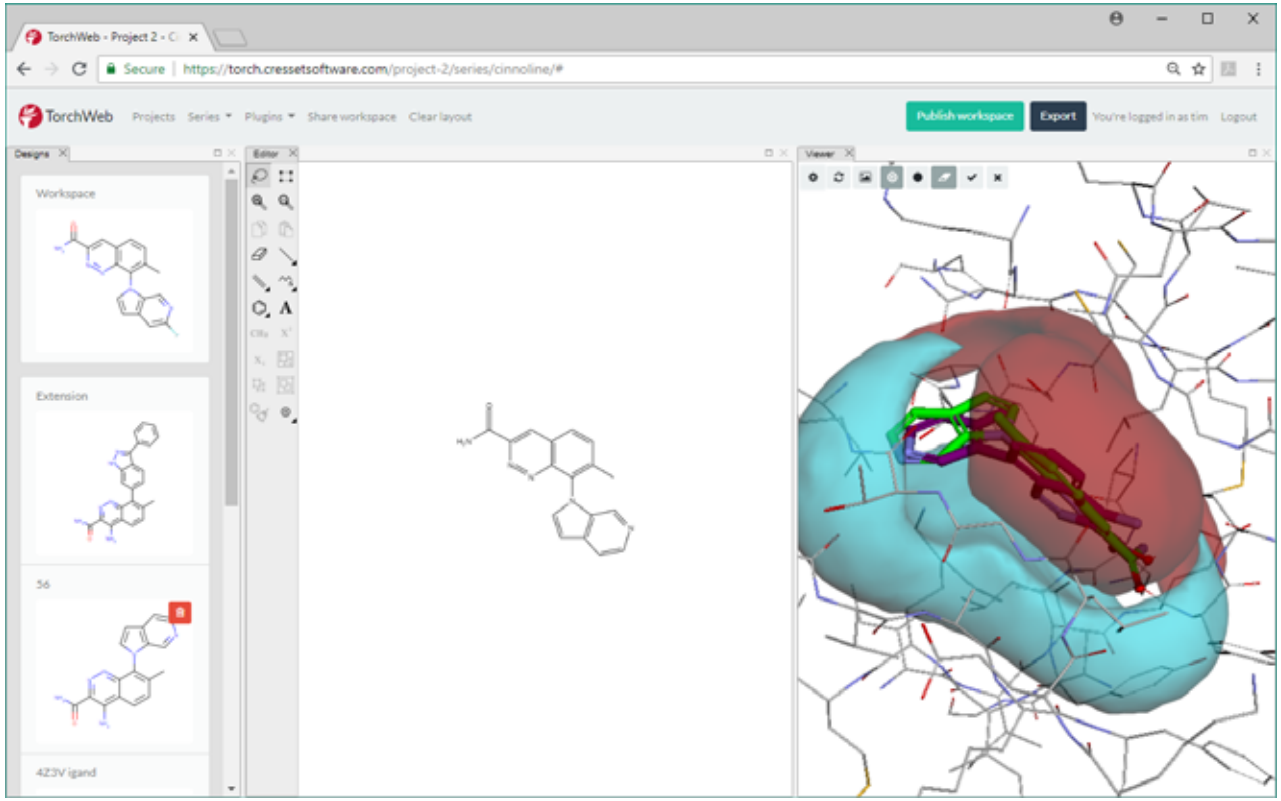
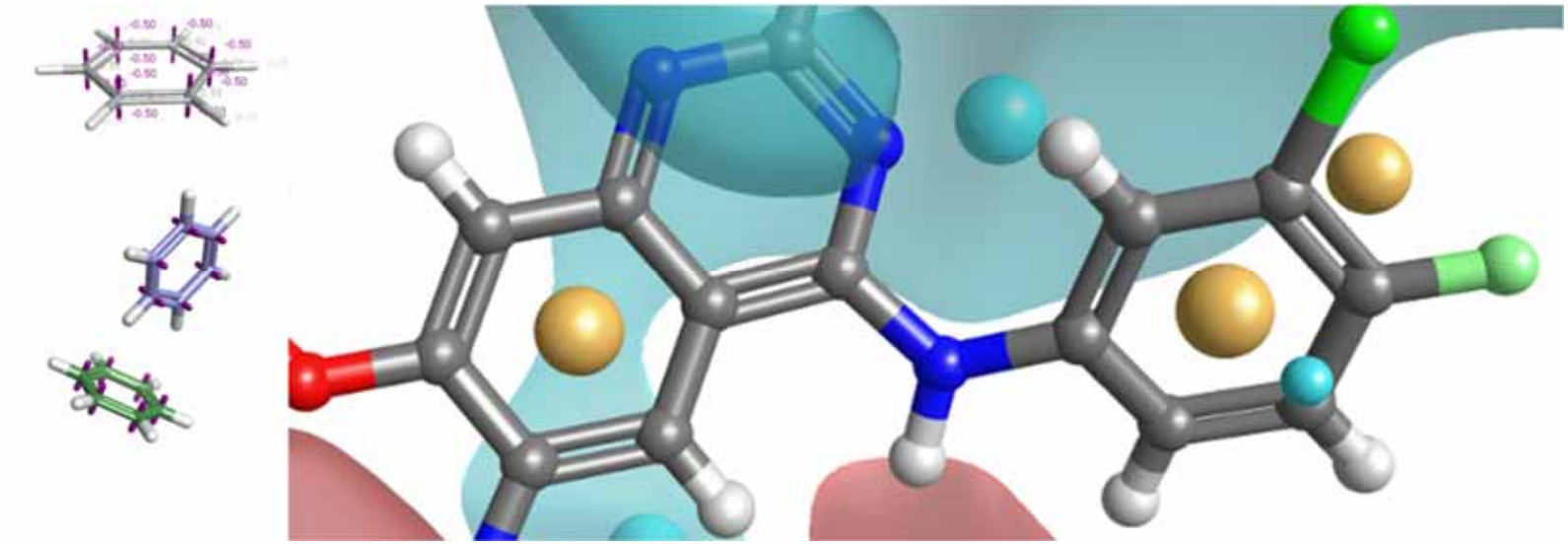
Torx™: Connected Chemistry

