J. Mex. Chem. Soc. **2025**, *69*(1)
Special Issue

ISSN-e 2594-0317

UAM-Ixachi: Desktop Tool for Massive Automated Molecular Docking

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Received May 25th, 2024; Accepted July 25th, 2024.

DOI for the article: http://dx.doi.org/10.29356/jmcs.v69i1.2299

Supplementary Information

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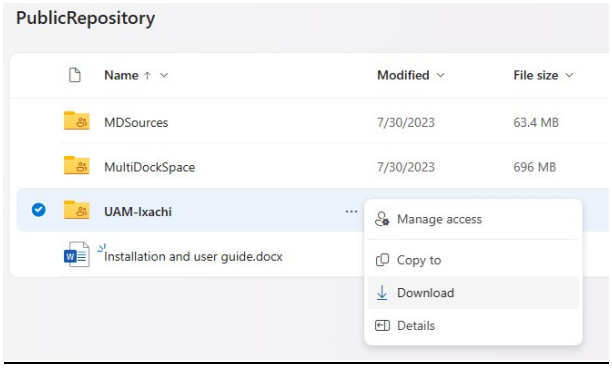
UAM-Ixachi Windows installation and user guide

Installation

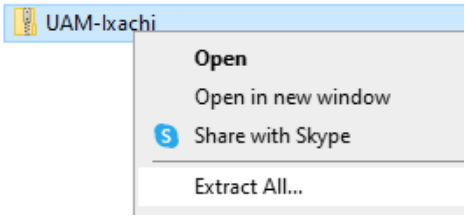
Download the tool in the repository:
https://1drv.ms/f/s!AiwrqGMGvesstXgOcz3Hn1Q2mfI9?e=903be7

Select only the UAM-Ixachi folder. MDSources and MultiDockSpace are demo sets that are not necessary for the tool's operation.

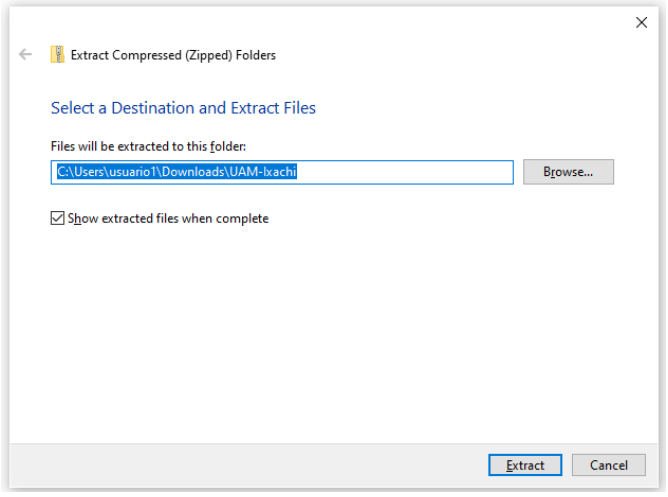


UAM-Ixachi uses OpenBabel 3.1.1, Python 3.11, and AutodockTools 1.5.7. The download package includes this versions. The total size is approximately 164 MB.

Once the folder is downloaded, right-click on it and then click “extract all”.



Choose a destiny and click “Extract”.



In the folder you have just extracted, look for the “Installer” file and double-click it.

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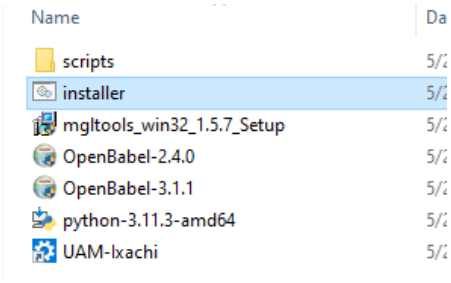
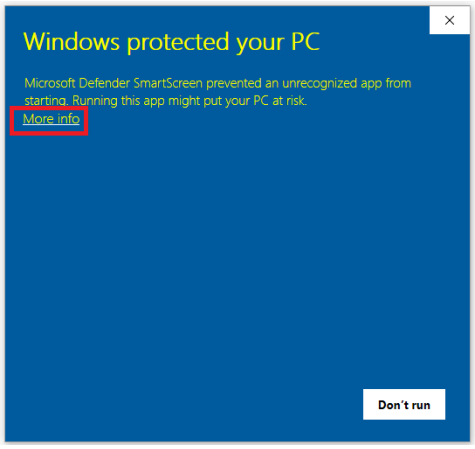
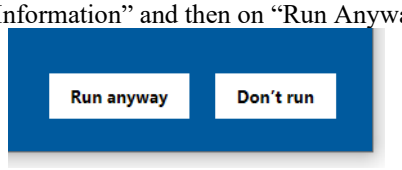


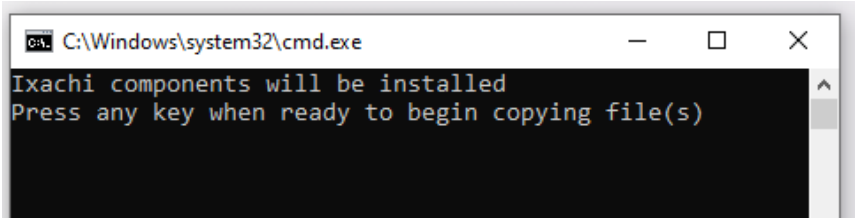
You may receive a warning about potential hazards. This is a false positive; the tool is open source and is free of malicious code.



