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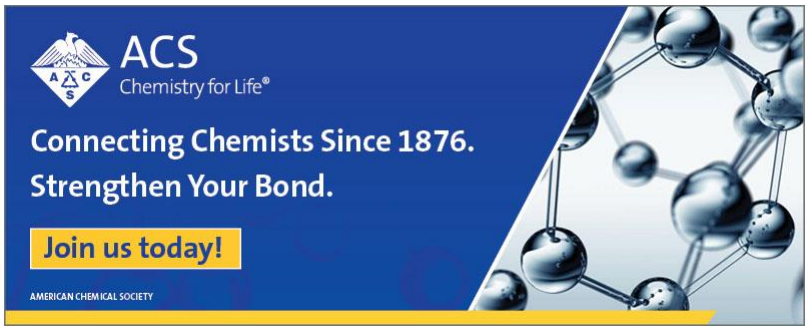

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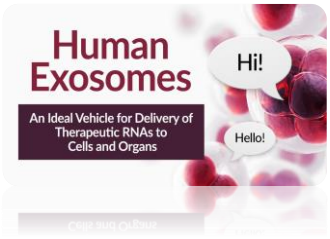
"The speaker gave an excellent presentation, he patiently and systematically introduced knowledge and nomenclature to the audience so each listener readily could understand the function and operation of exosomes. The science presented was captivating and served to launch innovative thought about how a scientist might harness the utility of exosomes."

Fan of the Week

Valarie Thomas



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ACS Heroes of Chemistry Award

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Deadline: Friday, Feb. 1, 2019

2018 Winners: AstraZeneca, DuPont, Pfizer, Seattle Genetics

www.acs.org/heroes

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Upcoming ACS Webinars

www.acs.org/acswebinars

Thursday, February 7, 2019 @ 2-3pm ET

Startups 101: From Lab Scientist to Entrepreneur

Co-produced with ACS Graduate & Postdoctoral Scholars Office

Experts

Naresh Sunkara
Nosocom Solutions, Inc.

Corrie Kuniyoshi
ACS Graduate & Postdoctoral Scholars Office

Thursday, February 14, 2019 @ 2-3pm ET

The Chemistry of Chocolate and Desire

Co-produced with ACS Division of Agricultural & Food Chemistry

Experts

Michael Tunick
Drexel University

Brian Guthrie
Cargill

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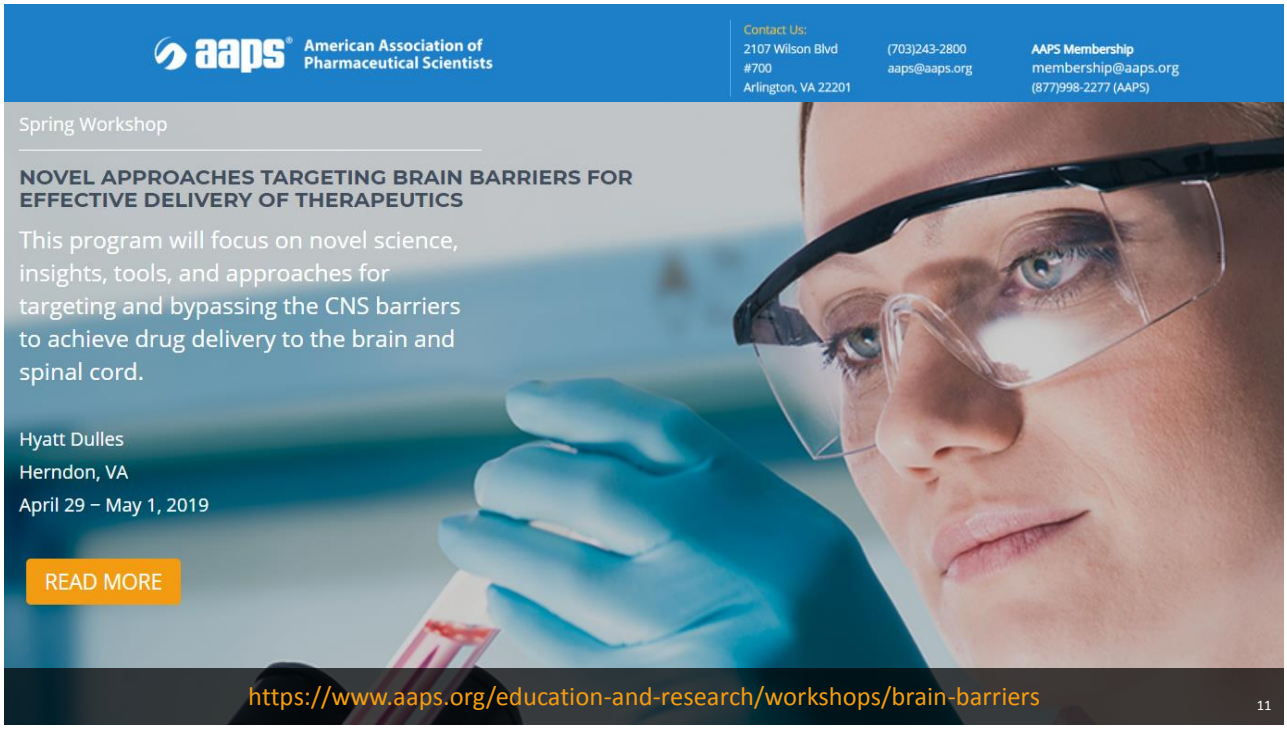

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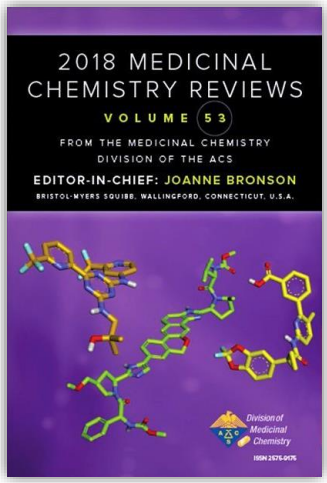

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Celebrating 5 years & 50 Drug Discovery Webinars!

