Dimensionality Reduction (Principal Component Analysis (PCA) and t-Distributed Stochastic Neighbor Embedding (t-SNE) for Ground Coffee

In [2]:
```
# Load packages
import os
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.preprocessing import LabelEncoder, StandardScaler
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE
```

In [3]:
```
# set the working directory
os.chdir('C:/Users/abc/OneDrive - UGent/Documenten/Derick Malavi_PhD Docs_UGent/Mar
```

In [4]:
```
# Read_data. Import the files for ground coffee
ground_raw = pd.read_csv('coffee_data_pycleaned.csv')
ground_msc_sg_1d = pd.read_csv('coffee_ground_msc_sg_1d.csv')
ground_msc_sg_2d = pd.read_csv('coffee_ground_msc_sg_2d.csv')
ground_snv_sg_1d = pd.read_csv('coffee_ground_snv_sg_1d.csv')
ground_snv_sg_2d = pd.read_csv('coffee_ground_snv_sg_2d.csv')
```

In [5]:
```
ground_raw.head()
```

Out[5]:

	sample_id	binary_class	three_class	adult_percent	cal_val	935.609985	939.059998	942.
0	Pure_Arabica_10	pure_arabica	pure_arabica	0	1	0.347876	0.349376	0.3
1	Pure_Arabica_3	pure_arabica	pure_arabica	0	1	0.332850	0.334093	0.3
2	Pure_Arabica_2	pure_arabica	pure_arabica	0	1	0.347639	0.349199	0.3
3	Pure_Arabica_2	pure_arabica	pure_arabica	0	1	0.338413	0.339599	0.3
4	Pure_Arabica_2	pure_arabica	pure_arabica	0	1	0.343888	0.345065	0.3

5 rows × 229 columns

In [6]:
```
# Select the X columns
X_raw = ground_raw.iloc[:,5:230]
X_msc_sg_1d = ground_msc_sg_1d.iloc[:,5:230]
X_msc_sg_2d = ground_msc_sg_2d.iloc[:,5:230]
X_snv_sg_1d = ground_snv_sg_1d.iloc[:,5:230]
X_snv_sg_2d = ground_snv_sg_2d.iloc[:,5:230]

print(X_raw.shape)
print(X_msc_sg_1d.shape)
print(X_msc_sg_2d.shape)
print(X_snv_sg_1d.shape)
print(X_msc_sg_2d.shape)
```

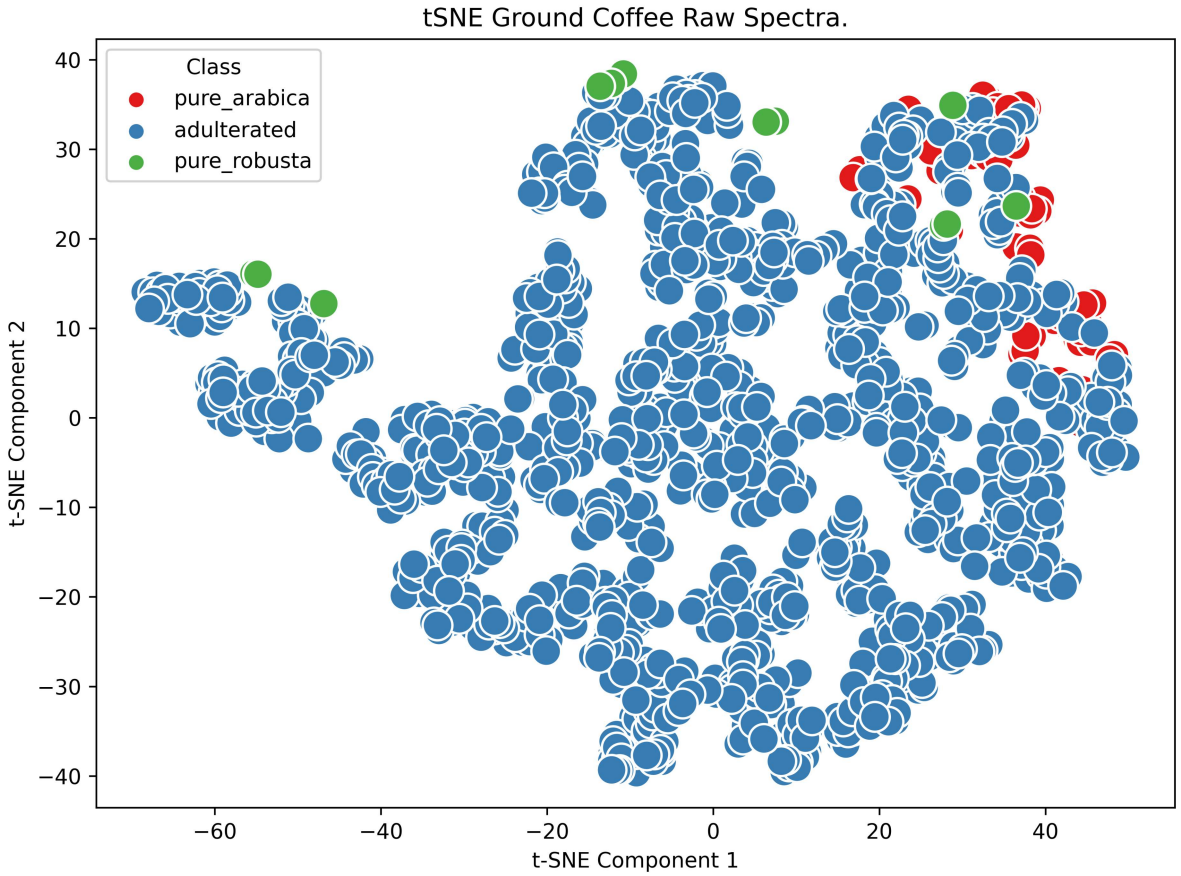
```
(1469, 224)
(1469, 224)
(1469, 224)
(1469, 224)
(1469, 224)
```

In [7]:
```python
# Subset the categorical variable
three_class = ground_raw['three_class']

# Subset the percentage adulteration
percent_adult = ground_raw['adult_percent']

print(three_class.shape)
```

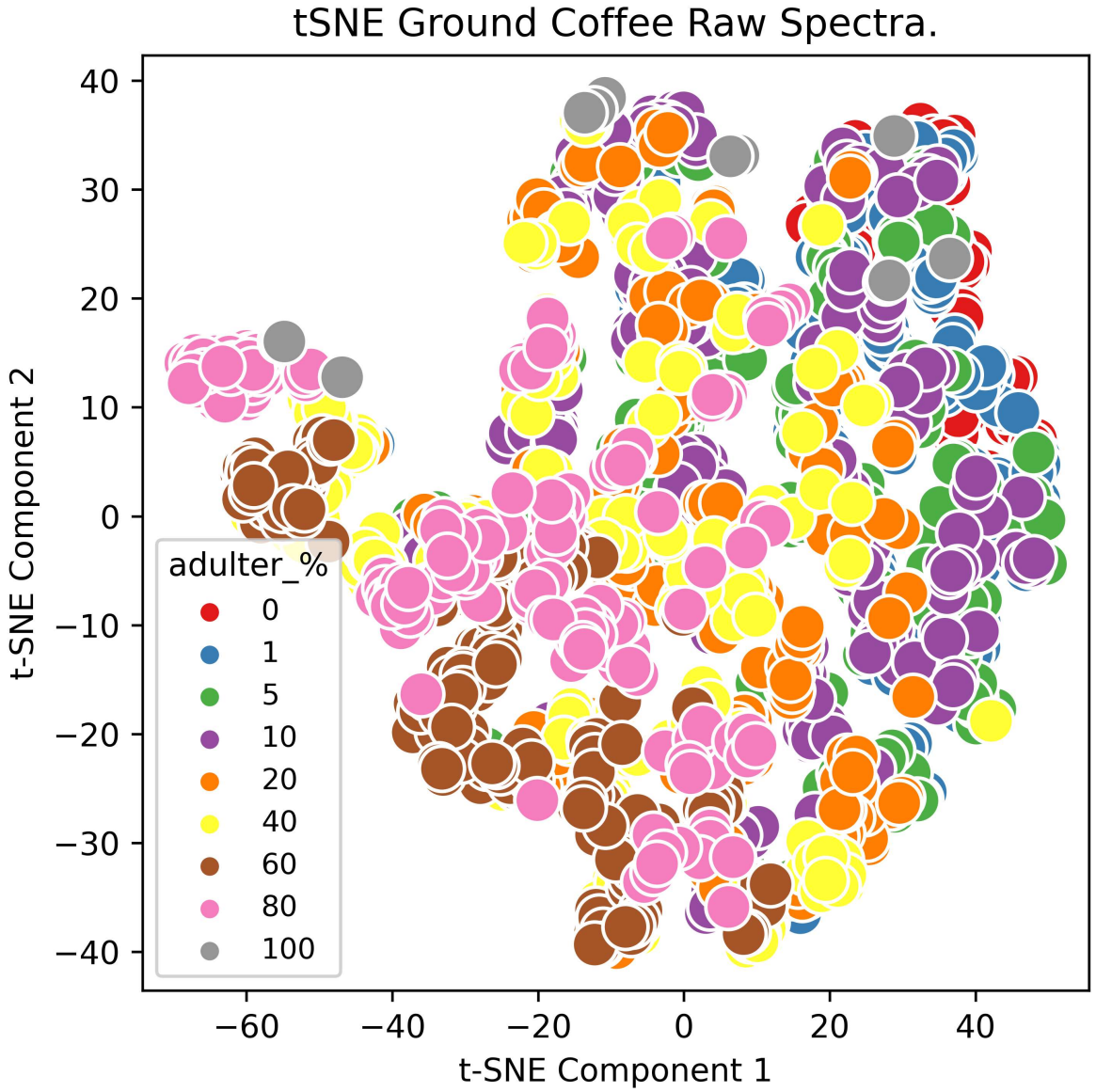
```
(1469,)
```

In [8]:
```python
# Raw Spectra Ground Coffee
# Apply t-SNE to reduce dimensions to 2D

# Scale the data
scaler = StandardScaler()
X_raw_scaled = scaler.fit_transform(X_raw)

tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,init=
X_tsne = tsne.fit_transform(X_raw_scaled)

# Convert to DataFrame for plotting
tsne_df = pd.DataFrame(X_tsne, columns=['TSNE1', 'TSNE2'])
tsne_df[['Class', 'adulter_percent']] = ground_raw[['three_class','adult_percent']]
```

