Computer-Based Problem Solving

Breaking Down Research Challenges

What We Did Last Time

You learned the fundamental building blocks:

- **Variables** for storing information
- **Loops** for repeating actions
- **Conditionals** for making decisions
- **Files** for permanent storage
- **Computational thinking** - systematic problem-solving approach

What We're Doing Today

Your mission:
- **Choose one** real drug development problem
- **Work in groups** to solve it together
- **Develop complete pseudocode** solution
- **Think through** all the logical steps and decisions

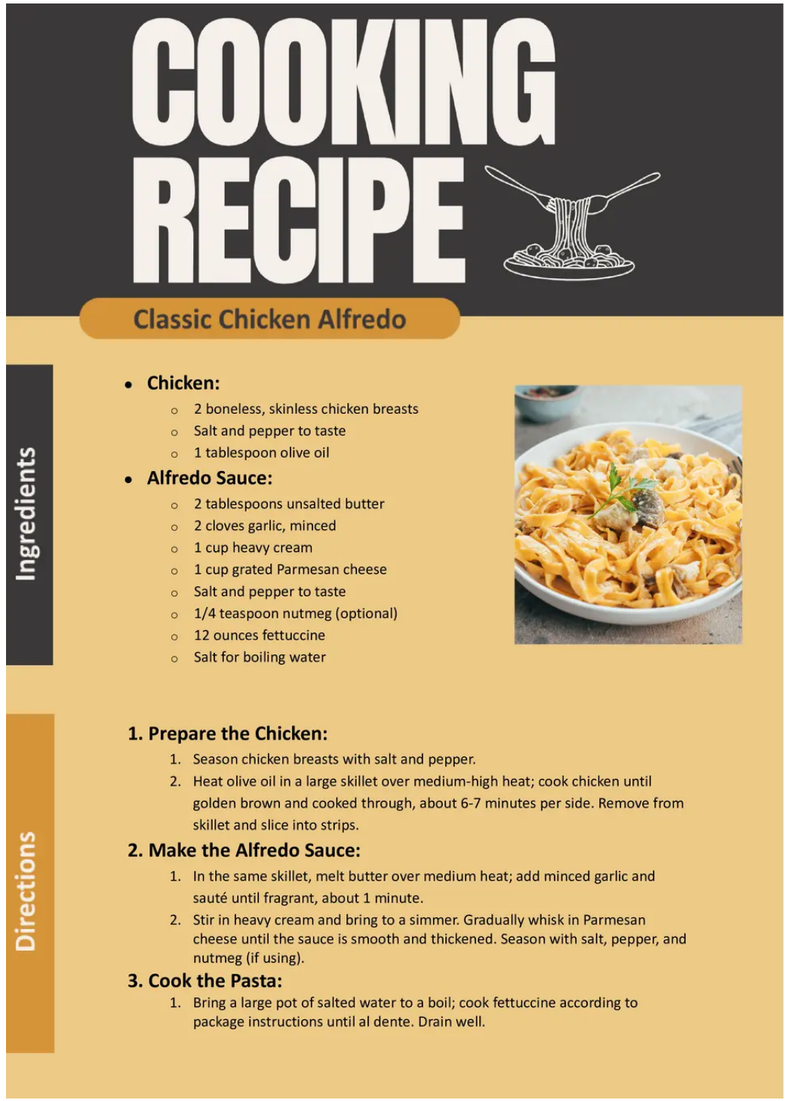
Timeline: You have about **60 minutes** to work on your chosen problem.

Key mindset: Do your best in the time available. This teaches you **time management** and **iterative problem-solving**. Perfect solutions aren't always necessary - focus on the best solution you can develop within the timeframe.

What is Pseudocode?

Pseudocode = Plain English instructions for solving a problem

- Detailed plan using everyday language
- Bridge between your ideas and actual programming code
- Like writing a recipe or instruction manual
- No programming syntax required



Why Pseudocode Matters

Learning progression over 3 weeks:
- **This week:** Develop pseudocode solutions
- **Next week:** Learn Python programming syntax
- **Week after:** Translate your pseudocode into working Python code

Benefit: When you learn Python syntax next week, you'll already know exactly what you want to accomplish.

How to Write Good Pseudocode

Key principles:

1. **Use simple, clear language** - avoid technical jargon
2. **Be specific about steps** - don't just say "process the data"
3. **Include decision points** - IF/THEN logic for different situations
4. **Plan for problems** - what if data is missing or strange?
5. **Specify inputs and outputs** - what files do you read and create?

