Supporting information Data 3

of thesis entitled

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

Submitted by

**ZHANG Jiawei**

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|  |  |
| --- | --- |
|  | NP Acute SSD All species |
| a |  |
|  | NP Acute SSD Native species |
| b |  |
|  | TBBPA Acute SSD Native species |
| c |  |

|  |  |
| --- | --- |
|  | NP Reproductive SSD Measured data of All species |
| d |  |
|  | NP Reproductive SSD Measured data of Native species |
| e |  |
|  | NP Reproductive SSD Measured and ACR data of Native species |
| f |  |
|  | NP Reproductive SSD Measured and ICE data of Native species |
| g |  |
|  | TBBPA Reproductive SSD Measured data of All species |
| h |  |
|  | TBBPA Reproductive SSD Measured data of Native species |
| i |  |
|  | TBBPA Reproductive SSD Measured and ACR data of Native species |
| j |  |
|  | TBBPA Reproductive SSD Measured and ICE data of Native species |
| k |  |

Figure S The visual goodness of fit of SSD models based on the log-normal, log-logistic, log-Gumbel, and Weibull distributions

Table S Selected acute toxicity data of NP

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Species** | **LC50/EC50 (μg/L)** | **Phylum** | **Family** | **Species taxa** | **Group** | **Reference** |
|  | *Acipenser brevirostrum* | 80 | Chordata | Acipenseridae |  | Fish | (Dwyer et al., 2005) |
|  | *Acipenser oxyrhynchus* | 50 | Chordata | Acipenseridae |  | Fish | (Dwyer et al., 2005) |
|  | *Alosa sapidissima* | 50 | Chordata | Clupeidae |  | Fish | (Dwyer et al., 2005) |
|  | *Anaxyrus boreas* | 120 | Chordata | Bufonidae |  | Amphibians | (Dwyer et al., 2005) |
|  | *Ankistrodesmus convolutus* | 1520 | Chlorophyta | Selenastraceae | Native species | Algae | (Sun, 2012) |
|  | *Brachionus calyciflorus* | 580 | Rotifera | Brachionidae | Native species | Invertebrates | (Radix et al., 2002) |
|  | *Bufo boreas* | 120 | Chordata | Bufonidae |  | Amphibians | (USEPA, 2005) |
|  | *Carassius auratus red variety* | 251.3 | Chordata | Cyprinidae | Native species | Fish | (Lv et al., 2012) |
|  | *Caridina sp.* | 366 | Arthropoda | Atyidae | Native species | Crustaceans | (Hong and Li, 2007) |
|  | *Ceriodaphnia cornuta* | 20 | Arthropoda | Daphniidae | Native species | Crustaceans | (Hong and Li, 2007) |
|  | *Ceriodaphnia dubia* | 92.4 | Arthropoda | Daphniidae | Native (Model) species | Crustaceans | (TenEyck and Markee, 2007) |
|  | *Chironomus riparius* | 688 | Arthropoda | Chironomidae | Native species | Insects | (Ha and Choi, 2008b) |
|  | *Chironomus tentans* | 1271 | Arthropoda | Chironomidae | Native species | Insects | (Ha and Choi, 2008a) |
|  | *Clarias gariepinus* | 3480 | Chordata | Clariidae | Native species | Fish | (Kumaran et al., 2011) |
|  | *Corbicula fluminea* | 1090 | Mollusca | Cyrenidae | Native species | Molluscs | (Zeng et al., 2014) |
|  | *Ctenopharyngodon idellus* | 155.8 | Chordata | Cyprinidae | Native species | Fish | (Lv et al., 2012) |
|  | *Cyprinodon bovinus* | 480 | Chordata | Cyprinodontidae |  | Fish | (Dwyer et al., 2005) |
