

Antonia F. Stepan, Ph.D.

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4070 Basel, Switzerland

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Employment

10/2018–present	Section Head Medicinal Chemistry, Roche, Basel, Switzerland
11/2017–09/2018	Principal Scientist, Immunology & Respiratory Medicinal Chemistry, Boehringer Ingelheim, Biberach an der Riß, Germany
04/2015–10/2017	Senior Principal Scientist, Neuroscience & Pain Medicinal Chemistry, Pfizer, Cambridge, USA
07/2012–03/2015	Principal Scientist, Neuroscience Medicinal Chemistry, Pfizer, Cambridge, USA
01/2010–06/2012	Senior Scientist, Neuroscience Medicinal Chemistry, Pfizer, Groton, USA
12/2008–01/2010	Senior Scientist, Antibacterials Medicinal Chemistry, Pfizer, Groton, USA

Education

10/2006–10/2008	The Scripps Research Institute, La Jolla, USA Postdoctoral research in the Professor K. C. Nicolaou group
05/2003–09/2006	University of Cambridge, UK Ph.D. research in the Professor Steven V. Ley group
10/2000–04/2003	ETH Zürich, Switzerland Diploma in Chemistry
04/1998–06/2000	Ruprecht-Karls-University Heidelberg, Germany Pre-Diploma ('Vordiplom') in Chemistry

Publications and Patents

Independent Career Publications (2008–present)

52. 'Late-Stage Functionalization and its Impact on Modern Drug Discovery'
David F. Nippa, Remo Hohler, [Antonia F. Stepan](#), Uwe Grether, David B. Konrad,* Rainer E. Martin*
Chimia **2022**, 76, 25
51. 'Small-Molecule Lead-Finding Trends across the Roche and Genentech Research Organizations'
Peter S. Dragovich,* Wolfgang Haap,* Melinda M. Mulvihill, Jean-Marc Plancher, [Antonia F. Stepan](#)
J. Med. Chem. **2022**, 65, 3606
50. 'Direct C–H Functionalization Approaches to Pharmaceutically Relevant Molecules'
James J. Mousseau, [Antonia F. Stepan](#)*
Green Chemistry in Drug Discovery, From Academia to Industry Springer Nature **2021**, 269
49. 'Cytochrome P450 Metabolism'
[Antonia F. Stepan](#),* R. Scott Obach
The Medicinal Chemist's Guide to Solving ADMET Challenges Royal Society of Chemistry **2021**, 173
48. 'The 2nd Alpine Winter Conference on Medicinal and Synthetic Chemistry'
Alessio Ciulli, Lawrence Hamann, Wolfgang Jahnke, Amit S. Kalgutkar, Thomas Magauer, Tobias Ritter, Vicky Steadman, Scott D. Williams, Georg Winter, Klemens Hoegenauer,* Karl Heinz Krawinkler,* [Antonia F. Stepan](#)*
ChemMedChem **2021**, 16, 2417
47. 'Phenyl bioisosteres in medicinal chemistry: discovery of novel γ -secretase modulators as a potential treatment for Alzheimer's disease'
Hasane Ratni,* Karlheinz Baumann, Peter Bellotti, Xinlan A. Cook, Luke G. Green, Thomas Luebbbers, Michael Reutlinger, [Antonia F. Stepan](#), Walter Vifian
RSC Med. Chem. **2021**, 12, 758
46. 'LRRK2 inhibitors induce reversible changes in nonhuman primate lungs without measurable pulmonary deficits'
Marco A. S. Baptista,* Kalpana Merchant, Ted Barrett, Sakshi Bhargava, Dianne K. Bryce, J. Michael Ellis, Anthony A. Estrada, Matthew J. Fell, Brian K. Fiske¹, Reina N. Fuji, Paul Galatsis, Anastasia G. Henry, Sue Hill, Warren Hirst, Christopher Houle, Matthew E. Kennedy, Xingrong Liu, Matthew L. Maddess, Carrie Markgraf, Hong Mei, William A. Meier, Elie Needle, Stephen Ploch, Christopher Royer, Karin Rudolph, Alok K. Sharma, [Antonia F. Stepan](#), Stefan Steyn, Craig Trost, Zhizhang Yin, Hongshi Yu, Xiang Wang, Todd B. Sherer
Science Translational Medicine **2020**, 20, eaav0820
45. 'A Central Role for LRRK2 in Idiopathic Parkinson Disease'
Roberto Di Maio, Eric K. Hoffman, Emily M. Rocha, Matthew T. Keeney, Laurie H. Sanders, Briana R. De Miranda, Alevtina Zharikov, Amber Van Laar, [Antonia F. Stepan](#), Thomas A. Lanz, Julia K. Kofler, Edward A. Burton, Dario R. Alessi, Teresa G. Hastings, J. Timothy Greenamyre*
Science Translational Medicine **2018**, 10, eaar5429/1

