optibrium

StarDrop™

Software that guides you to successful drug discovery

Break Free from Chemical Spreadsheets

Introducing Card View™

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Overview

- Introduction to Optibrium and StarDrop
- Compounds and data in the context of drug discovery
- Introducing Card View
- Live demonstration
  - Including clustering, activity cliff detection and matched pair analysis
- More information
- Q&A

Introduction to Optibrium
www.optibrium.com

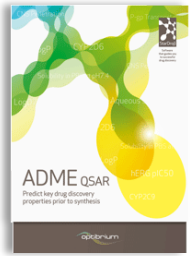
- Optibrium creates elegant software solutions for small molecule design, optimisation and data analysis
  - R&D of novel technologies to guide decisions and improve efficiency in drug discovery
- Global customer base from top-ten pharma to small biotech and academia
  - >60 StarDrop customers worldwide
  - Five of top-ten pharma
  - Adoption in other chemistry fields, e.g. agrochemicals, flavourings, etc.

Introduction to StarDrop

Guiding decisions from selection to design…

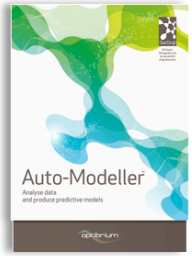
- Probabilistic Scoring – Multi-parameter optimisation
  - Define your property profile and quickly identify high quality compounds
- Chemical space and selection
  - Target quality compounds balanced with diversity to avoid missed opportunities
- Data visualisation and R-group analysis
  - Understand the structure-activity relationships in your chemical series
- Interactive design and Glowing Molecule
  - Guide the design of *balanced* compounds

StarDrop Plug-in Modules
Extend Core Capabilities



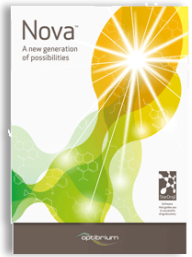
ADME QSAR

High quality predictive models of key ADME properties



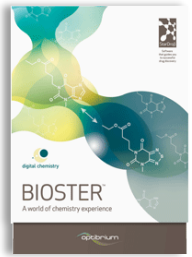
Auto-Modeller

Build and validate robust models tailored to your chemistry



Nova

Generate and prioritise new, relevant compound ideas



BIOSTER™

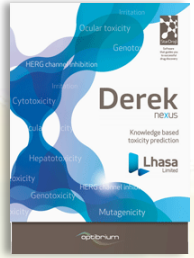
Explore >23k precedented transformations with the Nova module

