Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Development of molecularly imprinted polymer nanoarrays of N-acryloyl-2-mercaptobenzamide on silver electrode for ultratrace sensing of uracil and 5-fluorouracil

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Electronic Supplementary Information (ESI):

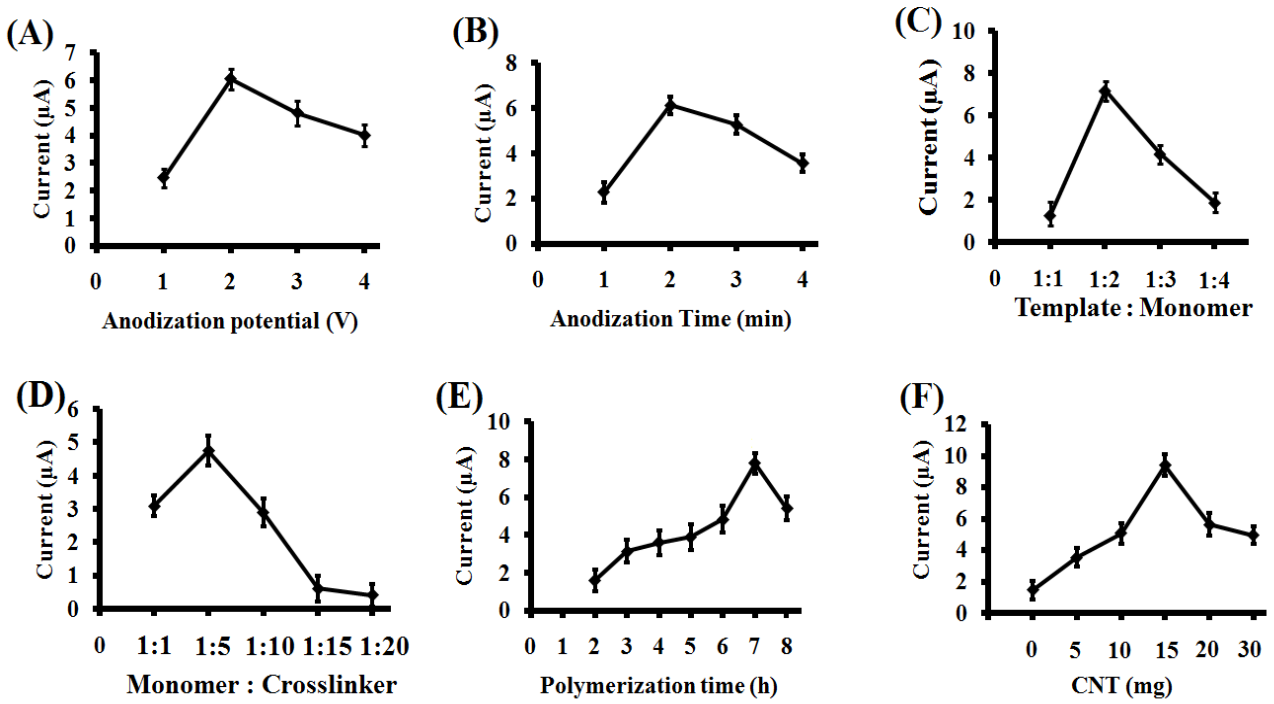

Fig. S1 Effect of anodization potential (A), anodization time (B), template: monomer molar ratio (C), monomer : cross-linker molar ratio (D), polymerization time (E), and CNT amount (F) on DPASV response of Ura/5-FU.

