**Determination of PCDD/F and DL-PCB pollution levels, source appointment and risk assessment of surface sediments in dam lakes in Istanbul, Turkey**

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**Table S1.** The instrumentation parameters of HR-GC/MS for each PCDD/Fs and DL-PCBs

|  |  |  |  |
| --- | --- | --- | --- |
| **Analytes** | **RT (min)** | **Cl35 Ion** | **Cl37 Ion** |
| **PCDD/Fs** |  |  |  |
| 2378-TCDF | 28.12 | 303.902 | 305.899 |
| 12378-PeCDF | 36.41 | 339.860 | 341.857 |
| 23478-PeCDF | 38.01 | 339.860 | 341.857 |
| 123478-HxCDF | 43.73 | 373.821 | 375.818 |
| 123678-HxCDF | 43.91 | 373.821 | 375.818 |
| 234678-HxCDF | 44.9 | 373.821 | 375.818 |
| 123789-HxCDF | 46.16 | 373.821 | 375.818 |
| 1234678-HpCDF | 48.91 | 407.782 | 409.779 |
| 1234789-HpCDF | 51.06 | 407.782 | 409.779 |
| OCDF | 55.77 | 441.743 | 443.74 |
| 2378-TCDD | 29.34 | 319.897 | 321.894 |
| 12378-PeCDD | 38.79 | 355.855 | 357.852 |
| 123478-HxCDD | 45.16 | 389.816 | 391.813 |
| 123678-HxCDD | 45.32 | 389.816 | 391.813 |
| 123789-HxCDD | 45.84 | 389.816 | 391.813 |
| 1234678-HpCDD | 50.47 | 423.777 | 425.774 |
| OCDD | 55.59 | 457.738 | 459.735 |
| 2378-TCDF | 28.12 | 303.902 | 305.899 |
| 12378-PeCDF | 36.41 | 339.860 | 341.857 |
| 23478-PeCDF | 38.01 | 339.860 | 341.857 |
| 123478-HxCDF | 43.73 | 373.821 | 375.818 |
| 123678-HxCDF | 43.91 | 373.821 | 375.818 |
| 13C12--2378-TCDF\* | 28.10 | 315.942 | 317.939 |
| 13C12-12378-PeCDF\* | 36.38 | 351.900 | 353.897 |
| 13C12-23478-PeCDF\* | 37.99 | 351.900 | 353.897 |
| 13C12-123478-HxCDF\* | 43.71 | 385.861 | 387.858 |
| 13C12-123678-HxCDF\* | 43.90 | 385.861 | 387.858 |
| 13C12-234678-HxCDF\* | 44.88 | 385.861 | 387.858 |
| 13C12-123789-HxCDF\* | 46.15 | 385.861 | 387.858 |
| 13C12-1234678-HpCDF\* | 48.90 | 419.822 | 421.819 |
| 13C12-1234789-HpCDF\* | 51.04 | 419.822 | 421.819 |
| 13C12-OCDF\* | 55.75 | 453.783 | 455.780 |
| 13C12-1234-TCDD\* | 28.97 | 331.937 | 333.934 |
| 13C12-2378-TCDD\* | 29.31 | 331.937 | 333.934 |
| 13C12-12378-PeCDD\* | 38.76 | 367.895 | 369.892 |
| 13C12-123478-HxCDD\* | 45.14 | 401.856 | 403.853 |
| 13C12-123678-HxCDD\* | 45.30 | 401.856 | 403.853 |
| 13C12-1234678-HpCDD\* | 50.45 | 435.817 | 437.814 |
| 13C12-OCDD\* | 55.57 | 469.778 | 471.775 |
| 13C12-123789-HxCDD\* | 45.82 | 401.856 | 403.853 |
| 13C12-2378-TCDF\* | 28.10 | 315.942 | 317.939 |
| **DL-PCBs** |  |  |  |
| PCB 81 | 18.64 | 289.9224 | 291.9194 |
| PCB 77 | 19.31 | 289.9224 | 291.9194 |
