Electronic Supplementary Material

Excitation-emission fluorescence matrix acquired from glutathione capped CdSeS/ZnS quantum dots in combination with chemometric tools for pattern-based sensing of neurotransmitters

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Scheme S.1. Schematical representation of procedure for Excitation-Emission Fluorescence data preparation. **(a)** Preparation of the Excitation-Emission Matrixes by arranging the appropriate emission spectra acquired during fluorescence measurements. **(b)** Arrangement of the Excitation-Emission Matrixes in a cube and their unfolding by combining the spectral modes.

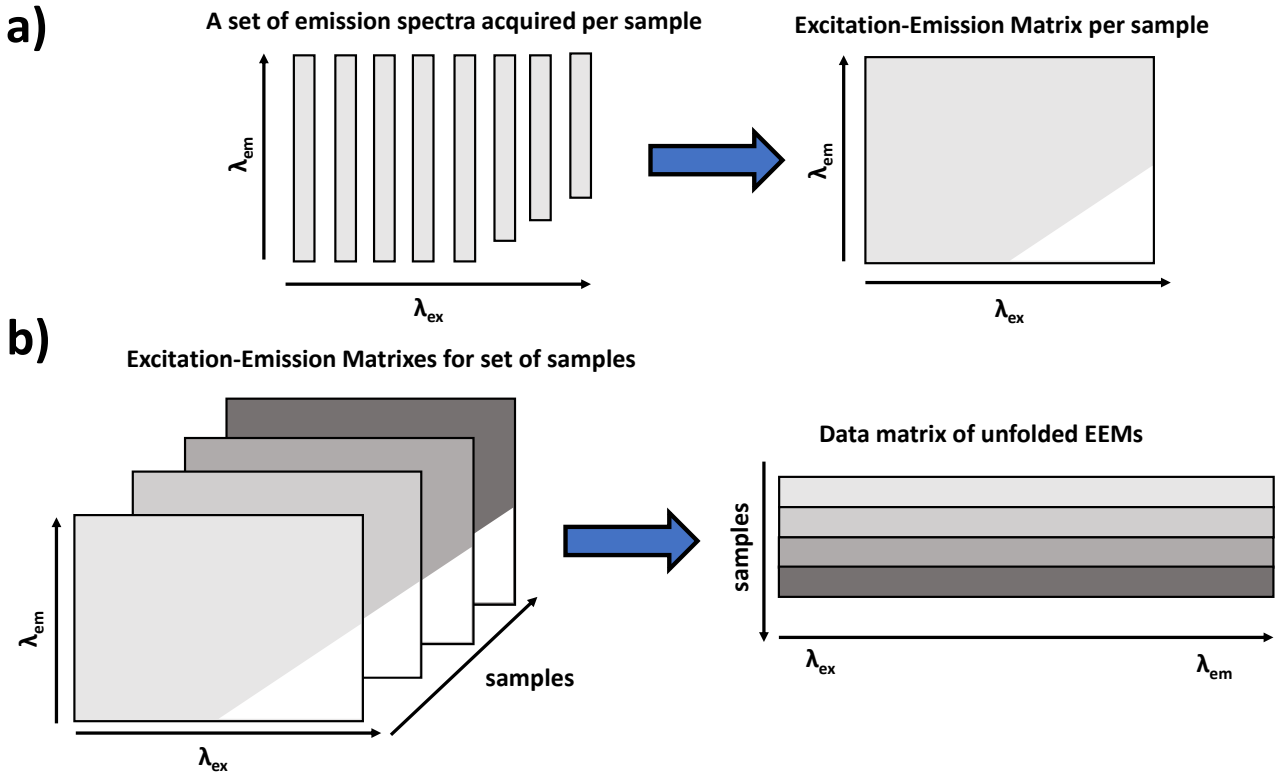

Table S.1. The measurement protocol used for acquisition of Excitation-Emission Matrixes.

Procedure step	λ_{ex} [nm]	λ_{em} [nm]
1	600	620 – 700
2	590	610 – 700
3	580	600 – 700
4	570	590 – 700
5	560	580 – 700
6	550	570 – 700
7	540	560 – 700
8	530	550 – 700
9	520	550 – 700
10	510	550 – 700
11	500	550 – 700
12	490	550 – 700
13	480	550 – 700
14	470	550 – 700
15	460	550 – 700
16	450	550 – 700
17	440	550 – 700
18	430	550 – 700
19	420	550 – 700
20	410	550 – 700
21	400	550 – 700
22	390	550 – 700
23	380	550 – 700
24	370	550 – 700
25	360	550 – 700
26	350	550 – 700
27	340	550 – 700
28	330	550 – 700
29	320	550 – 700
30	310	550 – 700
31	300	550 – 700
32	290	550 – 700
33	280	550 – 700
34	270	550 – 700

