Supporting information Data 2

of thesis entitled

Improving practicality and reliability of the ecological risk assessment of emerging contaminants: development of an integrated framework

Submitted by

ZHANG Jiawei

for the Degree of Doctor of Philosophy

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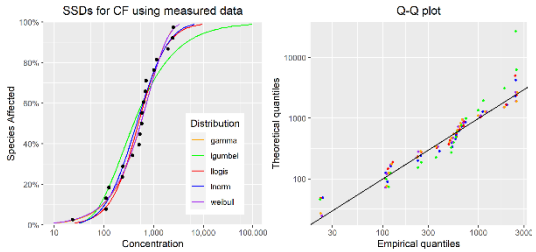
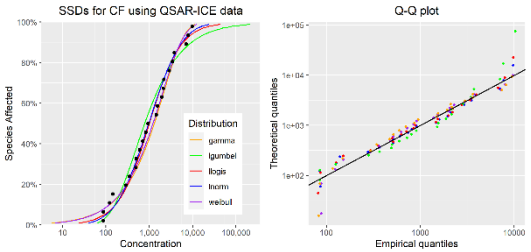
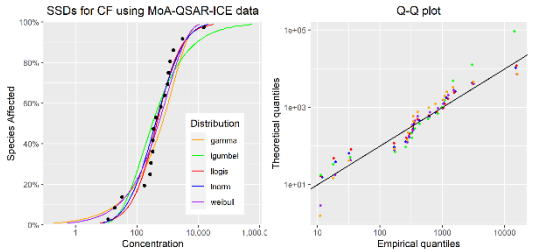
CF







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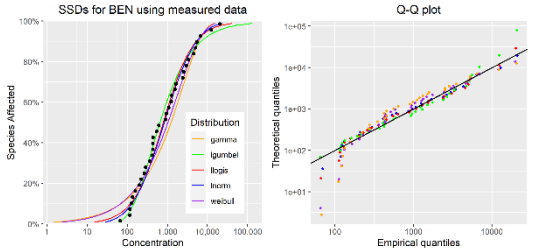

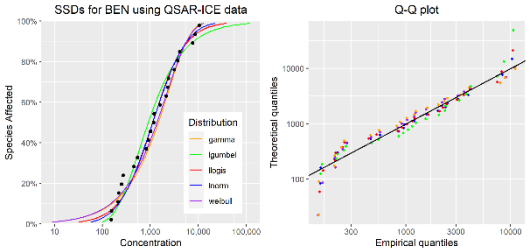

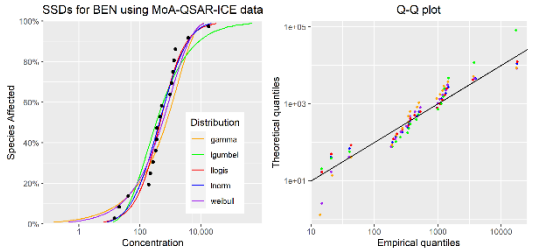

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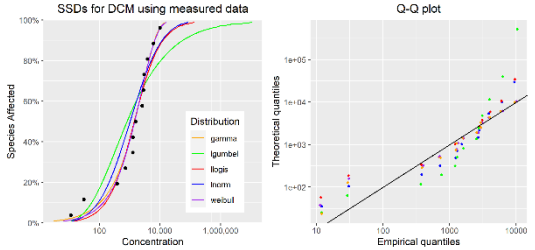

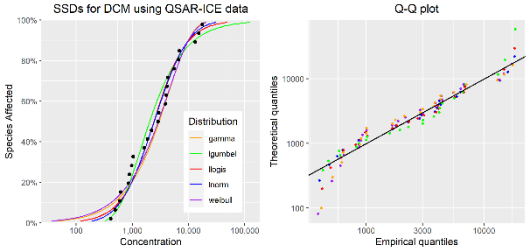

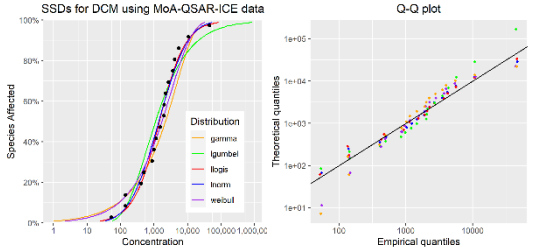

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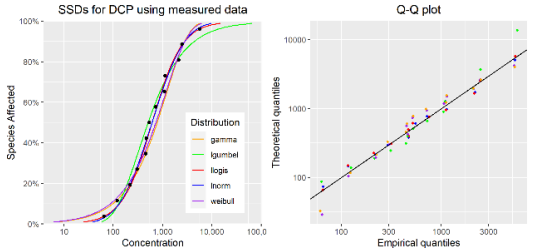

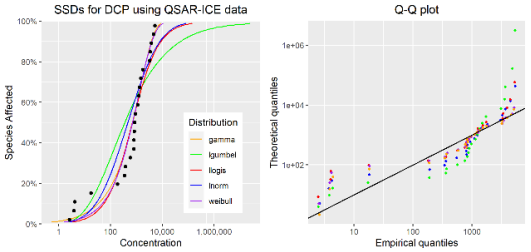

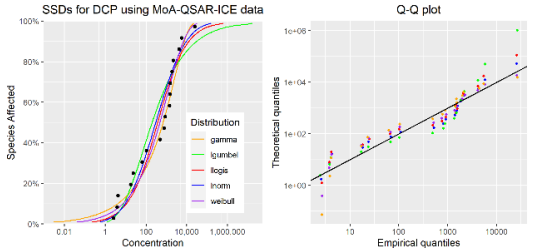

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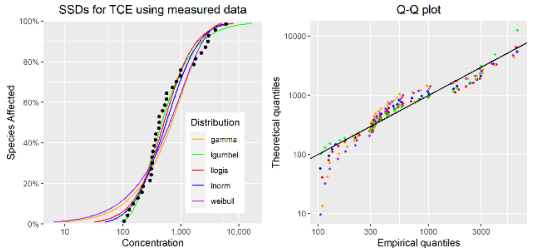

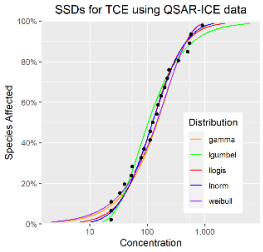

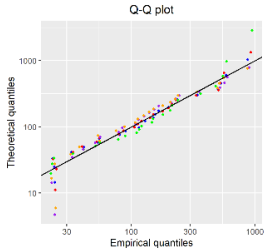

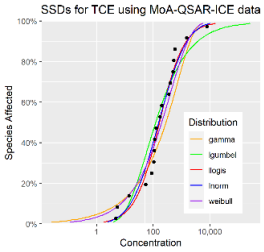

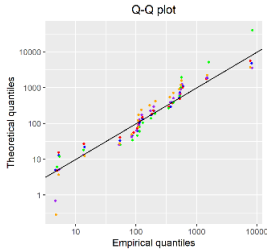

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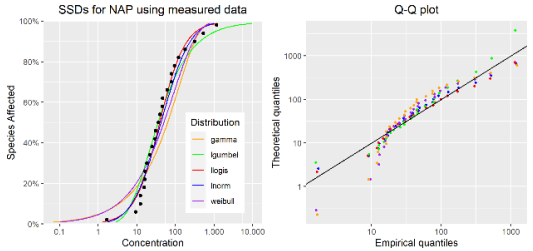

