```
In[ ]:= SetDirectory[
          "C:/Users/serha/OneDrive/Masaüstü/MyRepo/master_thesis_MMT003/210519_time_windows_and
            _OR_model/deleting_reactions"];

In[ ]:= Get["../../algoritm_packages/SingleNetworks-algorithm-package-2.wl"]
        (* ?SingleNetworks`* *)

In[ ]:= stoichioforhomosapiens =
          Drop[Import["../../210324_disc_time_windows_and_OR_model/iAT_PLT_636_stoichiomat.csv",
            HeaderLines → 1], None, {1}];
        SparseArray@stoichioforhomosapiens

Out[ ]= SparseArray[ Specified elements: 4006
                     Dimensions: {738, 1008} ]

In[ ]:= stoichiometricmatrix = stoichioforhomosapiens;
        metabolites = 738;
        fluxexchanges = 1008;
        steadystatevector = ConstantArray[{0, 0}, metabolites];
        first[a_] := First /@ GatherBy[Ordering@a, a[[#]] &] // Sort;

In[ ]:= subsetpositionsforsequences = Import["../cases/subsetpositionsforsequences.mx"];
        boundaries = Import["../cases/boundaries_-5and5_105.mx"];
        boundariespos = Flatten@Position[boundaries, {-5, 5}];
        objfunctions = Import[
           "C:/Users/serha/NonDrive/OR_model-objective_functions/-1+1objfunc_fxdbounds_-5and5_
             105pcs.mx"];

In[ ]:= boundariesa = ReplacePart[ConstantArray[{-500, 500}, fluxexchanges], MapThread[
            #1 → #2 &, {boundariespos, ConstantArray[{-0.5, 0.5}, Length@boundariespos]}]];

In[ ]:= syntheticseqgenerator[stoichiometricmatrix_, steadystatevector_, boundaries_,
          fluxexchanges_, subsetpositions_, objectivefunctions_] := Module[{solutionvectors},
          solutionvectors = Chop[Table[LinearProgramming[-objectivefunctions[[i]],
              stoichiometricmatrix, steadystatevector, boundaries],
             {i, Length@objectivefunctions}], 10^-5]]

In[ ]:= AbsoluteTiming[
         solutionvectorsminus1toplus1 = Quiet@Table[syntheticseqgenerator[stoichiometricmatrix,
              steadystatevector, boundariesa, fluxexchanges, i[[1]], i[[2]]],
             {i, MapThread[{#1, #2} &, {subsetpositionsforsequences, objfunctions}]}];]

Out[ ]= {4346.72, Null}

In[ ]:= Dimensions@solutionvectorsminus1toplus1

Out[ ]= {200, 300, 1008}
```

```
(*Export[
 "C:/Users/serha/NonDrive/OR_model-solution_vectors/-1+1solutionvectors_fxdcoeffs_-05
   and05_105pcs.mx",solutionvectorsminus1toplus1]*)
```

```
Out[]= C:/Users/serha/NonDrive/OR_model-solution_vectors/-1+1solutionvectors_fxdcoeffs_-05
   and05_105pcs.mx
```

```
In[]:= solutionvectors = Import[
    "C:/Users/serha/NonDrive/OR_model-solution_vectors/-1+1solutionvectors_fxdcoeffs_-05
      and05_105pcs.mx"];
```

```
In[]:= SeedRandom@25;
randomreactionlist =
  Table[Sort@RandomInteger[{1, fluxexchanges}, i], {i, Range[1008, 500, -50]}];
```

```
In[]:= solutionvectorsreactionsdeleted =
  Table[Partition[Flatten[solutionvectors, 1][[All, i]], 300], {i, randomreactionlist}];
```

