

Alexandre Varnek

LIST of SELECTED PUBLICATIONS

MONOGRAPH

A.Yu.Tsivadze, **A.A.Varnek**, V.E.Khutorsky

Coordination Compounds of Metals with Crown-Ligands (Russ), Nauka Publ. House, Moscow, 1991, 396 pp.

Edited Book

1. *Chemoinformatics Approaches to Virtual Screening*", **A. Varnek** and A. Tropsha, Eds., RSC Publishing, 2008
2. *Tutorials in Chemoinformatics*, Alexandre Varnek (Ed), WILEY, 2017

Text Books

1. T.I. Madzhidov, I.I. Baskin, I.A. Antipin and A.A. Varnek
Introduction into Chemoinformatics. Computer representation of chemical structures, (Russ)
University of Kazan, Kazan, 2013, 174 pp., ISBN 978-5-00019-131-6
2. T.I. Madzhidov, I.I. Baskin, and A.A. Varnek
Introduction into Chemoinformatics. Chemical Databases, (Russ)
University of Kazan, Kazan, 2015, 185 pp., ISBN 978-5-00019-429-4
3. I.I. Baskin, T.I. Madzhidov and A.A. Varnek
Introduction into Chemoinformatics. "Structure-Property" modeling, (Russ)
University of Kazan, Kazan, 2015, 302 pp., ISBN 978-5-00019-442-3
4. I.I. Baskin, T.I. Madzhidov and A.A. Varnek
Introduction into Chemoinformatics. Machine-Learning Methods (Russ)
University of Kazan, Kazan, 2016, 302 pp., ISBN 978-5-00019-442-3

Book Chapters

1. N.R.Streltsova, **A.A.Varnek**, A.S.Glebov, V.K.Belsky
Crystallochemistry of crown-ethers and their metal complexes.
In: *Problems of Crystallochemistry (Russ)*, M.Porii-Koshits Ed., Moscow, Nauka Publ. House, 1989, 47-84
2. **A.A.Varnek**, V.E.Khutorsky, A.S.Glebov
Complexation properties of Crown-Ethers
Deposit at VINITI (All-Union Institute of Scientific and Technical Information), Moscow, 1989, 109 pp.
3. **A. Varnek**, A.V. Goldberg
Monte-Carlo simulations of liquid-liquid CCl₄/water interface.
In: *Phase Transfer Catalysis: New Ideas and Methods*, Moscow, Russ. Ac. Sc., 1994, 9-11.
4. **A. Varnek**, A.V. Goldberg, O.I. Danilova, S.S. Yufit
Solvation of quaternary ammonium chlorides at the CCl₄/water interface with respect to their catalytic activity.
A theoretical and experimental study.
In: *Phase Transfer Catalysis: New Ideas and Methods*, Moscow, Russ. Ac. Sc., 1994, 11-14.
5. **A. Varnek**, G. Wipff
[Introduction to conformational analysis with the MacroModel software](#);
In: *"Crystallography of Supramolecular Compounds"*, NATO ASI Series,
G. Tsoucaris, J. L. Atwood., J. Lipkowski Eds., Kluwer Acad. Publ., Dordrecht, Boston, 1996, 461-463.

6. **A. Varnek**, E. Engler, M. Lauterbach, L. Troxler, G. Wipff
[Display of Dynamic Structures from Molecular Dynamics Simulations in aqueous/non-aqueous solutions. Comparison with X-ray structures](#), In: "*Crystallography of Supramolecular Compounds*", NATO ASI Series, G. Tsoucaris, J. L. Atwood., J. Lipkowski Eds., Kluwer Acad. Publ., Dordrecht, Boston, 1996, 465-470.
7. **A. Varnek**, C. Sirlin, G. Wipff
[Solvent and Dynamic Effects on the Structure of Alkali Cation Complexes of the t-butyl-calix\[4\]arene anion: MD and FEP Computer Investigations on the Na⁺ / Cs⁺ Binding Affinity](#).
In: "*Crystallography of Supramolecular Compounds*", NATO ASI Series G. Tsoucaris, J. L. Atwood., J. Lipkowski Eds., Kluwer Acad. Publ., Dordrecht, Boston, London, 1996, 67-99.
8. A.V. Solovyov, L.I. Atamas, O.V. Klimchuk, V.L. Rudzevich and V.I. Kalchenko, **A. Varnek** and G. Wipff.
[Ionophores Based on of Calix\[4\]arenes Phosphorylated at the Upper Rim](#)
In: *EURADWASTE 1999 "Radioactive Waste Management. Strategies and Issues"*, p. 523-526, 2000, Luxembourg. European Communities.
9. E. Stoyanov, I. Smirnov, **A. Varnek** and G. Wipff
[Microscopic Insights into Synergistic Effects: Sr\(II\) Extraction by a Mixture of Chlorinated Cobalt Dicarbolide and Polyethers](#).
In: *EURADWASTE 1999 "Radioactive Waste Management. Strategies and Issues"*, p. 519-522, 2000, Luxembourg. European Communities.
10. **A. Varnek**, D. Fourches, V. P. Solov'ev
In silico design of new compounds using fragment descriptors. In *QSAR and Molecular Modelling in Rational Drug Design of Bioactive Molecules*, E. Aki-Sener and I. Yalcin, Eds., CADD&D, Ankara, Turkey, 2004, pp. 342-345
11. Igor Baskin and **Alexandre Varnek**
[Fragment Descriptors in SAR/QSAR/QSPR Studies, Molecular Similarity Analysis and in Virtual Screening](#). In "*Cheminformatics Approaches to Virtual Screening*", A. Varnek and A. Tropsha, Eds., RSC Publishing, 2008
12. **Alexandre Varnek** and Vitaly Solov'ev
[Quantitative Structure-Property Relationships in Solvent Extraction and Complexation of Metals](#)
In "*Ion Exchange and Solvent Extraction*", Vol. 19, B. A. Moyer and A. K. Sengupta, Eds., Taylor and Francis: Philadelphia, 2009.
13. **Alexandre Varnek**
[Fragment Descriptors in Structure-Property Modeling and Virtual Screening](#),
In: "*Cheminformatics and Computational Chemical Biology*", J. Bajorath, Ed., Springer, 2010
14. **Varnek, Alexandre**
[Fragment descriptors in structure-property modeling and virtual screening](#).
Methods in molecular biology (Clifton, N.J.) 2011, Vol: 672, 213-43
15. Igor I. Baskin and **Alexandre Varnek**
[Building a Chemical Space Based on Fragment Descriptors](#)
In: *Advances in Combinatorial Chemistry & High Throughput Screening*,
Bentham Science Publishers, Rathnam Chaguturu, Ed., pp.36-59, 2014, ISBN: 978-1-60805-746-7
16. H el ena A. Gaspar, Pavel Sidorov , Dragos Horvath, Igor I. Baskin, Gilles Marcou, Alexandre Varnek Generative Topographic Mapping of Chemical Space
In "*Frontiers in Molecular Design and Chemical Information Science*", *ACS series book, 2016*, Chapter 11, pp. 211-241
17. H el ena A. Gaspar, Igor I. Baskin, Alexandre Varnek
Visualize a Multidimensional Descriptor Space,
In "*Frontiers in Molecular Design and Chemical Information Science*", *ACS series book, 2016*, Chapter 12, pp.242-267
18. Dragos Horvath, Gilles Marcou, Alexandre Varnek
Generative Topographic Mapping Approach to Chemical Space Analysis

In: "Challenges and Advances in Computational Chemistry and Physics. v. 24, Advances in QSAR Modeling", 2017, pp. 167-199

