CCPN

CCPN chemComp templates and force field parameters

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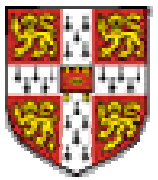

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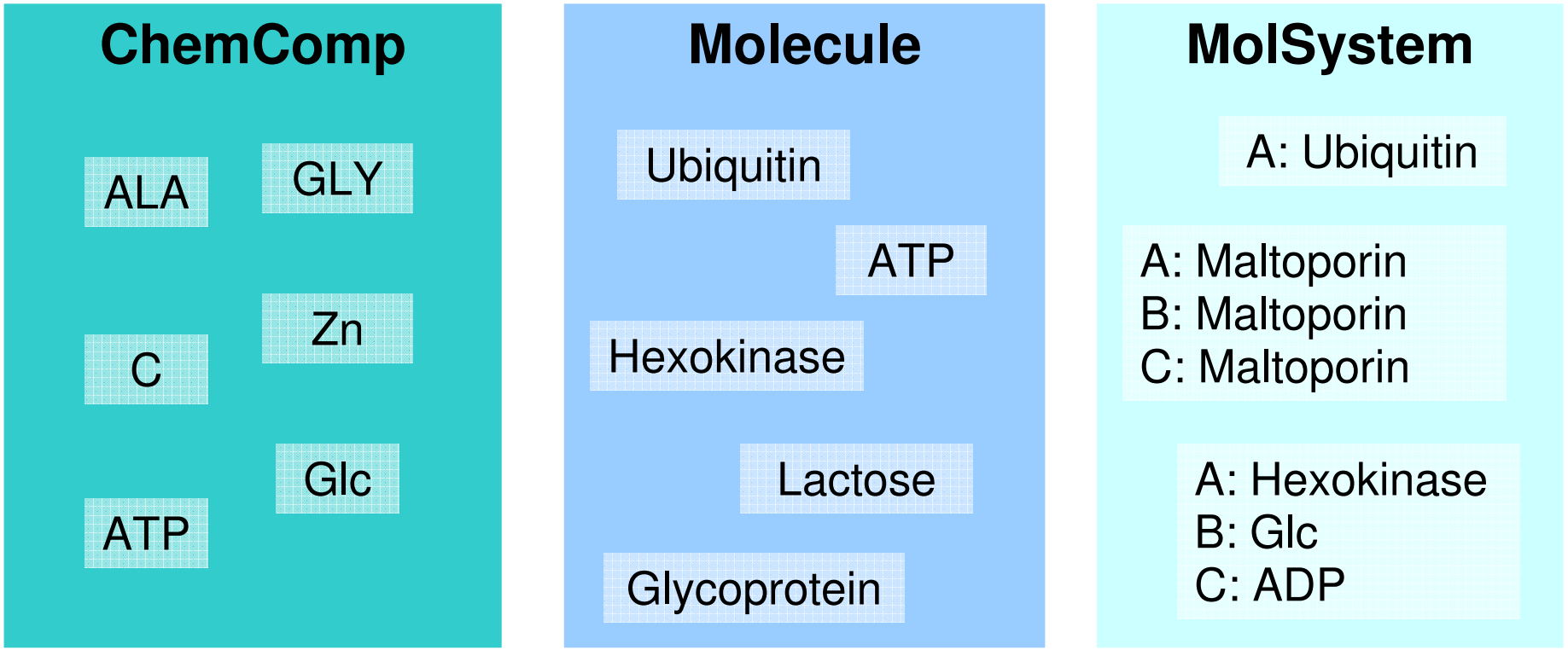
Molecule organisation



