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Wikipedia profile: http://en.wikipedia.org/wiki/Antony_John_Williams

Amazon Author Page: http://www.amazon.com/Antony-J.-Williams/e/B004YRPRV2

SUMMARY

SCIENTIST, ONLINE CHEMISTRY EVANGELIST AND SENIOR EXECUTIVE

- Experienced in senior leadership and management
- Expert at bridging science and community
- Thought leader and evangelist for "Open Access Chemistry"
- Prolific author, presenter and community engagement expert
- Experienced in distributed team management of software development
- Fellow of the Royal Society of Chemistry and Microsoft eScience Awardee

EXPERIENCE

Royal Society of Chemistry *2009-now*

Vice-President of Strategic Development and Cheminformatics Manager

The Royal Society of Chemistry is one of the world's pre-eminent scientific societies and acquired the ChemSpider platform to provide access to chemistry data to the public. At the RSC my role includes overseeing all eScience cheminformatics developments, management of multiple national (UK-based) and international (Europe) grant-based projects and developing community relationships to support our eScience activities. I manage a distributed team of ten people in the USA and UK offices to deliver ChemSpider and its related projects, Open PHACTS, PharmaSea and the UK National Chemical Database Service.

ChemZoo *2007-2009*

President of ChemZoo (www.chemspider.com)

ChemZoo ws the host of ChemSpider. ChemSpider is an Open Access website established with the intention of creating a structure centric community for chemists. The website delivers access to almost 25 million unique chemical structures. It is visited by over 6000 chemists per day and with over 100,000 transactions performed per day ChemSpider is fast becoming a primary resource for chemists around the world. ChemSpider is a valuable resource to assist chemists in sourcing chemicals from vendors, accessing Open Access literature and accessing information across over 400 data sources.

Advanced Chemistry Development (ACD/Labs) *1997 – 2007*

Ten years as the leader of the management and leadership team reporting directly to the president and shareholders. During this period the software product suite was expanded from 6 applications to over 50 individual modules. Gross revenues were increased by over a factor of 10.

VP of Scientific Development and Chief Science Officer (2004-2007)

Primary leadership role in company for setting vision and defining execution strategies. Management of the individual line managers for sales, marketing, product management, customer services and fulfillment. Direct management of three product lines. Primary responsibility for identifying strategic collaborations.

VP of Scientific Development and Marketing (2001-2004), Business Development and Marketing Manager (2000), Senior Product Manager (1997-2000)

Responsibilities included: Establishing vision and managing the product management and design and implementation team for chemistry-based software products including spectroscopy processing and management (NMR, MS, IR, UV-Vis), structure drawing, physicochemical property prediction and nomenclature generation. Project lead for a web-based sample management Laboratory Information Management System (LIMS). Technical consultant to sales staff and customers for all ACD/Labs software; Worldwide on-site consultant for software; Responsible for establishing and maintaining collaborative partnerships and relationships. Managed second line managers in marketing communication and technical support staff.

Eastman Kodak Company *1992-97*

Management of 7 professional NMR spectroscopists and 2 technicians. Management of multiple laboratory facilities ($3.2M budget) including operation and support of nine NMR spectrometers Co-designer of a web-based LIMS system for managing research samples and data within the Analytical Technology Division of Eastman Kodak. Support of Kodak spectroscopy needs including research, scale-up and manufacturing support. Established worldwide NMR team including cross divisional and geographical boundaries (including Europe). Developed, maintained and documented a collaborative partnership with Varian NMR Instruments for a period of five years (delivered over $1.2 million cost savings to Kodak during this time). Present teaching courses in NMR spectroscopy to Kodak research staff. Provide an environment appropriate to teamwork and development of group dynamics. Publication of research in peer-reviewed journals and internal to Kodak. Perform and guide research to maintain state-of-the-art NMR capabilities across Kodak worldwide. Adjunct faculty member at University of Buffalo, Medicinal Chemistry department.

1990-92

NMR Facility Director, University of Ottawa, Canada

1988-90

Postdoctoral fellow, National Research Council, Ottawa, Canada
Studies: Applications of Single Crystal Electron Paramagnetic Resonance

AWARDS

- Microsoft eScience Jim Gray Award (2012)
- Fellow of the Royal Society of Chemistry (2009)
- University of London Bourne Medal for best Chemistry Thesis (1988)
- Morris Ranger Undergraduate scholarship (1983)
- Shell Research Award Grant (fully funded PhD)

EDUCATION

1982-88

PhD, Department of Chemistry, University of London, United Kingdom 1988
Thesis: Applications of High Pressure NMR to the Studies of Alkyl Chains
BSc Hons I Chemistry, Department of Chemistry, Liverpool University, United Kingdom, 1985
Thesis: NMR Studies of Electron Exchange in Vitamin E Related Systems

ARTICLES

Book author, Patented, Peer Reviewed Publications, Public Speaker

- Book author: Practical Interpretation of P-31 NMR Spectra and Computer-Assisted Structure Verification; Collaborative Computational Technologies for Biomedical Research; NMR of Natural Products (3 volume series) in preparation
- >130 publications and book chapters
- >250 Lecture presentations at conferences
- >50 poster presentations at conferences
- 2 patents granted

PERSONAL

- Two children
- Memberships: RSC, ACS, IUPAC
- Editorial Boards: Pharmaceutical Research and Journal of Cheminformatics
- Interests: Exercise (running, weight training, triathlons), Reading, Writing, Theatre
- Adjunct Professor positions at UNC Chapel Hill and North Carolina State University

Antony Williams Scientific Publications (up to April 2014)

1989

1. F.L. Lee, K.F. Preston, **A.J. Williams**, L.H. Sutcliffe, A.J. Banister, S.T. Wait' A single-crystal electron paramagnetic resonance study of the 4-phenyl-1,2,3,5-dithiadiazolyl radical *Magn. Reson. Chem*. **27**, 1161-1165 (1989).

1990

2. D.G. Gillies, S.J. Matthews, L.H. Sutcliffe and **A.J. Williams**, The Evaluation of Two Correlation Times for Methyl Groups from Carbon-13 Spin-lattice Relaxation Times and nOe Data *J. Magn. Reson*., **86**, 371 (1990)

3. P.J. Bratt, D.G. Gillies, L.H. Sutcliffe and **A.J. Williams**, NMR Relaxation Studies of Internal Motions - A Comparison between Micelles and Related Systems, *J. Phys. Chem*., **94(7)**, 2727 (1990)

4. R.C. Hynes, J.R. Morton, J.A. Hriljac, Y. LePage, K.F. Preston, **A.J. Williams**, F. Evans, M.C. Grossel and L.H. Sutcliffe, Isolated Free Radical Pairs in Rb+TCNQ- 18-crown-6 Single Crystals, *J.Chem. Soc.,Chem. Commun.*, **5**, 439 (1990)

5. P.J. Krusic, J.R. Morton, K.F. Preston, **A.J. Williams** and F. Lee, EPR Spectrum of the $Fe_2(CO)_8$- Radical Trapped in Single Crystals of $PPN^+HFe_2(CO)_8^-$, *Organometallics* **9**, 697 (1990).

6. R. Hynes, K.F. Preston, J.J. Springs, and **A.J. Williams**, Single-crystal EPR Study of Radical Pairs in $[Fe(mesitylene)_2^{2+}]$ $\{C_3[C(CN)_2]^{3-}\}_2$, *J. Chem. Phys.* **93(4)**, 2222, 1990

7. R. Hynes, K.F. Preston, J.J. Springs, and **A.J. Williams**, EPR Studies of Radical Pairs $[M(CO)_5]_2$ (M = Cr, Mo, W) Trapped in Single Crystals of PPN^+ $HM(CO)_5$-, *Organometallics*, **9**, 2298 (1990)

8. R. Hynes, K.F. Preston, J.J. Springs, and **A.J. Williams**, Electron paramagnetic resonance study of the tetracarbonyl(trimethylphosphite)tungstate(1-) radical anion trapped in a single crystal of [N(PPh3)2][W(CO)4H{P(OMe)3}], Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) **12**, 3655-61(1990)

1991

9. R. Hynes, K.F. Preston, J.J. Springs, J. Tse and **A.J. Williams**, EPR Studies of $M(CO)_5^-$ Radicals (M = Cr, Mo, W) Trapped in Single Crystals of PPh_4^+ $HM(CO)_5^-$, *J. Chem. Soc. Faraday Trans*., **87(19)**, 3121 (1991)

