Supporting information Data 3

of thesis entitled

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

Submitted by

**ZHANG Jiawei**

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[Figure S1 Cumulative density curves and Q-Q plots of the SSD models 4](#_Toc122099880)

[Table S1 Selected acute toxicity data for BPA, PFOS, PBDEs, and their substitutes 6](#_Toc122099881)

[Table S2 Selected chronic (lethal effect) toxicity data for BPA, PFOS, PBDEs, and their substitutes 13](#_Toc122099882)

[Table S3 Selected chronic (reproductive effect) toxicity data for BPA, PFOS, PBDEs, and their substitutes 17](#_Toc122099883)

[Table S4 The goodness of fit of SSD models 20](#_Toc122099884)

[Table S5 SSD model parameters, HC5 values, and the results of K-S tests using measured data and extrapolated data by ICE 22](#_Toc122099885)

[Table S6 SSD model parameters and HC5 values using chronic data 23](#_Toc122099886)

|  |  |
| --- | --- |
| **Mesured acute toxicity data** | **ICE-based acute toxicity data** |
| **BPA** |  |
|  |  |
| **PFOS** |  |
|  |  |
| **TPHP** |  |
|  |  |
| **PBDEs** |  |
|  |  |
| **Chronic-lethal toxicity data** | **Chronic-reproductive toxicity data** |
| **BPA** |  |
|  |  |
| **PFOS** |  |
|  |  |
| **TPHP** |  |
|  |  |
| **PBDEs** |  |
|  |  |
| **Acute toxicity** | |
| **BPF** | **BPAF** |
|  |  |
| **BPS** | **PFBS** |
|  |  |
| **PFHxS** | **F-53B** |
|  |  |
| **6:2 FTS** | **TCEP** |
|  |  |
| **TCPP** | **TMP** |
|  |  |
| **TEP** | **TOCP** |
|  |  |

