Electronic Supplementary Material (ESI) for Analytical Methods.

Quantification of phosphatides in sunflower oils using potentiometric e-tongue

Regina Belugina[a,*], Anna Senchikhina[a], Sergey Volkov[b], Alexander Fedorov[a,b], Andrey Legin[a,c], Dmitry Kirsanov[a,c,*]

[a] ITMO University, St Petersburg, Russia

[b] All-Russian Research Institute of Fats (ARRIF), St Petersburg, Russia

[c] Institute of Chemistry, Saint Petersburg State University, St Petersburg, Russia

* Corresponding authors:

reginabelugina@yandex.ru (R. Belugina)

d.kirsanov@gmail.com (D. Kirsanov)

Supplementary material

Table S1. Sensor membrane compositions.

Sensor name	Membrane composition
S1	Polycrystalline mixture AgCl-Ag_2S
S2	Polycrystalline mixture AgBr-Ag_2S
S3	Polycrystalline mixture Ag_2S
S4	Polycrystalline mixture AgI-Ag_2S
S5	Metallic Au
S6	Metallic Sb
S7	Chalcogenide glass Cu-Ag-As-Se-Te
S8	Chalcogenide glass CdI_2-AgI-As_2S_3
S9	Chalcogenide glass Ag_2S-As_2S_3

Polycrystalline sensors were prepared from the pressed mixtures of salts according to [Mikhelson, K.N., 2013. Ion-Selective Electrodes. Springer, USA.}

Chalcogenide glass sensor membranes were synthesized according to [Vlasov, Y.G., Bychkov, E.A., Legin, A.V., 1994. Chalcogenide glass chemical sensors: research and analytical applications. Talanta 41 (6), 1059–1063]

Table S2. Root mean square errors for regression models recalculated into the concentration of phosphatides expressed in mg of phosphatides per 100 g of oil (validation).

	Whole database	Unrefined oil	Refined oil	Low concentration of PLs oil (0.0-0.1%)	High concentration of PLs oil (0.1-2.27%)
SVR	0.52	0.91	0.005	0.009	0.24
PLS	0.35	0.44	0.008	0.036	0.23
MLR	0.33	0.45	0.006	0.008	0.27

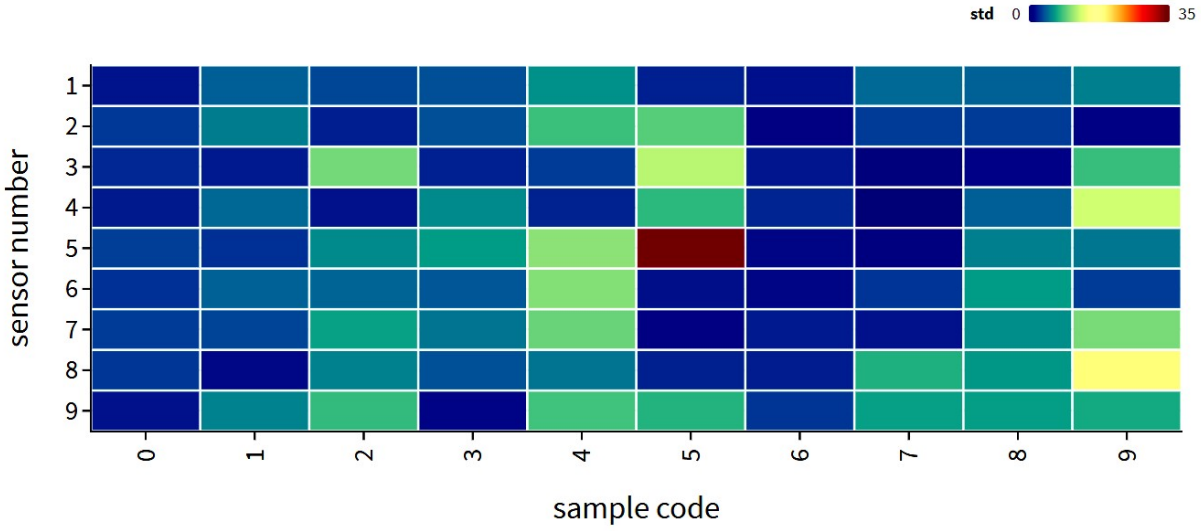


Figure S1. Heat map corresponding to standard deviations between three replicate measurements conducted in refined oils calculated for each sensor.

