```
hdbscan\ (gary)
   MenW rmsd
    └─ rmsd.txt
    MenY rmsd
    └─ rmsd.txt
    hdbscan men
       - hdbscan_MenW_100_1
           None-embedding-hdbscan.png
           - clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
        hdbscan_MenW_25_1
         — None-embedding-hdbscan.png
           clusters-hdbscan.txt
           results-hdbscan.txt
          — scatterplot-hdbscan.png
        hdbscan_MenW_50_1

    None-embedding-hdbscan.png

           clusters-hdbscan.txt
           results-hdbscan.txt
          scatterplot-hdbscan.png
        hdbscan_MenW_75_1

    None-embedding-hdbscan.png

           clusters-hdbscan.txt
           results-hdbscan.txt
          — scatterplot-hdbscan.png
        hdbscan_MenY_100_1

    None-embedding-hdbscan.png

           - clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
        hdbscan_MenY_25_1

    None-embedding-hdbscan.png

          clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
        hdbscan_MenY_50_1

    None-embedding-hdbscan.png

           clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
        hdbscan_MenY_75_1
         — None-embedding-hdbscan.png
           clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
    hdbscan rmsd
       MenW 100 1
          - MenW_100_1_cluster0
            └─ rmsd.txt
            MenW_100_1_cluster1
            └─ rmsd.txt
           - MenW_100_1_cluster2
```

```
└─ rmsd.txt
            MenW_100_1_cluster3
            └─ rmsd.txt
        MenW_25 1
           - MenW_25_1_cluster12
            └─ rmsd.txt
            MenW_25_1_cluster6
            └─ rmsd.txt
        MenW_50_1
           - MenW 50 1 cluster10
            └─ rmsd.txt
           - MenW_50_1_cluster5
            └─ rmsd.txt
        MenW 75 1
           - MenW_75_1_cluster0
            └─ rmsd.txt
           MenW_75_1_cluster2
            └─ rmsd.txt
            MenW_75_1_cluster3
            └─ rmsd.txt
            MenW_75_1_cluster4
            └─ rmsd.txt
        MenY_25_1_cluster4
          rmsd.txt
        MenY_50_1_cluster1
        └─ rmsd.txt
    hdbscan_test
       hdbscan_breastcancer_30_1_NEW
         — None-embedding-hdbscan.png
           clusters-hdbscan.txt
           scatterplot-hdbscan.png
        hdbscan_digits_50_1_NEW

    None-embedding-hdbscan.png

           clusters-hdbscan.txt
          — scatterplot-hdbscan.png
       hdbscan_iris_5_1_NEW

    None-embedding-hdbscan.png

           clusters-hdbscan.txt
          scatterplot-hdbscan.png
       hdbscan wine 14 1 NEW
          None-embedding-hdbscan.png
          clusters-hdbscan.txt
         — scatterplot-hdbscan.png
hdbscan\ (robyn)
   menW
       hdbmenW_70_1
           clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
      - hdbmenW 75 1
          - clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
       hdbmenW 95 1
```

```
clusters-hdbscan.txt
           results-hdbscan.txt
          scatterplot-hdbscan.png
   menY
       hdbmenY_30_1
         — clusters-hdbscan.txt
          - results-hdbscan.txt
          scatterplot-hdbscan.png
       hdbmenY_45_1
          clusters-hdbscan.txt
           results-hdbscan.txt
          scatterplot-hdbscan.png
      - hdbmenY_50_1
         — clusters-hdbscan.txt
           results-hdbscan.txt
         — scatterplot-hdbscan.png
    sflexneri6_6RU
       hdbSf6 2 1
          clusters-hdbscan.txt
           results-hdbscan.txt
          — scatterplot-hdbscan.png
        hdbSf6_55_1
          clusters-hdbscan.txt
           - results-hdbscan.txt
          scatterplot-hdbscan.png
        hdbSf6_5_1
          — clusters-hdbscan.txt
          results-hdbscan.txt
         — scatterplot-hdbscan.png
    sflexneriY_3RU
