WP9 Use case: From cells to molecules - integrating structural data

SurveyMonkey

1. Do you currently do any shape fitting?

	Response Percent	Response Count
Yes	**80.0%**	**36**
No, but would do if a web-service was available	13.3%	6
No, tools are not mature enough	0.0%	0
No, not enough data available	0.0%	0
No, I don't need it	4.4%	2
No – other reason	2.2%	1
	Comment	3
	answered question	**45**
	skipped question	**0**

2. If you answered "No" above, please describe what you would be looking for/need in terms of tools, data, web services or other resources.

	Response Count
	5
answered question	**5**
skipped question	**40**

3. What type(s) of shapes do you use?

	Response Percent	Response Count
Volume	80.5%	33
Sub-volume	53.7%	22
Atomic models	**82.9%**	**34**
Course-grained models	22.0%	9
Geometric shapes – cube, ellipsoid, drawn by hand, based on feature in volume	14.6%	6
Other (please specify)	9.8%	4
	answered question	**41**
	skipped question	**4**

4. What type(s) of volume data do you fit into?

	Response Percent	Response Count
EM single particle	**75.6%**	**31**
EM 2D crystals	4.9%	2
EM Helices	12.2%	5
ET Tomogram	24.4%	10
ET Sub tomogram averages	26.8%	11
SAXS	29.3%	12
SXT	0.0%	0
Other (please specify)	9.8%	4
	answered question	**41**
	skipped question	**4**

5. Which software are you using for shape matching (select all that you use)? Please note: while this is a long list, we have no doubt forgotten several software packages - please enter any that are missing below in the comments field.

	Response Percent	Response Count
Amira	2.6%	1
Chimera	**61.5%**	**24**
CoAn/BBHP	0.0%	0
DireX	5.1%	2
DockEM	7.7%	3
EMAN - foldhunter/helixhunter	12.8%	5
EMFIT	12.8%	5
Flex-EM	5.1%	2
Fold-EM	2.6%	1
MDFF (NAMD/VMD)	23.1%	9
MODELLER	7.7%	3
Mod-EM	2.6%	1
MOLREP	15.4%	6
NMFF	5.1%	2
NORMA	5.1%	2
Situs - CoLoRes/qplasty	28.2%	11
3SOM	2.6%	1
Veda/Urox	12.8%	5
Yup.scx	0.0%	0
Other (please specify)	46.2%	18
	answered question	**39**
	skipped question	**6**

6. Do you use a GUI or a command line script? Do you follow a documented or published protocol, or do you use an in-house protocol?

		Response Percent	Response Count
Use GUI		**68.3%**	**28**
Use command line script		65.9%	27
Follow documented or published protocol		31.7%	13
Follow in-house protocol		31.7%	13
No, each case is different		24.4%	10
		Comment	2
		answered question	**41**
		skipped question	**4**

7. What, if any, meta data does the software need (select all that apply)?

		Response Percent	Response Count
Resolution		**66.7%**	**24**
Density level representing surface (contour level)		38.9%	14
Density level above background scattering and/or masks		30.6%	11
Symmetry		61.1%	22
Grid sampling		55.6%	20
Other (please specify)		19.4%	7
		answered question	**36**
		skipped question	**9**

8. Any options/feature that is particularly useful with the software that you use?

		Response Percent	Response Count
Ease of use		**61.1%**	**22**
Features available - please use comment field		30.6%	11
Scriptable		44.4%	16
Availability		**61.1%**	**22**
Developed in-house		22.2%	8
		Comment	8

answered question	**36**
skipped question	**9**

9. What type of matching do you do (select all that apply)?

		Response Percent	Response Count
Manual fit		56.1%	23
Rigid body		**90.2%**	**37**
Flexible		58.5%	24
		Comment	2

answered question	**41**
skipped question	**4**

10. If your volume data have symmetry elements, such as in viruses, chaperons, helices etc., how do you handle the symmetry (select all that apply)?

		Response Percent	Response Count
Ignore symmetry		29.0%	9
Fit into each symmetry position		**54.8%**	**17**
Only fit into one symmetry position		51.6%	16
		Comment	11
		answered question	**31**
		skipped question	**14**

11. How do you evaluate the results (select all that apply)?

		Response Percent	Response Count
Visual inspection		**80.0%**	**32**
Cross correlation score		72.5%	29
Atom inclusion score		22.5%	9
Special scoring function different from matching/fitting function		25.0%	10
		Comment	1
		answered question	**40**
		skipped question	**5**

12. What is your role?

		Response Percent	Response Count
Principal investigator		**54.5%**	**24**
Staff scientist		18.2%	8
Postdoc		11.4%	5
Graduate student		15.9%	7
Undergraduate student		2.3%	1
Industry		0.0%	0
Government		2.3%	1
Management		0.0%	0
Other (please specify)		4.5%	2
		answered question	**44**
		skipped question	**1**