

Case study | Cortellis Drug Discovery Intelligence™

Discovery research starts with the data

Moscow professor then turns to sophisticated searches, analytics in quest for leads.

Professor Vladimir Poroikov, now a professor at the Institute of Biomedical Chemistry in Moscow, has long focused his research on the development and validation of ligandbased methods for computer-aided drug discovery.

He is one of the first researchers in the world to integrate data from Cortellis Drug Discovery Intelligence into his computational methods. It integrates biological, chemical and pharmacological data in a single, easy to use platform. He is one of the first researchers in the world to integrate data from Cortellis Drug Discovery Intelligence into his computational methods.

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His initial efforts involved searching Cortellis Drug Discovery Intelligence for information about pharmaceutical agents exhibiting a particular biological activity.

He needed data to build computational models of (Quantitative) Structure-Activity Relationships [(Q)SARs], which relate the chemical structure of a compound to its biological activity in the hopes of making specific, potent molecules to serve as drug leads.

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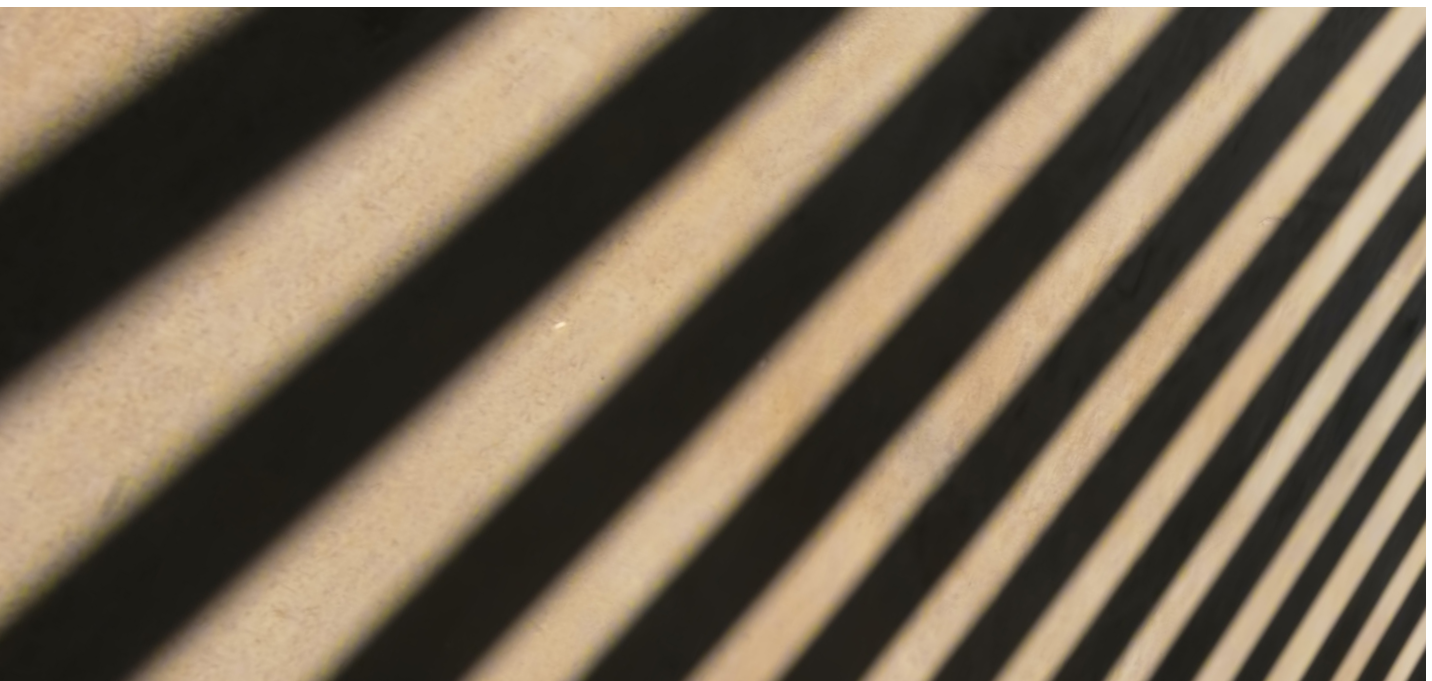
**Professor Vladimir Poroikov,
Institute of Biomedical Chemistry, Moscow**

An all-in-one tool

Another important part of Poroikov's work has been finding new biological activities for old drugs. Cortellis Drug Discovery Intelligence, which he calls an "all-in-one tool," has been an important part of this effort as well. The solution provides the perfect landscape view from which to begin his inquiry, backed by the reservoir of scientific data to deepen it. "If I start some study in a new field, I am going to [Cortellis Drug Discovery Intelligence] to obtain 'the first impression' about the general situation in this field," he said.