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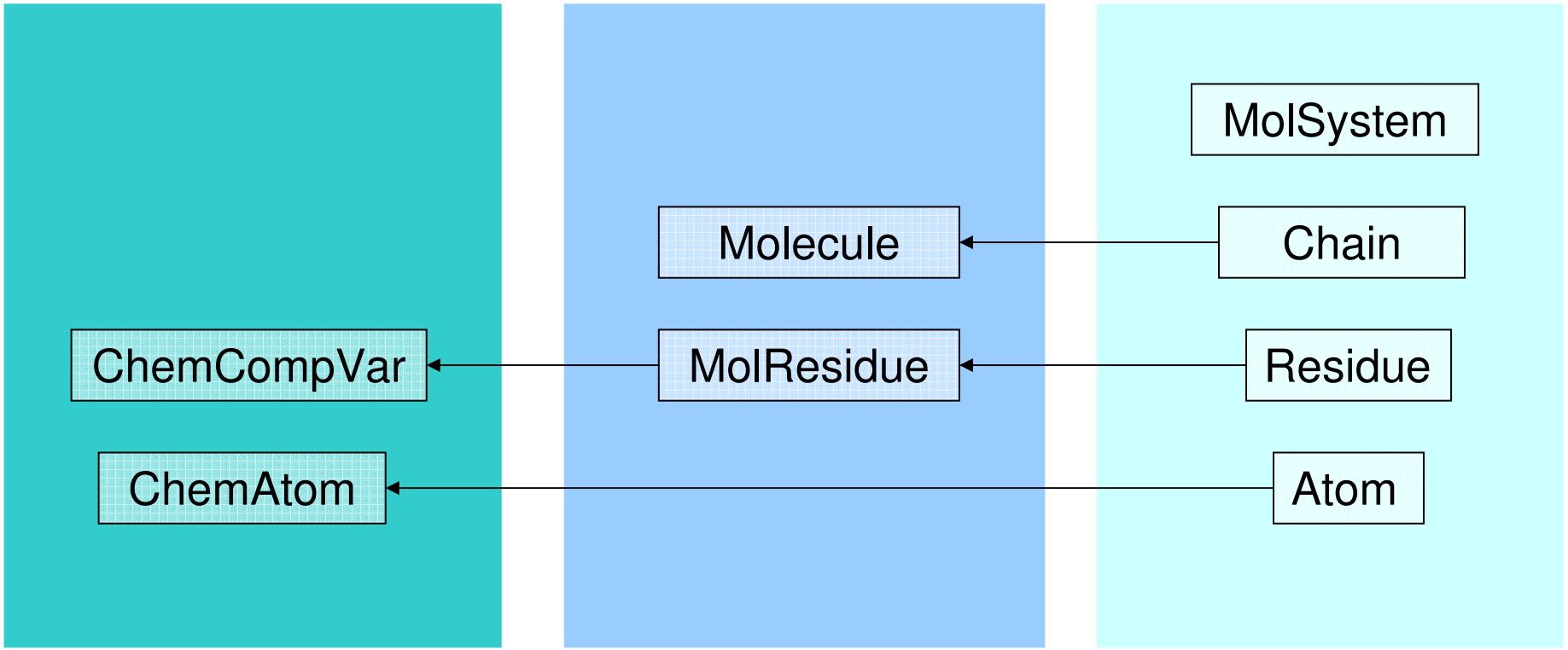
Molecule organisation



