CURRICULUM VITAE

Jürgen Bajorath

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PERSONAL

U.S. citizen

EDUCATION

Ph.D., Structural Biochemistry, Department of Chemistry, Free University Berlin, 1988

MS, Biochemistry (Dipl.-Biochem.), Department of Chemistry, Free University Berlin, 1986

PROFESSIONAL EXPERIENCE

RHEINISCHE FRIEDRICH-WILHELMS UNIVERSITY BONN — 2004-PRESENT

Full Professor and Chair of Life Science Informatics

UNIVERSITY OF WASHINGTON — 1995-PRESENT
DEPARTMENT OF BIOLOGICAL STRUCTURE

Affiliate Professor

MDS PANLABS, NEW CHEMICAL ENTITIES, ALBANY MOLECULAR RESEARCH — 1997-2004
BOTHELL RESEARCH CENTER (ACQUISITIONS)
Bothell, WA

Director, Senior Director - Computer-Aided Drug Discovery

BRISTOL-MYERS SQUIBB PHARMACEUTICAL RESEARCH INSTITUTE — 1991-1997
Seattle, WA

Principal Scientist – Drug Design

BIOSYM TECHNOLOGIES — 1989-1991

San Diego, CA

Postdoctoral Fellow

SCIENTIFIC ADVISORY BOARDS

Washington State University 1993-1995
Pullman, WA
Center for Analysis and Design in Molecular Sciences

Chemical Computing Group 1998- 2012
Montreal, Quebec, Canada

JADO Technologies 2009- 2013
Dresden, Germany

Astra Zeneca
Discovery Sciences External Science Panel
Alderly Park, UK 2012- 2015

eADMET
Munich, Germany 2014-2015

EDITOR

Associate Editor
Journal of Medicinal Chemistry 2008- PRESENT

EDITORIAL BOARDS

Editorial Board
Journal of Molecular Graphics & Modeling 2000-2003

Editorial Advisory Board
Targets 2001-2004

Editorial Advisory Board
Journal of Chemical Information and Computer Science 2001-2004

Editorial Advisory Board
The Open Drug Discovery Journal 2008- 2012

Editorial Board
The International Journal of High Throughput Screening 2009- 2016

Editorial Board
Research Reports in Medicinal Chemistry 2011- 2016

Editorial Advisory Board
Drug Discovery Today 2002- PRESENT

Editorial Advisory Board
Advances in Chemoinformatics and Computational Methods 2007- PRESENT

Editorial Board
The Open Applied Informatics Journal 2007- PRESENT

Editorial Board
Molecular Diversity 2007- PRESENT

Editorial Advisory Board
Chemical Biology and Drug Design 2008- PRESENT

Editorial Board
Expert Opinion on Drug Discovery 2011- PRESENT

Board of Editors
Journals of the American Computational Science Society 2011-PRESENT

Editorial Advisory Board
Systems Pharmacology 2012- PRESENT

Editorial Board
F1000 Research 2012- PRESENT

Editorial Advisory Board
Molecular Informatics 2014- PRESENT

HONORS

1989 Ernst-Reuter-Award

1996 Bristol-Myers Squibb Excellence Award

2008 Invited Professor, Faculté de Chimie, University of Strasbourg, France

2011 Novartis Chemistry Lecturer Award

2011 *Faculty of 1000* – Drug Discovery & Design

2011-Present *Highly Cited Scientist*, Chemistry, Thomson Reuters

2015 *Medicinal Chemistry Leader*, Future Science Group

2015 Herman-Skolnik-Award, American Chemical Society

2016 Invited Professor, Faculté de Chimie, University of Strasbourg, France

2016 Hansch-Fujita Award, Hansch-Fujita Foundation

PUBLICATIONS

1. 1. Bajorath J, Pal GP & Saenger W. Inhibition and autolysis of proteinase K, a subtilisin-related serine proteinase from the fungus *Tritirachium album Limber*. Biochem Biophys Acta 954, 176-182, 1988.

2. Bajorath J, Hinrichs W & Saenger W. The activity of proteinase K is controlled by calcium. Eur J Biochem 176, 441-447, 1988.

3. Betzel C, Bellemann M, Pal GP, Bajorath J, Saenger W & Wilson KS. X-ray and model building studies on the specificity of the active site of proteinase K. Proteins: Struct, Funct & Genet 4, 157-164, 1988.

4. Bajorath J, Raghunathan S, Hinrichs W & Saenger W. Long-range structural changes in proteinase K triggered by calcium ion removal. Nature 337, 481-484, 1989.

5. Wolf W, Bajorath J, Müller A, Raghunathan S, Singh TP, Hinrichs W & Saenger W. Inhibition of proteinase K by methoxysuccinyl-Ala-Ala-Pro-Ala-chloromethyl ketone. An X-ray study at 2.2 Å resolution. J Biol Chem 26, 17695-17699, 1991.

6. Bajorath J, Kitson DH, Fitzgerald G, Andzelm J, Kraut J & Hagler AT. Electron redistribution on binding of a substrate to an enzyme: Folate and dihydrofolate reductase. Proteins: Struct, Funct & Genet 9, 217-224, 1991.

7. Bajorath J, Kitson DH, Kraut J & Hagler AT. The electrostatic potential of *Escherichia coli* dihydrofolate reductase. Proteins: Struct, Funct & Genet 11, 1-12, 1991.

8. Bajorath J, Li Z, Fitzgerald G, Kitson DH, Farnum M, Fine RM, Kraut J & Hagler AT. Changes in the electron density of the cofactor NADPH on binding to *E. coli* dihydrofolate reductase. Proteins: Struct, Funct & Genet 11, 263-270, 1991.

9. Bajorath J, Kraut J, Li Z, Kitson DH & Hagler AT. Theoretical studies on the dihydrofolate reductase mechanism: Electronic polarization of bound substrates. Proc Natl Acad Sci USA 88, 6423-6426, 1991.

10. Fell HP, Gayle MA, Schieven GL, Yelton DE, Lipsich L, Hellström KE, Hellström I, Marken J, Aruffo A & Bajorath J. Chimeric L6 anti-tumor antibody. Genomic construction, expression, and characterization of the antigen binding site. J Biol Chem 267, 15552-15558, 1992.

11. Ganju RK, Smiley ST, Bajorath J, Novotny J & Reinherz E. Similarity between fluorescein-specific T cell receptor and antibody in chemical details of antigen recognition. Proc Natl Acad Sci USA 89, 11552-11556, 1992.

12. Bajorath J & Fine RM. On the use of minimization from many randomly generated loop structures in modeling antibody combining sites. Immunomethods 1, 137-146, 1992.

13. Aruffo A, Farrington M, Hollenbaugh D, Li X, Milatovitch A, Nonoyama S, Bajorath J, Grosmaire LS, Stenkamp R, Neubauer M, Roberts RL, Noelle RJ, Ledbetter JA, Francke U & Ochs HD. The CD40 ligand, gp39, is defective in activated cells from patients with X-linked hyper-IgM syndrome. Cell 72, 291-300, 1993.

14. Bajorath J, Stenkamp R & Aruffo A. Knowledge-based model building of proteins: Concepts and examples. Protein Sci 2, 1798-1810, 1993.

15. Hollenbaugh D, Bajorath J, Stenkamp R & Aruffo A. Interaction of P-selectin (CD62) and its cellular ligand: Analysis of critical residues. Biochemistry 32, 2960-2966, 1993.

16. Hsiao K, Bajorath J & Harris LJ. Humanization of 60.3, an anti-CD18 antibody; importance of the L2 loop. Protein Eng 7, 815-822, 1994.

17. Chang CY, Jeffrey PD, Bajorath J, Hellström I, Hellström KE & Sheriff S. Crystallization and preliminary X-ray analysis of the monoclonal anti-tumor antibody BR96 and its complex with the LeY determinant. J Mol Biol 235, 372-376, 1994.

18. Hayden MS, Linsley PS, Gayle MA, Bajorath J, Brady WA, Norris NA, Fell HP, Ledbetter JA & Gilliland LK. Single chain mono- and bispecific antibody derivatives with novel biological properties and anti-tumor activity from a COS cell transient expression system. Therapeutic Immunol 1, 3-15, 1994.

19. Marken JS, Bajorath J, Hellström I, Hellström KE & Aruffo A. Isolation of the human tumor-associated antigen L6: membrane topology of L6 and identification of the epitope region of an anti-L6 monoclonal antibody. J Biol Chem 269, 7397-7401, 1994.

20. Peach RJ, Bajorath J, Brady W, Leytze G, Greene J, Naemura J & Linsley PS. Conserved and non-conserved residues of CDR-analogous regions in CTLA-4 and CD28 determine the binding to B7-1. J Exp Med 180, 2049-2058, 1994.

21. Linsley PS, Greene JL, Brady W, Bajorath J, Ledbetter JA & Peach RJ. Human B7-1 (CD80) and B7-2 (CD86) bind with similar avidities but distinct kinetics to CD28 and CTLA-4 receptors. Immunity 1, 793-801, 1994.

22. Bajorath J, Hollenbaugh D, King G, Harte WE Jr, Darveau RP, Eustice D & Aruffo A. The CD62/P-selectin binding sites for HL-60 cells and sulfatides are overlapping. Biochemistry 33, 1332-1339, 1994.

23. Bajorath J & Aruffo A. Three-dimensional protein models: insights into structure, function, and molecular interactions. Bioconjug Chem 5, 173-181, 1994.

24. Bajorath J. Three-dimensional model structure of the BR96 monoclonal antibody variable fragment. Bioconjug Chem 5, 213-219, 1994.

25. Harte WE Jr & Bajorath J. Synergism of calcium and carbohydrate binding to a mammalian lectin suggested by a dynamic model. J Am Chem Soc 116, 10394-10398, 1994.

26. Linsley PS, Peach RJ, Gladstone P & Bajorath J. Extending the B7 gene family. Protein Sci 3, 1341-1343, 1994.

27. Stenzel-Johnson P, Yelton DE & Bajorath J. Identification of residues in the monoclonal anti-tumor antibody L6 important for the binding to tumor antigen. Biochemistry 33, 14400-14406, 1994.

28. Bajorath J, Peach RJ & Linsley PS. Immunoglobulin fold characteristics of B7-1 (CD80) and B7-2 (CD86). Protein Sci 3, 2148-2150, 1994.

29. Bajorath J & Aruffo A. Molecular model of the extracellular lectin-like domain in CD69. J Biol Chem 269, 32457-32463, 1994.

30. Harris L & Bajorath J. Profiles for the analysis of immunoglobulin sequences: Comparison of V gene subgroups. Protein Sci 4, 306-310, 1995.

31. Bajorath J, Stenkamp R & Aruffo A. Comparison of a protein model with its X-ray structure: the ligand binding domain in E-selectin. Bioconjug Chem 6, 3-6, 1995.

32. Bajorath J, Chalupny NJ, Marken JS, Siadak AW, Skonier J, Gordon M, Hollenbaugh D, Noelle RJ, Ochs HD & Aruffo A. Identification of residues on CD40 and its ligand which are critical for receptor-ligand interactions. Biochemistry 34, 1833-1844, 1995.

33. Jeffrey PD, Bajorath J, Chang CY, Yelton DE, Hellström I, Hellström KE & Sheriff S. The X-ray structure of an anti-tumour antibody in complex with antigen. Nature Struct Biol 2, 466-471, 1995.

34. Linsley PS, Ledbetter JA, Peach RJ & Bajorath J. CD28/CTLA-4 receptor structure, stoichiometry of ligand binding, and aggregation during T cell activation. Res Immunol 146, 130-140, 1995.

35. Bajorath J & Novotny J. Model building of antibody combining sites. Therapeutic Immunol 2, 95-103, 1995.

36. Linsley PS, Nadler S, Bajorath J, Peach RJ, Rogers J, Bradshaw J, Leung HT, Stebbins M, Leytze G, Brady W, Malacko AR, Marquardt H & Shaw S-Y. Binding stoichiometry of the cytotoxic T lymphocyte-associated molecule-4 (CTLA-4). A disulfide-linked homodimer binds two CD86 molecules. J Biol Chem 270, 15417-15424, 1995.

37. Bajorath J, Marken JS, Chalupny NJ, Spoon TL, Siadak AW, Gordon M, Noelle RJ, Hollenbaugh D & Aruffo A. Analysis of gp39/CD40 interactions using molecular models and site-directed mutagenesis. Biochemistry 34, 9884-9892, 1995.

38. Yelton DE, Rosok MJ, Cruz G, Cosand WL, Bajorath J, Hellström I, Hellström KE, Huse WD & Glaser SM. Affinity maturation of the BR96 anti-carcinoma antibody *in vitro* by codon-based mutagenesis. J Immunol 155, 1994-2004, 1995.

39. Peach RJ, Bajorath J, Naemura J, Leytze G, Aruffo A & Linsley PS. Both extracellular immunoglobulin-like domains of CD80 contain residues critical for binding to T-cell surface receptors CTLA-4 and CD28. J Biol Chem 270, 21181-21187, 1995.

40. Bajorath J, Bowen MA, Aruffo A. Molecular model of the N-terminal receptor-binding domain of the human CD6 ligand ALCAM. Protein Sci 4, 1644-1647, 1995.

41. Bajorath J, Harris L & Novotny J. Conformational similarity and systematic displacements of CDR loops in high-resolution X-ray structures. J Biol Chem 270, 22081-22084, 1995.

42. Edwards CP, Farr AG, Marken JS, Nelson A, Bajorath J, Hellström KE, Hellström I & Aruffo A. Cloning of the 12A8 antigen, the murine homolog of the tumor-associated antigen H-L6, and fine mapping of the epitope recognized by the anti-H-L6 monoclonal antibody L6. Biochemistry 34, 12653-12660, 1995.

43. Bajorath J & Aruffo A. A template for generation and comparison of three-dimensional selectin models. Biochem Biophys Res Comm 216, 1018-1023, 1995.

44. Lee N, Malacko AR, Ishitani A, Chen MC, Bajorath J, Marquardt H & Geraghty DE. The membrane-bound and soluble forms of HLA-G bind identical sets of endogenous peptides but differ with respect to TAP association. Immunity 3, 591-600, 1995.

45. Chalupny NJ, Aruffo A, Esselstyn JM, Chang PY, Bajorath J, Blake J, Gilliland LK, Ledbetter JA & Tepper MA. Specific binding of Fyn and phosphatidylinositol 3-kinase to the B cell surface glycoprotein CD19 through their src homology 2 domains. Eur J Immunol 25, 2978-2984, 1995.

46. Bajorath J & Sheriff S. Comparison of an antibody model with an X-ray structure: The variable fragment of BR96. Proteins: Struct, Funct & Genet 24, 152-157, 1996.

47. Siemers NO, Yelton DE, Bajorath J & Senter PD. Modifying the specificity of *Enterobacter cloacae* P99 ß-lactamase within an M13 phage vector. Biochemistry 35, 2104-2111, 1996.

48. Bajorath J & Aruffo A. Structure-based modeling of the ligand binding domain of the human cell surface receptor CD23 and comparison of two independently derived molecular models. Protein Sci 5, 240-247, 1996.

49. Bajorath J, Seyama K, Nonoyama S, Ochs HD & Aruffo A. Classification of mutations in the human CD40 ligand, gp39, which are associated with X-linked hyper IgM syndrome. Protein Sci 5, 531-534, 1996.

50. Sheriff S, Chang CY, Jeffrey PD & Bajorath J. X-ray structure of the uncomplexed anti-tumor antibody BR96 and comparison with its antigen-bound form. J Mol Biol 259, 938-946, 1996.

51. Bowen MA, Bajorath J, Siadak AW, Modrell B, Malacko AR, Marquardt H, Nadler SG & Aruffo A. The amino-terminal immunoglobulin-like domain of activated leukocyte cell adhesion molecule (ALCAM) binds specifically to the membrane-proximal scavenger receptor cysteine rich domain of CD6. J Biol Chem 271, 17390-17396, 1996.

52. Rosok MJ, Yelton DE, Harris LJ, Bajorath J, Hellström KE, Hellström I, Cruz GA, Kristensson K, Lin H, Huse WD & Glaser SM. Combinatorial libraries for the rapid humanization of anticarcinoma BR96 Fab. J Biol Chem 271, 22611-22618, 1996.

53. Foy TM, Aruffo A, Bajorath J, Buhlmann JE & Noelle RJ. Immune regulation by CD40 and its ligand gp39. Ann Rev Immunol 14, 591-617, 1996.

