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Table A1. Acyl Backbone Torsion Angles for Representative Structures of the Two Most Highly Populated Conformational Families of Arachidonic Acid



ARACHIDONIC ACID

	in vacuo		CHCl ₃		H,O	
· · · · ·	cls1	cls2	cls1	cls2	cls1	cls2
Torsion Angle	(deg)	(deg)	(deg)	(deg)	(deg)	(deg)
$\omega_1 = C1 - C2 - C3 - C4$	178.04	-173.98	-170.50	164.93	170.00	-154.03
$\omega_2 = C2 - C3 - C4 - C5$	67.56	74.37	-174.34	-62.59	-60.83	174.17
$\omega_3 = C3-C4-C5-C6$	-114.84	-131.17	-146.26	110.86	133.76	146.40
ω ₄ = C4-C5-C6-C7	1.14	1.13	0.75	0.78	1.02	1.12
$\omega_{s} = C5 - C6 - C7 - C8$	-140.71	-106.70	97.67	131.29	125.23	111.97
$\omega_{6} = C6 - C7 - C8 - C9$	114.06	107.59	102.98	100.05	153.33	104.14
$\omega_7 = C7 - C8 - C9 - C10$	0.00	0.05	1.63	1.55	-0.07	0.12
$\omega_{\rm s} = C8-C9-C10-C11$	- 95.19	-132.02	106.40	-129.62	-88.42	109.36
ω ₉ = C9-C10-C11-C12	-127.27	-126.15	-115.48	109.81	145.75	69.82
$\omega_{10} = C10-C11-C12-C13$	0.03	0.07	0.17	0.13	0.00	0.09
ω ₁₁ = C11-C12-C13-C14	116.40	-128.49	107.26	126.04	109.39	123.96
$\omega_{12} = C12 - C13 - C14 - C15$	91.02	130.99	137.72	136.79	121.05	107.63
$\omega_{_{13}} = C13 - C14 - C15 - C16$	1.10	1.18	0.26	0.23	1.14	1.10
ω ₁₄ = C14-C15-C16-C17	93.18	-117.84	127.88	-122.30	121.36	74.11
$\omega_{15} = C15 - C16 - C17 - C18$	174.25	61.89	73.83	-161.22	173.43	168.52
ω ₁₆ = C16-C17-C18-C19	-168.34	179.17	-164.84	-68.77	179.26	-68.59
ω ₁₇ = C17-C18-C19-C20	-172.79	75.79	-177.35	172.20	-176.28	166.15

*See Figure 3

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Table A2. Acyl Backbone Torsion Angles for Representative Structures of the Two Most Highly Populated Conformational Families of Anandamide



	ANANDAM	IDE (AEA)		
	CHCI		H₂O	
	cis1	cls2	cls1	cls2
Torsion Angle	(deg)	(deg)	(deg)	(deg)
$\omega_1 = C1 - C2 - C3 - C4$	167.90	150.13	175.58	172.47
$\omega_2 = C2 - C3 - C4 - C5$	54.95	160.04	61.94	174.25
$\omega_3 = C3-C4-C5-C6$	-127.46	91.94	-112.83	130.41
$\omega_4 = C4-C5-C6-C7$	-0.28	-0.26	-0.44	-0.34
$\omega_{5} = C5 - C6 - C7 - C8$	-133.95	-131.60	-89.54	-117.92
$\omega_{e} = C6-C7-C8-C9$	-106.72	-109.56	-117.85	93.32
$\omega_{7} = C7 - C8 - C9 - C10$	1.58	1.53	1.42	1.44
$\omega_{s} = C8-C9-C10-C11$	125.95	118.77	109.76	104.66
ω _a = C9-C10-C11-C12	115.10	-111.91	137.51	-144.53
$\omega_{10} = C10 - C11 - C12 - C13$	1.53	1.56	1.45	1.43 ک
$\omega_{1} = C11 - C12 - C13 - C14$	121.60	-109.88	94.13	-148.81
ω ₁₂ = C12-C13-C14-C15	130.68	-155.43	-130.70	-84.98
ω ₁₃ = C13-C14-C15-C16	-1.13	-1.26	-1.11	-1.11
ω ₄ = C14-C15-C16-C17	139.94	-148.09	-123.96	-129.71
$\omega_{15} = C15 - C16 - C17 - C18$	-68.24	-179.17	67.34	-173.86
ω _s = C16-C17-C18-C19	177.52	-178.76	-165.04	172.54
ω. = C17-C18-C19-C20	-172.01	167.53	67.76	178.22

*See Figure 4

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Table A3. Acyl Backbone Torsion Angles for Representative Structures of the Two Most HighlyPopulated Conformational Families of 2-AG



