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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Figures

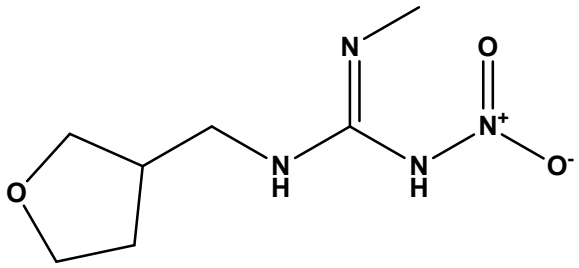

Figure S1. Chemical structure of dinotefuran (DNF).

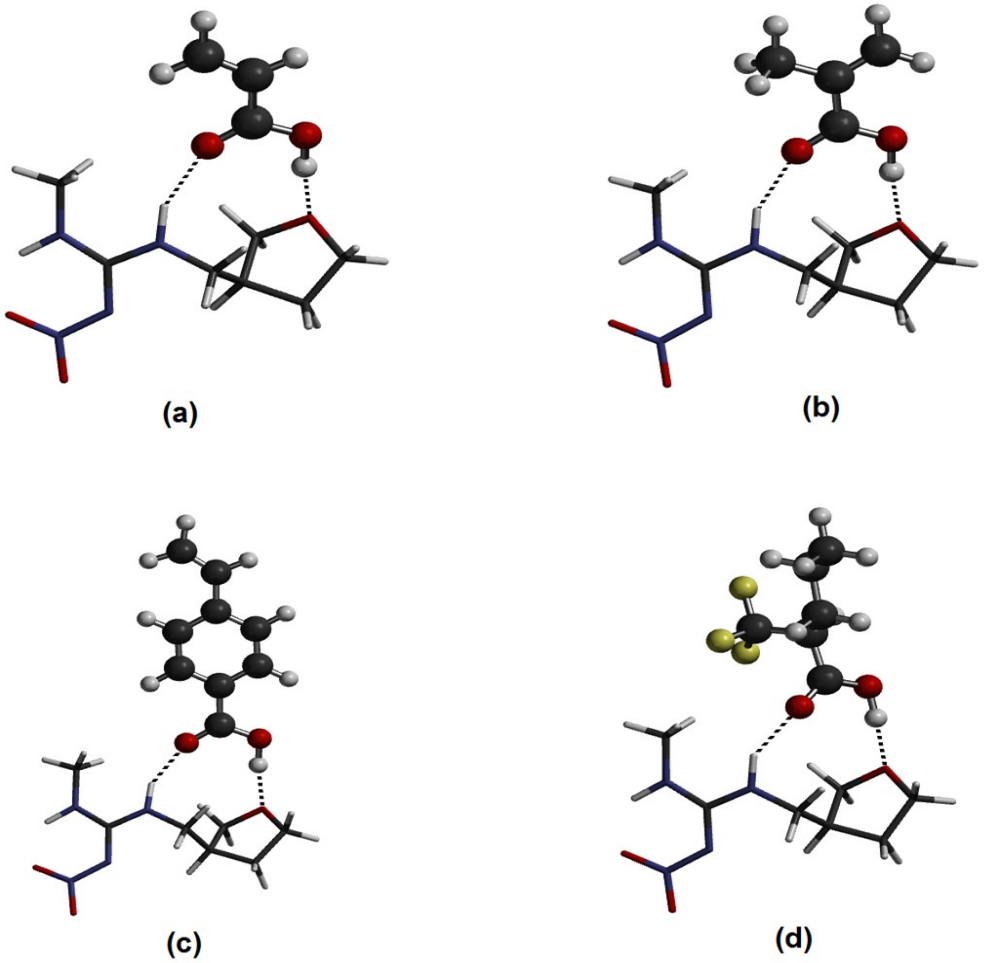

Figure S2. B3LYP/6-311G(d,p) optimized structures for the 1:1 FM/template complexes: (a) DNF-$(AA)_1$; (b) DNF-$(MAA)_1$; (c) $(DNF\text{-}APA)_1$; (d) DNF-$(TFMAA)_1$. The hydrogen bonds were drawn in dotted lines to ease the visualization.