10. R.C. Hynes, J.R. Morton, K.F. Preston, **A.J. Williams**, F. Evans, M.C. Grossel, L.H. Sutcliffe, and S.C. Weston, An EPR Study of Isolated Free Radical Pairs in M^+ 18-Crown-6 $TCNQ^-$ salts (TCNQ:7,7,8,8-tetracyanoquinodimethane; M=K, Rb), *J. Chem. Soc. Faraday Trans*., **87(14)**, 2229 (1991)

11. L.M. Bull, D.G. Gillies, S.J. Matthews, L.H. Sutcliffe, and **A.J. Williams**, Carbon-13 NMR Relaxation Study of the Overall and Internal Motions in Compounds Containing *n*-Octyl Chains, *Magn. Reson. Chem.*, **29**, 273 (1991)

12. K.F. Preston, J.J. Springs, and **A.J. Williams,** The EPR Spectrum of $(C_5Me_5)MoCl_2(PMe_3)$

in Solution and Trapped in Single Crystals of $(C_5Me_5)MoCl(PMe_3)(N_2)$, *Inorg. Chem.*, **30**, 113 (1991)

13. J.H. MacNeil, A.C. Chiverton, S. Fortier, M.C. Baird, R.C. Hynes, **A.J. Williams**, K.F. Preston and T. Ziegler, An X-ray Crystallographic and Single-Crystal EPR Investigation of the Cationic, Iron-Centred Radical Tricarbonylbis(triphenylphosphine)iron(I). A Theoretical Examination of the Structural Preferences of Five-Coordinated Seventeen-Electron Complexes, *J. Am. Chem. Soc.*, **113**, 9834 (1991)

14. R. Hynes, K.F. Preston, J.J. Springs, and **A.J. Williams**, EPR studies of chromium tungsten carbonyl sulfur dimer, S[M(CO)5]2-, radicals (M = chromium, tungsten) trapped in single crystals of bis(triphenylphosphino)imium salt, PPN+HS[M(CO)5]2-, Organometallics, 10, 180-5 (1991)

15. R. Hynes, K.F. Preston, J.J. Springs, and **A.J. Williams,** X-Ray Crystallographic, Single-Crystal EPR, and Theoretical Study of Metal-Centred Radicals of the Type $\{C_5R_5Cr(CO)_2L\}$ (R=H,Me; L=CO, Tertiary Phosphine), *J. Am. Chem. Soc*., **113**, 542 (1991)

16. R. Hynes, K.F. Preston, J.J. Springs, and **A.J. Williams**, EPR Spectra in gamma-irradiated PPN^+ $HFeW(CO)_9^-$ Crystals, *Magn. Reson. Chem.*, **29**, 476 (1991)

17. R. Roy, F.D. Tropper and **A.J. Williams**, ^1H and ^{13}C Chemical Shift Assignments of Para-Substituted O-aryl b-D-N-acetyl glucopyranosides, *Magn. Reson. Chem.*, **29**, 852 (1991)

18. R. Duchateau, **A.J. Williams**, S. Gambarotta and M.Y.Chiang, Carbon-Carbon Double-Bond Formation in the Intermolecular Acetonitrile Reductive Coupling Promoted by a Mononuclear Titanium (II) Compound. Preparation and Characterization of Two Titanium (IV) Imido Derivatives, *Inorg. Chem*. **30**, 4863 (1991)

1992

19. J. Milne and **A.J. Williams**, Exchange Processes in Diselenium and Selenium-sulphur Dihalides, Se_2X_2, $SeSX_2$ (X = Br, Cl). A ^{77}Se 2D-EXSY Study, *Inorg. Chem.*, **31**, 4534 (1992)

20. L.A. Denys, **A.J. Williams** and G. Sachs, 2D Hetero- and Homonuclear NMR Study of a K+ Competitive Fluorescent Inhibitor of the H,K-ATPase, *Bull. Magn. Reson.*, **15**, 89 (1992)

21. J-C. Bradley, T. Durst, and A. J. Williams, Thermolysis of 2-Benzylidenebenzocyclobutenols, *J. Org. Chem.*, **57**, 6575 (1992)

1993

22. R. Roy, F.D. Tropper, **A.J. Williams** and J.R. Brisson, Global and Internal Molecular Dynamics of Poly(acrylamide-co-allyl 2-acetamido-2-deoxy-D-glucopyranosides) Glycopolymers from ^{13}C NMR Relaxation Studies, *Can. J. Chem.*, **71**, 12 (1993)

1994

23. **A.J. Williams** and J.-C. Bradley, Analysis of the C13 and H1 Spectra of Mixtures of Benzylidene Derivatives, *Magn. Reson. Chem.* **32**, 496 (1994)

24. B. Antalek, S.Song, L. Oppeheimer, **A.J. Williams**, E. Garcia and J. Texter, Cosurfactant-Induced Electron Transfer in Highly Resistive Microemulsions, *Langmuir*, **9**, 2782 (1994)

25. D.D. Miller, W. Lenhart, B. Antalek, **A.J. Williams** and M.J. Hewitt, The Use of NMR to Study Sodium Dodecyl Sulfate-Gelatin Interactions, *Langmuir*, **10**, 68 (1994)

26. B. Antalek, **A.J. Williams**, E. Garcia and J. Texter, NMR Analysis of Interfacial Structure Transitions Accompanying Electron Transfer Threshold Transitions in Reverse Microemulsions, *Langmuir*, **10**, 4459, (1994)

1995

27. R. Hynes, P.J. Krusic, K.F. Preston, J.J. Springs, **A.J. Williams** and J.S. Miller, Single Crystal EPR Study of Triplet Excitons in Tetraethylammonium 2,3,5,6 Tetracyano-p-benzoquinone. Evidence for an Interdimer Triplet Exciton, *JACS*, **117**, 2547 (1995)

28. M.R. Detty, D. Young and **A.J. Williams**, A Mechanism for Heteroatom Scrambling in the Synthesis of Unsymmetrical Chalcogenpyrilium Trimethine Dyes, *J. Org. Chem*. **60**, 6631 (1995)

29. R. Roy, F. Tropper and **A.J. Williams**, Substituent-induced chemical shifts of aromatic carbon centers in a series of non-acetylated and peracetylated para-substituted aryl 2-N-acetamido-2-deoxy-b-D-glucopyranosides, *Magnetic Resonance in Chemistry* **33**, 981 (1995)

30. M.R. Detty, M.J. Hewitt, **A.J. Williams** and M. McMillan, H-1 NMR Exchange Reactions in Te(IV) Derivatives with Cleavage of Te-N Bonds, *Organometallics* **14**, 5258 (1995)

1996

31. R.Lok, R. Leone and **A.J. Williams**, Facile Rearrangements of Alkynylamino Heterocycles with Noble Metal Cations, *Journal of Organic Chemistry* **61(10)**, 3289 (1996)

32. B. Antalek, **A.J. Williams** and J. Texter, Self-diffusion near the percolation threshold in reverse microemulsions, *Phys Rev. E*. **54 (6)**, 5913 (1996)

1997

33. B. Antalek, **A.J. Williams**, J. Texter, J. Feldman, G. Yuri and N. Garti, Microstructure Analysis at the Percolation Threshold in Reverse Microemulsions, *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **128**, 1 (1997)

34. B. Antalek, **A.J. Williams** and J. Texter, Observation of a Reverse Micelle to Sponge Phase Transition, *J. Chem. Phys.* **106**, 7869-7872 (1997)

35. D.E. Brown, **A.J. Williams** and D. McLaughlin, WIMS - A Web-based Information Management System, *Trends in Analytical Chemistry*, **16**, 370 (1997)

1998

36. **A.J. Williams**, Combining Sample, Structural, and Spectral Information in an Information Management System, *Sci. Comput. Auto*. **15**, 60 (1998).

