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SUPPLEMENTARY INFORMATION

Fe_2O_3/NiO nanocomposite: Synthesis, characterization and roxarsone sensing by Fourier transform infrared photoacoustic spectroscopy

R. Suresh[1,2,3]*, Ángela Álvarez[1,4], Claudio Sandoval[1], Eimmy Ramírez[1], Paola Santander[5], R.V. Mangalaraja[6], Jorge Yáñez[1]*

[1]*Department of Analytical and Inorganic Chemistry, Faculty of Chemistry, University of Concepcion, Concepción, Chile.*
[2]*Department of Chemistry, Karpagam Academy of Higher Education, Coimbatore, Tamil Nadu, India*
[3]*Centre for Material Chemistry, Karpagam Academy of Higher Education, Coimbatore, Tamil Nadu, India*
[4]*Department of Chemistry and Biology, Basic Sciences Division, Universidad del Norte, Barranquilla 081007, Colombia*
[5]*Departamento de Ciencias del Ambiente, Facultad de Química y Biología, Universidad de Santiago de Chile*
[6]*Faculty of Engineering and Sciences, Adolfo Ibanez University, Diagonal las Torres 2640, Penalolén, Santiago, Chile*

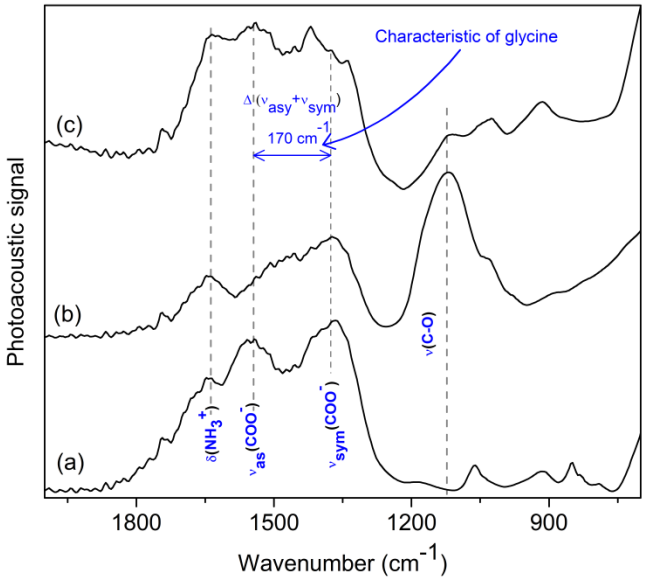

Fig. S1: FTIR-PA spectrum of (a) Fe_2O_3, (b) NiO and (c) Fe_2O_3/NiO nanocomposite in the range of 2000 to 700 cm^{-1}.

