Dimensionality Reduction (Principal Component Analysis (PCA) and t-Distributed Stochastic Neighbor Embedding (t-SNE) for Instant 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_U
```

In [4]:
```
# Read_data. Import the files for instant coffee
instant_raw = pd.read_excel('instant_coffee_raw.xlsx')
instant_msc_sg_1d = pd.read_excel('coffee_instant_msc_sg_1d.xlsx')
instant_msc_sg_2d = pd.read_excel('coffee_instant_msc_sg_2d.xlsx')
instant_snv_sg_1d = pd.read_excel('coffee_instant_snv_sg_1d.xlsx')
instant_snv_sg_2d = pd.read_excel('coffee_instant_snv_sg_2d.xlsx')
```

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

Out[5]:

	sample_name	binary_class	three_class	cal_val	perc_adulter	935.609985	939.0599
0	Arabica_10	pure_arabica	pure_arabica	1	0	0.530853	0.5336
1	Arabica_10	pure_arabica	pure_arabica	1	0	0.533290	0.5359
2	Arabica_10	pure_arabica	pure_arabica	1	0	0.531486	0.5342
3	Arabica_11	pure_arabica	pure_arabica	1	0	0.563388	0.5664
4	Arabica_11	pure_arabica	pure_arabica	1	0	0.560974	0.5639

5 rows × 229 columns

In [6]:
```
# Select the X columns
X_raw = instant_raw.iloc[:,5:230]
X_msc_sg_1d = instant_msc_sg_1d.iloc[:,5:230]
X_msc_sg_2d = instant_msc_sg_2d.iloc[:,5:230]
X_snv_sg_1d = instant_snv_sg_1d.iloc[:,5:230]
X_snv_sg_2d = instant_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)
```

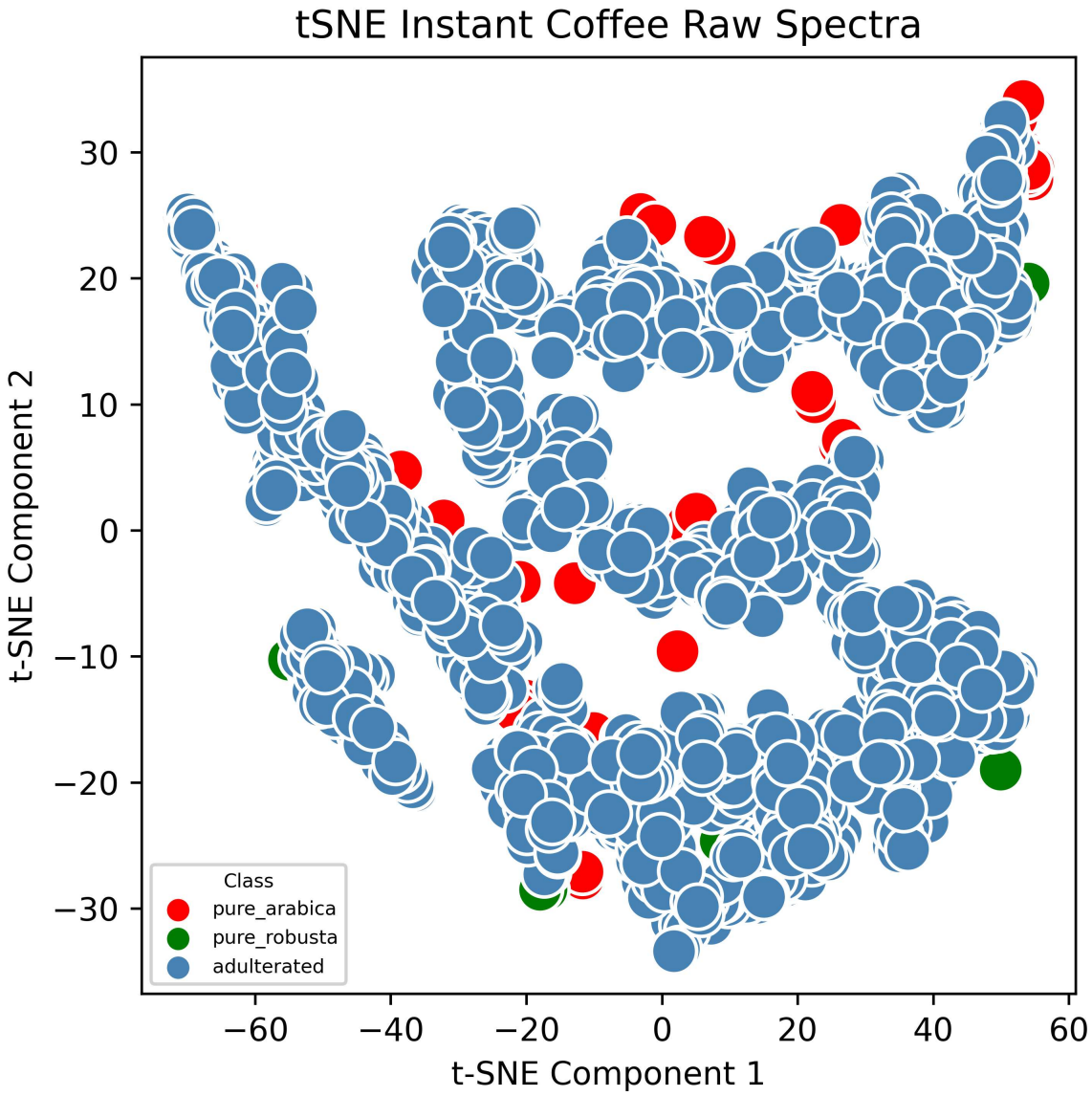
```
(1476, 224)
(1476, 224)
(1476, 224)
(1476, 224)
(1476, 224)
```

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

# Subset the percentage adulteration
percent_adult = instant_raw['perc_adulter']

print(three_class.shape)
```

```
(1476,)
```

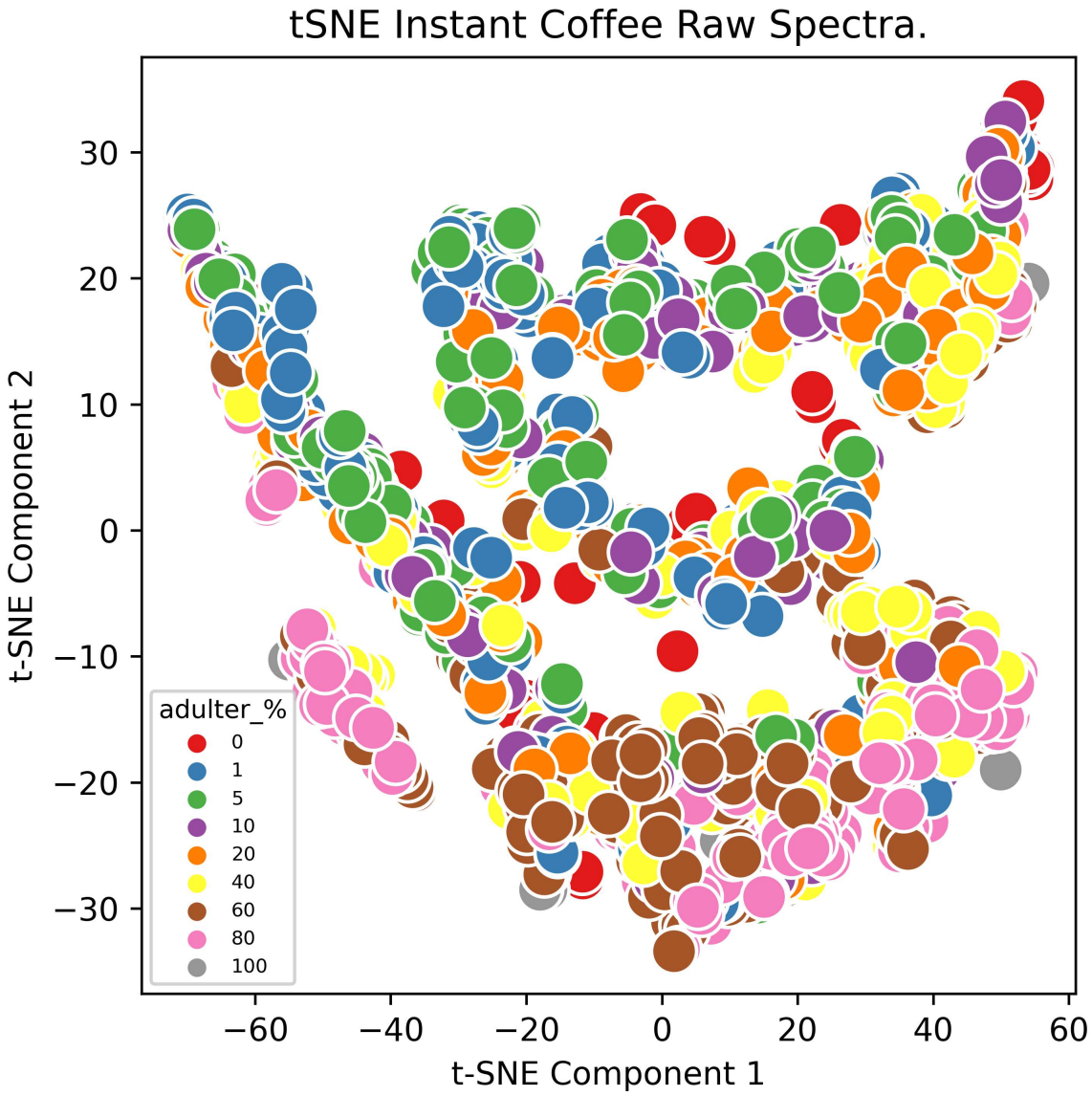
In [8]:
```python
# Raw Spectra Instant Coffee
# Apply t-SNE to reduce dimensions to 2D

# 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,in
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']] = instant_raw[['three_class','perc_adulter
```

