

Third-party publications with references to PASS

Chand, B., Malik, M.A. Biological-activity predictions, crystallographic comparison and role of packing interactions in androstane derivatives of steroids. (2011) *Journal of Chemical Crystallography*, 41 (3), pp. 255-275.

Deshmukh, V.K., Raviprasad, P., Kulkarni, P.A., Kuberkar, S.V. Design, synthesis and biological activities of novel 4H-pyrimido [2, 1-b] [1, 3] benzothiazole derivatives. (2011) *International Journal of ChemTech Research*, 3 (1), pp. 136-142.

Sapa, J., Nowaczyk, A., Kulig, K. Antiarrhythmic and antioxidant activity of novel pyrrolidin-2-one derivatives with adrenolytic properties. (2011) *Naunyn-Schmiedeberg's Archives of Pharmacology*, 383 (1), pp. 13-25.

Vasilevsky, S.F., Govdi, A.I., Sorokina, I.V., Tolstikova, T.G., Baev, D.S., Tolstikov, G.A., Mamatuyk, V.I., Alabugin, I.V. Rapid access to new bioconjugates of betulonic acid via click chemistry. (2011) *Bioorganic and Medicinal Chemistry Letters*, 21 (1), pp. 62-65.

Mashentseva, A.A., Seytembetov, T.S., Adekenov, S.M., Tuleuov, B.I., Loiko, O.P., Khalitova, A.I. Synthesis and biological activity of the pinostrobin oxime complex compounds with some d-metals. (2011) *Russian Journal of General Chemistry*, 81 (1), pp. 96-101.

Azhaguraj, R., Arokia Lenin, E., Viswanathan, C., Sangeetha, B., Selvanayagam, M. Predication of biological activity of algal antitumor drugs using pass (2010) *Pharmacologyonline*, 3, pp. 22-34.

Prasad, Y.R., Rajasekhar, K.K., Shankarananth, V., Pradeepkumar, G.S.S., Surya Teja, S.P., Rajeev Reddy, B. *In silico* biological activity evaluation of some 3-substituted-4-hydroxy-6-methyl-2Hpyran-2-ones. (2010) *Journal of Pharmacy Research*, 3 (10), pp. 2470-2472.

Babaev, E.V. Combinatorial chemistry in higher school: Ten-year experience of research, educational, and managerial projects (2010) *Russian Journal of General Chemistry*, 80 (12), pp. 2655-2670.

Xie, X.-Q.S. Exploiting PubChem for virtual screening (2010) *Expert Opinion on Drug Discovery*, 5 (12), pp. 1205-1220.

Zadorozhny, A.V., Turov, A.V., Kovtunencko, V.A. Synthesis of substituted 4-oxo-3, 4-dihydro-thieno[3, 4-d]pyrimidines and comparison of their properties with those of positionally isomeric thienopyrimidinones and benzo isosteres (2010) *Chemistry of Heterocyclic Compounds*, 46 (8), pp. 991-997.

- Potikha, L.M., Sypchenko, V.V., Kovtunenکو, V.A.
Condensed isoquinolines. 36*. Cyclization of N-alkyl-3-(2-benzoylbenzyl)azolium salts. A novel method of preparing azolo[b]isoquinolines
(2010) Chemistry of Heterocyclic Compounds, 46 (9), pp. 1096-1104.
- Zadorozhny, A.V., Kovtunenکو, V.A., Turov, A.V.
Condensed isoquinolines. 35*. Synthesis and reactions of 4h-thieno[3', 4':5, 6]pyrimido-[1, 2-b]isoquinoline-4, 11(5H)-dione
(2010) Chemistry of Heterocyclic Compounds, 46 (8), pp. 957-965.
- Potikha, L.M., Sypchenko, V.V., Kovtunenکو, V.A.
Condensed isoquinolines. 36. The cyclization of N-alkyl-3-(2-benzoylbenzyl) -azolium salts - A new method of synthesis of azolo[b]isoquinoline derivatives
(2010) Khimiya Geterotsiklicheskih Soedinenii, (9), pp. 1360-1371.
- Zadorozny, A.V., Kovtunenکو, V.A., Turov, A.V.
Condensed iso-quinolines. 35. The synthesis and transformation of 4H-thieno[3', 4':5, 6]pyrimido[1, 2-b]isoquinoline-4, 11(5H)-dione
(2010) Khimiya Geterotsiklicheskih Soedinenii, (8), pp. 1185-1195. Cited 1 time.
- Zadorozny, A.V., Turov, A.V., Kovtunenکو, V.A.
Synthesis of substituted 4-oxo-3, 4-dihydrothieno[3, 4-d]pyrimidines and comparison of their properties with properties of positionally isomeric thienopyrimidinones and benzene isomers
(2010) Khimiya Geterotsiklicheskih Soedinenii, (8), pp. 1227-1234.
- Pospieszny, T., Wyrzykiewicz, E.
Thio analogs of pyrimidine bases: Synthesis and spectroscopic study of new potentially biologically active disulfides of N, O-(N, N- or O, O-)-Di- and N, N, O-Tri-(o-, m-, and p-)bromobenzyl-2-thiouracils
(2010) Phosphorus, Sulfur and Silicon and the Related Elements, 185 (10), pp. 2101-2107.
- Kulakov, I.V., Turdybekov, D.M.
Synthesis and crystal structure of 5-methyl-2-(N-Anabasinyl)-5, 6-dihydro-1, 3-thiazin-4-one from the alkaloid anabasin
(2010) Chemistry of Natural Compounds, 46 (4), pp. 586-589.
- Zhao, H.-T., Soda, M., Endo, S., Hara, A., El-Kabbani, O.
Selectivity determinants of inhibitor binding to the tumour marker human aldose reductase-like protein (AKR1B10) discovered from molecular docking and database screening
(2010) European Journal of Medicinal Chemistry, 45 (9), pp. 4354-4357.
- Schuster, D.
3D pharmacophores as tools for activity profiling
(2010) Drug Discovery Today: Technologies, 7 (4), pp. e205-e211.
- Ursu, O., Oprea, T.I.
Model-free drug-likeness from fragments
(2010) Journal of Chemical Information and Modeling, 50 (8), pp. 1387-1394.
- Pospieszny, T., Małacka, I., Paryzek, Z.

A practical synthesis and spectroscopic study of new potentially biologically active S-lithocholic acid-substituted derivatives of 2-thiouracil
(2010) *Tetrahedron Letters*, 51 (32), pp. 4166-4169.

Bartkowiak, G., Wyrzykiewicz, E., Schroeder, G., Walkowiak, A., Szponar, A., Pawlak, I.
Thio analogues of pyrimidine bases: Syntheses and spectral study of new potentially biologically active 2, 4-di-ortho-(meta- and para-)bromo- (chloro and nitro)-benzylthio-5-bromouracils (and 6-methyluracils)
(2010) *Phosphorus, Sulfur and Silicon and the Related Elements*, 185 (7), pp. 1429-1436.

Ferdosiyan, M., Sardari, S.
In silico design and selection of anti-fungal AmB-polyene-analog lead molecules by virtual screening method
(2010) *Avicenna Journal of Medical Biotechnology*, 2 (3), pp. 137-143.

Torres-Piedra, M., Ortiz-Andrade, R., Villalobos-Molina, R., Singh, N., Medina-Franco, J.L., Webster, S.P., Binnie, M., Navarrete-Vázquez, G., Estrada-Soto, S.
A comparative study of flavonoid analogues on streptozotocin-nicotinamide induced diabetic rats: Quercetin as a potential antidiabetic agent acting via 11 β -Hydroxysteroid dehydrogenase type 1 inhibition
(2010) *European Journal of Medicinal Chemistry*, 45 (6), pp. 2606-2612.