44. 'Lead Diversification at the Nanomole Scale Using Liver Microsomes and Quantitative Nuclear Magnetic Resonance Spectroscopy: Application to Phosphodiesterase 2 Inhibitors'
R. Scott Obach,* Gregory S. Walker, Raman Sharma, Stephen Jenkinson, Tuan P. Tran, Antonia F. Stepan
Journal of Medicinal Chemistry **2018**, *61*, 3626
43. 'Preparation of novel imidazo[4,5-c]quinoline derivatives as LRRK2 inhibitors'
Michael A. Brodney, Thomas A. Chappie, Jinshan M. Chen, Jotham W. Coe, Karen J. Coffman, Paul Galatsis, Michelle R. Garnsey, Christopher J. Helal, Jaclyn L. Henderson, Bethany L. Kormos, Ravi G. Kurumbail, Luis A. Martinez-Alsina, Martin Y. Pettersson, Matthew R. Reese, Colin R. Rose, Antonia F. Stepan, Patrick R. Verhoest, Travis T. Wager, Joseph S. Warmus, Yuan Zhang
Patent WO**2018**163066
42. 'Synthesis and Applications of Highly Functionalized 1-Halo-3-Substituted Bicyclo[1.1.1]pentanes'
Dimitri F. J. Caputo, Carlos Arroniz, James J. Mousseau, Antonia F. Stepan, Steven J. Mansfield, Edward A. Anderson*
Chemical Science **2018**, *9*, 5295
41. 'Preparation of cyclic substituted imidazo[4,5-c]quinoline derivatives for treating diseases associated with LRRK2'
Thomas A. Chappie, Paul Galatsis, Michelle R. Garnsey, Christopher J. Helal, Jaclyn L. Henderson, Bethany L. Kormos, Ravi G. Kurumbail, Luis A. Martinez-Alsina, Martin Y. Pettersson, Antonia F. Stepan, Travis T. Wager
Patent WO**2018**163030
40. 'Late-Stage Microsomal Oxidation Reduces Drug-Drug Interaction and Identifies Phosphodiesterase 2A Inhibitor PF-06815189'
Antonia F. Stepan,* Tuan P. Tran, Christopher J. Helal, Maria S. Brown, Cheng Chang, Rebecca E. O'Connor, Michael De Vivo, Shawn D. Doran, Ethan L. Fisher, Stephen Jenkinson, David Karanian, Bethany L. Kormos, Raman Sharma, Gregory S. Walker, Ann S. Wright, Edward X. Yang, Michael A. Brodney, Travis T. Wager, Patrick R. Verhoest, R. Scott Obach
ACS Medicinal Chemistry Letters **2018**, *9*, 68
39. 'Discovery and Characterization of (R)-6-Neopentyl-2-(pyridin-2-ylmethoxy)-6,7-dihydropyrimido[2,1-c][1,4]oxazin-4(9H)-one (PF-06462894), an Alkyne-Lacking Metabotropic Glutamate Receptor 5 Negative Allosteric Modulator Profiled in both Rat and Nonhuman Primates'
Antonia F. Stepan,* Michelle M. Claffey, Matthew R. Reese, Gayatri Balan, Gabriela Barreiro, Jason Barricklow, Michael J. Bohanon, Brian P. Boscoe, Gregg D. Cappon, Lois K. Chenard, Julie Cianfrogna, Laigao Chen, Karen J. Coffman, Susan E. Drozda, Joshua R. Dunetz, Somraj Ghosh, Xinjun Hou, Christopher Houle, Kapil Karki, John T. Lazzaro, Jessica Y. Mancuso, John M. Marcek, Emily L. Miller, Mark A. Moen, Steven O'Neil, Isao Sakurada, Marc Skaddan, Vinod Parikh, Deborah L. Smith, Patrick Trapa, Jamison B. Tuttle, Patrick R. Verhoest, Daniel P. Walker, Annie Won, Ann S. Wright, Jessica Whritenour, Kenneth Zasadny, Margaret M. Zaleska, Lei Zhang, and Christopher L. Shaffer
Journal of Medicinal Chemistry **2017**, *60*, 7764
38. 'Mechanisms of Skin Toxicity Associated with Metabotropic Glutamate Receptor 5 Negative Allosteric Modulators'
Falgun Shah,* Antonia F. Stepan, Alison O'Mahony, Sharlene Velichko, Alexandra E. Foliass, Christopher Houle, Christopher L. Shaffer, John Marcek, Jessica Whritenour, Robert Stanton, Ellen L. Berg
Cell Chemical Biology **2017**, *24*, 858

