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Supplemental Material

Developmental Effects of the ToxCast™ Phase I and II Chemicals in *Caenorhabditis elegans* and Corresponding Responses in Zebrafish, Rats, and Rabbits

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Supplemental Code and Data Zip File

Excel Table S1. ToxCast Phase I mean log(EXT) values and weighted t-test Bonferoni-corrected p-values

Excel Table S2. Phase I and II *C. elegans* and zebrafish toxicity estimates

Table S1. Estimated Z-factors and summary statistics using 4% DMSO with vehicle control.

Plate Number	Z-factor	Standard Deviation (negative control)	Standard Deviation (positive control)	Mean (negative control)	Mean (positive control)
1	0.8113	0.0628	0.0640	5.8411	3.8252
2	0.3960	0.0572	0.3016	5.8322	4.0496
3	0.8762	0.0551	0.0416	5.9068	3.5642
4	0.8264	0.0618	0.0655	5.7675	3.5671
5	0.4678	0.0446	0.2511	5.7687	4.1021
6	0.8683	0.0295	0.0780	5.7737	3.3251
7	0.7080	0.0606	0.0669	5.8553	4.5454
8	0.6139	0.0771	0.0961	5.7169	4.3707
9	0.8395	0.0330	0.0775	5.8052	3.7388
10	0.5768	0.1079	0.2145	5.9039	3.6183

Using the 10 replicate plates in the preliminary experiment, the Z-factor and summary statistics were calculated using 4% DMSO as positive control. The summary statistics include standard deviations and means for the negative control (1% DMSO) as well as the positive control (4% DMSO).

Table S2. Estimated Z-factors and summary statistics using parathion.

Plate Number	Z-factor	Standard Deviation (negative control)	Standard Deviation (positive control)	Mean (negative control)	Mean (positive control)
1	0.7620	0.0628	0.1227	5.8411	3.5036
2	0.7310	0.0572	0.1557	5.8322	3.4572
3	0.8292	0.0551	0.0827	5.9068	3.4870
4	0.8065	0.0618	0.0895	5.7675	3.4228
5	0.7546	0.0446	0.1530	5.7687	3.3531
6	0.8618	0.0295	0.0801	5.7737	3.3938
7	0.7740	0.0606	0.1140	5.8553	3.5372
8	0.6805	0.0771	0.1814	5.7169	3.2893
9	0.8894	0.0330	0.0496	5.8052	3.5646
10	0.7020	0.1079	0.1360	5.9039	3.4490

Using the 10 replicate plates in the preliminary experiment, the Z-factor and summary statistics were calculated using 200 μ M parathion as positive control. The summary statistics include standard deviations and means for the negative control (1% DMSO) as well as the positive control (Parathion).

Table S3. Estimated Z-factors and summary statistics using dichlorvos.

Plate Number	Z-factor	Standard Deviation (negative control)	Standard Deviation (positive control)	Mean (negative control)	Mean (positive control)
1	0.8676	0.0628	0.0513	5.8411	3.2570
2	0.8565	0.0572	0.0657	5.8322	3.2618
3	0.8720	0.0551	0.0576	5.9068	3.2649
4	0.8309	0.0618	0.0786	5.7675	3.2781
5	0.8874	0.0446	0.0521	5.7687	3.1920
6	0.8713	0.0295	0.0772	5.7737	3.2864
7	0.8477	0.0606	0.0617	5.8553	3.4451
8	0.8431	0.0771	0.0551	5.7169	3.1873
9	0.9167	0.0330	0.0359	5.8052	3.3231
10	0.7922	0.1079	0.0746	5.9039	3.2689

Using the 10 replicate plates in the preliminary experiment, the Z-factor and summary statistics were calculated using 200 μ M dichlorvos, as positive control. The summary statistics include standard deviations and means for the negative control (1% DMSO) as well as the positive control (Dichlorvos).

Table S4. Description of chemicals in the lower panel of Figure 4.

Order (1-most toxic)	CASRN	Name in Figure 4	Chemical name	Classification
1	135080-03-4	Pharma CP-100829	6-chloro-3-[(4-chlorothiophen-2-yl)carbonyl]-5-fluoro-2-oxo-2,3-dihydro-1H-indole-1-carboxamide	failed pharmaceutical
2	71751-41-2	Abamectin	Abamectin	avermectin
3	155569-91-8	Emamectin benzoate	Emamectin benzoate	avermectin
4	76-87-9	Triphenyltin hydroxide	Fentin	organotin
5	NOCAS	Milbemectin	Milbemectin (mix of >70% Milbemycin A4 CAS 51596-11-3; <30% Milbemycin A3 CAS 51596-10-2)	avermectin
6	205-99-2	Benzo[b]fluoranthene	Benzo[b]fluoranthene	PAH
7	50471-44-8	Vinclozolin	Vinclozolin	fungicide/antiandrogenic
8	2921-88-2	Chlorpyrifos	Chlorpyrifos	OP pesticide
9	72-54-8	DDD	p,p'-DDD	OC metabolite
10	50-29-3	DDT	p,p'-DDT	OC pesticide
11	119446-68-3	Difenoconazole	Difenoconazole	fungicide
12	5598-15-2	Chlorpyrifos oxon	Chlorpyrifos oxon	OP metabolite
13	119168-77-3	Tebufenpyrad	Tebufenpyrad	pyrazole insecticide
14	1461-22-9	Tributyltin chloride	Tributyltin chloride	organotin
15	2155-70-6	Tributyltin methacrylate	Stannane, tributyl(2-methyl-1-oxo-2-propenyl)oxy-	organotin
16	42509-80-8	Isazofos	Isazofos	OP pesticide
17	124495-18-7	Quinoxifen	Quinoxifen	fungicide
18	548-62-9	Hexamethyl-p-rosaniline chloride	Hexamethyl-p-rosaniline chloride	crystal violet
19	111812-58-9	Fenpyroximate (Z,E)	(Z,E)-Fenpyroximate	pyrazole insecticide

