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Table S2	Predicted and Measured J couplings for r(CAAU)
Table S3	Predicted and Measured NOE distances for r(UCAAUC)
Table S4	Predicted and Measured J couplings for r(UCAAUC)
Table S5	Predicted and Measured NOE distances for d(CAAU)
Table S6	Predicted and Measured J couplings for d(CAAU)
Table S7	Predicted and Measured NOE distances for d(UCAAUC)
Table S8	Predicted and Measured J couplings for d(UCAAUC)
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Table S1. Predicted and Measured NOE distances for r(CAAU)

					OL3 Error				OL3			ROCRNA Error				ROCRNA	
rCAAU	low	NMR	high		ss1	ss2	ss3	ss4	Avg	stdev		ss1	ss2	ss3	ss4	Avg	stdev
C1H1'-C1H6	3.04	3.34	3.74		0.00	0.00	0.00	0.00	3.43	0.27		0.00	0.00	0.00	0.00	3.41	0.16
C1H1'-A2H8	4.20	5.10	6.60		0.10	0.00	0.00	0.00	6.27	0.37		0.00	0.00	0.00	0.00	5.28	0.09
C1H2'-C1H6	2.76	3.06	3.36		0.00	0.00	0.00	0.00	3.12	0.04		0.40	0.03	0.45	0.53	3.71	0.22
C1H2'-A2H1'	3.49	3.99	4.59		1.66	1.34	1.75	1.26	6.09	0.24		0.00	0.00	0.00	0.00	3.91	0.06
C1H2'-A2H8	2.67	2.97	3.27		0.79	0.47	0.89	0.58	3.95	0.19		0.00	0.00	0.00	0.00	3.09	0.05
C1H3'-C1H6	2.48	2.78	2.98		0.00	0.00	0.00	0.00	2.75	0.01		0.04	0.00	0.05	0.08	3.02	0.04
C1H4'-C1H6	3.85	4.45	5.75		0.00	0.00	0.00	0.00	4.31	0.02		0.00	0.00	0.00	0.00	4.20	0.02
C1H4'-A2H8	3.94	4.54	6.14		0.35	0.00	0.00	0.00	5.91	0.42		0.00	0.00	0.00	0.00	5.23	0.09
C1H6-A2H8	3.76	4.36	5.36		0.84	0.43	0.96	0.58	6.06	0.24		0.00	0.00	0.00	0.00	3.92	0.06
A2H1'-A2H2	3.67	4.17	4.97		0.00	0.00	0.00	0.00	4.84	0.03		0.00	0.00	0.00	0.00	4.67	0.03
A2H1'-A2H8	3.03	3.43	3.73		0.00	0.00	0.00	0.00	3.48	0.11		0.00	0.00	0.00	0.01	3.72	0.03
A2H1'-A3H8	3.84	4.54	5.94		0.00	0.00	0.00	0.00	4.69	0.25		0.00	0.00	0.00	0.00	5.06	0.06
A2H2'-A2H8	2.76	3.06	3.36		0.31	0.00	0.00	0.00	3.40	0.18		0.26	0.25	0.15	0.00	3.50	0.16
A2H2'-A3H1'	3.12	3.52	3.92		0.16	0.25	0.23	0.24	4.15	0.04		0.00	0.00	0.00	0.00	3.86	0.03
A2H2'-A3H4'	3.22	3.52	4.02		0.12	0.22	0.19	0.20	4.21	0.04		0.00	0.00	0.00	0.00	4.00	0.03
A2H2'-A3H8	2.30	2.50	2.80		0.00	0.00	0.00	0.00	2.43	0.03		0.00	0.00	0.00	0.00	2.64	0.06
A2H3'-A2H8	2.48	2.78	2.98		0.37	0.27	0.31	0.00	3.21	0.18		0.00	0.00	0.00	0.00	2.87	0.07
A2H3'-A3H8	2.30	2.50	2.80		-0.05	0.00	-0.02	0.00	2.30	0.04		0.00	0.00	0.00	0.00	2.56	0.06
A2H4'-A2H8	3.58	4.08	4.88		0.00	0.00	0.00	0.00	4.38	0.03		0.00	0.00	0.00	0.00	4.37	0.01
A2H2-A2H2'	4.02	4.82	6.62		0.00	0.00	0.00	0.00	4.31	0.04		0.00	0.00	0.00	0.00	4.63	0.08
A2H2-A3H1'	3.22	3.62	4.02		-0.44	-0.34	-0.40	-0.37	2.83	0.04		0.00	0.00	0.00	0.00	3.49	0.10
A3H1'-A3H2	4.11	5.01	6.61		0.00	0.00	0.00	0.00	4.70	0.03		0.00	0.00	0.00	0.00	4.59	0.02
A3H1'-A3H8	3.13	3.43	3.93		0.00	0.00	0.00	0.00	3.50	0.18		0.00	0.00	0.00	0.00	3.72	0.08
A3H2'-A3H8	2.67	2.97	3.27		0.51	0.00	0.29	0.36	3.56	0.22		0.27	0.20	0.30	0.03	3.47	0.12
A3H2'-U4H1'	3.67	4.27	5.07		2.64	2.28	2.82	2.25	7.56	0.28		0.07	0.12	0.00	0.13	5.14	0.06
A3H2'-U4H5	2.85	3.15	3.45		1.45	0.98	1.63	0.81	4.67	0.38		-0.09	0.00	-0.06	-0.04	2.82	0.07
A3H2'-U4H6	2.58	2.78	3.08		1.60	1.16	1.78	1.09	4.49	0.34		0.00	0.00	0.00	0.00	2.85	0.05
A3H3'-A3H8	2.30	2.50	2.80		0.10	0.14	0.17	0.10	2.93	0.03		0.00	0.00	0.00	0.00	2.60	0.03
A3H3'-U4H2'	2.58	2.78	3.08		0.28	0.17	0.30	0.14	3.30	0.08		-0.20	-0.10	-0.19	-0.17	2.42	0.05
A3H3'-U4H5	3.22	3.62	4.02		1.44	1.09	1.46	1.29	5.34	0.17		0.03	0.10	0.00	0.07	4.06	0.06
A3H3'-U4H6	2.58	2.88	3.18		1.11	0.79	1.09	0.90	4.15	0.15		0.00	0.00	0.00	0.00	2.88	0.05
A3H4'-A3H8	3.67	4.27	5.17		0.00	0.00	0.00	0.00	4.38	0.04		0.00	0.00	0.00	0.00	4.33	0.01
A3H4'-U4H2'	3.85	4.45	5.65		0.23	0.16	0.14	0.08	5.81	0.06		0.00	0.00	0.00	0.00	5.38	0.05
A3H2-U4H1'	3.67	4.17	4.97		3.79	1.47	2.59	1.40	7.29	1.13		0.00	0.00	0.00	0.00	4.52	0.14
A3H8-U4H2'	3.22	3.62	4.02		0.53	0.55	0.91	0.45	4.63	0.21		-0.47	-0.34	-0.45	-0.43	2.80	0.06
A3H8-U4H5	3.49	3.99	4.69		1.69	1.19	1.78	1.15	6.14	0.33		0.00	0.00	0.00	0.00	4.58	0.07
A3H8-U4H6	3.84	4.54	5.94		0.24	0.09	0.40	0.01	6.13	0.17		0.00	0.00	0.00	0.00	4.41	0.09
U4H1'-U4H6	3.04	3.34	3.74		0.00	0.00	0.00	0.00	3.60	0.02		0.00	0.00	0.00	0.00	3.46	0.14

Table S2. Predicted and Measured J couplings for r(CAAU)

		ff99+						ROC-RNA							Measured	range	range
		ss1	ss2	ss3	ss4	avg	stdev	ss1	ss2	ss3	ss4	avg	stdev		from Condon paper	low	high
C1	J(H1'-H2')	2.72	3.19	3.03	3.12	3.02	0.21	0.76	1.39	0.77	1.24	1.04	0.32		~1	0	3
	J(H2'-H3')	5.2	5.16	5.19	5.15	5.18	0.02	3.87	4.25	3.9	3.97	4.00	0.17		4.5	2.5	6.5
	J(H3'-H4')	10.88	10.42	10.57	10.38	10.56	0.23	10.65	10.51	10.62	10.22	10.50	0.20		8.4	6.4	10.4
	J(H5'-H4')	3.99	3.85	3.9	3.82	3.89	0.07	2.85	3	2.87	2.86	2.90	0.07		1.6	0	3.6
	J(H5''-H4')	4.48	4.36	4.43	4.31	4.40	0.08	6.27	6.21	6.26	6.24	6.25	0.03		~3.75	1.75	5.75
A2	J(H1'-H2')	0.7	1.26	1.21	0.8	0.99	0.28	0.76	0.82	0.86	1.22	0.92	0.21		~1	0	3
	J(H2'-H3')	4.53	4.59	4.61	4.56	4.57	0.04	4.18	4.3	4.2	4.23	4.23	0.05		4.6	2.6	6.6
	J(H3'-H4')	9.06	8.8	8.71	9.01	8.90	0.17	10.46	10.17	10.33	10.04	10.25	0.18		8.3	6.3	10.3
	J(H5'-H4')	3.54	7.59	3.52	3.51	4.54	2.03	3.32	7.05	3.29	3.23	4.22	1.89		~2.8	0.8	4.8
	J(H5''-H4')	3.38	3.93	3.42	3.39	3.53	0.27	4.03	3.48	4.26	4.01	3.95	0.33		~2.1	0.1	4.1
	J(P-H5')	3.38	3.31	3.37	3.39	3.36	0.04	6.09	5.52	5.93	6.33	5.97	0.34		3.7	1.7	5.7
	J(P-H5'')	1.91	2.06	1.98	1.97	1.98	0.06	2.67	3.01	2.95	2.53	2.79	0.23		2.2	0.2	4.2
	J(2P-1H3')	2.7	3.09	2.91	3.06	2.94	0.18	9.9	9.35	9.75	9.94	9.74	0.27		9.4-9.8	7.4	11.8
A3	J(H1'-H2')	0.39	1.49	0.86	0.9	0.91	0.45	0.63	0.78	0.65	0.89	0.74	0.12		1.4	0	3.4
	J(H2'-H3')	4.11	4.33	4.18	4.29	4.23	0.10	4.16	4.22	4.22	4.21	4.20	0.03		4.3	2.3	6.3
	J(H3'-H4')	10.41	9.78	10.04	10.23	10.12	0.27	10.46	10.38	10.42	10.11	10.34	0.16		8.2-8.4	6.2	10.4
	J(H5'-H4')	3.12	7.63	3.08	3.13	4.24	2.26	2.96	7.59	3.02	3.05	4.16	2.29		2	0	4
	J(H5''-H4')	3.74	3.44	3.83	3.77	3.70	0.17	4.1	3.24	4.21	4.21	3.94	0.47		1.3	0	3.3
	J(P-H5')	3.74	3.68	3.76	3.68	3.72	0.04	6.03	5.58	6.15	6.44	6.05	0.36		3.5	1.5	5.5
	J(P-H5'')	1.8	2.08	1.84	1.87	1.90	0.13	2.12	1.97	2.26	2.43	2.20	0.20		<1	0	3
	J(3P-2H3')	8.86	7.98	8.58	8.22	8.41	0.39	9.4	9.53	9.43	9.34	9.43	0.08		8.4	6.4	10.4
U4	J(H1'-H2')	6.46	6.85	6.5	6.65	6.62	0.18	6.94	7.09	6.95	7	7.00	0.07		3.7	1.7	5.7
	J(H2'-H3')	5.05	5.02	5.05	5.06	5.05	0.02	4.67	4.69	4.67	4.7	4.68	0.02		3.7	1.7	5.7
	J(H5'-H4')	3.28	3.23	3.25	3.23	3.25	0.02	2.1	2.06	2.11	2.18	2.11	0.05		1	0	3
	J(H5''-H4')	3.64	3.73	3.68	3.73	3.70	0.04	5.17	5.13	5.15	5.23	5.17	0.04		<1	0	3
	J(P-H5')	1.91	1.96	1.95	1.98	1.95	0.03	5.95	5.56	5.88	5.8	5.80	0.17		3.8-4.3	1.8	6.3
	J(P-H5'')	3.76	3.75	3.77	3.7	3.75	0.03	3.39	3.14	3.35	3.33	3.30	0.11		3.3	1.3	5.3
	J(4P-3H3')	5.3	5.36	5.3	5.26	5.31	0.04	8.78	8.87	8.75	8.74	8.79	0.06		8.3	6.3	10.3

Table S3. Predicted and Measured NOE distances for r(UCAAUC)

