In [23]:

```
def install_reqs():
#This defines a function named install_reqs.

  !pip install pandas
#Installs the pandas library, used for reading and manipulating tabular data (like .csv, .tsv).

  !pip install "matplotlib>=3.4"
#Installs matplotlib version 3.4 or higher, used for plotting graphs and visualizations.

  !pip install numpy
#Installs numpy, a fundamental package for numerical computations and arrays.

  !pip install statsmodels
#Installs statsmodels, a library used for statistical tests (e.g., t-tests, Wilcoxon), regression, and model fitting.

  !pip install scipy
#Installs scipy, which contains scientific computing tools, including statistical and optimization functions.

install_reqs()
# to install all the above dependencies uncomment the above line.
```

```
Requirement already satisfied: pandas in c:\users\user\anaconda3\lib\site-packages (2.2.3)
Requirement already satisfied: numpy>=1.26.0 in c:\users\user\anaconda3\lib\site-packages (from pandas) (2.1.3)
Requirement already satisfied: python-dateutil>=2.8.2 in c:\users\user\anaconda3\lib\site-packages (from pandas) (2.9.0.post0)
Requirement already satisfied: pytz>=2020.1 in c:\users\user\anaconda3\lib\site-packages (from pandas) (2024.1)
Requirement already satisfied: tzdata>=2022.7 in c:\users\user\anaconda3\lib\site-packages (from pandas) (2025.2)
Requirement already satisfied: six>=1.5 in c:\users\user\anaconda3\lib\site-packages (from python-dateutil>=2.8.2->pandas) (1.17.0)
Requirement already satisfied: matplotlib>=3.4 in c:\users\user\anaconda3\lib\site-packages (3.10.0)
Requirement already satisfied: contourpy>=1.0.1 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (1.3.1)
Requirement already satisfied: cycler>=0.10 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (0.11.0)
Requirement already satisfied: fonttools>=4.22.0 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (4.55.3)
Requirement already satisfied: kiwisolver>=1.3.1 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (1.4.8)
Requirement already satisfied: numpy>=1.23 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (2.1.3)
Requirement already satisfied: packaging>=20.0 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (24.2)
Requirement already satisfied: pillow>=8 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (11.1.0)
Requirement already satisfied: pyparsing>=2.3.1 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (3.2.0)
Requirement already satisfied: python-dateutil>=2.7 in c:\users\user\anaconda3\lib\site-packages (from matplotlib>=3.4) (2.9.0.post0)
Requirement already satisfied: six>=1.5 in c:\users\user\anaconda3\lib\site-packages (from python-dateutil>=2.7->matplotlib>=3.4) (1.17.0)
Requirement already satisfied: numpy in c:\users\user\anaconda3\lib\site-packages (2.1.3)
Requirement already satisfied: statsmodels in c:\users\user\anaconda3\lib\site-packages (0.14.4)
Requirement already satisfied: numpy<3,>=1.22.3 in c:\users\user\anaconda3\lib\site-packages (from statsmodels) (2.1.3)
Requirement already satisfied: scipy!=1.9.2,>=1.8 in c:\users\user\anaconda3\lib\site-packages (from statsmodels) (1.15.3)
Requirement already satisfied: pandas!=2.1.0,>=1.4 in c:\users\user\anaconda3\lib\site-packages (from statsmodels) (2.2.3)
Requirement already satisfied: patsy>=0.5.6 in c:\users\user\anaconda3\lib\site-packages (from statsmodels) (1.0.1)
Requirement already satisfied: packaging>=21.3 in c:\users\user\anaconda3\lib\site-packages (from statsmodels) (24.2)
Requirement already satisfied: python-dateutil>=2.8.2 in c:\users\user\anaconda3\lib\site-packages (from pandas!=2.1.0,>=1.4->statsmodels) (2.9.0.post0)
Requirement already satisfied: pytz>=2020.1 in c:\users\user\anaconda3\lib\site-packages (from pandas!=2.1.0,>=1.4->statsmodels) (2024.1)
Requirement already satisfied: tzdata>=2022.7 in c:\users\user\anaconda3\lib\site-packages (from pandas!=2.1.0,>=1.4->statsmodels) (2025.2)
Requirement already satisfied: six>=1.5 in c:\users\user\anaconda3\lib\site-packages (from python-dateutil>=2.8.2->pandas!=2.1.0,>=1.4->statsmodels) (1.17.0)
Requirement already satisfied: scipy in c:\users\user\anaconda3\lib\site-packages (1.15.3)
Requirement already satisfied: numpy<2.5,>=1.23.5 in c:\users\user\anaconda3\lib\site-packages (from scipy) (2.1.3)
```

In [24]:

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

In [25]:

```
from compass_analysis import cohens_d, wilcoxon_test, get_reaction_consistencies, get_metareactions, labeled_reactions, amino_acid_metab
```

In [26]:

```
from matplotlib import __version__ as matplotlibversion
if matplotlibversion < "3.4":
    print("Matplotlib versions older than 3.4 may not be able to generate figure 2E, as they do not support alpha arrays")
```

```
Matplotlib versions older than 3.4 may not be able to generate figure 2E, as they do not support alpha arrays
```

In [27]:

```
#import os
#os.system(
#     "compass --data expression.tsv "
#     "--model RECON2_mat --species homo_sapiens --media default-media --lambda 0.25 "
#     "--and-function mean --output-dir extdata/APOB --penalty-diffusion knn --num-neighbors 10 "
#     "--isoform-summing legacy --num-processes 50"
#)
```

In [28]:

```
import os
print(os.getcwd())
```

```
C:\Users\user\Desktop\Harshini\Human dataset_APOB_AIM\1_A vs D
```

In [29]:

```
reaction_penalties = pd.read_csv("reactions.tsv", sep="\t", index_col=0)
```

In [30]:

```
import pandas as pd

# Load reactions.tsv
reaction_penalties = pd.read_csv("reactions.tsv", sep="\t", index_col=0)

# Extract cell IDs from the columns
cell_ids = reaction_penalties.columns

# --- NEW FUNCTION: infer group based on suffix after "_" ---
def infer_group(cell_id):
    """
    Extracts the group label from a cell name like '1_A' or '15_C'.
    """
    if "_" in cell_id:
        return cell_id.split("_")[-1]   # A, B, C, or D
    else:
        return "Unknown"

# Create list of inferred groups for each cell
cell_groups = [infer_group(cell) for cell in cell_ids]

# Create metadata DataFrame
cell_metadata = pd.DataFrame({
    "cell_id": cell_ids,
    "group": cell_groups
}).set_index("cell_id")

# Save file
cell_metadata.to_csv("cell_metadata.csv")

print("Created cell_metadata.csv with the following group counts:")
print(cell_metadata["group"].value_counts())
```

```
Created cell_metadata.csv with the following group counts:
group
D    38
A    37
B    35
C    34
Name: count, dtype: int64
```

