SUPPLEMENTARY MATERIAL 1

```
# AutoDock Vina configuration file
# Defines the receptor, grid box parameters, and docking settings

# Receptor file in PDBQT format
receptor = InIA.pdbqt  # Replace with the name of your receptor file if different

# Grid box center coordinates (in Angstroms)
center_x = 5.017
center_y = 6.016
center_z = 149.855

# Grid box dimensions (in Angstroms)
size_x = 58
size_y = 58
size_z = 52

# Docking parameters
exhaustiveness = 8      # Search thoroughness (higher = more accurate, slower)
energy_range = 10       # Energy range (kcal/mol) for output poses
num_modes = 9           # Maximum number of binding modes to generate
```

SUPPLEMENTARY MATERIAL 2

```
:: Batch Docking Script for AutoDock Vina (Windows)
:: This script automates the docking process for multiple ligands using the same configuration file.
:: Place this script in the folder containing your 'ligandopdbqt' subfolder and 'config.txt'.

@echo off

:: Loop through all ligand PDBQT files in the 'ligandopdbqt' folder
for %%a in ("%~dp0\ligandopdbqt\*.pdbqt") do (
    echo Processing %%a >> output.txt

    :: Run AutoDock Vina for each ligand using the same config file
    "C:\Users\HP I5\Desktop\Docking Molecular\vina_1.2.5_win.exe" --ligand "%%a" --config config.txt >> output.txt

    echo. >> output.txt
)

:: Pause to view the final message in the terminal
pause
```