CCP CompMedChem workshop

Intro & catch-up

21 June 2017

Cambridge Chemistry

Frank von Delft

Objectives & recap

InnovateUK proposal

Actions

XCHEM Diamond Fragment Screening
SGC UNIVERSITY OF OXFORD
diamond

Objectives for the day

- Update on progress
- Identify (immediate) scientific gaps
- Consensus on strategy (community, ownership, etc.)
- Actions and timelines

Recap: March meeting

- Goals
  - Overall sanity check: does a "CCP" make sense?
  - Scope out ambition
    - for grant: who can commit
    - For community: who's missing
  - Actions & timelines

- Conclusions
  - There is a need for a "CCP" (minimally: standards, repository)
  - Other CCPs have lessons – assimilate them
  - Scientific scope is huge – pick an initial focus (XChem)

- Actions
  - Submit grant – **DONE**
  - Organise follow-up meeting – **DONE**
  - Think how to build community (CCP) – **ongoing**

What I call “community”

- Main lesson from CCP4: if you’re new, that’s where you turn to
  - Source of expertise (bulletin board, docs, workshops)
  - Software that just works (download, install, run)
  - All developers take it seriously – pushes limits, sets standards and trends
  - Training new developers

- Primary focus: naïve user. Everything flows from this.

- (CCP-CompMedChem – okay as name?)
  - CCP: Collaborative Computational Project
  - CMC: “compchem” means too many things (!!)

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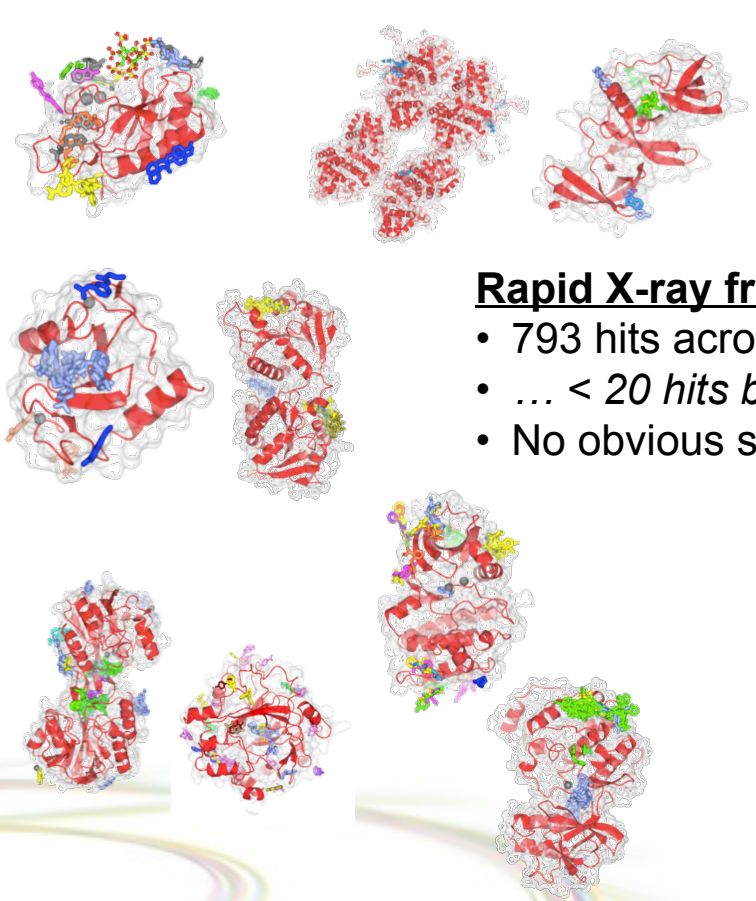
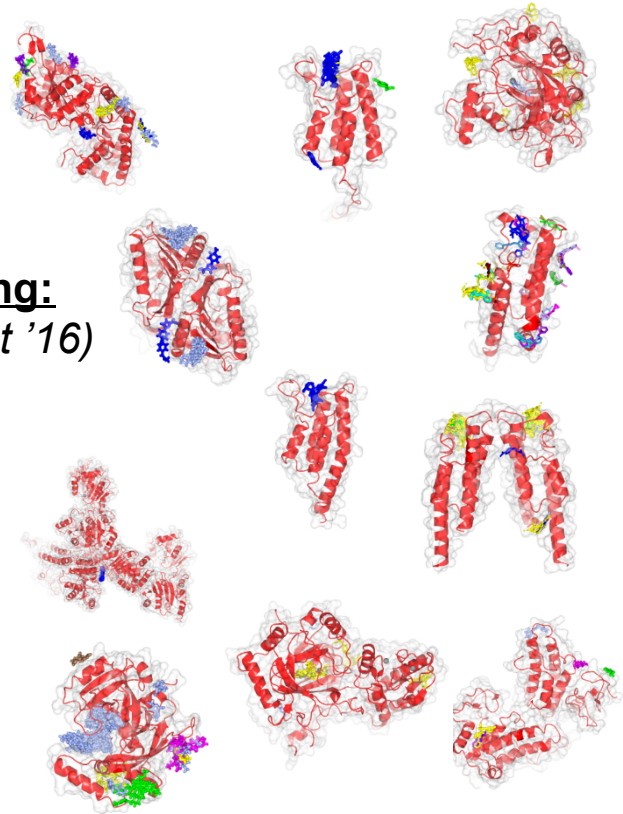
The immediate problem: XChem's output



