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Supplementary Data S1 - Compound List

	Chemical Name	Molecular Weight	CASNR	Supplier	Lot Number	CoA Purity (%)
1	Acetaminophen	151.16	103-90-2	Sigma-Aldrich	10018JE	98.7
2	Aflatoxin B1	312.27	1162-65-8	Toronto Research Chemicals, Inc.	21-GHZ-14-1	98
3	Aspirin	180.16	50-78-2	Sigma-Aldrich	048K0015	99.9
4	Benzo(a)pyrene	252.32	50-32-8	TCI America	2IGMD	98.6
5	Chenodeoxycholic acid	392.57	474-25-9	Sigma-Aldrich	058K1318	97.2
6	Chlorpromazine	318.87	50-53-3	Matrix Scientific	P24Q	95
7	Cyclophosphamide	279.1	6055-19-2	TCI America	PUGEG	99.5
8	Cyclosporine A	1202.64	59865-13-3	TCI America	66F3M	99.9
9	Diphenhydramine	291.82	147-24-0	Sigma-Aldrich	096K0036	100
10	Fenofibric acid	318.75	42017-89-0	Sigma-Aldrich	MKBV3048V	99.2
11	Levofloxacin	370.38	138199-71-0	Toronto Research Chemicals, Inc.	14-SSR-91-1	98
12	Menadione	172.18	58-27-5	Sigma-Aldrich	BCBP6090V	99.7
13	N-nitrosodimethylamine (DMN)	74.08	62-75-9	Sigma-Aldrich		
14	Omeprazole	345.42	73590-58-6	Spectrum Chemical Mfg. Corp.	XP3040	98.0
15	Potassium chloride	74.55	7447-40-7	Sigma-Aldrich	SLBN7927V	99.9
16	Rifampicin	822.94	13292-46-1	Sigma-Aldrich	087K18753	98
17	Ritonavir	720.95	155213-67-5	TCI America	2CMOG	99.4
18	Rosiglitazone	357.43	122320-73-4	TCI America	5MM4N	99.6
19	sucrose	342.2965	57-50-1	Sigma-Aldrich		
20	Tamoxifen	371.51	10540-29-1	Sigma-Aldrich	048K1239	99
21	Troglitazone	441.50	97322-87-7	Cayman Chemical Company	0449170	100.0
22	Trovafloxacin	512.46	147059-75-4	Toronto Research Chemicals Inc	14-ABY-17-1-PFZ	98
23	Valproic acid	144.21	99-66-1	Sigma-Aldrich	074K3654	99.9
24	Phenobarbital	254.22	57-30-7	Sigma-Aldrich		

Supplementary Data S2 -BMC Threshold Values

2D DIFF

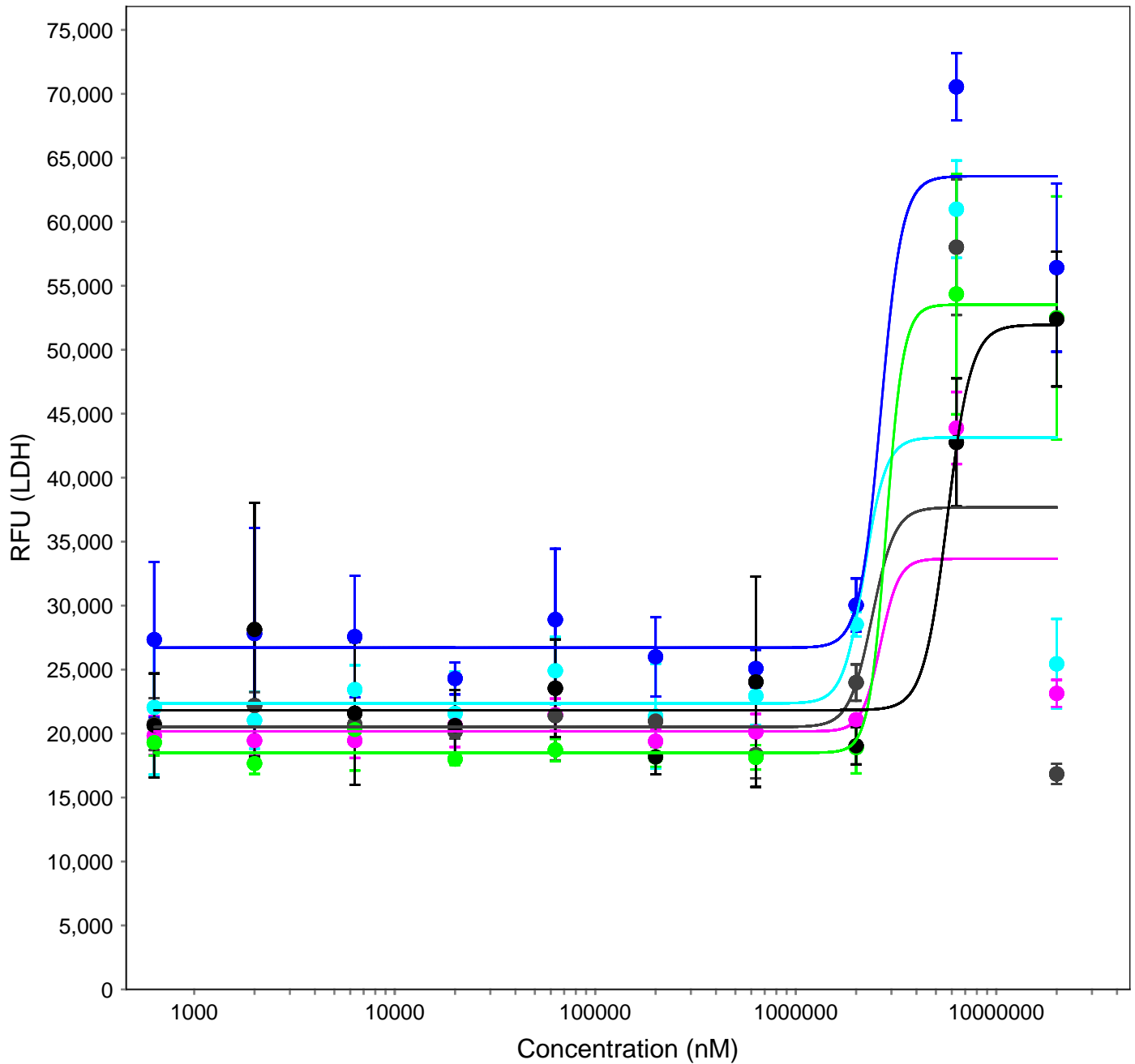
Compound Name-Top Concentration Evaluated	*Reference Human Plasma Concentrations (µM)	Mean Total BMC Number	SD Total BMC Number	Mean BMC#105 (µM)	SD BMC#105 (µM)	CILI 'Index' 10XCmax/BMC105	Mean LDH Emax/Emin (48h)	Mean LDH Leakage (48h) EC50 (µM)	Mean LDH Emax/Emin (96h)	Mean LDH Leakage (96h) EC50 (µM)	Mean LOEL-Morphology (µM, 96h)
afatoxin B1 (150µM)	0.000054	1,364	187	0.344	0.122	0.00	6.25	4.81	6.17	1.46	1.50
menadione (300µM)	7.40	1,350	187	18.8	6.65	3.93	3.44	27.2			49.0
troglitazone (300µM)	6.38	1,313	162	56.2	5.38	1.14	7.34	235	5.53	255	232
chlorpromazine (300µM)	0.470	1,267	400	18.1	7.10	0.26	6.32	30.6	2.61	8.37	23.2
acetaminophen (20,000µM)	132	1,175	224	845	127	1.57	2.55	3,727	1.81	2,413	4,883
tamoxifen (93.5µM)	0.323	1,007	369	19.0	6.19	0.17	9.09	69.3	9.06	59.8	50.9
benzo(a)pyrene (30µM)	0.0038	930	37.4	0.254	0.0190	0.15	1.74	3.36	9.27	9.63	9.49
ritonavir (298µM)	15.5	792	129	8.73	7.11	17.8	6.77	50.5	6.33	39.8	66.3
trovafloxacin (300µM)	5.28	764	118	3.04	1.81	17.4	2.90	41.6	4.90	30.6	300
rosiglitazone (300µM)	1.68	609	44.1	32.2	25.4	0.52					300
rifampicin (291µM)	13.0	540	70.4	49.1	53.6	2.65			2.73	178	137
omeprazole (300µM)	0.681	493	79.6	44.0	10.0	0.15			2.05	137	300
CDCA (200µM)	0.34400	432	91.5	53.1	7.46	0.06					200
diphenhydramine (200µM)	0.259	233	26.5	37.3	20.3	0.07			1.76	34.7	132
fenofibric acid (300µM)	38.7	78.7	36.5								
cyclophosphamide (300µM)	121	62.7	52.3								
valproic acid (301µM)	236	55.7	25.9								
aspirin (300µM)	133	54.3	19.0								
phenobarbital (1000µM)	23.7	49.7	24.5								
sucrose (300µM)	6,100	37.7	36.5								
N-nitrosodimethylamine (300µM)	0.0189	36.0	16.0								
levofloxacin (300µM)	12.5	36.0	13.2								
caffeine (300µM)	50.0	22.7	2.9								
potassium chloride (300µM)	5,500	12.7	10.7								

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Compound Name-Top Concentration Evaluated	*Reference Human Plasma Concentrations (µM)	Mean Total BMC Number	SD Total BMC Number	Mean BMC#105 (µM)	SD BMC#105 (µM)	CILI 'Index' 10XCmax/BMC105	Mean LDH Emax/Emin (48h)	Mean LDH Leakage (48h) EC50 (µM)	Mean LDH Emax/Emin (96h)	Mean LDH Leakage (96h) EC50 (µM)	Mean LOEL-Morphology (µM, 96h)	Mean LOEL-Attenuation of Proliferation (µM, 96h)
afatoxin B1 (150µM)	0.000054	1,435	173	0.219	0.147	0.00	2.83	3.61	NMR	NMR	0.224	1.16
menadione (300µM)	7.40	1,287	9	9.4	1.00	7.86	1.66	25.5	NMR	NMR	30.0	
troglitazone (300µM)	6.38	1,336	85	19.2	2.78	3.32	2.22	25.70			163	198
chlorpromazine (300µM)	0.470	1,313	117	5.20	3.26	0.90	2.47	10.6	NMR	NMR	2.32	23.2
acetaminophen (20,000µM)	132	1,443	143	581	70.0	2.28					20,000	6,324
tamoxifen (93.5µM)	0.323	1,138	215	7.0	0.558	0.46	6.25	48.30			5.09	29.6
benzo(a)pyrene (30µM)	0.0038	1,331	106.1	0.135	0.0320	0.28	3.01	2.47	NMR	NMR	1.42	1.63
ritonavir (298µM)	15.5	986	128	9.71	1.54	16.00	2.56	48.3	NMR	NMR	29.8	29.8
trovafloxacin (300µM)	5.28	543	43	1.32	0.820	40.03					9.49	23.2
rosiglitazone (300µM)	1.68	1355	214.2	15.2	6.01	1.10					30.0	30.0
rifampicin (291µM)	13.0	875	23.3	41.1	2.64	3.16					291	291
omeprazole (300µM)	0.681	573	57.2	19.1	7.20	0.36					163	300
CDCA (200µM)	0.34400	445	83.8	43.0	15.1	0.08						
diphenhydramine (200µM)	0.259	341	31.8	11.0	2.79	0.24					48.8	
fenofibric acid (300µM)	38.7	56	5.6									
cyclophosphamide (300µM)	121	8	2.5									
valproic acid (301µM)	236	34	4.2									
aspirin (300µM)	133	10	6.4									
phenobarbital (1000µM)	23.7	26	9.0									
sucrose (300µM)	6,100	33	12.7									
N-nitrosodimethylamine (300µM)	0.0189	26	5.7									
levofloxacin (300µM)	12.5	59	50.2									
caffeine (300µM)	50.0	21	13.0									
potassium chloride (300µM)	5,500	4	3.8									

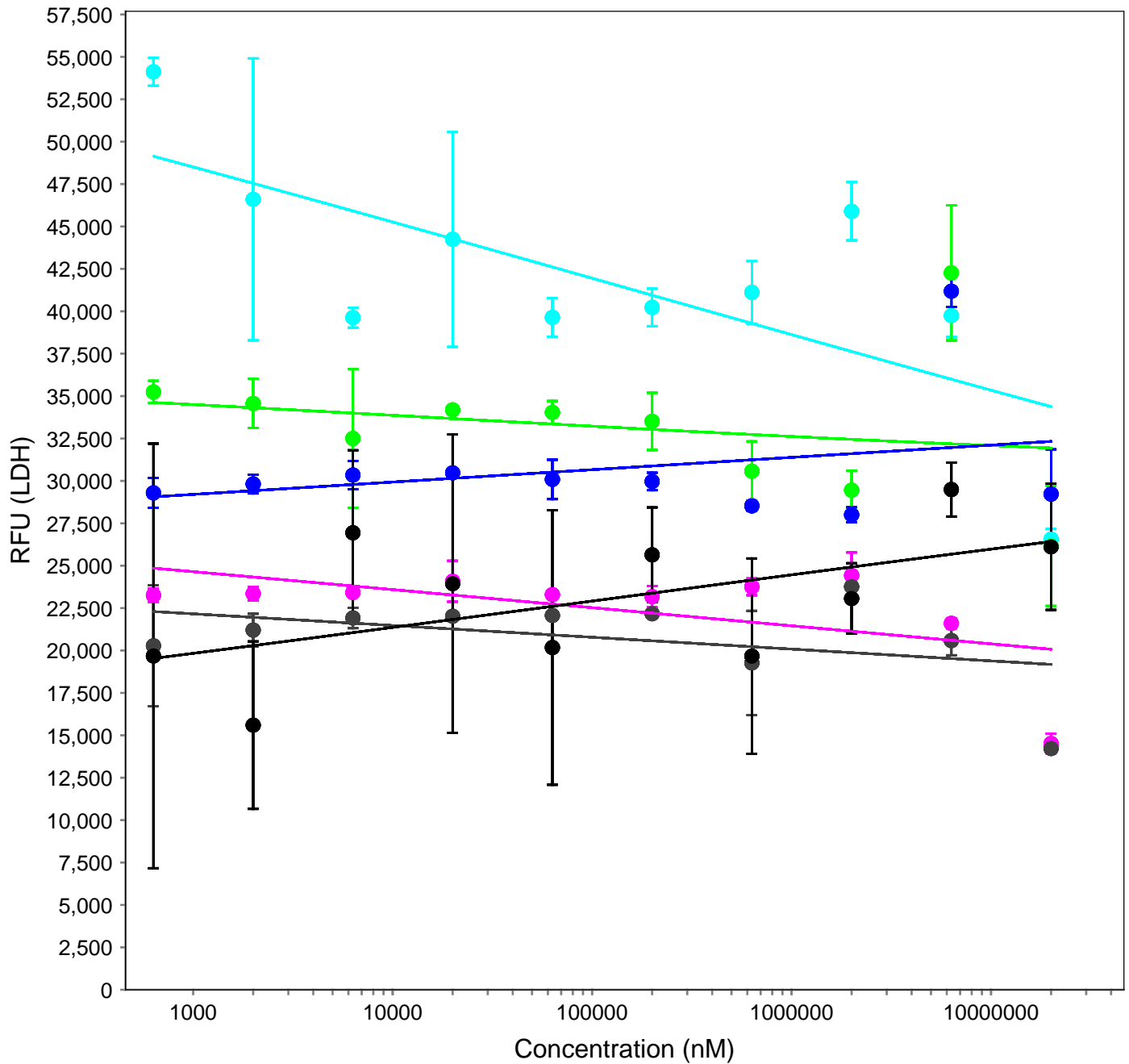
NMR: Non-monotonic response with LDH Leakage Response

Supplementary Data S3 - LDH Leakage Data



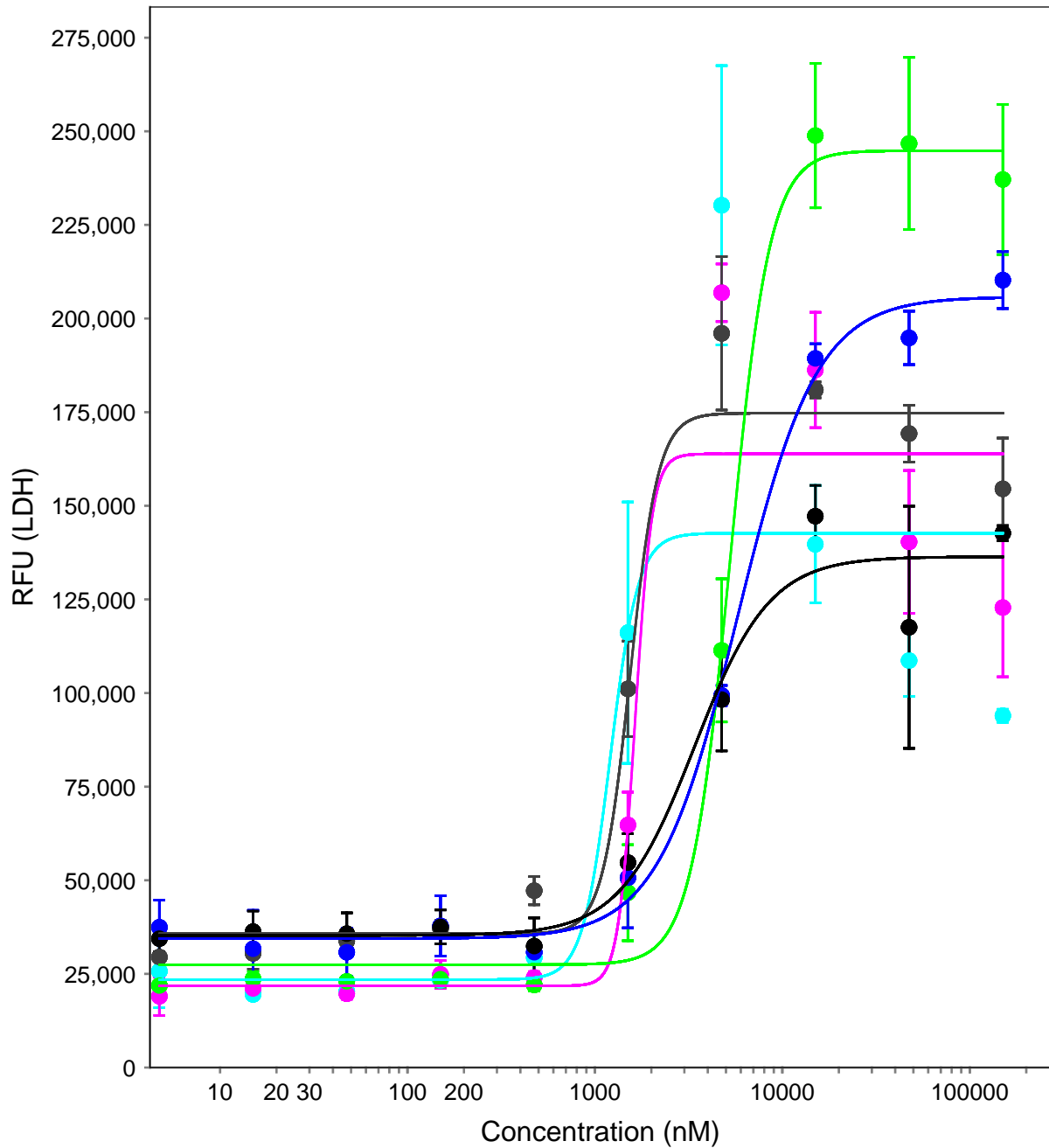
■	acetaminophen 2D-DIFF-R1 LDH 48h EMAX: 51900 EMIN: 21800 EC50: 5.70E6 R ² : 0.938
■	acetaminophen 2D-DIFF-R2 LDH 48h EMAX: 63600 EMIN: 26700 EC50: 2660000 R ² : 0.948
■	acetaminophen 2D-DIFF-R3 LDH 48h EMAX: 53500 EMIN: 18500 EC50: 2820000 R ² : 0.996
■	acetaminophen 2D-DIFF-R1 LDH 96h EMAX: 37700 EMIN: 20500 EC50: 2.40E6 R ² : 0.338
■	acetaminophen 2D-DIFF-R2 LDH 96h EMAX: 33700 EMIN: 20200 EC50: 2640000 R ² : 0.565
■	acetaminophen 2D-DIFF-R3 LDH 96h EMAX: 43100 EMIN: 22400 EC50: 2.20E6 R ² : 0.511

Supplementary Data S3 - LDH Leakage Data



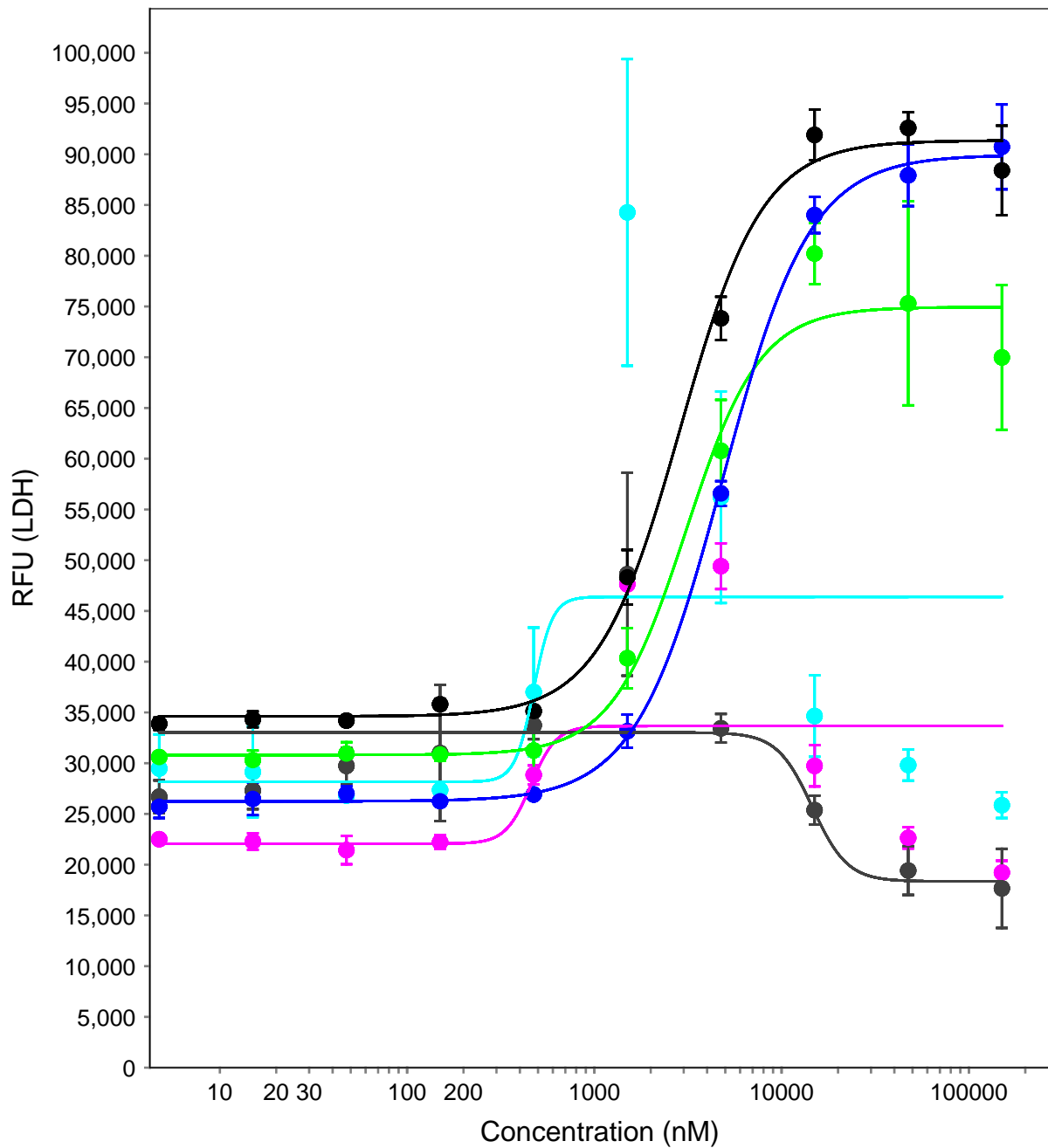
- acetaminophen | PROLIF-R1 | LDH | 48h | EMAX: 3.90E4 | EMIN: 6330 | EC50: 6.80E4 | R^2: 0.311
- acetaminophen | PROLIF-R2 | LDH | 48h | EMAX: 48900 | EMIN: 11600 | EC50: 29200 | R^2: 0.0888
- acetaminophen | PROLIF-R3 | LDH | 48h | EMAX: 37100 | EMIN: 30400 | EC50: 16600 | R^2: 0.0534
- acetaminophen | PROLIF-R1 | LDH | 96h | EMAX: 31500 | EMIN: 9250 | EC50: 3.90E5 | R^2: 0.166
- acetaminophen | PROLIF-R2 | LDH | 96h | EMAX: 4.10E4 | EMIN: 3.10E3 | EC50: 266000 | R^2: 0.303
- acetaminophen | PROLIF-R3 | LDH | 96h | EMAX: 76400 | EMIN: 6.30E3 | EC50: 152000 | R^2: 0.504

Supplementary Data S3 - LDH Leakage Data



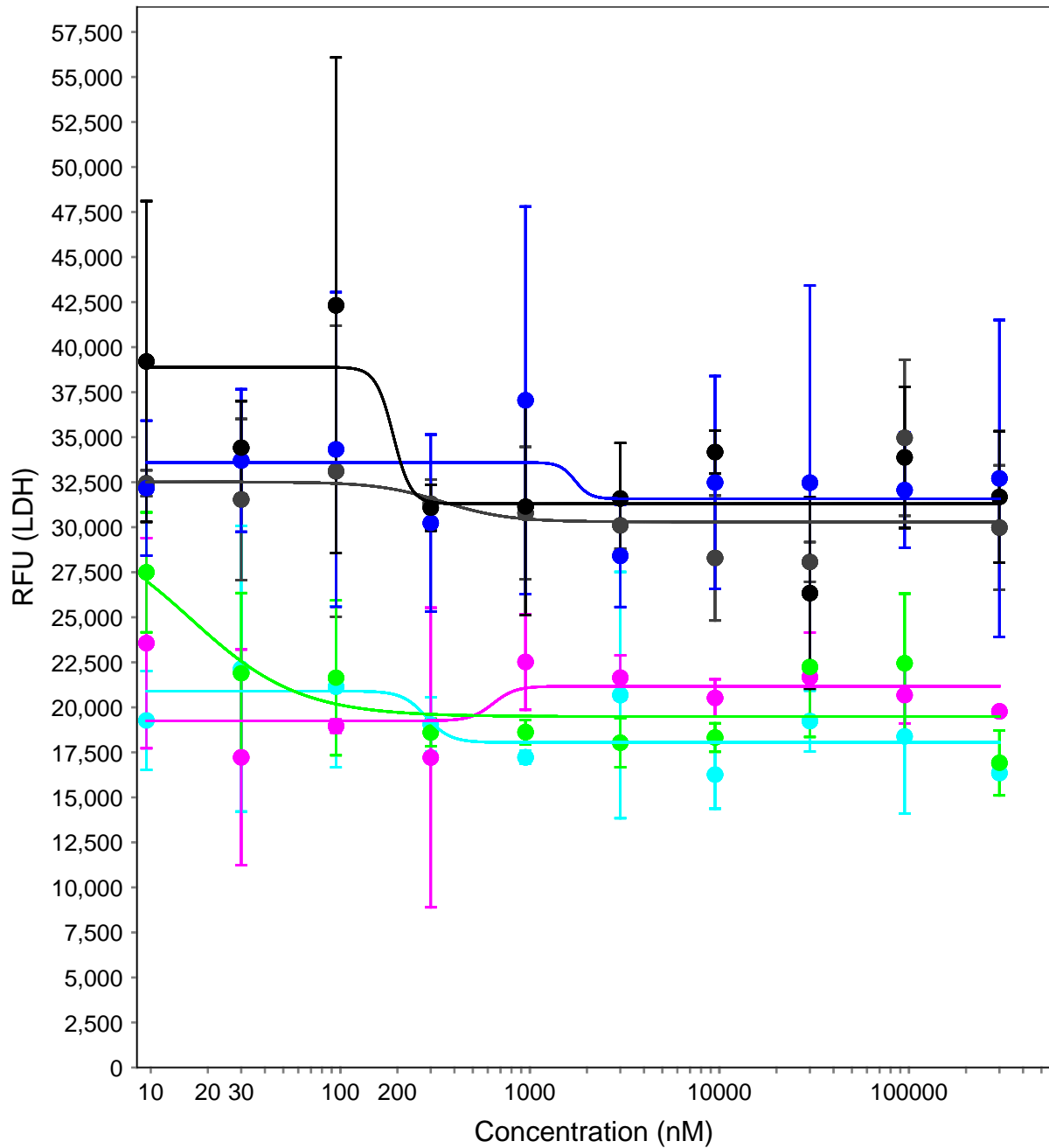
■	aflatoxin B1 2D-DIFF-R1 LDH 48h EMAX: 136000 EMIN: 35300 EC50: 3410 R ² : 0.967
■	aflatoxin B1 2D-DIFF-R2 LDH 48h EMAX: 206000 EMIN: 34400 EC50: 5750 R ² : 0.996
■	aflatoxin B1 2D-DIFF-R3 LDH 48h EMAX: 245000 EMIN: 27500 EC50: 5280 R ² : 0.994
■	aflatoxin B1 2D-DIFF-R1 LDH 96h EMAX: 175000 EMIN: 35700 EC50: 1540 R ² : 0.974
■	aflatoxin B1 2D-DIFF R2 LDH 96h EMAX: 164000 EMIN: 21800 EC50: 1640 R ² : 0.908
■	aflatoxin B1 2D-DIFF-R3 LDH 96h EMAX: 143000 EMIN: 23500 EC50: 1210 R ² : 0.746

Supplementary Data S3 - LDH Leakage Data



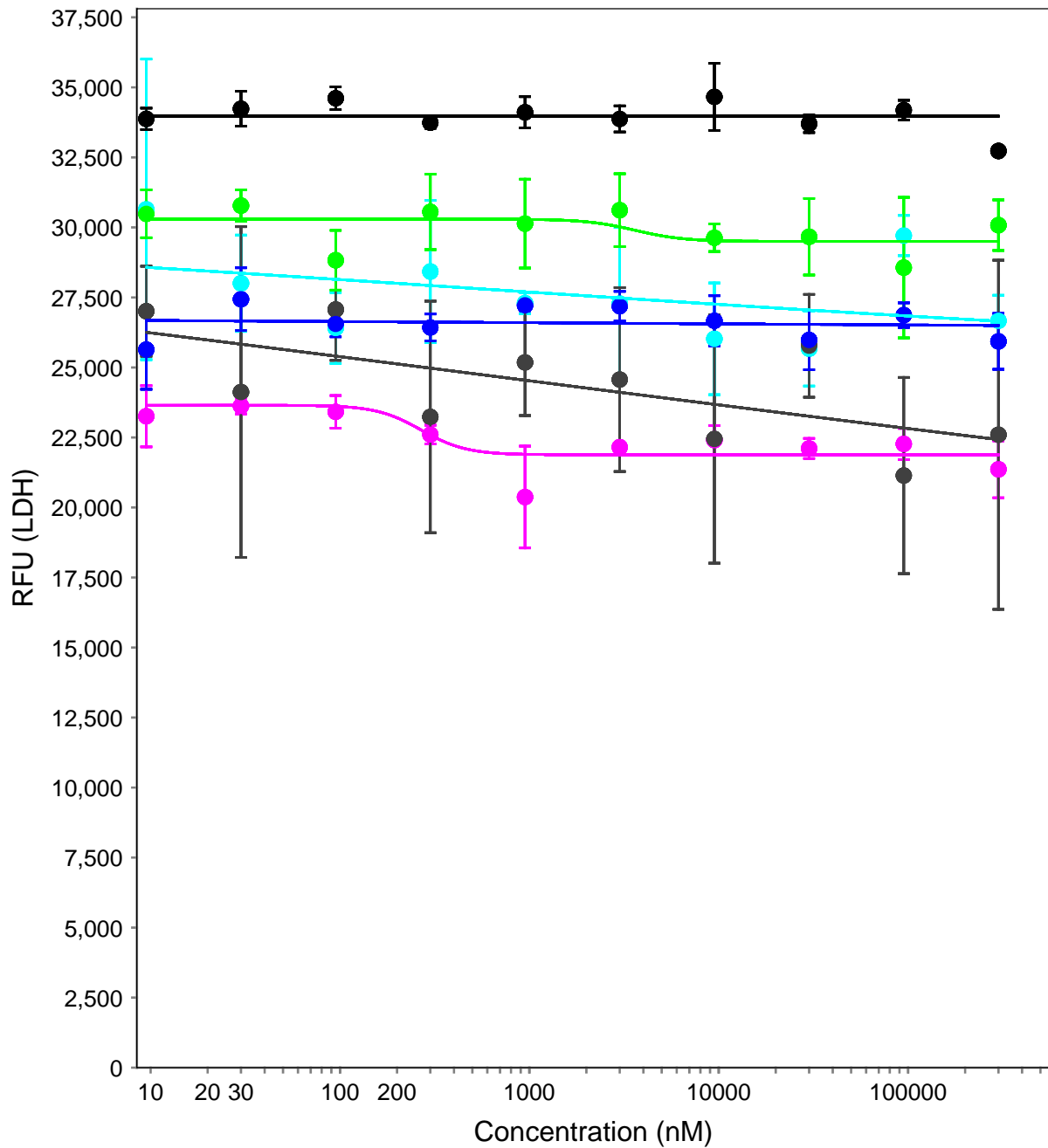
■	aflatoxin B1 PROLIF-R1 LDH 48h EMAX: 91400 EMIN: 34600 EC50: 2880 R ² : 0.996
■	aflatoxin B1 PROLIF-R2 LDH 48h EMAX: 89900 EMIN: 26200 EC50: 4860 R ² : 0.999
■	aflatoxin B1 PROLIF-R3 LDH 48h EMAX: 74900 EMIN: 30800 EC50: 3080 R ² : 0.981
■	aflatoxin B1 PROLIF-R1 LDH 96h EMAX: 3.30E4 EMIN: 18400 EC50: 14600 R ² : 0.504
■	aflatoxin B1 PROLIF-R2 LDH 96h EMAX: 33700 EMIN: 22100 EC50: 459 R ² : 0.275
■	aflatoxin B1 PROLIF-R3 LDH 96h EMAX: 46400 EMIN: 28200 EC50: 475 R ² : 0.232