|  | *Cyprinodon variegatus* | 460 | Chordata | Cyprinodontidae |  | Fish | (Dwyer et al., 2005) |
|  | *Cyprinus carpio* | 540 | Chordata | Cyprinidae | Native species | Fish | (Jung et al., 2020) |
|  | *Danio rerio Embroy* | 1500 | Chordata | Cyprinidae | Native (Model) species | Fish | (Stengel et al., 2017) |
|  | *Daphnia carinata* | 159 | Arthropoda | Daphniidae | Native species | Crustaceans | (Guo and Xie, 2009) |
|  | *Daphnia galeata* | 60.8 | Arthropoda | Daphniidae | Native species | Crustaceans | (Tanaka and Nakanishi, 2002) |
|  | *Daphnia magna* | 180 | Arthropoda | Daphniidae | Native (Model) species | Crustaceans | (Hirano et al., 2004) |
|  | *Daphnia pulex* | 140 | Arthropoda | Daphniidae | Native species | Crustaceans | (Ernst et al., 1980) |
|  | *Desmodesmus subspicatus* | 870 | Chlorophyta | Scenedesmaceae | Native species | Algae | (Hense et al., 2003) |
|  | *Dugesia japonica* | 508 | Platyhelminthes | Planariidae | Native species | Worms | (Hong and Li, 2007) |
|  | *Erimonax monachus* | 80 | Chordata | Cyprinidae |  | Fish | (Dwyer et al., 2005) |
|  | *Etheostoma fonticola* | 110 | Chordata | Percidae |  | Fish | (Dwyer et al., 2005) |
|  | *Etheostoma lepidum* | 190 | Chordata | Percidae |  | Fish | (USEPA, 2005) |
|  | *Etheostoma rubrum* | 110 | Chordata | Percidae |  | Fish | (USEPA, 2005) |
|  | *Eurytemora affinis* | 38 | Arthropoda | Temoridae |  | Crustaceans | (Forget-Leray et al., 2005) |
|  | *Fusconaia masoni* | 70 | Mollusca | Unionidae |  | Molluscs | (Black, 2003) |
|  | *Gila elegans* | 289.3 | Chordata | Cyprinidae |  | Fish | (USEPA, 2005) |
|  | *Hyalella azteca* | 38 | Arthropoda | Hyalellidae |  | Crustaceans | (Spehar et al., 2010) |
|  | *Hydra vulgaris* | 74 | Cnidaria | Hydridae | Native species | Invertebrates | (Pachura et al., 2005) |
|  | *Hypophthalmichthys molitrix* | 187 | Chordata | Cyprinidae | Native species | Fish | (Lv et al., 2012) |
|  | *Kirchneriella obesa* | 1310 | Chlorophyta | Selenastraceae | Native species | Algae | (Sun, 2012) |
|  | *Lampsilis cardium* | 1190 | Mollusca | Unionidae |  | Molluscs | (Milam et al., 2005) |
|  | *Lampsilis siliquoidea* | 490 | Mollusca | Unionidae |  | Molluscs | (Milam et al., 2005) |
|  | *Lasmigona subviridis* | 420 | Mollusca | Unionidae |  | Molluscs | (Black, 2003) |
|  | *Lepomis macrochirus* | 135 | Chordata | Centrarchidae | Native species | Fish | (Brooke, 1993a) |
|  | *Leptodea fragilis* | 570 | Mollusca | Unionidae | Native (Introduced) species | Molluscs | (Milam et al., 2005) |
|  | *Ligumia subrostrata* | 1040 | Mollusca | Unionidae |  | Molluscs | (Milam et al., 2005) |
|  | *Lithobates sphenocephalus* | 332 | Chordata | Ranidae | Native (Introduced) species | Amphibians | (Mayer et al., 2008) |
|  | *Lumbriculus variegatus* | 342 | Annelida | Lumbriculidae | Native species | Worms | (Brooke, 1993b) |
|  | *Megalonaias nervosa* | 560 | Mollusca | Unionidae | Native (Introduced) species | Molluscs | (Milam et al., 2005) |
|  | *Misgurnus anguillicaudatus* | 9740 | Chordata | Cobitidae | Native species | Fish | (Lei et al., 2014) |
