

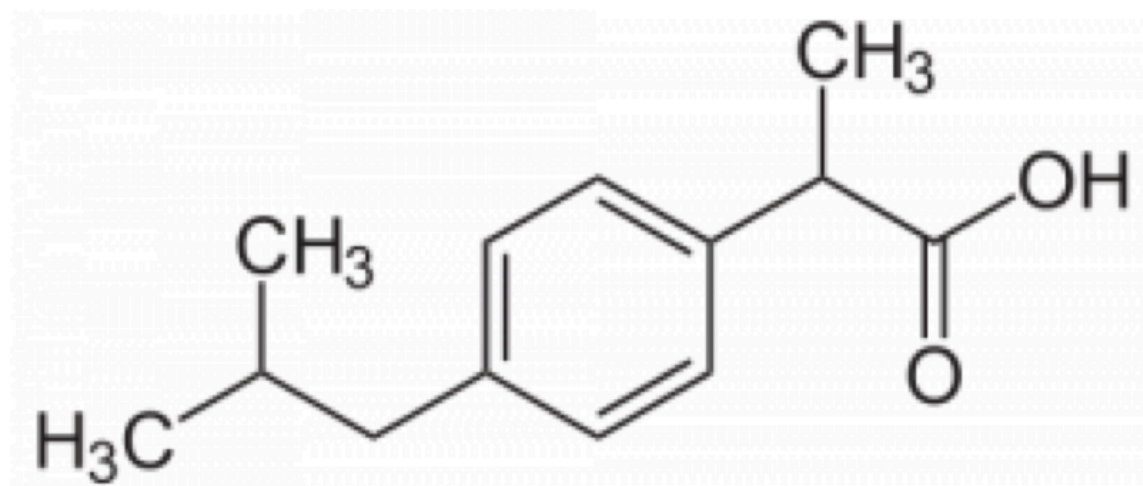
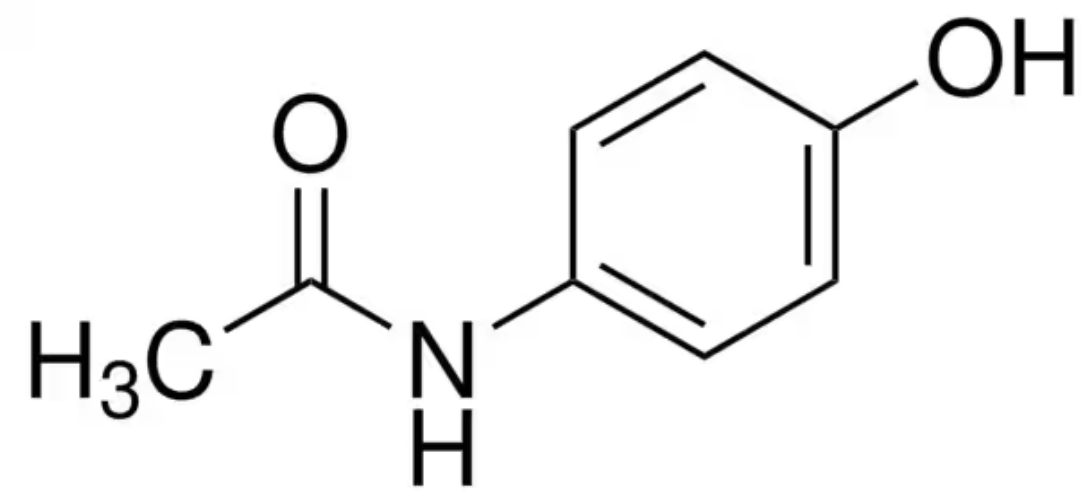
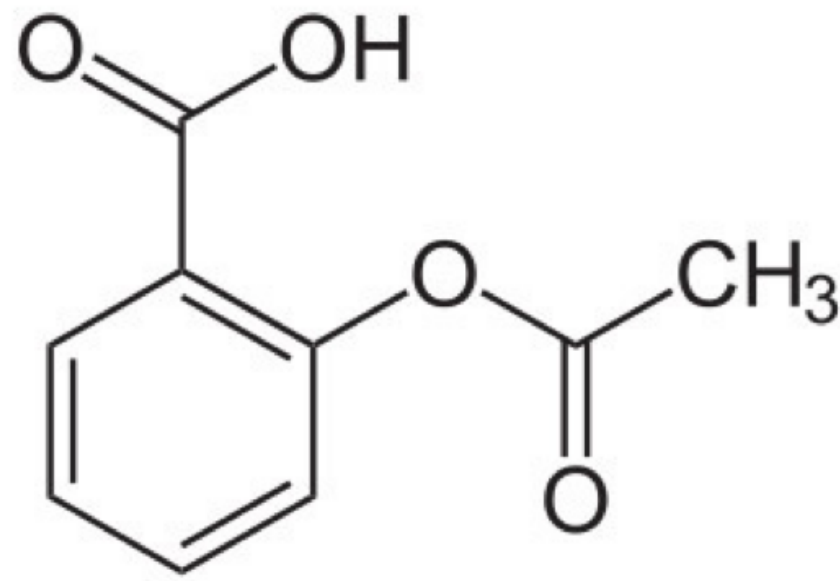
Inter-molecular Graph Pathfinder

**[Interactive Graph Mining]
Graph Mining Project Proposal**

성균관대학교 소프트웨어학과 김산
2023. 10. 11. 수요일.

