Minimal Patch for stab_ESM_IF.ipynb - Colab compatibility

This patch changes the **"PRELIMINARY OPERATIONS: Install dependencies"** cell in the original colab notebook. It fixes `ModuleNotFoundError` for `esm` and `torch_geometric`.

Why

After condacolab installs, `os.system("pip install ...")` and `conda install` can install to the wrong Python environment, causing `ModuleNotFoundError` for `esm` and `torch_geometric`.

Notes before applying

PRELIMINARY OPERATIONS: Install condalab – This cell installs the correct Python environment for the notebook. If running this cell leads to a disconnect and reconnect, that is normal because there is a kernel restart at the end. If unsure, run the cell again; it should print ✨🍰✨ `Everything looks OK!`

IMPORTANT: Replace the install block in dependencies

In the following block **PRELIMINARY OPERATIONS: Install dependencies**, replace the install block inside `if not os.path.isfile("finished_install")` with the code below.

Instructions:

1. Double-click the cell to open the code editor.
2. Delete the original install block (from the first `os.system(...)` to the last `os.system(...)`).
3. Paste the new code block (**tab-indentation required**).
4. Run the cell.

Original:

```
	os.system(f"conda install conda-forge::torch-scatter")
	os.system(f"conda install conda-forge::pytorch_sparse")
	os.system(f"conda install conda-forge::torch-cluster")
	os.system(f"conda install ostrokach-forge::torch-spline-conv")
	os.system(f'pip install torch_geometric')
	print('...finished torch dependencies')
	os.system(f"pip install biopython")
	os.system(f"pip install biotite")

	print("installing esmfold...")
	# install esmfold
	os.system(f"pip install git+https://github.com/matteo-
cagiada/esm.git")
	os.system("touch finished_install")
```

Replace with:

```
    # Use kernel's Python (os.system installs to wrong env with
condacolab)
    pip_install = [sys.executable, "-m", "pip", "install"]
    subprocess.run(pip_install + ["torch_geometric"], check=True)
    print('...finished torch dependencies')
    subprocess.run(pip_install + ["biopython", "biotite"], check=True)
    print("installing esmfold...")
    subprocess.run(pip_install + ["git+https://github.com/matteo-
cagiada/esm.git"], check=True)
    open("finished_install", "w").close()
```

Expected output of the patched cell

In the **PRELIMINARY OPERATIONS: Install dependencies** cell, when this patch runs successfully, you should see something like the following output:

```
installing libs...
...finished torch dependencies
installing esmfold...
importing the model
/usr/local/lib/python3.12/dist-packages/esm/pretrained.py:216:
UserWarning: Regression weights not found, predicting contacts will not
produce correct results.
  warnings.warn(
--> Installations succeeded
CPU times: user 12.1 s, sys: 2.81 s, total: 14.9 s
Wall time: 1min 2s
```

- The **Regression weights** warning is harmless (ESM-IF does not use contact prediction).
- Wall time becomes **faster than the expected 5–10 min** (e.g. ~1 min).

Tested results

Validated with values based on the spreadsheet:

Input	ΔG (likelihoods sum)	ΔG (kcal/mol)
YP_009724390.1_ref_RBD_AF2 (AlphaFold2 model 4, rank 1)	91.75509978423361	10.171060613370988
YP_009724390.1_ref_RBD_SWISS (SWISS-MODEL)	87.47504538903013	9.725362356565233

Both results closely match the original spreadsheet.