

## **Supporting Information**

### **Exploring the Thermodynamics of 7-Amino Actinomycin D Induced Single-Stranded DNA Hairpin by Spectroscopic Techniques and Computational Simulations**

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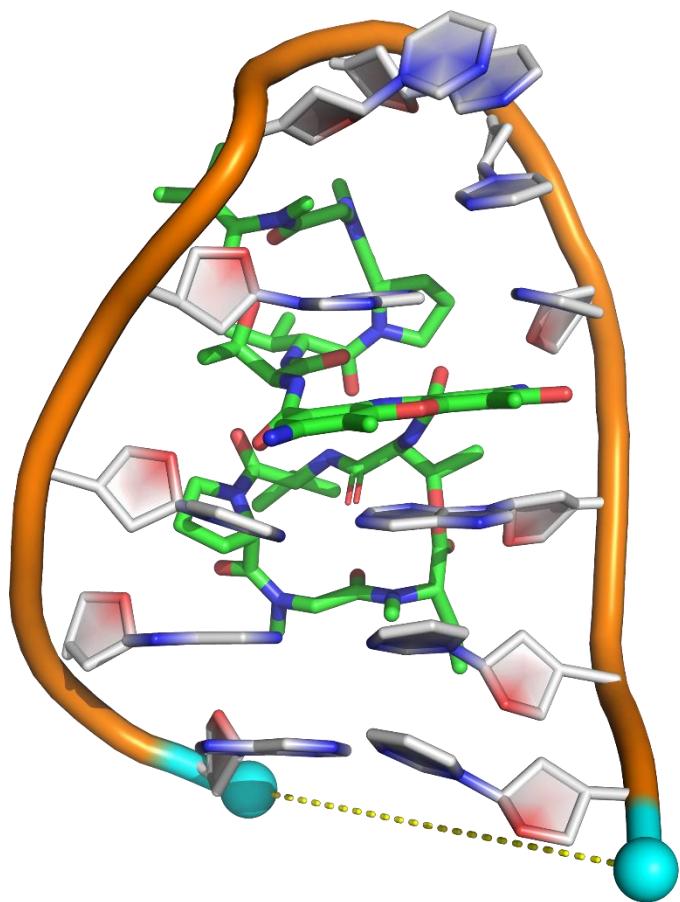
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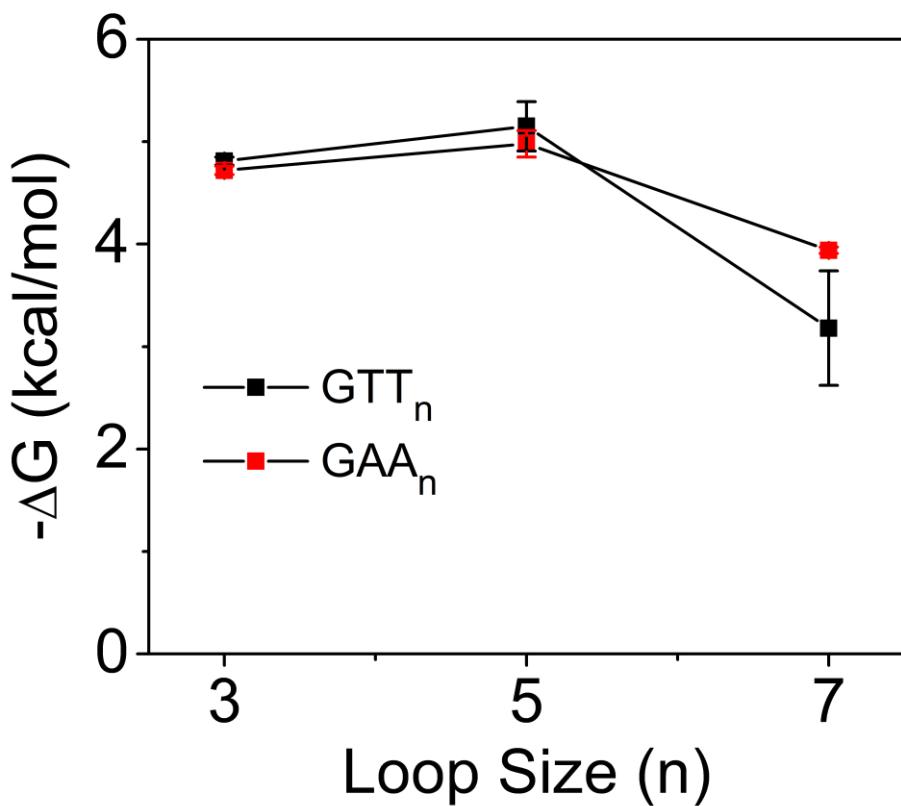
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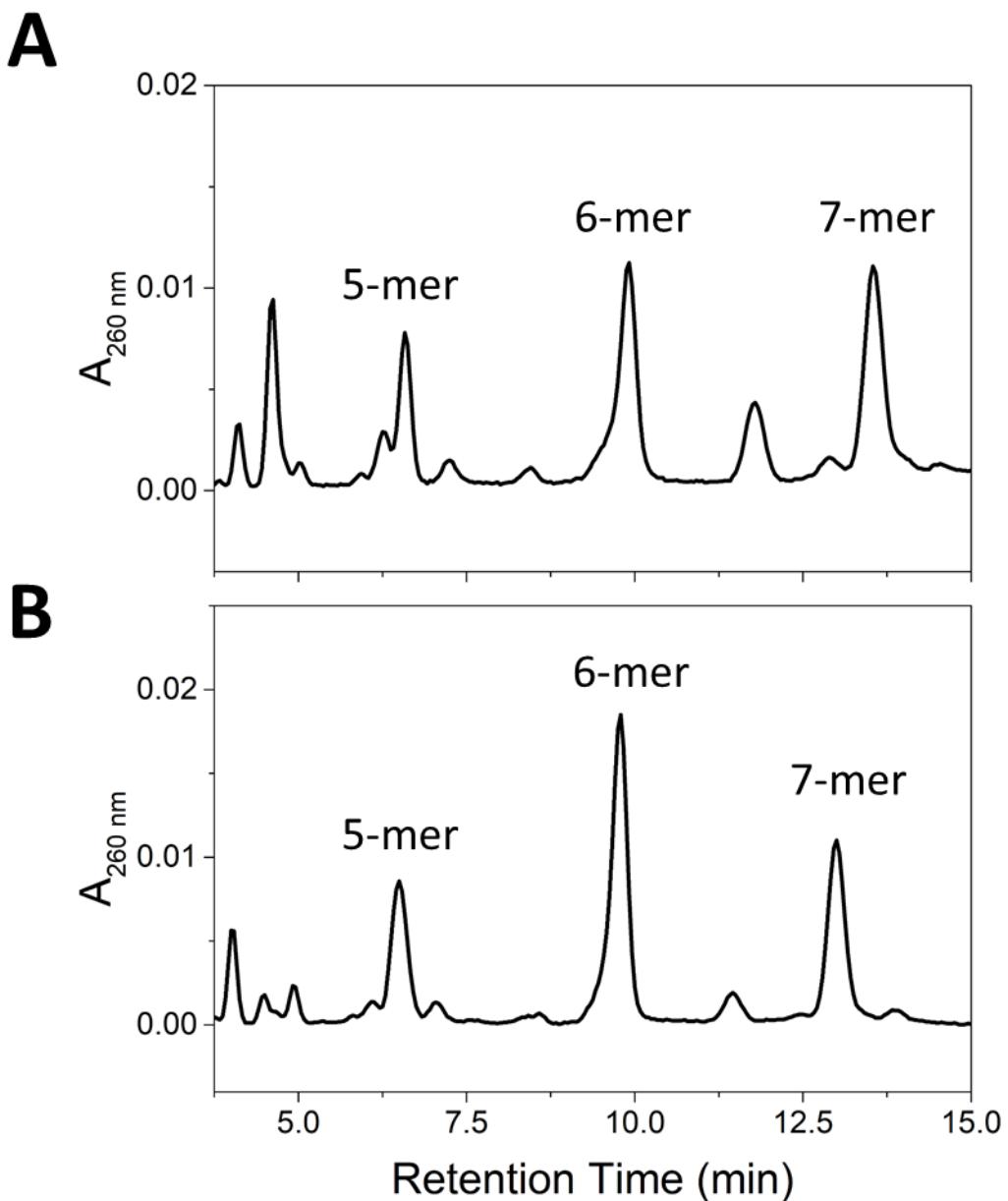
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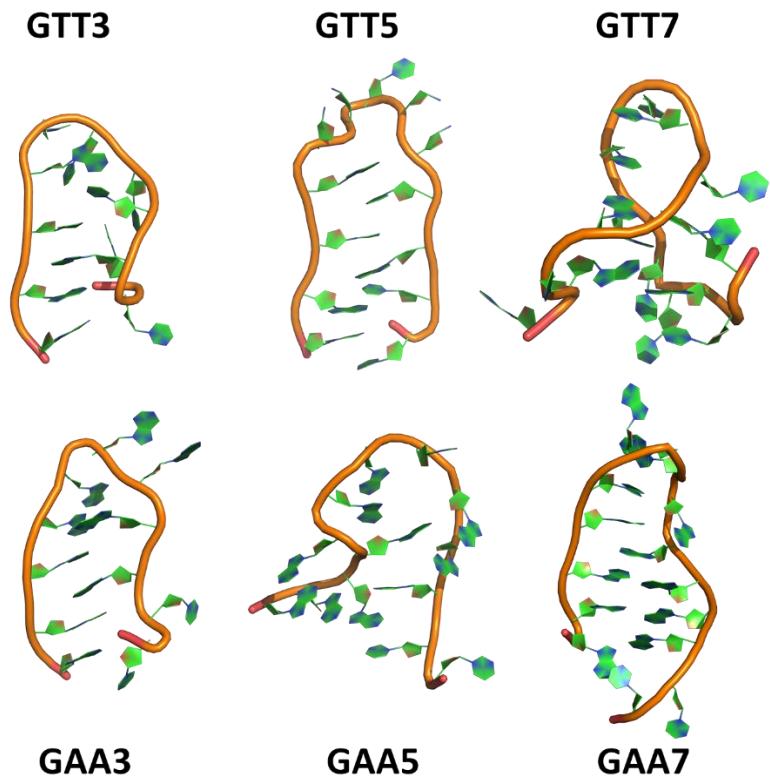
**Fig. S1. Reaction coordinate for unfolding simulations.** The reaction coordinate was defined as the distance between the oxygen atoms of the first base C and the last base G (yellow dashed line).



