NMR Inversion Recovery Analysis in Python

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Objective

In this notebook, we will learn the basics of working with scientific data in Python, focusing on an NMR inversion recovery experiment. We will import experimental data into a Pandas DataFrame, calculate the T_1 relaxation times and ideal an ideal d_1 delay time, and visualize the fitted data.

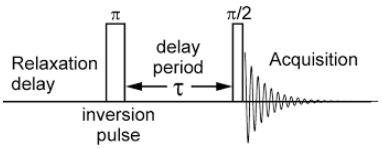
Inversion recovery experiment

The inversion-recovery experiment measures T1 relaxation times of any nucleus. If the net magnetization is placed along the -z axis, it will gradually return to its equilibrium position along the +z axis at a rate governed by T1. The equation governing this behavior as a function of the time t after its displacement is:

$M_z(t) = M_{z,\,eq} * (1 - 2\,e^{-t/T_1})$

The basic pulse sequence consists of an 180° pulse that inverts the magnetization to the -z axis. During the following delay, relaxation along the longitudinal plane takes place. Magnetization comes back to the original equilibrium z-magnetization. A 90° pulse creates transverse magnetization. The experiment is repeated for a series of delay values taken from a variable delay list. A 1D spectrum is obtained for each value of vd and stored in a pseudo 2D dataset. The longer the relaxation delay (d_1) is, the more precise the T_1 measurement is. An ideal relaxation time (d_1) can be calculated (aq = acquisition time):

$d_1 + aq = 5 * T_1$



More information: https://imserc.northwestern.edu/downloads/nmr-t1.pdf

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1. Importing Required Libraries

First, let's import the python libraries/packages we need to work with the data.

In [ ]:
```
import pandas as pd
import numpy as np
from scipy.optimize import curve_fit
import matplotlib.pyplot as plt
import re
import os

# Enable inline plotting
%matplotlib inline

# Set DataFrame precision to 3 decimal places
pd.set_option("display.precision", 3)
```

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2. Importing the Data

We will now import the NMR inversion recovery data from a CSV file to a Pandas Dataframe (the excel of Python).

The data file `Ibuprofen-C13-invrec-data.csv` contains columns:

Time	Peak<#>
Time of scan (s)	Signal for each carbon peak in ibuprofen

Pro Tip: In computer languages you always start counting at 0 so the first peak in our dataset is labeled `Peak0`.

In [ ]:
```
# Load the data from the CSV file
df = pd.read_csv('data/Ibuprofen-C13-invrec-data-mnova.csv', header=1)

# Formats MNOVA csv input and renames columns to peak chemical shift (ppm)
def rename_columns(df : pd.DataFrame):
    # Rename first column to time
    df = df.dropna(axis=1)
    df = df.drop([col for col in df.columns if "'" in col], axis=1)
    df = df.drop([col for col in df.columns if "#" in col], axis=1)
    df = df.rename(columns={'X(I)': 'Time'})


    # Regular expression to match "Integral(float1, float2)"
    pattern = r'Integral\((\d+\.\d+),(\d+\.\d+)\)'

    # Iterate over each column
    for col in df.columns:
        first_row_value = str(df[col].iloc[0])

        # Use regex to find the two float numbers in the string
```

```
        match = re.match(pattern, first_row_value)
        if match:
            float1 = float(match.group(1))
            float2 = float(match.group(2))
            # Calculate the median of the two floats
            median_value = round((float1 + float2) / 2, 1)
            # Rename the column
            df = df.rename(columns={col: f'{median_value}_ppm'})
    if any(index == 0 for index in df.index):
        df = df.drop(index=0, axis=0)
    df = df.astype(float)
    if '79.3_ppm' in df.columns:
        df = df.drop('79.3_ppm', axis=1)

    return df
df = rename_columns(df)

# Display the dataframe to understand its structure
df
```

Out[ ]:

	Time	183.7_ppm	143.4_ppm	139.3_ppm	132.3_ppm	130.3_ppm	47.5_ppm	24.9_ppm
1	0.062	-4684.675	-5499.795	-5036.193	-6258.796	-5560.295	-1331.859	-2792.253
2	0.125	-3658.109	-6311.520	-5046.871	-5070.044	-5501.243	-2232.157	-718.401
3	0.250	-3931.386	-4594.111	-6585.526	-4965.123	-4204.978	-4227.647	-2714.234
4	0.500	-3852.770	-3103.076	-4563.785	-3098.568	-3719.214	-2123.349	-399.047
5	1.000	-4292.297	-3898.902	-6335.422	-3270.550	-2361.015	600.839	234.864
6	2.000	-6274.636	-458.690	-4315.249	267.014	1098.219	2348.319	2742.474
7	4.000	-3083.688	632.667	-3011.320	2682.380	1102.794	4361.105	1551.448
8	8.000	-1456.791	339.541	1444.355	4345.313	3865.516	3288.270	1518.069
9	16.000	-1819.283	791.616	1181.459	4085.027	5653.630	3659.424	1841.427

---

3. Visualizing the Data

Let's create a function using MatPlotLib to visualize the raw data for all peaks.

Function : a module of code that is not run until called by subsequent code.

1. Define a function:

```
def <function_name>(arguments):
    <function_code>
```

2. Run a function:

```
<function_name>(arguments)
```

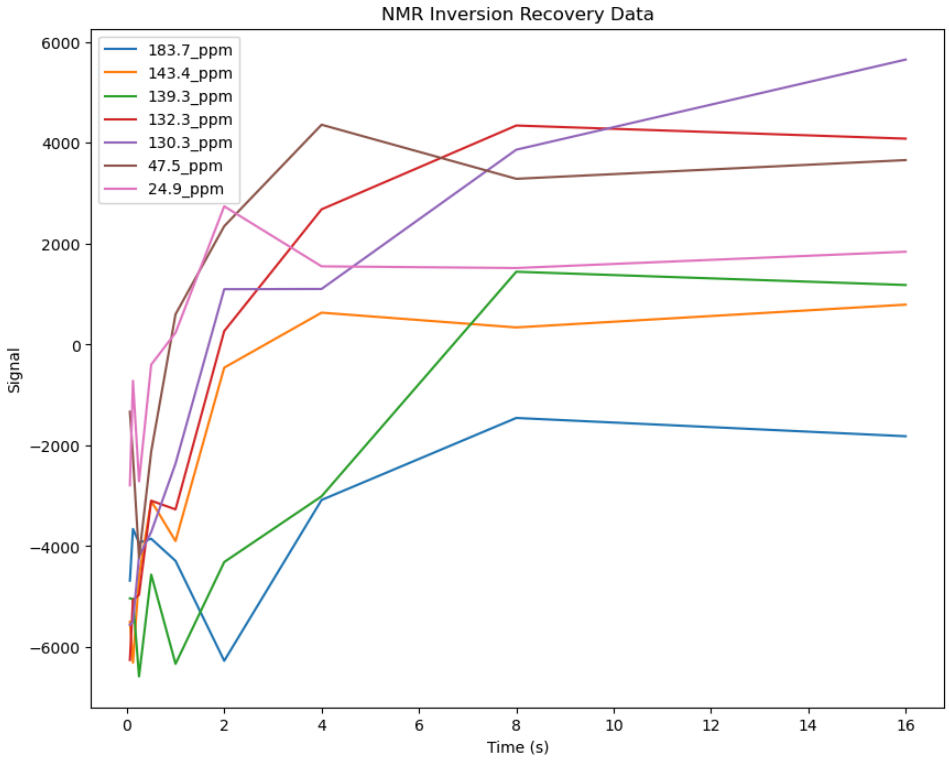
In [ ]:

```
def plot_nmr_data(df : pd.DataFrame):
    plt.figure(figsize=(10, 8))

    for column in df.columns:
        if column != 'Time':
            plt.plot(df['Time'], df[column], label=column)

    plt.xlabel('Time (s)')
    plt.ylabel('Signal')
    plt.title('NMR Inversion Recovery Data')
    plt.legend()
    plt.show()

# Visualize the data
plot_nmr_data(df)
```