In [9]:
```python
# Plotting
plt.figure(figsize=(8, 6), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
                palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee Raw Spectra.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class")
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_Raw.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```

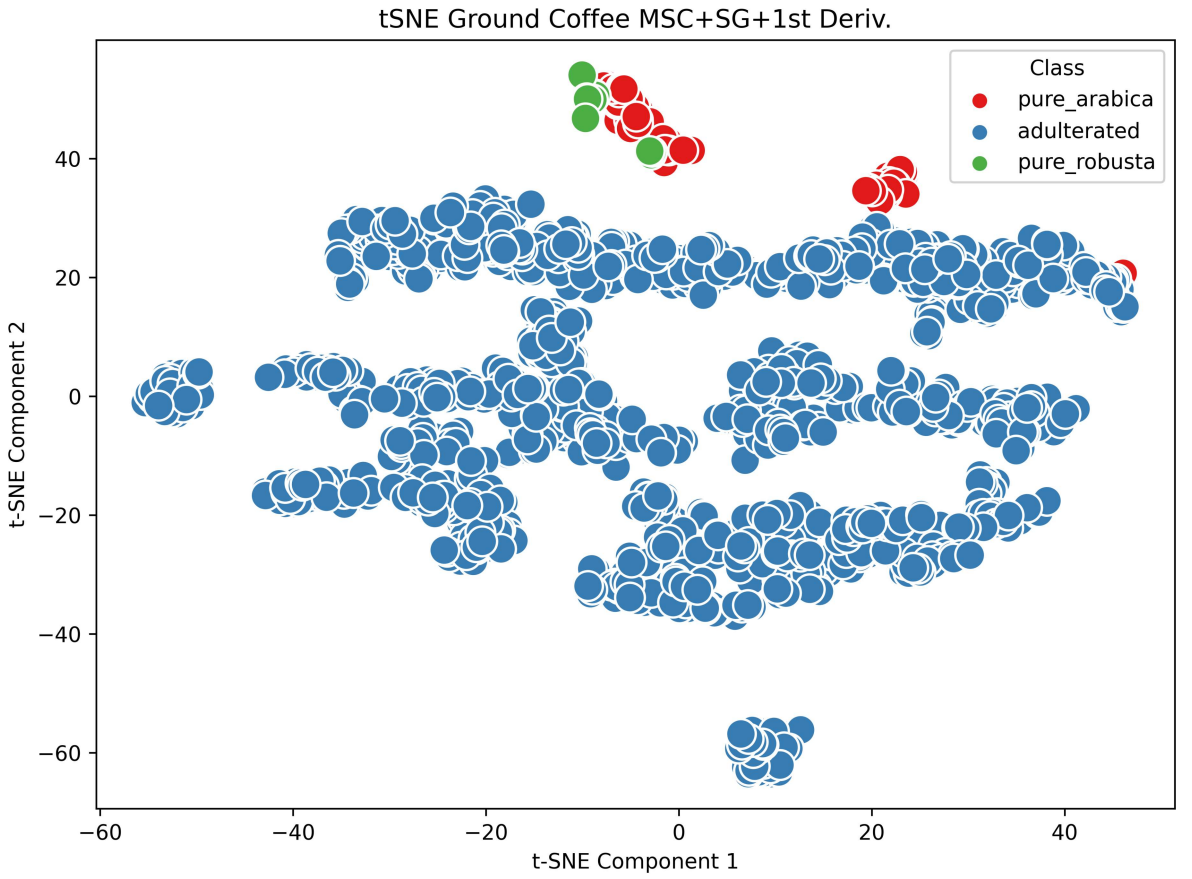


In [10]:
```
# Plotting-Adulteration percentage
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
                palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee Raw Spectra.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title='adulter_%', prop={'size': 9}, loc='best', markerscale=0.8)
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_Raw_adult_percent.png", dpi=600, bbox_inches="tight", form
plt.show()
```



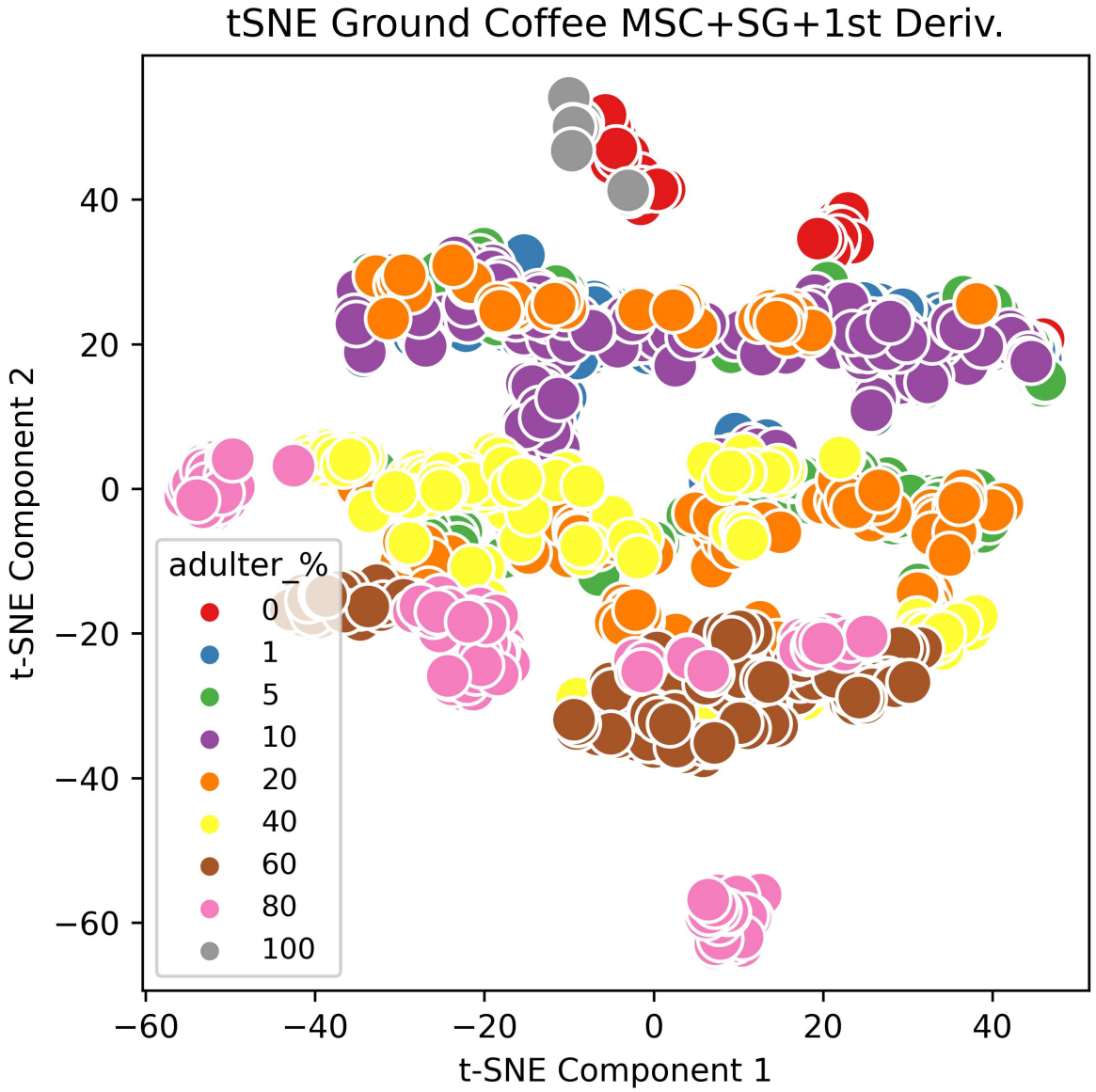
In [11]:
```
# MSC+SG+first derivative Ground Coffee

# Apply t-SNE to reduce dimensions to 2D
tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,init=
X_tsne = tsne.fit_transform(X_msc_sg_1d)

# Convert to DataFrame for plotting
tsne_df = pd.DataFrame(X_tsne, columns=['TSNE1', 'TSNE2'])
tsne_df[['Class', 'adulter_percent']] = ground_msc_sg_1d[['three_class','adult_perc
```

In [12]:
```
# Plotting
plt.figure(figsize=(8, 6), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
                palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee MSC+SG+1st Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class")
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_MSC_1D.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