					OL3 Error				OL3			ROCRNA Error				ROCRNA	
rUCAAUC	low	NMR	high		ss1	ss2	ss3	ss4	Avg	stdev		ss1	ss2	ss3	ss4	Avg	stdev
U1H1'-U1H4'	2.98	3.38	3.81		0.00	0.00	-0.02	-0.04	2.97	0.02		0.00	0.00	0.00	0.00	3.21	0.04
U1H2'H3'-U1H5''	2.53	2.84	3.15		0.00	0.00	0.00	0.00	2.70	0.04		0.00	0.00	0.00	0.00	2.79	0.02
U1H2'H3'-U1H5'	2.76	3.11	3.47		0.00	0.00	0.00	0.00	3.30	0.01		0.00	0.00	0.00	0.00	3.11	0.05
U1H2'H3'-U1H6	2.27	2.55	2.82		0.00	0.00	0.00	0.00	2.46	0.02		0.00	0.00	0.08	0.67	2.80	0.15
U1H2'H3'-C2H5'	2.37	2.66	2.94		0.11	0.13	0.04	0.09	3.03	0.04		0.00	0.00	0.00	0.00	2.49	0.04
U1H2'H3'-C2H6	2.31	2.59	2.86		0.00	0.00	0.00	0.00	2.70	0.06		-0.03	-0.03	-0.08	0.00	2.28	0.04
U1H2'H3'-A3H8	3.30	3.78	4.39		0.77	0.00	0.55	0.10	4.64	0.54		0.55	0.23	0.85	-0.25	4.47	0.98
U1H4'-U1H6	3.42	3.95	4.68		0.00	0.00	0.00	0.00	4.40	0.03		0.00	0.00	0.00	0.00	4.20	0.02
U1H5'H5''-U1H6	2.83	3.23	3.70		0.00	0.00	0.00	0.00	3.54	0.05		0.00	0.00	0.00	0.00	2.92	0.03
C2H1'-C2H6	2.89	3.26	3.66		0.00	0.01	0.00	0.00	3.60	0.07		0.00	0.00	0.00	0.00	3.60	0.01
C2H2'-C2H6	2.45	2.75	3.05		0.00	0.00	0.00	0.00	2.68	0.02		0.30	0.31	0.58	0.08	3.37	0.20
C2H2'-A3H1'	3.30	3.78	4.39		0.47	0.74	0.36	0.77	4.98	0.20		0.00	0.00	0.00	0.00	4.02	0.11
C2H2'-A3H5'H5''	2.26	2.54	2.82		0.30	0.19	0.36	0.54	3.17	0.15		0.00	0.00	0.00	0.00	2.63	0.06
C2H2'-A3H8	2.55	2.87	3.18		0.00	0.11	0.00	0.09	3.16	0.13		0.00	0.00	0.00	0.00	2.89	0.08
C2H3'-C2H6	2.36	2.65	2.93		0.00	0.00	0.00	0.00	2.59	0.09		0.00	0.00	0.00	0.00	2.85	0.05
C2H3'-A3H8	2.27	2.54	2.80		0.13	0.34	0.20	0.40	3.08	0.12		0.00	0.00	0.00	0.00	2.48	0.07
C2H4'-C2H6	3.20	3.65	4.19		0.12	0.10	0.11	0.14	4.31	0.02		0.00	0.00	0.00	0.04	4.20	0.02
C2H4'-A3H8	3.37	3.88	4.55		0.00	0.03	0.00	0.00	4.35	0.21		0.50	0.26	0.67	0.18	4.95	0.23
C2H5'H5''-C2H6	2.62	2.97	3.34		0.10	0.02	0.12	0.00	3.35	0.14		0.00	0.00	0.00	0.00	3.23	0.05
A3H1'-A3H8	2.92	3.30	3.71		0.00	0.00	0.00	0.00	3.23	0.18		0.00	0.00	0.00	0.04	3.71	0.02
A3H2'-A3H1'	2.32	2.61	2.88		0.00	0.00	0.00	0.00	2.81	0.04		0.00	0.00	0.00	0.00	2.77	0.04
A3H2'-A3H2	3.84	4.60	7.59		0.00	0.00	0.00	0.00	4.88	0.15		0.00	0.00	0.00	0.00	4.74	0.14
A3H2'-A3H8	2.69	3.02	3.36		0.00	0.00	0.00	0.00	2.76	0.08		-0.03	0.00	0.00	0.00	2.94	0.29
A3H2'-A4H1'	3.10	3.52	4.01		0.42	1.12	0.79	0.95	4.83	0.30		0.04	0.00	0.00	0.02	4.00	0.05
A3H2'-A4H3'	3.31	3.79	4.41		0.17	0.00	0.00	0.00	4.14	0.41		0.55	0.00	0.18	0.45	4.67	0.32
A3H2'-A4H5'H5''	2.41	2.72	3.02		0.00	0.36	0.10	0.07	3.12	0.20		0.00	0.00	0.00	0.00	2.84	0.09
A3H2'-A4H8	2.28	2.56	2.83		0.00	0.31	0.09	0.24	2.94	0.22		0.00	0.00	0.00	0.00	2.67	0.09
A3H1'-A3H3'	3.19	3.64	4.17		0.00	0.00	0.00	0.00	3.80	0.01		0.00	0.00	0.00	0.00	3.74	0.02
A3H3'-A3H5'H5''	2.12	2.37	2.62		0.05	0.00	0.00	0.00	2.61	0.06		0.00	0.00	0.02	0.04	2.62	0.05
A3H3'-A3H8	2.44	2.74	3.03		0.00	0.00	0.00	0.00	2.66	0.08		0.00	0.00	0.00	0.00	2.84	0.16
A3H3'-A4H8	2.27	2.54	2.80		0.00	0.28	0.33	0.30	3.03	0.16		0.03	0.00	0.00	0.00	2.71	0.10
A3H5'H5''-A3H8	2.50	2.82	3.15		0.49	0.50	0.43	0.50	3.63	0.03		0.15	0.00	0.00	0.00	3.16	0.10
A3H2-A4H1'	2.90	3.28	3.69		0.00	0.56	0.11	0.29	3.85	0.36		0.00	0.00	0.00	0.00	3.28	0.04
A4H1'-A4H3'	2.92	3.30	3.71		0.09	0.12	0.07	0.09	3.81	0.02		0.05	0.06	0.06	0.05	3.77	0.01
A4H1'-A4H2	3.64	4.28	5.45		0.00	0.00	0.00	0.00	4.68	0.06		0.00	0.00	0.00	0.00	4.72	0.02
A4H1'-A4H8	2.99	3.39	3.83		0.00	0.00	0.00	0.00	3.40	0.14		0.00	0.00	0.00	0.00	3.69	0.01
A4H2'-A4H8	2.48	2.78	3.08		0.00	0.00	0.00	0.00	2.73	0.15		0.62	0.34	0.20	0.00	3.31	0.36
A4H2'-U5H1'	3.63	4.26	5.39		0.00	0.00	0.00	0.00	4.92	0.28		0.00	0.00	0.00	0.00	3.99	0.10
A4H2'-U5H5'H5''	2.27	2.55	2.83		0.19	0.50	0.26	0.08	3.09	0.18		0.00	0.00	0.00	0.00	2.67	0.06
A4H2'-U5H5	3.31	3.79	4.41		0.00	0.00	0.00	0.00	3.87	0.05		0.00	0.00	0.00	0.00	4.15	0.08
A4H2'-U5H6	2.35	2.63	2.91		0.00	0.25	0.08	0.00	2.98	0.14		0.00	0.00	0.00	0.00	2.67	0.05
A4H3'-A4H8	2.35	2.63	2.91		0.00	0.00	0.00	0.00	2.82	0.06		0.10	0.10	0.13	0.14	3.03	0.02
A4H3'-U5H5'	2.68	3.01	3.35		0.25	0.57	0.00	0.00	3.45	0.38		0.29	0.27	0.38	0.44	3.70	0.08
A4H3'-U5H5	2.93	3.32	3.73		0.17	0.66	0.00	0.16	3.97	0.30		0.00	0.00	0.00	0.00	3.25	0.06
A4H3'-U5H6	2.48	2.78	3.08		0.03	0.43	0.01	0.00	3.20	0.21		0.00	0.00	0.00	0.00	2.54	0.04
A4H4'-A4H8	3.24	3.71	4.28		0.19	0.29	0.41	0.29	4.57	0.09		0.11	0.11	0.11	0.21	4.41	0.05
A4H5''-A4H8	2.91	3.29	3.70		0.52	0.68	0.87	0.74	4.40	0.14		0.00	0.00	0.00	0.00	3.31	0.27
A4H2-U5H1'	2.99	3.39	3.83		0.07	0.77	0.35	0.09	4.15	0.33		0.00	0.00	0.00	0.00	3.30	0.06
A4H8-U5H5	3.31	3.79	4.41		0.00	0.27	0.00	0.00	4.29	0.27		0.00	0.00	0.00	0.00	3.65	0.02
U5H1'-U5H2'	2.36	2.65	2.93		0.00	0.00	0.00	0.00	2.86	0.04		0.00	0.00	0.00	0.00	2.76	0.00
U5H1'-U5H3'	2.98	3.38	3.81		0.00	0.00	0.00	0.00	3.79	0.00		0.00	0.00	0.00	0.00	3.77	0.00
U5H1'-U5H6	2.96	3.35	3.77		0.00	0.00	0.00	0.00	3.20	0.06		0.00	0.00	0.00	0.00	3.61	0.03
U5H2'-U5H6	2.36	2.65	2.93		0.00	0.00	0.00	0.00	2.76	0.14		0.78	0.63	0.62	0.64	3.60	0.08
U5H2'-C6H6	2.45	2.75	3.05		0.12	0.54	0.17	0.09	3.28	0.21		0.00	0.00	0.00	0.00	2.88	0.03
U5H3'-U5H6	2.22	2.49	2.74		0.00	0.16	0.00	0.00	2.72	0.13		0.00	0.00	0.00	0.00	2.71	0.04
U5H3'-C6H2'	3.01	3.41	3.85		-0.24	0.00	-0.07	-0.02	2.95	0.13		-0.79	-0.70	-0.63	-0.68	2.31	0.07
U5H3'-C6H5	3.25	3.72	4.29		0.00	0.00	0.00	0.00	3.58	0.34		0.00	0.00	0.00	0.00	3.70	0.19
U5H3'-C6H6	2.64	2.97	3.30		0.00	0.14	0.00	0.00	3.11	0.23		0.00	0.00	0.00	0.00	2.68	0.03
U5H5''-U5H6	3.03	3.44	3.89		0.31	0.48	0.33	0.23	4.23	0.10		0.18	0.00	0.19	0.02	3.99	0.11
U5H6-C6H5	3.45	3.99	4.76		0.00	0.52	0.00	0.00	4.71	0.39		0.00	0.00	0.00	0.00	4.31	0.25
C6H1'-C6H3'	3.19	3.64	4.17		0.00	0.00	0.00	0.00	3.81	0.00		0.00	0.00	0.00	0.00	3.81	0.00
C6H2'-C6H6	2.55	2.87	3.18		0.00	0.00	0.00	0.00	2.72	0.07		0.00	0.00	0.00	0.00	2.73	0.02
C6H3'-C6H6	2.31	2.59	2.86		0.16	0.00	0.04	0.05	2.90	0.09		0.92	0.52	0.37	0.53	3.44	0.24
C6H5''-C6H6	3.08	3.50	3.97		0.37	0.26	0.28	0.28	4.27	0.05		0.31	0.22	0.00	0.03	4.07	0.20

Table S4. Predicted and Measured J couplings for r(UCAAUC)

	ol3					ROC-RNA					NMR	err=2				
	avg(Hz)	err(Hz)	C3'-endo	K 2°C	ΔG 2°C	avg(Hz)	err(Hz)	C3'-endo	K 2°C	ΔG 2°C	avg(Hz)	min(Hz)	max(Hz)	C3'-endo	K 2°C	ΔG 2°C
Pucker J(H1'-H2')/J(H3'-H4')					(kcal/mol)					(kcal/mol)						(kcal/mol)
U1	5.2/7.7	0.8/0.8	0.60	1.48	-0.21	1.2/10.4	0.3/0.1	0.90	9.01	-1.20	1.5/6.8	0/4.8	3.5/8.8	0.82	4.53	-0.83
C2	5.0/6.8	1.0/0.9	0.57	1.35	-0.16	1.9/9.7	1.0/1.0	0.83	5.05	-0.89	1.3/7.2	0/5.2	3.3/9.2	0.85	5.54	-0.94
A3	3.7/7.1	1.5/1.5	0.66	1.91	-0.35	2.6/8.8	1.8/1.6	0.77	3.43	-0.67	0.3/7.5	0/5.5	2.3/9.5	0.97	29.80	-1.86
A4	3.9/7.3	1.3/1.3	0.65	1.87	-0.34	1.7/9.5	1.1/1.1	0.85	5.69	-0.95	0.4/7.9	0/5.9	2.4/9.9	0.96	22.57	-1.70
U5	4.9/7.2	1.6/1.7	0.60	1.48	-0.21	1.0/10.5	0.2/0.2	0.91	10.33	-1.28	1.2/7.6	0/5.6	3.2/9.6	0.86	6.33	-1.01
C6	6.1/5.7	0.6/0.8	0.49	0.94	0.03	8.3/3.3	0.9/0.9	0.28	0.40	0.51	3.1/6.8	1.1/4.8	5.1/8.8	0.69	2.23	-0.44
Gamma J(H5'-H4')/J(H5''-H4')																
U1	3.5/3.8	0.1/0.1				2.6/5.8	0.1/0.2				2.1/3.4	0.1/1.4	4.1/5.4			
C2	3.3/3.9	0.2/0.2				3.0/4.2	0.1/0.1				<1.5/2.1	0/0.1	3.5/4.1			
A3	3.6/3.9	0.2/0.3				2.8/4.7	0.1/0.1				<1.5/3.8	0/1.75	3.5/5.8			
A4	3.3/3.7	0.3/0.3				3.2/4.7	0.3/0.5				<1.5/<1.5	0/0	3.5/3.5			
U5	--/4.1	--/0.2				--/3.9	--/0.2				--/<1.5	--/0	--/3.5			
C6	3.1/4.0	0.1/0.1				2.2/5.1	0.2/0.1				<1.5/<1.5	0/0	3.5/3.5			
Beta J(P-H5')/J(P-H5'')																
C2	3.4/2.3	0.1/0.1				5.8/2.7	0.6/0.2				4.2/1.0-2.0	2.2/0	6.2/4			
A3	3.2/2.8	0.1/0.3				5.2/3.4	0.2/0.7				2.8/3	0.8/1	4.8/5			
A4	3.2/2.6	0.2/0.2				6.4/4.5	0.8/1.8				2.7/1.0-2.0	0.7/0	4.7/4			
U5	3.7/2.6	0.4/0.4				5.9/2.0	0.3/0.4				2.0-3.0/1.0-2.0	0/0	5.0/4.0			
C6	2.7/3.2	0.1/0.2				6.8/2.9	0.2/0.2				2.0-3.0/1.0-2.0	0/0	5.0/4.0			
Epsilon J(nP-(n-1)H3')																
C2	6.2	0.2				9.3	0.4				8.8	6.8	10.8			
A3	6.1	0.2				9.6	0.2				8.5	6.5	10.5			
A4	6.2	0.4				8.9	0.2				8.7	6.7	10.7			
U5	6.7	0.2				9.5	0.2				8.6	6.6	10.6			
C6	6.1	0.3				9.0	0.1				8.8	6.8	10.8			
A3 J(H2'-H3')	4.6	0.1				4.0	0.1				4.6	2.6	6.6			

