

NAMD Survey 2000

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*Existing items: Items related to NAMD existing features.

*Planned items: Items related to NAMD planned features.



NAMD Questionnaire

The NAMD Questionnaire is at:

http://www.ks.uiuc.edu/Research/namd/survey/survey2000.html



Response Rates

NAMD 2000 survey was announced on May 12, 2000 to 383 registered users of NAMD 2.1. For convenience reasons the survey was mailed only to individuals who registered since January 7, 2000, and were included in our newly established database. Two reminders were sent to users on May 25 and June 6, leading to a 33.7% total response rate (129 responses).

Date survey notice sent	May 12	May 25	June 6	Total
Number of persons receiving notice by date	383	344	295	383
Responses up to date of next notice	41	52	36	129
Response rate for total population (all 383)	10.7%	13.6%	9.4%	33.7%
Cumulative response rate		24.3%	33.7%	33.7%

Those responses that were considered incomplete were deleted from our dataset. The deletions fell into two categories: Non-responsive and duplicates. Non-responsive records were those instances in which respondents did not answer most of the questions in the survey. Duplicates were those instances in which there was more than one response for a person, based on their e-mail address. After deletions, 109 records were used for further analyses.

Deletions	Non-Responsive	Duplicates	Total
	18	2	20
Number of records in dataset after removing deletions			109

NAMD

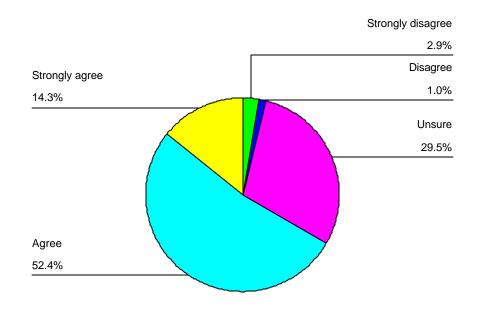


User Profile

An overwhelming majority of NAMD users are affiliated with academic institutions (80%) and use NAMD for research (80%). Over 63% of NAMD respondents reported moderate to very high levels of experience with molecular modeling. 11% of the respondents reported to be funded by NIH. 65% of NAMD users run the program on Linux-i686 or Origin2000. Most of our users first heard of NAMD via the web (48%) or from friends (31%), and they clearly prefer to be informed of NAMD news by Email (57%) or web announcements (43%). The respondents reported the majority of sites had one user (62%), though many sites had more than one user (38%).



Rating Distribution of Satisfaction



Means & Std Deviation Distribution

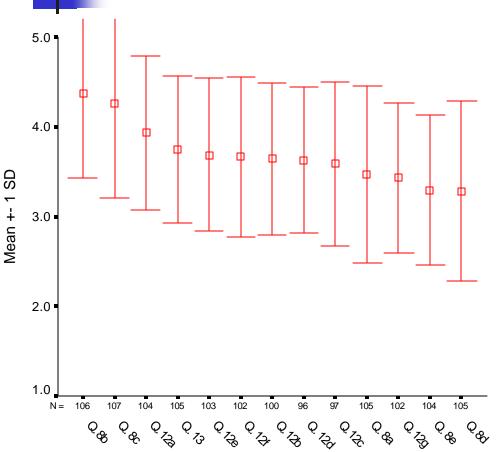
Question	Mean	Std Deviation
Q. 13 - Satisfied	3.74	.82

Frequency Distribution

Question Items	Frequency
Strongly disagree	3
Disagree	1
Unsure	31
Agree	55
Strongly agree	15
Total	105

•The mean response was 3.74 with a standard deviation of .82 on a 5-point scale (1=strongly disagree, 5=strongly agree).

