Gregory A. Landrum, Ph. D.

Spalenring 11, Basel 4055, Switzerland
tel: +41 79 445 8118
greg@landrumdecker.com
http://www.linkedin.com/pub/greg-landrum/1/422/276

Major Accomplishments

- Led a global team of chemists, cheminformaticians, software developers, and external partners to design, deliver, and support chemistry-centric informatics solutions that accelerate the drug-discovery process. Collaborated with scientists to design and implement cutting-edge tools to help drug-discovery project teams access their data and make decisions more effectively.
- Worked as co-lead in a global cross-functional initiative to develop and implement a multi-year cheminformatics strategy for a major pharmaceutical company; acted as project manager for the implementation of the strategy using a combination of in-house experts and contractors. Initiated and managed external partnerships to develop new algorithms and scientific tools supporting drug discovery.
- Invented new algorithms for machine learning, descriptor calculation, and library design for application to chemical and pharmaceutical discovery.
- Designed and led the implementation of the RDKit: an open source, object-oriented cheminformatics toolkit including scripting-language integration, a database cartridge, 2D depiction, and 3D structure generation and optimization. Created and supported an active community of contributors from academia and industry.
- Co-founded and managed a small discovery organization; developed and maintained partnerships with a number of pharmaceutical companies and research organizations for continuing development and support of novel, applied technologies for drug discovery. Helped invent, implement, and validate a powerful methodology for predictive ADME/Tox. Managed a successful multi-year R&D contract with the U.S. Air Force; developed expertise in writing and managing successful SBIR grants and contracts.

Employment History

Jan 2011 - Present: **Global Head Chemical Information Systems at Novartis Institutes for BioMedical Research in Basel Switzerland**
Direct management of a global team of chemists, cheminformaticians, software developers, and post-docs; member of CIO's Senior Leadership Team; evolved the strategy of the Chemical Information Systems group to move beyond supporting operational and LIMS systems and into informatics; responsibility for developing, deploying, and supporting software and informatics solutions for medicinal chemists and drug-discovery teams; managed relationships with external collaborators and vendors; drove implementation and global deployment of a new generation of query and reporting tools for drug-discovery project teams; other major projects under my leadership include: development of a new compound registration system, development of a new corporate reaction database, global replacement of ISIS software with other tools; worked across teams in the Research IT organization to help develop a new model for supporting global applications.

July 2006 – Dec 2010: **Senior Investigator I (from May 2010), Research Investigator II at Novartis Institutes for BioMedical Research in Basel Switzerland**
Direct management of three Ph.D. scientists (from Nov. 2009); leadership of a global matrix team to implement a multi-year cheminformatics strategy; worked at the interface of medicinal chemistry, analytical chemistry, computational chemistry, and research informatics to develop and deliver new algorithms and tools for drug discovery.

Oct 2000 – May 2006: **Co-founder of Rational Discovery LLC**
Designed and helped implement a suite of software tools for cheminformatics, combinatorial library design, machine learning, and chemical descriptor calculation. Proposed, planned, and managed government and private R&D grants and contracts. Worked collaboratively with scientists at client sites to define, and refine, project specifications. Recruited and led a team of scientists to develop new algorithms and technology for computational ADME/Tox, drug discovery, and material science.

Dec 1999 – May 2000: **Sr. Research Scientist at DuPont Pharmaceutical Research**

Laboratories (formerly CombiChem, Inc.) in Palo Alto, CA
Spearheaded a project to design and develop graphical tools for computational drug design. Collaborated with application scientists to design and implement computational-geometry and visualization tools as part of a combinatorial library design/analysis project. Responsible for the education of application scientists and management in the capabilities and use of object-oriented scripting and modeling tools.