Navarrete-Vázquez, G., Hidalgo-Figueroa, S., Torres-Piedra, M., Vergara-Galicia, J., Rivera-Leyva, J.C., Estrada-Soto, S., León-Rivera, I., Aguilar-Guardarrama, B., Rios-Gómez, Y., Villalobos-Molina, R., Ibarra-Barajas, M.
Synthesis, vasorelaxant activity and antihypertensive effect of benzo[d]imidazole derivatives
(2010) *Bioorganic and Medicinal Chemistry*, 18 (11), pp. 3985-3991.

Rayan, A., Marcus, D., Goldblum, A.
Predicting oral druglikeness by iterative stochastic elimination
(2010) *Journal of Chemical Information and Modeling*, 50 (3), pp. 437-445.

Rognan, D.
Structure-based approaches to target fishing and ligand profiling
(2010) *Molecular Informatics*, 29 (3), pp. 176-187.

Guha, R., Gilbert, K., Fox, G., Pierce, M., Wild, D., Yuan, H.
Advances in cheminformatics methodologies and infrastructure to support the data mining of large, heterogeneous chemical datasets
(2010) *Current Computer-Aided Drug Design*, 6 (1), pp. 50-67.

da Silva, C.H.T.d.P., da Silva, V.B., Resende, J., Rodrigues, P.F., Bononi, F.C., Benevenuto, C.G., Taft, C.A.
Computer-aided drug design and ADMET predictions for identification and evaluation of novel potential farnesyltransferase inhibitors in cancer therapy
(2010) *Journal of Molecular Graphics and Modelling*, 28 (6), pp. 513-523.

Mustafayeva, K., Giorgio, C.D., Elias, R., Kerimov, Y., Ollivier, E., De Méo, M.
DNA-damaging, mutagenic, and clastogenic activities of gentiopicroside isolated from *Cephalaria kotschyi* roots
(2010) *Journal of Natural Products*, 73 (2), pp. 99-103.

Blunt, J.W., Copp, B.R., Munro, M.H.G., Northcote, P.T., Prinsep, M.R.
Marine natural products
(2010) *Natural Product Reports*, 27 (2), pp. 165-237.

Prado-Prado, F.J., Ubeira, F.M., Borges, F., González-DÍAZ, H.
Unified QSAR & network-based computational chemistry approach to antimicrobials. II.
Multiple distance and triadic census analysis of antiparasitic drugs complex networks
(2010) *Journal of Computational Chemistry*, 31 (1), pp. 164-173.

Merlot, C.
Computational toxicology-a tool for early safety evaluation
(2010) *Drug Discovery Today*, 15 (1-2), pp. 16-22.

Raja, A.K., Vimalanathan, A.B., Raj, S.V., et al.
Indispensable chemical genomic approaches in novel systemic targeted drug discovery.
(2010) *Biology and Medicine*, 2 (3), pp. 26-37.

Zhao, J., Jiang, P., Zhang, W.
Molecular networks for the study of TCM pharmacology
(2009) *Briefings in Bioinformatics*, 11 (4), art. no. bbp063, pp. 417-430.

Riju, A., Sithara, K., Suja, S.N., et al.
In silico screening major spice phytochemicals for their novel biological activity and pharmacological fitness.
(2009) *Journal of Bioequivalence and Availability*, 1 (2), pp. 063-073.

Dearden, J.C., Hewitt, M., Geronikaki, A.A., Garibova, T.L., Macaev, F.Z., Voronina, T.A.
QSAR investigation of new cognition enhancers
(2009) *QSAR and Combinatorial Science*, 28 (10), pp. 1123-1129.

Ghadimi, S., Ebrahimi-Valmoozi, A.A.
Lipophilicity, electronic, steric and topological effects of some phosphoramidates on acetylcholinesterase inhibitory property
(2009) *Journal of the Iranian Chemical Society*, 6 (4), pp. 838-848.

Potikha, L.M., Turelyk, A.R., Kovtunenکو, V.A.
Synthesis and properties of Z-1, 3-bis(aryI)-4-bromo-2-buten-1-ones
(2009) *Khimiya Geterotsiklicheskikh Soedinenii*, (10), pp. 1478-1484.

Gorpinchenko, V.A., Petrov, D.V., Khursan, S.L., Dokichev, V.A., Tomilov, Yu.V.
Catalytic hydrogenation of methyl 3, 4-diazatricyclo[5.2.1.0 2, 6]dec-4-ene-5-carboxylate
(2009) *Khimiya Geterotsiklicheskikh Soedinenii*, (9), pp. 1301-1310.

Ellison, C.M., Enoch, S.J., Cronin, M.T.D., Madden, J.C., Judson, P.
Definition of the applicability domains of knowledge-based predictive toxicology expert systems by using a structural fragment-based approach
(2009) *ATLA Alternatives to Laboratory Animals*, 37 (5), pp. 533-545.

Potikha, L.M., Turelik, A.R., Kovtunenکو, V.A.
Synthesis and properties of Z-1, 3-bis- (aryl)-4-bromo-2-buten-1-ones
(2009) *Chemistry of Heterocyclic Compounds*, 45 (10), pp. 1184-1189.

- Balaji, S., Chempakam, B.
Pharmacokinetics prediction and drugability assessment of diphenylheptanoids from turmeric (*Curcuma longa* L)
(2009) *Medicinal Chemistry*, 5 (2), pp. 130-138.
- Gorpinchenko, V.A., Petrov, D.V., Khursan, S.L., Dokichev, V.A., Tomilov, Y.V.
Catalytic hydrogenation of methyl 3, 4-diazatricyclo-[5.2.1.0 2, 6]dec-4-ene-5-carboxylate
(2009) *Chemistry of Heterocyclic Compounds*, 45 (9), pp. 1039-1046.
- Ivanenkov, Ya.A., Bovina, E.V., Balakin, K.V.
Nonlinear mapping techniques for predicting the pharmacological properties of chemical compounds
(2009) *Russian Chemical Reviews*, 78 (5), pp. 465-483.
- Pokhodylo, N.T., Matiychuk, V.S., Obushak, M.D.
Synthesis of the 1H-1, 2, 3-triazole derivatives by the cyclization of arylazides with 1-(1, 3-benzothiazol-2-yl) acetone, 1, 3-benzothiazol-2-ylacetonitrile and (4-aryl-1, 3-thiazol-2-yl) acetonitrile
(2009) *Khimiya Geterotsiklicheskikh Soedinenii*, (4), pp. 612-618.
- Banewar, V.W., Raut, A.R., Thakre, V.D., Deahmukh, D.R.
Prediction of activity spectra and synthesis of some substituted coumarins
(2009) *Asian Journal of Chemistry*, 21 (7), pp. 5135-5139.
- Rastogi, R.P., Sinha, R.P.
Biotechnological and industrial significance of cyanobacterial secondary metabolites
(2009) *Biotechnology Advances*, 27 (4), pp. 521-539.
- Hernández-Núñez, E., Tlahuext, H., Moo-Puc, R., Torres-Gómez, H., Reyes-Martínez, R., Cedillo-Rivera, R., Nava-Zuazo, C., Navarrete-Vazquez, G.
Synthesis and in vitro trichomonocidal, giardicidal and amebicidal activity of N-acetamide(sulfonamide)-2-methyl-4-nitro-1H-imidazoles
(2009) *European Journal of Medicinal Chemistry*, 44 (7), pp. 2975-2984.
- Viña, D., Uriarte, E., Orallo, F., González-Díaz, H.
Alignment-free prediction of a drug-target complex network based on parameters of drug connectivity and protein sequence of receptors
(2009) *Molecular Pharmaceutics*, 6 (3), pp. 825-835.
- Benchabane, Y., Di Giorgio, C., Boyer, G., Sabatier, A.-S., Allegro, D., Peyrot, V., De Méo, M.
Photo-inducible cytotoxic and clastogenic activities of 3, 6-di-substituted acridines obtained by acylation of proflavine
(2009) *European Journal of Medicinal Chemistry*, 44 (6), pp. 2459-2467.
- Balaz, S.
Modeling kinetics of subcellular disposition of chemicals
(2009) *Chemical Reviews*, 109 (5), pp. 1793-1899.
- Carlsen, L., Kenessov, B.N., Batyrbekova, S.Ye.