|  | *Moina macrocopa* | 65 | Arthropoda | Moinidae | Native species | Crustaceans | (Hu et al., 2011) |
|  | *Moina micrura* | 126 | Arthropoda | Moinidae | Native species | Crustaceans | (Guo and Xie, 2009) |
|  | *Neocaridina denticulata* | 371 | Arthropoda | Atyidae | Native species | Crustaceans | (Hong and Li, 2007) |
|  | *Notropis mekistocholas* | 140 | Chordata | Cyprinidae |  | Fish | (Dwyer et al., 2005) |
|  | *Oncorhynchus apache* | 169.7 | Chordata | Salmonidae |  | Fish | (USEPA, 2005) |
|  | *Oncorhynchus clarki henshawi* | 166.6 | Chordata | Salmonidae |  | Fish | (USEPA, 2005) |
|  | *Oncorhynchus mykiss* | 221 | Chordata | Salmonidae | Native species | Fish | (Brooke, 1993b) |
|  | *Oreochromis aureus* | 264.6 | Chordata | Cichlidae | Native species | Fish | (Huang et al., 2006) |
|  | *Oryzias latipes* | 130 | Chordata | Adrianichthyidae | Native (Model) species | Fish | (Kashiwada et al., 2002) |
|  | *Paphia undulata* | 260 | Mollusca | Veneridae | Native species | Molluscs | (Gong, 2012) |
|  | *Physa virgata* | 774 | Mollusca | Physidae |  | Molluscs | (Brooke, 1993b) |
|  | *Physella acuta* | 319 | Mollusca | Physidae | Native species | Molluscs | (Hong and Li, 2007) |
|  | *Physella virgata* | 774 | Mollusca | Physidae |  | Molluscs | (Spehar et al., 2010) |
|  | *Pimephales promelas* | 128 | Chordata | Cyprinidae | Native (Model) species | Fish | (Brooke, 1993b) |
|  | *Poeciliopsis occidentalis* | 230 | Chordata | Poeciliidae |  | Fish | (USEPA, 2005) |
|  | *Pseudokirchneriella subcapitata* | 410 | Chlorophyta | Scenedesmaceae | Native (Model) species | Algae | (CMA, 1990) |
|  | *Ptychocheilus lucius* | 254.6 | Chordata | Cyprinidae |  | Fish | (USEPA, 2005) |
|  | *Puntius conchonius* | 379 | Chordata | Cyprinidae |  | Fish | (Xiao et al., 2007) |
|  | *Rana chensinensis* | 140 | Chordata | Ranidae | Native species | Amphibians | (Zheng and Zhang, 2008) |
|  | *Ruditapes philippinarum* | 469 | Mollusca | Veneridae | Native species | Molluscs | (Gong, 2012) |
|  | *Salmo salar* | 130 | Chordata | Salmonidae |  | Fish | (McLeese et al., 1981) |
|  | *Scaphirhynchus platorynchus* | 200 | Chordata | Acipenseridae |  | Fish | (Dwyer and Hardesty, 1999) |
|  | *Scenedesmus obliquus* | 6050 | Chlorophyta | Scenedesmaceae | Native species | Algae | (Zhao et al., 2006) |
|  | *Scenedesmus quadricauda* | 1300 | Chlorophyta | Scenedesmaceae | Native species | Algae | (Heidorn et al., 1996) |
|  | *Scenedesmus subspicatus* | 56 | Chlorophyta | Scenedesmaceae | Native species | Algae | (Kopf, 1997) |
|  | *Selenastrum capricornutum* | 979 | Chlorophyta | Selenastraceae | Native species | Algae | (Liu et al., 2018) |
|  | *Tetrahymena pyriformis* | 460 | Ciliophora | Tetrahymenidae |  | Invertebrates | (Yoshioka et al., 1985) |
|  | *Utterbackia imbecillis* | 390 | Mollusca | Unionidae | Native (Introduced) species | Molluscs | (Black, 2003) |
|  | *Xiphophorus helleri* | 205.98 | Chordata | Poeciliidae | Native species | Fish | (Kwak et al., 2001) |
|  | *Xyrauchen texanus* | 174.4 | Chordata | Catostomidae |  | Fish | (USEPA, 2005) |

