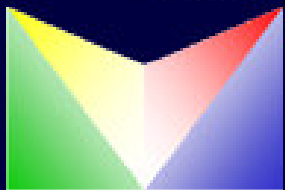




# Building a Comprehensive Chemical Supplier Catalogue:

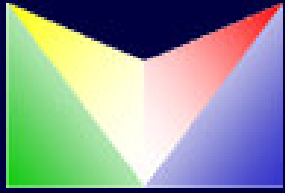
## Technical Challenges

*Craig A. James*  
*Modgraph Consultants Ltd*



# The Modgraph CSC

- What is it?
  - A complete system for integrating data from dozens or hundreds of chemical suppliers into a single, searchable chemical catalogue



# The Modgraph CSC

- Why Build It?
  - Existing Supplier Databases can be:
    - Incomplete
    - Inconsistent quality
    - Out-of-date information
    - Expensive when deployed widely
- But ... researchers *really need* a comprehensive supplier database



# The Modgraph CSC

- The need is there
  - We discovered *many* customers considered or tried to build their own supplier database systems
- A do-it-yourself CSC is difficult
  - Loading, searching applications must be built from scratch
  - Database schema is tricky, many pitfalls
  - Requires an ongoing high level of support



# Requirements for a Supplier Catalogue

## User Requirements

1. Consistent, Up-to-Date Chemistry
2. User-Friendly Front End
3. Fast Reagent Searching
4. Supplier Selection / Ordering

## Administration Requirements

1. Flexible, Powerful Loader
2. Maintainable with Modest Effort
3. Affordable



# Registration vs. CSC

- **Relational Database**
  - Basic Information Repository
  - High-performance
  - Reliable
  - Manages relations amongst data

**Chemical Registration**



**Chemical Cartridge**  
Chemistry for Oracle



**Relational Database**  
Information Repository



# Registration vs. CSC

- Chemistry Cartridge
  - Adds ability to store molecules
  - Indexing for fast search, retrieval and “joins” (chemical relationships)

**Chemical Registration**



**Chemical Cartridge**  
Chemistry for Oracle



**Relational Database**  
Information Repository



# Registration vs. CSC

- Chemical Registration
  - Deeper information about chemistry
  - Business Rules
  - Security
  - Amendments
  - Auditing