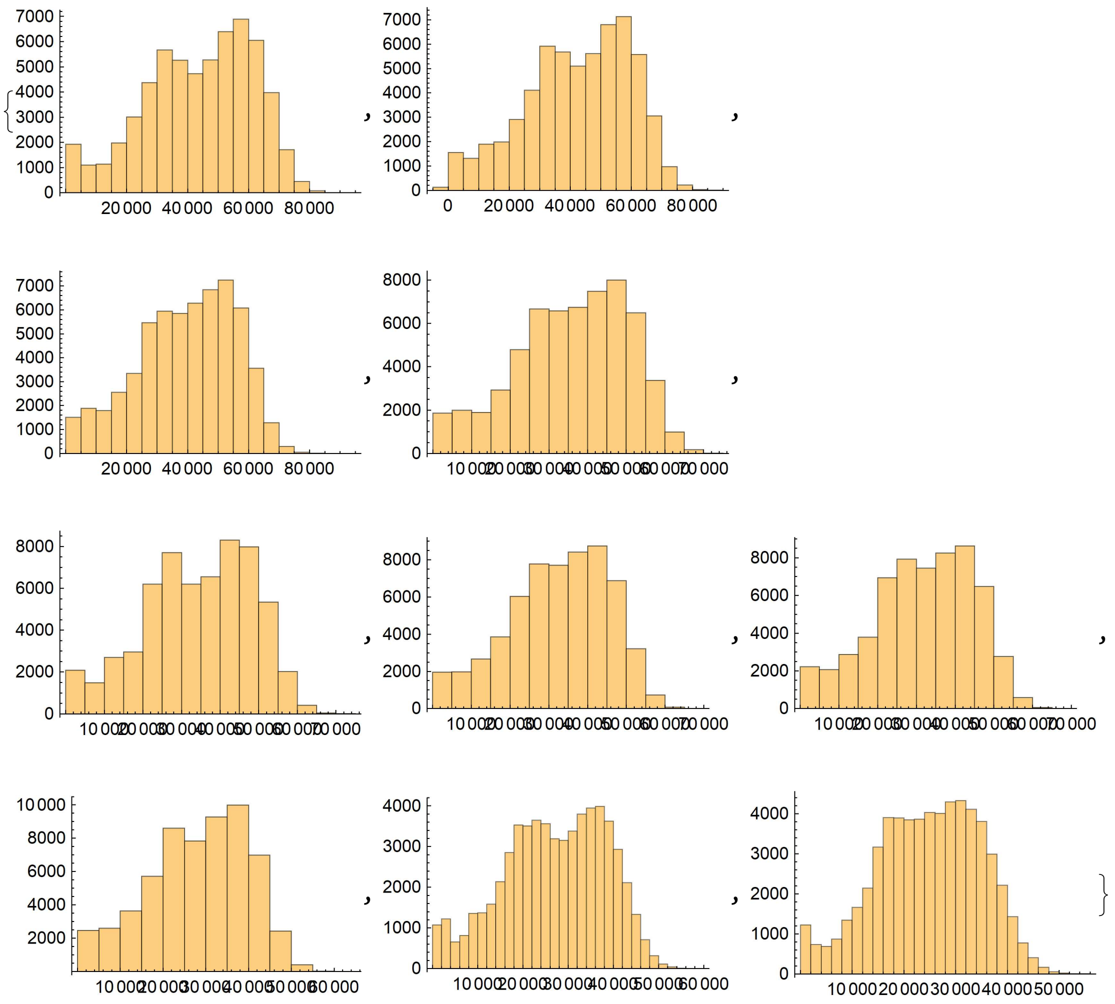
```
In[]:= objfunctionsreactionsdeleted =
  Table[Partition[Flatten[objfunctions, 1][[All, i]], 300], {i, randomreactionlist}];
```

```
In[]:= AbsoluteTiming[
 featuredatalist = Table[Table[MapThread[Dot, {objfunctionsreactionsdeleted[[j]][[i]],
       solutionvectorsreactionsdeleted[[j]][[i]]}], {i, 200}], {j, 10}];]
```

```
Out[]= {50.1076, Null}
```

```
In[ ]:= datafulllist = Table[Join[Partition[Range@60 000, 1],
            Partition[Flatten@Table[ConstantArray[i, 300], {i, 200}], 1],
            Partition[Flatten[featuredatalist[[j]], 1], 1], 2], {j, 10}];
        Table[Histogram@datafulllist[[i]][[All, 3]], {i, 10}]
```