The next generation chemistry platform

Update on ‘Project TorchWeb’



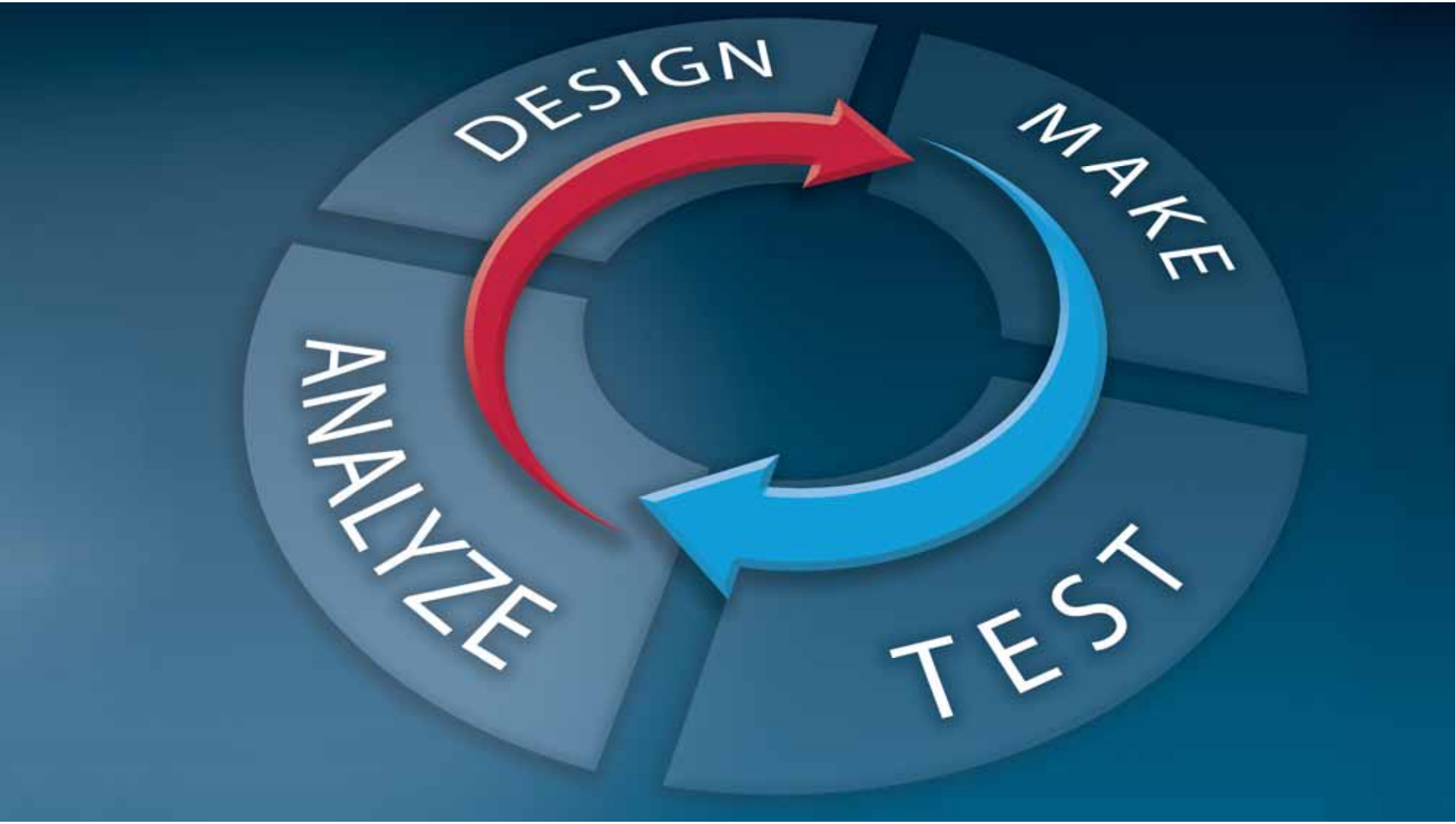
Cresset: The Science



blaze spark forge flare torch


torx
connected chemistry


torx
connected chemistry
cresset
software
innovative science • intuitive software
elixir


