**Air–water exchange and gas-particle partitioning of polycyclic aromatic hydrocarbons (PAHs) in coral reef areas of the South China Sea Ziyue Feng1,2,3, Chenglong Wang1,2,3, Wanzhi Wang1,2,3, Chuchu Zhang1,2,3, Jiajia Wang3, Xinqing Zou1,2,3,4,\*, Guanghe Fu1,2,3,\***

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Table S1 Concentrations (ng/L) of 16 PAHs in water phase

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Congener** | **W1** | **W2** | **W3** | **W4** | **W5** | **W6** | **W7** | **W8** | **W9** | **W10** | **W11** | **W12** | **W13** | **W14** | **W15** | **W16** |
| **Nap** | 15.10 | 36.84 | 10.56 | 35.29 | 10.47 | 14.73 | 3.70 | 24.39 | 10.44 | 13.61 | 21.93 | 7.75 | 7.42 | 9.31 | 36.02 | 38.96 |
| **Ace** | 1.64 | 0.00 | 0.31 | 0.00 | 0.30 | 0.40 | 0.60 | 0.00 | 0.57 | 0.57 | 1.56 | 0.00 | 0.27 | 0.39 | 1.90 | 1.31 |
| **Acy** | 0.44 | 0.53 | 0.33 | 0.51 | 0.33 | 0.40 | 0.30 | 0.45 | 0.36 | 0.36 | 0.42 | 0.44 | 0.28 | 0.34 | 0.53 | 0.52 |
| **Flo** | 3.30 | 4.97 | 1.68 | 4.32 | 1.19 | 1.88 | 1.38 | 3.27 | 1.91 | 1.56 | 3.00 | 4.11 | 1.07 | 1.68 | 4.67 | 4.55 |
| **Phe** | 0.00 | 0.14 | 0.00 | 0.00 | 1.37 | 0.00 | 1.32 | 0.00 | 1.81 | 0.00 | 0.00 | 0.03 | 0.00 | 0.00 | 0.05 | 0.10 |
| **Ant** | 0.02 | 4.12 | 0.00 | 3.98 | 0.00 | 0.14 | 0.00 | 2.87 | 0.00 | 0.00 | 0.07 | 3.85 | 0.00 | 0.00 | 3.88 | 5.11 |
| **Flu** | 0.96 | 0.47 | 0.24 | 0.32 | 0.20 | 0.38 | 0.14 | 0.23 | 0.29 | 0.18 | 0.32 | 0.36 | 0.14 | 0.24 | 0.36 | 0.75 |
| **Pyr** | 0.73 | 0.51 | 0.28 | 0.44 | 0.20 | 0.83 | 0.17 | 0.29 | 0.25 | 0.21 | 0.39 | 0.36 | 0.16 | 0.31 | 0.51 | 0.81 |
| **BaA** | 0.08 | 0.03 | 0.03 | 0.03 | 0.00 | 0.16 | 0.00 | 0.01 | 0.02 | 0.03 | 0.04 | 0.05 | 0.00 | 0.04 | 0.04 | 0.00 |
| **Chr** | 0.20 | 0.00 | 0.08 | 0.00 | 0.00 | 0.81 | 0.05 | 0.00 | 0.07 | 0.00 | 0.11 | 0.00 | 0.00 | 0.08 | 0.10 | 0.10 |
| **BbF** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **BkF** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **BaP** | 0.00 | 11.86 | 0.00 | 0.00 | 0.00 | 11.17 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **IndP** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **DahA** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **BghiP** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **∑16PAHs** | 22.48 | 59.46 | 13.52 | 44.89 | 14.05 | 30.89 | 7.65 | 31.52 | 15.73 | 16.50 | 27.84 | 16.94 | 9.36 | 12.38 | 48.05 | 52.20 |

