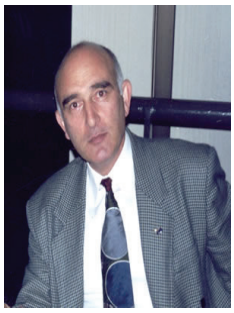
Europass Curriculum Vitae



Personal information

First name(s) / Surname(s)	**Ovanes Mekenyan**
Address(es)	L. Karavelov 57 8000 Bourgas (Bulgaria)
Telephone(s)	+359-56-818429 Mobile | +359-88-8225576
Fax(es)	+359-56-880230
E-mail(s)	omekenya@btu.bg
Nationality	Bulgarian
Gender	Male

Work experience

Dates	1989 →
Occupation or position held	Head of Laboratory of Mathematical Chemistry
Name and address of employer	University "Prof. As. Zlatarov" Bourgas Bulgaria
Dates	1992 →
Occupation or position held	Professor of Chemistry
Name and address of employer	University "Prof. As. Zlatarov" Bourgas, Bulgaria
Dates	1996 - 2000
Occupation or position held	Head of Department "Physical Chemistry"
Name and address of employer	University "Prof. Asen Zlatarov" Bourgas Bulgaria
Dates	1992 - 1994
Occupation or position held	Senior Scientist
Name and address of employer	Lake Superior Research Institute University of Wisconsin - Superior
Dates	1991 - 1992
Occupation or position held	Associate Scientist
Name and address of employer	Lake Superior Research Institute University of Wisconsin - Superior
Dates	1989 - 1991
Occupation or position held	Vice Dean of the Chemical Technology Faculty
Name and address of employer	University "Prof. As. Zlatarov" Bourgas Bulgaria
Dates	1985 - 1992
Occupation or position held	Associate Professor

Name and address of employer	University "Prof. As. Zlatarov" Bourgas Bulgaria
Dates	1975 - 1984
Occupation or position held	Assistant Professor
Name and address of employer	University "Prof. As. Zlatarov" Bourgas Bulgaria

Education and training

Dates	1980 - 1992
Title of qualification awarded	D. Sci.
Principal subjects / occupational skills covered	Theoretical Chemistry
Name and type of organisation providing education and training	Institute of Organic Chemistry Bulgarian Academy of Sciences, Sofia Bulgaria
Dates	1976 - 1980
Title of qualification awarded	Ph.D.
Principal subjects / occupational skills covered	Theoretical Chemistry
Name and type of organisation providing education and training	Institute of Organic Chemistry Bulgarian Academy of Sciences, Sofia Bulgaria
Dates	1967 - 1972
Title of qualification awarded	M.S.
Principal subjects / occupational skills covered	Organic Chemistry
Name and type of organisation providing education and training	University "Prof. As. Zlatarov" Bourgas Bulgaria
Dates	1967 - 1972
Title of qualification awarded	B.S.
Principal subjects / occupational skills covered	Organic Chemistry
Name and type of organisation providing education and training	University "Prof. As. Zlatarov" Bourgas Bulgaria

Personal skills and competences

Mother tongue(s) **Bulgarian**

Other language(s)

Self-assessment	Understanding				Speaking				Writing	
European level (*)	Listening		Reading		Spoken interaction		Spoken production			
English	C1	Proficient user	C1	Proficient user	C1	Proficient user	C1	Proficient user	C1	Proficient user
Russian	B2	Independent user	B2	Independent user	B2	Independent user	B2	Independent user	B2	Independent user
Armenian	B1	Independent user	B1	Independent user	B1	Independent user	A2	Basic User	A1	Basic User