Pseudocode Example

```
STEP 1: Read the data file
  Open the CSV file with compound data
  Store all the measurements in memory

STEP 2: Check data quality
  FOR each measurement:
    IF the value seems wrong (negative or too high):
      Flag it for review
      Decide whether to keep or exclude it
```

Pseudocode Example

```
STEP 3: Calculate results
  FOR each compound:
    Calculate the average of good measurements
    Determine if compound is active or inactive

STEP 4: Create output
  Write results to a new CSV file
  Create a chart showing active compounds
```

Using AI Tools (ChatGPT, Claude, etc.)

Let's be realistic: You're probably going to use AI tools regardless of what I say.

My approach: I **encourage** you to use them, but use them **strategically**.

Why this makes sense:
- You'll use AI in your professional research career
- Learning to work **with** AI tools effectively is a valuable skill
- Critical evaluation of AI output is more important than generating code from scratch

Requirements for Using AI Tools

If you use ChatGPT, Claude, or similar:

✅ **Document your prompts** - What did you ask the AI?
✅ **Understand every line** - Can you explain each step in your own words?
✅ **Identify potential problems** - What could go wrong with this approach?
✅ **Consider alternatives** - Could you solve this differently?
✅ **Plan for validation** - How would you test if this logic works?

When I visit your group, I'll ask you to explain the logic, not just show me the pseudocode.

Computational Thinking Reminder

The Five-Step Approach

1. Understand the Problem

- What exactly are you trying to find out?
- What data do you have available?
- What would success look like?

2. Break It Down (Decomposition)

- What smaller sub-problems can you identify?
- Which parts can be solved independently?
- What's the logical order for solving each piece?

Computational Thinking Reminder

The Five-Step Approach

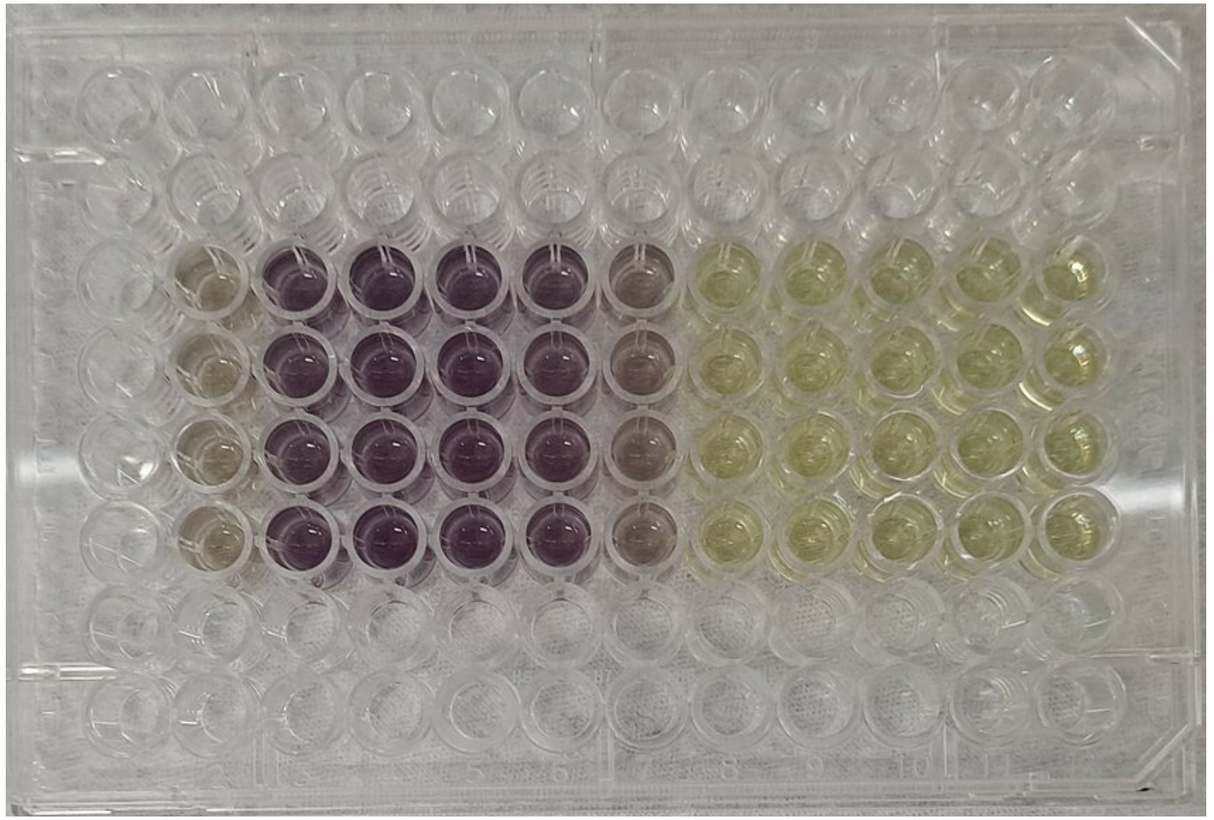
3. Identify Patterns (Pattern Recognition)
- Are there repeated calculations or processes?
- Which steps will need to be applied to multiple data points?