In [9]:
```python
# Plotting
plt.figure(figsize=(5, 5), dpi=600)
palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g
# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
               palette=palette, alpha=1.0, s=200)
plt.title("tSNE Instant Coffee Raw Spectra")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class", loc='lower left', fontsize=6, title_fontsize=6)
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Instant_Raw.png", dpi=600, bbox_inches="tight", format="png")
plt.show()
```



In [10]:

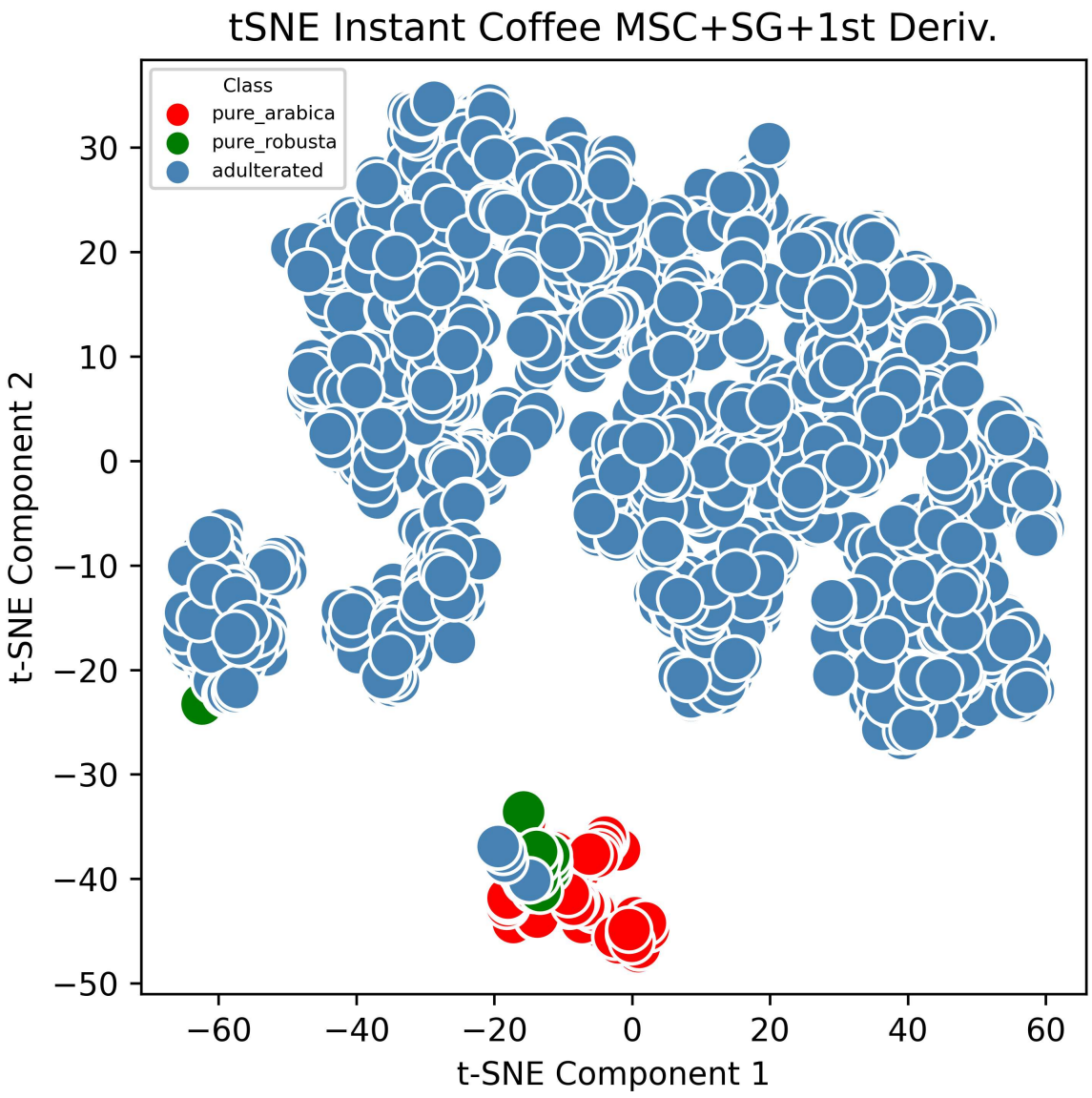
```
# Plotting-Adulteration percentage
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
               palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Instant Coffee Raw Spectra.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title='adulter_%', prop={'size': 6}, loc='best', markerscale=0.8, tit
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Instant_Raw_adult_percent.png", dpi=600, bbox_inches="tight",
plt.show()
```



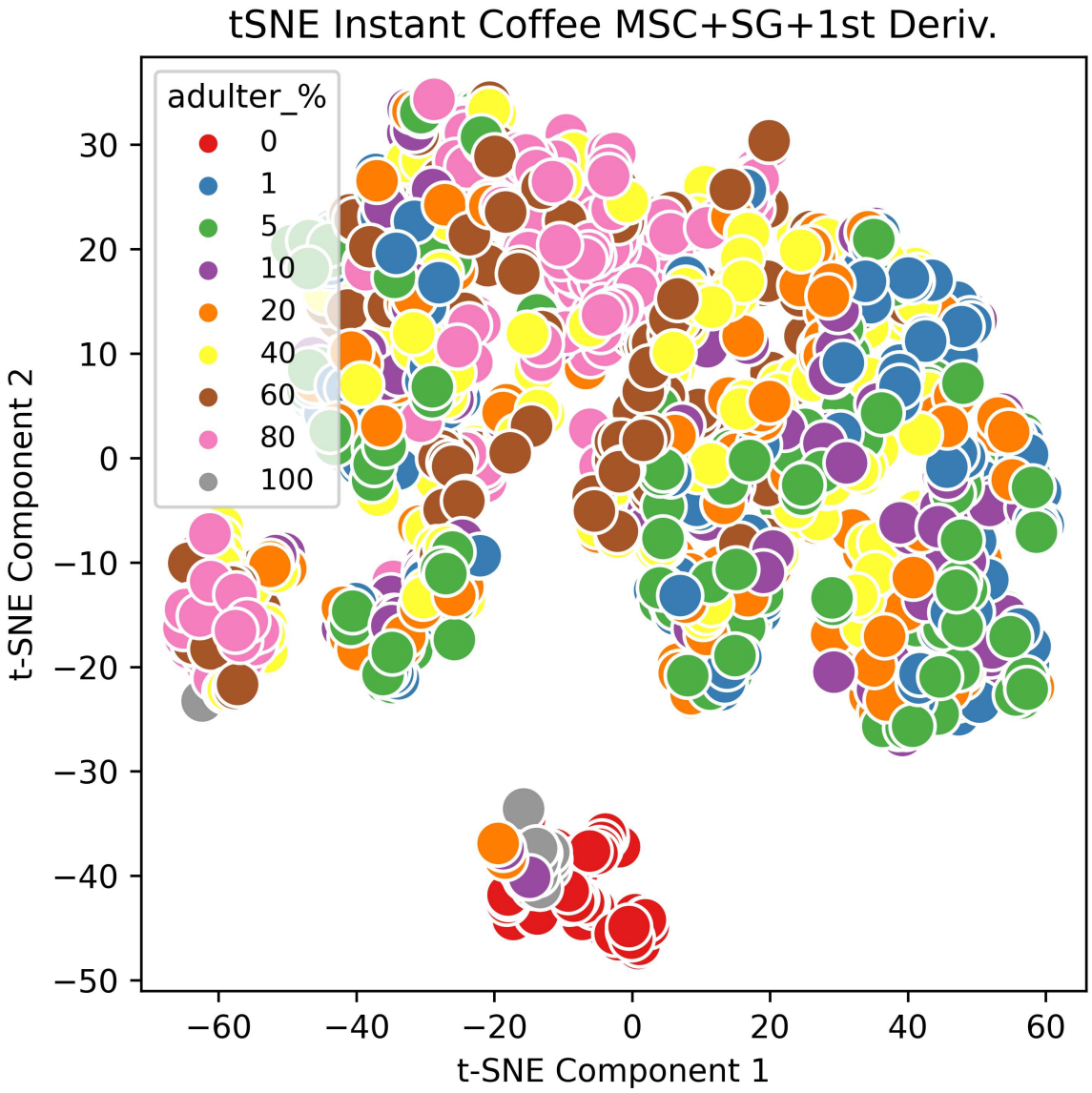
In [11]:
```
# MSC+SG+first derivative Instant Coffee

# Apply t-SNE to reduce dimensions to 2D
tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,in
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']] = instant_msc_sg_1d[['three_class','perc_a
```

