Molecular Structures
and
Thermodynamic Functions
of
Phospholipid Components

(Supplementary Materials)

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1. Z-Matrix and Input Variables

Table S1-1 Sample symbolic z-matrices of atom connectivity for various phospholipid size (Bolded lines represent variable atoms that change as the result of the addition and the substitution of other fragments)

	GLYCEROL (Fragment I)	GLYCEROL WITH PHOSPHATE (Fragments I + II)	GLYCEROL, PHOSPHATE, X-GROUP (Fragments I to III)	PHOSPHOLIPID First fatty acid included (Fragments I to IV)	PHOSPHOLIPID First and second fatty acid included (Fragments I to V)	
Glycerol and Phosphate Group (Fragment I and II)	0 1	0 1	+1 1	+1 1	+1 1	
	H	H	H	H	H	1
	C 1 R2	C 1 R2	C 1 R2	C 1 R2	C 1 R2	2
	C 2 R3 1 A3	C 2 R3 1 A3	C 2 R3 1 A3	C 2 R3 1 A3	C 2 R3 1 A3	3
	C 3 R4 2 A4 1 D4	C 3 R4 2 A4 1 D4	C 3 R4 2 A4 1 D4	C 3 R4 2 A4 1 D4	C 3 R4 2 A4 1 D4	4
	H 4 R5 3 A5 2 D5	H 4 R5 3 A5 2 D5	H 4 R5 3 A5 2 D5	H 4 R5 3 A5 2 D5	H 4 R5 3 A5 2 D5	5
	H 2 R6 3 A6 4 D6	H 2 R6 3 A6 4 D6	H 2 R6 3 A6 4 D6	H 2 R6 3 A6 4 D6	H 2 R6 3 A6 4 D6	6
	H 3 R7 2 A7 1 D7	H 3 R7 2 A7 1 D7	H 3 R7 2 A7 1 D7	H 3 R7 2 A7 1 D7	H 3 R7 2 A7 1 D7	7
	H 4 R8 3 A8 2 D8	H 4 R8 3 A8 2 D8	H 4 R8 3 A8 2 D8	H 4 R8 3 A8 2 D8	H 4 R8 3 A8 2 D8	8
	O 2 R9 3 A9 4 D9	O 2 R9 3 A9 4 D9	O 2 R9 3 A9 4 D9	O 2 R9 3 A9 4 D9	O 2 R9 3 A9 4 D9	9
	O 3 R10 2 A10 1 D10	O 3 R10 2 A10 1 D10	O 3 R10 2 A10 1 D10	O 3 R10 2 A10 1 D10	O 3 R10 2 A10 1 D10	10
	O 4 R11 3 A11 2 D11	O 4 R11 3 A11 2 D11	O 4 R11 3 A11 2 D11	O 4 R11 3 A11 2 D11	O 4 R11 3 A11 2 D11	11
	H 9 R12 2 A12 3 D12	P 9 R12 2 A12 3 D12	P 9 R12 2 A12 3 D12	P 9 R12 2 A12 3 D12	P 9 R12 2 A12 3 D12	12
	H 10 R13 3 A13 2 D13	H 10 R13 3 A13 2 D13	H 10 R13 3 A13 2 D13	H 10 R13 3 A13 2 D13	C 10 R13 3 A13 2 D13	13
	H 11 R14 4 A14 3 D14	H 11 R14 4 A14 3 D14	H 11 R14 4 A14 3 D14	C 11 R14 4 A14 3 D14	C 11 R14 4 A14 3 D14	14
		O 12 R15 9 A15 2 D15	O 12 R15 9 A15 2 D15	O 12 R15 9 A15 2 D15	O 12 R15 9 A15 2 D15	15
		O 12 R16 9 A16 2 D16	O 12 R16 9 A16 2 D16	O 12 R16 9 A16 2 D16	O 12 R16 9 A16 2 D16	16
		O 12 R17 9 A17 2 D17	O 12 R17 9 A17 2 D17	O 12 R17 9 A17 2 D17	O 12 R17 9 A17 2 D17	17
		H 17 R18 12 A18 9 D18	C 17 R18 12 A18 9 D18	C 17 R18 12 A18 9 D18	C 17 R18 12 A18 9 D18	18
		H 16 R19 12 A19 9 D19 (Alcoholic Group (Fragment III))	C 18 R19 17 A19 12 D19	C 18 R19 17 A19 12 D19	C 18 R19 17 A19 12 D19	19
			N 19 R20 18 A20 17 D20	N 19 R20 18 A20 17 D20	N 19 R20 18 A20 17 D20	20
			H 18 R21 17 A21 12 D21	H 18 R21 17 A21 12 D21	H 18 R21 17 A21 12 D21	21
			H 18 R22 17 A22 12 D22	H 18 R22 17 A22 12 D22	H 18 R22 17 A22 12 D22	22
			H 19 R23 18 A23 17 D23	H 19 R23 18 A23 17 D23	H 19 R23 18 A23 17 D23	23
			H 19 R24 18 A24 17 D24	H 19 R24 18 A24 17 D24	H 19 R24 18 A24 17 D24	24
			H 20 R25 19 A25 18 D25	H 20 R25 19 A25 18 D25	H 20 R25 19 A25 18 D25	25
			H 20 R26 19 A26 18 D26	H 20 R26 19 A26 18 D26	H 20 R26 19 A26 18 D26	26
			H 20 R27 19 A27 18 D27	H 20 R27 19 A27 18 D27	H 20 R27 19 A27 18 D27	27
			H 16 R28 12 A28 19 D28 (Fatty Acid (Fragment IV))	O 14 R28 11 A28 4 D28	O 14 R28 11 A28 4 D28	28
				C 14 R29 11 A29 4 D29	C 14 R29 11 A29 4 D29	29
				C 29 R30 14 A30 11 D30	C 29 R30 14 A30 11 D30	30
				C 30 R31 29 A31 14 D31	C 30 R31 29 A31 14 D31	31
				H 29 R32 14 A32 11 D32	H 29 R32 14 A32 11 D32	32
				H 29 R33 14 A33 11 D33	H 29 R33 14 A33 11 D33	33
				H 30 R34 29 A34 14 D34	H 30 R34 29 A34 14 D34	34
				H 30 R35 29 A35 14 D35	H 30 R35 29 A35 14 D35	35
				H 31 R36 30 A36 29 D36	H 31 R36 30 A36 29 D36	36
				H 31 R37 30 A11 29 D37	H 31 R37 30 A11 29 D37	37
				H 31 R38 30 A38 29 D38	H 31 R38 30 A38 29 D38	38
				H 16 R39 12 A39 9 D39 (Fatty Acid (Fragment IV))	O 13 R39 10 A39 3 D39	39
					C 13 R40 10 A40 3 D40	40
					C 40 R41 13 A41 10 D41	41
					C 41 R42 40 A42 13 D42	42
					H 40 R43 13 A43 10 D43	43
					H 40 R44 13 A44 10 D44	44
					H 41 R45 40 A45 13 D45	45
					H 41 R46 40 A46 13 D46	46
					H 42 R47 41 A47 40 D47	47
					H 42 R48 41 A48 40 D48	48
					H 42 R49 41 A49 40 D49	49
					H 16 R50 12 A50 9 D50	50

Table S1-2 Geometrical variables for the various Z-matrices of phospholipids

GLYCEROL (Fragment I)	GLYCEROL WITH PHOSPHATE (Fragment I + II)	GLYCEROL, PHOSPHATE, X-GROUP (Fragment I to III)	PHOSPHOLIPID First fatty acid included (Fragments I to IV	PHOSPHOLIPID First and second fatty acid included (Fragments I to V)
R2=1.1216	R2=1.126	R2=1.1281	R2=1.1283	R2=1.1252
R3=1.5315	R3=1.5329	R3=1.5317	R3=1.5328	R3=1.5352
R4=1.5296	R4=1.5356	R4=1.5316	R4=1.5284	R4=1.5335
R5=1.1221	R5=1.1219	R5=1.1226	R5=1.1211	R5=1.1203
R6=1.1224	R6=1.1262	R6=1.1243	R6=1.1246	R6=1.1253
R7=1.1258	R7=1.1257	R7=1.1267	R7=1.1265	R7=1.1285
R8=1.1214	R8=1.1225	R8=1.1212	R8=1.1208	R8=1.1205
R9=1.4106	R9=1.4068	R9=1.4136	R9=1.4131	R9=1.4091
R10=1.42	R10=1.4227	R10=1.4216	R10=1.4221	R10=1.4304
R11=1.419	R11=1.4126	R11=1.4171	R11=1.4311	R11=1.4332
R12=0.9668	**R12=1.7057**	**R12=1.6927**	**R12=1.6927**	**R12=1.7089**
R13=0.9662	**R13=0.9674**	**R13=0.9686**	**R13=0.9675**	**R13=1.3797**
R14=0.9638	**R14=0.967**	**R14=0.9652**	**R14=1.3815**	**R14=1.3781**
	R15=1.5521	R15=1.56	R15=1.5599	R15=1.5339
	R16=1.6807	R16=1.6757	R16=1.6757	R16=1.678
	R17=1.6792	R17=1.7129	R17=1.713	R17=1.7042
	R18=0.962	**R18=1.4015**	**R18=1.4014**	**R18=1.4061**
	R19=0.9631	R19=1.538	R19=1.5382	R19=1.5366
		R20=1.486	R20=1.4859	R20=1.4816
		R21=1.1262	R21=1.1262	R21=1.1299
		R22=1.1292	R22=1.1293	R22=1.1222
		R23=1.127	R23=1.127	R23=1.1287
		R24=1.1316	R24=1.1317	R24=1.1278
		R25=1.0221	R25=1.0222	R25=1.0346
		R26=1.0452	R26=1.0449	R26=1.0277
		R27=1.0219	R27=1.0219	R27=1.0269
		R28=0.9666	R28=1.2287	R28=1.2387
			R29=1.4938	R29=1.4879
			R30=1.5149	R30=1.5161
			R31=1.5064	R31=1.5065
			R32=1.1232	R32=1.1253
			R33=1.123	R33=1.1243
			R34=1.1223	R34=1.1221
			R35=1.1223	R35=1.1224
			R36=1.117	R36=1.117
			R37=1.1169	R37=1.1169
			R38=1.1171	R38=1.1175
			R39=0.9665	R39=1.2325
				R40=1.4934
				R41=1.5162
				R42=1.5069
				R43=1.1251
				R44=1.1223
				R45=1.1218
				R46=1.1228
				R47=1.117
				R48=1.1169
				R49=1.1172
				R50=0.9668

Table S1-2 Continue

GLYCEROL (Fragment I)	GLYCEROL WITH PHOSPHATE (Fragment I + II)	GLYCEROL, PHOSPHATE, X-GROUP (Fragment I to III)	PHOSPHOLIPID First fatty acid included (Fragments I to IV	PHOSPHOLIPID First and second fatty acid included (Fragments I to V)
A3=110.0974	A3=109.1725	A3=109.9195	A3=109.8414	A3=111.1376
A4=110.4478	A4=110.9072	A4=109.9386	A4=109.268	A4=112.1617
A5=110.3795	A5=111.0577	A5=110.6167	A5=111.5957	A5=110.5231
A6=109.8647	A6=110.6528	A6=111.2454	A6=111.1582	A6=110.4884
A7=110.2977	A7=109.4897	A7=110.442	A7=110.4361	A7=109.4902
A8=110.2439	A8=110.6323	A8=110.1218	A8=111.12	A8=111.3046
A9=111.1015	A9=110.3678	A9=110.2706	A9=110.2921	A9=109.2875
A10=106.2381	A10=106.8801	A10=106.6297	A10=106.6623	A10=109.6952
A11=106.1371	A11=110.35	A11=105.3672	A11=105.3623	A11=104.8915
A12=106.9957	**A12=111.7365**	**A12=112.4255**	**A12=112.35**	**A12=113.684**
A13=106.6503	**A13=107.0443**	**A13=107.6328**	**A13=107.4828**	**A13=117.2627**
A14=106.8514	**A14=107.3144**	**A14=107.1963**	**A14=116.4654**	**A14=118.8617**
	A15=115.1375	A15=118.8107	A15=118.7567	A15=116.2749
	A16=103.8712	A16=109.4897	A16=109.174	A16=101.5556
	A17=102.1326	A17=102.3787	A17=102.4541	A17=95.025
	A18=104.2327	A18=113.8763	A18=113.8057	A18=116.0671
	A19=105.1155	A19=113.1627	A19=113.2176	A19=109.7724
		A20=113.5057	A20=113.577	A20=113.4188
		A21=111.7025	A21=111.6973	A21=105.8982
		A22=103.6839	A22=103.6782	A22=113.1914
		A23=108.7264	A23=108.6905	A23=109.2299
		A24=109.4808	A24=109.4409	A24=108.4871
		A25=110.4825	A25=110.4682	A25=111.103
		A26=108.5398	A26=108.5081	A26=109.9291
		A27=110.1548	A27=110.1837	A27=111.368
		A28=107.3796	A28=116.8871	A28=109.0617
			A29=112.2085	A29=121.4404
			A30=111.2038	A30=111.8053
			A31=110.8594	A31=110.8326
			A32=108.4512	A32=108.3245
			A33=108.4818	A33=108.957
			A34=109.4151	A34=109.3823
			A35=109.4035	A35=109.3674
			A36=110.8532	A36=110.9053
			A37=110.8574	A37=110.9152
			A38=109.9225	A38=109.8288
			A39=107.2186	A39=116.9821
				A40=112.6202
				A41=111.0045
				A42=110.6798
				A43=107.1833
				A44=109.8654
				A45=109.5367
				A46=109.4027
				A47=110.8377
				A48=110.8593
				A49=109.8775
				A50=106.6959

Table S1-2 Continued

GLYCEROL (Fragment I)	**GLYCEROL WITH PHOSPHATE** (Fragment I + II)	GLYCEROL, PHOSPHATE, X-GROUP (Fragment I to III)	PHOSPHOLIPID First fatty acid included (Fragments I to IV)	2-CHAINS-PHOSPHOLIPID (Fragment I to V)
D4= -60.1588	D4= -53.7954	D4= -63.8902	D4= -66.5999	D4= 26.8253
D5= -59.1874	D5= -6.3298	D5= -54.5261	D5= -61.2505	D5= -179.811
D6= 61.3828	D6= 67.251	D6= 58.3345	D6= 55.4271	D6= 148.3108
D7= 61.3457	D7= 68.3508	D7= 57.6093	D7= 54.9113	D7= 149.334
D8= 62.1282	D8= 115.2874	D8= 67.1209	D8= 61.7809	D8= -56.8221
D9= -176.39	D9= -168.746	D9= -177.636	D9= 179.5192	D9= -88.8693
D10= 179.5268	D10= -173.729	D10= 175.2217	D10= 172.5609	D10= -89.5396
D11= **-178.533**	D11= -129.247	D11= -173.41	D11= -178.943	D11= 61.3632
D12= -55.3082	**D12= -99.5764**	**D12= -92.835**	**D12= -93.7806**	**D12= -96.1656**
D13= 175.5578	**D13= 178.6422**	**D13= 163.0249**	**D13= 163.5726**	**D13= -83.2318**
D14= 175.6388	**D14= 67.7852**	**D14= -178.446**	**D14= -169.178**	**D14= 173.5444**
	D15= -29.8477	D15= -36.5255	D15= -34.7588	D15= -50.5988
	D16= 100.7922	D16= 100.9108	D16= 102.5071	D16= 78.688
	D17= -153.691	D17= -151.425	D17= -149.719	D17= -175.649
	D18= 127.1654	**D18= -156.821**	**D18= -158.078**	**D18= -76.1666**
	D19= -69.5994	D19= -66.268	D19= -66.838	D19= 115.6701
		D20= -38.05	D20= -37.4747	D20= -62.6243
		D21= 55.7906	D21= 55.2686	D21= -128.593
		D22= 173.2979	D22= 172.7539	D22= -9.1516
		D23= -159.578	D23= -159.013	D23= 57.8023
		D24= 81.4758	D24= 81.9385	D24= 176.6851
		D25= -50.936	D25= -50.6133	D25= -51.628
		D26= 68.3443	D26= 68.6355	D26= 66.6063
		D27= -172.363	D27= -172.064	D27= -171.324
		D28= -30.827	D28= -0.3377	D28= 178.2039
			D29= 179.6415	D29= -2.0544
			D30= -179.953	D30= 174.0422
			D31= 179.9618	D31= 178.0883
			D32= -58.2419	D32= -64.6654
			D33= 58.3206	D33= 52.1424
			D34= -58.4292	D34= -60.4195
			D35= 58.3732	D35= 56.5049
			D36= -60.1931	D36= -60.7521
			D37= 60.2132	D37= 59.8156
			D38= -179.987	D38= 179.5414
			D39= -29.4313	D39= 2.9895
				D40= 181.7598
				D41= 141.2515
				D42= 174.0639
				D43= -98.3579
				D44= 18.5726
				D45= -64.73
				D46= 52.6464
				D47= -60.8242
				D48= 59.6213
				D49= 179.4392
				D50= -114.629

Table S1-3 Sample symbolic z-matrices of atom connectivity for various sizes of fats; Note that hydrocarbon chains are the only substituents on this molecule

	GLYCEROL (Fragment I)	FAT First fatty acid included (Fragments I + II)	FAT First and second fatty acid included (Fragments I to III)	FAT First, second and third fatty acid included (Fragments I to IV)
Glycerol Groups	0 1 H C 1 R2 C 2 R3 1 A3 C 3 R4 2 A4 1 D4 H 4 R5 3 A5 2 D5 H 2 R6 3 A6 4 D6 H 3 R7 2 A7 1 D7 H 4 R8 3 A8 2 D8 O 2 R9 3 A9 4 D9 O 3 R10 2 A10 1 D10 O 4 R11 3 A11 2 D11	0 1 H C 1 R2 C 2 R3 1 A3 C 3 R4 2 A4 1 D4 H 4 R5 3 A5 2 D5 H 2 R6 3 A6 4 D6 H 3 R7 2 A7 1 D7 H 4 R8 3 A8 2 D8 O 2 R9 3 A9 4 D9 O 3 R10 2 A10 1 D10 O 4 R11 3 A11 2 D11	0 1 H C 1 R2 C 2 R3 1 A3 C 3 R4 2 A4 1 D4 H 4 R5 3 A5 2 D5 H 2 R6 3 A6 4 D6 H 3 R7 2 A7 1 D7 H 4 R8 3 A8 2 D8 O 2 R9 3 A9 4 D9 O 3 R10 2 A10 1 D10 O 4 R11 3 A11 2 D11	0 1 H C 1 R2 C 2 R3 1 A3 C 3 R4 2 A4 A D4 H 4 R5 3 A5 2 D5 H 2 R6 3 A6 4 D6 H 3 R7 2 A7 1 D7 H 4 R8 3 A8 2 D8 O 2 R9 3 A9 4 D9 O 3 R10 2 A10 1 D10 O 4 R11 3 A11 2 D11
	H 9 R12 2 A12 3 D12 **H 10 R13 3 A13 2 D13** **H 11 R14 4 A14 3 D14**	**C 9 R12 2 A12 3 D12** **H 10 R13 3 A13 2 D13** **H 11 R14 4 A14 3 D14**	**C 9 R12 2 A12 3 D12** **H 10 R13 3 A13 2 D13** **C 11 R14 4 A14 3 D14**	**C 9 R12 2 A12 3 D12** **C 10 R13 3 A13 2 D13** **C 11 R14 4 A14 3 D14**
Fatty Acid (Fragment II)		O 12 R15 9 A15 2 D15 C 12 R16 9 A16 2 D16 C 16 R17 12 A17 9 D17 C 17 R18 16 A18 12 D18 H 16 R19 12 A19 9 D19 H 16 R20 12 A20 9 D20 H 17 R21 16 A21 12 D21 H 17 R22 16 A22 12 D22 H 18 R23 17 A23 16 D23 H 18 R24 17 A24 16 D24 H 18 R25 17 A25 16 D25	O 12 R15 9 A15 2 D15 C 12 R16 9 A16 2 D16 C 16 R17 12 A17 9 D17 C 17 R18 16 A18 12 D18 H 16 R19 12 A19 9 D19 H 16 R20 12 A20 9 D20 H 17 R21 16 A21 12 D21 H 17 R22 16 A22 12 D22 H 18 R23 17 A23 16 D23 H 18 R24 17 A24 16 D24 H 18 R25 17 A25 16 D25	O 12 R15 9 A15 2 D15 C 12 R16 9 A16 2 D16 C 16 R17 12 A17 9 D17 C 17 R18 16 A18 12 D18 H 16 R19 12 A19 9 D19 H 16 R20 12 A20 9 D20 H 17 R21 16 A21 12 D21 H 17 R22 16 A22 12 D22 H 18 R23 17 A23 16 D23 H 18 R24 17 A24 16 D24 H 18 R25 17 A25 16 D25
Fatty Acid (Fragment III)			O 14 R26 11 A26 4 D26 C 14 R27 11 A29 4 D29 C 27 R28 14 A30 11 D30 C 28 R29 27 A31 14 D31 H 27 R30 14 A32 11 D32 H 27 R31 14 A33 11 D33 H 28 R32 27 A34 14 D34 H 28 R33 27 A35 14 D35 H 29 R34 28 A36 27 D36 H 29 R35 28 A11 27 D37 H 29 R36 28 A36 27 D36	O 14 R26 11 A26 4 D26 C 14 R27 11 A29 4 D29 C 27 R28 14 A30 11 D30 C 28 R29 27 A31 14 D31 H 27 R30 14 A32 11 D32 H 27 R31 14 A33 11 D33 H 28 R32 27 A34 14 D34 H 28 R33 27 A35 14 D35 H 29 R34 28 A36 27 D36 H 29 R35 28 A11 27 D37 H 29 R36 28 A36 27 D36
Fatty Acid (Fragment IV)				O 13 R37 10 A37 3 D37 C 13 R38 10 A38 3 D38 C 38 R39 13 A39 10 D39 C 39 R40 38 A29 13 D40 H 38 R41 13 A41 10 D41 H 38 R42 13 A42 10 D42 H 39 R43 38 A43 13 D43 H 39 R44 38 A44 13 D44 H 40 R45 39 A45 38 D45 H 40 R46 39 A46 38 D46 H 40 R47 39 A47 38 D47

Table S1-4 Variables (Bond Distances, Bond Angles and Dihedral Values) of a fat molecule

GLYCEROL (Fragment I)	FAT First fatty acid included (Fragments I + II)	FAT First and second fatty acid included (Fragments I to III)	FAT First, second and third fatty acid included (Fragments I to IV)
R2=1.1216	R2=1.1205	R2=1.1204	R2=1.1221
R3=1.5315	R3=1.5325	R3=1.5334	R3=1.5302
R4=1.5296	R4=1.5306	R4=1.5288	R4=1.5306
R5=1.1221	R5=1.1223	R5=1.1203	R5=1.1219
R6=1.1224	R6=1.1206	R6=1.1213	R6=1.1205
R7=1.1258	R7=1.1257	R7=1.1264	R7=1.1253
R8=1.1214	R8=1.1214	R8=1.1202	R8=1.1197
R9=1.4106	R9=1.4284	R9=1.4282	R9=1.4284
R10=1.42	R10=1.4194	R10=1.4198	R10=1.4354
R11=1.419	R11=1.4192	R11=1.4357	R11=1.4335
R12=0.9668	**R12=1.3774**	**R12=1.3778**	**R12=1.3762**
R13=0.9662	**R13=0.9669**	**R13=0.966**	**R13=1.3732**
R14=0.9638	**R14=0.9636**	**R14=1.3725**	**R14=1.3721**
	R15=1.2308	R15=1.2305	R15=1.2309
	R16=1.4949	R16=1.4948	R16=1.4954
	R17=1.5148	R17=1.5148	R17=1.5147
	R18=1.5061	R18=1.5061	R18=1.5061
	R19=1.1229	R19=1.1229	R19=1.1228
	R20=1.1236	R20=1.1235	R20=1.1234
	R21=1.1225	R21=1.1224	R21=1.1225
	R22=1.1222	R22=1.1222	R22=1.1222
	R23=1.117	R23=1.117	R23=1.117
	R24=1.117	R24=1.117	R24=1.117
	R25=1.1169	R25=1.1169	R25=1.1169
		R26=1.2309	R26=1.2312
		R27=1.4957	R27=1.496
		R28=1.514	R28=1.5147
		R29=1.5063	R29=1.5066
		R30=1.1229	R30=1.1218
		R31=1.1226	R31=1.1239
		R32=1.1223	R32=1.1229
		R33=1.1223	R33=1.1219
		R34=1.117	R34=1.1169
		R35=1.117	R35=1.117
		R36=1.1169	R36=1.1169
			R37=1.2307
			R38=1.4964
			R39=1.5146
			R40=1.5065
			R41=1.1239
			R42=1.1218
			R43=1.1219
			R44=1.1229
			R45=1.1169
			R46=1.1169
			R47=1.117

Table S1-4 Continued

GLYCEROL (Fragment I)	FAT First fatty acid included (Fragments I + II)	FAT First and second fatty acid included (Fragments I to III)	FAT First, second and third fatty acid included (Fragments I to IV)
A3=110.0974	A3=110.8831	A3=111.1742	A3=109.142
A4=110.4478	A4=110.6974	A4=110.2722	A4=110.9223
A5=110.3795	A5=110.532	A5=111.7815	A5=110.1132
A6=109.8647	A6=109.6135	A6=109.6214	A6=110.7424
A7=110.2977	A7=110.1298	A7=110.0622	A7=110.6866
A8=110.2439	A8=109.4899	A8=110.8327	A8=111.8672
A9=111.1015	A9=105.914	A9=105.6611	A9=106.0801
A10=106.2381	A10=105.5937	A10=105.7309	A10=105.9291
A11=106.1371	A11=106.1792	A11=105.4591	A11=106.1598
A12=106.9957	**A12=117.5617**	**A12=117.5504**	**A12=117.5939**
A13=106.6503	**A13=106.2931**	**A13=106.3397**	**A13=117.8844**
A14=106.8514	**A14=106.8117**	**A14=116.5616**	**A14=116.5797**
	A15=111.6499	A15=111.6669	A15=111.8564
	A16=120.4212	A16=120.3534	A16=120.3786
	A17=111.4893	A17=111.4846	A17=111.5014
	A18=111.1289	A18=111.1301	A18=111.1598
	A19=109.1238	A19=109.0533	A19=109.0757
	A20=108.5296	A20=108.6015	A20=108.5406
	A21=109.2417	A21=109.2442	A21=109.2304
	A22=109.2872	A22=109.2763	A22=109.27
	A23=110.8344	A23=110.8325	A23=110.8349
	A24=110.8215	A24=110.8268	A24=110.8267
	A25=110.0297	A25=110.0259	A25=110.0358
		A26=117.8512	A26=118.0184
		A27=112.2647	A27=112.3912
		A28=111.3076	A28=111.1025
		A29=110.9926	A29=110.9567
		A30=108.3488	A30=109.7459
		A31=108.4598	A31=107.2226
		A32=109.3698	A32=109.2851
		A33=109.3481	A33=109.4675
		A34=110.803	A34=110.8037
		A35=110.8131	A35=110.7686
		A36=110.0289	A36=110.0437
			A37=118.3739
			A38=112.1131
			A39=111.1109
			A40=110.9469
			A41=107.1701
			A42=109.7047
			A43=109.4679
			A44=109.2902
			A45=110.0339
			A46=110.801
			A47=110.7749

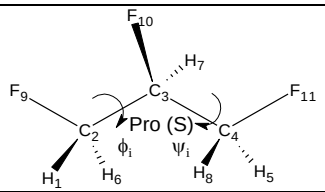
Table S1-4 Continued

GLYCEROL (Fragment I)	FAT First fatty acid included (Fragments I + II)	FAT First and second fatty acid included (Fragments I to III)	FAT First, second and third fatty acid included (Fragments I to IV)
D4= -60.1588	D4= 50.0202	D4= 33.5711	D4= -40.4434
D5= -59.1874	D5= -59.6731	D5= -64.5566	D5= -172.583
D6= 61.3828	D6= 171.6628	D6= 155.4752	D6= 81.8533
D7= 61.3457	D7= 171.1178	D7= 154.7339	D7= 82.8712
D8= 62.1282	D8= 61.5283	D8= 58.696	D8= -50.2572
D9= -176.39	D9= -68.8284	D9= -85.361	D9= -158.429
D10= 179.5268	D10= -70.6047	D10= -86.7687	D10= -157.321
D11= -178.533	D11= -178.502	D11= 177.3589	D11= 68.425
D12= -55.3082	**D12= -172.491**	**D12= -173.858**	**D12= -174.627**
D13= 175.5578	**D13= 171.6604**	**D13= 175.5582**	**D13= -152.01**
D14= 175.6388	**D14= -173.094**	**D14= -177.047**	**D14= 169.1387**
	D15= -178.179	D15= -179.617	D15= -179.818
	D16= 2.126	D16= 0.5728	D16= 0.3738
	D17= -174.732	D17= -175.643	D17= -174.592
	D18= -178.738	D18= -179.025	D18= -178.726
	D19= -53.0396	D19= -54.0308	D19= -52.9545
	D20= 64.0893	D20= 63.1131	D20= 64.2129
	D21= -56.9809	D21= -57.2687	D21= -56.9511
	D22= 59.5518	D22= 59.2594	D22= 59.5491
	D23= -60.0065	D23= -60.0304	D23= -59.9758
	D24= 60.2834	D24= 60.2674	D24= 60.3206
	D25= -179.871	D25= -179.885	D25= -179.834
		D26= -1.4399	D26= 3.5768
		D27= 178.6624	D27= -175.987
		D28= 179.6407	D28= -144.064
		D29= 179.8872	D29= -174.235
		D30= -58.6138	D30= -21.4036
		D31= 57.8167	D31= 95.3267
		D32= -58.4378	D32= -52.6243
		D33= 58.2292	D33= 64.3993
		D34= -60.1286	D34= -59.3163
		D35= 60.1401	D35= 60.9258
		D36= -179.989	D36= -179.235
			D37= -6.1713
			D38= 173.5907
			D39= 145.5699
			D40= 174.2472
			D41= -93.7769
			D42= 22.9409
			D43= -64.378
			D44= 52.6389
			D45= 179.2166
			D46= 59.3154
			D47= -60.9409

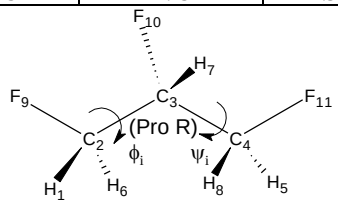
2. Tabulated Values Glycerol and Similar Models

2.1 Dihedral Values of 1,2,3-trifluoropropane and 1,2-difluoro-3-dihydroxylpropane

Table S2-1 **Dihedral angles (Degree) for all computed/attempted backbone conformer and total and relative energies of 1,2,3-trifluoropropane with F_{10} substitution in different enantiomeric arrangements**

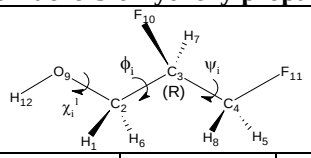


Conformation ϕ_i, ψ_i	ϕ_i	ψ_i	Total Energy	Relative Energy (Kcal · mol-1)
g^+g^+	46.991	59.372	-412.5620548790	0.000
g^+a	35.861	168.137	-412.5589035780	1.978
g^+g^-	52.473	-52.446	-412.5505691310	7.208
ag^+	-168.480	56.350	-412.5599287750	1.334
aa	-169.903	169.986	-412.5543521910	4.834
ag^-	-168.164	-35.900	-412.5589035860	1.978
g^-g^+	-47.777	85.673	-412.5554872840	4.121
g^-a	-56.377	168.480	-412.5599287930	1.334
g^-g^-	-59.413	-47.151	-412.5620551750	0.000

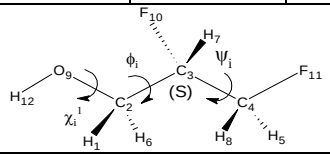


g^+g^+	59.360	47.209	-412.5620550200	0.000
g^+a	56.388	191.525	-412.5599288070	1.334
g^+g^-	85.644	-47.762	-412.5554872950	4.121
ag^+	168.182	35.950	-412.5589035710	1.978
aa	169.875	189.991	-412.5543521570	4.834
ag^-	168.469	-56.384	-412.5599288060	1.334
g^-g^+	-52.418	52.613	-412.5505692200	7.207
g^-a	-35.907	191.848	-412.5589035970	1.978
g^-g^-	-47.082	-59.372	-412.5620550500	0.000

Table S2-2 Dihedral angles (Degree) for all computed/attempted backbone conformer and total and relative energies of 12-difluoro-3-dihydroxylpropane at the R and S enantiomer



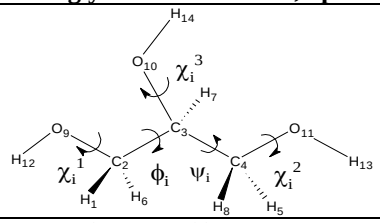
Conformation (ϕ_i, ψ_i, χ_i)	ϕ_i	ψ_i	χ_i^1	Total Energy (Hartrees)	Relative Energy (Kcal · mol^{-1})
R Configuration					
***g*$^+$*g*$^+$*g*$^+$**	62.9241	50.2006	89.341	-388.677989331	2.822
***g*$^+$*ag*$^+$**	61.0972	-167.106	83.292	-388.677753514	2.970
***g*$^+$*g*$^-$*g*$^+$**	24.311	-74.651	45.911	-388.677060952	3.403
***ag*$^+$*g*$^+$**	-177.6867	39.334	58.117	-388.679721754	1.735
***aag*$^+$**	-174.2237	-168.941	52.419	-388.676840259	3.543
***ag*$^-$*g*$^+$**	-178.0211	-55.184	57.917	-388.679705903	1.745
***g*$^-$*g*$^+$*g*$^+$**	-66.9891	40.563	49.374	-388.677430572	3.173
***g*$^-$*ag*$^+$**	Not Found				
***g*$^-$*g*$^-$*g*$^+$**	-34.9848	-43.865	78.170	-388.680031197	1.541
g*$^+$*g*$^+$*a	62.0719	46.707	-164.305	-388.680998523	0.934
g*$^+$*aa	59.8672	-170.132	177.586	-388.678670249	2.395
g*$^+$*g*$^-$*a	55.1832	-94.082	-178.105	-388.672634648	6.182
ag*$^+$*a	166.6145	37.071	152.988	-388.675122045	4.621
aaa	167.1333	-171.033	159.277	-388.670873420	7.287
ag*$^-$*a	167.5279	-56.220	172.461	-388.675712676	4.251
g*$^-$*g*$^+$*a	-43.9846	66.810	-165.476	-388.664383445	11.360
g*$^-$*aa	-38.7819	-166.369	-169.249	-388.676083778	4.018
g*$^-$*g*$^-$*a	-50.5513	-59.818	175.061	-388.678195138	2.693
***g*$^+$*g*$^+$*g*$^-$**	47.3994	31.305	-82.764	-388.682486294	0.000
***g*$^+$*ag*$^-$**	Not Found				
***g*$^+$*g*$^-$*g*$^-$**	75.8825	-49.266	-59.122	-388.681797850	0.432
***ag*$^+$*g*$^-$**	175.6926	37.353	-71.442	-388.672551201	6.234
***aag*$^-$**	179.7225	-167.464	-65.284	-388.669663632	8.046
***ag*$^-$*g*$^-$**	173.0188	-58.771	-76.009	-388.674532311	4.991
***g*$^-$*g*$^+$*g*$^-$**	Not Found				
***g*$^-$*ag*$^-$**	-56.4593	-174.434	-60.947	-388.679615054	1.801
***g*$^-$*g*$^-$*g*$^-$**	-61.0671	-65.397	-59.488	-388.682308717	0.111



Conformation (ϕ_i, ψ_i, χ_i)	ϕ_i	ψ_i	χ_i^1	Total Energy (Hartrees)	Relative Energy (Kcal · mol^{-1})
S Configuration					
***g*$^+$*g*$^+$*g*$^+$**	61.069	65.413	59.645	-388.682309409	0.111
***g*$^+$*ag*$^+$**	56.382	174.446	61.086	-388.679615115	1.802
***g*$^+$*g*$^-$*g*$^+$**	Not Found				
***ag*$^+$*g*$^+$**	-172.989	58.759	75.923	-388.674532456	4.991
***aag*$^+$**	-179.677	167.470	65.327	-388.669663613	8.046
***ag*$^-$*g*$^+$**	-175.693	-37.408	71.414	-388.672551074	6.234
***g*$^-$*g*$^+$*g*$^+$**	-75.866	49.299	59.093	-388.681797908	0.432
***g*$^-$*ag*$^+$**	Not Found				
***g*$^-$*g*$^-$*g*$^+$**	-47.415	-31.276	82.726	-388.682486282	0.000
g*$^+$*g*$^+$*a	50.553	59.766	-174.987	-388.678195063	2.693
g*$^+$*aa	38.838	166.297	169.054	-388.676083733	4.018
g*$^+$*g*$^-$*a	44.049	-66.777	165.513	-388.664383446	11.360
ag*$^+$*a	-167.589	56.207	-172.540	-388.675712553	4.251
aaa	-167.079	171.022	-159.185	-388.670873443	7.287
ag*$^-$*a	193.365	-37.075	151.743	-388.675122052	4.619
g*$^-$*g*$^+$*a	-55.276	94.070	178.135	-388.672634518	6.182
g*$^-$*aa	-59.990	169.993	-177.590	-388.678670635	2.394
g*$^-$*g*$^-$*a	-62.072	-46.705	164.298	-388.680998522	0.934
***g*$^+$*g*$^+$*g*$^-$**	34.732	43.971	-77.884	-388.680030949	1.541
***g*$^+$*ag*$^-$**	Not Found				
***g*$^+$*g*$^-$*g*$^-$**	66.940	-40.918	-49.017	-388.677430517	3.173
***ag*$^+$*g*$^-$**	177.966	55.325	-57.841	-388.679705987	1.745
***aag*$^-$**	174.218	168.942	-52.411	-388.676840283	3.543
***ag*$^-$*g*$^-$**	177.699	-39.241	-58.106	-388.679722261	1.734
***g*$^-$*g*$^+$*g*$^-$**	-18.952	72.541	-49.374	-388.677059216	3.406
***g*$^-$*ag*$^-$**	-58.434	167.099	-83.357	-388.677753515	2.970
***g*$^-$*g*$^-$*g*$^-$**	-62.902	-50.048	-89.364	-388.677989176	2.821

2.2 Dihedral Values of Found Conformation in Glycerol

Table S2-3 Dihedral angles (Degree) for all computed/attempted backbone conformer and total and relative energies of stable glycerol conformers, optimized at RHF 3-21g

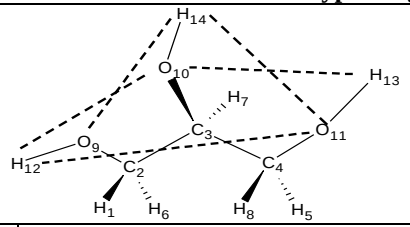


Conformations of found geometry							
Conformations (ϕ_i, ϕ_i, χ_i^1, χ_i^2, χ_i^3)	ϕ_i	ψ_i	χ_i^1	χ_i^2	χ_i^3	**Total Energy (Hartrees)**	**Relative Energy (Kcal · mol^{-1})**
g*$^+$*g*$^+$*g*$^+$*a	64.757	66.457	51.606	75.818	-177.803	-340.9141639030	5.22
***g*$^+$*g*$^+$*g*$^+$*g*$^-$**	65.012	64.835	42.684	80.923	-82.838	-340.9135957220	5.46
g*$^+$*g*$^+$*g*$^+$*aa	63.373	68.462	52.593	-158.013	-171.396	-340.9165790490	3.57
***g*$^+$*g*$^+$*g*$^+$*ag*$^-$**	63.665	65.655	44.876	-162.017	-86.727	-340.9160641750	3.94
g*$^+$*g*$^+$*g*$^-$*a	46.949	34.077	60.692	-71.354	-176.369	-340.9178920300	3.27
***g*$^+$*g*$^+$*g*$^+$*g*$^-$**	50.180	30.634	52.903	-71.065	-83.317	-340.9176228940	3.52
***g*$^+$*g*$^+$*ag*$^+$*g*$^+$**	70.391	61.327	-174.026	79.080	37.665	-340.917343882	3.23
g*$^+$*g*$^+$*ag*$^+$*a	52.731	62.375	-167.926	75.671	-178.949	-340.9047877150	10.34
***g*$^+$*g*$^+$*aag*$^+$**	69.352	62.214	-179.104	-176.747	37.721	-340.9179318310	2.88
***g*$^+$*g*$^+$*ag*$^-$*g*$^+$**	54.184	28.045	167.403	-72.781	49.068	-340.9164592180	4.14
***g*$^+$*g*$^+$*ag*$^-$*g*$^-$**	36.375	42.290	159.886	-75.998	-76.229	-340.9112656000	6.83
***g*$^+$*g*$^+$*g*$^-$*g*$^+$*g*$^+$**	67.549	53.993	-97.708	80.532	35.571	-340.9165815650	3.64
g*$^+$*g*$^+$*g*$^-$*g*$^+$*a	27.180	48.153	-68.093	75.728	-172.274	-340.9101847960	7.70
***g*$^+$*g*$^+$*g*$^-$*g*$^+$*g*$^-$**	35.635	41.763	-70.003	80.937	-54.266	-340.9117043870	6.68
***g*$^+$*g*$^+$*g*$^-$*ag*$^+$**	66.659	53.852	-96.064	170.127	35.450	-340.9166022690	3.61
g*$^+$*g*$^+$*g*$^-$*aa	22.648	53.070	-67.457	171.882	-165.443	-340.9104925610	7.50
***g*$^+$*g*$^+$*g*$^-$*ag*$^-$**	35.250	44.504	-71.143	168.823	-56.620	-340.9119925400	6.53
***g*$^+$*ag*$^+$*g*$^+$*g*$^-$**	61.347	-171.664	44.843	52.273	-85.660	-340.9175606660	3.33
g*$^+$*ag*$^+$*aa	61.639	-164.986	49.970	171.785	160.541	-340.9220523430	0.77
g*$^+$*ag*$^+$*g*$^-$*a	61.182	198.016	50.444	-84.432	153.227	-340.9205110270	1.70
***g*$^+$*aag*$^+$*g*$^+$**	67.268	-171.912	176.238	41.832	39.055	-340.9189571120	2.57
***g*$^+$*aag*$^+$*g*$^-$**	50.079	-178.397	-178.569	52.255	-63.167	-340.9097935660	7.55
***g*$^+$*aag*$^-$*g*$^-$**	47.391	171.632	177.907	-62.906	-64.751	-340.8988820990	13.76
***g*$^+$*ag*$^-$*g*$^+$*g*$^+$**	71.073	189.668	-96.563	40.079	33.802	-340.9164780270	3.92
***g*$^+$*g*$^-$*g*$^+$*g*$^+$*g*$^+$**	62.458	-73.011	68.303	58.450	105.928	-340.9239906530	0.00
***g*$^+$*g*$^-$*g*$^+$*g*$^+$*g*$^-$**	67.246	-53.600	46.312	32.585	-91.108	-340.9151064600	4.93
***g*$^+$*g*$^-$*ag*$^+$*g*$^+$**	44.548	-76.198	169.409	61.739	93.056	-340.9225734860	0.58
***g*$^+$*g*$^-$*g*$^-$*ag*$^+$**	76.166	-44.600	-61.679	-169.375	29.104	-340.9225735020	0.57
***g*$^+$*g*$^-$*g*$^-$*g*$^+$**	72.922	-62.554	-58.374	-68.163	14.135	-340.9239903620	0.00
g*$^+$*g*$^-$*g*$^-$*g*$^-$*a	53.507	-67.301	-32.405	-46.299	-148.188	-340.9151064670	4.93
***ag*$^+$*g*$^+$*g*$^+$*g*$^-$**	169.011	58.044	84.350	83.275	-36.213	-340.9146551840	4.67
***ag*$^+$*g*$^+$*ag*$^-$**	168.518	57.957	84.174	-179.589	-36.690	-340.9160817690	3.91
***ag*$^+$*ag*$^+$*g*$^-$**	172.107	55.972	184.197	79.078	-44.299	-340.9160563300	3.89
***ag*$^+$*aag*$^-$**	170.214	55.734	-178.747	179.170	-44.083	-340.9166774700	3.52
***ag*$^+$*g*$^-$*g*$^+$*g*$^+$**	179.054	55.700	-41.758	76.152	69.131	-340.9117035070	6.53
ag*$^+$*g*$^-$*g*$^+$*a	177.125	57.647	-52.597	73.853	-163.106	-340.9132857920	5.51
***ag*$^+$*g*$^-$*ag*$^+$**	176.902	57.077	-38.983	177.412	67.477	-340.9117028380	6.53

ag$^+$g$^-$aa	174.606	60.509	-50.684	-174.198	-158.300	-340.9142435380	4.94
ag$^+$g$^-$g$^-$g$^+$	175.683	60.167	-37.685	-94.307	71.940	-340.9090268310	7.94
aag$^+$g$^+$g$^-$	167.348	-173.082	82.272	47.933	-38.870	-340.9168267810	3.65
aaag$^+$g$^-$	170.669	-173.266	-174.897	46.713	-48.112	-340.9179959810	2.94
aag$^-$aa	173.278	-170.679	-46.755	175.058	169.934	-340.9179960090	2.94
aag$^-$g$^-$a	173.070	-167.326	-47.875	-82.370	160.739	-340.916826850	3.65
ag$^-$g$^+$aa	-171.635	-47.437	62.850	-177.647	-174.989	-340.8988820580	13.76
ag$^-$g$^+$g$^-$g$^-$	162.016	-61.135	84.410	-50.496	-34.478	-340.9205111200	1.70
ag$^-$ag$^-$g$^-$	164.967	-61.667	-171.784	-49.954	-41.860	-340.9220522900	0.77
ag$^-$g$^-$g$^+$g$^+$	170.395	-71.086	-40.093	96.661	88.499	-340.9164781620	3.92
ag$^-$g$^-$ag$^+$	171.922	-67.252	-41.873	-176.201	82.916	-340.9189571570	2.56
ag$^-$g$^-$aa	178.311	-50.011	-52.135	179.006	-175.787	-340.9097935060	7.55
ag$^-$g$^-$g$^-$a	171.651	-61.274	-52.257	-44.891	-155.186	-340.9175608500	3.32
g$^-$g$^+$g$^+$g$^+$g$^+$	-66.325	57.282	50.215	82.351	49.987	-340.9153998850	4.46
g$^-$g$^+$g$^+$g$^+$a	-67.582	58.094	53.864	78.288	-158.092	-340.9154038420	4.34
g$^-$g$^+$g$^+$g$^+$g$^-$	-69.106	57.373	52.981	84.193	-67.230	-340.9172134900	3.34
g$^-$g$^+$g$^+$ag$^+$	-70.954	54.707	45.969	175.539	47.163	-340.9154743480	4.33
g$^-$g$^+$g$^+$ag$^-$	-74.277	54.129	49.441	181.410	-70.793	-340.9181067390	2.79
g$^-$g$^+$ag$^-$g$^+$	-54.638	71.037	-175.583	-46.160	76.943	-340.9154745000	4.33
g$^-$g$^+$ag$^-$a	-54.172	74.244	178.434	-49.423	-169.176	-340.9181066890	2.79
g$^-$g$^+$g$^-$g$^-$g$^+$	-57.303	66.337	-82.375	-50.225	73.699	-340.9153998730	4.46
g$^-$g$^+$g$^-$g$^-$a	-57.428	69.132	-84.260	-52.878	-172.911	-340.9172131520	3.34
g$^-$g$^+$g$^-$g$^-$g$^-$	-58.017	67.660	-78.550	-53.958	-82.145	-340.9154037880	4.33
g$^-$ag$^+$g$^+$g$^+$	-60.149	-175.703	94.388	37.685	52.758	-340.909026847	7.94
g$^-$aag$^+$g$^+$	-57.052	-176.893	-177.717	39.056	56.942	-340.9117028420	6.53
g$^-$aag$^+$g$^-$	-60.513	-174.628	174.457	50.695	-81.588	-340.9142435080	4.94
g$^-$aaaa	-55.763	-170.079	-179.470	178.919	164.148	-340.9166772740	3.53
g$^-$aag$^-$a	-57.970	-168.516	179.536	-84.280	157.137	-340.9160817770	3.91
g$^-$ag$^-$g$^+$g$^+$	-55.611	-179.089	-76.286	41.889	55.287	-340.9117033280	6.53
g$^-$ag$^-$g$^+$g$^-$	-57.636	-177.148	-73.960	52.578	-76.836	-340.9132856220	5.51
g$^-$ag$^-$aa	-55.902	-172.072	-79.049	175.865	164.465	-340.9160561450	3.89
g$^-$ag$^-$g$^-$a	-58.083	-169.060	-83.150	-84.252	156.454	-340.9146551470	4.67
g$^-$g$^-$g$^+$ag$^+$	-27.983	-54.223	72.761	-167.286	72.023	-340.9164589670	4.14
g$^-$g$^-$g$^+$aa	-42.399	-36.264	76.086	-159.372	-164.011	-340.9112653030	6.82
g$^-$g$^-$g$^+$g$^-$a	-30.619	-50.177	71.052	-52.939	-159.555	-340.9176228810	3.52
g$^-$g$^-$g$^+$g$^-$g$^-$	-33.995	-46.993	71.292	-60.702	-66.250	-340.9178920950	3.27
g$^-$g$^-$ag$^+$g$^+$	-33.294	-53.436	-168.614	80.811	80.829	-340.9168595000	3.78
g$^-$g$^-$ag$^+$a	-44.497	-35.265	-168.776	71.178	175.808	-340.9119925110	6.53
g$^-$g$^-$ag$^+$g$^-$	-53.044	-22.670	-171.788	67.472	-74.347	-340.9104925660	7.50
g$^-$g$^-$aag$^+$	-62.278	-69.362	176.807	179.200	82.991	-340.9179319840	2.88
g$^-$g$^-$ag$^-$a	-65.647	-63.654	161.938	-44.876	-155.167	-340.916063160	3.94
g$^-$g$^-$ag$^-$g$^-$	-65.647	-68.480	157.719	-52.628	-70.536	-340.916579187	3.57
g$^-$g$^-$g$^-$g$^+$g$^+$	-33.703	-51.153	-81.410	79.654	78.8362	-340.9167237920	3.88
g$^-$g$^-$g$^-$g$^+$a	-41.729	-35.636	-80.845	69.911	172.720	-340.9117043410	6.68
g$^-$g$^-$g$^-$g$^+$g$^-$	-47.966	-27.312	-75.641	67.985	-68.756	-340.9101846300	7.70
g$^-$g$^-$g$^-$ag$^+$	-61.348	-70.388	-79.245	174.382	82.568	-340.9173438160	3.23
g$^-$g$^-$g$^-$ag$^-$	-62.354	-52.723	-75.716	167.851	-61.162	-340.9047877370	10.34
g$^-$g$^-$g$^-$g$^-$a	-64.812	-65.013	-81.053	-42.645	-159.391	-340.9135957750	5.46
g$^-$g$^-$g$^-$g$^-$g$^-$	-66.442	-64.721	-75.916	-51.571	-64.765	-340.9141640450	5.09