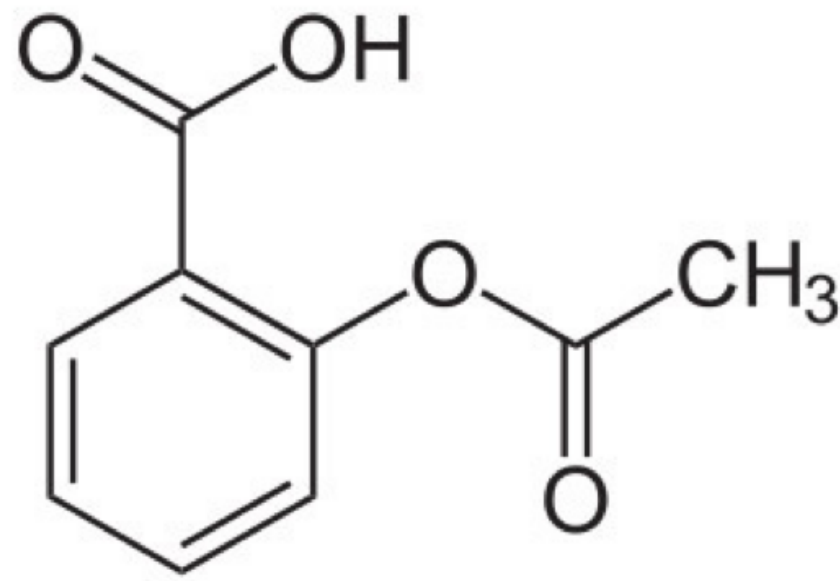
Introduction

Pharmaceutics :: 제약

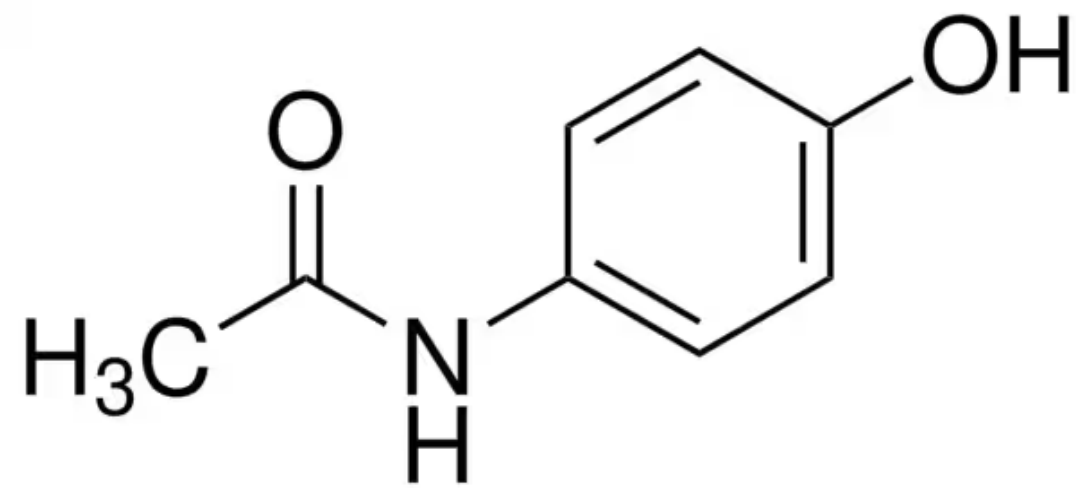


Introduction

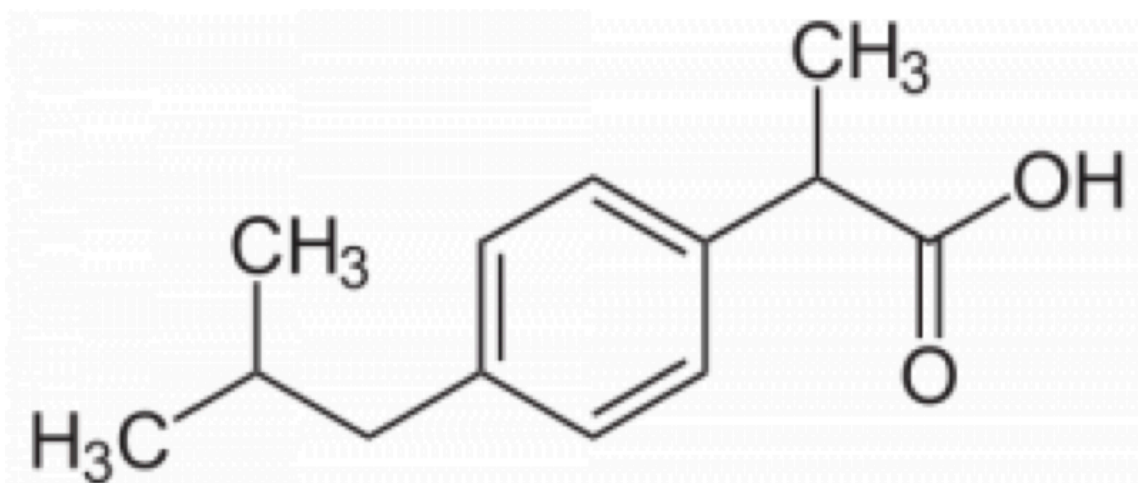
Pharmaceutics :: 제약