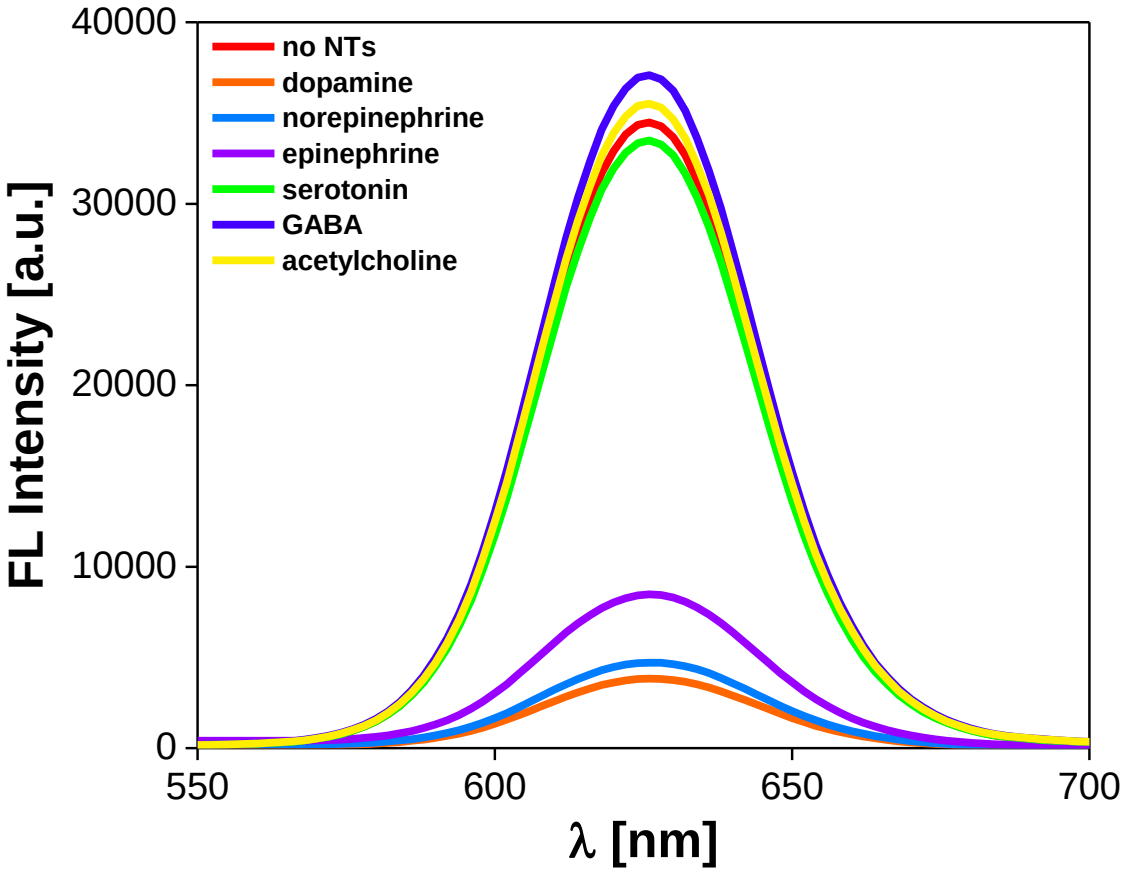

Fig S. 1. Fluorescence spectra (i.e. 1st-order fluorescence data) of GSH capped QDs without and with influence of neurotransmitters at 50 µM concentration acquired at λ_{ex} = 430 nm, $\lambda_{em} \in$ [550 nm, 700 nm].