In [12]:
```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)
palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g
# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
               palette=palette, alpha=1.0, s=200)
plt.title("tSNE Instant Coffee MSC+SG+1st Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class", loc = 'upper left',fontsize=6, title_fontsize=6)
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
```

```
plt.savefig("tSNE_Instant_MSC_1D.png", dpi=600, bbox_inches="tight", format="png
plt.show()
```



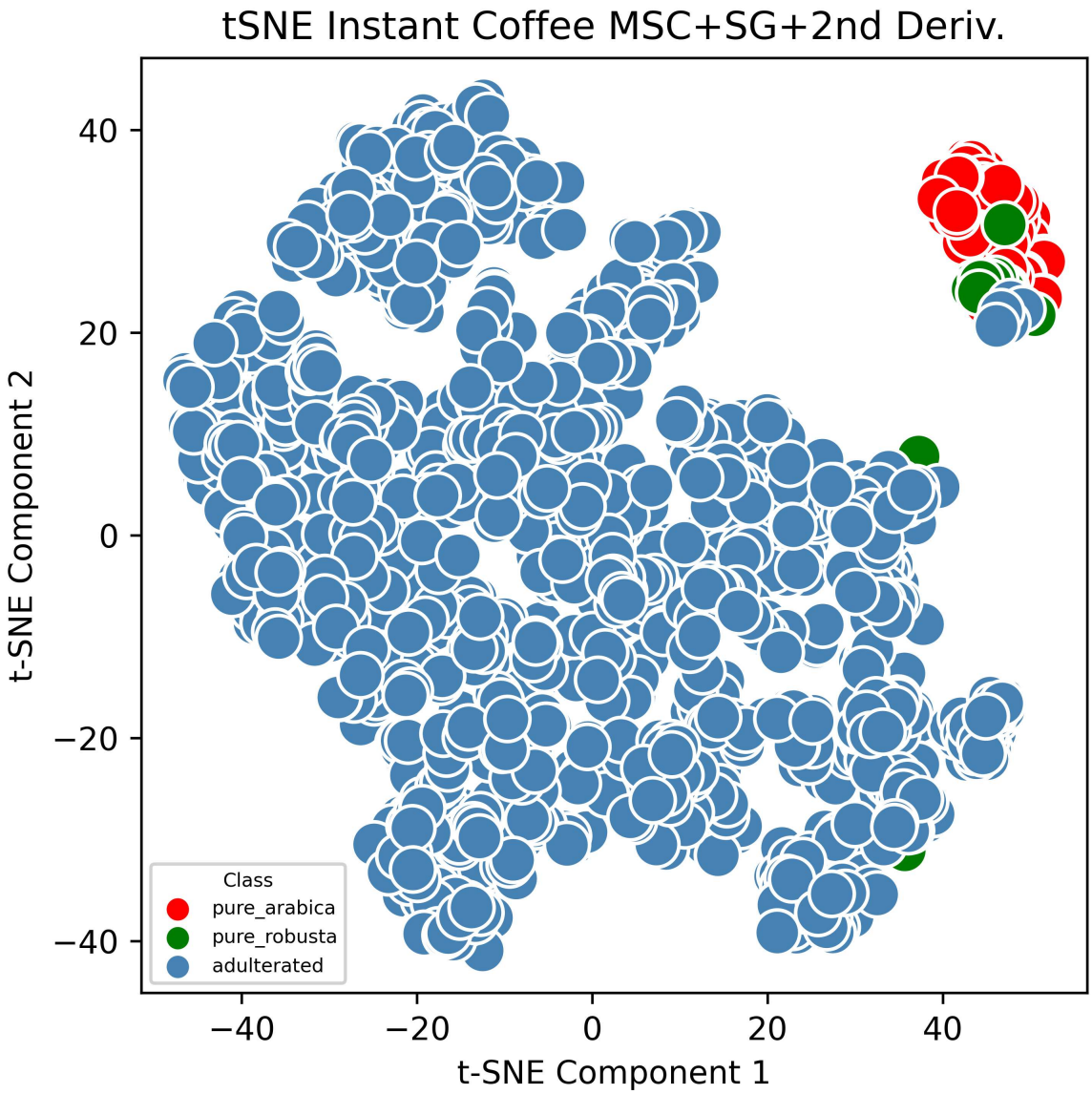
In [13]:
```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
               palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Instant 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_Instant_MSC_1D_adult_percent.png", dpi=600, bbox_inches="tight
plt.show()
```



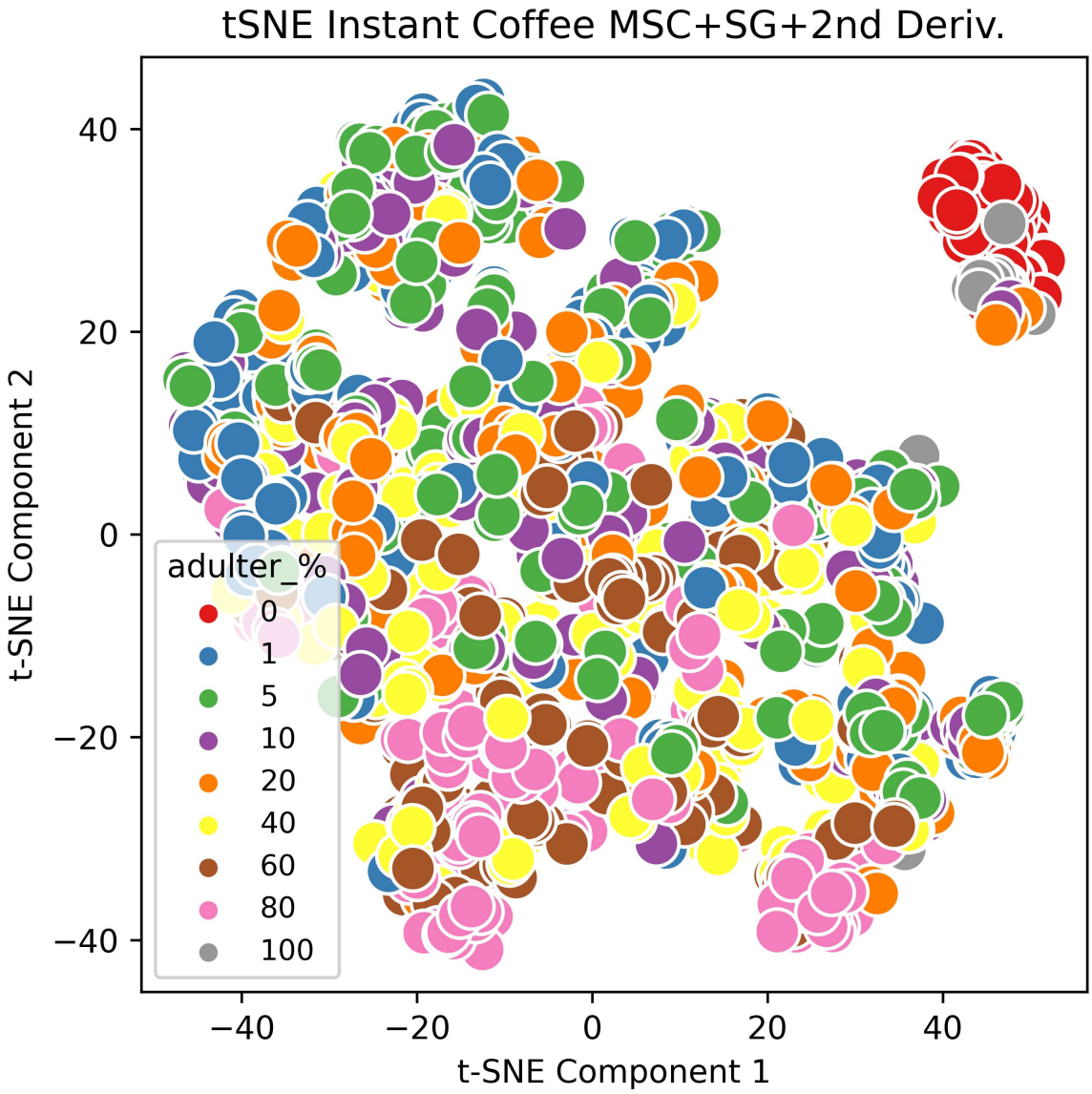
In [14]:
```
# MSC+SG+second derivative Instant Coffee

# Apply t-SNE to reduce dimensions to 2D
tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,in
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']] = instant_msc_sg_2d[['three_class','perc_a
```

In [15]:
```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g
# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
               palette=palette, alpha=1.0, s=200)
plt.title("tSNE Instant Coffee MSC+SG+2nd Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class",loc = 'lower left',fontsize=6, title_fontsize=6)
plt.grid(False)
plt.tight_layout()
```

```
# Save the figure with high resolution
plt.savefig("tSNE_Instant_MSC_2D.png", dpi=600, bbox_inches="tight", format="png
plt.show()
```



