Supplementary Material

**From Waters to Fish: A Multi-Faceted Analysis of Contaminants Pollution Sources, Distribution Patterns, Ecological and Human Health Consequences**

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Table S1. Retention time, monitored ion, linearity, and limits of detection (LOD) of OCPs for biota (mollusks and fish)

|  |  |  |  |
| --- | --- | --- | --- |
| OCPs | Retention Time | Linearity (R2) | LOD (µg/g) dwt\* |
| Hexachlorobenzene (HCB) | 3.176 | 0.9925 | 0.0005 |
| Lindane (γ-HCH) | 5.118 | 0.9909 | 0.0004 |
| Heptachlor | 7.060 | 0.9909 | 0.0003 |
| Aldrin | 7.886 | 0.9587 | 0.0003 |
| Dieldrin | 11.220 | 0.9860 | 0.0003 |
| Endrin | 12.200 | 0.9945 | 0.0004 |
| p,p’ dichlorodiphenyldichloroethylene (p,p'DDE) | 10.800 | 0.9751 | 0.0002 |
| p,p’ dichlorodiphenyldichloroethane (p,p’DDD) | 12.790 | 0.9917 | 0.0002 |
| p,p’dichloro-diphenyl-trichloroethane (p,p’DDT) | 15.100 | 0.9909 | 0.0002 |

*\*Dwt: dry weight tissue*

Table S 2. Retention time, monitored ion, linearity, and limits of detection (LOD) of PCBs for biota (mollusks and fish)

|  |  |  |  |
| --- | --- | --- | --- |
| PCBs | Retention Time | Linearity (R2) | LOD (µg/g) dwt |
| Polychlorobiphenyls 28 (PCB 28) | 18.827 | 0.9996 | 0.0004 |
| Polychlorobiphenyls 52 (PCB 52) | 20.801 | 0.9979 | 0.0003 |
| Polychlorobiphenyls 101 (PCB 101) | 25.880 | 0.9988 | 0.0006 |
| Polychlorobiphenyls 118(PCB 118) | 29.591 | 0.9992 | 0.0004 |
| Polychlorobiphenyls 138(PCB 138) | 30.819 | 0.9994 | 0.0006 |
| Polychlorobiphenyls 152(PCB 152) | 32.362 | 0.9952 | 0.0007 |
| Polychlorobiphenyls 180(PCB 180) | 36.257 | 0.9992 | 0.0003 |

Table S3. Retention time, monitored ion, linearity, and limits of detection (LOD) of PAHs for biota (mollusks and fish)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| PAHs | Retention Time | m/z | Linearity (R2) | LOD (µg/g) dwt |
| Naphthalene (Na) | 7.25 | 128 | 0.9885 | 0.0001 |
| Acenaphthylene (Ac) | 13.70 | 152 | 0.9937 | 0.0001 |
| Acenaphthene (Ace) | 14.50 | 154 | 0.9933 | 0.0001 |
| Fluorene (Flu) | 16.57 | 166 | 0.9945 | 0.0001 |
| Phenanthrene (Ph) | 20.36 | 178 | 0.9922 | 0.0001 |
| Anthracene (An) | 20.56 | 178 | 0.9968 | 0.0001 |
| Fluoranthene (Fln) | 25.04 | 202 | 0.9923 | 0.0001 |
| Pyrene (Pyr) | 25.87 | 202 | 0.9980 | 0.0001 |
| Benzo[a]anthracene (BaA) | 30.74 | 228 | 0.9972 | 0.0001 |
| Chrysene (Chr) | 30.90 | 228 | 0.9946 | 0.0001 |
| Benzo[b]fluoranthene (BbF) | 33.80 | 252 | 0.9840 | 0.0001 |
| Benzo[k]fluoranthene (BkF) | 34.00 | 252 | 0.9734 | 0.0001 |
| Benzo[a]pyrene (BaP) | 34.68 | 252 | 0.9858 | 0.0001 |
| Benzo[g,h,i]perylene (Bghi) | 37.20 | 276 | 0.9765 | 0.0001 |
| Dibenzo[a,h]anthracene (DahA) | 37.40 | 278 | 0.9823 | 0.0001 |
| Indeno[1,2,3 –cd] pyrene (IP) | 37.74 | 276 | 0.9756 | 0.0001 |

Table S 4. Variability of heavy metal concentrations in seawater from the Romanian Black Sea investigated during 2016 – 2023