Table S2 Concentrations (ng/m3) of 16 PAHs in gas phase

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Congener** | **W1** | **W2** | **W3** | **W4** | **W5** | **W6** | **W7** | **W8** | **W9** | **W10** | **W11** | **W12** | **W13** | **W14** | **W15** | **W16** |
| **Nap** | 1.771 | 2.713 | 2.178 | 3.954 | 5.462 | 4.263 | 2.832 | 4.190 | 5.051 | 2.378 | 11.782 | 1.769 | 2.041 | 1.259 | 1.887 | 2.202 |
| **Acy** | 0.367 | 0.162 | 0.123 | 0.185 | 0.729 | 1.383 | 0.088 | 0.120 | 0.227 | 0.111 | 0.466 | 0.121 | 0.036 | 0.034 | 0.152 | 0.110 |
| **Ace** | 0.249 | 0.313 | 0.220 | 0.253 | 0.380 | 0.697 | 0.073 | 0.173 | 0.183 | 0.106 | 0.114 | 0.213 | 0.047 | 0.062 | 0.086 | 0.189 |
| **Flo** | 1.376 | 2.406 | 1.797 | 1.106 | 2.418 | 4.171 | 0.951 | 2.425 | 1.519 | 1.690 | 0.806 | 2.531 | 0.545 | 0.606 | 1.343 | 1.200 |
| **Phe** | 11.592 | 14.289 | 16.579 | 10.752 | 22.505 | 52.470 | 19.650 | 13.497 | 27.843 | 15.756 | 7.873 | 24.445 | 9.951 | 12.520 | 14.376 | 25.824 |
| **Ant** | 1.504 | 2.007 | 2.163 | 1.748 | 3.173 | 7.096 | 2.960 | 0.000 | 4.132 | 2.458 | 1.337 | 4.268 | 1.410 | 1.665 | 2.309 | 3.828 |
| **Flu** | 3.675 | 6.480 | 7.258 | 8.963 | 8.611 | 25.381 | 8.771 | 6.407 | 36.470 | 12.487 | 5.606 | 10.281 | 3.913 | 8.265 | 10.076 | 12.645 |
| **Pyr** | 2.402 | 3.290 | 4.207 | 6.744 | 4.350 | 20.603 | 4.575 | 3.085 | 16.036 | 5.866 | 1.787 | 5.271 | 1.842 | 4.821 | 5.099 | 6.741 |
| **BaA** | 0.033 | 0.040 | 0.051 | 0.363 | 0.063 | 0.221 | 0.085 | 0.079 | 0.392 | 0.132 | 0.039 | 0.079 | 0.034 | 0.061 | 0.061 | 0.000 |
| **Chr** | 0.400 | 0.328 | 0.423 | 0.770 | 0.473 | 1.104 | 0.567 | 0.388 | 1.804 | 0.677 | 0.251 | 0.385 | 0.252 | 0.297 | 0.283 | 0.673 |
| **BbF** | 0.020 | 0.021 | 0.018 | 0.061 | 0.033 | 0.020 | 0.035 | 0.026 | 0.049 | 0.047 | 0.017 | 0.026 | 0.017 | 0.013 | 0.026 | 0.023 |
| **BkF** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **BaP** | 0.000 | 0.004 | 0.000 | 0.000 | 0.003 | 0.003 | 0.003 | 0.000 | 0.000 | 0.004 | 0.000 | 0.003 | 0.000 | 0.000 | 0.000 | 0.000 |
| **IndP** | 0.000 | 0.002 | 0.000 | 0.000 | 0.001 | 0.003 | 0.004 | 0.000 | 0.000 | 0.005 | 0.000 | 0.003 | 0.000 | 0.000 | 0.000 | 0.000 |
| **DahA** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 | 0.000 | 0.002 | 0.000 |
| **BghiP** | 0.008 | 0.006 | 0.006 | 0.000 | 0.007 | 0.007 | 0.008 | 0.004 | 0.004 | 0.010 | 0.000 | 0.006 | 0.001 | 0.000 | 0.000 | 0.000 |
| **∑16PAHs** | 23.397 | 32.062 | 35.022 | 34.900 | 48.210 | 117.423 | 40.602 | 30.394 | 93.709 | 41.727 | 30.078 | 49.400 | 20.090 | 29.604 | 35.701 | 53.437 |

