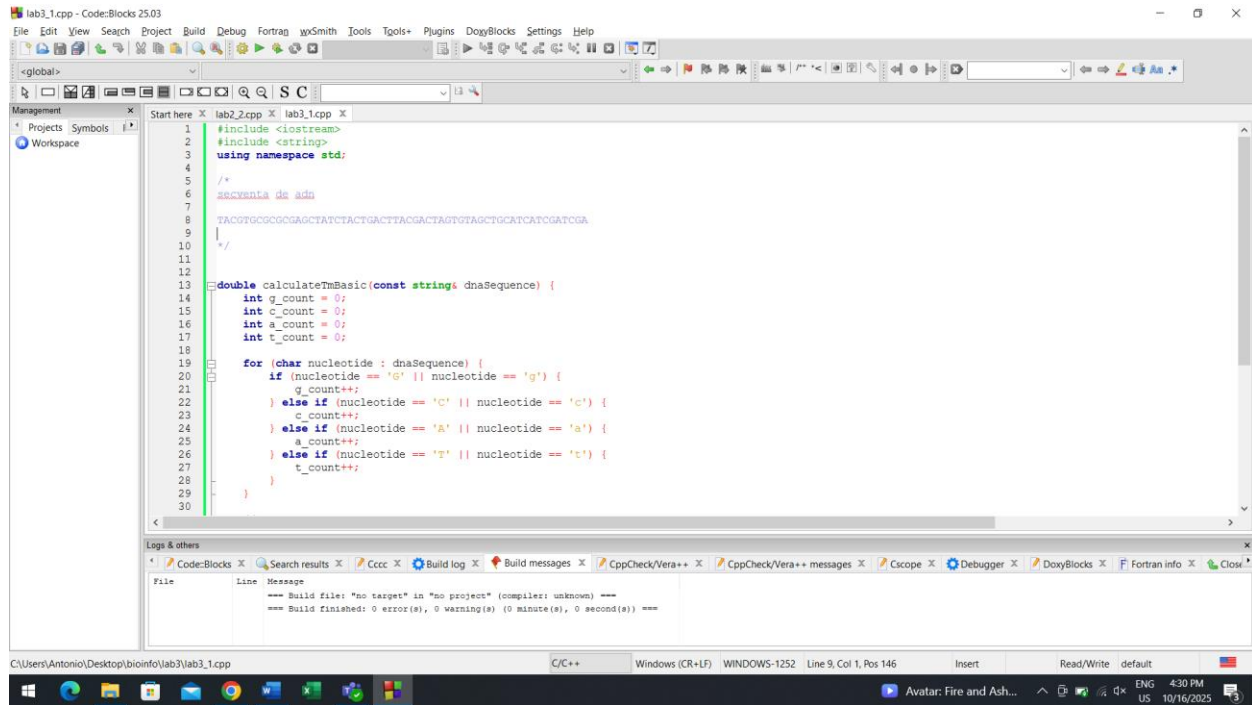


LABORATORY REPORT #3

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Bioinformatics, 4th year 1st semester, 2025-2026

