Environmental Science: Advances

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Development of diffusive gradients in thin-films with mixed binding gels for *in situ* monitoring of artificial sweeteners in waters

Hussain Ijaz, Jin-Xin Zi, Si-Si Liu,^{*} Qi-Si Cai, Sheng-Ming Cheng, Zong-Xi Zhao, Guang-Guo Ying, Andy J. Sweetman and Chang-Er Chen^{*}

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Shiwei Xie, Zhengkang Bai, Wei Shao, Chen Wang, Jianglong Qin, Ze Liu and Peng Liao*





PAPERS

 $\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \\ S_{31} & S_{32} \\ \vdots & \vdots \\ S_{m1} & S_{m2} \end{pmatrix}$

M₂ M₃ : $... S_{N_1}$ $... S_{N_2}$ $... S_{N_3}$

S.



 $S_{ij} =$ SMILES fragment CW = correlation weight

Henry's law constant = $C_0 + C_1 \times \sum CW(S_{ij})$

Monte Carlo method –

 $\begin{array}{c} CW(S_{11}) & CW(S_{12}) & \dots & CW(S_{N_1}) \\ CW(S_{21}) & CW(S_{22}) & \dots & CW(S_{N_2}) \\ CW(S_{31}) & CW(S_{32}) & \dots & CW(S_{N_2}) \end{array}$

 $CW(S_{m1})$ $CW(S_{m2})$... $CW(S_{N_m})$

Investigating the urinary concentrations and distribution of phthalate metabolites in cow urine distillate in India

Sachin B. Jorvekar, Jaya Ajay Singh, Manthan Sharma, Gayatri Narkhede, Rahul Moriya, Dhanashri Pimpare and Roshan M. Borkar*

Does the accounting of the local symmetry fragments in SMILES improve the predictive potential of the QSPR-model for Henry's law constants?

Andrey A. Toropov, Alla P. Toropova,* Alessandra Roncaglioni and Emilio Benfenati