

Supporting Information

Machine learning assisted discovery of interactions between pesticides, phthalates, phenols, and trace elements in child neurodevelopment

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Figure S1

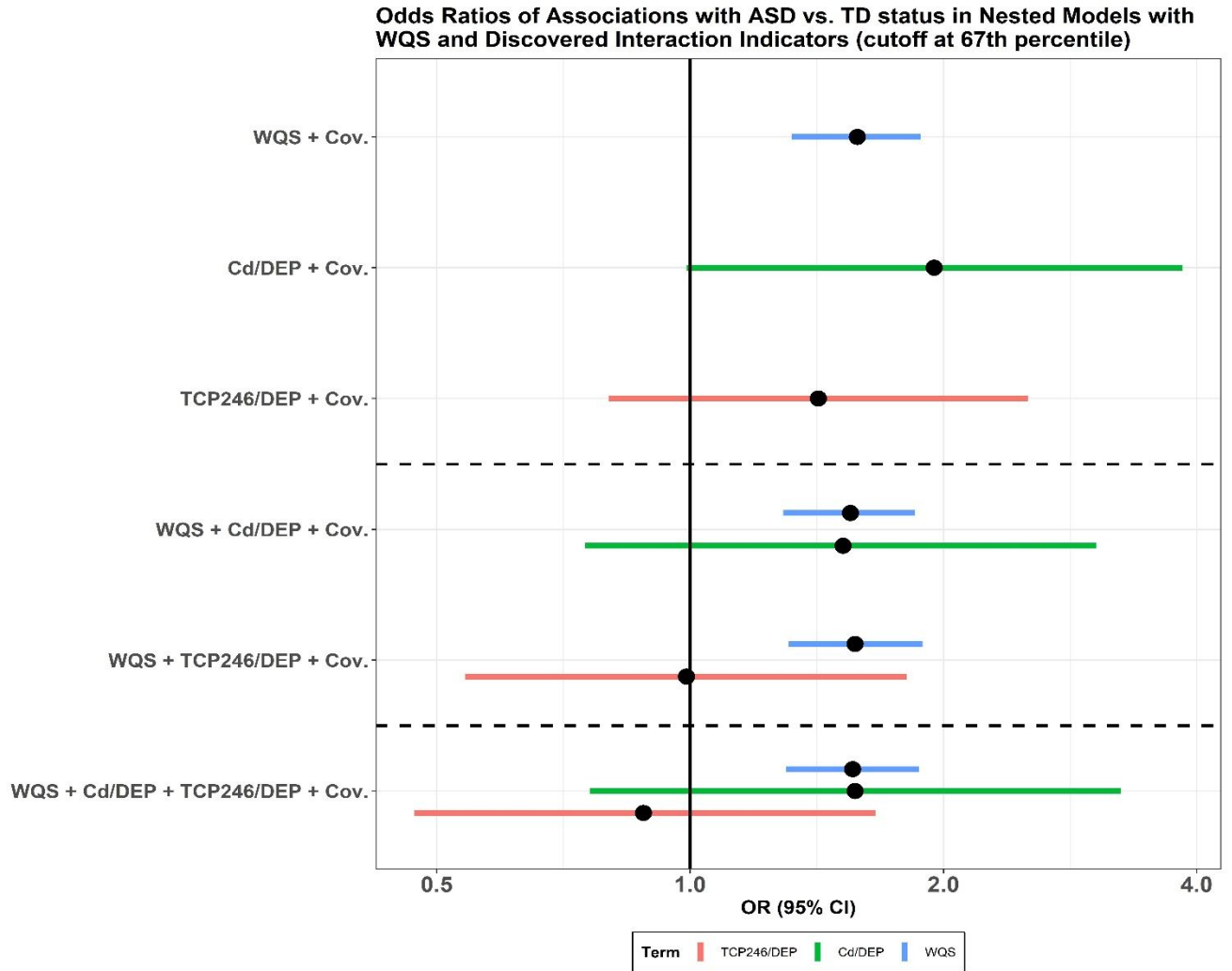


Figure S1: Results from nested linear models with WQS and discovered interaction indicators (cutoff set at 67th percentile) and WQS chemical mixture. In the top three models, the WQS chemical mixture and the two interaction indicators were used in separate models. Both interaction indicators were adjusted for the WQS chemical mixture in the following two models. In the last model, interaction indicators and the WQS chemical mixture were put in the same model. All models were adjusted for covariates.

Figure S2:

