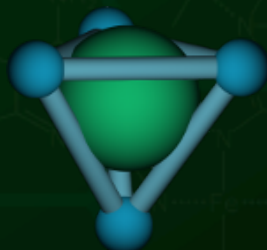


# **Pistoia Alliance App Strategy: *Apps for life sciences R&D***

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# Mobile apps

- The world of computing goes through periodic revolutions, e.g.
  - mainframes
  - minicomputers
  - personal computers
  - graphical user interfaces
  - network connectivity
  - wallet-sized computers
- Some revolutions are more revolutionary than others
  - does all the software have to be redesigned from scratch?
  - are the new ideas and expectations transformative?

# The future is mobile

- In case you haven't noticed...  
... people live their lives on their phones and tablets.
  - Applicable functionality keeps growing: email, browsing, scheduling, games, presentations, word processing...  
... and thousands of useful apps that have no equivalent in the desktop realm.
- 
- **Q:** Why would somebody waste their time trying to do chemistry on a mobile device?
  - **A:** Because if you can do *everything* else on mobile, do you really want to keep a PC around only for chemistry?

# Chemistry apps

- App producers have been busy building chemistry tools:



- But what do they do? Who makes them? What do people do with them? Are they toys, or industrial strength tools?

# Consumer bias

- Apps are delivered via company stores (iTunes, Google Play, etc.)
- Benefits relative to conventional software deployment:
  - platform vendor takes responsibility for many steps
  - delivery and billing all taken care of (for 30%)
  - review process stamp of approval is valuable
- Great fit for **consumer** apps; not so much for **vertical**:
  - expectation of low price: business only works at scale
  - limited options for evaluation
  - user feedback crude and inappropriate (comments, ratings)
  - no way to *find out who your customers are!*

# Apps for life sciences R&D

- Scientific discovery is *not a consumer market*
- The market has a **small headcount**: tens of thousands...  
...working on **big problems** (e.g. curing cancer)
- Vertical market apps should not necessarily be cheap
- The **scientists** who use the apps need to be actively involved:
  - could an app be used to solve this problem?
  - how could this app be improved to suit our needs?
- As do the **software engineers** to create them:
  - would this feature be useful to you?
  - what would you pay for it?

# Enter the Pistoia Alliance

The logo for the Pistoia Alliance, featuring a stylized blue outline of a building with a flag on top, positioned to the right of the text.

- Lowering the barriers to R&D software innovation...
- ... by bringing together life sciences companies, academic groups and software vendors for *precompetitive collaboration*
- This includes recognising emerging trends, and supporting ways to benefit all stakeholders
- The *Pistoia Alliance* recognised the value of mobile devices and cloud computing
- These will be as important to life sciences as they are to every other industry
- In 2012, the *app strategy* team was formally assembled

# Phase I: App Catalog

- There are many chemistry/biology apps on the iTunes AppStore and Google Play
  - many of them are irrelevant or useless for R&D
  - all of them are buried inside a massive catalog
- Solve the easiest problems first:
  - compile a directory of apps (<100 vs. >10<sup>6</sup>)
  - provide a forum for creators & users
- **Phase I** is a simple layer on top of the company stores for iPhone/iPod/iPad and Android devices



# The AirWatch platform

- Partnered with *Air Watch*, the leading provider of enterprise app catalogs and device management tools
- We use their hosted service to make the *Pistoia Alliance App Catalog* available to the public