Table S Selected acute toxicity data of TBBPA

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Species** | **LC50/EC50 (μg/L)** | **Phylum** | **Family** | **Species taxa** | **Group** | **Reference** |
|  | *Brachionus calyciflorus Pallas* | 2180 | Rotifera | Brachionidae | Native species | Invertebrates | (Zhang, 2014) |
|  | *Carassius auratus* | 3134 | Chordata | Cyprinidae | Native species | Fish | (Yang et al., 2012b) |
|  | *Chironomus plumosus* | 24576 | Arthropoda | Chironomidae | Native species | Insects | (Yang et al., 2012b) |
|  | *Danio rerio* | 5270 | Chordata | Cyprinidae | Native (Model) species | Fish | (Chow et al., 2013) |
|  | *Danio rerio Embryo* | 1090 | Chordata | Cyprinidae | Native (Model) species | Fish | (Chan and Chan, 2012) |
|  | *Daphnia magna* | 1336 | Arthropoda | Daphniidae | Native (Model) species | Crustaceans | (Yang et al., 2012b) |
|  | *Gammarus pulex* | 1174 | Arthropoda | Gammaridae | Native species | Crustaceans | (Mariager, 2001) |
|  | *Gobiocypris rarus* | 210 | Chordata | Cyprinidae | Native species | Fish | (Zhang, 2014) |
|  | *Lepomis macrochirus* | 510 | Chordata | Centrarchidae | Native species | Fish | (WHO/IPCS, 1995) |
|  | *Limnodrilus hoffmeisteri* | 7852 | Annelida | Naididae | Native species | Worms | (Yang et al., 2012b) |
|  | *Macrobrachium nipponense* | 1216 | Arthropoda | Palaemonidae | Native species | Crustaceans | (Yang et al., 2012b) |
|  | *Nitzschia palea* | 11095 | Bacillariophyta | Bacillariaceae | Native species | Algae | (Debenest et al., 2010) |
|  | *Oncorhynchus mykiss* | 1100 | Chordata | Salmonidae | Native species | Fish | (Wildlife International, LTD., 2003) |
|  | *Pimephales promelas* | 1040 | Chordata | Cyprinidae | Native (Model) species | Fish | (Brooke, 1991) |
|  | *Pseudokirchneriella subcapitata* | 7723 | Chlorophyta | Scenedesmaceae | Native species | Algae | (Debenest et al., 2010) |
|  | *Pseudorasbora parva* | 860 | Chordata | Cyprinidae | Native species | Fish | (Goodman et al., 1988) |
|  | *Rana limnocharis* | 1254 | Chordata | Ranidae | Native species | Amphibians | (Yang et al., 2012b) |
|  | *Scenedesmus quadricauda* | 1202 | Chlorophyta | Scenedesmaceae | Native species | Algae | (Yang et al., 2012b) |
|  | *Tubifex sinicus* | 2310 | Annelida | Naididae | Native species | Worms | (Zhang, 2014) |

