```
import networkx as nx
import numpy as np
import matplotlib.pyplot as plt
import random
import os
```

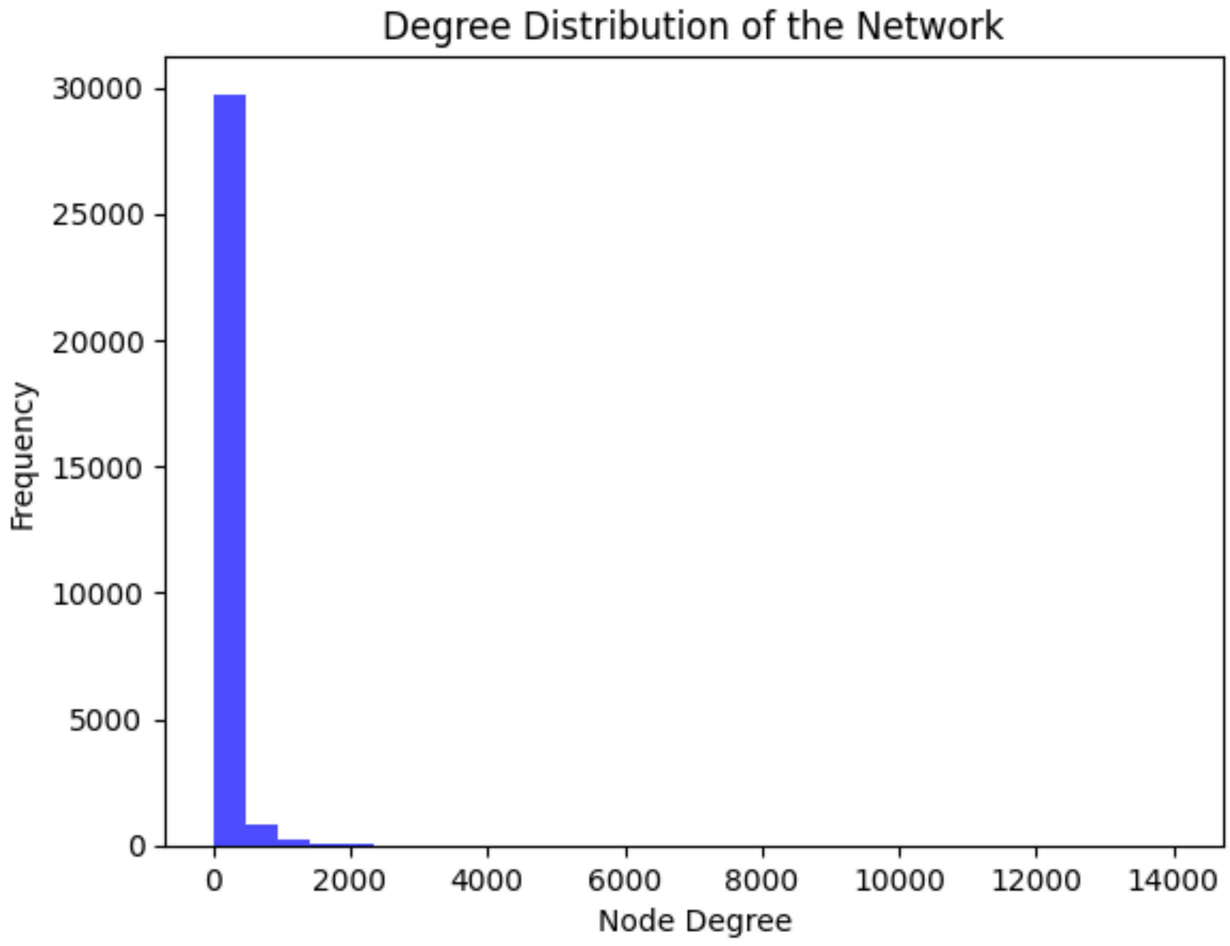
```
# Corrected File Path
file_path = "/content/PathwayCommons12.All.hgnc.sif"  # Adjust if needed

# Initialize an empty graph
G = nx.Graph()

# Read the SIF file and build the graph
with open(file_path, "r") as f:
    for line in f:
        parts = line.strip().split("\t")
        if len(parts) == 3:  # Ensure correct format (source, interaction, target
            source, interaction, target = parts
            G.add_edge(source, target)  # Adding only interacting proteins

# Check if graph loaded correctly
print(f"Loaded network with {G.number_of_nodes()} nodes and {G.number_of_edges()}
```

```
Loaded network with 30918 nodes and 1708952 edges
```

```
# Approximate Clustering for Faster Computation
sample_nodes = random.sample(list(G.nodes()), min(1000, len(G.nodes())))
approx_clustering_coeff = nx.average_clustering(G, nodes=sample_nodes)
print(f"Approximate Clustering Coefficient: {approx_clustering_coeff}")

# Global Clustering Coefficient (Faster Alternative)
global_clustering = nx.transitivity(G)
print(f"Global Clustering Coefficient: {global_clustering}")

# Compute Network Density
print(f"Network Density: {nx.density(G)}")
```

```
Approximate Clustering Coefficient: 0.27512942139385266
Global Clustering Coefficient: 0.0560354733068454
Network Density: 0.0035756180548324524
```

```
# Visualize Degree Distribution
degree_sequence = [d for n, d in G.degree()]
plt.hist(degree_sequence, bins=30, color="blue", alpha=0.7)
plt.xlabel("Node Degree")
plt.ylabel("Frequency")
plt.title("Degree Distribution of the Network")
plt.show()
```



```
!apt-get install -y mcl
```

```
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
mcl is already the newest version (1:14-137+ds-9build2).
