Metal Bioaccumulation Prediction via QSPR-q-RASPR Synergy and Cross-Species Risk Analysis

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Table S1. Summary of Y-randomization test results (50 Permutations) for QSPR and q-RASPR individual species models.

Species	***Model Type***	***Average R***	***Average R^2***	***Average Q^2(LOO)***	***cRp^2***
			Metal		
Algae	QSPR	0.48	0.28	-0.58	0.66
	q-RASPR	0.44	0.22	-0.75	0.56
Crustaceans	QSPR	0.46	0.27	-0.91	0.58
	q-RASPR	0.45	0.25	-0.74	0.75
Fish	QSPR	0.44	0.23	-0.64	0.80
	q-RASPR	0.43	0.22	-0.42	0.78
Mollusc	QSPR	0.44	0.23	-0.79	0.67
	q-RASPR	0.39	0.19	-1.15	0.64
Plant	QSPR	0.39	0.19	-0.76	**0.41**
	q-RASPR	0.45	0.25	-3.06	0.76
			Metal Halide		
Algae	QSPR	0.45	0.24	-0.57	0.61
	q-RASPR	0.52	0.31	-0.49	0.79
Crustaceans	QSPR	0.41	0.21	-0.52	0.66
	q-RASPR	0.45	0.25	-0.65	0.72
Fish	QSPR	0.45	0.24	-0.52	0.67
	q-RASPR	0.37	0.16	-0.50	0.64
Mollusc	QSPR	0.41	0.20	-9.22	0.70
	q-RASPR	0.41	0.20	-1.00	0.77
Plant	QSPR	0.44	0.26	-1.85	0.62
	q-RASPR	0.42	0.22	-1.70	0.78
			Metal Oxide		
Fish	QSPR	0.44	0.22	-0.73	0.72
	q-RASPR	0.44	0.24	-0.52	0.56

Values marked with bold are below the optimum threshold.

Table S2. Summary of Y-randomization test results (50 Permutations) for SbSDs models (QSPR and q-RASPR).

Species	***Model Type***	***Average R***	***Average R^2***	***Average Q^2(LOO)***	***cRp^2***
			Metal		
Mean	QSPR	0.37	0.18	-0.50	0.72
	q-RASPR	0.42	0.21	-0.53	0.78
SD	QSPR	0.40	0.20	-0.42	0.66
	q-RASPR	0.37	0.18	-0.47	0.70
HC5	q-RASPR	0.39	0.22	-0.97	0.91
			Metal Halide		
Mean	QSPR	0.38	0.19	-0.72	0.66
	q-RASPR	0.43	0.22	-0.73	0.75
SD	QSPR	0.44	0.22	-0.68	**0.39**
	q-RASPR	0.28	0.12	-0.37	0.78
HC5	q-RASPR	0.40	0.22	-1.87	0.90

Values marked with bold are below the optimum threshold.

Table S3. Mean and SD models representing SSDs modeling.

Sr.	**Equation**	**Ntrain**	**R^2**	**Q^2**	**$RMSE_c$**	**Ntest**	**Q^2_{F1}**	**Q^2_{F2}**	**Q^2_{F3}**	**$RMSE_P$**

No.										
					Metals					
1	$Mean\_p(BCF) = 7.54 + 0.0441 \times Electrons\_ActiveM -$	12	0.79	0.61	0.43	5	<0.5	<0.5	<0.5	0.78
2	$Mean\_p(BCF) = 3.48 + 1.8 \times gm(Euc)[Banerjee - Ro$	12	0.87	0.79	0.30	5	0.86	0.86	0.86	0.34
3	$SD\_p(BCF) = 4.43 + 0.0151 \times Neutons\_ActiveM - 0.7$	13	0.74	0.61	0.23	3	0.84	0.84	0.84	0.25
4	$SD\_p(BCF) = 1.15 + 0.342 \times MaxNeg(GK) + 1.01 \times$	12	0.76	0.60	0.18	5	0.80	0.80	0.81	0.28
					Metal Halides					
1	$Mean\_p(BCF) = 0.70 + 5.07 \times VWR\_ActivM + 0.646$	10	0.74	<0.50	0.19	2	<0.50	<0.50	<0.50	1.38
2	$Mean\_p(BCF) = 2.78 + 5.65 \times SD\ Activity(Euc) - 15.$	10	0.84	0.73	0.28	2	<0.50	<0.50	<0.50	1.38
3	$SD\_p(BCF) = - 0.387 - 0.381 \times logKow + 0.00989 \times$	10	<0.60	<0.50	0.29	2	<0.50	<0.50	<0.50	0.85
4	$SD_{p(BCF)} = 0.335 + 1.32 \times MaxPos(LK))$	10	0.81	0.72	0.18	1	0.60	NA	0.51	0.52

Table S4. Summary of applicability domain analysis towards QSPR, q-RASPR and SbSDs models.

Species	Compound type	Model	Ntotal	Outliers	Outside AD	%Training coverage	%Test coverage	Total (%)
Algae	Metal	QSPR	12	0	0	100	100	100
		q-RASPR	12	0	0	100	100	100
Crustaceans	Metal	QSPR	12	0	0	100	100	100
		q-RASPR	12	0	0	100	100	100
Fish	Metal	QSPR	16	0	0	100	100	100
		q-RASPR	16	0	0	100	100	100
Mollusc	Metal	QSPR	14	0	0	100	100	100
		q-RASPR	14	0	0	100	100	100
Plant	Metal	QSPR	10	0	-	100	-	100
		q-RASPR	10	0	-	100	-	100

