ADMEWORKS ModelBuilder List of Publications

- **Fujita, Masaharu, et al.**
  Development of a prediction method for skin sensitization using novel cysteine and lysine derivatives.
  Journal of pharmacological and toxicological methods 70.1 (2014): 94-105.
- **Marwaha, Rakesh Kumar, and A. K. Madan.**
  Fourth generation detour matrix–based topological descriptors for QSAR/QSPR-Part–2: application in development of models for prediction of biological activity.
  International journal of computational biology and drug design 7.1 (2014): 1-30.
- **Nicolotti, Orazio, et al.**
  REACH and< i> in silico methods: an attractive opportunity for medicinal chemists.
  Drug discovery today 19.11 (2014): 1757-1768.
- **Perekhoda, L. A.**
  Assessment of Quantitative Structure-Anticonvulsive Activity Relationships in a Series of Derivatives of 1, 2, 3-Triazole (1H), 1, 2, 4-Triazole (4H), 1, 3, 4-Oxadiazole (1H), and 1, 3, 4-Thiadiazole (1H).
  Pharmaceutical Chemistry Journal 47.11 (2014): 586-588.
- **Singh, Monika, et al.**
  Detour matrix–based adjacent path eccentric distance sum indices for QSAR/QSPR. Part I: development and evaluation.
  International journal of computational biology and drug design 7.4 (2014): 295-318.
- **Singh, Monika, Harish Dureja, and A. K. Madan.**
  Detour matrix–based adjacent path eccentric distance sum indices for (Q) SAR/QSPR. Part II: application in development of models for COX–2 inhibitory activity of indomethacin derivatives.
  International journal of computational biology and drug design 7.4 (2014): 319-340.
- **Yuta, Kohtarou.**
  Sample class prediction method, prediction program, and prediction apparatus.
  U.S. Patent No. 8,682,813. 25 Mar. 2014.
- **Gupta, Monika, and A. K. Madan.**
  Models for the prediction of melanocortin–4 receptor agonist activity of 4–substituted piperidin–4–ol.
  International journal of computational biology and drug design 6.4 (2013): 294-317.
- **Kotaro, Y. U. T. A.**
  Method, program, and apparatus for generating two-class classification/prediction model.
  U.S. Patent No. 8,352,390. 8 Jan. 2013.
- **Saka, Kanju, et al.**
  Relationship between the matrix effect and the physicochemical properties of analytes in gas chromatography.
  Analytical and bioanalytical chemistry 405.30 (2013): 9879-9888.
- **Venkatapathy, Raghuraman, and Nina Ching Y. Wang.**
  Developmental Toxicity Prediction.
  Computational Toxicology. Humana Press, 2013. 305-340.
- **Перехода, Л. А.**
  Количественное исследование взаимосвязи «структура—противосудорожная активность» в рядах производных 1, 2, 3-триазола (1 H), 1, 2, 4-триазола (4 H), 1, 3, 4-оксадиазола (1 H) и 1, 3, 4–тиадиазола (1 H).
  Химико-фармацевтический журнал 47.11 (2013): 16-18.