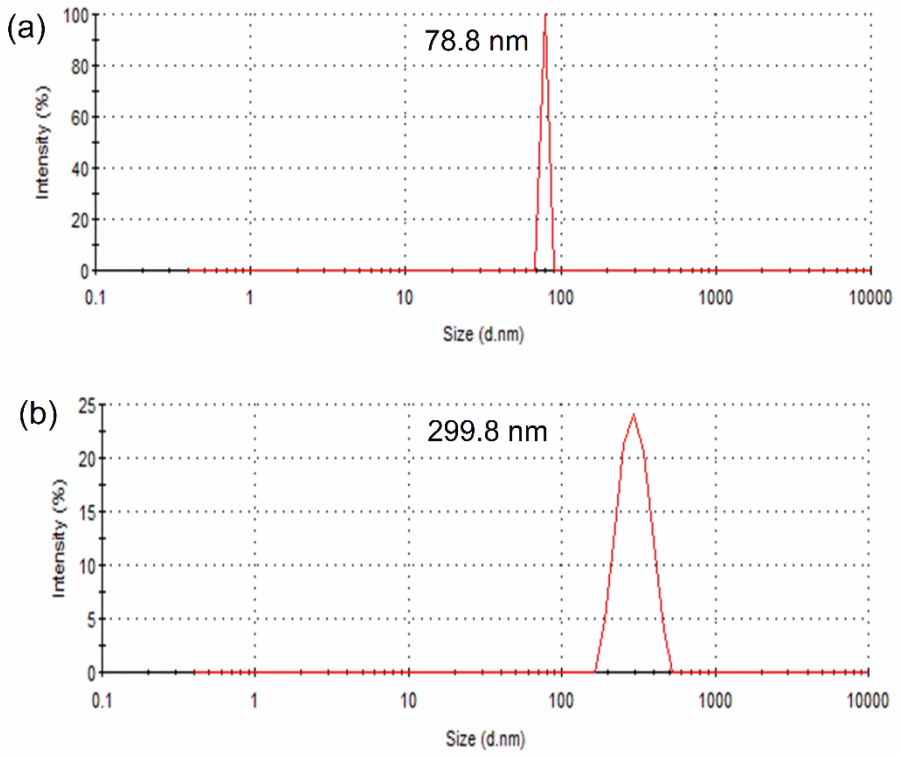

Fig. S2: Particle size distribution curve of (a) Fe_2O_3, and (b) NiO nanoparticles, prepared by glycine aided synthesis (450 °C, 4 h).