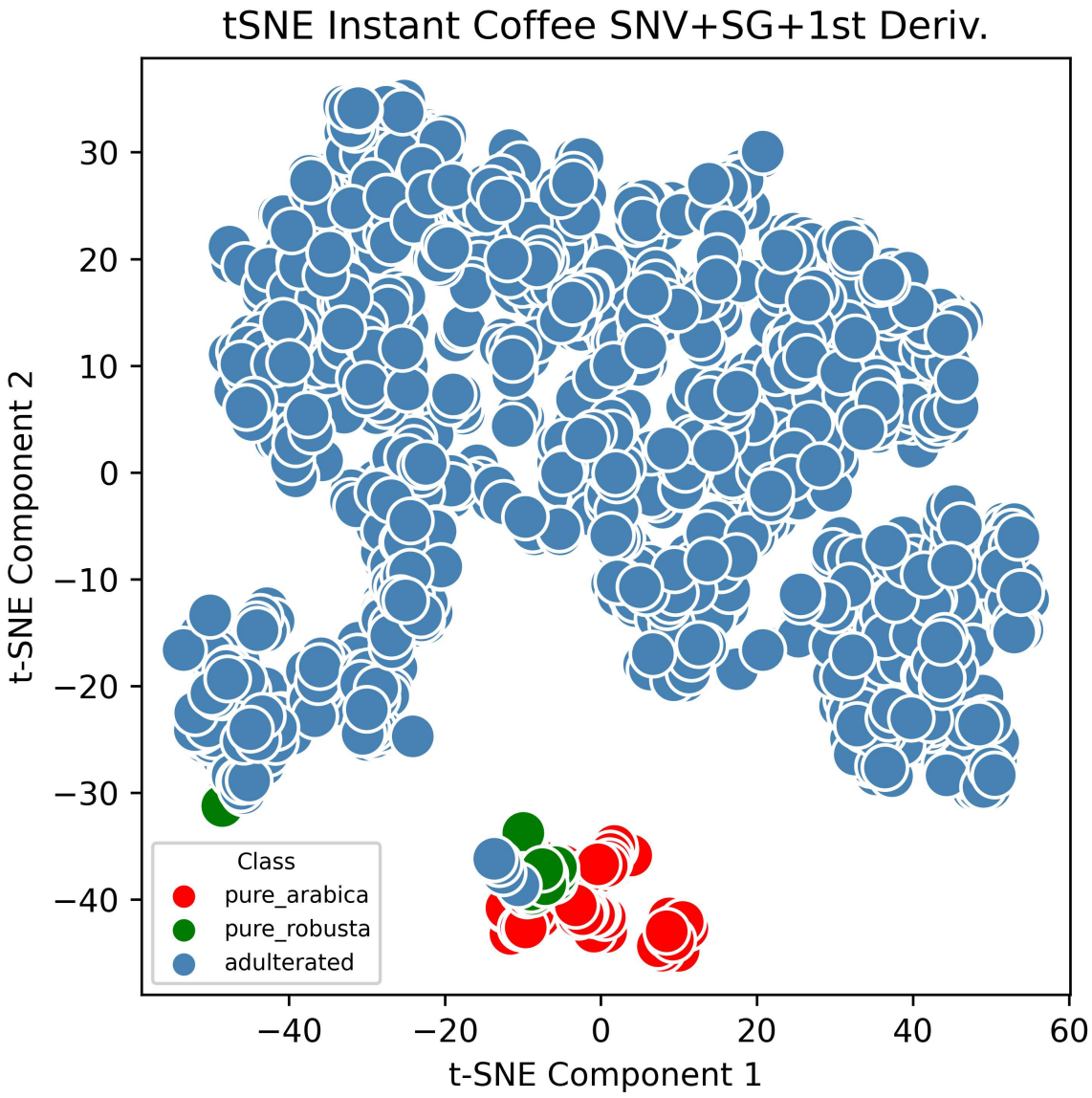
In [16]:
```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
               palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Instant 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_Instant_MSC_2D_adult_percent.png", dpi=600, bbox_inches="tight
plt.show()
```



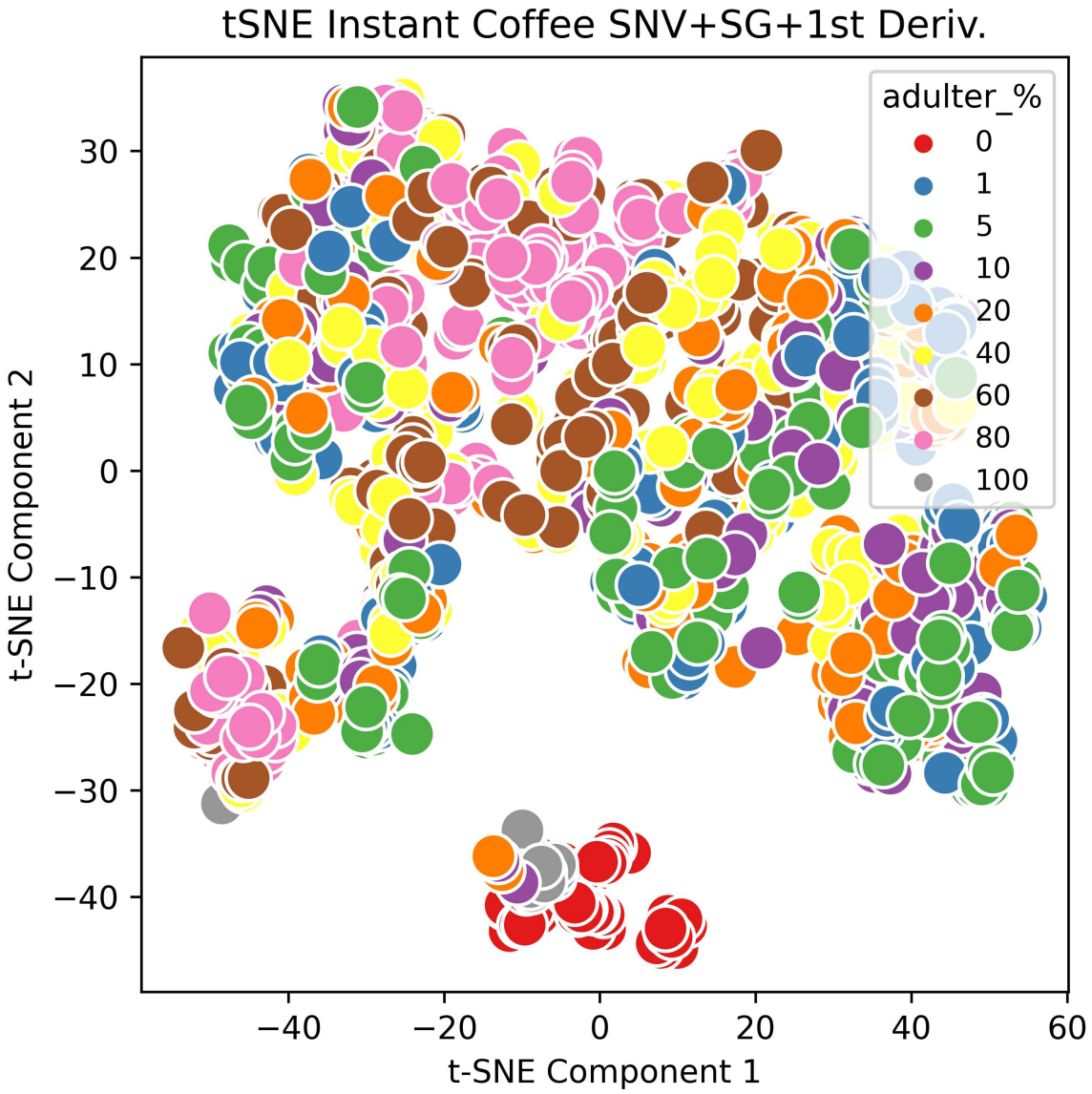
In [17]:
```
# SNV+SG+first derivative Instant Coffee

# Apply t-SNE to reduce dimensions to 2D
tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,in
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']] = instant_snv_sg_1d[['three_class','perc_a
```

In [18]:
```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g
# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
               palette=palette, alpha=1.0, s=200)
plt.title("tSNE Instant Coffee SNV+SG+1st Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class", fontsize=7, title_fontsize=7, loc='lower left')
plt.grid(False)
plt.tight_layout()
```

```
# Save the figure with high resolution
plt.savefig("tSNE_Instant_SNV_1D.png", dpi=600, bbox_inches="tight", format="png
plt.show()
```



