Clustering Canadian Crude: Unsupervised Learning for Oil Grade Classification

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Project Summary

This project applies unsupervised machine learning to predict and group the grades of Canadian crude oils based on their chemical and physical characteristics. The dataset includes four target categories—Light & Medium Sweet Crude Oil, Light & Medium Sour Crude Oil, Heavy Sour Crude Oil, and Sweet Synthetic Crude Oil—sourced from CrudeMonitor.ca. The goal is to determine whether natural patterns in the data support these four distinct classes or suggest fewer underlying groupings based on compositional similarities.

The central hypothesis is that the Light & Medium Sweet and Light & Medium Sour crude oils share nearly identical physical properties, differing mainly in sulfur content and related compounds. Therefore, they may not form truly distinct groups in an unsupervised context. If clustering algorithms naturally group these two together, it would indicate that the optimal structure of the data reflects three clusters rather than four—thus rejecting the null hypothesis that four separate groups best represent the dataset.

To test this, three unsupervised clustering methods—K-Means, Agglomerative Clustering, and Gaussian Mixture Models (GMM)—are applied to segment the data, with results visualized through PCA and t-SNE dimensionality reduction. Cluster quality is assessed using internal and external scoring metrics to evaluate cohesion and separation. To validate the findings, the results are compared against supervised learning models—Multinomial Logistic Regression, Support Vector Classifier, and Gradient Boosting Classifier—to determine how well unsupervised learning aligns with known class labels and to assess whether the data's natural structure supports three or four true crude oil groupings.

Data Summary

This section provides an initial overview of the dataset to establish a clear understanding of its structure and contents before any analysis begins. It outlines the data source, the number of records and features, and the types of variables included. Basic statistics are used to summarize the range of values, while data types are confirmed to distinguish between numerical and categorical columns.

Import Python Packages

In [80]:
```
import pandas as pd
import numpy as np
from IPython.display import display, Markdown, Image
from datetime import datetime
from dateutil import relativedelta
import requests

from sklearn.impute import KNNImputer
from sklearn.preprocessing import OneHotEncoder, StandardScaler, LabelEncoder
from sklearn.pipeline import Pipeline
from sklearn.compose import ColumnTransformer
from sklearn.cluster import MiniBatchKMeans, AgglomerativeClustering
from sklearn.metrics.cluster import contingency_matrix
from sklearn.mixture import GaussianMixture
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE
from sklearn.linear_model import LogisticRegressionCV
from sklearn.svm import SVC
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.metrics import (
    silhouette_score,
    davies_bouldin_score,
    calinski_harabasz_score,
    adjusted_rand_score,
    normalized_mutual_info_score,
    fowlkes_mallows_score,
    silhouette_samples,
    classification_report,
    confusion_matrix
)
from scipy.optimize import linear_sum_assignment

import altair as alt
import seaborn as sns
import matplotlib.pyplot as plt
import matplotlib.cm as cm

pd.set_option('future.no_silent_downcasting', True)
alt.data_transformers.disable_max_rows()
```

Out[80]:
```
DataTransformerRegistry.enable('default')
```

Data Source

The data for this project was obtained from CrudeMonitor.ca, a publicly available resource that provides detailed information on the quality characteristics of various crude oil grades produced in Western Canada.

Reference:
Crude Quality Inc. (n.d.). CrudeMonitor.ca. Retrieved October 16, 2025, from https://www.crudemonitor.ca/

Target Groups

For this project I've created a set of 4 target groups which each contain crude oil grades that have similar crude oil qualities. I'll use these groupings to evaluate the predictive quality of various unsupervised machine learning algorithms.

- Heavy Sour Crude Oils
  - Density range: 918 - 931 kg/m3
  - Quality range: 20 - 22 °API
  - Grades:
    - Bow River North (BRN)
    - Bow River South (BRS)
    - Fosterton (F)
    - Lloyd Blend (LLB)
    - Lloyd Kerrobert (LLK)
    - Seal Heavy (SH)
    - Smiley-Coleville (SC)
    - Wabasca Heavy (WH)
    - Western Canadian Blend (WCB)
    - Western Canadian Select (WCS)
- Sweet Synthetic Crude Oils
  - Density range: 836 - 866 kg/m3
  - Quality range: 32 - 38 °API
  - Grades:
    - CNRL Light Sweet Synthetic (CNS)
    - Husky Synthetic Blend (HSB)
    - Long Lake Light Synthetic (PSC)
    - Premium Albian Synthetic (PAS)
    - Shell Synthetic Light (SSX)
    - Suncor Synthetic A (OSA)
    - Syncrude Sweet Premium (SSP)
- Light & Medium Sour Crude Oils
  - Density range: 822 - 862 kg/m3
  - Quality range: 33 - 41 °API
  - Grades:
    - Hardisty Light (MBL)
    - Medium Gibson Sour (MGS)
    - Midale (MSM)
    - Peace Pipe Sour (SPR)
    - BC Light (BCL)
    - Boundary Lake (BDY)
    - Koch Alberta (CAL)
    - Moose Jaw Tops (MJT)
    - Pembina Light Sour (PLS)
- Light & Medium Sweet Crude Oils
  - Density range: 807 - 838 kg/m3
  - Quality range: 37 - 44 °API
  - Grades:
    - Federated (FD)
    - Light Smiley (MSY)
    - Peace (MPR)
    - Pembina (P)
    - Secure Sask Light (MSE)
    - Mixed Sweet Blend (MSW)
    - Rainbow (RA)

Create Dataset

In [81]:
```
# Function to create a dataframe from historical crude oil properties by crude_grade
def get_data(crude_grade, crude_oils_dict):
    # Create URL parts
    start_date = crude_oils_dict[crude_grade]['min_date'] # Start date is the min_date defined in the crude_oils_dict for each crude_grade
    end_date = datetime.now().date().strftime('%Y-%m-%d') # End date is the current date
    base_url = 'https://www.crudemonitor.ca/api/1.1/json.php?'
    crude_properties_url = '&crudeProperties%5B0%5D=crudes-BA&crudeProperties%5B1%5D=crudes-LE&crudeProperties%5B2%5D=crudes-HTSD'
    crudes_url = ''.join([f'&crudes%5B{i}%5D={x.replace(' ','+')}' for i, x in enumerate([k for k in crude_oils_dict[crude_grade]['grades'].keys()])])
    date_url = f'&date%5Bstart%5D={start_date}&date%5Bend%5D={end_date}'

    # Merge url parts into full url
    url = base_url + crudes_url + crude_properties_url + date_url

    # Request data from API
    response = requests.get(url)
    response.raise_for_status()

    # Create dataframe
```

```
    response_df = pd.DataFrame.from_dict(response.json())

    # Replace values
    response_df = response_df.replace({'': np.nan, 'ND': np.nan}).infer_objects(copy=False)

    # Correct Location names
    response_df['Location'] = response_df['Location'].str.replace(r'(?i)milk.+river', 'Milk River', regex=True)

    # Change numeric columns datatypes
    num_cols = response_df.columns[4:]
    response_df[num_cols] = response_df[num_cols].apply(pd.to_numeric, errors='coerce')

    # Downcast numeric columns where possible
    for col in response_df.select_dtypes(include=['float64']).columns:
        response_df[col] = pd.to_numeric(response_df[col], downcast='float')
    for col in response_df.select_dtypes(include=['int64']).columns:
        response_df[col] = pd.to_numeric(response_df[col], downcast='integer')

    # Convert Sample Date (yyyy-mm-dd) column to datetime
    response_df['Sample Date (yyyy-mm-dd)'] = pd.to_datetime(response_df['Sample Date (yyyy-mm-dd)'])

    # Add target labels to df
    response_df = response_df.assign(target_label=crude_oils_dict[crude_grade]['target_label'])

    return response_df
```

In [82]:
```
# Define dictionary of crude oil types & associated metadata
crude_oils_dict = {
    'Heavy Sour':{
        'target_label':0,
        'min_date':'2001-01-02',
        'grades':{
            'Bow River North':'BRN',
            'Bow River South':'BRS',
            'Fosterton':'F',
            'Lloyd Blend':'LLB',
            'Lloyd Kerrobert':'LLK',
            'Seal Heavy':'SH',
            'Smiley-Coleville':'SC',
            'Wabasca Heavy':'WH',
            'Western Canadian Blend':'WCB',
            'Western Canadian Select':'WCS'
        }
    },
    'Sweet Synthetic':{
        'target_label':1,
        'min_date':'2004-01-05',
        'grades':{
            'CNRL Light Sweet Synthetic':'CNS',
            'Husky Synthetic Blend':'HSB',
            'Long Lake Light Synthetic':'PSC',
            'Premium Albian Synthetic':'PAS',
            'Shell Synthetic Light':'SSX',
            'Suncor Synthetic A':'OSA',
            'Syncrude Sweet Premium':'SSP'
        }
    },
    'Light & Medium Sweet Crude Oils':{
        'target_label':2,
        'min_date':'1999-11-12',
        'grades':{
            'Federated':'FD',
            'Light Smiley':'MSY',
            'Peace':'MPR',
            'Pembina':'P',
            'Secure Sask Light':'MSE',
            'Mixed Sweet Blend':'MSW',
            'Rainbow':'RA'
        }
    },
    'Light & Medium Sour Crude Oils':{
        'target_label':3,
        'min_date':'1999-11-21',
        'grades':{
            'Hardisty Light':'MBL',
            'Medium Gibson Sour':'MGS',
            'Midale':'MSM',
            'Peace Pipe Sour':'SPR',
            'BC Light':'BCL',
            'Boundary Lake':'BDY',
            'Koch Alberta':'CAL',
            'Moose Jaw Tops':'MJT',
            'Pembina Light Sour':'PLS'
        }
    },
}
```

In [83]:
```
# Loop over crude_grade types and concatenate datasets into one
df = pd.concat(
    [get_data(crude_grade, crude_oils_dict) for crude_grade in crude_oils_dict.keys()],
    ignore_index=True,
    copy=False
)
```

```
# Display the dataset
df
```

Out[83]:

	Crude	Batch	Sample Date (yyyy-mm-dd)	Location	Density (kg/m^3) [ASTM D5002]	Gravity (°API) [ASTM D5002]	Sulphur (wt%) [ASTM D4294]	Micro Carbon Residue (wt%) [ASTM D4530]	Sediment (ppmw) [ASTM D4807]	Total Acid Number (mgKOH/g) [ASTM D664]	...	91 Mass% Recovered (°C) [ASTM D7169]	92 Mass% Recovered (°C) [ASTM D7169]	93 Mass% Recovered (°C) [ASTM D7169]	94 Mass% Recovered (°C) [ASTM D7169]	95 Mass% Recovered (°C) [ASTM D7169]	96 Mass% Recovered (°C) [ASTM D7169]
0	Bow River North	BR-030	2001-01-02	Hardisty	927.099976	21.000000	2.95	8.9	170.0	1.24	...	664.900024	676.0	689.400024	704.700012	733.200012	NaN
1	Bow River North	BR-073	2001-01-07	Hardisty	927.299988	21.000000	2.96	9.4	150.0	1.16	...	719.099976	NaN	NaN	NaN	NaN	NaN
2	Lloyd Blend	LLB-464	2001-01-03	Hardisty	920.799988	22.000000	3.17	9.4	230.0	0.75	...	NaN	NaN	NaN	NaN	NaN	NaN
3	Lloyd Blend	LLB-468	2001-01-18	Hardisty	922.500000	21.799999	3.11	9.6	300.0	0.91	...	NaN	NaN	NaN	NaN	NaN	NaN
4	Lloyd Kerrobert	LLK-062	2001-01-04	Kerrobert	926.299988	21.100000	2.80	9.6	230.0	1.56	...	NaN	NaN	NaN	NaN	NaN	NaN
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
5298	Pembina Light Sour	PLS-807	2019-02-05	Edmonton	850.299988	34.799999	1.28	4.3	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5299	Pembina Light Sour	PLS-813	2019-03-03	Edmonton	844.799988	35.799999	1.14	3.8	NaN	NaN	...	703.099976	NaN	NaN	NaN	NaN	NaN
5300	Pembina Light Sour	PLS-818	2019-04-05	Edmonton	841.900024	36.400002	1.08	3.8	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5301	Pembina Light Sour	PLS-825	2019-05-07	Edmonton	833.799988	38.000000	0.84	3.1	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5302	Pembina Light Sour	PLS-835	2019-06-05	Edmonton	842.099976	36.400002	1.04	3.7	NaN	NaN	...	665.000000	689.0	711.799988	NaN	NaN	NaN

5303 rows × 133 columns

Dataset Info

- `df.info()` provides a concise summary of a DataFrame, including the:
  - Number of rows
  - Column names
  - Data types
- It also shows the count of non-null entries for each column, which makes it easy to identify missing values.
- In addition, it displays the memory usage of the DataFrame, helping to assess the size and efficiency of the dataset in memory.