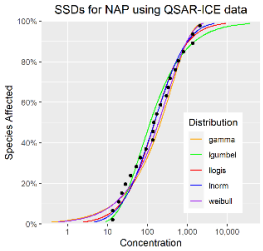

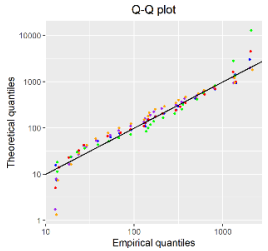

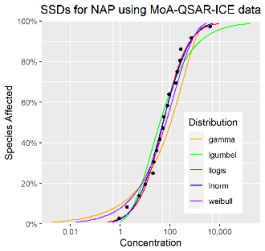

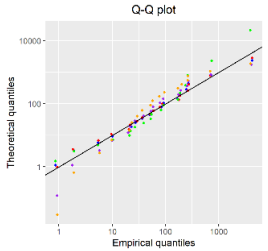

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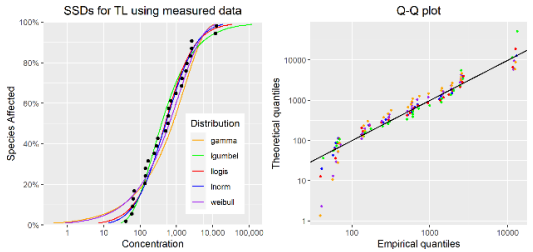

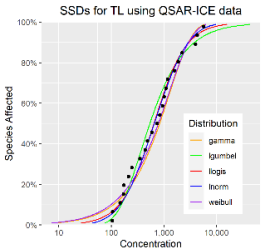

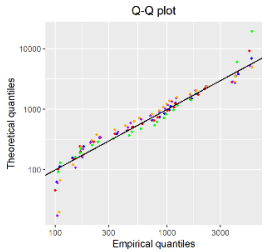

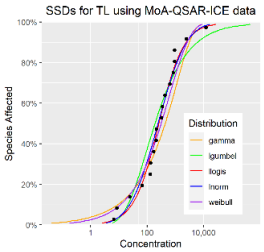

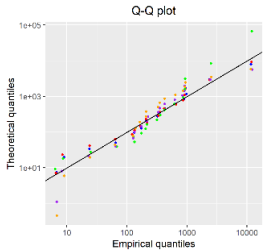

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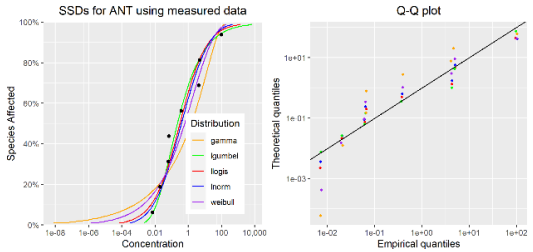
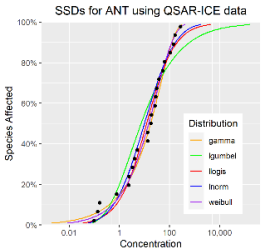
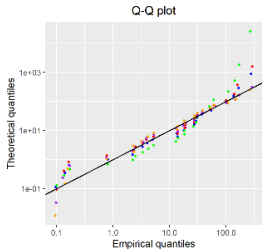
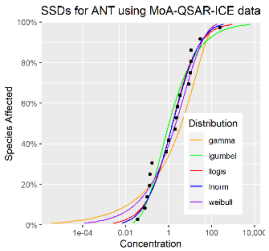
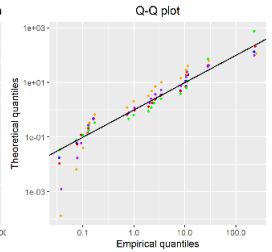