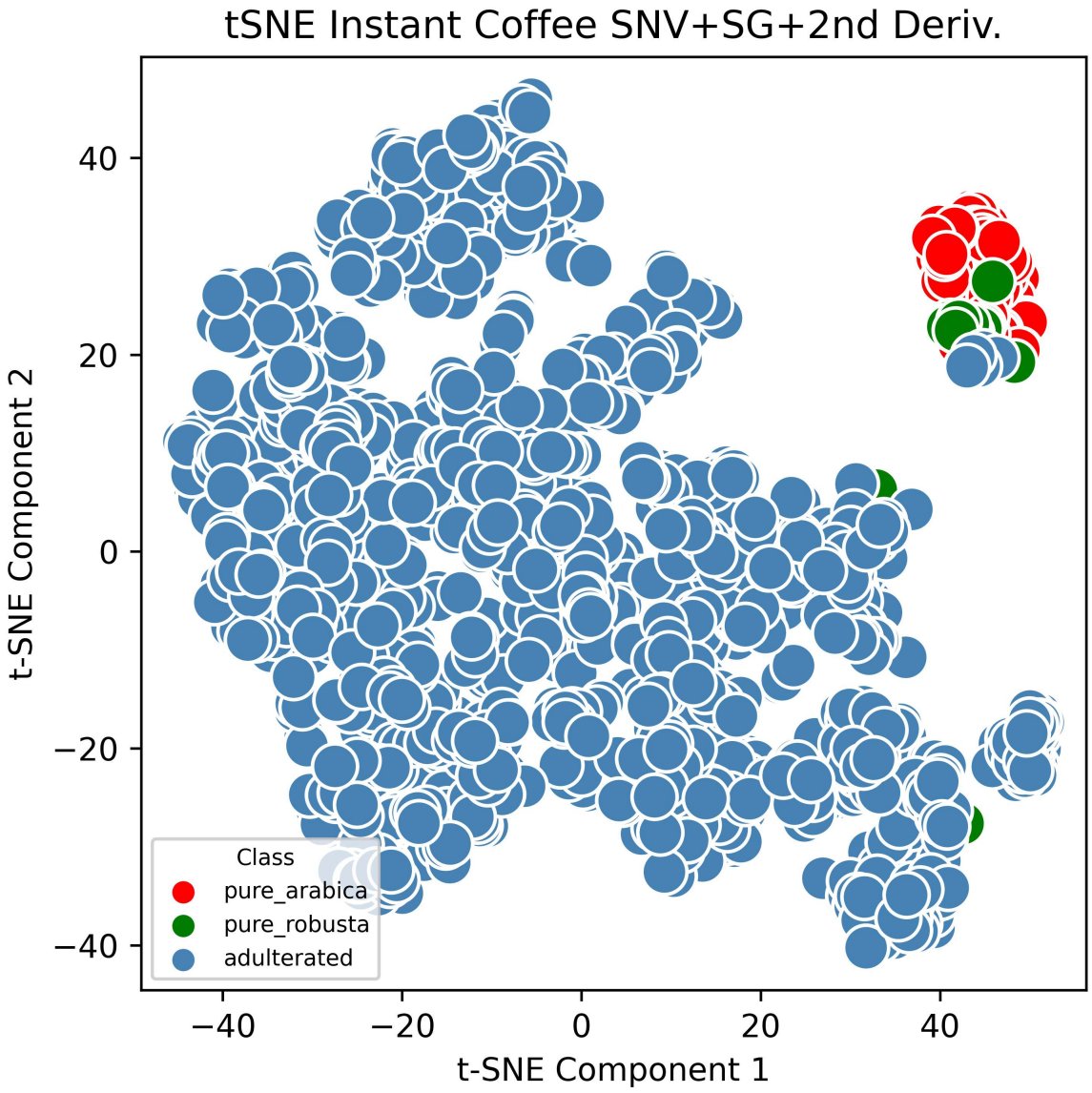
In [19]:
```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'adulter_percent',
                palette='Set1', alpha=1.0, s=200)
plt.title("tSNE Instant 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_Instant_SNV_1D_adult_percent.png", dpi=600, bbox_inches="tight
plt.show()
```



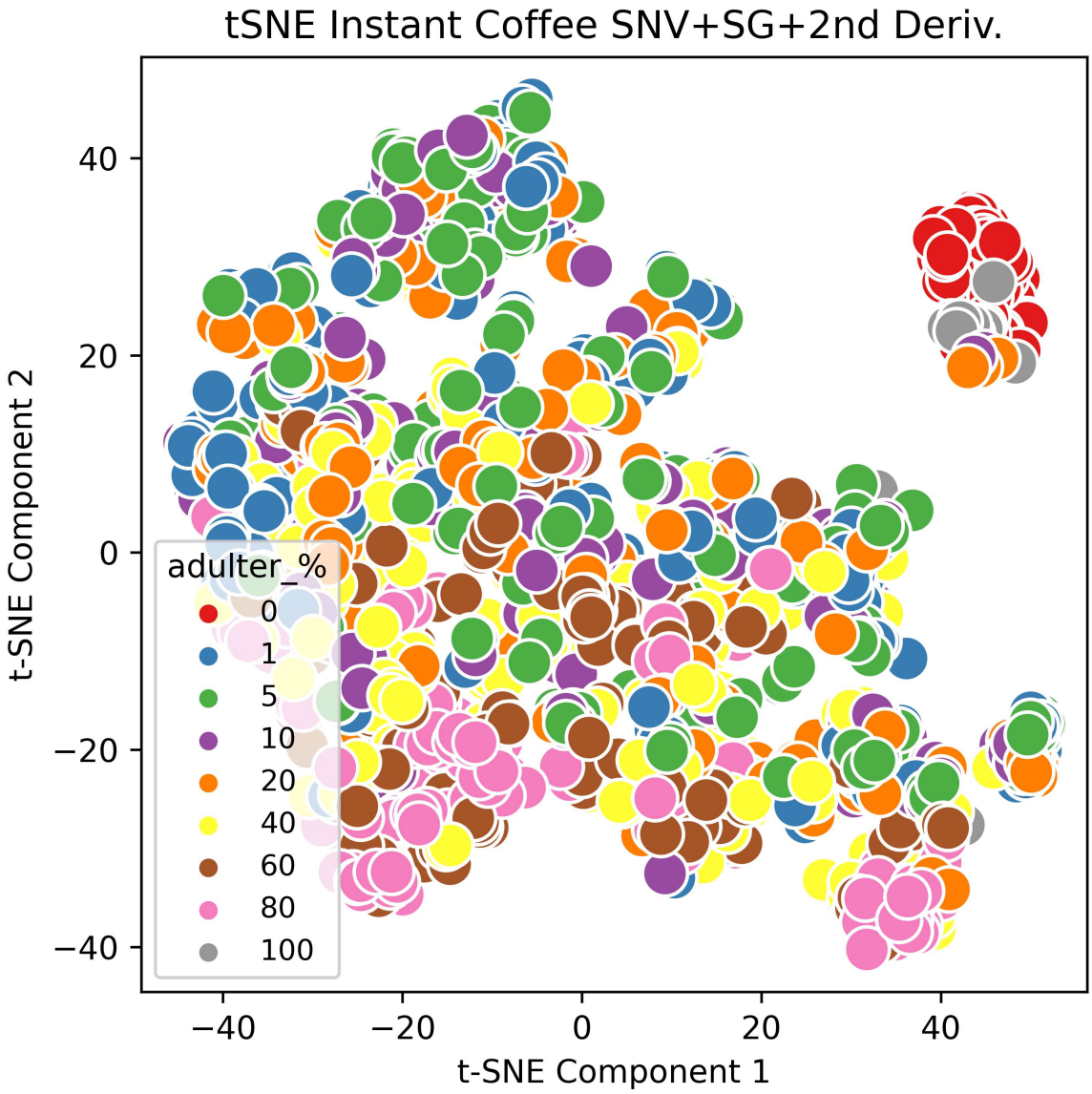
In [20]:
```
# SNV+SG+second derivative Instant Coffee

# Apply t-SNE to reduce dimensions to 2D
tsne = TSNE(n_components=2, perplexity=30, learning_rate=200, random_state=42,in
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']] = instant_snv_sg_2d[['three_class','perc_a
```

In [21]:
```
# Plotting
plt.figure(figsize=(5, 5), dpi=600)

palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g

# Scatterplot
sns.scatterplot(data=tsne_df, x='TSNE1', y='TSNE2',
                hue = 'Class',
               palette=palette, alpha=1.0, s=200)
plt.title("tSNE Instant Coffee SNV+SG+2nd Deriv.")
plt.xlabel("t-SNE Component 1")
plt.ylabel("t-SNE Component 2")
plt.legend(title="Class", prop={'size': 7}, loc = 'lower left', fontsize=7, titl
plt.grid(False)
```

```
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Instant_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 Instant 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='lower left', markerscale=0.
plt.grid(False)
plt.tight_layout()
# Save the figure with high resolution
plt.savefig("tSNE_Instant_SNV_2D_adult_percent.png", dpi=600, bbox_inches="tight
plt.show()
```



