**Ecological indicators and source diagnostic ratios of aliphatic and polyaromatic hydrocarbons in marine sediments of Qatar**

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Supplementary Table1: Physical and toxicity properties of 16 priority US EPA PAHs.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 16 Priority US EPA PAHs | Abbreviation | Physical Properties | | | Toxicity Properties | | |
| Benzene  Ring(s) | LogKow | Solubility in water at 25 °C (µg/L) | aAcute Toxicity  (ng∙g-1 or µg∙L-1) | aChronic Toxicity  (ng∙g-1 or µg∙L-1) | bRfD (mg/kg/day) |
| Naphthalene | NaP | 2 | 3.37 | 3.17 × 104 | 4870 | 970 | 0.02 |
| Acenaphthylene | Acl | 3 | 4.07 | 3.93 × 103 | 1181 | 180 | 0.03 |
| Acenaphthene | Ace | 3 | 3.92 | 3.4 × 103 | 1360 | 270 | 0.6 |
| Fluorene | Fl | 3 | 4.18 | 1.98 × 103 | 730 | 150 | 0.04 |
| Phenanthrene | Phe | 3 | 4.46 | 1.29 × 103 | 367 | 55 | 0.053 |
| Anthracene | Ant | 3 | 4.54 | 73 | 300 | 60 | 0.3 |
| Fluoranthene | Flu | 4 | 5.22 | 260 | 55 | 11 | 0.04 |
| Pyrene | Pyr | 4 | 5.18 | 135 | 61 | 12 | 0.03 |
| Benz[a]anthracene | BaA | 4 | 5.91 | 14 | 9.8 | 2.0 | 0.0003 |
| Chrysene | Chry | 4 | 5.86 | 2.0 | 11 | 2.2 | NA |
| Benzo[b]fluoranthene | BbF | 5 | 5.8 | 1.2 | 14 | 2.9 | 0.0003 |
| Benzo[k]fluoranthene | BkF | 5 | 6.0 | 0.76 | 8.6 | 1.7 | 0.0003 |
| Benzo[a]pyrene | BaP | 5 | 6.04 | 3.8 | 7.6 | 1.5 | 0.0003 |
| Indeno[1,2,3-cd]pyrene | InP | 6 | 7.0 | 62 | 0.64 | 0.13 | 0.0003 |
| Dibenz[a,h]anthracene | DahA | 5 | 6.75 | 0.5 | 1.3 | 0.25 | 0.0003 |
| Benzo[ghi]perylene | BghiP | 6 | 6.5 | 0.26 | 2.4 | 0.49 | NA |

aAcute and chronic toxicity data of PAH frequently found in crude and refined petroleum (Neff *et al.*, 2005).

bRfD: Reference dose is a maximum acceptable oral dose of a toxic substance by USEPA (2011).

Supplementary Table 2: The established Effect Range-Low (ERL) and Effect Range-Median (ERM) from NOAA and the Threshold Effects Level (TEL) and Probable Effects Level (PEL) of the PAH congeners in sediments.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **PAHs** | **NOAA** | | **CSQGs** | |
| **ERL** | **ERM** | **TEL** | **PEL** |
| Naphthalene | 160 | 2100 | 34.6 | 391 |
| Acenaphthylene | 44 | 640 | 5.87 | 128 |
| Acenaphthene | 16 | 500 | 6.71 | 88.9 |
| Fluorene | 19 | 540 | 21.2 | 144 |
| Phenanthrene | 240 | 1500 | 86.7 | 544 |
| Anthracene | 85.3 | 1100 | 46.9 | 245 |
| ΣLMW PAHs | 552.0 | 3160 | 312 | 1442 |
| Fluoranthene | 600 | 5100 | 113 | 1494 |
| Pyrene | 665 | 2600 | 153 | 1398 |
| Benzo(a)anthracene | 261 | 1600 | 74.8 | 693 |
| Chrysene | 384 | 2800 | 108 | 846 |
| Benzo(b)fluoranthene | - | - | - | - |
| Benzo(k)fluoranthene | - | - | - | - |
| Benzo(a)pyrene | 430 | 1600 | 88.8 | 763 |
| Indeno(1,2,3-cd)pyrene | - | - | - | - |
| Dibenz(a,h)anthracene | 63.4 | 260 | 6.22 | 135 |
| Benzo(g,h,i)perylene | - | - | - | - |
| ΣHMW PAHs | 1700 | 9600 | 655 | 6676 |
| ΣPAHs | 4022 | 44792 | 1684 | 16770 |
| NOAA: National Oceanic and Atmospheric Administration; CSQG: Canadian Sediment Quality Guidelines; ΣLMW: Low Molecular weight PAHs; ΣHMW: High Molecular Weight PAHs; ΣPAHs: sum of the 16 polycyclic aromatic hydrocarbons. Source: Buchman, 2008; CCME, 1999; Nascimento *et al.*, 2017. | | | | |

