DR. ERIC E. SIMANEK

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Current Interests: Organic and medicinal chemistry, science education, interdisciplinary studies, whiskey

Education

Post-doctoral Studies (8/96-5/98): Scripps Research Institute with Dr. Chi-Huey Wong

Research: Glycopeptide synthesis and conformation; anti-inflammatories

Ph.D., Chemistry (8/91-8/96): Harvard University with Dr. George M. Whitesides

Research: Molecular recognition; materials science

B.S., Chemistry (8/87-5/91): University of Illinois with Dr. Kenneth L. Rinehart, Jr.

Research: Bioassay development; synthesis

Professional Experience

Affiliated Faculty - TCU/UNTHSC Medical School, 2019-present

Affiliated Faculty - Women & Gender Studies, TCU, 2018-present

Affiliated Faculty - Comparative Race & Ethic Studies, TCU, 2018-present

Affiliated Faculty - John V. Roach Honors College, TCU, 2018-present

Chair, Department of Chemistry & Biochemistry, 2014-present

Director & founder, TCU IdeaFactory, 2012-2019

Robert A. Welch Chair of Chemistry, Texas Christian University, August 2010-present

Professor of Chemistry, Texas Christian University, August 2010-present

Professor of Chemistry, Texas A&M University, 2007-2010

Director of the First Year Chemistry Program (General Chemistry), 2006-2009

Associate Professor of Chemistry, Texas A&M University: 2004-2007 Assistant Professor of Chemistry, Texas A&M University: 1998-2004

Other Professional Experience

Abbott Laboratories, Summer Research Intern Anti-inflammatory discovery, Lake Forest, IL 1990,1991 USDA Northern Regional Laboratory, Summer Research Intern, Mycotoxins Unit, Peoria, IL 1989

Awards and Honors

Honors Professor of the Year, TCU 2019

Finalist, Honors Professor of the Year, TCU 2018

Sigma Xi Distinguished Lecturer, 2018-2020

Finalist for Best Wine Book, International Association of Culinary Professionals, 2017

Gourmand Hall of Fame Award for Shots of Knowledge: The Science of Whiskey, 2016

Coleman Fellow, Texas Christian University, 2011-2012

STEM Science Award from the Fort Worth Chapter of The Links, Inc. 2011

Robert A. Welch Chair of Chemistry, Texas Christian University, 2010

College of Science Distinguished Achievement Award from the Association of Former Students 2005

Texas A&M University Montague-Center for Teaching Excellence Scholar, 2003

Innovation Award, Research Corporation, 1999

Eli Lilly Predoctoral Fellowship, Harvard University, 1994-1995,

Teaching Fellow Awards, Harvard University (1992) and University of Illinois (1991)

Carl Shipp Marvel Research Award, University of Illinois, 1991

SERVICE & SUMMARIES

Professional/National Service

Organizing Committee, International Dendrimer Symposium 2011 Editorial Advisory Board, Molecular Pharmaceutics 2010-2014

Editor, Special Issues of Molecular Pharmaceutics (2006, 2008, 2010)

Advisory Committee, International Polymer Therapeutics Conference, Valencia 2010 N.I.H. Study Section

Member, Ad hoc (SBCA 2005, 2007, 2009; ZMDG, 2006; K99 2010)

NSF Panel Member (Educ: CCLI 2009; Sci: MSN 2010)

Selected Service from Texas Christian University

Member, Executive Committee Council of Department Chairs, 2018-present Chair, Department of Chemistry & Biochemistry, 2014-2020 Director, TCU IdeaFactory, 2012-2019 Faculty Senate, Texas Christian University, 2013-2016, 2019-present Member, Core Curriculum HMVV Committee, 2014-present Member, Dean search committees (Honors, 2016; Interdisciplinary Sciences, 2018)

Selected Service from Texas A&M University

Director of the First Year (General Chemistry) Program, 2006-2009
Chair, Promotion and Tenure Committee, 2009
Member, Academic Oversight Committee, 2006-2010
Member, Promotion and Tenure Committee, 2007-2009
Editor & author, general chemistry laboratory manuals, 2007 & 2008
Member, Graduate Admissions Committee, 2006
Chair, Mass Spec Users Group-TAMU, 2004-2006
Chair, Organic Division-TAMU, 2004-2005

Summary of Efforts as Director of the general chemistry program at Texas A&M University (2006-9)

Prior to volunteering for the position, the tenured, research active faculty were largely divorced from the general chemistry program-one that served more than 3500 students/semester-save for the few that rotated in occasionally to teach one section of general chemistry. There was no oversight or standardization of content in either lecture or labs. Lecturer and staff morale was poor due in part to the 'caste system' perceived to be in place. In short, 'external' leadership was required. Recognizing the challenges of large classes, the teaching load was normalized across the lecturers and class size was reduced from 313 to 250. Lab and lecture were separated into two distinct courses to increase efficiencies. An e-curriculum was adopted, described as the first in the country by the publisher, that saved students >\$250K/yr in textbook costs. The laboratory curriculum was revamped for the non-engineering majority and laboratory manuals were written and sold (at \$15 ea) with proceeds funding other activities of the program and by establishing a quasi-endowment that continues to grow to substantial corpus. Labs were outfitted with projectors and university-recycled benchtop computers for the students. Travel awards were instituted for teaching fellows and a teaching fellows lounge was built to provide space for grading and planning. Each member of the faculty was awarded \$2K annually for professional development. A lecture series was instituted with 3 mandatory talks each semester offered to the entire student population to underscore the relevancy of the curriculum and inspire examples of real world applications for the faculty to draw on. Most of these changes stand now almost a decade later.

Summary of Efforts as Department Chair at Texas Christian University (2014-2020)

My first term as chair focused on stewardship of the physical space. To this end, broken and unused equipment was purged from teaching labs and closets. Instrumentation was consolidated to afford opportunities for space reassignment leading to a new office for a new member of the instructional faculty (vide infra), an office for a safety officer, a definable space for the advanced inorganic laboratory and a suite for the chemistry club. Furniture was secured to provide study space for undergraduates in the hallways. A reassignment of research space put faculty in labs more suitable to the size of their groups and bench/hood needs. Teaching assistant awards were instituted. Salary inversions of the faculty were (and continue to be) addressed. The human infrastructure expanded to include

an organic laboratory coordinator. My second term has addressed pedagogoical and human infrastructure changes. An additional faculty office was created by equipment reorganization, and an additional 0.5 FTE to teach general chemistry to an ever-increasing enrollment was secured. Normalization of teaching and service loads is being addressed among this cohesive community of teacher-scholars is ongoing. Of particular note, we have addressed national trends in grade inflation without compromising TCU rigor.

