

Supporting Information

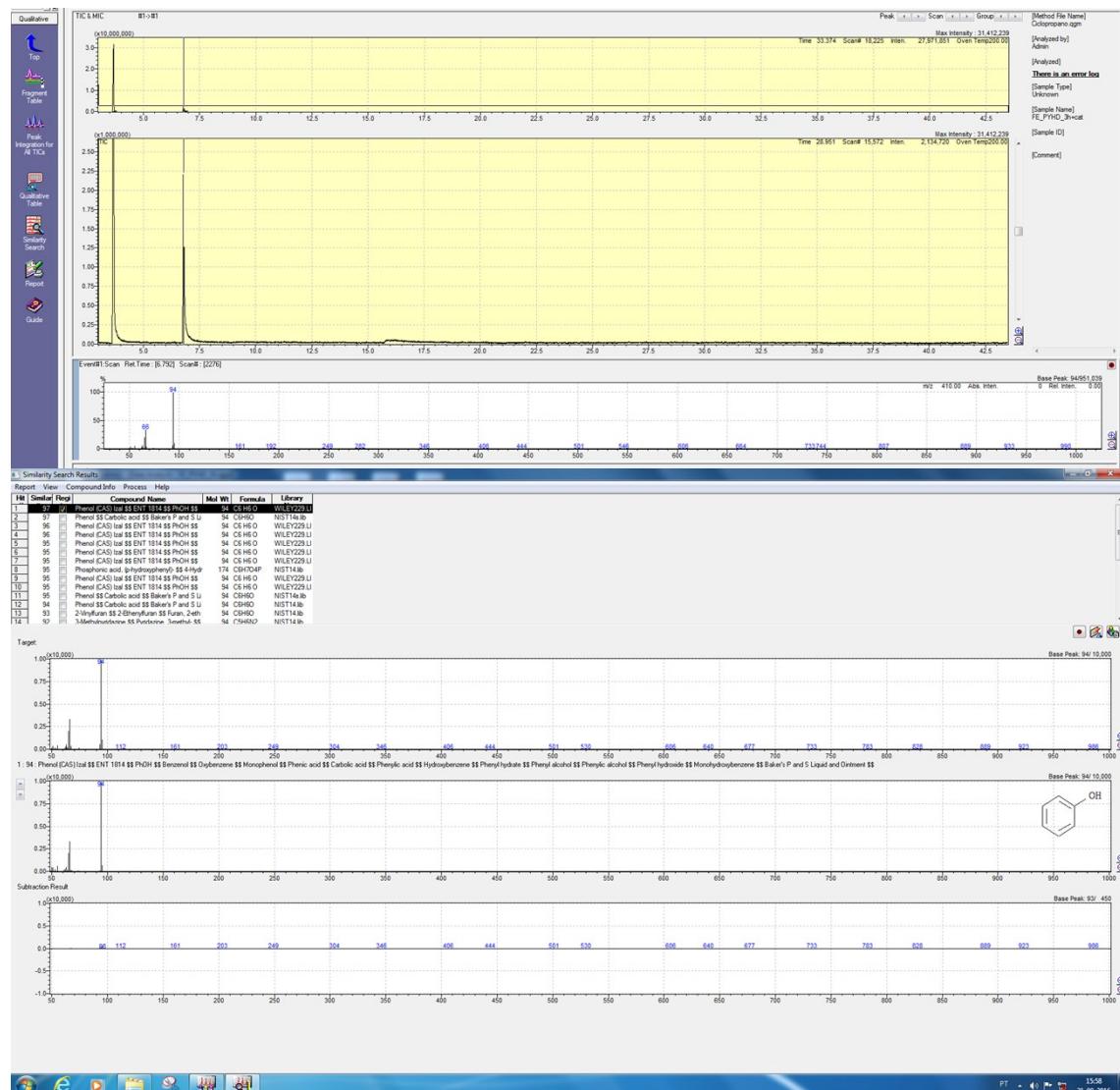


Fig. S1. Chromatogram obtained for the oxidation of benzene with hydrogen peroxide using $[\text{Fe}(\text{pyhd})\text{Cl}_2]$ as homogeneous catalyst after 3 hours of reaction at 50°C in acetonitrile, mass spectra for the major product peak at 6.8 min and result of corresponding search in the data base.

