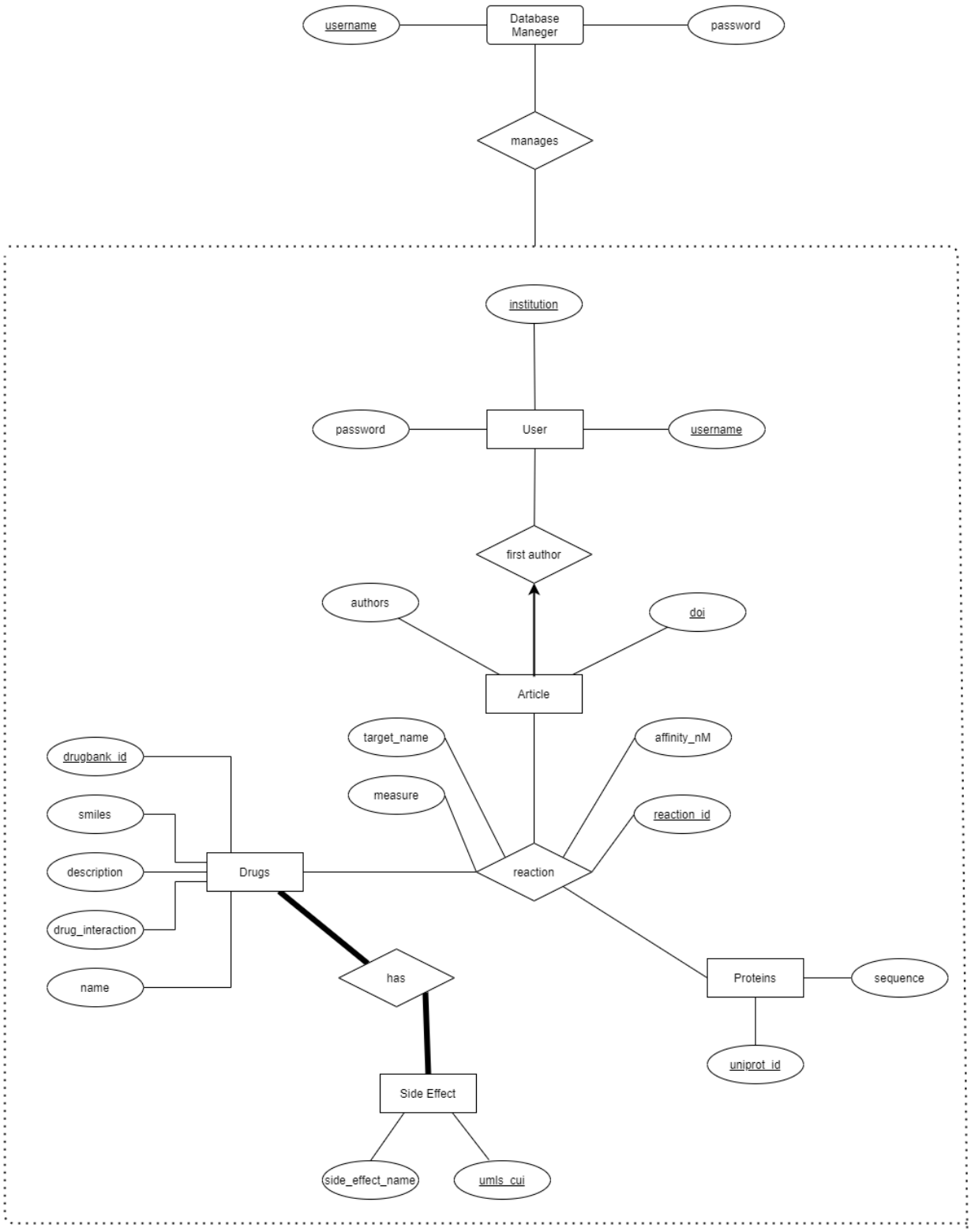
Part 1:

We designed ER according to relationships between entities and attributes. We tried to make it simple as possible. After designing ER diagram, we looked for participation constraints and key constraints. We draw arrows and bold lines accordingly.



Part 2:

Drug(drugbank_id:char(7),name:char(50),smiles:char(200),drug_interaction:char(100),description:char(1000))

User(username:char(50),institution:char(100),password:char(50))

Article(doi:char(100),authors:char(500),institution:char(100),username:char(50))