37. 'Novel imidazo[4,5-c]quinoline and imidazo[4,5-c][1,5]naphthyridine derivatives as Irrk2 inhibitors'
Paul Galatsis, Jaclyn L. Henderson, Bethany L. Kormos, Ravi G. Kurumbail, Matthew R. Reese, Antonia F. Stepan, Patrick R. Verhoest, Travis T. Wager, Martin Y. Pettersson, Michelle R. Garnsey
Patent US**2017**0073343
36. 'A Multi-endpoint Matched Molecular Pair (MMP) Analysis of 6-Membered Heterocycles'
George Chang,* Kim Huard, Gregory W. Kauffman, Antonia F. Stepan, Christopher E. Keefer
Bioorganic & Medicinal Chemistry **2017**, 25, 381
35. 'Discovery of cyclopropyl chromane-derived pyridopyrazine-1,6-dione γ -secretase modulators with robust central efficacy'
Martin Pettersson,* Douglas S. Johnson, Danica A. Rankic*, Gregory W. Kauffman, Christopher W. Am Ende, Todd W. Butler, Brian Boscoe, Edelweiss Evrard, Christopher J. Helal, John M. Humphrey, Antonia F. Stepan, Cory M. Stiff, Eddie Yang, Longfei Xie, Kelly R. Bales, Eva Hajos-Korcsok, Stephen Jenkinson, Betty Pettersen, Leslie R. Pustilnik, David S. Ramirez, Stefanus J. Steyn, Kathleen M. Wood, Patrick R. Verhoest
MedChemComm **2017**, 8, 730
34. 'Novel cyclopropabenzofuranyl pyridopyrazinediones'
Martin Y. Pettersson, Christopher J. Am Ende, Douglas S. Johnson, Gregory W. Kauffman, Antonia F. Stepan, Patrick R. Verhoest
Patent US**2016**0222007
33. 'Synthesis and Biopharmaceutical Evaluation of Imatinib Analogues Featuring Unusual Structural Motifs'
K. C. Nicolaou,* Dionisios Vourloumis,* Sotirios Totokotsopoulos, Athanasios Papakyriakou, Holger Karsunky, Hanan Fernando, Julia Gavrilyuk, Damien Webb, Antonia F. Stepan*
ChemMedChem **2016**, 11, 31
32. 'Oxidative diversification of amino acids and peptides by small-molecule iron catalysis'
Thomas J. Osberger, Donald C. Rogness, Jeffrey T. Kohrt, Antonia F. Stepan, M. Christina White*
Nature **2016**, 537, 214
31. 'Pyrido[1,2-a]pyrazinedione derivatives as γ -secretase modulators and their preparation and use for the treatment of Alzheimer's disease and Niemann-Pick disease type C'
Martin Y. Pettersson, Christopher J. Am Ende, John M. Humphrey, Douglas S. Johnson, Gregory W. Kauffman, Danica A. Rankic, Antonia F. Stepan, Patrick R. Verhoest
Patent US**2015**0274721
30. 'Preparation of novel 3,4-disubstituted-1h-pyrrolo[2,3-b]pyridines and 4,5-disubstituted-7h-pyrrolo[2,3-c]pyridazines as LRRK2 inhibitors'
Paul Galatsis, Matthew M. Hayward, Bethany L. Kormos, Travis T. Wager, Lei Zhang, Jaclyn L. Henderson, Ravi G. Kurumbail, Patrick R. Verhoest, Antonia F. Stepan
Patent WO**2015**092592
29. 'Preparation of novel bicyclic pyridinones as gamma-secretase modulators'

Martin Y. Pettersson, Douglas S. Johnson, Chakrapani Subramanyam, Christopher J. O'Donnell, Christopher J. Am Ende, Michael E. Green, Nandini C. Patel, Cory M. Stiff, Tuan P. Tran, Gregory W. Kauffman, [Antonia F. Stepan](#), Patrick R. Verhoest
Patent WO**2015**049616

28. 'Design of Pyridopyrazine-1,6-dione γ -Secretase Modulators that Align Potency, MDR Efflux Ratio, and Metabolic Stability'
Martin Pettersson,* Douglas S. Johnson, John M. Humphrey, Todd W. Butler, Christopher W. Am Ende, Benjamin A. Fish, Michael E. Green, Gregory W. Kauffman, Patrick B. Mullins, Christopher J. O'Donnell, [Antonia F. Stepan](#), Cory M. Stiff, Chakrapani Subramanyam, Tuan P. Tran, Beth Cooper Vetelino, Eddie Yang, Longfei Xie, Kelly R. Bales, Leslie R. Pustilnik, Stefanus J. Steyn, Kathleen M. Wood, Patrick R. Verhoest
ACS Medicinal Chemistry Letters **2015**, 6, 596