In [84]:
```
# Inspect column data types and size of the dataframe
df.info(verbose=True)
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 5303 entries, 0 to 5302
Data columns (total 133 columns):
 #    Column                                     Dtype
---   ------                                     -----
 0    Crude                                      object
 1    Batch                                      object
 2    Sample Date (yyyy-mm-dd)                   datetime64[ns]
 3    Location                                   object
 4    Density (kg/m³) [ASTM D5002]               float32
 5    Gravity (°API) [ASTM D5002]                float32
 6    Sulphur (wt%) [ASTM D4294]                 float32
 7    Micro Carbon Residue (wt%) [ASTM D4530]    float32
 8    Sediment (ppmw) [ASTM D4807]               float32
 9    Total Acid Number (mgKOH/g) [ASTM D664]    float32
 10   Salt (ptb) [ASTM D3230]                    float32
 11   Nickel (mg/kg) [ASTM D5708A]               float32
 12   Vanadium (mg/kg) [ASTM D5708A]             float32
 13   C1 Methane (vol%) [GC/FID]                 float32
 14   C2 Ethane (vol%) [GC/FID]                  float32
 15   C3 Propane (vol%) [GC/FID]                 float32
 16   iC4 iso-Butane (vol%) [GC/FID]             float32
 17   nC4 n-Butane (vol%) [GC/FID]               float32
 18   iC5 iso-Pentane (vol%) [GC/FID]            float32
 19   nC5 n-Pentane (vol%) [GC/FID]              float32
 20   C6 Hexanes (vol%) [GC/FID]                 float32
 21   C7 Heptanes (vol%) [GC/FID]                float32
 22   C8 Octanes (vol%) [GC/FID]                 float32
 23   C9 Nonanes (vol%) [GC/FID]                 float32
 24   C10 Decanes (vol%) [GC/FID]                float32
 25   Nitrogen - C4- (vol%) [GPA 2177M]          float32
 26   Carbon Dioxide - C4- (vol%) [GPA 2177M]    float32
 27   C1 Methane - C4- (vol%) [GPA 2177M]        float32
 28   C2 Ethane - C4- (vol%) [GPA 2177M]         float32
 29   C3 Propane - C4- (vol%) [GPA 2177M]        float32
 30   iC4 iso-Butane - C4- (vol%) [GPA 2177M]    float32
 31   nC4 n-Butane - C4- (vol%) [GPA 2177M]      float32
 32   IBP (°C) [ASTM D7169]                      float32
 33   1 Mass% Recovered (°C) [ASTM D7169]        float32
 34   2 Mass% Recovered (°C) [ASTM D7169]        float32
 35   3 Mass% Recovered (°C) [ASTM D7169]        float32
 36   4 Mass% Recovered (°C) [ASTM D7169]        float32
 37   5 Mass% Recovered (°C) [ASTM D7169]        float32
 38   6 Mass% Recovered (°C) [ASTM D7169]        float32
 39   7 Mass% Recovered (°C) [ASTM D7169]        float32
 40   8 Mass% Recovered (°C) [ASTM D7169]        float32
 41   9 Mass% Recovered (°C) [ASTM D7169]        float32
 42   10 Mass% Recovered (°C) [ASTM D7169]       float32
 43   11 Mass% Recovered (°C) [ASTM D7169]       float32
 44   12 Mass% Recovered (°C) [ASTM D7169]       float32
 45   13 Mass% Recovered (°C) [ASTM D7169]       float32
 46   14 Mass% Recovered (°C) [ASTM D7169]       float32
 47   15 Mass% Recovered (°C) [ASTM D7169]       float32
 48   16 Mass% Recovered (°C) [ASTM D7169]       float32
 49   17 Mass% Recovered (°C) [ASTM D7169]       float32
 50   18 Mass% Recovered (°C) [ASTM D7169]       float32
 51   19 Mass% Recovered (°C) [ASTM D7169]       float32
 52   20 Mass% Recovered (°C) [ASTM D7169]       float32
 53   21 Mass% Recovered (°C) [ASTM D7169]       float32
 54   22 Mass% Recovered (°C) [ASTM D7169]       float32
 55   23 Mass% Recovered (°C) [ASTM D7169]       float32
 56   24 Mass% Recovered (°C) [ASTM D7169]       float32
 57   25 Mass% Recovered (°C) [ASTM D7169]       float32
 58   26 Mass% Recovered (°C) [ASTM D7169]       float32
 59   27 Mass% Recovered (°C) [ASTM D7169]       float32
 60   28 Mass% Recovered (°C) [ASTM D7169]       float32
 61   29 Mass% Recovered (°C) [ASTM D7169]       float32
 62   30 Mass% Recovered (°C) [ASTM D7169]       float32
 63   31 Mass% Recovered (°C) [ASTM D7169]       float32
 64   32 Mass% Recovered (°C) [ASTM D7169]       float32
 65   33 Mass% Recovered (°C) [ASTM D7169]       float32
 66   34 Mass% Recovered (°C) [ASTM D7169]       float32
 67   35 Mass% Recovered (°C) [ASTM D7169]       float32
 68   36 Mass% Recovered (°C) [ASTM D7169]       float32
 69   37 Mass% Recovered (°C) [ASTM D7169]       float32
 70   38 Mass% Recovered (°C) [ASTM D7169]       float32
 71   39 Mass% Recovered (°C) [ASTM D7169]       float32
 72   40 Mass% Recovered (°C) [ASTM D7169]       float32
 73   41 Mass% Recovered (°C) [ASTM D7169]       float32
 74   42 Mass% Recovered (°C) [ASTM D7169]       float32
 75   43 Mass% Recovered (°C) [ASTM D7169]       float32
 76   44 Mass% Recovered (°C) [ASTM D7169]       float32
 77   45 Mass% Recovered (°C) [ASTM D7169]       float32
 78   46 Mass% Recovered (°C) [ASTM D7169]       float32
 79   47 Mass% Recovered (°C) [ASTM D7169]       float32
 80   48 Mass% Recovered (°C) [ASTM D7169]       float32
 81   49 Mass% Recovered (°C) [ASTM D7169]       float32
 82   50 Mass% Recovered (°C) [ASTM D7169]       float32
 83   51 Mass% Recovered (°C) [ASTM D7169]       float32
 84   52 Mass% Recovered (°C) [ASTM D7169]       float32
 85   53 Mass% Recovered (°C) [ASTM D7169]       float32
 86   54 Mass% Recovered (°C) [ASTM D7169]       float32
 87   55 Mass% Recovered (°C) [ASTM D7169]       float32
 88   56 Mass% Recovered (°C) [ASTM D7169]       float32
```

```
 89   57 Mass% Recovered (°C) [ASTM D7169]     float32
 90   58 Mass% Recovered (°C) [ASTM D7169]     float32
 91   59 Mass% Recovered (°C) [ASTM D7169]     float32
 92   60 Mass% Recovered (°C) [ASTM D7169]     float32
 93   61 Mass% Recovered (°C) [ASTM D7169]     float32
 94   62 Mass% Recovered (°C) [ASTM D7169]     float32
 95   63 Mass% Recovered (°C) [ASTM D7169]     float32
 96   64 Mass% Recovered (°C) [ASTM D7169]     float32
 97   65 Mass% Recovered (°C) [ASTM D7169]     float32
 98   66 Mass% Recovered (°C) [ASTM D7169]     float32
 99   67 Mass% Recovered (°C) [ASTM D7169]     float32
 100  68 Mass% Recovered (°C) [ASTM D7169]     float32
 101  69 Mass% Recovered (°C) [ASTM D7169]     float32
 102  70 Mass% Recovered (°C) [ASTM D7169]     float32
 103  71 Mass% Recovered (°C) [ASTM D7169]     float32
 104  72 Mass% Recovered (°C) [ASTM D7169]     float32
 105  73 Mass% Recovered (°C) [ASTM D7169]     float32
 106  74 Mass% Recovered (°C) [ASTM D7169]     float32
 107  75 Mass% Recovered (°C) [ASTM D7169]     float32
 108  76 Mass% Recovered (°C) [ASTM D7169]     float32
 109  77 Mass% Recovered (°C) [ASTM D7169]     float32
 110  78 Mass% Recovered (°C) [ASTM D7169]     float32
 111  79 Mass% Recovered (°C) [ASTM D7169]     float32
 112  80 Mass% Recovered (°C) [ASTM D7169]     float32
 113  81 Mass% Recovered (°C) [ASTM D7169]     float32
 114  82 Mass% Recovered (°C) [ASTM D7169]     float32
 115  83 Mass% Recovered (°C) [ASTM D7169]     float32
 116  84 Mass% Recovered (°C) [ASTM D7169]     float32
 117  85 Mass% Recovered (°C) [ASTM D7169]     float32
 118  86 Mass% Recovered (°C) [ASTM D7169]     float32
 119  87 Mass% Recovered (°C) [ASTM D7169]     float32
 120  88 Mass% Recovered (°C) [ASTM D7169]     float32
 121  89 Mass% Recovered (°C) [ASTM D7169]     float32
 122  90 Mass% Recovered (°C) [ASTM D7169]     float32
 123  91 Mass% Recovered (°C) [ASTM D7169]     float32
 124  92 Mass% Recovered (°C) [ASTM D7169]     float32
 125  93 Mass% Recovered (°C) [ASTM D7169]     float32
 126  94 Mass% Recovered (°C) [ASTM D7169]     float32
 127  95 Mass% Recovered (°C) [ASTM D7169]     float32
 128  96 Mass% Recovered (°C) [ASTM D7169]     float32
 129  97 Mass% Recovered (°C) [ASTM D7169]     float32
 130  98 Mass% Recovered (°C) [ASTM D7169]     float32
 131  99 Mass% Recovered (°C) [ASTM D7169]     float32
 132  target_label                            int64
dtypes: datetime64[ns](1), float32(128), int64(1), object(3)
memory usage: 2.8+ MB
```

> The dataset contains 133 columns and 5,298 rows* of data (*Note: new rows of data are added incrementally over time so this row count may be larger than the current count).
>
> - 3 columns are categorical (`Crude` , `Batch` , and `Location`)
> - 1 column is datetime (`Sample Date (yyyy-mm-dd)`)
> - 1 column is integer (`target_label`)
> - 128 columns are numeric

Feature Descriptions

- These are the key variables that will be used in the modeling process. Together, these variables represent a comprehensive characterization of crude oil samples, covering density, composition, impurities, metal content, acidity, and detailed distillation properties that collectively influence crude quality and processing behavior.

Feature	Description
Crude	Name of the crude oil grade.
Batch	Shipment or lot identifier for the sample.
Sample Date (yyyy-mm-dd)	Date the crude sample was collected.
Location	Site or facility where the sample was taken.
Density (kg/m^3) [ASTM D5002]	Mass per unit volume; indicates heaviness of crude.
Gravity (°API) [ASTM D5002]	Measure of crude lightness; inverse of density.
Sulphur (wt%) [ASTM D4294]	Sulphur content; affects refining and emissions.
Micro Carbon Residue (wt%) [ASTM D4530]	Carbon left after pyrolysis; indicator of coke-forming tendency.
Sediment (ppmw) [ASTM D4807]	Solid impurities or particles in crude.
Total Acid Number (mgKOH/g) [ASTM D664]	Measure of acidity; indicates corrosive potential.
Salt (ptb) [ASTM D3230]	Salt concentration; impacts corrosion and desalting needs.
Nickel (mg/kg) [ASTM D5708A]	Metal contaminant affecting catalyst life.
Vanadium (mg/kg) [ASTM D5708A]	Metal impurity impacting refining catalysts.
C1–C10 Components (vol%) [GC/FID]	Light hydrocarbon composition (methane to decane) by gas chromatography; indicates volatility and gas content.
iC4–nC5 (vol%) [GC/FID]	Branched and normal butane/pentane fractions; measure of light-end structure.
C6–C10 (vol%) [GC/FID]	Heavier paraffins; affect vapor pressure and yield profiles.

Feature	Description
Nitrogen – C4- (vol%) [GPA 2177M]	Nitrogen content in light gas fraction.
Carbon Dioxide – C4- (vol%) [GPA 2177M]	CO_2 concentration in gas fraction.
C1–nC4 – C4- (vol%) [GPA 2177M]	Light hydrocarbon breakdown (methane through butane) in gas stream.
IBP (°C) [ASTM D7169]	Initial boiling point; start of vaporization during distillation.
1–99 Mass% Recovered (°C) [ASTM D7169]	Distillation temperatures where 1–99% of sample mass is vaporized; describes boiling range and fractionation behavior.
target_label	Integer encoded variable to describe the crude grade groups (corresponds to `'target_label'` in the `crude_oils_dict`)

Data Summary - Conclusions/Discussions/Next Steps:

- The Data Summary confirmed that the combined dataset contains over 5,000 samples and 133 features covering physical, chemical, and compositional properties across four crude oil groups. It showed that most variables are numeric and suitable for quantitative analysis, while a few categorical and datetime columns provide sample context. Minor inconsistencies in text formatting and missing values were identified for later cleaning.
- With the dataset now organized and understood, the next step will be Exploratory Data Analysis (EDA) to examine feature distributions, detect missing values, assess correlations, and identify any outliers or patterns that may influence modeling.

EDA

For the Exploratory Data Analysis (EDA) we begin by organizing the dataset into logical column groups—categorical variables, crude quality features, and distillation temperature features—to simplify analysis. We then examine the numeric column distributions through histograms to visualize how the crude grade groups differ across key quality and distillation variables. After exploring these distributions, the analysis evaluates missing data patterns to identify incomplete or inconsistent features and concludes with a correlation assessment to detect relationships and redundancy among numeric features.

Column Groups

- These column groups will be used throughout the analysis and to aid in modeling

In [85]:
```
# Categorical columns
categorical_cols = ['Crude', 'Batch', 'Sample Date (yyyy-mm-dd)', 'Location', 'target_label']

# Columns that describe the quality of the crude oil
crude_quality_cols = df.loc[:,'Density (kg/m³) [ASTM D5002]':'IBP (°C) [ASTM D7169]'].columns.to_list()

# Columns that describe distillation temperatures for the crude oil
dist_temp_cols = df.loc[:,'1 Mass% Recovered (°C) [ASTM D7169]':'99 Mass% Recovered (°C) [ASTM D7169]'].columns.to_list()
```

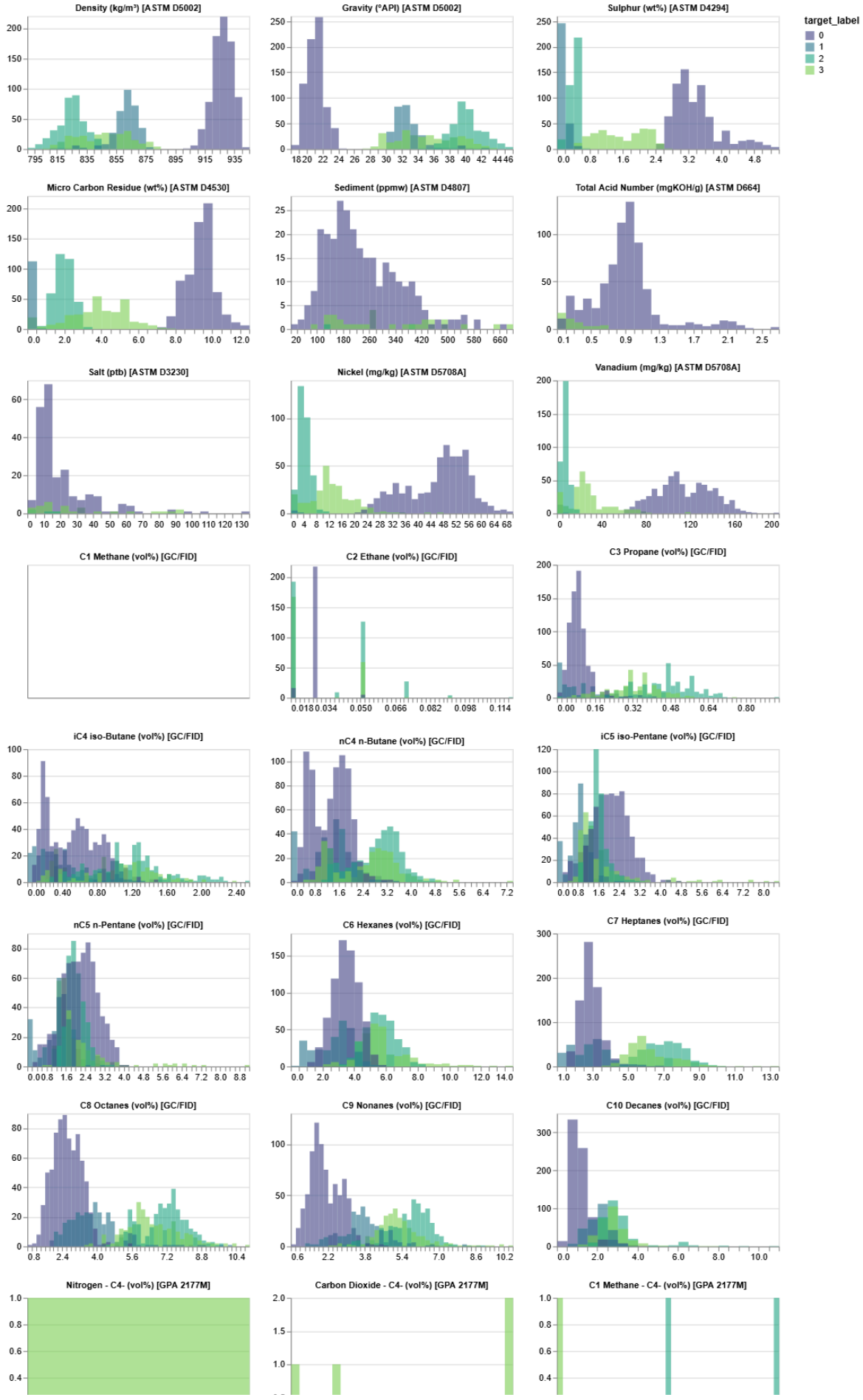
Crude Quality Histograms

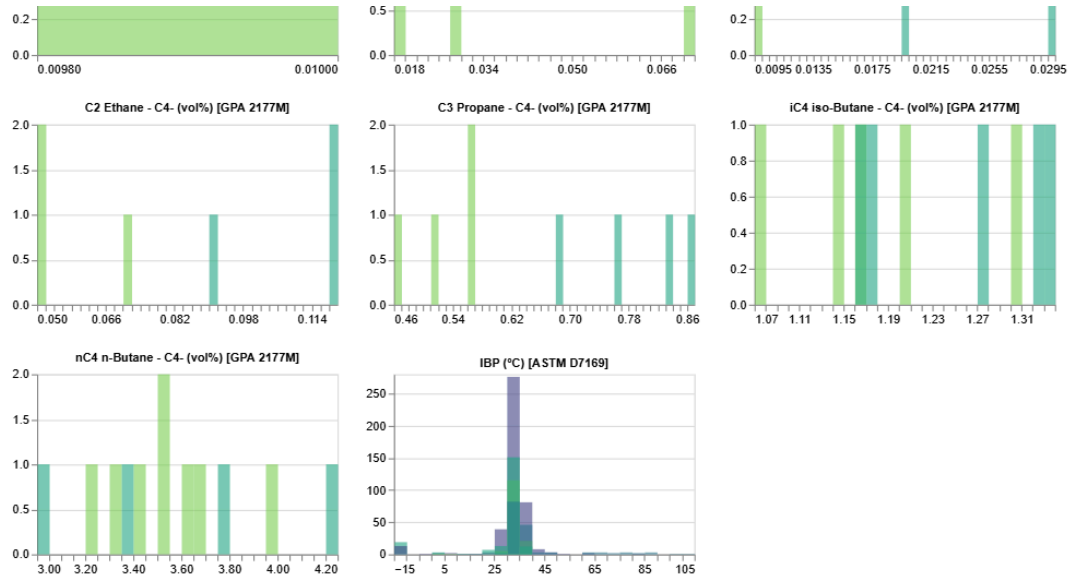
- These histograms give us a sense of the distribution of the `crude_quality_cols` .
- Note: To reduce memory usage for large sets of plots the dataset is temporarily reduced by randomly selecting a subset of data points. Histograms may look different depending on the size of the subset, but generally show the distributions by crude grades.