37. M. Foster, E. Kolovanov, S. Mabury, A. Marsella and **A.J. Williams,** Log P, partition coefficients of selected benzoylphenylurea insecticides, *EnviroAnalysis* **731** (1998)

1999

38. **A.J. Williams** and A. Yerin, The Need for Systematic Naming Software Tools for Exchange of Chemical Information, *Molecules*, **9**, 255 (1999)

2000

39. M.E. Elyashberg, K.A. Blinov and A.J. Williams, Computer-aided Molecular Structure Elucidation on the Basis of 1D and 2D NMR Spectra, *Applied Magnetic Resonance*, (May 2000)

40. **A.J. Williams**, Recent Advances in NMR Prediction and Automated Structure Elucidation Software, *Current Opinion in Drug Discovery & Development* **3**, 298 (2000)

41. **A.J. Williams** and S.G. Golotvin, Improved baseline correction and modeling of FT NMR spectra, *J. Magn. Reson,* **146**, 122 (2000)

2001

42. K.A. Blinov, M.E. Elyashberg, S.G. Molodtsov, **A.J. Williams** and E.R. Martirosian, An Expert System for Automated Structure Elucidation Utilizing ^{1}H-^{1}H, ^{13}C-^{1}H, and ^{15}N-^{1}H 2D NMR correlations, *Fresenius J. Anal. Chem*., **369**, 709 (2001)

43. **A.J. Williams**, V. Lashin and M. Lee, An integrated desktop mass spectrometry processing and molecular structure management system, *Spectroscopy* **16**, 38 (2001)

2002

44. G.E. Martin, C.E. Hadden, D.J. Russell, B.D. Kaluzny, J.E. Guido, W.K. Duholke, B.A. Stiemsma, T.J. Thamann, R.C. Crouch, K.A. Blinov, M.E. Elyashberg, E.R. Martirosian, S.G. Molodtsov, **A.J. Williams**, P.L. Schiff, Jr., Identification of Degradants of a Complex Alkaloid Using NMR Cryoprobe Technology and ACD/Structure Elucidator, *J. Heterocyclic Chem*. **39**, 1241 (2002)

45. M.E. Elyashberg, K.A. Blinov, **A.J. Williams**, E.R. Martirosian, S.G. Molodtsov, Application of a New Expert System for the Structure Elucidation of Natural Products from the 1D and 2D NMR Data, *J. Nat. Prod.*, **65**, 693 (2002)

46. S. Golotvin and **A.J. Williams**, A new approach to automated first-order multiplet analysis. *Magn Reson Chem*. **40**, 331 (2002)

47. G . E. Martin, C .E. Hadden, D. J. Russell, B. D. Kaluzny, J. E. Guido, W. K. Duholke, B. A. Stiemsma, T. J. Thamann, R. C. Crouch, K. A. Blinov, M. E. Elyashberg, E. R. Martirosian, S. G. Molodotsov, **A. J. Williams**, and P. L. Schiff, Jr., Identification of Degradants of a Complex Alkaloid Using NMR Cryoprobe Technology and ACD/Structure Elucidator, *J. Heterocyclic Chem.*, **39** 1241-1250 (2002).

2003

48. D. G. Gillies, L. H. Sutcliffe and **A. J. Williams**, Variable-temperature high-pressure investigation of the cobalt-59 NMR spectroscopy of aqueous potassium hexacyanocobaltate (III) *Magn Reson Chem.* **40**, 57 (2002)

49. **A. J. Williams**. Applications of Computer Software for the Interpretation and Management of Mass Spectrometry Data in Pharmaceutical Science, *Current Topics in Medicinal Chemistry*, **2**, 99 (2002)

2003

50. K. A. Blinov, D. Carlson, M. E. Elyashberg, G. E. Martin, E. R. Martirosian, S. Molodtsov, and **A. J. Williams**, Computer-Assisted Structure Elucidation of Natural Products with Limited 2D NMR Data: Applications of the StrucEluc System, *Magn. Reson. Chem.*, **41**, 359-372 (2003).

51. G. E. Martin, D. J. Russell, K. A. Blinov, M. E. Elyashberg and **A. J. Williams**, Applications and Advances in Cryogenic NMR Probes & Computer-Assisted Structure Elucidation. *Ann. Magn. Reson.*, **2**, 1-31 (2003)

52. **A.J. Williams**. Recent Advances in NMR Prediction and Automated Structure Elucidation Software. *Current Opinion in Drug Discovery & Development*, **3,** 298 (2003)

53. K. Blinov, M. Elyashberg, E. R. Martirosian, S. G. Molodtsov, **A. J. Williams**, M. H. M. Sharaf, P. L. Schiff, Jr., R. C. Crouch, G. E. Martin, C. E. Hadden, and J. E. Guido, "Quindolinocryptotackieine: The Elucidation of a Novel Indoloquinoline Alkaloid Structure through the Use of Computer-Assisted Structure Elucidation and 2D-NMR," *Magn. Reson. Chem.,* **41**, 577-584 (2003).

54. M. E. Elyashberg, K. A. Blinov, E. R. Martirosian, S. G. Molodtsov, **A. J. Williams**, and G. E. Martin, Automated Structure Elucidation – The Benefits of a Symbiotic Relationship between the Spectroscopist and the Expert System, *J. Heterocyclic Chem*., **40**, 1017-1029 (2003).

2004

55. M. E. Elyashberg, K. A. Blinov, **A. J. Williams**, S. G. Molodtsov, G. E. Martin, and E. R. Martirosian, *Structure Elucidator:* A Versatile Expert System for Molecular Structure Elucidation from 1D and 2D NMR Data and Molecular Fragments, *J. Chem. Inf. Comput. Sci.* **44**, 771-792 (2004).

56. A. J. Simpson, B. Lefebvre, A. Moser, **A.J. Williams**, N. Larin, M. Kvasha, W. L. Kingery and B. Kelleher. Identifying residues in natural organic matter through spectral prediction & 2D NMR datasets. *Magn. Reson. Chem.* **42**, 14 (2004)

57. S. G. Molodtsov, M. E. Elyashberg, K. A. Blinov, **A. J. Williams**, E. E. Martirosian, G. E. Martin, and B. Lefebvre. Structure Elucidation from 2D NMR Spectra Using the StrucEluc Expert System: Detection and Removal of Contradictions in the Data. *J. Chem. Inf. Comp. Sci.*, **44**, 1737-1751 (2004)

58. G. J. Sharman, I. C. Jones, M. P. Parnell, M. C. Willis, M. F. Mahon, D. V. Carlson, **A. J. Williams**, M. E. Elyashberg, K. A. Blinov, S. G. Molodtsov. Automated structure elucidation of two products in a reaction of an α,β-unsaturated pyruvate. *Magn. Reson. Chem.* **42**, 567 (2004)

59. J. Meiler, B. Lefebvre, **A.J Williams** and M. Hachey. Using neural networks for 13C NMR chemical shift prediction-comparison with traditional methods. *J. Magn. Reson*. **171**, 1 (2004)

2005

60. Y. D. Smurnyy, M. E. Elyashberg, K. A. Blinov, B. A. Lefebvre, G. E. Martin, and **A. J. Williams**, Computer-Aided Determination of Relative Stereochemistry and 3D Models of Complex Organic Molecules from 2D NMR Spectra, *Tetrahedron*, **61**, 9980-9989 (2005).

61. K. A. Blinov, N. I. Larin, M. P. Kvasha, A. Moser, **A. J. Williams**, and G. E. Martin, Analysis and Elimination of Artifacts in Indirect Covariance NMR Spectra *via* Unsymmetrical Processing, *Magn. Reson. Chem.*, **43**, 999 (2005).

2006

62. K. A. Blinov, N. I. Larin, **A. J. Williams**, K. A. Mills, and G. E. Martin, Unsymmetrical Covariance Processing of COSY or TOCSY and HSQC NMR Data to Obtain the Equivalent of HSQC-COSY and HSQC-TOCSY Spectra, *J. Heterocyclic Chem.*, **43**, 145-147 (2006).

63. S. S. Golotvin, E. Vodopianov, B. A. Lefebvre, **A. J. Williams**, and T. D. Spitzer. Automated structure verification based on 1H NMR prediction**.** *Magn. Reson. Chem.*, **44**, 524 (2006)

64. K. A. Blinov, N. I. Larin, **A. J. Williams**, M. Zell, and G. E. Martin, Long-Range Carbon-Carbon Connectivity *via* Unsymmetrical Indirect Covariance Processing of HSQC and HMBC NMR Data, *Magn. Reson. Chem.*, **44**, 143-147 (2006).

65. A.J. Simpson, B. Lam, M.L. Diamond, D.J. Donaldson, B. Lefebvre, A. Moser, **A.J. Williams**, N. Larin and M. Kvasha. Assessing the organic composition of urban surface films using nuclear magnetic resonance spectroscopy. *Chemosphere*, **63**, 142 (2006)

66. M. E. Elyashberg, K. A. Blinov, **A. J. Williams**, S. G. Molodtsov, and G. E. Martin, Are Deterministic Expert Systems for Computer-Assisted Structure Elucidation Obsolete? *J. Chem. Inf. Model.* **46**, 1643-1656 (2006).