| PCB 123 | 21.04 | 325.8804 | 327.8775 |
| PCB 118 | 21.23 | 325.8804 | 327.8775 |
| PCB 114 | 22.25 | 325.8804 | 327.8775 |
| PCB 105 | 23.63 | 325.8804 | 327.8775 |
| PCB 126 | 26.46 | 289.9224 | 327.8775 |
| PCB 167 | 27.71 | 359.8415 | 361.8385 |
| PCB 156 | 29.14 | 359.8415 | 361.8385 |
| PCB 157 | 29.47 | 359.8415 | 361.8385 |
| PCB 169 | 31.28 | 359.8415 | 361.8385 |
| PCB 189 | 33.20 | 393.8025 | 395.7995 |
| 13C12-PCB 81\* | 18.61 | 301.9626 | 303.9597 |
| 13C12-PCB 77\* | 19.28 | 301.9626 | 303.9597 |
| 13C12-PCB 123\* | 21.01 | 337.9207 | 339.9207 |
| 13C12-PCB 118\* | 21.19 | 337.9207 | 339.9207 |
| 13C12-PCB 114\* | 22.22 | 337.9207 | 339.9207 |
| 13C12-PCB 105\* | 23.59 | 337.9207 | 339.9207 |
| 13C12-PCB 126\* | 26.44 | 337.9207 | 339.9207 |
| 13C12-PCB 167\* | 27.69 | 371.8817 | 373.8788 |
| 13C12-PCB 156\* | 29.12 | 371.8817 | 373.8788 |
| 13C12-PCB 157\* | 29.45 | 371.8817 | 373.8788 |
| 13C12-PCB 169\* | 31.25 | 371.8817 | 373.8788 |
| 13C12-PCB 189\* | 33.17 | 405.8428 | 407.8398 |
| PCB70\* | 15.41 | 301.9626 | 303.9597 |
| PCB60\* | 16.6 | 301.9626 | 303.9597 |
| PCB111\* | 18.34 | 337.9207 | 339.9207 |
| PCB127\* | 23.59 | 337.9207 | 339.9207 |
| PCB159\* | 27.01 | 371.8817 | 373.8788 |
| PCB170\* | 33.17 | 405.8428 | 407.8398 |

\* Internal Standard (IS)

**Table S2.** The linearity, LOD and LOQ values for each PCDD/Fs and DL-PCBs

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Analytes** | **R2** | **Calibration Curve Equation**  **(y=ax+b)** | **LOD  (pg/g)** | **LOQ  (pg/g)** |
| **DL-PCBs** |  |  |  |  |
| PCB 81 | 0.9998 | y = 34184x - 5046.6 | 0.0533 | 0.1600 |
| PCB 77 | 0.9996 | y = 13031x - 2191.5 | 0.0687 | 0.2060 |
| PCB 123 | 0.9990 | y = 24918x - 6931.5 | 0.0196 | 0.0589 |
| PCB 118 | 0.9988 | y = 20290x - 8183.6 | 0.0185 | 0.0556 |
| PCB 114 | 0.9996 | y = 13031x - 2191.5 | 0.0202 | 0.0607 |
| PCB 105 | 0.9999 | y = 22962x - 363.87 | 0.0198 | 0.0593 |
| PCB 126 | 0.9994 | y = 32546x - 500.11 | 0.0460 | 0.1380 |
| PCB 167 | 0.9993 | y = 12673x - 3735.9 | 0.0158 | 0.0474 |
| PCB 156 | 0.9995 | y = 8716.6x - 2753.5 | 0.0156 | 0.0467 |
| PCB 157 | 0.9989 | y = 4559.6x - 1681.6 | 0.0154 | 0.0462 |
| PCB 169 | 0.9980 | y = 20845x - 11303 | 0.0430 | 0.1290 |
| PCB 189 | 0.9993 | y = 17912x – 5135.1 | 0.0114 | 0.0343 |
| **PCDD/Fs** |  |  |  |  |
| 2378-TCDF | 0.9997 | y=1.0191x -0.4372 | 0.0131 | 0.0394 |
| 12378-PeCDF | 0.9993 | y=1.034x -2.2128 | 0.0217 | 0.0651 |
| 23478-PeCDF | 0.9998 | y=1.0224x -4.7272 | 0.0204 | 0.0613 |
