



Editorial

Foreword — Chemometrics in Russia: The first five-year plan fulfilled

In October 1997 a group of scientists from different institutes and universities in Moscow decided to establish the Russian Chemometric Society (RCS) with the objective to create an organized scientific environment for spreading the ideas – and the spirit – of chemometrics in all of Russia. A few earlier chemometric contributions already existed in the former USSR and later in Russia. As far back as in the 1950s, studies dealing with mathematical description of equilibria were carried out under Kromar's [1] direction at the Kharkov State University while more recent publications include studies by Gribov and Elyashberg [2] on spectroscopic methods and some other publications of Russian scientists [3–6]. To illustrate the situation surrounding introduction of chemometrics in Russia, suffice to relate the following item from the 11th conference on: “Mathematical Methods in Chemistry and Technology” (June, 1998). The meeting was held at the Vladimir State University, not far from Moscow [5]. During this conference A. Pomerantsev and O. Rodionova decided to introduce chemometrics to their colleagues working in related areas, but an unexpected complication arose – the organizing committee, as well as the local university authorities, professed that they were uncomfortable with the term “chemometrics” – it was in fact considered that this word had something in common with *scientology* or some other *religious sect*. Such was the backdrop for the introduction of chemometrics in Russia — quite a challenge ahead.

At the beginning of the new millennium Alexey Pomerantsev, Oxana Rodionova and Kim H. Esbensen nevertheless decided to launch a 5-year DRUSHBAMETRICS project (“friendship-metrics”) bringing together foreign and Russian chemometricians at full blast. The main idea behind the DRUSHBAMETRICS concept was that young(er) Russian chemometricians get an opportunity to get together while learning chemometrics at a top international level, and will be able to create personal network-links as well as to start individual scientific collaborations early in their careers. Starting out as annual Winter Schools on Chemometrics (WSC), after 3 years the institution morphed naturally into “Winter Symposium on Chemometrics” beginning with WSC-4. Today, after the first five events, WSC has become a well-organized platform for presenting new ideas and fruitful discussions in a friendly, informal atmosphere (very informal at times). There are by now sufficient attendees from Russia contributing many new chemometric ideas which benefits greatly from being discussed in a professional, international forum; there

is always a minor, though highly significant international complement at the WSC. A representative selection of the state of the art of contributions was presented in the recent book: “Progress In Chemometrics Research” [16], comprising all peer-reviewed presentations from WSC-4. The present special issue of Chemometrics and Intelligent Laboratory Systems constitute the proceedings from WSC-5. This can be viewed as the crowning result from the DRUSHBAMETRICS project in particular and of the chemometric activity in Russia in general.

As a case in point: searching for the word “chemometrics” on the Russian speaking part of internet 7 years ago, one would get exactly one hit, the then newly established web-site of the Russian Chemometrics Society. A similar search today yields about 700 hits, including the following most recent publications of Russian scientists devoted to different aspects of chemometrics, e.g. works of Mar'yanov [7] on titrimetric analysis, Derendyaev and Vershinin [8] on computer identification of organic compounds and Zenkevich [9] on chromatography. The chemometric approach [10] is also a characteristic of the scientific school of Zolotov [11]. QSAR studies related to the laboratory headed by Zefirov are underway [12]. A research group comprising Legin, Rudlitskaya and Vlasov [13] at the St Petersburg State University is very active on electrochemical sensor array systems (‘electronic tongue’), while analogous systems for the ‘electronic nose’ are developed at the Voronezh Technological Academy [14]. Professor Razumov [15] and his colleagues from the Institute of Problems of Chemical Physics of the RAS (Chernogolovka) employ multivariate data analysis methods to solve problems of chemical kinetics. This year the prestigious Russian Chemical Reviews printed the first comprehensive review devoted to chemometrics [17]. Another significant event is that the Scientific Council on Analytical Chemistry of the Russian Academy of Sciences now organizes a Chemometrics section. There are today several well-established chemometric R&D groups in Russia, notably the group of Pomerantsev and Rodionova (in Moscow) [18,19], Zhilin and Kucheryavski (in Barnaul) [20], Romanenko (in Tomsk) [21] and Shabanova and Vasil'ev (in Irkutsk). [22]. While this evolution is highly satisfactory in a limited 5-year time horizon, it is of course only a beginning for such a big country. However all major goals of the DRUSHBAMETRICS project have been achieved.

For willingness to be involved in all these activities we want to thank not only the abovementioned, but also the members of

the various organizing committees as well as the approximately 125 active attendees of the first five WSC meetings. There is here an enthusiasm well worthy the adjective ‘chemometric’ in all its shapes and forms (scientific, educational, sociological ...). It is also timely to mention the significant complement of distinguished, established chemometricians who has contributed in leading roles for their great help to the Russian Chemometrics Society: Paul Geladi (Sweden), Pentti Minkkinen and Satu-Pia Reinikainen (Finland), Roma Tauler (Spain), Tormod Næs (Norway), Chris Marks (USA) and Kurt Varmuza (Austria) as well as Andrei Bogomolov, Lev Gribov, Sergei Kusherayvski and Vladimir Palulin (Russia).

Unfortunately, the meaning of the word “chemometrics” is still very much hidden for many Russian lecturers who are responsible for teaching chemistry, process technology, etc. Very often *chemometrics* is treated as elementary statistics in chemistry, and nothing more. Chemometric applications in industry are still very few. So: “while not absolutely all of the initial optimistic expectations have come true 100% and while there is a lot to do in the future – *status quo* is healthy and very satisfactory” – was the conclusion to a plenum discussion of the past, present and future of Russian chemometrics at the end of WSC5, 2006 (Samara).