2.3 Bond Length of Found Conformation in Glycerol

Table S2-4 Values for topologically probably conformations in under different types of geometry



Type	Conformation		Relative Energy (Kcal · mol^{-1})	Distance of H-bonds								
	ϕ_i ψ_i	$\chi_i^1 \chi_i^2 \chi_i^3$		$H_{12}-O_9$	$H_{12}-O_{10}$	$H_{12}-O_{11}$	$H_{13}-O_9$	$H_{13}-O_{10}$	$H_{13}-O_{11}$	$H_{14}-O_9$	$H_{14}-O_{10}$	$H_{14}-O_{11}$
	g+ g+	a g-g+	4.726	0.965	3.603	3.541	2.169	3.760	0.968	2.353	0.969	3.741
2 Non-Bonding O and H Atoms pairs with distances under 2.5A	g+ a	g+g+g-	4.035	0.969	2.188	4.005	4.150	2.210	0.968	3.290	0.966	3.408
		g+ a a	1.216	0.970	2.153	3.921	4.642	3.467	0.965	3.420	0.969	2.062
		g+g-a	2.183	0.969	2.165	3.924	4.780	3.205	0.966	3.364	0.970	2.072
		a g+g+	3.158	0.965	3.511	5.048	4.047	2.160	0.969	2.070	0.970	3.231
		g-g+g+	4.714	0.964	3.333	4.324	4.126	2.129	0.970	2.077	0.971	3.269
	a a	g+g+g-	4.495	0.967	3.238	5.140	4.654	2.168	0.969	2.161	0.968	3.625
		a g+g-	3.762	0.965	3.517	5.593	4.581	2.156	0.969	2.161	0.968	3.599
		g-a a	3.762	0.969	2.156	4.581	5.594	3.518	0.965	3.598	0.968	2.162
		g-g-a	4.494	0.969	2.168	4.653	5.141	3.238	0.967	3.625	0.968	2.161
	ag-	g+g-g-	2.183	0.966	3.204	4.780	3.925	2.167	0.969	2.072	0.970	3.365
		a g-g-	1.216	0.965	3.466	4.642	3.921	2.153	0.970	2.061	0.969	3.420
		g-g+g+	4.714	0.970	2.130	4.127	4.325	3.333	0.964	3.270	0.971	2.076
		g- a g+	3.158	0.969	2.160	4.047	5.049	3.511	0.965	3.231	0.970	2.071
		g-g- a	4.035	0.968	2.210	4.150	4.005	2.190	0.969	3.410	0.966	3.290
	g+ g+	g+g-a	3.827	0.968	2.475	3.375	2.119	3.739	0.970	3.724	0.966	4.061
		g+g-g-	3.996	0.969	2.391	3.301	2.124	3.679	0.969	3.429	0.966	4.394
	g+g-	g+g+g-	5.575	0.972	2.119	2.804	1.879	2.935	0.969	3.284	0.966	3.872
		g-g- a	5.575	0.969	2.935	1.879	2.806	2.118	0.972	3.873	0.966	3.284
		a g+g+	0.889	0.964	3.766	3.510	1.846	2.874	0.972	2.914	0.970	2.036
		g-a g+	0.889	0.972	2.873	1.846	5.086	3.766	0.965	2.036	0.968	2.913
	g-g-	g+ag+	4.726	0.968	3.758	2.168	3.541	3.602	0.965	3.740	0.969	2.351
		g+g-a	3.996	0.969	3.679	2.123	3.301	2.391	0.969	4.394	0.966	3.430
		g+g-g-	3.827	0.970	3.739	2.119	3.376	2.474	0.968	4.061	0.966	3.723
		a g+g+	4.475	0.965	4.369	3.652	2.258	3.414	0.968	3.769	0.970	2.374
		g-g+g+	4.560	0.965	4.161	3.586	2.241	3.443	0.969	3.802	0.970	2.429

Table S2-4 Continued

			Relative Energy (Kcal · mol^{-1})	Distance of H-bonds								
	ϕ_i ψ_i	$\chi_i^1\chi_i^2\chi_i^3$		$H_{12}-O_9$	$H_{12}-O_{10}$	$H_{12}-O_{11}$	$H_{13}-O_9$	$H_{13}-O_{10}$	$H_{13}-O_{11}$	$H_{14}-O_9$	$H_{14}-O_{10}$	$H_{14}-O_{11}$
Type 3 Glycerol folded into a ball	g+ g-	g+g+g+	0.000	0.968	2.402	2.949	1.956	2.831	0.972	2.857	0.970	2.051
		g-g-g+	0.000	0.969	2.830	1.955	2.948	2.399	0.965	2.051	0.968	2.856
Type 4 five-member ring	g+g+	g+g+a	6.166	0.968	2.153	4.116	4.364	4.032	0.966	3.549	0.965	3.992
		g+g+g-	6.523	0.969	2.155	4.005	4.379	4.012	0.966	3.231	0.966	4.379
		g+ a a	4.651	0.968	2.175	4.088	4.016	4.377	0.965	3.585	0.965	3.971
		g+a g-	4.974	0.969	2.172	3.975	4.026	4.327	0.965	3.285	0.966	4.308
		a g+g+	4.170	0.964	3.544	4.180	4.342	4.032	0.966	2.050	0.969	4.014
		a a g+	3.802	0.964	3.534	4.188	4.185	4.385	0.965	2.063	0.969	3.980
		g-g+g+	8.663	0.965	3.391	3.229	4.253	4.082	0.966	2.137	0.970	3.974
		g-a g+	4.636	0.965	3.390	3.168	4.193	4.377	0.965	2.150	0.970	3.938
	g+a	ag+g-	8.909	0.965	3.791	5.060	4.212	2.195	0.968	3.311	0.965	3.539
	a g+	g+g+g-	5.858	0.966	3.272	4.542	4.718	4.049	0.966	2.160	0.969	4.326
		g+a g-	4.963	0.966	3.258	4.441	5.104	4.343	0.965	2.147	0.969	4.263
		a g+g-	4.979	0.965	3.539	4.847	4.594	4.036	0.966	2.151	0.969	4.340
		a a g-	4.589	0.965	3.538	4.753	5.073	4.337	0.965	2.123	0.968	4.274
		g-g+g+	7.710	0.969	2.266	4.633	4.536	4.058	0.966	3.179	0.968	3.932
		g-g+a	6.717	0.968	2.249	4.678	4.539	4.061	0.966	3.494	0.966	4.087
		g-a g+	7.711	0.968	2.227	4.535	5.086	4.412	0.965	3.128	0.968	3.908
		g- a a	6.116	0.968	2.210	4.590	5.070	4.392	0.965	3.442	0.965	4.051
		g-g-g+	9.386	0.969	2.198	4.636	4.366	4.163	0.965	3.156	0.968	3.940
	ag-	g- a a	8.909	0.968	2.193	4.210	5.060	3.790	0.965	3.540	0.965	3.308
	g- a	g+g+g+	9.386	0.965	4.163	4.366	4.635	2.198	0.969	3.940	0.968	3.156
		a g+g+	7.711	0.965	4.412	5.086	4.535	2.228	0.969	3.908	0.968	3.127
		a g+g-	6.116	0.965	4.392	5.071	4.590	2.210	0.968	4.051	0.965	3.442
		a a a	4.589	0.965	4.337	5.073	4.753	3.538	0.965	4.275	0.968	2.121
		a g- a	4.963	0.965	4.343	5.104	4.441	3.259	0.966	4.262	0.969	2.147
		g-g+g+	7.710	0.966	4.058	4.537	4.633	2.267	0.969	3.932	0.968	3.179
		g-g+g-	6.717	0.966	4.062	4.540	4.678	2.248	0.968	4.087	0.965	3.493
		g- a a	4.979	0.966	4.037	4.594	4.848	3.540	0.965	4.341	0.969	2.152
		g-g-a	5.858	0.966	4.049	4.717	4.542	3.271	0.966	4.326	0.969	2.161
	g-g-	ag+g+	3.802	0.965	4.385	4.187	4.190	3.533	0.964	3.980	0.969	2.064
		a g- a	4.973	0.965	4.326	4.024	3.975	2.172	0.969	4.308	0.966	3.285
		ag-g-	4.649	0.965	4.377	4.013	4.088	2.176	0.968	3.969	0.965	3.584
		g-ag+	4.171	0.966	4.033	4.344	4.184	3.543	0.964	4.014	0.969	2.050
		g-g-a	6.523	0.966	4.013	4.380	4.004	2.155	0.969	4.380	0.966	3.229
		g-g-g-	6.166	0.966	4.033	4.364	4.115	2.152	0.968	3.993	0.965	3.549
		a g+ a	7.529	0.965	4.310	3.522	2.094	3.626	0.968	4.335	0.965	3.515
		+aa	7.985	0.968	3.830	2.074	3.578	3.786	0.965	4.398	0.966	3.651

Table S2-4 Continued

Type 5 **Six-member ring**		a g-g-	7.985	0.965	3.789	3.575	2.074	3.829	0.968	3.649	0.966	4.399
		g-g+a	8.663	0.969	3.680	2.044	3.472	4.103	0.966	4.054	0.967	4.048
		g-g+g-	7.707	0.969	3.615	2.065	3.507	4.090	0.965	3.488	0.966	4.375
		g- a a	8.470	0.968	3.722	2.050	3.445	4.391	0.965	4.121	0.966	4.032
	g-g+	g+g+g+	5.391	0.970	3.920	1.910	3.121	4.081	0.966	3.949	0.968	4.021
		g+g+ a	5.388	0.969	3.890	1.942	3.080	4.090	0.967	4.383	0.965	4.104
		g+g+g-	4.253	0.970	3.902	1.921	3.135	4.059	0.966	3.987	0.966	4.412
		g+a g+	5.344	0.970	3.909	1.859	3.539	4.398	0.964	3.947	0.968	3.985
		g+ag-	3.691	0.970	3.898	1.877	3.531	4.320	0.964	3.974	0.966	4.353
		a g-g+	5.344	0.964	4.398	3.539	1.859	3.910	0.970	3.986	0.968	3.946
		a g- a	3.692	0.964	4.320	3.530	1.877	3.899	0.970	4.354	0.966	3.974
		g-g-g+	5.391	0.966	4.081	3.122	1.911	3.920	0.970	4.021	0.968	3.949
		g-g-a	4.253	0.966	4.060	3.137	1.921	3.901	0.970	4.412	0.966	3.988
		g-g-g-	5.388	0.967	4.091	3.082	1.942	3.890	0.969	4.104	0.965	4.383
	g-g-	a g+g-	8.470	0.965	4.392	3.445	2.049	3.721	0.968	4.029	0.966	4.118
		g-g+a	7.710	0.965	4.090	3.506	2.064	3.614	0.969	4.376	0.966	3.488
		g-g+g-	8.663	0.966	4.104	3.469	2.041	3.677	0.969	4.048	0.967	4.053
Type 6 No Hydrogen Bonds	g+g+	a g+ a	12.050	0.965	3.733	3.891	4.113	4.030	0.966	3.688	0.966	3.963
	g+ a	a g-g-	15.756	0.965	3.793	5.059	4.638	3.295	0.966	3.370	0.966	3.742
	a g-	g+ a a	15.756	0.966	3.294	4.639	5.061	3.791	0.965	3.742	0.966	3.368
	g-g-	g- a g-	12.050	0.966	4.030	4.112	3.889	3.734	0.965	3.964	0.966	3.688

3. PUFA Model (Model 0) Values

Table S3-1 Relative Energies (in kcal mol^{-1})* and dihedral values of 2U for all possible *trans* isomers obtained at RHF/3-21G level of theory

Conformations	ϕ_{t1}	ϕ_1	ψ_1	ϕ_2	ψ_2	ϕ_{t2}	ΔE
+(++--)+	**120.599**	**117.031**	**116.916**	**-117.030**	**-116.969**	**120.301**	**0.0**[a]
+ (--++)+	120.270	-117.028	-116.940	116.988	117.026	120.612	0.0
-(++++)+	**-120.380**	**117.062**	**116.735**	**116.772**	**116.705**	**120.472**	**0.0**[a]
+(----)-	120.413	-116.869	-116.960	-116.982	-116.832	120.287	0.0
+(--+s$^-$)+	120.479	-116.896	-116.646	115.743	-16.939	120.444	0.8
+(++-s$^+$)+	120.694	116.982	116.673	-115.857	16.873	120.568	0.8
-(s$^+$-++)+	-120.447	16.947	-115.901	116.585	116.847	120.611	0.8
+(s$^-$+--)+	120.497	-16.803	115.890	-116.624	-116.880	120.274	0.8
+(--s$^-$+)+	120.466	-116.944	-116.776	-16.147	116.013	120.877	0.8
+(++s$^+$-)+	120.690	117.021	116.779	16.264	-116.050	120.028	0.8
+(-s$^+$++)	120.146	-116.011	16.162	116.609	116.880	120.576	0.8
+(-+++)+	120.449	-118.392	119.556	117.089	117.327	120.656	0.8
+(+++-)+	120.661	117.615	117.132	119.486	-118.296	120.342	0.8
-(+---)+	-120.416	118.411	-119.453	-117.157	-117.396	120.173	0.8
+(---+)+	120.297	-117.357	-117.134	-119.416	118.508	120.541	0.8
-(+-++)+	-120.440	118.761	-119.102	117.015	117.054	120.585	0.8
+(-+--)+	120.490	-118.771	119.164	-116.993	-117.092	120.105	0.8
+(--+-)+	120.407	-117.141	-117.081	119.079	-118.749	120.393	0.8
+(+s$^-$--)+	-120.107	116.042	-16.184	-116.738	-116.894	120.287	0.8
+(++-+)+	120.619	117.062	117.050	-119.139	118.744	120.457	0.9
+(--s$^+$-)+	120.460	-117.255	-116.985	16.319	-115.782	120.132	0.9
-(s$^+$---)+	-120.412	17.086	-116.043	-117.400	-117.085	120.327	0.9
+(+s$^-$++)+	120.835	115.801	-16.329	116.724	117.151	120.539	0.9
+(-s$^+$--)+	120.235	-115.734	16.312	-116.947	-117.151	120.307	0.9
-(+++s$^-$)+	-120.329	116.994	117.411	116.007	-17.169	120.436	0.9
+(---s$^+$)+	120.330	-116.991	-117.420	-116.006	17.169	120.557	0.9
+(s$^-$+++)+	120.502	-17.053	115.980	117.377	117.008	120.580	0.9
+(++s$^-$+)+	120.624	120.644	117.133	116.926	-16.277	115.852	0.9
-(s$^+$--s$^+$)+	-120.486	15.320	-115.980	-115.906	15.254	120.512	1.5
+(s$^-$++s$^-$)+	120.091	-15.206	115.929	115.869	-15.262	120.508	1.5
+(-++s$^-$)+	120.233	-118.488	116.297	113.709	-17.857	120.497	1.6
+(s$^-$++-)+	120.515	-17.827	113.578	116.258	-118.499	120.238	1.6
-(s$^+$--+)+	-120.464	17.763	-113.636	-116.439	118.486	120.619	1.6
+(+--s$^+$)+	-120.262	118.516	-116.433	-113.549	17.845	120.586	1.6
+(-s$^+$s$^+$-)+	120.091	-115.929	16.729	16.783	-115.896	119.911	1.6
-(+s$^-$s$^-$+)+	-120.054	115.947	-16.771	-16.623	115.868	120.870	1.6
+(+s$^-$s$^+$-)+	-120.262	116.039	-16.794	16.724	-115.928	120.071	1.6
+(-s$^+$s$^-$+)+	120.246	-115.892	16.753	-16.678	115.954	120.866	1.6
+(-s$^+$+-)+	120.126	-115.815	16.860	119.215	-118.991	120.384	1.6
+(+-s$^-$+)+	-120.332	119.038	-119.278	-16.940	115.911	120.924	1.6
+(-+s$^+$-)+	120.467	-118.907	119.285	16.861	-115.905	119.995	1.6
+(+s$^-$-+)+	-120.025	115.932	-16.936	-119.368	119.045	120.472	1.6
+(s$^+$-s$^-$+)+	120.455	16.374	-115.644	-16.893	115.610	120.870	1.6
+(-s$^+$-s$^+$)+	**120.147**	**-115.614**	**15.305**	**-115.885**	**15.930**	**120.467**	**1.6**[a]
+(s$^+$-s$^+$-)+	-120.490	15.886	-115.958	15.300	-115.741	120.137	1.6
+(s$^-$+s$^+$-)+	120.556	-16.361	115.727	16.823	-115.656	120.123	1.6
+(s$^+$-s$^-$+)+	-120.494	16.391	-115.736	-16.791	115.665	120.805	1.6
+(-s$^+$+s$^-$)+	120.165	-115.662	16.827	115.645	-16.418	120.531	1.6
+(s$^-$+s$^-$+)+	120.561	-15.878	115.962	-15.269	115.670	120.818	1.6
+(+s$^-$+s$^-$)+	-120.112	115.632	-15.282	115.832	-15.933	120.527	1.6
+(+s$^-$-s$^+$)	-120.119	115.693	-16.912	-115.686	16.391	120.456	1.6
+(-s$^+$-+)+	120.117	-115.457	16.860	-118.947	119.339	120.471	1.7
+(+-s$^+$-)+	-120.382	119.346	-118.979	16.778	-115.526	120.036	1.7
+(+s$^-$+-)+	120.973	115.541	-16.773	118.902	-119.192	120.402	1.7
-(s$^+$-+-)+	-120.482	16.761	-115.692	118.730	-118.712	120.384	1.7
+(-+s$^-$+)+	120.453	-119.247	118.997	-16.683	115.517	120.902	1.7
+(s$^-$+-+)+	120.558	-16.651	115.727	-118.676	118.665	120.468	1.7
-(s$^+$-+s$^-$)+	-120.443	16.805	-115.548	115.456	-16.872	120.476	1.7
-(+-+s$^-$)+	-120.426	118.730	-118.766	115.749	-16.746	120.459	1.7
+(-+-s$^+$)+	120.484	-118.630	118.816	-115.702	16.706	120.535	1.7
+(s$^-$+-s$^+$)+	120.493	-16.741	115.544	-115.563	16.814	16.814	1.7
+(-+-+)+	120.506	-119.008	119.161	-119.034	119.184	120.553	1.7
+(+-+-)+	120.461	118.968	-119.016	119.058	-118.923	120.338	1.7
+(+--+)+	-120.516	118.962	-119.412	-119.320	119.059	120.412	1.8
+(-++-)+	120.567	-118.950	119.433	119.315	-119.013	120.437	1.8

*Relative to trans (++++) conformation

Table S3-2 Dihedral values and relative energies kcal mol^{-1} of the *cis* isomers of 2U obtained at RHF/3-21G level of theory

Conformations	ϕ_{t1}	ϕ_1	ψ_1	ϕ_2	ψ_2	ϕ_{t2}	ΔE
+(----)+	121.185	-114.858	-114.891	-114.821	-114.872	121.126	5.5
+(++++)+	**120.625**	**114.776**	**114.873**	**114.892**	**114.825**	**120.636**	**5.5**[a]
+(++--)+	**-121.246**	**114.968**	**115.189**	**-115.154**	**-114.978**	**121.275**	**5.6**
+(--++)+	121.425	-114.996	-115.192	115.237	114.825	120.333	5.6
+(a^+-++)+	120.783	129.185	-89.532	105.818	114.278	120.723	6.2
+(--+a^-) +	120.984	-114.274	-105.894	89.469	-129.209	120.916	6.2
+(++-a^+)+	120.733	114.318	105.799	-89.572	129.165	120.728	6.2
+(a^-+--)+	121.002	-129.204	89.461	-105.842	-114.247	120.953	6.2
+(-+++)+	122.065	-119.824	117.625	113.935	115.058	120.414	6.2
+(---+)+	121.162	-115.189	-113.788	-117.512	119.989	119.522	6.2
+(-++-)+	122.292	-119.900	117.473	113.890	-119.413	120.489	6.2
+(+++-)+	120.569	115.040	113.700	117.383	-120.088	122.315	6.2
+(+---)+	119.610	120.122	-117.381	-113.749	-115.177	121.190	6.2
+(+a^-+a^-)+	113.724	90.144	-145.767	93.149	-133.742	123.919	6.7
+(a^-+a^++)+	**123.840**	**-133.642**	**93.249**	**-145.747**	**90.118**	**113.610**	**6.7**
+(a^+-a^+-)+	117.731	133.664	-93.042	145.839	-90.155	128.011	6.7
+(-a^+-a^+)+	128.138	-90.261	145.891	-92.883	133.716	117.765	6.7
+(a^-++a^-)	122.599	-134.339	97.934	97.881	-134.365	122.607	6.8
+(a^+--a^+)+	119.133	134.428	-97.766	-97.931	134.421	119.053	6.8
+(-$a^+$$a^-$+)	121.412	-122.702	128.528	-128.096	122.871	120.693	7.1
+(+$a^-$$a^+$-)+	120.306	123.136	-128.008	128.569	-122.468	121.351	7.1

a Conformers were selected to construct longer chains

Table S3-3 Dihedral Values for PUFA

Fragment Name		Conformation[a]	ϕ_{t1}	ϕ_1	ψ_1	ϕ_2	ψ_2	ϕ_3	ψ_3	ϕ_4	ψ_4	ϕ_5	ψ_5	ϕ_5	ψ_5	ϕ_{t2}
0U	*Cis*	++	-120.993													120.978
	Trans	–+	120.645													120.978
1U	*Cis*	–(–+)+	122.306	-124.331	123.701											119.509
		–(++)+	121.415	115.320	116.706											119.789
		–(—)–	120.701	-115.597	-116.829											122.314
	Trans	–(–s^+)+	-121.017	-119.037	13.117											120.704
		–(--)+	121.033	-116.948	-118.243											120.834
		–(++) –	-121.379	116.975	118.098											120.874
2U	*Cis* helix	–(a^-+ a^-+)–	-119.809	-125.336	127.812	-128.155	125.157									-121.987
	Cis extended	+(++++)+	-121.979	117.577	116.878	116.033	117.681									120.347
	Cis beta	–(++—)+	-121.779	116.886	118.557	-118.930	-117.097									121.749
	Trans helix	–(–s^+–s^+)–	120.386	-119.184	11.989	-118.876	12.750									-120.813
	Trans extended	+(++++)+	-120.028	118.429	118.740	118.717	117.599									120.799
	Trans beta	–(++—)+	121.030	118.432	118.376	-118.388	-118.433									120.297
3U	*Cis* helix	–(a^-+ a^-+ a^-+)–	123.503	-133.934	123.308	-144.282	109.899	-137.927	112.441							-125.060
	Cis extended	–(++++++)+	-121.390	116.248	115.489	116.152	116.199	115.938	116.848							120.556
	Cis beta	–(++—++)–	119.857	119.909	119.162	-119.679	-119.680	119.921	117.849							119.828
	Trans helix	–(–s^+–s^+–s^+)–	-121.641	-119.507	12.747	-118.963	11.845	-119.157	12.293							-120.925
	Trans extended	–(++++++)+	120.559	117.688	118.596	118.318	118.541	118.827	117.988							120.727
	Trans beta	–(++—++)+	120.889	117.811	117.543	-118.058	-118.050	117.552	117.827							120.888
4U	*Cis* helix	+(a^-+ a^-+ a^-+ a^-+)–	123.368	-132.165	121.353	-139.198	104.697	-153.065	116.041	-132.725	115.980					-122.636
	Cis extended	+(++++++++)–	120.333	116.052	117.385	114.948	115.881	115.851	114.953	117.431	116.607					120.364
	Cis beta	+(++—++—)+	120.319	117.448	119.192	-119.031	-118.141	118.141	119.032	-119.193	-117.448					121.772
	Trans helix	+(-s^+–s^+–s^+–s^+)+	120.287	-118.880	12.301	-118.810	11.195	-119.423	11.272	-119.745	12.715					120.594
	Trans extended	+(+++++++++)+	-120.470	117.912	118.290	117.715	117.477	117.454	117.710	118.283	117.894					120.875
	Trans beta	+(++—++—)–	121.065	118.585	119.996	-116.177	-117.810	118.108	118.687	-117.214	-118.275					120.334
5U	*Cis* helix	–(a^-+ a^-+ a^-+ a^-+ a^-+)–	123.800	-132.649	125.190	-143.564	114.373	-142.071	113.171	-147.114	111.176	-138.237	115.557			119.709
	Cis extended	+(++++++++++)+	120.488	116.967	116.490	118.531	116.360	117.203	117.783	116.543	117.337	117.127	120.447			120.447
	Cis beta	+(++—++—++)–	120.406	117.620	119.104	-117.938	-117.438	117.753	118.483	-117.943	-116.972	117.832	117.455			119.906
	Trans helix	–(–s^+–s^+–s^+–s^+–s^+)–	120.146	-119.273	12.013	-119.476	11.319	-119.487	11.570	-119.420	11.288	-119.351	12.440			120.659
	Trans extended	–(++++++++++)+	121.010	118.221	116.920	116.587	117.345	117.324	117.353	117.508	117.218	117.387	117.991			120.731
	Trans beta	–(++—++—++) –	122.335	119.386	114.094	-122.002	-115.822	120.098	116.480	-119.305	-117.192	119.162	118.007			120.871
6U	*Cis* helix	–(a^-+ a^-+ a^-+ a^-+ a^-+ a^- +)–	122.941	-131.521	129.033	-146.638	120.916	-142.194	114.654	-139.334	106.473	-157.289	116.938	-129.645	116.696	119.677
	Cis extended	+(++++++++++)+	120.290	116.902	117.339	116.057	116.745	115.890	116.120	116.138	115.888	116.755	116.078	117.344	116.906	120.304
	Cis beta	+(++—++—++)–	120.026	117.276	117.339	-118.127	-117.996	117.398	117.450	-117.451	-117.408	118.021	118.154	-118.105	-117.286	122.098
	Trans helix	–(–s^+–s^+–s^+–s^+–s^+)–	120.468	-118.650	11.249	-119.591	9.756	-120.428	10.642	-120.177	11.439	-119.774	11.460	-119.711	12.680	120.720
	Trans extended	–(++++++++++)+	120.854	117.797	118.150	117.876	118.302	118.219	118.085	117.983	118.080	118.013	118.055	118.106	117.816	120.865
	Trans beta	–(++—++—++)–	121.078	118.665	119.012	-117.084	-117.811	118.595	121.381	-114.909	-117.738	118.188	118.966	-117.151	-118.213	-121.008

[a] unit conformation are separated from terminal group by bracket

Table S3-4 Relative energy, enthalpy, free energy as well as the entropy of models 0U – 6U and DHA in kcal mol^{-1}

Fragments Name		ΔE^0 RHF/ 3-21G	ΔE^0 B3LYP/ 6-31G(d)	ΔE^0 [a] B3LYP/ 6-311 +G(2d,p)	ΔH^0 [a] B3LYP/ 6-311 +G(2d,p)	ΔG^0 [a] B3LYP/ 6-311 +G(2d,p)	S [b] B3LYP/ 6-31G(d)	ΔS_{ref}[b] B3LYP/ 6-31G(d)
0U	*Cis*	1.7	1.2	1.3	1.3	1.5	71.910	0.86
	Trans	0.0	0.0	0.0	0.0	0.0	71.054	0.00
1U	*Cis*	4.3	3.8	3.6	3.6	3.1	93.738	1.60
		3.6	3.3	3.2	3.2	2.8	93.325	1.18
		3.6	3.3	3.2	3.2	2.8	93.380	1.24
	Trans	0.8	0.6	0.7	0.7	0.8	91.582	-0.56
		0.0	0.0	0.0	0.0	0.0	92.038	-0.11
		0.0	0.0	0.0	0.0	0.0	92.143	0.00
2U	*Cis* helix	6.7	6.3	6.0	5.9	5.7	114.449	0.59
	Cis extended	5.5	5.1	5.1	5.0	4.5	115.314	1.46
	Cis beta	5.6	5.2	5.2	5.0	4.9	114.057	0.20
	Trans helix	1.6	1.3	1.6	1.5	2.0	111.912	-1.94
	Trans extended	0.0	0.1	0.0	0.0	0.1	113.727	-0.13
	Trans beta	0.0	0.0	0.0	0.0	0.0	113.855	0.00
3U	*Cis* helix	9.0	8.8	8.8	8.6	8.4	133.971	0.63
	Cis extended	7.5	6.9	6.9	6.7	6.5	134.149	0.81
	Cis beta	7.6	6.9	6.9	6.7	6.3	134.870	1.53
	Trans helix	2.4	1.8	2.2	2.1	2.3	132.742	-0.60
	Trans extended	0.0	0.1	0.1	0.0	0.4	131.948	-1.39
	Trans beta	0.0	0.0	0.0	0.0	0.0	133.343	0.00
4U	*Cis* helix	11.2	11.0	11.4	11.1	11.6	153.474	-1.61
	Cis extended	9.5	8.7	8.7	8.5	8.0	156.613	1.53
	Cis beta	9.6	8.7	8.8	8.5	8.0	156.795	1.71
	Trans helix	3.2	2.4	2.9	2.8	3.1	153.895	-1.19
	Trans extended	0.0	0.0	0.0	0.0	0.0	154.95	-0.14
	Trans beta	0.0	0.0	0.0	0.0	0.0	155.088	0.00
5U	*Cis* helix	13.5	13.3	13.9	13.5	14.7	172.561	-3.86
	Cis extended	11.4	10.4	10.5	10.2	9.8	177.909	1.49
	Cis beta	11.6	10.6	10.6	10.3	9.8	178.087	1.67
	Trans helix	4.0	2.9	3.5	3.4	4.2	173.924	-2.50
	Trans extended	0.1	0.0	0.0	-0.1	0.3	175.310	-1.11
	Trans beta	0.0	0.0	0.0	0.0	0.0	176.421	0.00
6U	*Cis* helix	15.9	15.4	16.4	16.0	16.9	191.140	-3.14
	Cis extended	13.5	11.8	12.2	11.9	9.6	199.147	4.86
	Cis beta	13.7	12.3	12.4	12.1	11.0	198.013	3.73
	Trans helix	4.9	3.6	4.3	4.1	4.7	192.309	-1.97
	Trans extended	0.1	0.0	0.0	-0.1	-0.7	196.353	2.07
	Trans beta	0.0	0.0	0.0	0.0	0.0	194.282	0.00

[a] Single point calculation using B3LYP/6-31G(d) geometries
[b] Entropy unit: cal (mol K)$^{-1}$

4. Data for DHA models

4.1 Dihedral Values for DHA Models (Model 1, Model 2 and PUFA)

Table S4-1 Dihedral values of each block of Model 1, 2 , SDA, EPA and DHA

		Dihedrals Indices	ϕ_1	ψ_1	ϕ_2	ψ_2	ϕ_3	ψ_3	ϕ_4	ψ_4	ϕ_5	ψ_5
4U'	Cis helix	+ –+–+–+–+ –	-136.387	124.676	-132.873	87.884	-161.261	116.890	-127.896	118.202		
	Cis extended	+ +++++++++ –	116.111	116.798	116.162	116.351	116.359	116.147	116.798	116.092		
	Cis strand	+ ++—++— +	115.662	118.038	-117.907	-117.733	118.023	117.277	-117.765	-118.325		
	Trans Helix	+ –s^+–s^+–s^+–s^+ +	-118.697	10.600	-119.990	10.836	-120.404	11.467	-112.726	12.658		
	Trans Extended	+ +++++++++ +	118.395	117.578	117.946	117.900	118.172	118.416	118.380	118.275		
	Trans beta	+ ++—++— –	117.822	118.181	-117.515	-117.996	117.868	117.966	-117.701	-117.670		
5U'' = 5U'	Cis helix	– –+–+–+–+–+ –	-134.942	128.274	-132.768	88.002	-148.621	103.855	-148.026	116.918	-135.686	115.078
	Cis extended	+ ++++++++++ +	115.737	114.7246	117.527	117.3891	116.2715	118.1984	116.4692	115.8657	117.896	114.8758
	Cis beta	+ ++—++—++ –	115.366	117.385	-116.985	-117.260	118.080	117.530	-116.730	-117.428	119.147	116.475
	Trans Helix	– –s^+–s^+–s^+–s^+–s^+ –	-119.487	12.168	-119.429	11.271	-119.113	10.798	-119.978	11.210	-119.759	13.412
	Trans Extended	– ++++++++++ +	118.180	117.636	117.472	117.411	117.220	117.228	117.404	117.470	117.633	118.187
	Trans beta	– ++—++—++ –	117.201	118.070	-117.690	-118.136	117.499	117.881	-117.768	-118.015	117.738	118.244
3U'''	Cis helix	+ –+–+–+–+ –	-136.898	123.6803	-138.063	109.9206	-137.337	82.4399				
	Cis extended	+ +++++++++ –	115.7556	116.0587	116.1902	113.1682	118.6378	115.0498				
	Cis strand	+ ++—++— +	115.3904	118.0734	-119.3338	-118.2427	116.3917	116.177				
	Trans Helix	+ –s^+–s^+–s^+–s^+ +	-118.5707	12.9924	-118.2156	11.6517	-119.3458	12.4954				
	Trans Extended	+ +++++++++ +	118.4188	119.6571	119.2665	118.9266	118.6932	117.7809				
	Trans beta	+ ++—++— –	118.2548	117.2192	-118.4963	-118.0668	117.7479	117.547				
4U''	Cis helix	– –+–+–+–+–+ –	-146.8321	119.7814	-124.0229	92.8969	-160.1463	114.2514	-130.5746	119.6628		
	Cis extended	+ ++++++++++ +	117.8569	118.487	114.9193	115.8573	118.1653	115.0057	119.4245	119.9688		
	Cis beta	+ ++—++—++ –	117.8565	116.9629	-117.4956	-118.8902	119.5025	117.2518	-117.2909	-119.1367		
	Trans Helix	– –s^+–s^+–s^+–s^+–s^+ –	-118.9463	11.5154	-119.8209	10.3792	-120.4933	10.8187	-120.5146	11.7671		
	Trans Extended	– ++++++++++ +	118.0341	118.3472	118.206	117.7644	117.5774	117.2615	116.975	117.7789		
	Trans beta	– ++—++—++ –	118.2602	118.1558	-117.7986	-117.9037	118.0243	118.3632	-117.4675	-118.2722		
SDA	Cis helix	+ –+–+–+–+ –	-137.5812	125.4062	-152.762	110.4865	-133.2151	102.4668				
	Cis extended	+ +++++++++ –	116.7561	116.785	117.3185	116.21	116.9482	116.8573				
	Cis strand	+ ++—++— +	115.9604	118.5332	-118.7716	-117.2331	118.1155	119.7026				
	Trans Helix	+ –s^+–s^+–s^+–s^+ +	-117.8155	11.8334	-118.5653	11.1419	-119.4387	12.3401				
	Trans Extended	+ +++++++++ +	117.8762	118.3783	118.4226	118.9011	119.3434	117.5381				
	Trans beta	+ ++—++— –	118.1625	117.5469	-118.2532	-118.6901	117.2759	117.6614				
EPA	Cis helix	– –+–+–+–+–+ –	-149.863	124.189	-143.353	129.416	-151.927	113.747	-138.048	92.375		
	Cis extended	+ ++++++++++ +	115.82479	115.96733	115.9114	115.96687	116.0427	114.51554	117.57561	114.88306		
	Cis beta	+ ++—++—++ –	115.975	116.822	-118.349	-120.682	118.601	118.026	-119.370	-118.648		
	Trans Helix	– –s^+–s^+–s^+–s^+–s^+ –	-119.135	11.372	-119.344	11.	-119.294	10.462	-120.070	11.757		
	Trans Extended	– ++++++++++ +	117.925	118.159	117.830	117.819	117.866	117.159	117.237	117.923		
	Trans beta	– ++—++—++ –	117.8796	118.085	-117.630	-117.796	117.818	118.238	-117.229	-117.836		
DHA	Cis helix	+ –+–+–+–+–+ –	-133.178	129.072	-134.696	84.920	-146.881	110.428	-145.648	99.615	-136.665	107.967
	Cis extended	+ ++++++++++ +	114.910	116.529	114.990	116.620	116.421	115.345	117.139	116.789	114.848	115.748
	Cis beta	+ —++—++—+	116.092	117.601	-117.226	-116.672	117.035	118.610	-117.914	-118.703	118.678	116.407
	Trans Helix	-(-s^+– s^+– s^+– s^+– s^+)–	-118.681	11.673	-119.556	12.147	-118.684	13.057	-118.463	11.758	-118.773	13.329
	Trans Extended	+ (++++++++++) +	118.180	117.883	117.839	118.674	118.526	118.296	118.142	119.223	118.713	118.946
	Trans beta	– ++ —++—++ –	118.413	118.197	-117.531	-118.313	117.169	118.291	-117.453	-118.966	116.725	118.398

Table S4-2 Dihedral values of the terminal group dihedrals

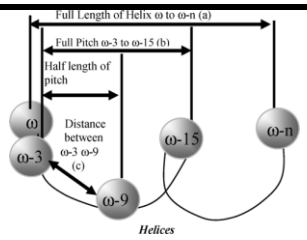
Structure and Model		Dihedral Indices	Terminal Group (Methyl End)		Terminal Group (Carboxyl End)				Carboxyl Group	
			$\phi_{t1'}$	ϕ_{t1}	ϕ_{t2}	$\phi_{t2'}$	$\phi_{t2''}$	$\phi_{t2'''}$	χ_1	χ_2
4U'	Cis helix	+ –+–+–+–+ –	177.285	131.834	116.460	176.901				
	Cis extended	+ +++++++++ –	-178.798	119.647	119.638	177.153				
	Cis strand	+ ++—++— +	-178.823	120.141	121.262	177.399				
	Trans Helix	+ –s^+–s^+–s^+–s^+ +	-179.121	118.676	119.177	178.091				
	Trans Extended	+ +++++++++ +	-179.186	119.269	119.116	176.974				
	Trans beta	+ ++—++— –	-179.222	119.228	119.384	178.023				
5U'	Cis helix	– –+–+–+–+–+ –	-178.133	130.503	117.572	177.076				
	Cis extended	+ ++++++++++ +	-178.809	118.839	118.946	176.973				
	Cis beta	+ ++—++—++ –	-178.849	119.458	119.435	177.046				
	Trans Helix	– –s^+–s^+–s^+–s^+–s^+ –	-179.214	118.319	119.216	178.004				
	Trans Extended	– ++++++++++ +	-179.416	119.312	119.300	177.976				
	Trans beta	– ++—++—++ –	-179.944	118.547	119.676	178.304				
3U'''	Cis helix	+ –+–+–+–+ –	57.199	128.630	-113.738	-176.901	-179.921	179.859		
	Cis extended	+ +++++++++ –	57.315	118.965	118.412	176.713	179.781	179.699		
	Cis strand	+ ++—++— +	57.065	118.325	-118.393	-177.263	-179.826	179.752		
	Trans Helix	+ –s^+–s^+–s^+–s^+ +	58.161	118.858	-118.592	-177.704	-179.934	177.988		
	Trans Extended	+ +++++++++ +	58.172	119.996	118.431	178.595	179.978	177.976		
	Trans beta	+ ++—++— –	58.295	119.388	-118.404	-178.121	179.956	-179.943		
4U''	Cis helix	– –+–+–+–+–+ –	61.9426	131.9116	-125.604	64.9645	58.2126			
	Cis extended	+ ++++++++++ +	62.535	-120.466	-119.514	-177.326	-179.819			
	Cis beta	+ ++—++—++ –	62.486	-120.669	120.023	176.984	-179.743			
	Trans Helix	– –s^+–s^+–s^+–s^+–s^+ –	61.360	-119.664	-119.077	-178.531	179.973			
	Trans Extended	– ++++++++++ +	58.147	119.241	118.484	178.421	179.878			
	Trans beta	– ++—++—++ –	58.205	119.588	-119.083	-177.999	-179.931			
SDA	Cis helix	+ –+–+–+–+ –	57.263	126.787	-106.462	179.816	-177.083	170.313	155.169	177.596
	Cis extended	+ +++++++++ –	57.237	118.275	115.405	176.694	179.464	179.893	179.791	179.977
	Cis strand	+ ++—++— +	57.229	118.766	-119.059	-177.218	-179.887	-179.507	-179.945	-179.626
	Trans Helix	+ –s^+–s^+–s^+–s^+ +	58.091	119.128	-118.436	-177.465	-179.766	-179.729	-179.270	-179.888
	Trans Extended	+ +++++++++ +	58.211	119.080	117.644	177.527	179.524	179.761	179.529	179.924
	Trans beta	+ ++—++— –	58.277	119.491	-118.252	-178.667	179.954	179.657	179.568	179.915
EPA	Cis helix	– –+–+–+–+–+ –	57.321	130.874	111.948	174.542	176.459		176.553	179.574
	Cis extended	+ ++++++++++ +	57.218	118.132	119.197	177.346	-179.010		-177.684	-179.676
	Cis beta	+ ++—++—++ –	57.042	118.774	120.081	177.283	-178.647		-177.180	-179.644
	Trans Helix	– –s^+–s^+–s^+–s^+–s^+ –	58.191	118.727	118.331	178.102	-179.078		-177.603	-179.703
	Trans Extended	– ++++++++++ +	58.282	119.584	119.142	178.076	-178.692		-176.778	-179.588
	Trans beta	– ++—++—++ –	58.246	119.325	119.013	178.593	-178.714		-177.096	-179.625
DHA	Cis helix	+ –+–+–+–+–+ –	-178.278	129.668	114.811	171.468			162.030	178.120
	Cis extended	+ ++++++++++ +	-178.882	119.853	118.189	176.744			179.739	-179.936
	Cis beta	+ —++—++—+	-178.821	120.081	120.006	176.884			179.836	-179.920
	Trans Helix	-(-s^+– s^+– s^+– s^+– s^+)–	-179.240	118.702	119.098	176.985			178.428	179.863
	Trans Extended	+ (++++++++++) +	-179.165	119.254	119.258	176.794			177.317	179.749
	Trans beta	– ++ —++—++ –	-179.216	119.891	118.615	176.887			176.777	179.770

Table S4-3 ZPE Corrected Relative Energy and Enthalpy, Gibbs Free Energy (kcal mol-1), and Entropy (cal (mol K)-1) for ω-3 PUFAs and Their Model Compounds Obtained by B3LYP Density Function Combined with 6-31G(d) (A) and 6-311+G(2d,p) Basis Sets

Model	Structure	ΔE_0 B3LYP/A	ΔE_0 B3LYP/B	ΔH_0 B3LYP/B	ΔG_0 B3LYP/B	S_0 B3LYP/A	ΔS_0 B3LYP/A
Model 1 Fixed Chain Length for Q (Me) with $M = 0$							
cis-**3U**'	helix	9.0	9.6	9.4	9.4	147.2	-3.1
	extended	7.1	7.1	7.0	6.0	150.3	-0.1
	beta	7.1	7.2	7.0	6.1	150.4	0.0
trans-**3U**'	helix	1.7	2.0	2.1	1.6	148.6	1.4
	extended	-0.1	-0.1	-0.1	-0.7	149.1	1.9
-585.983283, -585.631166[a]	beta	0.0	0.0	0.0	0.0	147.2	0.0
cis-4U'	helix	11.3	12.2	11.9	12.7	165.7	-5.8
	extended	8.8	8.9	8.7	7.7	171.4	-0.1
	beta	8.9	9.0	8.8	7.8	171.5	0.0
trans-4U'	helix	2.3	2.8	2.8	2.9	167.9	-0.4
	extended	0.0	-0.1	-0.1	-0.8	170.8	2.5
-702.693033, -702.279039[a]	beta	0.0	0.0	0.0	0.0	168.3	0.0
cis-**5U**' [b]	helix	13.6	15.1	14.7	15.9	184.9	-7.8
	extended	10.7	10.7	10.5	9.1	193.7	0.9
	beta	10.8	10.9	10.6	9.5	192.8	0.0
trans-**5U**' [b]	helix	2.9	3.5	3.4	3.4	189.5	0.3
	extended	0.0	0.0	-0.1	-0.6	191.1	1.8
-819.402809, -818.926900[a]	beta	0.0	0.0	0.0	0.0	189.2	0.0
Model 2 Variable Chain Length for Q with $M = 3$, 2, and 1							
cis-**3U**"'	helix	8.7	9.1	8.9	7.9	155.5	-3.3
	extended	7.1	7.2	6.9	6.3	157.9	-0.9
	beta	7.1	7.1	7.0	5.5	158.8	0.0
trans-**3U**"'	helix	1.8	2.2	2.1	2.6	156.1	1.2
	extended	0.0	0.0	-0.1	-0.4	157.0	2.1
-664.610897, -664.201574[a]	beta	0.0	0.0	0.0	0.0	154.9	0.0
cis-**4U**' '	helix	11.1	12.1	11.8	12.9	174.2	-5.6
	extended	8.9	9.0	8.7	8.6	178.5	-1.3
	beta	9.0	9.1	8.8	8.4	179.8	0.0
trans-**4U**' '	helix	2.4	2.9	2.8	3.1	177.3	-0.8
	extended	0.0	0.0	0.0	-0.2	178.6	0.5
-742.006937, -741.564445[a]	beta	0.0	0.0	0.0	0.0	178.1	0.0
cis-**5U**' ' [b]	helix	13.6	15.1	14.7	15.9	184.9	-7.8
	extended	10.7	10.7	10.5	9.1	193.7	0.9
	beta	10.8	10.9	10.6	9.5	192.8	0.0
trans-**5U**' ' [b]	helix	2.9	3.5	3.4	3.4	189.5	0.3
	extended	0.0	0.0	-0.1	-0.6	191.1	1.8
-819.402809, -818.926900[a]	beta	0.0	0.0	0.0	0.0	189.2	0.0
ω-3 Polyunsaturated Fatty Acids (PUFAs)							
cis-SDA	helix	8.2	9.8	9.4	11.5	175.5	-5.8
	extended	7.1	7.2	6.9	6.6	183.3	2.0
	beta	7.3	7.3	7.0	7.3	181.3	0.0
trans-SDA	helix	1.7	2.1	2.0	2.6	180.5	-1.8
	extended	0.1	0.1	0.0	0.2	181.4	-0.8
-853.176842, -852.752487[a]	beta	0.0	0.0	0.0	0.0	182.3	0.0
cis-EPA	helix	10.2	12.1	11.7	13.9	186.3	-10.5
	extended	9.0	9.1	8.8	8.3	195.3	-1.5
	beta	9.0	9.1	8.8	7.9	196.8	0.0
trans-EPA	helix	2.2	2.7	2.6	2.7	193.4	-0.3
	extended	-0.1	0.1	-0.1	-0.4	194.8	1.2
[a]-930.572706, -930.114895[a]	beta	0.0	0.0	0.0	0.0	193.7	0.0
cis-DHA	helix	12.9	15.5	14.9	17.2	198.0	-11.8
	extended	10.6	10.7	10.5	8.4	212.7	2.9
	beta	10.7	10.9	10.6	9.3	209.8	0.0
trans-DHA	helix	2.8	3.4	3.3	3.0	206.9	1.2
	extended	0.0	-0.1	-0.1	-1.3	209.7	4.0
-1007.964077, -1007.47330[a]	beta	0.0	0.0	0.0	0.0	205.7	0.0

[a] Energy (in hartree) of the *trans* beta conformation in all structures. Left: energy. Right: energy with zero point correction.[b] **5U**' and **5U**' ' models are identical

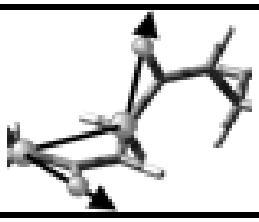
Table S4-4 Nanostructural Parameters (Length, Pitch, and Diameter in Å) for ω-3 PUFAs and Their Model Compounds



Model	Structure	Length of chain (*a*)	Pitch (*b*)	Distance between CΩ$_3$ and CΩ$_9$ (*c*)	Diameter (*d*)
Model 1 Fixed Chain Length for Q (Me) with *M* = 0					
cis-**3U**'	helix	5.9	5.3	5.9	5.3
	extended	14.9	-	-	-
	beta	14.7	-	-	-
trans-**3U**'	helix	11.4	9.2	6.4	4.4
	extended	14.3			
	beta	16.0			
cis-**4U**'	helix	7.3	5.3	5.8	5.2
	extended	18.1	-	-	-
	beta	17.9	-	-	-
trans-**4U**'	helix	12.9	10.2	6.8	4.5
	extended	14.4			
	beta	19.5			
cis-**5U**'	helix	9.5	6.0	5.9	5.1
	extended	21.3	-	-	-
	beta	21.3	-	-	-
trans-**5U**'	helix	15.6	9.2	6.3	4.3
	extended	20.3			
	beta	22.2			
Model 2 Variable Chain Length for Q with *M* = 3, 2, and 1					
cis-**3U**' '	helix	7.8	5.3	5.9	5.3
	extended	17.1	-	-	-
	beta	16.7	-	-	-
trans-**3U**' '	helix	13.6	9.3	6.3	4.3
	extended	16.4			
	beta	18.5			
cis-**4U**' '	helix	8.0	5.6	5.7	5.0
	extended	19.1	-	-	-
	beta	18.7	-	-	-
trans-**4U**' '	helix	14.1	9.0	6.3	4.4
	extended	18.4	-	-	-
	beta	20.4	-	-	-
CΩ-3 Polyunsaturated Fatty Acids (PUFAs)					
cis-SDA	helix	7.3	5.1	6.1	5.5
	extended	18.2	-	-	-
	beta	17.9	-	-	-
trans-SDA	helix	14.5	9.1	6.3	4.4
	extended	17.5	-	-	-
	beta	19.6	-	-	-
cis-EPA	helix	9.3	5.5	6.1	5.4
	extended	20.2	-	-	-
	beta	20.1	-	-	-
trans-EPA	helix	14.4	9.0	6.4	4.5
	extended	19.4	-	-	-
	beta	22.0	-	-	-
cis-DHA	helix	9.2	5.2	5.9	5.3
	extended	22.2	-	-	-
	beta	22.4	-	-	-
trans-DHA	helix	17.0	9.2	6.4	4.4
	extended	21.5	-	-	-
	beta	23.5	-	-	-

[a] **5U**' and **5U**' ' models are identical

Table S4-5 Average Plane Rotation Values and Standard Deviation (deg)



model	structure	av angle of plane rotation (deg)	std dev
Model 1 Fixed Chain Length for Q (Me) with *M* = 0			
cis-**3U**'	helix	34.5	8.2
	extended	-93.0	0.1
	beta	92.9	0.5
trans-**3U**'	helix	-105.5	0.6
	extended	93.4	0.2
	beta	93.2	0.2
cis-**4U**'	helix	35.6	16.4
	extended	-93.5	0.2
	beta	92.7	0.4
trans-**4U**'	helix	-105.4	0.9
	extended	93.2	0.2
	beta	93.1	0.1
cis-**5U**'	helix	29.5	16.4
	extended	-93.2	0.7
	beta	93.0	0.8
trans-**5U**'	helix	-105.5	1.2
	extended	92.5	0.5
	beta	93.0	0.2
Model 2 Variable Chain Length for Q with *M* = 3, 2, and 1			
cis-**3U**' '	helix	28.6	18.8
	extended	-94.3	0.5
	beta	93.1	1.6
trans-**3U**' '	helix	-105.4	1.3
	extended	94.1	0.3
	beta	93.0	0.5
cis-**4U**' '	helix	42.2	19.8
	extended	-93.0	1.1
	beta	92.4	0.5
trans-**4U**' '	helix	-105.3	0.7
	extended	92.6	0.2
	beta	92.7	1.3
ω-3 Polyunsaturated Fatty Acids (PUFAs)			
cis-SDA	helix	25.2	20.5
	extended	-93.1	0.1
	beta	92.3	0.8
trans-SDA	helix	-104.9	1.0
	extended	93.4	0.3
	beta	93.2	0.5
cis-EPA	helix	15.5	10.2
	extended	-94.2	0.3
	beta	92.1	1.3
trans-EPA	helix	-104.7	0.8
	extended	92.5	0.6
	beta	93.0	0.4
cis-DHA	helix	35.2	16.9
	extended	-94.1	0.4
	beta	92.8	0.5
trans-DHA	helix	-105.3	0.6
	extended	93.4	0.3
	beta	34.5	8.2

Table S4-6 Energy of *Trans* →*Cis* Isomerization and Energy of Folding for Model 1, Model 2, and PUFA

		trans →*cis* isomerization			folding beta →helix	
compound	structure	helix	extended	beta	*cis*	*trans*
	3U'	7.3	7.1	7.0	2.4	2.1
model 1	**4U**'	9.2	8.7	8.8	3.2	2.8
	5U'	11.2	10.5	10.6	4.1	3.4
	3U' '	6.8	7.0	7.0	1.9	2.1
model 2	**4U**' '	8.9	8.7	8.8	2.9	2.8
	5U' '	11.2	10.5	10.6	4.1	3.4
	SDA	7.4	7.0	7.0	2.4	2.0
PUFA	EPA	9.1	8.8	8.8	2.9	2.6
	DHA	11.6	10.5	10.6	4.4	3.3

Table S4-7 Linear Trends for All Helices' Trans-Cis Isomerization and Cis Folding of All Models[a]

thermodynamic function	model	*m*	*b*	R^2
Trans →*Cis* Isomerization for Helices				
ΔH	0[b]	1.8	1.4	1.00
	1	1.8	1.4	1.00
	2	1.8	1.4	1.00
	PUFA	1.8	1.4	1.00
ΔG	0[b]	1.7	1.1	0.99
	1	5.2	3.6	0.98
	2	2.4	0.5	0.99
	PUFA	2.7	0.7	0.99
ΔS	0[b]	-1.9	4.4	0.99
	1	-1.6	3.6	0.95
	2	-1.6	3.6	0.95
	PUFA	-2.0	0.8	1.00
Cis[c] Folding				
ΔH	0[b]	0.7	-0.1	0.98
	1	0.9	0.2	1.00
	2	1.1	-1.4	0.99
	PUFA	1.0	-0.8	0.92
ΔG	0[b]	0.8	-0.2	0.94
	1	1.5	1.1	1.00
	2	2.0	-3.5	0.99
	PUFA	1.9	-1.4	1.00
ΔS	0	-1.9	4.4	0.99
	1	-2.3	3.8	0.99
	2	-2.3	3.8	0.99
	PUFA	-3.0	2.7	0.91

[a] The linear fit equation is as follows: $y = mx + b$.[b] Helix, extended, and beta isomers follow the same trend
[c] *Cis* and *trans* isomers follow the same trend.