Summary of Efforts as Director of the TCU IdeaFactory (2012-2019)

The first special topics class I taught was inspired by the Dean's request to evaluate the IP strategies in place at TCU. What better way then to invent something. The success that a cohort of students had at 'inventing' a tool to teach plate tectonics, the Pangaea Mat & Cutter and its subsequent commercialization coupled with an NSF education grant led to the creation of the TCU IdeaFactory. Other education products followed. Notably, the Broadway-like show "Dance of the Continents." However, the scope of products now covers ideas from apps to social action. IdeaFactory acts as a doorstep to the Neeley School of Business and its entrepreneurship center for non-business students pursuing their own passions and ideas. Originally, students would be mentored to a prototype and draft pitch and business plan that they could take to Neeley. More recently, an academic framework, design thinking, has emerged as a foundation for our activities. While the unit's goal is to support students that are underserved by the traditional experience and instead engaged by their own ideas and dreams (including college athletes), IdeaFactory now is driving the goal of design thinking as a university-wide academic track. These efforts are facilitated with IdeaFactory's placement within the new School of Interdisciplinary Studies.

Summary of Consulting Efforts

Very little energy has been invested in the pursuit of external consulting. Most focuses on intellectual property where my role has been limited to that as an expert witness or appearing on behalf of an inventor in front of the patent office as an IP/patent consultant. The extent of consulting in education is limited to hosting individuals who wish to replicate the IdeaFactory at their home institutions, or traveling to talk about the unit.

Ocular Research of Boston, Inc. v. Allergan, Inc. Civil Action No. 2:07-cv-385-TJW (E.D. Tex. (2010) Johnson Matthey. Inc. v. Noven Pharm., Inc. et al. Civil Action No 2:07-cv-00260-CE (E.D. Tex.) (2008-9) Massey Research, Inc. lubricants (2006-7) including an appearance before the examiner in Alexandria VA.

Summary of Commercialization Efforts

Efforts in commercialization commenced with numerous disclosures and some provisional patents stemming from efforts at Texas A&M University on the dendrimers we produced because of potential applications in materials science, polymer chemistry and drug delivery. A license agreement was reached with Frontier Scientific (Logan UT) for the sale of our dendrimers for a period that last a few years, but was discontinued to the burden of just-intime synthesis. Continued interest in intellectual property protection at TAMU led to the founding of Lone Star Molecular, Inc. (2006). The company still exists and has pivoted to become a bookseller (*Shots of Knowledge: The Science of Whiskey*). At TCU, I was named a Coleman Fellow (to bring entreneurship into the classroom) and brought two products to market, the Pangaea Mat & Cutter and Plate Detective. The former has been available through Carolina Scientific for >5 years. We estimate it has reached more than 250,000 students on 6 continents. Through IdeaFactory, I serve as a consultant to students interested in early stage commercialization.

Summary of Efforts in Diversity, Equity & Inclusion

Efforts in DEI come in many forms. An early example was by winning am NSF GK-12 grant that allowed me to put 33 STEM graduate students in at-risk schools in Bryan, TX (while I was at Texas A&M). Other efforts stem from outreach activities through the IdeaFactory. The play we created to teach plate tectonics, Dance of the Continents, has been performed a dozen times with more than 1000 student actors to peer audiences numbering 5000. We target schools with diverse populations that are identified as 'at risk' as well as institutions that serve populations suffering from dyslexia and ADHD. Increasingly, the students that seek out the IdeaFactory are enriched in diverse students, increasingly student athletes. Most importantly, I believe, are the roles I play in strategically converting opportunities into policy initiatives that can be realized with consensus. For example, in 2016, HHMI called for proposals to diversify STEM education. Working with a colleague in student development, a proposal that put STEM counselors in the College of Science & Engineering was advanced. The completed proposal was never submitted by TCU, but in 2018, TCU announced the STEM scholars program realizing the goals of the first proposal. Another example opened through a different opportunity. With the shift to electronic annual reports, I led a group that proposed that activities listed on reports should be indicated as "DEI" when appropriate. I pitched the effort to

administration and now, through the click of a toggle button, we have a mechanism to identify, understand and ultimately support DEI activities of the faculty campus wide. While an e-transient modification, formal DEI inventories are now collected on campus. I have collaborated with the College of Education and TRIO (minority recruitment program) to offer a 4 week intensive research experience for high school seniors wherein sertraline is used as the basis for the construction of new molecules through multistep synthesis. My course, Whiskey: Science & History address many issues of DEI. Finally, I am an affiliated member of the Departments of Women & Gender Studies and Comparative Race & Ethnic Studies, where I hope to support their efforts and enhance the educational content of my class.

Summary of External Funding

Without substantive exception, my efforts have been externally funded continuously since the start of my independent career at Texas A&M University and continuing on to the present at TCU. I am grateful to the NIH for supporting much of our work in dendrimers through NIGMS and NCI. The NSF has richly supported education initiatives over this period as well as materials science collaborations through NTE. Other agencies include the USDA, Research Corporation, DARPA and most recently, the NIH through its SBIR initiative. During the first half of my career, much of the funding supported only our laboratory. With time, and owing in part to the maturation of the dendrimer chemistry we developed, funding has evolved to be highly collaborative and driven by clinicians and translationalists. With the emergence of a new research interest, self-assembling macrocycles, a return to unique support may be realized. A detailed summary of research support is available on request.

