

THEORETICAL AND COMPUTATIONAL BIOPHYSICS GROUP

2006 VMD SURVEY REPORT

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EXECUTIVE SUMMARY

The VMD 2006 Survey was announced on July 31 - August 3, 2006 to 26,079 registered users of VMD versions 1.8.3 and higher, and ran through August 7 of that year. Survey questions examined user satisfaction, the impact of the software on work quality, and user ratings of existing and planned features; demographic questions were asked as well.

- A total of 1,596 usable responses were returned by the survey, yielding a response rate of 6.1%. Using standard test percentages, sample size calculations indicate that it can be said with 95% confidence that results for a given question fall within a +/- 2.4% confidence interval (i.e., for any one question, the sample provides 95% confidence that the population response falls within plus or minus 2.4% of a given percentage). Please see the appendix on survey methodology below for more detail.
- Survey results indicate that the majority of VMD users are affiliated with academic institutions (90%) and use VMD for research purposes (91%) with approximately one-fifth indicating research funded at least in part by NIH (21%). Most VMD users are the sole VMD user at their site (34%). A majority of VMD users consider themselves to have an average level expertise with the software (52%) with slightly more users indicating a low level of expertise than a high level. Most survey respondents (63%) had downloaded more than one version of VMD.
- Most users are satisfied with VMD – 94% agreed or strongly agreed with the statement “I am satisfied with VMD”.
- VMD was judged to have a positive impact on work quality – 88% of respondents agreed or strongly agreed with the statement “VMD has improved the quality of my work”.
- A majority of users agree that not having VMD available would have a negative impact on their productivity – 78% agreed or strongly agreed with the statement “Not having VMD available (e.g., in case of discontinued funding of VMD development) would negatively impact my scientific productivity”.

OVERVIEW

VMD (Visual Molecular Dynamics) is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS-X, Unix, or Windows, is distributed free of charge, and includes source code. The VMD home page at the TCBG web site, <http://www.ks.uiuc.edu/Research/vmd/>, provides more information about the program. The VMD 2006 survey is part of an ongoing effort (similar surveys were conducted in 2000 and 2003) to ensure that VMD is up to date, relevant, and of high quality by collecting and analyzing user opinion about the application. VMD users were identified via registration records, and contacted via email with requests that they complete an on-line survey about VMD (see locations below for a copy of the survey) during August, 2006. The following report details the results and administration of the survey.

VMD 2006 Survey (complete copy)

A link to the survey form the users completed is available below; questions are also listed in the appendix. Note that for analysis, interpretation and review purposes all references to the items within the report are based on the numbering of the items as used in the original survey.

VMD 2006 Survey

<http://www.ks.uiuc.edu/Research/vmd/survey/report2006/>

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VMD USER PROFILE

User profile characteristics of those answering the survey are illustrated below:

- 90% of users have academic affiliations.
- 21% are funded at least partially by NIH.
- 91% use VMD for research purposes.
- 34% are the sole user of VMD at their site.
- 52% identified themselves as average-level users of the software.
- 56% indicated using VMD for all or most of their molecular visualization tasks.
- 26% of users also use NAMM.
- 62% have used the VMD tutorial.

Figure 1: VMD User Characteristics

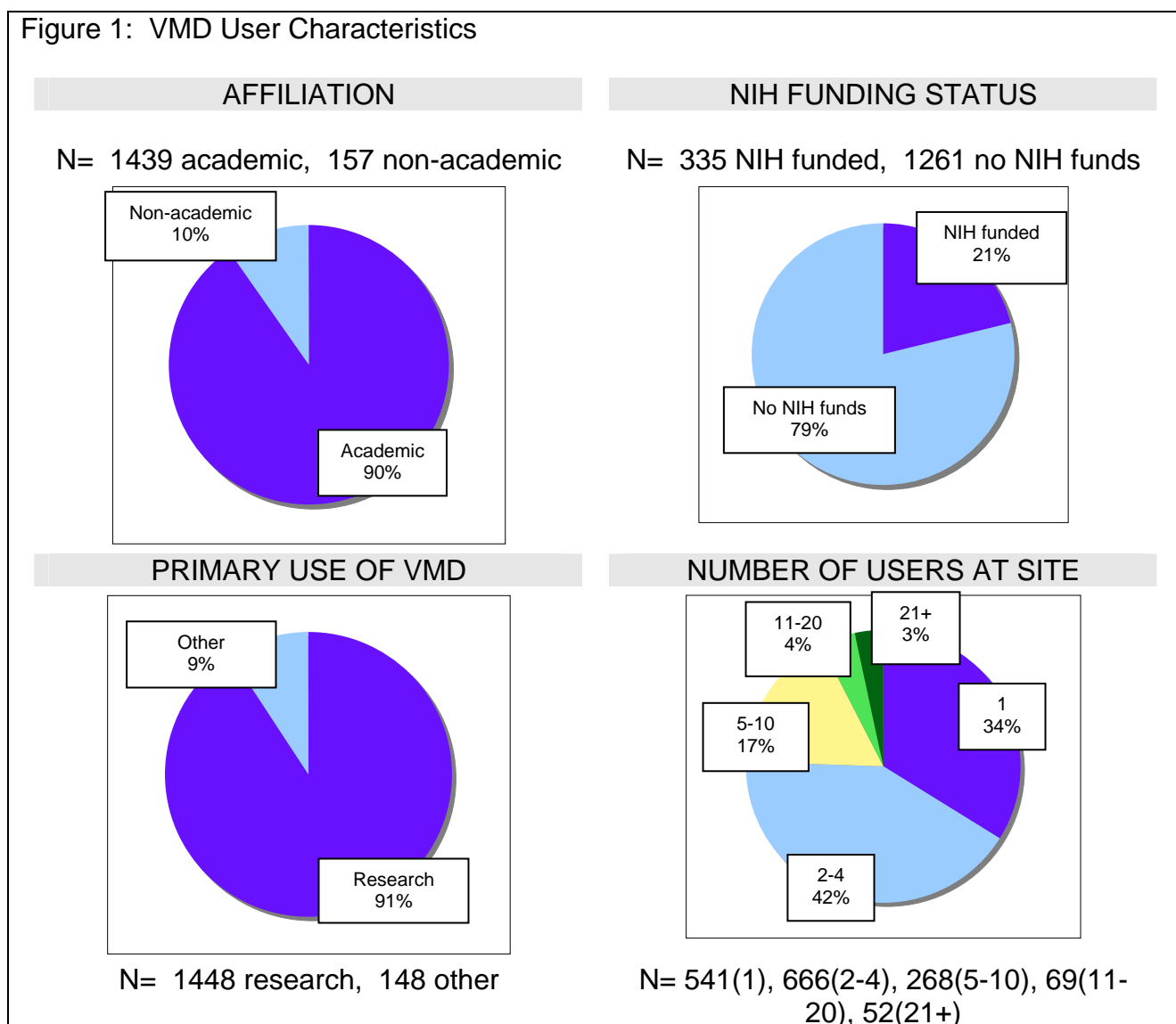
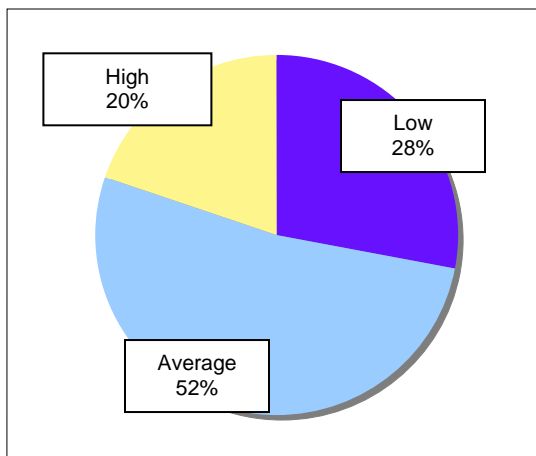


Figure 1: VMD User Characteristics, continued

SOFTWARE EXPERTISE

Q4: "My level of expertise in using VMD is..."