To fix this, click on "More Information" and then on "Run Anyway".



Follow the on-screen instructions.



OpenBabel 3.1.1 installation will start automatically; click "Yes" and follow the program's instructions with the default options.

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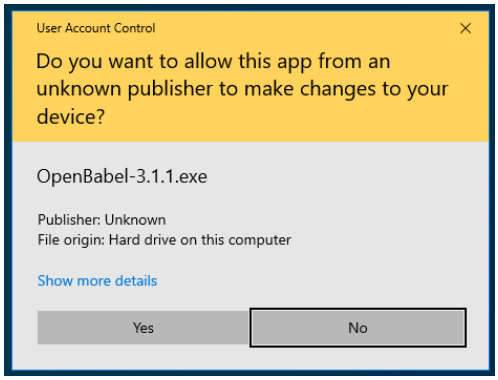
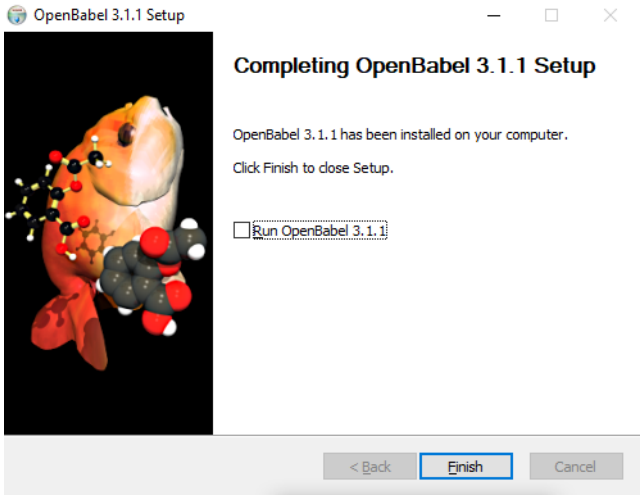
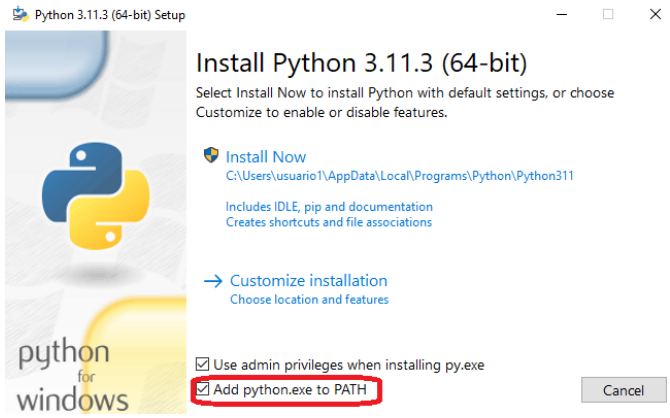


When finished, uncheck the "Run Openlabel" box and click "Finish".



The installation of Python 3.11.3 will be launched automatically. **Make sure to check "Add Python.exe to PATH** and then click "Install Now".



When asked, click "Yes", and wait for the process to be completed.

