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| --- | --- | --- |
| Figure | Script | Data |
| Figure 1 | total\_dataset.py  mononuclear.py | total\_dataset.xlsx  mononuclear\_1\_COMPONENT\_CN\_DIST.xlsx |
| Figure 2 | total\_dataset.py  mononuclear.py | total\_dataset.xlsx  mononuclear\_1\_COMPONENT\_CN\_DIST.xlsx |
| Figure 3 | element\_distribution.py | element\_distribution.xlsx |
| Figure 4 | screen\_pure\_organic\_ligand.py  screen\_pure\_inorganic\_ligand.py  differ\_org.py  differ\_inorg.py | organic\_ligand\_percentage.xlsx  inorganic\_ligand\_percentage.xlsx |
| Figure 5 | O identify.py | identify O count one element per time.xlsx |
| Figure 6 | element\_distribution new.py | identify C-O 1.xlsx |
| Figure 7 | Built-in software Conquest | commercial ex.xlsx |
| Figure 8 |
| Figure 9 |  |  |
| Figure 10 | La\_phenanthroline.py  La\_phenanthroline2.py  La\_phenanthroline3.py  La\_phenanthroline4.py  pythonLa\_phenanthroline.py  rename.py  txt\_to\_gcd.py | La\_phenanthroline\_OK\_1.gcd  La\_phenanthroline\_OK\_2.gcd  La\_phenanthroline\_OK\_3.gcd  La\_phenanthroline\_OK\_4.gcd  phen.xlsx |