Mean	Metal	QSPR	17	0	0	100	100	100
		q-RASPR	17	0	0	100	100	100
SD	Metal	QSPR	17	0	0	100	100	100
		q-RASPR	17	0	0	100	100	100
HC5	Metal	q-RASPR	17	1	1	93	75	89
Algae	Metal Halides	QSPR	11	0	0	100	100	100
		q-RASPR	11	0	0	100	100	100
Crustaceans	Metal Halides	QSPR	14	0	0	100	100	100
		q-RASPR	14	0	0	100	100	100
Fish	Metal Halides	QSPR	19	1	0	92.86	100	94.73
		q-RASPR	19	0	0	100	100	100
Mollusc	Metal Halides	QSPR	13	0	0	100	100	100
		q-RASPR	13	0	0	100	100	100
Plant	Metal Halides	QSPR	11	0	0	100	100	100
		q-RASPR	11	0	0	100	100	100
Mean	Metal Halides	QSPR	10	0	0	100	100	100
		q-RASPR	10	0	0	100	100	100
SD	Metal Halides	QSPR	11	0	0	100	100	100
		q-RASPR	11	0	0	100	100	100
HC5	Metal Halides	q-RASPR	10	0	0	100	100	100
Fish	Metal Oxide	QSPR	14	0	0	100	100	100
		q-RASPR	14	0	0	100	100	100

Table S5. Quantitative results obtained for QSPR and q-RASPR individual species models.

Species	*Model Type*	*Split*	*R2 test*	*Q2 (LOO)*	*RMSEc*	*Q2F1*	*Q2F2*	*Q2F3*	*RMSEP*
				Metals					
Algae	QSPR	Split 1	0.81	0.51	0.48	<0.50	<0.50	<0.50	2.25
		Split 2	0.68	<0.50	0.90	<0.50	<0.50	<0.50	1.07
		Split 3	0.68	<0.50	0.92	<0.50	<0.50	<0.50	0.94

	q-RASPR	Split 1	0.90	0.82	0.35	0.74	0.74	0.90	0.80
		Split 2	0.90	0.84	0.47	0.87	0.87	0.97	0.20
		Split 3	0.91	0.86	0.48	0.58	0.58	0.92	0.12
Crustaceans	QSPR	Split 1	0.68	<0.50	0.40	<0.50	<0.50	<0.50	1.48
		Split 2	0.66	<0.50	0.50	<0.50	<0.50	<0.50	1.33
		Split 3	0.62	<0.50	0.55	<0.50	<0.50	<0.50	1.18
	q-RASPR	Split 1	0.86	0.73	0.33	0.57	0.57	0.74	0.52
		Split 2	0.82	0.67	0.37	0.80	0.80	0.89	0.36
		Split 3	0.86	0.75	0.35	0.73	0.73	0.74	0.43
Fish	QSPR	Split 1	0.85	0.71	0.27	<0.50	<0.50	<0.50	2.39
		Split 2	0.78	<0.50	0.59	<0.50	<0.50	<0.50	2.37
		Split 3	0.71	0.53	0.79	<0.50	<0.50	<0.50	3.22
	q-RASPR	Split 1	0.88	0.73	0.72	<0.50	<0.50	<0.50	0.38
		Split 2	0.89	0.73	0.69	<0.50	<0.50	<0.50	0.58
		Split 3	0.87	0.71	0.71	<0.50	<0.50	0.73	0.45
Molluscs	QSPR	Split 1	0.73	0.59	0.73	0.64	0.64	0.66	0.67
		Split 2	0.75	0.61	0.69	0.52	0.52	0.57	0.81
		Split 3	0.77	0.52	0.65	0.55	0.55	0.55	0.93
	q-RASPR	Split 1	0.70	0.53	0.73	0.65	0.65	0.68	0.66
		Split 2	0.70	0.53	0.73	0.65	0.65	0.68	0.66
		Split 3	0.70	0.54	0.74	0.71	0.71	0.72	0.58
Plant		No Split				No Test Set			
					Metal halide				
Algae	QSPR	Split 1	0.71	0.50	0.36	0.72	NA	0.66	0.28
		Split 2	0.71	<0.50	0.36	0.79	NA	0.74	0.23
		Split 3	0.82	0.68	0.26	<0.50	NA	<0.50	0.89
	q-RASPR	Split 1	0.92	0.86	0.19	0.69	NA	0.62	0.23
		Split 2	0.91	0.85	0.20	0.91	NA	0.89	0.04
		Split 3	0.91	0.85	0.20	0.96	NA	0.95	0.10

Crustaceans	QSPR	Split 1	0.73	0.59	0.70	<0.50	<0.50	<0.50	2.57
		Split 2	0.68	0.53	0.77	<0.50	<0.50	<0.50	2.34
		Split 3	0.67	0.51	0.72	<0.50	<0.50	<0.50	2.36
	q-RASPR	Split 1	0.84	0.54	0.43	0.66	0.66	0.66	1.20
		Split 2	0.78	0.68	0.63	0.68	0.68	0.71	0.87
		Split 3	0.83	0.75	0.55	0.60	0.60	0.61	1.01
Fish	QSPR	Split 1	0.66	0.51	0.52	<0.50	<0.50	<0.50	1.69
		Split 2	0.60	<0.50	0.62	<0.50	<0.50	<0.50	1.27
		Split 3	<0.60	<0.50	0.76	<0.50	<0.50	<0.50	1.11
	q-RASPR	Split 1	0.81	0.60	0.43	0.54	0.54	0.55	0.94
		Split 2	0.75	0.59	0.54	0.53	0.53	0.53	0.84
		Split 3	0.72	0.58	0.56	0.64	0.64	0.65	0.75
Molluscs	QSPR	Split 1	0.79	0.53	0.57	0.57	0.57	0.73	0.50
		Split 2	0.80	0.65	0.49	0.61	0.61	0.62	1.01
		Split 3	0.79	0.59	0.57	0.55	0.55	0.71	0.47
	q-RASPR	Split 1	0.87	0.70	0.45	0.65	0.65	0.66	0.56
		Split 2	0.84	0.72	0.52	0.88	0.88	0.93	0.20
		Split 3	0.84	0.72	0.52	0.83	0.83	0.93	0.22
Plants	QSPR	Split 1	0.73	0.51	0.59	0.60	NA	0.51	0.36
		Split 2	0.80	0.55	0.46	<0.50	NA	<0.50	1.34
		Split 3	0.75	0.61	0.58	<0.50	NA	<0.50	0.58
	q-RASPR	Split 1	0.87	0.78	0.42	0.99	NA	0.99	0.06
		Split 2	0.87	0.78	0.42	0.99	NA	0.99	0.06
		Split 3	0.87	0.75	0.41	0.93	NA	0.92	0.22
				Metal Oxide					
Fish	QSPR	Split 1	0.80	0.51	0.42	<0.50	<0.50	<0.50	2.79
		Split 2	0.71	<0.50	0.50	<0.50	<0.50	<0.50	2.80
		Split 3	0.68	0.32	0.62	<0.50	<0.50	<0.50	3.00
	q-RASPR	Split 1	0.81	<0.50	0.86	<0.50	<0.50	<0.50	2.89