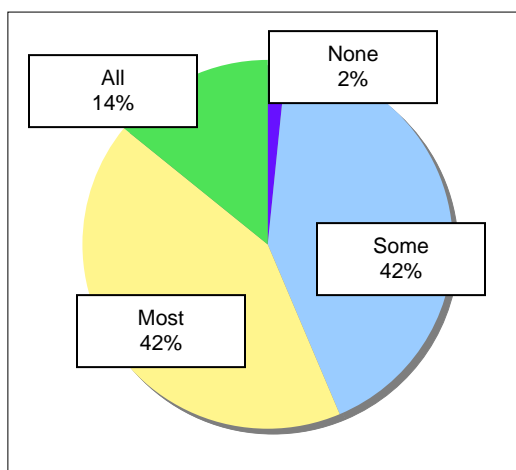
Approximately half, 52%, indicated an average level of expertise with the software. 20% indicated a high or very high level, and 28% indicated a low or very low level.



FREQUENCY OF USE

Q5: "I use VMD for _____ of my molecular visualization tasks..."

N = 228 all, 670 most, 672 some, 26 none



PLATFORM

Q6: "I primarily use VMD on..."

N = 689 Windows, 655 Linux, 228 MacOSX, 24 Other

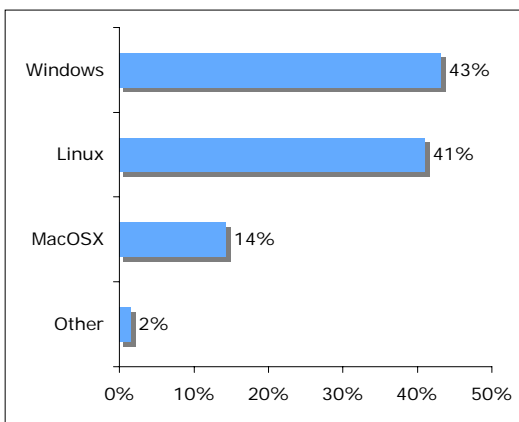
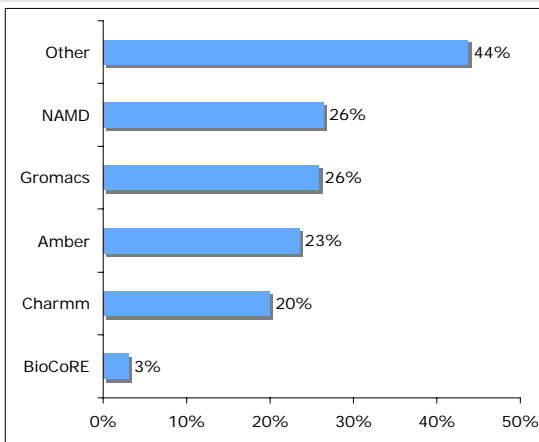


Figure 1: VMD User Characteristics, continued

USE OF OTHER PROGRAMS

Q12: "I am a user of (check all that apply)..."

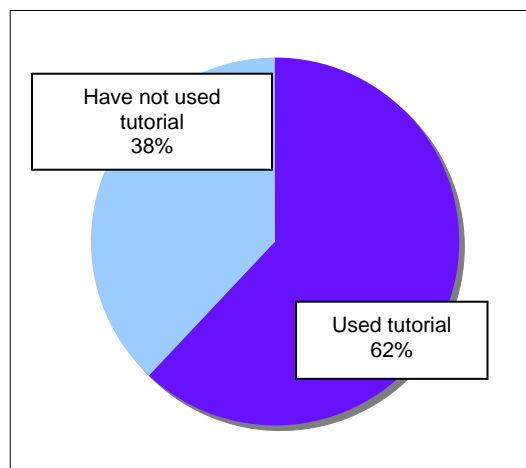
N = 48 BioCoRE, 319 Charmm, 375 Amber, 413 Gromacs, 421 NAMD, 698 other.



USE OF VMD TUTORIAL

Q13: "I have used the VMD tutorial..."

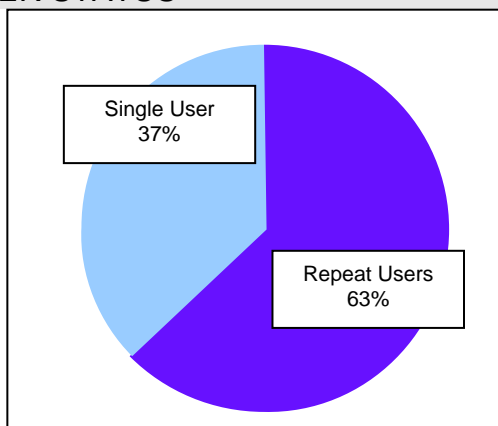
A majority of users, 62% (N=988) reported having used the VMD tutorial, while 39% (N=608) reported not having used it.



REPEAT USER STATUS

Repeat user status

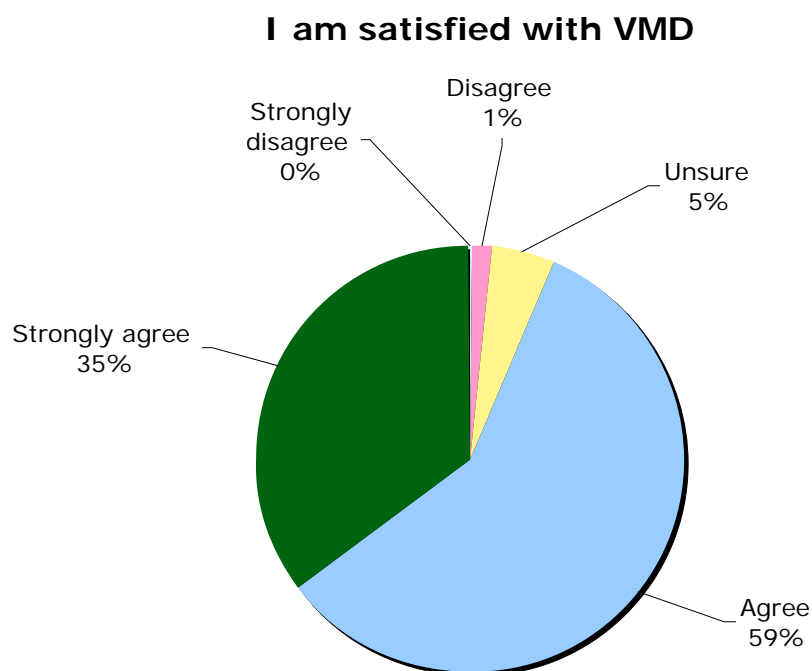
Repeat users had downloaded more than one version of VMD prior to the survey.



