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Databases of Porous Cages

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Updating the POC database

- Extract all REFCODEs associated with list of 23 authors using **ConQuest** OR CSD Python API
- Filter by:
  - Has 3D coordinates
  - Not organometallic
  - Crystal structures only
  - Published post 2015
- Visualize in ConQuest and keep only 'cage-like' structures
- Produces 108 cage structures (CDB41 has 41 structures) although this may not be exhaustive
- Applied the same process searching for metal–organic cages: 63 authors $\rightarrow$ 1131 "cage-like" structures

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Properties of crystal structures

- Visualize all structures and determine if:
  - Cage backbone is disordered
  - Solvent is present
  - Squeeze/Mask is used
- Using *pyWindow*:
  - Extract distinct cages and test if they are shape persistent
  - Remove solvent/guest molecules and return CIF with just cage network (defined by their pore diameter)
- Note that *pyWindow* does not handle disordered structures well

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Collaboration with Matthew Addicoat

- Topological analysis of the pore network of cage structures
- Use *pyWindow* to determine the COM of each cage and the COM of the windows of each cage