Table S4-8 The Relative Energy, Enthalpy, Gibbs Free Energy (kcal mol^{-1}), and Entropy (cal (mol K)$^{-1}$) for the Proton Transfer and Esterification Reactions of *cis*-DHA[a]

model	structure	ΔE_0 B3LYP/B	ΔH_0 B3LYP/B	ΔG_0 B3LYP/B	ΔS_0 B3LYP/A
R-COOH + $^{(-)}$OMe →R-COO$^{(-)}$ + HOMe					
cis-DHA-COO$^-$ + HOMe	helix	-43.5	-43.5	-43.1	-1.3
	extended	-38.7	-38.7	-38.4	-2.2
	beta	-38.6	-38.7	-38.3	1.7
R-COOH + $^{(-)}$OMe →R-COOMe + $^{(-)}$OH					
cis-DHA-COOCH$_3$ + $^-$OH	helix	6.4	7.1	8.5	-4.7
	extended	7.0	7.0	8.4	-6.2
	beta	7.0	7.0	8.4	-3.2

[a] Values for ΔS_0 were obtained by B3LYP density functional theory combined with the 6-31G(d) [A] basis set, and values for ΔE_0, ΔH_0, and ΔG_0 were calculated using the 6-311+G(2d,p) [B] basis set

5. Z-matrices for PUFA Models (Model 0)

5.1 Z-matrix for 1U PUFA structures

Table S5-1 Bond distances of 1U PUFA (Model 0)

Input Z-matrix 1U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Distances							
0 1	R2	1.09853744	1.0989132	1.09865963	1.09864636	1.0986	1.09842243
H	R3	1.50229597	1.50225803	1.50226413	1.50344143	1.5034	1.5033004
C 1 R2	R4	1.76088071	1.7758084	1.77526583	1.76057529	1.7599	1.76015376
C 2 R3 1 A3	R5	1.77492252	1.76174012	1.76129173	1.76994552	1.771	1.77039223
H 1 R4 2 A4 3 D4	R6	1.09218215	1.09218067	1.09206437	1.09090672	1.0909	1.09086006
H 1 R5 2 A5 3 D5	R7	1.33555503	1.33559788	1.33560048	1.33856538	1.3385	1.33782405
H 3 R6 2 A6 1 D6	R8	1.51071347	1.51071861	1.50487851	1.51223443	1.5123	1.51201024
C 3 R7 2 A7 1 D7	R9	1.51078432	1.5106862	1.51433119	1.51226029	1.5123	1.51196788
C 7 R8 3 A8 2 D8	R10	1.09169177	1.09169274	1.09188978	1.09035249	1.0904	1.0911287
C 8 R9 7 A9 3 D9	R11	1.09984017	1.09973511	1.10088364	1.0972949	1.0972	1.09265245
H 7 R10 3 A10 2 D10	R12	1.09973434	1.09982184	1.1024177	1.09724094	1.0973	1.10318155
H 8 R11 7 A11 3 D11	R13	1.09171498	1.09169726	1.09199884	1.09035511	1.0904	1.09112839
H 8 R12 7 A12 3 D12	R14	1.33553927	1.3356092	1.33530118	1.33849669	1.3385	1.33779423
H 9 R13 8 A13 7 D13	R15	1.50226919	1.50216664	1.50228895	1.50335693	1.5034	1.50329174
C 9 R14 8 A14 7 D14	R16	1.09216662	1.09215951	1.0904478	1.09092408	1.0909	1.09086776
C 14 R15 9 A15 8 D15	R17	1.09869701	1.09869683	1.0987688	1.09849968	1.0986	1.0986549
H 14 R16 9 A16 8 D16	R18	1.09533979	1.09864924	1.09872439	1.09861138	1.0985	1.09843173
H 15 R17 14 A17 9 D17	R19	1.09862442	1.09530972	1.09559039	1.09354513	1.0936	1.09345779
H 15 R18 14 A18 9 D18							
H 15 R19 14 A19 9 D19							

Table S5-2 Bond angles of 1U PUFA (Model 0)

Input Z-matrix		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.3209461	111.30183052	111.22559155	110.7475072	110.9241	110.77575265
H	A4	36.73802745	35.90956747	35.92979658	36.74260261	36.7819	36.76528789
C 1 R2	A5	35.93431848	36.71576578	36.71991331	36.05978241	36.0116	36.03245597
C 2 R3 1 A3	A6	116.04212461	116.05118784	116.0210466	114.70550033	114.7067	114.70645178
H 1 R4 2 A4 3 D4	A7	125.32396609	125.32964454	125.31710312	128.12568248	128.1187	128.11855558
H 1 R5 2 A5 3 D5	A8	125.12530496	125.16090189	125.18894787	127.96200099	127.9579	127.99296037
H 3 R6 2 A6 1 D6	A9	112.34667515	112.33757504	115.27609377	111.48174843	111.461	111.7953919
C 3 R7 2 A7 1 D7	A10	119.21697973	119.19426608	118.99381382	117.75010436	117.7541	117.49891165
C 7 R8 3 A8 2 D8	A11	108.91798591	109.91704848	109.65361175	110.34363236	109.1275	111.07004948
C 8 R9 7 A9 3 D9	A12	109.89398098	108.88432531	109.09692632	109.12848131	110.3505	108.26853701
H 7 R10 3 A10 2 D10	A13	115.57841959	115.58487542	115.05337085	114.22758786	114.2216	114.49897413
H 8 R11 7 A11 3 D11	A14	125.21700441	125.22603685	126.20275783	128.03017585	128.029	127.99524451
H 8 R12 7 A12 3 D12	A15	125.24954318	125.27275596	124.90233488	128.18486678	128.1815	128.12173233
H 9 R13 8 A13 7 D13	A16	118.67541686	118.64739914	118.80527332	117.13828326	117.1427	117.1751249
C 9 R14 8 A14 7 D14	A17	111.29623893	111.30832393	111.3629681	110.74668747	110.8259	110.868662
C 14 R15 9 A15 8 D15	A18	111.5083477	111.3456791	111.29332285	110.82908249	110.7469	110.73165165
H 14 R16 9 A16 8 D16	A19	111.33215278	111.51151402	111.59813553	113.0461496	113.0459	113.01402553
H 15 R17 14 A17 9 D17							
H 15 R18 14 A18 9 D18							
H 15 R19 14 A19 9 D19							

Table S5-3 Dihedral angles of 1U PUFA (Model 0)

Input Z-matrix		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	121.47139547	122.76552524	122.74013727	120.60386997	120.4906	120.62995366
H	D5	-122.75935943	-121.4434956	-121.48106873	-124.03751743	-124.2209	-124.08285223
C 1 R2	D6	-58.9391148	58.54041029	59.17048441	-59.34698749	-58.5468	-57.85001553
C 2 R3 1 A3	D7	121.03272554	238.62096716	238.98339643	120.70046099	121.4151	122.30597604
H 1 R4 2 A4 3 D4	D8	179.21723474	180.7501717	180.82930587	-0.6992889	0.7315	-0.21586681
H 1 R5 2 A5 3 D5	D9	-116.94746426	116.97506265	-119.03661215	-115.5964693	115.3201	-124.33128816
H 3 R6 2 A6 1 D6	D10	0.57146346	-0.63557122	0.63380469	180.74383511	179.2224	180.18235484
C 3 R7 2 A7 1 D7	D11	4.96652778	-121.53332958	4.76993112	5.75584093	-122.5062	0.35131653
C 7 R8 3 A8 2 D8	D12	121.58218461	-4.93620858	119.4479092	122.21867186	-6.033	116.51201572
C 8 R9 7 A9 3 D9	D13	60.71669649	-60.72409513	192.59992516	61.93390813	-62.0302	-55.85586454
H 7 R10 3 A10 2 D10	D14	-118.24331523	118.0978781	13.11671904	-116.82942914	116.7061	123.70123017
H 8 R11 7 A11 3 D11	D15	179.46443593	180.54104993	179.61470368	-0.72226423	0.7499	0.20631695
H 8 R12 7 A12 3 D12	D16	-0.57992228	0.74048414	-0.0116817	179.5431764	180.4783	180.04163749
H 9 R13 8 A13 7 D13	D17	239.525987	120.87398767	120.70354443	122.31439239	119.7894	119.50885227

C 9 R14 8 A14 7 D14 C 14 R15 9 A15 8 D15 H 14 R16 9 A16 8 D16 H 15 R17 14 A17 9 D17 H 15 R18 14 A18 9 D18 H 15 R19 14 A19 9 D19	D18 D19	0.15726584 120.83387855	-120.43822889 0.24031992	-120.6566272 0.00796851	-119.75287024 1.31684101	-122.2789 -1.2809	-122.50735549 -1.51433322

5.2 Z-matrix for 2U PUFA structures

Table S5-4 Bond distances for 2U PUFA (Model 0)

Input Z-matrix 2U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Distances							
H	R2	1.09865232	1.0986831	1.09862637	1.09850464	1.09849119	1.09865503
C 1 R2	R3	1.50218188	1.50224828	1.50221849	1.50339377	1.50326243	1.50315927
C 2 R3 1 A3	R4	1.76090449	1.77453037	1.76078686	1.77050531	1.77038065	1.76969942
H 1 R4 2 A4 3 D4	R5	1.77465921	1.761006	1.77453626	1.75994574	1.75968944	1.76069241
H 1 R5 2 A5 3 D5	R6	1.09220247	1.09217374	1.0920356	1.09087954	1.09088515	1.09081651
H 3 R6 2 A6 1 D6	R7	1.33556379	1.33555253	1.33556332	1.33848679	1.33853886	1.33768568
C 3 R7 2 A7 1 D7	R8	1.51069633	1.51072278	1.50486527	1.51217215	1.51222725	1.51170345
C 7 R8 3 A8 2 D8	R9	1.51066129	1.51069892	1.5140595	1.51219581	1.51219392	1.51208915
C 8 R9 7 A9 3 D9	R10	1.09169281	1.09168424	1.09179333	1.09040094	1.09037447	1.09115903
H 7 R10 3 A10 2 D10	R11	1.09963135	1.09977866	1.10076166	1.09726076	1.09731005	1.09280905
H 8 R11 7 A11 3 D11	R12	1.09981451	1.09967423	1.10246787	1.09746849	1.09747156	1.10343633
H 8 R12 7 A12 3 D12	R13	1.09181873	1.09178512	1.09189302	1.09047203	1.09046757	1.0912466
H 9 R13 8 A13 7 D13	R14	1.33566524	1.33561446	1.33536498	1.33867426	1.33867806	1.33727854
C 9 R14 8 A14 7 D14	R15	1.51066122	1.51069421	1.50514862	1.51217335	1.51214644	1.5121086
C 14 R15 9 A15 8 D15	R16	1.51069501	1.51077745	1.51427188	1.51210704	1.51222779	1.51167566
C 15 R16 14 A16 9 D16	R17	1.09181891	1.09176268	1.09017973	1.09055596	1.09054749	1.09124588
H 14 R17 9 A17 8 D17	R18	1.09963144	1.09974567	1.10096399	1.09740865	1.09726662	1.09280621
H 15 R18 14 A18 9 D18	R19	1.09981571	1.09960923	1.10250344	1.0973414	1.09745474	1.10345729
H 15 R19 14 A19 9 D19	R20	1.09169286	1.09169091	1.09202881	1.09039183	1.09036157	1.09116587
H 16 R20 15 A20 14 D20	R21	1.33556382	1.33554386	1.3353185	1.33849374	1.33849568	1.3376725
C 16 R21 15 A21 14 D21	R22	1.50218151	1.50223217	1.50246768	1.50339189	1.50330936	1.50315913
C 21 R22 16 A22 15 D22	R23	1.09864226	1.09867107	1.09873402	1.09851641	1.09854754	1.09838197
H 22 R23 21 A23 16 D23	R24	1.09220262	1.0921873	1.09036577	1.0908786	1.09090183	1.09082218
H 21 R24 16 A24 15 D24	R25	1.09865219	1.0986355	1.09563011	1.09856112	1.09852112	1.09350159
H 22 R25 21 A25 16 D25	R26	1.0953687	1.09531483	1.09878866	1.09351911	1.09341446	1.09863914
H 22 R26 21 A26 16 D26							

Table S5-5 Bond angle for 2U PUFA (Model 0)

Input Z-matrix 2U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
H	A3	111.28859079	111.30061725	111.28859079	110.72736517	110.82880258	36.07029432
C 1 R2	A4	36.73533596	35.95637028	36.73533596	36.03271905	36.03040262	36.73066662
C 2 R3 1 A3	A5	35.95970798	36.73109523	35.95970798	36.77117869	36.78345972	114.67379054
H 1 R4 2 A4 3 D4	A6	116.03622611	116.06111436	116.03622611	114.67396136	114.694577	128.16429434
H 1 R5 2 A5 3 D5	A7	125.3059025	125.27151948	125.3059025	128.19032204	128.1610693	128.09235809
H 3 R6 2 A6 1 D6	A8	125.13651428	125.15086217	125.13651428	127.96970946	127.99113652	111.76675173
C 3 R7 2 A7 1 D7	A9	115.37452615	112.41704729	115.37452615	111.54862747	111.53990001	117.47902825
C 7 R8 3 A8 2 D8	A10	118.99291853	119.22232908	118.99291853	117.73340729	117.74170284	111.18069213
C 8 R9 7 A9 3 D9	A11	109.69259071	109.87778171	109.69259071	109.09895902	109.10759754	108.23771593
H 7 R10 3 A10 2 D10	A12	109.13929804	108.91903126	109.13929804	110.32506864	110.36081173	114.4007196
H 8 R11 7 A11 3 D11	A13	114.97959219	115.66192694	114.97959219	114.11206081	114.12985901	128.25060262
H 8 R12 7 A12 3 D12	A14	126.30719475	125.117352	126.30719475	128.27365842	128.23482714	128.25381726
H 9 R13 8 A13 7 D13	A15	124.76484155	125.18899307	124.76484155	128.22297987	128.17766502	111.74961407
C 9 R14 8 A14 7 D14	A16	115.2358029	112.36701888	115.2358029	111.53464374	111.48757037	117.34852309
C 14 R15 9 A15 8 D15	A17	119.22345432	119.21005043	119.22345432	117.60224799	117.60971929	111.12551246
C 15 R16 14 A16 9 D16	A18	109.73199771	109.78386155	109.73199771	110.40536685	109.02606823	108.24961003
H 14 R17 9 A17 8 D17	A19	109.09815303	108.92817808	109.09815303	109.05459236	110.4106441	114.42125482
H 15 R18 14 A18 9 D18	A20	115.05254481	115.61881078	115.05254481	114.28877924	114.23771291	128.10478643
H 15 R19 14 A19 9 D19	A21	126.22008383	125.14414649	126.22008383	127.96587638	128.02243773	128.17561438
H 16 R20 15 A20 14 D20	A22	124.89389751	125.29042442	124.89389751	128.18697651	128.20542113	110.72132643
C 16 R21 15 A21 14 D21	A23	111.27764095	111.28551351	111.27764095	110.747797	110.79305143	117.15504259
C 21 R22 16 A22 15 D22	A24	118.86307101	118.66135003	118.86307101	117.13635898	117.12162556	113.03153393
H 22 R23 21 A23 16 D23	A25	111.6277107	111.32008946	111.6277107	110.81359924	110.77837597	110.87037684
H 21 R24 16 A24 15 D24	A26	111.35978751	111.53799695	111.35978751	113.06454017	113.04479496	
H 22 R25 21 A25 16 D25							
H 22 R26 21 A26 16 D26							

Table S5-6 Dihedral angle for 2U PUFA (Model 0)

Input Z-matrix 2U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
H	D4	121.46356302	122.71327691	121.46356302	124.12669684	124.1478253	124.11523517
C 1 R2	D5	-122.7500512	-121.5068998	-122.7500512	-120.53193961	-120.54541539	-120.54547971
C 2 R3 1 A3	D6	-59.35816473	59.69826577	-59.35816473	58.43432161	58.36799748	60.03902181
H 1 R4 2 A4 3 D4	D7	120.3863662	239.97208843	120.3863662	238.22088219	238.02062713	240.19101897
H 1 R5 2 A5 3 D5	D8	-179.04924749	180.33796938	-179.04924749	0.67275235	0.80651039	-0.14978643
H 3 R6 2 A6 1 D6	D9	-119.18377393	118.42893555	-119.18377393	116.88607925	117.57716365	-125.33596944
C 3 R7 2 A7 1 D7	D10	0.64451698	-0.7013659	0.64451698	179.45005839	179.62275843	180.15843513
C 7 R8 3 A8 2 D8	D11	4.5503159	-120.12171589	4.5503159	-120.84874073	-120.16177506	-0.51656046
C 8 R9 7 A9 3 D9	D12	119.2557435	-3.51524693	119.2557435	-4.44253457	-3.7215202	115.5719566
H 7 R10 3 A10 2 D10	D13	-168.32540898	-60.39078363	-168.32540898	-60.6627123	-61.76100103	-52.21722603
H 8 R11 7 A11 3 D11	D14	11.98872504	118.7400198	11.98872504	118.5573642	116.87842566	127.81170443
H 8 R12 7 A12 3 D12	D15	-179.51734413	180.87736675	-179.51734413	-0.06514902	1.43658596	-0.03161876
H 9 R13 8 A13 7 D13	D16	-118.8757497	118.71673192	-118.8757497	-118.92950805	116.03252258	-128.15453135
C 9 R14 8 A14 7 D14	D17	0.58194945	-0.00883459	0.58194945	180.74416221	179.81731202	179.95901625
C 14 R15 9 A15 8 D15	D18	4.92168693	-119.89627193	4.92168693	2.55463154	-121.86048605	-3.32425462
C 15 R16 14 A16 9 D16	D19	119.63800694	-3.31362348	119.63800694	118.98187545	-5.41860503	112.74764444
H 14 R17 9 A17 8 D17	D20	-167.82931752	-61.25377719	-167.82931752	61.72568805	-61.17323928	-54.53087644
H 15 R18 14 A18 9 D18	D21	12.7501495	117.59896264	12.7501495	-117.09715464	117.68068608	125.1565584
H 15 R19 14 A19 9 D19	D22	179.5585273	180.55137698	179.5585273	-0.68617923	0.7737886	0.12316213
H 16 R20 15 A20 14 D20	D23	-120.81282245	120.79926029	-120.81282245	121.74936433	120.34666084	-121.98681392
C 16 R21 15 A21 14 D21	D24	-0.10693819	0.74329909	-0.10693819	179.5439105	180.45923133	180.00592117
C 21 R22 16 A22 15 D22	D25	-0.14958813	239.46363712	-0.14958813	-120.33324497	-121.7293916	-1.00712393
H 22 R23 21 A23 16 D23	D26	120.55985226	0.14557319	120.55985226	0.7276045	-0.67423446	119.99817406
H 21 R24 16 A24 15 D24							
H 22 R25 21 A25 16 D25							
H 22 R26 21 A26 16 D26							

5.3 Z-matrix for 3U PUFA structures

Table S5-7 Bond Distance for 3U PUFA (Model 0)

Input Z-matrix 3U		*trans* Beta	*trans* Extended	*trans* Helix	*cis* Beta	*cis* Extended	*cis* Helix
Bond Distance							
0 1	R2	1.09866242	1.09867146	1.09849407	1.09856891	1.09851402	1.09821374
H	R3	1.50222833	1.50222593	1.50220170	1.50338947	1.50343778	1.50366406
C 1 R2	R4	1.76094805	1.76095869	1.77548808	1.76005991	1.09343799	1.76043469
C 2 R3 1 A3	R5	1.77471007	1.77464731	1.76032594	1.77019785	1.09849424	1.77195806
H 1 R4 2 A4 3 D4	R6	1.09216527	1.09217105	1.09201010	1.09085838	1.09088843	1.09075510
H 1 R5 2 A5 3 D5	R7	1.33555435	1.33557682	1.33557126	1.33848516	1.33849069	1.33845770
H 3 R6 2 A6 1 D6	R8	1.51074032	1.51069772	1.50493977	1.51202456	1.51227717	1.51204751
C 3 R7 2 A7 1 D7	R9	1.51068915	1.51077402	1.51414273	1.51217682	1.51216503	1.51162110
C 7 R8 3 A8 2 D8	R10	1.09166942	1.09169426	1.09184932	1.09040704	1.09034282	1.09093865
C 8 R9 7 A9 3 D9	R11	1.09961442	1.09956739	1.10074846	1.09743183	1.09725207	1.09312367
H 7 R10 3 A10 2 D10	R12	1.09976961	1.09977494	1.10242901	1.09747083	1.09738789	1.10361587
H 8 R11 7 A11 3 D11	R13	1.09177964	1.09176062	1.09194038	1.09050976	1.09041578	1.09120363
H 8 R12 7 A12 3 D12	R14	1.33564599	1.33562069	1.33537606	1.33866635	1.33864544	1.33736658
H 9 R13 8 A13 7 D13	R15	1.51070083	1.51077027	1.50498784	1.51207412	1.51220914	1.51477611
C 9 R14 8 A14 7 D14	R16	1.51070040	1.51080306	1.51411348	1.51207697	1.51229708	1.51204799
C 14 R15 9 A15 8 D15	R17	1.09175682	1.09173533	1.09014359	1.09058297	1.09049688	1.09051187
C 15 R16 14 A16 9 D16	R18	1.09964376	1.09956188	1.10251161	1.09750361	1.09732786	1.09379902
H 14 R17 9 A17 8 D17	R19	1.09964358	1.09959230	1.10084552	1.09750428	1.09735685	1.10261642
H 15 R18 14 A18 9 D18	R20	1.09175666	1.09173549	1.09196579	1.09058284	1.09047612	1.09109913
H 15 R19 14 A19 9 D19	R21	1.33564571	1.33563013	1.33539102	1.33866609	1.33867629	1.33705329
H 16 R20 15 A20 14 D20	R22	1.51068673	1.51073631	1.50499192	1.51217607	1.51214680	1.51375693
C 16 R21 15 A21 14 D21	R23	1.51074444	1.51070606	1.51417287	1.51202168	1.51219596	1.51212767
C 21 R22 16 A22 15 D22	R24	1.09177959	1.09175690	1.09014759	1.09050903	1.09050989	1.09083620
C 22 R23 21 A23 16 D23	R25	1.09976692	1.09977144	1.10098930	1.09747254	1.09723764	1.09309062
H 21 R24 16 A24 15 D24	R26	1.09961505	1.09960904	1.10258382	1.09743158	1.09743451	1.10291566
H 22 R25 21 A25 16 D25	R27	1.09167059	1.09169169	1.09207138	1.09040716	1.09032716	1.09119978
H 22 R26 21 A26 16 D26	R28	1.33555370	1.33557835	1.33532091	1.33848512	1.33850284	1.33766557
H 23 R27 22 A27 21 D27	R29	1.50223411	1.50222161	1.50251177	1.50339310	1.50338040	1.50287051
C 23 R28 22 A28 21 D28	R30	1.09866181	1.09865334	1.09873081	1.09857045	1.09852762	1.09821454
C 28 R29 23 A29 22 D29	R31	1.09216549	1.09216924	1.09033707	1.09085818	1.09088165	1.09105775
H 29 R30 28 A30 23 D30	R32	1.09861610	1.09860889	1.09561986	1.09845081	1.09850583	1.09290559
H 28 R31 23 A31 22 D31	R33	1.09531690	1.09532920	1.09879556	1.09349859	1.09346347	1.09920554
H 29 R32 28 A32 23 D32							
H 29 R33 28 A33 23 D33							

Table S5-8 Bond angle for 3U PUFA (Model 0)

Input Z-matrix 3U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.29155985	111.33948133	111.28061641	110.79125855	110.69316284	110.83478860
H	A4	36.73306556	36.73194154	35.91284957	36.76143218	107.76135717	36.75049359
C 1 R2	A5	35.94796192	35.95359640	36.76177016	36.04632781	106.48033544	35.97395409
C 2 R3 1 A3	A6	116.06846529	116.07275726	116.06746799	114.67119923	114.67576348	114.71734071
H 1 R4 2 A4 3 D4	A7	125.26176063	125.25069283	125.22138364	128.18693649	128.19727115	128.10621834
H 1 R5 2 A5 3 D5	A8	125.17675238	125.16262827	125.22786678	127.95831662	127.98419794	127.88264284
H 3 R6 2 A6 1 D6	A9	112.30717145	112.29892799	115.29483702	111.57486467	111.48208655	112.24789648
C 3 R7 2 A7 1 D7	A10	119.20842608	119.21167802	118.96216881	117.73546137	117.74570300	117.52832237
C 7 R8 3 A8 2 D8	A11	109.90529020	109.89515404	109.72766134	109.10087646	109.13341723	111.11978209
C 8 R9 7 A9 3 D9	A12	108.95363056	108.93846386	109.14057528	110.32634270	110.37058779	108.38484215
H 7 R10 3 A10 2 D10	A13	115.57721419	115.56450935	115.03462672	114.15495453	114.14659591	114.59803730
H 8 R11 7 A11 3 D11	A14	125.18988122	125.21841800	126.21657620	128.25833347	128.20182095	127.85302807
H 8 R12 7 A12 3 D12	A15	125.15870553	125.14311448	124.81388705	128.20570693	128.12106308	127.54809163
H 9 R13 8 A13 7 D13	A16	112.35838175	112.24443405	115.23027352	111.63129081	111.48981573	112.27193529
C 9 R14 8 A14 7 D14	A17	119.23135891	119.24978300	119.17642986	117.59223775	117.66265580	117.59657595
C 14 R15 9 A15 8 D15	A18	108.93631294	109.88481090	109.15578443	110.38218111	109.03827563	110.73964557
C 15 R16 14 A16 9 D16	A19	109.83479773	108.93653559	109.80935500	109.03996562	110.40291817	108.92806931
H 14 R17 9 A17 8 D17	A20	115.59834877	115.58825807	115.01626057	114.19916010	114.18295443	114.72093922
H 15 R18 14 A18 9 D18	A21	125.15864904	125.16055527	126.22405479	128.20594322	128.16794925	127.73777736
H 15 R19 14 A19 9 D19	A22	125.18992298	125.19693293	124.79515219	128.25825087	128.18435534	127.66025952
H 16 R20 15 A20 14 D20	A23	112.30800177	112.30374230	115.26425123	111.57469950	111.48095716	111.63981375
C 16 R21 15 A21 14 D21	A24	119.21762875	119.21779706	119.18789472	117.58347016	117.59696146	117.57748636
C 21 R22 16 A22 15 D22	A25	109.80445697	109.82330151	109.75861328	109.02062159	109.04686713	110.78952917
C 22 R23 21 A23 16 D23	A26	108.93951870	108.94223282	109.08994274	110.43678730	110.40595818	108.90791546
H 21 R24 16 A24 15 D24	A27	115.60522522	115.62656704	115.02708477	114.29812686	114.26041453	114.52543298
H 22 R25 21 A25 16 D25	A28	125.17642125	125.14705904	126.26142532	127.95844784	127.97743497	127.93731864
H 22 R26 21 A26 16 D26	A29	125.26257658	125.26640483	124.85777351	128.18730042	128.18849281	128.14669374
H 23 R27 22 A27 21 D27	A30	111.29067953	111.28736701	111.29648165	110.78912480	110.80130885	110.38920981
C 23 R28 22 A28 21 D28	A31	118.66928364	118.66489063	118.86649139	117.14090027	117.12881858	117.07771461
C 28 R29 23 A29 22 D29	A32	111.31414287	111.31837713	111.59663542	110.75705306	110.75731312	113.47329945
H 29 R30 28 A30 23 D30	A33	111.51973943	111.52214392	111.36096280	113.06630992	113.04889083	110.95940236
H 28 R31 23 A31 22 D31							
H 29 R32 28 A32 23 D32							
H 29 R33 28 A33 23 D33							

Table S5-9 Dihedral angle for 3U PUFA (Model 0)

Input Z-matrix 3U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	121.50693997	121.48434684	122.81518357	120.50195803	-124.09486113	120.55575997
H	D5	-122.70796380	122.74212985	-121.42855819	-124.14110853	120.51722651	-124.24701104
C 1 R2	D6	-59.31113675	-59.70844526	58.55781613	-59.81130479	58.79828447	-57.10466455
C 2 R3 1 A3	D7	120.88892639	120.55891057	-121.64093130	119.85739026	-121.39015940	123.50315668
H 1 R4 2 A4 3 D4	D8	-179.49165707	179.51499245	-179.09448640	0.72828259	0.72658702	-0.28889124
H 1 R5 2 A5 3 D5	D9	117.81088415	117.68741849	-119.50680732	117.81709299	116.24769985	-133.93392925
H 3 R6 2 A6 1 D6	D10	-0.66649140	-0.71250836	0.55927746	179.61505449	179.40665641	179.39578870
C 3 R7 2 A7 1 D7	D11	-120.74393477	120.84929618	4.22293539	-119.88667924	-121.53324510	-8.87398215
C 7 R8 3 A8 2 D8	D12	-4.06686659	-4.18513592	118.95801086	-3.52894833	-5.07810214	107.03493624
C 8 R9 7 A9 3 D9	D13	-61.02610826	-60.40601930	-167.59868918	-59.42241625	-62.97372957	-57.35133538
H 7 R10 3 A10 2 D10	D14	117.54270418	118.59617187	12.74738475	119.90860240	115.48883491	123.30811382
H 8 R11 7 A11 3 D11	D15	-179.86120757	178.84032200	-179.57847431	0.03803687	1.46904201	-1.29150057
H 8 R12 7 A12 3 D12	D16	-118.05766713	118.31826473	-118.96282947	-119.67928588	116.15227136	-144.28155219
H 9 R13 8 A13 7 D13	D17	1.43638158	0.12518571	0.52474269	-179.31493367	179.93711789	178.58633736
C 9 R14 8 A14 7 D14	D18	3.88017622	120.28687449	119.57494116	1.76587250	-121.65676801	-19.72554059
C 14 R15 9 A15 8 D15	D19	120.51687370	-3.60334117	4.79976094	118.09896994	-5.21981404	96.30271267
C 15 R16 14 A16 9 D16	D20	60.69283340	-60.47724180	-168.40847312	59.69785915	-62.35263771	-69.81899559
H 14 R17 9 A17 8 D17	D21	-118.05026087	118.54141211	11.84510379	-119.67956410	116.19906722	109.89889771
H 15 R18 14 A18 9 D18	D22	-179.86373387	178.87877014	-179.42860796	0.04636948	1.52085984	-1.43627871
H 15 R19 14 A19 9 D19	D23	117.55191832	118.82679860	-119.15729217	119.92108549	115.93795028	-137.92703088
H 16 R20 15 A20 14 D20	D24	-1.34086336	0.11839461	0.58401444	179.35609486	179.94146529	179.18840156
C 16 R21 15 A21 14 D21	D25	-121.05597695	119.79866230	4.67947935	-117.97739786	-121.96525070	-13.70253071
C 21 R22 16 A22 15 D22	D26	-4.44411084	-3.17995947	119.38686826	-1.60378153	-5.55789621	102.86258792
C 22 R23 21 A23 16 D23	D27	-61.03917257	-60.87391260	-168.19406154	-61.07176980	-61.91559488	-66.70630418
H 21 R24 16 A24 15 D24	D28	117.82712599	117.98829833	12.29337735	117.84889886	116.84823373	112.44091333
H 22 R25 21 A25 16 D25	D29	-179.49414173	179.45651696	179.64811094	0.73157011	0.75551548	-0.35759586
H 22 R26 21 A26 16 D26	D30	120.88761414	120.72727753	-120.92505143	119.82798634	120.55614980	-125.05954342
H 23 R27 22 A27 21 D27	D31	0.71040689	0.73002730	-0.02471073	-179.61143061	-179.49992530	179.87210375
C 23 R28 22 A28 21 D28	D32	-120.43421954	120.58990050	-0.27317347	-122.24954642	-121.52290832	-4.47380351
C 28 R29 23 A29 22 D29	D33	0.24243828	0.08550135	120.42009144	-1.19453309	-0.49842870	117.28616381
H 29 R30 28 A30 23 D30							
H 28 R31 23 A31 22 D31							
H 29 R32 28 A32 23 D32							
H 29 R33 28 A33 23 D33							

5.4 Z-matrix for 4U PUFA structures

Table S5-10 Bond Distances for 4U PUFA (Model 0)

Input Z-matrix 4U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Distance							
0 1	R2	1.09865057	1.09862386	1.09863214	1.09853945	1.09846566	1.09824532
H	R3	1.50212800	1.50218599	1.50215143	1.50334942	1.50344592	1.50351547
C 1 R2	R4	1.76086585	1.77476374	1.76060077	1.75998771	1.09848836	1.76024149
C 2 R3 1 A3	R5	1.77469705	1.76086929	1.77453466	1.77029276	1.09352668	1.77191556
H 1 R4 2 A4 3 D4	R6	1.09220705	1.09216521	1.09200412	1.09087094	1.09083661	1.09066408
H 1 R5 2 A5 3 D5	R7	1.33558160	1.33555825	1.33558179	1.33850154	1.33856705	1.33867607
H 3 R6 2 A6 1 D6	R8	1.51058033	1.51075251	1.50495930	1.51214287	1.51206213	1.51222242
C 3 R7 2 A7 1 D7	R9	1.51063193	1.51067654	1.51405245	1.51208613	1.51226427	1.51197008
C 7 R8 3 A8 2 D8	R10	1.09168490	1.09166888	1.09182395	1.09038615	1.09029668	1.09084734
C 8 R9 7 A9 3 D9	R11	1.09970122	1.09961922	1.10071069	1.09741062	1.09744622	1.09308318
H 7 R10 3 A10 2 D10	R12	1.09993006	1.09974737	1.10241951	1.09733666	1.09722333	1.10330451
H 8 R11 7 A11 3 D11	R13	1.09177374	1.09176656	1.09193923	1.09051185	1.09047610	1.09111740
H 8 R12 7 A12 3 D12	R14	1.33568355	1.33564041	1.33535228	1.33863018	1.33869568	1.33826838
H 9 R13 8 A13 7 D13	R15	1.51072798	1.51082065	1.50494576	1.51234107	1.51226399	1.51393054
C 9 R14 8 A14 7 D14	R16	1.51083730	1.51080358	1.51392090	1.51218515	1.51230288	1.51335231
C 14 R15 9 A15 8 D15	R17	1.09170303	1.09175483	1.09013493	1.09054490	1.09043867	1.09048030
C 15 R16 14 A16 9 D16	R18	1.09962862	1.09948945	1.10084755	1.09738844	1.09722934	1.09376262
H 14 R17 9 A17 8 D17	R19	1.09944217	1.09952207	1.10258941	1.09744748	1.09718495	1.10206270
H 15 R18 14 A18 9 D18	R20	1.09176900	1.09176837	1.09203336	1.09052371	1.09043520	1.09064720
H 15 R19 14 A19 9 D19	R21	1.33563384	1.33562283	1.33536222	1.33864700	1.33866532	1.33671345
H 16 R20 15 A20 14 D20	R22	1.51074606	1.51080491	1.50489236	1.51218465	1.51229277	1.51693007
C 16 R21 15 A21 14 D21	R23	1.51065693	1.51082154	1.51396168	1.51234196	1.51228596	1.51023567
C 21 R22 16 A22 15 D22	R24	1.09175516	1.09176805	1.09005136	1.09052379	1.09042771	1.09028109
C 22 R23 21 A23 16 D23	R25	1.09967190	1.09952079	1.10089877	1.09738828	1.09719336	1.09400899
H 21 R24 16 A24 15 D24	R26	1.09963279	1.09948856	1.10263004	1.09744723	1.09721907	1.10328976
H 22 R25 21 A25 16 D25	R27	1.09173542	1.09175442	1.09200102	1.09054439	1.09044719	1.09147651
H 22 R26 21 A26 16 D26	R28	1.33566539	1.33564095	1.33539354	1.33863012	1.33871701	1.33714605
H 23 R27 22 A27 21 D27	R29	1.51061907	1.51067845	1.50502292	1.51208612	1.51227402	1.51269544
C 23 R28 22 A28 21 D28	R30	1.51083278	1.51075289	1.51415465	1.51214177	1.51205539	1.51229241
C 28 R29 23 A29 22 D29	R31	1.09174976	1.09176756	1.09008499	1.09051238	1.09046810	1.09118594
C 29 R30 28 A30 23 D30	R32	1.09968195	1.09974694	1.10100890	1.09741064	1.09725570	1.09270001
H 28 R31 23 A31 22 D31	R33	1.09968483	1.09961699	1.10259377	1.09733622	1.09742059	1.10337247
H 29 R32 28 A32 23 D32	R34	1.09168520	1.09166930	1.09206503	1.09038681	1.09030684	1.09136518
H 29 R33 28 A33 23 D33	R35	1.33555071	1.33555739	1.33532703	1.33850144	1.33855792	1.33772510
H 30 R34 29 A34 28 D34	R36	1.50225735	1.50218878	1.50257665	1.50334950	1.50345651	1.50288230
C 30 R35 29 A35 28 D35	R37	1.09862713	1.09865847	1.09879821	1.09849540	1.09850898	1.09854160
C 35 R36 30 A36 29 D36	R38	1.09216981	1.09216656	1.09035574	1.09087103	1.09083356	1.09116934
H 36 R37 35 A37 30 D37	R39	1.09865533	1.09862469	1.09872759	1.09853890	1.09847938	1.09905711
H 35 R38 30 A38 29 D38	R40	1.09529421	1.09533863	1.09560658	1.09346897	1.09350589	1.09272802
H 36 R39 35 A39 30 D39							
H 36 R40 35 A40 30 D40							

Table S5-11 Bond angle for 4U PUFA (Model 0)

Input Z-matrix 4U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.28053199	111.31374612	111.27751509	110.79302383	110.80016364	110.83719687
H	A4	36.73742280	35.94602665	36.74295064	36.76631662	106.46317624	36.75783300
C 1 R2	A5	35.95013352	36.73818091	35.95953078	36.04003184	107.72822735	35.97147198
C 2 R3 1 A3	A6	116.04781293	116.06557247	116.02614841	114.66973266	114.67012649	114.70841570
H 1 R4 2 A4 3 D4	A7	125.32215076	125.28039698	125.30923527	128.20662072	128.20042122	128.17584775
H 1 R5 2 A5 3 D5	A8	125.06236743	125.14643494	125.15404750	127.96666524	127.94159722	127.91720090
H 3 R6 2 A6 1 D6	A9	112.47983709	112.31454240	115.33522088	111.52491645	111.53922124	112.08135625
C 3 R7 2 A7 1 D7	A10	119.23213694	119.22580015	118.99363931	117.73413679	117.74711207	117.49810236
C 7 R8 3 A8 2 D8	A11	109.96008060	109.90944998	109.71514679	109.12382281	109.13694061	111.11153812
C 8 R9 7 A9 3 D9	A12	108.87718819	108.93474127	109.14554304	110.32672104	110.30127177	108.42788407
H 7 R10 3 A10 2 D10	A13	115.62162076	115.59119506	115.02400018	114.16840921	114.16228815	114.56405772
H 8 R11 7 A11 3 D11	A14	125.16454997	125.17787580	126.23169333	128.27322240	128.23523019	127.94866568
H 8 R12 7 A12 3 D12	A15	125.12748606	125.18069472	124.77640204	128.23778910	128.14520090	127.61255257
H 9 R13 8 A13 7 D13	A16	112.25352103	112.21167492	115.25832234	111.52892022	111.46520112	112.30972275
C 9 R14 8 A14 7 D14	A17	119.22310650	119.23717552	119.18750908	117.59302756	117.62171329	117.59046396
C 14 R15 9 A15 8 D15	A18	108.94147800	109.85403197	109.80470267	110.43163394	109.07719440	110.72707489
C 15 R16 14 A16 9 D16	A19	109.88024528	108.96404660	109.19516938	109.02682281	110.38448191	108.90091799
H 14 R17 9 A17 8 D17	A20	115.52547292	115.55378494	115.00257675	114.20652290	114.17557924	115.28212607
H 15 R18 14 A18 9 D18	A21	125.26099495	125.19118806	126.24477895	128.19472728	128.20893274	126.80003847
H 15 R19 14 A19 9 D19	A22	125.08863947	125.19074889	124.77640549	128.19468144	128.20834482	126.74289929
H 16 R20 15 A20 14 D20	A23	112.39982592	112.21123476	115.26292939	111.52890533	111.46244161	112.11986103
C 16 R21 15 A21 14 D21	A24	119.25923596	119.24661326	119.21473940	117.59340978	117.60485963	117.90315093
C 21 R22 16 A22 15 D22	A25	109.85546945	109.85601039	109.82277980	109.06197163	109.01802600	110.36750275
C 22 R23 21 A23 16 D23	A26	108.90602885	108.98062796	109.17488071	110.39353324	110.44568647	109.06867265
H 21 R24 16 A24 15 D24	A27	115.61797137	115.57380077	114.99258299	114.16543716	114.21203655	114.41448304
H 22 R25 21 A25 16 D25	A28	125.15611120	125.18060665	126.27237783	128.23772865	128.15609186	128.20244382
H 22 R26 21 A26 16 D26	A29	125.14913302	125.17906060	124.78138345	128.27326074	128.24817990	128.20318527
H 23 R27 22 A27 21 D27	A30	112.32096737	112.31218751	115.26945680	111.52503679	111.53753375	111.36474963
C 23 R28 22 A28 21 D28	A31	119.21380671	119.22359484	119.23022843	117.55417715	117.58800418	117.31015376
C 28 R29 23 A29 22 D29	A32	108.91998384	109.82229708	109.75914336	110.42666347	108.99206206	111.37743848
C 29 R30 28 A30 23 D30	A33	109.81835742	108.93542849	109.08369677	109.03049738	110.46816488	108.52043583
H 28 R31 23 A31 22 D31	A34	115.59251271	115.61776523	115.03718904	114.28936588	114.30682413	114.46798632
H 29 R32 28 A32 23 D32	A35	125.18978501	125.14706291	126.26486050	127.96672997	127.93791444	128.04679126
H 29 R33 28 A33 23 D33	A36	125.26175013	125.28012920	124.83970925	128.20670162	128.19815243	128.21040395
H 30 R34 29 A34 28 D34	A37	111.31258911	111.29130256	111.35834489	110.74883592	110.80759645	110.42401812
C 30 R35 29 A35 28 D35	A38	118.67386330	118.65399212	118.88115836	117.12311112	117.13129841	117.03575026
C 35 R36 30 A36 29 D36	A39	111.29203968	111.31410760	111.30518362	110.79298615	110.75063692	110.78187627
H 36 R37 35 A37 30 D37	A40	111.51855876	111.53207650	111.58477120	113.07504771	113.07923060	113.43091546
H 35 R38 30 A38 29 D38							
H 36 R39 35 A39 30 D39							
H 36 R40 35 A40 30 D40							

Table S5-12 Dihedral angle for 4U PUFA (Model 0)

Input Z-matrix 4U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedrals							
0 1	D4	121.48525193	122.74171932	121.44736665	120.49030306	-120.50559332	120.49013841
H	D5	-122.74377285	-121.48834200	-122.75341994	-124.16080008	124.17041281	-124.30339801
C 1 R2	D6	-59.15799614	59.32085342	-59.43840931	-59.41032347	-59.36624031	-57.30625884
C 2 R3 1 A3	D7	121.06457186	-120.47000922	120.28647743	120.31862662	120.35019904	123.36802115
H 1 R4 2 A4 3 D4	D8	-179.56748310	-179.49069743	-179.01863946	0.73663053	0.73322266	-0.59588942
H 1 R5 2 A5 3 D5	D9	118.58500526	117.91148317	-118.87941488	117.44767265	116.78257084	-132.16454431
H 3 R6 2 A6 1 D6	D10	-0.63040350	-0.65612015	0.66308181	179.52584271	179.49918767	179.30883441
C 3 R7 2 A7 1 D7	D11	-119.87136959	-120.64196766	4.83522393	-120.28634319	-120.88737814	-7.13923378
C 7 R8 3 A8 2 D8	D12	-3.28597128	-3.98079965	119.55804179	-3.87803351	-4.48201941	108.85754643
C 8 R9 7 A9 3 D9	D13	-58.96289723	-60.72350863	-168.03404273	-60.03627282	-61.17125922	-59.18482554
H 7 R10 3 A10 2 D10	D14	119.99643109	118.29012428	12.30044681	119.19218154	117.45011723	121.35284908
H 8 R11 7 A11 3 D11	D15	179.56738625	-178.84716917	-179.59164719	0.06351261	1.52590854	-1.21859073
H 8 R12 7 A12 3 D12	D16	-116.17674449	117.71458907	-118.80968750	-119.03134160	115.04752214	-139.19805211
H 9 R13 8 A13 7 D13	D17	1.18373231	0.08614768	0.54575970	-179.18604727	179.83923448	178.82120623
C 9 R14 8 A14 7 D14	D18	5.61688535	-120.88827773	4.88650231	2.40918105	-122.72882037	-14.98845015
C 14 R15 9 A15 8 D15	D19	122.34349633	-4.17268006	119.67200178	118.80827136	-6.25766824	101.18933590
C 15 R16 14 A16 9 D16	D20	60.86454266	-61.44633460	-169.07378892	60.98776955	-62.61936443	-74.83021713
H 14 R17 9 A17 8 D17	D21	-117.80989149	117.47730494	11.19511528	-118.14080587	115.92333858	104.69655324
H 15 R18 14 A18 9 D18	D22	179.99705028	-178.72048776	-179.51595012	0.00000000	1.41804866	-1.08347353
H 15 R19 14 A19 9 D19	D23	118.10808051	117.45370351	-119.42342912	118.14123265	115.92481460	-153.06524524
H 16 R20 15 A20 14 D20	D24	-1.34211379	0.16387675	0.51963039	179.10323671	179.90858504	179.13842297
C 16 R21 15 A21 14 D21	D25	-120.42764141	-121.16934561	4.32901057	-119.62640396	-121.96576108	-28.72896336
C 21 R22 16 A22 15 D22	D26	-3.79912223	-4.44228122	119.11087161	-3.22837489	-5.49549938	87.39305001
C 22 R23 21 A23 16 D23	D27	-60.17704045	-61.25761179	-168.94546169	-60.23952919	-63.37197026	-63.71927587
H 21 R24 16 A24 15 D24	D28	118.68696137	117.71022629	11.27159826	119.03161357	114.98302469	116.04094203
H 22 R25 21 A25 16 D25	D29	179.71373320	-178.84487813	-179.31104521	-0.06354833	1.51080339	-0.99596443
H 22 R26 21 A26 16 D26	D30	-117.21395373	118.28272163	-119.74444290	-119.19271830	117.58517101	-132.72518316
H 23 R27 22 A27 21 D27	D31	1.25128319	0.13413554	0.62825426	-179.26959139	-179.88541594	179.54966120
C 23 R28 22 A28 21 D28	D32	4.74659168	-120.33273484	4.11400534	2.32035497	-120.39100053	-7.98779219
C 28 R29 23 A29 22 D29	D33	121.36475079	-3.71960163	118.82748860	118.73094791	-3.97880409	108.51270612
C 29 R30 28 A30 23 D30	D34	60.65685973	-60.97356370	-167.76792174	61.37630248	-62.09048959	-63.08637723
H 28 R31 23 A31 22 D31	D35	-118.27451731	117.89428547	12.71467143	-117.44809319	116.65363450	115.97995336
H 29 R32 28 A32 23 D32	D36	179.56380966	-179.48629981	179.69629879	-0.73652708	0.77644126	0.00000000
H 29 R33 28 A33 23 D33	D37	120.33379244	120.87511612	120.59409563	121.77232450	120.31296044	-122.63567247
H 30 R34 29 A34 28 D34	D38	-0.66804424	0.72774454	-0.01255144	179.54020794	-179.52612055	-179.81936317
C 30 R35 29 A35 28 D35	D39	-120.98818714	-120.45643153	-120.75578919	-120.31846553	-121.77610172	119.71296615
C 35 R36 30 A36 29 D36	D40	-0.33279617	0.22142969	-0.08550549	0.73100474	-0.75126327	-1.70691772
H 36 R37 35 A37 30 D37							
H 35 R38 30 A38 29 D38							
H 36 R39 35 A39 30 D39							
H 36 R40 35 A40 30 D40							

