

Environmental Science: Advances

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Cover

See Si-Si Liu, Chang-Er Chen *et al.*, pp. 837–847. Image reproduced by permission of Si-Si Liu from *Environ. Sci.: Adv.*, 2023, 2, 837.

PAPERS

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

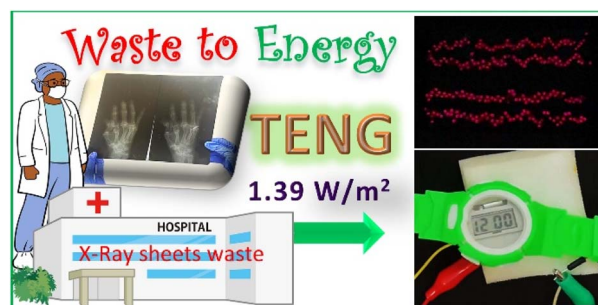
Hussain Ijaz, Jin-Xin Zi, Si-Si Liu,* Qi-Si Cai, Sheng-Ming Cheng, Zong-Xi Zhao, Guang-Guo Ying, Andy J. Sweetman and Chang-Er Chen*



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A medical waste X-ray film based triboelectric nanogenerator for self-powered devices, sensors, and smart buildings

M. Navaneeth, Supraja Potu, Anjaly Babu, Rakesh Kumar Rajaboina,* Uday Kumar K, Haranath Divi, Prakash Kodali and Balaji K.



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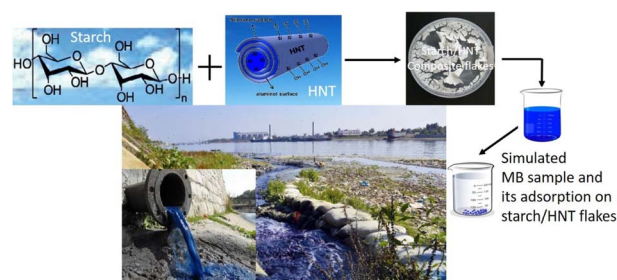
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A starch based sustainable bio-hybrid composite for surface assimilation of methylene blue: preparation, characterization, and adsorption study

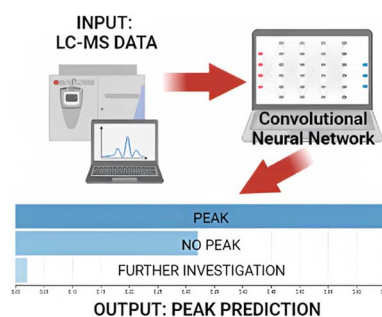
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Application of deep learning to support peak picking during non-target high resolution mass spectrometry workflows in environmental research

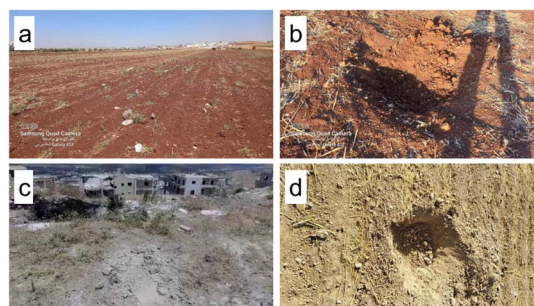
Kate Mottershead and Thomas H. Miller*



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A baseline survey of potentially toxic elements in the soil of north-west Syria following a decade of conflict

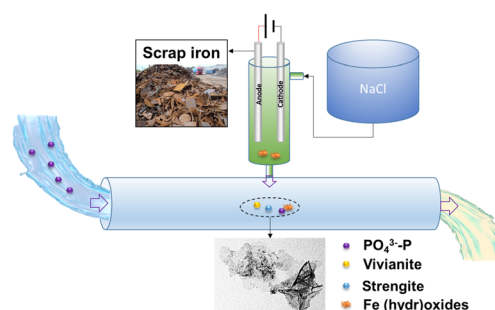
Miassar Alhasan, Abdulkarim Lakmes, Mohammad Gazy Alobaidy, Safwan AlHaeek, Muhammed Assaf, Lorna Dawson, Duncan Pirrie, Ziad Abdeldayem and Jonathan Bridge*



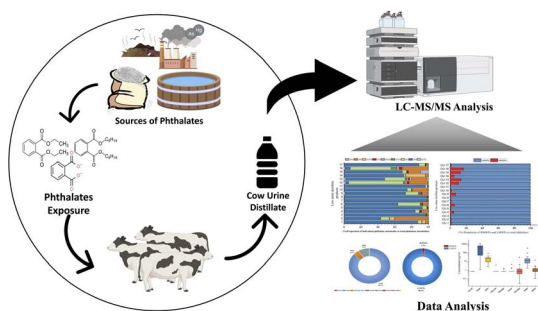
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Phosphate removal by *ex situ* generated Fe (hydr) oxides from scrap iron electrocoagulation: the critical role of coprecipitation

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



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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*

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M = molecule
 S_j = SMILES fragment
 CW = correlation weight

$$\begin{pmatrix} M_1 \\ M_2 \\ M_3 \\ \vdots \\ M_m \end{pmatrix} \rightarrow \begin{pmatrix} S_{11} & S_{12} & \dots & S_{N_1} \\ S_{21} & S_{22} & \dots & S_{N_2} \\ S_{31} & S_{32} & \dots & S_{N_3} \\ \vdots & \vdots & \ddots & \vdots \\ S_{m1} & S_{m2} & \dots & S_{N_m} \end{pmatrix} \xrightarrow{\text{Monte Carlo method}} \begin{pmatrix} CW(S_{11}) & CW(S_{12}) & \dots & CW(S_{N_1}) \\ CW(S_{21}) & CW(S_{22}) & \dots & CW(S_{N_2}) \\ CW(S_{31}) & CW(S_{32}) & \dots & CW(S_{N_3}) \\ \vdots & \vdots & \ddots & \vdots \\ CW(S_{m1}) & CW(S_{m2}) & \dots & CW(S_{N_m}) \end{pmatrix}$$

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

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