In [31]:

```
cell_metadata = pd.read_csv("cell_metadata.csv", sep=",")
cell_metadata.set_index("cell_id", inplace=True)
```

In [32]:

```
print(cell_metadata.columns.tolist())
print(cell_metadata.head())
```

```
['group']
        group
cell_id      
1_A         A
2_A         A
3_A         A
4_A         A
5_A         A
```

In [33]:

```
# Select cells by group
A_cells = cell_metadata.index[cell_metadata["group"] == "A"]
B_cells = cell_metadata.index[cell_metadata["group"] == "B"]
C_cells = cell_metadata.index[cell_metadata["group"] == "C"]
D_cells = cell_metadata.index[cell_metadata["group"] == "D"]

# Optional: print counts
print("Number of cells per group:")
print("A:", len(A_cells))
print("B:", len(B_cells))
print("C:", len(C_cells))
print("D:", len(D_cells))
```

```
Number of cells per group:
A: 37
B: 35
C: 34
D: 38
```

In [34]:

```
print(cell_metadata.columns.tolist())
```

```
['group']
```

In [35]:

```
print(cell_metadata.head())
print(cell_metadata.columns.tolist())
```

```
        group
cell_id      
1_A         A
2_A         A
3_A         A
4_A         A
5_A         A
['group']
```

In [36]:

```
reaction_metadata = pd.read_csv("reaction_metadata.csv", index_col = 0)
```

In [37]:

```
reaction_metadata.loc[['r0281']]
```

Out[37]:

	reaction_name	formula	associated_genes	subsystem	EC_number	confidence
reaction_no_direction						
r0281	Putrescine:oxygen oxidoreductase (deaminating)...	1.00 * Water [e] + 1.00 * O2 [e] + 1.00 * Putr...	AOC1	Methionine and cysteine metabolism	1.4.3.6	0.0

In [38]:

```
#This function is repeated here for clarity
def get_reaction_consistencies(compass_reaction_penalties, min_range=1e-3):
    """
        Converts the raw penalties outputs of compass into scores per reactions where higher numbers indicate more activity
    """
    df = -np.log(compass_reaction_penalties + 1)
    df = df[df.max(axis=1) - df.min(axis=1) >= min_range]
    df = df - df.min().min()
    return df
```

In [39]:

```
reaction_consistencies = get_reaction_consistencies(reaction_penalties)
```

In [40]:

```
common_cells = list(set(reaction_consistencies.columns).intersection(set(cell_metadata.index)))
reaction_consistencies = reaction_consistencies[common_cells]
```

In [41]:

```
# Select cells for groups A and B
A_cells = cell_metadata.index[cell_metadata["group"] == "A"]
B_cells = cell_metadata.index[cell_metadata["group"] == "D"]

# Run Wilcoxon test between A and B
wilcox_results = wilcoxon_test(reaction_consistencies, A_cells, D_cells)

# Add metadata reaction ID column
wilcox_results['metadata_r_id'] = ""

for r in wilcox_results.index:
    if r in reaction_metadata.index:
        wilcox_results.loc[r, 'metadata_r_id'] = r
    elif r[:-4] in reaction_metadata.index:  # handles possible suffixes
        wilcox_results.loc[r, 'metadata_r_id'] = r[:-4]
    else:
        print("Should not occur:", r)

# Optional: check the results
print(wilcox_results.head())
```

```
                  wilcox_stat  wilcox_pval  cohens_d  adjusted_pval  \
10FTHF5GLUtl_pos        923.0     0.020014  0.586732       0.046661   
10FTHF5GLUtm_pos        857.0     0.103807  0.206941       0.161212   
10FTHF6GLUtl_pos        925.0     0.018911  0.582505       0.044793   
10FTHF6GLUtm_pos        846.0     0.131018  0.267083       0.189929   
10FTHF7GLUtl_pos        920.0     0.021774  0.568015       0.048730   

                 metadata_r_id  
10FTHF5GLUtl_pos  10FTHF5GLUtl  
10FTHF5GLUtm_pos  10FTHF5GLUtm  
10FTHF6GLUtl_pos  10FTHF6GLUtl  
10FTHF6GLUtm_pos  10FTHF6GLUtm  
10FTHF7GLUtl_pos  10FTHF7GLUtl  
```

In [42]:

```
print(reaction_consistencies.columns.tolist()[:10])
```

```
['27_D', '33_D', '25_C', '25_A', '16_A', '3_D', '22_A', '33_B', '6_A', '11_D']
```

In [43]:

```
print(A_cells[:10])
```

```
Index(['1_A', '2_A', '3_A', '4_A', '5_A', '6_A', '7_A', '8_A', '9_A', '10_A'], dtype='object', name='cell_id')
```

In [44]:

```
# Select cells for groups A and B
A_cells = cell_metadata.index[cell_metadata["group"] == "A"]
B_cells = cell_metadata.index[cell_metadata["group"] == "D"]

# Run the Wilcoxon test between A and B
wilcox_results = wilcoxon_test(reaction_consistencies, A_cells, D_cells)

# Annotate metadata reaction IDs
wilcox_results['metadata_r_id'] = ""

for r in wilcox_results.index:
    if r in reaction_metadata.index:
        wilcox_results.loc[r, 'metadata_r_id'] = r
    elif r[:-4] in reaction_metadata.index:  # handles possible suffixes like '_x'
        wilcox_results.loc[r, 'metadata_r_id'] = r[:-4]
    else:
        print(f"Should not occur → {r}")

# Optional: check the results
print(wilcox_results.head())
```

```
                  wilcox_stat  wilcox_pval  cohens_d  adjusted_pval  \
10FTHF5GLUtl_pos        923.0     0.020014  0.586732       0.046661   
10FTHF5GLUtm_pos        857.0     0.103807  0.206941       0.161212   
10FTHF6GLUtl_pos        925.0     0.018911  0.582505       0.044793   
10FTHF6GLUtm_pos        846.0     0.131018  0.267083       0.189929   
10FTHF7GLUtl_pos        920.0     0.021774  0.568015       0.048730   

                 metadata_r_id  
10FTHF5GLUtl_pos  10FTHF5GLUtl  
10FTHF5GLUtm_pos  10FTHF5GLUtm  
10FTHF6GLUtl_pos  10FTHF6GLUtl  
10FTHF6GLUtm_pos  10FTHF6GLUtm  
10FTHF7GLUtl_pos  10FTHF7GLUtl  
```