Table S5. Predicted and Measured NOE distances for d(CAAU)

					BSC1 Error				BSC1	
	low	NMR	high		ss1	ss2	ss3	ss4	Avg	stdev
C1H1'-A2H5'	2.70	3.28	3.81		-0.32	-0.32	-0.31	-0.32	2.38	0.01
C1H2'-C1H6	2.39	2.88	3.29		-0.13	-0.13	-0.13	-0.12	2.26	0.00
C1H2''-A2H5'	2.88	3.52	4.18		0.00	0.00	0.00	0.00	2.93	0.01
C1H2'H2''-A2H8	2.78	3.46	4.32		-0.48	-0.48	-0.47	-0.48	2.30	0.00
A2H1'-A2H4'	2.71	3.30	3.84		0.00	0.00	0.00	0.00	3.02	0.00
A2H1'-A3H4'	3.45	4.46	5.47		0.00	0.00	0.00	0.00	3.97	0.03
A2H1'-A3H5'	2.43	2.93	3.35		-0.07	-0.07	-0.04	-0.06	2.37	0.01
A2H2'H2''-A2H8	1.92	2.31	2.62		0.00	0.00	0.00	0.00	2.25	0.01
A2H2''-A3H5'	2.86	3.49	4.13		0.00	0.00	0.00	0.00	3.24	0.01
A2H2'H2''-A3H8	2.33	2.83	3.27		-0.02	-0.01	0.00	0.00	2.34	0.03
A3H1'-A3H8	3.02	3.72	4.52		0.00	0.00	0.00	0.00	3.64	0.27
A3H1'-U4H5'	2.66	3.23	3.75		-0.27	-0.26	-0.28	-0.26	2.39	0.01
A3H2'H2''-A3H8	2.00	2.40	2.72		0.00	0.00	0.00	0.00	2.28	0.03
A3H2'H2''-U4H6	2.56	3.10	3.57		-0.25	-0.24	-0.25	-0.24	2.32	0.00
U4H1'-U4H6	2.80	3.42	4.02		0.00	0.00	0.00	0.00	3.73	0.00
U4H2'-U4H6	2.38	2.87	3.28		-0.11	-0.10	-0.11	-0.10	2.28	0.01
U4H3'-U4H6	2.63	3.19	3.69		0.04	0.06	0.02	0.05	3.74	0.02

Table S6. Predicted and Measured J couplings for d(CAAU)

dCAAU_noe800_pdec_									
J couplings from dCAAU data +-pdec at ~0C									
Pucker		ss1	ss2	ss3	ss4	MD avg	stdev	NMR avg	err
C1	J(H3'-H4')	1.15	1.17	1.19	1.16	1.17	0.01	3.5	2
A2	J(H3'-H4')	1.30	1.29	1.31	1.32	1.31	0.01	<2	2
A3	J(H3'-H4')	1.43	1.43	1.40	1.46	1.43	0.02	~2	2
U4	J(H3'-H4')	2.53	2.45	2.49	2.43	2.48	0.05	~4	2
Gamma									
C1	J(H5'-H4')	3.96	3.92	3.92	3.94	3.94	0.02	3.5	2
C1	J(H5''-H4')	3.82	3.84	3.83	3.83	3.83	0.01	3.5	2
A2	J(H5'-H4')	2.52	2.53	2.67	2.53	2.56	0.07	~2	2
A2	J(H5''-H4')	4.48	4.48	4.46	4.47	4.47	0.01	~2	2
A3	J(H5'-H4')	2.94	2.92	2.94	2.92	2.93	0.01	<2	2
A3	J(H5''-H4')	4.02	4.00	4.05	4.04	4.03	0.02	~2	2
U4	J(H5'-H4')	3.22	3.26	3.21	3.28	3.24	0.03	~2	2
U4	J(H5''-H4')	4.09	4.23	3.85	4.05	4.05	0.16	3	2
Beta									
A2	J(P-H5')	4.14	4.11	4.10	4.12	4.12	0.02	3.1	2
A2	J(P-H5'')	1.56	1.60	1.59	1.57	1.58	0.02	2.4	2
A3	J(P-H5')	4.24	4.24	4.21	4.24	4.23	0.01	4.5	2
A3	J(P-H5'')	1.78	1.63	1.70	1.66	1.69	0.07	~2	2
U4	J(P-H5')	3.95	3.93	3.85	3.89	3.91	0.04	5.6	2
U4	J(P-H5'')	3.34	4.11	2.34	3.43	3.31	0.73	4	2
Epsilon									
A2	J(2P-1H3')	4.05	4.06	4.27	4.07	4.11	0.10	~6	2
A3	J(3P-2H3')	3.12	3.10	3.26	3.14	3.16	0.07	~3.5	2

Table S7. Predicted and Measured NOE distances for d(UCAAUC)

					BSC1 Error				BSC1	
d(UCAAUC)	low	NMR	high		ss1	ss2	ss3	ss4	Avg	stdev
U1H1'-U1H6	3.23	3.71	4.60		0.00	0.00	0.00	0.00	3.68	0.11
U1H2'-U1H6	2.86	3.20	3.63		-0.57	-0.57	-0.57	-0.56	2.29	0.00
U1H2'-C2H5'H5''	3.27	3.76	4.77		0.00	0.00	0.00	0.00	4.40	0.00
U1H2''-U1H6	3.64	4.46	5.28		-0.09	-0.09	-0.08	-0.08	3.56	0.00
U1H2''-C2H6	3.53	4.21	4.90		-1.18	-1.18	-1.17	-1.18	2.35	0.00
U1H3'-U1H6	3.52	4.20	4.88		0.00	0.00	0.00	0.00	4.35	0.02
C2H1'-A3H5''	2.95	3.31	3.81		0.22	0.22	0.23	0.23	4.03	0.00
C2H2'-C2H6	2.42	2.67	2.95		-0.25	-0.25	-0.25	-0.25	2.17	0.00
C2H2'-A3H8	3.32	3.84	5.05		-0.20	-0.18	-0.21	-0.20	3.12	0.01
C2H2''-C2H6	3.08	3.49	4.10		0.00	0.00	0.00	0.00	3.31	0.00
C2H2''-A3H8	3.16	3.60	4.34		-0.78	-0.77	-0.78	-0.77	2.38	0.00
C2H3'-A3H8	3.35	3.89	5.27		0.00	0.00	0.00	0.00	4.35	0.06
C2H5'H5''-C2H6	3.19	3.64	4.43		0.00	0.00	0.00	0.00	4.16	0.02
A3H1'-A3H8	2.88	3.23	3.67		0.20	0.01	0.20	0.20	3.82	0.09
A3H1'-A4H5'	2.55	2.83	3.13		-0.16	-0.16	-0.14	-0.17	2.39	0.01
A3H1'-A4H5''	2.65	2.94	3.28		0.86	0.85	0.87	0.84	4.13	0.01
A3H2'-A3H8	2.20	2.42	2.64		0.00	0.00	0.00	0.00	2.28	0.00
A3H2'-A4H8	2.94	3.31	3.79		0.00	0.00	0.00	0.00	3.20	0.01
A3H2''-A3H8	2.66	2.95	3.29		0.12	0.13	0.13	0.12	3.42	0.00
A3H2''-A4H8	2.67	2.96	3.30		-0.31	-0.31	-0.29	-0.31	2.36	0.01
A3H3'-A3H5'	2.50	2.76	3.05		0.59	0.60	0.59	0.59	3.64	0.00
A3H3'-A3H5''	2.78	3.09	3.48		-0.26	-0.26	-0.26	-0.26	2.52	0.00
A3H3'-A3H8	3.14	3.57	4.28		0.16	0.16	0.16	0.18	4.44	0.01
A3H3'-A4H8	3.70	4.59	5.49		0.00	0.00	0.00	0.00	4.46	0.03
A3H4'-A3H8	3.77	4.82	5.87		0.00	0.00	0.00	0.00	5.15	0.00
A3H5'-A3H8	3.47	4.10	4.73		0.04	0.06	0.03	0.04	4.77	0.01
A3H2-A4H1'	3.82	4.98	6.13		0.00	0.00	0.00	0.00	4.70	0.02
A3H8-A4H8	3.62	4.40	5.19		0.00	0.00	0.00	0.00	4.03	0.02
A4H1'-A4H2'H2''	2.21	2.44	2.67		0.00	0.00	0.00	0.00	2.31	0.00
A4H1'-A4H2	3.81	4.93	6.05		0.00	0.00	0.00	0.00	4.47	0.00
A4H1'-A4H8	3.01	3.39	3.93		0.00	0.00	0.00	0.00	3.87	0.01
A4H1'-U5H5''	2.80	3.12	3.52		0.71	0.69	0.68	0.64	4.20	0.03
A4H2'H2''-A4H8	2.10	2.31	2.54		0.00	0.00	0.00	0.00	2.27	0.01
A4H2'H2''-U5H3'	3.49	4.14	4.78		0.00	0.00	0.00	0.00	4.09	0.06
A4H2'H2''-U5H5'	3.31	3.82	4.97		-0.01	-0.03	-0.20	-0.08	3.23	0.09
A4H2'H2''-U5H5	3.16	3.60	4.34		0.00	0.00	0.00	0.00	3.32	0.04
A4H2'H2''-U5H6	2.69	2.99	3.34		-0.29	-0.30	-0.32	-0.34	2.38	0.02
A4H2'H2''-C6H5	3.60	4.37	5.15		-0.58	-0.55	-0.42	-0.35	3.13	0.11
A4H3'-A4H8	3.34	3.87	5.17		0.00	0.00	0.00	0.00	4.38	0.02
A4H5'H5''-A4H8	3.34	4.24	5.13		0.00	0.00	0.00	0.00	4.22	0.08
U5H2'-U5H6	2.35	2.59	2.84		-0.07	-0.09	-0.09	-0.11	2.26	0.01
U5H2'-C6H5'	3.28	3.77	4.80		0.00	0.00	0.00	0.00	4.39	0.02
U5H2''-U5H6	3.03	3.42	3.98		0.00	0.00	0.00	0.00	3.46	0.02
U5H2''-C6H6	3.51	4.17	4.84		-1.09	-1.10	-1.10	-1.12	2.41	0.01
U5H3'-U5H5'	2.70	3.00	3.35		0.16	0.24	0.28	0.26	3.59	0.05
U5H3'-U5H5''	2.96	3.33	3.84		-0.44	-0.44	-0.44	-0.44	2.52	0.00
U5H3'-U5H6	2.92	3.28	3.75		0.48	0.50	0.45	0.43	4.21	0.03
U5H3'-C6H6	3.23	3.71	4.60		-0.29	-0.25	-0.27	-0.15	2.99	0.06
U5H4'-U5H6	3.82	4.97	6.12		0.00	0.00	0.00	0.00	4.71	0.03
U5H5''-U5H6	3.70	4.61	5.53		0.00	0.00	0.00	0.00	4.63	0.17
C6H1'-C6H6	3.37	3.93	5.48		0.00	0.00	0.00	0.00	3.72	0.00
C6H2'-C6H6	2.81	3.13	3.53		-0.51	-0.51	-0.49	-0.49	2.31	0.01
C6H3'-C6H5''	2.99	3.37	3.90		-0.47	-0.47	-0.46	-0.45	2.53	0.01
C6H3'-C6H6	3.11	3.53	4.20		0.00	0.00	0.00	0.00	3.83	0.01
C6H5'-C6H6	3.60	4.36	5.12		0.00	0.00	0.00	0.00	3.87	0.05
C6H5''-C6H6	3.55	4.25	4.96		0.00	0.00	0.00	0.00	4.20	0.13

Table S8. Predicted and Measured J couplings for d(UCAAUC)

dUCAAUC_noe800_pdec_									
J couplings from dUCAAUC data +-pdec at ~0C									
Pucker		ss1	ss2	ss3	ss4	MD avg	stdev	NMR avg	err
U1	J(H3'-H4')	1.17	1.17	1.20	1.16	1.17	0.02	3.5	2
C2	J(H3'-H4')	1.50	1.51	1.51	1.51	1.51	0.01	2.225	2
A3	J(H3'-H4')	1.31	1.35	1.36	1.32	1.34	0.02	<2.5	2
A4	J(H3'-H4')	1.46	1.44	1.40	1.45	1.44	0.02	<2.5	2
U5	J(H3'-H4')	1.46	1.48	1.57	1.64	1.54	0.08	3.0	2
C6	J(H3'-H4')	1.95	1.99	2.04	2.09	2.02	0.06	~4	2
Gamma									
U1	J(H5'-H4')	3.84	3.82	3.84	3.82	3.83	0.01	3.9	2
U1	J(H5''-H4')	3.85	3.84	3.84	3.85	3.85	0.01	3.1	2
C2	J(H5'-H4')	2.64	2.64	2.63	2.61	2.63	0.01	2.5	2
C2	J(H5''-H4')	4.41	4.43	4.43	4.43	4.42	0.01	2.5	2
A3	J(H5'-H4')	2.89	2.86	2.86	2.87	2.87	0.01	2.5	2
A3	J(H5''-H4')	4.05	4.07	4.08	4.07	4.07	0.01	<2.5	2
A4	J(H5'-H4')	2.92	2.95	2.97	2.92	2.94	0.02	<2.5	2
A4	J(H5''-H4')	4.05	4.05	4.03	4.03	4.04	0.01	<2.5	2
U5	J(H5'-H4')	3.05	3.03	3.03	3.03	3.03	0.01	2	2
U5	J(H5''-H4')	3.99	3.95	3.92	3.93	3.95	0.03	<2	2
C6	J(H5'-H4')	3.20	3.18	3.09	3.11	3.15	0.05	<2.5	2
C6	J(H5''-H4')	3.89	4.00	3.96	4.05	3.98	0.07	2.6	2
Beta									
A3	J(P-H5')	4.14	4.12	4.15	4.15	4.14	0.02	~1	2
A3	J(P-H5'')	1.60	1.58	1.57	1.60	1.59	0.01	~2	2
A4	J(P-H5')	4.40	4.37	4.33	4.33	4.36	0.04	~2	2
A4	J(P-H5'')	1.90	2.00	1.89	1.78	1.89	0.09	~1	2
U5	J(P-H5')	4.56	4.53	4.32	4.32	4.43	0.13	~1	2
U5	J(P-H5'')	2.25	1.93	1.84	1.87	1.97	0.19	~3.5	2
C6	J(P-H5')	3.68	3.66	3.66	3.71	3.68	0.02	~3	2
C6	J(P-H5'')	2.41	2.92	2.32	2.70	2.59	0.27	~3.5	2
Epsilon									
C2	J(2P-1H3')	4.28	4.27	4.37	4.30	4.30	0.05	6.3	2
A3	J(3P-2H3')	3.22	3.21	3.30	3.28	3.25	0.04	5.18	2
A4	J(4P-3H3')	3.43	3.38	3.52	3.29	3.40	0.10	4.5	2
C6	J(6P-5H3')	5.57	5.39	5.38	5.08	5.35	0.20	6.9	2