Figure S Cumulative density curves and Q-Q plots of the SSD models

Table S Selected acute toxicity data for BPA, PFOS, PBDEs, and their substitutes

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No. | Chemical | Species scientific name | Species common name | Group | Conc. (μmol/L) | Endpoint | Observed duration (days) | Klimisch code | Reference |
| 1 | BPA | Raphidocelis subcapitata | Green Algae | Algae | 13.579 | EC50 | 4 | 1 | (Alexander et al., 1988) |
| 2 | BPA | Scenedesmus acutus | Green Algae | Algae | 117.044 | EC50 | 4 | 2 | (Zhang et al., 2014) |
| 3 | BPA | Chlorella pyrenoidosa | Green Algae | Algae | 278.286 | EC50 | 4 | 2 | (Zhang et al., 2014) |
| 4 | BPA | Gammarus pulex | Scud | Crustaceans | 24.530 | LC50 | 2 | 1 | (Watts et al., 2001) |
| 5 | BPA | Asellus aquaticus | Aquatic Sowbug | Crustaceans | 41.614 | LC50 | 4 | 2 | (Plahuta et al., 2015) |
| 6 | BPA | Daphnia magna | Water Flea | Crustaceans | 56.069 | LC50 | 2 | 2 | (Hirano et al., 2004) |
| 7 | BPA | Chironomus tentans | Midge | Insects | 11.827 | LC50 | 4 | 1 | (Mihaich et al., 2009) |
| 8 | BPA | Dugesia japonica | Flatworm | Worms | 16.645 | LC50 | 4 | 2 | (Li, 2013) |
| 9 | BPA | Lumbriculus variegatus | Oligochaete, Worm | Worms | 23.216 | LC50 | 4 | 2 | (Ladewig et al., 2006) |
| 10 | BPA | Marisa cornuarietis | Snail | Molluscs | 9.812 | LC50 | 4 | 1 | (Mihaich et al., 2009) |
| 11 | BPA | Hydra vulgaris | Hydra | Invertebrates | 38.986 | LC50 | 2 | 2 | (Pascoe et al., 2002) |
| 12 | BPA | Xenopus laevis | African Clawed Frog | Amphibians | 25.362 | LC50 | 4 | 2 | (Ozmen et al., 2015) |
| 13 | BPA | Rhinella arenarum | Argentine Toad | Amphibians | 42.490 | LC50 | 2 | 2 | (Wolkowicz et al., 2014) |
| 14 | BPA | Pimephales promelas | Fathead Minnow | Fish | 20.150 | LC50 | 4 | 1 | (Alexander et al., 1988) |
| 15 | BPA | Oryzias latipes | Japanese Medaka | Fish | 22.340 | LC50 | 3 | 2 | (Kashiwada et al., 2002) |
| 16 | BPA | Cyprinus carpio | Common Carp | Fish | 28.604 | LC50 | 4 | 2 | (Jung et al., 2020) |
| 17 | BPA | Danio rerio | Zebra Danio | Fish | 35.218 | LC50 | 4 | 2 | (Chan and Chan, 2012) |
| 18 | BPA | Xiphophorus helleri | Green Swordtail | Fish | 78.540 | LC50 | 4 | 2 | (Kwak et al., 2001) |
| 1 | BPAF | Scenedesmus obliquus | Green Algae | Algae | 13.860 | EC50 | 3 | 1 | (Wang et al., 2018) |
| 2 | BPAF | Daphnia magna | Water Flea | Crustaceans | 8.030 | EC50 | 2 | 2 | (Tišler et al., 2016) |
| 3 | BPAF | Chironomus tentans | Midge | Insects | 1.933 | EC50 | 2 | 1 | (Wang et al., 2018) |
| 4 | BPAF | Marisa cornuarietis | Snail | Molluscs | 3.331 | LC50 | 4 | 1 | (Wang et al., 2018) |
| 5 | BPAF | Danio rerio | Zebra Danio | Fish | 5.800 | LC50 | 4 | 1 | (Mu et al., 2018) |
| 1 | BPF | Scenedesmus obliquus | Green Algae | Algae | 249.953 | EC50 | 3 | 1 | (Wang et al., 2018) |
| 2 | BPF | Daphnia magna | Water Flea | Crustaceans | 43.450 | EC50 | 2 | 1 | (Tatjana et al., 2016) |
| 3 | BPF | Chironomus tentans | Midge | Insects | 11.487 | EC50 | 2 | 1 | (Wang et al., 2018) |
| 4 | BPF | Marisa cornuarietis | Snail | Molluscs | 39.954 | LC50 | 4 | 1 | (Wang et al., 2018) |
| 5 | BPF | Danio rerio | Zebra Danio | Fish | 47.495 | LC50 | 4 | 1 | (Ren et al., 2017a) |
| 1 | PFOS | Raphidocelis subcapitata | Green Algae | Algae | 65.029 | EC50 | 3 | 1 | (Rosal et al., 2010) |
| 2 | PFOS | Chlorella vulgaris | Green Algae | Algae | 151.611 | EC50 | 4 | 2 | (Boudreau et al., 2003) |
| 3 | PFOS | Scenedesmus quadricauda | Green Algae | Algae | 165.992 | EC50 | 4 | 1 | (Yang et al., 2014) |
| 4 | PFOS | Scenedesmus acutus | Green Algae | Algae | 234.105 | EC50 | 4 | 2 | (Zhang et al., 2012b) |
| 5 | PFOS | Navicula pelliculosa | Diatom | Algae | 468.210 | EC50 | 4 | 1 | (Sutherland and Krueger, 2001) |
| 6 | PFOS | Chlorella pyrenoidosa | Green Algae | Algae | 594.552 | EC50 | 4 | 2 | (Zhang et al., 2012b) |
| 7 | PFOS | Daphnia carinata | Water Flea | Crustaceans | 16.350 | EC50 | 2 | 2 | (Logeshwaran et al., 2021) |
| 8 | PFOS | Neocaridina denticulata | Shrimp | Crustaceans | 18.580 | LC50 | 4 | 2 | (Li, 2009) |
| 9 | PFOS | Moina macrocopa | Water Flea | Crustaceans | 35.891 | EC50 | 2 | 2 | (Ji et al., 2008) |
| 10 | PFOS | Macrobrachium nipponense | Oriental River Shrimp | Crustaceans | 36.732 | LC50 | 4 | 1 | (Yang et al., 2014) |
| 11 | PFOS | Daphnia magna | Water Flea | Crustaceans | 42.379 | LC50 | 2 | 2 | (Yang et al., 2019) |