5.5 Z-matrix for 5U PUFA structures

Table S5-13 Bond Distances for 5U PUFA (Model 0)

Input Z-matrix 5U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Length							
0 1	R2	1.09854890	1.09863016	1.09863849	1.09853022	1.09850868	1.09811374
H	R3	1.50227354	1.50230103	1.50217149	1.50339272	1.50344511	1.50328886
C 1 R2	R4	1.75986627	1.76088287	1.76071929	1.76003595	1.76005936	1.09866351
C 2 R3 1 A3	R5	1.77505021	1.77500276	1.77461566	1.77026301	1.77025574	1.09362724
H 1 R4 2 A4 3 D4	R6	1.09208195	1.09214809	1.09202905	1.09086174	1.09087516	1.09056508
H 1 R5 2 A5 3 D5	R7	1.33554826	1.33556310	1.33556843	1.33848432	1.33852869	1.33838926
H 3 R6 2 A6 1 D6	R8	1.51094098	1.51082478	1.50491243	1.51217600	1.51216214	1.51184610
C 3 R7 2 A7 1 D7	R9	1.51075636	1.51074197	1.51404284	1.51211627	1.51215673	1.51128065
C 7 R8 3 A8 2 D8	R10	1.09166925	1.09167270	1.09180755	1.09037059	1.09034638	1.09103939
C 8 R9 7 A9 3 D9	R11	1.09966269	1.09973723	1.10073094	1.09743459	1.09741161	1.09327644
H 7 R10 3 A10 2 D10	R12	1.09947152	1.09948704	1.10246703	1.09735904	1.09723850	1.10386874
H 8 R11 7 A11 3 D11	R13	1.09175248	1.09181799	1.09193870	1.09052790	1.09049444	1.09103111
H 8 R12 7 A12 3 D12	R14	1.33563911	1.33562467	1.33534869	1.33868682	1.33871125	1.33784624
H 9 R13 8 A13 7 D13	R15	1.51084063	1.51080485	1.50494369	1.51237384	1.51214752	1.51395376
C 9 R14 8 A14 7 D14	R16	1.51049403	1.51088856	1.51387328	1.51218571	1.51218776	1.51124399
C 14 R15 9 A15 8 D15	R17	1.09184479	1.09176187	1.09015634	1.09053224	1.09049016	1.09051697
C 15 R16 14 A16 9 D16	R18	1.09943370	1.09943081	1.10079807	1.09727422	1.09739457	1.09387769
H 14 R17 9 A17 8 D17	R19	1.09993224	1.09948149	1.10261201	1.09737077	1.09745671	1.10330772
H 15 R18 14 A18 9 D18	R20	1.09175622	1.09170846	1.09196800	1.09051903	1.09049506	1.09116286
H 15 R19 14 A19 9 D19	R21	1.33566837	1.33562968	1.33536812	1.33863453	1.33864099	1.33790061
H 16 R20 15 A20 14 D20	R22	1.51063578	1.51087478	1.50501820	1.51227009	1.51214003	1.51388440
C 16 R21 15 A21 14 D21	R23	1.51063220	1.51088444	1.51387146	1.51226408	1.51222422	1.51214936
C 21 R22 16 A22 15 D22	R24	1.09183757	1.09171173	1.09009802	1.09052447	1.09047830	1.09058582
C 22 R23 21 A23 16 D23	R25	1.09974745	1.09947600	1.10083988	1.09733060	1.09740677	1.09356625
H 21 R24 16 A24 15 D24	R26	1.09954380	1.09947264	1.10257971	1.09738705	1.09743129	1.10285934
H 22 R25 21 A25 16 D25	R27	1.09174301	1.09174141	1.09200294	1.09051848	1.09049278	1.09106634
H 22 R26 21 A26 16 D26	R28	1.33566587	1.33563575	1.33537956	1.33859509	1.33860819	1.33702310
H 23 R27 22 A27 21 D27	R29	1.51066056	1.51079008	1.50502144	1.51231768	1.51215230	1.51497408
C 23 R28 22 A28 21 D28	R30	1.51065025	1.51083484	1.51387262	1.51232703	1.51217969	1.51132300
C 28 R29 23 A29 22 D29	R31	1.09181009	1.09170434	1.09010043	1.09049857	1.09048466	1.09054084
C 29 R30 28 A30 23 D30	R32	1.09955929	1.09948995	1.10087371	1.09732616	1.09746161	1.09339727
H 28 R31 23 A31 22 D31	R33	1.09973500	1.09949427	1.10264497	1.09735175	1.09741783	1.10340565
H 29 R32 28 A32 23 D32	R34	1.09174328	1.09173855	1.09199168	1.09051590	1.09049330	1.09135163
H 29 R33 28 A33 23 D33	R35	1.33565906	1.33563347	1.33539077	1.33868727	1.33865419	1.33702460
H 30 R34 29 A34 28 D34	R36	1.51060374	1.51069046	1.50509074	1.51213247	1.51213711	1.51377538
C 30 R35 29 A35 28 D35	R37	1.51065414	1.51086710	1.51417314	1.51226813	1.51208794	1.51146404
C 35 R36 30 A36 29 D36	R38	1.09180606	1.09175990	1.09014470	1.09049488	1.09051159	1.09109293
C 36 R37 35 A37 30 D37	R39	1.09986720	1.09963205	1.10095903	1.09731994	1.09732855	1.09270006
H 35 R38 30 A38 29 D38	R40	1.09964658	1.09959514	1.10258977	1.09737766	1.09746322	1.10264508
H 36 R39 35 A39 30 D39	R41	1.09166144	1.09167724	1.09207369	1.09037567	1.09033058	1.09155348
H 36 R40 35 A40 30 D40	R42	1.33558317	1.33554332	1.33530845	1.33845227	1.33850490	1.33776350
H 37 R41 36 A41 35 D41	R43	1.50220393	1.50228108	1.50251748	1.50329182	1.50338284	1.50292094
C 37 R42 36 A42 35 D42	R44	1.09862010	1.09864899	1.09879555	1.09847037	1.09348276	1.09866788
C 42 R43 37 A43 36 D43	R45	1.09218010	1.09216009	1.09036331	1.09087313	1.09087058	1.09118246
H 43 R44 42 A44 37 D44	R46	1.09534183	1.09860133	1.09875995	1.09351443	1.09851927	1.09274244
H 42 R45 37 A45 36 D45	R47	1.09863673	1.09529641	1.09561928	1.09855099	1.09850289	1.09914856
H 43 R46 42 A46 37 D46							
H 43 R47 42 A47 37 D47							

Table S5-14 Bond angle for 5U PUFA (Model 0)

Input Z-matrix 5U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.53599767	111.28100254	111.28715948	110.79186307	110.77729891	110.79508540
H	A4	36.78935536	36.73604595	36.73646645	36.76407831	36.76384269	106.52357523
C 1 R2	A5	35.92861853	35.93301074	35.95557599	36.04148964	36.03908215	107.89790934
C 2 R3 1 A3	A6	116.15008775	116.09216773	116.03014797	114.67771082	114.68257487	114.71731607
H 1 R4 2 A4 3 D4	A7	125.09185397	125.21243818	125.30011569	128.18624411	128.18793580	128.10065573
H 1 R5 2 A5 3 D5	A8	125.36516922	125.22254930	125.15357640	127.94127392	127.95501182	127.96052554
H 3 R6 2 A6 1 D6	A9	112.29929259	112.25690286	115.33726082	111.52854313	111.48013902	112.22161291
C 3 R7 2 A7 1 D7	A10	119.16115850	119.20515599	118.99791047	117.74549092	117.75733312	117.52373060
C 7 R8 3 A8 2 D8	A11	109.71199873	109.89005439	109.71474102	109.10951657	109.14261832	111.22708224
C 8 R9 7 A9 3 D9	A12	109.05306798	108.97819488	109.15618802	110.31605415	110.32321533	108.30170401
H 7 R10 3 A10 2 D10	A13	115.69212643	115.65118311	115.02024354	114.17572467	114.19965149	114.53457474
H 8 R11 7 A11 3 D11	A14	124.97158273	125.12972429	126.22123829	128.24526237	128.19128185	128.02479306
H 8 R12 7 A12 3 D12	A15	125.38047389	125.18271132	124.80365722	128.19599567	128.14362787	127.77445263
H 9 R13 8 A13 7 D13	A16	112.39815552	112.23195734	115.26290878	111.52967645	111.41791123	112.15210910
C 9 R14 8 A14 7 D14	A17	119.16566337	119.23118383	119.17429193	117.61260092	117.62902062	117.44591736
C 14 R15 9 A15 8 D15	A18	109.03727579	109.87935687	109.82011397	110.40489020	109.08762842	110.93735775
C 15 R16 14 A16 9 D16	A19	109.65665419	108.98432682	109.16166258	109.02522033	110.40931042	108.79457580
H 14 R17 9 A17 8 D17	A20	115.79321790	115.53610450	115.00848227	114.18199305	114.15832924	114.52921463
H 15 R18 14 A18 9 D18	A21	124.88962566	125.23035306	126.23627054	128.22387235	128.23906356	127.99771924
H 15 R19 14 A19 9 D19	A22	125.34758425	125.14630879	124.78322047	128.20636916	128.22693366	127.63555412
H 16 R20 15 A20 14 D20	A23	112.39046266	112.34292815	115.27045630	111.43886876	111.28476257	112.14254412
C 16 R21 15 A21 14 D21	A24	119.14563848	119.25145987	119.20522856	117.59225851	117.58385573	117.54026969
C 21 R22 16 A22 15 D22	A25	109.68032099	109.80645733	109.83519677	109.07784930	109.09635090	110.81205495
C 22 R23 21 A23 16 D23	A26	109.02645072	108.95266159	109.15046238	110.40379998	110.47118878	108.86157999
H 21 R24 16 A24 15 D24	A27	115.70689741	115.60766902	114.99849665	114.17537677	114.14801149	114.78999905
H 22 R25 21 A25 16 D25	A28	125.01063718	125.13368024	126.26379216	128.24031664	128.25340404	127.53116494
H 22 R26 21 A26 16 D26	A29	125.27342334	125.22469699	124.72601030	128.26727725	128.26459380	127.36694557
H 23 R27 22 A27 21 D27	A30	112.38276938	112.24315638	115.33574238	111.46411693	111.33984849	112.17078630
C 23 R28 22 A28 21 D28	A31	119.18264102	119.22119279	119.20022710	117.57209676	117.57691285	117.64243133
C 28 R29 23 A29 22 D29	A32	108.99054659	109.77777339	109.77769343	110.45853514	109.05572352	110.89773554
C 29 R30 28 A30 23 D30	A33	109.72444482	108.98821534	109.14683192	109.04405241	110.47280874	108.84297313
H 28 R31 23 A31 22 D31	A34	115.67472329	115.57154321	114.97562995	114.19951262	114.17807759	114.65942500
H 29 R32 28 A32 23 D32	A35	125.06076593	125.18687411	126.28689227	128.18228724	128.19315252	127.80724249
H 29 R33 28 A33 23 D33	A36	125.21870247	125.16131843	124.76486214	128.23603884	128.24203626	127.92301016
H 30 R34 29 A34 28 D34	A37	112.41669635	112.28121185	115.27328805	111.47473086	111.43572347	111.31532771
C 30 R35 29 A35 28 D35	A38	119.19538506	119.22244780	119.20911265	117.58088778	117.57668147	117.37073425
C 35 R36 30 A36 29 D36	A39	109.73962565	109.83371520	109.74596941	109.07888990	109.05749188	111.18630793
C 36 R37 35 A37 30 D37	A40	108.94556879	108.92671166	109.09889556	110.43193114	110.44007672	108.75565183
H 35 R38 30 A38 29 D38	A41	115.67759330	115.58179724	115.02483779	114.26323392	114.27220802	114.47984610
H 36 R39 35 A39 30 D39	A42	125.10220891	125.18983992	126.26220191	127.98811249	127.96584092	128.12308241
H 36 R40 35 A40 30 D40	A43	125.28465870	125.25555003	124.86650065	128.20872716	128.19376365	128.15288732
H 37 R41 36 A41 35 D41	A44	111.31108508	111.28381676	111.35927214	110.74094291	113.06339227	110.47439201
C 37 R42 36 A42 35 D42	A45	118.64799175	118.67496183	118.86376666	117.11890469	117.12820261	117.08981293
C 42 R43 37 A43 36 D43	A46	111.53200139	111.31563121	111.29331969	113.07326015	110.78447549	113.36737928
H 43 R44 42 A44 37 D44	A47	111.27897213	111.51660234	111.60955646	110.80154308	110.76118727	110.79792697
H 42 R45 37 A45 36 D45							
H 43 R46 42 A46 37 D46							
H 43 R47 42 A47 37 D47							

Table S5-15 Dihedral angles for 5U PUFA (Model 0)

Input Z-matrix 5U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedrals							
0 1	D4	121.47716516	121.49503038	121.44634093	120.50273239	120.51488354	-120.52101770
H	D5	-122.84480992	-122.72040866	-122.75681142	-124.13502108	-124.12006823	124.23995032
C 1 R2	D6	-58.22225278	-59.17921264	-59.61472312	-59.30723926	-59.19879979	-56.94151493
C 2 R3 1 A3	D7	122.33542654	121.00990977	120.14576008	120.40596198	120.48762597	123.70017319
H 1 R4 2 A4 3 D4	D8	179.84264646	-179.47436787	-179.06798933	0.72979697	0.81501873	-0.28557012
H 1 R5 2 A5 3 D5	D9	119.38557814	118.22117655	-119.27264117	117.61975243	117.55477090	-133.05108131
H 3 R6 2 A6 1 D6	D10	-0.96099077	-0.64985775	0.60695363	179.55866738	179.59047416	179.23475242
C 3 R7 2 A7 1 D7	D11	-119.40599331	-120.40064412	4.45112005	-120.13574983	-120.22357498	-7.82981237
C 7 R8 3 A8 2 D8	D12	-2.75102572	-3.69338514	119.17061303	-3.74114910	-3.78048069	108.04141733
C 8 R9 7 A9 3 D9	D13	-63.95222620	-61.90406452	-168.25380415	-60.05806386	-61.51234398	-53.08761641
H 7 R10 3 A10 2 D10	D14	114.09358860	116.92016271	12.01253164	119.10387722	116.96684858	128.05871610
H 8 R11 7 A11 3 D11	D15	-178.92469587	-178.56699347	-179.43213505	0.08738759	1.68412371	-1.33057287
H 8 R12 7 A12 3 D12	D16	-122.00169470	116.58669809	-119.47643240	-117.93760706	116.48992919	-144.20748908
H 9 R13 8 A13 7 D13	D17	1.73693572	0.20039266	0.57475353	-179.05991208	-179.92056526	178.18508908
C 9 R14 8 A14 7 D14	D18	0.30290554	-121.96714495	4.30037506	3.43426497	-121.32515898	-19.33007805
C 14 R15 9 A15 8 D15	D19	116.85072727	-5.20646447	119.06357996	119.86107783	-4.85549732	96.62876286
C 15 R16 14 A16 9 D16	D20	62.43042655	-61.73433384	-168.86302677	61.65065945	-60.07881446	-62.37978215
H 14 R17 9 A17 8 D17	D21	-115.82177079	117.34537342	11.31874340	-117.43821806	118.53112962	118.03414371
H 15 R18 14 A18 9 D18	D22	179.21839179	-179.03613149	-179.32431402	0.09520816	1.81516889	-1.25446137
H 15 R19 14 A19 9 D19	D23	120.09793722	117.32433592	-119.48724668	117.75284259	116.36001211	-142.05487045
H 16 R20 15 A20 14 D20	D24	-1.69041498	0.01618820	0.61754896	179.09381785	-179.97764001	178.70717849
C 16 R21 15 A21 14 D21	D25	-118.65423491	-121.27655773	4.30783093	-120.06477385	-121.49748229	-17.54962480
C 21 R22 16 A22 15 D22	D26	-2.07023225	-4.59781085	119.07955121	-3.60924174	-4.93586805	98.63881628
C 22 R23 21 A23 16 D23	D27	-61.96861707	-61.71668551	-168.60030664	-60.59716068	-61.19426369	-67.54310252
H 21 R24 16 A24 15 D24	D28	116.47956363	117.35275773	11.57026010	118.48320427	117.20291600	112.42949848
H 22 R25 21 A25 16 D25	D29	-179.54603122	-179.01631843	-179.28877218	0.06095504	1.81033403	-1.27428146
H 22 R26 21 A26 16 D26	D30	-119.30464623	117.50770174	-119.41970177	-117.94336951	117.78332281	-146.38088909
H 23 R27 22 A27 21 D27	D31	1.53114664	0.02576589	0.61934404	-179.02231118	-179.76240120	178.85277024
C 23 R28 22 A28 21 D28	D32	2.77963722	-121.12896445	4.35469381	3.50285571	-120.09317486	-21.80393186
C 28 R29 23 A29 22 D29	D33	119.38424430	-4.43728163	119.06911959	119.92345060	-3.57926955	94.40843014
C 29 R30 28 A30 23 D30	D34	61.38427207	-61.68051673	-168.95309233	62.05722766	-61.83997551	-67.30423616
H 28 R31 23 A31 22 D31	D35	-117.19149879	117.21775820	11.28827793	-116.97188218	116.54287472	112.55769095
H 29 R32 28 A32 23 D32	D36	179.76539942	-178.72418129	-179.40734221	0.07983127	1.77437260	-1.29049867
H 29 R33 28 A33 23 D33	D37	119.16192147	117.38669912	-119.35137192	117.83185622	117.33685243	-139.86424077
H 30 R34 29 A34 28 D34	D38	-1.44197004	0.14816723	0.57996128	179.03328472	-179.80076923	179.04894706
C 30 R35 29 A35 28 D35	D39	-119.48653084	-121.20090714	4.48821452	-120.05787093	-120.60010668	-15.26656024
C 35 R36 30 A36 29 D36	D40	-2.94232836	-4.56276542	119.20026622	-3.58667708	-4.14668890	100.82093139
C 36 R37 35 A37 30 D37	D41	-60.91186794	-60.88373125	-168.04018366	-61.42529456	-61.62619943	-64.13202488
H 35 R38 30 A38 29 D38	D42	118.00680553	117.99081493	12.43996333	117.45497970	117.12733938	114.76578923
H 36 R39 35 A39 30 D39	D43	-179.51852269	-179.48017012	179.65758197	0.65210131	0.82138843	0.07973118
H 36 R40 35 A40 30 D40	D44	-120.45873390	120.73117262	120.65946982	-122.18652427	-0.58859864	-122.00015762
H 37 R41 36 A41 35 D41	D45	0.69298964	0.71209689	-0.01291872	-179.61156166	-179.47031358	-179.68915277
C 37 R42 36 A42 35 D42	D46	0.21734343	-120.59146568	-120.69878232	-1.16463716	120.44646992	-1.03209681
C 42 R43 37 A43 36 D43	D47	120.87103577	0.08178605	-0.03907716	119.90568528	-121.63248656	120.36529941
H 43 R44 42 A44 37 D44							
H 42 R45 37 A45 36 D45							
H 43 R46 42 A46 37 D46							
H 43 R47 42 A47 37 D47							

5.6 Z-matrix for 6U PUFA structures

Table S5-16 Bond Length of 6U PUFA (Model 0)

Input Z-matrix 6U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Lengths							
0 1	R2	1.09863564	1.09865356	1.09861276	1.09855777	1.09854356	1.09819907
H	R3	1.50218431	1.50222633	1.50206485	1.50333435	1.50337218	1.50328870
C 1 R2	R4	1.76093900	1.09860537	1.76067057	1.09847913	1.09848869	1.76041314
C 2 R3 1 A3	R5	1.77478818	1.09533159	1.77456350	1.09347449	1.09352166	1.77209060
H 1 R4 2 A4 3 D4	R6	1.09216457	1.09217193	1.09204204	1.09086105	1.09086778	1.09060603
H 1 R5 2 A5 3 D5	R7	1.33556685	1.33556029	1.33558478	1.33847083	1.33850060	1.33871690
H 3 R6 2 A6 1 D6	R8	1.51062779	1.51074006	1.50494761	1.51227491	1.51210363	1.51152358
C 3 R7 2 A7 1 D7	R9	1.51065308	1.51069298	1.51394878	1.51208050	1.51226640	1.51157754
C 7 R8 3 A8 2 D8	R10	1.09169832	1.09167312	1.09184783	1.09035844	1.09033500	1.09110371
C 8 R9 7 A9 3 D9	R11	1.09965838	1.09962475	1.10070477	1.09736895	1.09748980	1.09337992
H 7 R10 3 A10 2 D10	R12	1.09985601	1.09970192	1.10246726	1.09733305	1.09729664	1.10387078
H 8 R11 7 A11 3 D11	R13	1.09181797	1.09178951	1.09199484	1.09049833	1.09050771	1.09089207
H 8 R12 7 A12 3 D12	R14	1.33565690	1.33563332	1.33532044	1.33868614	1.33867408	1.33764266
H 9 R13 8 A13 7 D13	R15	1.51077836	1.51072749	1.50490319	1.51239534	1.51222621	1.51435006
C 9 R14 8 A14 7 D14	R16	1.51059572	1.51075351	1.51370533	1.51219718	1.51226822	1.51064579
C 14 R15 9 A15 8 D15	R17	1.09175712	1.09176553	1.09005712	1.09053551	1.09048292	1.09056192
C 15 R16 14 A16 9 D16	R18	1.09958257	1.09954460	1.10078911	1.09735869	1.09739553	1.09409242
H 14 R17 9 A17 8 D17	R19	1.09958010	1.09957320	1.10274795	1.09736016	1.09727198	1.10354919
H 15 R18 14 A18 9 D18	R20	1.09179951	1.09174802	1.09197413	1.09052032	1.09047156	1.09116689
H 15 R19 14 A19 9 D19	R21	1.33565180	1.33564383	1.33535190	1.33863555	1.33864141	1.33799330
H 16 R20 15 A20 14 D20	R22	1.51046297	1.51082849	1.50508211	1.51232445	1.51219107	1.51415882
C 16 R21 15 A21 14 D21	R23	1.51069531	1.51072707	1.51367894	1.51233460	1.51225954	1.51196732
C 21 R22 16 A22 15 D22	R24	1.09178299	1.09173560	1.09008602	1.09051060	1.09046403	1.09053524
C 22 R23 21 A23 16 D23	R25	1.09967752	1.09955240	1.10075972	1.09735065	1.09731590	1.09354058
H 21 R24 16 A24 15 D24	R26	1.09987096	1.09953753	1.10273838	1.09728630	1.09726412	1.10295802
H 22 R25 21 A25 16 D25	R27	1.09176871	1.09175000	1.09198755	1.09051609	1.09045986	1.09112836
H 22 R26 21 A26 16 D26	R28	1.33567148	1.33564425	1.33539115	1.33859602	1.33863430	1.33789904
H 23 R27 22 A27 21 D27	R29	1.51076378	1.51069618	1.50491893	1.51233286	1.51226477	1.51362100
C 23 R28 22 A28 21 D28	R30	1.51092719	1.51078241	1.51373713	1.51232371	1.51219114	1.51319460
C 28 R29 23 A29 22 D29	R31	1.09168851	1.09174862	1.09009246	1.09051578	1.09046040	1.09057062
C 29 R30 28 A30 23 D30	R32	1.09959274	1.09952742	1.10084495	1.09735107	1.09726571	1.09363217
H 28 R31 23 A31 22 D31	R33	1.09933378	1.09956653	1.10267904	1.09728569	1.09732141	1.10274737
H 29 R32 28 A32 23 D32	R34	1.09174788	1.09175310	1.09200583	1.09051142	1.09046341	1.09077568
H 29 R33 28 A33 23 D33	R35	1.33561942	1.33562497	1.33542502	1.33863563	1.33864256	1.33681150
H 30 R34 29 A34 28 D34	R36	1.51075770	1.51073771	1.50497081	1.51219410	1.51226752	1.51729417
C 30 R35 29 A35 28 D35	R37	1.51066855	1.51079125	1.51368926	1.51239281	1.51222599	1.50915723
C 35 R36 30 A36 29 D36	R38	1.09173804	1.09173911	1.09005111	1.09052054	1.09047249	1.09042992
C 36 R37 35 A37 30 D37	R39	1.09966596	1.09953541	1.10092712	1.09736042	1.09727556	1.09372480
H 35 R38 30 A38 29 D38	R40	1.09965381	1.09958953	1.10267064	1.09736253	1.09739736	1.10242471
H 36 R39 35 A39 30 D39	R41	1.09173774	1.09176242	1.09196980	1.09053591	1.09048329	1.09177979
H 36 R40 35 A40 30 D40	R42	1.33565115	1.33561847	1.33542318	1.33868680	1.33867473	1.33727510
H 37 R41 36 A41 35 D41	R43	1.51063292	1.51069704	1.50519453	1.51207706	1.51226575	1.51244855
C 37 R42 36 A42 35 D42	R44	1.51080715	1.51079621	1.51404986	1.51228241	1.51210320	1.51220117
C 42 R43 37 A43 36 D43	R45	1.09174741	1.09177332	1.09013219	1.09049891	1.09050703	1.09138867
C 43 R44 42 A44 37 D44	R46	1.09967504	1.09971689	1.10101932	1.09736818	1.09729760	1.09244955
H 42 R45 37 A45 36 D45	R47	1.09970392	1.09958453	1.10259957	1.09733040	1.09748799	1.10334889
H 43 R46 42 A46 37 D46	R48	1.09168354	1.09169258	1.09206960	1.09035391	1.09033493	1.09136398
H 43 R47 42 A47 37 D47	R49	1.33556103	1.33555559	1.33533092	1.33847057	1.33850118	1.33778713
H 44 R48 43 A48 42 D48	R50	1.50224982	1.50219828	1.50253164	1.50333930	1.50336614	1.50303289
C 44 R49 43 A49 42 D49	R51	1.09864938	1.09866572	1.09874352	1.09347445	1.09854261	1.09847303
C 49 R50 44 A50 43 D50	R52	1.09216133	1.09218476	1.09031662	1.09086902	1.09086686	1.09116730
H 50 R51 49 A51 44 D51	R53	1.09531356	1.09861486	1.09565887	1.09847350	1.09849259	1.09288843
H 49 R52 44 A52 43 D52	R54	1.09862754	1.09532453	1.09879161	1.09855883	1.09351936	1.09921249
H 50 R53 49 A53 44 D53							
H 50 R54 49 A54 44 D54							

Table S5-17 Bond Angle of 6U PUFA

Input Z-matrix 6U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.29328032	111.30271406	111.28271240	110.80907210	110.80078740	110.79316195
H	A4	36.73358741	106.52753144	36.73986435	106.46791501	106.46266664	36.74736197
C 1 R2	A5	35.94441604	107.97881273	35.95964860	107.73721160	107.73076360	35.96950638
C 2 R3 1 A3	A6	116.07709209	116.05713194	116.01434671	114.68912266	114.68156501	114.70057763
H 1 R4 2 A4 3 D4	A7	125.25394646	125.28834560	125.33742119	128.17802214	128.18311752	128.12185973
H 1 R5 2 A5 3 D5	A8	125.12956013	125.14688367	125.07473427	127.95676824	127.94418329	128.01929331
H 3 R6 2 A6 1 D6	A9	112.40268419	112.34709123	115.40992596	111.51813810	111.48170352	112.20903736
C 3 R7 2 A7 1 D7	A10	119.20716235	119.22939163	119.01342694	117.75207299	117.75467997	117.50067377
C 7 R8 3 A8 2 D8	A11	109.92411268	109.89072129	109.67622819	109.09956196	109.12870448	111.27966367
C 8 R9 7 A9 3 D9	A12	108.92047871	108.93838875	109.17956273	110.34106575	110.32551892	108.21843375
H 7 R10 3 A10 2 D10	A13	115.59316364	115.58720784	114.95930427	114.18160497	114.16042265	114.60470327
H 8 R11 7 A11 3 D11	A14	125.17875282	125.18915141	126.30889468	128.24074951	128.23915931	127.90244624
H 8 R12 7 A12 3 D12	A15	125.14276929	125.14982984	124.70858100	128.18367998	128.14790117	127.64035908
H 9 R13 8 A13 7 D13	A16	112.34348964	112.28795498	115.32882888	111.47434831	111.44025947	112.37333002
C 9 R14 8 A14 7 D14	A17	119.23386088	119.23976560	119.21039826	117.62350565	117.61887909	117.47235021
C 14 R15 9 A15 8 D15	A18	108.93675526	109.87950303	109.78305897	110.40510195	109.08240036	110.91195626
C 15 R16 14 A16 9 D16	A19	109.84530922	108.94990288	109.22101718	109.06726045	110.37801925	108.72902260
H 14 R17 9 A17 8 D17	A20	115.56076516	115.57649259	114.94355683	114.18720556	114.16994001	114.49819858
H 15 R18 14 A18 9 D18	A21	125.25309968	125.19070428	126.30584878	128.22409288	128.20530496	128.06260343
H 15 R19 14 A19 9 D19	A22	124.99286073	125.14755981	124.74164949	128.22022538	128.16265829	127.71567087
H 16 R20 15 A20 14 D20	A23	112.49164176	112.31494383	115.28517012	111.45633389	111.44976875	111.97508266
C 16 R21 15 A21 14 D21	A24	119.25971609	119.24426602	119.21219782	117.58506533	117.61278840	117.49623732
C 21 R22 16 A22 15 D22	A25	109.94448097	109.83998439	109.80281744	109.05614255	109.06246748	110.83326618
C 22 R23 21 A23 16 D23	A26	108.84776449	108.94363411	109.18646182	110.42544011	110.40252666	108.86425937
H 21 R24 16 A24 15 D24	A27	115.61467713	115.59931606	114.99776075	114.19298870	114.19752217	114.59279850
H 22 R25 21 A25 16 D25	A28	125.17800056	125.15489908	126.25245354	128.19717535	128.16056283	127.86062226
H 22 R26 21 A26 16 D26	A29	125.09469020	125.18199443	124.76729090	128.19700480	128.16182120	127.62970107
H 23 R27 22 A27 21 D27	A30	112.21563092	112.27377338	115.32023717	111.45662269	111.44830838	112.17660775
C 23 R28 22 A28 21 D28	A31	119.23672404	119.23082507	119.20765963	117.60326508	117.62593515	117.56920503
C 28 R29 23 A29 22 D29	A32	108.94269500	109.83405962	109.81388662	110.41064094	109.04691174	110.85955839
C 29 R30 28 A30 23 D30	A33	109.89722193	108.97029489	109.14424128	109.05462672	110.43180843	108.83814958
H 28 R31 23 A31 22 D31	A34	115.48994109	115.58317793	114.99802925	114.18810071	114.20732407	115.30347742
H 29 R32 28 A32 23 D32	A35	125.30693081	125.17079655	126.28642607	128.22047211	128.16304251	126.64288847
H 29 R33 28 A33 23 D33	A36	125.04872039	125.16086659	124.72787889	128.22447613	128.20619436	126.71942071
H 30 R34 29 A34 28 D34	A37	112.40588148	112.28613747	115.35200966	111.47569263	111.43875185	112.04510626
C 30 R35 29 A35 28 D35	A38	119.27531615	119.23792669	119.23172109	117.58205002	117.60874302	117.75835711
C 35 R36 30 A36 29 D36	A39	109.87451613	109.83730015	109.80819518	109.06331447	109.02422006	110.48942560
C 36 R37 35 A37 30 D37	A40	108.88705157	108.94769161	109.12190551	110.42125617	110.46552605	109.17148586
H 35 R38 30 A38 29 D38	A41	115.61402527	115.57776967	114.98118285	114.18747218	114.21446632	114.42718443
H 36 R39 35 A39 30 D39	A42	125.16003741	125.17367837	126.32257223	128.18359499	128.14902011	128.30742289
H 36 R40 35 A40 30 D40	A43	125.14982169	125.18469507	124.72968216	128.24103954	128.23912107	128.12870679
H 37 R41 36 A41 35 D41	A44	112.32132045	112.33200778	115.27915368	111.51818588	111.48122412	111.39276048
C 37 R42 36 A42 35 D42	A45	119.21529181	119.22110278	119.25711066	117.57185508	117.58418017	117.38614066
C 42 R43 37 A43 36 D43	A46	108.91948406	109.80326970	109.73991146	110.41982395	109.02001402	111.29993360
C 43 R44 42 A44 37 D44	A47	109.81596242	108.92965899	109.08499814	109.04892065	110.46184565	108.47581253
H 42 R45 37 A45 36 D45	A48	115.60073292	115.61471309	115.05782349	114.28444498	114.28966936	114.51692170
H 43 R46 42 A46 37 D46	A49	125.18861180	125.15112763	126.25107632	127.95468878	127.94471140	128.02513389
H 43 R47 42 A47 37 D47	A50	125.24006920	125.28234878	124.85243779	128.18035900	128.18272287	128.18666078
H 44 R48 43 A48 42 D48	A51	111.29817089	111.29069364	111.29799136	113.04615338	110.80253824	110.48668497
C 44 R49 43 A49 42 D49	A52	118.68215654	118.65949833	118.88748009	117.13149653	117.13464540	117.08367843
C 49 R50 44 A50 43 D50	A53	111.50539528	111.30715933	111.60781537	110.74851474	110.75553211	113.35492147
H 50 R51 49 A51 44 D51	A54	111.31700912	111.53093415	111.35753929	110.81017150	113.05871325	110.81781195
H 49 R52 44 A52 43 D52							
H 50 R53 49 A53 44 D53							
H 50 R54 49 A54 44 D54							

Table S5-18 Dihedral Angles for 6U PUFA

Input Z-matrix 6U		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	121.51316648	-121.48564671	121.43441318	-120.50442343	-120.50023561	120.49329099
H	D5	-122.70317347	122.74002264	-122.77816629	124.14082766	124.14973874	-124.26471519
C 1 R2	D6	-59.15988548	-59.38117385	-59.29771008	-59.70131313	-59.43037989	-57.67443636
C 2 R3 1 A3	D7	121.07805955	120.85428839	120.46756390	120.02596314	120.28946027	122.94091226
H 1 R4 2 A4 3 D4	D8	-179.58323008	-179.54225979	-179.10205003	0.69186099	0.77935805	-0.16560178
H 1 R5 2 A5 3 D5	D9	118.66537869	117.79738684	-118.64995866	117.27603530	116.90206793	-131.52079927
H 3 R6 2 A6 1 D6	D10	-0.65405305	-0.67713660	0.60212662	179.50651995	179.50657416	179.27399259
C 3 R7 2 A7 1 D7	D11	-119.84224499	-120.74764179	4.99882760	-120.48771299	-120.81119561	-6.30576568
C 7 R8 3 A8 2 D8	D12	-3.22407813	-4.08882678	119.71871746	-4.07735200	-4.37933927	109.54265060
C 8 R9 7 A9 3 D9	D13	-59.75229145	-60.87193789	-169.06963659	-61.00991577	-61.17006990	-51.98961522
H 7 R10 3 A10 2 D10	D14	119.01199650	118.15027922	11.24930697	118.09594252	117.33907069	129.03256824
H 8 R11 7 A11 3 D11	D15	179.90714963	-178.89689569	-179.58472254	0.01486883	1.66280432	-0.93983832
H 8 R12 7 A12 3 D12	D16	-117.08414652	117.87564201	-119.59109835	-118.12727231	116.05674366	-146.63750945
H 9 R13 8 A13 7 D13	D17	1.31562485	0.08423363	0.45385752	-179.06066561	-179.98910916	178.30050749
C 9 R14 8 A14 7 D14	D18	4.75748537	-120.68487710	4.08442226	3.26068110	-121.71279520	-21.58867873
C 14 R15 9 A15 8 D15	D19	121.41371379	-3.99946707	118.84787916	119.68578370	-5.23962393	94.22432633
C 15 R16 14 A16 9 D16	D20	60.92594482	-60.79136983	-170.43761261	61.05603294	-61.78134777	-60.00308683
H 14 R17 9 A17 8 D17	D21	-117.81121663	118.30210649	9.75582053	-117.99623380	116.74517841	120.91638373
H 15 R18 14 A18 9 D18	D22	-179.90887106	-179.03011713	-179.37486629	-0.01127574	1.57700041	-1.75062640
H 15 R19 14 A19 9 D19	D23	118.59496226	118.21899544	-120.42793331	117.39809671	115.89013431	-142.19370011
H 16 R20 15 A20 14 D20	D24	-1.24698196	0.04667170	0.50699684	178.99751808	179.96757555	178.19132629
C 16 R21 15 A21 14 D21	D25	-119.82988885	-120.37408022	3.36472913	-120.44746481	-121.93233208	-17.60458260
C 21 R22 16 A22 15 D22	D26	-3.27077227	-3.70405405	118.12485804	-3.97938677	-5.45899541	98.59150214
C 22 R23 21 A23 16 D23	D27	-57.82069950	-61.01252394	-169.43520088	-61.58249086	-62.36552567	-65.40301438
H 21 R24 16 A24 15 D24	D28	121.38128169	118.08510643	10.64163872	117.45034820	116.12042694	114.65403919
H 22 R25 21 A25 16 D25	D29	179.23977253	-178.99739378	-179.08571975	0.00000000	1.54990331	-1.22883343
H 22 R26 21 A26 16 D26	D30	-114.90928000	117.98270118	-120.17721112	-117.45137047	116.13758991	-139.33356703
H 23 R27 22 A27 21 D27	D31	1.05644021	0.04259657	0.69825575	-179.00462045	179.99200044	179.00403879
C 23 R28 22 A28 21 D28	D32	6.81178911	-120.62513826	3.67042038	3.91818218	-121.73019906	-15.27234268
C 28 R29 23 A29 22 D29	D33	123.57846548	-3.94012221	118.40656393	120.37667801	-5.24945826	101.13443143
C 29 R30 28 A30 23 D30	D34	60.96014085	-60.97406573	-168.66378704	61.62985806	-62.54358212	-72.98798714
H 28 R31 23 A31 22 D31	D35	-117.73844489	118.08014619	11.43915267	-117.40748324	115.88834450	106.47250556
H 29 R32 28 A32 23 D32	D36	-179.94036358	-178.97719009	-179.13130594	0.00864900	1.58484209	-0.85137905
H 29 R33 28 A33 23 D33	D37	118.18771886	118.01279194	-119.77426382	118.02047135	116.75536404	-157.28854754
H 30 R34 29 A34 28 D34	D38	-1.30560756	0.04728967	0.66003893	179.03709830	-179.93647980	179.21458046
C 30 R35 29 A35 28 D35	D39	-120.32821327	-120.57548483	4.04801780	-119.81521259	-121.16365341	-32.88110481
C 35 R36 30 A36 29 D36	D40	-3.70204466	-3.91386762	118.76159329	-3.38411532	-4.67482832	82.61853991
C 36 R37 35 A37 30 D37	D41	-59.93351309	-60.99171774	-168.75474661	-60.95181028	-62.31597709	-62.70610041
H 35 R38 30 A38 29 D38	D42	118.96616417	118.05496533	11.46027401	118.15425339	116.07800854	116.93788557
H 36 R39 35 A39 30 D39	D43	179.67712548	-178.94715741	-179.29669600	-0.01694124	1.66885016	-0.94086875
H 36 R40 35 A40 30 D40	D44	-117.15117072	118.10562887	-119.71109394	-118.10492978	117.34438761	-129.64497400
H 37 R41 36 A41 35 D41	D45	1.22948416	0.04603564	0.62481263	-179.09831128	-179.86928477	179.76925839
C 37 R42 36 A42 35 D42	D46	4.81408969	-120.50278626	4.13656289	3.37008678	-120.61564569	-4.82479427
C 42 R43 37 A43 36 D43	D47	121.42967125	-3.89174862	118.83899879	119.79461962	-4.16930126	111.51912577
C 43 R44 42 A44 37 D44	D48	60.70829782	-61.06965088	-167.82345530	61.56500590	-61.85987682	-62.38347011
H 42 R45 37 A45 36 D45	D49	-118.21291627	117.81579008	12.67994291	-117.28591157	116.90587536	116.69627154
H 43 R46 42 A46 37 D46	D50	179.56321758	-179.51894806	179.66869353	-0.69139172	0.77700250	-0.02760622
H 43 R47 42 A47 37 D47	D51	-121.00796998	120.86487489	-120.63926143	1.07389027	120.30367147	-122.64814622
H 44 R48 43 A48 42 D48	D52	-0.67254008	0.71944920	-0.02403338	179.58960084	-179.50710243	-179.78937041
C 44 R49 43 A49 42 D49	D53	-0.35588749	-120.47265320	0.03348707	122.09756698	-121.78240401	-1.81711028
C 49 R50 44 A50 43 D50	D54	120.30256165	0.19947227	120.72001009	-119.98058433	-0.74715477	119.67682471
H 50 R51 49 A51 44 D51							
H 49 R52 44 A52 43 D52							
H 50 R53 49 A53 44 D53							
H 50 R54 49 A54 44 D54							

6. Z-matrix for Model I, II, and PUFA

6.1 Z-matrix for 3Up PUFA structures

Table S6-1 Bond distance for 5U PUFA (Model 0)

Input Z-matrix 3Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Distance							
0 1	R2	1.0968117	1.09674238	1.09674621	1.09669952	1.09673944	1.09558592
H	R3	1.5384785	1.53841862	1.53860403	1.53882835	1.53874532	1.53821711
C 1 R2	R4	1.50496554	1.50502045	1.50491444	1.50599678	1.50609422	1.50630919
C 2 R3 1 A3	R5	1.09608932	1.09603728	1.096046	1.09601453	1.0960516	1.09595125
C 3 R4 2 A4 1 D4	R6	1.09567995	1.09570039	1.09566658	1.09566197	1.09566178	1.09674422
H 2 R5 3 A5 4 D5	R7	1.09746661	1.09747736	1.09757313	1.09555013	1.09549833	1.09578737
H 2 R6 3 A6 4 D6	R8	1.10053036	1.10057381	1.10041533	1.10050336	1.10046248	1.100895
H 3 R7 2 A7 1 D7	R9	1.09314327	1.09310343	1.0929641	1.09196706	1.0919387	1.09186446
H 3 R8 2 A8 1 D8	R10	1.33570601	1.33574296	1.33573489	1.33873151	1.3387901	1.33889584
H 4 R9 3 A9 2 D9	R11	1.51085243	1.51089997	1.50500665	1.51251995	1.51237107	1.51194312
C 4 R10 3 A10 2 D10	R12	1.51068171	1.5106127	1.51412636	1.51220558	1.5121907	1.5116799
C 10 R11 4 A11 3 D11	R13	1.09174612	1.09174135	1.0919037	1.09050861	1.09049344	1.09126381
C 11 R12 10 A12 4 D12	R14	1.09961503	1.09967803	1.10070701	1.09731978	1.09738948	1.09321997
H 10 R13 4 A13 3 D13	R15	1.09970795	1.09967346	1.10242023	1.09729602	1.09732871	1.10384455
H 11 R14 10 A14 4 D14	R16	1.09179329	1.09184258	1.09194708	1.0904986	1.09051205	1.0911243
H 11 R15 10 A15 4 D15	R17	1.33563606	1.33563992	1.33534856	1.33863773	1.33863491	1.33851859
H 12 R16 11 A16 10 D16	R18	1.51071861	1.5106625	1.50500612	1.51229142	1.51222032	1.51498406
C 12 R17 11 A17 10 D17	R19	1.51071462	1.51066266	1.51396613	1.51237114	1.51222117	1.51725636
C 17 R18 12 A18 11 D18	R20	1.09175849	1.09180347	1.09012316	1.090521	1.09050038	1.09003768
C 18 R19 17 A19 12 D19	R21	1.0996365	1.09963908	1.10084131	1.09732504	1.09741269	1.09508003
H 17 R20 12 A20 11 D20	R22	1.09961013	1.09963911	1.10260473	1.09730734	1.09741422	1.10034767
H 18 R21 17 A21 12 D21	R23	1.09178643	1.09180345	1.09193304	1.09053371	1.0905015	1.09001993
H 18 R22 17 A22 12 D22	R24	1.33563478	1.33563992	1.33537338	1.3386733	1.33863172	1.33703993
H 19 R23 18 A23 17 D23	R25	1.510691	1.5106127	1.5051004	1.51219139	1.51219005	1.51333488
C 19 R24 18 A24 17 D24	R26	1.5108595	1.51089996	1.51430064	1.51257583	1.51236761	1.51229886
C 24 R25 19 A25 18 D25	R27	1.09180833	1.09184257	1.09010563	1.09054914	1.09051166	1.09091295
C 25 R26 24 A26 19 D26	R28	1.09973341	1.09967346	1.10097276	1.0971977	1.09733363	1.09275365
H 24 R27 19 A27 18 D27	R29	1.09959591	1.09967803	1.10257816	1.09738789	1.09739313	1.103283
H 25 R28 24 A28 19 D28	R30	1.09173062	1.09174137	1.09213225	1.09051584	1.09049355	1.09149862
H 25 R29 24 A29 19 D29	R31	1.33572557	1.33574295	1.33549419	1.33875887	1.33878582	1.33811443
H 26 R30 25 A30 24 D30	R32	1.50499906	1.50502053	1.5051223	1.50595772	1.50608549	1.50553746
C 26 R31 25 A31 24 D31	R33	1.09312476	1.09310342	1.09128251	1.09195895	1.09194232	1.09218431
C 31 R32 26 A32 25 D32	R34	1.0975124	1.10057383	1.09779782	1.09547134	1.10046505	1.09426738
H 31 R33 26 A33 25 D33	R35	1.10060712	1.09747734	1.1006999	1.10050262	1.095505	1.10049976
H 32 R34 31 A34 26 D34	R36	1.53838633	1.53841846	1.5385079	1.53887064	1.53874226	1.53903016
H 32 R35 31 A35 26 D35	R37	1.09677501	1.09674241	1.09675191	1.09672406	1.09674276	1.09693256
C 32 R36 31 A36 26 D36	R38	1.09568023	1.09570042	1.09570546	1.09570837	1.09566079	1.09536834
H 36 R37 32 A37 31 D37	R39	1.09604654	1.09603727	1.09619971	1.09599579	1.09605087	1.09614211
H 36 R38 32 A38 31 D38							
H 36 R39 32 A39 31 D39							

Table S6-2 Bond angel for 3Up PUFA (Model 1)

