

Supporting Information

Antibacterial nitrogen-containing mesostructured SBA-15-type materials: Insight on functional groups and surface polarity

Mohamed Amine Benzaouia,^a Othmane Dardari,^a Ghanem Hamdoun,^a Nadia Katir,^a
Abdelkrim El Kadib.^{a,b,*}

^a Euromed University of Fes, UEMF, Morocco.

^b Hassan II Academy of Science and Technology, Rabat, Morocco.

* Corresponding author

Email: a.elkadib@ueuromed.org

Figure S1. FTIR spectra and UV–Vis absorption spectra of 1-(3-trimethoxysilylpropyl)-4-(4-pyridyl)pyridinium bromide

Figure S2. ¹H NMR of 1-(3-trimethoxysilylpropyl)-4-(4-pyridyl)pyridinium bromide

Figure S3. ¹³C NMR of 1-(3-trimethoxysilylpropyl)-4-(4-pyridyl)pyridinium bromide

Figure S4. FTIR spectrum of organomodified mesoporous SBA-15 and HMDS passivated organosilica

Figure S5. Solid state NMR ¹³C spectra of SBA@NQS^{5%}

Figure S6. High resolution ¹H NMR spectra and COSY spectra of SBA@Pyr^{5%}

Figure S7. Thermogravimetric analysis (TGA) of organomodified mesoporous silica

Figure S8. Nitrogen sorption analysis of organosilica materials

Figure S9. SEM images of SBA@OH and SBA@NH₂^{5%}

Table S1. Quantification of anion exchange sites within the material

Figure S10. Removal of helianthine (methyl orange) using SBA@NQ^{5%} at different concentration.

Figure S11. Quercetin adsorption through organosilica and Quercetin release in water

Figure S1. FTIR spectra and UV–Vis absorption spectra of 1-(3-trimethoxysilylpropyl)-4-(4-pyridyl)pyridinium bromide