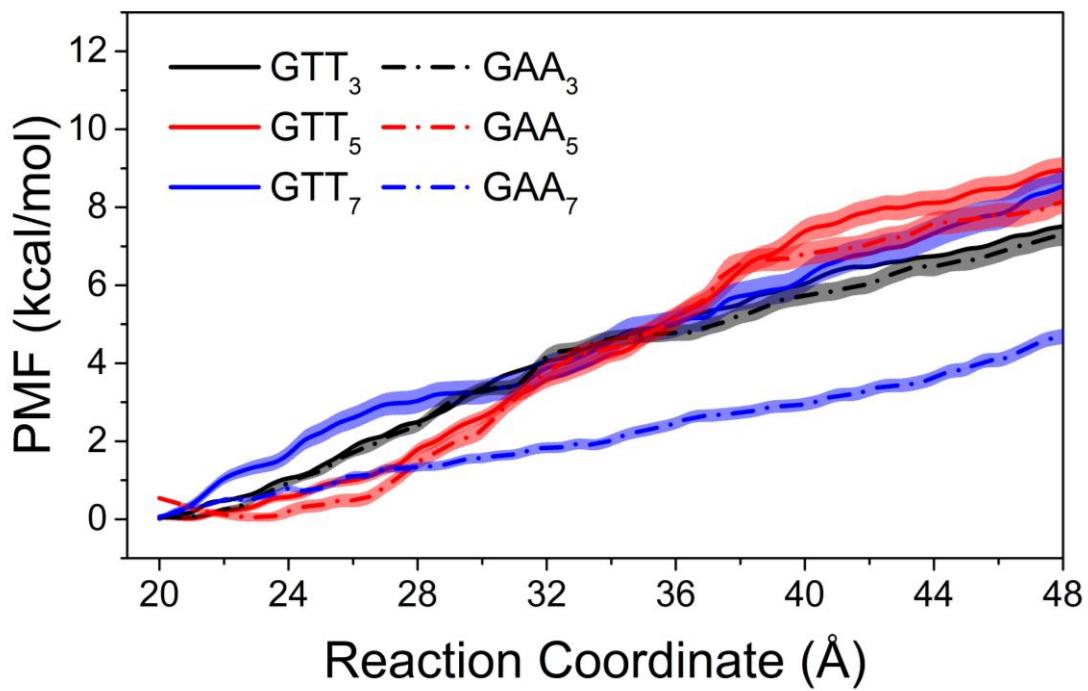
**Fig. S2.** Hairpin free energy [ $\Delta G$ ] at 20 °C versus the loop size of hairpin. The free energy of 7AACTD-induced hairpin was determined by van't Hoff analysis.



**Fig. S3. HPLC analysis of the mung bean nuclease digestion products of GTT<sub>3</sub> (A) and GTT<sub>3</sub>-7AACTD (B).** The digestion reactions were performed at 0 °C in 30 mM CH<sub>3</sub>COONa buffer (100 mM NaCl, 1 mM (CH<sub>3</sub>COO)<sub>2</sub>Zn and 5% glycerol, pH = 5.0). The digestion products were separated by ZORBAX Oligo column under denaturing condition (NaOH at pH = 12) with a gradient of 0-0.5 M NaCl. The length of digestion products were determined according to the calibration curve of retention time versus DNA length.



**Fig. S4. Conformations of GTT<sub>n</sub> and GAA<sub>n</sub> after MD simulations.** GTT<sub>n</sub> and GAA<sub>n</sub> were shown in orange ribbon with green sticks. All of them were mainly packed by base stacking interactions.



**Fig. S5. PMF profiles for the unfolding process of single-stranded  $\text{GTT}_n$  and  $\text{GAA}_n$ .** The reaction coordinate was defined as the distance between the oxygen atoms of the first base C and the last base G (see **Fig. S1**).

