Steps to extract and characterize single 3D large aggregates

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| **Step** | **Script** | **Input** | **Output** |
| **1** | main\_v3 >  main\_dataload.m | Path to rounds folder containing sample folders  (1 raw tif per sample folder) | xlsx table with metadata of each raw tif file  *dataset*\_metadata.xlsx |
| **2** | main\_v3 >  main\_aggregate.m | microscope name and xlsx files metadata table  sycamore  *dataset*\_metadata.xlsx | 3D image array with gain and offset applied, .mat files in datastore  image\_*rsid*.mat  binary mask voxels positions and numbers results  numbers\_result.csv  oligomer\_result.csv  non\_oligomer\_result.csv |
| **3** | nolig\_main\_nfp >  aggregate\_extraction.m | non\_oligomer\_result.csv  image\_*rsid*.mat  *dataset*\_metadata.xlsx | ‘Single aggregates’ folder with a tif stack of every single 3D aggregate extracted  *rsid*\_agg\_##.tif  csv file of the aggregates’ voxels’ positions in raw tif image  aggregates\_positions\_*rsid*.csv |
| **4** | nolig\_main\_nfp >  aggregate\_characterization3D.m | Tif stacks of 3D aggregates  *rsid*\_agg\_##.tif | If wanted, png figures of the aggregates  ##-*rsid*\_agg\_##.png  Table of all parameters for each aggregate  agg\_parameters\_3D.xlsx |
| **5** | nolig\_main\_nfp >  aggregate\_characterization2D.m | Tif stacks of 3D aggregates  *rsid*\_agg\_##.tif | If wanted, png figures of the 2D sub-aggregates found in each 3D aggregate  ##-*rsid*\_agg\_##.png  Table of all parameters for each aggregate  agg\_parameters\_2D.xlsx |
| **6** | nolig\_main\_nfp >  aggregate\_comparison.m | 3D aggs shape classification csv file  classmidrd.csv  Tables of all parameters for each aggregate  agg\_parameters\_3D.xlsx  agg\_parameters\_2D.xlsx | Figures wanted, t-sne plots and/or plots, currently no saving |