

Article

# Computational Design of a Molecularly Imprinted Polymer for the Biomonitoring of the Organophosphorous Metabolite Chlorferron

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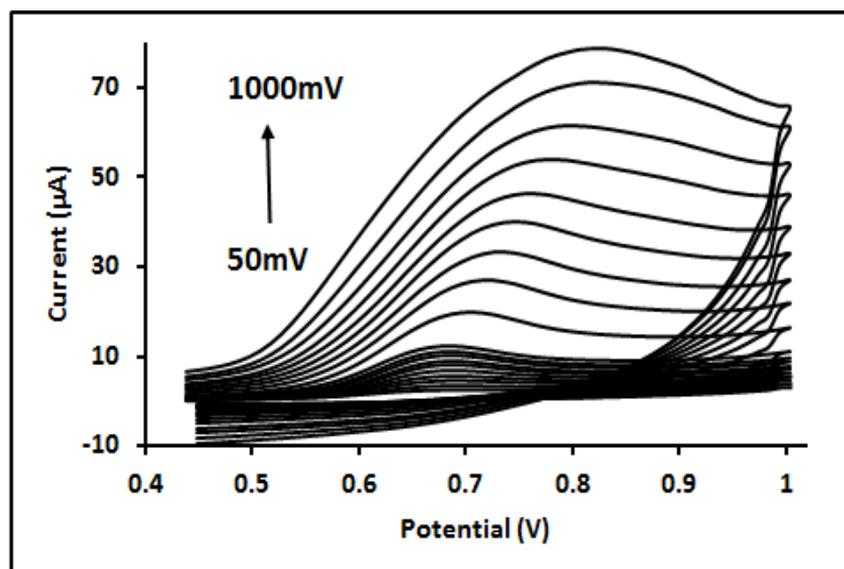
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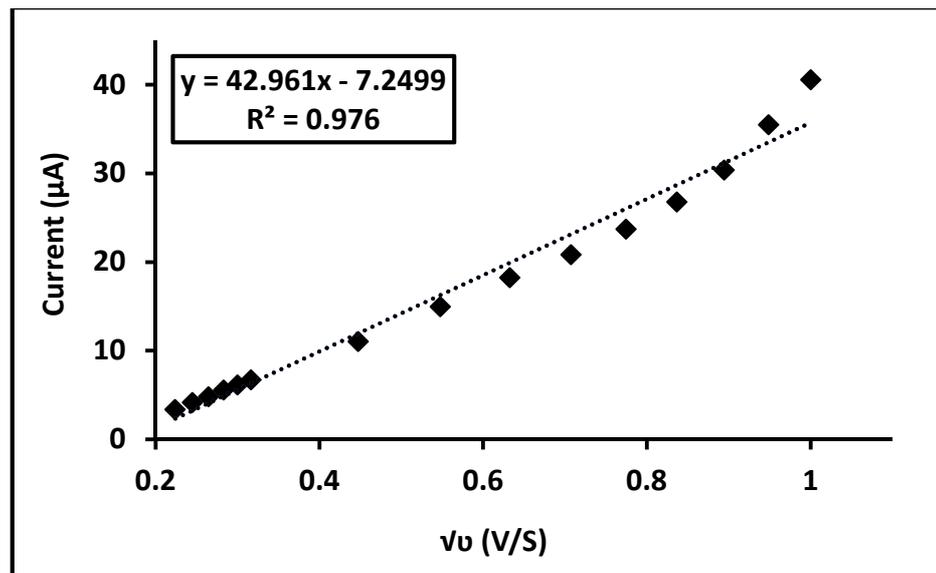
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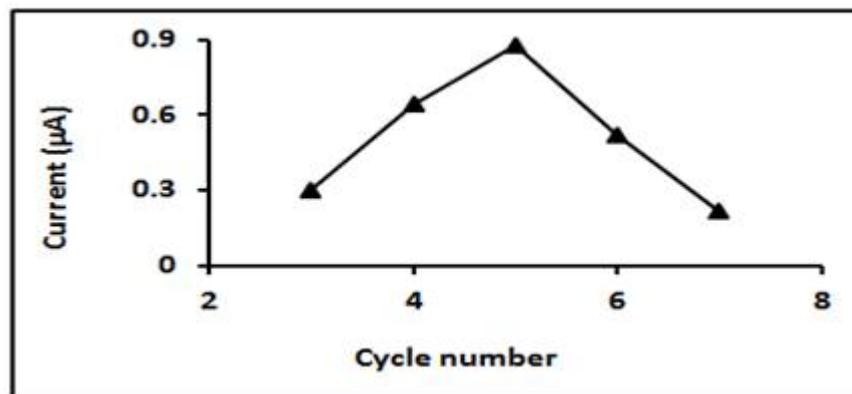
## Supplementary Materials:



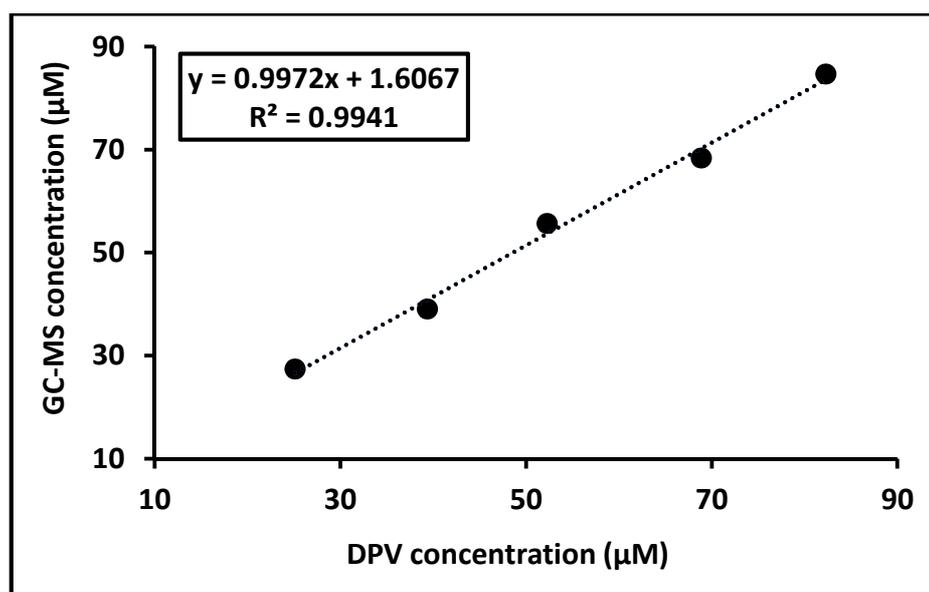
**Figure S1.** Cyclic voltammogram of 0.05mM CFN in 0.1M BR buffer solution (pH, 7) on bare GC electrode at scan rates ranging (50–1000) mV/s.



**Figure S2.** Relationship between peak current intensity of 0.05mM CFN and square root of scan rates ranging from 50–1000 mV/s.



**Figure S3.** Current response related to number of scan cycles used during electro polymerization of CFN-Py on GC electrode.



**Figure S4.** Comparison of concentration values 25, 40, 55, 70, and 85 µM CFN obtained in the experimental set with GC/MS and DPV on CFN-MIP sensor (n = 3 for each concentration).

The samples have been analysed by the two methods. If both methods are equivalent the slope is 1 and the intercept is 0. i.e.  $y=x$ . This would indicate both methods produce identical concentration values for the same sample.

**Table S1.** Intra-day and inter-day precision for seven concentrations of CFN using DPV measurements at CFN-MIP sensor.

Concentration (µM)	Intra-Day Precision		Inter-Day Precision	
	Mean ±SD (µM)	RSD (%)	Mean ±SD (µM)	RDS (%)
2	3.19±0.73	8.75%	2.98±0.73	13.1%
10	13.1±1.6	5.36%	11.6±0.58	10.3%
25	25.1±0.48	4.5%	21.1±0.38	8.17%
40	36.9±0.75	3.04%	36.5±2.9	3.58%
55	48.3±0.35	3.19%	49.8±0.54	4.88%
70	66.1± 0.47	3.13%	68.4±0.62	4.03%
85	91.2± 0.48	2.35%	87.7±0.64	3.22%

**Table S2.** Recovery experiments for various concentrations of CFN on CFN-MIP electrode using DPV measurements.

Concentration (µM)	Recovered Concentration (N=3)		
	Mean ±SD (µM)	RSD (%)	Recovered Percentage (%)
2	2.27±0.17	11.15%	80.61%
10	10.2±1.4	13.7%	102.02%
25	25.1±1.46	5.83%	100.42%
40	39.35±2.35	5.96%	98.37%
55	52.25±4.65	8.57%	98.64%
70	68.86±6.03	8.75%	98.38%
85	82.3±4.96	6.02%	96.82%