DESIGN
MAKE
TEST
ANALYZE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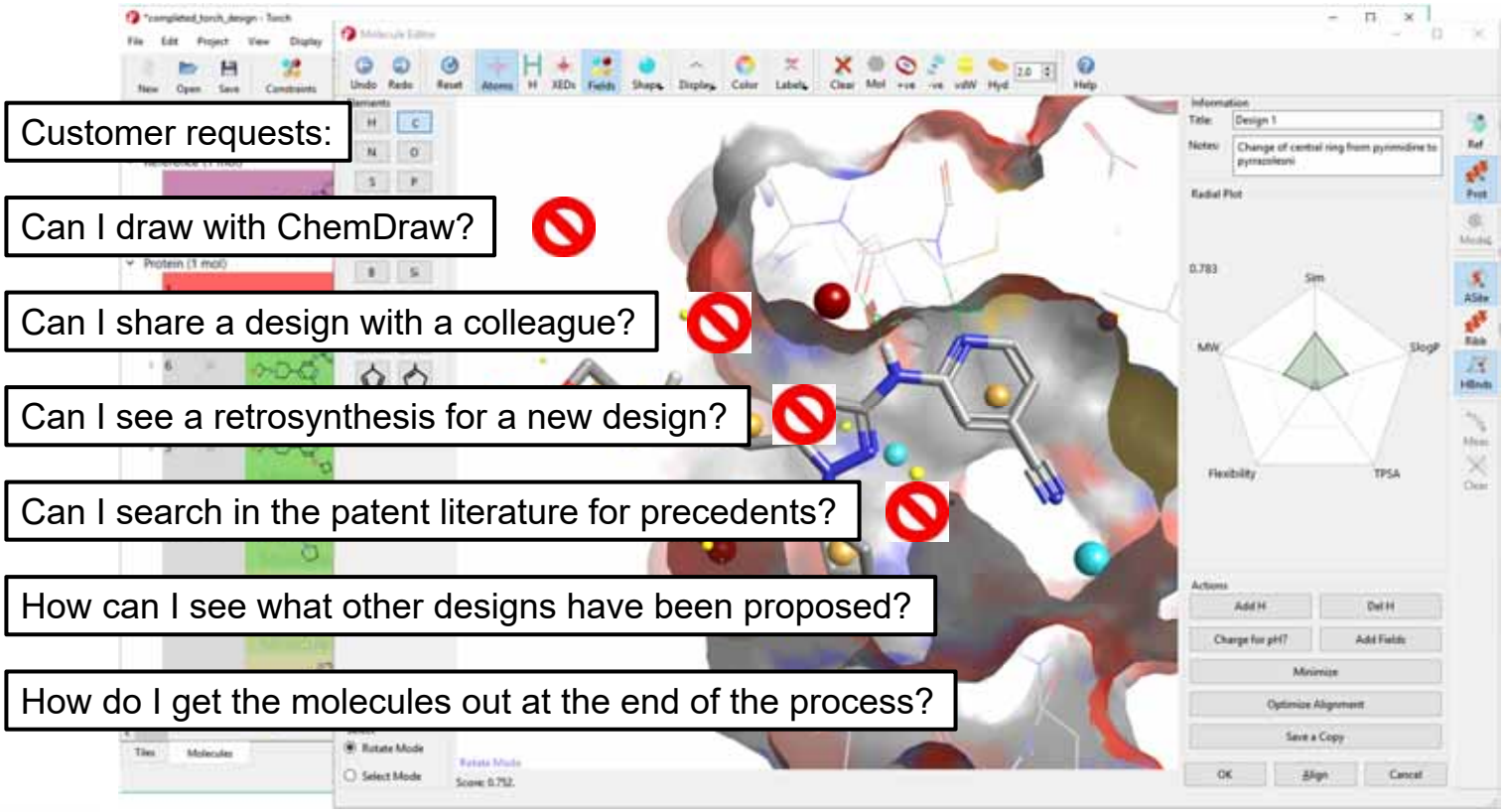
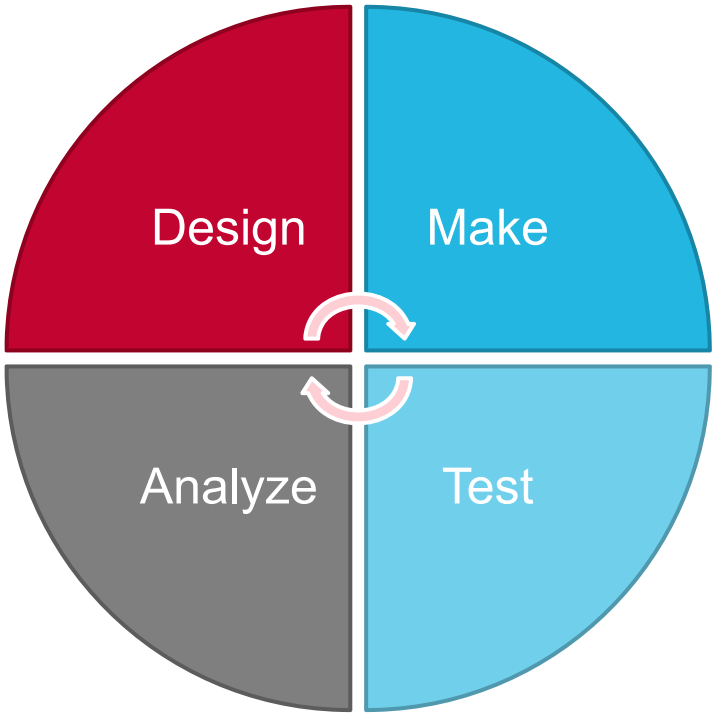
torx
connected chemistry

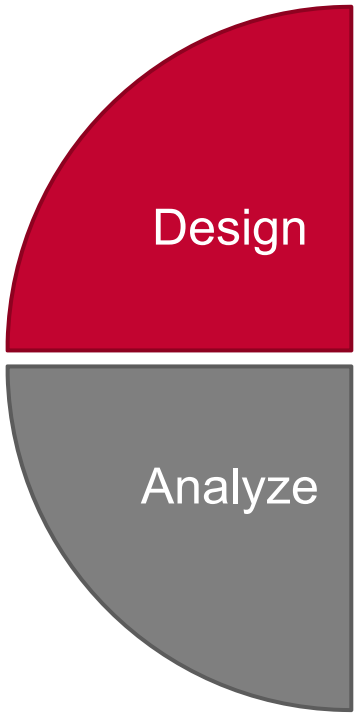
Torch™ – Molecule design using ligand alignment



The molecule discovery cycle & applications



Every task has specialist requirements

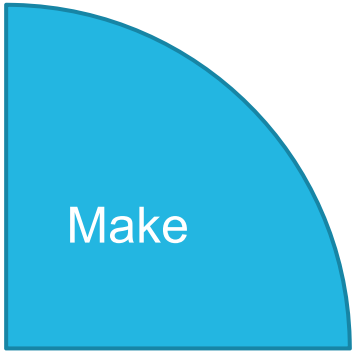


- Context
  - Protein, prior art, …
  - Hypothesis generation
- Novelty
- Precedent
- Properties & Predictions
- Redundancy

- Data fluidity
- Flexibility
  - 2D – charts, graphs etc
  - 3D – protein contexts, electrostatic and shape analysis
- Hypothesis satisfaction, knowledge advancement
  - Inspire new designs