Table S Selected reproductive toxicity data of NP

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Species** | **Value (μg/L)** | **Endpoint** | **Observed Duration (Days)** | **Phylum** | **Family** | **Species taxa** | **Group** | **Reference** |
|  | Alburnus tarichi | 200 | NOEC | 32 | Chordata | Cyprinidae |  | Fish | (Kaptaner and Ünal, 2011) |
|  | Americamysis bahia | 3 | NOEC | 14 | Arthropoda | Mysidae |  | Crustaceans | (Hirano et al., 2009) |
|  | Brachionus calyciflorus | 5 | NOEC | 4 | Rotifera | Brachionidae | Native Species | Invertebrates | (Preston et al., 2000) |
|  | Ceriodaphnia dubia | 125 | NOEC | 6 | Arthropoda | Daphniidae | Native (Model) species | Crustaceans | (Tatarazako et al., 2002) |
|  | Danio rerio | 30 | NOEC | 58 | Chordata | Cyprinidae | Native (Model) species | Fish | (Weber et al., 2003) |
|  | Danio rerio Embroy | 100 | NOEC | 6.83 | Chordata | Cyprinidae | Native (Model) species | Fish | (Wu et al., 2011) |
|  | Daphnia galeata | 17.3 | NOEC | 21 | Arthropoda | Daphniidae | Native Species | Crustaceans | (Tanaka and Nakanishi, 2002, 2001) |
|  | Daphnia magna | 77.3 | NOEC | 21 | Arthropoda | Daphniidae | Native (Model) species | Crustaceans | (Brooke, 1993b) |
|  | Eurytemora affinis | 7 | NOEC | 21 | Arthropoda | Temoridae |  | Crustaceans | (Forget-Leray et al., 2005) |
|  | Gammarus fossarum | 5 | NOEC | 21 | Arthropoda | Gammaridae |  | Crustaceans | (Geffard et al., 2010) |
|  | Gobiocypris rarus | 18.5 | NOEC | 21 | Chordata | Cyprinidae | Native Species | Fish | (Zha et al., 2008) |
|  | Lithobates pipiens | 10 | LOEC | 124 | Chordata | Ranidae |  | Amphibians | (Mackenzie et al., 2003) |
|  | Lithobates sylvaticus | 100 | NOEC | 47 | Chordata | Ranidae |  | Amphibians | (Mackenzie et al., 2003) |
|  | Lymnaea stagnalis | 100 | NOEC | 84 | Mollusca | Lymnaeidae | Native Species | Molluscs | (Czech et al., 2001) |
|  | Melanotaenia fluviatilis | 5000 | NOEC | 10 | Chordata | Melanotaeniidae |  | Fish | (Holdway et al., 2008) |
|  | Neomysis integer | 1 | NOEC | 4 | Arthropoda | Mysidae |  | Crustaceans | (Verslycke et al., 2004) |
|  | Oryzias latipes | 50.9 | NOEC | 21 | Chordata | Adrianichthyidae | Native (Model) species | Fish | (Kang et al., 2003) |
|  | Pelophylax nigromaculatus | 200 | NOEC | 45 | Chordata | Ranidae | Native Species | Amphibians | (Yang et al., 2005) |
|  | Pimephales promelas | 0.15 | NOEC | 28 | Chordata | Cyprinidae | Native (Model) species | Fish | (Schoenfuss et al., 2008) |
|  | Triturus carnifex | 19 | LOEC | 30.44 | Chordata | Salamandridae |  | Amphibians | (Capaldo et al., 2012) |
|  | Xenopus laevis | 22 | LOEC | 84 | Chordata | Pipidae | Native Species | Amphibians | (Kloas et al., 1999) |

Table S Selected reproductive toxicity data of TBBPA

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Species** | **Value (μg/L)** | **Endpoint** | **Observed Duration (Days)** | **Phylum** | **Family** | **Species taxa** | **Group** | **Reference** |
|  | *Brachionus calyciflorus* | 1000 | NOEC | 2 | Rotifera | Brachionidae | Native species | Invertebrates | (Zhang, 2014) |
|  | *Danio rerio* | 204 | NOEC | 79 | Chordata | Cyprinidae | Native (Model) species | Fish | (Kuiper et al., 2007b) |
|  | *Danio rerio Embryo* | 400 | LOEC | 5 | Chordata | Cyprinidae | Native (Model) species | Fish | (McCormick et al., 2010) |
|  | *Daphnia magna* | 16 | EC10 | 21 | Arthropoda | Daphniidae | Native (Model) species | Crustaceans | (Yang et al., 2012b) |
|  | *Pelophylax nigromaculatus* | 1.1 | NOEC | 14 | Chordata | Ranidae | Native species | Amphibians | (Zhang et al., 2018) |
|  | *Platichthys flesus* | 193 | NOEC | 105 | Chordata | Pleuronectidae |  | Fish | (Kuiper et al., 2007a) |
|  | *Salmo salar* | 0.05 | NOEC | 5 | Chordata | Salmonidae |  | Fish | (Lower, 2008) |