The most important task for the future is to continue and strengthen the WSC symposium series to become a prominent international scientific meeting place (a bi-annual event in the future). At WSC all attendees, old and new, get a possibility to contribute with a presentation, oral or as poster; participants may deliver not only final results but also discuss preliminary problem statements and methods, all in the distinguishing unofficial atmosphere. In this respect WSC is no longer only a local Russian event but is well on the path to becoming a significant element in the set of international chemometric symposia and conferences. Earlier WSC meetings have been reported in [23–26].

It is safe to say that Russia has by now become an equal partner in the international chemometrics community. We highly appreciate all interactions and contributions in continuing to develop chemometrics in Russia.

References

- [1] N.P. Kromar', *Osnovy Kachestvennogo Khimicheskogo Analiza* (Foundations of Qualitative Chemical Analysis), Kharkov State University, Kharkov, 1955.
- [2] M.E. Elyashberg, V.V. Serov, L.A. Gribiv, *Talanta* 21 (1987) 34.
- [3] M.S. Khots, V.I. Nazarov, A.A. Lyovin, *Chemometr. Intell. Lab. Syst.* 18 (1993) 281–284.
- [4] V.I. Dvorkin, *Chemometr. Intell. Lab. Syst.* 22 (1994) 127–146.
- [5] A.L. Pomerantsev, O.Ye. Rodionova, *Chemometr. Intell. Lab. Syst.* 48 (1999) 121–129.
- [6] E.B. Rudnyi, *Chemometr. Intell. Lab. Syst.* 34 (1996) 41–54.
- [7] B.M. Mar'yanov, A.G. Zarubin, S.V. Shumar, *Zh. Anal. Khim.* 58 (2003) 1126.
- [8] V.I. Vershinin, B.G. Derendyaev, K.S. Lebedev, *Metody Komp'yutnoi Identifikatsii Organicheskikh Soedinenii* (The Methods of Computer Identification of Organic Compounds), Nauka, Moscow, 2002.
- [9] I.G. Zenkevich, B. Kranicz, *Chemometr. Intell. Lab. Syst.* 67 (2003) 51.
- [10] I.V. Pletnev, V.V. Zernov, *Anal. Chim. Acta* 455 (2002) 131.
- [11] Yu.A. Zolotov, *Analiticheskaya Khimiya: Problemy I Dostizheniya* (Analytical Chemistry: Problems and Achievements), Nauka, Moscow, 1992.
- [12] N.M. Halberstam, I.I. Baskin, V.A. Palyulin, N.S. Zefirov, *Usp. Khim.* 72 (2003) 706 *Russ. Chem. Rev.* 72 (2003) 629.
- [13] Yu.G. Vlasov, A.V. Legin, A.M. Rudnitskaya, *Usp. Khim.* 75 (2006) 141 *Russ. Chem. Rev.* 75 (2006) 125.
- [14] A.V. Kalach, Ya.I. Korenman, F.I. Niftaliev, *Iskusstvennye Neironnye Seti - Vchera, segodnya, Zavtra* (Artificial Neuron Networks - Yesterday, Today and Tomorrow) Voronezh: State Technological Academy, 2002.
- [15] S.P. Kazakov, A.A. Rayabenko, V.F. Razumov, *Opt. Spektrosk.* 86 (1999) 537.
- [16] A.L. Pomerantsev (Ed.), *Progress in Chemometrics Research*, NovaScience Publishers, NY, 2005.
- [17] O.Ye. Rodionova, A.L. Pomerantsev, *Usp. Khim.* 75 (2006) 302 *Russ. Chem. Rev.* 75 (2006) 271.
- [18] O.Ye. Rodionova, K.H. Esbensen, A.L. Pomerantsev, *J. Chemom.* 18 (2004) 402–413.
- [19] A.L. Pomerantsev, O.Ye. Rodionova, A. Höskuldsson, *Chemometr. Intell. Lab. Syst.* 81 (2006) 165–179.
- [20] S. Kucheryavski, V. Polyakov, A. Govorov, in: A.L. Pomerantsev (Ed.), *Progress in Chemometrics Research*, NovaScience Publishers, New York, 2005.
- [21] S.V. Romanenko, A.G. Stromberg, E.V. Selivanova, E.S. Romanenko, *Chemometr. Intell. Lab. Syst.* 73 (2004) 7–13.
- [22] I.E. Vasil'ev, A.M. Kuznetsov, I.L. Vasil'eva, E.V. Shabanova, *Zh. Anal. Khim.* 52 (1997) 1238.
- [23] O.Ye. Rodionova, *Chemometr. Intell. Lab. Syst.* 67 (2003) 193–195.
- [24] K. Esbensen, O. Rodionova, A. Pomerantsev, O. Startsev, S. Kucheryavski, *J. Chemom.* 17 (2003) 422–423.
- [25] S. Kucheryavski, C. Marks, K. Varmuza, *Chemometr. Intell. Lab. Syst.* 78 (2005) 138–139.
- [26] K.H. Esbensen, A. Pomerantsev, O. Rodionova, S. Kucheryavski, *Chemometr. Intell. Lab. Syst.* 83 (2006) 180–181.

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