0 upgraded, 0 newly installed, 0 to remove and 29 not upgraded.
```

```
# Save the network in MCL-compatible format
edge_list_file = "network_mcl.txt"
nx.write_edgelist(G, edge_list_file, data=False)

print(f"Network saved to {edge_list_file} for MCL processing.")
```

```
Network saved to network_mcl.txt for MCL processing.
```

```
# Run MCL with default settings (adjust --I for inflation factor tuning)
!mcl network_mcl.txt --abc -o clusters.txt -I 1.8
```

```
............................................ 1M
..................................
[mcl] new tab created
[mcl] pid 9027
 ite -------------------  chaos  time hom(avg,lo,hi) m-ie m-ex i-ex fmv
  1  ................... 1753.50 46.13 1.76/0.00/17.96 112.24 12.20 12.20  78
  2  ................... 318.77 420.53 0.30/0.01/1.94 16.83 0.81 9.90  99
  3  ................... 124.72 233.98 0.44/0.03/2.34 11.33 0.16 1.55  99
  4  ...................  22.92  8.92 0.86/0.09/4.25 4.87 0.18 0.27  98
  5  ...................   9.31  0.61 0.93/0.23/2.93 2.08 0.25 0.07   0
  6  ...................   4.61  0.10 0.96/0.22/2.42 1.42 0.61 0.04   0
  7  ...................   2.54  0.06 0.97/0.32/1.84 1.08 0.84 0.03   0
  8  ...................   2.47  0.05 0.98/0.32/2.05 1.02 0.92 0.03   0
  9  ...................   2.10  0.05 0.99/0.43/1.39 1.01 0.96 0.03   0
 10  ...................   1.80  0.05 0.98/0.41/1.00 1.01 0.93 0.03   0
 11  ...................   1.32  0.04 0.94/0.43/1.00 1.00 0.99 0.03   0
 12  ...................   1.04  0.05 0.84/0.47/1.00 1.00 0.99 0.03   0
 13  ...................   1.16  0.04 0.71/0.52/1.00 1.00 1.00 0.03   0
 14  ...................   0.99  0.04 0.71/0.50/1.00 1.00 1.00 0.03   0
 15  ...................   0.75  0.04 0.89/0.68/1.00 1.00 0.99 0.03   0
 16  ...................   0.61  0.04 0.99/0.76/1.00 1.00 1.00 0.03   0
 17  ...................   0.23  0.04 1.00/0.77/1.00 1.00 0.32 0.01   0
 18  ...................   0.22  0.03 1.00/0.82/1.00 1.00 1.00 0.01   0
 19  ...................   0.25  0.03 1.00/0.76/1.00 1.00 1.00 0.01   0
 20  ...................   0.16  0.03 1.00/0.84/1.00 1.00 1.00 0.01   0
 21  ...................   0.23  0.03 1.00/0.81/1.00 1.00 1.00 0.01   0
 22  ...................   0.25  0.03 1.00/0.76/1.00 1.00 1.00 0.01   0
 23  ...................   0.15  0.03 1.00/0.85/1.00 1.00 1.00 0.01   0
 24  ...................   0.03  0.03 1.00/0.97/1.00 1.00 1.00 0.01   0
 25  ...................   0.00  0.03 1.00/1.00/1.00 1.00 1.00 0.01   0
 26  ...................   0.00  0.03 1.00/1.00/1.00 1.00 1.00 0.01   0
[mcl] jury pruning marks: <28,77,96>, out of 100
[mcl] jury pruning synopsis: <48.8 or off colour> (cf -scheme, -do log)
[mcl] output is in clusters.txt
```

```
[mcl] 467 clusters found
[mcl] output is in clusters.txt

Please cite:
    Stijn van Dongen, Graph Clustering by Flow Simulation.  PhD thesis,
    University of Utrecht, May 2000.