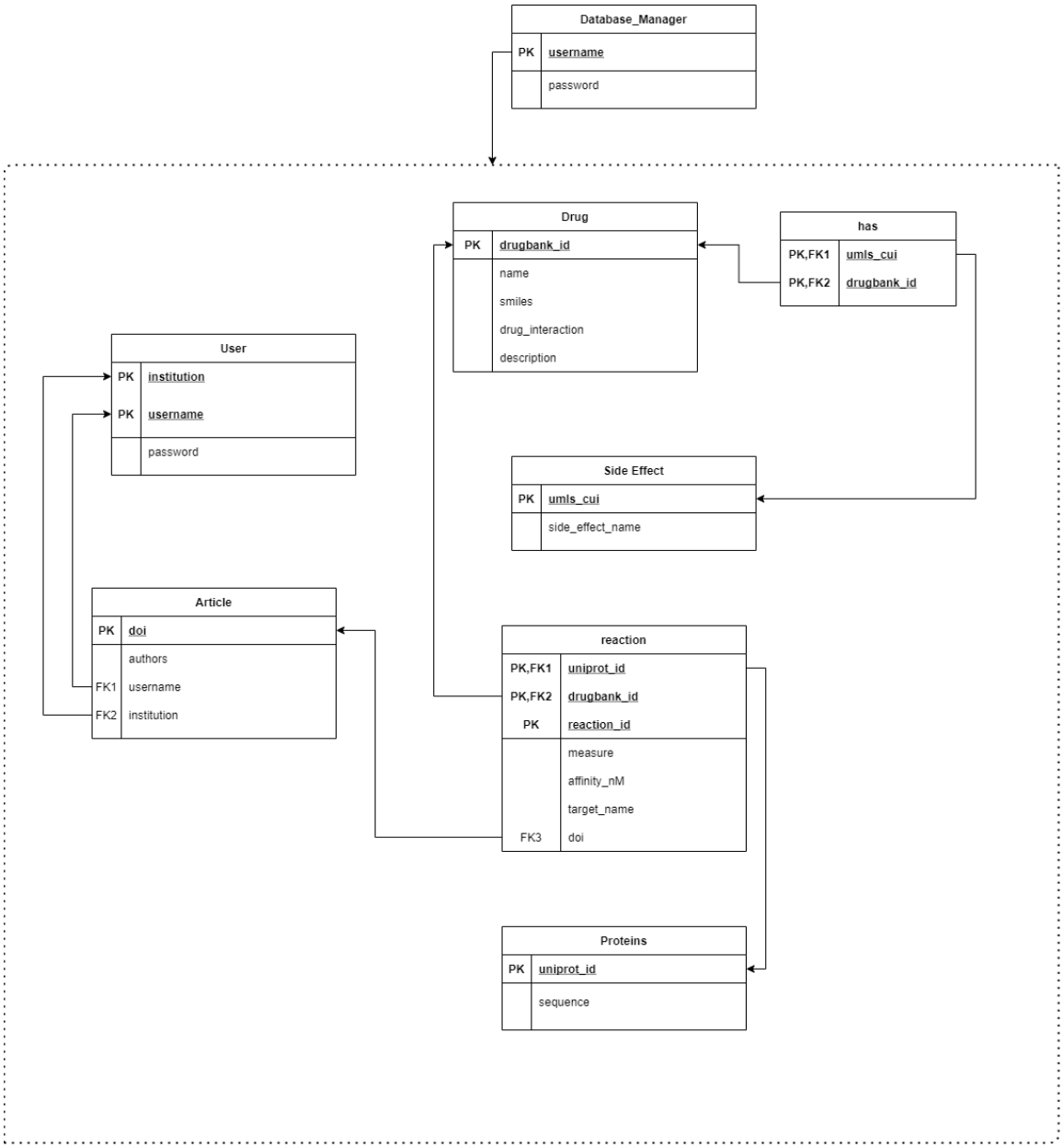
Proteins(uniprot_id:char(6),sequence:char(10000))

Side_Effect(umls_cui:char(8),side_effect_name: char(100))

Has(umls_cui:char(8), drugbank_id:char(7))

Reaction(uniprot_id:char(6),drugbank_id:char(7):reaction_id:char(8),measure:char(4),affinity_nM:real,target_name:char(1000),doi:char(100))

Database_Manager(username:char(50), password:char(50))



Part 3:

User entity:

User(username:char(50),institution:char(100),password:char(50))
username: U, institution: I, password: P
UI -> P
since U and I are primary keys it does not violate the BCNF

Article entity:

Article(doi:char(100),authors:char(500))
doi: D, authors: A
D -> A
since D is a primary key it does not violate BCNF

Drug entity:

Drug(drugbank_id:char(7),name:char(50),smiles:char(200),drug_interaction:char(100),description:char(1000))
drugbank_id : D name : N smiles : S drug_interaction : I description : R
D -> N D -> S D -> I D - > R so D -> NSIR

N -> D N -> S N -> I N -> R so N -> DSIR

S -> D S -> N S -> I S -> R so S -> DNIR

R -> D R -> N R -> I R -> S so R -> DNIS

Then D, S, N and R are candidate keys. We can choose D as primary key.

D -> NSIR So it does not violate BCNF rule.

Reaction relationship:

Reaction(uniprot_id:char(6),drugbank_id:char(7):reaction_id:char(8),measure:char(4),affinity_nM:real,target_name:char(1000),doi:char(100))
drugbank_id : D uniprot_id : U reaction_id : R measure : M affinity_nM : A target_name : T doi : Do
UDR -> MATDo
Since UDR are primary keys, it does not violate BCNF

Side_effect entity:

Side Effect(umls_cui:char(8),side_effect_name:char(100))
umls_cui : U side_effect_name : S
U -> S
since U is primary key, it does not violate BCNF

Proteins entity:

Proteins(uniprot_id:char(6),sequence:char(10000))
uniprot_id: U, sequence: Q
U -> Q
since U is primary key it does not violate BCNF

Database_Manager entity:

Database_Manager(username:char(50), password:char(50))

username: U password: P

U -> P

Since U is primary key it does not violate BCNF

Has relationship:

Has(umls_cui:char(8), drugbank_id:char(7))

There is no functional dependency in Has relation. (Between User and Side effect entities)

In conclusion, our database design is appropriate for BCNF rules. So we did not change anything in our database design.