lab3_1.cpp

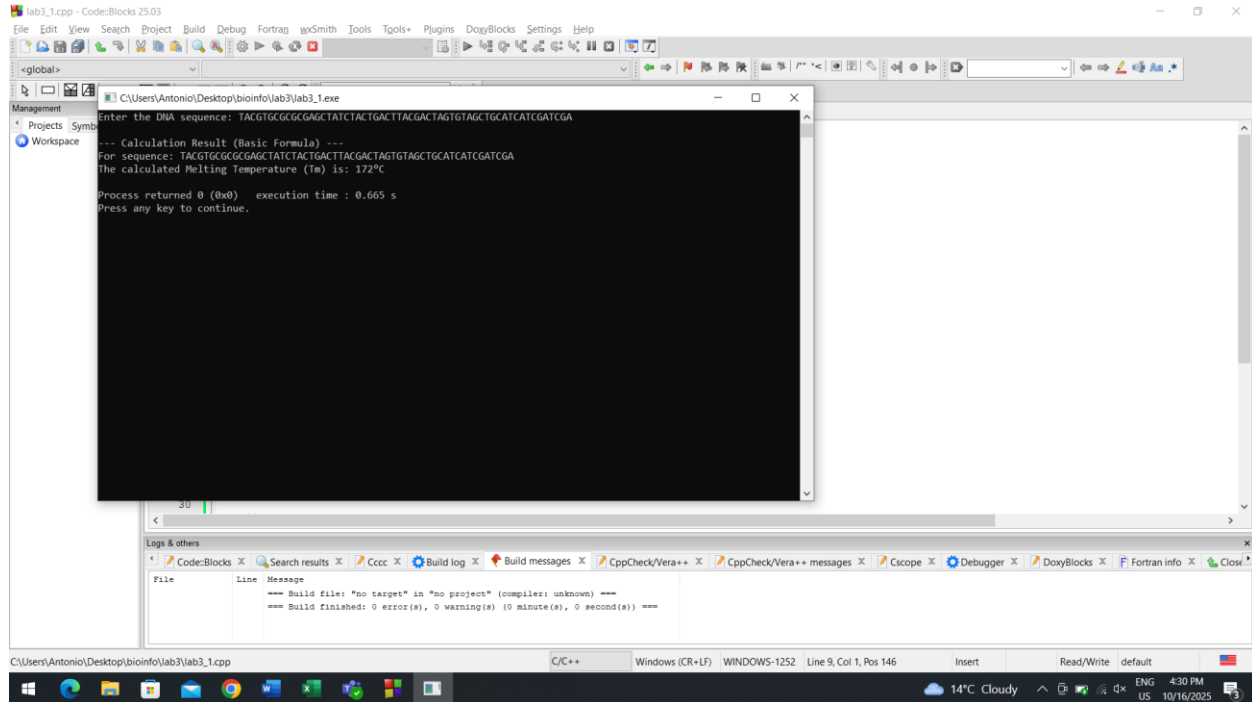


```
1 #include <iostream>
2 #include <string>
3 using namespace std;
4
5 /*
6  serventa de adn
7
8  TACGTGCGCGGAGCTATCTACTGACTTAAGACTAGTGTAGCTGCATCATCGATCGA
9
10 */
11
12
13 double calculateTmBasic(const string& dnaSequence) {
14     int g_count = 0;
15     int c_count = 0;
16     int a_count = 0;
17     int t_count = 0;
18
19     for (char nucleotide : dnaSequence) {
20         if (nucleotide == 'G' || nucleotide == 'g') {
21             g_count++;
22         } else if (nucleotide == 'C' || nucleotide == 'c') {
23             c_count++;
24         } else if (nucleotide == 'A' || nucleotide == 'a') {
25             a_count++;
26         } else if (nucleotide == 'T' || nucleotide == 't') {
27             t_count++;
28         }
29     }
30 }
```

Build file: "no target" in "no project" (compiler: unknown) ---
Build finished: 0 error(s), 0 warning(s) (0 minute(s), 0 second(s)) ---

