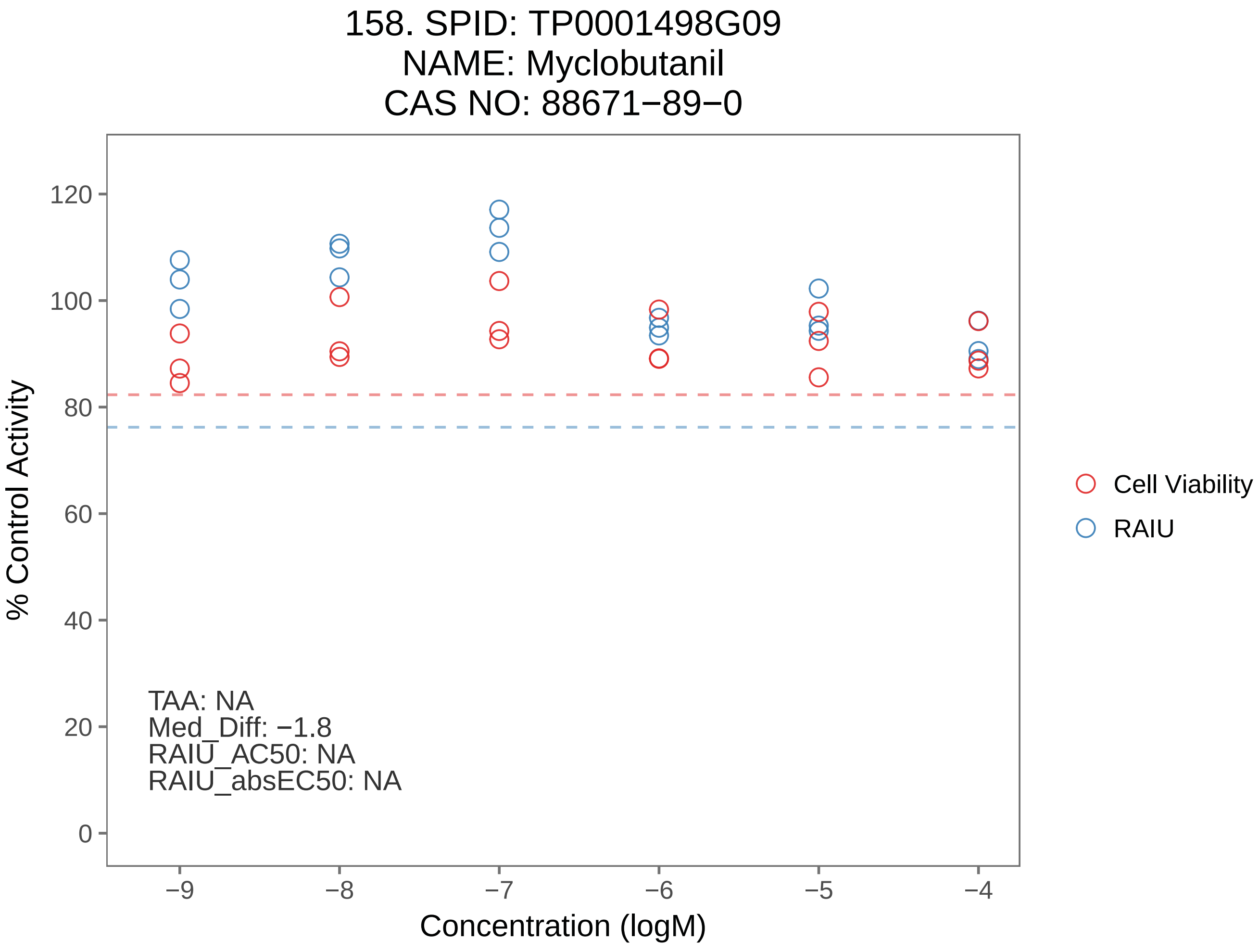

153. SPID: TP0001498D02
NAME: Chlorothalonil
CAS NO: 1897−45−6
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −6.23
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

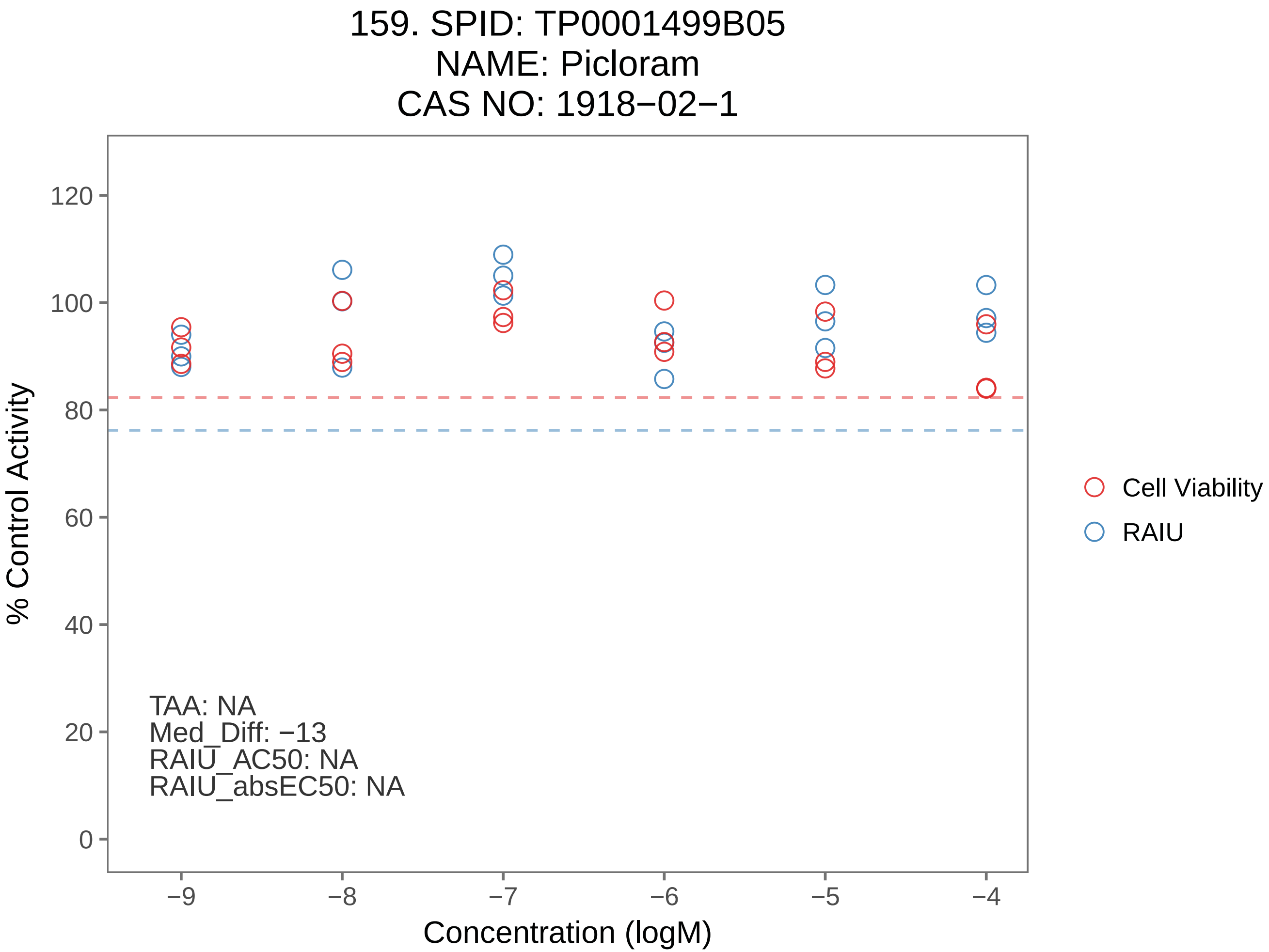

154. SPID: TP0001498E04
NAME: Nitrapyrin
CAS NO: 1929−82−4
% Control Activity
0
20
40
60
80
100
120
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: 6.98
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU


155. SPID: TP0001498F03
NAME: Napropamide
CAS NO: 15299−99−7
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: 0.69
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

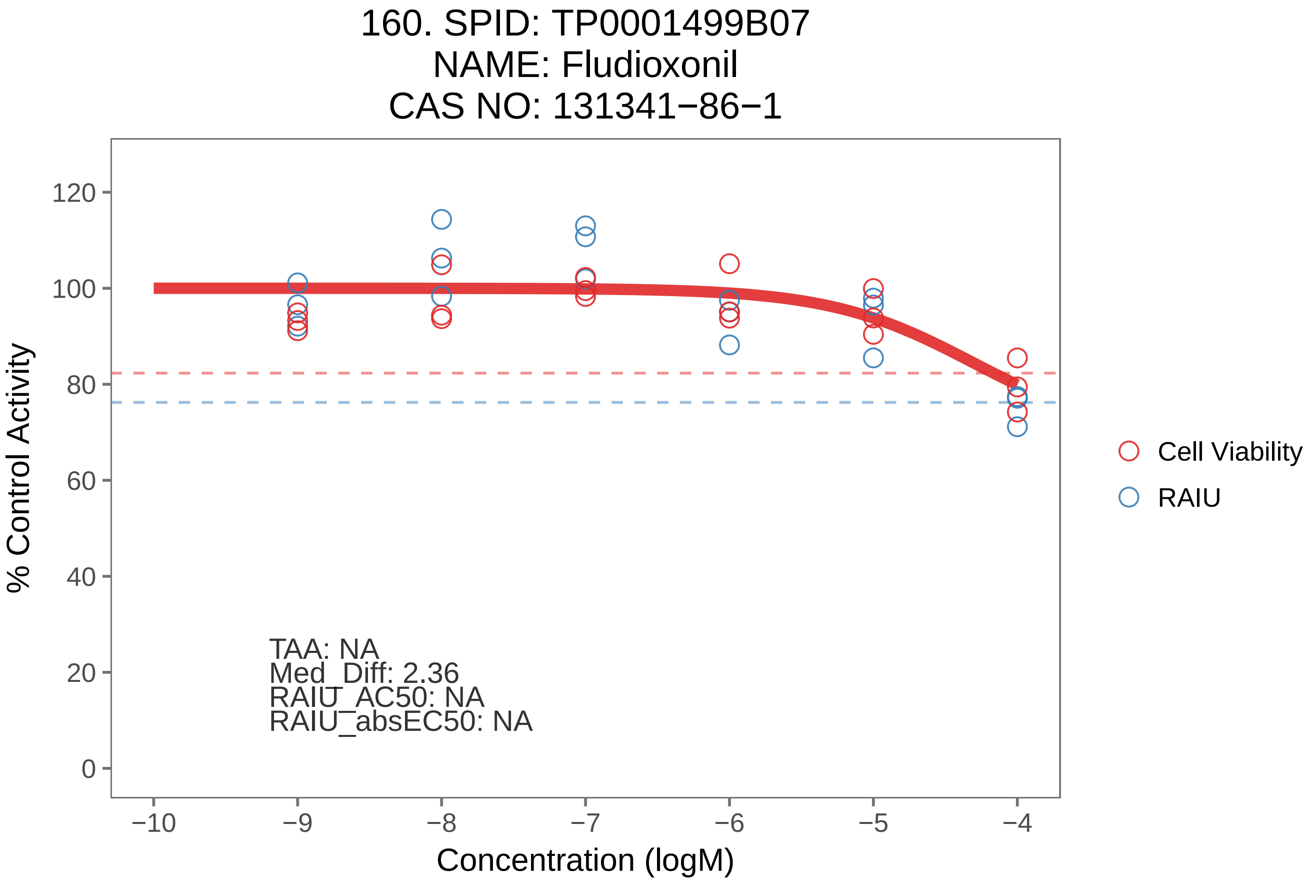

156. SPID: TP0001498G02
NAME: Propanil
CAS NO: 709−98−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −4.01
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

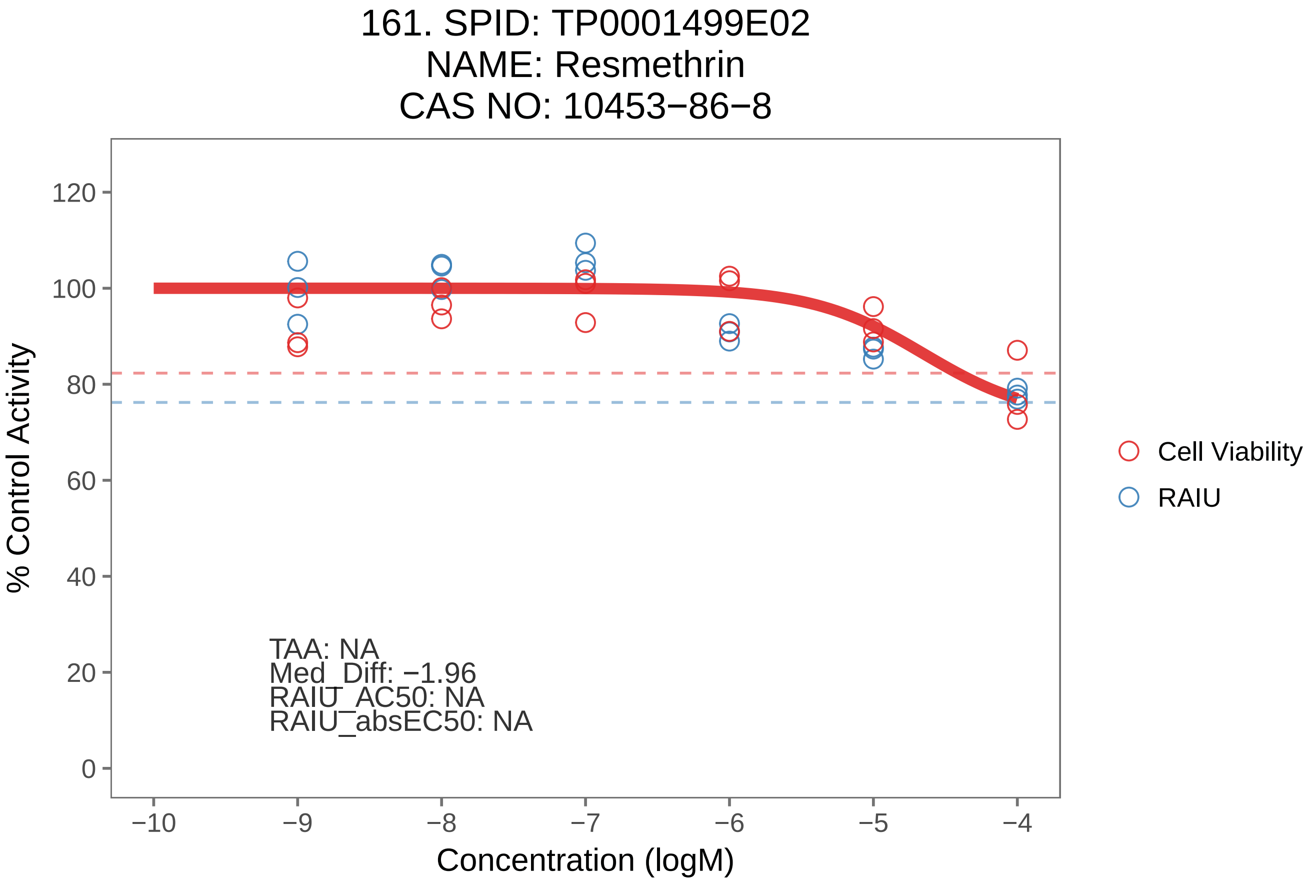

157. SPID: TP0001498G08
NAME: Propetamphos
CAS NO: 31218−83−4
% Control Activity
Concentration (logM)
Cell Viability
RAIU
TAA: NA
Med_Diff: 7.17
RAIU_AC50: NA
RAIU_absEC50: NA

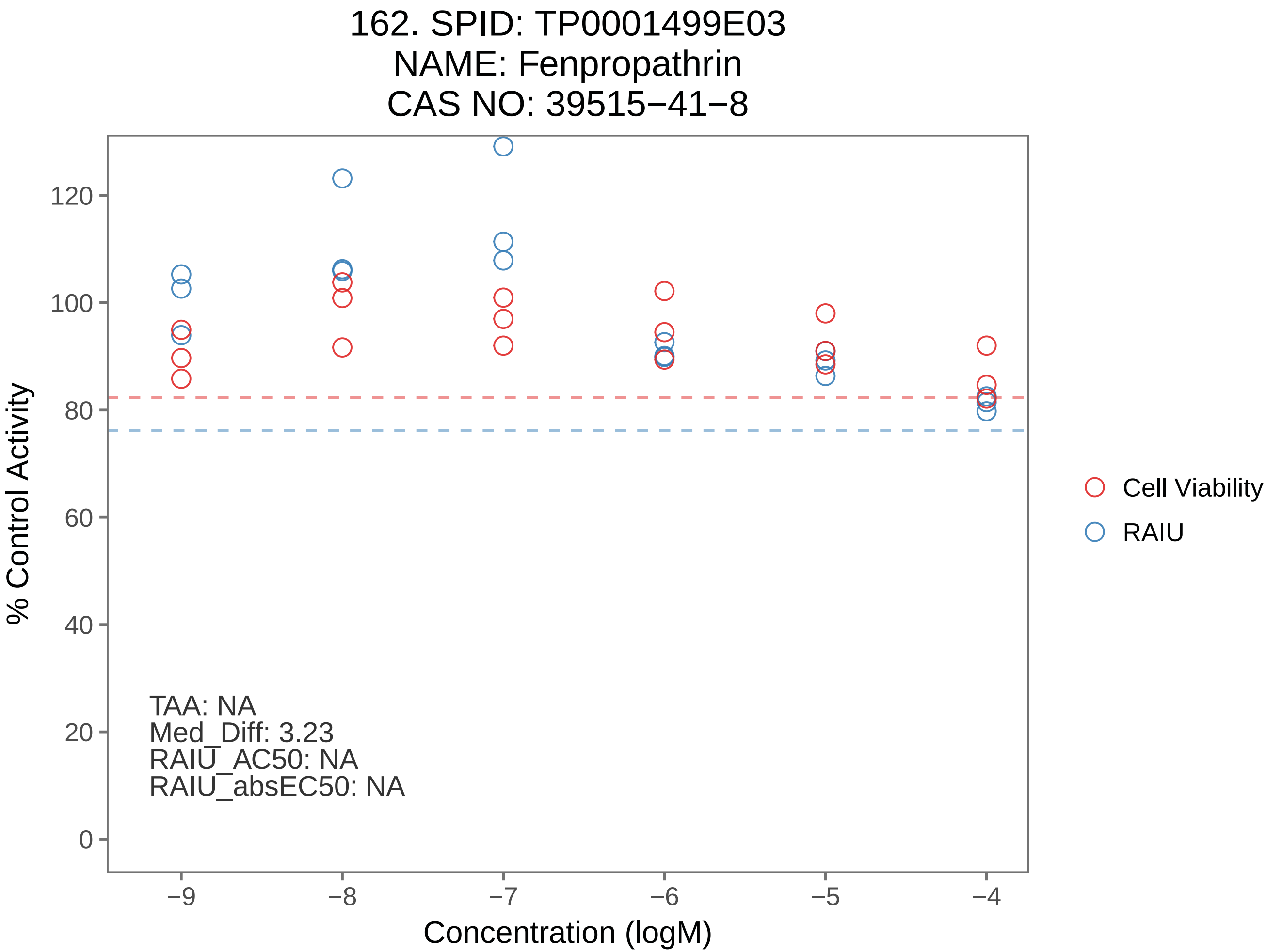

158. SPID: TP0001498G09
NAME: Myclobutanil
CAS NO: 88671−89−0
120
100
80
60
40
20
0
% Control Activity
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −1.8
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

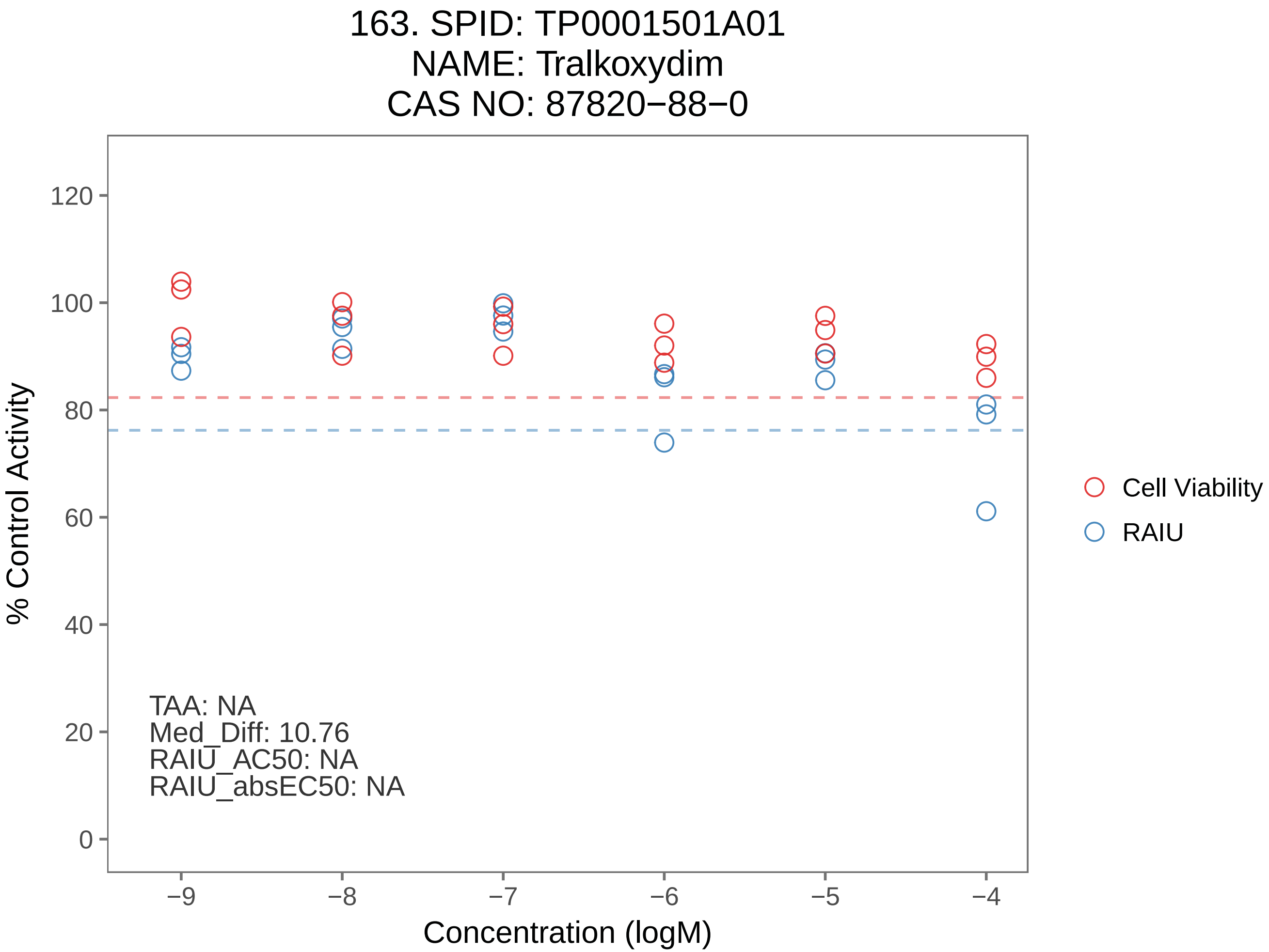


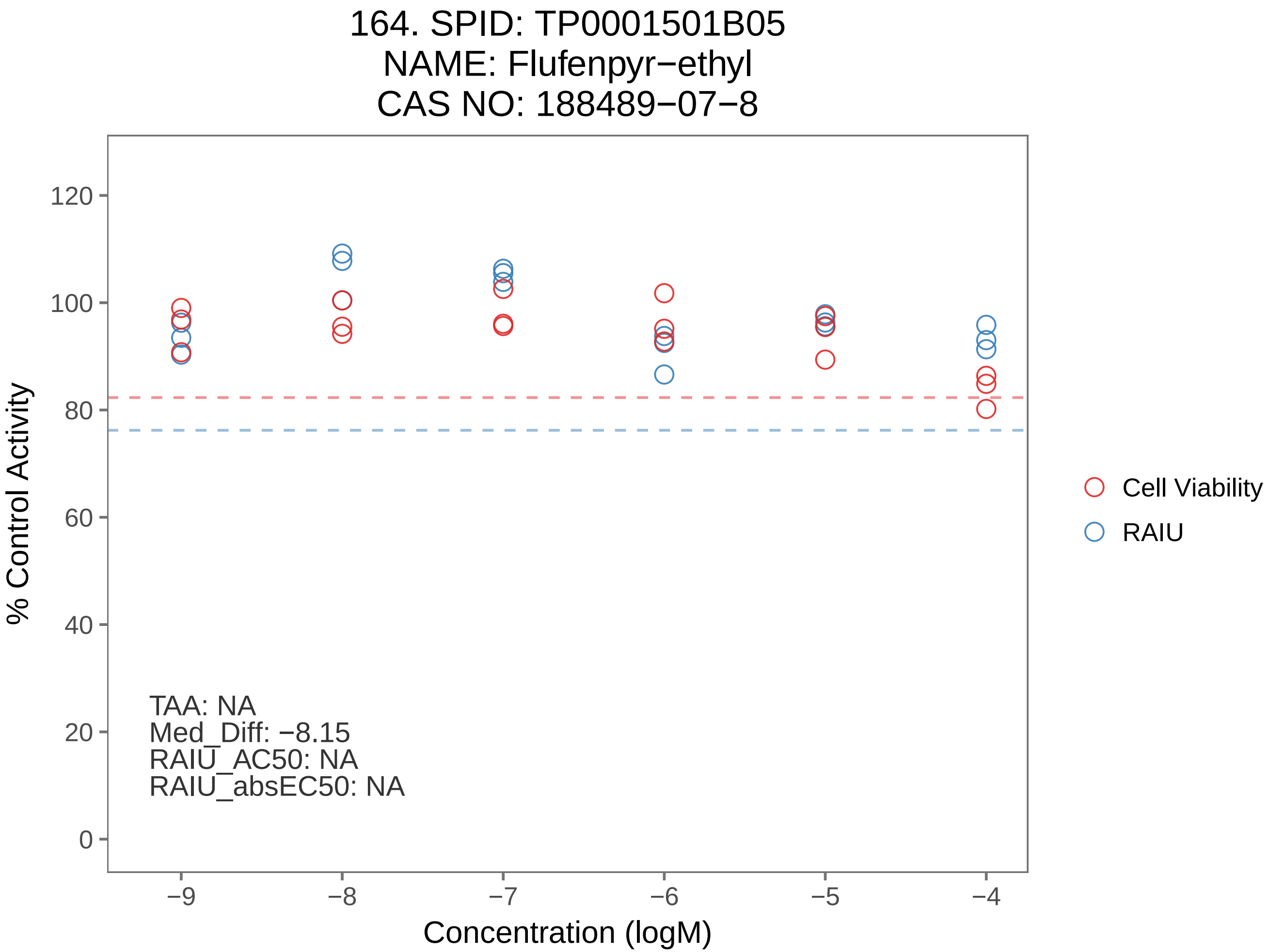
159. SPID: TP0001499B05
NAME: Picloram
CAS NO: 1918−02−1
% Control Activity
120
100
80
60
40
20
0
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU
TAA: NA
Med_Diff: −13
RAIU_AC50: NA
RAIU_absEC50: NA

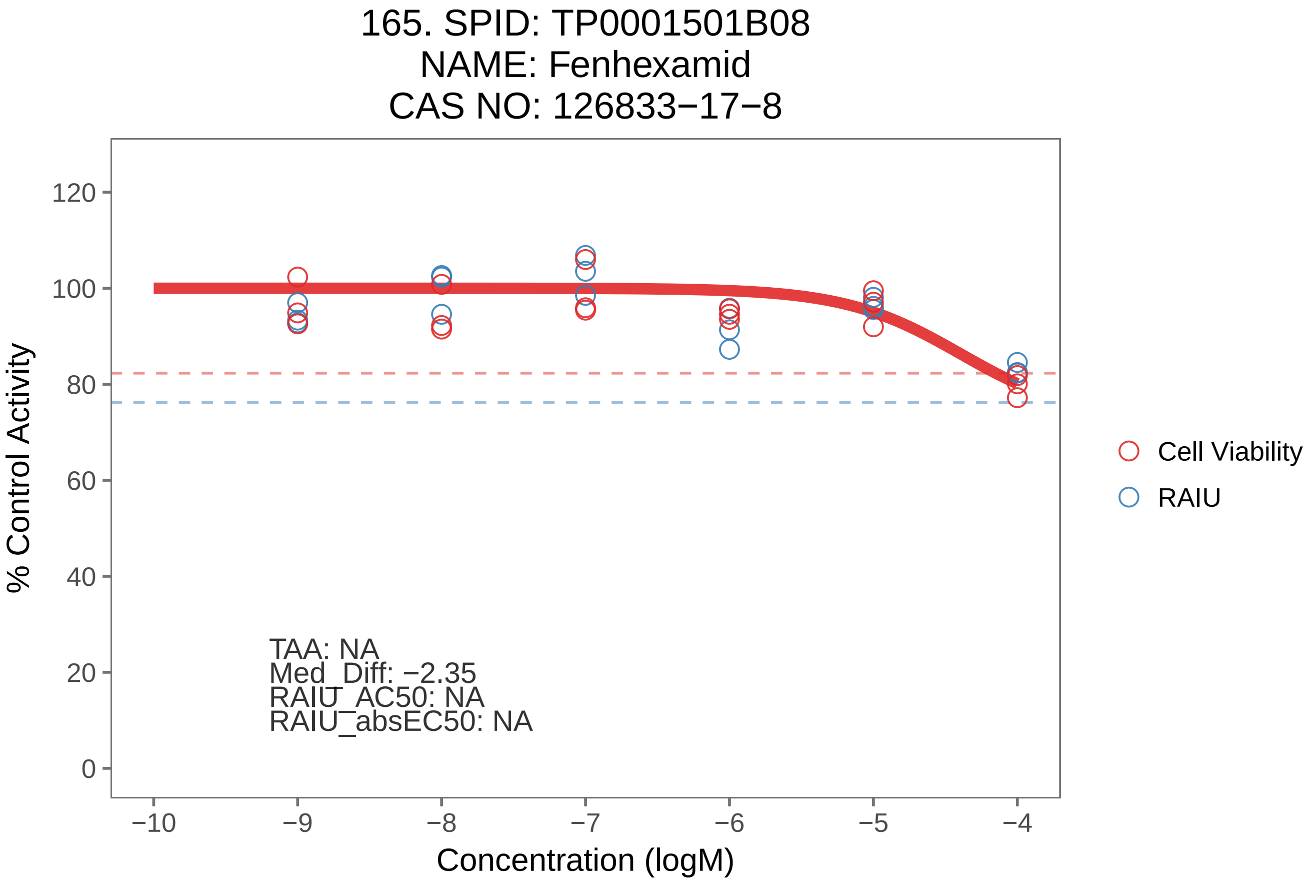

160. SPID: TP0001499B07
NAME: Fludioxonil
CAS NO: 131341−86−1
TAA: NA
Med_Diff: 2.36
RAIU_AC50: NA
RAIU_absEC50: NA
% Control Activity
Concentration (logM)
Cell Viability
RAIU

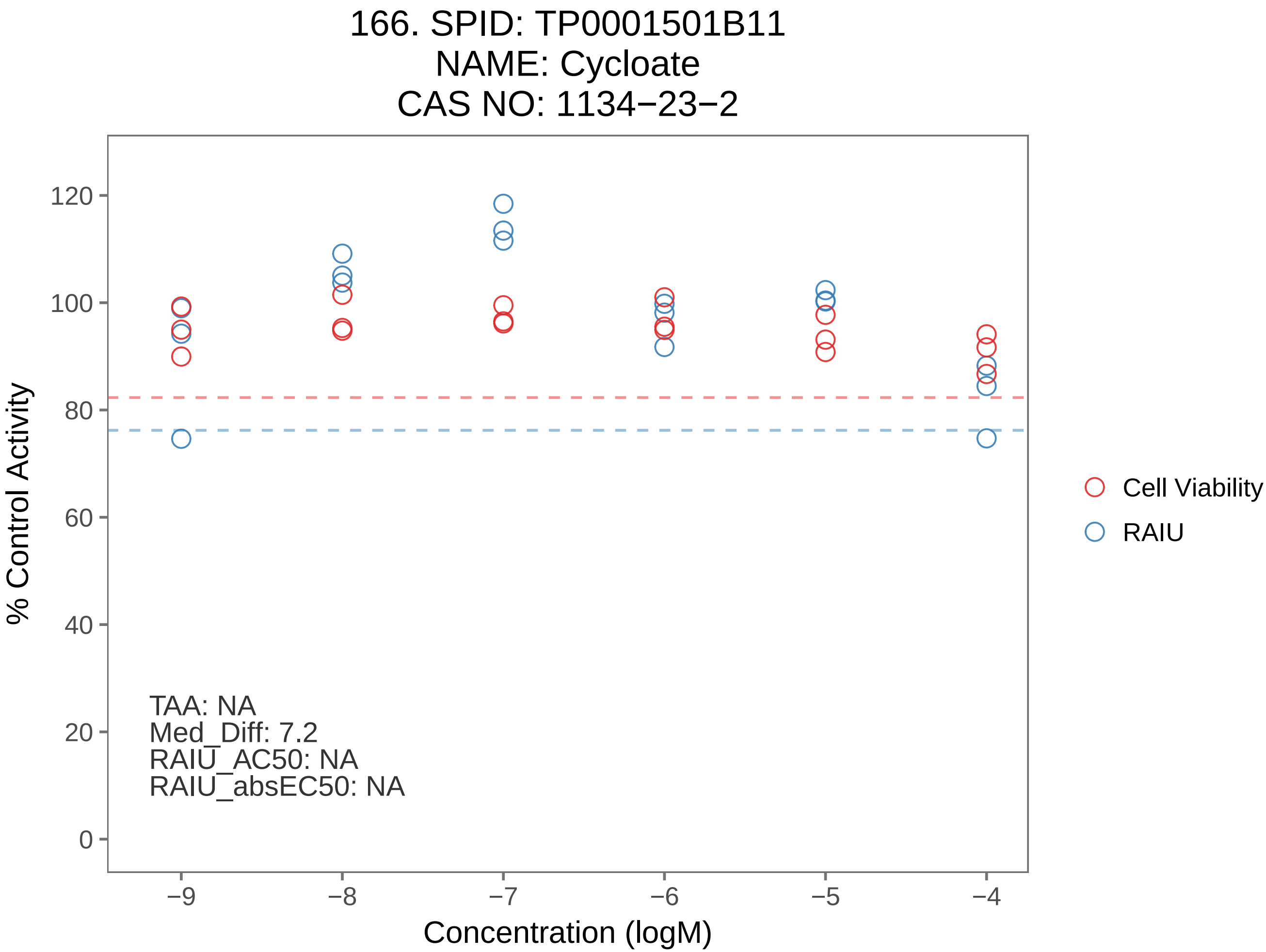

161. SPID: TP0001499E02
NAME: Resmethrin
CAS NO: 10453−86−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −1.96
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

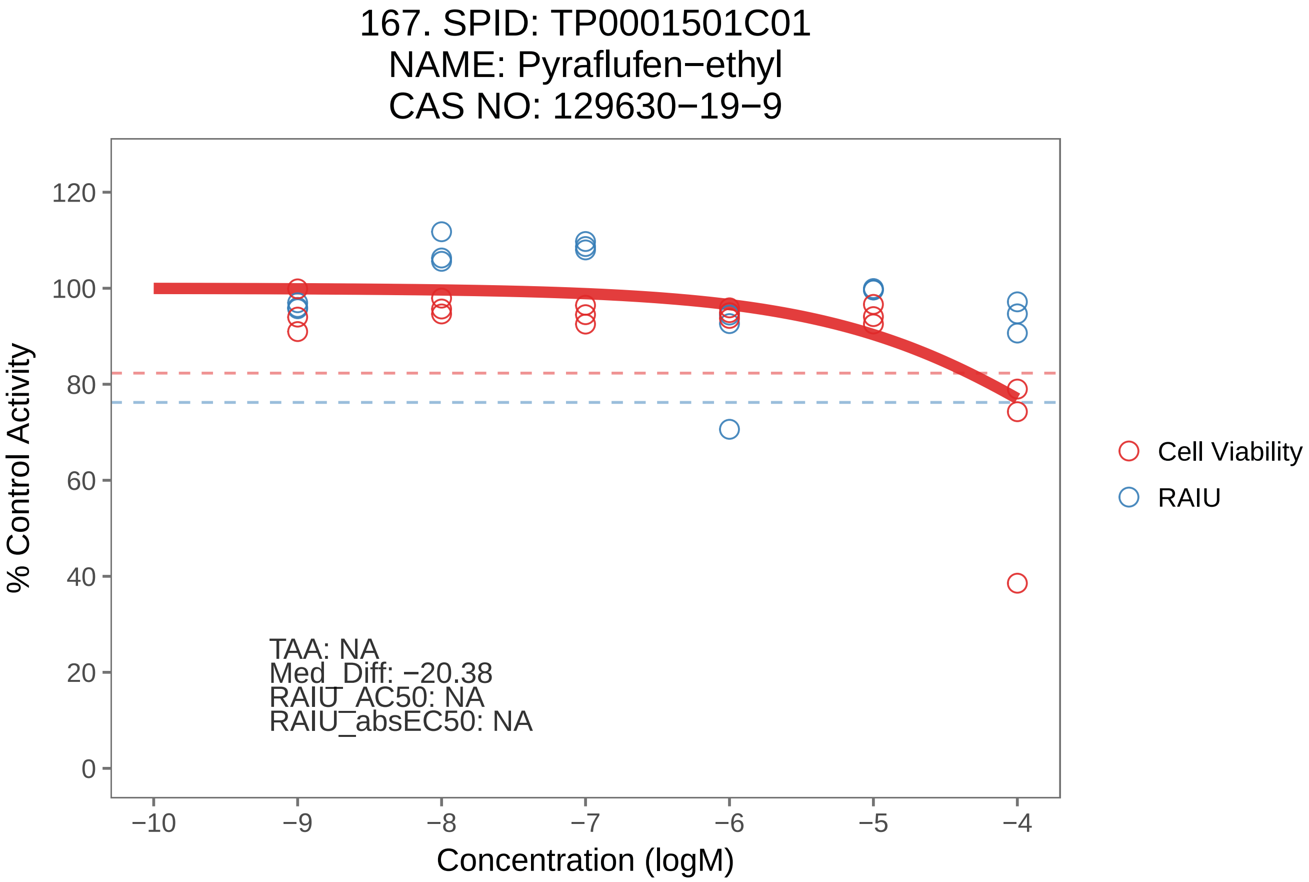

162. SPID: TP0001499E03
NAME: Fenpropathrin
CAS NO: 39515−41−8
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−9
−8
−7
−6
−5
−4
Cell Viability
RAIU
TAA: NA
Med_Diff: 3.23
RAIU_AC50: NA
RAIU_absEC50: NA

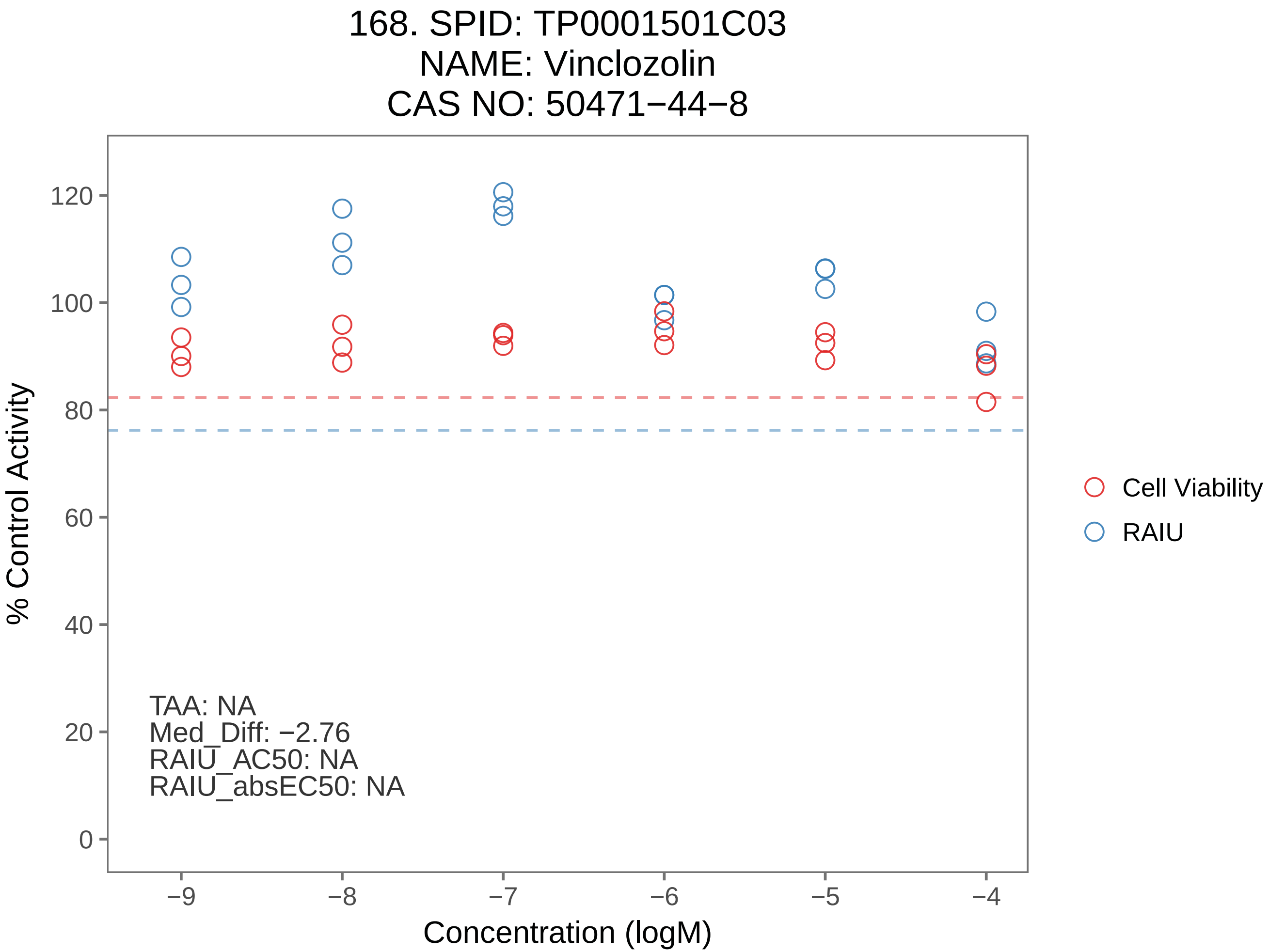

163. SPID: TP0001501A01
NAME: Tralkoxydim
CAS NO: 87820−88−0
% Control Activity
120
100
80
60
40
20
0
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: 10.76
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

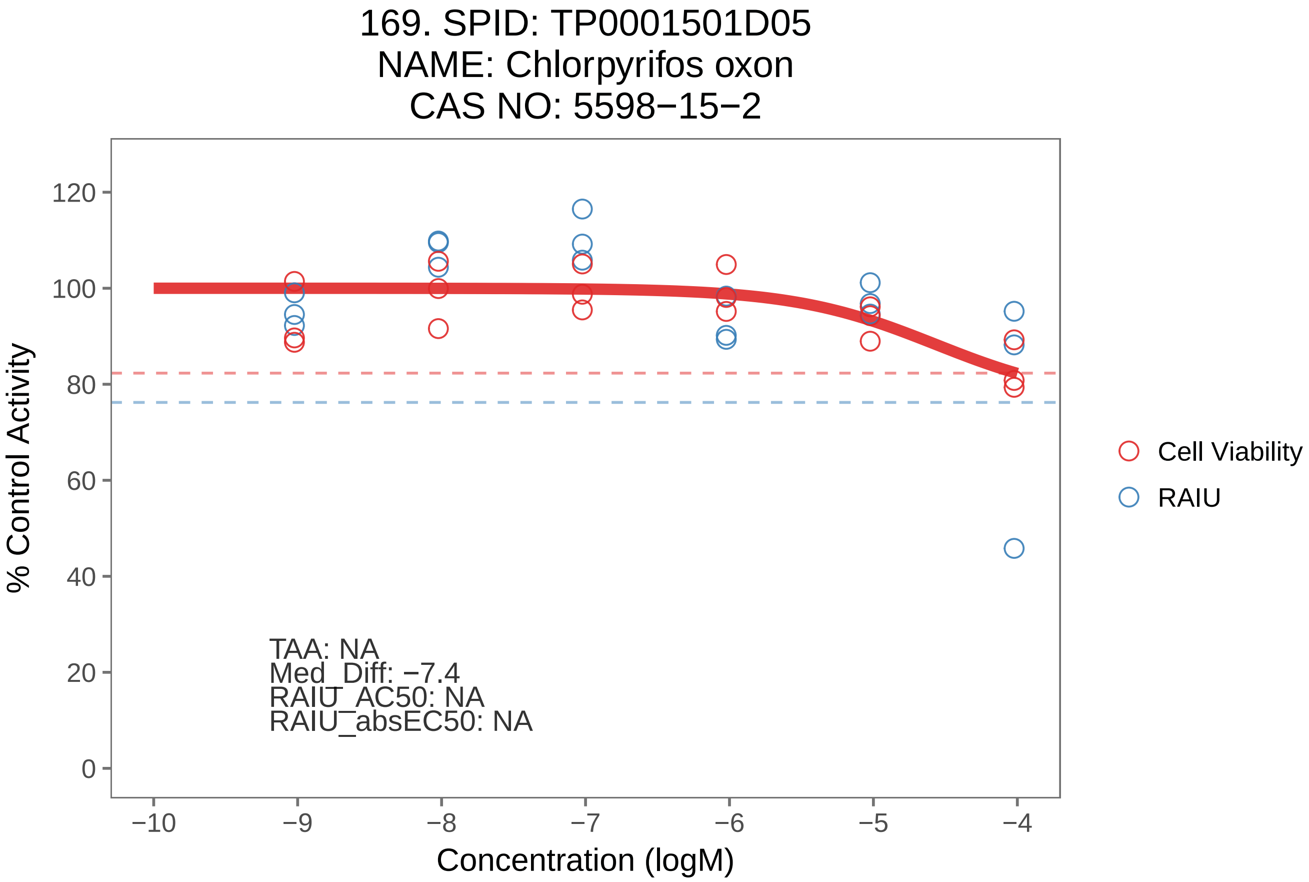

164. SPID: TP0001501B05
NAME: Flufenpyr−ethyl
CAS NO: 188489−07−8
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−9
−8
−7
−6
−5
−4
TAA: NA
Med_Diff: −8.15
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU


165. SPID: TP0001501B08
NAME: Fenhexamid
CAS NO: 126833−17−8
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −2.35
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

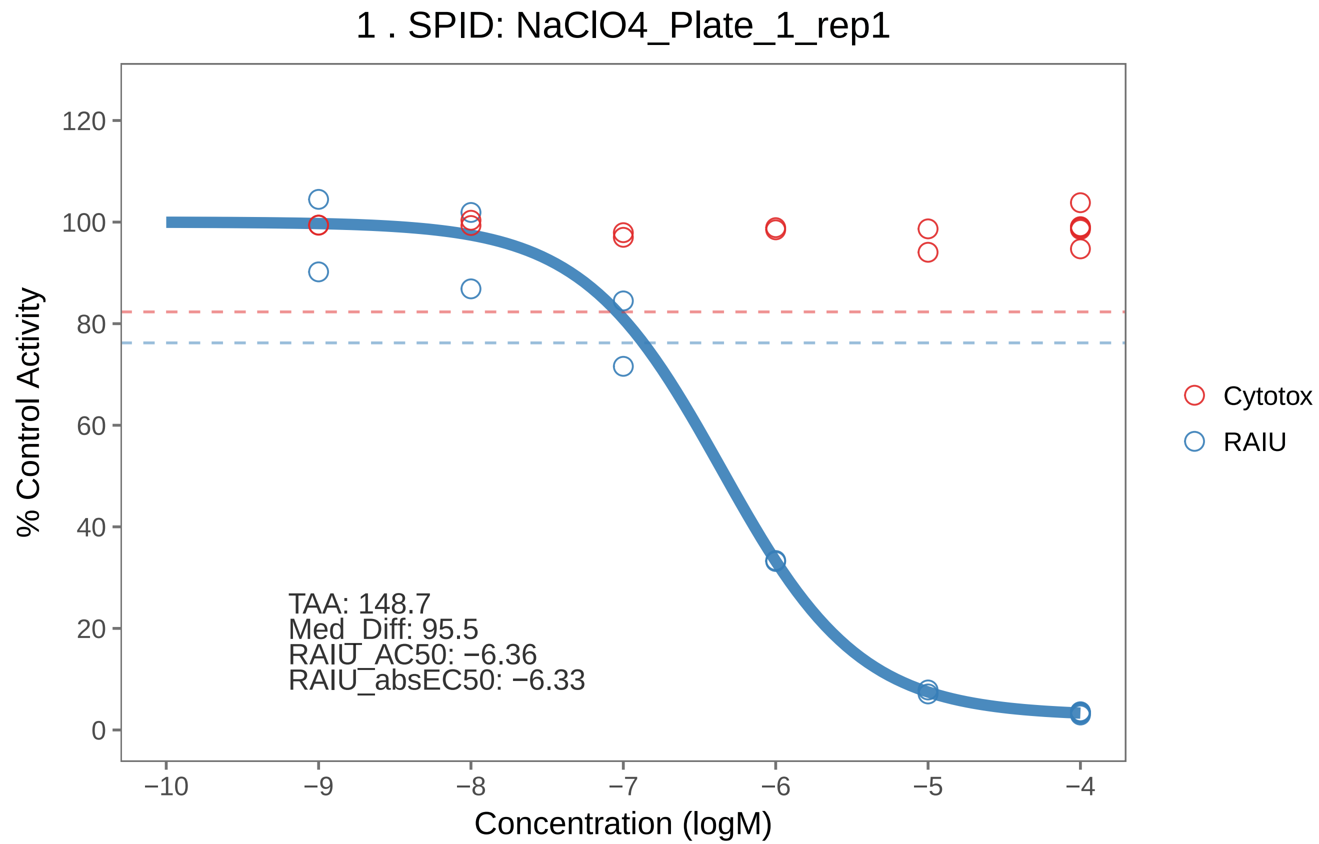

166. SPID: TP0001501B11
NAME: Cycloate
CAS NO: 1134−23−2
% Control Activity
120
100
80
60
40
20
0
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: 7.2
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

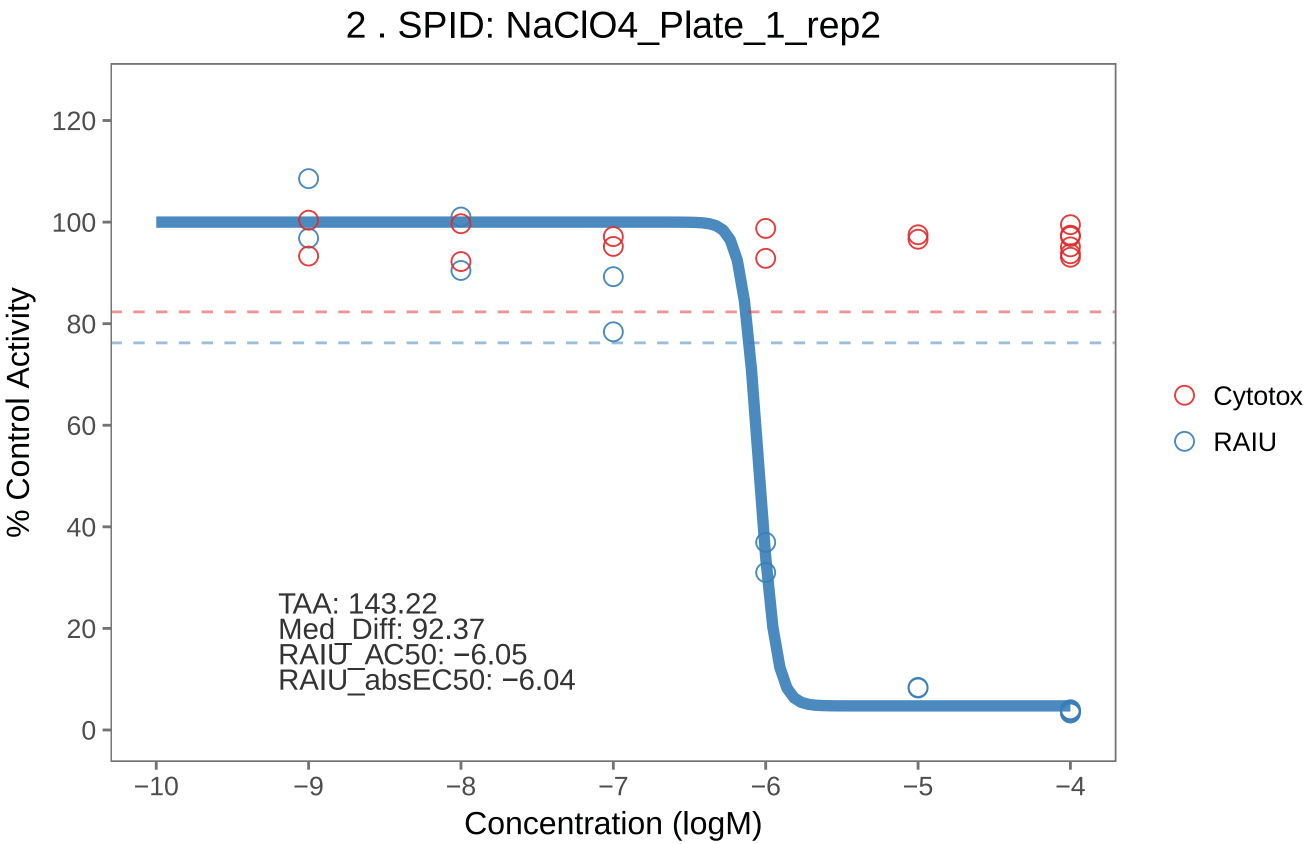

167. SPID: TP0001501C01
NAME: Pyraflufen−ethyl
CAS NO: 129630−19−9
% Control Activity
0
20
40
60
80
100
120
TAA: NA
Med_Diff: −20.38
RAIU_AC50: NA
RAIU_absEC50: NA
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cell Viability
RAIU

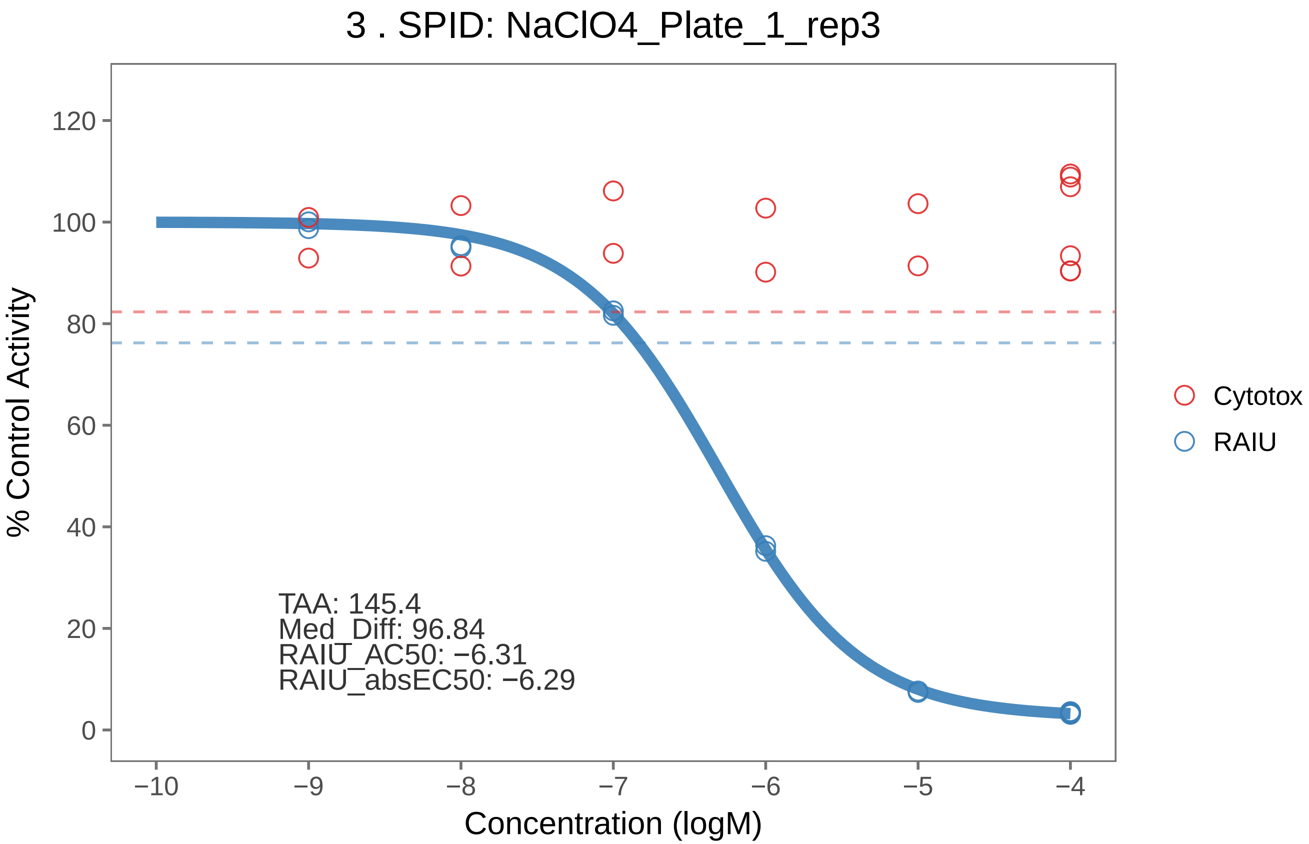

168. SPID: TP0001501C03
NAME: Vinclozolin
CAS NO: 50471−44−8
% Control Activity
0
20
40
60
80
100
120
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −2.76
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

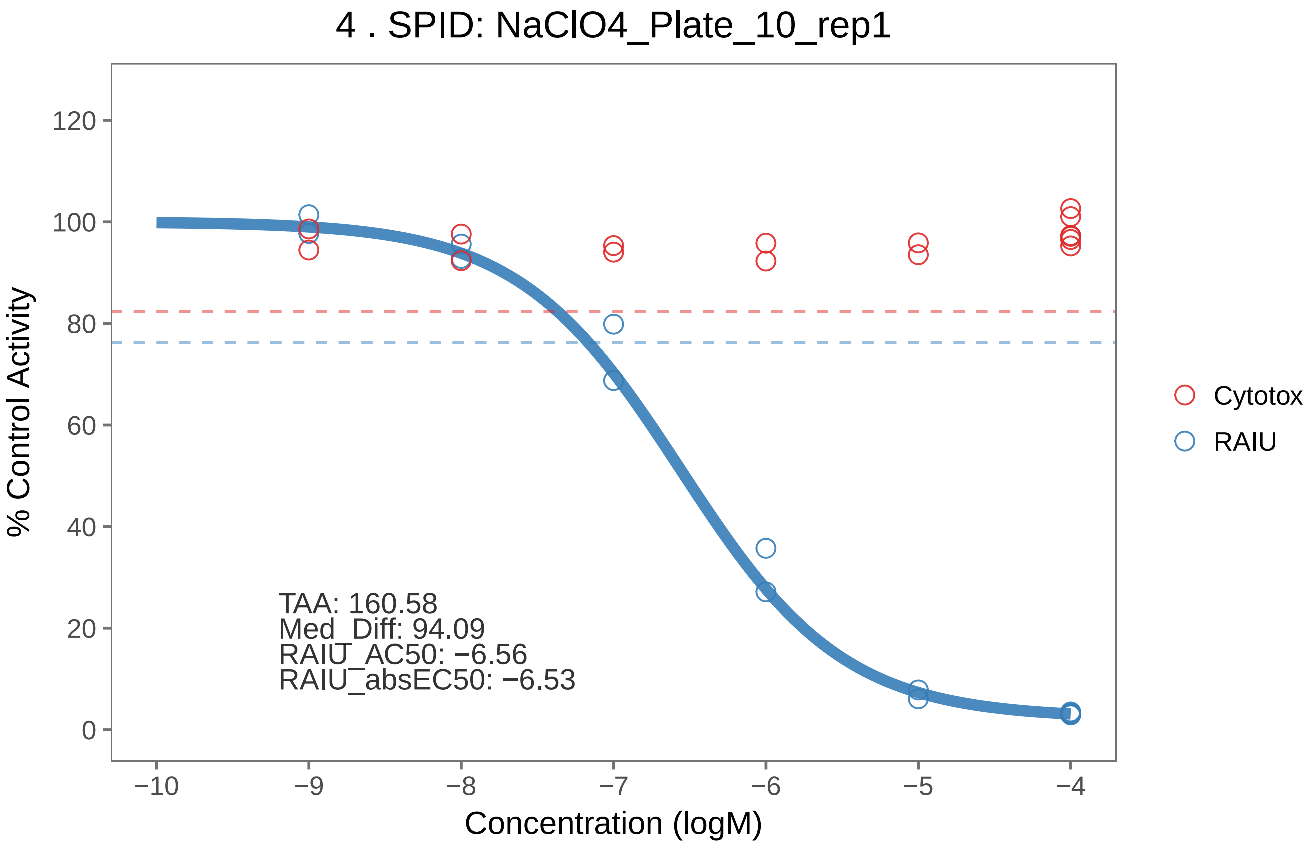

169. SPID: TP0001501D05
NAME: Chlorpyrifos oxon
CAS NO: 5598−15−2
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: NA
Med_Diff: −7.4
RAIU_AC50: NA
RAIU_absEC50: NA
Cell Viability
RAIU

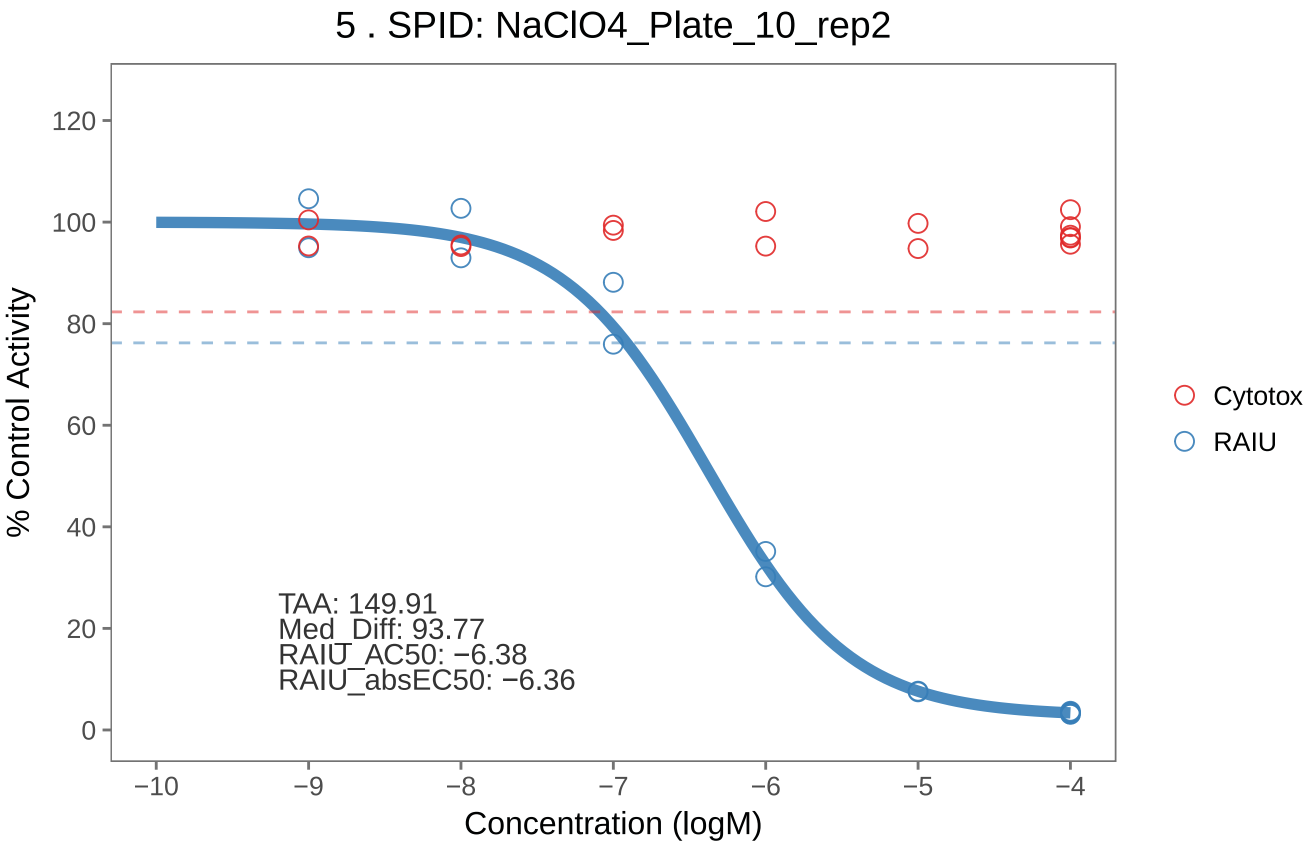
Part IV. Does-response of sodium perchlorate and DCNQ positive controls in multi-concentration screening


1 . SPID: NaClO4_Plate_1_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 148.7
Med_Diff: 95.5
RAIU_AC50: −6.36
RAIU_absEC50: −6.33
Cytotox
RAIU

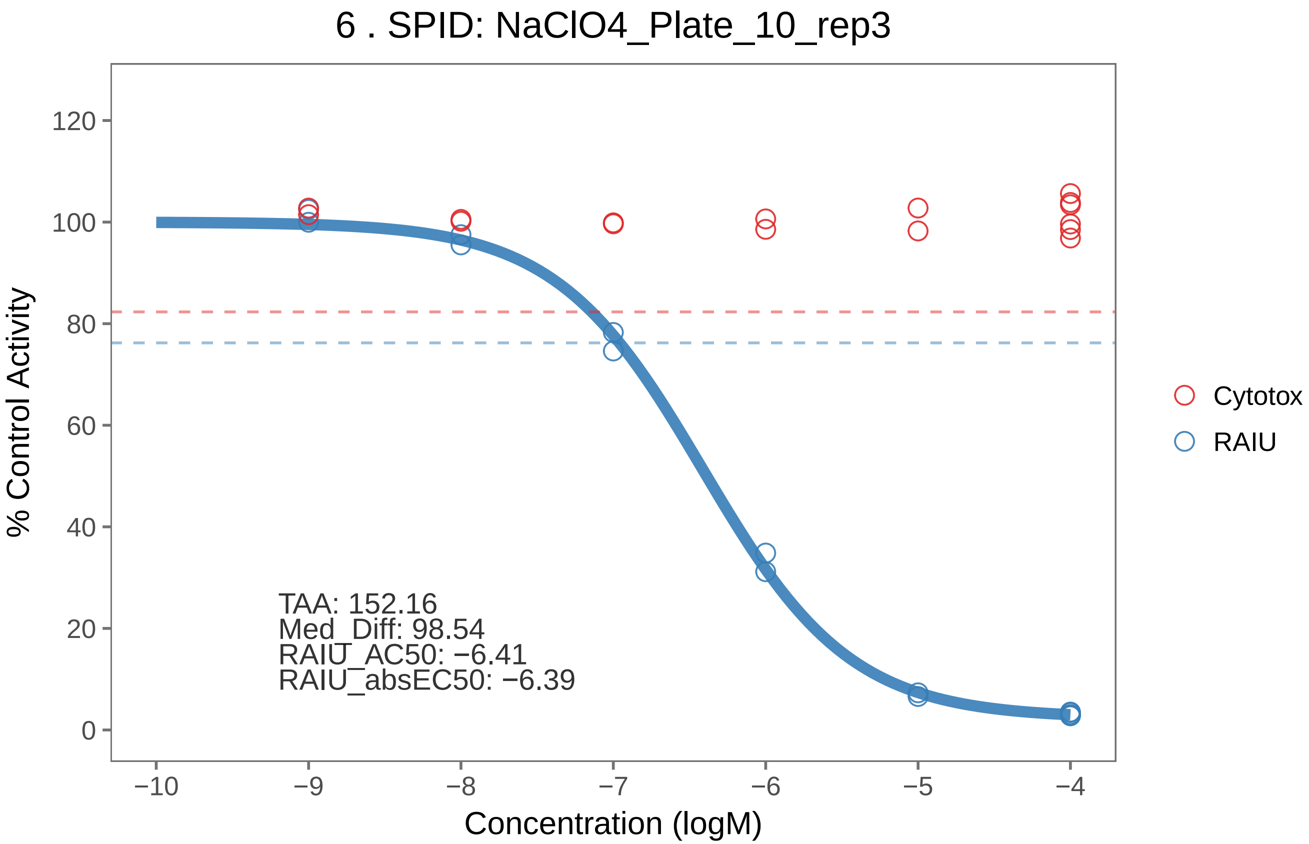

2 . SPID: NaClO4_Plate_1_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 143.22
Med_Diff: 92.37
RAIU_AC50: −6.05
RAIU_absEC50: −6.04
Cytotox
RAIU

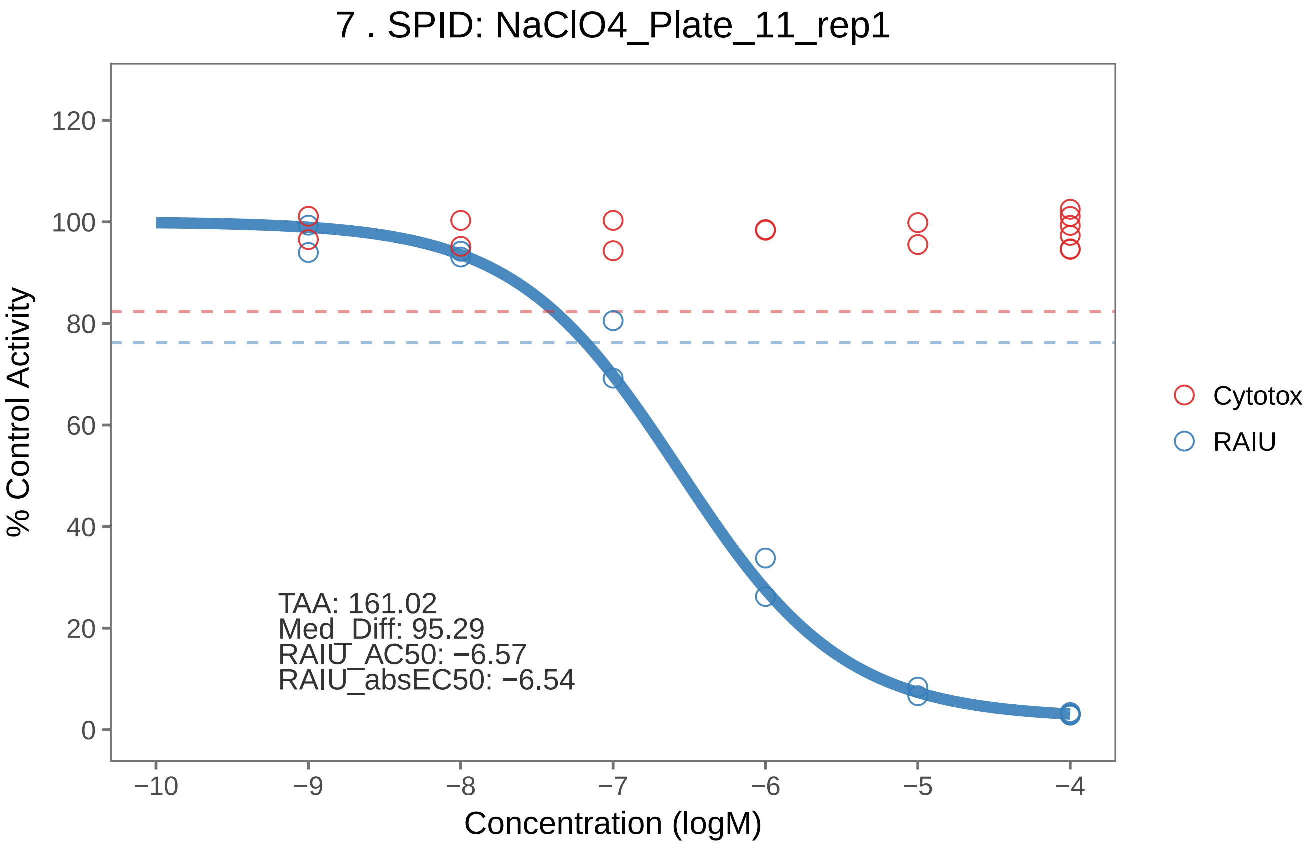

3 . SPID: NaClO4_Plate_1_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 145.4
Med_Diff: 96.84
RAIU_AC50: −6.31
RAIU_absEC50: −6.29
Cytotox
RAIU

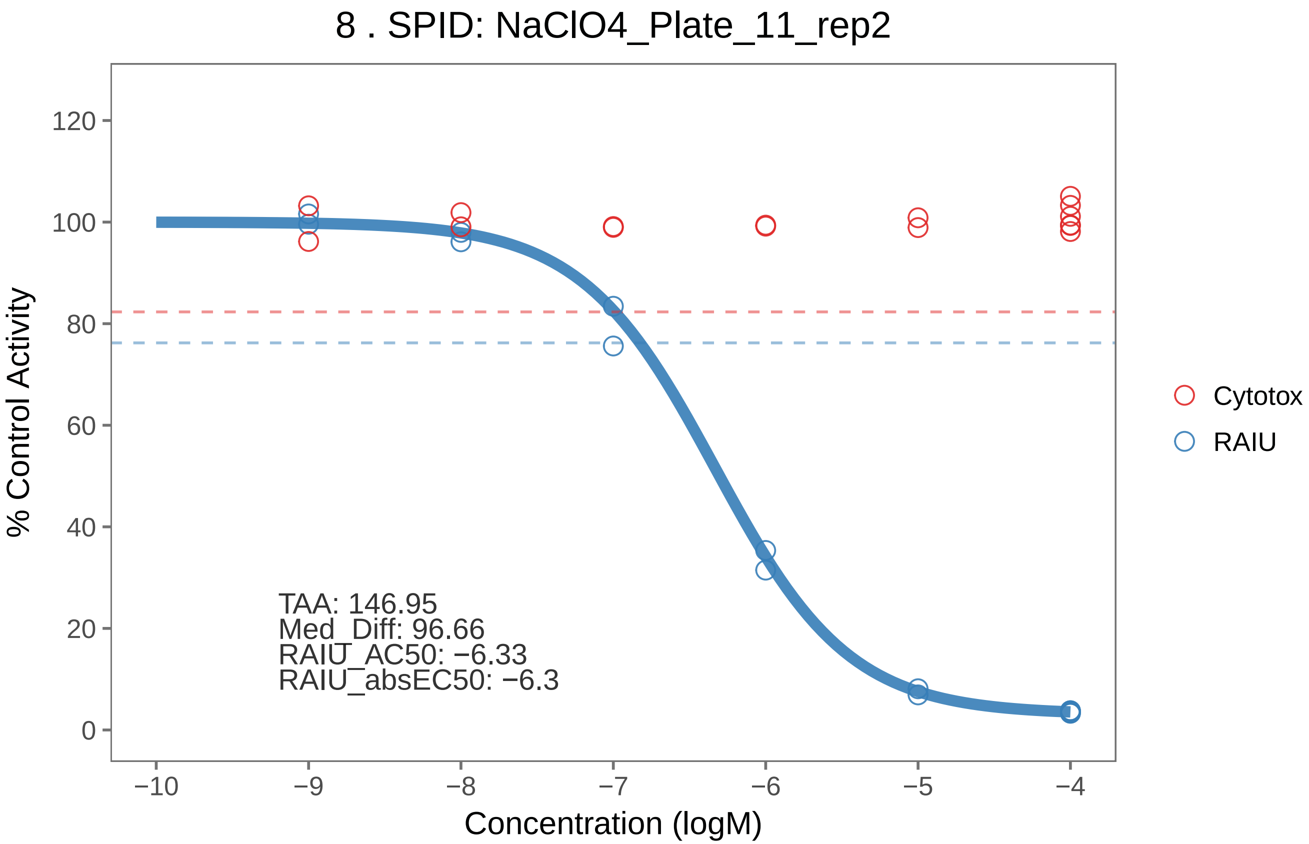

4 . SPID: NaClO4_Plate_10_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 160.58
Med_Diff: 94.09
RAIU_AC50: −6.56
RAIU_absEC50: −6.53
Cytotox
RAIU