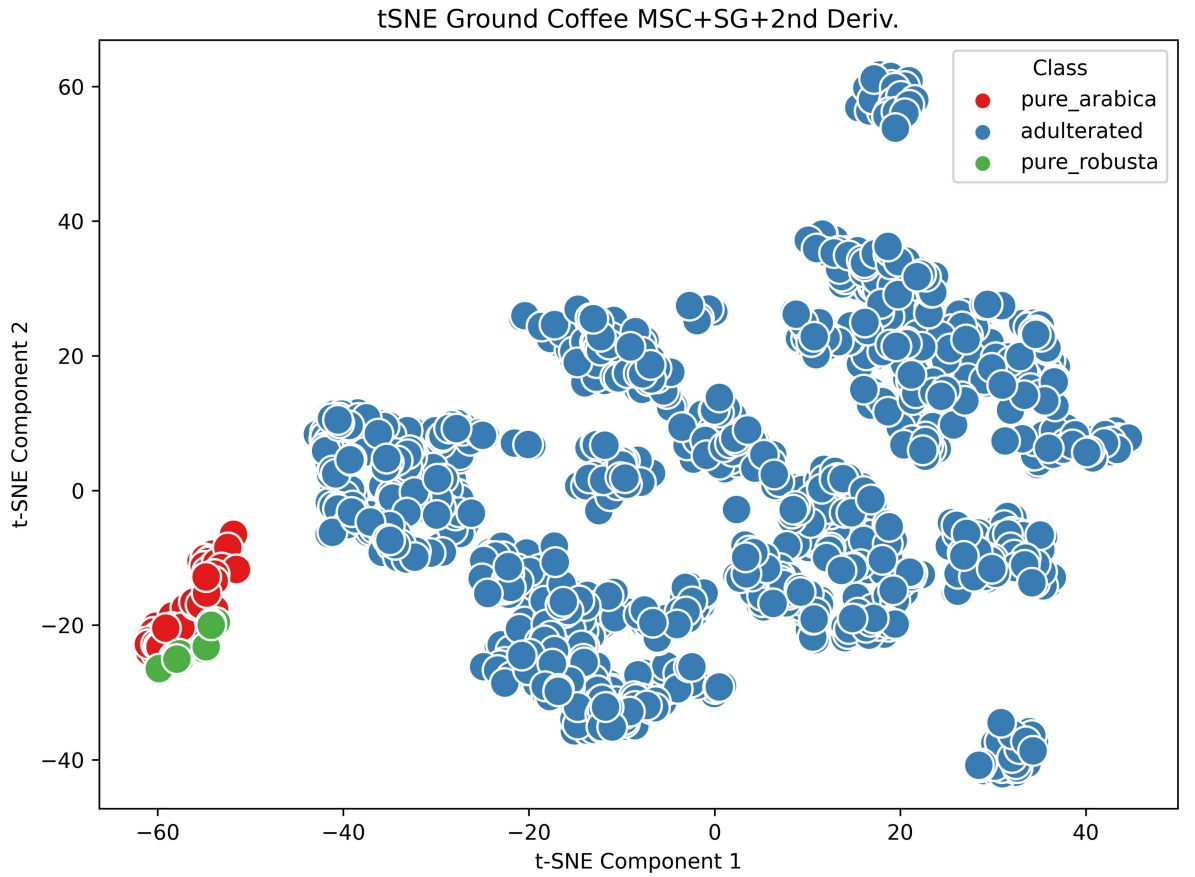
In [13]:

```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
               palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee MSC+SG+1st Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title='adulter_%', prop={'size': 9}, loc='best', markerscale=0.8)
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_MSC_1D_adult_percent.png", dpi=600, bbox_inches="tight", t
plt.show()
```



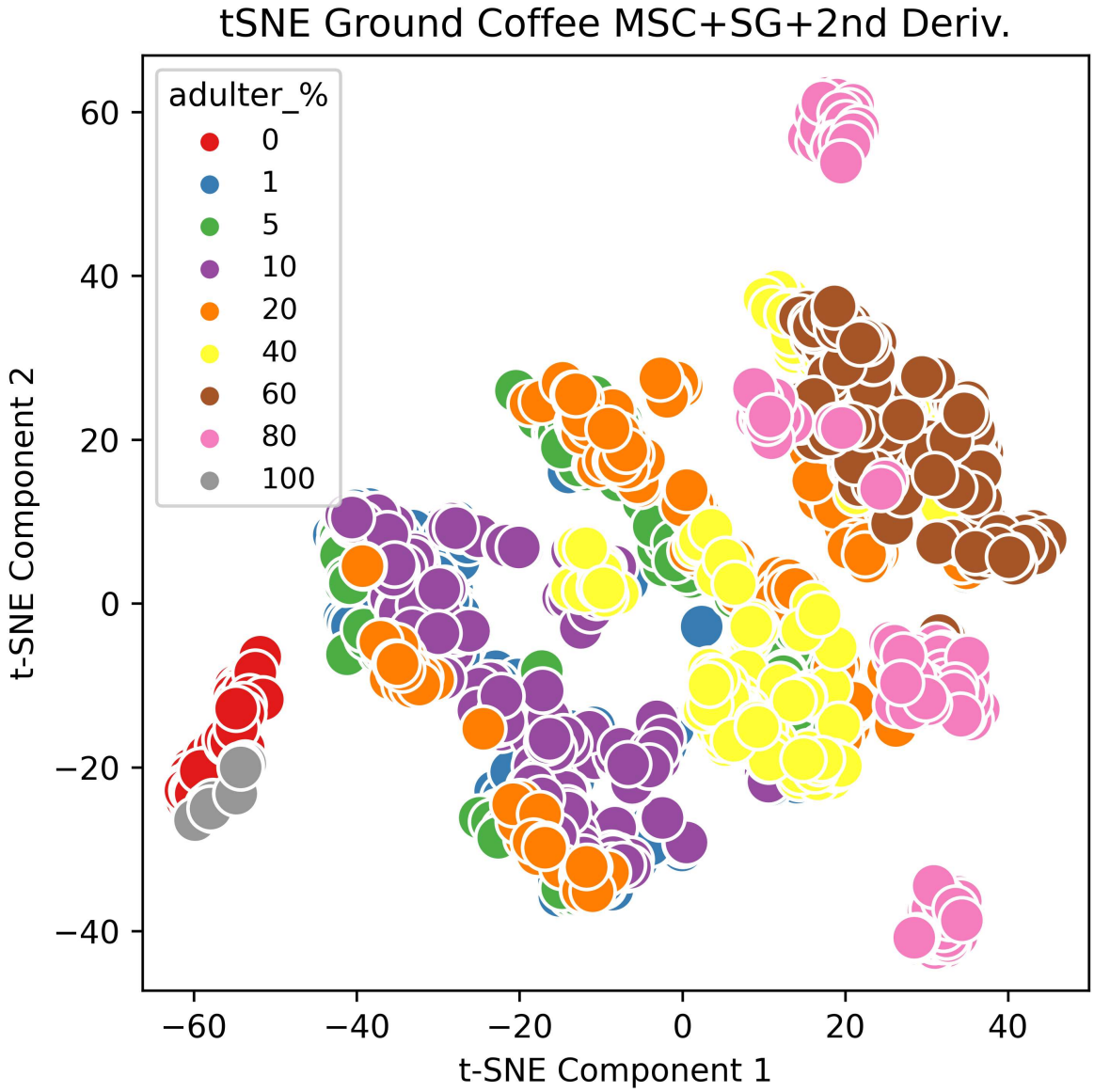
In [14]:
```
# MSC+SG+second derivative Ground Coffee

# Apply t-SNE to reduce dimensions to 2D
tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,init=
X_tsne = tsne.fit_transform(X_msc_sg_2d)

# Convert to DataFrame for plotting
tsne_df = pd.DataFrame(X_tsne, columns=['TSNE1', 'TSNE2'])
tsne_df[['Class', 'adulter_percent']] = ground_msc_sg_2d[['three_class','adult_perc
```