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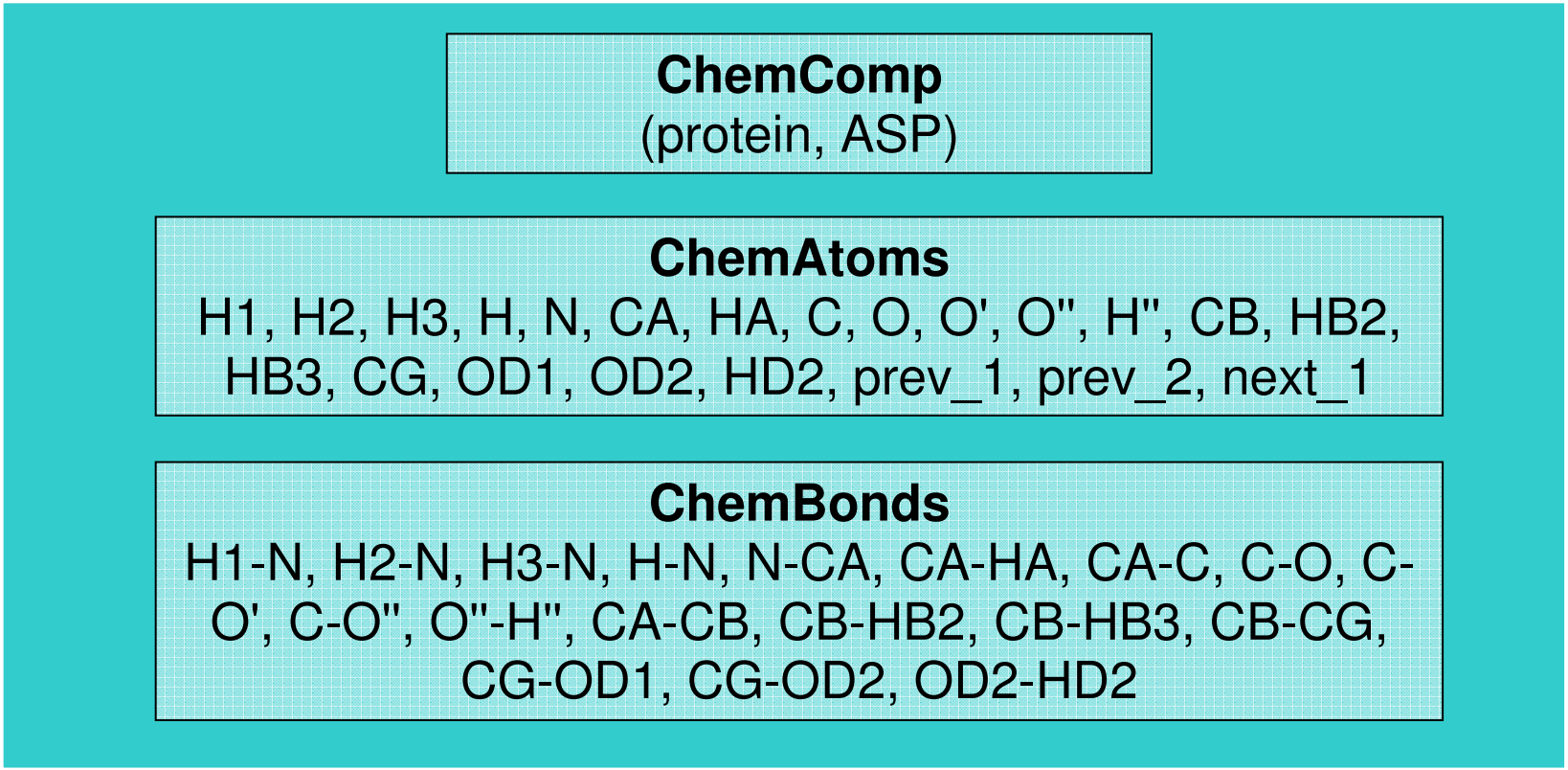
ChemComp organisation



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ChemComp organisation

ChemCompVar
linking: 'start'
descriptor: 'prot:H3;deprot:HD2'

Selected ChemAtoms