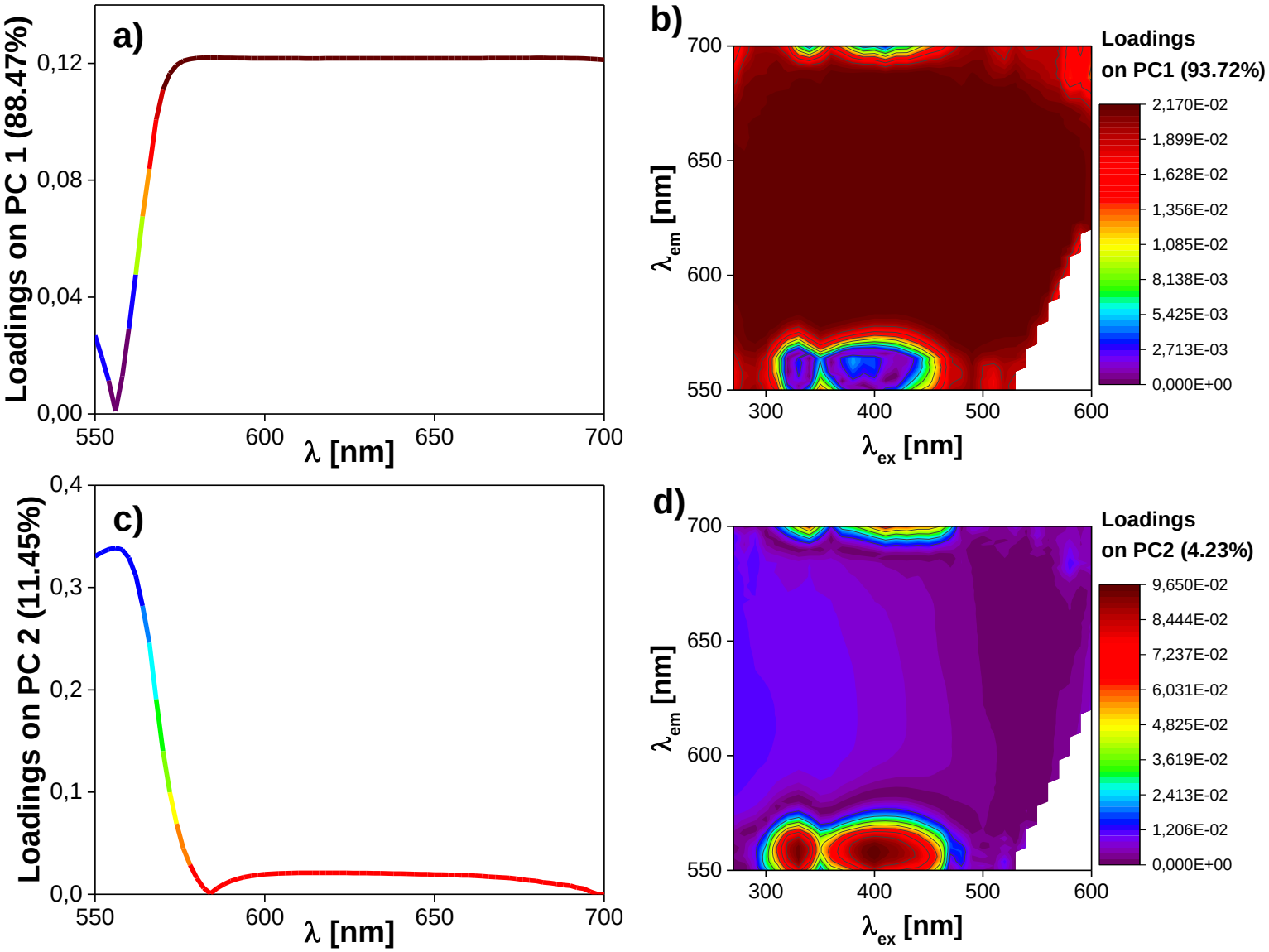

Fig S. 2. Loadings plots on **(a, b)** PC1 and **(c, d)** PC2 showing which variables correspond to clusterization of samples in PCA/UPCA models obtained with **(a, c)** 1st-order fluorescence data (i.e. emission spectra acquired at λ_{ex} = 430, $\lambda_{em} \in$ [550 nm, 700 nm] and **(b, d)** 2nd-order fluorescence data (i.e. Excitation-Emission Matrix acquired at $\lambda_{ex} \in$ [270 nm, 600 nm], $\lambda_{em} \in$ [550 nm, 700 nm]. For clarity, the absolute values of the loadings were presented.

Table S. 2. Definitions of quality performance metrics used to assess the quality of PLS-DA/UPLS-DA models **(a)** accuracy, **(b)** precision, **(c)** sensitivity, **(d)** specificity. TN – true negatives, FN – false negatives, FP – false positives, TP – true positives.