Table S9a. Predicted absent NOEs for r(CAAU)

absent NOE RNA CAAU OL3

	cutoff	OL3 ss1
C1H1'-U4H5	5.2	4.961
C1H5-A3H2'	4.6	3.242
C1H5-A3H3'	4.1	2.126
C1H5-A3H5''	4.6	4.470
C1H5-U4H2'	4.6	2.533
C1H5-U4H3'	5.2	2.967
C1H5-U4H5	4.6	3.646
C1H5-U4H5''	4.6	4.580
C1H6-A3H3'	4.1	3.808
C1H6-U4H2'	4.6	2.645
C1H6-U4H3'	5.2	3.403
C1H6-U4H5	4.6	4.137
A2H2-A3H4'	5.2	5.178
A2H3'-C1H2'	4.1	3.691
A2H5''-C1H5'	4.6	4.424
A2H5''-C1H5''	4.6	3.497
A3H4'-U4H5''	4.6	4.457
A3H8-C1H5	5.2	3.650
U4H2'-C1H5'	4.6	4.001
U4H6-C1H5	4.6	2.938

	cutoff	OL3 ss2
C1H1'-U4H5	5.2	5.087
C1H4'-A2H5''	4.6	4.534
C1H5-A3H2'	4.6	3.318
C1H5-A3H3'	4.1	2.192
C1H5-A3H5'	4.6	4.581
C1H5-U4H2'	4.6	2.604
C1H5-U4H3'	5.2	3.048
C1H5-U4H5	4.6	3.771
C1H6-A2H3'	4.1	3.870
C1H6-A3H3'	4.1	3.900
C1H6-U4H2'	4.6	2.724
C1H6-U4H3'	5.2	3.479
C1H6-U4H5	4.6	4.284
A2H1'-A3H5''	5.2	5.029
A2H2-C1H2'	5.2	5.002
A2H2-A3H2'	5.2	4.662
A2H3'-C1H2'	4.1	3.640
A2H4'-A3H2'	4.6	4.485
A2H5'-C1H5''	4.6	3.632
A2H5''-C1H5''	4.6	4.029
A3H2-A2H2'	5.2	4.791
A3H2-U4H2'	5.2	4.433
A3H2-U4H3'	5.8	4.726
A3H3'-U4H5'	4.1	4.072
A3H4'-U4H5''	4.6	4.359
A3H5'-U4H2'	4.6	4.315
A3H5'-U4H5'	4.6	4.519
A3H5'-U4H5''	4.6	3.117
A3H8-C1H5	5.2	3.790
U4H2'-C1H5'	4.6	4.114
U4H6-C1H5	4.6	3.036

	cutoff	OL3 ss3
C1H1'-U4H5	5.2	4.931
C1H5-A3H2'	4.6	3.283
C1H5-A3H3'	4.1	2.155
C1H5-A3H5''	4.6	4.533
C1H5-U4H2'	4.6	2.572
C1H5-U4H3'	5.2	3.002
C1H5-U4H5	4.6	3.691
C1H6-A3H3'	4.1	3.858
C1H6-U4H2'	4.6	2.681
C1H6-U4H3'	5.2	3.442
C1H6-U4H5	4.6	4.164
A2H2'-U4H3'	5.2	4.988
A2H3'-C1H2'	4.1	3.735
A2H4'-U4H3'	5.2	4.709
A2H5'-C1H5''	4.6	4.086
A2H5''-C1H5'	4.6	4.500
A2H5''-C1H5''	4.6	3.542
A3H2-U4H2'	5.2	4.822
A3H2-U4H3'	5.8	5.356
A3H4'-U4H5''	4.6	4.320
A3H8-C1H5	5.2	3.698
U4H2'-C1H5'	4.6	4.049
U4H5'-A3H5''	4.6	4.414
U4H6-C1H5	4.6	2.975

	cutoff	OL3 ss4
C1H1'-U4H5	5.2	5.075
C1H4'-A2H5''	4.6	4.530
C1H5-A3H2'	4.6	3.342
C1H5-A3H3'	4.1	2.184
C1H5-A3H5''	4.6	4.583
C1H5-U4H2'	4.6	2.627
C1H5-U4H3'	5.2	3.027
C1H5-U4H5	4.6	3.745
C1H6-A3H3'	4.1	3.911
C1H6-U4H2'	4.6	2.725
C1H6-U4H3'	5.2	3.473
C1H6-U4H5	4.6	4.238
A2H2'-U4H3'	5.2	4.887
A2H3'-C1H2'	4.1	3.772
A2H5'-C1H5''	4.6	4.445
A2H5''-C1H5''	4.6	3.569
A2H8-A3H2	5.8	5.639
A3H2-A2H2'	5.2	4.585
A3H2-U4H2'	5.2	4.126
A3H2-U4H3'	5.8	4.481
A3H4'-U4H5''	4.6	4.000
A3H8-C1H5	5.2	3.751
U4H2'-C1H5'	4.6	4.060
U4H6-C1H5	4.6	3.017

absent NOE RNA CAAU ROC-RNA

	cutoff	ROCRNA ss1
A2H1'-C1H5	5.2	4.679
A2H2-C1H5	5.2	5.104
A2H8-U4H3'	5.8	5.552
A3H2-U4H5	5.2	4.930
U4H6-A3H5'	4.6	4.542

	cutoff	ROCRNA ss2
C1H5-A3H2'	4.6	4.070
C1H5-A3H3'	4.1	2.800
C1H5-U4H2'	4.6	2.979
C1H5-U4H3'	5.2	4.200
C1H6-U4H2'	4.6	3.251
C1H6-U4H3'	5.2	4.562
A2H1'-C1H5	5.2	4.828
A2H1'-A3H5''	5.2	5.106
A2H3'-C1H2'	4.1	3.852
A2H5'-C1H5''	4.6	4.112
A3H2-U4H5	5.2	5.173
A3H5'-U4H2'	4.6	4.194
A3H5'-U4H5''	4.6	3.970
A3H8-C1H5	5.2	4.399
U4H1'-U4H5'	4.6	4.586
U4H2'-C1H5'	4.6	4.214
U4H6-C1H5	4.6	3.901

	cutoff	ROCRNA ss3
A2H1'-C1H5	5.2	4.677
A2H2-C1H5	5.2	5.153
A2H8-U4H2'	5.2	5.014
A2H8-U4H3'	5.8	5.123
A3H2-U4H2'	5.2	4.830
A3H2-U4H5	5.2	4.926
U4H5-A2H2'	4.6	4.333
U4H5-A3H5'	4.6	4.288
U4H6-A3H5'	4.6	4.108

	cutoff	ROCRNA ss4
C1H1'-A3H8	5.8	5.041
A2H1'-C1H5	5.2	4.767
A2H1'-U4H5	5.2	5.115
A2H2-C1H5	5.2	5.121
A2H2'-U4H3'	5.2	4.688
A2H3'-U4H3'	4.6	3.884
A2H8-U4H2'	5.2	4.571
A2H8-U4H3'	5.8	4.645
A3H2-U4H2'	5.2	5.068
A3H2-U4H5	5.2	4.960
A3H8-C1H1'	5.8	5.041
U4H5-A2H2'	4.6	3.998
U4H5-A3H5'	4.6	3.998
U4H6-A2H2'	4.6	4.564
U4H6-A3H5'	4.6	3.869

Table S9b. Predicted absent NOEs for r(UCAAUC)

	cutoff	OL3 ss1
U1H1'-C2H5'	5	4.863
C2H2'-U1H5''	4.4	3.480
C2H3'-U1H5'	4.4	3.856
C2H3'-U1H5''	4.4	3.651
C2H5-U1H4'	5	4.613
C2H5'-U1H5''	4.4	4.373
C2H5''-U1H5''	4.4	3.992
A3H1'-U1H1'	5.6	5.131
A3H1'-U1H5	5	4.823
A3H4'-U1H5'	4.4	4.388
A3H5'-U1H5'	4.4	3.843
A3H5'-U1H5''	4.4	4.308
A3H8-U1H5'	5	4.436
A4H2-A3H1'	5.6	5.513
A4H3'-C6H2'	4	3.686
A4H3'-C6H3'	4	3.967
A4H5''-U5H5''	4.4	3.363
A4H8-C6H2'	5	3.117
C6H1'-A4H1'	5	4.568

	cutoff	OL3 ss2
U1H1'-A3H2'	5	3.850
U1H6-A3H2'	4.4	4.318
C2H2'-U1H5''	4.4	4.273
C2H3'-U1H5'	4.4	4.202
C2H3'-U1H5''	4.4	3.523
C2H5'-U1H5''	4.4	4.146
C2H5''-U1H5''	4.4	3.415
A3H1'-U1H1'	5.6	5.374
A3H2-C2H4'	5	4.293
A3H2-A3H5'	5	4.773
A3H2'-U1H4'	5	3.662
A3H3'-C2H5'	4	3.947
A3H3'-C2H5''	4	3.200
A3H8-U1H5'	5	4.494
A3H8-U5H1'	5.6	5.267
A4H1'-U1H5	5	4.934
A4H1'-C6H2'	5	3.088
A4H1'-C6H3'	5	4.013
A4H2-A3H2'	5	4.910
A4H2-U5H5	5	4.768
A4H2-C6H2'	5	4.581
A4H3'-A3H5''	4	2.971
A4H4'-C6H2'	4.4	3.553
C6H2'-U5H5''	4.4	4.368
C6H6-A4H1'	5	4.865
C6H6-A4H4'	4.4	3.839

	nmr cutoff	OL3 ss3
U1H1'-C2H5'	5	4.796
U1H1'-A3H2'	5	4.363
C2H1'-U5H1'	5.6	4.369
C2H2'-U1H5''	4.4	3.566
C2H3'-U1H5'	4.4	3.743
C2H3'-U1H5''	4.4	3.758
C2H5'-U1H5''	4.4	4.288
C2H5''-U1H5''	4.4	4.272
A3H1'-U1H1'	5.6	5.467
A3H1'-U5H5''	5	4.691
A3H2-U5H1'	5.6	5.145
A3H2'-U1H4'	5	3.617
A3H2'-U5H5'	4.4	4.279
A3H3'-C2H5''	4	3.626
A3H8-U1H5'	5	4.106
A4H1'-C6H2'	5	4.642
A4H1'-C6H5'	5	4.416
A4H2-A3H1'	5.6	5.598
A4H2-C6H1'	5	4.426
A4H3'-A3H5''	4	3.682
U5H1'-C2H4'	5	4.148
C6H1'-A4H1'	5	3.729
C6H6-A4H1'	5	4.147

	nmr cutoff	OL3 ss4
U1H1'-C2H5'	5	4.937
U1H1'-A3H2'	5	4.206
C2H2'-U1H5''	4.4	3.695
C2H3'-U1H5'	4.4	3.882
C2H3'-U1H5''	4.4	3.703
C2H5'-U1H5''	4.4	4.164
C2H5''-U1H5''	4.4	4.201
C2H6-A4H1'	5	4.015
A3H1'-U1H1'	5.6	3.426
A3H2-U5H1'	5.6	5.209
A3H2'-U1H4'	5	3.639
A3H2'-U5H5'	4.4	3.600
A3H2'-U5H5''	4.4	4.064
A3H3'-C2H5'	4	3.902
A3H3'-C2H5''	4	3.382
A3H4'-U1H5'	4.4	3.629
A3H5'-U1H5'	4.4	4.238
A3H8-U1H5'	5	4.199
A3H8-U5H1'	5.6	5.044
A3H8-C6H5	5	4.476
A4H1'-U1H4'	5.6	4.586
A4H1'-C2H5	5	4.659
A4H2-U1H1'	5.6	5.582
A4H2-U1H5'	5	4.563
A4H2-C2H1'	5.6	5.060
A4H2-A3H1'	5.6	5.140
A4H2-A3H4'	5	3.492
A4H2-U5H5	5	4.995
A4H4'-U1H4'	5	4.882
C6H1'-A4H1'	5	4.384
C6H5-A4H1'	5	4.411
C6H6-A4H1'	5	4.801

	NMR cutoff	ROCRNA ss1
U1H5-C2H2'	4.4	3.560
U1H5-A3H5'	4.4	3.407
U1H6-C2H3'	4.4	3.519
U1H6-A3H2'	4.4	4.335
C2H1'-U1H5	5	4.861
C2H3'-U1H5''	4.4	4.285
A3H8-U1H5'	5	3.910
C6H2'-U5H5''	4.4	3.992