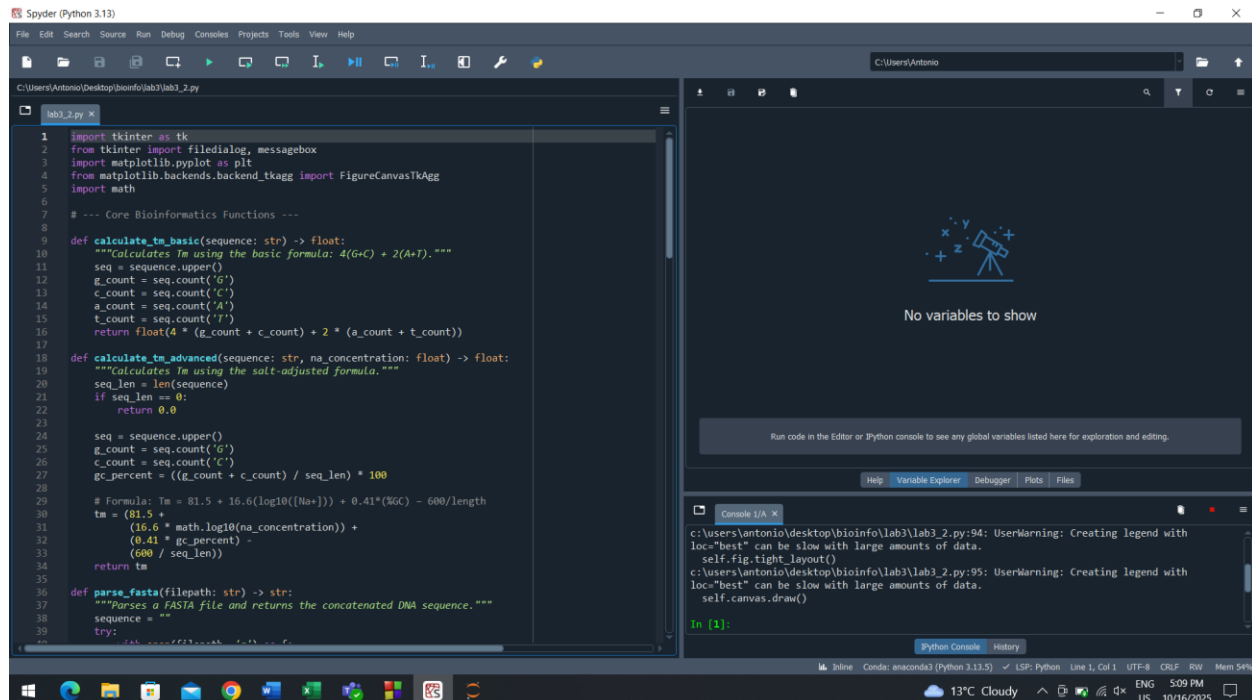
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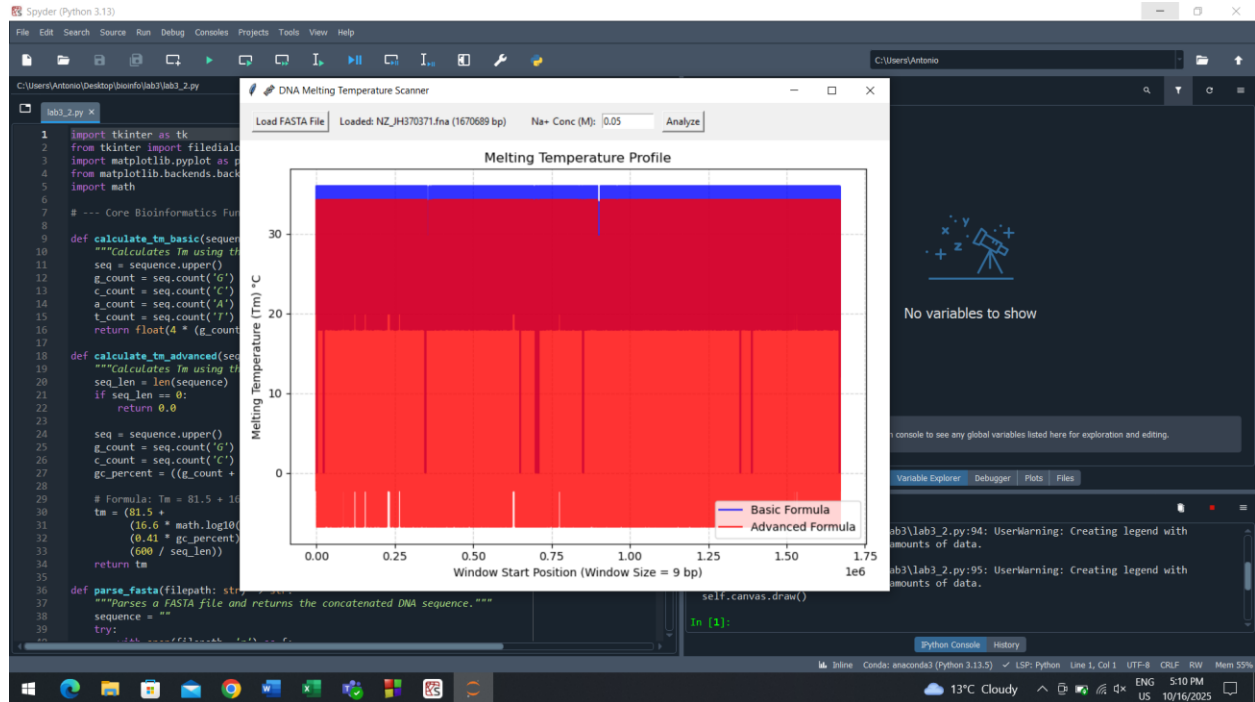
```
lab3_1.cpp - Code::Blocks 25.03
File Edit View Search Project Build Debug Fortran g++Smith Tools Tools+ Plugins DoxyBlocks Settings Help
<global>
C:\Users\Antonio\Desktop\bioinfo\lab3\lab3_1.exe
Enter the DNA sequence: TACGTGGCGCGAGCTATCTACTGACTTACGACTAGTGTAGCTGCATCATCGATCGA
--- Calculation Result (Basic Formula) ---
For sequence: TACGTGGCGCGAGCTATCTACTGACTTACGACTAGTGTAGCTGCATCATCGATCGA
The calculated Melting Temperature (Tm) is: 172°C
Process returned 0 (0x0)   execution time : 0.605 s
Press any key to continue.
Logs & others
Code::Blocks X Search results X Cccc X Build log X Build messages X CppCheck/Ver++ X CppCheck/Ver++ messages X Cscope X Debugger X DoxyBlocks X Fortran info X Close
File Line Message
--- Build file: "no target" in "no project" (compiler: unknown) ---
--- Build finished: 0 error(s), 0 warning(s) (0 minute(s), 0 second(s)) ---
C:\Users\Antonio\Desktop\bioinfo\lab3\lab3_1.cpp C/C++ Windows-CR+LF WINDOWS-1252 Line 9, Col 1, Pos 146 Insert Read/Write default ENG 4:30 PM 10/16/2025
```