RATINGS OF SATISFACTION

- Most users are satisfied with VMD – 94% agreed or strongly agreed with the statement “I am satisfied with VMD” (Q15). See Figure 2.
- Mean satisfaction was 4.27 on a 5-point scale (1=strongly disagree, 5=strongly agree). See Figure 2.

Figure 2: Satisfaction with VMD

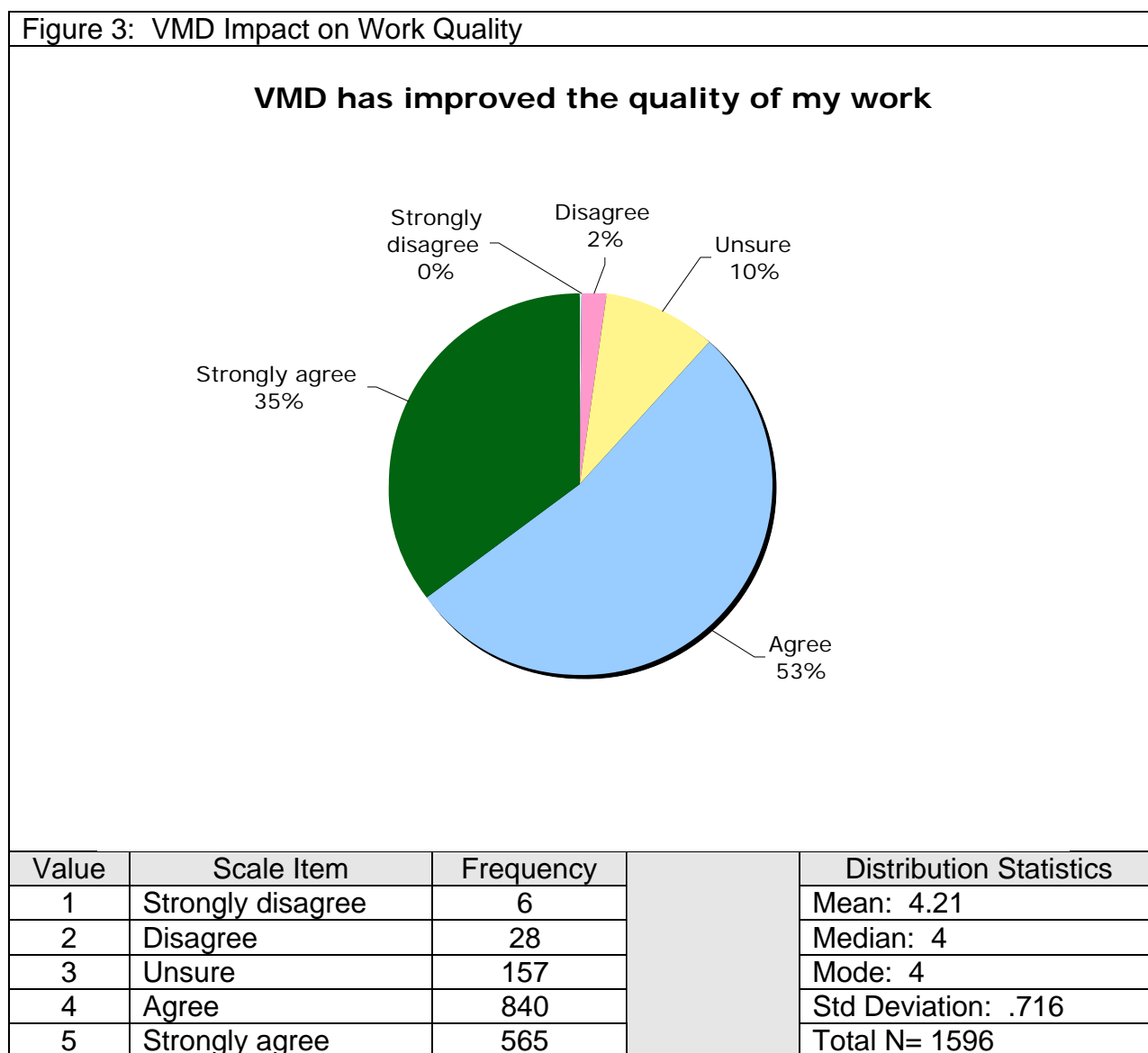


Value	Scale Item	Frequency		Distribution Statistics
1	Strongly disagree	3		Mean: 4.27
2	Disagree	22		Median: 4
3	Unsure	77		Mode: 4
4	Agree	931		Std Deviation: .632
5	Strongly agree	563	Total N= 1596	

RATINGS OF IMPACT ON WORK QUALITY

- VMD was judged to have a positive impact on work quality – 88% of respondents agreed or strongly agreed with the statement “VMD has improved the quality of my work” (Q16). See Figure 3.
- The mean response was 4.21 on a 5-point scale (1=strongly disagree, 5=strongly agree. See Figure 3.