Acetylsalicylic acid



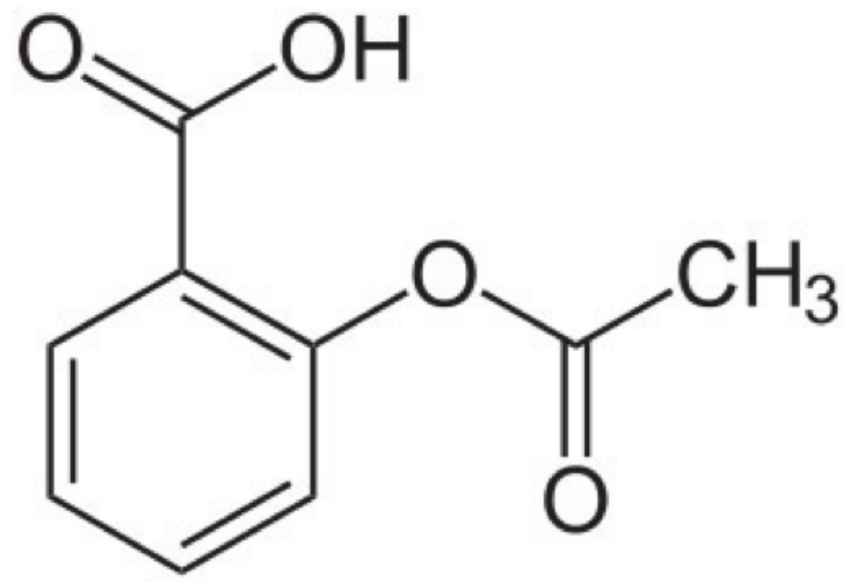
Acetaminophen



Ibuprofen

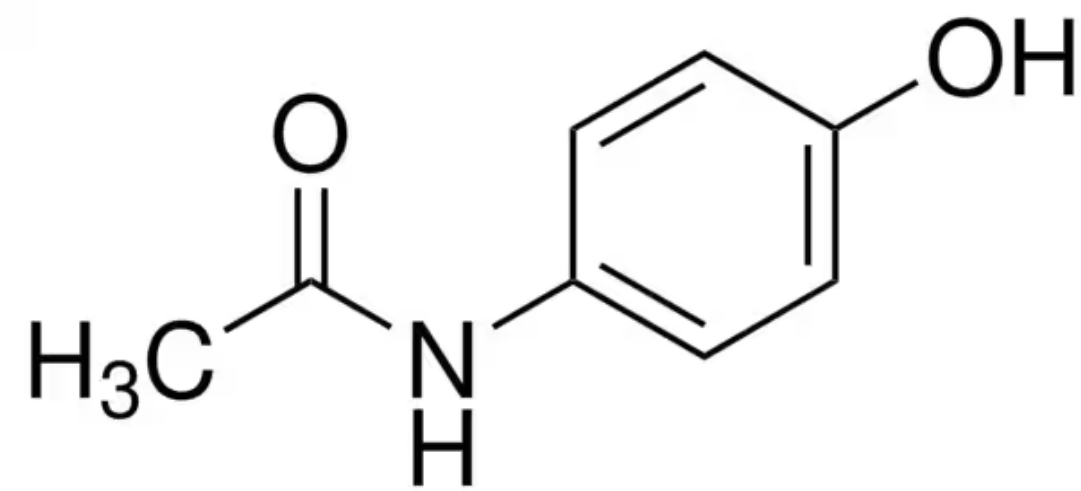
Introduction

Pharmaceutics :: 제약