		Split 2	0.69	<0.50	1.12	<0.50	<0.50	<0.50	1.91
		Split 3	0.62	<0.50	0.69	<0.50	<0.50	<0.50	2.33

Table S6. Quantitative results obtained for SbSDs models (QSPR and q-RASPR).

SbSD Type	***Model Type***	***Split***	***R2 test***	***Q2 (LOO)***	***RMSEc***	***Q2F1***	***Q2F2***	***Q2F3***	***RMSEP***
Metals									
Mean	QSPR	Split 1	0.68	0.53	0.51	<0.50	<0.50	<0.50	0.85
		Split 2	0.69	0.56	0.52	<0.50	<0.50	<0.50	0.84
		Split 3	0.70	0.56	0.51	<0.50	<0.50	<0.50	0.85
	q-RASPR	Split 1	0.90	0.83	0.29	0.73	0.73	0.73	0.35
		Split 2	0.91	0.85	0.28	0.69	0.69	0.72	0.35
		Split 3	0.81	0.68	0.27	0.89	0.80	0.88	0.43
SD	QSPR	Split 1	0.77	0.67	0.25	0.85	0.85	0.90	0.10
		Split 2	0.77	0.69	0.21	0.71	0.71	0.72	0.33
		Split 3	0.73	0.60	0.21	0.74	0.74	0.75	0.37
	q-RASPR	Split 1	0.89	0.81	0.16	0.70	0.70	0.72	0.28
		Split 2	0.75	0.59	0.18	0.84	0.84	0.85	0.27
		Split 3	0.82	0.73	0.22	0.89	0.89	0.90	0.11
HC5	q-RASPR	Split 1	0.87	0.65	0.83	0.98	0.98	0.98	1.28
		Split 2	0.98	0.89	0.84	0.78	0.78	0.82	0.87
		Split 3	0.98	0.89	0.75	0.68	0.68	0.73	1.14
Metal halide									
Mean	QSPR	Split 1	<0.60	<0.50	0.46	<0.50	<0.50	<0.50	0.85
		Split 2	<0.60	<0.50	0.5	<0.50	<0.50	<0.50	0.65
		Split 3	<0.60	<0.50	0.38	<0.50	<0.50	<0.50	0.89
	q-RASPR	Split 1	0.76	0.51	0.35	<0.50	<0.50	<0.50	0.88

		Split 2	0.76	<0.50	0.35	<0.50	<0.50	<0.50	0.95
		Split 3	0.72	<0.50	0.33	<0.50	<0.50	<0.50	0.86
SD	QSPR	Split 1	<0.60	<0.50	0.3	<0.50	<0.50	<0.50	0.8
		Split 2	<0.60	<0.50	0.41	<0.50	<0.50	<0.50	0.41
		Split 3	<0.60	<0.50	0.44	0.91	0.91	0.91	0.11
	q-RASPR	Split 1	0.75	0.64	0.22	0.84	NA	0.81	0.21
		Split 2	0.74	0.64	0.22	0.90	NA	0.88	0.16
		Split 3	0.75	0.63	0.23	0.99	NA	0.99	0.028
HC5	q-RASPR	Split 1	0.84	0.54	0.90	0.99	0.99	0.99	0.51
		Split 2	0.98	0.97	0.83	<0.50	<0.50	<0.50	0.82
		Split 3	0.98	0.92	0.75	0.89	0.89	0.89	1.14

Table S7. Quantitative metrics obtained for experiment-derived and synthetic-derived (SMOGN) QSPR and q-RASPR models.

Species	***Model Type***	N_{train}	R^2	***Q2 (LOO)***	$RMSE_c$	N_{test}	Q^2_{F1}	Q^2_{F2}	Q^2_{F3}	$RMSE_p$
					Metal					
Algae	*QSPR*	10	0.78	0.51	0.75	2	<0.5	<0.5	<0.5	1.75
	QSPR-SMOGN	10	0.78	0.51	0.75	10	0.66	0.66	0.67	1.12
	q-RASPR	10	0.91	0.84	0.43	2	0.82	0.82	0.91	0.51
	q-RASPR-SMOGN	10	0.91	0.84	0.43	11	0.83	0.83	0.86	0.64
Crustaceans	*QSPR*	10	0.69	0.54	0.38	2	<0.5	<0.5	<0.5	1.46
	QSPR-SMOGN	10	0.69	0.54	0.38	11	0.59	0.59	0.59	0.55
	q-RASPR	10	0.85	0.71	0.34	2	0.77	0.77	0.8	0.49
	q-RASPR-SMOGN	10	0.85	0.71	0.34	14	0.83	0.83	0.83	0.39
Fish	*QSPR*	10	0.9	0.67	0.41	8	<0.5	<0.5	<0.5	2.51