P450

QM simulations identify sites of metabolism and lability for major P450s

torch3D™

Understand and apply 3D SAR to identify and optimise novel actives



Derek Nexus™

Knowledge-based prediction of >40 toxicity endpoints

MPO Explorer™

Develop multi-parameter optimisation strategies

Compounds and Data in the Context of Drug Discovery

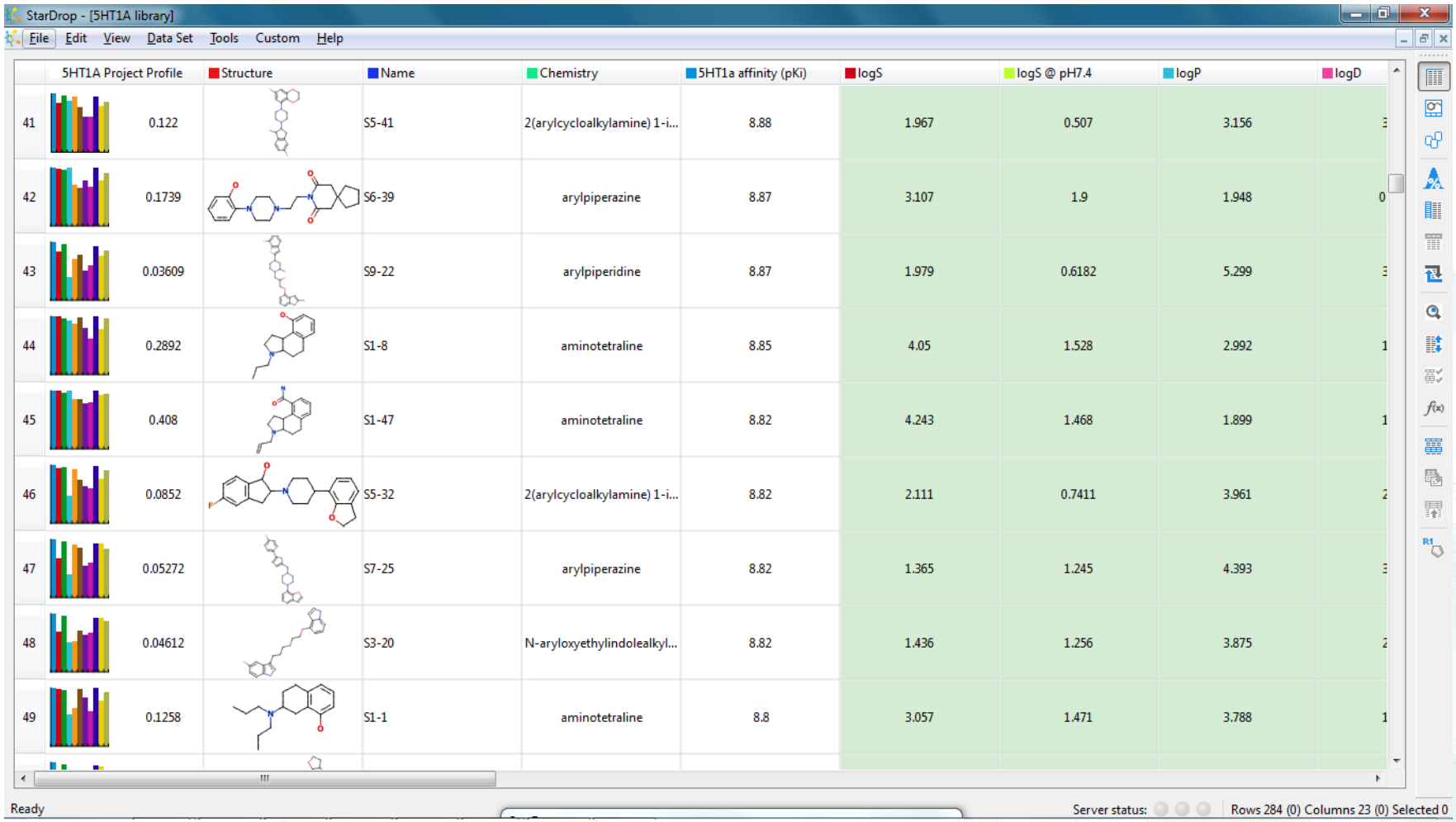
Thinking About Compounds
Some examples….

- Individual compounds
  - What are the properties of this compound?
  - How ‘good’ is it against my project’s objectives?
  - How ‘good’ is it relative to other compounds I am considering?
- Groups of compounds
  - Series, clusters, bins…
  - How ‘good’ is this series for my project?
  - Which is the ‘best’ series?
- Relationships between compounds
  - Project progress – retrospective analysis
  - Synthetic steps
  - Transformations or optimisation steps
  - Structure-activity relationships (SAR) – guide further optimisation