Out[ ]=

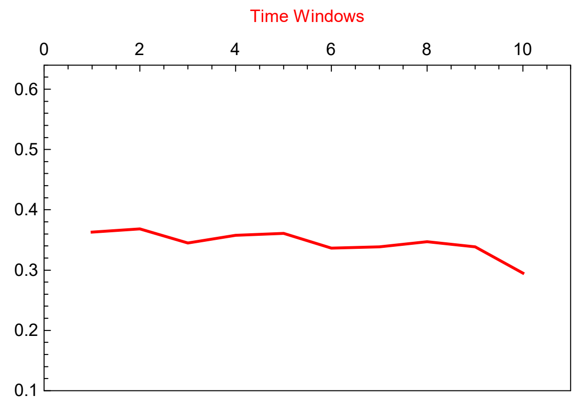


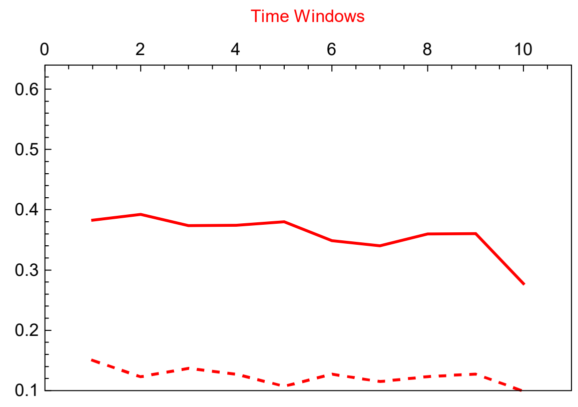
```
In[ ]:= thread = Thread[{Range@10, Range[2000, 1100, -100]}]

Out[ ]= {{1, 2000}, {2, 1900}, {3, 1800}, {4, 1700},
         {5, 1600}, {6, 1500}, {7, 1400}, {8, 1300}, {9, 1200}, {10, 1100}}

In[ ]:= AbsoluteTiming[widthdataFixedstep2 =
           Table[snetworkdatabinned[3, i[[2]], datafulllist[[i[[1]]]]], {i, thread}];]

Out[ ]= {38.9591, Null}

In[ ]:= graphsandnodenumbers12 = Table[snetworkgraph[widthdataFixedstep2[[i]][[1]],
            widthdataFixedstep2[[i]][[2]], 2, 7, 400, Green], {i, 10}];
        graphsandnodenumbers12[[All, 2]]

Out[ ]= {46, 47, 47, 44, 45, 46, 48, 46, 49, 51}
```

