Chemical composition and potential environmental impacts of water-soluble polar crude oil components inferred from ESI FT-ICR-MS

Supporting Information

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Log K_{ow} Estimation Method

We used the estimated octanol-water partition coefficients (log K_{ow}) of a series of pre-selected chemical structures to guide our further data interpretation. A total of 214 heteroatom-containing organic compounds were selected for estimating relationships between log K_{ow} and NSO:C (see examples in S4 Fig.). Log K_{ow} values and corresponding water solubility (S) values were estimated using the Estimation Program Interface (EPI) Suite obtained from the United States Environmental Protection Agency (EPA) (http://www.epa.gov/opptintr/exposure/pubs/episuite.htm) [1]. The KOWWIN package in the EPI suite estimated log K_{ow} based on the atom/fragment contribution method [2]. For example, 1-nitropyrene ($C_{16}H_9NO$) has 16 aromatic carbons and 1 nitro group fragment. Therefore, its log K_{ow} can be calculated as follows:

$$\log K_{ow\ \text{1-nitropyrene}} = 16 \times A + 1 \times B + 0.2290 \quad (1)$$

where A is the coefficient for an aromatic carbon (0.2940) and B is the coefficient for a nitro group (-0.1823) (see S3 Table). Hence, the log K_{ow} for 1-nitropyrene is 4.75. Experimentally determined log K_{ow} values were used when available from the EPI suite.

As shown above, heteroatom-containing functional groups tend to contribute negatively to the log K_{ow} calculation. A lower log K_{ow} corresponds to higher aqueous solubility. A significant correlation between log K_{ow} and NSO:C was observed (Pearson's $r = -0.81$, $p < 0.001$; S6 Fig.). Therefore, high NSO:C is expected to yield lower log K_{ow}. A linear regression relationship can be developed within the NSO:C range considered in this study (2).

$$\log K_{ow} = 5.81 - 9.48(\text{NSO:C}) \quad (2)$$

REFERENCES

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