Supplementary Data S3 - LDH Leakage Data



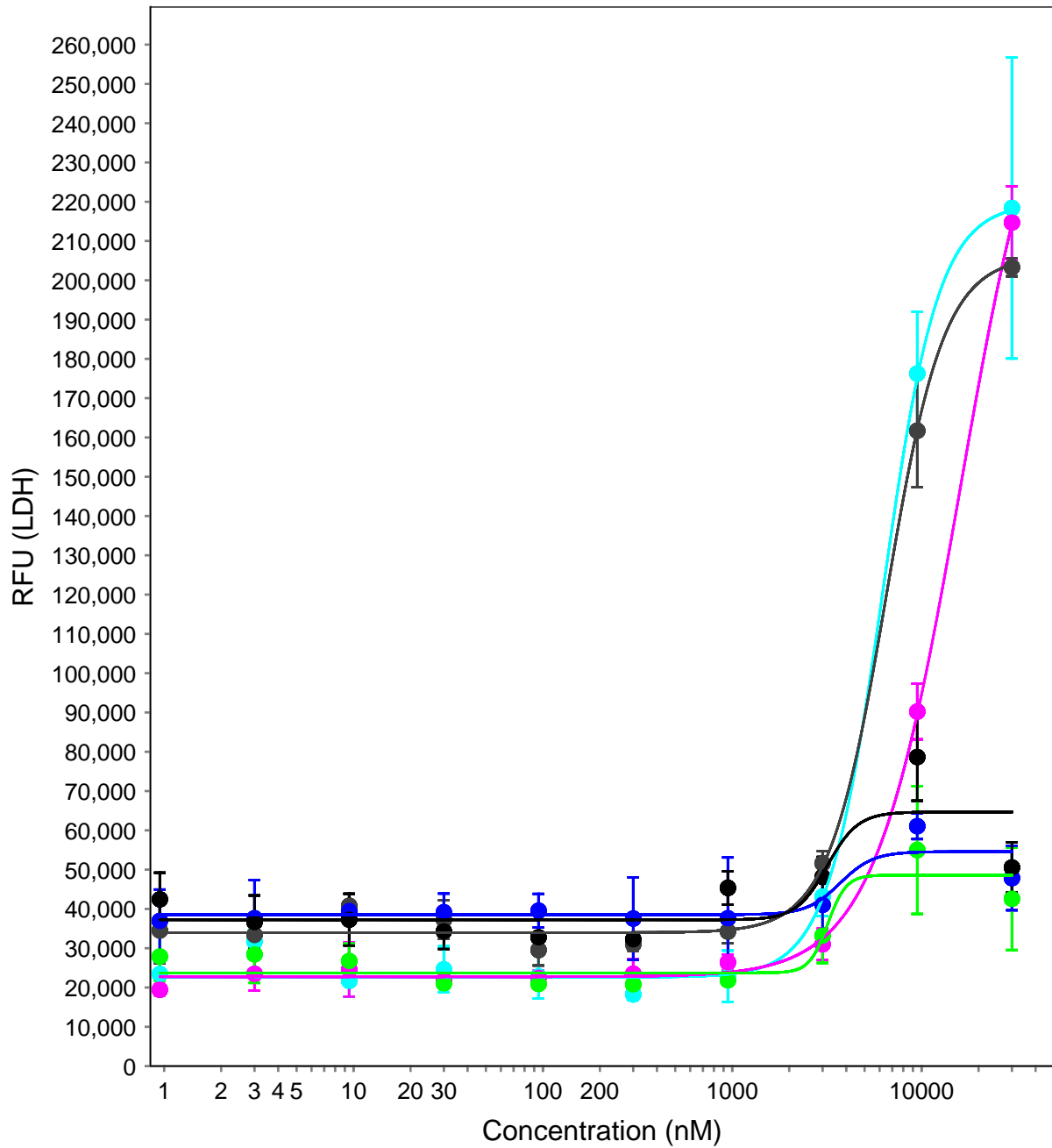
■	aspirin 2D-DIFF-R1 LDH 48h EMAX: 38900 EMIN: 31300 EC50: 190. R ² : 0.604
■	aspirin 2D-DIFF-R2 LDH 48h EMAX: 33600 EMIN: 31600 EC50: 1730 R ² : 0.181
■	aspirin 2D-DIFF-R3 LDH 48h EMAX: 30300 EMIN: 19500 EC50: 16.3 R ² : 0.654
■	aspirin 2D-DIFF-R1 LDH 96h EMAX: 32500 EMIN: 30300 EC50: 348 R ² : 0.195
■	aspirin 2D-DIFF-R2 LDH 96h EMAX: 21200 EMIN: 19300 EC50: 640. R ² : 0.205
■	aspirin 2D-DIFF-R3 LDH 96h EMAX: 20900 EMIN: 18100 EC50: 284 R ² : 0.450

Supplementary Data S3 - LDH Leakage Data



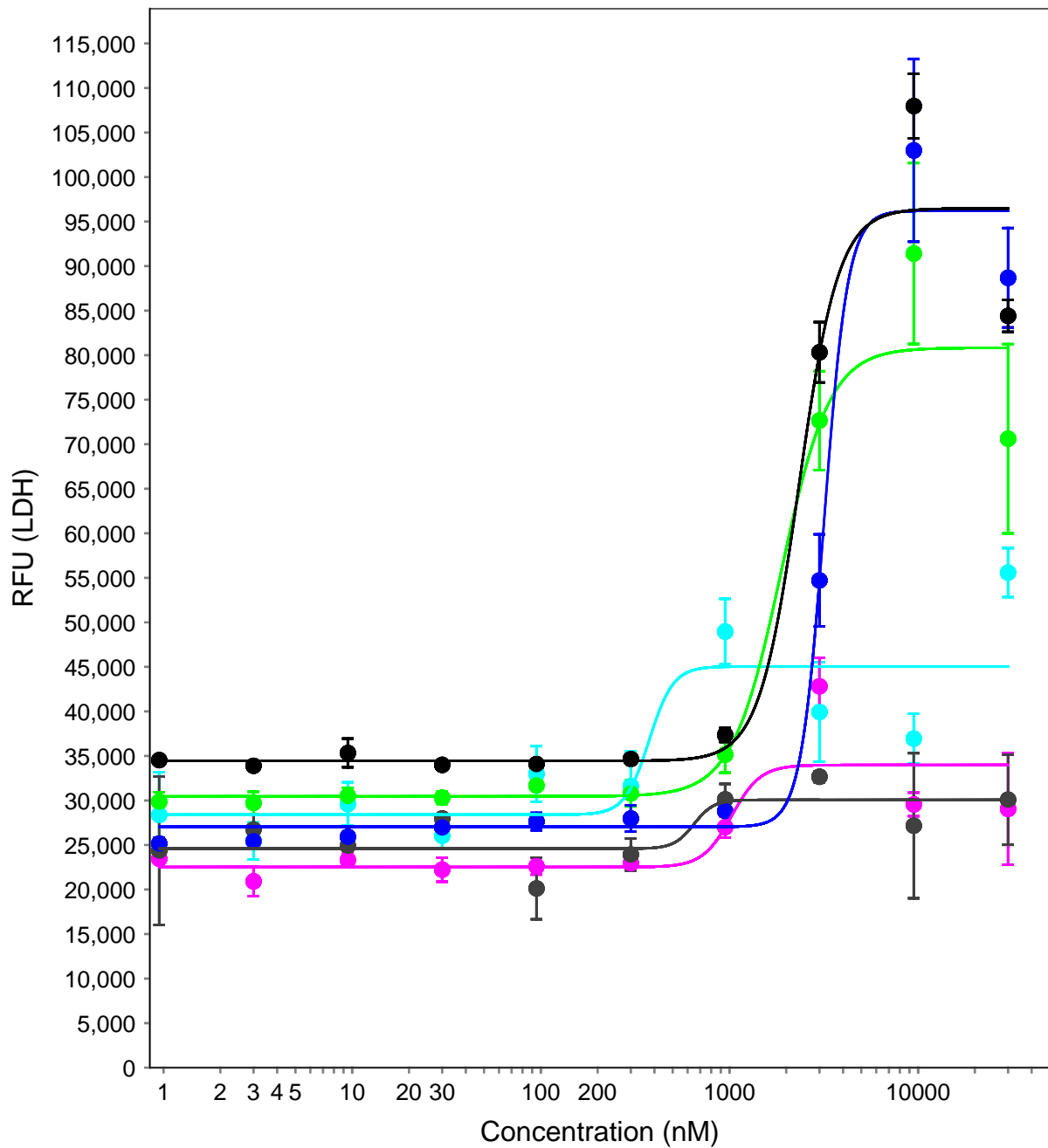
■	aspirin PROLIF-R1 LDH 48h EMAX: 68500 EMIN: 3.40E4 EC50: 1.49 R ² : -1.53E-6
■	aspirin PROLIF-R2 LDH 48h EMAX: 28800 EMIN: 24300 EC50: 2320 R ² : 0.0112
■	aspirin PROLIF-R3 LDH 48h EMAX: 30300 EMIN: 29500 EC50: 3620 R ² : 0.207
■	aspirin PROLIF-R1 LDH 96h EMAX: 34400 EMIN: 14800 EC50: 797 R ² : 0.418
■	aspirin PROLIF-R2 LDH 96h EMAX: 23600 EMIN: 21900 EC50: 269 R ² : 0.613
■	aspirin PROLIF-R3 LDH 96h EMAX: 30700 EMIN: 24900 EC50: 530. R ² : 0.161

Supplementary Data S3 - LDH Leakage Data



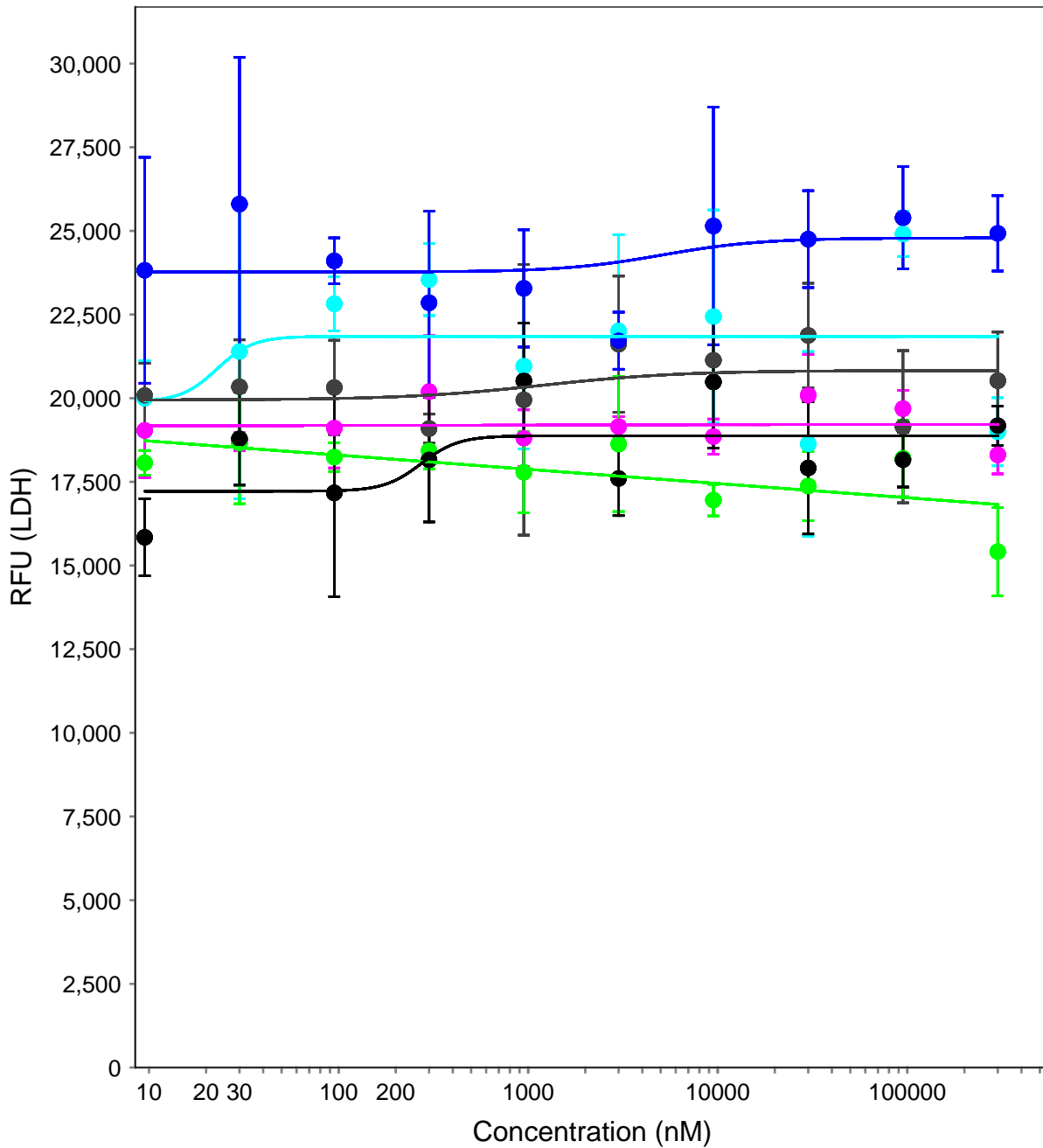
■	benzo(a)pyrene 2D-DIFF-R1 LDH 48h EMAX: 64700 EMIN: 37200 EC50: 3170 R ² : 0.684
■	benzo(a)pyrene 2D-DIFF-R2 LDH 48h EMAX: 54600 EMIN: 38500 EC50: 3710 R ² : 0.802
■	benzo(a)pyrene 2D-DIFF-R3 LDH 48h EMAX: 48600 EMIN: 23700 EC50: 3190 R ² : 0.864
■	benzo(a)pyrene 2D-DIFF-R1 LDH 96h EMAX: 206000 EMIN: 3.40E4 EC50: 6530 R ² : 0.95
■	benzo(a)pyrene 2D-DIFF R2 LDH 96h EMAX: 273000 EMIN: 22700 EC50: 16100 R ² : 0.9
■	benzo(a)pyrene 2D-DIFF-R3 LDH 96h EMAX: 2.20E5 EMIN: 22600 EC50: 6260 R ² : 0.998

Supplementary Data S3 - LDH Leakage Data



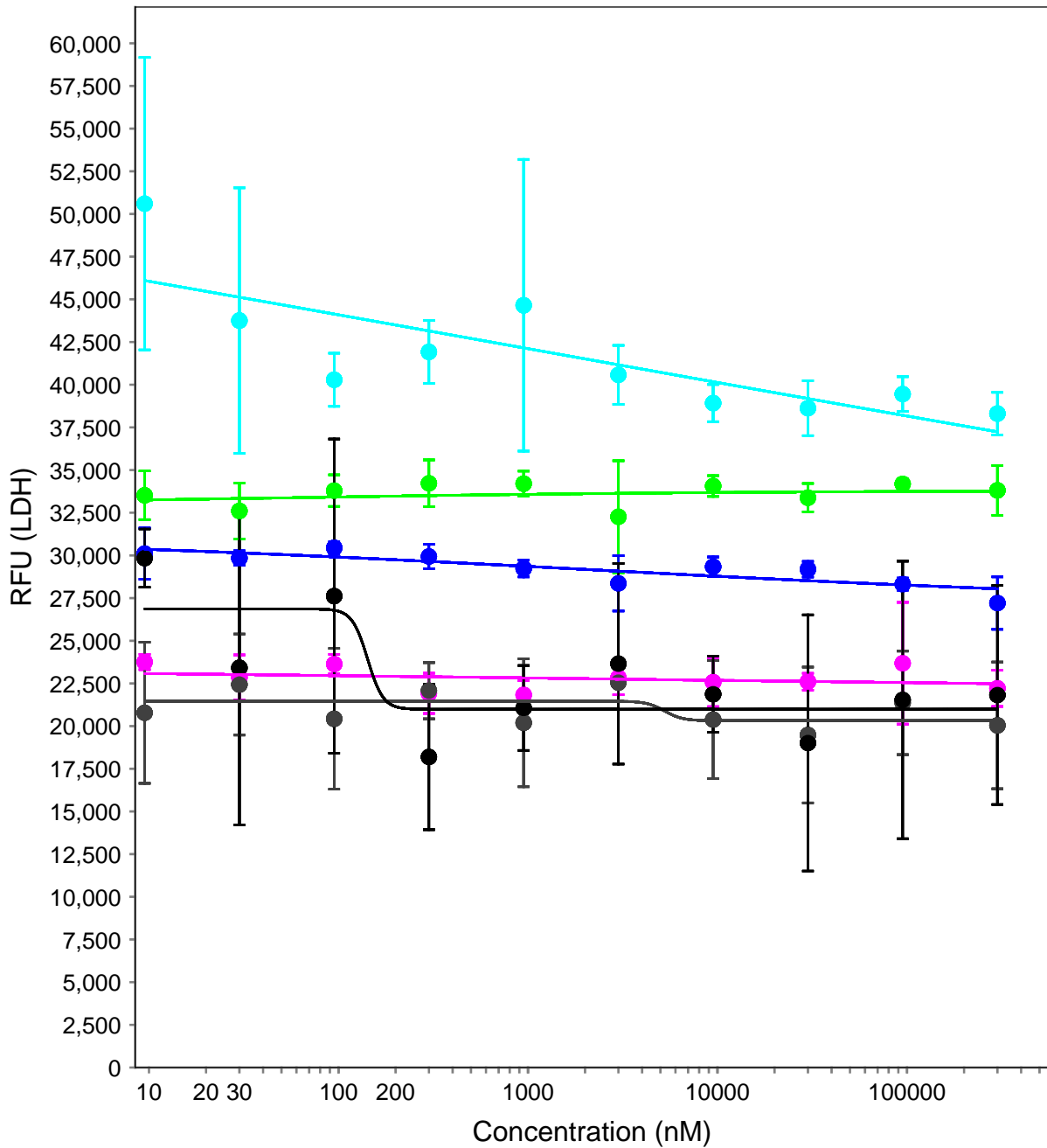
■	benzo(a)pyrene PROLIF-R1 LDH 48h EMAX: 96500 EMIN: 34400 EC50: 2340 R ² : 0.960
■	benzo(a)pyrene PROLIF-R2 LDH 48h EMAX: 96200 EMIN: 2.70E4 EC50: 3180 R ² : 0.985
■	benzo(a)pyrene PROLIF-R3 LDH 48h EMAX: 80800 EMIN: 30500 EC50: 1880 R ² : 0.955
■	benzo(a)pyrene PROLIF-R1 LDH 96h EMAX: 30100 EMIN: 24600 EC50: 647 R ² : 0.568
■	benzo(a)pyrene PROLIF-R2 LDH 96h EMAX: 3.40E4 EMIN: 22500 EC50: 1030 R ² : 0.665
■	benzo(a)pyrene PROLIF-R3 LDH 96h EMAX: 4.50E4 EMIN: 28400 EC50: 375 R ² : 0.718

Supplementary Data S3 - LDH Leakage Data



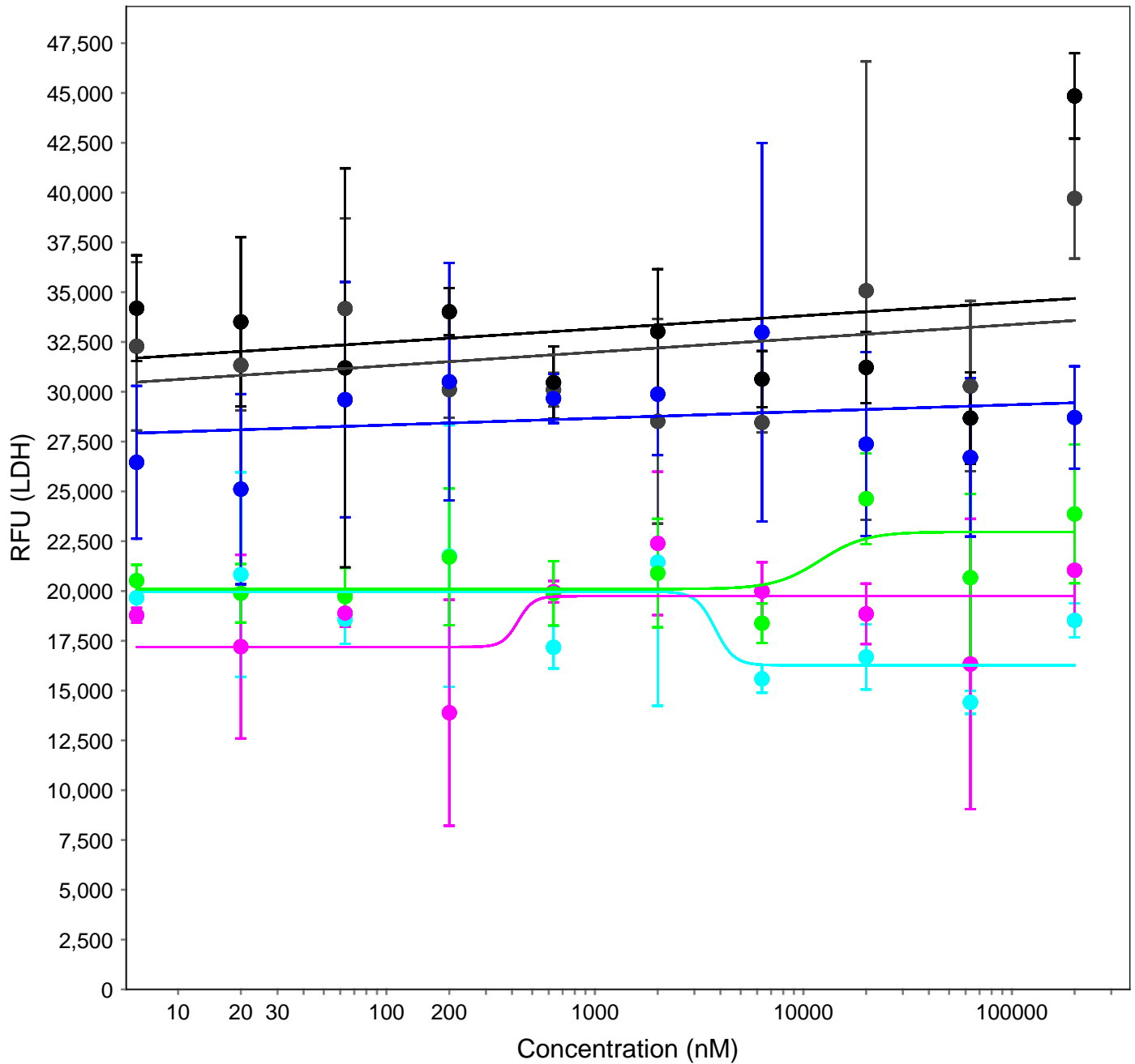
■	caffeine 2D-DIFF-R1 LDH 48h EMAX: 18900 EMIN: 17200 EC50: 273 R ² : 0.312
■	caffeine 2D-DIFF-R2 LDH 48h EMAX: 24800 EMIN: 23800 EC50: 5080 R ² : 0.202
■	caffeine 2D-DIFF-R3 LDH 48h EMAX: 31200 EMIN: 4130 EC50: 2730 R ² : 0.420
■	caffeine 2D-DIFF-R1 LDH 96h EMAX: 20800 EMIN: 19900 EC50: 1190 R ² : 0.152
■	caffeine 2D-DIFF-R2 LDH 96h EMAX: 19200 EMIN: 19200 EC50: 1340 R ² : 0.00287
■	caffeine 2D-DIFF-R3 LDH 96h EMAX: 21800 EMIN: 19900 EC50: 22.8 R ² : 0.0795

Supplementary Data S3 - LDH Leakage Data



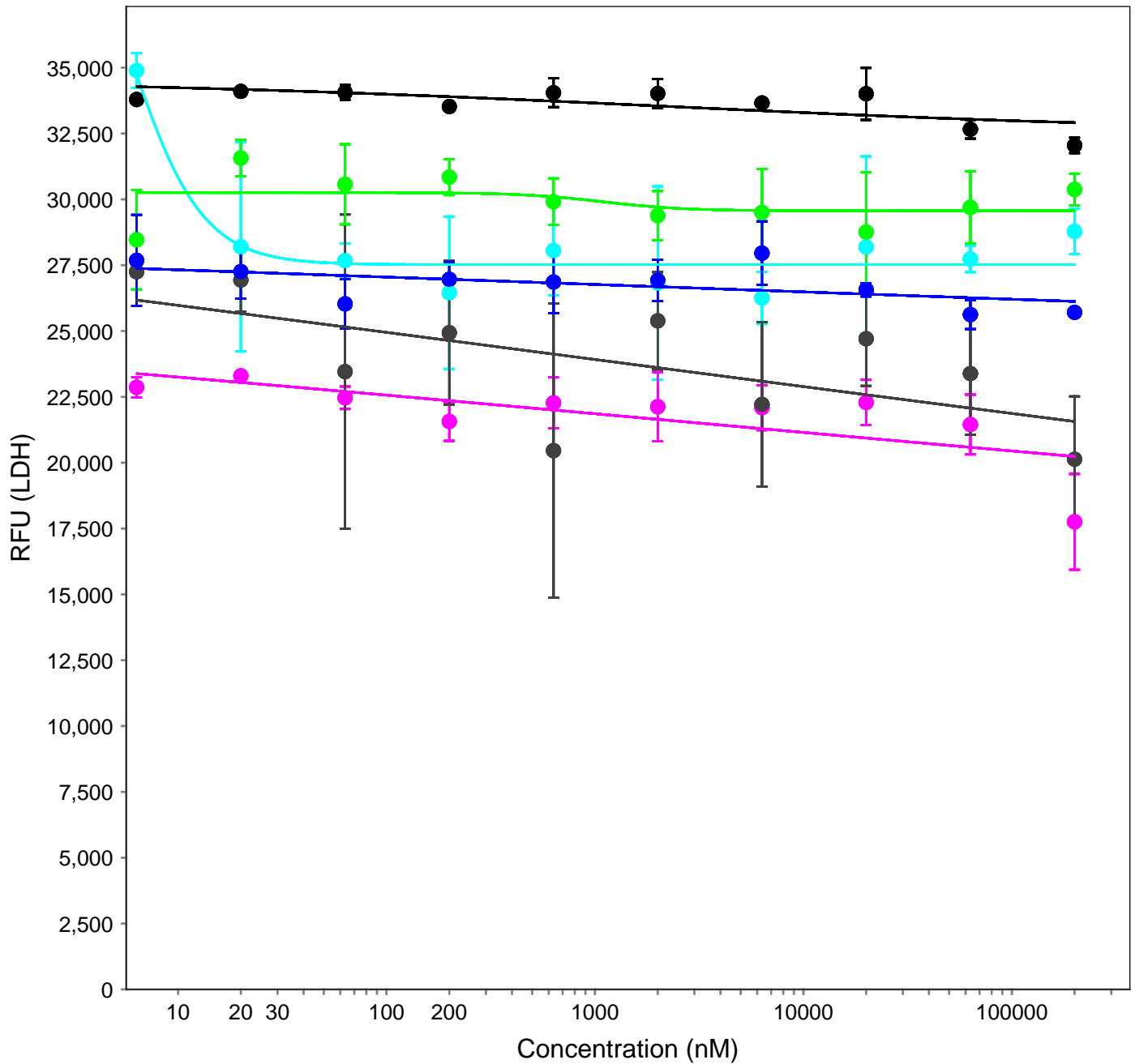
■	caffeine PROLIF-R1 LDH 48h EMAX: 26900 EMIN: 2.10E4 EC50: 142 R ² : 0.637
■	caffeine PROLIF-R2 LDH 48h EMAX: 31200 EMIN: 27100 EC50: 2140 R ² : 0.714
●	caffeine PROLIF-R3 LDH 48h EMAX: 33800 EMIN: 3.30E4 EC50: 54.0 R ² : 0.0534
●	caffeine PROLIF-R1 LDH 96h EMAX: 21500 EMIN: 20300 EC50: 5250 R ² : 0.275
●	caffeine PROLIF-R2 LDH 96h EMAX: 23500 EMIN: 2.20E4 EC50: 2840 R ² : 0.0650
●	caffeine PROLIF-R3 LDH 96h EMAX: 69700 EMIN: 14500 EC50: 1010 R ² : 0.616

Supplementary Data S3 - LDH Leakage Data



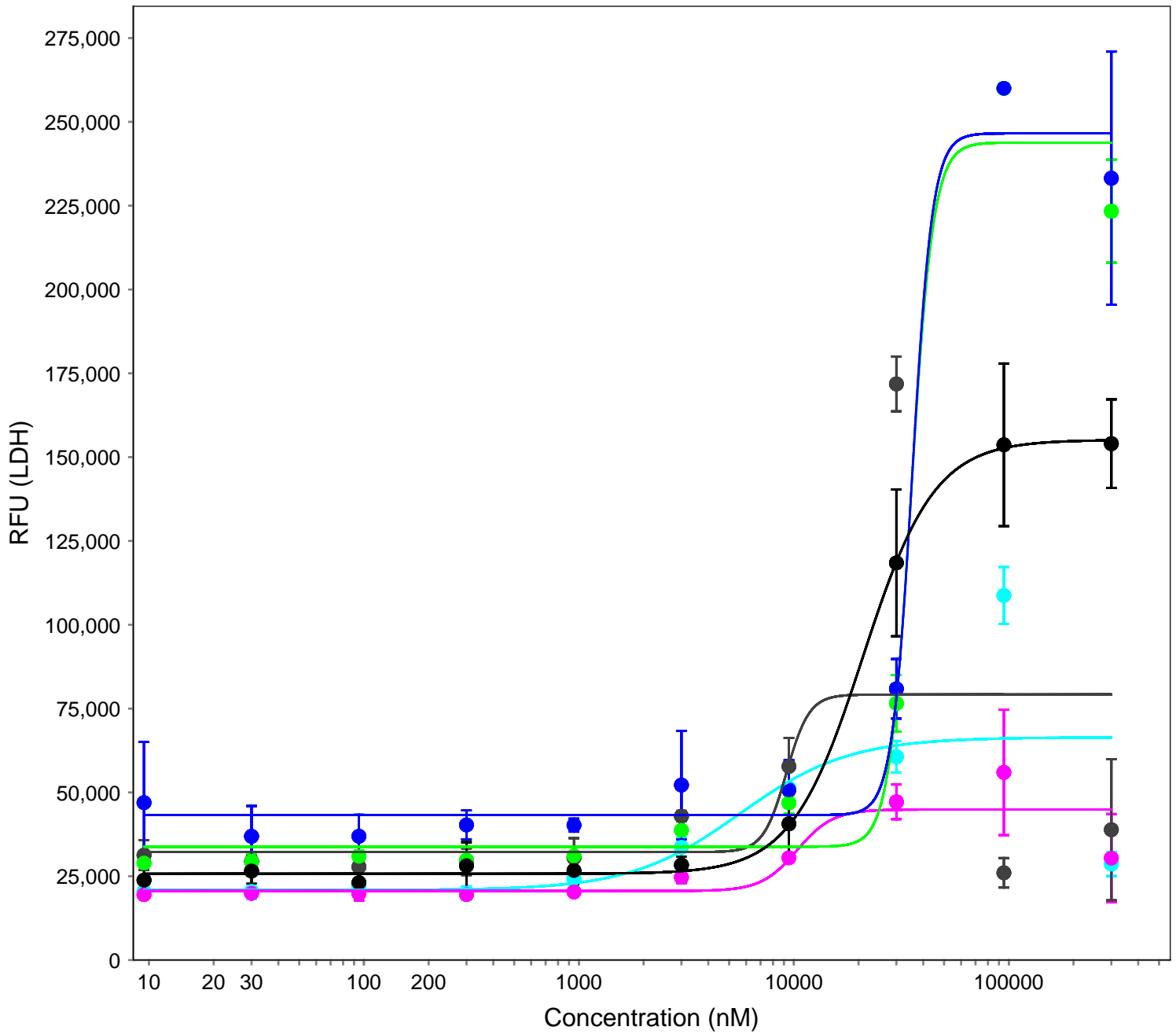
■	chenodeoxycholic acid 2D-DIFF-R1 LDH 48h EMAX: 51300 EMIN: 15500 EC50: 2640 R ² : 0.0502
■	chenodeoxycholic acid 2D-DIFF-R2 LDH 48h EMAX: 46900 EMIN: 9570 EC50: 56.2 R ² : 0.0488
■	chenodeoxycholic acid 2D-DIFF-R3 LDH 48h EMAX: 2.30E4 EMIN: 20100 EC50: 1.20E4 R ² : 0.476
■	chenodeoxycholic acid 2D-DIFF-R1 LDH 96h EMAX: 48600 EMIN: 16100 EC50: 3290 R ² : 0.0919
■	chenodeoxycholic acid 2D-DIFF R2 LDH 96h EMAX: 19700 EMIN: 17200 EC50: 427 R ² : 0.297
■	chenodeoxycholic acid 2D-DIFF-R3 LDH 96h EMAX: 2.00E4 EMIN: 16300 EC50: 3770 R ² : 0.552

Supplementary Data S3 - LDH Leakage Data



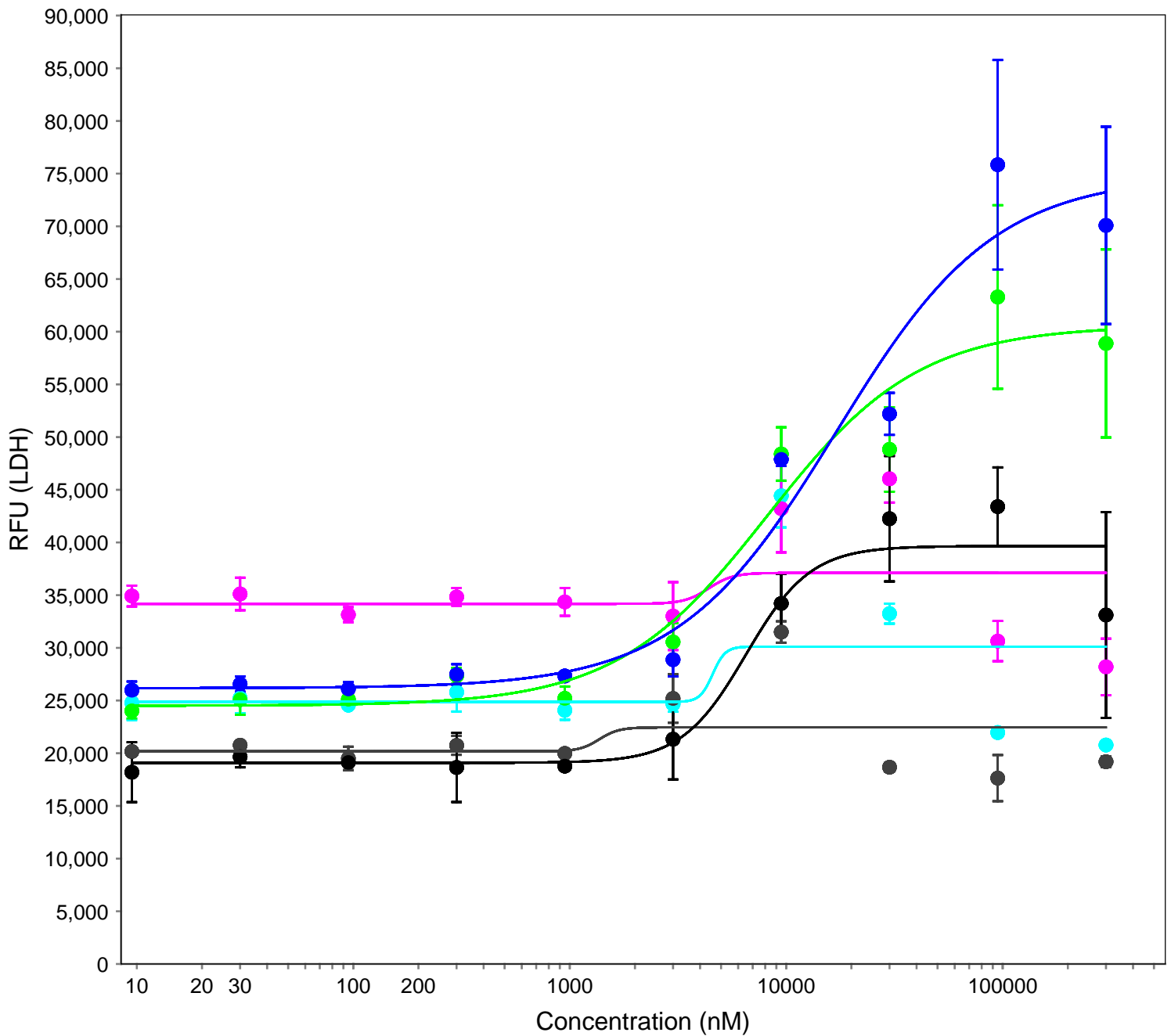
■	chenodeoxycholic acid PROLIF-R1 LDH 48h EMAX: 34600 EMIN: 32500 EC50: 2070 R ² : 0.458
■	chenodeoxycholic acid PROLIF-R2 LDH 48h EMAX: 30100 EMIN: 23200 EC50: 2040 R ² : 0.299
■	chenodeoxycholic acid PROLIF-R3 LDH 48h EMAX: 30300 EMIN: 29600 EC50: 1090 R ² : 0.161
■	chenodeoxycholic acid PROLIF-R1 LDH 96h EMAX: 4.20E4 EMIN: 6340 EC50: 585 R ² : 0.416
■	chenodeoxycholic acid PROLIF-R2 LDH 96h EMAX: 28800 EMIN: 14200 EC50: 2830 R ² : 0.490
■	chenodeoxycholic acid PROLIF-R3 LDH 96h EMAX: 44400 EMIN: 27500 EC50: 5.63 R ² : 0.896