67. A. J. Simpson, W. L. Kingery, B. Lefebvre, A. Moser, **A.J. Williams**, M. Kvasha and B.P. K8elleher. The application of 1H high-resolution magic-angle spinning NMR for the study of clay-organic associations in natural and synthetic complexes. *Langmuir* **22**, 4498 (2006)

68. G. M. Rishton, K. LaBonte, **A. J. Williams**, K. Kassam and E. Kolovanov. Computational approaches to the prediction of blood-brain barrier permeability: a comparative analysis of central nervous system drugs versus secretase inhibitors for Alzheimer's disease *Current Opinion in Drug Discovery & Development*, **9**, 303 (2006)

2007

69. K. A. Blinov, **A. J. Williams**, B. D. Hilton, P. A. Irish, and G. E. Martin, The Use of Unsymmetrical Indirect Covariance NMR Methods to Obtain the Equivalent of HSQC-NOESY Data, *Magn. Reson. Chem.*, **45**, 544-546 (2007). **10.1002/mrc.1998**

70. M. E. Elyashberg, K. A. Blinov, S. G. Molodtsov, **A. J. Williams**, and G. E. Martin, Fuzzy Structure Generation: An Efficient New Tool for Computer-Aided Structure Elucidation (CASE), *J. Chem. Inf. Model*., **47**, 1053-1066 (2007). **10.1021/ci600528g**

71. G. E. Martin, P. A. Irish, B. D. Hilton, K. A. Blinov, and **A. J. Williams**, Utilizing Unsymmetrical Indirect Covariance Processing to Define ^{15}N-^{13}C Connectivity Networks, *Magn. Reson. Chem.*, **45**, 624-627 (2007). **10.1002/mrc.2029**

72. G. E. Martin, B. D. Hilton, P. A. Irish, K. A. Blinov, and **A. J. Williams**, Application of Unsymmetrical Indirect Covariance NMR Methods to the Computation of ^{13}C-^{15}N HSQC-IMPEACH and ^{13}C-^{15}N HMBC-IMPEACH Correlation Spectra of the Alkaloid Vincamine, *Magn. Reson. Chem.*, **45**, 883-888 (2007).

73. G. E. Martin, B. D. Hilton, P. A. Irish, K. A. Blinov, and **A. J. William**s, ^{13}C-^{15}N Connectivity Networks *via* Unsymmetrical Indirect Covariance Processing of ^{1}H-^{13}C HSQC and ^{1}H-^{15}N IMPEACH Spectra, *J. Heterocyclic Chem.,* **44**, 1219-1222 (2007).

74. G. E. Martin, B. D. Hilton, P. A. Irish, K. A. Blinov, and **A. J. Williams**, Using Unsymmetrical Indirect Covariance Processing to Calculate GHSQC-COSY Spectra, *J. Nat. Prod*., **70**, 1393-1396 (2007). **10.1021/np070221j**

75. G. E. Martin, B. D. Hilton, K. A. Blinov, and **A. J. Williams**, ^{13}C-^{15}N Correlation *via* Unsymmetrical Indirect Covariance NMR: Application to Vinblastine, *J. Nat. Prod.,* **2007**, *70,* 1966-1970 **10.1021/np070361t**

76. S. S. Golotvin, E. Vodopianov, R. Pol, B. A. Lefebvre, **A. J. Williams**, R. D. Rutkowske and T. D. Spitzer, Automated structure verification based on a combination of 1D 1H NMR and 2D 1H–13C HSQC spectra, *Magn. Reson. Chem.* **2007**, *45*, 803–813

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M. Bayliss, V. Lashin, **A.J. Williams**, K. Owens, Advances in the extraction of spectra and the elucidation of MS and MS/MS data to help in the characterization of structure in metabolic and impurity studies, Aug. 31 - Sept. 5, 2003, IMSC, Edinburgh, Scotland

A.J. Williams, G.E. Martin, K.A. Blinov and M.E. Elyashberg, All Good Things to Those Who Wait: Solving a Structure Computationally After 10 Years of Human Effort, Jul. 16-18, 2003, The 44th Annual Meeting of the American Society of Pharmacognosy, Chapel Hill, NC

S. Golotvin, M. Kvasha, N. Larin, E. Vodopianov, B. Lefebvre, **A.J. Williams**, Spectroscopic Validation of Structures Assisted by Prediction and auto-assignment Algorithms - Verification Analysis of High-Resolution ^{1}H and ^{13}C NMR spectra, Mar. 31 - Apr. 4, 2003, ENC, Savannah, GA

D. Mityushev, M. Kvasha, B. Lefebvre, **A.J. Williams** and G.E. Martin, ^{15}N Chemical Shift Prediction Databases, Algorithms, and Applications, Mar. 31 - Apr. 4, 2003, ENC, Savannah, GA

K.A. Blinov, M.E. Elyashberg, **A.J. Williams**, G.E. Martin, C. Hadden and D. Russell, All Good Things to Those Who Wait the Application of Automated Structure ElucidationTools to Solve a Structure after 10 Years of Effort, Mar. 31 - Apr. 4, 2003, ENC, Savannah, GA

G.E. Martin, C.E. Hadden, D.J. Russell, K. Blinov, M. Elyashberg, and **A.J. Williams**, Dusting off the Data: Solving a Challenging Structural Problem a Decade Later, Mar. 30, 2003, ACD/Labs

ENC Seminar, Savannah, GA

A.J. Simpson, M. Simpson, B. Lefebvre, A. Moser, **A.J. Williams**, S. Golotvin, M. Kvasha, W.L Kingery and B. Kelleher, Identifying Residues in Natural Organic Matter through Spectral Prediction and Pattern Matching of 2-D datasets, Mar. 30, 2003, ACD/Labs ENC Seminar, Savannah, GA

M.R. Hachey, A.Y. Bogomolov, and **A.J. Williams**, Bringing Thermal Analysis Into the Fold, Mar. 9-14, 2003, Pittcon, Orlando, FL

A.J. Bogomolov, M.R. Hachey, E. Karpushkin, **A.J. Williams**, Progress in Making Structurally Aware Software across the Electromagnetic Spectrum with a Focus on IR, Mar. 9-14, 2003, Pittcon, Orlando, FL

2004

G. E. Martin, D. J. Russell, K. A. Blinov, and **A. J. Williams**, Applications and Advances with Cryoprobes and Computer Assisted Structure Elucidation, ANZMAG Meeting, Australia, February 16, 2004.

M. Boruta, M. Hachey, A. Bogomolov, E. Karpushkin and **A.J. Williams**, IR Verification and Interpretation, Oct.19-21, 2004, ACD/Labs 5th Annual European Users' Meeting 2004 (EUM)

M. Boruta, M. Hachey, A. Bogomolov, E. Karpushkin and **A.J. Williams**, Computer Assisted Structure Verification and Interpretation of Infrared and Raman Spectra, Oct. 3-7, 2004, FACSS, Portland, OR, USA

M. Boruta, M. Hachey and **A.J. Williams,** Infrared and Raman Spectroscopy - How to Capture and Retain the Knowledge We Acquire, Oct. 3-7, 2004, FACSS, Portland, OR, USA

M. Kvasha, D. Mityushev, B. Lefebvre, A. Moser and **A.J. Williams**, Utilizing the Power of ^{31}P NMR Prediction Software for Structural Validation and Data Storage, Sept. 12, 2004, SMASH 2004 Seminar, Beaver Run Resort, Breckenridge, CO

A.J. Williams and A. Anderson, ACD/Labs Workflow Management, Automation and Intranet Tools, Sept. 12, 2004, SMASH 2004 Seminar, Beaver Run Resort, Breckenridge, CO

A. Moser, **A.J. Williams**, A. Yerin, A Systematic Nomenclature Software Suite to Support the Naming of Phosphorus-based Compounds, Jul. 4-9, 2004, ICPC 2004 (16th International Conference on Phosphorus Chemistry), Birmingham, UK

M. Kvasha, D. Mityushev, B. Lefebvre, A. Moser and **A.J. Williams**, Utilizing the Power of ^{31}P NMR Prediction Software for Structural Validation and Data Storage, Jul. 4-9, 2004, ICPC 2004 (16th International Conference on Phosphorus Chemistry), Birmingham, UK

A.J. Williams, Automation Server and Web Librarian, Jun. 3, 2004, ACD/Labs RTP Seminar, Cary, NC, USA

G.E. Martin and **A.J. Williams**, Avoiding Fortuitous Serendipity - Using ^{15}N NMR Prediction as a tool for ^{1}H-^{15}N Heteronucleus Shift Correlation Experiments, Apr. 18, 2004, ACD/Labs ENC 2004 Seminar, Pacific Grove, CA, USA

B. Lefebvre, **A.J. Williams** and S. Golotvin, Quanalyst: Visualizing Relationships between Spectral Properties in NMR Data Series, Mar. 1-2, 2004, 1st International Meeting on NMR and Quantitative Analysis, Stockholm, Sweden

A. Bogomolov, M. Hachey and **A.J Williams**, Software for Interactive Curve Resolution using SIMPLISMA, Feb. 16-20, 2004, WSC-3, Pushkinskie Gory, Russia

2005

A.J. Williams, Extracting knowledge and delivering data: From the analytical laboratory to the chemist's desktop using web-enabled technologies. 229th ACS National Meeting, San Diego, CA, United States, March 13-17, 2005, CINF-016.