In [15]:
```
# Plotting
plt.figure(figsize=(8, 6), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
                palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee MSC+SG+2nd Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class")
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_MSC_2D.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



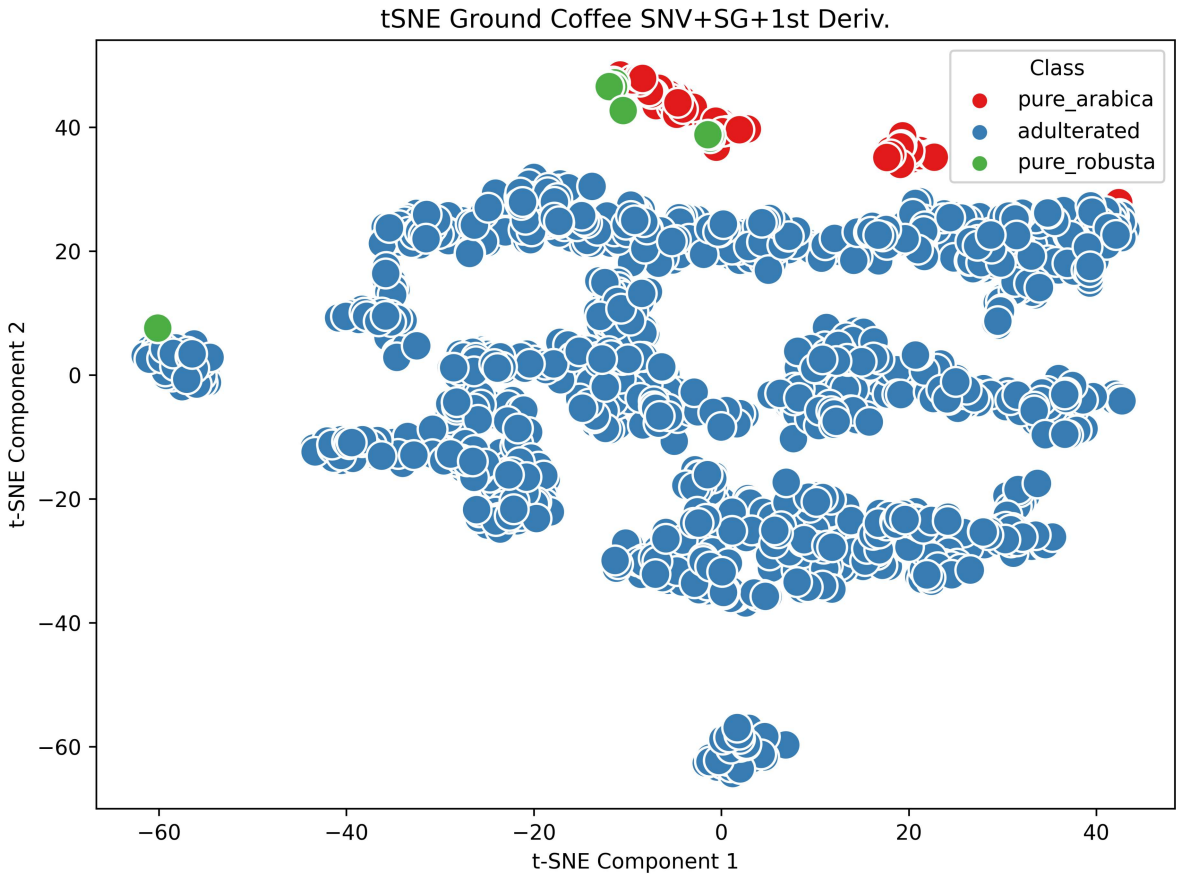
In [16]:

```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
               palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee MSC+SG+2nd Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title='adulter_%', prop={'size': 9}, loc='best', markerscale=0.8)
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_MSC_2D_adult_percent.png", dpi=600, bbox_inches="tight", t
plt.show()
```



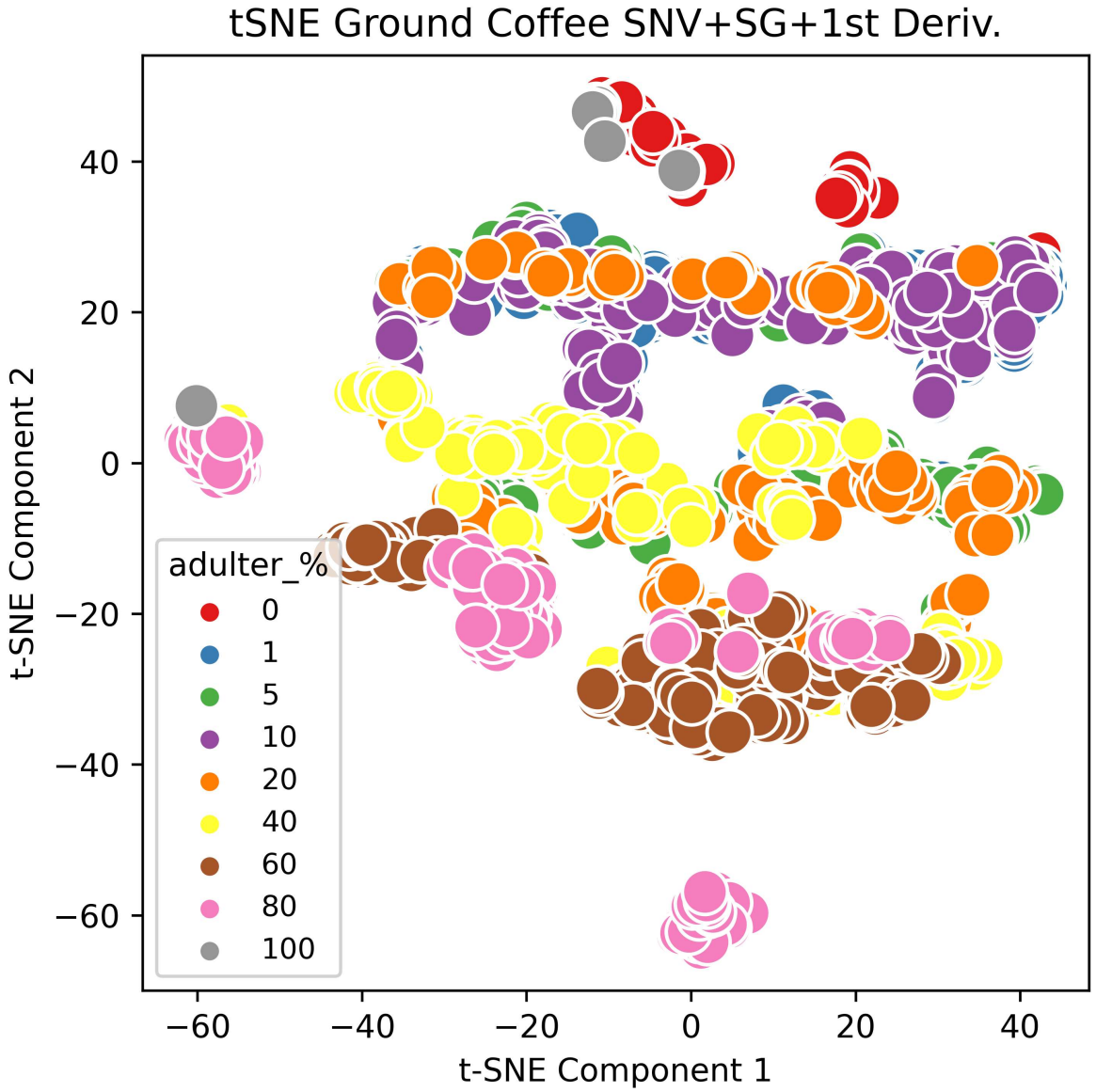
In [17]:
```python
# SNV+SG+first derivative Ground Coffee

# Apply t-SNE to reduce dimensions to 2D
tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,init=
X_tsne = tsne.fit_transform(X_snv_sg_1d)

# Convert to DataFrame for plotting
tsne_df = pd.DataFrame(X_tsne, columns=['TSNE1', 'TSNE2'])
tsne_df[['Class', 'adulter_percent']] = ground_snv_sg_1d[['three_class','adult_perc
```

In [18]:
```python
# Plotting
plt.figure(figsize=(8, 6), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
                palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee SNV+SG+1st Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class")
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_SNV_1D.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



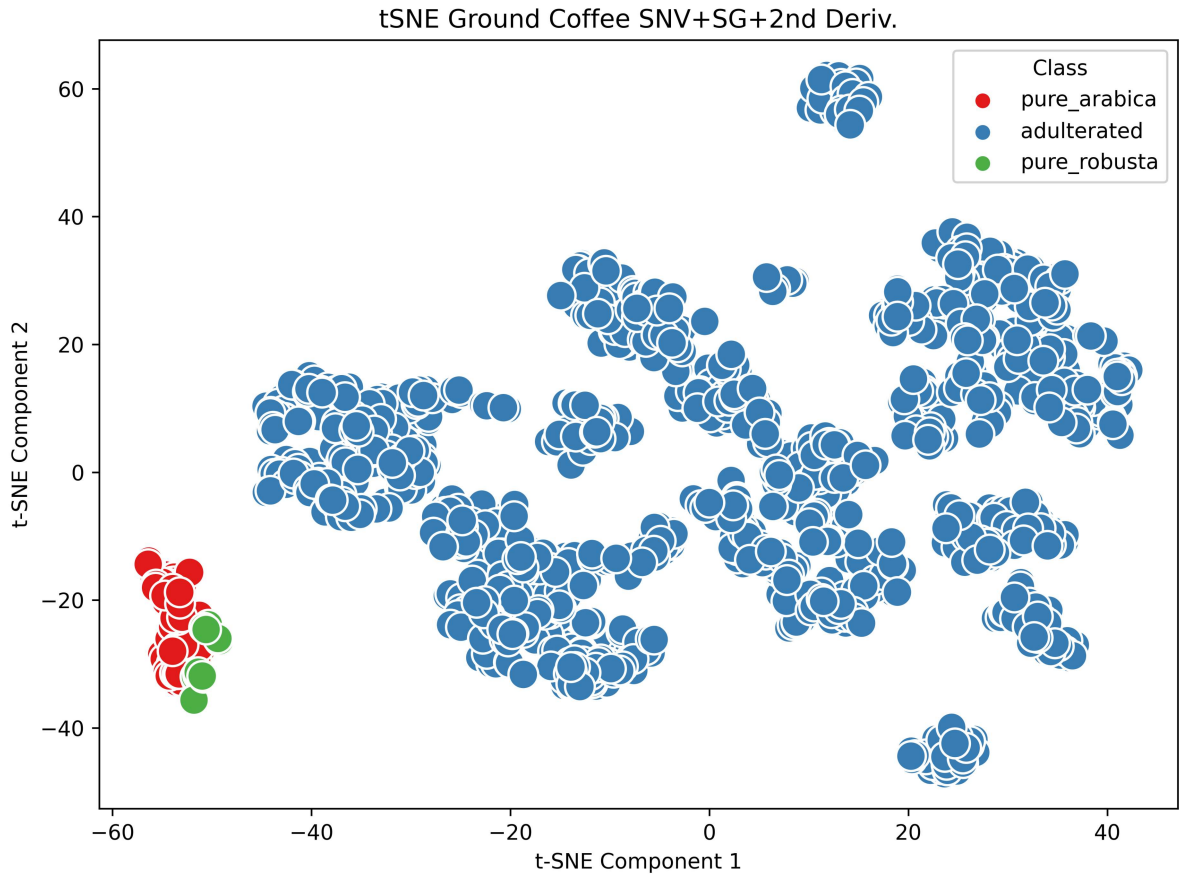
In [19]:

```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
               palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee SNV+SG+1st Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title='adulter_%', prop={'size': 9}, loc='best', markerscale=0.8)
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_SNV_1D_adult_percent.png", dpi=600, bbox_inches="tight", t
plt.show()
```