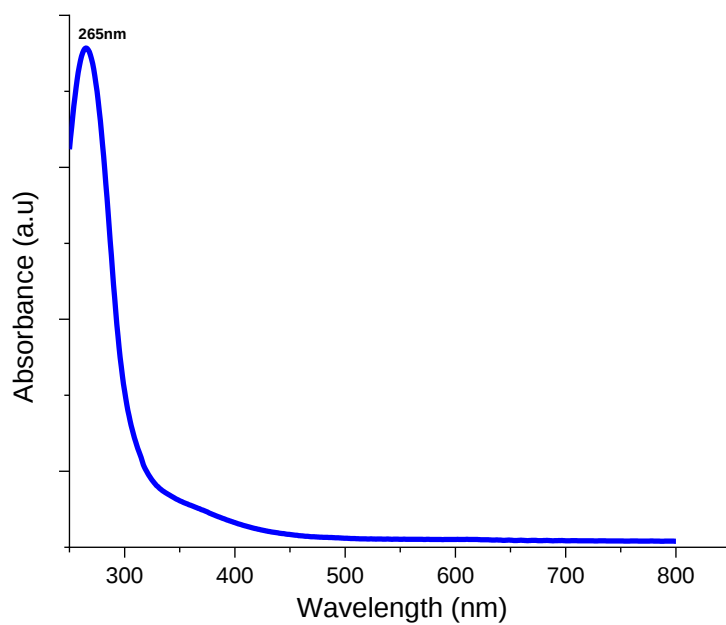
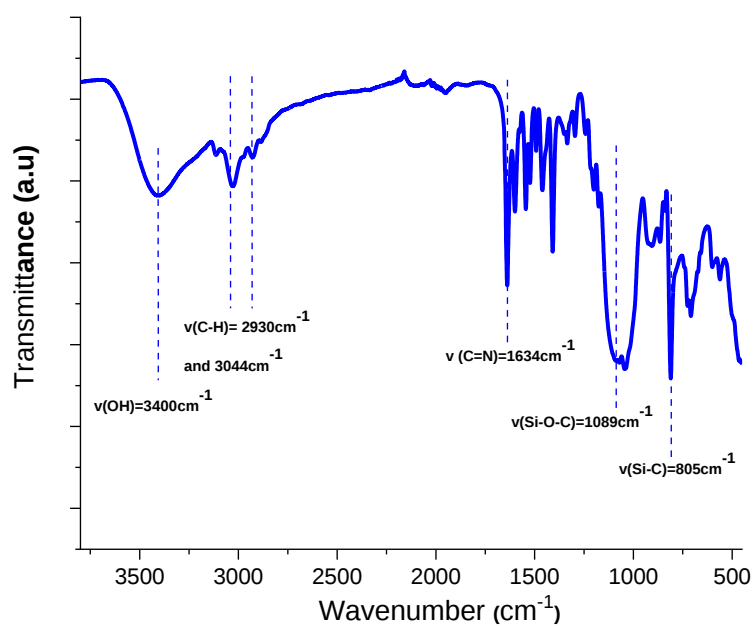
