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Member of the Council for Grants of the President of the Russian Federation, the Expert Board of the Skolkovo Foundation and the Expert Council of the Sirius University of Science and Technology; Expert of the Russian Academy of Sciences, the Russian Ministry of Science and High Education, the Russian Science Foundation. Member of the American Chemical Society, Russian Biochemical Society; Society of Russian Pharmacologists. <u>Editorial Board Member:</u> Big Data Mining and Analytics, SAR and QSAR in Environmental Research, Biomedical Chemistry, Pharmaceutical Chemistry Journal. <u>Reviewer:</u> Scientific Reports, Briefings in Bioinformatics, Molecular Informatics, Drug Discovery Today, Journal of Chemical Information and Modeling, ACS Pharmacology & Translational Sciences, ACS Omega, Chemical Research in Toxicology, Frontiers in Pharmacology, Expert Opinion on Drug Discovery, etc. Co-author of 350 publications in the peer-reviewed journals and book chapters with over 6,800 citations (Web of Science h-index is 40). For thirty years co-chaired the annual Symposium on Bioinformatics and Computer-Aided Drug Discovery (https://www.way2drug.com/dr/bcadd2024/). Scientific Advisory Board Member and/or Keynote/Invited/Oral Speaker of more than 12 International conferences and symposia in the past three years.

<u>Research interests</u>: Bioinformatics, Chemoinformatics, Computer-Aided Drug Design & Discovery, (Q)SAR, Molecular Modelling