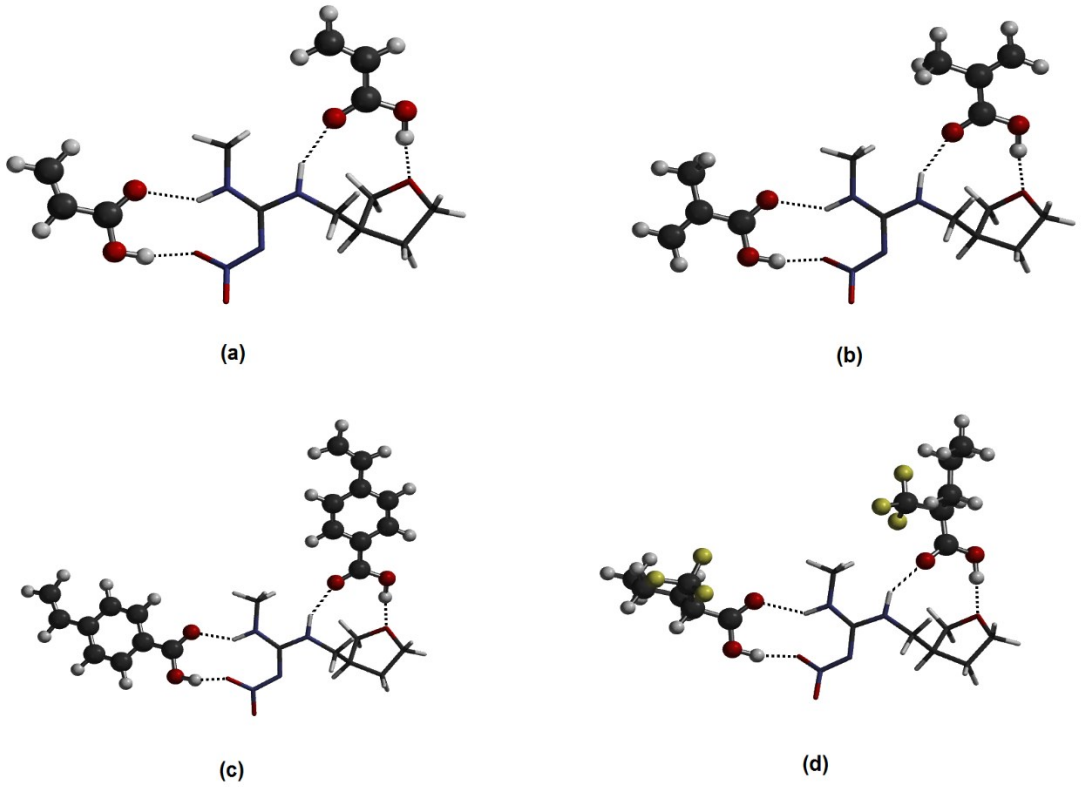

Figure S3. B3LYP/6-311G(d,p) optimized structures for the 1:2 FM/template complexes: (a) DNF-$(AA)_2$; (b) DNF-$(MAA)_2$; (c) $(DNF\text{-}APA)_2$; (d) DNF-$(TFMAA)_2$. The hydrogen bonds were drawn in dotted lines to ease the visualization.