	NMR cutoff	ROCRNA ss2
U1H5-C2H2'	4.4	4.097
U1H5-A3H5'	4.4	3.982
U1H6-C2H3'	4.4	4.103
C2H1'-U1H5	5	4.886
A3H8-U1H5'	5	4.442
A4H1'-U1H5'	5	4.344
C6H2'-U5H5''	4.4	4.123
C6H5-A4H1'	5	4.587

	NMR cutoff	ROCRNA ss3
C2H1'-U1H5	5	4.810
A3H8-C6H5''	5	4.695
A4H1'-C6H2'	5	3.646
A4H1'-C6H3'	5	4.203
A4H4'-C6H2'	4.4	4.359
U5H5-A3H5''	4.4	3.616
C6H2'-U5H5''	4.4	4.244
C6H5-A4H1'	5	4.609

	NMR cutoff	ROCRNA ss4
U1H5-A3H2'	4.4	3.428
U1H6-A3H2'	4.4	3.224
C2H5'-U1H5''	4.4	3.661
C2H5''-U1H5''	4.4	3.273
A3H1'-U1H5	5	3.874
A3H5''-A4H5''	4.4	3.700
A4H1'-C6H2'	5	4.241
A4H1'-C6H3'	5	4.639
A4H4'-U1H5''	4.4	3.996
A4H8-C6H2'	5	4.888
U5H5-A3H5''	4.4	4.334
C6H2'-U5H5''	4.4	4.147
C6H5-A4H1'	5	3.772

Table S10. Predicted absent NOEs for d(CAAU) and d(UCAAUC)

dUCAAUC		MD					
absent NOE	NMR cutoff	ss1	ss2	ss3	ss4	pred avg	err
U1H5''-U1H2'	3.749	3.485	3.502	3.510	3.498	3.499	0.010
A3H2-A4H4'	5.054	4.453	4.470	4.482	4.422	4.457	0.026
A4H1'-U5H2'	3.574	3.051	3.086	3.226	3.322	3.171	0.126

dCAAU							
absent NOE	nmr cutoff	ss1	ss2	ss3	ss4	pred avg	err
A2H2-C1H5	4.697	4.645	4.650	4.676	4.626	4.649	0.021
A2H2-A3H4'	5.272	4.420	4.419	4.475	4.456	4.443	0.028
A3H2-U4H4'	4.697	4.273	4.297	4.372	4.366	4.327	0.050
A3H2''-U4H2'	3.592	3.516	3.528	3.469	3.519	3.508	0.026
A2H8-A3H2	5.272			5.110			

Figure S1. Principal component projection for r(CAAU)

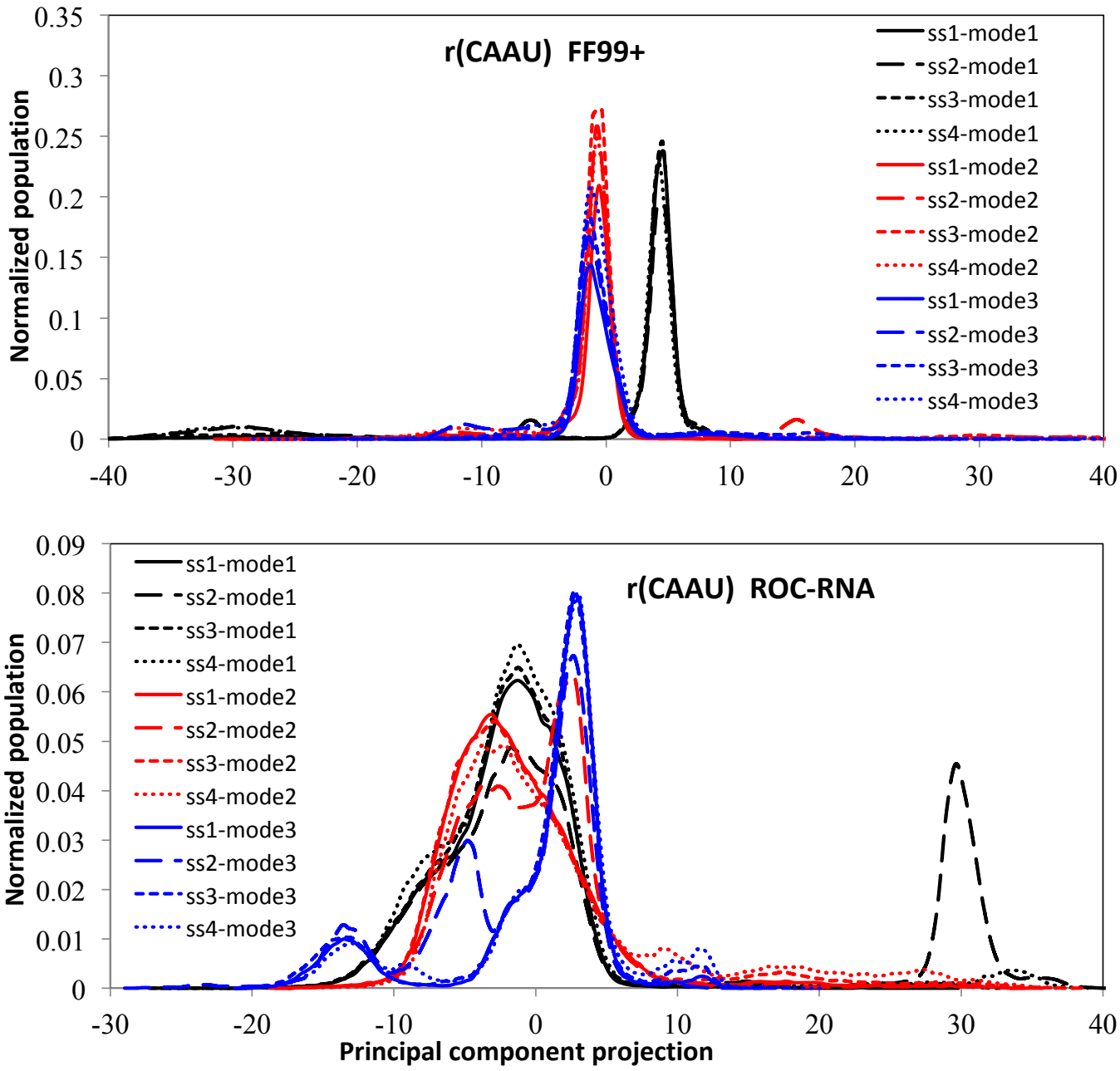


Figure S2. Principal component projection for r(UCAAUC)

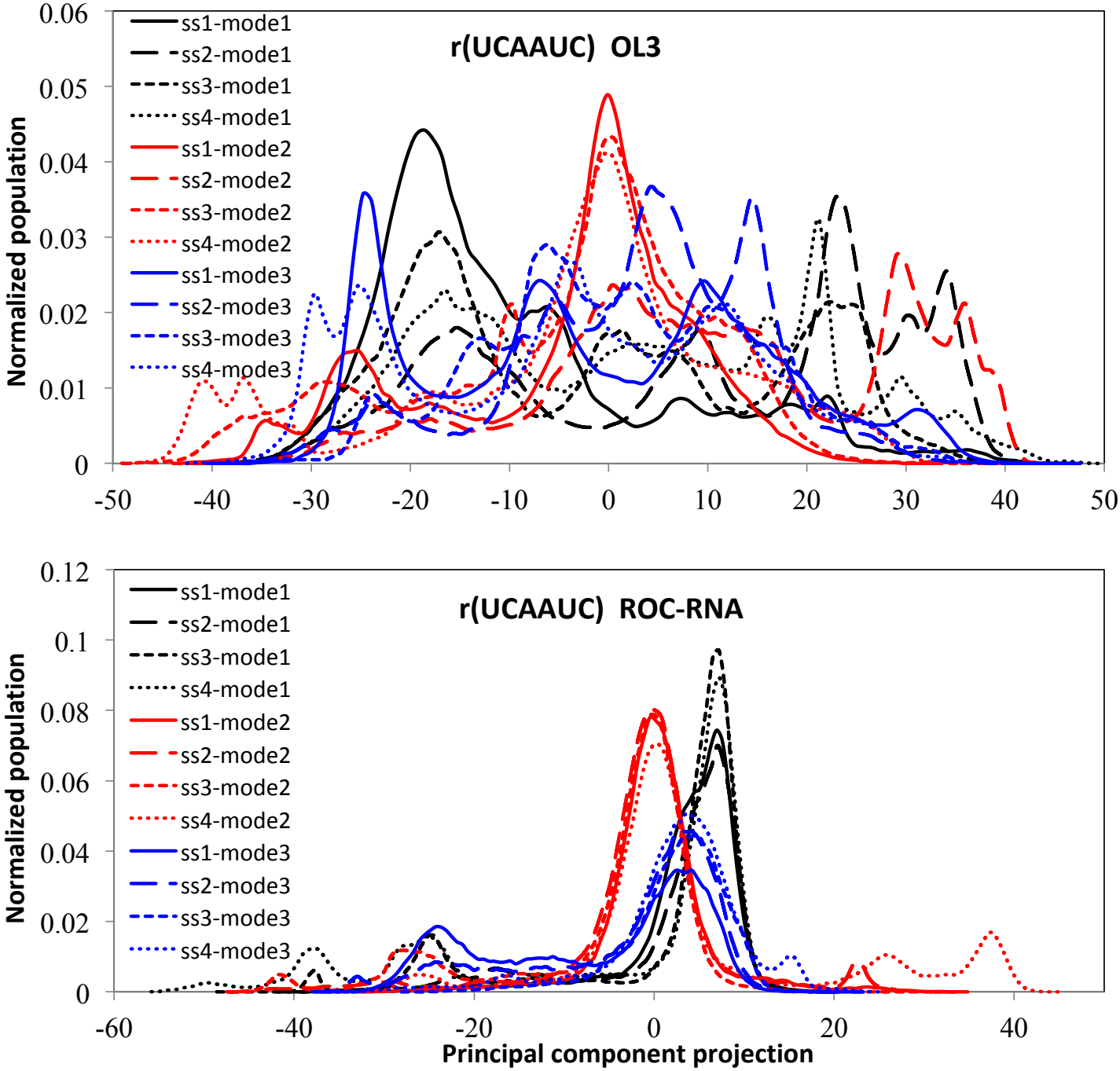


Figure S3. Principal component projection for d(CAAU) and d(UCAAUC)

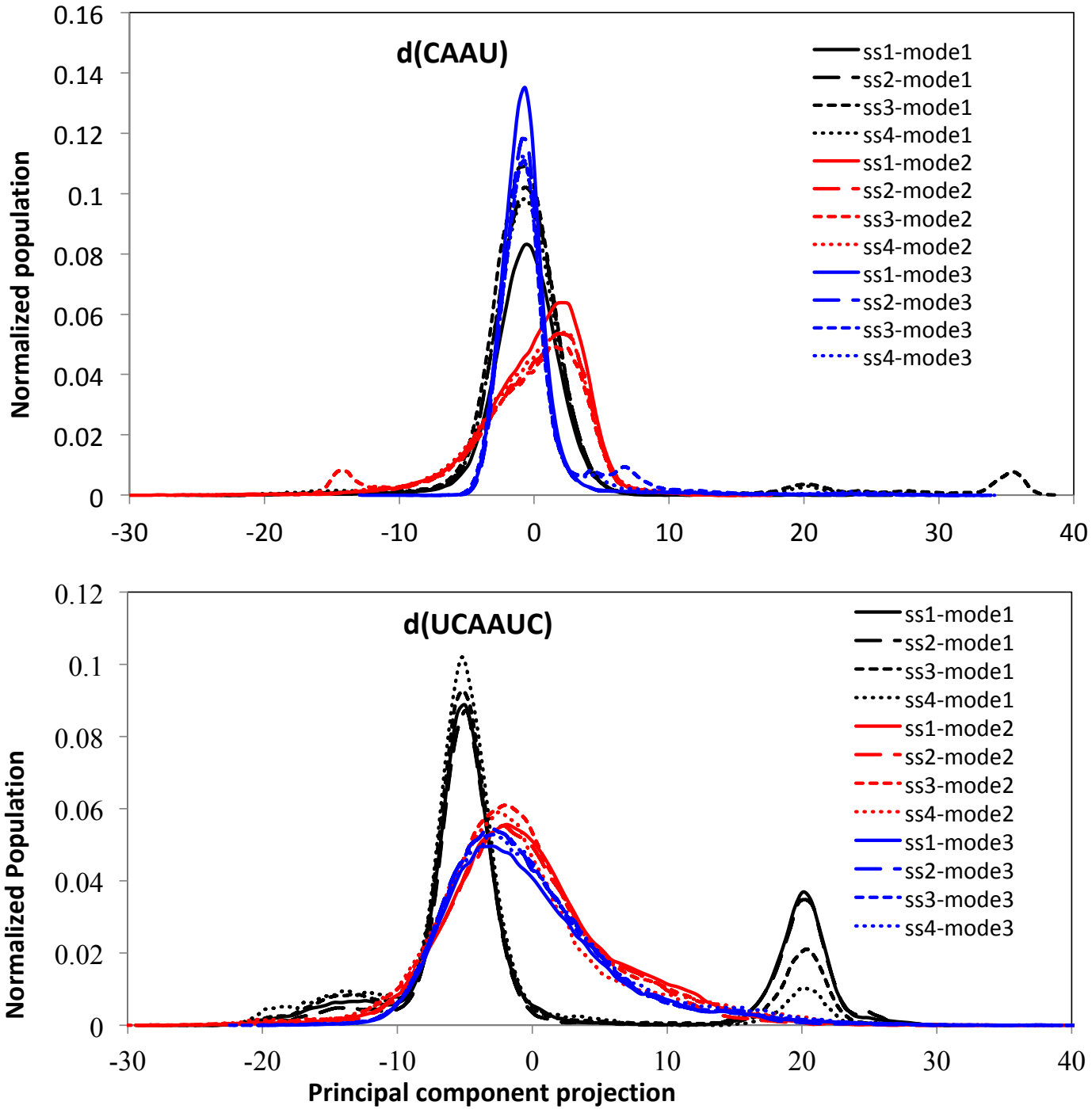


Figure S4. Comparison of NOE distances between water models for d(UCAAUC)