Rating Distribution of Existing Items



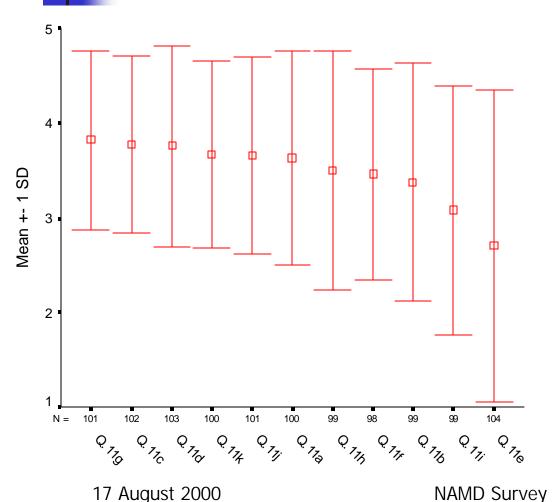
Means & Std Deviation Distributions

Question	Mean	Std Deviation
Q. 8b - Use Because Free	4.38	.95
Q. 8c - Use Because Source	4.25	1.06
Q. 12a - Well Written	3.93	.86
Q. 13 - Satisfied	3.74	.82
Q. 12e - Web Instructive	3.69	.85
Q. 12f - Docs Clear	3.67	.89
Q. 12b - Meets Needs	3.64	.85
Q. 12d - Support Meets Exp.	3.63	.81
Q. 12c - Devs Respond	3.59	.92
Q. 8a - Use Because Meets	3.47	.98
Q. 12g - Docs Complete	3.43	.84
Q. 8e - Use Because Better	3.30	.83
Q. 8d - Use Because Friendl	3.28	1.00

- •Mean responses range between 3.28 to 4.38 on a 5-point scale (1=strongly disagree, 5=strongly agree).
- •Standard deviations range from .81 to 1.06. The higher the std deviation, the higher the disagreement among respondents on the specific items.



Rating Distribution of Planned Items



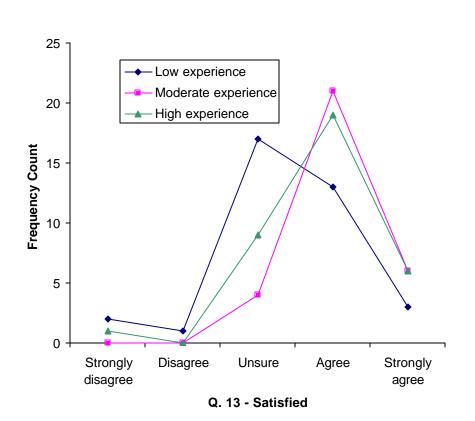
Means & Standard Deviations Distributions

Question	Mean	Std Deviation
Q. 11g - Need Structure	3.82	.94
Q. 11c - Need Timestep	3.77	.93
Q. 11d - Need Minimization	3.76	1.06
Q. 11k - Need Sampling	3.67	.99
Q. 11j - Need Mutation	3.65	1.04
Q. 11a - Need Serial	3.63	1.13
Q. 11h - Need Amber	3.51	1.26
Q. 11f - Need Scripting	3.46	1.11
Q. 11b - Need Scaling	3.37	1.26
Q. 11i - Need Gromacs	3.08	1.31
Q. 11e - Need Windows	2.70	1.65

- •Mean responses range between 2.70 to 3.82 on a 5-point scale (1=strongly disagree, 5=strongly agree).
- •Standard deviations range from .93 to 1.65. The higher the std deviation, the higher the disagreement among respondents on the specific item.



Satisfaction by Level of Molecular Modeling Experience



Mean and Std Deviation Distribution

Experience Level	Mean	Std Deviation
Low experience (N=36)	3.39	.90
Moderate experience (N=31)	4.06	.57
High experience (N=35)	3.83	.82

Frequency Distribution

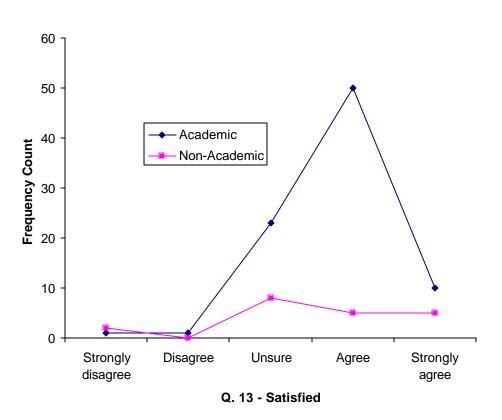
	Q. 3 - Experience, Three Categories			
Q. 13 - Satisfied	Low experience	Moderate experience	High experience	
Strongly disagree	2		1	
Disagree	1			
Unsure	17	4	9	
Agree	13	21	19	
Strongly agree	3	6	6	

- •Experience has an impact on user satisfaction: a significant difference was found between low-experience and moderate-experience groups; moderate-experience users reported higher satisfaction (F = 6.4).
- •A correlation analysis indicated a significant positive relationship between experience and satisfaction. (r=.22).

NAMD.