**Table S1. Free energy (enthalpy,  $\Delta H$ ) decomposition of 7AACTD binging to hairpin DNA (unit: kcal/mol).**  $E_{vdW}$  is the van der Waals contribution from the Molecular Mechanics (MM) force field.  $E_{elec}$  is the electrostatic contribution by the MM force field and the solvation free energy calculated by PBSA.  $E_{non-polar}$  is the nonpolar contribution to the solvation free energy. Numbers in parentheses present standard errors of mean.

	$E_{vdW}$	$E_{elec}$	$E_{non-polar}$	$\Delta H$
GTT <sub>3</sub>	-64.36(1.26)	26.00(3.32)	-5.29(0.10)	-43.65(0.85)
GTT <sub>5</sub>	-76.21(1.59)	28.57(3.80)	-6.00(0.12)	-53.64(1.13)
GTT <sub>7</sub>	-50.58(1.66)	19.14(4.33)	-4.14(0.14)	-35.58(1.17)
GAA <sub>3</sub>	-70.60(1.43)	28.72(3.55)	-5.46(0.11)	-47.34(0.97)
GAA <sub>5</sub>	-71.35(1.23)	26.35(3.05)	-5.68(0.10)	-50.67(0.89)
GAA <sub>7</sub>	-71.12(1.23)	27.29(2.85)	-5.66(0.10)	-49.49(0.86)

## Appendix (CHARMM parameter files for 7AACTD)

### 7AACTD.rtf

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DEFA FIRS NONE LAST NONE
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IC C1	C19	N	H	1.41	119.94	2.75	118.55	1.02	
IC C2	C1	C11	N10	1.41	118.94	177.53	120.74	1.35	
IC C2	C1	C11	C12	1.41	118.94	-2.47	120.00	1.41	
IC C2	C1	C19	N	1.41	119.63	119.76	119.94	1.34	
IC C2	C1	C19	O7	1.41	119.63	-55.69	118.42	1.23	
IC C2	C3	C4	C12	1.40	120.45	1.69	119.51	1.41	
IC C2	C3	C4	C15	1.40	120.45	-178.16	119.79	1.52	
IC C3	C2	C1	C11	1.40	120.62	3.01	118.94	1.41	
IC C3	C2	C1	C19	1.40	120.62	-174.47	119.63	1.41	
IC C3	C2	N2	HN21	1.40	118.17	1.45	120.30	1.01	
IC C3	C2	N2	HN22	1.40	118.17	-174.22	120.79	1.01	
IC C3	C4	C12	C11	1.40	119.51	-1.17	120.42	1.41	
IC C3	C4	C12	O5	1.40	119.51	178.60	118.84	1.35	
IC C3	C4	C15	H151	1.40	119.79	-1.13	110.75	1.09	
IC C3	C4	C15	H152	1.40	119.79	-121.20	109.85	1.09	
IC C3	C4	C15	H153	1.40	119.79	118.67	109.44	1.09	
IC C4	C3	C2	N2	1.40	120.45	179.47	118.17	1.34	
IC C4	C12	C11	N10	1.41	120.42	-178.42	119.26	1.35	
IC C4	C12	O5	C13	1.41	118.84	-178.94	119.16	1.35	
IC C6	C7	C8	C9	1.40	120.01	-4.84	121.30	1.41	

IC C6	C7	C8	H8	1.40	120.01	173.64	118.43	1.07
IC C6	C7	N01	H01	1.40	120.15	-178.83	119.99	1.01
IC C6	C7	N01	H02	1.40	120.15	1.20	119.97	1.01
IC C6	C13	C14	C9	1.41	120.50	-0.10	119.88	1.41
IC C6	C13	C14	N10	1.41	120.50	-176.49	119.19	1.34
IC C6	C13	O5	C12	1.41	118.72	175.86	119.16	1.35
IC C7	C6	C13	C14	1.40	119.45	1.35	120.50	1.42
IC C7	C6	C13	O5	1.40	119.45	-177.28	118.72	1.35
IC C7	C6	C16	H161	1.40	119.83	120.58	109.84	1.09
IC C7	C6	C16	H162	1.40	119.83	0.64	110.77	1.09
IC C7	C6	C16	H163	1.40	119.83	-119.42	109.59	1.09
IC C7	C8	C9	C14	1.40	121.30	6.01	118.62	1.41
IC C7	C8	C9	C'	1.40	121.30	-177.01	118.59	1.41
IC C8	C7	C6	C13	1.40	120.01	1.08	119.45	1.41
IC C8	C7	C6	C16	1.40	120.01	-177.73	119.83	1.52
IC C8	C7	N01	H01	1.40	119.79	-1.19	119.99	1.01
IC C8	C7	N01	H02	1.40	119.79	178.84	119.97	1.01
IC C8	C9	C14	N10	1.41	118.62	172.83	120.83	1.34
IC C8	C9	C14	C13	1.41	118.62	-3.51	119.88	1.42
IC C8	C9	C'	N6	1.41	118.59	137.31	121.40	1.35
IC C8	C9	C'	O'	1.41	118.59	-40.34	117.50	1.23
IC C9	C8	C7	N01	1.41	121.30	177.52	119.79	1.47
IC C9	C14	N10	C11	1.41	120.83	-175.76	120.79	1.35
IC C9	C14	C13	O5	1.41	119.88	178.50	120.77	1.35
IC C9	C'	N6	CA5	1.41	121.40	-176.60	122.76	1.47
IC C9	C'	N6	H2	1.41	121.40	-1.49	118.79	1.02
IC N10	C11	C1	C19	1.35	120.74	-5.04	121.38	1.41
IC N10	C11	C12	O5	1.35	119.26	1.81	120.75	1.35
IC N10	C14	C9	C'	1.34	120.83	-4.02	122.72	1.41
IC N10	C14	C13	O5	1.34	119.19	2.11	120.77	1.35
IC C11	C1	C2	N2	1.41	118.94	-179.17	121.17	1.34
IC C11	C1	C19	N	1.41	121.38	-57.65	119.94	1.34
IC C11	C1	C19	O7	1.41	121.38	126.90	118.42	1.23
IC C11	N10	C14	C13	1.35	120.79	0.60	119.19	1.42
IC C11	C12	C4	C15	1.41	120.42	178.68	120.70	1.52
IC C11	C12	O5	C13	1.41	120.75	0.83	119.16	1.35
IC C12	C4	C3	O3	1.41	119.51	-178.45	119.74	1.43
IC C12	C4	C15	H151	1.41	120.70	179.02	110.75	1.09
IC C12	C4	C15	H152	1.41	120.70	58.95	109.85	1.09
IC C12	C4	C15	H153	1.41	120.70	-61.18	109.44	1.09
IC C12	C11	C1	C19	1.41	120.00	174.96	121.38	1.41
IC C12	C11	N10	C14	1.41	119.26	-2.49	120.79	1.34
IC C12	O5	C13	C14	1.35	119.16	-2.76	120.77	1.42
IC C13	C6	C7	N01	1.41	119.45	178.71	120.15	1.47