**Chemical Registration**



**Chemical Cartridge**  
Chemistry for Oracle

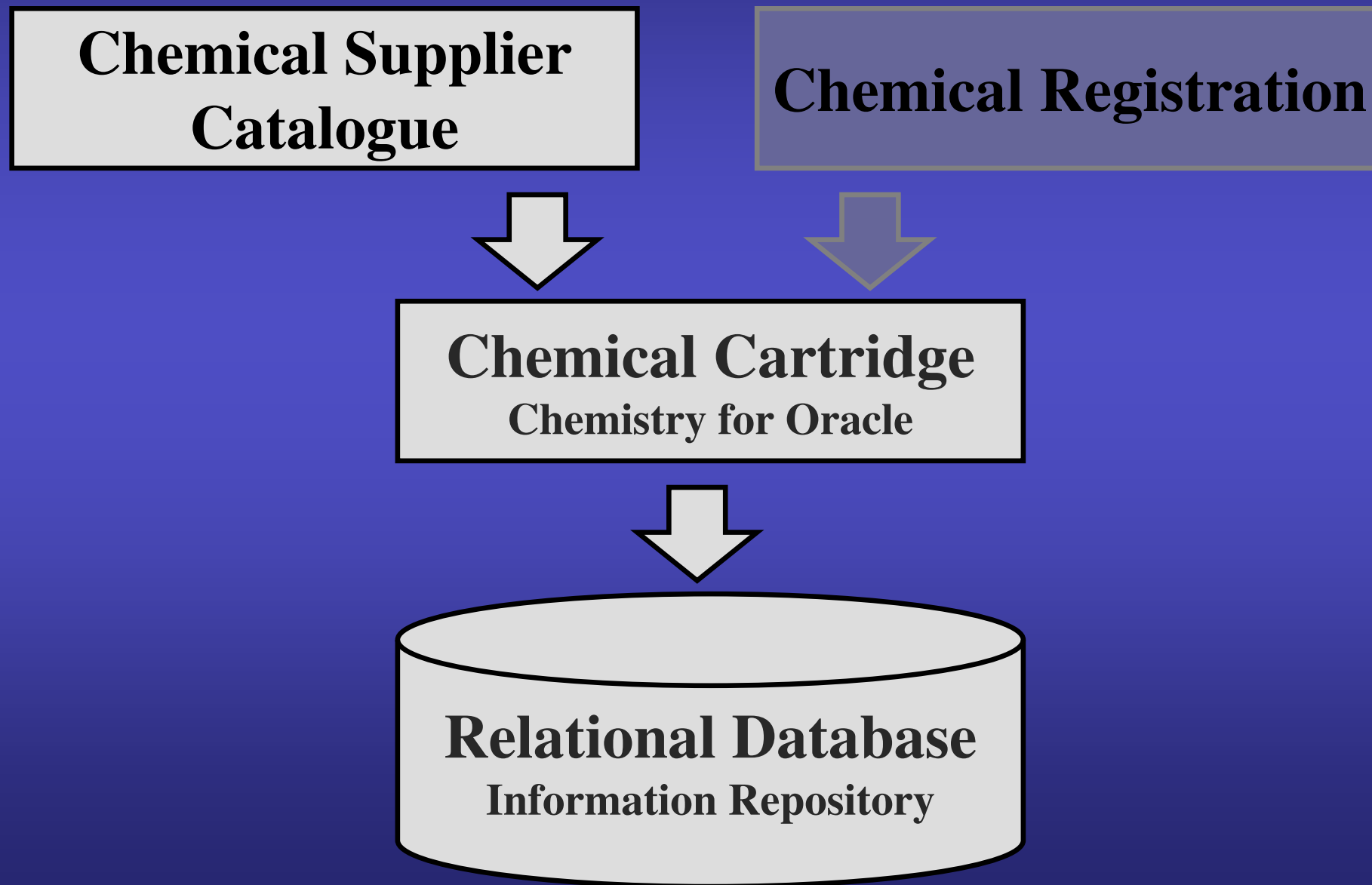


**Relational Database**  
Information Repository





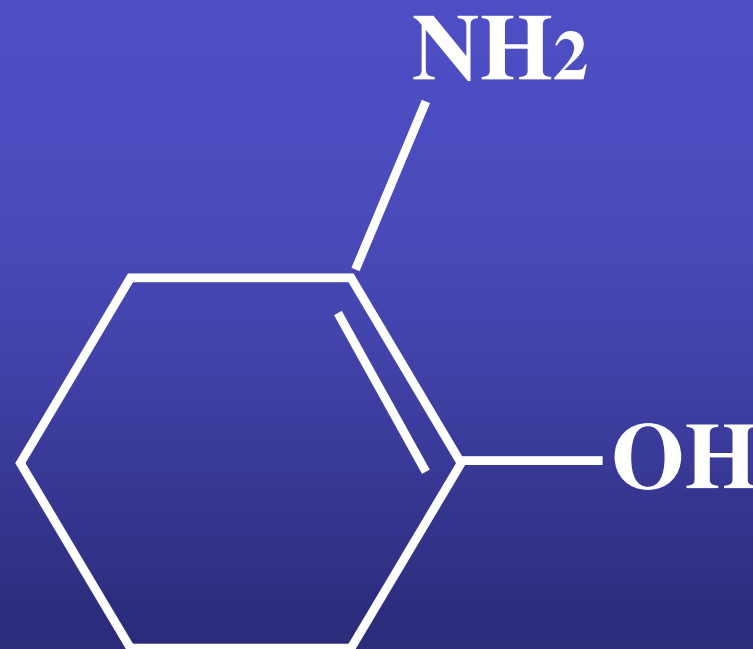
# Chemical Supplier Catalogue: Simple Chemical Registration