H1, H2, H3, N, CA, HA, C, O, CB, HB2, HB3, CG, OD1, OD2, next_1

ChemBonds included
H1-N, H2-N, H3-N, N-CA, CA-HA, CA-C, C-O, C-next_1, CA-CB, CB-HB2, CB-HB3, CB-CG, CG-OD1, CG-OD2

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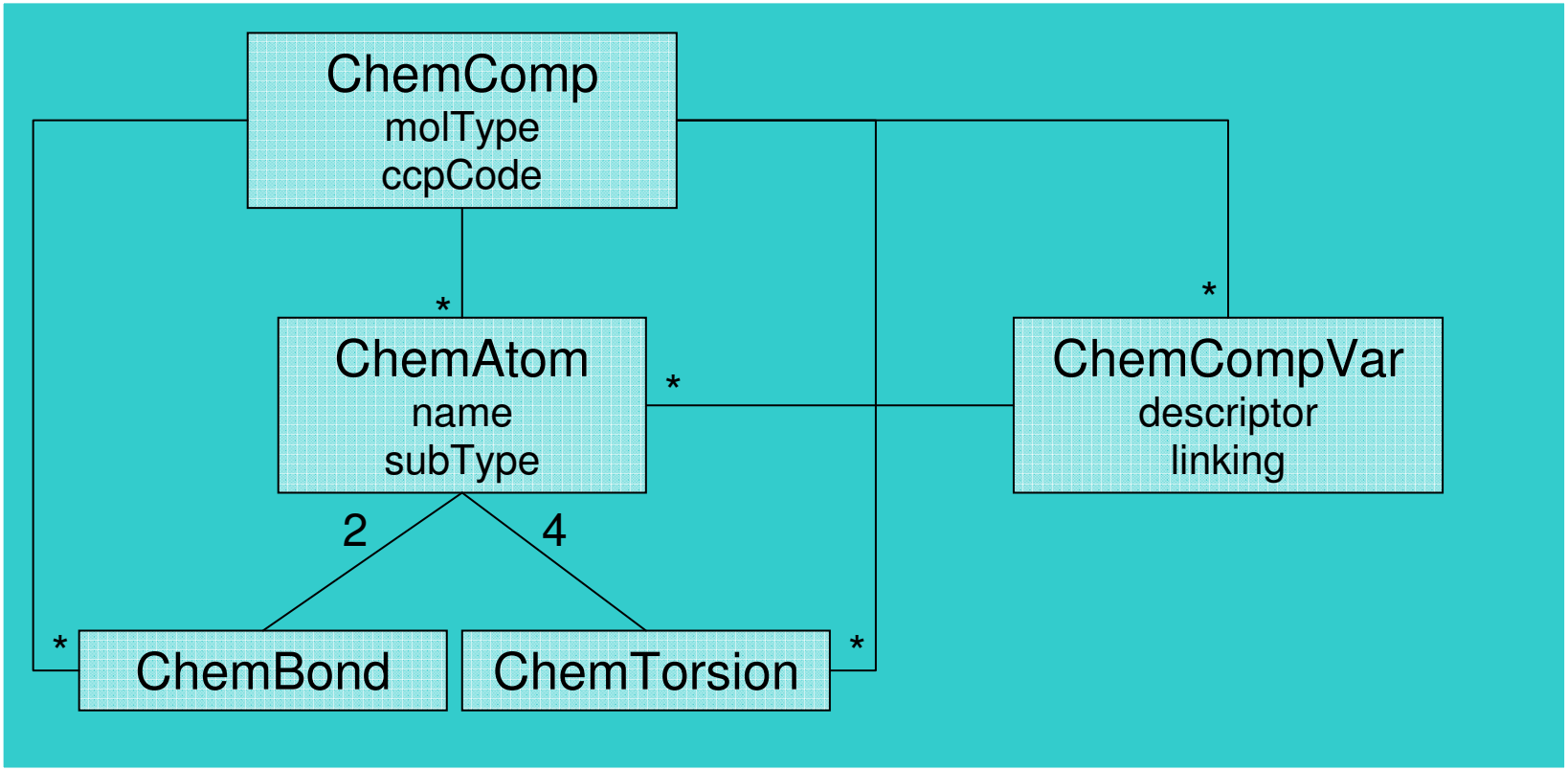
ChemComp organisation



