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# Supplementary Information

## Risk Simulation of Soil Contamination by Polycyclic Aromatic Hydrocarbons from Sewage Sludge used as Fertilizers

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**Table S1.** Conditions for the GC-EI-MS-MS analysis of PAHs

| PAHs compounds | Retention time / min | Parent ion / (*m/z*) | Wave-form type | ESL / (*m/z*) | CID amplitude / V |
|---|---|---|---|---|---|
| naphthalene | 9.14 | 128 | Resonant | 56 | 0.6 |
| acenaphthylene | 13.3 | 152 | Resonant | 48 | 0.2 |
| acenaphthene | 13.9 | 153 | Resonant | 67 | 0.2 |
| fluorene | 15.9 | 165 | Resonant | 73 | 0.2 |
| phenanthrene | 19.6 | 178 | Resonant | 78 | 0.2 |
| anthracene | 19.8 | 178 | Resonant | 78 | 0.2 |
| fluoranthene | 24.3 | 202 | Resonant | 89 | 0.2 |
| pyrene | 25.2 | 202 | Resonant | 89 | 0.2 |
| benzo(a)anthracene | 30.7 | 228 | Resonant | 101 | 0.2 |
| chrysene | 30.8 | 228 | Resonant | 101 | 0.2 |
| benzo(b)fluoranthene | 35.8 | 252 | Resonant | 111 | 0.2 |
| benzo(k)fluoranthene | 36.0 | 252 | Resonant | 111 | 0.2 |
| benzo(a)pyrene | 37.2 | 252 | Resonant | 111 | 0.2 |
| indeno(1,2,3-c,d)pyrene | 42.0 | 276 | Resonant | 122 | 0.6 |
| dibenzo(a,h)anthracene | 42.2 | 276 | Resonant | 122 | 0.6 |
| benzo(g,h,i)perylene | 42.9 | 276 | Resonant | 122 | 0.6 |

ESL = excitation storage level. CID = collision induced dissociation.

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**Table S2.** Polycyclic aromatic hydrocarbon (PAH) median, minimum and maximum concentrations in soil samples from the control plots (STEST), (n = 18)

| PAHs | Median / (μg kg$^{-1}$) | Minimum / (μg kg$^{-1}$) | Maximum / (μg kg$^{-1}$) | Occurence |
|---|---|---|---|---|
| naphthalene | < LOQ | < LOD | 6.3 | d.q. |
| acenaphthylene | < LOD | < LOD | < LOD | n.d. |
| acenaphthene | < LOD | < LOD | 1.3 | d.q. |
| fluorene | < LOQ | < LOD | 1.8 | d.q. |
| phenanthrene | 1.0 | < LOD | 3.7 | d.q. |
| anthracene | < LOQ | < LOD | 1.3 | d.q. |
| fluoranthene | < LOQ | < LOD | 1.9 | d.q. |
| pyrene | < LOD | < LOD | 1.5 | d.q. |
| benzo(a)anthracene | < LOQ | < LOD | 3.0 | d.q. |
| chrysene | < LOQ | < LOD | 2.3 | d.q. |
| benzo(b)fluoranthene | < LOQ | < LOD | < LOQ | d.n.q. |
| benzo(k)fluoranthene | < LOD | < LOD | < LOQ | d.n.q. |
| benzo(a)pyrene | < LOD | < LOD | < LOD | n.d. |
| indeno(1,2,3-c,d)pyrene | < LOD | < LOD | 4.5 | d.q. |
| dibenzo(a,h)anthracene | < LOD | < LOD | < LOQ | d.n.q. |
| benzo(g,h,i)perylene | < LOD | < LOD | < LOD | n.d. |

LOD = limit of detection; LOQ = limit of quantification; d.q. = detected and quantified; d.n.q. = detected and not quantified; n.d. = not detected.

**Table S3.** Polycyclic aromatic hydrocarbon (PAH) median, minimum and maximum concentrations in soil samples from the sewage sludge (SS) treated plots (SDL1N), n = 18

| PAHs | Median / (μg kg$^{-1}$) | Minimum / (μg kg$^{-1}$) | Maximum / (μg kg$^{-1}$) | Occurence |
|---|---|---|---|---|
| naphthalene | < LOQ | < LOQ | 3.27 | d.q. |
| acenaphthylene | < LOD | < LOD | < LOQ | d.n.q. |
| acenaphthene | < LOQ | < LOD | 1.66 | d.q. |
| fluorene | < LOQ | < LOD | 1.54 | d.q. |
| phenanthrene | 1.6 | < LOD | 2.74 | d.q. |
| anthracene | < LOQ | < LOD | 2.04 | d.q. |
| fluoranthene | 0.76 | < LOD | 2.81 | d.q. |
| pyrene | < LOD | < LOD | 2.63 | d.q. |
| benzo(a)anthracene | < LOQ | < LOD | 3.32 | d.q. |
| chrysene | 1.6 | < LOD | 4.47 | d.q. |
| benzo(b)fluoranthene | < LOQ | < LOD | 6.45 | d.q. |
| benzo(k)fluoranthene | < LOD | < LOD | < LOQ | d.n.q. |
| benzo(a)pyrene | < LOD | < LOD | < LOQ | d.n.q. |
| indeno(1,2,3-c,d)pyrene | < LOD | < LOD | 5.52 | d.q. |
| dibenzo(a,h)anthracene | < LOD | < LOD | 3.26 | d.q. |
| benzo(g,h,i)perylene | < LOD | < LOD | 3.34 | d.q. |

LOD = limit of detection; LOQ = limit of quantification; d.q. = detected and quantified; d.n.q. = detected and not quantified; n.d. = not detected.