       (  http://www.library.uu.nl/digiarchief/dip/diss/1895620/full.pdf
       or  http://micans.org/mcl/lit/svdthesis.pdf.gz)
OR
    Stijn van Dongen, A cluster algorithm for graphs. Technical
    Report INS-R0010, National Research Institute for Mathematics
    and Computer Science in the Netherlands, Amsterdam, May 2000.
       (  http://www.cwi.nl/ftp/CWIreports/INS/INS-R0010.ps.Z
       or  http://micans.org/mcl/lit/INS-R0010.ps.Z)
```

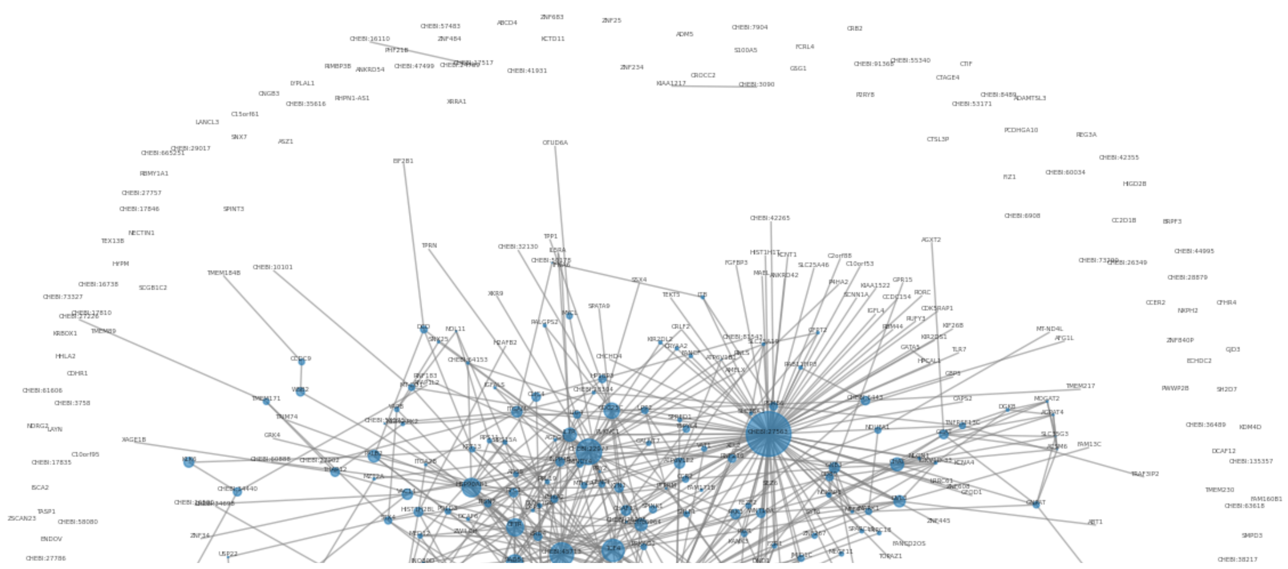
```python
# Read MCL clusters from the output file
clusters = []
with open("clusters.txt", "r") as f:
    for line in f:
        cluster = line.strip().split("\t")
        clusters.append(cluster)

# Print number of clusters detected
print(f"Number of clusters detected: {len(clusters)}")

# Display the first 5 clusters
for i, cluster in enumerate(clusters[:5]):
    print(f"Cluster {i+1}: {cluster}")
```

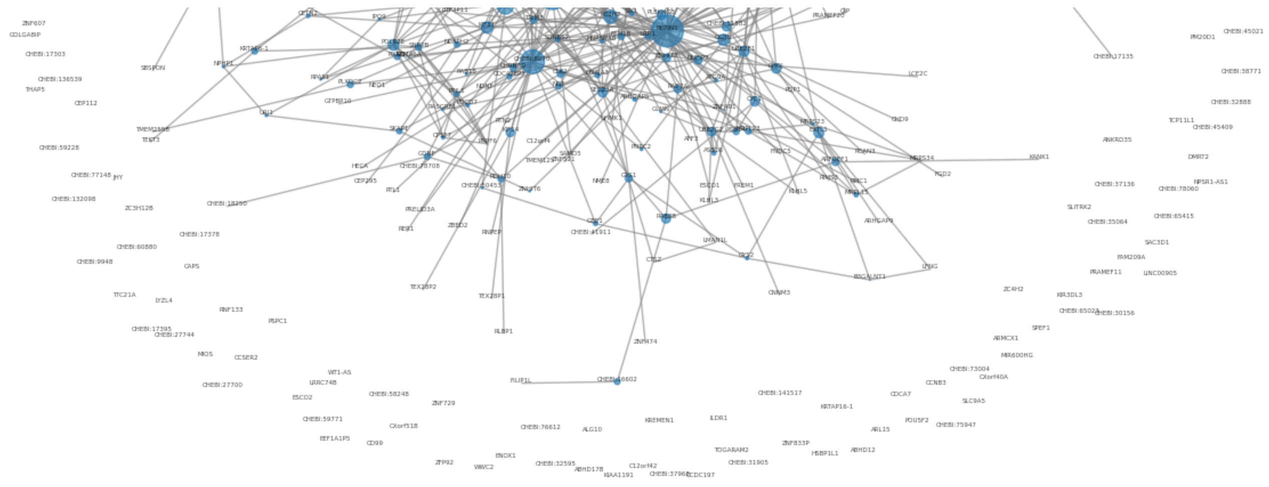
```
Number of clusters detected: 467
Cluster 1: ['A1BG', 'A2M', 'ADAM10', 'ADAM17', 'ADAM9', 'AGO1', 'ANXA7', 'CRI
Cluster 2: ['ABCC6', 'AKT1', 'CDKN1A', 'GCLC', 'CASP3', 'CASP9', 'CTSB', 'MMP
Cluster 3: ['CYP2C18', 'CYP2C8', 'LCAT', 'CHEBI:3687', 'CHEBI:5356', 'CYP2A13
Cluster 4: ['OR4S2', 'GNB1', 'GNGT1', 'OR14I1', 'OR6T1', 'REEP1', 'REEP4', 'R
Cluster 5: ['CPT2', 'HADHB', 'ACADS', 'CPT1A', 'HADHA', 'ELOVL5', 'PANK1', 'P
```

```python
import networkx as nx
import matplotlib.pyplot as plt
import numpy as np
import random

# Pick a sample cluster
sample_cluster_nodes = clusters[0]  # Select first cluster
subgraph = G.subgraph(sample_cluster_nodes)
```

```
# Ensure the cluster is connected (some clusters may be fragmented)
if nx.is_connected(subgraph):
    largest_cc = subgraph
else:
    largest_cc = max(nx.connected_components(subgraph), key=len)
    subgraph = G.subgraph(largest_cc)

# ⚡ **Speed Boost: Limit to 500 Nodes for Faster Visualization**
if len(subgraph.nodes()) > 500:
    sample_nodes = random.sample(list(subgraph.nodes()), 500)
    subgraph = G.subgraph(sample_nodes)

# ⚡ **Faster Layout Calculation with Better Node Spacing**
pos = nx.spring_layout(subgraph, seed=42, k=0.2)  # Higher k spreads nodes out

# ⚡ **Compute node centrality (betweenness) to scale node sizes**
centrality = nx.betweenness_centrality(subgraph)
node_sizes = np.array([centrality[n] for n in subgraph.nodes()]) * 5000  # Scale

# ⚡ **Optimized Plotting with Centrality-Based Node Sizing**
plt.figure(figsize=(12, 10))
nx.draw(subgraph, pos, with_labels=False, node_size=node_sizes, edge_color="gray"
nx.draw_networkx_labels(subgraph, pos, font_size=4, alpha=0.7, verticalalignment=

plt.title("Enhanced Visualization with Centrality-Based Node Sizing")
plt.show()
```

Enhanced Visualization with Centrality-Based Node Sizing





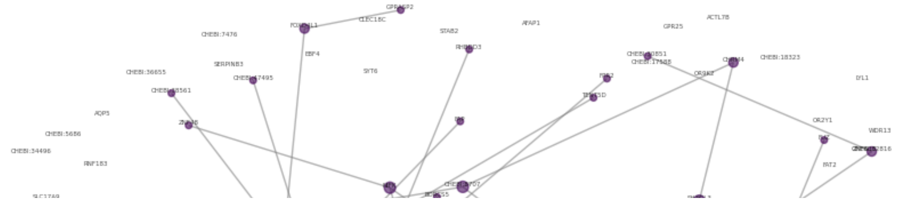
MCODE

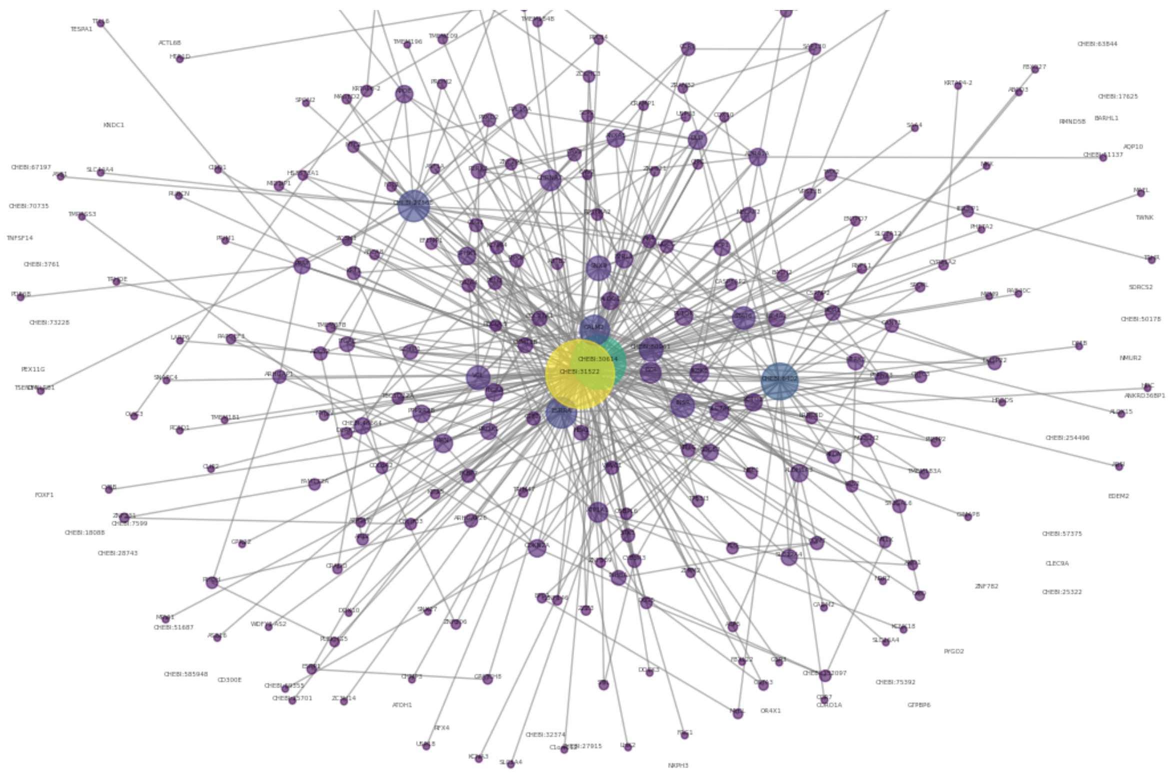
```
import networkx as nx
import numpy as np
import matplotlib.pyplot as plt
import random
import os
import matplotlib.cm as cm
from networkx.algorithms.community import k_clique_communities

# Corrected File Path
```

```
file_path = "/content/PathwayCommons12.All.hgnc.sif"  # Adjust if needed

# Initialize an empty graph
G = nx.Graph()

# Read the SIF file and build the graph
with open(file_path, "r") as f:
    for line in f:
        parts = line.strip().split("\t")
        if len(parts) == 3:  # Ensure correct format (source, interaction, target
            source, interaction, target = parts