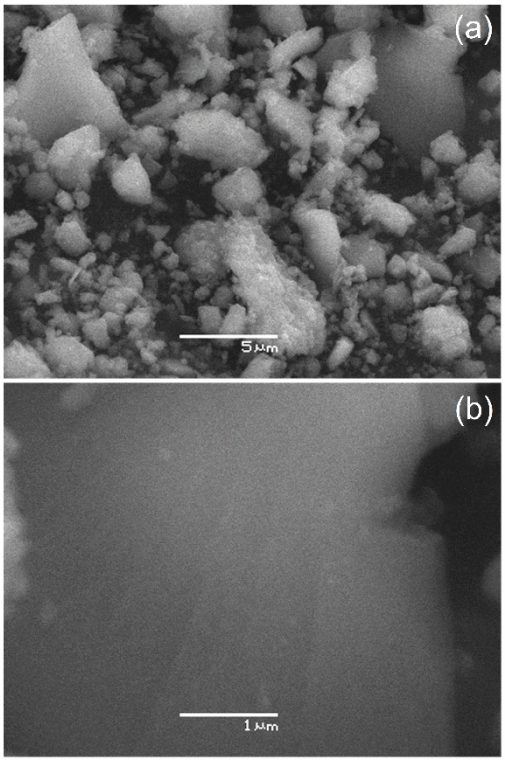

Fig. S3: SEM images of $Fe(OH)_3$

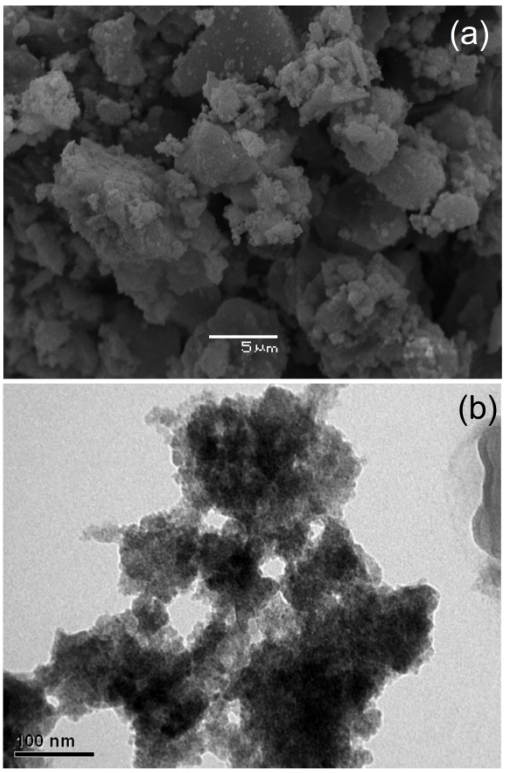

Fig. S4: (a) SEM and (b) TEM image of $Ni(OH)_2$

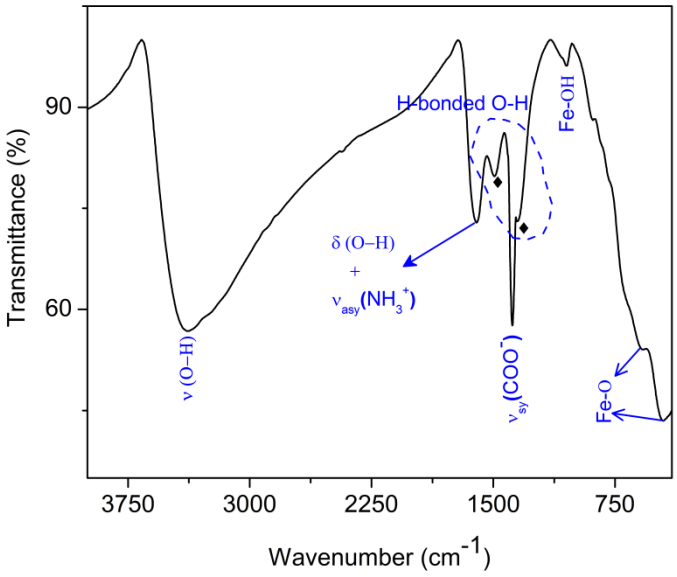

Fig. S5: FTIR spectrum of $Fe(OH)_3$

The FT-IR spectrum of $Fe(OH)_3$ shows broad band in the region of 3650-3000 cm^{-1} which is due to O-H stretching vibrations. The asymmetric stretching of NH_3^+ and deformation vibration of OH bond was observed as 1602 cm^{-1}. The bands at 1482 and 1336 cm^{-1} could be assigned to bending vibrations of NH_3^+ and CH_2 wagging vibration respectively [1]. The vibration of OH group in Fe-OH is observed at 1037 cm^{-1} [2]. The bands at 591 and 454 cm^{-1} are assigned to stretching vibration of Fe-O bond.

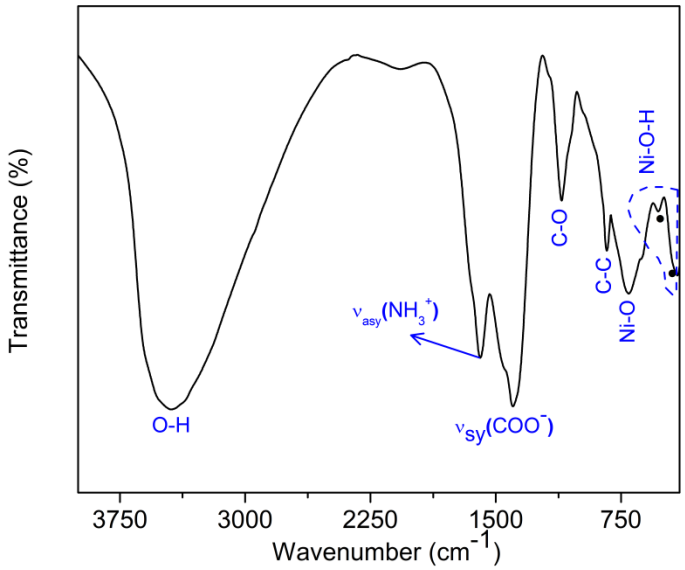

Fig. S6: FTIR spectrum of $Ni(OH)_2$

The broad band at 3443 cm^{-1} is corresponding to O-H stretching vibration. The asymmetric vibration of NH_3^+ is observed at 1592 cm^{-1}. The bands at 1402 and 1108 cm^{-1} are attributed to vibrations of carboxylate and C-O bond. The band at 827 cm^{-1} is due to C-C bending vibration [3]. The bands at 706 cm^{-1} is due to Ni-O bond [4]. The vibrations due related to Ni-O-H are observed at 537 and 413 cm^{-1} [5].