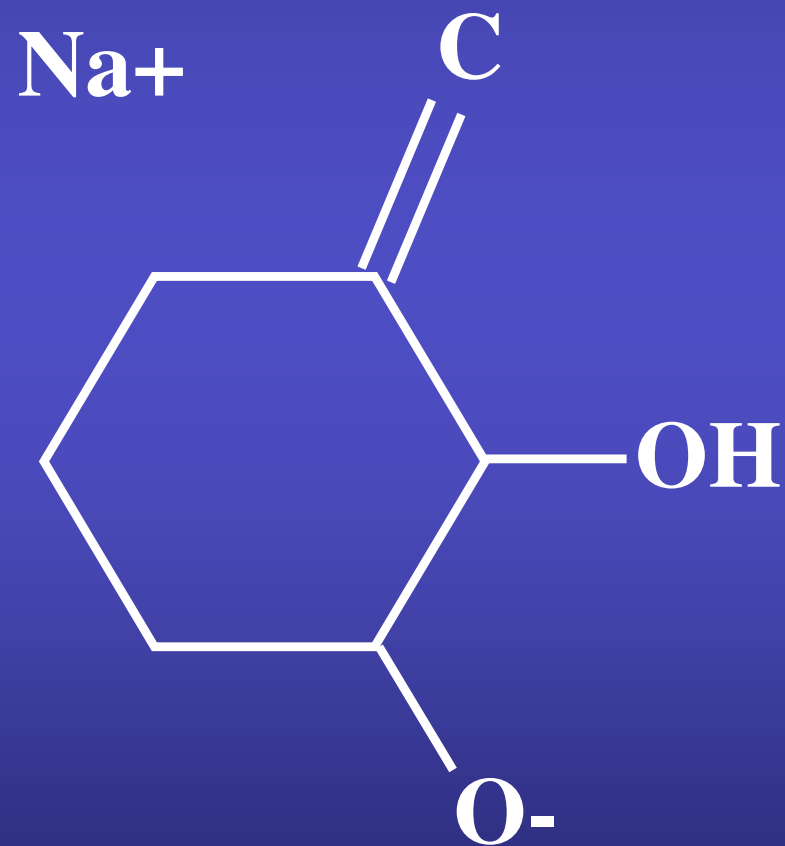
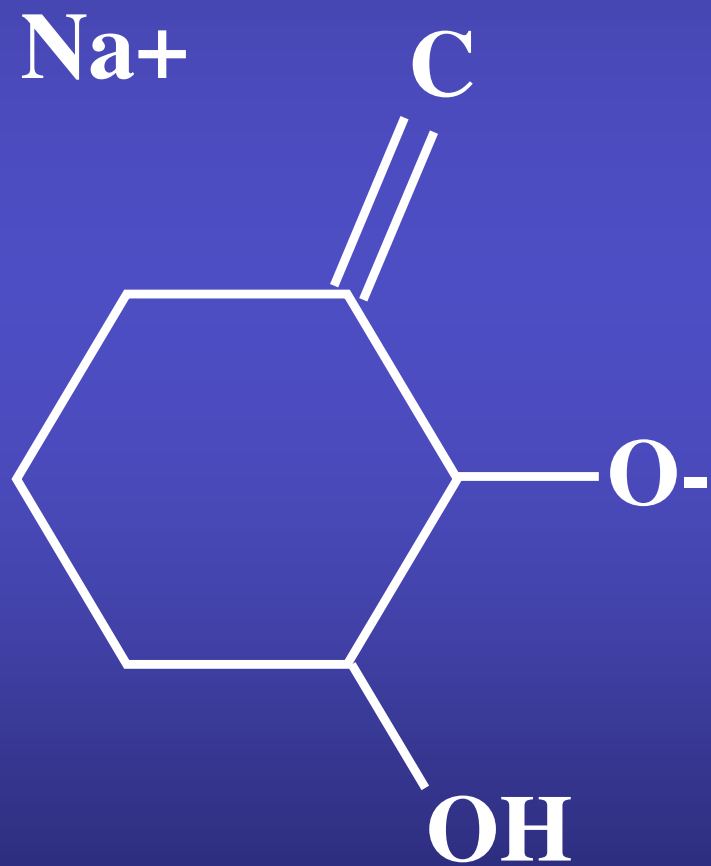
# Example: Bond Normalization

- Tautomers, electron / proton migration





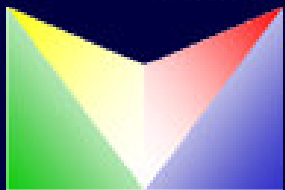
# Example: Charge Normalization





# Registration vs. CSC: Chemistry

<u>Feature</u>	<u>Registry</u>	<u>CSC</u>
bond normalization	yes	yes
charge normalization	yes	yes
mixtures / formulations	yes	no
uncertain stereo centers	yes	no
relative stereochemistry	yes	no
partial structures	yes	no



# Registration vs. CSC: Data Entry

<u>Feature</u>	<u>Registry</u>	<u>CSC</u>
draw & register single structs	yes	no
load batches of structures	yes	yes
workflow control / business process	yes	no
full audit trail	yes	optional
amendments	yes	no
link to assay data	yes	no