TEACHING, WORKSHOPS & EXTENDED EDUCATION

Non-traditional Coursework

Whiskey: Writing about Science & History (Writing intensive, SCIE 30303)

Cerebral Palsy & Dance (Undergraduate, SCIE 20303, TCU)

Whiskey: Science & History (Undergraduate & graduate, SCIE 20303 & 60203, TCU)

Recess (Special topics, Undergraduate, SCIE 20230)

Dance of the Continents I & II (Special topics, Undergraduate, SCIE 20230)

Commercialization and Education Outreach (Special topics, Undergraduate, Chem 50230, TCU)

Introduction to Research and Outreach (Special topics, Undergraduate, Chem 40200, TCU)

Traditional Coursework

General Chemistry 1 (Undergraduate, Chem 101, TAMU)

General Chemistry 2 (Undergraduate, Chem 102, TAMU)

Chemistry 1 & 2 (Undergraduate Chem 227 & Chem 228, TAMU)

Survey of Organic Chemistry (Undergraduate nonmajors, Chem 222, TAMU)

Organic Chemistry Lab for Majors (Undergraduate, Chem 238, TAMU)

Organic Chemistry Lab for Non-majors (Undergraduate, TAMU Chem 242)

Environmental Chemistry (Undergraduate, TAMU Chem 383)

Medicinal Chemistry (Graduate: Chem 689 TAMU) - 2005

Biochemistry (Graduate; Chem 647 TAMU) - 2004

Reactions & Mechanisms (Graduate; Chem 610 TAMU) - 1999, 2000

Workshops & Extended Education

Bourbon: Science & History - TCU Silver Frogs, Fa 2017 (1.5h x 4wk, Extended Ed)

Science of Scotch - TCU Silver Frogs, Spr 2017, (1.5h x 4wk, Extended Ed)

PUBLICATIONS (Updated March 2020)

Books (6)

- 6. Shots of Knowledge: The Science of Whiskey. Arnold, R. & Simanek, E. TCU Press, 2016.
- 4 & 5. Chem 112 Laboratory Manual(s). Texas A&M University, 2007, 2nd Ed. 2008
- 2 & 3. Chem 111 Laboratory Manual(s). Texas A&M University, 2007, 2nd Ed. 2008
- 1. Fundamentals of Organic Chemistry 6E. McMurry, J.E. & Simanek, E.E. Thompson/Brooks Cole, 2007.

Book chapters (5)

- 5. Chapter 10: Cationic Triazine Dendrimers: Synthesis, Characterization and Biological Applications. Enciso, A.E.; Simanek, E.E. In Cationic Polymers for Regenerative Medicine, 2015, S.K. Samal, Ed. RSC Publishing.
- 4. Chapter 17. Triazine dendrimers for DNA and siRNA delivery: Progress, challenges, and opportunities. Mintzer, M.A.; Merkel, O.M.; Kissel, T.; Simanek, E.E. in "Dendrimer-based drug delivery systems: from theory to practice Yien Chen, Editor. Wiley. 2012. doi: 10.1016/j.addr.2012.03.008. Review. PMID: 22465784
- 3. Dendrimers based on melamine: vehicles for drug delivery? Simanek, E. E. ACS Symposium Series 2006, 923(Polymeric Drug Delivery I), 121-136.
- 2. Carbohydrate Libraries in Solution Using Thioglycosides. From Multistep to Programmable, Orthogonal, One-pot Synthesis. Simanek, E.E.; Wong, C.-H. in Solid Support Oligosaccharide Synthesis and Combinatorial Carbohydrate Libraries. Ed. Peter Seeberger. Wiley and Sons. NY, NY. 2001.
- 1. Approaches to Synthesis Based on Non-covalent Bonds. Whitesides, G M.; Simanek, E.E.; Gorman, C. B. NATO Advanced Institute on Chemical Synthesis: Gnosis to Prognosis. (1994) American Chemical Society: Washington, DC.

Scientific Research Publications

- 105. Efficient syntheses of macrocycles ranging from 22-28 atoms through spontaneous dimerization to yield bis-hydrazones. Sharma, V.; Mehmood, A.; Janesko, B.G.; Simanek, E.E. RSC Advances, 2019, 10, 3217-3220. doi:10.1039/c9ra08056b
- 104. Tumor Uptake of Triazine Dendrimers Decorated with Four, Sixteen, and Sixty-Four PSMA-Targeted Ligands: Passive versus Active Tumor Targeting. Lim,J.; Guan,B.; Nham,K.; Hao,G.; Sun, X.; Simanek, E.E. Biomolecules **2019**, Aug 28;9(9). pii: E421. doi: 10.3390/biom9090421.
- 103. *In Vitro Skin Penetration of Dendrimer Nanoparticles*. Kraeling, M.E.K.; Topping, V.D.; Belgrave, K.R.; Schlick, K.; Simanek, E.E.; Man, S.; Dadiboyena, S.; Patri, A.K.; Sprando, R.L.; Yourick, J.J. *Applied In Vitro Toxicology* 2019, 5(3), 134-149. doi: 10.1089/aivt.2019.0004
- 102. Nanoparticle physicochemical properties determine the activation of intracellular complement. Ilinskaya, A.N.; Shah, A.; Enciso, A.E.; Chan, K.C.; Kaczmarczyk, J.A.; Blonder, J.; Simanek, E.E.; Dobrovolskaia M.A. Nanomedicine: Nanotechnology, Biology and Medicine, 2019, 17, 266-275.
- 101. Synthesis of Macrocycles Derived from Subsituted Triazines. Yepremyan, A.; Mehmood, A.; Asgari, P.; Janesko, B.G.; Simanek, E.E. ChemBioChem, 2019, 20, 241-246.
- 100. A new triazine bearing a pyrazolone group capable of copper, nickel, and zinc chelation. Yepremyan, A.; Mehmood, A.; Brewer, S.M.; Barnett, M.M.; Janesko, B.G.; Akkaraju, G.; Simanek, E.E.; Green, K.N. RSC Advances, 2018, 8, 3024-3035.
- 99. Intrinsic Fluorescence of Triazine Dendrimers Provides a New Approach to Study Dendrimer Structure and Conformational Dynamics. Raut, S.; Enciso, A. E.; Pavan, G. M.; Lee, C.; Yepremyan, A.; Tomalia, D. A.; Simanek, E. E. Gryczynski, Z. J. Phys. Chem. C, 2017, 12, 6946-54. DOI: 10.1021/acs.jpcc.6b11110.