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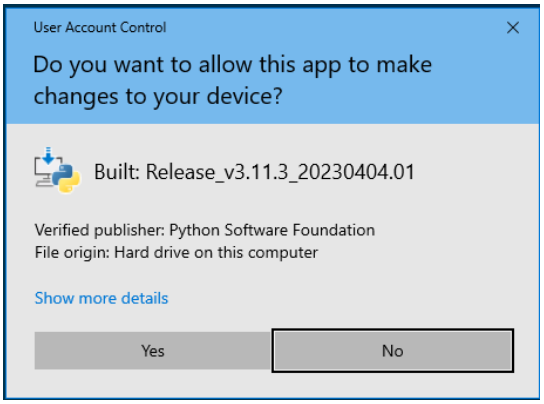
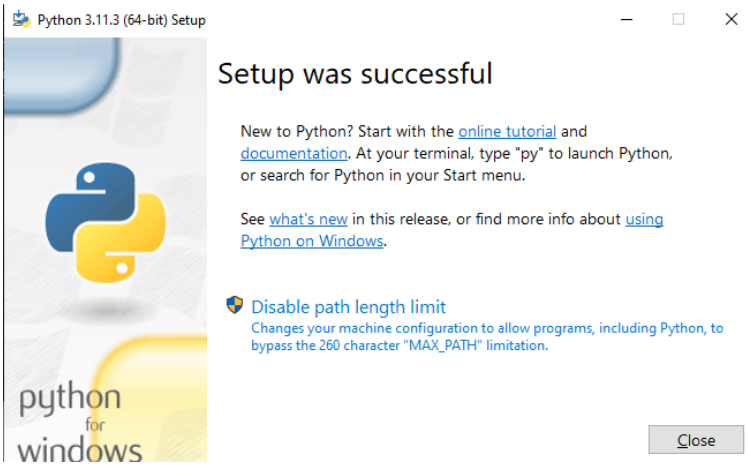
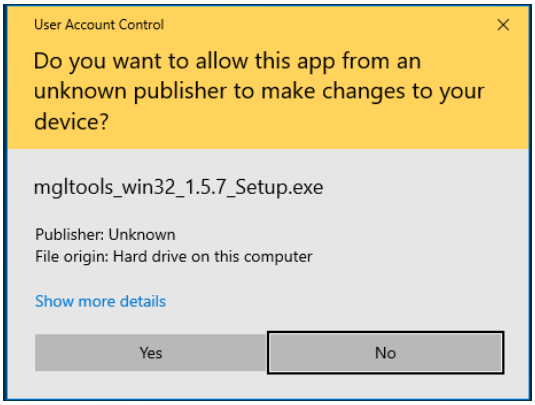


When the Python installation is complete, click “Close”.



The installation of AutoDockTools 1.5.7 will now be automatically launched. Click “Yes” and follow the on-screen instructions with the default settings.



When you finish installing AutoDockTools, click “OK”.

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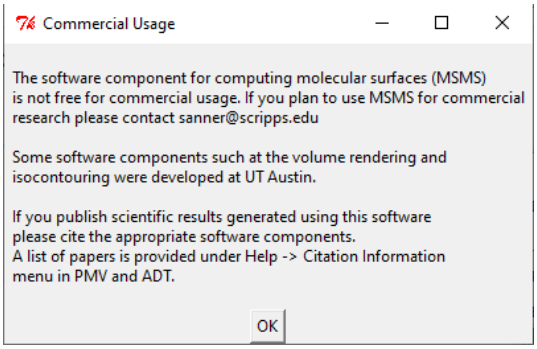
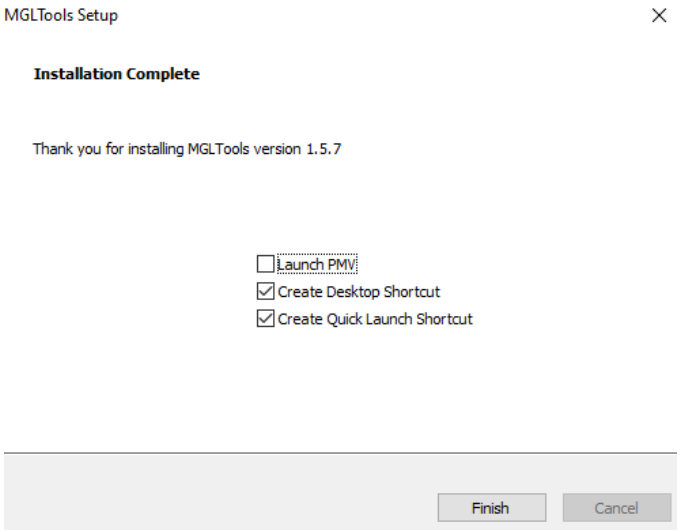
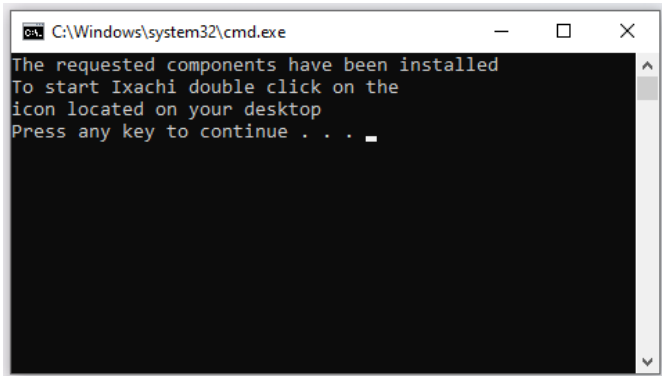


On the next screen, uncheck the "Launch PMV" box and click "Finish".



In turn, the UAM-Ixachi installer will notify you that the installation has been completed correctly.



Start a new project in UAM-Ixachi

On the desktop, you will find the Ixachi icon. Double-click on it to start.