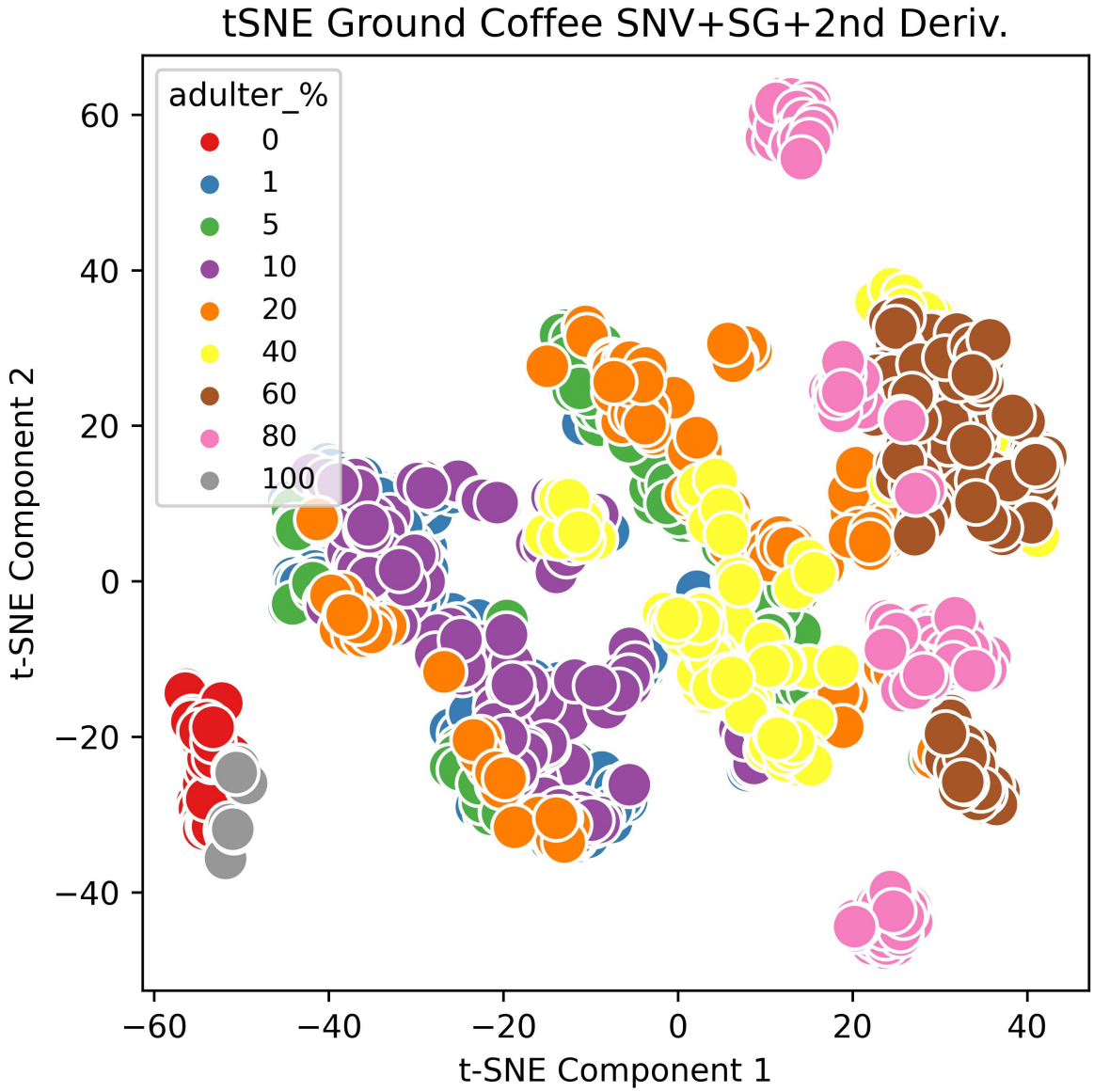
In [20]:
```
# SNV+SG+second derivative Ground Coffee

# Apply t-SNE to reduce dimensions to 2D
tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,init=
X_tsne = tsne.fit_transform(X_snv_sg_2d)

# Convert to DataFrame for plotting
tsne_df = pd.DataFrame(X_tsne, columns=['TSNE1', 'TSNE2'])
tsne_df[['Class', 'adulter_percent']] = ground_snv_sg_2d[['three_class','adult_perc
```

In [21]:
```
# Plotting
plt.figure(figsize=(8, 6), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
                palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee SNV+SG+2nd Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class")
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_SNV_2D.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



In [22]:

```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
               palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Ground Coffee SNV+SG+2nd Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title='adulter_%', prop={'size': 9}, loc='best', markerscale=0.8)
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Ground_SNV_2D_adult_percent.png", dpi=600, bbox_inches="tight", t
plt.show()
```



Principal Component Analysis

In [24]:
```
# Subset columns for aesthetics
columns = ground_raw[['binary_class','three_class','adult_percent']]
```

In [25]:
```
# Raw Spectra data

# Run PCA
pca = PCA(n_components=0.99)
pca_raw = pca.fit_transform(X_raw_scaled)

# Create a dataframe
pca_raw_df = pd.DataFrame(pca_raw, columns = ['PC1','PC2','PC3'])
pca_raw_df[['binary_class','three_class','adult_percent']] = columns

pca_raw_df.head(5)
```

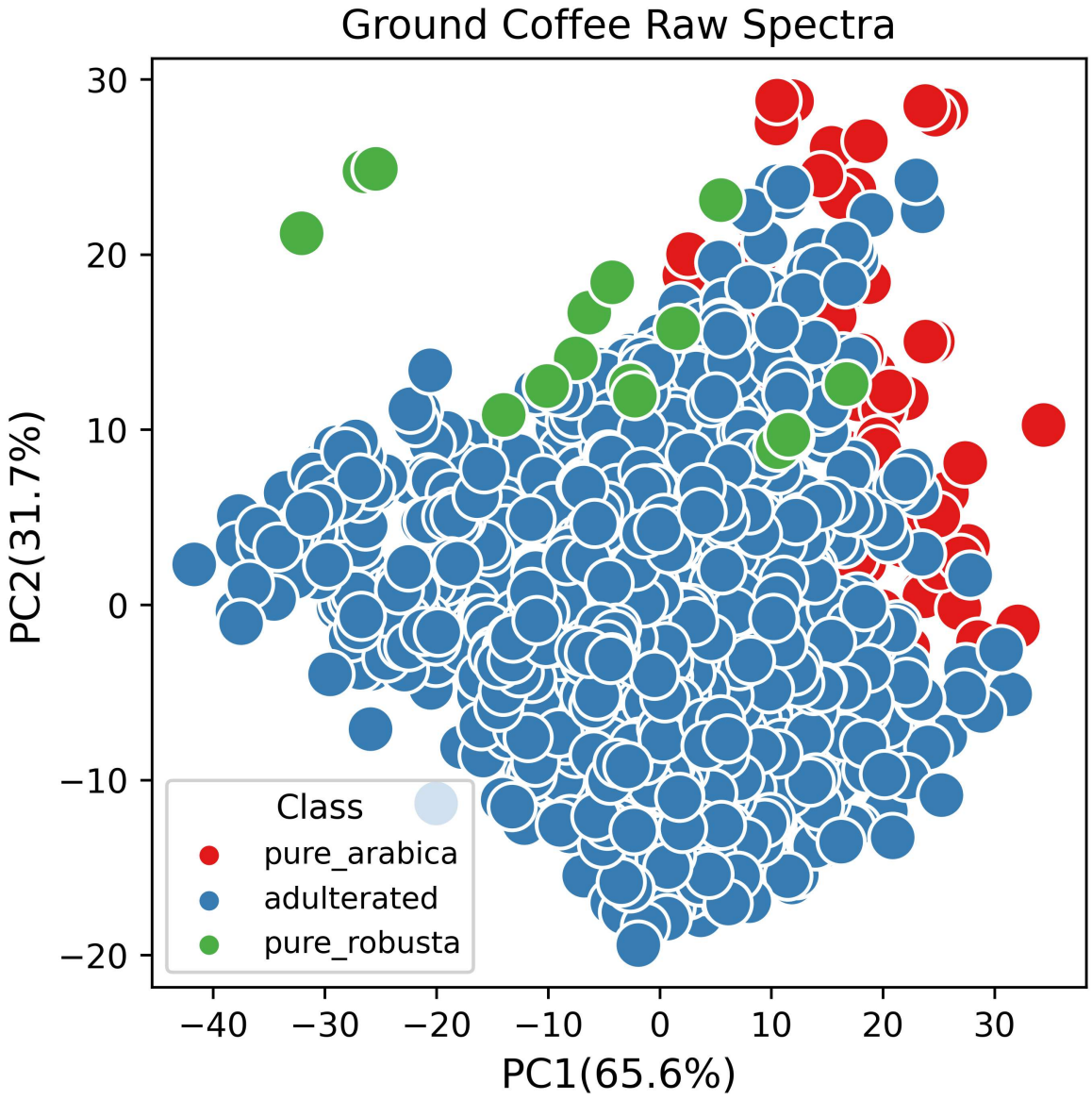
Out[25]:

	PC1	PC2	PC3	binary_class	three_class	adult_percent
0	9.551566	13.267316	0.652544	pure_arabica	pure_arabica	0
1	8.780026	20.034516	0.692442	pure_arabica	pure_arabica	0
2	16.737292	18.740437	2.952575	pure_arabica	pure_arabica	0
3	4.069887	11.888739	1.147600	pure_arabica	pure_arabica	0
4	11.655970	16.628360	1.907195	pure_arabica	pure_arabica	0

In [26]:
```
# Explained variance of each principal component
explained_variance = pca.explained_variance_ratio_
print(f"Explained variance by PC1: {explained_variance[0]:.3f}")
print(f"Explained variance by PC2: {explained_variance[1]:.3f}")
print(f"Explained variance by PC3: {explained_variance[2]:.3f}")
```

