Results SimID.2975901

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Disclaimer

This report has been auto-generated using paraprobe-autoreporter.
It is the responsibility of the author to check the validity and correctness of these results!

1 paraprobe-transcoder

Here is place for tool-specific comments.
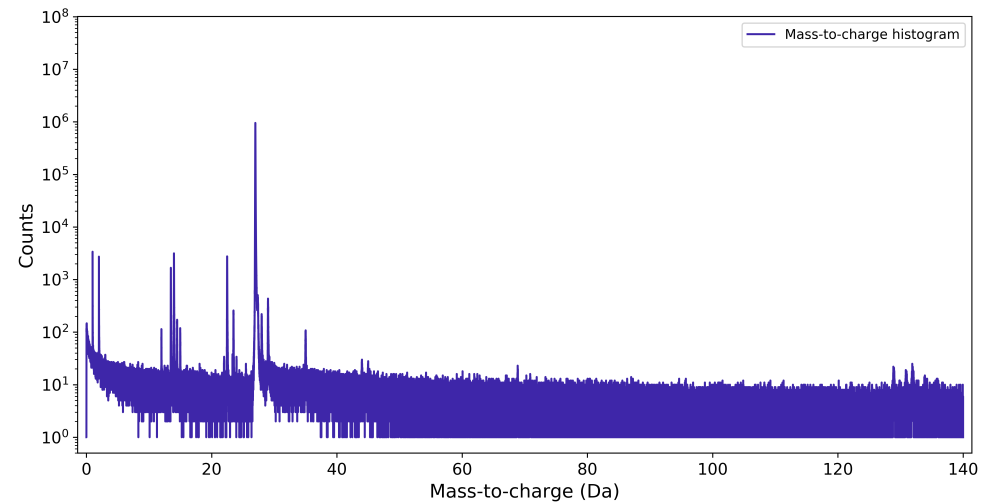The dataset contains 41431241 ions in total.

Table 1: Which XML settings were used for paraprobe-transcoder?

Keyword	Value	Unit	Description
Inputfile	R76_29759-v01.pos		
TranscodingMode	1		

2 paraprobe-ranger

Table 2: What is the composition of the dataset, i.e. how many ions with particular ion type labelled?

unknown	Al	Sc	Si	Mg	H:	C:	O:	Xe	AlO:	ScH:	AlH:	Total
1399307	39705921	109911	108819	6644	30881	1897	2017	10628	8421	9737	37058	41431241

(a)

Figure 1: What is the mass-to-charge histogram/diagram of the entire dataset?

Table 3: Which XML settings were used for paraprobe-ranger?

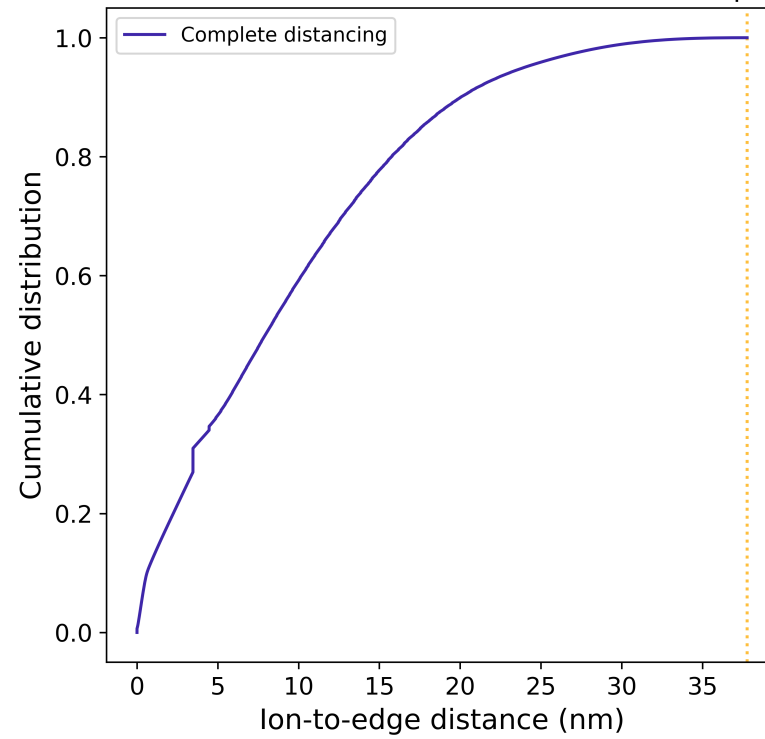| Keyword	Value	Unit	Description
Inputfile	R76_29759-v01.pos		
TranscodingMode	1		

3 paraprobe-surfacer

4 paraprobe-tessellator

5 paraprobe-spatstat

6 paraprobe-dbscan

PARAPROBE.Surfacer.Results.SimID.2975901.h5 α-shape, $\alpha = 3.589$

(a)