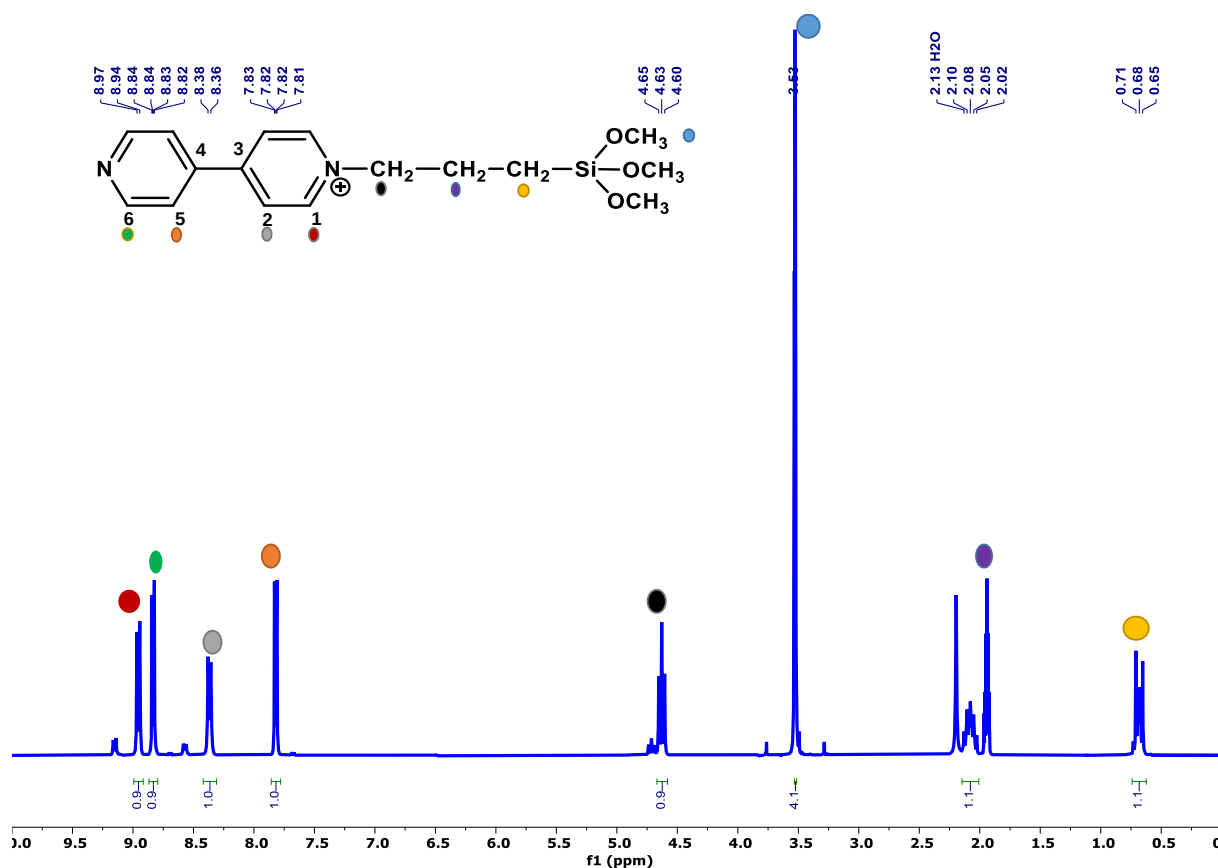
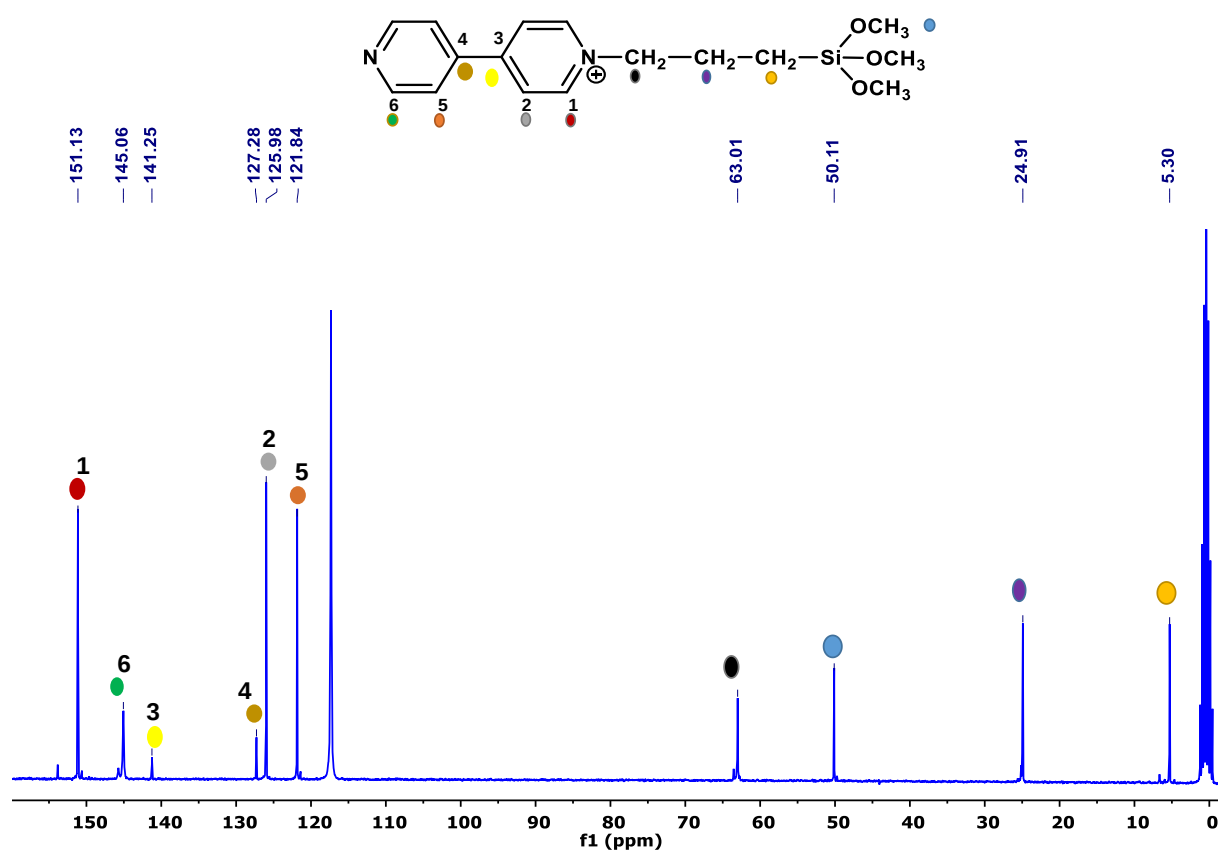