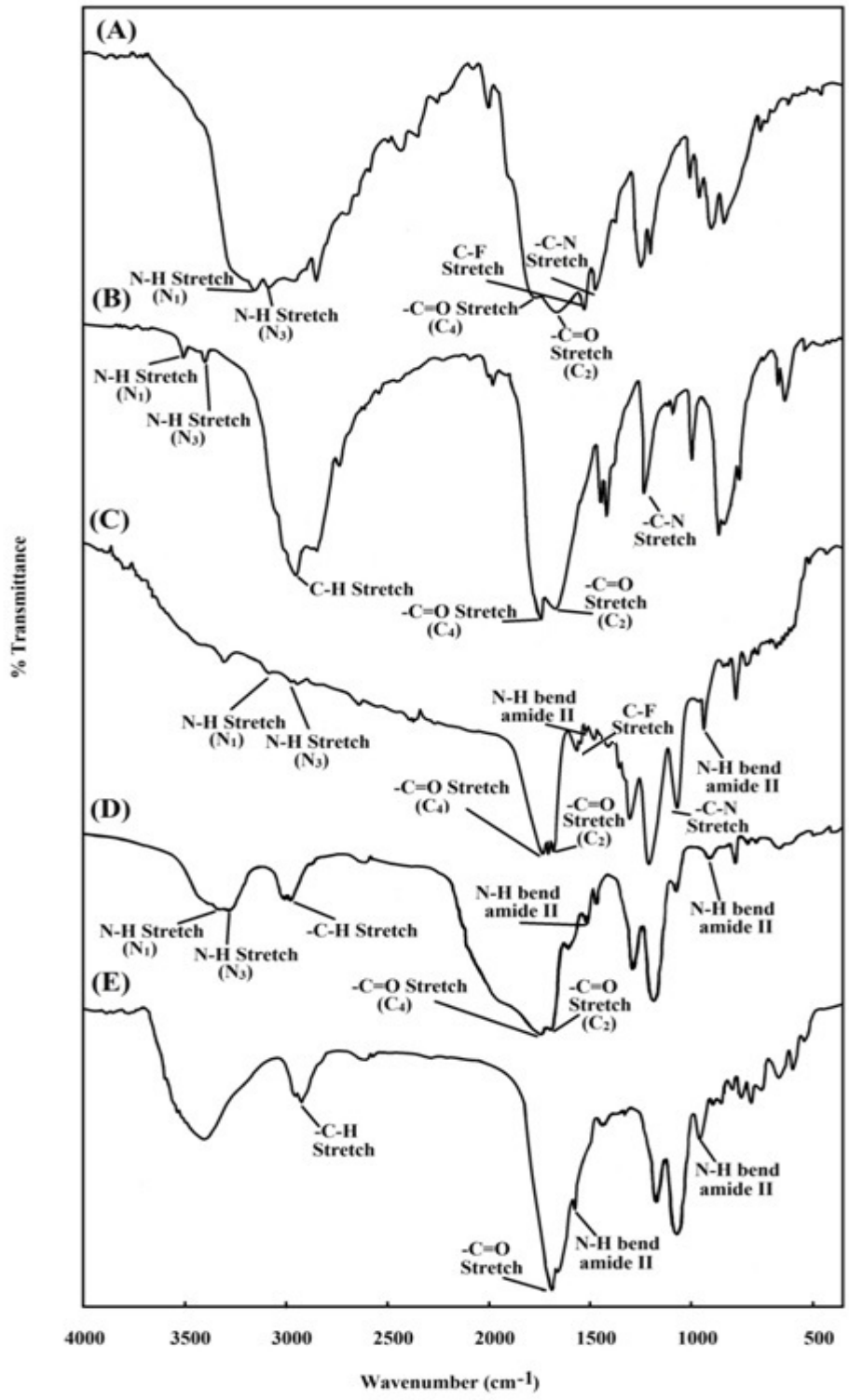

Fig. S2 FT-IR (KBr) spectra: (A) 5-FU, (B) Ura, (C) MIP-5-FU-adduct, (D) MIP-Ura adduct, and (E) MIP (5-FU or Ura).