| 123478-HxCDF | 0.9992 | y=1.0031x 1.6945 | 0.0173 | 0.0519 |
| 123678-HxCDF | 0.9999 | y=1.0011x -0.3776 | 0.0166 | 0.0497 |
| 234678-HxCDF | 0.9992 | y=1.0224x -3.5566 | 0.0169 | 0.0507 |
| 123789-HxCDF | 0.9999 | y=1.0107x 0.8833 | 0.0192 | 0.0575 |
| 1234678-HpCDF | 0.9998 | y=1.0105x 1.7550 | 0.0240 | 0.0721 |
| 1234789-HpCDF | 0.9998 | y=1.0295x -2.4324 | 0.0251 | 0.0752 |
| OCDF | 0.9990 | y=1.0128x -0.7245 | 0.0258 | 0.0774 |
| 2378-TCDD | 0.9999 | y=1.0084x 0.8191 | 0.0180 | 0.0541 |
| 12378-PeCDD | 0.9999 | y=1.0043x 0.885 | 0.0178 | 0.0535 |
| 123478-HxCDD | 0.9998 | y=1.0043x 2.0042 | 0.0251 | 0.0753 |
| 123678-HxCDD | 0.9989 | y=1.0044x 1.6706 | 0.0233 | 0.0699 |
| 123789-HxCDD | 0.9995 | y=1.0001x 5.2884 | 0.0242 | 0.0727 |
| 1234678-HpCDD | 0.9994 | y=1.0086x -0.6972 | 0.0242 | 0.0725 |
| OCDD | 0.9992 | y=1.0005x 4.4376 | 0.0347 | 0.1040 |

**Table S3.** The concentrations of each congener of PCDD/Fs and DL-PCBs in the sediments

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Samples** | **IS-1** | **IS-2** | **IS-3** | **IS-4** | **IS-5** | **IS-6** | **IS-7** | **IS-8** | **IS-9** | **IS-10** | **IS-11** | **IS-12** | **IS-13** | **IS-14** | **IS-15** | **IS-16** | **IS-17** | **IS-18** | **IS-19** | **IS-20** | **IS-21** | **IS-22** | **IS-23** |
| **PCDD/F (pg/g)** | | | | | | | | | | | | | | | | | | | | | | | |
| 2378-TCDF | 1.370 | 1.180 | 0.924 | 1.270 | 1.390 | 1.990 | 5.540 | 3.610 | 2.960 | 1.970 | 1.170 | 0.473 | 1.120 | 3.350 | 3.890 | 1.960 | 0.881 | 1.540 | 4.630 | 2.110 | 3.310 | 0.776 | 2.320 |
| 12378-PeCDF | 0.657 | 1.050 | 0.493 | 0.307 | 0.352 | 0.596 | 1.300 | 0.712 | 1.050 | 0.814 | 0.352 | 0.219 | 0.404 | 1.130 | 0.766 | 0.544 | 0.384 | 0.662 | 1.230 | 0.429 | 1.340 | 0.469 | 0.703 |
| 23478-PeCDF | 0.883 | 0.788 | 0.530 | 0.492 | 0.565 | 0.880 | 2.030 | 1.300 | 1.560 | 1.100 | 0.552 | 0.251 | 0.596 | 1.380 | 1.800 | 0.840 | 0.458 | 0.846 | 2.020 | 0.904 | 1.520 | 0.303 | 1.060 |
| 123478-HxCDF | 2.240 | 2.310 | 1.410 | 1.210 | 1.230 | 2.640 | 4.580 | 2.960 | 4.210 | 2.870 | 1.540 | 0.725 | 1.610 | 3.660 | 5.030 | 2.250 | 1.230 | 2.400 | 4.920 | 2.560 | 3.990 | 0.959 | 2.870 |
| 123678-HxCDF | 1.110 | 1.180 | 0.654 | 0.691 | 0.670 | 1.310 | 1.860 | 1.260 | 1.730 | 1.250 | 0.651 | 0.308 | 0.707 | 1.730 | 2.330 | 1.110 | 0.508 | 0.989 | 1.880 | 0.972 | 1.620 | 0.359 | 1.160 |
