



UNIVERSITY  
OF TRENTO - Italy  
Department of Information  
Engineering and Computer Science

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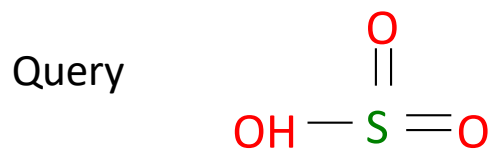
YAHOO!  
LABS

# Graph Query Reformulation with Diversity

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Francesco Bonchi, Yahoo Labs - Francesco Gullo, Yahoo Labs

# Pattern search



PubChem  
Compound

PubChem Compound

[Save search](#) [Limits](#) [Advanced](#)

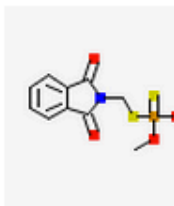
[Display Settings:](#)  Summary, 20 per page, Sorted by Default order

[Send to:](#)

Results: 1 to 20 of **510**

<< First < Prev Page  of 49 [Next >](#) [Last >>](#)

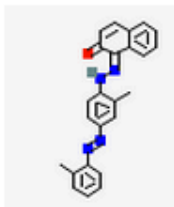
1.



- Too many matches
- Results are not grouped

[PubMed \(MeSH Keyword\)](#)

2.



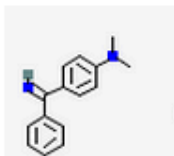
IUPAC name: (1Z)-1-[[[2-methoxy-4-[[2-methoxyphenyl]diazenyl]phenyl]hydrazinyl]...

Create Date: 2005-09-09

CID: 5876571

[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [PubMed \(MeSH Keyword\)](#) [Active in 7 of 209 BioAssays](#)

3.



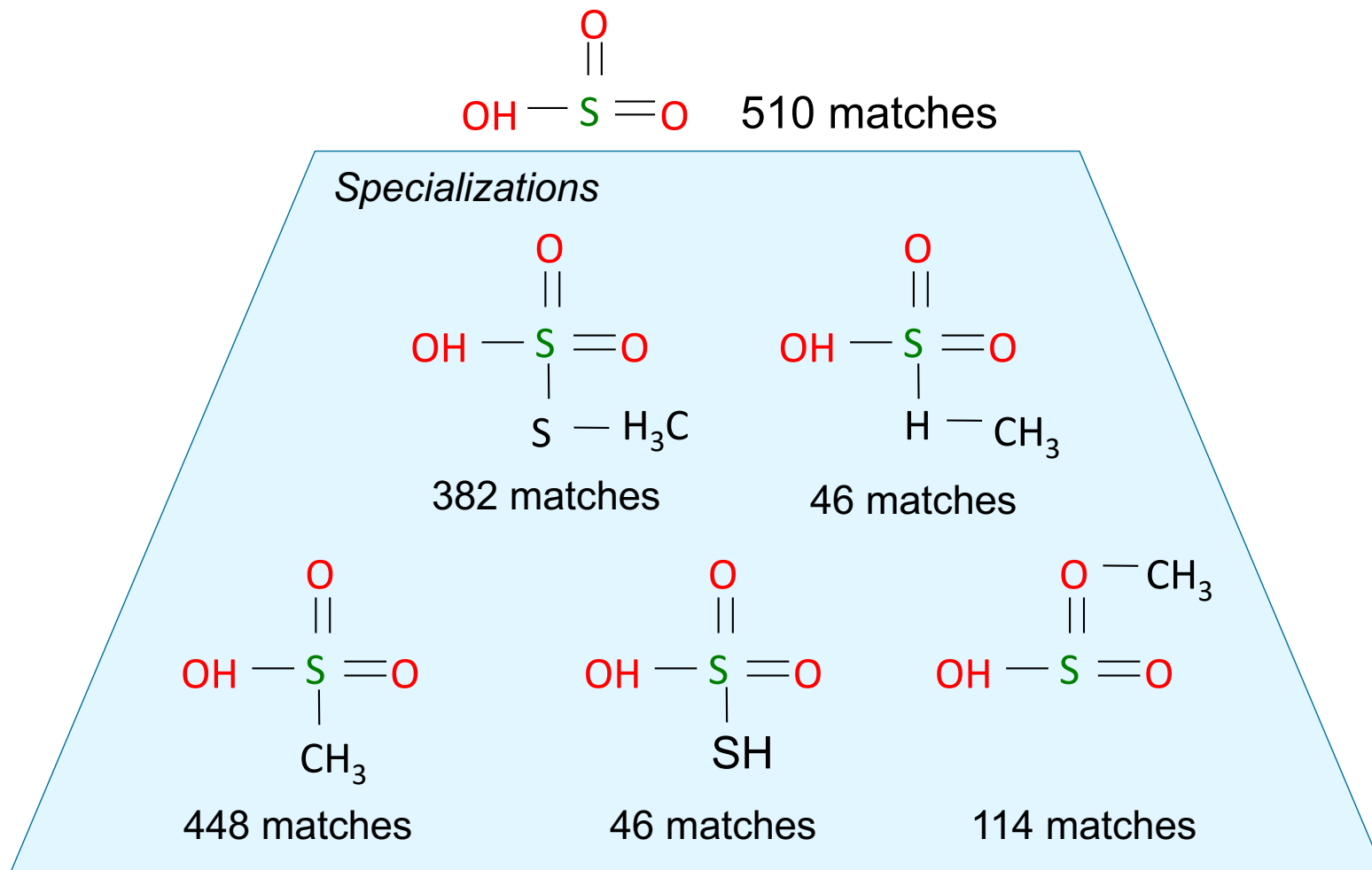
[Basic Yellow 2: Auramine O: Auramin ...](#)