In [86]:
```
# Function to plot a set of histograms for a subset of columns
def plot_column_histograms(input_df, subset, chart_title, col_count, row_sample_size):
    # Melt the numeric columns into one column
    df_melt = input_df[subset + ['target_label']].melt(id_vars='target_label', var_name='feature', value_name='value').sample(n=row_sample_size)

    # Create a base Altair histogram chart
    chart = alt.Chart(df_melt).mark_bar(opacity=0.6, binSpacing=0).encode(
        x = alt.X('value:Q').axis(title='').bin(maxbins=50),
        y = alt.Y('count():Q').axis(title='').stack(None),
        color = alt.Color('target_label:N').scale(scheme='viridis')
    ).properties(
        width=750 / col_count,
        height=150
    )

    # Display a histogram for each numeric_columns
    chart = alt.ConcatChart(
        title=alt.Title(f'{chart_title}', fontSize=20),
        concat=[chart.transform_filter(alt.datum.feature == value).properties(title=value) for value in subset],
        columns=col_count,
    ).configure_title(
        fontSize=10
    ).resolve_axis(
        x='independent',
        y='independent'
    ).resolve_scale(
        x='independent',
        y='independent'
    )

    return chart

plot_column_histograms(df, crude_quality_cols, 'Crude Quality Columns Data Distributions', 3, 50000)
```

Out[86]:

Crude Quality Columns Data Distributions



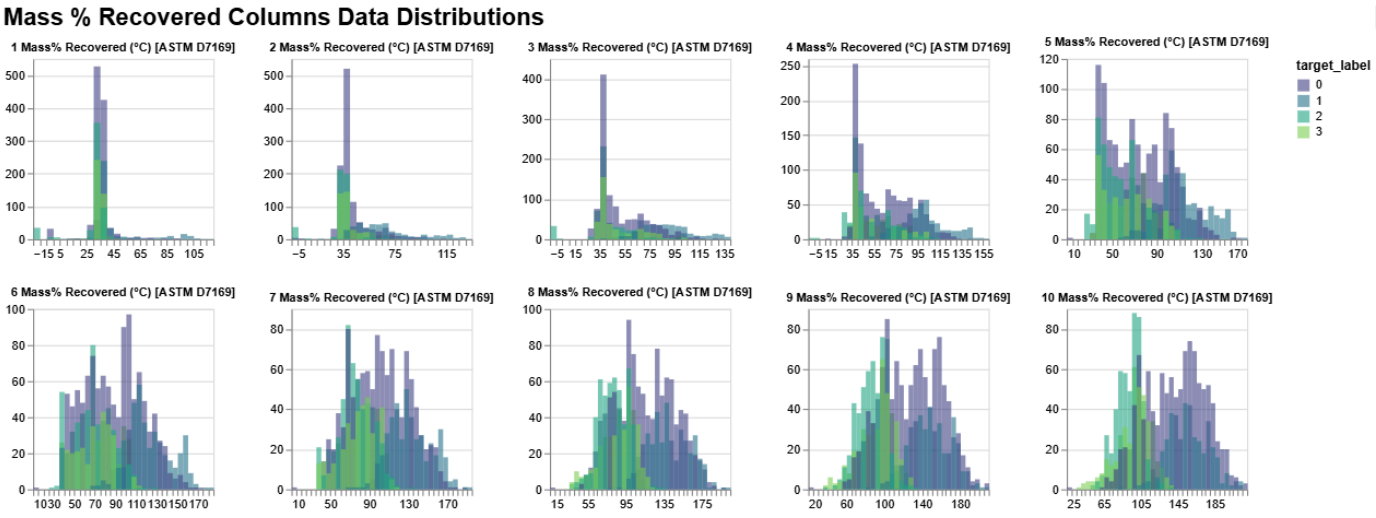


> The histograms show uneven data coverage across the crude grade groups, with several columns containing sparse or missing distributions for certain grades. Features such as Sediment, Total Acid Number, Salt, and the gas composition variables (e.g., C1 Methane, Nitrogen–C4–, CO_2–C4–, etc.) lack consistent representation and should be considered for removal during the Data Cleaning phase to prevent bias in model training.

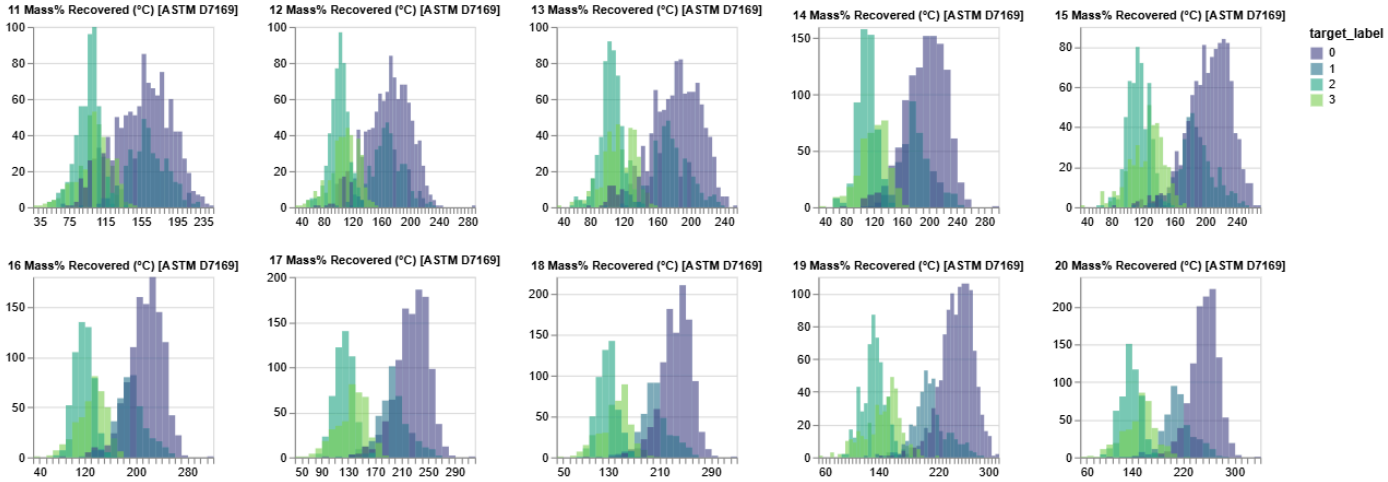
Distillation Temperature Histograms

- These histograms show how the distributions of crude oil grades vary across the dist_temp_cols as the mass percent recovered increases.
- NNote: To manage memory when generating multiple plots, a random subset of the dataset is used. The shapes of the histograms may vary slightly with different sample sizes but consistently illustrate the distribution patterns by crude grade.

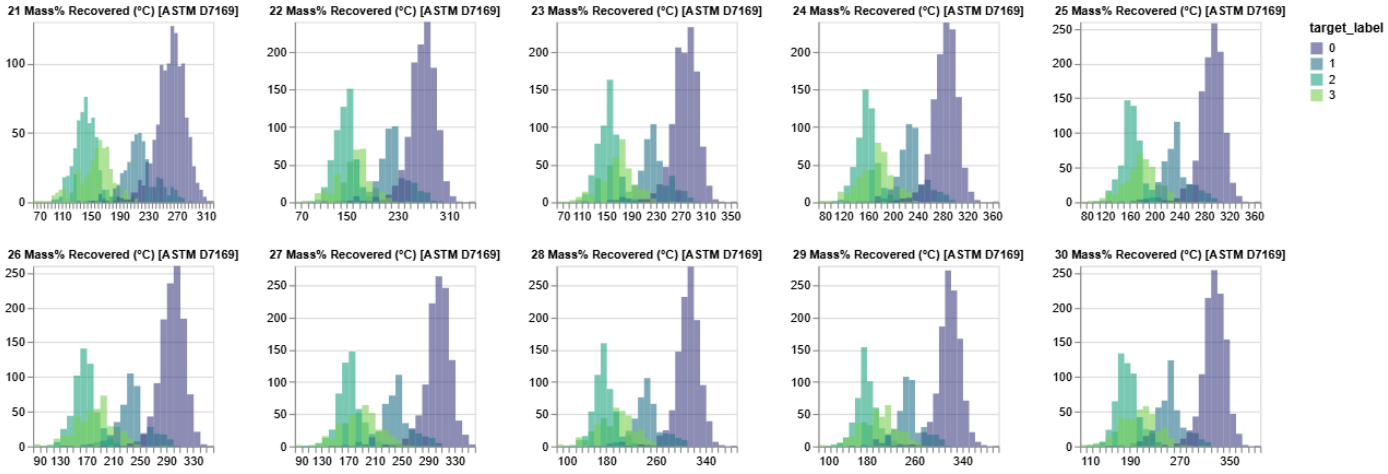
In [87]:
```
def chunk(seq, size):
    for i in range(0, len(seq), size):
        yield seq[i:i+size]

for subset in chunk(dist_temp_cols, 10):
    display(plot_column_histograms(df, subset, 'Mass % Recovered Columns Data Distributions', 5, 45000))
```



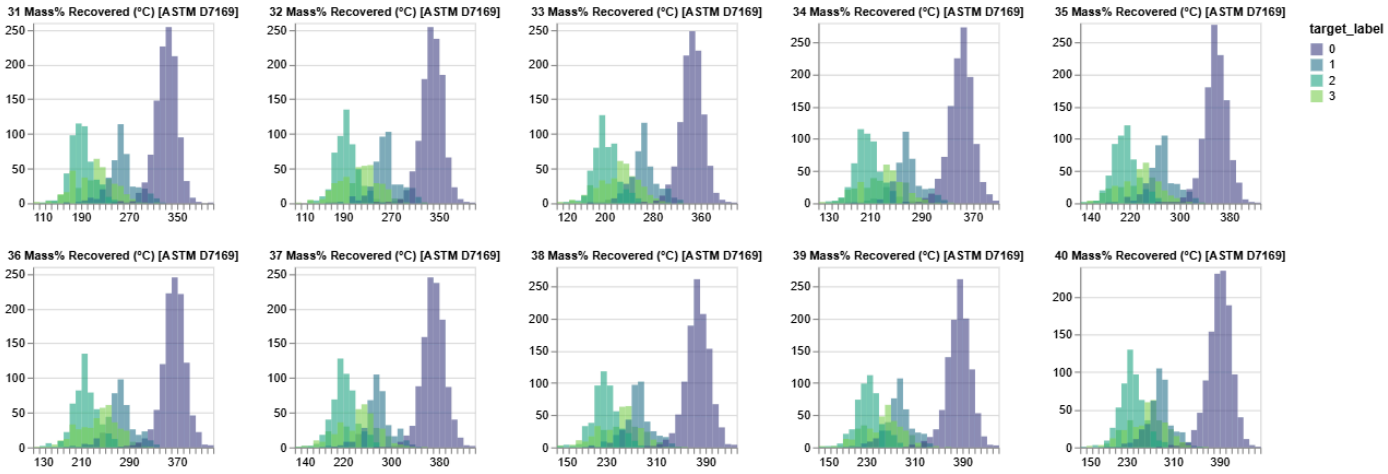
Mass % Recovered Columns Data Distributions



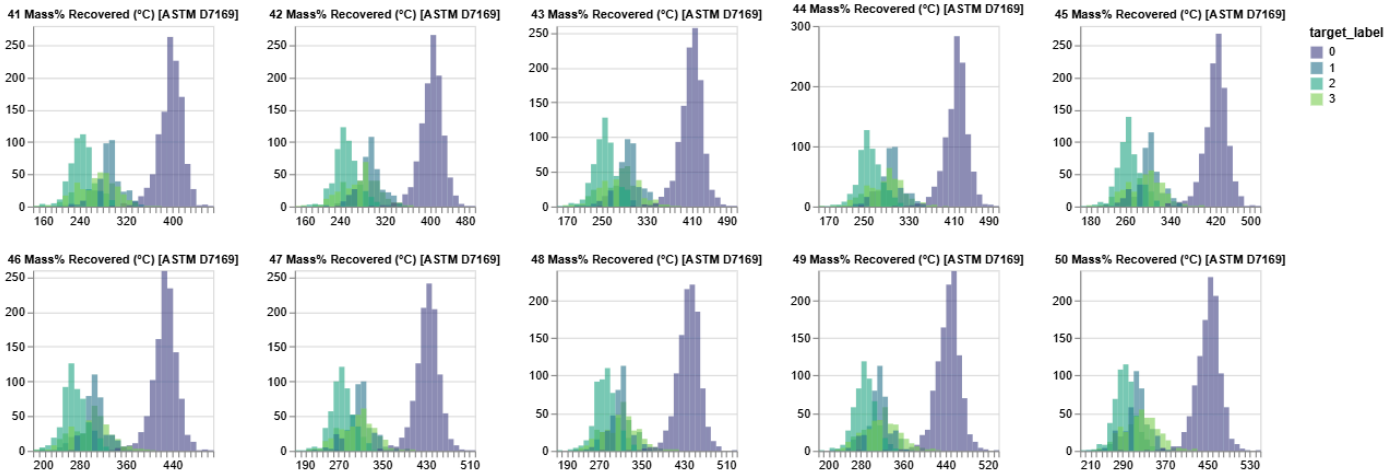
Mass % Recovered Columns Data Distributions



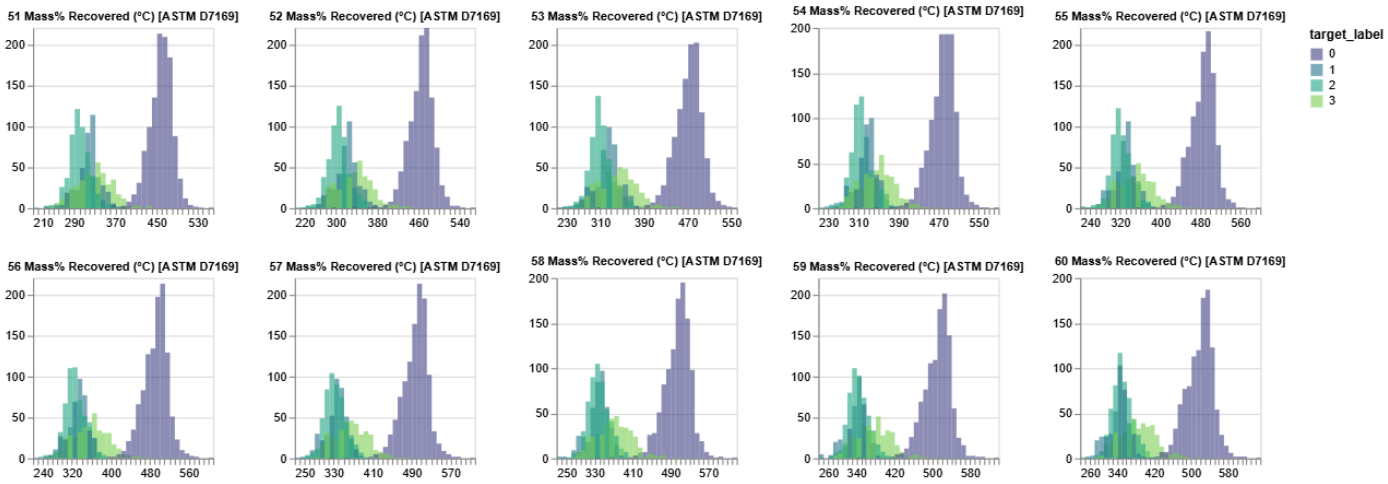
Mass % Recovered Columns Data Distributions



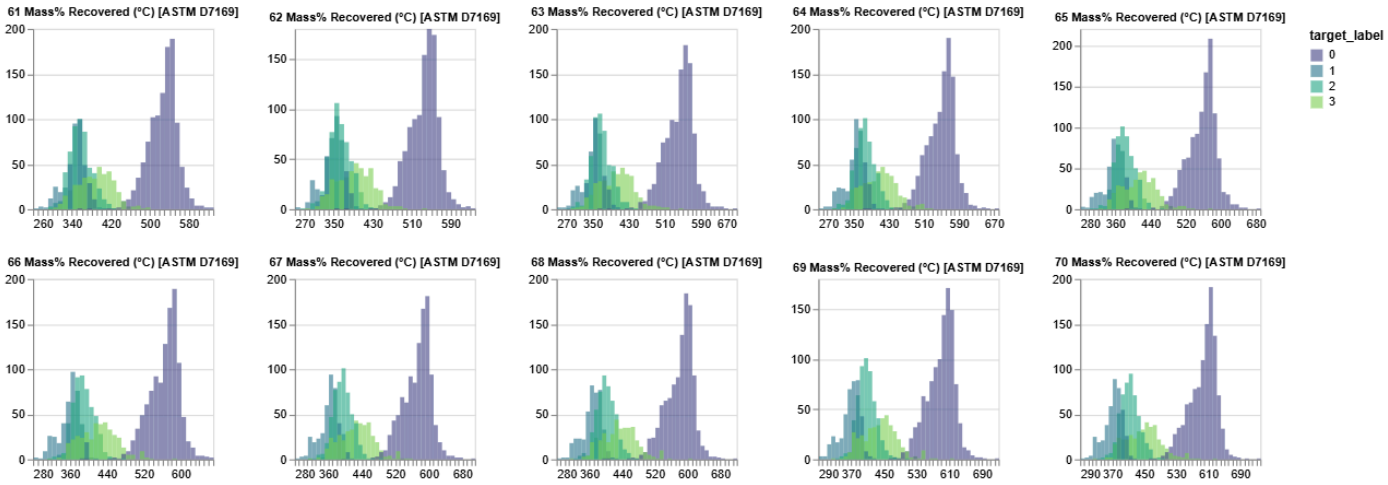
Mass % Recovered Columns Data Distributions