	QSPR-SMOGN	10	0.9	0.67	0.41	15	0.5	0.5	0.5	0.83
	q-RASPR	12	0.87	0.71	0.75	4	0.83	0.83	0.98	0.08
	q-RASPR-SMOGN	12	0.87	0.71	0.75	20	0.92	0.92	0.92	0.61
Molluscs	*QSPR*	10	0.77	0.65	0.6	3	0.57	0.54	0.56	1.11
	QSPR-SMOGN	10	0.77	0.65	0.6	16	0.66	0.66	0.66	0.83
	q-RASPR	11	0.72	0.59	0.75	3	0.57	0.57	0.66	0.44
	q-RASPR-SMOGN	11	0.72	0.59	0.75	17	0.69	0.69	0.69	0.68
Plant	*QSPR*	10	<0.6	=<0.5	0.64	NA	NA	NA	NA	NA
	QSPR-SMOGN	NA	NA	NA	NA	NA	NA	NA	NA	NA
	q-RASPR	10	0.86	0.64	0.34	NA	NA	NA	NA	NA
	q-RASPR-SMOGN	NA	NA	NA	NA	NA	NA	NA	NA	NA
				Metal Halide						
Algae	*QSPR*	10	0.71	0.51	0.37	1	0.91	0.91	0.91	0.04
	QSPR-SMOGN	10	0.71	0.51	0.37	12	0.71	0.71	0.71	0.34
	q-RASPR	10	0.93	0.87	0.17	1	0.8	NA	0.76	0.37
	q-RASPR-SMOGN	10	0.93	0.87	0.17	12	0.89	0.89	0.89	0.22
Crustaceans	*QSPR*	12	1	0.6	0.64	2	<0.5	<0.5	<0.5	2.49
	QSPR-SMOGN	12	0.75	0.6	0.64	14	0.6	0.6	0.61	0.83
	q-RASPR	10	0.83	0.72	0.55	4	0.62	0.62	0.62	1.04
	q-RASPR-SMOGN	10	0.83	0.72	0.55	18	0.71	0.71	0.71	0.8
Fish	*QSPR*	13	0.77	0.51	0.38	6	<0.5	<0.5	<0.5	1.62
	QSPR-SMOGN	13	0.77	0.51	0.38	14	0.62	0.62	0.62	0.57
	q-RASPR	14	0.71	0.58	0.63	5	0.72	0.72	0.72	0.51
	q-RASPR-SMOGN	14	0.71	0.58	0.63	24	0.71	0.71	0.71	0.58
Molluscs	*QSPR*	11	0.79	0.6	0.6	2	0.86	0.86	0.9	0.17
	QSPR-SMOGN	11	0.79	0.6	0.6	13	0.8	0.8	0.81	0.6
	q-RASPR	10	0.85	0.74	0.49	3	0.72	0.72	0.72	0.8
	q-RASPR-SMOGN	10	0.85	0.74	0.49	14	0.88	0.88	0.88	0.52
Plant	*QSPR*	10	0.72	0.57	0.6	1	0.98	NA	0.97	0.12
	QSPR-SMOGN	10	0.72	0.57	0.6	8	0.84	0.84	0.84	0.56

	q-RASPR	10	0.87	0.77	0.39	1	0.82	NA	0.78	0.51
	q-RASPR-SMOGN	10	0.87	0.77	0.39	8	0.88	0.88	0.88	0.44
				Metal Oxide						
Fish	*QSPR*	10	0.82	0.57	0.42	4	<0.5	<0.5	<0.5	2.9
	QSPR-SMOGN	10	0.82	0.57	0.42	11	0.63	0.63	0.63	0.86

Table S8. Quantitative metrics obtained for experiment-derived and synthetic-derived (SMOGN) various SbSD (QSPR and q-RASPR) models.

SbSD Type	***Model Type***	***N_{train}***	***R^2***	***Q2 (LOO)***	***$RMSE_c$***	***N_{test}***	***Q^2_{F1}***	***Q^2_{F2}***	***Q^2_{F3}***	***$RMSE_p$***
				Metals						
Mean	*QSPR*	12	0.79	0.61	0.43	5	<0.50	<0.50	<0.50	0.78
	QSPR-SMOGN	12	0.79	0.61	0.43	16	0.64	0.64	0.64	0.53
	q-RASPR	12	0.87	0.79	0.3	5	0.86	0.86	0.86	0.34
	q-RASPR-SMOGN	12	0.87	0.79	0.3	22	0.87	0.87	0.87	0.32
SD	*QSPR*	13	0.63	0.61	0.23	3	0.84	0.84	0.84	0.25
	QSPR-SMOGN	13	0.74	0.61	0.23	19	0.78	0.78	0.78	0.23
	q-RASPR	12	0.76	0.6	0.18	5	0.8	0.8	0.81	0.28
	q-RASPR-SMOGN	12	0.76	0.6	0.18	22	0.82	0.82	0.82	0.23
HC5	*q-RASPR*	13	0.98	0.91	0.77	4	0.92	0.92	0.92	1
	q-RASPR-SMOGN	13	0.98	0.91	0.77	16	0.95	0.95	0.95	1.13
				Metal Halide						
Mean	*QSPR*	10	0.74	<0.50	0.19	2	<0.50	<0.50	<0.50	1.38
	QSPR-SMOGN	10	0.74	<0.50	0.19	4	0.76	0.76	0.82	0.15
	q-RASPR	10	0.84	0.73	0.28	2	<0.50	<0.50	<0.50	
	q-RASPR-SMOGN	10	0.84	0.73	0.28	12	0.28	0.28	0.32	0.69
SD	*QSPR*	10	<0.60	<0.50	0.29	2	<0.50	<0.50	<0.50	0.85
	QSPR-SMOGN	10	<0.60	<0.50	0.29	9	0.59	0.59	0.59	0.26

	q-RASPR	10	0.81	0.73	0.18	1	0.6	NA	0.51	0.52
	q-RASPR-SMOGN	10	0.81	0.73	0.18	12	0.69	0.69	0.7	0.27
HC5	*q-RASPR*	10	0.81	0.58	3.17	2	<0.50	<0.50	<0.50	=>1.0
	q-RASPR-SMOGN	10	0.81	0.58	3.17	6	0.79	0.79	0.84	3.25

Table S9. Comparison of model BCF predictions with widely applied *in silico* tools.