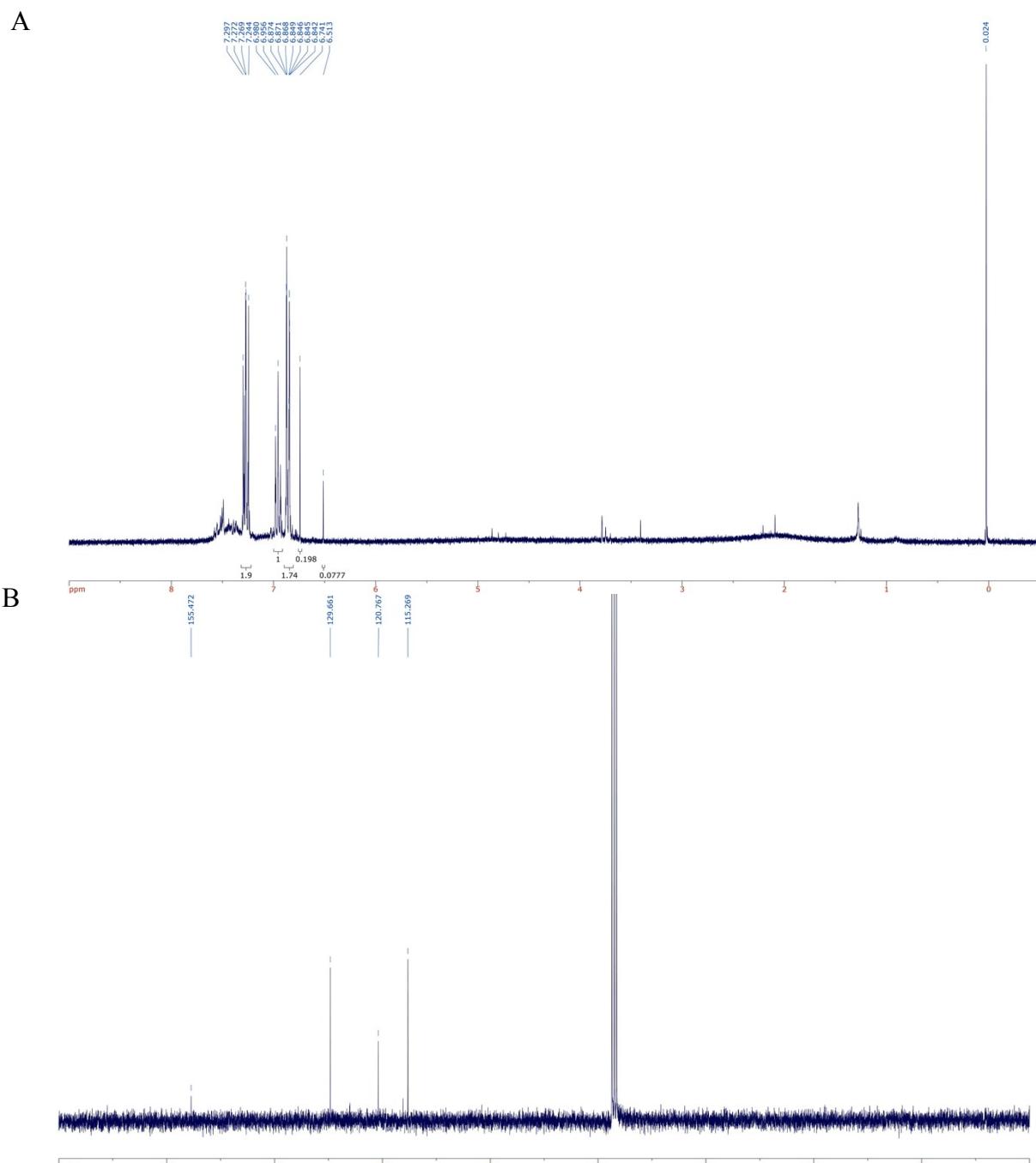


Fig. S2. NMR spectra in CDCl_3 for the phenol isolated by column chromatography using as eluent 20 petroleum ether: 80 ethyl acetate from the oxidation of benzene with hydrogen peroxide using $[\text{Fe}(\text{pyhd})\text{Cl}_2]$ as homogeneous catalyst after 3 hours of reaction at 50°C in acetonitrile: (A) ^1H and (B) ^{13}C .