| 12 | PFOS | Daphnia pulicaria | Water Flea | Crustaceans | 248.969 | EC50 | 2 | 2 | (Boudreau et al., 2003) |
| 13 | PFOS | Chironomus plumosus | Midge | Insects | 338.375 | LC50 | 4 | 1 | (Yang et al., 2014) |
| 14 | PFOS | Dugesia japonica | Flatworm | Worms | 42.733 | LC50 | 4 | 2 | (Li, 2009) |
| 15 | PFOS | Limnodrilus hoffmeisteri | Tubificid Worm, Oligochaete | Worms | 224.759 | LC50 | 4 | 1 | (Yang et al., 2014) |
| 16 | PFOS | Elliptio complanata | Mussel, Eastern Elliptio | Molluscs | 109.621 | LC50 | 4 | 1 | (Drottar and Krueger, 2000a) |
| 17 | PFOS | Unio ravoisieri | Freshwater Mussel | Molluscs | 122.441 | LC50 | 4 | 2 | (Amraoui et al., 2018) |
| 18 | PFOS | Ligumia recta | Black Sandshell | Molluscs | 283.326 | EC50 | 4 | 2 | (Hazelton et al., 2012) |
| 19 | PFOS | Lampsilis siliquoidea | Lamp-Mussel | Molluscs | 316.118 | EC50 | 4 | 2 | (Hazelton et al., 2012) |
| 20 | PFOS | Physella acuta | European Physa | Molluscs | 330.720 | LC50 | 4 | 2 | (Li, 2009) |
| 21 | PFOS | Cipangopaludina cathayensis | Freshwater Snail | Molluscs | 459.180 | LC50 | 4 | 1 | (Yang et al., 2014) |
| 22 | PFOS | Hyla versicolor | Gray Tree Frog | Amphibians | 47.988 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 23 | PFOS | Ambystoma texanum | Texas Salamander | Amphibians | 81.979 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 24 | PFOS | Bufo gargarizans | Asiatic Toad | Amphibians | 89.573 | LC50 | 4 | 1 | (Yang et al., 2014) |
| 25 | PFOS | Anaxyrus americanus | American Toad | Amphibians | 123.968 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 26 | PFOS | Ambystoma jeffersonianum | Jefferson's Salamander | Amphibians | 127.967 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 27 | PFOS | Ambystoma tigrinum | Tiger Salamander | Amphibians | 145.962 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 28 | PFOS | Lithobates pipiens | Leopard Frog | Amphibians | 145.962 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 29 | PFOS | Lithobates clamitans ssp. clamitans | Bronze Frog | Amphibians | 225.941 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 30 | PFOS | Lithobates sylvaticus | Wood Frog | Amphibians | 259.932 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 31 | PFOS | Rana catesbeiana | Bullfrog | Amphibians | 287.925 | LC50 | 4 | 2 | (Flynn et al., 2019) |
| 32 | PFOS | Pimephales promelas | Fathead Minnow | Fish | 17.651 | LC50 | 4 | 1 | (Drottar and Krueger, 2000a) |
| 33 | PFOS | Pseudorasbora parva | Motsuga, Stone Moroko | Fish | 125.859 | LC50 | 4 | 1 | (Yang et al., 2014) |
| 34 | PFOS | Lepomis macrochirus | Bluegill | Fish | 126.342 | LC50 | 4 | 2 | https://hero.epa.gov/hero/index.cfm/reference/details/reference\_id/3857455 |
| 35 | PFOS | Danio rerio | Zebra Danio | Fish | 141.963 | LC50 | 4 | 2 | (Ye et al., 2007) |
| 36 | PFOS | Carassius auratus | Goldfish | Fish | 150.831 | LC50 | 4 | 1 | (Yang et al., 2014) |
| 1 | PFHxS | Lithobates clamitans ssp. clamitans | Bronze Frog | Amphibians | 1729.764 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 2 | PFHxS | Rana catesbeiana | Bullfrog | Amphibians | 2521.622 | LC50 | 4 | 2 | (Tornabene et al., 2021) |
| 1 | PFBS | Raphidocelis subcapitata | Green Algae | Algae | 2956.830 | EC50 | 2 | 2 | (Kusk et al., 2018) |
| 2 | PFBS | Daphnia magna | Water Flea | Crustaceans | 6454.760 | EC50 | 2 | 1 | (Giesy et al., 2010) |
| 3 | PFBS | Danio rerio | Zebra Danio | Fish | 4121.821 | LC50 | 4 | 2 | (Wasel et al., 2021) |
| 4 | PFBS | Pimephales promelas | Fathead Minnow | Fish | 5730.337 | LC50 | 4 | 1 | (Giesy et al., 2010) |
| 5 | PFBS | Lepomis macrochirus | Bluegill | Fish | 19077.469 | LC50 | 4 | 1 | (Giesy et al., 2010) |
| 1 | 6:2 FTS | Raphidocelis subcapitata | Green Algae | Algae | 205.894 | EC50 | 3 | 1 | (Hoke et al., 2015) |
| 2 | 6:2 FTS | Daphnia magna | Water Flea | Crustaceans | 233.775 | LC50 | 2 | 1 | (Hoke et al., 2015) |
| 3 | 6:2 FTS | Danio rerio | Zebra Danio | Fish | 50.001 | LC50 | 6 | 2 | (Dasgupta et al., 2020) |
| 4 | 6:2 FTS | Oncorhynchus mykiss | Rainbow Trout | Fish | 229.486 | LC50 | 4 | 1 | (Hoke et al., 2015) |
| 1 | F-53B | Scenedesmus acutus | Green Algae | Algae | 70.619 | IC50 | 3 | 1 | (Liu et al., 2018) |
| 2 | F-53B | Daphnia magna | Water Flea | Crustaceans | 19.100 | LC50 | 2 | 2 | (Zhang et al., 2021) |
| 3 | F-53B | Danio rerio | Zebra Danio | Fish | 3.855 | LC50 | 4 | 2 | (Liu et al., 2021) |
| 4 | F-53B | Gobiocypris rarus | Chinese Rare Minnow | Fish | 36.448 | LC50 | 4 | 2 | (Liu et al., 2020) |
