Control of composition of mineral waters using Raman spectroscopy and artificial neural networks

A. Vervald, S. Burikov, E. Vervald, T. Dolenko, A. Efitorov,

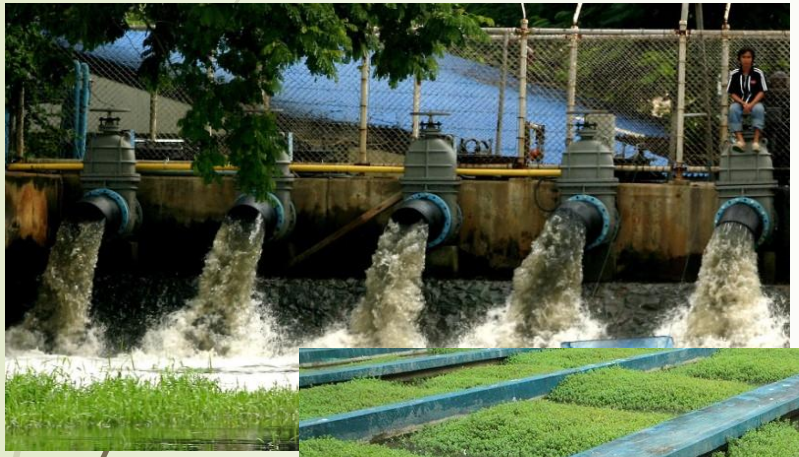
K. Laptinskiy, I. Plastinin, O. Sarmanova, and S. Dolenko

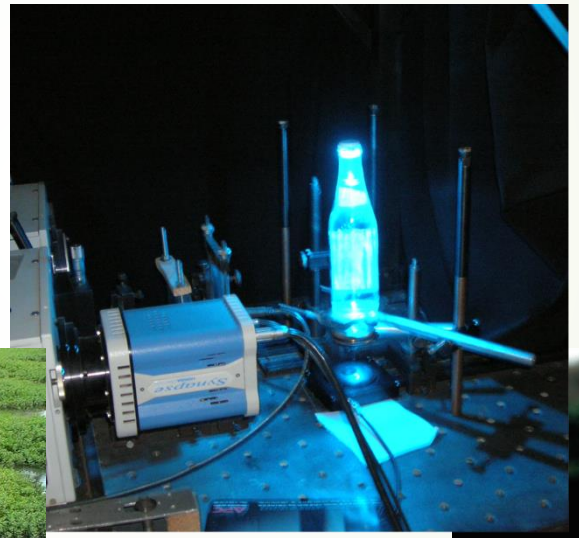
Physical Department, M.V. Lomonosov Moscow State University
D.V. Skobeltsyn Institute of Nuclear Physics, M.V. Lomonosov Moscow State University

Problem of composition determination

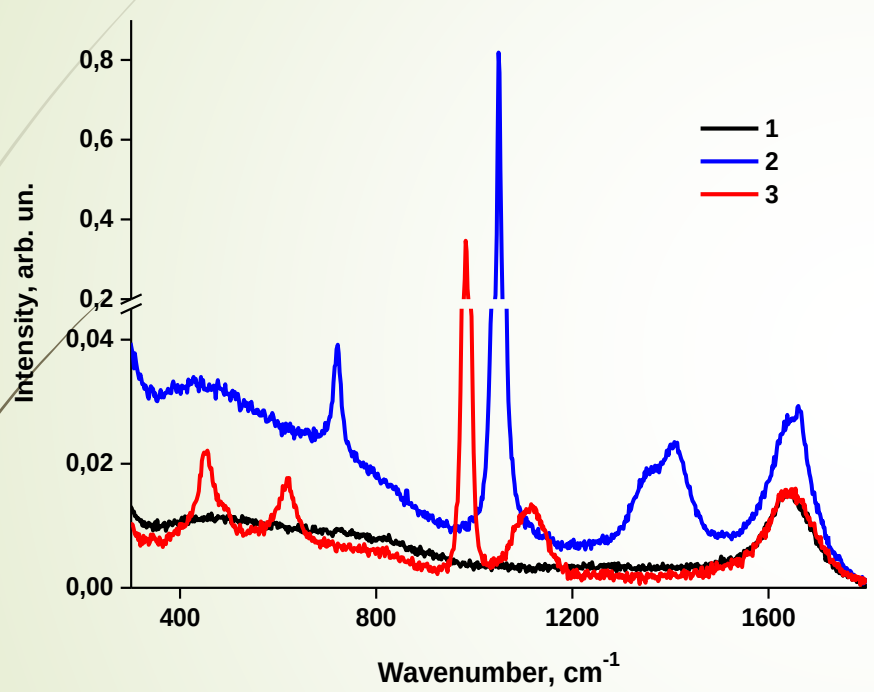
Multi-component water solution:

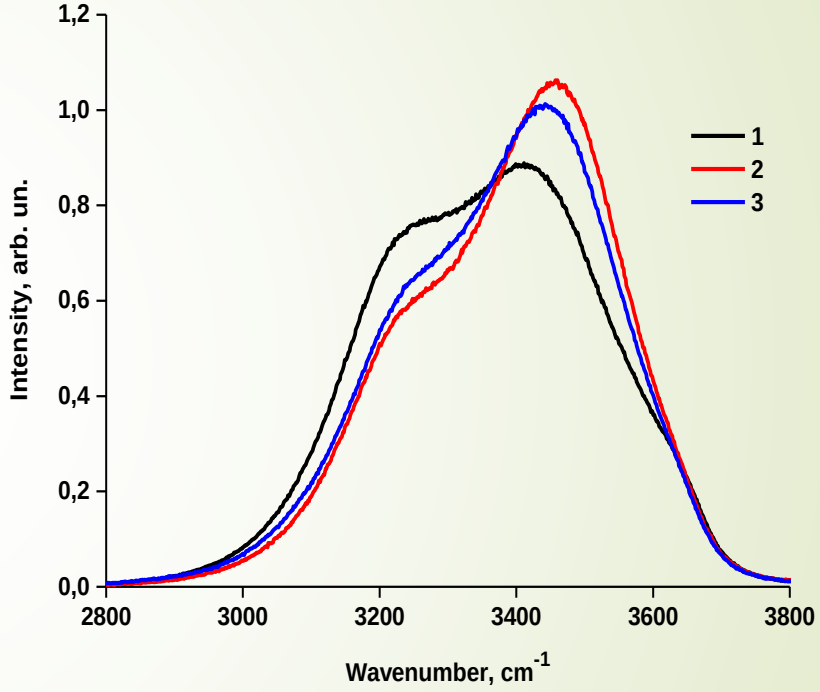
$MgSO_4$, $Mg(NO_3)_2$, LiCl, $LiNO_3$, NH_4F, $(NH_4)_2SO_4$, $KHCO_3$, KF, $NaHCO_3$, NaCl