TCB

PCE

PeCB

NP

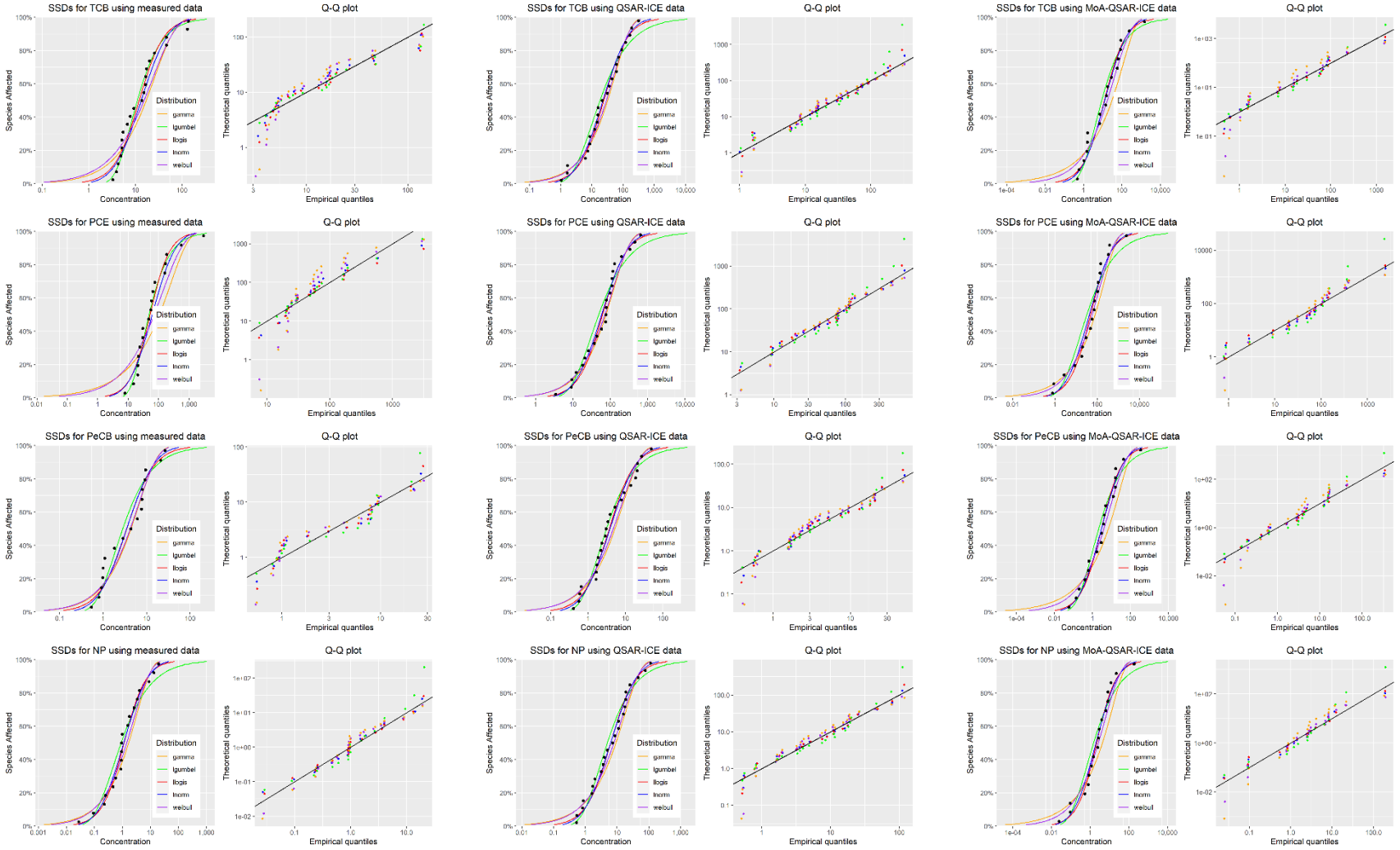
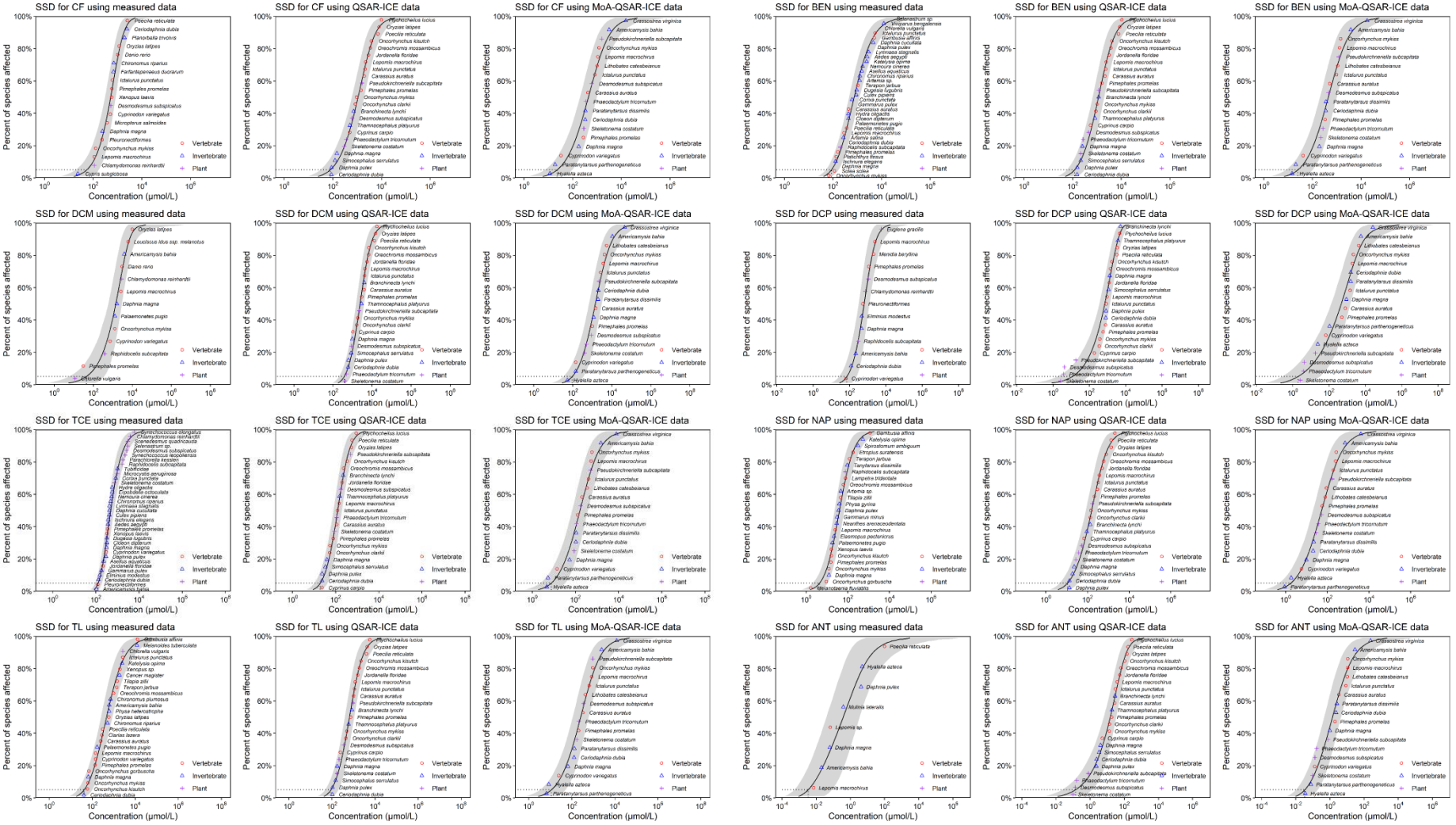
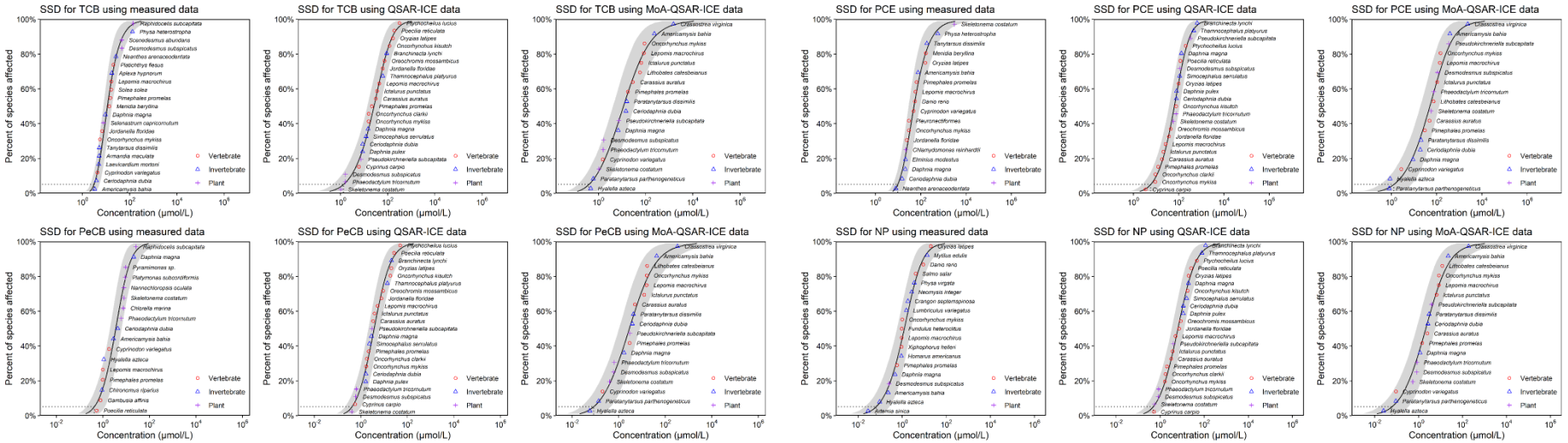