4. Design the Solution (Algorithm Design)
- What sequence of steps will solve each sub-problem?
- What decisions need to be made along the way?

5. Plan the Output (Results and Visualization)
- How will you present your findings?
- What files or reports need to be generated?

Problem A: Cell Viability Screening 🧪

Beginner-Friendly | Data Processing Focus



Research Context:
You're testing 20 potential anti-cancer compounds using an MTT viability assay. Each compound was tested at 5 concentrations in triplicate on HeLa cells.

Your Mission:
- Convert raw absorbance data to viability percentages
- Identify and handle outlier measurements appropriately
- Rank compounds by their cytotoxic potential
- Generate a summary report for follow-up studies

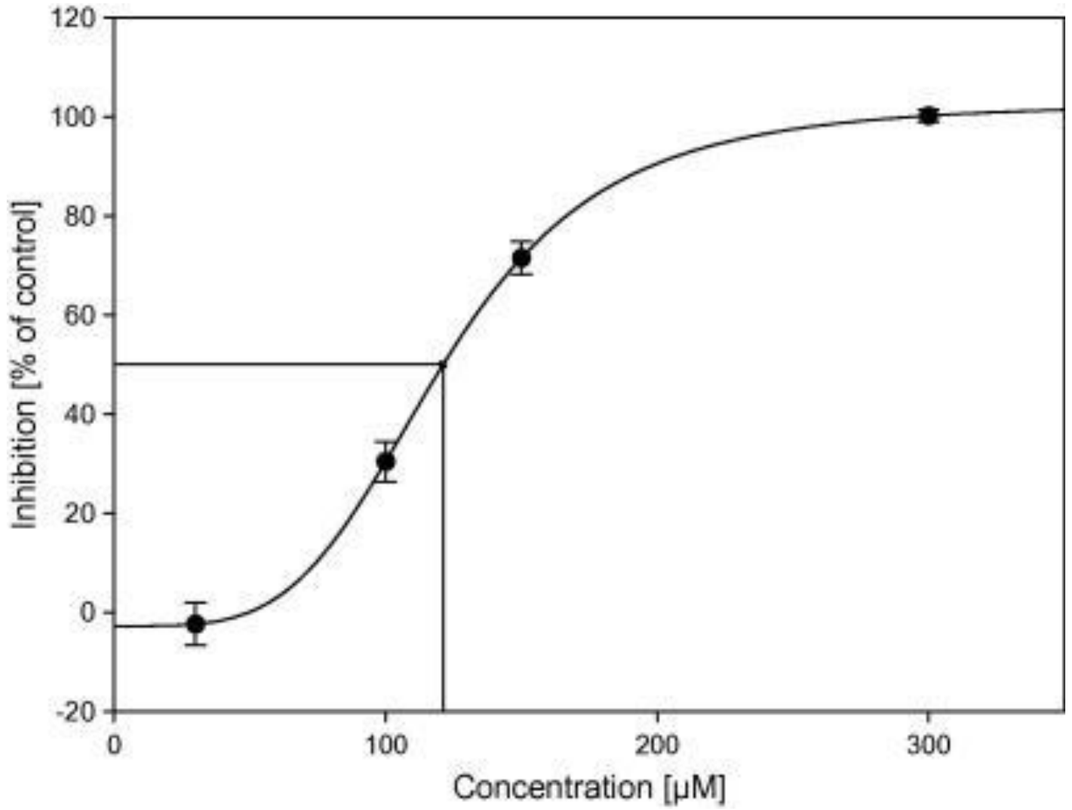
Problem A: Data Details

Available Data File: `viability_raw_data.csv`
- Contains: `compound_name`, `concentration`, `well_position`, `absorbance_reading`, `replicate_number`
- Includes DMSO controls (negative control, ~100% viability)
- Includes Doxorubicin controls (positive control, ~10% viability)
- Some wells may have experimental artifacts

