CHARMM36 CHOL **Layer 1: Raw simulation data** Available in open repository (e.g. Zenodo) Berger POPE GAEFLIPICH MM36 DOPS DHMDMAB GROMOS-CKP CER DOPC Slipids POPG ECClipids **Layer 2: Indexing of simulation data using** DAPC universal naming convetion MacRog https://github.com/NMRLipids/Databank Amber Lipid14/17 POPS DPPC Total number: 492 trajectories 0.0020 Total length: 231 micros **Layer 3: Applications** 0.0015 0.0010 0.0015 Graphical access: http://databank.nmrlipids.fi/ - Automated analyses (e.g. github.com/NMRLipids/DataBankManuscript, https://github.com/NMRLipids/DatabankExercises) 0.0005 0.0000 3000 2000 4000 5000 Simulation length (ns)