IC	C13	C6	C16	H161	1.41	120.71	-58.22	109.84	1.09
IC	C13	C6	C16	H162	1.41	120.71	-178.15	110.77	1.09
IC	C13	C6	C16	H163	1.41	120.71	61.79	109.59	1.09
IC	C13	C14	C9	C'	1.42	119.88	179.65	122.72	1.41
IC	C14	C9	C8	H8	1.41	118.62	-172.44	120.25	1.07
IC	C14	C9	C'	N6	1.41	122.72	-45.84	121.40	1.35
IC	C14	C9	C'	O'	1.41	122.72	136.51	117.50	1.23
IC	C14	C13	C6	C16	1.42	120.50	-179.86	120.71	1.52
IC	N	CA	C	N1	1.46	111.19	134.56	118.44	1.34
IC	N	CA	C	O	1.46	111.19	-50.14	119.00	1.22
IC	N	CA	CB	CG2	1.46	110.49	-63.14	113.30	1.53
IC	N	CA	CB	OG1	1.46	110.49	58.12	108.59	1.43
IC	N	CA	CB	HB	1.46	110.49	179.52	105.28	1.09
IC	N1	CA1	C5	N3	1.46	110.43	-107.63	120.13	1.35
IC	N1	CA1	C5	O1	1.46	110.43	73.00	118.80	1.23
IC	N1	CA1	CB1	CG1	1.46	109.18	177.98	111.36	1.53
IC	N1	CA1	CB1	CG7	1.46	109.18	57.42	111.02	1.54
IC	N1	CA1	CB1	HB1	1.46	109.18	-62.06	109.46	1.09
IC	N1	C	CA	CB	1.34	118.44	-104.56	107.23	1.54
IC	N1	C	CA	HA	1.34	118.44	13.06	108.36	1.09
IC	N3	CA2	C10	N4	1.46	111.62	147.55	120.22	1.35
IC	N3	CA2	C10	O2	1.46	111.62	-31.91	118.44	1.23
IC	N3	CA2	CB2	CG	1.46	105.33	28.85	103.15	1.53
IC	N3	CA2	CB2	HB2	1.46	105.33	149.86	112.75	1.09
IC	N3	CA2	CB2	HB3	1.46	105.33	-87.34	109.30	1.09
IC	N3	C5	CA1	CB1	1.35	120.13	130.51	111.93	1.54
IC	N3	C5	CA1	HA1	1.35	120.13	13.09	110.97	1.09
IC	N3	CD	CG	CB2	1.45	105.85	30.09	102.57	1.53
IC	N3	CD	CG	HG2	1.45	105.85	-85.97	109.44	1.09
IC	N3	CD	CG	HG3	1.45	105.85	151.18	112.29	1.09
IC	N4	CA3	C17	N5	1.47	112.61	-176.51	118.10	1.35
IC	N4	CA3	C17	O4	1.47	112.61	2.18	119.27	1.23
IC	N4	C10	CA2	CB2	1.35	120.22	-95.24	111.05	1.53
IC	N4	C10	CA2	HA4	1.35	120.22	26.00	112.39	1.08
IC	N5	CA4	C18	O6	1.48	114.05	-115.98	119.47	1.23
IC	N5	CA4	C18	OG1	1.48	114.05	66.32	114.57	1.37
IC	N5	CA4	CB3	CG4	1.48	112.08	-66.31	110.90	1.54
IC	N5	CA4	CB3	CG8	1.48	112.08	57.13	115.36	1.54
IC	N5	CA4	CB3	HB4	1.48	112.08	177.28	107.46	1.09
IC	N5	C17	CA3	HA2	1.35	118.10	-58.44	108.16	1.09
IC	N5	C17	CA3	HA3	1.35	118.10	57.92	110.43	1.09
IC	N6	CA5	C20	N7	1.47	112.73	176.83	115.63	1.34
IC	N6	CA5	C20	O8	1.47	112.73	-5.32	120.86	1.23
IC	N6	CA5	CB4	CG9	1.47	111.76	-51.84	112.89	1.53

IC N6	CA5	CB4	OG2	1.47	111.76	71.60	110.83	1.43
IC N6	CA5	CB4	HB5	1.47	111.76	-167.31	104.63	1.09
IC N7	CA6	C21	N8	1.46	111.42	-109.54	119.25	1.34
IC N7	CA6	C21	O9	1.46	111.42	70.75	119.07	1.23
IC N7	CA6	CB5	CG5	1.46	109.77	177.00	110.92	1.54
IC N7	CA6	CB5	CG10	1.46	109.77	56.63	111.76	1.54
IC N7	CA6	CB5	HB6	1.46	109.77	-63.37	109.58	1.09
IC N7	C20	CA5	CB4	1.34	115.63	-58.10	109.49	1.54
IC N7	C20	CA5	HA6	1.34	115.63	57.80	105.96	1.09
IC N8	CA7	C22	N9	1.46	111.53	159.78	119.18	1.35
IC N8	CA7	C22	O10	1.46	111.53	-21.58	119.19	1.23
IC N8	CA7	CB6	CG3	1.46	104.21	35.17	101.93	1.53
IC N8	CA7	CB6	HB8	1.46	104.21	156.18	112.73	1.09
IC N8	CA7	CB6	HB9	1.46	104.21	-80.67	109.91	1.09
IC N8	C21	CA6	CB5	1.34	119.25	127.19	111.84	1.54
IC N8	C21	CA6	HA7	1.34	119.25	9.69	110.89	1.08
IC N8	CD1	CG3	CB6	1.45	105.49	29.66	102.21	1.53
IC N8	CD1	CG3	HG15	1.45	105.49	-87.03	109.17	1.09
IC N8	CD1	CG3	HG34	1.45	105.49	150.20	112.84	1.08
IC N9	CA8	C23	N11	1.46	110.20	179.71	119.58	1.35
IC N9	CA8	C23	O11	1.46	110.20	-2.09	118.99	1.23
IC N9	C22	CA7	CB6	1.35	119.18	-85.26	109.74	1.53
IC N9	C22	CA7	HA8	1.35	119.18	36.19	111.94	1.09
IC N11	CA9	C24	O12	1.47	110.60	-128.43	118.58	1.23
IC N11	CA9	C24	OG2	1.47	110.60	50.33	115.98	1.38
IC N11	CA9	CB7	CG6	1.47	112.32	-159.33	109.76	1.54
IC N11	CA9	CB7	CG11	1.47	112.32	-40.12	112.55	1.54
IC N11	CA9	CB7	HB7	1.47	112.32	80.74	110.54	1.09
IC N11	C23	CA8	HA10	1.35	119.58	-60.80	108.18	1.09
IC N11	C23	CA8	HA11	1.35	119.58	56.49	111.60	1.09
IC CA	N	C19	O7	1.46	122.94	8.43	121.48	1.23
IC CA	C	N1	CA1	1.53	118.44	162.71	123.23	1.46
IC CA	C	N1	H1	1.53	118.44	-5.03	118.80	1.01
IC CA	CB	CG2	HG21	1.54	113.30	-53.13	110.26	1.09
IC CA	CB	CG2	HG22	1.54	113.30	67.96	110.44	1.09
IC CA	CB	CG2	HG23	1.54	113.30	-172.60	109.36	1.09
IC CA	CB	OG1	C18	1.54	108.59	137.67	114.22	1.37
IC CA1	N1	C	O	1.46	123.23	-12.43	122.38	1.22
IC CA1	C5	N3	CA2	1.54	120.13	2.89	127.45	1.46
IC CA1	C5	N3	CD	1.54	120.13	-178.96	122.37	1.45
IC CA1	CB1	CG1	HG11	1.54	111.36	60.04	110.86	1.09
IC CA1	CB1	CG1	HG12	1.54	111.36	179.42	109.55	1.09
IC CA1	CB1	CG1	HG13	1.54	111.36	-60.95	110.02	1.09
IC CA1	CB1	CG7	HG16	1.54	111.02	58.24	110.15	1.09