27. 'C-H Activation Approaches to Molecules'
Elisabeth M. Beck, [Antonia F. Stepan](#), Damien Webb*
Synthetic methods in drug discovery, Volume 1, Royal Society of Chemistry **2015**, 1, 274

26. 'Discovery of indole-derived pyridopyrazine-1,6-dione γ -secretase modulators that target presenilin'
Martin Pettersson,* Douglas S. Johnson, John M. Humphrey, Christopher W. Am Ende, Edelweiss Evrard, Ivan Efremov, Gregory W. Kauffman, [Antonia F. Stepan](#), Cory M. Stiff, Longfei Xie, Kelly R. Bales, Eva Hajos-Korcsok, Heather E. Murrey, Leslie R. Pustilnik, Stefanus J. Steyn, Kathleen M. Wood, Patrick R. Verhoest
Bioorganic & Medicinal Chemistry Letters **2015**, 25, 908

25. 'Preparation of novel bicyclic pyridinones as γ -secretase modulators'
Christopher W. Am Ende, Michael E. Green, Douglas S. Johnson, Gregory W. Kauffman, Christopher J. O'Donnell, Nandini C. Patel, Martin Y. Pettersson, [Antonia F. Stepan](#), Cory M. Stiff, Chakrapani Subramanyam, Tuan P. Tran, Patrick R. Verhoest
Patents WO**2014**045156 and US**2014**0088111

24. 'Preparation of novel 4-(substituted amino)-7H-pyrrolo[2,3-d]pyrimidines as LRRK2 inhibitors'
Paul Galatsis, Matthew M. Hayward, Bethany L. Kormos, Travis T. Wager, Lei Zhang, [Antonia F. Stepan](#), Jaclyn L. Henderson, Ravi G. Kurumbail, Patrick R. Verhoest
Patents US**2014**0005183 and WO**2014**001973

23. 'Discovery and Preclinical Characterization of 1-Methyl-3-(4-methylpyridin-3-yl)-6-(pyridin-2-ylmethoxy)-1H-pyrazolo-[3,4-b]-pyrazine (PF470): A Highly Potent, Selective, and Efficacious Metabotropic Glutamate Receptor 5 (mGluR5) Negative Allosteric Modulator'
Lei Zhang,* Gayatri Balan, Gabriela Barreiro, Brian P. Boscoe, Lois K. Chenard, Julie Cianfrogna, Michelle M. Claffey, Laigao Chen, Karen J. Coffman, Susan E. Drozda, Joshua R. Dunetz, Kari R. Fonseca, Paul Galatsis, Sarah Grimwood, John T. Lazzaro, Jessica Y. Mancuso, Emily L. Miller, Matthew R. Reese, Bruce N. Rogers, Isao Sakurada, Marc Skaddan, Deborah L. Smith, [Antonia F. Stepan](#), Patrick Trapa, Jamison B. Tuttle, Patrick R. Verhoest, Daniel P. Walker, Ann S. Wright, Margaret M. Zaleska, Kenneth Zasadny, Christopher L. Shaffer
Journal of Medicinal Chemistry **2014**, 57, 861

22. 'Fundamentals of Organic Chemistry as Applicable to the Biotransformation of Foreign Compounds'
[Antonia F. Stepan](#), Amit S. Kalgutkar*
Handbook of Metabolic Pathways of Xenobiotics **2014**, 1, 27