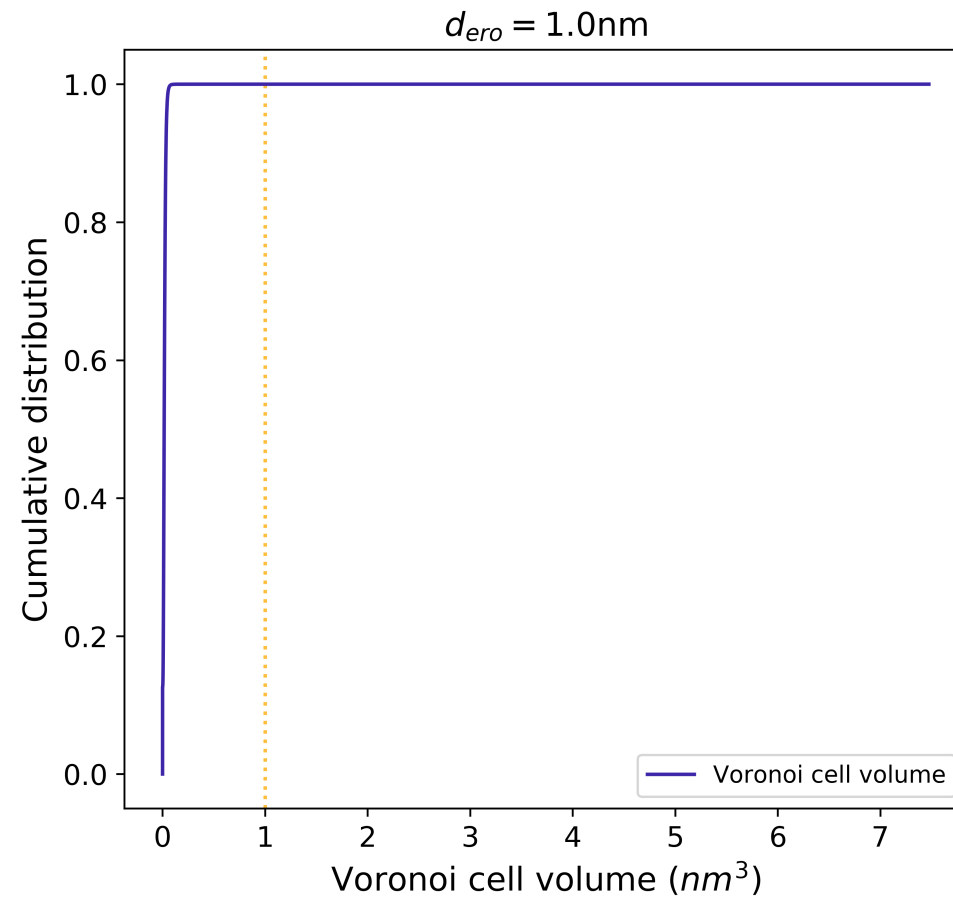Figure 2: How many ions are so and so far away from the dataset edge?

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Table 4: Which XML settings were used for paraprobe-surfacer?

Keyword	Value	Unit	Description
AdvDistanceBinWidthIncr	1	nm	
AdvDistanceBinWidthMax	1	nm	
AdvDistanceBinWidthMin	1	nm	
AdvIonPruneBinWidthIncr	1	nm	
AdvIonPruneBinWidthMax	1	nm	
AdvIonPruneBinWidthMin	1	nm	
AlphaShapeAlphaValue	0		
DistancingMode	1		
DistancingRadiusMax	0	nm	
InputfileReconstruction	PARAPROBE.Transcoder.Results.SimID.2975901.h5		
RequeryingThreshold	0		
SurfacingMode	1		

Table 5: Which XML settings were used for paraprobe-tessellator?