Satisfaction by Affiliation



Mean & Std Deviation Distribution

	Q. 2 - Affiliation	
Q. 13 -		Non-
Satisfied	Academic	Academic
Mean	3.79	3.55
Std Deviation	.71	1.19

Frequency Distribution

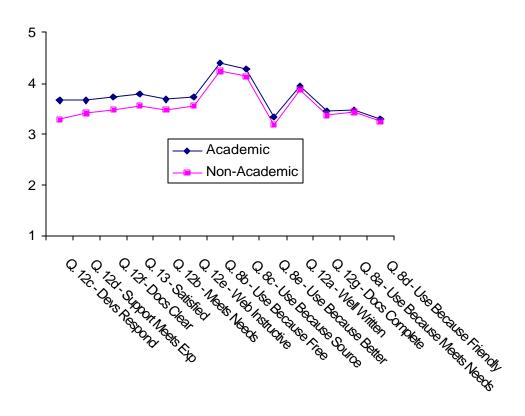
	Q. 2 - Affiliation		
Q. 13 - Satisfied	Academic	Non-Academic	
Strongly disagree	1	2	
Disagree	1		
Unsure	23	8	
Agree	50	5	
Stronlgy agree	10	5	
Total	85	20	

•Mean responses were 3.79 for academic users and 3.55 for non-academic users on a 5-point scale (1=strongly disagree, 5=strongly agree). No significant difference was found between the two groups.

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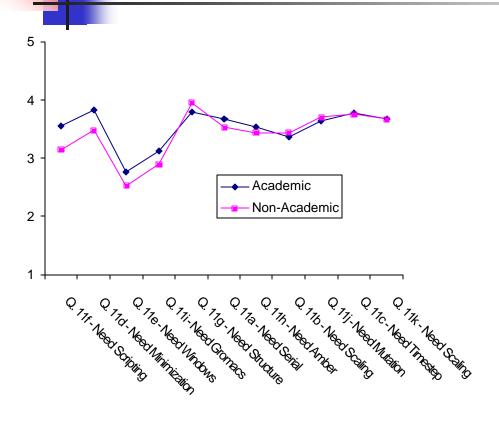


Mean Responses to Existing Items by Affiliation

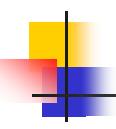


•No significant difference between academics and non-academics was found; clear pattern of slightly higher rating by academic users is indicated.

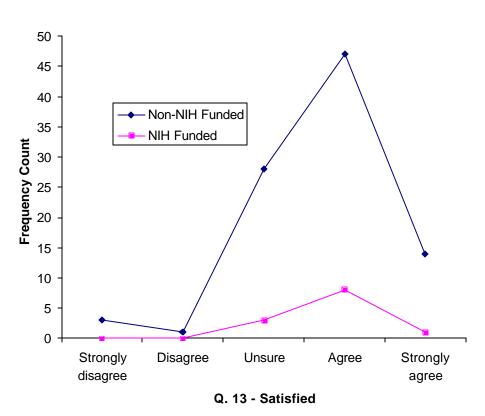
Mean Responses to Planned Items by Affiliation



•No significant difference was found between academic and non-academic users.



Satisfaction by Funding Source



Mean & Std Deviation Distribution

	Q. 4 - NIH Funded	
Q. 13 -		
Satisfied	No	Yes
Mean	3.73	3.83
Std Deviation	.85	.58

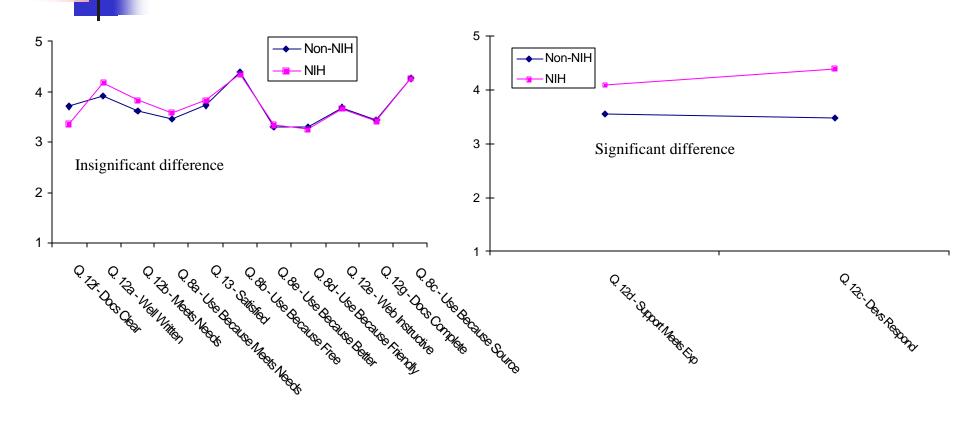
Frequency Distribution

	Q. 4 - NIH Funded		
Q. 13 - Satisfied	No	Yes	
Strongly disagree	3		
Disagree	1		
Unsure	28	3	
Agree	47	8	
Strongly agree	14	1	
Total	93	12	

•Mean responses were 3.73 for non-NIH users and 3.83 for NIH-funded users on a 5-point scale (1=strongly disagree, 5=strongly agree). No significant difference was found between the two groups.