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ACS Chemistry for Life®

2014

1. Drug Discovery Series #1 - Current Drug Discovery and Development Process (DDS #1) Watch this overview of the drug discovery and development process to learn the stages and challenges in every step.
2. Primer in Drug Target Classes (DDS #2) Listen in on a discussion on the big four druggable families and the difference between small molecule and biotherapeutic targets.
3. Key Concepts in Identifying Drug Leads (DDS #3) Discover how drug-likeness is a decisive concept, explore the Rule of Five, and show how lessons from the past may guide the present.
4. Lead Optimization - Building Efficacy & Safety (DDS #4) Learn strategies on how to effectively optimize small molecule hits and rapidly assess your findings.
5. Tips for Filing IND and Starting your Clinical Trials (DDS #5) What do you need to know when filing for Investigational New Drug submissions to the United States Food and Drug Administration?
6. The Role of Chemistry in Clinical Trials: The Big Expense & Lessons Learned (DDS #6) Learn how the properties of the candidate impact decisions in the discovery process.
7. Pharmacoeconomics and IP Strategies in Drug Development (DDS #7) Review the basic principles of Pharmacoeconomics in drug development strategies as well as its role in determining health insurance coverage of drug products.
8. Future of Drug Discovery - Challenges, Risks and Rewards (DDS #8) Explore how how risks and challenges will be dealt with in the future and the key skill sets required of future medicinal chemists.

2015

- Designing Better Drug Candidates (January) Learn various factors that can be used to improve candidate quality from Dr. Paul Leeson.
- Strategies to Improve Solubility of Drug Candidates (February) Learn a number of different strategies for improving drug solubility through structural modification.
- Fragment-Based Drug Design Strategies (March) Finding the right drug target is becoming increasingly difficult. Learn how focusing on the smaller picture can here big results.
- Screening Strategies (April) Learn the pros and cons of different screening strategies.
- Avoiding PAINS (pan-assay interference compounds) (May) Jonathan Baell shares some tips on how to avoid the dead ends of drug discovery.
- Accelerating CNS Positron Emission Tomography (PET) Ligand Discovery (June) Jon Lai Zhang as he lays out a set of preferred parameters for which has yielded successful PET ligands and reduced resources and timelines.
- X-ray Crystallography in Drug Discovery (July) Jon Mason and Miles Congreve describe what protein-ligand X-ray data can do for you.
- Choices and Trends in Solid Dosage Form Selection (August) Discover the pros and cons of the different solid state forms and what to consider when selecting.
- Delivery Options to Support Dose Escalation in Preclinical Toxicology and Pharmacodynamic Activity Studies (September) Gain an understanding of acceptable drug delivery approaches to support preclinical dose escalation.
- Pharmacokinetic Considerations in Drug Design and Development Learn about key pharmacokinetic concepts including clearance, volume of distribution, half life and protein binding.
- Prodrugs in Drug Discovery (November) John Higgins shares the utility of prodrugs, their general properties and prerequisites for optimal performance.

2016

I - Time: The Fourth Dimension in Drug Discovery

1. The Importance of Drug-Target Kinetics in Drug Design — Robert Copeland - Epizyme, Inc; Dan Evanson - Carmot Therapeutics
2. Long-Acting Injectable Medications: Strategies and Mechanistic Considerations — Jules Ramanjar - Alkermes; Annette Bak - Merck
3. Modified Release Formulations for Solubility Starved Compounds — Mangwei Hu - Merck; John Morrison - BMS
4. The Medicinal Chemist of Tomorrow (Special Topic) — Joel Barrish - Achillion; Ravi Nargund - Merck; Molly Schmid - Tech Coast Angels

II - Beyond Traditional Small Molecules

5. Design of Deliverable Macrocycles — Scott Lokey - UC Santa Cruz; Nicholas Meanwell - BMS
6. Dreaming Big and Thinking Small: Applying Medicinal Chemistry Strategy to Antibody-Drug-Conjugates — L. Nathan Tumey - Pfizer; Peter Senter - Seattle Genetics
7. Nucleic Acids Therapeutics: Making Sense of Antisense Oligonucleotides — Punit Seth - Ionis; Richard Olson - BMS
8. Crystallography as a Drug Design and Delivery Tool (Special Topic) — Robert Wanstrow - Crystal Pharmatech; Vincent Stoll - Abbvie; Andrew Bruntskill - Merck

III - Pharmacology Revisited

9. Dealing with Reactive Drug Metabolites in Drug Discovery: Can We Predict Toxicities of Drug Candidates that form Reactive Metabolites? — Deepak Dalvie - Pfizer; Frederick Peter Guengerich - Vanderbilt University
10. Rational Design of Small Molecules Targeting RNA — Matt Disney - Scripps Rl Florida; Amanda Garner - University of Michigan
11. Cell Penetrating Peptides to Improve Cellular Drug Uptake — Dehua Pei - The Ohio State University; Scott Hart - Bristol-Myers Squibb

