

Create Your Own Virtual Gel

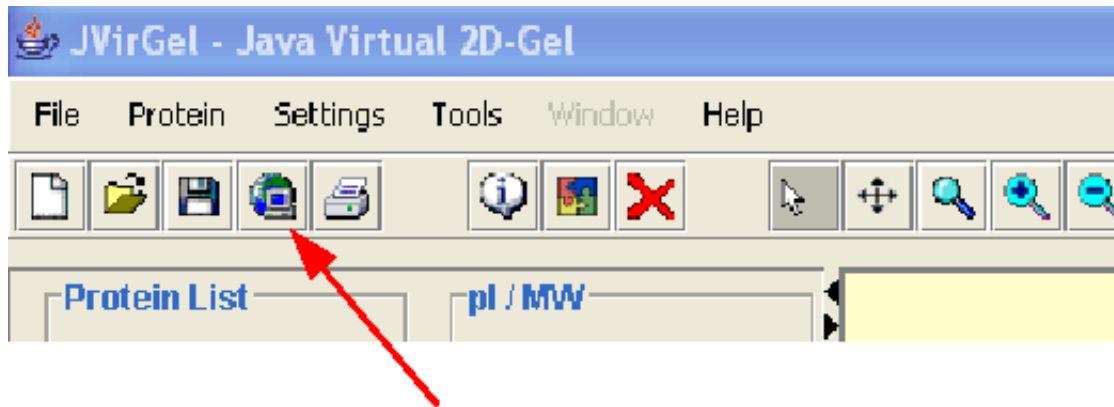
Karsten Hiller

There are three possibilities to import proteome sequence data into JVirGel:

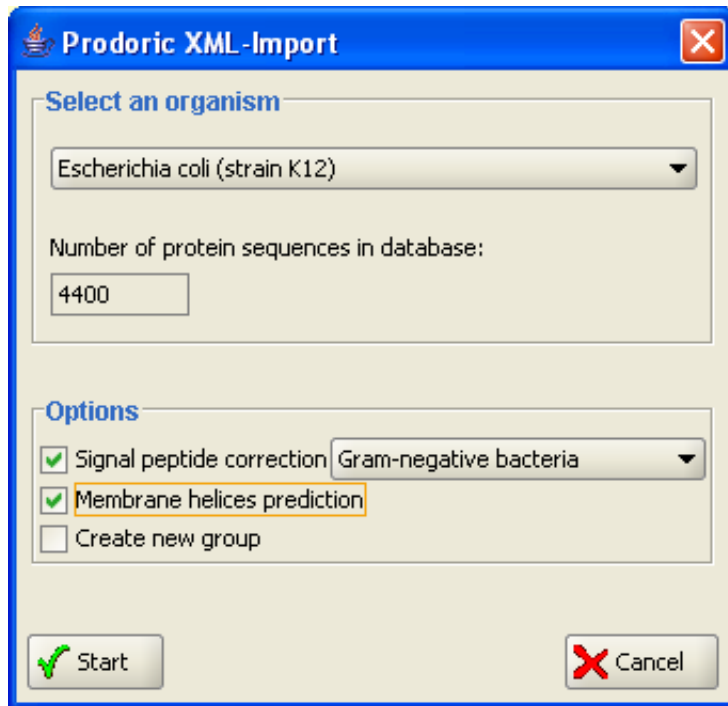
- Import data in XML format over the internet
- Import sequence files in FASTA format
- Import sequence files in EMBL format

1. Import Data in XML format over the Internet

1. The simplest way to import proteomic data is the **XML-Import** function of JVirGel. Just click on the computer icon in the toolbar to open the **XML-Import dialog**:

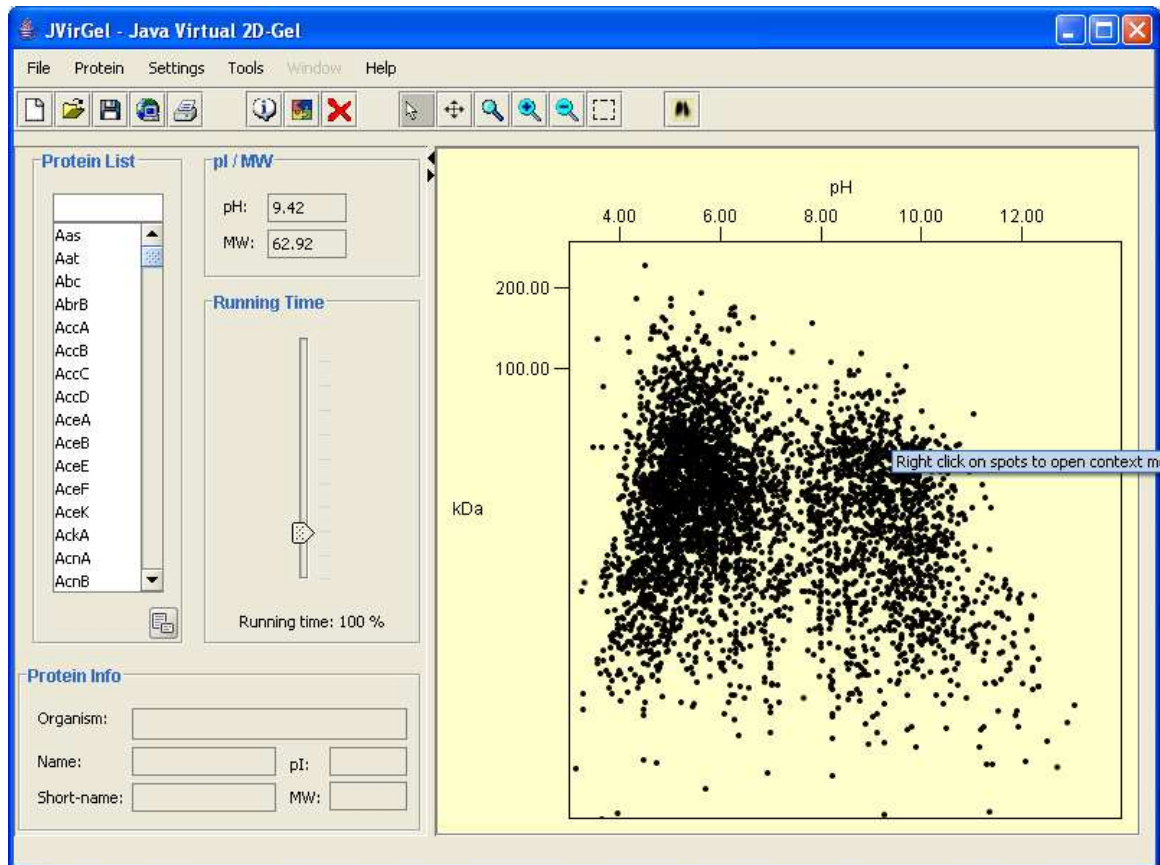


2. Select an organism. If you want JVirGel to predict the Sec-dependent secretome or the membrane subproteome enable **signal peptide prediction** and respectively **transmembrane helices prediction** by checking the corresponding checkboxes.



Note: The prediction of transmembrane helices may take some minutes depending on your hardware and the selected organism.

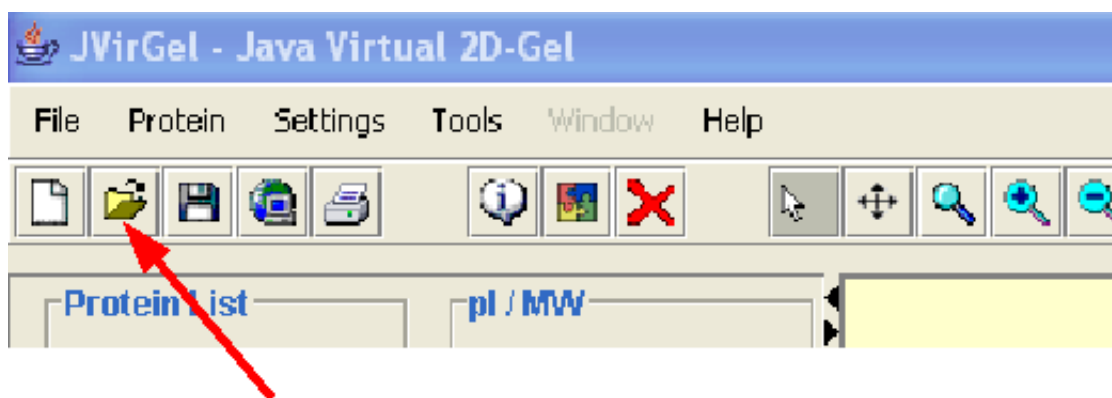
3. To start the XML-import just click the **Start button**. Be sure, that your firewall allows JVirGel to connect the database.



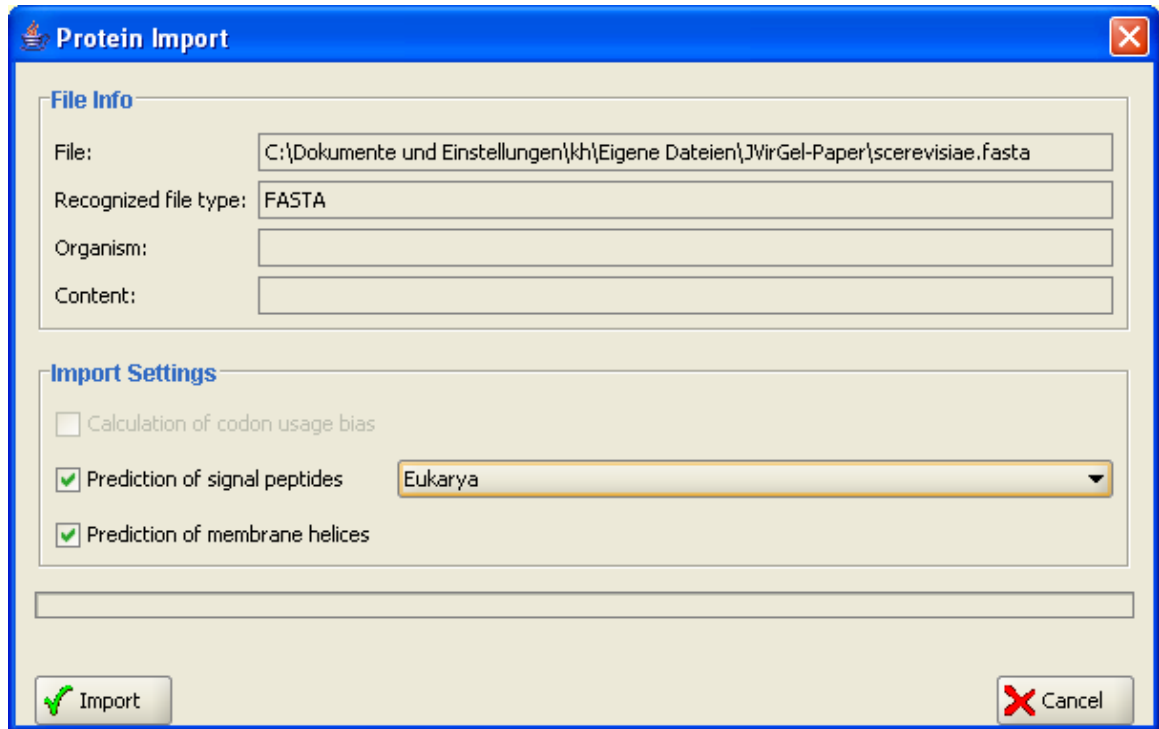
4. Congratulations, you have just created your first virtual gel !

2. Import Sequence Data in FASTA Format

1. In order to import your own sequence files in FASTA format, click on the **Open icon** in the toolbar. After selecting your FASTA-file the **FASTA-import dialog** appears:

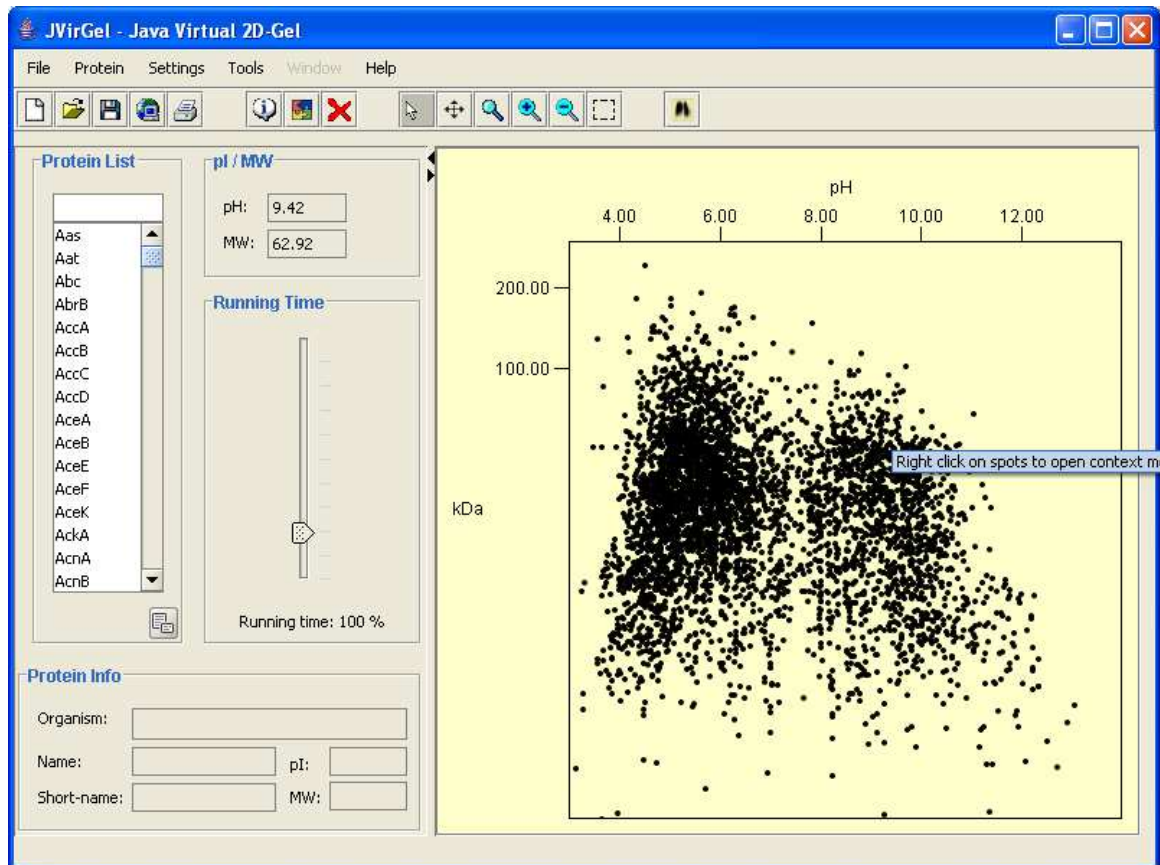


2. If you want JVirGel to predict the Sec-dependent secretome or the membrane subproteome enable **signal peptide prediction** and respectively **transmembrane helices prediction** by checking the corresponding checkboxes.



Note: The prediction of transmembrane helices may take some minutes depending on your hardware and the number of imported proteins.

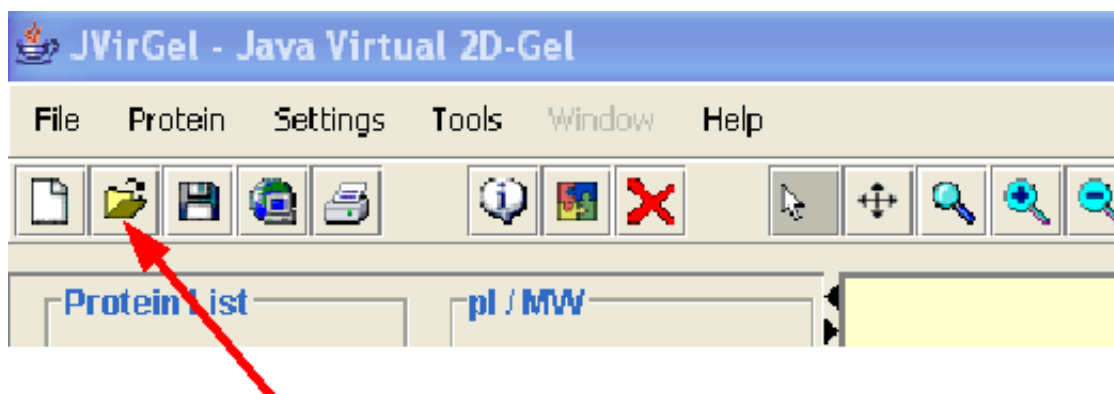
3. Congratulations, you have just created your first virtual gel !



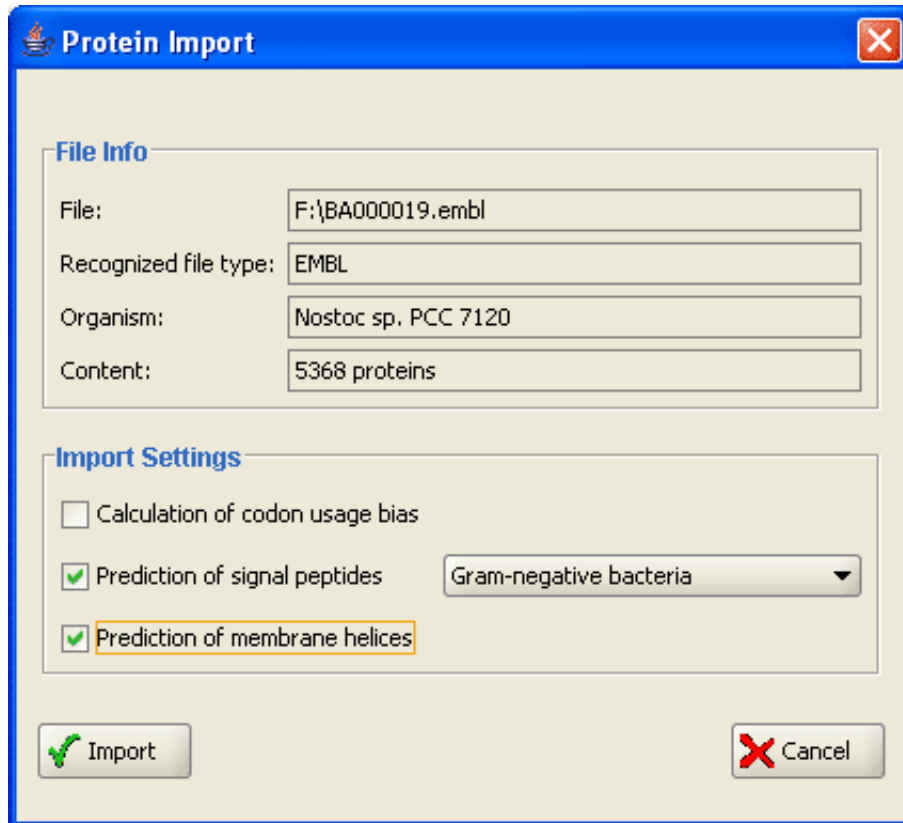
3. Import Sequence Data in EMBL Format

Note:

- We highly recommend to use **EMBL Genome Reviews** with JVirGel. You can download these files from the [EBI webservice](#).
 - The downloaded files need to be unzipped and renamed to "*.embl".
1. In order to import your own sequence files in EMBL format, click on the **Open icon** at the toolbar. After selecting an EMBL file the **EMBL-import dialog** appears:

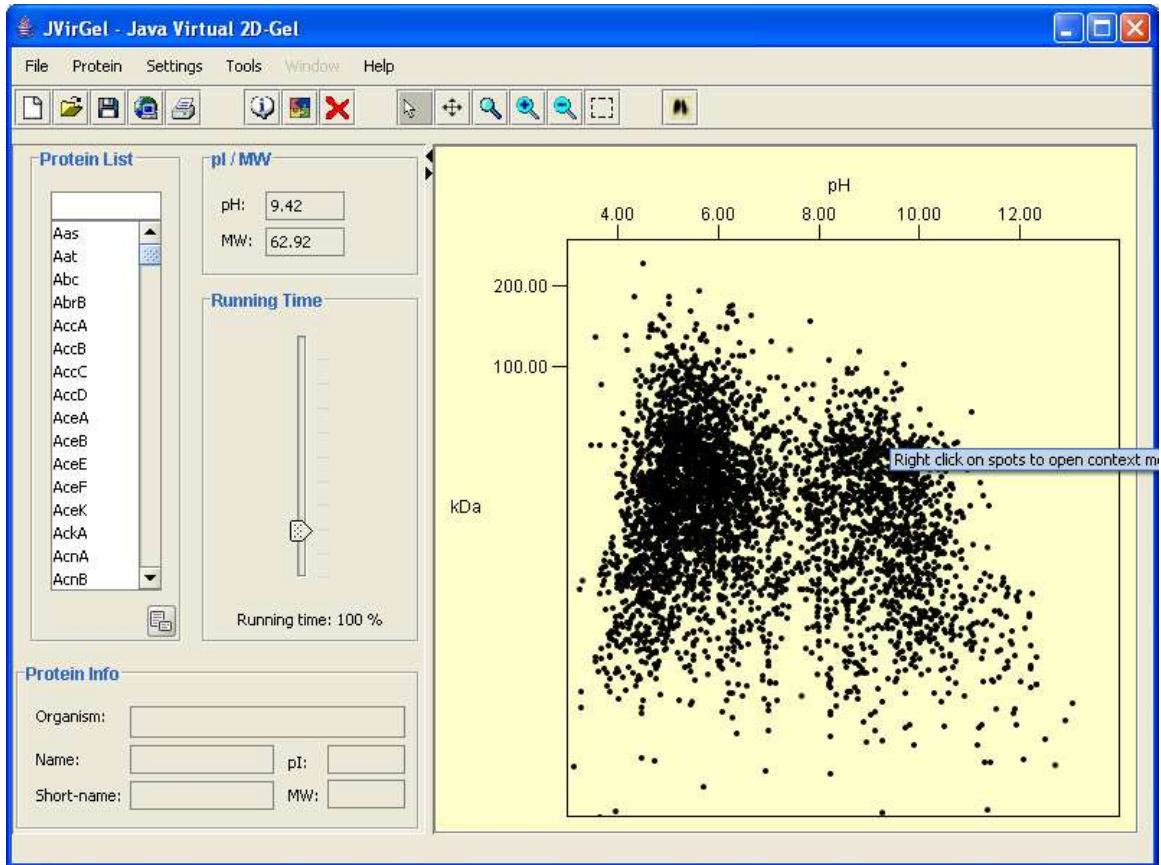


2. If you want JVirGel to predict the Sec-dependent secretome or the membrane subproteome enable **signal peptide prediction** and respectively **transmembrane helices prediction** by checking the corresponding checkboxes. Furthermore, JVirGel is able to predict **Codon Adaptation Indices (CAI)** if you check the appropriate checkbox.



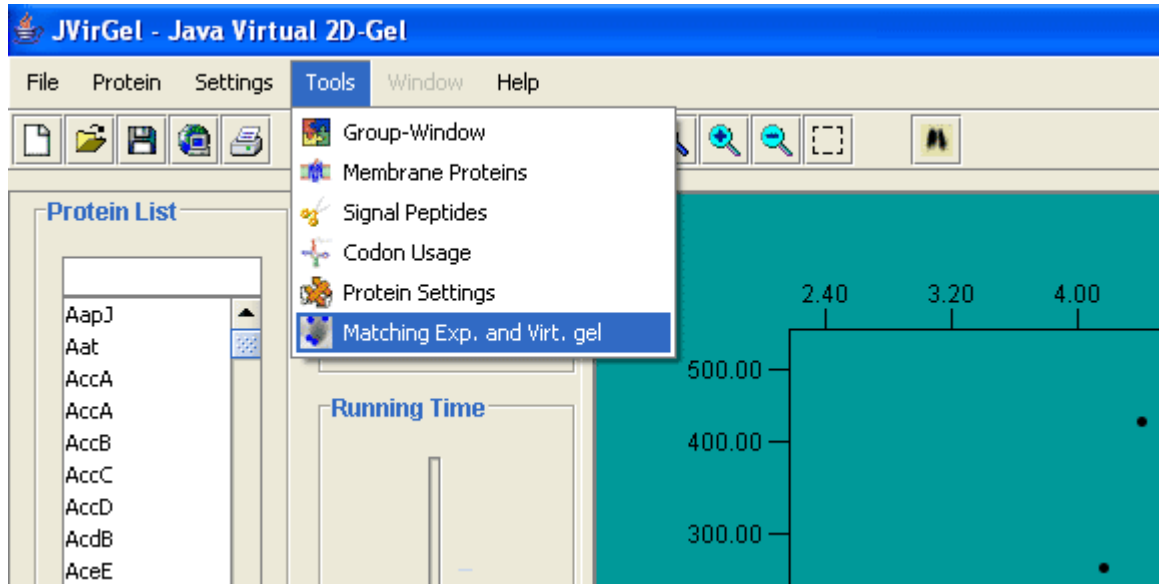
Note: The prediction of transmembrane helices may take some minutes depending on your hardware and the number of imported proteins.

3. Congratulations, you have just created your first virtual gel !



Matching of Experimental and Virtual 2D Gel

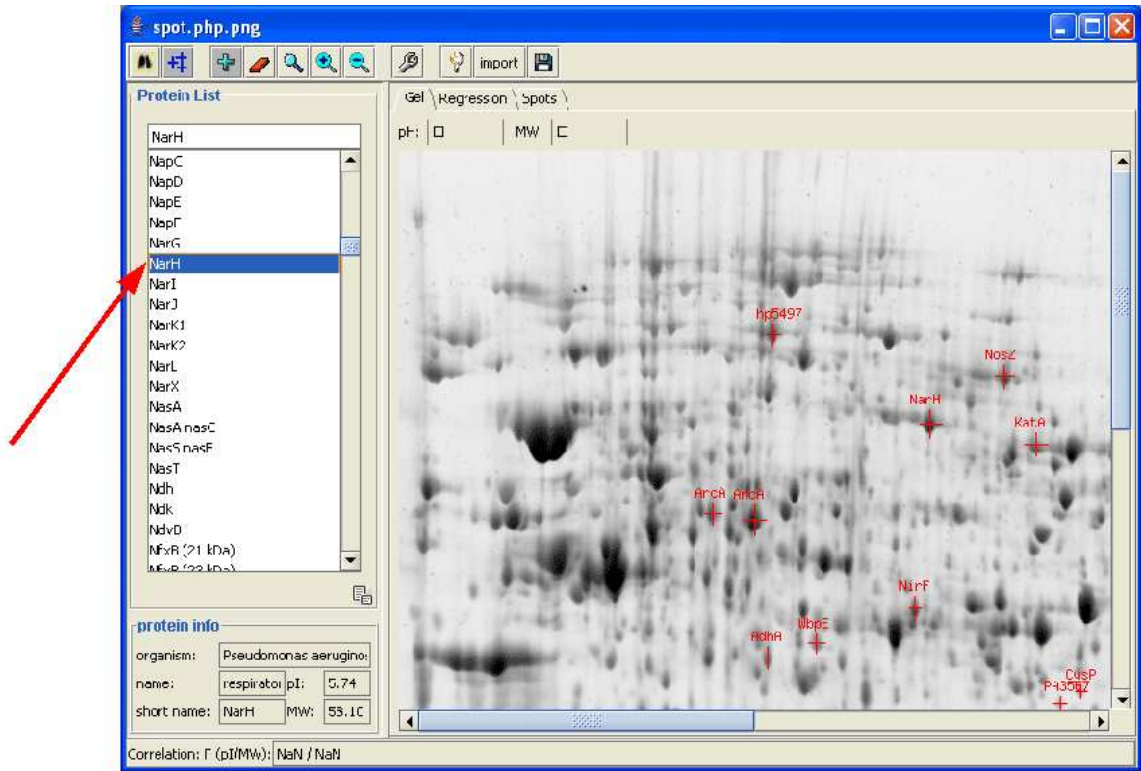
1. As a first step import a proteome
2. Choose **Tools->Matching Exp. and Vir. Gel:**



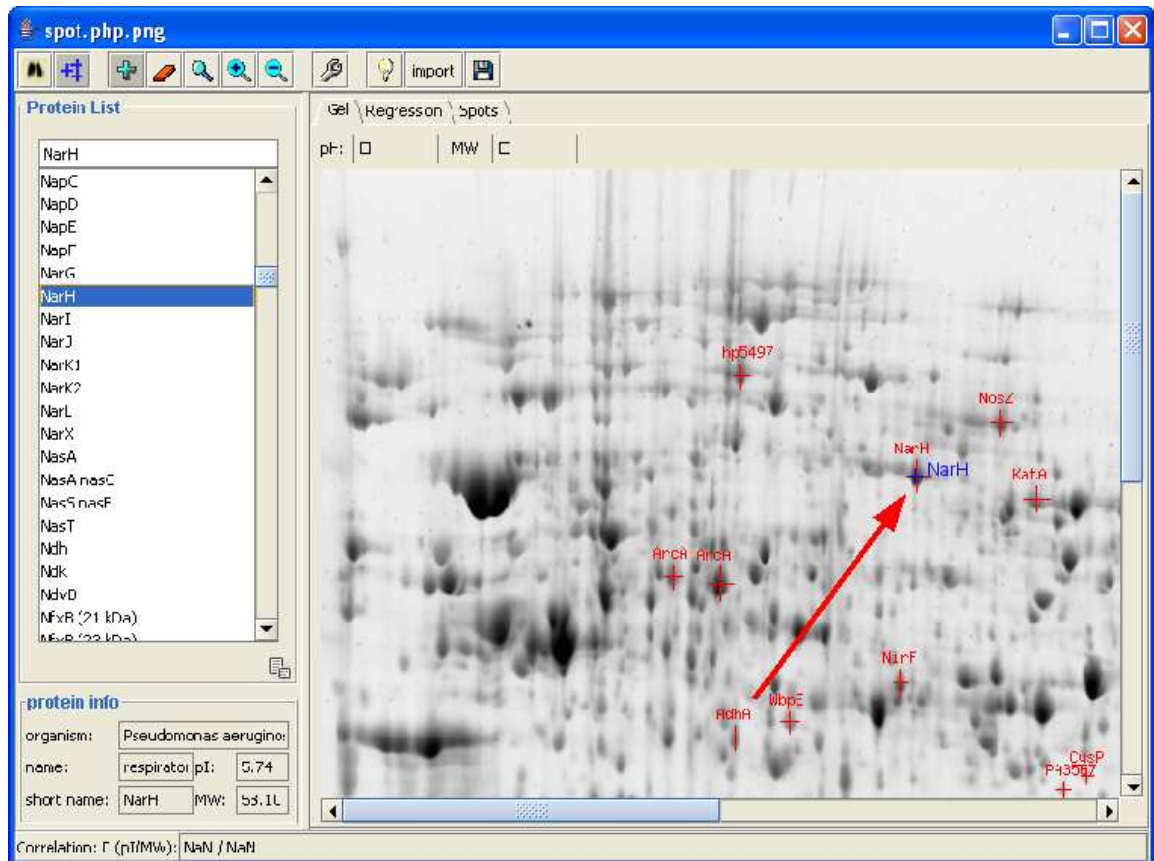
3. Select your experimental gel image

Note: Gel image must be in **.png, .jpg** or **.gif** format

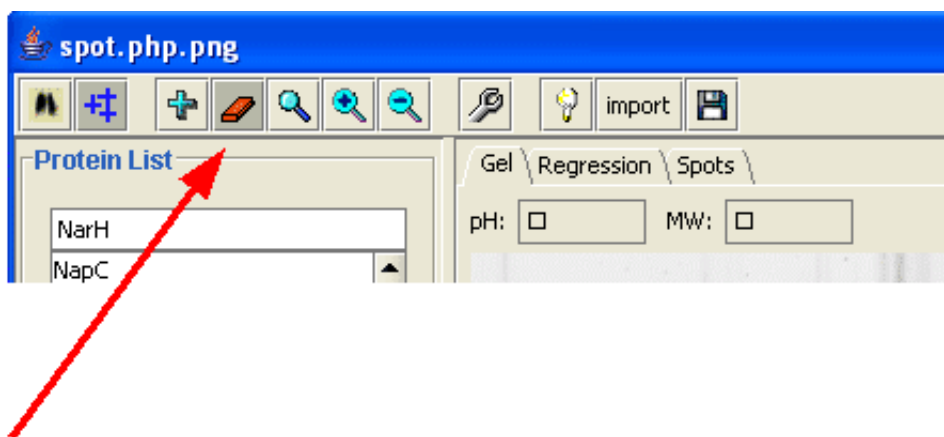
4. Select a protein that should be set as landmark from the list on the left side:



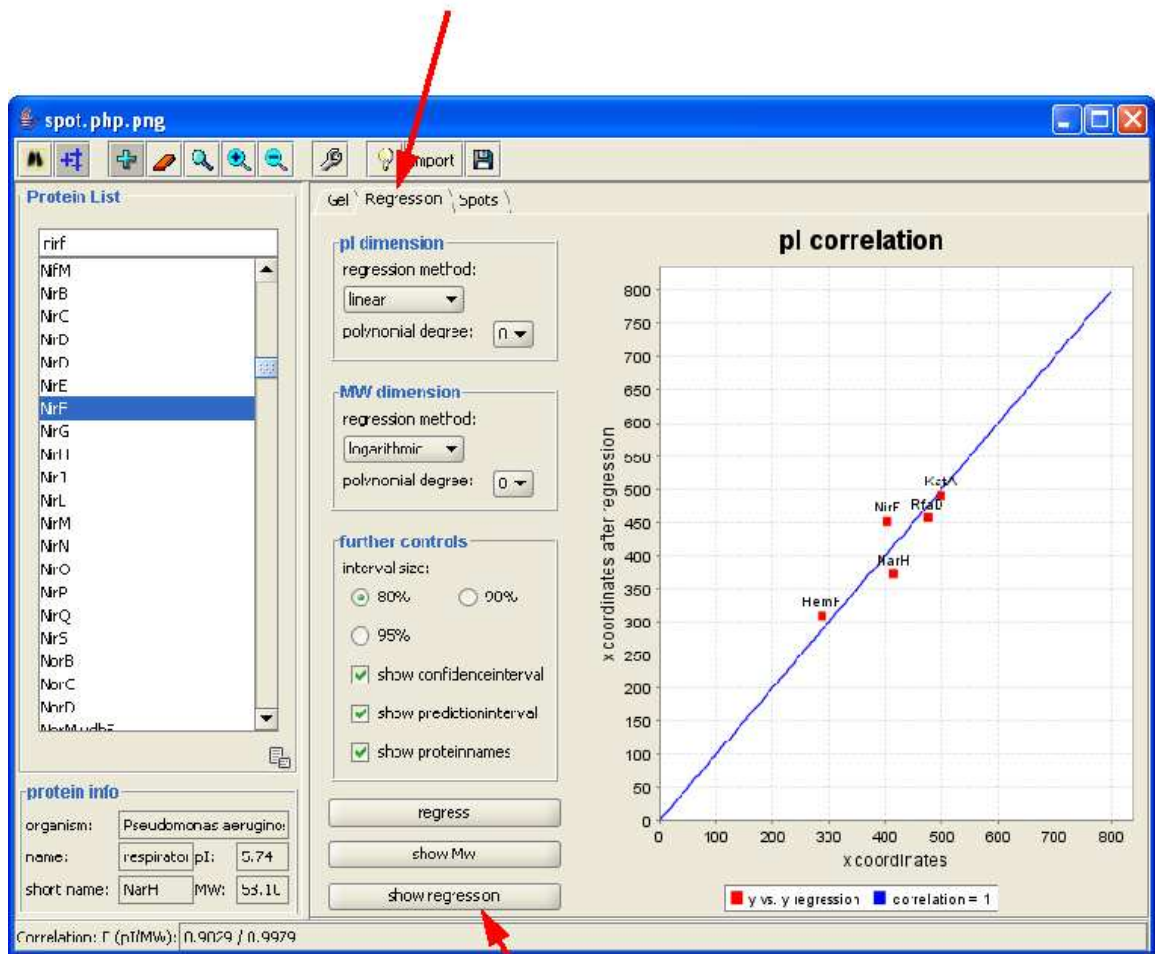
5. Click on the corresponding part of your experimental gel to set the landmark:



6. Repeat step 5 for defining **at least 5 landmarks equally distributed** throughout your experimental gel
7. Misplaced landmarks can be removed using the remove function:



8. The correlation between your landmarks and the predicted pI / MW can be checked by choosing the **Regression**-tab and clicking on **Show Regression**



9. In order to view the virtual 2D gel click the button **Virtual Gel** in the toolbar:



my selected proteins

File Protein View

Group:
my selected proteins

show whole group

103 Proteins:

Organism	Shortname	Name	pI(pH)	cpI(pH)	MW(kDa)
Pseudomon...	AidB	probable ac...	5,981	6,157	60,331
Pseudomon...	AntA	anthranilate...	5,868	6,495	52,472
Pseudomon...	AprF	alkaline prot...	5,778	5,615	54,464
Pseudomon...	AruD	succinylglut...	5,807	6,343	51,504
Pseudomon...	BetC	choline sulfa...	6,089	5,743	57,42
Pseudomon...	BioA	adenosylme...	5,834	5,887	52,472
Pseudomon...	CobJ	precorrin-3 ...	5,656	5,535	58,943
Pseudomon...	CobQ	cobyric acid ...	5,957	5,55	52,365
Pseudomon...	CreC	two-compon...	5,717	5,541	52,296
Pseudomon...	CysG	siroheme sy...	5,86	5,583	50,365
Pseudomon...	Dgt	deoxyguano...	6,063	5,792	56,735
Pseudomon...	Dht	dihydropyri...	5,744	5,688	52,206
Pseudomon...	FleR	two-compon...	5,948	7,298	51,228
Pseudomon...	GapB, gapN	probable gly...	5,964	6,617	59,953
Pseudomon...	Ggt	gamma-glut...	5,811	5,682	59,867
Pseudomon...	GltD	glutamate s...	6,042	5,229	52,619
Pseudomon...	HpaA	4-hydroxyp...	5,656	5,671	58,457
Pseudomon...	HpcC	5-carboxy-2...	5,964	6,653	52,991
Pseudomon...	HutU	urocanase	5,906	5,685	61,154
Pseudomon...	IlvA1	threonine d...	6,025	6,02	55,344
Pseudomon...	IlvA2	threonine d...	6,067	6,066	55,897
Pseudomon...	LeuC	3-isopropyl...	5,842	5,723	51,036
Pseudomon...	MdcA	malonate de...	5,98	5,535	61,417
Pseudomon...	MdoG	conserved h...	6,529	5,953	59,437
Pseudomon...	MmsA	methylmalon...	5,954	6,285	53,657

Table of Contents

Create Your Own Virtual Gel	1
1. Import Data in XML format over the Internet	1
2. Import Sequence Data in FASTA Format	3
3. Import Sequence Data in EMBL Format	5
Overlay Your Experimental 2D Gel with a Virtual One	8
Matching of Experimental and Virtual 2D Gel	8