```
Explained variance by PC1: 0.656
Explained variance by PC2: 0.317
Explained variance by PC3: 0.018
```

In [27]:
```
# Create figure
plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_raw_df, x='PC1', y='PC2', hue='three_class',
                palette='Set1', alpha=1.0, s=200)
plt.title('Ground Coffee Raw Spectra', fontsize=12)
plt.xlabel('PC1(65.6%)', fontsize=12)
plt.ylabel('PC2(31.7%)', fontsize=12)
plt.legend(title='Class', prop={'size': 9}, loc='best', markerscale=0.8)
plt.savefig("PCA_Ground_Raw.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



In [28]:
```
# MSC+SG+1st derivative Spectra

# Run PCA
pca = PCA(n_components=0.99)
pca_msc_1d = pca.fit_transform(X_msc_sg_1d)


# Create a dataframe
pca_msc_1d_df = pd.DataFrame(pca_msc_1d, columns = ['PC1','PC2','PC3','PC4','PC5'])
pca_msc_1d_df[['binary_class','three_class','adult_percent']] = columns

pca_msc_1d_df.head(5)
```

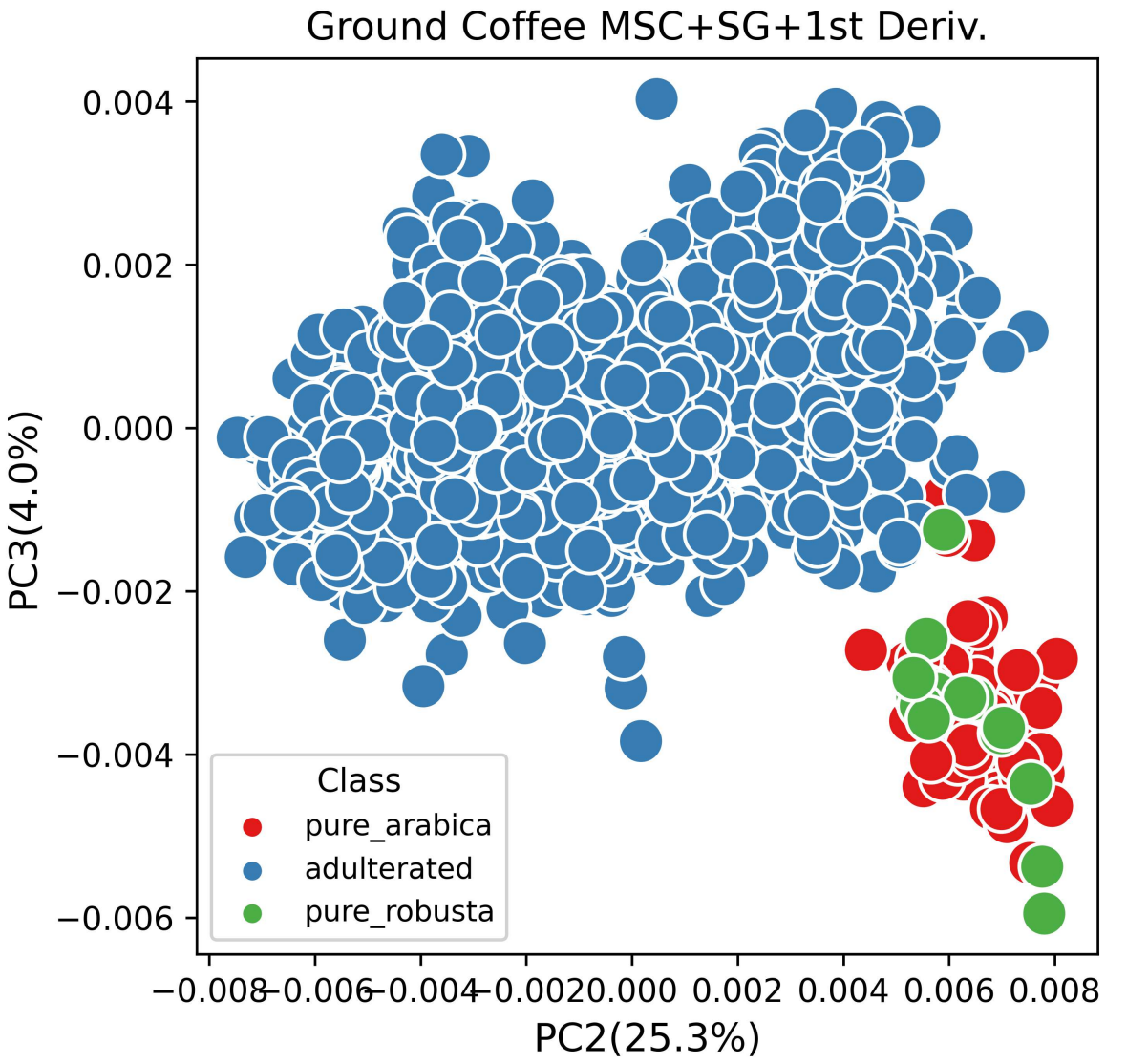
Out[28]:

	PC1	PC2	PC3	PC4	PC5	binary_class	three_class	adult_percent
0	-0.003665	0.006511	-0.003055	0.000389	-0.000330	pure_arabica	pure_arabica	0
1	-0.008059	0.007122	-0.004170	-0.000915	-0.000085	pure_arabica	pure_arabica	0
2	-0.004842	0.006300	-0.004060	0.000876	-0.000339	pure_arabica	pure_arabica	0
3	-0.005779	0.005513	-0.004391	0.000391	-0.001535	pure_arabica	pure_arabica	0
4	-0.005808	0.005693	-0.003282	0.000493	-0.001109	pure_arabica	pure_arabica	0

In [29]:
```
# Explained variance of each principal component
explained_variance = pca.explained_variance_ratio_
print(f"Explained variance by PC1: {explained_variance[0]:.3f}")
print(f"Explained variance by PC2: {explained_variance[1]:.3f}")
print(f"Explained variance by PC3: {explained_variance[2]:.3f}")
print(f"Explained variance by PC4: {explained_variance[3]:.3f}")
print(f"Explained variance by PC5: {explained_variance[4]:.3f}")
```

```
Explained variance by PC1: 0.663
Explained variance by PC2: 0.253
Explained variance by PC3: 0.040
Explained variance by PC4: 0.020
Explained variance by PC5: 0.015
```

In [30]:
```
# Create scatter plot
plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_msc_1d_df, x='PC2', y='PC3', hue='three_class',
                palette='Set1', alpha=1.0, s=200)
plt.title('Ground Coffee MSC+SG+1st Deriv.', fontsize=12)
plt.xlabel('PC2(25.3%)', fontsize=12)
plt.ylabel('PC3(4.0%)', fontsize=12)
plt.legend(title='Class', prop={'size': 9}, loc='best', markerscale=0.8)
plt.savefig("PCA_Ground_MSC_SG_1D.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



In [31]:
```
# MSC+SG+2nd derivative Spectra

# Run PCA
```

```
pca = PCA(n_components=0.99)
pca_msc_2d = pca.fit_transform(X_msc_sg_2d)