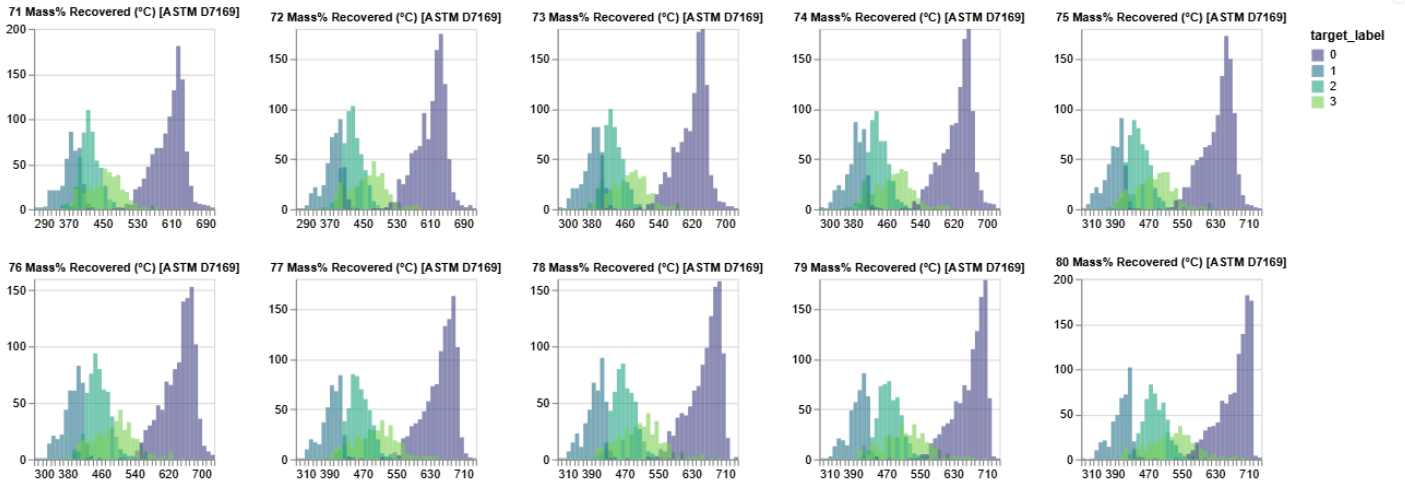


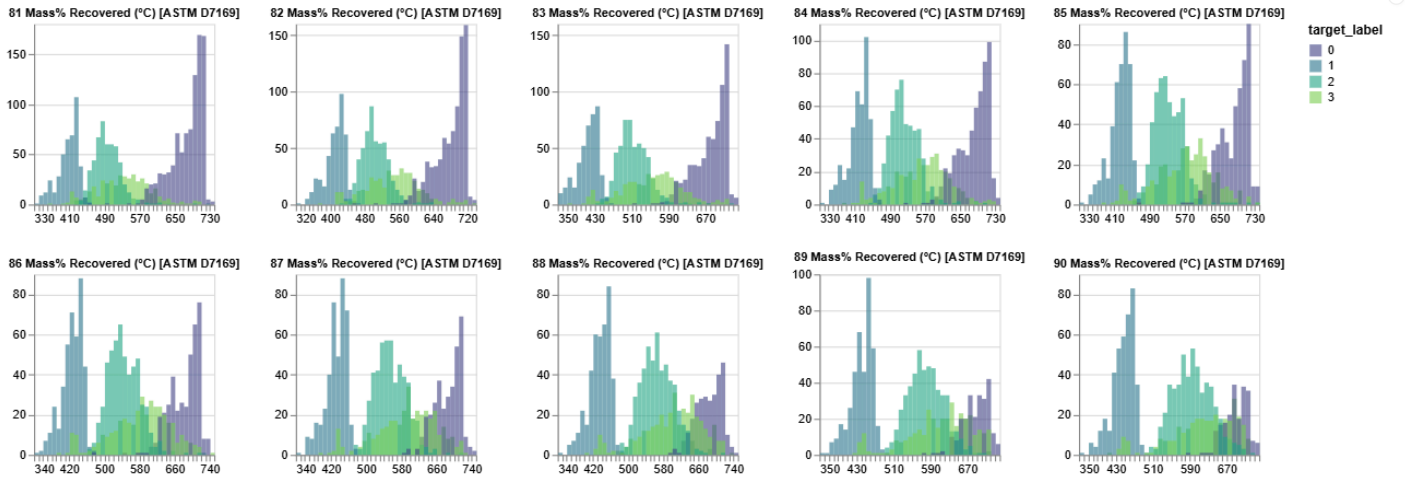
Mass % Recovered Columns Data Distributions

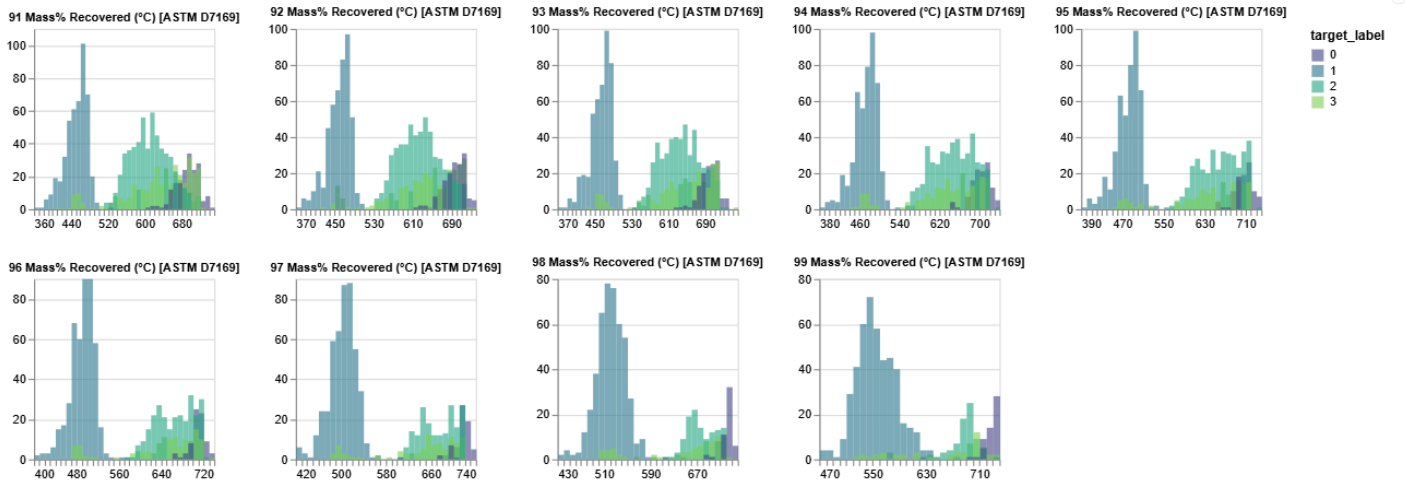


Mass % Recovered Columns Data Distributions









> The Mass % Recovered histograms show overlapping and mixed distributions at low recovery levels but become more distinct beyond roughly 5 % recovered. As recovery increases, the crude grade groups separate clearly, showing that distillation temperature profiles strongly differentiate the crude types even though some overlap persists at certain stages.

Check for Missing Values

- This step identifies missing data across all features and crude groups to assess dataset completeness and guide later cleaning and imputation decisions.

In [88]:
```
# Calculate the total number of values in the dataset
total_value_count = df.notna().sum().sum()
print(f'Total count of values in the dataset = {total_value_count:,d}')

# Calculate the number of missing values in the dataset
```

```
missing_value_count = df.isna().sum().sum()
print(f'Count of missing values in the dataset = {missing_value_count:,d}')

# Calculate the percent missing values in the dataset
percent_missing_values = missing_value_count / total_value_count * 100
print(f'Percent of values that are missing = {percent_missing_values:.1f}%')
```

```
Total count of values in the dataset = 380,970
Count of missing values in the dataset = 324,329
Percent of values that are missing = 85.1%
```

In [ ]:

```
# Create heatmap to visualize where data is missing in the dataset
fig, (ax1, ax2, ax3, ax4) = plt.subplots(1,4, figsize=(30,30), sharey=True)
plt.suptitle('Rows with Missing Values by Crude Grade', y=0.92, fontsize = 30)

sns.heatmap(df[df['target_label']==0].T.isna(), cmap=sns.color_palette('blend:#ffffff,#414487'), cbar=False, ax=ax1)
sns.heatmap(df[df['target_label']==1].T.isna(), cmap=sns.color_palette('blend:#ffffff,#2a788e'), cbar=False, ax=ax2)
sns.heatmap(df[df['target_label']==2].T.isna(), cmap=sns.color_palette('blend:#ffffff,#22a884'), cbar=False, ax=ax3)
sns.heatmap(df[df['target_label']==3].T.isna(), cmap=sns.color_palette('blend:#ffffff,#7ad151'), cbar=False, ax=ax4)

ax1.set_title('Heavy Sour Crude Oils', fontsize = 20)
ax2.set_title('Sweet Synthetic', fontsize = 20)
ax3.set_title('Light & Medium Sweet Crude Oils', fontsize = 20)
ax4.set_title('Light & Medium Sour Crude Oils', fontsize = 20)

plt.show()
```

> The missing values heatmap shows significant data gaps across all crude groups. As we found in the crude quality columns histograms the Sediment, Total Acid Number, Salt, and gas composition columns (C1 Methane, Nitrogen–C4–, CO_2–C4–, etc.) all have a large amount of missing values. These features are largely incomplete across samples and will likely need to be dropped or excluded in later cleaning steps to maintain dataset consistency.

- The `Location` column has one missing value:

In [12]:
```
# Find where the missing Location value is
df[df['Location'].isna()].index
```

Out[12]:
```
Index([5230], dtype='int64')
```

In [13]:
```
# Extract row where Location is missing
df.iloc[5230,:]
```

Out[13]:
```
Crude                                    Pembina Light Sour
Batch                                               PLS-685
Sample Date (yyyy-mm-dd)                2010-09-02 00:00:00
Location                                               None
Density (kg/m³) [ASTM D5002]                     825.200012
                                                    ...
96 Mass% Recovered (°C) [ASTM D7169]                702.0
97 Mass% Recovered (°C) [ASTM D7169]                  NaN
98 Mass% Recovered (°C) [ASTM D7169]                  NaN
99 Mass% Recovered (°C) [ASTM D7169]                  NaN
target_label                                            3
Name: 5230, Length: 133, dtype: object
```

In [14]:
```
# Check what the `Location` usually is for when `Crude`=='Pembina Light Sour'
df[df['Crude']=='Pembina Light Sour'].head(30)
```

Out[14]:

	Crude	Batch	Sample Date (yyyy-mm-dd)	Location	Density (kg/m³) [ASTM D5002]	Gravity (°API) [ASTM D5002]	Sulphur (wt%) [ASTM D4294]	Micro Carbon Residue (wt%) [ASTM D4530]	Sediment (ppmw) [ASTM D4807]	Total Acid Number (mgKOH/g) [ASTM D664]	...	91 Mass% Recovered (°C) [ASTM D7169]	92 Mass% Recovered (°C) [ASTM D7169]	93 Mass% Recovered (°C) [ASTM D7169]	94 Mass% Recovered (°C) [ASTM D7169]	95 Mass% Recovered (°C) [ASTM D7169]	96 Mass% Recovered (°C) [ASTM D7169]
5217	Pembina Light Sour	PLS-570	2010-05-04	Edmonton	830.700012	38.599998	0.92	2.2	NaN	NaN	...	600.500000	618.900024	639.400024	663.000000	694.599976	NaN
5218	Pembina Light Sour	PLS-026	2007-12-02	Edmonton	822.299988	40.400002	0.77	1.4	NaN	NaN	...	539.299988	552.799988	567.299988	582.400024	599.299988	619.000000
5219	Pembina Light Sour	PLS-042	2008-01-02	Edmonton	823.500000	40.200001	0.70	0.3	NaN	NaN	...	564.400024	579.200012	596.099976	615.599976	638.400024	669.200012
5220	Pembina Light Sour	PLS-317	2008-04-14	Edmonton	822.400024	40.400002	0.75	1.5	NaN	NaN	...	626.099976	651.400024	686.799988	NaN	NaN	NaN
5221	Pembina Light Sour	PLS-332	2008-05-14	Edmonton	823.700012	40.099998	0.74	1.3	NaN	NaN	...	618.900024	638.299988	661.000000	691.500000	NaN	NaN
5222	Pembina Light Sour	PLS-342	2008-06-04	Edmonton	821.900024	40.500000	0.69	1.6	NaN	NaN	...	576.099976	592.200012	610.200012	631.099976	655.500000	689.900024
5223	Pembina Light Sour	PLS-359	2008-07-08	Edmonton	828.099976	39.200001	0.79	1.5	NaN	NaN	...	576.000000	593.200012	612.599976	635.599976	664.599976	704.900024
5224	Pembina Light Sour	PLS-376	2008-08-12	Edmonton	822.000000	40.500000	0.74	1.5	NaN	NaN	...	643.400024	677.299988	719.500000	NaN	NaN	NaN
5225	Pembina Light Sour	PLS-501	2009-03-04	Edmonton	823.099976	40.299999	0.74	1.5	NaN	NaN	...	549.900024	565.000000	580.599976	597.799988	617.799988	641.099976
5226	Pembina Light Sour	PLS-352	2009-05-04	Edmonton	824.299988	40.000000	0.78	1.7	NaN	NaN	...	587.200012	604.799988	625.200012	649.400024	684.200012	NaN
5227	Pembina Light Sour	PLS-810	2009-09-02	Edmonton	826.900024	39.500000	0.83	1.6	NaN	NaN	...	549.700012	564.000000	578.500000	594.599976	612.599976	633.200012
5228	Pembina Light Sour	PLS-440	2009-11-02	Edmonton	822.599976	40.400002	0.77	1.6	NaN	NaN	...	554.400024	568.299988	583.099976	599.500000	618.700012	640.900024
5229	Pembina Light Sour	PLS-534	2010-03-01	Edmonton	831.000000	38.599998	0.85	2.1	NaN	NaN	...	604.200012	622.299988	642.200012	665.900024	695.500000	NaN
5230	Pembina Light Sour	PLS-685	2010-09-02	None	825.200012	39.799999	0.77	0.9	NaN	NaN	...	579.599976	596.500000	615.900024	638.500000	661.400024	702.000000
5231	Pembina Light Sour	PLS-713	2010-10-01	Edmonton	827.599976	39.299999	0.90	2.0	NaN	NaN	...	578.700012	595.500000	614.500000	636.200012	662.299988	696.000000
5232	Pembina Light Sour	PLS-744	2010-11-02	Edmonton	829.500000	38.900002	0.88	2.1	NaN	NaN	...	570.799988	586.500000	604.000000	624.299988	647.799988	678.299988
5233	Pembina Light Sour	PLS-594	2011-03-03	Edmonton	830.500000	38.700001	0.87	2.3	NaN	NaN	...	628.799988	649.700012	675.000000	703.099976	NaN	NaN
5234	Pembina Light Sour	PLS-645	2011-05-09	Edmonton	828.500000	39.099998	0.84	2.3	NaN	NaN	...	597.599976	614.900024	634.099976	655.400024	683.000000	710.599976
5235	Pembina Light Sour	PLS-283	2011-09-04	Edmonton	831.200012	38.599998	0.83	2.3	NaN	NaN	...	630.099976	649.900024	672.200012	696.099976	NaN	NaN
5236	Pembina Light Sour	PLS-357	2012-01-12	Edmonton	824.299988	40.000000	0.66	1.7	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5237	Pembina Light Sour	PLS-370	2012-02-07	Edmonton	824.400024	40.000000	0.67	2.0	NaN	NaN	...	551.599976	564.799988	577.799988	592.500000	608.400024	626.099976
5238	Pembina Light Sour	PLS-385	2012-03-06	Edmonton	836.500000	37.500000	0.68	1.8	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5239	Pembina Light Sour	PLS-430	2012-06-05	Edmonton	819.799988	41.000000	0.40	1.3	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN

	Crude	Batch	Sample Date (yyyy-mm-dd)	Location	Density (kg/m³) [ASTM D5002]	Gravity (°API) [ASTM D5002]	Sulphur (wt%) [ASTM D4294]	Micro Carbon Residue (wt%) [ASTM D4530]	Sediment (ppmw) [ASTM D4807]	Total Acid Number (mgKOH/g) [ASTM D664]	...	91 Mass% Recovered (°C) [ASTM D7169]	92 Mass% Recovered (°C) [ASTM D7169]	93 Mass% Recovered (°C) [ASTM D7169]	94 Mass% Recovered (°C) [ASTM D7169]	95 Mass% Recovered (°C) [ASTM D7169]	96 Mass% Recovered (°C) [ASTM D7169]
5240	Pembina Light Sour	PLS-460	2012-08-07	Edmonton	834.700012	37.900002	0.76	2.2	NaN	NaN	...	579.299988	593.799988	609.500000	627.000000	646.200012	668.700012
5241	Pembina Light Sour	PLS-176	2012-09-11	Edmonton	823.900024	40.099998	0.59	1.6	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5242	Pembina Light Sour	PLS-483	2012-10-02	Edmonton	828.700012	39.099998	0.59	2.1	NaN	NaN	...	570.900024	584.599976	599.200012	615.599976	633.599976	653.799988
5243	Pembina Light Sour	PLS-505	2012-11-05	Edmonton	828.799988	39.099998	0.77	2.2	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5244	Pembina Light Sour	PLS-516	2012-12-03	Edmonton	823.500000	40.200001	0.80	2.1	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5245	Pembina Light Sour	PLS-231	2013-01-01	Edmonton	827.799988	39.299999	0.78	2.2	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN
5246	Pembina Light Sour	PLS-241	2013-02-02	Edmonton	846.000000	35.599998	1.09	2.7	NaN	NaN	...	NaN	NaN	NaN	NaN	NaN	NaN

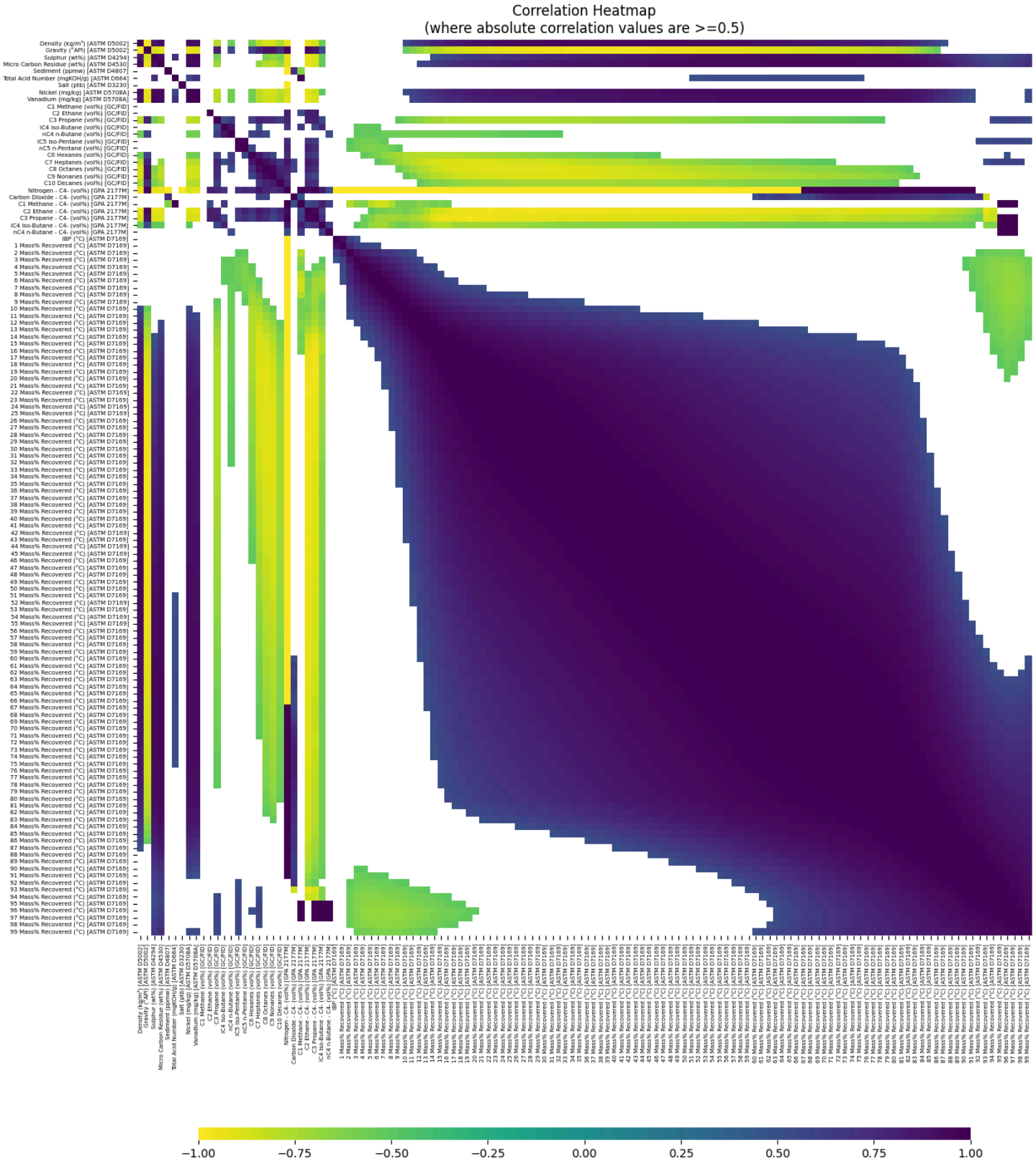
30 rows × 133 columns

In [15]:
```
# Location looks like it is always 'Edmonton', so I will impute this value
df.loc[df['Crude']=='Pembina Light Sour','Location'] = 'Edmonton'
```

Column Correlations

- We need to check if there exists strong correlations between the numeric features. If there are then we should consider dropping one or more of the correlated features from the dataset.
- To aid in this evaluation we will visualize the data using a heatmap, where values of `[-1,1]` indicate as strong correlation, and values close to `0` indicate a weak correlation.
  - Note: Only the correlation values between `[-1.0, -0.5]` and `[0.5, 1.0]` are colored in the heatmap in order to focus on the highly correlated variables.

In [98]:
```
# Correlation Heatmap
fig, ax = plt.subplots(figsize=(20, 20))
sns.heatmap(
    df[crude_quality_cols + dist_temp_cols].corr(),
    cmap='viridis_r',
    mask=abs(df[crude_quality_cols + dist_temp_cols].corr())<=0.5, # Plot only absolute correlation values that are >=0.5
    square=True,
    vmin=-1, vmax=1,
    xticklabels=True, yticklabels=True,
    cbar_kws={'location':'bottom', 'aspect':60, 'shrink':0.6}
)

plt.xticks(fontsize=5)
plt.yticks(fontsize=5)
plt.title('Correlation Heatmap\n(where absolute correlation values are >=0.5)')
plt.show()
```



> The correlation heatmap shows strong relationships among many of the Mass % Recovered columns, indicating high multicollinearity across distillation temperature features. Other notable correlations appear between related chemical and physical properties (e.g., Density, API Gravity, Sulphur), suggesting that several features convey overlapping information that may require dimensionality reduction or feature selection later in the analysis.

EDA - Conclusions/Discussions/Next Steps:

- The EDA revealed that while the dataset captures a wide range of crude oil properties, several features—such as Sediment, Total Acid Number, Salt, and gas composition variables—contain extensive missing data and inconsistent distributions across crude groups. Strong correlations were observed among the Mass % Recovered columns and between key physical properties like Density, API Gravity, and Sulphur, indicating potential redundancy.

- With these insights, the next step in the analysis will focus on Data Cleaning to prepare the dataset for modeling.

Data Cleaning

This section focuses on adding datetime-based features, removing low-quality or highly correlated columns, imputing missing values, and developing a preprocessing pipeline to ready the dataset for modeling.

Add Datetime Columns

- Add month number and year to the dataset to ensure effects of time are captured in the models.

In [17]:
```
# Add Months and Years columns
df['Months'] = (df['Sample Date (yyyy-mm-dd)'].dt.to_period('M') - df['Sample Date (yyyy-mm-dd)'].min().to_period('M')).apply(lambda x: x.n)
df['Year'] = df['Sample Date (yyyy-mm-dd)'].dt.year

# Update the crude_quality_cols list to add Months and Year columns
categorical_cols = categorical_cols + ['Months', 'Year']
```

Drop Columns

- The missing values analysis showed that several columns contained significant gaps across all four crude oil grades. Because the limited number of available observations would make mean imputation unreliable and potentially introduce bias, these columns were excluded from the dataset to preserve data integrity and modeling accuracy.
- I will aslo be dropping the `Crude`, `Batch`, and `Sample Date (yyyy-mm-dd)` columns from because they will not be used in this analysis.

In [18]:
```
# Define the set of crude_quality_cols to drop
crude_quality_cols_to_drop = [
    'Sediment (ppmw) [ASTM D4807]',
    'Total Acid Number (mgKOH/g) [ASTM D664]',
    'Salt (ptb) [ASTM D3230]',
    'C1 Methane (vol%) [GC/FID]',
    'Nitrogen - C4- (vol%) [GPA 2177M]',
    'Carbon Dioxide - C4- (vol%) [GPA 2177M]',
    'C1 Methane - C4- (vol%) [GPA 2177M]',
    'C2 Ethane - C4- (vol%) [GPA 2177M]',
    'C3 Propane - C4- (vol%) [GPA 2177M]',
    'iC4 iso-Butane - C4- (vol%) [GPA 2177M]',
    'nC4 n-Butane - C4- (vol%) [GPA 2177M]'
]

# Drop columns from dataset
df = df.drop(crude_quality_cols_to_drop, axis=1)

# Update the crude_quality_cols list to remove the crude_quality_cols_to_drop
crude_quality_cols = [col for col in crude_quality_cols if col not in crude_quality_cols_to_drop]
```

In [19]:
```
# Define categorical_cols to drop
categorical_cols_to_drop = [
    'Crude',
    'Batch',
    'Sample Date (yyyy-mm-dd)'
]

# Drop categorical columns
df = df.drop(categorical_cols_to_drop, axis=1)

# Update categorical_cols to remove the dropped columns
categorical_cols = [col for col in categorical_cols if col not in categorical_cols_to_drop]

categorical_cols
```

Out[19]:
```
['Location', 'target_label', 'Months', 'Year']
```

Impute Values

- Before imputing missing values, the following components in the Sweet Synthetic Crude Oil samples will be set to zero, as they are not expected to be present in this crude type:
  - `Nickel (mg/kg) [ASTM D5708A]`
  - `Vanadium (mg/kg) [ASTM D5708A]`
  - `C2 Ethane (vol%) [GC/FID]`
- After these adjustments, the remaining missing values will be imputed using a KNNImputer, which estimates missing entries based on the mean values of the nearest samples in feature space.
- There is also one missing value in the 'Location' column that will need to be imputed.

In [20]:
```
df.loc[df['target_label']==1, ['Nickel (mg/kg) [ASTM D5708A]', 'Vanadium (mg/kg) [ASTM D5708A]', 'C2 Ethane (vol%) [GC/FID]']] = 0
```

In [21]:
```
# Create a KNNImputer instance which uses the 10 nearest neighbors to the missing value to calculate an imputed mean value
imputer = KNNImputer(n_neighbors=10, weights='distance')

# Impute missing values for each crude type
for i in range(4):
    df.loc[df['target_label']==i, crude_quality_cols + dist_temp_cols] = imputer.fit_transform(df.loc[df['target_label']==i, crude_quality_cols + dist_temp_cols])
```

```
# Check that no missing values exist
df[crude_quality_cols + dist_temp_cols].isna().sum().sum()
```

Out[21]: np.int64(0)

Pre-Processing

something about Data Scaling and Encoding Pipeline, transforming X and defining the target y_true

In [22]:
```
# Define the feature matrix
X = df[['Months', 'Year', 'Location'] + crude_quality_cols + dist_temp_cols]

# Create a preprocessor
preprocessor = ColumnTransformer(
    [('num1', Pipeline([('scaler', StandardScaler())]), ['Months', 'Year']),
     ('num2', Pipeline([('scaler', StandardScaler())]), crude_quality_cols),
     ('num3', Pipeline([('scaler', StandardScaler())]), dist_temp_cols),
     ('cat', OneHotEncoder(drop='first', handle_unknown='ignore'), ['Location'])],
    remainder='drop'
).fit(X)

# Preprocess the feature matrix
X_transform = preprocessor.transform(X)

# Define the target label values
y_true = df['target_label']
```

Data Cleaning - Conclusions/Discussions/Next Steps:

- The Data Cleaning process successfully refined the dataset by removing unreliable or highly incomplete columns, such as Sediment, Total Acid Number, Salt, and gas composition variables. Datetime-based features were added to capture temporal effects, and missing values were handled through targeted zero-filling for specific synthetic crude components and KNN imputation for the remaining numeric data. All missing values were resolved, and a preprocessing pipeline was created to standardize numeric features and encode categorical ones.
- With a clean and fully prepared dataset, the next step is to begin cluster modeling to explore patterns and groupings among the crude oil samples.

Clustering Models

The Cluster Modeling section applies three unsupervised learning algorithms—K-Means, Agglomerative Clustering, and Gaussian Mixture Models (GMM)—to identify natural groupings within the crude oil dataset. Each model is tested across cluster sizes ranging from 2 to 6 to evaluate how well the data separates into meaningful clusters. Dimensionality reduction techniques, PCA and t-SNE, are used to visualize the cluster formations and assess their distinctness. Model performance is then compared using quantitative metrics and confusion matrices against the known crude grade labels, followed by a final comparison to supervised learning models to benchmark the clustering accuracy and interpretability.

Clustering Helper Functions

- The `results_plot` function is a modified version based on an example given by sklearn (https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html)
  - Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., & Duchesnay, É. (n.d.). K-means clustering and silhouette analysis example. scikit-learn documentation. Retrieved October 16, 2025, from https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html

In [23]:
```
# Function to calculate model performace metrics
def evaluate(X, labels, y_true=None):
    k = len(set(labels)) - (1 if -1 in labels else 0)
    metrics_dict = {
        'n_clusters': k,
        'Silhouette Score': silhouette_score(X, labels),
        'DBI': davies_bouldin_score(X, labels),
        'CHI': calinski_harabasz_score(X, labels),
        'ARI': adjusted_rand_score(y_true, labels) if y_true is not None else np.nan,
        'NMI': normalized_mutual_info_score(y_true, labels) if y_true is not None else np.nan,
        'FMI': fowlkes_mallows_score(y_true, labels) if y_true is not None else np.nan,
    }
    return metrics_dict

# Function to create a silhouette score plot, a PCA scatter plot, and a t-SNE scatter plot
def results_plot(X, labels, model_name, centers=None, random_state=10):
    # Prepare reductions
    pca = PCA(n_components=2, random_state=random_state)
    tsne = TSNE(n_components=2, random_state=random_state, perplexity=30, learning_rate='auto', init='pca')

    X_pca = pca.fit_transform(X)
    X_tsne = tsne.fit_transform(X)

    fig, (ax1, ax2, ax3) = plt.subplots(1, 3, figsize=(16, 5), gridspec_kw={'width_ratios': [1, 1, 1]})

    # Silhouette score plot
    k = len(set(labels)) - (1 if -1 in labels else 0)
    sil_avg = silhouette_score(X, labels)
    sil_vals = silhouette_samples(X, labels)
    ax1.set_xlim([-0.6, 1.0])
    ax1.set_ylim([0, X.shape[0] + (k + 1) * 10])
    y_lower = 10
    for i, cl in enumerate(sorted([c for c in set(labels) if c != -1])):
```