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4. Calculating T1 Relaxation Time

To calculate the T1 relaxation time for each peak, we will fit the data to the inversion recovery model:

$M_z(t) = M_{z,\,eq} * (1 - 2\,e^{-t/T1}) + C$

In [ ]:
```python
# Function to model the inversion recovery curve
def inversion_recovery(t, M, T1, C):
    return M * (1 - 2 * np.exp(-t / T1)) + C

# Function to calculate T1 relaxation time for a given nucleus
def calculate_T1(df : pd.DataFrame, x_col : str, y_col : str):
    t = df[x_col].values
    y = df[y_col].values

    # Initial guess for A, T1, and C
    initial_guess = [max(y), 1, min(y)]

    # Fit the curve
    popt, _ = curve_fit(inversion_recovery, t, y, p0=initial_guess)

    # Return the fitted parameters and T1 value
    return popt, popt[1]
```

---

5. Visualizing the Fitted Data

Let's create a function to plot the data and the fitted curve.

In [ ]:
```python
def plot_fitted_data(df : pd.DataFrame, x_col : str, y_col : str, popt : numpy.ndarray):
    t = df[x_col].values
    y = df[y_col].values

    plt.figure(figsize=(8, 6))
    plt.scatter(t, y, label=f'{y_col} Data')
    plt.plot(t, inversion_recovery(t, *popt), label=f'Fit: T1 = {popt[1]:.3f} s', color='red')
    plt.xlabel('Time (s)')
    plt.ylabel('Signal')
    plt.title(f'Inversion Recovery Fit for {y_col}')
    plt.legend()
    plt.show()
```