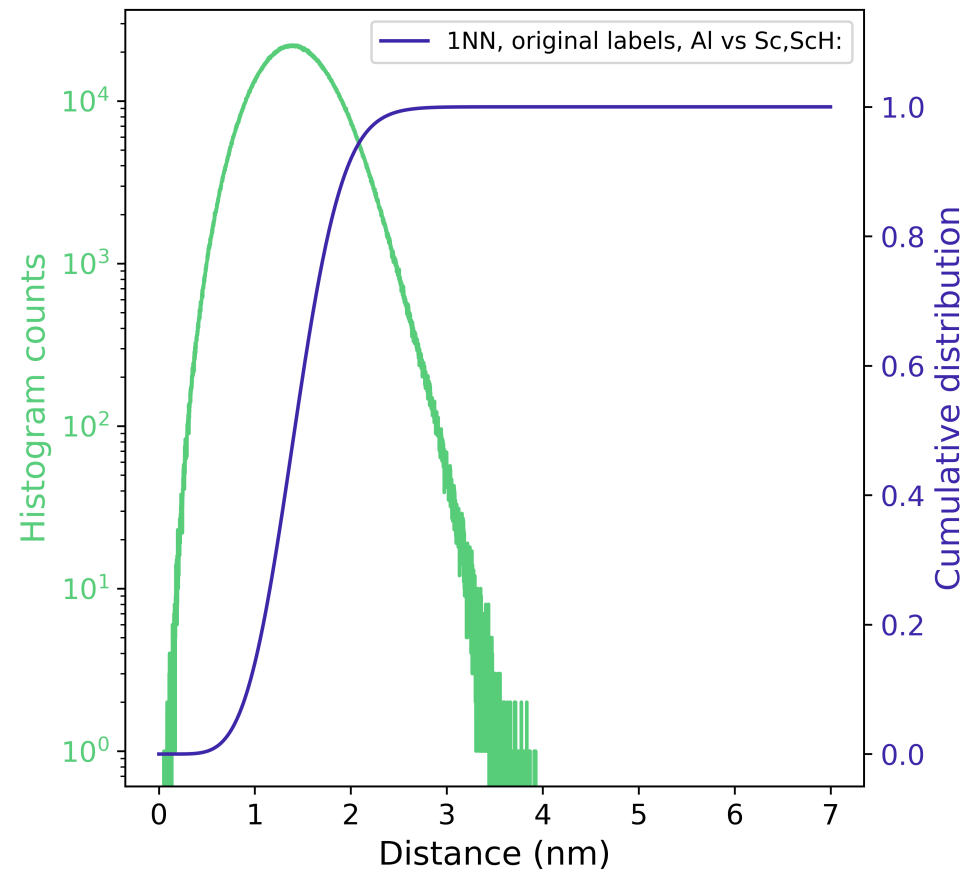| Keyword	Value	Unit	Description
CellErosionDistance	1	nm	
GuardZoneFactor	5		
IOCellNeighbors	0		
IOCellProfiling	1		
IOCellShape	0		
IOCellVolume	1		
InputfileDistances	PARAPROBE.Surfacer.Results.SimID.2975901.h5		
InputfilePSE	PARAPROBE.PeriodicTableOfElements.xml		
InputfileReconstruction	PARAPROBE.Transcoder.Results.SimID.2975901.h5		
IonsPerBlock	5		
SpatialSplittingMethod	0		

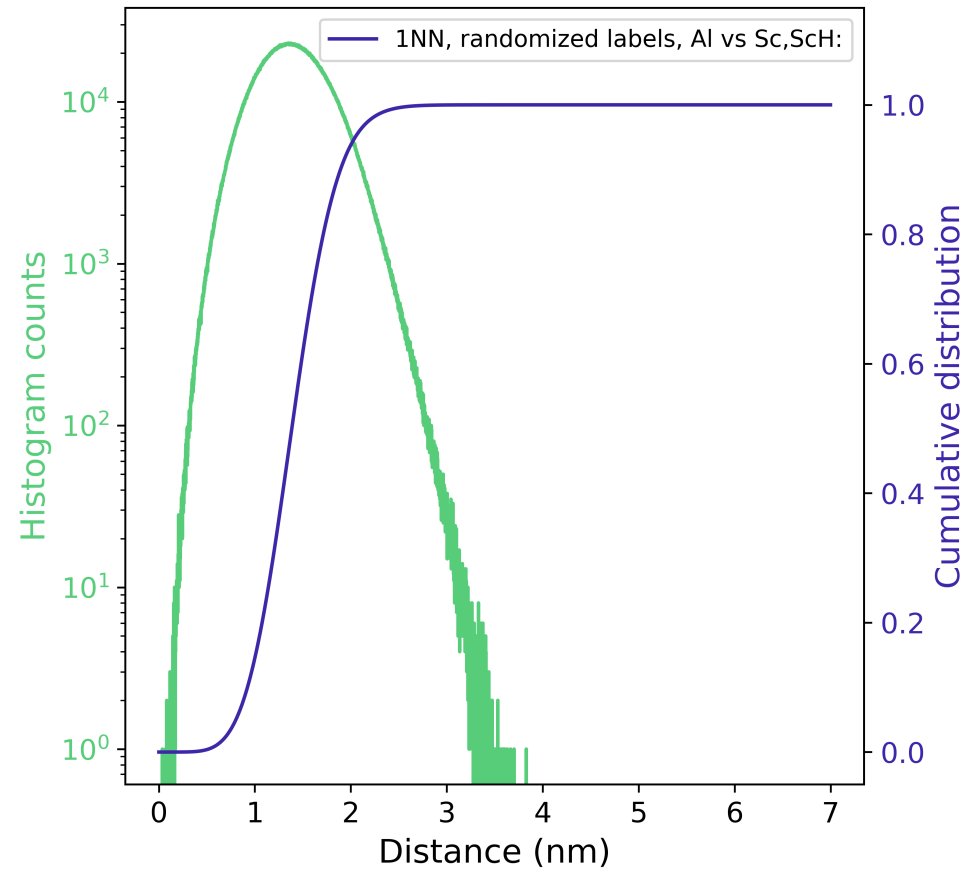Figure 3: What is the distribution of volume for the Voronoi cells?