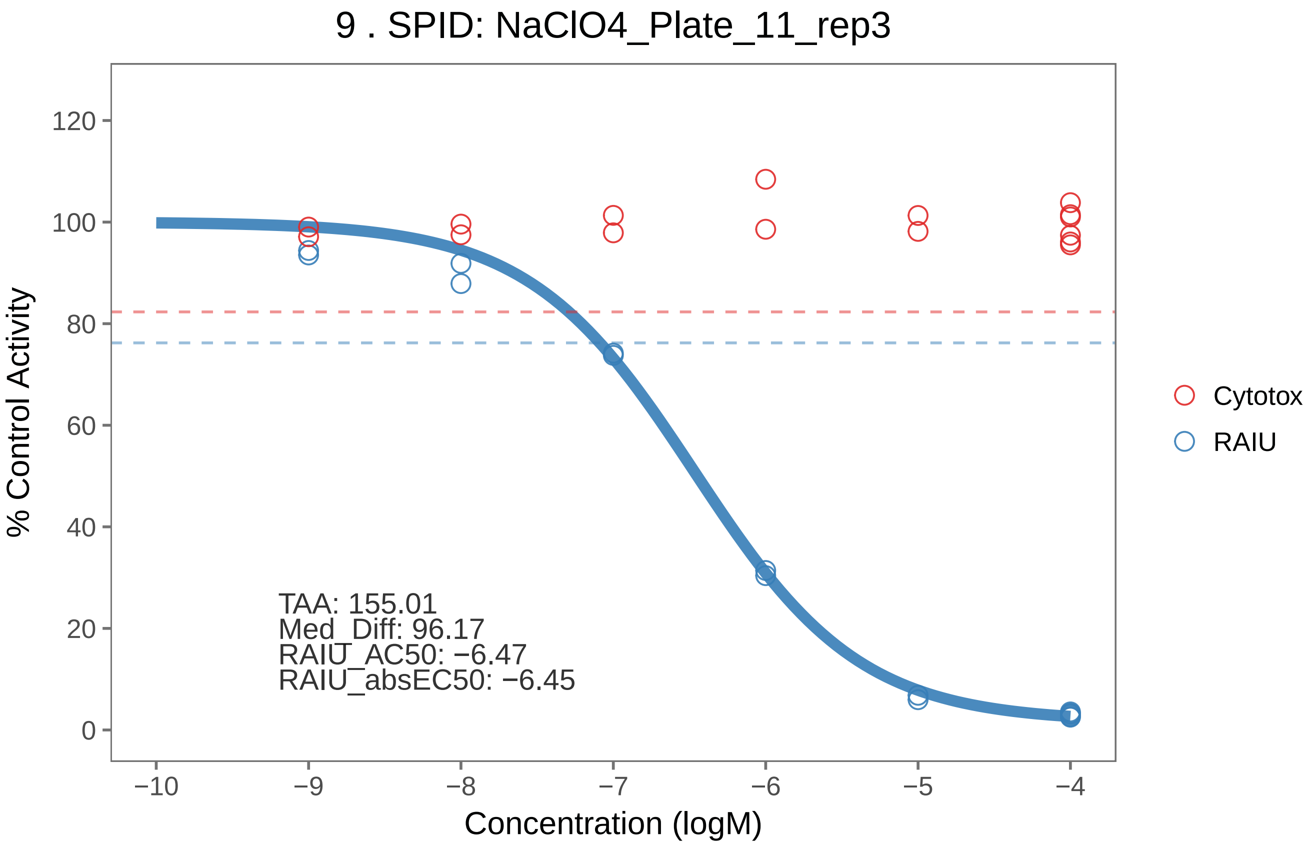


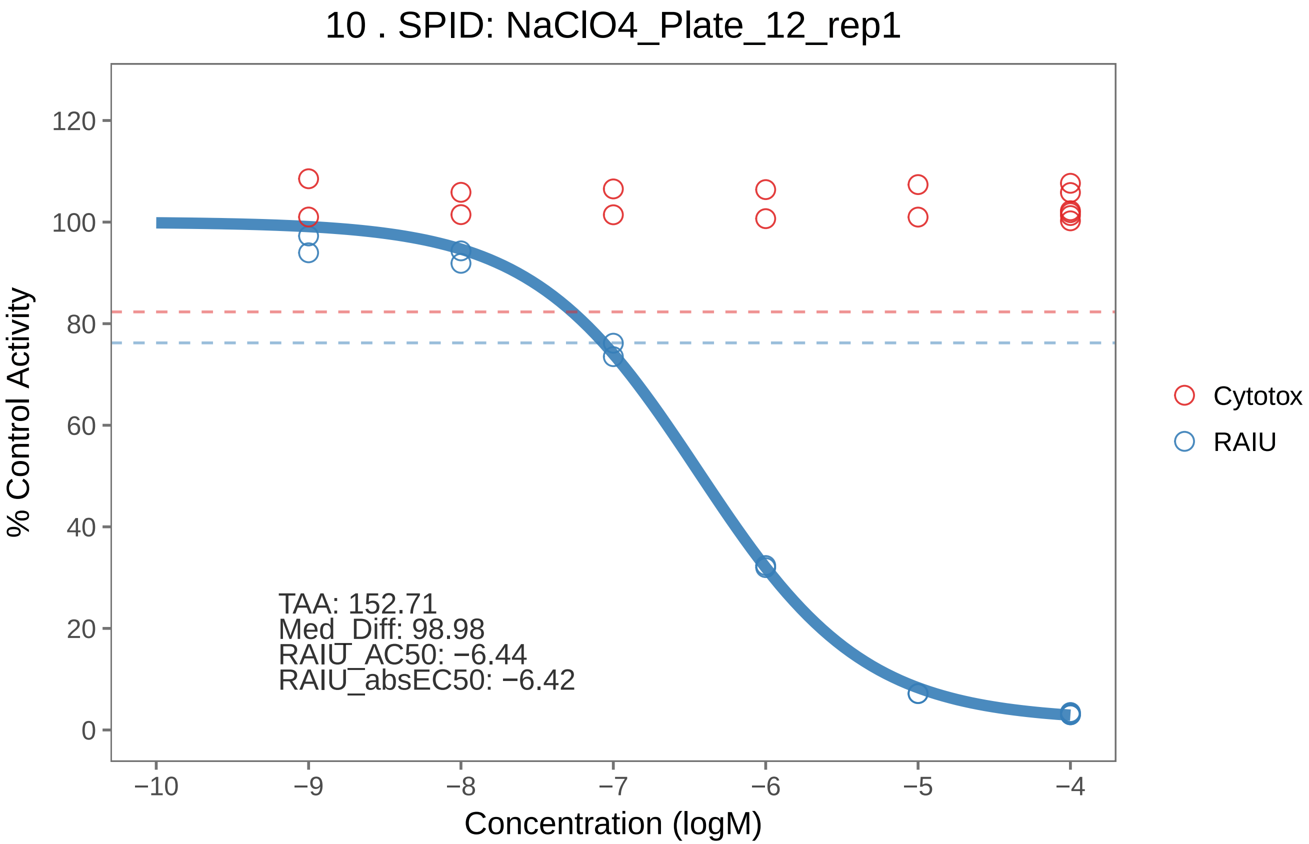
5 . SPID: NaClO4_Plate_10_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 149.91
Med_Diff: 93.77
RAIU_AC50: −6.38
RAIU_absEC50: −6.36
Cytotox
RAIU

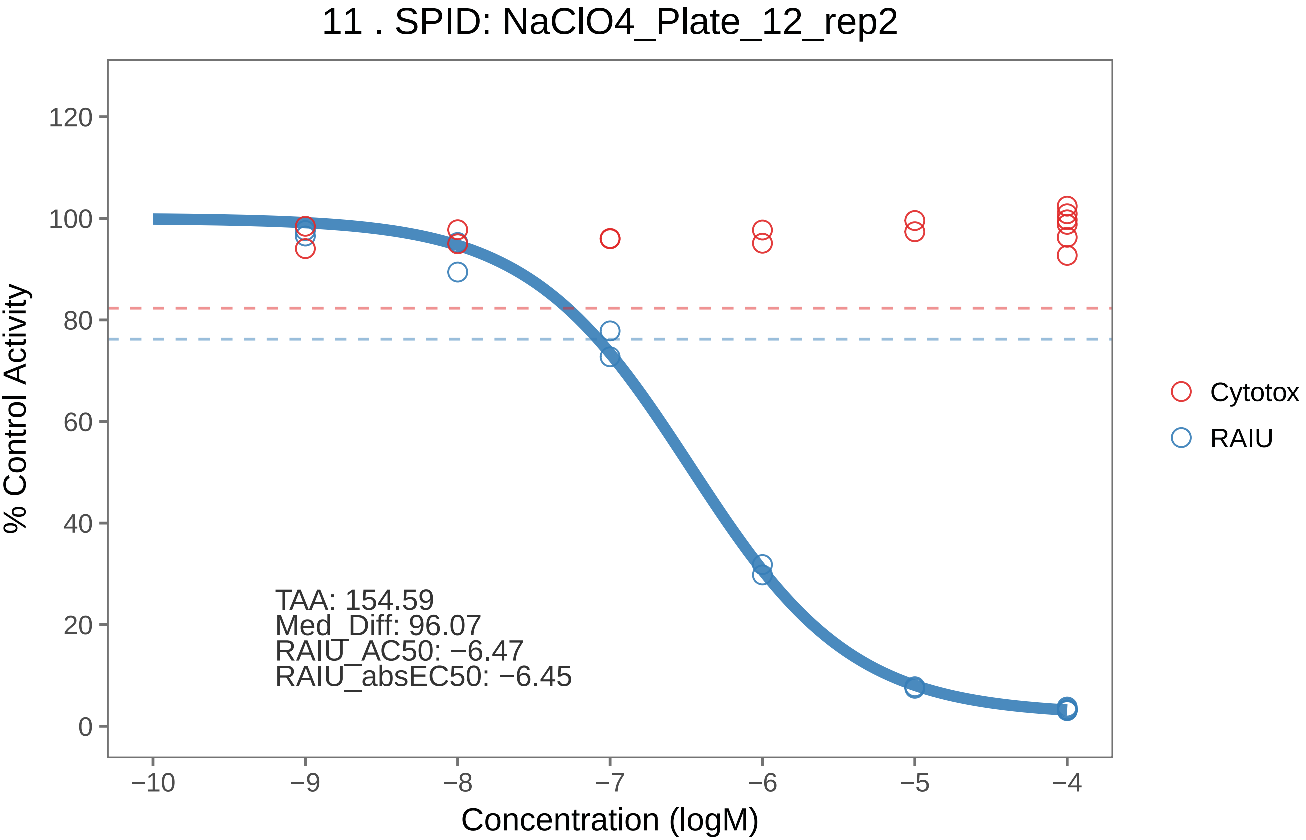

6 . SPID: NaClO4_Plate_10_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 152.16
Med_Diff: 98.54
RAIU_AC50: −6.41
RAIU_absEC50: −6.39
Cytotox
RAIU

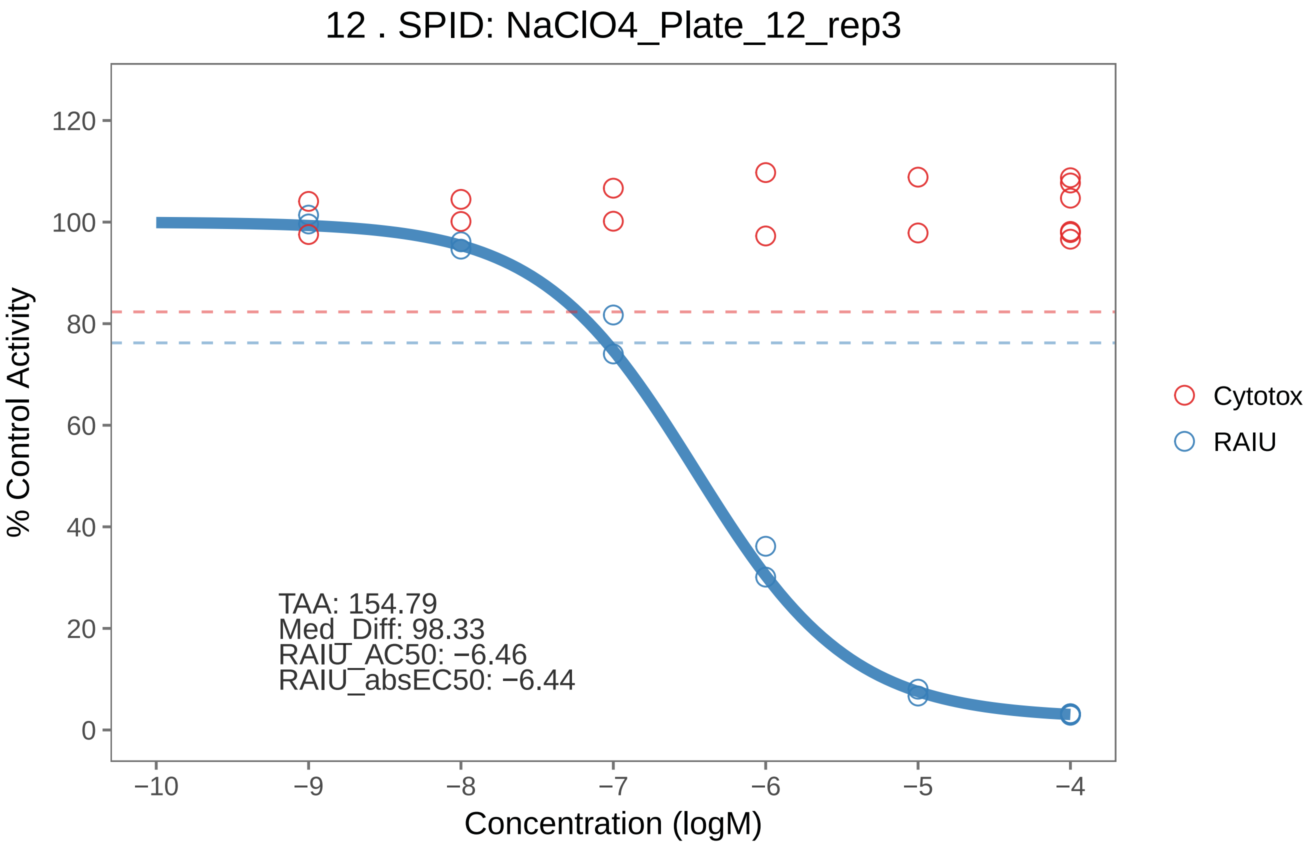

7 . SPID: NaClO4_Plate_11_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 161.02
Med_Diff: 95.29
RAIU_AC50: −6.57
RAIU_absEC50: −6.54
Cytotox
RAIU

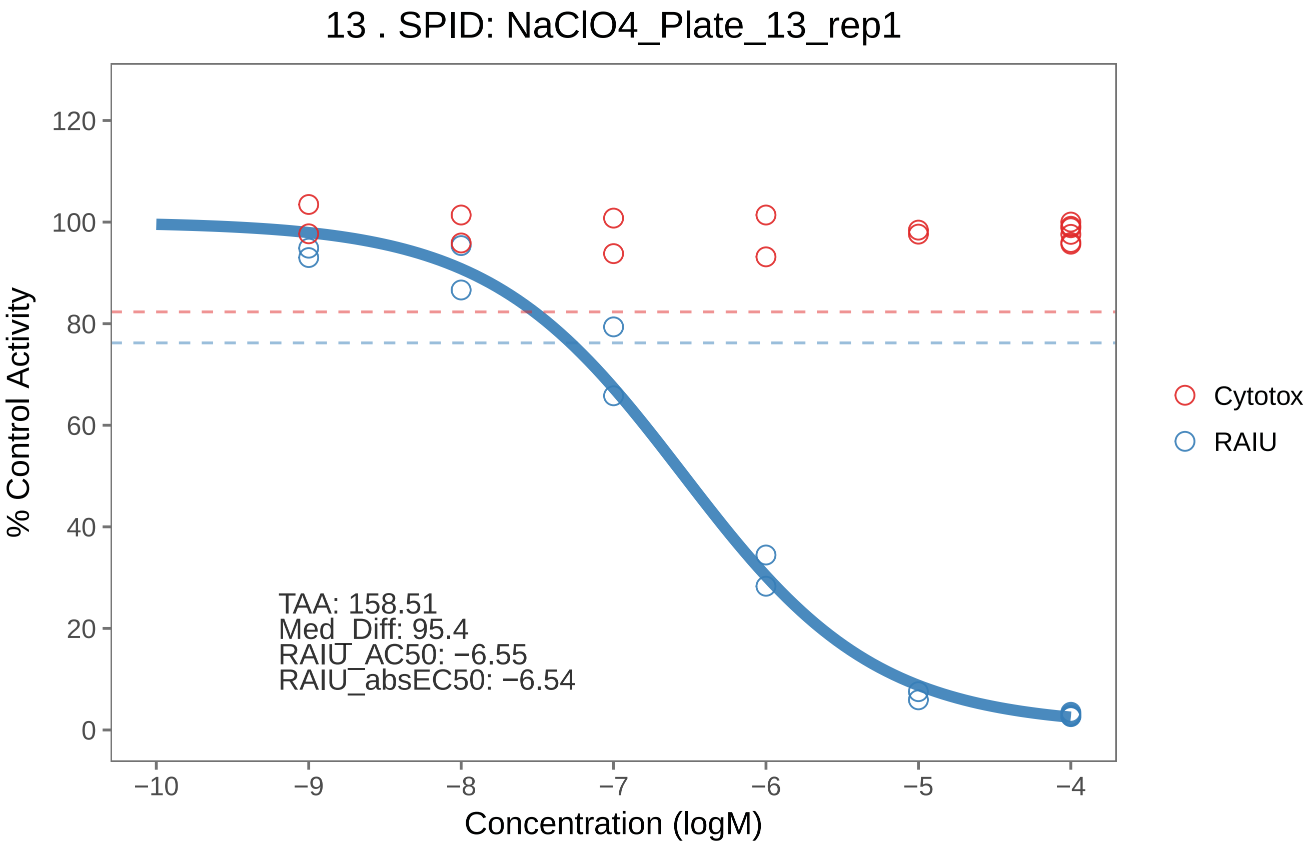

8 . SPID: NaClO4_Plate_11_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 146.95
Med_Diff: 96.66
RAIU_AC50: −6.33
RAIU_absEC50: −6.3
Cytotox
RAIU

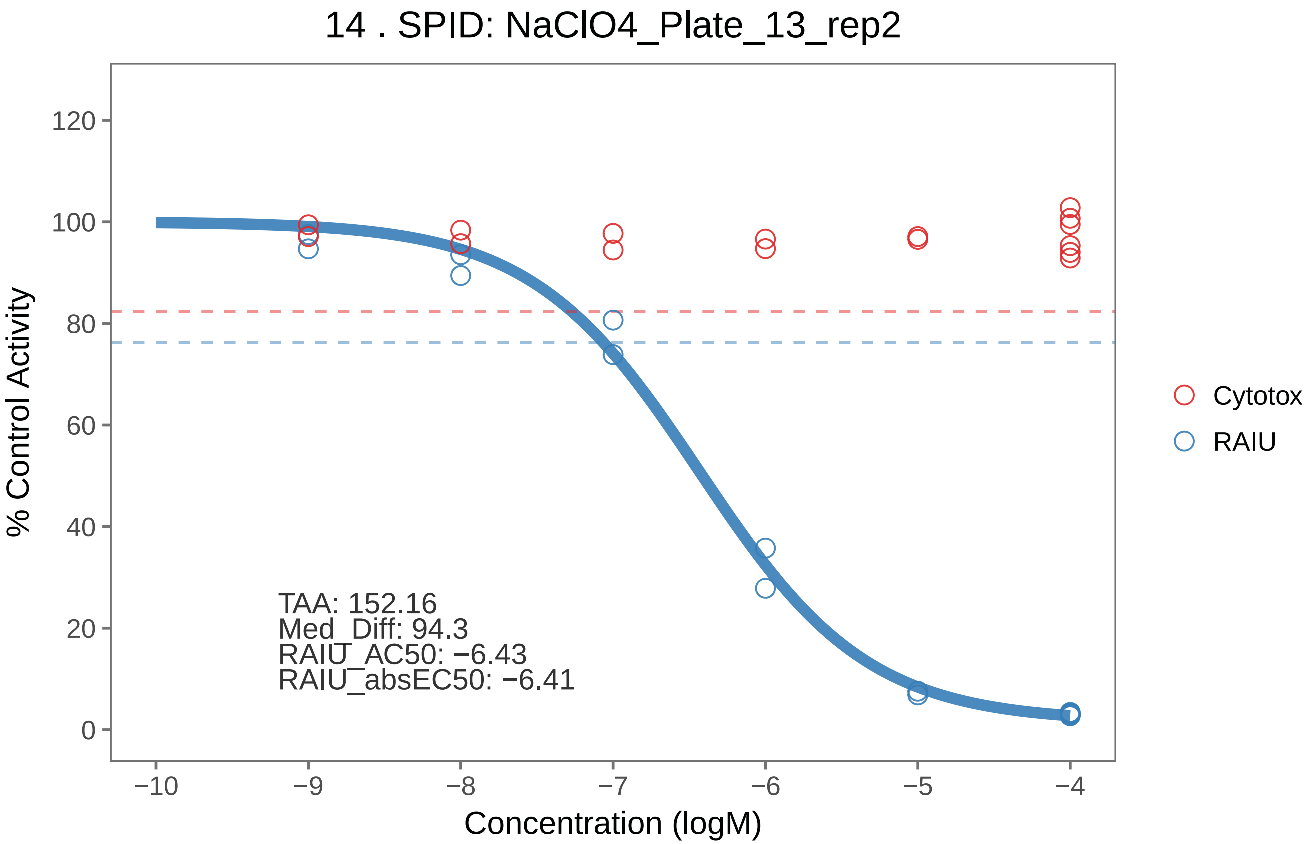

9 . SPID: NaClO4_Plate_11_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 155.01
Med_Diff: 96.17
RAIU_AC50: −6.47
RAIU_absEC50: −6.45
Cytotox
RAIU

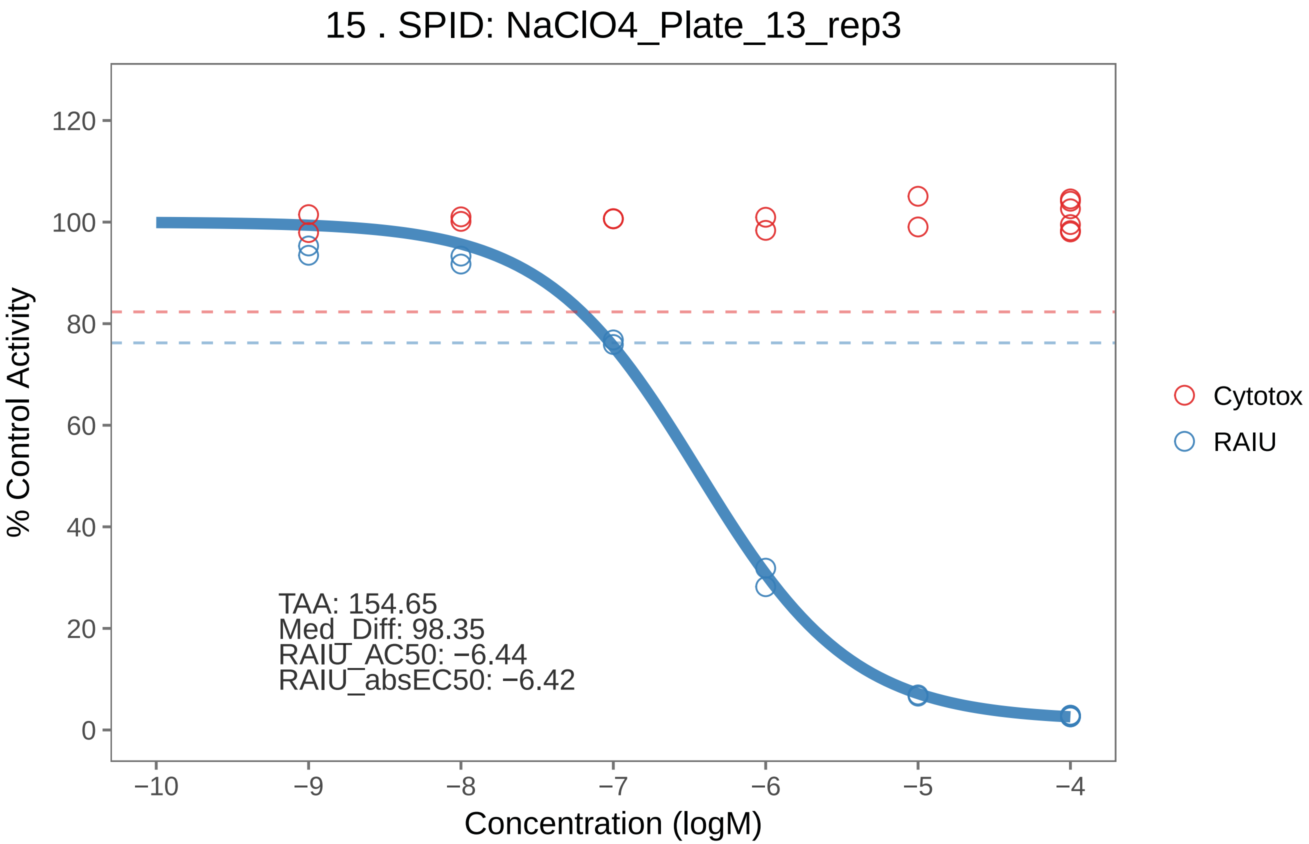

10 . SPID: NaClO4_Plate_12_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 152.71
Med_Diff: 98.98
RAIU_AC50: −6.44
RAIU_absEC50: −6.42
Cytotox
RAIU

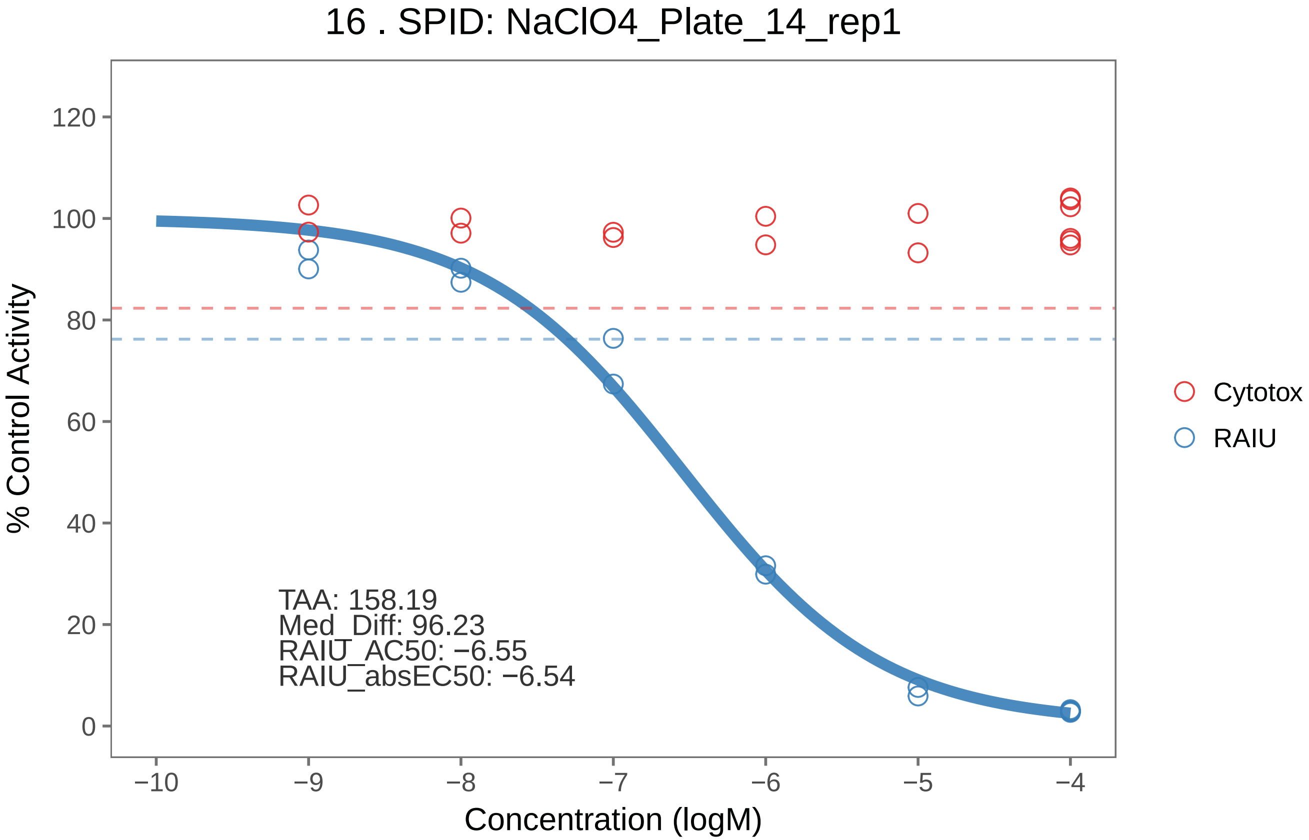

11 . SPID: NaClO4_Plate_12_rep2
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Cytotox
RAIU
TAA: 154.59
Med_Diff: 96.07
RAIU_AC50: −6.47
RAIU_absEC50: −6.45

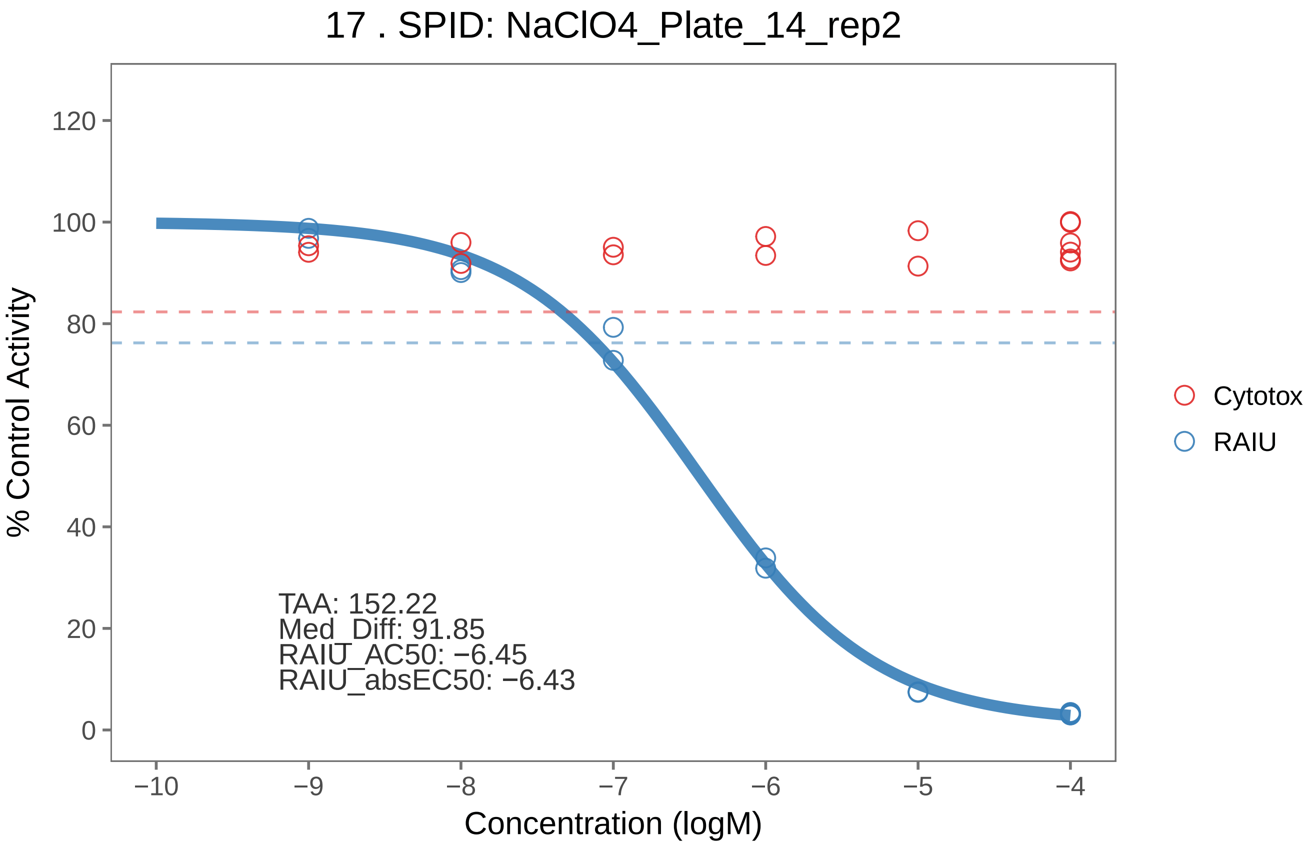

12 . SPID: NaClO4_Plate_12_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 154.79
Med_Diff: 98.33
RAIU_AC50: −6.46
RAIU_absEC50: −6.44


13 . SPID: NaClO4_Plate_13_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 158.51
Med_Diff: 95.4
RAIU_AC50: −6.55
RAIU_absEC50: −6.54

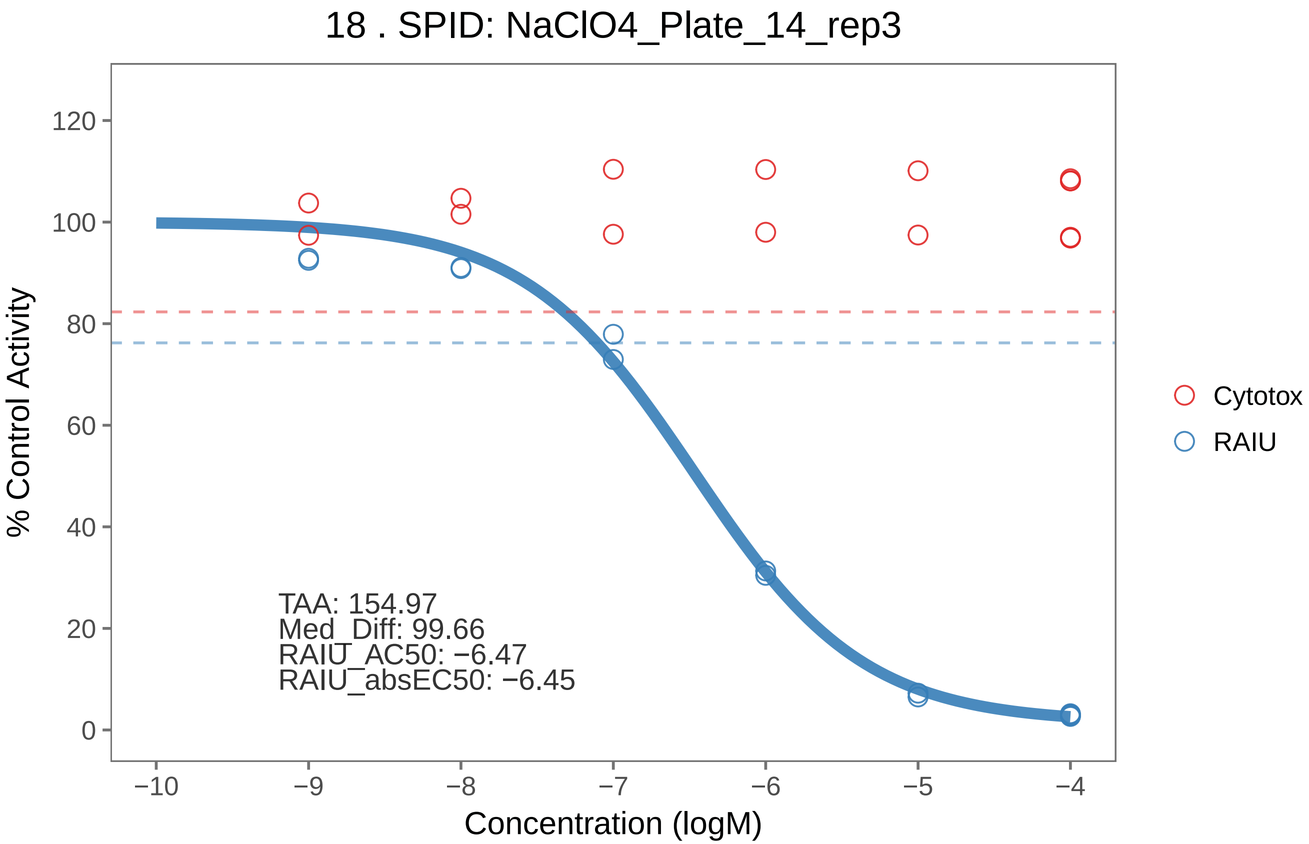

14 . SPID: NaClO4_Plate_13_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 152.16
Med_Diff: 94.3
RAIU_AC50: −6.43
RAIU_absEC50: −6.41
Cytotox
RAIU

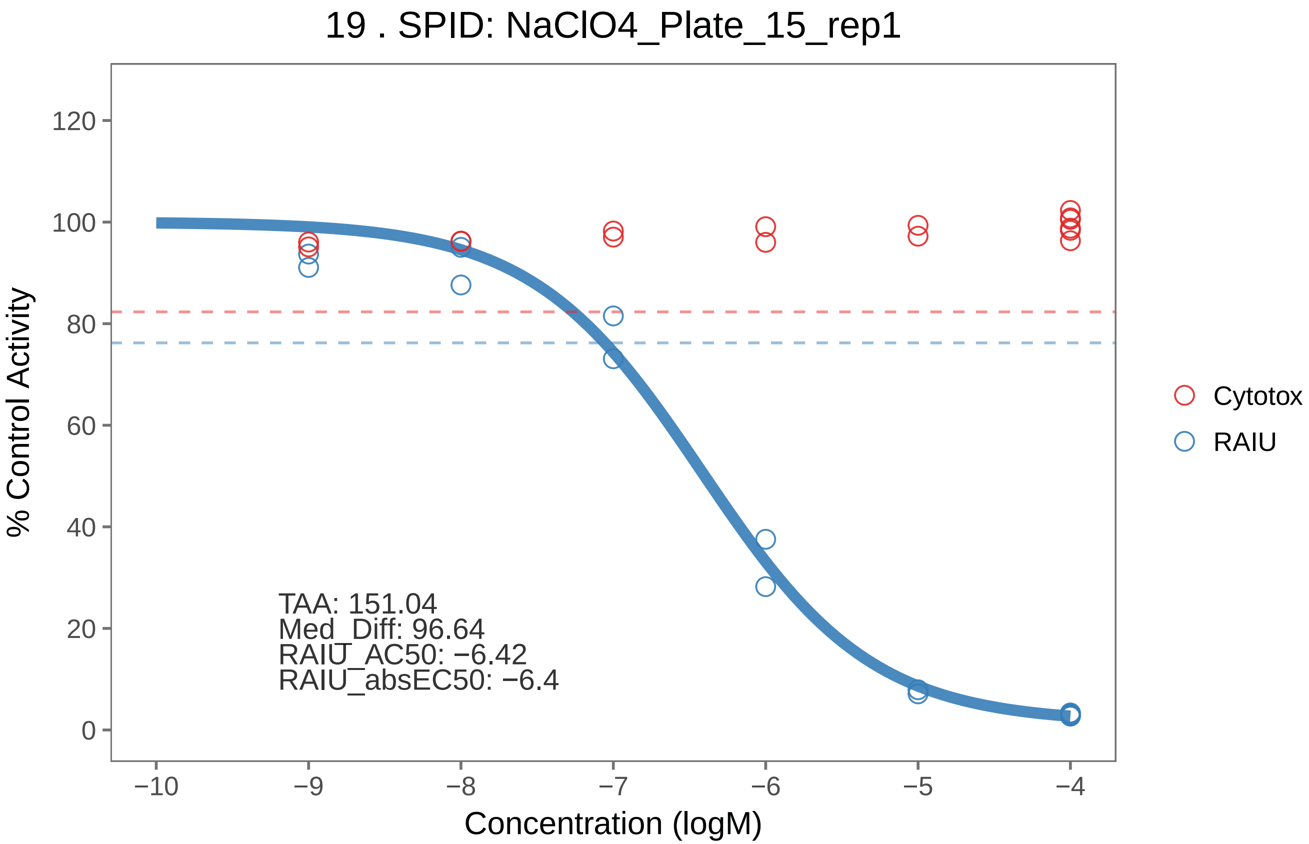

15 . SPID: NaClO4_Plate_13_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 154.65
Med_Diff: 98.35
RAIU_AC50: −6.44
RAIU_absEC50: −6.42
Cytotox
RAIU

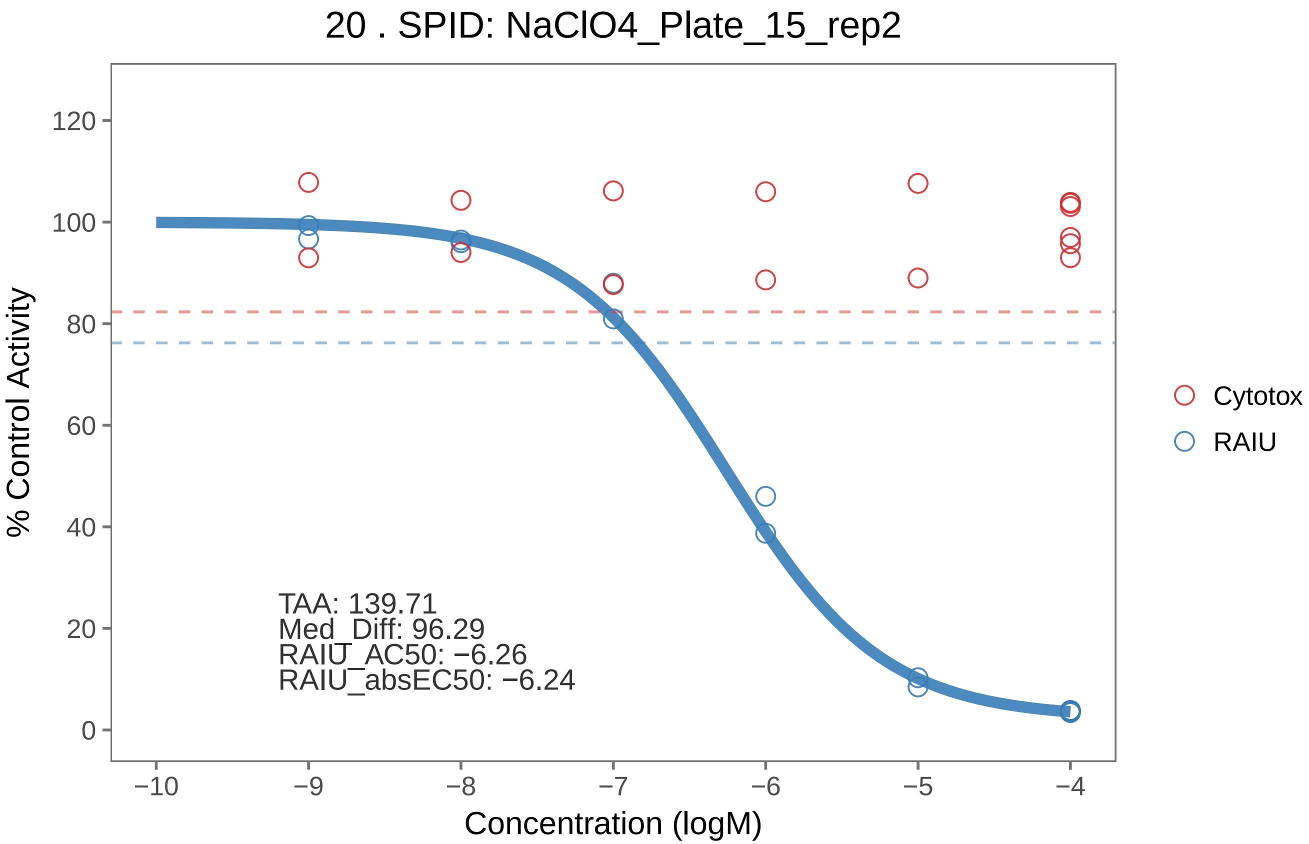

16 . SPID: NaClO4_Plate_14_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 158.19
Med_Diff: 96.23
RAIU_AC50: −6.55
RAIU_absEC50: −6.54
Cytotox
RAIU

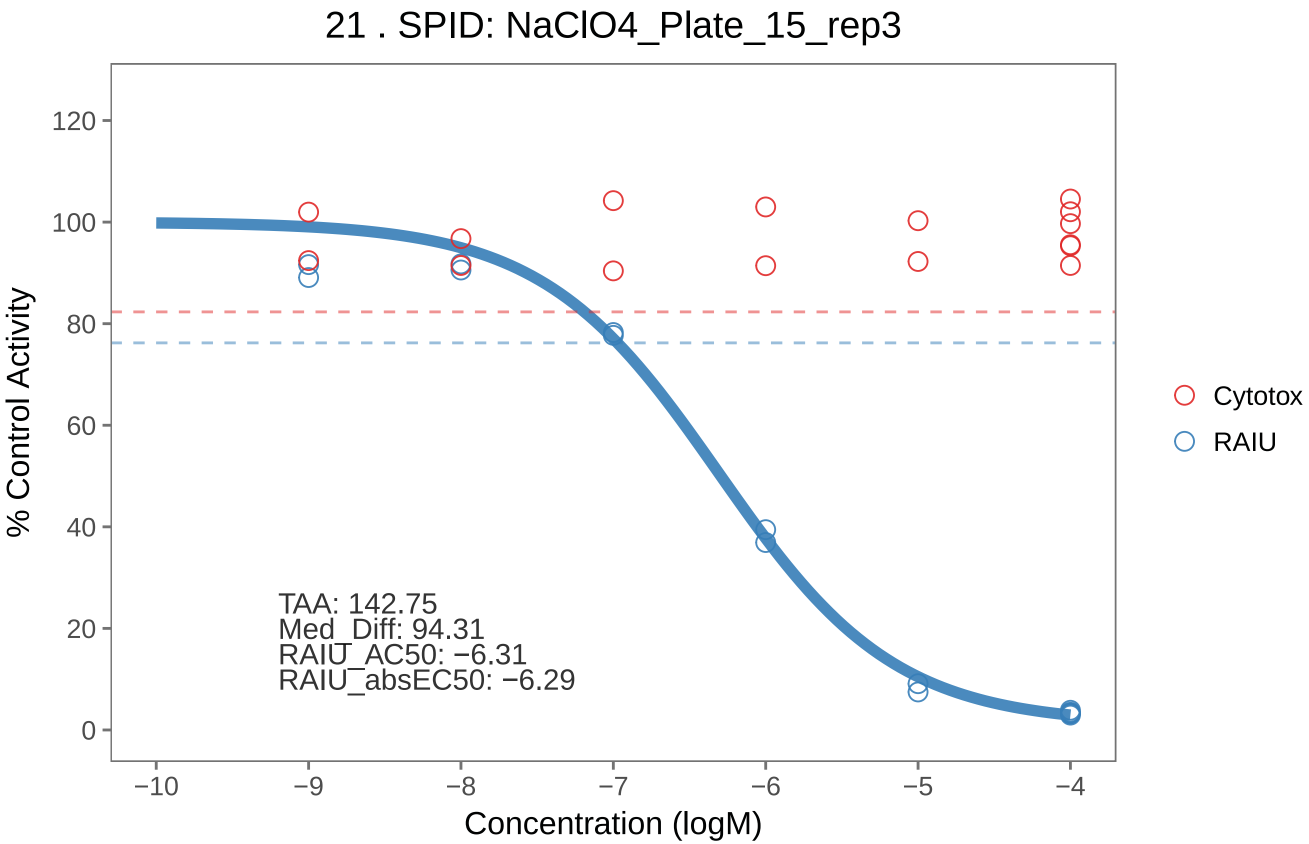


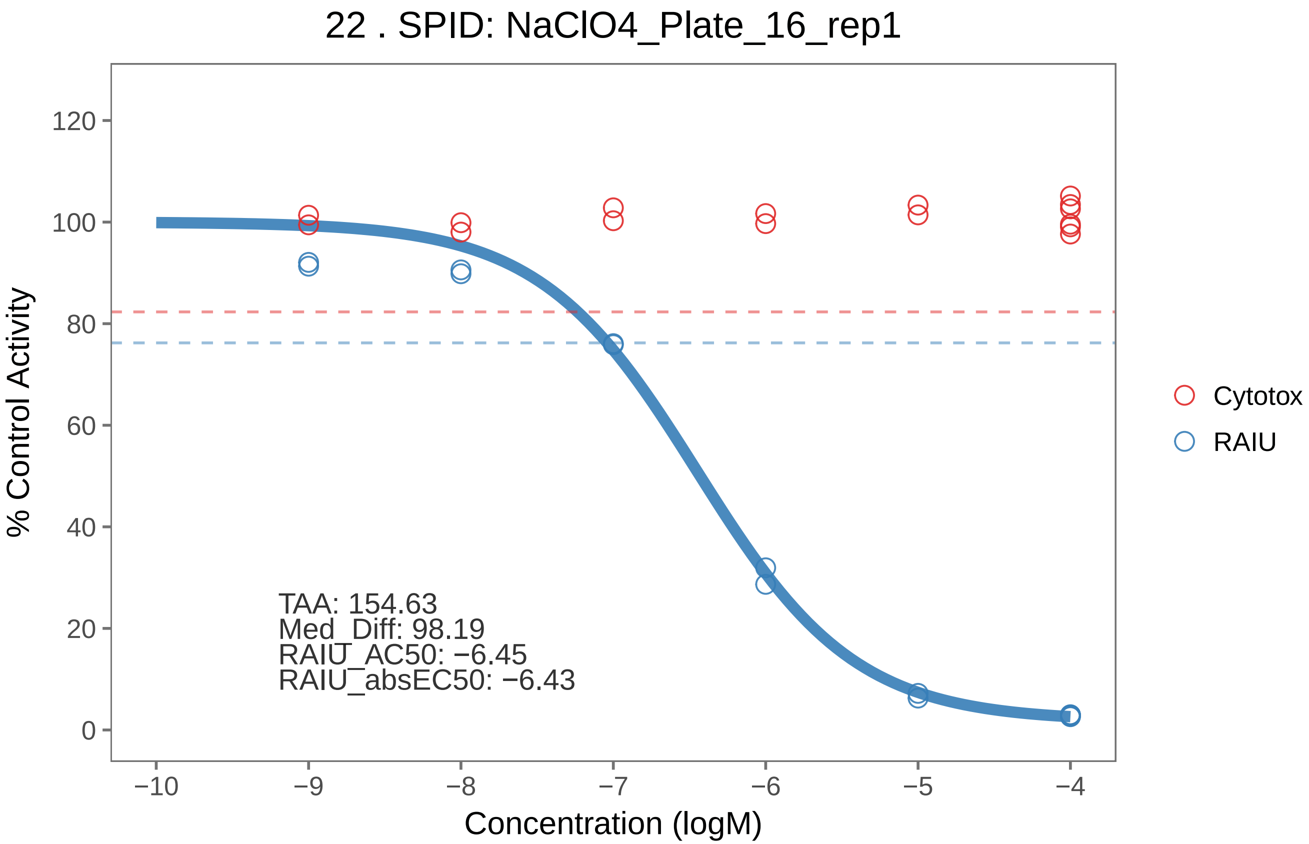
17 . SPID: NaClO4_Plate_14_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 152.22
Med_Diff: 91.85
RAIU_AC50: −6.45
RAIU_absEC50: −6.43
Cytotox
RAIU


18 . SPID: NaClO4_Plate_14_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 154.97
Med_Diff: 99.66
RAIU_AC50: −6.47
RAIU_absEC50: −6.45
Cytotox
RAIU

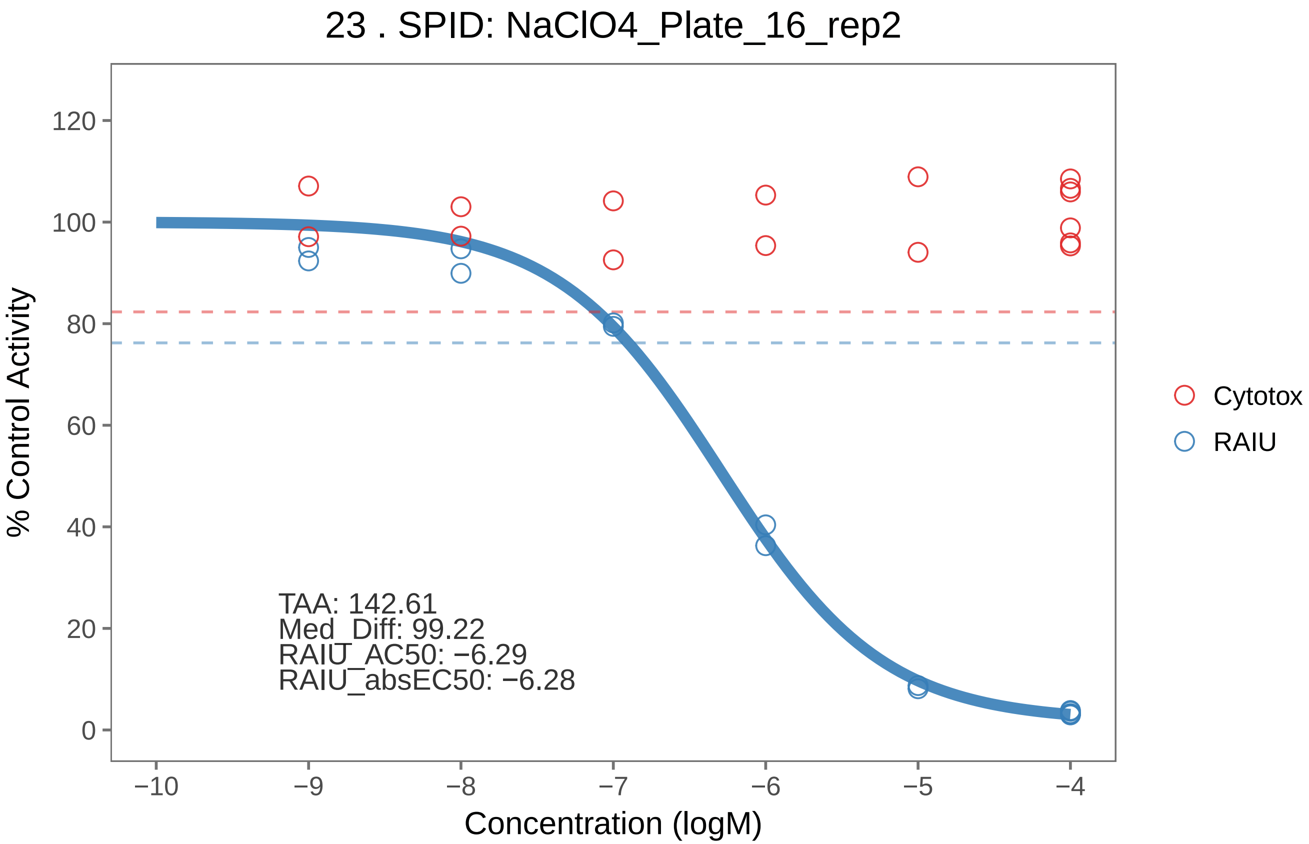

19 . SPID: NaClO4_Plate_15_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 151.04
Med_Diff: 96.64
RAIU_AC50: −6.42
RAIU_absEC50: −6.4
Cytotox
RAIU

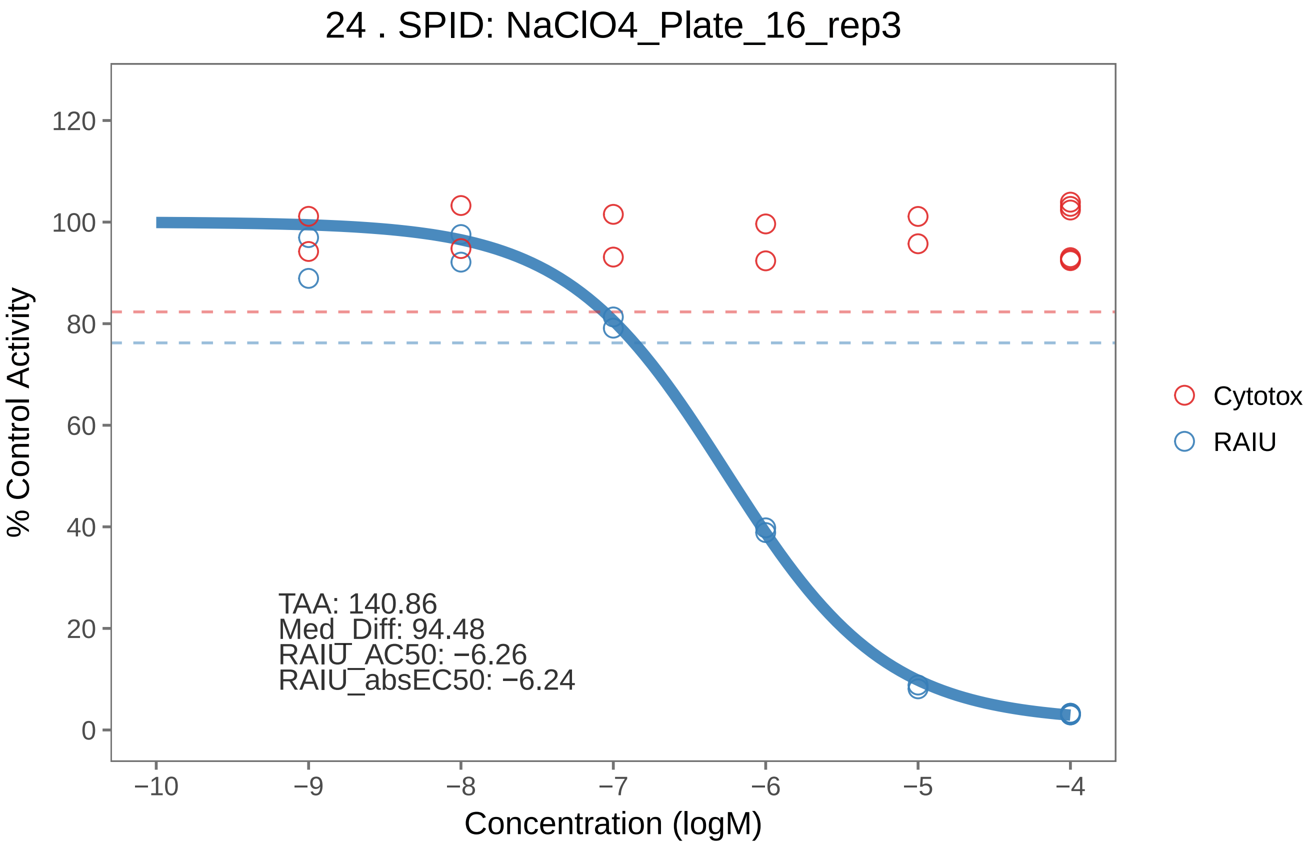

20 . SPID: NaClO4_Plate_15_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 139.71
Med_Diff: 96.29
RAIU_AC50: −6.26
RAIU_absEC50: −6.24
Cytotox
RAIU

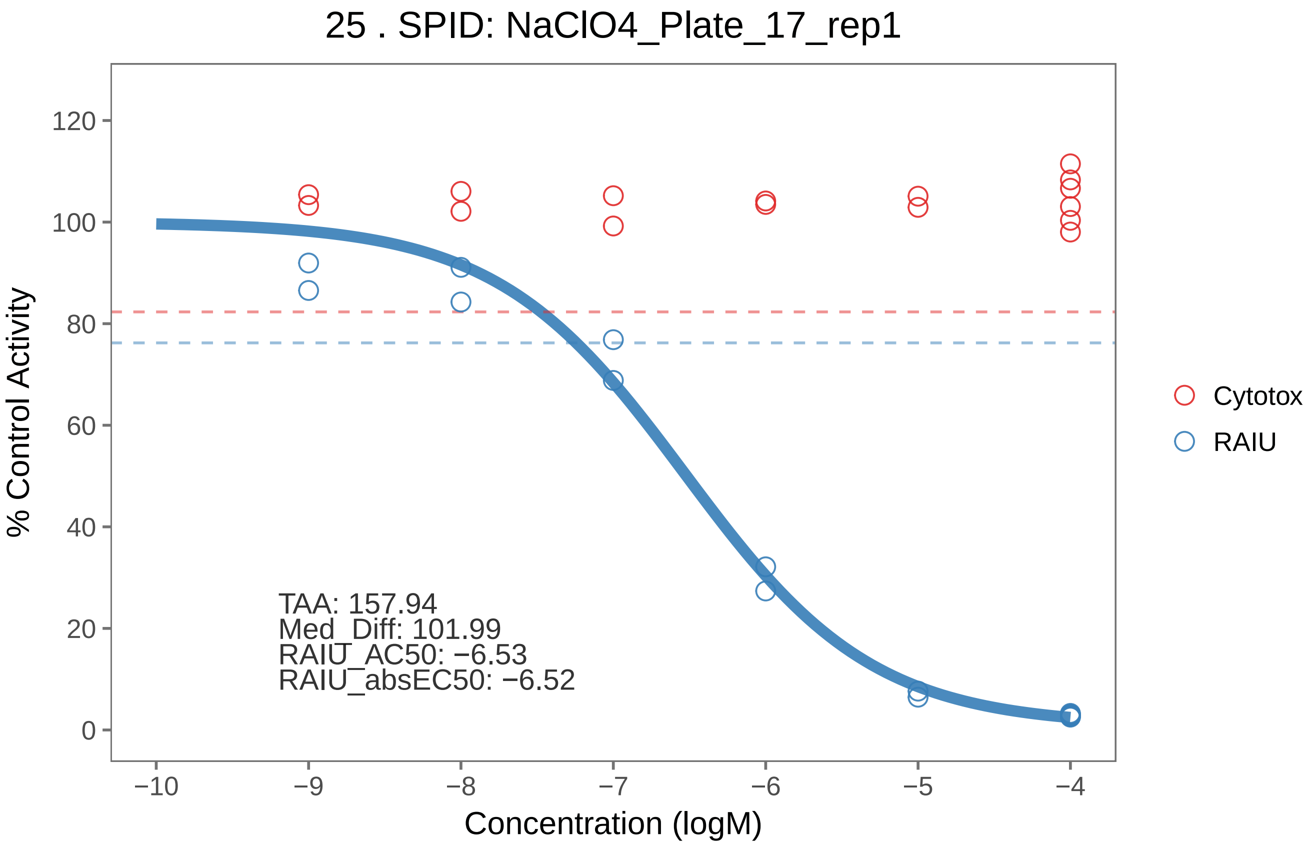

21 . SPID: NaClO4_Plate_15_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 142.75
Med_Diff: 94.31
RAIU_AC50: −6.31
RAIU_absEC50: −6.29

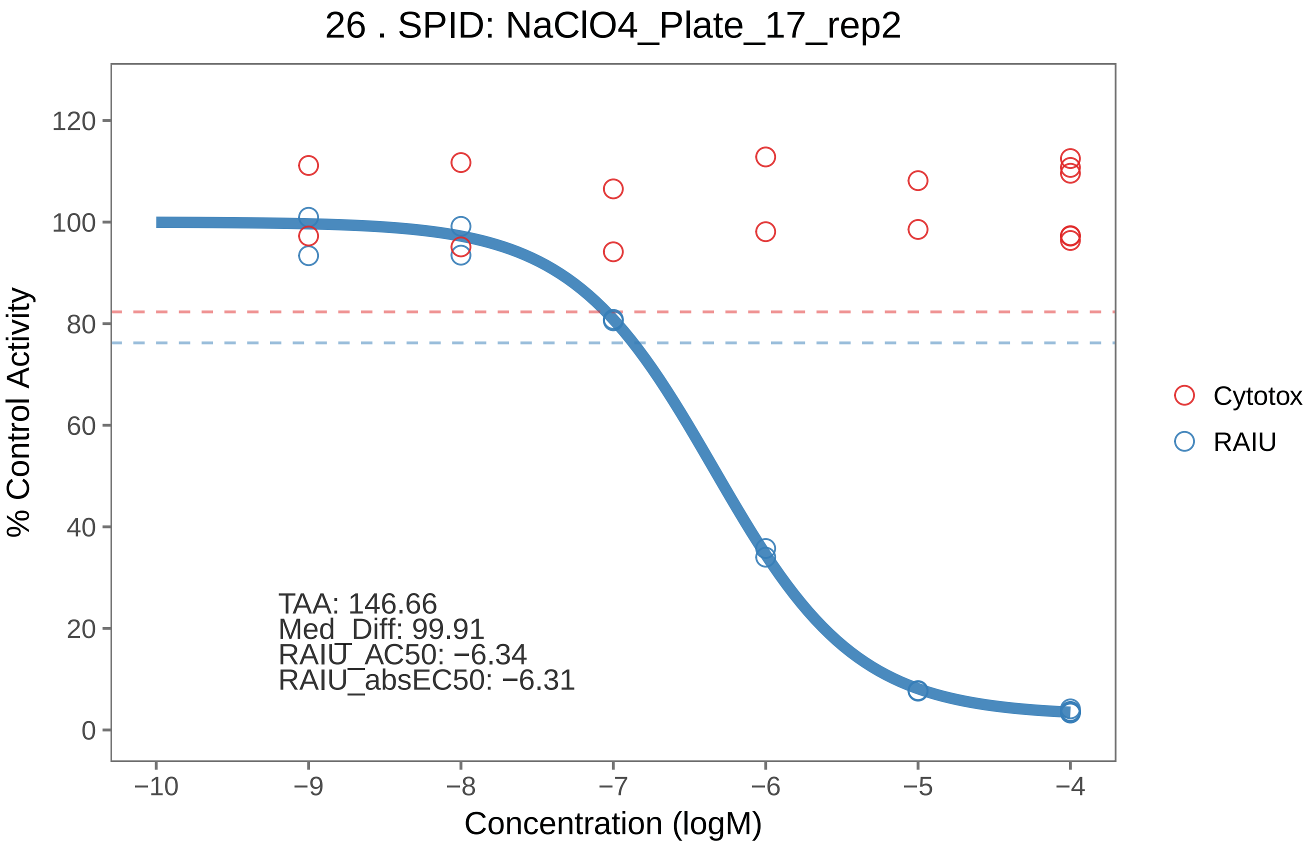


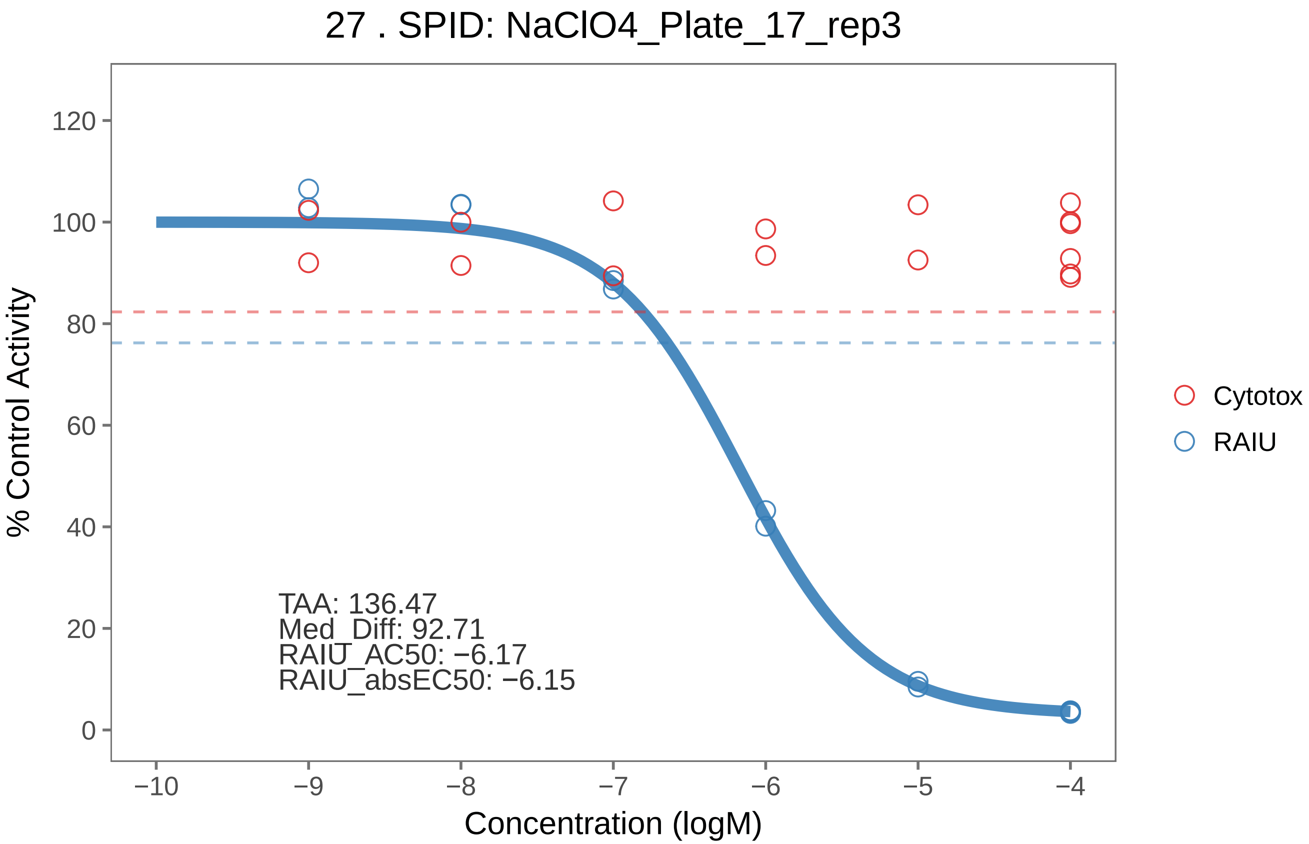
22 . SPID: NaClO4_Plate_16_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 154.63
Med_Diff: 98.19
RAIU_AC50: −6.45
RAIU_absEC50: −6.43
Cytotox
RAIU

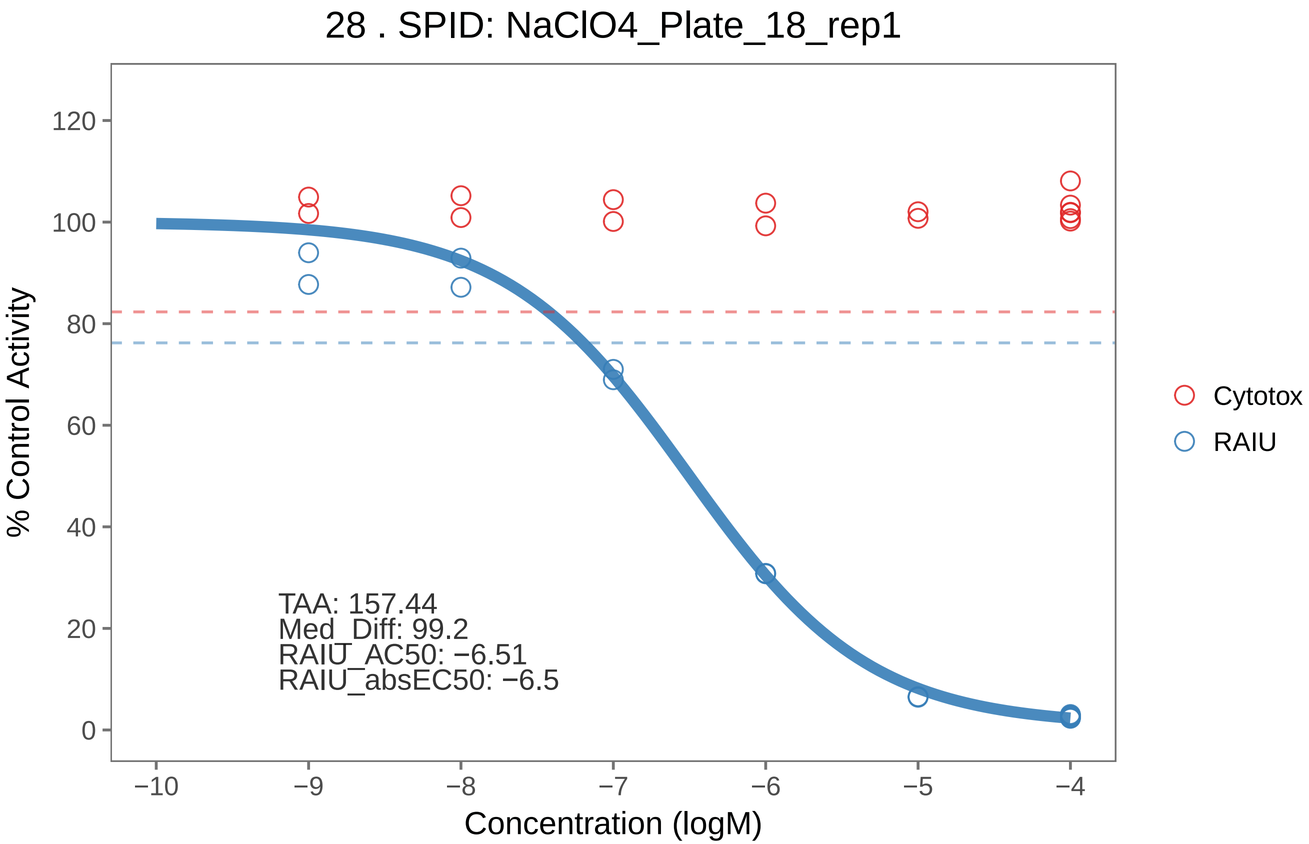

23 . SPID: NaClO4_Plate_16_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 142.61
Med_Diff: 99.22
RAIU_AC50: −6.29
RAIU_absEC50: −6.28

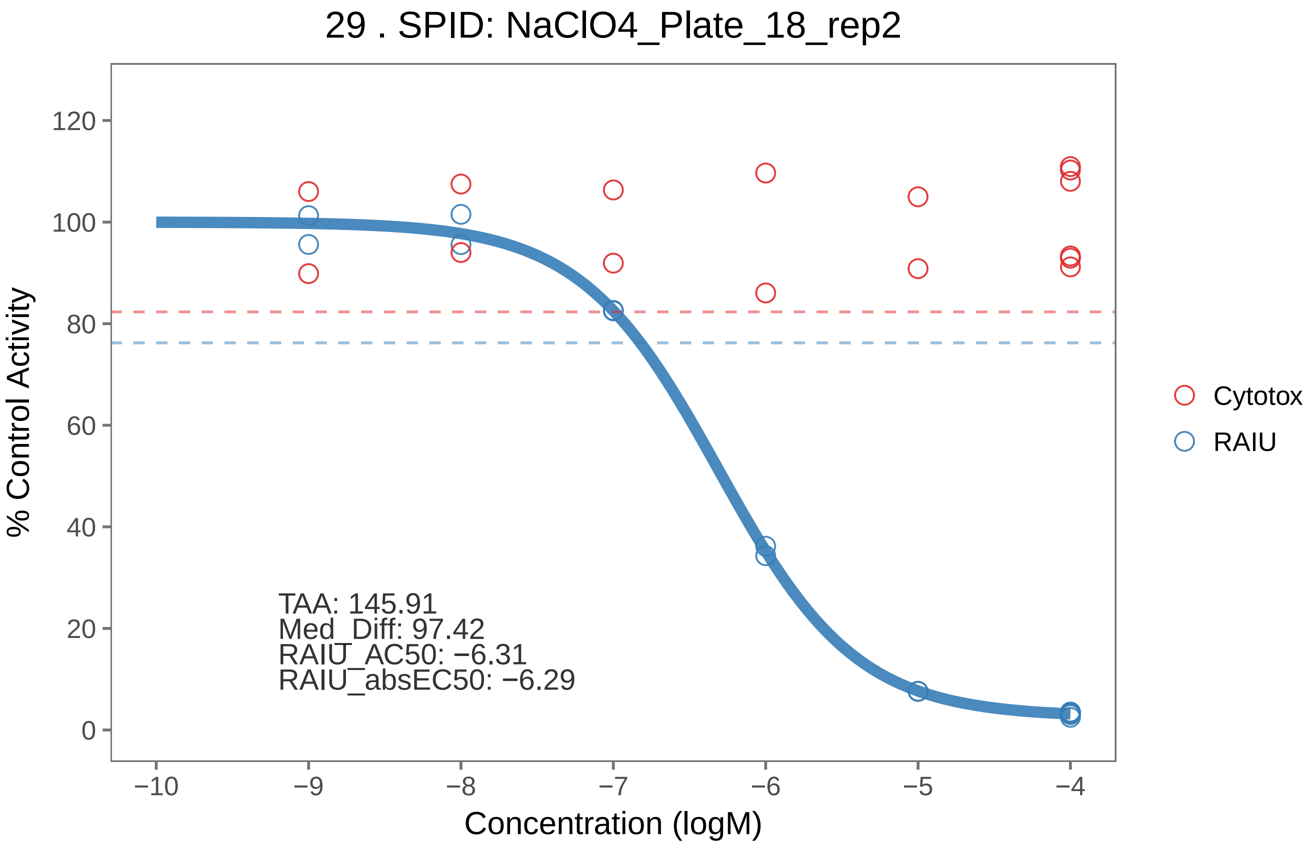

24 . SPID: NaClO4_Plate_16_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 140.86
Med_Diff: 94.48
RAIU_AC50: −6.26
RAIU_absEC50: −6.24
Cytotox
RAIU

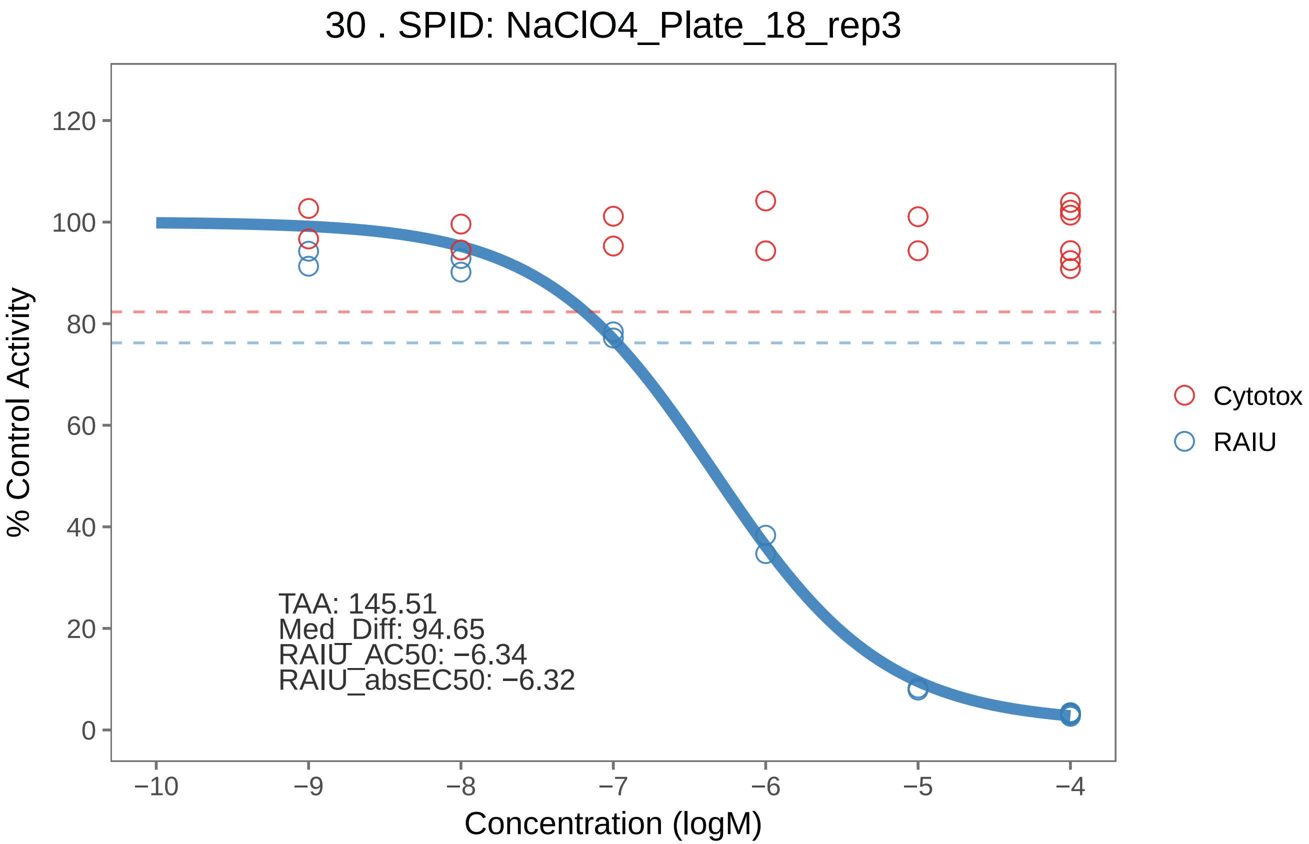

25 . SPID: NaClO4_Plate_17_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 157.94
Med_Diff: 101.99
RAIU_AC50: −6.53
RAIU_absEC50: −6.52
Cytotox
RAIU