MW: 303.829680 g/mol MF: C<sub>17</sub>H<sub>22</sub>ClN<sub>3</sub>

IUPAC name: 4-[4-(dimethylamino)benzenecarboximidoyl]-N,N-dimethylanilin...

Create Date: 2005-08-08

# Finding specializations



# Applications

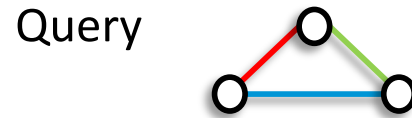
- Finding groups of molecules having a particular reagent
- Analyze a set of proteins to find diseases
- Workflow optimization
- Anomalies detection in a network
- Finding similar 3D shape search

# Dealing with specializations in web and relational data

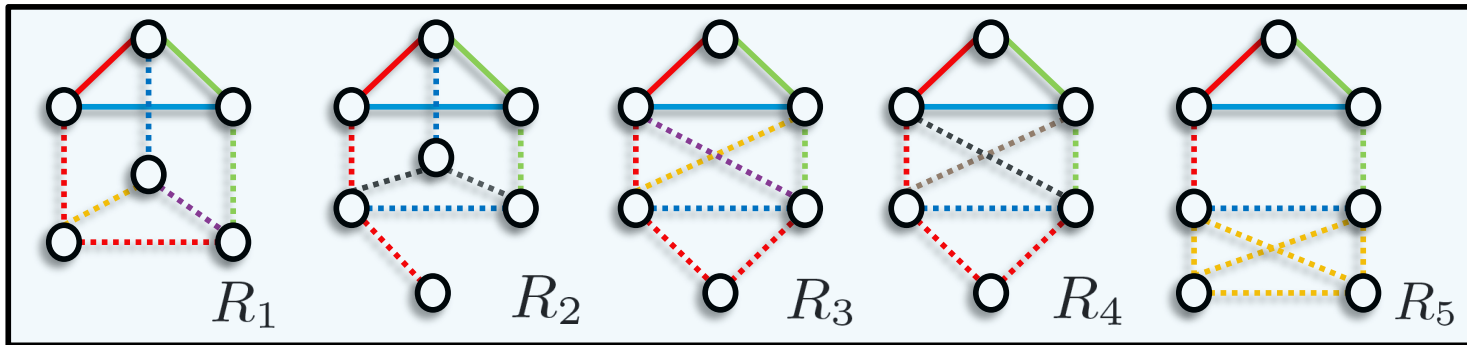
- Faceted Search
  - present aspects of the results [Roy08]
- **Query reformulation**
  - Modify some of the query conditions
    - In structured databases [Mishra09]
    - In web search [Dang10]