IC	CA1	CB1	CG7	HG24	1.54	111.02	178.02	109.62	1.09
IC	CA1	CB1	CG7	HG29	1.54	111.02	-62.61	110.96	1.09
IC	CA2	N3	C5	O1	1.46	127.45	-177.75	121.07	1.23
IC	CA2	N3	CD	CG	1.46	110.16	-12.53	105.85	1.53
IC	CA2	N3	CD	HD2	1.46	110.16	-132.74	111.77	1.09
IC	CA2	N3	CD	HD3	1.46	110.16	105.36	109.29	1.09
IC	CA2	C10	N4	CA3	1.54	120.22	2.71	125.93	1.47
IC	CA2	C10	N4	CN	1.54	120.22	-177.87	118.70	1.46
IC	CA2	CB2	CG	CD	1.53	103.15	-35.71	102.57	1.53
IC	CA2	CB2	CG	HG2	1.53	103.15	80.40	109.38	1.09
IC	CA2	CB2	CG	HG3	1.53	103.15	-156.60	112.56	1.09
IC	CA3	N4	C10	O2	1.47	125.93	-177.84	121.34	1.23
IC	CA3	N4	CN	HN1	1.47	115.37	-1.30	111.49	1.09
IC	CA3	N4	CN	HN2	1.47	115.37	-121.15	109.60	1.09
IC	CA3	N4	CN	HN3	1.47	115.37	119.12	109.74	1.09
IC	CA3	C17	N5	CA4	1.54	118.10	173.24	123.45	1.48
IC	CA3	C17	N5	CN1	1.54	118.10	-5.48	120.69	1.46
IC	CA4	N5	C17	O4	1.48	123.45	-5.40	122.62	1.23
IC	CA4	N5	CN1	HN4	1.48	115.85	120.89	109.75	1.09
IC	CA4	N5	CN1	HN7	1.48	115.85	1.36	112.36	1.09
IC	CA4	N5	CN1	HN10	1.48	115.85	-118.34	110.17	1.09
IC	CA4	C18	OG1	CB	1.54	114.57	-168.67	114.22	1.43
IC	CA4	CB3	CG4	HG1	1.55	110.90	67.82	110.52	1.09
IC	CA4	CB3	CG4	HG6	1.55	110.90	-53.11	110.50	1.09
IC	CA4	CB3	CG4	HG9	1.55	110.90	-172.55	109.48	1.09
IC	CA4	CB3	CG8	HG17	1.55	115.36	54.67	111.11	1.09
IC	CA4	CB3	CG8	HG25	1.55	115.36	173.88	109.14	1.09
IC	CA4	CB3	CG8	HG30	1.55	115.36	-67.01	110.68	1.09
IC	CA5	N6	C'	O'	1.47	122.76	0.96	121.05	1.23
IC	CA5	C20	N7	CA6	1.53	115.63	158.53	126.34	1.46
IC	CA5	C20	N7	H3	1.53	115.63	-12.39	116.94	1.01
IC	CA5	CB4	CG9	HG18	1.54	112.89	-53.99	110.12	1.09
IC	CA5	CB4	CG9	HG26	1.54	112.89	66.81	109.95	1.09
IC	CA5	CB4	CG9	HG31	1.54	112.89	-173.65	109.88	1.09
IC	CA5	CB4	OG2	C24	1.54	110.83	149.38	113.50	1.38
IC	CA6	N7	C20	O8	1.46	126.34	-19.26	123.48	1.23
IC	CA6	C21	N8	CA7	1.53	119.25	4.65	127.11	1.46
IC	CA6	C21	N8	CD1	1.53	119.25	-179.78	122.67	1.45
IC	CA6	CB5	CG5	HG4	1.54	110.92	60.60	110.88	1.09
IC	CA6	CB5	CG5	HG7	1.54	110.92	-179.97	109.62	1.09
IC	CA6	CB5	CG5	HG10	1.54	110.92	-60.31	109.89	1.09
IC	CA6	CB5	CG10	HG19	1.54	111.76	56.33	110.17	1.09
IC	CA6	CB5	CG10	HG27	1.54	111.76	176.05	109.61	1.09
IC	CA6	CB5	CG10	HG32	1.54	111.76	-64.69	111.21	1.09

IC	CA7	N8	C21	O9	1.46	127.11	-175.64	121.67	1.23
IC	CA7	N8	CD1	CG3	1.46	110.10	-7.85	105.49	1.53
IC	CA7	N8	CD1	HD1	1.46	110.10	-128.12	111.71	1.09
IC	CA7	N8	CD1	HD4	1.46	110.10	109.80	109.29	1.09
IC	CA7	C22	N9	CA8	1.54	119.18	-8.26	124.04	1.46
IC	CA7	C22	N9	CN2	1.54	119.18	176.83	119.55	1.46
IC	CA7	CB6	CG3	CD1	1.53	101.93	-39.38	102.21	1.53
IC	CA7	CB6	CG3	HG15	1.53	101.93	76.56	110.19	1.09
IC	CA7	CB6	CG3	HG34	1.53	101.93	-160.46	112.06	1.08
IC	CA8	N9	C22	O10	1.46	124.04	173.14	121.61	1.23
IC	CA8	N9	CN2	HN5	1.46	116.23	116.58	109.38	1.09
IC	CA8	N9	CN2	HN8	1.46	116.23	-3.80	111.50	1.09
IC	CA8	N9	CN2	HN11	1.46	116.23	-123.60	109.85	1.09
IC	CA8	C23	N11	CA9	1.54	119.58	173.41	120.95	1.47
IC	CA8	C23	N11	CN3	1.54	119.58	-4.48	124.66	1.46
IC	CA9	N11	C23	O11	1.47	120.95	-4.74	121.40	1.23
IC	CA9	N11	CN3	HN6	1.47	114.36	169.67	113.61	1.09
IC	CA9	N11	CN3	HN9	1.47	114.36	49.54	109.48	1.09
IC	CA9	N11	CN3	HN12	1.47	114.36	-68.97	109.02	1.09
IC	CA9	C24	OG2	CB4	1.54	115.98	171.00	113.50	1.43
IC	CA9	CB7	CG6	HG5	1.55	109.76	-57.56	111.30	1.09
IC	CA9	CB7	CG6	HG8	1.55	109.76	-177.26	109.51	1.09
IC	CA9	CB7	CG6	HG14	1.55	109.76	63.27	110.19	1.09
IC	CA9	CB7	CG11	HG20	1.55	112.55	66.68	111.16	1.09
IC	CA9	CB7	CG11	HG28	1.55	112.55	-54.46	109.98	1.09
IC	CA9	CB7	CG11	HG33	1.55	112.55	-174.07	109.68	1.09
IC	C	N1	CA1	C5	1.34	123.23	100.57	110.43	1.54
IC	C	N1	CA1	CB1	1.34	123.23	-135.96	109.18	1.54
IC	C	N1	CA1	HA1	1.34	123.23	-21.45	108.79	1.09
IC	C	CA	N	C19	1.53	111.19	-148.59	122.94	1.34
IC	C	CA	N	H	1.53	111.19	41.69	117.73	1.02
IC	C	CA	CB	CG2	1.53	107.23	175.54	113.30	1.53
IC	C	CA	CB	OG1	1.53	107.23	-63.20	108.59	1.43
IC	C	CA	CB	HB	1.53	107.23	58.20	105.28	1.09
IC	C5	N3	CA2	C10	1.35	127.45	-71.41	111.62	1.54
IC	C5	N3	CA2	CB2	1.35	127.45	167.98	105.33	1.53
IC	C5	N3	CA2	HA4	1.35	127.45	52.63	108.03	1.08
IC	C5	N3	CD	CG	1.35	122.37	169.03	105.85	1.53
IC	C5	N3	CD	HD2	1.35	122.37	48.82	111.77	1.09
IC	C5	N3	CD	HD3	1.35	122.37	-73.07	109.29	1.09
IC	C5	CA1	N1	H1	1.54	110.43	-91.48	116.89	1.01
IC	C5	CA1	CB1	CG1	1.54	111.93	-59.44	111.36	1.53
IC	C5	CA1	CB1	CG7	1.54	111.93	179.99	111.02	1.54
IC	C5	CA1	CB1	HB1	1.54	111.93	60.52	109.46	1.09

