

Article

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

Bakhtiyar Qader <sup>1,2</sup>, Issam Hussain <sup>3</sup>, Mark Baron <sup>2</sup>, Rebeca Jiménez-Pérez <sup>2,4</sup>, Guzmán Gil-Ramírez <sup>2</sup> and Jose Gonzalez-Rodriguez <sup>2,\*</sup>

<sup>1</sup> Sulaimani Medicolegal Institute, Qanat Street, Sulaimani, Sulaymaniyah, 46001, Kurdistan Regional Government, Iraq; bakhtyar88@gmail.com

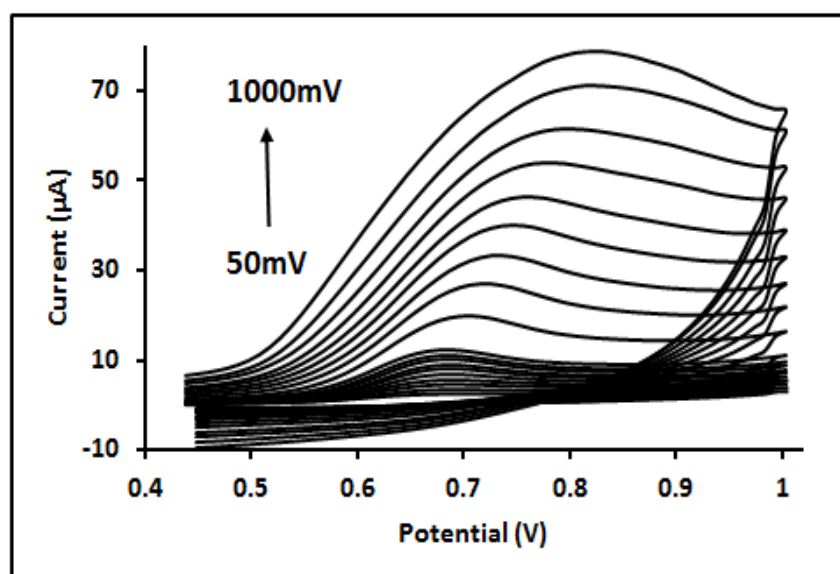
<sup>2</sup> Joseph Banks Laboratories, School of Chemistry, University of Lincoln, Lincoln LN6 7DL, UK; mbaron@lincoln.ac.uk (M.B.); Rebeca.Jimenez@uclm.es (R.J.-P.); GGilramirez@lincoln.ac.uk (G.G.-R.)

<sup>3</sup> School of Life Sciences, University of Lincoln, Brayford Pool, Lincoln LN6 7TS, UK; ihussain@lincoln.ac.uk

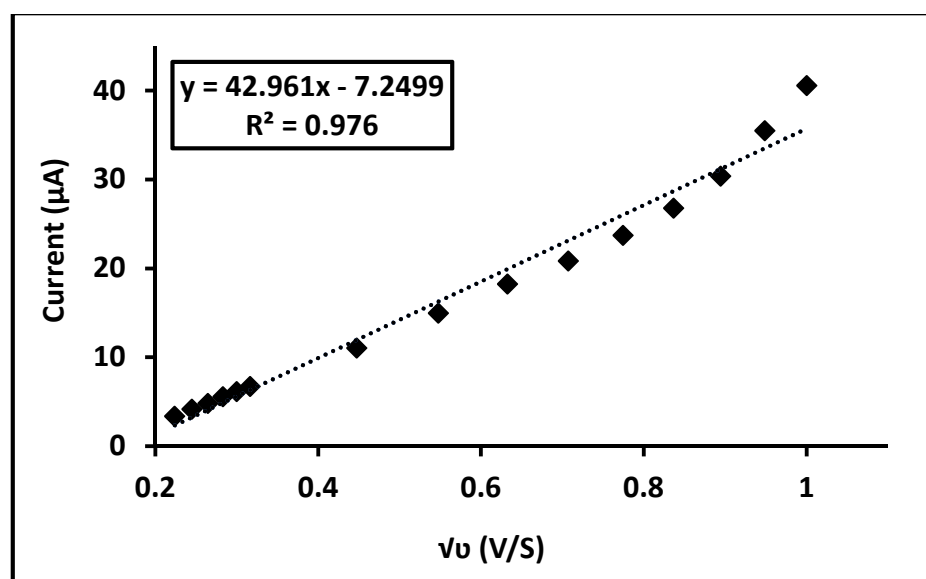
<sup>4</sup> Department of Physical Chemistry, Higher Technical School of Industrial Engineering, University of Castilla-La Mancha, Campus Universitario s/n, 02071 Albacete, Spain