## Frist Study of Problem on GRAPHS

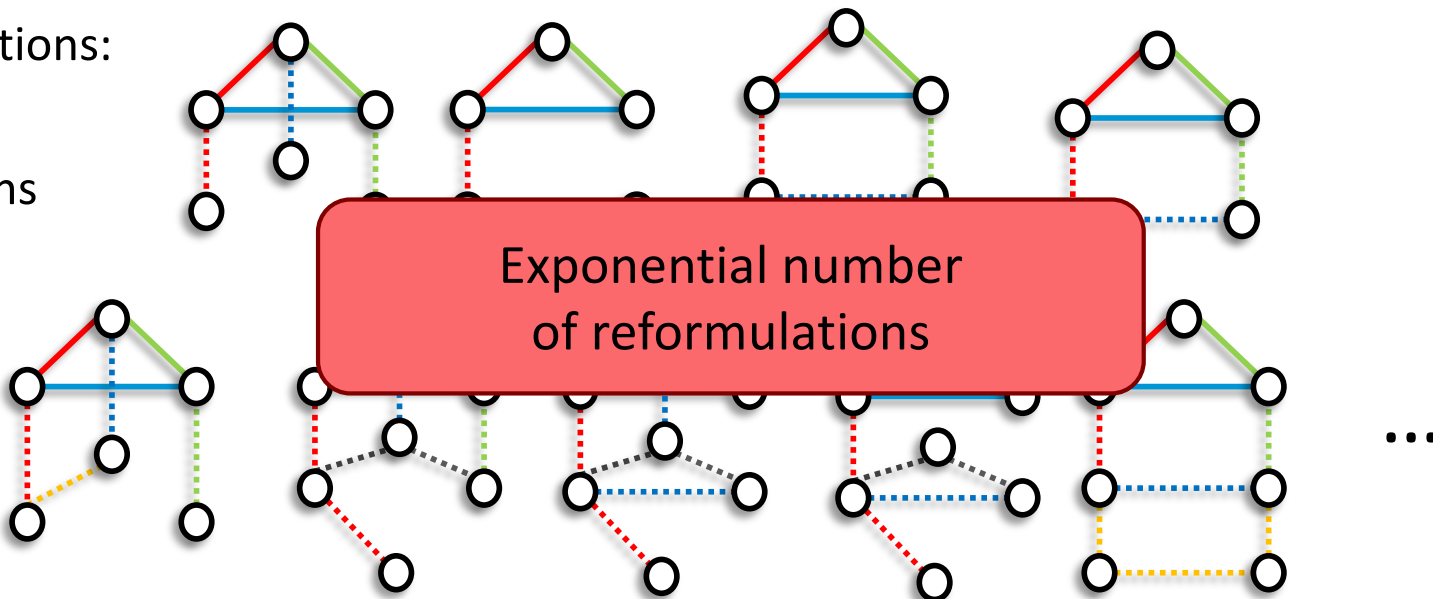
# Graph Query Reformulation



Results



Reformulations:  
query  
supergraphs



# Challenges

- The number of reformulation is exponential
- Quantify the interestingness of a reformulation
- Finding query reformulations is **NP**-complete

# Our Approach

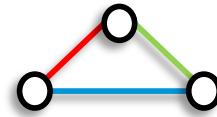
## Graph Query Reformulation with Diversity

- Finds  $k$  *meaningful* specializations efficiently



# Finding Meaningful Specializations

Query



Results

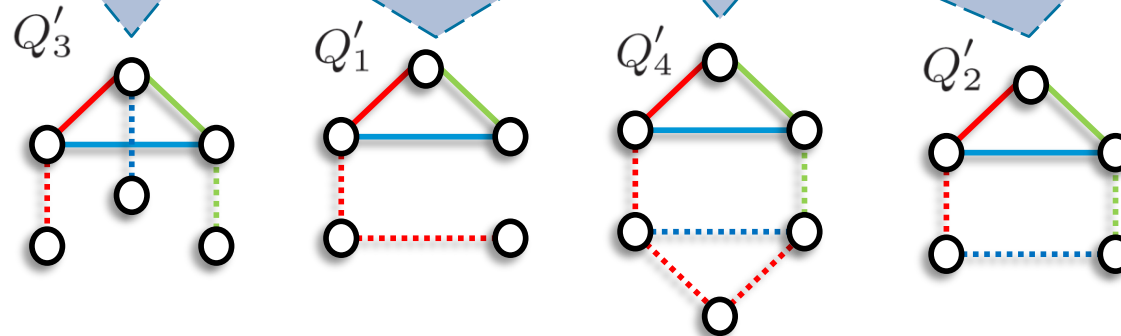
Find **k** meaningful specializations:

1. Span **all** the results
2. Present **different** aspects of the results

?