Supplementary Data S3 - LDH Leakage Data



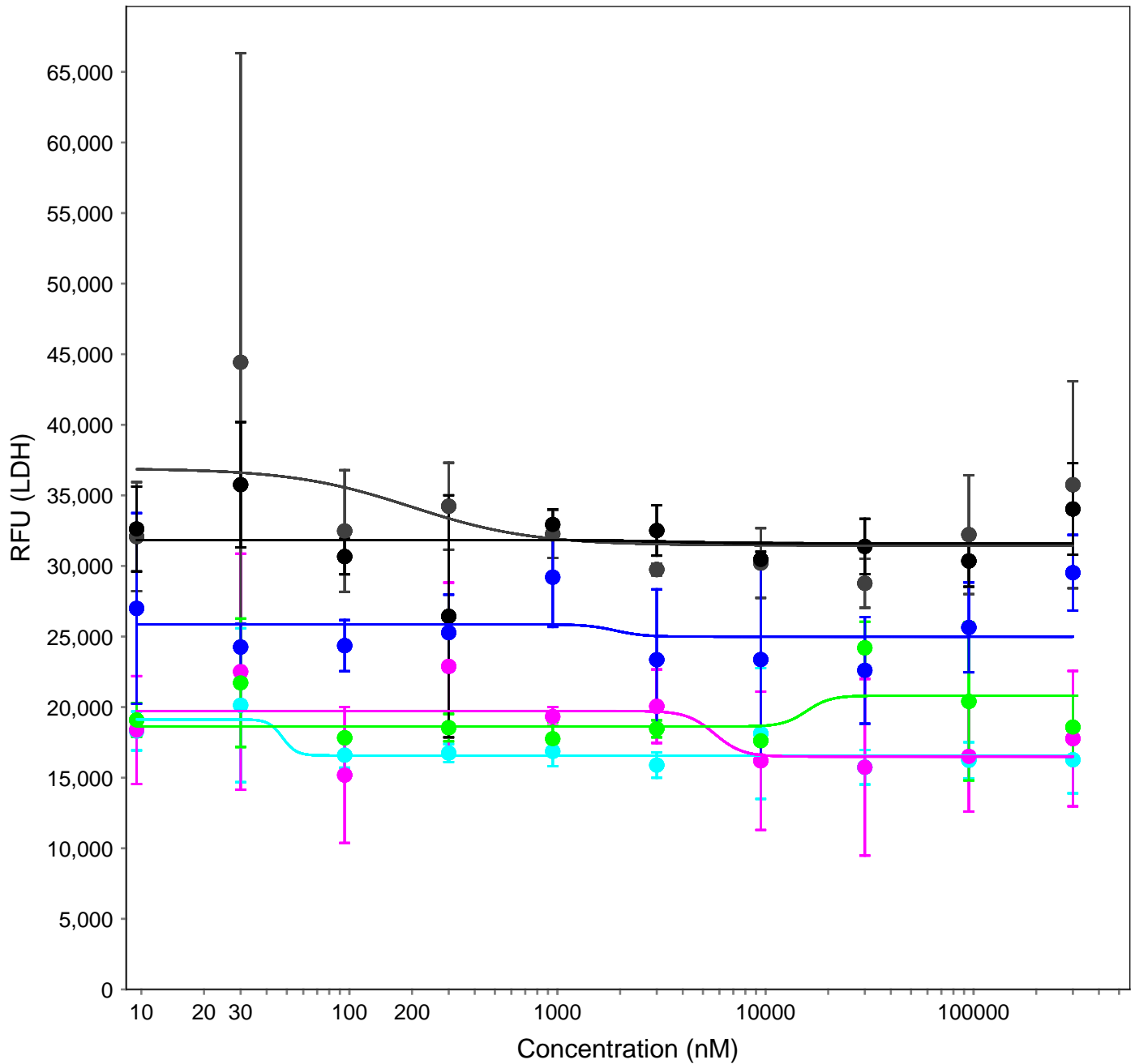
- chlorpromazine | 2D-DIFF-R1 | LDH | 48h | EMAX: 155000 | EMIN: 25700 | EC50: 2.10E4 | R^2: 0.999
- chlorpromazine | 2D-DIFF-R2 | LDH | 48h | EMAX: 247000 | EMIN: 43200 | EC50: 35600 | R^2: 0.991
- chlorpromazine | 2D-DIFF-R3 | LDH | 48h | EMAX: 244000 | EMIN: 33800 | EC50: 35100 | R^2: 0.986
- chlorpromazine | 2D-DIFF-R1 | LDH | 96h | EMAX: 79200 | EMIN: 32200 | EC50: 9220 | R^2: 0.255
- chlorpromazine | 2D-DIFF-R2 | LDH | 96h | EMAX: 44900 | EMIN: 20600 | EC50: 10300 | R^2: 0.761
- chlorpromazine | 2D-DIFF-R3 | LDH | 96h | EMAX: 66400 | EMIN: 20800 | EC50: 5.60E3 | R^2: 0.545

Supplementary Data S3 - LDH Leakage Data



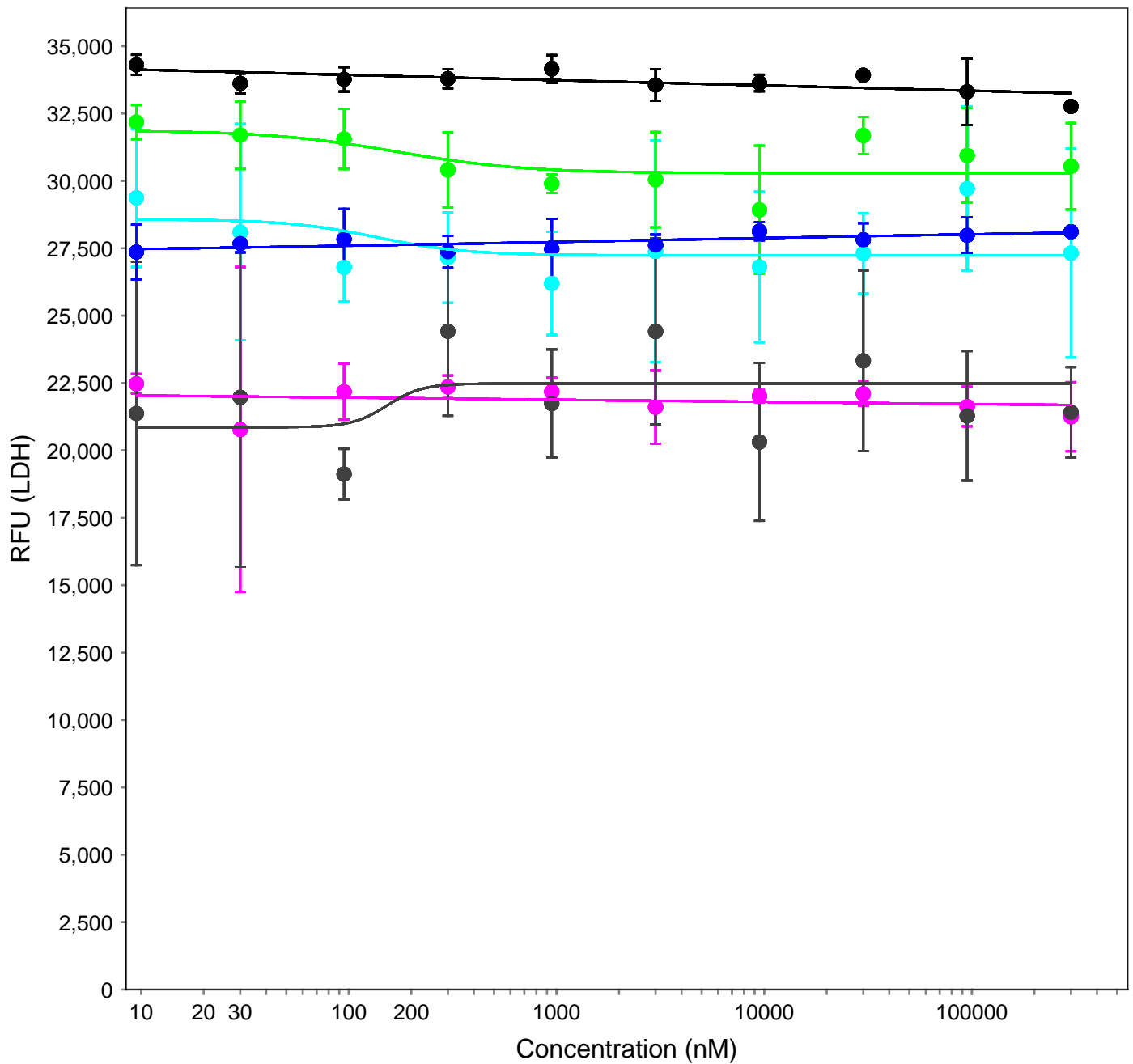
■	chlorpromazine	PROLIF-R1	LDH	48h	EMAX: 39700	EMIN: 19100	EC50: 6520	R ² : 0.930
■	chlorpromazine	PROLIF-R2	LDH	48h	EMAX: 74800	EMIN: 26200	EC50: 1.70E4	R ² : 0.961
■	chlorpromazine	PROLIF-R3	LDH	48h	EMAX: 60600	EMIN: 24500	EC50: 8180	R ² : 0.961
●	chlorpromazine	PROLIF-R1	LDH	96h	EMAX: 22400	EMIN: 20200	EC50: 1370	R ² : 0.0803
●	chlorpromazine	PROLIF-R2	LDH	96h	EMAX: 37100	EMIN: 34200	EC50: 4390	R ² : 0.0697
●	chlorpromazine	PROLIF-R3	LDH	96h	EMAX: 30100	EMIN: 24900	EC50: 4570	R ² : 0.152

Supplementary Data S3 - LDH Leakage Data



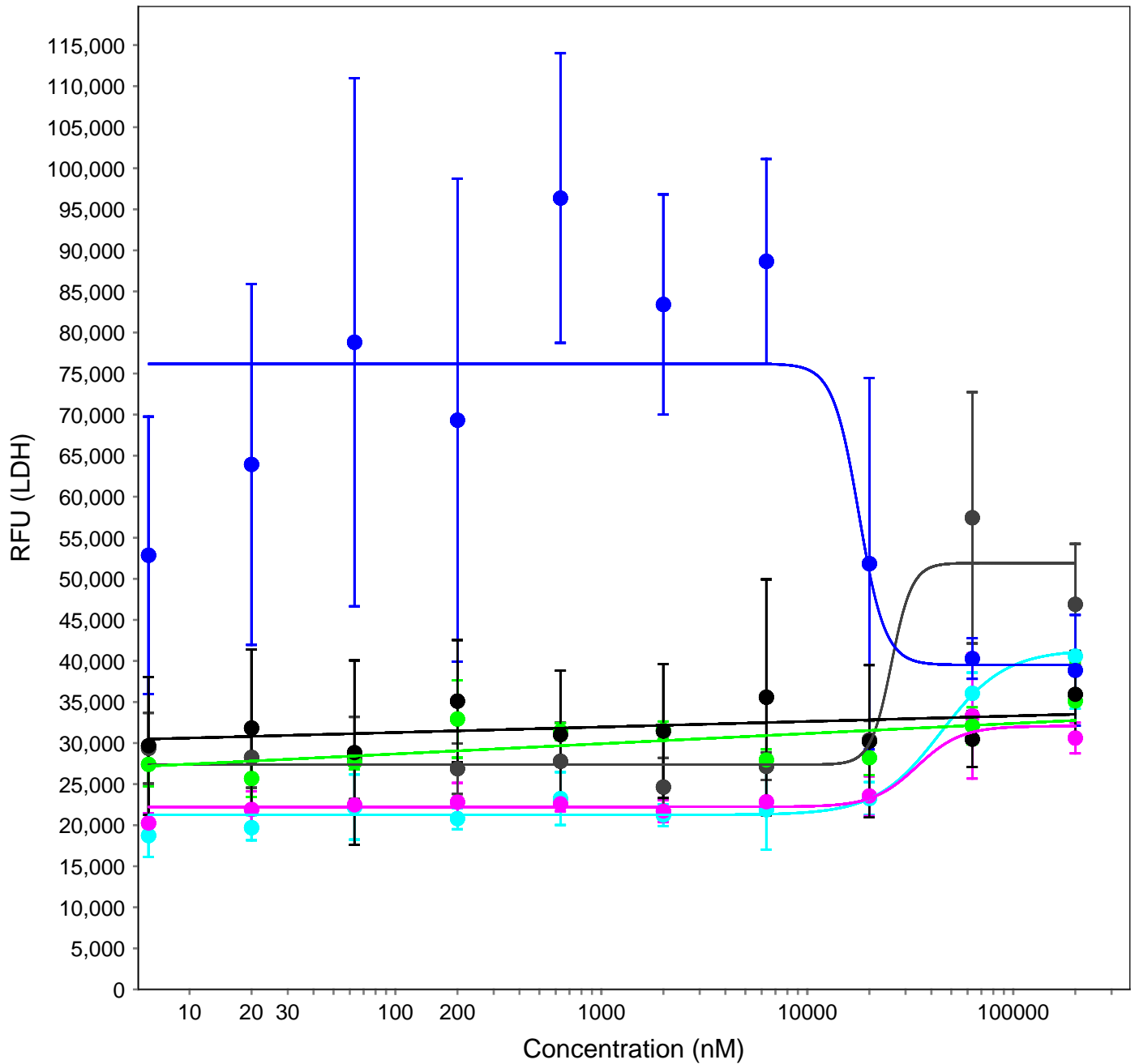
■	cyclophosphamide	2D-DIFF-R1	LDH	48h	EMAX: 31800	EMIN: 31600	EC50: 3560	R ² : -8.71E-4
■	cyclophosphamide	2D-DIFF-R2	LDH	48h	EMAX: 25900	EMIN: 2.50E4	EC50: 1890	R ² : 0.0519
■	cyclophosphamide	2D-DIFF-R3	LDH	48h	EMAX: 20800	EMIN: 18600	EC50: 15700	R ² : 0.276
■	cyclophosphamide	2D-DIFF-R1	LDH	96h	EMAX: 36900	EMIN: 31500	EC50: 199	R ² : 0.294
■	cyclophosphamide	2D-DIFF R2	LDH	96h	EMAX: 19700	EMIN: 16500	EC50: 5690	R ² : 0.359
■	cyclophosphamide	2D-DIFF-R3	LDH	96h	EMAX: 19100	EMIN: 16600	EC50: 47.7	R ² : 0.669

Supplementary Data S3 - LDH Leakage Data



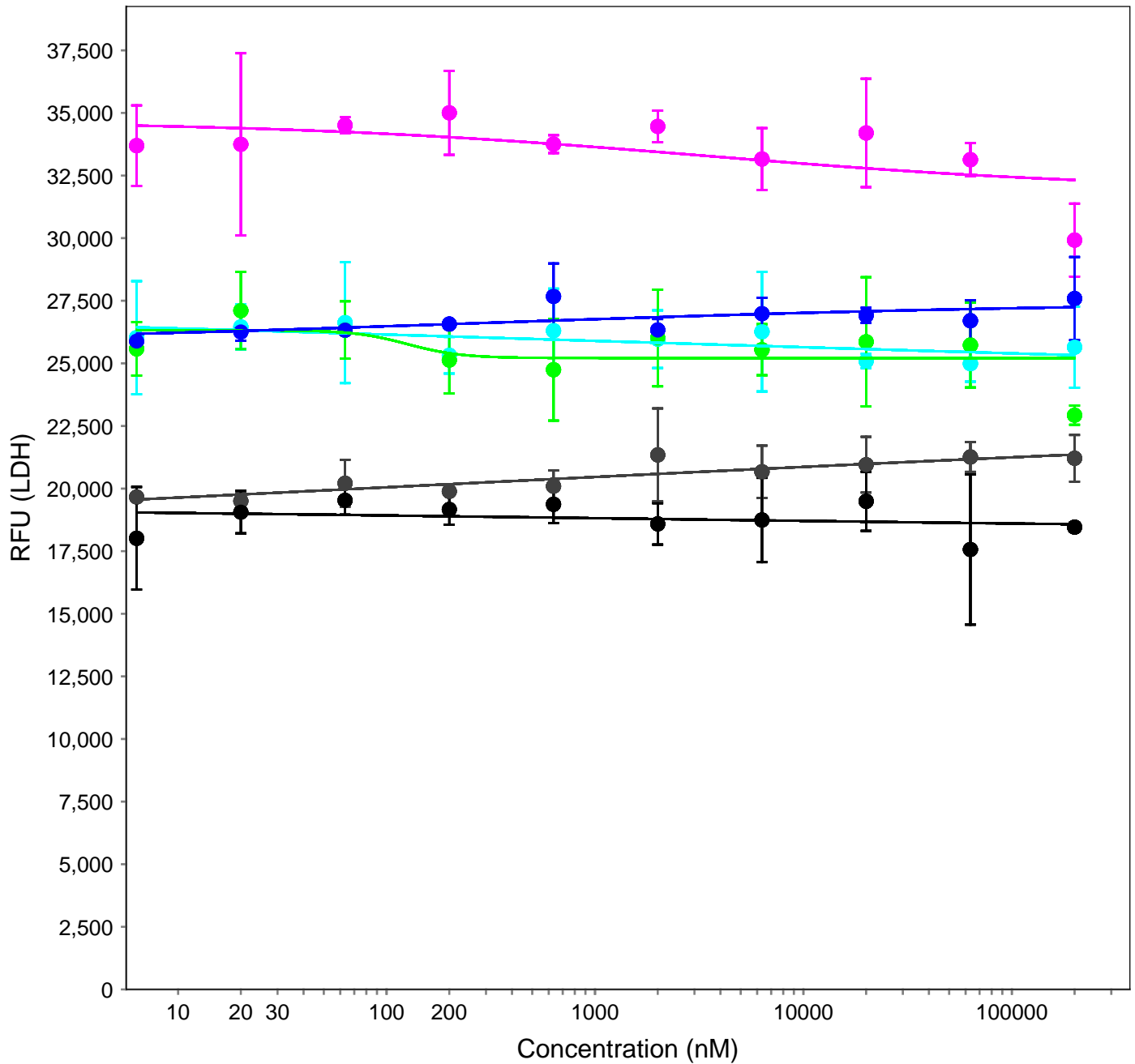
■	cyclophosphamide PROLIF-R1 LDH 48h EMAX: 4.30E4 EMIN: 24300 EC50: 3020 R ² : 0.478
■	cyclophosphamide PROLIF-R2 LDH 48h EMAX: 28400 EMIN: 27200 EC50: 2830 R ² : 0.504
■	cyclophosphamide PROLIF-R3 LDH 48h EMAX: 31900 EMIN: 30300 EC50: 171 R ² : 0.464
■	cyclophosphamide PROLIF-R1 LDH 96h EMAX: 22500 EMIN: 20900 EC50: 153 R ² : 0.180
■	cyclophosphamide PROLIF-R2 LDH 96h EMAX: 22600 EMIN: 21100 EC50: 2310 R ² : 0.0573
■	cyclophosphamide PROLIF-R3 LDH 96h EMAX: 28600 EMIN: 27200 EC50: 137 R ² : 0.112

Supplementary Data S3 - LDH Leakage Data



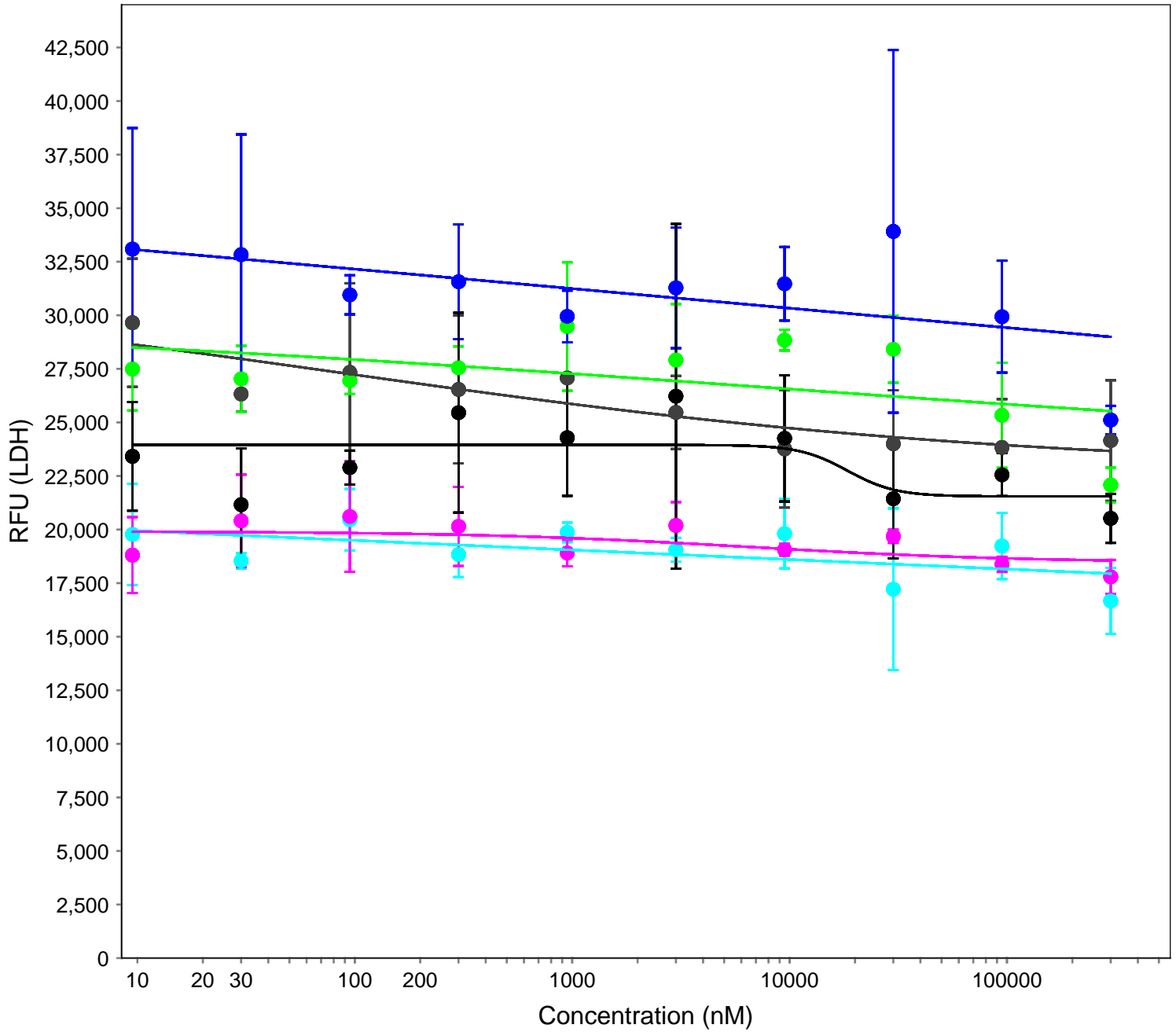
■	diphenhydramine 2D-DIFF-R1 LDH 48h EMAX: 56200 EMIN: 8140 EC50: 2160 R ² : 0.157
■	diphenhydramine 2D-DIFF-R2 LDH 48h EMAX: 76200 EMIN: 39500 EC50: 17800 R ² : 0.630
■	diphenhydramine 2D-DIFF-R3 LDH 48h EMAX: 49900 EMIN: 8970 EC50: 424 R ² : 0.386
■	diphenhydramine 2D-DIFF-R1 LDH 96h EMAX: 51900 EMIN: 27400 EC50: 25600 R ² : 0.932
■	diphenhydramine 2D-DIFF-R2 LDH 96h EMAX: 32100 EMIN: 22200 EC50: 34100 R ² : 0.930
■	diphenhydramine 2D-DIFF-R3 LDH 96h EMAX: 41400 EMIN: 21300 EC50: 44500 R ² : 0.970

Supplementary Data S3 - LDH Leakage Data



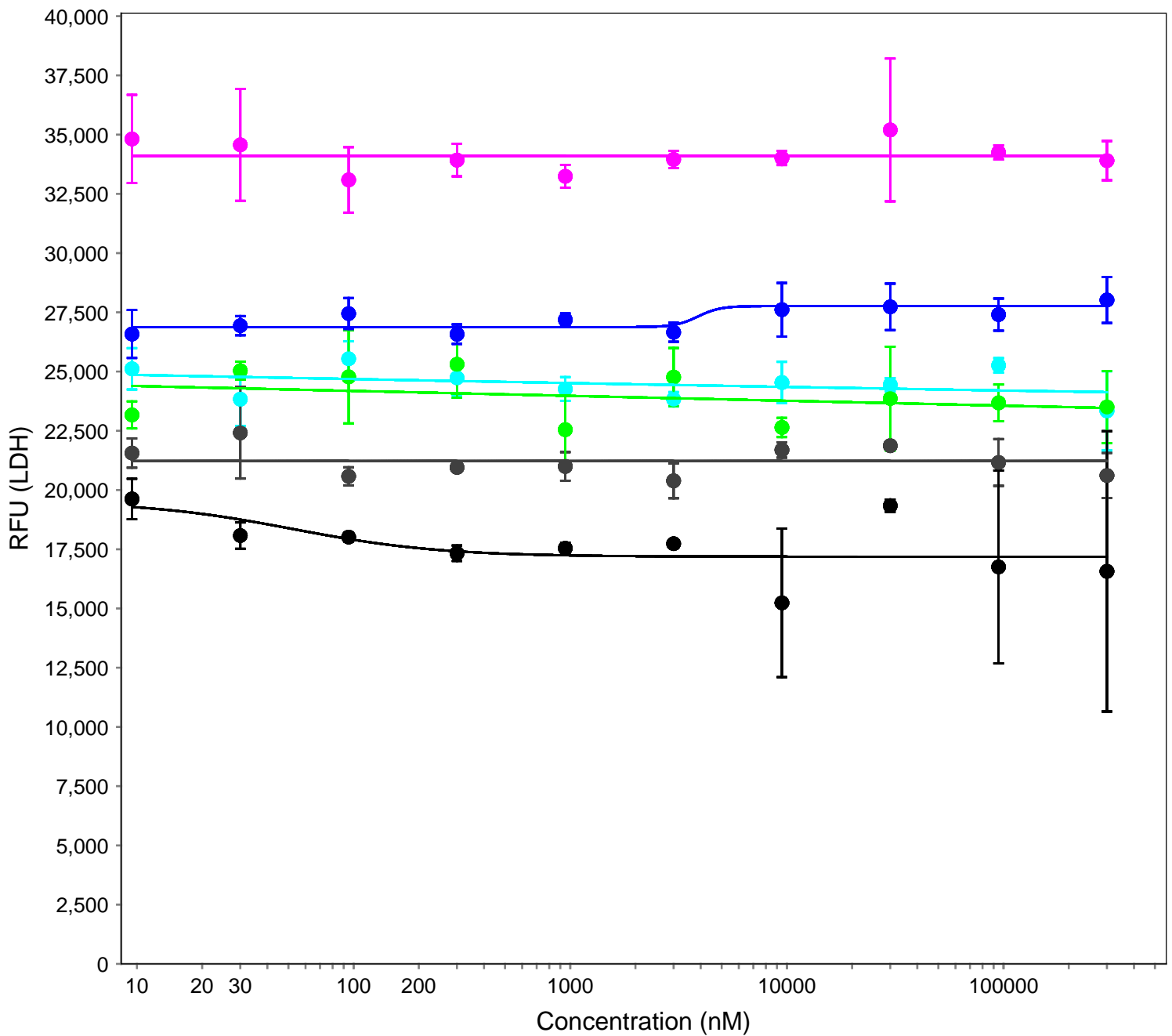
■ diphenhydramine | PROLIF-R1 | LDH | 48h | EMAX: 19400 | EMIN: 18200 | EC50: 1650 | R²: 0.0631
 ■ diphenhydramine | PROLIF-R2 | LDH | 48h | EMAX: 27500 | EMIN: 25700 | EC50: 275 | R²: 0.449
 ■ diphenhydramine | PROLIF-R3 | LDH | 48h | EMAX: 26300 | EMIN: 25200 | EC50: 126 | R²: 0.264
 ■ diphenhydramine | PROLIF-R1 | LDH | 96h | EMAX: 23600 | EMIN: 16600 | EC50: 137 | R²: 0.788
 ■ diphenhydramine | PROLIF-R2 | LDH | 96h | EMAX: 34700 | EMIN: 31900 | EC50: 3320 | R²: 0.371
 ■ diphenhydramine | PROLIF-R3 | LDH | 96h | EMAX: 2.80E4 | EMIN: 23800 | EC50: 1040 | R²: 0.354

Supplementary Data S3 - LDH Leakage Data



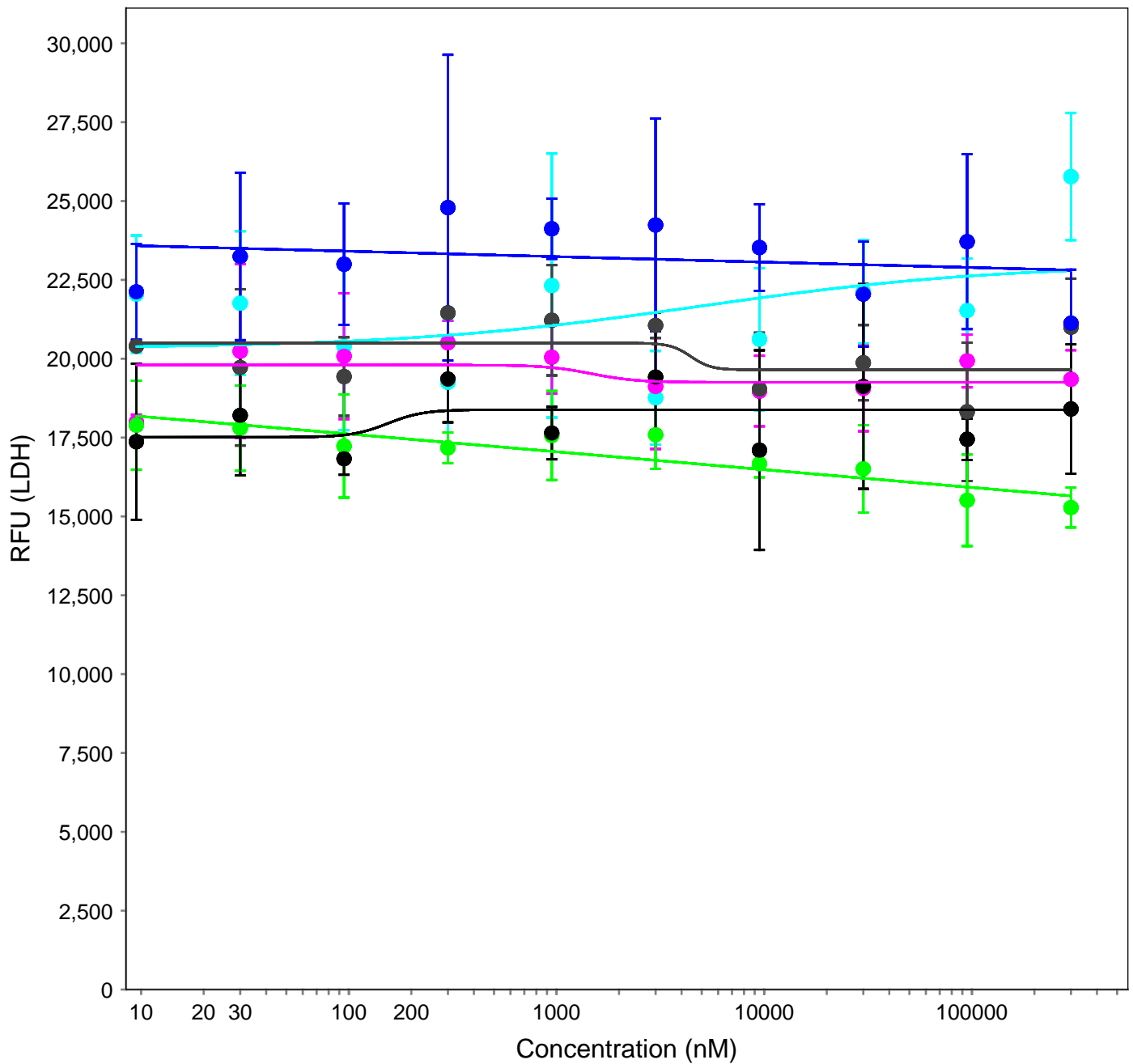
■ N-nitrosodimethylamine (DMN) | 2D-DIFF-R1 | LDH | 48h | EMAX: 23900 | EMIN: 21500 | EC50: 18500 | R²: 0.390
 ■ N-nitrosodimethylamine (DMN) | 2D-DIFF-R2 | LDH | 48h | EMAX: 44600 | EMIN: 17200 | EC50: 2440 | R²: 0.326
 ■ N-nitrosodimethylamine (DMN) | 2D-DIFF-R3 | LDH | 48h | EMAX: 3.00E4 | EMIN: 23300 | EC50: 7970 | R²: 0.211
 ■ N-nitrosodimethylamine (DMN) | 2D-DIFF-R1 | LDH | 96h | EMAX: 31900 | EMIN: 22800 | EC50: 83.0 | R²: 0.807
 ■ N-nitrosodimethylamine (DMN) | 2D-DIFF-R2 | LDH | 96h | EMAX: 19900 | EMIN: 18500 | EC50: 6610 | R²: 0.412
 ■ N-nitrosodimethylamine (DMN) | 2D-DIFF-R3 | LDH | 96h | EMAX: 30800 | EMIN: 7190 | EC50: 1270 | R²: 0.321