Input Z-matrix 3Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.14999665	111.11028784	111.15484527	111.12458321	111.12408805	111.16924851
H	A4	112.80752808	112.7862571	112.81548316	112.42283277	112.40645736	112.55554662
C 1 R2	A5	111.10476359	107.74255071	111.07341103	111.06051542	111.08710448	111.03343149
C 2 R3 1 A3	A6	110.90571478	107.6458582	110.91479603	110.97586291	110.94928028	111.06189127
C 3 R4 2 A4 1 D4	A7	109.76447641	109.79994804	109.73814087	109.50683767	109.5184701	109.65334786
H 2 R5 3 A5 4 D5	A8	108.61775355	108.60043327	108.61128938	108.58354904	108.60728263	108.54502619
H 2 R6 3 A6 4 D6	A9	115.79264563	115.77500185	115.77914712	114.3255092	114.36203678	114.32804423
H 3 R7 2 A7 1 D7	A10	125.43858377	125.49962267	125.43759188	128.51059159	128.47424218	128.52203607
H 3 R8 2 A8 1 D8	A11	125.22898373	125.17870094	125.22782456	128.04258325	128.02574006	128.04180426
H 4 R9 3 A9 2 D9	A12	112.35186034	112.37929936	115.32275941	111.47296829	111.43765802	112.29993291
C 4 R10 3 A10 2 D10	A13	119.19712991	119.21985271	118.96260031	117.75044162	117.76550979	117.49213962
C 10 R11 4 A11 3 D11	A14	109.87018534	109.8856981	109.72014763	109.04380378	109.08269186	111.12328235
C 11 R12 10 A12 4 D12	A15	108.94785203	108.91524044	109.13957549	110.37245246	110.37325981	108.27005319
H 10 R13 4 A13 3 D13	A16	115.57817529	115.6001875	114.99903581	114.13634589	114.14444794	114.62705984
H 11 R14 10 A14 4 D14	A17	125.18429189	125.17313141	126.2616328	128.2823843	128.25824777	127.84972605
H 11 R15 10 A15 4 D15	A18	125.15457514	125.16309654	124.78207182	128.24281602	128.23376802	127.45555866
H 12 R16 11 A16 10 D16	A19	112.35294854	112.39433746	115.27327316	111.42082828	111.33215039	112.96613086
C 12 R17 11 A17 10 D17	A20	119.23174162	119.23312597	119.19589734	117.58671799	117.5935031	117.6900745
C 17 R18 12 A18 11 D18	A21	108.94556872	109.81255108	109.80556304	110.42247668	109.06151465	110.30968156
C 18 R19 17 A19 12 D19	A22	109.82707153	108.94281572	109.15099275	109.07317567	110.46455908	108.98990195
H 17 R20 12 A20 11 D20	A23	115.59116832	115.59902321	114.97949617	114.18233939	114.1520299	115.65710845
H 18 R21 17 A21 12 D21	A24	125.16296316	125.16307806	126.27318405	128.2127973	128.23623094	126.66835662
H 18 R22 17 A22 12 D22	A25	125.18106027	125.17314001	124.78300424	128.25574902	128.26117506	127.04687764
H 19 R23 18 A23 17 D23	A26	112.38381117	112.37928163	115.25420519	111.45842228	111.43420525	111.34185345
C 19 R24 18 A24 17 D24	A27	119.22434616	119.22129018	119.2237447	117.56556321	117.58115983	117.88845922
C 24 R25 19 A25 18 D25	A28	109.76910607	109.79640893	109.76118153	109.08005551	109.04262938	110.5279048
C 25 R26 24 A26 19 D26	A29	108.93253695	108.93126555	109.09064213	110.4189802	110.4395496	108.82379211
H 24 R27 19 A27 18 D27	A30	115.58231974	115.59520218	115.02083109	114.18357989	114.19094678	114.28633137
H 25 R28 24 A28 19 D28	A31	125.20466069	125.17871906	126.27776089	128.05520768	128.02799552	128.23373079
H 25 R29 24 A29 19 D29	A32	125.45418758	125.49961069	125.04611379	128.52387127	128.47672797	128.61320278
H 26 R30 25 A30 24 D30	A33	118.75942987	118.72264426	118.95201954	117.15081541	117.15464006	116.98334102
C 26 R31 25 A31 24 D31	A34	109.6300224	109.38455015	109.71829828	111.09956621	108.84125818	111.57258547
C 31 R32 26 A32 25 D32	A35	109.36450047	109.63803551	109.44931773	108.8742869	111.08112852	108.85897779
H 31 R33 26 A33 25 D33	A36	112.82115059	112.7862536	112.77833239	112.39638173	112.40311887	112.10184967
H 32 R34 31 A34 26 D34	A37	111.13758983	111.11028218	111.12699078	111.15144293	111.12509253	111.34803676
H 32 R35 31 A35 26 D35	A38	110.92176972	110.92934555	110.89093944	110.96634562	110.94901581	110.68954775
C 32 R36 31 A36 26 D36	A39	111.09190725	111.09652194	111.13109954	111.05431316	111.08738297	110.9123731
H 36 R37 32 A37 31 D37							
H 36 R38 32 A38 31 D38							
H 36 R39 32 A39 31 D39							

Table S6-3 Dihedral angel for 3Up PUFA (Model 1)

Input Z-matrix 3Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	58.24983612	58.20596552	58.24675206	57.23576441	57.12620752	-62.45600905
H	D5	178.19971385	-121.91295609	178.18834105	177.1978989	177.10753556	177.12516699
C 1 R2	D6	-61.46188976	121.64337604	-61.48298119	-62.45294359	-62.53400963	57.27899026
C 2 R3 1 A3	D7	-179.19715641	-179.201031	-179.17112005	-178.72492397	-178.89429792	61.6808523
C 3 R4 2 A4 1 D4	D8	-63.20045066	-63.20809798	-63.16306113	-63.22610875	-63.36331368	177.04688689
H 2 R5 3 A5 4 D5	D9	-60.12474111	-59.73880452	-60.22705238	-59.21287235	-59.91196169	-53.69936722
H 2 R6 3 A6 4 D6	D10	119.25099914	119.6491262	118.73402426	119.74477196	118.94628051	126.47890601
H 3 R7 2 A7 1 D7	D11	-179.04193227	-179.04455438	-178.68754388	1.43427866	1.57250145	0.32045853
H 3 R8 2 A8 1 D8	D12	117.94040952	118.45041445	-118.67143535	115.54379108	115.78478545	-132.41813369
H 4 R9 3 A9 2 D9	D13	-0.02950699	0.00567348	1.23551577	179.89506799	-179.98919992	179.65952634
C 4 R10 3 A10 2 D10	D14	-120.60072064	-120.08036525	5.04967268	-122.24905491	-122.02229258	-7.2378124
C 10 R11 4 A11 3 D11	D15	-3.93702316	-3.43804236	119.79986815	-5.77203711	-5.53014219	108.5148533
C 11 R12 10 A12 4 D12	D16	-60.94739121	-60.71804333	-168.23604575	-61.24598161	-60.88281468	-52.60803645
H 10 R13 4 A13 3 D13	D17	117.68232932	118.42688858	12.03776217	117.82590724	117.65507828	128.43389138
H 11 R14 10 A14 4 D14	D18	-179.96621817	-179.18537182	-179.48159824	-0.02323406	1.73238867	-1.15134556
H 11 R15 10 A15 4 D15	D19	-117.96873431	118.44763551	-119.28267907	-118.04817168	116.42803009	-142.6792938
H 12 R16 11 A16 10 D16	D20	1.38530325	-0.01579069	0.57029228	-179.07189294	-179.96044126	178.47864055
C 12 R17 11 A17 10 D17	D21	3.95622822	-120.10977053	4.49775605	3.34027296	-121.42712931	-18.49880488
C 17 R18 12 A18 11 D18	D22	120.60975896	-3.49049394	119.24919826	119.81393075	-4.90033986	97.16663502
C 18 R19 17 A19 12 D19	D23	60.67370602	-60.74883273	-168.90376634	61.51663002	-61.87914575	-93.6371964
H 17 R20 12 A20 11 D20	D24	-118.02210643	118.44761771	11.33099988	-117.455151	116.48182461	85.67166188
H 18 R21 17 A21 12 D21	D25	-179.99793874	-179.18534608	-179.34946078	-0.029615	1.73252168	-1.0308056
H 18 R22 17 A22 12 D22	D26	117.87165017	118.42675458	-119.52687994	117.37419454	117.67126361	-136.79179742
H 19 R23 18 A23 17 D23	D27	-1.3695818	-0.06896303	0.62637973	178.94317674	-179.77436828	179.5931534
C 19 R24 18 A24 17 D24	D28	-120.71759656	-120.18721319	4.30005894	-120.54235165	-120.24208653	-12.70755813
C 24 R25 19 A25 18 D25	D29	-4.11160668	-3.58605985	119.01122138	-4.09038997	-3.73505794	104.04707324
C 25 R26 24 A26 19 D26	D30	-61.10265486	-60.63051527	-167.73136327	-61.22704372	-62.68067277	-63.70289068
H 24 R27 19 A27 18 D27	D31	117.64471719	118.45040656	12.61768583	117.77326395	115.80388089	115.19690178
H 25 R28 24 A28 19 D28	D32	179.96994167	-179.04460279	179.215511	0.03892944	1.57770162	-0.53152504
H 25 R29 24 A29 19 D29	D33	1.04784209	0.32692365	0.32729347	-179.35737759	-179.59373994	-179.13327455
H 26 R30 25 A30 24 D30	D34	3.5563232	-119.38254665	3.3757312	2.51662482	-120.67217459	6.16099676
C 26 R31 25 A31 24 D31	D35	119.88902286	-3.03444695	119.77172478	119.1058907	-4.13464807	123.15573532
C 31 R32 26 A32 25 D32	D36	-119.11311281	119.64915862	-119.26338869	-120.54637661	118.97342494	-116.61022148
H 31 R33 26 A33 25 D33	D37	-58.07121304	58.20595779	-58.24765478	-57.25985145	57.14092757	-56.68668311
H 32 R34 31 A34 26 D34	D38	61.62934423	-61.49987441	61.39862292	62.4290783	-62.51898163	63.19443825
H 32 R35 31 A35 26 D35	D39	-178.02359212	178.14492282	-178.23385164	-177.23863032	177.12265894	-176.76480793
C 32 R36 31 A36 26 D36							
H 36 R37 32 A37 31 D37							
H 36 R38 32 A38 31 D38							
H 36 R39 32 A39 31 D39							

6.2 Z-matrix for 3Upp PUFA structures

Table S6-4 Bond distance for 3U'' PUFA (Model 2)

Input Z-matrix 3U''		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Length							
0 1	R2	1.09681463	1.09675762	1.09673898	1.09671219	1.09673910	1.09561510
H	R3	1.53843337	1.53844483	1.53835072	1.53884439	1.53875414	1.53824507
C 1 R2	R4	1.50497259	1.50495482	1.50509609	1.50614801	1.50608430	1.50632420
C 2 R3 1 A3	R5	1.77097828	1.09602429	1.77106024	1.77143132	1.09603645	1.77375572
C 3 R4 2 A4 1 D4	R6	1.76972643	1.09571040	1.76963905	1.76907447	1.09564226	1.76897146
H 2 R5 1 A5 3 D5	R7	1.09747499	1.09749924	1.09760175	1.09551206	1.09552097	1.09609727
H 2 R6 1 A6 3 D6	R8	1.10057543	1.10060227	1.10045161	1.10039790	1.10045615	1.10108962
H 3 R7 2 A7 1 D7	R9	1.09312271	1.09311146	1.09291541	1.09192107	1.09193265	1.09187365
H 3 R8 2 A8 1 D8	R10	1.33570644	1.33572255	1.33568353	1.33878972	1.33879723	1.33857866
H 4 R9 3 A9 2 D9	R11	1.51085458	1.51084507	1.50516554	1.51254562	1.51253539	1.51274074
C 4 R10 3 A10 2 D10	R12	1.51069370	1.51065872	1.51433340	1.51221919	1.51220325	1.51158668
C 10 R11 4 A11 3 D11	R13	1.09172191	1.09173424	1.09182026	1.09053477	1.09047069	1.09101764
C 11 R12 10 A12 4 D12	R14	1.09960815	1.09962574	1.10075707	1.09725859	1.09739478	1.09329585
H 10 R13 4 A13 3 D13	R15	1.09970261	1.09979778	1.10233489	1.09727247	1.09719906	1.10369055
H 11 R14 10 A14 4 D14	R16	1.09178829	1.09178685	1.09197072	1.09050216	1.09050350	1.09130666
H 11 R15 10 A15 4 D15	R17	1.33563475	1.33564030	1.33533447	1.33866360	1.33863812	1.33855702
H 12 R16 11 A16 10 D16	R18	1.51071748	1.51073969	1.50489164	1.51240966	1.51250664	1.51337505
C 12 R17 11 A17 10 D17	R19	1.51068412	1.51071851	1.51422782	1.51215067	1.51227476	1.51298095
C 17 R18 12 A18 11 D18	R20	1.09176863	1.09177183	1.09021073	1.09054831	1.09047560	1.09071840
C 18 R19 17 A19 12 D19	R21	1.09961911	1.09966964	1.10081036	1.09735168	1.09738521	1.09318589
H 17 R20 12 A20 11 D20	R22	1.09967235	1.09962126	1.10249493	1.09743721	1.09709479	1.10250621
H 18 R21 17 A21 12 D21	R23	1.09176825	1.09174977	1.09197292	1.09057042	1.09047958	1.09098818
H 18 R22 17 A22 12 D22	R24	1.33564516	1.33565853	1.33536239	1.33863707	1.33866437	1.33789314
H 19 R23 18 A23 17 D23	R25	1.51067243	1.51071361	1.50500776	1.51234362	1.51231776	1.51446436
C 19 R24 18 A24 17 D24	R26	1.51089110	1.51090874	1.51447930	1.51254281	1.51217798	1.51855269
C 24 R25 19 A25 18 D25	R27	1.09179368	1.09178663	1.09011231	1.09054390	1.09047442	1.09025042
C 25 R26 24 A26 19 D26	R28	1.09970295	1.09972391	1.10094007	1.09717139	1.09742010	1.09462782
H 24 R27 19 A27 18 D27	R29	1.09962501	1.09959833	1.10253659	1.09734326	1.09732551	1.10010632
H 25 R28 24 A28 19 D28	R30	1.09171231	1.09171815	1.09209804	1.09051626	1.09051461	1.09007119
H 25 R29 24 A29 19 D29	R31	1.33580881	1.33582307	1.33556437	1.33878165	1.33884991	1.33876923
H 26 R30 25 A30 24 D30	R32	1.50461950	1.50463564	1.50478398	1.50560932	1.50564989	1.50473533
C 26 R31 25 A31 24 D31	R33	1.09299625	1.09300617	1.09121472	1.09179621	1.09180855	1.09183760
C 31 R32 26 A32 25 D32	R34	1.09831234	1.10143168	1.09861078	1.09638556	1.10132612	1.09501412
H 31 R33 26 A33 25 D33	R35	1.10152987	1.09833007	1.10164838	1.10128070	1.09632560	1.10072776
H 32 R34 31 A34 26 D34	R36	1.54074094	1.54074105	1.54061986	1.54137775	1.54142625	1.54229764
H 32 R35 31 A35 26 D35	R37	1.10008544	1.10010893	1.10009483	1.10003147	1.10001128	1.10036143
C 32 R36 31 A36 26 D36	R38	1.09892791	1.09904687	1.09900286	1.09897656	1.09899518	1.09850712
H 36 R37 32 A37 31 D37	R39	1.53384559	1.53364780	1.53388634	1.53387132	1.53362812	1.53368258
H 36 R38 32 A38 31 D38	R40	1.09945115	1.09952078	1.09943969	1.09944941	1.09951050	1.09858398
C 36 R39 32 A39 31 D39	R41	1.09930799	1.09935872	1.09948546	1.09944727	1.09944095	1.09962418
H 39 R40 36 A40 32 D40	R42	1.53210061	1.53205942	1.53206926	1.53197091	1.53206909	1.53211740
H 39 R41 36 A41 32 D41	R43	1.09695336	1.09604944	1.09608226	1.09701314	1.09700614	1.09721543
C 39 R42 36 A42 32 D42	R44	1.09702021	1.09697806	1.09704881	1.09694957	1.09605088	1.09707479
H 42 R43 39 A43 36 D43	R45	1.09614945	1.09701526	1.09698466	1.09601546	1.09695033	1.09630273
H 42 R44 39 A44 36 D44							
H 42 R45 39 A45 36 D45							

Table S6-5 Bond angle for 3U'' PUFA (Model 2)

Input Z-matrix 3U''		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angle							
0 1	A3	111.16207026	111.11727967	111.13832809	111.14789486	111.13294058	111.43549746
H	A4	112.84672846	112.79679761	112.78628551	112.46131667	112.43465593	112.73402123
C 1 R2	A5	36.12427017	107.74609917	36.11659611	36.09981289	107.76819973	35.97585599
C 2 R3 1 A3	A6	36.15897926	107.64615172	36.16114662	36.18259513	107.59239288	36.23677965
C 3 R4 2 A4 1 D4	A7	109.75467660	109.78722983	109.77270924	109.51021157	109.52121041	109.71285814
H 2 R5 1 A5 3 D5	A8	108.62307537	108.60061644	108.62968672	108.60554914	108.60251451	108.48395680
H 2 R6 1 A6 3 D6	A9	115.81245406	115.78174285	115.79116523	114.36208280	114.36402716	114.32107021
H 3 R7 2 A7 1 D7	A10	125.40846930	125.49959556	125.44587096	128.44042505	128.46945615	128.54160686
H 3 R8 2 A8 1 D8	A11	125.25960941	125.15468168	125.22768825	127.96749862	128.02574473	127.92181092
H 4 R9 3 A9 2 D9	A12	112.33924144	112.35654931	115.29343755	111.60580446	111.42027713	112.28762836
C 4 R10 3 A10 2 D10	A13	119.18245241	119.21500132	118.98232942	117.78192573	117.77563723	117.53279058
C 10 R11 4 A11 3 D11	A14	109.85105991	109.92546074	109.72846513	109.04041622	109.08414921	111.07602440
C 11 R12 10 A12 4 D12	A15	108.96184455	108.90406987	109.11025151	110.32095329	110.36613402	108.40521130
H 10 R13 4 A13 3 D13	A16	115.58390084	115.57838927	115.02013996	114.16604533	114.16021680	114.48013416
H 11 R14 10 A14 4 D14	A17	125.16904866	125.20940042	126.19614555	128.26057404	128.23766122	128.10008340
H 11 R15 10 A15 4 D15	A18	125.18013747	125.15095111	124.79862871	128.23363595	128.22106183	127.68334817
H 12 R16 11 A16 10 D16	A19	112.36899046	112.29348498	115.26026238	111.42287385	111.39824850	112.32585729
C 12 R17 11 A17 10 D17	A20	119.22453226	119.24555516	119.13645875	117.59623098	117.61182111	117.55471695
C 17 R18 12 A18 11 D18	A21	108.94779269	109.85968992	109.77911271	110.40803464	109.03846480	110.80211591
C 18 R19 17 A19 12 D19	A22	109.81395286	108.93052945	109.17855588	109.05856486	110.44863222	108.73594772
H 17 R20 12 A20 11 D20	A23	115.62291168	115.62087866	114.98584159	114.19923446	114.22462153	114.81054846
H 18 R21 17 A21 12 D21	A24	125.12828646	125.12598702	126.23750251	128.20251119	128.14599657	127.60620326
H 18 R22 17 A22 12 D22	A25	125.19937955	125.23337648	124.81592516	128.28279861	128.22459606	127.45922951
H 19 R23 18 A23 17 D23	A26	112.33998452	112.17746585	115.18733936	111.42106183	111.59033695	112.29540522
C 19 R24 18 A24 17 D24	A27	119.20823705	119.20240429	119.18685190	117.57145301	117.61920948	117.74814408
C 24 R25 19 A25 18 D25	A28	109.78422636	109.84206572	109.76337441	109.01427769	108.95734874	110.24796573
C 25 R26 24 A26 19 D26	A29	108.93331175	108.95942869	109.13049622	110.45707915	110.43374060	109.21679114
H 24 R27 19 A27 18 D27	A30	115.55676869	115.57788191	115.04080117	114.15531833	114.23278370	115.56026669
H 25 R28 24 A28 19 D28	A31	125.22500587	125.19612629	126.21757407	128.10551996	127.99006408	126.65798434
H 25 R29 24 A29 19 D29	A32	125.42236809	125.43357581	125.07650084	128.52427801	128.45293562	127.52879496
H 26 R30 25 A30 24 D30	A33	118.73330440	118.70706044	118.87587899	117.10457895	117.15020253	117.43382301
C 26 R31 25 A31 24 D31	A34	109.69577331	109.52863358	109.81911976	111.21132575	108.85388807	111.13055402
C 31 R32 26 A32 25 D32	A35	109.44167649	109.68224526	109.49821403	109.00181060	111.19923208	109.24453360
H 31 R33 26 A33 25 D33	A36	113.09782960	112.98116766	113.03130089	112.52874187	112.74937808	112.26795364
H 32 R34 31 A34 26 D34	A37	109.27217665	109.25822966	109.23387604	109.24261097	109.25758745	109.46849960
H 32 R35 31 A35 26 D35	A38	108.99293268	108.95982727	109.01291228	109.01223011	109.05067780	108.73145836
C 32 R36 31 A36 26 D36	A39	113.30543670	113.35703861	113.34224833	113.36426172	113.22756164	113.13623018
H 36 R37 32 A37 31 D37	A40	109.22445913	109.24930906	109.25251771	109.23429338	109.18847999	108.99915090
H 36 R38 32 A38 31 D38	A41	109.23136499	109.21045922	109.21914767	109.24241344	109.27042883	109.23127372
C 36 R39 32 A39 31 D39	A42	113.16579639	113.18798228	113.17631632	113.15781196	113.20255522	113.11601891
H 39 R40 36 A40 32 D40	A43	111.18801436	111.40951195	111.44582198	111.21187263	111.19525192	111.23598192
H 39 R41 36 A41 32 D41	A44	111.16733578	111.19496426	111.17172619	111.17273429	111.41035274	111.17918427
C 39 R42 36 A42 32 D42	A45	111.43191778	111.19079334	111.16419855	111.40678433	111.19663503	111.47031211
H 42 R43 39 A43 36 D43							
H 42 R44 39 A44 36 D44							
H 42 R45 39 A45 36 D45							

Table S6-6 Dihedral angle for 3U'' PUFA (Model 2)

Input Z-matrix 3U''		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedrals							
0 1	D4	58.29472721	58.17156571	58.16047875	57.06455456	57.31503702	-62.67135089
H	D5	121.93279290	-121.91160703	121.91124041	121.90870317	-121.91315044	-122.14549163
C 1 R2	D6	-121.64731581	121.64827100	-121.65295346	-121.66418270	121.66110091	121.86644294
C 2 R3 1 A3	D7	-179.14812224	-179.22889087	-179.26236765	-178.92584428	-178.70456103	61.65730308
C 3 R4 2 A4 1 D4	D8	-63.16813161	-63.24158509	-63.23300847	-63.40496828	-63.18421820	176.86776358
H 2 R5 1 A5 3 D5	D9	-60.05202839	-59.40579487	-60.03666359	-60.55058403	-59.90997832	-51.96849849
H 2 R6 1 A6 3 D6	D10	119.38816574	119.99570902	118.85764368	118.32492402	118.96483483	128.63017366
H 3 R7 2 A7 1 D7	D11	-179.16250554	-179.05586698	-178.56110519	1.36481784	1.53174885	0.05002755
H 3 R8 2 A8 1 D8	D12	118.25482020	118.41889156	-118.57066025	115.39046075	115.75557405	-136.89757594
H 4 R9 3 A9 2 D9	D13	-0.08271078	-0.01617471	1.34350819	179.91389041	179.95992972	179.29080969
C 4 R10 3 A10 2 D10	D14	-120.31823943	-120.09638369	5.15621273	-122.35885097	-122.05381175	-11.65534606
C 10 R11 4 A11 3 D11	D15	-3.65629495	-3.45821117	119.90509824	-5.94399798	-5.53769047	104.14068213
C 11 R12 10 A12 4 D12	D16	-61.32035322	-59.53456346	-167.34062828	-61.17836815	-62.33520156	-57.26615593
H 10 R13 4 A13 3 D13	D17	117.21916757	119.65719019	12.99236166	118.07335593	116.05867002	123.68029318
H 11 R14 10 A14 4 D14	D18	-179.83241120	-179.12333946	-179.63864718	-0.16956281	1.66315685	-1.19990554
H 11 R15 10 A15 4 D15	D19	-118.49629790	119.26648110	-118.21563648	-119.33383216	116.19022152	-138.06288605
H 12 R16 11 A16 10 D16	D20	1.44852663	0.00000000	0.55937797	-179.28971964	-179.95171665	178.62273810
C 12 R17 11 A17 10 D17	D21	3.48122300	-119.35272685	5.46276196	2.08000457	-121.70712906	-13.35469283
C 17 R18 12 A18 11 D18	D22	120.11660598	-2.70937942	120.23531740	118.55325588	-5.16784111	102.62123548
C 18 R19 17 A19 12 D19	D23	60.62622953	-60.11669542	-168.72333095	60.74738637	-64.99583807	-70.00491922
H 17 R20 12 A20 11 D20	D24	-118.06675987	118.92651500	11.65170882	-118.24267113	113.16827064	109.92062725
H 18 R21 17 A21 12 D21	D25	-179.95527098	-178.79794088	-179.65505311	-0.12589893	1.44869666	-1.80492057
H 18 R22 17 A22 12 D22	D26	117.74794483	118.69331994	-119.34577770	116.39168434	118.63780898	-137.33695144
H 19 R23 18 A23 17 D23	D27	-1.38729422	0.10148884	0.45831255	178.81676052	-179.70264220	179.02655009
C 19 R24 18 A24 17 D24	D28	-120.84264397	-119.99414915	4.43934509	-121.52118838	-119.28186774	-13.69817218
C 24 R25 19 A25 18 D25	D29	-4.22169323	-3.32579356	119.19928793	-5.04079230	-2.87828441	102.58325938
C 25 R26 24 A26 19 D26	D30	-61.12443128	-61.01531268	-167.80007180	-62.68161064	-63.42429382	-95.76430210
H 24 R27 19 A27 18 D27	D31	117.54706818	117.78086706	12.49543399	116.17704797	115.04987876	82.43984240
H 25 R28 24 A28 19 D28	D32	179.95949772	-178.45817836	179.20084880	-0.23538155	1.50593578	-0.71636515
H 25 R29 24 A29 19 D29	D33	1.07546046	0.61133430	0.31022581	-179.25941135	-179.62160425	-178.74670155
H 26 R30 25 A30 24 D30	D34	4.23923146	-120.55047640	4.06382937	4.61232964	-121.30805618	8.69212697
C 26 R31 25 A31 24 D31	D35	120.61442830	-4.11530216	120.49490346	121.30591384	-4.73824139	125.82029010
C 31 R32 26 A32 25 D32	D36	-118.40362488	118.43131784	-118.59174490	-118.39315032	118.41219994	-113.73802120
H 31 R33 26 A33 25 D33	D37	-55.98901346	56.42751758	-55.56789881	-55.06948850	54.59317236	-54.60592355
H 32 R34 31 A34 26 D34	D38	59.51364991	-59.04121161	59.88759538	60.35405804	-60.89261916	61.07645380
H 32 R35 31 A35 26 D35	D39	-178.12049950	178.59451108	-177.70425067	-177.26304607	176.71333660	-176.90082454
C 32 R36 31 A36 26 D36	D40	57.73039725	-57.77089241	-57.71934211	57.92209677	-57.98182701	-57.66896399
H 36 R37 32 A37 31 D37	D41	-57.82219688	57.77328393	57.82226769	-57.63827808	57.55423807	57.90871315
H 36 R38 32 A38 31 D38	D42	179.95580370	179.97838763	-179.93386261	-179.82546100	179.78078115	-179.92059113
C 36 R39 32 A39 31 D39	D43	59.91273696	179.98381508	179.94797450	-60.11989472	59.57428143	-60.00446357
H 39 R40 36 A40 32 D40	D44	-59.82098599	-59.89510348	-59.90462727	59.63253117	179.69875242	59.72429908
H 39 R41 36 A41 32 D41	D45	-179.94319026	59.86858697	59.79969757	179.75239767	-60.19213488	179.85888791
C 39 R42 36 A42 32 D42							
H 42 R43 39 A43 36 D43							
H 42 R44 39 A44 36 D44							
H 42 R45 39 A45 36 D45							

6.3 Z-matrix for 4Up PUFA structures

Table S6-7 Bond Lengths of 4Up (Model 1)

Input Z-matrix 4Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Lengths							
0 1	R2	1.09680448	1.09679475	1.09676411	1.09665043	1.09666190	1.09552194
H	R3	1.53844035	1.53836881	1.53841058	1.53890202	1.53884287	1.53786103
C 1 R2	R4	1.50499433	1.50502849	1.50490328	1.50599089	1.50616542	1.50666769
C 2 R3 1 A3	R5	1.77103332	1.77098463	1.77102365	1.77144475	1.77148428	1.77392529
C 3 R4 2 A4 1 D4	R6	1.76971831	1.76969761	1.76972382	1.76919258	1.76918407	1.76930286
H 1 R5 2 A5 3 D5	R7	1.09746460	1.09750279	1.09761891	1.09553045	1.09558173	1.09603113
H 1 R6 2 A6 3 D6	R8	1.10052371	1.10054538	1.10045820	1.10051266	1.10048869	1.10118348
H 3 R7 2 A7 1 D7	R9	1.09316104	1.09315196	1.09300507	1.09195825	1.09196776	1.09189954
H 3 R8 2 A8 1 D8	R10	1.33571365	1.33571168	1.33575641	1.33871292	1.33876931	1.33908466
H 4 R9 3 A9 2 D9	R11	1.51083183	1.51088450	1.50496558	1.51250816	1.51240940	1.51268911
C 4 R10 3 A10 2 D10	R12	1.51067736	1.51066307	1.51386602	1.51217852	1.51225145	1.51150263
C 10 R11 4 A11 3 D11	R13	1.09174247	1.09175113	1.09190641	1.09052110	1.09049443	1.09110046
C 11 R12 10 A12 4 D12	R14	1.09961939	1.09966281	1.10067203	1.09732028	1.09741760	1.09320507
H 10 R13 4 A13 3 D13	R15	1.09972709	1.09962553	1.10256886	1.09731641	1.09717507	1.10366536
H 11 R14 10 A14 4 D14	R16	1.09180093	1.09178026	1.09192862	1.09048635	1.09049397	1.09138797
H 11 R15 10 A15 4 D15	R17	1.33563948	1.33563506	1.33529010	1.33864130	1.33865862	1.33896493
H 12 R16 11 A16 10 D16	R18	1.51073427	1.51072502	1.50501850	1.51227714	1.51221785	1.51356245
C 12 R17 11 A17 10 D17	R19	1.51070547	1.51074358	1.51381690	1.51231521	1.51223533	1.51718580
C 17 R18 12 A18 11 D18	R20	1.09174749	1.09175409	1.09013460	1.09051939	1.09048301	1.09024519
C 18 R19 17 A19 12 D19	R21	1.09963351	1.09957788	1.10077160	1.09735233	1.09734231	1.09487046
H 17 R20 12 A20 11 D20	R22	1.09956771	1.09956258	1.10268596	1.09733481	1.09728068	1.10023247
H 18 R21 17 A21 12 D21	R23	1.09178661	1.09173474	1.09199096	1.09051125	1.09047831	1.08975825
H 18 R22 17 A22 12 D22	R24	1.33562697	1.33563928	1.33540786	1.33862557	1.33865305	1.33679763
H 19 R23 18 A23 17 D23	R25	1.51068340	1.51070803	1.50484854	1.51233719	1.51223659	1.51758955
C 19 R24 18 A24 17 D24	R26	1.51072499	1.51077148	1.51375124	1.51234532	1.51222685	1.50918478
C 24 R25 19 A25 18 D25	R27	1.09178539	1.09174712	1.09006749	1.09051898	1.09047631	1.09001445
C 25 R26 24 A26 19 D26	R28	1.09962451	1.09958281	1.10089897	1.09730631	1.09727615	1.09426699
H 24 R27 19 A27 18 D27	R29	1.09960250	1.09961330	1.10268932	1.09728813	1.09734395	1.10346787
H 25 R28 24 A28 19 D28	R30	1.09175934	1.09173502	1.09199446	1.09052860	1.09048214	1.09158535
H 25 R29 24 A29 19 D29	R31	1.33563394	1.33563303	1.33539626	1.33869780	1.33866453	1.33791845
H 26 R30 25 A30 24 D30	R32	1.51069063	1.51068964	1.50506643	1.51208047	1.51226468	1.51227058
C 26 R31 25 A31 24 D31	R33	1.51087888	1.51087472	1.51398407	1.51250105	1.51241188	1.51258804
C 31 R32 26 A32 25 D32	R34	1.09178665	1.09177159	1.09014918	1.09055494	1.09049081	1.09131959
C 32 R33 31 A33 26 D33	R35	1.09961559	1.09971067	1.10101778	1.09742096	1.09717374	1.09202383
H 31 R34 26 A34 25 D34	R36	1.09969224	1.09965675	1.10263106	1.09725813	1.09741002	1.10287892
H 32 R35 31 A35 26 D35	R37	1.09175635	1.09171746	1.09208397	1.09053294	1.09049201	1.09147868
H 32 R36 31 A36 26 D36	R38	1.33572115	1.33572353	1.33553666	1.33873791	1.33877153	1.33808331
H 33 R37 32 A37 31 D37	R39	1.50499116	1.50501755	1.50530757	1.50591566	1.50617370	1.50576018
C 33 R38 32 A38 31 D38	R40	1.53826853	1.53837287	1.53843591	1.53890441	1.53882684	1.53900942
C 38 R39 33 A39 32 D39	R41	1.09317409	1.09311547	1.09126293	1.09197204	1.09196778	1.09211524
C 39 R40 38 A40 33 D40	R42	1.09747428	1.10055528	1.10064830	1.10054542	1.10049592	1.10035927
H 38 R41 33 A41 32 D41	R43	1.10064647	1.09751625	1.09783328	1.09552616	1.09557926	1.09472211
H 39 R42 38 A42 33 D42	R44	1.09677841	1.09678764	1.09677335	1.09669167	1.09666291	1.09688393
H 39 R43 38 A43 33 D43	R45	1.09606000	1.09606292	1.09621137	1.09599811	1.09599839	1.09645247
H 40 R44 39 A44 38 D44	R46	1.09570233	1.09570077	1.09577596	1.09570675	1.09565632	1.09593871
H 40 R45 39 A45 38 D45							
H 40 R46 39 A46 38 D46							

Table 6-8 Bond Angles of 4Up (Model 1)

Input Z-matrix 4Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.14024184	111.15713072	111.15483187	111.09994634	111.10263810	111.39500677
H	A4	112.77617091	112.81814948	112.81073365	112.38970804	112.37469386	112.71340370
C 1 R2	A5	36.12163308	36.12253831	36.11918886	36.09637315	36.09453558	35.96570798
C 2 R3 1 A3	A6	36.15726229	36.15900649	36.15773135	36.17697571	36.17765997	36.22148048
C 3 R4 2 A4 1 D4	A7	109.77503127	109.76484377	109.75302749	109.51622459	109.51623791	109.72786932
H 1 R5 2 A5 3 D5	A8	108.62076987	108.62789080	108.61570092	108.57784787	108.58129184	108.50347657
H 1 R6 2 A6 3 D6	A9	115.78252756	115.79041132	115.75261224	114.30827561	114.32530770	114.35769904
H 3 R7 2 A7 1 D7	A10	125.46543308	125.43601536	125.49037169	128.53459275	128.52040974	128.53108828
H 3 R8 2 A8 1 D8	A11	125.19752694	125.26165710	125.14535584	128.05147487	128.02497519	127.92729797
H 4 R9 3 A9 2 D9	A12	112.34301610	112.28736117	115.41231519	111.45137383	111.44597466	112.19517281
C 4 R10 3 A10 2 D10	A13	119.20816294	119.19985251	118.98355492	117.74570070	117.75783151	117.51766996
C 10 R11 4 A11 3 D11	A14	109.91079824	109.87130079	109.69929192	109.04778662	109.09610040	111.03246439
C 11 R12 10 A12 4 D12	A15	108.93230974	108.97806196	109.15239325	110.37500025	110.32816008	108.33331906
H 10 R13 4 A13 3 D13	A16	115.56674037	115.60246103	114.95548678	114.13916659	114.16222402	114.44399171
H 11 R14 10 A14 4 D14	A17	125.20061966	125.16251679	126.30071245	128.27920529	128.21985862	128.20946549
H 11 R15 10 A15 4 D15	A18	125.13384831	125.18094656	124.75877767	128.22472572	128.15579739	127.84252473
H 12 R16 11 A16 10 D16	A19	112.34576268	112.28114377	115.24943635	111.45139341	111.45053090	112.37570592
C 12 R17 11 A17 10 D17	A20	119.23960951	119.22749668	119.19941679	117.59366491	117.62269232	117.55216707
C 17 R18 12 A18 11 D18	A21	108.94175248	109.85528820	109.78743493	110.42150351	109.07214640	110.49097230
C 18 R19 17 A19 12 D19	A22	109.83967454	108.96115779	109.19439953	109.07964031	110.39215444	108.90109437
H 17 R20 12 A20 11 D20	A23	115.57536096	115.59841909	115.00245340	114.17915482	114.19470030	116.09650512
H 18 R21 17 A21 12 D21	A24	125.18443267	125.16659778	126.24359797	128.23638308	128.16382452	125.68899441
H 18 R22 17 A22 12 D22	A25	125.14900407	125.15516687	124.78674251	128.23713483	128.16454398	125.78552691
H 19 R23 18 A23 17 D23	A26	112.37136392	112.33325781	115.32302513	111.45196200	111.45065666	112.51267266
C 19 R24 18 A24 17 D24	A27	119.23929585	119.23120241	119.21694941	117.58485122	117.62508952	118.28933881
C 24 R25 19 A25 18 D25	A28	109.81619201	109.83204779	109.82325882	109.06269834	109.05217170	110.00587136
C 25 R26 24 A26 19 D26	A29	108.93795615	108.93816114	109.11984215	110.42292388	110.42273303	108.92489139
H 24 R27 19 A27 18 D27	A30	115.60310070	115.61958136	114.97555905	114.20385119	114.20513180	114.45640856
H 25 R28 24 A28 19 D28	A31	125.14862964	125.14643986	126.30754883	128.17641508	128.15531884	128.22056069
H 25 R29 24 A29 19 D29	A32	125.17836451	125.18473254	124.74988147	128.23276940	128.21874370	128.25458243
H 26 R30 25 A30 24 D30	A33	112.33570072	112.31974964	115.30909682	111.50596449	111.44529094	111.48065244
C 26 R31 25 A31 24 D31	A34	119.22022576	119.21282102	119.24010263	117.57906288	117.60199624	117.26982962
C 31 R32 26 A32 25 D32	A35	108.94342082	109.81176355	109.75188705	110.40293574	109.03383542	111.30955719
C 32 R33 31 A33 26 D33	A36	109.78780756	108.93650995	109.09107598	109.06824950	110.44785520	108.37179457
H 31 R34 26 A34 25 D34	A37	115.56149387	115.59476129	115.00488193	114.17572208	114.20089349	114.46203306
H 32 R35 31 A35 26 D35	A38	125.22614191	125.19696296	126.34957360	128.06176154	128.02485407	128.00058935
H 32 R36 31 A36 26 D36	A39	125.45169497	125.45581470	124.99317281	128.54100747	128.52066579	128.36521025
H 33 R37 32 A37 31 D37	A40	112.86071540	112.80148453	112.83944743	112.37369240	112.37365772	112.43371434
C 33 R38 32 A38 31 D38	A41	118.76266754	118.74566388	119.01413598	117.15068029	117.14528432	117.15411512
C 38 R39 33 A39 32 D39	A42	109.61974387	109.38910359	109.37894957	108.88314397	108.84865792	108.61415573
C 39 R40 38 A40 33 D40	A43	109.33940735	109.61958699	109.71696843	111.12321643	111.12496075	111.32430086
H 38 R41 33 A41 32 D41	A44	111.15572904	111.15076844	111.11229845	111.13617002	111.10403077	111.26914116
H 39 R42 38 A42 33 D42	A45	111.07963072	111.08349597	111.14932016	111.06547386	111.06381425	111.08082025
H 39 R43 38 A43 33 D43	A46	110.93930844	110.91389981	110.89909438	110.97344531	110.96617848	110.93588947
H 40 R44 39 A44 38 D44							
H 40 R45 39 A45 38 D45							
H 40 R46 39 A46 38 D46							

Table S6-9 Dihedral Angles of 4Up (Model 1)

Input Z-matrix 4Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	58.23008477	58.25970924	58.26976220	57.13042732	57.18567250	-62.23818662
H	D5	121.93675398	121.91992459	121.90350181	121.89813726	121.89591939	-122.17934773
C 1 R2	D6	-121.63032790	-121.65212492	-121.66936679	-121.66741847	-121.65993250	121.84000841
C 2 R3 1 A3	D7	-179.22239142	-179.18626780	-179.12061156	-178.82270066	-178.79803786	62.02086484
C 3 R4 2 A4 1 D4	D8	-63.21396011	-63.19480494	-63.11956324	-63.31200497	-63.27467262	177.28469346
H 1 R5 2 A5 3 D5	D9	-60.08885624	-60.09765328	-60.23528284	-58.82353651	-59.18043336	-49.10086608
H 1 R6 2 A6 3 D6	D10	119.22768063	119.26849011	118.67638286	120.14096547	119.64734022	131.83352324
H 3 R7 2 A7 1 D7	D11	-178.91368839	-179.03378400	-178.59604904	1.45772185	1.64161581	-0.03566050
H 3 R8 2 A8 1 D8	D12	117.82180705	118.39479317	-118.69719137	115.66153678	116.11136537	-136.38674514
H 4 R9 3 A9 2 D9	D13	0.03571242	0.00912025	1.22520079	179.91521516	-179.93666506	178.92557214
C 4 R10 3 A10 2 D10	D14	-120.69061808	-120.21430721	4.97676823	-122.13656516	-121.66486367	-11.18433100
C 10 R11 4 A11 3 D11	D15	-4.02139234	-3.53364129	119.68405791	-5.65681700	-5.16492417	104.58871884
C 11 R12 10 A12 4 D12	D16	-60.50307292	-61.36063641	-169.68291351	-61.03173351	-61.69269703	-56.05579400
H 10 R13 4 A13 3 D13	D17	118.18062767	117.57783836	10.60045409	118.03817096	116.79813464	124.67589313
H 11 R14 10 A14 4 D14	D18	179.95928172	-178.85848990	-179.52717853	0.01339595	1.60695549	-1.12511893
H 11 R15 10 A15 4 D15	D19	-117.51445707	117.94639298	-119.99012549	-117.90685088	116.16157850	-132.87337111
H 12 R16 11 A16 10 D16	D20	1.35698646	0.14832089	0.52776091	-179.05476180	-179.97824979	179.01608017
C 12 R17 11 A17 10 D17	D21	4.37189406	-120.64524070	3.76506695	3.46842354	-121.66472179	-9.13015207
C 17 R18 12 A18 11 D18	D22	121.03882453	-3.96124951	118.53997050	119.91095063	-5.18974950	106.97438655
C 18 R19 17 A19 12 D19	D23	60.70856511	-61.14591756	-169.27556852	61.33314660	-62.13051311	-91.07033102
H 17 R20 12 A20 11 D20	D24	-117.99606506	117.89976642	10.83565729	-117.73304336	116.35072157	87.88350574
H 18 R21 17 A21 12 D21	D25	-179.98649108	-179.03117181	-179.13720683	0.02297186	1.57892630	-0.21761730
H 18 R22 17 A22 12 D22	D26	117.86753280	118.17201900	-120.40399364	118.02325732	116.35866021	-161.26123840
H 19 R23 18 A23 17 D23	D27	-1.33962476	0.05806214	0.63803221	179.04942403	-179.97987447	179.88227390
C 19 R24 18 A24 17 D24	D28	-120.69796074	-120.41637375	3.45896003	-119.85393893	-121.51830693	-36.82215164
C 24 R25 19 A25 18 D25	D29	-4.05697249	-3.77534144	118.18446038	-3.39512192	-5.03744830	78.82119832
C 25 R26 24 A26 19 D26	D30	-60.77198569	-60.69294281	-168.67790764	-61.73123786	-62.30891829	-62.62286574
H 24 R27 19 A27 18 D27	D31	117.96607141	118.41568127	11.46681212	117.27710616	116.14645119	116.88951734
H 25 R28 24 A28 19 D28	D32	179.88726492	-179.03810400	-179.16510809	0.03020325	1.61687553	-0.67929900
H 25 R29 24 A29 19 D29	D33	-117.70042139	118.38024401	-119.94445322	-117.76489168	116.79787193	-127.89634343
H 26 R30 25 A30 24 D30	D34	1.33470616	-0.00359866	0.67863794	-178.99011235	-179.94342804	-179.97494435
C 26 R31 25 A31 24 D31	D35	4.26794924	-120.23441771	3.91740651	3.65572699	-121.17267728	-2.89545761
C 31 R32 26 A32 25 D32	D36	120.90042514	-3.63108030	118.61223840	120.10288919	-4.64081882	113.33925193
C 32 R33 31 A33 26 D33	D37	61.03073907	-60.74105773	-167.99243816	60.77128890	-62.37075249	-61.04699330
H 31 R34 26 A34 25 D34	D38	-117.66976436	118.27455284	12.65841790	-118.32482917	116.09190234	118.20222104
H 32 R35 31 A35 26 D35	D39	179.90509192	-178.94614830	-179.88644204	0.02191788	1.65716345	0.63206190
H 32 R36 31 A36 26 D36	D40	119.38362035	119.11609282	119.17686742	121.26161042	119.63810799	116.46012102
H 33 R37 32 A37 31 D37	D41	-1.09372893	0.35251457	-0.37946733	179.46933770	-179.55195024	179.65906433
C 33 R38 32 A38 31 D38	D42	-3.30845857	-119.87059272	-119.85477630	-118.39601590	-120.05374916	-123.36062709
C 38 R39 33 A39 32 D39	D43	-119.61161666	-3.52298632	-3.48939445	-1.81202120	-3.47884456	-6.90330641
C 39 R40 38 A40 33 D40	D44	58.08374156	58.14267502	58.10017749	57.42876801	57.18659977	56.92244409
H 38 R41 33 A41 32 D41	D45	178.02325622	178.08716047	178.09145855	177.39908480	177.15330401	176.90096332
H 39 R42 38 A42 33 D42	D46	-61.63878281	-61.57873534	-61.53811017	-62.25479337	-62.48977121	-62.76084868
H 39 R43 38 A43 33 D43							
H 40 R44 39 A44 38 D44							
H 40 R45 39 A45 38 D45							
H 40 R46 39 A46 38 D46							

6.4 Z-matrix for 4Upp PUFA structures

Table S6-10 Bond Lengths of 4Upp (Model 2)

Input Z-matrix 4Upp		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Lengths							
0 1	R2	1.09681790	1.09678962	1.09570370	1.09568592	1.09667331	1.09546822
H	R3	1.53843211	1.53839109	1.53834833	1.53880519	1.53884372	1.53732992
C 1 R2	R4	1.50497261	1.50501185	1.50483447	1.50613461	1.50610334	1.50694186
C 2 R3 1 A3	R5	1.77100392	1.77110396	1.77508613	1.77495374	1.77143909	1.77253514
C 3 R4 2 A4 1 D4	R6	1.76969655	1.76974547	1.76949537	1.76901729	1.76920696	1.77007816
H 1 R5 2 A5 3 D5	R7	1.09747329	1.09751441	1.10057182	1.10051503	1.09550937	1.09630911
H 1 R6 2 A6 3 D6	R8	1.10055360	1.10054718	1.09757086	1.09543563	1.10050993	1.10138778
H 3 R7 2 A7 1 D7	R9	1.09313339	1.09314147	1.09300619	1.09195551	1.09195005	1.09179492
H 3 R8 2 A8 1 D8	R10	1.33573547	1.33570741	1.33580277	1.33874925	1.33877818	1.33933697
H 4 R9 3 A9 2 D9	R11	1.51083687	1.51085560	1.50495157	1.51261298	1.51242033	1.51496887
C 4 R10 3 A10 2 D10	R12	1.51063182	1.51067800	1.51393795	1.51222015	1.51223678	1.51063913
C 10 R11 4 A11 3 D11	R13	1.09173084	1.09174674	1.09190009	1.09051398	1.09050724	1.09080561
C 11 R12 10 A12 4 D12	R14	1.09963119	1.09962378	1.10071580	1.09742508	1.09739108	1.09380933
H 10 R13 4 A13 3 D13	R15	1.09971026	1.09970369	1.10249362	1.09715362	1.09718167	1.10342274
H 11 R14 10 A14 4 D14	R16	1.09181100	1.09178136	1.09195344	1.09052151	1.09048963	1.09148274
H 11 R15 10 A15 4 D15	R17	1.33565337	1.33560872	1.33531616	1.33870629	1.33867527	1.33853746
H 12 R16 11 A16 10 D16	R18	1.51069425	1.51078548	1.50492963	1.51220847	1.51228844	1.51336935
C 12 R17 11 A17 10 D17	R19	1.51071486	1.51076105	1.51370245	1.51222601	1.51226384	1.51515340
C 17 R18 12 A18 11 D18	R20	1.09175845	1.09175717	1.09008604	1.09054282	1.09048103	1.09046059
C 18 R19 17 A19 12 D19	R21	1.09961705	1.09957371	1.10080839	1.09733712	1.09735564	1.09440746
H 17 R20 12 A20 11 D20	R22	1.09957594	1.09956295	1.10272998	1.09738099	1.09730009	1.10037242
H 18 R21 17 A21 12 D21	R23	1.09177123	1.09173194	1.09199484	1.09054281	1.09047961	1.08995465
H 18 R22 17 A22 12 D22	R24	1.33565833	1.33564143	1.33538269	1.33856341	1.33864933	1.33763446
H 19 R23 18 A23 17 D23	R25	1.51069746	1.51080472	1.50492814	1.51232164	1.51221816	1.51948647
C 19 R24 18 A24 17 D24	R26	1.51068902	1.51080011	1.51370036	1.51218020	1.51224233	1.50758482
C 24 R25 19 A25 18 D25	R27	1.09177251	1.09173452	1.09005247	1.09053785	1.09048902	1.08951751
C 25 R26 24 A26 19 D26	R28	1.09962265	1.09951052	1.10085189	1.09743358	1.09740050	1.09633867
H 24 R27 19 A27 18 D27	R29	1.09961297	1.09951151	1.10273913	1.09735506	1.09729323	1.10106963
H 25 R28 24 A28 19 D28	R30	1.09176812	1.09174420	1.09197131	1.09054397	1.09048397	1.09128799
H 25 R29 24 A29 19 D29	R31	1.33565669	1.33564868	1.33544035	1.33868646	1.33868438	1.33848253
H 26 R30 25 A30 24 D30	R32	1.51063163	1.51072457	1.50500333	1.51203521	1.51215839	1.51306999
C 26 R31 25 A31 24 D31	R33	1.51083720	1.51093536	1.51381347	1.51257414	1.51238842	1.51291455
C 31 R32 26 A32 25 D32	R34	1.09180238	1.09177478	1.09005409	1.09052954	1.09050454	1.09115429
C 32 R33 31 A33 26 D33	R35	1.09963443	1.09954411	1.10100416	1.09754449	1.09726133	1.09213124
H 31 R34 26 A34 25 D34	R36	1.09966680	1.09959727	1.10274185	1.09719464	1.09741832	1.10204196
H 32 R35 31 A35 26 D35	R37	1.09173546	1.09175784	1.09208644	1.09053288	1.09050647	1.09118610
H 32 R36 31 A36 26 D36	R38	1.33581191	1.33580851	1.33560994	1.33881674	1.33885355	1.33831579
H 33 R37 32 A37 31 D37	R39	1.50441400	1.50445968	1.50485590	1.50543489	1.50561373	1.50565426
C 33 R38 32 A38 31 D38	R40	1.54112588	1.54110215	1.54083702	1.54149548	1.54156252	1.54199449
C 38 R39 33 A39 32 D39	R41	1.53161277	1.53159171	1.53177129	1.53162224	1.53168748	1.53155718
C 39 R40 38 A40 33 D40	R42	1.09304002	1.09302998	1.09115135	1.09184050	1.09181285	1.09189467
C 40 R41 39 A41 38 D41	R43	1.10159003	1.10154443	1.09878149	1.10148963	1.10136910	1.09608956
H 38 R42 33 A42 32 D42	R44	1.09842692	1.09840477	1.10177177	1.09644418	1.09643417	1.10146061
H 39 R43 38 A43 33 D43	R45	1.09797754	1.09911026	1.09802968	1.09900772	1.09896700	1.09917757
H 39 R44 38 A44 33 D44	R46	1.09914037	1.09801542	1.09903249	1.09800626	1.09795628	1.09756636
H 40 R45 39 A45 38 D45	R47	1.09592573	1.09595527	1.09716324	1.09592713	1.09593446	1.09628133
H 40 R46 39 A46 38 D46	R48	1.09697517	1.09713528	1.09599137	1.09709174	1.09712950	1.09655738
H 41 R47 40 A47 39 D47	R49	1.09709101	1.09699198	1.09705131	1.09703904	1.09705091	1.09744209
H 41 R48 40 A48 39 D48							
H 41 R49 40 A49 39 D49							