FULL PAPERS

1. R. P. Ozerov, V. G. Tsirel'son, **A. A. Varnek**, M. V. Krasheninnikov, E. V. Parini and L. A. Pozdnjakov
[Studies of the electron density and potential distribution as well as other properties of crystals from diffraction data](#)
Acta Cryst A., 1981, A37, C137
2. **A.A.Varnek**, V.G.Tsirel'son, R.P.Ozerov
[Calculation of energy characteristics of crystals from diffraction data by the method of density functional](#)
Dokladi Akademii Nauk SSSR (Proc. Ac. Sci. USSR, Russ.), 1981, **257**, 382-385
3. **A.A.Varnek**, M.V.Krasheninnikov, V.G.Tsirel'son, R.P.Ozerov
Electron density and electrostatic potential distribution of Diamond from X-ray diffraction data.
Khimicheskaya Physica (Chem. Physics, Russ), 1982, No 6, 716-720
4. **A.A.Varnek**, A.A.Baskakov, V.G.Tsirel'son, R.P.Ozerov
[A Program for the Molecular Electrostatic Potential calculation on the base of direct integration of Poisson equation](#)
Zh. Structurnoy Khimii (J. of Struct. Chem., Russ.), 1984; **25**, 135/ *Journal of structural chemistry* 25 (1985), S. 636-637
5. O.M. Petrukhin, R.P.Ozerov, **A.A.Varnek**, V.G.Tsirel'son, G.A.Yagodin
Extraction ability and electron density distribution in organic compounds.
Trudi MKhTI (Proc. of Moscow Mendeleev Institute, Russ.), 1984, **134**, 87-96
6. **A.A.Varnek** Electrostatic potential distribution in crystals from X-ray diffraction data. 1985, pp.196.
Ph.D. Theses, Kurnakov Institute of General and Inorganic Chemistry USSR Ac. Sci., Moscow
7. **Varnek, A.A.**; Kovan, O.E.; Ozerov, R.P.
[Estimation of the Hydrogen-Atom - Alpha-Vanadium Lattice Interaction Energy from the X-Ray-Diffraction Data](#)
Chemica Scripta, 1986, Volume: 26, Issue: 3, P. 478-478
8. **A.A.Varnek**, P.D. Bregestovski
[Molecular pumps based on the macrocyclic complexons](#)
Dokladi Akademii Nauk SSSR (Proc. Ac. Sci. USSR, Russ.), 1986, **289**, 1500-1503
9. **A.A.Varnek**, R.P.Ozerov, P.A.Zagorets, N.R.Ozerova
Electrostatic potential distribution and complexation properties of crown-ethers.
Koord. Khimiya (Coord. Chemistry, Russ.), 1986, **12**, 1599-1603
10. S.I. Orlov, **A.A. Varnek**, O.B. Sel, A.L. Chimichkyan
[Kinetics and mechanism of the phosgenation of aliphatic-alcohols .5. Quantum chemical study of the mechanism of the reaction of phosgene with methanol](#)
Zh. Org. Khimii (J.Org.Chem., Russ), 1987, **23**, 2412-2418
11. S.G.Kozhevatin, **A.A.Varnek**, M.V.Artamonova
Electronic structure of the light sensitive phase of copper halide photochromic glasses. Quantum mechanics studies by the extended Hueckel method.
Fiz. Khim. Stekla (Phys. Chem. Glass, Russ.), 1987, **13**, 55-59
12. **A.A.Varnek**, V.E.Khutorsky, A.S.Glebov
[The influence of solvation effects on the stability of complexes of dialkyldibenzo-18-crown-6 with potassium-ion.](#)
Dokladi Akademii Nauk SSSR (Proc. Ac. Sci. USSR, Russ.), 1988, **301**, 917-920
13. **A.A.Varnek**, A.S.Glebov, A.N.Kuznetsov
Charge density distribution, electrostatic potential and complex formation ability of some neutral agents

Portugal Phys., 1988, 59-61

14. **A.A.Varnek**, A.S.Glebov, O.M.Petrukhin, R.P.Ozerov, N.V. Kolycheva
[Selectivity of reactions of 18-crown-6 complexation with alkali-metals](#)
Koord. Khimiya (Coord. Chemistry, Russ.), 1989, **15** (5) , P 600-606
15. **A.A.Varnek**, A.S.Glebov, S.K. Norov, O.M.Petrukhin, R.P.Ozerov
[Study of complexation of dibenzo-18-crown-6 dialkyl-derivatives with alkali-metals by the molecular mechanics and quantum-chemistry technique](#)
Koord. Khimiya (Coord. Chemistry, Russ.), 1989, **15**, 740-746
16. **A.A.Varnek**, A.S.Glebov, Sh.K.Norov, O.M.Petrukhin .
Conformational analysis of dialkyl derivatives of dibenzo-18-crown-6.
Dokladi Akademii Nauk UzSSR (Proc. Ac. Sci. UzSSR, Russ.), 1989, N° **2**, 40-44
17. **A.A.Varnek**, Sh.K.Norov, A.S.Glebov, O.M.Petrukhin .
Analysis of ion-molecular interactions in the crown-ether - alkali cation systems
Dokladi Akademii Nauk UzSSR (Proc. Ac. Sci. UzSSR, Russ.), 1989, N° **5**, 42-44
18. Kuznetsov, A. N.; **Varnek, A. A.**; Petrukhin, O. M.; Ozerov, R. P.
[Electrostatic-potential distributions applied to estimating neutral organophosphorus compound extraction capacity](#)
Zh. Strukturnoy Khimii, 1989; **30**, 44-48/ *Journal of structural chemistry* 30 (1989), S. 392-396
19. V. E. Khutorskii, A. A. Kamenchuk, **A. A. Varnek**, Sh. K. Norov, A. S. Glebov, V. P. Kukhar'
[Investigation of hydration effects of dibenzodialkyl-18-crown-6 complexes with the potassium ion by the Monte-Carlo method](#)
Theoretical and Experimental Chemistry, March–April, 1990, Volume **26**, Issue 2, pp 221-224
20. S.I.Orlov, A.L.Sidelkovskii, L.N.Margolin, A.F.Vasil'ev, **A.A.Varnek**
[Kinetics of thiophosgene solvolysis in aliphatic alcohols.](#)
Org. React. (Tartu), 1990, **27**, 141-151
21. A.V.Goldberg, **A.A.Varnek**
[Program to calculate the structural and energetic properties of aqueous solutions of binary systems using the Monte Carlo method](#)
Zh. Strukturnoy Khimii (Journal of structural chemistry), 1990; **31**, 173 (S. 686-686)
22. **A.A.Varnek**, E.V.Ermakov, A.N.Kuznetsov, E.S.Stoyanov
[Quantum-chemical analysis of coordination properties of ligands with poo-groups and coo-groups based on lithium-salts of dialkylphosphoric and carboxylic-acids](#)
Koord. Khimiya (Coord. Chemistry, Russ.), 1991, **17**, 12-16
23. **Varnek, A. A.**; Kuznetsov, A. N.; Petrukhin, O. M.; Ozerov, R. P.
[Study of the geometrical and electronic characteristics of tri-n-butyl phosphate by the methods of molecular mechanics and quantum chemistry](#)
Zhurnal Strukturnoi Khimii, 1991, Vol. **32** (1), pp. 156–159, January–February, 1991/*Journal of structural chemistry* 32 (1991), S. 130-133
24. **A.A.Varnek**, A.N.Kuznetsov, O.M.Petrukhin
[Calculation of indexes of extractability of neutral organophosphorus reagent series in the method of electronic density functional](#)
Koord. Khimiya (Coord. Chemistry, Russ.), 1991, **17**, 1038-1041
25. **A.A.Varnek**, A.Yu.Tsivadze, A.S.Glebov, I.Ya.Kachkurova
[Unusual complexation properties of alkyl-crown-ethers](#)
Dokladi Akademii Nauk SSSR (Proc. Ac. Sci. USSR, Russ.), 1991, **316**, 375-378
26. A.V.Goldberg, **A.A.Varnek**, S.I.Stepanov, A.M. Chekmarev, R.P. Ozerov
[Structural and energetic characteristics of hydration of salts of quaternary ammonium bases .I. \(NH₄\)⁺, \(NOct₄\)⁺, \(NMeOct₃\)⁺ cations in infinite diluted solutions](#)