$cov(Q)$

$Q''$



# Graph Query Reformulation with Diversity

## Problem

Find a set  $\mathcal{Q}^*$  of  $k$  specializations of  $Q$  that maximize a combination of **coverage** and **diversity**

$$f(\mathcal{Q}) = cov(\mathcal{Q}) + \lambda \sum_{Q', Q'' \in \mathcal{Q}} div(Q', Q'')$$

$$\mathcal{Q}^* = \arg \max_{\mathcal{Q} \subseteq \mathcal{S}_Q} f(\mathcal{Q})$$

$$\text{subject to } |\mathcal{Q}| = k.$$

## Theorem (NP-hardness)

The problem reduces to **MAX-SUM Diversification** Problem, so it is NP-hard

# Solution: Greedy Algorithm

## Greedy

While k-specializations are not found

1. Find the specialization leading to the maximum increment of the objective function (marginal gain)
2. Add the specialization to the results

### Theorem

The algorithm is a  $\frac{1}{2}$ -approximation

Finding the maximum gain is #P-complete [Valiant79]

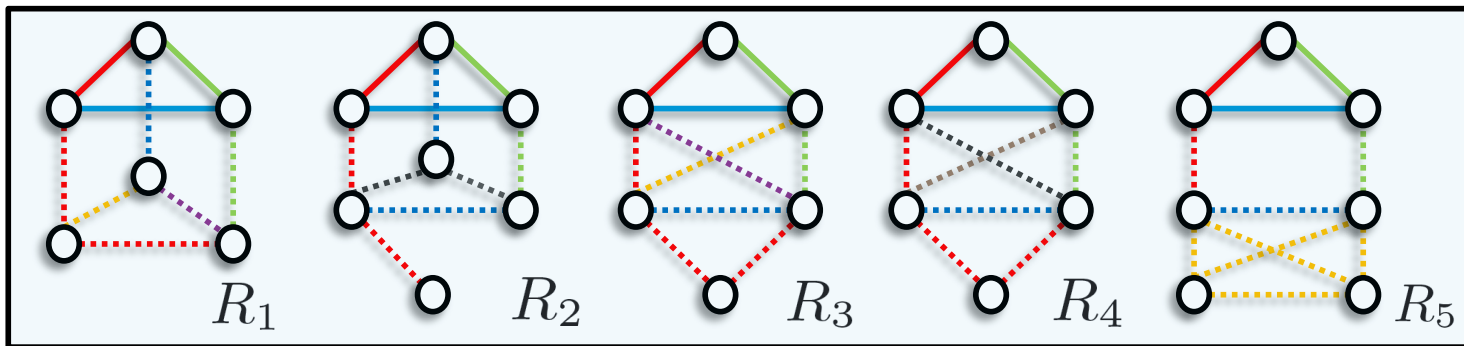
### Solution

**Fast\_MMPG:** Branch and bound algorithm with quality guarantees

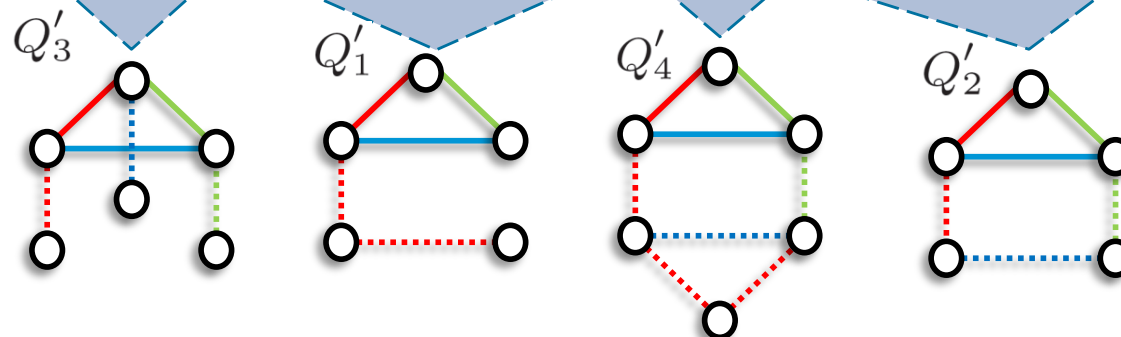
# The multiplicity vector

2	3	3	3	1
---	---	---	---	---

Results



Output set of specializations



# Upper bound on the Marginal gain

## Lemma

The marginal gain increases if the multiplicity of the considered item is  $\leq \frac{|Q|}{|Q|}$  where  $|Q|$  is the number of reformulations in the reformulated set constructed so far.

