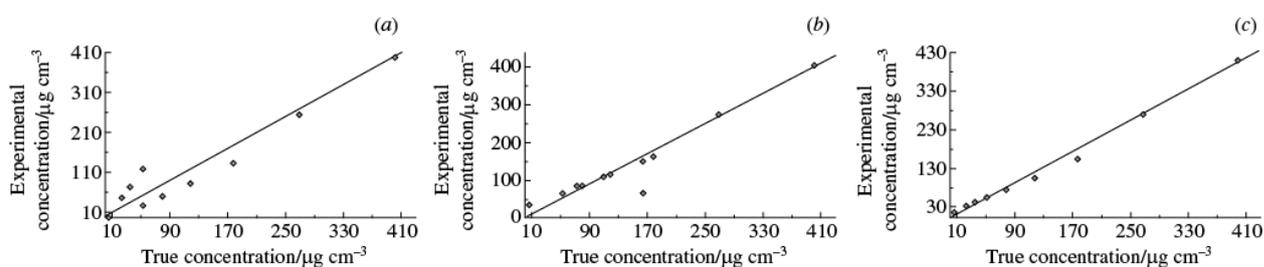


## Near IR spectroscopy of the solutions of a bacteriochlorin derivative as a quantitative method for the quality assurance of liquid products

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### Experimental

The solutions of compound **1** were prepared in *n*-butanol (reagent grade), AI95 gasoline (premium grade, Rosneft), and an equivolume mixture of gasoline and *n*-butanol. The spectra of strongly diluted solutions were recorded in cells with an optical path length of 1 cm. The spectra of more concentrated solutions were recorded through the lateral surface of a cylindrical tube with an internal diameter of 3 mm. The spectra were recorded on a Multi Bruker Purpose Analyzer FT-NIR spectrometer in standard configuration. The detection range was 15 000–4000  $\text{cm}^{-1}$ , the transmission mode with a spectral resolution of 8  $\text{cm}^{-1}$  and averaging of 32 interferograms was used. The absorption spectra in the visible region and a part of the NIR range were measured with a Perkin–Elmer Lambda instrument. The NIR spectra were processed using the OPUS 6.5 program package, including the Quant 1 and 2 programs for quantitative analysis. Calibration equations for prediction vs. true graphs were as follows: (a)  $y = -0.011982 + 0.000743x$ ; (b)  $y = 0.031023 + 0.000678x$ ; (c)  $y = 0.01511 + 0.056995x$ . The standard glass cylindrical tubes (internal diameter, 3 mm; height, 40 mm) were used to record the spectra of solution at concentrations from 400 to 53  $\mu\text{g cm}^{-3}$ , whereas more diluted solutions from 53 to 1.26  $\mu\text{g cm}^{-3}$  were studied in a 10-mm quartz cell.



**Figure S1** Calibration graphs of predicted value of compound **1** concentration vs. true value (as prepared) in the range from 6.28 to 400  $\mu\text{g cm}^{-3}$ : predicted value of concentrations for (a) measurements in a tube under assumption of optical path to be 3 mm; (b) measurements in a tube after correction of optical path by integral ratio factor at 53  $\mu\text{g cm}^{-3}$ ; (c) model with reference to solvent band as internal intensity standard.