J. Phys. Khimii (J.Phys.Chem., Russ.), 1991, **65**, 2397-3404

27. A.V.Goldberg, **A.A.Varnek**, S.I.Stepanov, A.M. Chekmarev, R.P. Ozerov
[Structural and energetic characteristics of hydration of salts of quaternary ammonium bases .II. Infinitely diluted solutions of tetraoctylammonium and methyltrioctylammonium fluorides](#)
J. Phys. Khimii (J.Phys.Chem., Russ.), 1992, **66**, 2446-2451

28. **A.A.Varnek**, G.Morosi, A.Gamba
[Molecular modelling of organophosphorus podands and their complexes with alkali metal cations](#)
J. Phys. Org. Chem., 1992, **5**, 109-118

29. **A.A.Varnek**, J.E.Ten Elschof, V.P.Solov'ev, V.E.Baulin, E.N.Tsvetkov
[Complexation of lithium and sodium cations with b-phosphorilate ethers, modelling terminal groups of organophosphorus podands. An experimental and theoretical study](#)
J. Mol. Structure, 1992, **271**, 311-325

30. A.V.Goldberg, **A.A.Varnek**, T.A. Zhdanova
[Structural and energy characteristics of complex hydration in the quaternary ammonium salt-water system - \(NOct₄\)⁺, \(NMeOct₃\)⁺chlorides and bromides in infinitely diluted aqueous-solutions](#)
Koord. Khimiya (Coord. Chemistry, Russ.), 1993, **19(2)**, 111-115

31. **A.A.Varnek**, A.Maia, D.Landini, A.Gamba, G.Morosi, G.Podda
[Catalytic activity of Polypodands and Glymes under Solid-Liquid Phase-Transfer Catalysis Conditions. A Molecular Mechanics Study.](#)
J. Phys. Org. Chem., 1993, **6**, 113-121

32. S.I. Orlov, L.N. Margolin, A.L. Sidelkovskii, **A.A. Varnek**
[Kinetics and mechanism of aliphatic-alcohols phosgenation .7. Kinetics of methanol phosgenation without solvent and the role of alcohol association with hydrogen-chloride.](#)
J. Org. Khimii (J. Org. Chem.,Russ.), 1993, **29**, 14-23

33. P.Guilbaud, **A.Varnek**, G.Wipff
[A MD study of tBu-calix\[4\]arene tetramide and its complexes with neutral and cationic guests. Influence of solvation on structures and stabilities](#)
J. Am. Chem. Soc., 1993, **115**, 8298-8312

34. **A.Varnek**, G.Wipff
[Dramatic Solvent Effect on the Ligand Wrapping around a Complexed Cation: a MD Study of p-tert-butylcalix\[4\]arene Tetramide and its Complexes with Alkali Cations and Eu³⁺ in Acetonitrile](#)
J. Phys. Chem. , 1993, **97**, 10840-10848.

35. **A.A. Varnek**, A.S. Glebov, D. Feil, G. Wipff
[An Application of Miertus-Scrocco-Tomasi Solvation Model in the Molecular Mechanics and Dynamics Simulations](#)
J. Comp. Chem., 1995, **16**, 1-19.

36. **A. Varnek**, G. Wipff
[Theoretical Calculations of Extraction Selectivity: Alkali Cation Complexes of Calix\[4\]-bis-crown6 in Pure Water, Chloroform and at the Water/Chloroform Interface](#)
J. Comp. Chem., 1996, **17**, 1520-1531.

37. **A. Varnek**, G. Wipff
[Solvent and Counterion Effects on the Na⁺ / Cs⁺ Complexation Selectivity by Conformationally Locked Calix\[4\]-bis-crown Ligands: MD and FEP Studies in Water and Methanol, Acetonitrile and Chloroform Solutions.](#)
J. Mol. Struct. (THEOCHEM), 1996, **363**, 67-85.

38. G. Wipff, E. Engler, P. Guilbaud, M. Lauterbach, L. Troxler, **A. Varnek**
[MD simulations on ionophores at a water-chloroform interface. Part I - Calix\[4\]arenes and the 222 cryptand uncomplexed.](#)
New. J. Chem., 1996, **20**, 403-417.

39. R. Abidi, M. V. Baker, J. M. Harrowfield, D. S-C. Ho, W. R. Richmond, B. W. Skelton, A. H. White, **A. Varnek**, G. Wipff
[Complexation of the *p*-t-butyl-calix\[4\]arene anion with alkali metal cations in polar, non-aqueous solvents: experimental and theoretical studies](#)
Inorganica Chim. Acta, 1996, 275-286.
40. R.J. Zauhar, **A. Varnek**
[A fast and space-efficient boundary element method for computing electrostatic and hydration effects in large molecules](#)
J. Comp. Chem., 1996, **17**, 864-877.
41. **A. Varnek**, L. Troxler, G. Wipff
[Adsorption of ionophores and of their complexes at the water/chloroform interface: a Molecular Dynamics study of a 2.2.2. cryptand and of phosphoryl-containing podands](#)
Chem. Eur. J., 1997, **3**, 552-560.
42. V. A. Varnek, **A. A. Varnek**
[To the nature of isomer shift in tin\(IV\) tetrachloride complexes with organic ligands from quantum-chemical calculation data.](#)
Zh. Strukt. Khimii (J. Structural Chemistry, Russ), 1997, **38**, 1160-1164
43. **A. Varnek**, S. Helissen, G. Wipff, A. Collet
[Van der Waals Host-Guest Complexes: Can one Predict the Complexation Selectivity of Neutral Guests by a Cryptophane ? MD-FEP Studies in the Gas Phase and in Chloroform Solution](#)
J. Comp. Chem., 1998, **17**, 820-832.
44. V.A. Varnek, **A.A. Varnek**
[Quantum-chemical analysis of outer sphere cation influence on the tin atom electronic state and isomer shift in hexafluorostannates](#)
Zh. Strukt. Khimii (J. Structural Chemistry, Russ), 1998, **39**, 154-157
45. V.P. Solov'ev, V.E. Baulin, N.N. Strakhova, V.P. Kazachenko, V.K. Belsky, **A.A. Varnek**, T.A. Volkova, G. Wipff
[Complexation of phosphoryl-containing mono-, bi- and tri-podands with alkali cations in acetonitrile. Structure of the complexes and binding selectivity](#)
J. Chem. Soc., Perkin Trans 2, 1998, 1489-1498
46. L. Gorb, A. Korokin, J. Leszczynski, **A. Varnek**, F. Mark, K. Schaffner
[Theoretical *an initio* and semi-empirical studies on biologically important di- and oligopyrrolic compounds - pyrromethenone and biliverdin](#)
J. Mol. Struct. (THEOCHEM), 1998, **425**, 137-145.
47. A.Y.Nazarenko, J.D.Lamb, V.E.Baulin, T. Volkova, **A.Varnek**, G.Wipff
[Solvent extraction of Metal Ion Picrates with Phosphine Oxide Podands](#)
J. Solvent Extract. Ion. Exch., 1999, **17**, 495-523
48. **A. Varnek**, G. Wipff
[Molecular Modelling in Solvent Extraction: Ionophores in Pure Solutions and at the Liquid/Liquid Interface](#)
J. Solvent Extract. Ion. Exch., **17** (6), 1999, 1493-1505.
49. **A. Varnek**, G. Wipff, A. Bilyk, J. Harrowfield
[Molecular Dynamics and Free Energy Perturbation Studies of Ca²⁺/Sr²⁺ Complexation Selectivities of the Macrocyclic Ionophores DOTA and TETA in Water](#)
J. Chem. Soc., Dalton Trans, 1999, Issue 23, 4155.
50. **A.A.Varnek**, B.Dietrich, G.Wipff, J.-M.Lehn, E.V.Boldyreva
[SUPRAMOLECULAR CHEMISTRY: computer assisted instruction in undergraduate and graduate chemistry courses](#)
J. Chem. Educat., 2000, **77**, 222-226.
51. **A. Varnek**, T. Volkova, O.M. Petrukhin, G. Wipff

[Switching of Ba²⁺/Ca²⁺ into Ba²⁺/Ca²⁺ Potentiometric Selectivities of Podands with Phosphoryl-Containing Terminal Groups. A Molecular Modelling Study.](#)

J. Incl. Phenom., 2000, **37**, 407-421

52. V. P. Solov'ev, **A. Varnek**, G. Wipff

[Modelling of Ion Complexation and Extraction of Organic Molecules Using Substructural Molecular Fragments](#)

Chem. Inf. Comp. Sci., 2000, **40**, 847-858.