A.J. Williams,. Battling the data avalanche: A chemical data management solution for the start-up company. 229th ACS National Meeting, San Diego, CA, United States, March 13-17, 2005, CINF-016.

K. A. Blinov, N. I. Larin, **A. J. Williams**, K. A. Mills, and G. E. Martin, Unsymmetrical Covariance Processing of COSY or TOCSY and HSQC NMR Data to Obtain the Equivalent of HSQC-COSY and HSQC-TOCSY Spectra, SMASH, 2005, Verona, Italy, September 25, 2005.

G.E. Martin and **A.J. Williams,** Acquiring ^{1}H-^{15}N Heteronuclear Shift Correlation Data, Oct. 18-20, 2005, EUM 2005, Obernai, France

G.E. Martin, D. Erdman, K. Blinov, A. Moser and **A.J. Williams**, Adventures with Structure Elucidator, Oct. 18-20, 2005, EUM 2005, Obernai, France

G.E. Martin, K.A. Blinov, N. Larin, M. Kvasha, A. Moser and **A.J. Williams**, M. Zell and K. Mills, Indirect Covariance NMR Spectroscopy, Oct. 18-20, 2005, EUM 2005, Obernai, France

M. O'Neil-Johnson, S. Tennant, **A.J. Williams** and R. Sasaki**,** When Should Computer-Assisted Structure Elucidation be Considered? Sept. 25, 2005, ACD/Labs SMASH 2005 Seminar, Verona, Italy

M. O'Neil-Johnson, S. Tennant, **A.J. Williams** and R. Sasaki**,** When Should Computer-Assisted Structure Elucidation be Considered? Jul. 23 - 27, 2005, 46th Annual Meeting of the American Society of Pharmacognosy, Oregon State University, Corvallis, Oregon, USA

M. Kvasha, D. Mityushev, B. Lefebvre, A. Moser and **A.J. Williams**, Utilizing the Power of ^{31}P NMR Prediction Software for Structural Validation and Data Storage, Apr. 10-15, 2005, ENC 2005 Seminar, Providence, RI, USA

M. Boruta, M. Hachey and **A.J. Williams,** Spectrum-Structure Correlation in Infrared and Raman Spectroscopy, a Corporate Resource, Feb. 28 - Mar. 4, 2005, Pittcon 2005, Orlando, FL, USA

2006

A.J. Williams, Iterative Steps Toward Automated Structural Analysis: Progress to Data and the Hurdles to Success, October 17 - 19, 2006, 7th Annual European Users' Meeting, Obernai, France

S.S. Golotvin, E. Vodopianov, R. Pol, B.A. Lefebvre, **A.J. Williams**, and T.D. Spitzer, Automated Evaluation of a Chemical Structure with Only 1D ^{1}H and 2D ^{1}H-^{13}C HSQC, September 10-13, 2006, ACD/Labs SMASH 2006 Seminar, Burlington, VT

Y.D. Smurnyy, K.A. Blinov, B.A. Lefebvre and **A.J. Williams**, The Effect of Structure Description

Schemes on Chemical Shift Prediction by Incremental and Neural Network Approaches, September 10-13, 2006, ACD/Labs SMASH 2006 Seminar, Burlington, VT

S.S. Golotvin, E. Vodopianov, R. Pol, B.A. Lefebvre, **A.J. Williams**, and T.D. Spitzer, Automated Evaluation of a Chemical Structure with only 1D ^{1}H and 2D ^{1}H-^{13}C HSQC, April 27, 2006, ACD/Labs ENC 2006, Pacific Grove, CA, USA

Y.D. Smurnyy, K.A. Blinov, B.A. Lefebvre and **A.J. Williams**, The Effect of Structure Description Schemes on Chemical Shift Prediction by Incremental and Neural Network Approaches, April 27, 2006, ACD/Labs ENC 2006, Pacific Grove, CA, USA

M. O'Neil-Johnson, S. Tennant, **A.J. Williams** and R. Sasaki, When Should Computer-Assisted Structure Elucidation be Considered? April 23, 2006, ACD/Labs ENC 2006 Academia Seminar, Pacific Grove, CA, USA

G.E. Martin, M. Zell, K.A. Mills, K.A. Blinov, N.I. Larin, M.P. Kvasha and **A.J. Williams**, Indirect Covariance NMR Spectroscopy, January 19, 2006, ACD/Labs NJ NMR Meeting, New Brunswick, NJ

2007

G. E. Martin, K. A. Blinov, and **A. J. Williams**, Unsymmetrical Indirect Covariance NMR, Experimental NMR Conference, Daytona, FL, April 23, 2007.

G. E. Martin, B. D. Hilton, P. A. Irish, K. A. Blinov, and **A. J. Williams**, NMR Outside of the Box: Unsymmetrical Indirect Covariance NMR Methods, 48th Annual Meeting of the American Society of Pharmacognosy, Portland, Maine, July 14-18, 2007, paper O16.

G. E. Martin, B. D. Hilton, P. A. Irish, K. A. Blinov, and **A. J. Williams**, NMR Outside of the Box: Applications of Indirect and Unsymmetrical Indirect Covariance NMR Processing Methods, NJ NMR Discussion Group, Iselin, NJ, September 20, 2007.

G.M. Rishton, K. LaBonte, **A.J. Williams**, K. Kassam, Karim, E. Kolovanov, Computational approaches to the prediction of blood-brain barrier permeability: Comparative analysis of CNS drugs vs. the secretase inhibitors for Alzheimer's disease. 233rd ACS National Meeting, Chicago, IL, United States, March 25-29, (2007)

R.R. Sasaki, S.S. Golotvin, B.A. Lefebvre, **A.J. Williams**, R.D. Rutkowske and T.D. Spitzer, Validating Automated Structure Confirmation in a Blind Study, September 16, 2007, ACD/Labs SMASH 2007 Seminar, Chamonix Mont-Blanc, France

B.A. Lefebvre, Y.D. Smurnyy, K.A. Blinov, M.E. Elyashberg and **A.J. Williams**, NMR Chemical Shift Prediction by Atomic Increment Based Algorithms, September 16, 2007, ACD/Labs SMASH 2007 Seminar, Chamonix Mont-Blanc, France

B.A. Lefebvre, Y.D. Smurnyy, K.A. Blinov, M.E. Elyashberg and **A.J. Williams**, NMR Chemical Shift Prediction by Atomic Increment Based Algorithms, April 22, 2007, ACD/Labs ENC 2007 Seminar, Daytona Beach, FL

R.R. Sasaki, S.S. Golotvin, B.A. Lefebvre, and **A.J. Williams**, Validating Automated Structure Confirmation in a Blind Study, April 22, 2007, ACD/Labs ENC 2007 Seminar, Daytona Beach, FL

G.E. Martin, K.A. Blinov, and **A.J. Williams**, NMR Outside of the Box: Unsymmetrical Indirect

Covariance, April 22, 2007, ACD/Labs ENC 2007 Seminar, Daytona Beach, FL

2008

B. D. Hilton, G. E. Martin, K. A. Blinov, and **A. J. Williams**, Covariance NMR Processing: Fundamentals, Applications, and Challenges, SMASH NMR Meeting, Santa Fe, NM, September, 2008.

G. E. Martin, B. D. Hilton, K. A. Blinov, and **A. J. Williams**, Covariance NMR Processing: Fundamentals, Applications, and Challenges, Eastern Analytical Symposium, New Brunswick, NJ, November 2008.

P.A. Johnson, J. Law, Z. Zsoldos, A. Simon and **A.J. Williams,** A new, automated retrosynthetic search engine: ARChem. 236th ACS National Meeting, Philadelphia, PA, United States, August 17-21 2008

K.A. Blinov, Y. Smurnyy, T. Churanova, and M. Elyashberg, B.E. Lefebvre and **A.J. Williams**, An Efficient Incremental Scheme for ^{15}N, ^{19}F, and ^{31}P Chemical Shift Prediction, March 9–14, 2008, ENC 2008, Pacific Grove, CA

A.J. Williams, Using text-mining and crowdsourced curation to build a structure centric community for chemists. Invited Presentation. 236th ACS National Meeting, Philadelphia, PA, United States, August 17-21, 2008

A.J. Williams, ChemSpider: Building a structure-centric community for chemists. Invited Presentation. 235th ACS National Meeting, New Orleans, LA, United States, April 6-10, 2008 (2008)

B. D. Hilton, G. E. Martin, K. A. Blinov, and **A. J. Williams**, Covariance NMR Processing: Fundamentals, Applications, and Challenges, Eastern Analytical Symposium. NJ, November, 2008.