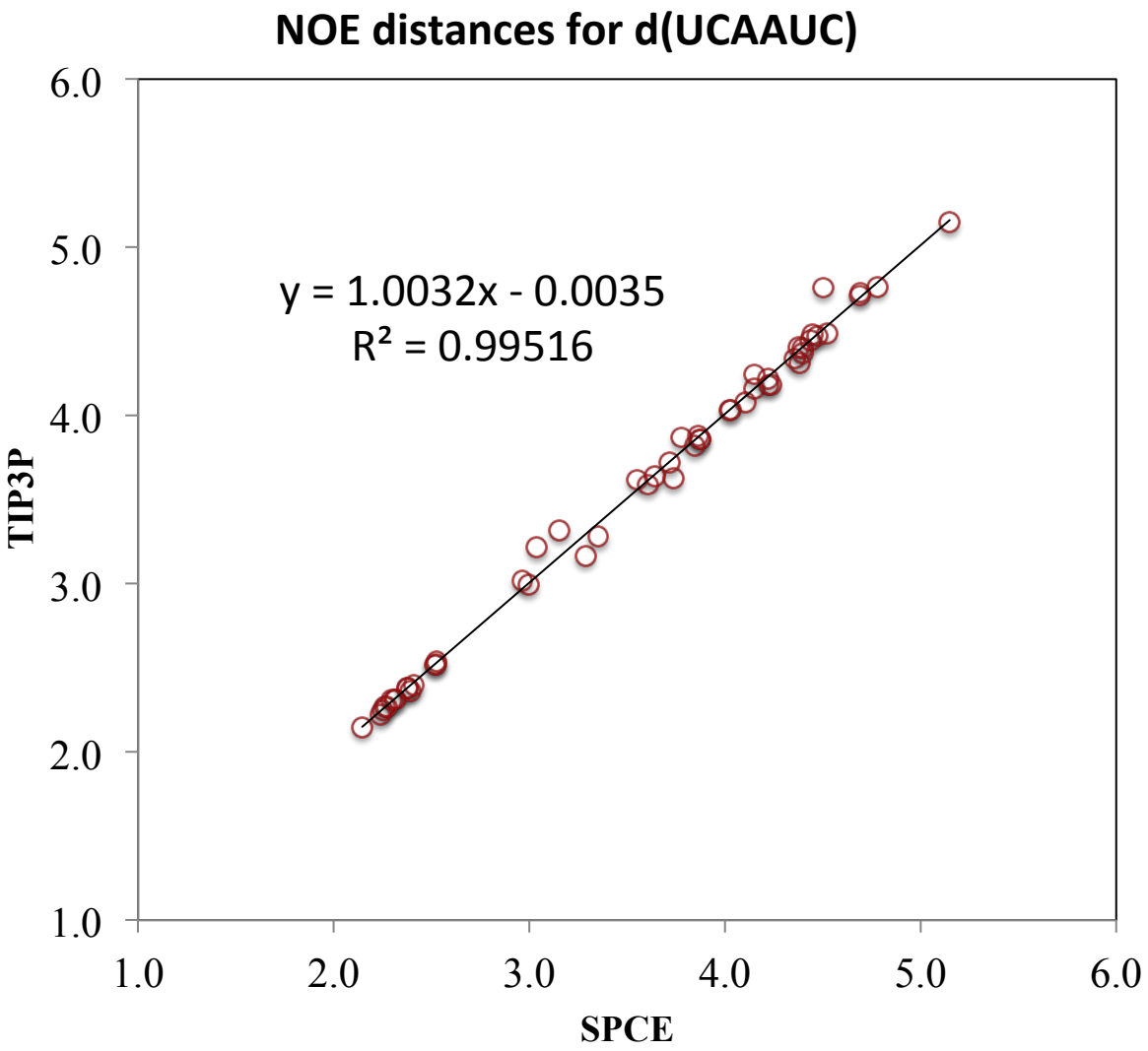


Table S11. Partial charges for deoxyU

dT	charges		dU	charges		diff
P	1.1659		P	1.1659		0.0000
OP1	-0.7761		OP1	-0.7761		0.0000
OP2	-0.7761		OP2	-0.7761		0.0000
O5'	-0.4954		O5'	-0.4954		0.0000
C5'	-0.0069		C5'	-0.0069		0.0000
H5'	0.0754		H5'	0.0754		0.0000
H5''	0.0754		H5''	0.0754		0.0000
C4'	0.1629		C4'	0.1629		0.0000
H4'	0.1176		H4'	0.1176		0.0000
O4'	-0.3691		O4'	-0.3691		0.0000
C3'	0.0713		C3'	0.0713		0.0000
H3'	0.0985		H3'	0.0985		0.0000
C2'	-0.0854		C2'	-0.0854		0.0000
H2'	0.0718		H2'	0.0718		0.0000
H2''	0.0718		H2''	0.0718		0.0000
O3'	-0.5232		O3'	-0.5232		0.0000
C1'	0.068		C1'	0.072125		-0.0041
H1'	0.1804		H1'	0.173473		0.0069
N1	-0.0239		N1	-0.001625		-0.0223
C6	-0.2209		C6	-0.081963		-0.1389
H6	0.2607		H6	0.230589		0.0301
C5	0.0025		C5	-0.383037		0.3855
C4	0.5194		C4	0.650378		-0.1310
O4	-0.5563		O4	-0.568656		0.0124
N3	-0.434		N3	-0.466716		0.0327
H3	0.342		H3	0.332807		0.0092
C2	0.5677		C2	0.567581		0.0001
O2	-0.5881		O2	-0.580214		-0.0079
C7	-0.2269		H5	0.176858		-0.4038
H71	0.077					
H72	0.077					
H73	0.077					

Figure S5. Blue: nH2′- nH6/8; Red: (n-1)H2′′- nH6/8 distances in d(UCAAUC) determined by different NMR methods. Distances on the horizontal and vertical axis are from NOESY (200 ms mix time) and ROESY (50 ms mix time) NMR experiments. Numbers next to symbols indicate residue (n) or residue pair (n-1, n).

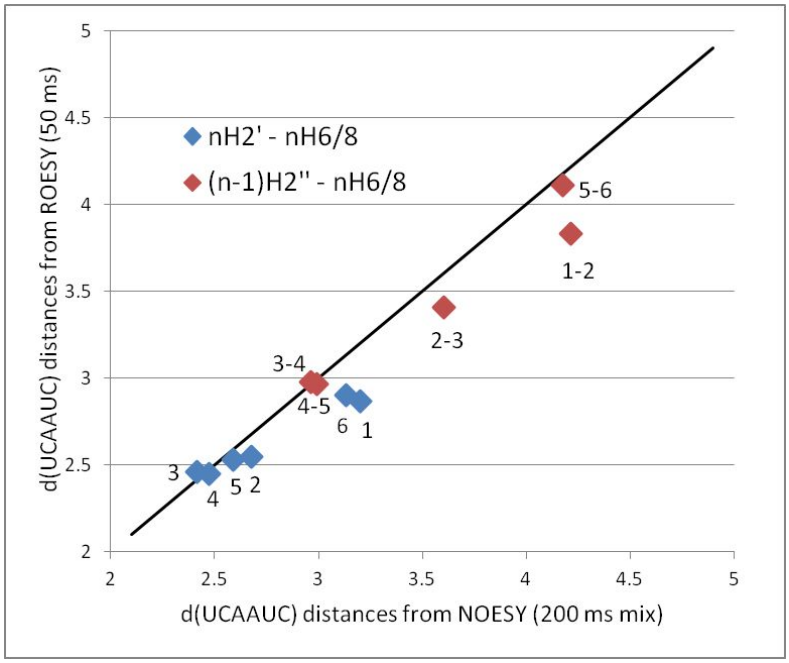


Table S12. ^{1}H chemical shifts at 1 °C for r(UCAAUC), d(CAAU), and d(UCAAUC). In DNA, the H2' and H2'' are assigned based on NOE cross-peak nH8/6-nH2' > nH8/6-nH2''; cytosine H41 and H42 are assigned based on NOE cross-peak H5-H42 > H5-H41 ; H5′ and H5′′ are not stereospecifically assigned.

Residue	**Atom ID**								
	H1'	H2'	H2''	H3'	H4'	H5'/H5''		H2/5	H6/8
rUCAAUC									
U1	5.68	4.44	na	4.45	4.24	3.91	3.79	5.64	7.83
C2	5.69	4.47	na	4.50	4.38	4.32	4.12	5.63	7.78
A3	5.85	4.76	na	4.67	4.50	4.37	4.20	7.83	8.22
A4	5.72	4.45	na	4.54	4.48	4.46	4.14	8.07	7.92
U5	5.46	4.15	na	4.36	4.32	4.34	4.04	5.34	7.44
C6	5.83	4.09	na	4.22	4.15	4.24	4.02	5.84	7.80
dCAAU									
C1	5.85	1.49	2.13	4.53	3.96	3.61	3.61	5.81	7.38
A2	5.95	2.62	2.74	4.95	4.32	3.91	4.01	7.89	8.19
A3	6.14	2.69	2.69	4.98	4.41	4.22	4.17	7.81	8.30
U4	5.99	2.19	2.22	4.51	4.03	4.21	4.05	5.51	7.56
dUCAAUC									
U1	6.10	2.15	2.43	4.66	4.09	3.68	3.73	5.76	7.72
C2	5.96	1.67	2.18	4.68	4.08	3.91	3.91	5.86	7.48
A3	5.93	2.58	2.73	4.94	4.31	4.03	3.93	7.86	8.18
A4	6.12	2.68	2.68	5.00	4.42	4.20	4.17	7.79	8.29
U5	5.97	2.12	2.36	4.74	4.18	4.09	4.22	5.49	7.46
C6	6.17	2.22	2.33	4.51	4.07	4.05	4.00	5.97	7.78

Chemical Shifts (ppm) of exchangeable protons in r(CAAU) and r(UCAAUC) were obtained from 1D spectra and 2D NOESY spectra (35 and 70 ms mixing time) of samples in 95% H_2O/5% D_2O:

r(CAAU): C1H41 (6.30), C1H42 (6.86)

r(UCAAUC): C2H41 (6.25), C2H42 (6.91), C6H41 (6.60), C6H42(7.27)

All sequences had a broad imino resonance at ~11.1 ppm.

Table S13a. ^{31}P and ^{13}C chemical shifts at 1 °C for r(UCAAUC), d(CAAU), and d(UCAAUC).

Residue	**Atom ID**							
	P	C1'	C2'	C3'	C4'	C5'	C2/5	C6/8
rUCAAUC								
U1	-	92.31	75.54	74.94	85.74	62.34	104.20	143.76
C2	-3.68	92.88	75.84	74.34	83.14	66.14	98.29	142.42
A3	-3.51	92.26	75.64	74.34	83.14	66.44	154.46	140.72
A4	-3.92	92.02	75.84	73.54	83.04	65.54	155.06	139.77
U5	-4.12	92.19	75.74	73.64	83.34	65.34	104.20	141.22
C6	-4.00	92.18	77.14	71.04	84.54	66.24	98.64	142.96
dCAAU								
C1	-	88.74	82.64	78.44	88.44	63.74	99.01	143.66
A2	-4.16	85.24	81.74	79.84	87.74	67.94	155.06	141.71
A3	-4.33	84.74	83.24	78.14	86.94	67.54	154.96	141.82
U4	-4.02	86.84	84.14	71.84	86.94	66.74	104.60	144.06
dUCAAUC								
U1	-	88.04	83.14	77.84	88.54	63.64	104.80	144.36
C2	-3.91	87.94	82.84	78.54	86.64	67.74	98.99	143.66
A3	-4.21	85.34	82.04	79.84	87.74	68.14	155.06	141.77
A4	-4.30	84.74	83.14	78.54	87.14	67.64	154.96	141.82
U5	-4.12	86.54	83.14	76.34	86.04	66.84	104.70	143.66
C6	-3.86	88.34	84.74	72.94	87.74	67.34	98.78	144.16

