A Chemometrics Approach for Simultaneous Determination of Cyanazine and Propazine Based on a Carbon Paste Electrode Modified by a Novel Molecularly Imprinted Polymer

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The Supporting Information includes two tables. Table S-1 summarizes the results of the theoretical study for finding the best monomer for preparation of the molecularly imprinted polymer. The second one (Table S-2) shows the design matrix based on fractional factorial design. The responses for each experiment have been included in Table S-2.

Page: 3

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Table S-1

Calculated interaction energies (E, kJ mol^{-1}) for 1:1 and 1:2 template–monomer complexes with and without BSSE correction in the gas-phase.

Complexes	$\Delta E_{non\ corr.}$	$\Delta E_{corr.}$
PR-(MAA)	-78.015	-62.769
PR-(TFMAA)	-75.939	-61.415
PR-(AA)	-72.693	-57.345
PR-(AAM)	-68.325	-53.466
PR-(4-VP)	-36.806	-26.732
PR-(MMA)	-34.884	-22.908
PR-(ACN)	-31.470	-22.805
PR-(MAA)2	-154.216	-123.870
PR-(MAAM)2	-149.759	-120.283
PR-(TFMAA)2	-148.677	-119.713
PR-(AA)2	-143.598	-113.060
PR-(AAM)2	-134.712	-105.055
PR-(4-VP)2	-72.660	-52.143
PR-(MMA)2	-68.839	-45.242
PR-(ACN)2	-61.604	-44.364

Page: 4

Table S-2

Design matrix of FFD for identifying the important factors and the responses obtained.

Experiment No.	Factor				Ip for cyanazine (µA)	Ip for propazine (µA)
	pH	E_{acc} (V)	v (mV.sec^{-1})	t_{acc} (sec)		
1	1.0	-0.8	100	100	0.21	0.85
2	2.5	-0.3	55	200	10.50	11.00
3	4.0	-0.8	10	100	3.20	3.90
4	4.0	-0.8	100	300	2.50	5.60
5	2.5	-0.3	55	200	11.20	10.00
6	1.0	0.2	10	100	0.49	0.19
7	1.0	0.2	100	300	0.55	0.18
8	4.0	0.2	100	100	2.80	2.80
9	4.0	0.2	10	300	2.90	3.70
10	1.0	-0.8	10	300	5.00	4.60
11	2.5	-0.3	55	200	12.00	9.20

Considering the absolute values of the coefficients of the linear terms in the models obtained by FFD, it is observed that those of v and tacc are small. This is also the case about the interaction factors containing v and tacc. On the other hand, the absolute values of coefficients Ph and Eacc in the linear terms and the term showing their interaction is very high. Therefore, ph and Eacc and interactions containing both of them are relevant factors and are relevant factors v and tacc are not.