2017

I - Fighting Cancer

1. Fighting Cancer: Targeting CNS Malignancy with Kinase Inhibitors — Timothy P. Heffron - Genentech; Mark Wittman - Bristol-Myers Squibb
2. Fighting Cancer: Epigenetic targets for Oncology — Stuart Conway - Oxford; Sharan Bagal - AstraZeneca
3. Fighting Cancer: Allostery and Targeting Cancer Cell Metabolism — Stefan Gross - Agios; Scott Edmundson - AstraZeneca

Special Broadcast

4. Cystic Fibrosis: Discovery of CFTR Modulators — Peter Grootenhuis - Vertex; Nick Meanwell - Bristol-Myers Squibb

II - Anti-Infectives

5. Anti-Infectives: Rational Approaches to the Design and Optimization — Jason Sello - Brown University; Courtney Aldrich - University of Minnesota
6. Tuberculosis: An Introduction for Medicinal Chemists — Carl Nathan - Weill Cornell Medicine; Christopher Boyce - Merck
7. Viral Hepatitis: The Search for a Cure — Mike Sofia - Arbutus Biopharma; Stephen Mason - CaroGen Corporation

Special Broadcast

8. Spinal Muscular Atrophy — Kevin Hodgetts - Harvard Medical School; Alyson Weidmann - ACS Publications

III - Immunology

9. Psoriasis: Treatment and Novel Approaches — Frank Narjes - AstraZeneca; John Morrison - Bristol-Myers Squibb
10. Lupus: Treatment and Novel Approaches — Laurence Menard - Bristol-Myers Squibb; Mary Struthers - Bristol-Myers Squibb

2018

- Jan 25 — A New Strategy in Drug Discovery: Protac-Induced Protein Degradation — Ian Churcher - Benevolentbio; Aaron Balog - Bristol-Myers Squibb
- Feb 22 — Women in Drug Discovery and Development: How to Succeed as a Female in Academia and Industry — Annette Bak - AstraZeneca; Donna Huryn - University of Pittsburgh; Erika Araujo - Bristol-Myers Squibb; Nurulain Zaveri - Astraea Therapeutics
- Mar 29 — A Nanomedicine Overview for mRNA Delivery: Innovative Methods Using Lipid Nanoparticles — Marianna Yanez Arteta - AstraZeneca; Dennis Luerig - Genentech
- Apr 26 — Nanomaterials for Fighting Antibiotic-Resistant Bacteria — Vincent Rotello - University of Massachusetts at Amherst; Christopher England - American Chemical Society
- May 31 — Advanced Nano-Delivery Systems: Facilitating Tumor Delivery and Mitigating Resistance — Mansoor Amiji - Northeastern University; Venkat Krishnamurthy - AstraZeneca
- Jun 28 — Pitfalls and Promise of Central Nervous System Drug Discovery — Valentin Gribkoff - Yale University; Nicholas Meanwell - Bristol-Myers Squibb
- Jul 26 — How to Optimize Central Nervous System Therapeutics: Med Chem Strategies, Tactics, and Workflows — Craig Lindsley - Vanderbilt Center for Neuroscience Drug Discovery; Amy Newman - Intramural Research Program, NIH
- Sept 20 — A Novel Strategy for the Treatment of Chronic Pain: Antagonising PAR2 with a Monoclonal Antibody — Pete Thornton - AstraZeneca; Nurulain Zaveri - Astraea Therapeutics
- Oct 18 — How to Predict Human CNS PK/PD: Preclinical Experiments and Advanced Mathematical Modelling — Elizabeth de Lange - Leiden Academic Center for Drug Research; Alexander Tropsha - University of North Carolina
- Nov 29 — Human Exosomes: An Ideal Vehicle for Delivery of Therapeutic RNAs to Cells and Organs — Hadi Valadi - University of Gothenburg; Alexander Kapustin - AstraZeneca

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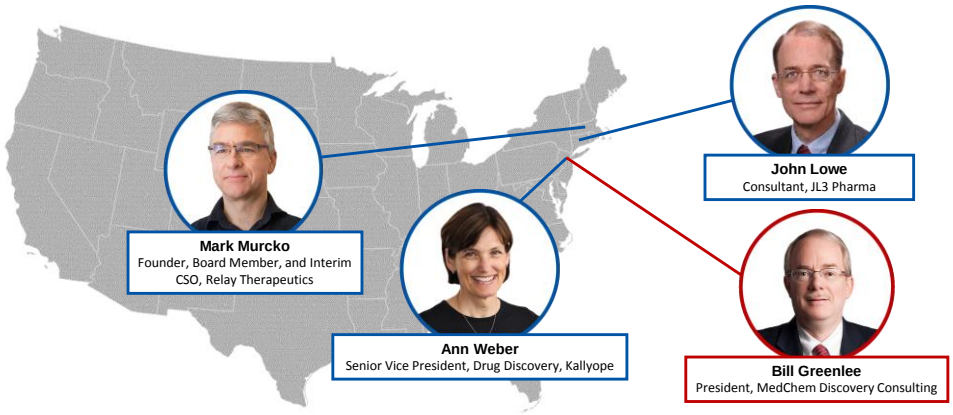
How to Succeed in Drug Discovery: Insight from Medicinal Chemists



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Bill Greenlee

President MedChem Discovery Consulting, LLC

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Today's Focus – How to Succeed in Medicinal Chemistry

- *What **skills** are **required***
- *What **behaviors** and **characteristics** are important*
- *What are the **best ways to acquire** these skills and characteristics*
- ***Advice** from our speakers, based on their successful careers*