- **Marwaha, Rakesh Kumar, et al.**
  Fourth generation detour matrix–based topological indices for QSAR/QSPR-Part–1: development and evaluation.
  International journal of computational biology and drug design 5.3 (2012): 335-360.
- **Mishra, Rahul, et al.**
  Synthesis and Anticonvulsant Activity of Some Novel 2-Methyl Imidazole Derivatives.
  Letters in Drug Design & Discovery 9.4 (2012): 402-408.
- **Tajima, Tomoyuki, et al.**
  Proton nuclear magnetic resonance and pattern recognition analysis of liver extracts from rats under different anesthetics.
  BMC medical imaging 12.1 (2012): 28.
- **Wawrzyniak, Rafał.**
  Separation of alicyclic and aromatic hydrocarbons on a PLOT column coated with 3-benzylketoiminepropyl group.
  Chemical Papers 66.7 (2012): 626-635.
- **Yuta, Kohtarou.**
  Method, apparatus, and program for generating prediction model based on multiple regression analysis.
  U.S. Patent No. 8,255,342. 28 Aug. 2012.
- **Mikael Harju, Solveig Ravnum, Elise Rundén Pran, Sonja Grossberndt, Lise Marie Fjellsbø, Maria Dusinska and Eldbjørg S. Heimstad.**
  Alternative approaches to standard toxicity testing.
  TQP ID 9 - OPTION - 257430181 - NILU
- **Yuta, Kohtarou.**
  Method, system, and program for generating prediction model based on multiple regression analysis.
  U.S. Patent Application 13/019,641.
- **A Mostrag-Szlichtyng, A Worth**
  Review of QSAR models and software tools for predicting biokinetic properties.
  Publications Office, 2010.
- **Chaudhry, Qasim, et al.**
  Global QSAR models of skin sensitisers for regulatory purposes.
  Chemistry Central Journal 4.Suppl 1 (2010): S5.
- **Kawaguchi, Hiroshi, et al.**
  Pattern recognition analysis of proton nuclear magnetic resonance spectra of brain tissue extracts from rats anesthetized with propofol or isoflurane.
  PloS one 5.6 (2010): e11172.
- **Mishra, Nitish K., Sandhya Agarwal, and Gajendra PS Raghava.**
  Prediction of cytochrome P450 isoform responsible for metabolizing a drug molecule.
  BMC pharmacology 10.1 (2010): 8.
- **Naik, Pradeep Kumar, Abhishek Dubey, and Rishay Kumar.**
  Development of Predictive Quantitative Structure-Activity Relationship Models of Epipodophyllotoxin Derivatives.
  Journal of biomolecular screening 15.10 (2010): 1194-1203.
- **Naik, Pradeep Kumar, et al.**
  Molecular Modeling and Structure-Activity Relationship of Podophyllotoxin and Its Congeners.
  Journal of biomolecular screening 15.5 (2010): 528-540.

- **Yuta, Kohtarou.**
  Generating two-class classification model for predicting chemical toxicity.
  U.S. Patent No. 7,725,413. 25 May 2010.
- **Szymański, Paweł, and Elżbieta Mikiciuk-Olasik.**
  The prediction of acetylcholinesterase inhibitor activity using a mathematical model: a new age in drug design
  Farm Przegl Nauk, 2009,12, 26-32
- **Sato et al.**
  Skin Sensitization Study by Quantitative Structure-Activity Relationships (QSAR)
  AATEX 14(3),940-946,2009
- **Franklin, Ronald B.**
  In silico studies in ADME/Tox: caveat emptor.
  Current Computer-Aided Drug Design 5.2 (2009): 128-138.
- **Heimstad, Eldbjørg Sofie, et al.**
  Quantitative structure–Photodegradation relationships of polybrominated diphenyl ethers, phenoxyphenols and selected organochlorines.
  Chemosphere 77.7 (2009): 914-921.
- **Hirakawa, Keiko, et al.**
  Experimental estimation of postmortem interval using multivariate analysis of proton NMR metabolomic data.
  Legal Medicine 11 (2009): S282-S285.
- **Naik, P. K., et al.**
  Quantitative structure–activity relationship (QSAR) for insecticides: development of predictive in vivo insecticide activity models.
  SAR and QSAR in Environmental Research 20.5-6 (2009): 551-566.
- **Srivastava, Mani, Harvinder Singh, and Pradeep Kumar Naik.**
  Quantitative structure–activity relationship (QSAR) of artemisinin: the development of predictive in vivo antimalarial activity models.
  Journal of Chemometrics 23.12 (2009): 618-635.
- **Wawrzyniak, Rafal.**
  Quantitative relationship and application of 3-benzylketoimine metal dichlorides in the analysis of volatile hydrocarbons.
  Journal of separation science 32.9 (2009): 1415-1424.
- **Engel, Thomas.**
  Was Döbereiner nicht wusste…
  Nachrichten aus der Chemie 56.2 (2008): 150-152.
- **Kah, Melanie, Sabine Beulke, and Colin D. Brown.**
  Factors influencing degradation of pesticides in soil.
  Journal of agricultural and food chemistry 55.11 (2007): 4487-4492.