| 234678-HxCDF | 0.861 | 0.950 | 0.563 | 0.448 | 0.462 | 1.010 | 1.770 | 1.130 | 1.550 | 1.090 | 0.612 | 0.294 | 0.636 | 1.460 | 2.250 | 0.915 | 0.484 | 0.932 | 2.210 | 1.070 | 1.450 | 0.372 | 1.040 |
| 123789-HxCDF | 0.115 | 0.157 | 0.070 | 0.059 | 0.051 | 0.116 | 0.167 | 0.135 | 0.152 | 0.094 | 0.066 | 0.042 | 0.078 | 0.120 | 0.175 | 0.068 | 0.060 | 0.067 | 0.160 | 0.106 | 0.214 | 0.039 | 0.174 |
| 1234678-HpCDF | 3.420 | 4.600 | 2.470 | 1.760 | 1.880 | 4.330 | 6.270 | 4.180 | 6.470 | 4.430 | 2.550 | 1.100 | 2.670 | 5.390 | 7.250 | 3.410 | 1.850 | 3.730 | 6.950 | 3.700 | 5.770 | 1.670 | 4.140 |
| 1234789-HpCDF | 0.300 | 0.316 | 0.191 | 0.136 | 0.153 | 0.353 | 0.603 | 0.409 | 0.654 | 0.454 | 0.232 | 0.117 | 0.275 | 0.537 | 0.715 | 0.341 | 0.201 | 0.386 | 0.726 | 0.425 | 0.776 | 0.223 | 0.579 |
| OCDF | 2.160 | 4.050 | 1.650 | 1.160 | 1.310 | 2.590 | 4.660 | 3.330 | 4.830 | 3.470 | 1.790 | 0.747 | 2.200 | 3.170 | 4.420 | 2.160 | 1.410 | 2.540 | 4.260 | 2.600 | 5.710 | 1.830 | 3.720 |
| 2378-TCDD | 0.155 | 0.088 | 0.062 | 0.191 | 0.175 | 0.255 | 0.098 | 0.063 | 0.227 | 0.095 | 0.047 | 0.036 | 0.073 | 0.186 | 0.162 | 0.121 | 0.044 | 0.075 | 0.521 | 1.040 | 0.097 | 0.031 | 0.064 |
| 12378-PeCDD | 0.438 | 0.294 | 0.231 | 0.493 | 0.493 | 0.891 | 0.411 | 0.322 | 0.818 | 0.409 | 0.136 | 0.108 | 0.227 | 0.453 | 0.517 | 0.381 | 0.178 | 0.222 | 1.020 | 1.970 | 0.355 | 0.103 | 0.376 |
| 123478-HxCDD | 0.631 | 0.381 | 0.308 | 0.605 | 0.572 | 1.150 | 0.412 | 0.323 | 1.340 | 0.570 | 0.199 | 0.153 | 0.336 | 0.514 | 0.543 | 0.410 | 0.250 | 0.368 | 0.954 | 1.810 | 0.439 | 0.137 | 0.561 |
| 123678-HxCDD | 0.928 | 0.581 | 0.420 | 0.758 | 0.749 | 1.400 | 0.837 | 0.644 | 1.680 | 0.831 | 0.280 | 0.174 | 0.405 | 0.813 | 0.914 | 0.600 | 0.291 | 0.446 | 1.480 | 2.840 | 0.770 | 0.196 | 0.885 |
| 123789-HxCDD | 2.270 | 1.100 | 0.803 | 1.730 | 1.790 | 3.430 | 1.470 | 1.130 | 4.160 | 1.860 | 0.509 | 0.369 | 0.886 | 1.780 | 1.920 | 1.230 | 0.686 | 0.982 | 4.240 | 9.390 | 1.580 | 0.386 | 2.210 |
| 1234678-HpCDD | 13.90 | 7.470 | 5.610 | 8.400 | 9.220 | 18.10 | 6.320 | 5.350 | 27.00 | 11.10 | 2.860 | 2.310 | 6.170 | 8.180 | 8.210 | 5.610 | 5.060 | 7.180 | 16.80 | 36.20 | 9.500 | 2.570 | 13.10 |
| OCDD | 160.0 | 64.00 | 57.50 | 50.10 | 86.90 | 108.0 | 49.80 | 45.50 | 397.0 | 157.0 | 15.30 | 20.70 | 59.10 | 67.60 | 79.20 | 36.20 | 86.80 | 144.0 | 122.0 | 379.0 | 82.80 | 19.20 | 164.0 |
| **DL-PCB (pg/g)** | | | | | | | | | | | | | | | | | | | | | | | |
| PCB 81 (3,4,4',5-TeCB) | 1.070 | 2.140 | 2.244 | 1.100 | 2.360 | 0.875 | 5.110 | 8.120 | 1.380 | 1.590 | 0.521 | 0.346 | 0.569 | 1.160 | 0.851 | 2.550 | 0.349 | 0.554 | 0.070 | 0.661 | 1.770 | 0.489 | 1.410 |