- 98. Facile synthesis of stable, water soluble, dendron-coated gold nanoparticles. Enciso, A.E.; Doni, G.; Nifosi, R.; Palazzesi, F.; Gonzalez, R.; Coffer, J. L.; Simanek, E. E.; Pavan, G. M.; Mohamed, A. A. Nanoscale, 2017, 9, 3128-32. DOI: 10.1039/c6nr09679d.
- 97. Thermoregulated Coacervation, Metal-encapsulation and Nanoparticle Synthesis in Novel Triazine Dendrimers. Enciso, A.; Ramirez-Crescencio, F.; Hasan, M.; Costa, V.; Annunziata, P.; Redon, R.; Coffer, J.L.; Simanek, E.E. Molecules 2016, 21, 599. doi:10.3390/molecules21050599. PMID: 27187331
- 96. Solid-phase Synthesis of Libraries of Triazine Dendrimers and Orthogonal Staining Methods for Tracking Reactions on Resin. Huang, A.Y.-T.; Patra, S.; Chen, H.-T.; Kao, K.-L.; Simanek, E.E. Asian J. Org. Chem. 2016, 5(7), 860-864. 10.1002/ajoc.201600085R1
- 95. Nanoparticle effects on human platelets in vitro: A comparison between PAMAM and Triazine dendrimers. Enciso, A.E; Neun, B.; Rodriguez, J.; Ranjan, A.P.; Dobrovolskaia, M.; Simanek, E.E. Molecules 2016, 21, 428; doi:10.3390/molecules21040428. PMID: 27043508
- 94. Functionalization of a dendrimer presenting four maleimide groups on the periphery and a DOTA group at the core. Lee, C.; Ji, K.; Simanek, E.E. Molecules 2016, 21(3). 335. doi:10.3390/molecules21030335. PMID: 26978338
- 93. Synthesis and Antimicrobial Activity of Triazine Dendrimers with DABCO Groups. Sreeperumbuduru, R.S.; Abid, Z.M.; Claunch, K.M.; Chen, H.-H.; McGillvray, S.; Simanek, E.E. RSC Advances 2016, 6, 8806-8810.
- 92. Accelerated Synthesis of Large Generation Triazine Dendrimers Using Microwave Assisted Reactions. Enciso, A. E.; Ramirez-Crescencio, F.; Zeiser, M. J.; Redon, R.; Simanek, E. E. Polymer J. 2015, 6, 5219-5224.
- 91. Triazine-Substituted and Acyl Hydrazones: Experiment and Computation Reveal a Stability Inversion at Low pH. Ji, K.; Lee, C.S.; Janesko, B.G.; Simanek, E.E. Molec. Pharm. 2015, 12, 2924-2927. doi: 10.1021/acs.molpharmaceut.5b00205. PMID: 26076408
- 90. Influence of linker groups on the solubility of triazine dendrimers. Enciso, A.E.; Garzoni, M.; Pavan, G.M.; Simanek, E.E. New J. Chem. 2015, 39, 1247-1252.
- 89. Light-fuelled transport of large dendrimers and proteins. Koskela, J.E.; Liljerstrom, V.; Lim, J.; Simanek, E.E.; Ras, R.H.A.; Priimagi, A.; Kostiainen, M.A. J. Am. Chem. Soc. 2014, 19, 6850-6853. doi: 10.1021/ja502623m. PMID: 24785836
- 88. Rapid, Semi-automated Convergent Synthesis of Low Generation Triazine Dendrimers using Microwave Assisted Reactions. Enciso, A.E.; Abid, Z.M.; Simanek, E.E. Polymer Chem. 2014, 5, 4635-40.
- 87. Design, Synthesis and Biological Assessment of a Triazine Dendrimer with Approximately 16 Paclitaxel Groups and 8 PEG Groups. Lee, C.S.; Lo, S.-T.; Lim, J.; da Costa, V.C.P.; Ramezani, S.; Oz, O.K.; Pavan, G.M.; Annunziata, O.; Sun, X.K.; Simanek, E.E. Mol. Pharmaceutics 2013, 10, 4452-4461. doi: 10.1021/mp400290u. PMID: 24134039
- 86. Computational design principles for the discovery of bioactive dendrimers: Triazines and other examples. Simanek, E.E.; Enciso, A.; Pavan, G.M. Expert Opin. Drug Disc. 2013, 8, 1057-1069. doi: 10.1517/17460441.2013.813479. Review. PMID: 23826946
- 85. Dendrimers Terminated with Dichlorotriazine Groups Provide a Route to Compositional Diversity. Patra, S.; Kozura, B.; Huang, A.-Y.; Enciso, A.E.; Sun, X.K.; Hsieh, J.T.; Kao, C.-L.; Chen, H.-T.Simanek, E.E. Org. Lett. 2013, 15, 3808-3811. doi: 10.1021/ol400811h. PMID: 23869522
- 84. Synthesis of Large Dendrimers with the Dimensions of Small Viruses. Lim, J.; Kostiainen, M.; Maly, J.; da Costa, C.P.; Annunziata,O.; Pavan, G.M.; Simanek, E.E. J. Am. Chem. Soc. 2013, 135, 4660-4663. doi: 10.1021/ja400432e.PMID: 23398590
- 83. Gadolinium MRI Contrast Agents Based on Triazine Dendrimers: Relaxivity and In Vivo Pharmacokinetics. Lim, J.; Turkbey, B.; Bernardo,M.; Bryant, L.H. Jr.; Garzoni,M.; Pavan, G.M.; Nakajima, T.; Choyke, P.L.; Simanek, E.E.; Kobayashi, H. Bioconj. Chem. 2012, 23, 2291-2299. doi: 10.1021/bc300461r. PMID: 23035964
- 82. *TAT-mediated photochemical internalization results in cell killing by causing the release of calcium into the cytosol of cells.* Muthukrishnan N.; Johnson, G.A.; Lim, J.; Simanek, E.E.; Pellois, J.P. Biochim. Biophys. Acta 2012, 1820, 1820,1734–1743. doi: 10.1016/j.bbagen.2012.06.020. PMID: 22771830

