Both sides now:
An intimate perspective on research collaborations

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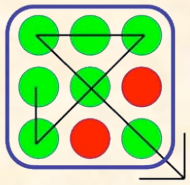
Outline

- Background
- Some Recent History
- Pros & Cons on Both Sides
- Lessons Learned

- There are only 22 slides

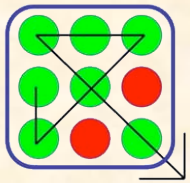


Motivation

Cheminformatics Implications of Collaborations between Academia and Industry

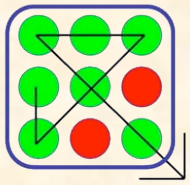
Why should we care?

Because it is where the most critical innovations come from.



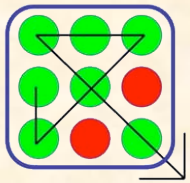
Who am I to Talk About It?

- 8.5 years in academia
- 10 years at Monsanto
  - biochemistry, synthesis & screening
- 13+ years at Tripos (International)
  - QSAR & combi-chem software development
  - applications research (Discovery Research)
  - algorithm & new methods development (IRC)
- Projects I have been intimately involved with
  - Advanced CoMFA® Consortium
  - OptiSim, OptiDock & OptDesign®
  - CScore™ for consensus scoring
  - Pharmacophore Tuplets™
  - GALAHAD®
  - …



Types of Collaboration at Tripos

- Software development
  - typically enterprise-scale projects
  - science is already known
  - application-specific
  - written to spec
  - “software consulting”: Schering, BMS, Wyeth…
- Applications research
  - science is already known
  - project-specific
  - Tripos Discovery Research, field scientists …
- Basic applied research
  - the problem is known but the solution isn’t



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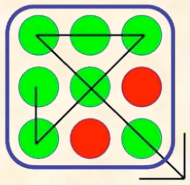
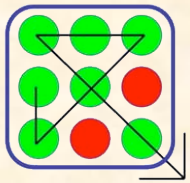


What is Research?

- It means many things to many people
  - Google yields 771,000,000 hits (“about”)
- It is not:
  - (very) predictable
  - easily budgeted ahead of time
  - carried out in the Boardroom
- But it can be:
  - very useful
  - very productive
  - very rewarding in intangible ways

**“If we knew what it was we were doing,
it would not be called research, would it?”**

-Albert Einstein



Caveat Auditor

- Names have been changed to protect the innocent

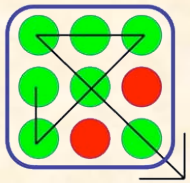
  …and the not-so-innocent

- Conclusions are generalized

  …but not overly so (I hope)

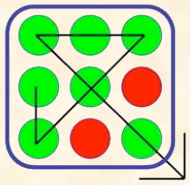
- Opinions expressed are solely my own

"The questions have been painstakingly researched,
but the answers have not"
– Michael Feldman, NPR



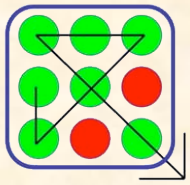
(Some) Collaborations I Have Known

- Pfizer, Inc.
  - 1998-2001 (Groton & Sandwich sites) → DAP
- Parke-Davis (→ Pfizer, too)
  - 2000-2003 (Ann Arbor) → CScore
- Novo Nordisk A/S
  - 2001-2003 (Copenhagen) → Tuplets
- University of Sheffield
  - 2002-2004 (Peter Willett & Nicola Richmond) → LAMDA
- Biovitrum AB
  - 2003-2004 (Stockholm) → GALAHAD
- Bayer HealthCare AG
  - 2005-2007+ (German & US sites) → PiX System



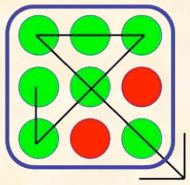
Types of Academic:Industrial Collaborations

- Good
  - everyone is happy at the end of the day
- Bad
  - good answer to the wrong problem
  - no publications
- Ugly
  - no useful code, nothing presentable
- Really ugly
- Really good
  - more often than not, for us
- “Fair to middling” is (surprisingly?) rare



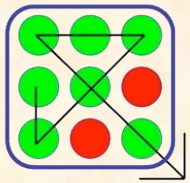
A Little History

- Mantras of the 90s
  - "New platforms & technologies are going to be the keys to drug discovery &development in the 21st Century."
  - "If you don't get there first, you won't get there at all."
  - "You can patent anything."
- Realities of the 90's
  - bigger is not always better
    - …and is only rarely *proportionately* better
  - strategic partnership management ⇒ fewer $$$ for collaboration
  - you do not have a patent until you have defended it
  - you can't patent everything
- Mantras of the 00's
  - "It is all about getting access to data"
    - … but try to keep the *informatics* in cheminformatics
  - "Outsource it if you can."