In [45]:

```
# Select cells for groups A and B
A_cells = cell_metadata.index[cell_metadata["group"] == "A"]
B_cells = cell_metadata.index[cell_metadata["group"] == "D"]

# Run the Wilcoxon test between A and B
wilcox_results = wilcoxon_test(reaction_consistencies, A_cells, D_cells)

# Annotate metadata reaction IDs
wilcox_results['metadata_r_id'] = ""

for r in wilcox_results.index:
    if r in reaction_metadata.index:
        wilcox_results.loc[r, 'metadata_r_id'] = r
    elif r[:-4] in reaction_metadata.index:  # handles possible suffixes like '_x'
        wilcox_results.loc[r, 'metadata_r_id'] = r[:-4]
    else:
        print(f"Should not occur → {r}")

# Optional: view top results
print(wilcox_results.head())
```

```
                 wilcox_stat  wilcox_pval  cohens_d  adjusted_pval  \
10FTHF5GLUtl_pos       923.0     0.020014  0.586732       0.046661   
10FTHF5GLUtm_pos       857.0     0.103807  0.206941       0.161212   
10FTHF6GLUtl_pos       925.0     0.018911  0.582505       0.044793   
10FTHF6GLUtm_pos       846.0     0.131018  0.267083       0.189929   
10FTHF7GLUtl_pos       920.0     0.021774  0.568015       0.048730   

                 metadata_r_id  
10FTHF5GLUtl_pos  10FTHF5GLUtl  
10FTHF5GLUtm_pos  10FTHF5GLUtm  
10FTHF6GLUtl_pos  10FTHF6GLUtl  
10FTHF6GLUtm_pos  10FTHF6GLUtm  
10FTHF7GLUtl_pos  10FTHF7GLUtl  
```

In [46]:

```
W = wilcox_results.merge(reaction_metadata, how='left',
                         left_on='metadata_r_id', right_index=True, validate='m:1')
W = W[W['confidence'].isin([0,4])]
W = W[~W['EC_number'].isna()]
W.loc[(W['formula'].map(lambda x: '[m]' not in x)) & (W['subsystem'] == "Citric acid cycle"), 'subsystem'] = 'Other'
```

In [47]:

```
wilcox_results.loc[['r0281_pos']]
```

Out[47]:

	wilcox_stat	wilcox_pval	cohens_d	adjusted_pval	metadata_r_id
r0281_pos	795.0	0.332224	0.255841	0.40657	r0281

In [48]:

```
reaction_metadata.loc['r0281']['formula']
```

Out[48]:

```
'1.00 * Water [e] + 1.00 * O2 [e] + 1.00 * Putrescine [e] --> 1.00 * Ammonium [e] + 1.00 * Hydrogen peroxide [e] + 1.00 * 4-Aminobutanal [e]\nAOC1'
```

In [49]:

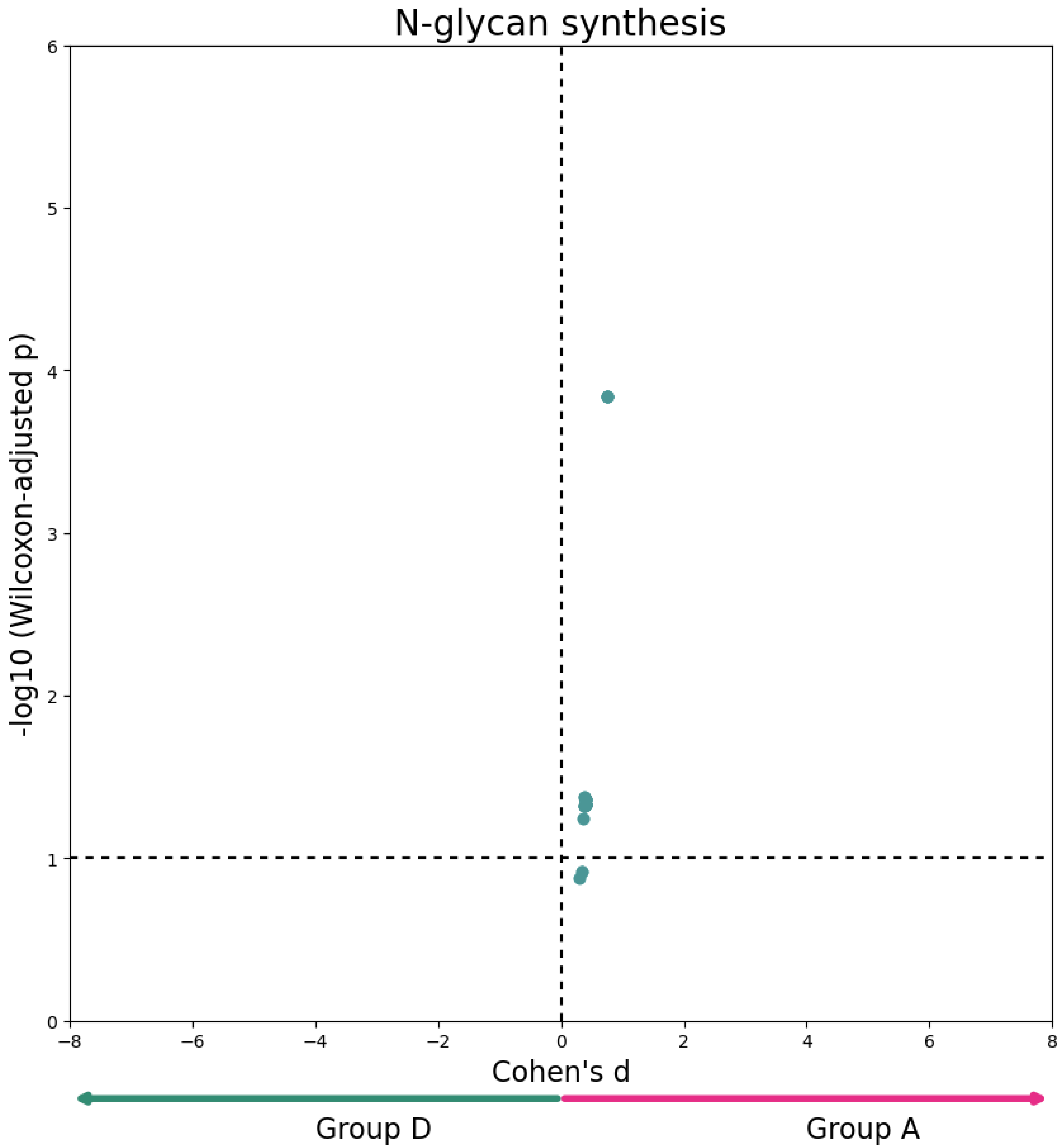
```
def plot_differential_scores(data, title, c):
    plt.figure(figsize=(10,10))
    axs = plt.gca()
    axs.scatter(data['cohens_d'], -np.log10(data['adjusted_pval']), c=c)
    axs.set_xlabel("Cohen's d", fontsize=16)
    axs.set_ylabel("-log10 (Wilcoxon-adjusted p)", fontsize=16)
    # Visual markers and title
    axs.set_xlim(-8, 8)
    axs.set_ylim(0, 6)
    axs.axvline(0, dashes=(3,3), c='black')
    axs.axhline(1, dashes=(3,3), c='black')
    axs.set_title(title, fontdict={'fontsize':20})

    # Arrows for group identity (A vs B)
    axs.annotate('', xy=(0.5, -0.08), xycoords='axes fraction', xytext=(0, -0.08),
                 arrowprops=dict(arrowstyle="<-", color='#348C73', linewidth=4))
    axs.annotate('Group A', xy=(0.75, -0.12), xycoords='axes fraction', fontsize=16)
    axs.annotate('', xy=(0.5, -0.08), xycoords='axes fraction', xytext=(1, -0.08),
                 arrowprops=dict(arrowstyle="<-", color='#E92E87', linewidth=4))
    axs.annotate('Group D', xy=(0.25, -0.12), xycoords='axes fraction', fontsize=16)

    # Dynamic annotation loop with variable offsets and labels
    for i, r in enumerate(data.index):
        if r in labeled_reactions:
            x = data.loc[r, 'cohens_d']
            y = -np.log10(data.loc[r, 'adjusted_pval'])

            dx = 30 if x >= 0 else -120  # horizontal offset
            dy = (i % 6) * 12 - 30       # vertical offset varies to reduce stacking

            axs.annotate(
                labeled_reactions[r],
                (x, y),
                xytext=(dx, dy),
                textcoords='offset pixels',
                arrowprops=dict(arrowstyle="-", shrinkA=6, shrinkB=4),
                fontsize=10,
                zorder=5,  # make sure text is on top
                bbox=dict(boxstyle="round,pad=0.3", fc="white", ec="gray", alpha=0.7)
            )
```