Supplementary Table 3: Concentration of individual PAH compounds (ng·g-1) and geochemical indices.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ring # | **Name** | **SD1** | **SD2** | **SD3** | **SD4** | **SD5** | **SD6** | **SD7** | **SD8** | **SD9** | **SD10** | **SD11** | **SD12** | **SD13** | **SD14** | **SD15** | **SD16** | **SD17** | **SD18** | **SD19** | **SD20** | **SUB** | **SZK** |
| 2 | Naphthalene (Phe) | 0.44 | <LOD | 0.52 | <LOD | <LOD | <LOD | 0.26 | 1.17 | 1.35 | 1.01 | 0.88 | 0.41 | <LOD | <LOD | <LOD | <LOD | 0.56 | <LOD | 0.15 | <LOD | <LOD | <LOD |
| 3 | Acenaphthylene (Acy) | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD |
| 3 | Acenaphthene (Ace) | 0.14 | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | 0.18 | 0.21 | 0.42 | 0.24 | <LOD | <LOD | <LOD | 0.25 | <LOD | 0.13 | <LOD | 0.18 | 0.10 | <LOD | <LOD |
| 3 | Fluorene (Fl) | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | 0.32 | <LOD | <LOD | 0.14 | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD |
| 3 | Phenanthrene (Phe) | 1.55 | 0.38 | 0.44 | <LOD | <LOD | <LOD | 0.86 | 0.13 | 0.22 | 5.14 | 0.37 | 0.17 | <LOD | <LOD | 0.61 | 0.46 | 2.24 | <LOD | 0.18 | 0.12 | <LOD | 0.10 |
| 3 | Anthracene (An) | 0.35 | 0.24 | 0.25 | <LOD | 0.11 | <LOD | 0.19 | 0.16 | 0.14 | 1.87 | 0.37 | 0.23 | <LOD | 0.17 | 0.42 | 0.11 | 0.41 | <LOD | 0.34 | 0.17 | 0.16 | 0.14 |
| 4 | Fluoranthene (Flu) | <LOD | 2.09 | 0.12 | <LOD | <LOD | <LOD | <LOD | <LOD | 0.27 | 11.02 | <LOD | <LOD | <LOD | <LOD | <LOD | 0.30 | 4.05 | <LOD | 0.16 | <LOD | <LOD | <LOD |
| 4 | Pyrene (Pyr) | 0.54 | 1.86 | 0.46 | <LOD | <LOD | <LOD | <LOD | <LOD | 0.30 | 9.20 | <LOD | <LOD | <LOD | <LOD | 0.39 | 0.22 | 2.36 | <LOD | 0.37 | <LOD | <LOD | 0.15 |
| 4 | Benz(a)anthracene (BaA) | 1.59 | 1.33 | 0.19 | <LOD | <LOD | <LOD | <LOD | <LOD | 0.14 | 3.88 | 0.13 | <LOD | <LOD | <LOD | 0.24 | 0.13 | 1.36 | <LOD | 0.23 | <LOD | <LOD | 0.78 |
| 4 | Chrysene (Cry) | 2.57 | 1.15 | 0.35 | <LOD | <LOD | <LOD | <LOD | <LOD | 0.26 | 3.14 | 0.30 | <LOD | <LOD | 0.10 | 0.54 | 0.26 | 1.47 | <LOD | 0.48 | <LOD | <LOD | 0.37 |
| 5 | Benzo(b)fluoranthene (BbFlu) | 3.89 | 1.53 | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | 4.17 | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | 1.04 | <LOD | 1.42 | <LOD | <LOD | <LOD |
| 5 | Benzo(k)fluoranthene (BkFlu) | 3.22 | 1.02 | 0.18 | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | 2.80 | 0.17 | <LOD | <LOD | <LOD | 0.66 | 0.12 | 2.14 | <LOD | 1.07 | <LOD | <LOD | <LOD |