54. Novotny J & Bajorath J. Computational biochemistry of antibodies and T-cell receptors. In: Advances in Protein Chemistry: Antigen binding molecules: Antibodies and T cell receptors. Adv Prot Chem 49, 147-258, 1996.

55. Skonier JE, Bowen MA, Emswiler J, Aruffo A & Bajorath J. Recognition of diverse proteins by members of the immunoglobulin superfamily: delineation of the receptor binding site in the human CD6 ligand ALCAM. Biochemistry 35, 12287-12291, 1996.

56. Sheriff S, Jeffrey PD & Bajorath J. Comparison of CH1 domains in different classes of murine antibodies. J Mol Biol 263, 385-389, 1996.

57. Greene JL, Leytze GM, Emswiler J, Peach R, Bajorath J, Cosand W & Linsley PS. Covalent dimerization of CD28/CTLA-4 and oligomerization of CD80/CD86 regulate T cell costimulatory interactions. J Biol Chem 271, 26762-26771, 1996.

58. Bajorath J. A molecular model of a macrophage lectin and analysis of its binding site. J Mol Graph 14, 297-301, 1996.

59. Skonier JE, Bowen MA, Emswiler J, Aruffo A & Bajorath J. Mutational analysis of the CD6 binding site in activated leukocyte cell adhesion molecule. Biochemistry 35, 14743-14748, 1996.

60. Shapiro RA, Cunningham MD, Ratcliffe K, Seachord C, Blake J, Bajorath J, Aruffo A & Darveau RP. Identification of CD14 residues involved in specific lipopolysaccharide recognition. Infect Immun 65, 293-297, 1997.

61. Stenkamp R, Aruffo A & Bajorath J. Protein superfamily members as targets for computer modeling: the carbohydrate recognition domain of a macrophage lectin. Pac Symp Biocomput 5, 432-440, 1997.

62. Bajorath J & Aruffo A. Construction and analysis of a detailed molecular model of the ligand binding domain of the human B cell receptor CD40. Proteins: Struct, Funct & Genet. 27, 59-70, 1997.

63. Bajorath J & Linsley PS. Molecular modeling of immunoglobulin superfamily proteins: predicting the three-dimensional structure of the extracellular domain of CTLA-4 (CD152). J Mol Modeling 3, 117-123, 1997.

64. Bajorath J & Klein TE. Modern concepts in molecular modeling. Pac Symp Biocomput 5, 4-5, 1997.

65. Hollenbaugh D, Bajorath J & Aruffo A. Cell adhesion molecules and their cellular targets, in: Bioorganic Chemistry: Carbohydrates, SM Hecht (Ed.), Oxford University Press, New York, 1997.

66. Bowen MA, Bajorath J & Aruffo A. CD166, in: Leukocyte Typing VI. New Adhesion Structures and CD Antigens, M Miyasaka (Ed.), Garland Publishing, Inc., New York, 129-131, 1997.

67. Bajorath J & Aruffo A. Prediction of the three-dimensional structure of the human Fas receptor by comparative molecular modeling. J Comp-Aided Mol Design 11, 3-8, 1997.

68. Bodian DL, Skonier JE, Bowen MA, Neubauer M, Siadak AW, Aruffo A & Bajorath J. Identification of residues in CD6 which are critical for ligand binding. Biochemistry 36, 2637-2641, 1997.

69. Loo DT, Chalupny NJ, Bajorath J, Shuford WW, Mittler RS & Aruffo A. Analysis of 4-1BBL and laminin binding to murine 4-1BB, a member of the tumor necrosis factor receptor superfamily, and comparison with human 4-1BB. J Biol Chem 272, 6448-6456, 1997.

70. Starling GC, Bajorath J, Ledbetter JA, Aruffo A & Kiener PA. Identification of amino acid residues important for ligand binding to Fas. J Exp Med 185, 1487-1492, 1997.

71. Bowen MA, Bajorath J, D'Egidio M, Whitney GS, Palmer D, Kobarg J, Starling GC, Siadak AW & Aruffo A. Characterization of mouse ALCAM (CD166): The CD6 binding site is conserved in different homologues and mediates cross-species binding. Eur J Immunol 27, 1469-1478, 1997.

72. Bajorath J. A molecular model of CD86 and analysis of mutations which disrupt receptor binding. J Mol Model 3, 216-223, 1997.

73. Metzler WJ, Bajorath J, Fenderson W, Shaw S-Y, Constantine KL, Naemura J, Leytze G, Peach RJ, Lavoie TB, Mueller L & Linsley PS. The solution structure of CTLA-4 identifies a binding site for CD80/CD86 which is conserved in CD28. Nature Struct Biol 4, 527-531, 1997.

74. Bajorath J, Linsley PS & Metzler WJ. Molecular modeling of immunoglobulin superfamily proteins: CTLA-4 (CD152) - Comparison of a predicted and experimentally determined structure. J Mol Model 3, 287-293, 1997.

75. Marinier A, Martel A, Banville J, Bachand C, Remillard R, Lapointe P, Turmel B, Menard M, Harte WE Jr, Wright JJK, Todderud G, Tramposch KM, Bajorath J, Hollenbaugh D & Aruffo A. Sulfated galactocerebrosides as potential anti-inflammatory agents. J Med Chem 40, 3234-3247, 1997.

76. Bajorath J, Metzler WJ & Linsley PS. Molecular modeling of CD28 and three-dimensional analysis of residue conservation in the CD28/CD152 family. J Mol Graph Model 15, 135-139, 1997.

77. Todderud G, Nair X, Lee D, Alford J, Davern L, Stanley P, Bachand C, Lapointe P, Marinier A, Martel A, Menard M, Wright JJK, Bajorath J, Hollenbaugh D, Aruffo A & Tramposch KM. BMS-190394, a selectin inhibitor, prevents rat cutaneous inflammatory reactions. J Pharmacol Exp Ther 282, 1298-1304, 1997.

78. Skonier JE, Bowen MA, Aruffo A & Bajorath J. CD6 recognizes the neural adhesion molecule BEN. Protein Sci 6, 1768-1770, 1997.

79. Aruffo A, Bowen M, Haynes B, Patel D, Starling G, Gebe JA & Bajorath J. Analysis of CD6-ligand interactions: A paradigm for SRCR domain function? Immunology Today 18, 498-504, 1997.

80. Bajorath, J. Antibody engineering. FEBS Lett 412, 646-647, 1997.

81. Skonier JE, Bodian DL, Emswiler J, Bowen MA, Aruffo A & Bajorath J. Mutational analysis of the CD6 ligand binding domain. Protein Eng 10, 943-947, 1997.

82. Rosok MJ, Eghtedarzadeh-Kandri M, Young K, Bajorath J, Glaser S & Yelton DE. Analysis of BR96 binding sites for antigen and anti-idiotype by codon-based scanning mutagenesis. J Immunol 160, 2353-2359, 1998.

83. Bajorath J. Cell surface receptors and adhesion molecules, three-dimensional structures, in: Encyclopedia of Immunology, 2nd Edition, PJ Delves & I Roitt (Eds.), Academic Press, London, 515-520, 1998.

84. Bajorath J, Klein TE & Lybrand TP. Molecular modeling in drug design and biotechnology. Pac Symp Biocomput 6, 303-304, 1998.

85. Bajorath J. Three-dimensional models of cell surface proteins and identification of binding sites. J Mol Model 4, 1-11, 1998.

86. Bajorath J. From tumor necrosis factor receptor to RANK, from selectins and link proteins to CD44: New molecular models of cell surface receptors and analysis of specificity determinants. J Mol Model 4, 239-249, 1998.

87. Bajorath J, Greenfield B, Munro SB, Day AJ & Aruffo A. Identification of CD44 residues important for hyaluronan binding. J Biol Chem 273, 338-343, 1998.

88. Starling GC, Kiener PA, Aruffo A & Bajorath J. Analysis of the ligand binding site in Fas (CD95) by site-specific mutagenesis and comparison with TNFR and CD40. Biochemistry 37, 3723-3726, 1998.

89. Bajorath J. Detailed comparison of two molecular models of the human CD40 ligand with an X-ray structure and assessment of model-based mutagenesis and residue mapping studies. J Biol Chem 273, 24603-24609, 1998.

90. Godden JW, Stahura F & Bajorath J. Evaluation of docking strategies for virtual screening of compound databases: cAMP-dependent Ser/Thr kinase as an example. J Mol Graph Model 16, 139-143, 1998.

91. Bajorath J, Klein TE, Lybrand TP, & Novotny J. Computer-aided drug discovery: From target proteins to drug candidates. Pac Symp Biocomput 7, 413-414, 1999.

92. Gao H, Williams C, Labute P & Bajorath, J. Binary QSAR analysis of estrogen receptor ligands. J Chem Inf Comput Sci 39, 164-168, 1999.

93. Gao H & Bajorath J. Comparison of binary and 2D QSAR analysis using inhibitors of human carbonic anhydrase II as a test case. Mol Divers 4, 115-130, 1999.

94. Cunningham MD, Bajorath J, Somerville JE & Darveau RP. Escherichia coli and Porphyromonas gingivalis interaction with CD14: implications for myeloid and non-myeloid cell activation. Clin Infect Dis 28, 497-504, 1999.

95. Xue L & Bajorath J. Distribution of molecular scaffolds and R-groups isolated from large compound databases. J Mol Model 5, 97-102, 1999.

96. Bajorath J. Analysis of Fas-ligand interactions using a molecular model of the receptor-ligand interface. J Comput-Aided Mol Des 13, 409-418, 1999.

97. Bajorath J. Identification of the ligand binding site in Fas (CD95) and analysis of Fas-ligand interactions. Proteins: Struct, Funct & Genet 35, 475-482, 1999.

98. Xue L, Godden JW, Gao H & Bajorath J. Identification of a preferred set of molecular descriptors for compound classification based on principal component analysis. J Chem Inf Comput Sci 39, 699-704, 1999.

99. Bajorath, J. A molecular model of inducible costimulator protein and three-dimensional analysis of its relation to the CD28 family of T cell-specific costimulatory receptors. J Mol Model 5, 169-176, 1999.

100. Xue L, Godden JW & Bajorath J. Database searching for compounds with similar biological activity using short binary bit string representations of molecules. J Chem Inf Comput Sci 39, 881-886, 1999.

101. Godden JW, Stahura F & Bajorath J. Statistical analysis of computational docking of large compound databases to distinct protein binding sites. J Comp Chem 20, 1634-1643, 1999.

102. Bajorath J. Three-dimensional analysis of CD6 mutagenesis and monoclonal antibody binding studies using the X-ray structure of the Mac-2 binding protein and a molecular model of the CD6 ligand binding domain. J Mol Model 5, 263-270, 1999.

103. Stahura FL, Xue L, Godden JW & Bajorath J. Molecular scaffold-based design and comparison of combinatorial libraries focused on the ATP binding site of protein kinases. J Mol Graph Model 17, 1-9, 1999.

104. Bajorath J. Specificity of the tumor necrosis factor receptor superfamily. J Mol Graph Model 17, 220-222, 1999.

105. Godden JW, Xue L, Stahura FL & Bajorath J. Searching for molecules with similar biological activity: analysis by fingerprint profiling. Pac Symp Biocomput 8, 566-575, 2000.

106. Bajorath J. Structure and function of CD44: characteristic molecular features and analysis of the hyaluronan binding site, in: Results and Problems in Cell Differentiation, Vol. 33. Mammalian Carbohydrate Recognition Systems. PR Crocker (Ed.), Springer-Verlag, Heidelberg New York, pp. 85-103, 2000.

107. Godden JW, Xue L & Bajorath J. Combinatorial preferences affect molecular similarity/diversity calculations using binary fingerprints and Tanimoto coefficients. J Chem Inf Comput Sci 40, 163-166, 2000.

108. Bajorath J. Combinatorial libraries and chemoinformatics in drug discovery. Investigational Drugs WH 5, 50-51, 2000.

109. Bajorath J. Molecular organization, structural features, and ligand binding characteristics of CD44, a highly variable cell surface glycoprotein with multiple functions. Proteins: Struct, Funct & Genet 39, 103-111, 2000.

110. Godden JW, Stahura, FL & Bajorath J. Variability of molecular descriptors in compound databases revealed by Shannon entropy calculations. J Chem Inf Comput Sci 40, 796-800, 2000.

111. Xue L & Bajorath J. Molecular descriptors for effective classification of biologically active compounds based on principal component analysis identified by a genetic algorithm. J Chem Inf Comput Sci 40, 801-809, 2000.

112. Godden JW & Bajorath J. Shannon entropy – A novel concept in molecular descriptor and diversity analysis. J Mol Graph Model 18, 73-76, 2000.

113. Bowen MA, Aruffo A & Bajorath J. Cell surface receptors and their ligands: in vitro analysis of CD6-CD166 interactions. Proteins: Struct, Funct & Genet 40, 420-428, 2000.

114. Xue L & Bajorath J. Molecular descriptors in chemoinformatics, computational combinatorial chemistry, and virtual screening, submitted. Combin Chem High Throuput Screen 3, 363-372, 2000.

115. Stahura FL, Xue L, Godden JW & Bajorath J. Design of array-type libraries that combine information from natural products and synthetic molecules. J Mol Model 6, 550-562, 2000.

116. Xue L, Godden JW & Bajorath J. Evaluation of descriptors and mini-fingerprints for the identification of molecules with similar activity. J Chem Inf Comput Sci 40, 1227-1234, 2000.

117. Bajorath J. Understanding the structural basis of T cell costimulation. J Mol Graph Model 18, 176-179, 2000.

118. Stahura FL, Godden JW, Xue L & Bajorath J. Distinguishing between natural products and synthetic molecules by Shannon descriptor entropy analysis and binary QSAR calculations. J Chem Inf Comput Sci 40, 1245-1252, 2000.

119. Xue L, Godden JW, Stahura FL & Bajorath J. A dual fingerprint-based approach for the design of focused combinatorial libraries and analogs. J Mol Model 7, 125-131, 2001.

120. Xue L, Stahura FL, Godden JW & Bajorath J. Fingerprint scaling increases the probability of identifying molecules with similar activity in systematic virtual screening calculations. J Chem Inf Comput Sci 41, 746-753, 2001.

121. Godden JW & Bajorath J. Differential Shannon entropy as a sensitive measure of differences in the variability of molecular descriptors. J Chem Inf Comput Sci 41, 1060-1066, 2001.

122. Bajorath J. Structural biology of T cell costimulatory molecules: new insights, more surprises. J Mol Graph Model 19, 619-623, 2001.

123. Bajorath J. Rational drug discovery revisited: interfacing experimental programs with bio- and chemoinformatics. Drug Discov Today 6, 989-995, 2001.

124. Bajorath J. Selected concepts and investigations in compound classification, molecular descriptor analysis, and virtual screening. J Chem Inf Comput Sci 41, 233-245, 2001.

125. Godden JW & Bajorath J. Chemical descriptors with distinct levels of information content and varying sensitivity to differences between selected compound databases identified by SE-DSE analysis. J Chem Inf Comput Sci 42, 87-93, 2002.

126. Bajorath J. Chemoinformatics methods for systematic comparison of molecules from natural and synthetic sources and design of hybrid libraries. Mol Divers 5, 305-313, 2002.

127. Bajorath J. Virtual screening: methods, expectations, and reality. Curr Drug Discov 2 (3), 24-28, 2002.

128. Wang S, Zhu G, Tamada K, Chen L & Bajorath J. Ligand binding sites of inducible costimulator and high avidity mutants with improved function. J Exp Med 195, 1033-1041, 2002.

129. Godden JW & Bajorath J. Computational molecular dynamics: challenges, methods, ideas - book review. Theor Chem Acc 107, 250-251, 2002.

130. Stahura FL, Godden JW & Bajorath J. Differential Shannon entropy analysis identifies molecular descriptors that predict aqueous solubility of synthetic compounds with high accuracy in binary QSAR calculations, J Chem Inf Comput Sci 42, 550-558, 2002.

131. Xue L & Bajorath J. Accurate partitioning of compounds in diverse activity classes. J Chem Inf Comput Sci 42, 757-764, 2002.

132. Stahura FL, Xue L, Godden JW & Bajorath J. Methods for compound selection focused on hits and application in drug discovery. J Mol Graph Model 20, 439-446, 2002.

133. Stahura FL & Bajorath J. Bio- and chemoinformatics beyond data management: Critical challenges and opportunities ahead. Drug Discov Today (Information Biotechnol Suppl), S41-S47, 2002.