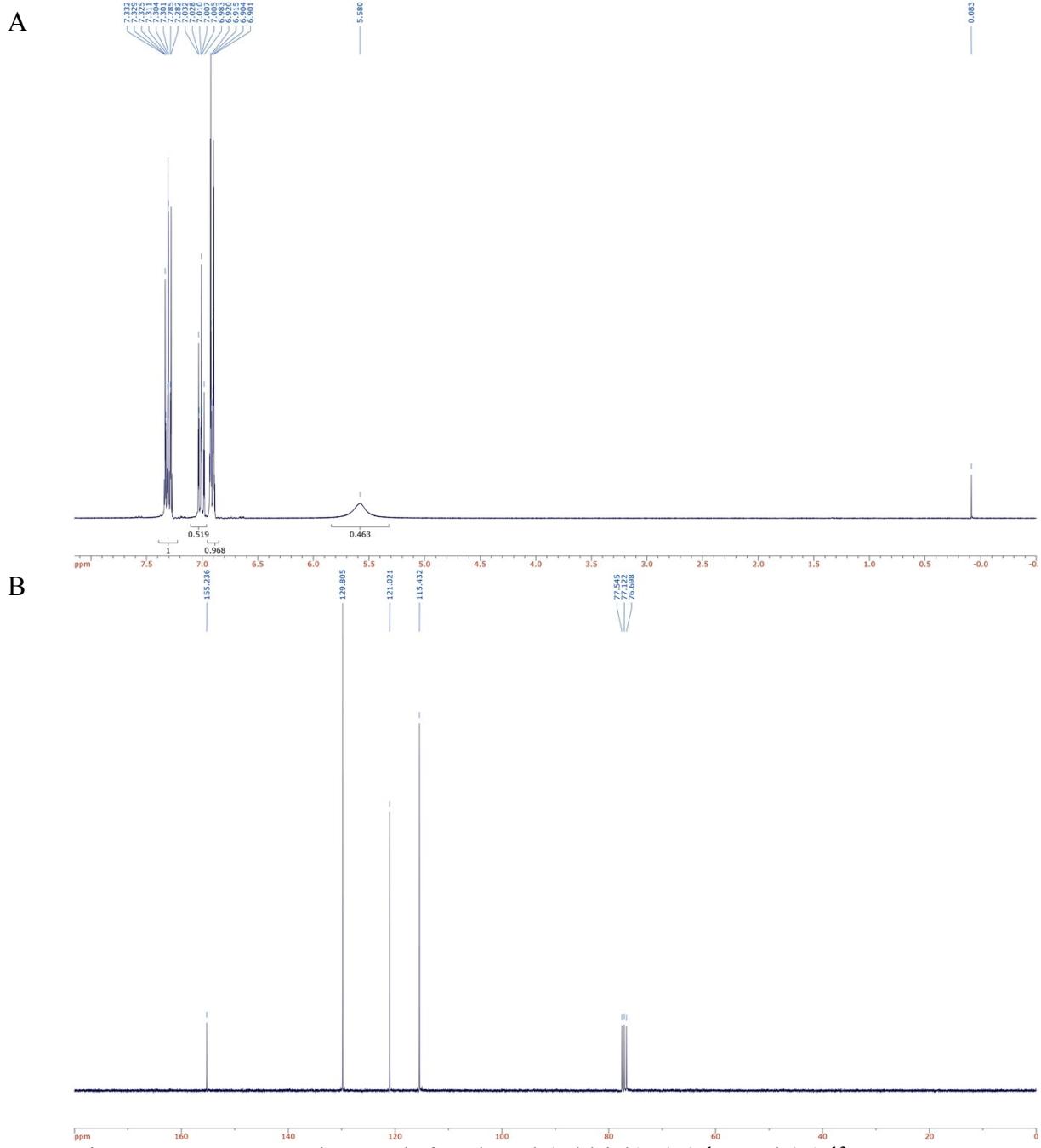


Fig. S3. NMR spectra in CDCl_3 for phenol (Aldrich): (A) ^1H and (B) ^{13}C .