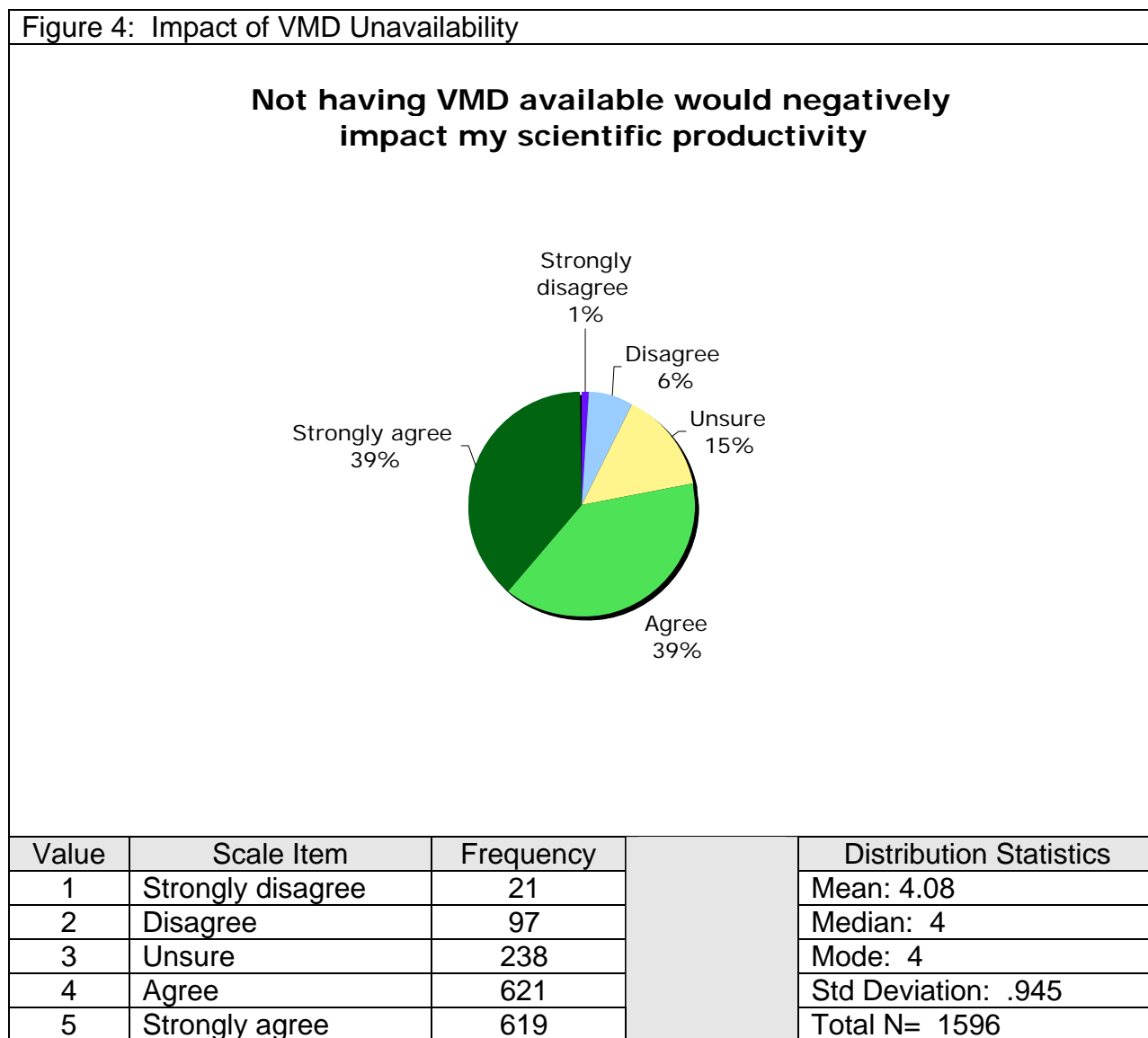
Figure 3: VMD Impact on Work Quality



RATINGS OF IMPACT OF VMD UNAVAILABILITY

- A majority of users agreed that not having VMD available would have a negative impact on their productivity – 78% agreed or strongly agreed with the statement “Not having VMD available (e.g., in case of discontinued funding of VMD development) would negatively impact my scientific productivity” (Q14). See Figure 4.
- The mean response was 4.08 on a 5-point scale (1=strongly disagree, 5=strongly agree). See Figure 4.

Figure 4: Impact of VMD Unavailability



RATINGS OF SUPPORT, DOCUMENTATION, AND OVERALL USABILITY

- Responses to usability, support and documentation items (Q9) indicated why respondents use VMD, and their agreement with statements about specific aspects of the program.
- The three highest rated qualities are: VMD is a useful program (M=4.58), VMD is a reliable program (M=4.35), and VMD is free (M=4.32). See Figures 5A and 5B.