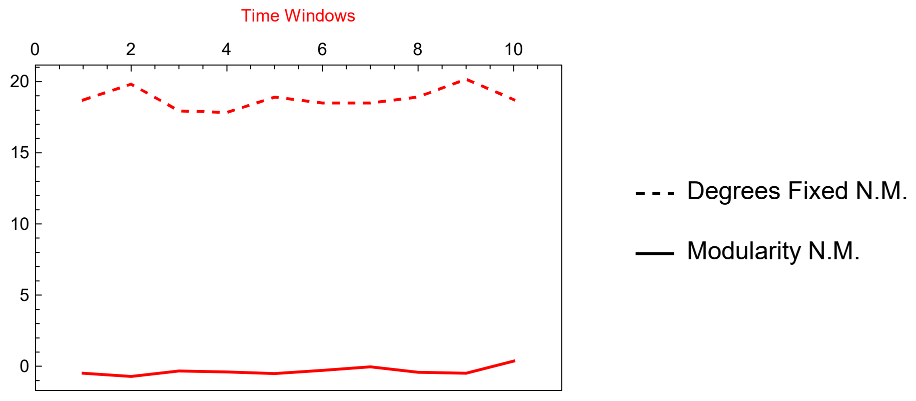
```
In[ ]:= modularityvalues12 = Table[N@GraphAssortativity[graphsandnodenumbers12[[i]][[1]],
           FindGraphCommunities[graphsandnodenumbers12[[i]][[1]]], "Normalized" → False],
        {i, Length@graphsandnodenumbers12}];

In[ ]:= singlerandomgraphsdegfxd12 =
          Table[randomizinggraphdegfxd[i], {i, graphsandnodenumbers12[[All, 1]]}];
        singlerandomerdrenmodularityvalues12 =
          Table[N@GraphAssortativity[singlerandomgraphsdegfxd12[[i]],
             FindGraphCommunities[singlerandomgraphsdegfxd12[[i]]], "Normalized" -> False],
           {i, Length@singlerandomgraphsdegfxd12}];
        singlerandomgraphscomm12 = Table[randomizinggraphmod[i],
           {i, graphsandnodenumbers12[[All, 1]]}];
        singlerandomcommmodularityvalues12 =
          Table[N@GraphAssortativity[singlerandomgraphscomm12[[i]],
             FindGraphCommunities[singlerandomgraphscomm12[[i]]], "Normalized" -> False],
           {i, Length@singlerandomgraphscomm12}];

In[ ]:= AbsoluteTiming[Zscoresmodularity12 =
           Table[zscorefunctionfortwonullmodels[i], {i, graphsandnodenumbers12[[All, 1]]}];]

Out[ ]= {110.433, Null}

In[ ]:= bucketnode12 = graphsandnodenumbers12[[All, 2]]

Out[ ]= {46, 47, 47, 44, 45, 46, 48, 46, 49, 51}
```

```
In[ ]:= modularityvaluestimewinsmall = modularityvalues12;
        randommodtimewinsmalldegreefxd = singlerandomerdrenmodularityvalues12;
        randommodtimewinsmallcomm = singlerandomcommmodularityvalues12;
        Zscoretimewinsmall = Zscoresmodularity12;
        modularityplotrange = {0.1, 0.64};
        (*MinMax[{modularityvalues1,singlerandomcommmodularityvalues1,
          singlerandomerdrenmodularityvalues1,modularityvalues12}]*)
        padding = 38;
        win2 = 10;
        Row[{ListLinePlot[Thread[{Range@win2, modularityvaluestimewinsmall}],
            Frame → True, ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
            FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}}, PlotStyle → Red,
            ImageSize → 350, PlotRange → {{0, win2 + 1}, modularityplotrange}],
          Row[{ListLinePlot[{Thread[{Range@win2, randommodtimewinsmalldegreefxd}],
                Thread[{Range@win2, randommodtimewinsmallcomm}]}, Frame → True,
              ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
              FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}},
              PlotStyle → {{Dashed, Red}, Red}, ImageSize → 350,
              PlotRange → {{0, win2 + 1}, modularityplotrange}],
            ListLinePlot[{Thread[{Range@win2, Zscoretimewinsmall[[All, 1]]}],
                Thread[{Range@win2, Zscoretimewinsmall[[All, 2]]}]}, Frame → True,
              ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
              FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}},
              PlotStyle → {{Dashed, Red}, Red}, ImageSize → 350,
              PlotRange → {{0, win2 + 1}, MinMax[Flatten[Zscoretimewinsmall], 1]}]}],
          LineLegend[{Dashed, Black}, {"Degrees Fixed N.M.", "Modularity N.M."},
            LegendMargins → 0, LegendMarkerSize → {20, 20}], Spacer@0.1}]
```