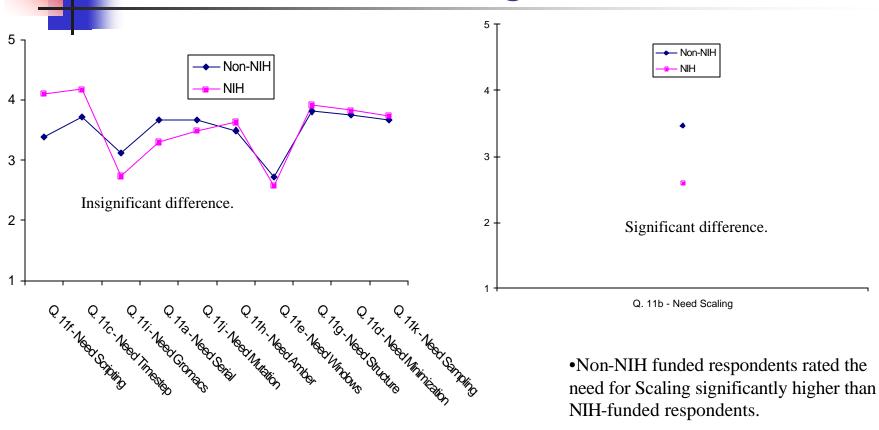
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- •NIH-funded respondents rated Support significantly higher than non-NIH funded respondents.
- •No other significant difference was found between the two groups.

Mean Responses to Planned Items by Funding Source



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•No other significant difference was found

between the two groups.

Correlations of Existing Items With Satisfaction

Evaluation Question	Correlations
Q. 12b - Meets Needs (N=100)	.675
Q. 12d - Support Meets Exp (N=96)	.644
Q. 12a - Well Written (N=103)	.619
Q. 8a - Use Because Meets Needs (N=102)	.575
Q. 12c - Devs Respond (N=97)	.524
Q. 8e - Use Because Better (N=102)	.448
Q. 8c - Use Because Source (N=103)	.412
Q. 12f - Docs Clear (N=101)	.378
Q. 8d - Use Because Friendly (N=103)	.377
Q. 12e - Web Instructive (N=102)	.369
Q. 8b - Use Because Free (N=102)	.283
Q. 12g - Docs Complete (N=102)	.279

•All ratings of existing items have a significant Pearson's correlation with satisfaction: the higher the ratings, the higher the satisfaction.



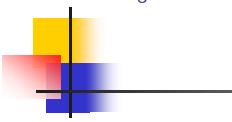
Summary of Findings

- The overall rating of NAMD is high. Existing features are rated higher than planned features. Responses to existing items indicate higher agreement among the respondents than responses to planned items.
- Overall satisfaction is high; experience in molecular modeling work has an impact on satisfaction of users. There is a significant positive relationship between experience and satisfaction: the higher the experience, the higher the satisfaction reported by the users.
- Academic and non-academic respondents rate existing and planned features similarly.
- In most cases, NIH-funded and non-NIH funded respondents rate existing features similarly. NIH-funded respondents rate Support significantly higher than non-NIH funded respondents.
- In general, NIH-funded and non-NIH funded respondents rate planned features similarly. Non-NIH funded respondents rate the need for Scaling higher than NIH-funded respondents.
- The responses to all existing features are significantly associated with overall satisfaction: the higher the rating, the higher the overall satisfaction.



Other analyses

Responses to Planned Items (Q. 4, 11) by Funding Source



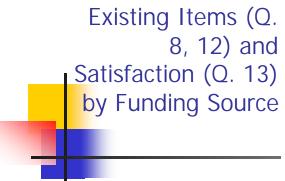
•Non-NIH funded respondents rate "Scaling on 100's of CPUs" as significantly more important (mean=3.46) than NIH funded respondents (mean=2.60).