Figure 4: How much accumulated volume of Voronoi cells remains when successively eroding Voronoi cells from the dataset edge towards the interior?
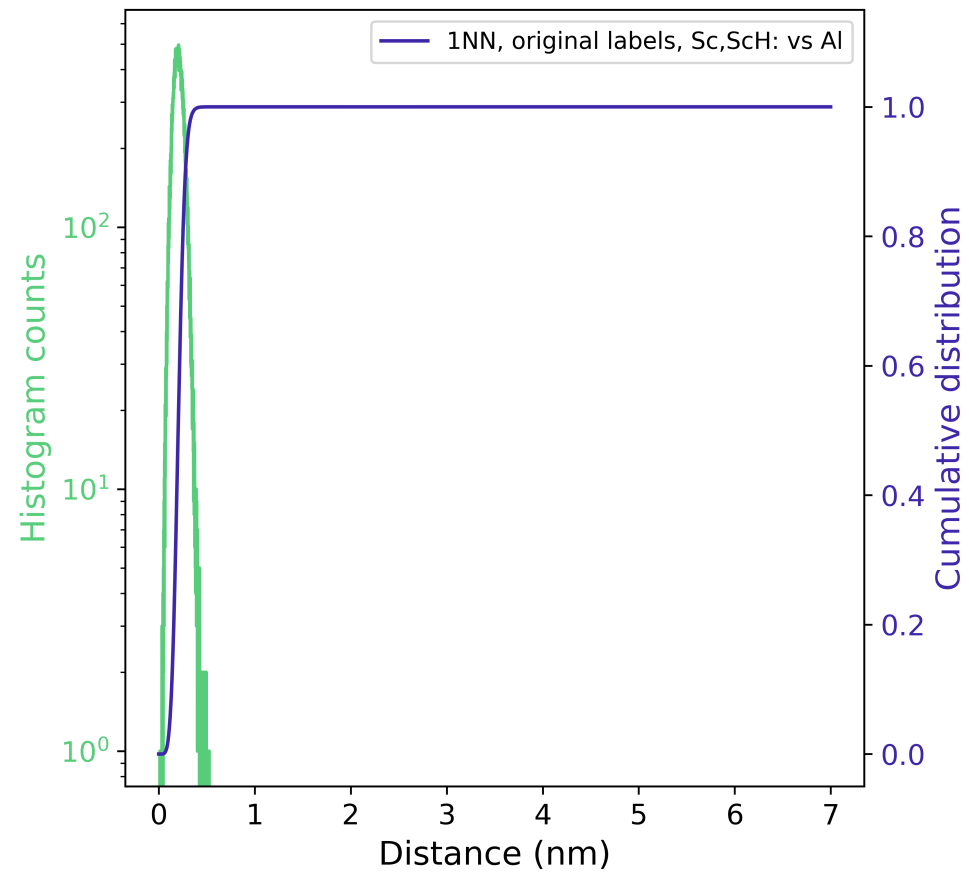
(a)

Figure 5: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?
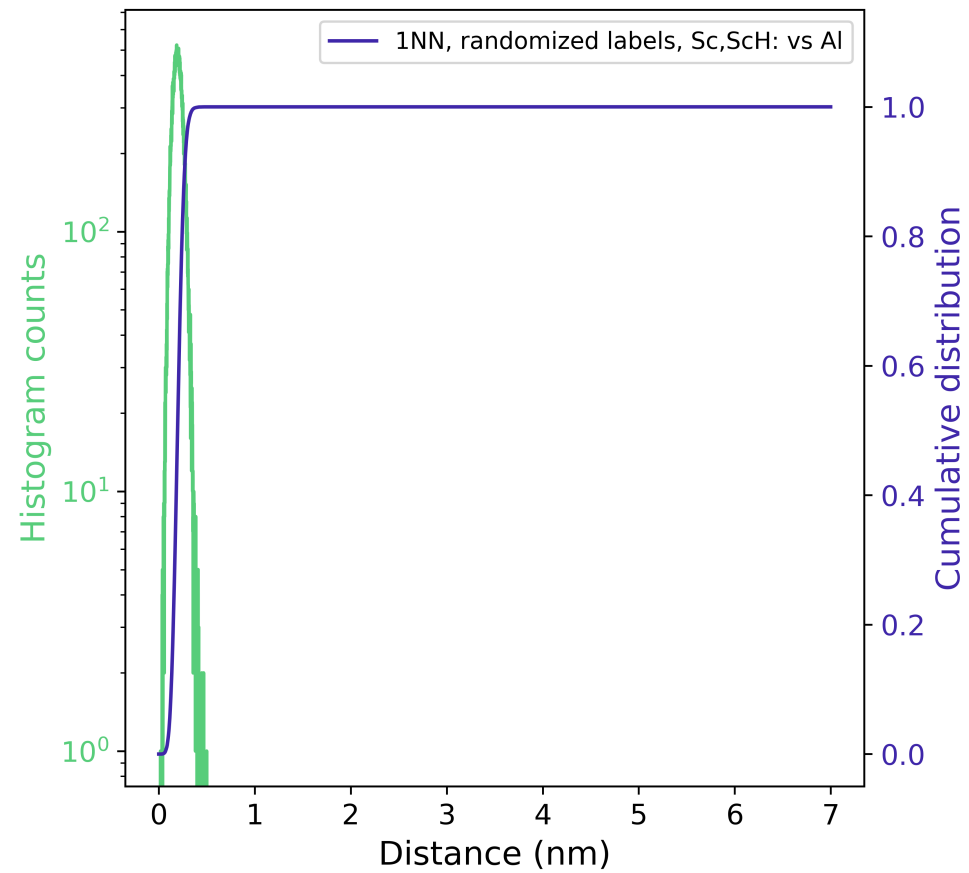
(a)