| 1 | TCPP | Scenedesmus subspicatus | Green Algae | Algae | 137.379 | EC50 | 4 | 2 | (Niu et al., 2019) |
| 2 | TCPP | Raphidocelis subcapitata | Green Algae | Algae | 222.860 | EC50 | 4 | 2 | (Niu et al., 2019) |
| 3 | TCPP | Daphnia magna | Water Flea | Crustaceans | 277.812 | EC50 | 2 | 2 | (Niu et al., 2019) |
| 4 | TCPP | Poecilia reticulata | Guppy | Fish | 91.586 | LC50 | 4 | 2 | (Niu et al., 2019) |
| 5 | TCPP | Pimephales promelas | Fathead Minnow | Fish | 155.697 | LC50 | 4 | 2 | (Niu et al., 2019) |
| 6 | TCPP | Oryzias latipes | Japanese Medaka | Fish | 164.855 | LC50 | 4 | 2 | (Niu et al., 2019) |
| 7 | TCPP | Danio rerio | Zebra Danio | Fish | 170.961 | LC50 | 4 | 2 | (Niu et al., 2019) |
| 8 | TCPP | Lepomis macrochirus | Bluegill | Fish | 256.442 | LC50 | 4 | 2 | (Niu et al., 2019) |
| 1 | TCEP | Scenedesmus subspicatus | Green Algae | Algae | 178.646 | EC50 | 4 | 2 | (Niu et al., 2019) |
| 2 | TCEP | Raphidocelis subcapitata | Green Algae | Algae | 409.836 | EC50 | 4 | 2 | (Niu et al., 2019) |
| 3 | TCEP | Daphnia magna | Water Flea | Crustaceans | 1155.948 | EC50 | 2 | 2 | (Niu et al., 2019) |
| 4 | TCEP | Moina macropoda | Water Flea | Crustaceans | 3502.872 | LC50 | 2 | 2 | (Niu et al., 2019) |
| 5 | TCEP | Oryzias latipes | Japanese Medaka | Fish | 231.190 | LC50 | 2 | 2 | https://hero.epa.gov/hero/index.cfm/reference/details/reference\_id/3617855 |
| 6 | TCEP | Carassius auratus | Goldfish | Fish | 315.259 | LC50 | 4 | 2 | (Niu et al., 2019) |
| 7 | TCEP | Leuciscus idus melanotus | Orfe | Fish | 700.574 | LC50 | 4 | 2 | (Niu et al., 2019) |
| 8 | TCEP | Danio rerio | Zebra Danio | Fish | 707.580 | LC50 | 4 | 2 | (Du et al., 2015) |
| 9 | TCEP | Oncorhynchus mykiss | Rainbow Trout | Fish | 872.215 | LC50 | 4 | 2 | (Niu et al., 2019) |
| 1 | TMP | Pimephales promelas | Fathead Minnow | Fish | 50046.405 | LC50 | 4 | 1 | (Geiger et al., 1990) |
| 1 | TPHP | Raphidocelis subcapitata | Green Algae | Algae | 6.130 | EC50 | 4 | 2 | (Mayer et al., 1981) |
| 2 | TPHP | Gammarus pseudolimnaeus | Scud | Crustaceans | 0.766 | EC50 | 4 | 1 | (Huckins et al., 1991) |
| 3 | TPHP | Daphnia magna | Water Flea | Crustaceans | 1.624 | LC50 | 2 | 2 | (Scanlan et al., 2015) |
| 4 | TPHP | Chironomus riparius | Midge | Insects | 1.103 | EC50 | 2 | 1 | (Huckins et al., 1991) |
| 5 | TPHP | Chironomus sp. | Midge | Insects | 4.904 | EC50 | 2 | 2 | ECOTOX database |
| 6 | TPHP | Chironomus tentans | Midge | Insects | 4.904 | EC50 | 2 | 2 | ECOTOX database |
| 7 | TPHP | Cyprinodon variegatus | Sheepshead Minnow | Fish | 0.919 | LC50 | 4 | 2 | (Mayer et al., 1981) |
| 8 | TPHP | Oncorhynchus mykiss | Rainbow Trout | Fish | 1.103 | LC50 | 4 | 2 | https://hero.epa.gov/hero/index.cfm/reference/details/reference\_id/7546266 |
| 9 | TPHP | Ictalurus punctatus | Channel Catfish | Fish | 1.287 | LC50 | 4 | 2 | (Mayer and Ellersieck, 1986) |
| 10 | TPHP | Gobiocypris rarus | Chinese Rare Minnow | Fish | 1.851 | LC50 | 4 | 2 | (Hong et al., 2018) |
| 11 | TPHP | Pimephales promelas | Fathead Minnow | Fish | 2.023 | LC50 | 4 | 2 | (Mayer et al., 1981) |
| 12 | TPHP | Carassius auratus | Goldfish | Fish | 2.145 | LC50 | 4 | 2 | (Sasaki et al., 1981) |
| 13 | TPHP | Lepomis macrochirus | Bluegill | Fish | 2.391 | LC50 | 4 | 1 | (Huckins et al., 1991) |
| 14 | TPHP | Oryzias latipes | Japanese Medaka | Fish | 3.678 | LC50 | 4 | 2 | (Sasaki et al., 1981) |
| 15 | TPHP | Danio rerio | Zebra Danio | Fish | 4.689 | LC50 | 4 | 2 | (Du et al., 2015) |
| 1 | PBDEs | Scenedesmus quadricanda | Green Algae | Algae | 2.012 | EC50 | 4 | 1 | (Lu et al., 2018) |
| 2 | PBDEs | Brachionus plicatilis |  | Invertebrates | 0.308 | EC50 | 2 | 1 | (Lu et al., 2018) |
| 3 | PBDEs | Sinocalanus sinensis |  | Invertebrates | 1.491 | EC50 | 2 | 1 | (Lu et al., 2018) |
| 4 | PBDEs | Daphnia magna | Water Flea | Invertebrates | 1.540 | EC50 | 2 | 1 | (Lu et al., 2018) |
| 5 | PBDEs | Macrobrachium nipponense | | Invertebrates | 2.210 | EC50 | 2 | 1 | (Lu et al., 2018) |
| 6 | PBDEs | Danio rerio | Zebra Danio | Vertebrates | 1.074 | LC50 | 4 | 1 | (Lu et al., 2018) |
| 7 | PBDEs | Pseudorasbora parva | Motsuga, Stone Moroko | Vertebrates | 3.266 | LC50 | 4 | 1 | (Lu et al., 2018) |
| 8 | PBDEs | Fejervarya limnocharis |  | Vertebrates | 9.603 | LC50 | 4 | 1 | (Lu et al., 2018) |
| 9 | PBDEs | Carassius carassius |  | Vertebrates | 16.446 | LC50 | 4 | 1 | (Lu et al., 2018) |