- 81. FRET Enhanced Fluorescent Nanodiamonds. Fudala, R.; Rout, S.; Maliwal, B.P.; Zerda, T.W.; Gryczynski, I.; Simanek, E.E.; Borejdo, J.; Rich, R.; Akopova, I.; Gryczynski, Z. Curr. Pharm. Biotechnology 2014, 14,1127-1133. PMID: 22394126
- 80. *Paclitaxel-triazine dendrimer constructs: Efficacy, toxicity, and characterization.* In Multifunctional Nanoparticles, Ed. S. Svenson and G. Prud'homme. Springer 2012.
- 79. Antitumor Activity and Molecular Dynamics Simulations of Paclitaxel-laden Triazine Dendrimers. Lim, J.; Lo, S.-T.; Hill, S.; Pavan, G.M.; Sun. X.; Simanek, E. E. Molecular Pharm. 2012, 9, 404-412. doi: 10.1021/mp2005017. PMID: 22260328
- 78. Experimental and Computational Evidence for an Inversion of Guest Capacity in High-Generation Triazine Dendrimer Hosts. Lim,J.; Pavan, G.M.; Annunziata, O.; Simanek, E.E. J. Am. Chem. Soc. 2012, 134, 1942-5. doi: 10.1021/ja210122z. PMID: 22239724
- 77. Computational design principles for bioactive dendrimer based constructs as antagonists of the TLR4-MD-2-LPS complex. Barata, T.; Teo, I.; Lalwani, S.; Zloh, M.; Shaunak, S. Biomaterials 2011, 32, 8702-11. PMID: 21864902
- 76. Encapsulation of Concanavalin A/Dendrimer Glucose Sensing Assay within Microporated Poly-Ethylene Glycol Microspheres. Cummins, B., Lim, J., Simanek, E.E., Pishko, M.V., and Coté, G.L. Biomedical Optics Express, 2011, 2, 1243-57. doi: 10.1364/BOE.2.001243. PMID: 21559135
- 75. Molecular modeling and in vivo imaging can identify successful flexible triazine dendrimer-based siRNA delivery systems. Merkel, O. M.; Zheng, M.; Mintzer, M. A.; Pavan, G.; Librizzi, D.; Maly, M.; Höffken, H.; Danani, A.; Simanek, E.E.; Kissel, T. J. Controlled Release, 2011, 153, 23-33. doi: 10.1016/j.jconrel.2011.02.016. PMID: 21342661
- 74. Conjugation to the Cell-Penetrating Peptide TAT Potentiates the Photodynamic Effect of Carboxytetramethyl-rhodamine. Muthukrishnan, N., Johnson, G.A.; Erazo-Oliveras, A.; Lim, J.; Pellois, J.P.; Lim, J.; Simanek, E.E. PLOS One, 2011, 6, e17732. doi: 10.1371/journal.pone.0017732. PMID: 21423812
- 73. Biological Assessment of Triazine Dendrimers as Candidate Platforms for Nanomedicine: Toxicological Profiles, Solution Behavior, Biodistribution, and Drug Release and Efficacy in a PEGylated, Paclitaxel Construct. Lo, S.-T.; Stern, S.; Clogston, J.D.; Zheng, J.; Adiseshaiah, P.P.; Dobrovolskaia, M.; Lim, J.; Patri, A.; Sun, X.; Simanek, E.E. Molec. Pharm. 2010, 7, 993-1006.
- 72. Synthesis and characterization of a triazine dendrimer that sequesters iron using twelve desferrioxamine B groups. Lim, J.; Venditto, V.J.; Simanek, E.E. Chem. Comm. 2010, 18, 5749-5753.
- 71. Triazine dendrimers as non-viral vectors for in vitro and in vivo RNAi: The effects of peripheral groups and core structure on biological activity. Merkel, O.M.; Mintzer, M.A.; Librizzi, D.; Samsonova, O.; Dicke, T.; Sproat, B.; Garn, H.; Barth, P.J.; Simanek, E.E.; Kissel, T. Mol. Pharmaceutics, 2010, 7, 969-983.
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- 69. Computational Insights into the Interactions between DNA and siRNA with "Rigid" and "Flexible" Triazine Dendrimers. Pavan, G. M.; Mintzer, M. A.; Simanek, E. E.; Merkel, O. M.; Kissel, T.; Danani, A. Biomacromol. 2010, 51, 1631-1634.
- 68. Divergent synthesis of triazine dendrimers using a trimethylene-dipiperidine linker that increases efficiency, simplifies analysis, and improves product solubility. Mintzer, M. A.; Perez, L. M.; Simanek, E. E. Tetrahedron Lett. 2010, 51, 1631–1634.
- 67. Mimicking PAMAM Dendrimers with Ampholytic, Hybrid Triazine Dendrimers: A Comparison of Dispersity and Stability. Lalwani, S.; Chouai ,A.; Perez,L.M.; Santiago,V.; Shaunak,S. Simanek, E.E. Macromolecules, 2009, 42, 6723–6732.
- 66. Intercepting triazine dendrimer synthesis with nucleophilic pharmacophores as a general strategy toward drug delivery vehicles. Venditto, V.J.; Allred, K.; Allred, C.D.; Simanek, E.E. Chem. Comm. 2009, 5541-5542.
- 65. Triazine dendrimers as non-viral gene delivery systems: Effects of molecular structure on biological activity. Merkel, O. M.; Mintzer, M. A.; Sitterberg, J.; Bakowsky, U.; Simanek, E. E.; Kissel, T. Bioconj. Chem. 2009, 20, 1799-1806.

- 64. Polycationic triazine-based dendrimers: Effect of peripheral groups on transfection efficiency. Mintzer, M.A.; Merkel, O.M.; Kissel, T.; Simanek, E.E. New J. Chem. 2009, 33, 1918-1925.
- 63. Design, Synthesis, and Characterization of Triazine Dendrimers Bearing Paclitaxel linked by Ester and Ester/Disulfide Linkages. Lim, J.; Chouai, A.; Lo, S-T.; Liu, W.; Sun, X.; Simanek, E.E. Bioconj. Chem. 2009, 20, 2154–2161.
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- 1. Self-Assembly Through Hydrogen Bonding: Preparation of a Supramolecular Aggregate Composed of 10 Molecules. Mathias, J.P.; Simanek, E.E.; Seto, C.T.; Whitesides, G.M. Angew. Chem., Int. Ed. Eng. 1993, 32, 1766-1769.