# Create a dataframe
pca_msc_2d_df = pd.DataFrame(pca_msc_2d, columns = ['PC1','PC2','PC3','PC4','PC5','
pca_msc_2d_df[['binary_class','three_class','adult_percent']] = columns

pca_msc_2d_df.head(5)
```

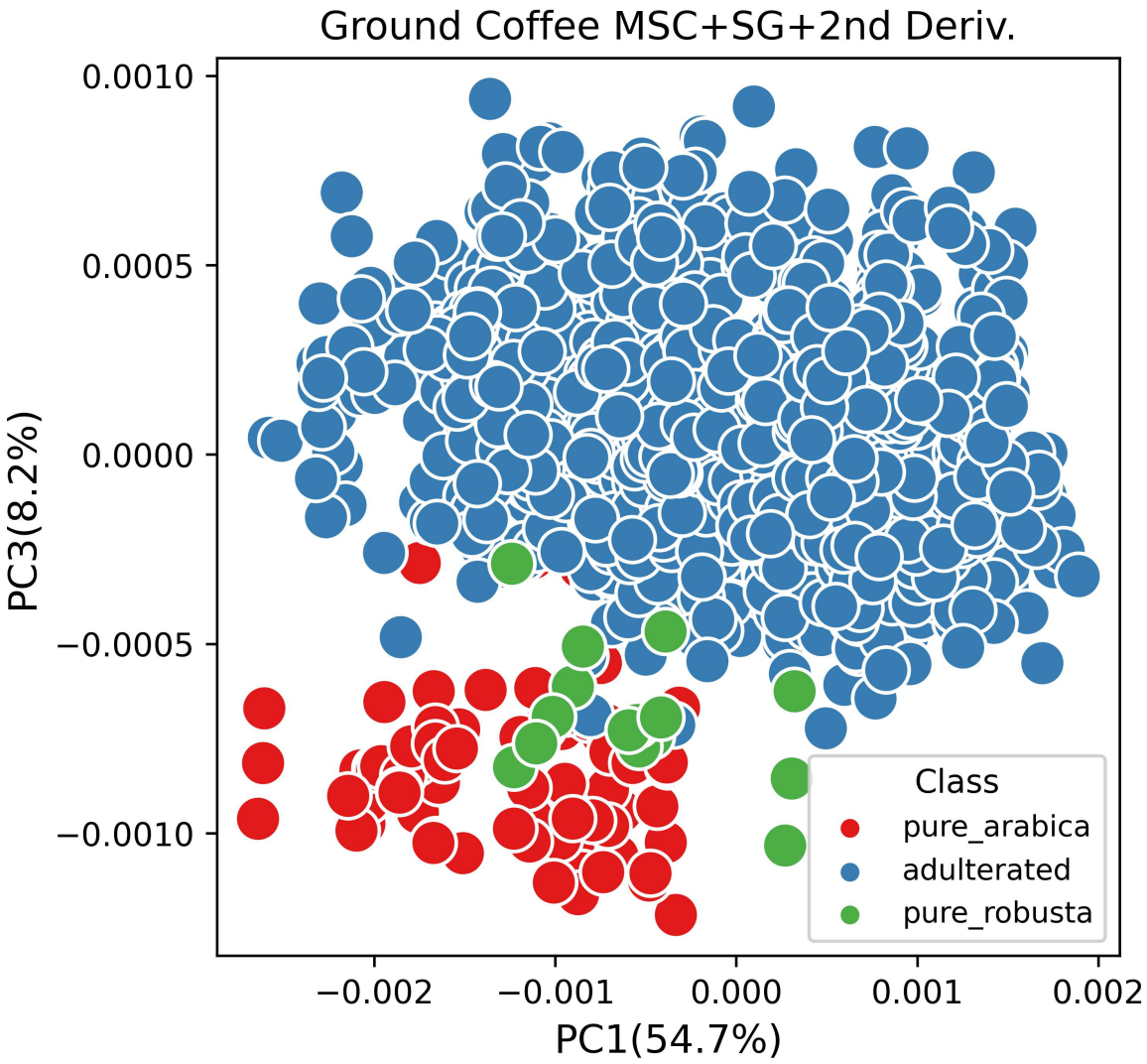
Out[31]:

	PC1	PC2	PC3	PC4	PC5	PC6	binary_class	three_class	adul
0	-0.000962	-0.001164	-0.000725	-0.000091	-0.000018	0.000018	pure_arabica	pure_arabica	
1	-0.000636	-0.001645	-0.000942	0.000026	-0.000021	-0.000046	pure_arabica	pure_arabica	
2	-0.000836	-0.001303	-0.001000	-0.000162	-0.000027	0.000090	pure_arabica	pure_arabica	
3	-0.000656	-0.001499	-0.001060	-0.000058	0.000134	0.000071	pure_arabica	pure_arabica	
4	-0.000669	-0.001425	-0.000754	-0.000101	0.000081	0.000053	pure_arabica	pure_arabica	

In [32]:
```
# Explained variance of each principal component
explained_variance = pca.explained_variance_ratio_
print(f"Explained variance by PC1: {explained_variance[0]:.3f}")
print(f"Explained variance by PC2: {explained_variance[1]:.3f}")
print(f"Explained variance by PC3: {explained_variance[2]:.3f}")
print(f"Explained variance by PC4: {explained_variance[3]:.3f}")
print(f"Explained variance by PC5: {explained_variance[4]:.3f}")
print(f"Explained variance by PC6: {explained_variance[5]:.3f}")
```

```
Explained variance by PC1: 0.547
Explained variance by PC2: 0.327
Explained variance by PC3: 0.082
Explained variance by PC4: 0.023
Explained variance by PC5: 0.011
Explained variance by PC6: 0.003
```

In [33]:
```
# Create scatter plot
plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_msc_2d_df, x='PC1', y='PC3', hue='three_class',
                palette='Set1', alpha=1.0, s=200)
plt.title('Ground Coffee MSC+SG+2nd Deriv.', fontsize=12)
plt.xlabel('PC1(54.7%)', fontsize=12)
plt.ylabel('PC3(8.2%)', fontsize=12)
plt.legend(title='Class', prop={'size': 9}, loc='best', markerscale=0.8)
plt.savefig("PCA_Ground_MSC_SG_2D.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



In [34]:
```
# SNV+SG+1st derivative Spectra

# Run PCA
pca = PCA(n_components=0.99)
pca_snv_1d = pca.fit_transform(X_snv_sg_1d)


# Create a dataframe
pca_snv_1d_df = pd.DataFrame(pca_snv_1d, columns = ['PC1','PC2','PC3','PC4','PC5','
pca_snv_1d_df[['binary_class','three_class','adult_percent']] = columns

pca_snv_1d_df.head(5)
```

Out[34]:

	PC1	PC2	PC3	PC4	PC5	PC6	binary_class	three_class	adult_
0	-0.044957	0.084259	-0.043836	0.013166	0.004019	-0.003347	pure_arabica	pure_arabica	
1	-0.110811	0.081966	-0.040079	0.030489	-0.011031	0.001585	pure_arabica	pure_arabica	
2	-0.062295	0.079499	-0.048865	0.027305	0.009931	-0.000988	pure_arabica	pure_arabica	
3	-0.073871	0.069315	-0.051821	0.031957	0.003146	-0.015806	pure_arabica	pure_arabica	
4	-0.075241	0.071144	-0.038900	0.023738	0.005004	-0.011423	pure_arabica	pure_arabica	

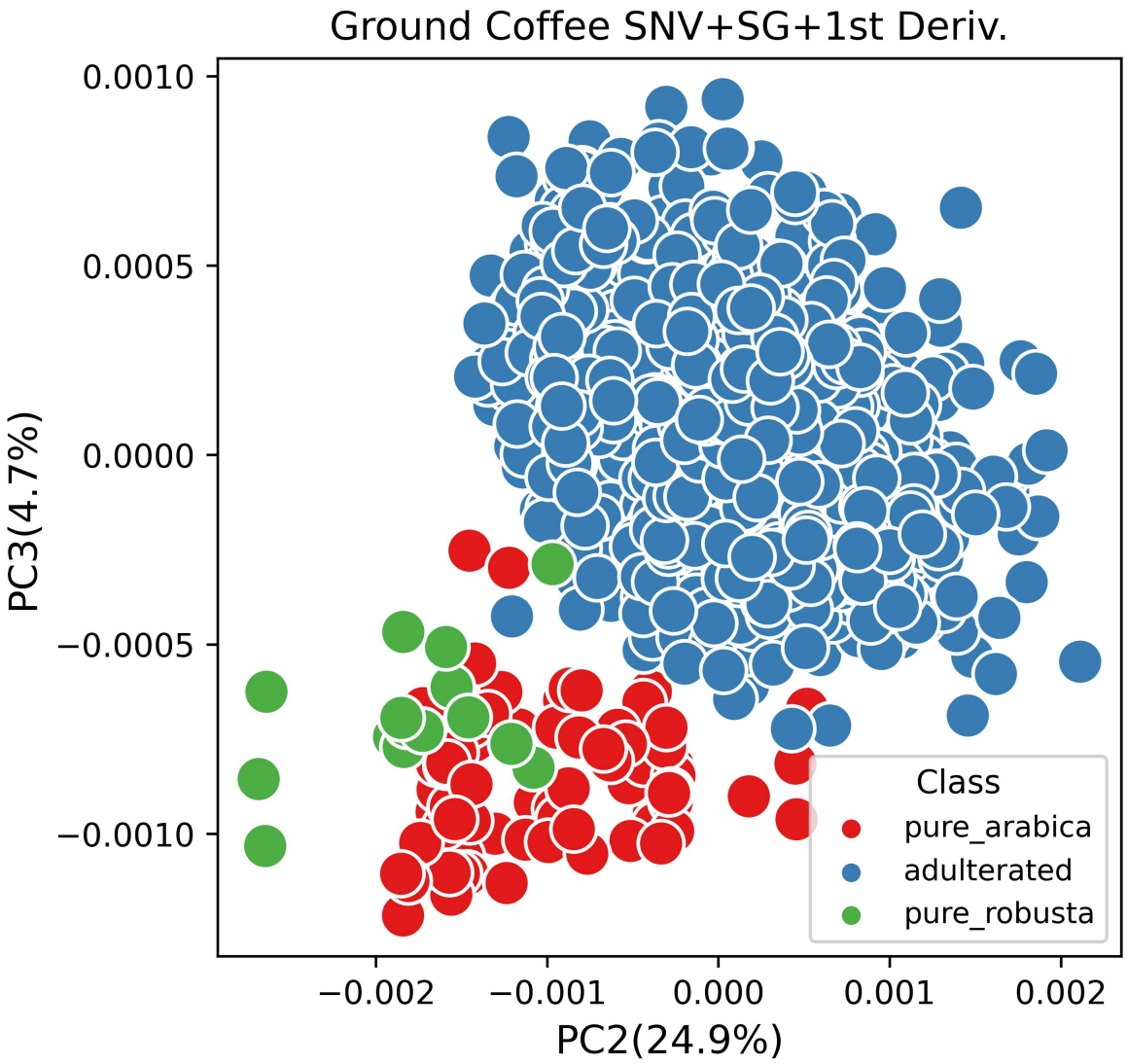
In [35]:
```
# Explained variance of each principal component
explained_variance = pca.explained_variance_ratio_
print(f"Explained variance by PC1: {explained_variance[0]:.3f}")
```

```
print(f"Explained variance by PC2: {explained_variance[1]:.3f}")
print(f"Explained variance by PC3: {explained_variance[2]:.3f}")
print(f"Explained variance by PC4: {explained_variance[3]:.3f}")
print(f"Explained variance by PC5: {explained_variance[4]:.3f}")
print(f"Explained variance by PC6: {explained_variance[5]:.3f}")
```

```
Explained variance by PC1: 0.635
Explained variance by PC2: 0.249
Explained variance by PC3: 0.047
Explained variance by PC4: 0.028
Explained variance by PC5: 0.020
Explained variance by PC6: 0.015
```