Table S3 Concentrations (ng/m3) of 16 PAHs in particle phase

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Congener** | **W1** | **W2** | **W3** | **W4** | **W5** | **W6** | **W7** | **W8** | **W9** | **W10** | **W11** | **W12** | **W13** | **W14** | **W15** | **W16** |
| **Nap** | 0.281 | 0.126 | 0.063 | 0.191 | 0.571 | 0.098 | 0.252 | 0.307 | 0.124 | 0.202 | 0.177 | 0.109 | 0.136 | 0.117 | 0.055 | 0.037 |
| **Acy** | 0.048 | 0.014 | 0.013 | 0.035 | 0.087 | 0.013 | 0.041 | 0.064 | 0.018 | 0.031 | 0.033 | 0.022 | 0.024 | 0.013 | 0.055 | 0.018 |
| **Ace** | 0.009 | 0.008 | 0.006 | 0.008 | 0.012 | 0.008 | 0.007 | 0.008 | 0.005 | 0.007 | 0.019 | 0.006 | 0.017 | 0.007 | 0.006 | 0.003 |
| **Flo** | 0.024 | 0.017 | 0.020 | 0.025 | 0.030 | 0.025 | 0.018 | 0.024 | 0.022 | 0.025 | 0.053 | 0.017 | 0.039 | 0.016 | 0.016 | 0.014 |
| **Phe** | 0.054 | 0.036 | 0.040 | 0.079 | 0.040 | 0.164 | 0.026 | 0.066 | 0.066 | 0.078 | 0.025 | 0.040 | 0.028 | 0.028 | 0.019 | 0.035 |
| **Ant** | 0.029 | 0.025 | 0.025 | 0.034 | 0.000 | 0.055 | 0.032 | 0.034 | 0.039 | 0.035 | 0.032 | 0.033 | 0.000 | 0.027 | 0.047 | 0.041 |
| **Flu** | 0.108 | 0.072 | 0.061 | 0.122 | 0.063 | 0.390 | 0.047 | 0.125 | 0.130 | 0.142 | 0.022 | 0.078 | 0.040 | 0.040 | 0.024 | 0.111 |
| **Pyr** | 0.072 | 0.050 | 0.040 | 0.090 | 0.057 | 0.621 | 0.027 | 0.078 | 0.094 | 0.093 | 0.021 | 0.049 | 0.031 | 0.029 | 0.021 | 0.075 |
| **BaA** | 0.015 | 0.014 | 0.011 | 0.067 | 0.031 | 0.326 | 0.009 | 0.072 | 0.066 | 0.067 | 0.004 | 0.000 | 0.011 | 0.000 | 0.009 | 0.034 |
| **Chr** | 0.084 | 0.064 | 0.051 | 0.153 | 0.088 | 1.338 | 0.037 | 0.158 | 0.230 | 0.156 | 0.017 | 0.074 | 0.030 | 0.023 | 0.030 | 0.121 |
| **BbF** | 0.074 | 0.033 | 0.029 | 0.184 | 0.047 | 0.222 | 0.035 | 0.141 | 0.176 | 0.123 | 0.009 | 0.023 | 0.023 | 0.012 | 0.008 | 0.030 |
| **BkF** | 0.081 | 0.045 | 0.039 | 0.177 | 0.087 | 0.232 | 0.055 | 0.141 | 0.179 | 0.121 | 0.029 | 0.040 | 0.035 | 0.030 | 0.046 | 0.062 |
| **BaP** | 0.026 | 0.008 | 0.008 | 0.106 | 0.021 | 0.065 | 0.009 | 0.082 | 0.035 | 0.063 | 0.000 | 0.002 | 0.008 | 0.003 | 0.000 | 0.006 |
| **IndP** | 0.047 | 0.016 | 0.017 | 0.156 | 0.031 | 0.084 | 0.024 | 0.092 | 0.100 | 0.079 | 0.001 | 0.005 | 0.012 | 0.004 | 0.000 | 0.012 |
| **DahA** | 0.000 | 0.000 | 0.000 | 0.036 | 0.000 | 0.030 | 0.000 | 0.024 | 0.014 | 0.019 | 0.000 | 0.000 | 0.001 | 0.000 | 0.000 | 0.000 |
| **BghiP** | 0.052 | 0.014 | 0.026 | 0.143 | 0.035 | 0.116 | 0.027 | 0.083 | 0.114 | 0.071 | 0.002 | 0.004 | 0.011 | 0.005 | 0.000 | 0.018 |
| **∑16PAHs** | 0.281 | 0.126 | 0.063 | 0.191 | 0.571 | 0.098 | 0.252 | 0.307 | 0.124 | 0.202 | 0.177 | 0.109 | 0.136 | 0.117 | 0.055 | 0.037 |