134. Godden JW, Xue L, Kitchen DB, Stahura FL, Schermerhorn EJ & Bajorath J. Median partitioning: A novel method for the selection of representative subsets from large compound pools. J Chem Inf Comput Sci 42, 885-893, 2002.

135. Bajorath J. Identification and validation of therapeutic target proteins. Targets 1, 45-46, 2002.

136. Bajorath J. Predicting proteins and their interactions. Drug Discov Today, 7, 945-946, 2002.

137. Godden JW, Xue L, Bajorath J. Classification of biologically active compounds by median partitioning. J Chem Inf Comput Sci 42, 1263-1269, 2002.

138. Bajorath J. Integration of virtual and high-throughput screening. Nature Rev Drug Discov 1, 882-894, 2002.

139. Bajorath J. Affinity fingerprints – leading the way? Drug Discov Today 7, 1035-1035, 2002.

140. Bajorath J. Chemoinformatics methods for systematic comparison of molecules from natural and synthetic sources and design of hybrid libraries. J Comput-Aided Mol Design 16, 5/6, 431-439, 2002.

141. Godden J, Furr JR & Bajorath J. Recursive median partitioning for virtual screening of large databases. J Chem Inf Comput Sci 43, 182-188, 2003.

142. Xue L, Godden JW & Bajorath J. Mini-fingerprints: design principles and generation of novel prototypes based on information theory. SAR QSAR Env Res 14, 27-40, 2003.

143. Wang S, Bajorath J, Flies DB, Dong H, Honjo T & Chen L. Molecular modeling and functional mapping of PD-1 ligands uncouple costimulatory function from PD-1 interaction. J Exp Med 197, 1083-1091, 2003.

144. Stahura FL & Bajorath J. Partitioning methods for the identification of active molecules. Curr Med Chem 8, 707-715, 2003.

145. Bajorath J. Structure prediction and binding site identification of members of the CD28 and B7 families of costimulatory immune cell surface proteins, in: The B7 Family and the Immune Response, L Chen (Ed.), Landes Bioscience, Georgetown, Texas, USA, 2003.

146. Godden JW & Bajorath J. An information-theoretic approach to descriptor selection for database profiling and QSAR modeling. QSAR Comb Sci 22, 487-497, 2003.

147. Xue L, Godden JW, Stahura FL & Bajorath J. Design and evaluation of a molecular fingerprint involving the transformation of property descriptor values into a binary classification scheme. J Chem Inf Comput Sci 43, 1151-1157, 2003.

148. Xue L, Godden JW, Stahura FL & Bajorath J. Profile scaling increases the similarity search performance of molecular fingerprints containing numerical descriptors and structural keys. J Chem Inf Comput Sci 43, 1218-1225, 2003.

149. Sica GL, Choi I-H, Zhu G, Tamada K, Wang, S-D, Tamura H, Chapoval AI, Flies DB, Bajorath J & Chen L. B7-H4, a new molecule of the B7 family, negatively regulates T cell immunity. Immunity 18, 849-861, 2003.

150. Bajorath J. Understanding chemoinformatics: a unifying approach. Drug Discov Today 9, 13-14, 2004.

151. Godden JW, Furr JR, Xue L, FL Stahura & Bajorath J. Molecular similarity analysis and virtual screening in binary-transformed chemical descriptor spaces with variable dimensionality. J Chem Inf Comput Sci 44, 21-29, 2004.

152. Xue L, Stahura FL & Bajorath J. Cell-based partitioning algorithms. Methods Mol Biol 275, 279-289, 2004.

153. Godden JW & Bajorath J. Partitioning in binary-transformed descriptor spaces. Methods Mol Biol 275, 291-300, 2004.

154. Kitchen DB, Stahura FL & Bajorath J. Computational techniques in diversity analysis and compound classification. Rev Med Chem 4, 1029-1039, 2004.

155. Bajorath J. Chemoinformatics and its role in pharmaceutical research. Pharmatech 2004, 76-82, 2004.

156. Stahura FL & Bajorath J. Virtual screening methods that complement HTS. Combin Chem High Throughput Screen 7, 259-269, 2004.

157. Xue L, Godden JW, Stahura FL & Bajorath J. Similarity search profiles as a diagnostic tool for the analysis of virtual screening calculations. J Chem Inf Comput Sci 1275-1281, 2004.

158. Shoda M, Harada T, Kogami Y, Tsujita R, Akashi H, Kouji H, Stahura FL, Xue L & Bajorath J. Identification of structurally diverse growth hormone secretagogue agonists by virtual screening and structure-activity relationship analysis of 2-formylamino-acetamide derivatives. J Med Chem 47, 4286-4290, 2004.

159. Kitchen DB, Decornez H, Furr JR, Bajorath J. Structure-based virtual screening and lead optimization: methods and applications. Nature Rev Drug Discov 3, 935-949, 2004.

160. Xue L, Stahura FL, Bajorath J. Similarity search profiling reveals effects of fingerprint scaling in virtual screening. J Chem Inf Comput Sci 44, 2032-2039, 2004.

161. Godden JW, Stahura FL & Bajorath J. POT-DMC – a virtual screening method for the identification of potent hits. J Med Chem 47, 5068-5611, 2004.

162. Xue L, Stahura FL & Bajorath J. Chemoinformatics: perspectives and challenges, in: Chemometrics and Chemoinformatics, BK Lavine (Ed.), ACS Symposiums Series No. 894, Oxford University Press, New York, USA, 41-53, 2005.

163. Larsen CP, Pearson TC, Adams AB, Tso P, Shirasugi N, Strobertm E, Anderson D, Cowan S, Price K, Naemura J, Emswiler J, Greene J, Turk LA, Bajorath J, Townsend R, Hagerty D, Linsley PS & Peach RJ. Rational development of LEA29Y (belatacept), a high-affinity variant of CTLA4-Ig with potent immunosuppressive properties. Am J Transplant 5, 443-453, 2005.

164. Stahura FL & Bajorath J. Novel methodologies for virtual screening. Curr Pharm Design 11, 1189-1202, 2005.

165. Bajorath J. Molecular similarity methods and QSAR models as virtual screening tools, in; Drug Discovery Handbook, Vol. 1, SC Gad (Ed.), John Wiley & Sons, Inc., Hoboken, New Jersey, USA, 87-122, 2005.

166. Bajorath J. Theoretical approaches in medicinal chemistry and drug discovery. Curr Top Med Chem 5, 737-738, 2005.

167. Bajorath J. Potency-scaled partitioning in descriptor spaces with increasing dimensionality. Curr Top Med Chem 5, 797-803, 2005.

168. Haffar O, Dubrovsky L, Lowe R, Berro R, Kashanchi F, Godden J, Vanpouille C, Bajorath J & Bukrinsky M. Oxadiazols: a new class of rationally designed anti-human immunodeficiency virus compounds targeting the nuclear localization signal of the viral matrix protein. J Virol 79, 13028-13036, 2005.

169. Godden JW, Stahura FL & Bajorath J. Anatomy of fingerprint search calculations on structurally diverse sets of active compounds. J Chem Inf Model 45, 1812-1819, 2005.

170. Lang TP, Kuntz ID, Maggiora GM & Bajorath J. Evaluating high-throughput screening computations. J Biomol Screen 10, 649-652, 2005.

171. Eckert H & Bajorath J. Determination and mapping of activity-specific descriptor value ranges for the identification of active compounds. J Med Chem 49, 2284-2293, 2006.

172. Godden JW & Bajorath J. A distance function for retrieval of active molecules from complex chemical space representations. J Chem Inf Model 46, 1094-1097, 2006.

173. Stahura FL & Bajorath J. Computational analysis of natural molecules and strategies for the design of natural product-based libraries, in: Combinatorial synthesis of natural product-based libraries, A Boldi (Ed.), Critical Reviews in Combinatorial Chemistry No. 2, Taylor & Francis, New York, USA, 53-64, 2006.

174. Eckert H, Vogt I & Bajorath J. Mapping algorithms for molecular similarity analysis and ligand-based virtual screening: design of DynaMAD and comparison with MAD and DMC, J Chem Inf Model 46, 1623-1634, 2006.

175. Parker CN, Shamu CE, Kraybill B, Austin CP, Bajorath J. Measure, mine, model, manipulate – the future for HTS and chemoinformatics? Drug Discov Today 11, 863-865, 2006.

176. Batista J, Godden JW & Bajorath J. Assessment of molecular similarity from the analysis of randomly generated structural fragment populations. J Chem Inf Model 46, 1937-1944, 2006.

177. Auer J & Bajorath J. Emerging chemical patterns: a new methodology for molecular classification and compound selection. J Chem Inf Model 46, 2502-2514, 2006.

178. Eckert H. & Bajorath J. Design and evaluation of a novel class-directed 2D fingerprint to search for structurally diverse compounds. J Chem Inf Model 46, 2515-2526, 2006.

179. Parker CN & Bajorath J. Towards unified compound screening strategies: a critical evaluation of error sources in experimental and virtual high-throughput screening. QSAR Comb Sci 25, 1153-1161, 2006.

180. Godden JW & Bajorath J. Analysis of chemical information content using Shannon entropy. Rev Comput Chem 23, 263-289, 2007.

181. Vogt M, Godden JW & Bajorath J. Bayesian interpretation of a distance function for navigating high-dimensional descriptor spaces. J Chem Inf Model 47, 39-46, 2007.

182. Tovar A, Eckert H & Bajorath J. Comparison of 2D fingerprint methods for multiple-template similarity searching on compound classes on increasing structural diversity. ChemMedChem 2, 208-217, 2007.

183. Batista J & Bajorath J. Chemical database mining through entropy-based molecular similarity assessment of randomly generated structural fragment populations. J Chem Inf Model 47, 59-68, 2007.

184. Eckert H & Bajorath J. Molecular similarity analysis in virtual screening: foundations, limitations, and novel approaches. Drug Discov Today 12, 225-233, 2007.

185. Vogt I & Bajorath J. Analysis of a high-throughput screening data set using potency-scaled molecular similarity algorithms. J Chem Inf Model 47, 367-375, 2007.

186. Vogt M & Bajorath J. Introduction of an information-theoretic method to predict recovery rates of active compounds for Bayesian in silico screening, J Chem Inf Model 47, 337-341, 2007.

187. Shoda M, Harada T, Stahura FL, Himeno T, Shioziri, S, Kogami Y, Kouji H & Bajorath J. Virtual screening leads to the discovery of an effective antagonist of lymphocyte function-associated antigen-1. ChemMedChem 2, 515-521, 2007.

188. Wang Y, Godden JW, Bajorath J. A novel histogram filtering method for database mining and the identification of active molecules. Lett Drug Design Discov 4, 286-292, 2007.

189. Peltason L & Bajorath J. Molecular similarity analysis uncovers heterogeneous structure-activity relationships and variable activity landscapes within active sites. Chem Biol 14, 489-497, 2007.

190. Wang Y, Eckert H & Bajorath J. Apparent asymmetric behavior of similarity search calculations is due to the molecular size dependence of conventional fingerprint representations. ChemMedChem 2, 1037-1042, 2007.

191. Yamazaki S, Tan L, Hartig JS, Mayer G, Song J-N, Reuter S, Restle T, Laufer S. D., Grohmann D, Kräusslich H-G, Bajorath J & Famulok M. Aptamer displacement identifies alternative small-molecule target sites that escape viral resistance. Chem Biol 14, 489-497, 2007.

192. Eckert H & Bajorath J. Exploring peptide-likeness of active molecules using 2D fingerprint methods. J Chem Inf Model 47, 1366-1378, 2007.

193. Batista J & Bajorath J. Mining of randomly generated molecular fragment populations uncovers activity-specific fragment hierarchies. J Chem Inf Model 47, 1405-1413, 2007.

194. Stumpfe D, Ahmed H, Vogt I & Bajorath J. Methods for computer-aided chemical biology, part 1: design of a benchmark system for the evaluation of compound selectivity. Chem Biol Drug Design 70, 182-194, 2007.

195. Vogt I, Stumpfe D, Ahmed H & Bajorath J. Methods for computer-aided chemical biology, part 2: evaluation of compound selectivity using 2D fingerprints. Chem Biol Drug Design 70, 195-205, 2007.

196. Vogt M & Bajorath J. Introduction of a generally applicable method to estimate retrieval of active molecules for similarity searching using fingerprints. ChemMedChem 2, 1311-1320, 2007.

197. Lounkine E, Batista J & Bajorath J. Mapping of activity-specific fragment pathways isolated from random fragment populations reveals the formation of coherent molecular cores. J Chem Inf Model 47, 2133-2139, 2007.

198. Peltason L & Bajorath J. SAR index: quantifying the nature of structure-activity relationships. J Med Chem 50, 5571-5578, 2007.

199. Auer J & Bajorath J. Simulation of sequential screening experiments using emerging chemical patterns. Med Chem 4, 80-90, 2008.

200. Vogt M & Bajorath J. Bayesian screening for active compounds in high-dimensional chemical spaces combining property descriptors and fingerprints. Chem Biol Drug Design 71, 8-14, 2008.

201. Batista J & Bajorath J. Similarity searching using compound class-specific combinations of substructures found in randomly generated molecular fragment populations. ChemMedChem 3, 67-73, 2008.

202. Wang Y & Bajorath J. Balancing complexity effects in fingerprint similarity searching. J Chem Inf Model 48, 75-84, 2008.

203. Vogt M & Bajorath J. Bayesian similarity searching in high-dimensional descriptor spaces combined with Kullback-Leibler descriptor divergence analysis. J Chem Inf Model 48, 247-255, 2008.

204. Bajorath J. Functional informatics in drug discovery. ChemMedChem 3, 502-503, 2008.

205. Bajorath J. Computational chemistry publications in the journal of medicinal chemistry. J. Med. Chem 51, 2327-2327, 2008.

206. Geppert H, Horvath T, Gärtner T, Wrobel S & Bajorath J. Support vector machine-based ranking significantly improves the effectiveness of similarity searching using 2D fingerprints and multiple reference compounds. J Chem Inf Model 48, 742-746, 2008.

207. Peltason, L & Bajorath J. Molecular similarity analysis in virtual screening, in: Chemoinformatics: An Approach to Virtual Screening, A Varnek & A Tropsha (Eds.), RSC Publishing, Cambridge, 120-149, 2008.

208. Wang Y, Geppert H & Bajorath J. Random reduction in fingerprint bit density improves compound recall in search calculations using complex reference molecules. Chem Biol Drug Design 71, 511-517, 2008.

209. Stumpfe D, Geppert H & Bajorath J. Methods for computer-aided chemical biology, part 3: analysis of structure-selectivity relationships through single- or dual-step selectivity searching and Bayesian classification. Chem Biol Drug Des 71, 518-528, 2008.

210. Auer J & Bajorath J. Molecular similarity concepts and search calculations. Methods Mol Biol 453, 327-347, 2008.

211. Eckert H & Bajorath J. Optimization of the MAD algorithm for virtual screening. Methods Mol Biol 453, 349-362, 2008.

212. Bajorath J. Computational analysis of ligand relationships within target families. Curr Opin Chem Biol 12, 352-358, 2008.

213. Lounkine E & Bajorath J. Core trees and fragment sequence alignments for molecular representation and similarity analysis. J Chem Inf Model 48, 1161-1166, 2008.

214. Vogt I, Ahmed H, Auer J & Bajorath J. Exploring structure-selectivity relationships of biogenic amine GPCR antagonists using similarity searching and dynamic compound mapping. Mol Divers 12, 25-40, 2008.

215. Batista J & Bajorath J. Distribution of randomly generated activity class characteristic substructures in diverse active and database compounds. Mol Divers 12, 77-83, 2008.

216. Vogt I & Bajorath J. Design and exploration of target-selective chemical space representations. J Chem Inf Model 48, 1389-1395, 2008.

217. Lounkine E, Batista J & Bajorath J. Random molecular fragment methods in computational medicinal chemistry. Curr Med Chem 15, 2108-2121, 2008.

218. Auer J & Bajorath J. Distinguishing between bioactive and modeled compound conformations through mining of emerging chemical patterns. J Chem Inf Model 48, 1747-1753, 2008.

219. Wang Y & Bajorath J. Bit silencing in keyed fingerprints enables the derivation of compound class-directed similarity metrics. J Chem Inf Model 48, 1754-1749, 2008.