Figure S2. ^1H NMR of 1-(3-trimethoxysilylpropyl)-4-(4-pyridyl)pyridinium bromide



^1H NMR (400 MHz, CD_3CN) δ 0.62-0.74 (m, 2H, $\text{CH}_2\text{-Si}$), 2.01-2.15 (m, 2H, $\text{CH}_2\text{-CH}_2\text{-Si}$), 3.53 (s, 9H, Si-O-CH_3), 4.63 (t, $^3J_{\text{HH}} = 7.3$ Hz, 2H, N-CH_2), 7.78-7.86 (m, 2H, H^5), 8.37 (d, $^3J_{\text{HH}} = 6.9$ Hz, 2H, H^2), 8.80-8.87 (m, 2H, H^6), 8.96 (d, $^3J_{\text{HH}} = 7$ Hz, 2H, H^1).

Figure S3. ^{13}C NMR of 1-(3-trimethoxysilylpropyl)-4-(4-pyridyl)pyridinium bromide



^{13}C NMR (101 MHz, CD_3CN): δ 5.3 ($\text{CH}_2\text{-Si}$), 24.9 ($\text{CH}_2\text{-CH}_2\text{-Si}$), 50.11 (Si-OCH_3), 63 (N-CH_2), 121.84 (C^5), 125.98 (C^2), 127.27 (C^4), 141.25 (C^3), 146.06 (C^6), 151.13 (C^1)

Figure S4. FTIR spectrum of organomodified mesoporous SBA-15 and HMDS passivated organosilica