2009

A.J. Williams, Crowdsourcing , Collaborations and Text Mining in a World of Open Chemistry, Conference on Semantics in Healthcare and Life Sciences, Cambridge, MA, United States, February 25-27 (2009)

A.J. Williams, Cleaning up chemistry for the pharma industry: delivering a flexible platform for interrogating the FDA DailyMed website. 237th ACS National Meeting, Salt Lake City, UT, United States, March 22-26, 2009 (2009)

A.J. Williams, Going a Mile InChI by InChI - Enabling Online Chemistry at ChemSpider, 237th ACS National Meeting, Salt Lake City, UT, United States, March 22-26, 2009 (2009)

A. J. Williams, Text Mining for Chemistry and Building a Public Platform for Document Markup, 237th ACS National Meeting, Salt Lake City, UT, United States, March 22-26, 2009 (2009)

A. J. Williams, Crowdsourcing , Collaborations and Text Mining in a World of Open Chemistry, Bio-IT Meeting, Boston, MA, United States, April 20-22 (2009)

A.J. Williams, ChemSpider as a Foundation for Crowdsourcing and Collaborations in Open Chemistry, Nature Publishing Group, New York, NY, United States May 7 (2009)

A.J. Williams, ChemSpider as a Foundation for Crowdsourcing and Collaborations in Open Chemistry, Triangle Chromatography Discussion Group, Raleigh, NC, United States, May 21 (2009)

A. J. Williams, ChemSpider: Building a Knowledge-Based Community for Chemists Using Social and Data Networking Technologies. 238th ACS National Meeting, Washington, DC, United States, August 16-20 (2009)

A. J. Williams, Building an integrated system for chemistry markup and online publishing integrated to online chemistry resources. 238th ACS National Meeting, Washington, DC, United States, August 16-20 (2009)

A. J. Williams, Oops and Downs of Resolving InChIs For the Chemistry Community. 238th ACS National Meeting, Washington, DC, United States, August 16-20 (2009)

A.J. Williams and V. Tkachenko, Enabling the World of Internet Based Chemistry Through ChemSpider, Bryn Mawr, PA, United States October 13-136 (2009)

A. J. Williams, Navigating the Complex Web of Chemistry Using ChemSpider. ACS NorthEast Regional Meeting, Hartford, CT, United States, October 7-10 (2009)

A.J. Williams, Navigating the Complex Web of Chemistry Using ChemSpider, Microsoft eScience Conference. Pittsburg, PA, United States, October 15-17 (2009)

A.J. Williams, How Internet Resources Are Providing a Collaborative Community for Chemistry, ICIC Meeting, Sitges, Spain, October 18-21 (2009)

A.J. Williams, Connecting Chemists to the Internet Through ChemSpider, RSC General Assembly, Birmingham, UK, November (2009). Invited Speaker.

A. J. Williams, Why Chemistry and the Web Will Benefit from a ChemSpider, University of Cambridge, Cambridge, UK, November (2009). Invited Speaker.

2010

A. J. Williams, Crowdsourced Chemistry – Why Online Chemistry Data Needs Your Help, ScienceOnline 2010, Research Triangle Park, North Carolina, January (2010)

A.J. Williams, ChemSpider: Collecting and Curating the World's Chemistry with the Community, Science Commons NorthWest Symposium, Microsoft Research Center, Redmond, Washington, February (2010) Invited Speaker

A. J. Williams, ChemSpider: Connecting and Curating Chemistry via Crowdsourcing. Syngenta, Jealotts Hill, Bracknell, UK, March (2010) Invited Speaker

A. J. Williams, RSC ChemSpider - Managing and Integrating Chemistry on the Internet to Build Community for Chemists, Lawrence Berkeley National Laboratory, March (2010) Invited Speaker

A.J. Williams and V. Tkachenko**,** Chemistry in your hand. Using mobile devices to access public chemistry compound data, American Chemical Society Meeting, Boston, August (2010)

A.J. Williams, ChemSpider – is this the future of linked chemistry on the internet? Boston area group for informatics and modeling, Boston, August (2010). Invited Speaker.

Sean Ekins, **A. J. Williams**, Z. Zsoldos, A. Simon, O. Ravitz and V. Tkachenko, LASSO-ing potential pregnane X receptor agonists, American Chemical Society Meeting, Boston, August (2010)

A.J. Williams, ChemSpider – A Platform to Gather, Host and Integrate Structure Based Data Across the Web, New Horizons in Toxicity Prediction, 2nd International Lhasa Symposium (October 2010), Invited Speaker

A.J. Williams, ChemSpider -Connecting and Curating Online Chemistry Resources, European Bioinformatics Institute, November (2010), Invited Speaker

A.J. Williams, ChemSpider as a Platform for Crowd Participation in Curating Chemistry, Internation Digital Curation Conference, December (2010), Invited Speaker

2011

A.J. Williams, V. Tkachenko and R. Kidd, Hosting a Compound Centric Community Resource for Chemistry Data, American Chemical Society Spring Meeting, CINF Session, Anaheim, March 2011

A.J. Williams, How the Internet Has Weaved a Web of Interlinked Chemistry Data, American Chemical Society Spring Meeting, Anaheim, March 2011, Invited Speaker

A.J. Williams, ChemSpider as an environment for teaching chemistry, American Chemical Society Spring Meeting, Anaheim, March 2011, Invited speaker

A.J. Williams, Sourcing High-Quality Online Data Resources for Computational Toxicology, Bio-IT World, Computational Toxicology Workshop 1, April 2011, Invited Speaker

J. Little, **A.J. Williams** and V. Tkachenko, Accurate Mass Measurements: Identifying "Known Unknowns" using ChemSpider, American Society of Mass Spectrometry, June 2011, Poster

A.J. Williams, ChemSpider: Integrating and Curating Internet-Based Chemistry Resources to Serve Life Scientists, PharmSciFair, Prague, Czech Republic. Keynote Presentation and invited speaker, June 2011

A.J. Williams, Mobile Chemistry and "Generation App", Infonortics ICIC 2011, Barcelona, October 2011, Invited Speaker

A.J. Williams, Navigating an Internet of Chemistry via ChemSpider, University of Arkansas Virtual Presentation

2012

A.J. Williams, Improving Online Chemistry One Structure at a Time, Astra-Zeneca, Loughborough, England, February 2012

A.J. Williams, Crowdsourcing Chemistry for the Community – 5 Years of Experiences, NFAIS Conference, “Born of Disruption: An Emerging New Normal for the Information Landscape”, February

A.J. Williams, V. Tkachenko, S. Ekins and A. Fant, ChemSpider as a Chemical Term Resolver, ACS San Diego, March 2012

A.J. Williams, The Great Promise of Navigating the Internet Using InChIs, ACS San Diego, March 2012

A.J. Williams, Social networking tools as public representations of a scientist, ACS San Diego, March 2012

A.J. Williams, Chemistry made mobile – the expanding world of chemistry in the hand, ACS San Diego, March 2012

A.J. Williams, A. Pshenichnov, V. Tkachenko and R. Oakley, Teaching NMR Spectroscopy Using Online Resources from the Royal Society of Chemistry, ACS San Diego, March 2012

A. Fant, E. Muratov, D. Fourches, D. Sharpe, **A.J. Williams** and A. Tropsha, On the Accuracy of Chemical Structures Found on the Internet, ACS San Diego, March 2012

A.J. Williams and S. Ekins, Towards a Gold Standard: Improving The Quality of Public Domain Chemistry Databases, ACS San Diego, March 2012

S. Ekins and **A.J. Williams**, Collaborative Computational Technologies for Biomedical Research: An Enabler of More Open Drug Discovery, ACS San Diego, March 2012

S. Ekins and **A.J. Williams**, Finding Promiscuous Old Drugs for New Uses, ACS San Diego, March 2012

D. Sharpe, **A.J. Williams**, A. Pshenichnov, V. Tkachenko, A. Day and S. Ekins, Serving up and consuming community content for chemists using wikis, ACS Philadelphia, August 2012

A.J. Williams, J-C. Bradley, A. Lang and V. Tkachenko, Feeding and consuming data to support open notebook science via the ChemSpider platform, ACS Philadelphia, August 2012

