

ReactionMap

An Efficient Atom-mapping Algorithm for Chemical Reactions

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1 Introduction

- Chemical Reactions
- Atom-Mapping
- Approaches

2 Methodology

- Maximum Common Graph
- Optimization Method
- Data

3 Results

- Accuracy
- Comparison
- Errors

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- Chemical Reactions
- Atom-Mapping
- Approaches

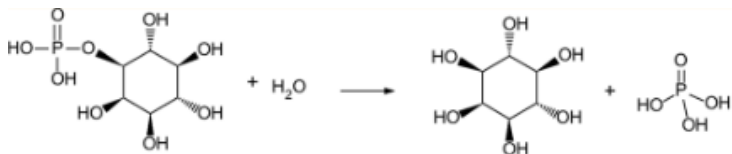
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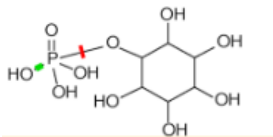
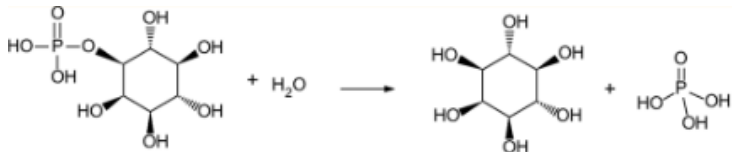
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Chemical Reactions



Chemical Reactions



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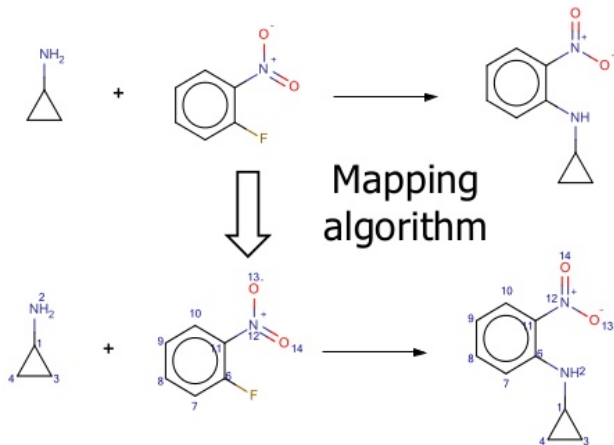
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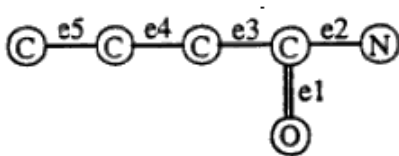
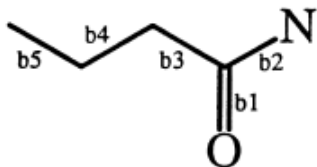
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Problem Definition



Graph representation



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- Maximum Common Subgraph

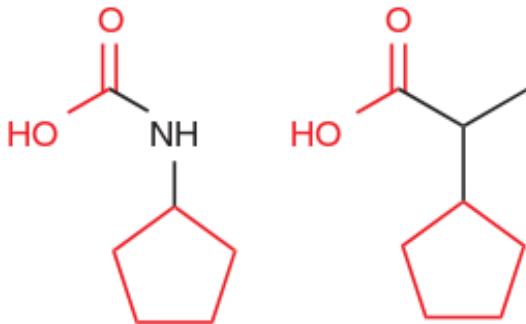
- Maximum Common Subgraph
- Maximum Common Edge Subgraph

- Maximum Common Subgraph
- Maximum Common Edge Subgraph
- Graph Isomorphism

- Maximum Common Subgraph
- Maximum Common Edge Subgraph
- Graph Isomorphism
- Optimization Problem

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Maximum Common Substructure



- Exact MCS with time limit (5 sec)
- Inexact MCS

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Matching remaining atoms

- Bipartite matching with cost function
 - Assignment of mapping costs according to a Reaction Rules database
 - Minimization of cost Mapping

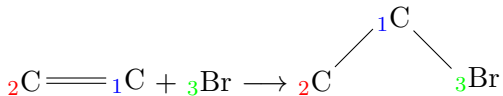
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- **SP05 set:**
 - SP05 test: 1000 reactions
 - SP05 training: 258595 reactions

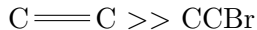
- **SP05 set:**
 - SP05 test: 1000 reactions
 - SP05 training: 258595 reactions
- **SP09 test:** 17996 reactions

Construction of the Reaction Rules database

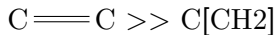
Reaction:



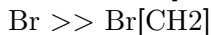
Reaction Rule for C¹:



Reaction Rule for C²:



Reaction Rule for Br³:



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Correctly Mapped **Reactions** with different algorithmic components

Algorithm	SP05_test (%)	SP09_test (%)
MCS only	78.2	89.7
Bipartite matching only	6.2	2.0
Combined	96.2	95.7

Correctly Mapped **Atoms** with different algorithmic components

Algorithm	SP05_test (%)	SP09_test (%)
MCS only	86.3	93.7
Bipartite matching only	49.8	44.9
Combined	99.4	98.8

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Comparison with other predictors

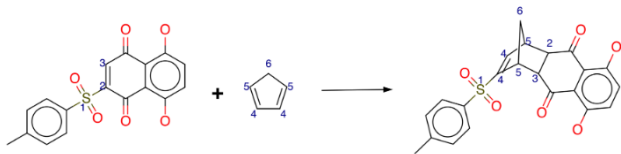
Algorithm	time per mapping (sec)	SP05_test (%)
ReactionMap	2	96.2
AutoMapper 5	0.03	60.7
AutoMapper 6.1	0.02	86.5
Dream	< 2	90.3

- **AutoMapper**: Search for isomorph subgraphs in reactant/product pairs
- **DREAM**: Edit-Distance Using Mixed Integer Linear Optimization

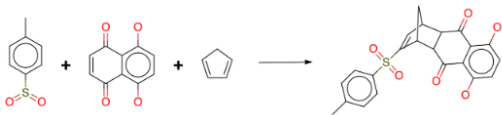
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Multi-step reactions

Incorrect mapping:



Correct Mapping:



- **Atom-Mapping** Problem approach
- Combination of **MCS and Optimization**
- **Superior** than previous techniques based on either MCS or Optimization.



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