

ID		rf	Dihedral Angle (°)			Selected Distances (Å)		
1°	2°		α_5	α_4	α_3	NH(21)-O(x)	Ar-choline(x)	O(x)-choline
1a	A	0.10	69 ± 92	-167 ± 50	-83 ± 80	2.73 ± 1.00 (60)	4.30 ± 1.57 (Me)	2.58 ± 1.13 (27)
1a	B	0.02	63 ± 7	92 ± 93	66 ± 79	2.72 ± 1.14 (59)	4.14 ± 1.47 (52)	2.47 ± 0.45 (27)
1a	C	0.02	-60 ± 9	152 ± 35	66 ± 55	2.81 ± 1.26 (59)	4.44 ± 1.78 (54)	3.07 ± 1.56 (27)
1b	A	0.07	64 ± 66	-166 ± 60	-70 ± 54	3.13 ± 1.04 (60)	4.16 ± 2.34 (Me)	2.73 ± 1.27 (27)
1b	B	0.05	-64 ± 8	139 ± 26	63 ± 44	2.83 ± 1.31 (59)	4.14 ± 1.93 (Me)	2.75 ± 1.30 (27)
1b	C	0.03	64 ± 9	76 ± 35	65 ± 99	3.00 ± 1.36 (59)	3.65 ± 2.25 (Me)	2.42 ± 0.66 (27)
1b	D	0.02	-63 ± 10	-107 ± 83	-90 ± 139	3.28 ± 1.94 (59)	4.57 ± 2.92 (Me)	2.49 ± 0.79 (27)
1b	E	0.01	62 ± 6	-141 ± 27	-158 ± 30	2.87 ± 1.15 (59)	3.94 ± 1.86 (Me)	2.56 ± 0.62 (27)
2	A	0.02	93 ± 162	-143 ± 35	-80 ± 149	3.24 ± 1.42 (59)	4.20 ± 3.26 (Me)	5.58 ± 4.57 (27)
2	B	0.01	64 ± 7	73 ± 7	56 ± 24	2.65 ± 1.42 (59)	5.59 ± 2.24 (52)	3.12 ± 2.49 (27)
2	C	<0.01	58 ± 6	167 ± 25	-67 ± 8	2.71 ± 1.22 (60)	4.89 ± 2.72 (Me)	2.94 ± 1.98 (27)
2	D	<0.01	-64 ± 11	152 ± 36	58 ± 82	3.10 ± 1.36 (59)	5.33 ± 4.50 (Me)	4.59 ± 4.93 (27)
2	E	<0.01	63 ± 4	163 ± 16	41 ± 4	2.94 ± 2.20 (59)	3.33 ± 0.88 (Me)	6.38 ± 0.60 (5)
3a	A	0.05	65 ± 28	-143 ± 29	-60 ± 37	3.48 ± 1.60 (59)	3.57 ± 1.32 (Me)	5.10 ± 5.61 (27)
3a	B	0.04	-63 ± 26	-80 ± 41	-51 ± 35	2.72 ± 0.66 (59)	3.13 ± 0.45 (Me)	2.43 ± 0.76 (27)
3a	C	0.01	-64 ± 21	154 ± 41	82 ± 90	3.73 ± 1.45 (59)	3.63 ± 1.82 (Me)	3.48 ± 3.95 (27)
3a	D	0.01	64 ± 7	78 ± 8	75 ± 86	3.21 ± 1.24 (59)	4.04 ± 2.56 (Me)	3.76 ± 4.38 (27)
3a	E	0.01	-67 ± 42	-167 ± 20	70 ± 93	2.67 ± 0.79 (59)	3.10 ± 1.69 (51)	2.40 ± 0.43 (27)
3a	F	<0.01	85 ± 137	161 ± 50	-74 ± 31	3.02 ± 1.79 (59)	3.47 ± 1.46 (Me)	6.28 ± 5.73 (27)
3a	G	<0.01	63 ± 13	164 ± 13	42 ± 50	2.72 ± 0.86 (59)	3.30 ± 1.20 (Me)	2.56 ± 1.24 (27)