Descriptives - Funding Source (NIH or Non-NIH) for Planned Items

							95% Confidence Interval for Mean			
			N	Mean	Std. Deviation	Std. Error	Lower Bound	Upper Bound	Minimum	Maximum
	Q. 11a - Need Serial	No	90	3.67	1.16	.12	3.42	3.91	1	5
		Yes	10	3.30	.82	.26	2.71	3.89	2	5
		Total	100	3.63	1.13	.11	3.40	3.86	1	5
	Q. 11b - Need Scaling	No	89	3.46	1.25	.13	3.20	3.72	1	5
		Yes	10	2.60	1.07	.34	1.83	3.37	1	5
•]		Total	99	3.37	1.26	.13	3.12	3.62	1	5
	Q. 11c - Need Timestep	No	90	3.72	.94	9.87E-02	3.53	3.92	1	5
		Yes	12	4.17	.83	.24	3.64	4.70	3	5
		Total	102	3.77	.93	9.23E-02	3.59	3.96	1	5
	Q. 11d - Need	No	91	3.75	1.03	.11	3.53	3.96	1	5
	Minimization	Yes	12	3.83	1.34	.39	2.98	4.68	1	5
		Total	103	3.76	1.06	.10	3.55	3.96	1	5
	Q. 11e - Need Windows	No	92	2.72	1.65	.17	2.38	3.06	1	5
		Yes	12	2.58	1.73	.50	1.48	3.68	1	5
		Total	104	2.70	1.65	.16	2.38	3.02	1	5
	Q. 11f - Need Scripting	No	88	3.39	1.12	.12	3.15	3.62	1	5
		Yes	10	4.10	.88	.28	3.47	4.73	3	5
		Total	98	3.46	1.11	.11	3.24	3.68	1	5
	Q. 11g - Need Structure	No	89	3.81	.96	.10	3.61	4.01	1	5
		Yes	12	3.92	.79	.23	3.41	4.42	3	5
		Total	101	3.82	.94	9.38E-02	3.64	4.01	1	5
	Q. 11h - Need Amber	No	88	3.49	1.29	.14	3.22	3.76	1	5
		Yes	11	3.64	1.12	.34	2.88	4.39	1	5
		Total	99	3.51	1.26	.13	3.25	3.76	1	5
	Q. 11i - Need Gromacs	No	88	3.13	1.32	.14	2.85	3.40	1	5
		Yes	11	2.73	1.19	.36	1.93	3.53	1	5
		Total	99	3.08	1.31	.13	2.82	3.34	1	5
	Q. 11j - Need Mutation	No	89	3.67	1.03	.11	3.46	3.89	1	5
		Yes	12	3.50	1.17	.34	2.76	4.24	1	5
		Total	101	3.65	1.04	.10	3.45	3.86	1	5
	Q. 11k - Need Sampling	No	89	3.66	1.01	.11	3.45	3.88	1	5
		Yes	11	3.73	.79	.24	3.20	4.26	3	5
		Total	100	3.67	.99	9.85E-02	3.47	3.87	1	5

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Descriptives - Funding Source (NIH or Non-NIH) for Evaluation Items



•NIH-funded respondents rated Responsiveness significantly higher (mean=4.40) than non-NIH funded respondents (mean=3.49).
•NIH-funded respondents rated Support significantly higher (mean=4.09) than non-NIH

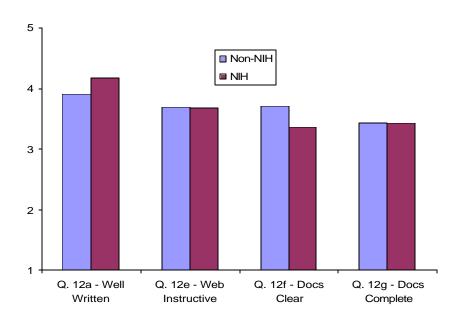
funded respondents (mean=3.56).