(*) Common European Framework of Reference (CEF) level

Social skills and competences	Team worker Easily adapting to international environment given the international travels and stayings abroad. Have easy and effective communication capabilities experienced as department and lab manager.
Organisational skills and competences	I have experience organizing and coordinating team work, heading projects and budgeting.
Technical skills and competences	I have been post doc in Polytechnica (Bucarest), Rudger Boshkovich (Zagreb), US EPA (Duluth, MN), Joint Research centre (Ispra, Italia), University Paris VII, etc.
Computer skills and competences	Experienced in using Microsoft Office (Word, Excel, PowerPoint) as well as basic knowledge in graphic design.
Artistic skills and competences	Playing the piano.
Driving licence(s)	Category B

Additional information

Dr. Mekenyan is an internationally recognized expert in the fields of mathematical chemistry and chemical informatics. He is knowledgeable of current physicochemical and mathematical (2D and 3D) methods to model molecular structure and properties of organic chemicals. He has built algorithms, methods and software for 3D modeling and 3D screening of large chemical inventories (3D Informational technology) since 1980. Dr. Mekenyan has introduced the molecular flexibility (4th dimension of chemical structures) and metabolic activation of chemicals in QSAR analysis and databasing. His is the leading developer of metabolic simulators for tissue and microbial biotransformations of chemicals. The metabolic simulators were used for predicting biodegradation, bioaccumulation, genotoxicity, skin sensitization, and receptor mediated endpoints. His lab developed the Centralized 3D database for all existing chemicals – conformationally multiplied and QC optimized. The 3D Database manager allows flexible searching of analogues and categorization of chemicals, accounting for their metabolic activation/deactivation. Dr. Mekenyan is the principal developer of the OASIS suite of programs for modeling biological (toxic) effects, which, according to some of the leading computer chemistry laboratories, is one of the most flexible and reliable programs for this purpose. Under his guidance the Laboratory of Mathematical Chemistry has developed the harmonized system for hazard assessment known currently as the OECD (Q)SAR Application Toolbox. The system is currently in use in all OECD member state countries and stake holders as well as in industry (1600 free downloads, so far). He has published about 200 papers (and 2 books) in internationally recognized journals. He holds the title of "Professor" in the Department of Physical Chemistry, and is Head of the Laboratory of Mathematical Chemistry, at Bourgas "Prof As. Zlatarov" University (Bulgaria), where he is lecturing extensively on physical chemistry and chemical reactivity approaches, and their application to real chemistry problems. Dr. Mekenyan has been a Senior Visiting Scientist at UW. Dr. Mekenyan is presently a consultant of the major industries, such as 3M, Procter and Gamble, DuPont, L'Oreal, Givaudan, Firmenich, ExxonMobil, BASF, Unilever, etc.

Annexes

LIST OF RELATED PUBLICATION OF PROF. DR. OVANES MEKENYAN

After 2000

I. SCIENTIFIC PUBLICATIONS IN THE FIELD OF MATHEMATICAL CHEMISTRY

1. O.G. Mekenyan, D. Dimitrov, N. Nikolova and S. Karabunarliev. Conformational Coverage by a Genetic Algorithm. Chem. Inf. Comput. Sci. 39/6, 997-1016 (1999).

2. V.Kamenska, J. Ivanov and O. Mekenyan. The COREPA Approach to lead generation: an application to ACE-inhibitors. European J. Med. Chem. 34, 687-699 (1999).

3. D. Dimov, Z. Nedyalkova, S. Haladjova, G. Schüürmann and O. Mekenyan. 2001. QSAR Modeling of Antimycobacterial Activity and Activity Against Other bacteria of 3-Formyl Rifamycin SV Derivatives. Quant. Struct.-Act. Relat. 20, 298-318 (2001).

4. O. Mekenyan. 2002. Dynamic QSAR Techniques: Applications in Drug Design and Toxicology. Curr. Pharm. Des. 8 (17) 1605-1624 (2002).

5. S. Karabunarliev, N. Nikolova. N. Nikolov and O.G. Mekenyan. 2003. Rule Interpreter: A Chemicals language that Implements Decision Rules Based on Molecular Structure . J. Mol. Structure (THEOCHEM), 622:53-62.