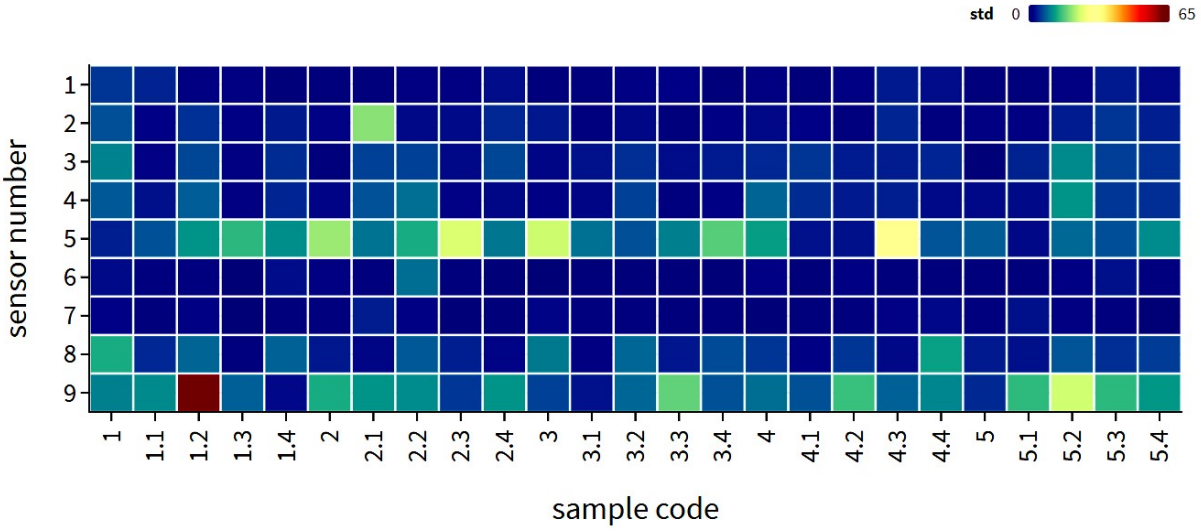
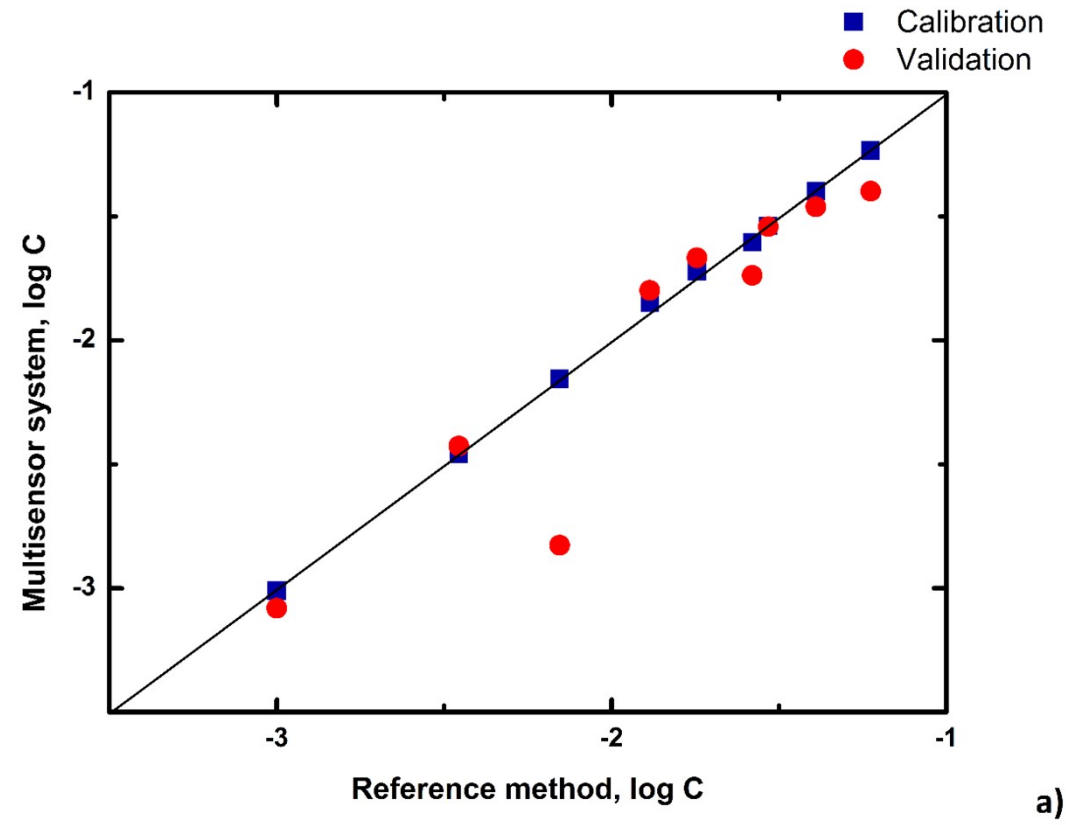


Figure S2. Heat map corresponding to standard deviations between three replicate measurements conducted in unrefined oils estimated for each sensor.