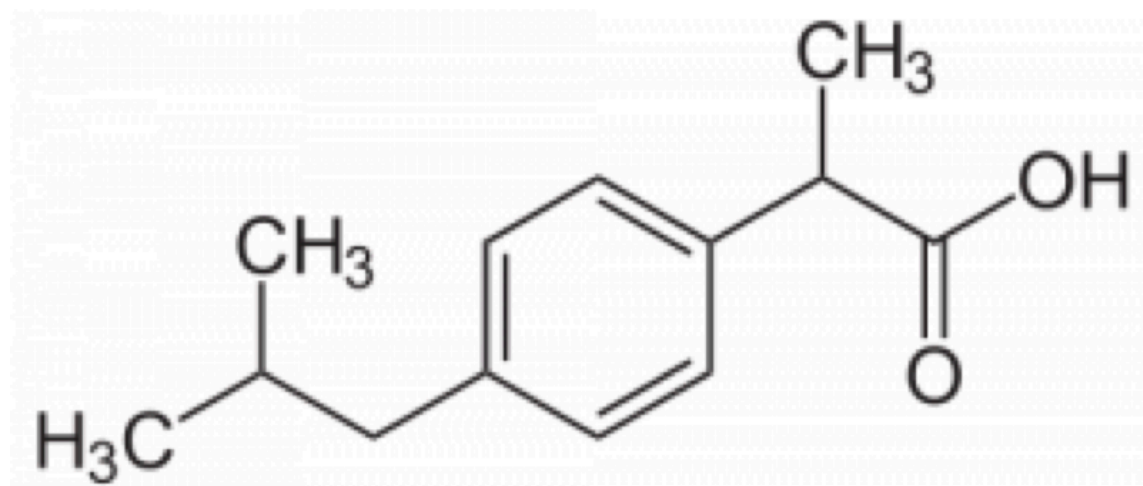
Acetylsalicylic acid

아세틸살리실산



Acetaminophen

아세트아미노펜

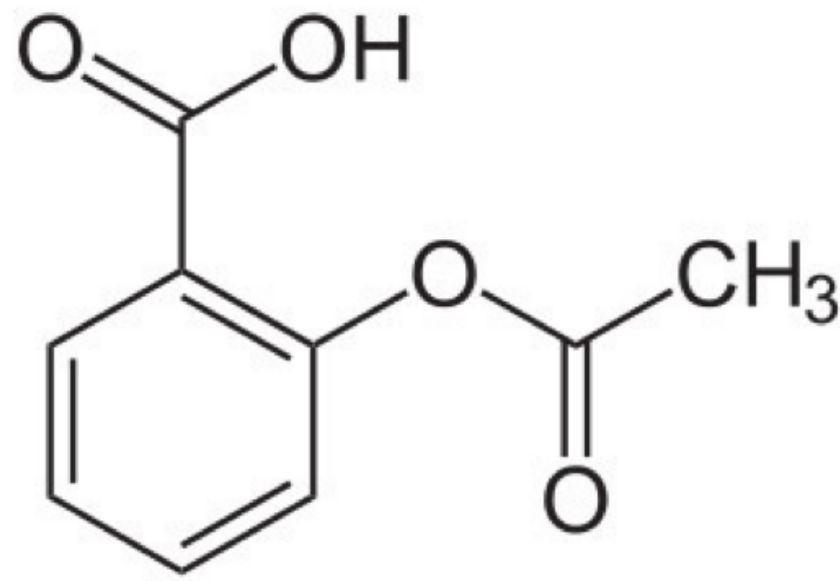


Ibuprofen

이부프로펜

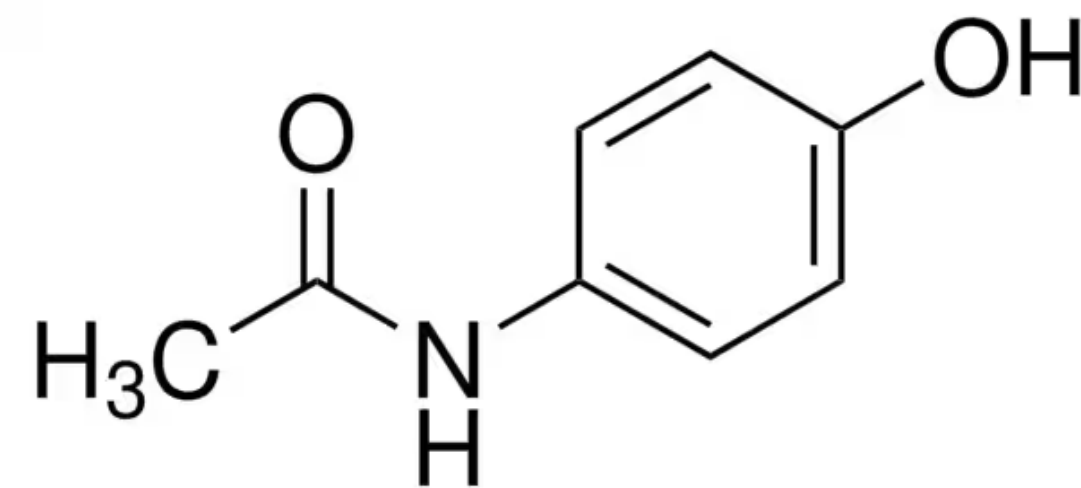
Introduction