21. 'Evaluating the Differences in Cycloalkyl Ether Metabolism Using the Design Parameter Lipophilic Metabolism Efficiency' (LipMetE) and a Matched Molecular Pairs Analysis'
Antonia F. Stepan,* Gregory W. Kauffman, Christopher Keefer, Patrick R. Verhoest, Martin Edwards
Journal of Medicinal Chemistry **2013**, 56, 6985
20. 'Novel γ -secretase modulators for the treatment of Alzheimer's disease: a review focusing on patents from 2010 to 2012'
Martin Pettersson, Antonia F. Stepan, Gregory W. Kauffman, Douglas S. Johnson*
Expert Opinion on Therapeutic Patents **2013**, 23, 1349
19. 'Metabolism-guided drug design'
Antonia F. Stepan, Vincent Mascitti, Kevin Beaumont, Amit S. Kalgutkar*
MedChemComm **2013**, 4, 631
18. 'Metabolic Stability and Analogue-Based Drug Discovery'
Amit S. Kalgutkar,* Antonia F. Stepan
Analogue-based Drug Discovery Vol. III **2013**, 37
17. 'Pd(II)-Catalyzed ortho- or meta-C-H Olefination of Phenol Derivatives'
Hui-Xiong Dai, Gang Li, Xing-Guo Zhang, Antonia F. Stepan, Jin-Quan Yu*
Journal of the American Chemical Society **2013**, 135, 7567
16. 'Discovery of Dap-3 Polymyxin Analogs for the Treatment of Multidrug-Resistant Gram-negative Nosocomial Infections'
Thomas V. Magee,* Matthew F. Brown, Jeremy T. Starr, David C. Ackley, Joseph Abramite, Jiri Aubrecht, Andrew Butler, Jared L. Crandon, Fadia Dib-Hajj, Mark Flanagan, Karl Granskog, Joel R. Hardink, Michael Huband, Rebecca Irvine, Michael Kuhn, Karen L. Leach, Bryan Li, Jian Lin, David Luke, Shawn H. MacVane, Alita Miller, Sandra P. McCurdy, James M. McKim, Jr., David P. Nicolau, Thuy-Trinh Nguyen, Mark C. Noe, John P. O'Donnell, Scott B. Seibel, Yue Shen, Antonia F. Stepan, Andrew P. Tomaras, Paul C. Wilga, Li Zhang, Jinfeng Xu, Jinshan Michael Chen
Journal of Medicinal Chemistry **2013**, 56, 5079
15. 'Application of the Bicyclo[1.1.1]pentane Motif as a Nonclassical Phenyl Ring Bioisostere in the Design of a Potent and Orally Active γ -Secretase Inhibitor'
Antonia F. Stepan,* Chakrapani Subramanyam, Ivan V. Efremov, Jason K. Dutra, Theresa J. O'Sullivan, Kenneth J. DiRico, W. Scott McDonald, Annie Won, Peter H. Dorff, Charles E. Nolan, Stacey L. Becker, Leslie R. Pustilnik, David R. Riddell, Gregory W. Kauffman, Bethany L. Kormos, Liming Zhang, Yasong Lu, Steven H. Capetta, Michael E. Green, Kapil Karki, Evelyn Sibley, Kevin P. Atchison, Andrew J. Hallgren, Christine E. Oborski, Ashley E. Robshaw, Blossom Sneed, and Christopher J. O'Donnell
Journal of Medicinal Chemistry **2012**, 55, 3414
14. 'Sequential Allylic C-H Amination/Vinyllic C-H Arylation: A Strategy for Unnatural Amino Acid Synthesis from α -Olefins'
Chao Jiang, Dustin J. Covell, Antonia F. Stepan, Mark S. Plummer, M. Christina White*
Organic Letters **2012**, 14, 1386

13. 'Quantitative Pharmacokinetic/Pharmacodynamic Analyses Suggest That 129/SVE Mouse Is A Suitable Preclinical Pharmacology Model For Identifying Small Molecule Gamma Secretase Inhibitors'
Yasong Lu,* Liming Zhang, Charles E. Nolan, Stacey L. Becker, Kevin Atchison, Ashley E. Robshaw, Leslie R. Pustilnik, Sarah M. Osgood, Emily H. Miller, Antonia F. Stepan, Chakrapani Subramanyam, Ivan Efremov, Andrew J. Hallgren, David Riddell

Journal of Pharmacology and Experimental Therapeutics **2011**, 339, 922

12. 'Structural Alert/Reactive Metabolite Concept as Applied in Medicinal Chemistry to Mitigate the Risk of Idiosyncratic Drug Toxicity: A Perspective Based on the Critical Examination of Trends in the Top 200 Drugs Marketed in the United States.'

Antonia F. Stepan, Daniel P. Walker, Jonathan Bauman, David A. Price, Thomas A. Baillie, Amit S. Kalgutkar,* Michael D. Aleo

Chemical Research in Toxicology **2011**, 24, 1345

11. 'Oxidative Metabolism of a Quinoxaline Derivative by Xanthine Oxidase in Rodent Plasma.'

Raman Sharma, Heather Eng, Gregory S. Walker, Gabriela Barreiro, Antonia F. Stepan, Kim F. McClure, Angela Wolford, Paul D. Bonin, Peter Cornelius, and Amit S. Kalgutkar*

Chemical Research in Toxicology **2011**, 24, 2207

10. 'Stereoselective Synthesis of Orthogonally Protected β -Hydroxy- α -, γ -diamino Butyric Acids'

Antonia F. Stepan,* Thuy-Trinh Nguyen, Dennis Anderson, Huang Liang, Qian Zhanshan, Thomas V. Magee
Synlett **2011**, 17, 2499

9. 'Metabolism-Directed Design of Oxetane-Containing Arylsulfonamide Derivatives as γ -Secretase Inhibitors.'

