



**Acelot, Inc.**

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U. S. DEPARTMENT OF HEALTH AND HUMAN SERVICES

National Institutes of Health



National Institutes of Health Commercialization Assistance Program  
(NIH-CAP)

## Company Profile

**Industry Sector:** Drug discovery

### Company Overview:

Acelot has developed innovative technology for lead identification and lead optimization. The technology is based on graph-based modeling of chemical compounds and has shown to be superior and complementary to existing methods deployed in the industry.

### Target Market(s):

Pharmaceuticals of all sizes.

## Key Value Drivers

### Technology\*:

Our unique graph-based mining software supports similarity queries and significance queries that can be used for finding all compounds containing a topological chemical fragment similar to a given one and all fragments that are significant in a given collection of compounds.

### Competitive Advantage:

Our topological characterization improves the current fingerprint-based technology by being sensitive to the spatial arrangement of atoms, bonds, and functional groups. We are currently conducting assays for identifying possible hits to the beta-secretase target.

### Plan & Strategy:

1. Partner with drug development effort at a pharmaceutical.
2. Offer services on the Internet.
3. Produce new leads.

\*Technology funded by the National Institute of Mental Health and being commercialized under the NIH-CAP

## Management

### Leadership:

Ambuj Singh, President

### Scientific Advisory Board:

Gilbert Rishton, CSUCI and ex-Amgen

## Product Pipeline

1. **FragmentFinder:** Finds all chemical compounds containing a given topological fragment. Tested on a collection of over a million compounds.
2. **SimFragmentFinder:** Finds all chemical compounds that contain a topological fragment similar to the given one. Tested on a collection of over a million compounds.
3. **SigFragmentFinder:** Finds all topological fragments occurring at a significance level much higher than random in a given collection. Tested on collections of chemical compounds as well as protein-ligand complexes.