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Silica nanoparticles-nylon 6 composites: synthesis, characterization and potential use as sorbent

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1. Chromatographic analyses

Two different systems were employed in this research. The optimization of the method was performed using a Waters AcquityTM Ultra Performance Liquid Chromatography system (Waters Corp., Madrid, Spain) using an Acquity UPLC®BEH C18 column (1.7 μm, 2.1 mm × 100 mm) maintained at 45 °C. The separation was performed under a gradient elution program using water (solvent A) and acetonitrile (solvent B) as mobile phase components. The elution started at 20% of solvent B and it was linearly increased up to 50% in 5 min. After that, the system was re-equilibrated for 2 min between analyses. During the separation, the flow rate was maintained at 0.4 mL/min and 5 μL was injected with partial loop mode. Detection was performed at 200 nm using a PDA eλ Detector (Waters). System control was performed with Empower software also from Waters. Since the extraction efficiency is calculated in relative terms (extraction recoveries and enrichment factors), the obtained values are independent of the employed instrument.

An Agilent 1260 Infinity HPLC system (Agilent, Palo Alto, CA, USA) coupled with mass spectrometric detector was employed for the validation of the method. It was equipped with a binary high-pressure pump for mobile phase delivery and an autosampler. Chromatographic separation was performed on a Zorbax Eclipse XDB-C18 (4.6 mm × 150 mm, 5 μm) column from Agilent, using LC-MS grade acetonitrile and water as mobile phase components in a 35/65 (v/v) ratio. A guard column (0.2 μm filter, 2.1 mm), also from Agilent, was used to preserve the integrity of the analytical column. The injection volume was 5 μL and the flow rate was maintained at 0.5 mL/min.

Quantification was performed on an Agilent 6420 Triple Quadrupole MS system equipped with an electrospray ionization source working in negative mode. Data

analyses were carried out using Agilent MassHunter Software (Version B.06.00). The mass spectrometer settings were fixed in order to improve the selected reaction monitoring signal. The flow and temperature of the drying gas (N2) were 8 L/min and 350 °C, respectively. The nebulizer pressure was 20 psi, and the capillary voltage was 5500 V. The analytes were detected using the selected reaction monitoring transitions. Table S1 summarizes the optimized parameters for each analyte.

Table S1. Transitions and optimized potentials for LC–MS/MS analysis, including fragmentor, collision energy (CE) and cell accelerator voltage (CAV).

Analyte	Transition	Fragmentor (V)	CE (eV)	CAV (V)
Estrone	269.2 → 145.2	133	37	7
β-Estradiol	271.3 → 145	130	40	7
	271.3 → 183.3	130	42	7
Estriol	287.3 → 145.1	137	47	7