Supplementary Information

Toward robust quantification of dopamine and serotonin in mixtures using nano-graphitic carbon sensors

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Fig. S1: The electrochemical pathway of 5-HT oxidation, illustrating the primary and secondary reactions.



Fig. S2: Top eight principal components (PCs) estimated from a training set of voltammograms collected from an NG sensor with the engineered N-shape waveform in a solution where [DA] and [5-HT] is varied. The first few PCs correspond to variations in voltammograms that correspond to the dynamics in analyte concentrations. The last few PCs correspond to data noise.



Fig. S3: Sample of voltammograms of a) 5-HT, b) DA, and c) ΔpH from 7.4 from sensor NG-A.



Fig. S4: Score plots for CVs collected from an NG sensor with the engineered N-shape waveform, where the training set consists of (a) CVs of DA and ΔpH only, (c) CVs of 5-HT and ΔpH only. The scores of (a) and (c) are computed from the first two principal components (PC1 and PC2) of the training data which are shown in (b) and (d), respectively. The near-orthogonal angles between the score vectors (72.54 and 88.65) indicate the ability of NG sensors to distinguish among DA, 5-HT and ΔpH .



Fig. S5: (a) First two principal components of FSCV data collected from CF with a traditional triangular waveform. (b) First two principal components of FSCV data collected from CF with the engineered N-shape waveform.

Solution	[DA] (nM)	[5-HT] (nM)
Pure	25	0
Pure	50	0
Pure	100	0
Pure	125	0
Pure	0	25
Pure	0	50
Pure	0	100
Pure	0	125
Mix	25	25
Mix	25	50
Mix	25	100
Mix	50	25
Mix	50	50
Mix	50	100
Mix	100	25
Mix	100	50
Mix	100	100

Table S1: Concentrations of DA and 5-HT used in the experiments described in Sections 2.4-2.5

Table S2: Prediction accuracy on same-sensor (NG-A) test data of a PCR model (num. PCs=3) trained from CVs of an NG sensor (NG-A) with the engineered N-shape waveform

Solution	[DA] (nM)	[5-HT] (nM)	Num. samples	Mean absolute error (nM)		Mean absolute	
				DA	5-HT	DA	5-HT
Pure	25	0	6	1.4	3.1	6%	-
Pure	50	0	10	6.4	1.3	13%	-
Pure	100	0	15	4.9	1.0	5%	-
Pure	125	0	16	4.1	0.4	3%	-
Pure	0	25	5	2.4	3.0	-	12%
Pure	0	50	7	3.2	4.0	-	8%
Pure	0	100	10	2.1	8.4	-	8%
Pure	0	125	10	2.1	4.0	-	3%
Mix	25	25	7	0.6	0.7	2%	3%
Mix	25	50	6	0.4	2.6	2%	5%
Mix	25	100	7	2.8	2.5	11%	3%
Mix	50	25	9	3.7	0.8	7%	3%
Mix	50	50	10	1.2	1.2	2%	2%
Mix	50	100	7	6.6	2.0	13%	2%
Mix	100	25	11	2.4	3.9	2%	16%
Mix	100	50	8	3.9	1.8	4%	4%
Mix	100	100	8	3.7	5.1	4%	5%
Average			3.0	2.7	6%	6%	

 Table S3:
 Prediction accuracy on same-sensor (NG-A) test data of a two-parameter model

 trained from CVs of an NG sensor (NG-A) with the engineered N-shape waveform

Solution	[DA]	[5-HT]	Num.	Mean absolute error (nM)		Mean absolute percentage error	
	(1111)	(NIVI)	samples	DA	5-HT	DA	5-HT
Pure	25	0	6	4.8	2.3	19%	-
Pure	50	0	10	6.5	5.2	13%	-
Pure	100	0	15	6.6	2.5	7%	-
Pure	125	0	16	3.3	4.6	3%	-
Pure	0	25	5	10.1	4.4	-	17%
Pure	0	50	7	5.6	4.9	-	10%
Pure	0	100	10	2.9	13.3	-	13%
Pure	0	125	10	8.3	2.5	-	2%
Mix	25	25	7	6.1	6.4	25%	25%
Mix	25	50	6	2.4	6.9	10%	14%
Mix	25	100	7	2.4	7.8	10%	8%
Mix	50	25	9	1.5	1.8	3%	7%
Mix	50	50	10	1.0	2.0	2%	4%
Mix	50	100	7	8.2	2.0	16%	2%
Mix	100	25	11	3.5	2.5	3%	10%
Mix	100	50	8	6.5	1.6	6%	3%
Mix	100	100	8	5.1	5.2	5%	5%
Average				5.0	4.5	9%	9%

Table S4: Prediction accuracy on cross-sensor (NG-B) test data of a PCR model	(num. I	PCs=3)
trained from CVs of an NG sensor (NG-A) with the engineered N-shape waveform		

Solution	[DA]	[5-HT]	Num.	Mean absolute error (nM)		Mean absolute percentage error	
	(NIVI)	(NIN)	samples	DA	5-HT	DA	5-HT
Pure	25	0	7	2.0	0.5	8%	-
Pure	50	0	10	11.6	1.4	23%	-
Pure	100	0	19	6.4	0.3	6%	-
Pure	125	0	16	9.8	2.6	6%	-
Pure	0	25	5	2.6	2.3	-	9%
Pure	0	50	7	3.3	4.3	-	9%
Pure	0	100	10	3.3	8.7	-	9%
Pure	0	125	10	1.6	6.3	-	5%
Mix	25	25	7	0.4	3.1	2%	12%
Mix	25	50	6	0.4	5.9	1%	12%
Mix	25	100	7	1.7	4.9	7%	5%
Mix	50	25	9	2.6	3.2	5%	13%
Mix	50	50	10	1.7	2.1	3%	4%
Mix	50	100	7	7.9	5.5	16%	5%
Mix	100	25	11	4.6	2.7	5%	11%
Mix	100	50	8	8.8	4.1	9%	8%
Mix	100	100	8	3.3	10.1	3%	10%
Average				4.2	4.0	7%	9%

Solution	[DA] (nM)	[5-HT] (nM)	Num. samples	Mean absolute error (nM)		Mean absolute percentage error	
				DA	5-HT	DA	5-HT
Pure	250	0	15	54.4	80.6	22%	-
Pure	500	0	15	68.9	45.2	14%	-
Pure	1000	0	20	62.9	68.3	6%	-
Pure	2000	0	19	64.5	53.0	3%	-
Pure	0	100	20	43.4	56.9	-	57%
Pure	0	200	10	11.6	58.0	-	29%
Pure	0	500	20	51.1	82.5	-	16%
Pure	0	1000	20	57.7	99.7	-	10%
Pure	0	1500	10	86.5	410.3	-	27%
			Average	55.7	106.1	11%	28%

Table S5: Prediction accuracy on same-sensor test data of a PCR model (num. PCs=8) trained from CVs of a CF microelectrode with the engineered N-shape waveform