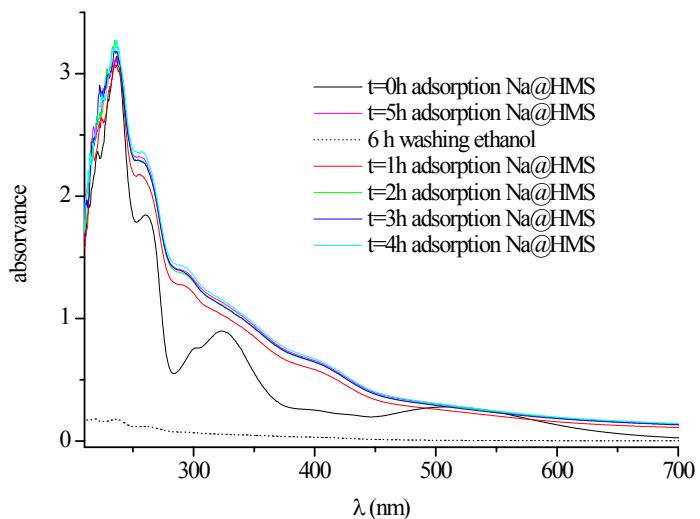
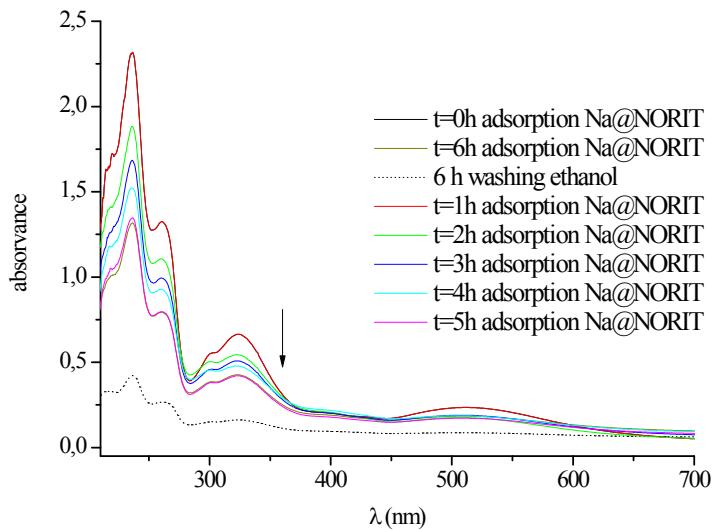


Fig. S4. UV-visible spectra of the adsorption of the [Fe(salhd)Cl] complex onto the Na@HMS and Na@AC materials in ethanol, as well as the washing ethanol solution of both materials.

Table S1. Elemental analysis for the silica and carbon materials

	%C	%H	%N	[Fe(salhd)] ($\mu\text{mol/g}$)
HMS	0.20	0.16		
Na@HMS	0.20	0.83		
[Fe(salhd)]@HMS	0.83	0.51	0.01	26 ^a
AC	86.13	0.55	0.47	
Na@AC	80.94	0.52	0.45	
[Fe(salhd)]@AC	82.13	0.40	0.69	86 ^b

^a Calculated from the variation in the %C, taking into consideration that the [Fe(salhd)] has 20 carbon atoms.

^b Calculated from the variation in the %N, taking into consideration that the [Fe(salhd)] has 2 nitrogen atoms. If the variation in the %C 50 $\mu\text{mol/g}$ of [Fe(salhd)] would be obtained.