20	96489-71-3	Pyridaben	Pyridaben	miticide/insecticide
21	85-01-8	Phenanthrene	Phenanthrene	PAH
22	78-48-8	Tributyl phosphorotrithioate	Tribufos	OP pesticide
23	122-39-4	Diphenylamine	Diphenylamine	Plant growth regulator; N containing
24	120-12-7	Anthracene	Anthracene	PAH
25	153233-91-1	Etoxazole	Etoxazole	miticide
26	129-00-0	Pyrene	Pyrene	PAH
27	101-20-2	Triclocarban	3,4,4'-Trichlorocarbanilide	antimicrobial in personal care products
28	56-72-4	Coumaphos	Coumaphos	OP pesticide
29	2104-64-5	EPN	O-Ethyl O-(p-nitrophenyl) phenylphosphonothioate	OP pesticide
30	62-38-4	Phenylmercuric acetate	Phenylmercuric acetate	organic mercury salt
31	191906	Captafol	Captafol	fungicide
32	72-55-9	DDE	p,p'-DDE	OC metabolite
33	42874-03-3	Oxyfluorfen	Oxyfluorfen	herbicide
34	2058-94-8	Henicosafuoroundecanoic acid	Perfluoroundecanoic acid	perfluoroalkyls; fluorosurfactant
35	309-00-2	Aldrin	Aldrin	OC pesticide
36	143-50-0	Kepone	Kepone (Chlordecone)	OC pesticide
37	1836-75-5	Nitrofen	2,4-dichloro-1-(4-nitrophenoxy)benzene	alkyl halide
38	NOCAS_47366	Pharma4736	5-fluoro-1-(3-fluorobenzyl)-N-(1H-indol-5-yl)-1H-indole-2-carboxamide	failed pharmaceutical
39	115-29-7	Endosulfan	Endosulfan	OC pesticide
40	173584-44-6	Indoxacarb	Indoxacarb	oxadiazine insecticide
41	76-44-8	Heptachlor	Heptachlor	OC pesticide
42	335-76-2	Perfluorodecanoic acid	Perfluorodecanoic acid	perfluoroalkyls; fluorosurfactant
43	2795-39-3	Potassium perfluorooctanesulfonate	Heptadecafluorooctanesulfonic acid potassium salt	perfluoroalkyls; fluorosurfactant

44	115-32-2	Dicofol	Dicofol	OC pesticide
45	7487-94-7	Mercuric chloride	Mercuric chloride	inorganic mercury salt
46	754-91-6	Perfluorooctanesulfonamide	Perfluorooctanesulfonamide	perfluoroalkyls; fluorosurfactant
47	57-74-9	Chlordane	Chlordane	OC pesticide
48	55285-14-8	Carbosulfan	Carbosulfan	carbamate
49	95737-68-1	Pyriproxyfen	Pyriproxyfen	pyridine pesticide (fleas)
50	56-55-3	Benz[a]anthracene	Benz[a]anthracene	PAH

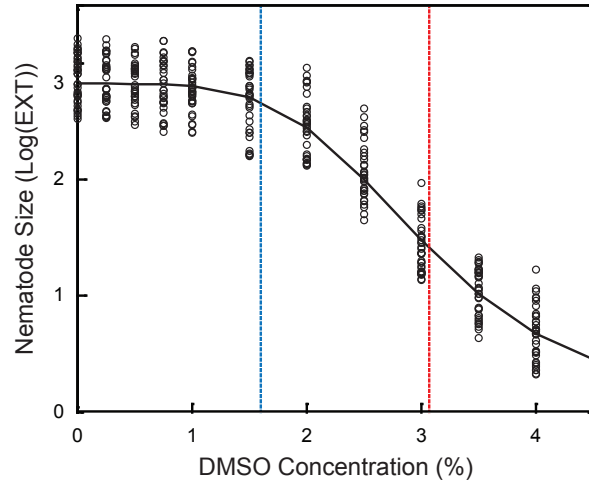


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