Education Research Publications (4)

- 4. Developing an Educational Tool to Model Food Chains. Blffi, D.; Hartwig, B.; de la Fuenta, Y.; Patterson, M.; Steward, M.; Simanek, E.E.; Weinburgh, M. Elect. J. Science Educ. **2016**, 20(1), 40-53.
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- 2. Scientists' Perspective on Introducing Authentic Inquiry to High School Teachers During an Intensive Three-Week Summer Professional Development Experience. Reubush, L.E.; Grossman, E.L.; Miller, S.A.; North, S.W.; Schielack, J.F.; Simanek, E.E. School Sci. Math. Journal **2009**, 109, 3: 162-174.
- 1. *Dendrimers. Branching Out of Polymer Chemistry.* Gonzalez, S.O.; Simanek, E.E. J. Chem. Ed. **2002**, 79, 1222-1231.

Reviews (8)

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- 7. *Perfectly shaped siRNA delivery.* Merkel, O.M.; Mintzer, M.A.; Simanek, E.E.; Kissel, T. Therapeutic Delivery 2010, 1, 737-742.
- 6. Cancer Therapies Utilizing the Camptothecins: A Review of in Vivo Literature. Venditto, V. J.; Simanek, E.E. Molec. Pharmaceutics, 2010, 7, 307–349.
- 5. The Eight Year Thicket of Triazine Dendrimers. Strategies, Targets, and Applications. Simanek, E.E.; Hanan A.; Lalwani, S.; Lim, J.; Mintzer, M.; Venditto, V.J.; Vittur, B. Proc. Royal Soc. A. 2010, 466, 1445-1468.
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- 1. *Noncovalent Synthesis: Using Physical Organic Chemistry to Make Aggregates.* Whitesides, G.M.; Simanek, E.E.; Mathias, J.P.; Seto, C.T.; Chin, D.; Mammen, M.; Gordon, D.M. Acc. Chem. Res. 1995, 28, 37-44.

LECTURES & PRESENTATIONS (UPDATED OCTOBER 2018)

Lectures for Scientific Audiences

University of Texas in Dallas, September 21, 2018, The Science of Whiskey

ICREA Conference on Functional Nanocontainers, 17-20 October 2017, Tarragona Spain, Dendrimers based on Triazines: From nano-Firkins to nano-Tuns for New Materials and Medicine

UNTHS Symposium for the Institute for Cancer Research, Fort Worth TX, 2015, Using Nano to Fight Cancer: A Chemist's Approach to Expanding the Arsenal and Targeting the Therapy

Biodendrimers International Conference, Lugano Switz., 2014, Dendrimers of Viral Dimensions

International Dendrimer Symposium-8, Madrid, Spain, 2013, The synthesis of large dendrimers

DFW Local ACS Section, Dallas TX, 2011, Recent Advances in Dendrimers Based on Triazines

Southwest Region Meeting of the ACS, 2011, Recent Progress in Triazine Dendrimers

Texas Tech University, Lubbock TX, 2011, From Flecks in the Flask to Kilograms in the Clinic: Progress toward Macromolecular Chemotherapeutics

Prostate Cancer Working Group UT Southwestern MC, Dallas TX, 2011, Towards Competitive Nanomedicines

Prostate Cancer Working Group UT Southwestern MC, TX, 2011, Paclitaxel-polymer constructions for Chemotherapy

American Chemical Society, National Meeting, Boston, 2010, Dendrimers Based on Melamine

Texas Lutheran University, Seguin TX, 2010, From Bench toward Clinic: Medical Applications of Triazine Dendrimers

American Chemical Society, Regional Meeting, New Orleans, 2009, Progress in the synthesis and applications of triazine dendrimers

American Chemical Society, Regional Meeting, New Orleans, 2009, Supramolecular chemistry and molecular recognition in triazine dendrimers

Phillips University, Marburg, Germany, 2009, Dendrimers Based on Melamine

Southern Methodist University, Dallas TX, 2009, Dendrimers Based on Melamine

American Chemical Society, National Meeting, Salt Lake City UT, 2009, Dendrimers Based on Melamine

International Dendrimer Symposium, Stockholm, Sweden, 2009, Dendrimers Based on Melamine

Texas Christian University, Fort Worth, TX, 2009, Dendrimers Based on Melamine

Interphase and Interphases Materials Conf., San Luis Obisbo, CA, 2008, Dendrimers Based on Melamine

7th Int. Symp. on Polymer Therapeutics, Valencia, Spain, 2008, Dendrimers Based on Melamine

Notre Dame University, South Bend IN, 2008, Dendrimers Based on Melamine

Frontier Scientific, Logan UT, 2008, Dendrimers Based on Melamine

Southern Methodist University, Dallas TX, 2008, Dendrimers Based on Melamine

University of Texas at Dallas, Dallas TX, 2008, Dendrimers Based on Melamine

UT Southwestern Medical Center, Dallas TX, 2008, Dendrimers Based on Melamine

International Polymer Therapeutics Symposium, Berlin Germany, 2007, Dendrimers Based on Melamine

MD Andersen Cancer Center, Houston TX, 2007, Dendrimers Based on Melamine

International Dendrimer Symposium 5, Toulouse France, 2007, Dendrimers Based on Melamine

University of St. Thomas, St. Paul MN, 2006, Dendrimers Based on Melamine

Trinity University, San Antonio TX, 2006, Dendrimers Based on Melamine

University of Texas-San Antonio, San Antonio TX, 2006, Dendrimers Based on Melamine