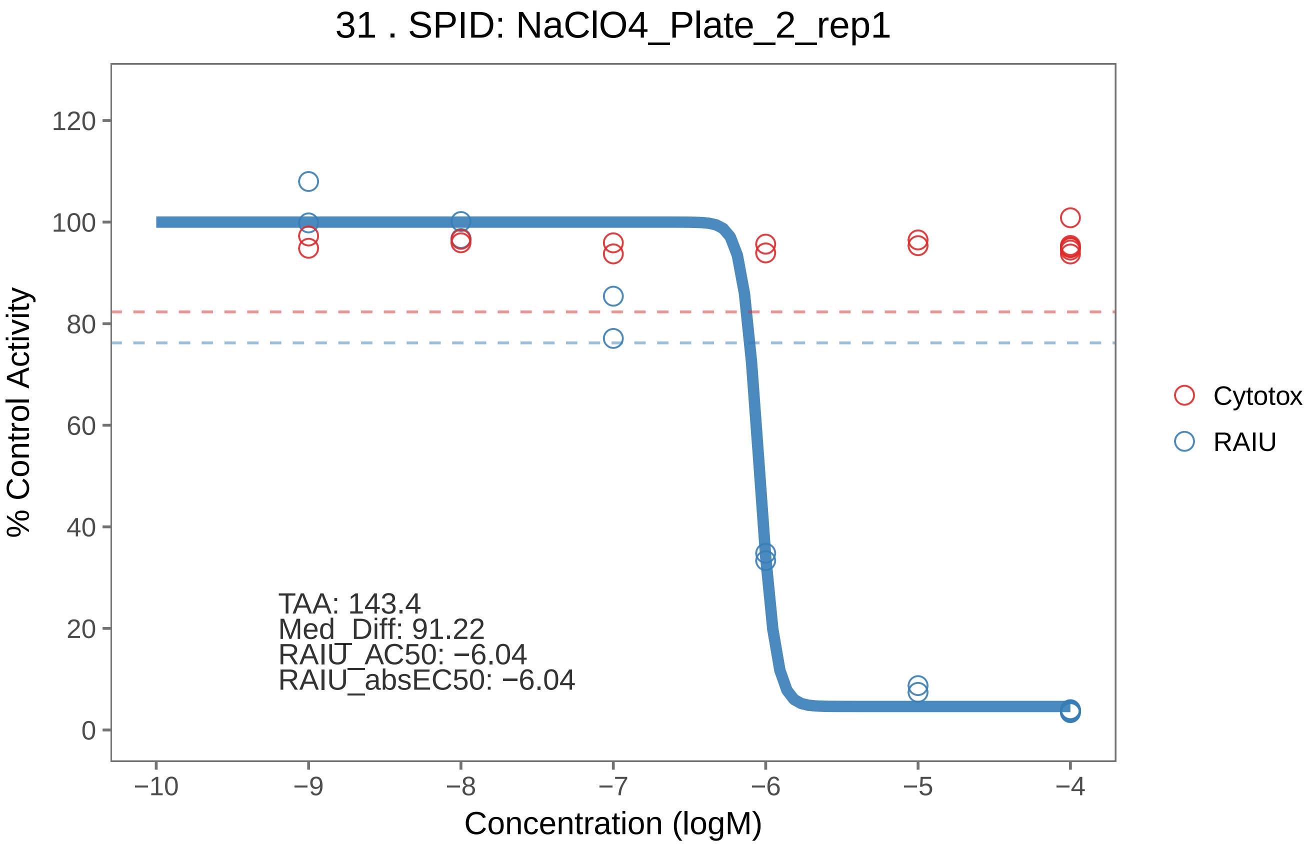

26 . SPID: NaClO4_Plate_17_rep2
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
TAA: 146.66
Med_Diff: 99.91
RAIU_AC50: −6.34
RAIU_absEC50: −6.31
Cytotox
RAIU

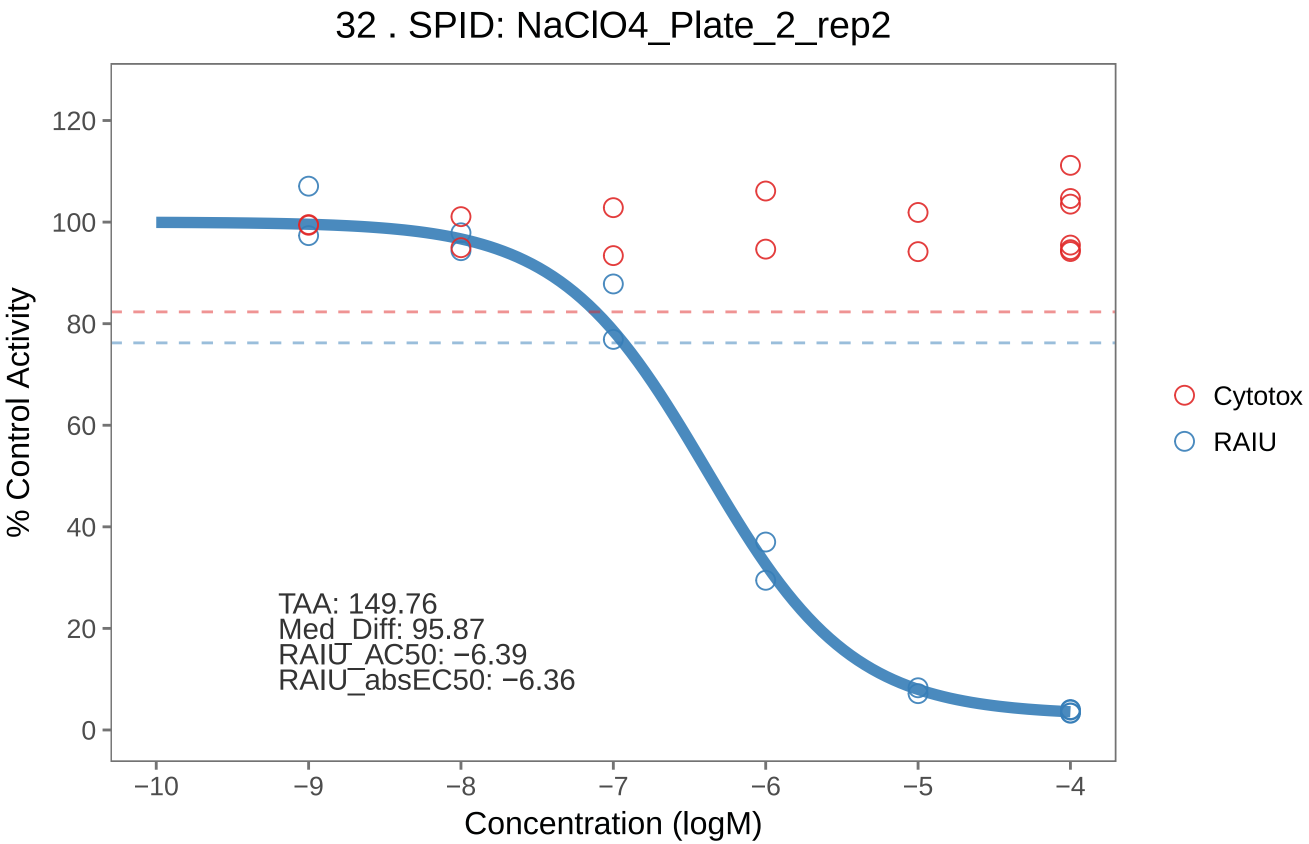

27 . SPID: NaClO4_Plate_17_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 136.47
Med_Diff: 92.71
RAIU_AC50: −6.17
RAIU_absEC50: −6.15

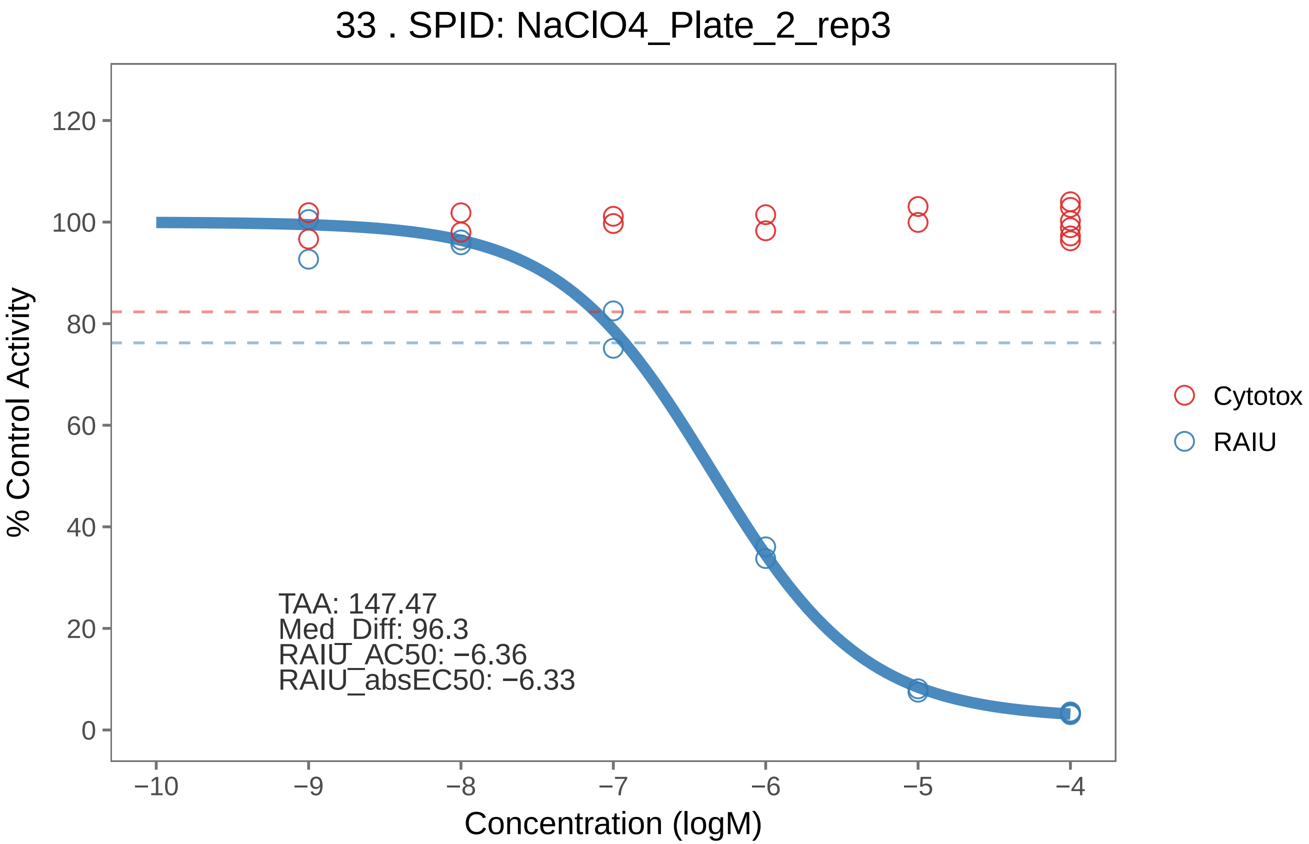

28 . SPID: NaClO4_Plate_18_rep1
120
100
80
60
40
20
0
% Control Activity
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 157.44
Med_Diff: 99.2
RAIU_AC50: −6.51
RAIU_absEC50: −6.5
Cytotox
RAIU

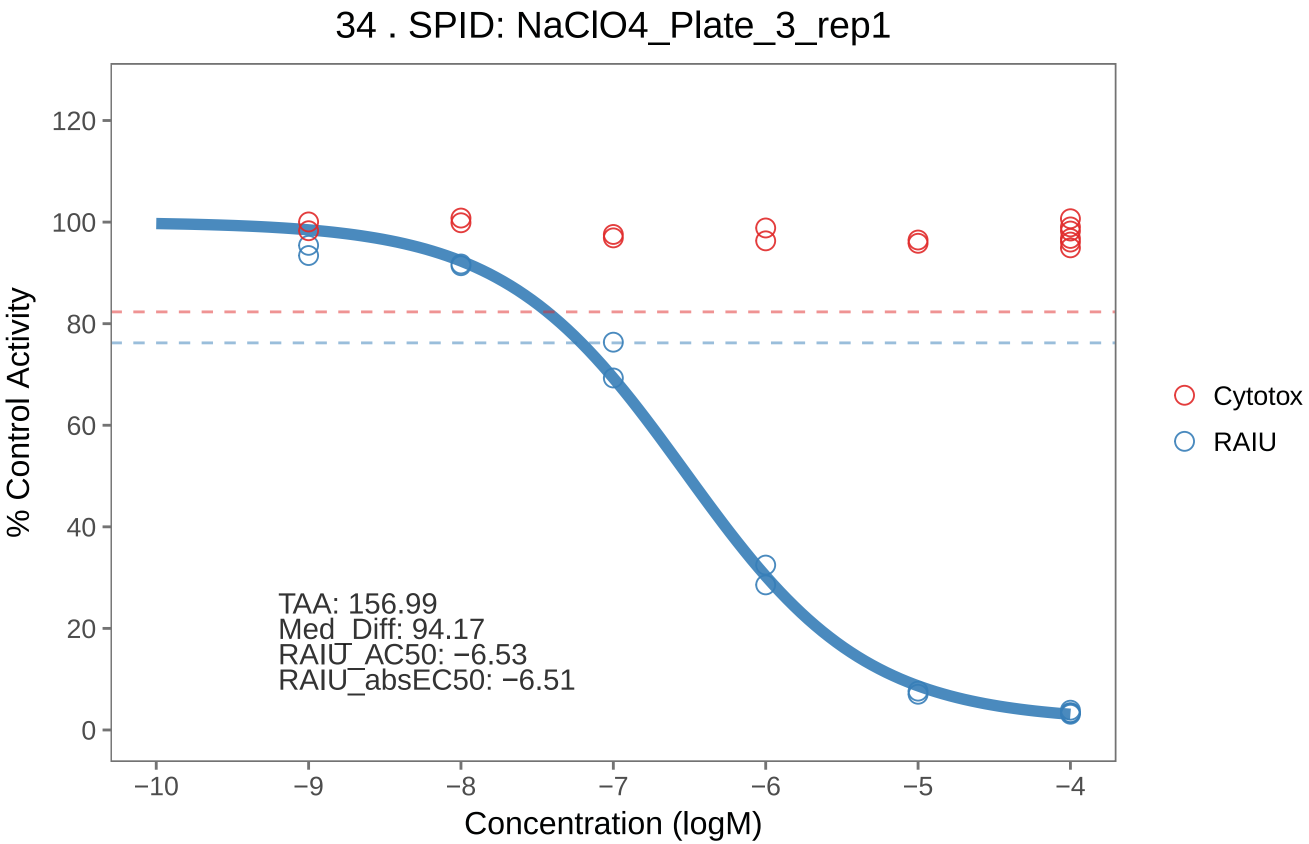

29 . SPID: NaClO4_Plate_18_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 145.91
Med_Diff: 97.42
RAIU_AC50: −6.31
RAIU_absEC50: −6.29
Cytotox
RAIU

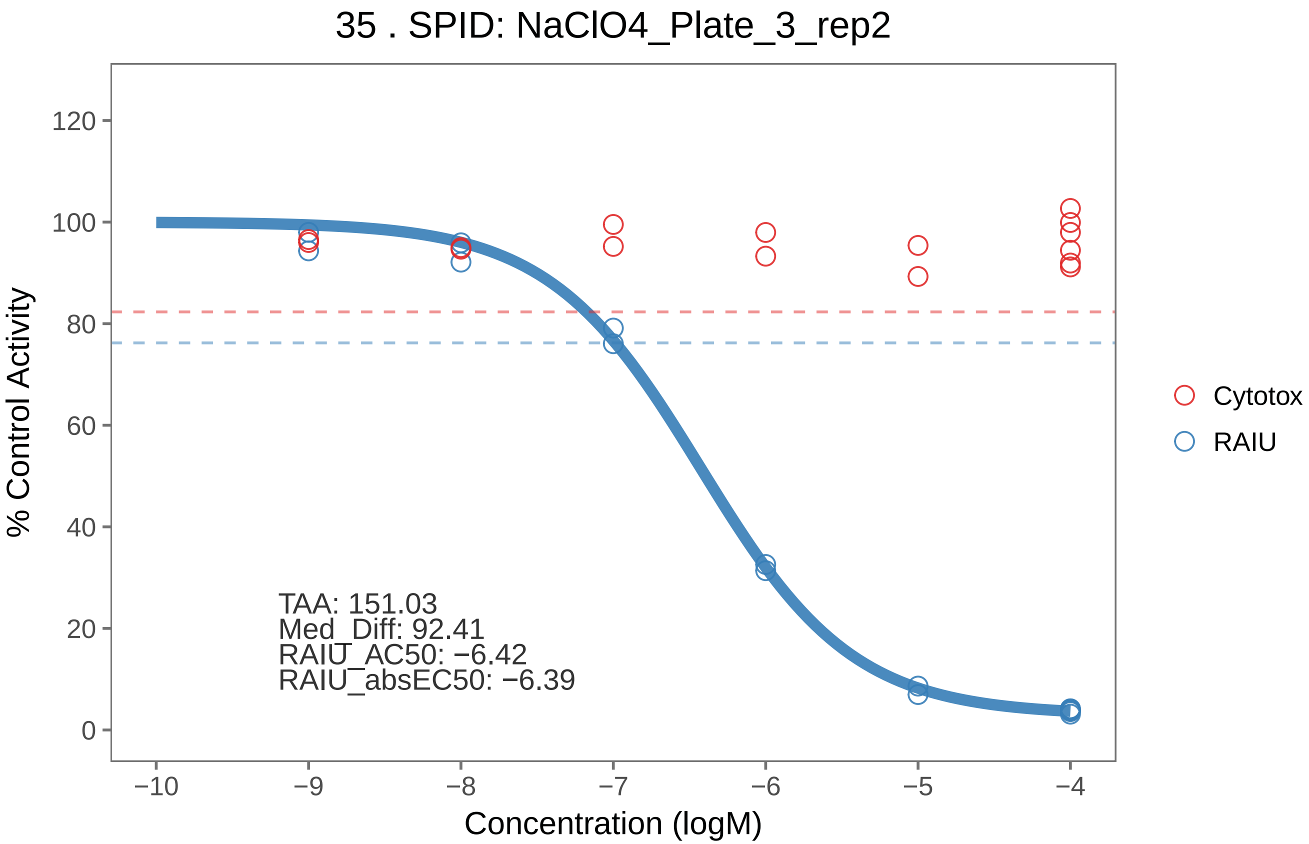

30 . SPID: NaClO4_Plate_18_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 145.51
Med_Diff: 94.65
RAIU_AC50: −6.34
RAIU_absEC50: −6.32
Cytotox
RAIU

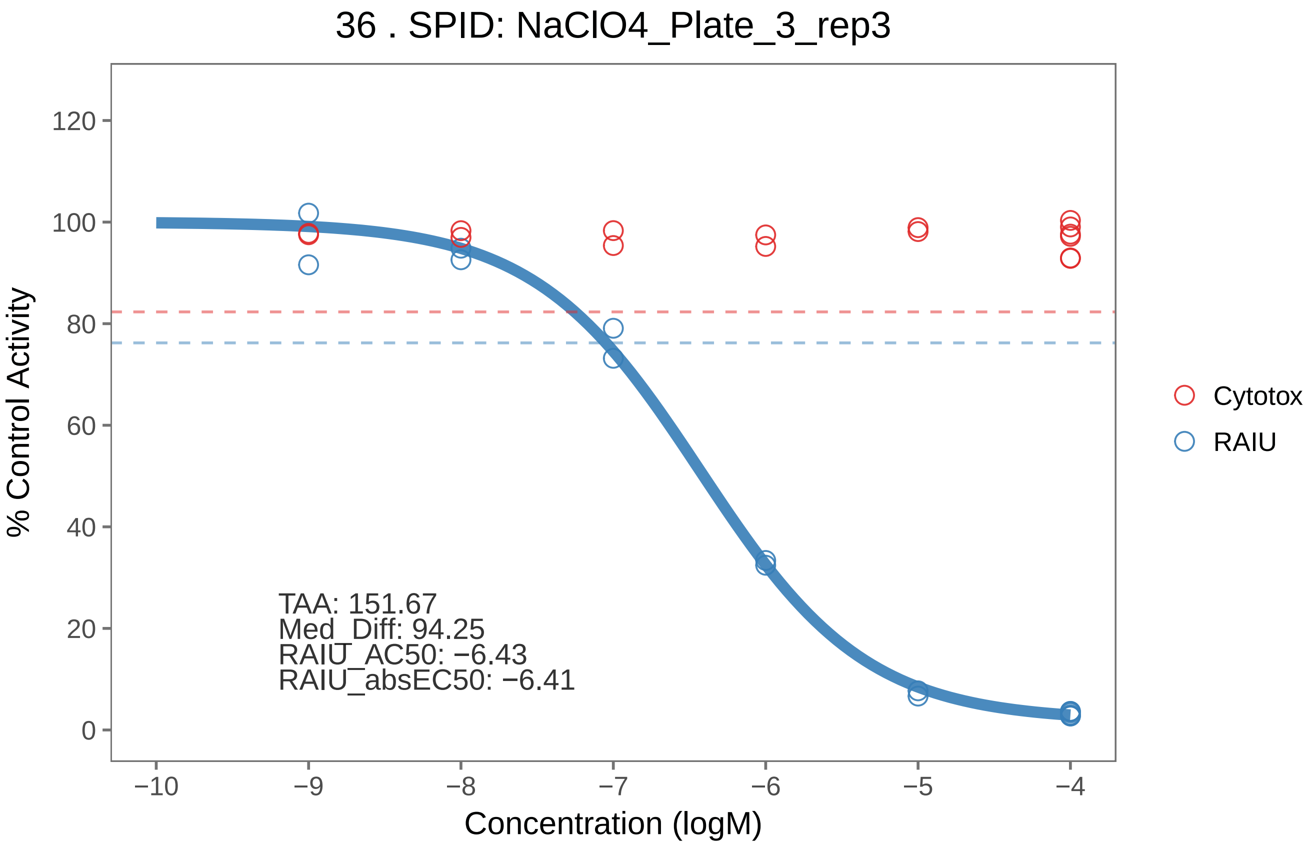

31 . SPID: NaClO4_Plate_2_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 143.4
Med_Diff: 91.22
RAIU_AC50: −6.04
RAIU_absEC50: −6.04

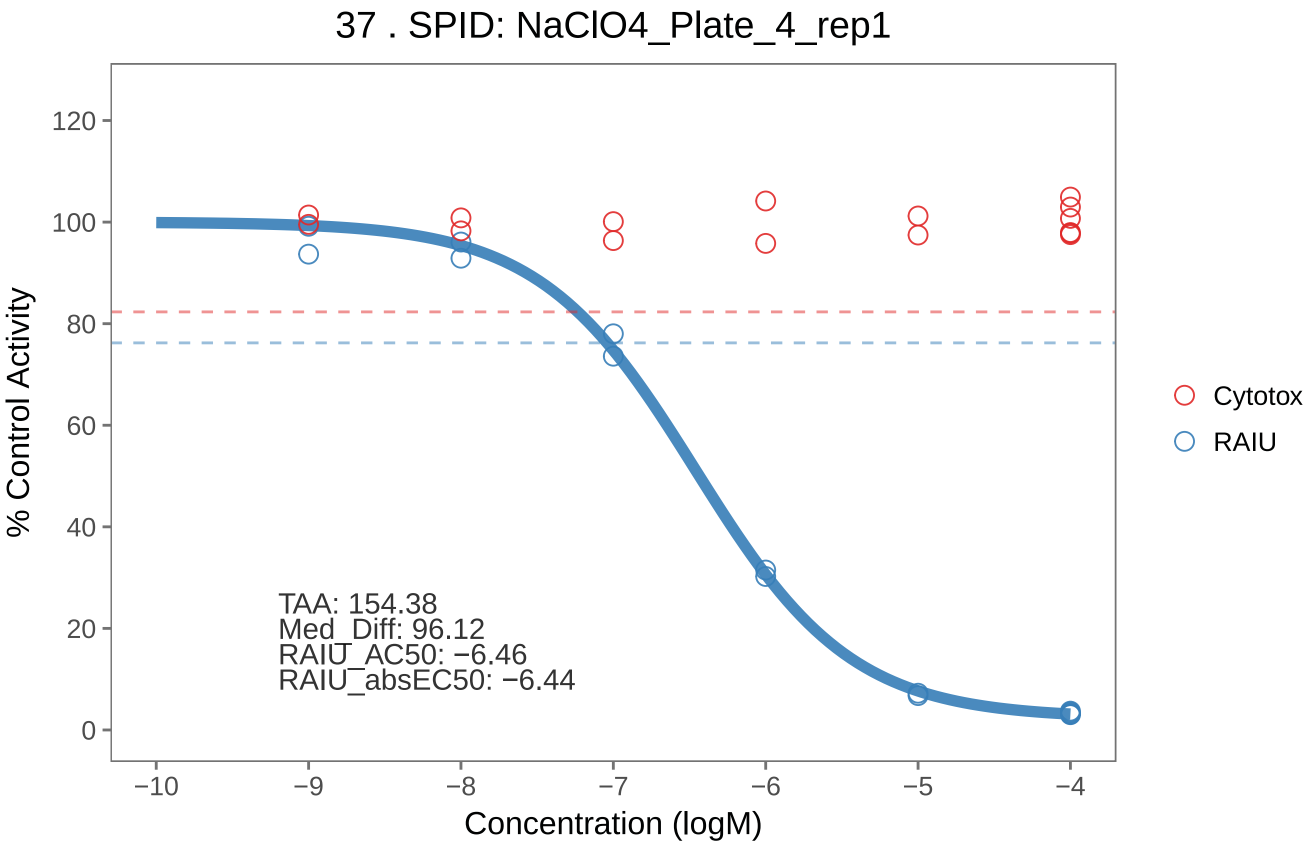

32 . SPID: NaClO4_Plate_2_rep2
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 149.76
Med_Diff: 95.87
RAIU_AC50: −6.39
RAIU_absEC50: −6.36
Cytotox
RAIU


33 . SPID: NaClO4_Plate_2_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 147.47
Med_Diff: 96.3
RAIU_AC50: −6.36
RAIU_absEC50: −6.33
Cytotox
RAIU

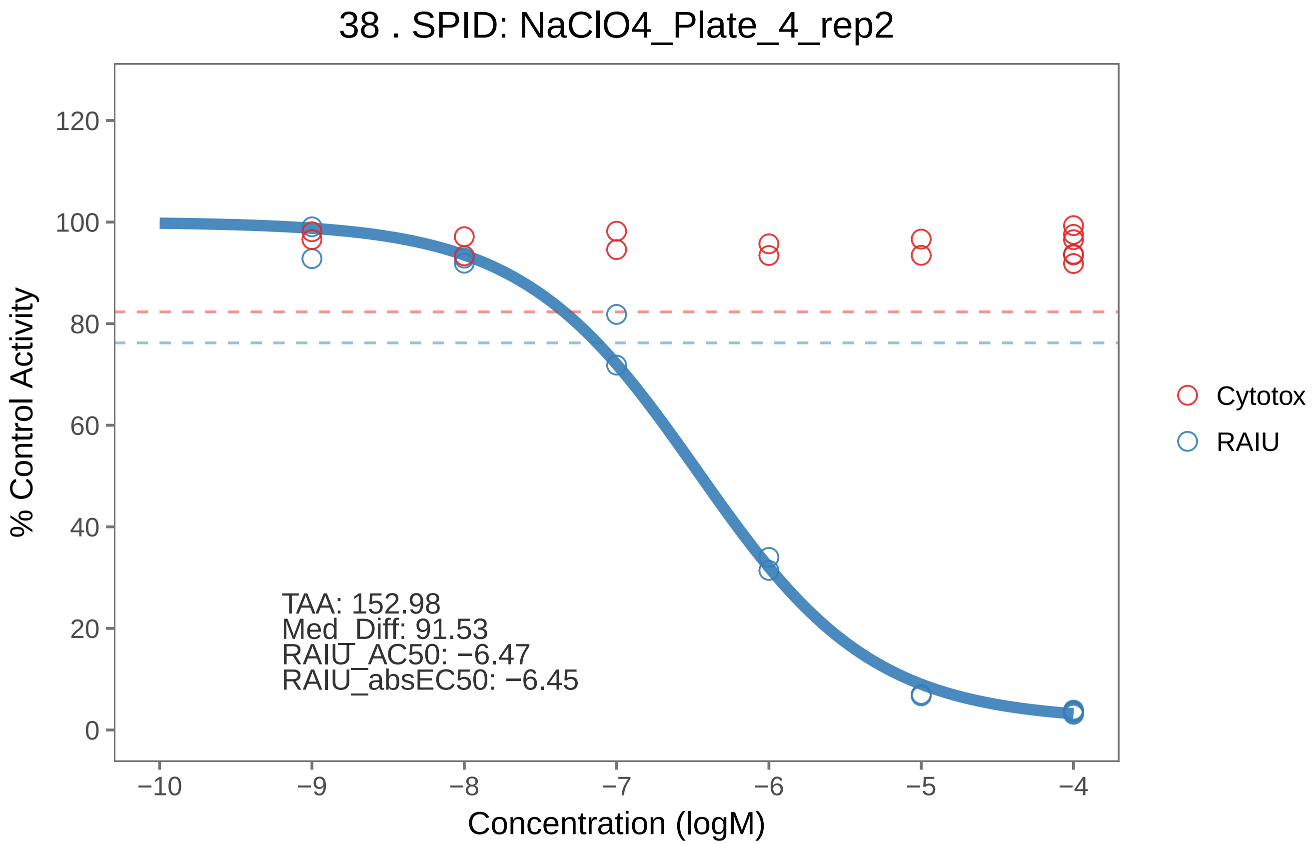

34 . SPID: NaClO4_Plate_3_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 156.99
Med_Diff: 94.17
RAIU_AC50: −6.53
RAIU_absEC50: −6.51
Cytotox
RAIU

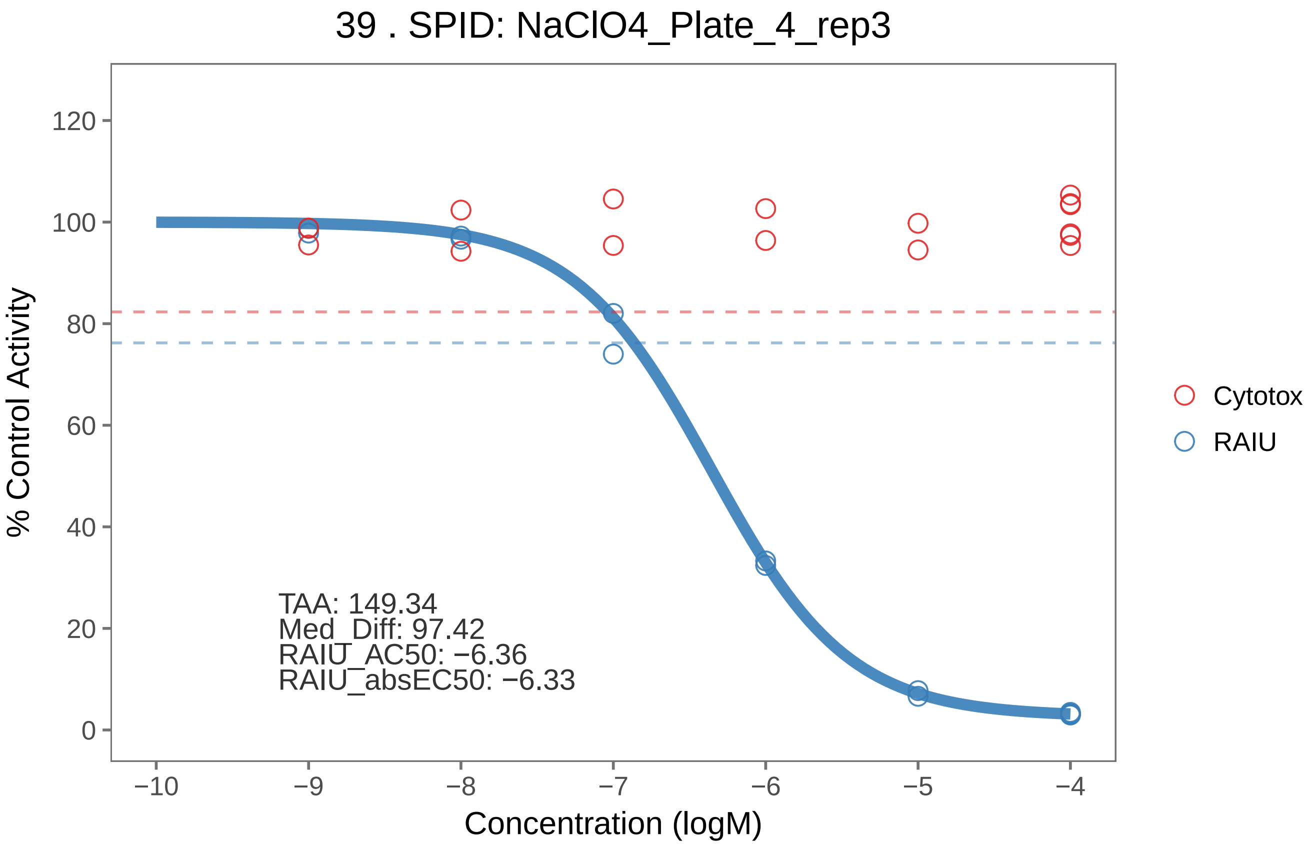

35 . SPID: NaClO4_Plate_3_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 151.03
Med_Diff: 92.41
RAIU_AC50: −6.42
RAIU_absEC50: −6.39

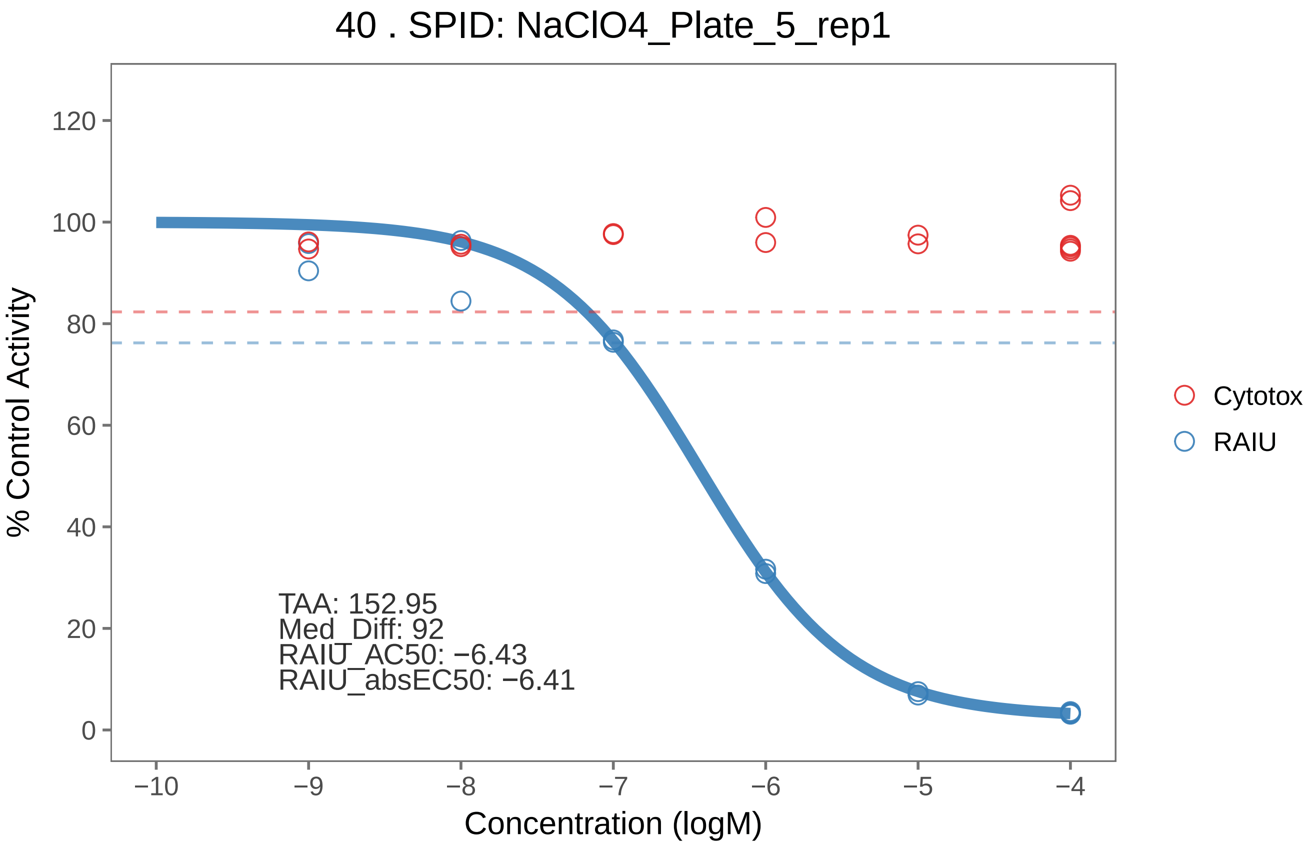

36 . SPID: NaClO4_Plate_3_rep3
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 151.67
Med_Diff: 94.25
RAIU_AC50: −6.43
RAIU_absEC50: −6.41



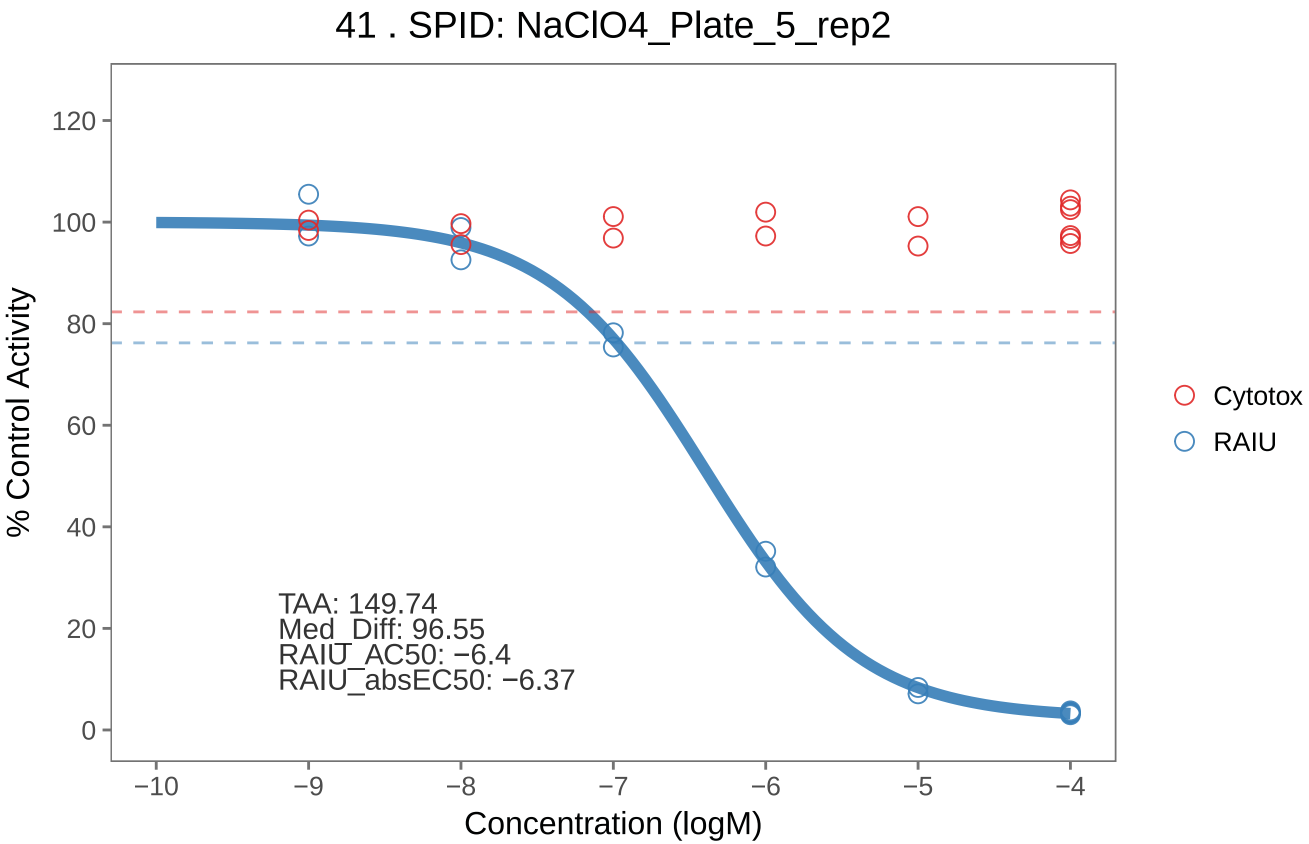
37 . SPID: NaClO4_Plate_4_rep1
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
TAA: 154.38
Med_Diff: 96.12
RAIU_AC50: −6.46
RAIU_absEC50: −6.44
Cytotox
RAIU

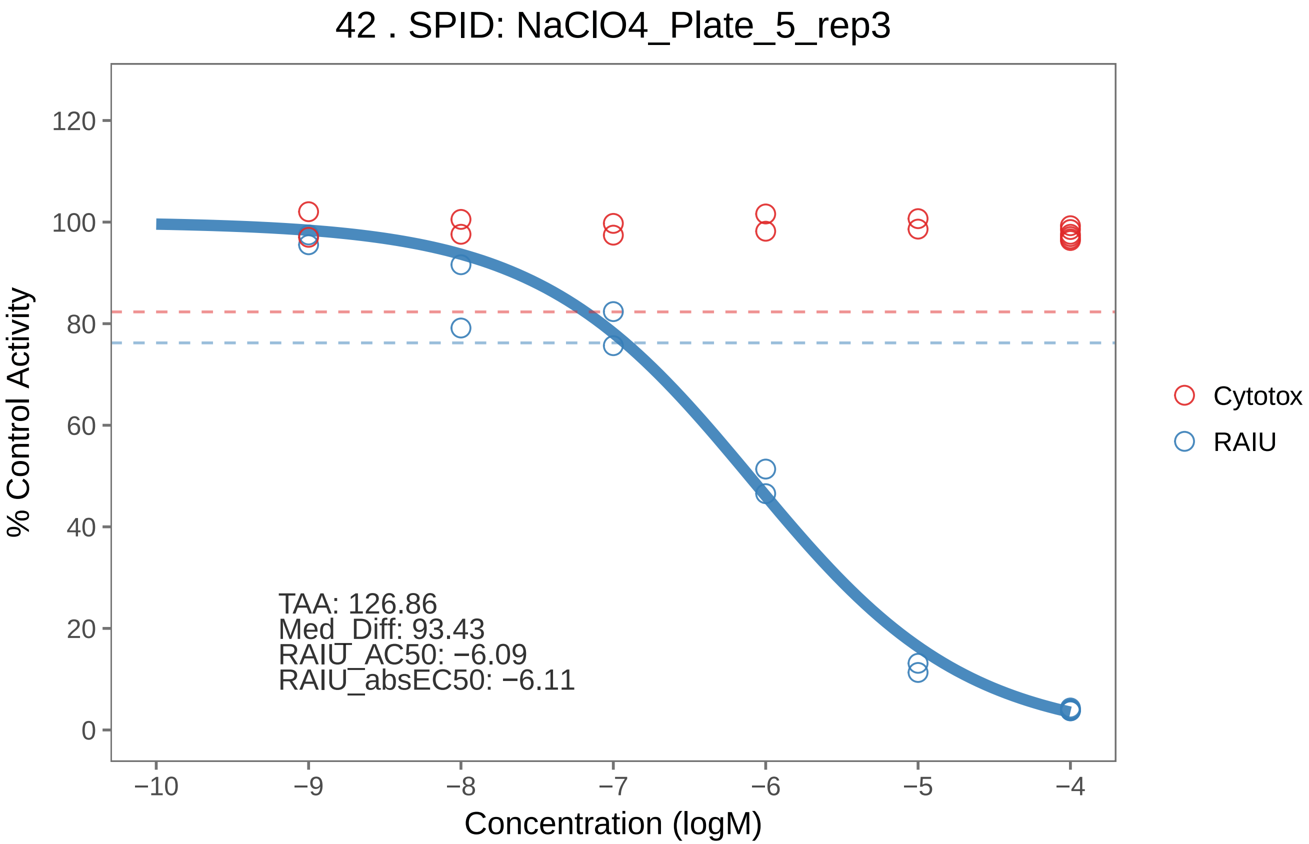

38 . SPID: NaClO4_Plate_4_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 152.98
Med_Diff: 91.53
RAIU_AC50: −6.47
RAIU_absEC50: −6.45
Cytotox
RAIU

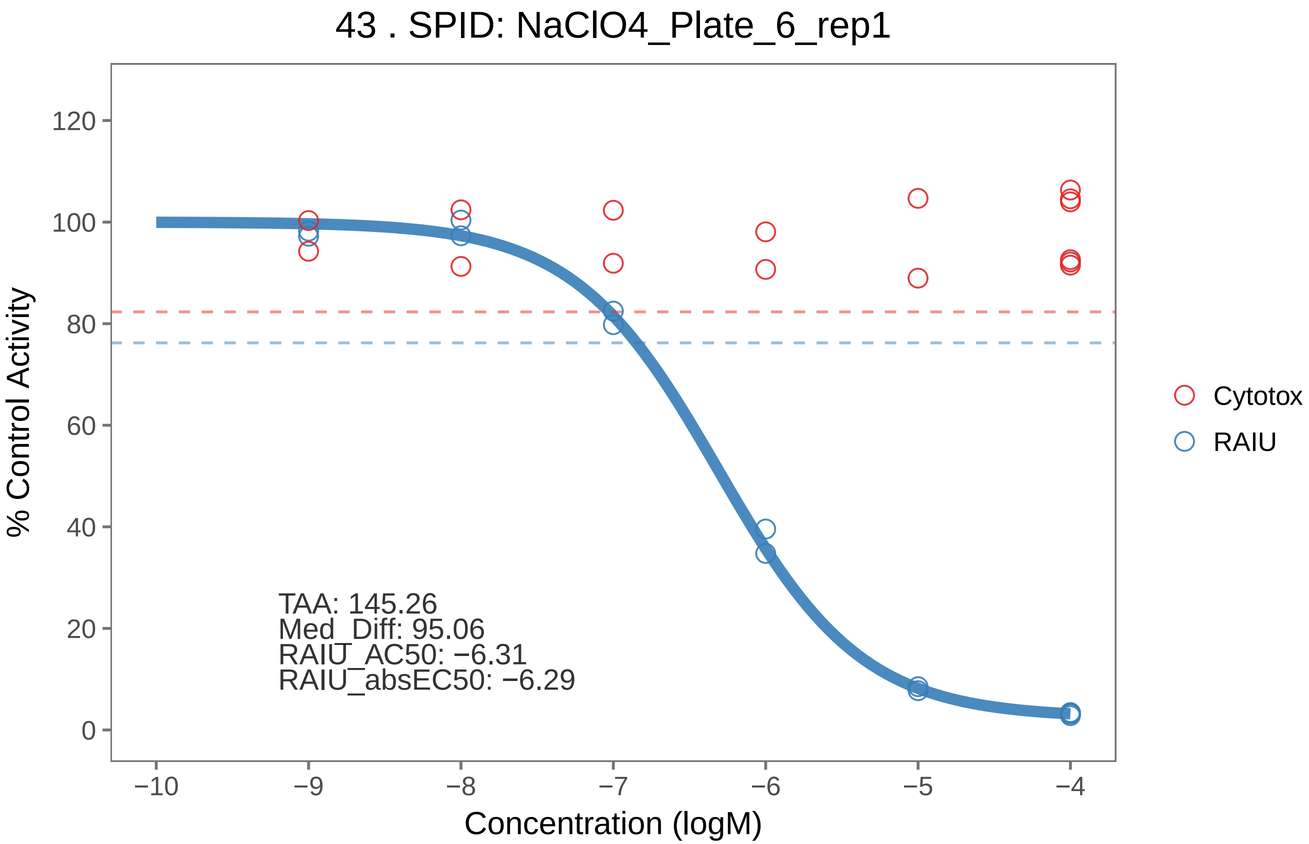

39 . SPID: NaClO4_Plate_4_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 149.34
Med_Diff: 97.42
RAIU_AC50: −6.36
RAIU_absEC50: −6.33
Cytotox
RAIU

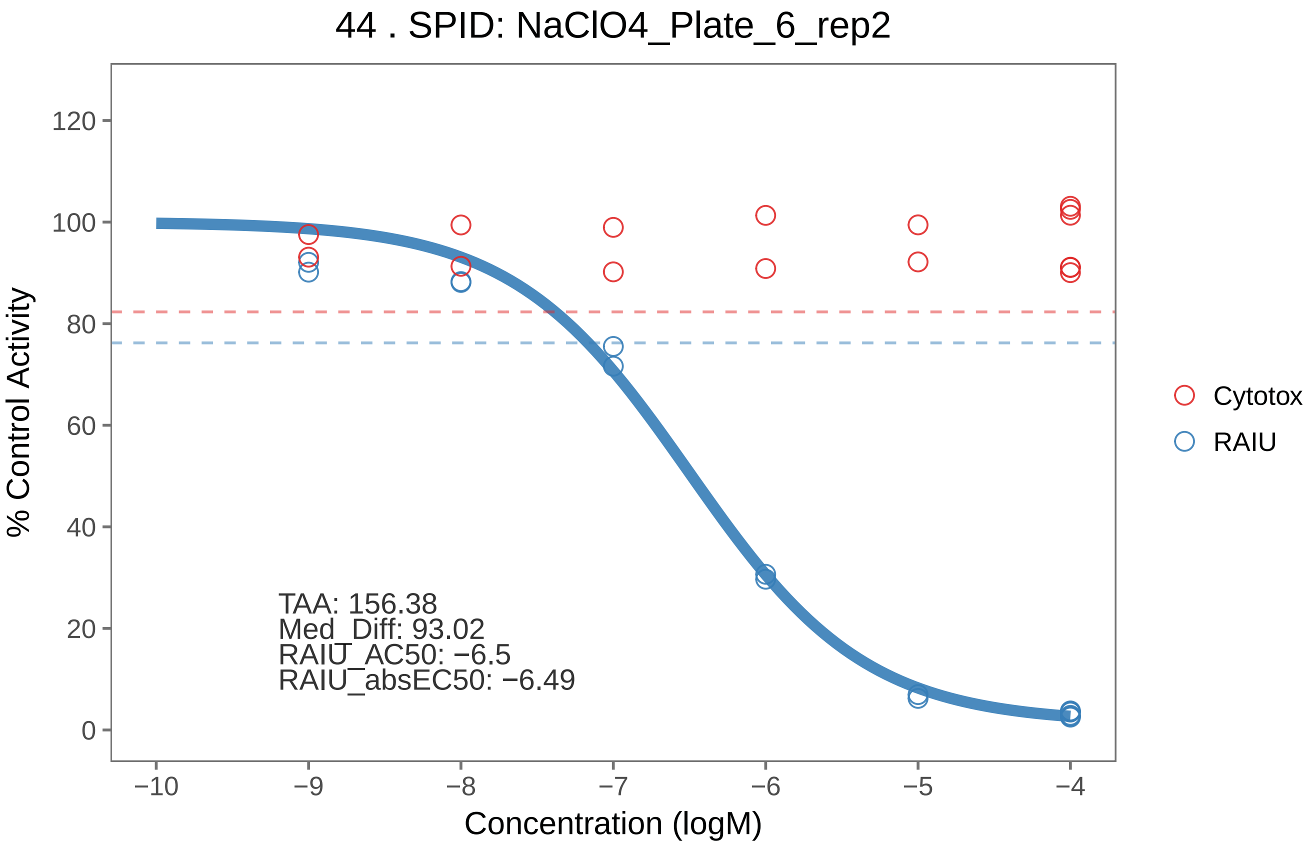


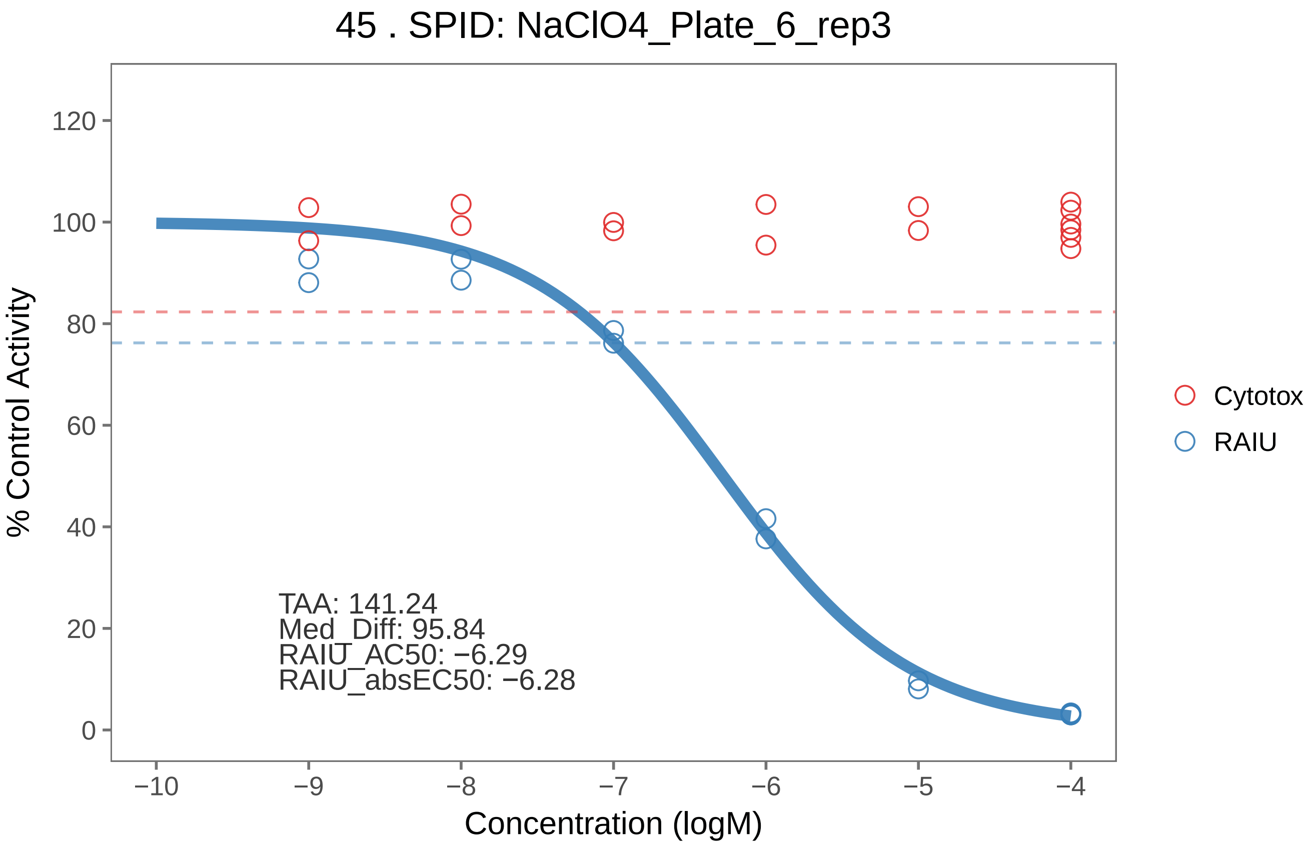
40 . SPID: NaClO4_Plate_5_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 152.95
Med_Diff: 92
RAIU_AC50: −6.43
RAIU_absEC50: −6.41

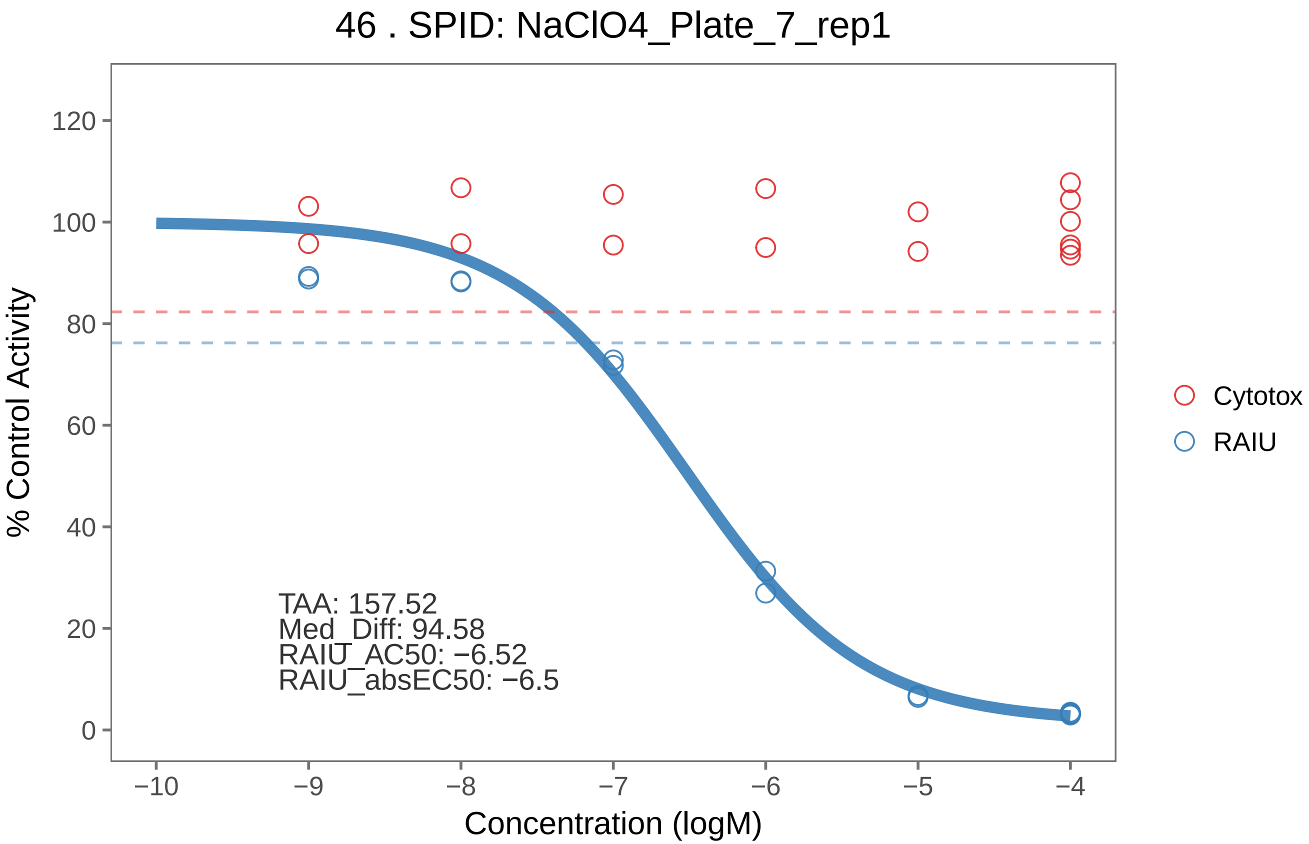

41 . SPID: NaClO4_Plate_5_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 149.74
Med_Diff: 96.55
RAIU_AC50: −6.4
RAIU_absEC50: −6.37

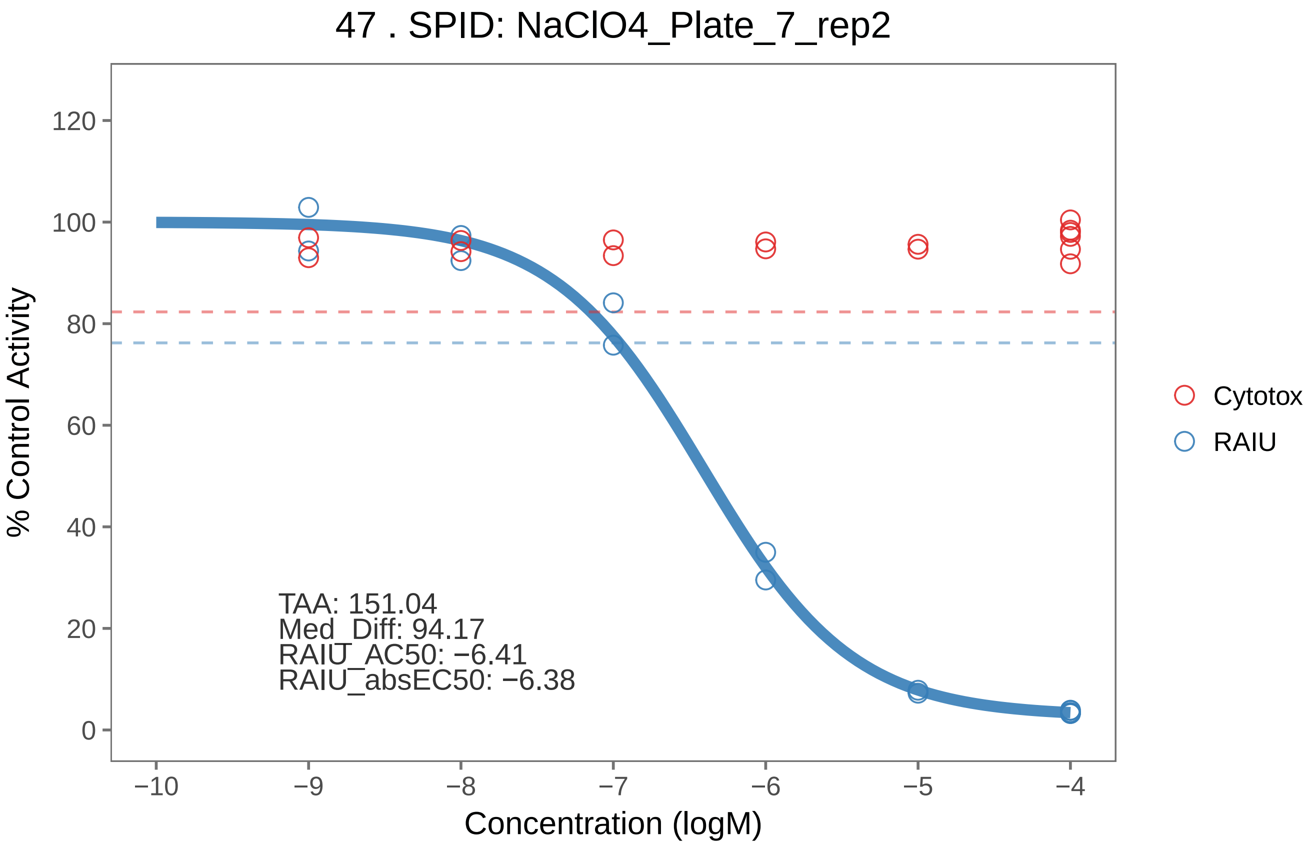

42 . SPID: NaClO4_Plate_5_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 126.86
Med_Diff: 93.43
RAIU_AC50: −6.09
RAIU_absEC50: −6.11
Cytotox
RAIU

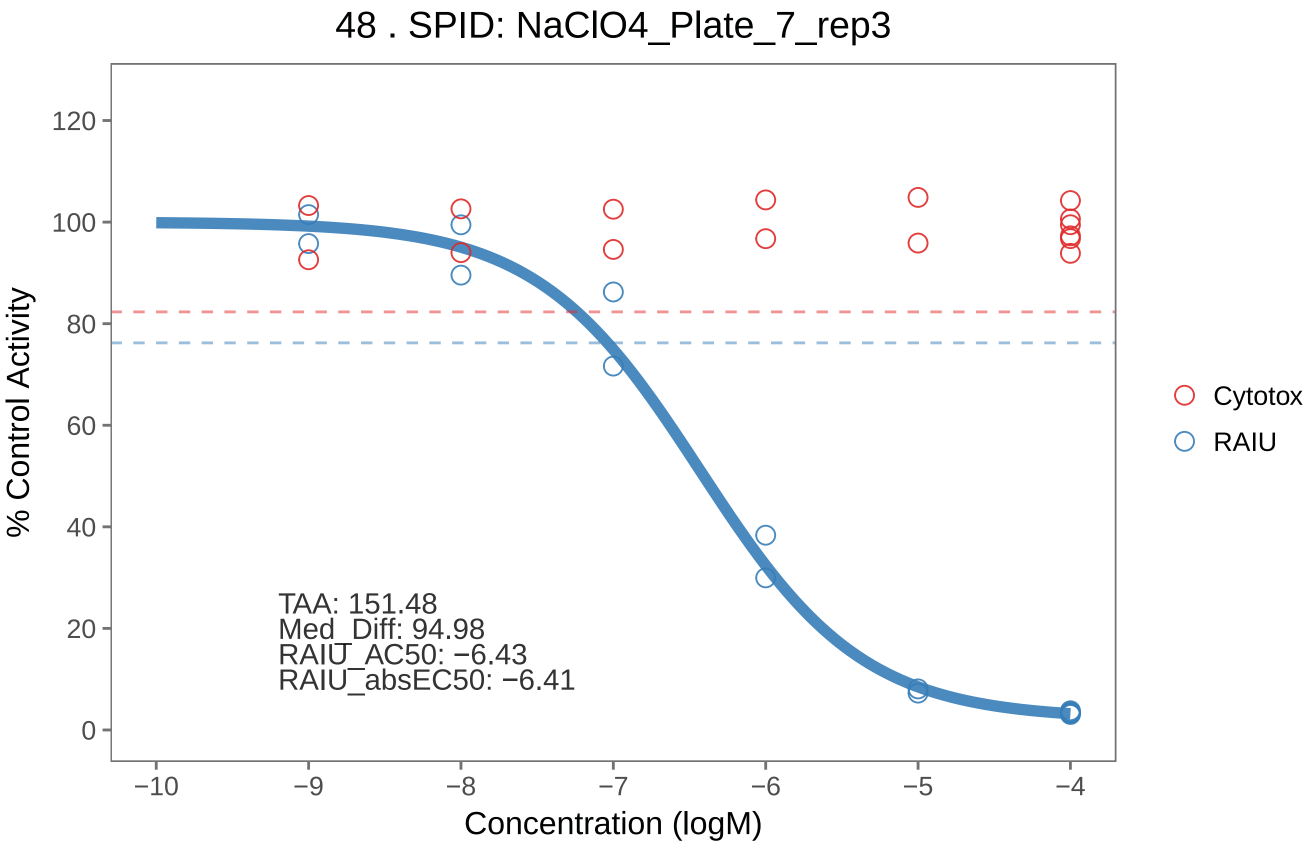

43 . SPID: NaClO4_Plate_6_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 145.26
Med_Diff: 95.06
RAIU_AC50: −6.31
RAIU_absEC50: −6.29
Cytotox
RAIU

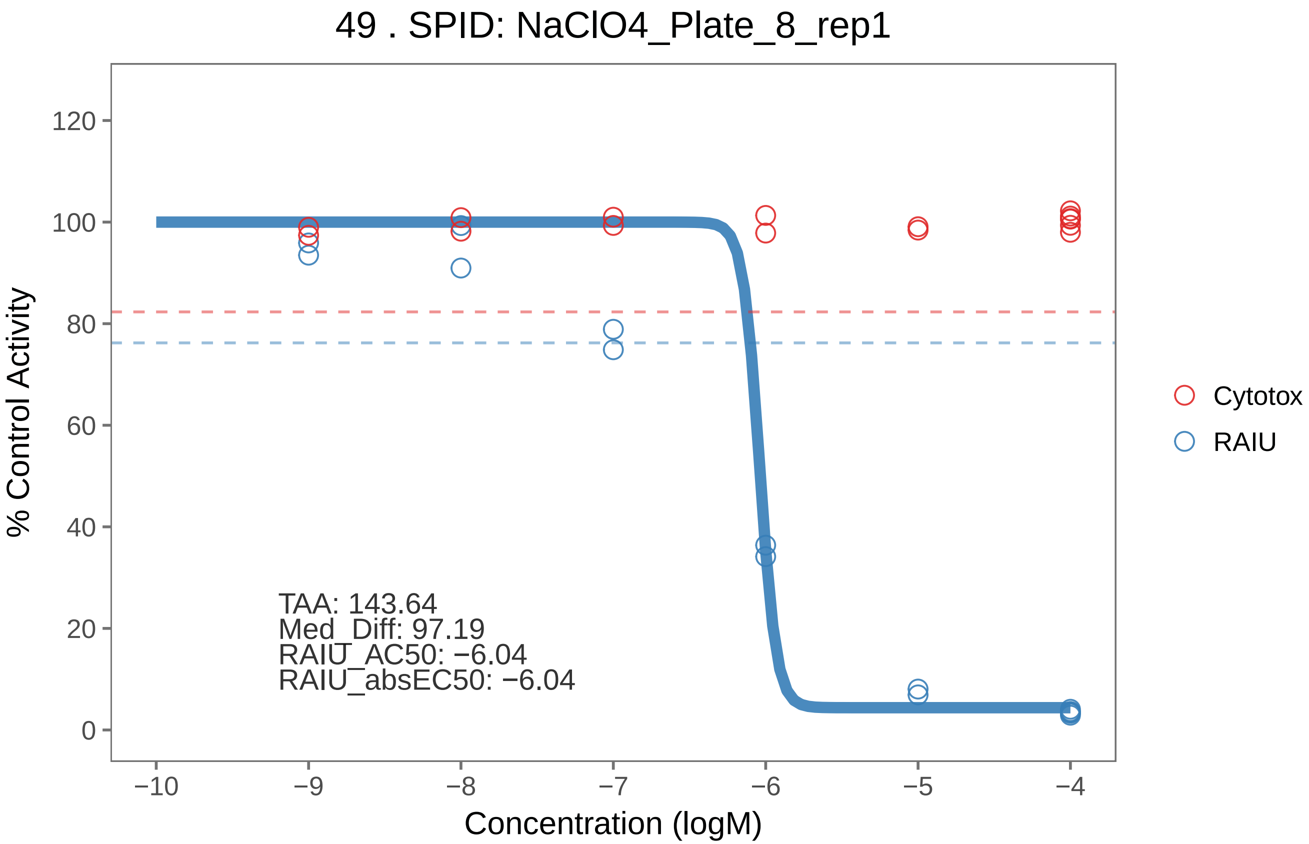

44 . SPID: NaClO4_Plate_6_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 156.38
Med_Diff: 93.02
RAIU_AC50: −6.5
RAIU_absEC50: −6.49
Cytotox
RAIU

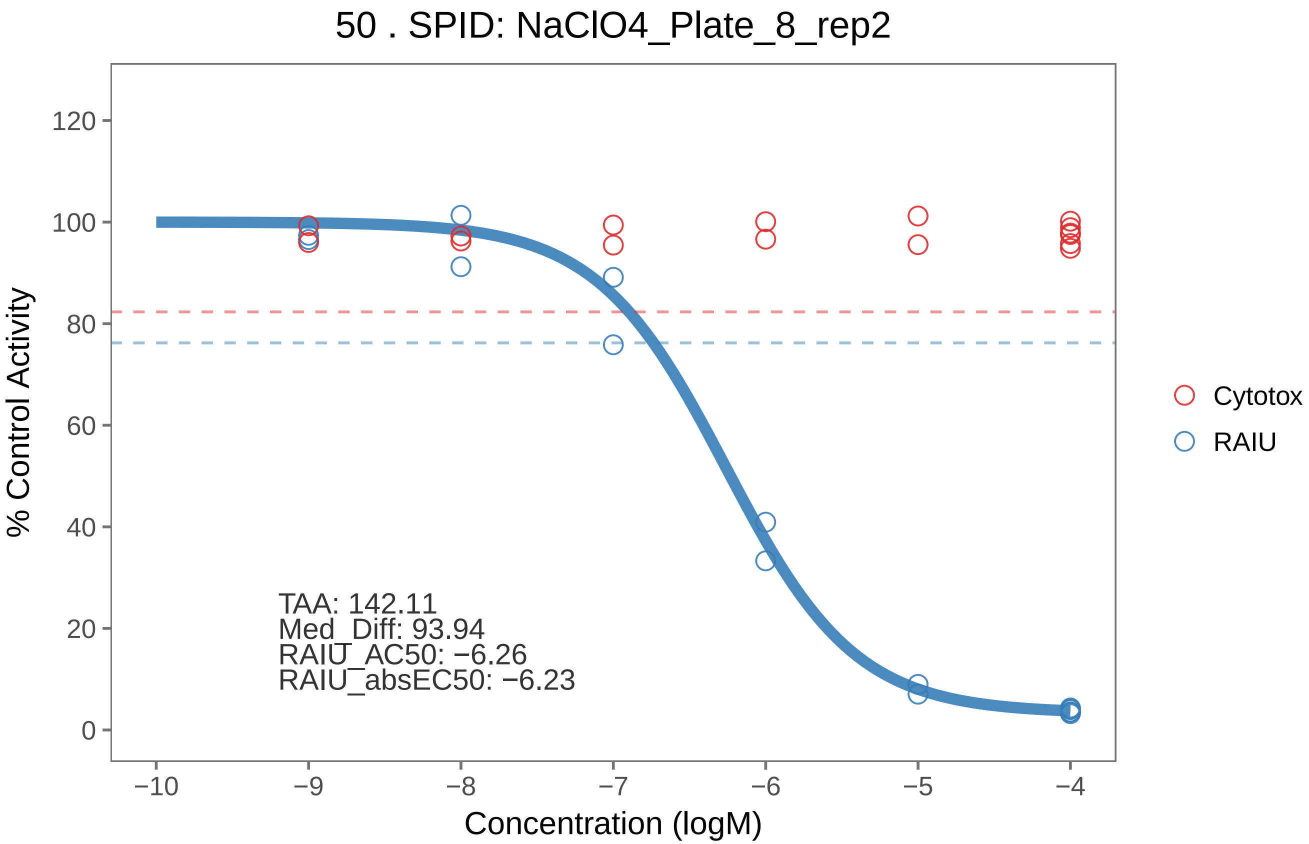

45 . SPID: NaClO4_Plate_6_rep3
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Cytotox
RAIU
TAA: 141.24
Med_Diff: 95.84
RAIU_AC50: −6.29
RAIU_absEC50: −6.28


46 . SPID: NaClO4_Plate_7_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 157.52
Med_Diff: 94.58
RAIU_AC50: −6.52
RAIU_absEC50: −6.5
Cytotox
RAIU

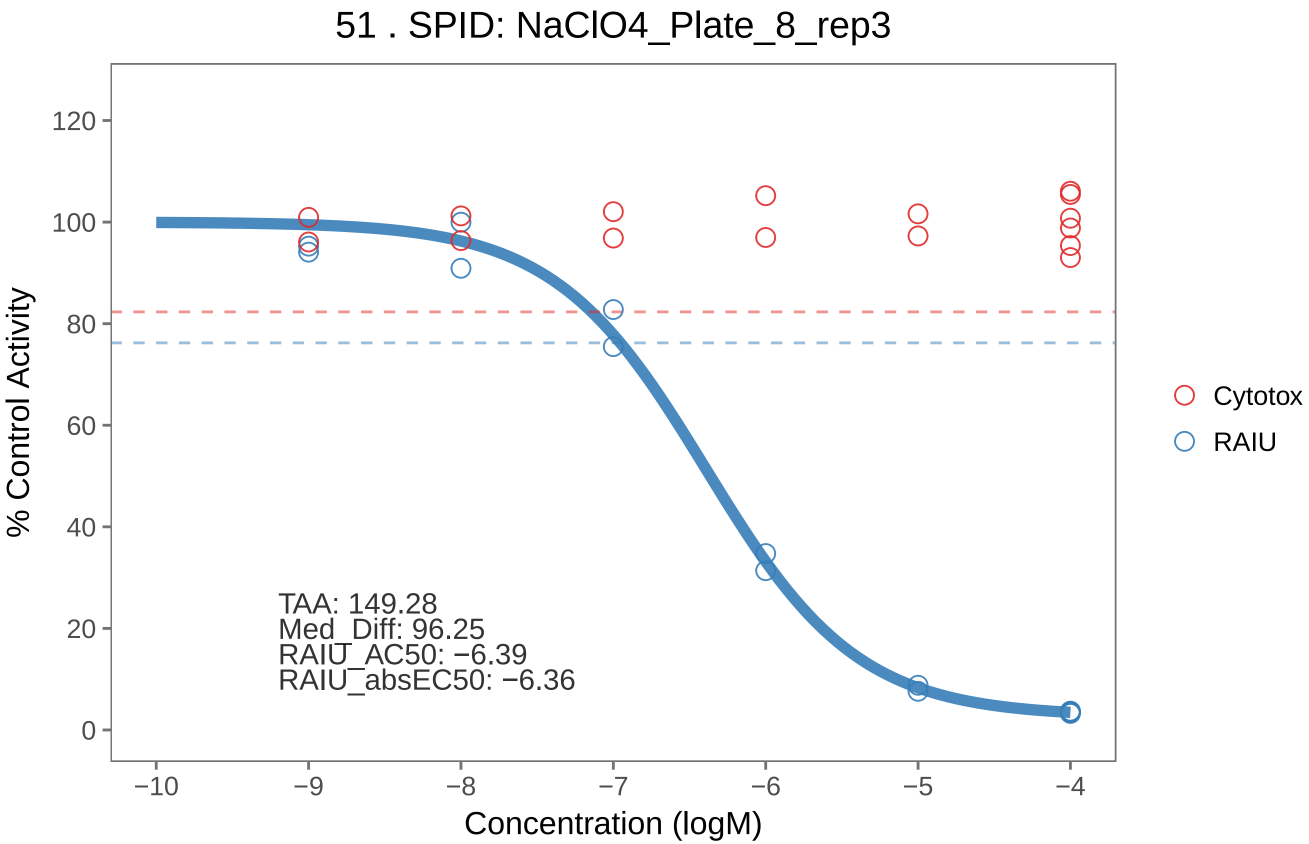

47 . SPID: NaClO4_Plate_7_rep2
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
TAA: 151.04
Med_Diff: 94.17
RAIU_AC50: −6.41
RAIU_absEC50: −6.38
Cytotox
RAIU