Chemical Name	**pBCF(Fish)_Exp**	**EPI Suite**	**TEST**	**OECD QSAR Toolbox**	**OCHEM Model**	**Present QSPR Models**	**Present q-RASPR Models**
				Metals			
Aluminum	1.56	0.5	0.5	0.5	0.53	1.56	5.42
Iron	0.86	0.5	0.5	0.5	0.53	1.90	0.14
Lead	0.53	0.5	0.5	0.5	0.53	3.07	0.14
Manganese	2.34	0.5	0.5	0.5	0.53	2.61	5.42
Mercury	4.43	0.5	0.5	0.5	0.53	3.66	5.42
Nickel	0.50	0.5	0.5	0.5	0.53	1.84	0.6
Silver	0.50	0.5	0.5	0.5	0.53	0.63	0.6
Antimony	-0.40	0.5	0.5	0.5	0.53	-0.75	0.14
Arsenic	0.62	0.5	0.5	0.5	0.53	0.58	0.6
Barium	0.50	0.5	0.5	0.5	0.53	0.81	0.6
Cadmium	1.10	0.5	0.5	0.5	0.53	1.90	0.6
Chromium	0.13	0.5	0.5	0.5	0.53	2.30	0.14
Cobalt	0.33	0.5	0.5	0.5	0.53	1.55	0.6
Copper	6.41	0.5	0.5	0.5	0.53	1.73	5.42
Vanadium	0.50	0.5	0.5	0.5	0.53	1.95	0.14
Zinc	-1.52	0.5	0.5	0.5	0.53	1.75	0.14
Calcium	0.50	0.5	0.5	0.5	0.53	0.10	0.6
Selenium	0.89	0.5	0.5	0.5	0.53	0.91	0.14

			Metal Halides				
Copper chloride	1.04	0.50	0.50	0.50	1.11	1.33	1.44
Mercury chloride	2.91	2.00	2.00	2.00	1.09	2.33	3.06
Lithium bromide	1.49	0.50	0.50	0.50	0.87	1.10	1.48
Cobalt chloride	-0.27	0.50	0.50	0.50	1.11	1.28	-0.52
Zinc chloride	1.65	0.50	0.50	0.50	1.10	1.20	1.44
Cesium chloride	0.91	0.50	0.50	0.50	0.84	1.97	1.39
Sodium fluoride	0.81	0.50	0.50	0.50	0.65	0.72	0.69
Nickel chloride	-1.12	0.50	0.50	0.50	1.11	1.30	-0.99
Iron chloride	1.15	0.50	0.50	0.50	1.11	1.25	1.12
Manganese chloride	1.35	0.50	0.50	0.50	1.11	1.28	1.12
Silver chloride	1.81	0.50	0.50	0.50	0.84	1.40	1.55
Beryllium chloride	-0.07	0.50	0.50	0.50	1.12	0.70	0.86
Indium chloride	1.96	0.43	0.43	0.43	1.36	2.28	1.53
Cadmium chloride	0.30	0.50	0.50	0.50	1.10	1.66	0.70
Mercury chloride	3.11	2.00	2.00	2.00	1.14	3.24	3.06
Barium chloride	1.78	0.50	0.50	0.50	1.09	2.21	2.22
Strontium chloride	1.77	0.50	0.50	0.50	1.10	1.72	1.72
Manganese chloride	-0.70	0.50	0.50	0.50	1.11	1.28	1.12
Iron chloride	2.30	0.50	0.50	0.50	1.40	1.57	1.12
			Metal Oxides				
Arsenic pentoxide	0.49	0.50	0.50	0.50	0.53	1.16	1.10
Cadmium oxide	1.76	0.50	0.50	0.50	0.52	1.71	0.48
Zinc oxide	0.36	0.68	0.68	0.68	0.49	-0.08	0.48
Lead oxide	2.37	0.50	0.50	0.50	0.57	2.15	2.49
Vanadium oxide	1.41	1.63	1.63	1.63	0.32	1.08	1.10
Lead oxide	1.63	0.50	0.50	0.50	0.54	2.15	0.48
Copper oxide	1.85	0.61	0.61	0.61	0.49	-0.01	2.49

Arsenic oxide	0.60	0.50	0.50	0.50	0.44	1.16	0.48
Chromium oxide	1.86	1.14	1.14	1.14	0.35	1.63	2.49
Titanium oxide	1.00	1.14	1.14	1.14	0.39	-0.12	1.10
Selenite	-0.22	0.50	0.50	0.50	0.38	1.78	1.10
Selenate	6.81	0.50	0.50	0.50	0.33	1.78	2.49
(T-4)-Vanadate	1.51	1.14	1.14	1.14	0.32	1.08	1.10
Mercury oxide	3.86	2.08	2.08	2.08	0.54	3.47	2.49