            G.add_edge(source, target)  # Adding only interacting proteins

# Check if graph loaded correctly
print(f"Loaded network with {G.number_of_nodes()} nodes and {G.number_of_edges()}

# **Step 1: Reduce Graph Size for Faster MCODE Execution**
num_nodes = 5000  # Adjust this number based on performance
sample_nodes = random.sample(list(G.nodes()), num_nodes)
subgraph = G.subgraph(sample_nodes)

print(f"Using subgraph with {subgraph.number_of_nodes()} nodes and {subgraph.numb

# **Step 2: Run MCODE Approximation (k-Clique Method) on Reduced Graph**
k = 3  # Smaller value = faster computation

# Run MCODE-like clustering
clique_communities = list(k_clique_communities(subgraph, k))

# Convert detected communities to list format
mcode_clusters = [list(community) for community in clique_communities]

print(f"Number of MCODE-like clusters detected: {len(mcode_clusters)}")

# Print first 5 detected clusters
for i, cluster in enumerate(mcode_clusters[:5]):
    print(f"MCODE Cluster {i+1}: {cluster}")

# **Step 3: Visualize a Sample MCODE Cluster**
# Pick a sample MCODE cluster
sample_mcode_nodes = mcode_clusters[0]  # Select first cluster
subgraph_mcode = subgraph.subgraph(sample_mcode_nodes)

# Ensure the cluster is connected
if nx.is_connected(subgraph_mcode):
    largest_cc_mcode = subgraph_mcode
else:
    largest_cc_mcode = max(nx.connected_components(subgraph_mcode), key=len)
    subgraph_mcode = subgraph.subgraph(largest_cc_mcode)

# ⚡ **Limit the number of nodes for better visualization**
if len(subgraph_mcode.nodes()) > 300:
    sample_nodes = random.sample(list(subgraph_mcode.nodes()), 300)
    subgraph_mcode = subgraph_mcode.subgraph(sample_nodes)

# Faster Layout Calculation
pos_mcode = nx.spring_layout(subgraph_mcode, seed=42, k=0.4)  # Higher k spreads