220. Lounkine E, Auer J & Bajorath J. Formal concept analysis for the identification of molecular fragment combinations specific for active and highly potent compounds. J Med Chem 51, 5342-5348, 2008.

221. Tan L, Geppert H, Sisay MT, Gütschow M & Bajorath J. Integrating structure-and ligand-based virtual screening: comparison of individual, parallel, and fused molecular docking and similarity search calculations on multiple targets. ChemMedChem 3, 1566-1571, 2008.

222. Wawer M, Peltason L, Weskamp N, Teckentrup A & Bajorath J. Structure-activity relationship anatomy by network-like similarity graphs and local structure-activity relationship indices. J Med Chem 51, 6075-6084, 2008.

223. Hu Y, Lounkine E, Batista J & Bajorath J. RelACCS-FP: a structural minimalist approach to fingerprint design. Chem Biol Drug Des 72, 341-349, 2008.

224. Crisman TJ, Sisay MT & Bajorath J. Ligand-target interaction-based weighting of substructures for virtual screening. J Chem Inf Model 48, 1955-1964, 2008.

225. Tan L, Lounkine E & Bajorath J. Similarity searching using fingerprints of molecular fragments involved in protein-ligand interactions. J Chem Inf Model 48, 2308-2312, 2008.

226. Bajorath J. Computational approaches in chemogenomics and chemical biology: current and future impact on drug discovery. Expert Opin Drug Discov 3, 1371-1376, 2008.

227. Bajorath J. Pharmacophore, in: Encyclopedia of Cancer, 2nd Edition, M Schwab (Ed.), Springer-Verlag, Heidelberg, 2310-2312, 2009.

228. Bajorath J. Quantitative structure activity relationship, in: Encyclopedia of Cancer, 2nd Edition, M Schwab (Ed.), Springer-Verlag, Heidelberg, 2506-2509, 2009.

229. Nisius B, Göller AH & Bajorath J. Combining cluster analysis, feature selection, and multiple support vector machine models for the identification of hERG channel blocking compounds. Chem Biol Drug Des 73, 17-25, 2009.

230. Stumpfe D, Frizler M, Sisay MT, Batista J, Vogt I, Gütschow M & Bajorath J. Hit expansion through selectivity searching. ChemMedChem 4, 52-54, 2009.

231. Bajorath J. Ligand-based methods for virtual screening. Frontiers Med Chem 4, 1-22, 2009.

232. Ahmed HEA, Geppert H, Stumpfe D, Lounkine E & Bajorath J. Methods for computer-aided chemical biology, part 4: selectivity searching for ion channel ligands and mapping of molecular fragments as selectivity markers. Chem Biol Drug Des 73, 273-282, 2009.

233. Lounkine E & Bajorath J. Topological fragment index for the analysis of molecular substructures and their topological environment in active compounds. J Chem Inf Model 49, 162-168, 2009.

234. Wawer M, Peltason L & Bajorath J. Elucidation of structure-activity relationship pathways in biological screening data. J Med Chem 52, 1075-1080, 2009.

235. Lounkine E, Hu Y, Batista J & Bajorath J. Relevance of feature combinations for similarity searching using general or activity class-directed molecular fingerprints. J Chem Inf Model 49, 561-570, 2009.

236. Wassermann A, Geppert H & Bajorath J. Searching for target-selective compounds using different combinations of multi-class support vector machine ranking methods, kernel functions, and fingerprint descriptors. J Chem Inf Model 49, 582-592, 2009.

237. Geppert H, Humrich J, Stumpfe D, Gärtner T & Bajorath J. Ligand prediction from protein sequence and small molecule information using support vector machines and fingerprint descriptors. J Chem Inf Model 49, 767-779, 2009.

238. Hu Y, Lounkine E & Bajorath J. Improving the performance of extended connectivity fingerprints through activity-oriented feature filtering and application of a bit density-dependent similarity function. ChemMedChem 4, 540-548, 2009.

239. Peltason L, Weskamp N, Teckentrup A & Bajorath J. Exploration of structure-activity relationship determinants in analogue series. J Med Chem 52, 3212-3224, 2009.

240. Tan L & Bajorath J. Utilizing target-ligand interaction information in fingerprint searching for ligands of related targets. Chem Biol Drug Des 74, 25-32, 2009.

241. Hu Y, Lounkine E & Bajorath J. Filtering and counting of extended connectivity fingerprint features maximizes compound recall and the structural diversity of hits. Chem Biol Drug Des 74, 92-98, 2009.

242. Nisius B, Vogt M & Bajorath J. Development of a fingerprint reduction approach for Bayesian similarity searching based on Kullback-Leibler divergence analysis. J Chem Inf Model 49, 1347-1358, 2009.

243. Lounkine E, Stumpfe D & Bajorath J. Molecular formal concept analysis for compound selectivity profiling in biologically annotated databases. J Chem Inf Model 49, 1359-1368, 2009.

244. Wang Y & Bajorath J. Development of a compound class-directed similarity coefficient that accounts for molecular complexity effects in fingerprint searching. J Chem Inf Model 49, 1369-1376, 2009.

245. Peltason L & Bajorath J. Systematic computational analysis of structure-activity relationships: concepts, challenges, and recent advances. Future Med Chem 1, 451-466, 2009.

246. Bajorath J, Peltason L, Wawer M, Guha R, Lajiness MS & van Drie J. Navigating structure-activity landscapes. Drug Discov Today 14, 698-705, 2009.

247. Krüger F, Lounkine E & Bajorath J. Fragment formal concept analysis accurately classifies compounds with closely related biological activities. ChemMedChem 4, 1174-1181, 2009.

248. Vogt M, Nisius B & Bajorath J. Predicting the similarity search performance of fingerprints and their combination with molecular property descriptors using probabilistic and information-theoretic modeling. Stat Anal Data Mining 2, 123-134, 2009.

249. Ahmed HEA & Bajorath J. Methods for computer-aided chemical biology, part 5: rationalizing the selectivity of cathepsin inhibitors on the basis of molecular fragments and topological feature distributions. Chem Biol Drug Des 74, 129-141, 2009.

250. Wang Y, Geppert H & Bajorath J. A Shannon entropy-based fingerprint similarity search strategy. J Chem Inf Model, 49, 1687-1691, 2009.

251. Sisay MT, Hautmann S, Mehner C, König GM, Bajorath J & Gütschow M. Brunsvicamides A-C: selective inhibitors of human leukocyte elastase. ChemMedChem 4, 1425-1429, 2009.

252. Wawer M & Bajorath J. Systematic extraction of structure-activity relationship information from biological screening data. ChemMedChem, 4, 1431-1438, 2009.

253. Wawer M & Bajorath J. Extraction of structure-activity relationship information from high-throughput screening data. Curr Med Chem 16, 4049-4057, 2009.

254. Tan L, Vogt M & Bajorath J. Three-dimensional protein-ligand interaction scaling of two-dimensional fingerprints. Chem Biol Drug Des 74, 449-456, 2009.

255. Nisius B & Bajorath J. Fingerprint recombination – generating hybrid fingerprints for similarity searching from different fingerprint types. ChemMedChem 4, 1859-1863, 2009.

256. Peltason L, Hu Y & Bajorath J. From structure-activity to structure-selectivity relationships: quantitative assessment, selectivity cliffs, and key compounds. ChemMedChem 4, 1864-1873, 2009.

257. Wassermann A, Geppert H & Bajorath J. Ligand prediction for orphan targets using support vector machines and various target-ligand kernels is dominated by nearest neighbor effects. J Chem Inf Model 49, 2155-2167, 2009.

258. Sisay MT, Peltason L & Bajorath J. Structural interpretation of activity cliffs revealed by systematic analysis of structure-activity relationships in analog series. J Chem Inf Model 49, 2179-2189, 2009.

259. Vogt M & Bajorath J. Data mining approaches for compound selection and iterative screening, in: Pharmaceutical Data Mining: Approaches and Applications for Drug Discovery, K. V. Balakin (Ed.), John Wiley & Sons, Hoboken, NJ, 115-143, 2009.

260. Nisius B & Bajorath J. Reduction and recombination of fingerprints of different design increase compound recall and the structural diversity of hits. Chem Biol Drug Design 75, 152-160, 2010.

261. Bajorath J. Computational studies, virtual screening, and theoretical molecular models. J Med Chem 53, 1-2, 2010.

262. Stumpfe D, Sisay MT, Frizler M,Vogt I, Gütschow M & Bajorath J. Inhibitors of cathepsin K and S identified using the DynaMAD virtual screening algorithm. ChemMedChem 5, 61-64, 2010.

263. Hu Y, Wassermann AM, Lounkine E & Bajorath J. Systematic analysis of public domain compound potency data identifies selective molecular scaffolds across druggable target families. J Med Chem 53, 752-758, 2010.

264. Lounkine E, Wawer M, Wassermann AM & Bajorath J. SARANEA – a freely available program to mine structure-activity and structure-selectivity relationship information in compound data sets. J Chem Inf Model 50, 68-78, 2010.

265. Hu Y & Bajorath J. Scaffold distributions in bioactive molecules, clinical trials compounds, and drugs. ChemMedChem 5, 187-190, 2010.

266. Batista J, Tan L & Bajorath J. Atom-centered interacting fragments and similarity search applications. J Chem Inf Model 50, 79-86, 2010.

267. Stumpfe D, Geppert H & Bajorath J. In silico screening, in: Lead Generation Approaches in Discovery, R. Morphy, Z. Rankovic (Eds.), John Wiley & Sons, Hoboken, NJ, 73-103, 2010.

268. Geppert H, Vogt M & Bajorath J. Current trends in ligand-based virtual screening: molecular representations, data mining methods, new application areas, and performance evaluation. J Chem Inf Model 50, 205-216, 2010.

269. Baqi Y, Lee S-Y, Iqbal J, Ripphausen P, Lehr A, Zimmermann H, Bajorath J & Müller CE. Development of potent and selective inhibitors of ecto-5'-nucleotidase based on an anthraquinone scaffold. J Med Chem 53, 2076-2086, 2010.

270. Wang Y & Bajorath J. Advanced fingerprint methods for similarity searching: balancing molecular complexity effects. Combin Chem High Throughput Screen 13, 220-228, 2010.

271. Behnke CA, Le Trong I, Godden JW, Merritt EA, Teller DC, Bajorath J & Stenkamp RA. Atomic resolution studies of carbonic anhydrase II. Acta Cryst D66, 616-627, 2010.

272. Wawer M, Sun S & Bajorath J. Computational characterization of SAR microenvironments in high-throughput screening data. Intl J High Throughput Screen 1, 15-27, 2010.

273. Batista J, Friedrichson T, Schlechtingen G, Braxmeier T, Jennings G & Bajorath J. Computational screening for membrane-directed inhibitors of mast cell activation. Eur J Med Chem 45, 2700-2704, 2010.

274. Ahmed HEA, Vogt M & Bajorath J. Design and evaluation of bonded atom pair descriptors. J Chem Inf Model 50, 487-499, 2010.

275. Hu Y & Bajorath J. Molecular scaffolds with high propensity to form multi-target activity cliffs. J Chem Inf Model 50, 500-510, 2010.

276. Wassermann AM, Vogt M & Bajorath J. Iterative Shannon entropy - a methodology to quantify the information content of value range dependent data distributions. Application to descriptor and compound selectivity profiling. Mol Inf 29, 432-440, 2010.

277. Hu Y & Bajorath J. Exploring target-selectivity patterns of molecular scaffolds. ACS Med Chem Lett 1, 54-58, 2010.

278. Geppert H & Bajorath J. Advances in 2D fingerprint similarity searching. Expert Opin Drug Discov 5, 529-542, 2010.

279. Wassermann AM, Peltason L & Bajorath J. Computational analysis of multi-target structure-activity relationships to derive preference orders for chemical modifications towards target selectivity. ChemMedChem 5, 847-858, 2010.

280. Nisius B & Bajorath J. Rendering conventional molecular fingerprints for virtual screening independent of molecular complexity and size effects. ChemMedChem 5, 859-868, 2010.

281. Peltason L, Iyer P & Bajorath J. Rationalizing three-dimensional activity landscapes and the influence of molecular representations on landscape topology and formation of activity cliffs. J Chem Inf Model 50, 1021-1033, 2010.

282. Tan L, Batista J & Bajorath J. Rationalization of the performance and target dependence of similarity searching incorporating protein-ligand interaction information. J Chem Inf Model 50, 1042-1052, 2010.

283. Wassermann AM & Bajorath J. Chemical substitutions that introduce activity cliffs across different compound classes and biological targets. J Chem Inf Model 50, 1248-1256, 2010.

284. Tan L, Batista J & Bajorath J. Computational methodologies for compound database searching that utilize experimental protein-ligand interaction information. Chem Biol Drug Des 76, 191-200, 2010.

285. Sisay MT, Steinmetzer T, Stirnberg M, Maurer E, Hammami M, Bajorath J & Gütschow M. Identification of the first low molecular weight inhibitors of matriptase-2. J Med Chem 53, 5523-5535, 2010.

286. Wawer M, Lounkine E, Wassermann AM & Bajorath J. Data structures and computational tools for the extraction of SAR information from large compound sets. Drug Discov Today 15, 630-639, 2010.

287. Vogt M, Stumpfe D, Geppert H & Bajorath J. Scaffold hopping using two-dimensional fingerprints: true potential, black magic, or a hopeless endeavor? Guidelines for virtual screening. J Med Chem 53, 5707-5715, 2010.

288. Wawer M & Bajorath J. Similarity-potency trees: a method to search for SAR information in compound data sets and derive SAR rules. J Chem Inf Model 50, 1395-1409, 2010.

289. Stumpfe D, Bill A, Novak N, Loch G, Blockus H, Geppert H, Becker T, Hoch M, Schmitz A, Kolanus W, Famulok M & Bajorath J. Targeting multi-functional proteins by virtual screening: structurally diverse cytohesin inhibitors with differentiated biological functions. ACS Chem Biol 5, 839-849, 2010.

290. Hu Y & Bajorath J. Structural and potency relationships between scaffolds of compounds active against human targets. ChemMedChem 5, 1681-1685, 2010.

291. Vogt M, Wassermann AM & Bajorath J. Application of information-theoretic concepts in chemoinformatics. Information 1, 60-73, 2010.

292. Vogt M & Bajorath J. Virtual screening methods based on Bayesian statistics, in: Chemoinformatics and Advanced Machine Learning Perspectives, H. Lodhi, Y. Yamanishi (Eds.), IGI Global, Hershey, PA, 190-211, 2010.

293. Hu Y & Bajorath J. Global assessment of scaffold hopping potential for current pharmaceutical targets. Med Chem Commun 1, 339-344, 2010.

294. Wassermann AM, Nisius B, Vogt M & Bajorath J. Identification of descriptors capturing compound class-specific features by mutual information analysis. J Chem Inf Model 50, 1935-1940, 2010.

295. Wassermann AM, Wawer M & Bajorath J. Activity landscape representations for structure-activity relationship analysis. J Med Chem 53, 8209-8223, 2010.

296. Ripphausen P, Nisius B, Peltason L & Bajorath J. Quo vadis, virtual screening? A comprehensive survey of prospective applications. J Med Chem 53, 8461-8467, 2010.

297. Hu Y & Bajorath J. Polypharmacology-directed compound data mining: identification of promiscuous chemotypes with different activity profiles and comparison to approved drugs. J Chem Inf Model 50, 2112-2118, 2010.

298. Peltason L & Bajorath J. Computational analysis of activity and selectivity cliffs. Methods Mol Biol 672, 119-132, 2011.

299. Vogt M & Bajorath J. Predicting the performance of fingerprint similarity searching. Methods Mol Biol 672, 159-174, 2011.

300. Stumpfe D, Lounkine E & Bajorath J. Molecular test systems for computational selectivity studies and systematic analysis of compound selectivity profiles. Methods Mol Biol 672, 503-516, 2011.

301. Wassermann AM, Geppert H & Bajorath J. Application of support vector machine-based ranking strategies to search for target-selective compounds. Methods Mol Biol 672, 517-530, 2011.

302. Stumpfe D & Bajorath J. Applied virtual screening: strategies, recommendations, and caveats, in: Methods and Principles in Medicinal Chemistry. Virtual Screening. Principles, Challenges, and Practical Guidelines. C. Sotriffer (Ed.), Wiley-VCH, Weinheim, 73-103, 2011.

303. Wassermann AM, Heikamp K & Bajorath J. Potency-directed similarity searching using support vector machines. Chem Biol Drug Des 77, 30-38, 2011.