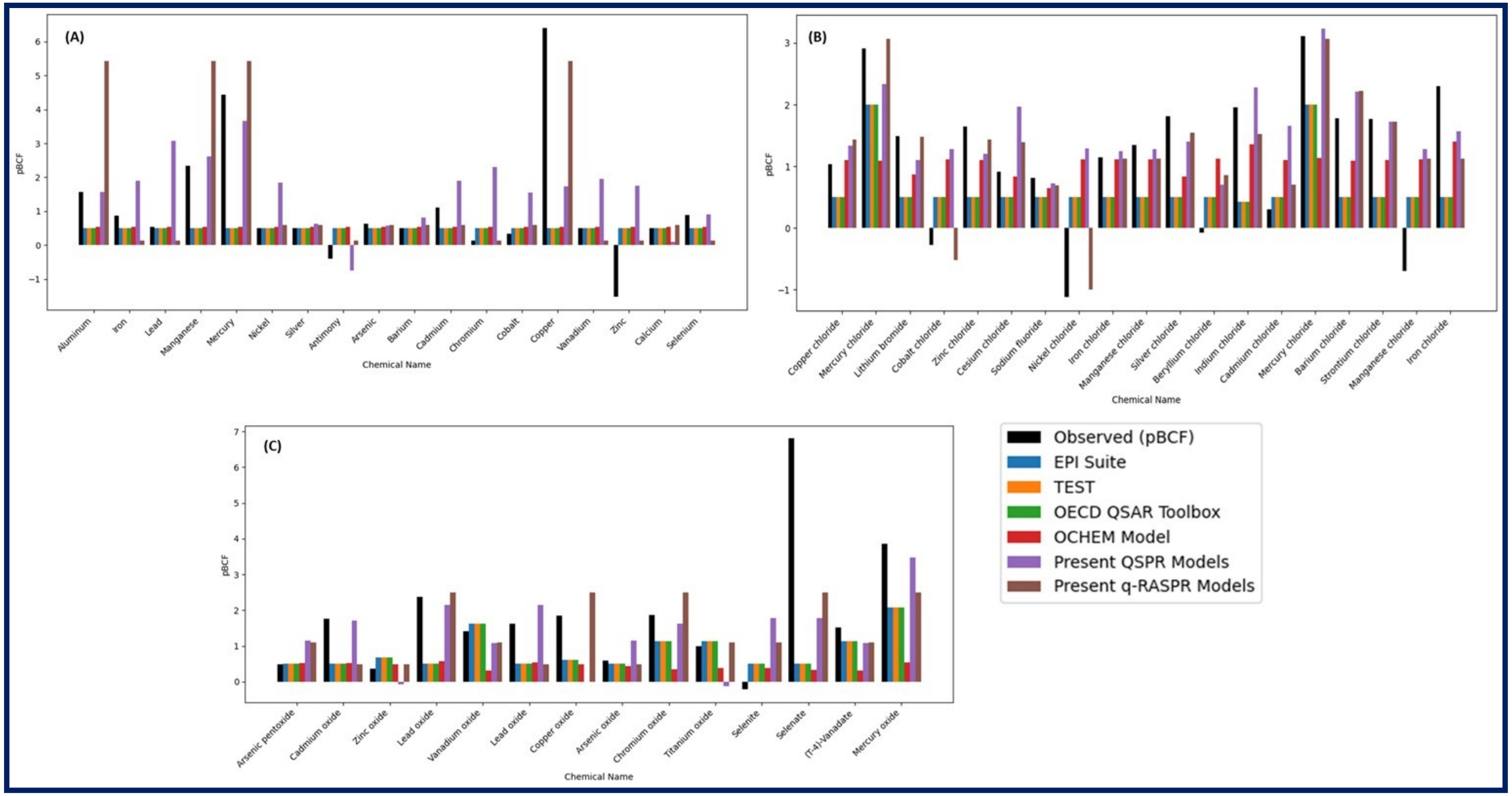
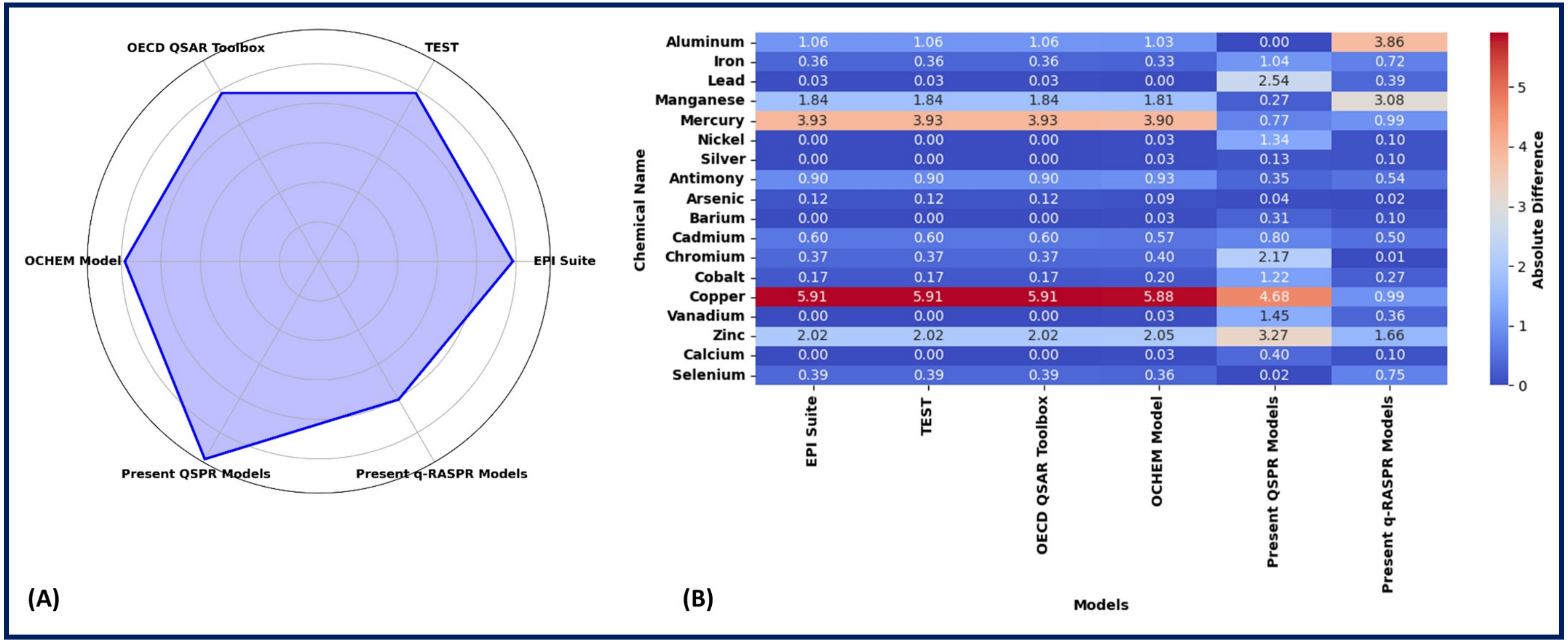
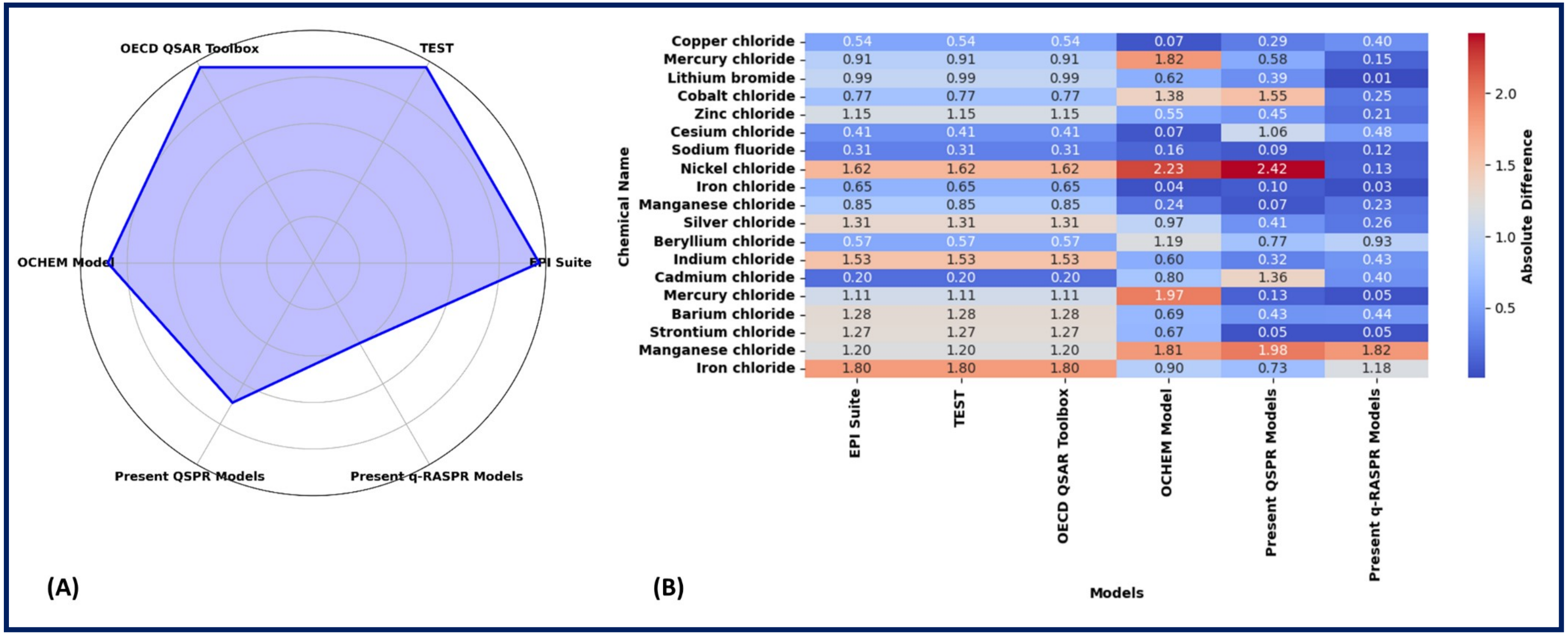