6. O. G. Mekenyan, T. Pavlov, V. Grancharov, M. Todorov, P. Schmieder and G. Veith. 2005. 2D-3D Migration of Large Chemical Inventories with Conformational Multiplication. Application of the Genetic Algorithm. J. Chem. Inf. Model., 45 (2), 283 -292.

7. N. Nikolov, V. Grancharov, G. Stoyanova, T. Pavlov, O. Mekenyan. 2006. Representation of Chemical Information in OASIS Centralized 3D Database for Existing Chemicals, J. Chem. Inf. Model., 46(6), 2537-2551.

8. Verginia Kamenska, Lyubomir Dourmishev, Assen Dourmishev, Rusi Vasilev and Ovanes Mekenyan. Quantitative Structure-Activity Relationship Modeling of Dermatomyositis Activity of Drug Chemicals. Arzneim. Forsch., 56, 856-865 (2006).

II. SCIENTIFIC PUBLICATIONS IN THE FIELD OF PREDICTIVE TOXICOLOGY

9. O. Mekenyan, N. Nikolova, S. Karabunarliev, S. Bradbury, G. Ankley, B Hansen. 1999. New Developments in a Hazard Identification Algorithm For Hormone Receptor Ligands: COREPA-C Quant. Struct.-Act. Relat. 18:139-153.35.

10. P.K. Schmieder, A.O. Aptula, E. J. Routledge, J.P. Sumpter, and O.G.Mekenyan. 2000. Estrogenicity of Alkylphenolic Compounds: A 3-D Structure Activity Evaluation of Gene Activation. Environ. Toxicol. Chem. 19(7):1727-1740.

11. S. Bradbury, V. Kamenska, P. Schmieder, G. Ankley, O. Mekenyan. 2000. A Computationally-Based Identification Algorithm for Estrogen Receptor Ligands.Part I. Predicting hER" Binding Affinity Toxicol. Sci. 58:253-269.

12. O. Mekenyan, V. Kamenska, P. Schmieder, G. Ankley, S. Bradbury. 2000. A Computationally-Based Identification Algorithm for Estrogen Receptor Ligands. Part II. Evaluation of a hER" Binding Affinity Model Toxicol.
Sci. 58: 270-281.

13. D. D. Dimitrov, O. G. Mekenyan, T.W. Schultz. 2000. Interspecies Modeling of Narcotics Toxicity to Aquatic Animals Bull. Environ. Toxicol. 65: 399-406.

14. T.W. Schultz and O.G. Mekenyan. Response-surface analyses: A comparison of two approaches to predicting acute toxicity. In: Walker J.(ed) Quantitative Structure Activity Relationships in Environmental Sciences - VIII. SETAC Press, Pensacola FL USA (in press).

15. O.Mekenyan, V. Kamenska, R.Serafimova, L.Poellinger, A. Brower, J. Walker. 2001. Development and Validation of an Average Mammalian Estrogen Receptor-Based QSAR Model. In: Mekenyan O. and Schultz T.W (eds.) Proceedings of Quantitative Structure Activity Relationships in Environmental Sciences - IX.; SAR and QSAR in Environ. Research 13 (6) 579-595 (2002).

16. G.T. Ankley, O.Mekenyan, V. Kamenska, P. Schmieder and S. Bradbury. Reactivity Profiles of Ligands of Mammalian Retinoic Acid Receptors:A Preliminary Corepa Analysis. In: Mekenyan O. and Schultz T.W (eds.) Proceedings of Quantitative Structure Activity Relationships in Environmental Sciences - IX.; SAR and QSAR in Environ. Research, 13 (2) 365-377 (2002).

17. R. Serafimova, J.Walker, O.Mekenyan. Androgen Receptor Binding Affinity of Pesticide "Active" Formulation Ingredients. QSAR Evaluation by COREPA Method. In: Mekenyan O. and Schultz T.W (eds.) Proceedings of Quantitative Structure Activity Relationships in Environmental Sciences - IX.; SAR and QSAR in Environ. Research, 13 (1) 127-134 (2002).