Analysing Compounds and Data
Chemoinformatics

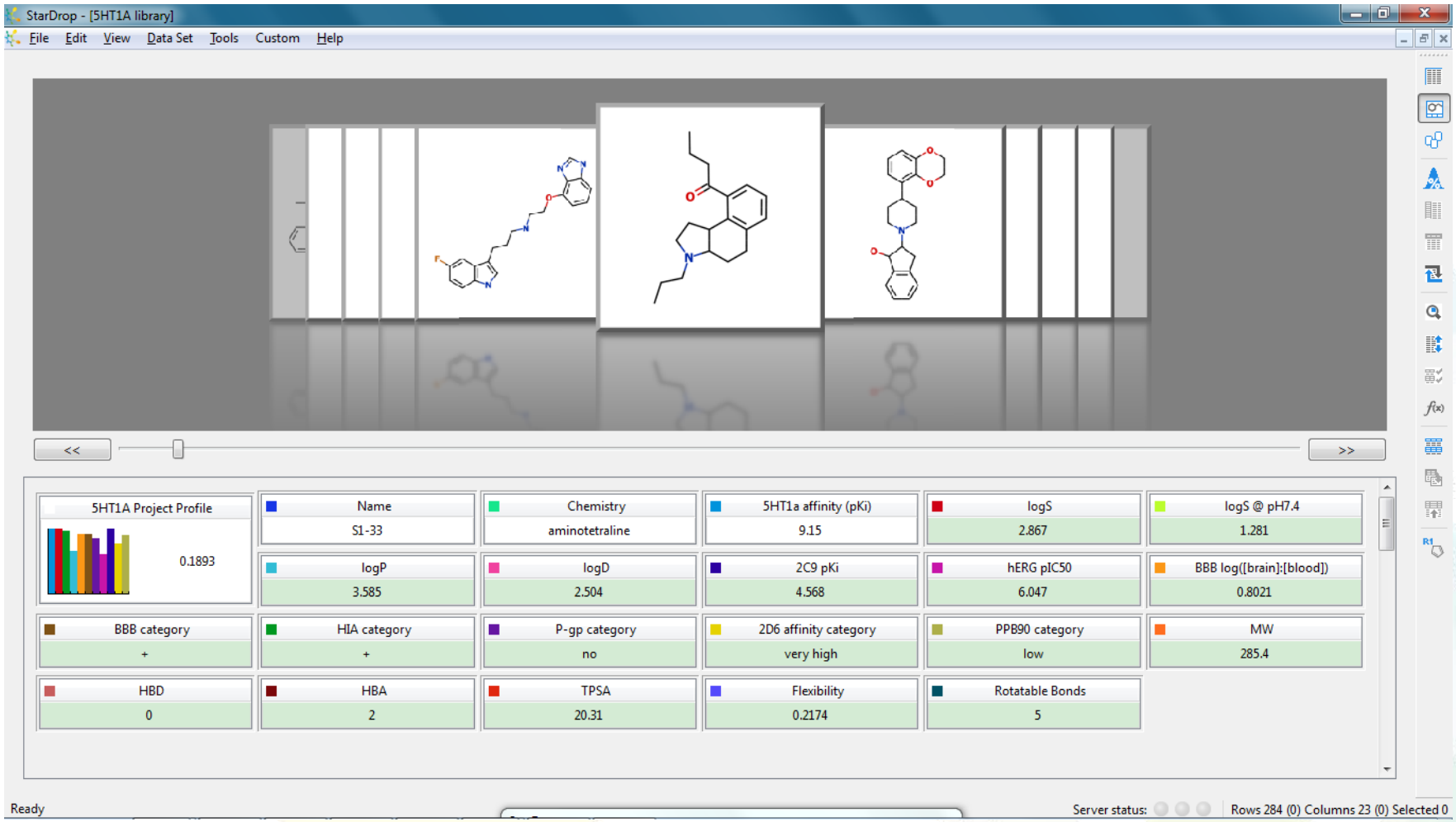
- Clustering
  - Group compounds by structural similarity, properties or substructure
- Activity landscapes
  - Find areas of interesting SAR or ‘flat’ spots with limited opportunities for optimisation
- Activity cliffs
  - Small changes in structure that lead to big changes in properties
  - Important SAR around a compound
- Matched molecular pair analysis
  - Learn from existing data to find transformations with consistent impact on properties

Representing Compounds and Data
Lists



	5HT1A Project Profile	Structure	Name	Chemistry	5HT1a affinity (pKi)	logS	logS @ pH7.4	logP	logD
41	0.122		S5-41	2(arylcycloalkylamine) 1-i...	8.88	1.967	0.507	3.156	
42	0.1739		S6-39	arylpiperazine	8.87	3.107	1.9	1.948	0
43	0.03609		S9-22	arylpiperidine	8.87	1.979	0.6182	5.299	
44	0.2892		S1-8	aminotetraline	8.85	4.05	1.528	2.992	1
45	0.408		S1-47	aminotetraline	8.82	4.243	1.468	1.899	1
46	0.0852		S5-32	2(arylcycloalkylamine) 1-i...	8.82	2.111	0.7411	3.961	
47	0.05272		S7-25	arylpiperazine	8.82	1.365	1.245	4.393	
48	0.04612		S3-20	N-aryloxyethylindolealkyl...	8.82	1.436	1.256	3.875	
49	0.1258		S1-1	aminotetraline	8.8	3.057	1.471	3.788	1