Pharmaceutics :: 제약



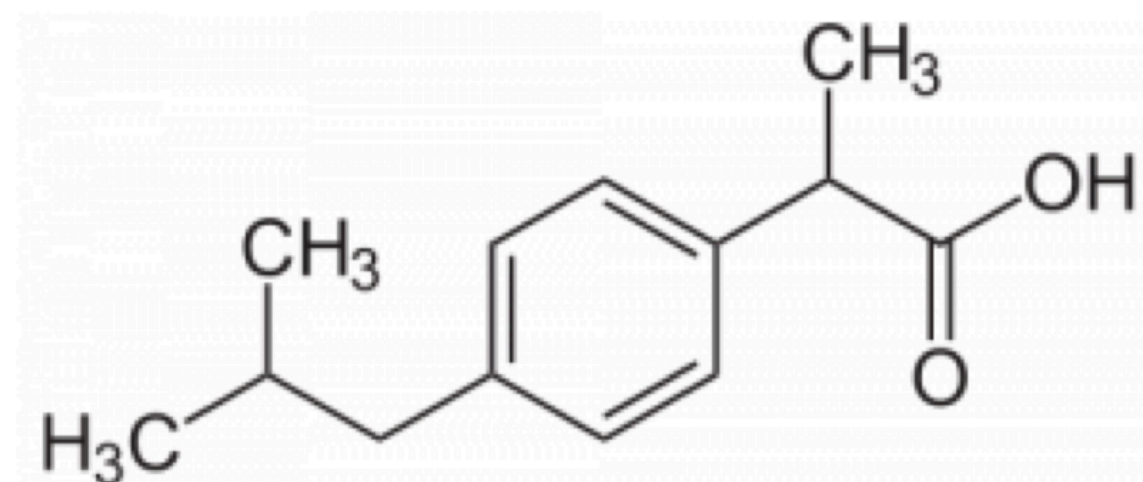
Acetylsalicylic acid

아세틸살리실산



Acetaminophen

아세트아미노펜



Ibuprofen

이부프로펜



Motivation

어떻게 chemical graphlet들을 찾을 수 있을까?

