

CURRICULUM VITAE

Stanislav K. Ignatov

Name: Stanislav Konstantinovich Ignatov

Date and place of birth: 1965, Nizhny Novgorod, Russia

Citizenship: Russian

Title: D.Sc. (д.х.н., Physical Chemistry, 2006)

Ph.D. (Physical Chemistry, 1995)

Professor (zvanie professor, 2019)



Position: Professor, Chair of Physical Chemistry, Department of Chemistry,

Lobachevsky State University of Nizhny Novgorod

Since 2021, additionally: Leading Scientist of the Laboratory of Molecular Modeling and Chemoinformatics, Lobachevsky State University of Nizhny Novgorod

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Education: 1982-1989 Department of Chemistry, University of Nizhny Novgorod

(Honor Diploma in Chemistry)

1991-1994 Ph.D. work (Aspirantura), Physical Chemistry Chair, University of Nizhny Novgorod, supervisor Prof. Yu.A.Alexandrov

Thesis: "Quantum-chemical treatment of the thermochemical, electronic, and structural parameters of organochromium compounds with the bipolar expansion technique for the Ohno potential"

Scientific interests:

1. Physico-chemical properties and molecular modeling of bioorganic structures including membranes, cell walls and biopolymer complexes.
2. Development of drugs with antibacterial, antiviral and anticancer activity on the basis of theoretical modeling including molecular dynamics, molecular docking, combined quantum-classical calculations and chemoinformatics.
3. Theoretical treatment of the metal clusters, weak complexes in organic and inorganic systems, studies of their reaction and dynamics in the gas-phase and on various interfaces.

Bibliometric data:

Hirsch index (WoS):	20
Number of publications(WoS)	74
Sum of the Times Cited:	1033
Citing Articles:	803

Selected Recent Publications

1. Savintseva L.A., Steshin I.S., Avdoshin A.A., Panteleev S.V., Rozhkov A.V., Shirokova E.A., Livshits G.D., Vasyankin A.V., Radchenko E.V., Ignatov S.K., Palyulin V.A. *Conformational dynamics and stability of bilayers formed by mycolic acids from the Mycobacterium tuberculosis outer membrane.* Molecules, 2023, **28**, 1347. Membrane. Molecules 2023, 28, 1347. <https://doi.org/10.3390/molecules28031347>
2. Radchenko E.V., Antoneyan G.V., Ignatov S.K., Palyulin V.A. *Machine Learning Prediction of Mycobacterial Cell Wall Permeability of Drugs and Drug-like Compounds.* Molecules. 2023, **28**, 633 (14 pages). <https://doi.org/10.3390/molecules28020633>
3. Avdoshin A, Naumov V., Colombi Ciacchi L., Ignatov S., Köppen S. *Atomistic Simulations of Chitosan as Possible Carrier System for miRNA Transport.* Materials Advances. 2023. ASAP article. <https://doi.org/10.1039/D2MA00830K>
4. Naumov V.S., Ignatov S.K. *Modification of 56A(CARBO) force field for molecular dynamic calculations of chitosan and its derivatives.* Journal of Molecular Modeling. 2017, **23**(8). DOI:10.1007/s00894-017-3421-x.
5. Naumov V.S., Ignatov S.K. *Dissolution of chitosan nanocrystals in aqueous media of different acidity. Molecular dynamic study.* Carbohydrate Polymers. 2019, **207**, 619-627. DOI:10.1016/j.carbpol.2018.12.019.
6. Savintseva L., Avdoshin A., Ignatov S., Novikov A. *Theoretical Study of Charge Mobility in Crystal Porphine and a Computer Design of a Porphine-Based Semiconductive Discotic Liquid Mesophase.* International Journal of Molecular Sciences. 2023, **24**, 736 (13 pages). <https://doi.org/10.3390/ijms24010736>.
7. Savintseva L. A., Avdoshin A. A., Ignatov S. K. *Charge Transport in Biomimetic Models of Organic Neuromorphous Materials.* Russian Journal of Physical Chemistry B, 2022, Vol. 16, No. 3, pp. 450–459. <https://doi.org/10.1134/S1990793122030216>.
8. Shchegrevina E.S., Maleev A.A., Ignatov S.K., Gracheva I.A., Stein A., Schmalz H.G., Gavryushin A.E., Zubareva A.A., Svirshchevskaya E.V., Fedorov A.Y. *Synthesis and biological evaluation of novel non-racemic indole-containing allocolchicinoids.* European Journal of Medicinal Chemistry. 2017, **141**, 51-60. DOI:10.1016/j.ejmech.2017.09.055.
9. Eliseeva T.I., Tush E.V., Krasilnikova S.V., Kuznetsova S.V., Larin R.A., Kubysheva N.I., Khaletskaya O.V., Potemina T.E., Ryazantsev S.V., Ignatov S.K. *Metabolism of the Extracellular Matrix in Bronchial Asthma (Review).* Sovremennye Tehnologii V Medicine. 2018, **10**(4), 220-232. DOI:10.17691/stm2018.10.4.25.
10. Tush E.V., Eliseeva T.I., Khaletskaya O.V., Krasilnikova S.V., Ovsyannikov D.Y., Potemina T.E., Ignatov S.K. *Extracellular Matrix Markers and Methods for Their Study (Review).* Sovremennye Tehnologii V Medicine. 2019, **11**(2), 133-147. DOI:10.17691/stm2019.11.2.20.