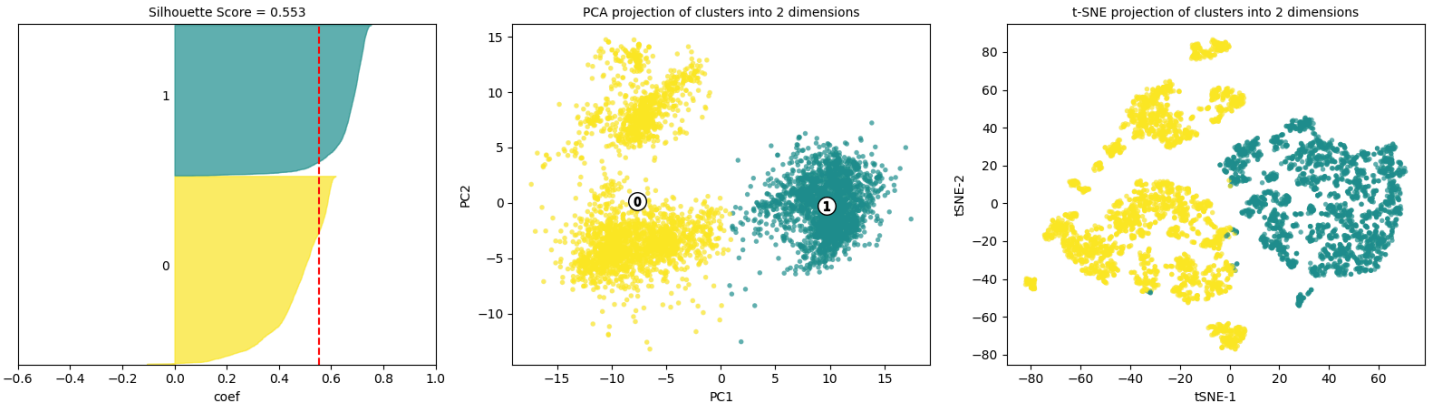
```
        vals = np.sort(sil_vals[labels == cl])
        y_upper = y_lower + vals.shape[0]
        color = cm.viridis_r(float(i) / max(k, 1))
        ax1.fill_betweenx(np.arange(y_lower, y_upper), 0, vals, facecolor=color, edgecolor=color, alpha=0.7)
        ax1.text(-0.05, y_lower + 0.5 * vals.shape[0], str(cl))
        y_lower = y_upper + 10
    ax1.axvline(x=sil_avg, color='red', linestyle='--')
    ax1.set_title(f'Silhouette Score = {sil_avg:.3f}', fontdict={'fontsize':10})
    ax1.set_xlabel('coef')
    ax1.set_yticks([])

    # common color map
    denom = (labels.max() + 1) if labels.max() >= 0 else 1
    colors = cm.viridis_r(labels.astype(float) / denom)

    # PCA scatterplot
    ax2.scatter(X_pca[:, 0], X_pca[:, 1], c=colors, s=15, lw=0, alpha=0.7, edgecolor='k')
    if centers is not None:
        centers_pca = pca.transform(centers)
        ax2.scatter(centers_pca[:, 0], centers_pca[:, 1], marker='o', c='white', s=200, edgecolor='k')
        for i, cpt in enumerate(centers_pca):
            ax2.scatter(cpt[0], cpt[1], marker=f'${i}$', s=50, edgecolor='k')
    ax2.set_title(f'PCA projection of clusters into 2 dimensions', fontdict={'fontsize':10})
    ax2.set_xlabel('PC1')
    ax2.set_ylabel('PC2')

    # t-SNE scatterplot
    ax3.scatter(X_tsne[:, 0], X_tsne[:, 1], c=colors, s=15, lw=0, alpha=0.7, edgecolor='k')
    ax3.set_title(f't-SNE projection of clusters into 2 dimensions', fontdict={'fontsize':10})
    ax3.set_xlabel('tSNE-1')
    ax3.set_ylabel('tSNE-2')

    plt.suptitle(f'{model_name}', horizontalalignment='left', x=0)
    plt.tight_layout()
    plt.show()
```

K-means Clustering

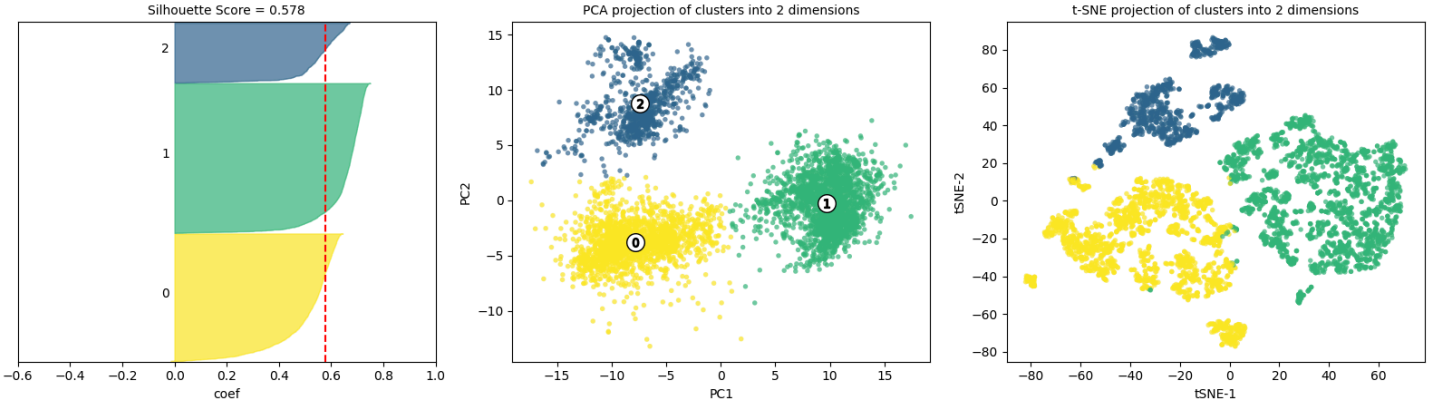
- K-Means partitions data into a predefined number of clusters by minimizing the variance within each cluster and assigning points to the nearest cluster centroid through iterative optimization.

In [24]:
```
# # Create empty dicts to store evaluation metrics for each model
results = []
confusion_data = {}

# Loop over various cluster sizes, fit model, and return evaluation plots
for k in [2, 3, 4, 5, 6]:
    # Fit the model
    model_name = f'K-means Clustering for {k} Clusters'
    kmeans_model = MiniBatchKMeans(n_clusters=k, batch_size=256*14, random_state=10)
    labels = kmeans_model.fit_predict(X_transform)

    # Plot the results
    centers = kmeans_model.cluster_centers_
    results_plot(X_transform, labels, model_name, centers=centers)

    # Add the model performace metrics to the results list
    clustering_metrics = evaluate(X_transform, labels, y_true)
    clustering_metrics.update({'Model': model_name})
    results.append(clustering_metrics)
```

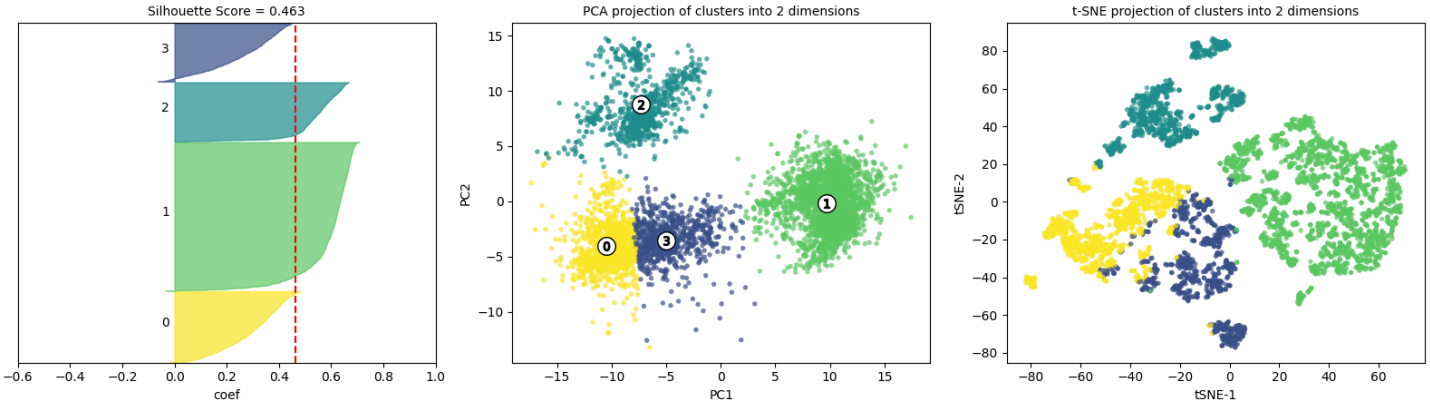
K-means Clustering for 2 Clusters



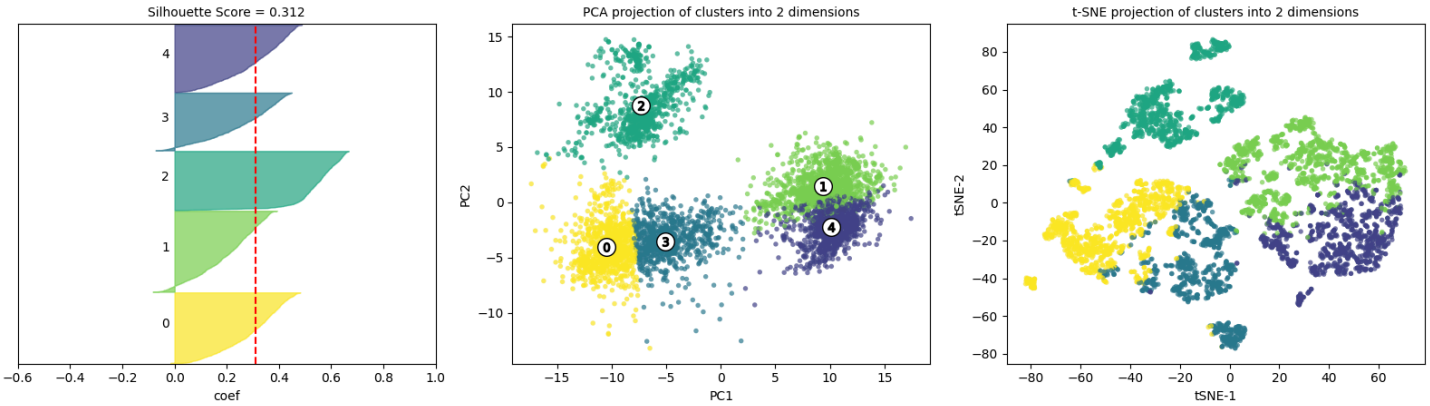
K-means Clustering for 3 Clusters



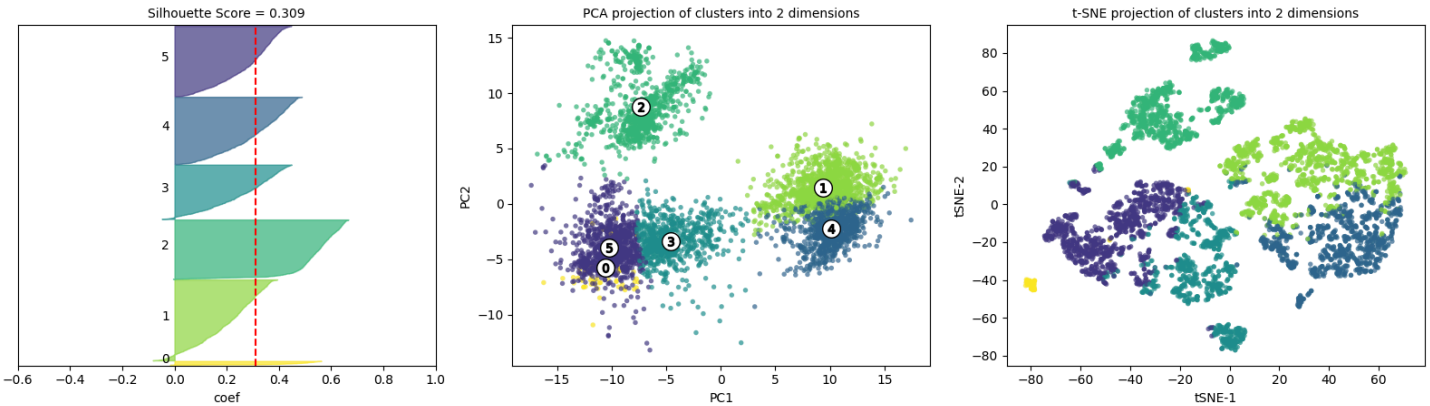
K-means Clustering for 4 Clusters



K-means Clustering for 5 Clusters



K-means Clustering for 6 Clusters



> Across cluster sizes 2–6, K-Means shows that the dataset begins with two broad, well-separated groups (silhouette = 0.553) and reaches its strongest structure with three clusters (silhouette = 0.578). This number of clusters aligns with my suspision that the light and medium crude oil groups may overlap. As cluster count increases beyond three,

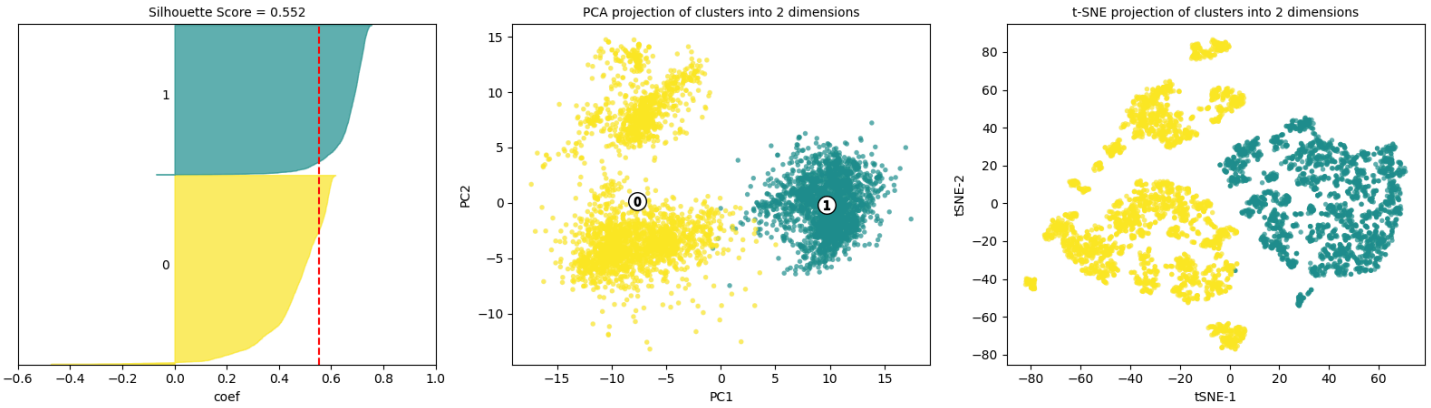
> the silhouette scores decline and boundaries blur, suggesting over-segmentation without meaningful separation. Overall, 3–4 clusters appear most representative of the underlying structure, consistent with the known four target classes and the suspected similarity between the light-medium crude categories.

Agglomerative Clustering

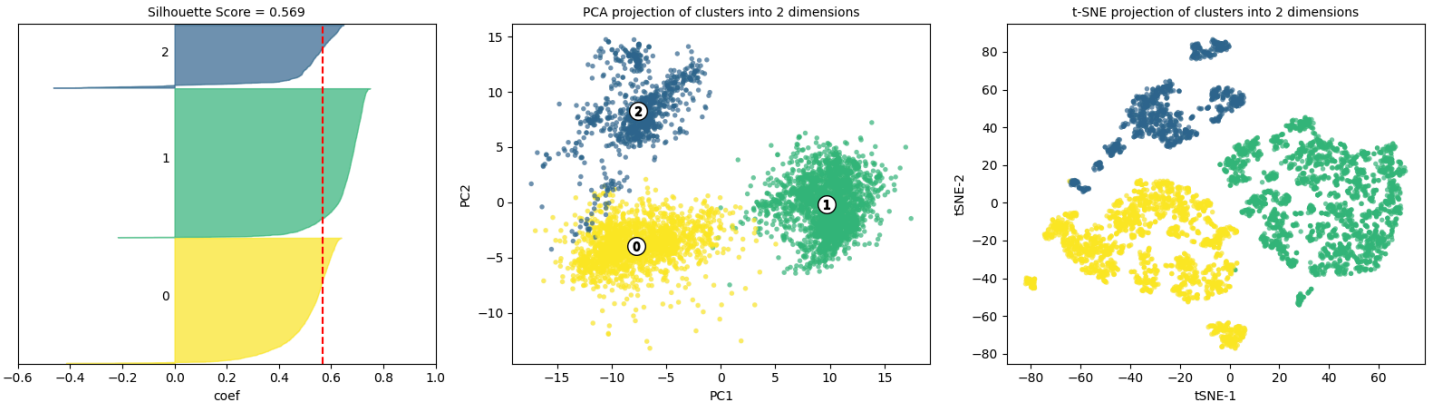
- Agglomerative Clustering is a hierarchical approach that starts with each data point as its own cluster and successively merges the most similar pairs based on linkage criteria until the desired number of clusters is reached.