# Opening the catalog





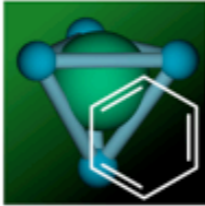









# Browsing the catalog

iPad 7:23 PM 100%

Pistoia Alliance App Catalog

Public All Categories

 <b>Approved Drugs</b> ★★★★★ Public Paid Install	 <b>ChemJuice G...</b> ★★★★★ Public Paid Install	 <b>ChemSpider</b> ★★★★★ Public Free Install
 <b>Green Solvents</b> ★★★★★ Public Free Install	 <b>Mobile Molec...</b> ★★★★★ Public Paid Install	 <b>Mobile Reage...</b> ★★★★★ Public Free Install
 <b>MolPrime</b> ★★★★☆ Public Free Install	 <b>MolPrime+</b> ★★★★★ Public Paid Install	 <b>MolSync</b> ★★★★★ Public Paid Install
 <b>ODDT</b> ★★★★★ Public Free Install	 <b>PyMOL</b> ★★★★☆ Public Free Install	 <b>Reaction101</b> ★★★★★ Public Paid Install

# Signing up

- If you have an iPhone/iPod/iPad, or an Android device:

<http://apps.pistoiaalliance.org>

- Gain access to the catalog
- We only list apps that are useful and relevant
- Installation of apps is done by the company store
  - some free, some paid
- Participate in discussions about existing apps:
  - everyone else is also a scientist, with similar interests
  - the app creators are actively involved: they *want* to know about your experiences
  - you can contact them/they can contact you offline

# Submitting an app

- Must already be listed on the company store (Google, Apple)
- Must be *directly relevant to lifesciences R&D* (broadly defined)
- Anyone can submit:

<http://www.pistoiaalliance.org/submitapp.html>

- Screening done by Pistoia members
- App creators are expected to participate in discussions

# Further developments

- More advanced discussion forum features (expected mid-late 2013)
- Encourage discussion of new app ideas, as well as comments on existing products
- Continued stimulation of new ideas at meetings, e.g. the *Pistoia Dragon's Den* (inspired the *Open Drug Discovery Teams* project)

# Phase 2: Deployment

- The biggest problems with vertical market apps relate to deployment:
  - traditional software is delivered by mailing a CD-ROM
  - web software is deployed by sending out a URL
  - apps have to be submitted & reviewed by a single authority
- There is no guarantee that an app will be allowed!
- Sales are always perpetual, no control
- There is only one price, and the vig is always 30%

# Deployment possibilities

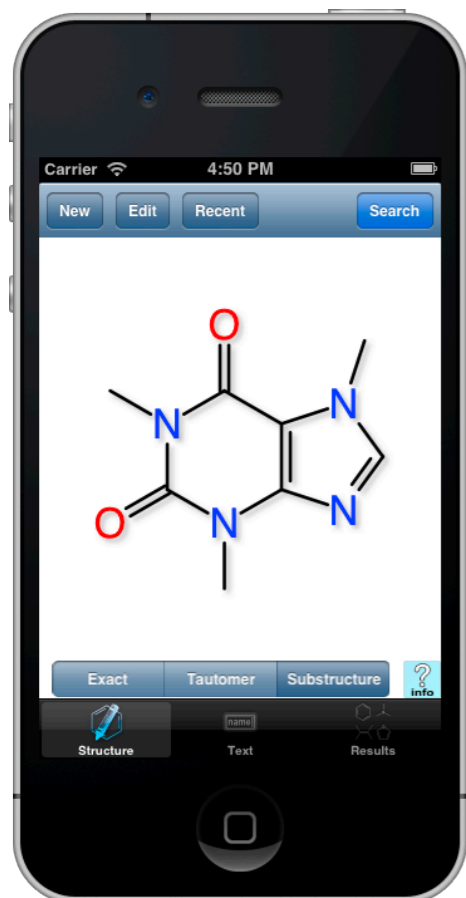
- **Android:**
  - direct loading of apps is permitted
  - can use the *AirWatch* platform to deliver Pistoia-mediated apps directly onto users' devices
- **Apple** (iPhone, iPod, iPad)
  - alternatives to the *iTunes AppStore* extremely restricted: directly circumventing the company store is not allowed
  - companies can setup their own *Enterprise AppStore*
  - the *Pistoia AppStore* could be used as a placeholder for non-public apps
  - private installation opens up many more deployment options