lab3_2.py



```
Spyder (Python 3.13)
File Edit Search Source Run Debug Consoles Projects Tools View Help
C:\Users\Antonio\Desktop\bioinfo\lab3\lab3_2.py
lab3_2.py
1 import tkinter as tk
2 from tkinter import filedialog, messagebox
3 import matplotlib.pyplot as plt
4 from matplotlib.backends.backend_tkagg import FigureCanvasTkAgg
5 import math
6
7 # --- Core Bioinformatics Functions ---
8
9 def calculate_tm_basic(sequence: str) -> float:
10     """Calculates Tm using the basic formula: 4(G+C) + 2(A+T)."""
11     seq = sequence.upper()
12     g_count = seq.count('G')
13     c_count = seq.count('C')
14     a_count = seq.count('A')
15     t_count = seq.count('T')
16     return float(4 * (g_count + c_count) + 2 * (a_count + t_count))
17
18 def calculate_tm_advanced(sequence: str, na_concentration: float) -> float:
19     """Calculates Tm using the salt-adjusted formula."""
20     seq_len = len(sequence)
21     if seq_len == 0:
22         return 0.0
23     seq = sequence.upper()
24     g_count = seq.count('G')
25     c_count = seq.count('C')
26     gc_percent = ((g_count + c_count) / seq_len) * 100
27
28     # Formula: Tm = 81.5 + 16.6(log10([Na+])) + 0.41*(%GC) - 600/length
29     tm = (81.5 +
30           (16.6 * math.log10(na_concentration)) +
31           (0.41 * gc_percent) -
32           (600 / seq_len))
33     return tm
34
35 def parse_fasta(filepath: str) -> str:
36     """Parses a FASTA file and returns the concatenated DNA sequence."""
37     sequence = ""
38     try:
39         with open(filepath, 'r') as file:
40             for line in file:
41                 if line.startswith('>'):
42                     continue
43                 sequence += line.strip()
44     except FileNotFoundError:
45         messagebox.showerror("File not found", f"File {filepath} does not exist.")
46     return sequence
47
48 if __name__ == '__main__':
49     # Create a Tkinter window
50     root = tk.Tk()
51     root.title("Lab3_2")
52     root.geometry("400x300")
53
54     # File selection
55     filepath = filedialog.askopenfilename()
56     if not filepath:
57         return
58
59     # Parse FASTA
60     sequence = parse_fasta(filepath)
61
62     # Calculate Tm
63     na_concentration = 0.1
64     tm_basic = calculate_tm_basic(sequence)
65     tm_advanced = calculate_tm_advanced(sequence, na_concentration)
66
67     # Display results
68     result_text = f"Basic Tm: {tm_basic}°C\nAdvanced Tm: {tm_advanced}°C"
69     label = tk.Label(root, text=result_text)
70     label.pack(pady=20)
71
72     # Plot Tm vs GC content
73     gc_percent = ((sequence.count('G') + sequence.count('C')) / len(sequence)) * 100
74     plt.figure(figsize=(10, 5))
75     plt.plot(gc_percent, tm_advanced)
76     plt.title("Tm vs GC content")
77     plt.xlabel("GC content (%)")
78     plt.ylabel("Tm (°C)")
79     canvas = FigureCanvasTkAgg(plt.gcf(), root)
80     canvas.get_tk_widget().pack(pady=20)
81
82     # Run button
83     def run():
84         messagebox.showinfo("Result", result_text)
85
86     button = tk.Button(root, text="Run", command=run)
87     button.pack(pady=10)
88
89     root.mainloop()
90
91 console
92 c:\users\antonio\desktop\bioinfo\lab3\lab3_2.py:94: UserWarning: Creating legend with loc="best" can be slow with large amounts of data.
93   self.fig.tight_layout()
94 c:\users\antonio\desktop\bioinfo\lab3\lab3_2.py:95: UserWarning: Creating legend with loc="best" can be slow with large amounts of data.
95   self.canvas.draw()
96 In [1]:
Python Console History
13°C Cloudy ENG 5:09 PM 10/16/2025
```

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lab3_3.py

