Type them into questions box!

“Why am I muted?”
Don’t worry. Everyone is muted except the presenter and host.
Thank you and enjoy the show.

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Robert Rittenhouse, Ph.D.
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Central Washington University, ACS member for 43 years strong!

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NOVEL APPROACHES TARGETING BRAIN BARRIERS FOR EFFECTIVE DELIVERY OF THERAPEUTICS

This program will focus on novel science, insights, tools, and approaches for targeting and bypassing the CNS barriers to achieve drug delivery to the brain and spinal cord.

Hyatt Dulles
Herndon, VA
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Women at the Interface of Computational Chemistry and Drug Discovery

Yvonne C. Martin  
Retired Computational Chemist, Previously of Abbott Laboratories

Kate Holloway  
Principal Scientist, Gfree Bio LLC

Shana Posy  
Principal Scientist, Computer-Aided Drug Discovery Group, Bristol-Myers Squibb

Zoe Courina  
Investigator – Assistant Professor Level Biomedical Research Foundation, Academy of Athens

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This ACS Webinar is co-produced with the ACS Division of Medicinal Chemistry and the American Association of Pharmaceutical Scientists
Please help us understand the current landscape of computational chemistry.

**Do you identify as:**

- Male
- Female
- Other

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

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**Women at the Interface of Computational Chemistry and Drug Discovery**

Yvonne C. Martin  
Retired Computational Chemist,  
Previously of Abbott Laboratories

Kate Holloway  
Principal Scientist,  
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Yvonne C. Martin
Retired Computational Chemist,
Previously of Abbott Laboratories

Career Path: Apply Chemical Insights to Biological Problems

Year


Computer Complexity

- BA
- Lab assistant
- PhD NU
- PK, DDI

yvonnecmartin@comcast.net
Career Path: Apply Chemical Insights to Biological Problems

yvonnecmartin@comcast.net

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yvonnecmartin@comcast.net
Career Path: Apply Chemical Insights to Biological Problems

Advice on Working in a Team

- **Provide what the team needs**, not what is most fun for you or what you already know how to do
- Interact with all team members, not just the leader
- Share your tools with whoever wants to use them
- Remember the problems that you couldn’t **solve**, because you might later find a solution to help someone else
- Listen to complaints and frustrations with what you provide as a hint for need capabilities
People who Can Help Advance Your Career

Career Mentor
A person who provides you with continuing advice on career decisions.

Guide Mentor
A person who helps you learn a new area of research.

Champion
A member of management who appreciates your contributions and looks out for you, often without totally understanding what you do.

Good Peer-reviewed Publications are Important

- Provides you with a check on your approach and methods
- Helps management and collaborators evaluate your work
- Introduces your work to others outside your institution
- Provides entry into discussions about the merits of different approaches, who is doing what, and ideas about where the field is moving
- Helps you meet collaborators or consultants
A Good Publication

- Provides evidence to contradict or refine current thinking.
  Do Structurally Similar Molecules Have Similar Biological Activity?
  Journal of Medicinal Chemistry  
  https://pubs.acs.org/doi/abs/10.1021/jm520155c

- Highlights a solution to a problem that we didn’t even know (or admit) we had.
  A Fast New Approach to Pharmacophore Mapping and its Application to Dopaminergic and Benzodiazepine Agonists
  SpringerLink  
  https://link.springer.com/article/10.1007%2FBF00141577

- Identifies a problem that the field needs to address. Let’s not Forget Tautomers
  PubMed  

Lessons Learned

- Focus on what the team or organization needs
- Share your expertise internally and externally
- Network to identify and cultivate capabilities beyond your own
- Champion initiatives that will move the organization forward
- Keep looking for opportunities to contribute in a different way
- Always keep learning new ways to do things
- Publish good papers
- Listen to complaints and advice
One of today’s speakers was named in a clue on the TV Show Jeopardy in the category “She Invented What?” Can you guess which one?

- Who is Yvonne Martin?
- Who is Kate Holloway?
- Who is Shana Posy?
- Who is Zoe Cournia?

* If your answer differs greatly from the choices above tell us in the chat!
How Did I Get Here?

Lesson #1

It’s OK to change your mind/major/direction/career/goal! The successful path isn’t always a straight one.

Lesson #2

It’s unlikely that today’s scientists will spend their entire career primarily at one company.
Computational Chemistry – 1980s

- Yes, we did have computers back in the 1980s
  - Although not PCs!
  - Instead, we used remote mainframes – think early "cloud computing"
  - BTW, FEP was the hot new method at the 1988 Gordon Research Conference on Computational Chemistry

- **Typical computational chemist background at that time**
  - Medicinal Chemistry
  - Molecular Mechanics
  - Quantum Mechanics
  - Molecular Dynamics
  - Biophysics

- **First woman in the modeling group at Merck in 1985** – now there are many more!

Lesson #3

Never be afraid to follow your interests despite any norms or barriers. There are no women’s/men’s fields/jobs/opportunities.

A Rising Tide of CompChem Women

- Good news - women’s participation in the CompChem community appears to be on the rise, as *conferees, speakers, session chairs, and officers*.

Lesson #4

Continue to push for diversity and inclusion. Track the progress.
Some Unique Issues for Women

- "2-body" problem
  - My husband also has a career ... as a computational chemist
  - In fact, we were sometimes in direct competition at different companies
  - Even as recently as the 1990s, many folk expected women to go out on maternity leave and never return
  - 3 maternity leaves = 3 months, 4 months, 6 months ... then part-time for 2 years
  - That put me on the "mommy track" but I was still working which was important to me
- Learning to seriously multitask, e.g.
  - Shh, don’t tell! - I organized a GRC program at my home computer in the summer of 1998 while simultaneously nursing my third son
  - We had a child diagnosed with a learning disability that required intensive testing/therapy/advocacy
  - We were often creatively piecing together after-school and summer childcare situations – aren’t we all?

Lesson #5
Compromise is key. Supportive partners/friends/bosses can be critical. It’s OK to sometimes wonder if you are making the right choices.

Lesson #6
"Life is what happens while you are busy making other plans" - John Lennon. Learn to relax and go with the flow.

Collaborators and Mentors

- We don’t make real chemical compounds, only virtual ones!
- So ... we have to convince someone of our good ideas in order to get them synthesized and tested
- As it happened, all of my key chemistry collaborators were male
  - Joe Vacca
  - Craig Coburn
  - Nigel Liverton
  - John McCauley
  - Mike Rudd

Lesson #7
Finding good collaborators/mentors is essential to success, especially as a "virtual chemist". It is critical to learn how to “win friends and influence people”.
Computer to Bedside

• Fortunate to have been involved in the design/identification of 4 marketed drugs
  - Crixivan – HIV protease inhibitor; approved 1996
  - Isentress – HIV integrase inhibitor; approved 2007
  - Vanihep – HCV protease inhibitor; approved Japan 2014
  - Zepatier – HCV protease inhibitor; approved 2016

• Although mighty oaks from acorns grow … it takes a village to develop and market a drug!

Lesson #8
Recognize that your work often represents just a small cog in a large machine. BUT … do make sure that your contributions are valued and rewarded equally as your male and experimental colleagues.

Get Out There!

Lesson #2
It’s unlikely that today’s scientists will spend their entire career primarily at one company.

Lesson #9
Establishing an internal reputation is critical to success at your current job. But establishing an external reputation and network are even more important when looking for your next job!

• Take advantage of the opportunity to present your work at internal project team meetings.
• Sit at the table at project team meetings and contribute to the discussion.
• Support other women’s comments/discussion/ideas.
• Volunteer to present a poster or give a talk at an internal/local/national scientific meeting.
• Volunteer to organize a symposium at an internal/local/national scientific meeting.
• Volunteer to serve as an officer of an internal/local/national organization.
• Make sure you have a LinkedIn profile and it is up to date.
• Always take advantage of the opportunity to network with other scientists virtually (e.g. on LinkedIn) or IRL at internal/local/national meetings.
• Take advantage of any mentor networks (as a mentee and/or mentor) available at your company or via membership in a national organization such as the ACS.
Audience Survey Question

How have you worked to develop an external reputation and network? (choose all that apply)

• A) Created a LinkedIn Profile and kept it up to date
• B) Availed myself of any mentor resources or social networking available at my company/university or through organizations like ACS
• C) Volunteered to present a poster or give a talk at a local/national scientific meeting
• D) Volunteered to organize a symposium at a local/national scientific meeting
• E) Volunteered to serve as an officer of a local/national organization

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

Shana Posy
Principal Scientist, Bristol-Myers Squibb
Key Behaviors for Success

• Aim for autonomy – work in an independent, proactive manner

• Save your time for activities that add value
Never Stop Learning

- Cultivate curiosity – learn things outside your domain
- Develop your own expertise – build on your strengths
- Create an environment where you can learn
  - Sit at the table, don’t be cut off, and help others’ voices be heard

Personal Behaviors for Success

- Act with integrity – build trust
- Develop a thick skin – most people mean well
Nurture an identity outside work

• Prevent burnout over the long term

• Enthusiasm, passion, and creativity spill over into work

• Being part of a community provides a healthier perspective

Take-Home Messages

➢ In thinking about next career steps, don’t be limited by your current skills. Where can you best apply your talents?

➢ Know your priorities and don’t be afraid to live a full life outside work. With good support you can achieve a lot!
A recent study of population genetics papers found that women were only 7.4% of the authors. What percent of women computer programmers were recognized in the acknowledgements section?

- Twenty-three percent
- Thirty-three percent
- Forty-three percent
- Fifty-three percent
- Sixty-three percent

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

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Zoe Cournia
Investigator – Assistant Professor Level
Biomedical Research Foundation, Academy of Athens

1996 - 2001
Chemistry, University of Athens
Greece

2001 - 2006
Ph.D. in Chemistry
Heidelberg University, Germany
Zoe Cournia

2006 - 2009 PostDoc
Chemistry Dept.
Yale University
New Haven, USA

Ph.D. in Chemistry (2006)
Heidelberg University

BRFAA
2009 - Date
Investigator
Founder, Ingredio

Current Responsibilities

Faculty at Biomedical Research Foundation, Academy of Athens
- Research Activities:
  - Understanding the function of oncogenes through biomolecular simulation
  - Allosteric computer-aided drug design working with academia & industry

Faculty at the University of Athens, Department of Informatics
- Teaching

American Chemical Society
- Associate Editor, Journal of Chemical Information and Modeling
- Editorial Advisory Board, ACS Medicinal Chemistry Letters
- Editorial Advisory Board, Journal of Chemical Theory and Computation

European Commission
- Member of the Infrastructure Advisory Group for the EuroHPC Joint Undertaking
- EC Expert Panels

Co-chair, Gordon Research Conference in Computational Chemistry 2020
Ingredio helps consumers identify chemicals in food

First find your target, then achieve it

Postdoc Advancement: Marketing Your Value

“The most important step towards success is to identify a goal that you are passionate about.

Create a realistic 5 and 10-year career plan based on your individual:

- Dreams
- Skills
- Talents
- Market needs
Hard work & research excellence, but…

**Basis to a successful pathway is:**
- Excellent technical skills & publication record
  - Strong background in physical chemistry
  - 31 peer-reviewed publications
- Hard work

**…But SOFT SKILLS required for EXCELLENCE**
- Practice **writing** skills
- Strong oral **presentation** skills
- Networking skills
- Marketing of your work, social networks
- Ability to work in diverse Teams
- Enthusiasm
- Flexibility
- Have a high tolerance for failure and criticism

“Everyone is talented, but having something to say, and the WAY to say it so that people listen to it, that’s a whole other bag”

More items to consider for success

- Find a mentor who is supportive
- Develop supportive network of peers
- Apply for independent grant and travel funding
  - Wrote 30 grant applications as a postdoc, got 3 grants
- Develop your niche
- Advocate for yourself – Ask for what you need!
- Support from partner/family is crucial
Be a role model yourself, give back to society

EMPOWERING WOMEN IN CHEMISTRY: A GLOBAL NETWORKING EVENT

Dr. P. Gkeka  
Permanent Scientist  
Sanofi, Paris

M.E. Liosi  
PhD Student  
Yale University

E. Lionta  
Permanent Scientist  
Pharmathen, Athens

M. Zavitsanou  
PhD Student  
Oxford University

Women in Computational Chemistry

Coming out in May 2019!

- Platform for us to disseminate seminal works
- Set inspiring examples of female role models
- Create a network of peers that will instigate change for the new generation of Women in Science in the field of Computational Chemistry

Women in Computational Chemistry

Guest Editors: Habibah Wahab, Rommie Amaro and Zoe Cournia

DEADLINE: DEC 1, 2018

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