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

at the University of Hong Kong

in December 2022

[Figure S1 The cumulative density curves and Q-Q plots of the developed SSD models 4](#_Toc122018381)

[Figure S2 SSD models for PCCs using measured / QSAR-ICE / MoA-QSAR-ICE data (averaging multiple distributions) 6](#_Toc122018382)

[Figure S3 HC values of SSD models using measured / QSAR-ICE / MoA-QSAR-ICE data (averaging multiple distributions) 7](#_Toc122018383)

[Figure S4 HC values of SSD models using measured / QSAR-ICE / MoA-QSAR-ICE data (log-normal distributions) 8](#_Toc122018384)

[Table S1 The goodness of fit of SSD models fitted by different methods 9](#_Toc122018392)

[Table S2 HC values of SSD models using measured / QSAR-ICE / MoA-QSAR-ICE data (averaging multiple distributions) 14](#_Toc122018393)

[Table S3 HC values of SSD models using measured / QSAR-ICE / MoA-QSAR-ICE data (log-normal distributions) 18](#_Toc122018394)

|  |  |  |  |
| --- | --- | --- | --- |
| CF |  |  |  |
| BEN |  |  |  |
| DCM |  |  |  |
| DCP |  |  |  |
| TCE |  |  |  |
| NAP |  |  |  |
| TL |  |  |  |
| ANT |  |  |  |
| TCB |  |  |  |
| PCE |  |  |  |
| PeCB |  |  |  |
| NP |  |  |  |

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

|  |  |
| --- | --- |
| 图形用户界面  描述已自动生成 | 图形用户界面, 图表  中度可信度描述已自动生成 |
| 图形用户界面  中度可信度描述已自动生成 | 图表  描述已自动生成 |
| 图形用户界面  中度可信度描述已自动生成 | 图表  低可信度描述已自动生成 |
| 图形用户界面  描述已自动生成 | 图形用户界面  中度可信度描述已自动生成 |
| 图表  中度可信度描述已自动生成 | 图表  中度可信度描述已自动生成 |
| 图形用户界面  中度可信度描述已自动生成 | 图形用户界面, 图表  中度可信度描述已自动生成 |

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

|  |  |  |  |
| --- | --- | --- | --- |
| 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 |
| 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 |
| 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 | 图表, 箱线图  描述已自动生成 |

**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)**

**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 |

**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 |

**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 |