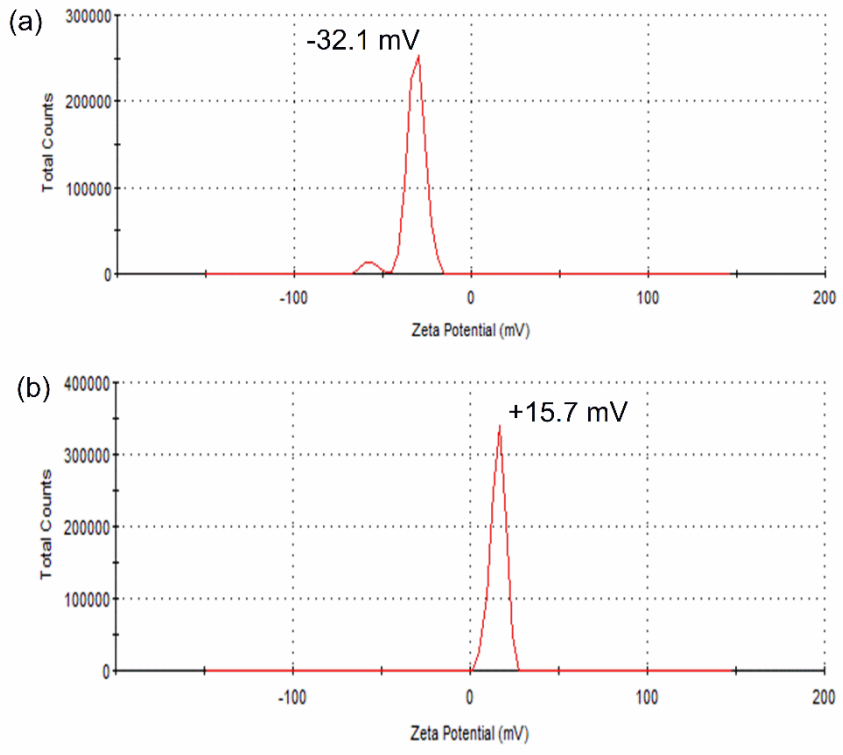

Fig. S7: Zeta potential curve of (a) Fe_2O_3, and (b) NiO nanoparticles, prepared by the glycine aided synthesis method (450 °C, 4 h).

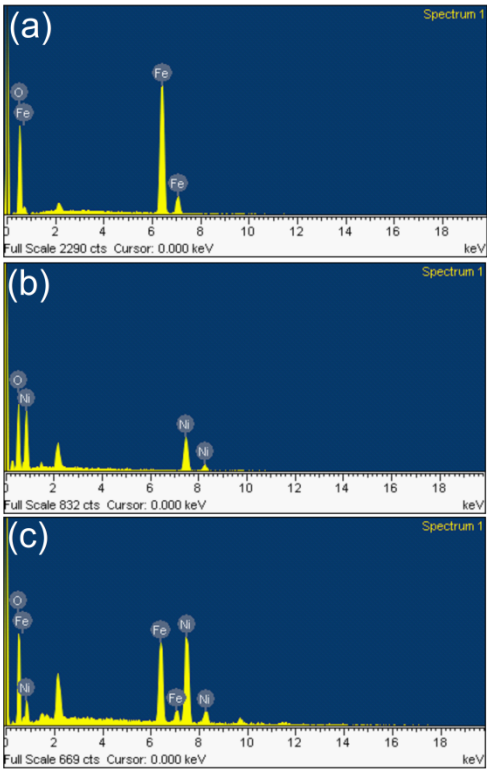

Fig. S8: EDS spectra of (a) Fe_2O_3, (b) NiO and (c) Fe_2O_3/NiO nanocomposite

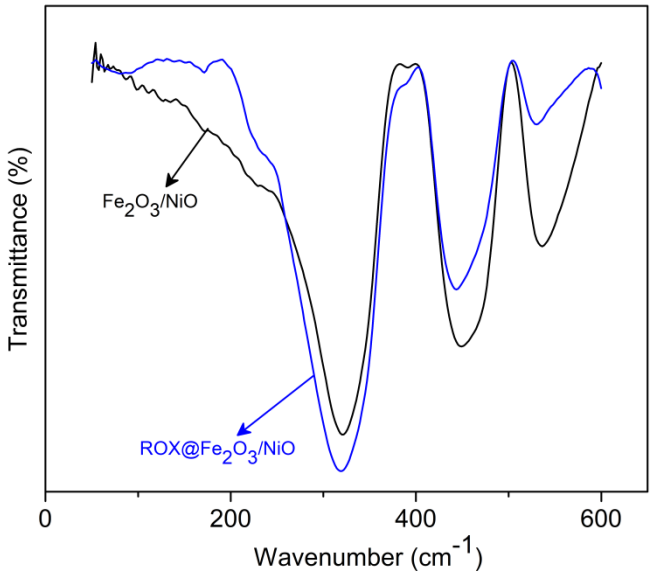

Fig. S9: Far FTIR spectra of (a) Fe_2O_3/NiO and (b) ROX adsorbed Fe_2O_3/NiO nanocomposite