A QSAR/QSTR study on the human health impact of the rocket fuel 1, 1-dimethyl hydrazine and its transformation products. Multicriteria hazard ranking based on partial order methodologies

(2009) *Environmental Toxicology and Pharmacology*, 27 (3), pp. 415-423.

Navarrete-Vazquez, G., Paoli, P., León-Rivera, I., Villalobos-Molina, R., Medina-Franco, J.L., Ortiz-Andrade, R., Estrada-Soto, S., Camici, G., Diaz-Coutiño, D., Gallardo-Ortiz, I., Martinez-Mayorga, K., Moreno-Díaz, H.

Synthesis, in vitro and computational studies of protein tyrosine phosphatase 1B inhibition of a small library of 2-arylsulfonylaminobenzothiazoles with antihyperglycemic activity

(2009) *Bioorganic and Medicinal Chemistry*, 17 (9), pp. 3332-3341.

Potikha, L.M., Gutsul, R.M., Kovtunenکو, V.A.

Condensed isoquinolines. 33. Synthesis of 1'-R-spiro[7H, 8H-2a, 7a- diaza-cyclopenta[fg]naphthacene-2, 4'(1'H))-pyridine]-1, 8(2H)-diones

(2009) *Khimiya Geterotsiklicheskikh Soedinenii*, (1), pp. 52-58.

Lukyanov, S.M., Bliznets, I.V., Shorshnev, S.V.

Synthesis of sterically hindered 3-(azolyl)pyridines

(2009) *Arkivoc*, 2009 (4), pp. 21-45.

Carlsen, L.

The interplay between QSAR/QSPR studies and partial order ranking and formal concept analyses

(2009) *International Journal of Molecular Sciences*, 10 (4), pp. 1628-1657.

Zadorozny, A.V., Kovtunenکو, V.A.

Condensed isoquinolines. 34. *Transformations of 4H-thieno-[3', 2':5, 6]- and 4H-thieno[2', 3':5, 6]pyrimido-[1, 2-b]isoquinolines

(2009) *Chemistry of Heterocyclic Compounds*, 45 (4), pp. 489-497.

Sashidhara, K.V., Kumar, A., Bhatia, G., Khan, M.M., Khanna, A.K., Saxena, J.K.

Antidyslipidemic and antioxidative activities of 8-hydroxyquinoline derived novel keto-enamine Schiff's bases

(2009) *European Journal of Medicinal Chemistry*, 44 (4), pp. 1813-1818.

Kondratovich, E.P., Zhokhova, N.I., Baskin, I.I., Palyulin, V.A., Zefirov, N.S.

Fragmental descriptors in (Q)SAR: Prediction of the assignment of organic compounds to pharmacological groups using the support vector machine approach

(2009) *Russian Chemical Bulletin*, 58 (4), pp. 657-662.

Mirzabekova, N.S., Kuz'Mina, N.E., Lukashov, O.I., Sokolova, N.A., Golosov, S.N.,

Kazakov, P.V., Perlova, T.G., Potapova, V.V., Kheinman, V.A., Ivanova, G.B.

Synthesis and biological activity of permethrin analogs containing various substituents in position 2 of the cyclopropane ring

(2009) *Russian Journal of Organic Chemistry*, 45 (3), pp. 355-359.

Emelina, E.E., Petrov, A.A.

α -aminoazoles in the Synthesis of heterocycles: V. Synthesis of azolo[1, 5-a]pyrimidines from 2-ethoxyvinyl trifluoromethyl ketones and 2, 2-diethoxyvinyl trifluoromethyl ketone

(2009) *Russian Journal of Organic Chemistry*, 45 (3), pp. 417-420.

- Gholivand, K., Oroujzadeh, N., Erben, M.F., Della Védova, C.O.
Synthesis, spectroscopy, computational study and prospective biological activity of two novel 1, 3, 2-diazaphospholidine-2, 4, 5-triones
(2009) *Polyhedron*, 28 (3), pp. 541-547.
- Strobl, J.S., Seibert, C.W., Li, Y., Nagarkatti, R., Mitchell, S.M., Rosypal, A.C., Rathore, D., Lindsay, D.S.
Inhibition of toxoplasma gondii and plasmodium falciparum infections in vitro by NSC3852, a redox active antiproliferative and tumor cell differentiation agent
(2009) *Journal of Parasitology*, 95 (1), pp. 215-223.
- Nigsch, F., Macaluso, N.J.M., Mitchell, J.B.O., Zmuidinavicius, D.
Computational toxicology: An overview of the sources of data and of modelling methods
(2009) *Expert Opinion on Drug Metabolism and Toxicology*, 5 (1), pp. 1-14.
- Potikha, L.M., Gutsul, R.M., Kovtunenکو, V.A.
Condensed isoquinolines 33*. Synthesis of 1?-R-spiro-[7H, 8H-2a, 7a- diazacyclopenta-[fg]naphthacene-2, 4?-(1?H)-pyridine]-1, 8(2H)-diones
(2009) *Chemistry of Heterocyclic Compounds*, 45 (1), pp. 42-47.
- Chandran, P.G.R., Balaji, S.
Phytochemical investigation and pharmacological studies of the flowers of *Pithecellobium Dulce*.
(2008) *Ethnobotanical Leaflets*, 12, pp. 245-253.
- De Britto, A.J., Raj, T.L.S., Chelliah, D.A.
Prediction of biological activity spectra for few anticancer drugs derived from plant sources.
(2008) *Ethnobotanical Leaflets*, 12, pp. 801-810.
- Maridass M., Raju G., Thangavel K., Ghanthikumar S.
Prediction of anti-HIV activity of flavanoid constituents through PASS.
(2008) *Ethnobotanical Leaflets*, 12, pp. 954-994.
- Koroleva L.S., Kuz'min V.E., Muratov E.N. et al. (2008). Artificial ribonucleases: quantitative analysis of the structure–activity relationship and a new insight into the strategy of design of highly efficient RNAse mimetics. *Rus. J. Bioorg. Chem.*, **34** (4): 442–452.
- Nigsch, F., Bender, A., Jenkins, J.L., Mitchell, J.B.O.
Ligand-target prediction using winnow and naive Bayesian algorithms and the implications of overall performance statistics
(2008) *Journal of Chemical Information and Modeling*, 48 (12), pp. 2313-2325.
- Agadzhanyan, V.S., Oganessian, E.T.
Applying quantum-chemical methods to interpretation of the antiradical activity in a series of hydroxy derivatives of cinnamic acid
(2008) *Pharmaceutical Chemistry Journal*, 42 (11), pp. 616-621.
- Rollinger, J.M., Stuppner, H., Langer, T.
Virtual screening for the discovery of bioactive natural products
(2008) *Progress in Drug Research*, 65, pp. 212-249.
- Nigsch, F., Mitchell, J.B.O.