| 5 | Benzo(a)pyrene (BaPyr) | 1.86 | 0.66 | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | 1.61 | <LOD | <LOD | <LOD | <LOD | 0.51 | <LOD | 1.68 | <LOD | 0.93 | <LOD | 1.12 | <LOD |
| 5 | Indeno(1,2,3-cd)pyrene (IP) | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD |
| 6 | Dibenz(a,h)anthracene (DahA) | <LOD | <LOD | 0.16 | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD |
| 6 | Benzo(g,h,i)perylene (BghiP) | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD | <LOD |
|  | Total ΣPAH | 16.15 | 10.27 | 2.67 | 0.00 | 0.11 | 0.00 | 1.64 | 1.64 | 2.89 | 44.41 | 2.46 | 0.81 | 0.00 | 0.27 | 3.63 | 1.61 | 17.45 | 0.00 | 5.52 | 0.40 | 1.28 | 1.54 |
|  | ΣLMW PAH | 2.47 | 0.62 | 1.21 | 0.00 | 0.11 | 0.00 | 1.64 | 1.64 | 1.92 | 8.58 | 1.87 | 0.81 | 0.00 | 0.17 | 1.28 | 0.58 | 3.34 | 0.00 | 0.85 | 0.40 | 0.16 | 0.24 |
|  | ΣHMW PAH | 13.68 | 9.65 | 1.46 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.97 | 35.82 | 0.59 | 0.00 | 0.00 | 0.10 | 2.35 | 1.04 | 14.12 | 0.00 | 4.67 | 0.00 | 1.12 | 1.30 |
|  | LMW/HMW | 0.18 | 0.06 | 0.83 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.97 | 0.24 | 3.16 | 0.00 | 0.00 | 1.60 | 0.54 | 0.55 | 0.24 | 0.00 | 0.18 | 0.00 | 0.14 | 0.19 |
|  | Ant/(Ant+Phe) | 0.18 | 0.39 | 0.37 | 0.00 | 0.00 | 0.00 | 0.18 | 0.56 | 0.38 | 0.27 | 0.50 | 0.58 | 0.00 | 0.00 | 0.41 | 0.20 | 0.16 | 0.00 | 0.66 | 0.59 | 0.00 | 0.59 |
|  | Fla/(Fla+Pyr) | 0.00 | 0.53 | 0.20 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.47 | 0.54 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.57 | 0.63 | 0.00 | 0.31 | 0.00 | 0.00 | 0.00 |
|  | Fla/(Fla+Pyr) | 0.00 | 0.53 | 0.20 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.47 | 0.54 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.57 | 0.63 | 0.00 | 0.31 | 0.00 | 0.00 | 0.00 |
|  | BaA/(BaA+Cry) | 0.38 | 0.54 | 0.35 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.35 | 0.55 | 0.30 | 0.00 | 0.00 | 0.00 | 0.30 | 0.34 | 0.48 | 0.00 | 0.32 | 0.00 | 0.00 | 0.68 |
|  | Fla/Pyr | 0.00 | 1.12 | 0.25 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.90 | 1.20 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.35 | 1.72 | 0.00 | 0.44 | 0.00 | 0.00 | 0.00 |
|  | An/(An+Phe) | 0.18 | 0.39 | 0.37 | 0.00 | 0.00 | 0.00 | 0.18 | 0.56 | 0.38 | 0.27 | 0.50 | 0.58 | 0.00 | 0.00 | 0.41 | 0.20 | 0.16 | 0.00 | 0.66 | 0.59 | 0.00 | 0.59 |
|  | Hazard Index | 6.52 | 3.12 | 1.06 | 0.00 | 0.00 | 0.00 | 0.02 | 0.01 | 0.25 | 9.42 | 0.31 | 0.01 | 0.00 | 0.05 | 1.15 | 0.31 | 4.70 | 0.00 | 2.13 | 0.01 | 0.75 | 0.57 |

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