IC C10	N4	CA3	C17	1.35	125.93	-104.82	112.61	1.54
IC C10	N4	CA3	HA2	1.35	125.93	136.45	107.03	1.09
IC C10	N4	CA3	HA3	1.35	125.93	20.09	111.66	1.09
IC C10	N4	CN	HN1	1.35	118.70	179.22	111.49	1.09
IC C10	N4	CN	HN2	1.35	118.70	59.37	109.60	1.09
IC C10	N4	CN	HN3	1.35	118.70	-60.36	109.74	1.09
IC C10	CA2	N3	CD	1.54	111.62	110.25	110.16	1.45
IC C10	CA2	CB2	CG	1.54	111.05	-92.14	103.15	1.53
IC C10	CA2	CB2	HB2	1.54	111.05	28.87	112.75	1.09
IC C10	CA2	CB2	HB3	1.54	111.05	151.67	109.30	1.09
IC C17	N5	CA4	C18	1.35	123.45	48.69	114.05	1.54
IC C17	N5	CA4	CB3	1.35	123.45	-83.22	112.08	1.55
IC C17	N5	CA4	HA5	1.35	123.45	161.56	108.37	1.09
IC C17	N5	CN1	HN4	1.35	120.69	-60.29	109.75	1.09
IC C17	N5	CN1	HN7	1.35	120.69	-179.83	112.36	1.09
IC C17	N5	CN1	HN10	1.35	120.69	60.47	110.17	1.09
IC C17	CA3	N4	CN	1.54	112.61	75.75	115.37	1.46
IC C18	CA4	N5	CN1	1.54	114.05	-132.53	115.85	1.46
IC C18	CA4	CB3	CG4	1.54	114.33	161.92	110.90	1.54
IC C18	CA4	CB3	CG8	1.54	114.33	-74.64	115.36	1.54
IC C18	CA4	CB3	HB4	1.54	114.33	45.51	107.46	1.09
IC C18	OG1	CB	CG2	1.37	114.22	-98.46	109.01	1.53
IC C18	OG1	CB	HB	1.37	114.22	21.19	113.10	1.09
IC C19	C1	C2	N2	1.41	119.63	3.36	121.17	1.34
IC C19	N	CA	CB	1.34	122.94	92.46	110.49	1.54
IC C19	N	CA	HA	1.34	122.94	-28.29	110.40	1.09
IC C20	N7	CA6	C21	1.34	126.34	59.54	111.42	1.53
IC C20	N7	CA6	CB5	1.34	126.34	-176.01	109.77	1.54
IC C20	N7	CA6	HA7	1.34	126.34	-61.91	107.12	1.08
IC C20	CA5	N6	C'	1.53	112.73	-141.28	122.76	1.35
IC C20	CA5	N6	H2	1.53	112.73	43.58	118.28	1.02
IC C20	CA5	CB4	CG9	1.53	109.49	-177.47	112.89	1.53
IC C20	CA5	CB4	OG2	1.53	109.49	-54.03	110.83	1.43
IC C20	CA5	CB4	HB5	1.53	109.49	67.06	104.63	1.09
IC C21	N8	CA7	C22	1.34	127.11	-82.93	111.53	1.54
IC C21	N8	CA7	CB6	1.34	127.11	158.74	104.21	1.53
IC C21	N8	CA7	HA8	1.34	127.11	41.82	109.89	1.09
IC C21	N8	CD1	CG3	1.34	122.67	175.91	105.49	1.53
IC C21	N8	CD1	HD1	1.34	122.67	55.64	111.71	1.09
IC C21	N8	CD1	HD4	1.34	122.67	-66.44	109.29	1.09
IC C21	CA6	N7	H3	1.53	111.42	-129.48	116.14	1.01
IC C21	CA6	CB5	CG5	1.53	111.84	-58.80	110.92	1.54
IC C21	CA6	CB5	CG10	1.53	111.84	-179.17	111.76	1.54
IC C21	CA6	CB5	HB6	1.53	111.84	60.84	109.58	1.09