Antonia F. Stepan,* Kapil Karki, W. Scott McDonald, Peter H. Dorff, Jason K. Dutra, Kenneth J. DiRico, Annie Won, Chakrapani Subramanyam, Ivan V. Efremov, Christopher J. O'Donnell, Charles E. Nolan, Stacey L. Becker, Leslie R. Pustilnik, Blossom Sneed, Hao Sun, Yasong Lu, Ashley E. Robshaw, David Riddell, Theresa J. O'Sullivan, Evelyn Sibley, Steven Capetta, Kevin Atchison, Andrew J. Hallgren, Emily Miller, Anthony Wood, R. Scott Obach

Journal of Medicinal Chemistry **2011**, 54, 7772

8. 'Divergent C-H Functionalizations Directed by Sulfonamide Pharmacophores: Late-stage Diversification as a Tool for Drug Discovery'

Xiong Dai, Antonia F. Stepan, Mark S. Plummer, Yang-Hui Zhang, Jin-Quan Yu*

Journal of the American Chemical Society **2011**, 133, 7222

7. 'The synthesis of C-13 functionalized pleuromutilins via C-H amidation and subsequent novel rearrangement product.'

Daniel P. Uccello,* Shawn M. Miller, Noah A. Dieterich, Antonia F. Stepan, Seung Won Chung, Kathleen A. Farley, Brian Samas, Jinshan Chen, Justin I. Montgomery

Tetrahedron Letters **2011**, 52, 4247

Postdoctoral Publications (2006–2008)

6. 'Design, Synthesis, and Biological Evaluation of Platensimycin Analogues with Varying Degrees of Molecular Complexity'

K. C. Nicolaou,* Antonia F. Stepan, Troy Lister, Ang Li, Ana Montero, G. Scott Tria, Craig I. Turner, Yefeng Tang,

Jianhua Wang, Ross M. Denton, David J. Edmonds
Journal of the American Chemical Society **2008**, *130*, 3110

5. 'Total Synthesis and Antibacterial Properties of Carbaplatensimycin'
K. C. Nicolaou,* Yefeng Tang, Jianhua Wang, Antonia F. Stepan, Ang Li, Ana Montero
Journal of the American Chemical Society **2007**, *129*, 14850

Graduate Research Publications and Patents (2003–2006)

4. 'Diastereoselective Aldol Reactions with Butane-2,3-Diacetal Protected Glyceraldehyde Derivatives'
Kristian Rahbek Knudsen, Antonia F. Stepan, Patrick Michel, Steven V. Ley*
Organic & Biomolecular Chemistry **2006**, *4*, 1471

3. 'Heterogeneous or Homogeneous? A Case Study Involving Palladium-Containing Perovskites in the Suzuki Reaction'
Stephen P. Andrews, Antonia F. Stepan, Hirohisa Tanaka, Steven V. Ley, Martin D. Smith*
Advanced Synthesis & Catalysis **2005**, *347*, 647

2. 'Method of Synthesizing Compounds and Catalysts for Synthesis Reaction.'
Steven V. Ley, Martin D. Smith, Chandrashekar Ramarao, Antonia F. Stepan, Hirohisa Tanaka
Patents US**2005**215804 and JP**2005**314355

1. 'Palladium-Containing Perovskites: Recoverable and Reusable Catalysts for Suzuki Couplings'
Martin D. Smith, Antonia F. Stepan, Chandrashekar Ramarao, Paul E. Brennan, Steven V. Ley*
Chemical Communications **2003**, 2652