Table S2. XPS analysis for the silica and carbon materials

	%C	%O	%Na	%Si	%Cl	%N	%Fe	[Fe(salhd)] ($\mu\text{mol/g}$) ^a
Na@HMS	3.54	68.38	0.02	28.05				
[Fe(salhd)]@HMS	6.86	67.27	0.54	24.27	0.07	0.16	0.83	44
Na@AC	91.75	7.06	0.36		0.09	0.75		
[Fe(salhd)]@AC	94.63	4.29	—		0.14	0.82	0.11	9.0

^a Calculated from the iron atomic%.

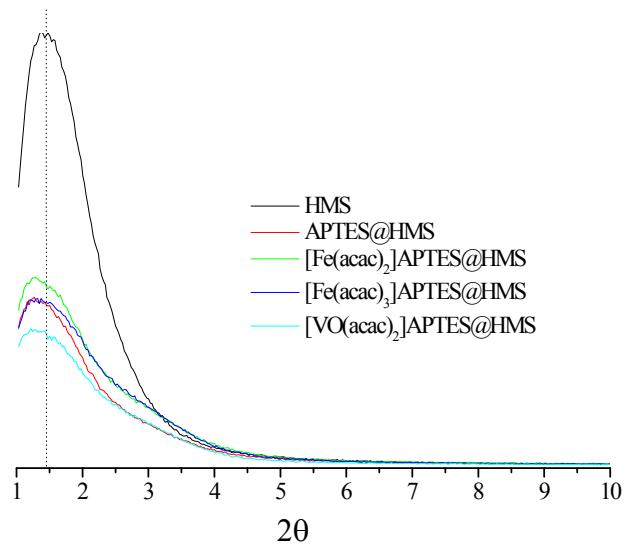


Fig. S5. XRD patterns for the HMS, APTES@HMS, $[\text{Fe}(\text{acac})_2]\text{APTES@HMS}$, $[\text{Fe}(\text{acac})_3]\text{APTES@HMS}$ and $[\text{VO}(\text{acac})_2]\text{APTES@HMS}$

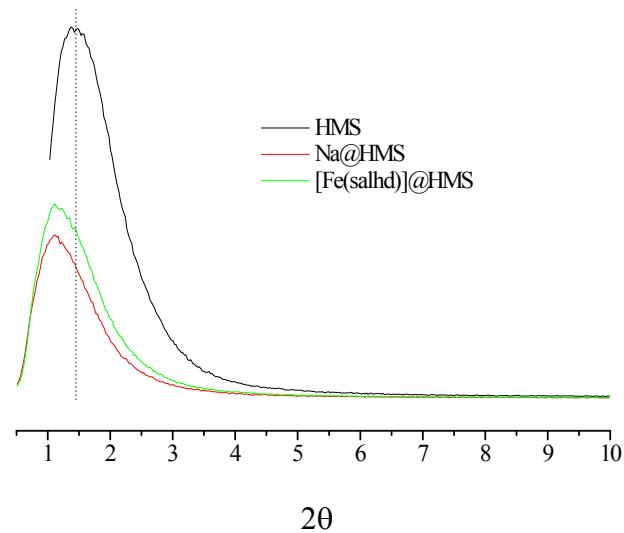


Fig. S6. XRD patterns for the HMS, Na@HMS and $[\text{Fe}(\text{salhd})]\text{@HMS}$ materials.

Table S3. d_{100} spacing and a_0 for the HMS materials

	d_{100} (nm)	a_0 (nm)
HMS	3.2	3.7
APTES@HMS	3.5	4.0
[Fe(acac) ₂]APTES@HMS	3.4	3.9
[Fe(acac) ₃]APTES@HMS	3.6	4.2
[VO(acac) ₂]APTES@HMS	3.6	4.2
Na@HMS	3.9	4.5
[Fe(salhd)]@HMS	3.9	4.5

^a Calculated using the Bragg equation.

^b Calculated using the equation: $a_0 = 2d_{100}/\sqrt{3}$.