Table S6-11 Bond Angles of 4Upp (Model 2)

Input Z-matrix 4Upp		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.14458575	111.14719218	110.91263142	110.95614030	111.10469548	111.54667329
H	A4	112.81104282	112.82367715	112.82728515	112.33853103	112.37364090	113.08554813
C 1 R2	A5	36.12273353	36.11548098	35.91915405	35.92440713	36.09707121	36.02645871
C 2 R3 1 A3	A6	36.16022861	36.15701221	36.20615233	36.22364679	36.17702040	36.18900188
C 3 R4 2 A4 1 D4	A7	109.77265252	109.76688185	108.62657890	108.60548258	109.51212860	109.77409462
H 1 R5 2 A5 3 D5	A8	108.61838558	108.61811860	109.78692435	109.53699320	108.57933541	108.46718744
H 1 R6 2 A6 3 D6	A9	115.79285410	115.79396030	115.78593241	114.33729433	114.31538797	114.56346368
H 3 R7 2 A7 1 D7	A10	125.44309499	125.46098309	125.46536992	128.53701621	128.54086918	128.15351453
H 3 R8 2 A8 1 D8	A11	125.21819365	125.20557985	125.18888627	128.06924779	128.04829443	127.47869886
H 4 R9 3 A9 2 D9	A12	112.36279398	112.33729210	115.38659090	111.47340228	111.43365445	112.40829588
C 4 R10 3 A10 2 D10	A13	119.19722847	119.20616944	118.98525187	117.75101690	117.75236380	117.63612581
C 10 R11 4 A11 3 D11	A14	109.89934546	109.89996782	109.72460220	109.09895233	109.09016374	110.76294625
C 11 R12 10 A12 4 D12	A15	108.93880970	108.94338384	109.14955786	110.35129778	110.35008573	108.49004952
H 10 R13 4 A13 3 D13	A16	115.59547460	115.57520034	114.96832987	114.18020058	114.16648999	114.33346997
H 11 R14 10 A14 4 D14	A17	125.16968187	125.21156940	126.30335846	128.23355960	128.22464351	128.44145817
H 11 R15 10 A15 4 D15	A18	125.14660378	125.15073397	124.72779384	128.16381514	128.16149363	128.06104497
H 12 R16 11 A16 10 D16	A19	112.35850530	112.33687844	115.32671062	111.49479949	111.39326826	111.34892917
C 12 R17 11 A17 10 D17	A20	119.22793341	119.25102238	119.20827784	117.61232788	117.62351352	117.43025392
C 17 R18 12 A18 11 D18	A21	108.93459807	109.82545738	109.78236467	110.37688530	109.06753115	110.58989635
C 18 R19 17 A19 12 D19	A22	109.83639283	108.94639859	109.19354444	109.11285128	110.40250113	108.92705329
H 17 R20 12 A20 11 D20	A23	115.58760445	115.61709069	114.95229041	114.15686307	114.17495945	115.98817859
H 18 R21 17 A21 12 D21	A24	125.17082267	125.12854157	126.32605458	128.27524964	128.20943327	125.66299241
H 18 R22 17 A22 12 D22	A25	125.14954149	125.21248021	124.72235671	128.28780207	128.20673673	125.70176508
H 19 R23 18 A23 17 D23	A26	112.33847012	112.20263217	115.32918192	111.47020714	111.41105319	112.67575298
C 19 R24 18 A24 17 D24	A27	119.23517692	119.22465954	119.24884333	117.56946934	117.60080508	118.33439119
C 24 R25 19 A25 18 D25	A28	109.84681316	109.82697065	109.79132624	109.00162746	109.05071935	109.50236103
C 25 R26 24 A26 19 D26	A29	108.93471348	108.98676799	109.16038636	110.45546254	110.42448339	109.25007451
H 24 R27 19 A27 18 D27	A30	115.60265263	115.57219061	114.96524116	114.21328373	114.20378055	114.71314619
H 25 R28 24 A28 19 D28	A31	125.16436524	125.19128770	126.33493637	128.17418467	128.15274504	127.76847750
H 25 R29 24 A29 19 D29	A32	125.14919974	125.16770811	124.71918120	128.24226122	128.21104014	127.91042721
H 26 R30 25 A30 24 D30	A33	112.38559527	112.20958985	115.38030156	111.43440244	111.47265016	111.35216949
C 26 R31 25 A31 24 D31	A34	119.22747770	119.23341451	119.25559867	117.58130976	117.59428754	117.43250758
C 31 R32 26 A32 25 D32	A35	108.91403096	109.85575815	109.74725825	110.44287940	109.06172948	111.12761915
C 32 R33 31 A33 26 D33	A36	109.79803206	108.93750222	109.06487157	109.08606160	110.41059964	108.25217641
H 31 R34 26 A34 25 D34	A37	115.54145116	115.48750689	114.96632573	114.15263607	114.20680786	114.58718135
H 32 R35 31 A35 26 D35	A38	125.25471673	125.31016052	126.41230814	128.09984911	128.01790765	127.76863408
H 32 R36 31 A36 26 D36	A39	125.40296307	125.37665434	124.90424242	128.52543729	128.48484223	128.42594283
H 33 R37 32 A37 31 D37	A40	113.20243442	113.13959459	113.18384804	112.74274985	112.64838948	112.63436452
C 33 R38 32 A38 31 D38	A41	112.91864977	112.93886890	112.94914020	112.92116491	112.93644258	112.81996680
C 38 R39 33 A39 32 D39	A42	118.73961760	118.75458426	119.01258691	117.07446390	117.11241601	117.11234225
C 39 R40 38 A40 33 D40	A43	109.45897604	109.52843555	109.78674065	108.93809152	108.98017453	111.33351009
C 40 R41 39 A41 38 D41	A44	109.71534762	109.71726966	109.54104551	111.22972061	111.24189676	108.92672210
H 38 R42 33 A42 32 D42	A45	108.92129921	109.19341317	108.92604785	109.13992003	109.15453309	109.18694395
H 39 R43 38 A43 33 D43	A46	109.18520714	108.88672906	109.17327011	108.98083071	108.93697022	108.86657903
H 39 R44 38 A44 33 D44	A47	111.35801659	111.36518664	111.21490906	111.34510676	111.35942767	111.26619780
H 40 R45 39 A45 38 D45	A48	111.19186601	111.22719038	111.38830793	111.18201138	111.19021126	110.90190728
H 40 R46 39 A46 38 D46	A49	111.19400505	111.18892509	111.16849109	111.26094218	111.23042806	111.28783690
H 41 R47 40 A47 39 D47							
H 41 R48 40 A48 39 D48							
H 41 R49 40 A49 39 D49							

Table S6-12 Dihedral Lengths of 4Upp (Model 2)

Input Z-matrix 4Upp		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	58.20463128	58.14724781	61.36003253	62.48614620	57.20126038	-63.1966683
H	D5	121.93819803	121.90241887	122.05194034	122.09149172	121.89701196	-122.0943505
C 1 R2	D6	-121.64291456	121.65604819	-121.78776404	-121.71562977	-121.66730051	121.9777491
C 2 R3 1 A3	D7	-179.23387781	179.28132516	-177.22695479	-177.01866443	-178.79119760	61.1964361
C 3 R4 2 A4 1 D4	D8	-63.23440295	-63.28949675	-61.24178584	-61.47158473	-63.26669212	176.3204781
H 1 R5 2 A5 3 D5	D9	-59.81969745	-60.14574148	59.80809930	58.72820395	-58.96809327	-47.2374434
H 1 R6 2 A6 3 D6	D10	119.58772718	119.24123652	-119.66363143	-120.66859214	119.86626804	134.4845887
H 3 R7 2 A7 1 D7	D11	-179.07282708	179.04074616	-179.49475908	-0.06643937	1.65477502	-0.3727593
H 3 R8 2 A8 1 D8	D12	118.26015608	118.03407441	-118.94632922	117.85649538	116.23745503	-146.8320689
H 4 R9 3 A9 2 D9	D13	-0.03212925	-0.01779097	0.02701419	178.95836559	-179.92513738	177.9468121
C 4 R10 3 A10 2 D10	D14	-120.28251124	120.48801509	4.76283563	-119.93448267	-121.57018546	-21.6458389
C 10 R11 4 A11 3 D11	D15	-3.63309968	-3.84144714	119.47786278	-3.51829625	-5.05456068	93.9892580
C 11 R12 10 A12 4 D12	D16	-60.52400586	-60.75794072	-168.79820079	-62.02022791	-61.49763706	-60.6936371
H 10 R13 4 A13 3 D13	D17	118.15576607	118.34721741	11.51544039	116.96291571	116.98902947	119.7814288
H 11 R14 10 A14 4 D14	D18	-179.98636526	179.11809914	-179.49810832	-0.06833139	1.66199149	-1.7361651
H 11 R15 10 A15 4 D15	D19	-117.79854757	118.20603543	-119.82092208	-117.49560182	116.20984790	-124.0228440
H 12 R16 11 A16 10 D16	D20	1.35322260	0.00000000	0.50135421	-178.99012497	-179.97072488	179.4485361
C 12 R17 11 A17 10 D17	D21	4.11300186	120.40166746	3.90487410	3.77637384	-121.61709719	-0.7870575
C 17 R18 12 A18 11 D18	D22	120.75871671	-3.74011769	118.66321459	120.24708531	-5.11224952	115.9325374
C 18 R19 17 A19 12 D19	D23	60.81520187	-61.27906590	-169.78437249	60.39587047	-62.08389086	-82.6686941
H 17 R20 12 A20 11 D20	D24	-117.90378619	117.76445215	10.37920541	-118.89019314	116.29674635	94.7005206
H 18 R21 17 A21 12 D21	D25	-179.94401331	178.91112296	-179.28952546	0.04749000	1.68316781	0.5983006
H 18 R22 17 A22 12 D22	D26	118.02436667	117.57736060	-120.49330128	119.50243100	117.34645601	170.8563650
H 19 R23 18 A23 17 D23	D27	-1.31807870	0.04771319	0.56613507	179.30078741	-179.83403646	-178.0423547
C 19 R24 18 A24 17 D24	D28	-120.55170181	121.05639560	3.32738264	-118.38195879	-120.53690924	-65.1838999
C 24 R25 19 A25 18 D25	D29	-3.90628221	-4.34475204	118.07235737	-1.94191000	-4.05808402	49.8244958
C 25 R26 24 A26 19 D26	D30	-60.37281060	-61.63180971	-169.26991047	-61.70432567	-62.11101349	-63.5086836
H 24 R27 19 A27 18 D27	D31	118.36325261	117.26153932	10.81871925	117.25172921	116.26329909	115.0944770
H 25 R28 24 A28 19 D28	D32	179.94144816	178.61293886	-179.03144255	0.00653312	1.70032082	-0.1027406
H 25 R29 24 A29 19 D29	D33	-117.46753907	116.97502016	-120.51457097	-117.29094107	117.77024306	-114.0191695
H 26 R30 25 A30 24 D30	D34	1.36291973	0.15725000	0.68566244	-178.91034714	-179.77860171	-178.4767141
C 26 R31 25 A31 24 D31	D35	4.48886255	121.58790050	3.39556925	4.14382070	-120.15635359	10.3605104
C 31 R32 26 A32 25 D32	D36	121.07997924	-4.90112103	118.04961684	120.61359845	-3.64220024	126.6869297
C 32 R33 31 A33 26 D33	D37	60.92410084	-61.22176958	-168.40746289	60.03095964	-61.57202860	-57.8972374
H 31 R34 26 A34 25 D34	D38	-118.27225607	117.77883810	11.76705598	-119.13669216	116.99032374	121.2422142
H 32 R35 31 A35 26 D35	D39	179.24208874	178.87102370	179.44077121	-0.01507614	1.74260584	-0.2876284
H 32 R36 31 A36 26 D36	D40	-119.08279447	118.48420275	-119.07709023	120.02259504	118.11198533	-115.8450704
H 33 R37 32 A37 31 D37	D41	-177.99877759	178.42064047	-178.53095465	176.98433130	177.04732394	-176.8418196
C 33 R38 32 A38 31 D38	D42	-0.25367074	0.42714222	0.41998172	179.51558348	-179.61368657	-179.0834897
C 38 R39 33 A39 32 D39	D43	119.93712603	120.51488884	3.55679635	-119.70954008	-121.62519030	7.1238515
C 39 R40 38 A40 33 D40	D44	3.56074510	-4.09260579	119.96030324	-3.10576127	-4.93118165	123.8510700
C 40 R41 39 A41 38 D41	D45	59.63206254	56.24789007	59.11462039	54.86412585	54.88642200	-54.5441949
H 38 R42 33 A42 32 D42	D46	-55.86557636	-59.22954431	-56.34716397	-60.58492020	-60.55666466	61.2011924
H 39 R43 38 A43 33 D43	D47	-179.93089304	179.87784650	59.80945481	-179.74264172	179.99273499	178.8915306
H 39 R44 38 A44 33 D44	D48	-59.83564471	-59.98487190	179.97335003	-59.63031015	-59.88622073	-61.2724917
H 40 R45 39 A45 38 D45	D49	59.93702764	59.79560413	-59.94022566	60.17338369	59.90307215	58.8248048
H 40 R46 39 A46 38 D46							
H 41 R47 40 A47 39 D47							
H 41 R48 40 A48 39 D48							
H 41 R49 40 A49 39 D49							

6.5 Z-matrix for 5Up PUFA structures

Table S6-13 Bond Lengths of 5Up (Model 1)

Input Z-matrix 5Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Length							
0 1	R2	1.09679536	1.09674693	1.09675089	1.09665740	1.09670173	1.09691906
H	R3	1.53843703	1.53841922	1.53854206	1.53896306	1.53889630	1.53810444
C 1 R2	R4	1.50499068	1.50505431	1.50498701	1.50593431	1.50598954	1.50658717
C 2 R3 1 A3	R5	1.77151150	1.77113775	1.77103895	1.77146792	1.09602682	1.76999694
C 3 R4 2 A4 1 D4	R6	1.76903233	1.76968256	1.76969365	1.76914831	1.09565854	1.76957379
H 1 R5 2 A5 3 D5	R7	1.09750992	1.09745355	1.09756988	1.09554495	1.09550720	1.09597389
H 1 R6 2 A6 3 D6	R8	1.10050183	1.10054185	1.10040107	1.10045033	1.10041699	1.10108401
H 3 R7 2 A7 1 D7	R9	1.09311830	1.09312397	1.09296016	1.09191764	1.09192528	1.09195056
H 3 R8 2 A8 1 D8	R10	1.33572066	1.33573122	1.33573979	1.33870976	1.33876398	1.33895500
H 4 R9 3 A9 2 D9	R11	1.51085847	1.51096636	1.50500605	1.51260118	1.51268550	1.51225071
C 4 R10 3 A10 2 D10	R12	1.51069972	1.51068221	1.51403795	1.51223239	1.51226816	1.51164147
C 10 R11 4 A11 3 D11	R13	1.09170742	1.09171180	1.09188486	1.09051524	1.09047598	1.09110349
C 11 R12 10 A12 4 D12	R14	1.09956634	1.09962199	1.10246333	1.09725059	1.09728012	1.09322757
H 10 R13 4 A13 3 D13	R15	1.09976876	1.09961359	1.10068984	1.09727159	1.09711111	1.10387024
H 11 R14 10 A14 4 D14	R16	1.09178875	1.09177618	1.09194597	1.09048139	1.09046340	1.09129078
H 11 R15 10 A15 4 D15	R17	1.33563170	1.33563580	1.33537448	1.33866728	1.33870083	1.33915766
H 12 R16 11 A16 10 D16	R18	1.51072721	1.51080927	1.50499500	1.51237833	1.51222878	1.51338705
C 12 R17 11 A17 10 D17	R19	1.51066624	1.51078289	1.51377856	1.51229347	1.51208717	1.51802586
C 17 R18 12 A18 11 D18	R20	1.09173085	1.09173943	1.09016447	1.09051406	1.09048920	1.09042303
C 18 R19 17 A19 12 D19	R21	1.09963224	1.09950802	1.10080908	1.09734626	1.09743043	1.09445248
H 17 R20 12 A20 11 D20	R22	1.09965145	1.09950395	1.10261626	1.09730582	1.09738627	1.10013670
H 18 R21 17 A21 12 D21	R23	1.09174887	1.09170119	1.09195443	1.09049560	1.09049131	1.08980144
H 18 R22 17 A22 12 D22	R24	1.33563064	1.33563280	1.33536813	1.33858004	1.33868940	1.33805083
H 19 R23 18 A23 17 D23	R25	1.51069086	1.51087156	1.50507790	1.51227722	1.51209841	1.51566378
C 19 R24 18 A24 17 D24	R26	1.51070214	1.51087777	1.51383106	1.51232212	1.51219415	1.51284039
C 24 R25 19 A25 18 D25	R27	1.09173512	1.09172480	1.09004575	1.09051618	1.09048173	1.09008968
C 25 R26 24 A26 19 D26	R28	1.09960181	1.09946137	1.10083790	1.09737016	1.09741089	1.09377482
H 24 R27 19 A27 18 D27	R29	1.09963349	1.09946132	1.10263136	1.09733503	1.09747582	1.10245916
H 25 R28 24 A28 19 D28	R30	1.09174532	1.09172463	1.09203478	1.09052529	1.09050079	1.09082882
H 25 R29 24 A29 19 D29	R31	1.33563205	1.33563192	1.33535535	1.33862125	1.33860814	1.33771745
H 26 R30 25 A30 24 D30	R32	1.51066237	1.51078626	1.50493605	1.51219568	1.51219767	1.51533271
C 26 R31 25 A31 24 D31	R33	1.51070090	1.51081120	1.51395367	1.51239769	1.51227859	1.51065322
C 31 R32 26 A32 25 D32	R34	1.09174564	1.09170090	1.09005454	1.09051413	1.09046711	1.09074183
C 32 R33 31 A33 26 D33	R35	1.09965405	1.09950376	1.10083950	1.09734660	1.09736897	1.09315364
H 31 R34 26 A34 25 D34	R36	1.09964325	1.09950568	1.10267432	1.09725428	1.09736640	1.10259530
H 32 R35 31 A35 26 D35	R37	1.09173966	1.09173981	1.09198943	1.09053017	1.09050144	1.09160101
H 32 R36 31 A36 26 D36	R38	1.33563406	1.33563545	1.33537643	1.33866645	1.33863698	1.33712966
H 33 R37 32 A37 31 D37	R39	1.51064201	1.51068180	1.50508517	1.51214880	1.51229309	1.51329042
C 33 R38 32 A38 31 D38	R40	1.51084028	1.51097018	1.51422177	1.51251398	1.51236763	1.51229773
C 38 R39 33 A39 32 D39	R41	1.09178615	1.09177734	1.09013223	1.09051166	1.09049056	1.09114923
C 39 R40 38 A40 33 D40	R42	1.09974597	1.09961225	1.10099644	1.09732074	1.09733654	1.09273637
H 38 R41 33 A41 32 D41	R43	1.09965940	1.09962110	1.10256366	1.09736266	1.09728394	1.10328694
H 39 R42 38 A42 33 D42	R44	1.09172033	1.09171068	1.09209469	1.09053071	1.09048060	1.09151574
H 39 R43 38 A43 33 D43	R45	1.33572017	1.33573178	1.33550951	1.33876140	1.33880124	1.33798171
H 40 R44 39 A44 38 D44	R46	1.50501544	1.50505574	1.50528127	1.50615375	1.50610526	1.50549001
C 40 R45 39 A45 38 D45	R47	1.53834717	1.53842209	1.53838249	1.53871882	1.53879407	1.53895560
C 45 R46 40 A46 39 D46	R48	1.09312156	1.09312297	1.09130065	1.09192206	1.09189765	1.09213590
C 46 R47 45 A47 40 D47	R49	1.10058086	1.10054110	1.10067824	1.10052083	1.10046322	1.10039489
H 45 R48 40 A48 39 D48	R50	1.09751894	1.09745375	1.09774616	1.09546345	1.09549184	1.09467364
H 46 R49 45 A49 40 D49	R51	1.09679789	1.09674731	1.09672612	1.09672977	1.09668417	1.09688614
H 46 R50 45 A50 40 D50	R52	1.09607440	1.09605618	1.09620479	1.09603613	1.09603450	1.09629663
H 47 R51 46 A51 45 D51	R53	1.09570527	1.09568509	1.09577137	1.09568392	1.09568482	1.09613773
H 47 R52 46 A52 45 D52							
H 47 R53 46 A53 45 D53							

Table S6-14 Bond Angle of 4Upp (Model 1)

Input Z-matrix 5Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.16871199	111.12121703	111.14984925	111.10379669	111.11332413	110.96989464
H	A4	112.73677188	112.78333390	112.78147469	112.40714497	112.40929480	112.60416163
C 1 R2	A5	36.09960799	36.11456798	36.11831613	36.09587451	107.77992064	36.16464237
C 2 R3 1 A3	A6	36.19120107	36.15861607	36.15669618	36.17819973	107.60334894	36.16763949
C 3 R4 2 A4 1 D4	A7	109.75672868	109.78986243	109.74708049	109.52699507	109.52230822	109.69957996
H 1 R5 2 A5 3 D5	A8	108.66812840	108.62434115	108.62825961	108.58252720	108.59338804	108.51234563
H 1 R6 2 A6 3 D6	A9	115.76739901	115.79597697	115.77380780	114.32991285	114.36487403	114.33547023
H 3 R7 2 A7 1 D7	A10	125.49404278	125.46461358	125.44347384	128.51715414	128.48039427	128.57842994
H 3 R8 2 A8 1 D8	A11	125.17811417	125.22834706	125.25681341	128.04706005	128.04871462	128.02435949
H 4 R9 3 A9 2 D9	A12	112.29623494	112.30010228	115.31750992	111.41732523	111.41969715	112.36671754
C 4 R10 3 A10 2 D10	A13	119.20755353	119.21135764	118.96947986	117.75356766	117.77743902	117.49318904
C 10 R11 4 A11 3 D11	A14	109.93311249	109.89630165	109.10144326	109.04805906	109.05278960	111.10682019
C 11 R12 10 A12 4 D12	A15	108.93832620	108.96612100	109.75349455	110.38180414	110.39460147	108.17246742
H 10 R13 4 A13 3 D13	A16	115.54658110	115.60938729	115.02086948	114.16193720	114.20244183	114.45908424
H 11 R14 10 A14 4 D14	A17	125.23193544	125.14964560	126.23071468	128.25430151	128.17982824	128.17522549
H 11 R15 10 A15 4 D15	A18	125.11829869	125.20445143	124.76827765	128.20923655	128.14486114	127.75274986
H 12 R16 11 A16 10 D16	A19	112.34953029	112.26047762	115.34602829	111.42272566	111.52321068	112.67017426
C 12 R17 11 A17 10 D17	A20	119.24610416	119.22597893	119.19511522	117.60261187	117.63820205	117.59696962
C 17 R18 12 A18 11 D18	A21	109.85560128	109.84945701	109.79878612	109.07807048	109.03536542	110.50542124
C 18 R19 17 A19 12 D19	A22	108.93393671	108.99082881	109.14511730	110.41457118	110.40074550	108.85091599
H 17 R20 12 A20 11 D20	A23	115.59428175	115.56536204	114.97247052	114.15174798	114.20003204	115.94517730
H 18 R21 17 A21 12 D21	A24	125.16856560	125.19683783	126.28459278	128.26947049	128.17794074	125.99650522
H 18 R22 17 A22 12 D22	A25	125.14987880	125.16293748	124.70702481	128.24763161	128.17571330	126.03654643
H 19 R23 18 A23 17 D23	A26	112.29179606	112.28897455	115.30761686	111.38569831	111.41378388	112.75437009
C 19 R24 18 A24 17 D24	A27	119.23043610	119.24024434	119.21606486	117.57777527	117.60488684	118.28984303
C 24 R25 19 A25 18 D25	A28	109.84703702	109.82540812	109.78411733	109.06557142	109.07611418	110.07905464
C 25 R26 24 A26 19 D26	A29	108.95365204	108.96002888	109.19937353	110.44382146	110.44030435	108.96936896
H 24 R27 19 A27 18 D27	A30	115.58564349	115.58917091	114.96849423	114.18438636	114.15266551	115.16584131
H 25 R28 24 A28 19 D28	A31	125.18061900	125.16358147	126.26783267	128.21444344	128.24828074	127.10117760
H 25 R29 24 A29 19 D29	A32	125.13363981	125.19635973	124.77919657	128.22158566	128.26243737	127.21940971
H 26 R30 25 A30 24 D30	A33	112.36751775	112.25988780	115.26355996	111.52101862	111.29483642	111.93023128
C 26 R31 25 A31 24 D31	A34	119.23671535	119.23175958	119.18183853	117.58813656	117.57552581	117.62290676
C 31 R32 26 A32 25 D32	A35	108.93953853	109.79429146	109.80490561	110.43093055	109.05697026	110.72998001
C 32 R33 31 A33 26 D33	A36	109.82554227	108.97298526	109.17030006	109.02544757	110.49327635	109.02903536
H 31 R34 26 A34 25 D34	A37	115.60207245	115.56149295	115.00212763	114.17548763	114.17041043	114.50953786
H 32 R35 31 A35 26 D35	A38	125.15740234	125.20431777	126.24071967	128.21408202	128.21509969	128.15693297
H 32 R36 31 A36 26 D36	A39	125.17988592	125.14997658	124.81940196	128.25712510	128.26399942	127.97372727
H 33 R37 32 A37 31 D37	A40	112.29125160	112.30001418	115.24926337	111.48099250	111.44878197	111.47791707
C 33 R38 32 A38 31 D38	A41	119.21827630	119.23313778	119.19637901	117.57662268	117.58270268	117.43680994
C 38 R39 33 A39 32 D39	A42	109.81554840	109.82766182	109.77141007	109.07673333	109.04690503	110.99422917
C 39 R40 38 A40 33 D40	A43	108.94091827	108.91481478	109.07991087	110.41944571	110.44350791	108.62698910
H 38 R41 33 A41 32 D41	A44	115.57097653	115.55323613	115.02731427	114.21469326	114.21830374	114.35782747
H 39 R42 38 A42 33 D42	A45	125.23765862	125.22740368	126.26898794	128.01263628	127.98962734	128.19915394
H 39 R43 38 A43 33 D43	A46	125.42886692	125.46535301	125.05451419	128.49110326	128.46054294	128.44395669
H 40 R44 39 A44 38 D44	A47	112.79469015	112.78188852	112.83150492	112.40968990	112.45640095	112.42903802
C 40 R45 39 A45 38 D45	A48	118.76956185	118.73597811	118.92124566	117.15254630	117.16339493	117.11553450
C 45 R46 40 A46 39 D46	A49	109.39730803	109.37673159	109.37917147	108.83006162	108.80932831	108.58142876
C 46 R47 45 A47 40 D47	A50	109.60558704	109.62528419	109.70914018	111.08544574	111.08545706	111.44519704
H 45 R48 40 A48 39 D48	A51	111.14980798	111.12038777	111.08261046	111.12348660	111.12737260	111.27515009
H 46 R49 45 A49 40 D49	A52	111.10053972	111.10833449	111.15388900	111.07559762	111.06608993	111.04752065
H 46 R50 45 A50 40 D50	A53	110.91151322	110.90600962	110.91109260	110.97218395	110.96289843	110.98723368
H 47 R51 46 A51 45 D51							
H 47 R52 46 A52 45 D52							
H 47 R53 46 A53 45 D53							

Table S6-15 Bond Lengths of 5Up (Model 1)

Input Z-matrix 5Up		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	57.51599823	58.01702531	58.22693667	57.10296201	57.19980674	57.73642250
H	D5	122.01294745	121.93535447	121.91296201	121.90753226	-121.91633313	121.60136973
C 1 R2	D6	-121.57280096	-121.61916603	-121.63852746	-121.65470685	121.64448701	-122.10772591
C 2 R3 1 A3	D7	-179.94346716	-179.41629771	-179.21440606	-178.84900496	-178.80870733	-178.13341973
C 3 R4 2 A4 1 D4	D8	-63.90925272	-63.40163208	-63.18922983	-63.33778744	-63.27954445	-62.80797982
H 1 R5 2 A5 3 D5	D9	-60.69351796	-60.05990316	-60.51142445	-59.50577832	-60.00491791	-50.04477297
H 1 R6 2 A6 3 D6	D10	118.54679499	119.31229747	118.31840688	119.45829586	118.83843386	130.50260232
H 3 R7 2 A7 1 D7	D11	-178.79410626	-178.98123040	-178.43798984	1.44528226	1.52966252	0.71581601
H 3 R8 2 A8 1 D8	D12	117.20122013	118.18024701	-119.48658241	115.36556881	115.73755952	-134.94241394
H 4 R9 3 A9 2 D9	D13	0.07052085	-0.01198860	1.32395179	179.87564537	179.98515785	179.52893514
C 4 R10 3 A10 2 D10	D14	-121.30044649	-120.41800329	119.06866654	-122.48578936	-122.14196455	-9.51520217
C 10 R11 4 A11 3 D11	D15	-4.60872756	-3.73184188	4.35027066	-5.99393116	-5.60783678	106.14327864
C 11 R12 10 A12 4 D12	D16	-60.60494627	-61.35182590	-167.97390117	-61.55902426	-63.53253442	-52.91293394
H 10 R13 4 A13 3 D13	D17	118.06987996	117.63616343	12.16819896	117.38472370	114.72460842	128.27440221
H 11 R14 10 A14 4 D14	D18	179.98783138	-178.86917987	-179.18444157	0.07632718	1.56586839	-1.49249231
H 11 R15 10 A15 4 D15	D19	-117.68965863	117.47158733	-119.42886396	-116.98470902	117.52702357	-132.76808324
H 12 R16 11 A16 10 D16	D20	1.35088744	0.06855006	0.70683305	-178.89757213	-179.77683162	178.39829624
C 12 R17 11 A17 10 D17	D21	120.85266853	-121.11164767	4.33496395	120.78772922	-120.29771093	-8.79531593
C 17 R18 12 A18 11 D18	D22	4.19935849	-4.38841303	119.06579432	4.34868908	-3.88770337	107.17329911
C 18 R19 17 A19 12 D19	D23	60.61449096	-61.63804923	-168.98428363	61.74704504	-61.19736644	-91.66840068
H 17 R20 12 A20 11 D20	D24	-118.13625939	117.41071907	11.27078183	-117.26020095	117.38909658	88.00236567
H 18 R21 17 A21 12 D21	D25	-179.87548931	-178.96198939	-179.50656872	0.06482122	1.65792564	-0.78717685
H 18 R22 17 A22 12 D22	D26	117.49903911	117.21967598	-119.11283596	118.08034912	116.27154706	-148.62140977
H 19 R23 18 A23 17 D23	D27	-1.30747924	0.03073655	0.52106807	179.02794001	179.99023237	179.13047656
C 19 R24 18 A24 17 D24	D28	-121.06981556	-121.37809170	4.56628150	-119.79614072	-121.53354501	-24.49863150
C 24 R25 19 A25 18 D25	D29	-4.39589633	-4.67618347	119.34166867	-3.30369115	-5.04771298	91.53271091
C 25 R26 24 A26 19 D26	D30	-60.79304718	-61.79914231	-169.46255780	-61.41582120	-60.43933577	-75.62822140
H 24 R27 19 A27 18 D27	D31	117.88139812	117.22808883	10.79803158	117.52965130	118.19837040	103.85525148
H 25 R28 24 A28 19 D28	D32	-179.97019969	-178.96177756	-179.48473736	0.13707316	1.71065275	-1.13708054
H 25 R29 24 A29 19 D29	D33	-117.76763565	117.40361631	-119.97829742	-116.72952015	116.46914010	-148.02568720
H 26 R30 25 A30 24 D30	D34	1.37328937	0.05340115	0.47422201	-178.85929161	179.96939033	179.15654843
C 26 R31 25 A31 24 D31	D35	4.15394568	-121.19574032	3.81017383	4.64092182	-121.43039024	-23.18554945
C 31 R32 26 A32 25 D32	D36	120.78945317	-4.51352881	118.57159023	121.07889210	-4.86386453	92.49045061
C 32 R33 31 A33 26 D33	D37	60.76084241	-61.50301610	-168.93822074	61.72734457	-62.42133161	-63.18537700
H 31 R34 26 A34 25 D34	D38	-118.01519307	17.47045081	11.21031010	-117.42786214	115.86575374	116.91801410
H 32 R35 31 A35 26 D35	D39	-179.82450839	-178.86893118	-179.21160396	0.14635211	1.76204511	-1.33115575
H 32 R36 31 A36 26 D36	D40	117.73765907	117.63260333	-119.75890187	119.14698458	117.89603159	-135.68635293
H 33 R37 32 A37 31 D37	D41	-1.29691906	0.08581867	0.69613914	179.24134363	-179.72417842	179.09311019
C 33 R38 32 A38 31 D38	D42	-120.86019448	-120.94906999	4.09199892	-118.75885041	-120.03785192	-10.94523355
C 38 R39 33 A39 32 D39	D43	-4.24497674	-4.33082595	118.81054086	-2.24021898	-3.52152545	105.46908332
C 39 R40 38 A40 33 D40	D44	-60.78377823	-60.81609794	-167.31640920	-62.09876540	-63.56932414	-63.84166260
H 38 R41 33 A41 32 D41	D45	118.24387655	118.18706175	13.41148741	116.47485311	114.87580128	115.07777051
H 39 R42 38 A42 33 D42	D46	-178.97687526	-178.97921129	-179.90759948	1.51577009	1.48250019	0.70513443
H 39 R43 38 A43 33 D43	D47	119.67613801	119.30042398	119.21648084	119.43487152	118.94583200	117.57154492
H 40 R44 39 A44 38 D44	D48	0.35701764	0.37333069	-0.42491857	-179.65100648	-179.60535207	179.90879879
C 40 R45 39 A45 38 D45	D49	-119.30637735	-119.70903960	-119.83872056	-120.23038881	-120.70684354	-122.33710415
C 45 R46 40 A46 39 D46	D50	-2.95930690	-3.35856346	-3.47913109	-3.68658091	-4.20076501	-5.90865953
C 46 R47 45 A47 40 D47	D51	58.35144908	58.01945215	58.01769826	57.07612247	56.99969143	57.05572118
H 45 R48 40 A48 39 D48	D52	178.30403583	177.97610663	178.00366323	177.04569363	176.97243029	177.07647370
H 46 R49 45 A49 40 D49	D53	-61.36341561	-61.67309921	-61.61534964	-62.60234060	-62.68165283	-62.60089640
H 46 R50 45 A50 40 D50							
H 47 R51 46 A51 45 D51							
H 47 R52 46 A52 45 D52							
H 47 R53 46 A53 45 D53							

6.6 Z-matrix for SDA structures

Table S6-16 Bond Lengths of SDA

Input Z-matrix SDA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Length							
0 1	R2	1.09681028	1.09678985	1.09672302	1.09671235	1.09673225	1.09590301
H	R3	1.53843943	1.53836206	1.53840122	1.53878750	1.53880458	1.53800269
C 1 R2	R4	1.50495839	1.50500732	1.50502478	1.50604356	1.50610195	1.50652865
C 2 R3 1 A3	R5	1.77096489	1.77105451	1.77102837	1.77144561	1.77141574	1.77443444
C 3 R4 2 A4 1 D4	R6	1.76974537	1.76971490	1.76966593	1.76909822	1.76906470	1.76825905
H 1 R5 2 A5 3 D5	R7	1.09747635	1.09751379	1.09758222	1.09553931	1.09554370	1.09608151
H 1 R6 2 A6 3 D6	R8	1.10055572	1.10053249	1.10047941	1.10044123	1.10040202	1.10102377
H 3 R7 2 A7 1 D7	R9	1.09312547	1.09314958	1.09294934	1.09192530	1.09195190	1.09191770
H 3 R8 2 A8 1 D8	R10	1.33573985	1.33573875	1.33570787	1.33874855	1.33877457	1.33919828
H 4 R9 3 A9 2 D9	R11	1.51085178	1.51084736	1.50514616	1.51249317	1.51240704	1.51317628
C 4 R10 3 A10 2 D10	R12	1.51065396	1.51064817	1.51420034	1.51210269	1.51213008	1.51125525
C 10 R11 4 A11 3 D11	R13	1.09171291	1.09173591	1.09183530	1.09052184	1.09049520	1.09012011
C 11 R12 10 A12 4 D12	R14	1.09962826	1.09964528	1.10069529	1.09735336	1.09743254	1.09380855
H 10 R13 4 A13 3 D13	R15	1.09968786	1.09968764	1.10237703	1.09734747	1.09723387	1.10388106
H 11 R14 10 A14 4 D14	R16	1.09181531	1.09177944	1.09197119	1.09051956	1.09048811	1.09072250
H 11 R15 10 A15 4 D15	R17	1.33564553	1.33563005	1.33534892	1.33864517	1.33865728	1.33831693
H 12 R16 11 A16 10 D16	R18	1.51069022	1.51069913	1.50506667	1.51238377	1.51230326	1.51740133
C 12 R17 11 A17 10 D17	R19	1.51064550	1.51071262	1.51420135	1.51223816	1.51223334	1.51122362
C 17 R18 12 A18 11 D18	R20	1.09178062	1.09174590	1.09010362	1.09053027	1.09048315	1.09051447
C 18 R19 17 A19 12 D19	R21	1.09966082	1.09962705	1.10080893	1.09729563	1.09741979	1.09427740
H 17 R20 12 A20 11 D20	R22	1.09962059	1.09965220	1.10254053	1.09733848	1.09734386	1.10254184
H 18 R21 17 A21 12 D21	R23	1.09177442	1.09172542	1.09197530	1.09051497	1.09045488	1.09127364
H 18 R22 17 A22 12 D22	R24	1.33564477	1.33564261	1.33533487	1.33872159	1.33868828	1.33773535
H 19 R23 18 A23 17 D23	R25	1.51073104	1.51078985	1.50499715	1.51220229	1.51221259	1.51403951
C 19 R24 18 A24 17 D24	R26	1.51078301	1.51069444	1.51425691	1.51242415	1.51231477	1.51425901
C 24 R25 19 A25 18 D25	R27	1.09173646	1.09180867	1.09010170	1.09059402	1.09046448	1.09079701
C 25 R26 24 A26 19 D26	R28	1.09967157	1.09975040	1.10095447	1.09723475	1.09722359	1.09319396
H 24 R27 19 A27 18 D27	R29	1.09958573	1.09953160	1.10252163	1.09740195	1.09739024	1.10160321
H 25 R28 24 A28 19 D28	R30	1.09171871	1.09168872	1.09206271	1.09049910	1.09045277	1.09092295
H 25 R29 24 A29 19 D29	R31	1.33577338	1.33576445	1.33549458	1.33877934	1.33885990	1.33828180
H 26 R30 25 A30 24 D30	R32	1.50468019	1.50464090	1.50491986	1.50558398	1.50593057	1.50553189
C 26 R31 25 A31 24 D31	R33	1.54074938	1.09295069	1.09119397	1.54110154	1.09168655	1.09152537
C 31 R32 26 A32 25 D32	R34	1.53309170	1.10107940	1.09833222	1.53305679	1.10080091	1.09569168
C 32 R33 31 A33 26 D33	R35	1.52975699	1.09808670	1.10133498	1.52963678	1.09612760	1.10016980
C 33 R34 32 A34 31 D34	R36	1.09298347	1.54081122	1.54054954	1.09175328	1.54143632	1.54274075
C 34 R35 33 A35 32 D35	R37	1.09809122	1.10008871	1.10006511	1.09614829	1.09995061	1.09990175
H 31 R36 26 A36 25 D36	R38	1.10119532	1.09893034	1.09900032	1.10109321	1.09894149	1.09824451
H 32 R37 31 A37 26 D37	R39	1.10008835	1.53324996	1.53318857	1.09999773	1.53302684	1.53252708
H 32 R38 31 A38 26 D38	R40	1.09893633	1.09712719	1.09721364	1.09899240	1.09720408	1.09432678
H 33 R39 32 A39 31 D39	R41	1.09725671	1.09715883	1.09718692	1.09721972	1.09718366	1.09869915
H 33 R40 32 A40 31 D40	R42	1.09707209	1.52967271	1.52959456	1.09719126	1.52968777	1.53206394
H 34 R41 33 A41 32 D41	R43	1.09854944	1.09842045	1.09868323	1.09862449	1.09860629	1.09545636
H 34 R42 33 A42 32 D42	R44	1.09849071	1.09865761	1.09842018	1.09845236	1.09843081	1.10040128
H 35 R43 34 A43 33 D43	R45	1.51325467	1.51325901	1.51324533	1.51331244	1.51333585	1.51349680
H 35 R44 34 A44 33 D44	R46	1.21111539	1.35869811	1.35894877	1.21113831	1.35862078	1.35691043
C 35 R45 34 A45 33 D45	R47	1.35871185	1.21110423	1.21116007	1.35859058	1.21112497	1.21341561
O 45 R46 35 A46 34 D46	R48	0.97577564	0.97577694	0.97577115	0.97578401	0.97578924	0.97619027
O 45 R47 35 A47 34 D47							
H 47 R48 45 A48 35 D48							

Table S6-17 Bond Angle of SDA

Input Z-matrix SDA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.15686635	111.15533406	111.13411160	111.12362674	111.14573520	111.11242183
H	A4	112.81915689	112.82644037	112.82371368	112.42356899	112.38618143	112.61552106
C 1 R2	A5	36.12400274	36.11743255	36.11596003	36.09808157	36.10190636	35.95468355
C 2 R3 1 A3	A6	36.15771493	36.15783240	36.15895406	36.18207583	36.18275145	36.26770946
C 3 R4 2 A4 1 D4	A7	109.76151859	109.76725074	109.78123378	109.52027915	109.49652458	109.63395972
H 1 R5 2 A5 3 D5	A8	108.62455776	108.62369056	108.60992732	108.60076459	108.61366690	108.50253471
H 1 R6 2 A6 3 D6	A9	115.80012634	115.79120776	115.76551942	114.35669447	114.34657483	114.37519877
H 3 R7 2 A7 1 D7	A10	125.42324413	125.44938857	125.47775642	128.48098044	128.49607259	128.54367974
H 3 R8 2 A8 1 D8	A11	125.24384242	125.21547881	125.17998627	128.02179673	128.04496015	127.46732677
H 4 R9 3 A9 2 D9	A12	112.31591853	112.33195173	115.32296747	111.53479786	111.46349499	112.32681746
C 4 R10 3 A10 2 D10	A13	119.18538068	119.20384080	118.97789996	117.75757544	117.76532864	117.81194415
C 10 R11 4 A11 3 D11	A14	109.89538295	109.89714249	109.70276954	109.05739227	109.05879760	111.32824531
C 11 R12 10 A12 4 D12	A15	108.95362835	108.94855413	109.16073506	110.36855914	110.37729753	108.38215455
H 10 R13 4 A13 3 D13	A16	115.58411545	115.57706506	115.00781817	114.16467084	114.17181206	114.57194293
H 11 R14 10 A14 4 D14	A17	125.18859842	125.20824873	126.22504500	128.27253805	128.22789941	127.51185768
H 11 R15 10 A15 4 D15	A18	125.13001440	125.11533531	124.81350221	128.23992843	128.19233934	127.13387688
H 12 R16 11 A16 10 D16	A19	112.37861730	112.41873308	115.18353447	111.48216980	111.47258866	112.50505653
C 12 R17 11 A17 10 D17	A20	119.22909602	119.23841169	119.15988223	117.59902453	117.61375589	117.76861061
C 17 R18 12 A18 11 D18	A21	108.91629832	109.85864561	109.81633138	110.44228034	109.05026139	110.45163037
C 18 R19 17 A19 12 D19	A22	109.86249513	108.91542961	109.20283794	109.05313671	110.41881486	109.10413957
H 17 R20 12 A20 11 D20	A23	115.60624675	115.61818949	115.02088199	114.21153920	114.19960435	114.56567783
H 18 R21 17 A21 12 D21	A24	125.15495053	125.13462630	126.16890995	128.17185539	128.17340499	128.09191206
H 18 R22 17 A22 12 D22	A25	125.15264463	125.21801733	124.85015988	128.17965791	128.15460875	127.82669535
H 19 R23 18 A23 17 D23	A26	112.31668552	112.37568344	115.21724672	111.48958979	111.54519754	111.26468259
C 19 R24 18 A24 17 D24	A27	119.23130054	119.20995783	119.13083667	117.57851551	117.62662820	117.52648794
C 24 R25 19 A25 18 D25	A28	109.83552145	109.74708577	109.79665698	109.09316089	109.06446376	110.61406071
C 25 R26 24 A26 19 D26	A29	108.93169613	108.95932740	109.12833068	110.34829817	110.37614881	109.06884698
H 24 R27 19 A27 18 D27	A30	115.55179785	115.64618542	115.03364720	114.16785364	114.21895271	114.78756696
H 25 R28 24 A28 19 D28	A31	125.25333351	125.11288217	126.22318982	128.11592276	128.01722963	127.54546984
H 25 R29 24 A29 19 D29	A32	125.30768658	125.43955689	125.04005706	128.41294545	128.31656730	127.69831064
H 26 R30 25 A30 24 D30	A33	112.99765734	118.70097420	118.89808635	112.65343106	117.16698033	117.31847557
C 26 R31 25 A31 24 D31	A34	112.89231692	109.56085341	109.87299193	112.83162371	109.00408595	111.24525756
C 31 R32 26 A32 25 D32	A35	112.60358750	109.77936312	109.57358725	112.68208297	111.17920143	109.39421642
C 32 R33 31 A33 26 D33	A36	118.77094736	112.91029983	112.90810689	117.12920737	112.57717564	112.20207022
C 33 R34 32 A34 31 D34	A37	109.70839556	109.21905778	109.18851189	111.19852418	109.23433260	109.58387422
C 34 R35 33 A35 32 D35	A38	109.57171855	108.92260048	108.95194873	108.99285556	108.91821755	108.42361030
H 31 R36 26 A36 25 D36	A39	109.22390565	112.92604394	112.95763105	109.21920263	112.90087255	112.57100090
H 32 R37 31 A37 26 D37	A40	108.92948879	109.97025107	109.98898237	108.99090708	109.98226597	109.49022471
H 32 R38 31 A38 26 D38	A41	110.00172984	109.97522171	109.96718733	109.96528401	109.99968592	109.98550613
H 33 R39 32 A39 31 D39	A42	109.96434877	112.58121357	112.59968659	109.97088811	112.62005900	112.62574824
H 33 R40 32 A40 31 D40	A43	111.26900597	111.29125725	111.26421999	111.29583435	111.31206032	112.13777699
H 34 R41 33 A41 32 D41	A44	111.30747417	111.27464978	111.31500447	111.31629032	111.28299559	109.88486383
H 34 R42 33 A42 32 D42	A45	113.20646232	113.21092024	113.22642500	113.14097323	113.17519052	113.21093907
H 35 R43 34 A43 33 D43	A46	126.25100146	111.42277968	111.44512350	126.22531327	111.43292760	111.80296444
H 35 R44 34 A44 33 D44	A47	111.42552812	126.25036258	126.27351695	111.44691144	126.23312230	126.28856181
C 35 R45 34 A45 33 D45	A48	105.90639452	105.91200448	105.86800121	105.90114398	105.91183581	105.95164140
O 45 R46 35 A46 34 D46							
O 45 R47 35 A47 34 D47							
H 47 R48 45 A48 35 D48							