Toxicological relationships between proteins obtained from protein target predictions of large toxicity databases
(2008) *Toxicology and Applied Pharmacology*, 231 (2), pp. 225-234.

Baskin, I., Varnek, A.
Building a chemical space based on fragment descriptors
(2008) *Combinatorial Chemistry and High Throughput Screening*, 11 (8), pp. 661-668.

Potikha, L.M., Gutsul, R.M., Kovtunenکو, V.A., Dubinina, G.G., Tolmachev, A.A.
Condensed isoquinolines. 30. Acylation and alkylation of 5, 13-dihydro-11H-isoquino[3, 2-b]quinazolin-11-one
(2008) *Khimiya Geterotsiklicheskikh Soedinenii*, (5), pp. 741-750.

Ghadimi, S., Ebrahimi Valmoozi, A.A., Pourayoubi, M., Asad Samani, K.
Structure-activity study of phosphoramido acid esters as acetylcholinesterase inhibitors
(2008) *Journal of Enzyme Inhibition and Medicinal Chemistry*, 23 (4), pp. 556-561.

Rajnikant, V., Dinesh, J., Bhavnaish, C.
Biological-activity predictions and hydrogen-bonding analysis of estrane derivatives of steroids
(2008) *Journal of Chemical Crystallography*, 38 (8), pp. 567-576.

Terent'ev, A.B., Vasil'eva, T.T., Chahovskaya, O.V., Mysova, N.E., Hambardzumyan, H.H., Kochetkov, K.A.
Pentafluorophenyl carbonyl compounds in the Reformatsky-type reactions promoted with Fe(CO)₅-based metal complex systems
(2008) *Journal of Fluorine Chemistry*, 129 (8), pp. 669-673.

Kirchmair, J., Distinto, S., Schuster, D., Spitzer, G., Langer, T., Wolber, G.
Enhancing drug discovery through in silico screening: Strategies to increase true positives retrieval rates
(2008) *Current Medicinal Chemistry*, 15 (20), pp. 2040-2053.

Ha, S., Seo, Y.-J., Kwon, M.-S., Chang, B.-H., Han, C.-K., Yoon, J.-H.
IDMap: Facilitating the detection of potential leads with therapeutic targets
(2008) *Bioinformatics*, 24 (11), pp. 1413-1415.

Kawai, K., Fujishima, S., Takahashi, Y.
Predictive activity profiling of drugs by topological-fragment-spectra- based support vector machines
(2008) *Journal of Chemical Information and Modeling*, 48 (6), pp. 1152-1160.

Guha, R., Schuřer, S.C.
Utilizing high throughput screening data for predictive toxicology models: Protocols and application to MLSCN assays
(2008) *Journal of Computer-Aided Molecular Design*, 22 (6-7), pp. 367-384.

Hranueli, D., Starčević, A., Źučko, J., Diminić, J., Škunca, N., Źeljeznak, V., Kovaček, D., Pavlinušić, D., Šimunković, J., Long, P.F., Cullum, J.
In silico design of 'un-natural' natural products [Oblikovanje novih prirodnih spojeva u uvjetima in silico]
(2008) *Kemija u industriji/Journal of Chemists and Chemical Engineers*, 57 (5), pp. 245-256.

Moreno-Díaz, H., Villalobos-Molina, R., Ortiz-Andrade, R., Díaz-Coutiño, D., Medina-Franco, J.L., Webster, S.P., Binnie, M., Estrada-Soto, S., Ibarra-Barajas, M., León-Rivera, I., Navarrete-Vázquez, G.

Antidiabetic activity of N-(6-substituted-1, 3-benzothiazol-2-yl)benzenesulfonamides
(2008) *Bioorganic and Medicinal Chemistry Letters*, 18 (9), pp. 2871-2877.

Abdou, W.M., Ganoub, N.A., Geronikaki, A., Sabry, E.

Synthesis, properties, and perspectives of gem-diphosphono substituted-thiazoles
(2008) *European Journal of Medicinal Chemistry*, 43 (5), pp. 1015-1024.

Musiol, R., Tabak, D., Niedbala, H., Podeszwa, B., Jampilek, J., Kralova, K., Dohnal, J., Finster, J., Mencil, A., Polanski, J.

Investigating biological activity spectrum for novel quinoline analogues 2: Hydroxyquinolinecarboxamides with photosynthesis-inhibiting activity
(2008) *Bioorganic and Medicinal Chemistry*, 16 (8), pp. 4490-4499.

Ghadimi, S., Mousavi, S.L., Javani, Z.

Synthesis, lipophilicity study and in vitro evaluation of some rodenticides as acetylcholinesterase reversible inhibitors
(2008) *Journal of Enzyme Inhibition and Medicinal Chemistry*, 23 (2), pp. 213-217.

Muster, W., Breidenbach, A., Fischer, H., Kirchner, S., Müller, L., Pähler, A.

Computational toxicology in drug development
(2008) *Drug Discovery Today*, 13 (7-8), pp. 303-310.

Schneider, N., Jäckels, C., Andres, C., Hutter, M.C.

Gradual in silico filtering for druglike substances
(2008) *Journal of Chemical Information and Modeling*, 48 (3), pp. 613-628.

Kotera, M., McDonald, A.G., Boyce, S., Tipton, K.F.

Functional group and substructure searching as a tool in metabolomics
(2008) *PLoS ONE*, 3 (2), art. no. e1537.

Kulakov, I.V., Ainabaev, A.A., Nurkenov, O.A., Gazaliev, A.M.

Synthesis of N-alkaloidacyl derivatives of phenothiazine
(2008) *Russian Journal of Applied Chemistry*, 81 (2), pp. 263-267.

Benigni, R., Bossa, C.

Predictivity and reliability of QSAR models: The case of mutagens and carcinogens
(2008) *Toxicology Mechanisms and Methods*, 18 (2-3), pp. 137-147.

Kulikov, O.V., Karaseva, T.L., Kabanova, T.A., Kostenko, E.A., Kuz'min, V.E., Andronati, S.A.

Pharmacological activity of 16-and 18-member dibenzodioxatetraaza macroheterocyclic compounds
(2008) *Pharmaceutical Chemistry Journal*, 42 (1), pp. 15-17.

Rajnikant, Dinesh, Chand, B.

Biological activity predictions, crystallographic comparison and hydrogen bonding analysis of cholane derivatives
(2007) *Indian Journal of Biochemistry and Biophysics*, 44 (6), pp. 458-469.