	CHCl		H₂O	
Torsion Angle	cls1 (deg)	cls2 (deg)	cls1 (deg)	cls2 (deg)
$\omega = C1 - C2 - C3 - C4$	-178.83	176.33	166.35	-170.07
$\omega_1 = C2 - C3 - C4 - C5$	54.11	-69.73	-161.83	-58.12
$\omega_{2} = C3-C4-C5-C6$	-121.12	140.50	146.26	-110.54
$\omega_{3} = C4-C5-C6-C7$	0.96	1.03	1.05	1.06
$\omega_{-} = C5 - C6 - C7 - C8$	-109.56	-101.47	108.64	107.11
$\omega_{s} = C6-C7-C8-C9$	-151.84	113.34	111.21	124.35
$\omega_{\rm e} = C7 - C8 - C9 - C10$	-0.28	-0.22	-0.68	-0.60
$\omega_{\rm r} = C8-C9-C10-C11$	-135.31	116.10	112.50	-89.14
$\omega_{\rm s} = C9 - C10 - C11 - C12$	-131.47	169.19	-92.62	-114.20
$\omega_{-} = C10 - C11 - C12 - C13$	-1.90	-1.88	-1.63	-1.60
$\omega_{10} = C11 - C12 - C13 - C14$	118.33	83.24	-103.46	-121.49
$\omega_{11} = C12 - C13 - C14 - C15$	176.25	-139.46	-162.88	108.39
$\omega_{12} = C13 - C14 - C15 - C16$	1.46	1.46	1.24	1.25
$\omega_{13} = C14 - C15 - C16 - C17$	-102.33	-116.13	-126.47	133.39
$\omega_{14} = C15 - C16 - C17 - C18$	155.40	-162.59	-172.35	178.51
$\omega_{15} = C16 \cdot C17 \cdot C18 \cdot C19$	165.89	-177.23	-168.78	175.39
$\omega_{16} = C17 - C18 - C19 - C20$	72.76	-73.02	-160.61	167.45

*See Figure 5

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Table A4. Acyl Backbone Torsion Angles for Representative Structures of the Two Most HighlyPopulated Conformational Families of DMH-AEA



· · · · · ·	DMH-AEA				
	CHCI		F	H₂O	
	cls1	cls2	cls1	cls2	
Torsion Angle	(deg)	(deg)	(deg)	(deg)	
$\omega_1 = C1-C2-C3-C4$	169.53	176.05	-177.92	178.88	
$\omega_2 = C2-C3-C4-C5$	56.35	-57.50	170.21	-73.71	
$\omega_3 = C3-C4-C5-C6$	99.29	107.74	-111.12	-121.20	
$\omega_{4} = C4-C5-C6-C7$	0.53	0.46	-1.31	-1.32	
$\omega_{\rm s} = C5 - C6 - C7 - C8$	95.58	111.24	-101.59	118.32	
$\omega_{6} = C6-C7-C8-C9$	-136.72	-164.74	145.36	-136.14	
$\omega_7 = C7 - C8 - C9 - C10$	-0.49	-0.60	0.62	0.61	
$\omega_{\rm s} = C8 - C9 - C10 - C11$	-77.54	91.84	92.52	-97.28	
ω _a = C9-C10-C11-C12	-145.43	120.91	162.89	-95.91	
$\omega_{10} = C10-C11-C12-C13$	0.07	0.03	-0.11	-0.07	
ω, = C11-C12-C13-C14	137.10	116.41	-112.41	-111.90	
$\omega_{12} = C12 - C13 - C14 - C15$	134.88	170.28	-142.04	-113.99	
ω ₁₂ = C13-C14-C15-C16	0.64	0.62	-0.34	-0.31	
ω, = C14-C15-C16-C17	-67.66	-53.49	-53.88	-56.76	
ω _{is} = C15-C16-C17-C18	-51.13	-57.99	-60.92	-58.91	
ω _w = C16-C17-C18-C19	167.32	163.26	-170.19	-177.72	
$\omega_{,7} = C17 - C18 - C19 - C20$	161.73	167.05	-56.54	-167.02	
ω _w = C18-C19-C20-C21	-169.60	161.60	-178.17	168.77	
$\omega_{19} = C19 - C20 - C21 - C22$	-168.80	172.14	-176.56	-159.17	

* See Figure 6

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Table A5. Acyl Backbone Torsion Angles for Representative Structures of the Most Highly Populated Conformational Families of PGB2-EA



PGB -EA

	CHCL		H ₂ O
	cls1	cls1	cls2
Torsion Angle	(deg)	(deg)	(deg)
	177.70	-154.86	-172.67
	68.63	-59.15	-169.92
	-135.86	-109.59	136.06
	0.00	0.33	0.37
	-142 24	-112.28	-145.87
C5-C6-C7-C8	80.73	113.59	90.63
C6-C7-C8-C9	0.42	0.65	0.58
C7-C8-C9-C10	172.00	144.37	-178.07
C8-C9-C10-C11	-1/3.90	170 1/	179.17
C9-C10-C11-C12	1/9.42	1/5.14	-117.28
C10-C11-C12-C13	-116.87		57 75
C11-C12-C13-C14	55.23	65.35	174.60
C12-C13-C14-C15	172.78	163.17	174.02
C13-C14-C15-C16	173.22	131.03	179.09
C14-C15-C16-C17	-164.47	177.79	177.28

*See Figure 7

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