- **Molecular graph**

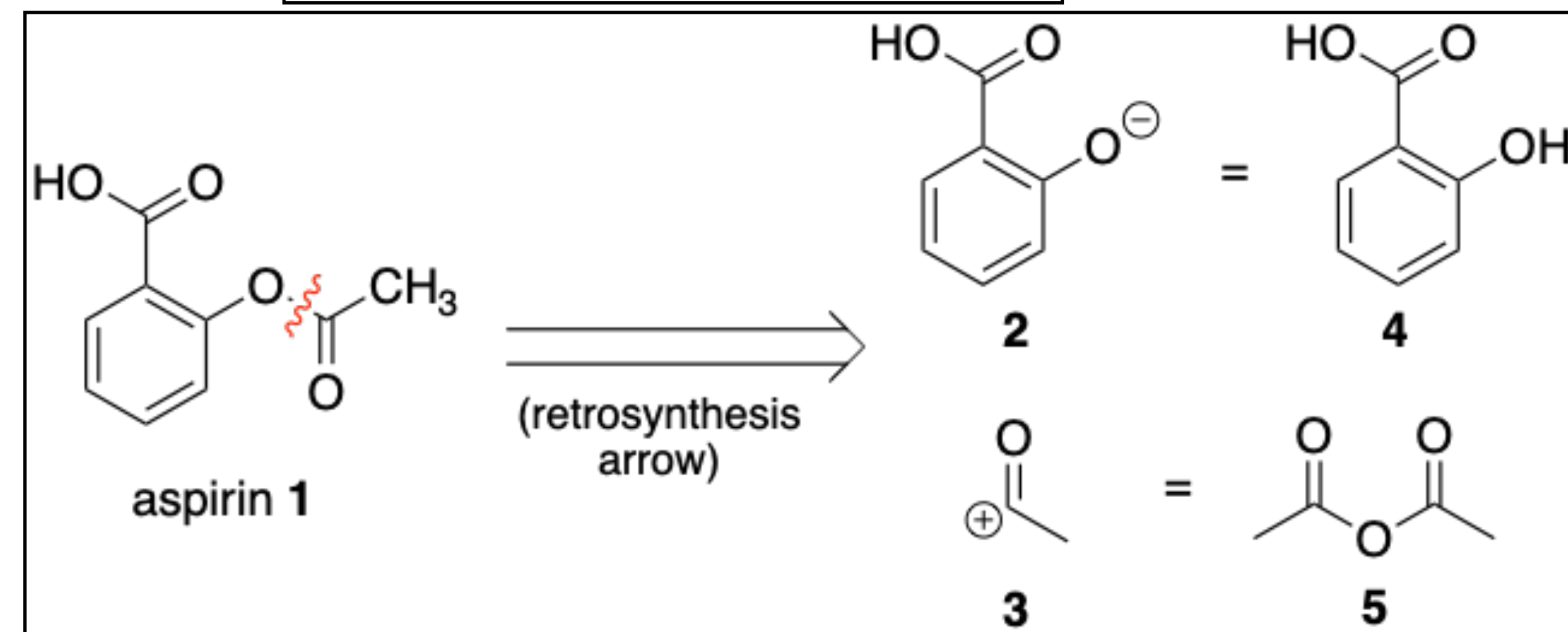
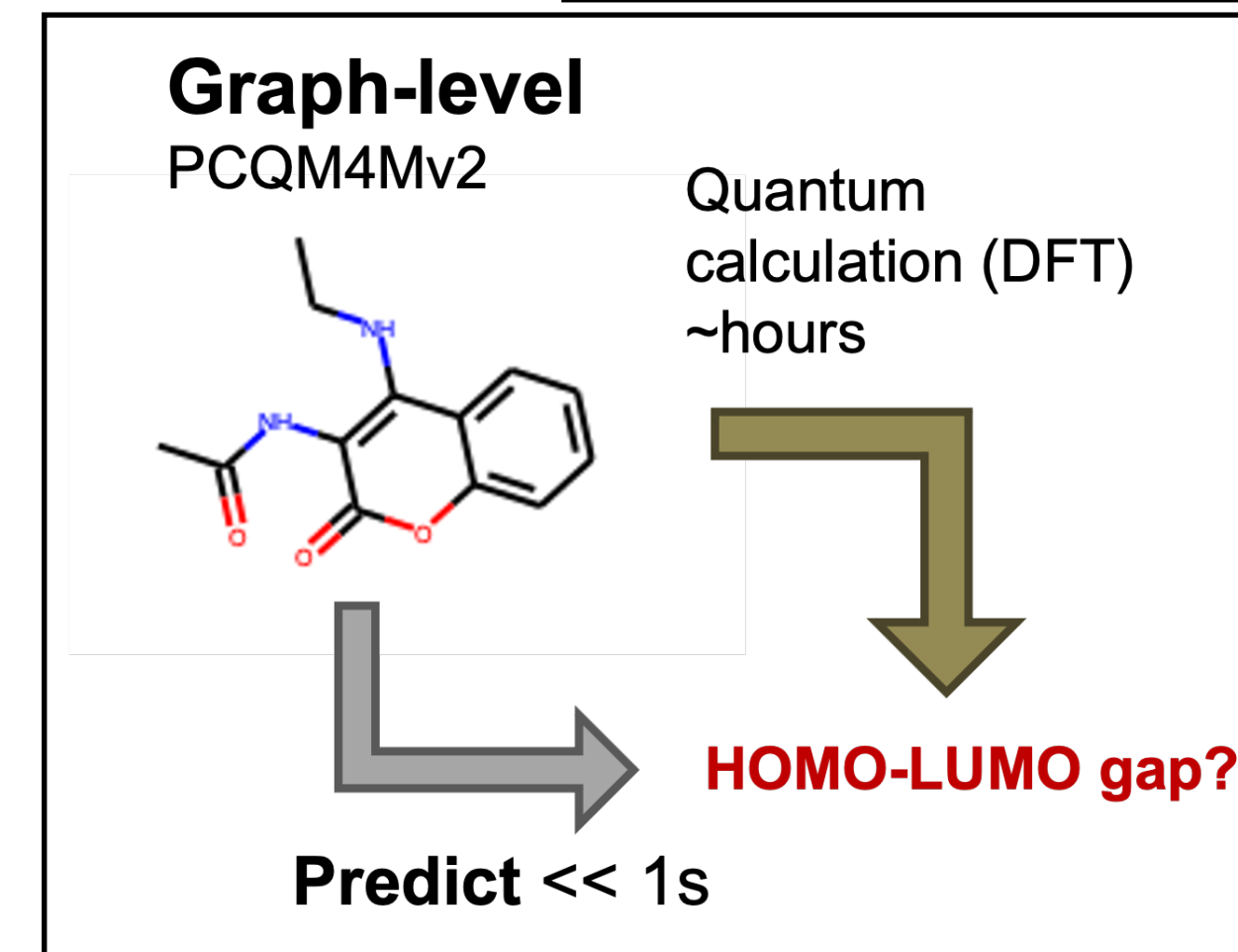