Principal Component Analyis

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

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)
```

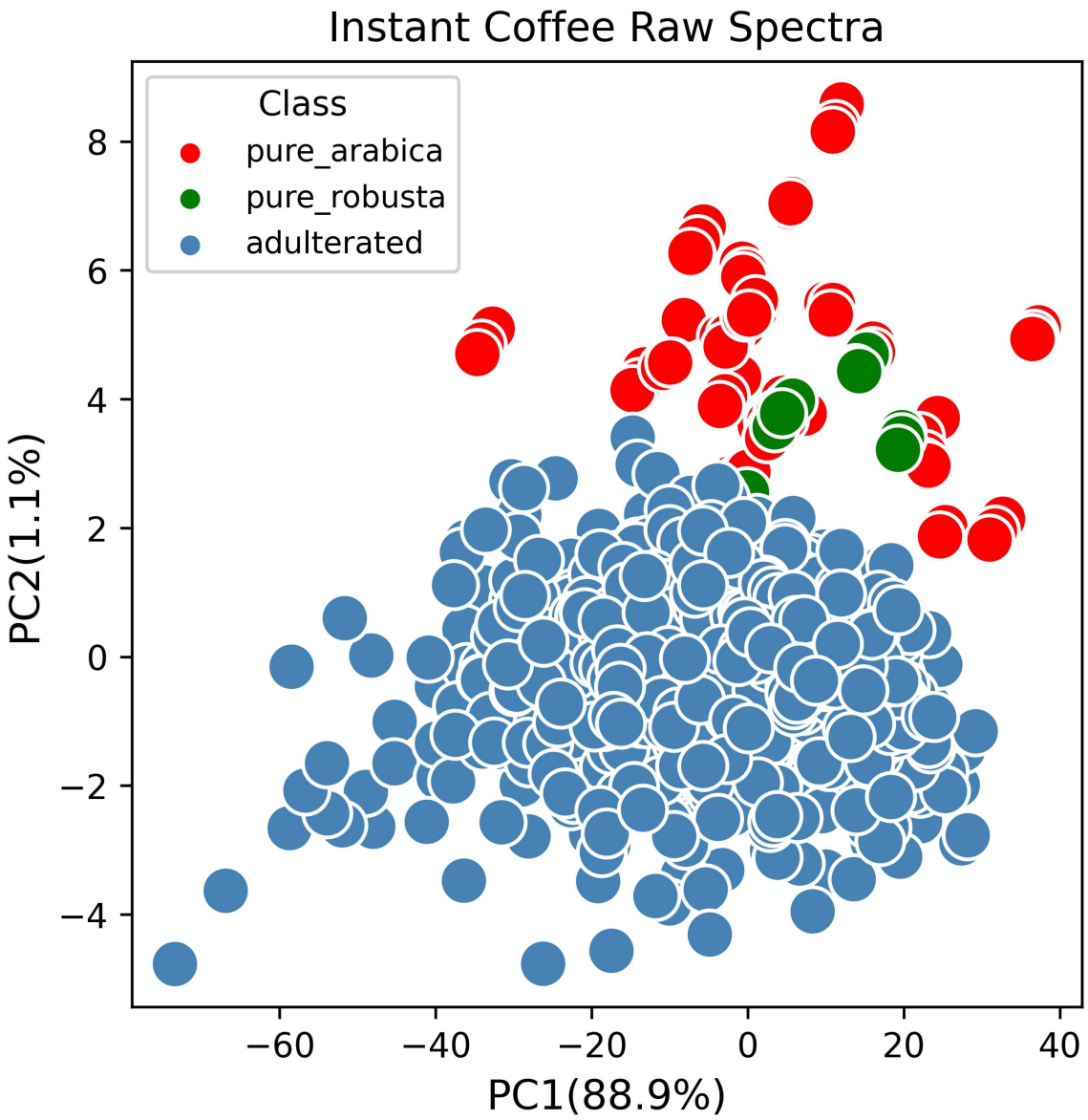
Out[25]:

	PC1	PC2	PC3	binary_class	three_class	adult_percent
0	10.067356	4.568623	5.484754	pure_arabica	pure_arabica	0
1	10.903091	4.372314	5.461795	pure_arabica	pure_arabica	0
2	10.641775	3.917128	5.313304	pure_arabica	pure_arabica	0
3	16.025809	8.960843	4.861415	pure_arabica	pure_arabica	0
4	15.282418	8.763996	4.695814	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: 0.889
Explained variance by PC2: 0.097
Explained variance by PC3: 0.011
```

In [27]:
```
# Create figure
palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g
plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_raw_df, x='PC1', y='PC3', hue='three_class',
                palette=palette, alpha=1.0, s=200)
plt.title('Instant Coffee Raw Spectra', fontsize=12)
plt.xlabel('PC1(88.9%)', fontsize=12)
plt.ylabel('PC2(1.1%)', fontsize=12)
plt.legend(title='Class', prop={'size': 9}, loc='upper left', markerscale=0.8)
plt.savefig("PCA_Instant_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)
```

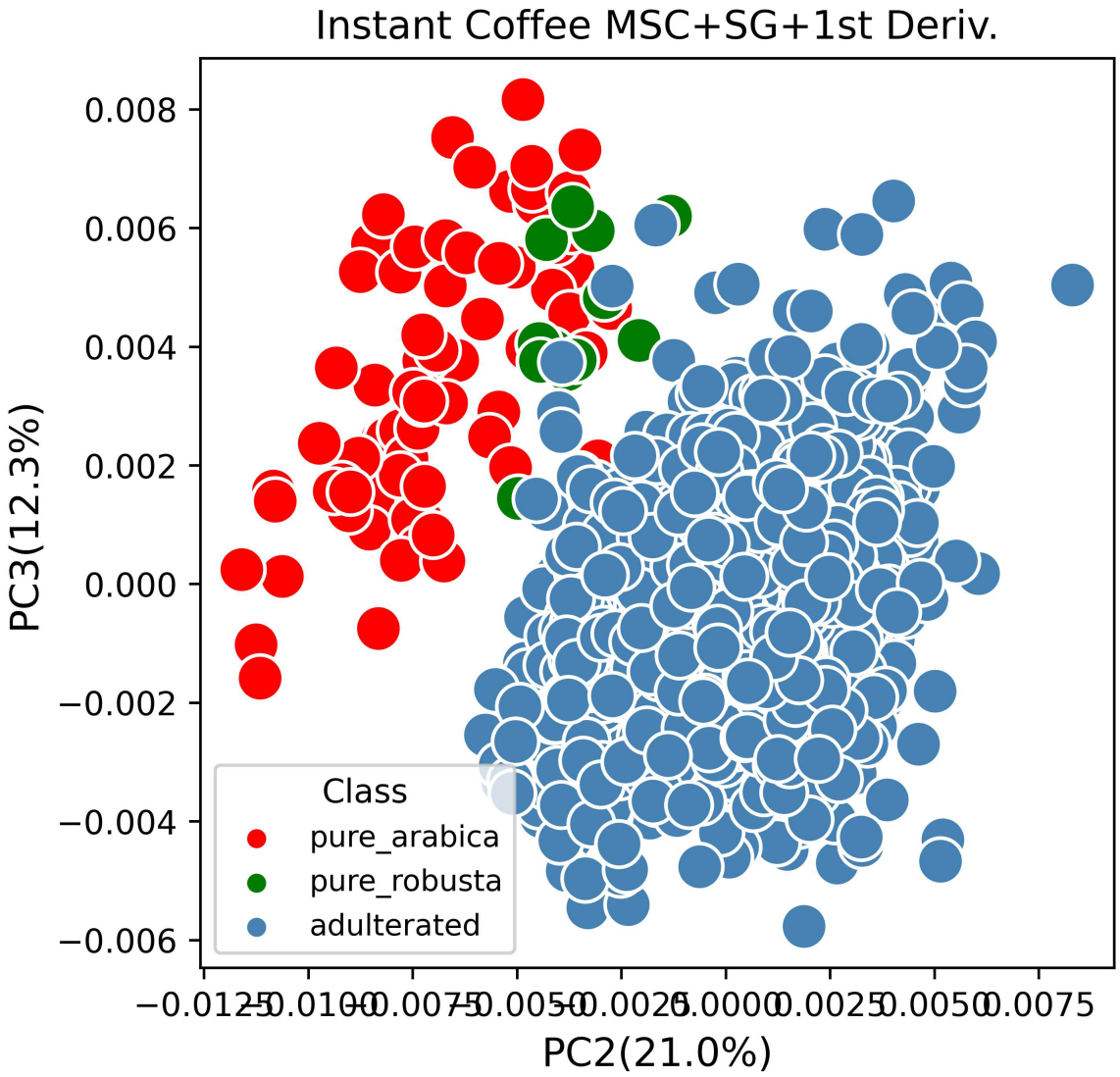
Out[28]:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	binary_class
0	-0.000778	-0.008225	0.002436	0.000213	-0.000730	0.001054	0.000304	pure_arabica
1	-0.000996	-0.008285	0.001533	-0.000600	-0.000353	0.001127	0.000610	pure_arabica
2	-0.001604	-0.008405	0.003351	-0.000587	-0.000251	0.000919	0.000607	pure_arabica
3	0.003513	-0.008114	0.002444	-0.000106	-0.000545	0.001167	0.000387	pure_arabica
4	0.003541	-0.007789	0.002584	-0.000666	-0.000334	0.001321	0.000504	pure_arabica

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}")
print(f"Explained variance by PC6: {explained_variance[5]:.3f}")
print(f"Explained variance by PC7: {explained_variance[6]:.3f}")
```