Table S Selected chronic (lethal effect) toxicity data for BPA, PFOS, PBDEs, and their substitutes

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No. | Chemical | Species scientific name | Species common name | Group | Conc. (μmol/L) | Endpoint | Observed duration (days) | Klimisch code | Reference |
| 1 | BPA | Chlorella pyrenoidosa | Green Algae | Algae | 219.020 | NOEC | 20 | 2 | (Zhang et al., 2014) |
| 2 | BPA | Chlorolobion braunii | Algae | Algae | 17.522 | NOEC | 4 | 2 | (Gattullo et al., 2012) |
| 3 | BPA | Scenedesmus acutus var. acutus | Green Algae | Algae | 219.020 | NOEC | 30 | 2 | (Zhang et al., 2014) |
| 4 | BPA | Asellus aquaticus | Aquatic Sowbug | Crustaceans | 8.761 | NOEC | 21 | 2 | (Plahuta et al., 2015) |
| 5 | BPA | Daphnia magna | Water Flea | Crustaceans | 21.902 | NOEC | 21 | 1 | (Tišler et al., 2016) |
| 6 | BPA | Gammarus fossarum | Scud | Crustaceans | 2.190 | NOEC | 103 | 2 | (Ladewig et al., 2006) |
| 7 | BPA | Chironomus tentans | Midge | Insects | 6.133 | NOEC | 4 | 1 | (Mihaich et al., 2009) |
| 8 | BPA | Potamopyrgus antipodarum | Snail | Molluscs | 0.438 | NOEC | 28 | 2 | (Gagnaire et al., 2009) |
| 9 | BPA | Valvata piscinalis | European Stream Valvata | Molluscs | 0.438 | NOEC | 28 | 2 | (Gagnaire et al., 2009) |
| 10 | BPA | Rhinella arenarum | Argentine Toad | Amphibians | 7.885 | NOEC | 14 | 2 | (Wolkowicz et al., 2014) |
| 11 | BPA | Xenopus laevis | African Clawed Frog | Amphibians | 0.100 | NOEC | 84 | 2 | (Kloas et al., 1999) |
| 12 | BPA | Danio rerio | Zebra Danio | Fish | 6.571 | NOEC | 21 | 1 | (Song et al., 2014) |
| 13 | BPA | Oryzias latipes | Japanese Medaka | Fish | 2.628 | NOEC | 44 | 2 | (Sun et al., 2014) |
| 14 | BPA | Pimephales promelas | Fathead Minnow | Fish | 0.569 | NOEC | 164 | 1 | (Mihaich et al., 2012) |
| 1 | BPAF | Daphnia magna | Water Flea | Crustaceans | 2.677 | NOEC | 21 | 1 | (Tišler et al., 2016) |
| 2 | BPAF | Danio rerio | Zebra Danio | Fish | 4.461 | NOEC | 21 | 1 | (Song et al., 2014) |
| 1 | BPF | Daphnia magna | Water Flea | Crustaceans | 33.462 | NOEC | 21 | 1 | (Tišler et al., 2016) |
| 2 | BPF | Danio rerio | Zebra Danio | Fish | 4.994 | NOEC | 4.8333 | 2 | (Qiu et al., 2018) |
| 1 | PFOS | Chlorella pyrenoidosa | Green Algae | Algae | 148.638 | NOEC | 4 | 2 | (Zhang et al., 2012a) |
| 2 | PFOS | Chlorella vulgaris | Green Algae | Algae | 15.235 | NOEC | 4 | 2 | (Boudreau et al., 2003) |
| 3 | PFOS | Scenedesmus acutus | Green Algae | Algae | 55.739 | NOEC | 30 | 2 | (Sanderson et al., 2002) |
| 4 | PFOS | Cyclops sp. | Cyclopoid Copepod | Crustaceans | 55.739 | NOEC | 7 | 2 | (Sanderson et al., 2002) |
| 5 | PFOS | Daphnia magna | Water Flea | Crustaceans | 21.367 | NOEC | 21 | 1 | (Drottar and Krueger, 2000b) |
| 6 | PFOS | Moina macrocopa | Water Flea | Crustaceans | 2.499 | NOEC | 7 | 2 | (Ji et al., 2008) |
| 7 | PFOS | Neocaridina denticulata | Shrimp | Crustaceans | 9.290 | NOEC | 4 | 2 | (Li, 2009) |
| 8 | PFOS | Chironomus tentans | Midge | Insects | 0.176 | NOEC | 20 | 1 | (MacDonald et al., 2004) |
| 9 | PFOS | Dugesia japonica | Flatworm | Worms | 18.580 | NOEC | 4 | 2 | (Li, 2009) |
| 10 | PFOS | Physella acuta | European Physa | Molluscs | 185.798 | NOEC | 4 | 2 | (Li, 2009) |
| 11 | PFOS | Bufo gargarizans | Asiatic Toad | Amphibians | 3.716 | EC10 | 30 | 1 | (Yang et al., 2014) |
| 12 | PFOS | Lithobates pipiens | Leopard Frog | Amphibians | 6.596 | NOEC | 105 | 1 | (Ankley et al., 2004) |
| 13 | PFOS | Rana catesbeiana | Bullfrog | Amphibians | 0.576 | NOEC | 72 | 2 | (Flynn et al., 2019) |
| 14 | PFOS | Xenopus laevis | African Clawed Frog | Amphibians | 0.200 | NOEC | 67 | 2 | (Cheng et al., 2011) |