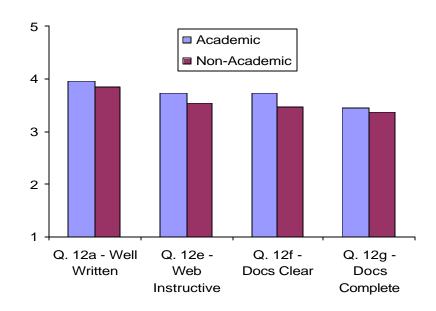
						95% Confidence Interval for			
						Me			
		N	Mean	Std. Deviation	Std. Error	Lower Bound	Upper Bound	Minimum	Maximum
Q. 8a - Use Because	No	93	3.45	.98	.10	3.25	3.65	1	5
Meets Needs	Yes	12	3.58	1.00	.29	2.95	4.22	2	5
	Total	105	3.47	.98	9.58E-02	3.28	3.66	1	5
Q. 8b - Use Because Free		94	4.38	.92	9.46E-02	4.20	4.57	1	5
	Yes	12	4.33	1.23	.36	3.55	5.12	1	5
	Total	106	4.38	.95	9.23E-02	4.19	4.56	1	5
Q. 8c - Use Because	No	95	4.25	1.06	.11	4.04	4.47	1	5
Source	Yes	12	4.25	1.06	.30	3.58	4.92	2	5
	Total	107	4.25	1.06	.10	4.05	4.45	1	5
Q. 8d - Use Because	No	93	3.28	1.04	.11	3.07	3.49	1	5
Friendly	Yes	12	3.25	.75	.22	2.77	3.73	2	4
	Total	105	3.28	1.00	9.81E-02	3.08	3.47	1	5
Q. 8e - Use Because	No	92	3.29	.85	8.82E-02	3.12	3.47	1	5
Better	Yes	12	3.33	.78	.22	2.84	3.83	2	5
	Total	104	3.30	.83	8.18E-02	3.14	3.46	1	5
Q. 12a - Well Written	No	92	3.90	.88	9.15E-02	3.72	4.08	1	5
	Yes	12	4.17	.72	.21	3.71	4.62	3	5
	Total	104	3.93	.86	8.45E-02	3.77	4.10	1	5
Q. 12b - Meets Needs	No	89	3.62	.85	8.97E-02	3.44	3.80	1	5
	Yes	11	3.82	.87	.26	3.23	4.41	3	5
	Total	100	3.64	.85	8.47E-02	3.47	3.81	1	5
Q. 12c - Devs Respond	No	87	3.49	.87	9.37E-02	3.31	3.68	1	5
	Yes	10	4.40	.97	.31	3.71	5.09	3	5
	Total	97	3.59	.92	9.36E-02	3.40	3.77	1	5
Q. 12d - Support Meets	No	85	3.56	.79	8.61E-02	3.39	3.74	1	5
Exp	Yes	11	4.09	.83	.25	3.53	4.65	3	5
	Total	96	3.63	.81	8.28E-02	3.46	3.79	1	5
Q. 12e - Web Instructive	No	91	3.69	.85	8.94E-02	3.51	3.87	1	5
	Yes	12	3.67	.89	.26	3.10	4.23	2	5
	Total	103	3.69	.85	8.40E-02	3.52	3.86	1	5
Q. 12f - Docs Clear	No	91	3.70	.88	9.18E-02	3.52	3.89	1	5
	Yes	11	3.36	1.03	.31	2.67	4.05	2	5
	Total	102	3.67	.89	8.85E-02	3.49	3.84	1	5
Q. 12g - Docs Complete	No	90	3.43	.81	8.52E-02	3.26	3.60	1	5
	Yes	12	3.42	1.08	.31	2.73	4.11	2	5
	Total	102	3.43	.84	8.30E-02	3.27	3.60	1	5
Q. 13 - Satisfied	No	93	3.73	.85	8.80E-02	3.56	3.91	1	5
	Yes	12	3.83	.58	.17	3.47	4.20	3	5
	Total	105	3.74	.82	8.01E-02	3.58	3.90	1	5

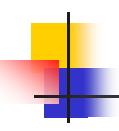
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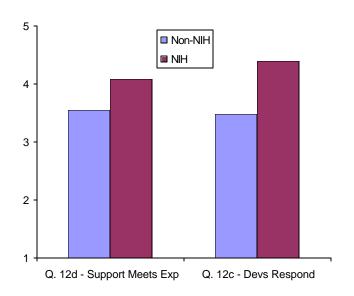
Documentation Items (Q.'s 12a, 12e, 12f, 12g) by Affiliation and Funding Source

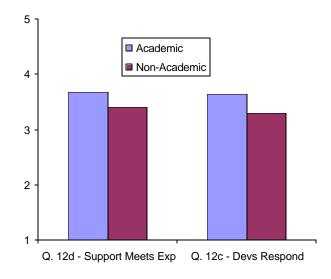






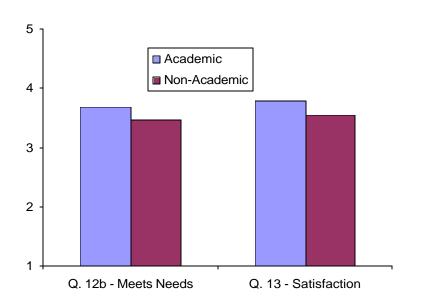
Support Items (Q.'s 12c, 12d) by Affiliation and Funding Source

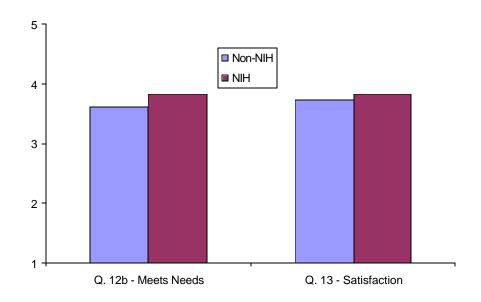






Meets Needs (Q. 12b) by Affiliation and Funding Source





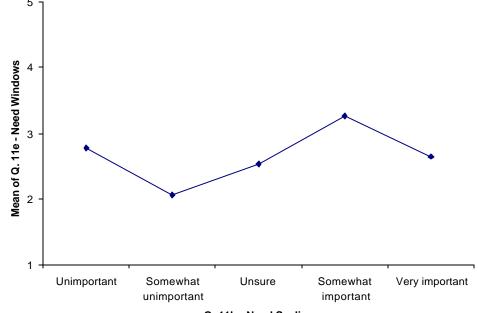
Need Scaling (Q. 11b) and Need Windows (Q. 11e): ANOVA