Every task has specialist requirements – make

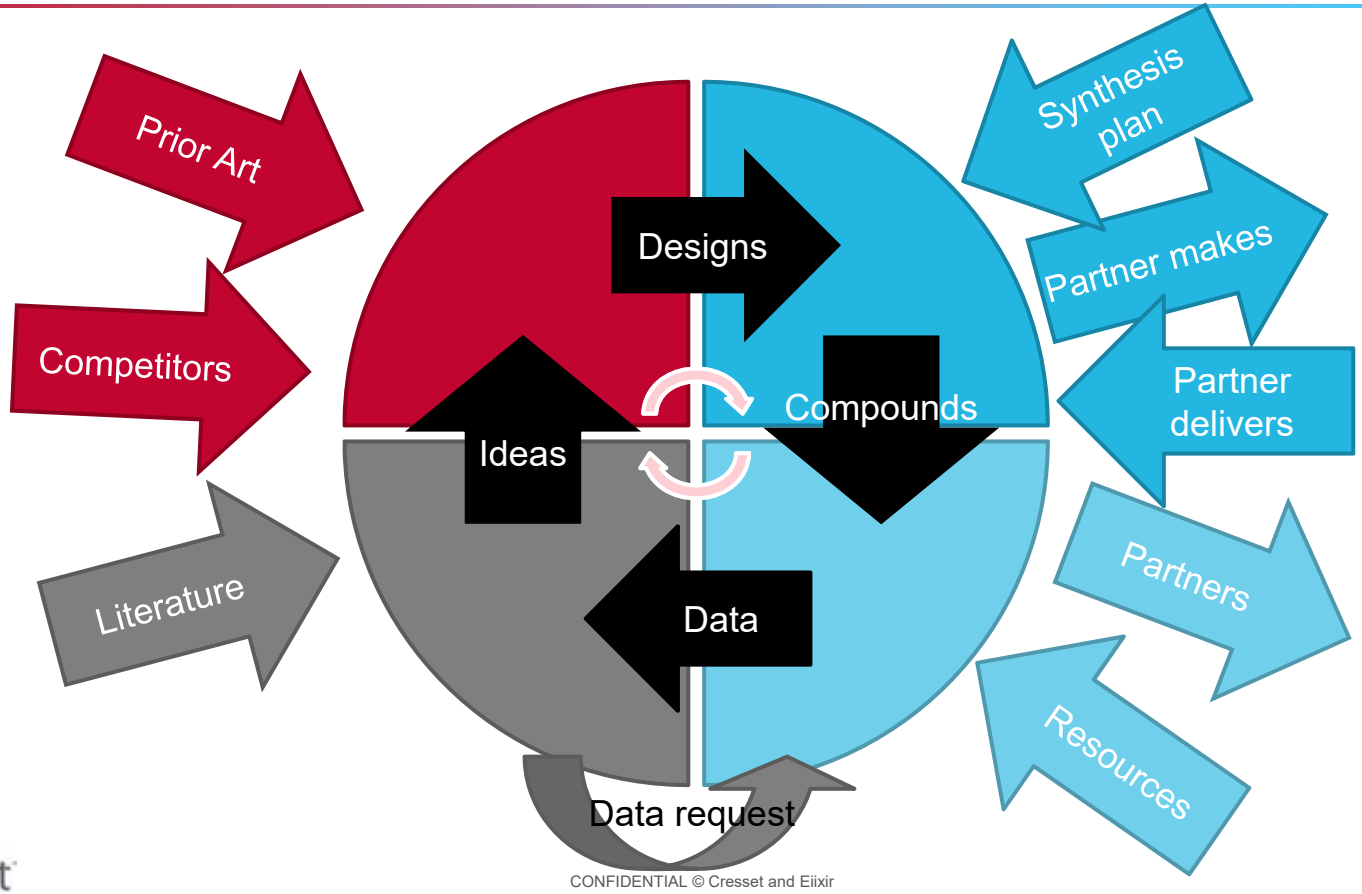
- Tracking compounds through synthesis
- Prioritize compounds
- Resource management
- Out-source management
  - Communication
  - Orchestration
- Re-prioritization



Every task has specialist requirements – test

- A Chemist's view of compounds & assays
  - Timelines
  - Capacity
  - Resources
- Portal to manage requests

Information flows in, out and around the cycle



Information sources increasing and diversifying

- Literature
- Patents
- Protein-ligand xrays
- Computer models
  - AI
  - QSAR
  - FEP
- Computational ideation
- Public databases
- Corporate databases
- Retro-synthetic analysis
- Reagent ordering
- CROs
  - Synthesis
  - ADME
  - Panel screening
- Progress reports
  - Multiple formats?
  - Multiple credentials
- Review meetings
  - Powerpoint slides
  - Excel spreadsheets
  - Email
- Monthly reports
  - Individual, project, team, department, ...