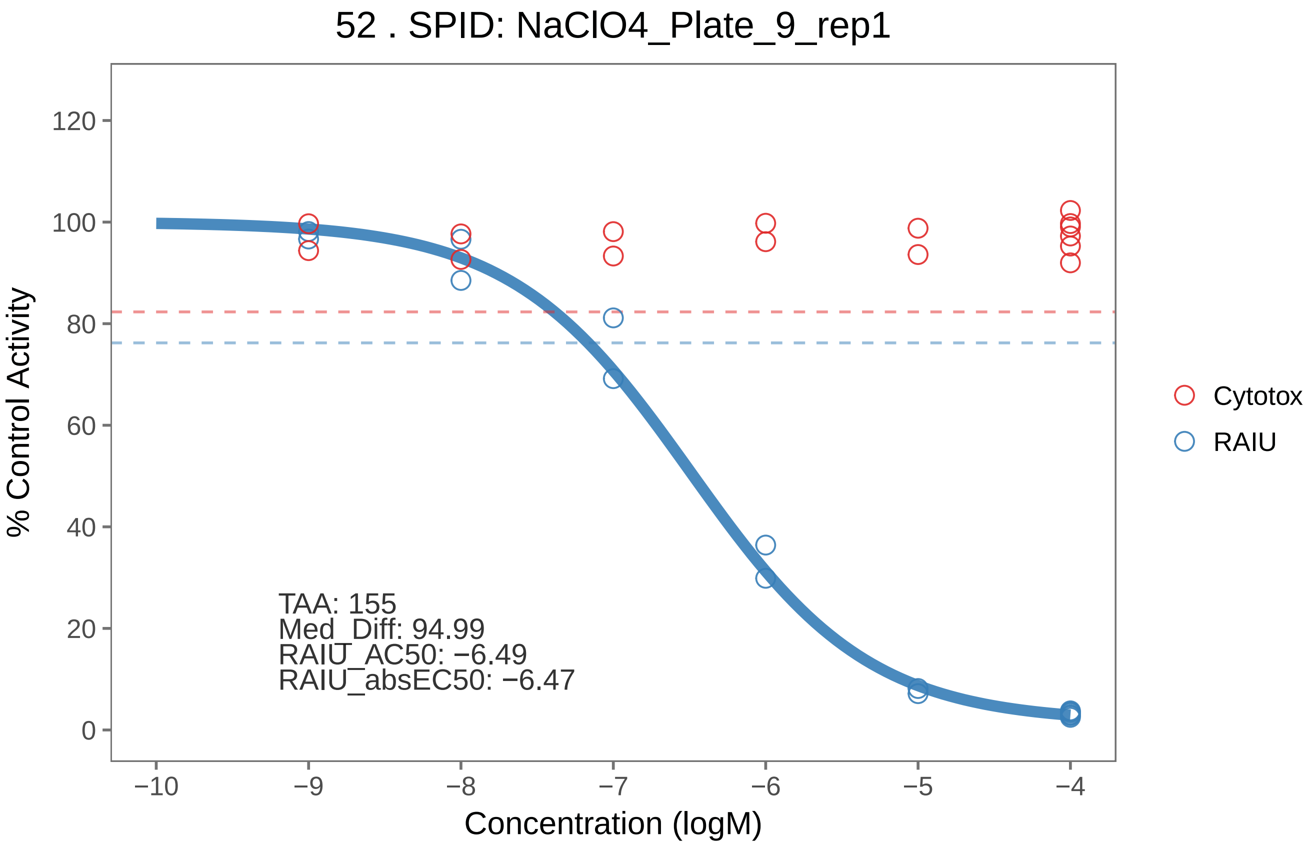

48 . SPID: NaClO4_Plate_7_rep3
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
TAA: 151.48
Med_Diff: 94.98
RAIU_AC50: −6.43
RAIU_absEC50: −6.41
Cytotox
RAIU

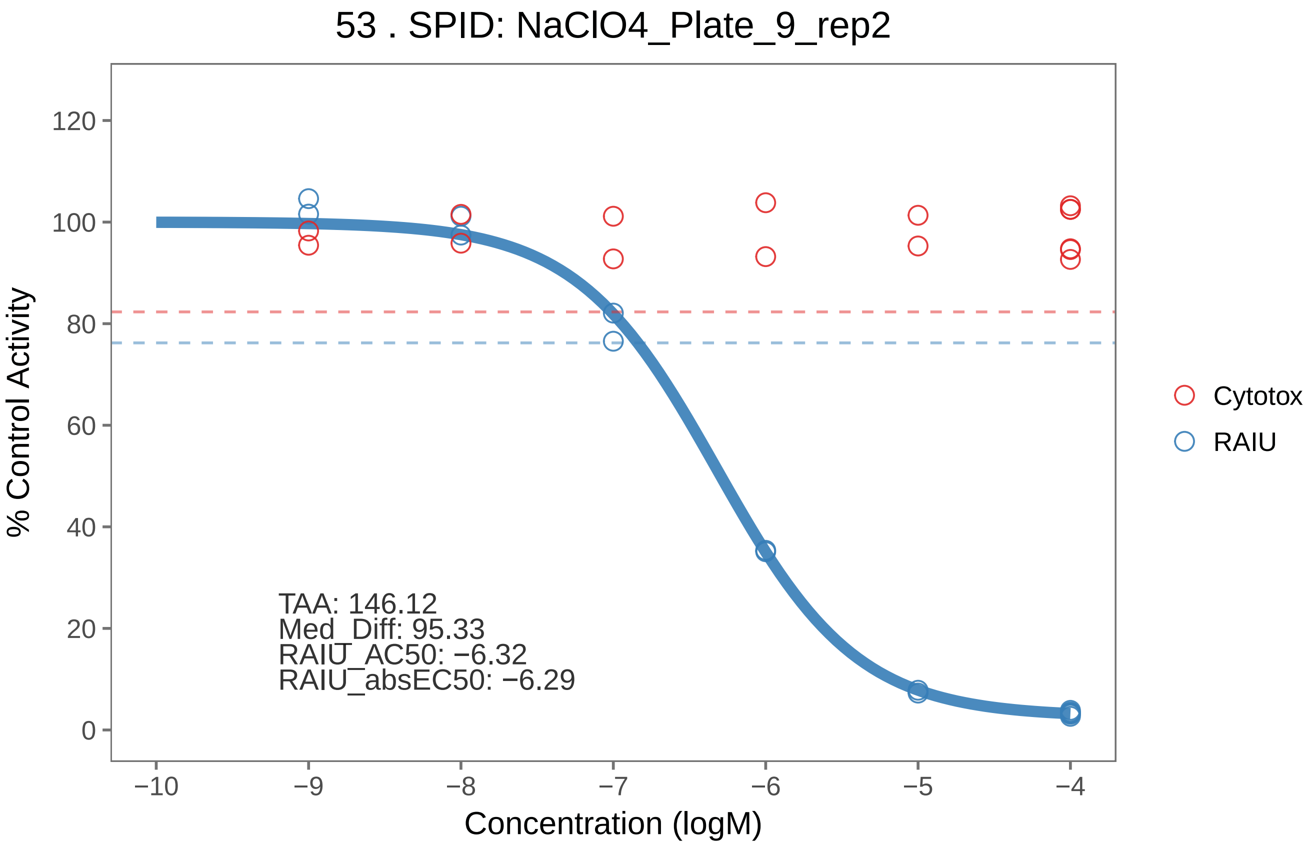

49 . SPID: NaClO4_Plate_8_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 143.64
Med_Diff: 97.19
RAIU_AC50: −6.04
RAIU_absEC50: −6.04
Cytotox
RAIU

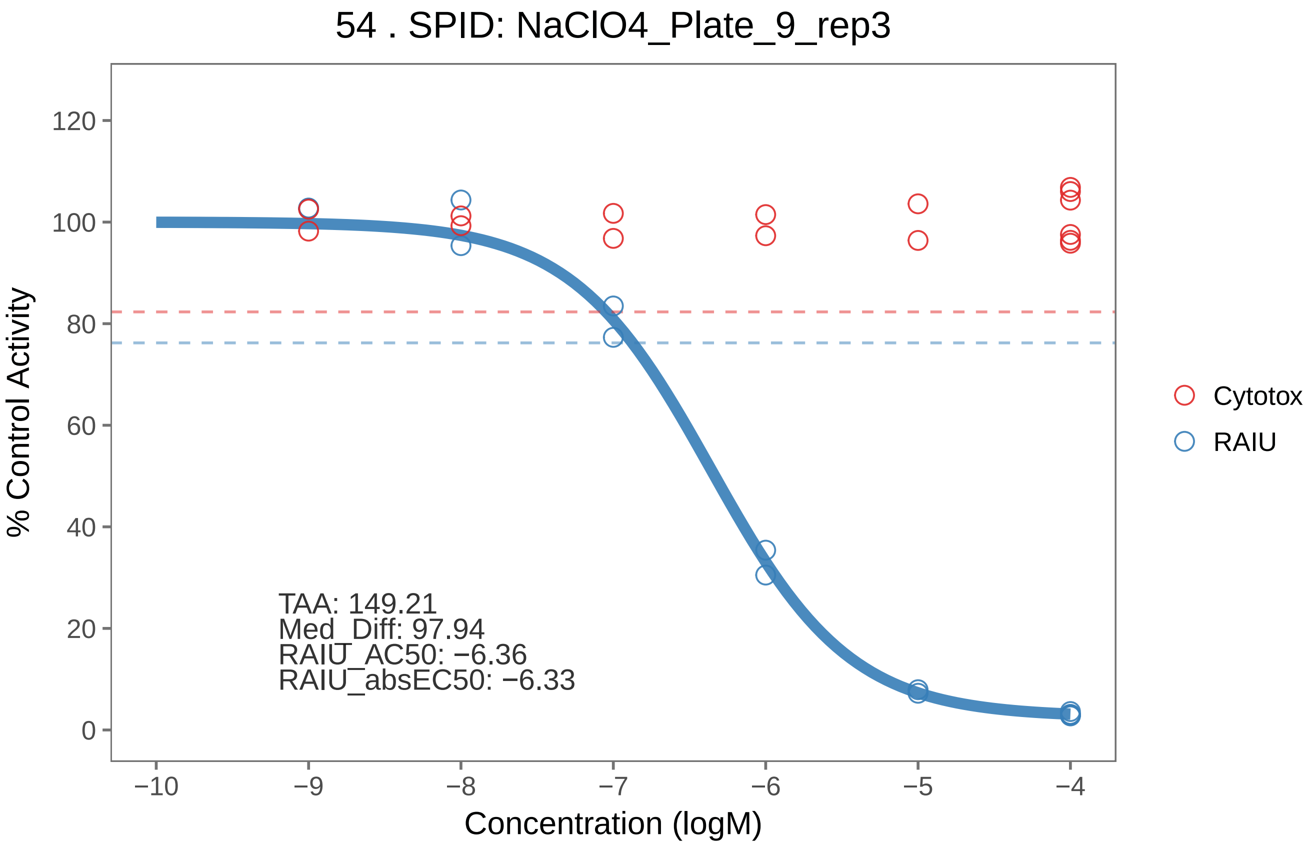


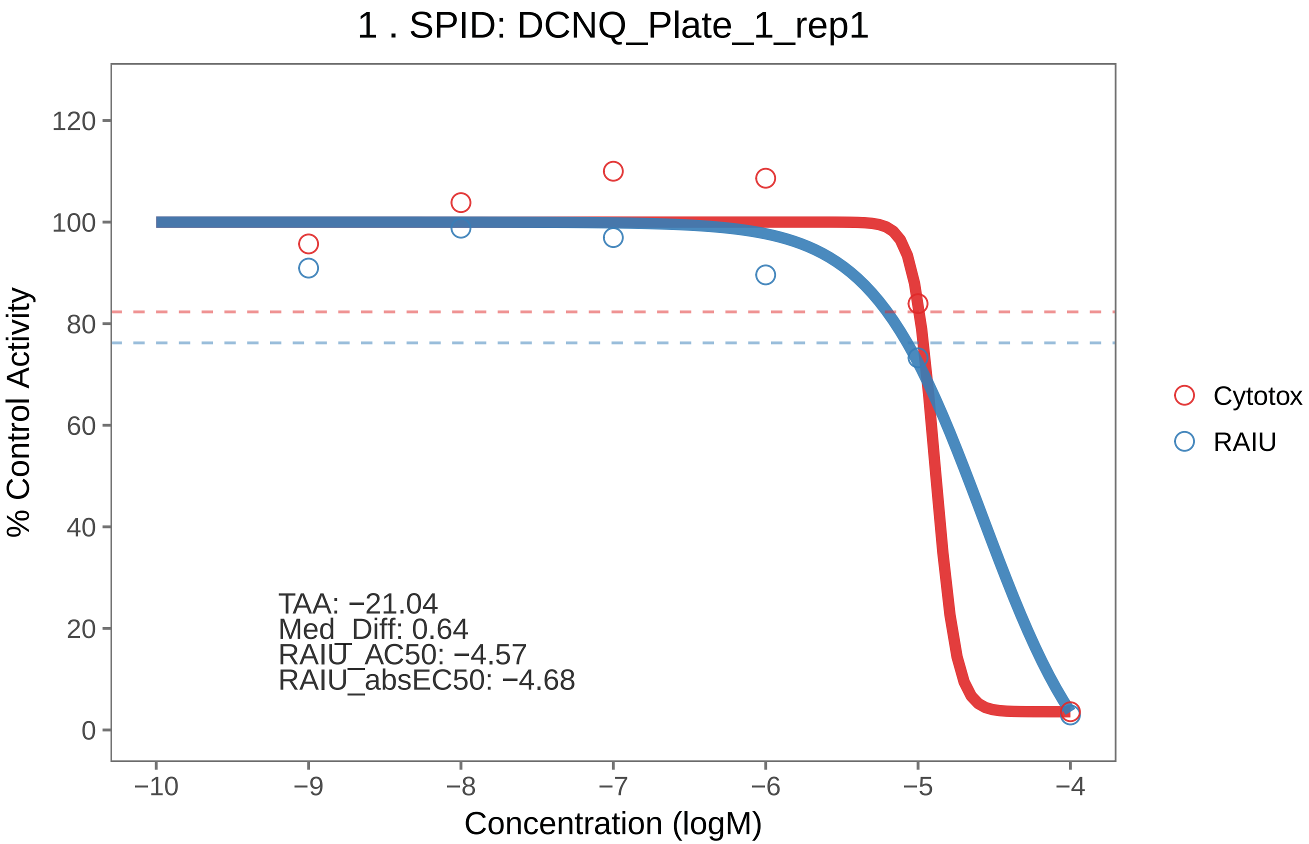
50 . SPID: NaClO4_Plate_8_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 142.11
Med_Diff: 93.94
RAIU_AC50: −6.26
RAIU_absEC50: −6.23
Cytotox
RAIU

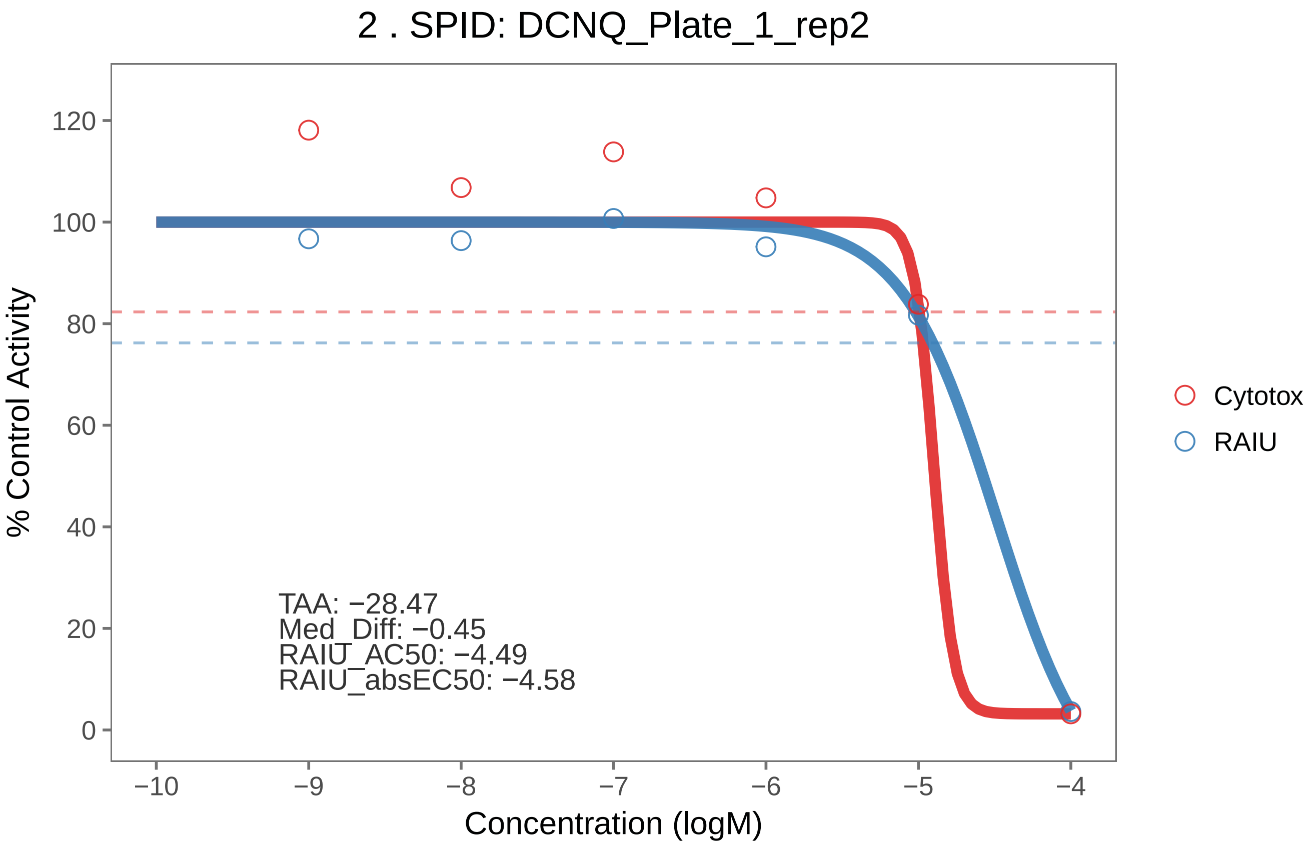

51 . SPID: NaClO4_Plate_8_rep3
% Control Activity
Concentration (logM)
Cytotox
RAIU
TAA: 149.28
Med_Diff: 96.25
RAIU_AC50: −6.39
RAIU_absEC50: −6.36
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4

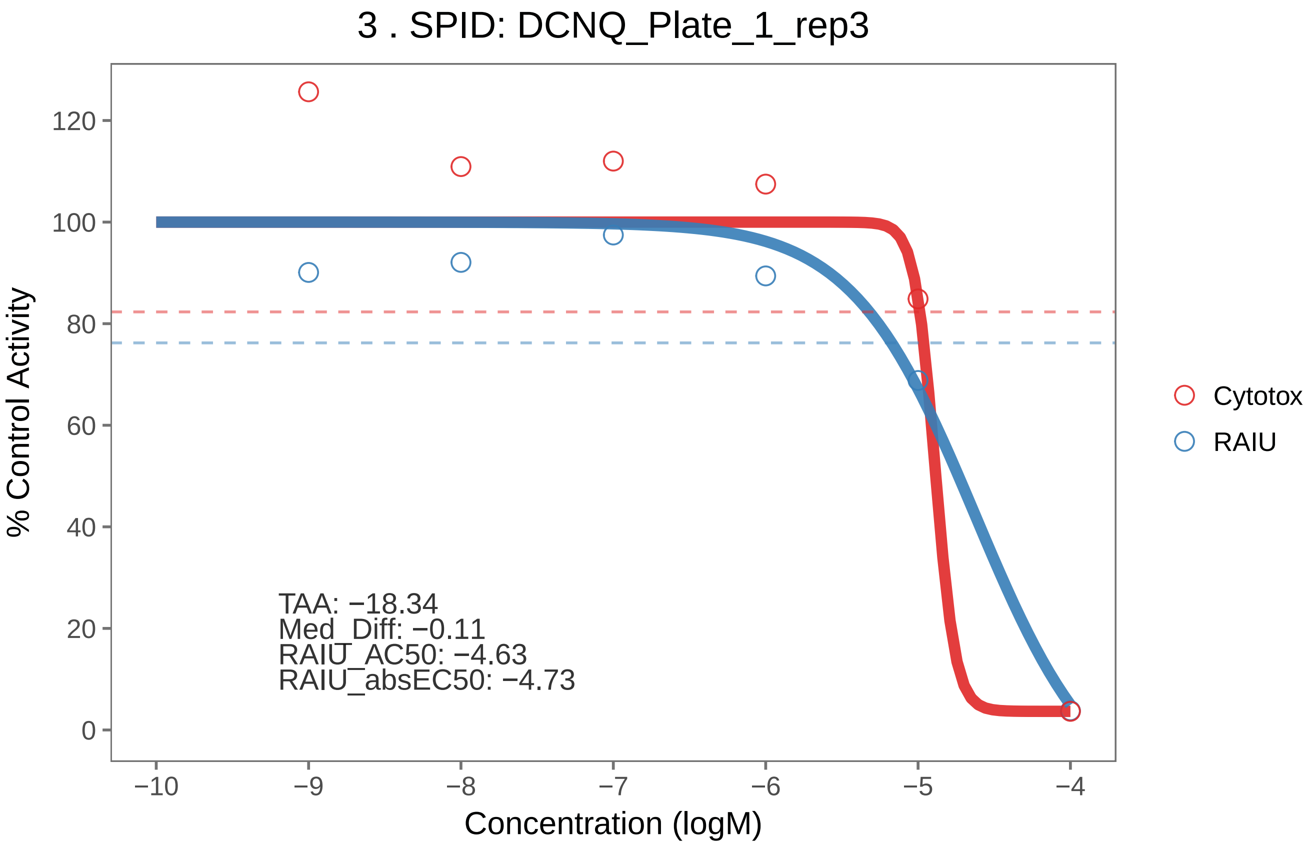

52 . SPID: NaClO4_Plate_9_rep1
% Control Activity
Concentration (logM)
Cytotox
RAIU
TAA: 155
Med_Diff: 94.99
RAIU_AC50: −6.49
RAIU_absEC50: −6.47
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4

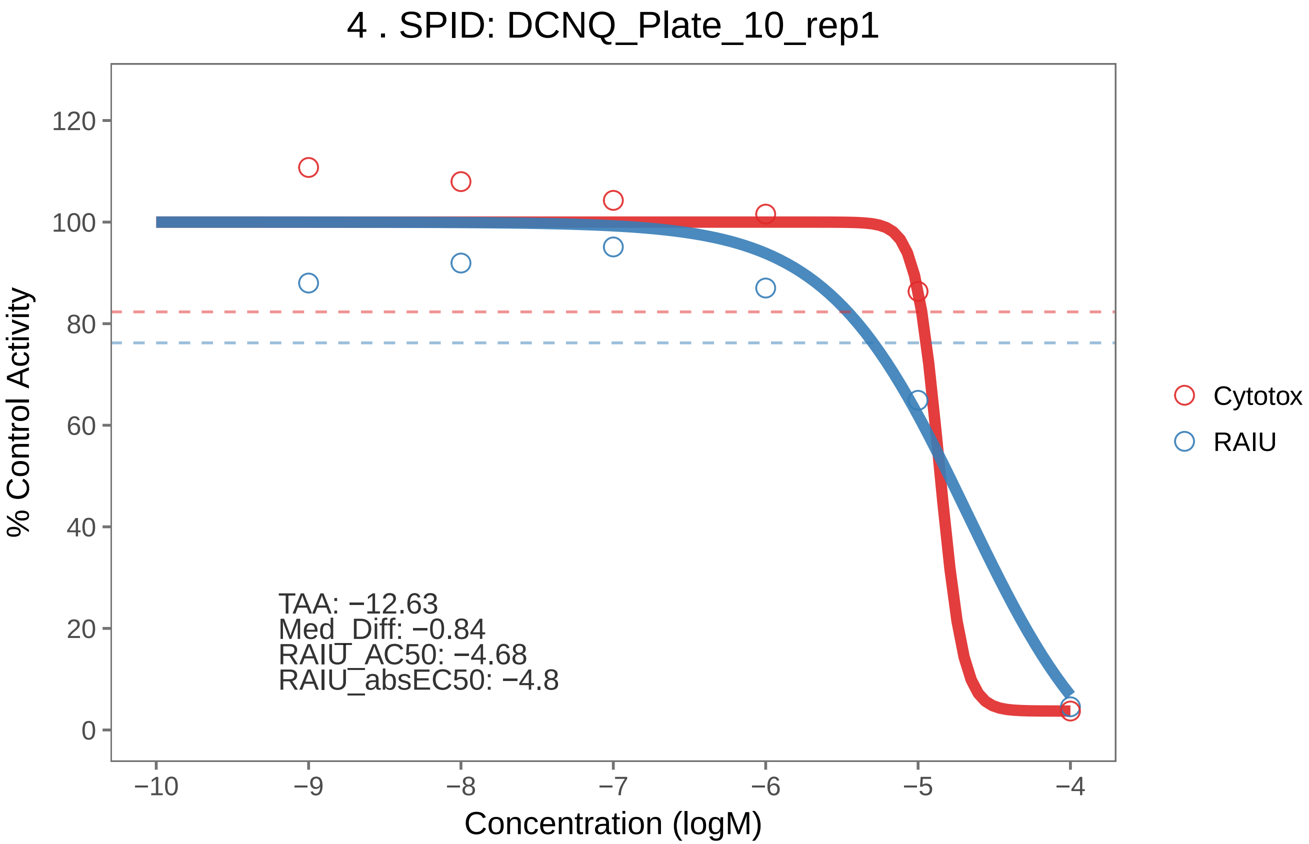

53 . SPID: NaClO4_Plate_9_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 146.12
Med_Diff: 95.33
RAIU_AC50: −6.32
RAIU_absEC50: −6.29
Cytotox
RAIU

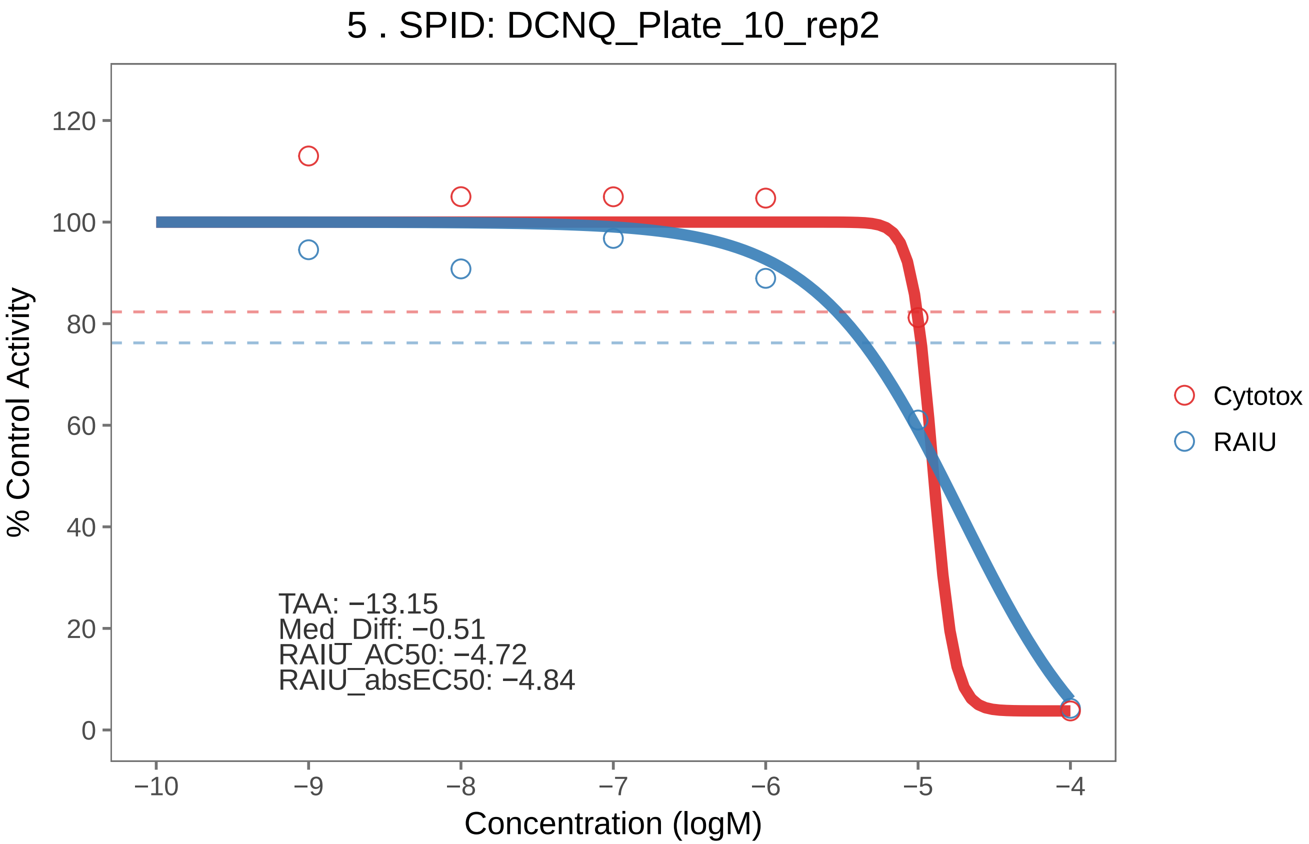

54 . SPID: NaClO4_Plate_9_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: 149.21
Med_Diff: 97.94
RAIU_AC50: −6.36
RAIU_absEC50: −6.33

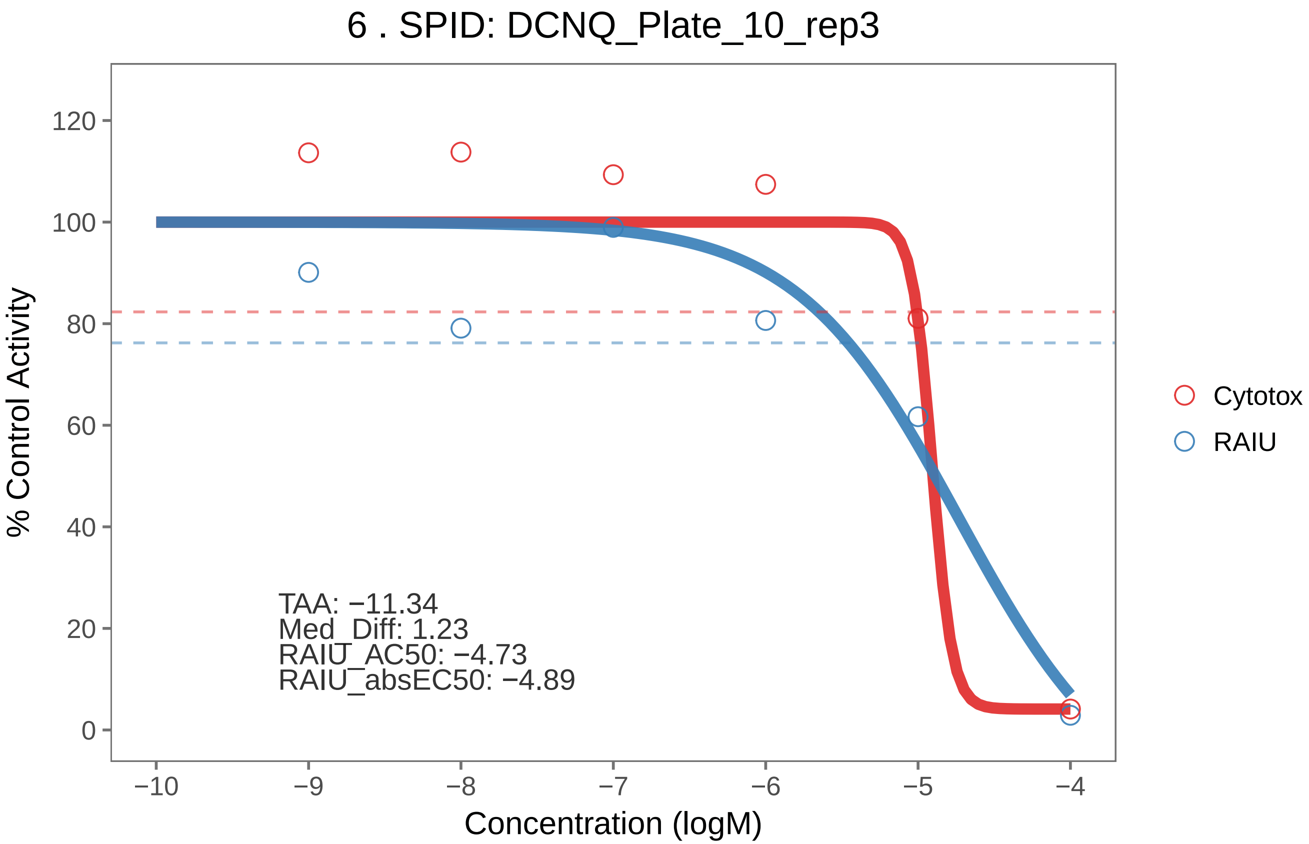

1 . SPID: DCNQ_Plate_1_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −21.04
Med_Diff: 0.64
RAIU_AC50: −4.57
RAIU_absEC50: −4.68
Cytotox
RAIU

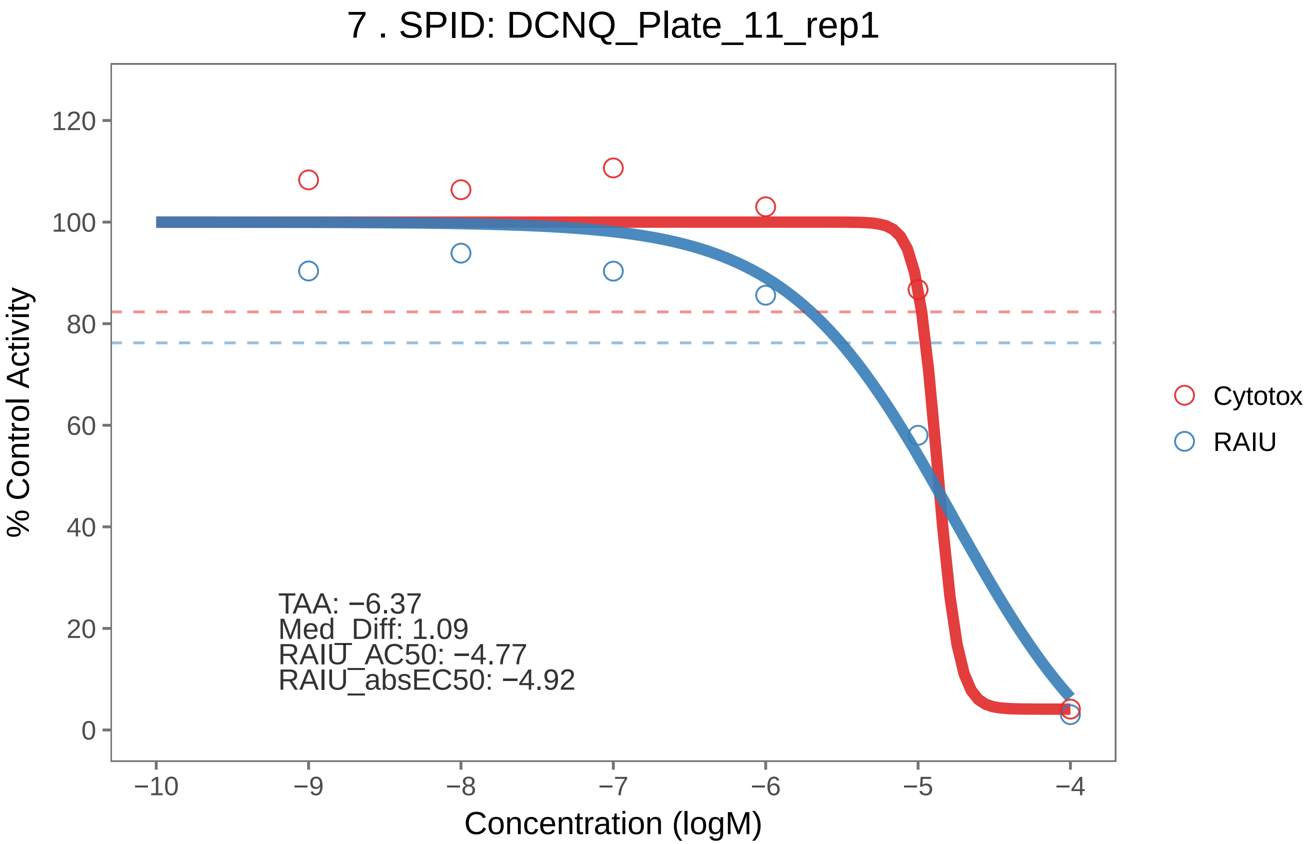

2 . SPID: DCNQ_Plate_1_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −28.47
Med_Diff: −0.45
RAIU_AC50: −4.49
RAIU_absEC50: −4.58

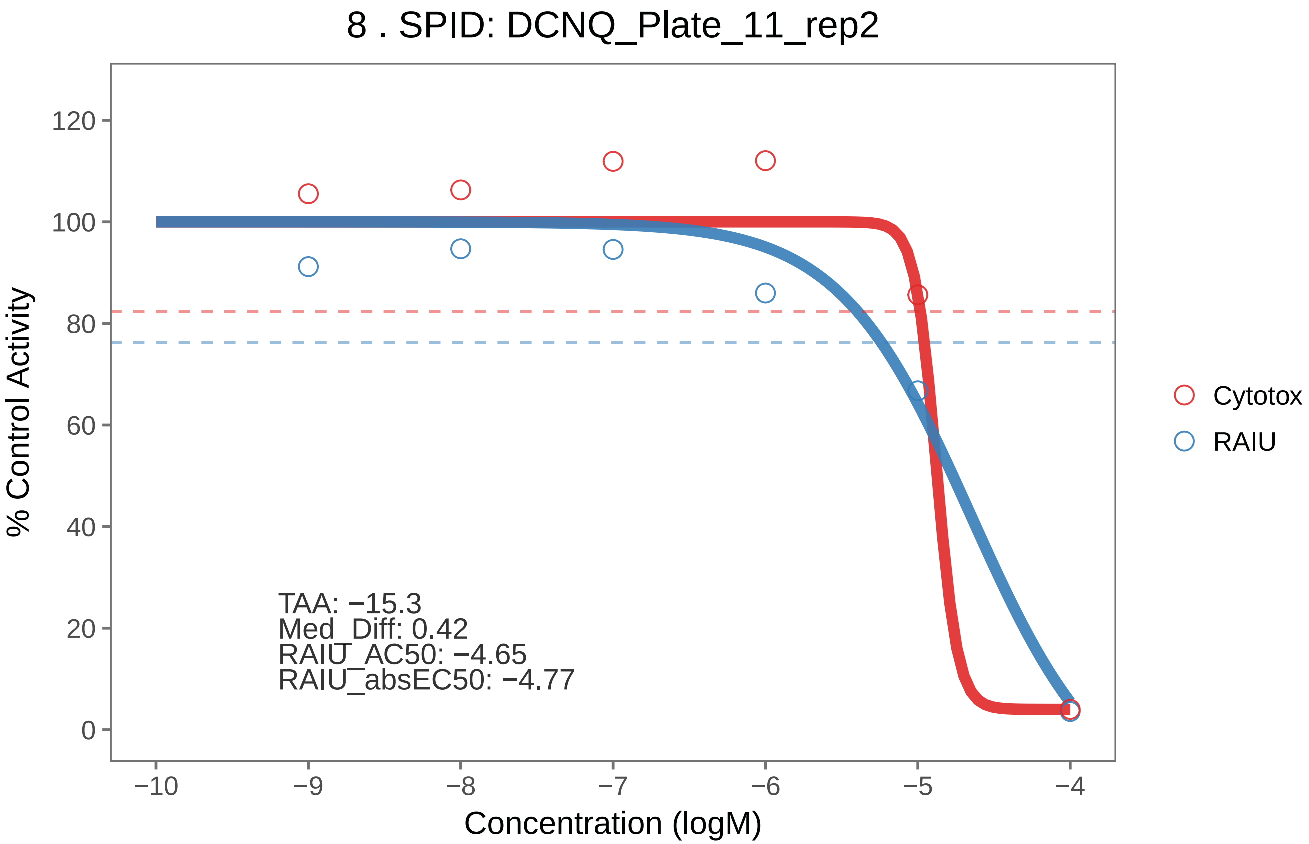

3 . SPID: DCNQ_Plate_1_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −18.34
Med_Diff: −0.11
RAIU_AC50: −4.63
RAIU_absEC50: −4.73
Cytotox
RAIU

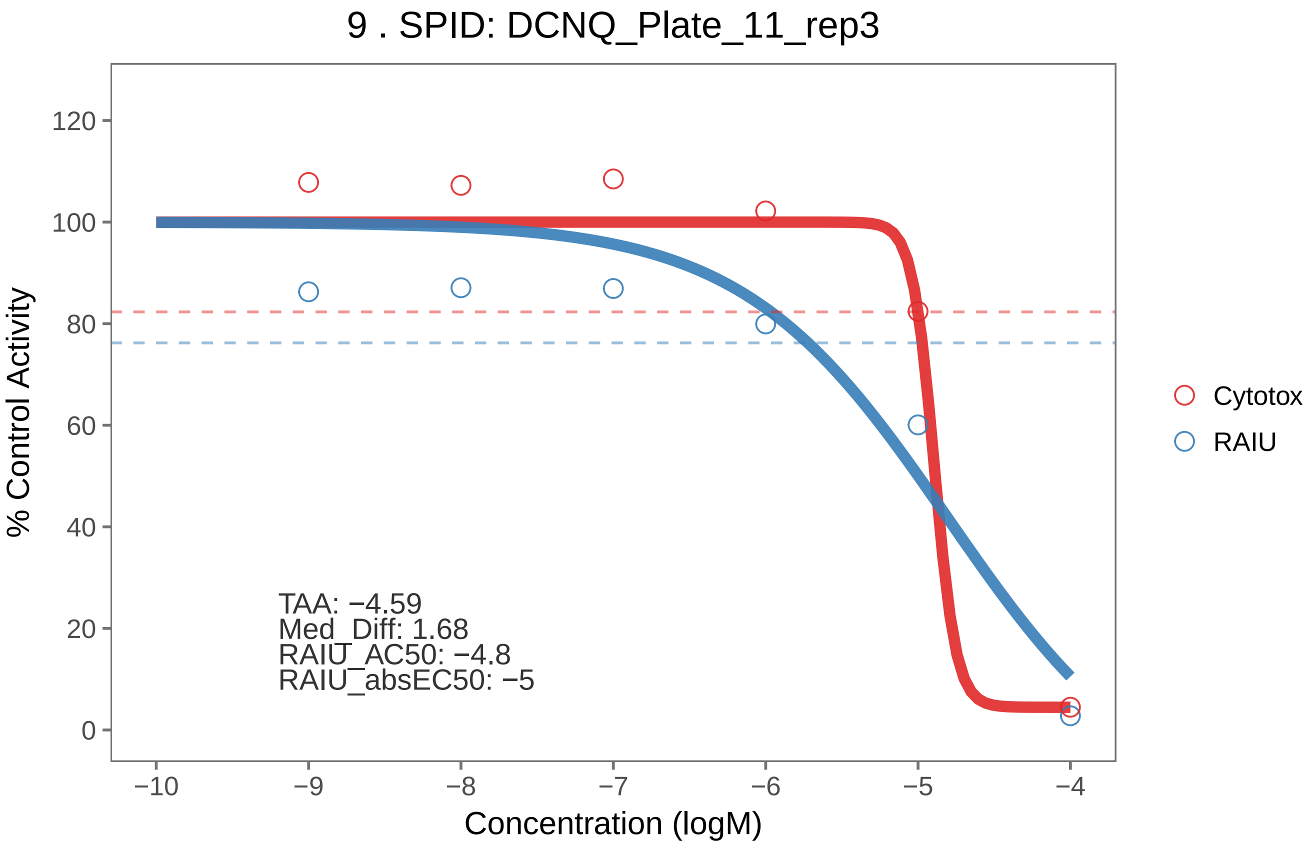

4 . SPID: DCNQ_Plate_10_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −12.63
Med_Diff: −0.84
RAIU_AC50: −4.68
RAIU_absEC50: −4.8
Cytotox
RAIU

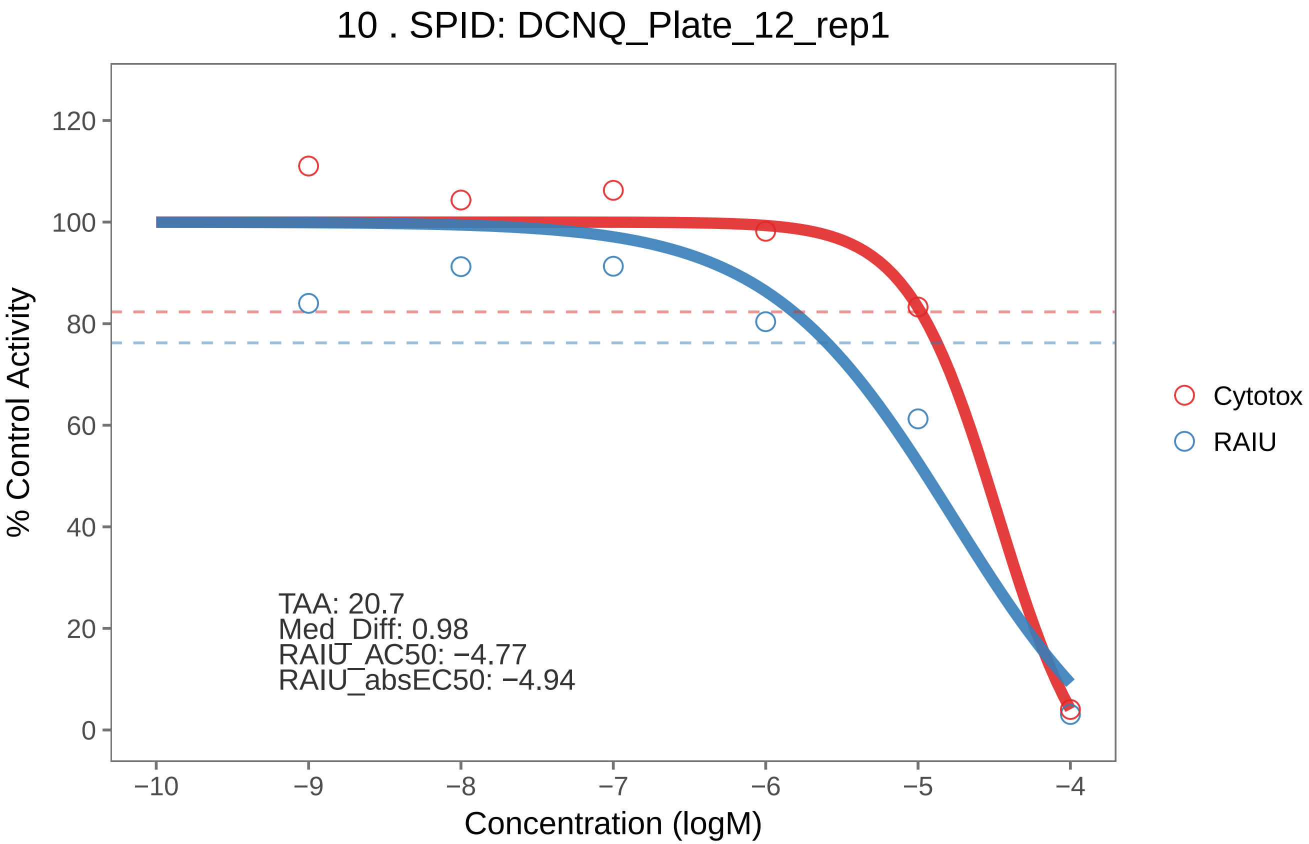

5 . SPID: DCNQ_Plate_10_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −13.15
Med_Diff: −0.51
RAIU_AC50: −4.72
RAIU_absEC50: −4.84
Cytotox
RAIU

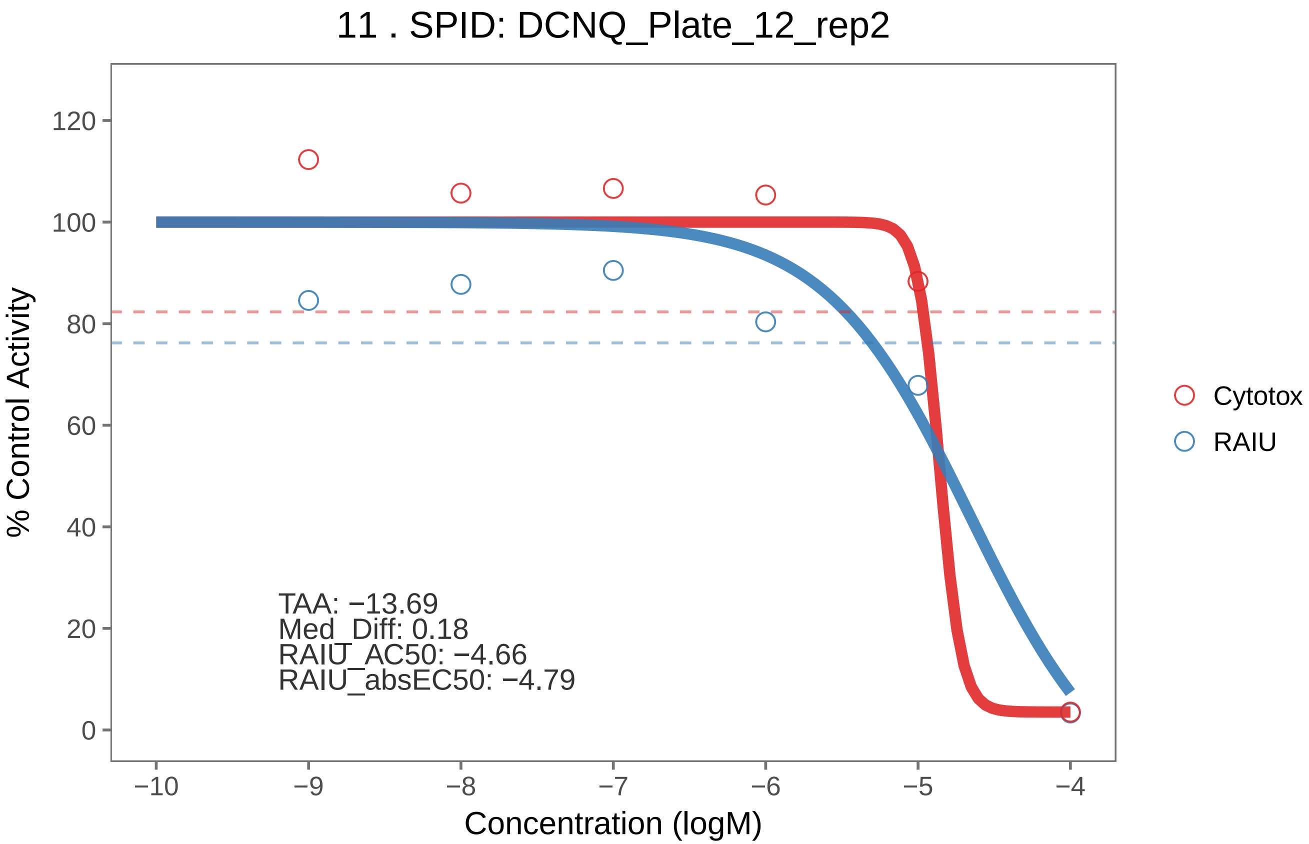

6 . SPID: DCNQ_Plate_10_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −11.34
Med_Diff: 1.23
RAIU_AC50: −4.73
RAIU_absEC50: −4.89
Cytotox
RAIU

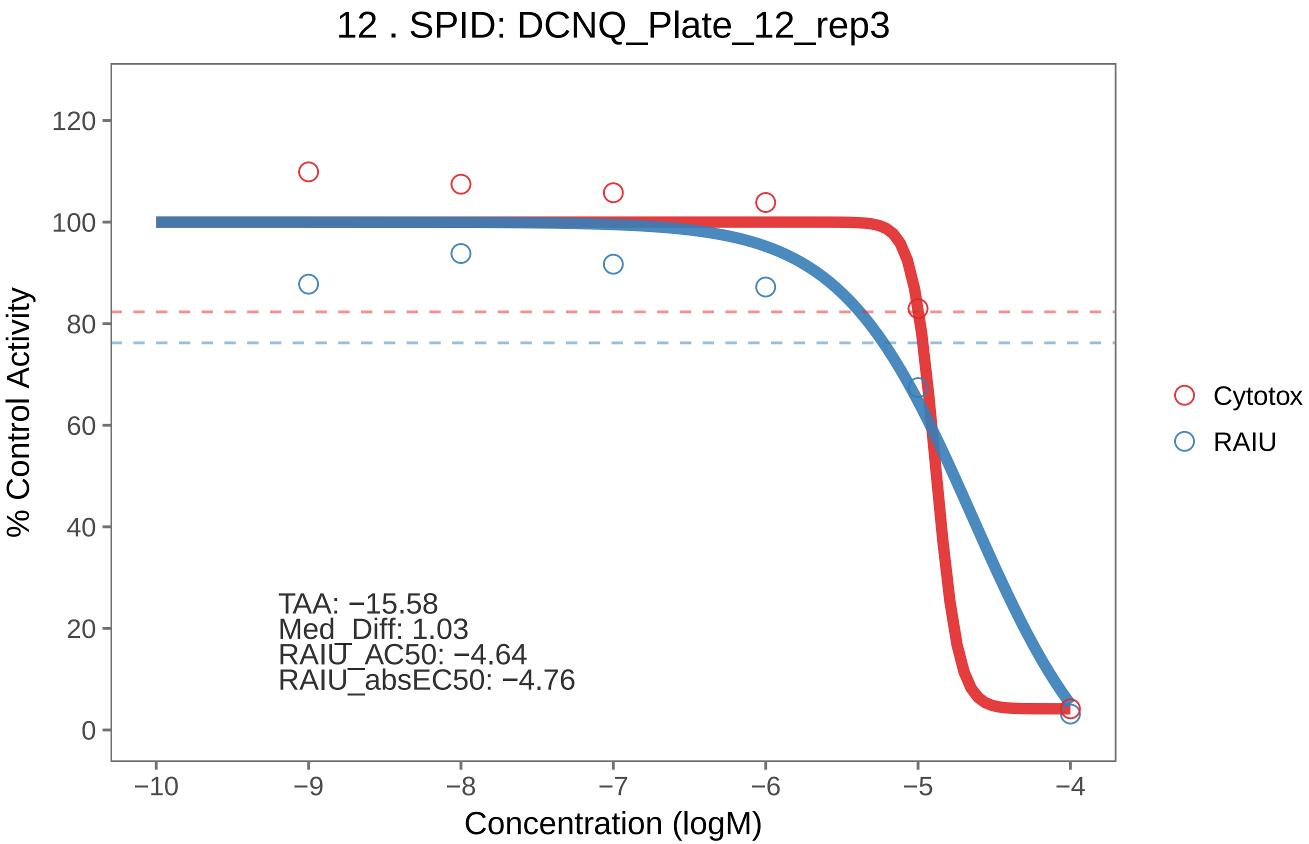

7 . SPID: DCNQ_Plate_11_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −6.37
Med_Diff: 1.09
RAIU_AC50: −4.77
RAIU_absEC50: −4.92
Cytotox
RAIU

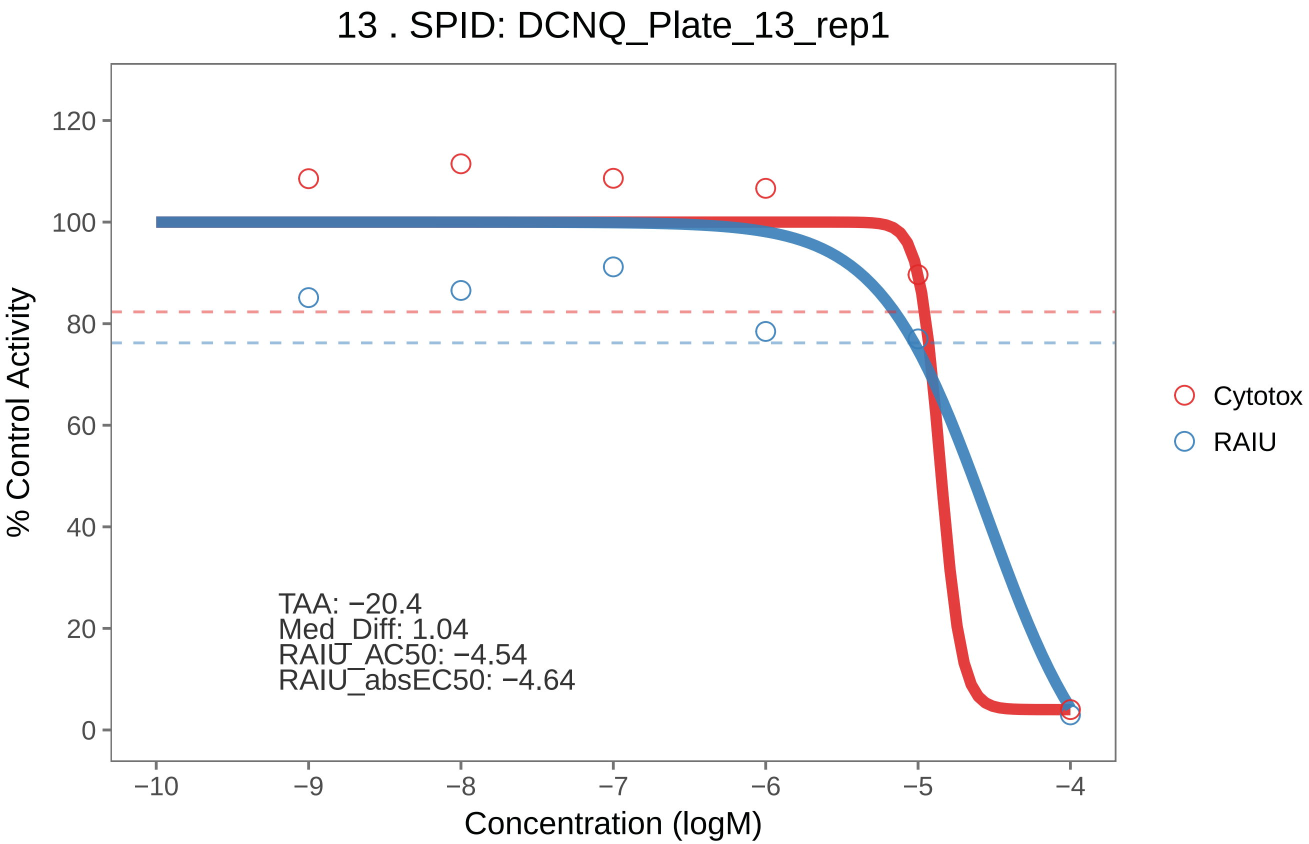

8 . SPID: DCNQ_Plate_11_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −15.3
Med_Diff: 0.42
RAIU_AC50: −4.65
RAIU_absEC50: −4.77
Cytotox
RAIU

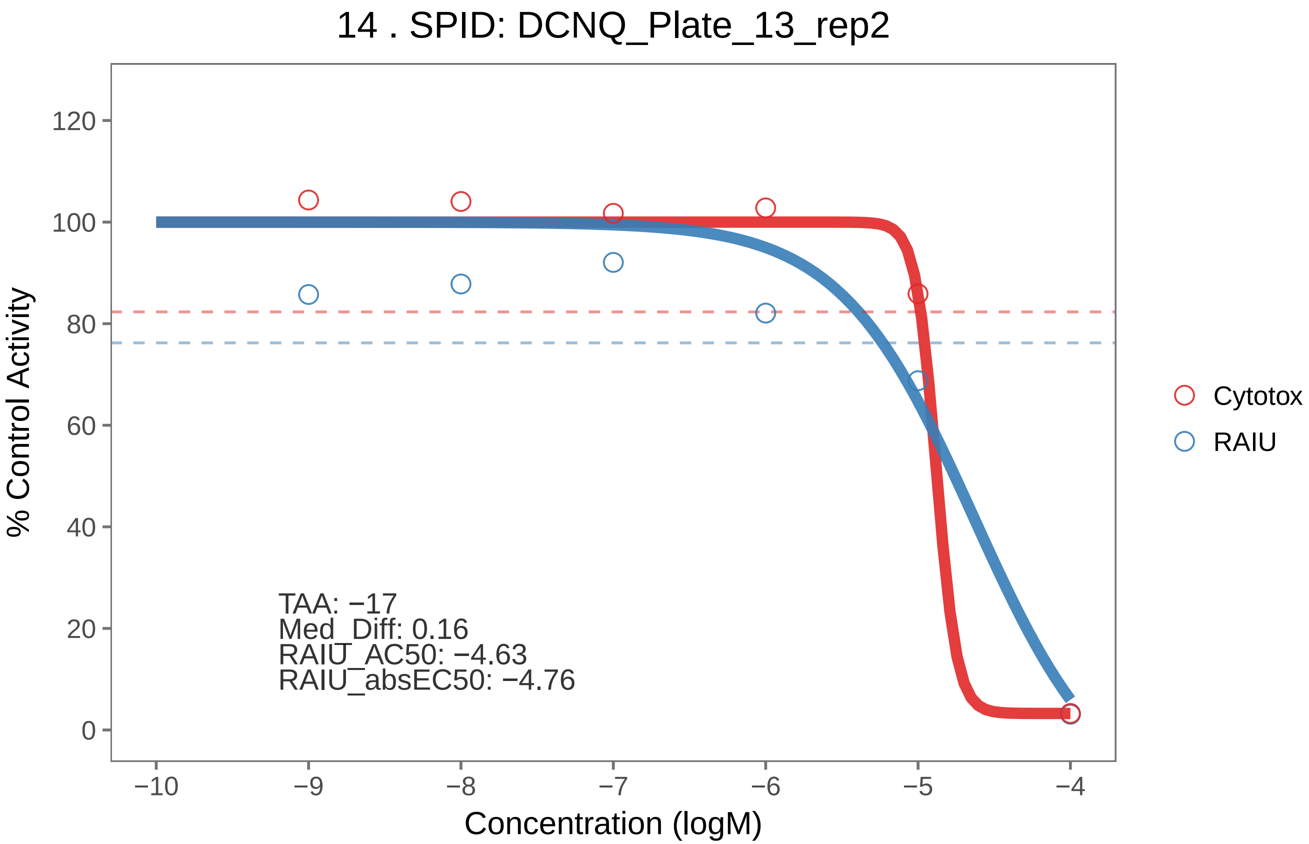

9 . SPID: DCNQ_Plate_11_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −4.59
Med_Diff: 1.68
RAIU_AC50: −4.8
RAIU_absEC50: −5

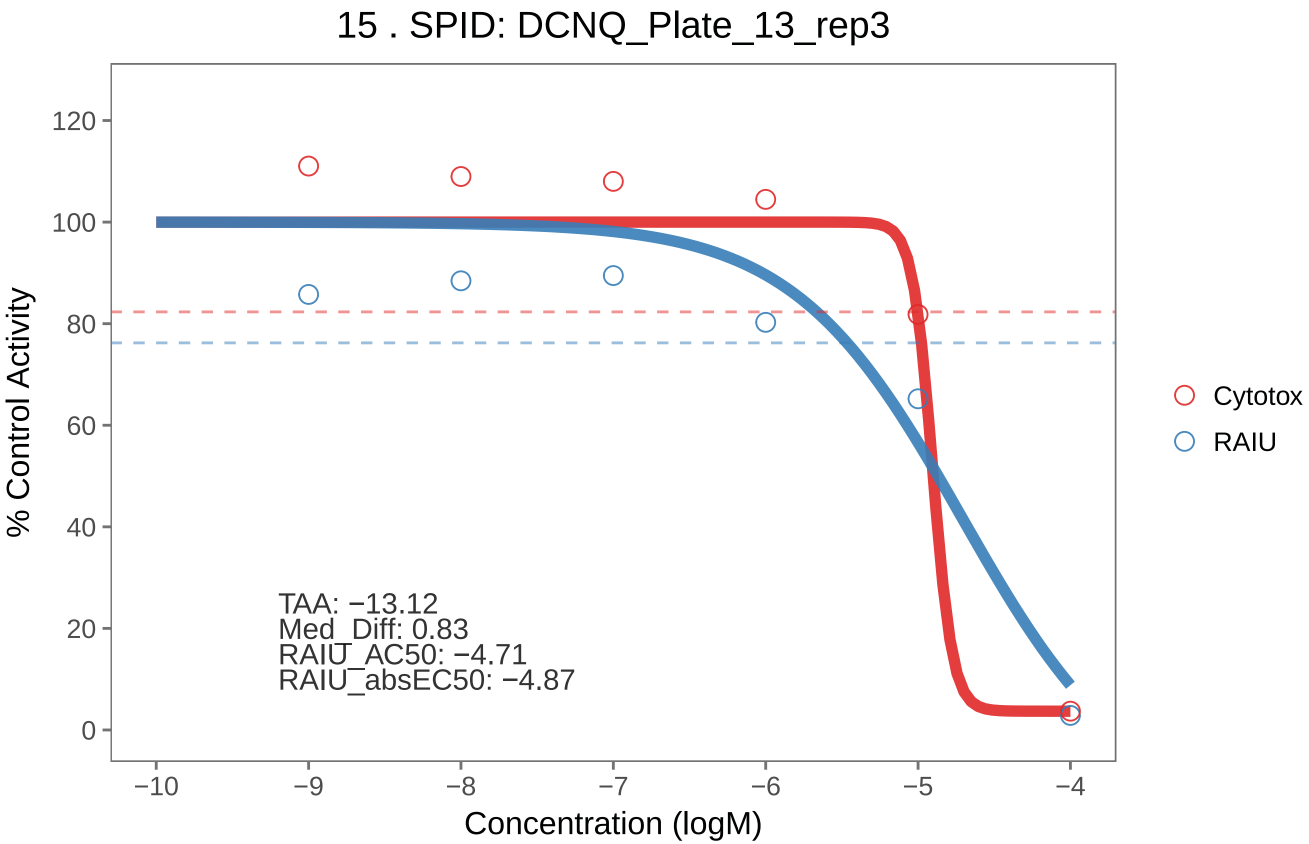

10 . SPID: DCNQ_Plate_12_rep1
% Control Activity
Concentration (logM)
Cytotox
RAIU
TAA: 20.7
Med_Diff: 0.98
RAIU_AC50: −4.77
RAIU_absEC50: −4.94
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4

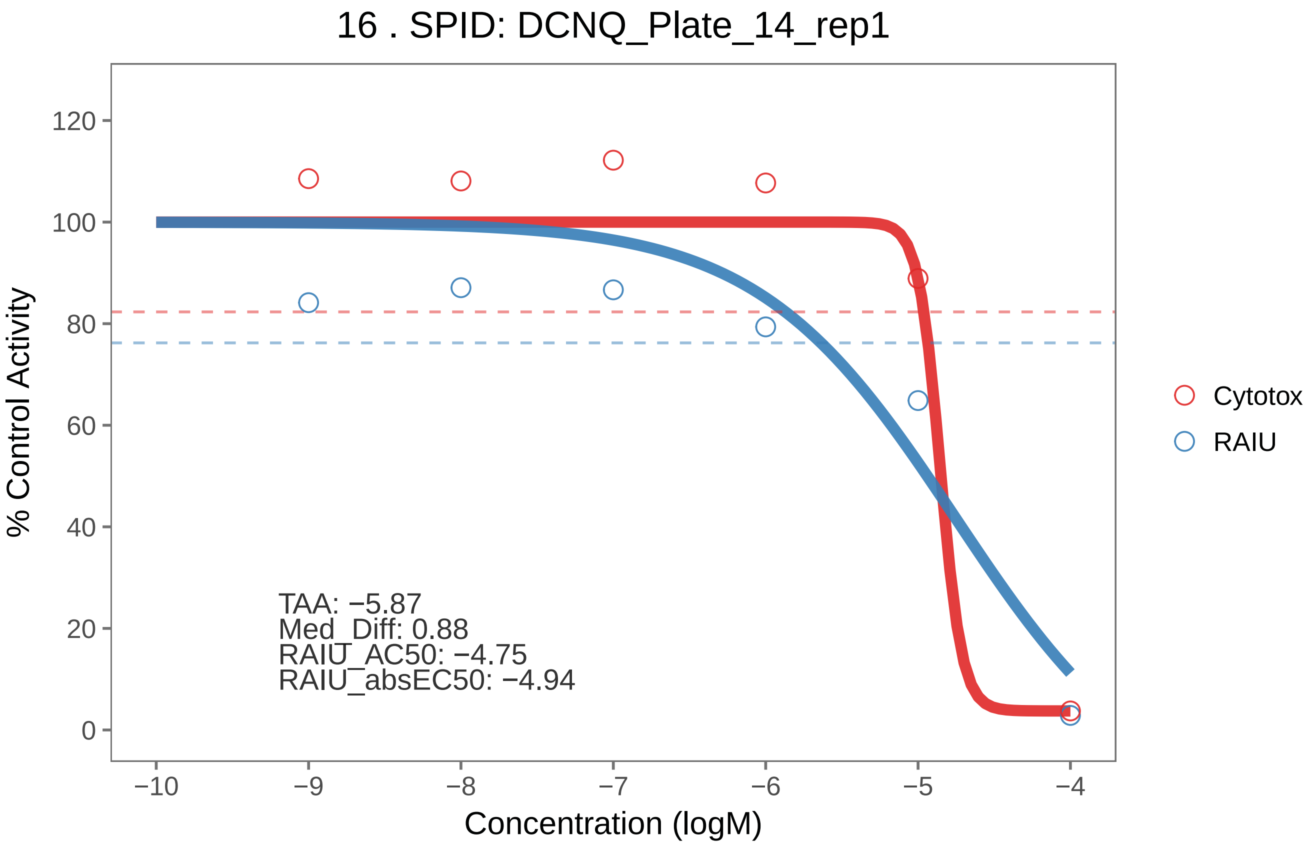

11 . SPID: DCNQ_Plate_12_rep2
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −13.69
Med_Diff: 0.18
RAIU_AC50: −4.66
RAIU_absEC50: −4.79
Cytotox
RAIU

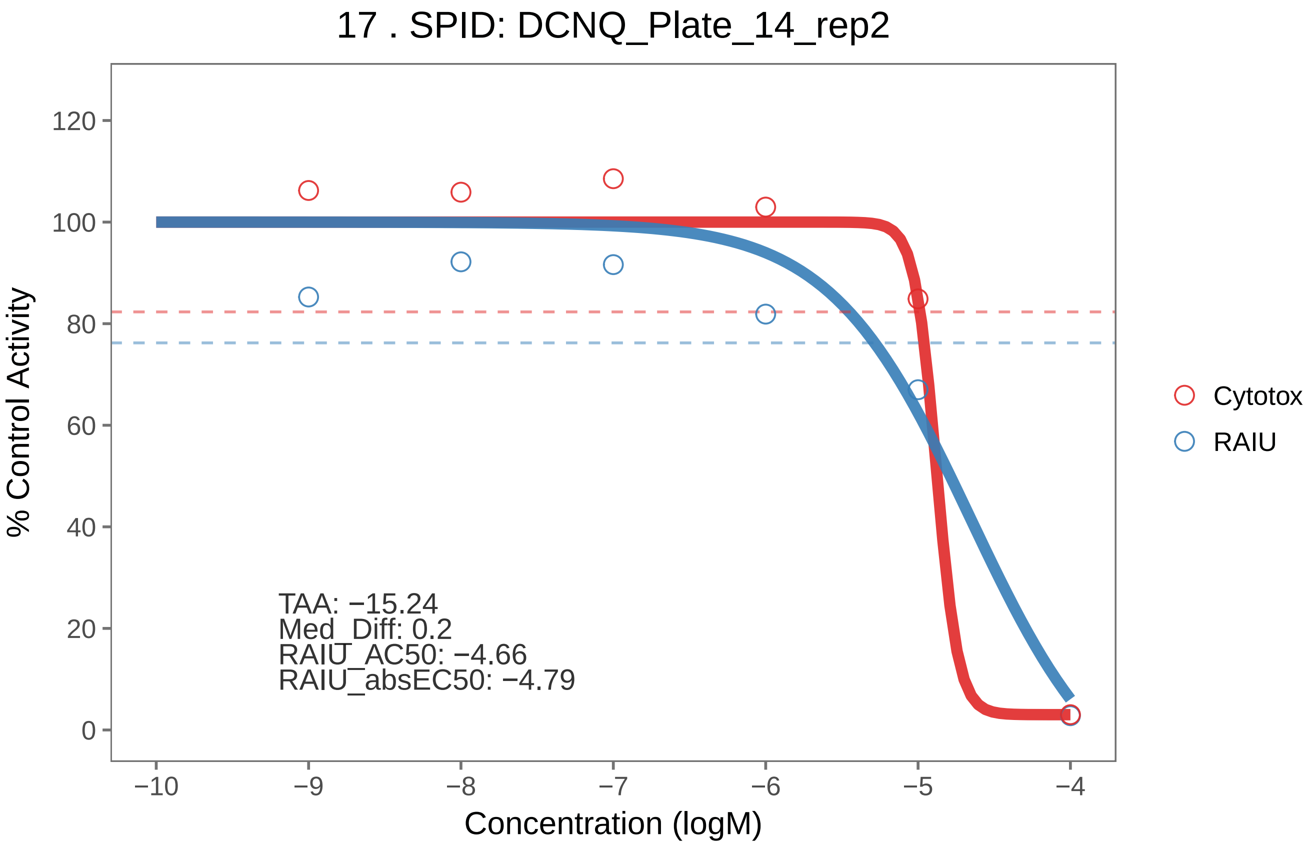

12 . SPID: DCNQ_Plate_12_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −15.58
Med_Diff: 1.03
RAIU_AC50: −4.64
RAIU_absEC50: −4.76
Cytotox
RAIU

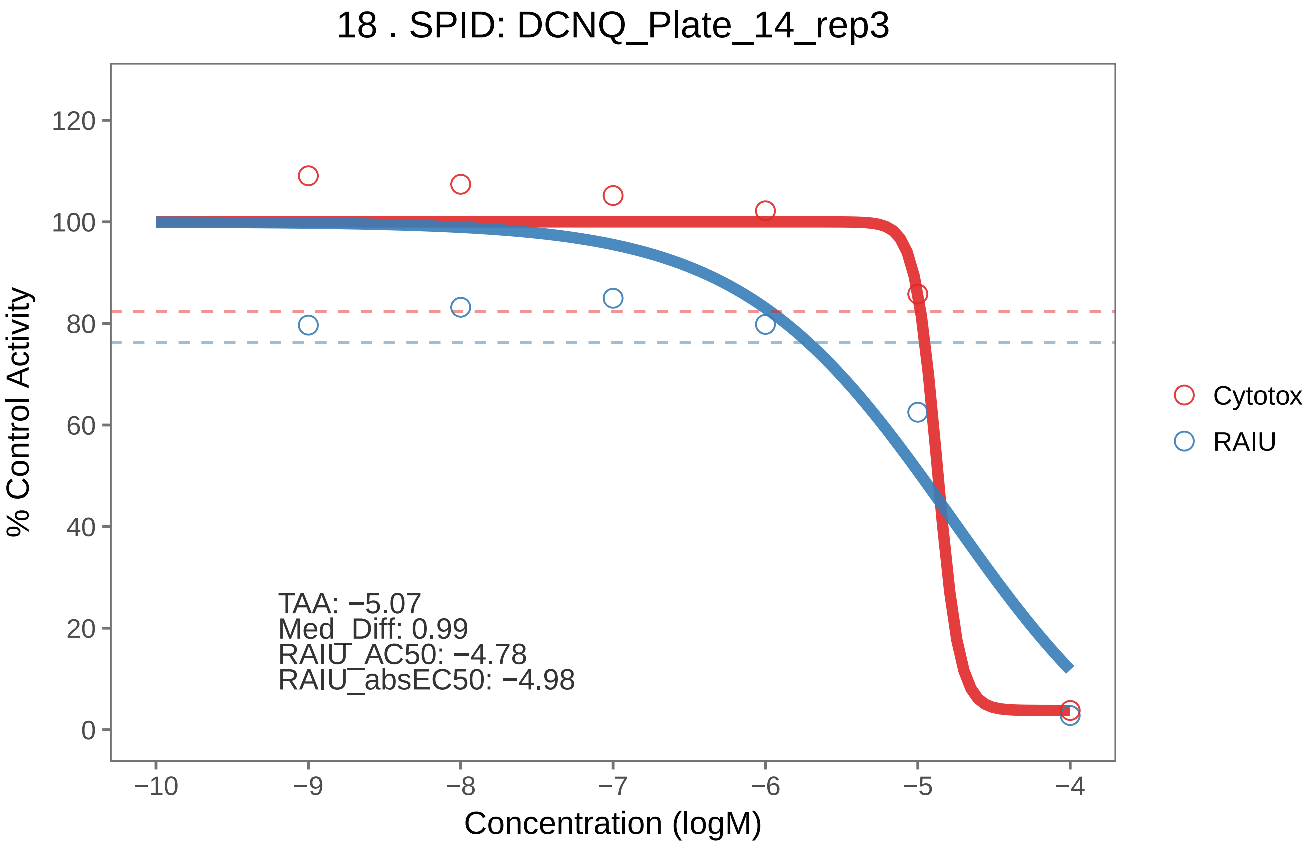

13 . SPID: DCNQ_Plate_13_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −20.4
Med_Diff: 1.04
RAIU_AC50: −4.54
RAIU_absEC50: −4.64