18. S. Dimitrov, O. Mekenyan, J. Walker. Non-Linear models for predicting bioconcentration and acute toxicity of narcotic chemicals. In: Mekenyan O. and Schultz T.W (eds.) Proceedings of Quantitative Structure Activity Relationships in Environmental Sciences - IX.; SAR and QSAR in Environ. Research, 13 (1) 177-184 (2002).

19. S. Dimitrov, R. Breton, D. Mackdonald, J. Walker and O. Mekenyan. Quantitative prediction of biodegradability, metabolite distribution and toxicity of stable metabolites. In: Mekenyan O. and Schultz T.W (eds.) Proceedings of Quantitative Structure Activity Relationships in Environmental Sciences - IX.; SAR and QSAR in Environ. Research,13 (3-4) 445-455 (2002).

20. D. T. Stanton, S. Dimitrov, V. Grancharov and O. Mekenyan. Charged partial surface area (CPSA) descriptors. QSAR Applications. In: Mekenyan O. and Schultz T.W (eds.) Proceedings of Quantitative Structure Activity Relationships in Environmental Sciences - IX.; SAR and QSAR in Environ. Research,13 (2) 341-353 (2002).

21. P. Schmieder, Y. Koleva and O. Mekenyan. 2001. A reactivity pattern for discrimination of ER agonism and antagonism based on 3-D molecular attributes. In: Mekenyan O. and Schultz T.W (eds.) Proceedings of Quantitative Structure Activity Relationships in Environmental Sciences - IX.; SAR and QSAR in Environ. Research, 13 (2) 353-364 (2002).

22. J. Jaworska, S. Dimitrov; N. Nikolova; P. Masscheleyn; O. Mekenyan. Probabilistic Assessment of Biodegradability Based on Metabolic Pathways: CATABOL System. In: Mekenyan O. and Schultz T.W (eds.) Proceedings of Quantitative Structure Activity Relationships in Environmental Sciences - IX.; SAR and QSAR in Environ. Research, 13 (2) 307-323 (2002).

23. S. D. Dimitrov, N. C. Dimitrova, J. D. Walker, G. D. Veith, and O. G. Mekenyan. Predicting bioconcentration factors of highly hydrophobic chemicals. Effects of molecular size, Pure Appl. Chem., 74, (10), 1823-1830 (2002).

24. S. D. Dimitrov, O.G. Mekenyan, S. Karabunarliev, G.D. Sinks and T. W. Schultz. 2003. Global Modeling of Narcotic Chemicals: Ciliate and Fish Toxicity. J. Mol. Structure (THEOCHEM), 622:63-70.

25. O. Mekenyan, N. Nikolova and P. Schmieder. 2003. Dynamic 3D QSAR techniques: application in toxicology, J. Mol. Structure (THEOCHEM), 622:147-165.

26. J. D. Walker, S. Dimitrov, O. Mekenyan. 2003. Using HPV Chemical Data to Develop QSARs for Non-HPV Chemicals: Opportunities to Promote More Efficient Use of Chemical Testing Resources, QSAR Comb. Sci., 22(3), 386-395.

27. S. D. Dimitrov, N. C. Dimitrova, J. D. Walker, G. D. Veith and O. G. Mekenyan. 2003. Bioconcentration potential predictions based on molecular attributes – an early warning approach for chemicals found in humans, birds, fish and wildlife, QSAR Comb. Sci., 22, 58-68.

28. Dimitrov S., Koleva Y., Lewis M., Breton R., Veith G. and Mekenyan O. 2003. Modeling mode of action of industrial chemicals: Application using chemicals on Canada's Domestic Substances List (DSL), QSAR Comb. Sci., 22, 5-17.