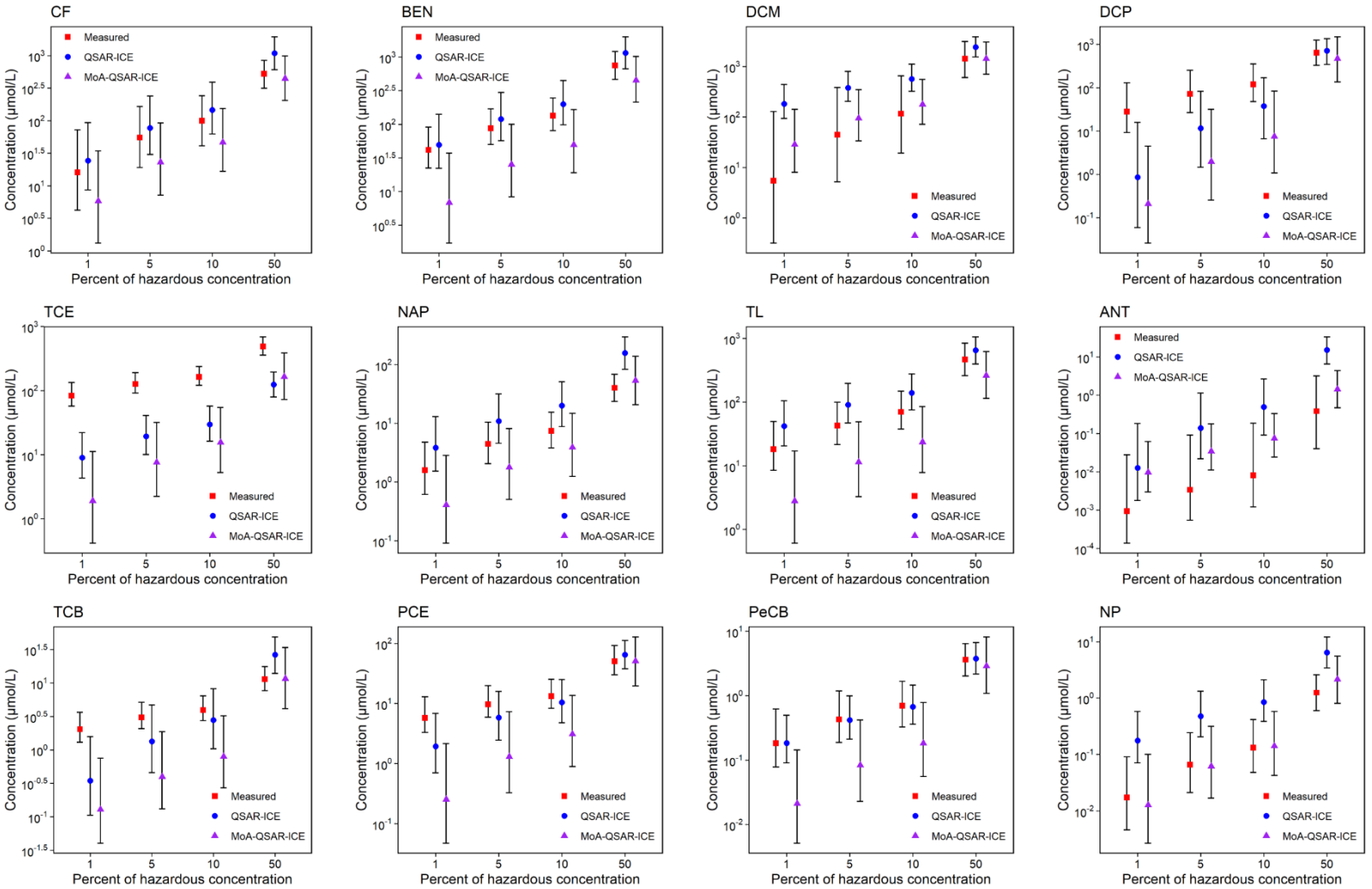
Figure S1 The cumulative density curves and Q-Q plots of the developed SSD models


SSD for CF using measured data
SSD for CF using QSAR-ICE data
SSD for CF using MoA-QSAR-ICE data
SSD for BEN using measured data
SSD for BEN using QSAR-ICE data
SSD for BEN using MoA-QSAR-ICE data
SSD for DCM using measured data
SSD for DCM using QSAR-ICE data
SSD for DCM using MoA-QSAR-ICE data
SSD for DCP using measured data
SSD for DCP using QSAR-ICE data
SSD for DCP using MoA-QSAR-ICE data
SSD for TCE using measured data
SSD for TCE using QSAR-ICE data
SSD for TCE using MoA-QSAR-ICE data
SSD for NAP using measured data
SSD for NAP using QSAR-ICE data
SSD for NAP using MoA-QSAR-ICE data
SSD for TL using measured data
SSD for TL using QSAR-ICE data
SSD for TL using MoA-QSAR-ICE data
SSD for ANT using measured data
SSD for ANT using QSAR-ICE data
SSD for ANT using MoA-QSAR-ICE data
Percent of species affected
Concentration (µmol/L)
Vertebrate
Invertebrate
Plant



29 **Figure S2 SSD models for PCCs using measured / QSAR-ICE / MoA-QSAR-ICE data (averaging multiple distributions)**

30



31 **Figure S3 HC values of SSD models using measured / QSAR-ICE / MoA-QSAR-ICE data (averaging multiple distributions)**

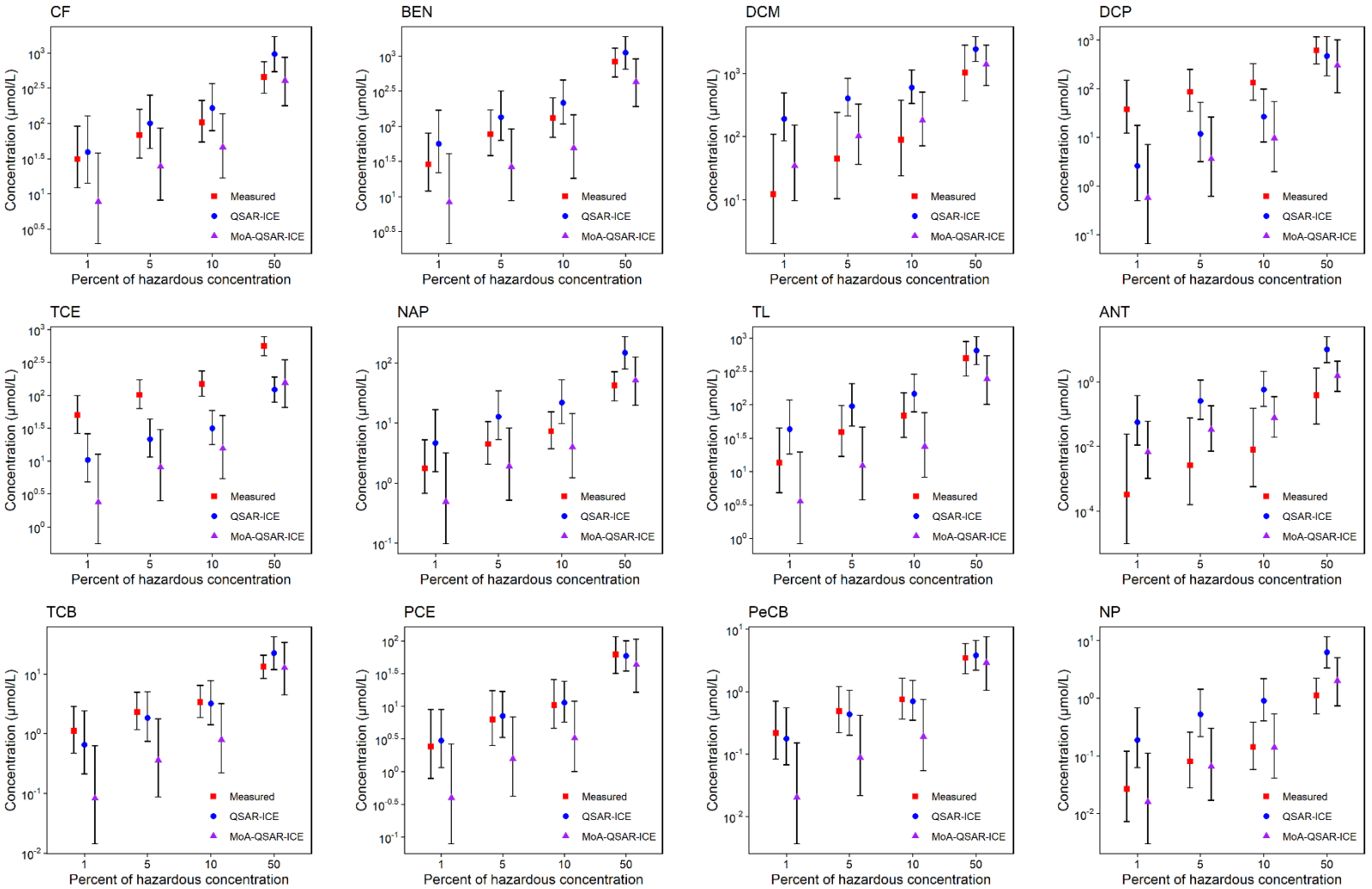


Figure S4 HC values of SSD models using measured / QSAR-ICE / MoA-QSAR-ICE data (log-normal distributions)

