

Supplementary Material

Selective Detection of Nucleotides in Infant Formula Using an N-Rich Covalent Triazine Porous Polymer

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Table S1. Adsorption energy between host and guest molecules ΔE_n .

CTF-DBF-analytes	ΔE_n / (kJ/mol)
CTF-DBF-UMP	−42.01
CTF-DBF-CMP	−55.60
CTF-DBF-AMP	−45.55
CTF-DBF-IMP	−27.95
CTF-DBF-GMP	−133.99

Note: Using the B3LYP method combined with the 6-31G basis.

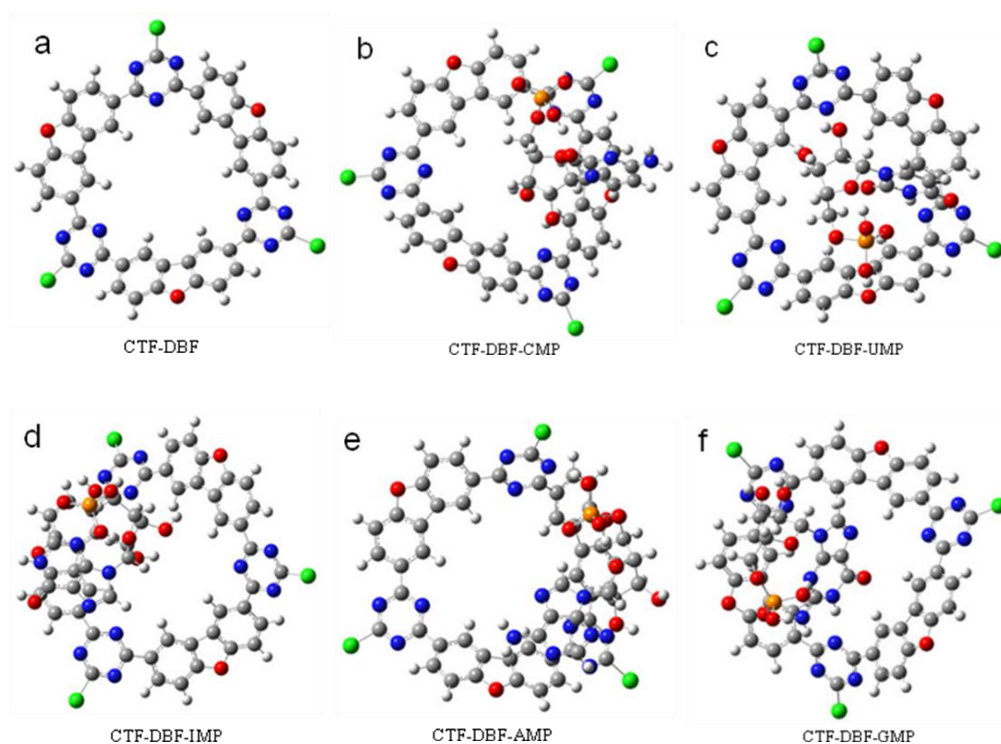


Figure S1. (a) Optimal structure of the host molecule CTF-DBF; (b–f) Optimal conformation of host and guest molecules; the optimization of the above structural models all use the B3LYP/6–31+G basis set; carbon atoms are gray, hydrogen atoms are white, oxygen atoms are red, nitrogen atoms are blue, and chlorine atoms are green.

Table S2. Relevant parameters of SPE-HPLC-UV method.

Analytes	Linear range/ ($\mu\text{g/mL}$)	Regression equation	<i>r</i>	LOD/ (mg/kg)	LOQ/ (mg/kg)
CMP	2–100	$y = 27.921x + 1.224$	0.9998	0.50	1.70
UMP	1–100	$y = 15.103x + 0.335$	0.9998	0.30	1.20
IMP	1.5–50	$y = 13.036x + 0.049$	0.9996	0.50	1.50
AMP	2–100	$y = 68.225x + 1.446$	0.9995	0.30	1.20
GMP	1–100	$y = 71.016x - 1.645$	0.9993	0.30	1.10

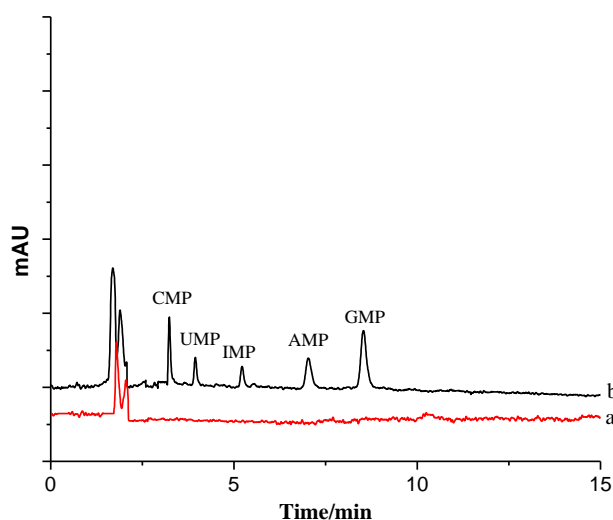


Figure S2. Chromatograms of five nucleotides after SPE treatment of blank and blank spiked samples. (a: Blank sample; b: Blank spiked sample 5.0 mg/kg).

The coordinates of the CTF-DBF:

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C 0.63673900 -5.80865674 -2.39955546
C 1.70970866 -5.63705625 -3.26274054
C 2.49193365 -4.50925822 -3.06282748
C 2.21910997 -3.52865083 -2.08669807
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