5a	A	0.05	72 ± 98	-154 ± 36	-58 ± 26	2.84 ± 1.58 (57)	4.58 ± 0.74 (52)	2.37 ± 0.19 (5)
5a	B	0.03	-98 ± 170	149 ± 54	60 ± 140	2.89 ± 0.75 (59)	4.56 ± 2.33 (54)	3.17 ± 2.52 (5)
10a	A	0.01	64 ± 14	-144 ± 27	-67 ± 73	3.07 ± 1.57 (59)	4.51 ± 3.27 (Me)	2.91 ± 1.67 (27)
10a	B	0.01	-64 ± 5	-76 ± 9	-68 ± 119	3.04 ± 0.69 (59)	3.82 ± 2.56 (Me)	2.38 ± 0.47 (27)
10a	C	0.01	62 ± 69	167 ± 13	-79 ± 18	2.62 ± 1.03 (59)	4.83 ± 1.34 (54)	2.89 ± 2.39 (27)
10a	D	0.01	64 ± 7	73 ± 9	55 ± 56	2.75 ± 2.24 (57)	4.12 ± 0.57 (Me)	2.36 ± 0.19 (27)
10a	E	<0.01	63 ± 7	-140 ± 30	-156 ± 29	2.70 ± 0.09 (59)	3.83 ± 1.15 (Me)	2.53 ± 0.41 (27)
10a	F	<0.01	-61 ± 10	148 ± 35	71 ± 34	3.36 ± 0.86 (60)	4.46 ± 2.72 (Me)	2.43 ± 0.48 (27)
10a	G	<0.01	-73 ± 8	136 ± 9	170 ± 1	2.99 ± 0.35 (59)	4.06 ± 1.29 (54)	2.67 ± 0.99 (27)
10a	H	<0.01	-58 ± 4	-169 ± 14	74 ± 22	2.45 ± 0.23 (59)	3.42 ± 1.40 (52)	2.64 ± 2.52 (27)
10b	A	0.01	63 ± 49	-169 ± 61	-63 ± 29	3.18 ± 1.39 (59)	4.67 ± 3.07 (Me)	4.60 ± 2.19 (5)
10b	B	0.01	-64 ± 7	137 ± 25	67 ± 42	2.54 ± 0.85 (59)	3.64 ± 1.02 (Me)	5.56 ± 1.88 (5)
10b	C	<0.01	75 ± 125	-157 ± 35	-163 ± 27	2.39 ± 0.77 (59)	3.60 ± 1.63 (Me)	5.79 ± 3.97 (27)
10b	D	<0.01	63 ± 8	84 ± 58	75 ± 112	2.85 ± 1.12 (59)	4.07 ± 1.84 (Me)	5.43 ± 1.34 (5)
10b	E	<0.01	-61 ± 11	-107 ± 82	-97 ± 172	2.71 ± 1.31 (59)	3.53 ± 0.55 (Me)	4.47 ± 2.74 (5)
10c	A	<0.01	77 ± 124	-152 ± 49	-70 ± 34	2.82 ± 1.18 (60)	5.24 ± 1.64 (Me)	3.20 ± 0.08 (27)
10c	B	<0.01	64 ± 5	-136 ± 25	-164 ± 28	2.46 ± 0.70 (60)	3.86 ± 0.54 (Me)	3.27 ± 0.12 (27)
10c	C	<0.01	61 ± 7	174 ± 11	-72 ± 6	2.44 ± 0.25 (60)	5.05 ± 0.90 (Me)	3.65 ± 1.14 (27)
10c	D	<0.01	-63 ± 5	139 ± 22	71 ± 97	2.76 ± 1.12 (59)	4.78 ± 1.63 (Me)	3.34 ± 0.20 (27)
10c	E	<0.01	78 ± 97	78 ± 88	53 ± 32	2.41 ± 0.98 (59)	5.33 ± 0.82 (Me)	3.20 ± 0.08 (27)