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ChemComp organisation

Actual ChemAtom keys for sidechain COOH
(CG, 1), (OD1, 1), (OD1, 2), (OD2, 1), (OD2, 2), (HD2, 1)

descriptor: 'prot: HD2'
ChemAtoms (CG,1) (OD1, 1) (OD2, 1) (HD2, 1)
ChemBond (CG, 1)-(OD1, 1) double
ChemBond (CG, 1)-(OD2, 1) single
ChemBond (CG, 1)-(HD2, 1) single

descriptor: 'deprot: HD2'
ChemAtoms (CG,1) (OD1, 2) (OD2, 2)
ChemBond (CG, 1)-(OD1, 2) singleplanar
ChemBond (CG, 1)-(OD2, 2) singleplanar

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ChemComp organisation

Specific linking

(protein, CYS)
Linking: 'middle', **descriptor**: 'link:SG'
Includes chemAtom SG_1, chemBond SG-SG_1

(carbohydrate,Glc)
Linking: 'link:C1,O3,O4', **descriptor**: 'neutral'
Includes chemAtoms C1_1, O3_1, O4_1,
chemBonds C1-C1_1, O3-O3_1, O4-O4_1

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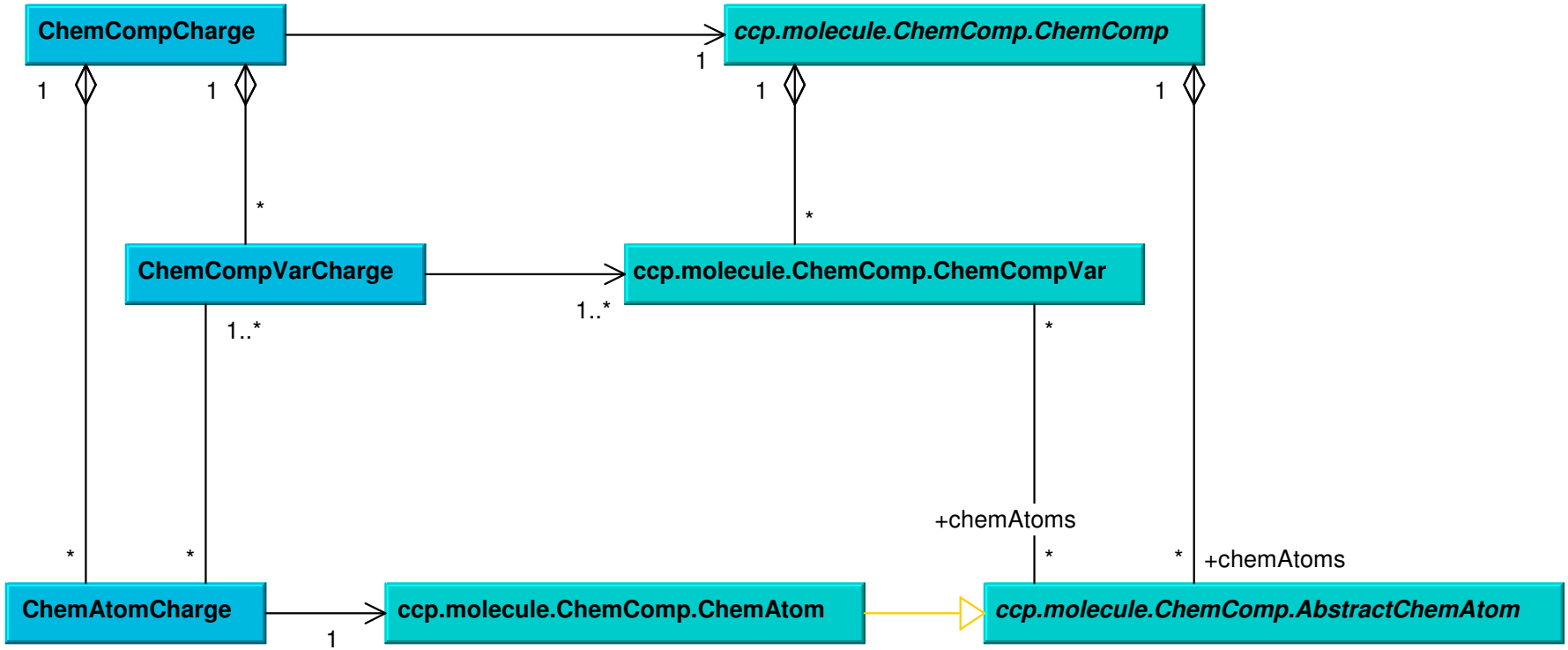
Other ChemComp information

- cifCode, code1Letter, isParamagnetic, …
- Angles
- Stereochemistry of groups of atoms
- Naming systems for atoms
- Atom sets

- Default coordinates, by source (Cactvs, corina, …)
- Charges, by source (Gasteiger, …)

ChemCompCharge



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ChemAtoms and force fields

- Atom topology descriptor string ('*shortVegaType*')
- Automatic generation of reasonable chemComp templates:
  - Atom topology mapping to force field energy types
  - Stereochemistry information
  - Default coordinate information
  - Relevant charge information

Current status

- Structure determination of complexes by NMR
- Testing:
  - For CNS calculations
  - Generating ‘new’ topology for standard proteins
  - Recalculating structures
  - Comparing with original calculations
- Extend mapping to all atom topology in current databank

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Reference data

- Molecule information from the MSD group (EBI)
  - Over 6000 reference ‘chemical components’ from PDB
    - E.g. ALA, ADP, GLC, Zn, …
    - Easily extendable to full range of organic molecules
  - Added information relevant for NMR:
    - Atom naming systems
    - NMR-equivalent atoms, protons that exchange with water, …
  - Continuity between CCPN and PDB codes

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Other molecules?

- Reference information contains all molecules in PDB
  - With default coordinates, atom names, bonds, …
  - Current effort to clean up this data at wwPDB
- Also possible to generate CCPN ‘chemComp’ building blocks from other sources
  - PDB, mol, mol2
- Scripts can be hacked for custom purposes

Acknowledgements

- University of Cambridge
  - Rasmus Fogh (*Data model*)
  - Wayne Boucher (*CcpNmr Analysis, CLOUDS, Data model*)
  - Tim Stevens (*CcpNmr Analysis, CLOUDS*)
  - Wolfgang Rieping (*ISD*)
  - Dan O'Donovan (*Bayesian analysis*)
  - Alan Wilter (*CCPNGrid*)
  - Ernest Laue
- MSD group (EBI, Cambridge)
  - Wim Vranken (*CcpNmr FormatConverter, Data model*)
  - John Ionides (*Data model*)
  - Anne Pajon (*Protein production, Data model*)
  - Kim Henrick

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Information and downloads

- CCPN Web Site :
  - www.ccpn.ac.uk/
- Downloads for all CCPN chemComps:
  - www.ebi.ac.uk/msd-srv/docs/NMR/chemCompXml

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