| 15 | PFOS | Danio rerio | Zebra Danio | Fish | 0.497 | NOEC | 180 | 1 | (Keiter et al., 2012) |
| 16 | PFOS | Oncorhynchus mykiss | Rainbow Trout | Fish | 1.858 | NOEC | 14 | 2 | (Oakes et al., 2005) |
| 17 | PFOS | Oryzias latipes | Japanese Medaka | Fish | 1.999 | NOEC | 14 | 2 | (Ji et al., 2008) |
| 18 | PFOS | Pimephales promelas | Fathead Minnow | Fish | 0.557 | NOEC | 47 | 1 | (Drottar and Krueger, 2000c) |
| 19 | PFOS | Pseudorasbora parva | Motsuga, Stone Moroko | Fish | 3.939 | EC10 | 30 | 1 | (Yang et al., 2014) |
| 1 | PFHxS | Chironomus dilutus | Midge | Insects | 2.334 | NOEC | 19 | 1 | (McCarthy et al., 2021) |
| 2 | PFHxS | Danio rerio | Zebra Danio | Fish | 11.747 | NOEC | 6 | 1 | (Menger et al., 2020) |
| 1 | PFBS | Selenastrum capricornutum | Green Algae | Algae | 842.697 | NOEC | 4 | 1 | (Giesy et al., 2010) |
| 2 | PFBS | Daphnia magna | Water Flea | Crustaceans | 2942.046 | NOEC | 21 | 1 | ECOTOX database |
| 3 | PFBS | Chironomus dilutus | Midge | Insects | 142.286 | NOEC | 19 | 1 | (McCarthy et al., 2021) |
| 4 | PFBS | Danio rerio | Zebra Danio | Fish | 73.309 | NOEC | 6 | 1 | (Menger et al., 2020) |
| 5 | PFBS | Lepomis macrochirus | Bluegill | Fish | 8027.794 | NOEC | 4 | 1 | (Giesy et al., 2010) |
| 6 | PFBS | Pimephales promelas | Fathead Minnow | Fish | 2625.665 | NOEC | 4 | 1 | (Giesy et al., 2010) |
| 1 | 6:2 FTS | Danio rerio | Zebra Danio | Fish | 184.510 | NOEC | 6 | 1 | (Menger et al., 2020) |
| 2 | 6:2 FTS | Oncorhynchus mykiss | Rainbow Trout | Fish | 18.659 | NOEC | 90 | 1 | (Hoke et al., 2015) |
| 1 | F-53B | Danio rerio | Zebra Danio | Fish | 0.088 | NOEC | 180 | 2 | (Shi et al., 2019) |
| 2 | TCPP | Dugesia japonica | Flatworm | Worms | 100.004 | NOEC | 12 | 2 | (Zhang et al., 2019b) |
| 1 | TCPP | Danio rerio | Zebra Danio | Fish | 7.425 | NOEC | 4.9167 | 1 | (Li et al., 2019) |
| 2 | TCEP | Dugesia japonica | Flatworm | Worms | 100.004 | NOEC | 12 | 2 | (Zhang et al., 2019a) |
| 1 | TCEP | Danio rerio | Zebra Danio | Fish | 8.711 | NOEC | 4.9167 | 1 | (Li et al., 2019) |
| 1 | TPHP | Daphnia magna | Water Flea | Crustaceans | 0.153 | NOEC | 21 | 2 | (Yuan et al., 2018) |
| 2 | TPHP | Dugesia japonica | Flatworm | Worms | 10.000 | NOEC | 12 | 2 | (Zhang et al., 2019b) |
| 3 | TPHP | Danio rerio | Zebra Danio | Fish | 1.532 | NOEC | 7 | 2 | (Kim et al., 2015) |
| 4 | TPHP | Oncorhynchus mykiss | Rainbow Trout | Fish | 0.004 | LOEC | 90 | 1 | (Mayer et al., 1981) |
| 5 | TPHP | Rana catesbeiana | Bullfrog | Ver | 0.052 | NOEC | 28 | 2 | (赵师晴, 2021) |
| 6 | TPHP | Macrobrachium nipponense | | Inver | 0.132 | NOEC | 28 | 2 | (赵师晴, 2021) |
| 7 | TPHP | Rhodeus sinensis |  | Ver | 0.555 | NOEC | 28 | 2 | (赵师晴, 2021) |
| 8 | TPHP | Oryzias melastigma | Medaka | Ver | 0.015 | NOEC | 20 | 2 | (钟代银, 2019) |
| 9 | TPHP | Pimephales promelas | Fathead Minnow | Fish | 0.267 | NOEC | 30 | 1 | (Mayer et al., 1981) |
| 1 | PBDEs | Raphidocelis subcapitata | Green Algae | Algae | 0.048 | NOEC | 6 | 2 | (Masekoameng, 2006) |
| 2 | PBDEs | Nitocra spinipes |  | Crustaceans | 0.005 | NOEC | 26 | 1 | (Breitholtz et al., 2008) |
| 3 | PBDEs | Daphnia magna | Water Flea | Crustaceans | 0.185 | NOEC | 21 | 1 | (Lu et al., 2018) |
| 4 | PBDEs | Dugesia japonica | Flatworm | Worms | 10 | NOEC | 12 | 2 | (Zhang et al., 2019b) |
| 5 | PBDEs | Danio rerio | Zebra Danio | Fish | 0.031 | NOEC | 21 | 2 | (Masekoameng, 2006) |
| 6 | PBDEs | Pseudorasbora parva | Motsuga, Stone Moroko | Vertebrates | 0.211 | NOEC | 30 | 1 | (Lu et al., 2018) |
| 7 | PBDEs | Fejervarya limnocharis |  | Vertebrates | 0.961 | NOEC | 30 | 1 | (Lu et al., 2018) |