# Compute node degree centrality for sizing and coloring
degree_centrality = nx.degree_centrality(subgraph_mcode)
node_sizes_mcode = np.array([degree_centrality[n] for n in subgraph_mcode.nodes()

# Normalize for colormap
norm = plt.Normalize(vmin=min(degree_centrality.values()), vmax=max(degree_centra
colors = [cm.viridis(norm(degree_centrality[n])) for n in subgraph_mcode.nodes()]

# Optimized Plot
plt.figure(figsize=(12, 10))
nx.draw(subgraph_mcode, pos_mcode, with_labels=False, node_size=node_sizes_mcode,
nx.draw_networkx_labels(subgraph_mcode, pos_mcode, font_size=4, alpha=0.7, vertic

plt.title("Enhanced Visualization of Sample MCODE Cluster")
plt.show()
```

```
Loaded network with 30918 nodes and 1708952 edges
Using subgraph with 5000 nodes and 46275 edges
Number of MCODE-like clusters detected: 20
MCODE Cluster 1: ['TAP1', 'YPEL4', 'KCTD10', 'CHEBI:17824', 'PRRC2C', 'RCCD1',
MCODE Cluster 2: ['CHEBI:15905', 'CHEBI:17677', 'CHEBI:17561']
MCODE Cluster 3: ['CHEBI:15820', 'GMPPA', 'CHEBI:18205']
MCODE Cluster 4: ['CHEBI:32816', 'CHEBI:16946', 'CHEBI:17442']
MCODE Cluster 5: ['CHEBI:31440', 'OR9A4', 'REEP2']
```

Enhanced Visualization of Sample MCODE Cluster





lets Perform biological analysis of the clusters.

```
# Check if clusters exist, otherwise reload from saved files
if 'clusters' not in globals():
    print("⚠️ MCL clusters not found! Reloading clusters from file...")
    clusters = []
    with open("clusters.txt", "r") as f:
        for line in f:
            cluster = line.strip().split("\t")
            clusters.append(cluster)

if 'mcode_clusters' not in globals():
    print("⚠️ MCODE clusters not found! Re-running MCODE clustering...")