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Descriptive Statistics (Seawater, 2016 - 2023) | | | | | | | | | | |
|  | **N** | **Mean** | **Median** | **Min** | **Max** | **25th percentile** | **75th percentile** | **Coef.**  **Var.** | **Skewness** | **Kurtosis** |
| **Cu (µg/L)** | 77 | 8.041 | 5.720 | 0.790 | 33.480 | 3.119 | 10.263 | 89.19 | 1.811 | 3.495 |
| **Cd (µg/L)** | 77 | 0.529 | 0.580 | 0.001 | 2.070 | 0.034 | 0.890 | 96.84 | 0.904 | 0.637 |
| **Pb (µg/L)** | 77 | 5.828 | 4.810 | 0.001 | 25.970 | 0.838 | 9.370 | 95.60 | 1.045 | 1.028 |
| **Ni (µg/L)** | 77 | 8.297 | 2.738 | 0.010 | 75.380 | 1.320 | 7.270 | 180.30 | 3.133 | 10.676 |
| **Cr (µg/L)** | 77 | 4.323 | 2.310 | 0.219 | 47.730 | 1.138 | 4.160 | 152.68 | 4.426 | 25.878 |

Table S5. Variability of heavy metal concentrations in sediments from the Romanian Black Sea investigated during 2016 – 2023

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Descriptive Statistics (Sediments, 2016 - 2023) | | | | | | | | | | |
|  | **N** | **Mean** | **Median** | **Min** | **Max** | **25th percentile** | **75th percentile** | **Coef.**  **Var.** | **Skewness** | **Kurtosis** |
| **Cu**  **(µg/g dw)** | 77 | 31.74 | 23.25 | 3.660 | 123.90 | 12.270 | 43.750 | 85.199 | 1.852 | 3.736 |
| **Cd**  **(µg/g dw)** | 77 | 0.546 | 0.336 | 0.030 | 4.345 | 0.177 | 0.518 | 143.98 | 3.593 | 13.883 |
| **Pb**  **(µg/g dw)** | 77 | 16.30 | 13.84 | 1.350 | 65.362 | 6.170 | 20.830 | 82.431 | 1.402 | 2.062 |
| **Ni**  **(µg/g dw)** | 77 | 48.59 | 39.63 | 5.630 | 160.20 | 21.320 | 60.960 | 76.066 | 1.497 | 2.297 |
| **Cr**  **(µg/g dw)** | 77 | 33.38 | 29.17 | 6.290 | 98.730 | 16.860 | 47.841 | 60.802 | 0.884 | 0.355 |

Table S6. Variability of OCPs concentrations in seawater from the Romanian Black Sea investigated during 2016 – 2023

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Descriptive Statistics (Water, 2016 - 2023) | | | | | | | | |
|  | N | Mean | Median | Min | Max | 25th percentile | 75th percentile | Coef.  Var. |
| HCB  (µg/L) | 72 | 0.029 | 0.004 | 0.004 | 0.895 | 0.004 | 0.004 | 0.124 |
| Lindane (µg/L) | 72 | 0.319 | 0.003 | 0.003 | 4.942 | 0.003 | 0.075 | 0.859 |
| Heptachlor (µg/L) | 72 | 0.069 | 0.003 | 0.003 | 1.464 | 0.003 | 0.003 | 0.256 |
| Aldrin (µg/L) | 72 | 0.615 | 0.003 | 0.003 | 7.320 | 0.003 | 0.032 | 1.561 |
| Dieldrin (µg/L) | 72 | 0.252 | 0.002 | 0.002 | 4.498 | 0.002 | 0.003 | 0.750 |
| Endrin (µg/L) | 72 | 0.142 | 0.003 | 0.003 | 3.989 | 0.003 | 0.003 | 0.577 |
| p,p' DDE (µg/L) | 72 | 0.294 | 0.002 | 0.002 | 4.274 | 0.002 | 0.005 | 0.892 |
| p,p' DDD (µg/L) | 72 | 1.048 | 0.002 | 0.002 | 19.837 | 0.002 | 0.002 | 3.250 |
| p,p' DDT (µg/L) | 72 | 0.367 | 0.002 | 0.002 | 5.855 | 0.002 | 0.006 | 1.212 |

Table S7. Variability of PCBs concentrations in seawater from the Romanian Black Sea investigated during 2016 – 2023

