Electronic Supporting Information

Influence of the Aromatic Surface on the Capacity of Adsorption of VOCs by Magnetite Supported Organic-Inorganic Hybrids


Structural Characterization

PMDI (1)

Figure S1. $^1$H-NMR spectrum of PMDI (1) in DMSO-d$_6$.

Figure S2. $^{13}$C-NMR spectrum of PMDI (1) in DMSO-d$_6$.
Figure S3. FTIR spectrum of PMDI (1), solid, KBr.

Figure S4. $^1$H-NMR spectrum of NDI (2) in DMSO-$d_6$. 
Figure S5. $^{13}$C-NMR spectrum of NDI (2) in DMSO-d$_6$.

Figure S6. FTIR spectrum of NDI (2), solid, KBr.
Figure S7. $^1$H-NMR spectrum of PDI (3) in $\text{D}_2\text{O}/\text{NaOD}$.

Figure S8. $^{13}$C-NMR spectrum of PDI (3) in $\text{D}_2\text{O}/\text{NaOD}$. 
**Figure S9.** FTIR spectrum of PDI (3), solid, KBr.

**PMDI-Fe₃O₄NP**

**Figure S10.** SEM Micrographic of PMDI-Fe₃O₄NP
Figure S11. (A) DLS size distribution and (B) Zeta potential of PMDI-Fe$_3$O$_4$NP in H$_2$O (pH=7.0) at 25°C. Hydrodynamic Size = 295.0 nm. Zeta potential = -43.3 mV.

Figure S12. FTIR of PMDI-Fe$_3$O$_4$NP (KBr).
Figure S13. Thermographic analysis of PMDI-Fe$_3$O$_4$NP.

NDI-Fe$_3$O$_4$NP

Figure S14. SEM Micrographic image of NDI-Fe$_3$O$_4$NP.
Figure S15. (A) DLS size distribution and (B) Zeta potential of NDI-Fe$_3$O$_4$NP in H$_2$O (pH=7.0) at 25°C. Hydrodynamic Size = 300.6 nm. Zeta potential = - 38.3 mV.

Figure S16. FTIR of NDI-Fe$_3$O$_4$NP (KBr).
Figure S17. Thermographic analysis of NDI-Fe$_3$O$_4$NP.

PDI-Fe$_3$O$_4$NP

Figure S18. SEM Micrographic of PDI-Fe$_3$O$_4$NP
Figure S19. (A) DLS size distribution and (B) Zeta potential of NDI-Fe₃O₄NP in H₂O (pH=7.0) at 25°C. Hydrodynamic Size = 335.2 nm. Zeta potential = -51.3 mV.

Figure S20. FTIR of PDI-Fe₃O₄NP (KBr).
**Figure S21.** Thermographic analysis of PDI-$\text{Fe}_3\text{O}_4\text{NP}$.

**Figure S22.** NDI hybrid nanoparticle in the presence (a) and absence (b) of the neodymium magnet.
Determination of number of molecules on FeNPs surface.

TGA curves shows two typical desorption zones for Fe$_3$O$_4$NP: the first zone (between 300-500 ºC) corresponds to physisorbed molecules, the second zone (between 500-1000 ºC) corresponds to chemisorbed molecules, the summary of this two desorption zones is used to determinate the total number of molecules on the surface. Applying the following equations, the number of molecules on a Fe$_3$O$_4$NPs surface can be determinated:

$$N = \frac{\pi D^3 \rho}{6 m_w}$$

$$\frac{1}{N} = \frac{\text{nanoparticles}}{\text{mol Fe}_3\text{O}_4}$$

Where $1/N$ refers to the number of Fe$_3$O$_4$NP for each mol of Fe$_3$O$_4$. $D$ is the average diameter of Fe$_3$O$_4$NP in cm (provided by TEM micrographs), $\rho$ is Fe$_3$O$_4$ density (5.196 g/cm$^3$) and $m_w$ is the molecular weight of Fe$_3$O$_4$ (231.53 g/mol).

In order to improve and clarify the number of substituents, we chose TGA method to determinate conjugation rate against mass loss due to decomposition. Experiments were performed with constant heating rate of 10 ºC/min from room temperature (25 ºC) to 1000 ºC. Using weight loss percentage values it is possible to quantify the number of molecules on Fe$_3$O$_4$NP surface applying previous equations.

<table>
<thead>
<tr>
<th>Weight loss (%)</th>
<th>Molecules on Fe$_3$O$_4$NP surface</th>
<th>$\xi$ (molecules per nm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMDI-Fe$_3$O$_4$NP</td>
<td>45.15</td>
<td>6.26 x 10$^{17}$</td>
</tr>
<tr>
<td>NDI-Fe$_3$O$_4$NP</td>
<td>47.07</td>
<td>2.65 x 10$^{18}$</td>
</tr>
<tr>
<td>PDI-Fe$_3$O$_4$NP</td>
<td>71.02</td>
<td>6.28 x 10$^{17}$</td>
</tr>
</tbody>
</table>

Table S1. Thermogravimetric values of Fe$_3$O$_4$-NPs.

<table>
<thead>
<tr>
<th>BET surface (m$^2$/g)</th>
<th>Maximum absorption (cm$^3$/g)</th>
<th>Pore diameter (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMDI-Fe$_3$O$_4$NP</td>
<td>78.39</td>
<td>118.0</td>
</tr>
<tr>
<td>NDI-Fe$_3$O$_4$NP</td>
<td>79.07</td>
<td>233.0</td>
</tr>
<tr>
<td>PDI-Fe$_3$O$_4$NP</td>
<td>20.67</td>
<td>52.0</td>
</tr>
</tbody>
</table>

Table S2. Values for specific surface BET essays of Fe$_3$O$_4$-NPs.

Calibration Plots

In the following figures we represent the calibration plots obtained for each analyte (VOC). We represent the range of concentration that the linear behavior
is maintained. Higher concentrations provoke the saturation of the tube and were used for the experiments where two tubes were connected in series and to measure the % of retention.

**PMDI-Fe₃O₄NP**

**Benzene (4)**

![Graph of Benzene (4)](image)

**Toluene (5)**

![Graph of Toluene (5)](image)

**Ethyl benzene (6)**
**Propyl benzene (7)**

**Butyl benzene (8)**

**Ethyl acetate (10)**
Propyl acetate (11)

Butyl acetate (12)

NDI-Fe$_3$O$_4$NP
**Butyl benzene (8)**

**Ethyl acetate (10)**

**Propyl acetate (11)**
**Butyl acetate (12)**

**PDI-Fe₃O₄NP**

**Benzene (4)**
**Toluene (5)**

![Graph for Toluene]

**Ethyl benzene (6)**

![Graph for Ethyl benzene]

**Propyl benzene (7)**

![Graph for Propyl benzene]

**Butyl benzene (8)**
**Butyl benzene**

![Graph showing the relationship between mg Butyl benzene and Area](image)

**Ethyl acetate (10)**

![Graph showing the relationship between mg Ethyl acetate and Area](image)

**Propyl acetate (11)**

![Graph showing the relationship between mg Propyl acetate and Area](image)
Butyl acetate (12)