IC C22	N9	CA8	C23	1.35	124.04	-87.82	110.20	1.54
IC C22	N9	CA8	HA10	1.35	124.04	153.39	109.34	1.09
IC C22	N9	CA8	HA11	1.35	124.04	36.01	110.55	1.09
IC C22	N9	CN2	HN5	1.35	119.55	-68.12	109.38	1.09
IC C22	N9	CN2	HN8	1.35	119.55	171.51	111.50	1.09
IC C22	N9	CN2	HN11	1.35	119.55	51.71	109.85	1.09
IC C22	CA7	N8	CD1	1.54	111.53	101.04	110.10	1.45
IC C22	CA7	CB6	CG3	1.54	109.74	-84.38	101.93	1.53
IC C22	CA7	CB6	HB8	1.54	109.74	36.63	112.73	1.09
IC C22	CA7	CB6	HB9	1.54	109.74	159.78	109.91	1.09
IC C23	N11	CA9	C24	1.35	120.95	65.68	110.60	1.54
IC C23	N11	CA9	CB7	1.35	120.95	-62.95	112.32	1.55
IC C23	N11	CA9	HA9	1.35	120.95	-176.03	107.89	1.08
IC C23	N11	CN3	HN6	1.35	124.66	-12.32	113.61	1.09
IC C23	N11	CN3	HN9	1.35	124.66	-132.44	109.48	1.09
IC C23	N11	CN3	HN12	1.35	124.66	109.04	109.02	1.09
IC C23	CA8	N9	CN2	1.54	110.20	87.25	116.23	1.46
IC C24	CA9	N11	CN3	1.54	110.60	-116.23	114.36	1.46
IC C24	CA9	CB7	CG6	1.54	114.01	73.85	109.76	1.54
IC C24	CA9	CB7	CG11	1.54	114.01	-166.94	112.55	1.54
IC C24	CA9	CB7	HB7	1.54	114.01	-46.07	110.54	1.09
IC C24	OG2	CB4	CG9	1.38	113.50	-85.33	109.65	1.53
IC C24	OG2	CB4	HB5	1.38	113.50	32.84	112.16	1.09
IC O	C	N1	H1	1.22	122.38	179.84	118.80	1.01
IC O	C	CA	CB	1.22	119.00	70.75	107.23	1.54
IC O	C	CA	HA	1.22	119.00	-171.63	108.36	1.09
IC O1	C5	N3	CD	1.23	121.07	0.40	122.37	1.45
IC O1	C5	CA1	CB1	1.23	118.80	-48.86	111.93	1.54
IC O1	C5	CA1	HA1	1.23	118.80	-166.27	110.97	1.09
IC O2	C10	N4	CN	1.23	121.34	1.58	118.70	1.46
IC O2	C10	CA2	CB2	1.23	118.44	85.30	111.05	1.53
IC O2	C10	CA2	HA4	1.23	118.44	-153.46	112.39	1.08
IC O4	C17	N5	CN1	1.23	122.62	175.88	120.69	1.46
IC O4	C17	CA3	HA2	1.23	119.27	120.25	108.16	1.09
IC O4	C17	CA3	HA3	1.23	119.27	-123.40	110.43	1.09
IC O6	C18	CA4	CB3	1.23	119.47	14.83	114.33	1.55
IC O6	C18	CA4	HA5	1.23	119.47	127.40	102.03	1.09
IC O6	C18	OG1	CB	1.23	125.91	13.80	114.22	1.43
IC O7	C19	N	H	1.23	121.48	178.06	118.55	1.02
IC O8	C20	N7	H3	1.23	123.48	169.82	116.94	1.01
IC O8	C20	CA5	CB4	1.23	120.86	119.75	109.49	1.54
IC O8	C20	CA5	HA6	1.23	120.86	-124.34	105.96	1.09
IC O9	C21	N8	CD1	1.23	121.67	-0.07	122.67	1.45
IC O9	C21	CA6	CB5	1.23	119.07	-52.53	111.84	1.54

IC O9	C21	CA6	HA7	1.23	119.07	-170.03	110.89	1.08
IC O10	C22	N9	CN2	1.23	121.61	-1.78	119.55	1.46
IC O10	C22	CA7	CB6	1.23	119.19	93.38	109.74	1.53
IC O10	C22	CA7	HA8	1.23	119.19	-145.17	111.94	1.09
IC O11	C23	N11	CN3	1.23	121.40	177.37	124.66	1.46
IC O11	C23	CA8	HA10	1.23	118.99	117.40	108.18	1.09
IC O11	C23	CA8	HA11	1.23	118.99	-125.31	111.60	1.09
IC O12	C24	CA9	CB7	1.23	118.58	-0.72	114.01	1.55
IC O12	C24	CA9	HA9	1.23	118.58	113.54	108.31	1.08
IC O12	C24	OG2	CB4	1.23	125.42	-10.34	113.50	1.43
IC CB	CA	N	H	1.54	110.49	-77.25	117.73	1.02
IC CB1	CA1	N1	H1	1.54	109.18	31.99	116.89	1.01
IC CB2	CA2	N3	CD	1.53	105.33	-10.36	110.16	1.45
IC CB2	CG	CD	HD2	1.53	102.57	151.21	110.38	1.09
IC CB2	CG	CD	HD3	1.53	102.57	-87.63	109.55	1.09
IC CB3	CA4	N5	CN1	1.55	112.08	95.56	115.85	1.46
IC CB3	CA4	C18	OG1	1.55	114.33	-162.87	114.57	1.37
IC CB4	CA5	N6	C'	1.54	111.76	94.89	122.76	1.35
IC CB4	CA5	N6	H2	1.54	111.76	-80.25	118.28	1.02
IC CB5	CA6	N7	H3	1.54	109.77	-5.03	116.14	1.01
IC CB6	CA7	N8	CD1	1.53	104.21	-17.29	110.10	1.45
IC CB6	CG3	CD1	HD1	1.53	102.21	150.62	110.64	1.09
IC CB6	CG3	CD1	HD4	1.53	102.21	-87.85	109.50	1.09
IC CB7	CA9	N11	CN3	1.55	112.32	115.15	114.36	1.46
IC CB7	CA9	C24	OG2	1.55	114.01	178.03	115.98	1.38
IC CG	CB2	CA2	HA4	1.53	103.15	144.14	108.10	1.08
IC CG3	CB6	CA7	HA8	1.53	101.93	152.56	109.22	1.09
IC CG1	CB1	CA1	HA1	1.53	111.36	61.27	105.38	1.09
IC CG1	CB1	CG7	HG16	1.53	108.14	-64.21	110.15	1.09
IC CG1	CB1	CG7	HG24	1.53	108.14	55.57	109.62	1.09
IC CG1	CB1	CG7	HG29	1.53	108.14	174.94	110.96	1.09
IC CG4	CB3	CA4	HA5	1.54	110.90	51.03	104.85	1.09
IC CG4	CB3	CG8	HG17	1.54	108.21	179.52	111.11	1.09
IC CG4	CB3	CG8	HG25	1.54	108.21	-61.26	109.14	1.09
IC CG4	CB3	CG8	HG30	1.54	108.21	57.85	110.68	1.09
IC CG5	CB5	CA6	HA7	1.54	110.92	61.87	105.53	1.08
IC CG5	CB5	CG10	HG19	1.54	107.83	-65.83	110.17	1.09
IC CG5	CB5	CG10	HG27	1.54	107.83	53.90	109.61	1.09
IC CG5	CB5	CG10	HG32	1.54	107.83	173.15	111.21	1.09
IC CG6	CB7	CA9	HA9	1.54	109.76	-43.39	103.21	1.08
IC CG6	CB7	CG11	HG20	1.54	107.12	-172.58	111.16	1.09
IC CG6	CB7	CG11	HG28	1.54	107.12	66.27	109.98	1.09
IC CG6	CB7	CG11	HG33	1.54	107.12	-53.34	109.68	1.09
IC CG2	CB	CA	HA	1.53	113.30	58.39	109.08	1.09

