Supplementary material

Rational design of a molecular imprinting polymer for dinotefuran: Theoretical and experimental studies aiming the development of an efficient adsorbent for microextraction by packed sorbent

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Figure S1. Chemical structure of dinotefuran (DNF).
Figure S2. B3LYP/6-311G(d,p) optimized structures for the 1:1 FM/template complexes: (a) DNF-(AA)$_1$; (b) DNF-(MAA)$_1$; (c) (DNF-APA)$_1$; (d) DNF-(TFMAA)$_1$. The hydrogen bonds were drawn in dotted lines to ease the visualization.
Figure S3. B3LYP/6-311G(d,p) optimized structures for the 1:2 FM/template complexes: (a) DNF-(AA)$_2$; (b) DNF-(MAA)$_2$; (c) (DNF-APA)$_2$; (d) DNF-(TFMAA)$_2$. The hydrogen bonds were drawn in dotted lines to ease the visualization.
Figure S4. B3LYP/6-311G(d,p) optimized structures for the 1:3 FM/template complexes: (a) DNF-(AA)$_3$; (b) DNF-(MAA)$_3$; (c) (DNF-APV)$_3$; (d) DNF-(TFMAA)$_3$. The hydrogen bonds were drawn in dotted lines to ease the visualization.
Figure S5. (A) Chromatogram referring to enantioseparation of dinotefuran employing 85% hexane, 5% ethanol, 10% methanol as mobile phase and flow rate of 1.2 mL min⁻¹; (B) Chromatogram referring to enantioseparation of dinotefuran employing 80% hexane, 10% ethanol, 10% methanol plus 0.1% diethylamine and flow rate of 1.2 mL min⁻¹; (C) Chromatogram referring to enantioseparation of dinotefuran employing 83% hexane, 11% ethanol, 6% methanol plus 0.25% diethylamine and flow rate of 1.2 mL min⁻¹. (1) (+)-(S)-DNF and (2) (−)-(R)-DNF.
Figure S6. Micrographs of the (A) NIP at magnifications of 180× and (B) MIP at magnifications of 200 × and TGA and DrTGA of (C) NIP and (D) MIP.