Table S4 Fugacity fractions (*ff*) of PAHs

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Congener** | **W1** | **W2** | **W3** | **W4** | **W5** | **W6** | **W7** | **W8** | **W9** | **W10** | **W11** | **W12** | **W13** | **W14** | **W15** | **W16** |
| **Nap** | 0.161 | 0.232 | 0.097 | 0.164 | 0.041 | 0.071 | 0.028 | 0.113 | 0.043 | 0.112 | 0.039 | 0.088 | 0.074 | 0.140 | 0.296 | 0.281 |
| **Ace** | 0.050 | 0.000 | 0.029 | 0.000 | 0.005 | 0.003 | 0.073 | 0.000 | 0.028 | 0.056 | 0.037 | 0.000 | 0.080 | 0.117 | 0.127 | 0.122 |
| **Acy** | 0.012 | 0.011 | 0.010 | 0.013 | 0.006 | 0.004 | 0.025 | 0.017 | 0.013 | 0.021 | 0.023 | 0.013 | 0.037 | 0.033 | 0.038 | 0.017 |
| **Flo** | 0.010 | 0.008 | 0.004 | 0.015 | 0.002 | 0.002 | 0.006 | 0.005 | 0.005 | 0.004 | 0.015 | 0.006 | 0.008 | 0.011 | 0.014 | 0.015 |
| **Phe** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **Ant** | 0.000 | 0.004 | 0.000 | 0.005 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.002 | 0.000 | 0.000 | 0.003 | 0.003 |
| **Flu** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **Pyr** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **BaA** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **Chr** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **BbF** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **BkF** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **BaP** | 0.000 | 0.213 | 0.000 | 0.000 | 0.000 | 0.212 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **InP** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **DBahA** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| **BghiP** | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |

Table S5 Air-water exchange fluxes (ng/m2/d) of PAHs

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Congener** | **W1** | **W2** | **W3** | **W4** | **W5** | **W6** | **W7** | **W8** | **W9** | **W10** | **W11** | **W12** | **W13** | **W14** | **W15** | **W16** |
| **Nap** | -0.09 | -0.17 | -0.17 | -0.25 | -0.39 | -0.13 | -0.05 | -0.17 | -0.09 | -0.04 | -0.20 | -0.03 | -0.06 | -0.11 | -0.11 | -0.14 |
| **Ace** | -0.04 | -0.03 | -0.02 | -0.03 | -0.10 | -0.08 | 0.00 | -0.01 | -0.01 | 0.00 | -0.01 | 0.00 | 0.00 | -0.01 | -0.02 | -0.02 |
| **Acy** | -0.05 | -0.09 | -0.06 | -0.06 | -0.09 | -0.07 | 0.00 | -0.02 | -0.01 | -0.01 | -0.01 | -0.01 | 0.00 | -0.02 | -0.03 | -0.06 |
| **Flo** | -0.41 | -1.07 | -0.79 | -0.43 | -0.89 | -0.67 | -0.08 | -0.55 | -0.13 | -0.15 | -0.07 | -0.22 | -0.09 | -0.31 | -0.68 | -0.60 |
| **Phe** | -7.10 | -13.04 | -14.95 | -8.69 | -16.93 | -17.06 | -3.42 | -6.24 | -4.86 | -2.75 | -1.38 | -4.27 | -3.22 | -12.99 | -14.92 | -26.80 |
| **Ant** | -0.85 | -1.68 | -1.80 | -1.30 | -2.20 | -2.13 | -0.48 | 0.00 | -0.67 | -0.40 | -0.22 | -0.69 | -0.42 | -1.60 | -2.20 | -3.66 |
| **Flu** | -6.08 | -15.97 | -17.67 | -19.55 | -17.49 | -22.27 | -4.06 | -7.99 | -16.92 | -5.80 | -2.60 | -4.77 | -3.42 | -23.15 | -28.22 | -35.42 |
| **Pyr** | -3.22 | -6.56 | -8.29 | -11.91 | -7.15 | -14.64 | -1.72 | -3.11 | -6.02 | -2.20 | -0.67 | -1.98 | -1.30 | -10.93 | -11.56 | -15.28 |
| **BaA** | -0.19 | -0.36 | -0.45 | -2.87 | -0.46 | -0.70 | -0.14 | -0.36 | -0.65 | -0.22 | -0.06 | -0.13 | -0.11 | -0.62 | -0.62 | 0.00 |
| **Chr** | -2.56 | -3.13 | -3.99 | -6.52 | -3.73 | -3.76 | -1.00 | -1.87 | -3.20 | -1.20 | -0.45 | -0.68 | -0.86 | -3.23 | -3.07 | -7.31 |
| **BbF** | -0.29 | -0.45 | -0.38 | -1.17 | -0.58 | -0.15 | -0.14 | -0.28 | -0.19 | -0.19 | -0.07 | -0.10 | -0.13 | -0.31 | -0.65 | -0.57 |
| **BkF** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **BaP** | 0.00 | -0.05 | 0.00 | 0.00 | -0.05 | -0.02 | -0.01 | 0.00 | 0.00 | -0.01 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 |
| **InP** | -0.02 | -0.10 | 0.00 | 0.00 | -0.05 | -0.06 | -0.04 | 0.00 | 0.00 | -0.05 | 0.00 | -0.03 | 0.00 | 0.00 | 0.00 | 0.00 |
| **DBahA** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.01 | 0.00 | 0.00 | 0.00 | 0.00 | -0.17 | 0.00 |
| **BghiP** | -0.22 | -0.27 | -0.26 | 0.00 | -0.23 | -0.10 | -0.06 | -0.08 | -0.03 | -0.07 | 0.00 | -0.04 | -0.02 | 0.00 | 0.00 | 0.00 |
| **∑16PAHs** | -21.12 | -42.97 | -48.83 | -52.78 | -50.34 | -61.82 | -11.21 | -20.68 | -32.76 | -13.10 | -5.74 | -12.98 | -9.64 | -53.27 | -62.25 | -89.85 |

Table S6 Physicochemical properties of sampling sites

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sampling sites** | **Longitude** | **Latitude** | **Air temperature(K)** | **Pressure(Pa)** | **Wind speed(m/s)** | **Gas**  **Volume(L)** |
| **W1** | 112.32°E | 16.80°N | 293.81 | 101528.90 | 5.79 | 244.76 |
| **W2** | 115.18°E | 10.10°N | 297.77 | 101328.16 | 6.97 | 247.12 |
| **W3** | 116.37°E | 10.32°N | 299.34 | 101231.11 | 6.91 | 232.21 |
| **W4** | 116.64°E | 10.42°N | 300.92 | 101186.40 | 6.51 | 203.76 |
| **W5** | 116.83°E | 10.57°N | 300.25 | 101147.57 | 6.30 | 177.66 |
| **W6** | 114.77°E | 11.13°N | 301.19 | 100941.09 | 4.59 | 212.24 |
| **W7** | 113.34°E | 13.93°N | 300.95 | 100932.88 | 4.01 | 234.13 |
| **W8** | 111.90°E | 16.70°N | 300.81 | 100878.44 | 5.13 | 228.17 |
| **W9** | 113.33°E | 13.10°N | 301.03 | 100813.85 | 3.25 | 236.99 |
| **W10** | 114.21°E | 11.03°N | 301.49 | 100887.21 | 3.05 | 250.78 |
| **W11** | 115.31°E | 9.50°N | 301.78 | 100926.91 | 3.28 | 230.08 |
| **W12** | 115.46°E | 9.37°N | 301.67 | 100876.72 | 3.88 | 339.88 |
| **W13** | 115.96°E | 9.33°N | 301.45 | 100829.85 | 4.58 | 229.10 |
| **W14** | 115.86°E | 9.73°N | 301.31 | 100933.00 | 7.44 | 233.82 |
| **W15** | 115.57°E | 9.85°N | 300.00 | 101000.00 | 7.44 | 237.76 |
| **W16** | 115.54°E | 9.90°N | 300.00 | 101000.00 | 7.44 | 226.17 |