53. S. Meyer, R. Louis, B. Metz, Y. Agnus, **A. Varnek**, M. Gross

[Unprecedented Role of Water in Self-Assembly of Potential Molecular Tweezers](#)

New J. Chem., 2000, **24**, 371-376.

54. **A. Varnek**, G. Wipff, V. P. Solov'ev

[Towards an information system on solvent extraction](#)

J. Solvent Extract. Ion. Exch., 2001, **19** (5), 791 - 837.

55. V. Torgov, S. Erenburg, N. Bausk, E. Stoyanov, V. Kalchenko, **A. Varnek**, G. Wipff

[The structure of new heterometallic Ru / M \(M = Cu, Ni, Co, Zn\) complexes investigated by combined spectroscopic and modelling studies](#)

J. Mol. Struct., 2002, **611**, 131-138.

56. **A. Varnek**, G. Wipff, A. Famulari, M. Raimondi, T. Vorobieva, E. Stoyanov

[Complexes of the H₅O₂⁺ and H₃O⁺ cations with polyethers in water saturated dichloroethane solutions. A combined IR spectroscopic and quantum mechanics study](#)

J. Chem. Soc., Perkin Trans. 2, 2002, 887-893.

57. **A. Varnek**, G. Wipff, V. P. Solov'ev

[Assessment of the macrocyclic effect for the complexation of crown-ethers with alkali cations using Substructural Molecular Fragments](#)

J. Chem. Inf. Comp. Sci., 2002, **42**, 812-829.

58. **A. Varnek**, G. Wipff, V. P. Solov'ev

Towards "in silico" design of new potential extractants using chemical informatics methods. International Solvent Extraction Conference, Cape Town, South Africa, Mar. 17-21, 2002, 481-486. South African Institute of Mining and Metallurgy, Marshalltown, S. Africa

59. **A. Varnek**, B. Dietrich, G. Wipff, J.-M. Lehn, E. V. Boldyreva

[Initiation à la Chimie Supramoléculaire assistée par Ordinateur.](#)

Technique de l'Ingénieur, 2002, AF 6 048-1 - AF 6 048-8

60. Yu. Rudzevich, A. Drapaylo, V. Rudzevich, V. Miroshnichenko, V. Kalchenko, I. Smirnov, V. Babain, **A. Varnek**, G. Wipff

[Synthesis and extraction properties of hexaphosphorilated calix\[6\]arenes.](#)

Russian J. General Chemistry, 2002, **72**, 1840-1846.

61. L. Atamas, O. Klimchuk, V. Rudzevich, V. Kalchenko, V. Pirozhenko, I. Smirnov, V. Babain, T. Efremova, **A. Varnek**, G. Wipff, F. Arnaud-Neu, M. Roch, M. Saadioui, V. Böhmer,

[New organophosphorus calix\[4\]arene ionophores for trivalent lanthanide and actinide cations.](#)

J. Supramol. Chem., 2002, **2**, 421-427.

62. V. P. Solov'ev, **A. Varnek**

[Anti-HIV Activity of HEPT, TIBO and Cyclic Urea Derivatives: Structure-Property Studies. Focused Combinatorial Library Generation and Hits Selection Using Substructural Molecular Fragments Method](#)

J. Chem. Inf. Comp. Sci., 2003, **43**, 1703 - 1719

63. Alan R. Katritzky, Dan C. Fara, Hongfang Yang, Mati Karelson, Takahiro Suzuki, Vitaly P. Solov'ev, **Alexandre Varnek**

[Quantitative Structure-Property Modeling of β - Cyclodextrin Complexation Free Energies](#)

J. Chem. Inf. Comp. Sci., 2004, **44**, 529-541

64. O. Klimchuk, L. Atamas, S. Miroshnichenko, V. Kalchenko, I. Smirnov, V. Babain, **A. Varnek**, G. Wipff

[New wide rim phosphomethylated calix\[4\]arenes in extraction of actinides and lanthanides](#)

J. Inclusion Phenom. Macrocyclic Chem., 2004, **49**, 47-56.

65. **Alexandre Varnek**, Denis Fourches, Vitaly P. Solov'ev, Vladimir E. Baulin, Alexandre Turanov, Vassily Karandashev, Alan R. Katritzky, Dan Fara

["In silico" design of new uranyl extractants based on phosphoryl-containing podands: QSPR studies, generation and screening of virtual combinatorial library and experimental tests.](#)

J. Chem. Inf. Comp. Sci., 2004, **44**, 1365-1382

66. V. P. Solov'ev, **A. Varnek**

[Structure – property modeling of metal binders using molecular fragments.](#)

Russian Chem. Bulletin, 2004, **56**, No. 7, 1380-1391

67. **A. Varnek**, V. P. Solov'ev,

["In silico" design of potential anti-HIV actives using fragment descriptors](#)

Combinatorial Chemistry & High Throughput Screening, 2005, **8**, 403-416.

68. V. Torgov, G. Kostin, T. Korda, E. Stoyanov, V. Kalchenko, A. Drapailo, O. Kasyan, G. Wipff, **A. Varnek**

[Upper rim thioether derivatives of calix\[4,6\]arenes: synthesis and extraction of fission Pd\(II\) and Ag\(I\).](#)

J. Solv. Extr. Ion Exch., 2005, **23**, № 6, P. 781-801.

69. A. R. Katritzky, M. Kuanar, D. C. Fara, M. Karelson, W. E. Acree, Jr., V. P. Solov'ev, **A. Varnek**

[QSAR Modeling of Blood:Air and Tissue:Air Partition Coefficients Using Theoretical Descriptors](#)

Bio-organic Medicinal Chemistry, 2005, **13** (23), 6450-6463

70. **A. Varnek**, D. Fourches, F. Hoonakker, V. P. Solov'ev

[Substructural fragments: an universal language to encode reactions, molecular and supramolecular structures.](#)

J. Computer-Aided Molecular Design, 2005, **19**, 693-703.

71. V. P. Solov'ev, N.V. Kireeva, A.Yu. Tsivadze, **A. A. Varnek**

[Structure – property modelling of complexation of strontium cation by organic ligands.](#)

J. Struct. Chem., 2006, **47**, 311-325

72. Igor V. Tetko, Vitaly P. Solov'ev, Alexey V. Antonov, Xiaojun Yao, Jean Pierre Doucet, Botao Fan, Frank Hoonakker, Denis Fourches, Piere Jost, Nicolas Lachiche and **Alexandre Varnek**

[Benchmarking of linear and non-linear approaches for quantitative structure-property relationship studies of metal complexation with ionophores](#)

J. Chem. Inf. Comp. Sci., 2006, **46**, 808-819.

73. A. R. Katritzky, D.A. Dobchev, D. C. Fara, E. Hür, K. Tämm, L. Kurunczi, M. Karelson, V. P. Solov'ev, **A. Varnek**

[Skin Permeation Rate as a Function of Chemical Structure](#)

J. Med. Chem., 2006, **49**, 3305-3314.

74. A. R. Katritzky, M. Kuanar, S. Slavov, D.A. Dobchev, D. C. Fara, M. Karelson, W. E. Acree, Jr., V. P. Solov'ev, **A. Varnek**

[Correlation of Blood: Brain Barrier Permeation Using Structural Descriptors.](#)

Bioorganic & Medicinal Chem., 2006, **14**, 4888-4917.