- Shaikh, S.A., Jain, T., Sandhu, G., Latha, N., Jayaram, B.
From drug target to leads-sketching a physicochemical pathway for lead molecule design in silico
(2007) *Current Pharmaceutical Design*, 13 (34), pp. 3454-3470.
- Dhagat, U., Carbone, V., Chung, R.P.T., Matsunaga, T., Endo, S., Hara, A., El-Kabbani, O.
A salicylic acid-based analogue discovered from virtual screening as a potent inhibitor of human 20 α -hydroxysteroid dehydrogenase
(2007) *Medicinal Chemistry*, 3 (6), pp. 546-550.
- Nichols, J., Erhardt, S., Dyer, S., James, M., Moore, M., Plotzke, K., Segner, H., Schultz, I., Thomas, K., Vasiluk, L., Weisbrod, A.
Use of in vitro absorption, distribution, metabolism, and excretion (ADME) data in bioaccumulation assessments for fish
(2007) *Human and Ecological Risk Assessment*, 13 (6), pp. 1164-1191.
- Marwaha, A., Goel, R.K., Mahajan, M.P.
PASS-predicted design, synthesis and biological evaluation of cyclic nitrones as nootropics
(2007) *Bioorganic and Medicinal Chemistry Letters*, 17 (18), pp. 5251-5255.
- Ghadimi, S., Khajeh, V.
Synthesis, characterization, and prediction of biological activity of phosphoramidate compounds
(2007) *Journal of the Iranian Chemical Society*, 4 (3), pp. 325-331.
- Ekins, S., Mestres, J., Testa, B.
In silico pharmacology for drug discovery: Methods for virtual ligand screening and profiling
(2007) *British Journal of Pharmacology*, 152 (1), pp. 9-20.
- Bender, A., Young, D.W., Jenkins, J.L., Serrano, M., Mikhailov, D., Clemons, P.A., Davies, J.W.
Chemogenomic data analysis: Prediction of small-molecule targets and the advent of biological fingerprints
(2007) *Combinatorial Chemistry and High Throughput Screening*, 10 (8), pp. 719-731.
- Kowalski, P., Kowalska, T., Bojarski, A.J., Duszyńska, B.
Synthesis and biological properties of 1, 8-naphthalimidebutylamines. Serotonin 5-HT_{1A} and 5-HT₇ binding data and PASS-assisted search
(2007) *Journal of Heterocyclic Chemistry*, 44 (4), pp. 889-893.
- Sangamwar, A.T., Deshpande, U.D., Pekamwar, S.S., Vadvalkar, S.M.
Improving decision making for drug candidates: A computational approach for benzothiazoles as antifungal
(2007) *Indian Journal of Biotechnology*, 6 (3), pp. 389-396.
- Prathipati, P., Dixit, A., Saxena, A.K.
Computer-aided drug design: Integration of structure-based and ligand-based approaches in drug design
(2007) *Current Computer-Aided Drug Design*, 3 (2), pp. 133-148.
- Roshchin, A.I., Kuznetsov, Yu.V., Polunin, E.V.

High-pressure-assisted addition of (methoxyphenyl)maleic anhydrides to dienes. Synthesis of 3a-aryltetrahydroisindole-1, 3-diones
(2007) Russian Chemical Bulletin, 56 (3), pp. 509-512.

Musiol, R., Jampilek, J., Kralova, K., Richardson, D.R., Kalinowski, D., Podeszwa, B., Finster, J., Niedbala, H., Palka, A., Polanski, J.
Investigating biological activity spectrum for novel quinoline analogues
(2007) Bioorganic and Medicinal Chemistry, 15 (3), pp. 1280-1288.

Omelyanchik, L.A., Gencheva, V.I., Fedoryak, D.M., et al.
Search of bioregulators with antioxidant action among S-derivatives of 4-merkaptoquinoline.
(2007) Ukrainica Bioorganica Acta, 2, pp. 17-24.

Shestakov, A.S., Sidorenko, O.E., Shikhaliev, Kh.S., Pavlenko, A.A.
Guanidines based on tryptamine and histamine in reactions with electrophiles.
(2007) Rus. J. General Chem., 77 (10), pp. 1749-1760.

Hutter, M.C.
Separating drugs from nondrugs: A statistical approach using atom pair distributions
(2007) Journal of Chemical Information and Modeling, 47 (1), pp. 186-194.

Dix, D.J., Houck, K.A., Martin, M.T., Richard, A.M., Setzer, R.W., Kavlock, R.J.
The ToxCast program for prioritizing toxicity testing of environmental chemicals
(2007) Toxicological Sciences, 95 (1), pp. 5-12.

Chen, B., Harrison, R.F., Papadatos, G., Willett, P., Wood, D.J., Lewell, X.Q., Greenidge, P., Stiefl, N.
Evaluation of machine-learning methods for ligand-based virtual screening
(2007) Journal of Computer-Aided Molecular Design, 21 (1-3), pp. 53-62.

Caldwell, J.S.
Cancer Cell-Based Genomic and Small Molecule Screens
(2006) Advances in Cancer Research, 96, pp. 145-173.

Balakin, K.V., Tkachenko, S.E., Kiselyov, A.S., Savchuk, N.P.
Focused chemistry from annotated libraries
(2006) Drug Discovery Today: Technologies, 3 (4), pp. 397-403.

Lukyanov, S.M., Bliznets, I.V., Shorshnev, S.V., et al.
Microwave-assisted synthesis and transformations of sterically hindered 3-(5-tetrazolyl)pyridines.
(2006) Tetrahedron, 62 (8), pp. 1849-1863.

Ivanov, A.S., Veselovsky, A.V., Dubanov, A.V., Skvortsov, V.S.
Bioinformatics Platform Development. From Gene to Lead Compound.
(2006) In: Methods in Molecular Biology, vol. 316: *Bioinformatics and Drug Discovery*, Edited by: R. S. Larson. Humana Press Inc., Totowa, NJ, pp. 389-431.

Stasevych, M.V., Chervetsova, V.G., Plotnikov, M.Yu., et al.
Synthesis and antimicrobial evaluation of novel 2-substituted-3-mercapto-1, 4-naphthoquinones.
(2006) Ukrainica Bioorganica Acta, 2, pp. 33-39.

Jenkins, J.L., Bender, A., Davies, J.W.

In silico target fishing: Predicting biological targets from chemical structure
(2006) *Drug Discovery Today: Technologies*, 3 (4), pp. 413-421.

Prabhakar, K.R., Veerapur, V.P., Bansal, P., Vipani, K.P., Reddy, K.M., Barik, A., Reddy, B.K.D., Reddanna, P., Priyadarsini, K.L., Unnikrishnan, M.K.

Identification and evaluation of antioxidant, analgesic/anti-inflammatory activity of the most active ninhydrin-phenol adducts synthesized

(2006) *Bioorganic and Medicinal Chemistry*, 14 (21), pp. 7113-7120.

Anzali, S., Mujica, T., Reiffen, K.-A., Kirchmayer, J., Buchholz, H.

Cosmetic discovery process (CDP): searching for novel skin-lighteners by virtual screening methods.

(2006) IFSCC Congress, Osaka, Japan.

Mestres, J., Martín-Couce, L., Gregori-Puigjané, E., Cases, M., Boyer, S.

Ligand-based approach to in silico pharmacology: Nuclear receptor profiling

(2006) *Journal of Chemical Information and Modeling*, 46 (6), pp. 2725-2736.

Richard, A.M.

Future of toxicology-predictive toxicology: An expanded view of "chemical toxicity"

(2006) *Chemical Research in Toxicology*, 19 (10), pp. 1257-1262.

Chen, X., Liang, Y., Xu, J.

Toward automated biochemotype annotation for large compound libraries

(2006) *Molecular Diversity*, 10 (3), pp. 495-509.

Saxena, A.K., Prathipati, P.

Collection and preparation of molecular databases for virtual screening

(2006) *SAR and QSAR in Environmental Research*, 17 (4), pp. 371-392.