Supplementary Data S3 - LDH Leakage Data



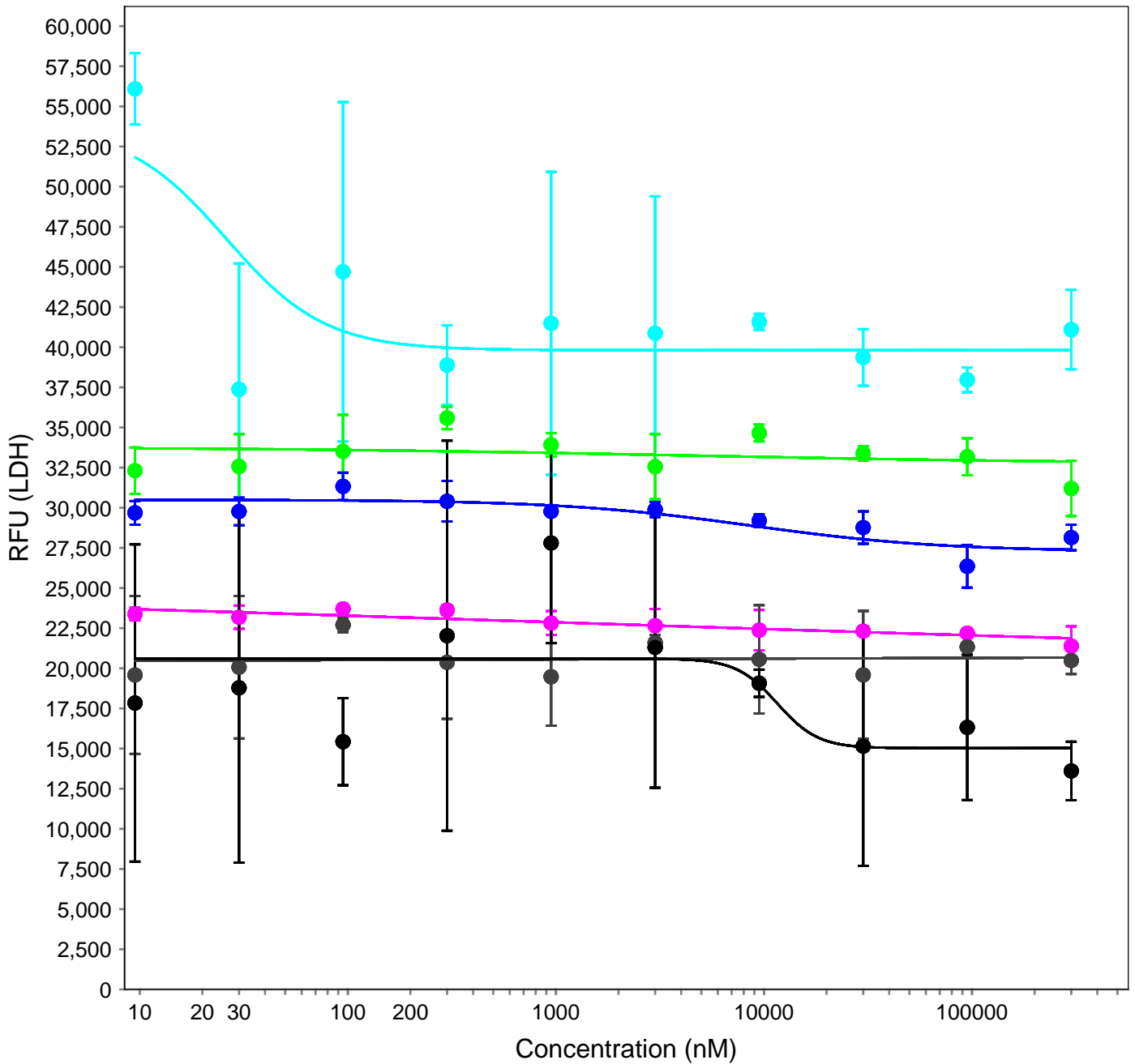
■	N-nitrosodimethylamine (DMN) PROLIF-R1 LDH 48h EMAX: 19500 EMIN: 17200 EC50: 52.5 R ² : 0.333
■	N-nitrosodimethylamine (DMN) PROLIF-R2 LDH 48h EMAX: 27800 EMIN: 26900 EC50: 3880 R ² : 0.612
■	N-nitrosodimethylamine (DMN) PROLIF-R3 LDH 48h EMAX: 38300 EMIN: 9.40E3 EC50: 3.70E3 R ² : 0.0964
■	N-nitrosodimethylamine (DMN) PROLIF-R1 LDH 96h EMAX: 22800 EMIN: 19600 EC50: 2430 R ² : -1.94E-8
■	N-nitrosodimethylamine (DMN) PROLIF-R2 LDH 96h EMAX: 37100 EMIN: 31100 EC50: 720. R ² : -1.70E-7
■	N-nitrosodimethylamine (DMN) PROLIF-R3 LDH 96h EMAX: 26700 EMIN: 23100 EC50: 3.75 R ² : 0.106

Supplementary Data S3 - LDH Leakage Data



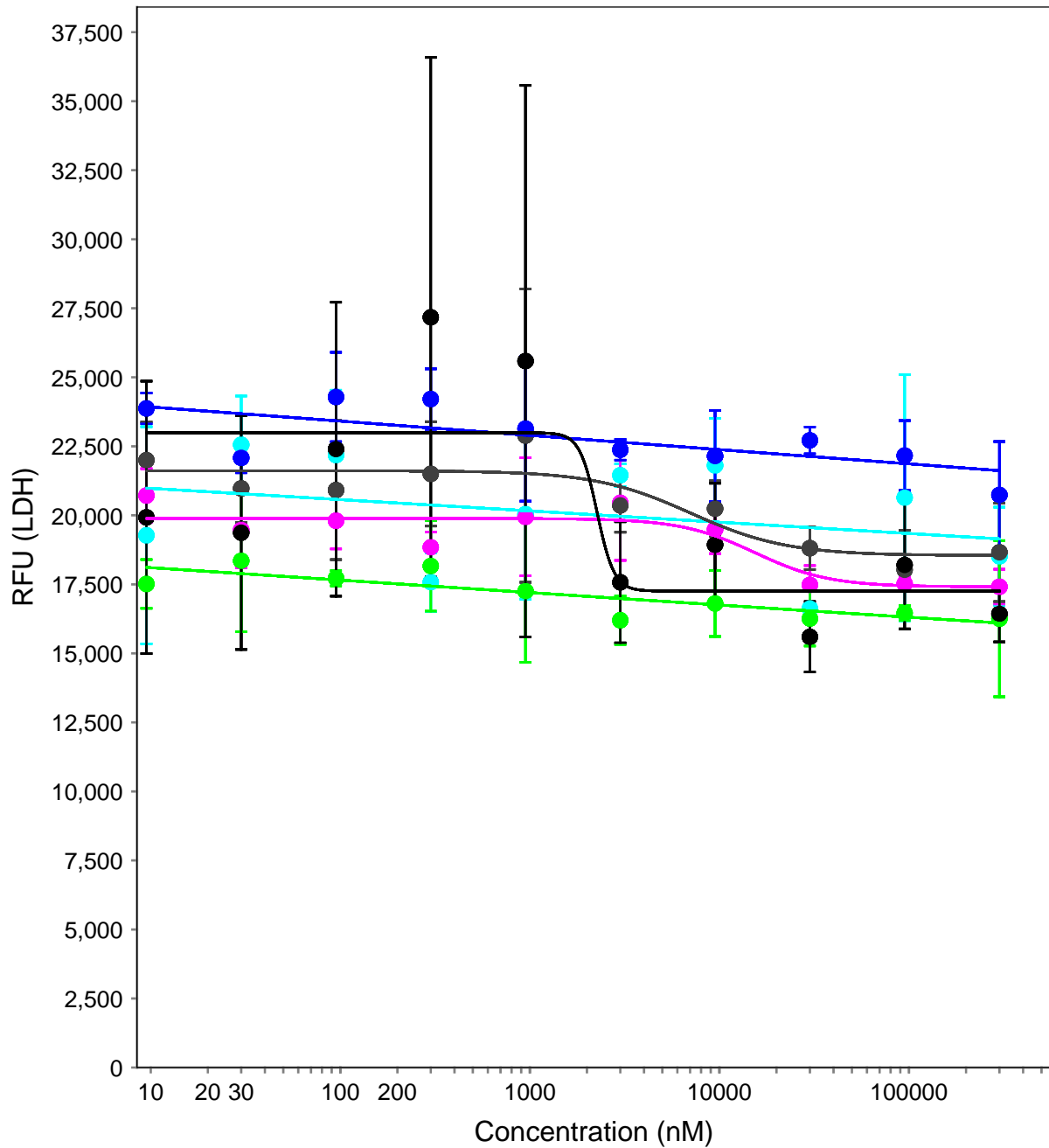
■	fenofibric acid 2D-DIFF-R1 LDH 48h EMAX: 18400 EMIN: 17500 EC50: 154 R ² : 0.180
■	fenofibric acid 2D-DIFF-R2 LDH 48h EMAX: 2.90E4 EMIN: 17300 EC50: 1790 R ² : 0.0515
■	fenofibric acid 2D-DIFF-R3 LDH 48h EMAX: 24700 EMIN: 8790 EC50: 3370 R ² : 0.788
■	fenofibric acid 2D-DIFF-R1 LDH 96h EMAX: 20500 EMIN: 19600 EC50: 4430 R ² : 0.232
■	fenofibric acid 2D-DIFF-R2 LDH 96h EMAX: 19800 EMIN: 19300 EC50: 1470 R ² : 0.0988
■	fenofibric acid 2D-DIFF-R3 LDH 96h EMAX: 2.30E4 EMIN: 20300 EC50: 4890 R ² : 0.197

Supplementary Data S3 - LDH Leakage Data



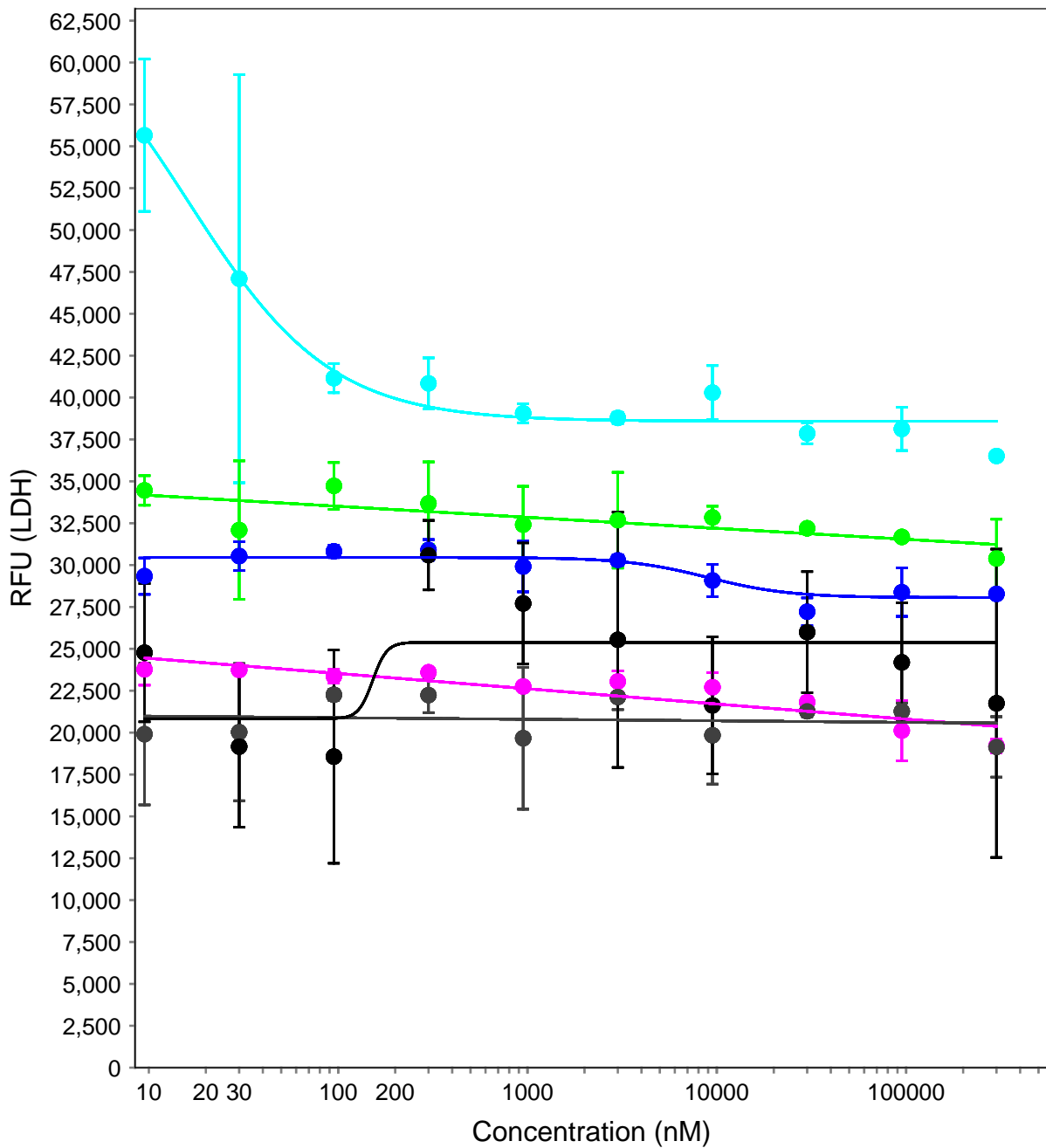
■	fenofibric acid PROLIF-R1 LDH 48h EMAX: 20600 EMIN: 1.50E4 EC50: 11600 R ² : 0.388
■	fenofibric acid PROLIF-R2 LDH 48h EMAX: 30500 EMIN: 27300 EC50: 8670 R ² : 0.706
■	fenofibric acid PROLIF-R3 LDH 48h EMAX: 33800 EMIN: 32700 EC50: 4360 R ² : 0.0419
■	fenofibric acid PROLIF-R1 LDH 96h EMAX: 20800 EMIN: 20300 EC50: 2620 R ² : 0.00438
■	fenofibric acid PROLIF-R2 LDH 96h EMAX: 25700 EMIN: 2.00E4 EC50: 1.20E3 R ² : 0.810
■	fenofibric acid PROLIF-R3 LDH 96h EMAX: 53700 EMIN: 39800 EC50: 26.0 R ² : 0.553

Supplementary Data S3 - LDH Leakage Data



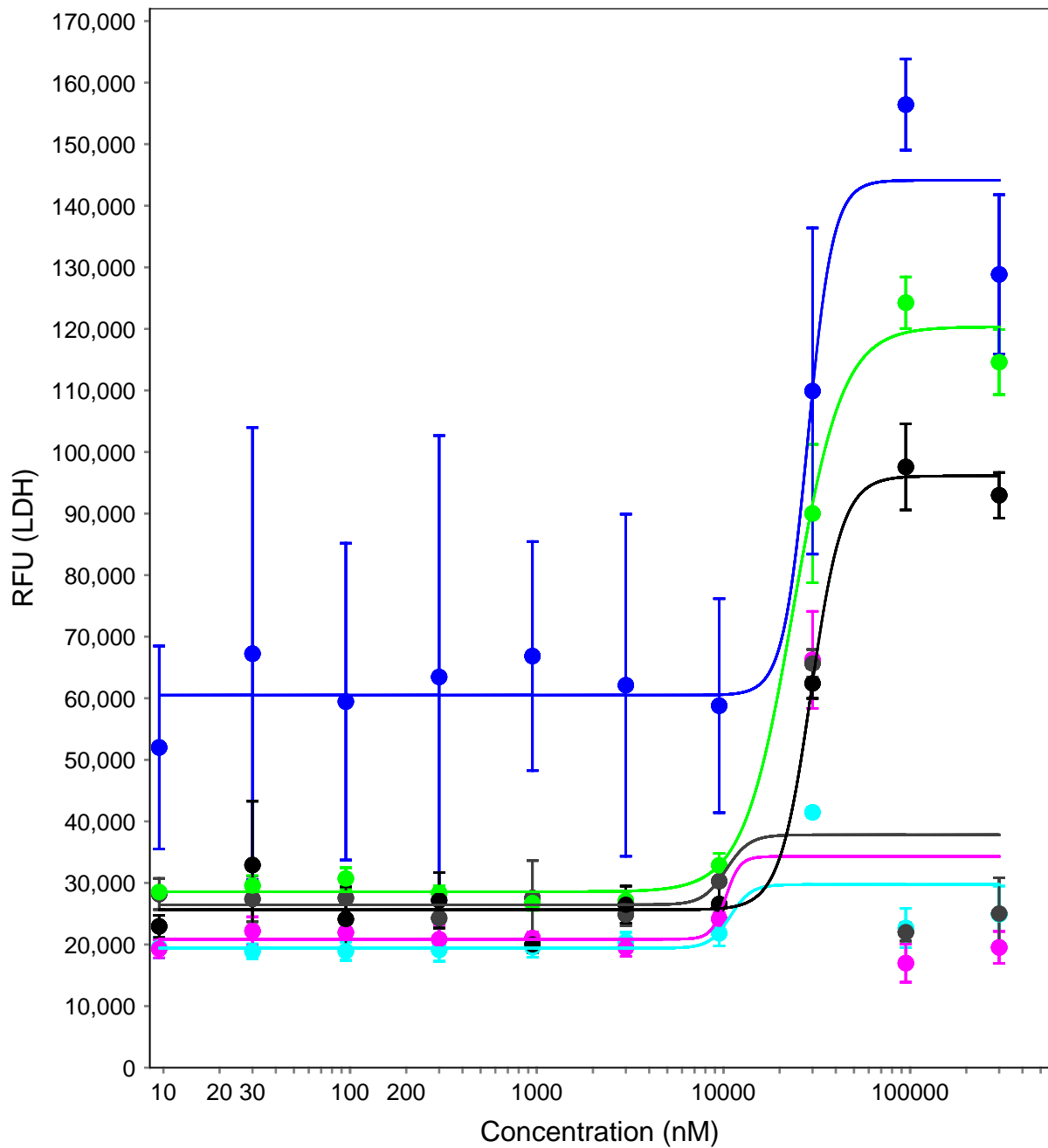
■	levofloxacin 2D-DIFF-R1 LDH 48h EMAX: 2.30E4 EMIN: 17300 EC50: 2260 R ² : 0.586
■	levofloxacin 2D-DIFF-R2 LDH 48h EMAX: 32700 EMIN: 12600 EC50: 2970 R ² : 0.486
■	levofloxacin 2D-DIFF-R3 LDH 48h EMAX: 24400 EMIN: 10600 EC50: 219 R ² : 0.691
■	levofloxacin 2D-DIFF-R1 LDH 96h EMAX: 21600 EMIN: 18500 EC50: 7060 R ² : 0.816
■	levofloxacin 2D-DIFF-R2 LDH 96h EMAX: 19900 EMIN: 17400 EC50: 15400 R ² : 0.816
■	levofloxacin 2D-DIFF-R3 LDH 96h EMAX: 38700 EMIN: 1250 EC50: 2820 R ² : 0.0946

Supplementary Data S3 - LDH Leakage Data



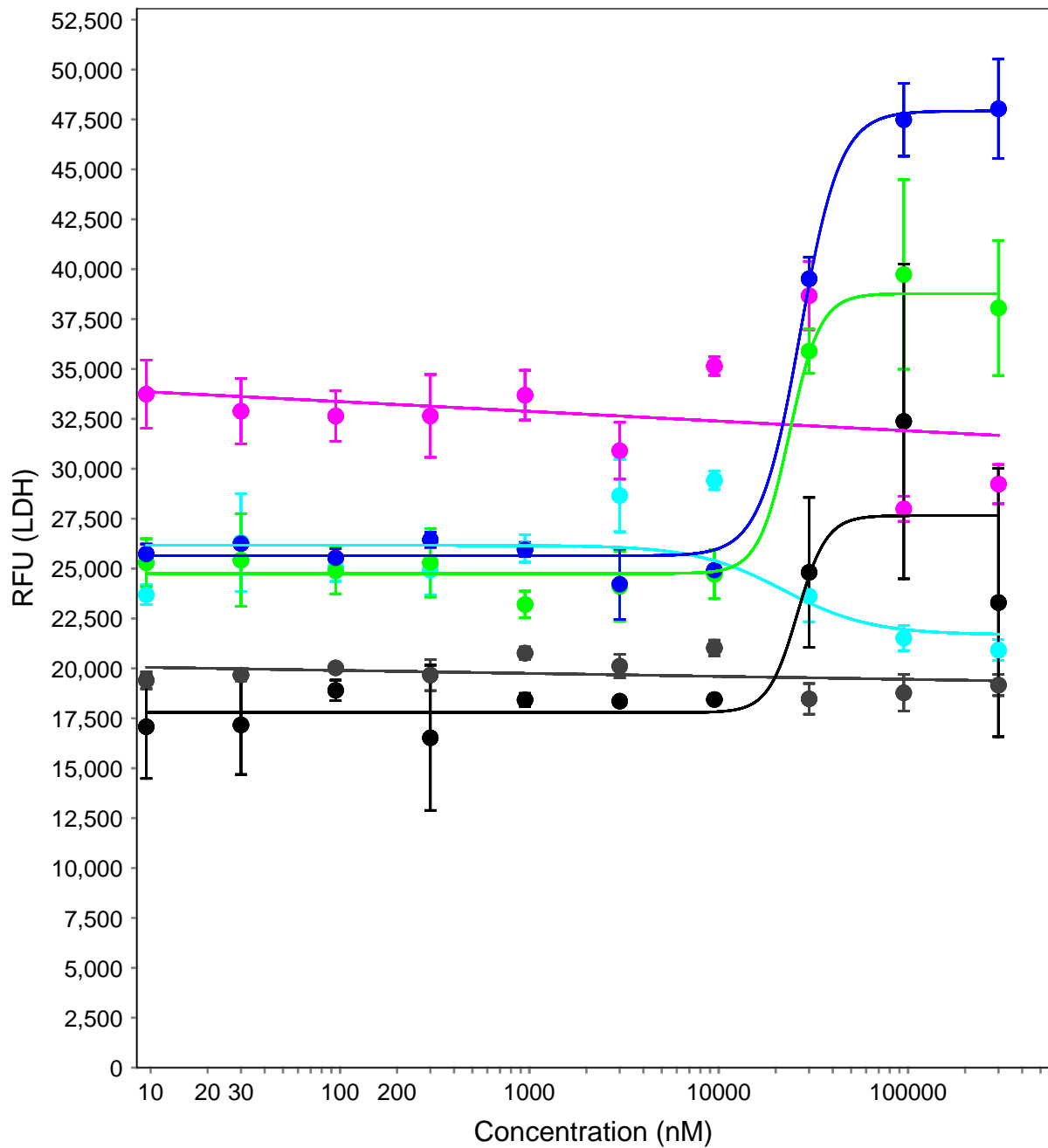
■	levo-floxacin PROLIF-R1 LDH 48h EMAX: 25400 EMIN: 20800 EC50: 152 R ² : 0.333
■	levo-floxacin PROLIF-R2 LDH 48h EMAX: 30500 EMIN: 28100 EC50: 8990 R ² : 0.775
■	levo-floxacin PROLIF-R3 LDH 48h EMAX: 52300 EMIN: 13600 EC50: 621 R ² : 0.586
■	levo-floxacin PROLIF-R1 LDH 96h EMAX: 2.70E4 EMIN: 14500 EC50: 1220 R ² : 0.0145
■	levo-floxacin PROLIF-R2 LDH 96h EMAX: 3.80E4 EMIN: 7540 EC50: 721 R ² : 0.789
■	levo-floxacin PROLIF-R3 LDH 96h EMAX: 64900 EMIN: 38600 EC50: 16.1 R ² : 0.966

Supplementary Data S3 - LDH Leakage Data



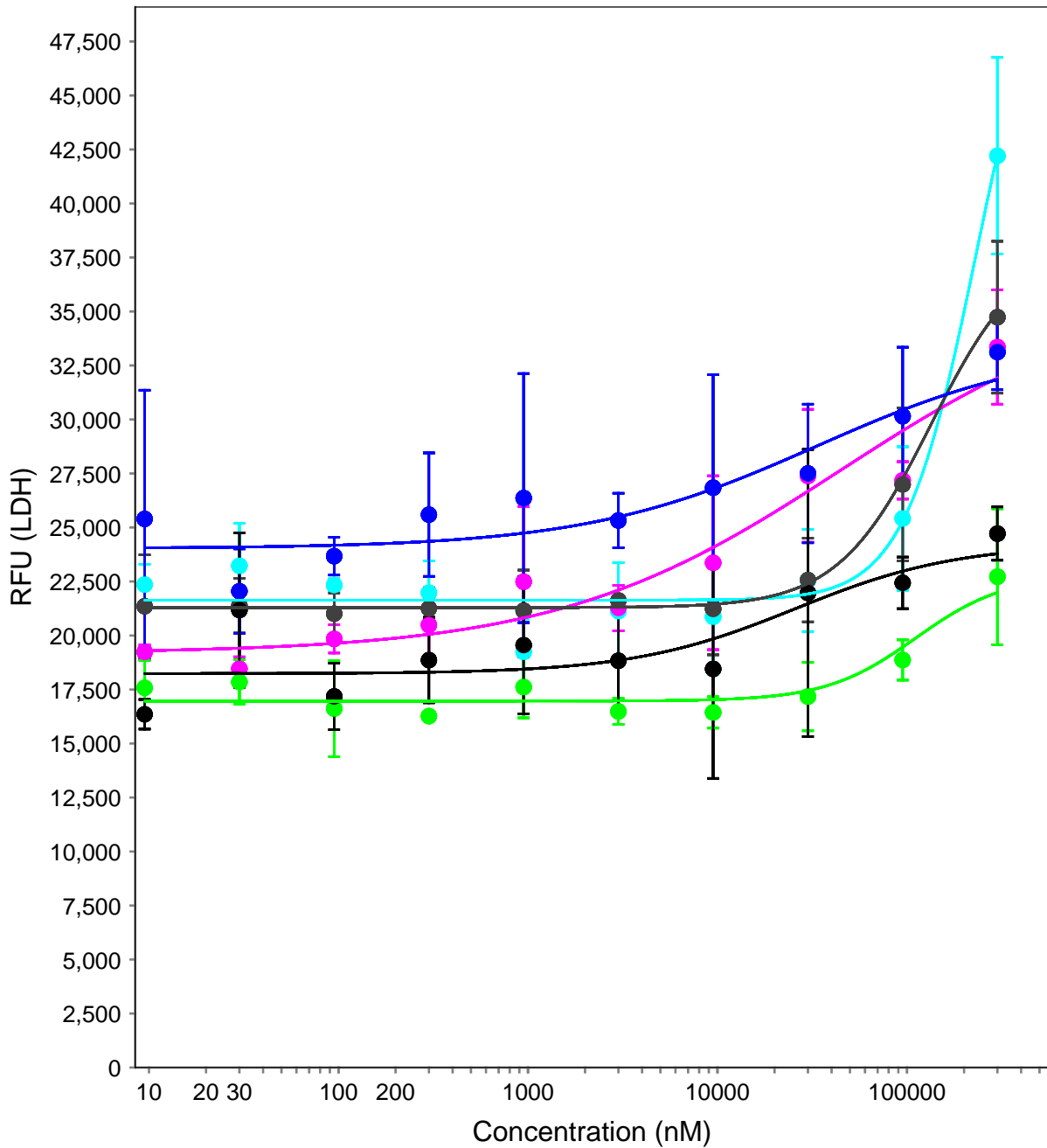
■	menadione 2D-DIFF-R1 LDH 48h EMAX: 96100 EMIN: 25600 EC50: 29500 R ² : 0.986
■	menadione 2D-DIFF-R2 LDH 48h EMAX: 144000 EMIN: 60500 EC50: 28400 R ² : 0.952
■	menadione 2D-DIFF-R3 LDH 48h EMAX: 1.20E5 EMIN: 28600 EC50: 23600 R ² : 0.995
■	menadione 2D-DIFF-R1 LDH 96h EMAX: 37800 EMIN: 26500 EC50: 10300 R ² : 0.165
■	menadione 2D-DIFF-R2 LDH 96h EMAX: 34300 EMIN: 20900 EC50: 10300 R ² : 0.190
■	menadione 2D-DIFF-R3 LDH 96h EMAX: 29700 EMIN: 19400 EC50: 10900 R ² : 0.499

Supplementary Data S3 - LDH Leakage Data



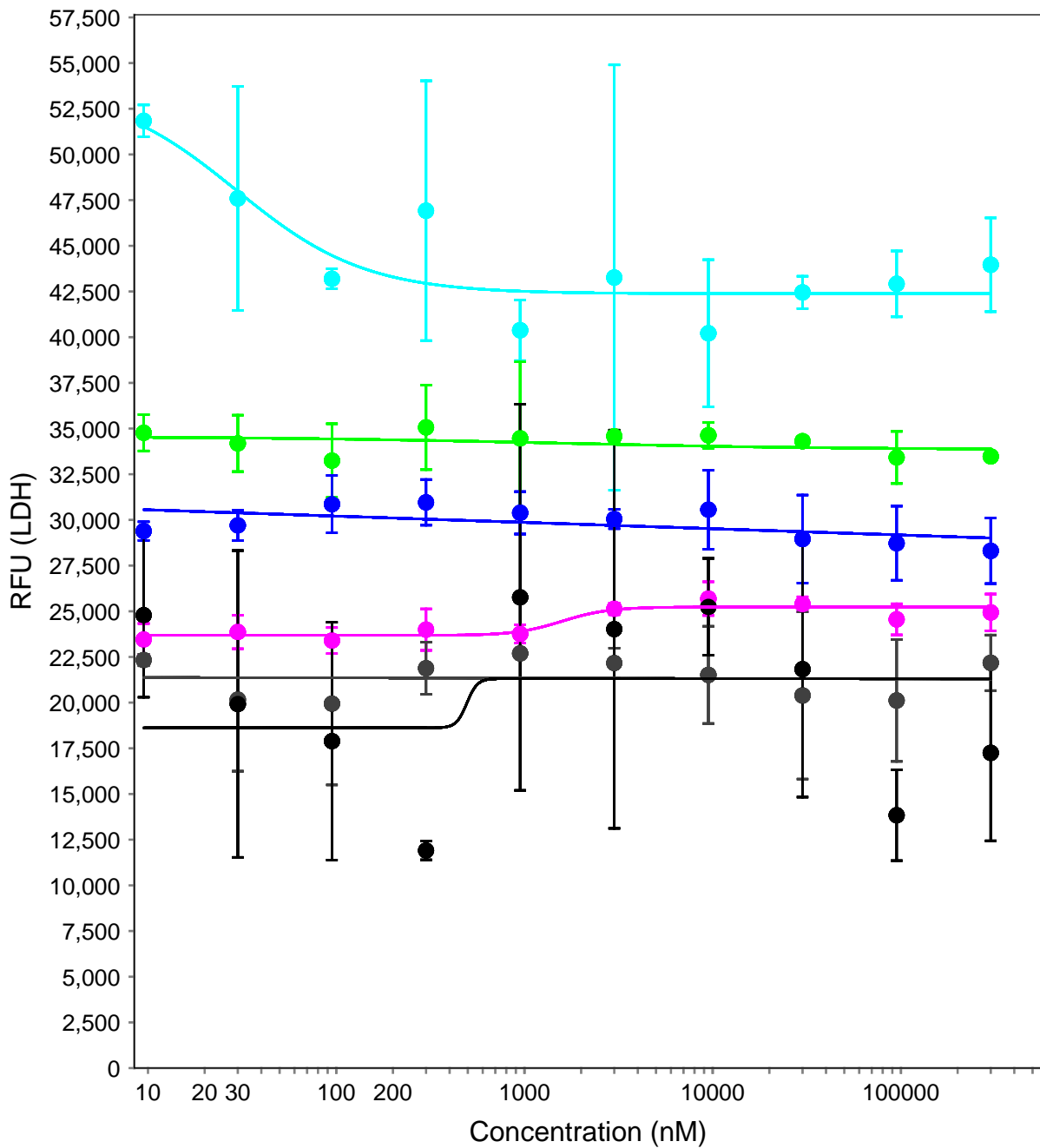
■	menadione PROLIF-R1 LDH 48h EMAX: 27700 EMIN: 17800 EC50: 2.60E4 R ² : 0.792
■	menadione PROLIF-R2 LDH 48h EMAX: 47900 EMIN: 25600 EC50: 26900 R ² : 0.995
■	menadione PROLIF-R3 LDH 48h EMAX: 38800 EMIN: 24800 EC50: 23600 R ² : 0.986
■	menadione PROLIF-R1 LDH 96h EMAX: 24100 EMIN: 15500 EC50: 739 R ² : 0.0831
■	menadione PROLIF-R2 LDH 96h EMAX: 39700 EMIN: 25800 EC50: 1830 R ² : 0.0591
■	menadione PROLIF-R3 LDH 96h EMAX: 26200 EMIN: 21700 EC50: 2.20E4 R ² : 0.516

Supplementary Data S3 - LDH Leakage Data



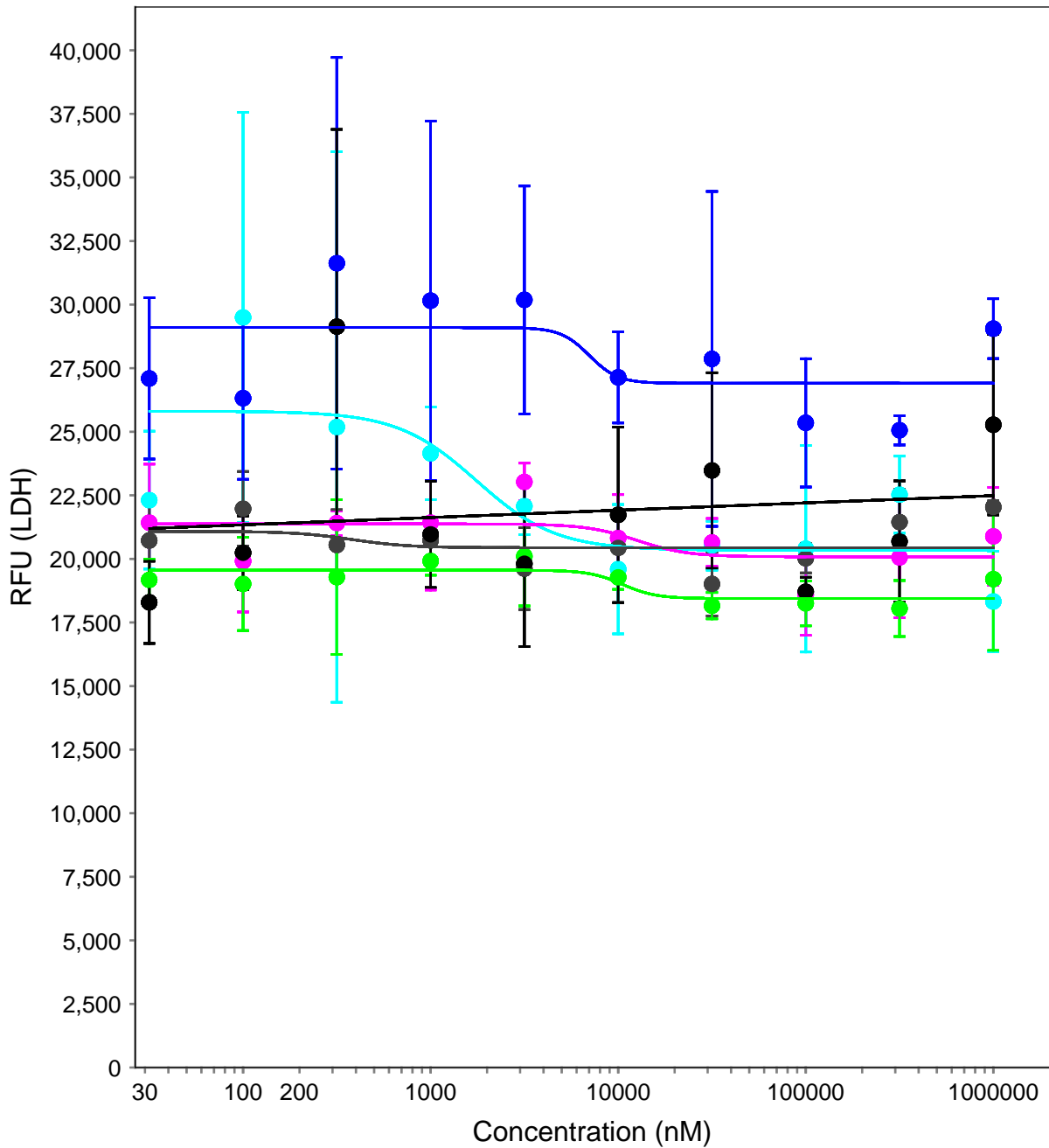
■	omeprazole 2D-DIFF-R1 LDH 48h EMAX: 24300 EMIN: 18200 EC50: 25800 R ² : 0.696
■	omeprazole 2D-DIFF-R2 LDH 48h EMAX: 33500 EMIN: 2.40E4 EC50: 33400 R ² : 0.851
■	omeprazole 2D-DIFF-R3 LDH 48h EMAX: 22800 EMIN: 1.70E4 EC50: 111000 R ² : 0.887
■	omeprazole 2D-DIFF-R1 LDH 96h EMAX: 38200 EMIN: 21300 EC50: 134000 R ² : 0.998
■	omeprazole 2D-DIFF-R2 LDH 96h EMAX: 36200 EMIN: 19200 EC50: 44900 R ² : 0.934
■	omeprazole 2D-DIFF-R3 LDH 96h EMAX: 53600 EMIN: 21600 EC50: 231000 R ² : 0.972