# Phase 3: Cloud computing

- Mobile devices are quite powerful, but:
  - not suitable for grinding through long calculations
  - not recommended for storing large collections of data
- Many mobile apps use webservices to provide functionality, e.g.
  - database search ([ChemSpider](#), [SPRESI](#), [Mobile Reagents](#))
  - property calculation ([MolPrime<sup>+</sup>](#), [SAR Table](#), [MMDS](#))
  - real time newsfeeds ([ODDT](#), [RSC Mobile](#))
  - sharing data ([MolSync](#), [Reaction101](#), [Yield101](#))
- But each app creator has to provide their own service...

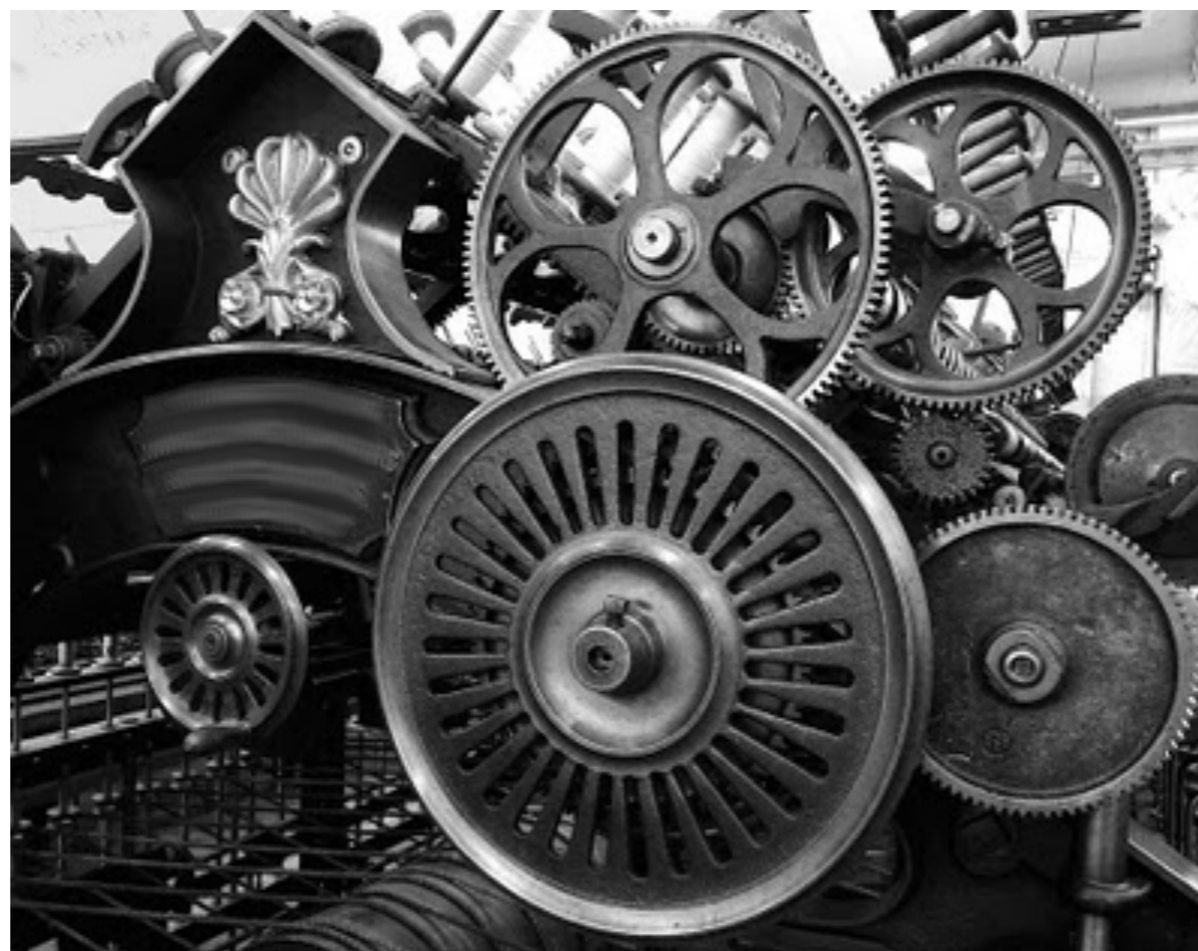
# Limited big data

- Can currently make use of big data under constrained workflow conditions



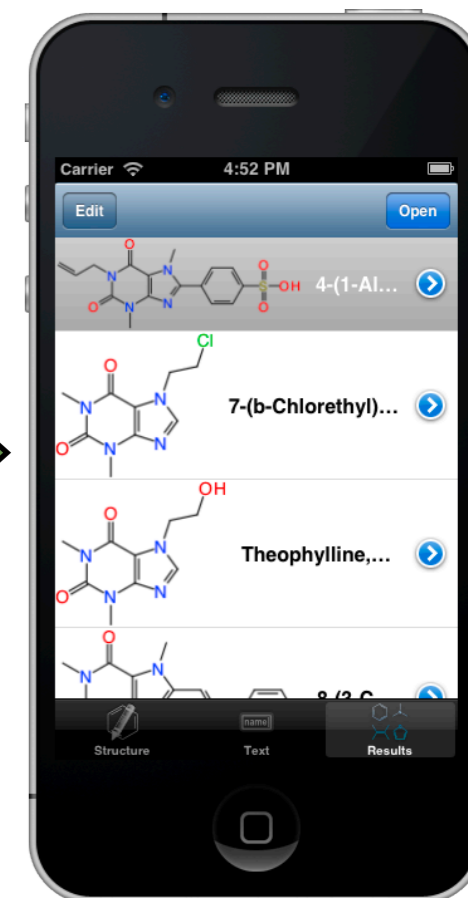
Search  
**Query**

small  
data



**ChemSpider**  
Database Engine

small  
data

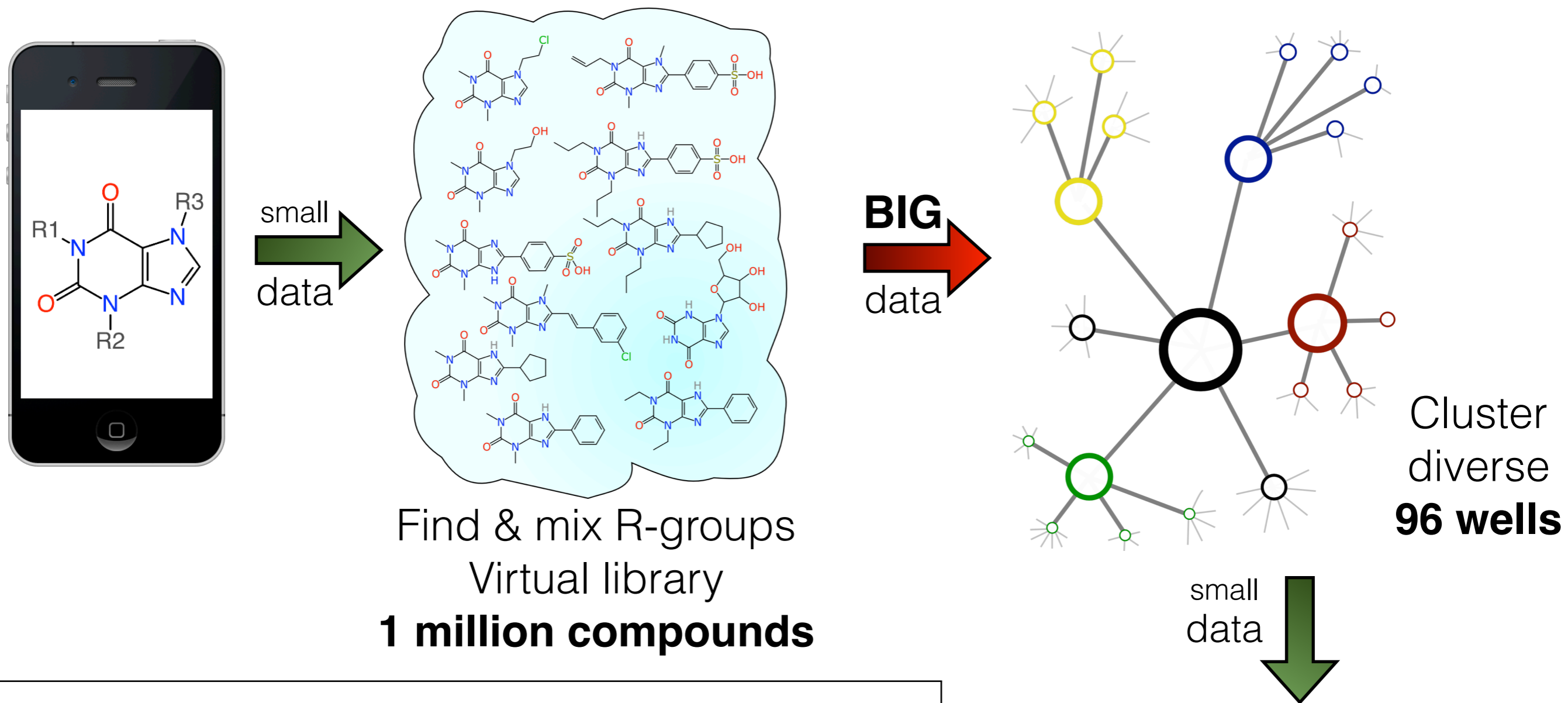


Search  