Betelina, I.B., Tyurina, L.A., Kirilan, S.A., Zarudii, F.S., Miftakhov, M.S., Ivanova, N.A., Baschenko, N.Zh., Kantor, E.A., Sementeeva, L.Sh.

Structure-biological activity relationship in prostaglandin analogs

(2006) *Pharmaceutical Chemistry Journal*, 40 (8), pp. 424-429.

Klekota, J., Brauner, E., Roth, F.P., Schreiber, S.L.

Using high-throughput screening data to discriminate compounds with single-target effects from those with side effects

(2006) *Journal of Chemical Information and Modeling*, 46 (4), pp. 1549-1562.

Estrada-Soto, S., Villalobos-Molina, R., Aguirre-Crespo, F., Vergara-Galicia, J., Moreno-Díaz, H., Torres-Piedra, M., Navarrete-Vázquez, G.

Relaxant activity of 2-(substituted phenyl)-1H-benzimidazoles on isolated rat aortic rings.

Design and synthesis of 5-nitro derivatives

(2006) *Life Sciences*, 79 (5), pp. 430-435.

Seibert, S.F., Eguereva, E., Krick, A., Kehraus, S., Voloshina, E., Raabe, G., Fleischhauer, J., Leistner, E., Wiese, M., Prinz, H., Alexandrov, K., Janning, P., Waldmann, H., König, G.M.

Polyketides from the marine-derived fungus *Ascochyta salicorniae* and their potential to inhibit protein phosphatases
(2006) *Organic and Biomolecular Chemistry*, 4 (11), pp. 2233-2240.

Rollinger, J.M., Langer, T., Stuppner, H.
Integrated in silico tools for exploiting the natural products' bioactivity
(2006) *Planta Medica*, 72 (8), pp. 671-678.

Richard, A.M., Gold, L.S., Nicklaus, M.C.
Chemical structure indexing of toxicity data on the Internet: Moving toward a flat world
(2006) *Current Opinion in Drug Discovery and Development*, 9 (3), pp. 314-325.

Nidhi, Glick, M., Davies, J.W., Jenkins, J.L.
Prediction of biological targets for compounds using multiple-category bayesian models trained on chemogenomics databases
(2006) *Journal of Chemical Information and Modeling*, 46 (3), pp. 1124-1133.

Cherkasov, A.
Can 'bacterial-metabolite-likeness' model improve odds of 'in silico' antibiotic discovery?
(2006) *Journal of Chemical Information and Modeling*, 46 (3), pp. 1214-1222.

Helma, C.
Lazy structure-activity relationships (lazar) for the prediction of rodent carcinogenicity and *Salmonella* mutagenicity
(2006) *Molecular Diversity*, 10 (2), pp. 147-158.

Petricci, E., Mugnaini, C., Radi, M., Togninelli, A., Bernardini, C., Manetti, F., Parlato, M.C., Renzulli, M.L., Alongi, M., Falciani, C., Corelli, F., Botta, M.
Towards new methodologies for the synthesis of biologically interesting 6-substituted pyrimidines and 4(3H)-pyrimidinones
(2006) *Arkivoc*, 2006 (7), pp. 1-27.

Solov'ev, V.P., Kireeva, N.V., Tsivadze, A.Yu., Varnek, A.A.
Structure-property modelling of complex formation of strontium with organic ligands in water
(2006) *Journal of Structural Chemistry*, 47 (2), pp. 298-311.

Lukyanov, S.M., Bliznets, I.V., Shorshnev, S.V., Aleksandrov, G.G., Stepanov, A.E., Vasil'ev, A.A.
Microwave-assisted synthesis and transformations of sterically hindered 3-(5-tetrazolyl)pyridines
(2006) *Tetrahedron*, 62 (8), pp. 1849-1863.

Gromova, V.P., Omeljanchik, L.O., Brazhko, O.A., et al.
Investigation of antioxidant activity of quinoline thioderivatives.
(2005) *Ukrainian Biochemical Journal*, 77 (3). Pp. 87-95.

Adekenov, S.M.
Synthesis and biological activity of new derivatives of arglabine and perspectives for production of original phytopharmaceuticals.
(2005) *Russian Biotherapeutical Journal*, 4 (2), pp. 7-14.

- Fioravanzo, E., Cazzolla, N., Durando, L., et al.
General and Independent Approaches to Predict hERG Affinity Values.
(2005). *Internet Electron. J. Mol. Des.*, **4** (9), pp. 625–646.
- Balakin, K.V., Ivanenkov, Y.A.
Computational methods for prediction of metabolism of physiologically active substances
(2005) *Biomeditsinskaya Khimiya*, **51** (4), pp. 384-412.
- Kogej, T., Muresan, S.
Database mining for pKa prediction
(2005) *Current Drug Discovery Technologies*, **2** (4), pp. 221-229.
- Katritzky, A.R., Kuanar, M., Fara, D.C., Karelson, M., Acree Jr., W.E., Solov'ev, V.P., Varnek, A.
QSAR modeling of blood:air and tissue:air partition coefficients using theoretical descriptors
(2005) *Bioorganic and Medicinal Chemistry*, **13** (23), pp. 6450-6463.
- Miller, G.G., Voronina, T.A.
Perspective technologies for design of therapeutics
(2005) *Antibiotiki i Khimioterapiya*, **50** (2-3), pp. 52-63.
- Klekota, J., Brauner, E., Schreiber, S.L.
Identifying biologically active compound classes using phenotypic screening data and sampling statistics
(2005) *Journal of Chemical Information and Modeling*, **45** (6), pp. 1824-1836.
- Faulon, J.-L., Brown, W.M., Martin, S.
Reverse engineering chemical structures from molecular descriptors: How many solutions?
(2005) *Journal of Computer-Aided Molecular Design*, **19** (9-10), pp. 637-650.
- Bock, J.R., Gough, D.A.
Virtual screen for ligands of orphan G protein-coupled receptors
(2005) *Journal of Chemical Information and Modeling*, **45** (5), pp. 1402-1414.
- Macaev, F., Rusu, G., Pogrebnoi, S., Gudima, A., Stingaci, E., Vlad, L., Shvets, N., Kandemirli, F., Dimoglo, A., Reynolds, R.
Synthesis of novel 5-aryl-2-thio-1, 3, 4-oxadiazoles and the study of their structure-anti-mycobacterial activities
(2005) *Bioorganic and Medicinal Chemistry*, **13** (16), pp. 4842-4850.
- Varnek, A., Solov'ev, V.P.
"In silico" design of potential anti-HIV actives using fragment descriptors
(2005) *Combinatorial Chemistry and High Throughput Screening*, **8** (5), pp. 403-416.
- Artiguenave, F., Lins, A., Maciel, W.D., Caldeira Jr., A.C., Nacif-Coelho, C., De Souza Linhares, M.M.R., De Oliveira, G.C., Barbosa, L.H.R., Lopes, J.C.D., Coelho Jr., C.N.
The Tropical Biominer Project: Mining old sources for new drugs
(2005) *OMICS A Journal of Integrative Biology*, **9** (2), pp. 130-138.
- Mayeno, A.N., Yang, R.S.H., Reifeld, B.
Biochemical reaction network modeling: Predicting metabolism of organic chemical mixtures

(2005) *Environmental Science and Technology*, 39 (14), pp. 5363-5371.

Kowalski, P., Nowak, K., Szpakiewicz, B.
Synthesis and prediction of bioactivity of new nitroimidazole derivatives
(2005) *Journal of Heterocyclic Chemistry*, 42 (5), pp. 883-888.

