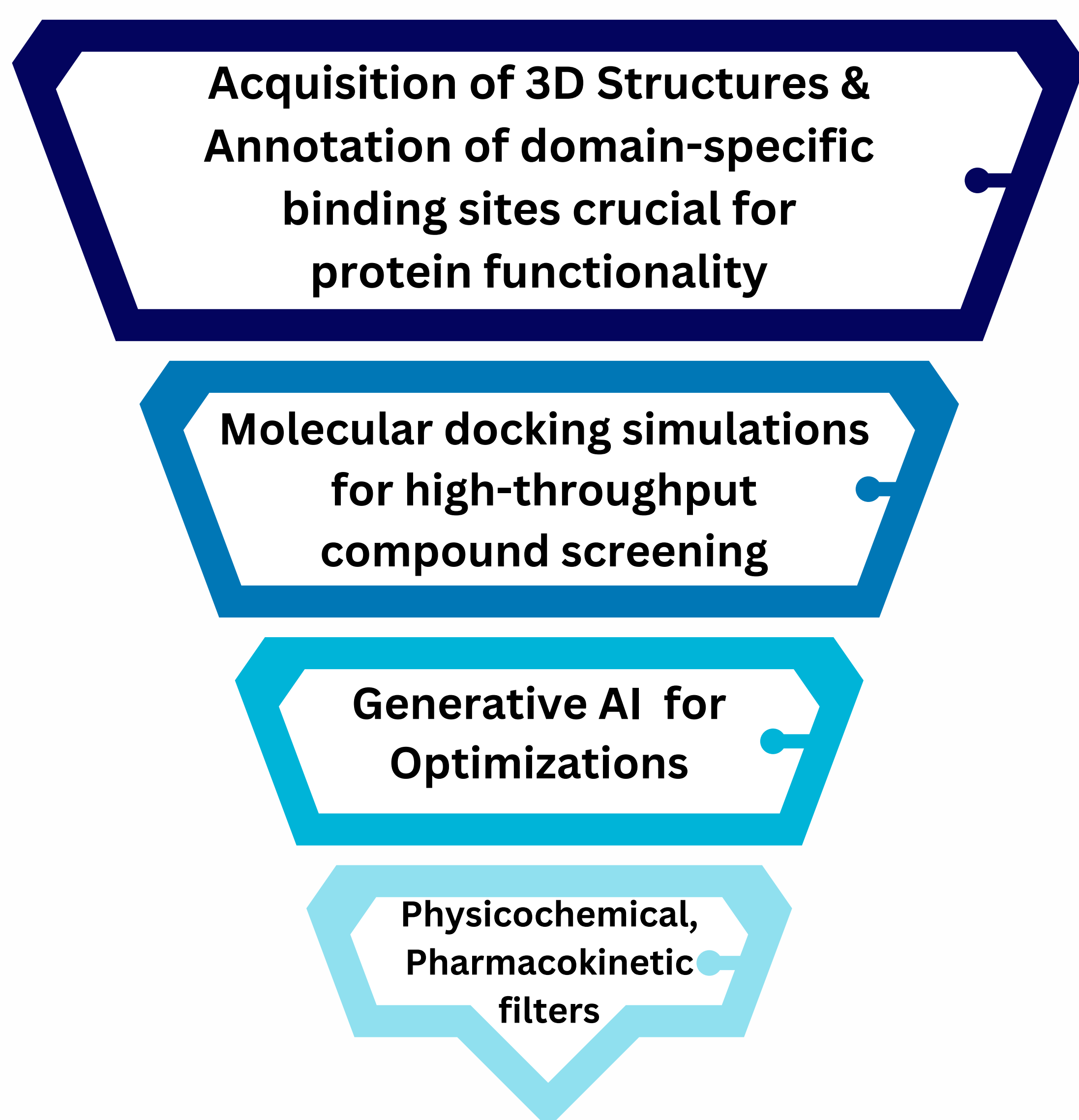




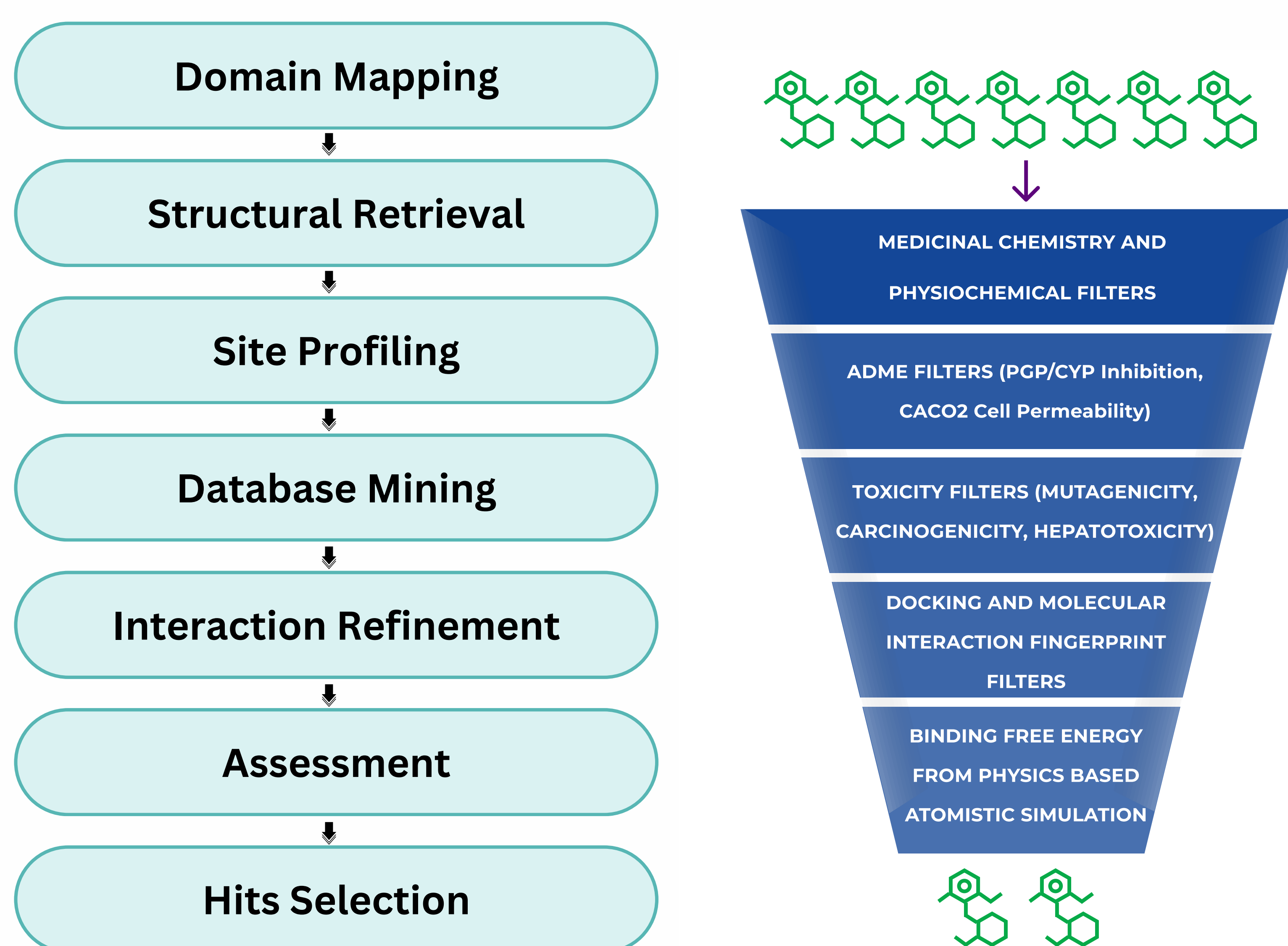
## CASE STUDY 1: Targeted Drug Repurposing through Domain-Specific Screening

- **Context:** Enhance chemotherapy and radiotherapy in TNBC Breast cancer patients by adjuvant therapy with repurposed drugs by selective inhibition of targets involved in DNA repair pathways for accelerated cancer cell death
- **Objective:** To repurpose clinically approved compounds for a protein domain implicated in cellular repair mechanisms using computational screening and domain-specific analysis

### Method



### Flow



### Results

- Several compounds were identified with a high binding affinity for a PPI domain in a target involved in DNA repair pathways identified for the indication of interest
- The compounds demonstrated enhanced interaction profiles, with several surpassing benchmark metrics
- Selected compounds showed compatibility with desirable **ADMET** properties, predicting a favourable in vivo response