75. **A. Varnek**, D. Fourches and N. Sieffert, V. P. Solov'ev, C. Hill, and M. Lecomte

[QSPR modeling of the AmIII / EuIII separation factor: How far can we predict ?](#)

J. Solv. Extr. Ion Exch., 2007, **25**, 1-26.

76. G.Kostin, A. Borodin, V. Emel'yanov, D. Naumov, A. Virovets, M.-M. Rohmer, **A. Varnek**

[Synthesis and structure of heterometallic compounds of \[RuNO\(NO₂\)₄OH\]²⁻ with triphenylphosphineoxide complexes of Co\(II\), Ni \(II\) and Zn\(II\).](#)

J. Mol. Structure, 2007, **837**, 63-71

77. **A. Varnek**, N. Kireeva, I. V. Tetko, I.I. Baskin, V. P. Solov'ev

[Exhaustive QSPR studies of large diverse set of ionic liquids: how accurately can we predict the melting point?](#)

J. Chem. Inf. Mod., 2007, **47**, 1111-1122

78. **A. Varnek**, D. Fourches, V. Solov'ev, O. Klimchuk, A. Ouadi, I. Billard
[Successful « In Silico » Design of New Efficient Uranyl Binders](#)
J. Solv. Extr. Ion Exch., 2007, **25**, N°4, 433–462.
79. D. Horvath, F. Bonachera, V. Solov'ev, C. Gaudin and **A. Varnek**
[Stochastic versus Stepwise Strategies for Quantitative Structure-Activity Relationship Generation – How much effort may the mining for successful QSAR models take?](#)
J. Chem. Inf. Mod., 2007, **47** (3), 927-939
80. Hao Zhu, Denis Fourches, **Alexandre Varnek**, Ester Papa, Paola Gramatica, Igor V. Tetko, Tomas Öberg, Artem Cherkasov and Alexander Tropsha
[Combinational QSAR Modeling of Chemical Toxicants Tested against *Tetrahymena pyriformis*](#)
J. Chem. Inf. Mod., 2008, **48**, 766–784
81. I. Baskin and **A. Varnek**
[Building a chemical space based on fragment descriptors](#)
Combinatorial Chemistry and High Throughput Screening, 2008, 11, No. 8
82. **A. Varnek**, D. Fourches, N. Kireeva, O. Klimchuk, G. Marcou, A. Tsivadze and V. Solov'ev
[Computer-aided design of new metal binders](#)
Radiochimica Acta, 2008, **96**, 505-511
83. Igor V. Tetko, Iurii Sushko, Anil Kumar Pandey, Hao Zhu, Alexander Tropsha, Ester Papa, Tomas Öberg, Roberto Todeschini, Denis Fourches, **Alexandre Varnek**
[Critical assessment of QSAR models of environmental toxicity against *Tetrahymena pyriformis*: Focusing on applicability domain and overfitting by variable selection](#)
J. Chem. Inf. Mod., 2008, **48**, 1733–1746
84. **A. Varnek**, D. Fourches, D. Horvath, O. Klimchuk, C. Gaudin, P. Vayer, V. Solov'ev, F. Hoonakker, I. V. Tetko, G. Marcou
[ISIDA - Platform for virtual screening based on fragment and pharmacophoric descriptors](#)
Current Computer-Aided Drug Design, 2008, **4** (3), 191-198.
85. **Varnek, A.**; Gaudin, C.; Marcou, G.; Baskin, I.; Pandey, A. K.; Tetko, I. V.
[Inductive transfer of knowledge: application of multi-task learning and feature net approaches to model tissue-air partition coefficients](#)
J. Chem. Inf. Model. 2009, **49** (1), 133-44.
86. Horvath Dragos, Marcou Gilles, and **Varnek Alexandre**
[Predicting the Predictability: A Unified Approach to the Applicability Domain Problem](#)
J. Chem. Inf. Mod., 2009, **49** (7), 1762–1776
87. Frank Hoonakker, Nicolas Lachiche, **Alexandre Varnek** and Alain Wagner
[A representation to apply usual data mining techniques to chemical reactions](#)
Trends in Applied Intelligent Systems (IEA/AIE'10), 2010, **6097**, 318-326.
88. Igor I. Baskin, Natalia Kireeva and Alexandre Varnek
[The One-Class Classification Approach to Data Description and to Models Applicability Domain.](#)
Mol. Informatics, 2010, 581-587
89. Iurii Sushko, Sergii Novotarskyi, Robert Korner, Anil Kumar Pandey, Jiazhong Li, Paola Gramatica, Katja Hansen, Timon Schroeter, Klaus-Robert Muller, Lili Xi, Huanxiang Liu, Xiaojun Yao, Tomas Oberg, Artem Cherkasov, Farhad Hormozdiari, Phuong Dao, Cenk Sahinalp, Roberto Todeschini, Pavel Polishchuk, Anatoliy Artemenko, Victor Kuz'min, Todd M. Martin, Douglas M. Young, Denis Fourches, Eugene Muratov, Alexander Tropsha, Igor Baskin, Dragos Horvath, Gilles Marcou, Christophe Muller, **Alexandre Varnek** and Igor V. Tetko
[Applicability domains for classification problems: benchmarking of distance to models for AMES mutagenicity set](#)
J. Chem. Inf. Model. 2010, **50** (12), 2094–2111
90. Fiorella Ruggiu, Gilles Marcou, **Alexandre Varnek** and Dragos Horvath

[ISIDA Property-labeled fragment descriptors](#)

Mol. Informatics, 2010, **29**, 855 – 868

91. G Marcou, N Lachiche, L Brillat, J-M Paris and **A Varnek**

[Learning antibacterial activity against *S. Aureus* on the Chimiothèque Nationale dataset](#)

Journal of Cheminformatics, 2010, Volume 2, Supplement 1, P30

92. Torgov V.G., Kostin G.A, Us T.V., Korda T.M., Klimchuk O.V., Miroshnichenko S.I., Suwinska K., **Varnek A.A.**, Kalchenko V. I.

[Calixarenes grafted with Bu₂P\(O\)CH₂O binding groups at the narrow rim. Synthesis, structure and extraction of heterometallic Ru/Zn complexes.](#)

J. Inclusion Phenomena and Macrocyclic Chemistry, 2011, **71** (1), 67-77

93. Gilles Marcou, Isabelle Billard, Ali Ouadi and **Alexandre Varnek**

[In silico design of new ionic liquids \(ILs\) based on QSPR models of ILs viscosity](#)

J. Phys. Chem. B, 2011, **115** (1), 93–98

94. **Alexandre Varnek** and Igor I. Baskin

[Chemoinformatics as a theoretical chemistry discipline.](#)

Mol. Informatics, 2011, **30**, 20 – 32

95. Christian Koch, Gisbert Schneider, Gilles Marcou, **Alexandre Varnek**, Dragos Horvath

[Local Neighborhood Behavior: Study of a Combinatorial Library Context](#)

J. Computer-Aided Molecular Design, 2011, **25**:237–252

96. Iurii Sushko, Anil Kumar Pandey, Sergii Novotarskyi, Robert Körner, Matthias Rupp, Wolfram Teetz, Stefan Brandmaier, Ahmed Abdelaziz, Volodymyr V. Prokopenko, Vsevolod Y. Tanchuk, Roberto Todeschini, **Alexander Varnek** Gilles Marcou, Peter Ertl, Vladimir Potemkin, Maria Grishina, Johann Gasteiger, Igor I. Baskin, Vladimir A. Palyulin, Eugene V. Radchenko, William J. Welsh, Vladyslav Kholodovych, Dmitriy Chekmarev Artem Cherkasov, Joao Aires-de-Sousa, Qing-You Zhang, Andreas Bender, Florian Nigsch, Luc Patiny, Igor V. Tetko

[Online Chemical Modeling Environment \(OCHEM\): Web Platform for Data Storage, Model Development and Publishing of Chemical Information](#)

J. Computer-Aided Molecular Design, 2011, **25** (6), 533-54.

97. Frank Hoonakker, Nicolas Lachiche, **Alexandre Varnek** and Alain Wagner

[Condensed Graph of Reaction: considering a chemical reaction as one single pseudo molecule](#)