Figure 6: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?

(a)

Figure 7: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?

(a)

Figure 8: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?

(a)

Figure 9: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?

(a)

Figure 10: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?
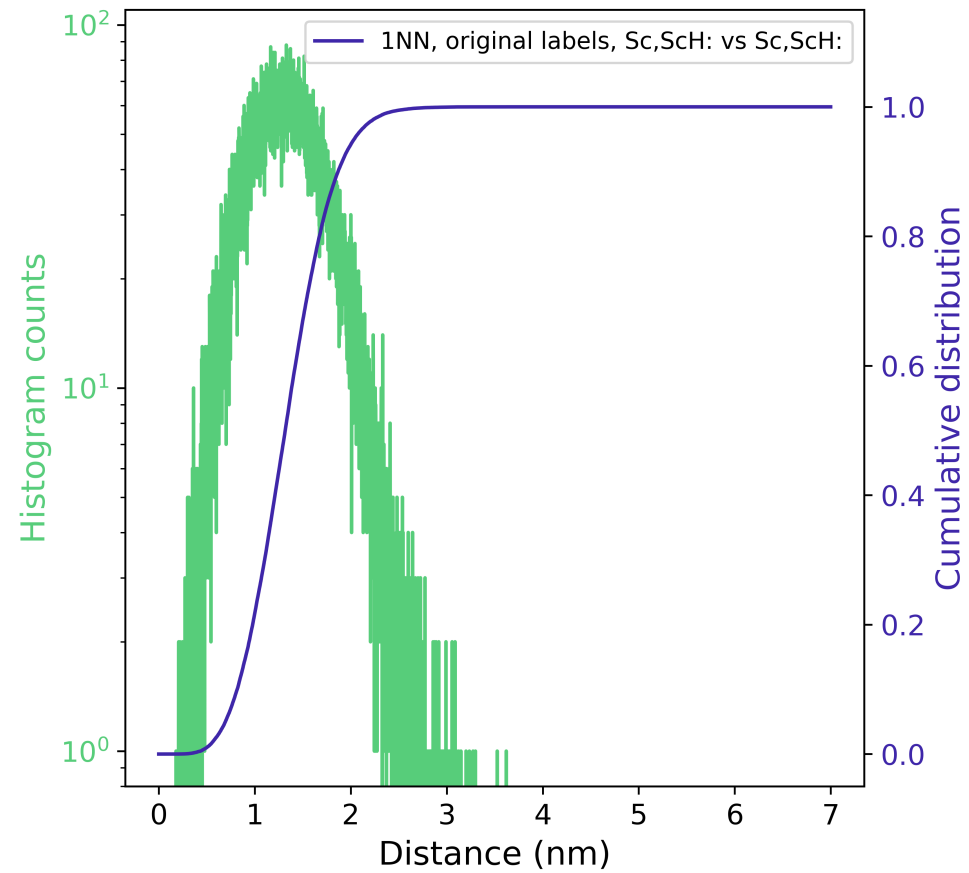
(a)

Figure 11: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?