Aug 1999 – Dec 1999: **Research Scientist at Aperion Technologies LLC/CombiChem, Inc., in Palo Alto, CA**
Participated in a multi-disciplinary team involving four companies and academic collaborators to define and plan an Advanced Technology Program-funded project to develop an integrated computational/experimental program for combinatorial catalyst discovery. Key contributor to a team developing a strategy for applying computational methods from the pharmaceutical industry to the material-science arena.

Aug 1997 – Aug 1999: **Postdoctoral Research Scientist at the Rheinisch-Westfälische Technische Hochschule Aachen, Germany**
Worked with solid-state chemists and materials scientists to understand and predict experimental data. Helped manage the computational-chemistry subgroup of a large research group. Trained and supervised undergraduate researchers. Developed and taught a computational chemistry mini-course for undergraduates.

Education

- Ph.D. in Chemistry, Cornell University, Ithaca NY. Thesis title: *Electronic Structure and Bonding in Molecules, Intermetallic Phases, and Other Extended Systems*. Advisor: Prof. Roald Hoffmann
- B.S. with Honors in Chemistry/Computer Science Track, Carnegie-Mellon University, Pittsburgh PA. Thesis title: *A Ligand Field Model for Magnetic Circular Dichroism Spectra of Biological Cupric Complexes.* Advisor: Prof. James Whittaker

References

Available upon request

Open-source Software Projects

3. KNIME: http://www.knime.org Contributor since 2011
2. RDKit: http://www.rdkit.org Project owner since 2006
1. YAeHMOP: http://yaehmop.sourceforge.net Project owner since 1996

Scientific Publications and Presentations

ORCID profile: http://orcid.org/0000-0001-6279-4481

Publications

35. Riniker, S; Landrum, G. A. “Similarity maps - a visualization strategy for molecular fingerprints and machine-learning methods” submitted to *Journal of Cheminformatics* 2013.
34. Riniker, S; Landrum, G. A. “Open-source platform to benchmark fingerprints for ligand-based virtual screening” *Journal of Cheminformatics* 2013 **5** 26. http://dx.doi.org/10.1186/1758-2946-5-26
33. Landrum, G. A.; Stiefl N. “Is that a scientific publication or an advertisement? Reproducibility, source code and data in the computational chemistry literature” *Future Medicinal Chemistry* 2012 **4** 1885-1887. [Invited editorial]
32. Hariharan, R.; Jankiraman, A.; Nilakantan R.; Singh, B.; Varghese S.; Landrum, G.A.; Schuffenhauer A. “MultiMCS: A Fast Algorithm for the Maximum Common Substructure Problem on Multiple Molecules.” *Journal of Chemical Information and Modeling* 2011 **51** 788-806.
31. Vulpetti, A.; Landrum, G. A.; Rüddiser S.; Erbel, P.; Dalvit, C. “19F NMR Chemical Shift Prediction with Fluorine Fingerprint Descriptor” *Journal of Fluorine Chemistry* 2010 **131** 570-577.
30. Zécri, F. J.; Albert, R.; Landrum, G. A.; Hinterding, K.; Cooke, N. G.; Guerini, D.; Streiff, M.; Bruns, C.; Nuesslein-Hildesheim, B. “Pyrazole derived from (+)-3-Carene; a Novel Potent and

Selective Scaffold for Sphingosine-1-Phosphate ($S1P_1$) Receptor Agonists" *Bioorganic & Medicinal Chemistry Letters* 2010 **20** 35-37.

