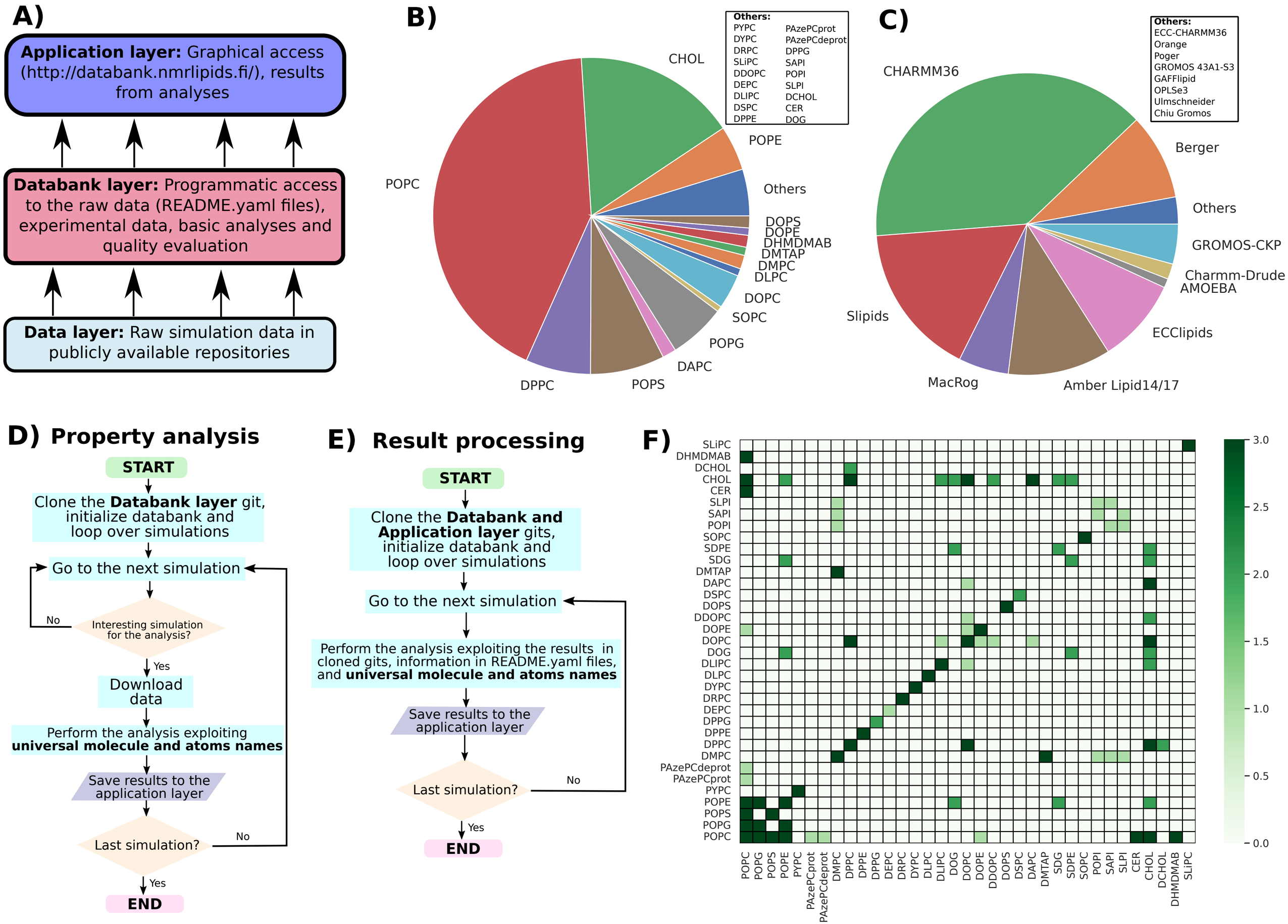
A)
Application layer: Graphical access (http://databank.nmrlipids.fi/), results from analyses
Databank layer: Programmatic access to the raw data (README.yaml files), experimental data, basic analyses and quality evaluation
Data layer: Raw simulation data in publicly available repositories
B)
Others:
PYPC
DYPC
DRPC
SLiPC
DDOPC
DEPC
DLIPC
DSPC
DPPE
PAzePCprot
PAzePCdeprot
DPPG
SAPI
POPI
SLPI
DCHOL
CER
DOG
CHOL
POPE
Others
DOPS
DOPE
DHMDMAB
DMTAP
DMPC
DLPC
DOPC
SOPC
POPG
DAPC
POPS
DPPC
POPC
C)
Others:
ECC-CHARMM36
Orange
Poger
GROMOS 43A1-S3
GAFFlipid
OPLSe3
Ulmschneider
Chiu Gromos
CHARMM36
Berger
Others
GROMOS-CKP
Charmm-Drude
AMOEBA
ECClipids
Amber Lipid14/17
MacRog
Slipids
D) Property analysis
START
Clone the Databank layer git, initialize databank and loop over simulations
Go to the next simulation
Interesting simulation for the analysis?
No
Yes
Download data
Perform the analysis exploiting universal molecule and atoms names
Save results to the application layer
Last simulation?
No
Yes
END
E) Result processing
START
Clone the Databank and Application layer gits, initialize databank and loop over simulations
Go to the next simulation
Perform the analysis exploiting the results in cloned gits, information in README.yaml files, and universal molecule and atoms names
Save results to the application layer
Last simulation?
No
Yes
END
F)
SLiPC
DHMDMAB
DCHOL
CHOL
CER
SLPI
SAPI
POPI
SOPC
SDPE
SDG
DMTAP
DAPC
DSPC
DOPS
DDOPC
DOPE
DOPC
DOG
DLIPC
DLPC
DYPC
DRPC
DEPC
DPPG
DPPE
DPPC
DMPC
PAzePCdeprot
PAzePCprot
PYPC
POPE
POPS
POPG
POPC
3.0
2.5
2.0
1.5
1.0
0.5
0.0