D. Sharpe, C. Batchelor, K. Karapetyan, V. Tkachenko and **A.J. Williams**, ChemValidator – an online service for validating and standardizing chemical structure files, ACS Philadelphia, August 2012

A.J. Williams, S.Ekins, V.Tkachenko, Mining public domain data as a basis for drug repurposing, ACS Philadelphia, August 2012

A.J. Williams, S. Ekins and V. Tkachenko, The Possibilities and Pitfalls of Internet-Based Chemical Data, ACS Philadelphia, August 2012

D. Sharpe, V. Tkachenko, C. Batchelor and **A.J. Williams**, Approaches for extraction and digital chromatography of chemical data, ACS Philadelphia, August 2012

A.J. Williams, ChemSpider – The Free Chemistry Database for the Community, Duke University, September 2012

A.J. Williams, ChemSpider SyntheticPages and the benefits of publishing chemical syntheses online. University of Southampton, UK, September 2012

A.J. Williams, S. Ekins and A. Clark, Mobile Apps for Drug Discovery, ACS San Diego, March 2012

A.J. Williams, The Possibilities and Pitfalls of Internet-Based Chemical Data, Microsoft eScience Meeting, Jim Gray Award presentation, October 2012

A.J. Williams, Chemistry Apps in the Wild and at the Royal Society of Chemistry, Pistoia Alliance Meeting, Morristown, NJ, October 2012

A.J. WIlliams, ChemSpider – The Vision and Challenges Associated with Building a Free Online Community Resource for Chemists, Merck, NJ October 2012

Sean Ekins, Joe Olechno and **A.J. Williams,** Data Quality Issues that can Impact Drug Discovery, SERMACS Meeting, Raleigh, NC, November 2012

A.J. Williams and V. Tkachenko, Connecting Chemistry Across the Internet Using ChemSpider, SERMACS Meeting, Raleigh, NC, November 2012

K. Karapetyan, C. Batchelor, V. Tkachenko and **A.J. Williams**, The Royal Society of Chemistry chemical validation and standardization platform, SERMACS Meeting, Raleigh, NC, November 2012

V. Tkachenko, Alexey Pshenichnov, Ken Karapetyan, Colin Batchelor, Jon Steele, David Sharpe and **A.J. Williams**, Creating one of the pillars of the semantic web for chemistry by curating public chemistry databases

A.J. Williams, V. Tkachenko and A. Pshenichnov, Structure verification and elucidation using the ChemSpider database, SERMACS Meeting, Raleigh, NC, November 2012

A.J. Williams, RSC ChemSpider is the online chemistry database where community contributions counts, William Patterson University, November 2012

A.J. Williams, ChemSpider – Traveling the Internet via Chemical Structures, Drexel University Online Cheminformatics Course, November 2012

2013

A.J. Williams and S.Ekins, Leading Scientists into Openness, ScienceOnline2013, Raleigh, NC

A.J. Williams, ChemSpider: a Chemistry Centric Hub to Navigate the Internet, The OBR Review, February 2013

J. Olechno, S. Ekins and **A.J. Williams**, Liquid Handling Processes Impact Computational Modeling in Drug Discovery, Pittcon, March 2013

V. Tkachenko and **A.J. Williams**, How ACDLabs Software Tools are used by the Royal Society of Chemistry, ACD/Labs User Meeting, Loughborough, UK, February

A.J. Williams, Engaging participation from the chemistry community, Board on Mathematical Sciences, National Research Council, Washington, DC, February 2013

A.J. Williams, Chemical Database Projects Delivered by RSC eScience, at the FDA Meeting regarding the "Development of a Freely Distributable Data System for the Registration of Substances", Maryland, February 2013

K. Karapetyan, V. Tkachenko, C. Batchelor, D. Sharpe and **A.J. Williams**, The RSC chemical validation and standardization platform, a potential path to quality-conscious databases, ACS Spring Meeting, New Orleans, April 2013

V. Tkachenko, C. Batchelor, K. Kapapetyan, D. Sharpe and **A.J. Williams**, ChemSpider reactions – delivering a free community resource of chemical syntheses, ACS Spring Meeting, New Orleans, April

C. Batchelor, K. Karapetyan, A. Pshenichnov, D. Sharpe, J. Steele, V. Tkachenko and **A.J. Williams,** Data Enhancing the RSC Archive, ACS Spring Meeting, New Orleans, April 2013

A. J. Williams, V. Tkachenko, A. Pshenichnov, S. Ekins, A.Day and M. Walker, Navigating scientific resources using wiki-based resources ACS Spring Meeting, New Orleans, April 2013

S. Ekins, J. Olechno and **A. J. Williams**, Dispensing Processes Profoundly Impact Biological Assays and Computational and Statistical Analyses, ACS Spring Meeting, New Orleans, April 2013

A. J. Williams, V.Tkachenko, A. Pshenichnov, W. Russell, J. Rumble and D. Leeming, Challenging, cajoling and rewarding the community for their contributions to online chemistry, ACS Spring Meeting, New Orleans, April 2013

A. J. Williams, V. Tkachenko,K. Karapetyan, A. Pshenichnov, D. Ivanov, C. Batchelor, J. Steele and D. Sharpe, ChemSpider: Disseminating data and enabling an abundance of chemistry platforms, ACS Spring Meeting, New Orleans, April 2013

E. L. Willighagen, C. Brenninkmeijer, C.T. Evelo, L. Harland, A. J. Gray, C. Goble, A. Waagmeester and **A. J. Williams,** Open PHACTS: Meaningful linking of preclinical drug discovery knowledge, ACS Spring Meeting, New Orleans, April 2013

A.J. Williams, V. Tkachenko, C. Batchelor, D. Sharpe and J. Steele, Engaging students in publishing on the internet early in their careers, ACS Spring Meeting, New Orleans, April 2013

C. Southan, **A. J. Williams** and S. Ekins, Challenges and recommendations for obtaining chemical structures of industry-provided repurposing candidates, ACS Spring Meeting, New Orleans, April 2013

C. Batchelor, K. Karapetyan, D. Sharpe, V. Tkachenko and **A.J. Williams,** Carbohydrate Structure Representation and Public Chemistry Databases, ACS Spring Meeting, New Orleans, April 2013

A.J. Williams, The Future of Scientific Information and Communication, Invited Presentation, Potsdam Academic Festival, Potsdam University, New York, April 2013

A.J. Williams, The expansive reach of ChemSpider as a resource for the chemistry community, University of Oregon, Eugene, April 2013

A.J. Williams, How to build an online profile as a scientist**,** University of Oregon, Eugene, April 2013

A.J. Williams, ChemSpider – A Combination Platform of Free Chemistry Database, Free Prediction Engines and Crowdsourcing Environment, University of Oregon, Eugene, April 2013

A.J. Williams, eScience at the Royal Society of Chemistry and our current initiatives, Cornell University, Ithaca NY. May 2013

A.J. Williams, Online social networking for the chemical sciences, Cornell University, Ithaca NY. May 2013

A.J. Williams, Royal Society of Chemistry projects underpinning Open Innovation, RSC Open Innovation Day for the Public, London, June 2013

C. Batchelor, K. Karapetyan, V. Tkachenko and **A.J. Williams**, Validation and standardization of molecular structures in general and sugars in particular: a case study, 6th Joint Sheffield Conference on Chemoinformatics, July 2013

A. Gray, C. Brenninkmeijer, C. Evelo, C. Goble, P. Groth, S. Pettifer, R. Stevens, **A.J. Williams,** E. Willighagen, K. Wolstencroft, Scientific Lenses: An Approach to Dynamically Vary the Relationship between Datasets, 21st Annual International Conference on Intelligent Systems for Molecular Biology, July 2013

A.J. Williams (on behalf of the Open PHACTS symposium), Practical semantics in the pharmaceutical industry – the Open PHACTS project, ACS Fall Meeting, Indianapolis, September 2013

K. Karapetyan, C.Batchelor, V.Tkachenko and **A.J. Williams**, An investigation of tautomerization and its impact on the content and data model for RSC ChemSpider, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, V. Tkachenko, C. Batchelor and A. Pshenichnov, Accessing chemical health and safety data online using Royal Society of Chemistry resources, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, @ChemConnector and my personal experiences in participating in the expanding social networks for science, ACS Fall Meeting, Indianapolis, September 2013

V. Tkachenko, A. Pshenichnov, Jon Steele and **A.J. Williams**, The importance of standards for data exchange and interchange on the Royal Society of Chemistry eScience platforms, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, V. Tkachenko, D. Ivanov and A. Pshenichnov, Acknowledging and rewarding participation of the community in developing online resources for chemistry, ACS Fall Meeting, Indianapolis, September 2013