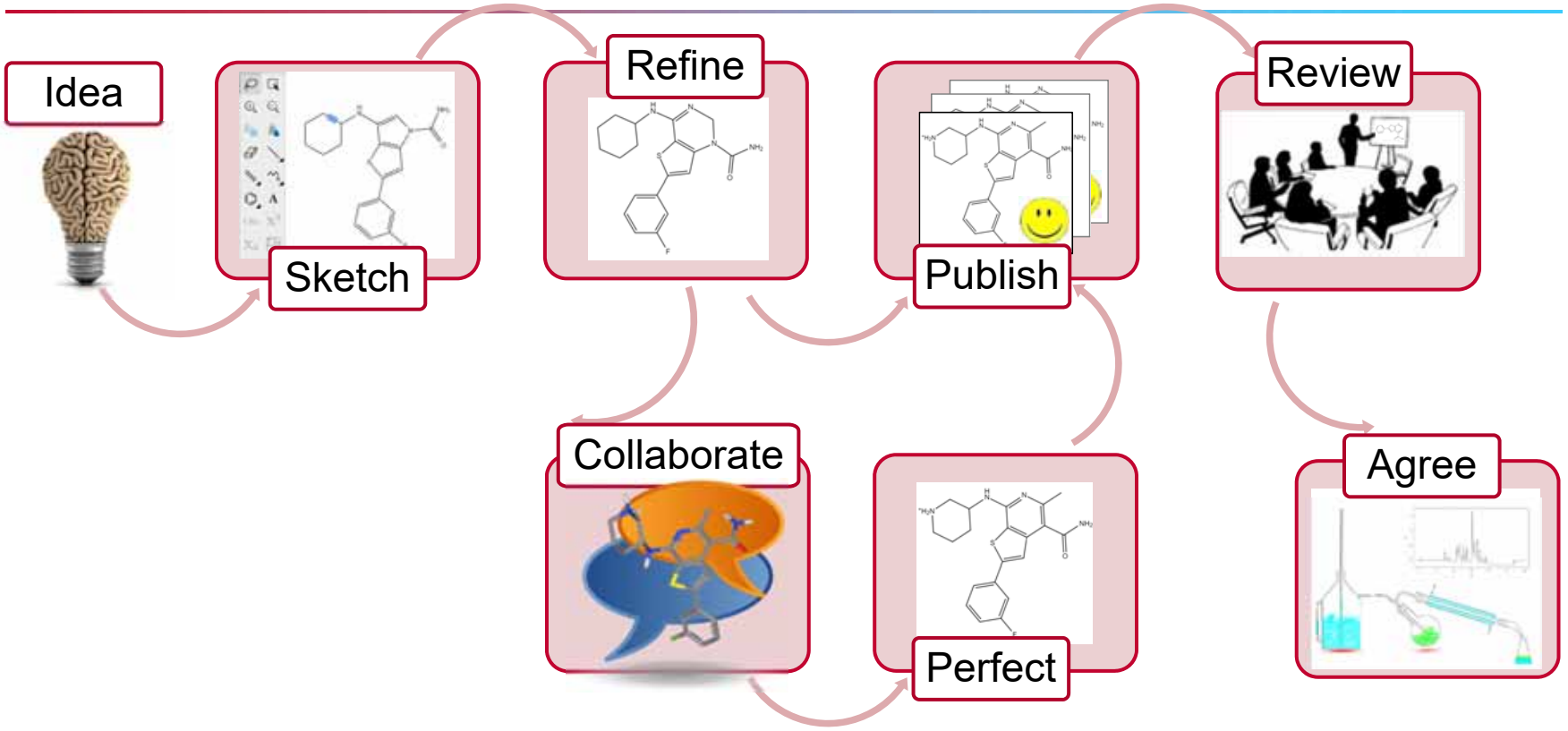
Torx: A central platform for all small molecule discovery chemistry

- Web based application
  - Easy integration of DMTA modules
  - Integration of 3rd party tools (Patent searching, Retrosynthesis, …)
- Dedicated applications for each part of the DMTA process
- Detailed recording of ideas, decisions and contributions
- Team working as a central theme
  - Connecting internal and external resources throughout the drug discovery process
- Modular construction to enable staged uptake and deployment