In [50]:

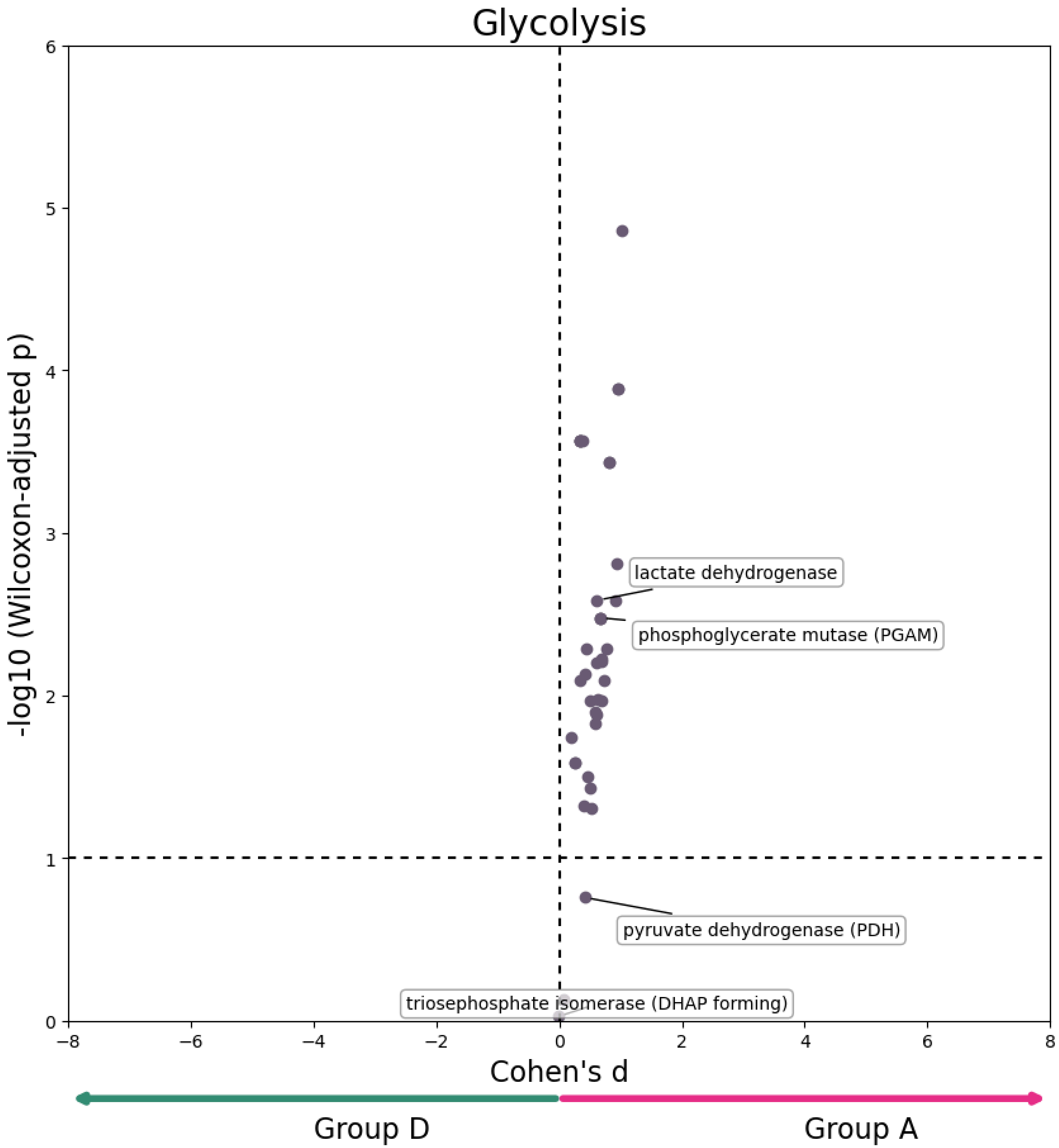
```
filtered_data = pd.concat([
    W[W['subsystem'] == "Glycolysis/gluconeogenesis"],
    W[W['subsystem'] == "Citric acid cycle"],
    W[W['subsystem'].isin(amino_acid_metab)],
    W[W['subsystem'] == "N-glycan synthesis"],
    W[W['subsystem'] == "Fatty acid oxidation"]
])
```