**Upper bound** : is the value of the objective function considering only results with multiplicity  $\leq \frac{|Q|}{2}$

## Theorem

For a reformulation  $Q' \in \mathcal{S} \setminus Q$  it holds that

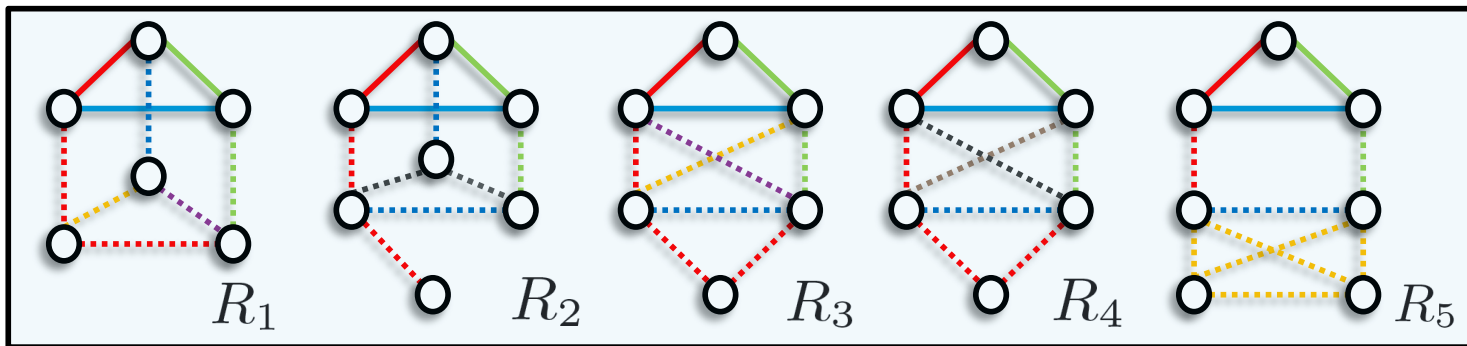
$$\begin{aligned} \max_{Q'' \in \mathcal{T}_{Q'}} \Delta_f(Q, Q'') &\leq \overline{\Delta}_f(Q, Q') = \\ &= \frac{1}{2} \vec{u}_Q \cdot \vec{x}_{Q^*} + \lambda (\|\vec{m}_Q\| + |Q| \times \|\vec{x}_{Q^*}\| - 2\vec{m}_Q \cdot \vec{x}_{Q^*}). \end{aligned}$$