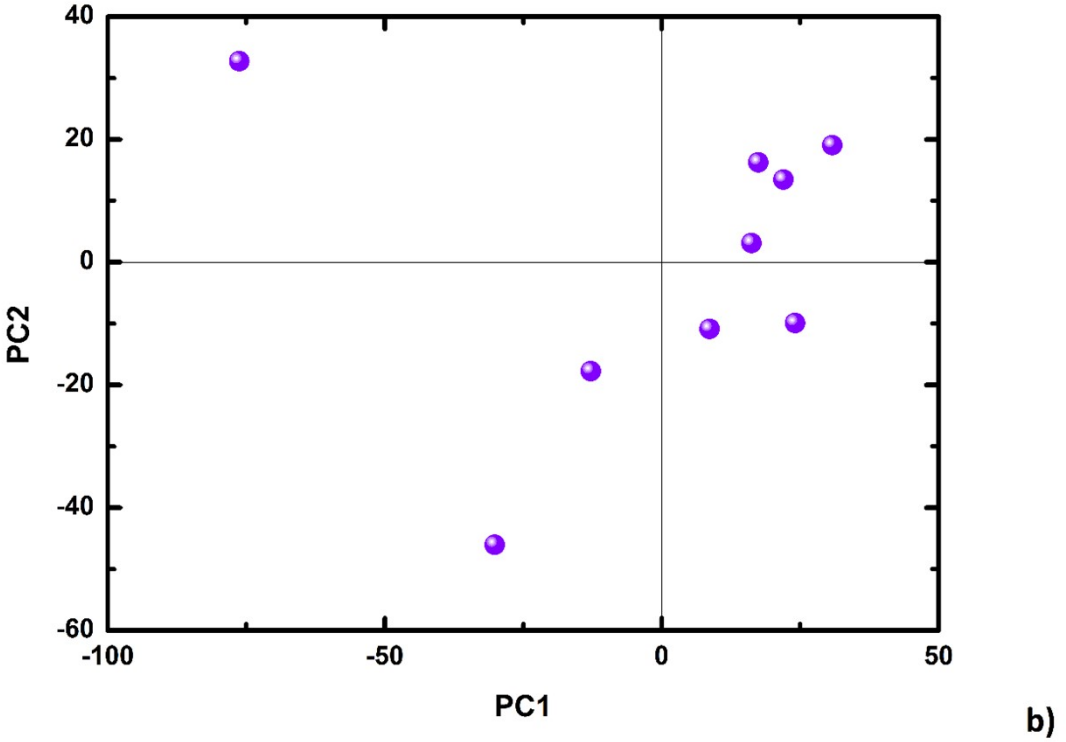


Figure S3. Results of refined oil samples data analysis. a - PLS regression model for determination of phosphatide logarithmic concentrations in refined sunflower oils; b – PCA score plots for PC1 and PC2 based on the potentiometric ET data

