**Facile synthesis of MIL-100 metal-organic framework via heatless technique**

 **for the adsorptive treatment of cationic and anionic pollutants**

K.L. Tan, K.Y. Foo\*

River Engineering and Urban Drainage Research Center (REDAC)

Universiti Sains Malaysia, 14300 Nibong Tebal,

Penang, Malaysia

\*Corresponding author: Tel: +60 45996539, Fax: +60 45996926

E-mail: k.y.foo@usm.my (K.Y. Foo)

**Table S1**:Molecular **s**tructure and physicochemical properties of MB and NPX.

|  |  |  |
| --- | --- | --- |
| **Property** | **MB** | **NPX** |
| Chemical formula | C16H18ClN3S | C14H14O3 |
| Category (sub-category) | Dye (basic dye) | Drug (NSAID) |
| CAS no.  | 61-73-4 | 22204-53-1 |
| Molecular weight | 319.85 | 230.26 |
| Solubility (g/L at 20 °C) | 44  | 0.03  |
| pKa | − | 4.19 |
| Log Kow | 0.75 | 3.18 |
| λmax (nm) | 664 | 232 |
| Molecular size (nm)\* | 1.41 x 0.54 x 0.19 | 1.14 x 0.53 x 0.40 |
| Structure |  |  |
|  |  |  |
|  |  |  |

**\***Measured by Chem3D on MM2 method-optimized configuration.

**Table S2**: Elemental analysis of MIL-100(FeSO4).

|  |  |
| --- | --- |
|  | **Weight% (dry basis)** |
| C | 30.22 |
| H |  1.55 |
| N |  0.00 |
| S |  0.14 |
| (O+Ash)\* | 68.09 |
|  |  |

\*Estimated by difference.

**Table S3**: Compositions of the simulated MB dye wastewater.

|  |  |  |
| --- | --- | --- |
| **Constituent** | **Concentration (mg/L)** | **Function** |
| MB |  100 | Coloring agent |
| Sodium bicarbonate (NaHCO3) | 1000 | Fixing agent  |
| Sodium carbonate (Na2CO3) | 1000 | Fixing agent |
| Sodium chloride (NaCl) | 1500 | Fixing agent |
| Sodium hydroxide (NaOH) | 1000 | Fabric hydrolysis  |
| Starch  | 2500 | Sizing agent |
| Sulfuric acid (H2SO4) | 1500 | pH neutralization |

**Table S4**:Chemical constituents of the simulated NPX pharmaceutical wastewater.

|  |  |
| --- | --- |
| **Constituent** | **Concentration (mg/L)** |
| NPX | 100 |
| Glucose (C6H12O6) | 400 |
| Iron (II) sulfate (FeSO4) | 15 |
| Magnesium sulfate (MgSO4) | 20 |
| Monopotassium phosphate (KH2PO4) | 20 |
| Sodium acetate (CH3COONa) | 50 |
| Urea (CH4N2O) | 35 |