Figure 5A: Support, Documentation, and Overall Usability

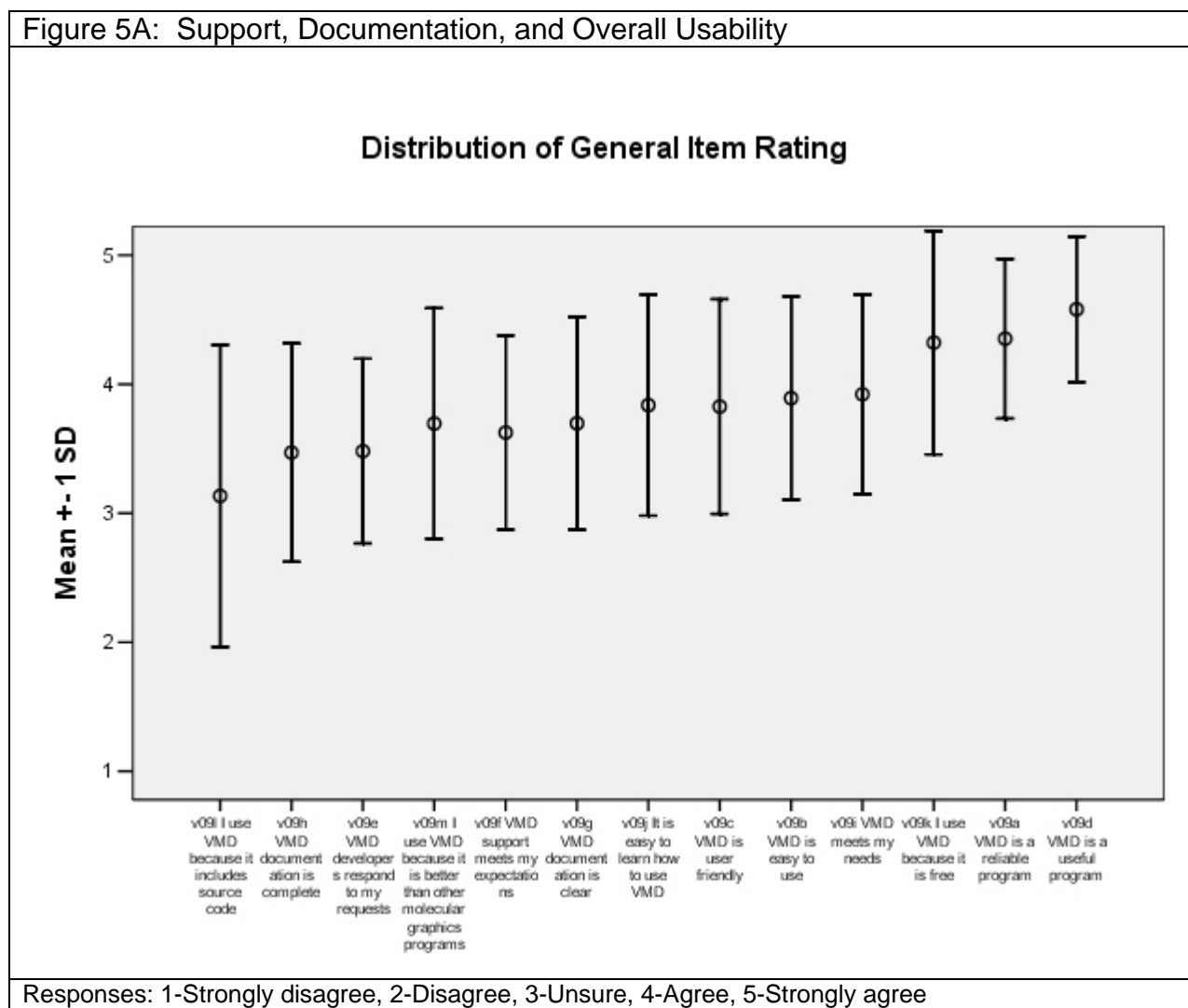


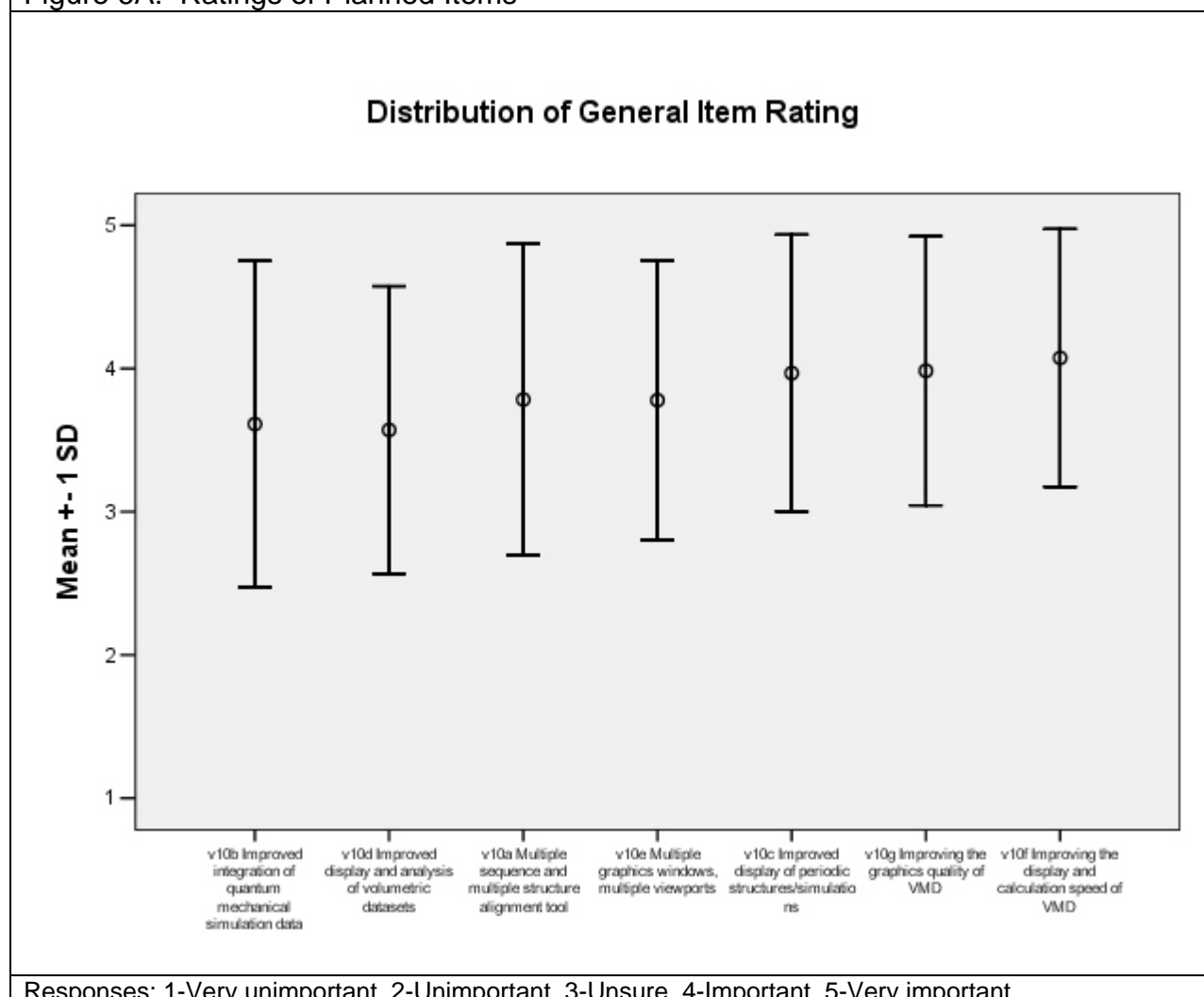
Figure 5B: Support, Documentation, and Overall Usability		
Question Stem	Mean [†]	Std Deviation [†]
Q9 Indicate your level of agreement with the statements below:		
9a VMD is a reliable program	4.35	.62
9b VMD is easy to use	3.89	.79
9c VMD is user friendly	3.83	.83
9d VMD is a useful program	4.58	.56
9e VMD developers respond to my requests	3.48	.72
9f VMD support meets my expectations	3.63	.75
9g VMD documentation is clear	3.70	.825
9h VMD documentation is complete	3.47	.85
9i VMD meets my needs	3.92	.77
9j It is easy to learn how to use VMD	3.84	.86
9k I use VMD because it is free	4.32	.87
9l I use VMD because it includes source code	3.13	1.17
9m I use VMD because it is better than other molecular graphics programs	3.69	.89

[†]Figures based on a 5-point scale, with responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.

RATINGS OF PLANNED ITEMS

- Users were asked to rate the importance of features planned for VMD as a means of identifying priority items for future development. In Q10, a list of 7 potential VMD features was provided to respondents, who were asked to “Rate the importance of these planned features to your work” using a 5-point scale (1-very unimportant, 5-very important). In Q11, participants were asked to “Select the PLANNED feature that should have the highest priority for development.”
- The three highest rated planned items are: improving the display and calculation speed (M=4.07), improving the graphics quality (M=3.98), and improving the display of periodic structures/simulations (M=3.97). See Figures 6A and 6B. When asked to choose the highest priority item, most (24%) chose the multiple sequence and multiple structure alignment tool. See Figure 6C.