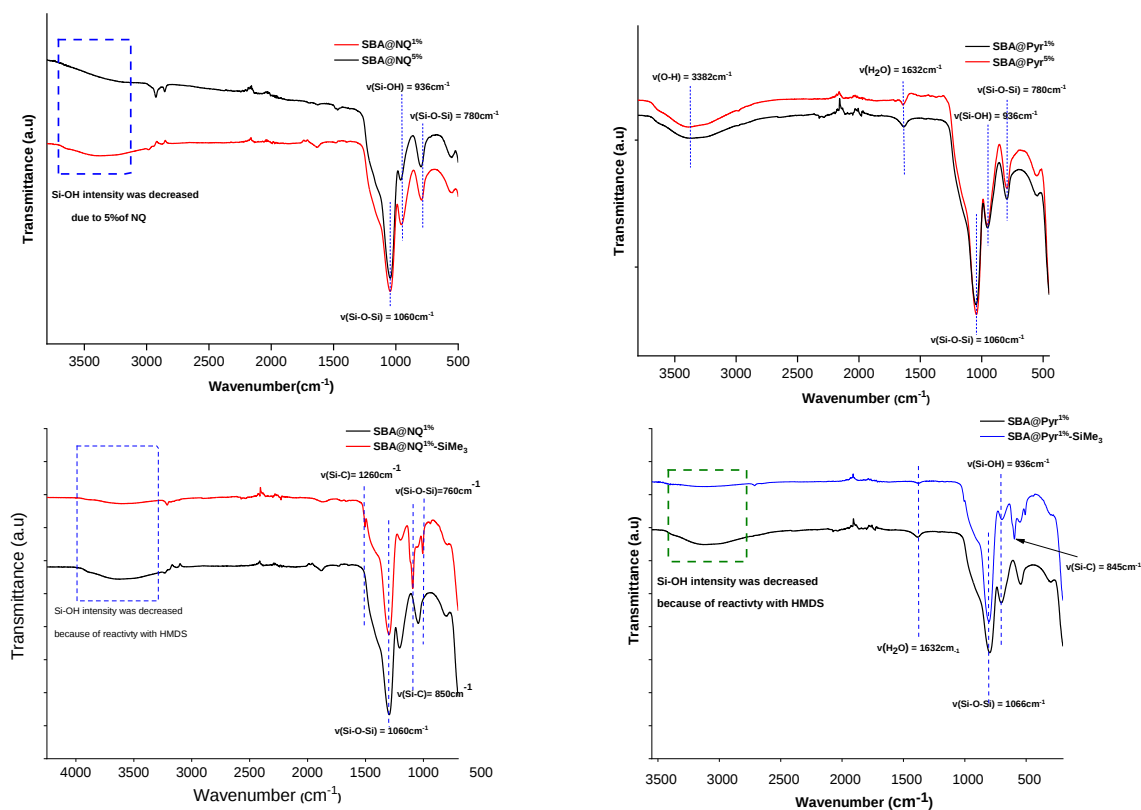


Figure S5. Solid state NMR ^{13}C spectra of SBA@NQ 5%

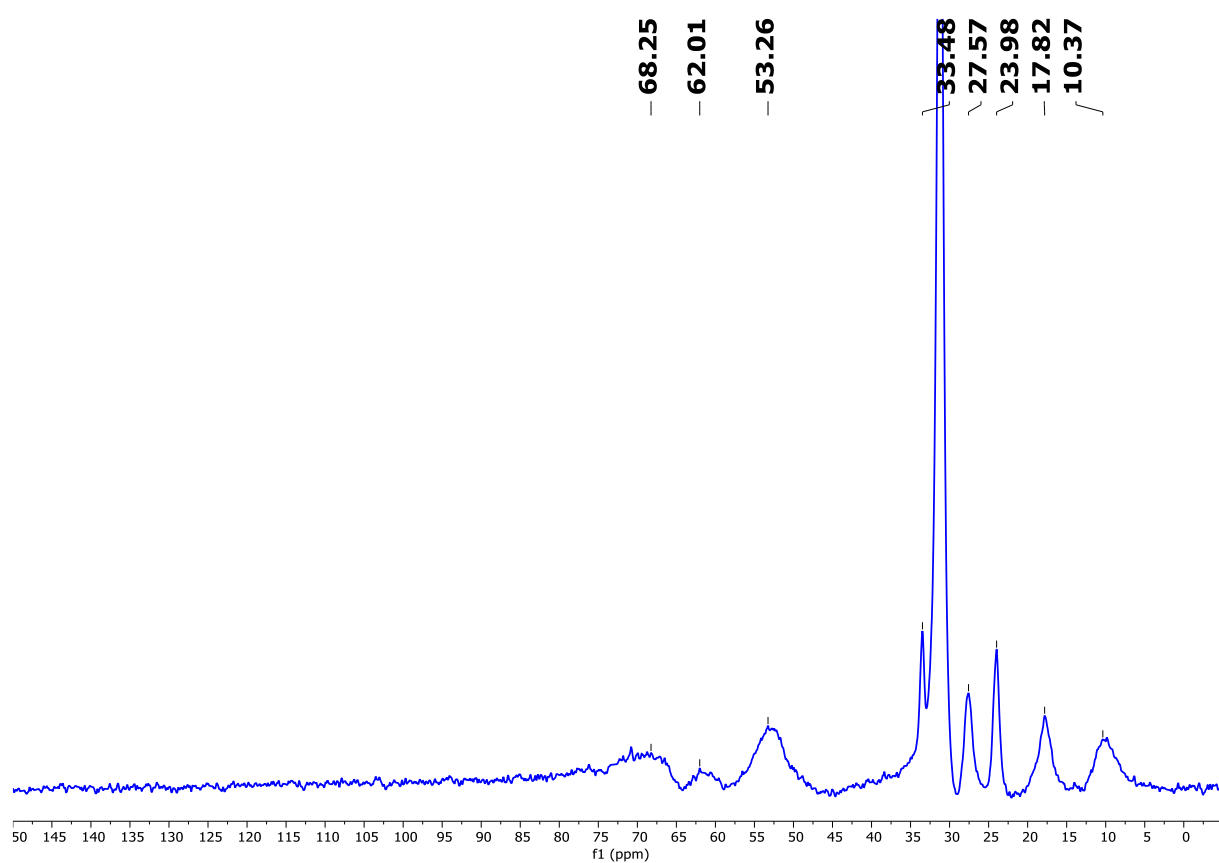


Figure S6. High resolution ^1H NMR spectra and COSY spectra of SBA@Pyr^{5%}

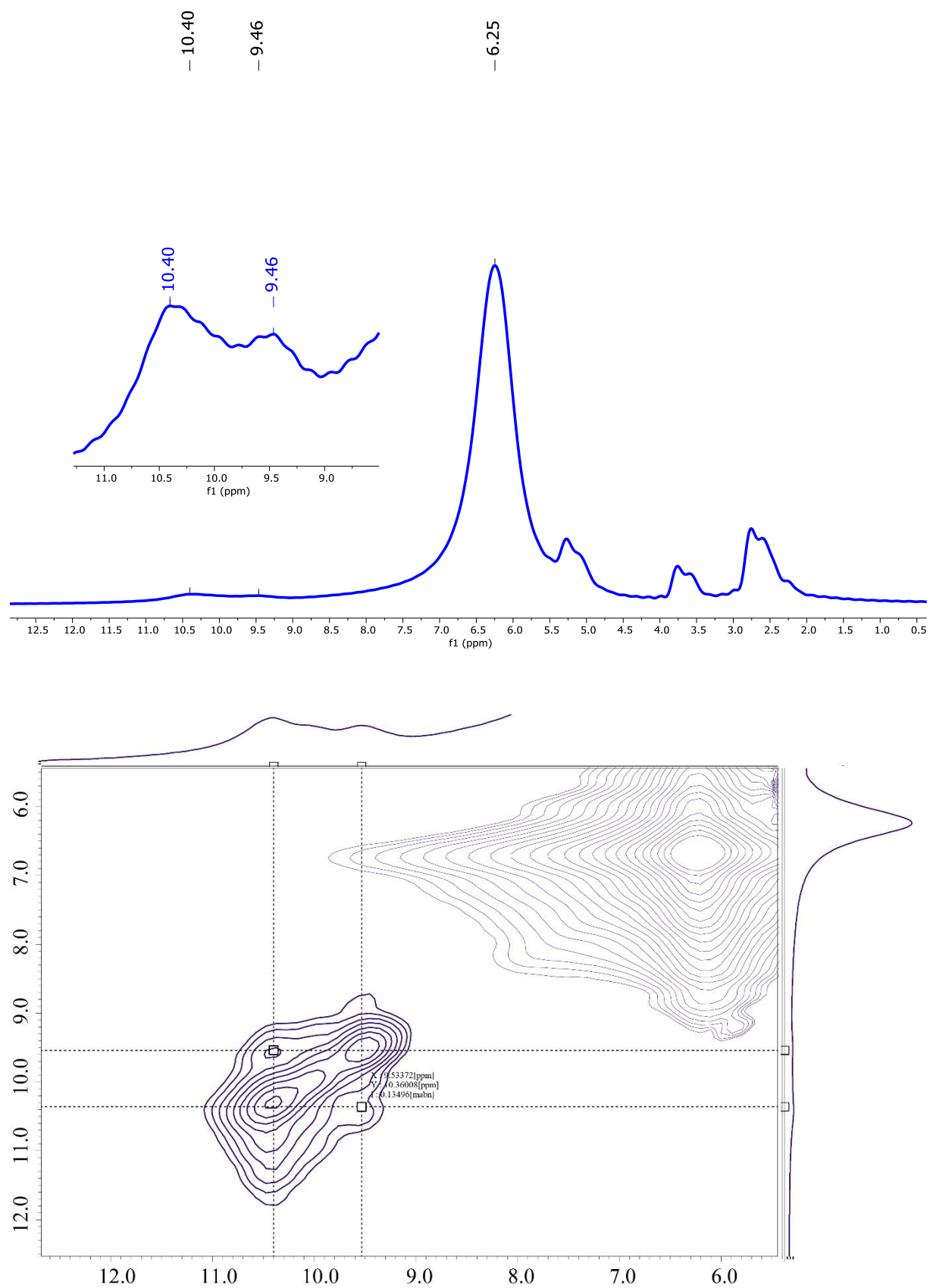


Figure S7. Thermogravimetric analysis (TGA) of organomodified mesoporous silica

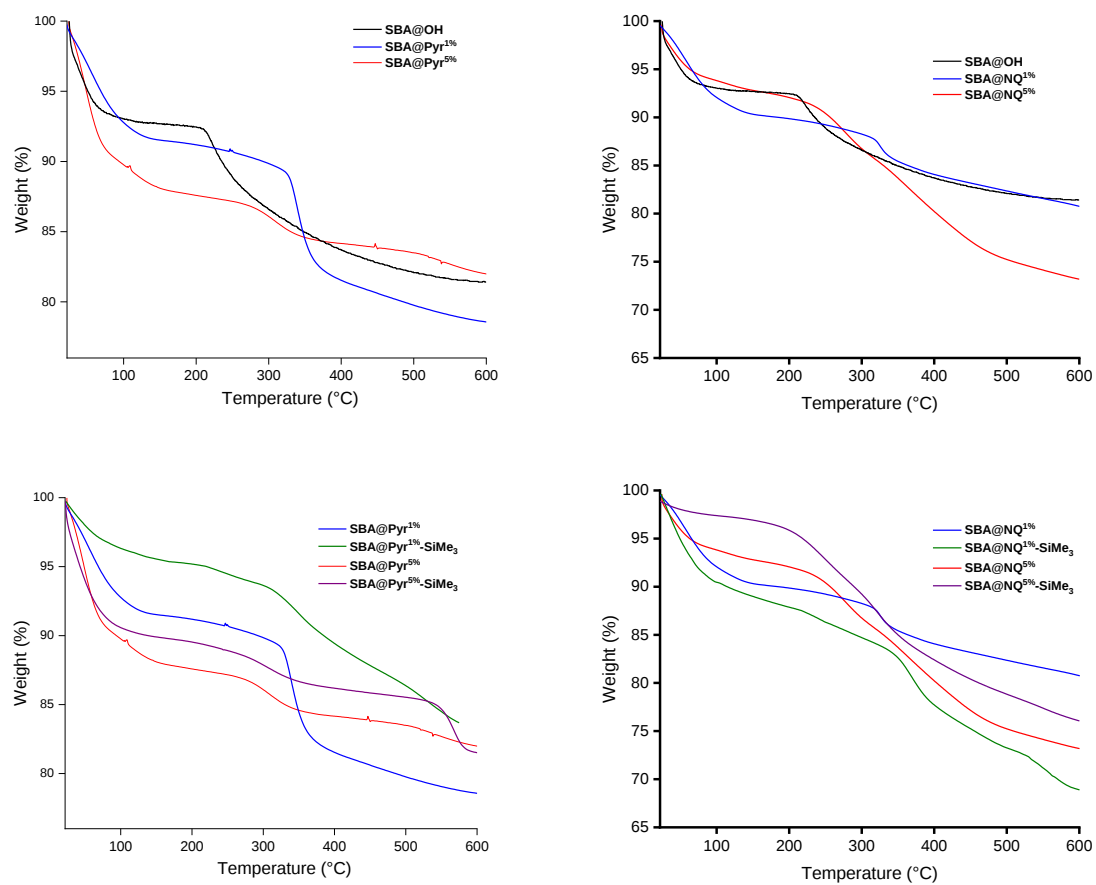