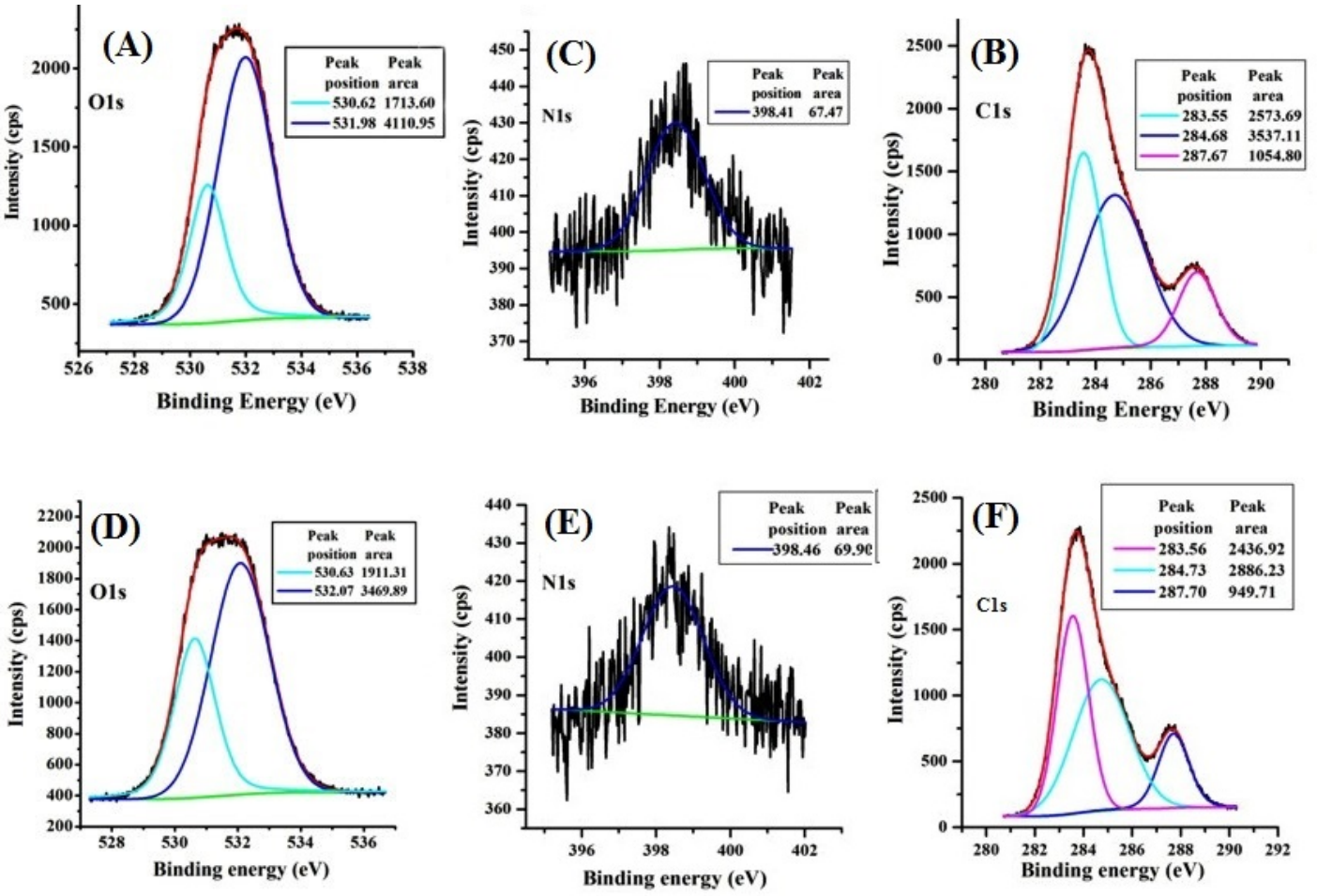

Fig. S3 Deconvoluted XPS spectra of various elements (O, N, C) of MIP Ura/5FU (A-C) and NIP (D-F).