Moderator Background

– B.S. - **Ohio State**; M.S./Ph.D. - **Harvard**; Postdoc – **Columbia**

– **Merck** in Rahway, NJ (cardiovascular, metabolic, ID, inflammation) – *Sr. Director*

– **Schering-Plough**, Kenilworth, NJ (cardiovascular, CNS, high-throughput synthesis, external collaborations) – *Sr. Director/VP of Chemistry*

– **Merck**, post-merger; Kenilworth, Rahway

– **Consulting** since 2011

Other Involvement in Medicinal Chemistry

Member of ACS since 1972

ACS Technical Division
Medicinal Chemistry (MEDI)

- Division of Medicinal Chemistry (MEDI), Program Chair, Division Chair, Councilor (2000 – present)
- Perspectives Editor for *Journal of Medicinal Chemistry* (2006-2017)

Journal of Medicinal Chemistry

Co-organizer, Drew University Residential School on Medicinal Chemistry and Biology in Drug Discovery (2002 – present)

ResMed

How to Become a Great Medicinal Chemist?

Journal of Medicinal Chemistry

ACS AuthorChoice

Perspective

Cite This: *J. Med. Chem.* 2018, 61, 7419–7424

pubs.acs.org/jmc

What Makes a Great Medicinal Chemist? A Personal Perspective

Miniperspective

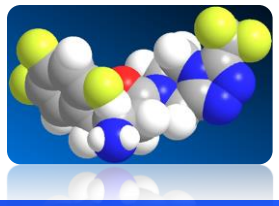
Mark A. Murcko*

Relay Therapeutics Inc., 215 First Street, Cambridge, Massachusetts 02142-1213, United States

https://pubs.acs.org/doi/abs/10.1021/acs.jmedchem.7b01445

Important Roles of Medicinal Chemists in Drug Discovery

- Help set the objectives for a drug discovery program and define the target candidate profile
- Select the very best hit structures to begin a medicinal chemistry program
- Design and synthesize new drug-like molecules to develop structure-activity relationships (SAR) for the program
- Deliver a survivable drug candidate, with optimized properties, for development
- Serve as a project champion/problem solver for the program



Medicinal Chemists – Skills/Characteristics for Success

A deep and critical understanding of medicinal chemistry – including a sense of what is a drug-like molecule, and an intuition for what compound to make next in a program. A long-term commitment to medicinal chemistry is required to acquire these skills.

- Read relevant medicinal chemistry papers from the top journals
- Follow the patent literature for your project *(and related projects)*
- Attend (and present at) medicinal chemistry meetings (*ACS National Meetings, Medicinal Chemistry Gordon Conference, ACS National Medicinal Chemistry Symposium, Frontiers in Medicinal Chemistry*)
- Attend seminars at your organization and outside
- Publish your work *(if possible)*

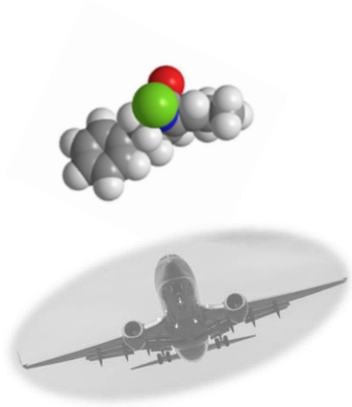
PLOS

Ten Simple Rules for Developing Good Reading Habits During Graduate School and Beyond, M. Menendez, *PLOS Computational Biology* 2018.
https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1006467

Medicinal Chemists – Skills/Characteristics for Success

Experienced and innovative medicinal chemists are essential for successful drug discovery and development.

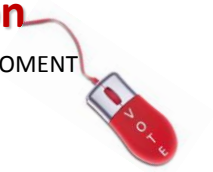
- All molecular and physical properties of a drug are determined by its structure, and are locked in when a development decision is made
- Changing a single atom in a drug molecule will affect every physical/chemical property of that molecule, along with its potency and selectivity



If we designed airplanes like we design drugs…, *J. Comput. Aided Mol. Des.*, 2012, **26**: 159-163.
https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3268976/

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



What stage are you currently in concerning medicinal chemistry career?

- I am in graduate school or preparing to enter the field
- I am new to the field *(ex. two to three years into my career)*
- I am in the beginning stages *(ex. five years into my career)*
- I am well into my career *(ex. ten to fifteen years into my career)*
- I could be a panelist for this webinar *(ex. over twenty years into my career)*

** If your answer differs greatly from the choices above tell us in the chat!*

Drug Discovery: A Calling

Mark Murcko

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"Drug discovery: aiming for the moon?"
Drug Discovery Today, 20 Aug 2009

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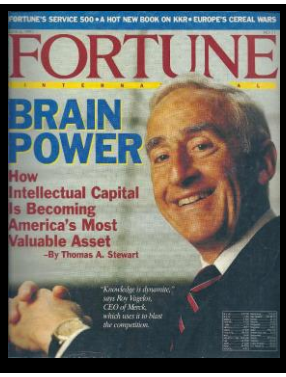
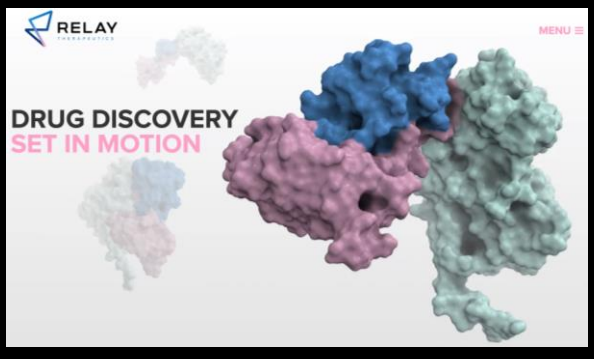
TIME