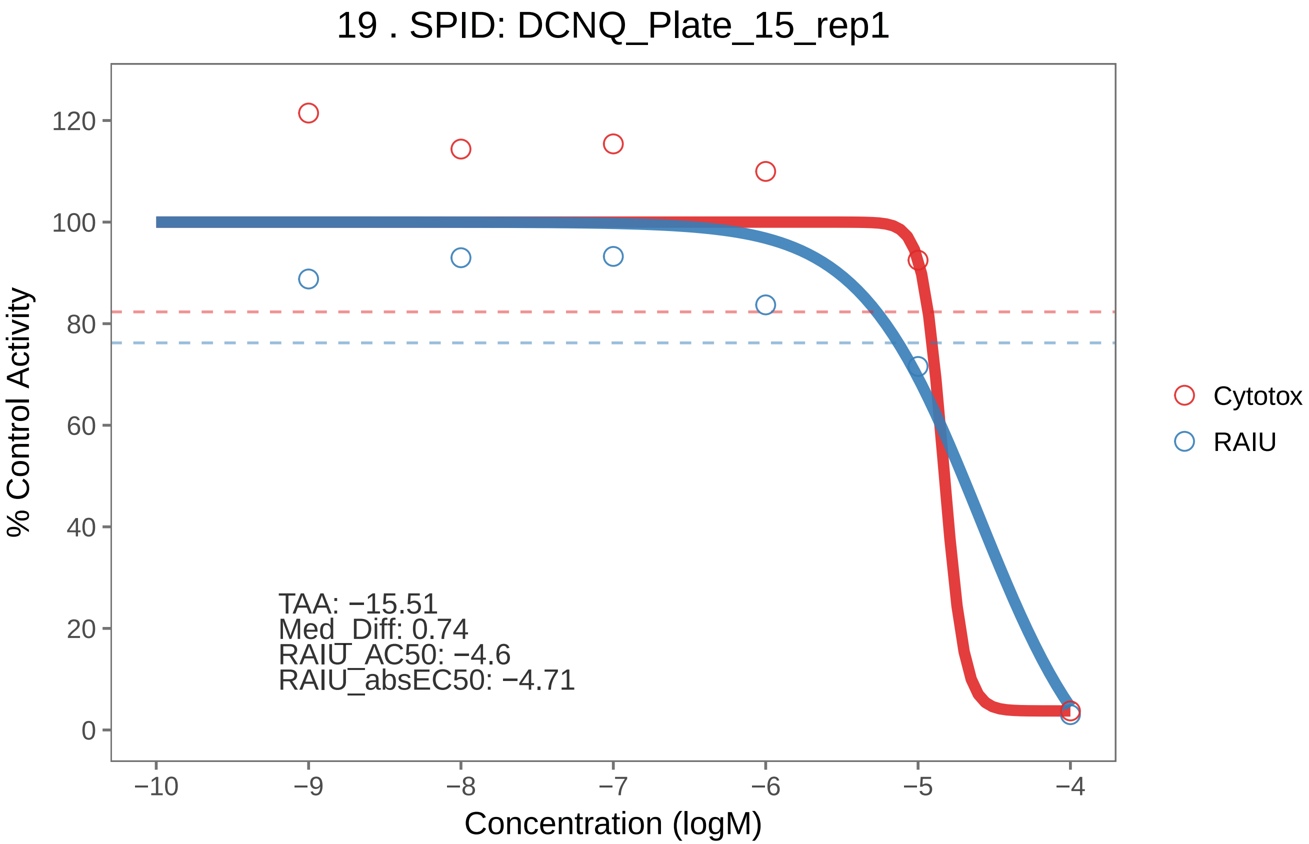

14 . SPID: DCNQ_Plate_13_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −17
Med_Diff: 0.16
RAIU_AC50: −4.63
RAIU_absEC50: −4.76


15 . SPID: DCNQ_Plate_13_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −13.12
Med_Diff: 0.83
RAIU_AC50: −4.71
RAIU_absEC50: −4.87
Cytotox
RAIU

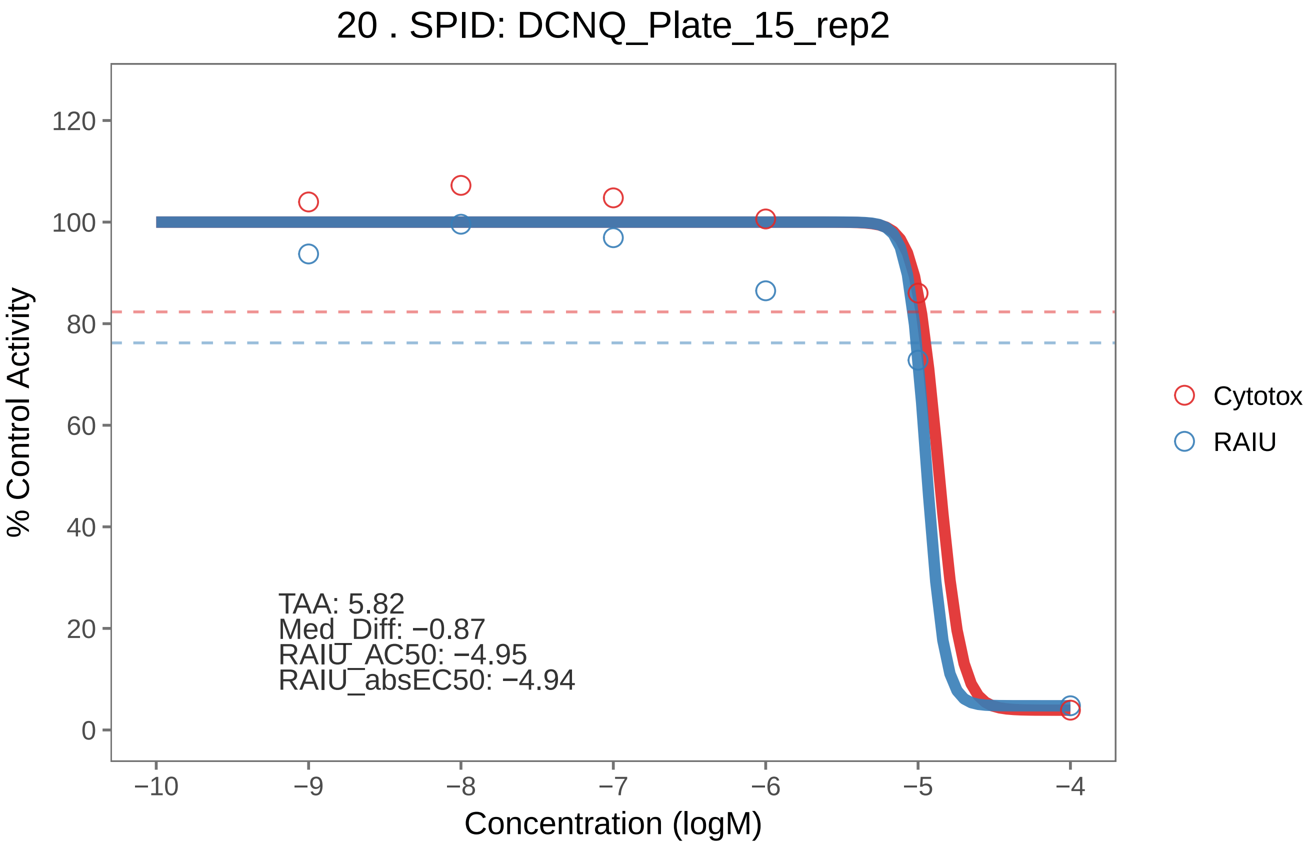

16 . SPID: DCNQ_Plate_14_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −5.87
Med_Diff: 0.88
RAIU_AC50: −4.75
RAIU_absEC50: −4.94
Cytotox
RAIU

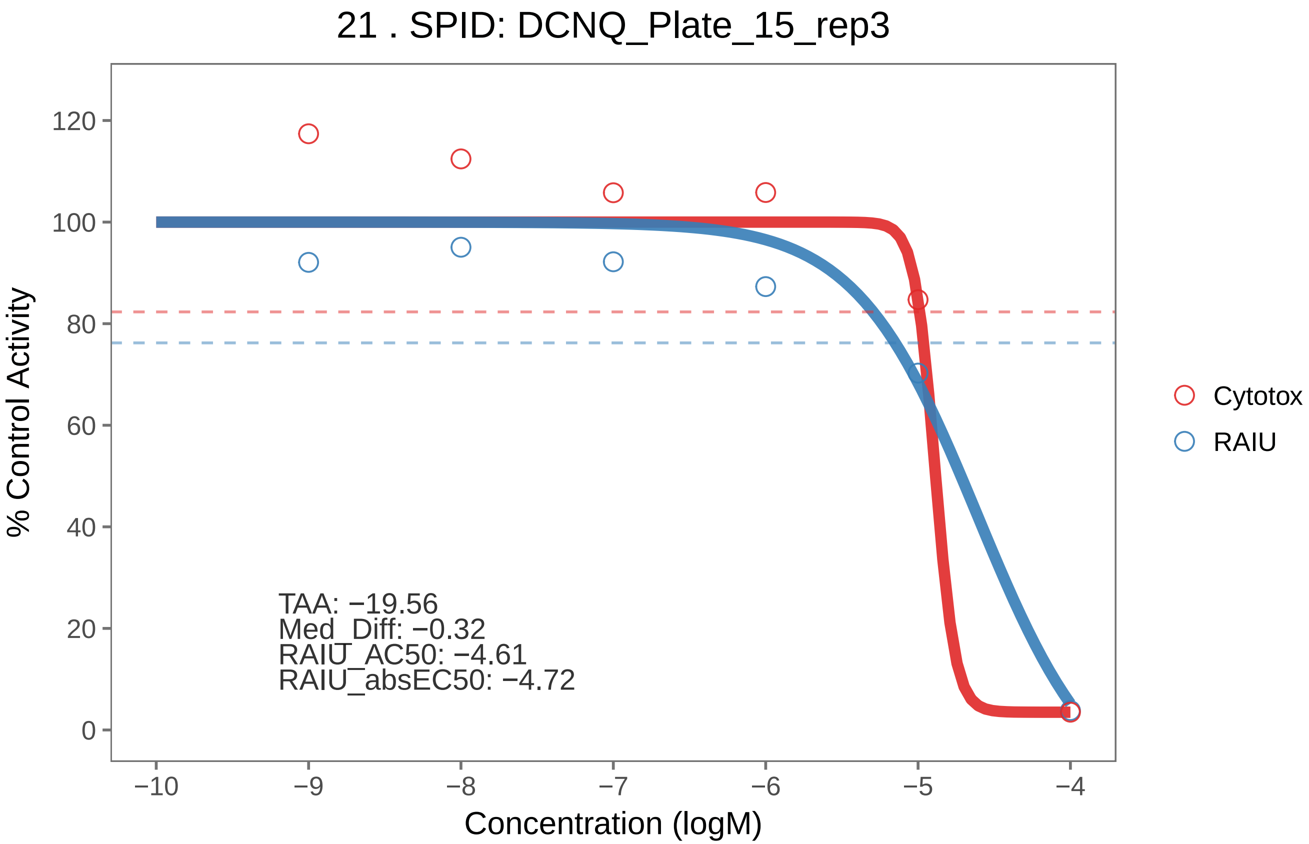

17 . SPID: DCNQ_Plate_14_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −15.24
Med_Diff: 0.2
RAIU_AC50: −4.66
RAIU_absEC50: −4.79

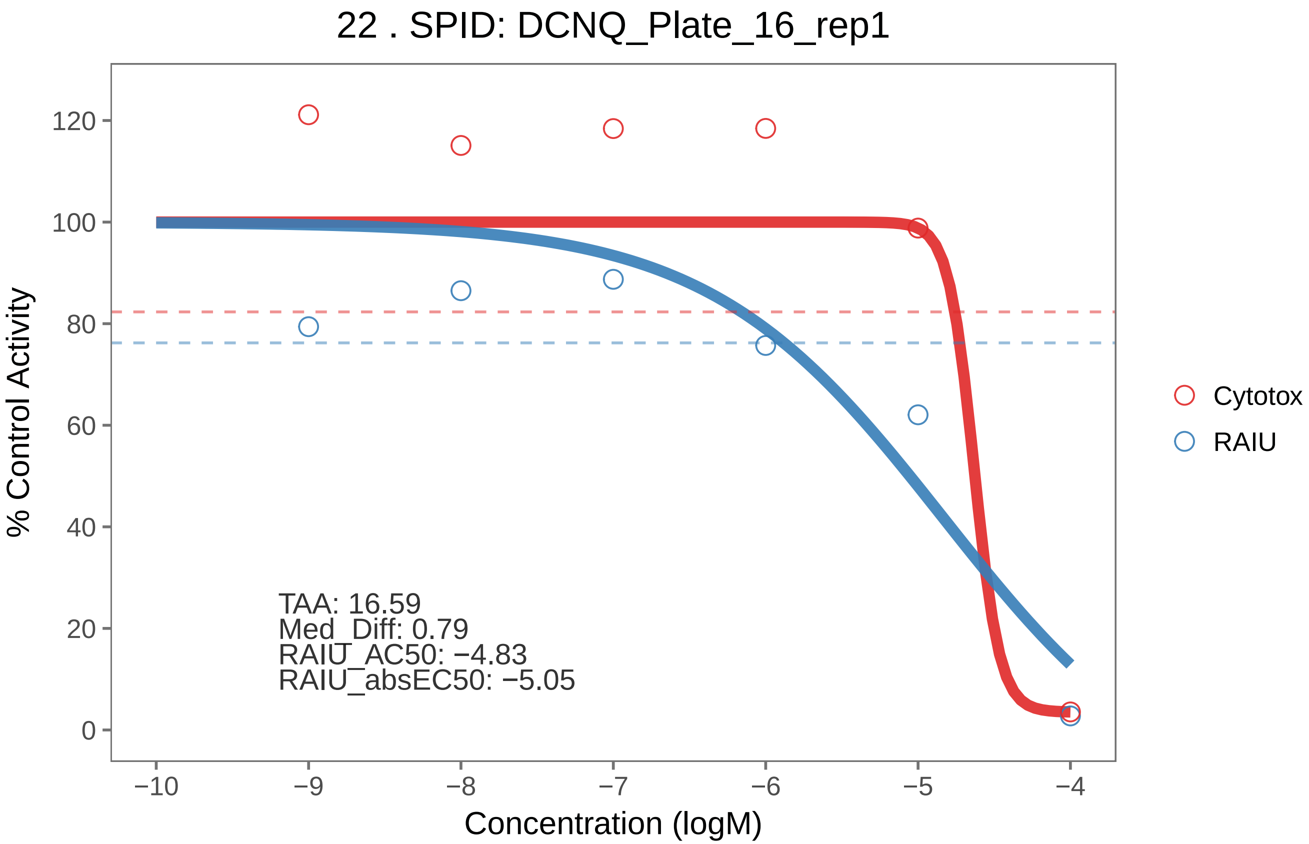

18 . SPID: DCNQ_Plate_14_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −5.07
Med_Diff: 0.99
RAIU_AC50: −4.78
RAIU_absEC50: −4.98
Cytotox
RAIU

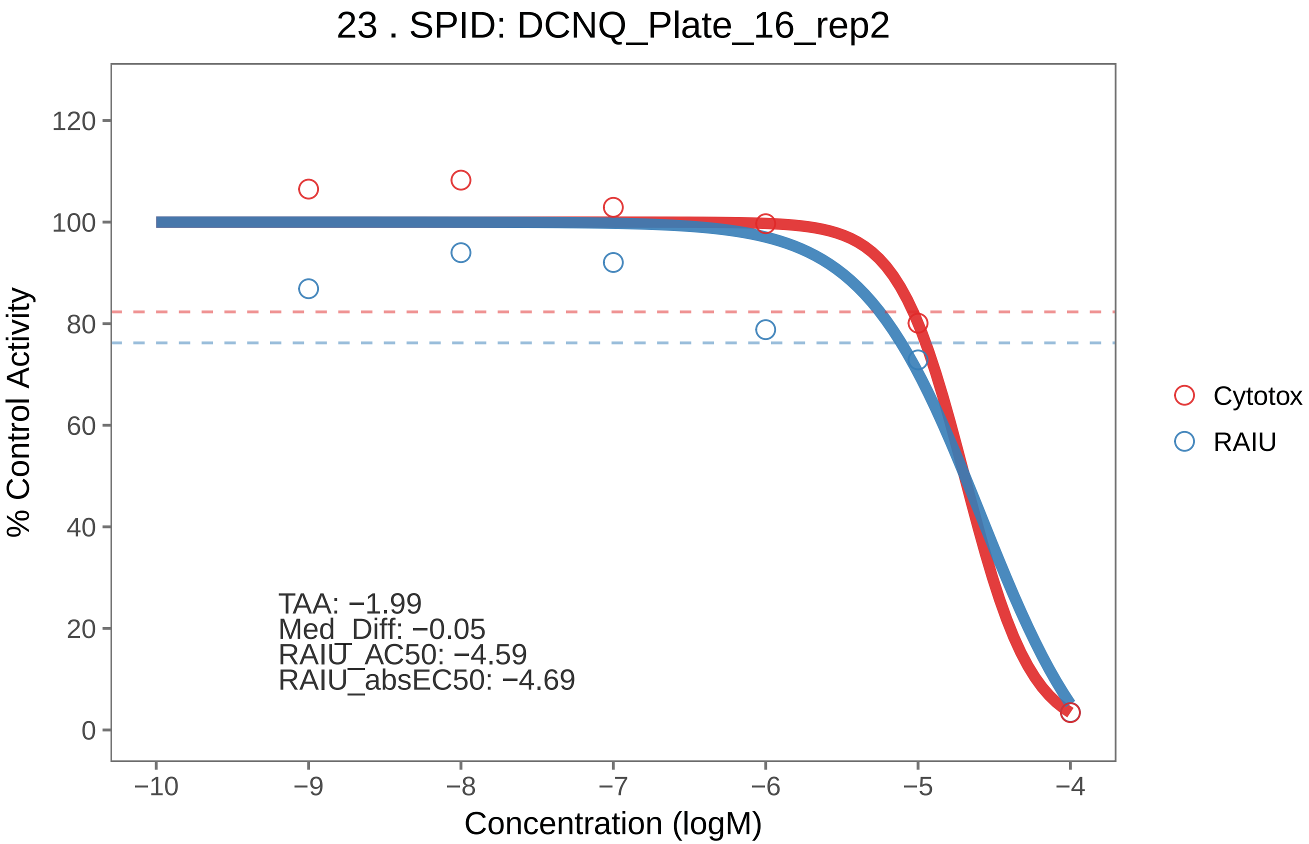


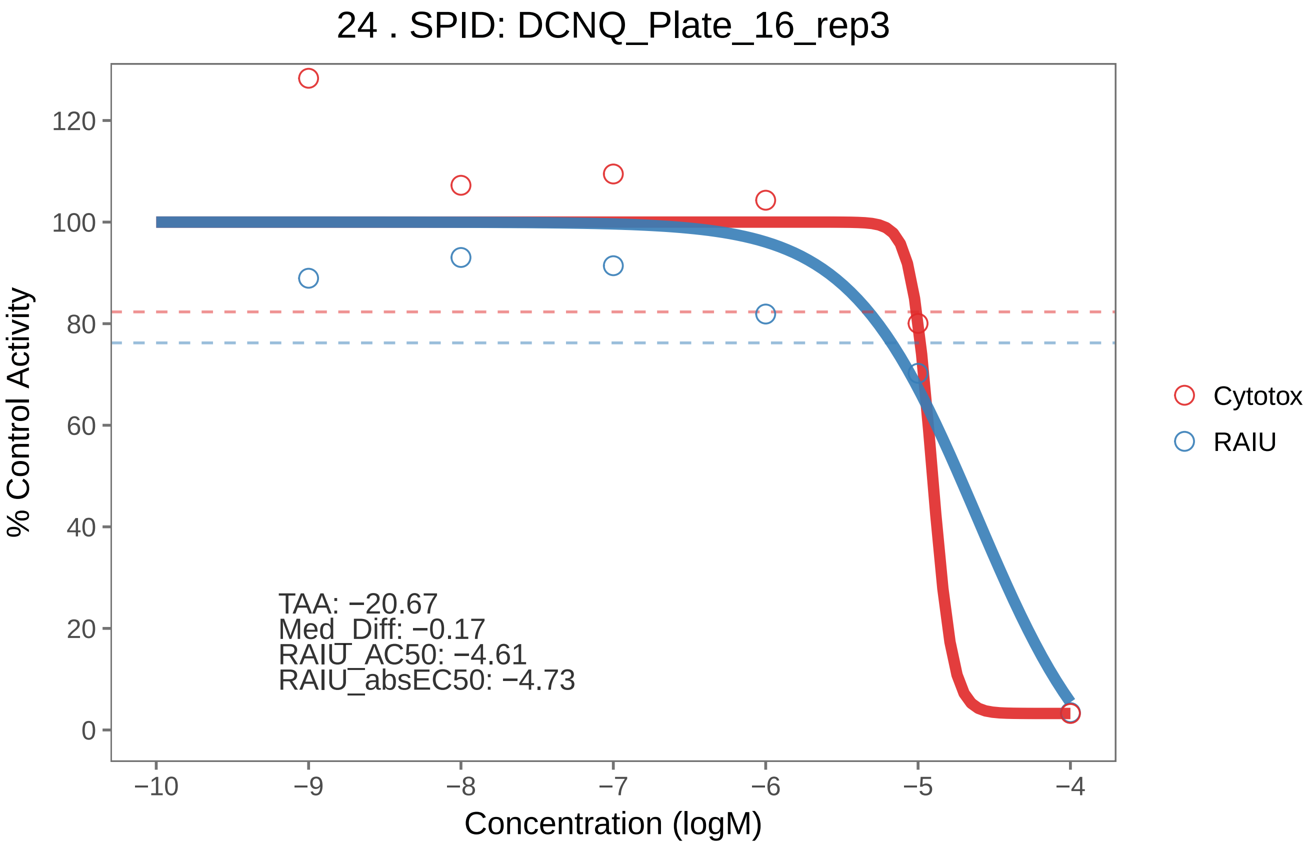
19 . SPID: DCNQ_Plate_15_rep1
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Cytotox
RAIU
TAA: −15.51
Med_Diff: 0.74
RAIU_AC50: −4.6
RAIU_absEC50: −4.71

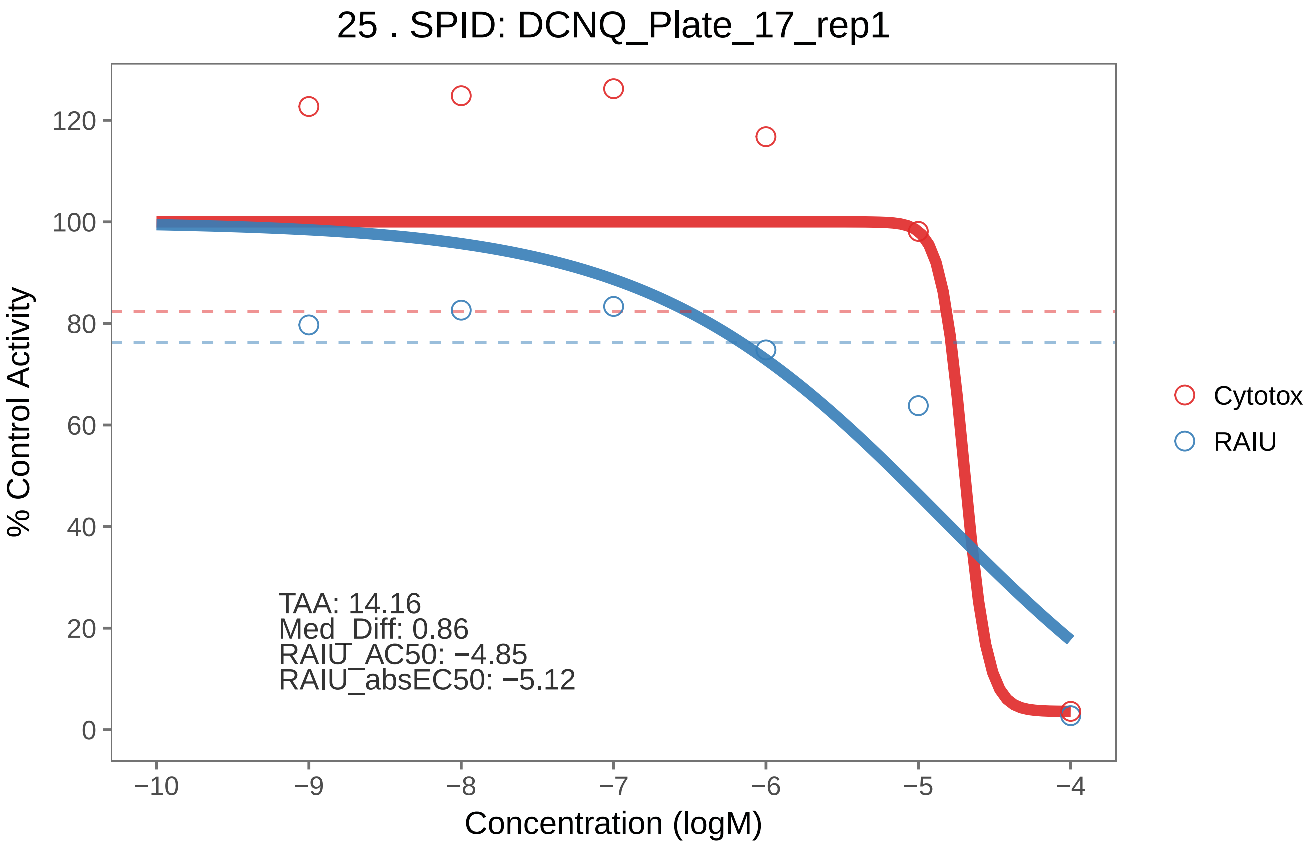

20 . SPID: DCNQ_Plate_15_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 5.82
Med_Diff: −0.87
RAIU_AC50: −4.95
RAIU_absEC50: −4.94
Cytotox
RAIU

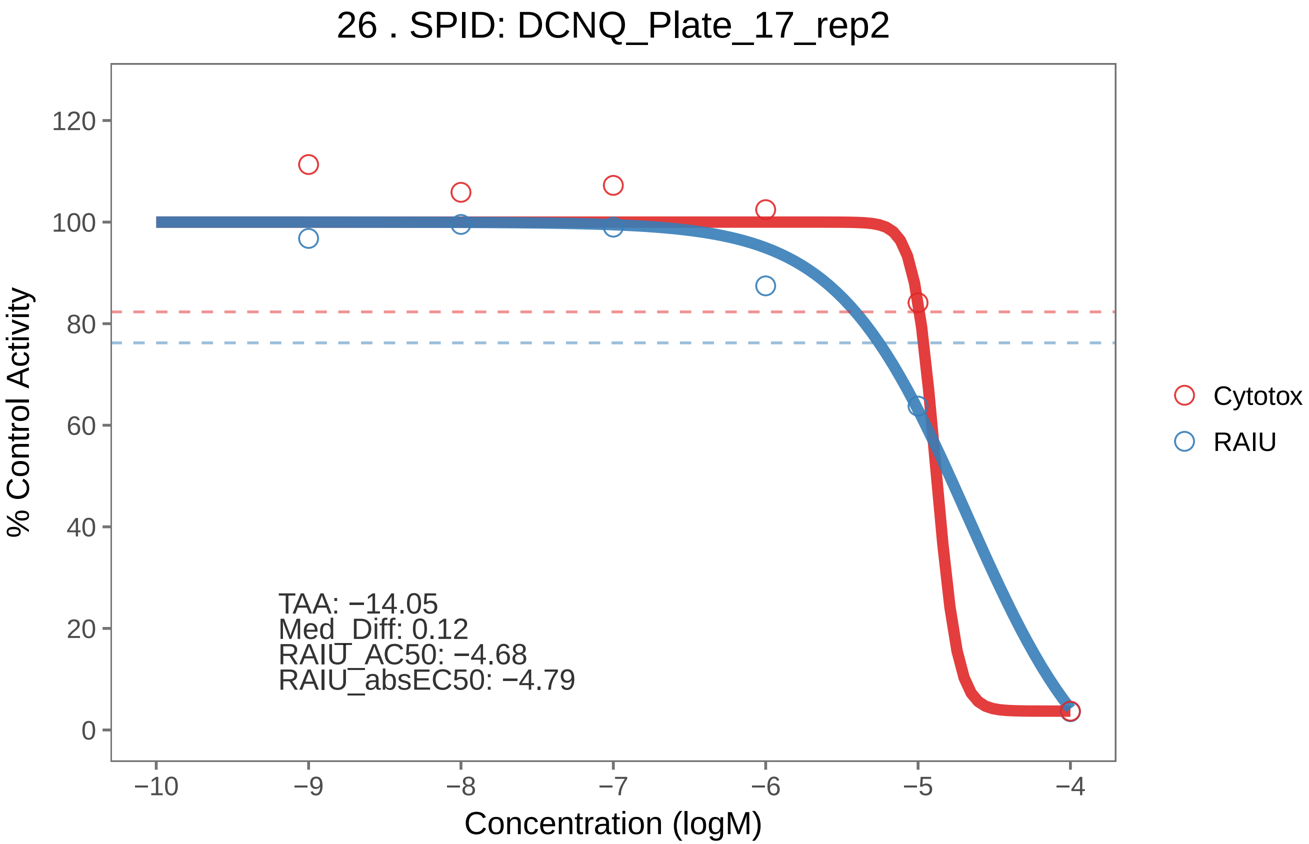

21 . SPID: DCNQ_Plate_15_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −19.56
Med_Diff: −0.32
RAIU_AC50: −4.61
RAIU_absEC50: −4.72
Cytotox
RAIU

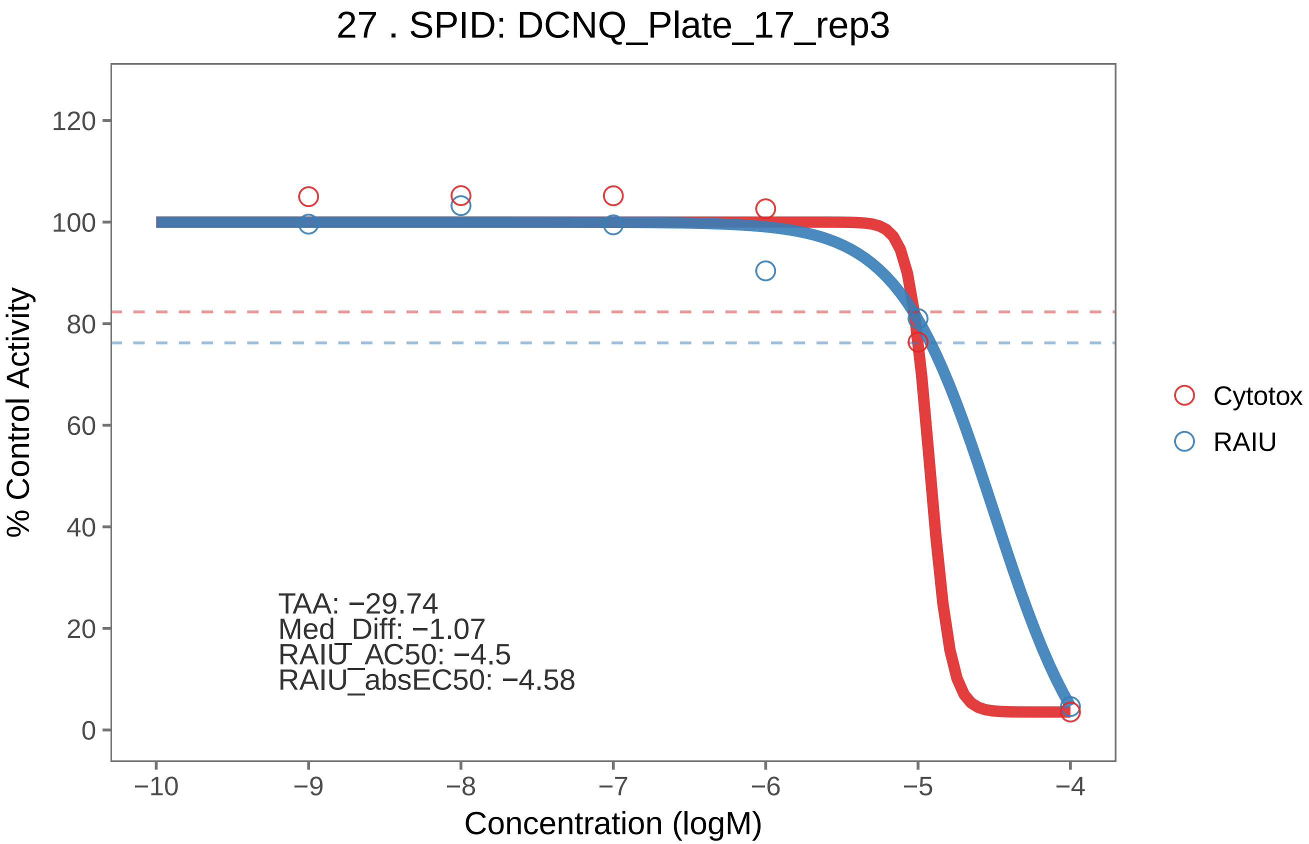

22 . SPID: DCNQ_Plate_16_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 16.59
Med_Diff: 0.79
RAIU_AC50: −4.83
RAIU_absEC50: −5.05
Cytotox
RAIU

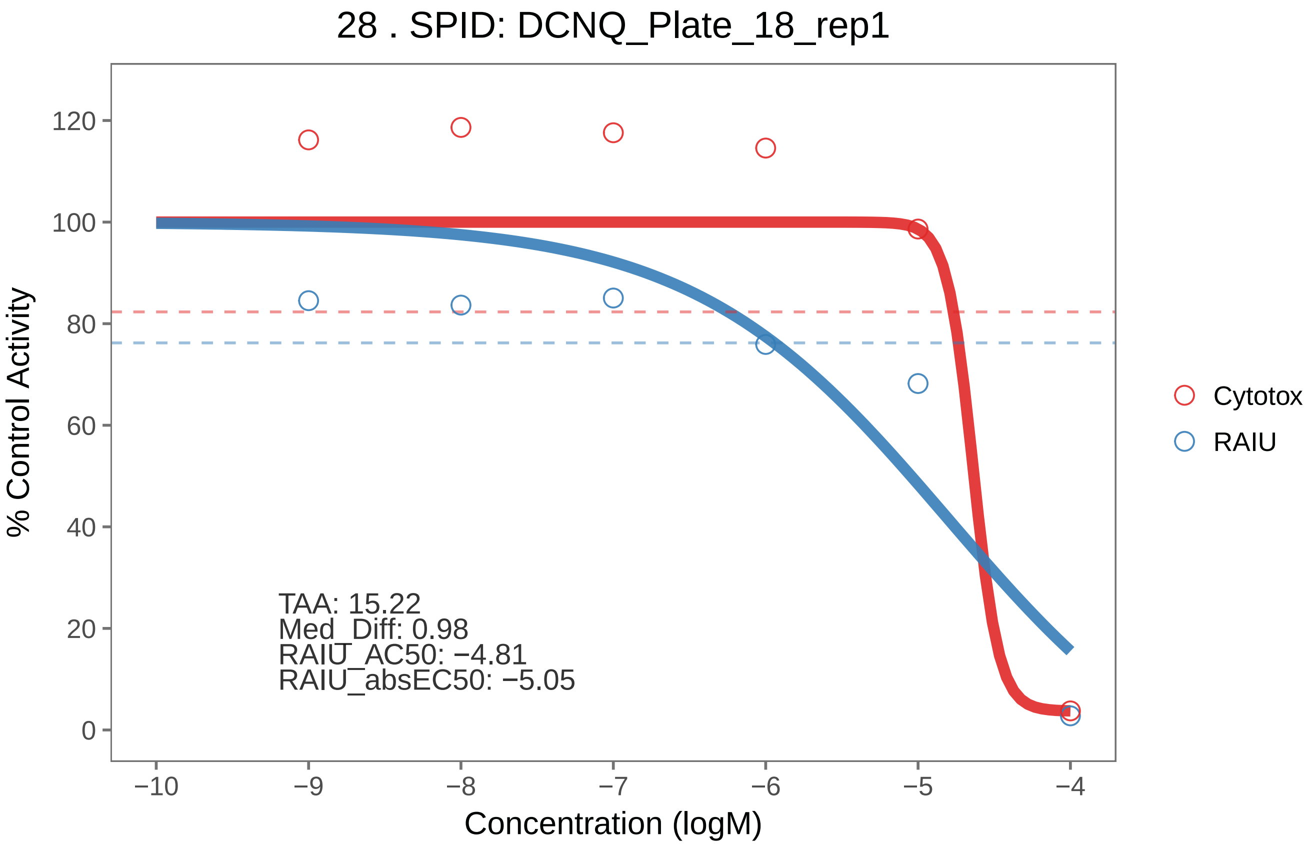

23 . SPID: DCNQ_Plate_16_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −1.99
Med_Diff: −0.05
RAIU_AC50: −4.59
RAIU_absEC50: −4.69

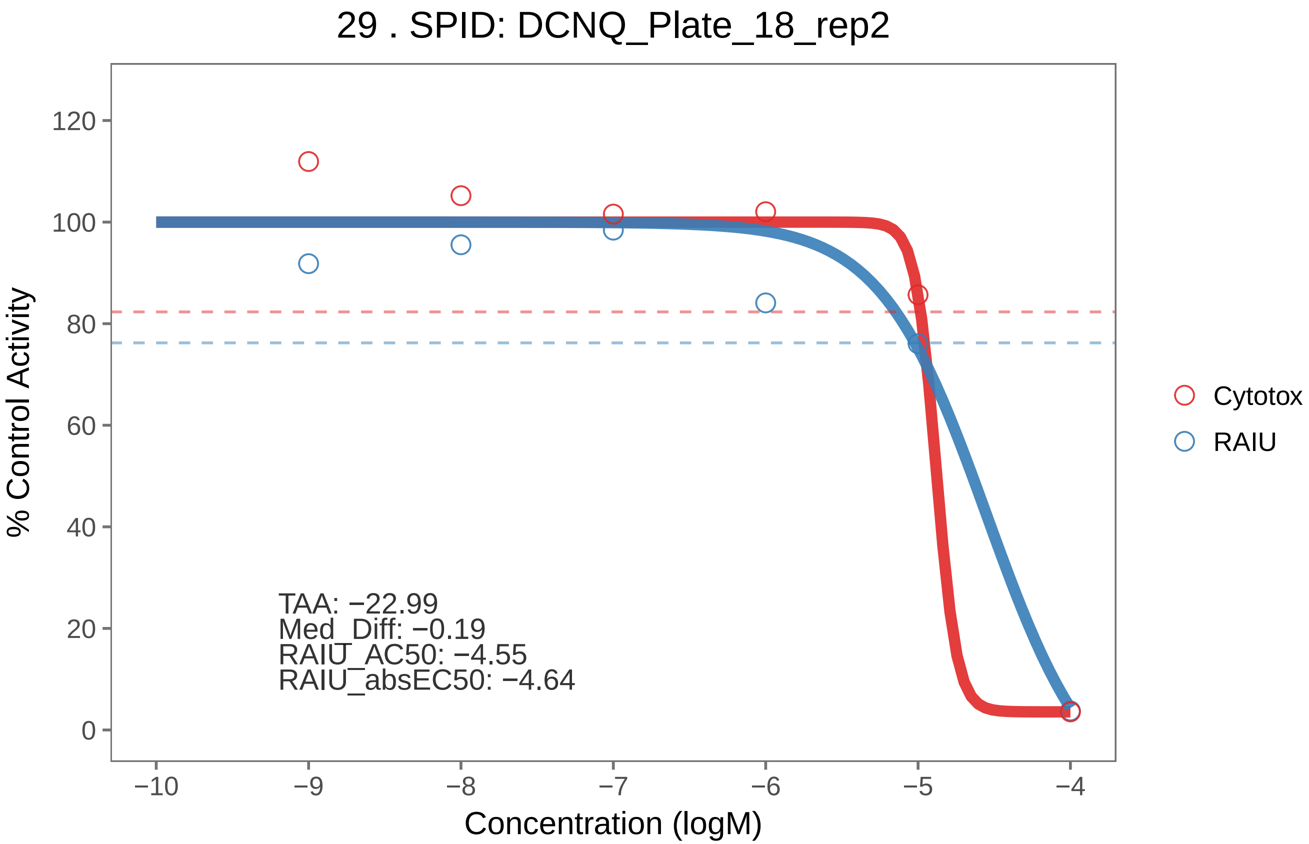

24 . SPID: DCNQ_Plate_16_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −20.67
Med_Diff: −0.17
RAIU_AC50: −4.61
RAIU_absEC50: −4.73
Cytotox
RAIU


25 . SPID: DCNQ_Plate_17_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 14.16
Med_Diff: 0.86
RAIU_AC50: −4.85
RAIU_absEC50: −5.12
Cytotox
RAIU

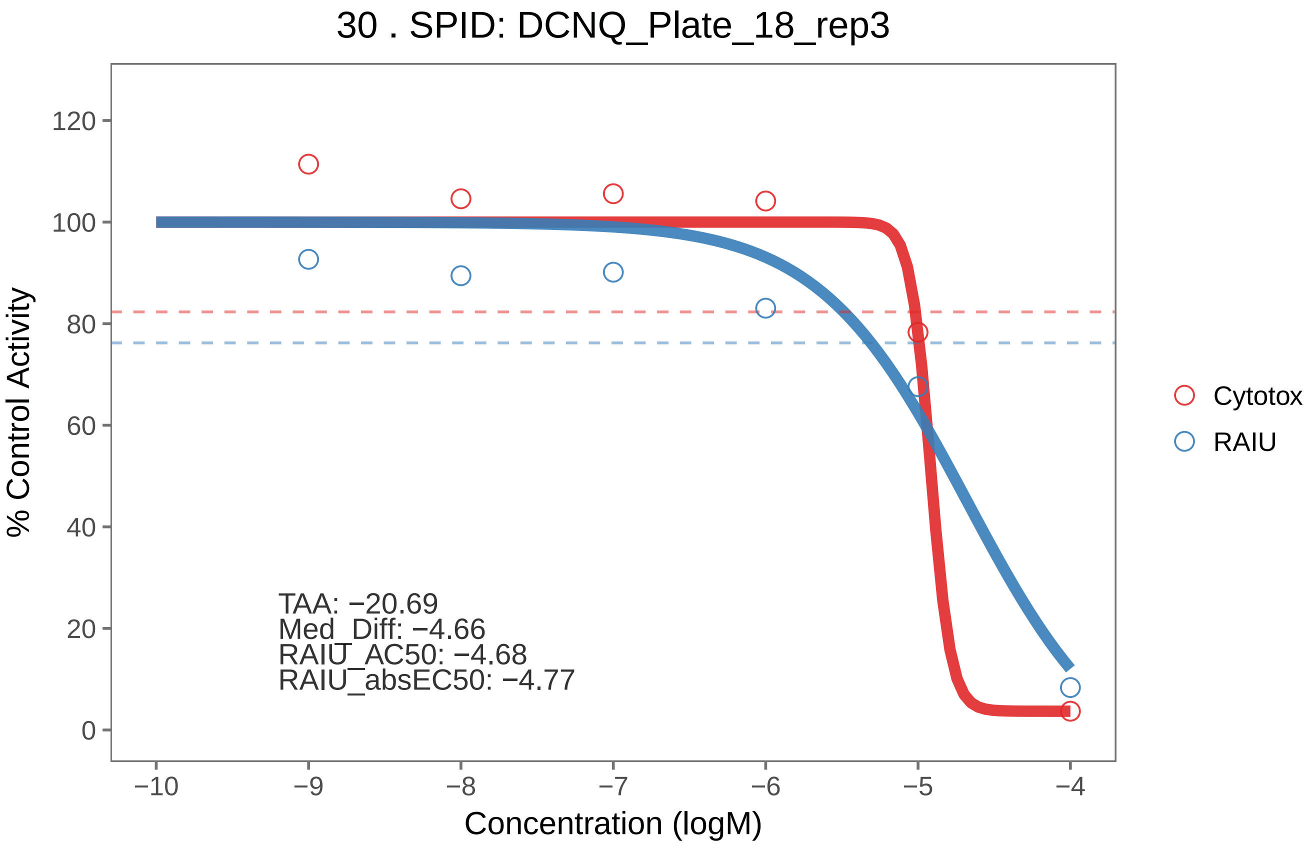

26 . SPID: DCNQ_Plate_17_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −14.05
Med_Diff: 0.12
RAIU_AC50: −4.68
RAIU_absEC50: −4.79
Cytotox
RAIU

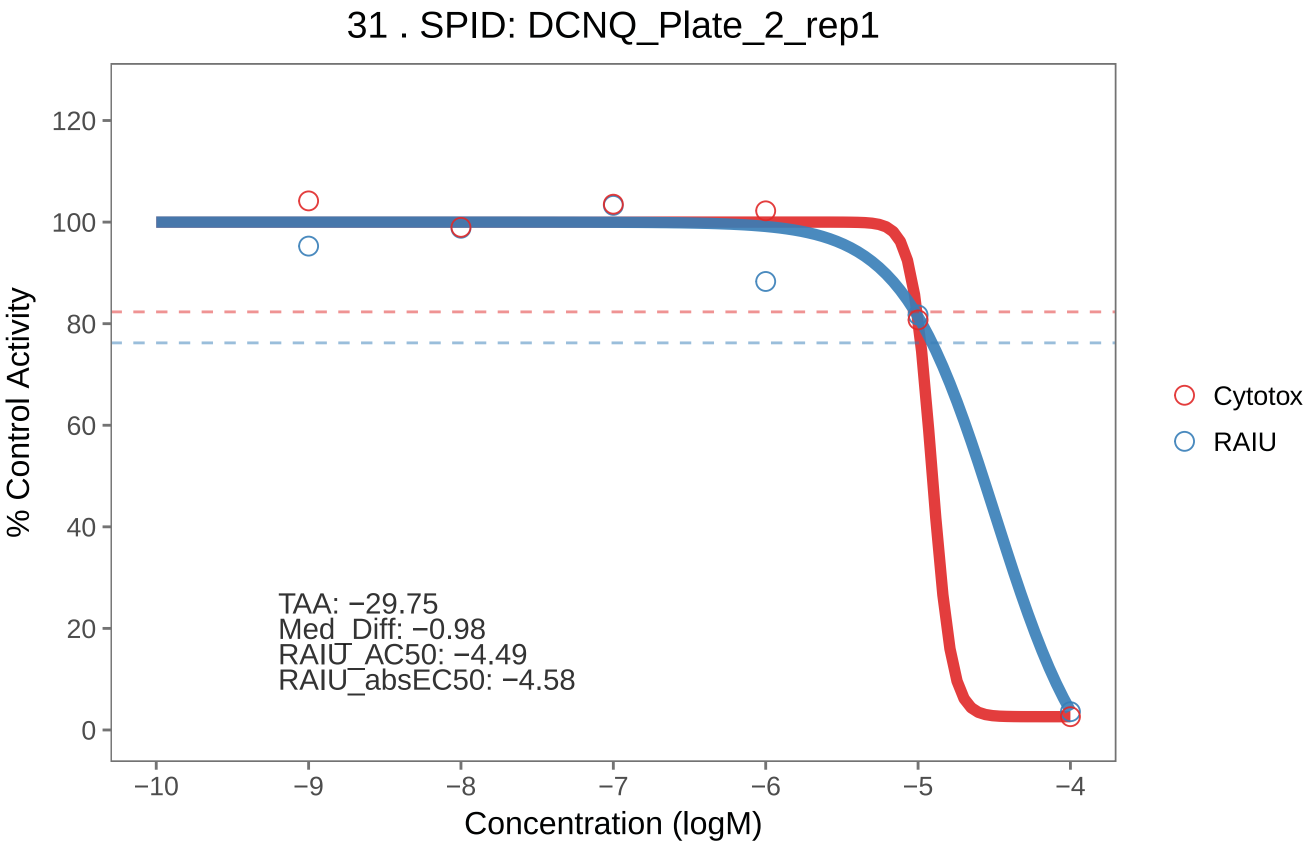

27 . SPID: DCNQ_Plate_17_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −29.74
Med_Diff: −1.07
RAIU_AC50: −4.5
RAIU_absEC50: −4.58
Cytotox
RAIU


28 . SPID: DCNQ_Plate_18_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 15.22
Med_Diff: 0.98
RAIU_AC50: −4.81
RAIU_absEC50: −5.05
Cytotox
RAIU

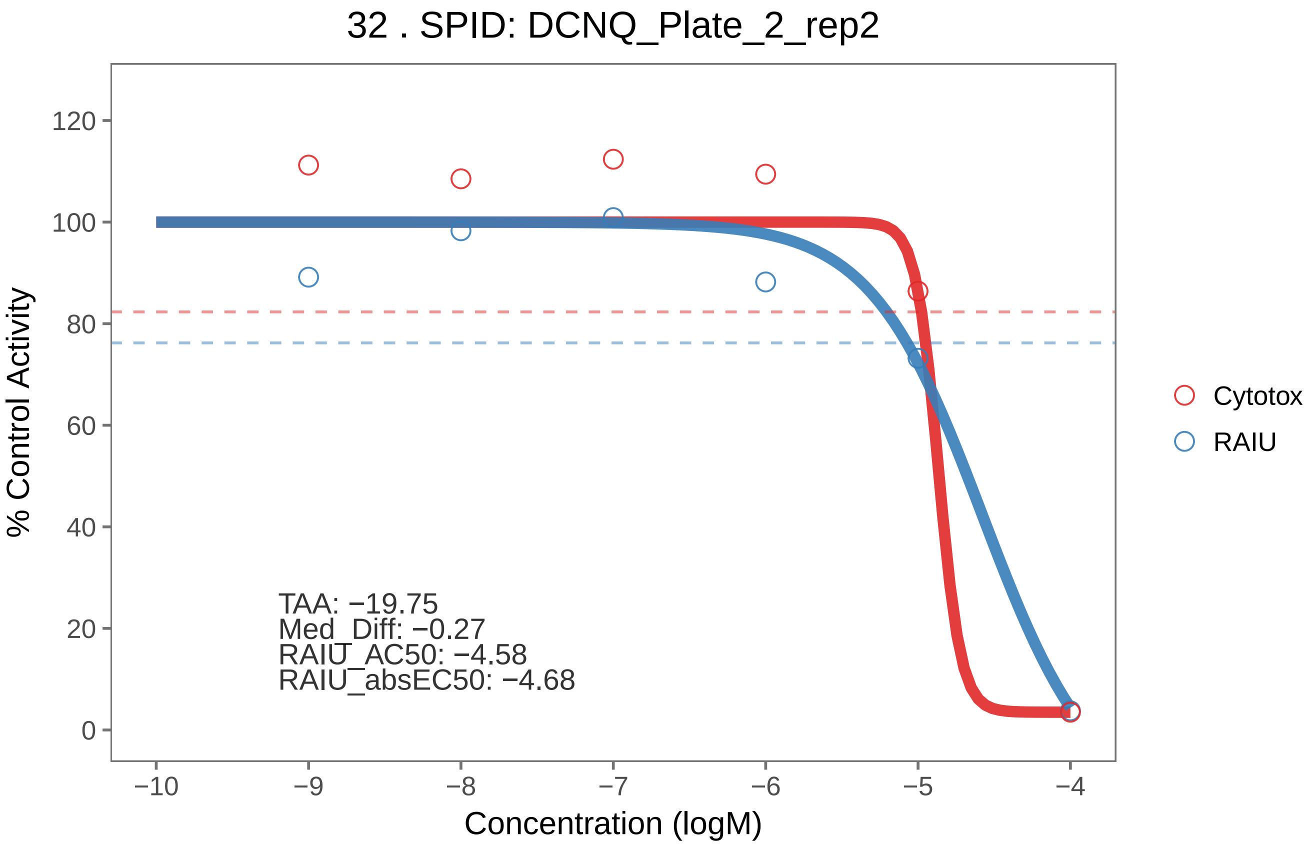


29 . SPID: DCNQ_Plate_18_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −22.99
Med_Diff: −0.19
RAIU_AC50: −4.55
RAIU_absEC50: −4.64

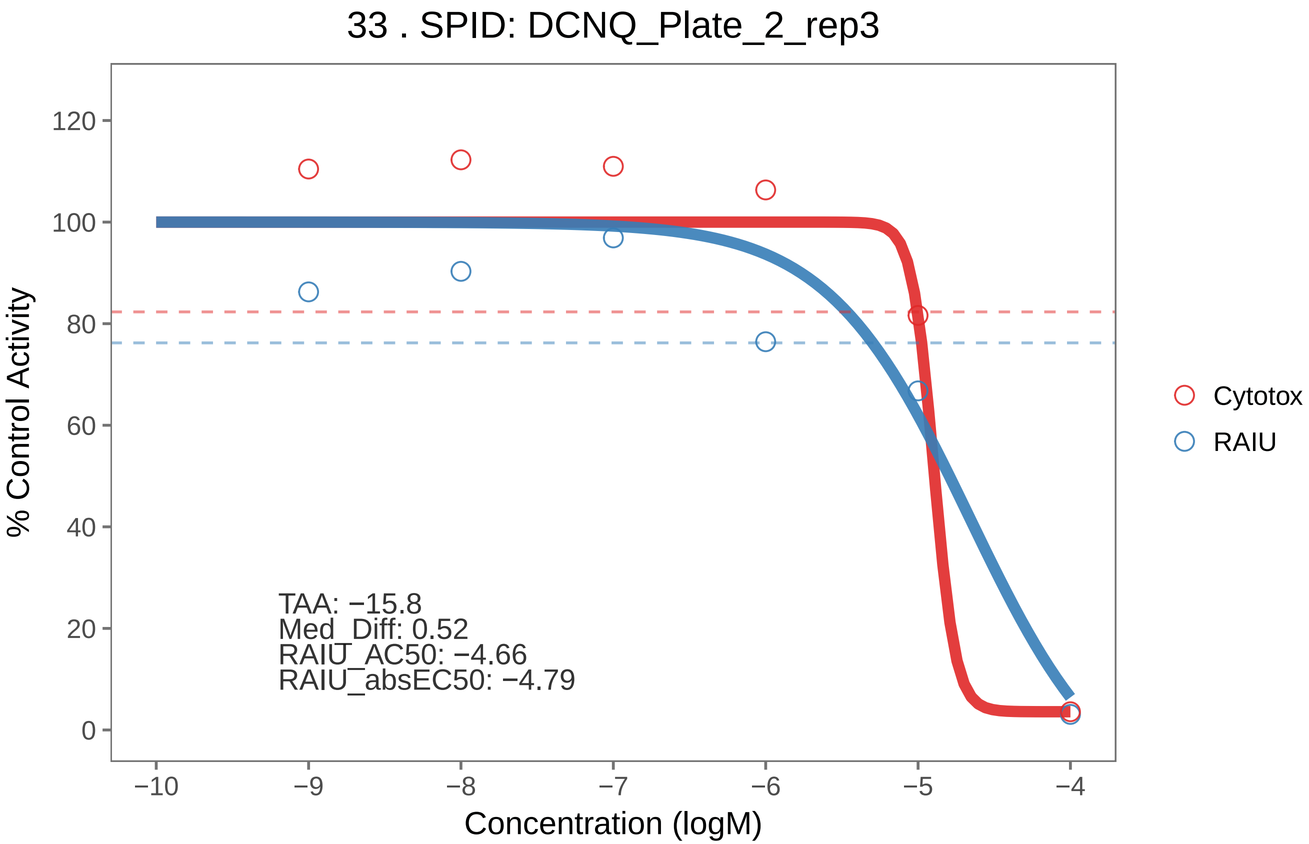

30 . SPID: DCNQ_Plate_18_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −20.69
Med_Diff: −4.66
RAIU_AC50: −4.68
RAIU_absEC50: −4.77
Cytotox
RAIU

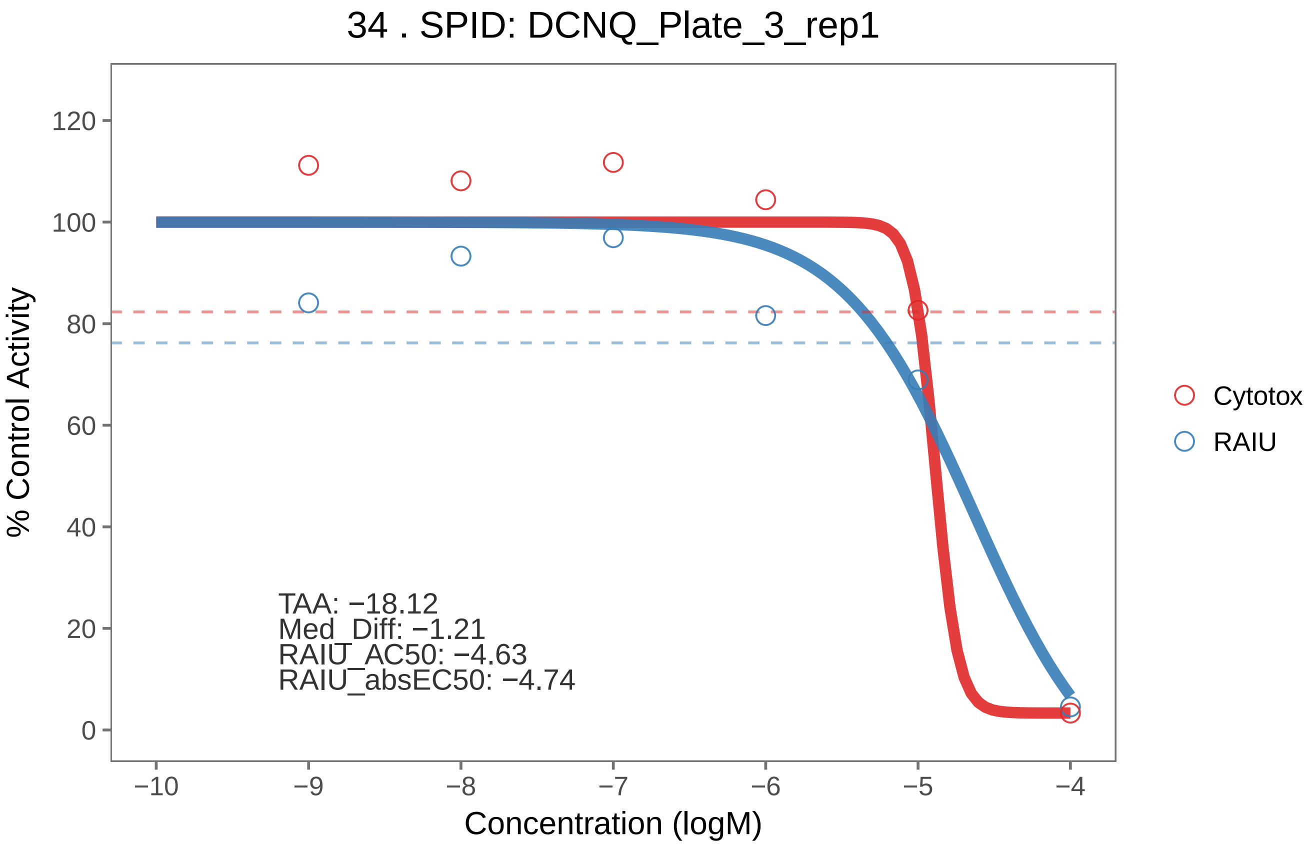


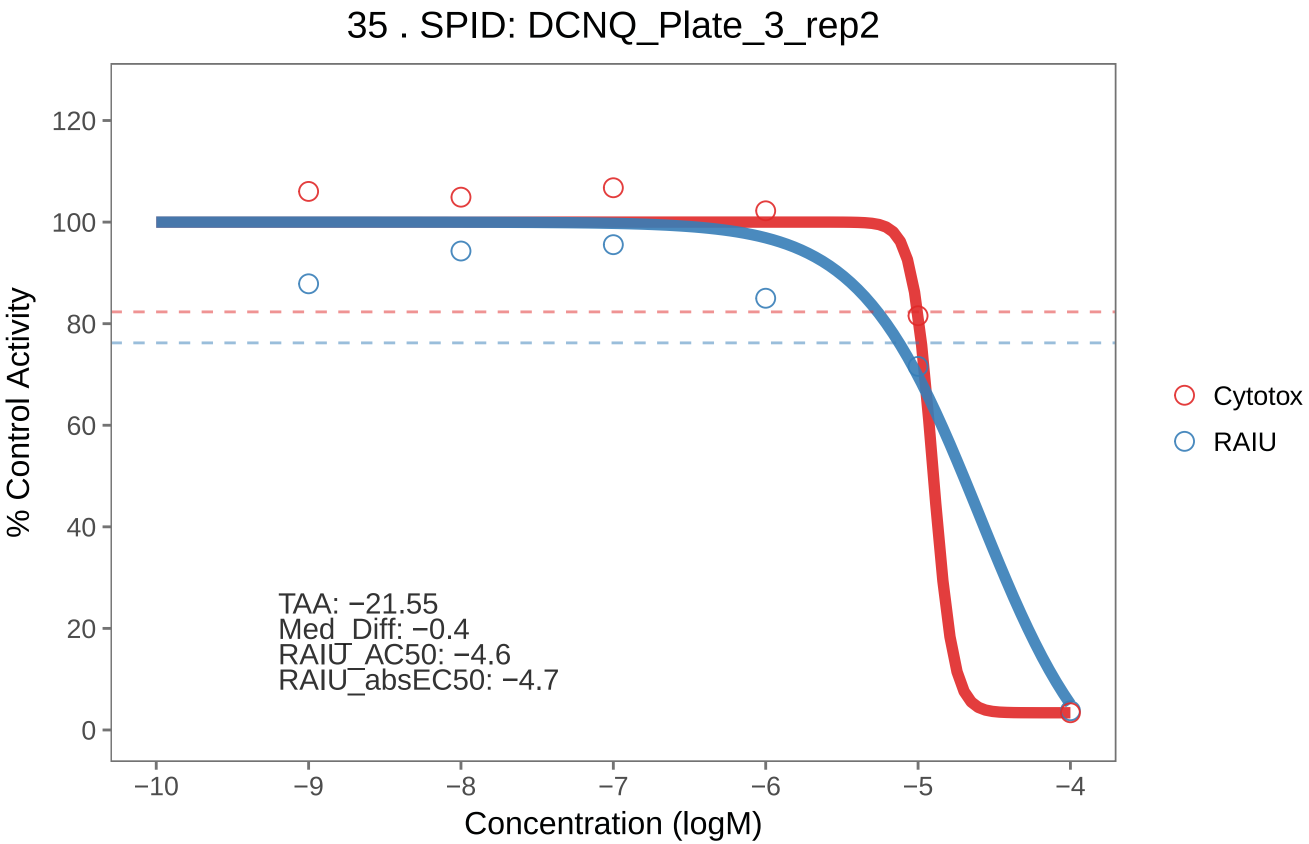
31 . SPID: DCNQ_Plate_2_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −29.75
Med_Diff: −0.98
RAIU_AC50: −4.49
RAIU_absEC50: −4.58
Cytotox
RAIU

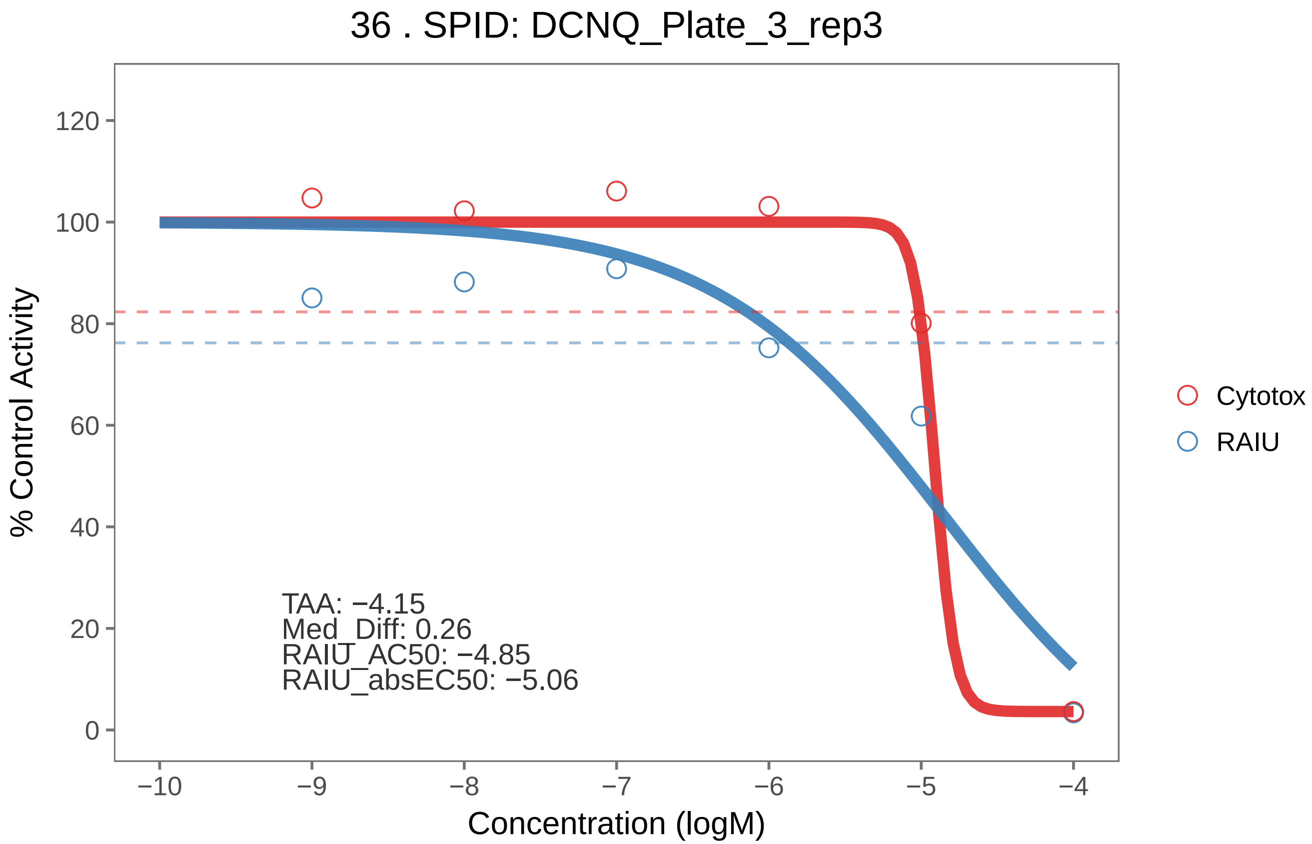


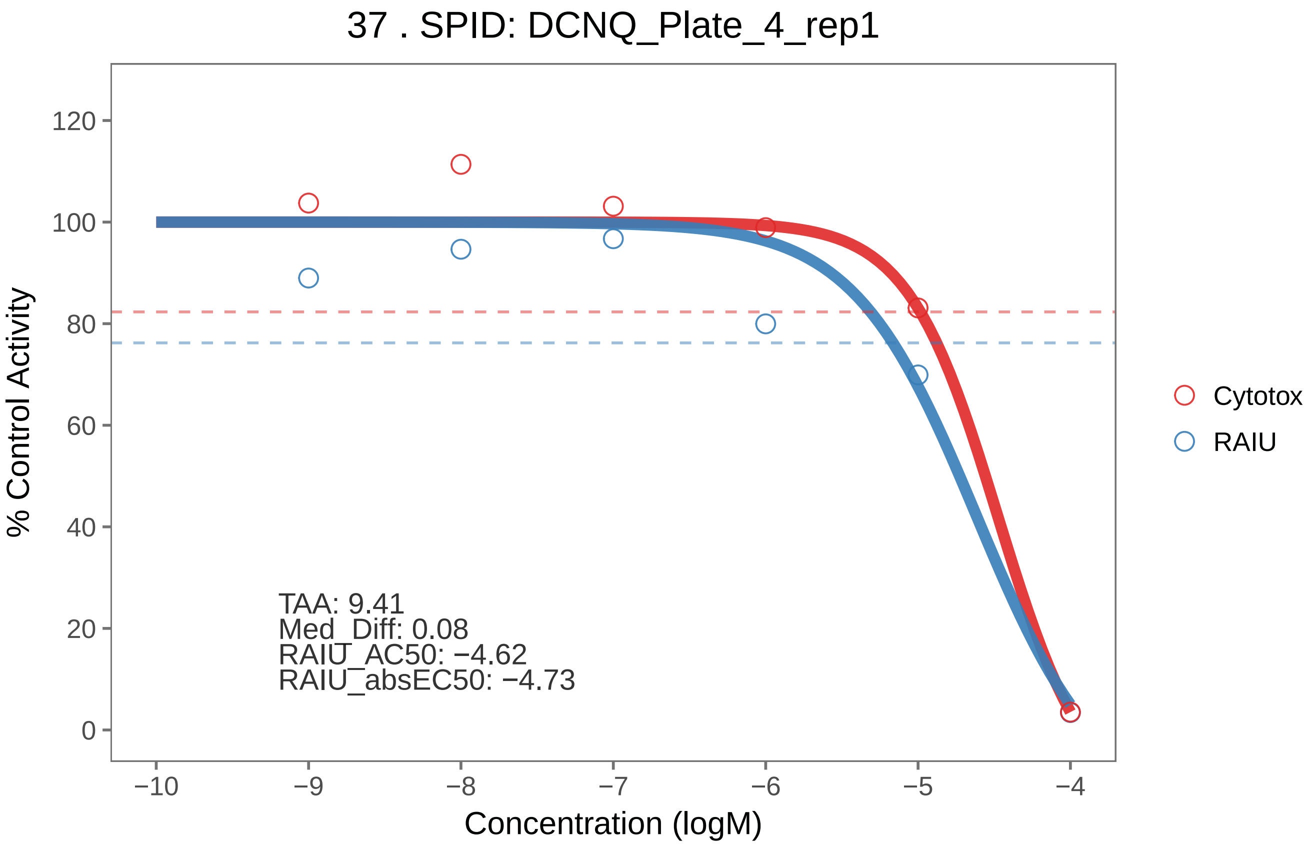
32 . SPID: DCNQ_Plate_2_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −19.75
Med_Diff: −0.27
RAIU_AC50: −4.58
RAIU_absEC50: −4.68
Cytotox
RAIU


33 . SPID: DCNQ_Plate_2_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −15.8
Med_Diff: 0.52
RAIU_AC50: −4.66
RAIU_absEC50: −4.79
Cytotox
RAIU

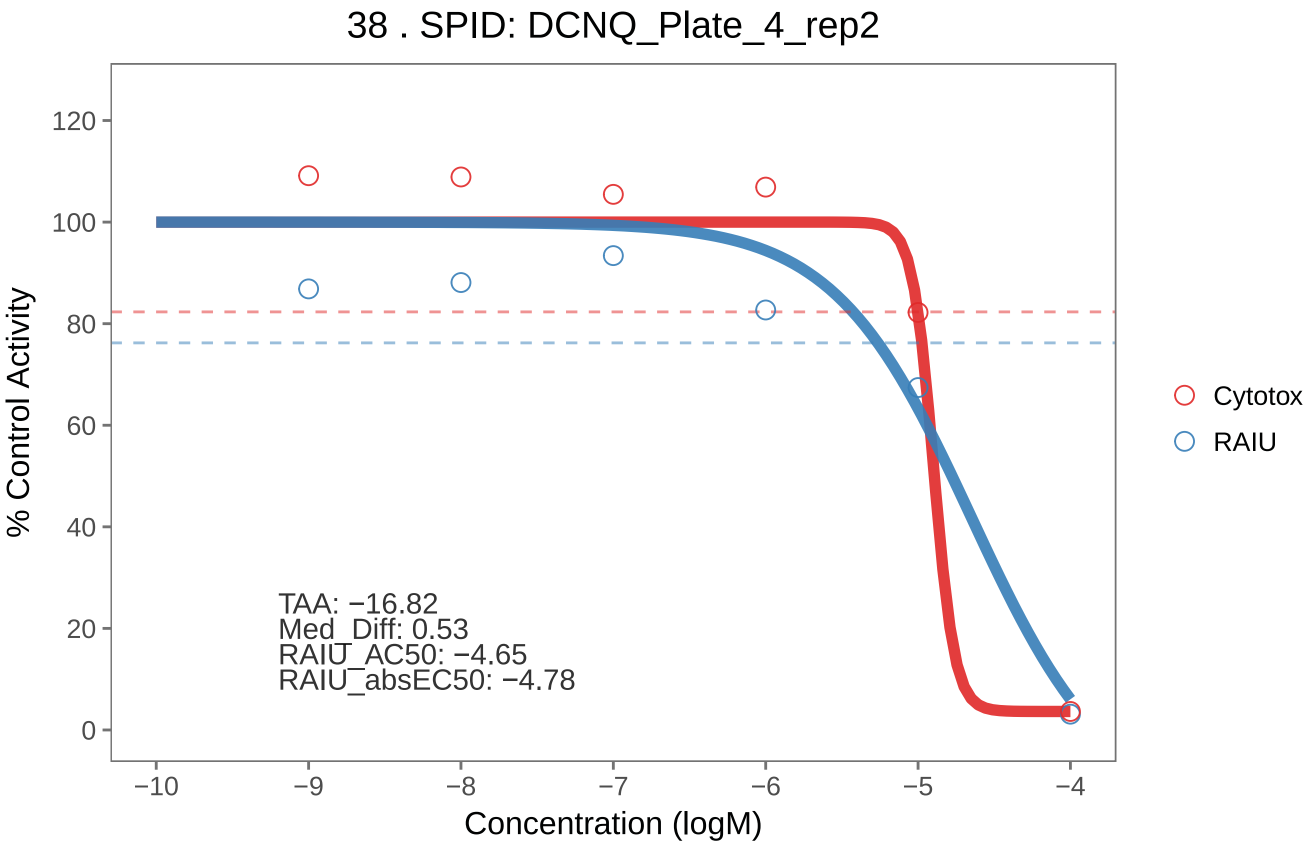

34 . SPID: DCNQ_Plate_3_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −18.12
Med_Diff: −1.21
RAIU_AC50: −4.63
RAIU_absEC50: −4.74
Cytotox
RAIU


35 . SPID: DCNQ_Plate_3_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −21.55
Med_Diff: −0.4
RAIU_AC50: −4.6
RAIU_absEC50: −4.7
Cytotox
RAIU

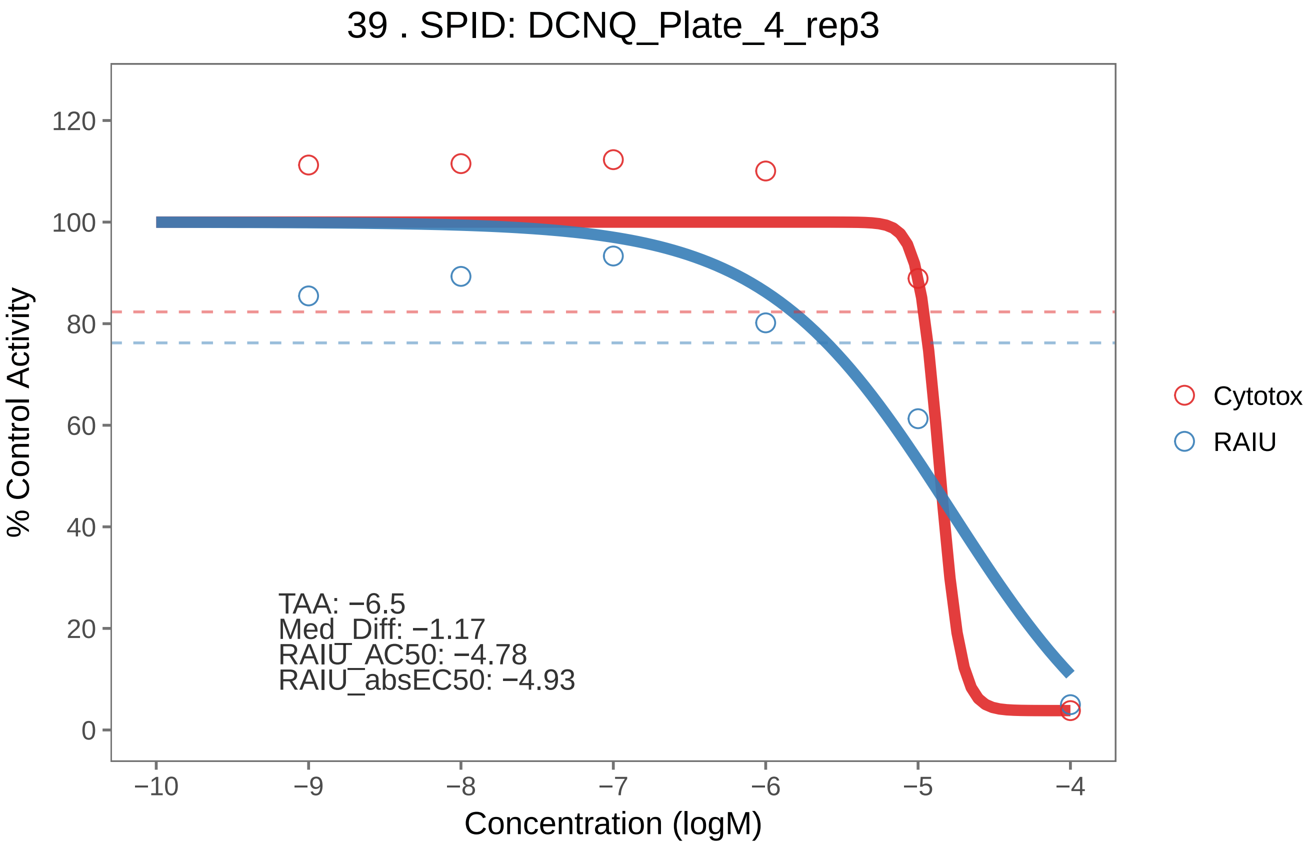

36 . SPID: DCNQ_Plate_3_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −4.15
Med_Diff: 0.26
RAIU_AC50: −4.85
RAIU_absEC50: −5.06