Table S The goodness of fit of SSD models

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| SSD models | Data set | Distributions | Anderson-Darling test | Kolmogorov-Smirnov test | Akaike Information Criterion (AIC) | Akaike Information Criterion corrected for small sample size (AICc) |
| NP Acute | All species | lnorm | 0.323354 | 0.056799 | 1110.972 | 1111.134 |
|  |  | llogis | 0.275396 | 0.053897 | 1110.761 | 1110.923 |
|  |  | lgumbel | 0.46473 | 0.073838 | 1112.245 | 1112.407 |
|  |  | weibull | 2.288641 | 0.121432 | 1135.432 | 1135.594 |
|  | Native species | lnorm | 0.299072 | 0.080347 | 692.4547 | 692.7338 |
|  |  | llogis | 0.220213 | 0.063218 | 692.0917 | 692.3708 |
|  |  | lgumbel | 0.408783 | 0.099288 | 694.7085 | 694.9876 |
|  |  | weibull | 1.473511 | 0.144551 | 705.7178 | 705.9969 |
| TBBPA Acute | Native species | lnorm | 0.677878 | 0.216358 | 350.9652 | 351.7152 |
|  |  | llogis | 0.658113 | 0.19906 | 351.2092 | 351.9592 |
|  |  | lgumbel | 0.573984 | 0.171029 | 351.2632 | 352.0132 |
|  |  | weibull | 1.0057 | 0.226319 | 355.6526 | 356.4026 |
| NP Reproductive | Measured data of All species | lnorm | 0.320078 | 0.119237 | 231.3024 | 231.9691 |
|  |  | llogis | 0.241205 | 0.101543 | 230.4743 | 231.1409 |
|  |  | lgumbel | 0.75411 | 0.168325 | 235.8662 | 236.5328 |
|  |  | weibull | 0.716399 | 0.161416 | 235.5564 | 236.2231 |
|  | Measured data of Native species | lnorm | 0.774806 | 0.238065 | 132.1192 | 133.4525 |
|  |  | llogis | 0.478756 | 0.14233 | 130.2504 | 131.5837 |
|  |  | lgumbel | 1.356797 | 0.293125 | 138.8346 | 140.168 |
|  |  | weibull | 0.309278 | 0.137307 | 126.6309 | 127.9643 |
|  | Measured and ACR data of Native species | lnorm | 0.946774 | 0.149356 | 400.1728 | 400.5062 |
|  |  | llogis | 0.321581 | 0.089007 | 393.3848 | 393.7181 |
|  |  | lgumbel | 3.243587 | 0.227275 | 421.6915 | 422.0248 |
|  |  | weibull | 1.4182 | 0.155208 | 402.7449 | 403.0782 |
|  | Measured and ICE data of Native species | lnorm | 0.866547 | 0.236003 | 144.5119 | 144.4418 |
|  |  | llogis | 0.501226 | 0.132472 | 142.1038 | 142.0337 |
|  |  | lgumbel | 1.543301 | 0.29476 | 152.207 | 152.1369 |
|  |  | weibull | 0.296513 | 0.128952 | 138.1154 | 138.0453 |
| TBBPA Reproductive | Measured data of All species | lnorm | NA | NA | 87.47737 | 90.47737 |
|  |  | llogis | NA | NA | 87.82778 | 90.82778 |
|  |  | lgumbel | NA | NA | 89.52105 | 92.52105 |
|  |  | weibull | NA | NA | 85.72264 | 88.72264 |
|  | Measured data of Native species | lnorm | NA | NA | 69.43008 | 75.43008 |
|  |  | llogis | NA | NA | 69.8152 | 75.8152 |
|  |  | lgumbel | NA | NA | 70.59009 | 76.59009 |
|  |  | weibull | NA | NA | 68.49637 | 74.49637 |
|  | Measured and ACR data of Native species | lnorm | 0.36482 | 0.164323 | 266.6518 | 267.4018 |
|  |  | llogis | 0.373177 | 0.166926 | 267.479 | 268.229 |
|  |  | lgumbel | 0.491311 | 0.157815 | 268.7081 | 269.4581 |
|  |  | weibull | 0.546144 | 0.191786 | 268.8529 | 269.6029 |
|  | Measured and ICE data of Native species | lnorm | 0.337597 | 0.204756 | 101.3225 | 103.7225 |
|  |  | llogis | 0.340222 | 0.220724 | 101.9483 | 104.3483 |
|  |  | lgumbel | 0.397868 | 0.207404 | 102.6649 | 105.0649 |
|  |  | weibull | 0.313372 | 0.241687 | 101.0932 | 103.4932 |

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