34 **Table S1 The goodness of fit of SSD models fitted by different methods**

Chemical	No.	Distribution	AD test	KS test	AIC	Type
CF	1	lnorm	0.406	0.172	296	Measured
	2	llogis	0.346	0.146	296	Measured
	3	lgumbel	0.919	0.197	302	Measured
	4	weibull	0.318	0.142	294	Measured
	5	gamma	0.317	0.141	294	Measured
	6	lnorm	0.235	0.092	400	QSAR-ICE
	7	llogis	0.239	0.088	402	QSAR-ICE
	8	lgumbel	0.522	0.125	404	QSAR-ICE
	9	weibull	0.250	0.095	401	QSAR-ICE
	10	gamma	0.334	0.113	402	QSAR-ICE
	11	lnorm	0.523	0.187	290	MoA-QSAR-ICE
	12	llogis	0.417	0.151	290	MoA-QSAR-ICE
	13	lgumbel	1.014	0.247	294	MoA-QSAR-ICE
	14	weibull	0.550	0.154	292	MoA-QSAR-ICE
	15	gamma	0.915	0.198	295	MoA-QSAR-ICE
BEN	1	lnorm	0.308	0.111	583	Measured
	2	llogis	0.346	0.104	585	Measured
	3	lgumbel	0.283	0.088	582	Measured
	4	weibull	0.673	0.121	589	Measured
	5	gamma	1.101	0.151	592	Measured
	6	lnorm	0.321	0.126	404	QSAR-ICE
	7	llogis	0.328	0.124	405	QSAR-ICE
	8	lgumbel	0.498	0.127	405	QSAR-ICE
	9	weibull	0.380	0.104	406	QSAR-ICE
	10	gamma	0.483	0.124	406	QSAR-ICE
	11	lnorm	0.430	0.152	292	MoA-QSAR-ICE
	12	llogis	0.348	0.118	292	MoA-QSAR-ICE
	13	lgumbel	0.847	0.215	296	MoA-QSAR-ICE
	14	weibull	0.574	0.172	295	MoA-QSAR-ICE
	15	gamma	1.025	0.235	298	MoA-QSAR-ICE
DCM	1	lnorm	0.867	0.238	238	Measured
	2	llogis	0.638	0.167	237	Measured
	3	lgumbel	1.295	0.259	243	Measured
	4	weibull	0.360	0.158	233	Measured
	5	gamma	0.301	0.159	233	Measured
	6	lnorm	0.325	0.131	432	QSAR-ICE
	7	llogis	0.345	0.132	434	QSAR-ICE
	8	lgumbel	0.427	0.138	433	QSAR-ICE

	9	weibull	0.446	0.122	435	QSAR-ICE
	10	gamma	0.515	0.137	435	QSAR-ICE
	11	lnorm	0.241	0.112	332	MoA-QSAR-ICE
	12	llogis	0.196	0.099	332	MoA-QSAR-ICE
	13	lgumbel	0.578	0.174	335	MoA-QSAR-ICE
	14	weibull	0.424	0.128	335	MoA-QSAR-ICE
	15	gamma	0.793	0.181	337	MoA-QSAR-ICE
DCP	1	lnorm	0.125	0.099	212	Measured
	2	llogis	0.123	0.090	213	Measured
	3	lgumbel	0.267	0.161	214	Measured
	4	weibull	0.238	0.132	214	Measured
	5	gamma	0.295	0.148	214	Measured
	6	lnorm	1.868	0.245	389	QSAR-ICE
	7	llogis	1.436	0.179	387	QSAR-ICE
	8	lgumbel	2.542	0.281	399	QSAR-ICE
	9	weibull	0.902	0.179	379	QSAR-ICE
	10	gamma	0.715	0.176	378	QSAR-ICE
	11	lnorm	0.686	0.194	296	MoA-QSAR-ICE
	12	llogis	0.661	0.168	297	MoA-QSAR-ICE
	13	lgumbel	0.927	0.225	300	MoA-QSAR-ICE
	14	weibull	0.422	0.134	295	MoA-QSAR-ICE
	15	gamma	0.448	0.142	296	MoA-QSAR-ICE
TCE	1	lnorm	0.829	0.151	549	Measured
	2	llogis	0.741	0.119	550	Measured
	3	lgumbel	0.363	0.103	546	Measured
	4	weibull	1.541	0.197	558	Measured
	5	gamma	1.822	0.223	559	Measured
	6	lnorm	0.243	0.083	293	QSAR-ICE
	7	llogis	0.246	0.088	295	QSAR-ICE
	8	lgumbel	0.432	0.135	295	QSAR-ICE
	9	weibull	0.378	0.105	295	QSAR-ICE
	10	gamma	0.427	0.103	295	QSAR-ICE
	11	lnorm	0.408	0.154	258	MoA-QSAR-ICE
	12	llogis	0.329	0.124	257	MoA-QSAR-ICE
	13	lgumbel	0.833	0.216	261	MoA-QSAR-ICE
	14	weibull	0.537	0.166	260	MoA-QSAR-ICE
	15	gamma	1.049	0.237	264	MoA-QSAR-ICE
NAP	1	lnorm	0.398	0.111	277	Measured
	2	llogis	0.281	0.097	277	Measured
	3	lgumbel	0.556	0.139	280	Measured
	4	weibull	1.057	0.158	284	Measured

	5	gamma	1.601	0.209	288	Measured
	6	lnorm	0.241	0.085	318	QSAR-ICE
	7	llogis	0.256	0.084	320	QSAR-ICE
	8	lgumbel	0.419	0.145	320	QSAR-ICE
	9	weibull	0.314	0.095	320	QSAR-ICE
	10	gamma	0.464	0.120	320	QSAR-ICE
	11	lnorm	0.163	0.103	222	MoA-QSAR-ICE
	12	llogis	0.126	0.081	222	MoA-QSAR-ICE
	13	lgumbel	0.474	0.165	225	MoA-QSAR-ICE
	14	weibull	0.374	0.135	225	MoA-QSAR-ICE
	15	gamma	1.030	0.219	229	MoA-QSAR-ICE
TL	1	lnorm	0.334	0.094	441	Measured
	2	llogis	0.351	0.094	442	Measured
	3	lgumbel	0.429	0.122	441	Measured
	4	weibull	0.616	0.113	446	Measured
	5	gamma	1.091	0.156	449	Measured
	6	lnorm	0.258	0.104	375	QSAR-ICE
	7	llogis	0.271	0.105	376	QSAR-ICE
	8	lgumbel	0.385	0.123	375	QSAR-ICE
	9	weibull	0.404	0.106	377	QSAR-ICE
	10	gamma	0.502	0.119	378	QSAR-ICE
	11	lnorm	0.308	0.141	274	MoA-QSAR-ICE
	12	llogis	0.238	0.110	274	MoA-QSAR-ICE
	13	lgumbel	0.721	0.203	278	MoA-QSAR-ICE
	14	weibull	0.431	0.161	277	MoA-QSAR-ICE
	15	gamma	0.918	0.229	280	MoA-QSAR-ICE
ANT	1	lnorm	0.311	0.217	29	Measured
	2	llogis	0.300	0.200	30	Measured
	3	lgumbel	0.248	0.187	28	Measured
	4	weibull	0.398	0.214	31	Measured
	5	gamma	0.702	0.246	33	Measured
	6	lnorm	0.528	0.162	212	QSAR-ICE
	7	llogis	0.435	0.128	212	QSAR-ICE
	8	lgumbel	1.090	0.194	218	QSAR-ICE
	9	weibull	0.199	0.091	209	QSAR-ICE
	10	gamma	0.208	0.087	209	QSAR-ICE
	11	lnorm	0.379	0.162	101	MoA-QSAR-ICE
	12	llogis	0.397	0.164	102	MoA-QSAR-ICE
	13	lgumbel	0.511	0.159	101	MoA-QSAR-ICE
	14	weibull	0.458	0.132	104	MoA-QSAR-ICE
	15	gamma	1.180	0.235	109	MoA-QSAR-ICE