Table S7 Details about analytical method

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Congener** | **Retention time (min)** | **Mass** | **Product mass** | **Collision energy** |
| **Nap** | 5.70 | 128/128 | 76.6/102.1 | 30/20 |
| **Acy** | 8.38 | 152/152 | 126/151.1 | 25/15 |
| **Ace-D10** | 8.69 | 164/164 | 80/160 | 30/30 |
| **Ace** | 8.74 | 153/153 | 126.6/151.9 | 25/20 |
| **Flo** | 9.78 | 166/166 | 115/165 | 40/15 |
| **Phe-D10** | 11.92 | 188/188 | 80/160 | 30/30 |
| **Phe** | 11.97 | 178/178 | 151.9/176 | 20/25 |
| **Ant** | 12.09 | 178/178 | 151.9/176.1 | 20/25 |
| **Flu** | 15.81 | 101/202 | 88/200.1 | 10/35 |
| **Pyr** | 16.64 | 101/202 | 88/200 | 10/35 |
| **BaA** | 22.16 | 228/228 | 201.9/226.1 | 25/30 |
| **Chr-D12** | 22.24 | 240/240 | 120/236 | 30/30 |
| **Chr** | 22.36 | 113/228 | 112.5/226.1 | 10/30 |
| **BbF** | 27.51 | 126/252 | 113/250.2 | 10/35 |
| **BkF** | 27.63 | 126/252 | 113/250.3 | 10/35 |
| **BaP** | 28.98 | 126/252 | 113/250.1 | 10/35 |
| **Pyr-D12** | 29.26 | 264/264 | 130/260 | 30/35 |
| **InP** | 33.97 | 138/276 | 125/374.1 | 15/40 |
| **DBahA** | 34.17 | 139/278 | 125.9/246.3 | 10/35 |
| **BghiP** | 34.97 | 138/276 | 137.2/274.2 | 15/40 |

Table S8 Physico-chemical properties of PAH congeners

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Congener** | **Ring** | **Henry’s law consistent**  **(Pa/m3/mol)** | **Molar mass *(*g/mol)** | **Molar volume(cm3/mol)** |
| **Nap** | 2 | 55 | 128 | 123.5 |
| **Acy** | 3 | 16 | 152 | 128 |
| **Ace** | 3 | 29 | 154 | 134 |
| **Flo** | 3 | 10 | 166 | 148 |
| **Phe** | 3 | 4.8 | 178 | 157 |
| **Ant** | 3 | 5.2 | 178 | 157 |
| **Flu** | 4 | 1.7 | 202 | 162 |
| **Pyr** | 4 | 2.1 | 202 | 162 |
| **BaA** | 4 | 0.45 | 228 | 191 |
| **Chr** | 4 | 0.42 | 228 | 191 |
| **BbF** | 5 | 0.18 | 252 | 196 |
| **BkF** | 5 | 0.17 | 252 | 196 |
| **BaP** | 5 | 0.21 | 252 | 196 |
| **IndP** | 5 | 0.07 | 276 | 200 |
| **DahA** | 5 | 0.05 | 278 | 225 |
| **BghiP** | 6 | 0.09 | 276 | 200 |

