# Supporting information for

# A review of the predictive models estimating association of neutral and ionizable organic chemicals with dissolved organic carbon

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## S1. LSER descriptors and Log $K_{OW}$ of the target contaminants

**Table S1.** LSER descriptors and Log $K_{OW}$ of the target chemicals.

| Chemical | CAS | E[1] | S[1] | A[1] | B[1] | V[1] | Log $K_{OW}$[2] |
|---|---|---|---|---|---|---|---|
| **PCBs** | | | | | | | |
| PCB 1 | 2051-60-7 | 1.48 | 1.97 | 0.00 | 0.20 | 1.45 | 1.48 |
| PCB 15 | 2050-68-2 | 1.65 | 1.18 | 0.00 | 0.16 | 1.57 | 1.65 |
| PCB 28 | 7012-37-5 | 1.76 | 1.33 | 0.00 | 0.15 | 1.69 | 1.76 |
| PCB 52 | 35693-99-3 | 1.90 | 1.48 | 0.00 | 0.15 | 1.81 | 1.90 |
| PCB 101 | 37680-73-2 | 2.04 | 1.61 | 0.00 | 0.13 | 1.94 | 2.04 |
| PCB 153 | 35065-27-1 | 2.18 | 1.74 | 0.00 | 0.11 | 2.06 | 2.18 |
| PCB 180 | 35065-29-3 | 2.29 | 1.87 | 0.00 | 0.09 | 2.18 | 2.29 |
| PCB 201 | 40186-71-8 | 2.43 | 2.00 | 0.00 | 0.06 | 2.30 | 2.43 |
| PCB 206 | 53742-07-7 | 2.60 | 2.13 | 0.00 | 0.04 | 2.43 | 2.60 |
| PCB 209 | 2051-24-3 | 2.72 | 2.26 | 0.00 | 0.02 | 2.55 | 2.72 |
| **PAHs** | | | | | | | |
| Naphthalene | 91-20-3 | 1.34 | 0.92 | 0.00 | 0.20 | 1.09 | 3.45 |
| Anthracene | 120-12-7 | 2.29 | 1.34 | 0.00 | 0.28 | 1.45 | 4.68 |
| Pyrene | 129-00-0 | 2.81 | 1.71 | 0.00 | 0.28 | 1.58 | 5.17 |
| Benzo[a]pyrene | 50-32-8 | 3.63 | 1.96 | 0.00 | 0.37 | 1.95 | 6.40 |
| Benzo[g,h,i]perylene | 191-24-2 | 4.07 | 1.90 | 0.00 | 0.45 | 2.08 | 6.89 |

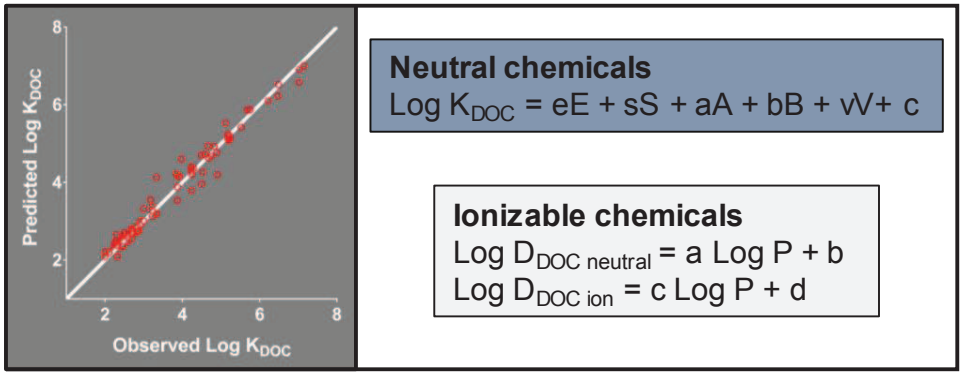
[1]UFZ-LSER database (Ulrich *et al.*, 2017). [2]ChemSpider database (2018), using predicted values by ACD software.

**References**

ChemSpider, 2018. ChemSpider database [Internet]. Accessed on 03.01.2019. Available from http://www.chemspider.com/

Ulrich, N., Endo, S., Brown, T.., Watanabe, N., Bronner, G., Abraham, M.., Goss, K., 2017. UFZ-LSER database v 3.2.1 [Internet], Leipzig, Germany, Helmholtz Centre for Environmental Research-UFZ. Accessed on 27.10.2018. Available from http://www.ufz.de/lserd

**Paper IV: Predicting dissolved organic carbon partition and distribution coefficients of neutral and ionizable organic chemicals**

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*Science of The Total Environment* 658 (2019), 1056-1063

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