304. Nisius B & Bajorath J. Mapping of pharmacological space. Expert Opin Drug Discov 6, 1-7, 2011.

305. Stahl M & Bajorath J. Computational medicinal chemistry. J Med Chem 54, 1-2, 2011.

306. Iyer P, Wawer M & Bajorath J. Comparison of two- and three-dimensional activity landscape representations for different compound data sets. Med Chem Commun 2, 113-118, 2011.

307. Hu Y & Bajorath J. Combining horizontal and vertical substructure relationships in scaffold hierarchies for activity prediction. J Chem Inf Model 51, 248-257, 2011.

308. Dimova D, Wawer M, Wassermann AM & Bajorath J. Design of multi-target activity landscapes that capture hierarchical activity cliff distributions. J Chem Inf Model 51, 258-266, 2011.

309. Wawer M & Bajorath J. Extracting SAR information from a large collection of anti-malarial screening hits by NSG-SPT analysis. ACS Med Chem Lett 2, 201-206, 2011.

310. Stumpfe D & Bajorath J. Similarity searching. WIRES Comp Mol Sci 1, 260-282, 2011.

311. Iyer P, Hu Y & Bajorath J. SAR monitoring of evolving compound data sets using activity landscapes. J Chem Inf Model 51, 532-540, 2011.

312. Wassermann AM & Bajorath J. Large-scale exploration of bioisosteric replacements on the basis of matched molecular pairs. Future Med Chem 3, 425-436, 2011.

313. Fustero S, Rodrigo V, Sánchez-Roselló M, del Pozo C, Timoneda J, Frizler M, Sisay MT, Bajorath J, Calle LP, Cañada FJ, Jiménez-Barbero J & Gütschow M. New cathepsin inhibitors to explore the fluorophilic properties of the S^2 pocket of cathepsin B: design, synthesis and biological evaluation. Chem Eur J 17, 5256-5260, 2011.

314. Ripphausen P, Nisius B, Wawer M & Bajorath J. Rationalizing the role of SAR tolerance for ligand-based virtual screening. J Chem Inf Model 51, 837-842, 2011.

315. Wawer M & Bajorath J. Local structural changes, global data views: graphical substructure-activity relationship trailing. J Med Chem 54, 2944-2951, 2011.

316. Batista J, Schlechtingen G, Friedrichson, T, Braxmeier T & Bajorath J. Lipid-like sulfoxides and amine oxides as inhibitors of mast cell activation. Eur J Med Chem 46, 2147-2151, 2011.

317. Ripphausen P, Nisius B & Bajorath J. State-of-the-art in ligand-based virtual screening. Drug Discov Today 16, 372-376, 2011.

318. Bill A, Blockus H, Stumpfe D, Bajorath J, Schmitz A & Famulok M. A homogeneous FRET-system for monitoring the activation of a protein switch in real time. J Am Chem Soc 133, 8372-8379, 2011.

319. Wassermann AM & Bajorath J. BindingDB and ChEMBL - online compound databases for drug discovery. Expert Opin Drug Discov 6, 683-687, 2011.

320. Bajorath J, Barreca ML, Bender A, Bryce R, Hutter M, Laggner C, Laughton C, Martin Y, Mitchell J, Padova A, Renner S, Selzer PM, Sherman W, Sippl W, Taft C, Tuccinardi T, Vistoli G & Willett P. Ask the experts: focus on computational chemistry. Future Med Chem 3, 909-921, 2011.

321. Iyer P, Stumpfe D & Bajorath J. Molecular mechanism-based network-like similarity graphs reveal relationships between different types of receptor ligands and structural changes that determine agonistic, inverse-agonistic, and antagonistic effects. J Chem Inf Model 51, 1281-1286, 2011.

322. Wassermann AM & Bajorath J. Identification of target family-directed bioisosteric replacements. Med Chem Commun 2, 601-606, 2011.

323. Hu Y & Bajorath J. Chemical transformations that yield compounds with distinct activity profiles. ACS Med Chem Lett 2, 523-527, 2011.

324. Wassermann AM, Dimova D & Bajorath J. Comprehensive analysis of single- and multi-target activity cliffs formed by currently available bioactive compounds. Chem Biol Drug Des 78, 224-228, 2011.

325. Namasivayam V, Iyer P & Bajorath J. Extraction of discontinuous structure-activity relationships from compound data sets through particle swarm optimization. J Chem Inf Model 51, 1545-1551, 2011.

326. Hu Y, Stumpfe D & Bajorath J. Lessons learned from molecular scaffold analysis. J Chem Inf Model 51, 1742-1753, 2011.

327. Heikamp K & Bajorath J. Large-scale similarity search profiling of CHEMBL compound data sets. J Chem Inf Model 51, 1831-1839, 2011.

328. Vogt M, Huang Y & Bajorath J. From activity cliffs to activity ridges: informative data structures for SAR analysis. J Chem Inf Model 51, 1848-1856, 2011.

329. Wassermann AM & Bajorath J. A data mining method to facilitate SAR transfer. J Chem Inf Model 51, 1857-1866, 2011.

330. Heikamp K & Bajorath J. How do 2D fingerprints detect structurally diverse active compounds? Revealing compound subset-specific fingerprint features through systematic selection. J Chem Inf Model 51, 2254-2265, 2011.

331. Iyer P & Bajorath J. Representation of multi-target activity landscapes through target pair-based compound encoding in self-organizing maps. Chem Biol Drug Des 78, 778-786, 2011.

332. Ripphausen P, Wassermann AM & Bajorath J. REPROVIS-DB: a benchmark system for ligand-based virtual screening derived from reproducible prospective applications. J Chem Inf Model 51, 2467-2473, 2011.

333. Vogt M & Bajorath J. Introduction of the conditional correlated Bernoulli model of similarity value distributions and its application to the prospective prediction of fingerprint search performance J Chem Inf Model 51, 2496-2506, 2011.

334. Li R, Stumpfe D, Vogt, M, Geppert H & Bajorath J. Development of a method to consistently quantify the structural distance between scaffolds and to assess scaffold hopping potential. J Chem Inf Model 51, 2507-2514, 2011.

335. Hu Y & Bajorath J. Activity profile sequences: a concept to account for the progression of compound activity in target space and extract SAR information from analog series with multiple target annotations. ChemMedChem 6, 2150-2154, 2011.

336. Stumpfe D & Bajorath J. Assessing the confidence level of public domain compound activity data and the impact of alternative potency measurements on SAR analysis. J Chem Inf Model 51, 3131-3137, 2011.

337. Hu Y & Bajorath J. Target family-directed exploration of scaffolds with different SAR profiles. J Chem Inf Model 51, 3138-3148, 2011.

338. Vogt M & Bajorath J. Statistical methods for predicting compound recovery rates for ligand-based virtual screening and assessing the probability of activity, in: Statistical Modeling of Molecular Descriptors in QSAR/QSPR. D. Bonchev, M. Dehmer, K. Varmuza (Eds.), Wiley-VCH, Weinheim, 229-243, 2012.

339. Maurer E, Sisay MT, Stirnberg M, Steinmetzer T, Bajorath J & Gütschow M. Insights into matriptase-2 substrate binding and inhibition mechanisms by analyzing active site-mutated variants. ChemMedChem 7, 68-72, 2012.

340. Namasivayam V, Iyer P & Bajorath J. Exploring SAR continuity in the vicinity of activity cliffs. Chem Biol Drug Des 79, 22-29, 2012.

341. Wassermann AM, Nisius B, Vogt M & Bajorath J. Information entropic functions for molecular descriptor profiling. Methods Mol Biol 819, 43-55, 2012.

342. Stumpfe D & Bajorath J. Methods for SAR visualization. RSC Adv 2, 369-378, 2012.

343. Wassermann AM & Bajorath J. Directed R-group combination graph: a methodology to uncover structure-activity relationship patterns in series of analogs. J Med Chem 55, 1215-1226, 2012.

344. Bajorath J. Computational chemistry in pharmaceutical research: at the crossroads. J Comput-Aided Mol Des 26, 11-12, 2012.

345. Auer J, Vogt M &Bajorath J. Emerging chemical patterns - theory and applications. in: Contrast Data Mining: Concepts, Algorithms, and Applications. G. Dong, J. Bailey (Eds.), Data Mining and Knowledge Discovery Series, Chapman & Hall / CRC, Boca Raton, 243-260, 2012.

346. Dimova D & Bajorath J. Computational chemical biology: identification of small molecular probes that discriminate between members of target families. Chem Biol Drug Des 79, 369-375, 2012.

347. Iyer P & Bajorath J. Mechanism-based bipartite matching molecular series graphs to identify structural modifications of receptor ligands that lead to mechanism hopping. Med Chem Commun 3, 441-448, 2012.

348. Hu Y & Bajorath J. Many structurally related drugs bind different targets whereas distinct drugs display significant target overlap. RSC Adv 2, 3481-3489, 2012.

349. Stumpfe D, Ripphausen P & Bajorath J. Virtual compound screening in drug discovery. Future Med Chem 4, 593-602, 2012

350. Ripphausen P, Stumpfe D & Bajorath J. Analysis of structure-based virtual screening studies and characterization of identified active compounds. Future Med Chem 4, 603-616, 2012.

351. Hu Y & Bajorath J. Exploration of 3D activity cliffs on the basis of compound binding modes and comparison of 2D and 3D cliffs. J Chem Inf Model 52, 670-677, 2012.

352. Stumpfe D & Bajorath J. Exploring activity cliffs in medicinal chemistry. J Med Chem 55, 2932-2942, 2012.

353. Namasivayam V & Bajorath J. Searching for coordinated activity cliffs using particle swarm optimization. J Chem Inf Model 52, 927-934, 2012.

354. Gupta-Ostermann D, Wawer M, Wassermann AM & Bajorath J. Graph mining for SAR transfer series. J Chem Inf Model 52, 935-942, 2012.

355. Bajorath J. Progress in computational medicinal chemistry. J Med Chem 55, 3593-3594, 2012.

356. Bajorath J. Modeling of activity landscapes for drug discovery. Expert Opin Drug Discov 7, 463-473, 2012.

357. Hu X, Hu Y, Vogt M, Stumpfe D & Bajorath J. MMP-cliffs: systematic identification of activity cliffs on the basis of matched molecular pairs. J Chem Inf Model 52, 1138-1145, 2012.

358. Gupta-Ostermann D, Hu Y & Bajorath J. Introducing the LASSO graph for compound data set representation and structure-activity relationship analysis. J Med Chem 55, 5546-5553, 2012.

359. Hu Y, Furtmann N, Gütschow M & Bajorath J. Systematic identification and classification of three-dimensional activity cliffs. J Chem Inf Model 52, 1490-1498, 2012.

360. Wassermann AM, Haebel P, Weskamp N & Bajorath J. SAR matrices: automated extraction of information-rich SAR tables from large compound data sets. J Chem Inf Model 52, 1769-1776, 2012.

361. Hu Y & Bajorath J. Extending the activity cliff concept: structural categorization of activity cliffs and systematic identification of different types of cliffs in the ChEMBL database. J Chem Inf Model 52, 1806-1811, 2012.

362. Ripphausen P, Freundlieb M, Brunschweiger A, Zimmermann H, Müller C & Bajorath J. Virtual screening identifies novel sulfonamide inhibitors of ecto-5'-nucleotidase. J Med Chem 55, 6576-6581, 2012.

363. Hu Y & Bajorath J. Freely available compound data sets and software tools for chemoinformatics and computational medicinal chemistry applications. F1000Research 1:11 (doi: 10.3410/f1000research.1-11.v1), 2012.

364. Iyer P, Dimova D, Vogt M & Bajorath J. Navigating high-dimensional activity landscapes: design and application of the ligand-target differentiation map. J Chem Inf Model 52, 1962-1969, 2012.

365. Bajorath J. Chemoinformatics: recent advances at the interfaces between computer and chemical information sciences, chemistry, and drug discovery. Bioorg Med Chem 20, 5316-5316, 2012.

366. Vogt M & Bajorath J. Chemoinformatics: a view of the field and current trends in method development. Bioorg Med Chem 20, 5317-5323, 2012.

367. Stumpfe D & Bajorath J. Frequency of occurrence and potency range distribution of activity cliffs in bioactive compounds. J Chem Inf Model 52, 2348-2353, 2012.

368. Heikamp K, Hu X, Yan A & Bajorath J. Prediction of activity cliffs using support vector machines. J. Chem Inf Model 52, 2354-2365, 2012.

369. Hu Y & Bajorath J. Rationalizing structure and target relationships between current drugs. AAPS J 14, 764-771, 2012.

370. Hu Y & Bajorath J. Growth of ligand-target interaction data in ChEMBL is associated with increasing and measurement-dependent compound promiscuity. J Chem Inf Model 52, 2550-2558, 2012.

371. Gupta-Ostermann D & Bajorath J. Identification of multi-target activity ridges in high-dimensional bioactivity space. J. Chem Inf Model 52, 2579-2586, 2012.

372. Heikamp K & Bajorath J. Fingerprint design and engineering strategies: rationalizing and improving similarity search performance. Future Med Chem 4, 1945-1959, 2012.

373. Li R & Bajorath J. Systematic assessment of scaffold distances in ChEMBL: prioritization of compound data sets for scaffold hopping analysis in virtual screening. J Comput-Aided Mol Des 26, 1101-1109, 2012.

374. Namasivayam V & Bajorath J. Multi-objective particle swarm optimization: automated identification of SAR-informative compounds with favorable physicochemical properties. J Chem Inf Model 52, 2848-2855, 2012.

375. de la Vega de León A & Bajorath J. Design of a three-dimensional multi-target activity landscape. J Chem Inf Model 52, 2876-2883, 2012.

376. Dimova D, Hu Y & Bajorath J. Matched molecular pair analysis of small molecule microarray data identifies promiscuity cliffs and reveals molecular origins of extreme compound promiscuity. J Med Chem 55, 10220-10228, 2012.

377. Wassermann AM, Dimova D, Iyer P & Bajorath J. Advances in computational medicinal chemistry - matched molecular pair analysis. Drug Dev Res 73, 518-527, 2012.

378. Zhang B, Wassermann AM, Vogt M & Bajorath J. Systematic assessment of compound series with SAR transfer potential. J Chem Inf Model 52, 3138-3143, 2012.

379. Dimova D, Iyer P, Vogt M,Totzke F, Kubbutat MHG, Schächtele C, Laufer S & Bajorath J. Assessing the target differentiation potential of imidazole-based protein kinase inhibitors. J Med Chem 55, 11067-11071, 2012.

380. Heikamp K & Bajorath J. The future of virtual compound screening. Chem Biol Drug Des 81, 33-40, 2013.

381. Hu Y & Bajorath J. How promiscuous are pharmaceutically relevant compounds? A data-driven assessment. AAPS J 15, 104-111, 2013.

382. Hu Y & Bajorath J. Systematic identification of scaffolds representing compounds active against individual targets and single or multiple target families. J Chem Inf Model 53, 312-326, 2013.

383. Elagawany M, Ibrahim MA, Ahmed HEA, El-Etrawy AS, Ghiaty A, El-Feky SA, Abdel-Samii ZK & Bajorath J. Design, synthesis, and molecular modelling of pyridazinone and phthalazinone derivatives as protein kinase inhibitors. Bioorg Med Chem Lett 23, 2007-2013, 2013.

384. Hu Y, Maggiora GM & Bajorath J. Activity cliffs in PubChem confirmatory bioassays taking inactive compounds into account. J Comput-Aided Mol Des 227, 115-124, 2013.

385. Hu Y & Bajorath J. Introduction of target cliffs as a concept to identify and describe complex molecular selectivity patterns. J Chem Inf Model 53, 545-552, 2013.

386. Ahmadi M, Vogt M, Iyer P, Bajorath J & Fröhlich H. Predicting potent compounds via model-based global optimization. J Chem Inf Model 53, 553-559, 2013.

387. Bajorath J. Virtual screening methods, in: Diversity-Oriented Synthesis: Basics and Applications in Organic Synthesis, Drug Discovery, and Chemical Biology. A. Trabocchi (Ed.), Wiley-Blackwell, Hoboken, 483-506, 2013.

388. Bajorath J. Structure-activity relationship data analysis: activity landscapes and activity cliffs, in: Diversity-Oriented Synthesis: Basics and Applications in Organic Synthesis, Drug Discovery, and Chemical Biology. A. Trabocchi (Ed.), Wiley-Blackwell, Hoboken, 507-532.