Invited Presentations

- 04/2021 'Vignettes on C–H Functionalization Collaborations'
Basel Chemical Society Online Lecture Series
- 08/2019 'Use of Aliphatic Bioisosteres in Medicinal Chemistry':
260th ACS National Meeting & Exposition, Session: 'Development of New Strategies for the Synthesis & Functionalization of Strained Rings for Applications as Bioisosteres in Biologically Active Compounds', San Diego, CA, USA
- 08/2017 'Strategies towards Increasing the 3-Dimensionality of the Medicinal Chemistry Design Space':
Plenary talk at the EFMC International Symposium on Advances in Synthetic and Medicinal Chemistry, Vienna, Austria
- 01/2017 'C–H Functionalization Methods as Cutting-Edge Synthesis Tools for Medicinal Chemists':
13th Winterconference on Bioorganic and Medicinal Chemistry, Session: 'Advances in Modern Synthetic Methods', Steamboat, CO, USA
- 08/2016 'Strategies towards Increasing the 3-Dimensionality of the Medicinal Chemistry Design Space':
252nd ACS National Meeting & Exposition, Session: 'Emerging Isosteric Replacement Methods: A Fundamental Strategy in Drug Design, Philadelphia, PA, USA
- 08/2016 'A LipMetE Assessment of Bioisosteres in Medicinal Chemistry':
252nd ACS National Meeting & Exposition, Session: 'Medicinal Chemists Toolbox: Scaffolds & Privileged Scaffolds in Drug Design', Philadelphia, PA, USA
- 04/2016 'Use of the Bicyclo[1.1.1]pentane Motif as a Nonclassical Phenyl Bioisostere with Increased 3-Dimensionality':
SpiroChem AG, ETH Zürich, Switzerland
- 03/2015 'Discovery and Adverse Safety Findings of Two New mGluR5 NAM Chemotypes':
249th ACS National Meeting & Exposition, Session: 'Young Investigator in Medicinal Chemistry', Denver, CO, USA
- 03/2015 'C–H Functionalization: Can We Leverage Cutting-Edge Synthetic Methods to Enhance Drug Discovery?':
249th ACS National Meeting & Exposition, Session: 'Development of Direct/C–H Functionalization Processes towards the Synthesis of Biologically Active Compounds', Denver, CO, USA
- 01/2015 'Reactive Metabolites in Drug-Induced Liver Injury':
12th Winterconference on Bioorganic and Medicinal Chemistry, Session: 'Mitigating Drug Induced Liver Injury (DILI) in Drug Discovery', Steamboat, CO, USA

- 11/2014 'The Impact of Oxetane and Bicyclo[1.1.1]pentane Motifs on Biopharmaceutical Properties – A γ -Secretase Inhibitors Study':
BIT's 12th Annual Congress of International Drug Discovery, Science & Technology, Session: 'Neuroscience and Drug Discovery', Suzhou, China
- 10/2014 'The Impact of Oxetane and Bicyclo[1.1.1]pentane Motifs on Biopharmaceutical Properties – A γ -Secretase Inhibitors Study':
East Cambridge Drug Discovery Working Group Meeting, Cambridge, MA, USA
- 03/2014 'Use of the Bicyclo[1.1.1]pentane Motif as a Nonclassical Phenyl Bioisostere with Increased 3-Dimensionality':
Professor K.C. Nicolaou Group Meeting, Rice University, Houston, TX, USA
- 03/2014 'Use of the Bicyclo[1.1.1]pentane Motif as a Nonclassical Phenyl Bioisostere with Increased 3-Dimensionality':
247th ACS National Meeting & Exposition, Session: 'Breaking the Plane: Exploiting the 3rd Dimension in Drug Design', Dallas, TX, USA
- 03/2014 'The Discovery of Immune-Mediated Hypersensitivities with Two Distinct mGluR5 NAM Chemotypes':
Applied Pharmaceutical Chemistry, Session: 'Optimizing Properties - Where Should We Focus?', Cambridge, MA, USA
- 01/2013 'The Impact of Oxetane and Bicyclo[1.1.1]pentane Motifs on Biopharmaceutical Properties':
11th Winterconference on Bioorganic and Medicinal Chemistry, Session: 'New Frontiers in Medicinal Chemistry', Steamboat, CO, USA
- 11/2012 'Case Studies of Preclinical Research at Pfizer':
College of Pharmacy, University of Arizona, Tucson, AZ, USA
- 05/2012 'The Impact of Oxetane and Bicyclo[1.1.1]pentane Motifs on Biopharmaceutical Properties – A γ -Secretase Inhibitors Case Study':
ACS 33rd National Medicinal Chemistry Symposium, Session: 'Professional Development', Tucson, AZ, USA
- 02/2012 'The Impact of Oxetane and Bicyclo[1.1.1]pentane Motifs on Biopharmaceutical Properties – A γ -Secretase Inhibitors Case Study':
Nottingham University, UK
- 07/2009 'Transition-Metal Catalyzed C–H Functionalization – An Enabling Tool for Lead Diversification in Medicinal Chemistry?':
WuXi, Shanghai, China
- 06/2006 'Studies Towards the Total Synthesis of Leustroducsin B':
Merck Graduate Symposium, University of Cambridge, UK
- 04/2006 'Studies Towards the Total Synthesis of Leustroducsin B':

Humboldt Graduate Symposium, University of Hannover, Germany

07/2005 'New Methodologies and Their Application in a Synthesis Towards Leustroducsin B':
Novartis, Horsham, UK