Tulane University, New Orleans LA, 2006, Dendrimers Based on Melamine UT Southwestern Medical Center, Dallas TX, 2005, Dendrimers Based on Melamine Henderson State, Arkedelphia AK, 2005, Dendrimers Based on Melamine Ouichita Baptist College, Arkedelphia, AK, 2005, Dendrimers Based on Melamine American Chemical Society National Meeting - San Diego, 2005, Dendrimers Based on Melamine Vanderbilt University, Nashville TN, 2005, Dendrimers Based on Melamine National Institutes of Health, Bethesda MD, 2005, Dendrimers Based on Melamine Southern Illinois University, Carbondale IL, 2005, Dendrimers Based on Melamine University of Texas-Dallas, Dallas TX, 2005, Dendrimers Based on Melamine Colorado State, Fort Collins CO, 2004, Dendrimers Based on Melamine University of Colorado, Boulder CO, 2004, Dendrimers Based on Melamine University of Konstanz, Konstanz Germany, 2004, Dendrimers Based on Melamine University of Dortmund, Dortmund Germany, 2004, Dendrimers Based on Melamine University of Hamburg, Hamburg Germany, 2004, Dendrimers Based on Melamine University of Berlin, Berlin Germany, 2004, Dendrimers Based on Melamine University of Massachusetts, Amherst MA, 2004, Dendrimers Based on Melamine University of Wisconsin, Madison WI, 2004, Dendrimers Based on Melamine International Drug Delivery Symposium, Cardiff Wales, 2004, Dendrimers Based on Melamine Gordon Research Conference - Drug Delivery, Boseman MT, 2004, Dendrimers Based on Melamine American Chemical Society National Meeting, NY NY, 2003, Dendrimers Based on Melamine Macalester College, Minneapolis MN, 2003, Dendrimers Based on Melamine Carleton College, Northfield MN, 2003, Dendrimers Based on Melamine American Chemical Society Regional Meeting, Oklahoma City OK, 2003, Dendrimers Based on Melamine Duke University, Raleigh NC, 2003, Dendrimers Based on Melamine North Carolina State University, Raleigh NB, 2003, Dendrimers Based on Melamine University of North Carolina, Raleigh NC, 2003, Dendrimers Based on Melamine Abbott Laboratories, Lake Forest IL, 2003, Dendrimers Based on Melamine S. F. Austin State University, Nacogdoches TX, 2003, Dendrimers Based on Melamine University of Chicago, Chicago IL, 2003, Dendrimers Based on Melamine University of Maryland, College Park MD, 2003, Dendrimers Based on Melamine Germany-US Polymer Conference, Bayreuth Germany, 2003, Dendrimers Based on Melamine University of Minnesota, Minneapolis MN, 2003, Dendrimers Based on Melamine James Madison University, Harrisonburgh VA, 2003, Dendrimers Based on Melamine Virginia Military Institute, Lexington VA, 2003, Dendrimers Based on Melamine Drug Delivery Symposium, Hawaii, 2003, Dendrimers Based on Melamine American Chemical Society National Meeting, New York NY, Strategies for Remediation

Brown University, Providence RI, 2002, Dendrimers Based on Melamine Smith College, Northampton MA, 2002, Dendrimers Based on Melamine

St. Olaf College, Northfield MN, 2002, Dendrimers Based on Melamine Emory University, Atlanta GA, 2002, Dendrimers Based on Melamine Georgia Institute of Technology, Atlanta GA, 2002, Dendrimers Based on Melamine Tulane University, New Orleans LA, 2002, Dendrimers Based on Melamine Indiana University, Bloomington IN, 2002, Dendrimers Based on Melamine University of Akron, Akron OH, 2002, Dendrimers Based on Melamine Lindsay Lecture - Texas A&M University, College Station TX, 2002, Dendrimers Based on Melamine University of California San Diego, San Diego CA, 2002, Dendrimers Based on Melamine Louisiana State University, Baton Rouge LA, 2002, Dendrimers Based on Melamine University of Connecticut, Storrs CT, 2002, Dendrimers Based on Melamine Michigan State University, East Lansing MI, 2002, Dendrimers Based on Melamine University of Illinois - Chicago, Chicago IL, 2002, Dendrimers Based on Melamine Northwestern University, Evanston IL, 2002, Dendrimers Based on Melamine University of Michigan, Ann Arbor MI, 2002, Dendrimers Based on Melamine Notre Dame University, South Bend IN, 2002, Dendrimers Based on Melamine Purdue University, South Bend IN, 2002, Dendrimers Based on Melamine Ohio State University, Columbus OH, 2002, Dendrimers Based on Melamine University of Minnesota, Minneapolis MN, 2002, Dendrimers Based on Melamine University of Texas - Austin, Austin TX, 2002, Dendrimers Based on Melamine University of Wisconsin, Madison WI, 2002, Dendrimers Based on Melamine San Diego State University, San Diego CA, 2002, Dendrimers Based on Melamine Wayne State University, Detroit MI, 2002, Dendrimers Based on Melamine The Scripps Research Institute, La Jolla CA, 2002, Dendrimers Based on Melamine American Chemical Society National Meeting, San Diego CA, 2001, Dendrimers Based on Melamine Sam Houston State University, Huntsville TX, 2001, Dendrimers Based on Melamine American Chemical Society Regional Meeting, San Antonio TX, 2001, Dendrimers Based on Melamine University of Houston, Houston TX, 2001, Dendrimers Based on Melamine American Chemical Society National Meeting, Washington D.C., 2000, Dendrimers Based on Melamine Texas Christian University, 2000, Dendrimers Based on Melamine Polymers Gordon Research Conf. (Poster), 2000, Dendrimers Based on Melamine University of Texas - San Antonio, San Antonio TX, 2000, Dendrimers Based on Melamine Southern Methodist University, Dallas TX, 2000, Dendrimers Based on Melamine Trinity University, San Antonio TX, 1999, Protein Glycosylation

Lectures for the General Public (including Sigma Xi Lectures)

Texas Lutheran University, Seguin TX, 1999, Protein Glycosylation

University of New Mexico – Albuquerque, NM, November 15, 2018, Shots of Knowledge: The Science of Whiskey

Texas A&M University – College Station, TX, October 22, 2018, Shots of Knowledge: The Science of Whiskey

Marietta College, Marietta, OH, October 16, 2018, Shots of Knowledge: The Science of Whiskey

University of West Virginia – Morgantown, WV, October 15, 2018, Shots of Knowledge: The Science of Whiskey

University of Texas - Dallas, TX, September 21, 2018, Shots of Knowledge: The Science of Whiskey

Copia (Culinary Institute of America), Napa CA, November 3, 2017, Shots of Knowledge: The Science of Whiskey