389. Heikamp K & Bajorath J. Prediction of compounds with closely related activity profiles using weighted support vector machine linear combinations. J Chem Inf Model 53, 791-801, 2013.

390. Anighoro A, Stumpfe D, Heikamp K, Bajorath J & Rastelli G. Targeting the Hsp90 interactome using in silico polypharmacology approaches. Chim Ind 3/13, 105-106, 2013.

391. Dimova D, Heikamp K, Stumpfe D & Bajorath J. Do medicinal chemists learn from activity cliffs? A systematic evaluation of cliff progression in evolving compound data sets. J Med Chem 56, 3339-3345, 2013.

392. Stumpfe D, Dimova D, Heikamp & Bajorath J. Compound pathway model to capture SAR progression: comparison of activity cliff-dependent and -independent pathways. J Chem Inf Model 53, 1067-1072, 2013.

393. Bajorath J. Large-scale SAR analysis. Drug Discov Today: Tech 10, e419-e426, 2013.

394. de la Vega de León A & Bajorath J. Compound optimization through data set-dependent chemical transformations. J Chem Inf Model 53, 1263-1271, 2013.

395. Namasivayam V, Hu Y, Balfer J & Bajorath J. Classification of compounds with distinct or overlapping multi-target activities and diverse molecular mechanisms using emerging chemical patterns. J Chem Inf Model 53, 1272-1281, 2013.

396. Hu Y & Bajorath J. What is the likelihood of an active compound to be promiscuous? Systematic assessment of compound promiscuity on the basis of PubChem confirmatory bioassay data. AAPS J 15, 808-815, 2013.

397. Hu Y & Bajorath J. Compound promiscuity - what can we learn from current data? Drug Discov Today 18, 644-650, 2013.

398. Bajorath J. Machine learning and similarity-based virtual screening techniques, in: In Silico Drug Discovery and Design Techniques. M. A. Lill (Ed.), Future Science Ltd., London, 3-14, 2013.

399. Hu Y & Bajorath J. High-resolution view of compound promiscuity. F1000Research 2:144 (doi: 10.12688/f1000research.2-144.v2), 2013.

400. Iyer P, Stumpfe D, Vogt M, Bajorath J & Maggiora GM. Activity landscapes, information theory, and structure-activity relationships. Mol Inf 32, 421-430, 2013.

401. Zhang B, Hu Y & Bajorath J. SAR transfer across different targets. J Chem Inf Model 53, 1589-1594, 2013.

402. Bajorath J. Hiking trails in activity landscapes - data visualization in medicinal chemistry. Lab&More 2/13, 9-13, 2013.

403. Heikamp K & Bajorath J. Comparison of inactive and randomly selected compounds as negative training examples in support vector machine-based virtual screening. J Chem Inf Model 53, 1595-1601, 2013.

404. Vogt M, Iyer P, Maggiora GM & Bajorath J. Conditional probabilities of activity landscape features for individual compounds. J Chem Inf Model 53, 1602-1612, 2013.

405. Vogt M & Bajorath J. Similarity searching for potent compounds using feature selection. J Chem Inf Model 53, 1613-1619, 2013.

406. Hu Y & Bajorath J. Promiscuity profiles of bioactive compounds: potency range and difference distributions and the relation to target numbers and families. Med Chem Commun 4, 1196-1201, 2013.

407. Lentz CS, Stumpfe D, Bajorath J, Famulok M, Hoerauf A & Pfarr KM. New chemotypes for wALADin1-like inhibitors of delta-aminoevulinic acid dehydratase from *Wolbachia* endobacteria. Bioorg Med Chem Lett 23, 5558-5562, 2013.

408. Bajorath J. Chemoinformatics: from methods and models to pharmaceutical applications, in: Chemoinformatics for Drug Discovery. J. Bajorath (Ed.), John Wiley and Sons, Hoboken, vii, 2013.

409. Stumpfe D & Bajorath J. Critical assessment of virtual screening for hit identification, in: Chemoinformatics for Drug Discovery. J. Bajorath (Ed.), John Wiley and Sons, Hoboken, 113-130, 2013.

410. Gupta-Ostermann D, Hu Y & Bajorath J. Systematic mining of analog series with related core structures in multi-target activity space. J Comput-Aided Mol Des 27, 665-674, 2013.

411. Balfer J, Vogt M & Bajorath J. Searching for closely related ligands with different mechanism-of-action using machine learning and mapping algorithms. J Chem Inf Model 53, 2252-2274, 2013.

412. Dimova D, Stumpfe D & Bajorath J. Quantifying the fingerprint descriptor dependence of structure-activity relationship information on a large scale. J Chem Inf Model, 2275-2281, 2013.

413. Hu Y & Bajorath J. Activity profile relationships between structurally similar promiscuous compounds. Eur J Med Chem 69, 393-398, 2013.

414. Iqbal J, Saeed A, Raza R, Matin A, Hameed A, Furtmann N, Lecka J, Sévigny J & Bajorath J. Identification of sulfonic acids as efficient ecto-5'-nucleotidase inhibitors. Eur J Med Chem 70, 685-691, 2013.

415. Bajorath J. Molecular crime scene investigation - dusting for fingerprints. Drug Discov Today: Tech, e491-e498, 2013.

416. Furtmann N & Bajorath J. Evaluation of molecular model-based discovery of ecto-5'-nucleotidase inhibitors on the basis of X-ray structures. Bioorg Med Chem 21, 6616-6622, 2013.

417. Hu Y, Stumpfe D & Bajorath J. Advancing the activity cliff concept. F1000Research 2:199 (doi: 10.12688/f1000research.2-199.v1), 2013.

418. Hu Y, Stumpfe D & Bajorath J. Visualization of activity landscapes and chemogenomics data. Mol Inf 32, 954-963, 2013.

419. Bajorath J. A perspective on computational chemogenomics. Mol Inf 32, 1025-1028, 2013.

420. Namasivayam V, Iyer P & Bajorath J. Prediction of individual compounds forming activity cliffs using emerging chemical patterns. J Chem Inf Model 53, 3131-3139, 2013.

421. Hu Y & Bajorath J. Scaffold mining of publicly available compound data, in: Scaffold Hopping in Medicinal Chemistry. N. Brown (Ed.). Methods and Principles in Medicinal Chemistry 58, Wiley-VCH, Weinheim, 61-81, 2014.

422. Heikamp K & Bajorath J. Support vector machines for drug discovery. Expert Opin Drug Discov 9, 93-104, 2014.

423. Wysocka M, Gruba N, Miecznikowska A, Popow-Stellmaszyk J, Gütschow M, Stirnberg M, Furtmann N, Bajorath J, Lesner A, Rolka K. Substrate specificity of human matriptase-2. Biochimie 97, 121-127, 2014.

424. de la Vega de León A & Bajorath J. Matched molecular pairs derived by retrosynthetic fragmentation. Med Chem Commun 5, 64-67, 2014.

425. Stumpfe D, Hu Y, Dimova D & Bajorath J. Recent progress in understanding activity cliffs and their utility in medicinal chemistry. J Med Chem 57, 18-28, 2014.

426. Hu Y, Gupta-Ostermann D & Bajorath J. Exploring compound promiscuity patterns and multi-target activity spaces. Comput Struct Biotech J 9, e201401003, 2014.

427. Hu Y, de la Vega de León A, Zhang & Bajorath J. Matched molecular pair-based data sets for computer-aided medicinal chemistry [v2; ref status: indexed, http://f1000r.es/2w9] F1000Research 3:36 (doi: 10.12688/f1000research.3-36.v2), 2014.

428. Kayastha S, Dimova D, Iyer P, Vogt M & Bajorath J. Large-scale assessment of activity landscape feature probabilities of bioactive compounds. J Chem Inf Model 54, 442-450, 2014.

429. Stumpfe D, Dimova D & Bajorath J. Composition and topology of activity cliff clusters formed by bioactive compounds. J Chem Inf Model 54, 451-461, 2014.

430. de la Vega de León A & Bajorath J. Formation of activity cliffs is accompanied by systematic increases in ligand efficiency from lowly to highly potent compounds. AAPS J 16, 335-341, 2014.

431. Hu Y & Bajorath J. Many drugs contain unique scaffolds with varying structural relationships to scaffolds of currently available bioactive compounds. Eur J Med Chem 76, 427-434, 2014.

432. Bajorath J. Improving data mining strategies for drug design. Future Med Chem 6, 255-257, 2014.

433. Laufer S & Bajorath J. New frontiers in kinases: second generation inhibitors. J Med Chem 57, 2167-2168, 2014.

434. Gupta-Ostermann D, Shanmugasundaram V & Bajorath J. Neighborhood-based prediction of novel active compounds from SAR matrices. J Chem Inf Model 54, 801-809, 2014.

435. Aslam S, Zaib S, Ahmad M, Gardiner JM, Ahmad A, Hameed A, Furtmann N, Gütschow M, Bajorath J & Iqbal J. Novel structural hybrids of pyrazolobenzothiazines with benzimidazoles as cholinesterase inhibitors. Eur J Med Chem 78, 106-117, 2014.

436. Stumpfe D, de la Vega de León A, Dimova D & Bajorath J (2014) Advancing the activity cliff concept, part II [v1; ref status: indexed, http://f1000r.es/34p] F1000Research 3:75 (doi: 10.12688/f1000research.4057), 2014.

437. Hu Y & Bajorath J. Learning from 'big data': compounds and targets. Drug Discov Today 19, 357-360, 2014.

438. Hu Y & Bajorath J. Compound data sets and software tools for chemoinformatics and medicinal chemistry applications: update and data transfer [v1; ref status: indexed, http://f1000r.es/32j] F1000Research 3:69 (doi: 10.12688/f1000research.3979), 2014.

439. Mertens MM, Schmitz J, Horn M, Furtmann N, Bajorath J, Mares M & Gütschow M. A coumarin-labeled vinyl sulfone as tripeptidomimetic activity-based probe for cysteine cathepsins. ChemBioChem 15, 955-959, 2014.

440. de la Vega de León A, Hu Y & Bajorath J. Systematic identification of matching molecular series and mapping of screening hits. Mol Inf 33, 257-263, 2014.

441. Maggiora G, Vogt M, Stumpfe D & Bajorath J. Molecular similarity in medicinal chemistry. J Med Chem 57, 3186-3204, 2014.

442. Namasivayam V, Gupta-Ostermann D, Balfer J, Heikamp K & Bajorath J. Prediction of compounds in different local structure-activity relationship environments using emerging chemical patterns. J Chem Inf Model 54, 1301-1310, 2014.

443. Dimova D, Stumpfe D & Bajorath J. Specific chemical changes leading to consistent potency increases in structurally diverse active compounds. Med Chem Commun 5, 742-749, 2014.

444. Gupta-Ostermann D & Bajorath J. The 'SAR Matrix' method and its extensions for applications in medicinal chemistry and chemogenomics [v2; ref status: indexed, http://f1000r.es/3gh] F1000Research 3:113 (doi: 10.12688/f1000research.4185.2), 2014.

445. Bajorath J. Exploring activity cliffs from a chemoinformatics perspective. Mol Inf 33, 438-442, 2014.

446. Balfer J, Heikamp K, Laufer S & Bajorath J. Modeling of compound profiling experiments using support vector machines. Chem Biol Drug Des 84, 75-85, 2014.

447. Hu Y, Lounkine E & Bajorath J. Many approved drugs have bioactive analogs with different target annotations. AAPS J 16, 847-849, 2014.

448. Maggiora G & Bajorath J. Chemical space networks - a powerful new paradigm for the description of chemical space. J Comput-Aided Mol Des 28, 795-802, 2014.

449. Balfer J, Hu Y & Bajorath, J. Compound structure-independent activity prediction in high-dimensional target space. Mol Inf 33, 544-558, 2014.

450. Dimova D, Stumpfe D & Bajorath J. Method for the evaluation of structure-activity relationship information associated with coordinated activity cliffs. J Med Chem 57, 6553-6563, 2014.

451. Saeed A, Tehseen Y, Rafique H, Furtmann N, Bajorath J, Flörke U & Iqbal J. Benzothiazolyl substituted iminothiazolidinones and benzamido-oxothiazolidines as potent and partly selective aldose reductase inhibitors. Med Chem Commun 5, 1371-1380, 2014.

452. Stumpfe D & Bajorath J. Activity cliff networks for medicinal chemistry. Drug Dev Res 75, 291-298, 2014.

453. Balfer J & Bajorath J. Introduction of a methodology for visualization and graphical interpretation of Bayesian classification models. J Chem Inf Model 54, 2451-2468, 2014.

454. Anighoro A, Bajorath J & Rastelli G. Polypharmacology: challenges and opportunities in drug discovery. J Med Chem 57, 7874-7887, 2014.

455. Bajorath J. Activity artifacts in drug discovery and different facets of compound promiscuity [v1; ref status: indexed, http://f1000r.es/4gz] F1000Research 3:233 (doi: 10.12688/f1000research.5426.1), 2014.

456. Zhang B, Vogt M & Bajorath J. Design of an activity landscape view taking compound-based feature probabilities into account. J Comput-Aided Mol Des 28, 919-926, 2014.

457. Khan I, Ibrar A, Zaib S, Ahmad S, Furtmann N, Hameed S, Simpson J, Bajorath J & Iqbal J. Active compounds from a diverse library of triazolothiadiazole and triazolothiadiazine scaffolds: synthesis, crystal structure determination, cytotoxicity, cholinesterase inhibitory activity, and binding mode analysis. Bioorg Med Chem 22, 6163-6173, 2014.

458. Hu Y & Bajorath J. Monitoring drug promiscuity over time [v2; ref status: indexed, http://f1000r.es/4bh] F1000Research 3:218 (doi: 10.12688/f1000research.5250.1), 2014.

459. Dimova D & Bajorath J. Extraction of structure-activity relationship information from activity cliff clusters via matching molecular series. Eur J Med Chem 87, 454-460, 2014.

460. de la Vega de León A & Bajorath J. Prediction of compound potency changes in matched molecular pairs using support vector regression. J Chem Inf Model 54, 2654-2663, 2014.

461. Bajorath J. Evolution of the activity cliff concept for SAR analysis and drug discovery. Future Med Chem 6, 1545-1549, 2014.

462. Bajorath J. On data sharing in computational drug discovery and the need for data notes [v1; ref status: not peer reviewed, http://f1000r.es/4qi] F1000Research 3:280 (doi: 10.12688/f1000research.5742.1), 2014.

463. Zhang B, Hu Y & Bajorath J. AnalogExplorer – a new method for graphical analysis of analog series and associated structure-activity relationship information. J Med Chem 57, 9184-9194, 2014.

464. Hu Y & Bajorath J. Influence of search parameters and criteria on compound selection, promiscuity, and pan assay interference characteristics. J Chem Inf Model 54, 3056-3066, 2014.

465. Dimova D, Stumpfe D & Bajorath J. Systematic assessment of coordinated activity cliffs formed by kinase inhibitors and detailed characterization of activity cliff clusters and associated SAR information. Eur J Med Chem 90, 414-427, 2015.

466. Laufer S & Bajorath J. Advancing the kinase field: new targets and second generation inhibitors. J. Med Chem 58, 1-1, 2015.

467. Hu Y, Furtmann N & Bajorath J. Current compound coverage of the kinome. J Med Chem 58, 30-40, 2015.

468. Furtmann N, Hu Y & Bajorath J. Comprehensive analysis of three-dimensional activity cliffs formed by kinase inhibitors with different binding modes and cliff mapping of structural analogs. J Med Chem 58, 252-264, 2015.

469. Hu Y & Bajorath J. Exploring the scaffold universe of kinase inhibitors. J Med Chem 58, 315-332, 2015.

470. Zwierzyna M, Vogt M, Maggiora GM & Bajorath J. Design and characterization of chemical space networks for different compound data sets. J Comput-Aided Mol Des 29, 113-125, 2015.

471. Bajorath J. Entering new publication territory in chemoinformatics and chemical information science [v1; ref status: not peer reviewed, http://f1000r.es/51g] F1000Research 4:35 (doi: 10.12688/f1000research.6101.1), 2015.

472. Bajorath J, Jiang H, Shoichet BK, Walters WP. Computational methods for medicinal chemistry. J Med Chem 58, 1019-1019, 2015.

473. Kayastha S, Dimova D, Stumpfe D & Bajorath J. Structural diversity and potency range distribution of scaffolds from compounds active against current pharmaceutical targets. Future Med Chem 7, 111-122, 2015.