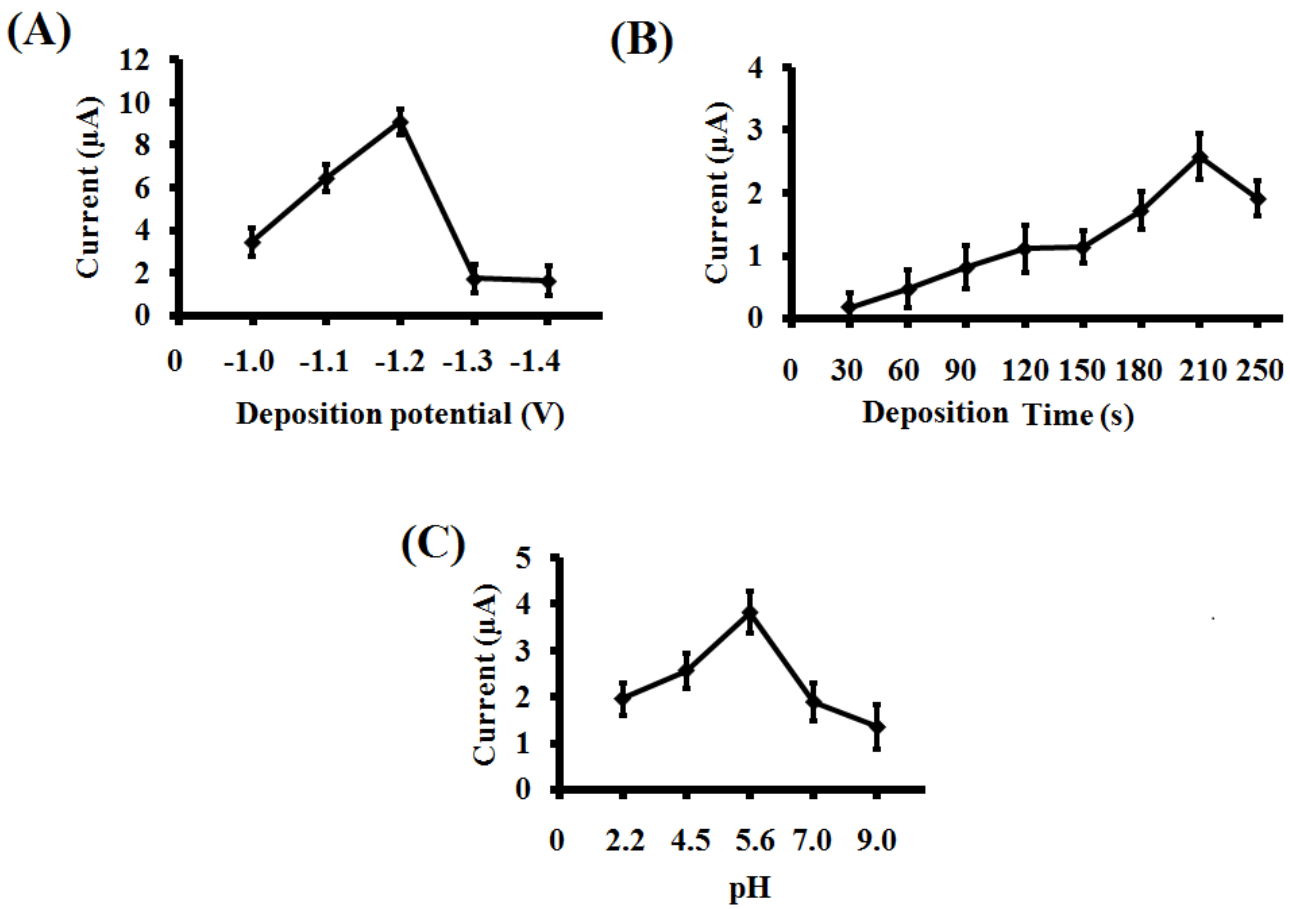

Fig. S4 Effect of deposition potential (A), deposition time (B), and pH (C) on DPASV response of Ura/5-FU.