```
Explained variance by PC1: 0.609
Explained variance by PC2: 0.210
Explained variance by PC3: 0.123
Explained variance by PC4: 0.024
Explained variance by PC5: 0.012
Explained variance by PC6: 0.009
Explained variance by PC7: 0.005
```

In [30]:
```
# Create scatter plot
palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g

plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_msc_1d_df, x='PC2', y='PC3', hue='three_class',
                palette=palette, alpha=1.0, s=200)
plt.title('Instant Coffee MSC+SG+1st Deriv.', fontsize=12)
plt.xlabel('PC2(21.0%)', fontsize=12)
plt.ylabel('PC3(12.3%)', fontsize=12)
plt.legend(title='Class', prop={'size': 9}, loc='lower left', markerscale=0.8)
plt.savefig("PCA_Instant_MSC_SG_1D.png", dpi=600, bbox_inches="tight", format="p
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)
```

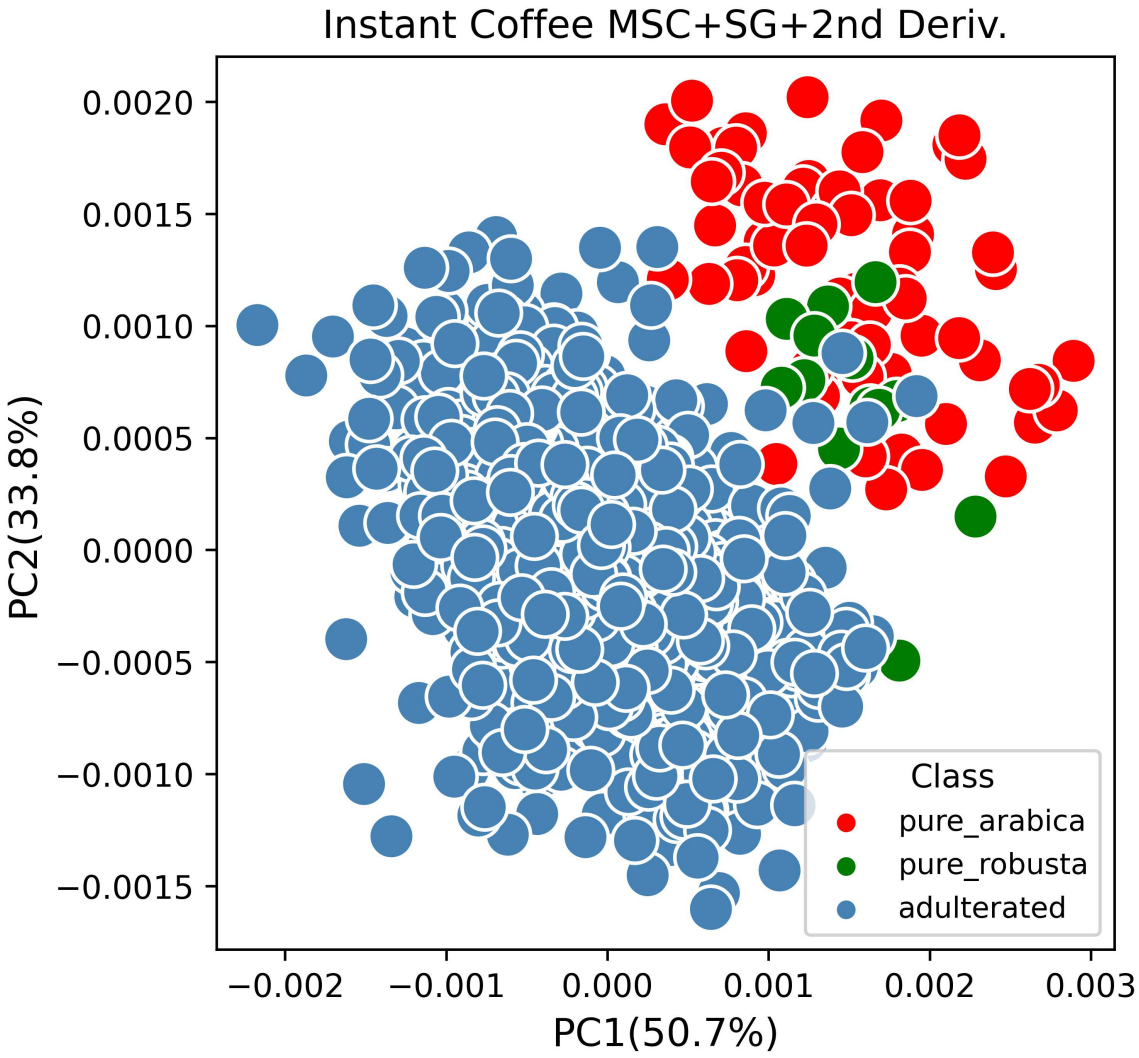
Out[31]:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	bi
0	0.001462	0.001061	0.000132	-0.000137	0.000152	0.000186	0.000021	-0.000102	pu
1	0.001444	0.000851	0.000193	-0.000032	0.000198	0.000247	-0.000033	-0.000099	pu
2	0.001652	0.001177	0.000013	-0.000019	0.000183	0.000226	-0.000043	-0.000057	pu
3	0.001024	0.001369	0.000231	-0.000094	0.000146	0.000244	0.000021	-0.000026	pu
4	0.000976	0.001376	0.000204	-0.000012	0.000177	0.000270	-0.000015	-0.000023	pu

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}")
print(f"Explained variance by PC7: {explained_variance[6]:.3f}")
print(f"Explained variance by PC8: {explained_variance[7]:.3f}")
```

```
Explained variance by PC1: 0.507
Explained variance by PC2: 0.338
Explained variance by PC3: 0.083
Explained variance by PC4: 0.022
Explained variance by PC5: 0.020
Explained variance by PC6: 0.011
Explained variance by PC7: 0.005
Explained variance by PC8: 0.004
```

In [33]:
```
# Create scatter plot
palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g
plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_msc_2d_df, x='PC1', y='PC2', hue='three_class',
                palette=palette, alpha=1.0, s=200)
plt.title('Instant Coffee MSC+SG+2nd Deriv.', fontsize=12)
plt.xlabel('PC1(50.7%)', fontsize=12)
plt.ylabel('PC2(33.8%)', fontsize=12)
plt.legend(title='Class', prop={'size': 9}, loc='best', markerscale=0.8)
plt.savefig("PCA_Instant_MSC_SG_2D.png", dpi=600, bbox_inches="tight", format="p
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)
```

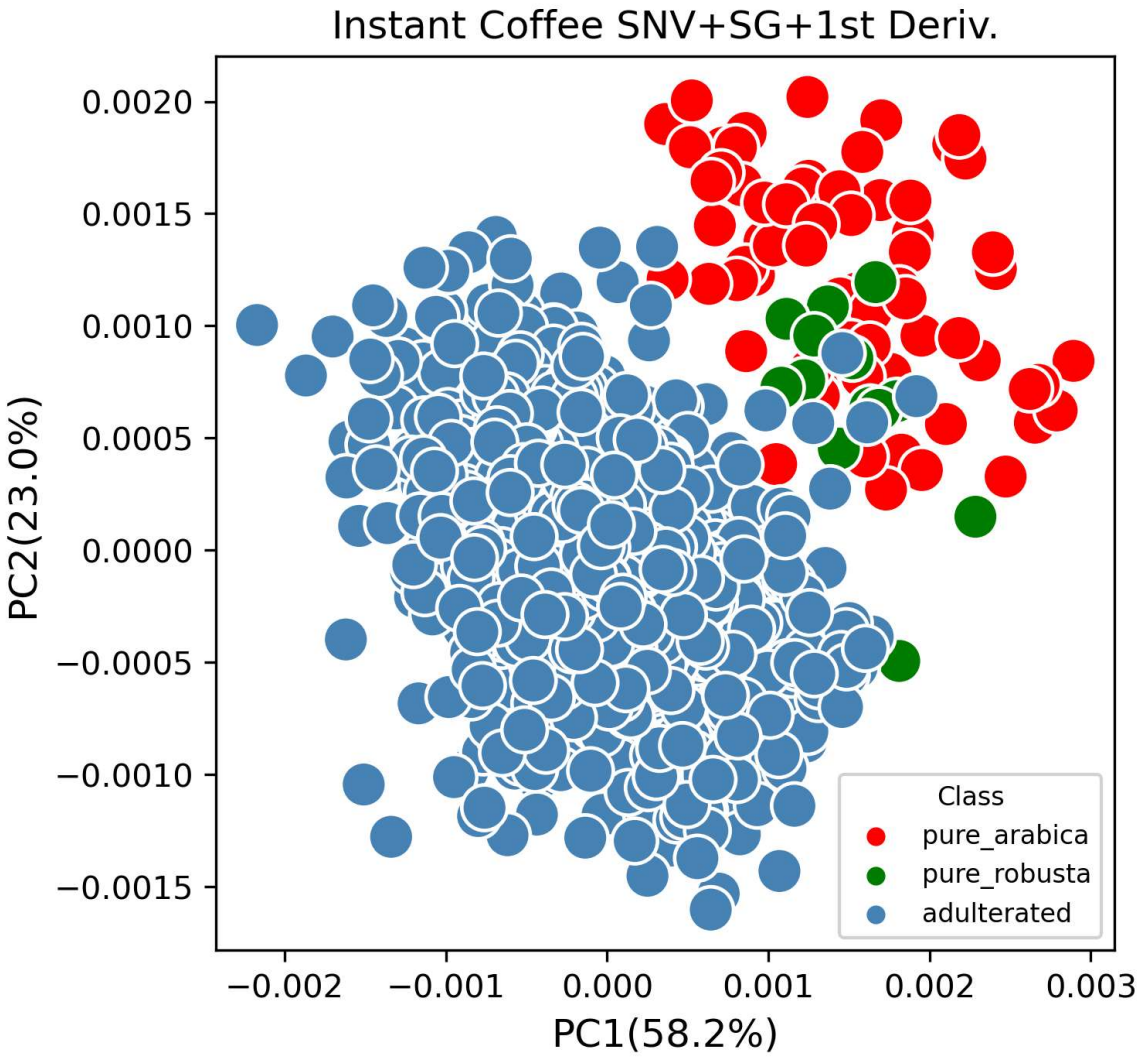
Out[34]:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	k
0	-0.010814	-0.095460	0.040670	-0.002646	-0.010207	0.014427	0.004153	-0.002640	p
1	-0.013590	-0.096666	0.030016	-0.012961	-0.005647	0.014255	0.007979	-0.004193	p
2	-0.020998	-0.096150	0.052267	-0.012014	-0.004286	0.011568	0.007532	-0.004674	p
3	0.043309	-0.101981	0.035705	-0.002139	-0.006525	0.013042	0.006647	-0.001740	p
4	0.043620	-0.097360	0.037339	-0.008917	-0.004102	0.014095	0.008525	-0.002507	p