| PCB 77 (3,3',4,4'-TeCB) | 2.080 | 5.270 | 4.644 | 2.100 | 4.920 | 2.920 | 13.30 | 14.40 | 4.590 | 3.820 | 2.510 | 0.714 | 1.760 | 3.590 | 2.840 | 5.670 | 1.390 | 2.260 | 13.300 | 3.210 | 13.10 | 2.060 | 8.880 |
| PCB 123 (2',3,4,4',5-PeCB) | 1.190 | 1.060 | 1.187 | 0.604 | 0.528 | 0.828 | 4.520 | 4.350 | 0.769 | 0.732 | 0.362 | 0.332 | 0.979 | 1.330 | 0.696 | 1.400 | 0.682 | 0.835 | 2.340 | 1.520 | 1.830 | 0.674 | 1.550 |
| PCB 118 (2,3',4,4',5-PeCB) | 20.80 | 16.30 | 23.33 | 11.30 | 10.70 | 16.10 | 152.0 | 99.90 | 26.40 | 18.00 | 13.50 | 5.22 | 14.50 | 26.90 | 21.40 | 28.60 | 11.50 | 16.50 | 37.80 | 18.40 | 46.70 | 10.90 | 31.70 |
| PCB 114 (2,3,4,4',5-PeCB) | 0.481 | 0.377 | 0.580 | 0.304 | 0.275 | 0.441 | 3.830 | 2.630 | 0.575 | 0.415 | 0.322 | 0.128 | 0.335 | 0.765 | 0.469 | 0.750 | 0.255 | 0.352 | 0.959 | 0.416 | 1.250 | 0.328 | 0.836 |
| PCB 105 (2,3,3',4,4'-PeCB) | 7.360 | 7.800 | 10.18 | 4.380 | 4.560 | 6.740 | 74.40 | 47.10 | 15.00 | 7.250 | 12.40 | 2.180 | 6.490 | 12.10 | 8.710 | 11.40 | 5.550 | 5.460 | 18.20 | 9.180 | 23.50 | 4.740 | 15.70 |
| PCB 126 (3,3',4,4',5-PeCB) | 0.176 | 0.462 | 0.413 | 0.467 | 3.200 | 0.556 | 3.490 | 3.440 | 0.965 | 0.959 | 0.470 | 0.213 | 0.570 | 1.060 | 0.947 | 1.620 | 0.389 | 0.445 | 1.580 | 0.691 | 1.240 | 0.364 | 0.757 |
| PCB 167 (2,3',4,4',5,5'-HxCB) | 5.490 | 6.280 | 6.244 | 2.720 | 3.140 | 3.840 | 49.80 | 32.50 | 11.90 | 5.610 | 12.50 | 1.640 | 6.710 | 7.780 | 7.410 | 8.240 | 6.150 | 5.830 | 14.90 | 11.50 | 15.00 | 3.770 | 8.730 |
| PCB 156 (2,3,3',4,4',5-HxCB) | 3.110 | 2.890 | 3.489 | 1.590 | 1.900 | 2.350 | 25.20 | 18.40 | 4.270 | 2.980 | 2.260 | 0.942 | 3.300 | 4.440 | 4.260 | 4.840 | 2.370 | 2.900 | 8.540 | 5.480 | 9.170 | 2.170 | 5.050 |
| PCB 157 (2,3,3',4,4',5'-HxCB) | 0.618 | 0.626 | 0.756 | 0.374 | 0.430 | 0.661 | 5.610 | 4.000 | 0.948 | 0.629 | 0.482 | 0.207 | 0.824 | 0.947 | 0.976 | 1.010 | 0.601 | 0.695 | 1.870 | 1.090 | 1.880 | 0.471 | 1.040 |
| PCB 169 (3,3',4,4',5,5'-HxCB) | 0.154 | 4.210 | 0.269 | 0.144 | 11.90 | 0.698 | 0.362 | 0.277 | 0.259 | 0.249 | 0.139 | 0.092 | 0.178 | 0.300 | 0.281 | 0.222 | 0.132 | 0.178 | 0.360 | 0.201 | 0.272 | 0.112 | 0.204 |
| PCB 189 (2,3,3',4,4',5,5'-HpCB) | 0.566 | 0.500 | 0.578 | 0.264 | 6.340 | 0.446 | 2.430 | 2.000 | 0.681 | 0.463 | 0.352 | 0.179 | 0.613 | 0.667 | 0.573 | 0.559 | 0.414 | 0.482 | 1.530 | 1.110 | 1.430 | 0.355 | 0.681 |