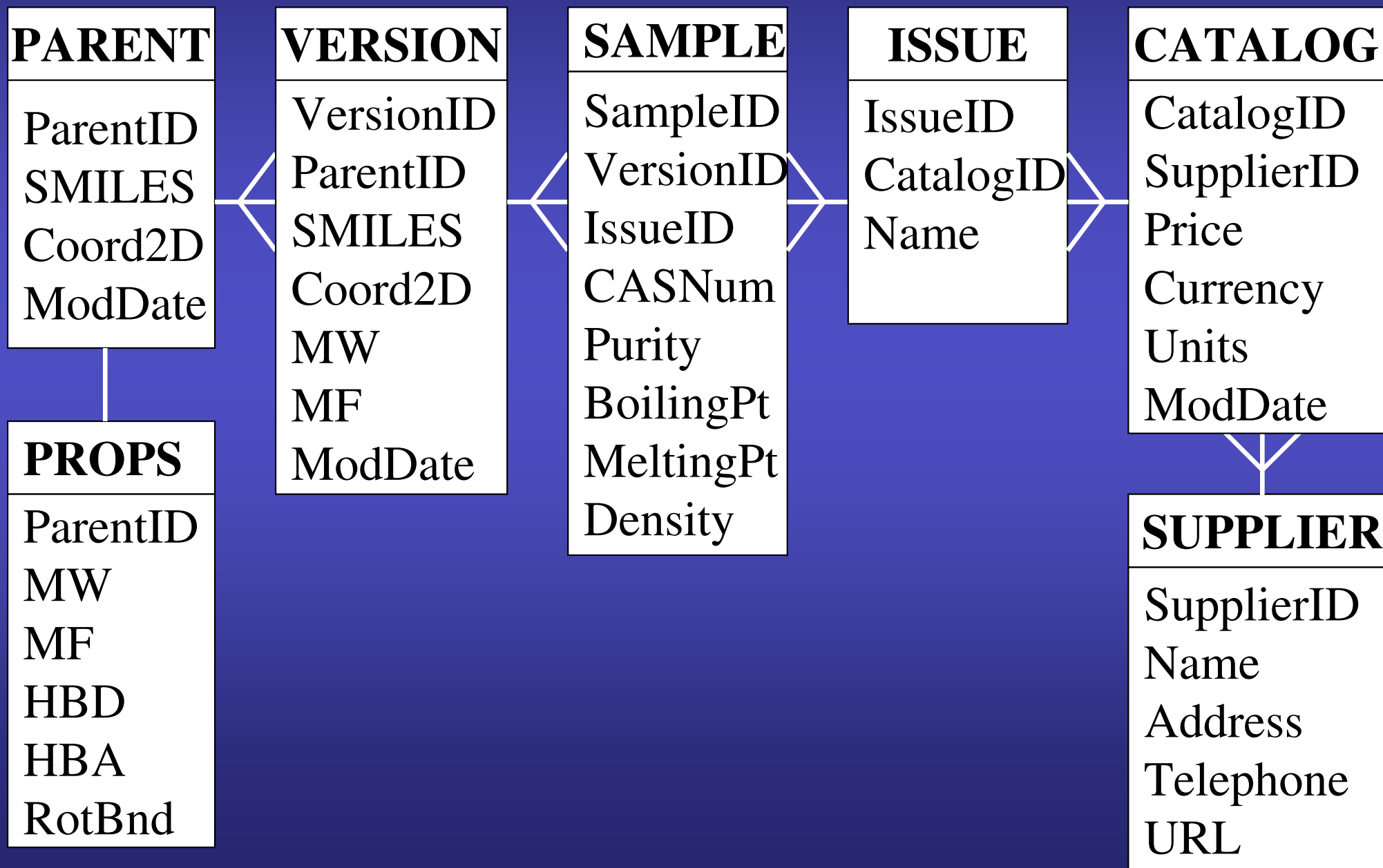


# Registration vs. CSC Searching

<u>Feature</u>	<u>Registry</u>	<u>CSC</u>
substructure & similarity	yes	yes
partial & relative stereochemistry	yes	no
mixtures & formulations	yes	no
physical properties	yes	yes
reagent selection	no	yes
supplier selection	no	yes



# CSC Database "Schema"





# Modgraph CSC Demo

- René: Key features for CSC
  - Web interface
  - Hitlist concept
  - Very large databases





# Modgraph CSC Demo

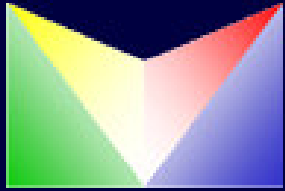
- René : Special Features for CSC
  - Reagent Selection
  - Supplier Selection
  - Supplier / Catalogue Management
  - Holding Table
  - Salt Table



# Modgraph CSC Demo

- Steps in Loading Data
  - *[optional]* Create Supplier
  - *[optional]* Create Catalogue
  - Create Issue
  - Browse for SD File
  - Analyze SD File
  - *[optional]* Map datatypes
  - Load
  - Approve & Update

MODGRAPH



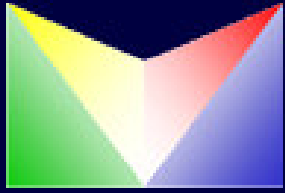
# Modgraph CSC

- Demo...



# Modgraph CSC

- Concluding Remarks
  - Solves the problem of creating and maintaining a comprehensive, current, searchable chemical catalogue
  - Uses simplified registration technology
  - Daylight powers chemical searches
  - Affordable
  - Simple but powerful user interface



# Acknowledgements

- Thanks to:
  - Rashmi Mistry, Mike Wainwright, Dave Taylor, David Digby (Modgraph)
- And of course...
  - Jack Delany and the Daylight gang



# Contact

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