\* Correspondence: jgonzalezrodriguez@lincoln.ac.uk

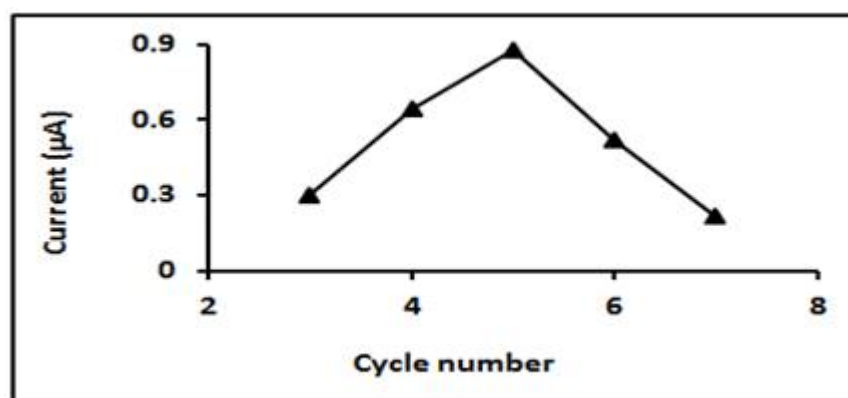
## Supplementary Materials:



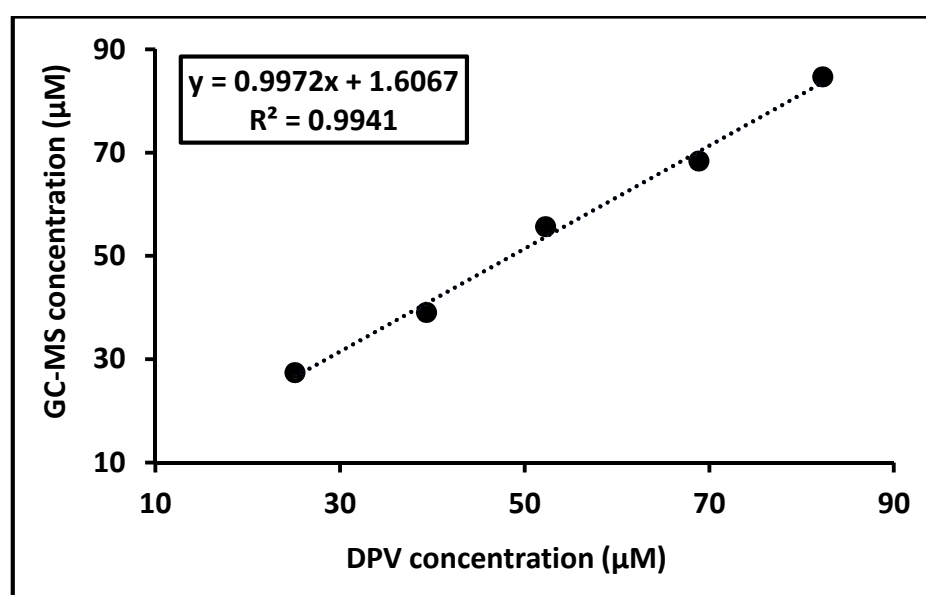
**Figure S1.** Cyclic voltammogram of 0.05mM CFN in 0.1M BR buffer solution (pH, 7) on bare GC electrode at scan rates ranging (50–1000) mV/s.



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

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

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