**Results**

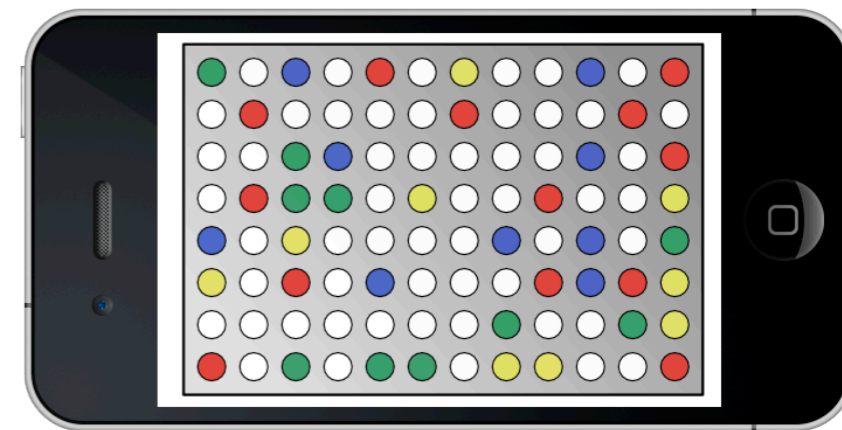
# Server support

- Using webservices is simple if:
  - requests are completed quickly
  - security is not an issue
  - dealing with **small** documents, easily transmitted
- **Large** documents are much more difficult:
  - stored on centralised server
  - need to access in small chunks
  - need to execute operations on large chunks
  - security and concurrency are important issues
  - sharing data can be tricky

