



J | A | C | S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc., 1998, 120(35), 9106-9107, DOI:[10.1021/ja982310b](https://doi.org/10.1021/ja982310b)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society

- S2 -

Supplementary Table 1. Alignment tensor of ubiquitin-SH₆ as a function of pH.^a

pH	conc. ^c	α	β	γ	$10^4 A_{zz}$	$10^4 A_{yy}$	$10^4 A_{xx}$
4.65	5%	37.5	21.2	34.4	-6.20	3.76	2.44
6.18	4.8%	33.0	23.2	29.6	-7.48	4.88	2.60
6.75	4.6%	32.0	27.5	25.5	-7.26	4.77	2.49
7.50	5.0%	31.3	31.1	27.8	-10.86	7.02	3.84

^a Using bicelles in 93% H₂O, 7% D₂O, with a 30:10:1 ratio of DMPC:DHPC:CTAB, at 310 K.

The Euler angles α , β , and γ define the alignment tensor relative to the coordinate frame of the 1.8-Å X-ray structure.¹⁶

^b Molar ratios of lipids. M = [DMPC]; H = [DHPC]; C = [CTAB]; MA = [myristic acid].^c Weight by volume for M+H+C in water.**Supplementary Table 2.** Alignment tensor of aprotinin in charged bicelles.^a

M:H:C ^b	conc. ^c	α	β	γ	$10^4 A_{zz}$	$10^4 A_{yy}$	$10^4 A_{xx}$
30:10:0	5%	153.3	92.7	58.7	5.47	-0.93	-4.54
30:10:1	3.5%	154.6	86.0	77.1	1.92	-0.58	-1.33
30:10:2	4.5%	154.8	77.8	93.6	2.53	-0.51	-2.02

^a Using bicelles in 93% H₂O, 7% D₂O, at pH 6.75, 310 K. The Euler angles α , β , and γ define the alignment tensor relative to the coordinate frame of the crystal X-ray/neutron structure (Wlodawer, A.; Walter, J.; Huber, R.; Sjolín, L. *J. Mol. Biol.* **1984**, *180*, 301-329).

^b Molar ratios of lipids. M = [DMPC]; H = [DHPC]; C = [CTAB].^c Weight by volume for M+H+C+MA in water.

- S3 -

Supplementary Table 3. Angles of intersection for the two cones of N-H vector orientations compatible with the D_{NH} dipolar couplings measured in ubiquitin in liquid crystalline phases consisting of 3:1:0 and 30:10:1 ratios of DMPC:DHPC:CTAB. Only the angle for the intersection closest to the true N-H orientation is given.

Q2	1		
I3	-25		
F4	32		
V5	19		
K6	-3		
T7	-14		
L8	2		
G10	73		
K11	11	D58	-26
T12	-19	Y59	-21
I13	6	N60	-23
T14	-25	I61	-2
L15	29	Q62	-15
E16	-14	K63	-24
V17	-6	E64	-53
E18	1	S65	-8
S20	12	T66	45
D21	-13	L67	42
T22	63	H68	-51
I23	-83	L69	-43
N25	-9	V70	-55
V26	-2	L71	44
K27	-59		
A28	31		
K29	0		
I30	-84		
D32	-28		
K33	24		
E34	-64		
G35	-17		
I36	-3		
D39	-43		
Q40	-29		
Q41	14		
R42	83		
L43	29		
I44	72		
F45	21		
G47	-77		
K48	-9		
Q49	-9		
L50	-73		
E51	-4		
D52	-50		
R54	9		
T55	1		
L56	50		
S57	-27		

- S5 -

Supplementary Table 4. Angles of intersection for the two cones of N-H vector orientations compatible with the D_{NH} dipolar couplings measured in aprotinin in liquid crystalline phases consisting of 3:1:0 and 15:5:1 ratios of DMPC:DHPC:CTAB. Only the angle for the intersection closest to the true N-H orientation is given.

Residue	Angle (°)
F4	16
C5	-3
L6	51
E7	47
Y10	61
G12	-34
C14	50
A16	-31
R17	-33
I18	25
I19	-13
R20	-80
Y21	24
F22	2
Y23	72
N24	5
A25	22
K26	25
A27	20
G28	15
L29	-32
C30	17
Q31	-37
T32	-47
F33	79
V34	-52
Y35	56
G36	-6
C38	13
A40	-30
K41	57
R42	17
N43	28
N44	7
F45	11
S47	-25
A48	18
E49	-8
D50	9
C51	-17
M52	5
R53	-1
T54	15
C55	18
G56	47