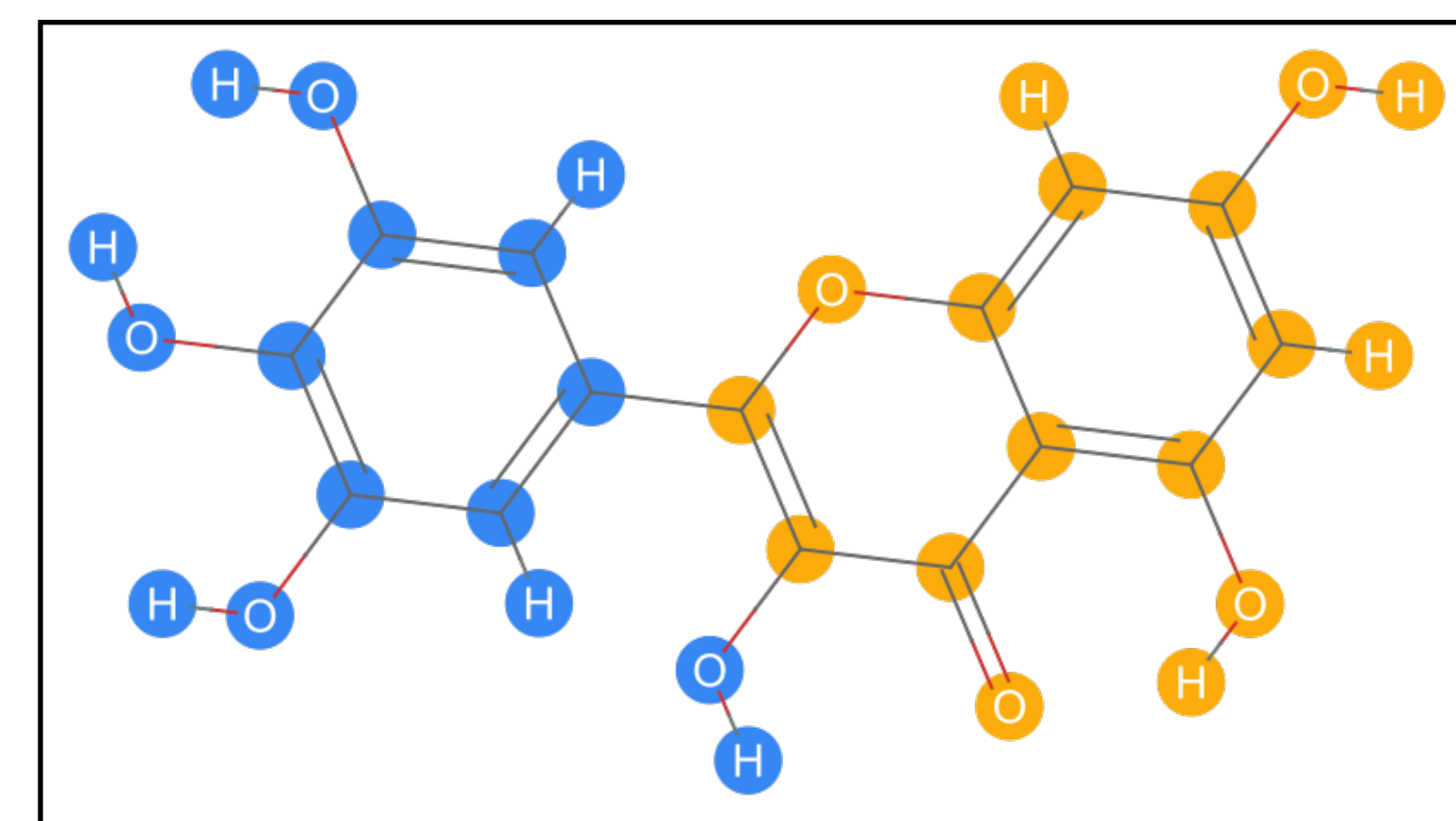
- Node = atom + atomic feature
- Edge = bond + bond feature