a)

$$accuracy = \frac{(TP + TN)}{(TP + TN + FP + FN)}$$

b)

$$precision = \frac{TP}{(TP + FP)}$$

c)

$$sensitivity = \frac{TP}{(TP + FN)}$$

d)

$$specificity = \frac{TN}{(TN + FP)}$$

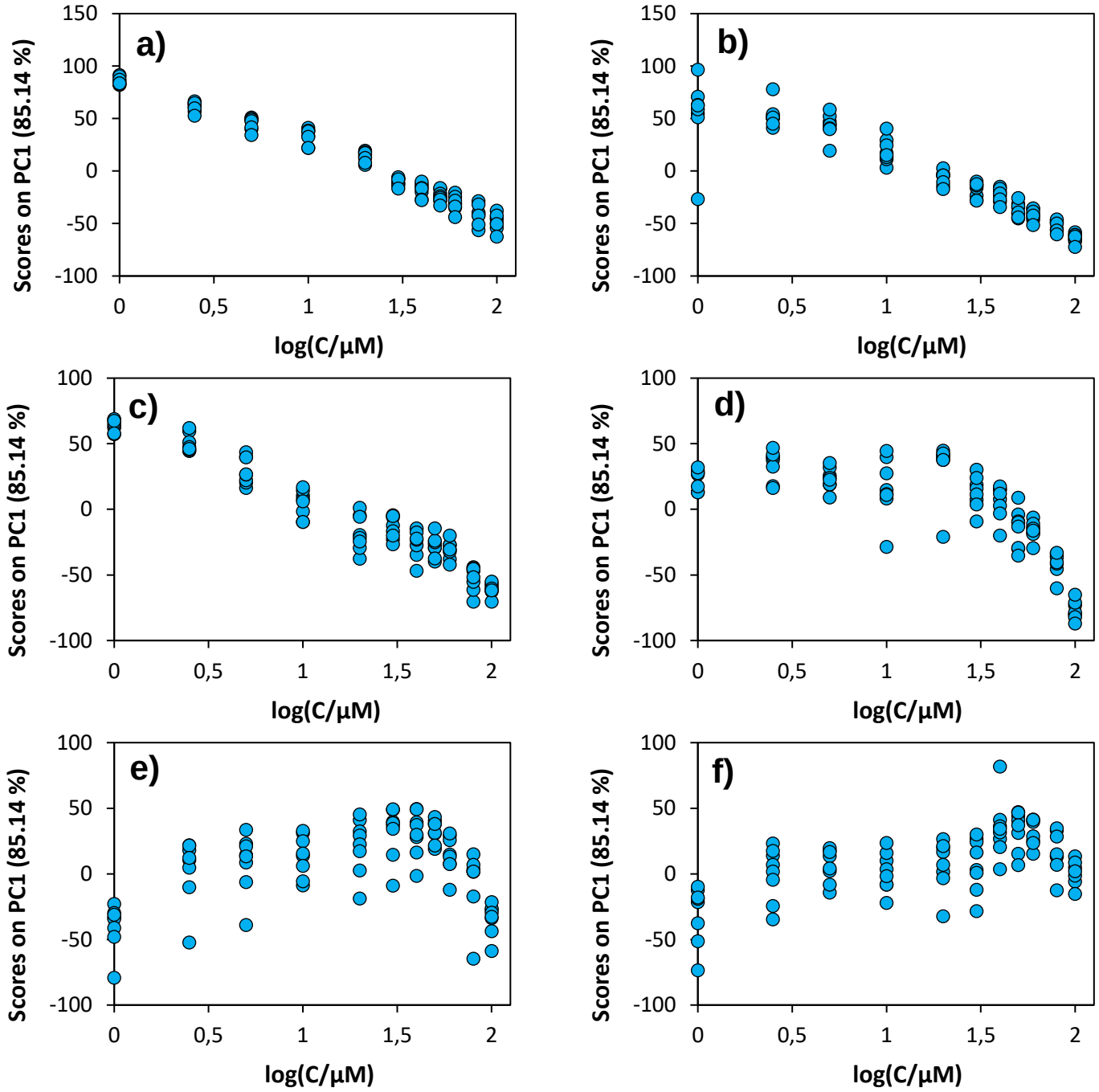

Fig S. 3. Relationship between the logarithms of concentration (µM) of neurotransmitters and scores on PC1 for **(a)** dopamine**, (b)** norepinephrine, **(c)** epinephrine, **(d)** serotonin, **(e)** GABA, **(f)** acetylcholine.