29. O. Mekenyan, S. Dimitrov, P. Schmieder, and G. Veith. 2003. In Silico Modelling of Hazard Enpoints: Current Problems and Perspectives. SAR and QSAR in Environ. Research, 14 (5-6), 361-371.

30. O. G. Mekenyan, N. Nikolova, P. Schmieder and G.D. Veith. 2004. COREPA-M: A Multi-Dimensional Formulation of COREPA, QSAR & Combinatorial Science, 23, 5-18.

31. S. D. Dimitrov, V.B.Kamenska, J. D. Walker, W. Windle, R. Purdy M. Lewis and O. G. Mekenyan. 2004. Predicting the biodegradation products of perfluorinated chemicals using CATABOL. SAR and QSAR in Environ. Research 15(1), 69-82.

34. P. Schmieder, O. Mekenyan, S. Bradbury and G. Veith. 2004. QSAR Prioritization of Chemical Inventories for Endocrine Disruptor Testing. Proceedings of the SCOPE/IUPAC International Symposium on Endocrine Active Substances, Yokohama, Japan, Nov. 17-21, 2002 (in press).

35. O. G. Mekenyan, S.D. Dimitrov, T. S. Pavlov, and G. D. Veith. 2004. A Systems Approach to Simulating Metabolism in Computational Toxicology. I. The TIMES Heuristic Modelling Framework. Current Pharmaceutical Design 10 (11), 1273-1293.

36. Mekenyan, O.G., S. Dimitrov, R. Serafimova, E. Thompson, S. Kotov, N. Dimitrova, J. Walker. 2004. Identification of the structural requirements for mutagencitiy, by incorporating molecular flexibility and metabolic activation of chemicals I. TA100 Model. Chem. Res.Toxicol. 17(6):753-766 (2004).

37. Walker JD, Dimitrova N, Dimitrov S, Mekenyan OG and Plewak D. 2004. Use of QSAR to promote More Cost Effective Use of Chemical Monitoring Resources. 2. Screening Chemicals for Half Lives, Henry's Low Constants, Ultimate Biodegradation Potential, Modes of Toxic Action and Bioavailability. Water Qual. Res J Canada 39(1):41-50.

38. K. Thomas, J. Balam, M. Hurst, Z. Nedyalkova and O. Mekenyan. Potency and characterization of estrogen-receptor agonists in United Kingdom estuarine sediments, Environmental Toxicology and Chemistry, Vol. 23, No. 2, pp. 471–479, 2004.

39. O. G. Mekenyan, S.D. Dimitrov, T.S. Pavlov, and G.D. Veith. 2005. POPs: A QSAR system for creating PBT profiles of chemicals and their metabolites. SAR and QSAR in Environ. Research, 16 (1-2), 102-133.

40. S.D. Dimitrov, L.K. Low, G.Y. Patlewicz, P.S. Kern, G. D. Dimitrova, M.H.I. Comber, R.D. Phillips, J. Niemela, P.T. Bailey, O.G. Mekenyan. 2004. Modeling Based on Skin Metabolism Simulation and Formation of Protein Conjugates, Internatational Journal of Toxicology, 24, 189-204.

41. S.D. Dimitrov, G. D. Dimitrova, T. Pavlov, N. Dimitrova, G.Y. Patlewicz, J. Niemela, O.G. Mekenyan. 2005. A stepwise approach for defining applicability domain of SAR and QSAR models, J. Chem. Inf. Modeling 45(4) 839-849.

42. Dimitrov A, N. Dimitrova A, T. Parkerton, M. Comber, M. Bonnell, O. Mekenyan, Base-line model for identifying the bioaccumulation potential of chemicals. 2005 SAR and QSAR in Environ. Research, 16 (6), 531 - 554.

43. Mekenyan, O.G., S. Dimitrov, N. Dimitrova, G. Dimitrova, T. Pavlov, G, Chankov, S. Kotov, K. Vasilev and R. Vasilev. 2006. Metabolic activation of chemicals: in-silico simulation, 17/1, 107-120.

