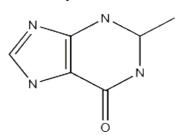
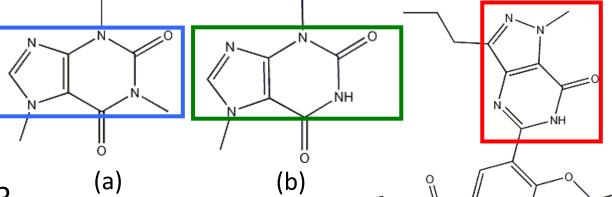


## Application II: Support Substructure Similarity Search

- ☐ Find graphs in a graph DB containing substructures similar to a given query graph
- Ex. Data: A chemical compound DB
  - A query graph q:





(c)

- How to do similarity search efficiently?
  - No indexing? Sequential scan + computing subgraph similarity – too costly!
  - Build graph indices to support approximate search?
    - Need an explosive number of subgraphs to cover all the similar subgraphs!
- ☐ An elegant solution (Yan, Yu, & Han, SIGMOD'05):
  - Keep the graph index structure, but select features in the query space

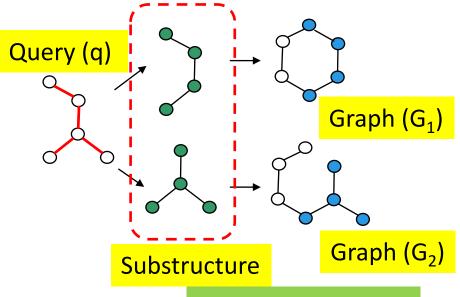
## Feature-Based Similarity Search

- Decompose a query graph into a set of features
- Feature-based similarity measure
  - Each graph is represented as a feature vector  $X = \{x_1, x_2, ..., x_n\}$
  - Similarity is defined by the distance of their corresponding vectors
- If graph G contains the major part of a query graph q,
  G should share a number of common features with q
  - Given a relaxation ratio, one can calculate the maximal number of features that can be missed!

Assume: Query graph has 5 features

Relaxation threshold: Can miss at most 2 features

Then: G<sub>1</sub>, G<sub>2</sub>, G<sub>3</sub> are pruned



## **Graphs in database**

	$G_1$	$G_2$	$G_3$	$G_4$	$G_5$
$f_1$	0	1	0	1	1
f <sub>2</sub>	0	1	0	0	1
$f_3$	1	0	1	1	1
f <sub>4</sub>	1	0	0	0	1
$f_5$	0	0	1	1	0