International Journal on Artificial Intelligence Tools, 2011, **20**, (2), 253-270

98. Andrei A. Krysko, Georgiy V. Samoilenko, Pavel G. Polishchuk, Sergei A. Andronati, Tatyana A. Kabanova, Tetiana M. Khristova, Victor E. Kuz'min, Vladimir M. Kabanov, Olga L. Krysko, **Alexandre A. Varnek** and Ruslan Ya. Grygorash

[RGD mimetics containing phthalimidine fragment, novel ligands of fibrinogen receptor.](#)

Bioorganic & Medicinal Chemistry Letters, 2011, **21**, 5971–5974

99. Vitaly P. Solov'ev, Ioana Oprisiu, Gilles Marcou and **Alexandre Varnek**

[QSPR Modeling of Normal Boiling Point Temperature and Composition of Binary Azeotropes](#)

Industrial & Engineering Chemistry Research, 2011, **50** (24), 14162–14167

100. Vitaly P. Solov'ev, Igor V. Sukhno, Vladimir Yu. Buzko, Aleksey A. Polushin, Gilles Marcou, Aslan Yu. Tsivadze, **Alexandre Varnek**

[QSPR modeling of stability constants of the complexes of Zn²⁺, Cd²⁺, and Hg²⁺ with organic ligands in water](#)

J. Inclusion Phenomena and Macrocyclic Chemistry, 2012, **72**, 309-321

101. Paul N. W. Baxter, Abdelaziz Al-Ouahabi, Jean-Paul Gisselbrecht, Lydia Brelot, André De Cian, **Alexandre Varnek**

[Electronic, Spectroscopic, Ion-Binding and Structural Property Screening of a Dehydro\[m\]pyrido\[n\]annulene Library: A Strategy for the Discovery of Optimal Candidates for Supramolecular Materials Engineering.](#)

J. Org. Chem, 2012, **77** (1), 126–142

102. N. Kireeva, I.I. Baskin, H. A. Gaspar a, D. Horvath, G. Marcou and **A. Varnek**

[Generative Topographic Maps \(GTM\): universal tool for data visualization, structure-activity modeling and database comparison.](#)

Mol. Informatics, 2012, **31**, 201-312

103. Fanny Bonachera,; Gilles Marcou,; Natalia Kireeva, **Alexandre Varnek**, Dragos Horvath

[Using Self-Organizing Maps to Accelerate Similarity Search](#)

Bioorganic Medicinal Chemistry, 2012, **20**, 5396–5409

104. **Alexandre Varnek** and Igor Baskin

[Machine Learning Methods for Property Prediction in Chemoinformatics: Quo Vadis ?](#)

J. Chem. Inf. Model. 2012, **52**, 1413–1437

105. I. Oprisiu, E. Varlamova, E. Muratov, A. Artemenko, G. Marcou, P. Polishchuk, V. Kuz'min, **A. Varnek**
[QSPR approaches to predict non-additive properties of mixtures. Application to bubble point temperatures of binary mixtures of liquids.](#)

Mol. Informatics, 2012, **31**, 491 – 502

106. G. Marcou, D. Horvath, V. Solov'ev, A. Arrault, P. Vayer, **A. Varnek**

[Interpretability of SAR/QSAR models of any complexity by atomic contributions](#)

Mol. Informatics, 2012, **31**(9), 639–642

107. Aurélie de Luca, Dragos Horvath, Gilles Marcou, Vitaly P. Solov'ev and **Alexandre Varnek**

[Mining Chemical Reactions Using Neighborhood Behavior and Condensed Graphs of Reactions Approaches](#)

J. Chem. Inf. Model. 2012, **52** (9), 2325–2338

108. Vitaly Solov'ev, Gilles Marcou, **Alexandre Varnek** and Aslan Tsivadze

[Complexation of Mn²⁺, Fe²⁺, Y³⁺, La³⁺, Pb²⁺, and UO₂²⁺ with Organic Ligands: QSPR Ensemble Modeling of Stability Constants](#)

Industrial & Engineering Chemistry Research, 2012, **51**, 13482–13489

109. Christophe Muller, Gilles Marcou, Dragos Horvath, João Aires-de-Sousa, **Alexandre Varnek**

[Models for identification of erroneous atom-to-atom mapping of reactions performed by automated algorithms.](#)

J. Chem. Inf. Model. 2012, **52** (12), 3116–3122

110. Evgeny Kondratovich, Igor I. Baskin and **Alexandre Varnek**

[Transductive Support Vector Machines: promising approach to model small, unbalanced and diverse datasets](#)

Mol. Inf., 2012, **32** (3), 261-266

111. V. P. Solov'ev, N. Kireeva, A. Yu. Tsivadze and **A. Varnek**,

[QSPR Consensus Models for Alkaline-Earth Metal Complexation](#)

J. Inclusion Phenomena and Macrocyclic Chemistry, 2013, **76**(1), 159-171

112. Vitaly Solov'ev, Aslan Tsivadze, **Alexandre Varnek**

[New Approach for Accurate QSPR Modeling of Metal Complexation: Application to Stability Constants of Lanthanide Ions Ln³⁺, Ag⁺, Zn²⁺, Cd²⁺ and Hg²⁺ with Organic Ligands in Water](#)

Macroheterocycles (Russ), 2012, **5** (4-5), 404-410

113. Ioana Oprisiu, Gilles Marcou, Dragos Horvath, Damien Bernard Brunel, Fabien Rivollet, **Alexandre Varnek**

[Publicly available models to predict normal boiling points of organic compounds.](#)

Thermochimica Acta, 2013, **553**, 60– 67

114. Vladimir Chupakhin, Gilles Marcou, Igor Baskin, **Alexandre Varnek**, and Didier Rognan

[Predicting ligand binding modes from neural networks trained on protein-ligand interaction fingerprints](#)

J. Chem. Inf. Model., 2013, **53** (4), 763-772

115. Horvath, Dragos; Marcou, Gilles; **Varnek, Alexandre**

[Do not hesitate to use Tversky – and other hints for successful active analogue searches with feature count descriptors.](#)