Supplementary Data S3 - LDH Leakage Data



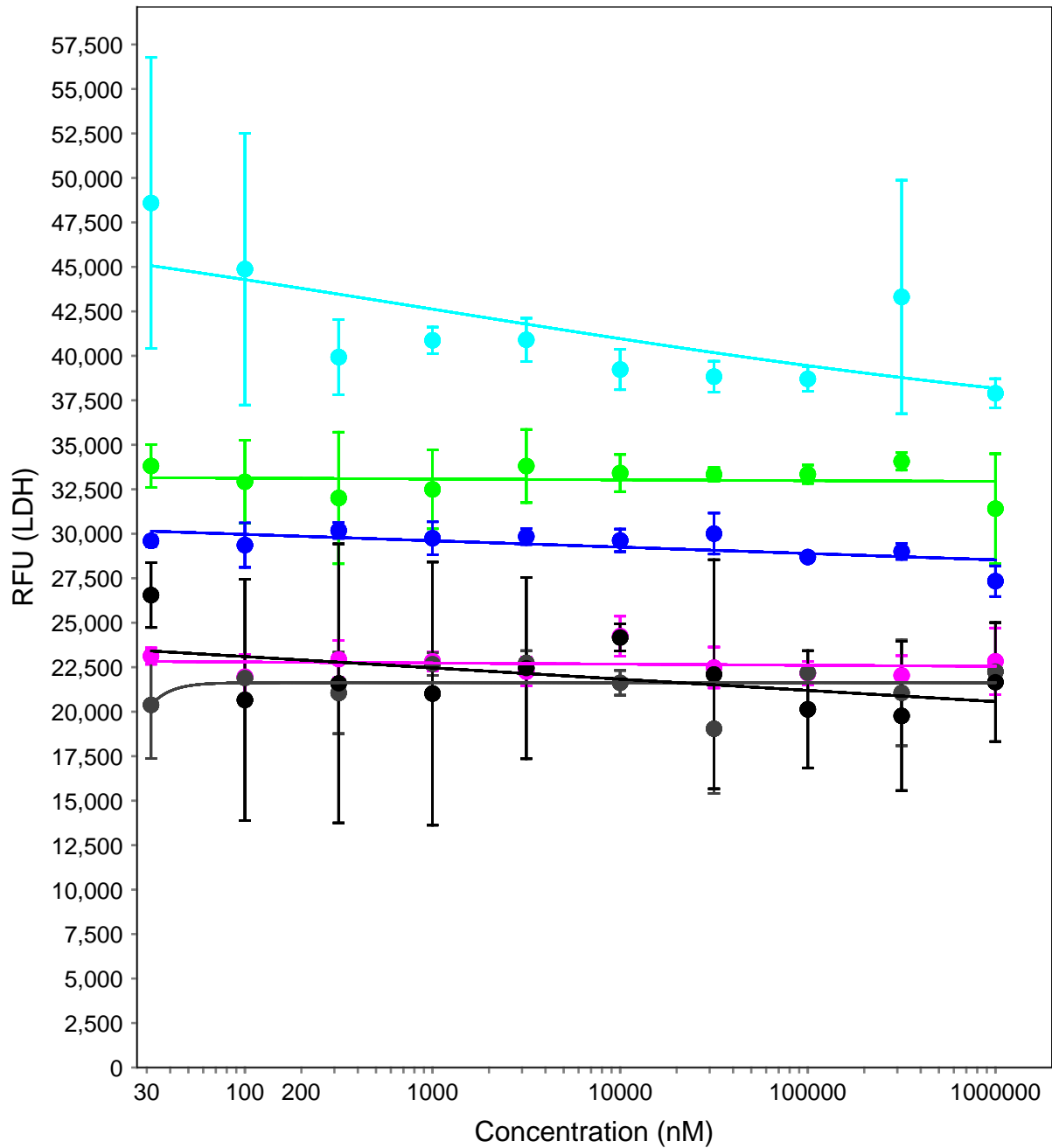
■	omeprazole PROLIF-R1 LDH 48h EMAX: 21300 EMIN: 18600 EC50: 494 R ² : 0.0799
■	omeprazole PROLIF-R2 LDH 48h EMAX: 54200 EMIN: 5540 EC50: 838 R ² : 0.299
■	omeprazole PROLIF-R3 LDH 48h EMAX: 34600 EMIN: 33800 EC50: 1520 R ² : 0.0940
■	omeprazole PROLIF-R1 LDH 96h EMAX: 21500 EMIN: 21200 EC50: 1940 R ² : 2.81E-4
■	omeprazole PROLIF-R2 LDH 96h EMAX: 25200 EMIN: 23700 EC50: 1580 R ² : 0.829
■	omeprazole PROLIF-R3 LDH 96h EMAX: 53700 EMIN: 42400 EC50: 29.4 R ² : 0.733

Supplementary Data S3 - LDH Leakage Data



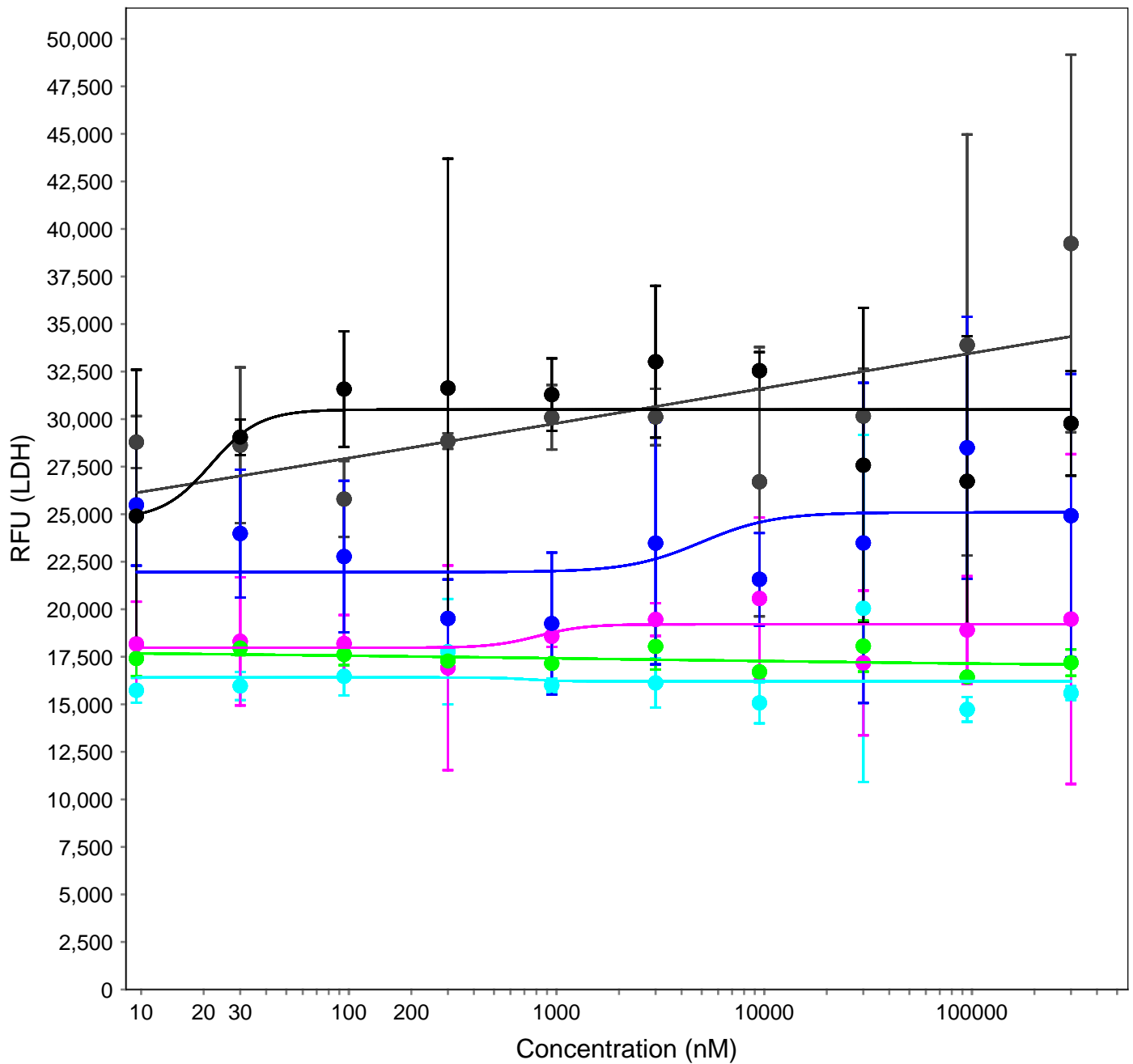
■	phenobarbital 2D-DIFF-R1 LDH 48h EMAX: 27100 EMIN: 16400 EC50: 1950 R ² : 0.0164
■	phenobarbital 2D-DIFF-R2 LDH 48h EMAX: 29100 EMIN: 26900 EC50: 7010 R ² : 0.272
■	phenobarbital 2D-DIFF-R3 LDH 48h EMAX: 19600 EMIN: 18400 EC50: 10500 R ² : 0.585
■	phenobarbital 2D-DIFF-R1 LDH 96h EMAX: 21100 EMIN: 20400 EC50: 381 R ² : 0.113
■	phenobarbital 2D-DIFF-R2 LDH 96h EMAX: 21400 EMIN: 20100 EC50: 12600 R ² : 0.347
■	phenobarbital 2D-DIFF-R3 LDH 96h EMAX: 25800 EMIN: 20300 EC50: 1760 R ² : 0.612

Supplementary Data S3 - LDH Leakage Data



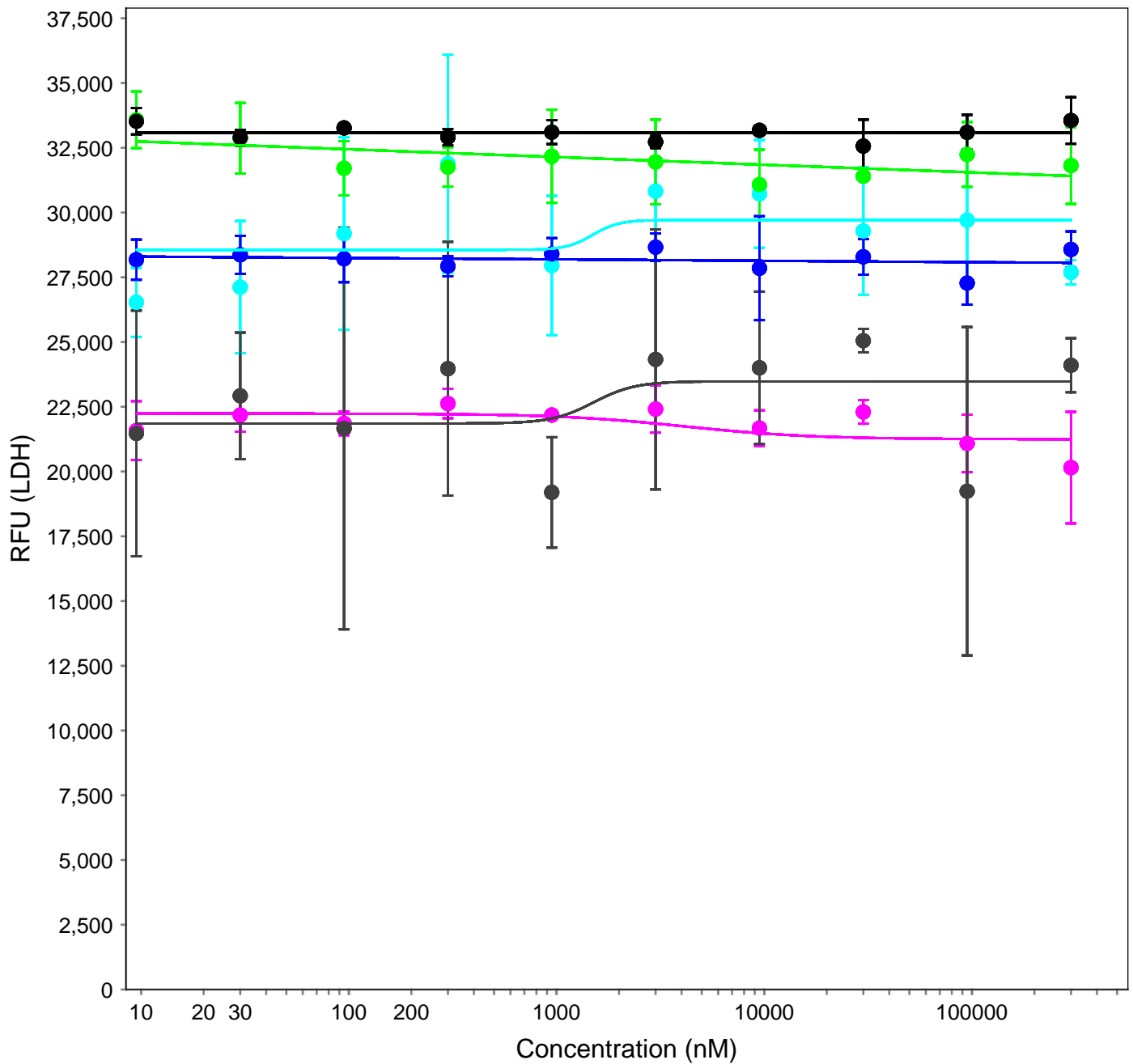
■	phenobarbital		PROLIF-R1		LDH		48h		EMAX: 36100		EMIN: 8240		EC50: 2960		R ² : 0.225
■	phenobarbital		PROLIF-R2		LDH		48h		EMAX: 54100		EMIN: 4470		EC50: 7220		R ² : 0.426
■	phenobarbital		PROLIF-R3		LDH		48h		EMAX: 33700		EMIN: 32400		EC50: 3540		R ² : 0.00931
■	phenobarbital		PROLIF-R1		LDH		96h		EMAX: 21600		EMIN: 9950		EC50: 19.6		R ² : 0.115
■	phenobarbital		PROLIF-R2		LDH		96h		EMAX: 34500		EMIN: 10900		EC50: 1470		R ² : 0.0193
■	phenobarbital		PROLIF-R3		LDH		96h		EMAX: 50400		EMIN: 34900		EC50: 1010		R ² : 0.454

Supplementary Data S3 - LDH Leakage Data



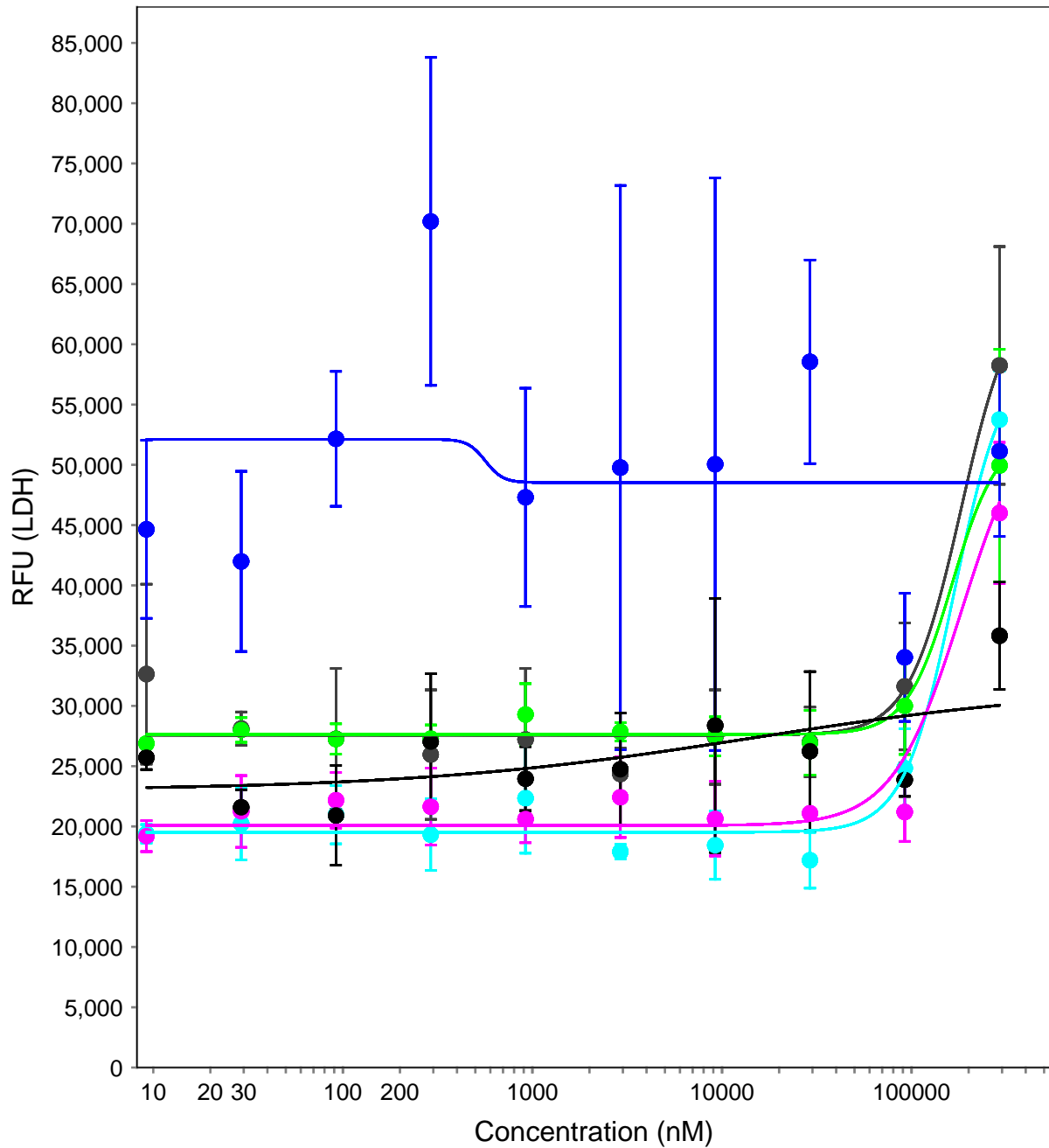
■	potassium chloride 2D-DIFF-R1 LDH 48h EMAX: 30500 EMIN: 24700 EC50: 21.7 R ² : 0.436
■	potassium chloride 2D-DIFF-R2 LDH 48h EMAX: 25100 EMIN: 2.20E4 EC50: 4980 R ² : 0.209
■	potassium chloride 2D-DIFF-R3 LDH 48h EMAX: 17900 EMIN: 16800 EC50: 2.10E3 R ² : 0.142
■	potassium chloride 2D-DIFF-R1 LDH 96h EMAX: 54500 EMIN: 8150 EC50: 6910 R ² : 0.489
■	potassium chloride 2D-DIFF R2 LDH 96h EMAX: 19200 EMIN: 1.80E4 EC50: 813 R ² : 0.292
■	potassium chloride 2D-DIFF-R3 LDH 96h EMAX: 16400 EMIN: 16200 EC50: 732 R ² : 0.00299

Supplementary Data S3 - LDH Leakage Data



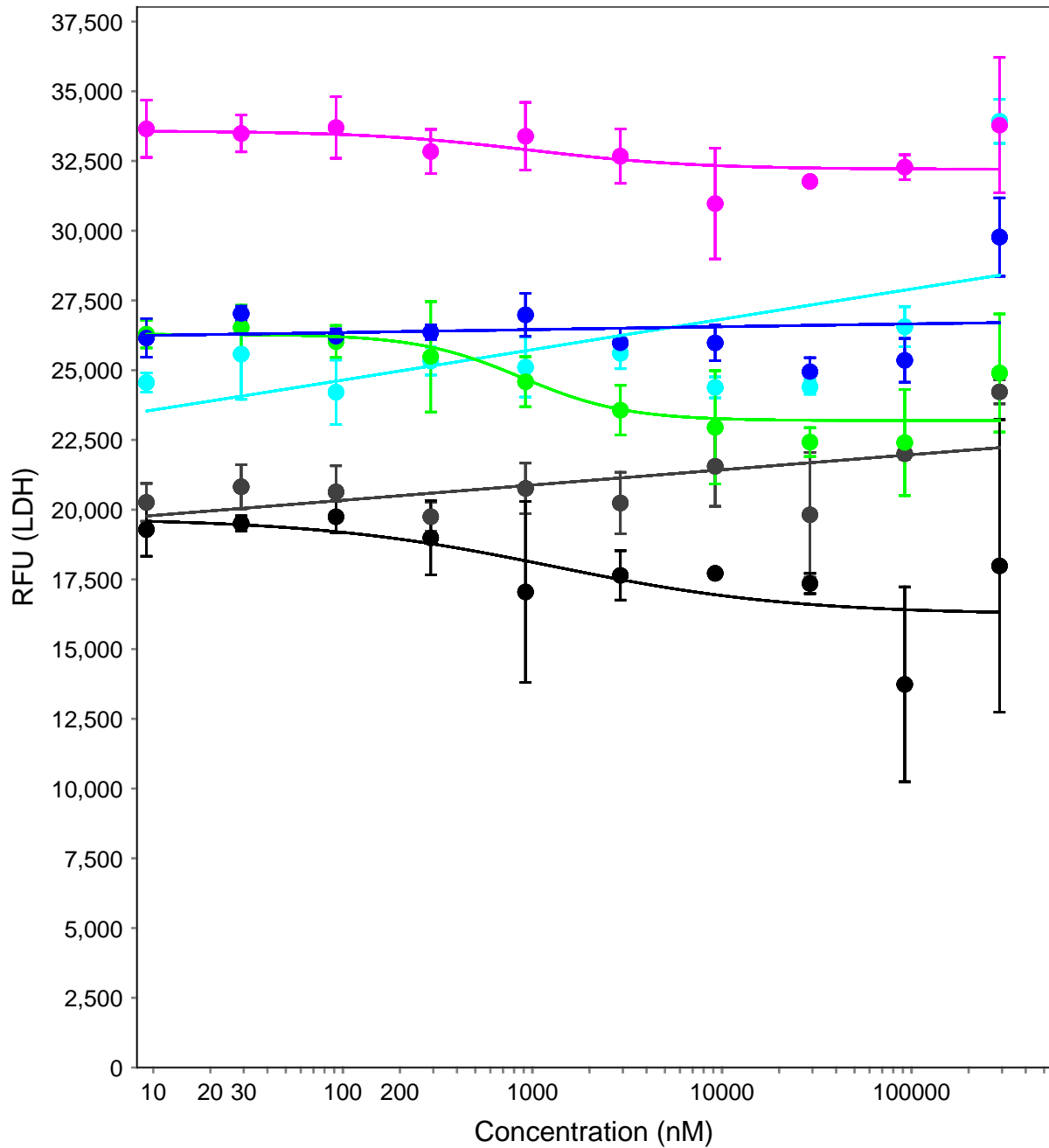
■	potassium chloride PROLIF-R1 LDH 48h EMAX: 3.60E4 EMIN: 30200 EC50: 2240 R^2: -5.27E-4
■	potassium chloride PROLIF-R2 LDH 48h EMAX: 28800 EMIN: 27600 EC50: 1240 R^2: 0.0269
■	potassium chloride PROLIF-R3 LDH 48h EMAX: 39900 EMIN: 25200 EC50: 30.0 R^2: 0.376
■	potassium chloride PROLIF-R1 LDH 96h EMAX: 23500 EMIN: 21900 EC50: 1510 R^2: 0.108
■	potassium chloride PROLIF-R2 LDH 96h EMAX: 22200 EMIN: 21200 EC50: 4140 R^2: 0.320
■	potassium chloride PROLIF-R3 LDH 96h EMAX: 29700 EMIN: 28600 EC50: 1490 R^2: 0.108

Supplementary Data S3 - LDH Leakage Data



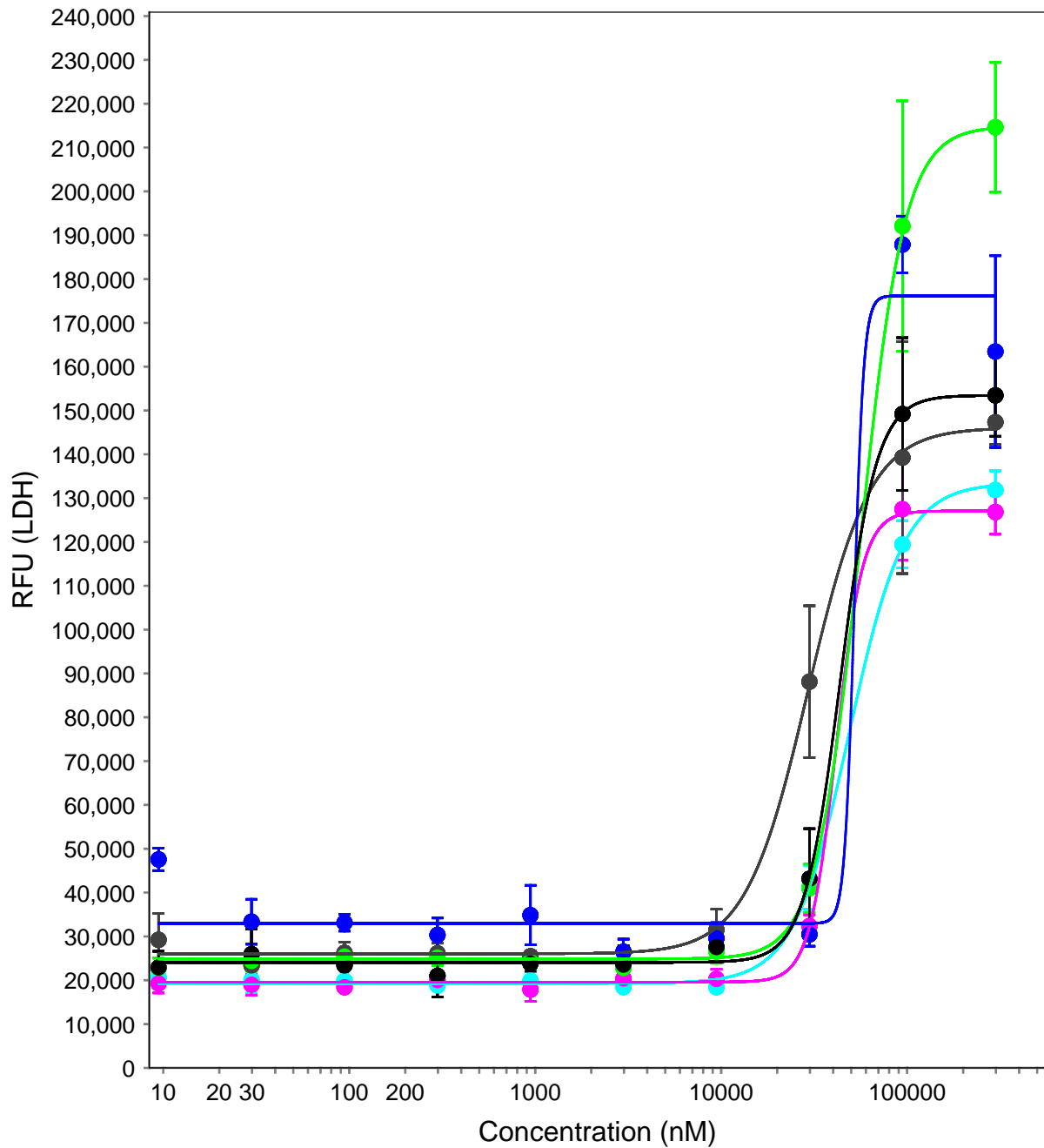
■	rifampicin		2D-DIFF-R1		LDH		48h		EMAX: 31700		EMIN: 2.30E4		EC50: 14600		R ² : 0.406
■	rifampicin		2D-DIFF-R2		LDH		48h		EMAX: 52100		EMIN: 48500		EC50: 565		R ² : 0.0401
■	rifampicin		2D-DIFF-R3		LDH		48h		EMAX: 52600		EMIN: 27600		EC50: 163000		R ² : 0.990
■	rifampicin		2D-DIFF-R1		LDH		96h		EMAX: 65200		EMIN: 27600		EC50: 183000		R ² : 0.955
■	rifampicin		2D-DIFF-R2		LDH		96h		EMAX: 55700		EMIN: 20100		EC50: 184000		R ² : 0.934
■	rifampicin		2D-DIFF-R3		LDH		96h		EMAX: 59400		EMIN: 19500		EC50: 168000		R ² : 0.981

Supplementary Data S3 - LDH Leakage Data



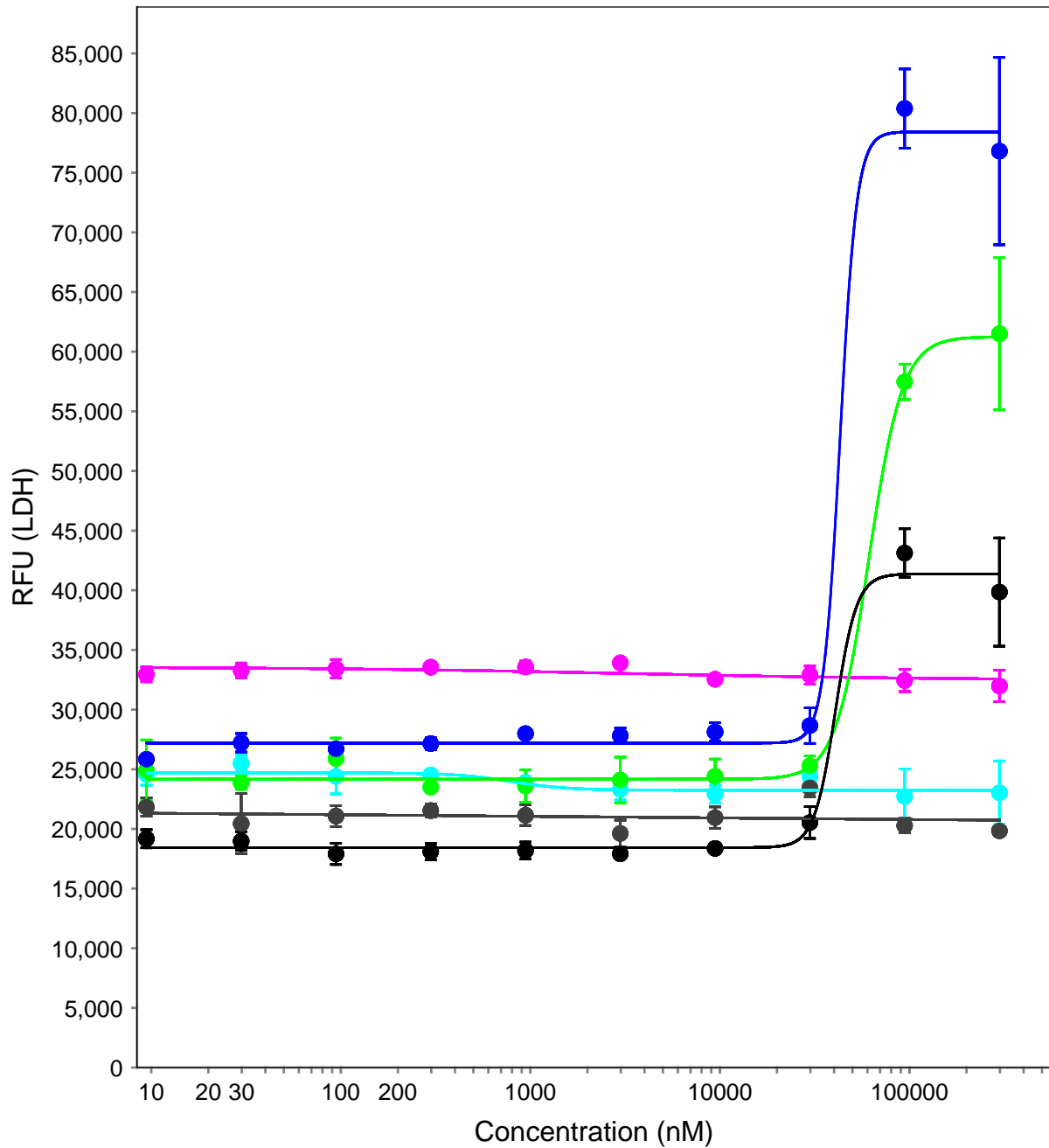
■	rifampicin	PROLIF-R1	LDH	48h	EMAX: 19700	EMIN: 16200	EC50: 1280	R ² : 0.537
■	rifampicin	PROLIF-R2	LDH	48h	EMAX: 27200	EMIN: 25700	EC50: 582	R ² : 0.0240
■	rifampicin	PROLIF-R3	LDH	48h	EMAX: 26300	EMIN: 23200	EC50: 875	R ² : 0.804
■	rifampicin	PROLIF-R1	LDH	96h	EMAX: 32300	EMIN: 9170	EC50: 592	R ² : 0.377
■	rifampicin	PROLIF-R2	LDH	96h	EMAX: 33600	EMIN: 32200	EC50: 971	R ² : 0.364
■	rifampicin	PROLIF-R3	LDH	96h	EMAX: 39400	EMIN: 12600	EC50: 1740	R ² : 0.323

Supplementary Data S3 - LDH Leakage Data



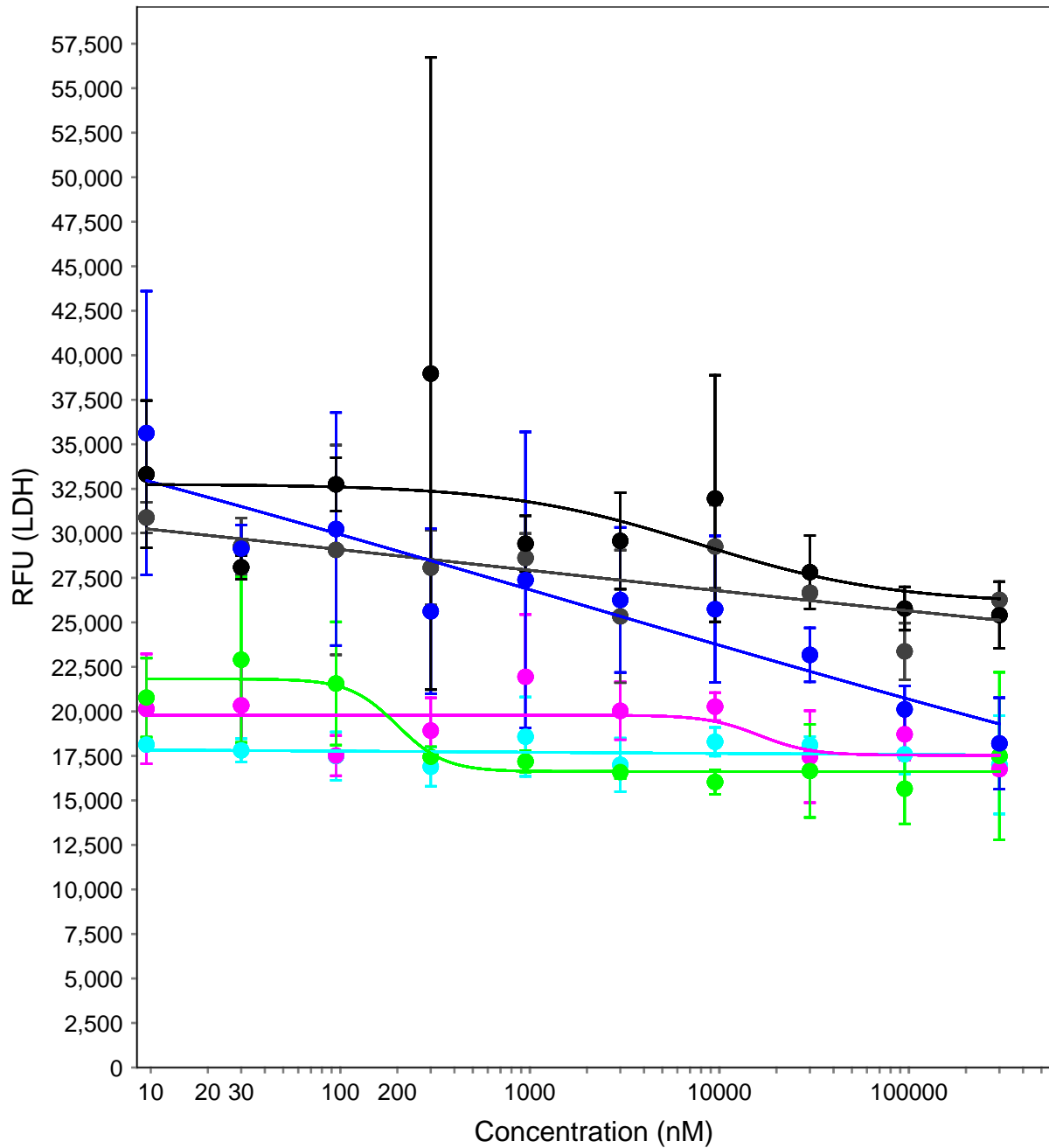
■	ritonavir 2D-DIFF-R1 LDH 48h EMAX: 153000 EMIN: 24100 EC50: 43800 R ² : 0.999
■	ritonavir 2D-DIFF-R2 LDH 48h EMAX: 176000 EMIN: 3.30E4 EC50: 51900 R ² : 0.982
■	ritonavir 2D-DIFF-R3 LDH 48h EMAX: 215000 EMIN: 24900 EC50: 55800 R ² : 1.00
■	ritonavir 2D-DIFF-R1 LDH 96h EMAX: 146000 EMIN: 2.60E4 EC50: 29300 R ² : 0.999
■	ritonavir 2D-DIFF-R2 LDH 96h EMAX: 127000 EMIN: 19600 EC50: 41500 R ² : 1.00
■	ritonavir 2D-DIFF-R3 LDH 96h EMAX: 133000 EMIN: 19300 EC50: 48700 R ² : 1.00