(a)

Figure 12: What is the kth nearest neighbor distribution function for particular ion types about specific ion types?
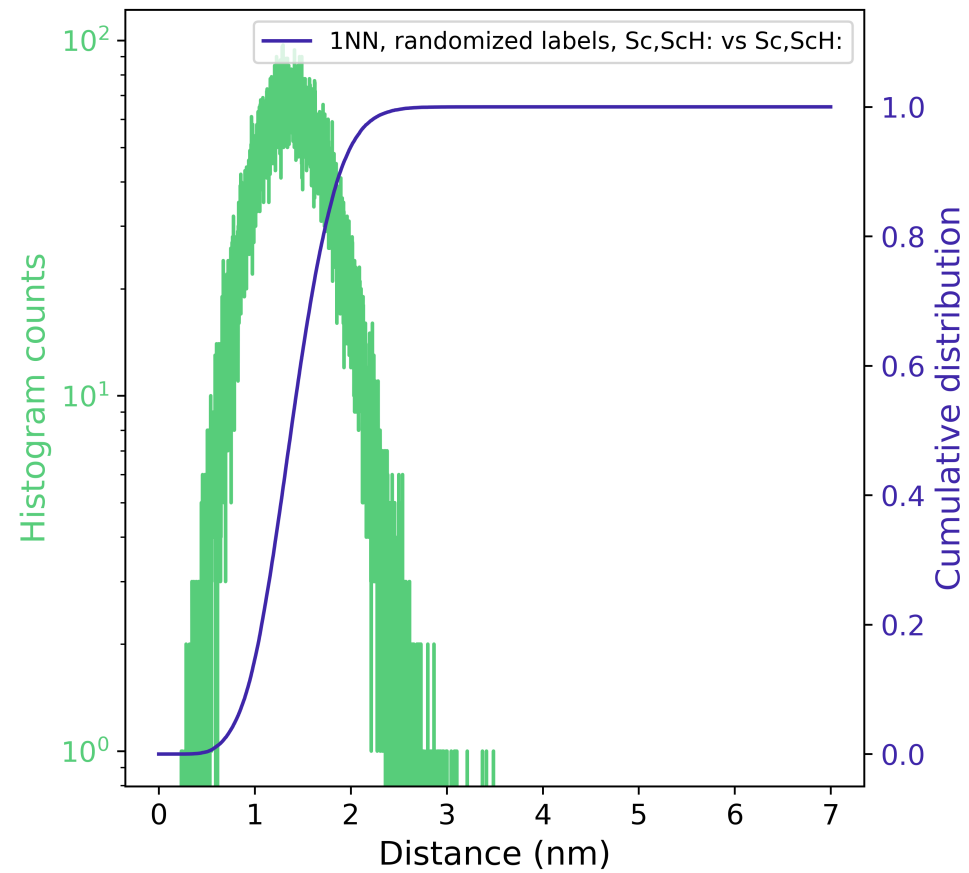