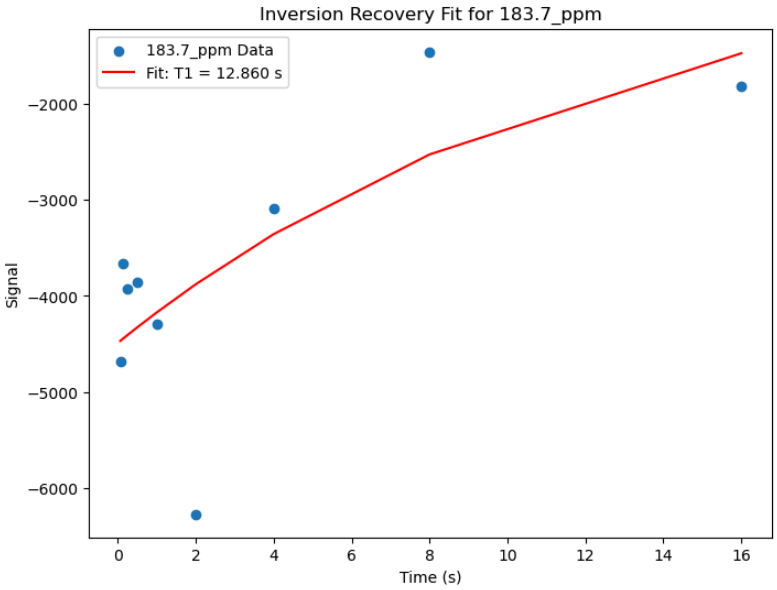
---

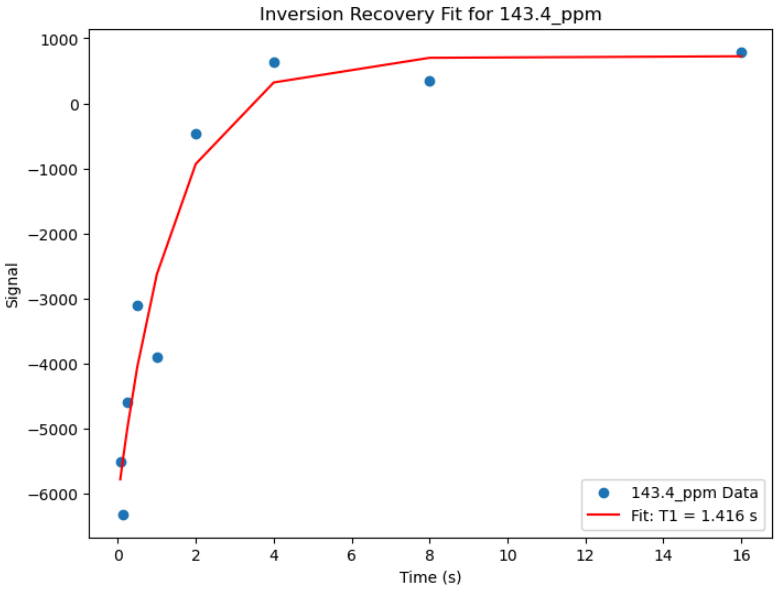
6. Analyzing and Summarizing T1 Times for All Nuclei

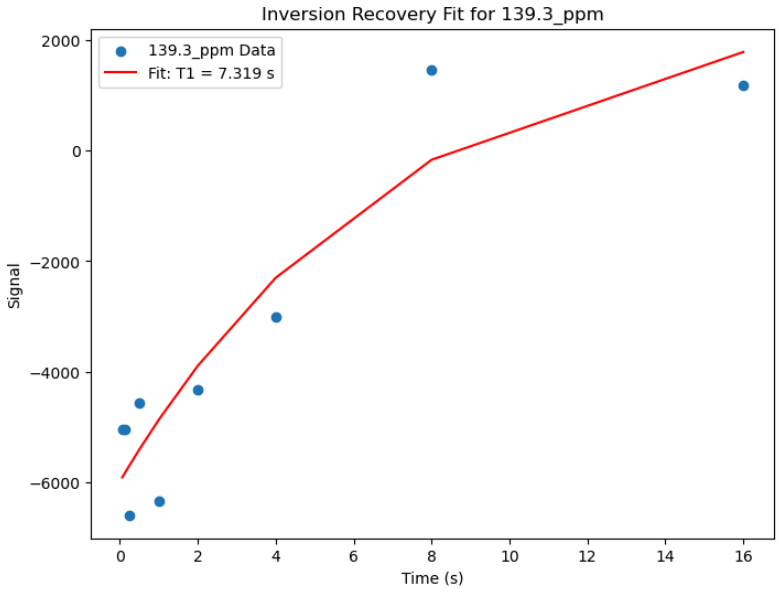
Now, let's use the functions we created to calculate the T1 relaxation time for each nucleus and visualize the fits.

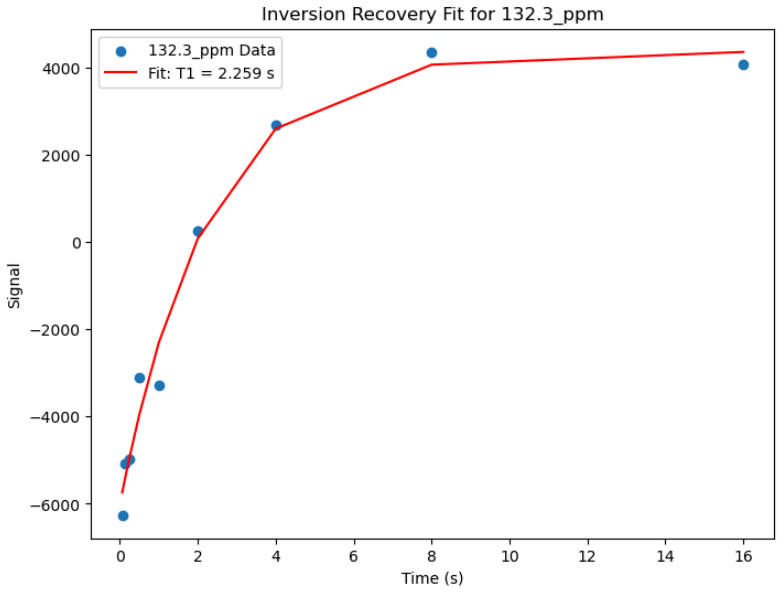
In [ ]:
```python
# Dictionary to store the T1 times
T1_times = {}
```