Figure S1. Comparative bar plot of observed and predicted pBCF values for various metals (A), metal halides (B), and metal oxides (C). Predictions from six computational models are shown alongside experimental (observed pBCF) values, enabling visual assessment of model accuracy across different chemicals.



Chemical Name	EPI Suite	TEST	OECD QSAR Toolbox	OCHEM Model	Present QSPR Models	Present q-RASPR Models
Aluminum	1.06	1.06	1.06	1.03	0.00	3.86
Iron	0.36	0.36	0.36	0.33	1.04	0.72
Lead	0.03	0.03	0.03	0.00	2.54	0.39
Manganese	1.84	1.84	1.84	1.81	0.27	3.08
Mercury	3.93	3.93	3.93	3.90	0.77	0.99
Nickel	0.00	0.00	0.00	0.03	1.34	0.10
Silver	0.00	0.00	0.00	0.03	0.13	0.10
Antimony	0.90	0.90	0.90	0.93	0.35	0.54
Arsenic	0.12	0.12	0.12	0.09	0.04	0.02
Barium	0.00	0.00	0.00	0.03	0.31	0.10
Cadmium	0.60	0.60	0.60	0.57	0.80	0.50
Chromium	0.37	0.37	0.37	0.40	2.17	0.01
Cobalt	0.17	0.17	0.17	0.20	1.22	0.27
Copper	5.91	5.91	5.91	5.88	4.68	0.99
Vanadium	0.00	0.00	0.00	0.03	1.45	0.36
Zinc	2.02	2.02	2.02	2.05	3.27	1.66
Calcium	0.00	0.00	0.00	0.03	0.40	0.10
Selenium	0.39	0.39	0.39	0.36	0.02	0.75

Figure S2. (A)Spider plot depicting the mean absolute deviations between predicted and observed pBCF values for various predictive models applied to metals. A smaller distance from the center indicates higher predictive accuracy. (B) Heatmap showing the absolute differences between predicted and experimentally observed pBCF values across various predictive models for selected metal compounds. Lower values indicate closer agreement with experimental data, highlighting model performance and reliability.



Chemical Name	EPI Suite	TEST	OECD QSAR Toolbox	OCHEM Model	Present QSPR Models	Present q-RASPR Models
Copper chloride	0.54	0.54	0.54	0.07	0.29	0.40
Mercury chloride	0.91	0.91	0.91	1.82	0.58	0.15
Lithium bromide	0.99	0.99	0.99	0.62	0.39	0.01
Cobalt chloride	0.77	0.77	0.77	1.38	1.55	0.25
Zinc chloride	1.15	1.15	1.15	0.55	0.45	0.21
Cesium chloride	0.41	0.41	0.41	0.07	1.06	0.48
Sodium fluoride	0.31	0.31	0.31	0.16	0.09	0.12
Nickel chloride	1.62	1.62	1.62	2.23	2.42	0.13
Iron chloride	0.65	0.65	0.65	0.04	0.10	0.03
Manganese chloride	0.85	0.85	0.85	0.24	0.07	0.23
Silver chloride	1.31	1.31	1.31	0.97	0.41	0.26
Beryllium chloride	0.57	0.57	0.57	1.19	0.77	0.93
Indium chloride	1.53	1.53	1.53	0.60	0.32	0.43
Cadmium chloride	0.20	0.20	0.20	0.80	1.36	0.40
Mercury chloride	1.11	1.11	1.11	1.97	0.13	0.05
Barium chloride	1.28	1.28	1.28	0.69	0.43	0.44
Strontium chloride	1.27	1.27	1.27	0.67	0.05	0.05
Manganese chloride	1.20	1.20	1.20	1.81	1.98	1.82
Iron chloride	1.80	1.80	1.80	0.90	0.73	1.18