Supplementary Data S3 - LDH Leakage Data



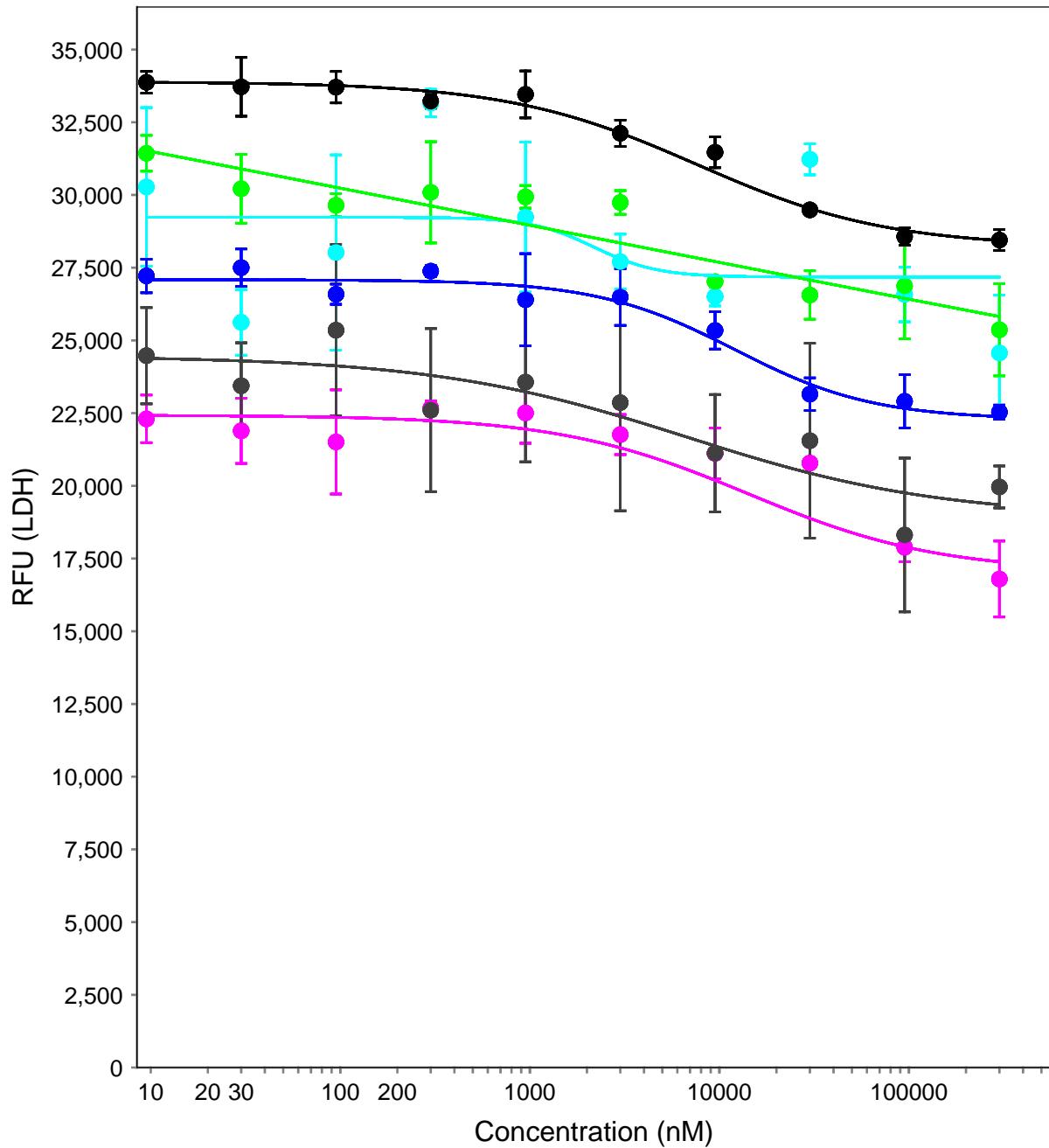
■	ritonavir PROLIF-R1 LDH 48h EMAX: 41400 EMIN: 18400 EC50: 40700 R ² : 0.992
■	ritonavir PROLIF-R2 LDH 48h EMAX: 78400 EMIN: 27200 EC50: 4.30E4 R ² : 0.998
■	ritonavir PROLIF-R3 LDH 48h EMAX: 61300 EMIN: 24200 EC50: 61100 R ² : 0.998
■	ritonavir PROLIF-R1 LDH 96h EMAX: 21800 EMIN: 20300 EC50: 998 R ² : 0.0275
■	ritonavir PROLIF-R2 LDH 96h EMAX: 33600 EMIN: 32500 EC50: 3.40E3 R ² : 0.435
■	ritonavir PROLIF-R3 LDH 96h EMAX: 24700 EMIN: 23200 EC50: 794 R ² : 0.653

Supplementary Data S3 - LDH Leakage Data



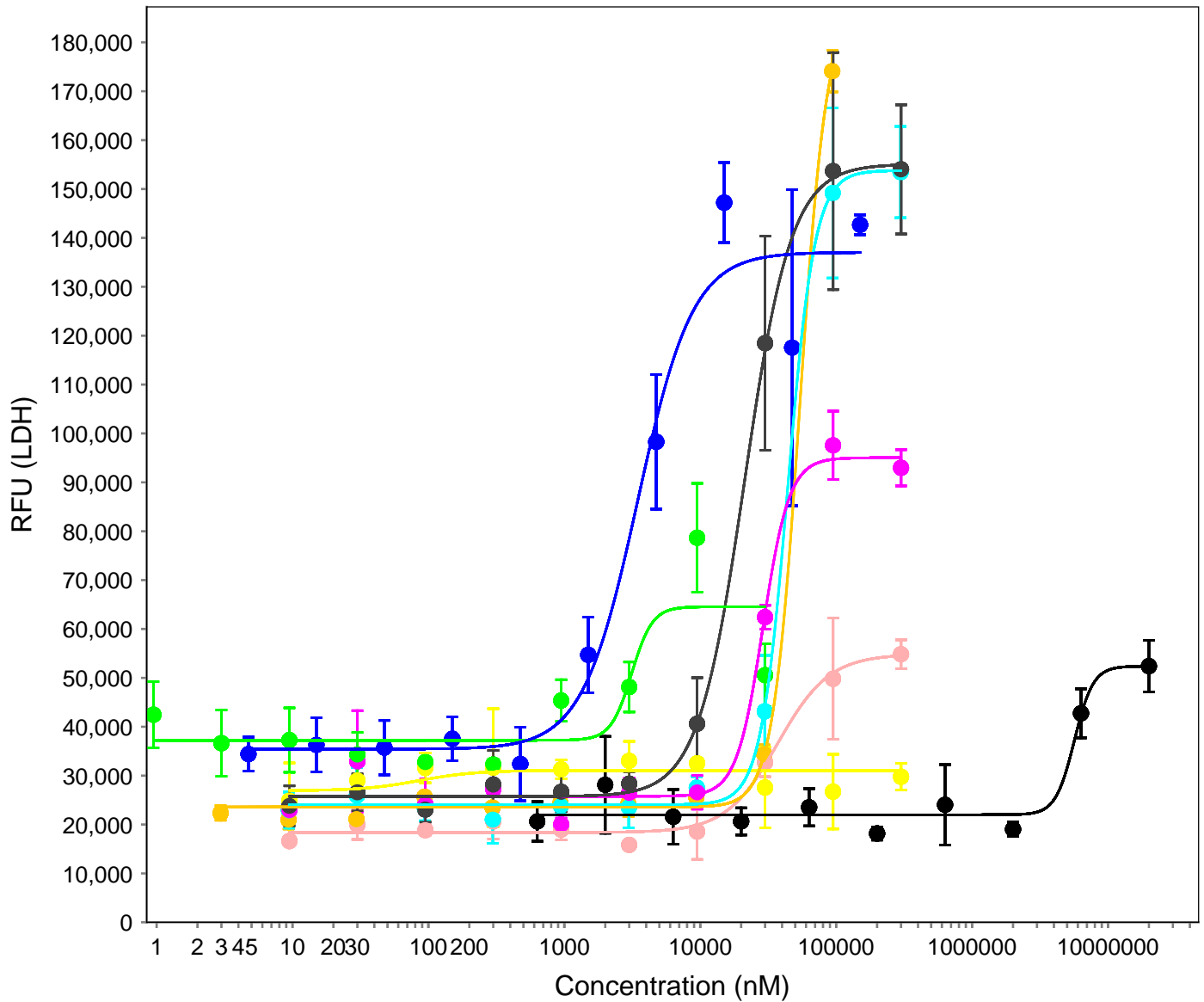
■	rosiglitazone 2D-DIFF-R1 LDH 48h EMAX: 32800 EMIN: 2.60E4 EC50: 7770 R ² : 0.452
■	rosiglitazone 2D-DIFF-R2 LDH 48h EMAX: 49300 EMIN: 3090 EC50: 1620 R ² : 0.875
■	rosiglitazone 2D-DIFF-R3 LDH 48h EMAX: 21800 EMIN: 16600 EC50: 200. R ² : 0.920
■	rosiglitazone 2D-DIFF-R1 LDH 96h EMAX: 38800 EMIN: 17400 EC50: 666 R ² : 0.599
■	rosiglitazone 2D-DIFF-R2 LDH 96h EMAX: 19800 EMIN: 17500 EC50: 16200 R ² : 0.415
■	rosiglitazone 2D-DIFF-R3 LDH 96h EMAX: 1.80E4 EMIN: 17400 EC50: 1.90E3 R ² : 0.030

Supplementary Data S3 - LDH Leakage Data



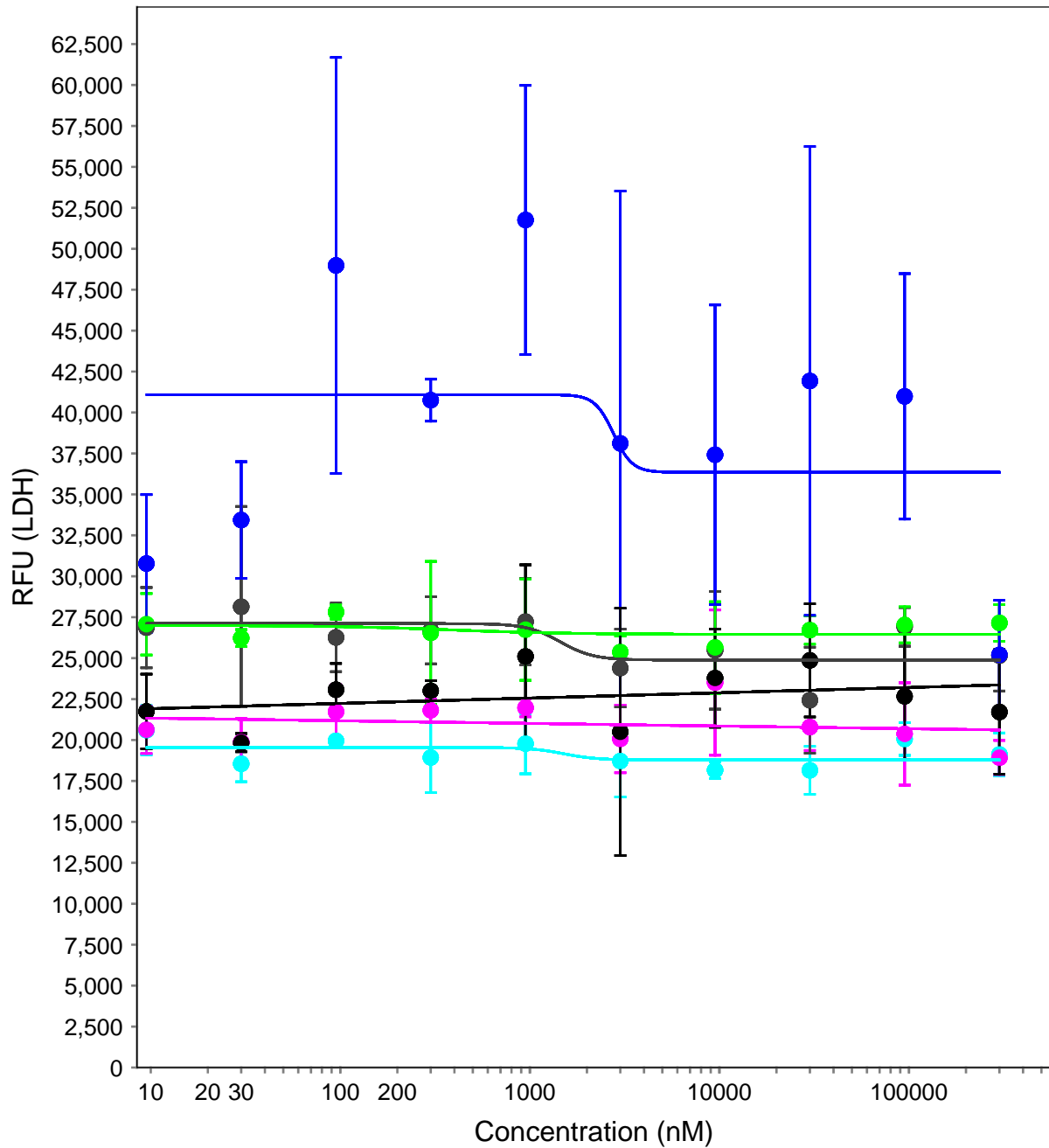
■	rosiglitazone PROLIF-R1 LDH 48h EMAX: 33900 EMIN: 28200 EC50: 7610 R ² : 0.982
■	rosiglitazone PROLIF-R2 LDH 48h EMAX: 27100 EMIN: 22300 EC50: 12100 R ² : 0.968
■	rosiglitazone PROLIF-R3 LDH 48h EMAX: 47200 EMIN: 10400 EC50: 1350 R ² : 0.864
■	rosiglitazone PROLIF-R1 LDH 96h EMAX: 24500 EMIN: 18900 EC50: 6670 R ² : 0.809
■	rosiglitazone PROLIF-R2 LDH 96h EMAX: 22400 EMIN: 1.70E4 EC50: 14200 R ² : 0.818
■	rosiglitazone PROLIF-R3 LDH 96h EMAX: 29200 EMIN: 27200 EC50: 2180 R ² : 0.146

Supplementary Data S3 - LDH Leakage Data



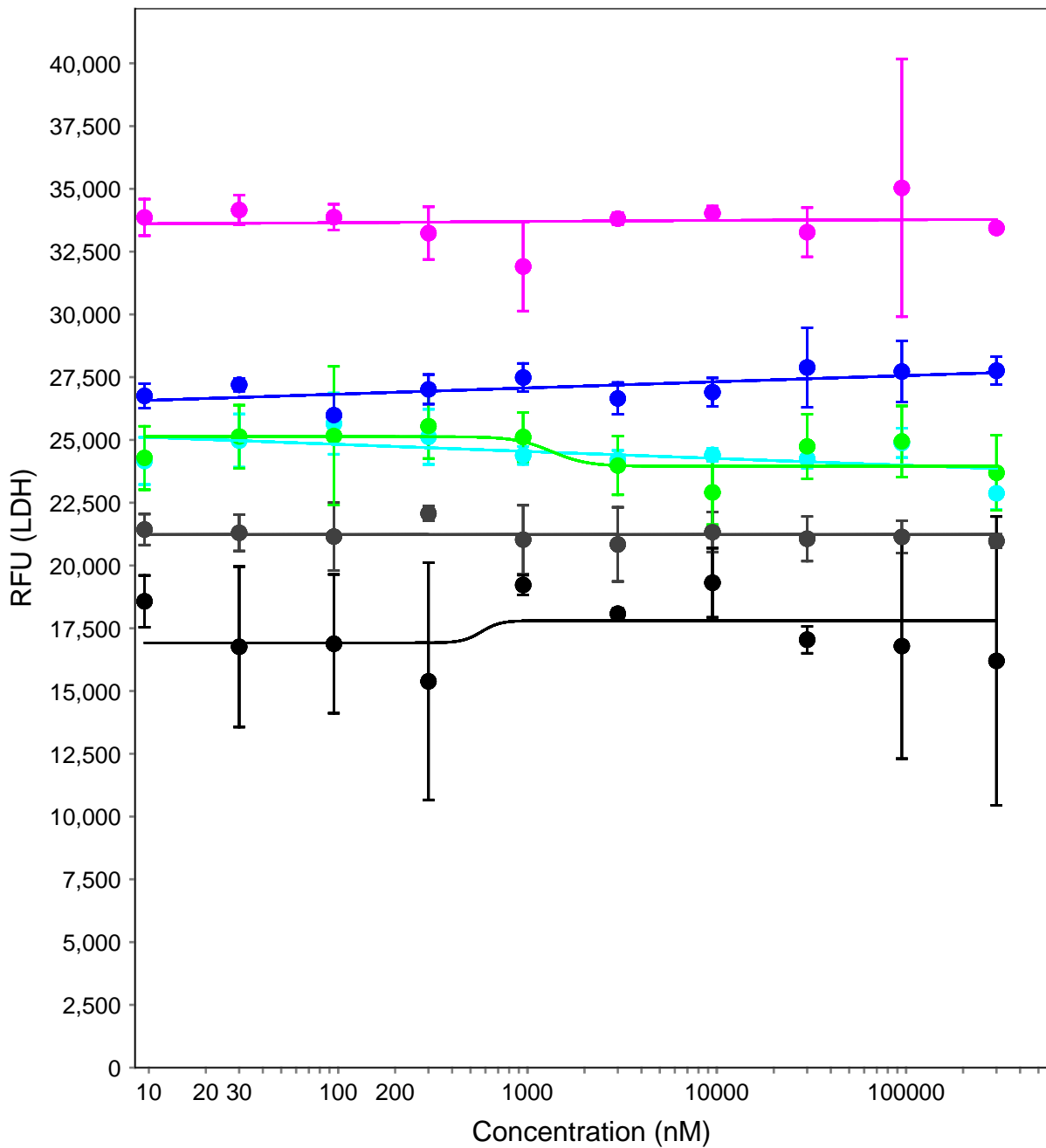
- acetaminophen | 2D-DIFF-R1 | LDH | 48h | EMAX: 52400 | EMIN: 2.20E4 | EC50: 5660000 | R²: 0.938
- aflatoxin B1 | 2D-DIFF-R1 | LDH | 48h | EMAX: 137000 | EMIN: 35400 | EC50: 3470 | R²: 0.967
- benzo(a)pyrene | 2D-DIFF-R1 | LDH | 48h | EMAX: 64600 | EMIN: 37200 | EC50: 3130 | R²: 0.684
- chlorpromazine | 2D-DIFF-R1 | LDH | 48h | EMAX: 155000 | EMIN: 25700 | EC50: 21200 | R²: 0.999
- menadione | 2D-DIFF-R1 | LDH | 48h | EMAX: 9.50E4 | EMIN: 25800 | EC50: 28900 | R²: 0.986
- ritonavir | 2D-DIFF-R1 | LDH | 48h | EMAX: 154000 | EMIN: 2.40E4 | EC50: 4.40E4 | R²: 0.999
- tamoxifen | 2D-DIFF-R1 | LDH | 48h | EMAX: 188000 | EMIN: 23600 | EC50: 54100 | R²: 0.999
- potassium chloride | 2D-DIFF-R1 | LDH | 48h | EMAX: 31100 | EMIN: 26900 | EC50: 85.4 | R²: 0.203
- trovafloxacin | 2D-DIFF-R1 | LDH | 48h | EMAX: 54800 | EMIN: 18400 | EC50: 37100 | R²: 0.988

Supplementary Data S3 - LDH Leakage Data



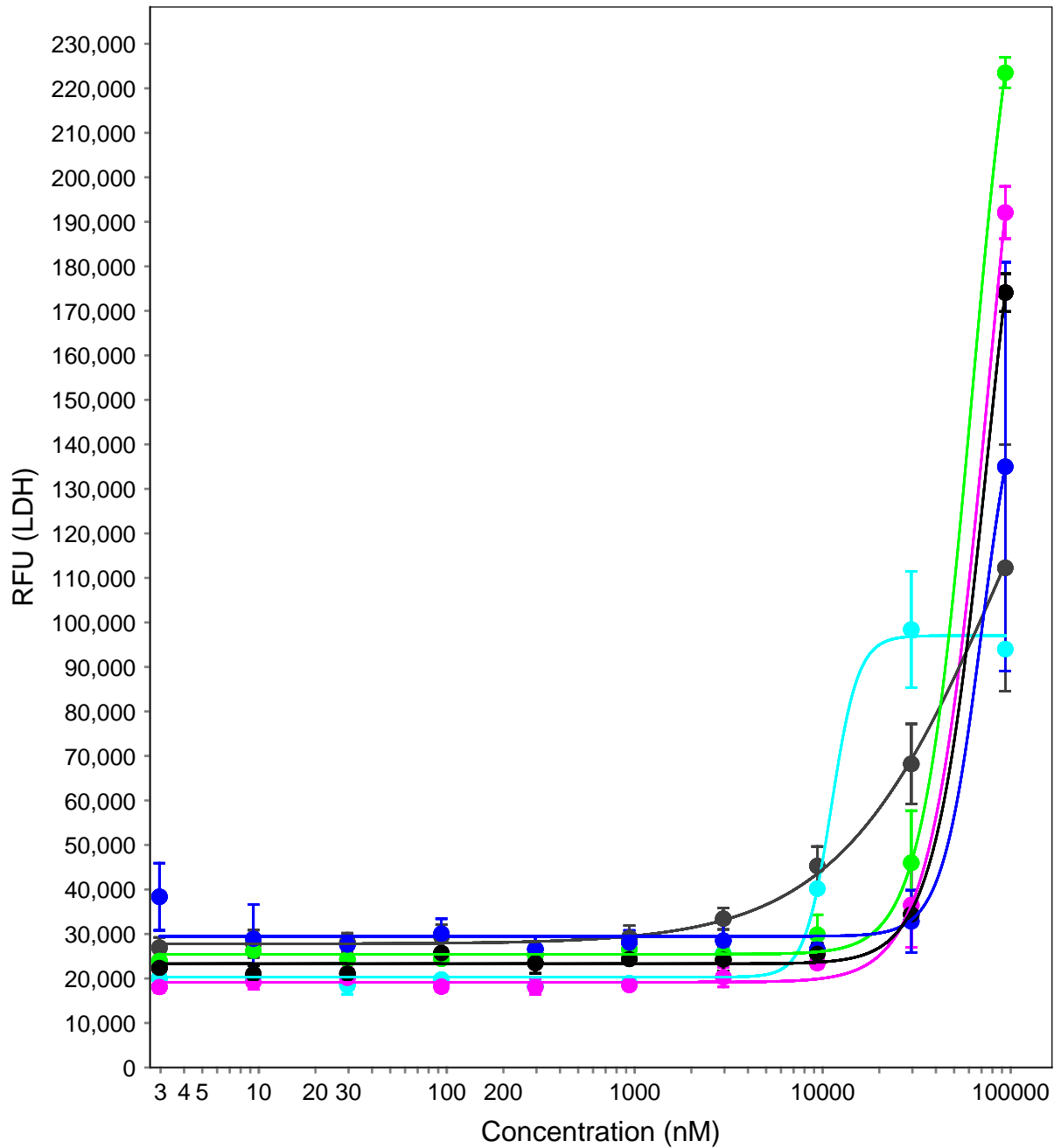
■	sucrose 2D-DIFF-R1 LDH 48h EMAX: 31900 EMIN: 13300 EC50: 1590 R ² : 0.0778
■	sucrose 2D-DIFF-R2 LDH 48h EMAX: 41100 EMIN: 36300 EC50: 2760 R ² : 0.0894
■	sucrose 2D-DIFF-R3 LDH 48h EMAX: 2.70E4 EMIN: 26500 EC50: 385 R ² : 0.114
■	sucrose 2D-DIFF-R1 LDH 96h EMAX: 27100 EMIN: 24900 EC50: 1450 R ² : 0.470
■	sucrose 2D-DIFF-R2 LDH 96h EMAX: 33900 EMIN: 8190 EC50: 593 R ² : 0.0347
■	sucrose 2D-DIFF-R3 LDH 96h EMAX: 19500 EMIN: 18800 EC50: 1510 R ² : 0.191

Supplementary Data S3 - LDH Leakage Data



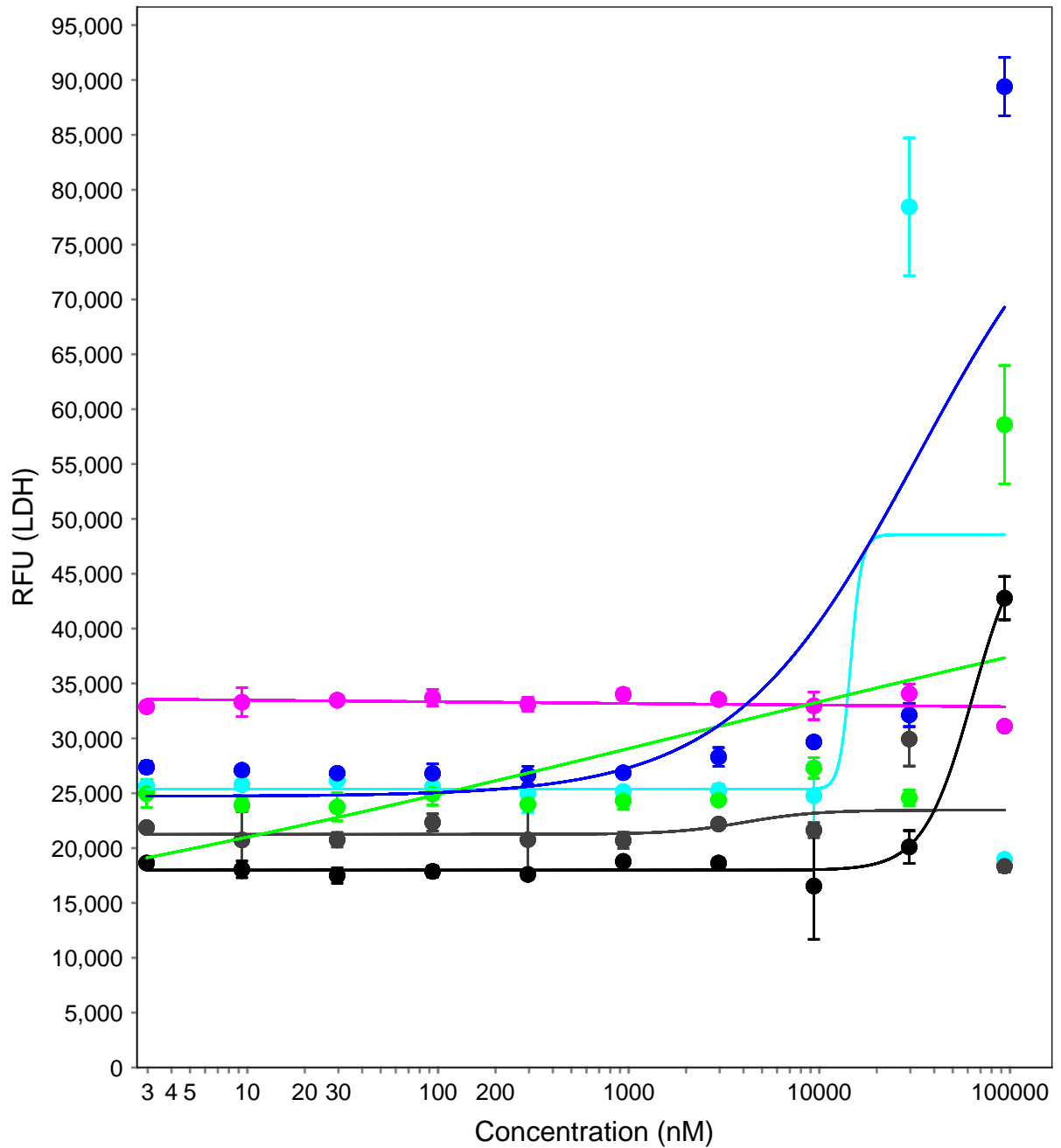
■	sucrose PROLIF-R1 LDH 48h EMAX: 17800 EMIN: 16900 EC50: 571 R ² : 0.116
■	sucrose PROLIF-R2 LDH 48h EMAX: 3.10E4 EMIN: 23100 EC50: 750. R ² : 0.420
■	sucrose PROLIF-R3 LDH 48h EMAX: 25100 EMIN: 2.40E4 EC50: 1340 R ² : 0.391
■	sucrose PROLIF-R1 LDH 96h EMAX: 34600 EMIN: 7910 EC50: 2040 R ² : -2.90E-6
■	sucrose PROLIF-R2 LDH 96h EMAX: 33800 EMIN: 33600 EC50: 402 R ² : -2.18E-5
■	sucrose PROLIF-R3 LDH 96h EMAX: 29100 EMIN: 20700 EC50: 55.0 R ² : 0.278

Supplementary Data S3 - LDH Leakage Data



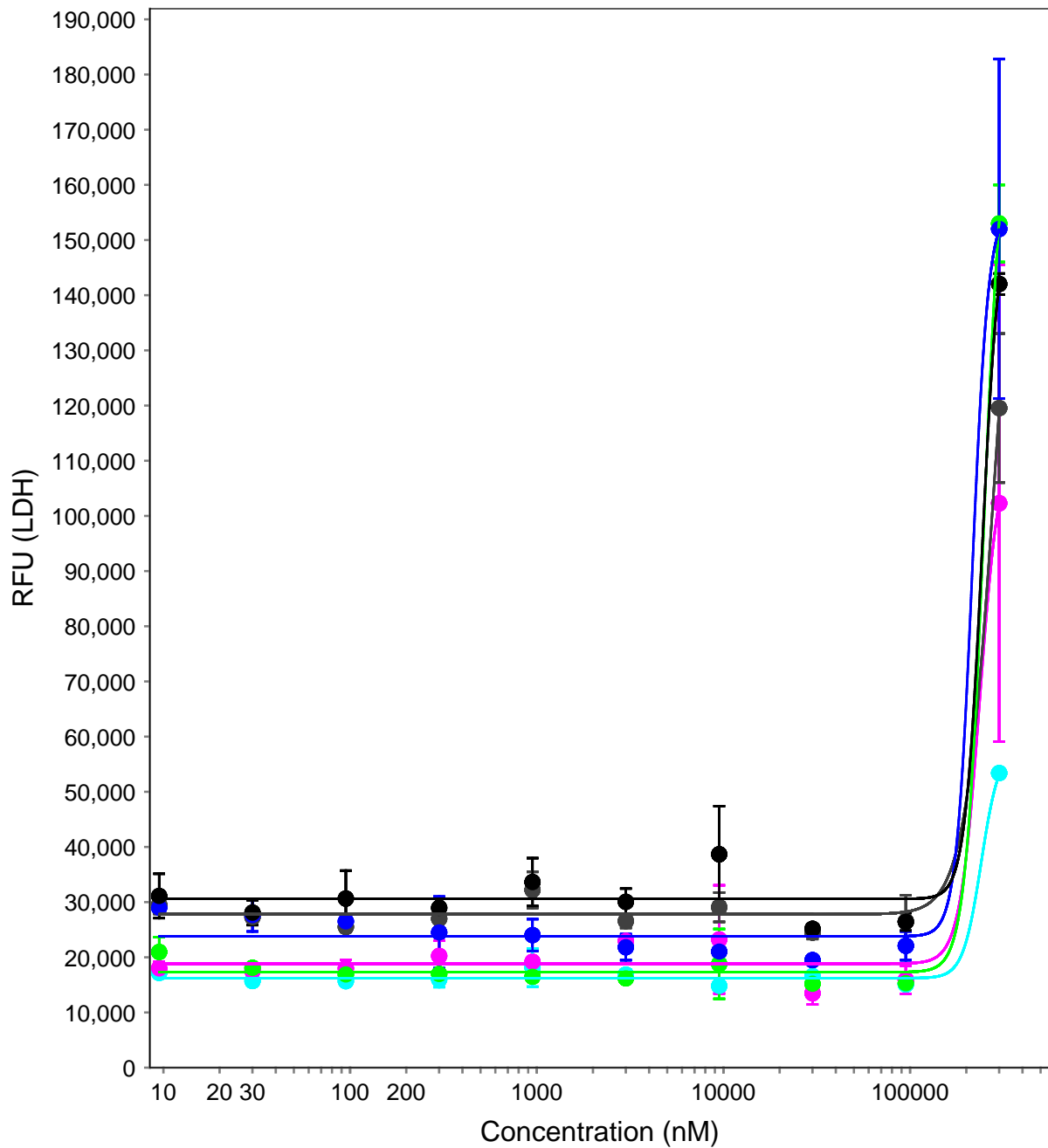
■	tamoxifen		2D-DIFF-R1		LDH		48h		EMAX: 251000		EMIN: 23300		EC50: 75300		R ² : 0.999
■	tamoxifen		2D-DIFF-R2		LDH		48h		EMAX: 167000		EMIN: 29500		EC50: 70200		R ² : 0.990
■	tamoxifen		2D-DIFF-R3		LDH		48h		EMAX: 276000		EMIN: 25500		EC50: 62300		R ² : 0.999
■	tamoxifen		2D-DIFF-R1		LDH		96h		EMAX: 196000		EMIN: 27800		EC50: 90600		R ² : 0.998
■	tamoxifen		2D-DIFF-R2		LDH		96h		EMAX: 295000		EMIN: 19200		EC50: 77800		R ² : 0.999
■	tamoxifen		2D-DIFF-R3		LDH		96h		EMAX: 9.70E4		EMIN: 20300		EC50: 11100		R ² : 0.995