Sernov, L.N., Skachilova, S.Ya., Blinov, D.S., Druzhinina, V.V., Kostin, Ya.V., Shilova, E.V.
Synthesis and antiarrhythmic activity of 2-diethylamino-2', 6'- dimethylphenylacetamide derivatives
(2005) *Pharmaceutical Chemistry Journal*, 39 (7), pp. 350-353.

Ósk Jónsdóttir, S., Jørgensen, F.S., Brunak, S.
Prediction methods and databases within chemoinformatics: Emphasis on drugs and drug candidates
(2005) *Bioinformatics*, 21 (10), pp. 2145-2160.

Goel, R.K., Singh, A., Naidu, P.S., Mahajan, M.P., Kulkarni, S.K.
PASS assisted search and evaluation of some azetidin-2-ones as C.N.S. active agents
(2005) *Journal of Pharmacy and Pharmaceutical Sciences*, 8 (2), pp. 182-189.

Goel, R.K., Kumar, V., Mahajan, M.P.
Quinazolines revisited: Search for novel anxiolytic and GABAergic agents
(2005) *Bioorganic and Medicinal Chemistry Letters*, 15 (8), pp. 2145-2148.

Labanauskas, L., Brukstus, A., Udrenaite, E., Bucinskaite, V., Susvilo, I., Urbelis, G.
Synthesis and anti-inflammatory activity of 1-acylaminoalkyl-3, 4- dialkoxybenzene derivatives
(2005) *Farmaco*, 60 (3), pp. 203-207.

Carbone, V., Ishikura, S., Hara, A., El-Kabbani, O.
Structure-based discovery of human L-xylulose reductase inhibitors from database screening and molecular docking
(2005) *Bioorganic and Medicinal Chemistry*, 13 (2), pp. 301-312.

Fliri, A.F., Loging, W.T., Thadeio, P.F., Volkmann, R.A.
Biological spectra analysis: Linking biological activity profiles to molecular structure
(2005) *Proceedings of the National Academy of Sciences of the United States of America*, 102 (2), pp. 261-266.

Cherkasov, A.
Inductive QSAR descriptors. Distinguishing compounds with antibacterial activity by artificial neural networks
(2005) *International Journal of Molecular Sciences*, 6 (1), pp. 63-86.

Helma, C.
In silico predictive toxicology: The state-of-the-art and strategies to predict human health effects
(2005) *Current Opinion in Drug Discovery and Development*, 8 (1), pp. 27-31.

Kuznetsov S.O.

Galois Connections in Data Analysis: Contributions from the Soviet Era and Modern Russian Research.

(2005) In: Formal Concept Analysis, Ganter B. et al. (Eds.), Berlin Heidelberg: Springer-Verlag, pp. 196–225.

Hongmao S.

Predicting ADMET Properties by Projecting onto Chemical Space? Benefits and Pitfalls.

(2005) Current Computer-Aided Drug Design, 1 (2), pp. 179-193.

Toshihiko H.

Chromatography and Computational Chemical Analysis for Drug Discovery.

(2005) Current Medicinal Chemistry, 12 (5), pp. 501-525.

Kuzmin, V.E., Grishchuk, L.V., Ivanov, L.I.

Virtual screening of biological activity of 1, 2-dihydroquinoline-2-ones derivatives by the computer system PASS.

(2004) Bulletin of Odessa National University, 9 (3): pp. 87-97.

Von Grotthuss, M., Koczyk, G., Pas, J., Wyrwicz, L.S., Rychlewski, L.

Ligand.Info small-molecule meta-database

(2004) Combinatorial Chemistry and High Throughput Screening, 7 (8), pp. 757-761.

Pirard, B.

Computational methods for the identification and optimisation of high quality leads.

(2004) Combinatorial Chemistry & High Throughput Screening, 7 (4), pp. 271-280.

Raevsky, O.A.

Physicochemical Descriptors in Property-Based Drug Design.

(2004) Mini Reviews in Medicinal Chemistry, 4 (10), pp. 1041-1052.

Parthasarathi, R., Subramanian, V., Roy, D.R., Chattaraj, P.K.

Electrophilicity index as a possible descriptor of biological activity

(2004) Bioorganic and Medicinal Chemistry, 12 (21), pp. 5533-5543.

Pogrebnyak, A.V., Oganessian, É.T., Kononov, D.A., Glushko, A.A.

Medicinal plants: A theoretical method based on a matrix algorithm for predicting biological activity of total medicinal plant extracts

(2004) Pharmaceutical Chemistry Journal, 38 (9), pp. 483-486.

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

Structure - Property modeling of metal binders using molecular fragments

(2004) Russian Chemical Bulletin, 53 (7), pp. 1434-1445.

Piclin, N., Pintore, M., Wechman, C., Chrétien, J.R.

Classification of a large anticancer data set by Adaptive Fuzzy Partition

(2004) Journal of Computer-Aided Molecular Design, 18 (7-9), pp. 577-586.

Weaver, D.C.

Applying data mining techniques to library design, lead generation and lead optimization

(2004) Current Opinion in Chemical Biology, 8 (3), pp. 264-270.

Zakharov, N.A., Polunina, I.A., Polunin, K.E., Rakitina, N.M., Kochetkova, E.I., Sokolova, N.P., Kalinnikov, V.T.

Calcium hydroxyapatite for medical applications
(2004) *Inorganic Materials*, 40 (6), pp. 641-648.

Mestres, J.

Computational chemogenomics approaches to systematic knowledge-based drug discovery
(2004) *Current Opinion in Drug Discovery and Development*, 7 (3), pp. 304-313.

Shitikov, V.K., Zinchenko, T.D., Golovatyuk, L.V.

Assessing surface water quality based on indicator zoobenthos species
(2004) *Water Resources*, 31 (3), pp. 323-332.

Katritzky, A.R., Fara, D.C., Yang, H., Karelson, M., Suzuki, T., Solov'ev, V.P., Varnek A., A.

Quantitative structure - Property relationship modeling of β -cyclodextrin complexation free energies
(2004) *Journal of Chemical Information and Computer Sciences*, 44 (2), pp. 529-541.

Di Giorgio, C., Delmas, F., Ollivier, E., Elias, R., Balansard, G., Timon-David, P.

In vitro activity of the β -carboline alkaloids harmine, harmine, and harmaline toward parasites of the species *Leishmania infantum*
(2004) *Experimental Parasitology*, 106 (3-4), pp. 67-74.

Shahkeldyan, I.V., Melekhina, E.K., Atroshchenko, Yu.M. et al.

Synthesis of heterocyclic analogs of gamma-aminobutyric acid from 3, 5-dinitrobenzoic acid.
(2003) *Russian Journal of Organic Chemistry*, **39** (4), pp. 589-595.

Artamkina, G.A., Petrov, A.R., Serushkina, O.V., et al.

Arylation of Substituted Anilines Catalyzed by Palladium.
(2003) *Russian Journal of Organic Chemistry*, **39** (6), pp. 846-859.

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

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
(2003) *Journal of Chemical Information and Computer Sciences*, 43 (5), pp. 1703-1719.

Dolzhenko, A.V. et al. (2003).

Substituted amides and hydrazides of dicarboxylic acids. Part 14. Synthesis and antimicrobial and antiinflammatory activity of 4-antipyrylamides, 2-thiazolylamides, and 1-triazolylamides of some dicarboxylic acids.
(2003) *Pharmaceutical Chemistry Journal*, 37, pp. 149-151.