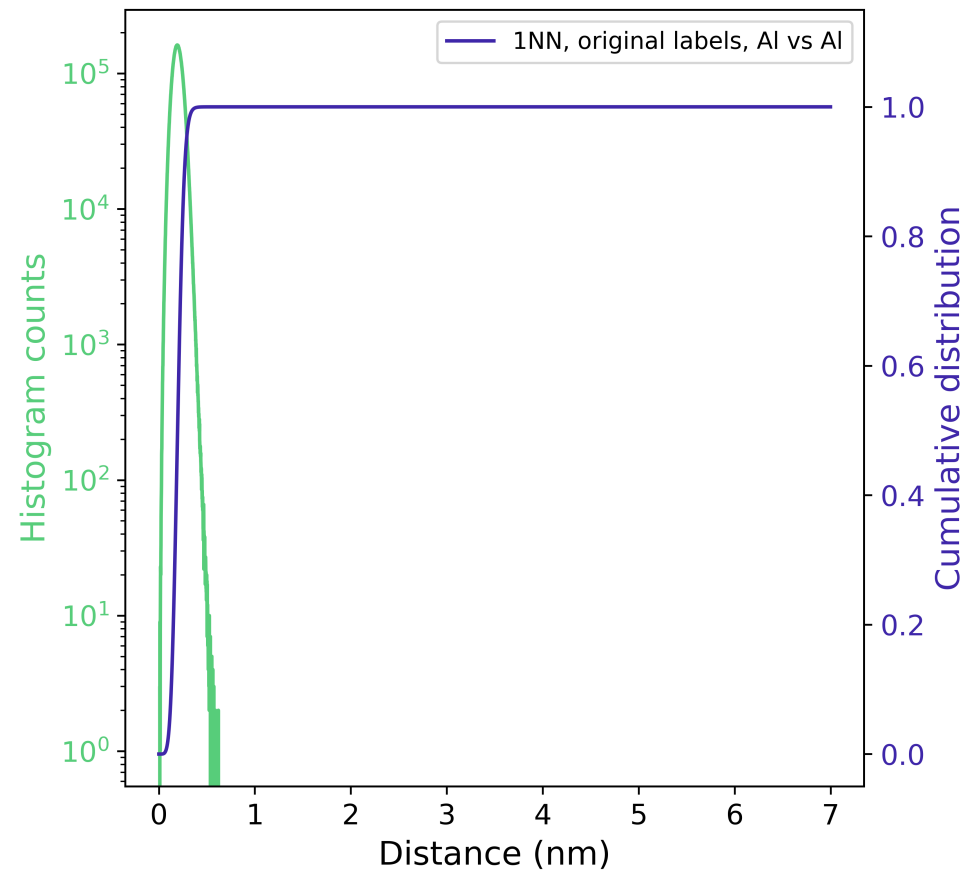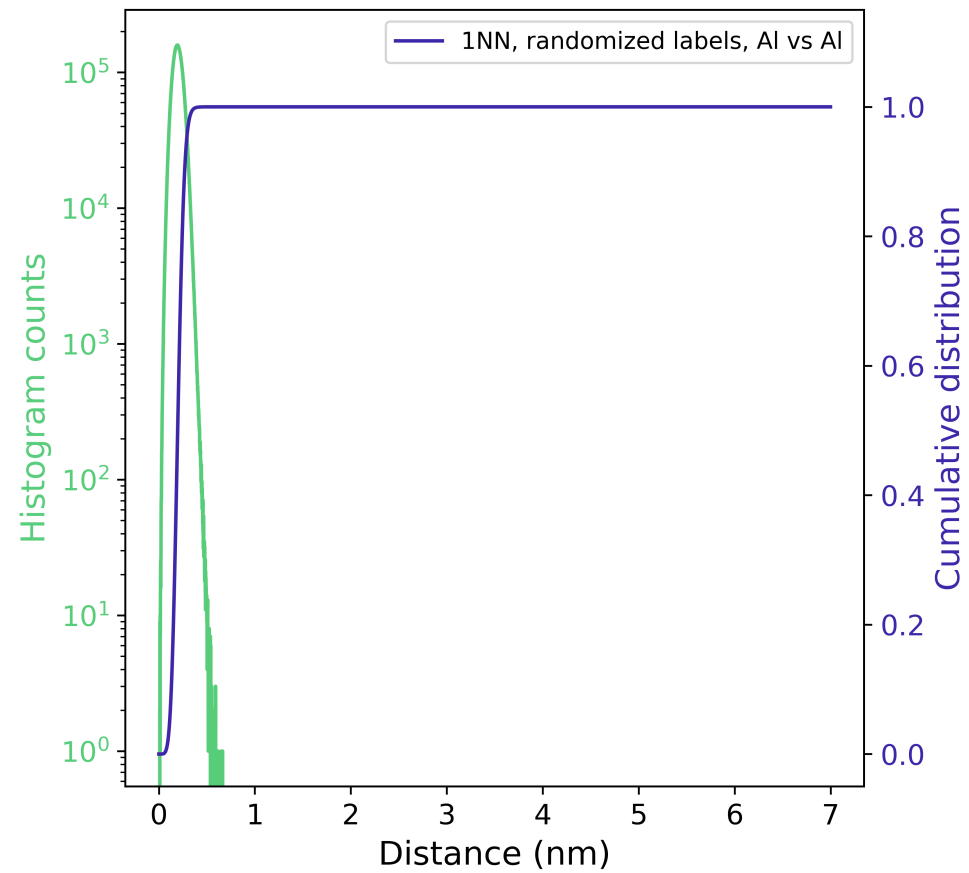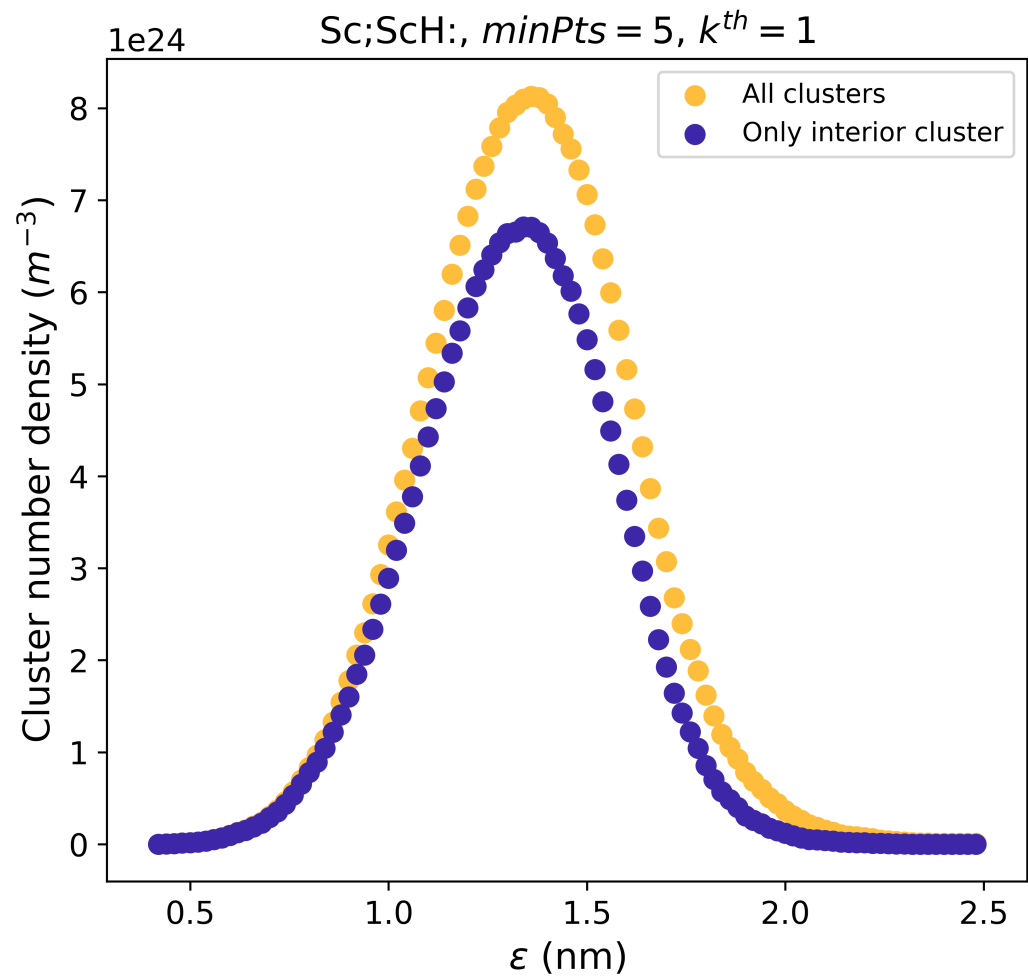
Table 6: Which XML settings were used for paraprobe-spatstat?

