

Twenty five years in cheminformatics – a career path through a diverse series of roles and responsibilities

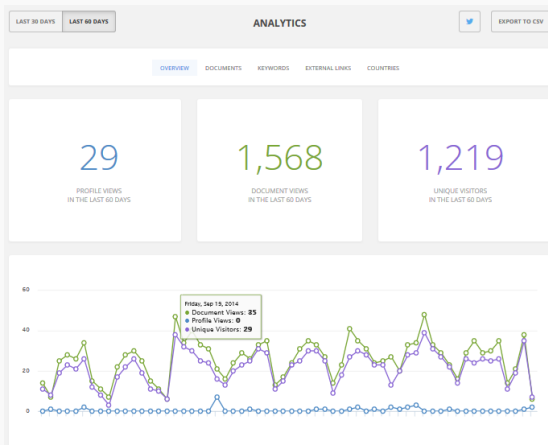
Antony Williams

*National Center for Computational Toxicology
U.S. Environmental Protection Agency, RTP, NC*

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

*April 2017
ACS Spring Meeting, San Francisco, CA*

Being Data Driven...about me



Antony John Williams

Vice President of Strategic Development, Royal Society of Chemistry
 Chemistry, Cheminformatics, Nuclear Magnetic Resonance, Drug Discovery
 Verified email at rsc.org - Homepage
 My profile is public

Change photo

<input type="checkbox"/> Title	<input type="checkbox"/> Add	<input type="checkbox"/> More	1-20	Cited by	Year
<input type="checkbox"/> ChemSpider: an online chemical information resource				104	2010
<input type="checkbox"/> HE Penoe, A Williams Journal of Chemical Education 87 (11), 1123-1124					
<input type="checkbox"/> In silico repositioning of approved drugs for rare and neglected diseases				75	2011
<input type="checkbox"/> S Ekins, AJ Williams, MD Krasovski, JS Freundlich Drug discovery today 16 (7), 298-310					
<input type="checkbox"/> Open PHACTS: semantic interoperability for drug discovery				72	2012
<input type="checkbox"/> AJ Williams, L Harland, P Groth, S Pettifer, C Chichester, EL Willighagen, ... Drug discovery today 17 (21), 1188-1198					
<input type="checkbox"/> Internet-based tools for communication and collaboration in chemistry				66	2008
<input type="checkbox"/> AJ Williams Drug discovery today 13 (11), 502-506					

Google Scholar

Citation indices	All	Since 2009
Citations	2939	2010
h-index	32	24
i10-index	92	67



Co-authors Edit...

Kirill Blinov

Sean Ekins

Mikhail Elyashberg

Gary E. Martin

Valery Tkachenko

Yann Smeuninx

PLUMX

Antony Williams

Connections in Chemistry



Artifact Summary

<input type="checkbox"/> Presentation: 266	<input type="checkbox"/> Data Set: 4
<input type="checkbox"/> Article: 127	<input type="checkbox"/> Unknown: 3
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<input type="checkbox"/> Video: 28	<input type="checkbox"/> Patent: 2
<input type="checkbox"/> Figure: 11	<input type="checkbox"/> Media: 2
<input type="checkbox"/> Book: 9	<input type="checkbox"/> Web Page: 1
<input type="checkbox"/> Chapter: 7	<input type="checkbox"/> Conference Paper: 1

Recent Artifacts

- ☐ Bigger data, collaborative tools and the future of predictive drug discovery.
- ☐ The Royal Society of Chemistry and the delivery of chemistry data repositories for the community.
- ☐ Accessing 3D Printable Structures Online
- ☐ Open innovation contributions from RSC resulting from the Open Phacts project
- ☐ Who knew I would get here from there and how I became the ChemConnector final

see details



Antony John Williams

PhD

VP Strategic Development

The Royal Society of Chemistry · Chemistry

Add your publications

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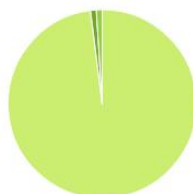
OVERVIEW CONTRIBUTIONS INFO STATS RG SCORE

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RG Score

A new way to measure
scientific reputation.

The RG Score takes all your
research and turns it into a
source of reputation.

- PUBLICATIONS
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Your score is higher than 97.5% of
ResearchGate members'.



Key profile metrics

1.7M impressions on
192 articles

16.9k views on
192 articles

248.8k impressions on
58 slide decks

54.8k impressions on
7 datasets

- Worked in
 - Government lab as postdoc
 - Academia as NMR Facility Manager
 - Fortune 500 Company as NMR Tech Leader
 - Small start-up company as product manager, marketing manager, Chief Science Officer
 - Consultant – chemistry informatics industry
 - Company owner – created ChemSpider
 - Royal Society of Chemistry (bought ChemSpider)
 - US-EPA – cheminformatician and “connector”

Who am I today?