       hdbSfY_15_1
           clusters-hdbscan.txt
           results-hdbscan.txt
          scatterplot-hdbscan.png
       hdbSfY 25 1
         — clusters-hdbscan.txt
          - results-hdbscan.txt
          scatterplot-hdbscan.png
       hdbSfY_5_1
          - clusters-hdbscan.txt
           results-hdbscan.txt
          scatterplot-hdbscan.png
hierarchical
   MenW_hierarchical_average
      - RMSD-matrix.png
      - clusters-hierarchical.txt
      - dendrogram-clustering-average-W.png
       results-hierarchical.txt
      scatterplot-hierarchical.png
   MenW hierarchical complete
      - RMSD-matrix.png
       clusters-hierarchical.txt

    dendrogram-clustering-complete-W.png

      results-hierarchical.txt
```

```
scatterplot-hierarchical.png
   MenW_hierarchical_single
      - RMSD-matrix.png
       clusters-hierarchical.txt
       dendrogram-clustering-single-W.png
      scatterplot-hierarchical.png
   MenW_hierarchical_ward
      - RMSD-matrix.png
      clusters-hierarchical.txt
      - dendrogram-clustering-ward-W.png
       results-hierarchical.txt
      scatterplot-hierarchical.png
   MenY_hierarchical_average
     — RMSD-matrix.png
      clusters-hierarchical.txt
     dendrogram-clustering-average-Y.png
      results-hierarchical.txt
     scatterplot-hierarchical.png
   MenY_hierarchical_complete
      RMSD-matrix.png
      clusters-hierarchical.txt
      dendrogram-clustering-complete-Y.png
      results-hierarchical.txt
      - scatterplot-hierarchical.png
   MenY_hierarchical_single
      - RMSD-matrix.png
      clusters-hierarchical.txt
     dendrogram-clustering-single-Y.png
     — results-hierarchical.txt
      scatterplot-hierarchical.png
   MenY_hierarchical_ward
      - RMSD-matrix.png
      clusters-hierarchical.txt
      dendrogram-clustering-ward-Y.png
      results-hierarchical.txt
      scatterplot-hierarchical.png
   dendograms

    dendrogram-clustering-average-W.png

      dendrogram-clustering-average-Y.png
      dendrogram-clustering-complete-W.png
      dendrogram-clustering-complete-Y.png
      dendrogram-clustering-single-W.png
      dendrogram-clustering-ward-W.png
     — dendrogram-clustering-ward-Y.png
imwk-means
  - menW
      clusters-imwkmeans.txt
       results-imwkmeans.txt
      scatterplot-imwkmeans.png
   menY
      clusters-imwkmeans.txt
       results-imwkmeans.txt
       scatterplot-imwkmeans.png
   sflexneri6 6RU
```

```
clusters-imwkmeans.txt
       results-imwkmeans.txt
      scatterplot-imwkmeans.png
   sflexneriY 3RU
      clusters-imwkmeans.txt
       results-imwkmeans.txt
       scatterplot-imwkmeans.png
output.txt
qt
  - MenW(1.5)
      – RMSD-matrix.png
      - clusters-qt.txt
      — results-qt.txt
       - rmsd-vs-frame.png
      scatterplot-qt.png
    MenW(2.5)
      RMSD-matrix.png
      — clusters-qt.txt
      - results-qt.txt
       - rmsd-vs-frame.png
      — scatterplot-qt.png
    MenW(3.5)
      RMSD-matrix.png
       - clusters-qt.txt
      — results-qt.txt
       - rmsd-vs-frame.png
     — scatterplot-qt.png
    MenW(4.5)
     — RMSD-matrix.png
      - clusters-qt.txt
       results-qt.txt
       - rmsd-vs-frame.png
      — scatterplot-qt.png
    MenY(1.5)
      RMSD-matrix.png
       - clusters-qt.txt
       - results-qt.txt
       - rmsd-vs-frame.png
      scatterplot-qt.png
   - MenY(2.5)
      RMSD-matrix.png
      - clusters-qt.txt
      - results-qt.txt
       - rmsd-vs-frame.png
       scatterplot-qt.png
    MenY(3.5)
       - RMSD-matrix.png
       - clusters-qt.txt
       - results-qt.txt
        rmsd-vs-frame.png
      scatterplot-qt.png
    MenY(4.5)
       - RMSD-matrix.png
       - clusters-qt.txt
```

```
- results-qt.txt