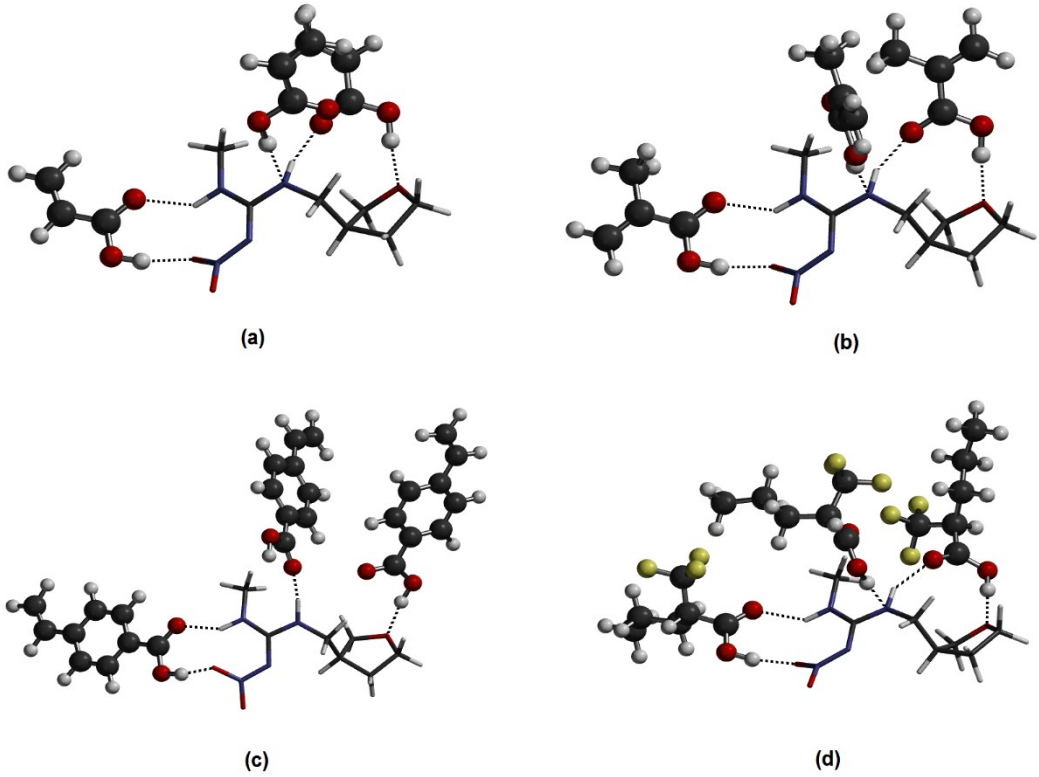

Figure S4. B3LYP/6-311G(d,p) optimized structures for the 1:3 FM/template complexes: (a) DNF-$(AA)_3$; (b) DNF-$(MAA)_3$; (c) $(DNF\text{-}APV)_3$; (d) DNF-$(TFMAA)_3$. The hydrogen bonds were drawn in dotted lines to ease the visualization.

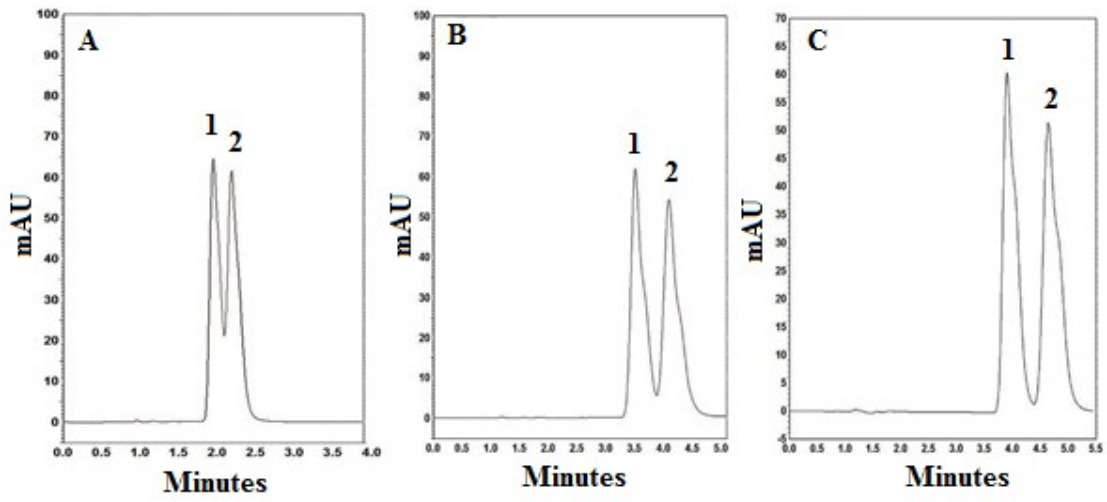

Figure S5. (A) Chromatogram referring to enantioseparation of dinotefuran employing 85% hexane, 5% ethanol, 10% methanol as mobile phase and flow rate of 1.2 mL min^{-1}; (B) Chromatogram referring to enantioseparation of dinotefuran employing 80% hexane, 10% ethanol, 10% methanol plus 0.1% diethylamine 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.