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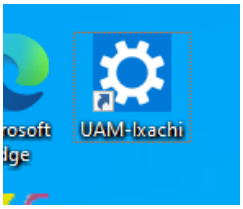
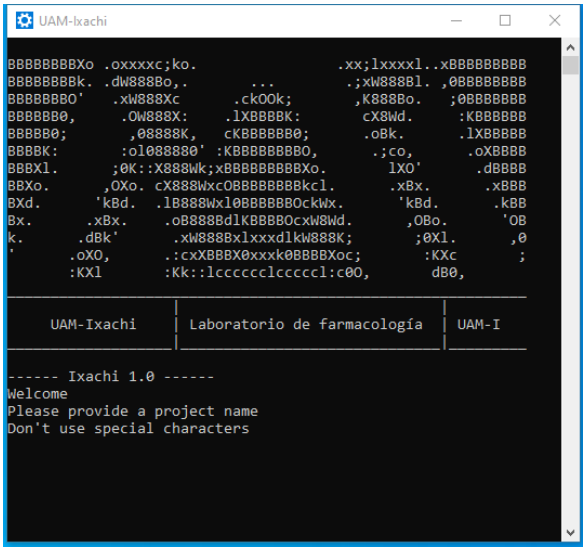


You will see a console screen. If this is the first time you are running the tool, it will ask you to name the project. Be sure not to use special characters to avoid errors related to the Windows file system. If you use special characters, the tool may try to remove them and will notify you of the change. By default, the tool will remove spaces from project names and replace them with underscores.



Follow the console's instructions, which will ask you: We need to know how many processors can be used at the same time, the size of the simulation box (grid), how many runs there are for each simulation, the full path to the plain text file (notepad, not Word; the file extension must be given, usually.txt) with the PDB codes, and the full path to the folder with your experimental ligands in mol2 or sdf format. The tool will guide you through each of these steps. The plain text file should contain PDB codes, one for each line, as shown in the example file in the following images. For each point on each axis, the grid size is expressed in units equivalent to 0.375 Å.

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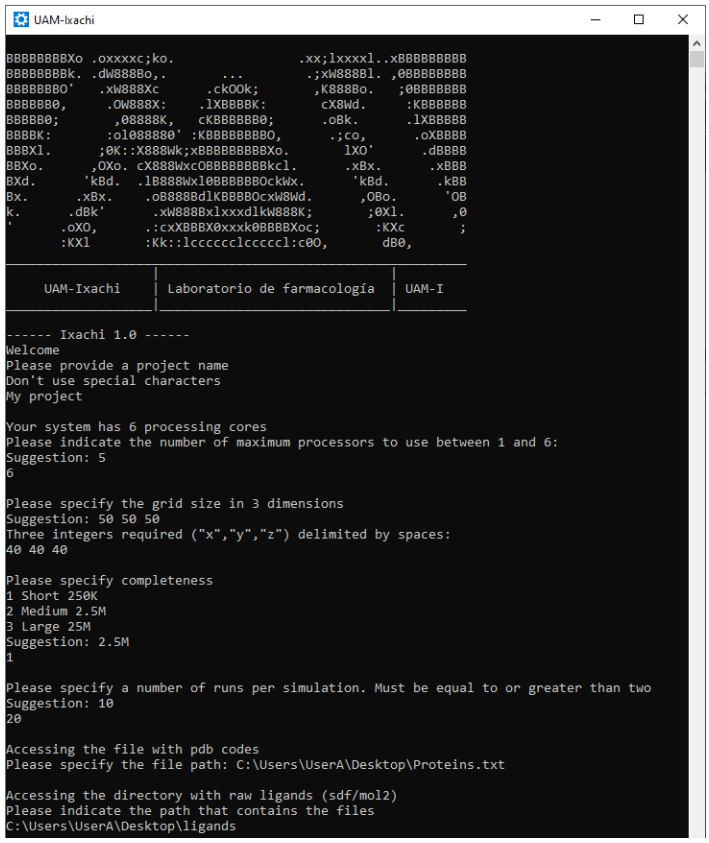

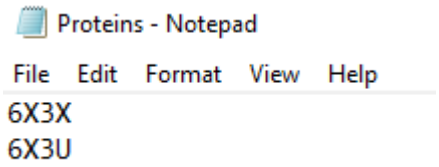

Once you have provided all the information to the tool, it will begin automatically downloading the PDB models from the online database. If this is your first time running the tool, you may receive a notification about the installation of "Requests". If so, follow the instructions and wait for the installation to finish. The process is automatic if you have correctly followed the UAM-Ixachi installation instructions. If the installation of "Requests" fails, the tool will not be able to download the models. If this is your case, exit UAM-Ixachi, then repeat the installation of Python 3.11.3 and make sure to check the "Add python.exe to PATH" box. Then run UAM-Ixachi, which will continue from the last step.

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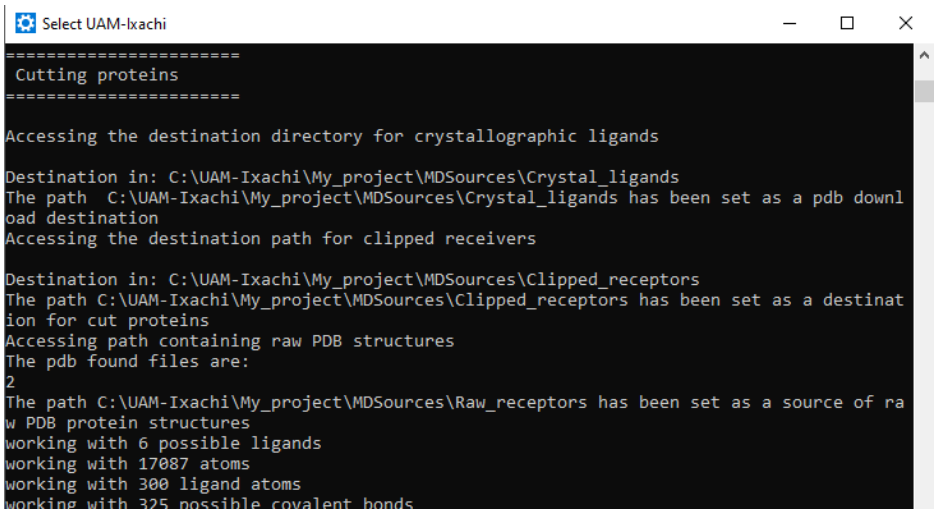
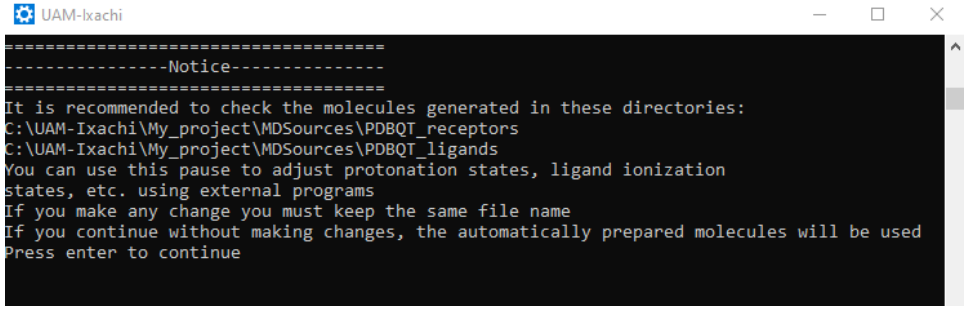
You will then receive notices about UAM-Ixachi activities: “Trimming receptors”, “Minimizing ligand geometry”, “Converting PDBQT”, etc. The tool will automatically identify ligands docked to protein models and prepare docking simulations of your experimental ligands at the same binding sites.



Once preparations are complete, the tool will pause before starting simulations. The pause is there so the user can change the models that the tool makes, like the protonation state of amino acid residues, the rotatable bonds of ligands, charges, or other things (by using outside programs). If you do not want to make any adjustments, just press “enter”.



From this point forward, the tool is autonomous. Be patient and wait for all processes to be complete.

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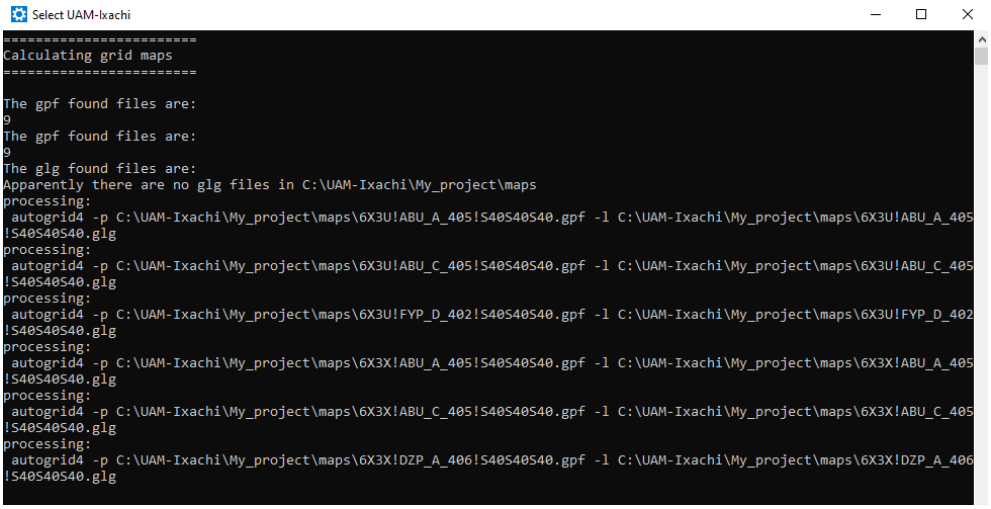
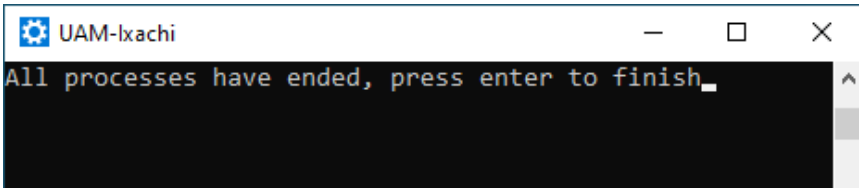
The time to complete will depend on your computer's hardware resources, the number of target proteins, the number of ligands, the level of completeness chosen, and the number of runs requested.



Once all the processes have been completed, the tool will issue a notice and wait for confirmation before closing the program.



Additional working modes

The next time you run UAM-Ixachi, it will automatically recognize the last project you worked on, display the previously configured parameters, and offer three work options.

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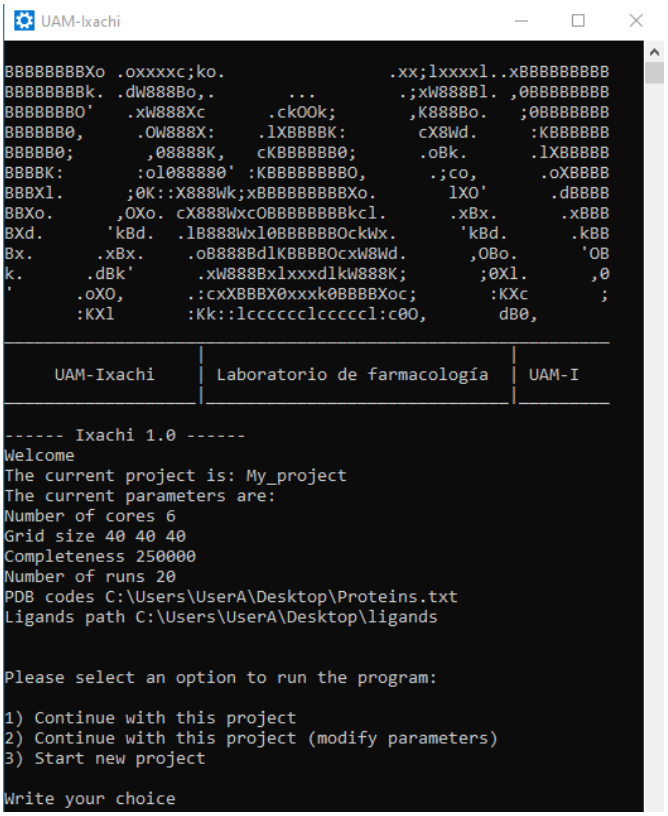

If you choose the first option, it will search for new PDB codes in the file and new ligands in the corresponding directory. It will then run the new docking simulations according to the previously configured parameters and add them to the results.

If you choose the second option, it will act the same as in the previous point but will request new parameters such as grid size, number of runs, etc. The new parameters will only influence the new docking simulations since the tool does not repeat previously successful simulations.

If you choose the third option, you will start a new project that will request all parameters and sources of molecules.

Consult results

The results are stored in files that are formatted as row and column reports. They are compatible with Excel and other spreadsheet programs. To consult these reports, enter the C:\UAM-Ixachi\ directory, where you will find a folder with the name of your project. Inside this, you will find three reports: Failreport.csv, Hbond_report.csv, and Report.csv.

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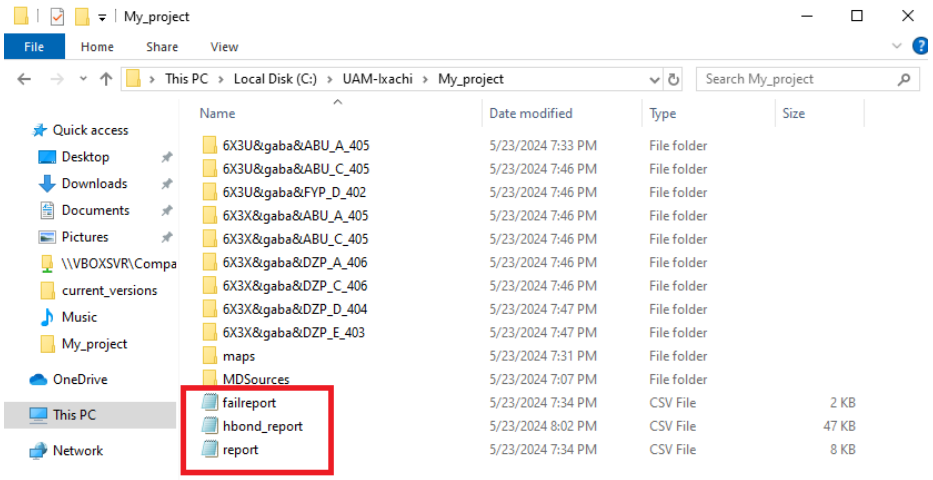

In Failreport.csv, you can check the success or failure of each simulation. The "Status" column identifies successful simulations with "True" and failed simulations with "False." The "Cause" column helps identify failure sources. Information about the complete simulation path, time, and date, among others, is included. To make this report easier to consult, use the filter functions of your spreadsheet.

	A	B	C	D	E	F	G	H	I	J
1	Path	Status	Cause	Hour:Min	Second	Period	Date(m/d/y)	Protein	Ligand	Site
2	C:\UAM-Ixachi\My_project\6X3U&gaba&ABU_A_405\6X3U&gaba&ABU_A_405.dlg	True	autodock4: S	07:32	33	p.m.	05/23/2024	6X3U	gaba	ABU_A_405
3	C:\UAM-Ixachi\My_project\6X3U&gaba&ABU_C_405\6X3U&gaba&ABU_C_405.dlg	True	autodock4: S	07:32	06	p.m.	05/23/2024	6X3U	gaba	ABU_C_405
4	C:\UAM-Ixachi\My_project\6X3U&gaba&FYP_D_402\6X3U&gaba&FYP_D_402.dlg	True	autodock4: S	07:32	34	p.m.	05/23/2024	6X3U	gaba	FYP_D_402
5	C:\UAM-Ixachi\My_project\6X3X&gaba&ABU_A_405\6X3X&gaba&ABU_A_405.dlg	True	autodock4: S	07:32	33	p.m.	05/23/2024	6X3X	gaba	ABU_A_405
6	C:\UAM-Ixachi\My_project\6X3X&gaba&ABU_C_405\6X3X&gaba&ABU_C_405.dlg	True	autodock4: S	07:32	33	p.m.	05/23/2024	6X3X	gaba	ABU_C_405
7	C:\UAM-Ixachi\My_project\6X3X&gaba&DZP_A_406\6X3X&gaba&DZP_A_406.dlg	True	autodock4: S	07:32	06	p.m.	05/23/2024	6X3X	gaba	DZP_A_406
8	C:\UAM-Ixachi\My_project\6X3X&gaba&DZP_C_406\6X3X&gaba&DZP_C_406.dlg	True	autodock4: S	07:32	34	p.m.	05/23/2024	6X3X	gaba	DZP_C_406
9	C:\UAM-Ixachi\My_project\6X3X&gaba&DZP_D_404\6X3X&gaba&DZP_D_404.dlg	True	autodock4: S	07:33	03	p.m.	05/23/2024	6X3X	gaba	DZP_D_404
10	C:\UAM-Ixachi\My_project\6X3X&gaba&DZP_E_403\6X3X&gaba&DZP_E_403.dlg	True	autodock4: S	07:33	04	p.m.	05/23/2024	6X3X	gaba	DZP_E_403

The user's premature termination of UAM-Ixachi is a common cause of failure. The “Status” column will contain the word “truncated”. In this case, run the tool again, let it finish, and it will correct the incomplete simulations.

Another cause of failure is the lack of grid maps (Indicated in the “Cause” column). This may be due to adding new ligands to the project that contain types of atoms not previously calculated. To fix this, go into your project directory and delete the “maps” folder. Then run UAM-Ixachi; this will allow the maps to be calculated correctly.

In the "Report.csv" file, you will find the concentrated results of all your project's simulations up to the cluster level. Use the spreadsheet program's filtering functions to isolate the best energies, cluster sizes, binding sites, etc. The "DlgPath" column contains the full path of the dlg result, which can be parsed with AutoDock tools.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Clusterings													
2	ClusterRa	MinEnergy	Run	AverageEnerg	ClusterSiz	Control	#Runs	Exhaust	Protein	Ligand	Site	ProteinPa	DlgPath	
3	1	-5.91	14	-5.2	20	##########	20	250000	6X3X	gaba	ABU_C_405	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
4	1	-6.07	11	-5.84	18	##########	20	250000	6X3X	gaba	ABU_A_405	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
5	1	-2.25	2	-1.86	14	##########	20	250000	6X3U	gaba	FYP_D_402	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
6	1	-5.23	4	-4.38	13	##########	20	250000	6X3U	gaba	ABU_A_405	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
7	1	-5.35	9	-4.76	12	##########	20	250000	6X3U	gaba	ABU_C_405	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
8	1	-2.25	5	-1.9	10	##########	20	250000	6X3X	gaba	DZP_A_406	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
9	2	-4.1	10	-3.3	8	########	20	250000	6X3U	gaba	ABU_C_405	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
10	2	-3.33	5	-3.1	7	#######	20	250000	6X3U	gaba	ABU_A_405	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
11	1	-1.92	6	-1.46	6	######	20	250000	6X3X	gaba	DZP_C_406	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
12	5	-2.02	5	-1.6	6	######	20	250000	6X3X	gaba	DZP_D_404	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
13	3	-1.67	14	-1.34	6	######	20	250000	6X3X	gaba	DZP_E_403	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	
14	6	-1.27	9	-1.08	5	#####	20	250000	6X3X	gaba	DZP_C_406	C:\UAM-Ixacl	C:\UAM-Ixachi\My_pr	

In the “Hbond_report.csv” file, you will find the results of your project up to the run level, and for each one, an approximation of the hydrogen bonds formed with their respective amino acid residues is offered. We strongly recommend that you check for hydrogen bonds using third-party programs such as Discovery or

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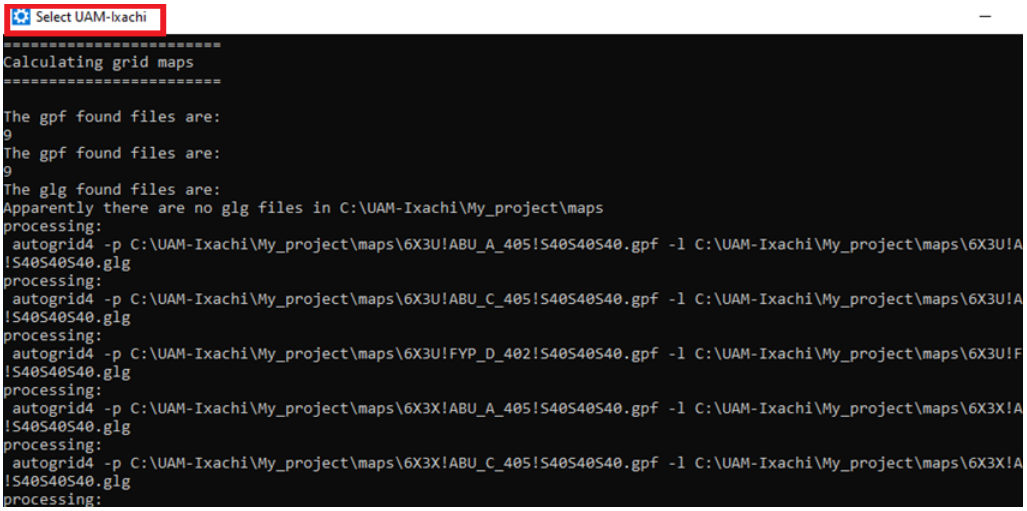
PyMOL. This report has the advantage of specifying the full path to the specific run file, i.e., a single-molecule conformation docked by simulation in PDBQT format. If you want, for example, to analyze the protein-ligand complex in Discovery, just open the protein path ("ProteinPath" column) and the ligand conformation path ("RunPath" column).

Run	Rank	Subrank	Energy	ClusterSiz	#Runs	Ligand	ProteinCo	Exhaust	ProteinPa	RunPath	DlgPath	Site	H-bonds				
11	1	1	-6.07	18	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_A_405	ARG B 67	GLU A 155	THR A 202	TYR A 97	
6	1	2	-6.01	18	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_A_405	ARG B 67	GLU A 155	SER A 156	THR A 202	
15	1	3	-5.96	18	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_A_405	ARG B 67	GLU A 155	THR A 202	TYR A 97	
5	1	4	-5.96	18	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_A_405	ARG B 67	GLU A 155	THR A 202	TYR A 97	
12	1	5	-5.93	18	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_A_405	ARG B 67	GLU A 155	THR A 202	TYR A 97	
17	1	6	-5.93	18	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_A_405	ARG B 67	GLU A 155	THR A 202	TYR A 97	
14	1	8	-5.91	18	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_A_405	ARG B 67	GLU A 155	THR A 202	TYR A 97	
7	1	7	-5.91	18	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_A_405	ARG B 67	GLU A 155	SER A 156	THR A 202	TYR A 97
14	1	1	-5.91	20	20	gaba	6X3X	250000	C:\UAM-Ixac	C:\UAM-Ixac	C:\UAM-Ixac	ABU_C_405	ARG D 67	GLU C 155	SER C 156	THR C 202	

The following is a known issue and may appear to be a bug (although it is not). If UAM-Ixachi has been running for a long time with no apparent progress, it may be in pause mode. This happens when, while running the tool, you click inside the console, then it pauses. Check the window title bar; it should not contain the word "select". If so, click on the console and press "enter" until the word "select" disappears.



If the tool still takes a long time, be patient. Some projects can take hours or days if you have requested many ligands and target proteins, or if the parameters you have configured are very exhaustive.

If you have found bugs or want to send comments about the tool, please contact the developers at e-mail ipn_2nv4@hotmail.com