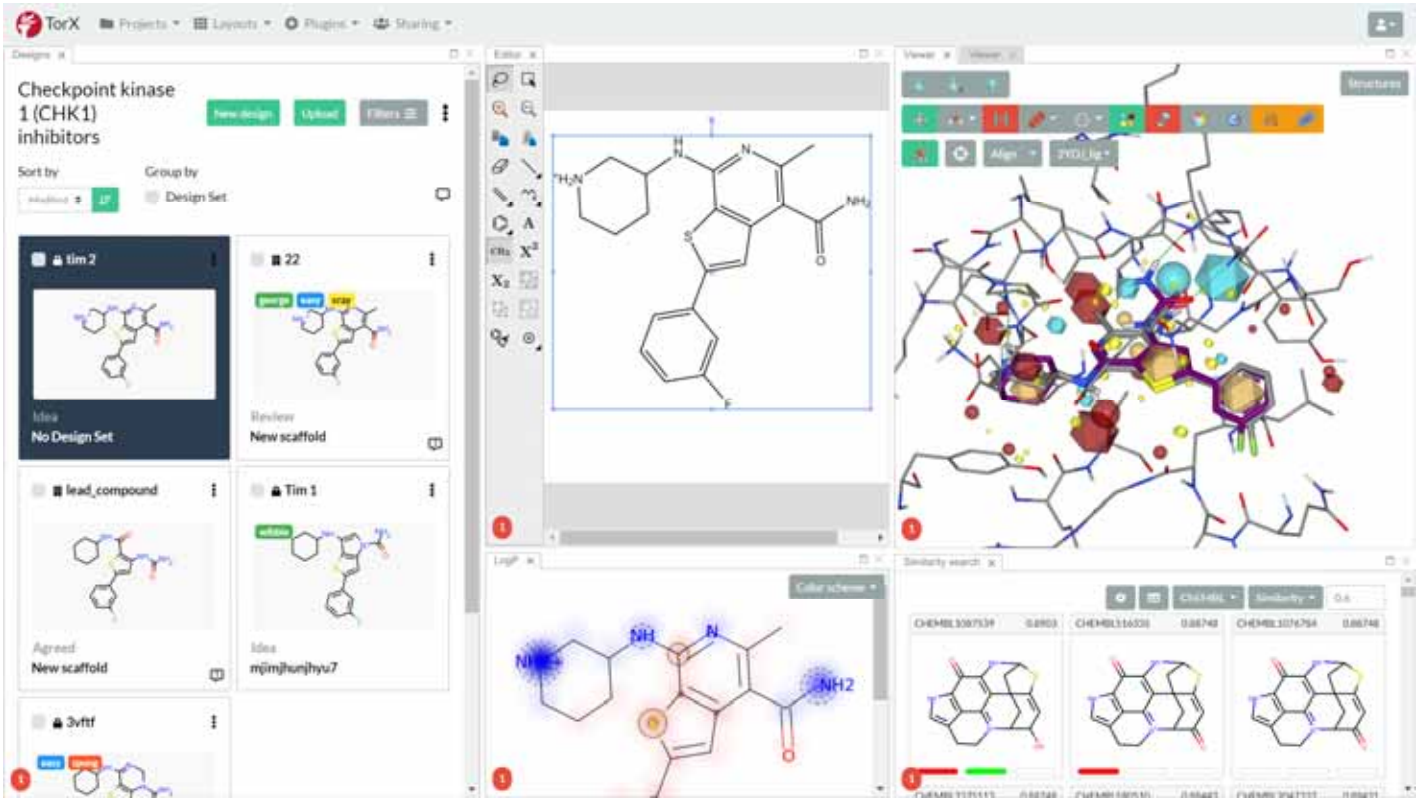
Torx Design

2D and 3D design with all vital information on tap

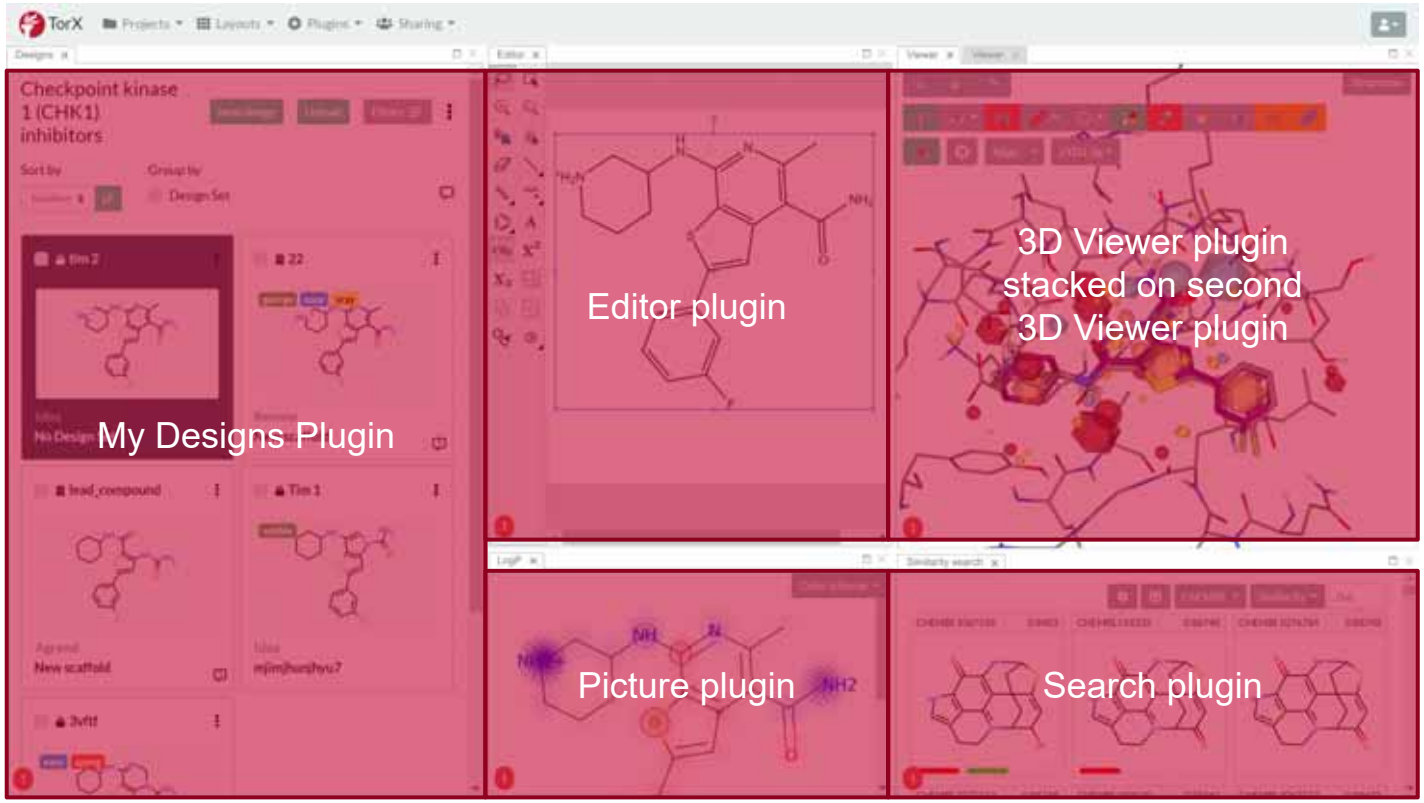
Torx design workflow



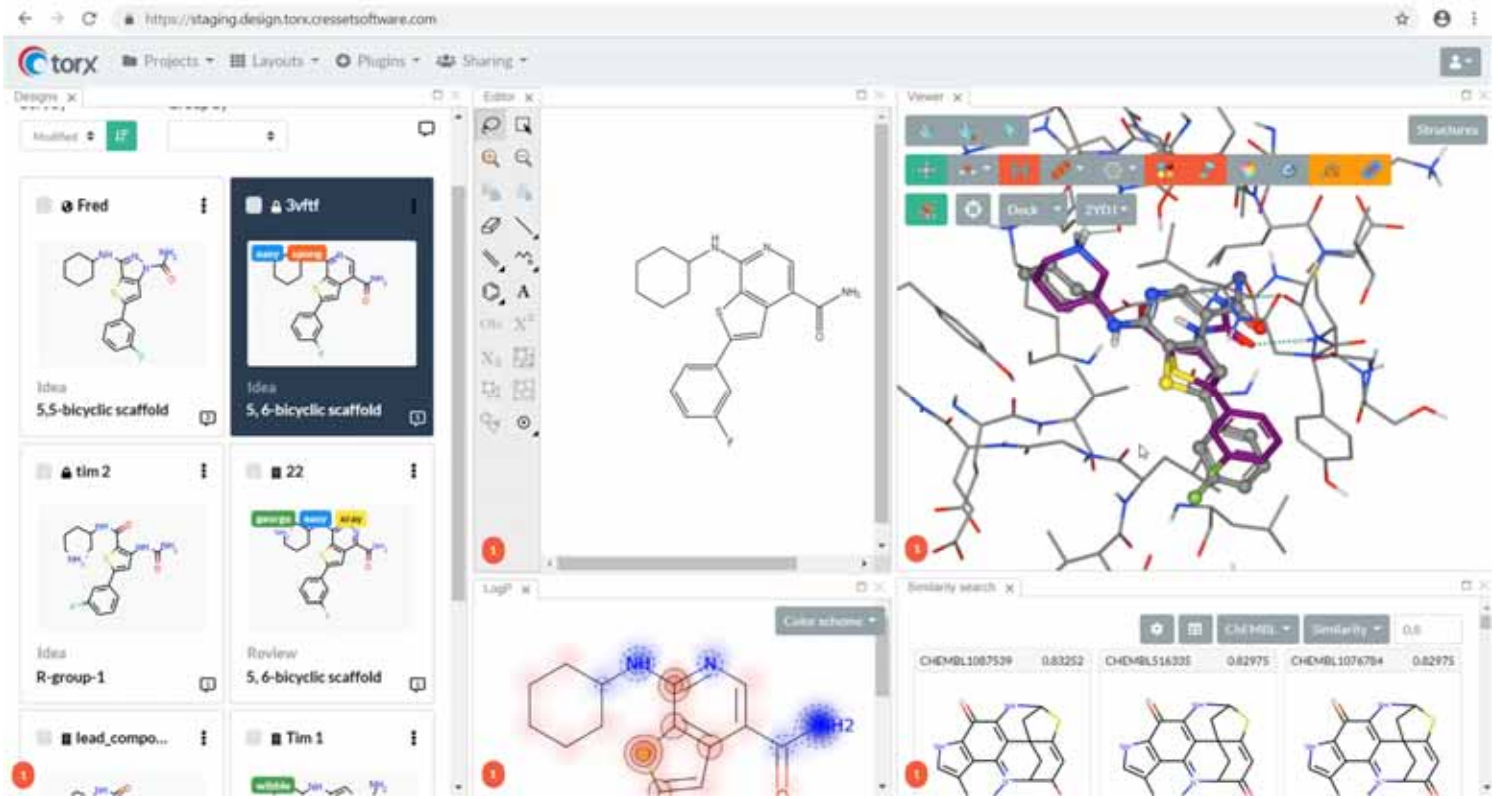
Flexible GUI in a web browser



Flexible information presentation



Design and Review in shared sessions



Design and collaborate in an information rich environment

Flexible canvas that holds ‘plugins’

- Cresset developed plugins
  - ‘My Designs’
  - Design ‘Review’
  - Database ‘Search’
  - 2D ‘Editor’
  - 3D ‘Viewer’
  - Physico-chemical ‘Properties’
- Additional actions
  - Customizable list of actions from any molecule
- Custom plugins
  - SDK with templates for plugin development