# Upper bound

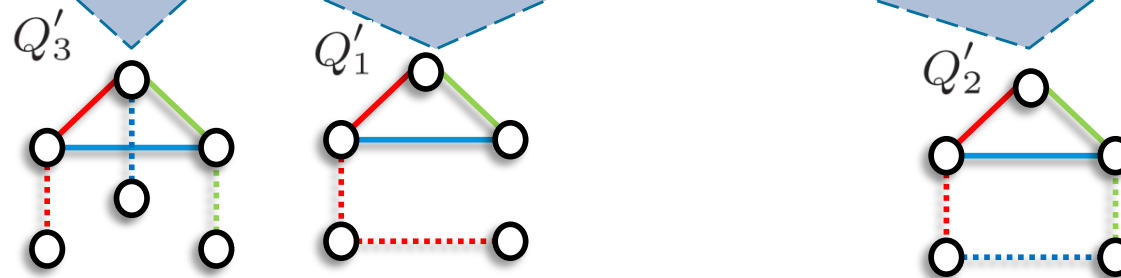
$$\leq \frac{|Q|}{2}$$



Results

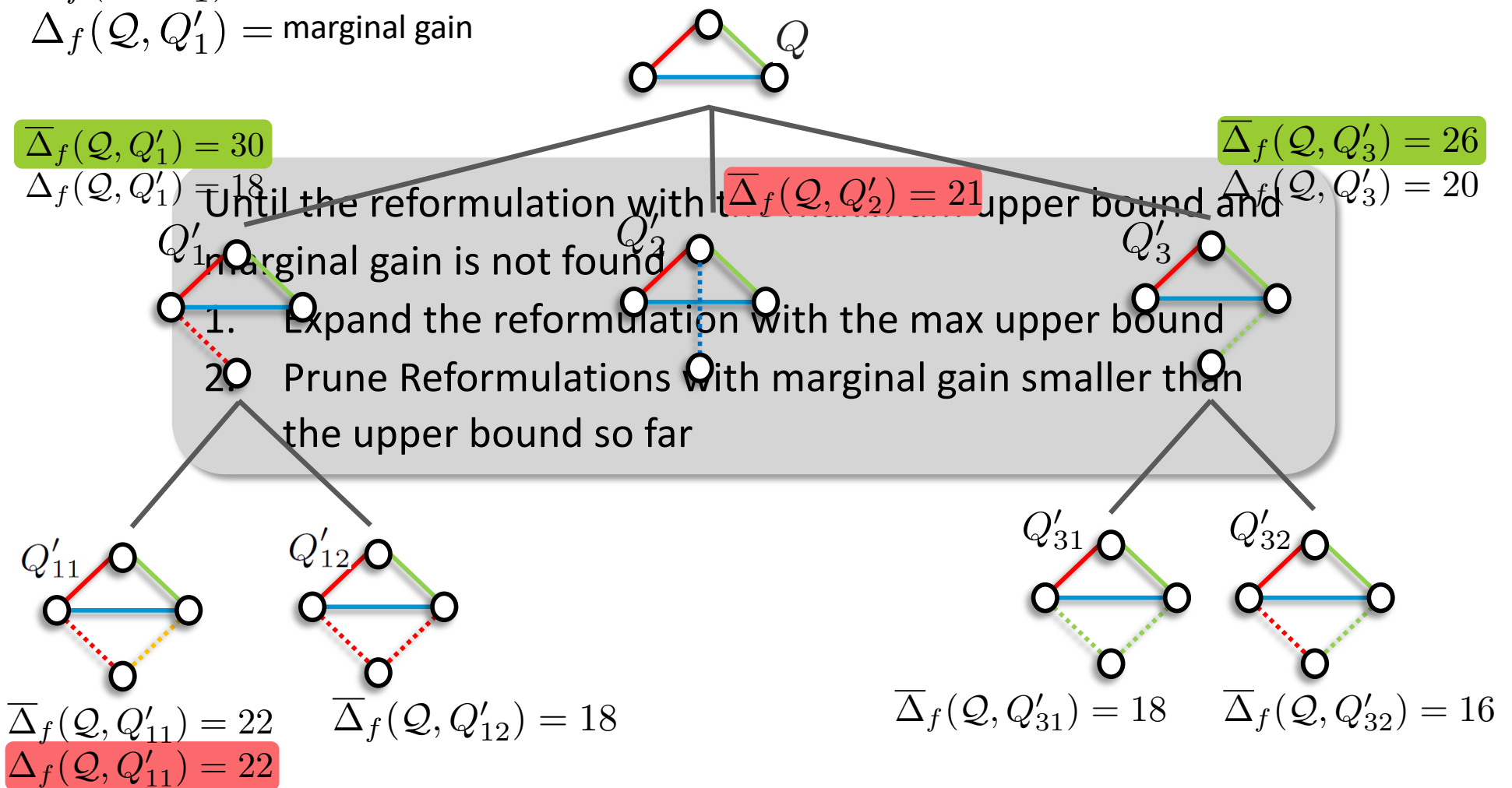


Output set of reformulations



# The Fast\_MMPG Algorithm

$\bar{\Delta}_f(Q, Q'_1) = \text{upper bound}$   
 $\Delta_f(Q, Q'_1) = \text{marginal gain}$



# Experimental Setup

- **Datasets:**

- AIDS: 10k chemical compounds
- Financial: 17k transaction workflows
- Web: 13k interactions with a recommender system