Supplementary Data S3 - LDH Leakage Data



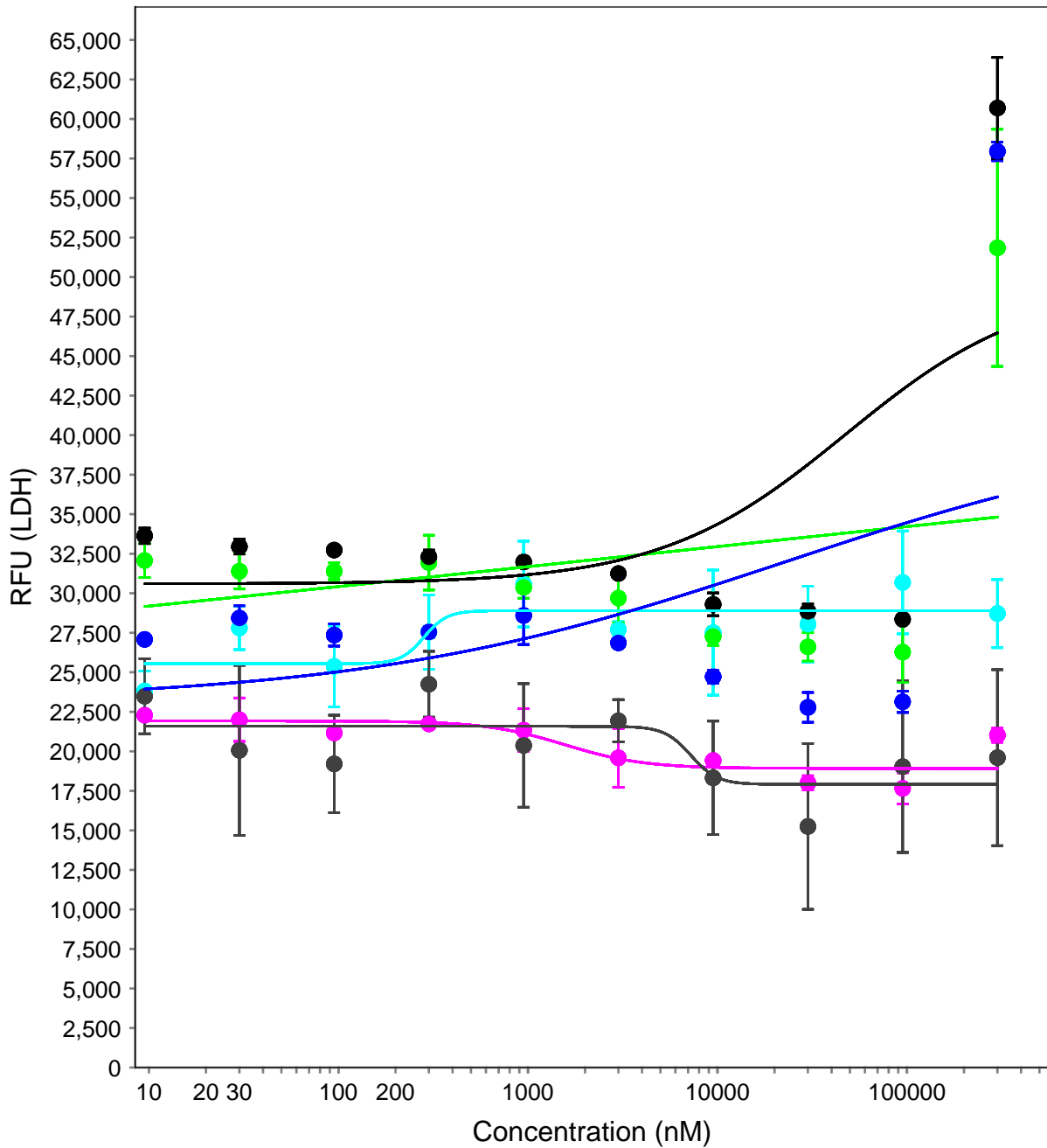
■	tamoxifen PROLIF-R1 LDH 48h EMAX: 49600 EMIN: 1.80E4 EC50: 63600 R^2: 0.993
■	tamoxifen PROLIF-R2 LDH 48h EMAX: 86800 EMIN: 24700 EC50: 32900 R^2: 0.699
■	tamoxifen PROLIF-R3 LDH 48h EMAX: 56600 EMIN: 4530 EC50: 2260 R^2: 0.309
■	tamoxifen PROLIF-R1 LDH 96h EMAX: 23500 EMIN: 21300 EC50: 4060 R^2: 0.114
■	tamoxifen PROLIF-R2 LDH 96h EMAX: 39300 EMIN: 27400 EC50: 114 R^2: 0.0761
■	tamoxifen PROLIF-R3 LDH 96h EMAX: 48600 EMIN: 25400 EC50: 14600 R^2: 0.329

Supplementary Data S3 - LDH Leakage Data



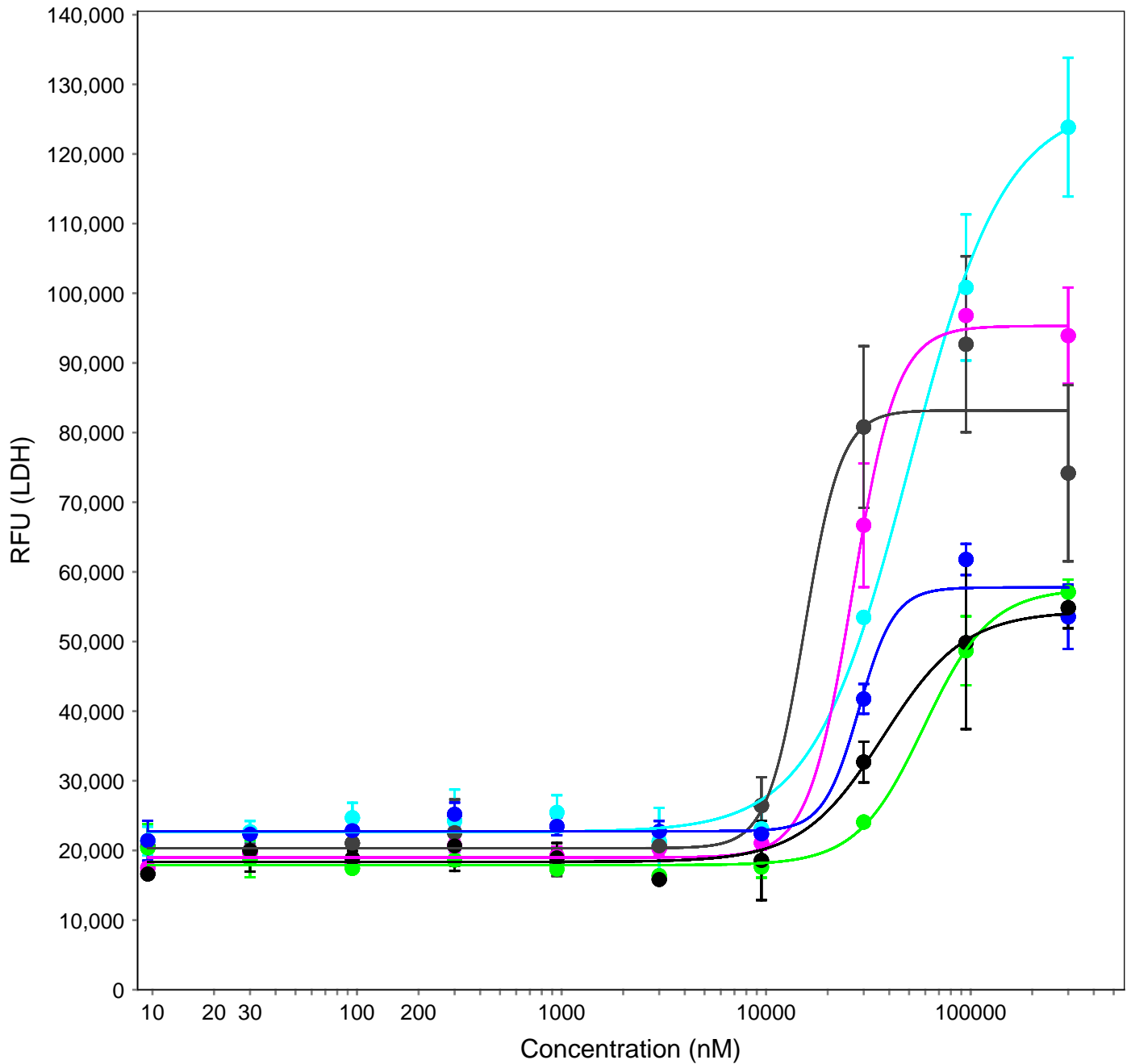
■	troglitazone		2D-DIFF-R1		LDH		48h		EMAX: 157000		EMIN: 30600		EC50: 243000		R ² : 0.988
■	troglitazone		2D-DIFF-R2		LDH		48h		EMAX: 156000		EMIN: 23800		EC50: 215000		R ² : 0.994
■	troglitazone		2D-DIFF-R3		LDH		48h		EMAX: 179000		EMIN: 17300		EC50: 248000		R ² : 0.998
■	troglitazone		2D-DIFF-R1		LDH		96h		EMAX: 193000		EMIN: 27800		EC50: 288000		R ² : 0.994
■	troglitazone		2D-DIFF R2		LDH		96h		EMAX: 114000		EMIN: 18800		EC50: 236000		R ² : 0.988
■	troglitazone		2D-DIFF-R3		LDH		96h		EMAX: 58100		EMIN: 16200		EC50: 2.40E5		R ² : 0.993

Supplementary Data S3 - LDH Leakage Data



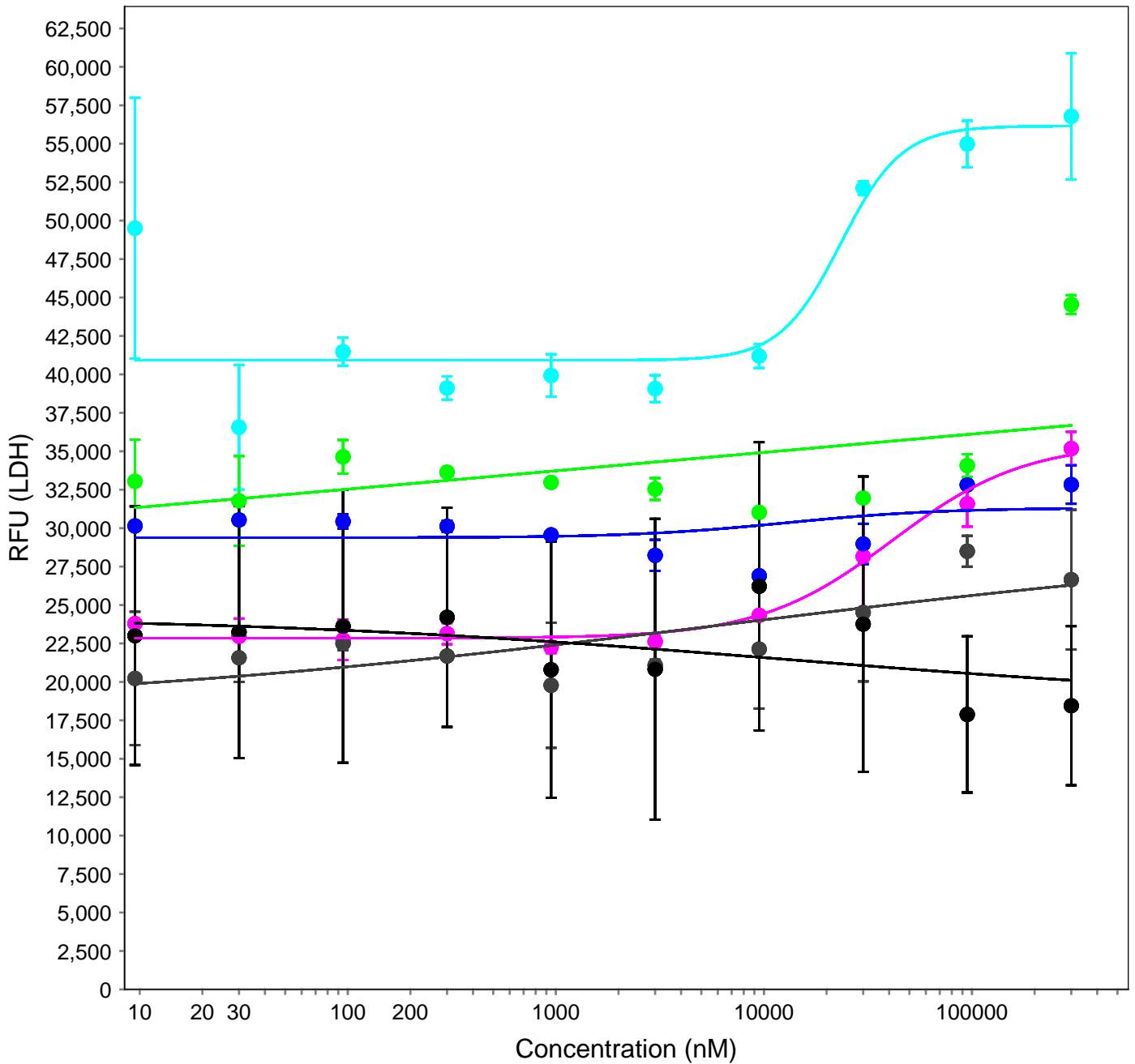
■	troglitazone		PROLIF-R1		LDH		48h		EMAX: 49600		EMIN: 30600		EC50: 47700		R ² : 0.325
■	troglitazone		PROLIF-R2		LDH		48h		EMAX: 40900		EMIN: 23100		EC50: 22800		R ² : 0.180
●	troglitazone		PROLIF-R3		LDH		48h		EMAX: 50100		EMIN: 15300		EC50: 6450		R ² : 0.0669
●	troglitazone		PROLIF-R1		LDH		96h		EMAX: 21600		EMIN: 17900		EC50: 7240		R ² : 0.484
●	troglitazone		PROLIF-R2		LDH		96h		EMAX: 21900		EMIN: 18900		EC50: 1560		R ² : 0.683
●	troglitazone		PROLIF-R3		LDH		96h		EMAX: 28900		EMIN: 25500		EC50: 283		R ² : 0.530

Supplementary Data S3 - LDH Leakage Data



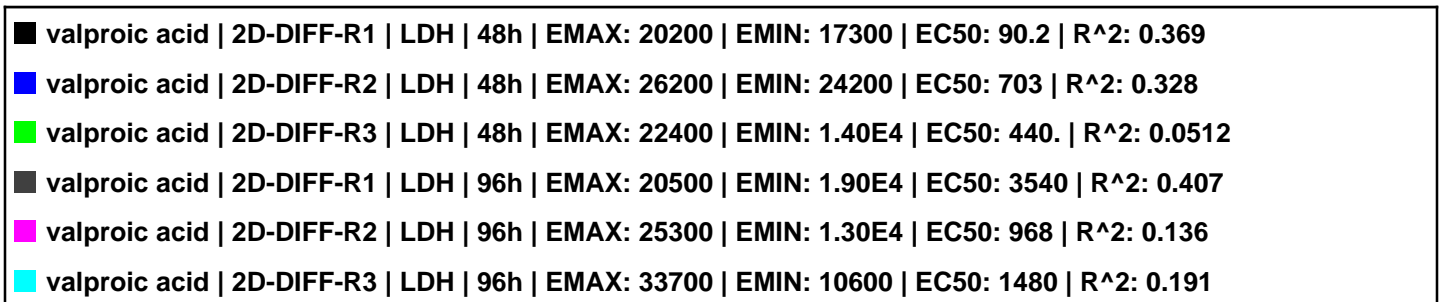
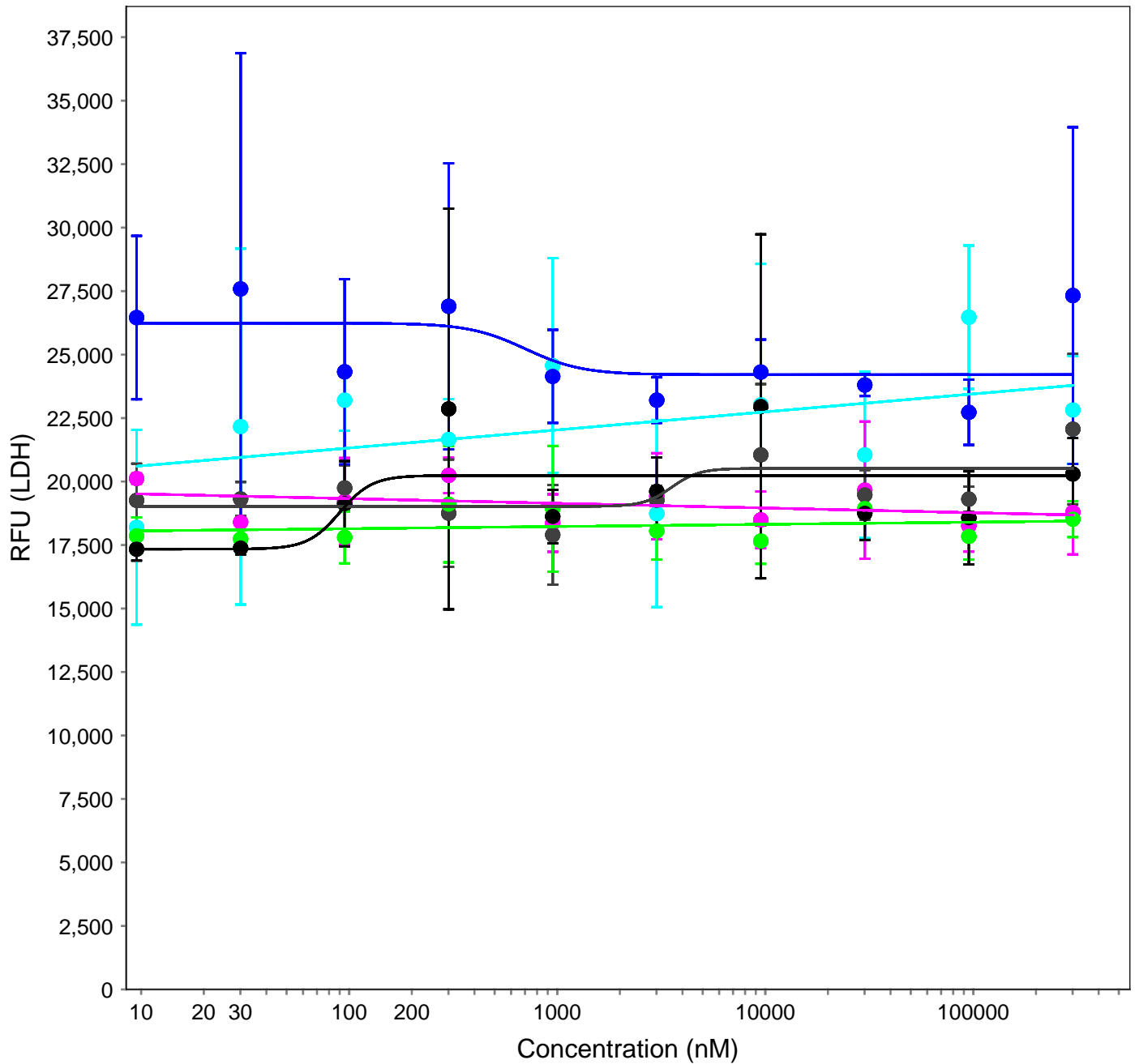
■	trovafloxacin 2D-DIFF-R1 LDH 48h EMAX: 54300 EMIN: 18400 EC50: 37300 R ² : 0.988
■	trovafloxacin 2D-DIFF-R2 LDH 48h EMAX: 57800 EMIN: 22800 EC50: 28400 R ² : 0.978
■	trovafloxacin 2D-DIFF-R3 LDH 48h EMAX: 57600 EMIN: 17900 EC50: 59100 R ² : 0.994
■	trovafloxacin 2D-DIFF-R1 LDH 96h EMAX: 83200 EMIN: 20300 EC50: 15400 R ² : 0.977
■	trovafloxacin 2D-DIFF-R2 LDH 96h EMAX: 95300 EMIN: 1.90E4 EC50: 26500 R ² : 0.999
■	trovafloxacin 2D-DIFF-R3 LDH 96h EMAX: 127000 EMIN: 22700 EC50: 49900 R ² : 0.997

Supplementary Data S3 - LDH Leakage Data

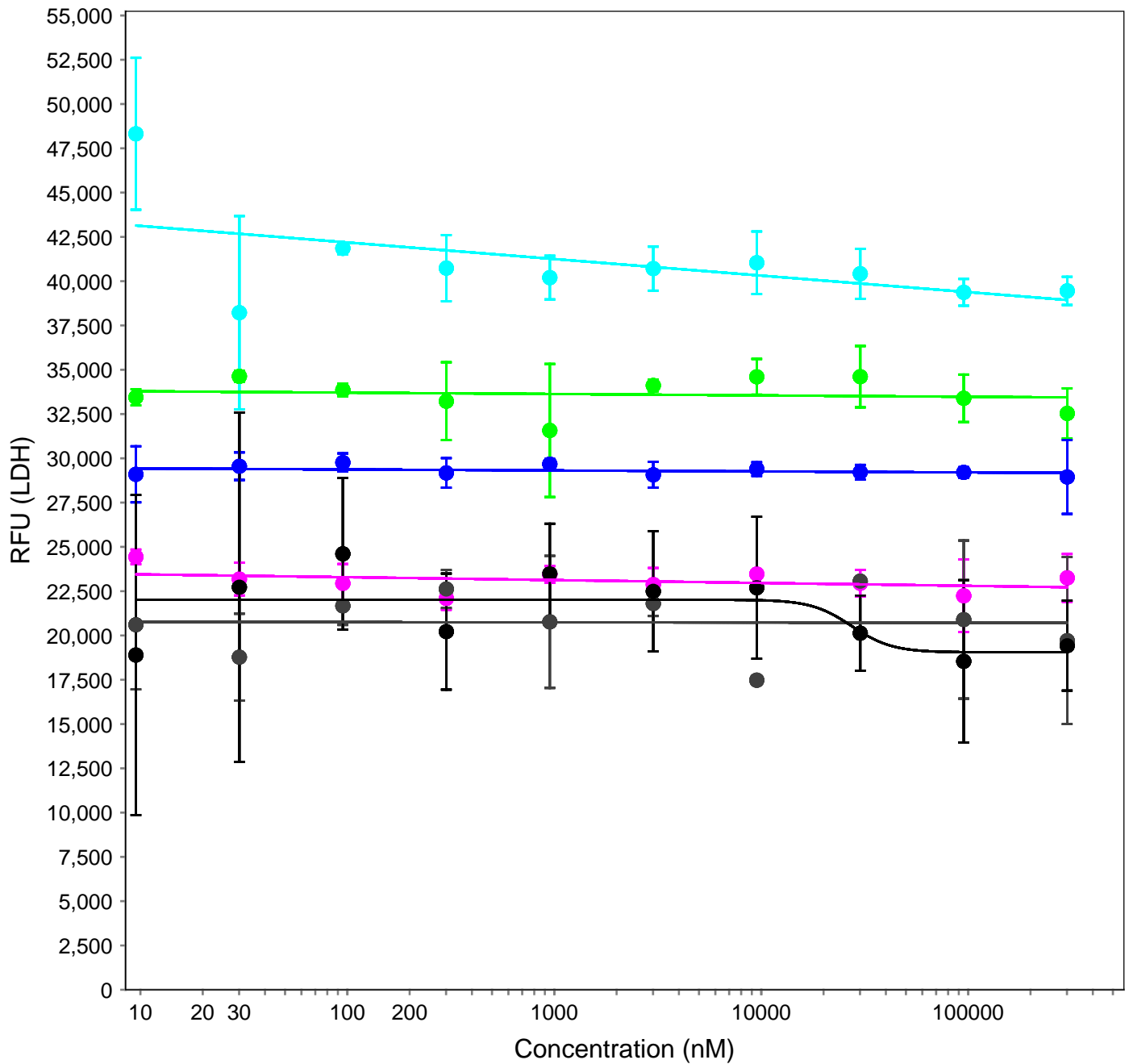


■	trovafloxacin	PROLIF-R1	LDH	48h	EMAX: 24300	EMIN: 18600	EC50: 12800	R ² : 0.273
■	trovafloxacin	PROLIF-R2	LDH	48h	EMAX: 31300	EMIN: 29400	EC50: 12800	R ² : 0.180
■	trovafloxacin	PROLIF-R3	LDH	48h	EMAX: 52900	EMIN: 15700	EC50: 2930	R ² : 0.217
■	trovafloxacin	PROLIF-R1	LDH	96h	EMAX: 29500	EMIN: 1.80E4	EC50: 6760	R ² : 0.623
■	trovafloxacin	PROLIF-R2	LDH	96h	EMAX: 35600	EMIN: 22800	EC50: 41500	R ² : 0.984
■	trovafloxacin	PROLIF-R3	LDH	96h	EMAX: 56200	EMIN: 40900	EC50: 23400	R ² : 0.795

Supplementary Data S3 - LDH Leakage Data



Supplementary Data S3 - LDH Leakage Data



■	valproic acid PROLIF-R1 LDH 48h EMAX: 2.20E4 EMIN: 1.90E4 EC50: 27300 R ² : 0.421
■	valproic acid PROLIF-R2 LDH 48h EMAX: 30200 EMIN: 28400 EC50: 2740 R ² : 0.170
■	valproic acid PROLIF-R3 LDH 48h EMAX: 35300 EMIN: 31900 EC50: 1.80E3 R ² : 0.0137
■	valproic acid PROLIF-R1 LDH 96h EMAX: 21700 EMIN: 19800 EC50: 1230 R ² : 2.54E-5
■	valproic acid PROLIF-R2 LDH 96h EMAX: 25100 EMIN: 2.10E4 EC50: 3120 R ² : 0.142
■	valproic acid PROLIF-R3 LDH 96h EMAX: 65400 EMIN: 17400 EC50: 677 R ² : 0.267

Supplementary Data S4 - LDH Leakage and Morphology LOELs

Compound Name	Model-Run#	Assay	Treatment Period	Emax (RFU)	Emin (RFU)	Emax/Emin	Mean Emax/Emin	EC50 (nM)	Mean EC50 (µM)	R ²	LOEL-Morphology Cell stress/death-96h (nM)	Mean LOEL-Morphology Cell stress/death-96h (nM)	LOEL-Attenuation of Proliferation-96h (nM)	Mean LOEL-Attenuation of Proliferation-96h (nM)
acetaminophen	2D-DIFF-R1	LDH	48h	51900	21800	2.4	2.55	5,700,000	3,727	0.938				
acetaminophen	2D-DIFF-R2	LDH	48h	63600	26700	2.4	2.55	2,660,000	3,727	0.948				
acetaminophen	2D-DIFF-R3	LDH	48h	53500	18500	2.9	2.55	2,820,000	3,727	0.996				
acetaminophen	2D-DIFF-R1	LDH	96h	37700	20500	1.8	1.81	2,400,000	2,413	0.338	2000000.00	4883036.88		
acetaminophen	2D-DIFF-R2	LDH	96h	33700	20200	1.7	1.81	2,640,000	2,413	0.565	6324555.32			
acetaminophen	2D-DIFF-R3	LDH	96h	43100	22400	1.9	1.81	2,200,000	2,413	0.511	6324555.32			
acetaminophen	PROLIF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
acetaminophen	PROLIF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
acetaminophen	PROLIF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
acetaminophen	PROLIF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR	2000000.00	2000000.00	6324555.32	6324555.32
acetaminophen	PROLIF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR	2000000.00		6324555.32	
acetaminophen	PROLIF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR	2000000.00		6324555.32	
afatoxin B1	2D-DIFF-R1	LDH	48h	136000	35300	3.9	6.25	3,410	4.81	0.967				
afatoxin B1	2D-DIFF-R2	LDH	48h	206000	34400	6.0	6.25	5,750	4.81	0.996				
afatoxin B1	2D-DIFF-R3	LDH	48h	245000	27500	8.9	6.25	5,280	4.81	0.994				
afatoxin B1	2D-DIFF-R1	LDH	96h	175000	35700	4.9	6.17	1,540	1.46	0.974	1499.72	1499.72		
afatoxin B1	2D-DIFF-R2	LDH	96h	164000	21800	7.5	6.17	1,640	1.46	0.908	1499.72			
afatoxin B1	2D-DIFF-R3	LDH	96h	143000	23500	6.1	6.17	1,210	1.46	0.746	1499.72			
afatoxin B1	PROLIF-R1	LDH	48h	91400	34600	2.6	2.83	2,880	3.61	0.996				
afatoxin B1	PROLIF-R2	LDH	48h	89900	26200	3.4	2.83	4,860	3.61	0.999				
afatoxin B1	PROLIF-R3	LDH	48h	74900	30800	2.4	2.83	3,080	3.61	0.981				
afatoxin B1	PROLIF-R1	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	47.43	223.88	474.25	1157.90
afatoxin B1	PROLIF-R2	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	149.97		1499.72	
afatoxin B1	PROLIF-R3	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	474.25		1499.72	
aspirin	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	PROLIF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	PROLIF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	PROLIF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	PROLIF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	PROLIF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
aspirin	PROLIF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
benzo(a)pyrene	2D-DIFF-R1	LDH	48h	64700	37200	1.7	1.74	3,170	3.36	0.684				
benzo(a)pyrene	2D-DIFF-R2	LDH	48h	54600	38500	1.4	1.74	3,170	3.36	0.802				
benzo(a)pyrene	2D-DIFF-R3	LDH	48h	48600	23700	2.1	1.74	3,190	3.36	0.864				
benzo(a)pyrene	2D-DIFF-R1	LDH	96h	206000	34000	6.1	9.27	6,530	9.63	0.99	9486.69	9486.69		
benzo(a)pyrene	2D-DIFF-R2	LDH	96h	273000	23700	11.5	9.27	16,100	9.63	0.99	9486.69			
benzo(a)pyrene	2D-DIFF-R3	LDH	96h	220000	22600	9.7	9.27	6,260	9.63	0.998	9486.69			
benzo(a)pyrene	PROLIF-R1	LDH	48h	96500	34400	2.8	3.01	2,340	2.47	0.96				
benzo(a)pyrene	PROLIF-R2	LDH	48h	96200	27000	3.6	3.01	3,180	2.47	0.985				
benzo(a)pyrene	PROLIF-R3	LDH	48h	80800	30500	2.6	3.01	1,880	2.47	0.955				
benzo(a)pyrene	PROLIF-R1	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	948.67	1416.21	948.67	1632.43
benzo(a)pyrene	PROLIF-R2	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	2999.95		2999.95	
benzo(a)pyrene	PROLIF-R3	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	300.00		948.67	
caffeine	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	PROLIF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	PROLIF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	PROLIF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	PROLIF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	PROLIF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
caffeine	PROLIF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR	200037.13	200037.13		
chenodeoxycholic acid	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR	200037.13			
chenodeoxycholic acid	PROLIF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	PROLIF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	PROLIF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	PROLIF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	PROLIF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chenodeoxycholic acid	PROLIF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
chlorthalimide	2D-DIFF-R1	LDH	48h	155000	25700	6.0	6.32	21,000	30.6	0.999				
chlorthalimide	2D-DIFF-R2	LDH	48h	247000	43200	5.7	6.32	35,600	30.6	0.991				
chlorthalimide	2D-DIFF-R3	LDH	48h	244000	32800	7.4	6.32	35,100	30.6	0.986				
chlorthalimide	2D-DIFF-R1	LDH	96h	79200	32200	2.5	2.61	9,220	8.37	0.255	30002.19	23163.97		
chlorthalimide	2D-DIFF-R2	LDH	96h	44900	20600	2.2	2.61	10,300	8.37	0.761	30002.19			
chlorthalimide	2D-DIFF-R3	LDH	96h	66400	20800	3.2	2.61	5,600	8.37	0.545	9487.52			
chlorthalimide	PROLIF-R1	LDH	48h	39700	19100	2.1	2.47	6,520	10.6	0.93				
chlorthalimide	PROLIF-R2	LDH	48h	74800	26200	2.9	2.47	17,000	10.6	0.961				
chlorthalimide	PROLIF-R3	LDH	48h	60600	24500	2.5	2.47	8,180	10.6	0.961				
chlorthalimide	PROLIF-R1	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	3000.22	2316.40	30002.19	23163.97
chlorthalimide	PROLIF-R2	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	3000.22		30002.19	
chlorthalimide	PROLIF-R3	LDH	96h	NMR	NMR	NMR	NMR	NMR	NMR	NMR	948.75		9487.52	
cyclophosphamide	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	PROLIF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	PROLIF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	PROLIF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	PROLIF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	PROLIF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
cyclophosphamide	PROLIF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
diphenhydramine	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
diphenhydramine	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
diphenhydramine	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
diphenhydramine	2D-DIFF-R1	LDH	96h	32100	22200	1.4	1.76	34,100	34.7	0.93	63244.66			
diphenhydramine	2D-DIFF-R2	LDH	96h	41400	21300	1.9	1.76	44,500	34.7	0.97	199997.18			
diphenhydramine	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
diphenhydramine	PROLIF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
diphenhydramine	PROLIF-R2	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
diphenhydramine	PROLIF-R3	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				
diphenhydramine	PROLIF-R1	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR	63244.66	48829.68		
diphenhydramine	PROLIF-R2	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR	63244.66			
diphenhydramine	PROLIF-R3	LDH	96h	LDR	LDR	LDR	LDR	LDR	LDR	LDR	199997.18			
fenofibric acid	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR	LDR	LDR	LDR	LDR				

Supplementary Data S4 - LDH Leakage and Morphology LOELs

Compound Name	Model-Run#	Assay	Treatment Period	Emax (RFU)	Emin (RFU)	Emax/Emin	Mean Emax/Emin	EC50 (nM)	Mean EC50 (µM)	R ²	LOEL-Morphology Cell stress/death-96h (nM)	Mean LOEL-Morphology Cell stress/death-96h (nM)	LOEL-Attenuation of Proliferation-96h (nM)	Mean LOEL-Attenuation of Proliferation-96h (nM)
fenofibric acid	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
fenofibric acid	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
levofloxacin	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
menadione	2D-DIFF-R1	LDH	48h	96100	25600	3.8	3.44	29,500	27.2	0.986				
menadione	2D-DIFF-R2	LDH	48h	144000	60500	2.4	3.44	28,400	27.2	0.952				
menadione	2D-DIFF-R3	LDH	48h	120000	28600	4.2	3.44	23,600	27.2	0.995				
menadione	2D-DIFF-R1	LDH	96h	NMR	NMR	NMR		NMR	NMR	NMR	22031.67	48964.99		
menadione	2D-DIFF-R2	LDH	96h	NMR	NMR	NMR		NMR	NMR	NMR	94864.50			
menadione	2D-DIFF-R3	LDH	96h	NMR	NMR	NMR		NMR	NMR	NMR	29998.79			
menadione	PROLIF-R1	LDH	48h	27700	17800	1.6	1.66	26,000	25.5	0.792				
menadione	PROLIF-R2	LDH	48h	47900	25600	1.9	1.66	26,900	25.5	0.995				
menadione	PROLIF-R3	LDH	48h	38800	24800	1.6	1.66	23,600	25.5	0.986				
menadione	PROLIF-R1	LDH	96h	NMR	NMR	NMR		NMR	NMR	NMR	29998.79	29998.79		
menadione	PROLIF-R2	LDH	96h	NMR	NMR	NMR		NMR	NMR	NMR	29998.79		29998.79	
menadione	PROLIF-R3	LDH	96h	NMR	NMR	NMR		NMR	NMR	NMR	29998.79			29998.79
N-nitrosodimethylamine (DMN)	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
N-nitrosodimethylamine (DMN)	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
omeprazole	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
omeprazole	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
omeprazole	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
omeprazole	2D-DIFF-R1	LDH	96h	38200	21300	1.8	2.05	134,000	136.6	0.998	299967.94	299967.94		
omeprazole	2D-DIFF-R2	LDH	96h	36200	19200	1.9	2.05	44,900	136.6	0.934	299967.94			
omeprazole	2D-DIFF-R3	LDH	96h	53600	21600	2.5	2.05	231,000	136.6	0.972	299967.94			
omeprazole	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
omeprazole	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
omeprazole	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
omeprazole	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	94858.19	163228.11	299967.94	299967.94
omeprazole	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	94858.19		299967.94	
omeprazole	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	299967.94		299967.94	
phenobarbital	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
phenobarbital	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
potassium chloride	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
rifampicin	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rifampicin	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rifampicin	2D-DIFF-R3	LDH	48h	52600	27600	1.9		163,000	163.0	0.99				
rifampicin	2D-DIFF-R1	LDH	96h	65200	27600	2.4	2.73	183,000	178.3	0.955	291007.03	137377.41		
rifampicin	2D-DIFF-R2	LDH	96h	55700	20100	2.8	2.73	184,000	178.3	0.934	29100.70			
rifampicin	2D-DIFF-R3	LDH	96h	59400	19500	3.0	2.73	168,000	178.3	0.981	92024.50			
rifampicin	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rifampicin	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rifampicin	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rifampicin	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	291007.03	291007.03	291007.03	291007.03
rifampicin	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	291007.03		291007.03	
rifampicin	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	291007.03		291007.03	
ritonavir	2D-DIFF-R1	LDH	48h	153000	24100	6.3	6.77	43,800	50.5	0.999				
ritonavir	2D-DIFF-R2	LDH	48h	176000	33000	5.3	6.77	51,900	50.5	0.982				
ritonavir	2D-DIFF-R3	LDH	48h	215000	24900	8.6	6.77	55,800	50.5	1				
ritonavir	2D-DIFF-R1	LDH	96h	146000	26000	5.6	6.33	29,300	39.8	0.999	139254.33	66295.55		
ritonavir	2D-DIFF-R2	LDH	96h	127000	19600	6.5	6.33	41,500	39.8	1	29816.15			
ritonavir	2D-DIFF-R3	LDH	96h	133000	19300	6.9	6.33	48,700	39.8	1	29816.15			
ritonavir	PROLIF-R1	LDH	48h	41400	18400	2.3	2.56	40,700	48.3	0.992				
ritonavir	PROLIF-R2	LDH	48h	78400	27200	2.9	2.56	43,000	48.3	0.998				
ritonavir	PROLIF-R3	LDH	48h	61300	24200	2.5	2.56	61,100	48.3	0.998				
ritonavir	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	29816.15	29816.15	29816.15	29816.15
ritonavir	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	29816.15			
ritonavir	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	29816.15			