    from networkx.algorithms.community import k_clique_communities
    k = 3  # Minimum clique size
    clique_communities = list(k_clique_communities(G, k))
    mcode_clusters = [list(community) for community in clique_communities]
```

```python
from collections import Counter

# Function to extract hub nodes from a cluster
def get_hub_nodes(cluster, G, top_n=5):
    degrees = {node: G.degree(node) for node in cluster}
    sorted_nodes = sorted(degrees.items(), key=lambda x: x[1], reverse=True)
    return [node for node, _ in sorted_nodes[:top_n]]

# Get top 5 clusters from MCL and MCODE
top_mcl_clusters = clusters[:5]  # From MCL
top_mcode_clusters = mcode_clusters[:5]  # From MCODE

# Extract hub nodes
hub_nodes_mcl = [get_hub_nodes(cluster, G) for cluster in top_mcl_clusters]
hub_nodes_mcode = [get_hub_nodes(cluster, G) for cluster in top_mcode_clusters]

# Print hub nodes
for i, hubs in enumerate(hub_nodes_mcl):
    print(f"🔷 MCL Cluster {i+1} Hub Nodes: {hubs}")

for i, hubs in enumerate(hub_nodes_mcode):
    print(f"🔷 MCODE Cluster {i+1} Hub Nodes: {hubs}")
```

```
🔷 MCL Cluster 1 Hub Nodes: ['CHEBI:39867', 'CHEBI:4667', 'CHEBI:60654', 'CHE
🔷 MCL Cluster 2 Hub Nodes: ['PTK2', 'CASP3', 'RELA', 'AKT1', 'PARP1']
🔷 MCL Cluster 3 Hub Nodes: ['CYP3A4', 'CYP2C19', 'CYP2C9', 'CYP2D6', 'NCOA1'
🔷 MCL Cluster 4 Hub Nodes: ['GNB1', 'GNGT1', 'GNAL', 'REEP4', 'REEP5']
🔷 MCL Cluster 5 Hub Nodes: ['ACSL1', 'HADHB', 'CHEBI:57287', 'CPT1A', 'HADHA
🔷 MCODE Cluster 1 Hub Nodes: ['CHEBI:60654', 'CHEBI:31522', 'CHEBI:31440', '
🔷 MCODE Cluster 2 Hub Nodes: ['CHEBI:17677', 'CHEBI:17561', 'CHEBI:15905']
🔷 MCODE Cluster 3 Hub Nodes: ['GMPPA', 'CHEBI:15820', 'CHEBI:18205']
🔷 MCODE Cluster 4 Hub Nodes: ['CHEBI:32816', 'CHEBI:16946', 'CHEBI:17442']
🔷 MCODE Cluster 5 Hub Nodes: ['CHEBI:31440', 'REEP2', 'OR9A4']
```

Next to compare MCL and MCODE Clustering

Let's compare the number of clusters, average cluster size, and density for MCL and MCODE.

```python
# Function to calculate basic cluster statistics
def cluster_statistics(cluster_list, G):
    cluster_sizes = [len(cluster) for cluster in cluster_list]
    avg_size = sum(cluster_sizes) / len(cluster_sizes)
    max_size = max(cluster_sizes)
    min_size = min(cluster_sizes)

    densities = [nx.density(G.subgraph(cluster)) for cluster in cluster_list if l
    avg_density = sum(densities) / len(densities) if densities else 0

    return len(cluster_list), avg_size, max_size, min_size, avg_density

# Compute stats for MCL
num_mcl, avg_mcl_size, max_mcl, min_mcl, avg_mcl_density = cluster_statistics(clu

# Compute stats for MCODE
num_mcode, avg_mcode_size, max_mcode, min_mcode, avg_mcode_density = cluster_stat

# Print the results
print(f"🔷 MCL Clustering Stats:")
print(f"- Number of Clusters: {num_mcl}")
print(f"- Avg Cluster Size: {avg_mcl_size:.2f}")
print(f"- Max Cluster Size: {max_mcl}")
print(f"- Min Cluster Size: {min_mcl}")
print(f"- Avg Cluster Density: {avg_mcl_density:.4f}\n")

print(f"🔷 MCODE Clustering Stats:")
print(f"- Number of Clusters: {num_mcode}")
print(f"- Avg Cluster Size: {avg_mcode_size:.2f}")
print(f"- Max Cluster Size: {max_mcode}")
print(f"- Min Cluster Size: {min_mcode}")
print(f"- Avg Cluster Density: {avg_mcode_density:.4f}")
```

```
🔷 MCL Clustering Stats:
- Number of Clusters: 467
- Avg Cluster Size: 66.21
- Max Cluster Size: 21541
- Min Cluster Size: 1
- Avg Cluster Density: 0.5219

🔷 MCODE Clustering Stats:
- Number of Clusters: 20
- Avg Cluster Size: 157.20
- Max Cluster Size: 3079
- Min Cluster Size: 3
- Avg Cluster Density: 0.8871
```

```
import os
import networkx as nx
from networkx.algorithms.community import k_clique_communities

# Ensure the graph is loaded
if 'G' not in globals():
    raise ValueError("⚠️ Graph (G) is not defined. Please reload the graph before

# Reload MCL Clusters if missing
if 'clusters' not in globals():
    if os.path.exists("clusters.txt"):
        print("⚠️ MCL clusters not found in memory! Reloading from file...")