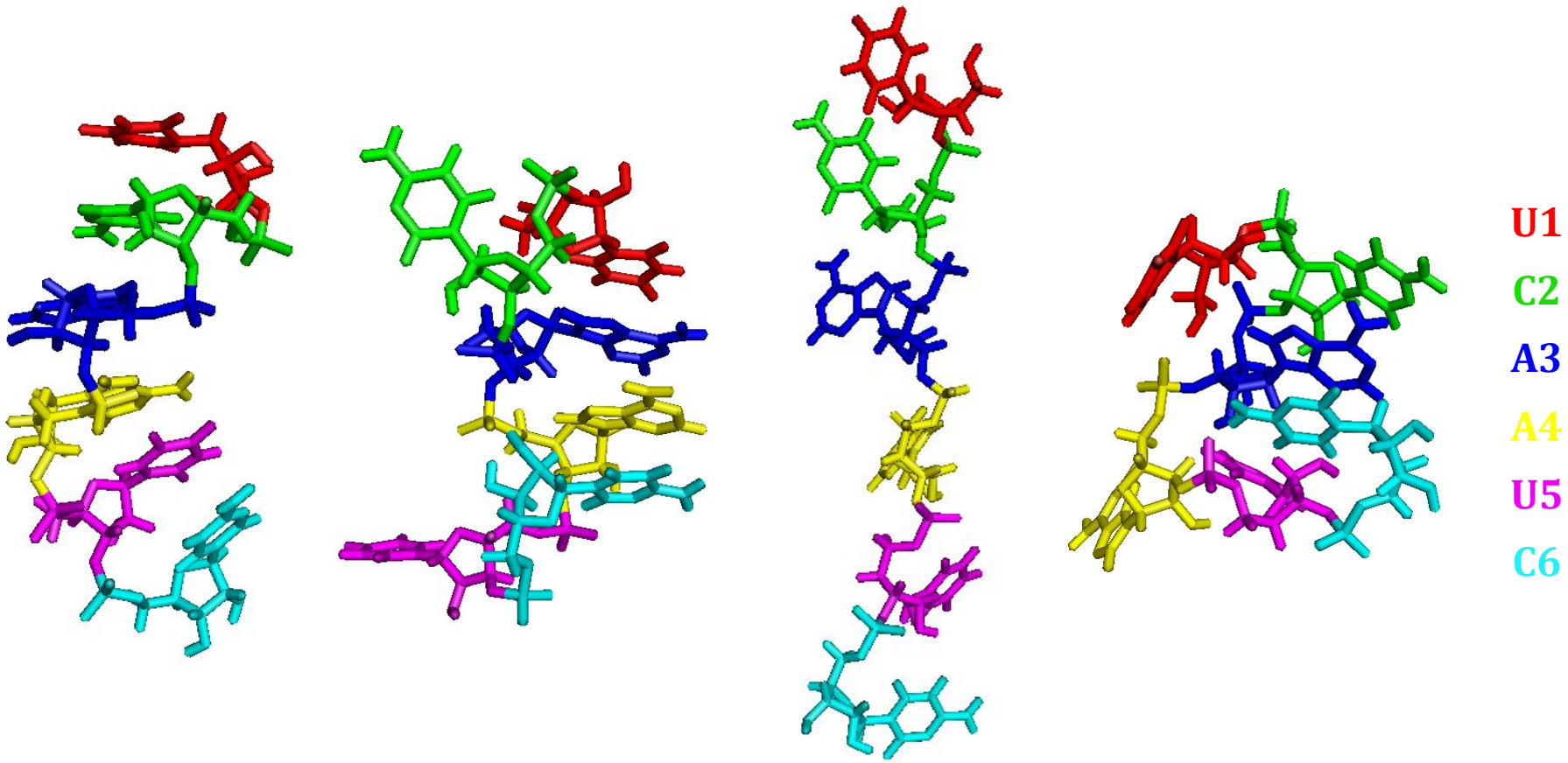
Table S13b. ^{1}H and ^{31}P chemical shifts at 1 °C for Duplex-d(UCAAUC). Duplex-d(UCAAUC) is d5′A**UCAAUC**A/3′AGUUAG. Shifts are listed only for the residues that correspond to single-strand d(UCAAUC). The difference between shifts in Duplex-d(UCAAUC) and d(UCAAUC) are given beneath each entry for atoms nearest the backbone; differences greater than 0.3 ppm are highlighted.

Residue	**Atom ID**									
	H1'	H2'	H2''	H3'	H4'			H2/5	H6/8	P
1 2 3 4 5 6 d5'AUCAAUCA3' 3'AGUUAG5'										
U1	5.86 0.24	2.25 -0.10	2.45 -0.02	4.80 -0.14	4.22 -0.13			5.62	7.69 0.03	-4.04
C2	5.26 0.70	2.05 -0.38	2.31 -0.12	4.80 -0.12	4.09 -0.01			5.76	7.56 -0.08	-3.98 0.07
A3	5.96 -0.03	2.81 -0.23	2.94 -0.22	5.06 -0.13	4.42 -0.11			7.28	8.28 -0.10	-3.66 -0.55
A4	6.08 0.04	2.59 0.09	2.78 -0.10	4.99 0.00	4.44 -0.02			7.59	8.16 0.14	-4.21 -0.10
U5	5.83 0.14	1.94 0.17	2.41 -0.05	4.76 -0.02	4.13 0.05			5.01	7.31 0.15	-4.13 0.00
C6	5.88 0.29	2.06 0.16	2.42 -0.09	4.76 -0.27	4.11 -0.05			5.55	7.44 0.34	-4.08 0.21

Table S14. H1'-H4' distances from crystal structures

H1'-H4'	nt	H1'-H4'	nt	H1'-H4'	nt	H1'-H4'	nt	H1'-H4'	nt	H1'-H4'	nt		H1'-H4'	nt
	1pjg		3SJ2		4PCO		4RBQ		5C5W		5NXT			1em0
3.261	C1	3.231	U2	3.191	G2	3.091	G2	3.249	C3	3.21	G31		3.112	T21
3.402	G5	3.263	G3	3.174	U3	3.233	A3	3.17	U4	3.251	U32		3.238	A22
3.273	A6	3.215	G4	3.219	G4	3.009	G4	3.096	G5	3.205	U33		2.737	G23
3.207	A7	3.241	G5	3.26	G5	3.224	A5	3.353	A6	3.368	C34		2.877	T3
3.39	A8	3.245	C6	3.236	C6	3.267	A6	3.161	G7	3.201	U35		3.234	G5
3.335	A9	3.116	C7	3.204	U7	3.171	G7	3.211	U13	3.206	C36		3.157	T9
	3nd3	3.328	G8	3.281	G8	3.221	A8	3.192	U14	3.185	U37		3.235	A10
3.306	A1	3.255	G9	3.229	U9	3.17	A9	3.187	C15	3.019	A38		2.732	G11
3.257	G2	3.224	C10	3.205	G2	3.259	A10	3.212	U16	3.21	C39		2.875	T15
3.279	A3	3.316	G11	3.178	U3	3.252	G11	3.104	A17	3.212	G40		3.202	G17
3.145	G4	3.29	G12	3.31	G4	3.232	G12	3.182	G18	3.191	A41			1ENE
3.248	A5	3.253	C13	3.258	G5	3.204	G13		5K8H	3.25	A42		3.405	A3
3.282	A6	3.242	G14	3.221	C6	3.223	A14	3.244	A1	3.15	G43		2.963	T8
3.013	G7	3.246	G15	3.241	U7	3.193	A15	3.278	A2	3.181	A44		3.458	G9
3.224	A8	3.225	G16	3.247	G8	3.221	A16		5MRX	3.24	A45			5MVL
3.255	U9	3.251	U17	3.177	U3	3.216	U17	3.126	C2652	3.204	C46		2.684	C4
3.207	U10	3.208	C18	3.181	G4	3.201	U18	3.183	U2653					284D
3.205	U11	3.236	G4	3.231	G5	3.197	U19	3.237	U2656				3.331	C4
3.23	U12	3.223	G5	3.213	C6	3.188	U20	3.103	A2657				3.407	A5
3.234	U13	3.196	C6	3.228	U7	3.232	U21	3.2	C2658				3.208	T3
3.199	U14	3.202	C7	3.21	G8	3.236	U22	3.217	G2659	avg	3.222		3.266	A15
3.252	U15	3.307	G8	3.215	U9	3.179	U23	3.185	A2660	stdev	0.059		3.244	C14
	3NJ6	3.294	G9	3.238	G2	3.199	U24	3.223	G2661				3.251	T13
3.334	G1	3.245	C10	3.283	U3	3.186	U25	3.246	A2662	RNA x-ray resolution < 1.5			3.222	T7
3.28	G2	3.233	G11	3.196	G4	3.193	U26	3.347	G2663	all c3'-endo			3.436	C8
3.182	C3	3.25	G12	3.234	G5	3.211	U27	3.268	G2664				3.39	A1
3.204	A4	3.215	C13	3.191	C6	3.181	U28	3.366	A2665				3.122	T17
3.28	G5	3.272	G14	3.244	U7	3.206	U29	3.204	C2666				3.248	C18
3.227	C6	3.219	G15	3.148	G8	3.176	U30	3.223	C2667				3.439	A11
3.314	A7	3.186	G16					3.262	G2668					
3.207	G8	3.212	U17					3.163	G2669				avg	3.172
3.233	C9	3.165	C18					3.235	A2670				stdev	0.228
								3.146	G2671					
								3.203	U2672				DNA x-ray resolution < 1.5	

Figure S6. Four starting structures for UCAAUC simulations



A-form **C2 & U5 flip out** **random coil** **frame from ff99+ simulation**

Four CAAU starting structures in Condon et. al (JCTC 2015, 11, 2729-2742) were used for CAAU simulations. For d(UCAAUC), B-form replaces A-form and 2'-H replaces 2'-OH.

Table S15. r(CAAU) Chemical Shifts, measured by NMR and predicted by NUCHEMICS

				r(CAAU) Chemical Shifts predicted by NUCHEMICS			
			NMR	A-form	error	intercalation	error
CYT	1	H1'	5.632	5.495	0.192	5.609	0.213
CYT	1	H2'	4.585	4.583	0.460	4.627	0.358
CYT	1	H3'	4.413	4.677	0.193	4.589	0.120
CYT	1	H4'	4.299	4.416	0.082	4.376	0.201
CYT	1	H5'	4.001	4.438	0.083	4.333	0.181
CYT	1	H5''	3.895	4.172	0.072	4.094	0.096
CYT	1	H5	5.499	5.445	0.607	5.388	0.321
CYT	1	H6	7.8	7.899	0.254	7.574	0.216
ADE	2	H1'	5.828	5.702	0.288	5.806	0.285
ADE	2	H2'	4.742	4.530	0.543	4.980	0.557
ADE	2	H3'	4.713	4.682	0.160	4.639	0.195
ADE	2	H4'	4.515	4.484	0.083	4.554	0.080
ADE	2	H5'	4.422	4.490	0.083	4.556	0.086
ADE	2	H5''	4.225	4.192	0.051	4.200	0.097
ADE	2	H2	7.875	7.838	0.434	8.046	0.278
ADE	2	H8	8.223	8.180	0.190	8.520	0.172
ADE	3	H1'	5.806	5.811	0.449	5.542	0.464
ADE	3	H2'	4.363	4.378	0.381	4.625	0.331
ADE	3	H3'	4.624	4.453	0.279	4.571	0.200
ADE	3	H4'	4.486	4.470	0.090	4.510	0.110
ADE	3	H5'	4.521	4.475	0.070	4.534	0.108
ADE	3	H5''	4.162	4.135	0.060	4.186	0.066
ADE	3	H2	8.134	8.333	0.176	8.361	0.140
ADE	3	H8	8.031	7.780	0.324	7.465	0.403
URI	4	H1'	5.693	5.734	0.157	5.796	0.123
URI	4	H2'	4.055	4.210	0.414	4.571	0.173
URI	4	H3'	4.185	4.491	0.302	4.663	0.087
URI	4	H4'	4.19	4.268	0.078	4.369	0.035
URI	4	H5'	4.29	4.262	0.086	4.370	0.040
URI	4	H5''	4.048	4.014	0.083	4.118	0.040
URI	4	H6	7.596	7.719	0.333	7.975	0.181
URI	4	H5	5.348	5.161	0.557	5.349	0.338

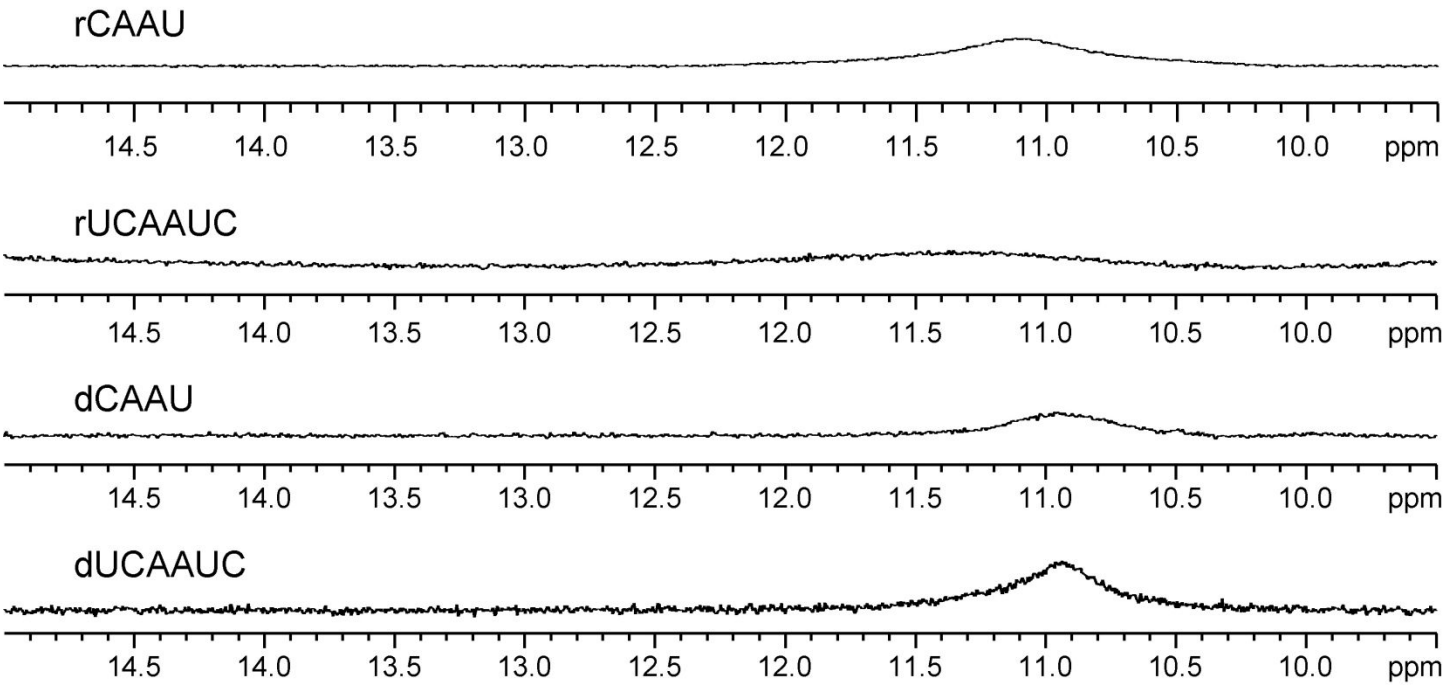
Table S16. nH2'-nH6/8 and nH2''-(n+1)H6/8 distances from crystal structures