Representing Compounds and Data
Lists



Representing Compounds and Data
Visualisation

	5HT1A Project Profile	Structure	5HT1a affinit	logS	logP	hERG pIC50	BBB log([brai	BBB category	HIA category	P-gp categor	2C9 pKi	2D6 affinity c	PPB90 categ
129	0.09091		7.04	2.562	3.584	6.184	0.02164	+	+	yes	4.636	high	low
130	0.08962		8.04	1.354	4.236	5.6	0.1691	+	+	yes	5.065	medium	high
131	0.08951		8.7	1.541	3.946	5.319	0.0381	+	+	yes	5.173	medium	high
132	0.08819		7	1.98	3.173	6.589	0.1233	+	+	no	4.518	high	high
133	0.08644		8.74	1.868	4.777	5.992	0.346	+	+	yes	5.208	medium	high
134	0.08566		7.06	2.531	2.464	5.606	0.0244	-	+	no	4.487	high	low
135	0.0852		8.82	2.111	3.961	6.468	0.7654	+	+	yes	4.83	very high	low
136	0.08297		7.31	1.889	3.503	6.091	0.3864	-	+	yes	5.355	medium	high
137	0.0813		6.87	2.495	2.997	5.759	0.145	+	+	no	4.561	high	high

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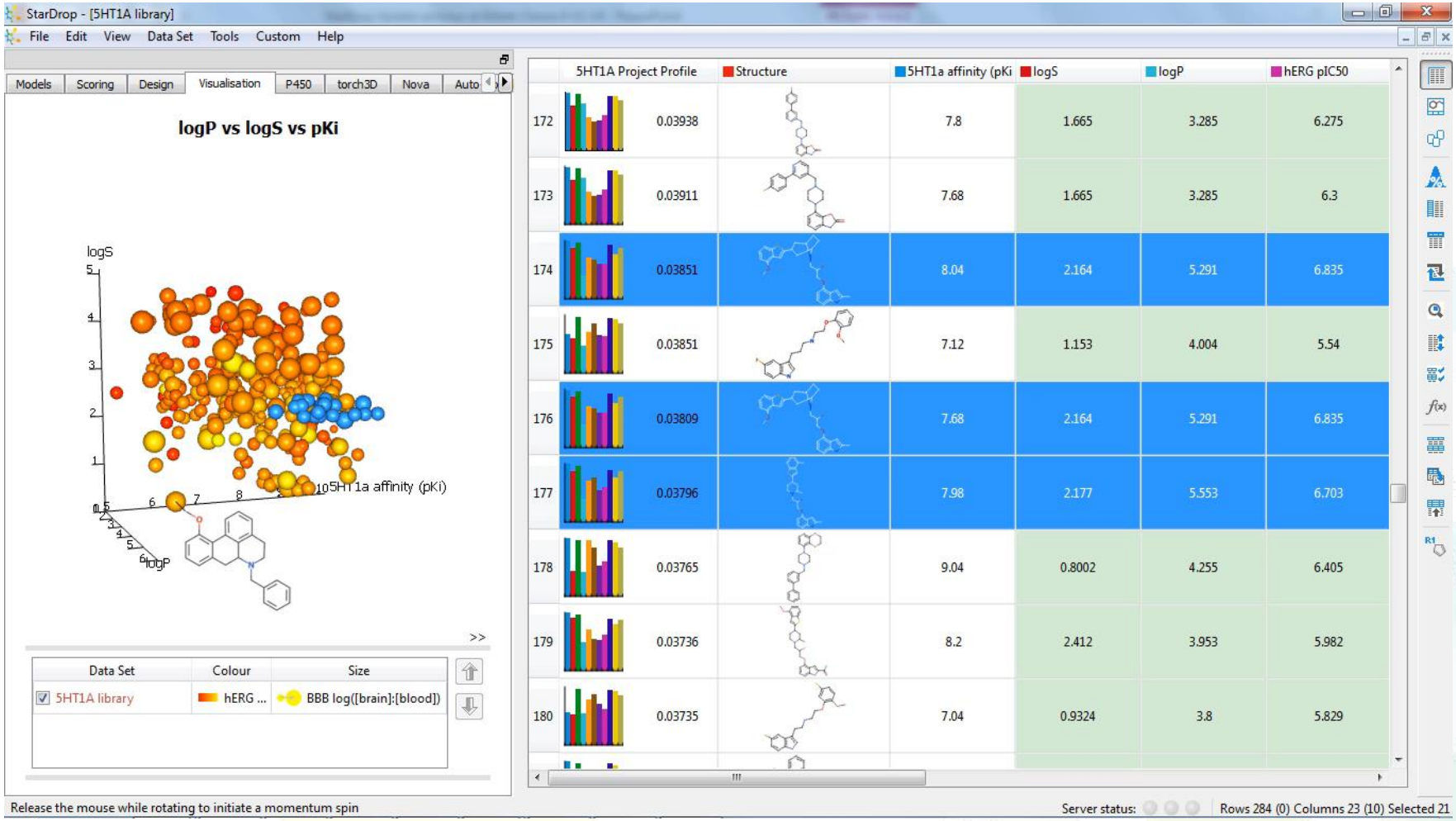