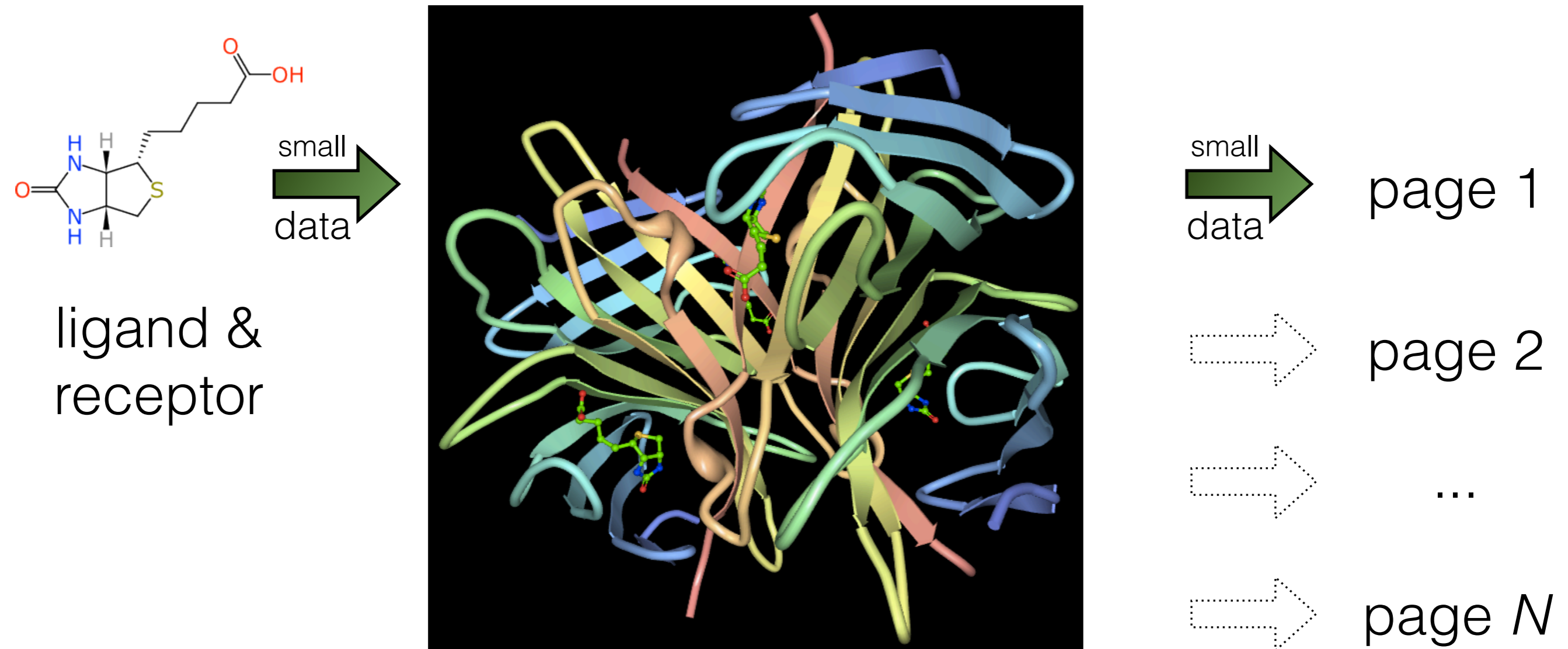
# Unlimited big data



- Tools available from different vendors
- Apps operate on bite-sized chunks
- Big data generation, or multiple steps, requires new infrastructure



# Paged Data Access



- Setup molecular dynamics docking run
- Thousands of frames generated
- Access results as available, optionally cancel

# Proposed solution

- Working with *TM Forum* and its member organisations



- Propose to create a cloud-hosted server platform for:
  - large datasets
  - cheminformatics/bioinformatics tools
  - an API for accessing data & executable tasks
- By providing a single platform with a common API, multiple software products can be hosted on the same environment
- A many-to-many relationship between apps & data/computation

# Conclusion

- The Pistoia Alliance has executed **Phase I** of its *App Strategy*:
  - curated catalog of relevant lifesciences R&D apps
  - bringing app creators & app users together
- **Phase 2** will address deployment issues
- **Phase 3** will provide a cloud-based support framework

# Acknowledgments

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