DNA	nt	nH2'-nH6/8	nH2''-(n+1)H6/8
1EN3	C1	2.484	2.726
	C2	2.068	3.467
	A3	2.209	2.89
	A4	2.405	2.528
	C5	2.262	2.266
	G6	2.502	2.43
	T7	2.465	2.783
	T8	2.089	3.509
	G9	2.112	2.708
1ENE	C2	2.086	3.663
	A3	2.106	3.2
	G4	2.379	3.119
	C5	2.175	2.318
	G6	2.631	2.511
	C7	2.466	2.955
	T8	2.067	3.615
	G9	2.165	2.839
1EN8	C2	2.075	3.525
	A3	2.19	2.86
	A4	2.418	2.84
	C5	2.067	2.562
	G6	2.207	2.528
	T7	2.102	2.514
	T8	2.081	3.545
	G9	2.151	2.835
1EN9	C2	2.032	3.659
	A3	2.127	3.046
	G4	2.264	3.352
	C5	2.098	2.152
	G6	2.154	2.64
	C7	2.374	2.934
	T8	2.045	3.605
	G9	2.138	2.723
AVG		2.218	2.935
STDEV		0.164	0.447

Table S17. Fractions of BII substates predicted by BSC1

		BII fraction
d(UCAAUC)	U1-C2	0.018
	C2-A3	0.002
	A3-A4	0.040
	A4-U5	0.011
	U5-C6	0.036
d(CAAU)	C1-A2	0.003
	A2-A3	0.017
	A3-U4	0.028

Figure S7. NMR spectra of imino proton region at 1 °C of rCAAU, rUCAAUC, dCAAU, and dUCAAUC



Sample calculation of estimated fraction of U5 extruded structure in d(UCAAUC)

General calculations are:

$$\boldsymbol{V_{NOE} = \frac{C}{r_{NOE}^6}}$$

$$\boldsymbol{V_{NMR} = f \times V_{minor} + (1 - f) \times V_{AB}}$$

$$\boldsymbol{\frac{1}{r_{NMR}^6} = f \times \frac{1}{r_{minor}^6} + (1 - f) \times \frac{1}{r_{AB}^6}}$$

Where *f*=fraction of the minor structure, i.e. extruded or inverted

r_{NMR}=measured NOE distance

r_{minor}=simulation predicted NOE distance for the minor structure

r_{AB}=NOE distance in A-form RNA or B-form DNA

For example, in NMR experiment, d(UCAAUC) has *f* fraction of U5 extruded, the measured NOE distance C6H5-A4H2'/H2'' is 4.38 Å. In B-form DNAs, C6H5-A4H2'/H2'' is 5.51 Å; in U5 extruded structures, C6H5-A4H2'/H2'' is predicted to be 2.45 Å in MD simulations.

$$\boldsymbol{\frac{1}{4.38^6} = f \times \frac{1}{2.45^6} + (1 - f) \times \frac{1}{5.51^6}}$$

$$\boldsymbol{f = 0.023}$$

Table S18. Predicted NOE distances for d(CAAU) by OL15

NOE dCAAU	low	NMR	high	OL15	
C1H1'-A2H5'	2.7	3.28	3.81	2.47	outlier
C1H2'-C1H6	2.39	2.88	3.29	2.5	agree
C1H2'H2''-A2H8	2.78	3.46	4.32	2.5	outlier
C1H2''-A2H5'	2.88	3.52	4.18	3.18	agree
A2H1'-A2H4'	2.71	3.3	3.84	2.94	agree
A2H1'-A3H4'	3.45	4.46	5.47	4.07	agree
A2H1'-A3H5'	2.43	2.93	3.35	2.5	agree
A2H2'H2''-A2H8	1.92	2.31	2.62	2.29	agree
A2H2''-A3H5'	2.86	3.49	4.13	3.35	agree
A2H2'H2''-A3H8	2.33	2.83	3.27	2.51	agree
A3H1'-A3H8	3.02	3.72	4.52	3.2	agree
A3H1'-U4H5'	2.66	3.23	3.75	2.44	outlier
A3H2'H2''-A3H8	2	2.4	2.72	2.29	agree
A3H2'H2''-U4H6	2.56	3.1	3.57	2.41	outlier
U4H1'-U4H6	2.8	3.42	4.02	3.19	agree
U4H2'-U4H6	2.38	2.87	3.28	2.33	outlier
U4H3'-U4H6	2.63	3.19	3.69	3.45	agree

Combined simulation length is 20 μs with four starting structures.

Table S19. Predicted NOE distances for d(UCAAUC) by OL15

NOE dUCAAUC	low	NMR	high	OL15	
U1H1'-U1H6	3.23	3.71	4.60	2.31	outlier
U1H2'-U1H6	2.86	3.20	3.63	2.96	agree
U1H2'-C2H5'H5''	3.27	3.76	4.77	4.48	agree
U1H2''-U1H6	3.64	4.46	5.28	3.65	agree
U1H2''-C2H6	3.53	4.21	4.90	2.44	outlier
U1H3'-U1H6	3.52	4.20	4.88	4.85	agree
C2H1'-A3H5''	2.95	3.31	3.81	4.09	outlier
C2H2'-C2H6	2.42	2.67	2.95	2.17	outlier
C2H2'-A3H8	3.32	3.84	5.05	3.31	agree
C2H2''-C2H6	3.08	3.49	4.10	3.30	agree
C2H2''-A3H8	3.16	3.60	4.34	2.53	outlier
C2H3'-A3H8	3.35	3.89	5.27	4.47	agree
C2H5'H5''-C2H6	3.19	3.64	4.43	4.16	agree
A3H1'-A3H8	2.88	3.23	3.67	3.85	outlier
A3H1'-A4H5'	2.55	2.83	3.13	2.42	outlier
A3H1'-A4H5''	2.65	2.94	3.28	4.14	outlier
A3H2'-A3H8	2.20	2.42	2.64	2.26	agree
A3H2'-A4H8	2.94	3.31	3.79	3.37	agree
A3H2''-A3H8	2.66	2.95	3.29	3.37	outlier
A3H2''-A4H8	2.67	2.96	3.30	2.45	outlier
A3H3'-A3H5'	2.50	2.76	3.05	3.56	outlier
A3H3'-A3H5''	2.78	3.09	3.48	2.51	outlier
A3H3'-A3H8	3.14	3.57	4.28	4.26	agree
A3H3'-A4H8	3.70	4.59	5.49	4.56	agree
A3H4'-A3H8	3.77	4.82	5.87	5.19	agree
A3H5'-A3H8	3.47	4.10	4.73	4.79	outlier
A3H2-A4H1'	3.82	4.98	6.13	4.89	agree
A3H8-A4H8	3.62	4.40	5.19	4.20	agree
A4H1'-A4H2''	2.21	2.44	2.67	2.37	agree
A4H1'-A4H2	3.81	4.93	6.05	4.48	agree
A4H1'-A4H8	3.01	3.39	3.93	3.86	agree
A4H1'-U5H5''	2.80	3.12	3.52	4.13	outlier
A4H2'H2''-A4H8	2.10	2.31	2.54	2.23	agree
A4H2'H2''-U5H3'	3.49	4.14	4.78	4.41	agree
A4H2'H2''-U5H5	3.16	3.60	4.34	3.15	outlier
A4H2'H2''-U5H5'	3.31	3.82	4.97	3.23	outlier
A4H2'H2''-U5H6	2.69	2.99	3.34	2.38	outlier
A4H2'H2''-C6H5	3.60	4.37	5.15	4.84	agree
A4H3'-A4H8	3.34	3.87	5.17	4.25	agree
A4H5'H5''-A4H8	3.34	4.24	5.13	4.31	agree
U5H2'-U5H6	2.35	2.59	2.84	2.25	outlier
U5H2'-C6H5'	3.28	3.77	4.80	4.52	agree
U5H2''-U5H6	3.03	3.42	3.98	3.49	agree
U5H2''-C6H6	3.51	4.17	4.84	2.57	outlier
U5H3'-U5H5'	2.70	3.00	3.35	3.59	outlier
U5H3'-U5H5''	2.96	3.33	3.84	2.55	outlier
U5H3'-U5H6	2.92	3.28	3.75	3.85	outlier
U5H3'-C6H6	3.23	3.71	4.60	3.68	agree
U5H4'-U5H6	3.82	4.97	6.12	4.78	agree
U5H5''-U5H6	3.70	4.61	5.53	4.90	agree
C6H1'-C6H6	3.37	3.93	5.48	3.33	outlier
C6H2''-C6H6	2.81	3.13	3.53	3.53	agree
C6H3'-C6H5''	2.99	3.37	3.90	2.59	outlier
C6H3'-C6H6	3.11	3.53	4.20	3.32	agree
C6H5'-C6H6	3.60	4.36	5.12	4.26	agree
C6H5''-C6H6	3.55	4.25	4.96	4.70	agree

Combined simulation length is 17 μs with four starting structures.

Table S20. Predicted absent NOE distances for d(CAAU) and d(UCAAUC) by OL15

Absent NOE		
	cutoff	dCAAU
C1H6-A2H4'	4.7	4.266
C1H6-A2H5'	4.2	4.104
A2H2-C1H2'	4.2	3.842
A2H2-C1H2''	4.2	4.094
A2H2-C1H5	4.7	3.991
A2H2-A3H4'	5.3	4.835
A2H8-C1H5	4.7	4.475
A2H8-A3H2	5.3	4.772
A3H2-U4H4'	4.7	4.665
A3H8-A2H2	5.3	5.066
	cutoff	dUCAAUC
U1H6-C2H4'	4.5	4.003
U1H6-C2H5'	4.5	3.700
A3H2-A4H4'	5.1	4.709
C6H3'-U5H5''	4.0	3.807

Table S21. Predicted stacking fraction for d(CAAU) and d(UCAAUC) by OL15

d(CAAU)		d(UCAAUC)	
		U1-C2	**0.845**
		U1-A3	0.000
		U1-A4	0.017
		U1-U5	0.000
		U1-C6	0.000
C1-A2	**0.838**	**C2-A3**	**0.798**
C1-A3	0.000	C2-A4	0.000
C1-U4	0.000	C2-U5	0.000
		C2-C6	0.000
A2-A3	**0.814**	**A3-A4**	**0.836**
A2-U4	0.006	A3-U5	0.000
		A3-C6	0.008
A3-U4	**0.851**	**A4-U5**	**0.853**
		A4-C6	0.012
		U5-C6	**0.647**

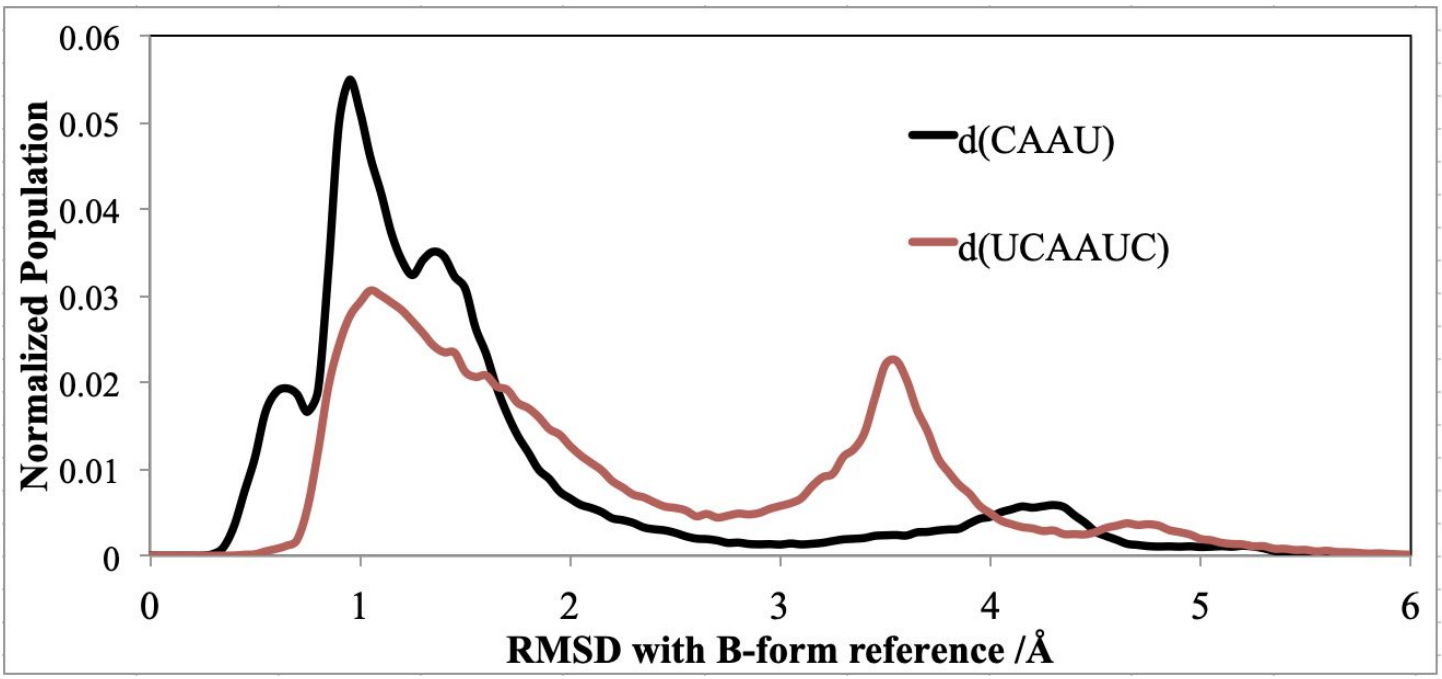



Figure S8. RMSD population with B-form reference for d(CAAU), and d(UCAAUC) predicted by OL15