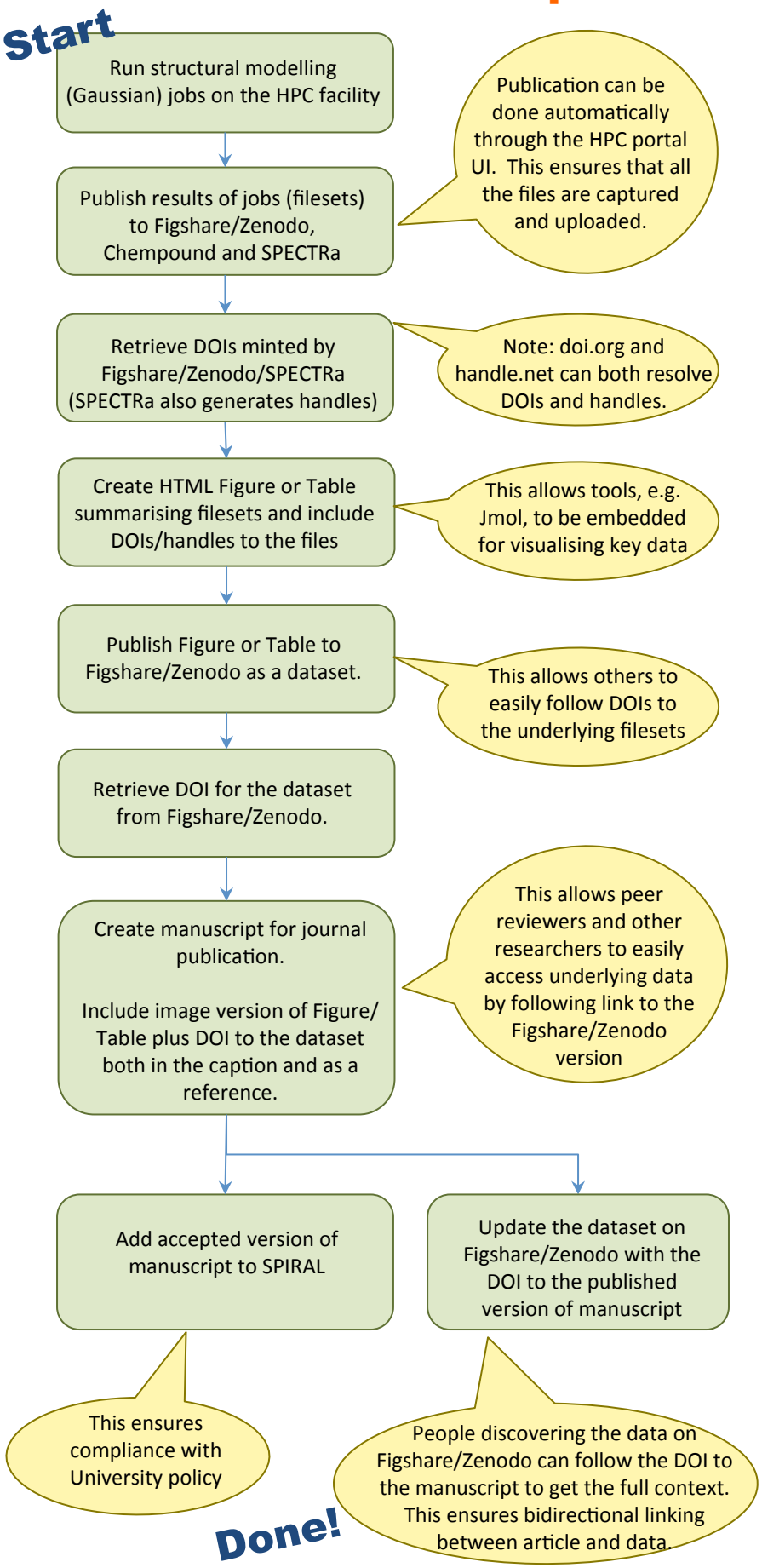
Use of DOIs for computational chemistry data



Tools and Services

HPC Portal
Imperial College HPC facility
https://www.imperial.ac.uk/admin-services/ict/self-service/research-support/hpc/

Gaussian
Software tool for chemical structure simulations
http://www.gaussian.com/

Chempound
Imperial college Chemical Database (Chempound)
http://www.chempound.net/

SPECTRa
Imperial College Data Repository (DSpace)
https://spectradspace.lib.imperial.ac.uk:8443/

SPIRAL
Imperial College Publication Repository (Dspace)
https://spiral.imperial.ac.uk/

Jmol
3D Chemical Structure Viewer
http://jmol.sourceforge.net/

Figshare
Public data sharing platform
http://figshare.com/

Zenodo
Public data sharing platform
https://zenodo.org/

Example

Journal Publication (Manuscript)
The Houk–List transition states for organocatalytic mechanisms revisited
A. Armstrong, R. A. Boto, P. Dingwall, J. Contreras-García, M. J. Harvey, N. J. Mason and H. S. Rzepa, Chem. Sci., 2014, 5, 2057
DOI: 10.1039/C3SC53416B

Table (Dataset)
Rzepa, Henry S.; Harvey, M J; Mason, Nicholas; Dingwall, Paul; Armstrong, Alan; Contreras-García, Julia; Boto, Roberto (2013): Table 8. Houk-List Transition state analogues. figshare.
DOI: 10.6084/m9.figshare.832543

Gaussian Simulation (Fileset)
dc.title C 17 H 22 N 2 O 3
dc.type Gaussian job archive
dc.identifier.uri
http://hdl.handle.net/10042/25119
dc.identifier.uri
DOI: 10.14469/ch/19080