J. Chem. Inf. Model., 2013, **53** (7), 1543-1562

116. Krysko, A. A., Samoylenko, G. V.; Polishchuk, P.G.; Fonari, M. S; Kravtsov, V. C; Andronati, S. A; Kabanova, T. A; Lipkowski, J; Khristova, T. M; Kuz'min, V. E; Kabanov, V. M; Krysko, O. L; **Varnek, A. A.** [Synthesis, biological evaluation, X-ray molecular structure and molecular docking studies of RGD mimetics containing 6-amino-2,3-dihydroisoindolin-1-one fragment as ligands of integrin alpha\(IIb\)beta\(3\)](#) *Bioorganic & Medicinal Chemistry*, 2013, **21**(15), 4646-4661
117. Paul N. W. Baxter, Jean-Paul Gisselbrecht, Lydia Brelot, **Alexandre Varnek** and Lionel Allouche [Synthesis of a Strained Acetylenic Macrocyclic Incorporating a para-Oligo\[2\]cruciform Bridge Bent over Nanoscopic Dimensions: Structural, Electronic, Spectroscopic and Ion-Sensing Properties.](#) *Chem. Eur. J.*, 2013, **19** (37), 12336-12349
118. P.G. Polishchuk, T.I. Madzhidov, **A. Varnek** [Estimation of the size of drug-like chemical space based on GDB-17 data](#) *J. Comput. Aided Mol. Des.*, 2013, **27**:675–679
119. Denis Beltrami, Alexandre Chagnes, Mansour Haddad, **Alexandre Varnek**, Hamid Mokhtari, Bruno Courtaud, Gérard Cote [Recovery of uranium \(VI\) from concentrated phosphoric acid by mixtures of new bis\(1,3- dialkylxypropan-2-yl\) phosphoric acids and tri-n-octylphosphine oxide](#) *Hydrometallurgy*, 2013, **140** 28–33
120. Héléna A. Gaspar, Gilles Marcou, Alban Arault, Sylvain Lozano, Philippe Vayer, **Alexandre Varnek** [GTM-based classification models and their applicability domain: application to the Biopharmaceutics Drug Disposition Classification System \(BDDCS\)](#) *J. Chem. Inf. Model.*, 2013, **53** (12), 3318-25; DOI: 10.1021/ci400423c
121. A. Cherkasov, E. Muratov, D. Fourches, **A. Varnek**, I. Baskin, M. Cronin, J. Dearden, P. Gramatica, Y. Martin, R. Todeschini, V. Consonni, V. Kuz'min, R. Cramer, R. Benigni, C Yang, A. Richard, L. Terfloth, J. Gasteiger, and A. Tropsha [QSAR Modeling: Where have you been? Where are you going to?](#) *J. Med. Chem.*, 2014, **57** (12), 4977-5010
122. Fiorella Ruggiu, Patrick Gizzi, Jean-Luc Galzi, Marcel Hibert, Jacques Haiech, Igor Baskin, Dragos Horvath, Gilles Marcou, **Alexandre Varnek** [QSPR modelling – a valuable support in HTS quality control](#) *Anal.Chem.* 2014, **86** (5) 2510-2520
123. T. I. Madzhidov, P. G. Polishchuk, R. I. Nugmanov, A.V. Bodrov, A.I. Lin, I.I. Baskin, I.S. Antipin, **A.A. Varnek** [Structure-reactivity relationships in terms of the condensed graphs of reactions](#) *Russ. J. Org. Chem.*, 2014, **50** (4), 459-463
124. Vitaly Solov'ev, **Alexandre Varnek**, Aslan Tsivadze [QSPR Ensemble Modelling of the 1:1 and 1:2 Complexation of Co²⁺, Ni²⁺, and Cu²⁺ with Organic Ligands. Relationships between Stability Constants](#) *Computer Aided Mol. Design*, 2014, **28**,549–564
125. J. B. Brown, Yasushi Okuno, Gilles Marcou, **Alexandre Varnek**, and Dragos Horvath [Computational chemogenomics - is it more than inductive transfer?](#) *J. Computer Aided Mol. Design*, 2014, **28**, 597–618
126. Vladimir Chupakhin, Gilles Marcou, Helena Gaspar, **Alexandre Varnek** [Simple Ligand-Receptor Interaction Descriptor \(SILIRID\) for alignment-free binding sites comparison](#) *Computational and Structural Biotechnology Journal*, 2014, **10** (16), 33–37
127. Fiorella Ruggiu, Vitaly Solov'ev, Gilles Marcou, Dragos Horvath, Jerome Graton, Jean-Yves Le Questel, **Alexandre Varnek** [Individual hydrogen-bond strength QSPR modelling with ISIDA local descriptors: a step towards polyfunctional molecules](#) *Mol. Informatics*, 2014, **33**, 477 – 487

128. Dragos Horvath, Michael Lisurek, Bernd Rupp, Ronald Khne, Edgar Specker, Jens von Kries, Didier Rognan, C. David Andersson, Fredrik Almqvist, Mikael Elofsson, Per-Anders Enqvist, Anna-Lena Gustavsson, Nikita Remez, Jordi Mestres, Gilles Marcou, **Alexandre Varnek**, Marcel Hibert, Jordi Quintana, Ronald Frank [Design of a General-Purpose European Compound Screening Library for EU-OPENSREEN](#) *ChemMedChem*, 2014, **9**, 2309 – 2326, DOI: 10.1002/cmdc.201402126
129. Didier Rognan, **Alexandre Varnek** [A Summer School for Structuring the Chemoinformatics Community](#) *Mol. Informatics*, 2014, **33** (6-7), 390
130. R.I. Nugmanov, T.I. Madzhidov, G.R. Haliullina, I.I. Baskin, I.S. Antipin, **A. Varnek** Development of "structure-reactivity" models for nucleophilic substitution reactions with participation of azides *J. Struct. Chem. (Russ)*, 2014, **55** (6), 1080 – 1087
131. Gleb V. Sitnikov, Nelly I. Zhokhova, Yury A. Ustynyuk, **Alexandre Varnek**, Igor I. Baskin Continuous [Indicator Fields – A Novel Universal Type of Molecular Fields](#) *J. Computer Aided Mol. Design*, 2014, **29**(3), DOI 10.1007/s10822-014-9818-z
132. Dragos Horvath, J.B. Brown, Gilles Marcou and **Alexandre Varnek** [An Evolutionary Optimizer of libsvm Models](#) *Challenges*, 2014, **5**(2), 450-472; doi:10.3390/challe5020450
133. Mourad Elhabiri, Pavel Sidorov, Elena Cesar Rodo, Gilles Marcou, Don Antoine Lanfranchi, Elisabeth Davioud-Charvet, Dragos Horvath, and **Alexandre Varnek** [Electrochemical Properties of Substituted 2-Methyl-1,4-Naphthoquinones \(Vitamin K3\): How to Predict their Redox Behavior](#) *Chemistry Eur. J.*, 2014, **21**, 3415–3424, DOI: 10.1002/chem.201403703
134. C. Muller, D. Pekthong, C. Desbans, E. Alexandre, G. Marcou, L. Richert and **A. Varnek** Prediction of DILI using molecular and biological descriptors *Combinatorial Chemistry & High Throughput Screening*, 2015, **18**(3). DOI:10.2174/1386207318666150305144650
135. Héléna Gaspar, Igor I. Baskin, Gilles Marcou, Dragos Horvath and **Alexandre Varnek** [Chemical Data Visualization and Analysis with Incremental GTM: Big Data Challenge](#) *J. Chem. Inf. Model.*, 2015, **55** (1), 84–94
136. H. A. Gaspar, I. I. Baskin, G. Marcou, D. Horvath, **A. Varnek** GTM-based QSAR models and their applicability domains *Mol. Informatics*, 2015, **34** (6-7), 348-356
137. T. Khristova, P. Polishchuk, A. Varnek, V. Kuzmin Computer-aided design of new antagonists of thromboxane receptors acting as anti-aggregation agents *Dopovidi NASU. (ukr)*, 2014, N⁹, 103-108
138. G. Marcou, J. Aires de Sousa, D. Latino, A. Deluca, D. Horvath, V. Rietsch, and A. Varnek Towards an expert system for predicting reaction conditions: the Michael reaction case. *J. Chem. Inf. Model.*, 2015, **55**, 239–250; DOI: 10.1021/ci500698a
139. Laurent Hoffer, Camelia Chira, Gilles Marcou, Alexandre Varnek and Dragos Horvath S4MPLE – Sampler For Multiple Protein-Ligand Entities. I. Methodology & Rigid-Site Docking Benchmarking *Molecules*, 2015, **20**, 8997-9028; DOI:10.3390/molecules20058997
140. Christophe Muller, Ana G. Maldonado, Alexandre Varnek, Benoit Creton Prediction of optimal salinities for surfactant formulations using QSPR approaches. *Energy and Fuels*, 2015, **29** (7), 4281–4288.
141. Pavel G. Polishchuk, Georgiy V. Samoylenko, Tetiana M. Khristova, Olga L. Krysko, Tatyana A. Kabanova, Vladimir M. Kabanov, Alexander Yu. Korniylov, Olga Klimchuk, Thierry Langer, Sergei A. Andronati, Victor E. Kuz'min, Andrei A. Krysko, Alexandre Varnek Virtual screening, design and synthesis of antagonists of α IIb β 3 as antiplatelet agents