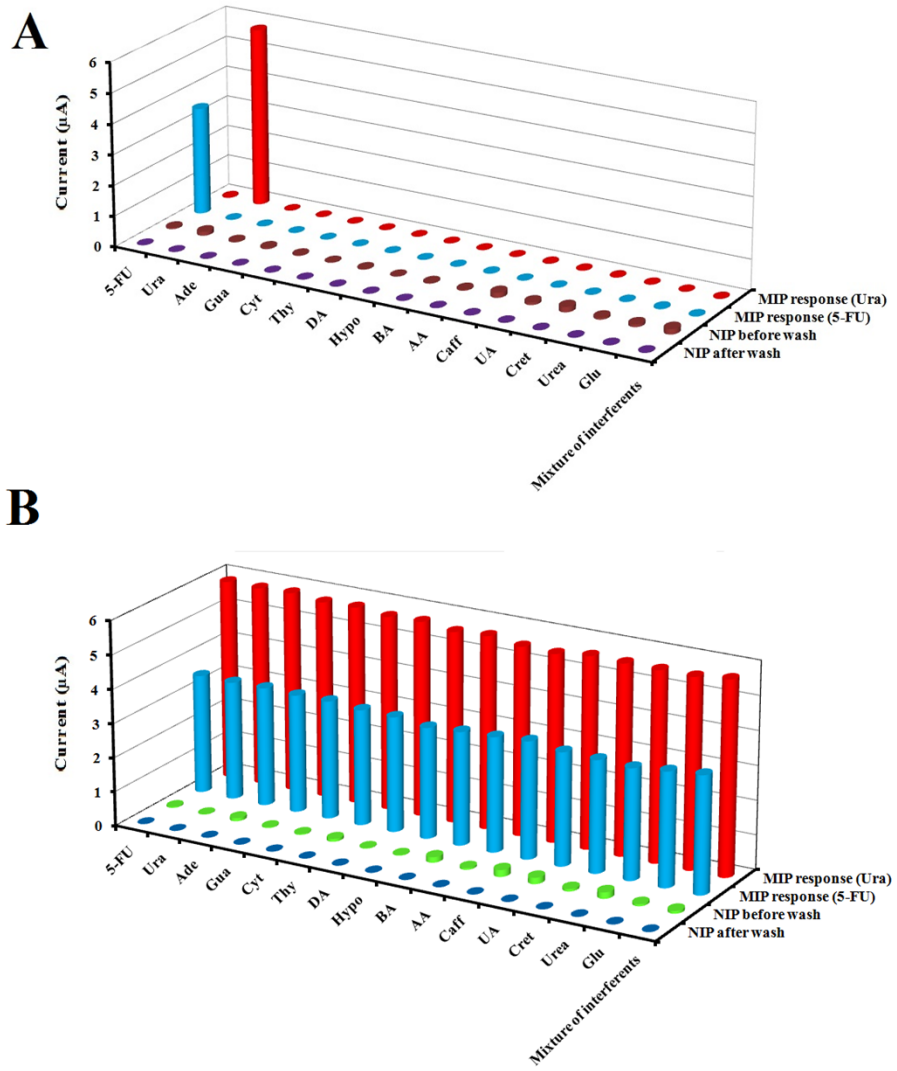

Fig. S5 (A) DPASV response for analyte and interferents [when studied individually (each 19.607 ng mL^{-1})] after water-washing and before water-washing at NIP modified nanoarrays electrode and for analyte and interferents(s) (each having concentration 19.607 ng mL^{-1}) in individual capacity at MIP-Ura/5-FU modified nanoarrays silver electrode.

(B) DPASV response of 19.607 ng mL^{-1} 5-FU in binary mixture with interferents [19.607 ng mL^{-1}(Ura, DA, Cret); 196.0 ng mL^{-1} (Ade, Gua, Cyt, Thy, Hypo, BA, AA, Caff); 588.2 ng mL^{-1}

(Urea); 19.607 µg mL^{-1} (Glu)]. DPASV response of 19.607 ng mL^{-1} Ura in binary mixture with interferents [58.823 ng mL^{-1}(Ade); 19.607 ng mL^{-1} (5-FU, Gua, Cyt, Thy, DA); 98.039 ng mL^{-1} (Hypo); 19.607 ng mL^{-1} (BA, AA, Caff); 19.6 µg mL^{-1} (UA, Cret); 196.0 µg mL^{-1} (Urea); 490.2 µg mL^{-1} (Glu). The multiple sample examined was consisted of 19.607 ng mL^{-1} plus mixture of the interferents, each having clinically relevant aforementioned concentrations.