Rapid X-ray fragment screening:

- 793 hits across 20 targets (*Oct '16)*
- *… < 20 hits being pursued …*
- No obvious software routes



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Current state of tools

Standalone app

Code and install instructions

Webservices

Virtual Machines

Workflows

Commercial tool providers

Best practice????

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Grant update: InnovateUK – F2LCP

- Partners: Diamond, Informatics Matters, GSK, CCDC, U. Oxford
- Timelines
  - Decision: end June
  - Duration: Sept 2017 for 2 years
- Budget:
  - 6 people (Diamond – 2; IM – 1; CCDC – 0.7; UOx – 2)
  - In kind: beamtime, CPU, compounds (Diamond); active projects (GSK)
- Goals
  - Technology: make Squonk routine tool – infrastructure, workflows, hardening
  - Science: look hard at visualisation & scoring
  - Partners: follow-up workflows (GSK), scoring (CCDC)
- Management
  - Diamond's project management team

Grant: sections

- Section 1: need or challenge
- Section 2: approach or innovation:
  - Deploy as regular tool for analysing XChem results and designing follow-up
  - Squonk platform has uniquely comprehensive features
  - Improve methods with GSK, CCDC & UOx
- Team and resources
  - Diamond: FvD, Anthony
  - Informatics Matters: Tim Dudgeon
  - CCDC: Jason Cole
  - GSK: Darren Green, Ian Wall
  - Oxford: Brian Marsden, Garrett Morriss
  - *Extensive collaborative network via XChem users and SGC's open access*

Grant: sections

- Section 4: market awareness
- Section 5: outcomes and route to market
  - Diamond: already has industrial users
  - IM: exposure through XChem users
  - CCDC: novel tools, access to customers
  - GSK: improved productivity
  - Dissemination: 2 workshops costed
  - Longer term: CCP-CMC
- Section 6: wider impacts – “People are sick. Very sick.”

Grant: sections

- Section 7: project management
  - WP1: Project management (Diamond)
  - WP2: Core software development (IM)
  - WP3: Protein-fragment docking validation (Diamond)
  - WP4: Protein-fragment complex preparation (Diamond)
  - WP5: Protein-fragment hit follow-up workflows (Diamond)
- Section 8: risks
  - Recruitment
  - Validating workflows
  - Complex project
  - Security
  - Competitor
- Section 9: Additionality (why do you need our money?)
- Section 10: Costs and value for money

Long term implications

- Active development into open-source platform
- Long-term home for code
- Transition to CCP-CMD
  - Academic funding – convince UKRI – longer time-spans
  - Establish income stream (*cf.* CCP4)
- Goal: self-sustaining dynamic

Actions

- Who are the women we're not inviting??
- Trainathon – who, when, where
- Next meeting
  - where?
  - how to structure?
  - audio problem
- Too early to formalise?
  - constitution
  - executive, etc.
- PlanB if InnovateUK fails
  - Talk to UKRI / WT (these minutes are evidence)
  - Scope – still fragments?
- How do we translate the actions?