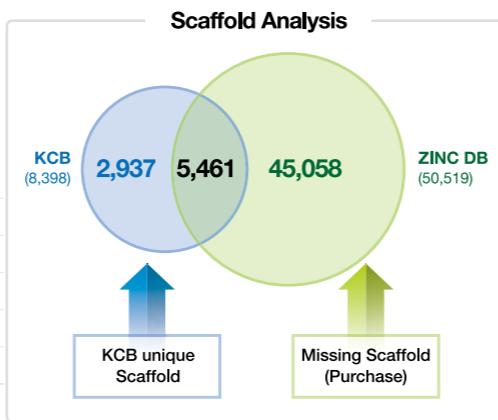
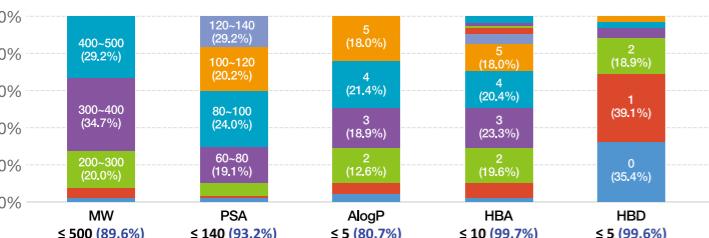


# 09. Diverse Chemical Libraries for Hit Identification

유효물질 검색을 위한 화합물 라이브러리

## Diversity of KCB compound library

ZINC DB (35M compounds): classified to 50,519 scaffolds  
 KCB DB (0.34 compounds): classified to 8,398 scaffolds  
 KCB unique scaffolds: 2,937 Drug-Likeness and Physico-chemical properties of KCB library

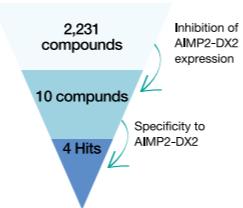


## Library types served by KCB

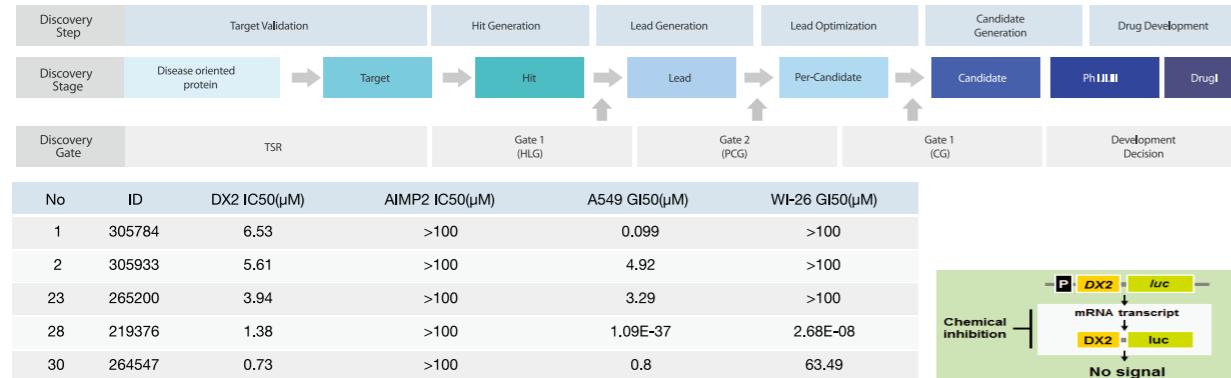
Library	No of compounds
Total Library	340,000
Diversity Set	8,400
Clinical Collection Set	2,300
Kinase Library	3,200
Fragment Library	1,000
Natural Product	1,200
PharmaCore collection	As requested
GPCR, PPI Library	On preparation

## DX2 hits from libraries & optimization

**763 DR Libraries**  
**DX2 luciferase**  
**AIMP2 luciferase**  
**Cell viability**  
**30 hits**  
**IC50 on DX2, AIMP2**  
**GI50 on A549, WI-26**  
**5 leads**



## Decision gate

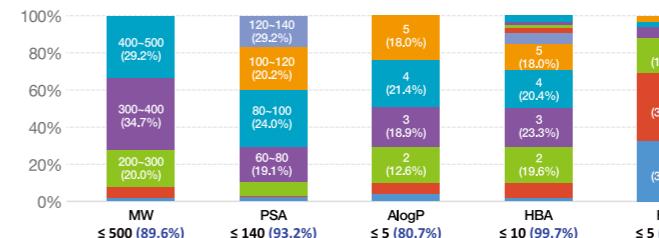


## Publication / Patents

- Leei et al. Biochemical J. 454:411-416, 2013
- Novel maleic acid derivatives, preparation method thereof, and anti-cancer compositions containing them, PCT/KR2014/004933

## 한국 화합물 은행의 다양성

가상 데이터베이스 (350만종): 50,519 골격 구조 한국화합물은행 (34만종): 8,398 골격구조 한국화합물은행 고유의 독창적 구조: 2,937 골격구조 한국화합물은행 화합물의 약물성 분석

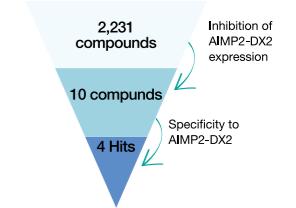


## 한국화합물은행의 라이브러리 분류

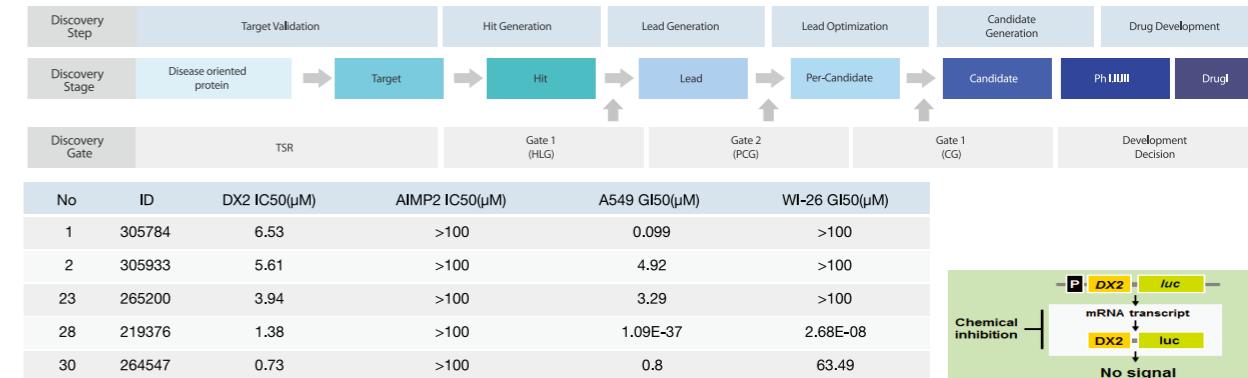
Library	No of compounds
Total Library	340,000
Diversity Set	8,400
Clinical Collection Set	2,300
Kinase Library	3,200
Fragment Library	1,000
Natural Product	1,200
PharmaCore collection	As requested
GPCR, PPI Library	On preparation

## 라이브러리에서 히트발굴 및 최적화

**763 DR Libraries**  
**DX2 luciferase**  
**AIMP2 luciferase**  
**Cell viability**  
**30 hits**  
**IC50 on DX2, AIMP2**  
**GI50 on A549, WI-26**  
**5 leads**



## 신약개발 관문



## 논문 / 특허

- Leei et al. Biochemical J. 454:411-416, 2013
- 말레인산 유도체 PCT/KR2014/004933