Challenges

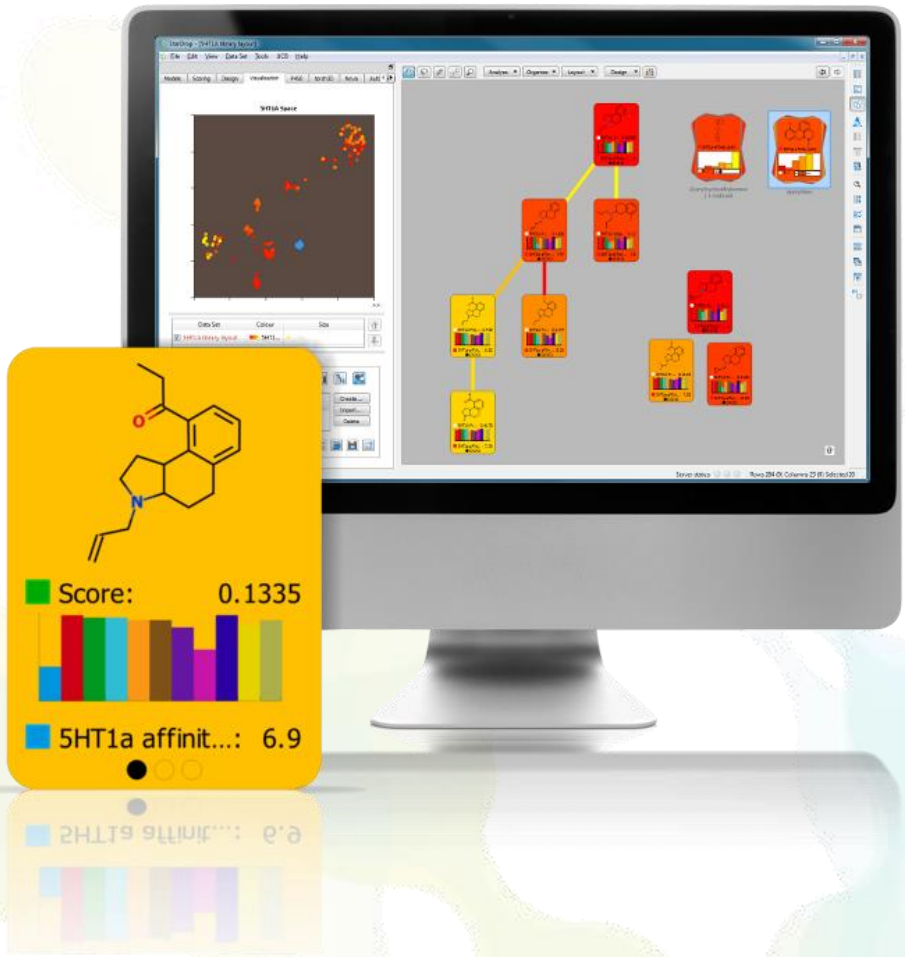
- Organise compounds and data to reflect the way we are thinking about them
  - Interactive
  - Intuitive
- Represent the output of complex analyses to more easily interpret and act on the output
  - Combine strengths of algorithms and experts
- Share and present results easily
  - Flexible – different disciplines are interested in different data