       rmsd-vs-frame.png
       scatterplot-qt.png
    S3RUY(2.5)
      RMSD-matrix.png
      - clusters-qt.txt
       results-qt.txt
       rmsd-vs-frame.png
      scatterplot-qt.png
    S3RUY(3.5)
      - RMSD-matrix.png
      – clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
      scatterplot-qt.png
    S3RUY(4.5)
      - RMSD-matrix.png
      - clusters-qt.txt
      - results-qt.txt
      - rmsd-vs-frame.png
      — scatterplot-qt.png
    S6RU6(6.5)
      RMSD-matrix.png
      clusters-qt.txt
     - results-qt.txt
      - rmsd-vs-frame.png
     — scatterplot-qt.png
    S6RU6(7)
     — RMSD-matrix.png
      - clusters-qt.txt
       results-qt.txt
      - rmsd-vs-frame.png
      scatterplot-qt.png
    S6RU6(7.5)
      - RMSD-matrix.png
      clusters-qt.txt
      - results-qt.txt
       rmsd-vs-frame.png
      - scatterplot-qt.png
gtvector
   MenW(1.5)
      RMSD-matrix.png
      clusters-qtvector.txt
      results-qtvector.txt
      - rmsd-vs-frame.png
      scatterplot-qtvector.png
   MenW(2.5)
      - RMSD-matrix.png
      clusters-qtvector.txt
      results-qtvector.txt
       rmsd-vs-frame.png
       scatterplot-qtvector.png
   MenW(3.5)
      RMSD-matrix.png
```

```
clusters-qtvector.txt
   results-qtvector.txt
    rmsd-vs-frame.png
   scatterplot-qtvector.pnq
MenW(4.5)
  — RMSD-matrix.png
   - clusters-qtvector.txt
   results-qtvector.txt
   - rmsd-vs-frame.png
  scatterplot-qtvector.png
MenY(1.5)
  RMSD-matrix.png
   clusters-qtvector.txt
   results-qtvector.txt
   - rmsd-vs-frame.png
  scatterplot-qtvector.png
MenY(2.5)
   RMSD-matrix.png
   - clusters-qtvector.txt
  - results-qtvector.txt
   - rmsd-vs-frame.png
  — scatterplot-qtvector.png
MenY(3.5)
   – RMSD–matrix.png
   clusters-qtvector.txt
   results-qtvector.txt
   - rmsd-vs-frame.png
  scatterplot-qtvector.png
MenY(4.5)
   – RMSD-matrix.png
   clusters-qtvector.txt
   results-qtvector.txt
   - rmsd-vs-frame.png
  scatterplot-qtvector.png
S3RUY(2.5)
  — RMSD-matrix.png
   - clusters-qtvector.txt
   results-qtvector.txt
   - rmsd-vs-frame.png
  scatterplot-qtvector.png
S3RUY(3.5)
  RMSD-matrix.png
   clusters-qtvector.txt
   - results-qtvector.txt
   - rmsd-vs-frame.png
   scatterplot-qtvector.png
S3RUY(4.5)
   - RMSD-matrix.png
   clusters-qtvector.txt
   results-qtvector.txt
   - rmsd-vs-frame.png
   scatterplot-qtvector.png
S6RU6(6.5)
   RMSD-matrix.png
```

```
clusters-qtvector.txt
        results-qtvector.txt
        rmsd-vs-frame.png
        scatterplot-qtvector.png
    S6RU6(7)
      RMSD-matrix.png
       clusters-qtvector.txt
        results-qtvector.txt
        rmsd-vs-frame.png
      scatterplot-qtvector.pnq
    S6RU6(7.5)
      - RMSD-matrix.png
        clusters-qtvector.txt
        results-qtvector.txt
       rmsd-vs-frame.png
      scatterplot-qtvector.png
umap
    umap_men
        umap_hdbscan_MenW_100_1_100_2
           - clusters-hdbscan.txt
            results-hdbscan.txt
           scatterplot-hdbscan.png
           umap-embedding-hdbscan.png
        umap_hdbscan_MenW_100_1_100_30
           clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
           umap-embedding-hdbscan.png
        umap_hdbscan_MenW_100_1_50_2
           clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
           umap-embedding-hdbscan.png
        umap_hdbscan_MenW_100_1_50_30
           clusters-hdbscan.txt
           results-hdbscan.txt
            scatterplot-hdbscan.png
           umap-embedding-hdbscan.png
        umap_hdbscan_MenW_50_1_100_2
           clusters-hdbscan.txt
           results-hdbscan.txt
           scatterplot-hdbscan.png
            umap-embedding-hdbscan.png
        umap_hdbscan_MenW_50_1_100_30