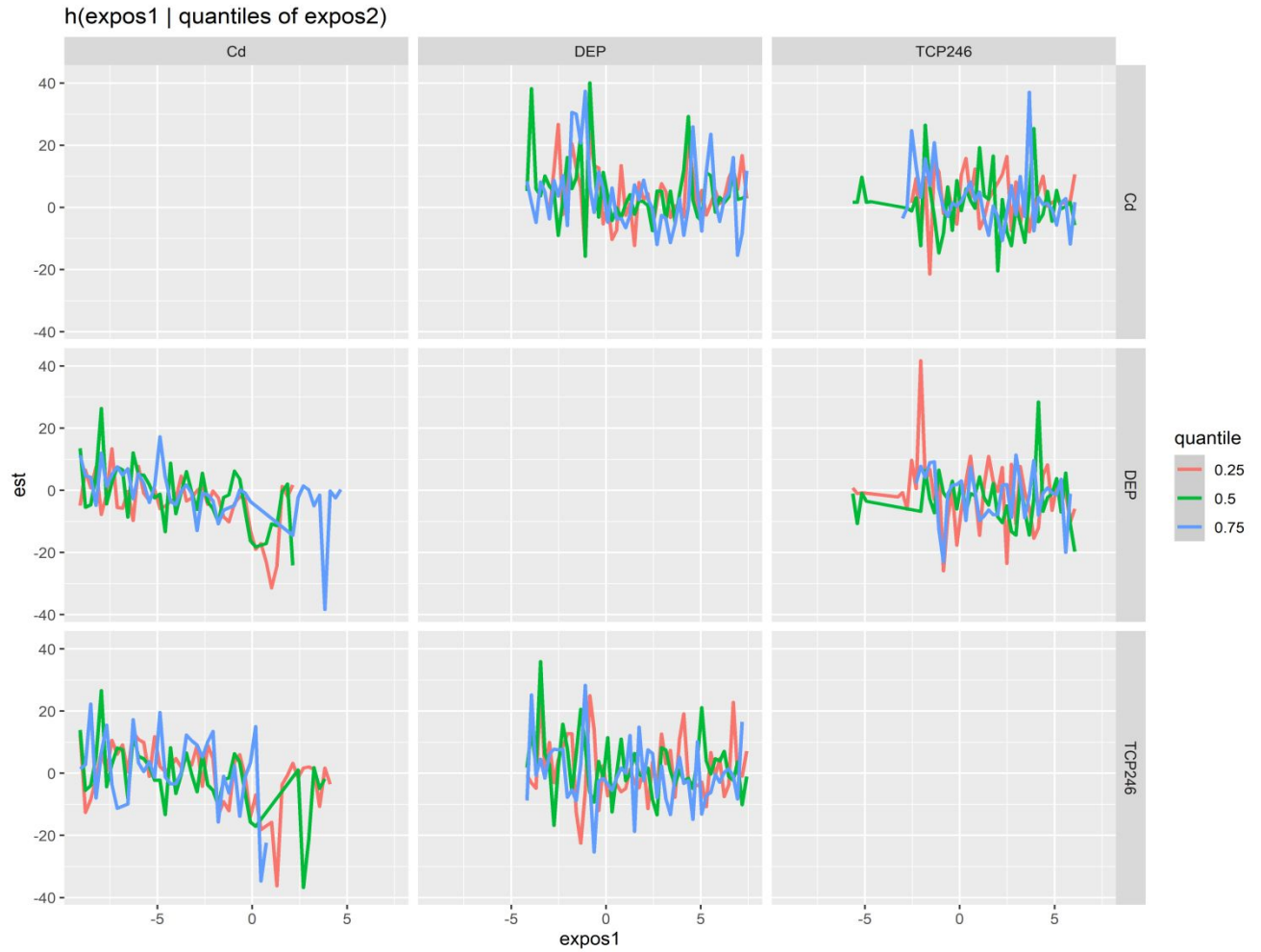


Figure S2: Plot for pair-wise interactions at quantiles 25th, 50th, and 75th between Diethyl-phosphate (DEP), Cadmium (Cd), and 2,4,6-Trichlorophenol (TCP-246) obtained from Bayesian Kernel Machine Regression (BKMR) model (adjusted for covariates)

Table S1: Chemical names and abbreviations*

Chemical class	Chemical Abbreviation	Chemical Full Name
Phenols and Parabens	BP1	Benzophenone-1
	BP2	2,2',4,4'-tetrahydroxybenzophenone
	BP3	Benzophenone-3
	BP8	2,2'-dihydroxy-methoxybenzophenone
	BPA	Bisphenol A
	BPAF	4,4'-(hexafluoroisopropylidene)-dephenol
	BPAP	4,4'-(1-phenylethylidene)bisphenol
	BPB	2,2'-bis(4-hydroxyphenyl)butane
	BPF	Bisphenol F
	BPP	4,4'-(1,4-Phenylenediisopropylidene)bisphenol
	BPS	Bisphenol S
	BPZ	4,4'-cyclo-hexylidenebisphenol
	BUPB	Butyl paraben
	BZPB	Benzyl paraben
	DCP24	2,4-Dichlorophenol
	DCP25	2,5-Dichlorophenol
	DHB34	3,4-Dihydroxy benzoic acid
	ETPB	Ethyl paraben
	HB4	4-Hydroxybenzoic acid
	HEPB	Heptyl paraben
	MEPB	Methyl Paraben
	OH4BP	4-hydroxybenzophenone
	OHETP	Protocatechuic acid ethyl ester
	OHMEP	3,4-Dihydroxy-benzoic acid methyl ester
	PCP	Pentachlorophenol
	PRPB	Propyl paraben
	TCC	Triclocarban
	TCP245	2,4,5-Trichlorophenol
	TCP246	2,4,6-Trichlorophenol
	TCS	Triclosan
Phthalates	MBZP	mono-benzyl phthalate
	MCHP	Monocyclohexyl phthalate
	MCHPP	mono(7-carboxyheptyl)phthalate
	MCINP	mono-carboxy isononyl phthalate
	MCIOP	mono-carboxy isooctyl phthalate
	MCMHP	Mono-2-(carboxymethyl) hexyl phthalate
	MCPP	mono (3-carboxypropyl) phthalate (multiple)
	MECPP	mono-(2-ethyl-5-carboxypentyl) phthalate
	MEHHP	mono (2-ethyl-5-hydroxyhexyl) phthalate
	MEOHP	mono (2-ethyl-5-oxohexyl) phthalate
	MEP	monoethyl phthalate (DEP)
	MHPP	mono-2-heptyl phthalate
	MHXP	mono-hexyl phthalate
	MIBP	mono-isobutyl phthalate (DiBP)
	MINP	mono-isononyl phthalate
	MIPP	Mono-isopropyl phthalate
	MMP	mono-methyl phthalate
	MNBP	mono-n-butylphthalate (BzBP, DnBP)
	MOP	Mono-n-octyl phthalate
	MPEP	mono-pentyl phthalate

Pesticides	DMP	Dimethylphosphate
	DEP	Diethylphosphate
	DMTP	Dimethylthiophosphate
	DETP	Diethylthiophosphate
	DMDP	Dimethyldithiophosphate
	DEDP	Diethyldithiophosphate
Trace Elements	As	Arsenic
	Be	Beryllium
	Cd	Cadmium
	Mo	Molybdenum
	Tl	Thallium
	U	Uranium

* From (Bennett et al. 2022)

Table S2: Limit of detection (LOD) for individual chemicals and percent detection above the LOD by chemical classes

Phenols (N=479)			Phthalates (N=479)			Pesticides (N=479)			Trace Elements (N=479)		
Chemical	LOD	% above LOD	Chemical	LOD (ng/ml)	% above LOD	Chemical	LOD (ng/ml)	% above LOD	Chemical	LOD (ng/ml)	% above LOD
BP1	0.05	100	MBZP	0.02	99.25	DMP	0.05	99.55	As	0.059	100
BP2	0.2	11.19	MCHP	0.50	07.46	DEP	0.10	99.25	Be	0.022	6.57
BP3	0.5	100	MCHPP	0.10	26.57	DMTP	0.05	95.82	Mo	0.45	100
BP8	0.02	80.90	MCINP	0.01	98.66	DETP	0.02	98.51	Cd	0.006	72.84
BPA	0.05	98.66	MCIOP	0.01	99.85	DMDP	0.02	91.79	Tl	0.005	100
BPAF	0.05	0.75	MCMHP	0.02	98.81	DEDP	0.05	3.73	U	0.0007	99.55
BPAP	0.1	89.25	M CPP	0.05	99.85						
BPB	0.05	50.75	MECPP	0.02	99.70						
BPF	0.5	89.40	MEHHP	0.20	100						
BPP	0.01	76.72	MEOHP	0.01	100						
BPS	0.05	94.78	MEP	0.10	100						
BPZ	0.05	1.19	MHPP	0.50	74.18						
BUPB	0.05	92.84	MHXP	0.50	57.16						
BZPB	0.1	14.48	MIBP	0.01	100						
DCP24	0.02	95.07	MINP	0.01	0						
DCP25	0.02	88.06	MIPP	0.50	2.69						
DHB34	0.2	100	MMP	5.0	41.34						
ETPB	0.02	99.1	MNBP	0.20	99.85						
HB4	1	100	MOP	0.50	1.64						
HEPB	0.1	0.30	MPEP	1.0	2.69						
MEPB	0.05	99.85									
OH4BP	0.2	98.81									
OHETP	0.1	65.67									
OHMEP	0.1	96.12									
PCP	0.05	96.27									
PRPB	0.1	98.51									
TCC	0.1	07.91									
TCP245	0.1	51.75									
TCP246	0.02	99.85									
TCS	0.1	96.87									