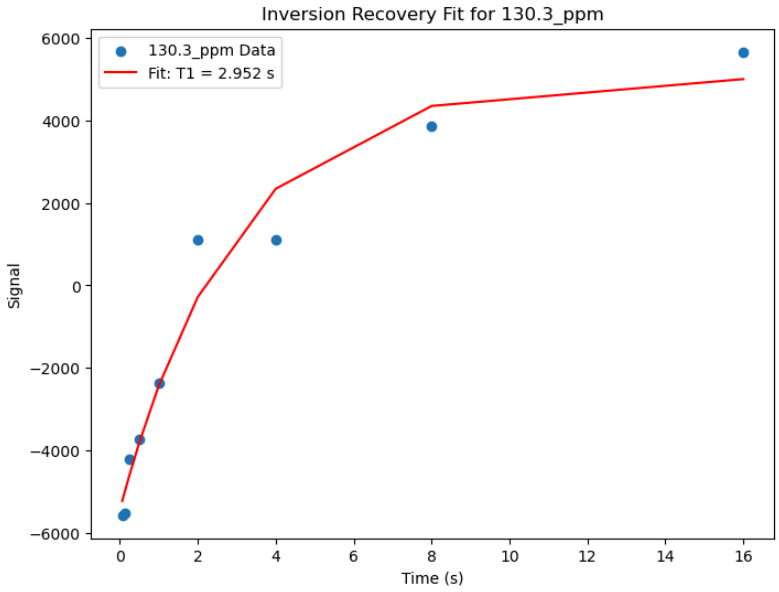
```
# Calculate T1 for each nucleus and plot the fit
for column in df.columns:
    if column != 'Time':
        popt, T1 = calculate_T1(df, 'Time', column)
        T1_times[column] = T1
        plot_fitted_data(df, 'Time', column, popt)

# Create a summary table of T1 times
T1_df = pd.DataFrame(list(T1_times.items()), columns=['Peak', 'T1_Time'])
T1_df
```