Figure 6A: Ratings of Planned Items



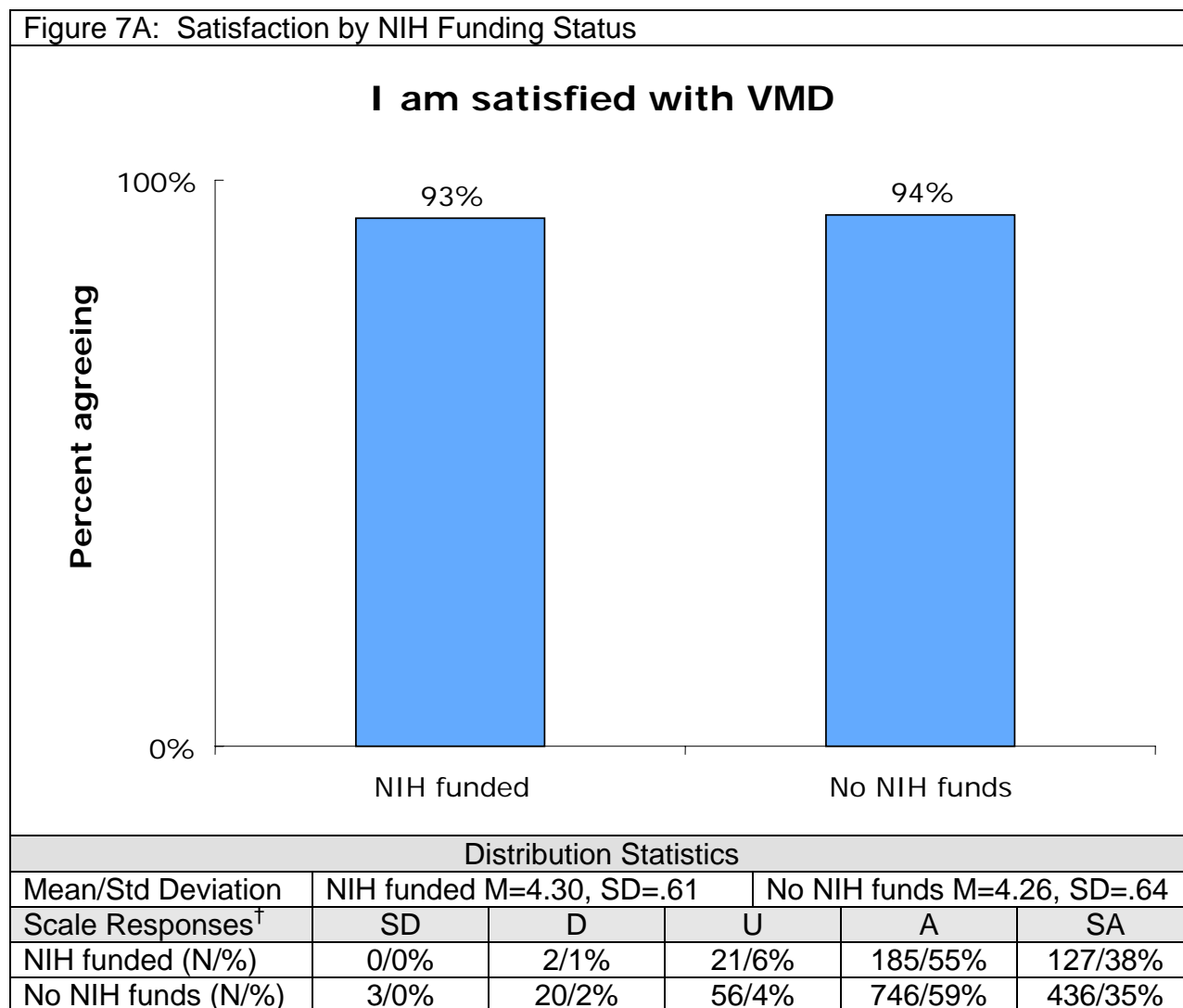
Question Stem	Mean [†]	Std Deviation [†]
Q10 Rate the importance of these PLANNED features to your work:		
10a Multiple sequence and multiple structure alignment tool	3.78	1.09
10b Improved integration of quantum mechanical simulation data	3.61	1.14
10c Improved display of periodic structures/simulations	3.97	.97
10d Improved display and analysis of volumetric datasets	3.57	1.00
10e Multiple graphics windows, multiple viewports	3.78	.98
10f Improving the display and calculation speed of VMD	4.07	.90
10g Improving the graphics quality of VMD	3.98	.94

[†]Figures based on a 5-point scale, with responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.

Question Stem	Count	Percent
Q11 Select the PLANNED feature that should have the highest priority for development:		
10a Multiple sequence and multiple structure alignment tool	383	24.0%
10b Improved integration of quantum mechanical simulation data	301	18.9%
10c Improved display of periodic structures/simulations	223	14.0%
10d Improved display and analysis of volumetric datasets	113	7.1%
10e Multiple graphics windows, multiple viewports	113	7.1%
10f Improving the display and calculation speed of VMD	253	15.9%
10g Improving the graphics quality of VMD	210	13.2%

RATINGS BY NIH FUNDING STATUS

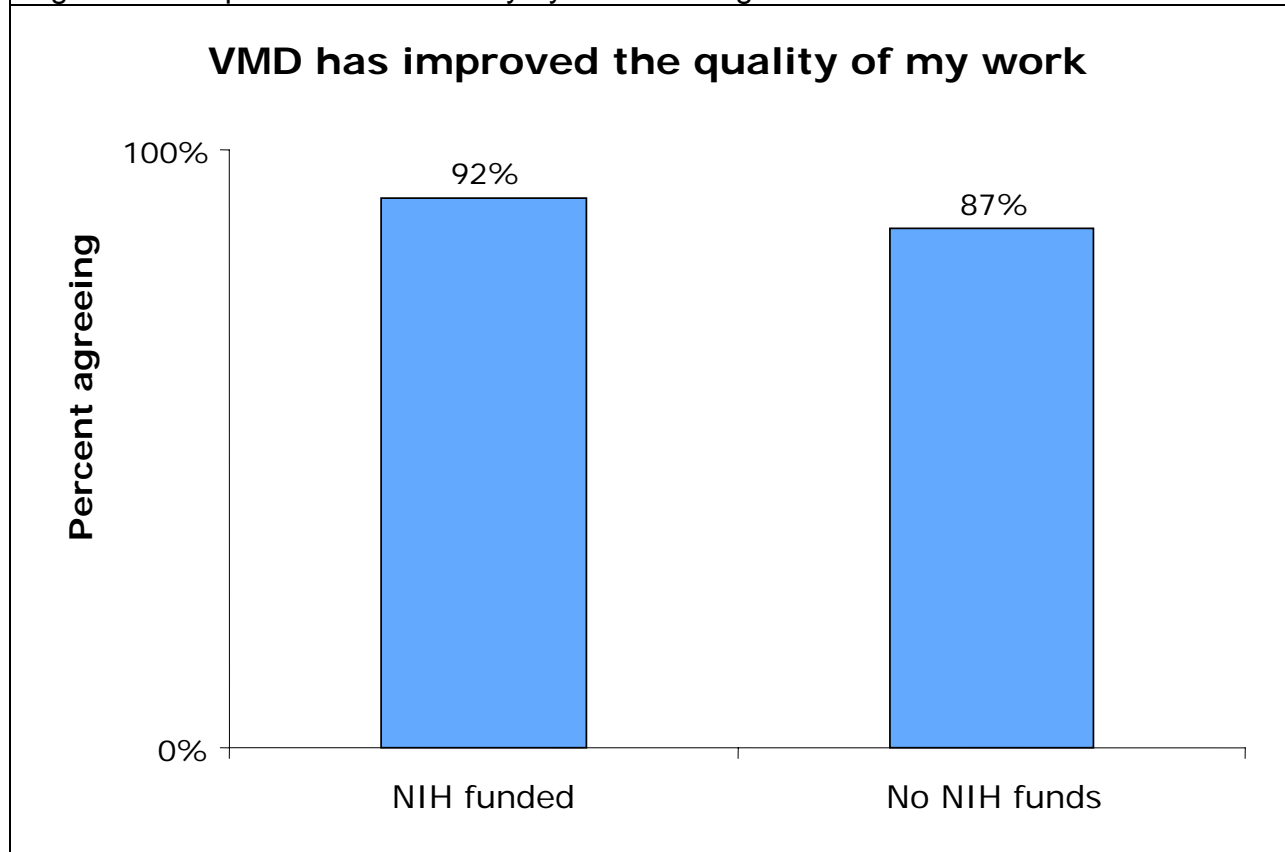
- Users were asked to answer ‘yes’ or ‘no’ to the question “The work I do with VMD is funded (at least partially) by NIH” (Q3).
- Most users, regardless of NIH funding, agreed or strongly agreed with the statement “I am satisfied with VMD” (Q15). See Figure 7A.
- A majority of both NIH funded (92%) and those with no NIH funds (87%) agreed or strongly agreed with the statement “VMD has improved the quality of my work” (Q16). See Figure 7B.