Table S3: Distribution of log-transformed (base=2) specific gravity-adjusted urinary phenol, phthalate, and trace element biomarker concentrations (ng/ml) among 479 participants included in the analysis

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phenols</i>					
BP1	0.76	2.58	4.00	5.91	12.75
BP2	-3.84	-3.53	-3.16	-2.54	-0.96
BP3	2.75	4.32	5.82	7.64	10.51
BP8	-6.75	-3.51	-1.87	-0.10	3.45
BPA	-1.53	0.15	1.16	1.98	3.52
BPAF	-5.87	-5.60	-5.30	-4.82	-4.32
BPAP	-4.09	-2.58	-1.64	-0.88	0.40
BPB	-5.70	-5.16	-4.32	-3.24	-1.94
BPF	-2.22	0.41	1.65	3.07	4.44
BPP	-7.92	-6.39	-3.50	-2.14	-0.38
BPS	-4.32	-2.56	-1.30	-0.09	2.03
BPZ	-5.87	-5.60	-5.30	-4.82	-4.32
BUPB	-4.46	-2.51	-1.34	0.03	3.75
BZPB	-4.84	-4.54	-4.13	-3.43	-1.90
DCP24	-4.38	0.32	1.40	2.48	3.68
DCP25	-6.66	0.61	1.83	2.73	5.88
DHB34	5.17	6.48	7.39	8.10	9.12
ETPB	-2.13	-0.84	0.32	1.68	5.62
HB4	9.20	10.06	10.55	11.24	12.75
HEPB	-4.87	-4.60	-4.30	-3.84	-3.32
MEPB	2.14	3.63	5.41	7.55	11.29
OH4BP	-1.11	0.35	0.97	1.67	3.71
OHETP	-4.62	-3.57	-1.51	-0.02	1.97
OHMEP	-2.28	0.63	2.16	3.71	6.61
PCP	-2.53	-0.75	0.05	0.91	2.14
PRPB	-1.16	0.95	2.60	4.73	8.52
TCC	-4.85	-4.58	-4.20	-3.65	-1.51
TCP245	-4.70	-4.16	-3.32	-2.38	-0.89
TCP246	-1.07	-0.01	0.56	1.28	2.61
TCS	-1.34	1.49	2.98	4.72	7.42

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phthalates</i>					
MBZP	2.15	3.88	4.97	6.13	8.04
MCHP	-2.52	-2.25	-1.88	-1.33	-0.34
MCHPP	-4.84	-4.49	-3.93	-3.29	3.90
MCINP	0.47	1.81	2.54	3.30	4.84
MCIOP	2.07	3.59	4.37	5.20	6.81
MCMHP	1.20	3.13	4.08	5.08	6.51
MCPP	0.40	1.66	2.45	3.27	4.50
MECPP	2.97	4.27	5.04	6.06	7.59
MEHHP	3.32	4.64	5.48	6.50	8.34

MEOHP	1.98	3.30	4.24	5.33	7.03
MEP	3.64	4.62	5.41	6.31	8.34
MHPP	-2.11	-1.00	0.43	1.69	3.72
MHXP	-2.38	-1.73	-0.56	3.56	7.12
MIBP	2.32	3.47	4.31	5.14	6.59
MINP	-8.19	-7.92	-7.62	-7.16	-6.64
MIPP	-2.52	-2.28	-1.95	-1.43	-1.00
MMP	0.89	1.34	2.10	2.98	4.84
MNBP	3.53	4.65	5.45	6.19	7.39
MOP	-2.55	-2.28	-1.95	-1.48	-1.00
MPEP	-1.52	-1.28	-0.95	-0.48	0.00

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Pesticides</i>					
DMP	0.22	1.82	3.16	4.34	6.06
DEP	-0.63	0.88	2.02	3.18	4.78
DMTP	-3.39	0.19	1.81	3.68	5.62
DETP	-4.10	-2.25	-1.03	0.32	2.52
DMDP	-6.12	-3.23	-1.69	0.01	2.99
DEDP	-5.85	-5.57	-5.24	-4.75	-4.32

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Trace Elements</i>					
As	1.99	2.83	3.47	4.11	5.57
Be	-7.03	-6.77	-6.42	-5.86	-5.51
Mo	5.02	6.04	6.62	7.18	8.25
Cd	-8.81	-7.43	-5.46	-4.37	-3.03
Tl	-3.53	-2.71	-2.25	-1.78	-0.98
U	-8.48	-7.35	-6.62	-5.68	-4.26

Table S4: Distribution of log-transformed (base =2) and specific gravity-adjusted urinary phenol, phthalate, and trace element biomarker concentrations (ng/ml) among 231 ASD participants included in the analysis

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phenols</i>					
BP1	0.75	2.43	3.56	5.60	12.61
BP2	-3.87	-3.53	-3.16	-2.37	-0.96
BP3	2.64	3.96	5.67	7.47	10.37
BP8	-6.87	-3.76	-2.01	-0.40	3.40
BPA	-2.05	0.05	1.17	1.99	3.57
BPAF	-5.89	-5.62	-5.24	-4.65	-4.32
BPAP	-4.11	-2.77	-1.83	-0.94	0.57
BPB	-5.70	-5.16	-4.32	-3.12	-1.81
BPF	-2.15	0.68	1.94	3.24	4.47
BPP	-7.89	-5.58	-3.39	-2.15	-0.49
BPS	-4.28	-2.28	-0.98	0.29	1.94
BPZ	-5.89	-5.62	-5.27	-4.65	-4.32
BUPB	-4.39	-2.50	-1.45	-0.03	3.33
BZPB	-4.87	-4.49	-3.97	-3.32	-1.68
DCP24	-1.23	0.51	1.57	2.49	3.60
DCP25	-6.72	0.43	1.59	2.63	5.60
DHB34	5.68	6.54	7.49	8.29	9.23
ETPB	-1.93	-0.60	0.43	1.83	6.02
HB4	9.34	10.08	10.7	11.39	12.66
HEPB	-4.89	-4.62	-4.27	-3.68	-3.32
MEPB	2.58	3.86	6.04	8.33	11.38
OH4BP	-0.77	0.42	0.97	1.70	3.47
OHETP	-4.62	-3.65	-1.81	-0.16	1.76
OHMEP	-1.66	0.63	1.91	3.64	6.79
PCP	-2.44	-0.83	0.03	0.81	1.96
PRPB	-0.78	1.29	3.05	5.34	8.63
TCC	-4.89	-4.60	-4.20	-3.43	-1.58
TCP245	-4.70	-4.20	-3.32	-2.43	-1.10
TCP246	-1.25	0.00	0.62	1.31	2.54
TCS	-0.99	1.45	3.04	4.77	7.48