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Descriptive Statistics (Water, 2016 - 2023) | | | | | | | | |
|  | N | Mean | Median | Min | Max | 25th percentile | 75th percentile | Coef.  Var. |
| PCB28 (µg/L) | 72 | 0.031 | 0.004 | 0.004 | 0.343 | 0.004 | 0.012 | 0.067 |
| PCB52 (µg/L) | 72 | 0.060 | 0.006 | 0.006 | 0.925 | 0.006 | 0.006 | 0.166 |
| PCB101 (µg/L) | 72 | 0.084 | 0.006 | 0.006 | 3.799 | 0.006 | 0.006 | 0.470 |
| PCB118 (µg/L) | 72 | 0.098 | 0.004 | 0.004 | 5.789 | 0.004 | 0.004 | 0.685 |
| PCB153 (µg/L) | 72 | 0.019 | 0.009 | 0.009 | 0.591 | 0.009 | 0.009 | 0.069 |
| PCB138 (µg/L) | 72 | 0.024 | 0.007 | 0.007 | 1.007 | 0.007 | 0.007 | 0.118 |
| PCB180 (µg/L) | 72 | 0.013 | 0.003 | 0.003 | 0.160 | 0.003 | 0.004 | 0.028 |

Table S8. Variability of OCPs concentrations in sediments from the Romanian Black Sea investigated during 2016 – 2023

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Descriptive Statistics (Sediment, 2016 - 2023) | | | | | | | | |
|  | N | Mean | Median | Min | Max | 25th percentile | 75th percentile | Coef.  Var. |
| HCB (µg/g dw) | 72 | 0.3071 | 0.0044 | 0.0003 | 3.5759 | 0.0003 | 0.1268 | 0.6848 |
| Lindane (µg/g dw) | 72 | 0.3978 | 0.0003 | 0.0003 | 7.3846 | 0.0003 | 0.0239 | 1.3077 |
| Heptachlor (µg/g dw) | 72 | 0.0265 | 0.0002 | 0.0002 | 0.7473 | 0.0002 | 0.0002 | 0.1266 |
| Aldrin (µg/g dw) | 72 | 0.2419 | 0.0002 | 0.0002 | 3.5977 | 0.0002 | 0.0036 | 0.7549 |
| Dieldrin (µg/g dw) | 72 | 0.0111 | 0.0002 | 0.0002 | 0.6222 | 0.0002 | 0.0002 | 0.0737 |
| Endrin (µg/g dw) | 72 | 0.4387 | 0.0003 | 0.0003 | 12.1924 | 0.0003 | 0.0027 | 2.1008 |
| p,p' DDE (µg/g dw) | 72 | 0.0622 | 0.0003 | 0.0002 | 3.2469 | 0.0002 | 0.0030 | 0.3838 |
| p,p' DDD (µg/g dw) | 72 | 0.2691 | 0.0002 | 0.0002 | 8.7926 | 0.0002 | 0.0042 | 1.1544 |
| p,p' DDT (µg/g dw) | 72 | 0.0964 | 0.0002 | 0.0002 | 2.3954 | 0.0002 | 0.0002 | 0.4011 |

Table S9. Variability of PCBs concentrations in sediments from the Romanian Black Sea investigated during 2016 – 2023

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Descriptive Statistics (Sediment, 2016 - 2023) | | | | | | | | |
|  | N | Mean | Median | Min | Max | 25th percentile | 75th percentile | Coef.  Var. |
| PCB28 (µg/g dw) | 72 | 0.0183 | 0.0009 | 0.0004 | 0.3363 | 0.0004 | 0.0090 | 0.0575 |
| PCB52 (µg/g dw) | 72 | 0.0301 | 0.0003 | 0.0003 | 0.4780 | 0.0003 | 0.0204 | 0.0808 |
| PCB101 (µg/g dw) | 72 | 0.0011 | 0.0006 | 0.0006 | 0.0102 | 0.0006 | 0.0006 | 0.0018 |
| PCB118 (µg/g dw) | 72 | 0.0265 | 0.0004 | 0.0004 | 1.5632 | 0.0004 | 0.0004 | 0.1846 |
| PCB153 (µg/g dw) | 72 | 0.0023 | 0.0006 | 0.0006 | 0.0330 | 0.0006 | 0.0006 | 0.0061 |
| PCB138 (µg/g dw) | 72 | 0.0016 | 0.0007 | 0.0007 | 0.0161 | 0.0007 | 0.0008 | 0.0024 |
| PCB180 (µg/g dw) | 72 | 0.0130 | 0.0003 | 0.0003 | 0.3091 | 0.0003 | 0.0022 | 0.0526 |

A map of the ocean showing the temperature

Description automatically generated with medium confidence

Figure S1. Distribution of cadmium in biota, during 2016-2023