        clusters = []
        with open("clusters.txt", "r") as f:
            for line in f:
                cluster = line.strip().split("\t")
                clusters.append(cluster)
    else:
        raise ValueError("⚠️ clusters.txt file not found! You need to rerun MCL c

# Reload MCODE Clusters if missing
if 'mcode_clusters' not in globals():
    print("⚠️ MCODE clusters not found! Re-running MCODE clustering...")
    k = 3  # Adjust k for density
    clique_communities = list(k_clique_communities(G, k))
    mcode_clusters = [list(community) for community in clique_communities]

print(f"✅ MCL Clusters Loaded: {len(clusters)} clusters")
print(f"✅ MCODE Clusters Loaded: {len(mcode_clusters)} clusters")
```

```
✅ MCL Clusters Loaded: 467 clusters
✅ MCODE Clusters Loaded: 20 clusters
```

```
import random

# Extract a subgraph for faster computation (limit to 5000 nodes)
if len(G.nodes) > 5000:
    sampled_nodes = random.sample(list(G.nodes), 5000)
    subG = G.subgraph(sampled_nodes).copy()
    print(f"⚡ Using subgraph with {len(subG.nodes)} nodes and {len(subG.edges)} e
else:
    subG = G  # Use full graph if it's already small
```

```
⚡ Using subgraph with 5000 nodes and 48854 edges
```

```
import time

# Measure MCL execution time
start_time = time.time()
mcl_clusters = clusters[:5]  # Use only the first 5 clusters for efficiency
mcl_time = time.time() - start_time

# Measure MCODE execution time
start_time = time.time()
k = 3  # Minimum clique size
mcode_clusters = [list(community) for community in k_clique_communities(subG, k)]
mcode_time = time.time() - start_time

# Print results
print(f"⏳ Execution Time for MCL (Top 5 Clusters): {mcl_time:.2f} seconds")
print(f"⏳ Execution Time for MCODE (Limited Subgraph): {mcode_time:.2f} seconds"
```

```
⏳ Execution Time for MCL (Top 5 Clusters): 0.00 seconds
⏳ Execution Time for MCODE (Limited Subgraph): 911.56 seconds
```

```
# Function to calculate basic cluster statistics
def cluster_statistics(cluster_list, G):
    cluster_sizes = [len(cluster) for cluster in cluster_list]
    avg_size = sum(cluster_sizes) / len(cluster_sizes) if cluster_sizes else 0
    max_size = max(cluster_sizes) if cluster_sizes else 0
    min_size = min(cluster_sizes) if cluster_sizes else 0

    densities = [nx.density(G.subgraph(cluster)) for cluster in cluster_list if len
    avg_density = sum(densities) / len(densities) if densities else 0
    return len(cluster_list), avg_size, max_size, min_size, avg_density

# Compute stats for MCL
num_mcl, avg_mcl_size, max_mcl, min_mcl, avg_mcl_density = cluster_statistics(clust

# Compute stats for MCODE
num_mcode, avg_mcode_size, max_mcode, min_mcode, avg_mcode_density = cluster_statis

# Print the results
print(f"🔷 MCL Clustering Stats (Top 5 Clusters):")
print(f"- Number of Clusters: {num_mcl}")
print(f"- Avg Cluster Size: {avg_mcl_size:.2f}")
print(f"- Max Cluster Size: {max_mcl}")
print(f"- Min Cluster Size: {min_mcl}")
print(f"- Avg Cluster Density: {avg_mcl_density:.4f}\n")

print(f"🔷 MCODE Clustering Stats (Top 5 Clusters):")
print(f"- Number of Clusters: {num_mcode}")
print(f"- Avg Cluster Size: {avg_mcode_size:.2f}")
print(f"- Max Cluster Size: {max_mcode}")
print(f"- Min Cluster Size: {min_mcode}")
print(f"- Avg Cluster Density: {avg_mcode_density:.4f}")
```

```
🔷 MCL Clustering Stats (Top 5 Clusters):
- Number of Clusters: 5
- Avg Cluster Size: 4686.80
- Max Cluster Size: 21541
- Min Cluster Size: 337
- Avg Cluster Density: 0.0536

🔷 MCODE Clustering Stats (Top 5 Clusters):
- Number of Clusters: 5
- Avg Cluster Size: 622.60
- Max Cluster Size: 3100
- Min Cluster Size: 3
- Avg Cluster Density: 0.7686
```

Start coding or generate with AI.