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phthalates</i>					
MBZP	2.13	3.82	4.92	6.07	8.01
MCHP	-2.54	-2.25	-1.88	-1.11	-0.09
MCHPP	-4.84	-4.43	-3.84	-2.96	4.01
MCINP	0.47	1.85	2.62	3.43	4.55
MCIOP	1.83	3.50	4.41	5.36	6.99
MCMHP	0.58	3.00	3.91	5.11	6.93
MCPP	0.26	1.56	2.45	3.34	4.75
MECPP	2.50	4.22	4.96	6.09	7.94
MEHHP	3.21	4.54	5.46	6.64	8.54

MEOHP	1.77	3.22	4.24	5.40	7.25
MEP	3.35	4.61	5.43	6.31	8.33
MHPP	-2.30	-1.15	0.18	1.49	3.89
MHXP	-2.39	-1.77	-1.00	4.05	7.25
MIBP	2.36	3.54	4.40	5.25	6.74
MINP	-8.21	-7.95	-7.59	-7.05	-6.64
MIPP	-2.57	-2.28	-1.91	-1.28	-1.00
MMP	0.88	1.34	2.22	3.05	4.96
MNBP	3.56	4.58	5.45	6.27	7.59
MOP	-2.57	-2.30	-1.95	-1.33	-1.00
MPEP	-1.57	-1.28	-0.91	-0.33	0.00

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Pesticides</i>					
DMP	0.21	1.88	3.31	4.41	6.38
DEP	-0.94	1.33	2.39	3.65	5.04
DMTP	-4.54	0.12	1.67	3.79	5.62
DETP	-4.18	-2.13	-0.8	0.79	2.66
DMDP	-6.02	-3.09	-1.69	-0.03	3.49
DEDP	-5.89	-5.60	-5.20	-4.65	-4.32

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Trace Elements</i>					
As	1.98	2.90	3.60	4.29	5.70
Be	-7.07	-6.78	-6.38	-5.70	-5.36
Mo	4.86	6.08	6.65	7.34	8.29
Cd	-8.76	-8.00	-5.53	-4.40	-2.94
Tl	-3.56	-2.63	-2.23	-1.67	-0.90s
U	-8.39	-7.26	-6.41	-5.35	-3.94

Table S5: Distribution of log-transformed (base =2) and specific gravity-adjusted urinary phenol, phthalate, and trace element biomarker concentrations (ng/ml) among 248 TD participants included in the analysis

Chemical	5 th Percentile	25 th Percentile	Median	75 th Percentile	95 th Percentile
<i>Phenols</i>					
BP1	0.90	2.78	4.41	6.13	12.89
BP2	-3.84	-3.52	-3.15	-2.64	-0.97
BP3	2.76	4.53	6.06	7.83	10.57
BP8	-6.62	-3.29	-1.62	0.12	3.61
BPA	-1.16	0.19	1.16	1.97	3.50
BPAF	-5.84	-5.60	-5.33	-4.89	-4.32
BPAP	-3.96	-2.37	-1.56	-0.88	-0.06
BPB	-5.67	-5.16	-4.32	-3.34	-1.99
BPF	-2.20	0.27	1.40	2.95	4.36
BPP	-7.97	-6.64	-3.70	-2.14	-0.35
BPS	-4.32	-2.67	-1.64	-0.38	2.09
BPZ	-5.84	-5.60	-5.33	-4.88	-4.32
BUPB	-4.47	-2.58	-1.27	0.08	3.80
BZPB	-4.84	-4.54	-4.22	-3.65	-2.24
DCP24	-5.87	0.06	1.35	2.41	3.93
DCP25	-6.55	0.89	2.05	2.85	6.50
DHB34	4.88	6.41	7.27	7.91	9.01
ETPB	-2.25	-0.96	0.17	1.52	5.50
HB4	9.08	10.03	10.45	11.1	12.76
HEPB	-4.84	-4.60	-4.33	-3.89	-3.32
MEPB	1.91	3.49	4.87	7.11	10.92
OH4BP	-1.16	0.25	0.97	1.64	3.94
OHETP	-4.56	-3.54	-1.35	0.02	2.11
OHMEP	-3.32	0.64	2.28	3.75	6.34
PCP	-2.67	-0.63	0.09	0.99	2.23
PRPB	-1.64	0.79	2.32	4.01	8.25
TCC	-4.84	-4.54	-4.22	-3.70	-1.55
TCP245	-4.70	-4.14	-3.32	-2.37	-0.78
TCP246	-0.95	-0.05	0.54	1.22	2.90
TCS	-3.11	1.50	2.93	4.71	7.30

Chemical	5 th Percentile	25 th Percentile	Median	75 th Percentile	95 th Percentile
<i>Phthalates</i>					
MBZP	2.23	3.95	5.00	6.24	8.21
MCHP	-2.51	-2.23	-1.91	-1.47	-0.76
MCHPP	-4.84	-4.49	-4.01	-3.32	3.84
MCINP	0.54	1.76	2.39	3.21	4.86
MCIOP	2.29	3.63	4.33	5.06	6.47
MCMHP	1.43	3.32	4.17	5.02	6.13
MCPP	0.52	1.72	2.46	3.20	4.29

MECPP	3.19	4.31	5.10	6.02	7.13
MEHHP	3.45	4.73	5.52	6.48	7.89
MEOHP	2.28	3.44	4.24	5.28	6.66
MEP	3.70	4.67	5.37	6.31	8.33
MHPP	-1.90	-0.63	0.50	1.77	3.45
MHXP	-2.37	-1.66	-0.23	2.85	6.95
MIBP	2.27	3.42	4.14	5.07	6.29
MINP	-8.16	-7.92	-7.66	-7.21	-6.64
MIPP	-2.52	-2.28	-2.00	-1.52	-1.00
MMP	0.92	1.34	1.99	2.91	4.34
MNBP	3.51	4.72	5.41	6.10	7.18
MOP	-2.52	-2.28	-2.00	-1.52	-1.00
MPEP	-1.52	-1.28	-1.00	-0.52	0.00