- **Baseline algorithms:**

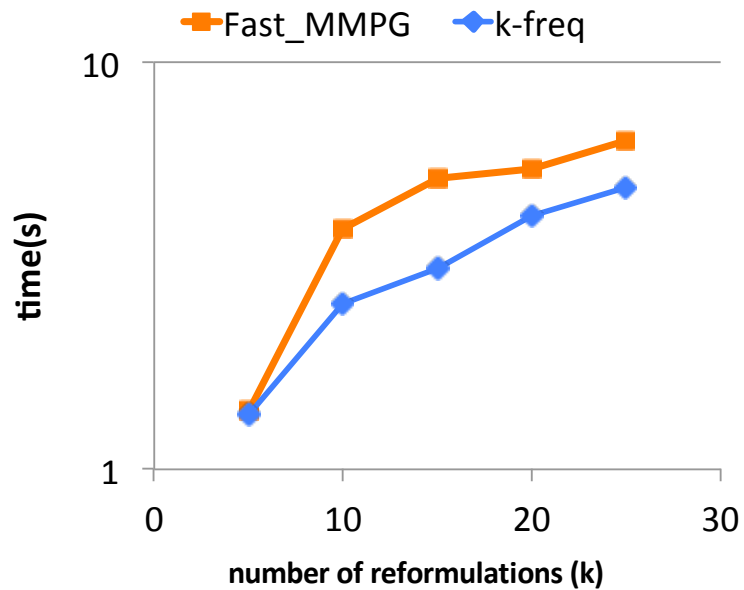
- k-freq: returns top-k frequent supergraphs of a query
- LIndex: informative patterns index

- **Experiments:**

- Time and objective function value varying k, query size,  $\lambda$
- Anecdotal
- Scalability

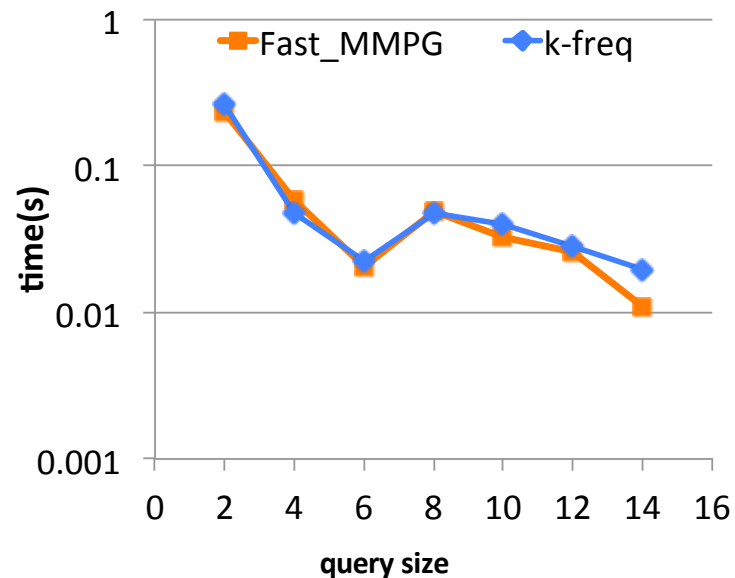


# Time Comparison



## Number of reformulations

1. k-freq runs only slightly faster
2. Time increases linearly in k
3. Fast\_MMPG has real-time performance



## Query size

1. Fast\_MMPG comparable to k-freq
2. Time decreases with query size (less reformulations)

# Objective function gain

	$\lambda$				
	0	0.01	0.05	0.1	0.5
Fast_MMPG	433	613	1 345	2 260	9 566
k-freq	409	540	1 063	1718	6 954
<i>gain (%)</i>	6	12	21	24	27

## Analysis

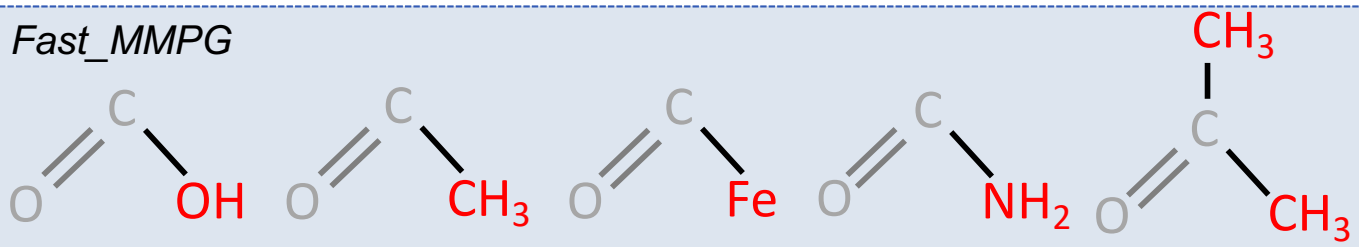
1. Lambda correctly moves the objective function towards diversity
2. k-freq only captures coverage

$$f(\mathcal{Q}) = cov(\mathcal{Q}) + \lambda \sum_{Q', Q'' \in \mathcal{Q}} div(Q', Q'')$$