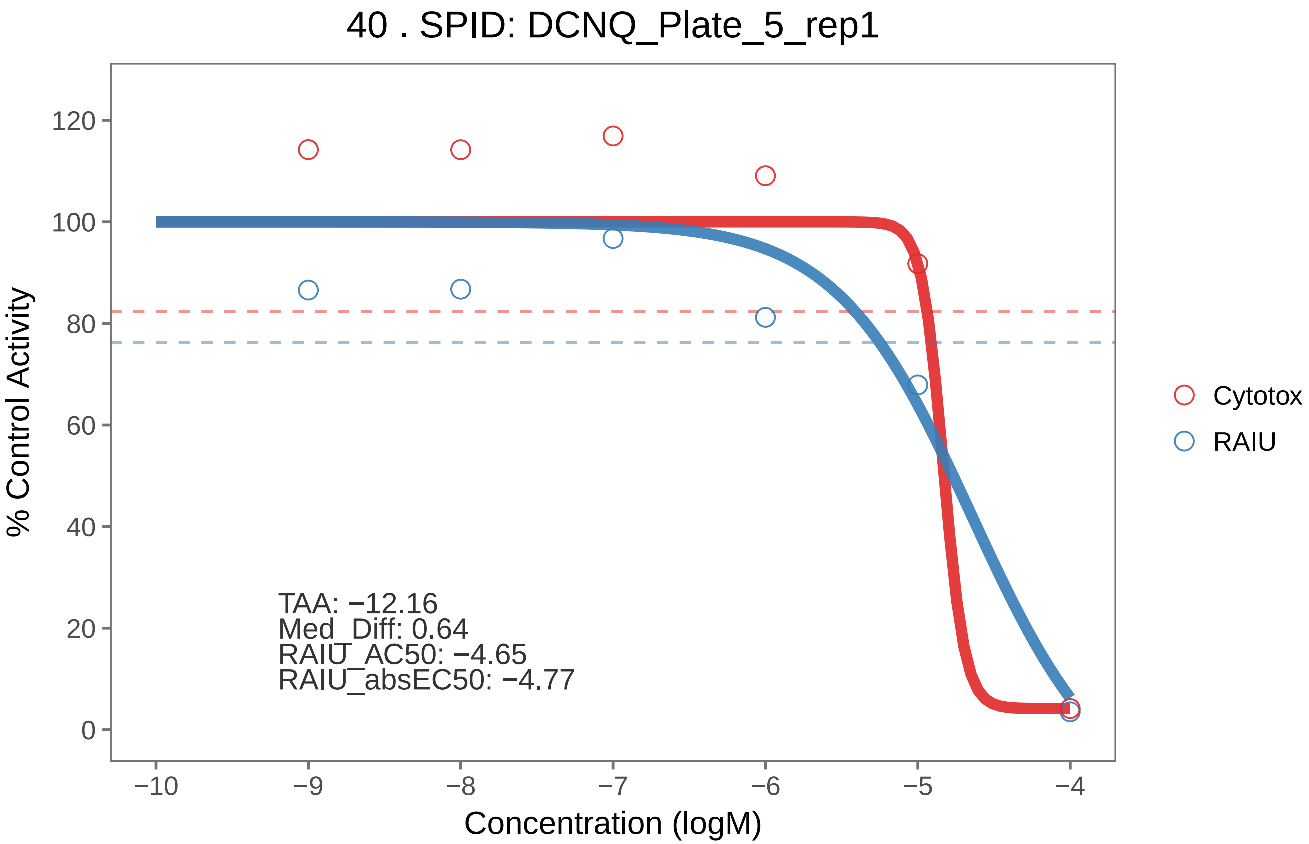


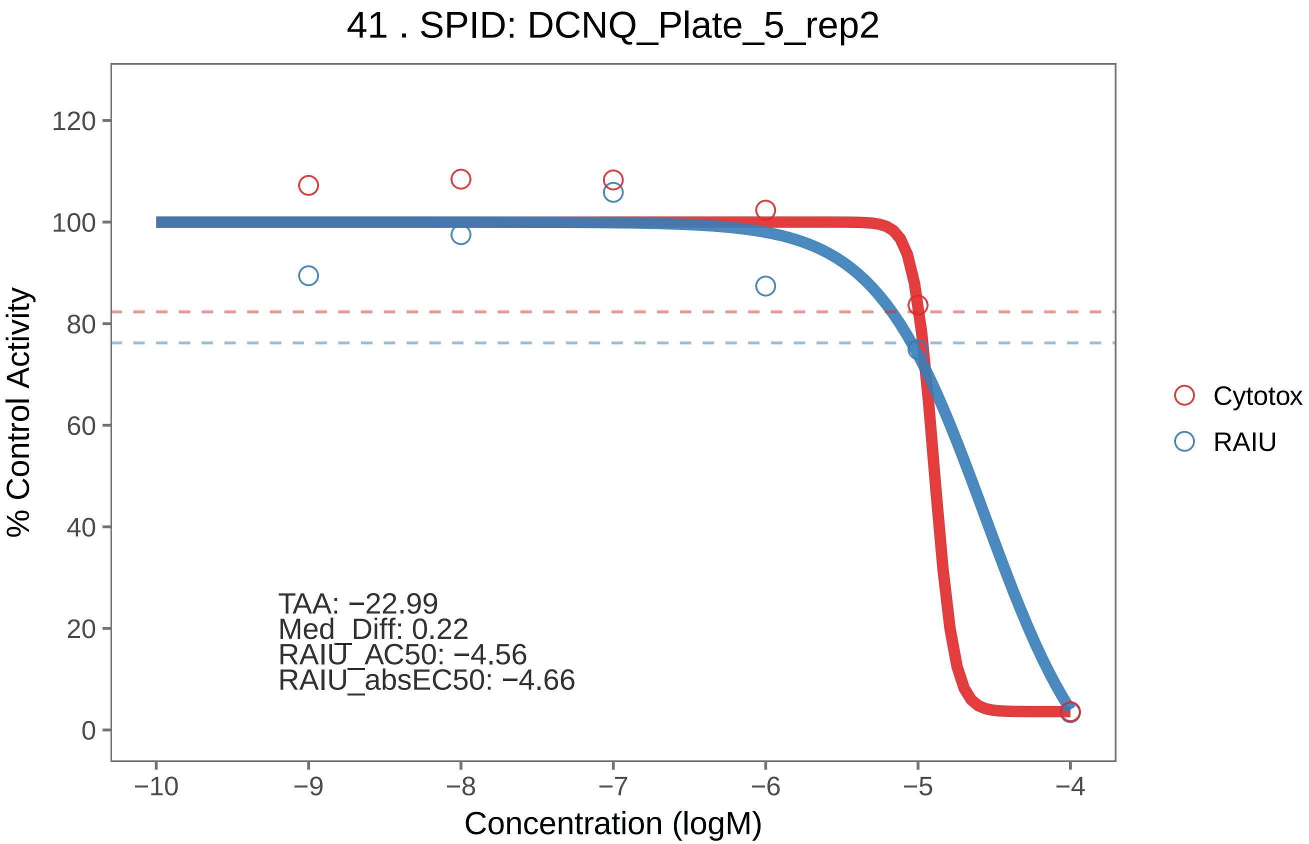
37 . SPID: DCNQ_Plate_4_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 9.41
Med_Diff: 0.08
RAIU_AC50: −4.62
RAIU_absEC50: −4.73
Cytotox
RAIU

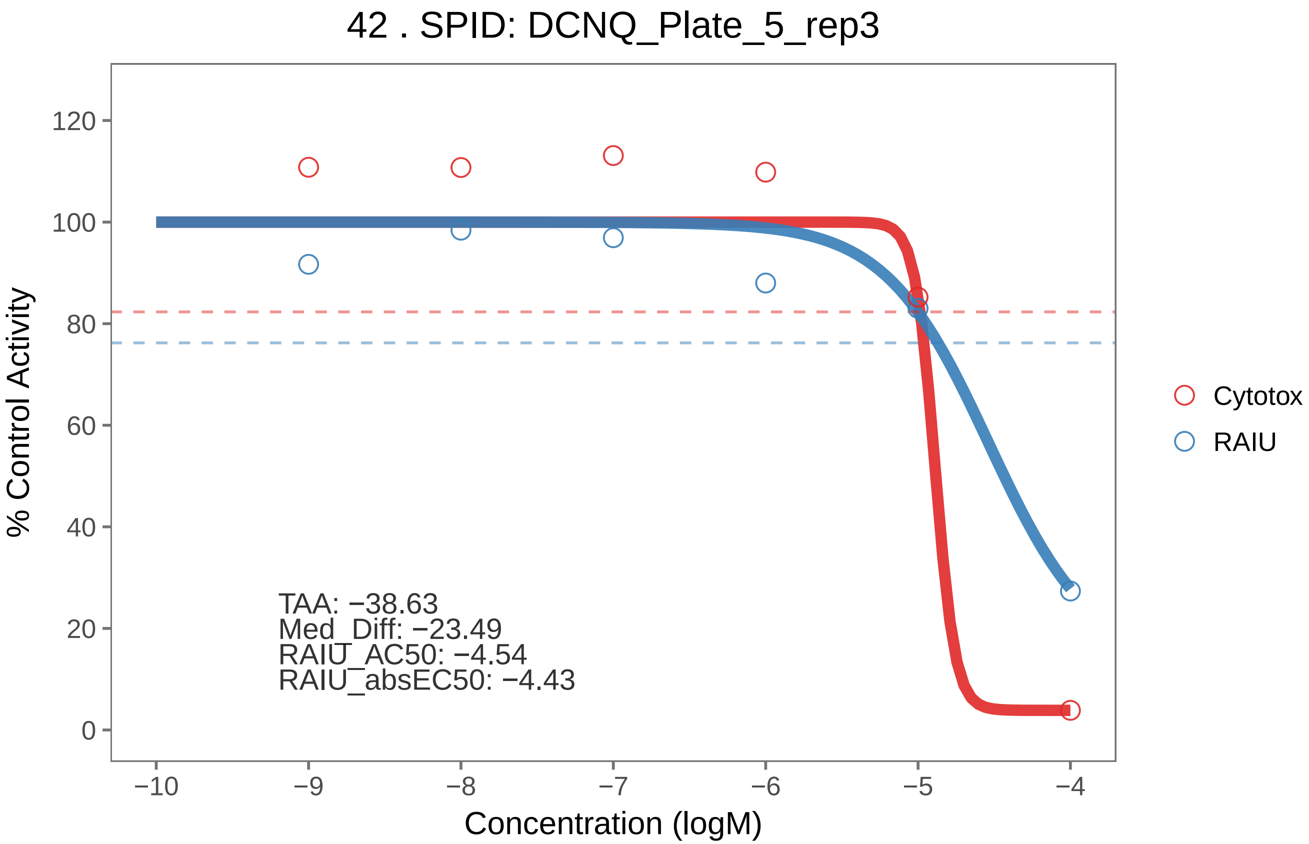


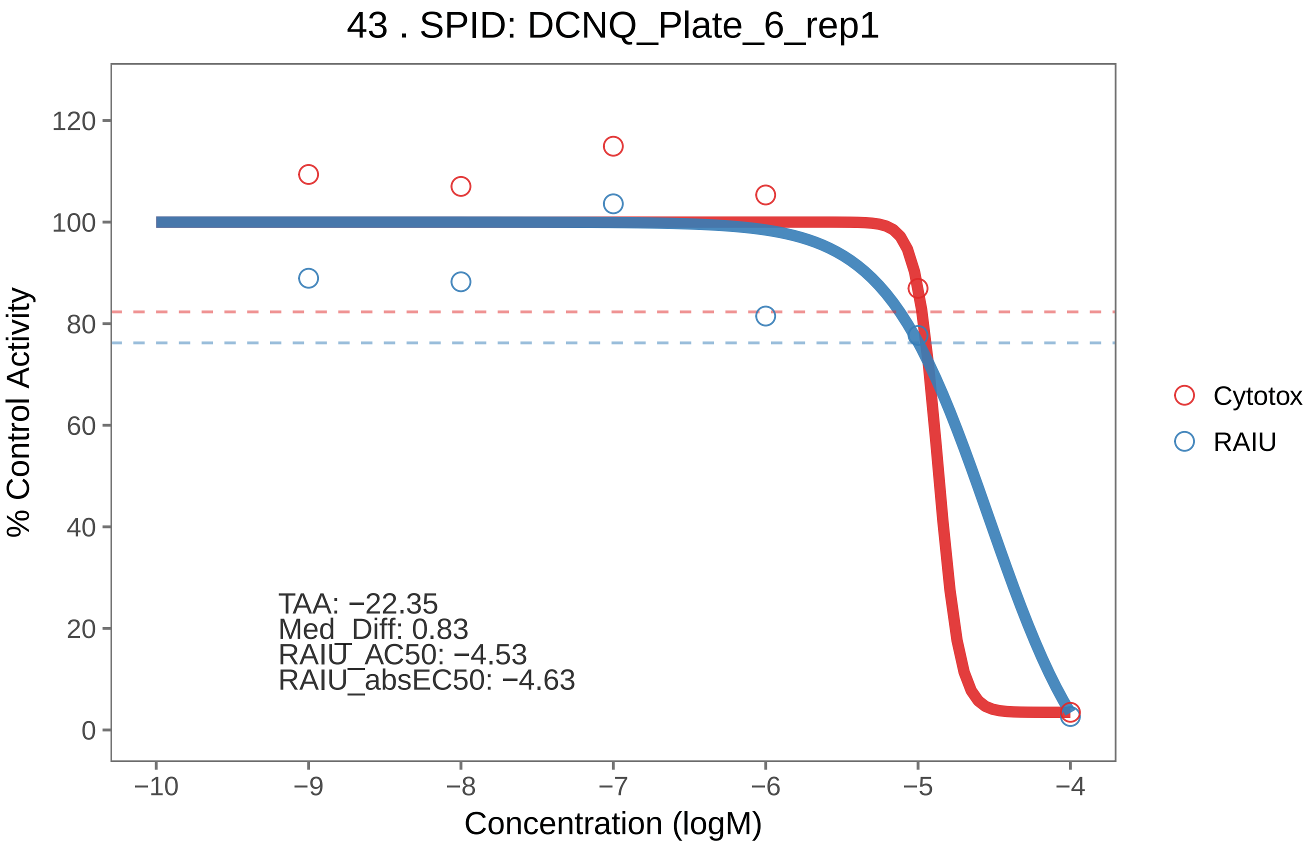
38 . SPID: DCNQ_Plate_4_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −16.82
Med_Diff: 0.53
RAIU_AC50: −4.65
RAIU_absEC50: −4.78
Cytotox
RAIU

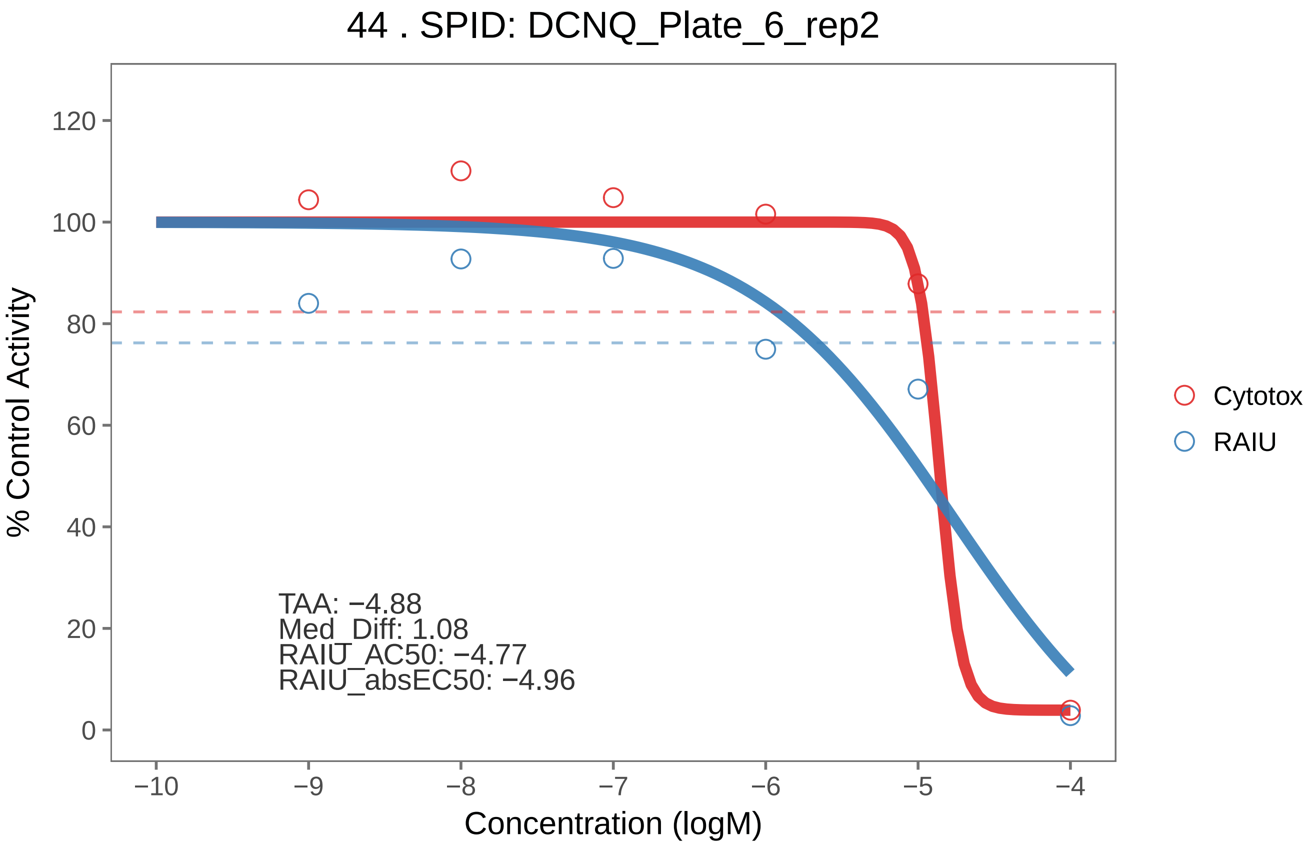

39 . SPID: DCNQ_Plate_4_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −6.5
Med_Diff: −1.17
RAIU_AC50: −4.78
RAIU_absEC50: −4.93
Cytotox
RAIU

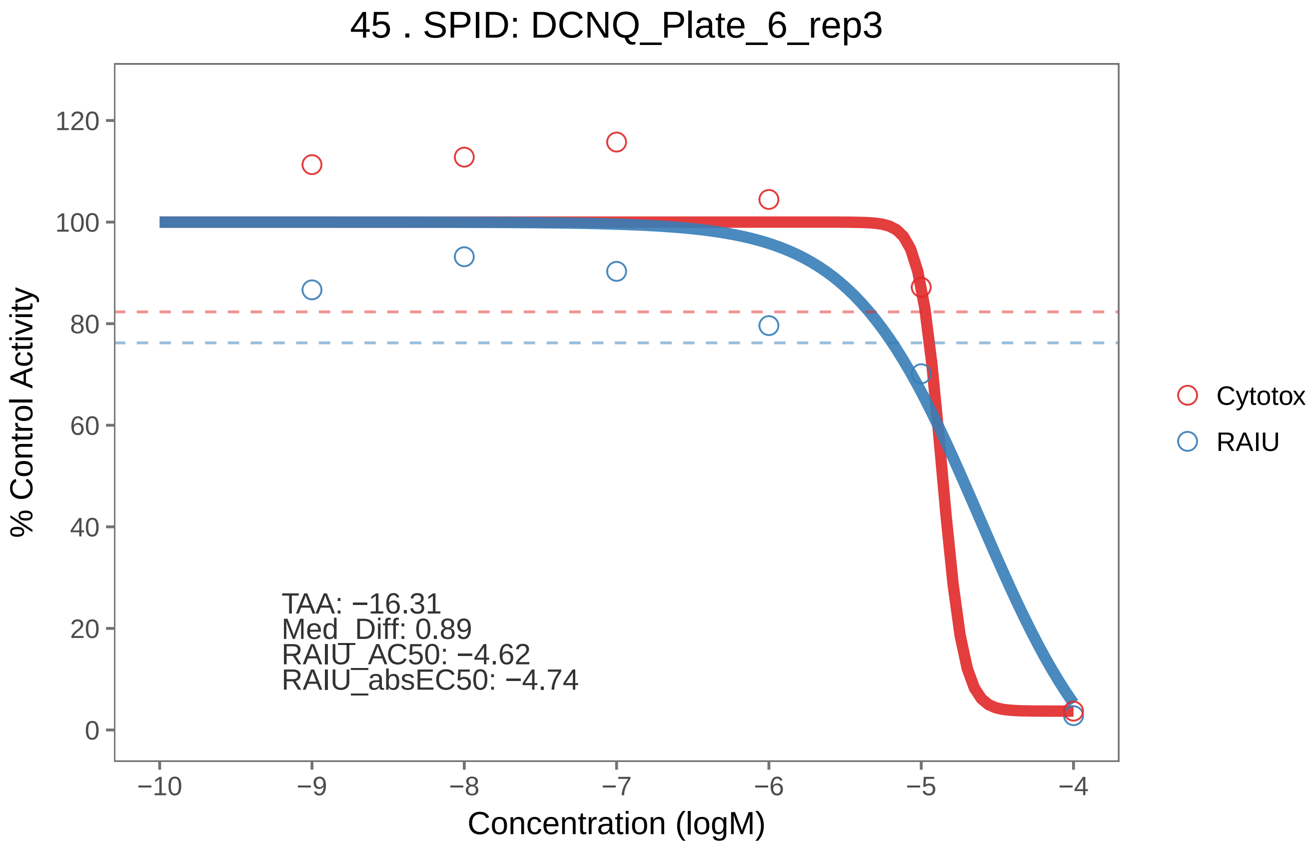

40 . SPID: DCNQ_Plate_5_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −12.16
Med_Diff: 0.64
RAIU_AC50: −4.65
RAIU_absEC50: −4.77
Cytotox
RAIU

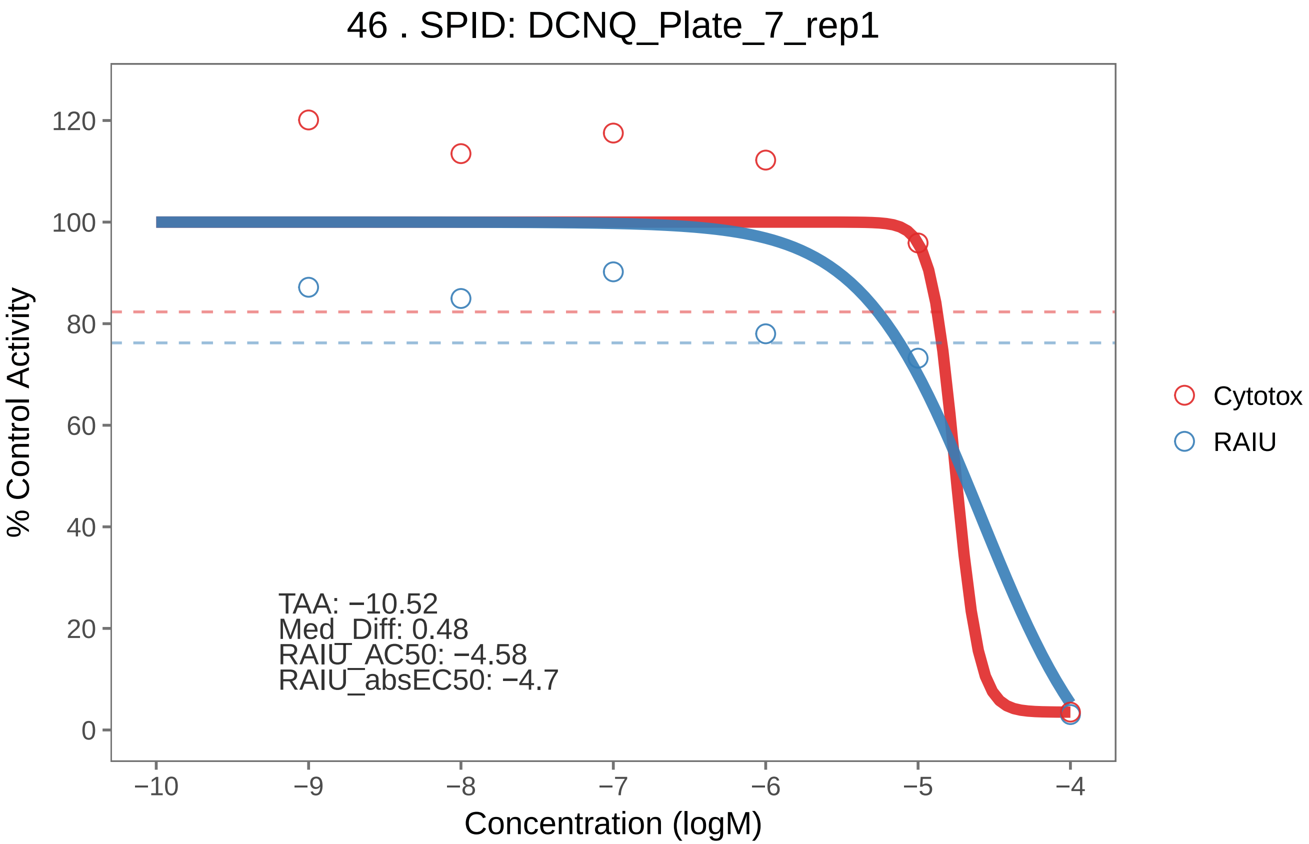

41 . SPID: DCNQ_Plate_5_rep2
% Control Activity
120
100
80
60
40
20
0
TAA: −22.99
Med_Diff: 0.22
RAIU_AC50: −4.56
RAIU_absEC50: −4.66
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU

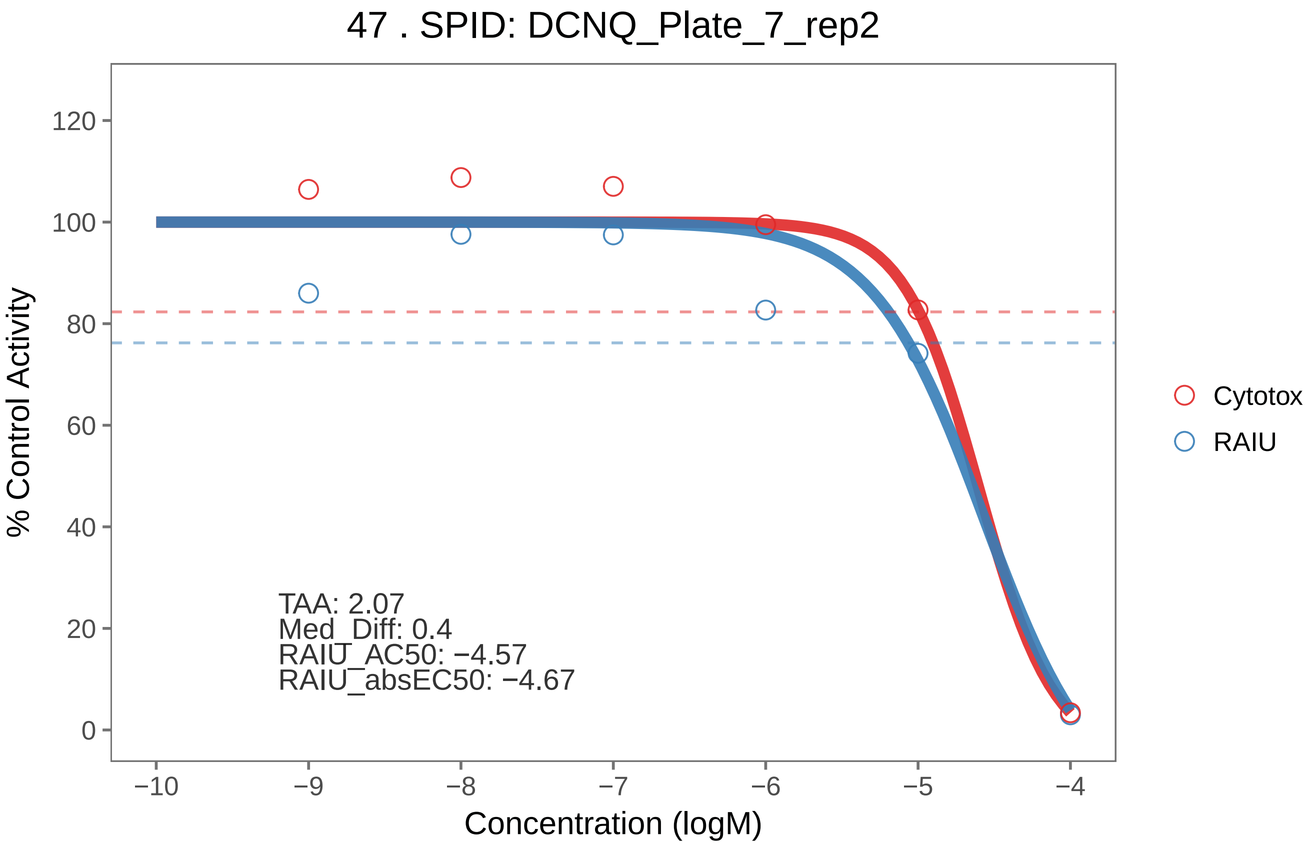

42 . SPID: DCNQ_Plate_5_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −38.63
Med_Diff: −23.49
RAIU_AC50: −4.54
RAIU_absEC50: −4.43
Cytotox
RAIU

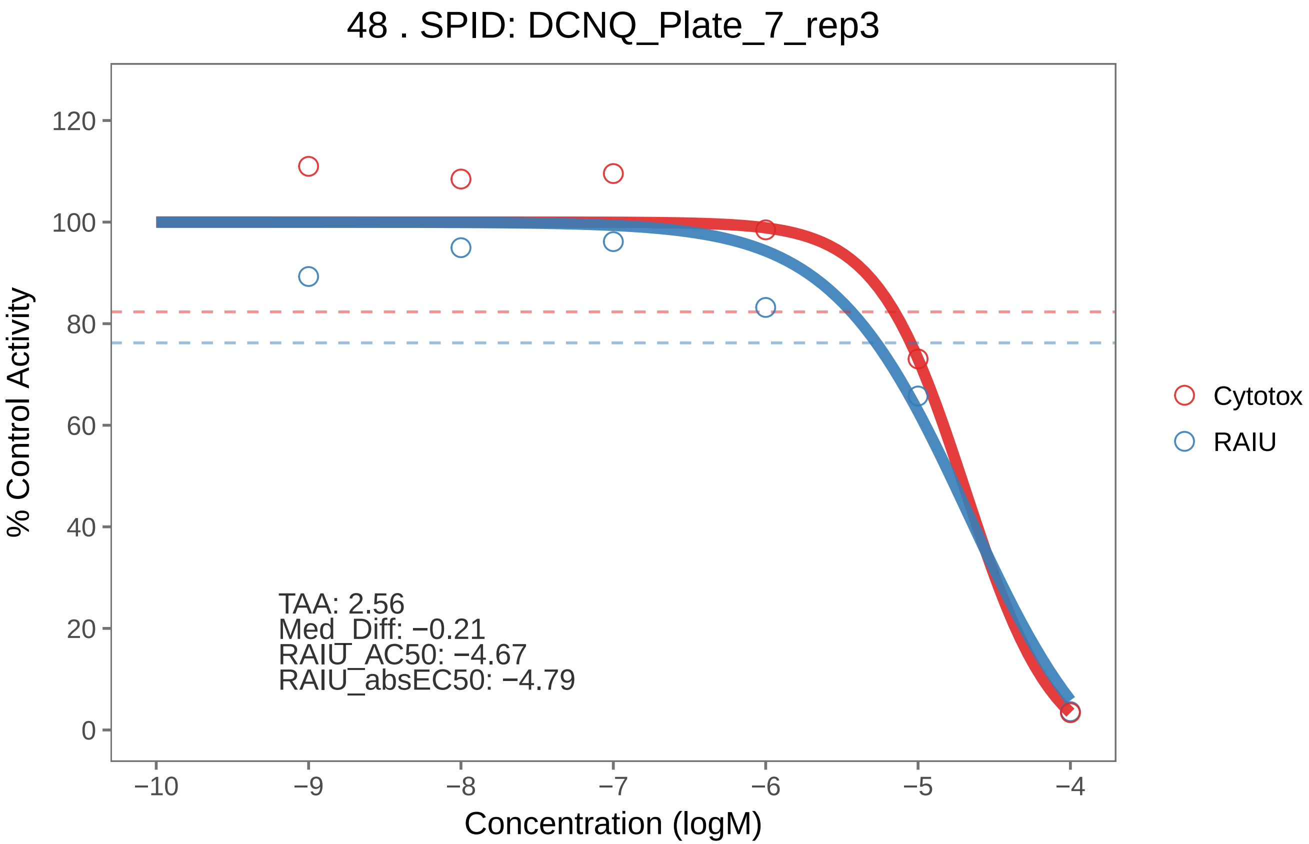

43 . SPID: DCNQ_Plate_6_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −22.35
Med_Diff: 0.83
RAIU_AC50: −4.53
RAIU_absEC50: −4.63
Cytotox
RAIU

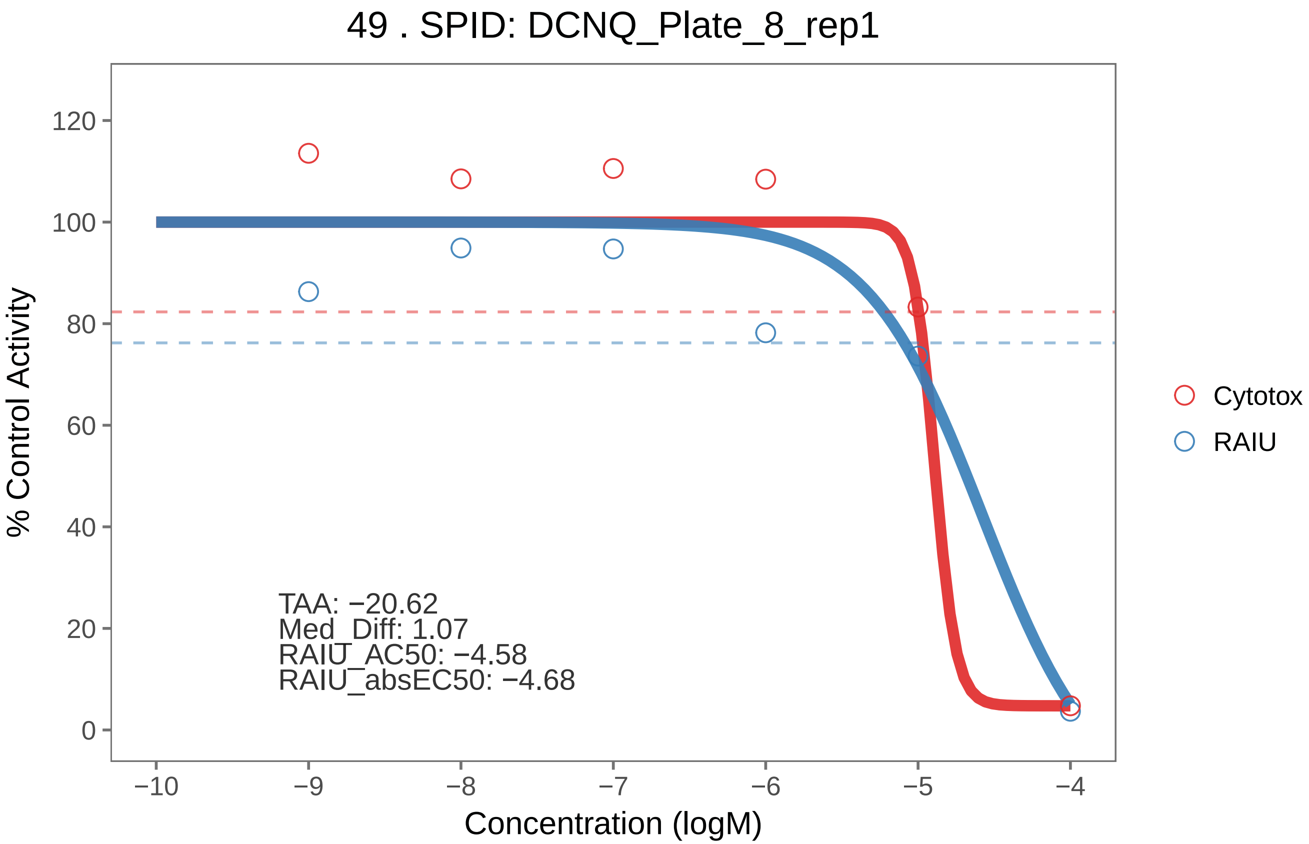

44 . SPID: DCNQ_Plate_6_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −4.88
Med_Diff: 1.08
RAIU_AC50: −4.77
RAIU_absEC50: −4.96
Cytotox
RAIU


45 . SPID: DCNQ_Plate_6_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −16.31
Med_Diff: 0.89
RAIU_AC50: −4.62
RAIU_absEC50: −4.74
Cytotox
RAIU

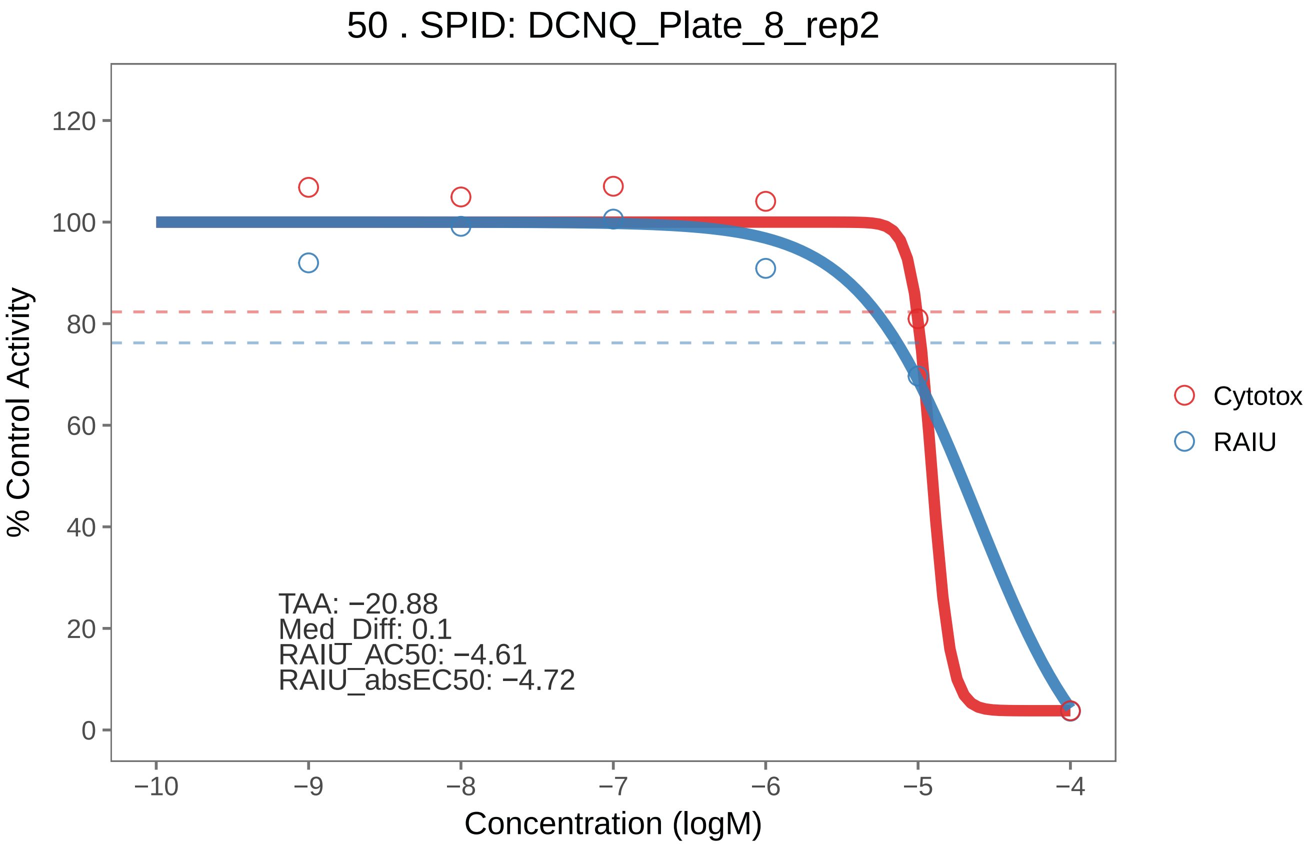

46 . SPID: DCNQ_Plate_7_rep1
% Control Activity
Concentration (logM)
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Cytotox
RAIU
TAA: −10.52
Med_Diff: 0.48
RAIU_AC50: −4.58
RAIU_absEC50: −4.7


47 . SPID: DCNQ_Plate_7_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 2.07
Med_Diff: 0.4
RAIU_AC50: −4.57
RAIU_absEC50: −4.67
Cytotox
RAIU

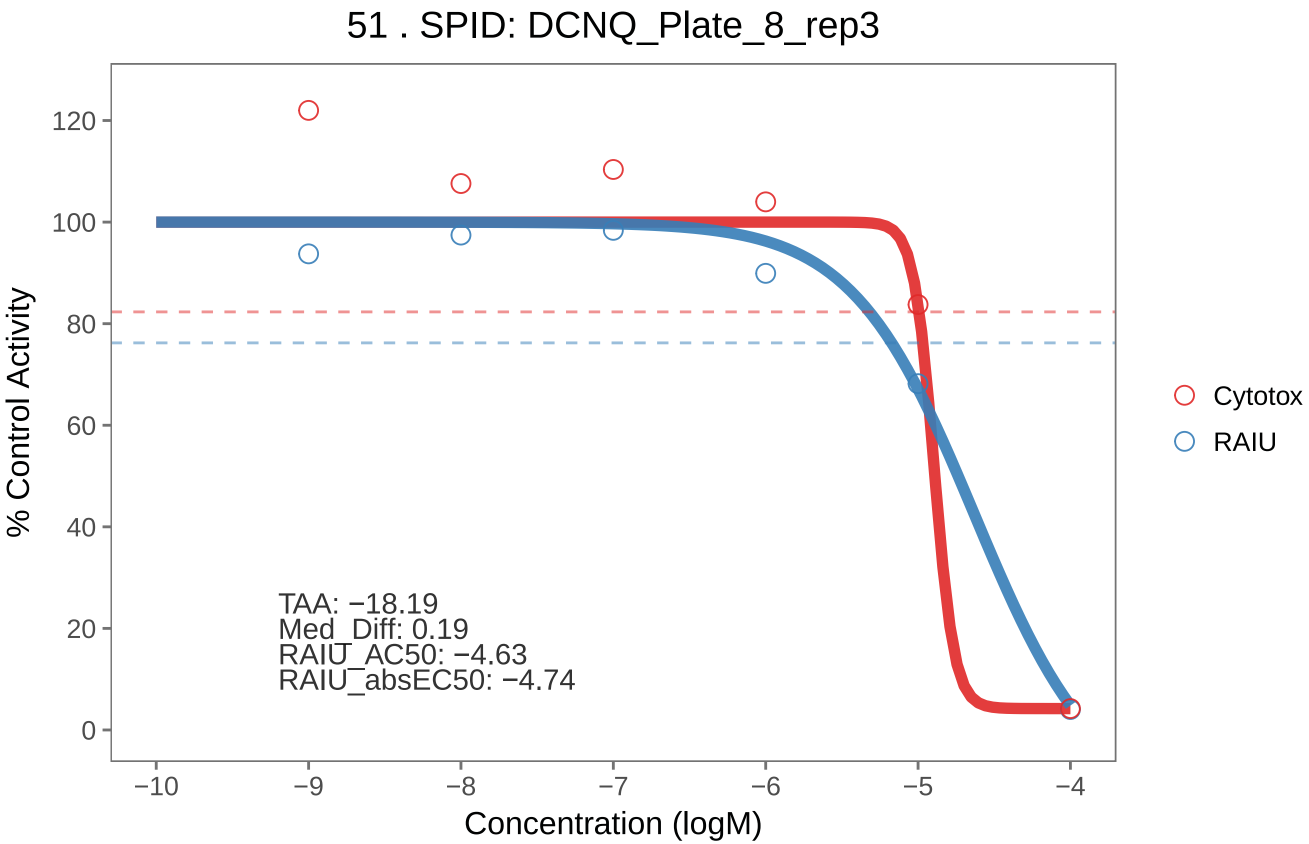

48 . SPID: DCNQ_Plate_7_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 2.56
Med_Diff: −0.21
RAIU_AC50: −4.67
RAIU_absEC50: −4.79
Cytotox
RAIU

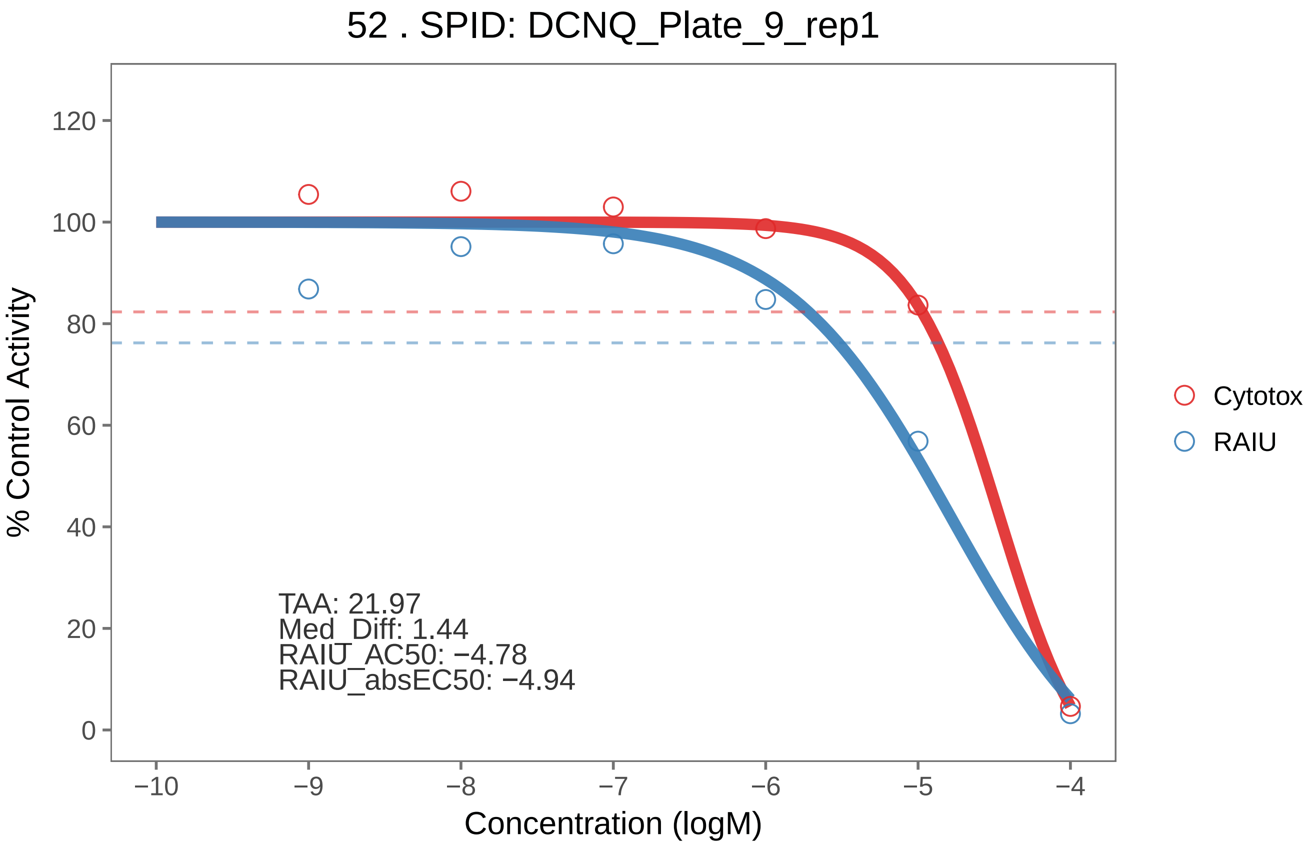


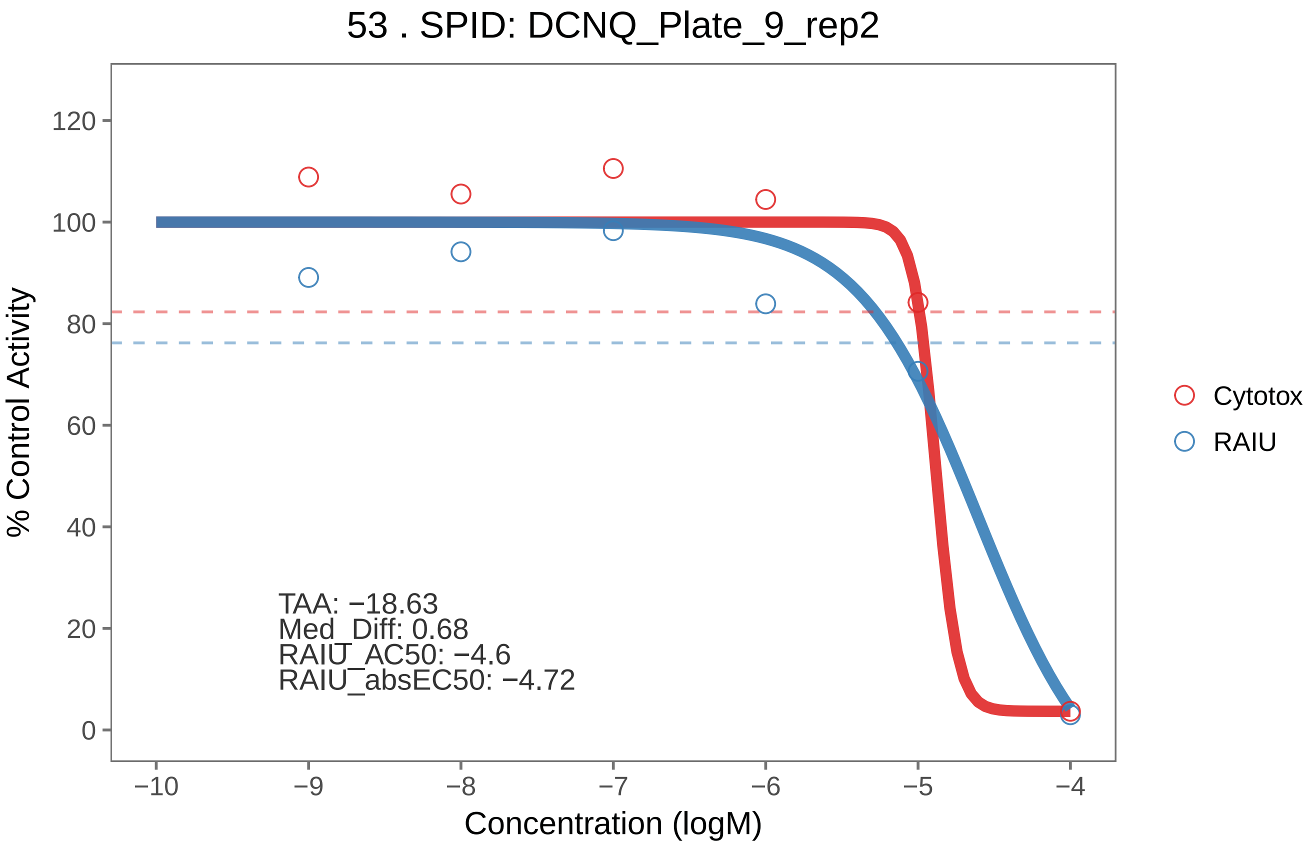
49 . SPID: DCNQ_Plate_8_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −20.62
Med_Diff: 1.07
RAIU_AC50: −4.58
RAIU_absEC50: −4.68
Cytotox
RAIU



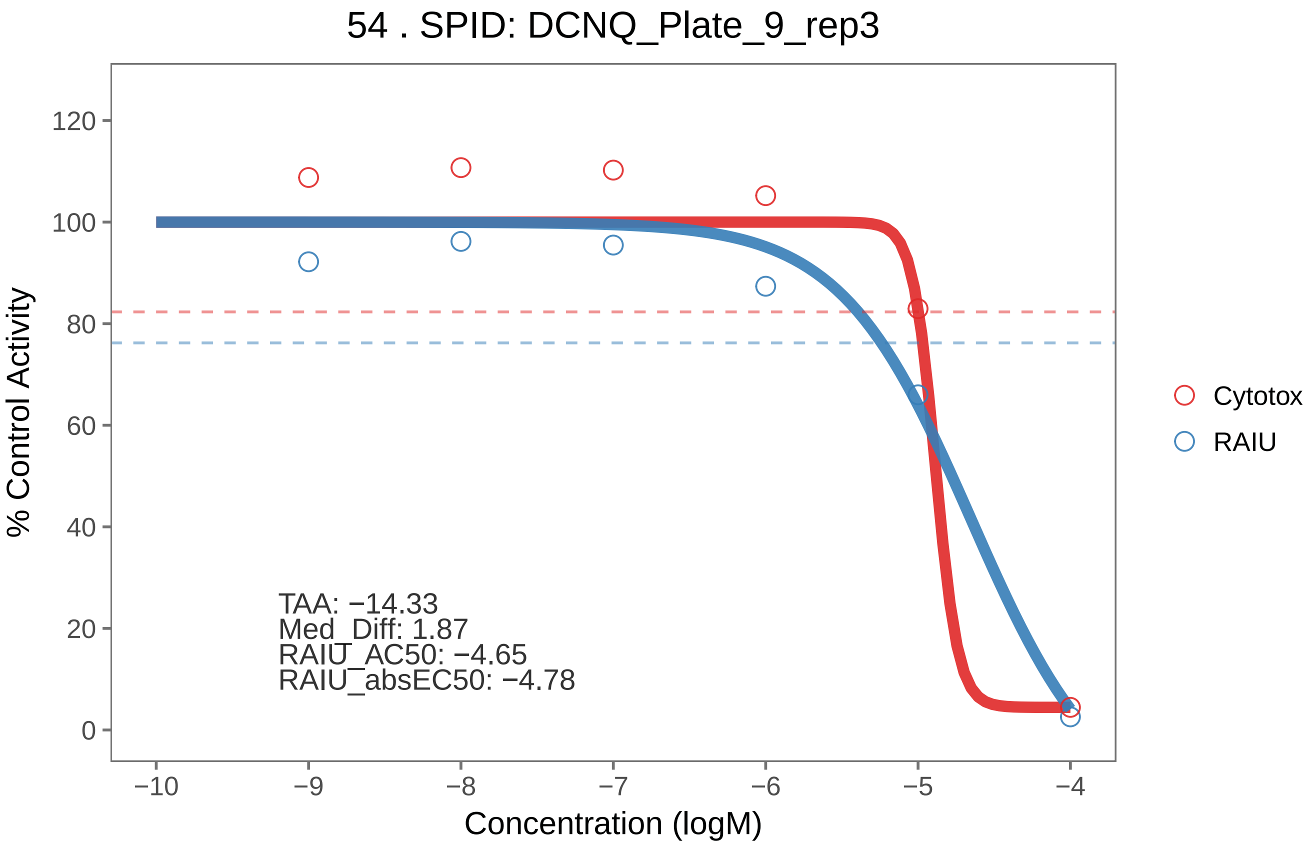
50 . SPID: DCNQ_Plate_8_rep2
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
TAA: −20.88
Med_Diff: 0.1
RAIU_AC50: −4.61
RAIU_absEC50: −4.72


51 . SPID: DCNQ_Plate_8_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −18.19
Med_Diff: 0.19
RAIU_AC50: −4.63
RAIU_absEC50: −4.74
Cytotox
RAIU

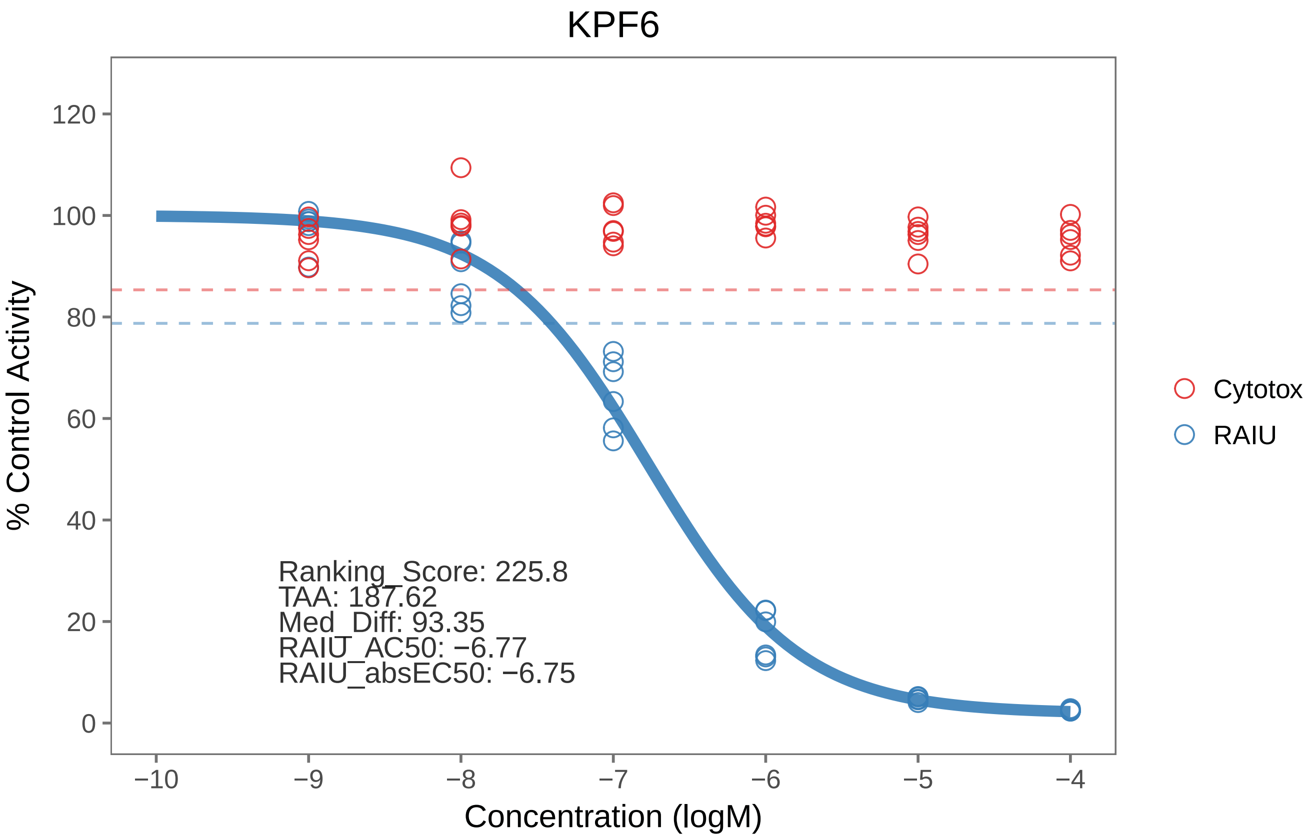

52 . SPID: DCNQ_Plate_9_rep1
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: 21.97
Med_Diff: 1.44
RAIU_AC50: −4.78
RAIU_absEC50: −4.94
Cytotox
RAIU

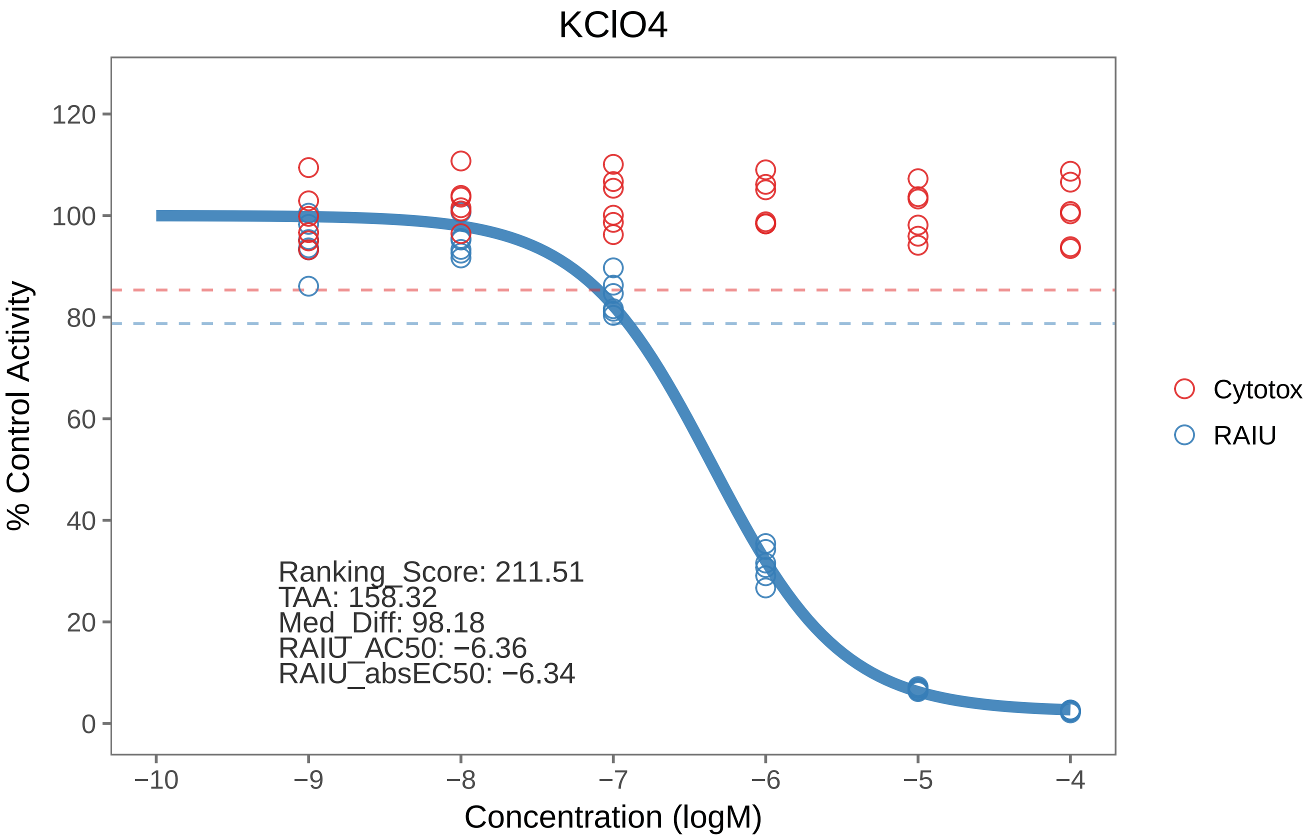


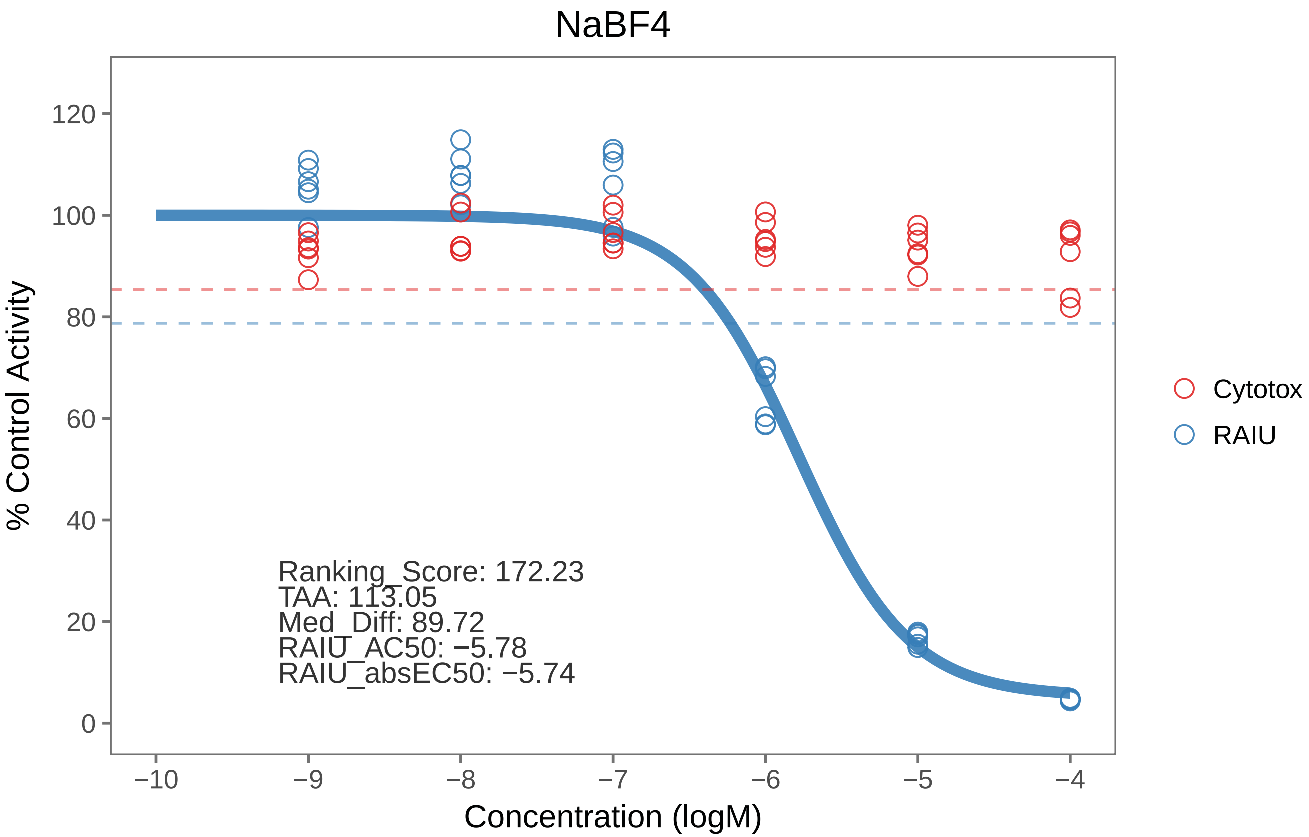
53 . SPID: DCNQ_Plate_9_rep2
% Control Activity
Concentration (logM)
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
TAA: −18.63
Med_Diff: 0.68
RAIU_AC50: −4.6
RAIU_absEC50: −4.72
Cytotox
RAIU

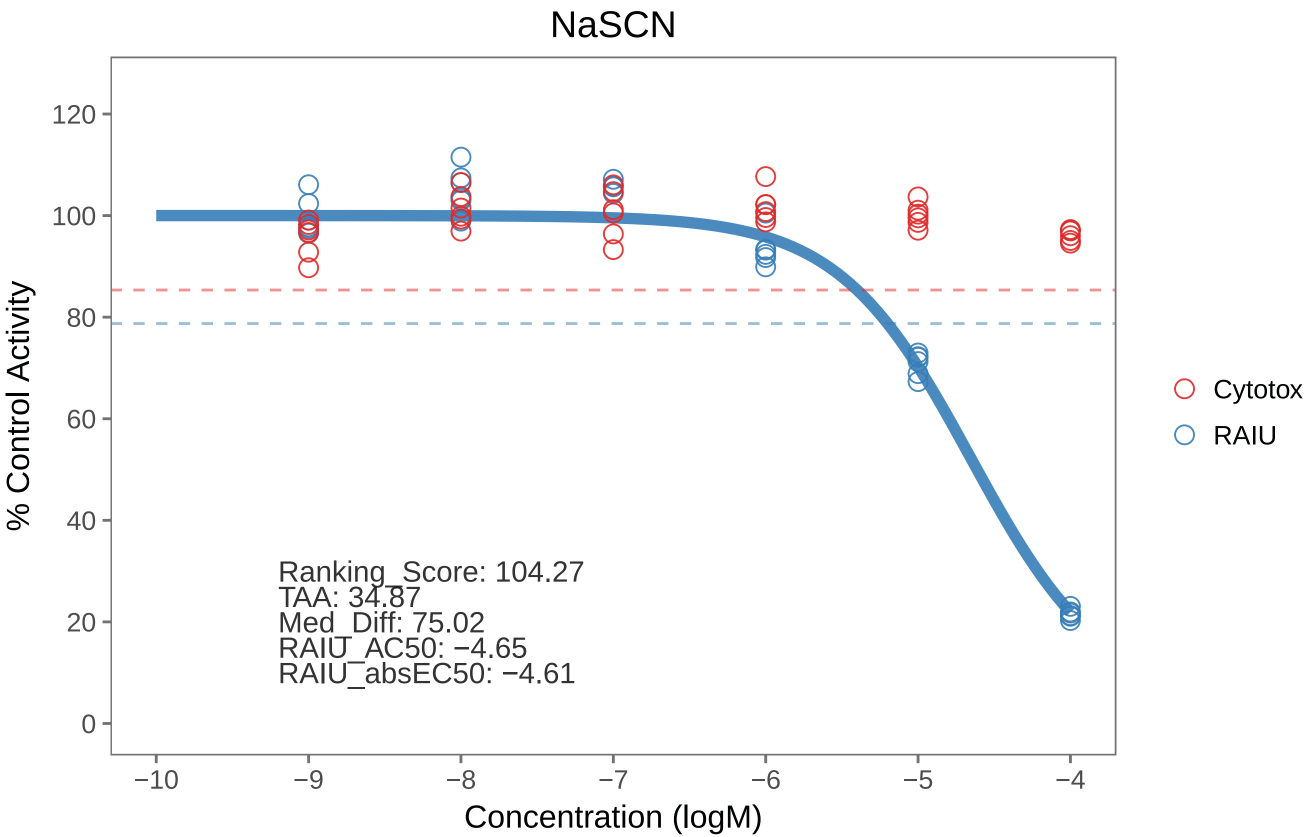

54 . SPID: DCNQ_Plate_9_rep3
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
TAA: −14.33
Med_Diff: 1.87
RAIU_AC50: −4.65
RAIU_absEC50: −4.78
Cytotox
RAIU

Part V. Dose-response of reanalyzed reference chemicals


KPF6
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
Ranking_Score: 225.8
TAA: 187.62
Med_Diff: 93.35
RAIU_AC50: −6.77
RAIU_absEC50: −6.75


KClO4
% Control Activity
120
100
80
60
40
20
0
Ranking_Score: 211.51
TAA: 158.32
Med_Diff: 98.18
RAIU_AC50: −6.36
RAIU_absEC50: −6.34
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU


NaBF4
% Control Activity
0
20
40
60
80
100
120
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
Ranking_Score: 172.23
TAA: 113.05
Med_Diff: 89.72
RAIU_AC50: −5.78
RAIU_absEC50: −5.74


NaSCN
% Control Activity
120
100
80
60
40
20
0
−10
−9
−8
−7
−6
−5
−4
Concentration (logM)
Cytotox
RAIU
Ranking_Score: 104.27
TAA: 34.87
Med_Diff: 75.02
RAIU_AC50: −4.65
RAIU_absEC50: −4.61

Part VI. Documented data analysis in R markdown

Part VI. Documented Data Analysis in R

Introduction

This report includes all the R code in the analysis of ToxCast Phase 1_v2 chemical library screening results from the NIS radioactive iodide uptake (RAIU) assay. With the aim of reproducible data analysis, this document was written in rmarkdown format and generated by R's `knitr` and `bookdown` package.

A web book version of this document (easier to navigate), in addition with interactive dose-response plots is also available at this link:https://njekin.github.io/NIS-RAIU-assay-ToxCast-Phase1_v2-screening-analysis/index.html.

Key R functions written in this analysis were compiled as an R package `toxplot`, and version 0.1.0 is available on CRAN. To get the most up-to-date source code please go to github. At the end of this document the source code of these functions used in this analysis is also provided.

Single-Conc Analysis

```
rm(list=ls())
library(plotly)
library(ggthemes)
library(RColorBrewer)
library(stringr)
library(readxl)
library(grid)
library(gridExtra)
library(devtools)
load_all("../../toxplot")
library(tidyverse)
session_info()
```

```
##  setting  value
##  version  R version 3.3.0 (2016-05-03)
##  system   x86_64, mingw32
##  ui       RTerm
##  language (EN)
##  collate  English_United States.1252
##  tz       America/New_York
##  date     2018-03-29
##
##  package      * version  date       source
##  assertthat     0.1      2013-12-06 CRAN (R 3.3.0)
##  backports      1.1.2    2017-12-13 CRAN (R 3.3.3)
##  base64enc      0.1-3    2015-07-28 CRAN (R 3.3.0)
##  chron          2.3-47   2015-06-24 CRAN (R 3.3.1)
##  colorspace     1.2-6    2015-03-11 CRAN (R 3.3.0)
##  data.table     1.9.6    2015-09-19 CRAN (R 3.3.1)
##  DBI            0.5-1    2016-09-10 CRAN (R 3.3.1)
##  devtools     * 1.12.0   2016-06-24 CRAN (R 3.3.1)
##  digest         0.6.10   2016-08-02 CRAN (R 3.3.1)
##  dplyr        * 0.5.0    2016-06-24 CRAN (R 3.3.1)
```

```
##  evaluate       0.9      2016-04-29 CRAN (R 3.3.1)
##  formatR        1.4      2016-05-09 CRAN (R 3.3.1)
##  ggplot2      * 2.2.1    2016-12-30 CRAN (R 3.3.3)
##  ggthemes     * 3.2.0    2016-07-11 CRAN (R 3.3.1)
##  gridExtra    * 2.2.1    2016-02-29 CRAN (R 3.3.0)
##  gtable         0.2.0    2016-02-26 CRAN (R 3.3.0)
##  htmltools      0.3.5    2016-03-21 CRAN (R 3.3.0)
##  htmlwidgets    0.7      2016-08-02 CRAN (R 3.3.1)
##  httr           1.2.1    2016-07-03 CRAN (R 3.3.1)
##  jsonlite       1.1      2016-09-14 CRAN (R 3.3.1)
##  knitr          1.14     2016-08-13 CRAN (R 3.3.1)
##  lazyeval       0.2.0    2016-06-12 CRAN (R 3.3.1)
##  magrittr       1.5      2014-11-22 CRAN (R 3.3.1)
##  memoise        1.0.0    2016-01-29 CRAN (R 3.3.0)
##  munsell        0.4.3    2016-02-13 CRAN (R 3.3.0)
##  numDeriv       2016.8-1 2016-08-27 CRAN (R 3.3.1)
##  plotly       * 3.6.0    2016-05-18 CRAN (R 3.3.1)
##  plyr           1.8.4    2016-06-08 CRAN (R 3.3.0)
##  purrr        * 0.2.2    2016-06-18 CRAN (R 3.3.1)
##  R6             2.1.3    2016-08-19 CRAN (R 3.3.1)
##  RColorBrewer * 1.1-2    2014-12-07 CRAN (R 3.3.0)
##  Rcpp           0.12.7   2016-09-05 CRAN (R 3.3.1)
##  readr        * 1.0.0    2016-08-03 CRAN (R 3.3.1)
##  readxl       * 0.1.1    2016-03-28 CRAN (R 3.3.1)
##  rmarkdown      1.8      2017-11-17 CRAN (R 3.3.3)
##  RMySQL         0.10.9   2016-05-08 CRAN (R 3.3.1)
##  roxygen2       5.0.1    2015-11-11 CRAN (R 3.3.1)
##  rprojroot      1.3-2    2018-01-03 CRAN (R 3.3.3)
##  RSQLite        1.0.0    2014-10-25 CRAN (R 3.3.1)
##  scales         0.5.0    2017-08-24 CRAN (R 3.3.3)
##  stringi        1.1.6    2017-11-17 CRAN (R 3.3.3)
##  stringr      * 1.1.0    2016-08-19 CRAN (R 3.3.1)
##  tcpl           1.2.2    2016-05-18 CRAN (R 3.3.1)
##  tibble       * 1.2      2016-08-26 CRAN (R 3.3.1)
##  tidyr        * 0.6.0    2016-08-12 CRAN (R 3.3.1)
##  tidyverse    * 1.0.0    2016-09-09 CRAN (R 3.3.2)
##  toxplot      * 0.1.0    <NA>       local
##  viridis        0.3.4    2016-03-12 CRAN (R 3.3.0)
##  withr          1.0.2    2016-06-20 CRAN (R 3.3.1)
##  yaml           2.1.13   2014-06-12 CRAN (R 3.3.0)
```

Define basic assay info

```
  #define the names of the primary and toxicity assay.
  #names should match what's provided in the <assay> column of the input dataframe
assay_info <- list(
  prim_assay = "RAIU",
  toxi_assay = "Cytotox"
)
```

Data Import

```
dt_sc <- read_csv("./input data files/NIS_ph1_v2_sc_lvl0_for_tcpl.csv")
```

Normalization

Each sample well is normalized as percentage of the DMSO median on each plate.

```
dt_sc_norm <- toxplot::normalize_per_plate(dt_sc, nctrl = "DMSO")
```

Threshold of Significance

Now calculating 3bMAD and 3sigma value for the DMSO control in the single concentration assay as a whole.

```
sig_cutoff_sc <- dt_sc_norm %>%
    filter(spid == "DMSO") %>%
    summarize(bMAD = mad(nval_median, na.rm=TRUE),
              three_bMAD = 3*mad(nval_median, na.rm=TRUE))
knitr::kable(sig_cutoff_sc, digits = 2)
```

bMAD	three_bMAD
6.83	20.5

QC of Single-conc assay

Assay quality control measures were calculated by each 96-well plate.