Table S6-18 Dihedral angles of SDA

Input Z-matrix SDA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	58.27669336	58.21093890	58.09070117	57.22879351	57.23671079	-62.34801288
H	D5	121.93170042	121.90599010	121.88883985	121.90892223	121.92792983	-122.22938298
C 1 R2	D6	-121.64765887	-121.65646560	-121.67274418	-121.65276447	-121.63725311	121.71614966
C 2 R3 1 A3	D7	-179.16687237	-179.21923708	-179.28074205	-178.75376281	-178.77870191	61.83595052
C 3 R4 2 A4 1 D4	D8	-63.17090113	-63.23458602	-63.27210158	-63.23838157	-63.24931150	177.06898310
H 1 R5 2 A5 3 D5	D9	-59.91407874	-60.28670253	-59.86273472	-60.08865424	-60.45478878	-53.57865204
H 1 R6 2 A6 3 D6	D10	119.49128968	119.08006890	119.12747643	118.76564682	118.27453466	126.78689951
H 3 R7 2 A7 1 D7	D11	-179.05625016	-179.00842361	-178.79173039	1.46743381	1.52600446	0.02944732
H 3 R8 2 A8 1 D8	D12	118.16250703	117.87618520	-117.81552562	115.96045590	116.75608925	-137.58116884
H 4 R9 3 A9 2 D9	D13	-0.04240052	-0.01823911	1.22525292	179.98807042	-179.85906700	179.79080313
C 4 R10 3 A10 2 D10	D14	-120.40227543	-120.65804515	5.82547517	-121.83092739	-121.06050497	-12.28884202
C 10 R11 4 A11 3 D11	D15	-3.72557735	-3.99567604	120.57374285	-5.39835916	-4.58896925	103.62419927
C 11 R12 10 A12 4 D12	D16	-61.01447231	-60.71457915	-168.54430785	-60.68934022	-61.66091433	-55.33049025
H 10 R13 4 A13 3 D13	D17	117.54686948	118.37823383	11.83340103	118.53318894	116.78502415	125.40616828
H 11 R14 10 A14 4 D14	D18	-179.87752421	-179.13318433	-179.79335236	-0.02326397	1.57727098	-1.59911223
H 11 R15 10 A15 4 D15	D19	-118.25326589	118.42260914	-118.56532737	-118.77155187	117.31848130	-152.76199148
H 12 R16 11 A16 10 D16	D20	1.42501080	0.01710539	0.47481711	-179.20186037	-179.87032269	177.95427863
C 12 R17 11 A17 10 D17	D21	3.66990369	-120.11176135	5.11860402	2.64055528	-120.50165527	-28.15927244
C 17 R18 12 A18 11 D18	D22	120.29903192	-3.49891077	119.91712888	119.10068054	-4.05118913	87.62648242
C 18 R19 17 A19 12 D19	D23	60.09510232	-60.36746390	-169.10077280	61.78822660	-62.22693134	-69.35356929
H 17 R20 12 A20 11 D20	D24	-118.69008555	118.90114905	11.14189228	-117.23309083	116.21004412	110.48648190
H 18 R21 17 A21 12 D21	D25	-179.83010264	-179.39184120	-179.46927005	-0.01577409	1.54958346	-1.84851348
H 18 R22 17 A22 12 D22	D26	117.27587371	119.34332092	-119.43872889	118.11552625	116.94829150	-133.21511468
H 19 R23 18 A23 17 D23	D27	-1.31796254	-0.10806877	0.53230739	179.04855852	-179.89861569	179.24093898
C 19 R24 18 A24 17 D24	D28	-121.27615251	-119.31340403	4.36378649	-119.70833194	-120.90408663	-9.39207725
C 24 R25 19 A25 18 D25	D29	-4.62040241	-2.72900662	119.10920687	-3.26666216	-4.43784207	107.34426768
C 25 R26 24 A26 19 D26	D30	-61.00081548	-61.46747395	-167.90574965	-59.50232527	-61.78092492	-75.49522621
H 24 R27 19 A27 18 D27	D31	117.66135162	117.53809655	12.34002746	119.70262028	116.85729456	102.46673052
H 25 R28 24 A28 19 D28	D32	179.95757772	-178.81378821	179.25626804	0.05897471	1.59697844	-0.82365819
H 25 R29 24 A29 19 D29	D33	-118.25189348	0.46109512	0.33075075	-119.05924352	-179.80749545	-178.26088696
H 26 R30 25 A30 24 D30	D34	-178.66678098	-121.38447986	4.14991569	-177.21784488	-124.25128543	15.39272591
C 26 R31 25 A31 24 D31	D35	179.95362270	-4.85620652	120.67211939	-179.88677273	-7.55064601	132.65559818
C 31 R32 26 A32 25 D32	D36	1.02608044	117.64349461	-118.43580704	-179.50663248	115.40479211	-106.46228306
C 32 R33 31 A33 26 D33	D37	4.27669567	55.38114488	-55.32266898	3.99390774	54.48829134	-57.12799296
C 33 R34 32 A34 31 D34	D38	120.74003462	-60.05192984	60.07681837	120.60815948	-60.89490127	58.57912178
C 34 R35 33 A35 32 D35	D39	-56.46871071	177.52679108	-177.46483628	-55.04496621	176.69383792	179.81641313
H 31 R36 26 A36 25 D36	D40	58.97951936	-58.51947632	-57.84729111	60.37476053	-58.57773416	-55.77882833
H 32 R37 31 A37 26 D37	D41	57.99752469	57.62100271	58.28428896	58.13471199	57.55571936	60.66387980
H 32 R38 31 A38 26 D38	D42	-58.15031406	179.52416152	-179.76638337	-57.96607921	179.46348932	-177.08255911
H 33 R39 32 A39 31 D39	D43	58.26073268	-58.73528429	-58.37225912	-58.56712561	58.47437747	-65.96206143
H 33 R40 32 A40 31 D40	D44	-58.86605827	58.37516989	58.74115099	58.58305966	-58.66803838	51.62353908
H 34 R41 33 A41 32 D41	D45	179.65688712	179.76052115	-179.72859227	-179.94446141	179.89343135	170.31321786
H 34 R42 33 A42 32 D42	D46	-0.46275512	179.52941681	-179.27014948	0.40800542	179.79095235	155.16871355
H 35 R43 34 A43 33 D43	D47	179.56836734	-0.52357722	0.79943439	-179.62614470	-0.22464731	-26.42727590
H 35 R44 34 A44 33 D44	D48	179.91461452	179.92399871	-179.88824977	-179.95090233	179.97727102	177.59575336
C 35 R45 34 A45 33 D45							
O 45 R46 35 A46 34 D46							
O 45 R47 35 A47 34 D47							
H 47 R48 45 A48 35 D48							

6.7 Z-matrix for EPA structures

Table S6-19 Bond Lengths of EPA

Input Z-matrix EPA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Length							
0 1	R2	1.09678571	1.09679431	1.09673960	1.09670609	1.09666190	1.09560593
H	R3	1.53836348	1.53843084	1.53843254	1.53881548	1.53884287	1.53734680
	R4	1.50504867	1.50492256	1.50499747	1.50602787	1.50616542	1.50632450
C 1 R2	R5	1.77105302	1.77100673	1.77106727	1.77144000	1.09599746	1.77443914
C 2 R3 1 A3	R6	1.76972935	1.76975065	1.76965830	1.76916921	1.09565628	1.76815799
C 3 R4 2 A4 1 D4	R7	1.09746860	1.09751525	1.09757309	1.09549273	1.09558173	1.09635084
H 2 R5 3 A5 4 D5	R8	1.10055736	1.10057550	1.10048220	1.10045413	1.10048869	1.10124264
H 2 R6 3 A6 4 D6	R9	1.09315712	1.09309687	1.09297302	1.09190395	1.09196776	1.09148103
H 3 R7 2 A7 1 D7	R10	1.33571924	1.33573526	1.33576309	1.33872834	1.33876931	1.33890303
H 3 R8 2 A8 1 D8	R11	1.51084720	1.51085601	1.50502434	1.51265333	1.51240940	1.51572004
H 4 R9 3 A9 2 D9	R12	1.51070474	1.51066311	1.51398385	1.51218632	1.51225145	1.50979429
C 4 R10 3 A10 2 D10	R13	1.09171272	1.09171682	1.09188993	1.09052956	1.09049443	1.08988743
C 10 R11 4 A11 3 D11	R14	1.09960734	1.09960869	1.10065787	1.09735613	1.09741760	1.09440059
C 11 R12 10 A12 4 D12	R15	1.09973051	1.09968987	1.10247558	1.09718921	1.09717507	1.10390396
H 10 R13 4 A13 3 D13	R16	1.09177630	1.09176022	1.09185981	1.09045406	1.09049397	1.09133161
H 11 R14 10 A14 4 D14	R17	1.33564843	1.33566228	1.33532331	1.33866769	1.33865862	1.33855415
H 11 R15 10 A15 4 D15	R18	1.51076837	1.51076028	1.50503113	1.51210545	1.51221785	1.51311355
H 12 R16 11 A16 10 D16	R19	1.51064964	1.51075273	1.51376651	1.51238564	1.51223533	1.51106670
C 12 R17 11 A17 10 D17	R20	1.09172104	1.09174807	1.09012585	1.09054746	1.09048301	1.09118415
C 17 R18 12 A18 11 D18	R21	1.09960419	1.09956515	1.10069986	1.09752014	1.09734231	1.09399699
C 18 R19 17 A19 12 D19	R22	1.09958365	1.09953549	1.10261606	1.09741479	1.09728068	1.10408608
H 17 R20 12 A20 11 D20	R23	1.09176611	1.09175387	1.09203294	1.09050439	1.09047831	1.09126138
H 18 R21 17 A21 12 D21	R24	1.33563507	1.33561376	1.33533866	1.33860139	1.33865305	1.33770914
H 18 R22 17 A22 12 D22	R25	1.51068119	1.51075378	1.50503410	1.51219442	1.51223659	1.51604028
H 19 R23 18 A23 17 D23	R26	1.51072257	1.51076717	1.51376619	1.51212190	1.51222685	1.51115929
C 19 R24 18 A24 17 D24	R27	1.09174455	1.09174960	1.09007661	1.09050445	1.09047631	1.09031054
C 24 R25 19 A25 18 D25	R28	1.09960558	1.09950617	1.10083234	1.09739199	1.09727615	1.09436330
C 25 R26 24 A26 19 D26	R29	1.09961717	1.09947612	1.10269210	1.09736882	1.09734395	1.10284801
H 24 R27 19 A27 18 D27	R30	1.09172869	1.09175235	1.09204436	1.09049412	1.09048214	1.09121001
H 25 R28 24 A28 19 D28	R31	1.33564044	1.33565147	1.33536200	1.33864480	1.33866453	1.33753214
H 25 R29 24 A29 19 D29	R32	1.51078696	1.51075271	1.50500590	1.51221140	1.51226468	1.51393866
H 26 R30 25 A30 24 D30	R33	1.51063823	1.51068587	1.51387227	1.51218280	1.51241188	1.51612379
C 26 R31 25 A31 24 D31	R34	1.09174330	1.09166975	1.09002404	1.09050337	1.09049081	1.09037217
C 31 R32 26 A32 25 D32	R35	1.09950145	1.09951568	1.10091912	1.09744292	1.09717374	1.09422307
C 32 R33 31 A33 26 D33	R36	1.09958092	1.09956667	1.10259877	1.09742883	1.09741002	1.10093877
H 31 R34 26 A34 25 D34	R37	1.09173020	1.09174345	1.09215943	1.09043046	1.09049201	1.09031720
H 32 R35 31 A35 26 D35	R38	1.33560018	1.33560526	1.33536834	1.33865362	1.33877153	1.33759860
H 32 R36 31 A36 26 D36	R39	1.50489226	1.50478910	1.50490111	1.50589500	1.50617370	1.50555848
H 33 R37 32 A37 31 D37	R40	1.53982328	1.53996652	1.53996040	1.54052722	1.53882684	1.54085954
C 33 R38 32 A38 31 D38	R41	1.52954319	1.52955391	1.52950258	1.52941758	1.54000000	1.52954458
C 38 R39 33 A39 32 D39	R42	1.09268336	1.09267082	1.09083647	1.09148349	1.09196778	1.09139999
C 39 R40 38 A40 33 D40	R43	1.09841339	1.10169636	1.10172700	1.10157592	1.10049592	1.10121008
C 40 R41 39 A41 38 D41	R44	1.10168263	1.09846510	1.09878342	1.09637175	1.09557926	1.09607416
H 38 R42 33 A42 32 D42	R45	1.09673796	1.09672961	1.09680932	1.09664718	1.09666291	1.09736225
H 39 R43 38 A43 33 D43	R46	1.09606051	1.09605705	1.09607563	1.09609529	1.09565632	1.09544411
H 39 R44 38 A44 33 D44	R47	1.09900486	1.09900171	1.09834470	1.09896702	1.07000000	1.09810791
H 40 R45 39 A45 38 D45	R48	1.09818733	1.09815995	1.09896336	1.09821592	1.07000000	1.09828142
H 40 R46 39 A46 38 D46	R49	1.51330497	1.51332723	1.51318425	1.51343275	1.54000000	1.51057113
H 41 R47 40 A47 39 D47	R50	1.21101229	1.21102894	1.21109833	1.21098281	1.23026900	1.21264730
H 41 R48 40 A48 39 D48	R51	1.35866547	1.35862789	1.35897683	1.35860147	1.35698563	1.36028365
C 41 R49 40 A49 39 D49	R52	0.97579686	0.97579279	0.97576554	0.97580627	0.97116469	0.97590352
O 49 R50 41 A50 40 D50							
O 49 R51 41 A51 40 D51							
H 51 R52 49 A52 41 D52							

Table S6-20 Bond Angles of EPA

Input Z-matrix EPA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.14057432	111.15301568	111.13834351	111.12456026	111.10263810	111.07383666
H	A4	112.78545805	112.84326417	112.81698357	112.43170265	112.37469386	112.80043222
C 1 R2	A5	36.11938803	36.12073205	36.11719099	36.09984514	111.06380058	35.94561499
C 2 R3 1 A3	A6	36.15735353	36.15727894	36.16013022	36.17953138	110.96740709	36.25921346
C 3 R4 2 A4 1 D4	A7	109.77489236	109.76893676	109.76250382	109.52945063	109.51623791	109.74716395
H 2 R5 3 A5 4 D5	A8	108.62722244	108.61502748	108.61710220	108.59474473	108.58129184	108.51084396
H 2 R6 3 A6 4 D6	A9	115.79168080	115.82003240	115.78622331	114.34788821	114.32530770	114.68715701
H 3 R7 2 A7 1 D7	A10	125.46086744	125.42172432	125.44269255	128.49777840	128.52040974	128.12953138
H 3 R8 2 A8 1 D8	A11	125.19740144	125.21563348	125.20616722	128.05499218	128.02497519	127.06524354
H 4 R9 3 A9 2 D9	A12	112.30324238	112.35794172	115.36203515	111.50453559	111.44597466	112.80167695
C 4 R10 3 A10 2 D10	A13	119.20564562	119.19037592	118.96035772	117.75940631	117.75783151	117.50444585
C 10 R11 4 A11 3 D11	A14	109.92550077	109.87803023	109.72082448	109.01921427	109.09610040	110.95858691
C 11 R12 10 A12 4 D12	A15	108.93465717	108.94230686	109.14227163	110.38431271	110.32816008	108.60738775
H 10 R13 4 A13 3 D13	A16	115.55977516	115.59048898	114.97115054	114.16332902	114.16222402	114.64623597
H 11 R14 10 A14 4 D14	A17	125.20156828	125.20369642	126.26947150	128.23944857	128.21985862	128.13453347
H 11 R15 10 A15 4 D15	A18	125.13958043	125.13487349	124.71446772	128.15964529	128.15579739	127.88092423
H 12 R16 11 A16 10 D16	A19	112.38342539	112.39049056	115.27646830	111.45656205	111.45053090	112.22154164
C 12 R17 11 A17 10 D17	A20	119.24364475	119.24712987	119.21296696	117.60656381	117.62269232	117.40305349
C 17 R18 12 A18 11 D18	A21	108.94292913	109.82310634	109.78472866	110.37821096	109.07214640	111.03917863
C 18 R19 17 A19 12 D19	A22	109.82043826	108.93824606	109.20836972	109.10778278	110.39215444	108.60708411
H 17 R20 12 A20 11 D20	A23	115.59781883	115.59803047	114.98185629	114.15915777	114.19470030	114.59408561
H 18 R21 17 A21 12 D21	A24	125.16136176	125.14242767	126.27172503	128.25678503	128.16382452	127.82549047
H 18 R22 17 A22 12 D22	A25	125.13934733	125.20685821	124.70309096	128.20701763	128.16454398	127.37851548
H 19 R23 18 A23 17 D23	A26	112.30744098	112.33215176	115.31861132	111.63677627	111.45065666	112.45836524
C 19 R24 18 A24 17 D24	A27	119.23564357	119.22874365	119.18705036	117.58697719	117.62508952	117.55682923
C 24 R25 19 A25 18 D25	A28	109.86429770	109.78091189	109.77644122	108.97659383	109.05217170	110.59767094
C 25 R26 24 A26 19 D26	A29	108.93200190	108.98374638	109.22272318	110.39200782	110.42273303	108.89793339
H 24 R27 19 A27 18 D27	A30	115.57996145	115.60859306	114.96764696	114.22017472	114.20513180	114.56971192
H 25 R28 24 A28 19 D28	A31	125.17817734	125.16117450	126.28147705	128.19952896	128.15531884	127.91425466
H 25 R29 24 A29 19 D29	A32	125.13439927	125.11523794	124.73109979	128.21368481	128.21874370	127.47991126
H 26 R30 25 A30 24 D30	A33	112.35144924	112.34646630	115.25539100	111.46016066	111.44529094	112.35687402
C 26 R31 25 A31 24 D31	A34	119.24064423	119.25864281	119.22333413	117.60376812	117.60199624	117.67065082
C 31 R32 26 A32 25 D32	A35	108.95844909	109.82892618	109.78422272	110.43501648	109.03383542	110.48173669
C 32 R33 31 A33 26 D33	A36	109.82637342	108.94638083	109.19813094	109.09717084	110.44785520	109.14418037
H 31 R34 26 A34 25 D34	A37	115.55115167	115.54614430	115.01157480	114.20176516	114.20089349	115.40240521
H 32 R35 31 A35 26 D35	A38	125.22514992	125.23216156	126.25745702	128.11946416	128.02485407	126.76564731
H 32 R36 31 A36 26 D36	A39	125.25687271	125.27387830	124.91527348	128.33415893	128.52066579	127.35266032
H 33 R37 32 A37 31 D37	A40	112.72571549	112.83390533	112.69374391	112.36826373	112.37365772	112.91662237
C 33 R38 32 A38 31 D38	A41	112.41322069	112.32793973	112.46196748	112.33431361	111.06381425	111.74646838
C 38 R39 33 A39 32 D39	A42	118.86326295	118.86148516	119.04704083	117.25425250	117.14528432	117.63947250
C 39 R40 38 A40 33 D40	A43	109.61771357	109.42233445	109.47877833	108.90631960	108.84865792	108.34770624
C 40 R41 39 A41 38 D41	A44	109.46861889	109.63593256	109.77508090	111.11404538	111.12496075	111.00463523
H 38 R42 33 A42 32 D42	A45	109.96022538	109.97243765	109.92769944	109.96596543	111.10403077	110.12515800
H 39 R43 38 A43 33 D43	A46	109.62729014	109.65930567	109.60671877	109.67388256	110.96617848	109.58156630
H 39 R44 38 A44 33 D44	A47	111.19509709	111.14630987	111.40727042	111.16413818	109.47120255	111.59717221
H 40 R45 39 A45 38 D45	A48	111.41409397	111.41262918	111.21149632	111.43774632	109.47123134	110.60787416
H 40 R46 39 A46 38 D46	A49	113.15226482	113.18273453	113.19378603	113.14816136	109.47120255	113.46246259
H 41 R47 40 A47 39 D47	A50	126.24688023	126.24470760	126.28421519	126.23235348	130.07326412	126.57966209
H 41 R48 40 A48 39 D48	A51	111.40991737	111.41003988	111.43031248	111.41514450	112.29471685	111.53923545
C 41 R49 40 A49 39 D49	A52	105.90725344	105.91285131	105.86854100	105.90134369	110.60791865	105.77259906
O 49 R50 41 A50 40 D50							
O 49 R51 41 A51 40 D51							
H 51 R52 49 A52 41 D52							

Table S6-21 Dihedral Angles of EPA

Input Z-matrix EPA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	58.24566920	58.28167826	58.19104305	57.04191589	57.18567250	-62.27413561
H	D5	121.92461126	121.91463665	121.91719503	121.90956012	177.15205134	-122.20542246
C 1 R2	D6	-121.63946204	-121.65494323	-121.64552864	-121.66510871	-62.49041299	121.67186372
C 2 R3 1 A3	D7	-179.20737511	-179.15229087	-179.22239120	-178.92090812	178.79803786	61.99131581
C 3 R4 2 A4 1 D4	D8	-63.20317839	-63.16585295	-63.21431890	-63.40733394	-63.27467262	177.17874517
H 2 R5 3 A5 4 D5	D9	-59.98671167	-59.88813431	-60.22689487	-60.11768654	-59.18043336	-50.29289896
H 2 R6 3 A6 4 D6	D10	119.32499370	119.58411742	118.72706813	118.77411815	119.64734022	130.87373893
H 3 R7 2 A7 1 D7	D11	-178.88712093	-179.14606390	-178.61346262	1.37018136	1.64161581	-0.08429180
H 3 R8 2 A8 1 D8	D12	117.87916162	117.92507705	-119.13528957	115.97537932	116.11136537	-149.86318323
H 4 R9 3 A9 2 D9	D13	0.03595449	-0.10563388	1.19815805	179.94618570	179.93666506	178.52352697
C 4 R10 3 A10 2 D10	D14	-120.65047356	-120.61189802	4.60060166	-121.80747769	121.66486367	-24.51498483
C 10 R11 4 A11 3 D11	D15	-3.96057737	-3.94992873	119.32191019	-5.36471043	-5.16492417	91.06551455
C 11 R12 10 A12 4 D12	D16	-60.52609273	-60.94307643	-168.86256851	-62.20650885	-61.69269703	-57.01095072
H 10 R13 4 A13 3 D13	D17	118.08463008	118.15934596	11.37219495	116.82183706	116.79813464	124.18857462
H 11 R14 10 A14 4 D14	D18	-179.89498872	-179.11072452	-179.42000574	-0.07812048	1.60695549	-1.46739727
H 11 R15 10 A15 4 D15	D19	-117.63030984	117.83013897	-119.34416489	-118.34852433	116.16157850	-143.35285109
H 12 R16 11 A16 10 D16	D20	1.42386670	0.00000000	0.62903536	-179.10954468	179.97824979	177.73096259
C 12 R17 11 A17 10 D17	D21	4.27591006	-120.72646618	4.33317334	3.00090878	121.66472179	-18.45257034
C 17 R18 12 A18 11 D18	D22	120.93155638	-4.06929748	119.13266811	119.43810983	-5.18974950	97.49064595
C 18 R19 17 A19 12 D19	D23	60.92947326	-61.36714896	-169.24141816	58.57433289	-62.13051311	-52.02286473
H 17 R20 12 A20 11 D20	D24	-117.79620150	117.81913401	11.00054951	-120.68204377	116.35072157	129.41602678
H 18 R21 17 A21 12 D21	D25	-179.87866125	-179.25541434	-179.51799074	-0.26100095	1.57892630	-1.36779624
H 18 R22 17 A22 12 D22	D26	117.81751625	117.86610504	-119.29355985	118.60138997	116.35866021	-151.92747172
H 19 R23 18 A23 17 D23	D27	-1.31015079	-0.05781659	0.52788467	179.13205219	179.97987447	177.96187383
C 19 R24 18 A24 17 D24	D28	-120.73736476	-120.73546001	4.36942816	-119.18470377	121.51830693	-27.13420227
C 24 R25 19 A25 18 D25	D29	-4.05908251	-4.06677025	119.14161982	-2.87002216	-5.03744830	88.59481040
C 25 R26 24 A26 19 D26	D30	-60.43881440	-61.88156249	-169.77729577	-61.16379374	-62.30891829	-66.29573685
H 24 R27 19 A27 18 D27	D31	118.23827749	117.15906856	10.46177299	118.02570973	116.14645119	113.74688397
H 25 R28 24 A28 19 D28	D32	179.98833140	-179.02249612	-179.45730548	-0.06834963	1.61687553	-1.72484909
H 25 R29 24 A29 19 D29	D33	-117.22928842	117.23786300	-120.07016952	-119.37028982	116.79787193	-138.04800203
H 26 R30 25 A30 24 D30	D34	1.38623768	0.01107939	0.50313759	-179.21913935	179.94342804	178.98386066
C 26 R31 25 A31 24 D31	D35	4.63901942	-121.29061298	3.70403542	2.06915411	121.17267728	-14.21393087
C 31 R32 26 A32 25 D32	D36	121.31035627	-4.62444756	118.50361305	118.49162550	-4.64081882	102.13745263
C 32 R33 31 A33 26 D33	D37	60.94525164	-61.20420112	-168.80549379	60.38715778	-62.37075249	-86.37830706
H 31 R34 26 A34 25 D34	D38	-117.83594292	117.92358200	11.75699254	-118.64822343	116.09190234	92.37500404
H 32 R35 31 A35 26 D35	D39	-179.93732240	-179.33335934	-179.74095034	-0.16975249	1.65716345	-0.18018182
H 32 R36 31 A36 26 D36	D40	119.01267932	119.14188501	118.33141209	120.08085884	119.63810799	111.94825520
H 33 R37 32 A37 31 D37	D41	178.59254657	178.07563640	178.10150065	177.28252527	177.15330401	174.54241980
C 33 R38 32 A38 31 D38	D42	-0.99635511	0.23559779	-0.31629633	179.34006290	179.55195024	179.41403307
C 38 R39 33 A39 32 D39	D43	-3.63168912	-119.84074482	-120.70583270	-119.55708215	120.05374916	-127.47015854
C 39 R40 38 A40 33 D40	D44	-119.95163415	-3.56909524	-4.31464285	-3.03211817	-3.47884456	-11.53661716
C 40 R41 39 A41 38 D41	D45	56.74568677	56.27482975	56.23299660	55.43353018	57.18659977	52.44862259
H 38 R42 33 A42 32 D42	D46	-59.32510599	-59.83895671	-59.79557616	-60.62405211	-62.48977121	-64.09021684
H 39 R43 38 A43 33 D43	D47	-57.58880287	-57.58605005	59.27632683	-57.51608540	-54.28876340	-61.20510047
H 39 R44 38 A44 33 D44	D48	59.58113236	59.55387168	-57.87470401	59.65520414	65.71122920	56.29763965
H 40 R45 39 A45 38 D45	D49	-178.71401558	-178.69212907	-179.07824085	-178.64654289	174.28877820	176.45876484
H 40 R46 39 A46 38 D46	D50	3.15165688	3.48457634	2.58291038	3.05477557	-0.00311965	-4.43910156
H 41 R47 40 A47 39 D47	D51	-177.09570501	-176.77763983	-177.60273910	-177.18043485	180.00000000	176.55302777
H 41 R48 40 A48 39 D48	D52	-179.62480742	-179.58754659	-179.70316201	-179.64411240	180.00000000	179.57423496
C 41 R49 40 A49 39 D49							
O 49 R50 41 A50 40 D50							
O 49 R51 41 A51 40 D51							
H 51 R52 49 A52 41 D52							

6.8 Z-matrix for DHA structures

Table S6-22 Bond Length of DHA

Input Z-matrix DHA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Lengths							
0 1	R2	1.09679275	1.09679714	1.09673824	1.09679275	1.09679714	1.09673824
H	R3	1.53834940	1.53842520	1.53850094	1.53834940	1.53842520	1.53850094
C 1 R2	R4	1.50501940	1.50497899	1.50498464	1.50501940	1.50497899	1.50498464
C 2 R3 1 A3	R5	1.77101290	1.77099777	1.77109662	1.77101290	1.77099777	1.77109662
C 3 R4 2 A4 1 D4	R6	1.76969913	1.76969893	1.76967737	1.76969913	1.76969893	1.76967737
H 1 R5 2 A5 3 D5	R7	1.09749519	1.09752078	1.09756377	1.09749519	1.09752078	1.09756377
H 1 R6 2 A6 3 D6	R8	1.10060014	1.10055182	1.10043212	1.10060014	1.10055182	1.10043212
H 3 R7 2 A7 1 D7	R9	1.09311391	1.09310050	1.09297797	1.09311391	1.09310050	1.09297797
H 3 R8 2 A8 1 D8	R10	1.33571770	1.33575197	1.33571395	1.33571770	1.33575197	1.33571395
H 4 R9 3 A9 2 D9	R11	1.51089083	1.51091572	1.50494471	1.51089083	1.51091572	1.50494471
C 4 R10 3 A10 2 D10	R12	1.51061277	1.51063495	1.51397424	1.51061277	1.51063495	1.51397424
C 10 R11 4 A11 3 D11	R13	1.09171862	1.09172781	1.09187647	1.09171862	1.09172781	1.09187647
C 11 R12 10 A12 4 D12	R14	1.09966071	1.09963049	1.10069238	1.09966071	1.09963049	1.10069238
H 10 R13 4 A13 3 D13	R15	1.09972756	1.09965249	1.10243322	1.09972756	1.09965249	1.10243322
H 11 R14 10 A14 4 D14	R16	1.09179162	1.09174582	1.09192770	1.09179162	1.09174582	1.09192770
H 11 R15 10 A15 4 D15	R17	1.33563585	1.33565531	1.33533124	1.33563585	1.33565531	1.33533124
H 12 R16 11 A16 10 D16	R18	1.51070520	1.51076786	1.50505001	1.51070520	1.51076786	1.50505001
C 12 R17 11 A17 10 D17	R19	1.51069754	1.51071835	1.51388531	1.51069754	1.51071835	1.51388531
C 17 R18 12 A18 11 D18	R20	1.09172950	1.09173764	1.09018527	1.09172950	1.09173764	1.09018527
C 18 R19 17 A19 12 D19	R21	1.09965665	1.09956163	1.10078786	1.09965665	1.09956163	1.10078786
H 17 R20 12 A20 11 D20	R22	1.09958598	1.09956467	1.10251503	1.09958598	1.09956467	1.10251503
H 18 R21 17 A21 12 D21	R23	1.09174897	1.09174091	1.09193960	1.09174897	1.09174091	1.09193960
H 18 R22 17 A22 12 D22	R24	1.33564043	1.33561976	1.33542210	1.33564043	1.33561976	1.33542210
H 19 R23 18 A23 17 D23	R25	1.51076287	1.51078611	1.50515213	1.51076287	1.51078611	1.50515213
C 19 R24 18 A24 17 D24	R26	1.51064308	1.51066889	1.51422932	1.51064308	1.51066889	1.51422932
C 24 R25 19 A25 18 D25	R27	1.09171967	1.09173333	1.09013753	1.09171967	1.09173333	1.09013753
C 25 R26 24 A26 19 D26	R28	1.09958144	1.09957235	1.10089505	1.09958144	1.09957235	1.10089505
H 24 R27 19 A27 18 D27	R29	1.09960719	1.09955649	1.10234905	1.09960719	1.09955649	1.10234905
H 25 R28 24 A28 19 D28	R30	1.09173117	1.09175297	1.09200228	1.09173117	1.09175297	1.09200228
H 25 R29 24 A29 19 D29	R31	1.33561541	1.33561912	1.33549690	1.33561541	1.33561912	1.33549690
H 26 R30 25 A30 24 D30	R32	1.51069692	1.51074186	1.50500762	1.51069692	1.51074186	1.50500762
C 26 R31 25 A31 24 D31	R33	1.51064706	1.51063609	1.51406265	1.51064706	1.51063609	1.51406265
C 31 R32 26 A32 25 D32	R34	1.09170503	1.09172344	1.09010600	1.09170503	1.09172344	1.09010600
C 32 R33 31 A33 26 D33	R35	1.09966921	1.09955026	1.10085370	1.09966921	1.09955026	1.10085370
H 31 R34 26 A34 25 D34	R36	1.09958900	1.09958720	1.10244202	1.09958900	1.09958720	1.10244202
H 32 R35 31 A35 26 D35	R37	1.09172245	1.09175435	1.09195792	1.09172245	1.09175435	1.09195792
H 32 R36 31 A36 26 D36	R38	1.33561988	1.33556803	1.33537814	1.33561988	1.33556803	1.33537814
H 33 R37 32 A37 31 D37	R39	1.51084342	1.51077024	1.50509028	1.51084342	1.51077024	1.50509028
C 33 R38 32 A38 31 D38	R40	1.51051570	1.51051794	1.51401016	1.51051570	1.51051794	1.51401016
C 38 R39 33 A39 32 D39	R41	1.09176528	1.09179073	1.09017405	1.09176528	1.09179073	1.09017405
C 39 R40 38 A40 33 D40	R42	1.09963008	1.09966775	1.10084340	1.09963008	1.09966775	1.10084340
H 38 R41 33 A41 32 D41	R43	1.09947028	1.09950952	1.10235446	1.09947028	1.09950952	1.10235446
H 39 R42 38 A42 33 D42	R44	1.09152837	1.09157901	1.09193627	1.09152837	1.09157901	1.09193627
H 39 R43 38 A43 33 D43	R45	1.33564594	1.33563785	1.33540354	1.33564594	1.33563785	1.33540354
H 40 R44 39 A44 38 D44	R46	1.50456235	1.50449838	1.50471167	1.50456235	1.50449838	1.50471167
C 40 R45 39 A45 38 D45	R47	1.53571873	1.53573858	1.53576728	1.53571873	1.53573858	1.53576728
C 45 R46 40 A46 39 D46	R48	1.09287899	1.09295430	1.09116298	1.09287899	1.09295430	1.09116298
C 46 R47 45 A47 40 D47	R49	1.09824056	1.09826664	1.09841093	1.09824056	1.09826664	1.09841093
H 45 R48 40 A48 39 D48	R50	1.09575199	1.09572501	1.09588713	1.09575199	1.09572501	1.09588713
H 46 R49 45 A49 40 D49	R51	1.09867103	1.09863591	1.09845873	1.09867103	1.09863591	1.09845873
H 46 R50 45 A50 40 D50	R52	1.09710929	1.09715516	1.09734726	1.09710929	1.09715516	1.09734726
H 47 R51 46 A51 45 D51	R53	1.51337249	1.51336180	1.51299888	1.51337249	1.51336180	1.51299888
H 47 R52 46 A52 45 D52	R54	1.35818516	1.35817969	1.35872586	1.35818516	1.35817969	1.35872586
C 47 R53 46 A53 45 D53	R55	1.21113773	1.21112080	1.21121287	1.21113773	1.21112080	1.21121287
O 53 R54 47 A54 46 D54	R56	0.97585985	0.97585058	0.97582917	0.97585985	0.97585058	0.97582917
O 53 R55 47 A55 46 D55							
H 54 R56 53 A56 47 D56							

Table S6-23 Bond Angles of DHA

Input Z-matrix DHA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Bond Angles							
0 1	A3	111.13772400	111.15927582	111.13958686	111.13772400	111.15927582	111.13958686
H	A4	112.80909061	112.81243608	112.80102624	112.80909061	112.81243608	112.80102624
C 1 R2	A5	36.11865006	36.12170277	36.11425403	36.11865006	36.12170277	36.11425403
C 2 R3 1 A3	A6	36.15927001	36.15936618	36.15775834	36.15927001	36.15936618	36.15775834
C 3 R4 2 A4 1 D4	A7	109.79092986	109.75941313	109.75489761	109.79092986	109.75941313	109.75489761
H 1 R5 2 A5 3 D5	A8	108.61910470	108.62686112	108.61280780	108.61910470	108.62686112	108.61280780
H 1 R6 2 A6 3 D6	A9	115.78252565	115.82593223	115.76695570	115.78252565	115.82593223	115.76695570
H 3 R7 2 A7 1 D7	A10	125.45227673	125.39747273	125.48126995	125.45227673	125.39747273	125.48126995
H 3 R8 2 A8 1 D8	A11	125.21440083	125.25439005	125.18364632	125.21440083	125.25439005	125.18364632
H 4 R9 3 A9 2 D9	A12	112.31939624	112.29614899	115.38520033	112.31939624	112.29614899	115.38520033
C 4 R10 3 A10 2 D10	A13	119.19332574	119.16913842	118.98217545	119.19332574	119.16913842	118.98217545
C 10 R11 4 A11 3 D11	A14	109.92253368	109.88478576	109.71400579	109.92253368	109.88478576	109.71400579
C 11 R12 10 A12 4 D12	A15	108.93493277	108.96421188	109.13875995	108.93493277	108.96421188	109.13875995
H 10 R13 4 A13 3 D13	A16	115.57636278	115.59904803	114.94599743	115.57636278	115.59904803	114.94599743
H 11 R14 10 A14 4 D14	A17	125.19865323	125.18713022	126.31499574	125.19865323	125.18713022	126.31499574
H 11 R15 10 A15 4 D15	A18	125.13471411	125.12567783	124.77791394	125.13471411	125.12567783	124.77791394
H 12 R16 11 A16 10 D16	A19	112.32890499	112.32242516	115.22347040	112.32890499	112.32242516	115.22347040
C 12 R17 11 A17 10 D17	A20	119.23628020	119.23647430	119.23190676	119.23628020	119.23647430	119.23190676
C 17 R18 12 A18 11 D18	A21	108.93123427	109.86768534	109.81571697	108.93123427	109.86768534	109.81571697
C 18 R19 17 A19 12 D19	A22	109.86631671	108.92953950	109.17034986	109.86631671	108.92953950	109.17034986
H 17 R20 12 A20 11 D20	A23	115.57808911	115.58977363	115.03893160	115.57808911	115.58977363	115.03893160
H 18 R21 17 A21 12 D21	A24	125.19652049	125.17152007	126.20349868	125.19652049	125.17152007	126.20349868
H 18 R22 17 A22 12 D22	A25	125.09851532	125.16821905	124.80706259	125.09851532	125.16821905	124.80706259
H 19 R23 18 A23 17 D23	A26	112.32919965	112.26652670	115.19961819	112.32919965	112.26652670	115.19961819
C 19 R24 18 A24 17 D24	A27	119.24803190	119.23060534	119.22671467	119.24803190	119.23060534	119.22671467
C 24 R25 19 A25 18 D25	A28	109.88579481	109.84334662	109.83407693	109.88579481	109.84334662	109.83407693
C 25 R26 24 A26 19 D26	A29	108.92177036	108.95795534	109.15146050	108.92177036	108.95795534	109.15146050
H 24 R27 19 A27 18 D27	A30	115.56507094	115.59572008	115.06589197	115.56507094	115.59572008	115.06589197
H 25 R28 24 A28 19 D28	A31	125.21958535	125.18089276	126.17752688	125.21958535	125.18089276	126.17752688
H 25 R29 24 A29 19 D29	A32	125.07117202	125.10304029	124.76147532	125.07117202	125.10304029	124.76147532
H 26 R30 25 A30 24 D30	A33	112.31298792	112.29792044	115.26832336	112.31298792	112.29792044	115.26832336
C 26 R31 25 A31 24 D31	A34	119.25647542	119.23970852	119.16456353	119.25647542	119.23970852	119.16456353
C 31 R32 26 A32 25 D32	A35	108.91117094	109.91321206	109.83058718	108.91117094	109.91321206	109.83058718
C 32 R33 31 A33 26 D33	A36	109.90855686	108.92259911	109.18570318	109.90855686	108.92259911	109.18570318
H 31 R34 26 A34 25 D34	A37	115.57063888	115.54997052	115.02718216	115.57063888	115.54997052	115.02718216
H 32 R35 31 A35 26 D35	A38	125.21265628	125.22763678	126.21253969	125.21265628	125.22763678	126.21253969
H 32 R36 31 A36 26 D36	A39	125.07723278	125.11866313	124.79359667	125.07723278	125.11866313	124.79359667
H 33 R37 32 A37 31 D37	A40	112.34145678	112.37653293	115.20350288	112.34145678	112.37653293	115.20350288
C 33 R38 32 A38 31 D38	A41	119.25167117	119.24979428	119.17312388	119.25167117	119.24979428	119.17312388
C 38 R39 33 A39 32 D39	A42	109.88376857	109.85361742	109.82373167	109.88376857	109.85361742	109.82373167
C 39 R40 38 A40 33 D40	A43	108.93294033	108.94557733	109.21151401	108.93294033	108.94557733	109.21151401
H 38 R41 33 A41 32 D41	A44	115.59393286	115.63448132	115.09023398	115.59393286	115.63448132	115.09023398
H 39 R42 38 A42 33 D42	A45	125.23126208	125.15994556	126.18134863	125.23126208	125.15994556	126.18134863
H 39 R43 38 A43 33 D43	A46	125.11386096	125.20037355	124.81701616	125.11386096	125.20037355	124.81701616
H 40 R44 39 A44 38 D44	A47	112.28116369	112.17223300	112.15546528	112.28116369	112.17223300	112.15546528
C 40 R45 39 A45 38 D45	A48	118.79656493	118.76746642	118.93081454	118.79656493	118.76746642	118.93081454
C 45 R46 40 A46 39 D46	A49	110.24226122	110.25425560	110.23580634	110.24226122	110.25425560	110.23580634
C 46 R47 45 A47 40 D47	A50	110.27103466	110.32038093	110.44553574	110.27103466	110.32038093	110.44553574
H 45 R48 40 A48 39 D48	A51	111.19270260	111.16629349	111.15547225	111.19270260	111.16629349	111.15547225
H 46 R49 45 A49 40 D49	A52	111.11238296	111.10196377	111.05271945	111.11238296	111.10196377	111.05271945
H 46 R50 45 A50 40 D50	A53	112.85793354	112.93513578	112.99996856	112.85793354	112.93513578	112.99996856
H 47 R51 46 A51 45 D51	A54	111.44574744	111.41476533	111.44706457	111.44574744	111.41476533	111.44706457
H 47 R52 46 A52 45 D52	A55	126.16923121	126.18507528	126.23721574	126.16923121	126.18507528	126.23721574
C 47 R53 46 A53 45 D53	A56	105.92954765	105.94766768	105.88674128	105.92954765	105.94766768	105.88674128
O 53 R54 47 A54 46 D54							
O 53 R55 47 A55 46 D55							
H 54 R56 53 A56 47 D56							

Table S6-24 Dihedral Angles of DHA

Input Z-matrix DHA		Trans Beta	Trans Extended	Trans Helix	cis Beta	cis Extended	cis Helix
Dihedral Angles							
0 1	D4	58.21594492	58.30021294	58.16536429	58.21594492	58.30021294	58.16536429
H	D5	121.91044651	121.93092464	121.90470013	121.91044651	121.93092464	121.90470013
C 1 R2	D6	-121.65331304	-121.64132943	-121.65492460	-121.65331304	-121.64132943	-121.65492460
C 2 R3 1 A3	D7	-179.21548048	-179.16484124	-179.23977719	-179.21548048	-179.16484124	-179.23977719
C 3 R4 2 A4 1 D4	D8	-63.21760845	-63.17203329	-63.22410112	-63.21760845	-63.17203329	-63.22410112
H 1 R5 2 A5 3 D5	D9	-59.49516890	-60.10636134	-60.20029585	-59.49516890	-60.10636134	-60.20029585
H 1 R6 2 A6 3 D6	D10	119.89089080	119.25427474	118.70232781	119.89089080	119.25427474	118.70232781
H 3 R7 2 A7 1 D7	D11	-179.02183635	-178.97952362	-178.58897083	-179.02183635	-178.97952362	-178.58897083
H 3 R8 2 A8 1 D8	D12	118.41345445	118.17990553	-118.68103475	118.41345445	118.17990553	-118.68103475
H 4 R9 3 A9 2 D9	D13	-0.02849788	-0.00388219	1.28096101	-0.02849788	-0.00388219	1.28096101
C 4 R10 3 A10 2 D10	D14	-120.12758365	-120.39557904	5.03682938	-120.12758365	-120.39557904	5.03682938
C 10 R11 4 A11 3 D11	D15	-3.45221664	-3.71292042	119.76947699	-3.45221664	-3.71292042	119.76947699
C 11 R12 10 A12 4 D12	D16	-60.44901792	-61.11956141	-168.59317326	-60.44901792	-61.11956141	-168.59317326
H 10 R13 4 A13 3 D13	D17	118.19665050	117.88330878	11.67328183	118.19665050	117.88330878	11.67328183
H 11 R14 10 A14 4 D14	D18	179.99573836	-178.94455812	-179.45930626	179.99573836	-178.94455812	-179.45930626
H 11 R15 10 A15 4 D15	D19	-117.53058903	117.83870748	-119.55630507	-117.53058903	117.83870748	-119.55630507
H 12 R16 11 A16 10 D16	D20	1.39387683	0.10302202	0.57748578	1.39387683	0.10302202	0.57748578
C 12 R17 11 A17 10 D17	D21	4.34405068	-120.71308886	4.23249536	4.34405068	-120.71308886	4.23249536
C 17 R18 12 A18 11 D18	D22	121.01473837	-4.03532011	119.02148440	121.01473837	-4.03532011	119.02148440
C 18 R19 17 A19 12 D19	D23	60.42272113	-60.48135359	-168.01111947	60.42272113	-60.48135359	-168.01111947
H 17 R20 12 A20 11 D20	D24	-118.31284388	118.67384526	12.14732617	-118.31284388	118.67384526	12.147326177
H 18 R21 17 A21 12 D21	D25	-179.86896477	-179.11758233	-179.36734442	-179.86896477	-179.11758233	-179.36734442
H 18 R22 17 A22 12 D22	D26	117.16929698	118.52609982	-118.68403469	117.16929698	118.52609982	-118.68403469
H 19 R23 18 A23 17 D23	D27	-1.32963248	0.01092353	0.66402259	-1.32963248	0.01092353	0.66402259
C 19 R24 18 A24 17 D24	D28	-121.33685513	-120.07244932	5.07362701	-121.33685513	-120.07244932	5.07362701
C 24 R25 19 A25 18 D25	D29	-4.65257410	-3.39674217	119.87859281	-4.65257410	-3.39674217	119.87859281
C 25 R26 24 A26 19 D26	D30	-60.49056957	-60.74743781	-167.22473280	-60.49056957	-60.74743781	-167.22473280
H 24 R27 19 A27 18 D27	D31	118.29078118	118.29593457	13.05676948	118.29078118	118.29593457	13.05676948
H 25 R28 24 A28 19 D28	D32	179.79071509	-178.89500766	-179.51075660	179.79071509	-178.89500766	-179.51075660
H 25 R29 24 A29 19 D29	D33	-117.45318922	118.14217521	-118.46297195	-117.45318922	118.14217521	-118.46297195
H 26 R30 25 A30 24 D30	D34	1.26781200	0.09518298	0.47337382	1.26781200	0.09518298	0.47337382
C 26 R31 25 A31 24 D31	D35	4.37258824	-120.34576711	5.23552042	4.37258824	-120.34576711	5.23552042
C 31 R32 26 A32 25 D32	D36	121.05002418	-3.66784556	120.03689820	121.05002418	-3.66784556	120.03689820
C 32 R33 31 A33 26 D33	D37	59.82801613	-60.02281318	-168.54867290	59.82801613	-60.02281318	-168.54867290
H 31 R34 26 A34 25 D34	D38	-118.96566429	119.22284942	11.75798923	-118.96566429	119.22284942	11.75798923
H 32 R35 31 A35 26 D35	D39	-179.84397267	-179.28559536	-179.58772140	-179.84397267	-179.28559536	-179.58772140
H 32 R36 31 A36 26 D36	D40	116.72497074	118.71258915	-118.77320632	116.72497074	118.71258915	-118.77320632
H 33 R37 32 A37 31 D37	D41	-1.29686235	-0.04851435	0.50336096	-1.29686235	-0.04851435	0.50336096
C 33 R38 32 A38 31 D38	D42	-121.74335344	-119.81252154	4.91617720	-121.74335344	-119.81252154	4.91617720
C 38 R39 33 A39 32 D39	D43	-5.06917035	-3.18271427	119.76523830	-5.06917035	-3.18271427	119.76523830
C 39 R40 38 A40 33 D40	D44	-60.92483848	-60.38435554	-167.55830659	-60.92483848	-60.38435554	-167.55830659
H 38 R41 33 A41 32 D41	D45	118.39768178	118.94559392	13.32862883	118.39768178	118.94559392	13.32862883
H 39 R42 38 A42 33 D42	D46	-179.83352275	-179.72174149	179.50358266	-179.83352275	-179.72174149	179.50358266
H 39 R43 38 A43 33 D43	D47	118.61460910	119.25751456	119.09834920	118.61460910	119.25751456	119.09834920
H 40 R44 39 A44 38 D44	D48	0.18222037	0.25908848	-0.42875987	0.18222037	0.25908848	-0.42875987
C 40 R45 39 A45 38 D45	D49	-120.52765957	-119.94581391	-120.18716835	-120.52765957	-119.94581391	-120.18716835
C 45 R46 40 A46 39 D46	D50	-3.63953941	-3.00431575	-3.19560075	-3.63953941	-3.00431575	-3.19560075
C 46 R47 45 A47 40 D47	D51	55.83209684	55.71494613	55.75329983	55.83209684	55.71494613	55.75329983
H 45 R48 40 A48 39 D48	D52	-61.29488257	-61.37166128	-61.24819402	-61.29488257	-61.37166128	-61.24819402
H 46 R49 45 A49 40 D49	D53	176.88692552	176.79401529	176.98492122	176.88692552	176.79401529	176.98492122
H 46 R50 45 A50 40 D50	D54	176.77683957	177.31701341	178.42779156	176.77683957	177.31701341	178.42779156
H 47 R51 46 A51 45 D51	D55	-3.37537803	-2.83126932	-1.65005130	-3.37537803	-2.83126932	-1.65005130
H 47 R52 46 A52 45 D52	D56	179.76961023	179.74857821	179.86274069	179.76961023	179.74857821	179.86274069
C 47 R53 46 A53 45 D53							
O 53 R54 47 A54 46 D54							
O 53 R55 47 A55 46 D55							
H 54 R56 53 A56 47 D56							

7. Hartree Fock Method

7.1 Generation of Hartree Fock Equation and coefficient matrix

A many electron wavefunction (7-1)

$$\Phi(1,2,...,N) \tag{7-1}$$

becomes (7-2):

$$\Phi(1) = u(1) \tag{7-2}$$

when N=1.