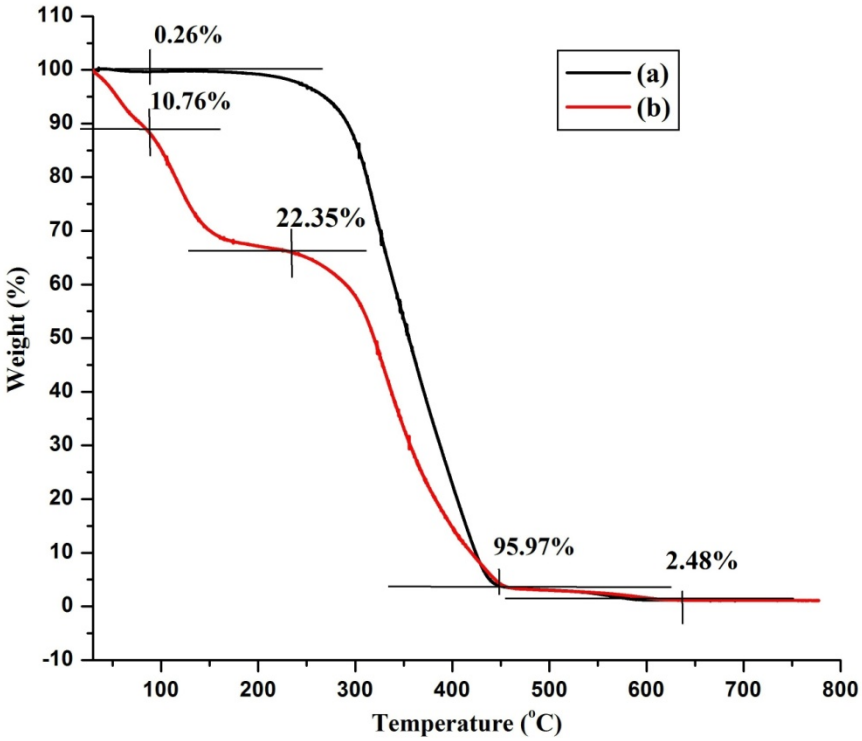

Fig. S6 TG Curves of MIP (a), and MIP-adduct (b).

Table S1 Binding energies, *ΔE,* of the optimized complexes of Ura and 5-FU with APD, HPP and AMB at MP2/6-31+G (d, p) basis set.

Complex	**Δ*E* (kJ mol^{-1})**	
	1:1	**1:2**
Ura-APD	-33.86	-69.31
Ura-HPP	-26.25	-73.51
Ura-AMB	-65.63	-133.90
5-FU-APD	-34.13	-70.88
5-FU-HPP	-27.77	-44.63
5-FU-AMB	-66.42	-139.41

Table S2 Comparison of different methods for the determination of Ura and 5-FU.

S. N.	Method	Determination range (ng mL^{-1})		Limit of detection (ng mL^{-1})		Comments	Reference
		Ura	5-FU	Ura	5-FU		
1.	Electrochemical oxidation at pyrolytic graphite electrode	14.56× 10^3-112.07× 10^3	13.00× 10^3-85.84× 10^3	-	-	No interference study and no real sample analysis	[1]
2.	MIP polymer brushes grafted to SPME fiber	1.0- 70.00	1.00- 80.00	0.02	0.04	Interference and real sample studies	[2]
3.	Non-hydrolytic sol–gel derived Composite-fiber	1.99–75.0	9.99–426.46	0.56	1.30	Interference and real sample studies	[3]
4.	HPLC assay with UV detection	2.5–80.00	-	-	-	No interference study	[4]
5.	HPLC method	6.25-100.0	-	0.62	-	No interference study	[5]
6.	Measurement by liquid chromatography tandem mass spectrometry	0.5–100	-	-	-	No interference study	[6]
7.	MIP membranes prepared by phase separation	14.34×10^2	-	-	-	No interference study and no real samples analysis	[7]

8.	MIP membranes functionalized by phase inversion imprinting	134.48 885.35	-	-	-	No interference study and no real sample analysis	[8]
9.	MIP (RNA-type Nucleobase pairing) electrochemical sensor	-	-	-	7.28	No interference study	[9]
10.	Present work	1.49-278.76	1.33-401.15	0.50	0.33	Interference and real sample studies	

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