           clusters-hdbscan.txt
            results-hdbscan.txt
           scatterplot-hdbscan.png
           - umap-embedding-hdbscan.png
        umap_hdbscan_MenW_50_1_50_2
           - clusters-hdbscan.txt
            results-hdbscan.txt
           scatterplot-hdbscan.png
           umap-embedding-hdbscan.png
        umap_hdbscan_MenW_50_1_50_30
```

```
clusters-hdbscan.txt
        results-hdbscan.txt
        scatterplot-hdbscan.png
       umap-embedding-hdbscan.png
    umap_hdbscan_MenY_100_1_100_2
      clusters-hdbscan.txt
        results-hdbscan.txt
        scatterplot-hdbscan.png
      umap-embedding-hdbscan.png
   umap_hdbscan_MenY_100_1_100_30
      clusters-hdbscan.txt
      results-hdbscan.txt
       scatterplot-hdbscan.png
      - umap-embedding-hdbscan.png
   umap_hdbscan_MenY_100_1_50_2
      clusters-hdbscan.txt
      results-hdbscan.txt
      scatterplot-hdbscan.png
       umap-embedding-hdbscan.png
    umap_hdbscan_MenY_100_1_50_30
      clusters-hdbscan.txt
       results-hdbscan.txt
      scatterplot-hdbscan.png
      umap-embedding-hdbscan.png
    umap_hdbscan_MenY_50_1_100_2
      - clusters-hdbscan.txt
      results-hdbscan.txt
       scatterplot-hdbscan.png
       umap-embedding-hdbscan.png
    umap_hdbscan_MenY_50_1_100_30
       clusters-hdbscan.txt
       results-hdbscan.txt
      scatterplot-hdbscan.png
      umap-embedding-hdbscan.png
    umap_hdbscan_MenY_50_1_50_2
      clusters-hdbscan.txt
       results-hdbscan.txt
      - scatterplot-hdbscan.png
      umap-embedding-hdbscan.png
   umap hdbscan MenY 50 1 50 30
      clusters-hdbscan.txt
      results-hdbscan.txt
      - scatterplot-hdbscan.png
      umap-embedding-hdbscan.png
umap_rmsd
   MenW_100_1_100_2_cluster1
      rmsd.txt
   MenW_100_1_100_2_cluster2
     — rmsd.txt
   MenW_100_1_100_2_cluster5
    └─ rmsd.txt
   MenW_100_1_100_30_cluster0
      rmsd.txt
   MenW_100_1_100_30_cluster1
```

```
└─ rmsd.txt
MenW_100_1_100_30_cluster6
└─ rmsd.txt
MenW_100_1_50_2_cluster0
└─ rmsd.txt
MenW_100_1_50_2_cluster3
└─ rmsd.txt
MenW_100_1_50_2_cluster5
└─ rmsd.txt
MenW_100_1_50_30_cluster0
└─ rmsd.txt
MenW_100_1_50_30_cluster2
└─ rmsd.txt
MenW_100_1_50_30_cluster5
└─ rmsd.txt
MenW_100_1_50_30_cluster6
└─ rmsd.txt
MenW_100_1_50_30_cluster7
└─ rmsd.txt
MenW_50_1_100_2_cluster1
└─ rmsd.txt
MenW_50_1_100_2_cluster2
└─ rmsd.txt
MenW_50_1_100_2_cluster5
└─ rmsd.txt
MenW_50_1_100_30_cluster0
└─ rmsd.txt
MenW_50_1_100_30_cluster1
└─ rmsd.txt
MenW_50_1_100_30_cluster7
└─ rmsd.txt
MenW_50_1_50_2_cluster0
└─ rmsd.txt
MenW_50_1_50_2_cluster4
└─ rmsd.txt
MenW_50_1_50_30_cluster0
└─ rmsd.txt
MenW_50_1_50_30_cluster2
└─ rmsd.txt
MenW_50_1_50_30_cluster5
└─ rmsd.txt
MenW_50_1_50_30_cluster9
└─ rmsd.txt
MenY_100_1_100_2_cluster1
└─ rmsd.txt
MenY_100_1_100_30_cluster1
└─ rmsd.txt
MenY_100_1_50_2_cluster1
└─ rmsd.txt
MenY_100_1_50_30_cluster1
└─ rmsd.txt
MenY_50_1_100_2_cluster3
└─ rmsd.txt
MenY_50_1_100_30_cluster2
```

```
└─ rmsd.txt
   MenY_50_1_50_2_cluster3
    └─ rmsd.txt
   MenY_50_1_50_30_cluster2
    └─ rmsd.txt
umap_test
  - umap_hdbscan_breastcancer_150_1_20_2
      - clusters-hdbscan.txt
      results-hdbscan.txt
      scatterplot-hdbscan.png
     — umap-embedding-hdbscan.png
   umap_hdbscan_digits_100_1_15_2
     — clusters-hdbscan.txt
     — results-hdbscan.txt
      scatterplot-hdbscan.png
      — umap-embedding-hdbscan.png
   - umap_hdbscan_iris_30_1_20_2
     — clusters-hdbscan.txt
      - results-hdbscan.txt
      scatterplot-hdbscan.png
      — umap-embedding-hdbscan.png
   umap_hdbscan_wine_30_1_30_2
      - clusters-hdbscan.txt
      results-hdbscan.txt
     scatterplot-hdbscan.pngumap-embedding-hdbscan.png
```

156 directories, 409 files