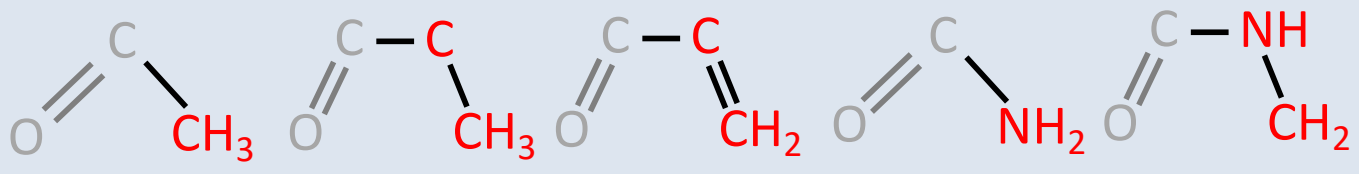
# Qualitative evaluation

Query  $C=O$

*Fast\_MMPG*



*k-freq*

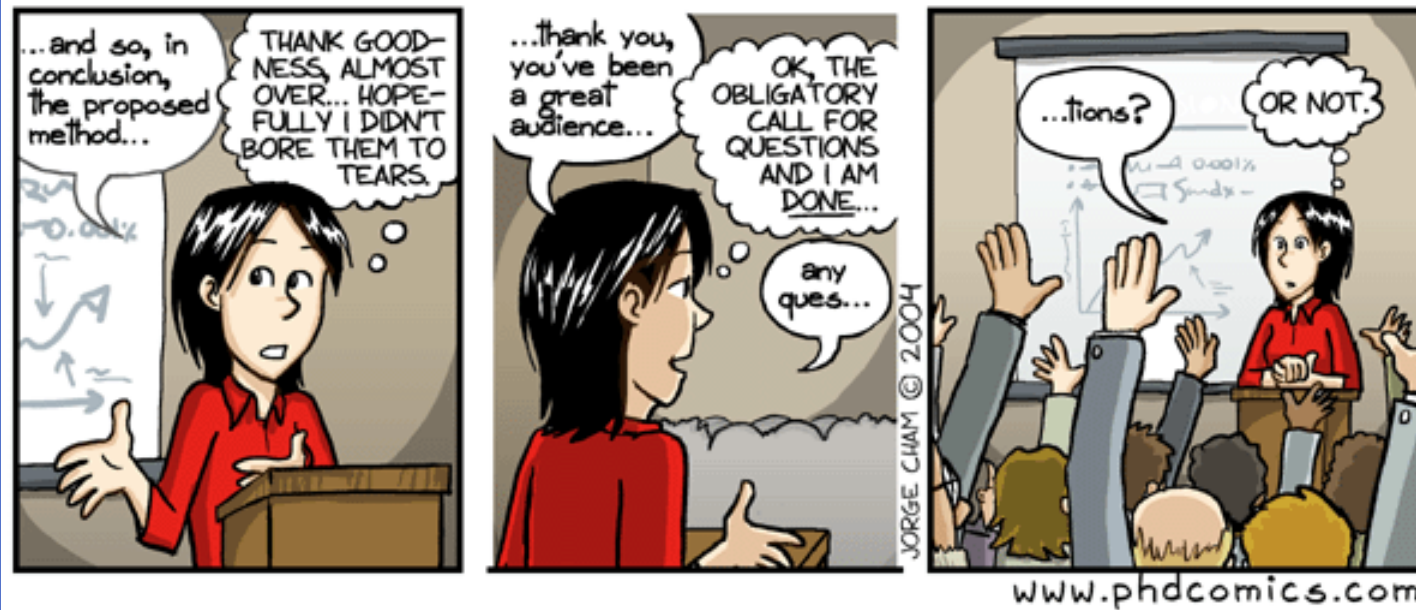


## Analysis

- k-freq finds reformulation of the same superquery
- Fast\_MMPG returns reformulations with more diversified structures

# Conclusions

- First study of the problem in **graph databases**
- **Principled** objective function optimizing **coverage** and **diversity**
- Algorithmic solutions **with quality guarantees** and **real time responses**



Thank you!  
**Questions?**