Introducing Card View

Interacting with data just got interesting…

Card View™
Interacting with data just got interesting…

- Freedom from the constraints of ‘chemical spreadsheets’
  - Work the way **you** think
- Cards
  - Show compound data you choose
  - Position how you want
- Stacks
  - Group compounds
  - Summarise and compare data
- Links
  - Highlight compound relationships
- Intuitive visualisation of analyses
  - Clustering, activity landscapes, matched molecular pairs…
  - Extend with your own methods



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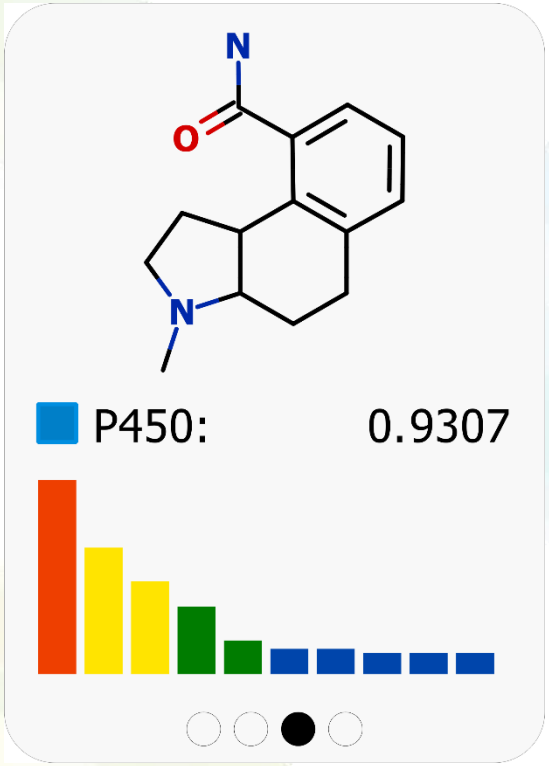

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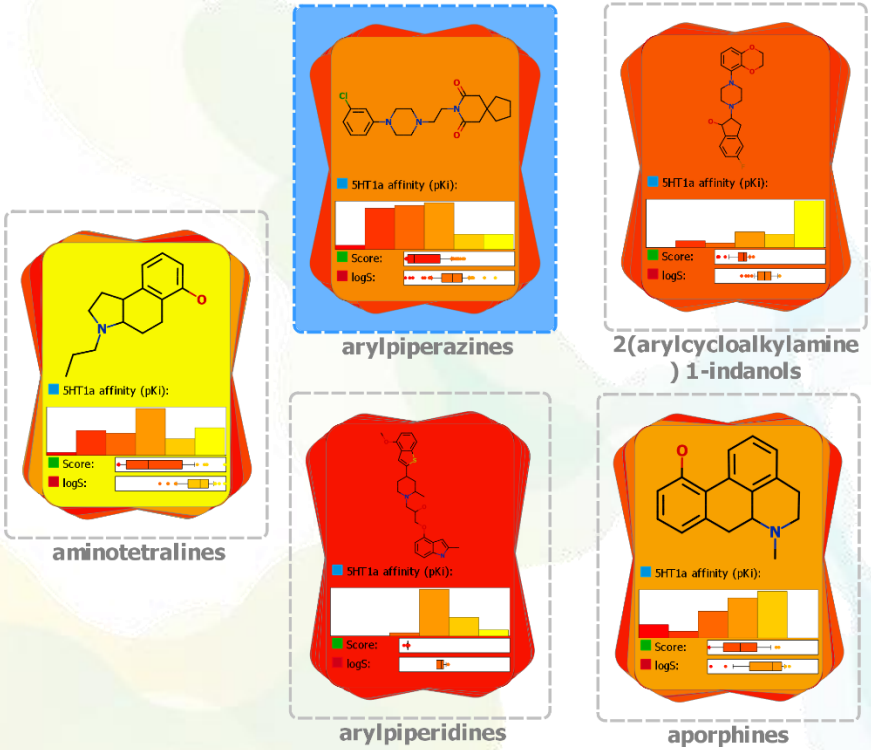