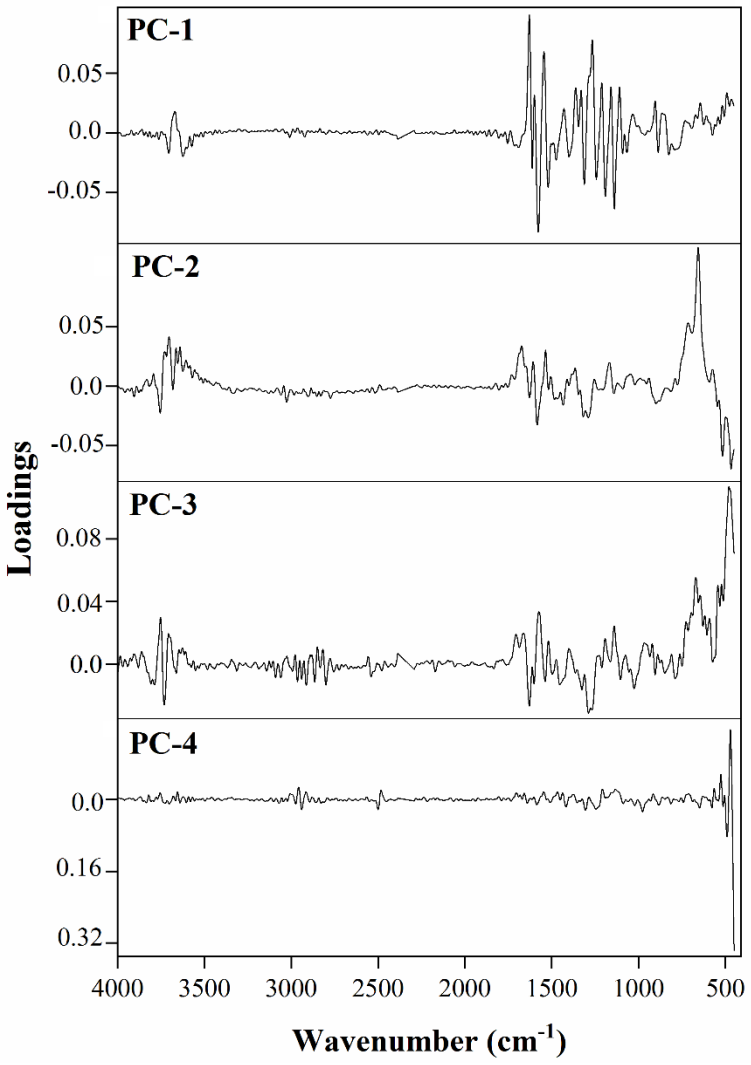

Fig. S10: Loading plots for the first four PCs

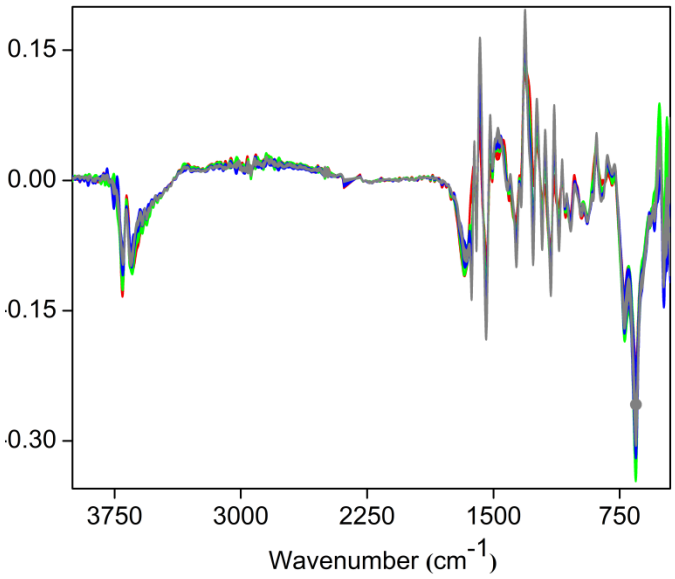

Fig. S11. First derivative FTIR-PA spectra of 10 mg L^{-1} (red), 20 mg L^{-1} (green), 30 mg L^{-1} (blue) and 40 mg L^{-1} (gray) ROX adsorbed Fe_2O_3/NiO nanocomposites

