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Chemical structure-based predictive model for the oxidation of trace organic contaminants by sulfate radical

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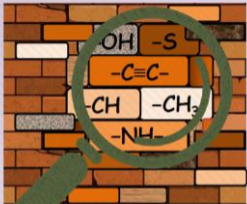
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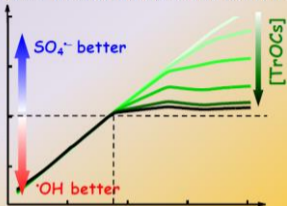
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Group Contribution Method

TrOCs in environmental matrix



Removal efficiency
 $\text{SO}_4^{\cdot-}$ vs. $\cdot\text{OH}$



ethanol:



$$k_{\text{SO}_4^{\cdot-}} = a_0 + a_{-\text{CH}_3} \times n_{-\text{CH}_3} + \dots$$

0.28
 $k_{\text{SO}_4^{\cdot-}} / k_{\text{HO}^{\cdot}}$

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