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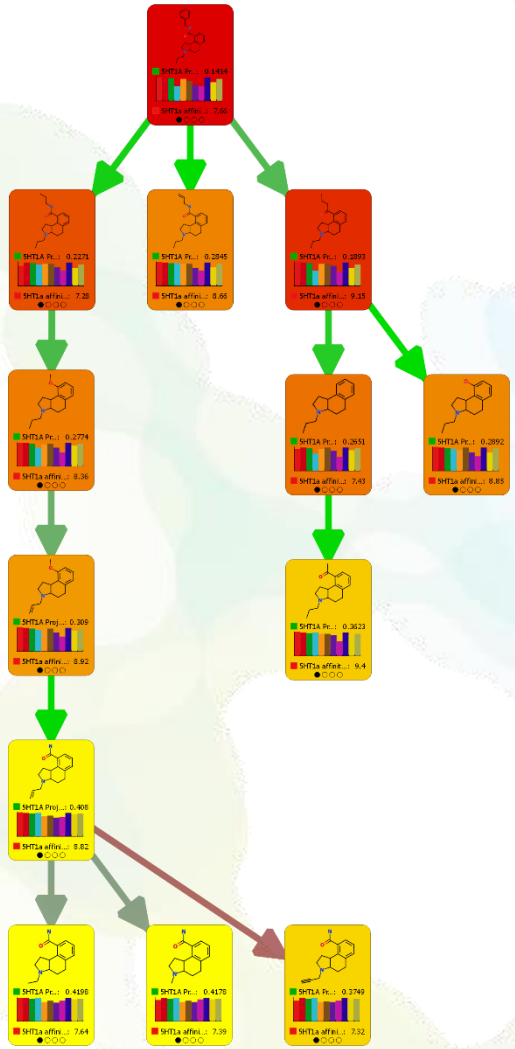

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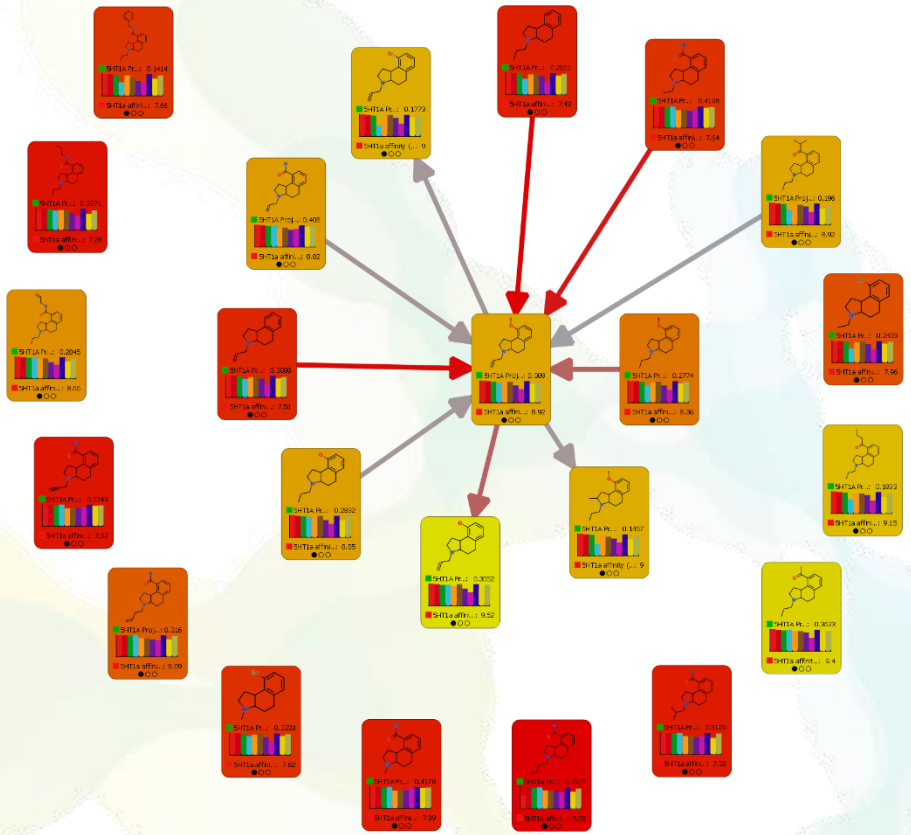