  - Standard templates for web page display, multi-molecule display, picture rendering

Detailed live sharing of molecules

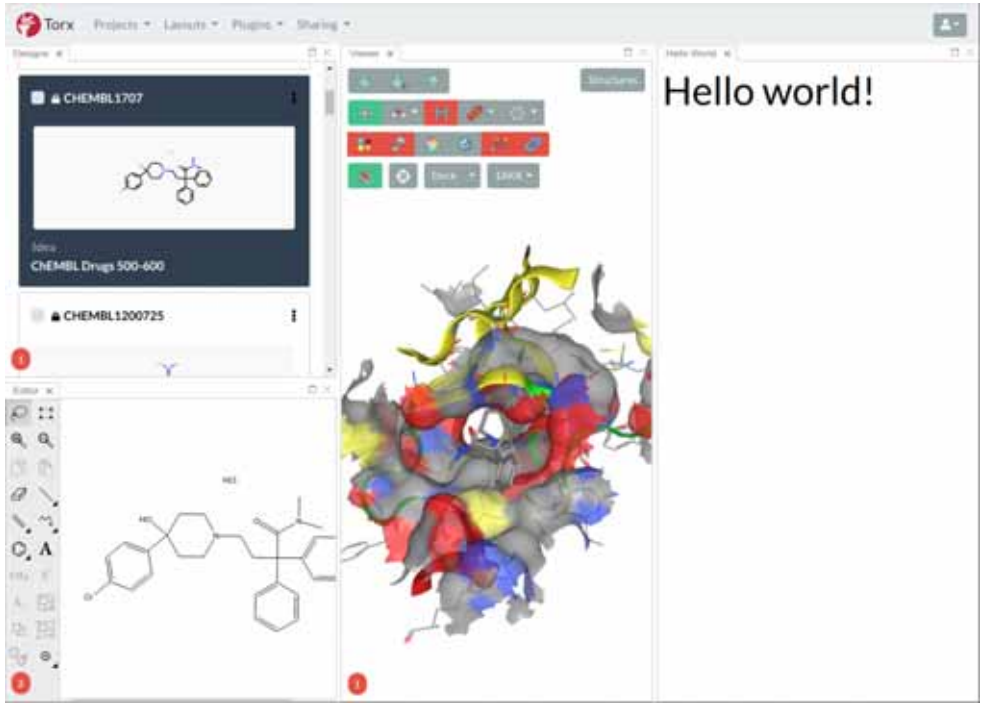
- Shared sessions provide team working environment
- Share molecules not screens – your environment remains unchanged
- Create a personal view while sharing
- Permissions on molecules and plugins prevents inadvertent information leakage

Easy plugin development

- Plugins are Vue.js components
  - See https://vuejs.org/v2/guide/ for a guide using Vue
- Development of a new plugin is straightforward
- We will provide templates and componentry to cover most common use cases
  - Render an external web page
  - Image rending
  - Tile view of molecules
  - Etc..