To assesss the quality of assay for each 96 well plate, the following metrics were used:

- CV of DMSO controls
- Z' score

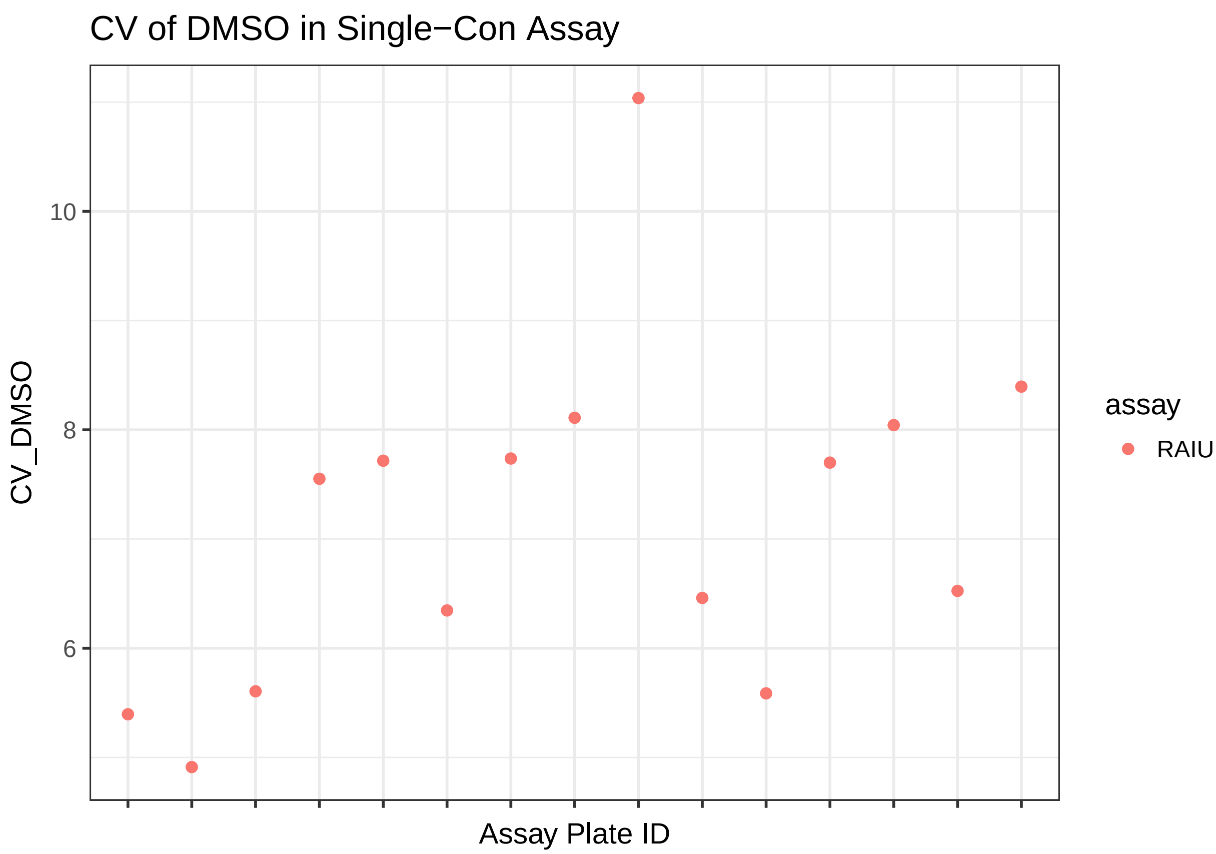
The negative control DMSO wells' raw readings were used to calculate mean, standard deviation and CV for each plate.

Z' factor is calculated as follows:

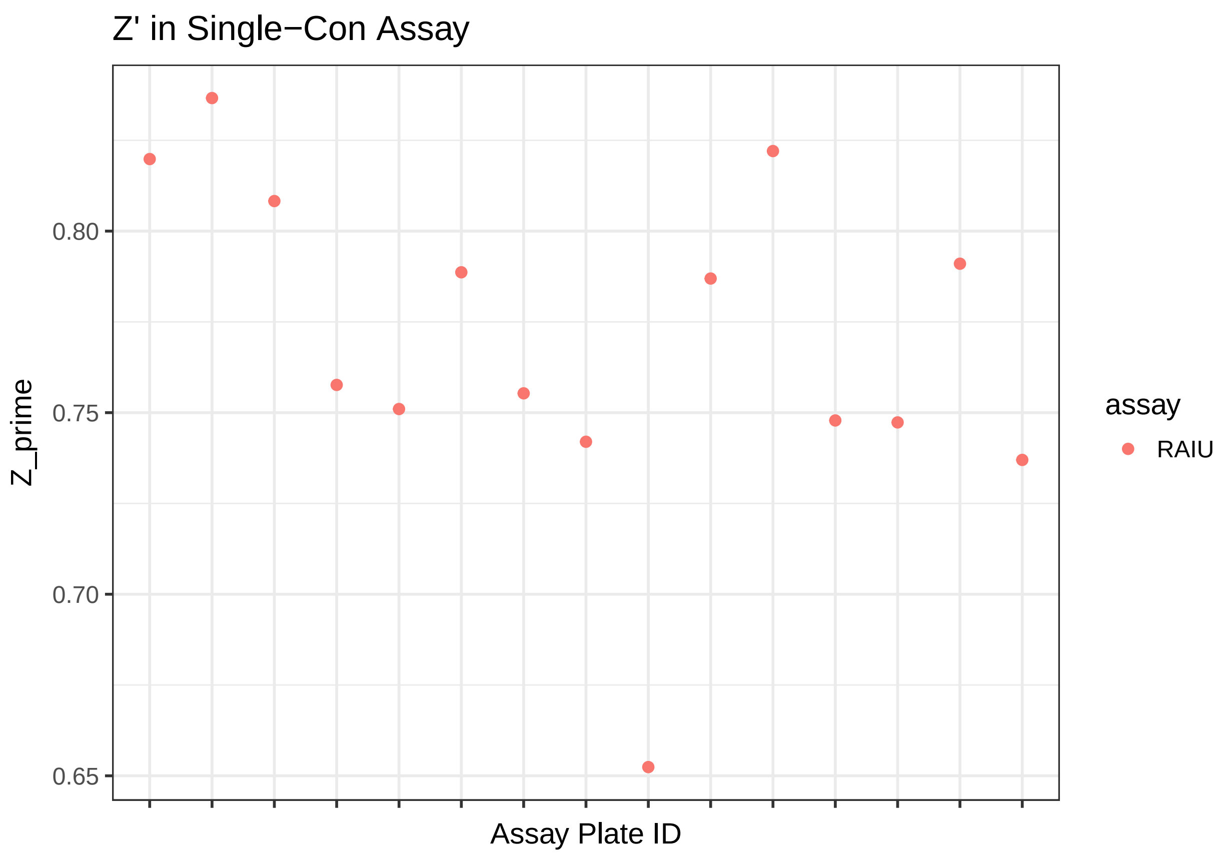
$$Z' = 1 - \frac{3\sigma_{positive\ control} + 3\sigma_{DMSO\ control}}{|\mu_{positive\ control} - \mu_{DMSO\ control}|}$$

Note that in Z' calculation, because we only had one well of cytotox positive control, therefore sigma wasn't calculatable. Hence the Z' calculated for cytotox is unusable.

```
qc_sc <- qc_per_plate(dt_sc_norm, assay_info, resp = "nval_median")

qplot(unique_id, CV_DMSO, data = qc_sc$qc, color = assay) +
    ggtitle("CV of DMSO in Single-Con Assay") +
    xlab("Assay Plate ID") +
    scale_x_discrete(labels = NULL) +
    theme_bw()
```




```r
qplot(unique_id, Z_prime, data = qc_sc$qc, color = assay) +
    ggtitle("Z' in Single-Con Assay") +
    xlab("Assay Plate ID") +
    scale_x_discrete(labels = NULL) +
    theme_bw()
```



QC Summary of Single-Con assay

```
library(psych)
qc_sc_t <- qc_sc$qc %>%
    dplyr::select(CV_DMSO, Z_prime) %>%
    describe
knitr::kable(qc_sc_t, digits = 2,  caption = "Summary Single-Con Assay QC Metrics")
```

Table 2: Summary Single-Con Assay QC Metrics

	vars	n	mean	sd	median	trimmed	mad	min	max	range	skew	kurtosis	se
apid*	1	15	NaN	NA	NA	NaN	NA	Inf	-Inf	-Inf	NA	NA	NA
CV_DMSO	2	15	7.14	1.56	7.55	7.01	1.52	4.91	11.04	6.13	0.68	0.19	0.40
Z_prime	3	15	0.77	0.05	0.76	0.77	0.04	0.65	0.84	0.18	-0.72	0.40	0.01

All single-con QC metrics in a table

```
knitr::kable(dplyr::select(qc_sc$qc, apid, CV_DMSO, Z_prime),
             digits = 2,
             col.names = c("Plate", "CV of DMSO", "Z'"),
             caption = "QC metrics in Single-Conc Screening")
```

Table 3: QC metrics in Single-Conc Screening

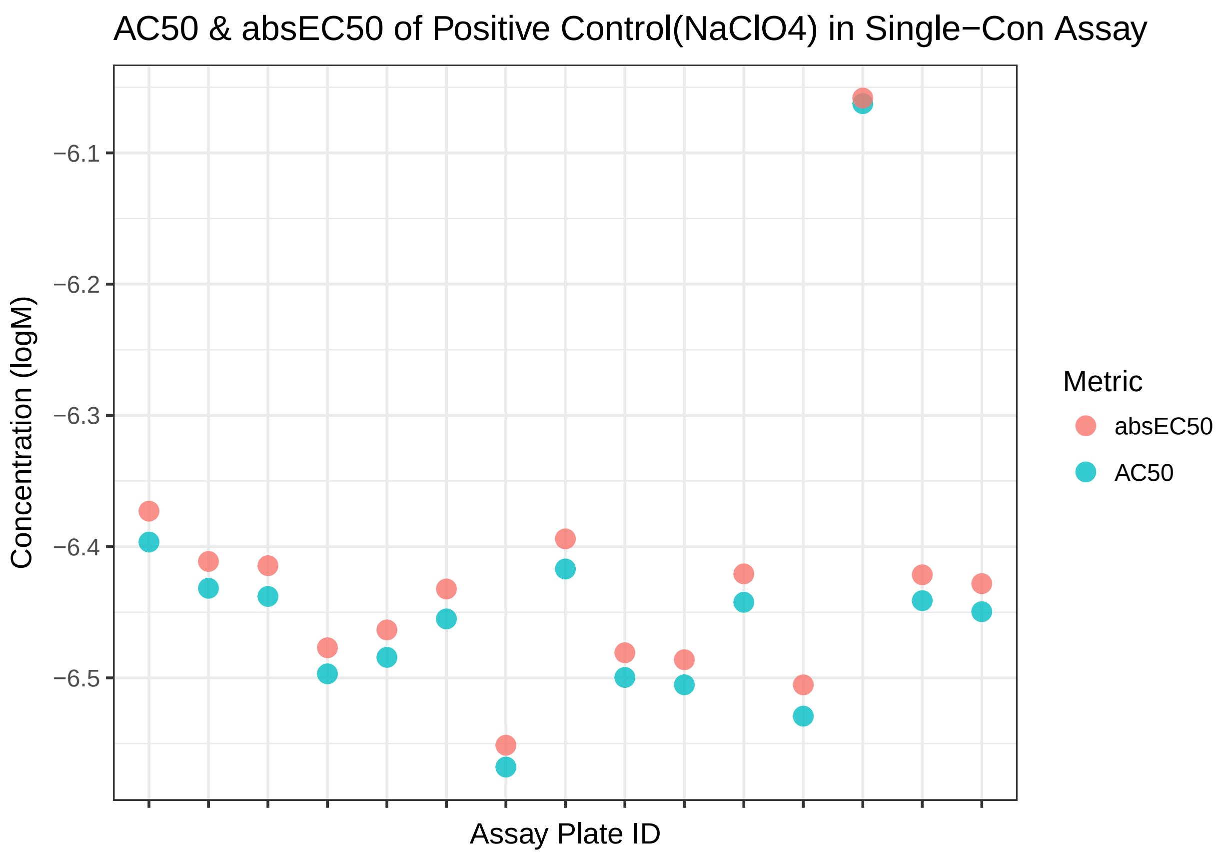
Plate	CV of DMSO	Z'
TP0001498_rep1	5.40	0.82
TP0001498_rep2	4.91	0.84
TP0001498_rep3	5.61	0.81
TP0001499_rep1	7.55	0.76
TP0001499_rep2	7.72	0.75
TP0001499_rep3	6.35	0.79
TP0001500_rep1	7.74	0.76
TP0001500_rep2	8.11	0.74
TP0001500_rep3	11.04	0.65
TP0001501_rep1	6.46	0.79
TP0001501_rep2	5.59	0.82
TP0001501_rep3	7.70	0.75
TP0001502_rep1	8.04	0.75
TP0001502_rep2	6.53	0.79
TP0001502_rep3	8.40	0.74

Single-Con Positive Control QC

```
## model single-con controls on each plate
sc_pos_raiu <- dt_sc_norm %>%
    filter(spid == "NaClO4") %>%
    mutate(spid = paste(spid, apid)) # change spid to distinguish NaClO4 on each plate.

sc_raiu_pos_md <- toxplot::fit_curve_tcpl(sc_pos_raiu,
                                          assay_info = list(prim_assay = "RAIU",
                                                            toxi_assay = NULL))
```

```
## Processing 15 samples(spid)....
## NaClO4 TP0001498_rep1 ||NaClO4 TP0001498_rep2 ||NaClO4 TP0001498_rep3 ||NaClO4 TP0001499_rep1 ||NaCl
## Curve Fitting Completed!
## Calculation time: 1.7 secs
```

```
sc_raiu_pos_sum <- toxplot::summary_tcpl(sc_raiu_pos_md)

##plot AC50 for pos controls together
st <- sc_raiu_pos_sum %>%
    dplyr::select(AC50_prim, absEC50_prim, spid) %>%
    rename(AC50 = AC50_prim, absEC50 = absEC50_prim) %>%
    gather(key=Metric, value= value, AC50, absEC50)

ggplot(st, aes(spid, value)) +
    geom_point(aes(color=Metric), alpha=0.8, size=3)+
    #facet_grid(Metric~., scale="free")+
    scale_x_discrete(labels=NULL)+
    ggtitle("AC50 & absEC50 of Positive Control(NaClO4) in Single-Con Assay")+
    xlab("Assay Plate ID") +
    ylab("Concentration (logM)") +
    theme(plot.title = element_text(hjust=0.5)) +
    theme_bw()
```




```
    #theme(legend.position = "none")

#summary
library(psych)
sc_pos_sum_raiu <- sc_raiu_pos_sum %>%
    dplyr::select(AC50_prim, absEC50_prim) %>%
    rename(AC50=AC50_prim, absEC50 = absEC50_prim) %>%
    describe
knitr::kable(sc_pos_sum_raiu, digits = 2,
             caption="Summary of single-con RAIU positive control IC50s")
```

Table 4: Summary of single-con RAIU positive control IC50s

	vars	n	mean	sd	median	trimmed	mad	min	max	range	skew	kurtosis	se
AC50	1	15	-6.44	0.11	-6.45	-6.46	0.05	-6.57	-6.06	0.51	2.28	5.19	0.03
absEC50	2	15	-6.42	0.11	-6.43	-6.44	0.05	-6.55	-6.06	0.49	2.18	4.85	0.03

Single-Con Controls

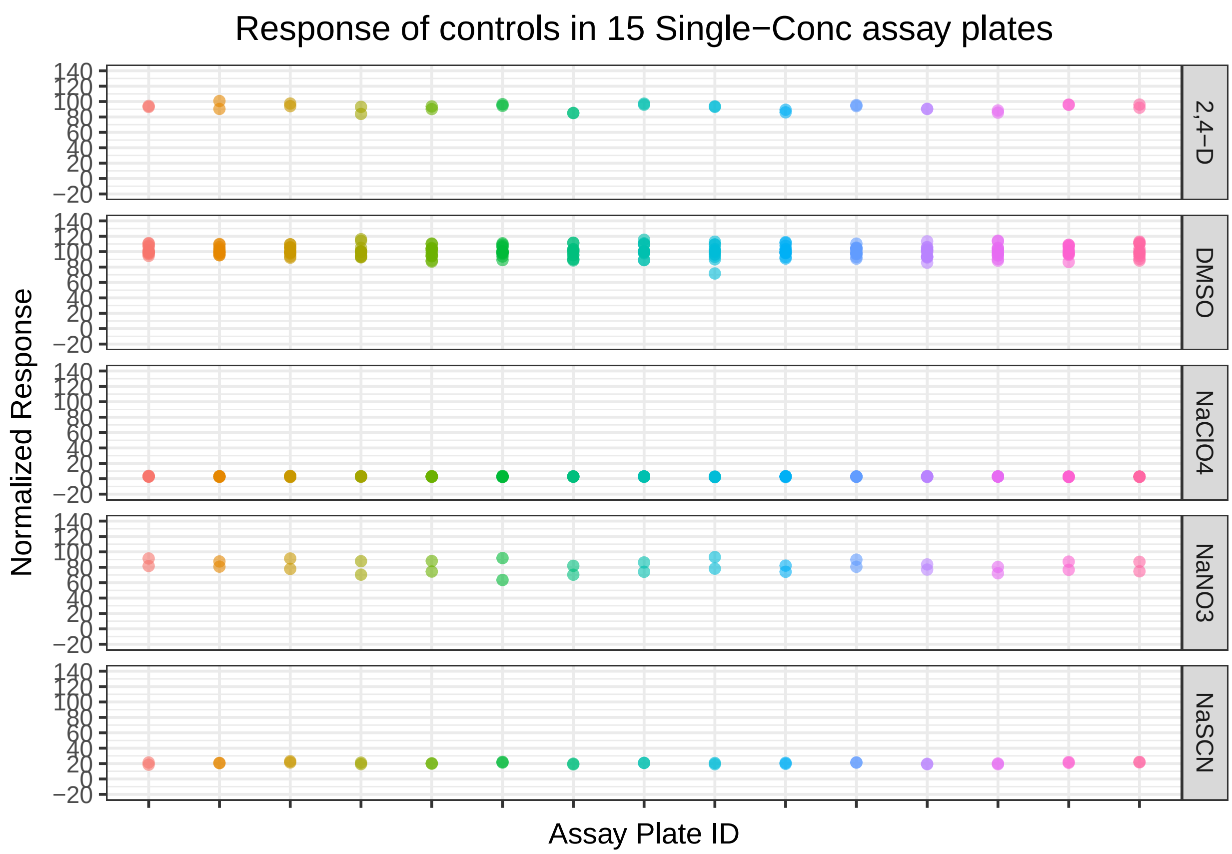
```
#only take the NaClO4 wells at 1E-4M
s1 <- dt_sc_norm %>% filter(wllt!="t", spid!="NaClO4")
s2 <- dt_sc_norm %>% filter(spid=="NaClO4", conc== 1E-4)
s3 <- bind_rows(s1, s2)
```

```
sc_ctrl_sum <- s3 %>%
    filter(wllt !="t") %>%
    mutate(resp=nval_median) %>%
    #rename("NaClO4(1E-4M)F"=NaClO4) %>%
    group_by(spid) %>%
    summarize(mean = mean(resp),
              sd = sd(resp),
              min = min(resp),
              max = max(resp),
              CV = sd/mean*100)
knitr::kable(sc_ctrl_sum, digits =2, caption="Single-Con control summary stats")
```

Table 5: Single-Con control summary stats

spid	mean	sd	min	max	CV
2,4-D	92.41	4.24	83.91	100.71	4.59
DMSO	100.63	7.11	71.69	116.19	7.06
NaClO4	2.85	0.36	2.08	3.84	12.60
NaNO3	81.25	7.56	63.47	93.21	9.31
NaSCN	20.64	1.12	18.56	23.05	5.41

```
# plot all sc controls
ggplot(filter(s3, wllt !="t"), aes(apid, nval_median)) +
    geom_point(aes(color=apid),alpha=0.6) +
    facet_grid(spid~.) +
    scale_y_continuous(limits= c(-20,140), breaks= seq(from=-20, to=140, by=20)) +
    #scale_x_discrete(breaks=NULL)+
    scale_x_discrete(labels=NULL)+
    ylab("Normalized Response") +
    xlab("Assay Plate ID")+
    ggtitle("Response of controls in 15 Single-Conc assay plates")+
    theme_bw()+
    theme(legend.position = "none") +
    theme(plot.title=element_text(hjust=0.5))
```

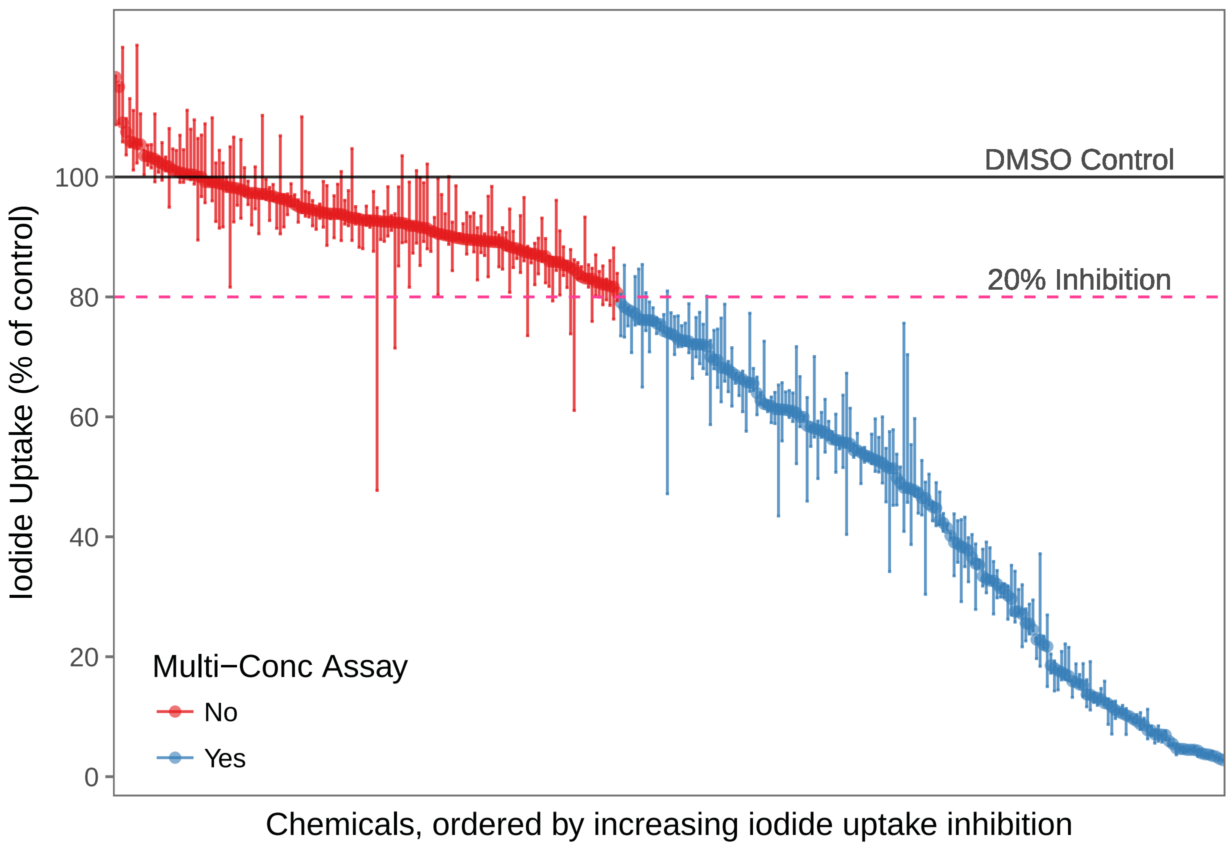


Visualize the single concentration data

A total of 310 chemical samples was tested in the single-con and 169 were further tested in multi-concentration. The plot below showed the median, max, and min value for each tested chemical, and coloring shows which chemical were carried on to the multi-con assay. Because the assay has 3 replicates, so all three replicate's data are actually plotted in this figure.

```
#calculate median, max and min value
sc_median <- dt_sc_norm %>% ungroup() %>%
    filter(str_detect(dt_sc_norm$spid, "^TP*")) %>%
    mutate(welltype = "sample") %>%
    group_by(pid, spid) %>%
    summarize(
        median = median(nval_median),
        up_range = max(nval_median),
        lo_range = min(nval_median),
        range = max(nval_median) - min(nval_median)
    ) %>%
    ungroup() %>%
    mutate(mc_test = ifelse(median < 80, "Yes", "No")) %>%
    arrange(median)
##Plot single con median+range plot.


fig2 <- ggplot(sc_median, aes(x=reorder(spid, -median), y=median, color=mc_test)) +
```

```
    geom_point(size=1.5, alpha=0.6) +
    geom_errorbar(aes(ymax=up_range, ymin=lo_range), alpha=0.8, size = 0.5) +
    xlab("Chemicals, ordered by increasing iodide uptake inhibition") +
    ylab("Iodide Uptake (% of control)")+scale_x_discrete(breaks=NULL) +
    #ggtitle("Median and Response of Test Chemicals")+
    geom_hline(yintercept = 80, linetype="dashed", color="violetred1") +
    geom_hline(yintercept = 100, alpha=0.8) +
    geom_text(data = NULL, x = 270, y = 103, label = "DMSO Control", color = "grey30")+
    geom_text(data = NULL, x = 270, y = 83, label = "20% Inhibition", color = "grey30")+
    scale_y_continuous(breaks = seq(from = 0, to =100, by=20))+
    scale_color_brewer(palette="Set1", name= "Multi-Conc Assay", labels= c("No", "Yes")) +
    theme_few(base_size = 12) +
    theme(legend.position = c(0.15, 0.1), legend.background = element_blank())
fig2
```




```
#ggsave("./output plots/fig2.tiff", fig2, dpi = 900, width = 7, height = 5, compression = "lzw")
```

Multi-Conc Analysis

Import MC data

```
#Get the spid of the 169 chemicals entering multi-con test.
dt_mc_ls <- read_csv("./input data files/NIS_ph1_v2_mc_lvl0_for_tcpl_raiu.csv", na = "NA") %>%
```

```
    select(spid)
mc_chem_list <- unique(dt_mc_ls$spid)[-(1:6)]
ls169 <- sc_median %>%
    filter(mc_test=="Yes") %>%
    dplyr::select(spid)

ls11 <- data.frame(mc_chem_list) %>%
    mutate(flag = (mc_chem_list %in% ls169$spid)) %>%
    filter(flag==FALSE) %>%
    dplyr::select(mc_chem_list) %>% rename(spid=mc_chem_list)

spid_chnm_table <- read_excel("./raw data files/EPA_11700_EPA-SLaws_ph1v2_150ul_20170125_key.xlsx")

spid_chnm_table <- spid_chnm_table %>%
    dplyr::select(EPA_Sample_ID, CASRN, Preferred_Name)
# rename the column title to be compatible with tcpl package.
names(spid_chnm_table) <- c("spid", "casn", "chnm")

# Import MC data (look at the 169 chemicals)
mc_lvl0_raiu_update <-
    read_csv("./input data files/NIS_ph1_v2_mc_lvl0_for_tcpl_raiu.csv") %>%
    filter(!(spid %in% ls11$spid))

mc_lvl0_cyto_update <-
    read_csv("./input data files/NIS_ph1_v2_mc_lvl0_for_tcpl_cytotox.csv") %>%
    filter(!(spid %in% ls11$spid))

dt_mc <- bind_rows(mc_lvl0_cyto_update, mc_lvl0_raiu_update)
```

Normalization

Normalize raw response to the median of DMSO controls, calculated per plate.

```
dt_mc_norm <- toxplot::normalize_per_plate(dt_mc)
```

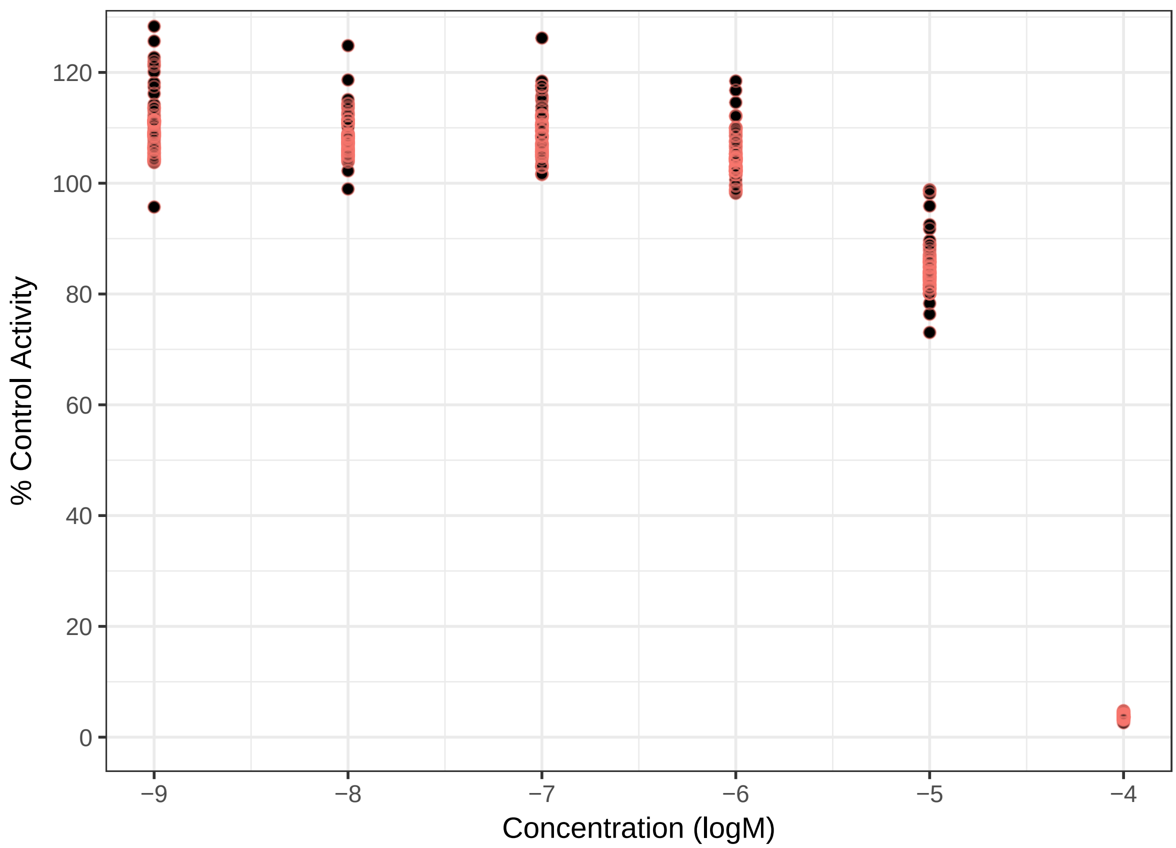
3bMAD of MC

```
#create concentration index
dt_mc_norm <- dt_mc_norm %>%
    group_by(spid) %>%
    mutate(cndx = generate_index(conc)) %>%
    ungroup
sig_mc <- dt_mc_norm %>%
  mutate(neg_nval_median= 100 - nval_median) %>%
  group_by(assay) %>%
  dplyr::filter(wllt == "t") %>%
  dplyr::filter(cndx == 1 | cndx == 2) %>%
  summarise(bMAD = mad(neg_nval_median, na.rm = TRUE),
            three_bMAD=3*mad(neg_nval_median, na.rm = TRUE))
knitr::kable(sig_mc, digits =2)
```

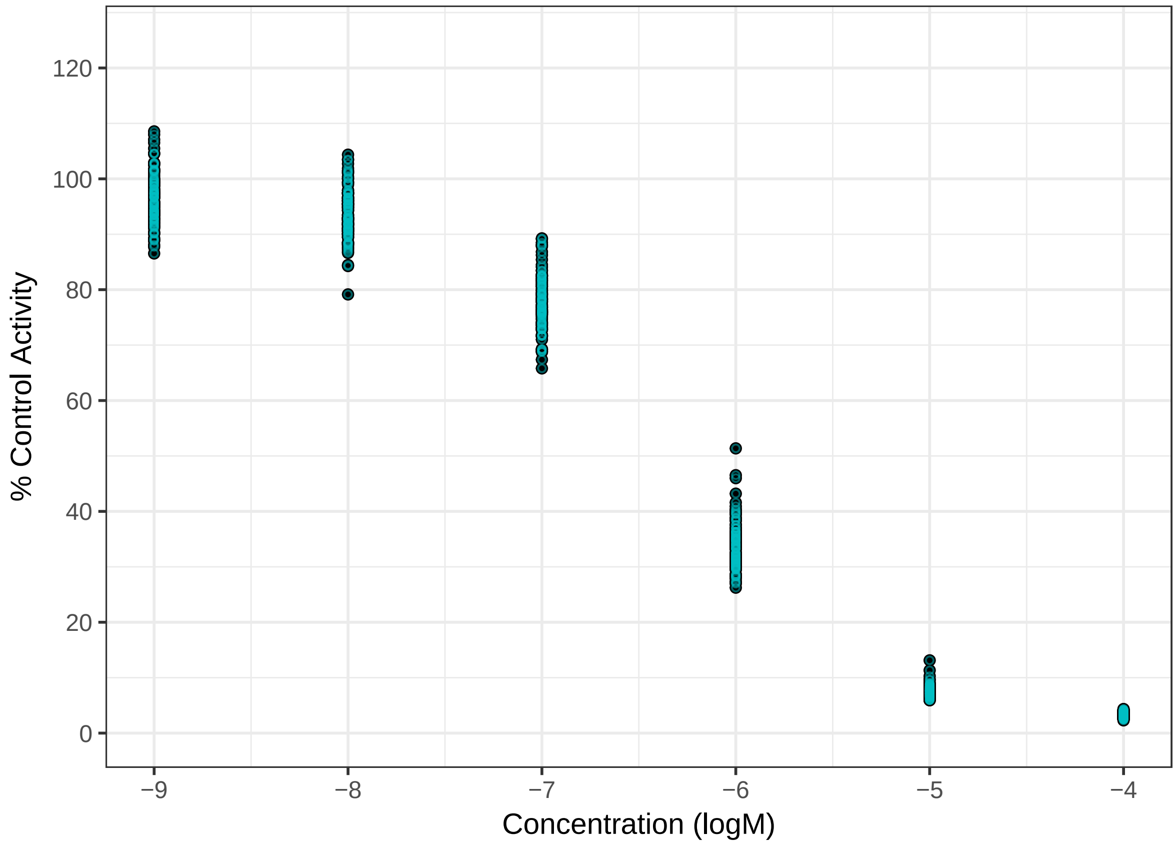
assay	bMAD	three_bMAD
Cytotox	5.89	17.68
RAIU	7.93	23.78

Multi-Con QC

```
##extract mc related data frame
d_pos_cyto <- dt_mc_norm %>% filter(assay == "Cytotox", wllt== "pc")
d_pos_raiu <- dt_mc_norm %>% filter(assay == "RAIU", wllt=="pr")

d_neg_cyto <- dt_mc_norm %>% filter(assay == "Cytotox", wllt=="nrc")
d_neg_raiu <- dt_mc_norm %>% filter(assay == "RAIU", wllt=="nrc")
d_ec80_raiu <- dt_mc_norm %>% filter(assay == "RAIU", wllt=="pr_ec80")
d_ec20_raiu <- dt_mc_norm %>% filter(assay == "RAIU", wllt=="pr_ec20")

##plot all DCNQ in multi-con
g_cyto_pos <- qplot(data=d_pos_cyto, x=log10(conc), y=nval_median) +
    labs(
        x = "Concentration (logM)",
        y = "% Control Activity"
    ) +
    geom_point(
        color = "#F8766D",
        shape = 1,
        alpha = 0.5,
        size = 1.8
    ) +
    coord_fixed(
        ylim = c(0, 125),
        xlim = c(-9, -4),
        ratio = 2 / 70
    ) +
    scale_y_continuous(breaks = seq(
        from = 0,
        to = 120,
        by = 20
    )) +
    theme_bw() +
    theme(legend.title = element_blank())+
    theme(plot.title=element_text(hjust=0.5))
g_cyto_pos
```




```
##plot all NaClO4 in multi-con
g_raiu_pos <- qplot(data=d_pos_raiu, x=log10(conc), y=nval_median) +
    labs(
        x = "Concentration (logM)",
        y = "% Control Activity"
    ) +
    geom_point(
        color = "#00BFC4",
        shape = 1,
        alpha = 0.5,
        size = 1
    ) +
    coord_fixed(
        ylim = c(0, 125),
        xlim = c(-9, -4),
        ratio = 2 / 70
    ) +
    scale_y_continuous(breaks = seq(
        from = 0,
        to = 120,
        by = 20
    )) +
    theme_bw() +
    theme(legend.title = element_blank())+
    theme(plot.title=element_text(hjust=0.5))
g_raiu_pos
```




```
# Obtain AC50 adn absEC50 for the positive controls

d_pos_raiu <- mutate(d_pos_raiu, spid = paste(spid, apid, sep = "_"))
pos_raiu_md <- toxplot::fit_curve_tcpl(df = d_pos_raiu,
                                       assay_info = list(prim_assay = "RAIU",
                                                         toxi_assay = NULL))
```

```
## Processing 54 samples(spid)....
## NaClO4_Plate_1_rep1 ||NaClO4_Plate_1_rep2 ||NaClO4_Plate_1_rep3 ||NaClO4_Plate_10_rep1 ||NaClO4_Plat
## Curve Fitting Completed!
## Calculation time: 7.2 secs
```

```
raiu_pos_tbl <- toxplot::summary_tcpl(pos_raiu_md)
d_pos_cyto <- mutate(d_pos_cyto, spid = paste(spid, apid, sep = "_"))
pos_cyto_md <- toxplot::fit_curve_tcpl(df = d_pos_cyto,
                                       assay_info = list(prim_assay = NULL,
                                                         toxi_assay = "Cytotox"))
```

```
## Processing 54 samples(spid)....
## DCNQ_Plate_1_rep1 ||DCNQ_Plate_1_rep2 ||DCNQ_Plate_1_rep3 ||DCNQ_Plate_10_rep1 ||DCNQ_Plate_10_rep2
## Curve Fitting Completed!
## Calculation time: 3.9 secs
```

```
cyto_pos_tbl <- toxplot::summary_tcpl(pos_cyto_md)
#this is the modelling results for all mc positive
pos_tbl <- bind_rows(cyto_pos_tbl, raiu_pos_tbl)
```

Summarize AC50s of positive controls in multi-con assay.

```
##summarizing AC50s of positive controls.
library(psych)
pos_sum_raiu <- raiu_pos_tbl %>%
    dplyr::select(AC50_prim, absEC50_prim) %>%
    describe

pos_sum_cyto <- cyto_pos_tbl %>%
    dplyr::select(AC50_toxi, absEC50_toxi) %>%
    describe

knitr::kable(pos_sum_raiu, digits = 2,
             caption="Summary of RAIU positive control IC50s")
```

Table 7: Summary of RAIU positive control IC50s

	vars	n	mean	sd	median	trimmed	mad	min	max	range	skew	kurtosis	se
AC50_prim	1	54	-6.38	0.13	-6.41	-6.40	0.11	-6.57	-6.04	0.53	1.04	0.83	0.02
absEC50_prim	2	54	-6.36	0.13	-6.39	-6.38	0.10	-6.54	-6.04	0.51	0.89	0.52	0.02

```
knitr::kable(pos_sum_cyto, digits = 2,
             caption="Summary of Cytotox positive control IC50s")
```

Table 8: Summary of Cytotox positive control IC50s

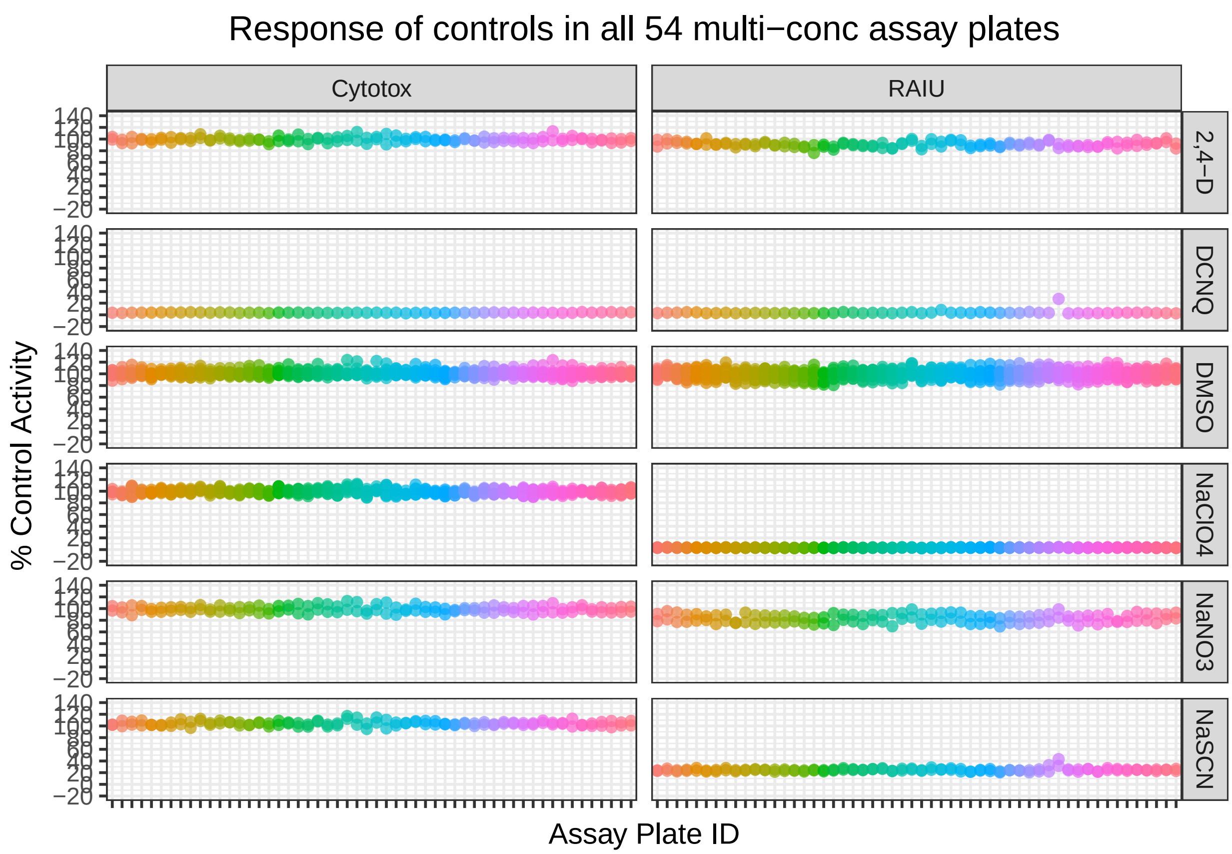
	vars	n	mean	sd	median	trimmed	mad	min	max	range	skew	kurtosis	se
AC50_toxi	1	54	-4.83	0.12	-4.88	-4.86	0.03	-4.92	-4.47	0.45	1.98	2.87	0.02
absEC50_toxi	2	54	-4.83	0.10	-4.88	-4.85	0.03	-4.92	-4.55	0.37	1.75	1.74	0.01

Multi-Con Controls

Visualize all controls in MC. NaClO4 and DCNQ are plotted using the 1E-4M concentration wells.

```
m3 <- dt_mc_norm %>%
    filter(!wllt %in% c("t")) %>%
    filter(!(spid %in% c("NaClO4", "DCNQ")))

m4 <- dt_mc_norm %>%
    filter(spid %in% c("NaClO4", "DCNQ")) %>%
    filter(conc == 1e-4)

m31 <- bind_rows(m3, m4)

## facet plots of all controls' data points
ggplot(m31, aes(apid, nval_median)) +
    geom_point(aes(color=apid),alpha=0.7) +
    facet_grid(spid~assay) +
    scale_y_continuous(limits= c(-20,140), breaks= seq(from=-20, to=140, by=20)) +
    scale_x_discrete(labels=NULL)+
    ylab("% Control Activity") +
    xlab("Assay Plate ID")+
```

```
    ggtitle("Response of controls in all 54 multi-conc assay plates")+
    theme_bw()+
    theme(legend.position = "none",
          plot.title=element_text(hjust=0.5))
```




```
##print the control stats table.
mc_ctrl_sum <- m31 %>%
    filter(wllt != "t") %>%
    mutate(resp=nval_median) %>%
    group_by(assay, spid) %>%
    summarize(mean = mean(resp),
              sd = sd(resp),
              min = min(resp),
              max = max(resp),
              CV = sd/mean*100)
knitr::kable(mc_ctrl_sum, digits = 2,
             caption = "Multi-Conc Control Summary Stats")
```

Table 9: Multi-Conc Control Summary Stats

assay	spid	mean	sd	min	max	CV
Cytotox	2,4-D	99.34	4.21	90.92	113.31	4.24
Cytotox	DCNQ	3.72	0.38	2.62	4.76	10.33
Cytotox	DMSO	100.92	5.41	87.82	123.66	5.36
Cytotox	NaClO4	99.19	4.69	89.12	112.51	4.73
Cytotox	NaNO3	98.95	5.43	88.64	112.92	5.49

assay	spid	mean	sd	min	max	CV
Cytotox	NaSCN	104.30	3.98	94.83	117.03	3.81
RAIU	2,4-D	90.86	4.49	76.22	101.30	4.94
RAIU	DCNQ	3.92	3.37	2.58	27.36	85.98
RAIU	DMSO	99.50	8.28	80.77	119.46	8.32
RAIU	NaClO4	3.28	0.38	2.30	4.33	11.47
RAIU	NaNO3	83.08	7.17	69.45	98.80	8.63
RAIU	NaSCN	24.69	2.71	20.47	43.17	10.99

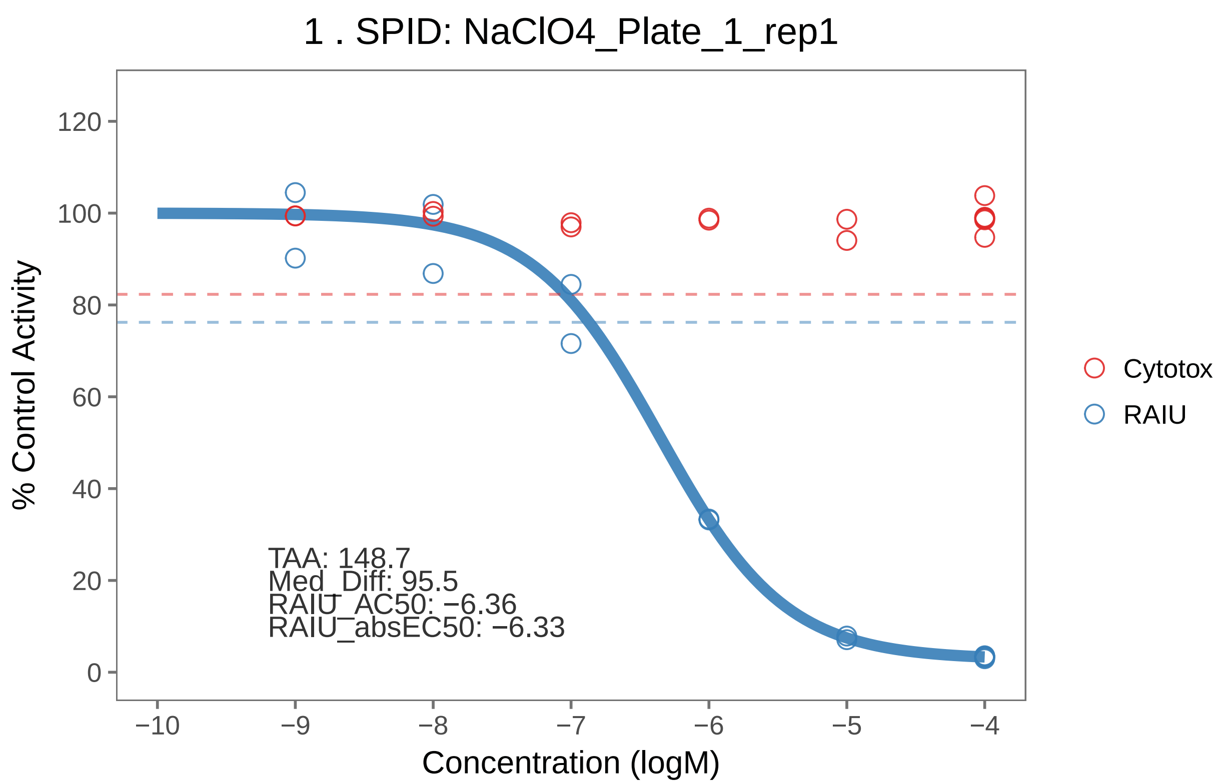
Sodium Perchlorate & DCNQ

On each assay plate, sodium perchlorate and DCNQ were included in six concentrations to serve as positive controls for RAIU and Cytotox assay. Here they are modelled separately by each assay plate.

```
# perchlorate
dt_perchlorate <- dt_mc_norm %>% filter(spid == "NaClO4") %>%
    mutate(spid = paste(spid, pid, rep, sep = "_"))
#dt_perchlorate <- dt_mc_norm %>% filter(spid == "NaClO4")
perchlorate_md <- fit_curve_tcpl(dt_perchlorate,
                                 assay_info = list(prim_assay = "RAIU",
                                                   toxi_assay = "Cytotox"),
                                 prim_cutoff = 23.78165,
                                 toxi_cutoff = 17.68251)
```

```
## Processing 54 samples(spid)....
## NaClO4_Plate_1_rep1 ||NaClO4_Plate_1_rep2 ||NaClO4_Plate_1_rep3 ||NaClO4_Plate_10_rep1 ||NaClO4_Plat
## Curve Fitting Completed!
## Calculation time: 7.9 secs
```

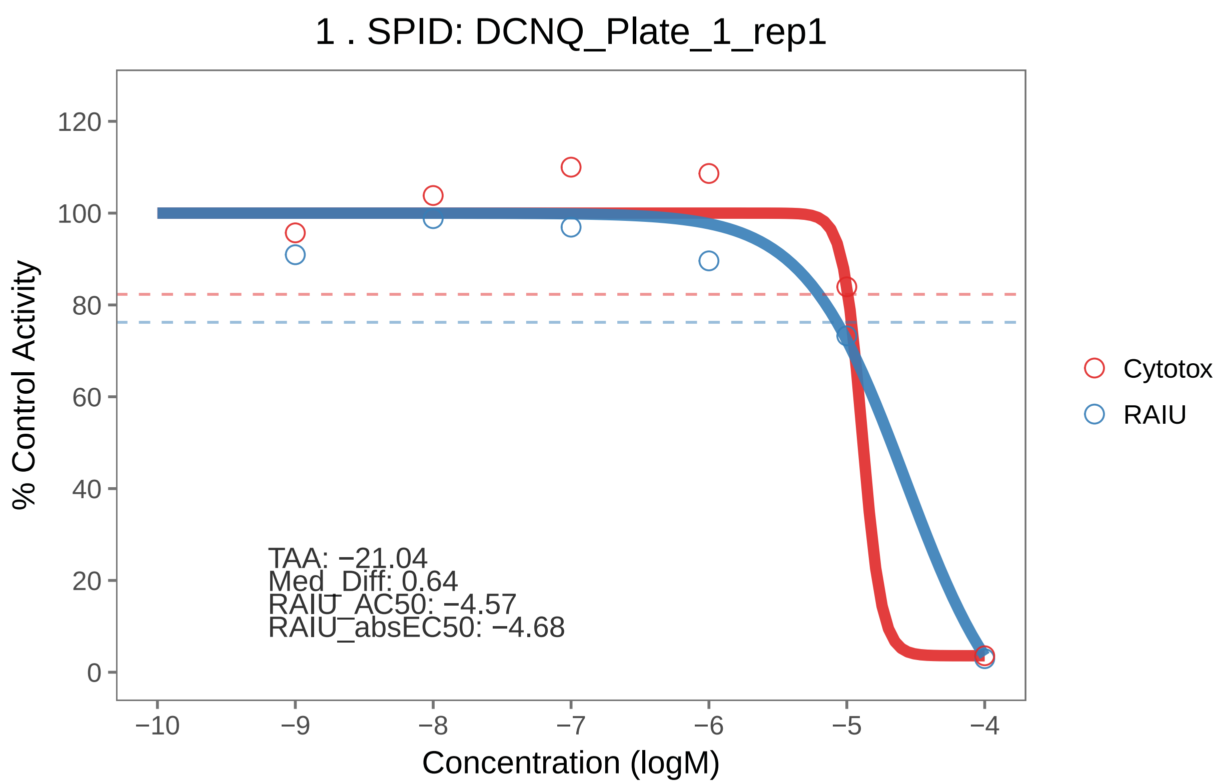
```
perchlorate_rank <- rank_tcpl(perchlorate_md)
#perchlorate_rank$taa %>% median
perchlorate_plots <- plot_tcpl(perchlorate_md, perchlorate_rank, notation = T)
perchlorate_plots[[1]]
```




```
# DCNQ
dt_dcnq <- dt_mc_norm %>% filter(spid == "DCNQ") %>%
    mutate(spid = paste(spid, pid, rep, sep = "_"))
dcnq_md <- fit_curve_tcpl(dt_dcnq,
                          assay_info = list(prim_assay = "RAIU",
                                            toxi_assay = "Cytotox"),
                          prim_cutoff = 23.78165,
                          toxi_cutoff = 17.68251)
```

```
## Processing 54 samples(spid)....
## DCNQ_Plate_1_rep1 ||DCNQ_Plate_1_rep2 ||DCNQ_Plate_1_rep3 ||DCNQ_Plate_10_rep1 ||DCNQ_Plate_10_rep2
## Curve Fitting Completed!
## Calculation time: 8.5 secs
```

```
dcnq_rank <- rank_tcpl(dcnq_md)
dcnq_plots <- plot_tcpl(dcnq_md, dcnq_rank, notation = T)
dcnq_plots[[1]]
```




```
# Export all Sodium Perchlorate and DCNQ plots into one pdf supplemental file
l3 <- append(perchlorate_plots, dcnq_plots)
# save_plot_pdf(l3, "./output plots/perchlorate_dcnq_curves.pdf")
```

Dose-response modeling

The model used here is the Hill model provided in `tcpl` R package.

$$f(x) = \frac{tp}{1 + 10^{(ga-x)gw}}$$

Where x is the log concentration, tp is the top asymptote, ga is the AC50 (the log concentration where the modeled activity equals 50% of the top asymptote), and gw is the hill coefficient. The Hill model provided in the tcpl R package constrains the three parameters as following:

- (1) 0 <= tp <= 1.2 times the maximum response value
- (2) (minimum log concentration minus 2) <= ga <= (maximum log concentration plus 0.5)
- (3) 0.3 <= gw <= 8

The modelling is done using a wrapper function `fit_curve_tcpl` in `ToxPlot` package, which serves as an convenient interface to use the `tcplFit` function in the `tcpl` package, and returns a list object containing all data and modeling results.

```
mc_model <- fit_curve_tcpl(df = filter(dt_mc_norm, wllt == "t"),
                           assay_info = list(prim_assay = "RAIU", toxi_assay = "Cytotox"),
                           prim_cutoff = 23.78165, toxi_cutoff = 17.68251)
```

```
## Processing 169 samples(spid)....
## TP0001498A01 ||TP0001498B02 ||TP0001498B05 ||TP0001498B07 ||TP0001498B08 ||TP0001498B09 ||TP0001498B
## Curve Fitting Completed!
## Calculation time: 26.5 secs
```

Rank Chemicals

To prioritize the chemicals for potential NIS inhibition activity, a ranking score was calculated using two metrics that take into account the potential confounding impact of cytotoxicity on identifying RAIU inhibition activity: 1) toxicity-adjusted area (TAA) and 2) the difference of median responses of RAIU and cytotoxicity at maximum tested concentration (Median-Difference). TAA was defined by the maximum concentration vertical line (right border), the significant threshold horizontal line for RAIU assay (top border), and the dose-response curves of RAIU and cell viability results. The numeric value of TAA is penalized when a chemical demonstrates strong cytotoxicity. Median-Difference was calculated using the median of cell viability responses minus the median of RAIU responses at the maximum testing concentration (usually 100 µM). Larger separations between RAIU and cytotoxicity are reflected in larger Median-Difference values. To rank test chemicals, NaClO4 was used as the reference to normalize the TAA and Median-Difference of each test chemical. Specifically, the TAA and Median-Difference values of NaClO4 positive control included on each of the 54 multi-concentration testing plates were first calculated to obtain the median of NaClO4 TAA and Median-Difference (150.03 and 95.67 respectively). Then the TAA and Median-Difference of test chemicals were normalized as the percentage of the median NaClO4 TAA and Median-Difference separately and then summed to obtain a chemical ranking score. The ranking score of 200 represents the potency of the referenced NaClO4.

```
median(perchlorate_rank$taa)
```

```
## [1] 151.0348
```

```
median(perchlorate_rank$med_diff)
```

```
## [1] 95.66618
```

```
# calculate ranking metrics, normalize to sodium perchlorate
sum_tbl <- toxplot::rank_tcpl(mc_model, spid_chnm_table,
                              med_taa = median(perchlorate_rank$taa),
                              med_med_diff = median(perchlorate_rank$med_diff))

#write_csv(sum_tbl, "./output data files/Phase1_rank_table.csv")
```

Ranking Score Plot (Fig.2)

Use color to indicate chemicals that have significant RAIU but no significant cytotoxicity at any given concentration.

```
#check each concentration, find concentrations that have sig RAIU but no sig cytotoxicity.
#get the median response for each chemical on each concentration
median_responses <- dt_mc_norm %>%
    filter(wllt == "t") %>%
    group_by(spid, conc, assay) %>%
    summarize(med = median(nval_median)) %>% ungroup
```

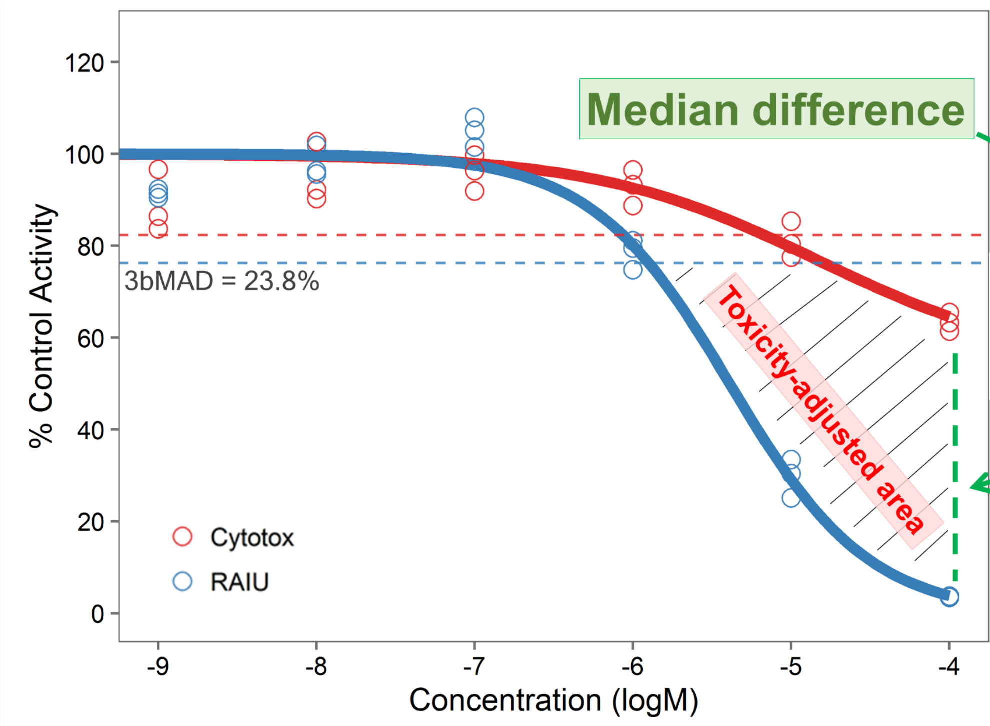
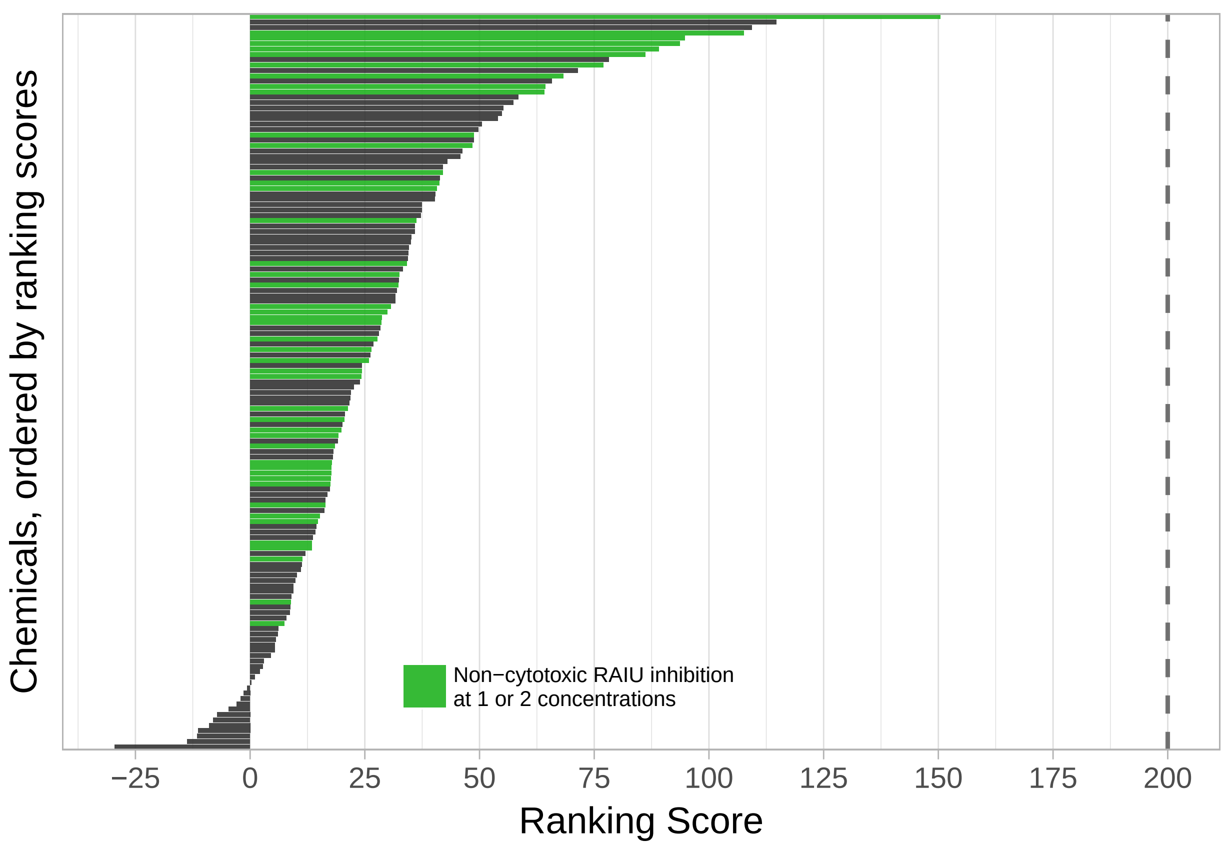


Figure 1: Demonstration of TAA and Median-Difference

```
cyto_positives <- median_responses %>%
    filter(assay == 'Cytotox') %>%
    mutate(positive_cyto = ifelse((med < 100 - sig_mc[[1,3]]), 1, 0))
raiu_positives <- median_responses %>%
    filter(assay == 'RAIU') %>%
    mutate(positive_raiu = ifelse((med < 100 - sig_mc[[2,3]]), 1, 0))

raiu_1_cyto_0 <- left_join(cyto_positives, raiu_positives, by = c("spid", "conc")) %>%
    mutate(separation = ifelse((positive_raiu == 1 & positive_cyto == 0), 1, 0))

separation_spid <- raiu_1_cyto_0 %>%
    filter(separation == 1) %>%
    select(spid) %>%
    unique %>%
    mutate(sep = "Yes")


sum_tbl5 <- left_join(sum_tbl, separation_spid, by = "spid") %>%
    mutate(sep = ifelse(is.na(sep), "No", "Yes")) %>%
    filter(!(is.na(taa_norm)))
sum_tbl6 <- left_join(sum_tbl, separation_spid, by = "spid") %>%
    mutate(sep = ifelse(is.na(sep), "-", "+")) %>%
    filter(!(is.na(taa_norm)))
write.csv(sum_tbl6, "./output data files/sum_tble_for_paper_new_ranking_add_separation.csv")

rs_plot2 <- ggplot(sum_tbl5) +
    geom_col(aes(x=reorder(spid, ranking_score), y = ranking_score, fill = sep),
```

```
            alpha = 0.9, linetype = "solid") +
    theme_light(base_size = 14) +
    xlab("Chemicals, ordered by ranking scores") +
    ylab("Ranking Score") +
    geom_hline(yintercept = 200, alpha = 0.8, size = 0.8,
               linetype = "dashed", color = "gray32") +
    theme(axis.text.y = element_blank(),
          axis.ticks.y = element_blank()) +
    scale_fill_manual(name = "",
                      values = c("gray20", "#21B321"),
                      breaks = c("","Yes"),
                      labels = c("No", "Non-cytotoxic RAIU inhibition\nat 1 or 2 concentrations")
                      )+
    theme(legend.justification = c(0,1), legend.position = c(0.28, 0.18),
          legend.title = element_text(size = rel(0.7)),
          legend.text = element_text(size = rel(0.6)),
          legend.background = element_blank()) +
    coord_flip() +
    scale_x_discrete(breaks = NULL) +
    scale_y_continuous(breaks = seq(-25, 200, by = 25))


rs_plot2
```



Results Table for publication

Table S1

```
multi_results <- sum_tbl %>%
    dplyr::select(spid, chnm, casn, AC50_prim, absEC50_prim, cyto_lim, ranking_score)

## merge sum-tbl with spid_chnm_table, to include all single and multi-con results
spid_chnm_table <-
read_excel("./raw data files/EPA_11700_EPA-SLaws_ph1v2_150ul_20170125_key.xlsx")
#rename the column title to be compatible with tcpl package.

spid_chnm_table <-
    spid_chnm_table %>%
    dplyr::select(EPA_Sample_ID, Aliquot_Concentration, CASRN, Preferred_Name)
names(spid_chnm_table) <- c("spid", "aliquot_conc", "casn", "chnm")
#calculate the actual cocnentration tested in single-con screening
#the unit will be convert from mM to Molar
spid_chnm_table <- spid_chnm_table %>%
    mutate(test_conc = aliquot_conc / 2E5)
single_con_results <- spid_chnm_table %>%
    mutate(hitc = ifelse(spid %in% ls169$spid, "+", "-"))

final_sum_tbl <- full_join(single_con_results, multi_results,
                           by = c("spid", "chnm", "casn")) %>%
    dplyr::select(spid, chnm, casn, test_conc, hitc, everything()) %>%
    dplyr::select(-aliquot_conc) %>%
    arrange(desc(ranking_score), desc(hitc))

colnames(final_sum_tbl) <- c("SPID", "Chemical", "CAS NO.", "Max Conc(M)",
                             "Tested in Multi-Conc", "AC50", "absEC50",
                             "Cytotox Point", "Ranking Score")
knitr::kable(final_sum_tbl, caption = "List of chemicals and screening results" )
```

Table 10: List of chemicals and screening resul

SPID	Chemical	CAS NO.	Max Conc(M)	T
TP0001500G04	Etoxazole	153233-91-1	1.0e-04	+
TP0001502E10	Triphenyltin hydroxide	76-87-9	1.0e-04	+
TP0001501D03	Niclosamide	50-65-7	5.0e-05	+
TP0001502G01	3-Iodo-2-propynyl-N-butylcarbamate	55406-53-6	1.0e-04	+
TP0001501E07	PFOS	1763-23-1	8.0e-05	+
TP0001498G01	PFOS	1763-23-1	8.0e-05	+
TP0001498B02	Cyprodinil	121552-61-2	1.0e-04	+
TP0001501G03	Rotenone	83-79-4	1.0e-04	+
TP0001501C09	Pyridaben	96489-71-3	1.0e-04	+
TP0001500E11	Methoxyfenozide	161050-58-4	1.0e-04	+
TP0001500E05	2-(Thiocyanomethylthio)benzothiazole	21564-17-0	1.0e-04	+
TP0001500D09	Oxyfluorfen	42874-03-3	1.0e-04	+
TP0001499D08	Captan	133-06-2	9.5e-05	+
TP0001502F03	Fipronil	120068-37-3	1.0e-04	+
TP0001502E07	Fluroxypyr-meptyl	81406-37-3	1.0e-04	+
TP0001500D03	Cyhalofop-butyl	122008-85-9	9.5e-05	+

SPID	Chemical	CAS NO.	Max Conc(M)
TP0001499A01	Fenpyroximate (Z,E)	111812-58-9	1.0e-04
TP0001498C01	Thiobencarb	28249-77-6	1.0e-04
TP0001500E07	Emamectin benzoate	155569-91-8	1.0e-04
TP0001499C08	Diphenylamine	122-39-4	1.0e-04
TP0001499G03	Folpet	133-07-3	1.0e-04
TP0001499B03	Endosulfan	115-29-7	1.0e-04
TP0001498C04	Prometryn	7287-19-6	1.0e-04
TP0001502F02	Zoxamide	156052-68-5	1.0e-04
TP0001499E01	Cyazofamid	120116-88-3	1.0e-04
TP0001501E01	Parathion	56-38-2	1.0e-04
TP0001498F01	Fenthion	55-38-9	1.0e-04
TP0001499G11	Mancozeb	8018-01-7	5.0e-05
TP0001502F04	Bifenazate	149877-41-8	1.0e-04
TP0001502F09	Clorophene	120-32-1	1.0e-04
TP0001499F10	Trifloxystrobin	141517-21-7	1.0e-04
TP0001500D07	Triclosan	3380-34-5	1.0e-04
TP0001502B03	Methoxychlor	72-43-5	9.5e-05
TP0001499F01	Quinoxyfen	124495-18-7	1.0e-04
TP0001499G01	Triflumizole	68694-11-1	1.0e-04
TP0001501E11	Prallethrin	23031-36-9	9.5e-05
TP0001499C01	S-Bioallethrin	28434-00-6	1.0e-04
TP0001502B10	Coumaphos	56-72-4	1.0e-04
TP0001502F07	Chlorpyrifos-methyl	5598-13-0	1.0e-04
TP0001498D10	Fluoxastrobin	361377-29-9	1.0e-04
TP0001501C11	Triclosan	3380-34-5	1.0e-04
TP0001498H12	Pyraclostrobin	175013-18-0	1.0e-04
TP0001502G11	Fenoxaprop-ethyl	66441-23-4	1.0e-04
TP0001501D10	Fenoxycarb	72490-01-8	1.0e-04
TP0001500G01	Hexaconazole	79983-71-4	1.0e-04
TP0001499E10	Diclosulam	145701-21-9	1.0e-04
TP0001499D01	Clorophene	120-32-1	1.0e-04
TP0001498D08	Tebupirimfos	96182-53-5	1.0e-04
TP0001501C02	Abamectin	71751-41-2	1.0e-04
TP0001500E08	Pyriproxyfen	95737-68-1	1.0e-04
TP0001498B11	Triclosan	3380-34-5	1.0e-04
TP0001502C11	Carfentrazone-ethyl	128639-02-1	1.0e-04
TP0001498A01	Pirimiphos-methyl	29232-93-7	1.0e-04
TP0001502G02	Dibutyl phthalate	84-74-2	1.0e-04
TP0001498C09	Methylene bis(thiocyanate)	6317-18-6	1.0e-04
TP0001502D03	Bisphenol A	80-05-7	1.0e-04
TP0001498B08	Dithiopyr	97886-45-8	9.5e-05
TP0001500D05	Tebufenpyrad	119168-77-3	1.0e-04
TP0001502D04	Diclofop-methyl	51338-27-3	1.0e-04
TP0001500G11	Dibutyl phthalate	84-74-2	1.0e-04
TP0001498G03	Lactofen	77501-63-4	1.0e-04
TP0001500C09	Piperonyl butoxide	51-03-6	1.0e-04
TP0001500B08	Buprofezin	69327-76-0	1.0e-04
TP0001502G03	Cloprop	101-10-0	1.0e-04
TP0001498C10	Flutolanil	66332-96-5	1.0e-04
TP0001500G03	Cinmethylin	87818-31-3	1.0e-04
TP0001502D09	Chlorpropham	101-21-3	1.0e-04
TP0001499C09	Clodinafop-propargyl	105512-06-9	1.0e-04

SPID	Chemical	CAS NO.	Max Conc(M)	T
TP0001501G11	Phosalone	2310-17-0	1.0e-04	
TP0001502F05	Allethrin	584-79-2	1.0e-04	
TP0001501G10	Disulfoton	298-04-4	1.0e-04	
TP0001502B05	Flumiclorac-pentyl	87546-18-7	1.0e-04	
TP0001502D11	Forchlorfenuron	68157-60-8	1.0e-04	
TP0001500F07	Flumetralin	62924-70-3	1.0e-04	
TP0001501E03	Ethalfluralin	55283-68-6	1.0e-04	
TP0001500B09	Lindane	58-89-9	1.0e-04	
TP0001500G08	Fluazinam	79622-59-6	9.0e-05	
TP0001501D02	Cyfluthrin	68359-37-5	1.0e-04	
TP0001499D02	Tri-allate	2303-17-5	1.0e-04	
TP0001502G07	Imazalil	35554-44-0	1.0e-04	
TP0001502E08	Cypermethrin	52315-07-8	1.0e-04	
TP0001500F09	Amitraz	33089-61-1	1.0e-04	
TP0001499E11	Tetraconazole	112281-77-3	9.5e-05	
TP0001502C07	Thiazopyr	117718-60-2	1.0e-04	
TP0001502E02	Trifluralin	1582-09-8	1.0e-04	
TP0001500F11	Tebufenozide	112410-23-8	1.0e-04	
TP0001502B07	Azoxystrobin	131860-33-8	1.0e-04	
TP0001501B01	Mancozeb	8018-01-7	5.0e-05	
TP0001500F01	Fluazifop-butyl	69806-50-4	1.0e-04	
TP0001502F10	Fenarimol	60168-88-9	1.0e-04	
TP0001499B11	Allethrin	584-79-2	1.0e-04	
TP0001498E08	Maneb	12427-38-2	1.0e-04	
TP0001498D07	Flusilazole	85509-19-9	1.0e-04	
TP0001499B01	Bisphenol A	80-05-7	1.0e-04	
TP0001498G05	Ametryn	834-12-8	1.0e-04	
TP0001499G10	Fluazifop-P-butyl	79241-46-6	1.0e-04	
TP0001500E10	Diniconazole	83657-24-3	1.0e-04	
TP0001501G09	Pendimethalin	40487-42-1	1.0e-04	
TP0001501F07	Fenitrothion	122-14-5	1.0e-04	
TP0001502B04	Isazofos	42509-80-8	1.0e-04	
TP0001502B01	Oxadiazon	19666-30-9	1.0e-04	
TP0001498D11	Hexythiazox	78587-05-0	1.0e-04	
TP0001500E09	Fenamidone	161326-34-7	1.0e-04	
TP0001498F05	Difenoconazole	119446-68-3	1.0e-04	
TP0001501F01	Azoxystrobin	131860-33-8	1.0e-04	
TP0001502C04	Fluthiacet-methyl	117337-19-6	1.0e-04	
TP0001498E01	Oryzalin	19044-88-3	1.0e-04	
TP0001501E05	Thidiazuron	51707-55-2	1.0e-04	
TP0001500B05	Famoxadone	131807-57-3	1.0e-04	
TP0001502E04	Dicofol	115-32-2	1.0e-04	
TP0001500F02	Propargite	2312-35-8	1.0e-04	
TP0001501E02	2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane	2971-36-0	1.0e-04	
TP0001502G09	Propiconazole	60207-90-1	1.0e-04	
TP0001498E11	Chlorethoxyfos	54593-83-8	1.0e-04	
TP0001502G04	Thiodicarb	59669-26-0	1.0e-04	
TP0001500D04	Ethofumesate	26225-79-6	1.0e-04	
TP0001498F07	Bensulide	741-58-2	1.0e-04	
TP0001500G09	Prodiamine	29091-21-2	1.0e-04	
TP0001501D04	Bensulide	741-58-2	1.0e-04	
TP0001500C04	Bisphenol A	80-05-7	1.0e-04	