Out[ ]=





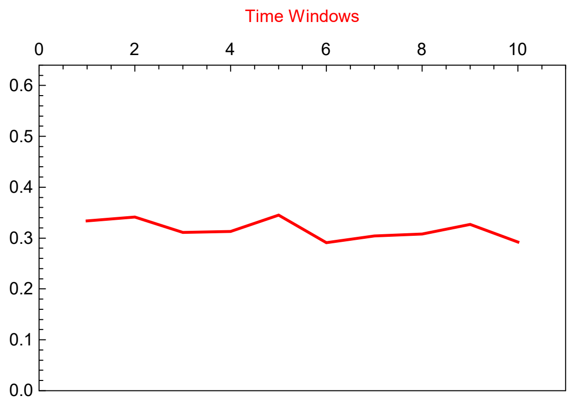


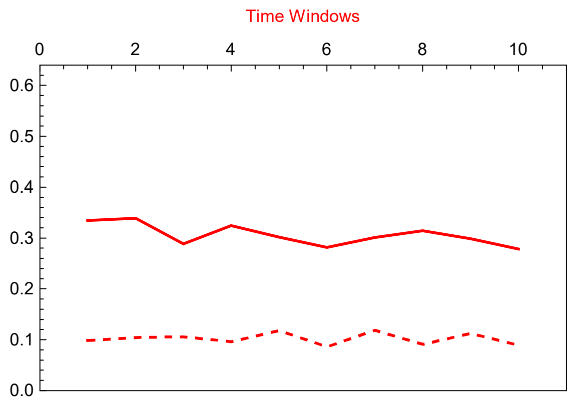
```
In[ ]:= AbsoluteTiming[widthdataFixedbucket2 =
           Table[snetworkdatafxdbucket[3, bucketnode12[[i]], datafulllist[[i]]], {i, 10}];]
Out[ ]= {19.1707, Null}
```

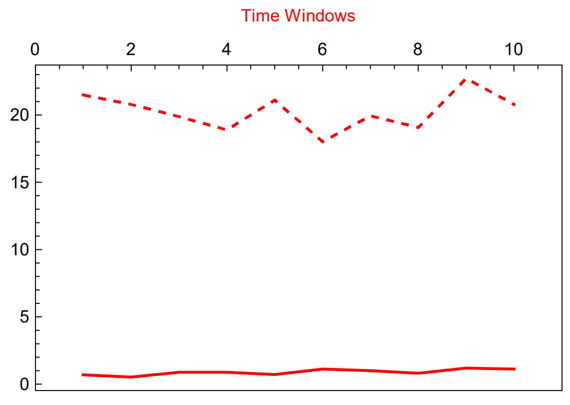
```
In[ ]:= graphsandnodenumbers32 = Table[snetworkgraph[widthdataFixedbucket2[[i]][[1]],
            widthdataFixedbucket2[[i]][[2]], 1.5, 7, 400, Green], {i, 10}];
        modularityvalues32 = Table[N@GraphAssortativity[graphsandnodenumbers32[[i]][[1]],
             FindGraphCommunities[graphsandnodenumbers32[[i]][[1]]], "Normalized" → False],
           {i, Length@graphsandnodenumbers32}];

In[ ]:= singlerandomgraphsdegfxd32 =
          Table[randomizinggraphdegfxd[i], {i, graphsandnodenumbers32[[All, 1]]}];
        singlerandomerdrenmodularityvalues32 =
          Table[N@GraphAssortativity[singlerandomgraphsdegfxd32[[i]],
             FindGraphCommunities[singlerandomgraphsdegfxd32[[i]]], "Normalized" -> False],
           {i, Length@singlerandomgraphsdegfxd32}];
        singlerandomgraphscomm32 = Table[randomizinggraphmod[i],
           {i, graphsandnodenumbers32[[All, 1]]}];
        singlerandomcommmodularityvalues32 =
          Table[N@GraphAssortativity[singlerandomgraphscomm32[[i]],
             FindGraphCommunities[singlerandomgraphscomm32[[i]]], "Normalized" -> False],
           {i, Length@singlerandomgraphscomm32}];

In[ ]:= AbsoluteTiming[Zscoresmodularity32 =
           Table[zscorefunctionfortwonullmodels[i], {i, graphsandnodenumbers32[[All, 1]]}];]

Out[ ]= {119.858, Null}
```