Torx Plugin Development

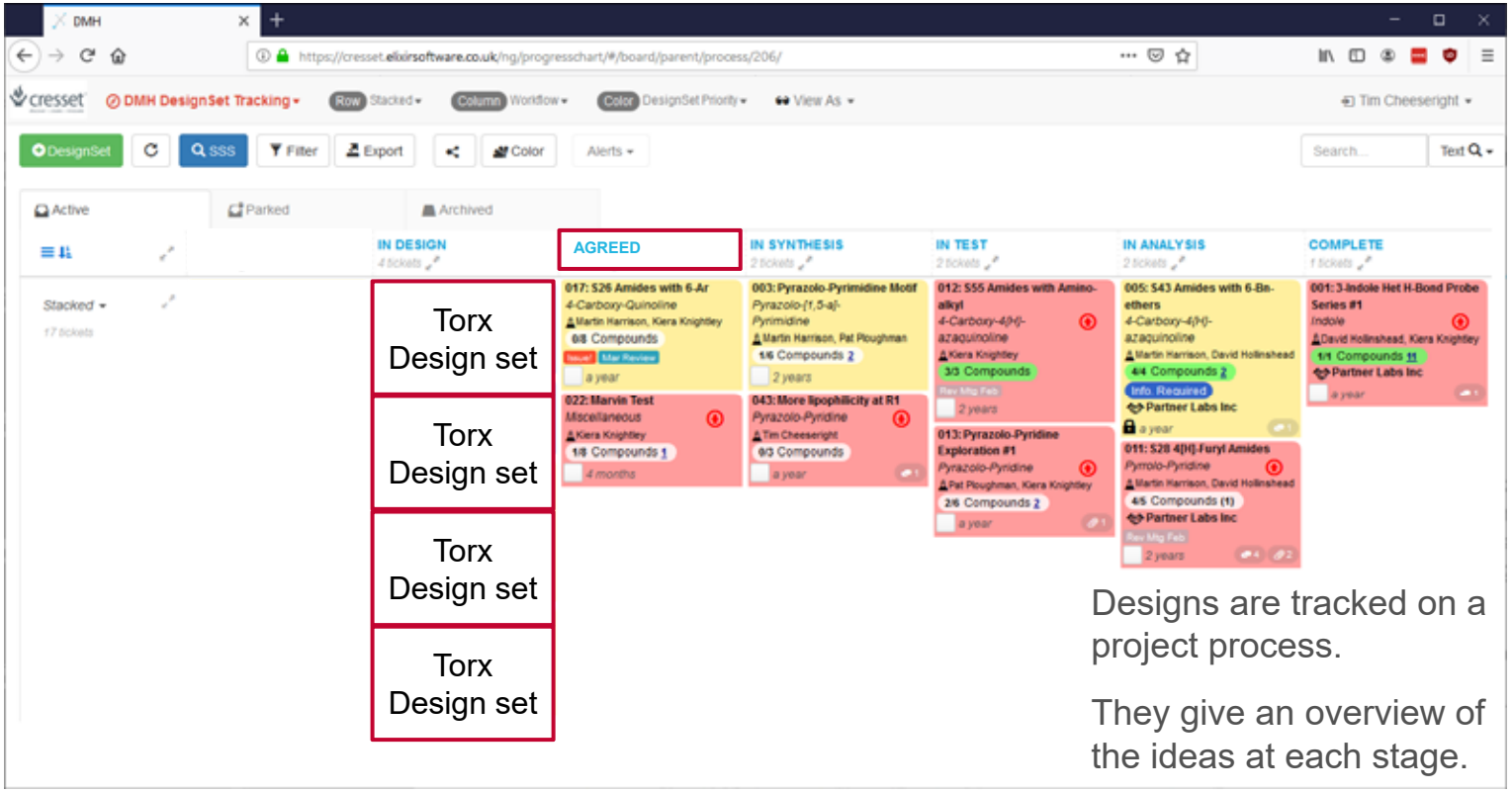
```vue
<template>
  <div class="plugin">
    <h1>Hello world!</h1>
  </div>
</template>

<script type="text/ecmascript-6">
  import Base from '../base/Base.vue'

  export default {

    // Declare that plugin extends the base plugin
    extends: Base

  }
</script>

<style lang="scss" scoped>
  .plugin {
    padding: 6px;
  }
</style>
```



Torx Make

chemTraX

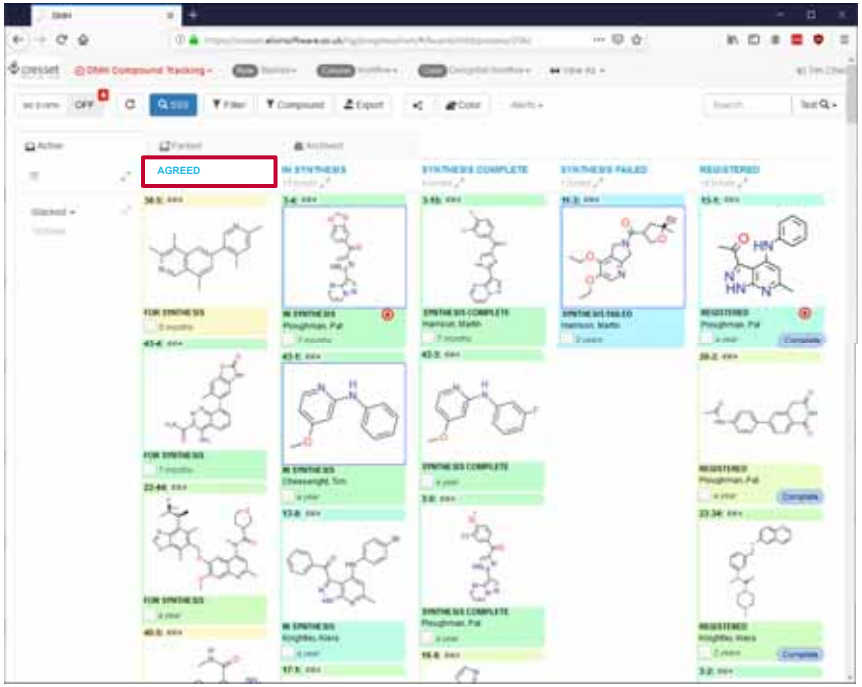
Design Tracking



Designs are tracked on a project process.

They give an overview of the ideas at each stage.

Synthesis View



> Compound tracking provides an overview of all target molecules at each stage of planning & synthesis

> It gives a visual overview of chemistry assignments for resourcing and prioritization

Torx Analysis

Analysis and design are symbiotic

Multi-faceted analysis

- Data analysis
  - Chart/Plot driven
- Binding analysis
  - 3D derived

Personal & Public

- Create personal insights
  - Graph, plot, 3D view, MMP, …
- Share with the project team
- Pick from existing insights

Application to design

- View key insights at design time
- Apply insights to new designs
- Ensure knowledge is gained – avoid learning twice

Flexible data

- Static & dynamic datasets
- Use queries to live update
- Combine & manipulate datasets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Team working platform

> Interactive review and design process

> No more Excel or Powerpoint in meetings

> Efficient, effective communication with CROs

> Accessible anytime anywhere

Improved communications

- Save time in meetings
  - More time in the lab
- Live interactive chemistry tools
- Faster turnaround times to active chemistry
- Never miss a decision, never decide blind

Questions

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