TCB	1	lnorm	0.615	0.131	175	Measured
	2	llogis	0.522	0.118	175	Measured
	3	lgumbel	0.399	0.138	171	Measured
	4	weibull	1.098	0.178	182	Measured
	5	gamma	1.351	0.207	182	Measured
	6	lnorm	0.240	0.094	232	QSAR-ICE
	7	llogis	0.232	0.094	233	QSAR-ICE
	8	lgumbel	0.627	0.115	236	QSAR-ICE
	9	weibull	0.225	0.122	232	QSAR-ICE
	10	gamma	0.319	0.141	233	QSAR-ICE
	11	lnorm	0.301	0.161	175	MoA-QSAR-ICE
	12	llogis	0.317	0.161	176	MoA-QSAR-ICE
	13	lgumbel	0.406	0.150	175	MoA-QSAR-ICE
	14	weibull	0.446	0.126	178	MoA-QSAR-ICE
	15	gamma	1.148	0.214	183	MoA-QSAR-ICE
PCE	1	lnorm	0.600	0.163	215	Measured
	2	llogis	0.424	0.121	214	Measured
	3	lgumbel	0.222	0.112	211	Measured
	4	weibull	1.298	0.209	224	Measured
	5	gamma	2.096	0.286	229	Measured
	6	lnorm	0.279	0.143	268	QSAR-ICE
	7	llogis	0.277	0.134	269	QSAR-ICE
	8	lgumbel	0.632	0.174	273	QSAR-ICE
	9	weibull	0.344	0.138	269	QSAR-ICE
	10	gamma	0.434	0.153	270	QSAR-ICE
	11	lnorm	0.410	0.136	216	MoA-QSAR-ICE
	12	llogis	0.331	0.109	216	MoA-QSAR-ICE
	13	lgumbel	0.875	0.186	220	MoA-QSAR-ICE
	14	weibull	0.334	0.147	216	MoA-QSAR-ICE
	15	gamma	0.718	0.214	219	MoA-QSAR-ICE
PeCB	1	lnorm	0.618	0.185	100	Measured
	2	llogis	0.619	0.182	102	Measured
	3	lgumbel	0.700	0.191	101	Measured
	4	weibull	0.542	0.171	101	Measured
	5	gamma	0.586	0.181	102	Measured
	6	lnorm	0.365	0.102	144	QSAR-ICE
	7	llogis	0.374	0.105	145	QSAR-ICE
	8	lgumbel	0.379	0.130	145	QSAR-ICE
	9	weibull	0.593	0.158	147	QSAR-ICE
	10	gamma	0.765	0.185	148	QSAR-ICE
	11	lnorm	0.210	0.112	121	MoA-QSAR-ICE

	12	llogis	0.220	0.111	122	MoA-QSAR-ICE
	13	lgumbel	0.371	0.168	122	MoA-QSAR-ICE
	14	weibull	0.411	0.144	124	MoA-QSAR-ICE
	15	gamma	1.168	0.242	129	MoA-QSAR-ICE
NP	1	lnorm	0.234	0.132	80	Measured
	2	llogis	0.202	0.118	80	Measured
	3	lgumbel	0.598	0.184	84	Measured
	4	weibull	0.393	0.159	81	Measured
	5	gamma	0.611	0.192	82	Measured
	6	lnorm	0.215	0.084	173	QSAR-ICE
	7	llogis	0.238	0.090	174	QSAR-ICE
	8	lgumbel	0.397	0.117	174	QSAR-ICE
	9	weibull	0.330	0.099	175	QSAR-ICE
	10	gamma	0.549	0.129	177	QSAR-ICE
	11	lnorm	0.276	0.111	106	MoA-QSAR-ICE
	12	llogis	0.218	0.105	106	MoA-QSAR-ICE
	13	lgumbel	0.659	0.174	110	MoA-QSAR-ICE
	14	weibull	0.417	0.128	109	MoA-QSAR-ICE
	15	gamma	1.129	0.220	114	MoA-QSAR-ICE

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Table S2 HC values of SSD models using measured / QSAR-ICE / MoA-QSAR-ICE data (averaging multiple distributions)

Chemical	HC percent	Type	HC value	95% CI lower limit	95% CI upper limit
CF	1	Measured	16.038	4.210	71.821
	5	Measured	54.876	19.066	164.539
	10	Measured	98.889	40.651	241.553
	50	Measured	525.074	313.420	843.789
	1	QSAR-ICE	24.305	8.608	93.074
	5	QSAR-ICE	77.489	30.015	239.283
	10	QSAR-ICE	146.044	62.289	389.886
	50	QSAR-ICE	1082.672	604.936	1943.799
	1	MoA-QSAR-ICE	5.834	1.310	34.269
	5	MoA-QSAR-ICE	23.003	7.174	92.100
	10	MoA-QSAR-ICE	46.223	16.558	153.713
	50	MoA-QSAR-ICE	443.758	203.867	983.383
BEN	1	Measured	41.402	22.352	90.884
	5	Measured	86.891	49.857	169.914
	10	Measured	134.691	80.384	244.681
	50	Measured	748.861	463.823	1206.992
	1	QSAR-ICE	49.307	22.087	140.569
	5	QSAR-ICE	119.725	56.770	296.606
	10	QSAR-ICE	199.053	98.260	445.606
	50	QSAR-ICE	1150.198	668.224	2005.490
	1	MoA-QSAR-ICE	6.776	1.699	37.143
	5	MoA-QSAR-ICE	25.235	8.339	99.836
	10	MoA-QSAR-ICE	49.458	18.879	165.007
	50	MoA-QSAR-ICE	450.723	213.271	1015.418
DCM	1	Measured	5.441	0.316	128.351
	5	Measured	44.687	5.141	386.094
	10	Measured	116.465	19.266	650.339
	50	Measured	1428.486	604.683	3112.842
	1	QSAR-ICE	181.509	93.466	439.150
	5	QSAR-ICE	376.826	203.003	796.758
	10	QSAR-ICE	570.089	323.508	1108.306
	50	QSAR-ICE	2437.301	1542.943	3889.285
	1	MoA-QSAR-ICE	28.355	7.993	141.466
	5	MoA-QSAR-ICE	94.496	33.293	349.007
	10	MoA-QSAR-ICE	177.177	71.059	551.110