Table S Selected chronic (reproductive effect) toxicity data for BPA, PFOS, PBDEs, and their substitutes

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| No. | Chemical | Species scientific name | Species common name | Group | Conc. (μmol/L) | Endpoint | Observed duration (days) | Klimisch code | Reference |
| 1 | BPA | Ceriodaphnia dubia | Water Flea | Crustaceans | 4.118 | NOEC | 7 | 2 | (Tatarazako et al., 2002) |
| 2 | BPA | Daphnia magna | Water Flea | Crustaceans | 3.504 | NOEC | 21 | 2 | (Brennan et al., 2006) |
| 3 | BPA | Gammarus fossarum | Scud | Crustaceans | 2.190 | NOEC | 103 | 2 | (Ladewig et al., 2006) |
| 4 | BPA | Hyalella azteca | Scud | Crustaceans | 2.146 | NOEC | 42 | 1 | (Mihaich et al., 2009) |
| 5 | BPA | Potamopyrgus antipodarum | Snail | Molluscs | 0.438 | NOEC | 28 | 2 | (Gagnaire et al., 2009) |
| 6 | BPA | Valvata piscinalis | European Stream Valvata | Molluscs | 0.438 | NOEC | 28 | 2 | (Gagnaire et al., 2009) |
| 7 | BPA | Xenopus laevis | African Clawed Frog | Amphibians | 0.010 | NOEC | 120 | 2 | (Levy et al., 2004) |
| 8 | BPA | Cyprinella sp. | Satinfin Shiners | Fish | 5.607 | LOEC | 15 | 2 | (Ward and Blum, 2012) |
| 9 | BPA | Danio rerio | Zebra Danio | Fish | 1.752 | NOEC | 180 | 2 | (Keiter et al., 2012) |
| 10 | BPA | Gasterosteus aculeatus | Threespine Stickleback | Fish | 0.235 | NOEC | 165 | 1 | (de Kermoysan et al., 2013) |
| 11 | BPA | Gobiocypris rarus | Chinese Rare Minnow | Fish | 0.056 | NOEC | 63 | 1 | (Zhu et al., 2020) |
| 12 | BPA | Oryzias latipes | Japanese Medaka | Fish | 3.000 | NOEC | 21 | 2 | (Shioda and Wakabayashi, 2000) |
| 13 | BPA | Pimephales promelas | Fathead Minnow | Fish | 2.484 | NOEC | 164 | 1 | (Mihaich et al., 2012) |
| 14 | BPA | Poecilia reticulata | Guppy | Fish | 1.200 | LOEC | 21 | 2 | (Haubruge et al., 2000) |
| 15 | BPA | Salmo trutta ssp. fario | Brown Trout | Fish | 0.011 | NOEC | 60.88 | 2 | (Lahnsteiner et al., 2005) |
| 1 | BPAF | Daphnia magna | Water Flea | Crustaceans | 0.684 | NOEC | 21 | 1 | (Tišler et al., 2016) |
| 2 | BPAF | Danio rerio | Zebra Danio | Fish | 0.074 | NOEC | 120 | 2 | (Shi et al., 2015) |
| 1 | BPF | Daphnia magna | Water Flea | Crustaceans | 4.195 | NOEC | 21 | 1 | (Tišler et al., 2016) |
| 1 | PFOS | Daphnia magna | Water Flea | Crustaceans | 13.805 | NOEC | 21 | 1 | (Yang et al., 2014) |
| 2 | PFOS | Moina macrocopa | Water Flea | Crustaceans | 0.625 | NOEC | 7 | 2 | (Ji et al., 2008) |
| 3 | PFOS | Lampsilis siliquoidea | Lamp-Mussel | Molluscs | 0.139 | NOEC | 36 | 1 | (Hazelton et al., 2012) |
| 4 | PFOS | Carassius auratus | Goldfish | Fish | 2.787 | NOEC | 16 | 2 | (Han et al., 2009) |
| 5 | PFOS | Catostomus commersoni | White Sucker | Fish | 5.574 | NOEC | 21 | 2 | (Oakes et al., 2005) |
| 6 | PFOS | Danio rerio | Zebra Danio | Fish | 0.199 | NOEC | 316 | 1 | (Keiter et al., 2012) |
| 7 | PFOS | Oryzias latipes | Japanese Medaka | Fish | 1.999 | LOEC | 21 | 2 | (Kang et al., 2019) |
| 8 | PFOS | Pimephales promelas | Fathead Minnow | Fish | 0.522 | NOEC | 45 | 1 | (Ankley et al., 2005) |
| 9 | PFOS | Xiphophorus helleri | Green Swordtail | Fish | 0.186 | NOEC | 90 | 2 | (Han and Fang, 2010) |
| 1 | PFHxS | Pimephales promelas | Fathead Minnow | Fish | 2.825 | NOEC | 42 | 1 | (Suski et al., 2021) |
| 1 | PFBS | Daphnia magna | Water Flea | Crustaceans | 1484 | NOEC | 21 | 1 | ECOTOX database |
| 1 | 6:2 FTS | Oncorhynchus mykiss | Rainbow Trout | Fish | 5.619 | NOEC | 90 | 1 | (Hoke et al., 2015) |
| 1 | F-53B | Danio rerio | Zebra Danio | Fish | 0.085 | NOEC | 180 | 1 | (Shi et al., 2018) |
| 1 | TCPP | Danio rerio | Zebra Danio | Fish | 7.425 | NOEC | 4.9167 | 1 | (Li et al., 2019) |
| 1 | TCEP | Danio rerio | Zebra Danio | Fish | 8.711 | NOEC | 4.9167 | 1 | (Li et al., 2019) |
| 2 | TCEP | Oryzias latipes | Japanese Medaka | Fish | 21.9 | NOEC | 14 | 2 | (Sun et al., 2016) |
| 1 | TPHP | Daphnia magna | Water Flea | Crustaceans | 0.153 | NOEC | 21 | 2 | (Yuan et al., 2018) |
| 2 | TPHP | Danio rerio | Zebra Danio | Fish | 1.532 | NOEC | 7 | 2 | (Kim et al., 2015) |
| 3 | TPHP | Oryzias latipes | Japanese Medaka | Fish | 0.000 | NOEC | 100 | 1 | (Li et al., 2018) |
| 4 | TPHP | Oryzias melastigma | Medaka | Fish | 0.015 | NOEC | 20 | 2 | (钟代银, 2019) |
| 5 | TPHP | Gobiocypris rarus | Chinese Rare Minnow | Fish | 0.037 | NOEC | 28 | 1 | (Chen et al., 2020) |
| 6 | TPHP | Pimephales promelas | Fathead Minnow | Fish | 0.705 | NOEC | 30 | 1 | (Bionomics and Bionomics, 1979) |
| 1 | PBDEs | Nitocra spinipes |  | Crustaceans | 0.005 | NOEC | 26 | 1 | (Breitholtz et al., 2008) |
| 2 | PBDEs | Ceriodaphnia dubia | Water Flea | Crustaceans | 0.140 | NOEC | 21 | 1 | (Lu et al., 2018) |
| 3 | PBDEs | Daphnia magna | Water Flea | Crustaceans | 0.071 | NOEC | 21 | 1 | (Lu et al., 2018) |
| 4 | PBDEs | Brachionus plicatilis | Rotifer | Rotifera | 0.094 | NOEC | 17 | 1 | (Zhang et al., 2016) |
| 5 | PBDEs | Danio rerio | Zebra Danio | Fish | 0.104 | NOEC | 91 | 2 | (Chen et al., 2017) |
| 6 | PBDEs | Pimephales promelas | Fathead Minnow | Fish | 0.179 | NOEC | 28 | 1 | (Lu et al., 2018) |
| 7 | PBDEs | Oryzias latipes | Japanese Medaka | Fish | 1.158 | NOEC | 28 | 1 | (Lu et al., 2018) |