- Computational chemist at the US-EPA – **scientist**
- Responsibility for cheminformatics projects, internal & external collaborations, “product marketing” – **cheminformatician**
- Work with a team of people developing software solutions – “**product & project manager**”
- Scientific publications, books, blogger – **author**; I am @ChemConnector – **social networker**

Being philosophical...



What have I learned in my career?

- Much time is spent working - not enjoying it is not an option for me
- It is called “work” for a reason – if you enjoyed every moment it would be a hobby
- Continue to sharpen your toolset as time and projects allow. Don’t fear going outside the box

What have I learned in my career?

- “Playing it safe” is a perfectly valid option – but rarely effects change and innovation
- Use your head & heart to make career choices
- Say what you are going to do and do what you say – it defines your reputation as an employee
- Careers are **made** – they don’t just happen

“Work” versus “Passion”

- We all need to work but choose to work on things that give you a **good** emotional response... stimulate interest, lack of sleep, joy, obsession...
- Develop new skills, step out of the box and extend yourself. What you know now is never enough...
- Balance logical decisions with gut-level responses
- Work somewhere that supports your passion(s)

- I always found Chemistry interesting....but never found it easy!
- Master of crystallization and yield
- Almost **bottom** of my class for PhysChem! – spectroscopy made no sense but was **fascinating!**
- Self-realization – “Beat the Challenge” – had to study it until I got it.

What brings you joy?

- **Figure out early** what brings you joy if you can (**not so easy!**) what drives you and what brings you joy? The list below fits for classical chemistry and for me:
 - Creating solutions to difficult problems
 - Building and playing with functional teams
 - Communicating complexities
 - Acts of service for my community
 - Working with people more skilled than me

- Multiple offers for NMR Postdocs in USA (PhD studies)
- One offer for ESR/EPR Postdoc in Canada
- Why Canada?
- Emotional decision...
 - Exploration is fun
 - Out of the box motivates

- **Business Driver:** Do more analyses faster and with higher quality. Walk-up automation for analytical support, Get data to chemists
- **Business Driver:** Improve NMR Data analysis- **can software outperform people for analysis?**
- **Business Driver:** Sample tracking – LIMS as the internet was born
- I entered cheminformatics for BUSINESS REASONS

ACD/Labs Start-up 1997-2007

Commercial Cheminformatics

- Creativity at its best – new products, new markets, design work, marketing, good science
- From NMR spectroscopist to deeply understanding chemical **nomenclature**, **structure** representation and **databasing**, data integration, and the **web**
- My greatest **joys** – solving problems for people and innovating scientific solutions with computers
- My driver – “Help OTHER people be more successful”

Can software outperform people?

- Chemistry skills into software – YES, software can outperform people in so many areas!!!

REVIEW

www.rsc.org/npr | Natural Product Reports

Structural revisions of natural products by Computer-Assisted Structure Elucidation (CASE) systems

Mikhail Elyashberg,^a Antony J. Williams^{† *b} and Kirill Blinov^a

Received 2nd February 2010

DOI: 10.1039/c002332a

- Nomenclature generation, PhysChem prediction, NMR analysis, Structure Elucidation

A HOBBY PROJECT just because

– Skills and Passion

- Use technology to spider the internet for chemicals
- Hobby project built in a basement – thousands of visitors a day.
- Judged harshly in the blogosphere but “beat the challenge” by engaging in it...
- Acquired by RSC – chose them as the best partner to define the world of web-based chemistry