Figure S8. Nitrogen sorption analysis of organosilica materials

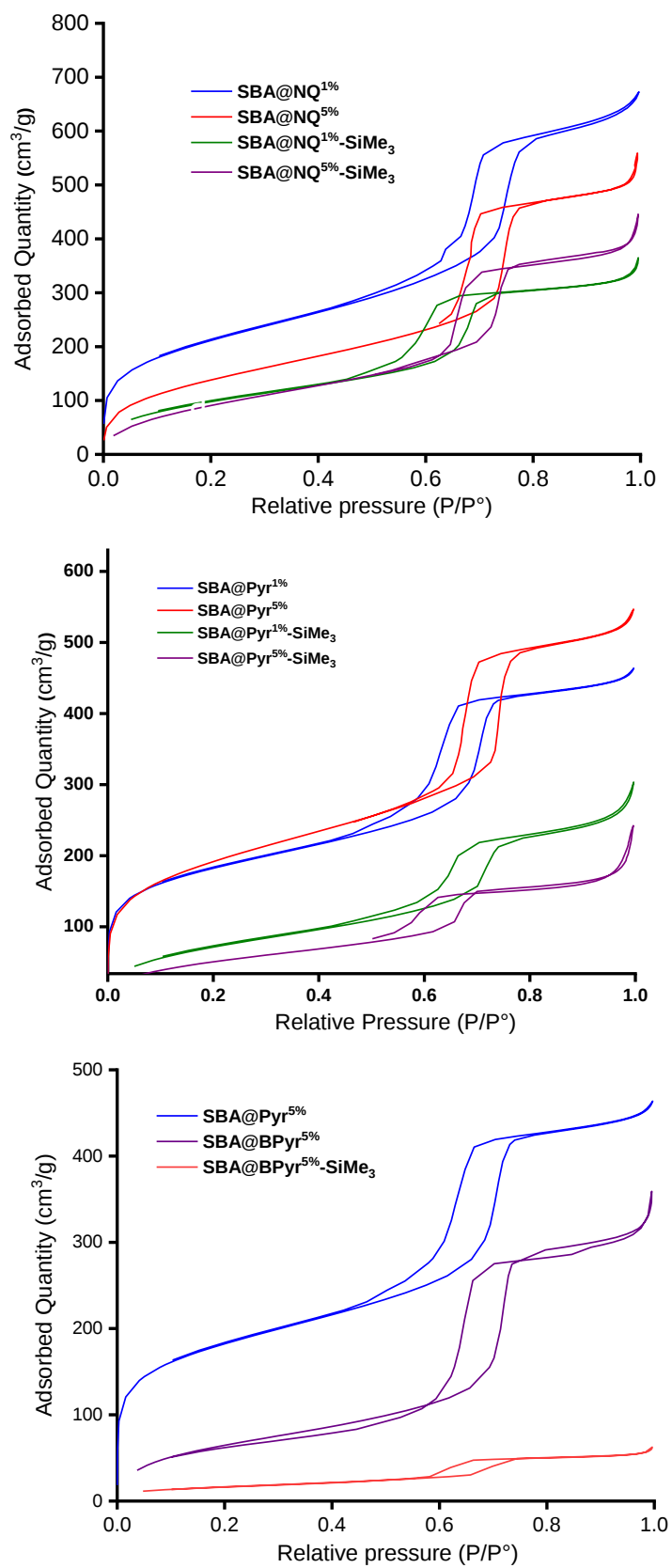


Figure S9. SEM images of SBA@OH and SBA@NH₂^{5%}

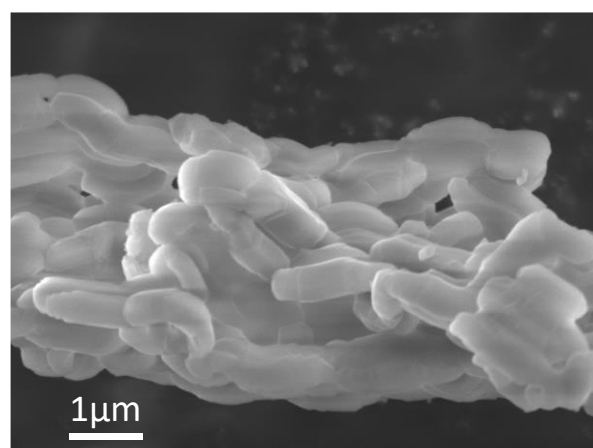
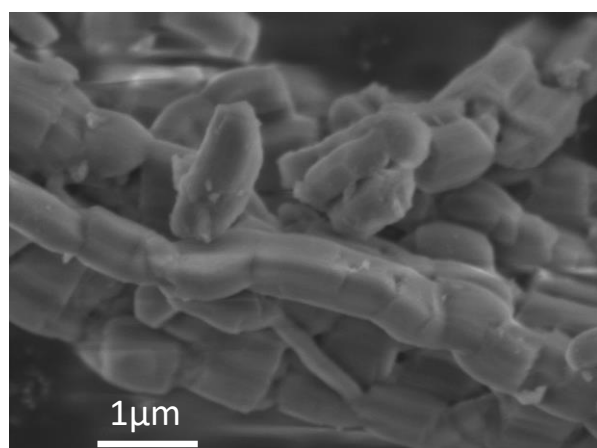
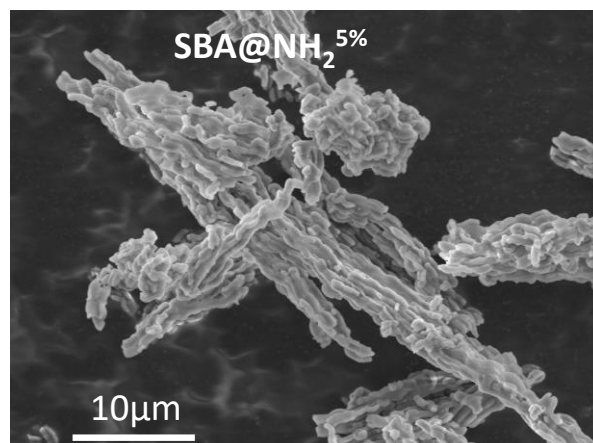
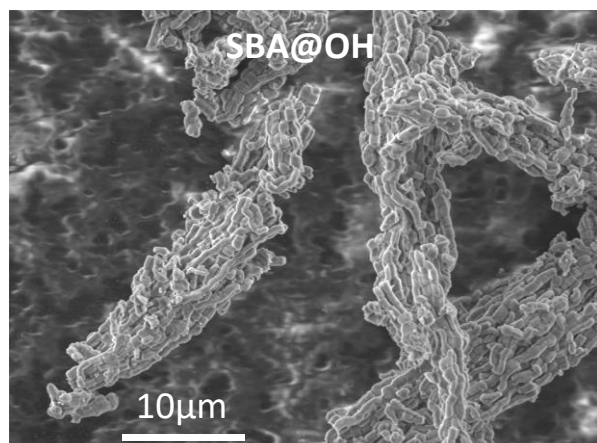


Table S1. Quantification of anion exchange sites within the material