Chemical	5 th Percentile	25 th Percentile	Median	75 th Percentile	95 th Percentile
<i>Pesticides</i>					
DMP	0.23	1.76	3.00	4.22	5.67
DEP	-0.58	0.73	1.66	2.80	4.29
DMTP	-2.05	0.27	1.88	3.64	5.54
DETP	-4.10	-2.32	-1.16	0.06	2.33
DMDP	-6.26	-3.31	-1.85	0.02	2.45
DEDP	-5.84	-5.57	-5.27	-4.80	-4.32

Chemical	5 th Percentile	25 th Percentile	Median	75 th Percentile	95 th Percentile
<i>Trace Elements</i>					
As	2.01	2.77	3.40	4.02	5.33
Be	-7.03	-6.76	-6.45	-5.98	-5.51
Mo	5.13	6.03	6.59	7.03	7.83
Cd	-8.82	-6.72	-5.38	-4.35	-3.21
Tl	s-3.51	-2.77	-2.25	-1.82	-1.08
U	-8.70	-7.47	-6.68	-5.90s	-4.54

Table S6: Distribution of log-transformed (base =2) and specific gravity-unadjusted urinary phenol, phthalate, and trace element biomarker concentrations (ng/ml) among 479 participants included in the analysis

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phenols</i>					
BP1	0.52	2.39	3.88	5.90	12.71
BP2	-3.32	-3.32	-3.32	-3.32	-0.94
BP3	2.41	4.14	5.72	7.70	10.64
BP8	-6.64	-3.74	-1.96	-0.13	3.58
BPA	-1.99	0.16	1.06	2.02	3.48
BPAF	-5.32	-5.32	-5.32	-5.32	-5.32
BPAP	-4.32	-2.63	-1.78	-1.02	0.16
BPB	-5.32	-5.32	-5.32	-3.36	-1.94
BPF	-2.00	0.36	1.53	2.79	4.26
BPP	-7.64	-6.42	-3.54	-2.31	-0.71
BPS	-5.32	-2.69	-1.45	-0.20	1.81
BPZ	-5.32	-5.32	-5.32	-5.32	-5.32
BUPB	-5.32	-2.79	-1.37	-0.06	3.33
BZPB	-4.32	-4.32	-4.32	-4.32	-1.90
DCP24	-4.09	0.17	1.34	2.45	3.70
DCP25	-6.64	0.53	1.71	2.68	5.75
DHB34	5.05	6.32	7.20	8.08	8.98
ETPB	-2.54	-0.84	0.23	1.58	5.63
HB4	8.64	9.92	10.5	11.15	12.62
HEPB	-4.32	-4.32	-4.32	-4.32	-4.32
MEPB	1.78	3.58	5.22	7.37	11.15
OH4BP	-1.04	0.14	0.79	1.63	3.61
OHETP	-4.32	-4.32	-1.60	0.01	2.02
OHMEP	-2.54	0.40	2.11	3.70	6.65
PCP	-3.39	-0.90	-0.07	0.88	2.23
PRPB	-1.44	0.87	2.41	4.46	8.47
TCC	-4.32	-4.32	-4.32	-4.32	-1.62
TCP245	-4.32	-4.32	-4.32	-2.45	-1.02
TCP246	-1.52	-0.21	0.52	1.28	2.77
TCS	-1.98	1.30	2.80	4.67	7.48

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phthalates</i>					
MBZP	2.01	3.75	4.87	6.11	8.14
MCHP	-2.00	-2.00	-2.00	-2.00	-0.38
MCHPP	-4.32	-4.32	-4.32	-3.15	3.95
MCINP	-0.09	1.66	2.41	3.27	4.81
MCIOP	1.63	3.37	4.26	5.25	6.73
MCMHP	0.85	2.98	3.96	5.00	6.39
MCPP	-0.08	1.45	2.42	3.28	4.55
MECPP	2.25	4.08	5.02	6.04	7.72
MEHHP	2.89	4.45	5.42	6.54	8.18

MEOHP	1.42	3.15	4.21	5.21	6.92
MEP	3.22	4.41	5.38	6.29	8.25
MHPP	-2.00	-2.00	0.32	1.48	3.88
MHXP	-2.00	-2.00	-0.55	3.44	7.32
MIBP	1.97	3.38	4.25	5.11	6.40
MINP	-7.64	-7.64	-7.64	-7.64	-7.64
MIPP	-2.00	-2.00	-2.00	-2.00	-2.00
MMP	1.32	1.32	1.32	2.96	4.86
MNBP	2.85	4.43	5.33	6.22	7.51
MOP	-2.00	-2.00	-2.00	-2.00	-2.00
MPEP	-1.00	-1.00	-1.00	-1.00	-1.00s

Chemical	5 th Percentile	25 th Percentile	Median	75 th Percentile	95 th Percentile
<i>Pesticides</i>					
DMP	-0.17	1.68	3.04	4.34	6.17
DEP	-1.04	0.74	1.92	3.20	4.81
DMTP	-3.96	-0.01	1.69	3.65	5.63
DETP	-4.42	-2.43	-1.05	0.34	2.40
DMDP	-6.64	-3.48	-1.84	-0.04	2.79
DEDP	-5.32	-5.32	-5.32	-5.32	-5.32

Chemical	5 th Percentile	25 th Percentile	Median	75 th Percentile	95 th Percentile
<i>Trace Elements</i>					
As	1.37	2.69	3.45	4.15	5.42
Be	-6.51	-6.51	-6.51	-6.51	-5.37
Mo	4.33	5.80	6.55	7.20s	8.22
Cd	-8.43	-8.43	-5.64	-4.44	-3.18
Tl	-3.91	-2.89	-2.25	-1.77	-0.91
U	-8.78	-7.48	-6.67	-5.75	-4.24

Table S7: Distribution of log-transformed (base =2) and specific gravity-unadjusted urinary phenol, phthalate, and trace element biomarker concentrations (ng/ml) among 231 ASD participants included in the analysis

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phenols</i>					
BP1	0.54	2.11	3.47	5.76	12.53
BP2	-3.32	-3.32	-3.32	-3.32	-0.96
BP3	2.41	3.89	5.48	7.51	10.36
BP8	-6.64	-4.05	-2.27	-0.34	3.54
BPA	-2.07	0.14	1.02	1.89	3.49
BPAF	-5.32	-5.32	-5.32	-5.32	-5.32
BPAP	-4.32	-2.81	-2.00	-1.02	0.09
BPB	-5.32	-5.32	-5.32	-3.31	-1.88
BPF	-2.00	0.57	1.75	2.88	4.41
BPP	-7.64	-5.39	-3.45	-2.25	-0.86
BPS	-4.08	-2.49	-1.03	0.08	1.81
BPZ	-5.32	-5.32	-5.32	-5.32	-5.32
BUPB	-5.32	-2.83	-1.48	-0.02	2.97
BZPB	-4.32	-4.32	-4.32	-4.32	-1.70
DCP24	-1.78	0.38	1.55	2.47	3.68
DCP25	-6.64	-0.13	1.52	2.46	5.42
DHB34	5.21	6.46	7.31	8.22	9.10
ETPB	-2.04	-0.66	0.42	1.61	6.01
HB4	8.73	9.91	10.61	11.35	12.65
HEPB	-4.32	-4.32	-4.32	-4.32	-4.32
MEPB	2.25	3.71	5.80	7.94	11.48
OH4BP	-0.91	0.12	0.80	1.50	3.15
OHETP	-4.32	-4.32	-1.83	-0.18	1.91
OHMEP	-1.85	0.46	1.81	3.52	6.83
PCP	-2.91	-0.99	-0.15	0.73	2.05
PRPB	-1.12	0.89	3.00	5.31	8.50
TCC	-4.32	-4.32	-4.32	-4.32	-1.74
TCP245	-4.32	-4.32	-4.32	-2.46	-1.21
TCP246	-1.61	-0.31	0.53	1.31	2.62
TCS	-1.50	1.26	2.88	4.67	7.74