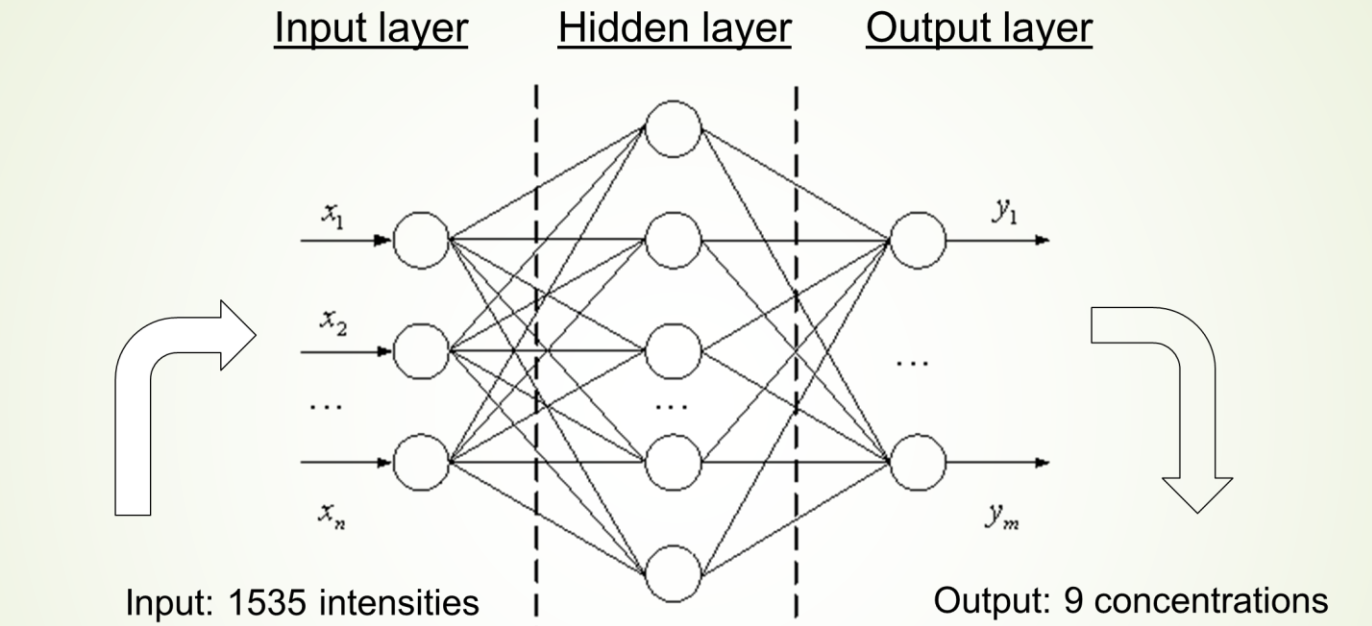
Methods: Raman spectroscopy



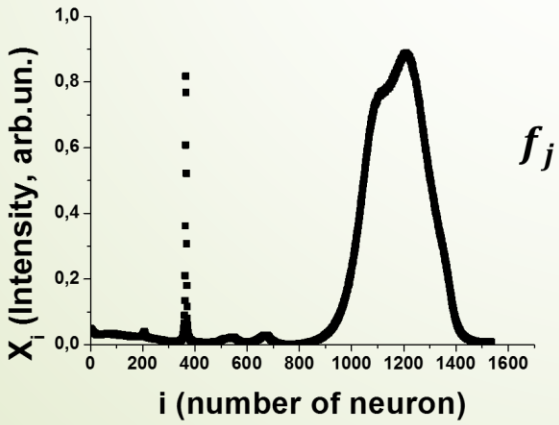


Raman spectra of water and aqueous solutions of different inorganic salts
(Left) in the 300-1800 cm^{-1} spectral: 1 - water, 2 - KNO_3 - 1 M, 3 - Li_2SO_4 - 1M; and
(Right) Raman stretching bands: 1 - water, 2 - CsI - 2M, 3 - NaCl, NH4Br, Li_2SO_4 - 0.4 M, KNO_3 and CsI - 0.6 M.