In [51]:

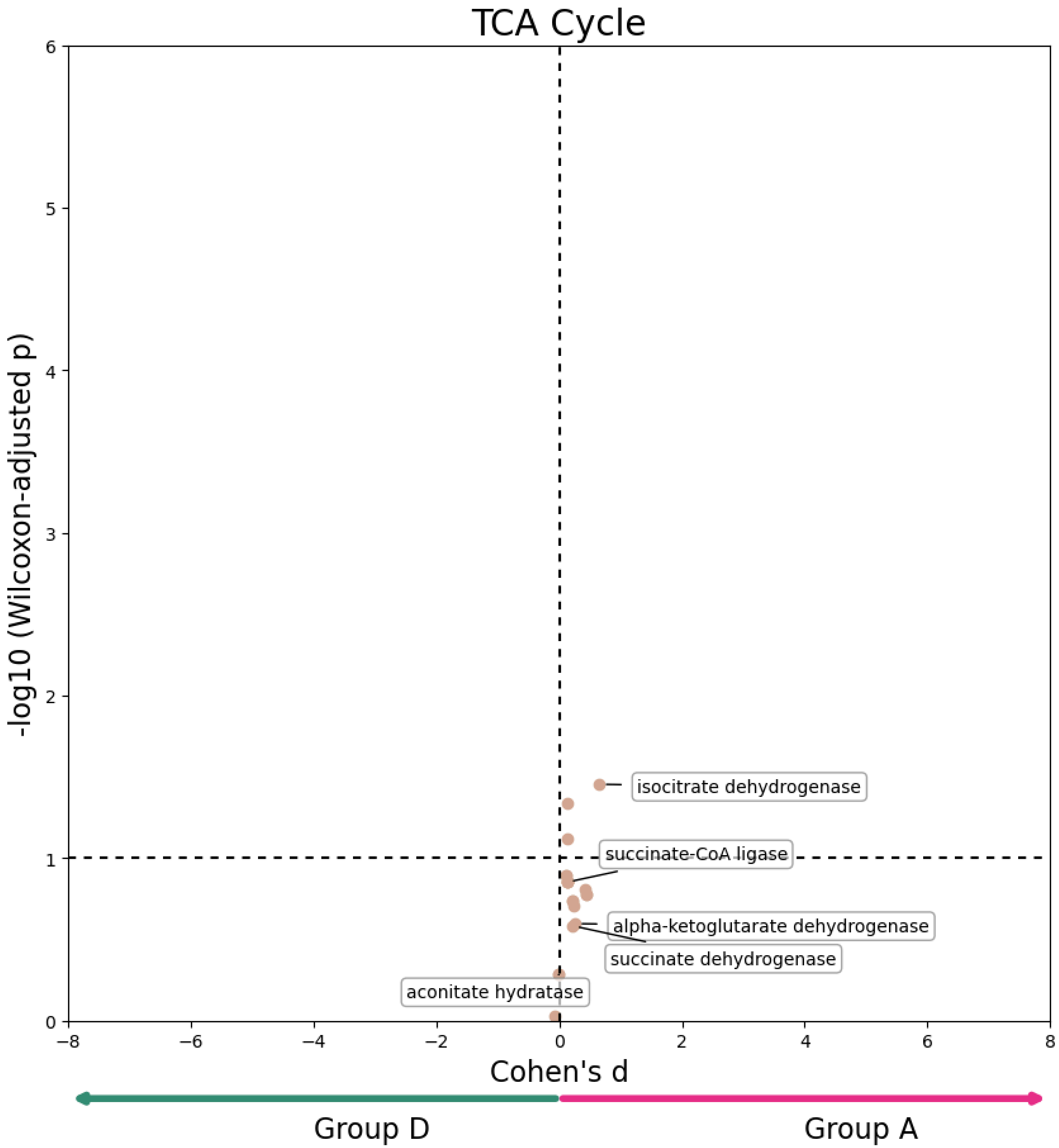
```
data = W[W['subsystem'] == "N-glycan synthesis"]
plot_differential_scores(data, title='N-glycan synthesis', c="#4C9A9A")
```