FORTUNE'S SERVICE 500 • A HOT NEW BOOK ON KKR • EUROPE'S CEREAL WARS
FORTUNE
BRAIN POWER
How Intellectual Capital Is Becoming America's Most Valuable Asset
–By Thomas A. Stewart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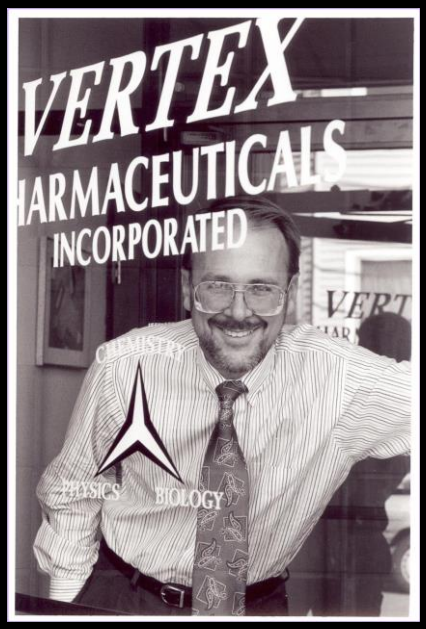
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A Starting Point For A Discussion

Perspective

What Makes a Great Medicinal Chemist? A Personal Perspective

Miniperspective

Mark A. Murcko*
Relay Therapeutics Inc., 215 First Street, Cambridge, Massachusetts 02142-1213, United States

J. Med. Chem., **2018**, *61* (17), pp 7419–7424
DOI: 10.1021/acs.jmedchem.7b01445
Publication Date (Web): May 10, 2018

*Phone: 508-282-6797. E-mail: mark.murcko@gmail.com.

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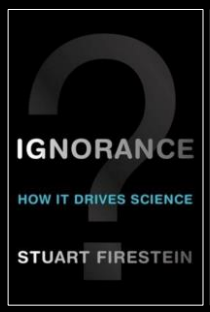

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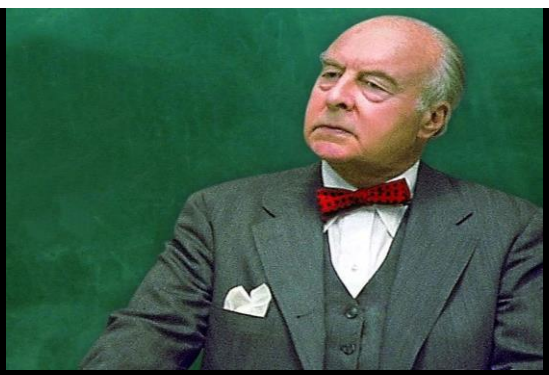

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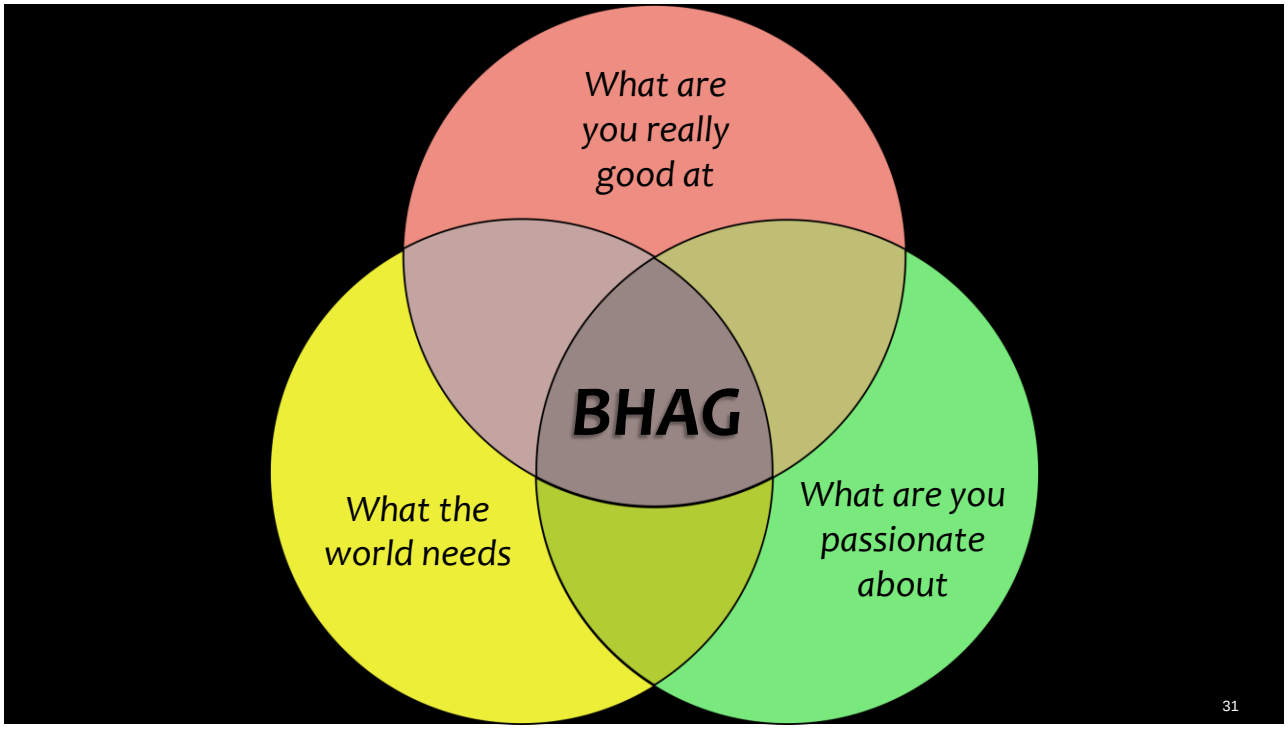
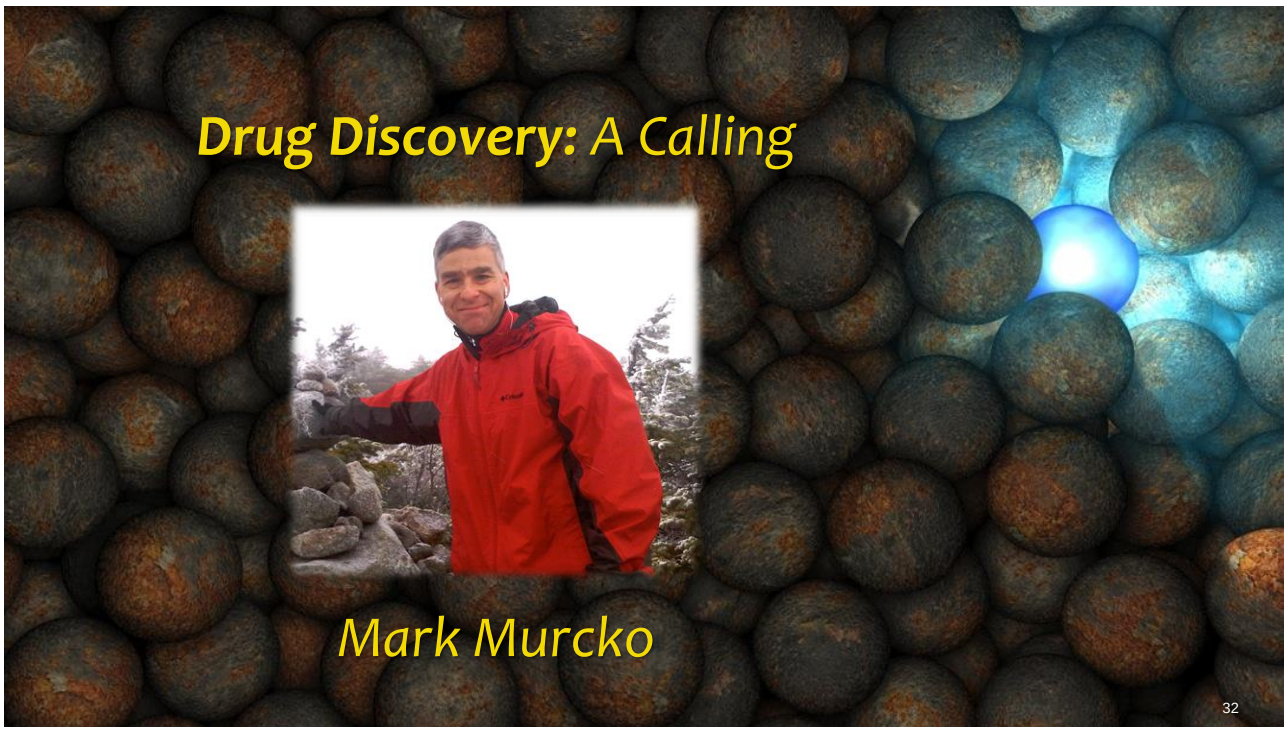

What are you really good at
BHAG
What the world needs
What are you passionate about
31


Drug Discovery: A Calling
Mark Murcko
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Audience Survey Question

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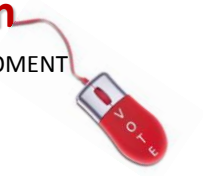
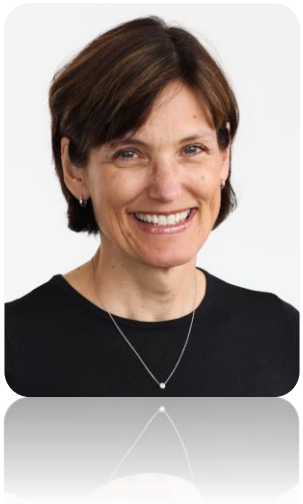


How many employers have you worked for during your medicinal chemistry career?

- I have never worked for an employer in the field
- I have worked for one employer
- I have worked for several employers
- I have worked for three or four employers
- I have worked for over five employers

** If your answer differs greatly from the choices above tell us in the chat!*



Ann E. Weber

Kallyope Inc.

My Career Path

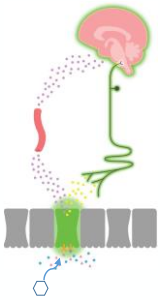
Education

- BS, chemistry, University of Notre Dame
- PhD, synthetic organic chemistry, Harvard

Dave Evans

Merck

- From Sn Research Chemist in 1987
- To VP of Lead Optimization Chemistry in 2015



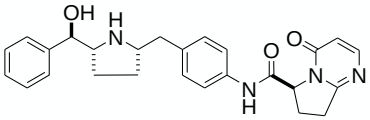
Life after Merck

- Ann Weber Pharma Consulting: Dec 2015
- Kallyope Inc: Oct 2016 – present

From Bench to Bedside

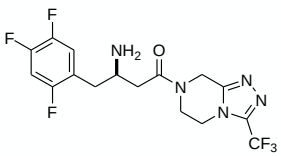
- β_3 adrenergic receptor agonists for obesity – and overactive bladder