J. Med. Chem., 2015, **58** (19), pp 7681–7694, DOI 10.1021/acs.jmedchem.5b00865

142. H. A. Gaspar, I. I. Baskin, G. Marcou, D. Horvath, A. Varnek
Stargate GTM: bridging descriptor and activity spaces.
J. Chem. Inf. Model., 2015, **55** (11), 2403–2410, DOI: 10.1021/acs.jcim.5b00398
143. T. Madzhidov, A. Bodrov, T. Gimadiev, R. Nugmanov, I. Antipin, A. Varnek
Obtaining structure-reactivity relationships for bimolecular elimination reactions with Condensed Reaction Graph approach
J. Struct. Chem. (Russ), 2015, **56** (7), 1227–1234; DOI: 10.1134/S002247661507001X
144. Marta Glavatskikh, Timur Madzhidov, Vitaly Solov'ev, Gilles Marcou, Dragos Horvath, Jérôme Graton, Jean-Yves Le Questel, Alexandre Varnek
Predictive models for halogen-bond basicity of binding sites of polyfunctional molecules
Mol. Informatics, 2016, **35**, 70-80; DOI: 10.1002/minf.201500116
145. P. Sidorov, H. A. Gaspar, Helena; A. Varnek, G. Marcou, D. Horvath
Mappability of drug-like space: towards a polypharmacologically competent map of drug-relevant compounds
J Comput Aided Mol Des. 2015, **29**(12):1087-1108
146. T. Madzhidov, R. Nugmanov, T. Gimadiev, A. Lin, I. Antipin, A. Varnek
Consensus approach to atom-to-atom mapping in chemical reactions
Butlerov Communications 11/2015; 44(12):170-176
147. Gilles Marcou, Dragos Horvath, and Alexandre Varnek
Kernel Target Alignment parameter – a new modelability measure for regression tasks
J. Chem. Inf. Model., 2016, **56** (1), 6–11
148. Sidorov P., Desta I. Chessé M., Horvath D., Marcou G., Varnek A., Davioud-Charvet E., Elhabiri M.
Redox Polypharmacology as an Emerging Strategy to Combat Malarial Parasites
ChemMedChem, 2016, **11**, 1-14, DOI: 10.1002/cmdc.201600009
149. Kamel Mansouri, Ahmed Abdelaziz, Aleksandra Rybacka, Alessandra Roncaglioni, Alexander Tropsha, **Alexandre Varnek**, Alexey Zakharov, Andrew Worth, Ann M. Richard, Christopher M. Grulke, Daniela Trisciuzzi, Denis Fourches, Dragos Horvath, Emilio Benfenati, Eugene Muratov, Eva Bay Wedebye, Francesca Grisoni, Giuseppe F. Mangiatordi, Giuseppina M. Incisivo, Huixiao Hong, Hui W. Ng, Igor V. Tetko, Ilya Balabin, Jayaram Kancharla, Jie Shen, Julien Burton, Marc Nicklaus, Matteo Cassotti, Nikolai G. Nikolov, Orazio Nicolotti, Patrik L. Andersson, Qingda Zang, Regina Politi, Richard D. Beger, Roberto Todeschini, Ruili Huang, Sherif Farag, Sine A. Rosenberg, Svetoslav Slavov, Xin Hu, and Richard S. Judson
CERAPP: Collaborative Estrogen Receptor Activity Prediction Project
Environ Health Perspect, 2016, *accepted*, DOI: 10.1289/ehp.1510267
150. Birgit Viira, Thibault Gendron, Don Antoine Lanfranchi, Sandrine Cojean, Dragos Horvath, Gilles Marcou, Alexandre Varnek, Louis Maes, Uko Maran, Philippe Loiseau, Elisabeth Davioud-Charvet
In Silico Mining for Antimalarial Structure-Activity Knowledge and Discovery of Novel Antimalarial Curcuminoids
Molecules, 2016, **21**(7), 853, DOI:10.3390/molecules21070853
151. Marta Glavatskikh, Timur Madzhidov, Vitaly Solov'ev, Gilles Marcou, Dragos Horvath and Alexandre Varnek
Predictive Models for the Free Energy of Hydrogen Bonded Complexes with Single and Cooperative Hydrogen Bonds
Mol. Informatics, 2016, **35** (11-12), 629-638, DOI: 10.1002/minf.201600070
152. Klimenko Kyrylo, Gilles Marcou, Dragos Horvath, Alexandre Varnek
Chemical space mapping and structure-activity analysis of the ChEMBL antiviral compound set.
J. Chem. Inf. Model., 2016, **56**, 1438–1454
153. Pavel Polishchuk, Oleg Tinkov, Tatiana Khristova, Ludmila Ognichenko, Anna Kosinskaya, Alexandre Varnek, Victor Kuz'min
Structural and physico-chemical interpretation (SPCI) of QSAR models and its comparison with MMP analysis

J. Chem. Inf. Model., 2016, **56**, 1455–1469

154. Timur R. Gimadiev, Timur I. Madzhidov, Gilles Marcou, Alexandre Varnek
Generative Topographic Mapping approach to modeling and chemical space visualization of Human Intestinal Transporters
BioNanoScience, 2016, **6** (4), 464-472, DOI: 10.1007/s12668-016-0246-5

155. Dragos Horvath, Gilles Marcou, Alexandre Varnek, Shilva Kayastha, Antonio de la Vega de León, Jürgen Bajorath
Prediction of Activity Cliffs Using Condensed Graphs of Reaction Representations, Descriptor Recombination, Support Vector Machine Classification, and Support Vector Regression
J. Chem. Inf. Model., 2016, **56** (9), 1631–1640

156. Arkadii I. Lin, Timur I. Madzhidov, Olga Klimchuk, Ramil I. Nugmanov, Igor S. Antipin and Alexandre Varnek
Assessment of protective group reactivity from big data analysis
J. Chem. Inf. Model., 2016, **56** (11), 2140–2148, DOI: 10.1021/acs.jcim.6b00319

157. Маджидов Т. И., Гимадиев Т. Р., Малахова Дарья Андреевна, Нугманов Рамиль Ирекович, Антипин Игорь Сергеевич и Варнек Александр
Соотношение «структура–реакционная способность» в реакциях Дильса-Альдера с использованием подхода конденсированных графов реакций
J. Struct. Chem (Russ.), 2016, **58** (4)

158. Pavel Sidorov, Birgit Viira, Elisabeth Davioud-Charvet, Uko Maran, Gilles Marcou, Dragos Horvath, Alexandre Varnek
QSAR modeling and chemical space analysis of antimalarial compounds
J. Computer-Aided Molecular Design, 2017, **31** (5), 441-45, DOI: 10.1007/s10822-017-0019-4

159. Dragos Horvath, Igor Baskin, Gilles Marcou, Alexandre Varnek
Generative Topographic Mapping of Conformational Space
Mol. Informatics, accepted 30.03.17

160. Shilva Kayastha, Dragos Horvath, Erik Gilberg, Michael Gütschow, Jürgen Bajorath, Alexandre Varnek
Privileged Structural Motif Detection and Analysis using Generative Topographic Maps
J. Chem. Inf. Model., 2017, **56** (5), 1218-1232

161. Igor I. Baskin, Vitaly P. Solov'ev, Alexander A. Bagaturyans and Alexandre Varnek
Predictive Cartography of Metal Binders Using Generative Topographic Mapping
J. Computer-Aided Molecular Design, 2017, accepted

162. Kyrylo Klimenko, Sergei Lyakhov, Marina Shibinskaya, Alexander Karpenko, Gilles Marcou, Dragos Horvath, Marina Zenkova, Elena Goncharova, Rinat Amirkhanov, Sergei Andronati, Pavel Polishchuk, Victor Kuz'min, and Alexandre Varnek
Virtual screening, synthesis and biological evaluation of DNA intercalating antiviral agents
Bioorganic & Medicinal Chemistry Letters, 2017, accepted

163. G. Marcou, D. Horvath and A. Varnek
Neighboring structure visualization on a grid-based layout
Mol. Informatics, 2017, accepted

164. Pavel Polishchuk, Timur Madzhidov, Timur Gimadiev, Andrey Bodrov, Ramil Nugmanov, Alexandre Varnek
Structure-reactivity modeling using mixture-based representation of chemical reactions
J. Computer-Aided Molecular Design, 2017, accepted

Patent

Frank Hoonakker, **Alexandre Varnek** and Alain Wagner

[A computer based method for calculate similarity between two reactions based on the concept of Condensed Graph of Reactions.](#)

US 11/779 255, PCT/IB2008/052851 from 17.07.2008