[†]Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.

Total N: NIH funded, 335; no NIH funds, 1261.

Figure 7B: Impact on Work Quality by NIH Funding Status

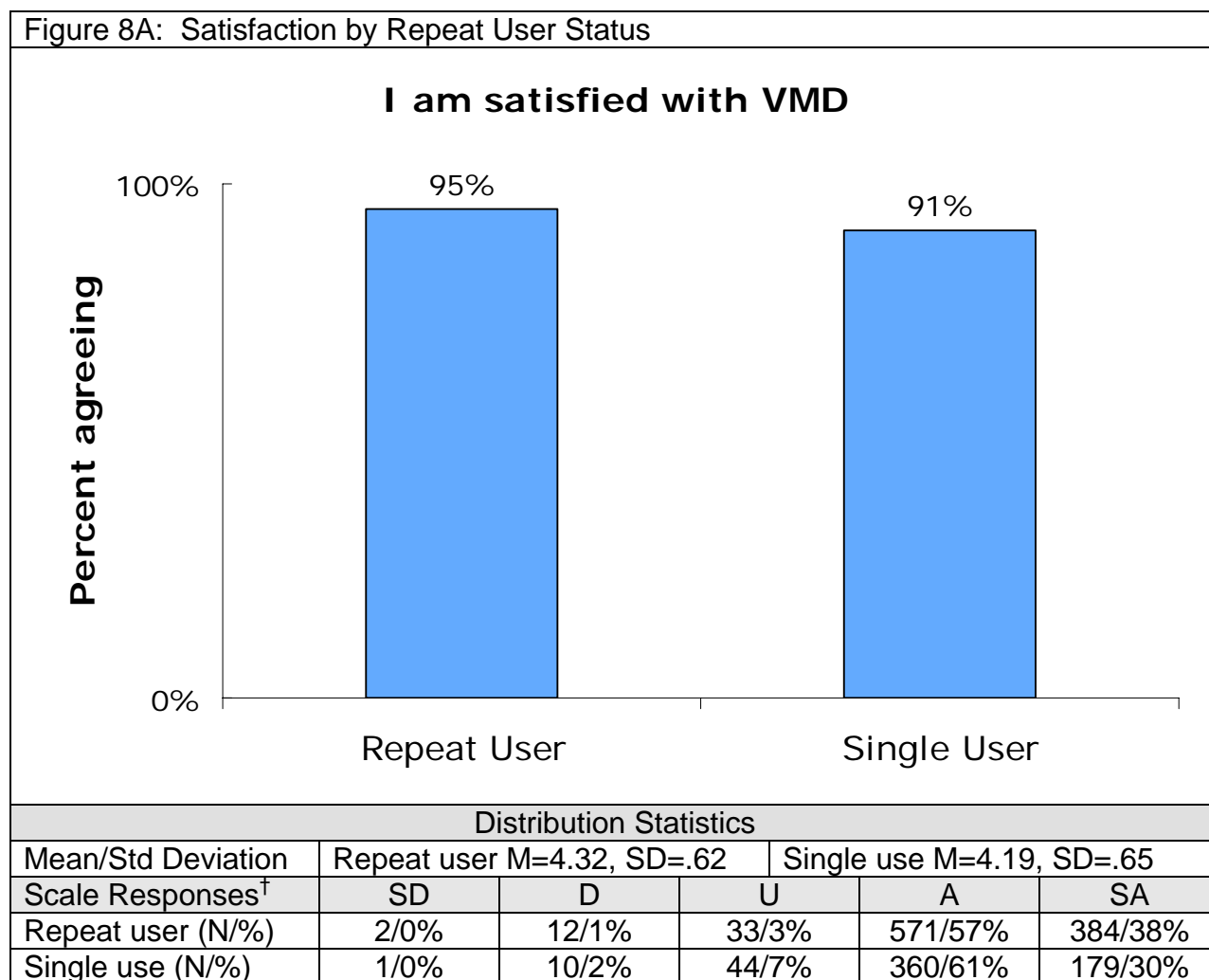


Distribution Statistics					
Mean/Std Deviation	NIH funded M= 4.34, SD=.64			No NIH funds M=4.17, SD=.73	
Scale Responses [†]	SD	D	U	A	SA
NIH funded (N/%)	0/0%	2/1%	25/7%	164/49%	144/43%
No NIH funds (N/%)	6/0%	26/2%	132/11%	676/54%	421/33%

[†]Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
 Total N: NIH funded, 335; no NIH funds, 1261.