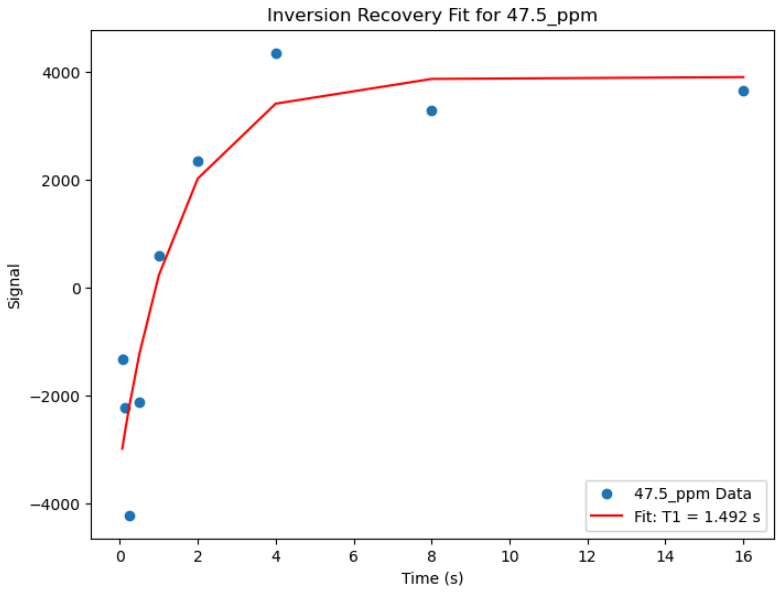


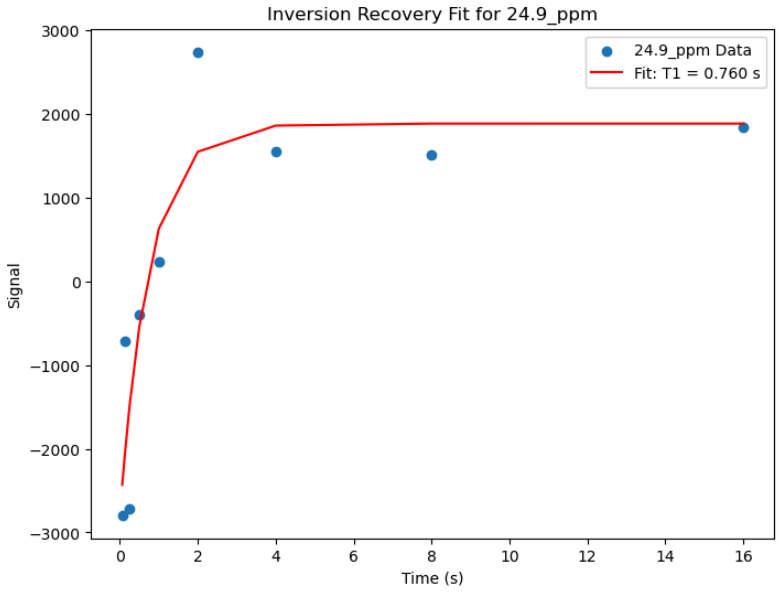



Inversion Recovery Fit for 139.3_ppm
139.3_ppm Data
Fit: T1 = 7.319 s
Signal
Time (s)


Inversion Recovery Fit for 132.3_ppm
132.3_ppm Data
Fit: T1 = 2.259 s
Signal
Time (s)


Inversion Recovery Fit for 130.3_ppm
130.3_ppm Data
Fit: T1 = 2.952 s
Signal
Time (s)





Out[ ]:

	Peak	T1_Time
0	183.7_ppm	12.860
1	143.4_ppm	1.416
2	139.3_ppm	7.319
3	132.3_ppm	2.259
4	130.3_ppm	2.952
5	47.5_ppm	1.492
6	24.9_ppm	0.760

---

7. Calculate an ideal delay time (d_1)

Now, let's calculate an ideal delay time (d_1) for future NMR experiments on ibuprofen based on the (T_1) times we measured.

$d_1 + aq = 5 * T_1$

aq = acquisition time = 1.3 seconds for ibuprofen

Relaxation time (d_1) can not be shorter than 0 seconds:

- if $d_1 > 0$ seconds:

  $d_1 = (5 * T_1) - aq$

- else:

  $d_1 = 0$ seconds

In [ ]:
```python
# Define the conditional logic for calculating the relaxation time (d1)
def calculate_d1_time(t1_time : float, aq : float):
    d1 = 5 * t1_time - aq
    if d1 > 0:
        return d1
    else:
        return 0

T1_df['D1_Time'] = T1_df['T1_Time'].apply(calculate_d1_time, aq=1.3)

# Find the largest D1
max_d1 = T1_df['D1_Time'].max()

# Round d1 time to nearest second
max_d1 = round(max_d1)

# Print the ideal d1 time using an f-string
print(f'Ideal d1 time: {max_d1} (s)')
T1_df
```

```
Ideal d1 time: 63 (s)
```

Out[ ]:

	Peak	T1_Time	D1_Time
0	183.7_ppm	12.860	63.001
1	143.4_ppm	1.416	5.779
2	139.3_ppm	7.319	35.293
3	132.3_ppm	2.259	9.995
4	130.3_ppm	2.952	13.458
5	47.5_ppm	1.492	6.161
6	24.9_ppm	0.760	2.499

---

8. Export results

We can save the T_1 and d_1 values we calculated by exporting our summary DataFrame as a .csv file.

You can open the .csv file in excel.

In [ ]:
```python
# Define output directory
directory = 'results'

# Make sure the parent directory exists
if not os.path.isdir(directory):
    os.makedirs(directory)

# Export DataFrame to a .csv file
T1_df.to_csv(f'{directory}/ibprofen_t1_d1_summary.csv')
```