Methods: Artificial Neuron Networks

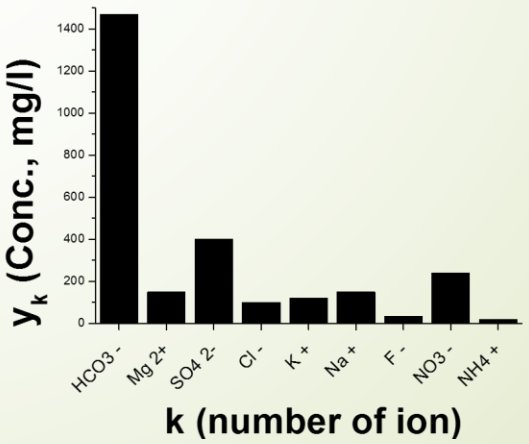


Input: 1535 intensities



$$f_j\left(\sum_{i=1}^{1535} x_i * w_{ij}\right)$$

Output: 9 concentrations



Methods: Application of ANNs

1. Training of ANN:

– training set

2. Test of quality of ANN being trained:

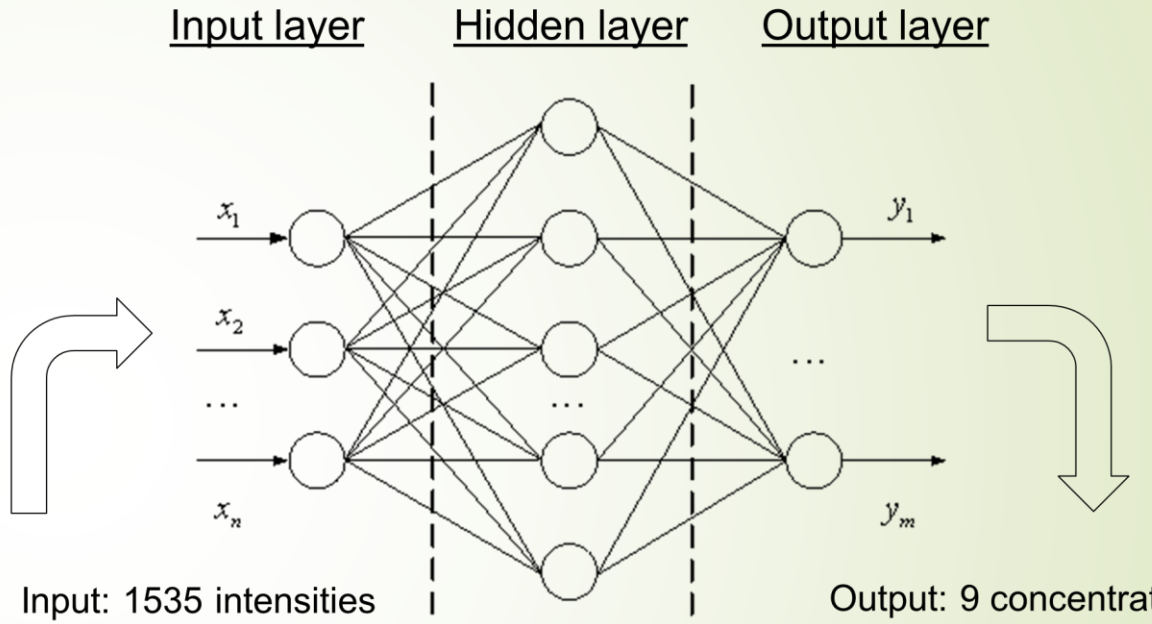
– validation set

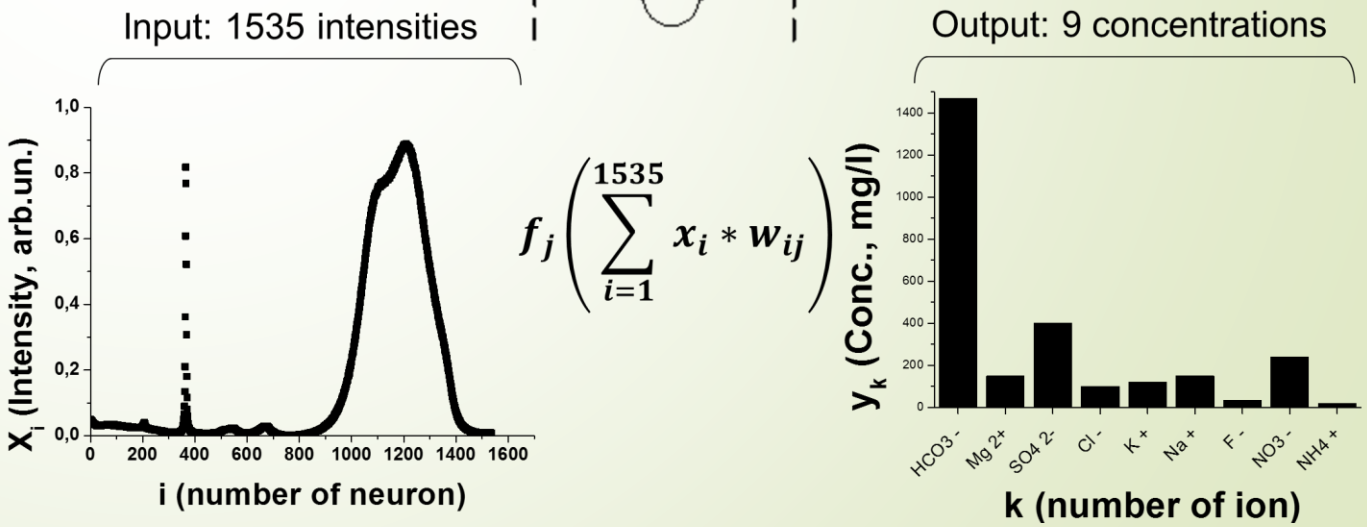
3. Evaluation of accuracy of determination of target parameters by a trained ANN:

– examination set

Training set – 70%, validation set – 20%, examination set – 10%

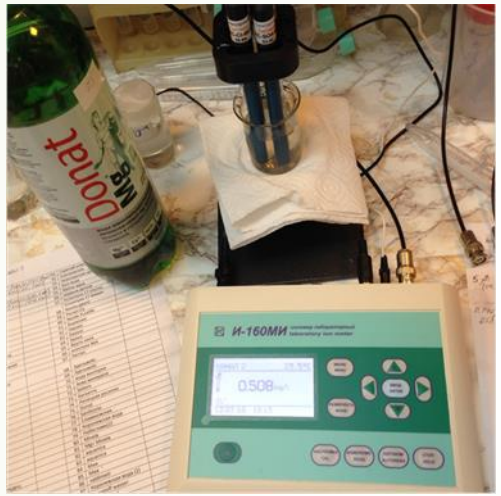
Perceptron with 3 hidden layers (64, 32, 16 neurons)