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}")
print(f"Explained variance by PC7: {explained_variance[6]:.3f}")
print(f"Explained variance by PC8: {explained_variance[7]:.3f}")
```

```
Explained variance by PC1: 0.582
Explained variance by PC2: 0.230
Explained variance by PC3: 0.124
Explained variance by PC4: 0.025
Explained variance by PC5: 0.012
Explained variance by PC6: 0.009
Explained variance by PC7: 0.005
Explained variance by PC8: 0.004
```

In [36]:
```
# Create scatter plot
palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g
plt.figure(figsize=(5, 5), dpi=300)
sns.scatterplot(data=pca_msc_2d_df, x='PC1', y='PC2', hue='three_class',
                palette=palette, alpha=1.0, s=200)
plt.title('Instant Coffee SNV+SG+1st Deriv.', fontsize=12)
plt.xlabel('PC1(58.2%)', fontsize=12)
plt.ylabel('PC2(23.0%)', fontsize=12)
plt.legend(title='Class', prop={'size': 8}, loc='lower right', fontsize=8, title
plt.savefig("PCA_Instant_SNV_SG_1D.png", dpi=300, bbox_inches="tight", format="p
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)
```

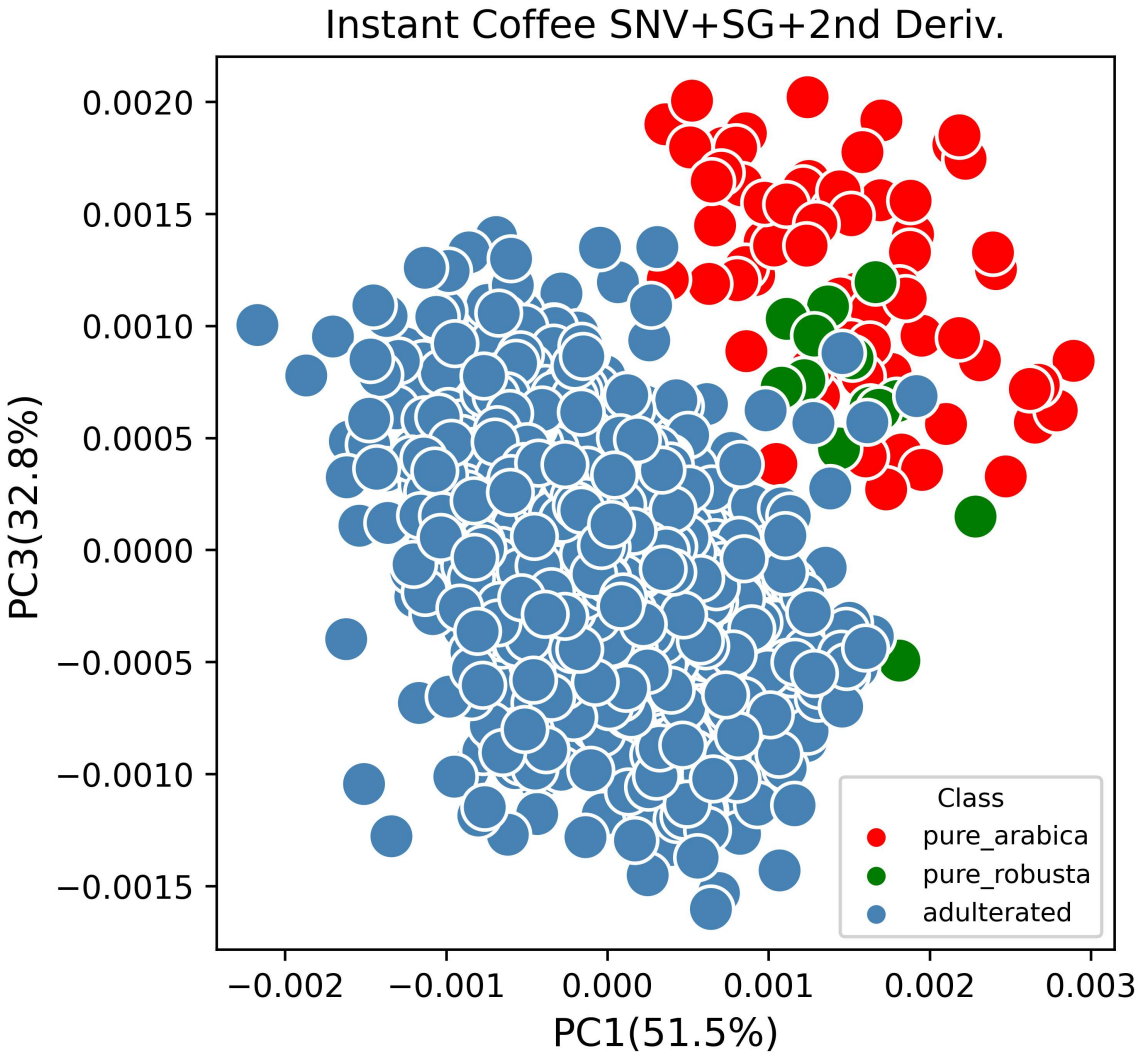
Out[37]:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	b
0	0.018174	0.012510	0.000946	-0.000622	0.002345	0.002375	0.000171	-0.001450	p
1	0.017870	0.009927	0.001615	0.000815	0.002508	0.003123	-0.000492	-0.001409	p
2	0.020488	0.013866	-0.000634	0.000844	0.002248	0.002872	-0.000609	-0.000878	p
3	0.013736	0.016172	0.003175	-0.000591	0.002255	0.002779	0.000242	-0.000293	p
4	0.013114	0.016280	0.002797	0.000468	0.002314	0.003088	-0.000186	-0.000232	p

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}")
print(f"Explained variance by PC7: {explained_variance[6]:.3f}")
print(f"Explained variance by PC8: {explained_variance[7]:.3f}")
```

```
Explained variance by PC1: 0.515
Explained variance by PC2: 0.328
Explained variance by PC3: 0.086
Explained variance by PC4: 0.022
Explained variance by PC5: 0.020
Explained variance by PC6: 0.011
Explained variance by PC7: 0.005
Explained variance by PC8: 0.004
```

In [39]:
```
# Create scatter plot
palette = {"adulterated": "steelblue", "pure_arabica": "red", "pure_robusta": "g
plt.figure(figsize=(5, 5), dpi=600)
sns.scatterplot(data=pca_msc_2d_df, x='PC1', y='PC2', hue='three_class',
                palette=palette, alpha=1.0, s=200)
plt.title('Instant Coffee SNV+SG+2nd Deriv.', fontsize=12)
plt.xlabel('PC1(51.5%)', fontsize=12)
plt.ylabel('PC3(32.8%)', fontsize=12)
plt.legend(title='Class', prop={'size': 8}, loc='lower right', markerscale=0.8,
plt.savefig("PCA_Instant_SNV_SG_2D.png", dpi=600, bbox_inches="tight", format="p
plt.show()
```


Instant Coffee SNV+SG+2nd Deriv.
PC3(32.8%)
PC1(51.5%)
0.0020
0.0015
0.0010
0.0005
0.0000
−0.0005
−0.0010
−0.0015
−0.002
−0.001
0.000
0.001
0.002
0.003
Class
pure_arabica
pure_robusta
adulterated