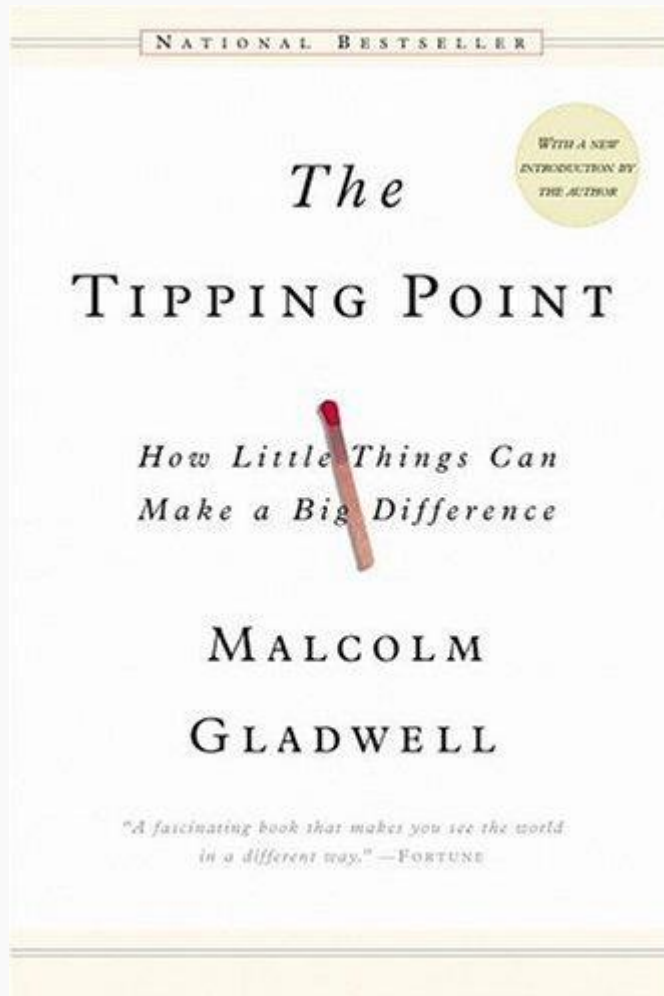


- Bringing my cheminformatics skills to bear
 - Publishing (how to enrich publications with data)
 - Large European Projects
 - Open PHACTS (drug discovery data and the semantic web)
 - PharmaSea Natural Products Discovery
 - National Chemical Database Service
 - Building a user community for ChemSpider – to over 50,000 users a day by education, sharing and engagement (i.e. connecting)
 - Delivering tools to support the community

- Whatever your chemistry interests, if you like applying computational science there are possibilities
 - Spectroscopy (analysis, prediction, elucidation)
 - Synthesis (databasing, representation, retrosynthesis)
 - Drug design (docking, screening, property prediction)
 - Nanomaterials (databasing, design, QSAR)
- Where are computers NOT having an impact in chemistry...

- The majority of us are passionate about ODSOS – Open Data, Open Source and Open Standards
- My passion for supporting Openness was not being fulfilled so I joined a government laboratory with full support for public domain data
- Your impact can be much broader when contributing code, data and to standards

It finally made sense...



- This book brought it into perspective for me...

It might be useful...

- <http://www.productiveflourishing.com/maven-connector-or-salesperson-whats-your-archetype>

Maven, Connector, or Salesperson: What's Your Archetype?

BY CHARLIE GILKEY ON APRIL 4, 2012 — 46 COMMENTS



I might be a connector..

<http://www.productiveflourishing.com/maven-connector-or-salesperson-whats-your-archetype>


- *You might be a connector if:*
- You are constantly referring people to the right expert or service to solve their problem.
- You love networking and talking with people, just for the sake of doing it.
- When you're talking to people, they say, "Wow – you know everyone!"
- The stories you tell always focus on the *people*, not the ideas or the sizzle.





A Personal Interest Social Networking in Science




- I think you should ALL take part in “connecting” yourselves to the growing network
- Career-wise, **NOT** having a personal presence online is likely already a detriment
 - Establishing a public profile
 - Getting on the record
 - Collaborative Science
 - Demonstrating a skill set
 - Measured using alternative metrics
 - Contributing to the public peer review process

- <https://www.slideshare.net/AntonyWilliams/building-an-online-profile-social-networking-and-amplification-tools-for-scientists>

ORCID ID:0000-0002-2668-4821



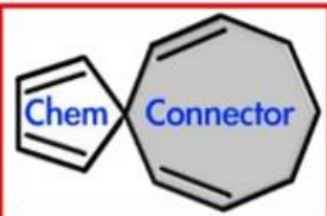




Building an Online Profile: Social Networking and Amplification Tools for Scientists

Antony Williams,
February 22nd 2017, NC State University

Presentation: 1:00-3:00pm



Conclusions...what worked for me..

- I LOVE Chemistry – never want to synthesize again!
- Career choices should be head & heart decisions
- Decide what motivates, excites and stimulates you over what puts food on the table. (Clearly driven by the need to eat also!!!)

Conclusions...what worked for me..

- You are responsible for your reputation – build it and maintain it - and with online tools take charge of it!
- Not every decision is a good one – but not making decisions is crippling in terms of your career
- In cheminformatics there are very few limits to participation
 - Always something to learn
 - Contribute and share data, code and skills openly
 - Get into the network – Wikipedia, StackOverflow, many networks
 - Join the ACS Division of Chemical Information and participate

Coming Soon....

ACS CINF ONLINE WEBINAR

**“Profile Building, Research Sharing and
Data Proliferation using Social Media
Tools for Scientists”**

May 1st 2pm EST