Poroikov's use of Cortellis Drug Discovery Intelligence has expanded significantly over time as both the biological and chemical information in the database itself has been enhanced continually over the years.

Expansion of Cortellis Drug Discovery Intelligence content, coupled with new analytics and increasingly sophisticated search capabilities, have helped in his research. Also contributing, he added: "My personal development that leads to the more complicated understanding of chemical-biological interactions in general."



More complex searches

As his scientific questions become more complex, so do his searches, Poroikov noted. He can use the structure of a molecule, or even a sub structure, and retrieve information about groups of molecules. Additional fields added in Cortellis Drug Discovery Intelligence have allowed for deeper interpretation of chemical-biological interactions.

"Sometimes, I use more complex queries to limit the results of the informational search for the particular need," he explained. Asked if he could remember a single query that has yielded the most fruitful results via Cortellis Drug Discovery Intelligence, he hesitated, and then demurred. "I use many different queries depending on the particular research interest. And all of them are 'the most useful' for a particular case," he said.

Poroikov shared one example of his research, which leaned heavily on Cortellis Drug Discovery Intelligence for support:

"In 2001 we published predictions of new pharmacotherapeutic effects for eight medicines from a list of Top 200 Drugs.¹ In particular, we predicted that Sertraline could be applied for cocaine dependency treatment, Amlodipine could be an antineoplastic enhancer, Oxaprozin could be an interleukin-1 antagonist and Ramipril could exhibit an anti-arthritic action."

He said a recent analysis of the published literature has shown that all of these predictions have been confirmed either by experiment or by clinical studies.²⁻⁵

Poroikov said he has had experience with other commercially-available databases, but Cortellis Drug Discovery Intelligence provides what he described as "extended (multi-aspect) coverage of the information" exceeding the capabilities of its competitors. He and his colleagues have tried other research databases, including those in the public domain, but have always come back to Cortellis Drug Discovery Intelligence. "In my opinion, [Cortellis Drug Discovery Intelligence] provides more carefully curated information in the field of human medicines," he said.

A big part of his appreciation for Cortellis Drug Discovery Intelligence has been the support and guidance he has received over time from Clarivate to drive the maximum results from Cortellis Drug Discovery Intelligence. He said free training webinars "clarified the optimal ways of informational search in Cortellis" and the company's scientific support staff "very quickly sent me the answers to my questions."

An enthusiastic Cortellis Drug Discovery Intelligence fan, Poroikov has recommended the solution to many of his scientific colleagues both in Russia and abroad. He has harnessed the tool in presentations made at scientific conferences as well as to graduate students at the Russian National Medical Research University. He said he has emphasized that Cortellis Drug Discovery Intelligence provides "the most reliable multi-faceted information about human medicines under study from a single source."

¹ Poroikov V. et al. Top 200 Medicines: Can New Actions Be Discovered Through Computer-Aided Predictions? SAR and QSAR Environ Res, 2001, 12: 327-344

² Mancino M.J. et al. Clinical Efficacy of Sertraline Alone and Augmented with Gabapentin in Recently Abstinent Cocaine-Dependent Patients with Depressive Symptoms. J Clin Psychopharmacol, 2014, 34: 234- 239

³ Takara K. et al. Differential Effects of Calcium Antagonists on ABCG2/BCRP-Mediated Drug Resistance and Transport in SN-38-Resistant HeLa Cells. Mol Med Rep, 2012, 5: 603-609

⁴ Rainsford K.D. et al. Recent Pharmacodynamic and Pharmacokinetic Findings on Oxaprozin. Inflammopharmacology, 2002, 10: 185-239

⁵ Shi Q. et al. Ramipril Attenuates Lipid Peroxidation and Cardiac Fibrosis in an Experimental Model of Rheumatoid Arthritis. Arthritis Res Ther, 2012, 14: R223

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