- **작용기 (Functional group)**

- Graphlets, Inter-molecular feature

- **역합성 (Retrosynthesis)**

- 제약, 화학공학



Dataset

QM7 dataset → Inter-molecular graph

- Quantum Machines 9 (QM9) dataset

- Nodes
 - Atoms
- Edges
 - Molecular bonds
(Valence Shell Electron Pair Repulsion theory based)
- # of graphs
 - 7165 graphs(= molecules)
 - MAX 23 nodes(= atoms) per graph
 - MAX 7 heavy atoms per graph

- Inter-molecular graph

- Nodes
 - Molecules
- Edges
 - **Subgraph relations ($\Delta_{\text{atom}} = 1$)**
- 1 large graph
 - 7165 nodes(= molecules)

Purpose

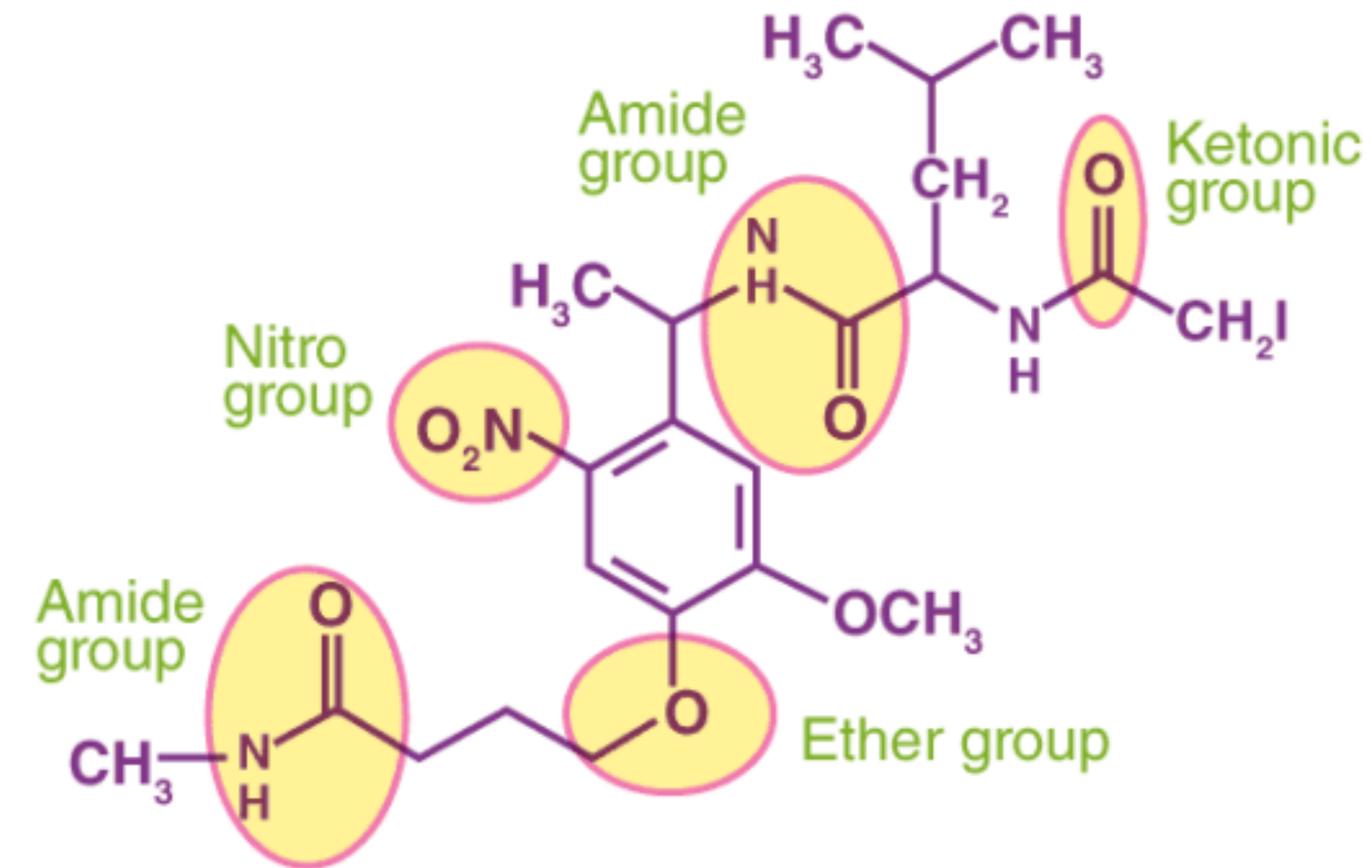
Reveal undefined functional groups

- 작용기 확인하기

- Functional group은 화학적으로 안정하면서도
- 자주 나타나기 때문에 molecular graph의 edge feature를 수집해 발견할 수 있음

- 작용기를 분류하기 :: Inter-molecular feature

- 기존에 알려진 작용기들과 비슷한 빈도로 등장하면서
- 특별한 기능으로 명명되지 않았던 작용기를 계층적으로 분류해 inter-molecular feature로 사용할 수 있음



Method

Sample pathways from Eigen-central nodes

- **Inter-molecular graph**의 Eigenvector-centrality 계산
 - 주요 backbone 분자구조 indentify
 - 모든 path를 계산하는건 computational/physical 문제가 있기 때문에 중심노드 선정
- **Path 정보 수집**
 - Eigenvector-center로 부터 커지는 방향으로 원자들을 붙여나가면서 지나가는 edge 정보 수집
- **Path dataset 분석**
 - Hierarchical clustering을 통해 자주 등장하는 path를 hierarchical 분류

Expected Result & Conclusion

Hierarchical clustering of functional groups

- 예상 결과
 - **Inter-molecular graph**를 정의하고 구축
 - Chemical path를 hierarchical clustering
 - 기존에 알려진 작용기와 비교 분석
- 의의
 - **Inter-molecular** feature를 **graph** mining 기법으로 발견하려는 시도
 - Path를 역으로 밟아 retrosynthesis software에 응용 가능