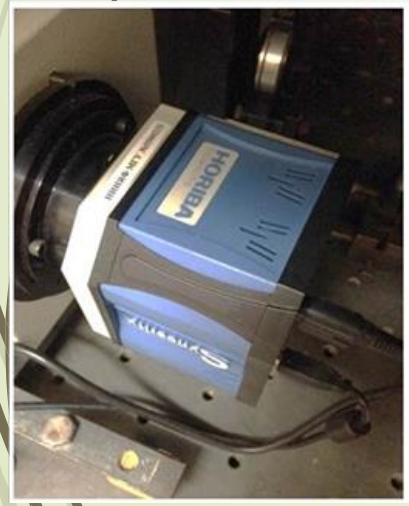


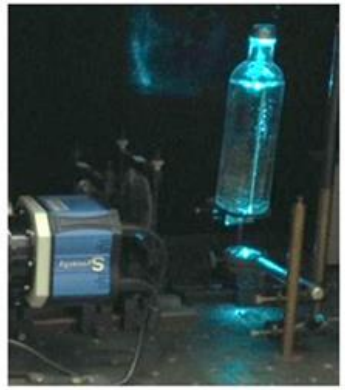


Training of ANN

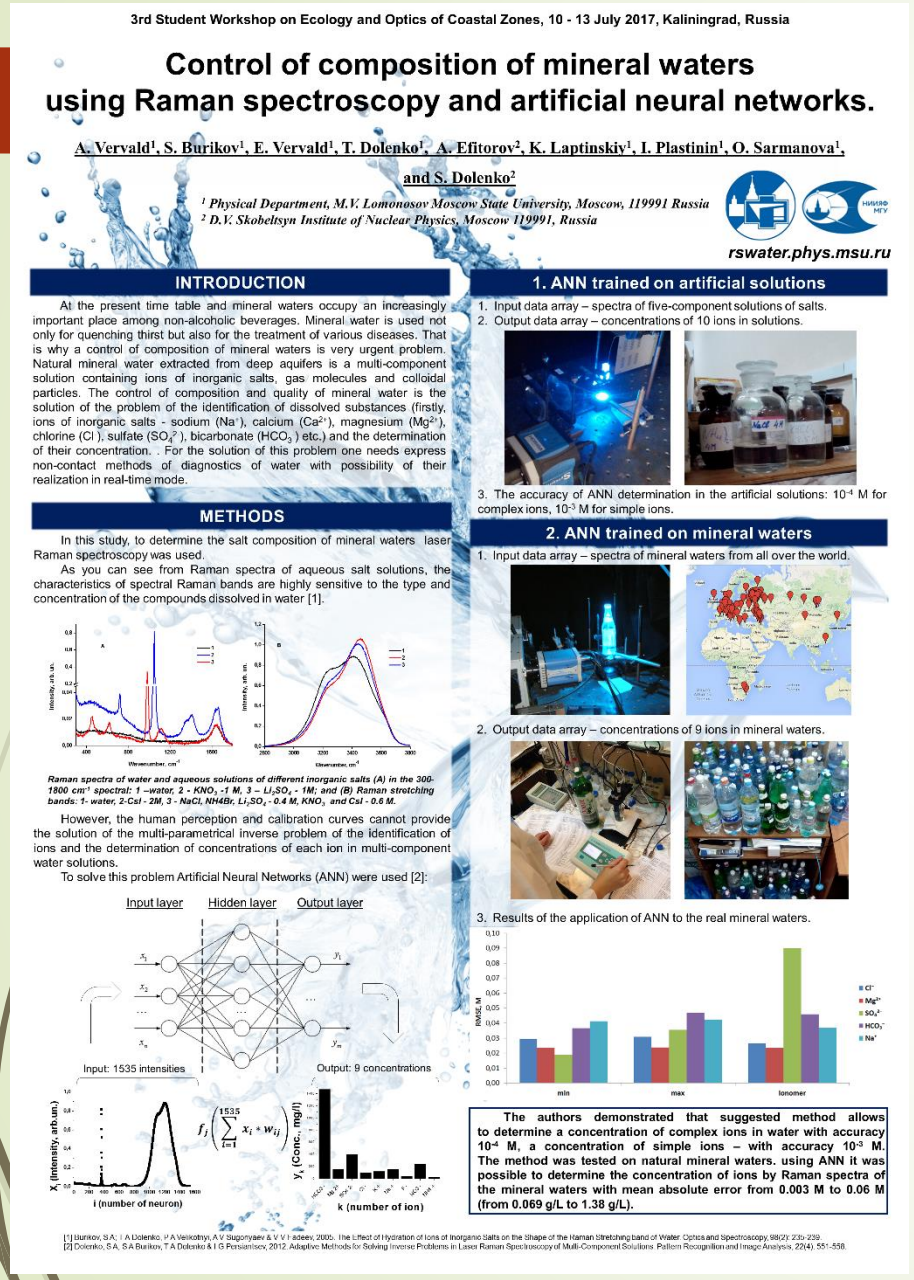
160 mineral waters of various manufacturers from various points of the globe