ANOVA

Q. 11e - Need Windows

	Sum of Squares	df	Mean Square	F	Sig.
Between Groups	12.426	4	3.107	1.178	0.326
Within Groups	247.897	94	2.637		
Total	260.323	98			

•Ratings of 'Need Scaling' was not found to explain the ratings of 'Need Windows'

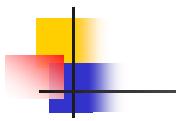


Q. 11b - Need Scaling

Q. 11b - Need Scaling (mean responses)

		Somewhat		Somewhat	
	Unimportant	unimportant	Unsure	important	Very important
Q. 11e - Need Windows	2.78	2.07	2.53	3.26	2.64

Responses to Existing Items by Affiliation



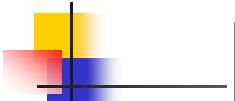
•No significant differences were found.

Descriptives for Affiliation (Academic or Non-Academic) by Evaluation Items

						95% Confiden Me			
		N	Mean	Std. Deviation	Std. Error	Lower Bound	Upper Bound	Minimum	Maximum
Q. 8a - Use Because Meets Needs	Academic	84	3.48	.94	.10	3.27	3.68	1	5
	Non-Academic	21	3.43	1.16	.25	2.90	3.96	1	5
	Total	105	3.47	.98	9.58E-02	3.28	3.66	1	5
Q. 8b - Use Because Free	Academic	85	4.41	.89	9.66E-02	4.22	4.60	1	5
	Non-Academic	21	4.24	1.18	.26	3.70	4.77	2	5
	Total	106	4.38	.95	9.23E-02	4.19	4.56	1	5
Q. 8c - Use Because Source	Academic	85	4.28	.98	.11	4.07	4.49	1	5
	Non-Academic	22	4.14	1.32	.28	3.55	4.72	1	5
	Total	107	4.25	1.06	.10	4.05	4.45	1	5
Q. 8d - Use Because Friendly	Academic	84	3.29	1.00	.11	3.07	3.50	1	5
	Non-Academic	21	3.24	1.04	.23	2.76	3.71	1	5
	Total	105	3.28	1.00	9.81E-02	3.08	3.47	1	5
Q. 8e - Use Because Better	Academic	83	3.33	.78	8.59E-02	3.15	3.50	1	5
	Non-Academic	21	3.19	1.03	.22	2.72	3.66	1	5
	Total	104	3.30	.83	8.18E-02	3.14	3.46	1	5
Q. 12a - Well Written	Academic	83	3.95	.85	9.37E-02	3.77	4.14	1	5
	Non-Academic	21	3.86	.91	.20	3.44	4.27	1	5
	Total	104	3.93	.86	8.45E-02	3.77	4.10	1	5
Q. 12b - Meets Needs	Academic	81	3.68	.83	9.27E-02	3.49	3.86	1	5
	Non-Academic	19	3.47	.90	.21	3.04	3.91	1	5
	Total	100	3.64	.85	8.47E-02	3.47	3.81	1	5
Q. 12c - Devs Respond	Academic	80	3.65	.84	9.43E-02	3.46	3.84	2	5
	Non-Academic	17	3.29	1.21	.29	2.67	3.92	1	5
	Total	97	3.59	.92	9.36E-02	3.40	3.77	1	5
Q. 12d - Support Meets Exp	Academic	79	3.67	.69	7.80E-02	3.52	3.83	3	5
	Non-Academic	17	3.41	1.23	.30	2.78	4.04	1	5
	Total	96	3.63	.81	8.28E-02	3.46	3.79	1	5
Q. 12e - Web Instructive	Academic	83	3.72	.85	9.28E-02	3.54	3.91	2	5
	Non-Academic	20	3.55	.89	.20	3.13	3.97	1	5
	Total	103	3.69	.85	8.40E-02	3.52	3.86	1	5
Q. 12f - Docs Clear	Academic	81	3.72	.90	9.97E-02	3.52	3.91	2	5
	Non-Academic	21	3.48	.87	.19	3.08	3.87	1	5
	Total	102	3.67	.89	8.85E-02	3.49	3.84	1	5
Q. 12g - Docs Complete	Academic	83	3.45	.86	9.43E-02	3.26	3.63	1	5
·	Non-Academic	19	3.37	.76	.17	3.00	3.74	1	4
	Total	102	3.43	.84	8.30E-02	3.27	3.60	1	5
Q. 13 - Satisfied	Academic	85	3.79	.71	7.69E-02	3.64	3.94	1	5
	Non-Academic	20	3.55	1.19	.27	2.99	4.11	1	5
	Total	105	3.74	.82	8.01E-02	3.58	3.90	1	5

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Responses to Planned Items by Affiliation



•No significant differences were found.