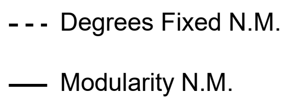
```
In[ ]:= modularityvaluestimewinsmall = modularityvalues32;
        randommodtimewinsmalldegreefxd = singlerandomerdrenmodularityvalues32;
        randommodtimewinsmallcomm = singlerandomcommmodularityvalues32;
        Zscoretimewinsmall = Zscoresmodularity32;
        modularityplotrange = {0, 0.64};
        (*MinMax[{modularityvalues1,singlerandomcommmodularityvalues1,
          singlerandomerdrenmodularityvalues1,modularityvalues12}]*)
        padding = 38;
        win2 = 10;
        Row[{ListLinePlot[Thread[{Range@win2, modularityvaluestimewinsmall}],
            Frame → True, ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
            FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}}, PlotStyle → Red,
            ImageSize → 350, PlotRange → {{0, win2 + 1}, modularityplotrange}],
          Row[{ListLinePlot[{Thread[{Range@win2, randommodtimewinsmalldegreefxd}],
               Thread[{Range@win2, randommodtimewinsmallcomm}]}, Frame → True,
              ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
              FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}},
              PlotStyle → {{Dashed, Red}, Red}, ImageSize → 350,
              PlotRange → {{0, win2 + 1}, modularityplotrange}],
             ListLinePlot[{Thread[{Range@win2, Zscoretimewinsmall[[All, 1]]}],
               Thread[{Range@win2, Zscoretimewinsmall[[All, 2]]}]}, Frame → True,
              ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
              FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}},
              PlotStyle → {{Dashed, Red}, Red}, ImageSize → 350,
              PlotRange → {{0, win2 + 1}, MinMax[Flatten[Zscoretimewinsmall], 1]}]}],
          LineLegend[{Dashed, Black}, {"Degrees Fixed N.M.", "Modularity N.M."},
           LegendMargins → 0, LegendMarkerSize → {20, 20}], Spacer@0.1}]
```

Out[•]=


Time Windows
0
2
4
6
8
10
0.6
0.5
0.4
0.3
0.2
0.1
0.0


Time Windows
0
2
4
6
8
10
0.6
0.5
0.4
0.3
0.2
0.1
0.0


Time Windows
0
2
4
6
8
10
20
15
10
5
0


- - - Degrees Fixed N.M.
—— Modularity N.M.

```
In[ ]:= Export["plot_values/fxd_coeffs/-05+05_105_(-1,1)-modularityvalues-fss.mx",
         modularityvalues12]
        Export["plot_values/fxd_coeffs/-05+05_105_(-1,1)-singrand-erd-modularityvalues-fss.mx",
         singlerandomerdrenmodularityvalues12]
        Export["plot_values/fxd_coeffs/-05+05_105_(-1,1)-singrand-comm-modularityvalues-fss.mx",
         singlerandomcommmodularityvalues12]
        Export["plot_values/fxd_coeffs/-05+05_105_(-1,1)-zscores-fss.mx", Zscoresmodularity12]
        Export["plot_values/fxd_coeffs/-05+05_105_(-1,1)-modularityvalues-fbs.mx",
         modularityvalues32]
        Export["plot_values/fxd_coeffs/-05+05_105_(-1,1)-singrand-erd-modularityvalues-fbs.mx",
         singlerandomerdrenmodularityvalues32]
        Export["plot_values/fxd_coeffs/-05+05_105_(-1,1)-singrand-comm-modularityvalues-fbs.mx",
         singlerandomcommmodularityvalues32]
        Export["plot_values/fxd_coeffs/-05+05_105_(-1,1)-zscores-fbs.mx", Zscoresmodularity32]

Out[ ]= plot_values/fxd_coeffs/-05+05_105_(-1,1)-modularityvalues-fss.mx

Out[ ]= plot_values/fxd_coeffs/-05+05_105_(-1,1)-singrand-erd-modularityvalues-fss.mx

Out[ ]= plot_values/fxd_coeffs/-05+05_105_(-1,1)-singrand-comm-modularityvalues-fss.mx

Out[ ]= plot_values/fxd_coeffs/-05+05_105_(-1,1)-zscores-fss.mx

Out[ ]= plot_values/fxd_coeffs/-05+05_105_(-1,1)-modularityvalues-fbs.mx

Out[ ]= plot_values/fxd_coeffs/-05+05_105_(-1,1)-singrand-erd-modularityvalues-fbs.mx

Out[ ]= plot_values/fxd_coeffs/-05+05_105_(-1,1)-singrand-comm-modularityvalues-fbs.mx

Out[ ]= plot_values/fxd_coeffs/-05+05_105_(-1,1)-zscores-fbs.mx
```