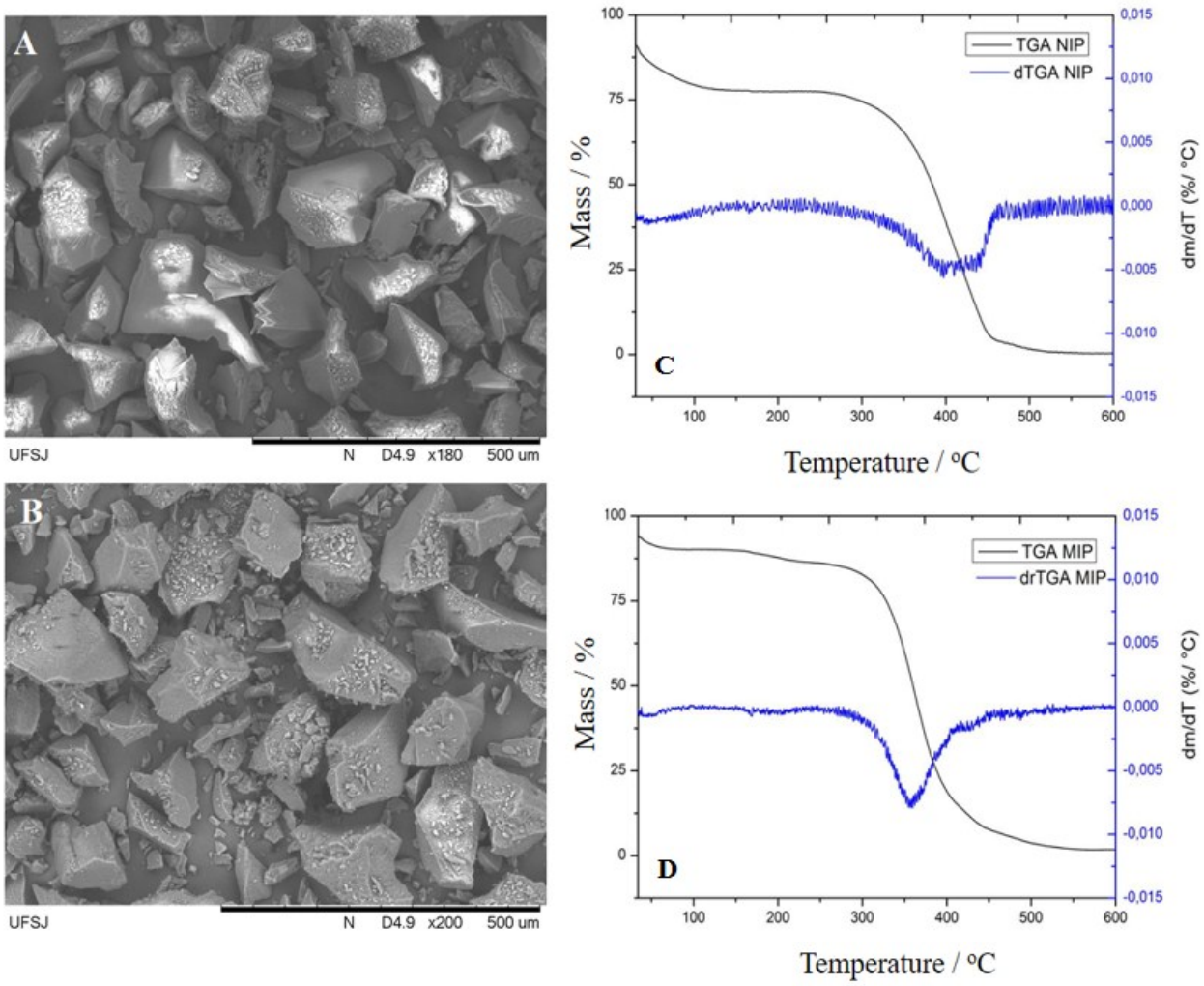

Figure S6. Micrographs of the (A) NIP at magnifications of 180× and (B) MIP at magnifications of 200 × and TGA and DrTGA of (C) NIP and (D) MIP.