SPID	Chemical	CAS NO.	Max Conc(M)	T
TP0001500G05	Flumioxazin	103361-09-7	1.0e-04	+
TP0001502A01	Methidathion	950-37-8	1.0e-04	+
TP0001498B05	Azoxystrobin	131860-33-8	1.0e-04	+
TP0001498B09	Butralin	33629-47-9	1.0e-04	+
TP0001498D01	Dicloran	99-30-9	1.0e-04	+
TP0001500D11	Oryzalin	19044-88-3	1.0e-04	+
TP0001501B10	Fenbuconazole	114369-43-6	1.0e-04	+
TP0001499E09	Thiram	137-26-8	1.0e-04	+
TP0001500B02	Tetramethrin	7696-12-0	1.0e-04	+
TP0001498D05	Profenofos	41198-08-7	5.0e-05	+
TP0001501D01	Quizalofop-ethyl	76578-14-8	8.5e-05	+
TP0001498D03	Prochloraz	67747-09-5	1.0e-04	+
TP0001501C04	Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3)	NOCAS_34742	9.5e-05	+
TP0001498B07	Captafol	2425-06-1	1.0e-04	+
TP0001499G02	Tribufos	78-48-8	1.0e-04	+
TP0001499C07	Benfluralin	1861-40-1	1.0e-04	+
TP0001500E01	MGK-264	113-48-4	1.0e-04	+
TP0001498D02	Chlorothalonil	1897-45-6	1.0e-04	+
TP0001498G02	Propanil	709-98-8	1.0e-04	+
TP0001498C03	Bromoxynil	1689-84-5	8.0e-05	+
TP0001498F03	Napropamide	15299-99-7	1.0e-04	+
TP0001498E04	Nitrapyrin	1929-82-4	1.0e-04	+
TP0001498G08	Propetamphos	31218-83-4	1.0e-04	+
TP0001498G09	Myclobutanil	88671-89-0	1.0e-04	+
TP0001498C11	Malathion	121-75-5	1.0e-04	+
TP0001499E02	Resmethrin	10453-86-8	1.0e-04	+
TP0001499E03	Fenpropathrin	39515-41-8	1.0e-04	+
TP0001499B05	Picloram	1918-02-1	1.0e-04	+
TP0001499B07	Fludioxonil	131341-86-1	1.0e-04	+
TP0001500A01	Acibenzolar-S-methyl	135158-54-2	1.0e-04	+
TP0001500G02	Azinphos-methyl	86-50-0	1.0e-04	+
TP0001500F03	Mancozeb	8018-01-7	5.0e-05	+
TP0001500F04	Boscalid	188425-85-6	1.0e-04	+
TP0001500C05	Butachlor	23184-66-9	1.0e-04	+
TP0001500B07	Tefluthrin	79538-32-2	1.0e-04	+
TP0001500G07	Butafenacil	134605-64-4	1.0e-04	+
TP0001501A01	Tralkoxydim	87820-88-0	1.0e-04	+
TP0001501C01	Pyraflufen-ethyl	129630-19-9	1.0e-04	+
TP0001501G02	Prometon	1610-18-0	1.0e-04	+
TP0001501C03	Vinclozolin	50471-44-8	1.0e-04	+
TP0001501F04	2-Phenylphenol	90-43-7	1.0e-04	+
TP0001501G04	Clomazone	81777-89-1	1.0e-04	+
TP0001501B05	Flufenpyr-ethyl	188489-07-8	1.0e-04	+
TP0001501D05	Chlorpyrifos oxon	5598-15-2	9.5e-05	+
TP0001501B08	Fenhexamid	126833-17-8	1.0e-04	+
TP0001501B11	Cycloate	1134-23-2	1.0e-04	+
TP0001502E01	Naled	300-76-5	1.0e-04	+
TP0001502E03	Linuron	330-55-2	1.0e-04	+
TP0001502C09	EPTC	759-94-4	1.0e-04	+
TP0001498B01	Bifenthrin	82657-04-3	1.0e-04	-
TP0001498C02	Bentazone	25057-89-0	1.0e-04	-
TP0001498E02	Mesotrione	104206-82-8	1.0e-04	-

SPID	Chemical	CAS NO.	Max Conc(M)	T
TP0001498F02	Esfenvalerate	66230-04-4	1.0e-04	-
TP0001498B03	Thiophanate-methyl	23564-05-8	1.0e-04	-
TP0001498E03	Trichlorfon	52-68-6	1.0e-04	-
TP0001498B04	Carbaryl	63-25-2	1.0e-04	-
TP0001498D04	2,4-Dichlorophenoxyacetic acid	94-75-7	1.0e-04	-
TP0001498F04	Boric acid	10043-35-3	1.0e-04	-
TP0001498G04	Dichlorprop	120-36-5	1.0e-04	-
TP0001498C05	Dicrotophos	141-66-2	1.0e-04	-
TP0001498E05	Butylate	2008-41-5	1.0e-04	-
TP0001498C07	Dimethylarsinic acid	75-60-5	1.0e-04	-
TP0001498E07	Dichlorvos	62-73-7	5.0e-05	-
TP0001498G07	Malaoxon	1634-78-2	1.0e-04	-
TP0001498C08	Cyanazine	21725-46-2	1.0e-04	-
TP0001498F08	Methomyl	16752-77-5	1.0e-04	-
TP0001498D09	PFOA	335-67-1	1.0e-04	-
TP0001498E09	Propoxur	114-26-1	1.0e-04	-
TP0001498F09	Imazethapyr	81335-77-5	1.0e-04	-
TP0001498B10	Imidacloprid	138261-41-3	1.0e-04	-
TP0001498E10	Fenamiphos	22224-92-6	1.0e-04	-
TP0001498F10	Clopyralid	1702-17-6	1.0e-04	-
TP0001498G10	Metalaxyl	57837-19-1	1.0e-04	-
TP0001498F11	Monocrotophos	6923-22-4	1.0e-04	-
TP0001498G11	Indoxacarb	173584-44-6	8.0e-05	-
TP0001499B02	Acephate	30560-19-1	1.0e-04	-
TP0001499C02	Anilazine	101-05-3	1.0e-04	-
TP0001499F02	Diuron	330-54-1	1.0e-04	-
TP0001499C03	Clofentezine	74115-24-5	1.0e-04	-
TP0001499D03	Methamidophos	10265-92-6	1.0e-04	-
TP0001499F03	Thiamethoxam	153719-23-4	1.0e-04	-
TP0001499B04	Formetanate hydrochloride	23422-53-9	1.0e-04	-
TP0001499C04	Fluometuron	2164-17-2	1.0e-04	-
TP0001499D04	Difenzoquat metilsulfate	43222-48-6	1.0e-04	-
TP0001499E04	Bendiocarb	22781-23-3	1.0e-04	-
TP0001499F04	Alachlor	15972-60-8	1.0e-04	-
TP0001499G04	Dimethenamid	87674-68-8	1.0e-04	-
TP0001499C05	2,4-Dichlorophenoxyacetic acid	94-75-7	1.0e-04	-
TP0001499D05	Ethylene thiourea	96-45-7	1.0e-04	-
TP0001499E05	Azamethiphos	35575-96-3	1.0e-04	-
TP0001499F05	Dazomet	533-74-4	1.0e-04	-
TP0001499G05	Pyrimethanil	53112-28-0	1.0e-04	-
TP0001499D07	Propyzamide	23950-58-5	1.0e-04	-
TP0001499E07	Triadimenol	55219-65-3	1.0e-04	-
TP0001499F07	Pirimicarb	23103-98-2	1.0e-04	-
TP0001499G07	Isoxaben	82558-50-7	1.0e-04	-
TP0001499B08	Acetochlor	34256-82-1	1.0e-04	-
TP0001499E08	Acifluorfen	50594-66-6	1.0e-04	-
TP0001499F08	Tepraloxydim	149979-41-9	1.0e-04	-
TP0001499G08	Clopyralid-olamine	57754-85-5	1.0e-04	-
TP0001499B09	2,4-DB	94-82-6	1.0e-04	-
TP0001499D09	Hexazinone	51235-04-2	1.0e-04	-
TP0001499F09	Tebuthiuron	34014-18-1	1.0e-04	-
TP0001499G09	Iprodione	36734-19-7	1.0e-04	-

SPID	Chemical	CAS NO.	Max Conc(M)	T
TP0001499B10	Dicamba	1918-00-9	1.0e-04	-
TP0001499C10	Methyl parathion	298-00-0	1.0e-04	-
TP0001499D10	Fluroxypyr	69377-81-7	1.0e-04	-
TP0001499C11	Dimethomorph	110488-70-5	1.0e-04	-
TP0001499D11	Benomyl	17804-35-2	1.0e-04	-
TP0001499F11	Monomethyl phthalate	4376-18-5	1.0e-04	-
TP0001499H12	Diazinon	333-41-5	1.0e-04	-
TP0001500B01	Cyclanilide	113136-77-9	1.0e-04	-
TP0001500C01	Cyanamide	420-04-2	1.0e-04	-
TP0001500D01	Ethoprop	13194-48-4	1.0e-04	-
TP0001500C02	Penoxsulam	219714-96-2	1.0e-04	-
TP0001500D02	Clothianidin	210880-92-5	1.0e-04	-
TP0001500E02	Di(2-ethylhexyl) phthalate	117-81-7	1.0e-04	-
TP0001500B03	Acetamiprid	135410-20-7	1.0e-04	-
TP0001500C03	Novaluron	116714-46-6	1.0e-04	-
TP0001500E03	Isoxaflutole	141112-29-0	1.0e-04	-
TP0001500B04	Imazamox	114311-32-9	1.0e-04	-
TP0001500E04	Sulfentrazone	122836-35-5	1.0e-04	-
TP0001500F05	Cyproconazole	94361-06-5	9.5e-05	-
TP0001500C07	Pymetrozine	123312-89-0	1.0e-04	-
TP0001500C08	Spiroxamine	118134-30-8	1.0e-04	-
TP0001500D08	Quinclorac	84087-01-4	1.0e-04	-
TP0001500F08	Triclopyr	55335-06-3	1.0e-04	-
TP0001500B10	Propamocarb hydrochloride	25606-41-1	1.0e-04	-
TP0001500C10	Monobutyl phthalate	131-70-4	1.0e-04	-
TP0001500D10	Pentachloronitrobenzene	82-68-8	1.0e-04	-
TP0001500F10	Flufenacet	142459-58-3	1.0e-04	-
TP0001500G10	Imazapyr	81334-34-1	1.0e-04	-
TP0001500B11	Trifloxysulfuron-sodium	199119-58-9	1.0e-04	-
TP0001500C11	Propazine	139-40-2	1.0e-04	-
TP0001500H12	Thiacloprid	111988-49-9	1.0e-04	-
TP0001501G01	2-Methoxyethanol	109-86-4	1.0e-04	-
TP0001501B02	Chloridazon	1698-60-8	1.0e-04	-
TP0001501F02	Asulam	3337-71-1	1.0e-04	-
TP0001501B03	Pyrithiobac-sodium	123343-16-8	1.0e-04	-
TP0001501F03	Deisopropylatrazine	1007-28-9	1.0e-04	-
TP0001501B04	Molinate	2212-67-1	1.0e-04	-
TP0001501E04	Oxytetracycline dihydrate	6153-64-6	1.0e-04	-
TP0001501C05	Spirodiclofen	148477-71-8	1.0e-04	-
TP0001501F05	Carboxin	5234-68-4	1.0e-04	-
TP0001501G05	Oxamyl	23135-22-0	1.0e-04	-
TP0001501B07	Symclosene	87-90-1	1.0e-04	-
TP0001501C07	Fosthiazate	98886-44-3	1.0e-04	-
TP0001501D07	Sethoxydim	74051-80-2	1.0e-04	-
TP0001501G07	Dimethoate	60-51-5	1.0e-04	-
TP0001501C08	MCPA	94-74-6	1.0e-04	-
TP0001501D08	Paclobutrazol	76738-62-0	1.0e-04	-
TP0001501E08	Dipropyl 2,5-pyridinedicarboxylate	136-45-8	1.0e-04	-
TP0001501F08	Methyl isothiocyanate	556-61-6	1.0e-04	-
TP0001501G08	DEET	134-62-3	1.0e-04	-
TP0001501B09	Cyromazine	66215-27-8	1.0e-04	-
TP0001501D09	Imazaquin	81335-37-7	1.0e-04	-

SPID	Chemical	CAS NO.	Max Conc(M)	T
TP0001501E09	Metribuzin	21087-64-9	1.0e-04	-
TP0001501F09	Flumetsulam	98967-40-9	1.0e-04	-
TP0001501C10	Triadimefon	43121-43-3	1.0e-04	-
TP0001501E10	Metolachlor	51218-45-2	1.0e-04	-
TP0001501F10	Permethrin	52645-53-1	1.0e-04	-
TP0001501D11	Terbacil	5902-51-2	1.0e-04	-
TP0001501F11	Triadimenol	55219-65-3	1.0e-04	-
TP0001501H12	Etridiazole	2593-15-9	1.0e-04	-
TP0001502C01	Propoxycarbazone-sodium	181274-15-7	1.0e-04	-
TP0001502D01	Mevinphos	7786-34-7	1.0e-04	-
TP0001502F01	Bromacil	314-40-9	1.0e-04	-
TP0001502B02	Metam-sodium hydrate	6734-80-1	1.0e-04	-
TP0001502C02	2,4-Dichlorophenoxyacetic acid	94-75-7	1.0e-04	-
TP0001502D02	Thiabendazole	148-79-8	1.0e-04	-
TP0001502C03	Atrazine	1912-24-9	1.0e-04	-
TP0001502C05	2-Phenoxyethanol	122-99-6	1.0e-04	-
TP0001502D05	Icaridin	119515-38-7	1.0e-04	-
TP0001502E05	Imazapic	104098-48-8	1.0e-04	-
TP0001502G05	Aldicarb	116-06-3	1.0e-04	-
TP0001502D07	Triticonazole	131983-72-7	9.5e-05	-
TP0001502B08	Diazoxon	962-58-3	1.0e-04	-
TP0001502C08	Maleic hydrazide	123-33-1	1.0e-04	-
TP0001502D08	Daminozide	1596-84-5	1.0e-04	-
TP0001502F08	Mepiquat chloride	24307-26-4	1.0e-04	-
TP0001502G08	Norflurazon	27314-13-2	1.0e-04	-
TP0001502B09	Chloroneb	2675-77-6	1.0e-04	-
TP0001502E09	Ethephon	16672-87-0	1.0e-04	-
TP0001502C10	Iodosulfuron-methyl-sodium	144550-36-7	1.0e-04	-
TP0001502D10	Simazine	122-34-9	1.0e-04	-
TP0001502G10	MEHP	4376-20-9	1.0e-04	-
TP0001502B11	Cymoxanil	57966-95-7	1.0e-04	-
TP0001502E11	Diquat dibromide monohydrate	6385-62-2	5.0e-05	-
TP0001502F11	Dimethyl phthalate	131-11-3	1.0e-04	-
TP0001502H12	Dichlobenil	1194-65-6	1.0e-04	-

Export supplemental summary table that includes all potency metrics.

```r
sup_sum_tbl <- full_join(single_con_results, sum_tbl, by = c("spid", "chnm", "casn")) %>%
    dplyr::select(spid, chnm, casn, test_conc, hitc, everything()) %>%
    dplyr::select(-aliquot_conc, -index) %>%
    arrange(desc(ranking_score), desc(hitc))

colnames(sup_sum_tbl) <- c("Sample ID", "Chemical", "CAS NO.", "Max Conc(M)",
                           "Hit Call", "TAA", "Median_Difference", "AC50_Cytotox",
                           "AC50_RAIU", "absEC80_Cytotox", "absEC50_Cytotox",
                           "absEC80_RAIU", "absEC50_RAIU", "Cytotox_point",
                           "TAA_Normalized", "Median_Difference_Normalized",
                           "Ranking Score")

#write_csv(sup_sum_tbl, "./output data files/Supplemental_summary_table.csv")
```

ToxCast Internal Replicates

Single-con internal Replicate performance

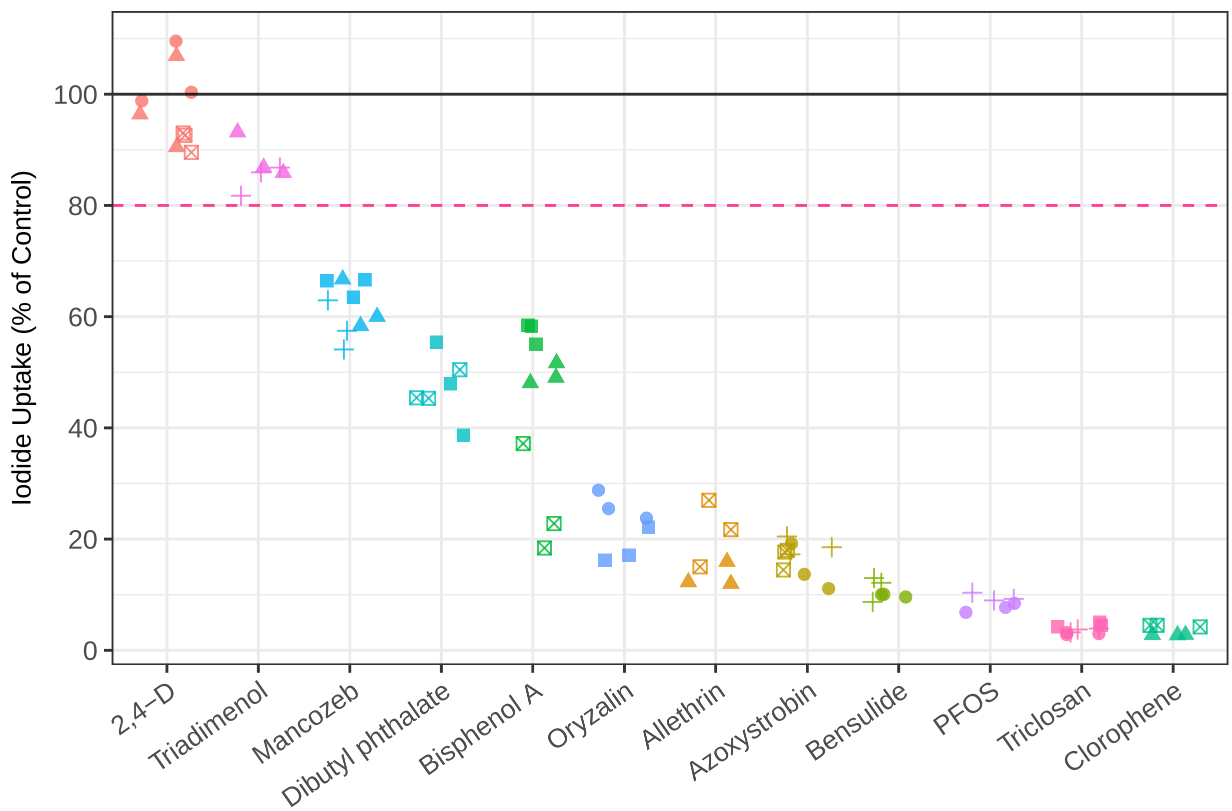
ToxCast Ph1_v2 library included internal replicates. They are the same chemical but under different sample id, therefore tested blindly with each sample repliated three times. .

There are 12 chemicals been repeated, showed in the following table

```
name_code <- spid_chnm_table %>% dplyr::select(spid, casn, chnm)
#check which chemical is repeated in toxcast ph1_v2 library
chnm_freq <- data.frame(table(name_code$chnm)) %>% arrange(desc(Freq))
internal_rep <- head(chnm_freq, 12)
knitr::kable(internal_rep)
```

Var1	Freq
2,4-Dichlorophenoxyacetic acid	3
Azoxystrobin	3
Bisphenol A	3
Mancozeb	3
Triclosan	3
Allethrin	2
Bensulide	2
Clorophene	2
Dibutyl phthalate	2
Oryzalin	2
PFOS	2
Triadimenol	2

```
##add chnm to sc data
sc_unblind <- left_join(dt_sc_norm, name_code, by= "spid")
## get sc data for interval replicates
sc_rep <- sc_unblind %>% dplyr::filter(chnm %in% internal_rep$Var1)
sc_rep$chnm <- str_replace(sc_rep$chnm, "2,4-Dichlorophenoxyacetic acid", "2,4-D")

library(RColorBrewer)
ggplot(sc_rep, aes(x=reorder(chnm, -nval_median), y=nval_median) ) +
    geom_point(size=2, alpha = 0.8, aes(shape=pid, color=chnm),
               position = position_jitter(width=0.3)) +
    xlab("") +
    ylab("Iodide Uptake (% of Control)")+
    geom_hline(yintercept = 80, linetype="dashed", color="violetred1") +
    geom_hline(yintercept = 100, alpha=0.8) +
    scale_y_continuous(breaks = seq(from = 0, to =100, by=20))+
    theme_bw(base_size = 12) +
    theme(axis.text.x  = element_text(angle=35, vjust=1, hjust=1),
          axis.title = element_text(size = rel(0.8)))+
    theme(legend.position="none")
```



Multi-con internal controls replication performance

```
##add chnm to mc data
mc_unblind <- left_join(dt_mc_norm, name_code, by= c("spid"="spid"))

##gettting reps's metrics
mc_rep_sum <-
    sum_tbl %>% filter(chnm %in% internal_rep$Var1)

## getting range of ac50s
mc_rep_sum %>%
    filter(!is.na(AC50_prim)) %>%
    group_by(chnm) %>%
    summarize(min = min(AC50_prim),
              max= max(AC50_prim),
              range = min - max) %>%
    arrange(desc(range)) %>%
    knitr::kable(digits = 2, caption = "Range of AC50 for internal replicates")
```

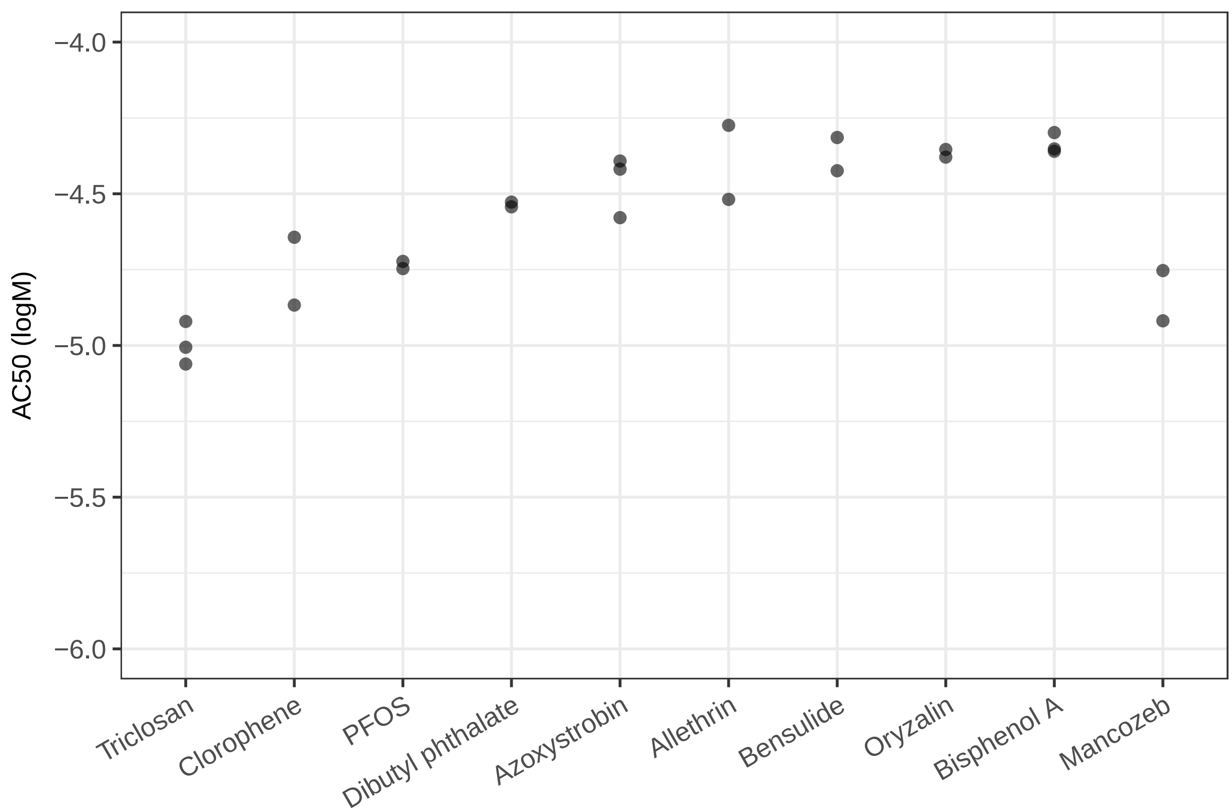
Table 12: Range of AC50 for internal replicates

chnm	min	max	range
Dibutyl phthalate	-4.54	-4.53	-0.02
PFOS	-4.75	-4.72	-0.02

chnm	min	max	range
Oryzalin	-4.38	-4.35	-0.03
Bisphenol A	-4.36	-4.30	-0.06
Bensulide	-4.42	-4.31	-0.11
Triclosan	-5.06	-4.92	-0.14
Mancozeb	-4.92	-4.75	-0.17
Azoxystrobin	-4.58	-4.39	-0.19
Clorophene	-4.87	-4.64	-0.22
Allethrin	-4.52	-4.27	-0.24

```r
##plot all points of ac50
ggplot(mc_rep_sum, aes(x=reorder(chnm, AC50_prim), y=AC50_prim) ) +
    geom_point(size = 2, alpha = 0.6, shape = 16) +
    xlab("") +
    ylab("AC50 (logM)")+
    ylim(-6, -4)+
    theme_bw(base_size = 12) +
    theme(axis.text.x  = element_text(angle=30, vjust=1, hjust=1),
          #axis.text.y = element_text(size = 5),
          legend.position = "none",
          axis.title = element_text(size = rel(0.8))
          #plot.margin = NULL
          )
```

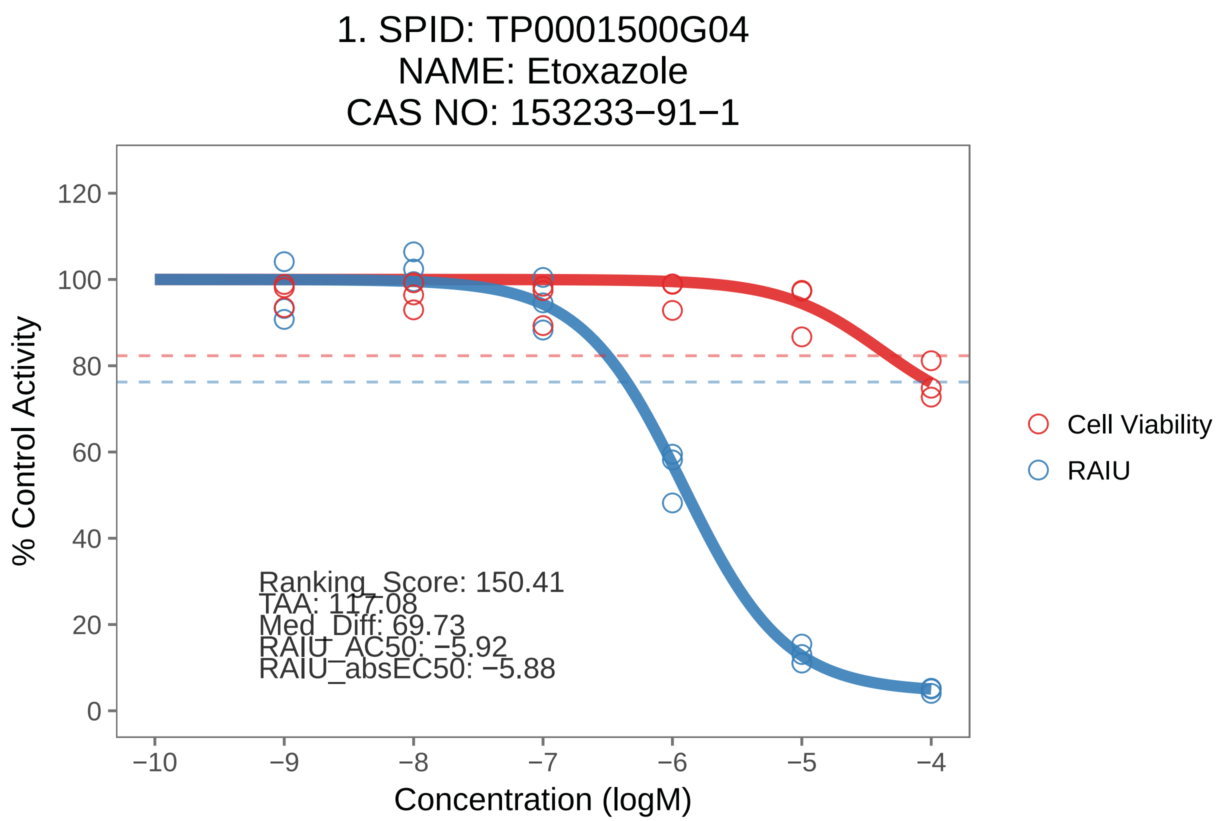
```
## Warning: Removed 1 rows containing missing values (geom_point).
```



Export Dose-Response Curve

Make plots

```
#plot all
allplot <- toxplot::plot_tcpl(mc_model, sum_tbl, spid_chnm_table, notation = T)
# allplot[[1]] + scale_color_manual(values=c("#e02929", "#377eb8"),
#                                    labels = c("Cell Viability", "RAIU"))

for (i in 1:length(allplot)) {
    allplot[[i]] <- allplot[[i]] + scale_color_manual(values=c("#e02929", "#377eb8"),
                                   labels = c("Cell Viability", "RAIU"))
}

allplot[[1]]
```



Export as PDF file.

```
# Export plots as pdf file
save_plot_pdf(allplot,"./output plots/ranked_dose_response_plots.pdf")
```

Fig. 3

```r
# Top 15 samples graphs group
ap_mini <- toxplot::plot_tcpl_minimal(mc_model, sum_tbl, spid_chnm_table, notation = T)

tiff('./output plots/top15v6.tiff', units="px",
     width=750*12.5, height=1000*12.5, res=900, compression = "lzw")
multiplot(ap_mini[[1]],ap_mini[[2]],ap_mini[[3]],
          ap_mini[[4]],ap_mini[[5]],ap_mini[[6]],
          ap_mini[[7]],ap_mini[[8]],ap_mini[[9]],
          ap_mini[[10]],ap_mini[[11]],ap_mini[[12]],
          ap_mini[[13]],ap_mini[[14]],ap_mini[[15]],
          layout = matrix(c(1,2,3,4,5,6,7,8,9,10,11,12,13,14,15), nrow=5, byrow=TRUE))
dev.off()

# three graphs for ETC disruption
tiff('./output plots/3_ETC_Disruption.tiff', units="px",
     width=750*12.5, height=200*12.5, res=900, compression = "lzw")
multiplot(ap_mini[[17]],ap_mini[[58]], ap_mini[[42]],
          layout = matrix(c(1,2,3), nrow=1, byrow=TRUE))
dev.off()
```

R source code in `ToxPlot` package

Main R functions written for this analysis were compiled as an R package `ToxPlot`, and version 0.1.0 is available on CRAN.
For the most up-to-date version please go to the github link.

Below is the source code of `ToxPlot` ver.0.1.0 used in this analysis.

```r
#' normalize per plate
#'
#' normalize raw readings as percent of median vehicle control wells
#'
#' @param dt data.frame contains essential columns with the raw data.
#' @param nctrl the name (spid) of the vehicle/solvent control used for calculation
#'
#' @return data.frame with normalized value columns. 'nval_mean' column is the normalized value
#' calculated using the mean of vehicle control wells, 'nval_median' column is the normalized value
#' calculated using the median of vehicle control wells.
#' @import dplyr
#'
#' @examples
#' ## normalize demo data
#' demo_mc_norm <- normalize_per_plate(demo_mc, nctrl = "DMSO")
#'
#' @export

normalize_per_plate <- function(dt, nctrl = "DMSO") {

  # claim variables for passing R CMD Check
  assay <- spid <- apid <- rval <- NULL


  output <- data.frame()
```

```r
  #iterate through each assay, calculate separately
  for (as in unique(dt$assay)) {
    df_t <- normalize_single_assay(dplyr::filter(dt, assay == as), nctrl)
    output <- dplyr::bind_rows(output, df_t)
  }

  return(output)

}

#' normalize per plate (from single assay data)
#'
#' normalize raw readings as percent of median/mean vehicle control wells, per assay, per plate.
#' This function is called by normalize_per_plate, should not be called directly by user.
#' #'
#' @param dt data.frame contains essential columns with the raw data.
#' @param nctrl the name (spid) of the vehicle/solvent control used for calculation
#'
#' @return data.frame with normalized value columns. 'nval_mean' column is the normalized value
#' calculated using the mean of vehicle control wells, 'nval_median' column is the normalized value
#' calculated using the median of vehicle control wells.
#' @import dplyr
#
normalize_single_assay <- function(dt, nctrl) {

  # claim variables for passing R CMD Check
  assay <- spid <- apid <- rval <- NULL


  #calculate the mean and median value for negative control
  ctrl_avg <- dt %>%
    dplyr::filter(spid == nctrl) %>%
    dplyr::group_by(apid) %>%
    dplyr::summarize(mean_DMSO = mean(rval, na.rm = TRUE),
                     median_DMSO = stats::median(rval, na.rm = TRUE))

  #iterate through the data table to calculate normalized percent activity
  #normalization was done using both mean and median separately.

  temp <- data.frame()
  for (id in ctrl_avg$apid){
    med <- dplyr::filter(ctrl_avg, apid == id)$median_DMSO
    avg <- dplyr::filter(ctrl_avg, apid == id)$mean_DMSO
    t <- dplyr::filter(dt, apid == id) %>%
      mutate(nval_mean = 100 * rval/avg,
             nval_median = 100 * rval/med)
    temp <- bind_rows(temp, t)
  }
  return(temp)
}

#' Quality-control metrics calculation
#'
```

```
#' Calculate QC metrics, includin Z' score, CV of DMSO negative control, per assay plate.
#'
#' @param d data.frame contains essential columns with the raw data.
#' @param resp response type, specify either 'nval_median' or 'nval_mean' for QC calculation
#' @param assay_info assay_info list, contains names of primary and cytotox assay, names must match
#' what are provided in the raw data, under the column 'assay'.
#'
#' @examples
#' ## calculate QC measures from demo data
#' assay_info <- list(prim_assay = "Primary",toxi_assay = "Cytotox")
#' demo_mc_norm <- normalize_per_plate(demo_mc, nctrl = "DMSO")
#' qc <- qc_per_plate(demo_mc_norm, assay_info)
#'
#' @return three dataframe each representing negative control stats, positive control stats and QC metr
#' @export
# QC measures are calculated per 96-well palte. 'apid' plus 'assay' column can serve as the ID to disti

qc_per_plate <- function(d, assay_info, resp = "nval_median") {

  # claim variables for passing R CMD Check
  assay <- apid <- wllt <- conc <- CV_DMSO <- SSMD <- Z_prime <- logc <- mean_DMSO <- mean_positive <- 
  sd_positive <- sd_DMSO <- unique_id <- NULL



  # choose which normalized value to use (median based or mean based)
  if (resp == "nval_mean") {
    d$resp <- d$nval_mean
  } else if (resp == "nval_median") {
    d$resp <- d$nval_median
  } else {
    stop("specify either nval_median or nval_mean for QC calculation")
  }

  # create unique ID for each plate (apid + assay)
  # (can also distinguish between primary and cytotox assays)
  # group by the unique ID.
  d <- d %>% #dplyr::mutate(uid = paste(apid, assay)) %>%
      # dplyr::group_by(pid, assay, repi)
      dplyr::group_by(apid, assay)

  # calculate vehicle control (e.g., DMSO etc.) qc stats
  # use welltype = n to identify vehicle control
  n_ctrl_sum <- d %>%
    dplyr::filter(wllt == "n") %>%
    dplyr::summarize(count_DMSO = n(),                          #count of DMSO control wells on each plate
                     count_DMSO_NA = sum(is.na(resp)),          #count of DMSO control wells with missing va
                     mean_DMSO = mean(resp, na.rm = TRUE),
                     sd_DMSO = stats::sd(resp, na.rm = TRUE),
                     CV_DMSO = 100 * stats::sd(resp, na.rm = TRUE) / mean(resp, na.rm = TRUE)
                     # median_DMSO= median(resp, na.rm=TRUE),
                     # mad_DMSO= mad(resp, constant = 1, na.rm=TRUE),
                     # bmad_DMSO= mad(resp, constant = 1.4826, na.rm=TRUE),
```

```
                    # three_bmad = 3*bmad_DMSO
                    )


  # calculate positive control stats
  pctrl_prim <-  d %>%
    dplyr::filter(assay == assay_info$prim_assay,
                  wllt == "pr") %>%
    dplyr::filter(conc == max(conc)) %>%
    dplyr::summarize(sd_positive = stats::sd(resp, na.rm = TRUE),
                     mean_positive= mean(resp, na.rm = TRUE))

  pctrl_toxi <-  d %>%
    dplyr::filter(assay == assay_info$toxi_assay,
                  wllt == "pc") %>%
    dplyr::filter(conc == max(conc)) %>%
    dplyr::summarize(sd_positive = stats::sd(resp, na.rm = TRUE),
                     mean_positive = mean(resp, na.rm = TRUE))

  p_ctrl_sum <- bind_rows(pctrl_prim, pctrl_toxi)
  remove(pctrl_toxi, pctrl_prim)


  # calculate Z', SSMD

  qc <- dplyr::left_join(p_ctrl_sum, n_ctrl_sum,
                          by=c("apid"="apid", "assay"="assay")) %>%
       #replace NaN with 0 in sd_positive
       dplyr::mutate(sd_positive = (ifelse(is.na(sd_positive), 0, sd_positive))) %>%
       dplyr::mutate(Z_prime = 1 - 3*(sd_positive + sd_DMSO) / (abs(mean_positive - mean_DMSO)),
                     SSMD = (abs(mean_positive - mean_DMSO) / sqrt(sd_positive^2 + sd_DMSO^2))) %>%
       dplyr::mutate(unique_id = paste(apid, assay, sep = "_")) %>%
       dplyr::select(unique_id, apid, assay, CV_DMSO, Z_prime, SSMD)



  list(neg_ctrl_sum = n_ctrl_sum,
       pos_ctrl_sum = p_ctrl_sum,
       qc = qc)
}



#' save plots in pdf
#'
#' save ggplot2 plots generated in a list to a pdf file
#'
#' @param plot_list  the r list object contains all ggplot2 objects
#' @param filename  the output file name, including the file directory
#'
#' @examples
#' ## start from raw data
#' # define assay
```

```r
#' assay_info <- list(prim_assay = "Primary",toxi_assay = "Cytotox")
#' # data normalization
#' demo_mc_norm <- normalize_per_plate(demo_mc, nctrl = "DMSO")
#' # filter out two test chemicals
#' demo_mc_norm <- dplyr::filter(demo_mc_norm, spid %in% c("TP0001502B05", "TP0001502B01"))
#' # fit curve with default 20% threshold
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info)
#' # calculate TAA and Med_diff only
#' demo_rank <- rank_tcpl(demo_md, med_taa = NULL, med_med_diff = NULL)
#' #produce plots with notations
#' demo_plots <- plot_tcpl_minimal(demo_md, demo_rank, notation = TRUE)
#'
#' ## save all the plots as pdf
#' # save_plot_pdf(demo_plots, ".\output plots\all_plots.pdf")
#'
#' ## save the 1st plot as pdf
#' # save_plot_pdf(demo_plots[1], ".\output plots\plot1.pdf")
#'
#'
#'
#' @export
#'

save_plot_pdf <- function(plot_list, filename) {
  # claim variables for passing R CMD Check
  assay <- spid <- apid <- rval <- NULL

  grDevices::pdf(filename)
  cat("Preparing file...\n")
  invisible(lapply(plot_list, print))
  grDevices::dev.off()
  cat("Finished!")
}



#' round digits of numbers
#'
#' round numbers in a datafram to specified digits
#'
#' @param df the dataframe input
#' @param digits  the specified number of digits
#' @return a dataframe
#'
#'
round_df <- function(df, digits) {
  nums <- vapply(df, is.numeric, FUN.VALUE = logical(1))
  df[,nums] <- round(df[,nums], digits = digits)
  df
}


# -----------------------------------------------------
```

```r
# function to scale dataset from 0 to 100
# -----------------------------------------------------

rescale_0_100 <- function(x) {
  y <- scale(x, center = min(x, na.rm = T), scale = diff(range(x, na.rm = T)))
  as.vector(y) * 100
}



## function to generate index for concentrations

## both are targeting unique(x), 'match' provide the position of each x value on the list of unique(x),
## while 'rank' provide the ordering index that is exported for each component of unique(x)

generate_index <- function(x) {
  uls <- unique(x)
  index <- rank(uls)[match(x, uls)]
  return(as.integer(index))
}

#' hill mode in ToxCast tcpl package
#'
#' @param p a vector containing the Hill model parameters: top, log AC50, hill coefficient
#' @param x a vector of log concentrations
#' @return calculated y value based on the x and model parameters
#'
hill_model <- function(p, x) {
  y <- p[1] / (1 + 10 ^ ((p[2] - x) * p[3]))
  return(y)
}

# ##========inversed hill model (using 100- the Y value)=======##
# hill_model_inverse <- function(p, x) {
#   ###   p:      a numeric vector of length 4 containg the starting values for
#   ###           the hill model, in order: top, log AC50, hill
#   ###           coefficient
#   ###   x: a numeric vector containing the log concentration values
#
#   y <- 100 - (p[1] / (1 + 10 ^ ((p[2] - x) * p[3])))
#   return(y)
# }

#' calculate absolute EC_anything based on tcpl hill model
#'
#' @param p a vector containing the Hill model parameters: top, log AC50, hill coefficient
#' @param y the y value
#' @return calculated x value

log_abs_ec <- function(p, y) {
  ## y value is the absolute response value
  ##p[1] is top parameter
  ##p[2] is ga, logac50
```

```
  ##p[3] is gw, hillslope
  suppressWarnings(x <- p[2] - log10((p[1] - y) / y) / p[3])
  if (is.nan(x)) {x <- NA}
  return(x)
}


#' function to calculate Area Under the Curve (AUC) of the hill model
#'
#' @param p a vector containing the Hill model parameters: top, log AC50, hill coefficient
#' @param lower lower boundary of x for integration
#' @param upper upper boundary of x for integration
#' @return calculated area under the curve (AUC) value
#'
auc_hill_tcpl <- function(p, lower, upper) {
  # if (is.na(lower)){
  #   cat("lower boundary is NA")
  # } else if (is.nan(lower)){
  #   cat("lower boudary is NaN")
  # }
  #
  # if (is.na(upper)){
  #   cat("upper boundary is NA")
  # } else if (is.nan(upper)){
  #   cat("upper boudary is NaN")
  # }

  #define the hill model function
  hill <- function(x) {
    p[1] / (1 + 10 ^ ((p[2] - x) * p[3]))
  }
  a <- stats::integrate(hill, lower = lower, upper = upper)
  return(a[[1]])
}




#' fit dose-resopnse curve using tcpl hill model
#'
#' Curve fitting using the tcplFit function in `tcpl` package.
#' Chemicals are modelled based on spid.
#' If you want to model the same chemical (e.g. positive controls),
#' then assign different spid to this chemical so the function can separate them out.
#' Absolute IC20 and absolute IC50 are calculated as well.
#'
#' @param df input data contain normalized assay readings
#' @param assay_info predefined names for primary and cytotoxicity assays,
#' use NULL if either one of the assay does not need to be modeled.
#' @param prim_cutoff significance cutoff for primary assay (eg. 3sigma or 3bMAD)
#' @param toxi_cutoff significance cutoff for cytotoxicity assay (eg. 3sigma or 3bMAD)
#'
#' @return A list object containing modeling results, the corresponding data for each chemical.
```

```r
#'
#' @examples
#' ## fit curve with default significant threshold 20
#'
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info =
#' list(prim_assay = "Primary", toxi_assay = "Cytotox"))
#'
#' ## start from raw data
#' # define assay
#' assay_info <- list(prim_assay = "Primary",toxi_assay = "Cytotox")
#' # data normalization
#' demo_mc_norm <- normalize_per_plate(demo_mc, nctrl = "DMSO")
#' # filter out two test chemicals
#' demo_mc_norm <- dplyr::filter(demo_mc_norm, spid %in% c("TP0001502B05", "TP0001502B01"))
#' # fit curve with default 20% threshold
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info)
#'
#' ## fit curve with specified significance threshold
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info, prim_cutoff = 25, toxi_cutoff = 25)
#'
#'
#' @import dplyr
#' @export

fit_curve_tcpl <- function(df, assay_info, prim_cutoff = 20, toxi_cutoff = 20) {

  # claim variables for passing R CMD Check
  conc <- spid <- assay <- apid <- NULL

  st_time <- Sys.time()
  r_list <- list()
  c_list <- list()
  bmad_prim <- prim_cutoff/3
  bmad_toxi <- toxi_cutoff/3
  # get log concentration
  df <- df %>% dplyr::mutate(logc = log10(conc))
  spid_list <- unique(df$spid)
  if (is.null(assay_info$prim) & is.null(assay_info$toxi_assay)) {
    stop("assay_info cannot be NULL for both primary and cytotoxicity assay")
  }
  n <- 1
  prim_md <- toxi_md <- model_list <- list()
  cat("Processing", length(unique(df$spid)), "samples(spid)....\n")
  # process by each spid
  for (id in unique(df$spid)) {
    #d <- df %>% dplyr::filter(spid == i)
    cat(id, "||")
    # model raiu data
    # check if toxi assay data is available, if not, skip modeling
    if (is.null(assay_info$prim_assay)) {
      prim_md <- NA
      prim_dt <- NA
    } else {
```

```
    prim_dt <- df %>% dplyr::filter(spid == id, assay == assay_info$prim_assay)
    m <- tcpl::tcplFit(logc = prim_dt$logc, resp = 100 - prim_dt$nval_median, bmad_prim)
    absIC50 <- log_abs_ec(c(m$hill_tp, m$hill_ga, m$hill_gw), 50)
    absIC20 <- log_abs_ec(c(m$hill_tp, m$hill_ga, m$hill_gw), 20)
    m[["absIC20"]] <- absIC20
    m[["absIC50"]] <- absIC50
    m[["apid"]] <- prim_dt[[1,1]]
    m[["assay"]] <- assay_info$prim_assay
    m[["spid"]] <- id
    #prim_md <- dplyr::bind_rows(prim_md, m)
    # print(m)
    prim_md <- data.frame(m) %>% dplyr::select(apid, assay, spid, everything())
  }

  # model cytotox data
  # check if toxi assay data is available, if not, skip modeling
  if (is.null(assay_info$toxi_assay)) {
    toxi_md <- NA
    toxi_dt <- NA
  } else {
    toxi_dt <- df %>% dplyr::filter(spid == id, assay==assay_info$toxi_assay)
    m <- tcpl::tcplFit(logc = toxi_dt$logc, resp = 100 - toxi_dt$nval_median, bmad_toxi)
    absIC50 <- log_abs_ec(c(m$hill_tp, m$hill_ga, m$hill_gw), 50)
    absIC20 <- log_abs_ec(c(m$hill_tp, m$hill_ga, m$hill_gw), 20)
    m[["absIC20"]] <- absIC20
    m[["absIC50"]] <- absIC50
    m[["apid"]] <- toxi_dt[[1,1]]
    m[["assay"]] <- assay_info$toxi_assay
    m[["spid"]] <- id
    #toxi_md <- dplyr::bind_rows(toxi_md, m)

    toxi_md <- data.frame(m) %>% dplyr::select(apid, assay, spid, everything())

  }

  #build final model list
  model_list[[n]] <- list(spid = id,
                          model_prim = prim_md,
                          model_toxi = toxi_md,
                          data_prim = prim_dt,
                          data_toxi = toxi_dt,
                          cutoff_prim = prim_cutoff,
                          cutoff_toxi = toxi_cutoff,
                          assay_info = assay_info)

  n <- n + 1

}

time <- difftime(Sys.time(), st_time) %>% round(1)
cat("\nCurve Fitting Completed!\nCalculation time:", paste(unclass(time), units(time)), "\n\n")
```

```r
  return(model_list)
}



#' function to calculate ranking score, TAA, med_diff, EC values based on tcpl hill model
#'
#' calculate ranking score, TAA, med_diff, absolute EC values, AC50, based on the hill model in tcpl pa
#'
#' @param tcpl_models the list object returned by 'fit_curve_tcpl' function
#' @param spid_chnm_table a reference table with 'spid' and the corresponding chemical name 'chnm' colu
#' and the CAS number 'casn' column.
#' @param med_taa the median TAA value from reference chemical, if not supplied, then ranking score won
#' @param med_med_diff the median Median-Difference from reference chemical, if not supplied, then rank
#' @return a dataframe containing ranking metrics for each chemical (spid)
#'
#' @examples
#' ## start with normalized data
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info =
#' list(prim_assay = "Primary", toxi_assay = "Cytotox"))
#' demo_rank <- rank_tcpl(demo_md)
#'
#'
#' ## start from raw data
#' # define assay
#' assay_info <- list(prim_assay = "Primary",toxi_assay = "Cytotox")
#' # data normalization
#' demo_mc_norm <- normalize_per_plate(demo_mc, nctrl = "DMSO")
#' # filter out two test chemicals
#' demo_mc_norm <- dplyr::filter(demo_mc_norm, spid %in% c("TP0001502B05", "TP0001502B01"))
#' # fit curve with default 20% threshold
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info)
#' # calculate TAA and Med_diff only
#' demo_rank <- rank_tcpl(demo_md, med_taa = NULL, med_med_diff = NULL)
#'
#' ## calculate ranking score with specified median TAA and meidan Med_Difference
#' demo_rank <- rank_tcpl(demo_md, med_taa = 150, med_med_diff = 92)
#'
#' @export
#'
rank_tcpl <- function(tcpl_models, spid_chnm_table = NULL, med_taa = NULL, med_med_diff = NULL) {

  # claim variables for passing R CMD Check
  taa_norm <- med_diff_norm <- ranking_score <- spid <- logc <- nval_median <- NULL

  df <- data.frame()
  ##iterate through each spid
  for (i in seq_along(tcpl_models)) {
    #get chemical sample id 'spid'
    .spid <- tcpl_models[[i]]$spid
    # print(i)
    # print(.spid)
    #get chnm
```

```
  if (!is.null(spid_chnm_table)) {
    chnm <- dplyr::filter(spid_chnm_table, spid == .spid)$chnm
    casn <- dplyr::filter(spid_chnm_table, spid == .spid)$casn
  } else {
    chnm <- NA
    casn <- NA
  }

  assay_info <- tcpl_models[[i]]$assay_info
  if (is.null(assay_info$toxi_assay)) {
    stop("No toxi_assay, ranking score is not calculable!")
  }
  #extract modelling results
  m_toxi <- tcpl_models[[i]]$model_toxi
  m_prim <- tcpl_models[[i]]$model_prim

  #cutoff
  cutoff_prim <- tcpl_models[[i]]$cutoff_prim
  cutoff_toxi <- tcpl_models[[i]]$cutoff_toxi

  #
  #calculate med_diff at max(logc)
  max_prim <- tcpl_models[[i]]$data_prim %>%
    dplyr::filter(logc == max(logc)) %>%
    dplyr::summarize(median = stats::median(nval_median))
  max_toxi <- tcpl_models[[i]]$data_toxi %>%
    dplyr::filter(logc == max(logc)) %>%
    dplyr::summarize(median = stats::median(nval_median))
  med_diff <- max_toxi$median - max_prim$median

  ##get auc, logEC_3bmadprim, for prim
  ##first check if significant response was present and hill model was fitted
  if (!is.na(m_prim$hill) & m_prim$hill == 1) {
    para_prim <- c(m_prim$hill_tp, m_prim$hill_ga, m_prim$hill_gw)
    #get auc
    ## check if the modeled curve pass through the cutoff line.
    ## if not, then assign 0 to area.
    if (hill_model(para_prim,m_prim$logc_max) >= cutoff_prim) {
      lr <- log_abs_ec(para_prim, cutoff_prim)
      aa_prim <-
        auc_hill_tcpl(para_prim, lower = lr, upper = m_prim$logc_max) - cutoff_prim * (m_prim$logc_ma
    } else {
      aa_prim <- 0
      lr <- -3
    }
    # lr <- log_abs_ec(para_prim, cutoff_prim)
    #
    # aa_prim <-
    #   auc_hill_tcpl(para_prim, lower = lr, upper = m_prim$logc_max) - cutoff_prim * (m_prim$logc_ma
    #get AC50
    AC50_prim <- m_prim$hill_ga
    #get absEC
    if (hill_model(para_prim,m_prim$logc_max) > 50) {
```

```
      absEC50_prim <- log_abs_ec(para_prim, 50)
      absEC80_prim <- log_abs_ec(para_prim, 20)
    } else if (hill_model(para_prim,m_prim$logc_max) > 20) {
      absEC50_prim <- NA
      absEC80_prim <- log_abs_ec(para_prim, 20)
    } else {
      absEC80_prim <- NA
      absEC50_prim <- NA
    }
  } else {
    aa_prim <- NA
    lr <- NA
    absEC80_prim <- NA
    absEC50_prim <- NA
    AC50_prim <- NA
  }

  ##get auc, logEC_3bmadprim, for tox
  if (!is.na(m_toxi$hill) & m_toxi$hill == 1) {
    para_toxi <- c(m_toxi$hill_tp, m_toxi$hill_ga, m_toxi$hill_gw)
    #get AC50
    AC50_toxi <- m_toxi$hill_ga
    #get aa_toxi
    if (hill_model(para_toxi,m_prim$logc_max) > cutoff_prim) {
      lc <- log_abs_ec(para_toxi, cutoff_prim)
      aa_toxi <-
        auc_hill_tcpl(para_toxi,lower = lc, upper = m_prim$logc_max) - cutoff_prim * (m_prim$logc_max
    } else {
      aa_toxi <- NA
      lc <- -3
    }

    #calculate absEC
    if (hill_model(para_toxi,m_prim$logc_max) > 50) {
      absEC50_toxi <- log_abs_ec(para_toxi, 50)
      absEC80_toxi <- log_abs_ec(para_toxi, 20)
    } else if (hill_model(para_toxi,m_prim$logc_max) > 20) {
      absEC50_toxi <- NA
      absEC80_toxi <- log_abs_ec(para_toxi, 20)
    } else {
      absEC80_toxi <- NA
      absEC50_toxi <- NA
    }
    #get cytotox limit (absEC_cutoff_toxi)
    absEC_ct_toxi <- log_abs_ec(para_toxi, cutoff_toxi)
  } else {
    aa_toxi <- NA
    lc <- -3
    absEC80_toxi <- NA
    absEC50_toxi <- NA
    AC50_toxi <- NA
    absEC_ct_toxi <- NA
  }
```

```
  ##calculate taa
  if (is.na(aa_prim)) {
    taa <- NA
  } else if (is.na(aa_toxi)) {
    taa <- aa_prim
  } else {
    taa <- aa_prim - aa_toxi
  }

  ##calculate selectivity based logEC value at 3bmad of prim assay.
  if (is.na(lr)) {
    selectivity_3bmad <- NA
  } else {
    selectivity_3bmad <- lc - lr
  }

  ##calculate selectivity based on logAC50 (original method)
  if (is.na(m_prim$hill_ga)) {
    selectivity_AC50 <- NA
  } else if (is.na(m_toxi$hill_ga)) {
    selectivity_AC50 <- -3 - m_prim$hill_ga
  } else {
    selectivity_AC50 <- m_toxi$hill_ga - m_prim$hill_ga
  }

  ##gather taa and selectivity into one table
  t <- data.frame(
    index = i,
    spid = .spid,
    chnm = chnm,
    casn = casn,
    # aa_toxi = aa_toxi,
    # aa_prim = aa_prim,
    taa = taa,
    # sel_3bMAD = selectivity_3bmad,
    # sel_AC50 = selectivity_AC50,
    med_diff = med_diff,
    AC50_toxi = AC50_toxi,
    AC50_prim = AC50_prim,
    absEC80_toxi = absEC80_toxi,
    absEC50_toxi = absEC50_toxi,
    absEC80_prim = absEC80_prim,
    absEC50_prim = absEC50_prim,
    cyto_lim = absEC_ct_toxi
  )

  df <- base::rbind(df, t)

}

#calculate ranking_score
#this done by adding 0-100 rescaled TAA value an med_diff value
# df <- df %>%
```

```
  #   dplyr::mutate(taa_rescale = rescale_0_100(taa),
  #                 med_diff_rescale = rescale_0_100(med_diff),
  #                 ranking_score = taa_rescale + med_diff_rescale ) %>%
  #   dplyr::arrange(desc(ranking_score))
  if (is.null(med_taa)&is.null(med_med_diff)) {
    df <- df %>%
      dplyr::mutate(ranking_score = NA)
  } else {
    df <- df %>%
      dplyr::mutate(taa_norm = taa/med_taa*100,
                    med_diff_norm = med_diff/med_med_diff*100,
                    ranking_score = taa_norm + med_diff_norm ) %>%
      dplyr::arrange(desc(ranking_score))

  }



  return(df)
}





#' function to summarize curve fitting results
#'
#' @param tcpl_models the list object returned by 'fit_curve_tcpl' function
#' @param spid_chnm_table a reference table with 'spid' and the corresponding chemical name 'chnm' colu
#' and the CAS number 'casn' column.
#' @return a data.frame contains summarized metrics for each chemical (spid)
#'
#' @examples
#' ## supply models as the essential argument. spid_chnm_table is optional.
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info =
#' list(prim_assay = "Primary", toxi_assay = "Cytotox"))
#' demo_sum <- summary_tcpl(demo_md)
#'
#'
#' ## start from raw data
#' # define assay
#' assay_info <- list(prim_assay = "Primary",toxi_assay = "Cytotox")
#' # data normalization
#' demo_mc_norm <- normalize_per_plate(demo_mc, nctrl = "DMSO")
#' # filter out two test chemicals
#' demo_mc_norm <- dplyr::filter(demo_mc_norm, spid %in% c("TP0001502B05", "TP0001502B01"))
#' # fit curve with default 20% threshold
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info)
#' # obtain summary table
#' demo_sum <- summary_tcpl(demo_md)
#'
#' @export
#'
summary_tcpl <- function(tcpl_models, spid_chnm_table = NULL) {
```

```r
# claim variables for passing R CMD Check
spid <- NULL


df <- data.frame()
##iterate through each spid
for (i in seq_along(tcpl_models)) {
  #get chemical sample id 'spid'
  .spid <- tcpl_models[[i]]$spid
  # print(i)
  # print(.spid)
  #get chnm
  if (!is.null(spid_chnm_table)) {
    chnm <- dplyr::filter(spid_chnm_table, spid == .spid)$chnm
    casn <- dplyr::filter(spid_chnm_table, spid == .spid)$chnm
  } else {
    chnm <- NA
  }

  #extract modelling results
  m_toxi <- tcpl_models[[i]]$model_toxi
  m_prim <- tcpl_models[[i]]$model_prim

  #cutoff
  cutoff_prim <- tcpl_models[[i]]$cutoff_prim
  cutoff_toxi <- tcpl_models[[i]]$cutoff_toxi

  #get assay_info
  assay_info <- tcpl_models[[i]]$assay_info

  ##get metrics for prim
  if (is.null(assay_info$prim_assay)) {
    absEC80_prim <- NA
    absEC50_prim <- NA
    AC50_prim <- NA
  } else {
    if (!is.na(m_prim$hill) & m_prim$hill == 1) {
      para_prim <- c(m_prim$hill_tp, m_prim$hill_ga, m_prim$hill_gw)
      #get AC50
      AC50_prim <- m_prim$hill_ga
      #get absEC
      if (hill_model(para_prim, m_prim$logc_max) > 50) {
        absEC50_prim <- log_abs_ec(para_prim, 50)
        absEC80_prim <- log_abs_ec(para_prim, 20)
      } else if (hill_model(para_prim,m_prim$logc_max) > 20) {
        absEC50_prim <- NA
        absEC80_prim <- log_abs_ec(para_prim, 20)
      } else {
        absEC80_prim <- NA
        absEC50_prim <- NA
      }
    } else {
      absEC80_prim <- NA
```

```
      absEC50_prim <- NA
      AC50_prim <- NA
    }
  }

  ##get metrics for toxi

  if (is.null(assay_info$toxi_assay)) {
    absEC80_toxi <- NA
    absEC50_toxi <- NA
    AC50_toxi <- NA
  } else {
    if (!is.na(m_toxi$hill) & m_toxi$hill == 1) {
      para_toxi <- c(m_toxi$hill_tp, m_toxi$hill_ga, m_toxi$hill_gw)
      #get AC50
      AC50_toxi <- m_toxi$hill_ga
      #calculate absEC
      if (hill_model(para_toxi,m_toxi$logc_max) > 50) {
        absEC50_toxi <- log_abs_ec(para_toxi, 50)
        absEC80_toxi <- log_abs_ec(para_toxi, 20)
      } else if (hill_model(para_toxi,m_toxi$logc_max) > 20) {
        absEC50_toxi <- NA
        absEC80_toxi <- log_abs_ec(para_toxi, 20)
      } else {
        absEC80_toxi <- NA
        absEC50_toxi <- NA
      }
    } else {
      absEC80_toxi <- NA
      absEC50_toxi <- NA
      AC50_toxi <- NA
    }

  }

  ##gather taa and selectivity into one table
  t <- data.frame(
    index = i,
    spid = .spid,
    chnm = chnm,
    AC50_toxi = AC50_toxi,
    AC50_prim = AC50_prim,
    absEC80_toxi = absEC80_toxi,
    absEC50_toxi = absEC50_toxi,
    absEC80_prim = absEC80_prim,
    absEC50_prim = absEC50_prim
  )

  df <- base::rbind(df, t)

}
```

```
  return(df)
}




#' Plot dose-resonse curves based on the tcpl hill model
#'
#' Produce the plot for the dose-response curves and data points for both primary and toxicity assay.
#' The direction of the data and dose-resonse curves are presented as the original data, rather than
#' the uptrend direction required by the 'tcpl' function. Plots are sorted by the ranking_score.
#'
#' @param tcpl_models the list object created by 'fit_curve_tcpl' function
#' @param rank_table the data.frame output from 'rank_tcpl' function
#' @param spid_chnm_table the spid, chnm, casn info table
#' @param notation value can be TRUE or FALSE, determine whehter to show potency metrics on the plot
#' @param cunit  the unit of concentration, on default is "M" (molar).
#'
#' @return list of ggplot2 objects, each corresponding to one spid.
#' @import ggthemes ggplot2
#'
#' @examples
#' ## produce plots without notations
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info =
#' list(prim_assay = "Primary", toxi_assay = "Cytotox"))
#' plots <- plot_tcpl(demo_md)
#'
#'
#' ## start from raw data
#' # define assay
#' assay_info <- list(prim_assay = "Primary",toxi_assay = "Cytotox")
#' # data normalization
#' demo_mc_norm <- normalize_per_plate(demo_mc, nctrl = "DMSO")
#' # filter out two test chemicals
#' demo_mc_norm <- dplyr::filter(demo_mc_norm, spid %in% c("TP0001502B05", "TP0001502B01"))
#' # fit curve with default 20% threshold
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info)
#' # calculate TAA and Med_diff only
#' demo_rank <- rank_tcpl(demo_md, med_taa = NULL, med_med_diff = NULL)
#' #produce plots with notations
#' demo_plots <- plot_tcpl(demo_md, demo_rank, notation = TRUE)
#'
#' ##produce plots with notations, with changed concentration unit displayed on the plot
#' demo_plots <- plot_tcpl(demo_md, demo_rank, notation = TRUE, cunit = "uM")
#'
#' @export
#'
#'
plot_tcpl <-
  function(tcpl_models, rank_table=NULL, spid_chnm_table = NULL, notation = FALSE, cunit = "M") {

    # claim variables for passing R CMD Check
    spid <- nval_median <- logc <- resp <- pred <- assay <- NULL
```

```r
#initiate empty output plot list
plot_list <- list()
#reorder if rank is available
if (!is.null(rank_table)) {
  tcpl_models <- tcpl_models[rank_table$index]
}

#loop through tcpl_models's unique spid.
#note tcpl_models is the level 4 output from tcpl package, including all the modelling results
for (i in seq_along(tcpl_models)) {
  #get chemical sample id and chemical name
  .spid <- tcpl_models[[i]]$spid
  #print(.spid)
  if (!is.null(spid_chnm_table)) {
    chnm <- dplyr::filter(spid_chnm_table, spid == .spid)$chnm
    casn <- dplyr::filter(spid_chnm_table, spid == .spid)$casn
  } else {
    chnm <- NA
    casn <- NA
  }

  #cutoff
  cutoff_prim <- tcpl_models[[i]]$cutoff_prim
  cutoff_toxi <- tcpl_models[[i]]$cutoff_toxi
  #assay_info
  assay_info <- tcpl_models[[i]]$assay_info

  #get normalized resonse value (cytotox and raiu together)
  #and use 100 minus the response value (inverse the plot)
  d <- dplyr::bind_rows(tcpl_models[[i]]$data_prim, tcpl_models[[i]]$data_toxi) %>%
    dplyr::mutate(resp = nval_median) #%>%
  #mutate(assay = ifelse(aeid == 1, assay_info$toxi_assay, assay_info$prim_assay))

  #determine left and right x boundary of the plot
  if ( round(max(d$logc)) < max(d$logc) ) {
    rb <- round(max(d$logc)) + 1
  } else { rb <- round(max(d$logc))}

  lb <- round(min(d$logc))-1

  #initiate basic plot with data points.
  g <- ggplot(d, aes(x = logc, y = resp))

  if (!is.null(spid_chnm_table)){
    g <- g + labs(
      title = paste(i, ". SPID: ", .spid, "\nNAME: ", chnm, "\nCAS NO: ", casn, sep = ""),
      x = paste("Concentration (log", cunit, ")", sep = ""),
      y = "% Control Activity"
      )
  } else {
    g <- g + labs(
      title = paste(i, ". SPID:" , .spid),
      x = paste("Concentration (log", cunit, ")", sep = ""),
```

```r
      y = "% Control Activity"
    )
  }

    # labs(
    #   title = paste(i, "\nSPID: " , .spid, "\nNAME: ", chnm, "\nCAS NO: ", casn, sep = ""),
    #   x = "Concentration (logM)",
    #   y = "% Control Activity"
    # )

  #extract modelling results
  m_toxi <- tcpl_models[[i]]$model_toxi
  m_prim <- tcpl_models[[i]]$model_prim

  #create 100 concentrations
  s <- expand.grid(logc = seq(lb, rb, length = 130))

  #test and plot cytotox model
  if (!is.na(m_toxi$hill) & m_toxi$hill == 1) {
    para_cyto <- c(m_toxi$hill_tp, m_toxi$hill_ga, m_toxi$hill_gw)
    p1 <- 100 - hill_model(para_cyto, s)
    p1 <- dplyr::bind_cols(s, data.frame(p1))
    names(p1) <- c("logc", "pred")
    g <- g + geom_line(
      data = p1,
      aes(x = logc, y = pred),
      size = 2,
      alpha = 0.9,
      color = "#e02929"
    )
    #plot the vertical line at 3bmad cutoff
    #g <- g+ geom_vline(xintercept = log_abs_ec(para_cyto, 3*m_toxi$bmad) )
  }

  #test and plot raiu model
  if (!is.na(m_prim$hill) & m_prim$hill == 1) {
    para_raiu <- c(m_prim$hill_tp, m_prim$hill_ga, m_prim$hill_gw)

    p2 <- 100 - hill_model(para_raiu, s)
    p2 <- bind_cols(s, data.frame(p2))
    names(p2) <- c("logc", "pred")
    g <- g + geom_line(
      data = p2,
      aes(x = logc, y = pred),
      size = 2,
      alpha = 0.9,
      color = "#377eb8"
    )
  }

  #draw 3bmad cutoff line for cytotox and raiu respectively
  g <- g +
    geom_hline(
```

```
      yintercept = 100 - cutoff_toxi,
      alpha = 0.5,
      size = 0.5,
      linetype = "dashed",
      color = "#e02929"
    )

  g <- g +
    geom_hline(
      yintercept = 100 - cutoff_prim,
      alpha = 0.5,
      size = 0.5,
      linetype = "dashed",
      color = "#377eb8"
    )

  #plot data points
  #aesthetics fixes
  g <- g +
    geom_point(
      aes(color = assay),
      shape = 21,
      alpha = 0.9,
      size = 3
    ) +
    coord_fixed(
      ylim = c(0, 125),
      #xlim = c(-10, -4),
      ratio = 4 / 120   #used to be 2/70, when x axis was from -9 to -4.
    ) +
    scale_y_continuous(breaks = seq(
      from = 0,
      to = 120,
      by = 20
    )) +
    scale_x_continuous(breaks = seq(
      from = lb,
      to = rb,
      by = 1
    )) +
    theme_few() +
    theme(legend.title = element_blank()) +
    scale_color_manual(values=c("#e02929", "#377eb8"))+
    theme(plot.title=element_text(hjust=0.5))

  ##adding annotations
  if (!is.null(rank_table) & notation == TRUE) {
    #Get ec and ranking info
    ds <- rank_table %>% dplyr::filter(spid==.spid)
    ds <- round_df(ds, digits=2)

    #annotate with text info
    if (is.na(ds$ranking_score)) {
```

```
        line1 <- ""} else {
        line1 <- paste("Ranking_Score:", ds$ranking_score)
      }

      line2 <- paste("TAA:", ds$taa)
      line3 <- paste("Med_Diff:", ds$med_diff)
      line4 <- paste(assay_info$prim_assay, "_AC50: ", ds$AC50_prim, sep = "")
      line5 <- paste(assay_info$prim_assay, "_absEC50: ", ds$absEC50_prim, sep = "")
      #line6 <- paste(assay_info$prim_assay, "_absEC80: ", ds$absEC80_prim, sep = "")
      g <- g +
        annotate("text", x= lb + 0.8, y = 30, alpha = 0.8, hjust=0, label=line1) +
        annotate("text", x= lb + 0.8, y = 25, alpha = 0.8, hjust=0, label= line2) +
        annotate("text", x= lb + 0.8, y = 20, alpha = 0.8, hjust=0, label= line3) +
        annotate("text", x= lb + 0.8, y = 15, alpha = 0.8, hjust=0, label= line4) +
        annotate("text", x= lb + 0.8, y = 10, alpha = 0.8, hjust=0, label= line5)
        #annotate("text", x= lb + 0.8, y = 5, alpha = 0.8, hjust=0, label= line6)

    }

    #collect all plots into a list
    plot_list[[i]] <- g

  }

  return(plot_list)

}



#' Plot dose-resonse curves with minimal text annotation
#' This funciton plots dose-response curve with minimal text annotation,
#' no x and y axis label, 0 borders. Useful when need to present several plots
#' together.
#' @param tcpl_models the list object created by 'fit_curve_tcpl' function
#' @param rank_table the data.frame output from 'rank_tcpl' function
#' @param spid_chnm_table the spid, chnm, casn info table
#' @param notation value can be TRUE or FALSE, determine whehter to show potency metrics on the plot
#' @param cunit  the unit of concentration, on default is "M" (molar).
#'
#' @return list of ggplot2 objects, each corresponding to one spid.
#' @import ggthemes ggplot2
#'
#' @examples
#' ## produce plots without notations
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info =
#' list(prim_assay = "Primary", toxi_assay = "Cytotox"))
#' plots_minimal <- plot_tcpl_minimal(demo_md)
#'
#' ## start from raw data
#' # define assay
#' assay_info <- list(prim_assay = "Primary",toxi_assay = "Cytotox")
#' # data normalization
```

```r
#' demo_mc_norm <- normalize_per_plate(demo_mc, nctrl = "DMSO")
#' # filter out two test chemicals
#' demo_mc_norm <- dplyr::filter(demo_mc_norm, spid %in% c("TP0001502B05", "TP0001502B01"))
#' # fit curve with default 20% threshold
#' demo_md <- fit_curve_tcpl(demo_mc_norm, assay_info)
#' # calculate TAA and Med_diff only
#' demo_rank <- rank_tcpl(demo_md, med_taa = NULL, med_med_diff = NULL)
#' #produce plots with notations
#' demo_plots <- plot_tcpl_minimal(demo_md, demo_rank, notation = TRUE)
#'
#' ##produce plots with notations, with changed concentration unit displayed on the plot
#' demo_plots <- plot_tcpl_minimal(demo_md, demo_rank, notation = TRUE, cunit = "uM")
#'
#'
#'
#'
#' @export
#'
#'
plot_tcpl_minimal <-
  function(tcpl_models, rank_table = NULL, spid_chnm_table = NULL, notation = FALSE, cunit = "M") {

    # claim variables for passing R CMD Check
    spid <- nval_median <- logc <- resp <- pred <- assay <- NULL

    #initiate empty output plot list
    plot_list <- list()

    #reorder if rank is available
    if (!is.null(rank_table)) {
      tcpl_models <- tcpl_models[rank_table$index]
    }

    #loop through tcpl_models's unique spid.
    #note tcpl_models is the level 4 output from tcpl package, including all the modelling results
    for (i in seq_along(tcpl_models)) {
      #get chemical sample id and chemical name
      .spid <- tcpl_models[[i]]$spid
      #print(.spid)
      if (!is.null(spid_chnm_table)) {
        chnm <- dplyr::filter(spid_chnm_table, spid == .spid)$chnm
        casn <- dplyr::filter(spid_chnm_table, spid == .spid)$casn
      } else {
        chnm <- NA
        casn <- NA
      }

      #cutoff
      cutoff_prim <- tcpl_models[[i]]$cutoff_prim
      cutoff_toxi <- tcpl_models[[i]]$cutoff_toxi
      #assay_info
      assay_info <- tcpl_models[[i]]$assay_info
```

```
#get normalized resonse value (cytotox and raiu together)
#and use 100 minus the response value (inverse the plot)
d <- dplyr::bind_rows(tcpl_models[[i]]$data_prim, tcpl_models[[i]]$data_toxi) %>%
  dplyr::mutate(resp = nval_median) #%>%
#mutate(assay = ifelse(aeid == 1, assay_info$toxi_assay, assay_info$prim_assay))

#determine left and right x boundary of the plot
if ( round(max(d$logc)) < max(d$logc) ) {
  rb <- round(max(d$logc)) + 1
} else { rb <- round(max(d$logc))}

lb <- round(min(d$logc))-1

#initiate basic plot with data points.
g <- ggplot(d, aes(x = logc, y = resp))

if (!is.null(spid_chnm_table)){
  g <- g + labs(
    title = paste(chnm, sep = ""),
    x = paste("Concentration (log", cunit, ")", sep = ""),
    y = "% Control Activity"
  )
} else {
  g <- g + labs(
    title = paste(i, ". SPID:" , .spid),
    x = paste("Concentration (log", cunit, ")", sep = ""),
    y = "% Control Activity"
  )
}

# labs(
#   title = paste(i, "\nSPID: " , .spid, "\nNAME: ", chnm, "\nCAS NO: ", casn, sep = ""),
#   x = "Concentration (logM)",
#   y = "% Control Activity"
# )

#extract modelling results
m_toxi <- tcpl_models[[i]]$model_toxi
m_prim <- tcpl_models[[i]]$model_prim

#create 100 concentrations
s <- expand.grid(logc = seq(lb, rb, length = 130))

#test and plot cytotox model
if (!is.na(m_toxi$hill) & m_toxi$hill == 1) {
  para_cyto <- c(m_toxi$hill_tp, m_toxi$hill_ga, m_toxi$hill_gw)
  p1 <- 100 - hill_model(para_cyto, s)
  p1 <- dplyr::bind_cols(s, data.frame(p1))
  names(p1) <- c("logc", "pred")
  g <- g + geom_line(
    data = p1,
    aes(x = logc, y = pred),
    size = 2,
```

```
      alpha = 0.9,
      color = "#e02929"
    )
    #plot the vertical line at 3bmad cutoff
    #g <- g+ geom_vline(xintercept = log_abs_ec(para_cyto, 3*m_toxi$bmad) )
  }

  #test and plot raiu model
  if (!is.na(m_prim$hill) & m_prim$hill == 1) {
    para_raiu <- c(m_prim$hill_tp, m_prim$hill_ga, m_prim$hill_gw)

    p2 <- 100 - hill_model(para_raiu, s)
    p2 <- bind_cols(s, data.frame(p2))
    names(p2) <- c("logc", "pred")
    g <- g + geom_line(
      data = p2,
      aes(x = logc, y = pred),
      size = 2,
      alpha = 0.9,
      color = "#377eb8"
    )
  }

  #draw 3bmad cutoff line for cytotox and raiu respectively
  g <- g +
    geom_hline(
      yintercept = 100 - cutoff_toxi,
      alpha = 0.5,
      size = 0.5,
      linetype = "dashed",
      color = "#e02929"
    )

  g <- g +
    geom_hline(
      yintercept = 100 - cutoff_prim,
      alpha = 0.5,
      size = 0.5,
      linetype = "dashed",
      color = "#377eb8"
    )

  #plot data points
  #aesthetics fixes
  g <- g +
    geom_point(
      aes(color = assay),
      shape = 21,
      alpha = 0.9,
      size = 3
    ) +
    coord_fixed(
      ylim = c(0, 125),
```

```
          xlim = c(-9, -4),
          ratio = 2 / 70   #used to be 2/70, when x axis was from -9 to -4.
        ) +
        scale_y_continuous(breaks = seq(
          from = 0,
          to = 120,
          by = 20
        )) +
        scale_x_continuous(breaks = seq(
          from = lb,
          to = rb,
          by = 1
        )) +
        theme_few() +
        theme(axis.title.x = element_blank()) +
        theme(axis.title.y = element_blank()) +
        theme(legend.title = element_blank(),
              legend.position = "none") +
        theme(legend.margin=unit(0, "null")) +
        scale_color_manual(values=c("#e02929", "#377eb8"))+
        theme(plot.title=element_text(hjust=0.5, size = 16))

      ##adding annotations
      if (!is.null(rank_table) & notation == TRUE) {
        #Get ec and ranking info
        ds <- rank_table %>% dplyr::filter(spid==.spid)
        ds <- round_df(ds, digits=2)

        #annotate with text info
        line1 <- paste("Ranking_Score:", ds$ranking_score)
        # line2 <- paste("TAA:", ds$taa)
        # line3 <- paste("Med_Diff:", ds$med_diff)
        line4 <- paste("AC50: ", ds$AC50_prim, sep = "")
        line5 <- paste("absEC50: ", ds$absEC50_prim, sep = "")
        # line6 <- paste(assay_info$prim_assay, "_absEC80: ", ds$absEC80_prim, sep = "")
        g <- g +
          annotate("text", x= lb + 0.8, y = 34, alpha = 0.8, hjust=0, label=line1) +
          # annotate("text", x= lb + 0.8, y = 25, alpha = 0.8, hjust=0, label= line2) +
          # annotate("text", x= lb + 0.8, y = 20, alpha = 0.8, hjust=0, label= line3) +
          annotate("text", x= lb + 0.8, y = 22, alpha = 0.8, hjust=0, label= line4) +
          annotate("text", x= lb + 0.8, y = 10, alpha = 0.8, hjust=0, label= line5)
          # annotate("text", x= lb + 0.8, y = 5, alpha = 0.8, hjust=0, label= line6)

      }

      #collect all plots into a list
      plot_list[[i]] <- g

    }

    return(plot_list)

  }
```