29. Vulpetti, A.; Hommel, U.; Landrum G. A.; Lewis R.; Dalvit C. "Design and NMR-based screening of LEF, a library of chemical fragments with different local environment of fluorine" *Journal of the American Chemical Society* 2009 **36** 12949-12959.
28. Landrum, G. A., Penzotti, J. E., Putta S. "Feature-map vectors: a new class of informative descriptors for computational drug discovery" *Journal of Computer-Aided Molecular Design* 2007 **20** 751-762. (Invited Paper)
27. Putta, S.; Landrum, G. A.; Penzotti, J. E. "Conformation mining: an algorithm for finding biologically relevant conformations" *Journal of Medicinal Chemistry* 2005 **48** 3313-3318.
26. Landrum, G. A.; Penzotti, J. E.; Putta, S. "Machine-learning models for combinatorial catalyst discovery" *Measurement Science and Technology* 2005 **16** 270-277. (Invited Paper)
25. Landrum, G. A.; Penzotti, J. E.; Putta, S. "Machine-learning models for combinatorial catalyst discovery" *Materials Research Society Symposium Series* 2004 **804** Paper JJ11.5. (Invited Paper)
24. Penzotti, J. E.; Landrum, G. A., Putta, S. "Building predictive ADMET models for early decisions in drug discovery." *Current Opinions in Drug Discovery and Development* 2004 **7** 49-61. (Invited Paper)
23. Landrum, G. A.; Genin, H. "Application of machine-learning methods to solid-state chemistry: ferromagnetism in transition metal alloys." *Journal of Solid State Chemistry* 2003 **176** 587-593. (Invited Paper)
22. Landrum, G. A.; Genin, H. "The Rational Discovery Framework: A Novel Tool for Computationally Guided High-Throughput Discovery" *Materials Research Society Symposium Series* 2002 **700** Paper S7.6.
21. Landrum, G. A.; Dronskowski, R. "Reply to: 'Itinerant Ferromagnetism of the Transition Metals -- our Present Understanding' by Gernot Stollhoff, or: The Limits of Reductionism." *Angewandte Chemie* 2000 **112** 4647-4649;*Angewandte Chemie International Edition* 2000 **39** 4475-4476.
20. Decker, A.; Landrum, G. A.; Dronskowski, R. "Peierls and Spin-Peierls Distortions in the Elements (B): The Antiferromagnetism of Chromium." *Zeitschrift für anorganische und allgemeine Chemie* 2002 **628** 303-309.
19. Decker, A.; Landrum, G. A.; Dronskowski, R. "Peierls and Spin-Peierls Distortions in the Elements (A): The Crystal Structure of Tellurium." *Zeitschrift für anorganische und allgemeine Chemie* 2002 **628** 295-302.
18. Landrum, G. A.; Dronskowski, R. "The orbital origins of magnetism: from atoms to molecules to ferromagnetic alloys." *Angewandte Chemie* 2000 **112** 1598-1627; *Angewandte Chemie International Edition* 2000 **39** 1560-1585. (Invited Paper)
17. Zumdick, M. F.; Landrum, G. A.; Dronskowski, R.; Hoffmann, R.-D.; Pöttgen, R.; "Structure, Chemical Bonding, and Properties of $ZrIn_2$, $IrIn_2$, and $Ti_3Rh_2In_3$." *Journal of Solid State Chemistry* 2000, **150** 19-30.
16. Landrum, G. A.; Dronskowski, R. "Ferromagnetism in Transition Metals: A Chemical Bonding Approach." *Angewandte Chemie* 1999 **111** 1481-1485; *Angewandte Chemie International Edition* 1999 **38** 1389-1393.
15. Landrum, G. A.; Dronskowski, R.; Niewa, R.; DiSalvo, F. J. "Electronic Structure and Bonding in Ce (Nitride) Compounds: Trivalent versus Tetravalent Cerium." *Chemistry, A European Journal* 1998 **5** 515-522.
14. Hoffmann, R.-D.; Pöttgen, R.; Landrum, G. A.; Dronskowski, R.; Künnen, B.; Kotzyba, G. "Syntheses, Structure, Chemical Bonding and Properties of $CaTIn_2$ (T=Pd, Pt, Au)" *Zeitschrift für anorganische und allgemeine Chemie* 1998 **625** 789-798.
13. Landrum, G. A.; Eck, B.; Dronskowski, R. "Why is Nitrogen so Different?" Structure, Bonding, and Magnetic Properties of Some Model Nitrides, Carbides, and Phosphides." *Materials Science Forum* 2000 **325-326** 105-110.
12. Landrum, G. A.; Evers, J.; Boysen, H.; Hoffmann, R. "The TiNiSi Family of Compounds: Structure and Bonding." *Inorganic Chemistry* 1998 **37** 5754-5763.
11. Landrum, G. A.; Goldberg, N.; Hoffmann, R.; Minyaev, R. M. "Intermolecular Interactions