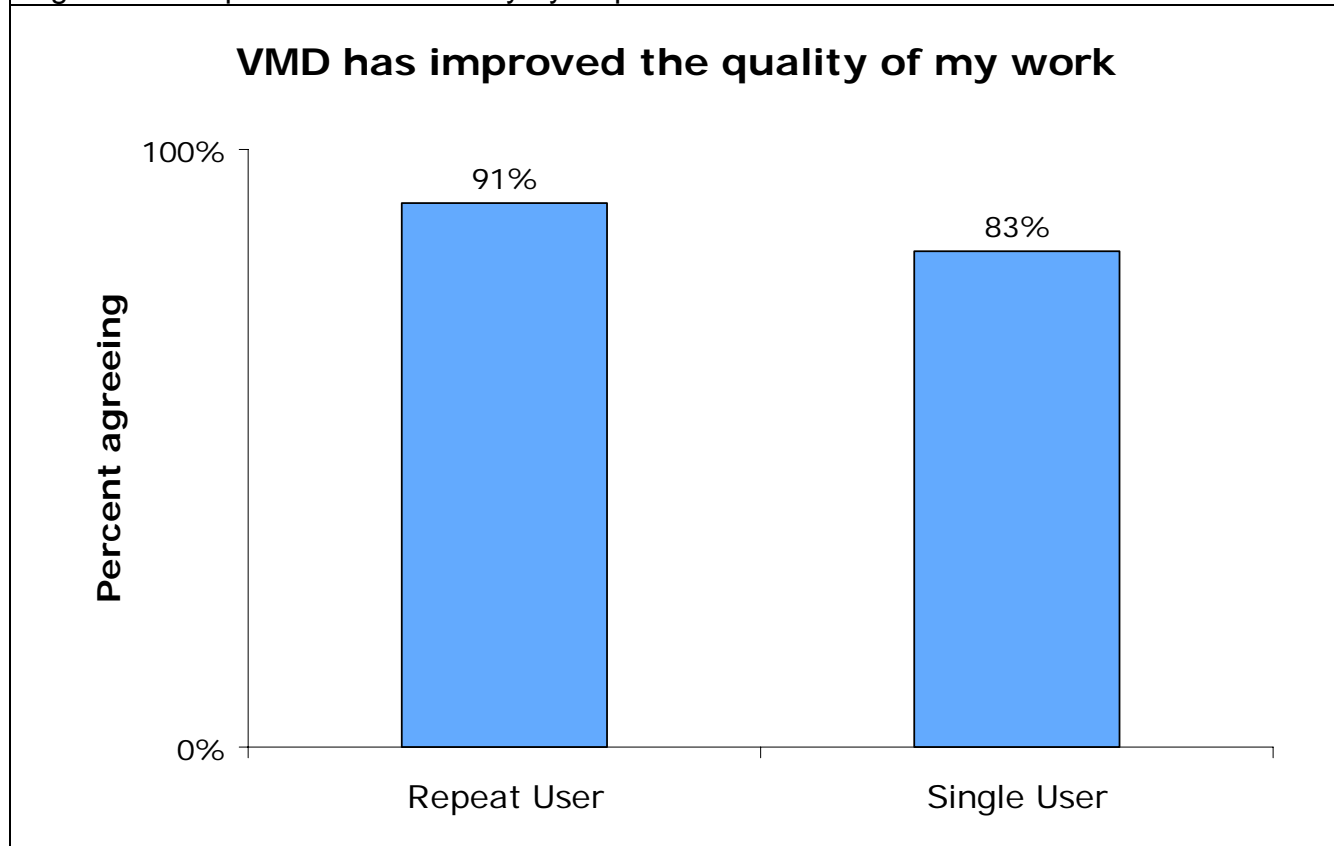
RATINGS BY REPEAT USER STATUS

- Repeat users are those survey respondents who downloaded more than one version of VMD, while single users had at the time of the survey downloaded only one version of VMD.
- Most users, regardless of having used multiple or single versions of VMD, agreed or strongly agreed with the statement “I am satisfied with VMD” (Q15). See Figure 8A.
- A majority of both repeat (91%) and single users of VMD (83%) agreed or strongly agreed with the statement “VMD has improved the quality of my work” (Q16). See Figure 8B.



[†]Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: Repeat users, 1002; single users, 594.

Figure 8B: Impact on Work Quality by Repeat User Status



Distribution Statistics					
Mean/Std Deviation	Repeat user M= 4.29, SD=.70			Single use M=4.07, SD=.73	
Scale Responses [†]	SD	D	U	A	SA
Repeat user (N/%)	2/0%	17/2%	76/8%	499/50%	408/41%
Single user (N/%)	4/1%	11/2%	81/14%	341/57%	157/26%

[†]Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
 Total N: Repeat users, 1002; single users, 594.

APPENDIX: SURVEY METHODOLOGY

Following are details about the administration of the survey, including survey method, target population, survey schedule and response rates, sample validity, and questions used on the survey.

Survey Method

The 2006 VMD User Survey was conducted with the assistance of a commercial survey service (QuestionPro, www.questionpro.com). Population members received an e-mail solicitation asking them to complete an on-line survey, with the link to the survey containing information about the user. Participants were required to complete all items on the survey form and submit their responses; upon submission, participants were thanked for their participation.

Target Population

The target population was defined as those downloading VMD versions 1.8.3 or higher. Version 1.8.3 was released in February, 2005; the current version of VMD is 1.8.4.

Survey Schedule and Response Rates

The target population of 26,079 registered VMD users was contacted over the July 31 – August 3 period to complete the survey. The survey software required lists smaller than the total population, hence a small test sample was sent out initially on August 31, followed by two larger lists on August 2 and August 3. By August 7, 2006, 1608 responses had been collected, representing a sufficient sample size for the population, and a response rate of 6.2 percent.

Data Editing

- 12 Duplicate responses were deleted from the dataset. Duplicates were those instances in which there was more than one response for a person, based on an assigned ID number incorporated in the e-mail solicitation. There were no incomplete records, as the survey software required that all questions be filled.

Deletions left 1596 (out of a total of 1608) valid records for analyses.

- The final response rate, after accounting for deleted records, is 6.1%.

Sample Validity

The validity of a sample size for representing an entire population is always a concern in survey research. Sample size calculators can provide measures of confidence intervals

(+/- figures, i.e. 'margin of error') and confidence level measures (how certain you can be that an answer falls within a confidence interval). For a sample of 1596 and a population of 26079, using a standard test percentage of 50%, sample size calculations indicate that it can be said with 95% confidence that a given result for a question falls within a +/- 2.38% confidence interval. (Figures were generated using Survey System sample size calculator: <http://www.surveysystem.com/sscalc.htm>).

Question Sets

To aid in interpreting survey results, it is useful to view the question stems viewed by survey participants. Below are the survey questions, grouped by purpose:

Demographic/User Information Questions:

Q. #	Topic	Question Stem	Scale
1	E-mail address	Auto-completed, but users could change	Text box
2	Affiliation	Academic, Government, Industry, Other (specify)	Select one, Text box (other)
3	Funding	My work in BioCoRE is funded (at least partially) by NIH	Select Yes or No
4	VMD expertise	My level of expertise in using VMD is	1-5 scale, very low to very high
5	Frequency of use	I use VMD for ____ of my (molecular dynamics or molecular) visualization tasks: none, some, most, all	Select one
6	Platform	I primarily use VMD on: Windows, MacOS X, Linux, Other	Select one
7	Primary use	I use VMD primarily for: Research, Teaching, Business, Personal	Select one
8	Number of users	The number of people using VMD at my site is: 1, 2-4, 5-10, 11-20, 21 or more	Select one

Evaluation Questions:

Q. #	Question Stem	Scale
14	Not having VMD available (e.g., in case of discontinued funding of VMD development) would negatively impact my scientific productivity	1-5 scale, strongly agree to strongly disagree
15	I am satisfied with VMD	
16	VMD has improved the quality of my work	
17	What suggestions do you have for improving VMD and VMD support:	Text area

Ratings of Support, Documentation, and Overall Usability: All ratings of existing items used the same 1-5 scale, ranging from strongly disagree to strongly agree.

Q. #	Question Stem
9	Rate your agreement with each the following statements:
9a	VMD is a reliable program
9b	VMD is easy to use
9c	VMD is user friendly
9d	VMD is a useful program
9e	VMD developers respond to my requests
9f	VMD support meets my expectations
9g	VMD documentation is clear
9h	VMD documentation is complete
9i	VMD meets my needs
9j	It is easy to learn how to use VMD
9k	I use VMD because it is free
9l	I use VMD because it includes source code
9m	I use VMD because it is better than other molecular graphics programs

Importance of Planned Features: All planned items used the same 1-5 scale ranging from very unimportant to very important.

Q. #	Question Stem
10	Rate the importance of VMD planned features to your work:
10a	Multiple sequence and multiple structure alignment tool
10b	Improved integration of quantum mechanical simulation data
10c	Improved display of periodic structures/simulations
10d	Improved display and analysis of volumetric datasets
10e	Multiple graphics windows, multiple viewports
10f	Improving the display and calculation speed of VMD
10g	Improving the graphics quality of VMD