44. K. Thomas, J. Balam, M. Hurst, Z. Nedyalkova and O. Mekenyan. Potency and characterization of estrogen-receptor agonists in United Kingdom estuarine sediments, Environmental Toxicology and Chemistry, Vol. 23, No. 2, pp. 471–479, 2004.

45. R. Serafimova, M. Todorov, D. Nedelcheva, T. Pavlov, Y. Akahori, M. Nakai and O. Mekenyan, QSAR and mechanistic interpretation of estrogen receptor binding, SAR and QSAR in Environ. Research, 18, 1-33 (2007).

46. A. Weisbrod, L. Burkhard, J. Arnot, O. Mekenyan, P. Howard, C. Russom, R. Boethling, Y. Sakuratani, T. Traas, T. Bridges, C. Lutz, M. Bonnell, K. Woodburn. Workgroup Report: Review of Fish Bioaccumulation Databases Used to Identify Persistent, Bioaccumulative, Toxic Substances, Environ. Health Presp. 115, 255-261 (2007).

47. R. Serafimova, M. Todorov, T. Pavlov, S. Kotov, E. Jacob, A.Aptula, O. Mekenyan. Identification of the Structural Requirements for Mutagencitiy, by Incorporating Molecular Flexibility and Metabolic Activation of Chemicals. II. General Ames Mutagenicity Model, Chem. Res. Toxicol., 20 (4), 662 -676, 2007.

48. Patlewicz, G., Dimitrov, S., Low, L., Kern, P., Dimitrova, G., Comber, M., Aptula, A., Philips, R., Niemela, J., Madsen, C., Wedebye, E., Roberts, D., Bailey, P., Mekenyan, O. TIMES-SS – A promising tool for the assessment of skin sensitization hazard. A characterization with respect to the OECD validation principles for (Q)SARs and an external evaluation for predictivity. Regulatory

Toxicology and Pharmacology 48 (2007) 225-239.

49. Roberts, D., Patlewicz, G., Dimitrov, S., Low, L., Aptula, A., Kern, P., Dimitrova, G., Comber, M., Philips, R., Niemela, J., Madsen, C., Wedebye, E., Bailey, P., Mekenyan, O. TIMES-SS – A mechanistic evaluation of an external validation study using reaction chemistry principles. Chem. Res. Toxicol. (2007) (published on web 05/23/2007)

50. O. Mekenyan, M. Todorov, R. Serafimova, S. Stoeva, A. Aptula, R. Finking, Elard Jacob, Identification of the structural requirements for genotoxicity, by incorporating molecular flexibility and metabolic activation of chemicals: (iii) Chromosomal Aberration, Chem. Res. Toxicol., 20 (12), 1927–1941.

51. M.N. Jacobs, W. Janssens, U. Bermauer, E. Brandon, S Coecke, R. Combes, P. Edwards, A. Freidig, A. Freiberger, R. Lolanczyk, C. McArdle, O. Mekenyan, P. Schmieder, T. Schrader, M. Takeyoshi, B. van der Burg. The Use of Metabolizing Systems for In Vitro Testing of Endocrine Disruptors. Curr. Drug Metabolism, 9, 796-826 (2008).

52. Petko I. Petkov, J. C. Rowlands, R. Budinsky, B. Zhao, M. S. Denison, O.Mekenyan, Mechanism based common reactivity pattern (COREPA) modeling of AhR binding affinity, SAR and QSAR in Environ. Research, 20, 657-678 (2009).

53. Hristo Aladjov, Milen Todorov, Patricia Schmieder, Rossitsa Serafimova, Ovanes Mekenyan and Gilman Veith. Strategic selection of chemicals for testing. Part I. Functionalities and performance of basic selection methods. SAR and QSAR in Environ. Research, 20, 159-183 (2009).