	50	MoA-QSAR-ICE	1433.586	700.937	3064.461
DCP	1	Measured	28.002	9.151	129.828
	5	Measured	71.677	26.629	250.924
	10	Measured	119.564	47.700	350.160
	50	Measured	640.866	327.450	1244.229
	1	QSAR-ICE	0.856	0.059	15.849
	5	QSAR-ICE	11.683	1.450	82.701
	10	QSAR-ICE	37.459	6.603	168.596
	50	QSAR-ICE	710.737	341.356	1343.321
	1	MoA-QSAR-ICE	0.209	0.026	4.451
	5	MoA-QSAR-ICE	1.966	0.252	31.559
	10	MoA-QSAR-ICE	7.425	1.069	83.479
	50	MoA-QSAR-ICE	469.903	134.840	1498.315
TCE	1	Measured	82.934	57.022	133.229
	5	Measured	126.973	91.491	190.711
	10	Measured	164.047	120.281	237.481
	50	Measured	487.315	355.493	690.474
	1	QSAR-ICE	8.973	4.313	21.949
	5	QSAR-ICE	19.412	10.032	40.950
	10	QSAR-ICE	29.683	16.222	57.525
	50	QSAR-ICE	124.963	79.367	194.958
	1	MoA-QSAR-ICE	1.898	0.415	11.231
	5	MoA-QSAR-ICE	7.620	2.224	31.693
	10	MoA-QSAR-ICE	15.568	5.251	54.417
	50	MoA-QSAR-ICE	163.863	72.663	386.991
NAP	1	Measured	1.591	0.611	4.749
	5	Measured	4.433	2.034	10.407
	10	Measured	7.424	3.800	15.379
	50	Measured	40.040	23.604	68.379
	1	QSAR-ICE	3.847	1.525	12.997
	5	QSAR-ICE	10.906	4.571	31.408
	10	QSAR-ICE	19.920	8.788	50.975
	50	QSAR-ICE	157.728	83.047	295.912
	1	MoA-QSAR-ICE	0.406	0.090	2.841
	5	MoA-QSAR-ICE	1.773	0.502	8.135
	10	MoA-QSAR-ICE	3.867	1.237	14.797
	50	MoA-QSAR-ICE	53.344	20.627	138.003
TL	1	Measured	18.084	8.404	49.142
	5	Measured	42.288	21.261	98.632
	10	Measured	69.624	37.523	148.396
	50	Measured	464.210	257.857	835.827

	1	QSAR-ICE	41.908	20.401	104.231
	5	QSAR-ICE	90.184	46.510	194.670
	10	QSAR-ICE	139.523	74.507	275.002
	50	QSAR-ICE	651.788	395.905	1055.435
	1	MoA-QSAR-ICE	2.783	0.603	16.916
	5	MoA-QSAR-ICE	11.337	3.254	48.584
	10	MoA-QSAR-ICE	23.474	7.769	84.250
	50	MoA-QSAR-ICE	259.906	113.695	621.159
ANT	1	Measured	0.001	0.000	0.028
	5	Measured	0.003	0.001	0.089
	10	Measured	0.008	0.001	0.182
	50	Measured	0.382	0.040	3.169
	1	QSAR-ICE	0.013	0.002	0.181
	5	QSAR-ICE	0.139	0.022	1.126
	10	QSAR-ICE	0.487	0.089	2.611
	50	QSAR-ICE	15.147	6.422	33.142
	1	MoA-QSAR-ICE	0.010	0.003	0.061
	5	MoA-QSAR-ICE	0.034	0.011	0.177
	10	MoA-QSAR-ICE	0.074	0.024	0.329
	50	MoA-QSAR-ICE	1.424	0.470	4.339
TCB	1	Measured	2.034	1.304	3.659
	5	Measured	3.065	2.080	5.113
	10	Measured	3.930	2.726	6.374
	50	Measured	11.361	7.637	17.563
	1	QSAR-ICE	0.344	0.105	1.576
	5	QSAR-ICE	1.342	0.453	4.679
	10	QSAR-ICE	2.789	1.036	8.158
	50	QSAR-ICE	26.377	13.789	48.911
	1	MoA-QSAR-ICE	0.128	0.040	0.749
	5	MoA-QSAR-ICE	0.397	0.131	1.866
	10	MoA-QSAR-ICE	0.793	0.269	3.209
	50	MoA-QSAR-ICE	11.610	4.137	34.095
PCE	1	Measured	5.738	3.288	12.937
	5	Measured	9.618	5.878	19.688
	10	Measured	13.174	8.252	25.164
	50	Measured	50.307	29.727	91.596
	1	QSAR-ICE	1.924	0.701	6.821
	5	QSAR-ICE	5.819	2.436	15.812
	10	QSAR-ICE	10.395	4.727	24.888
	50	QSAR-ICE	64.552	37.384	110.205
	1	MoA-QSAR-ICE	0.253	0.047	2.146

	5	MoA-QSAR-ICE	1.296	0.324	7.232
	10	MoA-QSAR-ICE	3.063	0.887	13.590
	50	MoA-QSAR-ICE	50.393	19.443	127.440
PeCB	1	Measured	0.183	0.078	0.617
	5	Measured	0.426	0.188	1.176
	10	Measured	0.693	0.327	1.672
	50	Measured	3.604	2.015	6.386
	1	QSAR-ICE	0.184	0.091	0.496
	5	QSAR-ICE	0.418	0.212	0.986
	10	QSAR-ICE	0.673	0.359	1.454
	50	QSAR-ICE	3.755	2.151	6.654
	1	MoA-QSAR-ICE	0.021	0.005	0.144
	5	MoA-QSAR-ICE	0.083	0.023	0.418
	10	MoA-QSAR-ICE	0.181	0.055	0.780
	50	MoA-QSAR-ICE	2.876	1.080	8.136
NP	1	Measured	0.017	0.005	0.090
	5	Measured	0.065	0.021	0.243
	10	Measured	0.131	0.048	0.415
	50	Measured	1.244	0.595	2.563
	1	QSAR-ICE	0.175	0.070	0.574
	5	QSAR-ICE	0.478	0.204	1.320
	10	QSAR-ICE	0.847	0.384	2.100
	50	QSAR-ICE	6.386	3.384	12.090
	1	MoA-QSAR-ICE	0.013	0.003	0.100
	5	MoA-QSAR-ICE	0.061	0.017	0.312
	10	MoA-QSAR-ICE	0.140	0.042	0.573
	50	MoA-QSAR-ICE	2.132	0.801	5.494

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Table S3 HC values of SSD models using measured / QSAR-ICE / MoA-QSAR-ICE data (log-normal distributions)

Chemical	HC percent	Type	HC value	95% CI lower limit	95% CI upper limit
CF	1	Measured	31.149	12.140	91.193
	5	Measured	68.307	32.109	157.614
	10	Measured	103.816	53.999	210.808
	50	Measured	454.521	266.303	746.446
	1	QSAR-ICE	39.060	14.085	126.963
	5	QSAR-ICE	100.059	44.174	249.396
	10	QSAR-ICE	165.211	78.311	367.754
	50	QSAR-ICE	968.890	542.271	1704.274
	1	MoA-QSAR-ICE	7.696	1.960	37.845
	5	MoA-QSAR-ICE	24.554	8.065	85.467
	10	MoA-QSAR-ICE	45.573	16.770	136.234
	50	MoA-QSAR-ICE	403.811	178.155	863.291
BEN	1	Measured	28.735	11.907	79.603
	5	Measured	77.024	38.328	171.061
	10	Measured	130.290	69.605	254.838
	50	Measured	832.117	502.295	1296.004
	1	QSAR-ICE	56.333	21.820	168.592
	5	QSAR-ICE	135.102	63.162	315.864
	10	QSAR-ICE	215.369	107.570	453.261
	50	QSAR-ICE	1115.783	650.415	1886.496
	1	MoA-QSAR-ICE	8.337	2.139	40.631
	5	MoA-QSAR-ICE	26.425	8.734	91.344
	10	MoA-QSAR-ICE	48.878	18.087	145.223
	50	MoA-QSAR-ICE	427.852	189.625	910.816
DCM	1	Measured	12.300	2.038	108.635
	5	Measured	44.918	10.391	241.027
	10	Measured	89.598	23.960	376.194
	50	Measured	1023.593	369.495	2805.925
	1	QSAR-ICE	191.296	85.240	486.904
	5	QSAR-ICE	403.160	210.890	831.427
	10	QSAR-ICE	599.900	331.991	1131.098
	50	QSAR-ICE	2437.433	1538.763	3813.369
	1	MoA-QSAR-ICE	34.626	9.698	152.395
	5	MoA-QSAR-ICE	101.898	36.167	325.192
	10	MoA-QSAR-ICE	181.160	71.469	501.802
	50	MoA-QSAR-ICE	1379.041	644.072	2796.320