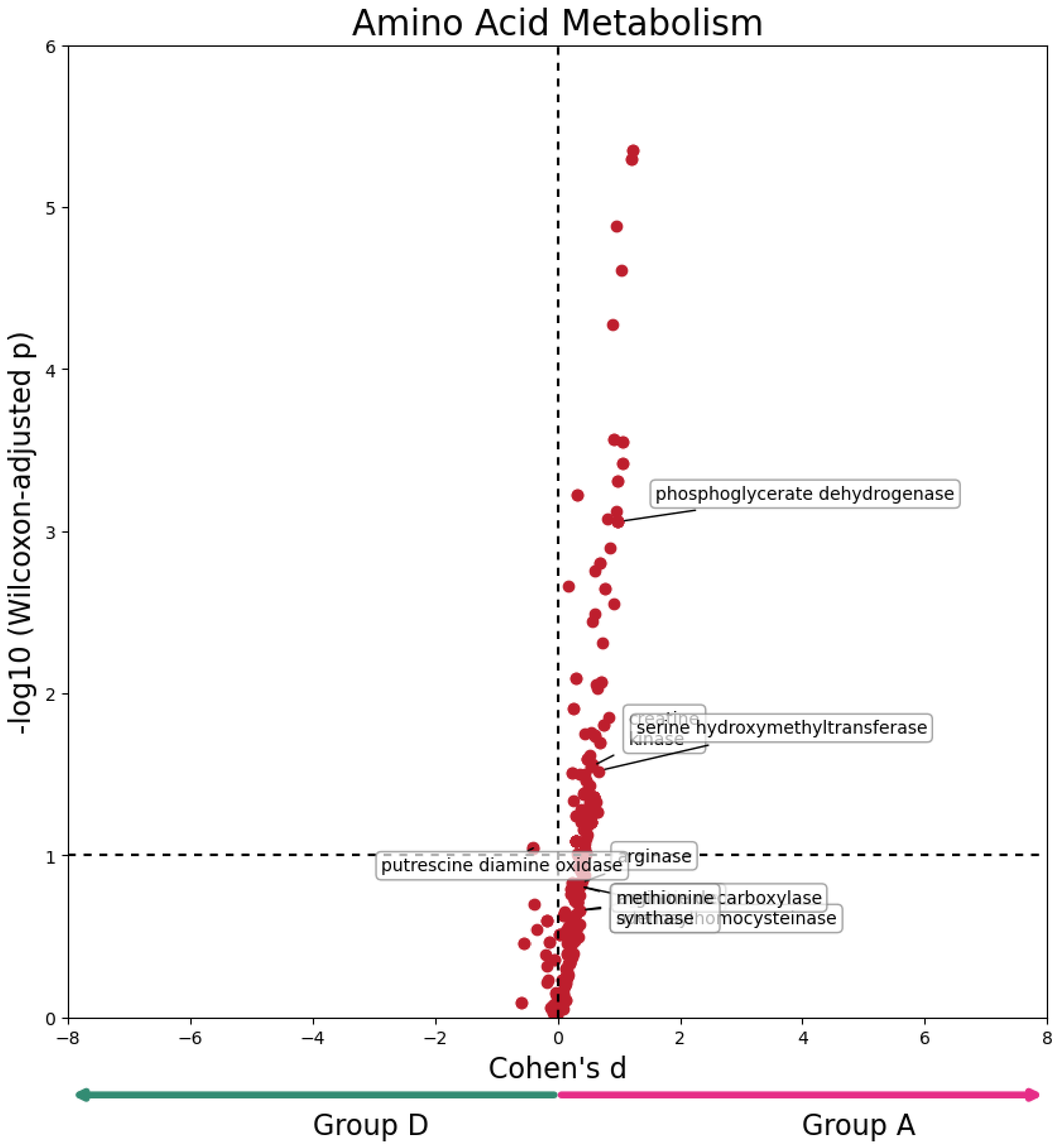
```
In [52]: data = W[W['subsystem'] == "Glycolysis/gluconeogenesis"]
         plot_differential_scores(data, title='Glycolysis', c="#695D73")
```



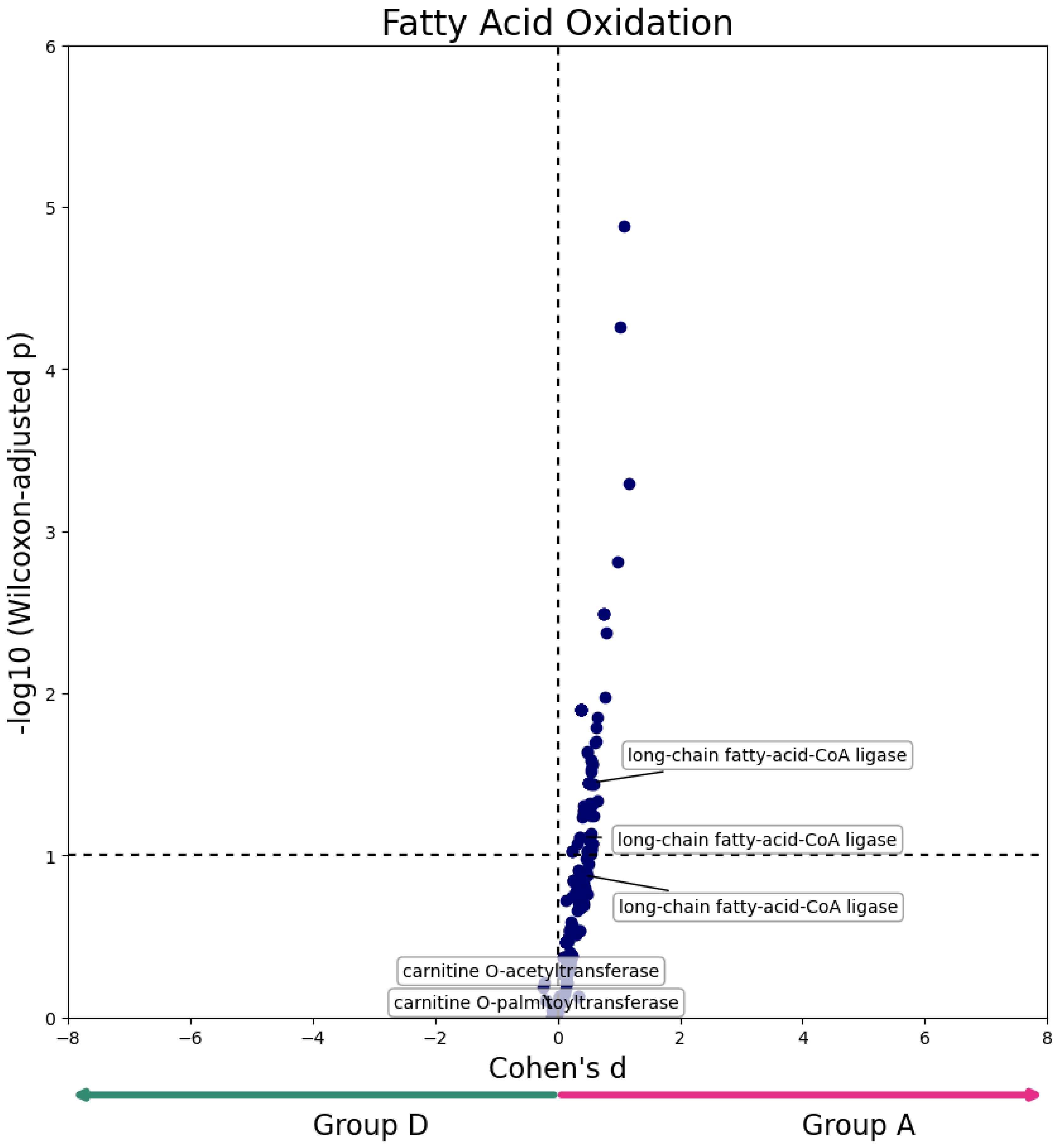
```
In [53]: data = W[W['subsystem'] == "Citric acid cycle"]
         plot_differential_scores(data, title="TCA Cycle", c="#D3A991")
```



```
In [54]: data = W[W['subsystem'].isin(amino_acid_metab)].copy()
         data['adjusted_pval'] = data['adjusted_pval'].clip(1e-12)
         plot_differential_scores(data, "Amino Acid Metabolism", c="#BF1E2E")
```



```
In [55]: data = W[W['subsystem'] == "Fatty acid oxidation"]
         plot_differential_scores(data, "Fatty Acid Oxidation", c="#040772")
```