In a given wave function, the electrons (e), include both a space function ϕ and spin function (α or β) ((7-3)

$$\mathrm{u}(1) = \begin{cases} \phi_1(1)\alpha(1) \\ \phi_1(1)\beta(1) \end{cases} \tag{7-3}$$

Many-electron wave functions may be constructed as products of one-electron functions or spin-orbitals (7-4)

$$= \frac{1}{\sqrt{N!}} \sum_{\nu=1}^{N!} (-1)^{\nu} \hat{P}_{\nu} u_1(1) u_2(2)..u_N(N) = \frac{1}{\sqrt{N!}} \sum_{\nu=1}^{N!} (-1)^{\nu} \hat{P}_{\nu} u_1(1) u_2(2)..u_N(N) \tag{7-4}$$

which equivalent to the formula for a determinant. (7-5) and (7-6):

$$\Phi(1,2,...,N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(1) & \Lambda & u_N(1) \\ \mathrm{M} & & \mathrm{M} \\ u_1(N) & \Lambda & u_N(N) \end{vmatrix} \tag{7-5}$$

$$\Phi(1,2,...,2M) = \frac{1}{\sqrt{(2M)!}} \begin{vmatrix} \phi_1(1)\alpha(1) & \phi_1(1)\beta(1) & \Lambda & \phi_M(1)\alpha(1) & \phi_M(1)\beta(1) \\ \mathrm{M} & \mathrm{M} & & \mathrm{M} & \mathrm{M} \\ \phi_1(2M)\alpha(2M) & \phi_1(2M)\beta(2M) & \Lambda & \phi_M(2M)\alpha(2M) & \phi_M(2M)\beta(2M) \end{vmatrix} \tag{7-6}$$

This is known as the Slater determinant.
Given the Schrödinger equation (7-7) which is a function for many electrons:

$$\hat{H}\Psi = \mathrm{E}\Psi \tag{7-7}$$

Applying the variation theorem, the Slater determinant can be converted to a set of equations called the Hartree Fock equations. (7-8)

$$\text{Many one-electron wave-equations} \begin{cases} \hat{F}(1)\Phi_1(1) = \varepsilon_{11}(1)\Phi_1(1) \\ \hat{F}(1)\Phi_2(1) = \varepsilon_{22}(1)\Phi_2(1) \\ \text{M} \\ \hat{F}(1)\Phi_N(1) = \varepsilon_{NN}(1)\Phi_N(1) \end{cases} \tag{7-8}$$

Hartree-Fock equation leads to the matrix equations where the matrix elements of the Fock operator have the following from (7-9):

$$F^{\phi}{}_{ij} = \int \phi_j \hat{F} \phi_i d\tau = \varepsilon_{ii} \int \phi_j \phi_i d\tau = \varepsilon_{ij} S_{ij}^{\Phi} \tag{7-9}$$

However, it is convenient to write (7-9) in the form of a matrix equation (7-10)

$$\underline{\underline{F}}^{\phi} = \underline{\underline{S}}^{\phi} \underline{\underline{\varepsilon}} \tag{7-10}$$

Where the ith,jth elements of S_{ij}^{ϕ} defined as $<\phi_i|\phi_j>$. For an orthonormal set of functions $\{\phi_i\} S_{ij}^{\phi}$ will become S_{ij}, which is 1 if $i = j$ and 0 if $i \neq j$. The orthonormal set of MOs can be expanded in terms of a set of known AOs $\{\eta\}$. Therefore, (7-11)

$$\langle \phi | \equiv (\underbrace{\phi_1 \phi_2 \Lambda \phi_M}_{\text{occupied}} \overbrace{\phi_{M+1} \Lambda \phi_N}^{\text{HOMO LUMO}}) = (\eta_1, \eta_2, \Lambda\ \eta_N) \underbrace{\begin{pmatrix} c_{11} & c_{12} & \Lambda & c_{1M} & c_{1M+1} & \Lambda & c_{1N} \\ c_{21} & c_{22} & \Lambda & c_{2M} & c_{2M+1} & \Lambda & c_{2N} \\ \text{M} & \text{M} & & \text{M} & \text{M} & & \text{M} \\ c_{N1} & c_{N2} & \Lambda & c_{NM} & c_{NM+1} & \Lambda & c_{NN} \end{pmatrix}}_{\text{Coeficients for the M doubly occupied MO}} \tag{7-11}$$

in vector notation is (7-12):

$$\langle \phi | = \langle \eta | \underline{\underline{C}} \tag{7-12}$$

Hartree-Fock equation assumes the following form (7-13)

$$\underbrace{\begin{pmatrix} \varepsilon_{11} & 0 & 0 & 0 \\ 0 & \varepsilon_{22} & 0 & 0 \\ 0 & 0 & O & 0 \\ 0 & 0 & 0 & \varepsilon_{NN} \end{pmatrix}}_{\text{Diagonal}} = \begin{pmatrix} c_{11} & c_{21} & \Lambda & c_{N1} \\ c_{21} & c_{22} & \Lambda & c_{N2} \\ \text{M} & \text{M} & & \text{M} \\ c_{1N} & c_{2N} & \Lambda & c_{NN} \end{pmatrix} \underbrace{\begin{pmatrix} F_{11}^{\eta} & F_{12}^{\eta} & \Lambda & F_{1N}^{\eta} \\ F_{21}^{\eta} & F_{22}^{\eta} & \Lambda & F_{2N}^{\eta} \\ \text{M} & \text{M} & & \text{M} \\ F_{N1}^{\eta} & F_{N2}^{\eta} & \Lambda & F_{NN}^{\eta} \end{pmatrix}}_{\text{Real\_symmetric}} \begin{pmatrix} c_{11} & c_{12} & \Lambda & c_{1N} \\ c_{21} & c_{22} & \Lambda & c_{2N} \\ \text{M} & \text{M} & & \text{M} \\ c_{1N} & c_{2N} & \Lambda & c_{NN} \end{pmatrix} \tag{7-13}$$

From the coefficients of the M doubly occupied MO we may generate the density matrix(r) (7-14) and (7-15)

$$\underline{\underline{C}}_M \underline{\underline{C}}_M^{\dagger} = \underline{\underline{\rho}} \tag{7-14}$$

$$\underbrace{\begin{pmatrix} c_{11} & c_{12} & \Lambda & c_{1M} \\ c_{21} & c_{22} & \Lambda & c_{2M} \\ \text{M} & \text{M} & & \text{M} \\ c_{N1} & c_{N2} & \Lambda & c_{NM} \end{pmatrix}}_{NxM} \underbrace{\begin{pmatrix} c_{11} & c_{12} & \Lambda & c_{1N} \\ c_{21} & c_{22} & \Lambda & c_{2N} \\ \text{M} & \text{M} & & \text{M} \\ c_{1M} & c_{2N} & \Lambda & c_{NM} \end{pmatrix}}_{MXN} = \underbrace{\begin{pmatrix} \rho_{11} & \rho_{21} & \Lambda & \rho_{N1} \\ \rho_{21} & \rho_{22} & \Lambda & \rho_{N2} \\ \text{M} & \text{M} & & \text{M} \\ \rho_{1N} & \rho_{2N} & \Lambda & \rho_{NM} \end{pmatrix}}_{NXN\ \text{Re}al\_Symmetric} \tag{7-15}$$

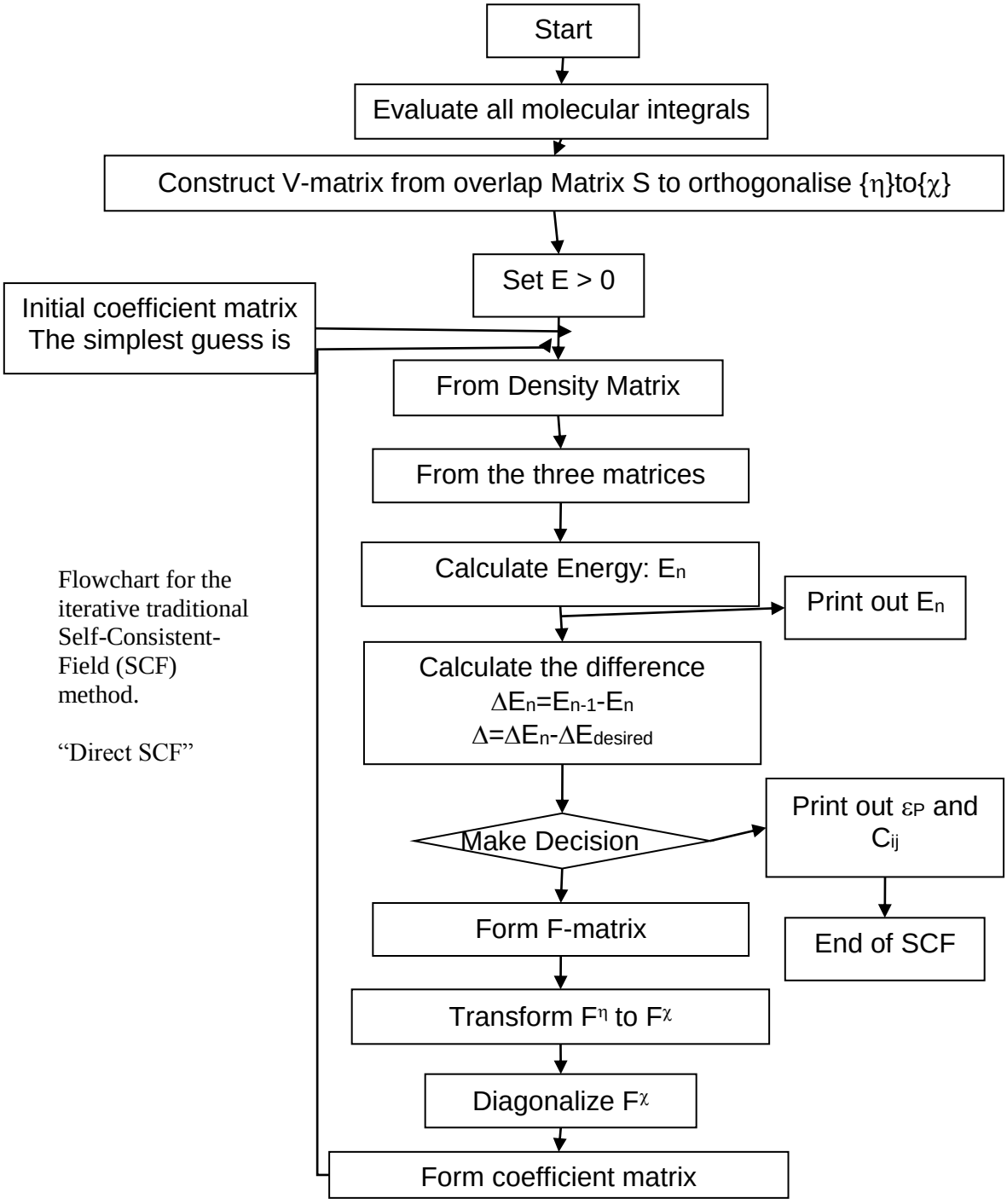
The elements of the Fock matrix F_{ij}^{η} the (h_{ij}^{η}), (J_{ij}^{η}) and (K_{ij}^{η}) integrals are evaluated (7-16),

$$F_{ij}^{\eta} = h_{ij}^{\eta} + 2J_{ij}^{\eta} - K_{ij}^{\eta} = h_{ij}^{\eta} + \sum_{k=1}^{N}\sum_{l=1}^{N}\left[2\left\{\eta_i\eta_j\middle|\eta_k\eta_l\right\} - \left\{\eta_i\eta_k\middle|\eta_j\eta_l\right\}\right]\rho_{kl} \tag{7-16}$$

The total electronic energy (E) (7-17):

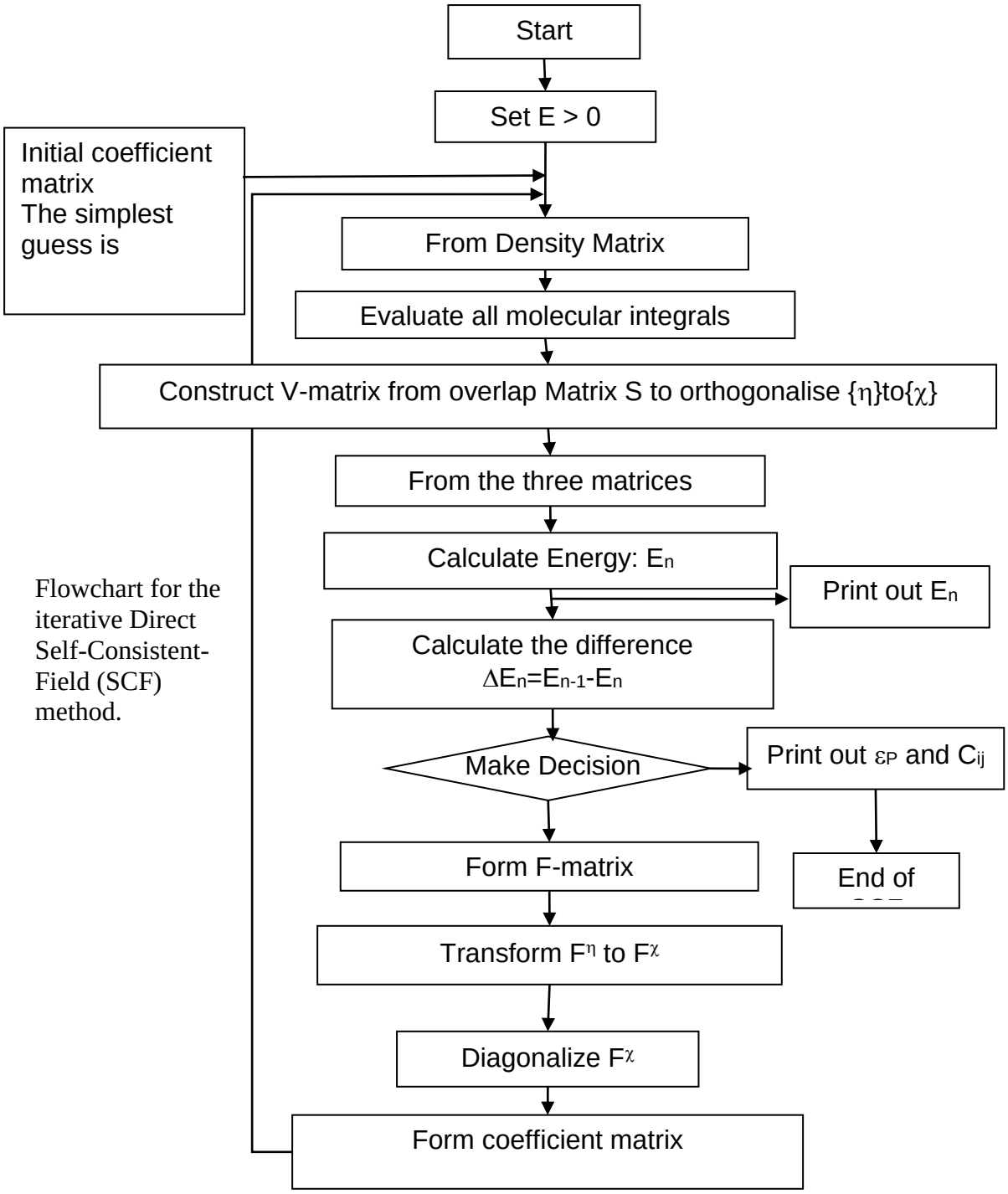
$$E = 2\sum_{i=1}^{N}\sum_{j=1}^{N}\rho_{ij}^{(1)}h_{ij}^{\eta} + \sum_{i=1}^{N}\sum_{j=1}^{N}\rho_{ij}^{(1)}\left[2J_{ij}^{\eta} - K_{ij}^{\eta}\right] \tag{7-17}$$

7.2 The Hartree Fock Method is summarized in the flowchart below



Flowchart for the iterative traditional Self-Consistent-Field (SCF) method.

"Direct SCF"



Flowchart for the iterative Direct Self-Consistent-Field (SCF) method.

8. Atomic Orbital expansion of Molecular Orbital

The term "orbital" is a synonym for the term "One-Electron" Function (OEF). A single centered OEF is synonymous with "Atomic Orbital". A multi centered OEF is synonymous with "Molecular Orbital". Therefore, Orbital = OEF. There are three ways to express a mathematical function:

1. Explicitly in analytical form :
   (hydrogen-like AOs)
2. As a table of numbers:
   (Hartree-Fock type AOs for numerous atoms)

x	f(x)
0.0	1.000
0.1	1.105
0.2	1.221

3. In the form of an expansion (expression of an MO in terms of a set of AO) (8-1) to (8-3):

$$f(x) = e^x \tag{8-1}$$

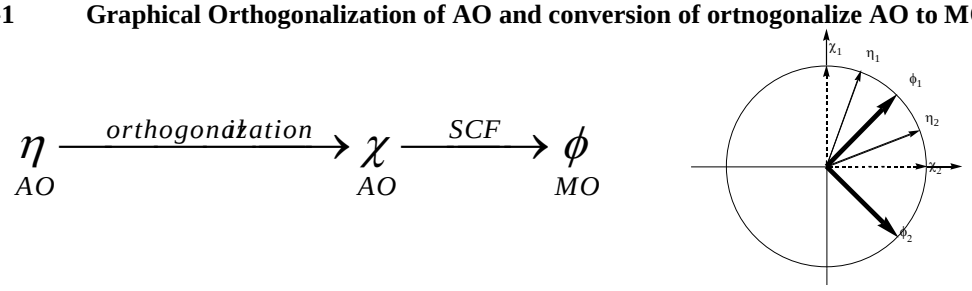
$$f(x) \equiv e^x = C_0 x^0 + C_1 x^1 + C_2 x^2 + C_3 x^3 + \mathrm{K} = \frac{f(0)}{0!} x^0 + \frac{f'(0)}{1!} x^1 + \frac{f''(0)}{2!} x^2 + \frac{f'''(0)}{3!} x^3 + = \mathrm{K} \tag{8-2}$$

By analyzing the MO expansion in terms of AOs, MO has the form as shown in (8-3):

$$\phi = C_0\eta_0 + C_1\eta_1 + C_2\eta_2 + C_3\eta_3 + \mathrm{K} \tag{8-3}$$

The generation of MOs (ϕ-s) from AOs (η-*s*) is equivalent to the transformation of an N-dimensional vector space where $\{\eta\}$is the original set of non-orthogonal functions. After orthogonalization of the non-orthogonal AO basis set $\{\eta\}$ the orthogonal set $\{\chi\}$ is rotated to another orthogonal set $\{\phi\}$ (**Figure 8-1**).

Figure 8-1 Graphical Orthogonalization of AO and conversion of ortnogonalize AO to MO



There are certain differences between the shape of numerical Hartree-Fock atomic orbitals (HF-AO), the analytic Slater type orbitals (**STO**) and the analytic Gaussian type functions (**GTF**). However, these differences are irrelevant to the final results as the MO can be expanded in terms of any of these complete sets of functions to any desired degree of accuracy.

8.1 Atomic Orbital Basis Sets

The generation of MO from AO requires the generation and transformation of the Fock matrix into diagonal form. The elements of the Fock matrix are assembled from integrals in the following fashion (8-4):

$$f_{ij} = \left\langle i\left|\hat{h}\right|j\right\rangle + \sum_{k}^{N}\sum_{l}^{N}\left[2\{ij|kl\} - \{ik|jl\}\right] \tag{8-4}$$

Where the first term is a one-electron integral and the latter terms are two-electron integrals as shown in (8-5) and (8-6) .

$$\left\langle i\left|\hat{h}\right|j\right\rangle \equiv \left\langle \eta_i\left|\hat{h}\right|\eta_j\right\rangle \equiv \int_1 \eta_i(1)\hat{h}_1\eta_j(1)d\tau_1 \tag{8-5}$$

$$\{ij|kl\} \equiv \left\langle \eta_i\eta_k\left|\frac{1}{r_{12}}\right|\eta_l\eta_j\right\rangle \equiv \int_1\int_2 \eta_i(1)\eta_l(2)\eta_j(1)d\tau_1 = \int_1 \eta_i(1)\left\{\int_2 \eta_k(2)\frac{1}{r_{12}}\eta_l'(2)d\tau_2\right\} \quad \eta_z(l)d\tau_1 \tag{8-6}$$

Therefore, the number of integrals can be generated as shown in equations (8-7) and (8-8)

$$\text{Number of 1-electron integrals} : p = \frac{N(N+1)}{2} \tag{8-7}$$

$$\text{Number of 2-electron integrals} : q = \frac{p(p+1)}{2} \tag{8-8}$$

From **Table 8-1**, it can be seen that the number of integrals generated becomes very large very quickly.

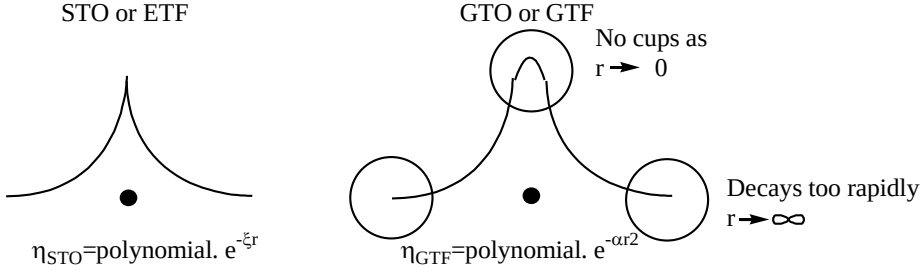
Table 8-1 **Number of integrals generated using the above questions**

N	p	q
1	1	1
10	55	1,540
50	1,275	814,725
100	5.050	12,751,250
150	11,325	64,133,475
200	20100	202,015,050
300	45150	1,019,261,250

To solve this problem, two types of analytic functions are used for molecular computations.

1) Slater-type orbital (**STO**) or exponential type functions.(**ETF**) in **Figure 8-2, left**.
2) Gaussian-type orbital (**GTO**) or Gaussian-type function (**GTF**) in **Figure 8-2, right**.

Figure 8-2 **Representation of ETF function (left) and GTF function (right)**



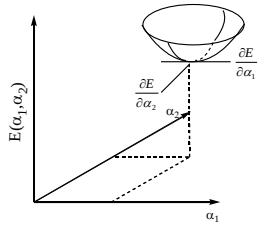
The GTF are more popular as it is possible to compute the integrals over Gaussian very quickly, but only relative large N gives accurate results. These AO basis sets need to be optimized for molecular calculation. This may be achieved by minimizing the electronic energy with respect to all orbital exponents.

The orbital case is shown in **Figure 8-3**

Figure 8-3 Graphic representation optimum orbital exponents (α_1, α_2) in a two dimesional AO vectorspan

$$\eta_1 = polynomial_1.e^{-\alpha_1 r^2}$$

$$\eta_2 = polynomial_2.e^{-\alpha_2 r^2}$$



Sometimes STOs are expanded in terms of GTFs or, in other words, a GTF basis set is contracted to a set of STO. The contraction of a set of three Gaussian-type functions to single Slater function used to be very popular (STO-3G) (8-9) (8-9):

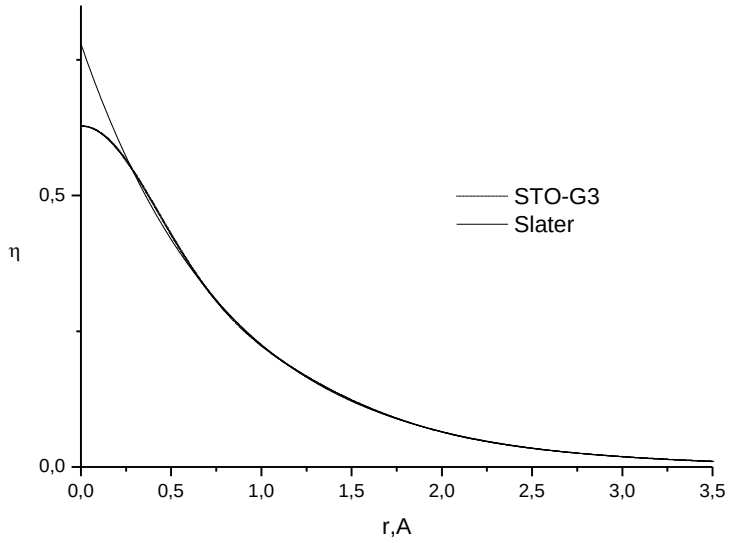
$$\eta_i^{STO} = d_{i1}\eta_1^{GTF} + d_{i2}\eta_2^{GTF} + d_{i3}\eta_3^{GTF} \tag{8-9}$$

This means that the total number of integrals to be stored can be reduced by contraction as illustrated bellow (8-10):

$$\begin{aligned}
&\left\langle \eta_i^{STO} \middle| \hat{h} \middle| \eta_j^{STO} \right\rangle = \\
&\left\langle d_{i1}\eta_1^{GTF} + d_{i2}\eta_2^{GTF} + d_{i3}\eta_3^{GTF} \middle| \hat{h} \middle| d_{i1}\eta_1^{GTF} + d_{i2}\eta_2^{GTF} + d_{i3}\eta_3^{GTF} \right\rangle \\
&d_{i1}d_{j1}\left\langle \eta_1^{GTF} \middle| \hat{h} \middle| \eta_1^{GTF} \right\rangle \\
&+ d_{i2}d_{j1}\left\langle \eta_2^{GTF} \middle| \hat{h} \middle| \eta_1^{GTF} \right\rangle \\
&+ d_{i3}d_{j1}\left\langle \eta_3^{GTF} \middle| \hat{h} \middle| \eta_1^{GTF} \right\rangle \\
&\text{M} \\
&d_{i2}d_{j3}\left\langle \eta_3^{GTF} \middle| \hat{h} \middle| \eta_3^{GTF} \right\rangle = \\
&\sum_k^3 \sum_l^3 d_{ik}d_{jl}\left\langle \eta_k^{GTF} \middle| \hat{h} \middle| \eta_l^{GTF} \right\rangle
\end{aligned} \tag{8-10}$$

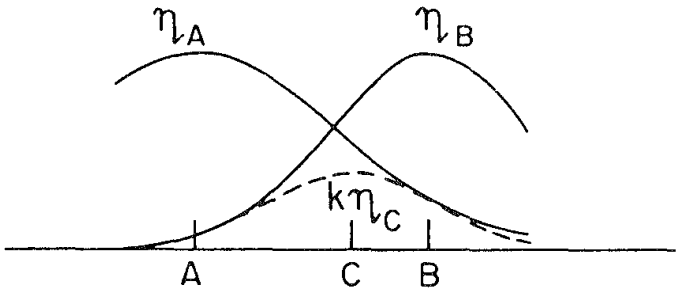
The contraction of basis set reduces the size of the Fock matrix which will be more manageable to find the solution. In the above case 9 integrals have been evaluated, but only their sum total, that is, a single integral, is stored. The STO-3G basis function is a contracted Gaussian consisting of three primitive Gaussians. Typically, an ab initio basis function consists of a set of primitive Gaussians bundled together with a set of contraction coefficient.

Figure 8-4 Comparison of STO and Slater basis function



The basic advantage of Gaussian type functions is due to the fact that the product of any two Gaussian is also a Gaussian with its centre on a line between the centres of the two original Gaussian functions (Figure 8-5).

Figure 8-5 Overlapping of two Gaussian functions



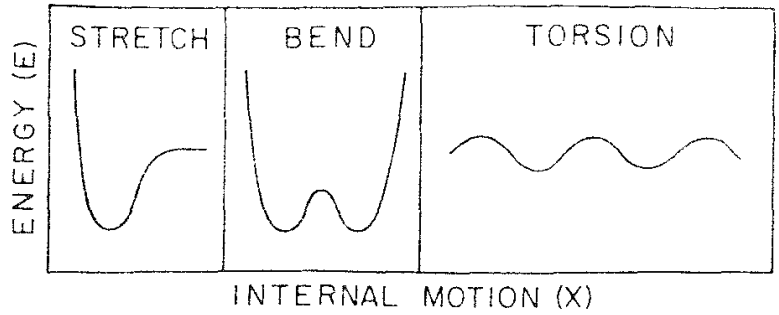
Consequently, all integrals have explicit analytical expressions and may be evaluated rapidly. A similar theorem does not exist for STO. The principal disadvantages of GTF are their smooth behaviour (lack of cusp) at the nucleus and their too rapid (by rather than by) decrease at large distances. This improper asymptotic behaviour requires the use of a larger number of GTF than STO for equivalent accuracy. However, the much greater speed per integral

evaluation in terms of GTF as opposed to STO allows for this greater total number of integrals.

9. Potential Energy Surfaces

There are three types of internal motions of molecules: stretch, bend and torsion. The torsion is a periodic motion even if its periodicity low so that it repeats itself only after a 360° rotation. The bending motion usually governs a double-well potential. If the bonds that undergo bending motion are attached to N or O then the barrier to inversion is quite low (from a few to a few tens kcal/mol) but if it involves C then the inversion potential is very high as the inversion would pass through a planar carbon.

Figure 9-1 Internal motions of a molecule



If we knew the potential curves that are characteristic to a given molecular system then we could determine the whereabouts of the minimum energy points that in fact correspond to the equilibrium geometry. Unfortunately, these potential functions are not only unknown but they change from molecule to molecule and from bond to bond. However, we do know that they may be approximated, near any of their minima by same quadratic potential, since quadratic and true functions osculate at the minimum.

The quadratic function is the traditional Hooke's law (9-1):

$$E = E_m + \frac{1}{2}G(x - x_m)^2 \tag{9-1}$$

where G, the second derivative of E with respect to x, is the force constant usually denoted by k (9-2):

$$\frac{d^2E}{dx^2} = G \equiv k \tag{9-2}$$

The minimum energy point is denoted by E_m and x_m. For a multi-dimensional problem the generalized Hooke's law may be written as follows (9-3) and (9-4):

$$E = E + \frac{1}{2}(x - x^m)^{\dagger}\mathbf{G}(x - x^m) \tag{9-3}$$

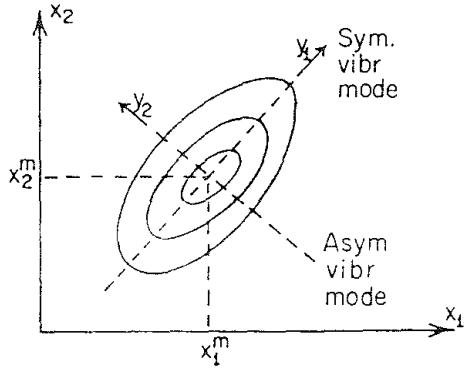
$$E = E_m + \frac{1}{2}\left(\left[x_1 - x_1^m\right]\left[x_2 - x_2^m\right]\mathrm{K}\right)\begin{bmatrix} G_{11} & G_{12} & \Lambda \\ \mathrm{M} & G_{22} & \Lambda \\ \mathrm{M} & \mathrm{M} & \mathrm{O} \end{bmatrix}\begin{bmatrix} \left[x_1 - x_1^m\right] \\ \left[x_2 - x_2^m\right] \\ \mathrm{M} \end{bmatrix} \tag{9-4}$$

where $(x\text{-}x_m)$ is the displacement vector and G, the Hessian matrix, collects all diagonal and off-diagonal or interaction force constants (9-5).

$$\begin{bmatrix} \frac{\partial^2 E}{\partial x_1^2} & \frac{\partial^2 E}{\partial x_1 \partial x_2} & \Lambda \\ \mathrm{M} & \frac{\partial^2 E}{\partial x_2^2} & \Lambda \\ \mathrm{M} & \mathrm{M} & \mathrm{O} \end{bmatrix} = \begin{bmatrix} G_{11} & G_{12} & \Lambda \\ \mathrm{M} & G_{22} & \Lambda \\ \mathrm{M} & \mathrm{M} & \mathrm{O} \end{bmatrix} = \mathbf{G} \tag{9-5}$$

A schematic illustration of a two-dimensional potential energy surface: $E= E(x_1, x_2)$ in terms of energy levels contours. Note that the normal coordinates $\{y_i\}$ are different from the internal coordinates $\{x_i\}$(**Figure 9-2**)

Figure 9-2 Potential surface representation of equation (9-5)



Molecular geometry optimization involves the finding of the minimum energy (E_m) point or in other words locating x_{1m}, x_{2m}; . . .This can most effectively be done by evaluating the gradient vector (9-6):

$$\langle g| \equiv g = \left(\frac{\partial E}{\partial x_1}, \frac{\partial E}{\partial x_2}, \ldots..\right) \tag{9-6}$$

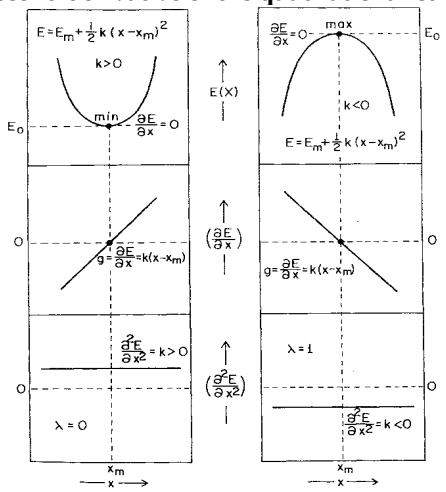
and searching for the point where the gradient vector is a zero vector since at the minimum the gradient vanishes (9-7)

$$\langle g| = (0,0,\ldots..) \tag{9-7}$$

9.1 Critical Points: Minimum, Maximum, Saddle Point

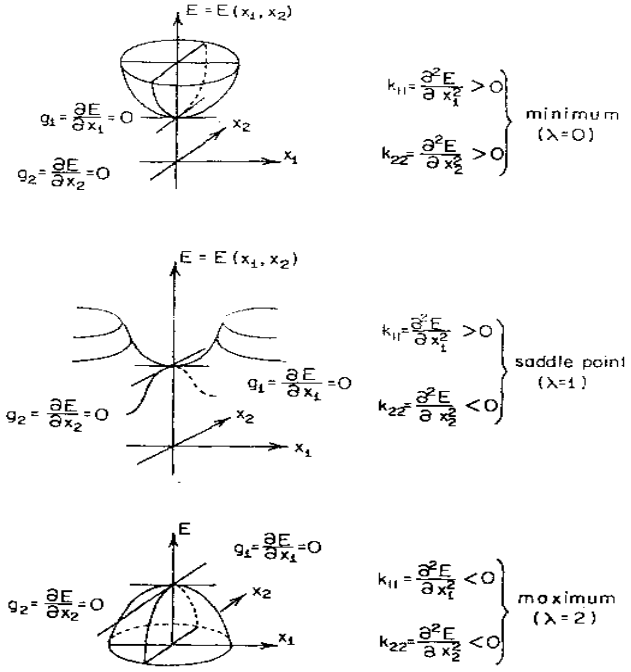
Characteristics of minima and maxima of a potential energy curve, (Note that *g* is the gradient, k is the force constant of the potential energy function and λ is the index of the critical point in question.

Figure 9-3 **Top Panel: A quadratic function; Middle Panel: First derivative of quadratic function; Bottom Panel: Second derivative of the quadratic function.**



There are three types of critical points of a potential energy surface and their characteristics in terms of second partial derivatives. This is shown in Figure 9-4 (Note that the index (λ) of a critical point is the number of negative second derivatives.)

Figure 9-4 **Three types of critical points**



This predicted $E(x_m)$ is the minimum energy of the quadratic function. This value can be compared to $E(x_m)$ calculated from the function. Note also that an estimate of the force constant, the parameter a, is readily obtained (9-8).

$$\frac{\partial^2 E}{\partial x^2} = a \equiv k \equiv G \tag{9-8}$$

9.2 Characteristics of potential energy surface critical points

The force constant or the Hessian matrix is a real symmetric matrix. In diagonal form the diagonal elements are the eigenvalues of the Hessian. Sometime all of these eigenvalues are positive, other times some of them are negative while some of them are positive and other times all of the eigenvalues are negative. This is a general case, for a particular critical point, where the first λ diagonal elements are negative and the rest of them are positive. Of course; l may assume values between 0 and n (9-9).

$$G^{diag} = \begin{bmatrix} -a_1^2 & & & & & & \\ & -a_2^2 & & & & 0 & \\ & & \mathrm{O} & & & & \\ & & & -a_\lambda^2 & & & \\ & & & & +a_{\lambda+1}^2 & & \\ & 0 & & & & \mathrm{O} & \\ & & & & & & +a_n^2 \end{bmatrix} \tag{9-9}$$

The parameter λ; the number of negative eigenvalues, is called the index of the particular point. For a minimum $\lambda = 0$, that is all diagonal elements of G_{diag} are positive. For a saddle point, corresponding to a chemical transition state $\lambda = 1$. For a maximum $\lambda = n$. **Table 9-1** shows a few different types of critical points possible.

Table 9-1 **This table shows the kind of critical point obtain with different number of –ve G_{diag}**

	Number of independent variables (n)			
Index	1a	2b	3c	4c
l=0	min	min	min	min
l=1	max	1°saddle	1°saddle	1°saddle
l=2		Max	2°saddle	2°saddle
l=3			Max	3°saddle
l=4				max

a) potential energy curve
b) potential energy surface
c) potential energy hyper surface

Since the fundamental frequency is related to the square root of the force constant (9-10)

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \tag{9-10}$$

Or , in a multidimensional case , for the m^{th} diagonal element of G_{diag} (9-11)

$$\nu_m \sim \frac{1}{2\pi}\sqrt{\frac{\pm a^2 m}{\mu}} \tag{9-11}$$

Therefore, the first λ eigenvalues of G_{diag} correspond to imaginary frequency. For m>λ we obtain (9-12)

$$\nu_m \sim \frac{1}{2\pi}\sqrt{\frac{-a^2 m}{\mu}} = \frac{a_m}{2\pi\sqrt{\mu}}\sqrt{-1} = \frac{a_m}{2\pi\sqrt{\mu}}i \tag{9-12}$$

At the end of the optimization it is advisable to check the order (λ) of the critical point. If λ = 0 then we can rest assured that the critical point in our optimization we have converged to is indeed a minimum.

10. Geometric Optimization

First of all, from the start position, one should find the minimum along the first direction(x_1). Subsequently, one must cycle through the remaining independent variables, (x_2, x_3, ..., x_n), fitting parabolas to sets of 3 points in each direction in turn. To reach M1, the best point after the l[st] cycle through all the parameters (**Figure 10-1**).

Figure 10-1 Potential Surface describing optimization steps

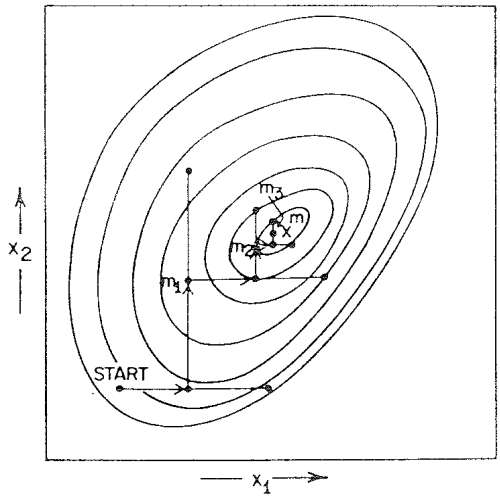
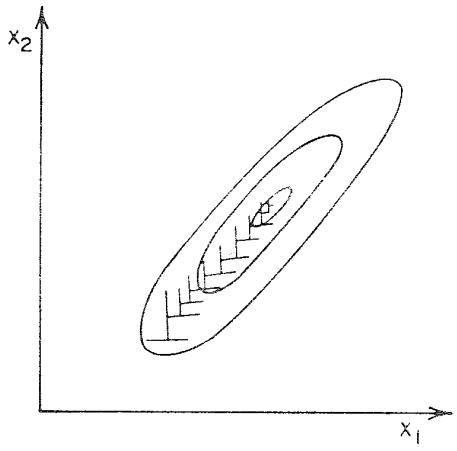


Figure 10-1 is a typical parabolic interpolation optimization of E(x_l,x_2). (Note that after the start position, m_i: end of cycle i, m: true minimum.) If m_i and m_{i-1} are sufficiently close to each other then quit. Alternatively use m_i as the new start position, and continue. As the optimization progresses, it is desirable to cut down the step size d. While this type of sequential optimization along one internal coordinate before the next one is a working method but it is rather pedestrian. Also, if the variables are coupled, as they very often are, the method is very inefficient (**Figure 10-2**).

Figure 10-2 Potential Surface describing optimization steps where x_1 is related to x_2



10.1 General introduction to gradient methods of optimization

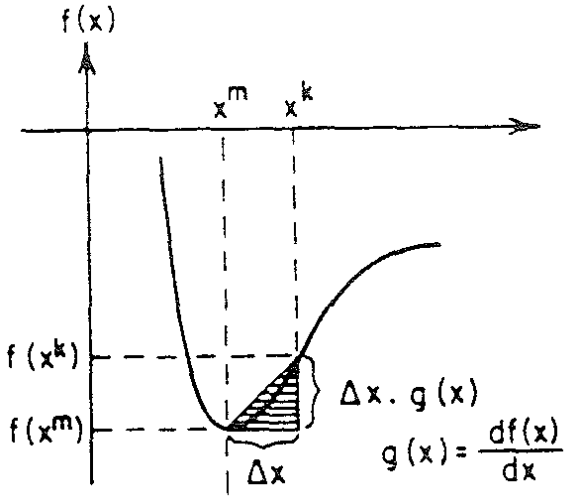
Methods for unconstrained optimization of a variables (n dimensions) are designed to produce the answer in a finite number of steps when the function, f(x), is quadratic. It is then hoped that the method will be efficient on more general functions, but especially those with slowly varying second derivatives. For a general function the notation f(x) is used rather than the E(x) specified before. This is done to emphasize that the method is applicable to any routine differentiable function. At the minimum or very close to it the functions have quadratic form, in addition to the constant $f(x^m)$, without a linear term. This function may be written, as show in (10-1):

$$f(x) = f(x^m) + \frac{1}{2}(x - x^m)^{\dagger}\mathbf{G}(x - x^m) \qquad (10\text{-}1)$$

However, some distance away from the minimum at point x_k the `inclusion of a linear term is advisable as specified by the next equation (10-2). **Figure 10-3** is a diagram of the Morse potential, showing the locations of the variables.

$$f_k(x) = \frac{1}{2}(x - x^k)^{\dagger}\mathbf{G}(x - x^k) + (x - x^k)^{\dagger} g_k + f(x^k) \qquad (10\text{-}2)$$

Figure 10-3 Diagram of Morse potential



The components of the gradient vector g(x) are the first partial derivatives of f(x) as shown in (10-3)

$$grad\ f(x) = \nabla f(x) = g = \langle g| = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ... \right) \tag{10-3}$$

In general, the objective function f(x) is shown in (10-4)

$$f_k(x) = f_m + \sum_{i=1}^{n} a_i x_i + \frac{1}{2} \sum_{i,j}^{n} G_{ij} x_i x_j \tag{10-4}$$

or in Dirac notation (10-5):

$$f_k(x) = f_m + < x|a > + \frac{1}{2} < x|\mathbf{G}|x > \tag{10-5}$$

Where *G* can be written as in (10-6):

$$G_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j} \tag{10-6}$$

The gradient of f(x), g(x) is shown in (10-7) and (10-8):

$$g_i(x) = a_i + \sum_j G_{ij} x_j \tag{10-7}$$

$$|g >= |a > + |\mathbf{G}|x > \tag{10-8}$$

where $g_i(x)$ is the ith component of |g>. At the extremum of f:

$$|g >= 0$$

Letting $|x_m>$ be the coordinates of the extremum and using (10-9), (10-10) is obtained:

$$|a> + \mathbf{G}|x_m> = 0 \tag{10-9}$$

$$|x_m> = -\mathbf{G}^{-1}|a> \tag{10-10}$$

Substitute for |a>=|g>-G|x>

$$\begin{aligned} |x_m> &= -\mathbf{G}^{-1}\left[|g> - \mathbf{G}|x>\right] \\ &= -\mathbf{G}^{-1}|g> + \mathbf{G}^{-1}\mathbf{G}|x> \\ &= -\mathbf{G}^{-1}|g> + |x> \end{aligned}$$

(10-11) is obtained:

$$|x_m> = |x> - \mathbf{G}^{-1}|g> \tag{10-11}$$

Which is the Newton (or Newton-Raphson) equation. Given exact G and |g>, the minimum can be found in one step for a quadratic function. Methods which do not use an exact G often use an approximate matrix H (a positive definite symmetric matrix) such that:

$$\mathbf{HG}=\mathbf{1} \tag{10-12}$$

In these cases, the step size is usually written as in (10-13):

$$|x^{(i+1)}> = |x^{(i)}> - \lambda_i \mathbf{H}|g^{(i)}> \tag{10-13}$$

where λ_i is to be determined

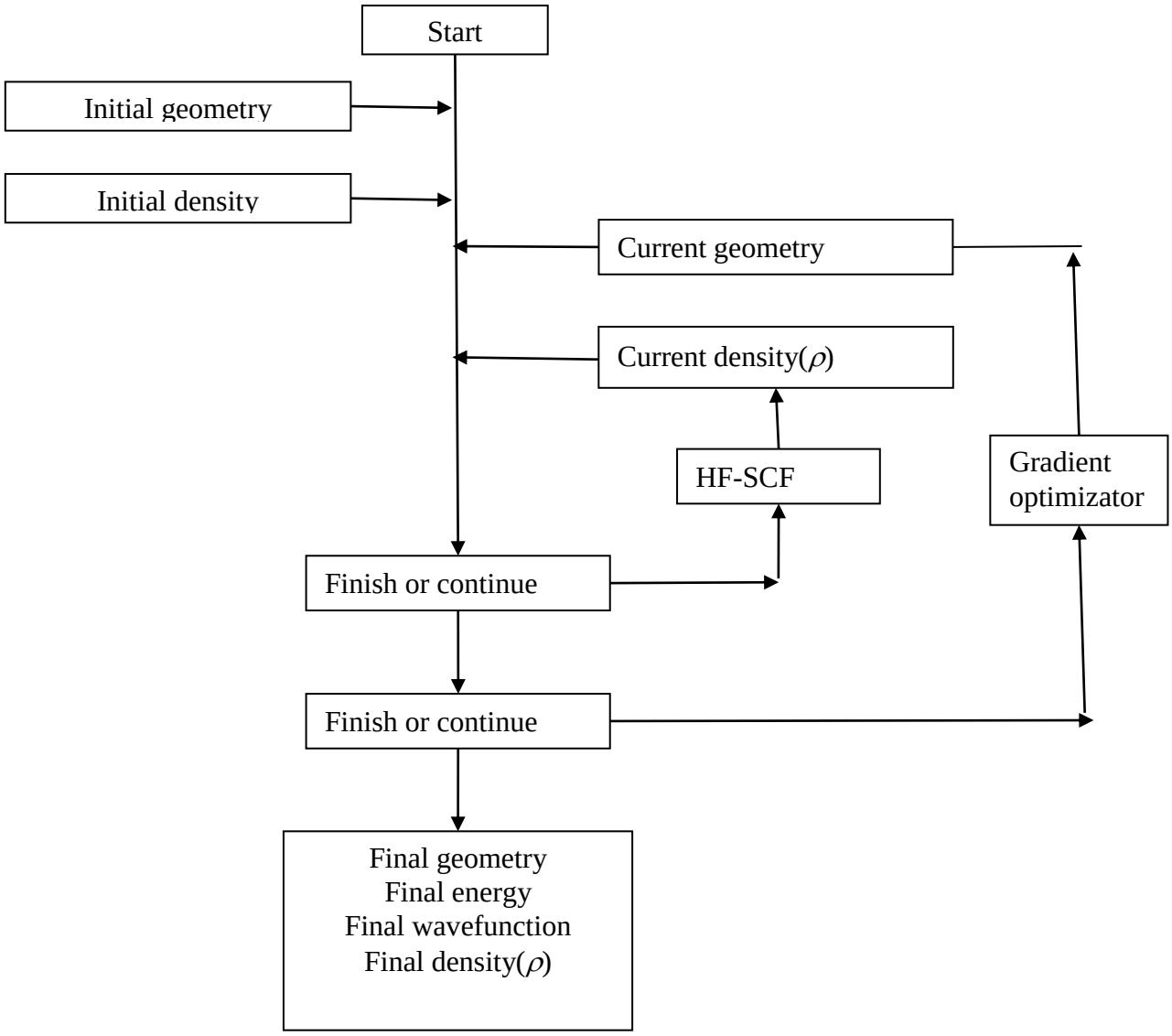
Note that $|x^{(i+1)}>$ will not necessarily be the extremum desired for any value of λ_i, as H is not exact. Besides if f is not quadratic, (10-11) is not valid anyways so (10-14) is always used in practice. Such methods, based on (10-15), are called quasi-Newton methods.

10.2 Steepest descend

A very simple optimization method called steepest descents arises from (10-13). by assuming H is the unit matrix, so that the search direction is always -|g(i)>. A line search is carried out along the direction -|g(i)> to obtain λi. This method however, poses some problems. Subsequent search directions tend to be linearly dependent, so only a small subspace of the

total space is explored. Directions with large components of |g(i)> are always favoured whereas progress can sometimes be made by searching in orthogonal directions to reach a part of the surface that would allow better progress. Also, the method converges very slowly near the minimum as g(x) is getting smaller in that vicinity. Flowchart for non-empirical (ab-initio) and semi-empirical (AM1 or PM3) Molecular orbital (MO)computations with geometry optimization.

10.3 Summary of Optimization process



11. Entropy Calculation

In general, there are three molecular motions contributing to the entropy:

The first one is translation (11-1):

$$S_t = \mathrm{R}(\ln(\mathrm{q}_t \mathrm{e}) + \mathrm{T}\left(\frac{3}{2T}\right)) = R(\ln q_t + 1 + \frac{3}{2}) \tag{11-1}$$

where q_t can be written as (11-2):

$$q_t = \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} \frac{k_B T}{P} \tag{11-2}$$

Rotation also contributes to the entropy as shown (11-3):

$$S_r = \mathrm{R}(\ln \mathrm{q}_r + \mathrm{T}\left(\frac{\partial \ln q_r}{\partial T}\right)_v) = R(\ln q_r + \frac{3}{2}) \tag{11-3}$$

where q_r can be represented by (11-4) :

$$q_r = \frac{\pi^{1/2}}{\sigma_r}\left(\frac{T^{3/2}}{(\Theta_{r,x}\Theta_{r,y}\Theta_{r,z})^{1/2}}\right) \tag{11-4}$$

where Θ's are the eigenvalues of the rotational moment of inertia tensor. Vibrational is the third factor contributing to the entropy (11-5):

$$\begin{aligned} S_v &= \mathrm{R}(\ln \mathrm{q}_v + \mathrm{T}\left(\frac{\partial \ln q}{\partial T}\right)_v) = R(\ln q_v + T\left(\sum_K \frac{\Theta_{v,k}}{2T^2} + \sum_K \frac{(\Theta_{v,k}/T^2)e^{-\Theta_{v,K}/T}}{1-e^{-\Theta_{v,K}/T}}\right)) \\ &= R\left(\sum_K \frac{\Theta_{\mathrm{v,k}}}{2\mathrm{T}} + \ln(1-e^{-\Theta_{v,K}/T}) + T\left(\sum_K \frac{\Theta_{v,k}}{2T^2} + \sum_K \frac{(\Theta_{v,k}/T^2)e^{-\Theta_{v,K}/T}}{1-e^{-\Theta_{v,K}/T}}\right)\right) \\ &= R\left(\sum_K \ln(1-e^{-\Theta_{v,K}/T}) + \left(\sum_K \frac{(\Theta_{v,k}/T)e^{-\Theta_{v,K}/T}}{1-e^{-\Theta_{v,K}/T}}\right)\right) \\ &= R\sum_K\left(\frac{\Theta_{v,K}/T}{e^{\Theta_{v,K}/T}-1} - \ln(1-e^{-\Theta_{v,K}/T})\right) \end{aligned} \tag{11-5}$$

where Θ_K is as follows (11-6):

$$\Theta_K = \frac{h\nu_K}{k_B} = \frac{h\nu_K}{R/N} \tag{11-6}$$

Therefore, the total entropy for the electronic ground state is (11-7):

$$S_{total} = S_t + S_r + S_v \tag{11-7}$$