DCP	1	Measured	37.726	12.170	148.648
	5	Measured	85.256	33.927	245.478
	10	Measured	131.670	57.402	324.873
	50	Measured	610.028	321.218	1150.854
	1	QSAR-ICE	2.593	0.498	17.440
	5	QSAR-ICE	11.867	3.164	51.954
	10	QSAR-ICE	26.697	7.985	97.348
	50	QSAR-ICE	466.166	182.399	1161.678
	1	MoA-QSAR-ICE	0.575	0.066	7.127
	5	MoA-QSAR-ICE	3.597	0.619	25.824
	10	MoA-QSAR-ICE	9.559	1.969	53.958
	50	MoA-QSAR-ICE	300.502	82.450	998.537
TCE	1	Measured	50.039	26.115	98.786
	5	Measured	101.587	62.365	171.837
	10	Measured	148.178	95.904	234.164
	50	Measured	561.178	397.143	774.730
	1	QSAR-ICE	10.455	4.783	25.815
	5	QSAR-ICE	21.507	11.490	43.320
	10	QSAR-ICE	31.591	17.823	58.346
	50	QSAR-ICE	122.628	78.584	189.077
	1	MoA-QSAR-ICE	2.361	0.556	12.699
	5	MoA-QSAR-ICE	8.041	2.480	30.029
	10	MoA-QSAR-ICE	15.454	5.375	49.142
	50	MoA-QSAR-ICE	154.875	65.244	345.608
NAP	1	Measured	1.773	0.679	5.255
	5	Measured	4.487	2.075	10.631
	10	Measured	7.359	3.738	15.399
	50	Measured	42.169	23.524	71.513
	1	QSAR-ICE	4.660	1.550	16.630
	5	QSAR-ICE	12.861	5.321	34.464
	10	QSAR-ICE	22.097	9.872	52.409
	50	QSAR-ICE	149.104	79.694	274.287
	1	MoA-QSAR-ICE	0.492	0.099	3.197
	5	MoA-QSAR-ICE	1.923	0.520	8.326
	10	MoA-QSAR-ICE	3.977	1.229	14.398
	50	MoA-QSAR-ICE	51.606	19.733	125.998
TL	1	Measured	13.576	4.793	44.811
	5	Measured	39.161	16.792	97.333
	10	Measured	68.883	32.502	151.264
	50	Measured	504.967	272.713	886.541
	1	QSAR-ICE	43.470	18.376	117.584

	5	QSAR-ICE	96.171	48.228	207.903
	10	QSAR-ICE	146.854	78.198	288.565
	50	QSAR-ICE	653.716	400.514	1052.999
	1	MoA-QSAR-ICE	3.564	0.828	19.489
	5	MoA-QSAR-ICE	12.285	3.746	46.469
	10	MoA-QSAR-ICE	23.761	8.180	76.411
	50	MoA-QSAR-ICE	243.510	101.727	547.646
ANT	1	Measured	0.000	0.000	0.024
	5	Measured	0.003	0.000	0.075
	10	Measured	0.008	0.001	0.149
	50	Measured	0.385	0.049	2.612
	1	QSAR-ICE	0.056	0.011	0.375
	5	QSAR-ICE	0.256	0.068	1.114
	10	QSAR-ICE	0.574	0.172	2.084
	50	QSAR-ICE	9.932	3.897	24.686
	1	MoA-QSAR-ICE	0.007	0.001	0.059
	5	MoA-QSAR-ICE	0.033	0.007	0.181
	10	MoA-QSAR-ICE	0.076	0.019	0.342
	50	MoA-QSAR-ICE	1.519	0.495	4.306
TCB	1	Measured	1.110	0.473	2.860
	5	Measured	2.295	1.172	4.917
	10	Measured	3.382	1.860	6.468
	50	Measured	13.262	8.393	20.681
	1	QSAR-ICE	0.654	0.212	2.401
	5	QSAR-ICE	1.846	0.749	5.056
	10	QSAR-ICE	3.210	1.409	7.761
	50	QSAR-ICE	22.596	11.911	42.131
	1	MoA-QSAR-ICE	0.082	0.014	0.625
	5	MoA-QSAR-ICE	0.360	0.087	1.765
	10	MoA-QSAR-ICE	0.792	0.222	3.197
	50	MoA-QSAR-ICE	12.762	4.499	33.600
PCE	1	Measured	2.409	0.786	8.875
	5	Measured	6.228	2.503	17.290
	10	Measured	10.333	4.558	25.326
	50	Measured	61.643	31.547	114.821
	1	QSAR-ICE	2.974	1.152	8.902
	5	QSAR-ICE	7.134	3.335	16.680
	10	QSAR-ICE	11.372	5.680	23.936
	50	QSAR-ICE	58.926	34.348	99.632
	1	MoA-QSAR-ICE	0.399	0.079	2.618
	5	MoA-QSAR-ICE	1.570	0.421	6.856

	10	MoA-QSAR-ICE	3.261	1.001	11.895
	50	MoA-QSAR-ICE	42.954	16.332	105.428
PeCB	1	Measured	0.218	0.083	0.703
	5	Measured	0.490	0.219	1.212
	10	Measured	0.754	0.362	1.638
	50	Measured	3.461	1.940	5.884
	1	QSAR-ICE	0.178	0.067	0.549
	5	QSAR-ICE	0.438	0.200	1.047
	10	QSAR-ICE	0.707	0.346	1.518
	50	QSAR-ICE	3.832	2.201	6.575
	1	MoA-QSAR-ICE	0.020	0.004	0.150
	5	MoA-QSAR-ICE	0.087	0.022	0.417
	10	MoA-QSAR-ICE	0.190	0.054	0.749
	50	MoA-QSAR-ICE	2.924	1.048	7.582
NP	1	Measured	0.027	0.007	0.120
	5	Measured	0.081	0.028	0.257
	10	Measured	0.144	0.058	0.385
	50	Measured	1.120	0.533	2.232
	1	QSAR-ICE	0.190	0.063	0.686
	5	QSAR-ICE	0.529	0.217	1.431
	10	QSAR-ICE	0.914	0.405	2.184
	50	QSAR-ICE	6.276	3.335	11.610
	1	MoA-QSAR-ICE	0.016	0.003	0.112
	5	MoA-QSAR-ICE	0.066	0.017	0.302
	10	MoA-QSAR-ICE	0.140	0.041	0.533
	50	MoA-QSAR-ICE	2.004	0.739	5.060

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