Materials	C (mol/L)	n_{ads} (mmol/g)			n_{Sites} (mmol/g)	Fraction of occupied sites F (%)		
		pH = 2	pH = 6.5	pH = 9.5		pH = 2	pH = 6.5	pH = 9.5
SBA@NH₂ ^{5%}	10 ⁻⁴	0.0163	0.0143	0.00049	0.36	4.5	4	0.14
SBA@Pyr ^{5%}	10 ⁻⁴	0.0133	0.00202	0.00306	0.47	2.8	0.43	0.65
SBA@Bpyr ^{5%}	10 ⁻⁴	0.0235	0.0220	0.00713	0.47	5	4.7	1.5
SBA@NQ ^{5%}	10 ⁻⁴	0.0504	0.0504	0.0504	0.41	12.3	12.3	12.3
SBA@NQ ^{5%}	5.10 ⁻⁴	0.231			0.41	56		
SBA@NQ ^{5%}	10 ⁻³	0,375			0.41	90		

Figure S10. Removal of helianthine (methyl orange) using **SBA@NQ^{5%}** at different concentration. a) Percentage of Helianthine removal, b) Adsorption capacity (Q_e , mg/g)

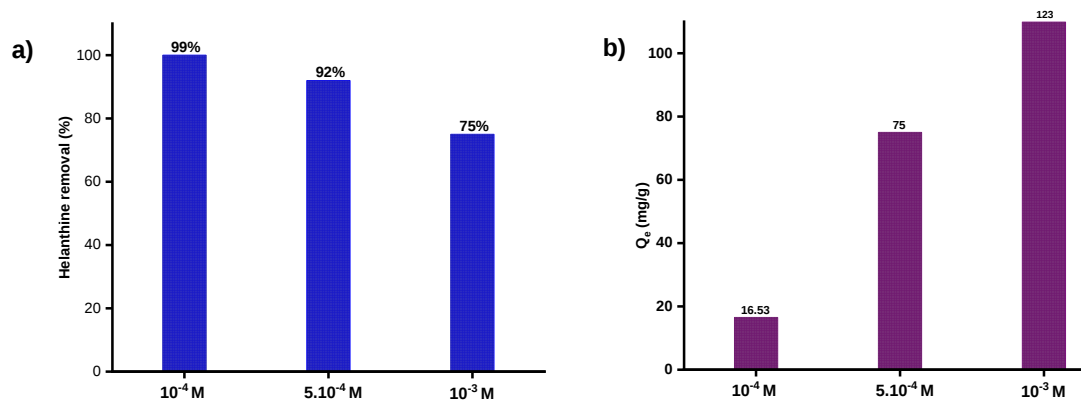


Figure S11. Quercetin adsorption through organosilica and Quercetin release in water