**Table S4.** Polycyclic aromatic hydrocarbon (PAH) median, minimum and maximum concentrations in soil samples from the sewage sludge (SS) treated plots (SDL8N), n = 18

| PAHs | Median / (μg kg$^{-1}$) | Minimum / (μg kg$^{-1}$) | Maximum / (μg kg$^{-1}$) | Occurence |
|---|---|---|---|---|
| naphthalene | < LOQ | < LOD | < LOQ | d.n.q. |
| acenaphthylene | < LOQ | < LOD | 2.4 | d.q. |
| acenaphthene | < LOQ | < LOD | 2.2 | d.q. |
| fluorene | < LOQ | < LOD | 1.8 | d.q. |
| phenanthrene | 2.9 | < LOD | 3.9 | d.q. |
| anthracene | 1.5 | < LOD | 2.4 | d.q. |
| fluoranthene | < LOD | < LOD | 4.4 | d.q. |
| pyrene | < LOD | < LOD | 3.3 | d.q. |
| benzo(a)anthracene | 3.8 | < LOD | 5.0 | d.q. |
| chrysene | 6.7 | < LOD | 10.4 | d.q. |
| benzo(b)fluoranthene | 9.6 | < LOD | 11.65 | d.q. |
| benzo(k)fluoranthene | < LOQ | < LOD | 8.0 | d.q. |
| benzo(a)pyrene | < LOQ | < LOD | < LOQ | d.n.q. |
| indeno(1,2,3-c,d)pyrene | 7.3 | < LOD | 14.0 | d.q. |
| dibenzo(a,h)anthracene | < LOQ | < LOD | 11.0 | d.q. |
| benzo(g,h,i)perylene | 6.4 | < LOD | 10.2 | d.q. |

LOD = limit of detection; LOQ = limit of quantification; d.q. = detected and quantified; d.n.q. = detected and not quantified; n.d. = not detected.

**Table S5.** Polycyclic aromatic hydrocarbon (PAH) median, minimum and maximum concentrations in the sewage sludge used in SDL1N and SDL8N plots, n = 18

| PAHs | Average / (μg kg$^{-1}$) | Minimum / (μg kg$^{-1}$) | Median / (μg kg$^{-1}$) | Maximum / (μg kg$^{-1}$) |
|---|---|---|---|---|
| naphthalene | 51.65 | 20.6 | 49.35 | 88.8 |
| acenaphthylene | 13.52 | < LOD | < LOD | 81.1 |
| acenaphthene | 33.07 | < LOD | 33.5 | 80.8 |
| fluorene | 74.55 | < LOD | 79.65 | 124.3 |
| phenanthrene | 387.42 | 84.5 | 415.7 | 622.9 |
| anthracene | 25.27 | 8.8 | 15.4 | 82.0 |
| fluoranthene | 78.52 | < LOD | 93.4 | 123.3 |
| pyrene | < LOD | < LOD | < LOD | 161.7 |
| benzo(a)anthracene | 41.05 | < LOD | 43.25 | 90.5 |
| chrysene | 112.93 | 62.2 | 103.2 | 173.4 |
| benzo(b)fluoranthene | 107.95 | < LOD | 123.15 | 183.0 |
| benzo(k)fluoranthene | 47.32 | < LOD | 47.8 | 100.5 |
| benzo(a)pyrene | 143.93 | 83.5 | 157.3 | 175.2 |
| indeno(1,2,3-c,d)pyrene | 52.57 | < LOD | 35.65 | 122.2 |
| dibenzo(a,h)anthracene | 18.13 | < LOD | 6.05 | 81.3 |
| benzo(g,h,i)perylene | 63.37 | < LOD | 42.7 | 176.2 |

**Table S6.** Simulation of soil PAH concentrations after ten years of yearly successive applications of sewage sludge rates and simulation of soil PAH limit concentrations in μg $kg^{-1}$

| PAHs | $C_0^{PAH}$ | $C_{10}^{PAH}$ | $C_\infty^{PAH}$ |
|---|---|---|---|
| naphthalene | 1.83 | 1.84 | 1.84 |
| acenaphthylene | 0.50 | 0.51 | 0.51 |
| acenaphthene | 1.22 | 1.33 | 1.33 |
| fluorene | 2.77 | 2.81 | 2.81 |
| phenanthrene | 14.47 | 20.16 | 20.16 |
| anthracene | 0.94 | 2.22 | 2.23 |
| fluoranthene | 2.94 | 6.71 | 6.73 |
| pyrene | 1.54 | 9.03 | 12.18 |
| benzo(a)anthracene | 1.54 | 4.79 | 4.90 |
| chrysene | 4.24 | 17.33 | 18.79 |
| benzo(b)fluoranthene | 4.05 | 11.74 | 11.93 |
| benzo(k)fluoranthene | 1.78 | 11.04 | 15.93 |
| benzo(a)pyrene | 5.40 | 14.11 | 14.23 |
| indeno(1,2,3-c,d)pyrene | 1.97 | 6.53 | 6.74 |
| dibenzo(a,h)anthracene | 0.68 | 2.69 | 2.88 |
| benzo(g,h,i)perylene | 2.38 | 7.23 | 7.38 |
| $\sum_{j=1-16} PAH_j$ | 48.25 | 120.07 | 130.57 |