IdeaFestival, Louisville KY, November 3, 2017, Shots of Knowledge: The Science of Whiskey

Reata (restaurant), Fort Worth, TX, August 16, 2017, Shots of Knowledge: The Science of Whiskey

Read Between the Lines, Dallas TX, June 14, 2017, Shots of Knowledge: The Science of Whiskey

Elixir, San Francisco CA, May 26, 2017, Shots of Knowledge: The Science of Whiskey

Trinity Hall Pub, Dallas TX, May 20, 2017, Shots of Knowledge: The Science of Whiskey

TCU Leadership Series (x2), Fort Worth TX, April 28, 2017, Shots of Knowledge: The Science of Whiskey

Friends of the TCU Library, Fort Worth TX, April 4, 2017, Shots of Knowledge: The Science of Whiskey

PUBlic Knowledge, FW Museum of Science & History at World of Beer, Fort Worth TX, March 7, 2017, Shots of Knowledge: The Science of Whiskey

Faculty Favorite Lecture Series, TCU, Fort Worth TX, February 21, 2017, Shots of Knowledge: The Science of Whiskey

Fort Worth Museum of Science & History, Fort Worth TX, December 2016, Shots of Knowledge: The Science of Whiskey

TCU Development, Fort Worth TX, 2011 Nanomedicines (x2)

Texas A&M Chem. Open House, CS TX, 2009, Big Fights in Little Medicines: Using Nano to Fight Cancer First Year Program Lecture Series, TAMU, 2009, Big Fights in Little Medicines: Using Nano to Fight Cancer

Lectures on Education, Administration and Public Action

Endowed Chairs Banquet of TCU, Fort Worth TX, 2015, The Science of Water - A Poem

Endowed Chairs Banquet of TCU, Fort Worth TX, 2011, Nanomedicines

Retiree's Luncheon at TCU, Fort Worth TX, 2011, Dance of the Continents

South Dakota School of Mines and Technology, Rapid City SD, 2015, TCU IdeaFactory

A.C.S. Natl Mtg, Salt Lake City UT, 2009, Strategies for Sustainability in a General Chemistry Program

NSF CCLI Annual Mtg, Washington DC, 2008, Strategies for Sustainability in a General Chemistry Program

University of Texas as Dallas, 2008, Strategies for Sustainability in a General Chemistry Program

ACS National Meeting (CHED), 2007, Texas A&M and the FYP: Investment, Change, and Sustainability

NSF GK-12 Annual Meeting, DC, 2007, Organizational strategies for educational outreach programs

College Station Park District, College Station TX, 2007, Proposal for Wolf Pen Creek Science Park

Bryan Rotary Club, Bryan TX, 2007, Proposal for Wolf Pen Creek Science Park

College Station Rotary Club, College Station TX, 2006, Proposal for Wolf Pen Creek Science Park

Exec. Board of the Convention and Visitors Bureau, College Station TX, 2006 Proposal for Wolf Pen Creek Science Park

College Station City Council/Independent School District Joint Meeting, 2006, Proposal for Wolf Pen Creek Science Park

Wolf Pen Creek Oversight (TIF) Board, College Station TX, 2006, Proposal for Wolf Pen Creek Science Park

Poster Presentations - Science, Education and Outreach

Cerebral Palsy and Dance. Momentis Conference, Boston MA, June 2018.

Two Decades of Dendrimer Chemistry. International Polymer Conference, Barcelona Spain, March 2018.

Dendrimers of Viral Dimensions. International Polymer Conference, Riva Italy, May 2015.

- Cost-effective, high volume strategy for teaching the atom to K-7 students" Zachary M. Abid, Nicholas A. Bigham, Kevin S. Chatley, Sandi B. Dang, Abby R. Moore, Katelyn E. Poole, Derek P. Royer, Eric E. Simanek. Regional Meeting of the American Chemical Society, New Orleans, December 1, 2010.
- Synthesis of Hyperbranched Polymers. Zachary M. Abid, Nicholas A. Bigham, Kevin S. Chatley, Sandi B. Dang, Abby R. Moore, Katelyn E. Poole, Derek P. Royer, Eric E. Simanek. Regional Meeting of the American Chemical Society, New Orleans, December 1, 2010.
- Food Chain Jenga: Using Models to Test Predictions. Biffi D, Hartweg B, Patterson M, Stewart M, de la Fuente Y, Simanek E, & Weinburg M. 2015. ASTE. Denton, Texas, USA.
- Food Chain Jenga: Using Models to Test Predictions. Biffi D, Hartweg B, Patterson M, Stewart M, Simanek E, & Weinburg M. 2015. SSMA Annual Convention. Oklahoma City, Oklahoma, USA.

Writing for the General Public

Whiskey and Cherry Blossoms. Distiller Magazine (Fall 2018 issue)

Teaching Whiskey to College Students, Washington Post, Aug 24, 2018

Twenty Bars in Two Days: A Whiskey Professor Sips San Francisco Fort Worth Inc. Jan/Feb 2018

Shots of Knowledge: The Science of Whiskey. Arnold, R. & Simanek, E. TCU Press, 2016.

<u>Interviews - Print & Online</u>

- "2 Arkansas Chemistry Professors Face Charges of Making Meth" by Johnny Diaz Nov 17, 2019 for The New York Times. https://www.nytimes.com/2019/11/17/us/arkansas-chemistry-professor-meth.html
- "THE PIVOT TO WHISKEY: Artificial whiskey is coming, and one company is betting you'll drink up" by Alan Goldfarb Aug 23, 2018 for The Verge. Article link.
- "Not So Neat: Why You Should Add Water to Your Whiskey" by Marcus Woo for *Science Insider*, Aug 17, 2017
- "10x10" in Malibu Magazine, May-June Issue 2017

Interviews - Television

"The Bookmark" hosted by Christine Brown, public television, KAMU, College Station TX*

Interviews - Radio

"Think" hosted by Krys Boyd on public radio, KERA, Dallas TX* aired December 20, 2017

The Science Behind the Drink with Chemist Eric Simanek, WFPL Radio hosted by Ashlie Stevens on WFPL, Louisville KY, as part of the IdeaFestival in 2017