11	A	0.05	65 ± 47	-153 ± 53	-69 ± 97	3.60 ± 1.65 (59)	4.15 ± 2.09 (51)	5.07 ± 5.09 (27)
11	B	0.01	-61 ± 9	139 ± 12	54 ± 14	4.19 ± 2.00 (60)	2.88 ± 0.25 (Me)	6.42 ± 0.68 (5)
11	C	0.01	-63 ± 13	172 ± 13	61 ± 32	3.22 ± 2.19 (58)	4.97 ± 3.01 (Me)	2.93 ± 1.99 (27)
11	D	0.01	-65 ± 11	-169 ± 17	77 ± 132	2.86 ± 1.10 (59)	4.53 ± 4.27 (Me)	5.34 ± 2.27 (5)
11	E	0.01	-62 ± 10	-82 ± 34	-57 ± 69	2.82 ± 0.78 (59)	4.44 ± 2.99 (52)	3.58 ± 4.59 (27)
11	F	<0.01	-67 ± 14	140 ± 32	154 ± 31	2.97 ± 0.78 (60)	3.59 ± 0.83 (Me)	2.48 ± 0.50 (27)
11	G	<0.01	63 ± 8	82 ± 32	82 ± 66	3.65 ± 1.07 (60)	3.76 ± 2.31 (51)	4.26 ± 5.40 (27)
13	A	0.06	61 ± 10	-165 ± 46	-63 ± 38	3.66 ± 1.67 (59)	4.43 ± 2.12 (52)	2.45 ± 0.28 (27)
13	B	0.03	65 ± 6	75 ± 18	52 ± 65	3.41 ± 1.49 (59)	4.26 ± 1.97 (Me)	2.84 ± 1.52 (27)
13	C	<0.01	-65 ± 8	-74 ± 9	-62 ± 61	3.94 ± 2.09 (59)	3.27 ± 1.55 (52)	3.25 ± 1.68 (5)
13	D	<0.01	-63 ± 0	-167 ± 3	77 ± 74	2.37 ± 0.89 (60)	3.21 ± 0.43 (Me)	2.37 ± 0.23 (5)
13	E	<0.01	-62 ± 5	144 ± 19	61 ± 45	3.96 ± 1.01 (59)	4.01 ± 0.16 (Me)	2.61 ± 0.91 (5)
14	A	0.05	-64 ± 33	-178 ± 65	77 ± 119	2.83 ± 1.58 (59)	6.36 ± 1.28 (52)	2.45 ± 0.47 (27)
14	B	0.04	68 ± 58	-139 ± 30	-53 ± 43	2.84 ± 1.00 (59)	3.95 ± 2.72 (55)	6.14 ± 2.58 (5)
14	C	0.01	62 ± 10	90 ± 55	69 ± 101	3.32 ± 1.61 (59)	4.23 ± 0.77 (Me)	2.29 ± 0.23 (27)
14	D	<0.01	-61 ± 6	140 ± 23	-167 ± 17	2.62 ± 0.53 (59)	4.47 ± 2.50 (Me)	2.89 ± 2.29 (27)
14	E	<0.01	61 ± 16	173 ± 12	-70 ± 33	3.18 ± 1.09 (60)	4.68 ± 1.45 (52)	2.60 ± 0.39 (27)
15	A	<0.01	60 ± 7	82 ± 16	75 ± 39	4.00 ± 1.42 (59)	5.72 ± 1.29 (Me)	3.34 ± 0.17 (5)
15	B	<0.01	59 ± 6	-141 ± 24	-71 ± 19	2.92 ± 1.21 (59)	5.45 ± 1.17 (Me)	4.08 ± 2.38 (5)
15	C	<0.01	-63 ± 4	138 ± 20	56 ± 97	3.45 ± 1.28 (59)	5.58 ± 1.47 (Me)	3.26 ± 0.14 (5)
15	D	<0.01	61 ± 7	-131 ± 3	150 ± 7	2.38 ± 0.04 (58)	5.43 ± 0.07 (Me)	3.31 ± 0.12 (5)