Descriptives - Affiliation (Academic or Non-Academic) for Planned Items

						95% Confidence Interval for Mean			
		N	Mean	Std. Deviation	Std. Error	Lower Bound	Upper Bound	Minimum	Maximum
Q. 11a - Need Serial	Academic	79	3.66	1.05	.12	3.42	3.89	1	5
	Non-Academic	21	3.52	1.44	.31	2.87	4.18	1	5
	Total	100	3.63	1.13	.11	3.40	3.86	1	5
Q. 11b - Need Scaling	Academic	78	3.36	1.26	.14	3.08	3.64	1	5
	Non-Academic	21	3.43	1.29	.28	2.84	4.01	1	5
	Total	99	3.37	1.26	.13	3.12	3.62	1	5
Q. 11c - Need Timester	Academic	81	3.78	.84	9.30E-02	3.59	3.96	1	5
	Non-Academic	21	3.76	1.26	.28	3.19	4.34	1	5
	Total	102	3.77	.93	9.23E-02	3.59	3.96	1	5
Q. 11d - Need	Academic	82	3.83	.97	.11	3.62	4.04	1	5
Minimization	Non-Academic	21	3.48	1.36	.30	2.86	4.10	1	5
	Total	103	3.76	1.06	.10	3.55	3.96	1	5
Q. 11e - Need Windows	Academic	83	2.75	1.61	.18	2.39	3.10	1	5
	Non-Academic	21	2.52	1.81	.39	1.70	3.35	1	5
	Total	104	2.70	1.65	.16	2.38	3.02	1	5
Q. 11f - Need Scripting	Academic	77	3.55	1.02	.12	3.31	3.78	1	5
	Non-Academic	21	3.14	1.39	.30	2.51	3.77	1	5
	Total	98	3.46	1.11	.11	3.24	3.68	1	5
Q. 11g - Need Structure	Academic	80	3.79	.92	.10	3.58	3.99	1	5
	Non-Academic	21	3.95	1.02	.22	3.49	4.42	1	5
	Total	101	3.82	.94	9.38E-02	3.64	4.01	1	5
Q. 11h - Need Amber	Academic	78	3.53	1.30	.15	3.23	3.82	1	5
	Non-Academic	21	3.43	1.16	.25	2.90	3.96	1	5
	Total	99	3.51	1.26	.13	3.25	3.76	1	5
Q. 11i - Need Gromacs	Academic	79	3.13	1.30	.15	2.83	3.42	1	5
	Non-Academic	20	2.90	1.33	.30	2.28	3.52	1	5
	Total	99	3.08	1.31	.13	2.82	3.34	1	5
Q. 11j - Need Mutation	Academic	81	3.64	1.05	.12	3.41	3.87	1	5
	Non-Academic	20	3.70	1.03	.23	3.22	4.18	1	5
	Total	101	3.65	1.04	.10	3.45	3.86	1	5
Q. 11k - Need Sampling	Academic	79	3.67	.98	.11	3.45	3.89	1	5
	Non-Academic	21	3.67	1.02	.22	3.20	4.13	1	5
	Total	100	3.67	.99	9.85E-02	3.47	3.87	1	5



Additional Analyses

- No significant correlation found between 'need windows' and 'need scaling' (r=.083).
- No significant interaction was found for 'funding source' and 'need scaling' on the dependent variable 'need windows' when the former two items were entered in a GLM univariate analysis as fixed factors (significance for interaction term was .772).
- No significant differences were found when 'need windows' was the dependent variable and 'platform' was entered as the single factor in a one-way ANOVA (significance value was .555).
- No significant interaction was found when 'funding source' and 'platform' were entered as fixed factors in a GLM univariate analysis with 'need windows' as the dependent variable (significance for interaction term was .656).
- A small, positive correlation (.208) was found between 'need windows' and 'need minimization', and a small, negative correlation (-.205) was found between 'need windows' and 'well written'. However, there is also a small, positive correlation (.202) between 'need minimization' and 'well written'.