Number of solutions/spectra: 776



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[1] Physical Department, M.V. Lomonosov Moscow State University, Moscow, 119991 Russia
[2] D.V. Skobeltsyn Institute of Nuclear Physics, Moscow 119991, Russia

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INTRODUCTION

At the present time table and mineral waters occupy an increasingly important place among non-alcoholic beverages. Mineral water is used not only for quenching thirst but also for the treatment of various diseases. That is why a control of composition of mineral waters is very urgent problem. Natural mineral water extracted from deep aquifers is a multi-component solution containing ions of inorganic salts, gas molecules and colloidal particles. The control of composition and quality of mineral water is the solution of the problem of the identification of dissolved substances (firstly, ions of inorganic salts - sodium (Na^+), calcium (Ca^{2+}), magnesium (Mg^{2+}), chlorine (Cl^-), sulfate (SO_4^{2-}), bicarbonate (HCO_3^-) etc.) and the determination of their concentration. . For the solution of this problem one needs express non-contact methods of diagnostics of water with possibility of their realization in real-time mode.

METHODS

In this study, to determine the salt composition of mineral waters laser Raman spectroscopy was used.

As you can see from Raman spectra of aqueous salt solutions, the characteristics of spectral Raman bands are highly sensitive to the type and concentration of the compounds dissolved in water [1].

Raman spectra of water and aqueous solutions of different inorganic salts (A) in the 300-1800 cm^{-1} spectral: 1 –water, 2 - KNO_3 -1 M, 3 – Li_2SO_4 - 1M; and (B) Raman stretching bands: 1- water, 2-CsI - 2M, 3 - NaCl, NH4Br, Li_2SO_4 - 0.4 M, KNO_3 and CsI - 0.6 M.

However, the human perception and calibration curves cannot provide the solution of the multi-parametrical inverse problem of the identification of ions and the determination of concentrations of each ion in multi-component water solutions.

To solve this problem Artificial Neural Networks (ANN) were used [2]:

1. ANN trained on artificial solutions

1. Input data array – spectra of five-component solutions of salts.
2. Output data array – concentrations of 10 ions in solutions.

3. The accuracy of ANN determination in the artificial solutions: 10^{-4} M for complex ions, 10^{-3} M for simple ions.

2. ANN trained on mineral waters

1. Input data array – spectra of mineral waters from all over the world.

2. Output data array – concentrations of 9 ions in mineral waters.

3. Results of the application of ANN to the real mineral waters.

The authors demonstrated that suggested method allows to determine a concentration of complex ions in water with accuracy 10^{-4} M, a concentration of simple ions – with accuracy 10^{-3} M. The method was tested on natural mineral waters. using ANN it was possible to determine the concentration of ions by Raman spectra of the mineral waters with mean absolute error from 0.003 M to 0.06 M (from 0.069 g/L to 1.38 g/L).

[1] Burikov, S.A.; I.A.Dolenko, I.P.A.Velikotnyi, A.V.Sugonyaev & V.V.Tadeev, 2005. The Effect of Hydration of Ions of Inorganic Salts on the Shape of the Raman Stretching Band of Water. Optics and Spectroscopy, 98(2): 235-239.
[2] Dolenko, S.A.; S.A.Burikov, T.A.Dolenko & I.G.Persiantsev, 2012. Adaptive Methods for Solving Inverse Problems in Laser Raman Spectroscopy of Multi-Component Solutions. Pattern Recognition and Image Analysis, 22(4): 551-558.

Thank you for your attention.
See you at the poster session.

Using ANN it was possible to determine the concentration of ions by Raman spectra of real mineral waters with mean absolute error from 0.003 M to 0.06 M (from 0.069 g/L to 1.38 g/L).