BEOVA® (vibegron)

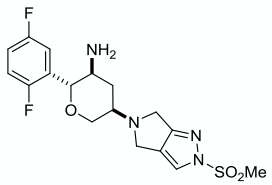


- DPP-4 inhibitors for type 2 diabetes

Nancy Thornberry



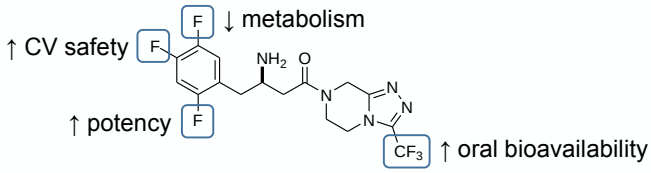
Januvia (sitagliptin phosphate)



MARIZEV® (omarigliptin)

How to Succeed: What's Worked for Me

- Maintaining a healthy skepticism around new data, but being open to new ideas
- Doing the key Go / No Go experiments
- Killing compounds quickly and cheaply
- Making every atom count



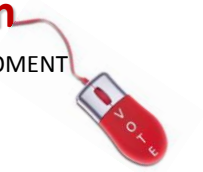
- Learning drug development

Lessons Learned

- Actively seek out mentors and sponsors
- Ask lots of questions
- Don't be afraid to make mistakes
- If it isn't working, try something else (Plan B)
- Diversity matters: be the best version of yourself
- Trust your gut

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



Do you work currently in teams as a medicinal chemist?

(Select all possible answers that apply.)

- I do not work on a team
- I work in a small interdepartmental team *(ex. less than five people)*
- I work in a large interdepartmental team *(ex. more than twenty people)*
- I work across multiple departments within my organization
- I work across multiple external organizational teams for my employer

** If your answer differ greatly from the choices above tell us in the chat!*

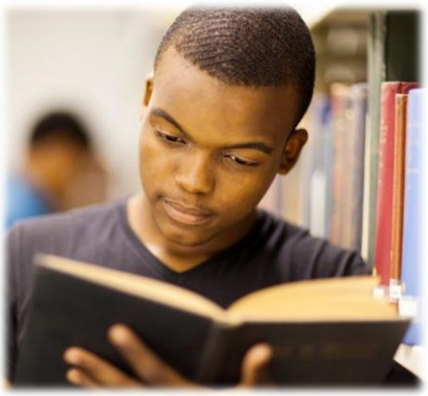
John Lowe

Background and Career Path

- Trained with Mike Jung at UCLA as a synthetic chemist
- Medicinal chemistry lab supervisor at Pfizer for 30 years
- Transitioned to consulting 10 years ago

Reading the Literature

- **Discipline journals**
  - Journal of Medicinal Chemistry — https://pubs.acs.org/journal/jmcmar
  - ACS Medicinal Chemistry Letters — https://pubs.acs.org/journal/amclct
- **Read more broadly**
  - nature — https://www.nature.com/
  - Science Journals AAAS — https://www.sciencemag.org/
  - nature reviews drug discovery — https://www.nature.com/nrd/
  - PNAS Proceedings of the National Academy of Sciences of the United States of America — https://www.pnas.org/cell_biology
- **General reading**
  - History of science
  - Biographies of scientists



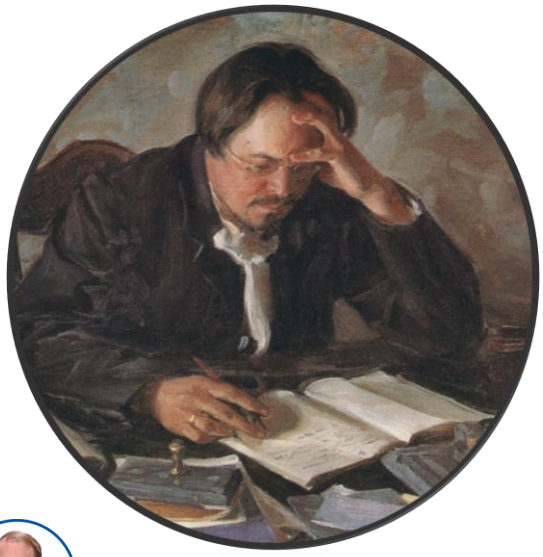
Working in a Team

- Listening to others' ideas
- Respect your team members' needs and requests, so they will respect yours
- Learning from colleagues in other disciplines

Backup Plans

- Unanticipated failures are common
- You can never have too many backup options
- Don't be afraid to try something new

Writing Well



- What do you know now that you wish you knew earlier in your career?
- I do not write well – many of my publications were spoiled because they were poorly written
- Taking a writing course would have helped me immensely

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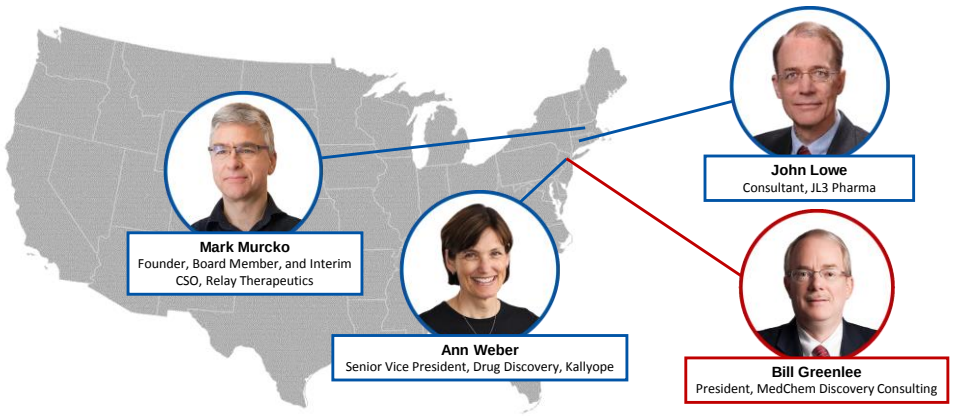

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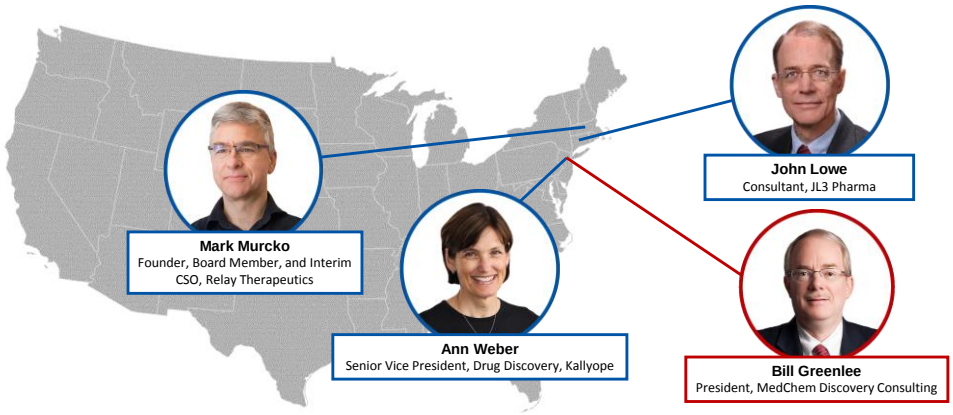

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Fan of the Week

Valarie Thomas

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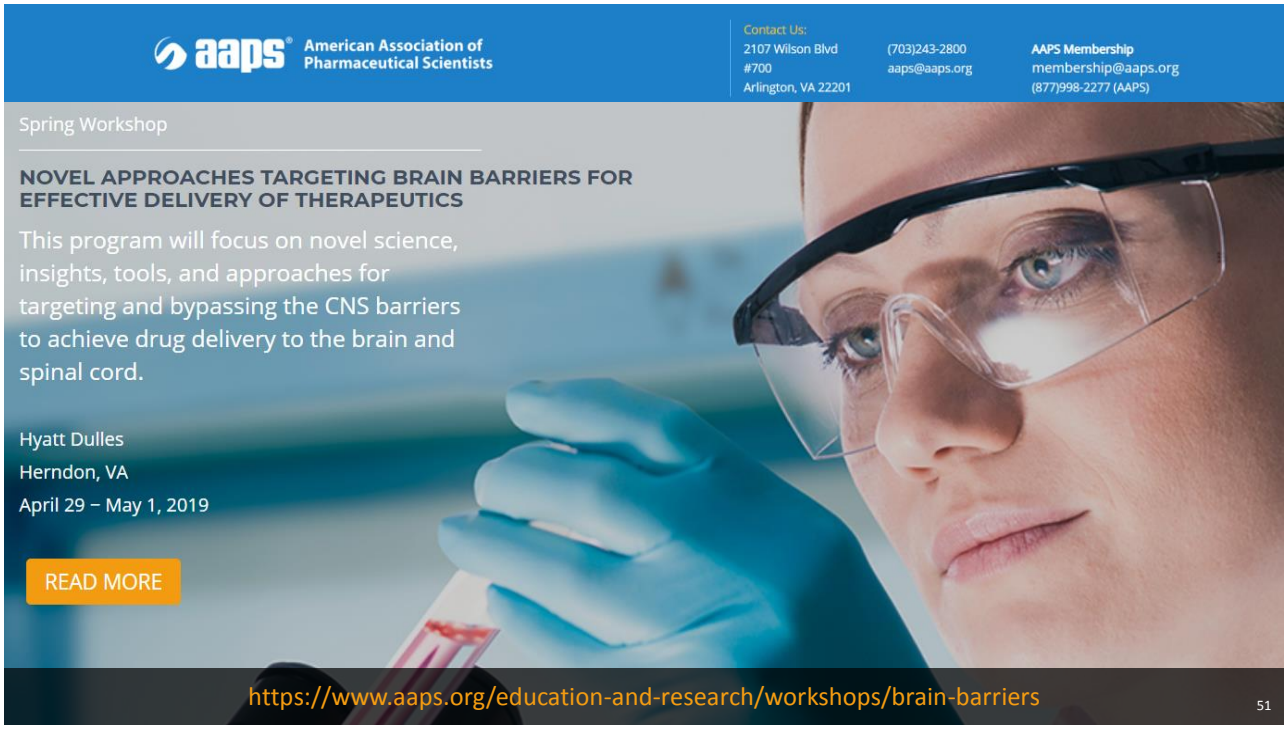

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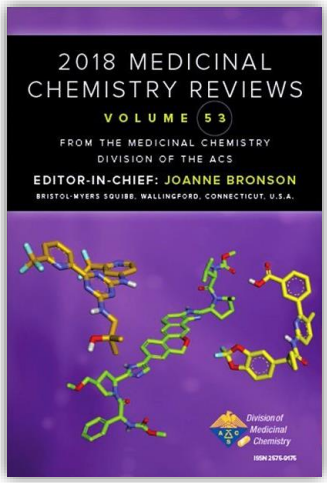

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