Table S9 LogKp (m3/ μg) of PAHs

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Congener** | **W1** | **W2** | **W3** | **W4** | **W5** | **W6** | **W7** | **W8** | **W9** | **W10** | **W11** | **W12** | **W13** | **W14** | **W15** | **W16** |
| **Nap** | -2.22 | -2.76 | -2.97 | -2.74 | -2.41 | -3.06 | -2.48 | -2.56 | -3.04 | -2.50 | -3.25 | -2.63 | -2.60 | -2.46 | -2.96 | -3.20 |
| **Ace** | -2.31 | -2.50 | -2.39 | -2.15 | -2.35 | -3.46 | -1.76 | -1.70 | -2.53 | -1.98 | -2.57 | -2.17 | -1.60 | -1.84 | -1.87 | -2.22 |
| **Acy** | -2.88 | -3.03 | -2.98 | -2.90 | -2.91 | -3.36 | -2.46 | -2.75 | -2.95 | -2.60 | -2.21 | -2.94 | -1.86 | -2.38 | -2.59 | -3.16 |
| **Flo** | -3.19 | -3.58 | -3.39 | -3.08 | -3.34 | -3.64 | -3.16 | -3.43 | -3.26 | -3.26 | -2.61 | -3.61 | -2.57 | -2.99 | -3.35 | -3.37 |
| **Phe** | -3.76 | -4.02 | -4.04 | -3.56 | -4.17 | -3.93 | -4.30 | -3.74 | -4.05 | -3.73 | -3.93 | -4.21 | -3.98 | -4.08 | -4.30 | -4.29 |
| **Ant** | -3.14 | -3.32 | -3.36 | -3.14 | 0.00 | -3.53 | -3.39 | 0.00 | -3.45 | -3.27 | -3.04 | -3.54 | 0.00 | -3.22 | -3.11 | -3.39 |
| **Flu** | -2.96 | -3.38 | -3.50 | -3.29 | -3.56 | -3.24 | -3.70 | -3.14 | -3.87 | -3.37 | -3.84 | -3.54 | -3.41 | -3.74 | -4.04 | -3.48 |
| **Pyr** | -2.95 | -3.24 | -3.45 | -3.30 | -3.31 | -2.95 | -3.66 | -3.02 | -3.66 | -3.23 | -3.36 | -3.46 | -3.20 | -3.65 | -3.82 | -3.38 |
| **BaA** | -1.75 | -1.87 | -2.08 | -2.16 | -1.74 | -1.26 | -2.38 | -1.47 | -2.20 | -1.72 | -2.39 | 0.00 | -1.92 | 0.00 | -2.26 | 0.00 |
| **Chr** | -2.10 | -2.14 | -2.35 | -2.13 | -2.15 | -1.34 | -2.61 | -1.81 | -2.32 | -2.06 | -2.60 | -2.14 | -2.35 | -2.54 | -2.40 | -2.17 |
| **BbF** | -0.86 | -1.23 | -1.21 | -0.95 | -1.27 | -0.38 | -1.42 | -0.69 | -0.87 | -1.01 | -1.70 | -1.48 | -1.29 | -1.44 | -1.94 | -1.31 |
| **BkF** | 0.00 | -1.07 | 0.00 | 0.00 | -0.59 | -0.16 | -0.97 | 1.66 | 0.00 | -0.18 | 0.00 | -1.45 | 0.00 | 0.00 | 0.00 | 0.00 |
| **BaP** | 0.56 | -0.46 | 3.15 | 0.00 | -0.02 | -0.02 | -0.67 | 0.00 | 0.00 | -0.27 | 0.00 | -1.24 | 0.00 | 0.00 | 0.00 | 0.00 |
| **InP** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | -0.09 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **DBahA** | -0.61 | -1.09 | -0.81 | 0.00 | -0.70 | -0.18 | -0.91 | -0.11 | 0.09 | -0.56 | -0.54 | -1.56 | -0.48 | 0.00 | 0.00 | 0.00 |
| **BghiP** | -2.22 | -2.76 | -2.97 | -2.74 | -2.41 | -3.06 | -2.48 | -2.56 | -3.04 | -2.50 | -3.25 | -2.63 | -2.60 | -2.46 | -2.96 | -3.20 |