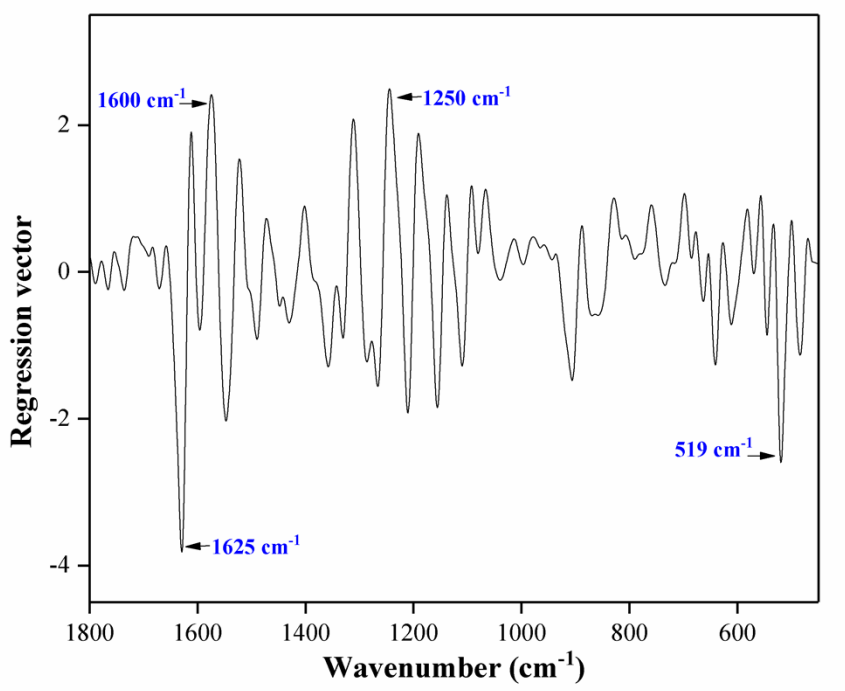

Fig. S12: Regression vector in the PLS model

Table S1

Significant factor analysis of the four concentration ROX analyzed by FTIR-PAS

Range spectral (cm^{-1})	Components	Absolute variance	Percentage variance (%)	Cumulative variance (%)	Press Cal
4000-450	PC 1	6.9	44.1	44.1	8.7
	PC 2	4.0	25.7	69.9	4.7
	PC 3	1.4	9.3	79.1	3.3
	PC 4	0.5	3.4	82.5	2.7
1800-450	PC 1	6.7	47.9	47.9	7.3
	PC 2	3.5	24.9	72.8	3.8
	PC 3	1.4	9.8	82.6	2.4
	PC 4	0.5	3.6	86.3	1.9

Table S2

Summary of PLS parameters in training and testing sets.

PLS parameters	*Training set*	
	n	40
	Validation	Cross validation LOO
	Latent variables	4
	Cumulative variance (%)	84.5
	RMSEC	1.31
	R^2 Cal	0.99
	RMSECV	1.81
	R^2Val	0.99
	Testing set	
	n	19
	Validation	External validation
	Latent variables	4
	RSEP	1.42
	R^2	0.99

References

1. N.C. Feitoza, T.D. Goncalves, J.J. Mesquita, J.S. Menegucci, M.K.M.S. Santos, J.A. Chaker, R.B. Cunha, A.M.M. Medeiros, J.C. Rubim and M.H. Sousa, *J. Hazard. Mater.* 2014, **264**, 153–160.
2. X. Yang, Y. Li, H. Gao, C. Wang, X. Zhang and H. Zhou, *Int. J. Biol. Macromol.* 2018, **117**, 30–41.
3. G. Fischer, X. Cao, N. Cox and M. Francis, *Chem. Phys.* 2005, **313**, 39–49.
4. M. Rajamathi, P.V. Kamath and R. Seshadri, *J. Mater. Chem.* 2000, **10**, 503-506.
5. S. Krehula, M. Ristic, C. Wu, X. Li, L. Jiang, J. Wang, G. Sun, T. Zhang, M. Perovic, M. Boskovic, B. Antic, L.K. Krehula, B. Kobzi, S. Kubuki and S. Music, *J. Alloys Compd.* 2018, **750**, 687-695.