Figure S3. (A) Spider plot depicting the mean absolute deviations between predicted and observed pBCF values for various predictive models applied to metal halides. A smaller distance from the center indicates higher predictive accuracy. (B) Heatmap showing the absolute differences between predicted and experimentally observed pBCF values across various predictive models for selected metal compounds. Lower values indicate closer agreement with experimental data, highlighting model performance and reliability.

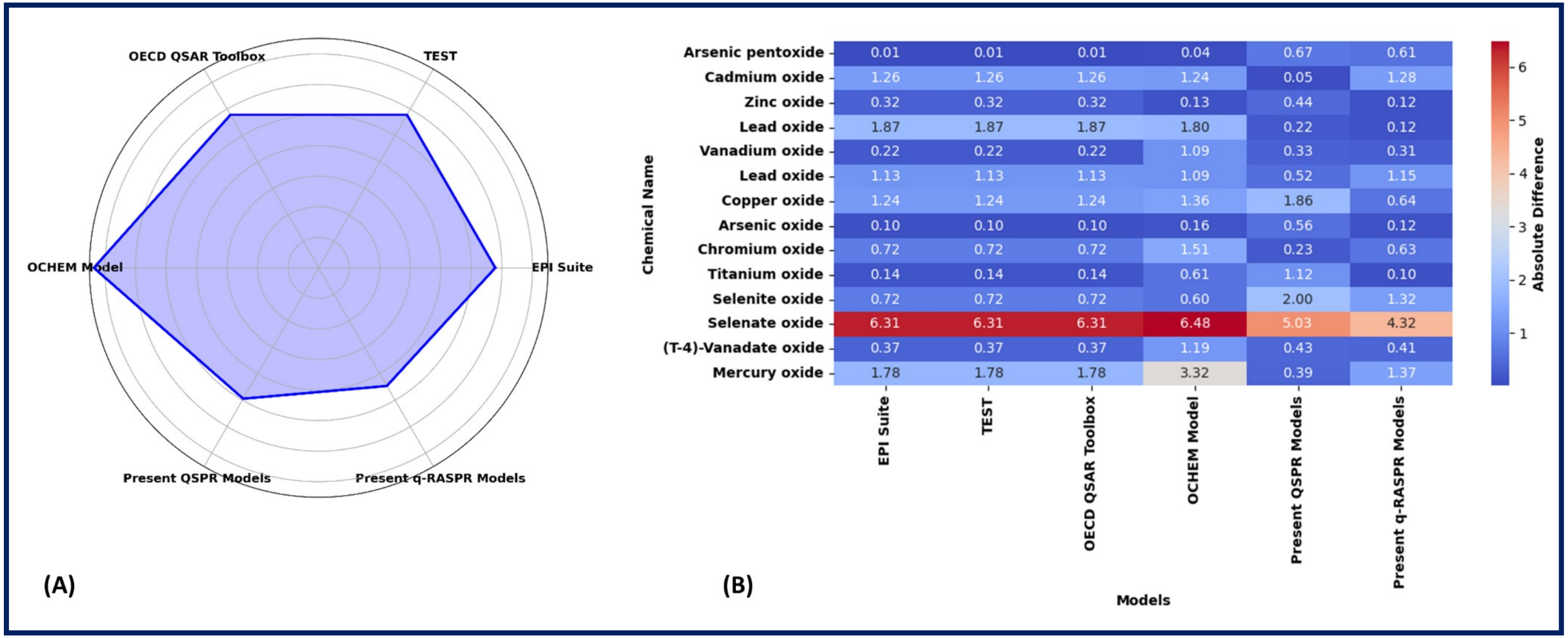


Figure S4. (A) Spider plot depicting the mean absolute deviations between predicted and observed pBCF values for various predictive models applied to metal oxides. A smaller distance from the center indicates higher predictive accuracy. (B) Heatmap showing the absolute differences between predicted and experimentally observed pBCF values across various predictive models for selected metal compounds. Lower values indicate closer agreement with experimental data, highlighting model performance and reliability.

Table S10. Results of paired Student's *t*-tests between experimentally measured and *in silico* predicted pBCF(Fish) values. Statistically significant differences are highlighted in red.

	EPI Suite	TEST	OECD QSAR Toolbox	OCHEM Model	Present QSPR Models	Present q-RASPR Models
Metals						
df	17	17	17	17	17	17
$t_{critical}$ for α=0.05	2.110	2.110	2.110	2.110	2.110	2.110
t-test value	1.424	1.424	1.424	1.352	1.166	1.293
p-value	0.173	0.173	0.173	0.194	0.260	0.213
Standard error of difference	0.421	0.421	0.421	0.421	0.396	0.304
Metal Halides						
df	18	18	18	18	18	18
$t_{critical}$ for α=0.05	2.101	2.101	2.101	2.101	2.101	2.101
t-test value	2.327	2.327	2.327	0.369	1.954	0.732
p-value	0.032	0.032	0.032	0.716	0.066	0.474
Standard error of difference	0.221	0.221	0.221	0.260	0.206	0.139
Metal Oxides						
df	13	13	13	13	13	13
$t_{critical}$ for α=0.05	2.160	2.160	2.160	2.160	2.160	2.160
t-test value	2.051	2.051	2.051	2.890	1.067	1.052
p-value	0.061	0.061	0.061	0.013	0.306	0.312
Standard error of difference	0.466	0.466	0.466	0.472	0.425	0.368