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phthalates</i>					
MBZP	2.01	3.63	4.87	5.95	8.06
MCHP	-2.00	-2.00	-2.00	-2.00	-0.14
MCHPP	-4.32	-4.32	-4.32	-2.88	3.68
MCINP	-0.28	1.70	2.53	3.37	4.65
MCIOP	1.12	3.28	4.33	5.33	6.95
MCMHP	0.45	2.65	3.79	5.14	6.75
MCPP	-0.30	1.28	2.35	3.36	4.77
MECPP	2.05	3.90	4.96	6.10	8.01
MEHHP	2.47	4.27	5.39	6.58	8.82

MEOHP	1.06	3.03	4.10	5.36	7.23
MEP	3.12	4.37	5.28	6.28	8.31
MHPP	-2.00	-2.00	0.20	1.27	4.19
MHXP	-2.00	-2.00	-0.89	3.81	7.38
MIBP	1.84	3.50	4.36	5.16	6.53
MINP	-7.64	-7.64	-7.64	-7.64	-7.64
MIPP	-2.00	-2.00	-2.00	-2.00	-2.00
MMP	1.32	1.32	1.32	3.00	4.94
MNBP	2.71	4.34	5.30	6.29	7.74
MOP	-2.00	-2.00	-2.00	-2.00	-2.00
MPEP	-1.00	-1.00	-1.00	-1.00	-1.00

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Pesticides</i>					
DMP	-0.44	1.77	3.17	4.37	6.26
DEP	-1.27	1.13	2.28	3.43	4.87
DMTP	-5.32	-0.04	1.60	3.63	5.52
DETP	-4.42	-2.30	-0.88	0.70	2.52
DMDP	-6.64	-3.39	-1.84	-0.08	3.06
DEDP	-5.32	-5.32	-5.32	-5.32	-5.32

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Trace Elements</i>					
As	1.32	2.78	3.50	4.38	5.70
Be	-6.51	-6.51	-6.51	-6.51	-5.26
Mo	4.13	5.76	6.60	7.37	8.30
Cd	-8.43	-8.43	-5.65	-4.62	-2.90s
Tl	-3.98	-2.87	-2.28	-1.69	-0.84
U	-8.67	-7.30	-6.57	-5.58	-4.13

Table S8: Distribution of log-transformed (base =2) and specific gravity-unadjusted urinary phenol, phthalate, and trace element biomarker concentrations (ng/ml) among 248 TD participants included in the analysis

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phenols</i>					
BP1	0.53	2.73	4.31	6.04	12.79
BP2	-3.32	-3.32	-3.32	-3.32	-0.89
BP3	2.63	4.35	6.01	7.76	10.67
BP8	-6.64	-3.43	-1.82	0.18	3.72
BPA	-1.58	0.16	1.08	2.11	3.34
BPAF	-5.32	-5.32	-5.32	-5.32	-5.32
BPAP	-4.32	-2.45	-1.66	-1.02	0.25
BPB	-5.32	-5.32	-5.32	-3.48	-2.11
BPF	-2.00	0.15	1.39	2.61	4.20
BPP	-7.64	-7.64	-3.71	-2.38	-0.65
BPS	-5.32	-2.86	-1.63	-0.42	1.87
BPZ	-5.32	-5.32	-5.32	-5.32	-5.32
BUPB	-5.32	-2.68	-1.3	-0.14	3.40
BZPB	-4.32	-4.32	-4.32	-4.32	-2.32
DCP24	-6.64	-0.13	1.22	2.44	3.69
DCP25	-6.64	0.81	1.85	2.84	6.37
DHB34	4.86	6.27	7.05	7.83	8.83
ETPB	-2.85	-0.89	0.08	1.5	5.48
HB4	8.44	9.92	10.42	10.97	12.52
HEPB	-4.32	-4.32	-4.32	-4.32	-4.32
MEPB	1.54	3.46	4.75	6.89	10.82
OH4BP	-1.22	0.14	0.79	1.74	3.71
OHETP	-4.32	-4.32	-1.45	0.09	2.08
OHMEP	-4.32	0.3	2.33	3.85	6.30
PCP	-3.42	-0.83	-0.02	0.99	2.26
PRPB	-1.89	0.85	2.19	4.15	7.98
TCC	-4.32	-4.32	-4.32	-4.32	-1.54
TCP245	-4.32	-4.32	-3.31	-2.42	-0.64
TCP246	-1.43	-0.19	0.48	1.26	2.81
TCS	-2.86	1.34	2.73	4.67	7.40

Chemical	5th Percentile	25th Percentile	Median	75th Percentile	95th Percentile
<i>Phthalates</i>					
MBZP	2.06	3.90	4.89	6.38	8.13
MCHP	-2.00	-2.00	-2.00	-2.00	-0.81
MCHPP	-4.32	-4.32	-4.32	-4.32	4.04
MCINP	0.08	1.62	2.32	3.15	5.02
MCIOP	2.05	3.48	4.24	5.22	6.51
MCMHP	1.15	3.20	4.14	4.94	6.20
MCPP	0.24	1.53	2.49	3.21	4.34
MECPP	2.72	4.22	5.09	5.89	7.42
MEHHP	2.97	4.65	5.53	6.50	7.98

MEOHP	1.62	3.29	4.26	5.16	6.72
MEP	3.54	4.42	5.44	6.32	8.13
MHPP	-2.00	-0.61	0.51	1.64	3.75
MHXP	-2.00	-2.00	-0.39	3.12	7.03
MIBP	2.04	3.23	4.15	5.03	6.20
MINP	-7.64	-7.64	-7.64	-7.64	-7.64
MIPP	-2.00	-2.00	-2.00	-2.00	-2.00
MMP	1.32	1.32	1.32	2.89	4.52
MNBP	3.28	4.58	5.38	6.19	7.28
MOP	-2.00	-2.00	-2.00	-2.00	-2.00
MPEP	-1.00	-1.00	-1.00	-1.00	-1.00s