Keyword	Value	Unit	Description
AnalyzeKNN	1		
AnalyzeRDF	1		
AnalyzeRandomize	1		
AnalyzeSDM	0		
InputfileHullAndDistances	PARAPROBE.Surfacer.Results.SimID.2975901.h5		
InputfilePSE	PARAPROBE.PeriodicTableOfElements.xml		
InputfileReconstruction	PARAPROBE.Transcoder.Results.SimID.2975901.h5		
IontypeCombi0	Targets;Al;Neighbors;Al		
IontypeCombi1	Targets;Al;Neighbors;Sc,ScH:		
IontypeCombi2	Targets;Sc,ScH:;Neighbors;Al		
IontypeCombi3	Targets;Sc,ScH:;Neighbors;Sc,ScH:		
KOrderForKNN	1		
KOrderForSDM			
MaxSizeCachedResPerNode	17179869184		
PRNGType	MT19937		
PRNGWarmup	700000		
PRNGWorldSeed	18446744073697205938		
ROIRadiiKNNIncr	0.001	nm	
ROIRadiiKNNMax	7	nm	
ROIRadiiKNNMin	0	nm	
ROIRadiiRDFIncr	0.001	nm	
ROIRadiiRDFMax	7	nm	
ROIRadiiRDFMin	0	nm	
ROIRadiiSDMIncr	1	nm	
ROIRadiiSDMMax	0	nm	
ROIRadiiSDMMin	0	nm	
ROIVolumeInsideOnly	1		

Figure 13: What are the number of clusters per unit volume, quantified using high-throughput studies of the DBScan/maximum separation clustering parameter?

Table 7: Which XML settings were used for paraprobe-dbscan?

Keyword	Value	Unit	Description
ClusteringMethod	2		
DBScanEpsilonIncr	0.02	nm	
DBScanEpsilonMax	7	nm	
DBScanEpsilonMin	0.2	nm	
DBScanMinPtsIncr	1		
DBScanMinPtsMax	1		
DBScanMinPtsMin	1		
DatasetEdgeThresholdDistance	1	nm	
IOStoreClusterIDs	0		
IOStoreClusters	1		
InputfileHullAndDistances	PARAPROBE.Surfacer.Results.SimID.2975901.h5		
InputfilePSE	PARAPROBE.PeriodicTableOfElements.xml		
InputfileReconstruction	PARAPROBE.Transcoder.Results.SimID.2975901.h5		
IontypeCombi0	Targets;Sc,ScH:		
MaxSepNumberOfIonsIncr	10		
MaxSepNumberOfIonsMax	5		
MaxSepNumberOfIonsMin	5		
MaxSizeCachedResPerNode	17179869184		

Table 8: How many MPI processes times OpenMP threads respectively were used, and what was the elapsed time for each tool run?

Toolname	#MPI	#OMP	$t_{elapsed}^{max}$ (s)
Transcoder	1	1	insignificant
Ranger	1	1	insignificant
Surfacer	1	40	10858.0
Tessellator	1	40	42.0
Spatstat	1	40	3413.0
DBScan	1	40	101.0