Dolzhenko, A.V. et al.

Substituted amides and hydrazides of dicarboxylic acids. Part 16. Synthesis and antibacterial activity of some amides and acylhydrazides of succinic acid
(2003) *Pharmaceutical Chemistry Journal*, 37, pp. 229-231.

Veselovsky, A.V., Ivanov, A.S.

Strategy of computer-aided drug design
(2003) *Current Drug Targets - Infectious Disorders*, 3 (1), pp. 33-40.

Wilton, D., Willett, P., Lawson, K., Mullier, G.
Comparison of ranking methods for virtual screening in lead-discovery programs
(2003) *Journal of Chemical Information and Computer Sciences*, 43 (2), pp. 469-474.

van de Waterbeemd, H., Gifford, E.
ADMET in silico modelling: Towards prediction paradise?
(2003) *Nature Reviews Drug Discovery*, 2 (3), pp. 192-204.

Di Giorgio, C., Delmas, F., Filloux, N., Robin, M., Seferian, L., Azas, N., Gasquet, M.,
Costa, M., Timon-David, P., Galy, J.-P.

In vitro activities of 7-substituted 9-chloro and 9-amino-2-methoxyacridines and their bis-
and tetra-acridine complexes against *Leishmania infantum*
(2003) *Antimicrobial Agents and Chemotherapy*, 47 (1), pp. 174-180.

Artemenko, N.V., Baskin, I.I., Palyulin, V.A., Zefirov, N.S.
Artificial neural network and fragmental approach in prediction of physicochemical
properties of organic compounds
(2003) *Russian Chemical Bulletin*, 52 (1), pp. 20-29.

Bulanova, A.V., Yegorova, K.V., Polyakova, Yu.L., et al.
The connection "biological activity physical and chemical properties" of imidazolides and
triazolides of sulfonic acids.
(2002) *Bulletin of Samara State University, Special issue*, pp. 124-131.

Pogrebnyak, A.V., Oganessian, E.T., Glushko, A.A.
MATRIX, a new algorithm for predicting biological activity of organic molecules based on
multidimensional analysis of physicochemical descriptors of modern pharmaceuticals: I.
General principles
(2002) *Russian Journal of Organic Chemistry*, 38 (11), pp. 1564-1575.

Ren, S.
Classifying class I and class II compounds by hydrophobicity and hydrogen bonding
descriptors
(2002) *Environmental Toxicology*, 17 (5), pp. 415-423.

Pogrebnyak, A.V., Vasilenko, Yu.K., Oganessian, É.T., Glushko, A.A., Suzdalev, K.F.,
Pogrebnyak, L.V.
Computer prognosis and targeted synthesis of a new betulin derivative possessing
antituberculous properties
(2002) *Pharmaceutical Chemistry Journal*, 36 (10), pp. 535-537.

Zefirov, N.S., Palyulin, V.A.
Fragmental approach in QSPR
(2002) *Journal of Chemical Information and Computer Sciences*, 42 (5), pp. 1112-1122.

Manallack, D.T., Pitt, W.R., Gancia, E., Montana, J.G., Livingstone, D.J., Ford, M.G.,
Whitley, D.C.
Selecting screening candidates for kinase and G protein-coupled receptor targets using neural
networks
(2002) *Journal of Chemical Information and Computer Sciences*, 42 (5), pp. 1256-1262.

- Van de Waterbeemd, H.
High-throughput and in silico techniques in drug metabolism and pharmacokinetics
(2002) *Current Opinion in Drug Discovery and Development*, 5 (1), pp. 33-43.
- Root, D.E., Kelley, B.P., Stockwell, B.R.
Global analysis of large-scale chemical and biological experiments
(2002) *Current Opinion in Drug Discovery and Development*, 5 (3), pp. 355-360.
- Clark, D.E., Grootenhuys, P.D.J.
Progress in computational methods for the prediction of ADMET properties
(2002) *Current Opinion in Drug Discovery and Development*, 5 (3), pp. 382-390.
- Ruicker, C., Ruicker, G., Meringer, M.
Exploring the limits of graph invariant- and spectrum-based discrimination of (sub)structures
(2002) *Journal of Chemical Information and Computer Sciences*, 42 (3), pp. 640-650.
- Delmas, F., Di Giorgio, C., Robin, M., Azas, N., Gasquet, M., Detang, C., Costa, M., Timon-David, P., Galy, J.-P.
In vitro activities of position 2 substitution-bearing 6-nitro- and 6-amino-benzothiazoles and their corresponding anthranilic acid derivatives against *Leishmania infantum* and *Trichomonas vaginalis*
(2002) *Antimicrobial Agents and Chemotherapy*, 46 (8), pp. 2588-2594.
- Ihlenfeldt, W.-D., Voigt, J.H., Bienfait, B., Oellien, F., Nicklaus, M.C.
Enhanced CACTVS browser of the open NCI database
(2002) *Journal of Chemical Information and Computer Sciences*, 42 (1), pp. 46-57.
- Nikiforova, E.G., Korolev, M.A., Shakhkel'dyan, I.V., et al.
3-Azabicyclo[3.3.1]nonane Derivatives: V. Synthesis of 7-Polyfluoroalkoxy-1, 5-dinitro-3-azabicyclo[3.3.1]non-6-enes.
(2001) *Russian Journal of Organic Chemistry*, **37** (5), pp. 734-738.
- Polyakova, Yu.L., Bulanova, A.V., Vartapetyan, R.Sh.
Hydrolysis of some imidazoles, benzimidazole, and 1, 2, 3-benzotriazole derivatives according to HPLC and NMR spectroscopy data.
(2001) *Russian Chemical Bulletin*, **50** (5), pp. 820-822.
- Gedeck, P., Willett, P.
Visual and computational analysis of structure-activity relationships in high-throughput screening data
(2001) *Current Opinion in Chemical Biology*, 5 (4), pp. 389-395.
- Cambria, A., Raudino, A., Geronikaki, A., Buemi, G., Raciti, G., Mazzone, P., Guccione, S., Ragusa, S.
Thiazole derivatives as inhibitors of purified bovine liver mitochondrial monoamine oxidase-B: Structure-activity relationships and theoretical study
(1999) *Journal of Enzyme Inhibition*, 14 (4), pp. 307-321.
- Gaidarova, E.L., Borisenko, A.A., Chumakov, T.I., Mel'nikov, A.V., Orlov, I.S., Grishina, G.V.
A simple and convenient route to 1, 2, 3, 4, 5, 6, 7, 8-octahydro-1, 6- naphthyridines

(1998) Tetrahedron Letters, 39 (42), pp. 7767-7770.

Rozantsev, G.G., Frolovskii, V.A., Studnev, Yu.N.
New principle of search for compounds possessing anticonvulsive properties
(1998) Pharmaceutical Chemistry Journal, 32 (7), pp. 345-351.

Maiboroda, D.A., Babaev, E.V., Goncharenko, L.V.
Synthesis and study of spectral and pharmacological properties of 1-amino-4/5-aryloxolyl-
2)-butadiens-1, 3.
(1998) Pharmaceutical Chemistry Journal, **32** (6), pp.24-28.

Islyaikin, M.K., Danilova, E.A., Kudrik, E.V., Smirnov, R.P., Budunova, A.P., Kinzirkii,
A.S.
Synthesis and study of antitumor activity of macroheterocyclic compounds and their
metallocomplexes
(1997) Pharmaceutical Chemistry Journal, 31 (8), pp. 409-412.