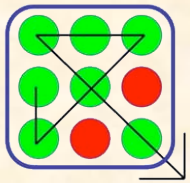
A Little More History

- New technologies did not deliver
  - HTS & combinatorial chemistry
  - molecular diversity
  - *in silico* ADME/Tox
- Effects at the industrial bottom lines:
  - too few new drugs are being produced
  - a lot of new tech is (too?) expensive
- Too little attention was paid to (flexible) validation benchmarks along the way
  - should have been built in from day one
  - courses changed without being able to measure how much things improved…if, in fact, they did
  - stakeholders, committees & nice guys took over



Bureaucracy

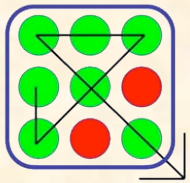
- Strategic partnership management
  - puts you cheek-to-jowl with outsourcing projects
  - accounting pressure to look to the lowest-cost “provider”
- Getting IT/IS departments involved
  - essential for enterprise-scale projects
  - performance & cost outrank features as criteria
  - linked to a “revenue sink”
    - … chemist support is critical but it’s not sexy
- Intellectual property problems
  - University wants downstream commitments
  - invention vs work-for-hire
  - Industry limits on data sharing
  - cross-licensing hassles & open source



Collaboration

- What does industry bring to the table?
  - experience in medicinal chemistry & drug discovery
  - a large quantity of data
  - high quality data

    …but usually not both at the same time
- What do academics bring to the table?
  - naiveté about the problem
  - innocence about what "won't" work
  - scholarship: "How come you *know* stuff like that?"



Collaboration

- What ***can*** industry bring to the table?
  - experience in medicinal chemistry & drug discovery
  - a large quantity of data
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- What ***can*** academics bring to the table?
  - naiveté about the problem
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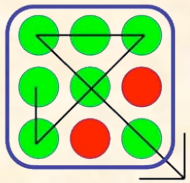
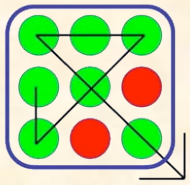


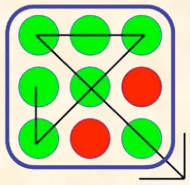
"What we have here is a failure to collaborate!"*

- What academics should ***not*** do
  - expect blue skies & ivory towers to be encouraged
  - broadcast that "We're here to tell you how to do it right!"
  - be lazy about making sure that programs are robust
  - think that the relationship is exclusive or forever
    - you haven't gotten married
- What industry should ***not*** do
  - plan on having a "product" at the end of the project
  - expect delivery of industrial-strength code
    - be wary of freeware, open source and Matlab
  - be *too* promiscuous
    - you are committed to living together for a while



Some Take-Home Lessons

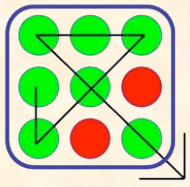
- Optimize communication
  - that's what committees are really good for
- The more the merrier…
  - …but there is strength in small numbers
- Each project needs a champion…
  - …on both sides of the collaboration
  - …in it for the long term
- Aim for publishability from the start
  - essential on the academic side
  - (very) valuable on the industrial side
  - a useful reality check in any case
- The "co" in collaboration is critical
  - cultivate a sense of group & individual ownership
- Do not plan on failing, but be prepared to do so



Some More Take-Home Lessons

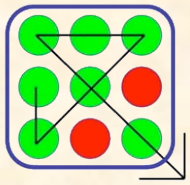
- Share everything.
- Play fair.
- Don't hit people.
- Put things back where you found them.
- Clean up your own mess.
- Don't take things that aren't yours.
- Say “Sorry!” when you hurt somebody.
- Wash your hands before you eat.
- Flush.
- Warm cookies and cold milk are good for you.
- Live a balanced life.

“All I Ever Really Needed to Know I Learned in Kindergarten”
- Robert Fulgham



A Few of the People Who Have Made Things Work...

- Tripos
  - Peter Fox
  - Frank Stahl
  - Lakshmi Akella
  - Charlene Abrams
  - Philippa Wolohan
  - Michael Berthold
  - Dave Patterson
  - Alex Strizhev
  - Andreas Witte
  - Roman Dorfman
  - Fred Soltanshahi
  - Edmond Abrahamian
- Biovitrum
  - Evert Homan
  - Jerk Vallgårda
  - Anna-Lena Gustavsson
  - Maria Wirstam
  - Peter Brandt
- University of Sheffield
  - Peter Willett
  - Nicola Richmond
  - John Holliday
  - Val Gillet
- UCSF
  - Ajay Jain
- Parke-Davis
  - Christine Humblet
  - George Cowan
  - Dan Ortwine
  - Alain Calvet
  - Jack Bikker
  - Mark Snow
  - Dave Mack
  - Jim Dunbar
- Bayer AG
  - Andreas Goeller
  - Stefan Mundt
  - Peter Nell
  - Jill Wood
- Novo Nordisk
  - Lars Nærum
  - Inge Christensen
  - Henning Thøgersen
- Pfizer
  - Jim Matthew
  - Mike Miller
  - Jim Blake
  - Erin Duffy
  - Kate Burt
  - Kelly Longo
  - Matt Wessel
  - Frank DiCapua



Conclusion

"I've looked at clouds from both sides now,
From up and down and still somehow,
It's clouds illusions that I recall,
I really don't know clouds…at all."

"[V]iew the boundary between the [academic] and [industrial] cultures not as a territorial line but as a broad and mostly unexplored terrain awaiting cooperative entry from both sides."

- *paraphrased from E.O. Wilson*

Thank you…

…for your kind attention.