54. Ovanes Mekenyan and Rossitsa Serafimova. Mechanism based modeling of ER binding affinity: A COREPA implementation. Endocrine Disruption Modeling, Ed. J. Devillers, pp. 259-294. 2009

55. Petko Petkov, Stanislav Temelkov, Daniel L. Villeneuve, Gerald T. Ankley, Ovanes G. Mekenyan1, Mechanism-Based Categorization of Aromatase Inhibitors: A Potential Discovery and Screening Tool, and QSAR in Environ. Research, 20(7), 657 - 678 (2009).

56. S. Dimitrov, D. Nedelcheva, N. Dimitrova, O. Mekenyan. Development of a biodegradation model for the prediction of metabolites in soil. Science of the Total Environment, 408 (18), 3811-3816, 2010.

57. N. Dimitrova, S. Dimitrov, D. Georgieva, C.A.M. Van Gestel, P. Hankard, D. Spurgeon, H. Li, O. Mekenyan. Elimination kinetic model for organic chemicals in earthworms, Science of the Total Environment, Volume 408 (18), 3787-3793, 2010.

58. Ovanes Mekenyan, Grace Patlewicz, Gergana Dimitrova, Chanita Kuseva, Milen Todorov, Stoyanka Stoeva, Stefan Kotov, E Maria Donner, Bhaskar Gollapudi. The use of genotoxicity information in the development of Integrated Testing Strategies (ITS) for skin sensitization. Chemical Research in Toxicology 1519 – 1540, 2010

59. Grace Patlewicz, Ovanes Mekenyan, Gergana Dimitrova, Chanita Kuseva, Milen Todorov, Stefan Kotov, Stoyanka Stoeva, E. Maria Donner, Bhaskar Gollapudi. The use of genotoxicity information in the development of Integrated Testing Strategies (ITS) for skin sensitization II. SAR and QSAR in Environ. Research, 21: 7, 619 — 656, 2010

60. Stephanie Ringeissen, Lauren Marrot, Reine Note1, Anita Labarussiat, Stéphane Imbert, Gladys Ouedraogo, Milen Todorov, Ovanes Mekenyan, Jean-Roch Meunier. Integrated in silico – in vitro approach for the detection of phototoxic chemicals. Refinement of an historic mechanistic model developed for PAHs. Toxicology in Vitro, 25(1), 324-334, 2011

61. Todorov M, Mombelli E, Ait-Aissa S, Mekenyan O. Androgen receptor binding affinity: a QSAR evaluation. SAR QSAR Environ Res. 22(3), 265-91, 2011.

62. S. Dimitrov, T. Pavlov, G. Veith and O. Mekenyan, Simulation of chemical metabolism for fate and hazard assessment. I. Approach for simulating metabolism, SAR and QSAR in Environmental Research, DOI:10.1080/1062936X.2011.623323 (Available online:14 Oct 2011).

63. S. Dimitrov, T. Pavlov, N. Dimitrova, D. Georgieva, D. Nedelcheva, A. Kesova, R. Vasilev and O. Mekenyan, Simulation of chemical metabolism for fate and hazard assessment. II CATALOGIC

simulation of abiotic and microbial degradation, SAR and QSAR in Environmental Research, DOI:10.1080/1062936X.2011.623322 (Available online:14 Oct 2011).

64. S. Dimitrov, N. Dimitrova, D. Georgieva, K. Vasilev, T. Hatfield, J. Straka and O. Mekenyan, Simulation of Chemical Metabolism for Fate and Hazard Assessment. III. New Developments of BCF Base-line Model, SAR and QSAR in Environmental Research, (In press).

65. S. Karabunarliev, S. Dimitrov, T. Pavlov, D. Nedelcheva, and O. Mekenyan, Simulation of Chemical Metabolism for Fate and Hazard Assessment. IV. Computer-based Derivation of Metabolic Simulators from Documented Metabolism Maps, SAR and QSAR in Environmental Research, (In press).