In [36]:

```
# Create scatter plot
plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_msc_2d_df, x='PC2', y='PC3', hue='three_class',
                palette='Set1', alpha=1.0, s=200)
plt.title('Ground Coffee SNV+SG+1st Deriv.', fontsize=12)
plt.xlabel('PC2(24.9%)', fontsize=12)
plt.ylabel('PC3(4.7%)', fontsize=12)
plt.legend(title='Class', prop={'size': 9}, loc='best', markerscale=0.8)
plt.savefig("PCA_Ground_SNV_SG_1D.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



In [37]:

```
# SNV+SG+1st derivative Spectra

# Run PCA
pca = PCA(n_components=0.99)
pca_snv_2d = pca.fit_transform(X_snv_sg_2d)
```

```
# Create a dataframe
pca_snv_2d_df = pd.DataFrame(pca_snv_2d, columns = ['PC1','PC2','PC3','PC4','PC5','
pca_snv_2d_df[['binary_class','three_class','adult_percent']] = columns

pca_snv_2d_df.head(5)
```

Out[37]:

	PC1	PC2	PC3	PC4	PC5	PC6	binary_class	three_class	adul
0	-0.013907	-0.013725	-0.009423	-0.001721	0.000372	-0.000517	pure_arabica	pure_arabica	
1	-0.008653	-0.020852	-0.011875	0.000260	-0.000368	-0.000291	pure_arabica	pure_arabica	
2	-0.012068	-0.015792	-0.012897	-0.002467	-0.000357	0.000340	pure_arabica	pure_arabica	
3	-0.009972	-0.018439	-0.013678	-0.001501	0.001917	0.000781	pure_arabica	pure_arabica	
4	-0.009949	-0.017543	-0.009709	-0.001838	0.001096	0.000513	pure_arabica	pure_arabica	

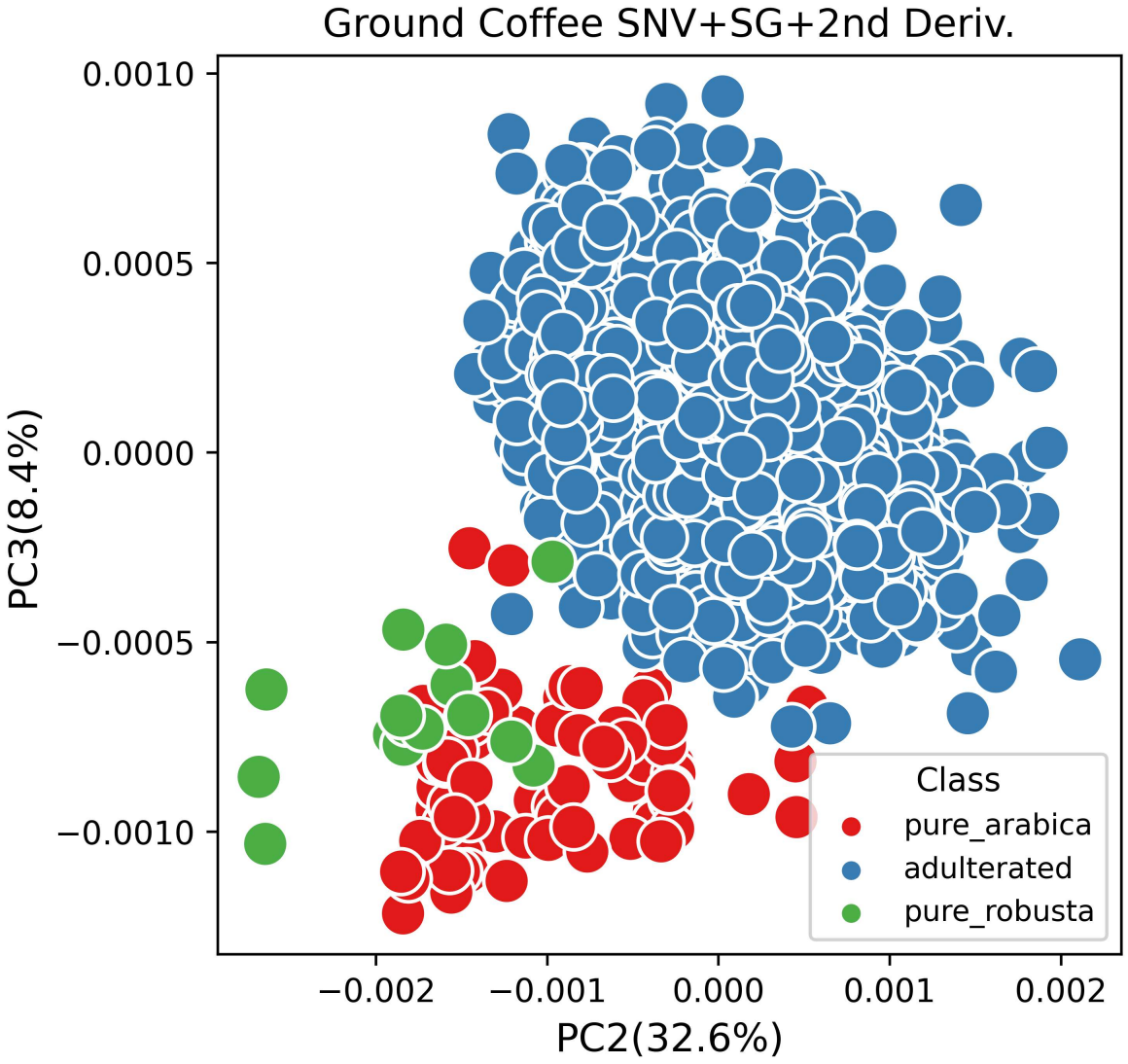
In [38]:

```
# Explained variance of each principal component
explained_variance = pca.explained_variance_ratio_
print(f"Explained variance by PC1: {explained_variance[0]:.3f}")
print(f"Explained variance by PC2: {explained_variance[1]:.3f}")
print(f"Explained variance by PC3: {explained_variance[2]:.3f}")
print(f"Explained variance by PC4: {explained_variance[3]:.3f}")
print(f"Explained variance by PC5: {explained_variance[4]:.3f}")
print(f"Explained variance by PC6: {explained_variance[5]:.3f}")
```

```
Explained variance by PC1: 0.538
Explained variance by PC2: 0.326
Explained variance by PC3: 0.084
Explained variance by PC4: 0.024
Explained variance by PC5: 0.014
Explained variance by PC6: 0.005
```

In [39]:

```
# Create scatter plot
plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_msc_2d_df, x='PC2', y='PC3', hue='three_class',
                palette='Set1', alpha=1.0, s=200)
plt.title('Ground Coffee SNV+SG+2nd Deriv.', fontsize=12)
plt.xlabel('PC2(32.6%)', fontsize=12)
plt.ylabel('PC3(8.4%)', fontsize=12)
plt.legend(title='Class', prop={'size': 9}, loc='best', markerscale=0.8)
plt.savefig("PCA_Ground_SNV_SG_2D.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```


Ground Coffee SNV+SG+2nd Deriv.
0.0010
0.0005
0.0000
−0.0005
−0.0010
PC3(8.4%)
−0.002
−0.001
0.000
0.001
0.002
PC2(32.6%)
Class
pure_arabica
adulterated
pure_robusta

In [ ]: