

DOG Manual

Domain Graph

Version 2.0 11/06/2011

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Statement

1. **Implementation**. The softwares of the CUCKOO Workgroup are implemented in JAVA (J2S E). Usually, both of online service and local stand-alone packages will be provided.

2. Availability. Our softwares are freely available for academic researches. For non-profit users, you can copy, distribute and use the softwares for your scientific studies. Our softwares are not free for commercial usage.

3. **GPS**. Previously, we used the GPS to denote our Group-based Phosphorylation Scoring algorithm. Currently, we are developing an integrated computational platform for post-translational modifications (PTMs) of proteins. We re-denote the GPS as Group-based Prediction Systems. This software is an indispensable part of GPS.

4. **Usage**. Our softwares are designed in an easy-to-use manner. Also, we invite you to read the manual before using the softwares.

5. **Updation**. Our softwares will be updated routinely based on users' suggestions and advices. Thus, your feedback is greatly important for our future updation. Please do not hesitate to contact with us if you have any concerns.

6. Citation. Usually, the latest published articles will be shown on the software websites. We wish you could cite the article if the software has been helpful for your work.

7. Acknowledgements. The work of CUCKOO Workgroup is supported by grants from the National Basic Research Program (973 project) (2007CB947401, 2010CB945400), National Natural Science Foundation of China (90919001, 30700138, 30830036, 30900835, 31071154),

Introduction

Schematic diagram of protein domain structures with functional motifs/sites is an important part in a large proportion of scientific articles which are focused on molecular and cellular researches. Diagram of protein domain/motif structures in an attractive, concise and precise manner is greatly helpful for a broad readership to grasp the old and novel functions of proteins rapidly.

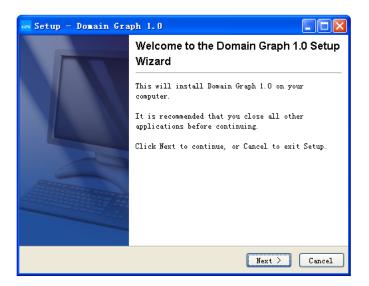
Usually, experimentalists could draw a protein domain graph with Microsoft PowerPoint, PhotoShop or other graphic softwares. However, the scale of a functional domain is often approximately decided by eyes. Thus, diagram of protein domain structures in exact proportions is almost unavailable. Also, the position of a specific motif or functional sites (e.g., a phosphorylation site) could be only roughly pointed. In this regard, preparation of an exquisite figure is quite time-consuming by hand-drawing. On the other hand, the protein domain graphs could be automatically generated by a dozen of computational programs. For example, the Pfam, SMART, PROSITE, InterPro and other related databases or online tools could predict out the functional domains organization of a given protein sequence, and generate the result into a figure. However, these tools couldn't help experimentalists to design their own graphs. Taken together, a software to generate user-defined protein domain graphs will be a great help for experimentalists to prepare their manuscripts.

Now, we present a software of DOG (<u>Domain Graph</u>, version 2.0) for experimentalists, to prepare publication-quality figures of protein domain structures. The scale of a protein domain and the position of a functional motif/site will be precisely calculated. The DOG 2.0 was written in JAVA 1.5 (J2SE 5.0) and packed with Install4j 4.0.8. Thus, the DOG 2.0 could be easily installed on a computer. Then we developed several packages to support three major Operating Systems (OS), including Windows, Unix/Linux and Mac. The Windows XP, Fedora Core 6 OS (Linux), Apple Mac OS X 10.4 (Tiger) and 10.5 (Leopard) were chosen to test the stability of DOG 2.0 software. For Windows and Linux systems, a Java Runtime Environment 6 (JRE) package of Sun Microsystems was also included.

Download & Installation

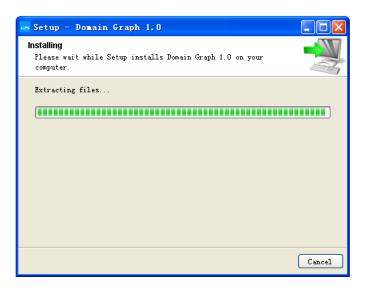
The DOG 2.0 software was implemented in JAVA 1.5 (J2SE 5.0), and could be installed on three major Operating Systems (OS), including Windows, Linux/Unix or Mac OS X systems. The local stand-alone packages of DOG 2.0 can be freely available at <u>http://dog.biocuckoo.org/software.php</u>. We recommend that users could download the latest release.

Please choose the proper package to download. After downloading, please double-click on the software package to begin installation, following the user prompts through the installation. And snapshots of the setup program for windows are shown below:



🔤 Setup - Domain Graph 1.0
Select Destination Directory Where should Domain Graph 1.0 be installed?
Select the folder where you would like Domain Graph 1.0 to be installed, then click Next.
C:\Program Files\DOG Browse
The program requires at least 63.66 MB of disk space.
<pre></pre>

an Setup - Domain Graph 1.0
Select Start Menu Folder Where should Setup place the program's shortcuts?
Select the Start Menu folder in which you would like Setup to create the program's shortcuts, then click Next.
Domain Graph 1.0
PHP Home Edition 2
Real tek SoundMAX
UltraEdit UltraISO
WinRAR
✓ Create shortcuts for all users
🗌 Don't create a Start Menu folder
<pre>Sack Next > Cancel</pre>

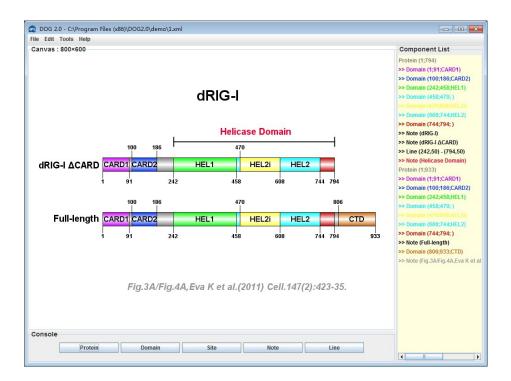




Finally, please click on the Finish button to complete the setup program.

The DOG work environment

When you open DOG for the first time, DOG activates the work environment, including the Canvas, Console panel, Component List and Menus. Also, there are 34 examples included in the software. Randomly, the schematic diagram of dRIG-I domain structures is shown below.



Canvas

Display the graph of the current project. You can use the keyboard **UP/DOWN** or mouse **Wheel Up/Wheel Down** to zoom in/out the graph. You can also use the Right-Click popup menu to adjust the graph.

Edit	
Add	•
Duplicate	
Delete	
Canvas Size	t l
Zoom In	Up
Zoom Out	Down
Fit Width	
Save Projec	t
Export Imag	е

Console

This panel contains four option buttons for drawing protein domain structures.

- 1. **Protein** button: Define the basic properties of the current protein.
- 2. **Domain** button: Add a functional domain to the current protein.
- 3. **Site** button: Add short motif (usually<15aa) or functional site to the current protein.
- 4. Note button: Add name of the current protein or some other comments.
- 5. Line button: Add line , Arrow , DoubleArrow or Scales.

Component List

List all the components of the current project, including protein, domain, site and note. Different components could be marked in different colors and major properties.

You can use the Right-Click popup menu to edit, delete or duplicate the selected component.

Edit	;sfsf)
Duplicate	
Move 🕨 🕨	Up
Delete	Down

You can also double click a component to edit it.

Menus

File menu



New project

Open a new and untitled DOG project.

Open project

Display a dialog box allowing you to open an existing DOG project file and display the contents in a new canvas.

Save

Save the contents of the current project in XML format as a file in the current directory or folder on the disk. If this is the first time that you are saving the file, you must enter a file name. If the file has been saved before, the existing file name is used.

Caution: The Save command will overwrite any file with the same name that is in the same directory or folder! If you do not want to do this, choose **File -> Save As** and give the file a different name.

Save As...

Display a dialog box allowing you to save the contents of the current project in XML format as a file, with a file name that you provide.

Export Image

Export image in PNG, JPEG, TIFF or SVG format to a file on the disk.

Exit

Close the current project and exits the current DOG session. A dialog asks if you want to save or abandon the changes, or cancel the command.

Edit Menu



Add Protein

Add a new protein.

Add Domain

Add a functional domain to the current protein.

Add Site

Add short motif (usually<15aa) or functional site to the current protein.

Add Note

Add name of the current protein or some other comments.

Add Line

Add lines of 4 types: Line, Arrow, DoubleArrow, Scale.

Canvas size

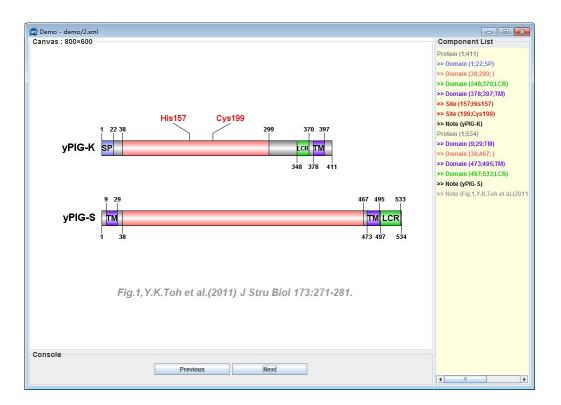
Set the size of current canvas.

Tools menu

Tools	
Demo	Ctrl-D
Batch Export Images	Ctrl-B
Image Format	Ctrl-F

Demo

We randomly re-drew domain graphs for 35 distinct proteins from four journals, including Cell, Molecular Cell, The Journal Structure Biology (JSB), Structure. These instances could be browsed in online or software demos.



Batch Export Images

🐵 Batch Export Images	
DOG Project List	Image Parameter
C:\Program Files (x86)\DOG2.0\demo\1.xml	Width 800 pix -
C:\Program Files (x86)\DOG2.0\demo\10.xml	
C:\Program Files (x86)\DOG2.0\demo\11.xml	
C:\Program Files (x86)\DOG2.0\demo\12.xml	Height 600 pix
C:\Program Files (x86)\DOG2.0\demo\13.xml	
C:\Program Files (x86)\DOG2.0\demo\14.xml	Image Format IPG (72dpi)
C:\Program Files (x86)\DOG2.0\demo\15.xml	Image Format JPG (72dpi)
C:\Program Files (x86)\DOG2.0\demo\16.xml	
	Export Folder C:\Program Files (x86)\DOG2.0\export
Remove All Remove Add File	Cancel Export

With this tool, you can batch export images form DOG projects into JPG(72dpi), PNG(72dpi), TIFF(300/600dpi) or SVG(vector image).

Image Format

💿 Image Format	
Load Image	
	>>
Close	Convert

With this tool, you can convert image in JPG, PNG or GIF format to TIFF format with 300-1200dpi.

Illustration of Protein Domain Structures

New Protein

When you click the *Protein* button or choose **File -> New Project**, a new protein feature dialog box will appear as shown below:

💿 New Protein				_X
Preview	Option			
	Start	1	Down -	
	End		Down -	
	Height	30	Color	
i 200	Vertical Position	0	Font Size	12
	Horizontal Position	0	Locked	
	Cancel			ОК

The right area of the property dialog box contains the following settings for the protein:

- 1. Sequence length of the protein
- 2. Display height of the protein
- 3. Display color of the protein
- 4. Font size of the position number
- 5. Vertical position in the canvas
- 6. Horizontal position in the canvas. When the checkbox **Locked** be unselected, the protein can be set at any position in the canvas.

Note: For convenience, the "Preview" panel shows the effect of current figure.

The DOG version 2.0 supports multi-protein display. You can add two or more proteins in a canvas.

Canvas : 800×600				Component List Protein (1:520) >> Domain (1:341;)
	PRC1			>> Domain (341;466;) >> Note (GFP-) >> Note (GFP-PRC1-FL)
GFP-PRC1-FL	341	466	620	>> Note (PRC1) Protein (1;486) >> Domain (1;341;)
GFP-PRC1-NSAC		406		>> Domain (341;466;) >> Note (GFP-PRC1-NS∆C) >> Note (GFP-) Protein (1;468) >> Domain (1;341;)
GFP- GFP-PRC1-NS		466		>> Domain (341;466;) >> Note (GEP-PRC1-NS) >> Note (GEP-) >> Note (Fig.1A.Radhika S et a
GFP-	1999 1997			
Fig.1A.Radhika	a S et al. (2011) Cell. 142(3,	:433-43.		
Console				

Add Domain

When you click the *Domain* button or choose **Edit -> Add Domain**, a domain property dialog box will appear as shown below:

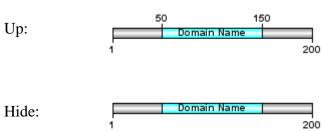
🐵 Add Domain			×
Preview	Option		
	Start		Down 💌
	End		Down 💌
Domain Name	Name		Center -
1 50 150 200	Color		
	Font Size	20	
	Cancel		ОК

The right area of the property dialog box contains the following settings for the domain:

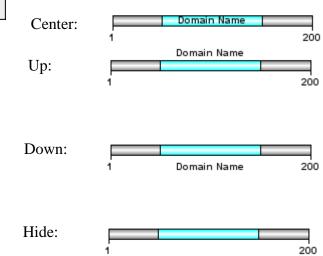
- 1. Start position of the domain.
- 2. End position of the domain.
- 3. Name of the domain.
- 4. Display color of the domain.
- 5. Font size of the text

Note:

Down 💌	You can use the position direction combo box to set the start and end position texts display above or under the domain or not display at all.
Down	
Up	
Hide	Down: Domain Name
	1 50 150 200



Center Center Up Down Hide Use the name **Direction** combo box to set the name of domain display above, under or inside the domain or not display at all.



Add Site

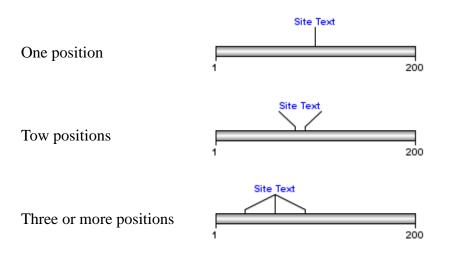
When you click the *Site* button or choose **Edit** -> **Add Site**, a site property dialog box will appear as shown below:

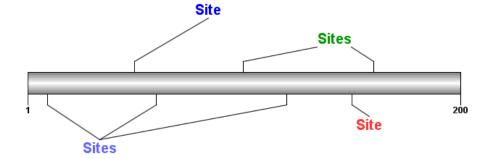
e Add Site Preview	Option Position(s)	123;234	(delimited with	semicolons)
Site Text	Text	123	Font Size	20
1 200	Text Color		Show Position	
	Delta X	0	Delta Y	50
	Cancel			ОК

The right area of the property dialog box contains the following settings for the site:

- 1. Positions of the site.
- 2. Text of the site
- 3. Font size of the text.
- 4. Display Color of the text.
- 5. Display position of the site text.

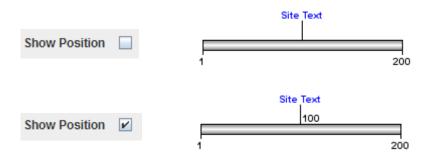
If you have more than one position to draw, please delimit the positions with <u>semicolons</u>. There are three different display ways based on the number of the positions.





You can use the mouse drag the text to a proper position in the canvas.

Use the Show Position check box to set the line display with or without position text.



Add Note

When you click the *Note* button or choose **Edit -> Add Note**, a note property dialog box will appear as shown below:

🐵 Add Note	
Preview	Option
	Text
Note Text	Font Size 32 Text Color
1 200	Font Style Bold Angle 0
	Delta X 0 Delta Y 60
	Cancel OK

The right area of the property dialog box contains the following settings for the note:

- 1. Text of the note.
- 2. Font size of the text.
- 3. Color of the text.
- 4. Font style of the text.

5. Display position in the canvas

You can use the mouse drag the text to a proper position in the canvas.

Add Line

When you click the *Line* button or choose **Edit -> Add Line**, a note property dialog box will appear as shown below:

🙉 Add Line			.
Preview	Options		
	Line Weight	1	Color
	Style	Line 💌	
1 200	X1	0	Y1 60
	X2	150	Y2 60
	Cancel		ОК

- 1. Weight of the Line.
- 2. Color of the Line.
- 3. Line Style:

Line	-
Line	
Arrow	
DoubleArr	ow
Scale	

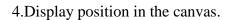
There are four styles of line:

1). Line

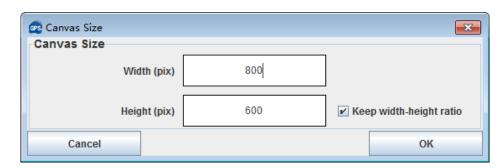


- 3). DoubleArrow
- 4). Scale





Canvas size



- 1. Set the width of current canvas(pix).
- 2. Set the height of current canvas(pix).

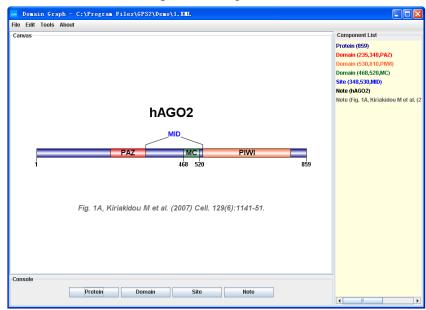
Keep width-height ratio

keep the width-height ratio when setting the canvas.

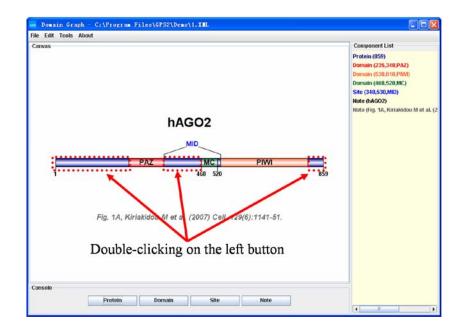
Mouse-clicking

3.

For convenience, we add a new function of mouse-clicking. Here, we used hAGO2 (1.xml in demo) as an instance to depict the usage.



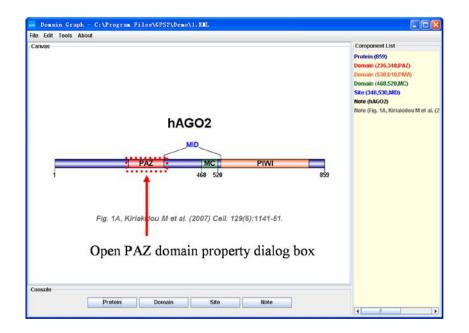
For further editing of protein parameters (e.g., color, length, and font size, etc), you can directly double-click the left button on the marker region below:



Then the protein feature dialog box will appear as shown below:

🚗 Domain Graph - C:	\Program Files\GPS2\Demo\1.XML		🛛
File Edit Tools About			
Canvas			Component List
			Protein (859)
			Domain (235,348,PAZ)
			Domain (530,810,PIWI)
			Domain (468,520,MC)
			Site (348,530,MID)
	as Edit Protein	5	Note (hAGO2) Note (Fig. 1A, Kiriakidou M et al. (2
	Preview	Option	Note (Fig. 1A, Riffaktuou M et al. (2
	Treview	option	
		Protein Length 859	
		Height 28	
		·	
1		200 Color	
	'	200	
		Font Size 16	
		·	
F	ig. 1/		
	9. 17	OK Cancel	
	1		-
Console			
	Protein Domain	Site Note	

If you want to edit a protein domain, please double-click the left button on the marker region below:



Then the PAZ domain property dialog box will appear as shown below:

am Domain Graph -	C:\Program Files\GPS2\Demo\1.	X III.		
File Edit Tools Abou	rt			
Canvas				Component List
				Protein (859)
				Domain (235,348,PAZ)
				Domain (530,810,PIMI) Domain (468,520,MC)
				Site (348,530,MID)
				Note (hAGO2)
	🚥 Edit Domian			(Fig. 1A, Kiriakidou M et al. (2
	Preview		Option	
			Start 235 Hide	•
			End 348 Hide	
1	Domain Name		Name PAZ Center	-
	1	200	,	
			Color Font Size 20	
	Fi		OK Cancel	
			Calica	
Console				
	Protein Domain	Site	Note	

Also, you can use similar method to edit Site or Note information.

Release Note

- 1. Feb. 2nd, 2008, the final packages of online demo and local stand-alone softwares of DOG 1.0 are released.
- 2. Mar. 25th, 2008, a bug on opening project was found and fixed.
- 3. Apr. 19th, 2008, Dr. Fernan Aguero (San Martin, Argentina), had contacted and reminded us that our software could not be installed or worked under Linux/Unix systems. We have re-complied the package of DOG 1.0 for Linux/Unix to fix the bug.
- 4. May 18th, 2008, a new function of "Mouse-clicking" was added in the software. And the figure format was extended to be exported in JPEG format.
- 5. Aug. 28th, 2008, rebuild the GUI with NetBeans 6.1.
- 6. Jan. 3rd, 2009, DOG version 1.0.3 was released. We fixed a bug that cannot create a new file under Mac OS X. The Acknowledgement list and contact information were added into the new version.
- 7. Jan. 19th, 2009, DOG web server was moved to new website (<u>http://dog.biocuckoo.org</u>) and a new GPS logo was put into use.
- 8. Apr. 7th, 2009, DOG version 1.0.4 was released. The DOG image can be exported in TIFF format with 300 or 600dpi. **Image Format** was added in **Tools** menu.
- 9. Jun. 10th, 2009, DOG version 1.0.5 was released. Express the domain length with relative length instead of absolute length.
- 10. Jan. 6th, 2011, DOG 2.0 beta version released. The new version supports multi-protein display and SVG (Scalable Vector Graphics) image output.
- 11. Nov. 6th, 2011, the official version of DOG 2.0 was released. In contrast to the previous version of DOG, the new version supports more functions, including multi-protein display, SVG (Scalable Vector Graphics) image output, canvas resize and draw line or arrow.