Live Demonstration

Conclusions
Card view provides…

- A flexible and dynamic way to work with your compounds and data
  - Organise your information the way **you** think about it
- Intuitive interpretation of analyses of compounds and data
  - Quickly identify high quality compounds and key SAR
  - Extensible through an API to add your own methods
- An easy way to present and share your findings

Quickly reach good decisions to achieve your project objectives

More information

- StarDrop - www.optibrium.com/stardrop
- Card View - www.optibrium.com/stardrop/card-view.php
- Online community: www.optibrium.com/community
  - Videos
    - Introductions to Card View and other StarDrop features
    - Hints and tips on using Card View and StarDrop
  - Tutorials, including video walk-throughs
  - Publications, presentations and posters by Optibrium team, StarDrop users and others
  - Download free add-ons for StarDrop: scripts, models, etc.
  - FAQs, forums, etc.
- For more information or to arrange a demo or trial, please email:
  - info@optibrium.com

Questions and Answers

Sentira™
Visualise your compound data

- Powerful, yet easy-to-use, data visualisation for chemists
  - Plot types include 2- and 3-D scatter plots, histograms, box plots, pie charts, radar plots…
  - Dynamic links between all plots and data set
- Chemically aware
  - Generate R-group analyses and visualise SAR
  - Annotate plots with structures and data
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  - Copy and paste into slides and reports
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Creative compound exploration and design on the iPad®

Science at your fingertips

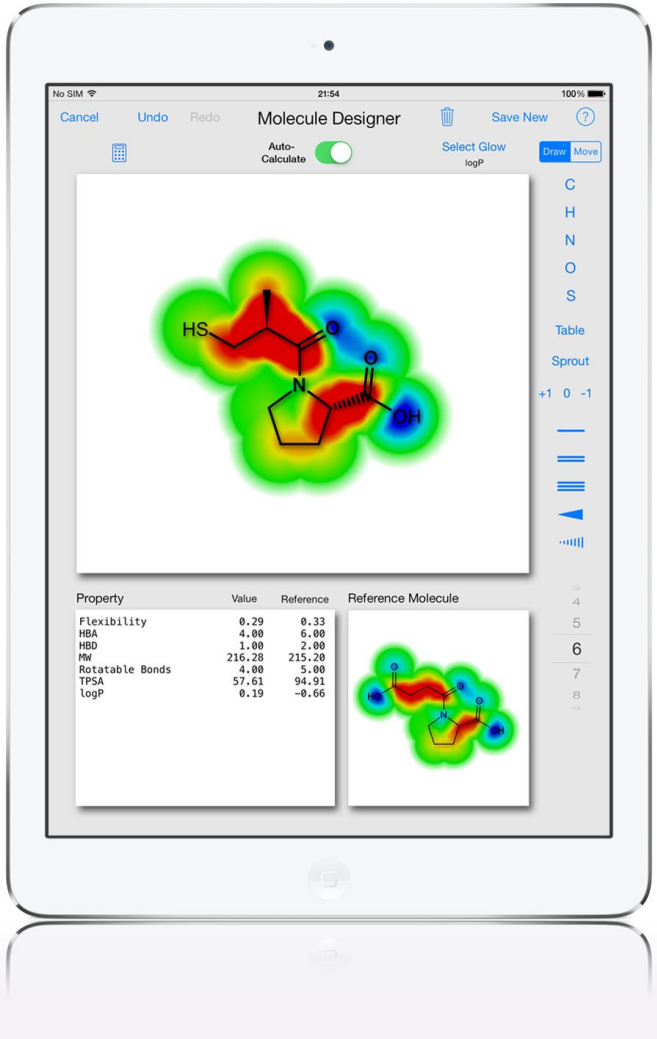
Asteris uses patent pending chemical drawing tools developed in Chirys Draw™ and optimized specifically for the touch environment

Seeing and believing

Glowing Molecule™ technology will provide you with a visual link between structures and predicted properties

Predictive confidence

Providing you with a more intuitive process, backed by rigorously validated models from StarDrop's™ industry-leading platform



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