In [27]:
```
for k in [2, 3, 4, 5, 6]:
    # Fit the model
    model_name = f'Agglomerative Clustering for {k} Clusters'
    agglo_model = AgglomerativeClustering(n_clusters=k, linkage='ward')
    labels = agglo_model.fit_predict(X_transform)

    # Plot the results
    cl_ids = sorted(set(labels))
    centers = np.vstack([X_transform[labels == c].mean(axis=0) for c in cl_ids if np.any(labels == c)])
    results_plot(X_transform, labels, model_name, centers=centers)

    # Add the model performace metrics to the results list
    clustering_metrics = evaluate(X_transform, labels, y_true)
    clustering_metrics.update({'Model': model_name})
    results.append(clustering_metrics)
```

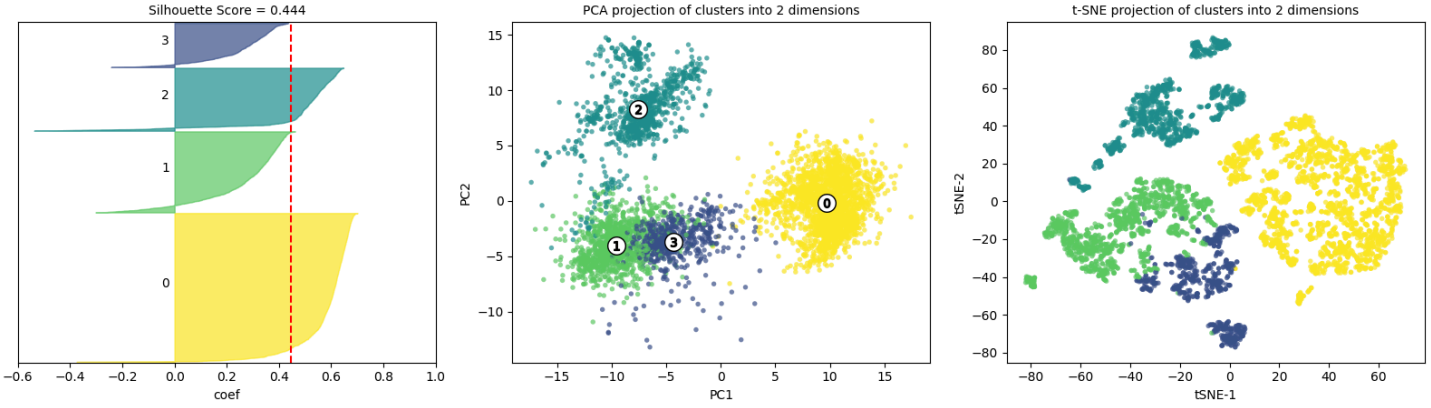
Agglomerative Clustering for 2 Clusters



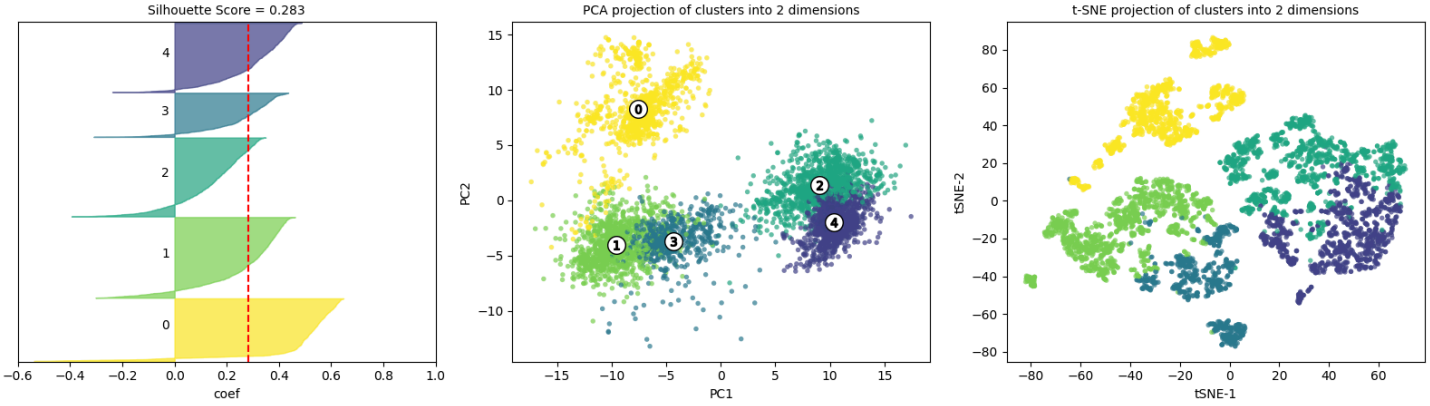
Agglomerative Clustering for 3 Clusters



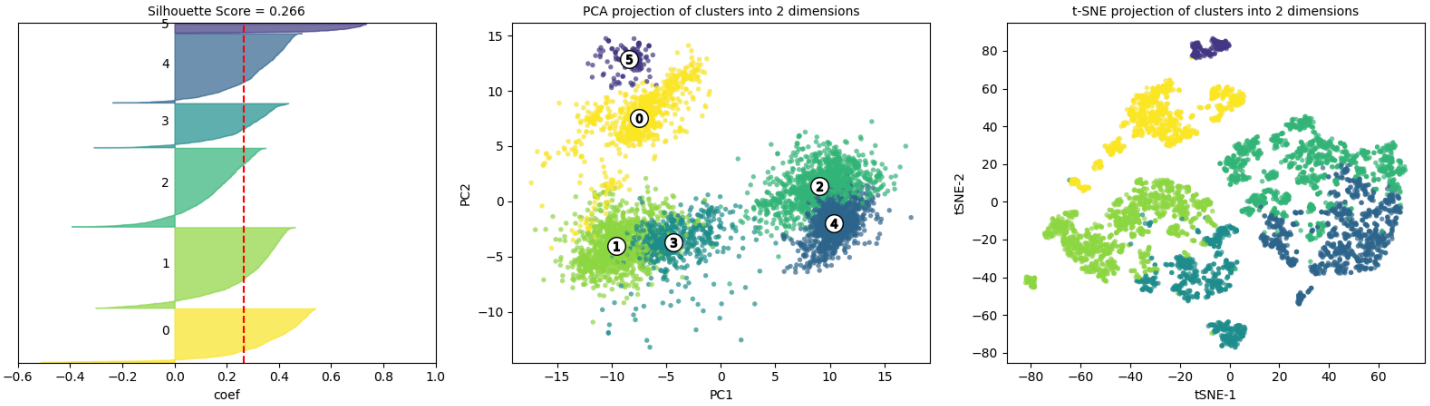
Agglomerative Clustering for 4 Clusters



Agglomerative Clustering for 5 Clusters



Agglomerative Clustering for 6 Clusters



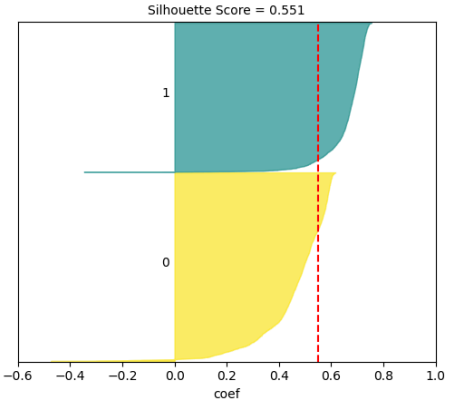
> Across cluster sizes 2–6, Agglomerative Clustering produces patterns similar to K-Means, with clear separation emerging at 3 clusters (silhouette = 0.569). The 2-cluster result shows two large, well-defined groups, while the 3-cluster structure best captures distinctions among heavy, synthetic, and combined light/medium crudes—supporting the hypothesis that light and medium sour/sweet grades are closely related. As clusters increase beyond 3, the structure fragments and silhouette scores decline, suggesting that 3–4 clusters most accurately represent the underlying relationships among the crude oil samples.

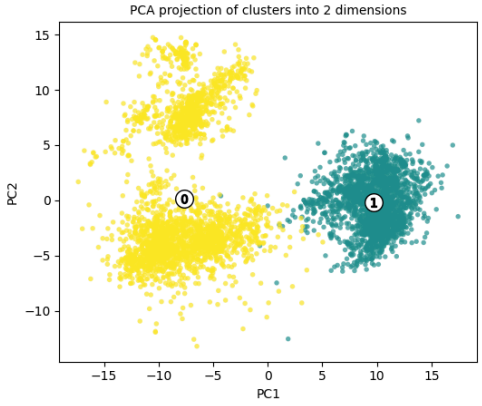
Gaussian Mixture Model Clustering

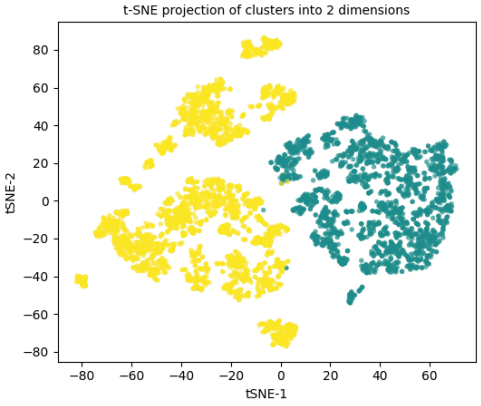
- Gaussian Mixture Models (GMM) assume that the data is generated from a mixture of Gaussian distributions, using probabilistic assignment of points to clusters to capture overlapping or non-spherical group structures more flexibly than K-Means.

In [28]:
```
for k in [2, 3, 4, 5, 6]:
    # Fit the model
    model_name = f'Gaussian Mixture Model Clustering for {k} Clusters'
    gmm_model = GaussianMixture(n_components=k, covariance_type='full', random_state=10)
    gmm_model.fit(X_transform)
    labels = gmm_model.predict(X_transform)

    # Plot the results
    centers = gmm_model.means_
    results_plot(X_transform, labels, model_name, centers=centers)

    # Add the model performace metrics to the results list
    clustering_metrics = evaluate(X_transform, labels, y_true)
    clustering_metrics.update({'Model': model_name})
    results.append(clustering_metrics)
```

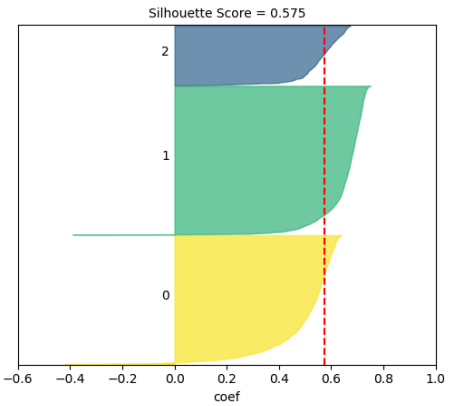
Gaussian Mixture Model Clustering for 2 Clusters

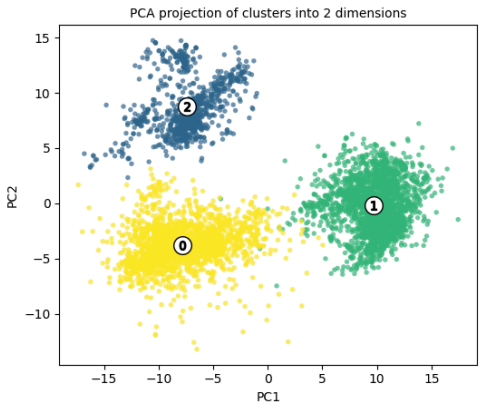


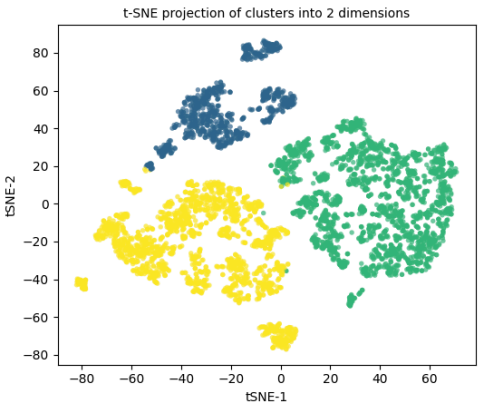




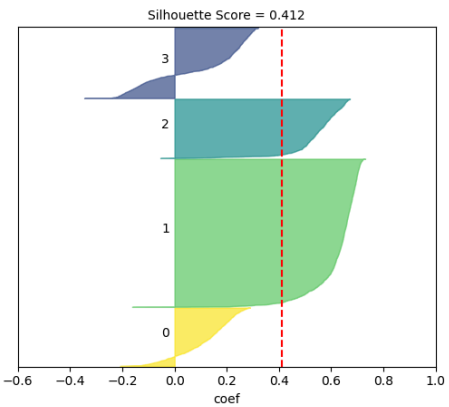
Gaussian Mixture Model Clustering for 3 Clusters

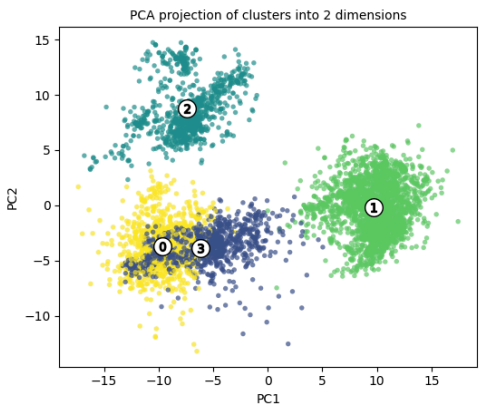


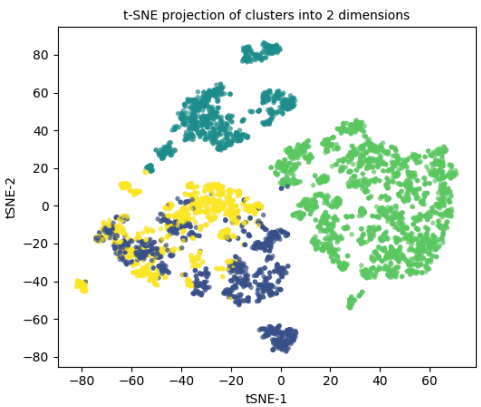




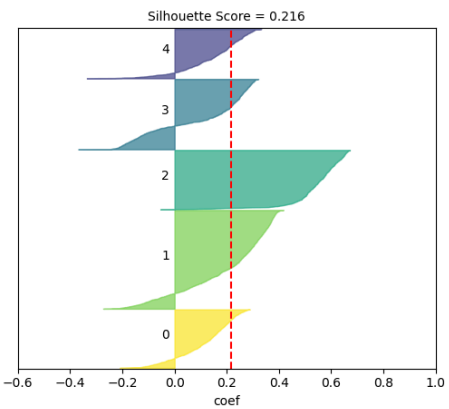
Gaussian Mixture Model Clustering for 4 Clusters

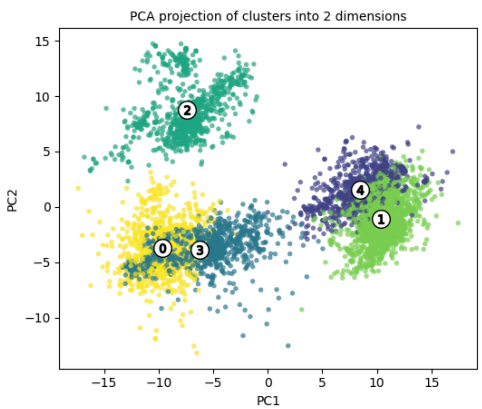


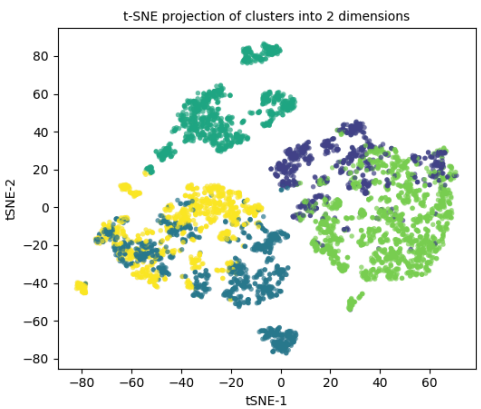




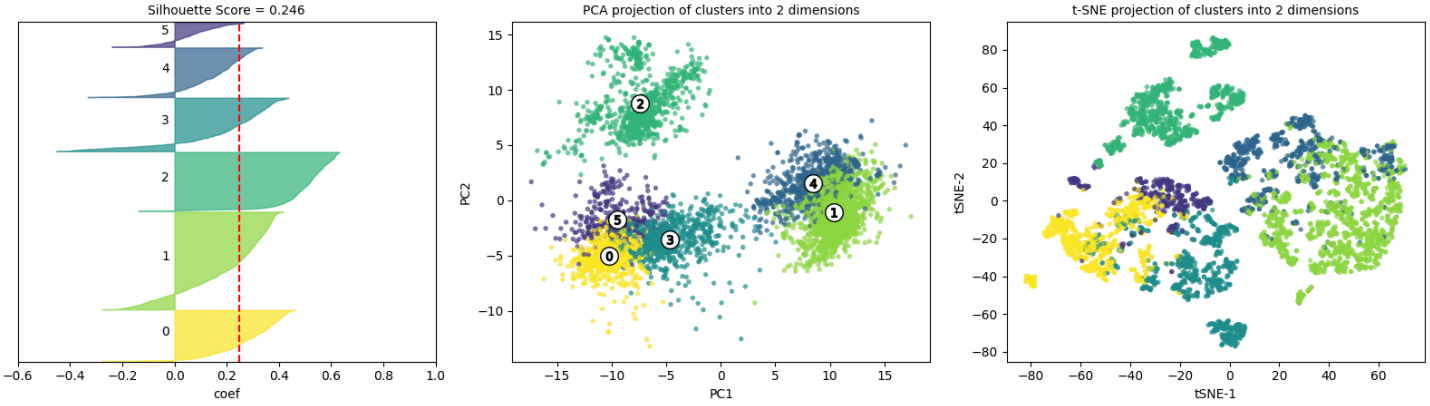
Gaussian Mixture Model Clustering for 5 Clusters







Gaussian Mixture Model Clustering for 6 Clusters



> The Gaussian Mixture Model results closely mirror K-Means and Agglomerative outcomes, with the most coherent separation appearing at 3 clusters (silhouette = 0.575). At 2 clusters, the model forms two dominant groups, while at 3 clusters it captures distinct heavy, synthetic, and combined light/medium crude categories—supporting the expected overlap between the sour and sweet light-medium grades. Beyond 3 clusters, performance declines as the algorithm overfits and splits natural groups into smaller, less meaningful segments. Overall, the GMM effectively models the probabilistic overlap among crudes, with 3–4 clusters best reflecting the underlying structure of the dataset.