Teaching

02/2017 'C–H Functionalization Methods as Cutting-Edge Synthesis Tools for Medicinal Chemists':
Institute for Organic Chemistry, Karlsruhe Institute of Technology, Germany

02/2017 'Oxetane and Bicyclo[1.1.1]pentane Motifs in Medicinal Chemistry – A γ -Secretase Inhibitor
Case Study':
Institute for Organic Chemistry, Karlsruhe Institute of Technology, Germany

04/2016 'Oxetane and Bicyclo[1.1.1]pentane Motifs in Medicinal Chemistry –
A γ -Secretase Inhibitor Case Study':
Professor Bräse Group Seminar, Karlsruhe Institute of Technology, Germany

08/2015 'Structural Alerts and Reactive Metabolites: A Medicinal Chemistry Perspective on How to
Navigate this Minefield':
Medicinal Chemistry Gordon Research Seminar (GRS), New London, NH, USA

03/2015 'A – Structural Alerts and the Risk of Reactive Metabolites; B – mGluR5 Case Study': MedChem
Navigator Course MC 1.02, Groton, CT, USA (Pfizer internal)

Contributions to Abstracts and Poster Presentations

08/2018 'Synthesis and cross-coupling of 1-halo-3-substituted bicyclo[1.1.1]pentanes: En route to 1,
4-disubstituted phenyl bioisosteres':
256th ACS National Meeting & Exposition, Boston, MA, USA

08/2017 'A Platform for Late-Stage Functionalization in Medicinal Chemistry':
66th Gordon Research Conference on Natural Products and Bioactive Compounds, Andover,
NH, USA

04/2017 'Discovery of clinical candidate PF-06648671: A potent, highly brain penetrant gamma
secretase modulator for the treatment of Alzheimer's disease':
253rd ACS National Meeting & Exposition, San Francisco, CA, USA

08/2016 'Synthesis of Pyrazole-Fused Piperazines by Double Alkylation of Amines':
65th Gordon Research Conference on Natural Products & Bioactive Compounds, Andover, NH,
USA

08/2015 'Synthetic optimization of MDW941 enables the development of a high content
glucocerebrosidase assay':
250th ACS National Meeting & Exposition, Boston, MA, USA

- 09/2014 'Development of a high content assay to measure glucocerebrosidase in Gaucher patient fibroblasts':
1st Annual Conference for the Society of Biomolecular Imaging and Informatics,
Boston, MA, USA
- 08/2014 'Process work on two synthetic routes of PF-06416495, a mGluR5 negative allosteric modulator':
248th ACS National Meeting & Exposition, San Francisco, CA, USA
- 05/2014 'Discovery of Novel Pyridopyrazine-1,6-diones as γ -Secretase Modulators and Development of Photoaffinity Probes to Study their Mechanism of Action':
34rd ACS National Medicinal Chemistry Symposium, Charleston, SC, USA
- 07/2013 'Clinical γ -Secretase inhibitors (GSIs) alter A β 40/42 ratio in brain and show CSF Abeta rebound in vivo':
Alzheimer's Association International Conference, Boston, MA, USA
- 04/2013 'New polymyxin analogs for the treatment of multidrug-resistant gram-negative nosocomial pathogens':
245th ACS National Meeting & Exposition, New Orleans, LA, USA
- 03/2013 'Diverse effects of aggregate-prone proteins and small molecules on autophagy flux in cell-based assays and primary neurons':
The 11th International Conference on Alzheimer's and Parkinson's Disease, Florence, Italy
- 10/2012 'Autophagy enhancers as potential therapeutics for neurodegenerative diseases: using a flow cytometry based assay to monitor autophagy flux':
Society for Neuroscience Meeting, New Orleans, LA, USA
- 09/2011 'Biocatalysis-enabled optimization of a bicyclo[1.1.1]pentane motif':
242nd ACS National Meeting & Exposition, Denver, CO, USA
- 09/2011 'Substituted cyclic ether arylsulfonamides as potent inhibitors of γ -secretase':
242nd ACS National Meeting & Exposition, Denver, CO, USA
- 10/2011 'Unusual Oxidative Instability of a Quinoxaline Derivative in Rodent Plasma: Role of Xanthine Oxidase':
17th North American ISSX Meeting, Atlanta, GA, USA
- 08/2006 'Studies Towards the Total Synthesis of Leustroductin B':
1st European Chemistry Congress, Budapest, Hungary
- 08/2004 'Palladium-Containing Perovskites: A New Class of Catalysts for Organic Synthesis':
IUPAC ICOS-15 conference, Nagoya, Japan
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