Expected Output:
- Processed data with viability percentages
- List of promising compounds ranked by activity
- Visualizations showing results clearly

Problem B: IC50 Determination 📈

Moderate Challenge | Statistical Analysis Focus



Research Context:
You've selected 15 promising compounds for detailed dose-response analysis. Each compound was tested at 8 concentrations in triplicate to generate full dose-response curves.

Your Mission:
- Analyze dose-response data to estimate IC50 values
- Assess the quality of each dose-response relationship
- Classify compounds by potency ranges
- Identify problematic datasets that need repeat testing

Problem B: Data Details

Available Data File: `dose_response_data.csv`
- Contains: `compound_name`, `concentration_uM`, `percent_inhibition`, `replicate_number`
- Each compound tested across 8 concentrations in triplicate
- Some compounds may not reach 50% inhibition at highest concentration
- Some curves may have unusual shapes or high variability

Expected Output:
- IC50 values with confidence measures
- Potency classification for each compound
- Quality assessment of each dose-response curve
- Recommendations for follow-up experiments

Problem C: Compound Selection 🎯

Advanced Challenge | Multi-Criteria Optimization

Research Context:
You have comprehensive data for 50 compounds but budget only allows testing 8 compounds in expensive animal studies. You need to select the optimal combination considering multiple criteria.

Your Mission:
- Develop systematic approach for multi-criteria ranking
- Balance potency, selectivity, safety, and drug-like properties
- Ensure chemical diversity in final selection (avoid selecting very similar compounds)
- Provide clear justification for selections and rejections

Key Challenges: How do you weight different criteria? How do you measure "chemical similarity"? How do you balance individual compound quality with portfolio diversity?

Problem C: Data Details

Available Data File: `compound_profiles.csv`
- Contains: `compound_name`, `ic50_uM`, `selectivity_ratio`, `cytotox_ic50`, `solubility_uM`, `admet_score`, `chemical_fingerprint`
- All compounds have IC50 < 10 μM (pre-filtered for activity)
- ADMET scores: 0-100 scale where >70 = drug-like, >85 = excellent drug-like properties
- Chemical fingerprints: Enable similarity calculations (research Tanimoto similarity or similar metrics)
- Some compounds may have missing data points

Research Notes: Consider both individual compound merit AND portfolio diversity. Look up multi-criteria decision analysis methods if needed.

Expected Output:
- Systematic scoring methodology with clear weighting rationale
- Final 8-compound selection with diversity assessment
- Risk/benefit analysis of selected portfolio
- Documentation suitable for research team review
- Final 8-compound selection with clear rationale
- Risk assessment of selected portfolio
- Documentation suitable for research team review

Self-Assessment Checklist

Before you finish, ensure your pseudocode addresses:

✅ **Data input:** How will you read and organize the data?
✅ **Quality control:** How will you identify and handle problematic data?
✅ **Core processing:** What are the main computational steps?
✅ **Decision points:** Where do you need to make choices or apply thresholds?
✅ **Edge cases:** What unusual situations might occur?
✅ **Output generation:** What results will you produce and in what format?
✅ **Validation:** How will you check that your solution is working correctly?

Quality Check Questions

Test your pseudocode by asking:

- Could another student follow your pseudocode to solve the problem?
- Are all your decision points clearly explained with reasoning?
- Have you planned for the most common edge cases and data problems?
- Is your planned output useful and clearly defined?
- Would your approach handle real experimental data reliably?

If you answer "no" to any question, refine your pseudocode before finishing.

Get Started!

Choose your problem and begin working.

Research approach: You're starting with information that may be incomplete - this mimics real research. If you don't understand something, **use ChatGPT or look online** to learn the context. I'm here to guide your research process and give feedback on your approach.

When to ask for help: If your group is stuck for more than **10 minutes**, call me over.

Remember: Focus on the logic and decision-making. Don't worry about programming syntax - that comes in the following weeks.