Chemical	5 th Percentile	25 th Percentile	Median	75 th Percentile	95 th Percentile
<i>Pesticides</i>					
DMP	0.09	1.65	2.96	4.31	6.13
DEP	-0.82	0.53	1.58	2.91	4.39
DMTP	-2.23	0.05	1.91	3.66	5.72
DETP	-4.42	-2.49	-1.23	0.08	1.97
DMDP	-6.64	-3.59	-1.88	0.06	2.52
DEDP	-5.32	-5.32	-5.32	-5.32	-5.32

Chemical	5 th Percentile	25 th Percentile	Median	75 th Percentile	95 th Percentile
<i>Trace Elements</i>					
As	1.37	2.60	3.36	4.03	5.10
Be	-6.51	-6.51	-6.51	-6.51	-6.51
Mo	4.67	5.91	6.53	7.03	7.90s
Cd	-8.43	-6.82	-5.61	-4.42	-3.28
Tl	-3.87	-2.90	-2.23	-1.83	-1.21
U	-8.83	-7.57	-6.79	-5.93	-4.55

Table S9: Univariate associations between ASD diagnosis and log-transformed (base =2), specific gravity-adjusted urinary phenol, phthalate, and trace element biomarker concentrations

Chemical	OR	95% CI	pvalue
BP1	0.96	(0.91, 1.02)	0.183
BP2	0.99	(0.82, 1.21)	0.953
BP3	0.97	(0.9, 1.05)	0.415
BP8	0.94	(0.89, 1.01)	0.080
BPA	0.98	(0.87, 1.11)	0.780
BPAF	1.33	(0.93, 1.9)	0.119
BPAP	0.94	(0.81, 1.08)	0.374
BPB	1.10	(0.95, 1.28)	0.212
BPF	1.12	(1.01, 1.24)	0.034
BPP	1.02	(0.94, 1.1)	0.631
BPS	1.06	(0.95, 1.18)	0.297
BPZ	1.23	(0.88, 1.73)	0.224
BUPB	1.01	(0.93, 1.09)	0.799
BZPB	1.24	(1.01, 1.52)	0.039
DCP24	1.10	(1.01, 1.2)	0.029
DCP25	0.98	(0.92, 1.04)	0.567
DHB34	1.19	(1.02, 1.4)	0.03
ETPB	1.05	(0.98, 1.14)	0.186
HB4	1.15	(0.97, 1.35)	0.098
HEPB	1.30	(0.9, 1.87)	0.166
MEPB	1.13	(1.06, 1.22)	<0.001
OH4BP	0.98	(0.85, 1.12)	0.74
OHETP	0.89	(0.81, 0.97)	0.011
OHMEP	1.00	(0.93, 1.08)	0.921
PCP	0.99	(0.88, 1.13)	0.922
PRPB	1.09	(1.02, 1.16)	0.011
TCC	0.95	(0.83, 1.1)	0.497
TCP245	0.94	(0.81, 1.1)	0.466
TCP246	0.95	(0.82, 1.11)	0.544
TCS	1.05	(0.97, 1.12)	0.214
MBZP	1.01	(0.91, 1.12)	0.841
MCHP	1.32	(1.03, 1.7)	0.027
MCHPP	1.04	(0.96, 1.12)	0.301
MCINP	1.00	(0.9, 1.12)	0.961
MCIOP	1.05	(0.92, 1.19)	0.502
MCMHP	0.97	(0.89, 1.07)	0.597
MCPP	1.02	(0.88, 1.19)	0.751
MECPP	1.07	(0.95, 1.21)	0.287
MEHHP	1.10	(0.97, 1.26)	0.140
MEOHP	1.10	(0.97, 1.25)	0.133
MEP	0.99	(0.87, 1.12)	0.821
MHPP	0.97	(0.87, 1.09)	0.661
MHXP	1.07	(1, 1.14)	0.039
MIBP	1.13	(0.98, 1.3)	0.102

MINP	1.26	(0.86, 1.84)	0.243
MIPP	1.40	(1.02, 1.91)	0.036
MMP	1.05	(0.91, 1.21)	0.545
MNBP	1.11	(0.95, 1.3)	0.177
MOP	1.18	(0.87, 1.59)	0.290
MPEP	1.40	(1, 1.96)	0.048
DMP	1.05	(0.95, 1.16)	0.374
DEP	1.14	(1.02, 1.27)	0.023
DMTP	0.97	(0.91, 1.05)	0.462
DETP	1.09	(0.99, 1.2)	0.077
DMDP	1.04	(0.97, 1.12)	0.273
DEDP	1.11	(0.86, 1.45)	0.423
As	1.24	(1.03, 1.49)	0.021
Be	1.49	(1.08, 2.07)	0.016
Mo	1.11	(0.92, 1.35)	0.285
Cd	0.92	(0.84, 1.01)	0.079
Tl	1.20	(0.94, 1.53)	0.139
U	1.25	(1.08, 1.45)	0.003

All models were adjusted for covariates. Pvalues are not adjusted for multi-comparison error.

Table S10: Univariate associations between ASD diagnosis and log-transformed (base =2), specific gravity-unadjusted urinary phenol, phthalate, and trace element biomarker concentrations

Chemical	OR	95% CI	pvalue
BP1	0.96	(0.91, 1.02)	0.152
BP2	0.93	(0.75, 1.14)	0.473
BP3	0.96	(0.89, 1.04)	0.310
BP8	0.94	(0.88, 1)	0.062
BPA	0.97	(0.87, 1.08)	0.578
BPAP	0.91	(0.79, 1.05)	0.205
BPB	1.06	(0.91, 1.22)	0.450
BPF	1.11	(0.99, 1.23)	0.065
BPP	1.01	(0.93, 1.09)	0.806
BPS	1.04	(0.94, 1.15)	0.473
BPZ	1.19	(0.57, 2.52)	0.642
BUPB	1.00	(0.92, 1.08)	0.995
BZPB	1.20	(0.96, 1.5)	0.108
DCP24	1.08	(1, 1.17)	0.057
DCP25	0.98	(0.92, 1.04)	0.458
DHB34	1.14	(0.97, 1.32)	0.106
ETPB	1.04	(0.97, 1.12)	0.282
HB4	1.09	(0.93, 1.27)	0.287
MEPB	1.12	(1.05, 1.2)	0.001
OH4BP	0.95	(0.84, 1.09)	0.493
OHETP	0.88	(0.81, 0.97)	0.006
OHMEP	1.00	(0.93, 1.07)	0.891
PCP	0.97	(0.87, 1.09)	0.660
PRPB	1.08	(1.01, 1.15)	0.022
TCC	0.91	(0.78, 1.07)	0.255
TCP245	0.92	(0.79, 1.07)	0.258
TCP246	0.93	(0.81, 1.07)	0.324
TCS	1.03	(0.96, 1.11)	0.350
MBZP	1.00	(0.9, 1.1)	0.927
MCHP	1.29	(0.97, 1.73)	0.083
MCHPP	1.03	(0.96, 1.11)	0.408
MCINP	0.99	(0.9, 1.1)	0.892
MCIOP	1.02	(0.9, 1.14)	0.793
MCMHP	0.97	(0.88, 1.06)	0.470
MCPP	0.99	(0.87, 1.13)	0.929
MECPP	1.04	(0.93, 1.17)	0.465
MEHHP	1.07	(0.95, 1.2)	0.291
MEOHP	1.07	(0.95, 1.2)	0.273
MEP	0.97	(0.86, 1.09)	0.611
MHPP	0.96	(0.86, 1.07)	0.466
MHXP	1.06	(1, 1.13)	0.062
MIBP	1.08	(0.95, 1.23)	0.240
MINP	0.96	(0.59, 1.55)	0.857
MIPP	1.51	(0.89, 2.57)	0.128