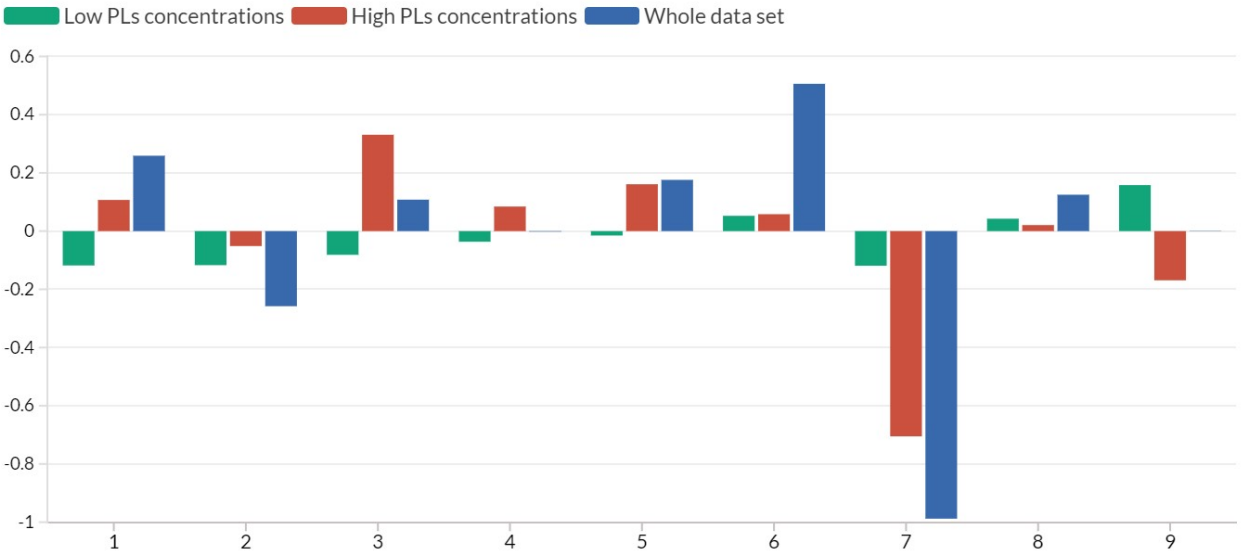


Figure S4. PLS Regression Coefficients for the models for determination of phosphatide concentrations in all sunflower oils (whole data set), sunflower oils with low concentration of PLs (0.0-0.1 %), and sunflower oils with high concentration of PLs (0.1-2.27 %).

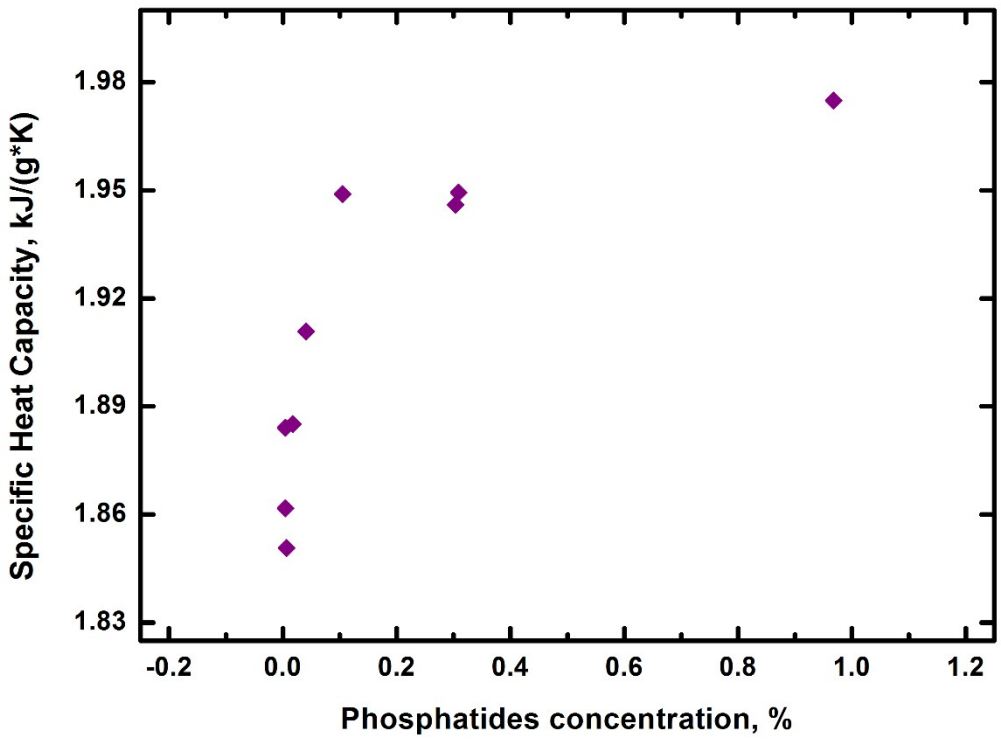


Figure S5. Dependence of specific heat capacity of sunflower oil samples on phosphatide concentrations. The temperature is 25 °C.

The measurement of specific heat capacity was based on the differential scanning calorimetry technique using Netzsch DSC 204 Phoenix F1. The parameters of studied oils were compared with etalon (sapphire). Each oil sample was measured in three physically different replicas. The results were

averaged. Temperature – time dependence was registered in temperature interval from 0 to 150 °C with the heating rate 10 °C per minute. Nitrogen was used as purge and protective gas with respective flow rates set at 20 and 50 mL per minute respectively. An empty reference pan was used to calibrate the equipment using sapphire with known thermal properties, which was placed in sample pan and studied.