Between Hypervalent Molecules: Ph_2IX and XF_3 (X=Cl, Br, I) Dimers." *New Journal of Chemistry* 1998 883-890.

10. Landrum, G. A.; Hoffmann, R. "Secondary Bonding between Chalcogens or Pnicogens and Halogens." *Angewandte Chemie* 1998 **110** 1989-1992; *Angewandte Chemie International Edition* 1998 **37** 1887-1890.
9. Landrum, G. A.; Goldberg, N.; Hoffmann, R. "Bonding in the Trihalides (X_3^-), Mixed Trihalides (X_2Y^-), and Hydrogen Bihalides (X_2H^-). The Connection Between Hypervalent, Electron-Rich Three-Center, Donor-Acceptor, and Strong Hydrogen Bonding." *Journal of the Chemical Society: Dalton Transactions* 1997 3605-3613.
8. Landrum, G. A.; Goldberg, N.; Hoffmann, R. "The Electronic Structure of $[Te_{15}Br_4][MoOBr_4]_2$ and Some General Aspects of Bonding in 'Classical' and Hypervalent Tellurium Halides." *Chemische Berichte* 1997 **130** 463-471.
7. Wang, S.; Mitzi, D. B.; Landrum, G. A.; Genin, H.; Hoffmann, R. "Synthesis and Solid State Chemistry of CH_3BiI_2: A Structure with an Extended One-Dimensional Organometallic Framework." *Journal of the American Chemical Society* 1996 **119** 724-732.
6. Nuspl, G.; Polborn, K.; Evers, J.; Landrum, G. A.; Hoffmann, R. "The Four-Connected Net in the $CeCu_2$ Structure and its Ternary Derivatives -- its Electronic and Structural Properties." *Inorganic Chemistry* 1996 **35** 6922-6932.
5. Röder, H.; Silver, R. N.; Kress, J. D.; Landrum, G. A.; Drabold, D.; Dong, J. J. "The Kernel Polynomial Method for Non-Orthogonal Electronic Structure Calculations." *Simulation Multiconference, 1996 Proceedings*, 1996.
4. Chu, F.; Jian, Q.X.; Landrum, G. A.; Wu, X. D.; Hawley, M.; Mitchell, T.E. "Microstructures and Electrical Properties of $SrRuO_3$ Thin Films on $LaAlO_3$ Substrates." *Journal of Electronic Materials* 1996 **25** 1754-1759.
3. Landrum, G. A. "YAeHMOP: Yet Another extended Hückel Molecular Orbital Package." A package for performing eHT calculations on molecules and extended systems and visualizing the results. YAeHMOP is freely distributed and is in use in a number of research groups around the world, 1995.
2. Landrum, G. A.; Ekberg, C.A.; Whittaker, J.W. "A Ligand Field Model for MCD Spectra of Biological Cupric Complexes." *Biophysical Journal* 1995 **69** 674-689.
1. Gassner, T. G.; Ballou, D. P.; Landrum, G. A.; Whittaker J. W., "Magnetic Circular Dichroism Studies on the Ferrous Active Site of Phthalate Dioxygenase from *Pseudomonas cepacia* Show a Change of Ligation State on Substrate Binding." *Biochemistry* 1993 **32** 4820-4825.