NMR: Non-monotonic response, poor fit to Hill model
LDR: Low dynamic range of response [i.e., flat]

Supplementary Data S4 - LDH Leakage and Morphology LOELs

Compound Name	Model-Run#	Assay	Treatment Period	Emax (RFU)	Emin (RFU)	Emax/Emin	Mean Emax/Emin	EC50 (nM)	Mean EC50 (µM)	R^2	LOEL-Morphology Cell stress/death-96h (nM)	Mean LOEL-Morphology Cell stress/death-96h (nM)	LOEL-Attenuation of Proliferation-96h (nM)	Mean LOEL-Attenuation of Proliferation-96h (nM)
rosiglitazone	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rosiglitazone	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rosiglitazone	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rosiglitazone	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	300049.84	300049.84		
rosiglitazone	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
rosiglitazone	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	300049.84			
rosiglitazone	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rosiglitazone	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rosiglitazone	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
rosiglitazone	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	30004.98	30004.98	30004.98	30004.98
rosiglitazone	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	30004.98		30004.98	
rosiglitazone	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	30004.98			
sucrose	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
sucrose	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
tamoxifen	2D-DIFF-R1	LDH	48h	251000	23300	10.8	9.09	75,300	69.3	0.999				
tamoxifen	2D-DIFF-R2	LDH	48h	167000	29500	5.7	9.09	70,200	69.3	0.99				
tamoxifen	2D-DIFF-R3	LDH	48h	276000	25500	10.8	9.09	62,300	69.3	0.999				
tamoxifen	2D-DIFF-R1	LDH	96h	196000	27800	7.1	9.06	90,600	59.8	0.998	93572.12	50917.44		
tamoxifen	2D-DIFF-R2	LDH	96h	295000	19200	15.4	9.06	77,800	59.8	0.999	29590.10			
tamoxifen	2D-DIFF-R3	LDH	96h	97000	20300	4.8	9.06	11,100	59.8	0.995	29590.10			
tamoxifen	PROLIF-R1	LDH	48h	49600	18000	2.8	6.25	63,600	48.3	0.993				
tamoxifen	PROLIF-R2	LDH	48h	86800	24700	3.5	6.25	32,900	48.3	0.699				
tamoxifen	PROLIF-R3	LDH	48h	56600	4530	12.5	6.25	2,260	48.3	0.309				
tamoxifen	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	2959.01	5091.74	29590.10	29590.10
tamoxifen	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	9357.21			
tamoxifen	PROLIF-R3	LDH	96h	48600	25400	1.9		14,600	LDR	LDR	2959.01		29590.10	
trogliatone	2D-DIFF-R1	LDH	48h	157000	30600	5.1	7.34	243,000	235.3	0.988				
trogliatone	2D-DIFF-R2	LDH	48h	156000	23800	6.6	7.34	215,000	235.3	0.994				
trogliatone	2D-DIFF-R3	LDH	48h	179000	17300	10.3	7.34	248,000	235.3	0.998				
trogliatone	2D-DIFF-R1	LDH	96h	193000	27800	6.9	5.53	288,000	254.7	0.994	300115.97	231712.31		
trogliatone	2D-DIFF-R2	LDH	96h	114000	18800	6.1	5.53	236,000	254.7	0.988	94905.00			
trogliatone	2D-DIFF-R3	LDH	96h	58100	16200	3.6	5.53	240,000	254.7	0.993	300115.97			
trogliatone	PROLIF-R1	LDH	48h	49600	30600	1.6	2.22	47,700	25.7	0.325				
trogliatone	PROLIF-R2	LDH	48h	40900	23100	1.8	2.22	22,800	25.7	0.18				
trogliatone	PROLIF-R3	LDH	48h	50100	15300	3.3	2.22	6,450	25.7	0.0669				
trogliatone	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	300115.97	163308.66	300115.97	197510.49
trogliatone	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	94905.00		94905.00	
trogliatone	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	94905.00			
trovafloxacin	2D-DIFF-R1	LDH	48h	54300	18400	3.0	2.90	37,300	41.6	0.988				
trovafloxacin	2D-DIFF-R2	LDH	48h	57800	22800	2.5	2.90	28,400	41.6	0.978				
trovafloxacin	2D-DIFF-R3	LDH	48h	57600	17900	3.2	2.90	59,100	41.6	0.994				
trovafloxacin	2D-DIFF-R1	LDH	96h	83200	20300	4.1	4.90	15,400	30.6	0.977	30000.85	30000.85		
trovafloxacin	2D-DIFF-R2	LDH	96h	95300	19000	5.0	4.90	26,500	30.6	0.999	30000.85			
trovafloxacin	2D-DIFF-R3	LDH	96h	127000	22700	5.6	4.90	49,900	30.6	0.997	30000.85			
trovafloxacin	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
trovafloxacin	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
trovafloxacin	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
trovafloxacin	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	9487.10	9487.10	9487.10	23162.93
trovafloxacin	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	9487.10		30000.85	
trovafloxacin	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR	9487.10		30000.85	
valproic acid	2D-DIFF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	2D-DIFF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	2D-DIFF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	2D-DIFF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	2D-DIFF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	2D-DIFF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	PROLIF-R1	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	PROLIF-R2	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	PROLIF-R3	LDH	48h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	PROLIF-R1	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	PROLIF-R2	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				
valproic acid	PROLIF-R3	LDH	96h	LDR	LDR	LDR		LDR	LDR	LDR				

NMR: Non-monotonic response, poor fit to Hill model

LDR: Low dynamic range of response (i.e., flat)

Supplementary Data S5 - EC50 Values of Nuclear Receptor Functionality in HepaRG cells

Compound	Reference Pathway	Mode	Inter-run Mean E _{max}	Inter-run Mean E _{min}	E _{max} /E _{min}	Inter-run Mean EC ₅₀ (μM)
Omeprazole	AhR	2D-DIFF	865	5	166	61.7
Omeprazole	AhR	PROLIF	3050	147	20.8	25.8
Phenobarbital	CAR	2D-DIFF	51.5	5.4	9.47	463
Phenobarbital	CAR	PROLIF	11.9	4.2	2.8	306
Rifampicin	PXR	2D-DIFF	9607	185	51.9	1.31
Rifampicin	PXR	PROLIF	484	37	12.9	64.3
chenodeoxycholic acid	FXR	2D-DIFF	716	6	117	207
chenodeoxycholic acid	FXR	PROLIF	189	6	30	110
Fenofibric acid	PPARα	2D-DIFF	73.5	16.1	4.57	88.8
Fenofibric acid	PPARα	PROLIF	27.5	8.5	3.25	9.87

Supplementary Data S6 - Cell Morphology and Cytotoxicity Assessment & BMD Analysis File

Files can be accessed from the link below:

<https://doi.org/10.22427/NTP-DATA-002-00058-0001-0000-6>

Description of the link:

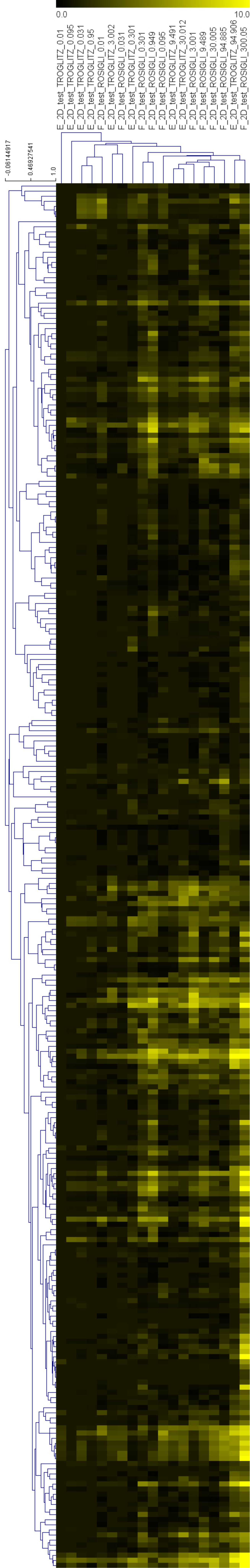
1. In the above weblink you will find data related to cell morphology and cytotoxicity assessments. Cell morphology pictures of all the treatments before, during and after the exposure regimens can be accessed from the link.
2. Raw data and calculations of LDH leakage assays are also available under 'cell morphology and cytotoxicity assessments'.
3. BMD analysis file (.bm2) (24 chemical HepaRG BMD Analysis File) - includes the entire dataset (24 chemicals/ 10 concentrations/ 3 independent runs). Raw expression data, Normalized data (Williams Trend test), benchmark dose analysis, gene and biological pathway-level accumulation plots can be accessible by following the steps below.

Steps:

- a) Download BMDExpress 2.2 from: <https://github.com/auerbachs/BMDExpress-2>.
- b) After installing the software package, double click on the desktop icon to open BMDExpress 2.2.
- c) Go to file - open project and select the .bm2 file - 24 chemical HepaRG BMD Analysis File.
- d) Below the file tab, you can see dropdown menu to visualize, raw expression data, normalized data, BMD analysis and pathway analysis. Additional information including video tutorials to analyze the data can be found in the link mentioned in step (a) - <https://github.com/auerbachs/BMDExpress-2>.
- e) Follow the instructions in the materials and methods section (BMDExpress 2.2 analysis of gene- and pathway-level benchmark concentrations) for additional settings to filter the data.

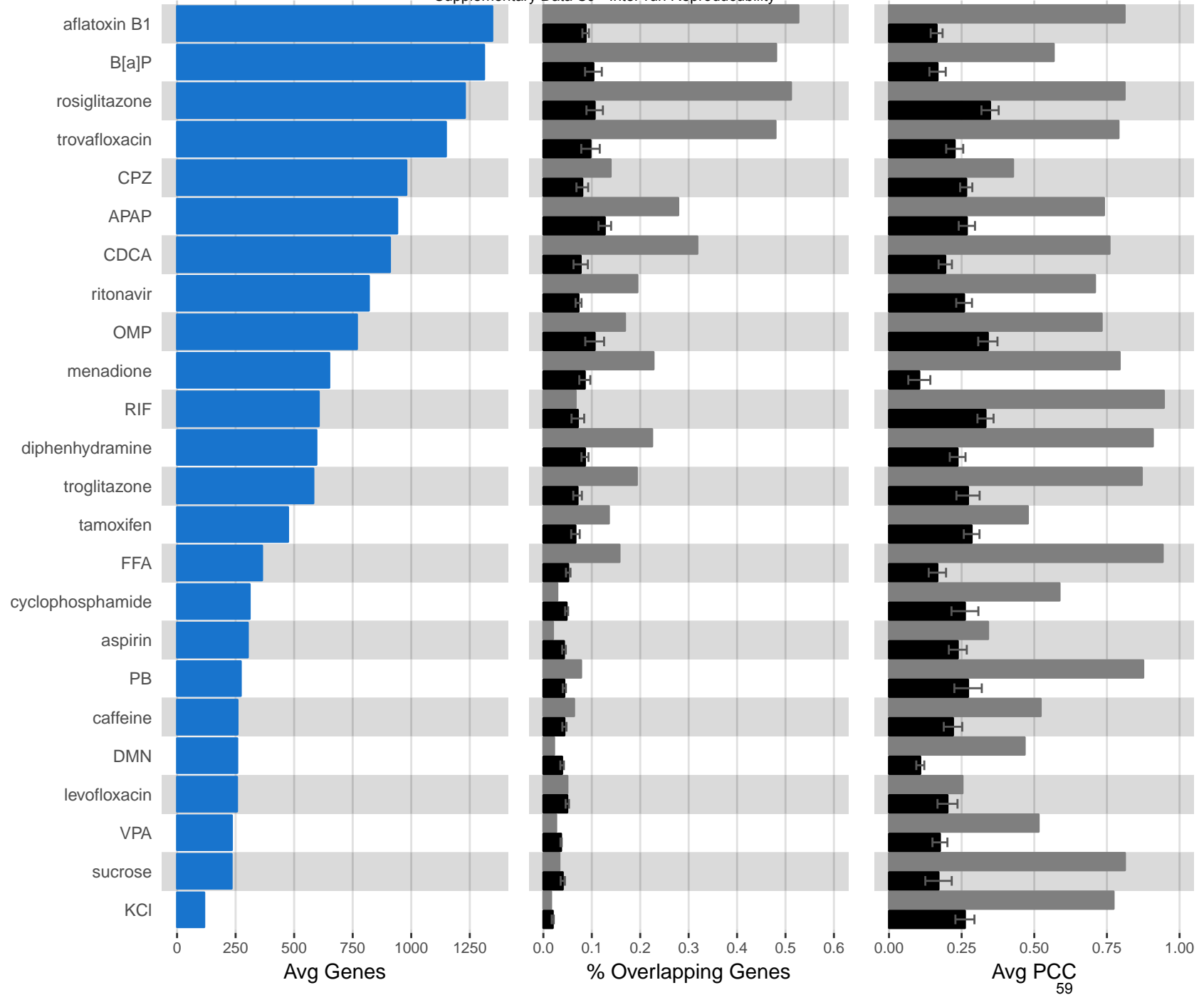
Supplementary Data S7 - BMCs of Signaling Pathways

Compound	Culture Model	Pathway set	Pathway (or Gene) Name	BMC-R1	BMC-R2	BMC-R3	Mean BMC	SD BMC
aflatoxin B1	2D-DIFF	GO Biol Proc	apoptotic process	78.7	358	231	222	140
aflatoxin B1	2D-DIFF	GO Biol Proc	cell cycle	50.4	207	143	133	78.7
aflatoxin B1	2D-DIFF	GO Biol Proc	cellular response to dna damage stimulus	95.0	228	224	182	75.7
aflatoxin B1	2D-DIFF	GO Biol Proc	signal transduction by p53 class mediator	53.3	189	199	147	81.5
aflatoxin B1	2D-DIFF	KEGG	Pathways in cancer	93.7	536	240	290	225
aflatoxin B1	2D-DIFF	Reactome	PPARa activates gene expression	34.2	432	173	213	202
aflatoxin B1	PROLIF	GO Biol Proc	apoptotic process	37.3	97	127	87.1	45.7
aflatoxin B1	PROLIF	GO Biol Proc	cell cycle	18.5	45	127	63.7	56.6
aflatoxin B1	PROLIF	GO Biol Proc	cellular response to dna damage stimulus	25.7	62	140	75.9	58.3
aflatoxin B1	PROLIF	GO Biol Proc	signal transduction by p53 class mediator	9.5	79	126	71.2	58.3
aflatoxin B1	PROLIF	KEGG	Pathways in cancer	46.2	71	149	88.7	53.5
aflatoxin B1	PROLIF	Reactome	PPARa activates gene expression	7.20	104	103	71.5	55.7
benzo(a)pyrene	2D-DIFF	GO Biol Proc	apoptotic process	1187	801	558	849	317
benzo(a)pyrene	2D-DIFF	GO Biol Proc	cell cycle	821	446	622	629	188
benzo(a)pyrene	2D-DIFF	GO Biol Proc	cellular response to dna damage stimulus	1454	806	721	994	401
benzo(a)pyrene	2D-DIFF	GO Biol Proc	signal transduction by p53 class mediator	2038	728	682	1149	770
benzo(a)pyrene	2D-DIFF	KEGG	Pathways in Cancer	2370	951	834	1385	855
benzo(a)pyrene	2D-DIFF	Reactome	PPARa activates gene expression	1117	561	1069	916	308
benzo(a)pyrene	PROLIF	GO Biol Proc	apoptotic process	226	309	301	279	45.8
benzo(a)pyrene	PROLIF	GO Biol Proc	cell cycle	181	298	293	257	66.2
benzo(a)pyrene	PROLIF	GO Biol Proc	cellular response to dna damage stimulus	230	304	281	272	37.9
benzo(a)pyrene	PROLIF	GO Biol Proc	signal transduction by p53 class mediator	225	275	360	287	68.3
benzo(a)pyrene	PROLIF	KEGG	Pathways in Cancer	227	321	314	287	52.4
benzo(a)pyrene	PROLIF	Reactome	PPARa activates gene expression	164	270	340	258	88.8
menadione	2D-DIFF	GO Biol Proc	signal transduction involved in DNA damage check	12953	7951	12681	11195	2813
menadione	2D-DIFF	GO Biol Proc	cellular response to reactive oxygen species	7932	8793	9596	8774	832
menadione	2D-DIFF	GO Biol Proc	response to oxidative stress	6613	8774	8563	7983	1191
menadione	2D-DIFF	GO Biol Proc	apoptotic process	6449	8066	11522	8679	2591
menadione	2D-DIFF	GO Biol Proc	glycolytic process through glucose-6-phosphate	4541	28344	3990	4266	389
trovafloxacin	2D-DIFF	GO Biol Proc	lipid hydroxylation	2805	5301	1031	3045	2145
trovafloxacin	2D-DIFF	GO Biol Proc	cellular response to oxidative stress	2689	8615	5473	5592	2965
trovafloxacin	2D-DIFF	GO Biol Proc	cellular response to DNA damage stimulus	6044	6965	11112	8040	2700
trovafloxacin	2D-DIFF	GO Biol Proc	cell cycle process	5318	6807	10017	7380	2401
trovafloxacin	2D-DIFF	GO Biol Proc	apoptotic process	5934	6647	10767	7783	2609
trovafloxacin	2D-DIFF	GO Biol Proc	regulation of cell killing	9085	9506	8652	9081	427
trovafloxacin	2D-DIFF	GO Biol Proc	necrotic cell death	1703	5263	32734	13233	16981
trovafloxacin	2D-DIFF	GO Biol Proc	antibacterial humoral response	5774	3628	5939	5114	1289
trovafloxacin	PROLIF	GO Biol Proc	cellular response to oxidative stress	2171	3509	2518	2733	695
trovafloxacin	PROLIF	GO Biol Proc	cellular response to DNA damage stimulus	3089	4841	4078	4003	878
trovafloxacin	PROLIF	GO Biol Proc	cell cycle process	2634	4335	3825	3598	873
trovafloxacin	PROLIF	GO Biol Proc	apoptotic process	2504	3777	1952	2744	936
trovafloxacin	PROLIF	GO Biol Proc	regulation of cell killing	6646	3032	467	3382	3104
trovafloxacin	PROLIF	GO Biol Proc	necrotic cell death	1504	1957	2955	2139	742
trovafloxacin	PROLIF	GO Biol Proc	antibacterial humoral response		914	2540	1727	1150
troglitazone	2D-DIFF	GO Biol Proc	DNA damage response, detection of dna damage	35.0	FBMC	28.3	31.6	4.75
troglitazone	2D-DIFF	GO Biol Proc	regulation of programmed cell death	3158	545	7095	3599	3297
troglitazone	2D-DIFF	GO Biol Proc	cell cycle process	100	588	133	274	272
troglitazone	2D-DIFF	GO Biol Proc	response to toxic substance	16974	1498	8999	9157	7739
troglitazone	2D-DIFF	C2	wang classic adipogeneci targets of pparg	374	410	175	319	127
troglitazone	2D-DIFF	RBS curated	PPAR signaling pathway	533	713	1287	844	394
troglitazone	2D-DIFF	Gene-Level	FABP4	NoBMC	20.4	0.276	10.3	14.2
troglitazone	2D-DIFF	Gene-Level	ADIPOQ	641	713	113	489	327
troglitazone	2D-DIFF	Gene-Level	PEX11A	373	1628	122	708	807
troglitazone	2D-DIFF	Gene-Level	CEBPA	FBMC	48691	38654	43672	7098
rosiglitazone	2D-DIFF	GO Biol Proc	DNA damage response, detection of dna damage	127936	152632	57247	112605	49506
rosiglitazone	2D-DIFF	GO Biol Proc	regulation of programmed cell death	128614	118745	156269	134543	19452
rosiglitazone	2D-DIFF	GO Biol Proc	cell cycle process	118312	119917	86092	108107	19082
rosiglitazone	2D-DIFF	GO Biol Proc	response to toxic substance	166687	152751	133815	151084	16499
rosiglitazone	2D-DIFF	C2	wang classic adipogeneci targets of pparg	225097	120970	51104	132390	87557
rosiglitazone	2D-DIFF	RBS curated	PPAR signaling pathway	185412	3592	146961	111988	95822
rosiglitazone	2D-DIFF	Gene-Level	FABP4	0.353	0.560	0.169	0.361	0.196
rosiglitazone	2D-DIFF	Gene-Level	ADIPOQ	3.45	29.1	6.80	13.1	13.9
rosiglitazone	2D-DIFF	Gene-Level	PEX11A	250551	248743	272505	257266	13228
rosiglitazone	2D-DIFF	Gene-Level	CEBPA	289736	187044	65276	180685	112365



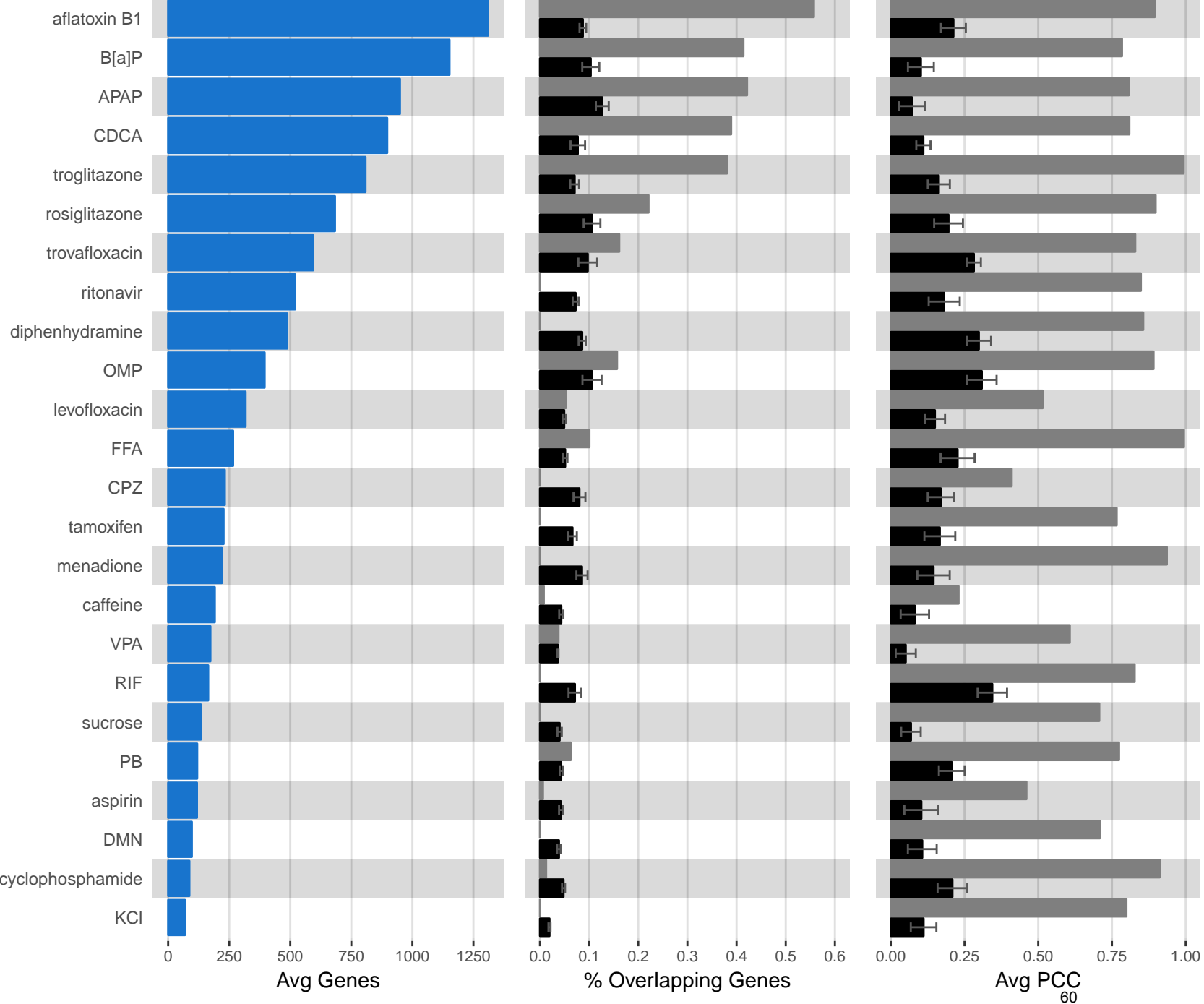
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- 1.0
- Rac Signaling
- dTMP De Novo Biosynthesis
- Stearate Biosynthesis I (Animals)
- Methylglyoxal Degradation III
- Histidine Degradation VI
- Pregnenolone Biosynthesis
- Ubiquinol-10 Biosynthesis (Eukaryotic)
- Regulation of Cellular Mechanics by Calpain Protease
- BER Pathway
- Agrin Interactions at Neuromuscular Junction
- Amyloid Processing
- Reelin Signaling in Neurons
- SAPK/JNK Signaling
- Interferon Signaling
- iNOS Signaling
- IL-15 Production
- "Role of JAK1, JAK2 and TYK2 in Interferon Signaling"
- Sumoylation Pathway
- CDK5 Signaling
- T Helper Cell Differentiation
- Signaling by Rho Family GTPases
- IL-1 Signaling
- Tec Kinase Signaling
- Hepatic Cholestasis
- Leukocyte Extravasation Signaling
- Cholecystokinin/Gastrin-mediated Signaling
- Opioid Signaling Pathway
- Activation of IRF by Cytosolic Pattern Recognition Receptors
- Crosstalk between Dendritic Cells and Natural Killer Cells
- Estrogen-Dependent Breast Cancer Signaling
- Lymphotxin ? Receptor Signaling
- IL-15 Signaling
- Role of IL-17A in Arthritis
- Differential Regulation of Cytokine Production in Intestinal Epithelial Cells by IL-17A and IL-17F
- Differential Regulation of Cytokine Production in Macrophages and T Helper Cells by IL-17A and IL-17F
- Tight Junction Signaling
- P2Y Purinergic Receptor Signaling Pathway
- GNRH Signaling
- RAR Activation
- Regulation of IL-2 Expression in Activated and Anergic T Lymphocytes
- Inflammasome pathway
- IL-10 Signaling
- Toll-like Receptor Signaling
- Phospholipase C Signaling
- Altered T Cell and B Cell Signaling in Rheumatoid Arthritis
- TREM1 Signaling
- PPAR Signaling
- PPAR?/RXR? Activation
- Neuroinflammation Signaling Pathway
- Dendritic Cell Maturation
- Role of IL-17F in Allergic Inflammatory Airway Diseases
- HMO51 Signaling
- Type I Diabetes Mellitus Signaling
- Role of Pattern Recognition Receptors in Recognition of Bacteria and Viruses
- Type II Diabetes Mellitus Signaling
- Agranulocyte Adhesion and Diapedesis
- Granulocyte Adhesion and Diapedesis
- VDR/RXR Activation
- Granzyme A Signaling
- Mitochondrial Dysfunction
- BMP signaling pathway
- FAK Signaling
- G?12/13 Signaling
- PAK Signaling
- 4-1BB Signaling in T Lymphocytes
- April Mediated Signaling
- B Cell Activating Factor Signaling
- Antioxidant Action of Vitamin C
- CD40 Signaling
- Growth Hormone Signaling
- LPS-stimulated MAPK Signaling
- fMLP Signaling in Neutrophils
- G?q Signaling
- NF-?B Activation by Viruses
- CD28 Signaling in T Helper Cells
- iCOS-iCOSL Signaling in T Helper Cells
- Role of NFAT in Regulation of the Immune Response
- OX40 Signaling Pathway
- Nitric Oxide Signaling in the Cardiovascular System
- VEGF Family Ligand-Receptor Interactions
- Role of JAK1 and JAK3 in ?Cytokine Signaling
- Th2 Pathway
- Corticotropin Releasing Hormone Signaling
- IL9 Signaling
- JAK/Stat Signaling
- Erythropoietin Signaling
- Role of JAK2 in Hormone-like Cytokine Signaling
- Oncostatin M Signaling
- TNFR2 Signaling
- Fatty Acid ?-oxidation
- Putrescine Degradation III
- "Tryptophan Degradation X (Mammalian, via Tryptamine)"
- PDGF Signaling
- Neurotrophin/TRK Signaling
- Aldosterone Signaling in Epithelial Cells
- Calcium-induced T Lymphocyte Apoptosis
- Caveolar-mediated Endocytosis Signaling
- Melanoma Signaling
- Protein Ubiquitination Pathway
- Mouse Embryonic Stem Cell Pluripotency
- UVB-Induced MAPK Signaling
- EGF Signaling
- GDNF Family Ligand-Receptor Interactions
- IL-2 Signaling
- Virus Entry via Endocytic Pathways
- Acute Myeloid Leukemia Signaling
- CXCR4 Signaling
- Factors Promoting Cardiogenesis in Vertebrates
- Mechanisms of Viral Exit from Host Cells
- ?-Adrenergic Signaling
- CCR3 Signaling in Eosinophils
- 14-3-3-mediated Signaling
- CCR5 Signaling in Macrophages
- Thrombin Signaling
- Salvage Pathways of Pyrimidine Deoxyribonucleotides
- Mismatch Repair in Eukaryotes
- Glioma Invasiveness Signaling
- Mitotic Roles of Polo-Like Kinase
- 3-phosphoinositide Biosynthesis
- Superpathway of Inositol Phosphate Compounds
- UVB-Induced MAPK Signaling
- Ethanol Degradation IV
- Oxidative Ethanol Degradation III
- Phagosome Formation
- Estrogen Receptor Signaling
- Nucleotide Excision Repair Pathway
- Systemic Lupus Erythematosus Signaling
- 3-phosphoinositide Degradation
- "D-myo-inositol (1,4,5,6)-Tetrakisphosphate Biosynthesis"
- "D-myo-inositol (3,4,5,6)-tetrakisphosphate Biosynthesis"
- D-myo-inositol-5-phosphate Metabolism
- Role of 14q19ARF in Tumor Suppression
- CREB Signaling in Neurons
- Hereditary Breast Cancer Signaling
- FGF Signaling
- UVA-Induced MAPK Signaling
- Cell Cycle Regulation by BTF5 Family Proteins
- Antiproliferative Role of TOB in T Cell Signaling
- Cell Cycle: G1/S Checkpoint Regulation
- Estrogen-mediated S-phase Entry
- p38 MAPK Signaling
- STAT3 Pathway
- Prolactin Signaling
- TGF-? Signaling
- Ethanol Degradation II
- Noradrenaline and Adrenaline Degradation
- ATM Signaling
- Cell Cycle: G2/M DNA Damage Checkpoint Regulation
- DNA damage-induced 14-3-3? Signaling
- GADD45 Signaling
- Cyclins and Cell Cycle Regulation
- Role of CHK Proteins in Cell Cycle Checkpoint Control
- Cell Cycle Control of Chromosomal Replication
- Pyridoxal 5'-phosphate Salvage Pathway
- Salvage Pathways of Pyrimidine Ribonucleotides
- Breast Cancer Regulation by Stathmin1
- Bladder Cancer Signaling
- HER-2 Signaling in Breast Cancer
- Chronic Myeloid Leukemia Signaling
- Molecular Mechanisms of Cancer
- Pancreatic Adenocarcinoma Signaling
- Aryl Hydrocarbon Receptor Signaling
- PTEN Signaling
- Apoptosis Signaling
- Prostate Cancer Signaling
- Small Cell Lung Cancer Signaling
- Androgen Signaling
- B Cell Receptor Signaling
- ILK Signaling
- Regulation of the Epithelial-Mesenchymal Transition Pathway
- Osteoarthritis Pathway
- Hepatic Fibrosis / Hepatic Stellate Cell Activation
- NF-?B Signaling
- "Role of Macrophages, Fibroblasts and Endothelial Cells in Rheumatoid Arthritis"
- Maturity Onset Diabetes of Young (MODY) Signaling
- Colorectal Cancer Metastasis Signaling
- Protein Kinase A Signaling
- Wnt/?-catenin Signaling
- Glioma Signaling
- Graft-versus-Host Disease Signaling
- Cardiac Hypertrophy Signaling
- Role of NFAT in Cardiac Hypertrophy
- IL-17A Signaling in Gastric Cells
- NGF Signaling
- IL-17 Signaling
- IL-17A Signaling in Airway Cells
- MIF Regulation of Innate Immunity
- PEDF Signaling
- Renin-Angiotensin Signaling
- Adipogenesis pathway
- IGF-1 Signaling
- "Role of Osteoblasts, Osteoclasts and Chondrocytes in Rheumatoid Arthritis"
- Induction of Apoptosis by HIV1
- IL-17A Signaling in Fibroblasts
- Acute Phase Response Signaling
- IL9 Signaling
- Atherosclerosis Signaling
- LXR/RXR Activation
- IL-12 Signaling and Production in Macrophages
- Production of Nitric Oxide and Reactive Oxygen Species in Macrophages
- AMPK Signaling
- Role of Tissue Factor in Cancer
- Death Receptor Signaling
- FXR/RXR Activation
- Sirtuin Signaling Pathway
- Cancer Drug Resistance By Drug Efflux
- PI3K/AKT Signaling
- Serotonin Degradation
- Phagosome Maturation
- Coagulation System
- Extrinsic Prothrombin Activation Pathway
- Non-Small Cell Lung Cancer Signaling
- Regulation of eIF4 and p70S6K Signaling
- Amyotrophic Lateral Sclerosis Signaling
- eNOS Signaling
- Insulin Receptor Signaling
- Ovarian Cancer Signaling
- Endometrial Cancer Signaling
- Thyroid Cancer Signaling
- Dopamine Degradation
- Intrinsic Prothrombin Activation Pathway
- Polyamine Regulation in Colon Cancer
- GP6 Signaling Pathway
- Gap Junction Signaling
- Thyroid Hormone Metabolism II (via Conjugation and/or Degradation)
- Inhibition of Matrix Metalloproteases
- Hypoxia Signaling in the Cardiovascular System
- Clathrin-mediated Endocytosis Signaling
- p53 Signaling
- NRF2-mediated Oxidative Stress Response
- EIF2 Signaling
- Glycolysis I
- "Phenylalanine Degradation IV (Mammalian, via Side Chain)"
- Melatonin Degradation II
- Tumoricidal Function of Hepatic Natural Killer Cells
- Antigen Presentation Pathway
- Unfolded protein response
- PI3K Signaling in B Lymphocytes
- Myc Mediated Apoptosis Signaling
- VEGF Signaling
- Angiopoietin Signaling
- "Bile Acid Biosynthesis, Neutral Pathway"
- EhB2-EhB3 Signaling
- Neuregulin Signaling
- Estrogen Biosynthesis
- Acetone Degradation I (to Methylglyoxal)
- Bupropion Degradation
- Nicotine Degradation II
- Nicotine Degradation III
- Melatonin Degradation I
- Superpathway of Melatonin Degradation
- Docosahexaenoic Acid (DHA) Signaling
- Fatty Acid ?-oxidation I
- mTOR Signaling
- Renal Cell Carcinoma Signaling
- Glucocorticoid Receptor Signaling
- Huntington's Disease Signaling
- Th1 and Th2 Activation Pathway
- Th1 Pathway
- TNFR1 Signaling
- ERK/MAPK Signaling
- TR/RXR Activation
- ErbB Signaling
- Sertoli Cell-Sertoli Cell Junction Signaling
- IL7 Signaling Pathway
- Inhibition of Angiogenesis by TSP1
- HIF1? Signaling
- IL8 Signaling
- Glioblastoma Multiforme Signaling
- LXR/RXR Activation
- LPS/IL-1 Mediated Inhibition of RXR Function
- Xenobiotic Metabolism Signaling

Supplementary Data S9 - Inter-run Reproducibility



Randomized Random Original

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