474. Furtmann N & Bajorath J. Structural and modeling studies on ecto-5'-nucleotidase aiding in inhibitor design. Mini Rev Med Chem 15, 34-40, 2015.

475. Gupta-Ostermann D, Balfer J & Bajorath J. Hit expansion from screening data based upon conditional probabilities of activity derived from SAR matrices. Mol Inf 34, 134-146, 2015.

476. Jasial S, Balfer J, Vogt M & Bajorath J. Determination of meta-parameters for support vector machine linear combinations. Mol Inf 34, 127-133, 2015.

477. Balfer J & Bajorath J. Systematic artifacts in support vector regression-based compound potency prediction revealed by statistical and activity landscape analysis. PLoS One 10, e0119301, 2015.

478. Garnett R, Gärtner T, Vogt M & Bajorath J. Introducing the 'active search' method for iterative virtual screening. J Comput-Aided Mol Des 29, 305-314, 2015.

479. Anighoro A, Stumpfe D, Heikamp K, Beebe K, Neckers LM, Bajorath J & Rastelli G. Computational polypharmacology analysis of the heat shock protein 90 interactome. J Chem Inf Model 55, 676-686, 2015.

480. Gupta-Ostermann D, Hirose Y, Odagami T, Kouji H & Bajorath J. Follow-up: Prospective compound design using the 'SAR Matrix' method and matrix-derived conditional probabilities of activity [v2; ref status: indexed, http://f1000r.es/59v] F1000Research 4:75 (doi: 10.12688/f1000research.6271.1), 2015.

481. Dimova D, Stumpfe D, Hu Y & Bajorath J. Activity cliff clusters as a source of structure-activity relationship information. Expert Opin Drug Discov 10, 441-447, 2015.

482. Hu Y & Bajorath. Structural and activity profile relationships between drug scaffolds. AAPS J 17, 609-619, 2015.

483. Furtmann N, Hu Y, Gütschow M & Bajorath J. Identification and analysis of currently available high-confidence three-dimensional activity cliffs. RSC Adv 5, 43660-43668, 2015.

484. Hu Y, Furtmann N & Bajorath J. Extension of three-dimensional activity cliff information through systematic mapping of active analogs. RSC Adv 5, 43006-43015, 2015.

485. Hu Y & Bajorath J. Quantifying the tendency of therapeutic target proteins to bind promiscuous or selective compounds. PLoS One 10, e0126838, 2015.

486. Hu Y, Jasial S & Bajorath J. Promiscuity progression of bioactive compounds over time [v2; ref status: indexed, http://f1000r.es/5h4] F1000Research 4(Chem Inf Sci):118 (doi: 10.12688/f1000research.6473.1), 2015.

487. Stumpfe D, Dimova D & Bajorath J. Systematic assessment of scaffold hopping versus activity cliff formation across bioactive compound classes following a molecular hierarchy. Bioorg Med Chem 23, 3183-3191, 2015.

488. Kayastha S, de la Vega de León A, Dimova D & Bajorath J. Target-based analysis of ionization states of bioactive compounds. Med Chem Commun 6, 1030-1035, 2015.

489. Balfer J & Bajorath J. Visualization and interpretation of support vector machine activity predictions. J Chem Inf Model 55, 1136-1147, 2015.

490. Hu Y, Furtmann N, Stumpfe D & Bajorath J. Comprehensive knowledge base of two- and three-dimensional activity cliffs for medicinal and computational chemistry [v1; ref status: indexed, http://f1000r.es/5ir] F1000Research 4(Chem Inf Sci):168 (doi: 10.12688/f1000research.6661.1), 2015.

491. Hameed A, Khan K, Zehra S, Ahmed R, Shafiq Z, Bakht S, Yaqub M, Hussain M, de la Vega de León A, Furtmann N, Bajorath J, Ahmad H, Tahir M & Iqbal J. Synthesis, biological evaluation and molecular docking of N-phenyl thiosemicarbazones as urease inhibitors. Bioorg Chem 61, 51-57, 2015.

492. Zhang B, Vogt M, Maggiora GM & Bajorath J. Comparison of bioactive chemical space networks generated using substructure- and fingerprint-based measures of molecular similarity. J Comput-Aided Mol Des 29, 595-608, 2015.

493. Schmitz J, Furtmann N, Ponert M, Frizler M, Löser R, Bartz U, Bajorath J & Gütschow M. Active site mapping of human cathepsin F with dipeptide nitrile inhibitors. ChemMedChem 10, 1365-1377, 2015.

494. Hu Y, Zhang B & Bajorath J. Method for systematic assessment of chemical changes in molecular scaffolds with conserved topology and application to the analysis of scaffold-activity relationships. Mol Inf 34, 531-549, 2015.

495. de la Vega de León A, Kayastha S, Dimova D, Schultz T & Bajorath J. Visualization of multi-property landscapes for compound selection and optimization. J Comput-Aided Mol Des 29, 695-705, 2015.

496. Bajorath J. Computer-aided drug discovery [v1; ref status: indexed, http://f1000r.es/5ij] F1000Research 4(F1000 Faculty Rev):630 (doi: 10.12688/f1000research.6653.1), 2015.

497. Stumpfe D & Bajorath J. Monitoring global growth of activity cliff information over time and assessing activity cliff frequencies and distributions. Future Med Chem 7, 1565-1579, 2015.

498. Ghareeb D, Khalil S, Hafez HS, Bajorath J, Ahmed HEA, Sarhan E, El-Wakeel E & El-Demellawy MA. Berberine reduces neurotoxicity related to non-alcoholic steatohepatitis in rats. Evid Based Complement Alternat Med 2015, e361847, 2015.

499. Dimova D, Stumpfe D & Bajorath J. Identification of orthologous target pairs with shared active compounds and comparison of organism-specific activity patterns. Chem Biol Drug Des 86, 1105-1114, 2015.

500. Hameed A, Zehra ST, Shah SJA, Khan KM, Alharthy RD, Furtmann N, Bajorath J, Tahir MN & Iqbal J. Syntheses, cholinesterases inhibition and molecular docking studies of pyrido[2,3-b]pyrazine derivatives. Chem Biol Drug Des 86, 1115-1120, 2015.

501. Kohl F, Schmitz J, Furtmann N, Schulz-Fincke A-C, Mertens MD, Küppers J, Benkhoff M, Tobiasch E, Bartz U, Bajorath J, Stirnberg M & Gütschow M. Design, characterization and cellular uptake studies of fluorescence-labeled prototypic cathepsin inhibitors. Org Biomol Chem 13, 10310-10323, 2015.

502. Zhang B, Vogt M, Maggiora GM & Bajorath J. Design of chemical space networks using a Tanimoto similarity variant based upon maximum common substructures. J Comput-Aided Mol Des 29, 937-950, 2015.

503. Hu Y, Zhang B, Vogt M and Bajorath J. AnalogExplorer2 – Stereochemistry sensitive graphical analysis of large analog series [version 1; referees: 2 approved] F1000Research 4(Chem Inf Sci):1031 (doi: 10.12688/f1000research.7146.1), 2015.

504. Furtmann N, Hu Y, Gütschow M & Bajorath J. Identification of interaction hotspots in structures of drug targets on the basis of three-dimensional activity cliff information. Chem Biol Drug Des 86, 1458-1465, 2015.

505. Walters WP & Bajorath J. On the evolving open peer review culture for chemical information science [version 1; referees: not peer reviewed] F1000Research 4(Chem Inf Sci):1350 (doi: 10.12688/f1000research.7460.1), 2015.

506. Bajorath J. Pushing the boundaries of computational approaches: special focus issue on computational chemistry and computer-aided drug discovery. Future Med Chem 7, 2415-2417, 2015.

507. Furtmann N, Häußler D, Scheidt T, Stirnberg M, Steinmetzer T, Bajorath J & Gütschow M. Limiting the number of potential binding modes by introducing symmetry into ligands: structure-based design of inhibitors for trypsin-like serine proteases. Chemistry 22, 610-625, 2016.

508. Tropsha A & Bajorath J. Computational methods for drug discovery and design. J Med Chem 59, 1-1, 2016.

509. Hameed A, Zehra ST, Abbas S, Nisa RU, Mahmmod T, Ayub K, Al-Rashida M, Bajorath J, Khan KM & Iqbal J. One-pot synthesis of tetrazole-1,2,5,6-tetrahydronicotinonitriles and cholinesterase inhibition: probing the plausible reaction mechanism via computational studies. Bioorg Chem 65, 38-47, 2016.

510. Wu M, Vogt M, Maggiora GM & Bajorath J. Design of chemical space networks on the basis of Tversky similarity. J Comput-Aided Mol Des 30, 1-12, 2016.

511. Ghosh A, Dimova D & Bajorath J. Classification of matching molecular series on the basis of SAR phenotypes and structural relationships. Med Chem Commun 7, 237-246, 2016.

512. Dimova D, Stumpfe D & Bajorath J. Systematic assessment of analog relationships between bioactive compounds and promiscuity of analog sets. Med Chem Commun 7, 230-236, 2016.

513. Jasial S, Hu Y & Bajorath J. Assessing the growth of bioactive compounds and scaffolds over time: implications for lead discovery and scaffold hopping. J Chem Inf Model 56, 300-307, 2016.

514. Anighoro A & Bajorath J. Three-dimensional similarity in molecular docking: prioritizing ligand poses on the basis of experimental binding modes. J Chem Inf Model 56, 580-587, 2016.

515. Vogt M, Stumpfe D, Maggiora GM & Bajorath J. Lessons learned from the design of chemical space networks and opportunities for new applications. J Comput-Aided Mol Des 30, 191-208, 2016.

516. Beckmann A-M, Maurer E, Lülsdorff V, Wilms A, Furtmann N, Bajorath J, Gütschow M & Stirnberg M. En route to new therapeutic options for iron overload diseases: matriptase-2 as a target for Kunitz-type inhibitors. ChemBioChem 17, 595-604, 2016.

517. Jasial S, Hu Y, Vogt M and Bajorath J. Activity-relevant similarity values for fingerprints and implications for similarity searching. F1000Research 5(Chem Inf Sci):591, 2016.

518. Jasial S, Hu Y & Bajorath J. Determining the degree of promiscuity of extensively assayed compounds. PLoS One, 11, e0153873, 2016.

519. Dimova D & Bajorath J. Advances in activity cliff research. Mol Inf 35, 181-191, 2016.

520. Shoichet BK, Walters WP, Jiang H & Bajorath J. Advances in computational medicinal chemistry: a reflection on the evolution of the field and perspective going forward. J Med Chem 59, 4033-4034, 2016.

521. Hu Y, Stumpfe D & Bajorath J. Computational exploration of molecular scaffolds in medicinal chemistry. J Med Chem 59, 4062-4076, 2016.

522. Shanmugasundaram V, Zhang L, Kayastha S, de la Vega de León A, Dimova D & Bajorath J. Monitoring the progression of structure-activity relationship information during lead optimization. J Med Chem 59, 4235-4244, 2016.

523. Dimova D & Bajorath J. Systematic design of analogs of active compounds covering more than 1000 targets. Med Chem Commun 7, 859-863, 2016.

524. Häußler D, Mangold M, Furtmann N, Braune A, Blaut M, Bajorath J, Stirnberg M & Gütschow M. Phospho bisbenzguanidines as irreversible dipeptidomimetic inhibitors and activity-based probes of matriptase-2. Chemistry 22, 8525-8535, 2016.

525. Stumpfe D & Bajorath J. Recent developments in SAR visualization. Med Chem Commun 7, 1045-1055, 2016.

526. Hu Y & Bajorath J. Analyzing compound activity records and promiscuity degrees in light of publication statistics. F1000Research 5(Chem Inf Sci):1227, 2016.

527. Hu Y & Bajorath J. Systematic assessment of molecular selectivity at the level of targets, bioactive compounds, and structural analogs. ChemMedChem 11, 1362-1370, 2016.

528. Bajorath J. Computational methods for chemical biology. Understanding biological pathways through computer-aided chemistry. GIT Lab J Eur 7/8, 14-18, 2016.

529. Beckmann A-M, Gilberg E, Gattner S, Huang TL, Vanden Eynde JJ, Mayence A, Bajorath J, Stirnberg M & Gütschow M. Evaluation of bisbenzamidines as inhibitors for matriptase-2. Bioorg Med Chem Lett 26, 3741-3745, 2016.

530. Anighoro A & Bajorath J. Binding mode similarity measures for ranking of docking poses - a case study on the adenosine A2A receptor. J Comput-Aided Mol Des 30, 447-456, 2016.

531. Bajorath J. Pharmacophore, in: Encyclopedia of Cancer, 4th Edition, Springer-Verlag, Heidelberg, in press.

532. Bajorath J. QSAR, in: Encyclopedia of Cancer, 4th Edition, Springer-Verlag, Heidelberg, in press.

533. Bajorath J. Molecular similarity concepts for informatics applications. Methods Mol Biol, in press.

534. Bajorath J. Compound data mining for drug discovery. Methods Mol Biol, in press.

535. Hu Y & Bajorath J. Exploring molecular promiscuity from a ligand and target perspective, in: Frontiers in Molecular Design and Chemical Information Science, ACS Books, in press.

536. Hu Y & Bajorath J. Network variants for analyzing ligand-target interactions, in: Frontiers in Molecular Design and Chemical Information Science, ACS Books, in press.

537. Bajorath J. Complexity and heterogeneity of data for chemical information science, in: Frontiers in Molecular Design and Chemical Information Science, ACS Books, in press.

538. de la Vega de León A & Bajorath J. Chemical space visualization: transforming multi-dimensional chemical spaces into similarity-based molecular networks. Future Med Chem, in press.

539. Bajorath J. Analyzing promiscuity at the level of active compounds and targets. Mol Inf, in press.

540. Bajorath J. Extending accessible chemical space for the identification of novel leads. Expert Opin Drug Discov, in press.

541. Stumpfe D, Dimova D & Bajorath J. Computational method for the systematic identification of analog series and key compounds representing series and their biological activity profiles. J Med Chem, in press.

BOOKS

Bajorath J (Ed.) Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery, in: Methods in Molecular Biology, Humana Press, Totowa, New Jersey, USA, 2004.

Bunin B, Morales G, Siesel B, Bajorath J. Chemoinformatics: Theory, Practice, Products. Springer, Dordrecht, The Netherlands, 2007.

Bajorath J (Ed.) Chemoinformatics and Computational Chemical Biology, Humana Press, Springer Science Media, New York, New York, USA, 2011.

Bajorath J (Ed.) Chemoinformatics for Drug Discovery. John Wiley and Sons, Hoboken, New Jersey, USA, 2013.

SELECTED ABSTRACTS & CONFERENCE PUBLICATIONS

1. Hayden MS, Gayle M, Gilliland LK, Bajorath J, Ledbetter JA & Linsley PS. Single chain mono- and bi-specific antibodies with novel biological properties. J Cell Biochem 17B, 180, 1993

2. McAndrew SJ, Glaser S, Webb SM, Yelton D, Bajorath J & Cosand WL. A single amino acid substitution in CDR loop H3 improves the affinity of the BR96 single-chain antibody fragment. J Cell Biochem 18B, 192, 1994.

3. Sheriff S, Chang CY, Jeffrey PD & Bajorath J. Structures of the monoclonal anti-tumor antibody BR96 and its complex with the Lewis Y determinant. Am Crystallogr Assoc Abstr 22, H07, 57, 1994.

4. Sheriff S, Jeffrey PD, Chang C & Bajorath J. Structures of the monoclonal anti-tumor antibody BR96 and its complex with the Lewis Y determinant. Protein Sci 3S, 143, 1994.

5. Seyama K, Bajorath J, Nonoyama S, Ganggsass I, Aruffo A & Ochs HD. X-linked hyper IgM syndrome and mutations of the CD40 gene. FASEB J 10, 1208, 1996.

6. Sheriff S, Chang CY, Jeffrey PD & Bajorath J. The anti-tumor antibody BR96: X-ray structures of its antigen-bound and free forms. Acta Cryst. A 52, 1996.

7. Bowen MA, Bajorath J, Skonier JE, Emswiler J, Nadler SG & Aruffo A. Analysis of domain-domain interactions between CD6 and Activated Leukocyte Cell Adhesion Molecule (ALCAM). Tissue Antigens 48, 360, 1996.