V. Tkachenko, C. Batchelor, J. Steele, A. Pshenichnov, **A.J. Williams**, Building support for the semantic web for chemistry at the Royal Society of Chemistry, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, D. Lowe, C. Batchelor and V. Tkachenko, ChemSpider reactions – developing the world's largest free access online resource of chemical syntheses, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, V. Tkachenko, A. Pshenichnov, R. Kidd, J. Stevens, D. Ging and D. James, The national chemical database service of the United Kingdom, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, V. Tkachenko, D. Ivanov, W. Russell, A. Clark and S. Ekins, Apps and approaches to mobilizing chemistry from the Royal Society of Chemistry, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, G.E. Martin, V. Tkachenko and A. Pshenichnov, The importance of standards in supporting articles of the future, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, The social profile of a chemist online – the potential profits of participation, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, C. Batchelor, W. Brouwer and V. Tkachenko, Digitizing documents to provide a public spectroscopy database, ACS Fall Meeting, Indianapolis, September 2013

A.J. Williams, The Big Data Challenges Associated with Building a National Data Repository for Chemistry, ICIC Meeting, Venice, October 2013

A.J. Williams, Facilitating Scientific Discovery through Crowdsourcing and Distributed Participation, NETTAB (Network Tools and Applications in Biology), Venice, October 2013

A.J. Williams, eScience Resources for the Chemistry Community from the Royal Society of Chemistry, North Carolina State University, Raleigh, NC, October 2013

A.J. Williams, Online Social Networking for the Sciences: How an Average Scientist Makes Himself Visible, North Carolina State University, Raleigh, NC, November 2013

C. Goble, A. J. G. Gray, L. Harland, K. Karapetyan, A. Loizou, Y. Rankka, S. Senger, V. Tkachenko, **A.J. Williams** and E. Willighagen, Incorporating Private and Commercial Data into an Open Linked Data Platform for Drug Discovery, The 12th International Semantic Web Conference and the 1st Australasian Semantic Web Conference, 21-25 October 2013, Sydney, Australia

A. Day, A. Pshenichnov, K. Karapetyan, C. Batchelor, P. Corbett, J. Steele, V. Tkachenko and **A.J. Williams** , Royal Society of Chemistry Activities to Develop a Data Repository for Chemistry-Specific Data, ACS Spring Meeting, Dallas, March 2014

A.J. Williams, C. Batchelor, P. Corbett, J. Steele and V. Tkachenko, Ontology work at the Royal Society of Chemistry, ACS Spring Meeting, Dallas, March 2014 (Invited Talk)

A. Day, A. Pshenichnov, K. Karapetyan, C. Batchelor, P. Corbett, J. Steele, V. Tkachenko and **A.J. Williams** , Royal Society of Chemistry developments to support open drug discovery ACS Spring Meeting, Dallas, March 2014 (Invited Talk)

S. Ekins, R.C. Reynolds, **A.J. Williams**, A.M. Clark and J.S. Freundlich, Looking Back at *Mycobacterium tuberculosis* Mouse Efficacy Testing To Move New Drugs Forward, ACS Spring Meeting, Dallas, March 2014 (Invited Talk)

A.J. Williams, A. Pshenichnov and V. Tkachenko, Accessing Royal Society of Chemistry resources and making chemistry mobile, ACS Spring Meeting, Dallas, March 2014

A.J. Williams, C. Batchelor, P. Corbett, K. Karapetyan and V. Tkachenko, Data enhancing the Royal Society of Chemistry publication archive, ACS Spring Meeting, Dallas, March 2014

A.J Williams, V. Tkachenko and R. Kidd, The UK National Chemical Database Service – an integration of commercial and public chemistry services to support chemists in the United Kingdom, ACS Spring Meeting, Dallas, March 2014

D. Hinks, N. Vinueza, D.C. Muddiman and **A.J. Williams**, Cheminformatics for Dye Chemistry Research: Bringing Online an Unprecedented 100,000 Sample Dye Library, POSTER, ACS Spring Meeting, Dallas, March 2014

D. Hinks, N. Vinueza and **A.J. Williams**, Cheminformatics for Dye Chemistry Research: Bringing Online an Unprecedented 100,000 Sample Dye Library, ACS Spring Meeting, Dallas, March 2014

V. Tkachenko, K. Karapetyan, J. Steele, A. Pshenichnov and **A.J. Williams**, The application of cloud computing to royal society of chemistry data platforms, ACS Spring Meeting, Dallas, March 2014

V. Tkachenko, C. Batchelor, P. Corbett, K. Karapetyan, A. Pshenichnov and **A.J. Williams**, Building a semantic chemistry platform with the royal society of chemistry, ACS Spring Meeting, Dallas, March 2014

Patents

United States Patent	2003-382461
Dugdale , et al.	APPLICATION

Apparatus and method for encoding chemical structure information.

Abstract
A method of encoding chem. information into a symbol, like a bar code, is provided such that the generated symbol represents the chem. structure information. A processor can be used to generate a string that describes chem. structure information. The string can then be sent to a homogenizer, which creates a standardized data format. The standardized data format can then be passed to a symbol generating function, which creates a symbol that encodes the chem. structural information. A scanner can then be used to decode the symbol, revealing the chem. structural information.

Inventors: Dugdale; Ian, Tkachenko; Valery, Williams; Antony J.

Assignee: Advanced Chemistry Development

Appl. No.: 02003-382461

Filed: March, 3 2003

United States Patent 6,040,129
Godleski , et al. March 21, 2000

Photographic emulsion having an improved speed, photographic element containing said emulsion, and method

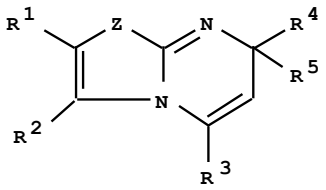
Abstract
A photographic emulsion comprising dispersed in a binder sensitized silver halide grains wherein the emulsion is sensitized from an organometallic compound of formula: wherein M is a metal selected from the group consisting of lead, tin, boron, bismuth and thallium, each R is independently an alkyl group, a cycloalkyl group, an aryl group, a heterocyclic group, an alkenyl group or a alkynyl group, each X is independently halogen, hydroxy, or alkoxy, n is 1 to 4 and m is 0 to 3, with the proviso that when M is lead or tin, n is 1 to 4 and m+n is 4, when M is boron or bismuth, n is 1 to 3 and m+n is 3 and when M is thallium, either n is 1 and m is 0, or n is 1 to 3 and n+m is 3.

Inventors: Godleski; Stephen A. (Fairport, NY), Dickinson; David A. (Brockport, NY), Williams; Antony J. (West Henrietta, NY)
Assignee: Eastman Kodak Company (Rochester, NY)
Appl. No.: 09/288,900
Filed: April 9, 1999

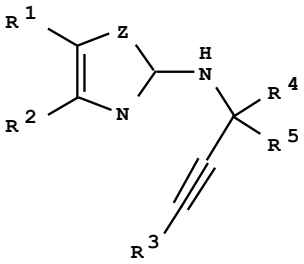
United States Patent 5,576,432
Lok , et al. November 19, 1996

Process for the manufacture of dihydropyrimidines

Abstract
A process of preparing a dihydropyrimidine compound of the structure (I): I wherein R.sup.1 and R.sup.2 are bonded together to form an aromatic or heterocyclic ring, which may be substituted or unsubstituted, or are individually selected from the group consisting of hydrogen, or a substituted or unsubstituted aliphatic, carbocyclic, or heterocyclic group; R.sup.3, R.sup.4 and R.sup.5 are individually selected from the group consisting of hydrogen or a substituted or unsubstituted aliphatic, carbocyclic or heterocyclic group; and X represents the atoms necessary to form a 5 or 6 membered heterocyclic ring, and is selected from the group consisting of oxygen, sulfur, selenium, II wherein R.sup.6, R.sup.7, and R.sup.8 are individually selected from the group consisting of a substituted or unsubstituted aliphatic, carbocyclic or heterocyclic group; comprising combining a compound (A) of the structure: ##STR3## wherein X, R.sup.1, R.sup.2, R.sup.3, R.sup.4, R.sup.5, R.sup.6, R.sup.7, and R.sup.8 are as previously defined, with a catalytic amount of a Group 11 or 12 metal cation catalyst at a temperature of less than about 50.degree. C. and in the presence of an organic solvent, to form compound (I).



I



II

Inventors: Lok; Roger (Rochester, NY), Williams; Antony J. (Rochester, NY)
Assignee: Eastman Kodak Company (Rochester, NY)
Appl. No.: 08/363,148
Filed: December 23, 1994