Presentations

24. "From a walled-off flood to a public explosion: chemical data for the life sciences." Public Symposium on Data Analysis in the Life Sciences, Konstanz Germany, June 2013. (Invited)
23. "Reproducibility in cheminformatics and computational chemistry research: Certainly we can do better than this." 8th German Conference on Cheminformatics, Goslar Germany, November 2012. American Chemical Society 2013 Spring Meeting, New Orleans LA, April 2013. (Invited)
22. "A new system for searching legacy and ELN reaction data." ChemAxon UGM, Budapest Hungary, May 2012. (Invited)
21. "It doesn't have to be a one-way street: Open-source software for drug discovery from big pharma." American Chemical Society 2012 Spring Meeting, San Diego CA, March 2012. (Invited)
20. "KNIME in NIBR: Stories from Industry." 2012 KNIME Users Group Meeting, Zurich CH, February 2012. (Invited)
19. "The RDKit and PostgreSQL: an open-source database system for chemistry." 5th Meeting on US Government Chemical Databases and Open Chemistry, Frederick MD, Aug 2011. (Invited)
18. "RDKit, PostgreSQL, and Knime: Open-source cheminformatics in big pharma." MIOSS 2011, Hinxton UK, May 2011. (Invited)
17. "The RDKit: open source cheminformatics now for Knime too!" 2011 KNIME Users Group Meeting, Zurich CH, March 2011. (Invited)
16. "Making sure there's a 'give' associated with the 'take': producing and using open-source

software in a large pharma company" 6th German Conference on Cheminformatics, Goslar Germany, November 2010.

15. "Application of computational methods to the design and optimization of selective S1P1 receptor agonists" American Chemical Society 2010 Spring Meeting, San Francisco CA, March 2010.
14. "The Snake that Fits Your Brain" American Chemical Society 2009 Fall Meeting, Washington DC, August 2009. (Invited)
13. "Feature-map vectors: A new family of informative and interpretable descriptors for drug discovery." American Chemical Society 2006 Spring Meeting, Atlanta GA, March 2006. (invited)
12. "Learning From Library Design" American Chemical Society 2005 Spring Meeting, San Diego CA, March 2005.
11. "Predictive models for CDK2 inhibition: Using crystal structures, machine learning, and novel pharmacophore descriptors to build models for library design." EChemInfo 2004, October 2004. (Invited)
10. "Machine-Learning Models for Combinatorial Catalyst Discovery" American Chemical Society 2004 Spring Meeting, Anaheim CA. April 2004. (Invited)
9. "Machine-Learning Models for Combinatorial Catalyst Discovery" Materials Research Society 2003 Fall Meeting, Boston MA. December, 2003. (Invited)
8. "Machine-learning Models for High-Throughput Materials Discovery" American Chemical Society 2003 Spring Meeting, New Orleans LA. March, 2003.
7. "A Life Preserver for the Data Flood" American Chemical Society 2003 Spring Meeting, New Orleans LA. March, 2003.
6. "Machine-learning Models for Predicting Chemical Toxicity" with Julie Penzotti. American Chemical Society 2003 Spring Meeting, New Orleans LA. March, 2003.
5. "A Machine-Learning Methodology for High-throughput Discovery" Gordon Research Conference: Combinatorial and High Throughput Materials Science, Meriden NH. July, 2002. (Invited)
4. "The Rational Discovery Framework: A Novel Tool for Computationally Guided High-Throughput Discovery" Materials Research Society 2001 Fall Meeting, Boston. November, 2001.
3. "Ferromagnetism in Transition Metals: A Chemical Bonding View" Fifth World Conference of Theoretically Oriented Chemists, London, UK. August, 1999.
2. "Why is Nitrogen so Different?" Structure, Bonding, and Magnetic Properties of Some Model Nitrides, Carbides, and Phosphides." International Symposium on Nitrides II, Limerick, Ireland. June, 1998.
1. "Ce^{3+} versus Ce^{4+}, the Importance of d-orbitals." Hemdsärmel Kolloquium (German Solid State Chemistry Conference), Giessen, Germany. March, 1998.