Table S The goodness of fit of SSD models

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Distribution | A-D test | K-S test | AIC |  | Distribution | A-D test | K-S test | AIC |
| BPA |  |  |  |  | **PFOS** |  |  |  |  |
| Acute | | | | | **Acute** | | | | |
| 1 | lnorm | 0.869 | 0.765 | 172.890 | **1** | lnorm | 0.559 | 0.336 | 448.498 |
| 2 | llogis | 0.973 | 0.990 | 172.266 | **2** | llogis | 0.648 | 0.666 | 449.470 |
| 3 | gamma | 0.346 | 0.267 | 179.246 | **3** | gamma | 0.929 | 0.854 | 445.195 |
| 4 | weibull | 0.343 | 0.344 | 180.092 | **4** | weibull | 0.949 | 0.901 | 445.164 |
| Chronic-lethal | | | | | **Chronic-lethal** | | | | |
| 5 | lnorm | 0.939 | 0.985 | 109.206 | **5** | lnorm | 0.982 | 0.955 | 147.007 |
| 6 | llogis | 0.954 | 0.977 | 109.776 | **6** | llogis | 0.979 | 0.963 | 148.395 |
| 7 | gamma | 0.363 | 0.388 | 113.983 | **7** | gamma | 0.575 | 0.667 | 151.049 |
| 8 | weibull | 0.725 | 0.830 | 111.396 | **8** | weibull | 0.889 | 0.930 | 148.974 |
| Chronic-reproductive | | | | | **Chronic-reproductive** | | | | |
| 9 | lnorm | 0.354 | 0.453 | 54.730 | **9** | lnorm | 0.918 | 0.882 | 36.649 |
| 10 | llogis | 0.447 | 0.719 | 54.797 | **10** | llogis | 0.927 | 0.932 | 37.501 |
| 11 | gamma | 0.708 | 0.640 | 48.724 | **11** | gamma | 0.799 | 0.654 | 38.591 |
| 12 | weibull | 0.594 | 0.623 | 49.791 | **12** | weibull | 0.891 | 0.799 | 38.004 |
| TPHP |  |  |  |  | **PBDEs** |  |  |  |  |
| Acute | | | | | **Acute** | | | | |
| 1 | lnorm | 0.845 | 0.878 | 56.571 | **1** | lnorm | 0.917 | 0.887 | 46.295 |
| 2 | llogis | 0.856 | 0.890 | 57.988 | **2** | llogis | 0.940 | 0.942 | 46.416 |
| 3 | gamma | 0.728 | 0.866 | 57.331 | **3** | gamma | 0.687 | 0.548 | 47.888 |
| 4 | weibull | 0.697 | 0.814 | 57.992 | **4** | weibull | 0.754 | 0.657 | 47.775 |
| Chronic-lethal | | | | | **Chronic-lethal** | | | | |
| 5 | lnorm | 1.000 | 0.998 | 12.453 | **5** | lnorm | NA | NA | 9.848 |
| 6 | llogis | 1.000 | 0.998 | 12.801 | **6** | llogis | NA | NA | 10.129 |
| 7 | gamma | 0.698 | 0.685 | 15.506 | **7** | gamma | NA | NA | 12.735 |
| 8 | weibull | 0.970 | 0.966 | 13.764 | **8** | weibull | NA | NA | 11.238 |
| Chronic-reproductive | | | | | Chronic-reproductive | | | | |
| 9 | lnorm | NA | NA | (1.120) | **9** | lnorm | NA | NA | (2.737) |
| 10 | llogis | NA | NA | (0.848) | **10** | llogis | NA | NA | (3.166) |
| 11 | gamma | NA | NA | (2.150) | **11** | gamma | NA | NA | (2.313) |
| 12 | weibull | NA | NA | (1.922) | **12** | weibull | NA | NA | (2.684) |
| BPAF |  |  |  |  | **BPF** |  |  |  |  |
| 1 | lnorm | 0.908 | 0.832 | 107.529 | **1** | lnorm | 0.980 | 0.985 | 167.241 |
| 2 | llogis | 0.965 | 0.867 | 107.058 | **2** | llogis | 0.994 | 0.996 | 167.355 |
| 3 | gamma | 0.926 | 0.721 | 107.241 | **3** | gamma | 0.759 | 0.674 | 169.065 |
| 4 | weibull | 0.896 | 0.669 | 107.587 | **4** | weibull | 0.746 | 0.711 | 169.510 |
| BPS |  |  |  |  | **PFBS** |  |  |  |  |
| 1 | lnorm | 0.168 | 0.096 | 229.960 | **1** | lnorm | 0.346 | 0.304 | 284.677 |
| 2 | llogis | 0.193 | 0.245 | 231.182 | **2** | llogis | 0.441 | 0.402 | 282.838 |
| 3 | gamma | 0.114 | 0.033 | 234.084 | **3** | gamma | 0.319 | 0.176 | 285.573 |
| 4 | weibull | 0.145 | 0.055 | 233.796 | **4** | weibull | 0.233 | 0.112 | 287.744 |
| PFHxS |  |  |  |  | **F-53B** |  |  |  |  |
| 1 | lnorm | 0.918 | 0.847 | 272.211 | **1** | lnorm | 0.590 | 0.351 | 126.968 |
| 2 | llogis | 0.971 | 0.927 | 271.590 | **2** | llogis | 0.813 | 0.816 | 125.679 |
| 3 | gamma | 0.797 | 0.834 | 273.203 | **3** | gamma | 0.978 | 0.786 | 122.729 |
| 4 | weibull | 0.584 | 0.787 | 275.550 | **4** | weibull | 0.983 | 0.848 | 122.663 |
| 6:2 FTS |  |  |  |  | **TCEP** |  |  |  |  |
| 1 | lnorm | 0.309 | 0.314 | 185.306 | **1** | lnorm | 0.981 | 0.992 | 141.838 |
| 2 | llogis | 0.397 | 0.599 | 184.307 | **2** | llogis | 0.990 | 0.950 | 142.085 |
| 3 | gamma | 0.425 | 0.392 | 181.481 | **3** | gamma | 0.804 | 0.899 | 143.906 |
| 4 | weibull | 0.494 | 0.475 | 178.864 | **4** | weibull | 0.813 | 0.910 | 144.250 |
| TCPP |  |  |  |  | **TMP** |  |  |  |  |
| 1 | lnorm | 0.972 | 0.979 | 91.975 | **1** | lnorm | 0.895 | 0.767 | 374.702 |
| 2 | llogis | 0.979 | 0.949 | 92.334 | **2** | llogis | 0.901 | 0.818 | 374.952 |
| 3 | gamma | 0.976 | 0.936 | 91.727 | **3** | gamma | 0.633 | 0.530 | 377.659 |
| 4 | weibull | 0.959 | 0.770 | 91.689 | **4** | weibull | 0.610 | 0.664 | 378.607 |
| TEP |  |  |  |  | **TOCP** |  |  |  |  |
| 1 | lnorm | 0.781 | 0.695 | 315.647 | **1** | lnorm | 0.994 | 0.931 | 140.639 |
| 2 | llogis | 0.827 | 0.794 | 315.723 | **2** | llogis | 0.991 | 0.965 | 141.564 |
| 3 | gamma | 0.487 | 0.363 | 318.926 | **3** | gamma | 0.926 | 0.726 | 141.904 |
| 4 | weibull | 0.474 | 0.415 | 320.050 | **4** | weibull | 0.864 | 0.706 | 143.182 |

Table S SSD model parameters, HC5 values, and the results of K-S tests using measured data and extrapolated data by ICE

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Method | μ (meanlog) | σ (sdlog) | HC5 value (μmol/L) | Two-sample K-S test |
| BPA | SSD using measured data | 3.48 | 0.81 | 8.60 | D = 0.0707, p = 0.967 |
|  | SSD using extrapolated data by ICE | 3.45 | 0.64 | 10.9 |  |
| PFOS | SSD using measured data | 4.82 | 0.92 | 27.2 | D = 0.253, p = 0.00350 |
|  | SSD using extrapolated data by ICE | 4.23 | 0.95 | 14.4 |  |
| TPHP | SSD using measured data | 0.75 | 0.65 | 0.729 | D = 0.111, p = 0.577 |
|  | SSD using extrapolated data by ICE | 0.93 | 0.66 | 0.854 |  |
| PBDEs | SSD using measured data | 0.82 | 1.11 | 0.371 | D = 0.172, p = 0.108 |
|  | SSD using extrapolated data by ICE | 0.38 | 1.08 | 0.246 |  |

Table S SSD model parameters and HC5 values using chronic data

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Compound | Data | μ (meanlog) | σ (sdlog) | HC5 value (μmol/L) |
| BPA | lethal | 1.56 | 2.17 | 0.135 |
|  | reproductive | -0.427 | 2.01 | 0.0238 |
| PFOS | lethal | 1.62 | 2.06 | 0.171 |
|  | reproductive | -0.0369 | 1.54 | 0.0765 |
| TPHP | lethal | -1.74 | 2.21 | 0.00465 |
|  | reproductive | -2.85 | 2.72 | 0.000662 |
| PBDEs | lethal | -1.83 | 2.29 | 0.00372 |
|  | reproductive | -2.30 | 1.49 | 0.00856 |

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