William Lindstrom
Acelot, Inc.

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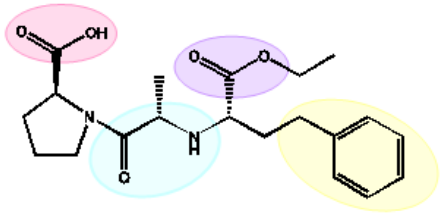
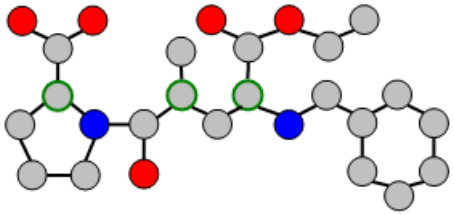
Acelot Core Technologies

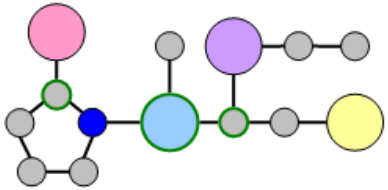
- Graph algorithms and graph-based data mining techniques



- SimFinder
  - Topological Similarity Search
  - Integrated as InstantJChem Plug-in



- SigFinder
  - Significant Substructure Mining



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SimFinder – Topological Similarity Search

- Alternative to fingerprint- or descriptor-based similarity search
- Similarity based upon well-defined notion of *edit distance*
- Isomorphism heuristics and ordering of chemical graphs allows index construction and fast similarity queries

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SimFinder InstantJChem Plug-in

Instant JChem 2.4.3.1

File Edit View Search Data Lists Tools Window Help

2 / 20 Reset Windows

Projects | **Lists and queries**

- BriemLessel
- Query_169164_20R
- Structures
- Query_141330_20R
- Query_141330_20R 2
- Query_158562_20R
  - Grid view for Query_158562_20R

Analysis Window | **GraphSig Window** | **Query Window**

CTree \Ambuj\Documents\demo_data\BriemLessel.ctj Browse

Results 20 Query

Mapper nbm Create CTree Index

Use abstract nodes

Abstract Nodes File

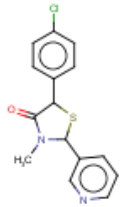
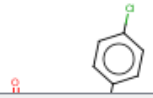
Browse

Query As Text [No query]

No query specified.

...ssel | Grid view for Query_141330_20R 2 | Grid view for Query_158562_20R

Query Browse

...	C...	Structure	Mol We...	Formula	ID	Similarity	Edit distance (1)
1	10		208.28	C10H12N2OS	141330	30.00	0.00
2	16		304.80	C15H13ClN2OS	140828	28.00	13.00
				C19H20ClN3O	163689		

Query_141330_20R 2: 20 out of 20 rows.

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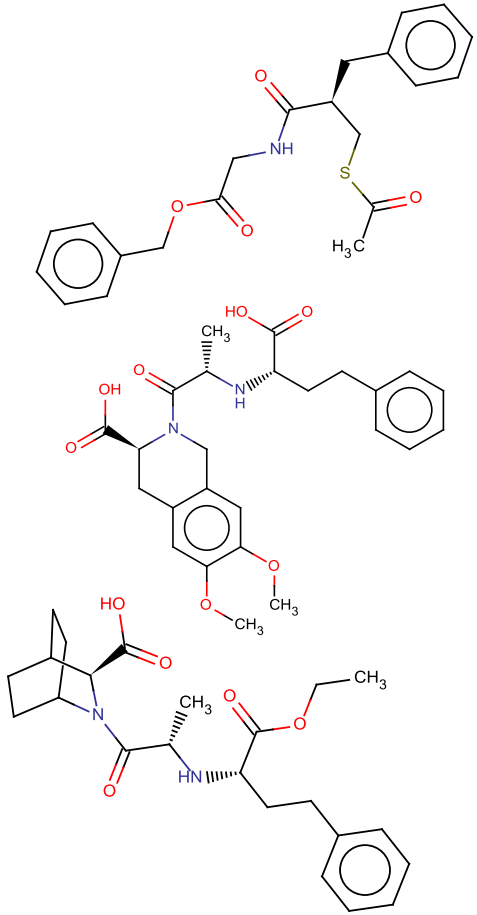
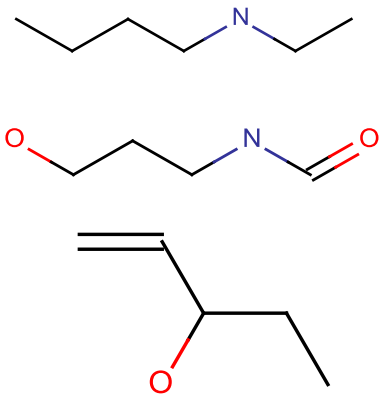
SigFinder – Substructure Mining



Automatic
Substructure
Mining

SigFinder

Significant Substructures



Mines significant substructures based on a unique statistical model – identifies unique and interesting substructures leading to specific physical/chemical property.

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Feature/Benefit Summary

Feature	**Benefits**	**Novel technology**
Similarity Searching: ***SimFinder***	• Intuitive notion of chemical similarity • Parameterized chemical distance functions • Search hits distinct from fingerprint-based queries	• Topology-based searching • Scalable index structure
Active substructure identification: ***SigFinder***	• Identification of active substructures for lead identification and optimization • Mining of protein-ligand complexes	• Significance model based on graph analysis

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More information

- www.acelot.com
- Partner Exhibition Table

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