8. Seyama K, Nonoyama S, Hollenbaugh D, Bajorath J, Hasle H, Kobayashi R, Apter A, Aruffo A & Ochs HD. X-linked hyper IgM syndrome (XHIM) mutation analysis, CD40L function and clinical phenotype. AAAI/AAI Abstr, No. 09507, 1996.

9. Bajorath J. Antibody modeling and engineering using canonical structures. Keystone Symposia on Molecular and Cellular Biology, Exploring and Exploiting Antibody and Ig Superfamily Combining Sites. Taos, NM, 1996.

10. Sheriff S, Chang CY, Jeffrey PD, Bajorath J & Yelton DE. Exploring and exploiting the anti-tumor monoclonal antibody BR96. Keystone Symposia on Molecular and Cellular Biology, Exploring and Exploiting Antibody and Ig Superfamily Combining Sites, 007, 13, 1996.

11. Sheriff S, Jeffrey PD, Bajorath J & Yelton DE. Exploring and exploiting the anti-tumor monoclonal antibody BR96. Immunotechnology 2, 264, 1996.

12. Stenkamp R, Aruffo A & Bajorath J. Members of protein superfamilies as targets for computer modeling. Pacific Symposium on Biocomputing , PSB Abstracts, 105, 1997.

13. Godden J, Stahura F & Bajorath J. Evaluation of protein-ligand docking strategies and scoring functions. J Mol Graph Model 16, 242, 1998.

14. Gao H, Godden J, Bajorath J. Molecular descriptors for compound clustering. 217th American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 103, 1999.

15. Bajorath J & Xue L. Molecular descriptors and fingerprints to identify molecules with similar biological activity. 219th American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 122, 2000.

16. Behnke C, Le Trong I, Godden J, Bajorath J & Stenkamp RE. Ultra high-resolution studies of human carbonic anhydrase-inhibitor complexes. 50th American Crystallographic Association National Meeting, Abstr. No W0204, 2000.

17. Bajorath J. Combinatorial libraries and chemoinformatics in drug discovery. Investigational Drugs WH 5, 50-51, 2000.

18. Stahura FL, Xue L & Bajorath J. Methods for compound selection focused on hits and application in drug discovery. 221th American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 56, 2001.

19. Owens J & Bajorath J. Integrating disciplines in the drug discovery industry. Targets 2, 45-47, 2003.

20. Furr JR, Kitchen DB, Godden JW & Bajorath J. Median partitioning for compound selection and virtual screening. 31st Northeast Regional Meeting of the American Chemical Society (NERM '03) Abstr. No 5, 49-50, 2003.

21. Godden JW & Bajorath J. Median partitioning for diversity selection, compound classification, and virtual screening. SIAM Conference on Computational Science and Engineering. MS1-Mathematical and Computational Challenges in Drug Discovery, 2003.

22. Bajorath J. Diverse fingerprints. Modern Drug Discov 2, 11, 2004.

23. Bajorath J. Novel methods for molecular similarity analysis and ligand-based virtual screening. Drugs Future 31, Suppl A, L78, 33, 2006.

24. Sisay M, Gütschow M & Bajorath J. Homology modeling and structural analysis of the catalytic domain of matriptase-2. Proceedings DPhG Annual Meeting, C03, 102, 2007.

25. Bajorath J. Foundations of molecular similarity analysis. Chem Centr J 2, S1, 2008.

26. Bajorath J. Understanding holistic approaches in molecular similarity analysis. 236th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 30, 2008.

27. Bajorath J. Systematic computational SAR analysis. Chem Centr J 3, S1, O2, 2009.

28. Lounkine E, Auer J & Bajorath J. Assessment of complex SARs using formal concept analysis of fragment combinations. Chem Centr J 3, S1, P3, 2009.

29. Stumpfe D, Geppert H & Bajorath J. Analysis of structure-selectivity relationships through single- or dual step selectivity searching using 2D molecular fingerprints. Chem Centr J 3, S1, P4, 2009.

30. Wang Y, Geppert H & Bajorath J. Complexity effects in fingerprint similarity searching. Chem Centr J 3, S1, P5, 2009.

31. Peltason L, Wawer M & Bajorath J. Quantification and visualization of structure-activity relationships at multiple levels of detail. Chem Centr J 3, S1, P6, 2009.

32. Peltason L, Hu Y & Bajorath J. From structure-activity to structure-selectivity relationships: quantitative assessment, selectivity cliffs, and key compounds. ChemMedChem 4, 1766, 2009.

33. Bajorath J. Privileged substructures revisited: target community-selective scaffolds. 240th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 41, 2010.

34. Bajorath J. Engineering and 3D protein-ligand interaction scaling of 2D fingerprints. 240th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 53, 2010.

35. Bajorath J. Analysis of activity landscapes, activity cliffs, and selectivity cliffs. 240th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 70, 2010.

36. Bajorath J. Virtual screening – success stories and challenges. XXIst International Symposium on Medicinal Chemistry, L19. Drugs of the Future 35 Suppl A, 13-14, 2010.

37. Sisay MT, Frizler M, Rodrigo V, Fustero S, Bajorath J & Gütschow M. Molecular modeling studies on the fluorophilic properties of the S2 pocket of cathepsin B. Proceedings DPhG Annual Meeting, C164, 127, 2010.

38. Lounkine E & Bajorath J. Adaptation of formal concept analysis for the systematic exploration of structure-activity and structure-selectivity relationships. J Cheminf 2, S1, P21, 2010.

39. Wawer M, Peltason L & Bajorath J. Systematic extractions of structure-activity relationship information from biological screening data. J Cheminf 2, S1, P22, 2010.

40. Bajorath J & Hu Y. Compound-centric mapping of protein-ligand interactions following molecular hierarchies. 242nd American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 164, 2011.

41. Wassermann AM & Bajorath J. A computational method to facilitate structure-activity relationship transfer. J Cheminf 4, S1, O3, 2012.

42. Dimova D & Bajorath J. Design of multi-target activity landscapes that capture hierarchical activity cliff distributions. J Cheminf 4, S1, P4, 2012.

43. Heikamp K, Wassermann AM & Bajorath J. Potency-directed similarity searching using support vector machines. J Cheminf 4, S1, P12, 2012.

44. Stumpfe D & Bajorath J. High-dimensional activity landscape representations. 244th American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 118, 2012.

45. Maggiora GM, Stumpfe D, Vogt M, Iyer P & Bajorath J. Activity cliffs, information theory, and QSAR. Corwin Hansch Symposium, 19th EuroQSAR Meeting, 2012.

46. Vogt M & Bajorath J. Statistical modeling of value distributions of similarity coefficients in virtual screening and its application to predict fingerprint search performance. J Cheminf 5, S1, O5, 2013.

47. Wawer M, Jaramillo D, Li K, Gustafsdottir S, Ljosa V, Bodycombe N, Parkin M, Sokolnicki K, Bray M-A, Winchester E, Grant G, Hon C, Duvall J, Bittker J, Dancik V, Narayan R, Subramanian A, Winckler W, Golub T, Carpenter A, Schreiber S, Shamji A, Bajorath J & Clemons P. Automated structure-activity relationship mining: connecting chemical structure to biological profiles. 245th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 5, 2013.

48. Shanmugasundaram V, Heck S, Montgomery J, Iyer P, Dimova D & Bajorath J. Characterizing activity landscapes using network-like similarity graphs to mine antibacterial data. 245th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 35, 2013.

49. Brodney MR, Heck SD, Milbank JJ, Iyer P, Dimova D, Bajorath J & Shanmugasundaram V. Multiple-property based network-like similarity graphs. 246th American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 347, 2013.

50. Bajorath J. Compound data mining in systems chemical biology: exploring multi-target activity spaces and compound promiscuity patterns. Second Annual Conference, International Chemical Biology Society, ICBS2013, Kyoto, Program, 19, 2013.

51. Bajorath J. Exploring activity cliffs in chemoinformatics and medicinal chemistry. Autumn School of Chemoinformatics, Nara, 2-5, 2013.

52. de la Vega de León A & Bajorath J. Compound optimization through data set-dependent chemical transformations. J Cheminf 6, S1, P5, 2014.

53. Furtmann N & Bajorath J. Evaluation of molecular model-based discovery of ecto-5'-nucleotidase inhibitors on the basis of X-ray structures. J Cheminf 6, S1, P13, 2014.

54. Bajorath J. Activity cliff analysis and SAR visualization. Frontiers in Medicinal Chemistry, GDCH Annual Meeting, Tübingen, Program, 38, 2014.

55. Zhang L, Starr J, Dimova D, Iyer P, Gupta-Ostermann D, de la Vega de Leon A, Bajorath J & Shanmugasundaram V. Novel applications of SAR matrices in pharmaceutical research. 247th American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 7, 2014.

56. Bajorath J. Exploring activity cliffs from a chemoinformatics perspective. Proceedings of the 4th Strasbourg Summer School on Chemoinformatics, L4, 12, 2014.

57. Namasivayam V & Bajorath J. Application of swarm intelligence to extract SAR-informative compounds with favorable physicochemical property distributions from large data sets. 248th American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 300, 2014.

58. Maggiora G, Vogt M, Iyer P & Bajorath J. Conditional structure-activity-similarity (SAS) maps. 248th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 133, 2014.

59. Müller G, Benningshof J, van Meurs P, Stumpfe D, de la Vega de León A, Furtmann N, Dimova D & Bajorath J. Synthetic and cheminformatic exploration of macrocyclic and peptidomimetic medicinal chemistry space. ChemMedChem, EFMC-ISMC, N019, 222, 2014.

60. Furtmann N, Häußler D, Bajorath J & Gütschow M. Structure-based design, synthesis, and biological evaluation of symmetrical bisbenzamidines as inhibitors of matriptase-2. ChemMedChem, EFMC-ISMC, Y019, 418, 2014.

61. Namasivayam V, Gupta-Ostermann D, Balfer J & Bajorath J. Development of prediction models for purinergic receptor compounds in different local SAR environments using emerging chemical patterns, in: Abstracts from Purines 2014. Purinergic Signal 10, 657-854, 2014.

62. Namasivayam V, Gupta-Ostermann D, Balfer J & Bajorath J. Expert system for predicting different local structure-activity relationship environments using the concept of emerging chemical patterns. 249th American Chemical Society National Meeting. Division of Computers in Chemistry, Abstr. No 136, 2015.

63. Dimova D & Bajorath J. Visualization of structure-activity relationship patterns and compound design using the SAR Matrix method. 250th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 28, 2015.

64. Vogt M, Maggiora GM & Bajorath J. Design and characterization of chemical space networks. 250th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 30, 2015.

65. Bajorath J. Complexity and heterogeneity of data for chemical information science. 250th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 110, 2015.

66. Stumpfe D, Dimova D & Bajorath J. Frequency of activity cliffs and distribution over different potency ranges. 250th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 126, 2015.

67. Dimova D, Stumpfe D & Bajorath J. Extraction of structure-activity relationship information from activity cliff clusters. 250th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 152, 2015.

68. Vogt M & Bajorath J. Improving virtual screening performance through identification of molecular descriptor features sensitive to specific biological activities. 250th American Chemical Society National Meeting. Division of Chemical Information, Abstr. No 167, 2015.

69. Bajorath J. SAR visualization, compound design, and activity predictions. 4th Autumn School of Chemoinformatics, Tokyo, 2-7, 2015.

PATENTS

1. Norinder U, Bajorath J & Stearns JF. Receptor ligands. US5567728, issued 10-22-1996.

2. Norinder U, Bajorath J & Stearns JF. 3,5,3'-triiodothyronine receptor ligands. US5585404, issued 12-17-1996.

3. Ledbetter JA, Hayden M, Linsley PS, Gilliland LK, Bajorath J & Fell HP. Expression vectors encoding bispecific fusion proteins and methods of producing biologically active bispecific fusion protein in a mammalian cell. US5637481, issued 06-10-1997.

4. Siadak A, Hollenbaugh D, Gilliland LK, Gordon M, Bajorath J & Aruffo A. Monoclonal antibodies specific for different epitopes of human gp39 and methods for their use in diagnosis and therapy. EP807175A2, issued 11-19-1997.

5. Siadak A, Hollenbaugh D, Gilliland LK, Gordon M, Bajorath J & Aruffo A. Monoclonal antibodies specific for different epitopes of human gp39 and methods for their use in diagnosis and therapy. US5876950, issued 03-02-1999.

6. Harris LJ, Bajorath J & Hsiao K-C. Humanized monoclonal antibodies. EP578515A3, issued 05-10-1999.

7. Aruffo A, Hollenbaugh D, Siadak AW, Berry K, Harris LJ, Thorne BA, Bajorath J, Wu H, Huse, WD & Watkins JD. Antibodies against human CD40. WO9942075, issued 08-28-1999.

8. Reed G, Harris L, Bajorath J, Matsueda G, Hsu M-Y & Novotny J. Chimeric, humanized and single-chain antibodies to alpha-2-antiplasmin. EP941345A2, issued 09-15-1999.

9. Starling GC, Siadak AW, Bowen MA, Aruffo A, Bajorath J, Bodian DL & Skonier JE. Monoclonal antibodies to human CD6. EP977991A1, issued 02-09-2000.

10. Peach RJ, Naemura JA, Linsley PS & Bajorath J. Soluble CTLA-4 mutant molecules and uses thereof. EP988047A1, issued 03-29-2000.

11. Aruffo AA, Hollenbaugh D, Siadak AW, Berry KK, Harris L, Thorne BA & Bajorath J. Antibodies against human CD40. US6051228, issued 4-18-2000.

12. Linsley PS, Ledbetter JA, Bajorath J, Peach RJ & Brady W. CTLA-4 molecules and IL-4 molecules and uses thereof. US6090914, issued 07-18-2000.

13. Reed G, Harris L, Bajorath J, Matsueda G, Hsu M-Y & Novotny J. Composition and method for enhancing fibrinolysis. US6114506, issued 09-05-2000.

14. Ledbetter JA, Hayden M, Linsley PS, Gilliland LK, Bajorath J & Fell HP. Expression vectors encoding bispecific fusion proteins and methods of producing biologically active bispecific fusion protein in a mammalian cell. US6132992, issued 10-17-2000.

15. Aruffo A, Hollenbaugh D, Siadak AW, Berry K, Harris LJ, Thorne BA, Bajorath J, Wu H, Huse, WD & Watkins JD. Antibodies against human CD40. US6312693, issued 11-06-2001.

16. Starling GC, Siadak AW, Bowen MA, Aruffo A, Bajorath J, Bodian DL & Skonier JE. Monoclonal antibodies to human CD6. US6372215, issued 4-16-2002.

17. Aruffo A, Hollenbaugh D, Siadak AW, Berry K, Harris L, Thorne B & Bajorath J. Methods of using antibodies against human CD40. US6413514, issued 07-02-2002.

18. Aruffo A, Hollenbaugh D, Siadak AW, Berry K, Harris L, Thorne B, Bajorath J, Huse WD, Wu H & Watkins JD. Antibodies against human CD40. US312693, issued 11-06-2002.

19. Peach RJ, Naemura J, Linsley PS & Bajorath J. Soluble CTLA-4 mutant molecules. US7094874, issued 08-22-2006.

20. Linsley PS, Ledbetter JA, Bajorath J, Peach RJ, Brady W & Damle N. Soluble CTLA-4 mutant molecules and uses thereof. US7105166, issued 12-09-2006.

21. Chen L & Bajorath J. ICOS mutants. US7235631, issued 06-26-2007.

22. Larsen CP, Pearson TC, Adams AB, Peach RJ, Linsley PS, Naemura JR & Bajorath J. Methods for protecting allogeneic islet transplant using soluble CTLA-4 mutant molecules. US7304033, issued 12-04-2007.

23. Peach RJ, Naemura JR, Linsley PS & Bajorath J. Methods for treatment using CTLA-4 mutant molecules. US7439230, issued 10-21-2008.

24. Cohen R, Peach RJ, Hagerty D, Carr S, Becker J-C, Linsley PS, Naemura JR & Bajorath J. Methods for treating immune diseases using a soluble CTLA-4 molecule. US7455835, issued 11-25-2008.

25. Famulok M, Bill A, Schmitz A & Bajorath J. Phenyl diamides and a pharmaceutical preparation comprising phenyl diamides. WO2012045734, issued 04-12-2012.

26. Peach RJ, Naemura JR, Linsley PS & Bajorath J. Soluble CTLA-4 mutant molecules and uses thereof. EP15197082.9-1408, issued 03-16-2016.