Performance Evaluation

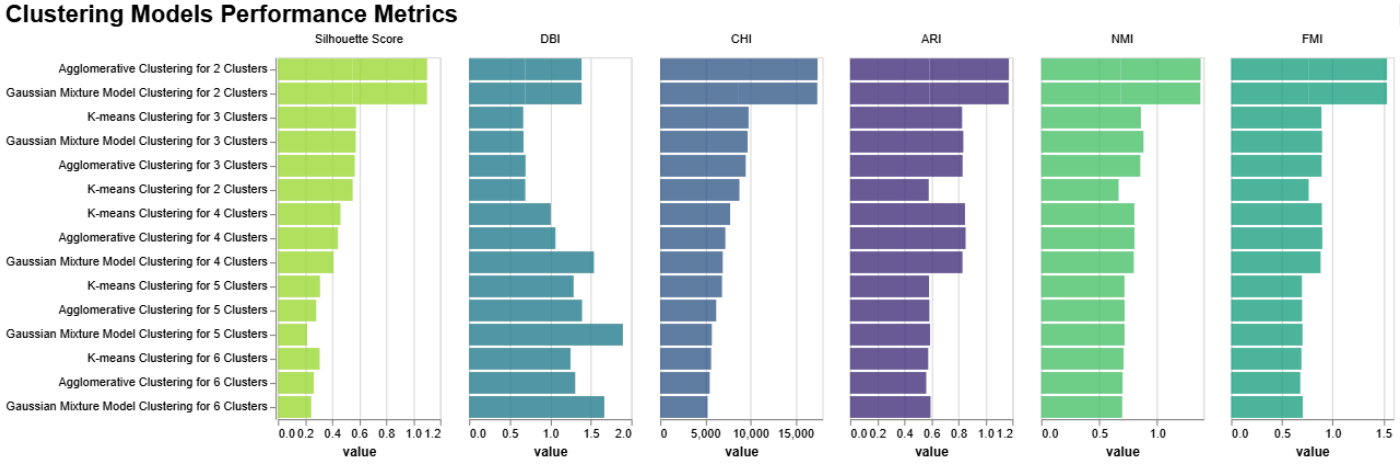
Clustering performance is assessed using **internal** and **external** validation metrics.

- *Internal Metrics* - evaluate the quality of the clusters based solely on the structure of the data, without using any true labels:
  - **Silhouette Score:** Measures how similar each sample is to its own cluster compared to other clusters (higher = better).
  - **Davies–Bouldin Index (DBI):** Average similarity ratio of each cluster to the most similar one (lower = better).
  - **Calinski–Harabasz Index (CHI):** Ratio of between-cluster dispersion to within-cluster dispersion (higher = better).
- *External Metrics* - compare the clustering results to known ground truth labels to measure how well the clusters align with the actual classes:
  - **Adjusted Rand Index (ARI):** Quantifies agreement between predicted clusters and true labels, adjusted for chance.
  - **Normalized Mutual Information (NMI):** Measures the amount of shared information between cluster assignments and true labels.
  - **Fowlkes–Mallows Index (FMI):** Geometric mean of precision and recall between predicted clusters and true labels.

In [105…

```
# Create a dataframe from the model results list
results_df = pd.DataFrame(results)[['Model', 'n_clusters', 'Silhouette Score', 'DBI', 'CHI', 'ARI', 'NMI', 'FMI']]

# Plot performance of models
alt.Chart(results_df, title=alt.Title('Clustering Models Performance Metrics', fontSize=20)).transform_fold(
    ['Silhouette Score', 'DBI', 'CHI', 'ARI', 'NMI', 'FMI']
).mark_bar(opacity=0.8).encode(
    alt.X('value:Q'),
    alt.Y('Model:N').title(None).sort('-x').axis(labelLimit=500),
    alt.Facet('key:N').sort(['Silhouette Score', 'DBI', 'CHI', 'ARI', 'NMI', 'FMI']).title(None),
    alt.Color('key:N').legend(None).scale(scheme='viridis')
).resolve_axis(
    x='independent',
    y='shared'
).resolve_scale(
    x='independent',
    y='shared'
).properties(width=135)
```

Out[105…



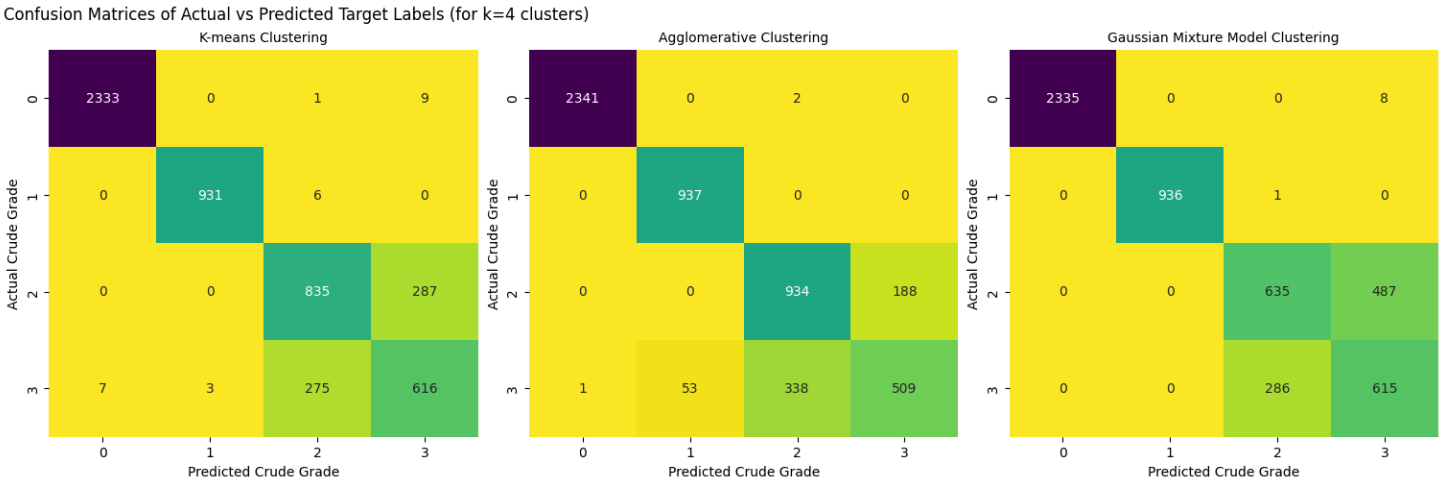
> Across all clustering models, the best overall performance occurs at 3 clusters, where the Gaussian Mixture Model and Agglomerative Clustering both achieve the highest Silhouette, ARI, NMI, and FMI scores while maintaining low DBI values. K-Means performs comparably but shows slightly less separation between clusters. As the number of

> clusters increases beyond three, all models show reduced cohesion and weaker external validation scores. Based on the combined internal and external metrics, the Gaussian Mixture Model with 3 clusters provides the best balance of cluster compactness, separation, and alignment with the true crude oil groupings.

Classification Confusion Matrices

- A set of confusion matrices are used to compare the clustering model performance wehen compared to actual crude grade labels for 4 clusters

In [99]:
```
def fit_and_align(model, X, y_true):
    # Fit and predict
    le = LabelEncoder()
    y_int = le.fit_transform(np.asarray(y_true))
    class_names = le.classes_
    if isinstance(model, GaussianMixture):
        model.fit(X)
        z = model.predict(X)
    else:
        z = model.fit_predict(X)

    # Create contingency matrix
    C = contingency_matrix(y_true, z)
    r_ind, c_ind = linear_sum_assignment(C.max() - C)
    mapping = {c: r for r, c in zip(r_ind, c_ind)}
    z_map = np.vectorize(lambda k: mapping.get(k, k))(z)

    # Confusion table
    df_cm = pd.crosstab(pd.Series(le.inverse_transform(y_true), name='Actual'),
                        pd.Series(le.inverse_transform(z_map), name='Predicted'),
                        rownames=['Actual'],
                        colnames=['Predicted'])
    return df_cm

# Run model for k=4
models_4 = {
    'K-means Clustering': MiniBatchKMeans(n_clusters=4, batch_size=256*14, random_state=10),
    'Agglomerative Clustering': AgglomerativeClustering(n_clusters=4, linkage='ward'),
    'Gaussian Mixture Model Clustering': GaussianMixture(n_components=4, covariance_type='full', random_state=10),
}

# build heatmaps
fig, axes = plt.subplots(1, 3, figsize=(15, 5), constrained_layout=True)

for ax, (name, mdl) in zip(axes, models_4.items()):
    cm_df = fit_and_align(mdl, X_transform, y_true)
    sns.heatmap(cm_df, annot=True, fmt='d', cmap='viridis_r', cbar=False, ax=ax)
    ax.set_title(f'{name}', fontdict={'fontsize':10})
    ax.set_xlabel('Predicted Crude Grade')
    ax.set_ylabel('Actual Crude Grade')

plt.suptitle('Confusion Matrices of Actual vs Predicted Target Labels (for k=4 clusters)', horizontalalignment='left', x=0)
plt.show()
```

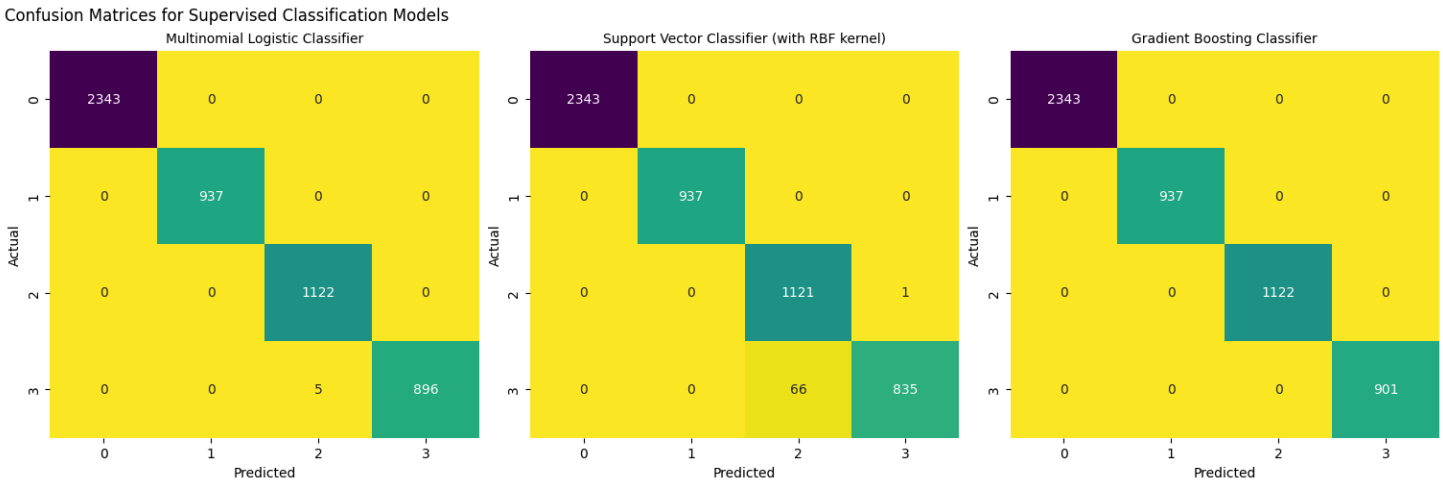


> All three models—K-Means, Agglomerative, and Gaussian Mixture—accurately identify the Heavy Sour and Sweet Synthetic crude groups but consistently confuse the Light & Medium Sweet and Light & Medium Sour categories. This overlap appears in each confusion matrix as significant cross-prediction between the 2nd and 3rd targets, indicating that these two groups share similar chemical and distillation characteristics. The consistent misclassification across models reinforces the earlier observation that the light and medium sour/sweet grades are closely related and may represent a single broader class rather than two distinct ones.

Compare to Supervised Classification Models

In [102…
```
# Define supervised model types
supervised_models = {
    'Multinomial Logistic Classifier': LogisticRegressionCV(solver='lbfgs', penalty='l2', cv=5, max_iter=5000, n_jobs=-1, random_state=10),
    'Support Vector Classifier (with RBF kernel)': SVC(kernel='rbf', gamma='scale', C=1.0, random_state=10),
    'Gradient Boosting Classifier': HistGradientBoostingClassifier(random_state=10)
```

```
}

# Fit and predict models
le = LabelEncoder()
y_int = le.fit_transform(np.asarray(y_true))
class_names = le.classes_
confusion_dict = {}
for model_name, supervised_model in supervised_models.items():
    supervised_model.fit(X_transform, y_true)
    y_pred = supervised_model.predict(X_transform)
    confusion_mat = confusion_matrix(y_true, y_pred, labels=np.arange(len(class_names)))
    confusion_dict[model_name] = pd.DataFrame(confusion_mat, index=class_names, columns=class_names)

# Plot confusion matrices
fig, axes = plt.subplots(1, 3, figsize=(15, 5), constrained_layout=True)
for ax, (model_name, confusion_df) in zip(axes, confusion_dict.items()):
    sns.heatmap(confusion_df, annot=True, fmt='d', cmap='viridis_r', cbar=False, ax=ax)
    ax.set_title(model_name, fontsize=10)
    ax.set_xlabel('Predicted'); ax.set_ylabel('Actual')

plt.suptitle('Confusion Matrices for Supervised Classification Models', x=0, ha='left')
plt.show()
```



> All three supervised models—**Multinomial Logistic Regression**, **Support Vector Classifier (RBF kernel)**, and **Gradient Boosting Classifier**—achieve near-perfect classification, cleanly separating all four crude groups with minimal or no misclassification. This contrasts sharply with the unsupervised models, which consistently confused the Light & Medium Sweet and Light & Medium Sour categories. The key difference is that supervised models are trained with explicit label guidance, allowing them to learn subtle, high-dimensional boundaries between similar classes that unsupervised models cannot infer on their own. However, this also highlights an advantage of unsupervised learning: its ability to reveal natural similarities—in this case, the close relationship between the two light/medium crude groups—which may indicate that the labeled classes are less distinct in practice than defined.

Modeling - Conclusions/Discussions/Next Steps:

- The modeling results confirmed the initial hypothesis that the dataset naturally forms three to four meaningful clusters, supporting the idea that the Light & Medium Sweet and Light & Medium Sour crude groups are closely related and may belong to a single broader category.
- Among the clustering methods, **the Gaussian Mixture Model with three clusters** achieved the strongest overall performance across both internal and external validation metrics. In contrast, the supervised models accurately classified all four target classes, demonstrating that labeled data can separate even highly similar crude types.
- The next step in the analysis will be to present the final discussion and conclusions, summarizing key insights, comparing supervised and unsupervised performance, and outlining the broader implications of these findings for crude quality classification.

Discussion & Conclusion

Learning and Takeaways

This project demonstrated how unsupervised learning techniques can uncover meaningful structure in high-dimensional industrial datasets, even without labeled outcomes. By integrating clustering, dimensionality reduction, and supervised benchmarking, the analysis showed that Canadian crude oil grades can be grouped effectively by chemical and physical properties. The results confirmed that the four labeled crude categories largely align with the natural data patterns, though the **Light & Medium Sweet** and **Light & Medium Sour** groups exhibit strong overlap, suggesting their compositional boundaries are more fluid than categorical. The project also reinforced the importance of robust preprocessing—handling missing data, scaling, and feature selection—before model training, as these steps significantly influence model interpretability and performance.

Why Something Didn't Work

Unsupervised models struggled to distinguish between the **Light & Medium Sweet** and **Light & Medium Sour** groups, which repeatedly appeared blended in the clustering outputs. This limitation stems from the inherent similarity of their feature distributions, where overlapping density, API gravity, and distillation temperature characteristics reduced cluster separability. The models, lacking label information, were unable to infer the subtle chemical differences that supervised methods later captured. Additionally, incomplete or uneven data coverage across certain features—such as Sediment, Total Acid Number, and gas composition columns—likely weakened the clustering accuracy by introducing noise and bias into the feature space.

Suggestions for Improvement

Future work could enhance model precision by incorporating **domain-informed feature engineering**, such as grouping variables into process-relevant ratios (e.g., sulfur-to-density or distillation slope metrics). Expanding the dataset with additional time periods or refinery assay data could also improve model generalization and balance across crude grades. Applying **semi-supervised learning** or **latent variable models** may bridge the gap between unsupervised discovery and supervised precision, allowing the model to leverage known class structures while maintaining flexibility. Finally, visual analytics dashboards or interactive tools could make the clustering insights more accessible to engineers and decision-makers, translating technical findings into actionable refinery and marketing strategies.