Fatty Acid Oxidation
-log10 (Wilcoxon-adjusted p)
0
1
2
3
4
5
6
−8
−6
−4
−2
0
2
4
6
8
Cohen's d
long-chain fatty-acid-CoA ligase
long-chain fatty-acid-CoA ligase
long-chain fatty-acid-CoA ligase
carnitine O-acetyltransferase
carnitine O-palmitoyltransferase
Group D
Group A

In [56]:

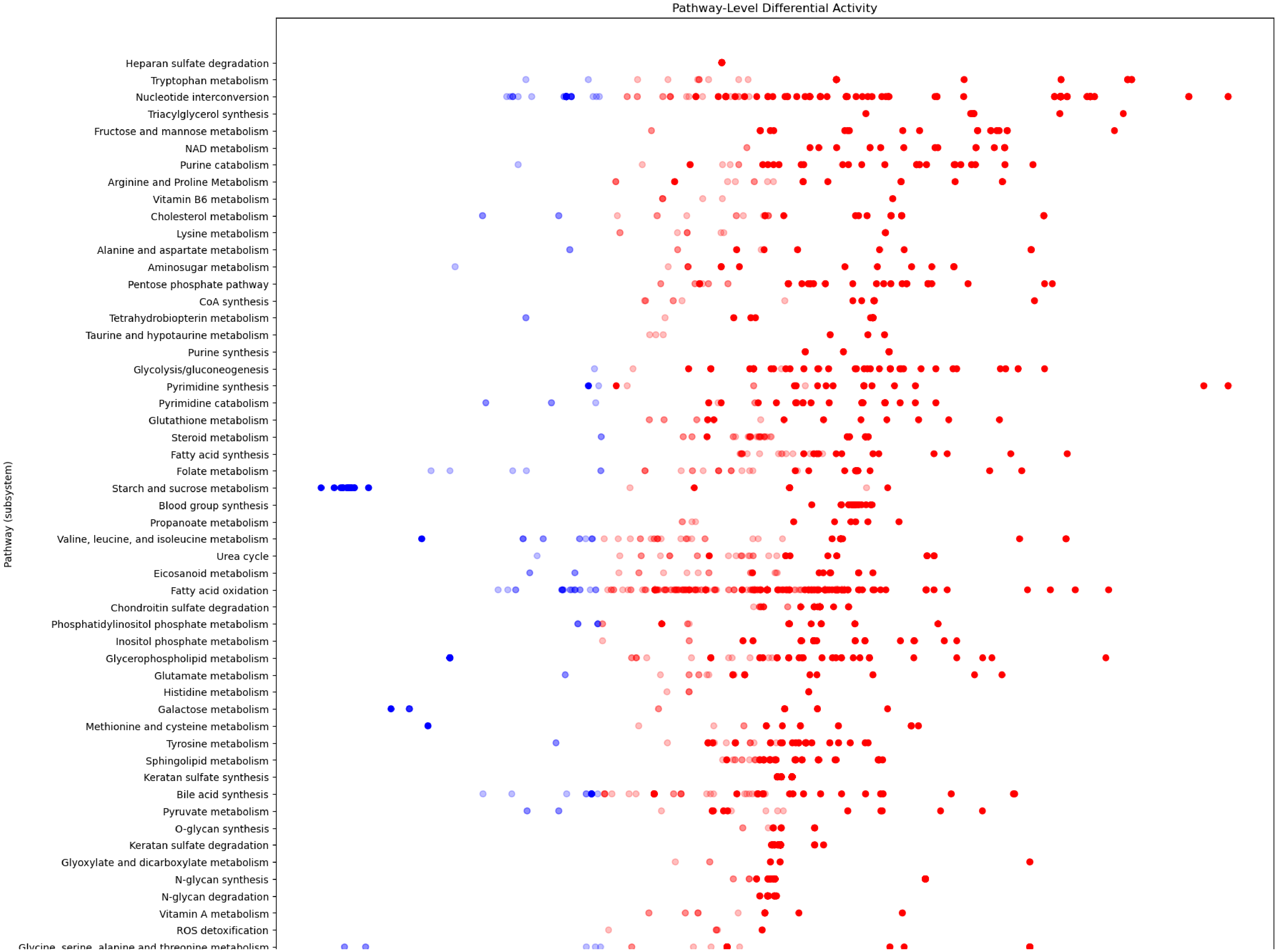
```
data = W[~W['subsystem'].isin(["Miscellaneous", "Unassigned"])]
data = data[~data['subsystem'].map(lambda x: "Transport" in x or "Exchange" in x or x == "Other")]
items, counts = np.unique(data['subsystem'], return_counts=True)
items = [items[i] for i in range(len(items)) if counts[i] > 5] #filter(n() > 5) %>%
data = data[data['subsystem'].isin(items)]
```

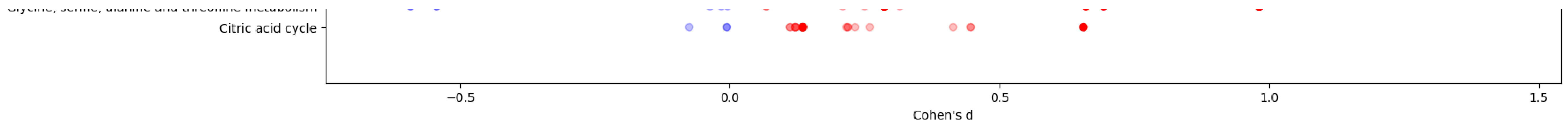
In [57]:

```
import matplotlib.pyplot as plt

plt.figure(figsize=(18, 18))
axs = plt.gca()

d = data[data['adjusted_pval'] < 0.1].groupby('subsystem')['cohens_d'].median().abs()

d_sorted = d.sort_values()

axs.scatter(d_sorted, d_sorted.index, alpha=0)

color = data['cohens_d'].map(lambda x: 'r' if x >= 0 else 'b')
alpha = data['adjusted_pval'].map(lambda x: 1.0 if x < 0.1 else 0.25)

axs.scatter(data['cohens_d'], data['subsystem'], c=color, alpha=alpha)

axs.set_xlabel("Cohen's d")
axs.set_ylabel("Pathway (subsystem)")
axs.set_title("Pathway-Level Differential Activity")
```