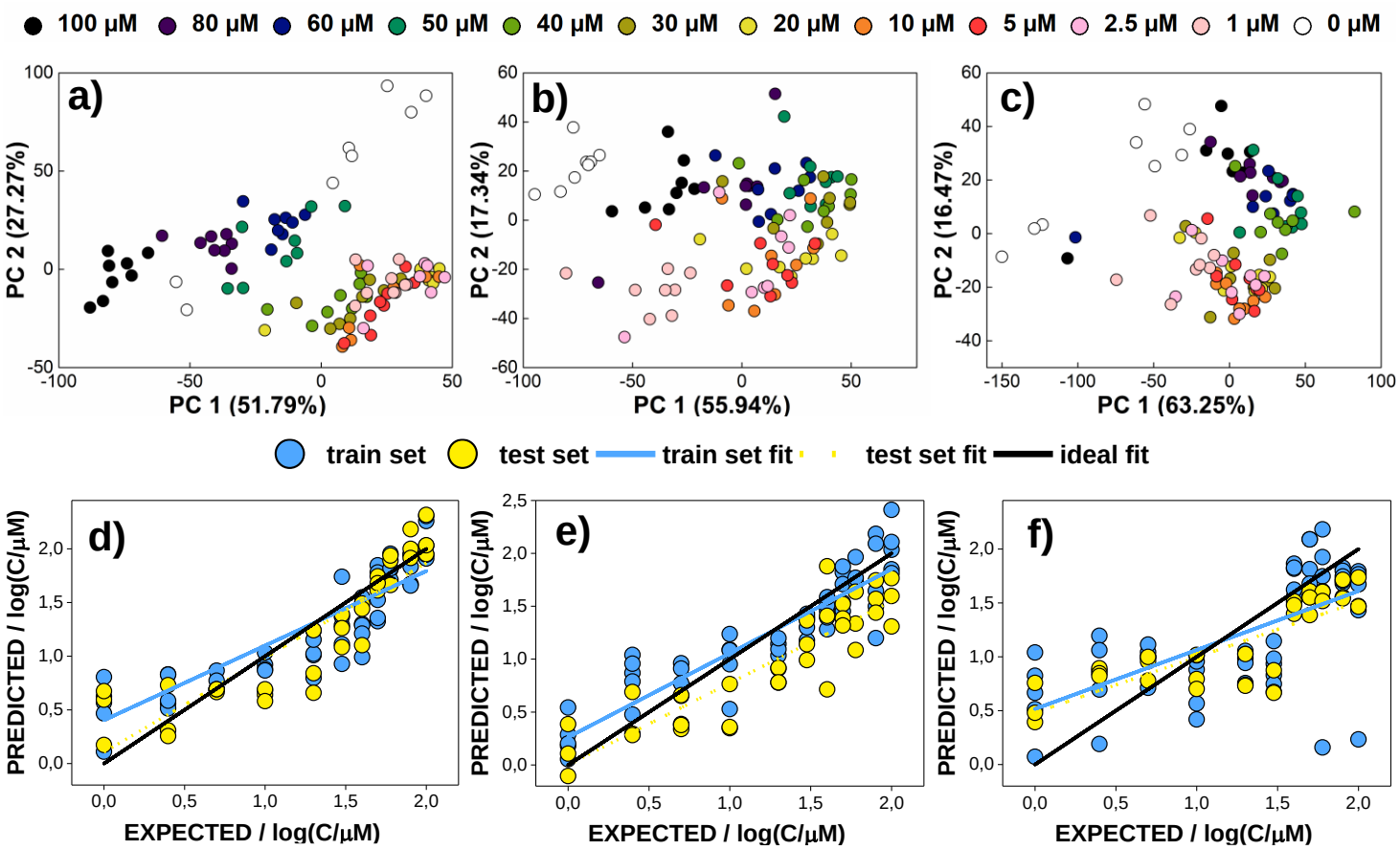

Fig S. 4. Quantitative analysis of catecholamine neurotransmitters. Differentiation of samples at various concentration levels visible on UPCA score plots for **(a)** serotonin, **(b)** GABA, **(c)** acetylcholine. UPLS model performances shown as linear fit of the predicted vs. real logarithm of concentrations for **(d)** serotonin, **(e)** GABA, **(f)** acetylcholine.

Table S. 3. Parameters of linear fit of real and UPLS-predicted logarithms of concentration (μM) for non-catecholamine neurotransmitters.

	serotonin	GABA	acetylcholine
RMSE	0.093	0.071	0.277
RMSEP	0.289	0.404	0.409
	train set		
a	0.695 ± 0.078	0.7946 ± 0.052	0.547 ± 0.093
b	0.404 ± 0.110	0.2614 ± 0.073	0.516 ± 0.130
R2	0.602 ± 0.360	0.817 ± 0.240	0.397 ± 0.429
	test set		
a	0.881 ± 0.079	0.773 ± 0.072	0.515 ± 0.069
b	0.106 ± 0.111	0.001 ± 0.101	0.482 ± 0.097
R2	0.800 ± 0.284	0.791 ± 0.257	0.641 ± 0.249