MMP	1.01	(0.88, 1.16)	0.883
MNBP	1.06	(0.92, 1.21)	0.413
MOP	1.07	(0.69, 1.64)	0.775
MPEP	2.08	(0.92, 4.7)	0.077
DMP	1.03	(0.94, 1.13)	0.564
DEP	1.11	(1, 1.23)	0.056
DMTP	0.97	(0.9, 1.04)	0.340
DETP	1.07	(0.97, 1.17)	0.157
DMDP	1.03	s(0.96, 1.11)	0.401
DEDP	1.00	(0.73, 1.37)	0.997
As	1.15	(0.97, 1.35)	0.100
Be	1.89	(1.11, 3.22)	0.020
Mo	1.04	(0.88, 1.23)	0.631
Cd	0.91	(0.82, 1)	0.043
Tl	1.07	(0.88, 1.32)	0.488
U	1.21	(1.05, 1.39)	0.010

All models were adjusted for covariates. Pvalues are not adjusted for multi-comparison error.

Table S11: Results of SiRF from the three different data partitions

- 70% training and 30% testing data

Interactions	Prevalence	Precision	Stability
DEP+_U+	0.069	0.555	0.884
DEP+_TCP246+	0.065	0.473	0.568
Cd+_DEP+	0.109	0.447	0.944
BPAP+_DEP+	0.115	0.448	0.928

- 75% training and 25% testing data

Interactions	Prevalence	Precision	Stability
DEP+_Mo+	0.076	0.558	0.936
DEP+_MEPB+	0.053	0.573	0.696
DEP+_U+	0.049	0.547	0.620
DEP+_TCP246+	0.083	0.480	0.792
Cd+_DEP+	0.100	0.460	0.848
BPAP+_DEP+	0.117	0.449	0.928

- 80% training and 20% testing data

Interactions	Prevalence	Precision	Stability
DEP+_MEPB+	0.052	0.565	0.672
DEP+_TCP246+	0.098	0.484	0.908
Cd+_DEP+	0.117	0.464	0.956
Cd+_TCP246+	0.078	0.448	0.512

Table S12: Results of SiRF from the three different data partitions without chemicals whose % of detection above LOD was less than 60%

- 70% training and 30% testing data

Interactions	Prevalence	Precision	Stability
DEP+_U+	0.062	0.553	0.868
DEP+_DETP+	0.055	0.506	0.660
DEP+_TCP246+	0.067	0.474	0.624
DEP+_MCMHP+	0.074	0.447	0.708
Cd+_DEP+	0.085	0.445	0.756
BPAP+_DEP+	0.108	0.443	0.884

- 75% training and 25% testing data

Interactions	Prevalence	Precision	Stability
DEP+_Mo+	0.069	0.564	0.864
DEP+_MEPB+	0.049	0.566	0.664
DEP+_U+	0.042	0.542	0.528
DEP+_TI+	0.051	0.527	0.576
DEP+_TCP246+	0.078	0.480	0.764
DEP+_MCP+	0.052	0.461	0.504
DEP+_MCMHP+	0.061	0.449	0.596
Cd+_DEP+	0.078	0.456	0.708
BPAP+_DEP+	0.094	0.444	0.792

- 80% training and 20% testing data

Interactions	Prevalence	Precision	Stability
DEP+_TCP246+	0.086	0.485	0.808
Cd+_DEP+	0.093	0.461	0.856
DEP+_MCMHP+	0.071	0.444	0.628
BPAP+_DEP+	0.090	0.450	0.724

Table S13: Results of SiRF when the whole dataset was used to test the model trained on 75% data

Interactions	Prevalence	Precision	Stability
DEP+_Mo+	0.076	0.558	0.936
DEP+_MEPB+	0.053	0.573	0.696
DEP+_U+	0.049	0.547	0.620
DEP+_TCP246+	0.083	0.480	0.792
Cd+_DEP+	0.100	0.460	0.848
BPAP+_DEP+	0.117	0.449	0.928

Tuning Parameters for WQS-SiRF

1. **WQS:** $q = 10$, $\text{signal} = \text{"t2"}$, $b = 500$, $\text{rs} = \text{T}$, $n_vars = 12$, $\text{rh} = 100$, $\text{validation} = 0.25$, $\text{seed} = 123123123$, $b1_pos = \text{T}$, $\text{family} = \text{"binomial"}$, $\text{plan_strategy} = \text{"multicore"}$
2. **SiRF:** seed was set at $\text{set.seed}(123456)$ and $n.\text{iter}=5$, $n.\text{core}=1$, $\text{select.iter} = \text{T}$, $n.\text{bootstrap}=500$
3. **Selection of training and testing data**

- **70% training and 30% testing data:**

```
set.seed(123456)
train.id <- sample(seq(1,n), ceiling(n*70/100))
test.id <- setdiff(1:n, train.id)
```

- **75% training and 25% testing data:**

```
set.seed(123456)
train.id <- sample(seq(1,n), ceiling(n*75/100))
test.id <- setdiff(1:n, train.id)
```

- **80% training and 20% testing data:**

```
set.seed(123456)
train.id <- sample(seq(1,n), ceiling(n*80/100))
test.id <- setdiff(1:n, train.id)
```

References

Bennett, D. H., Busgang, S. A., Kannan, K., Parsons, P. J., Takazawa, M., Palmer, C. D., Schmidt, R. J., Doucette, J. T., Schweitzer, J. B., Gennings, C., and Hertz-Picciotto, I. (2022), "Environmental exposures to pesticides, phthalates, phenols and trace elements are associated with neurodevelopment in the CHARGE study," *Environ Int*, 161, 107075. DOI: 10.1016/j.envint.2021.107075.