Out[57]:

```
Text(0.5, 1.0, 'Pathway-Level Differential Activity')
```


Pathway-Level Differential Activity
Pathway (subsystem)
Heparan sulfate degradation
Tryptophan metabolism
Nucleotide interconversion
Triacylglycerol synthesis
Fructose and mannose metabolism
NAD metabolism
Purine catabolism
Arginine and Proline Metabolism
Vitamin B6 metabolism
Cholesterol metabolism
Lysine metabolism
Alanine and aspartate metabolism
Aminosugar metabolism
Pentose phosphate pathway
CoA synthesis
Tetrahydrobiopterin metabolism
Taurine and hypotaurine metabolism
Purine synthesis
Glycolysis/gluconeogenesis
Pyrimidine synthesis
Pyrimidine catabolism
Glutathione metabolism
Steroid metabolism
Fatty acid synthesis
Folate metabolism
Starch and sucrose metabolism
Blood group synthesis
Propanoate metabolism
Valine, leucine, and isoleucine metabolism
Urea cycle
Eicosanoid metabolism
Fatty acid oxidation
Chondroitin sulfate degradation
Phosphatidylinositol phosphate metabolism
Inositol phosphate metabolism
Glycerophospholipid metabolism
Glutamate metabolism
Histidine metabolism
Galactose metabolism
Methionine and cysteine metabolism
Tyrosine metabolism
Sphingolipid metabolism
Keratan sulfate synthesis
Bile acid synthesis
Pyruvate metabolism
O-glycan synthesis
Keratan sulfate degradation
Glyoxylate and dicarboxylate metabolism
N-glycan synthesis
N-glycan degradation
Vitamin A metabolism
ROS detoxification
Glycine, serine, alanine and threonine metabolism



In [58]:
```
reaction_penalties = pd.read_csv("reactions.tsv", sep="\t", index_col = 0)
reaction_penalties[reaction_penalties <= 1e-4] = 0
reaction_penalties = reaction_penalties[np.all(reaction_penalties != 0, axis=1)]
```

In [59]:
```
reaction_penalties = reaction_penalties[reaction_penalties.max(axis=1) - reaction_penalties.min(axis=1) != 0]
```

In [60]:
```
meta_rxns_map = get_metareactions(reaction_penalties)
meta_rxns = reaction_penalties.join(pd.DataFrame(meta_rxns_map, columns=["meta_rxn_id"], index = reaction_penalties.index)).groupby("meta_rxn_id").mean()
```

In [61]:
```
meta_rxn_consistencies = get_reaction_consistencies(meta_rxns)
```

In [62]:
```
# Select cells for groups A and D
A_cells = cell_metadata.index[cell_metadata["group"] == "A"]
B_cells = cell_metadata.index[cell_metadata["group"] == "D"]

# Run Wilcoxon test between these two groups
wilcox_meta_rxn_results = wilcoxon_test(meta_rxn_consistencies, A_cells, D_cells)

# Optional: check the top results
print(wilcox_meta_rxn_results.head())
```

```
             wilcox_stat  wilcox_pval  cohens_d  adjusted_pval
meta_rxn_id
1                  695.0     0.936652 -0.098665       0.958395
2                  723.0     0.836287 -0.106541       0.877642
3                  711.0     0.936652 -0.172778       0.958395
4                  987.0     0.002662  0.301696       0.011133
5                 1013.0     0.001039  0.621489       0.005668
```

In [63]:
```
wilcox_meta_rxn_results.iloc[0:1]
```

Out[63]:

	wilcox_stat	wilcox_pval	cohens_d	adjusted_pval
meta_rxn_id				
1	695.0	0.936652	-0.098665	0.958395

In [64]:
```
wilcox_meta_rxn_expanded = pd.DataFrame(index=reaction_penalties.index, columns=wilcox_meta_rxn_results.columns)
for i in range(len(wilcox_meta_rxn_expanded.index)):
    if (meta_rxns_map[i] in wilcox_meta_rxn_results.index):
        wilcox_meta_rxn_expanded.loc[wilcox_meta_rxn_expanded.index[i]] = wilcox_meta_rxn_results.loc[meta_rxns_map[i]]
wilcox_meta_rxn_expanded = wilcox_meta_rxn_expanded.dropna().astype('float64')
```

In [65]:

```
wilcox_meta_rxn_expanded['metadata_r_id'] = ""
for r in wilcox_meta_rxn_expanded.index:
    if r in reaction_metadata.index:
        wilcox_meta_rxn_expanded.loc[r, 'metadata_r_id'] = r
    elif r[:-4] in reaction_metadata.index:
        wilcox_meta_rxn_expanded.loc[r, 'metadata_r_id'] = r[:-4]
    else:
        print("Should not occur")
```

In [66]:

```
wilcox_meta_rxn_expanded.iloc[0:1]
```

Out[66]:

	wilcox_stat	wilcox_pval	cohens_d	adjusted_pval	metadata_r_id
10FTHF5GLUtl_pos	923.0	0.020014	0.580328	0.049009	10FTHF5GLUtl

In [67]:

```
outputs = {
    "wilcox_results.csv": wilcox_results,
    "reaction_consistencies.csv": reaction_consistencies,
    "reaction_metadata.csv": reaction_metadata,
    "wilcox_meta_rxn_results.csv": wilcox_meta_rxn_results,
    "wilcox_meta_rxn_expanded.csv": wilcox_meta_rxn_expanded,
    "final_stats_with_metadata.csv": W,
}

for name, df in outputs.items():
    df.to_csv(name)
```

In [68]:

```
import zipfile

with zipfile.ZipFile("A vs D.zip", "w") as zipf:
    for filename in outputs:
        zipf.write(filename)
```

In [69]:

```
from IPython.display import FileLink
FileLink("A vs D.zip")
```

Out[69]: A vs D.zip