IC	CG7	CB1	CA1	HA1	1.54	111.02	-59.29	105.38	1.09
IC	CG7	CB1	CG1	HG11	1.54	108.14	-177.72	110.86	1.09
IC	CG7	CB1	CG1	HG12	1.54	108.14	-58.34	109.55	1.09
IC	CG7	CB1	CG1	HG13	1.54	108.14	61.29	110.02	1.09
IC	CG8	CB3	CA4	HA5	1.54	115.36	174.47	104.85	1.09
IC	CG8	CB3	CG4	HG1	1.54	108.21	-59.64	110.52	1.09
IC	CG8	CB3	CG4	HG6	1.54	108.21	179.43	110.50	1.09
IC	CG8	CB3	CG4	HG9	1.54	108.21	59.99	109.48	1.09
IC	CG9	CB4	CA5	HA6	1.53	112.89	67.74	107.72	1.09
IC	CG10	CB5	CA6	HA7	1.54	111.76	-58.50	105.53	1.08
IC	CG10	CB5	CG5	HG4	1.54	107.83	-176.73	110.88	1.09
IC	CG10	CB5	CG5	HG7	1.54	107.83	-57.30	109.62	1.09
IC	CG10	CB5	CG5	HG10	1.54	107.83	62.36	109.89	1.09
IC	CG11	CB7	CA9	HA9	1.54	112.55	75.82	103.21	1.08
IC	CG11	CB7	CG6	HG5	1.54	107.12	179.95	111.30	1.09
IC	CG11	CB7	CG6	HG8	1.54	107.12	60.26	109.51	1.09
IC	CG11	CB7	CG6	HG14	1.54	107.12	-59.21	110.19	1.09
IC	OG1	C18	CA4	HA5	1.37	114.57	-50.30	102.03	1.09
IC	OG1	CB	CA	HA	1.43	108.59	179.65	109.08	1.09
IC	OG1	CB	CG2	HG21	1.43	109.01	-174.16	110.26	1.09
IC	OG1	CB	CG2	HG22	1.43	109.01	-53.07	110.44	1.09
IC	OG1	CB	CG2	HG23	1.43	109.01	66.37	109.36	1.09
IC	OG2	C24	CA9	HA9	1.38	115.98	-67.71	108.31	1.08
IC	OG2	CB4	CA5	HA6	1.43	110.83	-168.82	107.72	1.09
IC	OG2	CB4	CG9	HG18	1.43	109.65	-178.09	110.12	1.09
IC	OG2	CB4	CG9	HG26	1.43	109.65	-57.28	109.95	1.09
IC	OG2	CB4	CG9	HG31	1.43	109.65	62.26	109.88	1.09
IC	CD	N3	CA2	HA4	1.45	110.16	-125.70	108.03	1.08
IC	CD	CG	CB2	HB2	1.53	102.57	-157.22	112.00	1.09
IC	CD	CG	CB2	HB3	1.53	102.57	80.49	109.30	1.09
IC	CD1	N8	CA7	HA8	1.45	110.10	-134.21	109.89	1.09
IC	CD1	CG3	CB6	HB8	1.53	102.21	-160.45	112.65	1.09
IC	CD1	CG3	CB6	HB9	1.53	102.21	76.90	109.30	1.09
IC	CN	N4	CA3	HA2	1.46	115.37	-42.98	107.03	1.09
IC	CN	N4	CA3	HA3	1.46	115.37	-159.34	111.66	1.09
IC	CN1	N5	CA4	HA5	1.46	115.85	-19.66	108.37	1.09
IC	CN2	N9	CA8	HA10	1.46	116.23	-31.54	109.34	1.09
IC	CN2	N9	CA8	HA11	1.46	116.23	-148.92	110.55	1.09
IC	CN3	N11	CA9	HA9	1.46	114.36	2.06	107.89	1.08
IC	N2	C2	C3	O3	1.34	118.17	-0.39	119.81	1.43
IC	O3	C3	C4	C15	1.43	119.74	1.70	119.79	1.52
IC	O5	C12	C4	C15	1.35	118.84	-1.55	120.70	1.52
IC	O5	C13	C6	C16	1.35	118.72	1.52	120.71	1.52
IC	C16	C6	C7	N01	1.52	119.83	-0.10	120.15	1.47

IC C'	C9	C8	H8	1.41	118.59	4.54	120.25	1.07
IC C'	N6	CA5	HA6	1.35	122.76	-23.99	108.90	1.09
IC O'	C'	N6	H2	1.23	121.05	176.07	118.79	1.02
IC N01	C7	C8	H8	1.47	119.79	-4.00	118.43	1.07
IC H	N	CA	HA	1.02	117.73	162.00	110.40	1.09
IC H1	N1	CA1	HA1	1.01	116.89	146.50	108.79	1.09
IC H2	N6	CA5	HA6	1.02	118.28	160.87	108.90	1.09
IC H3	N7	CA6	HA7	1.01	116.14	109.07	107.12	1.08
IC HA	CA	CB	HB	1.09	109.08	-58.94	105.28	1.09
IC HA1	CA1	CB1	HB1	1.09	105.38	-178.77	109.46	1.09
IC HA4	CA2	CB2	HB2	1.08	108.10	-94.85	112.75	1.09
IC HA4	CA2	CB2	HB3	1.08	108.10	27.95	109.30	1.09
IC HA5	CA4	CB3	HB4	1.09	104.85	-65.38	107.46	1.09
IC HA6	CA5	CB4	HB5	1.09	107.72	-47.73	104.63	1.09
IC HA7	CA6	CB5	HB6	1.08	105.53	-178.49	109.58	1.09
IC HA8	CA7	CB6	HB8	1.09	109.22	-86.43	112.73	1.09
IC HA8	CA7	CB6	HB9	1.09	109.22	36.72	109.91	1.09
IC HA9	CA9	CB7	HB7	1.08	103.21	-163.32	110.54	1.09
IC HB	CB	CG2	HG21	1.09	107.61	62.84	110.26	1.09
IC HB	CB	CG2	HG22	1.09	107.61	-176.07	110.44	1.09
IC HB	CB	CG2	HG23	1.09	107.61	-56.64	109.36	1.09
IC HB1	CB1	CG1	HG11	1.09	108.49	-60.49	110.86	1.09
IC HB1	CB1	CG1	HG12	1.09	108.49	58.89	109.55	1.09
IC HB1	CB1	CG1	HG13	1.09	108.49	178.52	110.02	1.09
IC HB1	CB1	CG7	HG16	1.09	108.28	178.42	110.15	1.09
IC HB1	CB1	CG7	HG24	1.09	108.28	-61.80	109.62	1.09
IC HB1	CB1	CG7	HG29	1.09	108.28	57.57	110.96	1.09
IC HB4	CB3	CG4	HG1	1.09	106.82	-175.38	110.52	1.09
IC HB4	CB3	CG4	HG6	1.09	106.82	63.69	110.50	1.09
IC HB4	CB3	CG4	HG9	1.09	106.82	-55.75	109.48	1.09
IC HB4	CB3	CG8	HG17	1.09	107.73	-65.33	111.11	1.09
IC HB4	CB3	CG8	HG25	1.09	107.73	53.88	109.14	1.09
IC HB4	CB3	CG8	HG30	1.09	107.73	172.99	110.68	1.09
IC HB5	CB4	CG9	HG18	1.09	106.56	60.31	110.12	1.09
IC HB5	CB4	CG9	HG26	1.09	106.56	-178.88	109.95	1.09
IC HB5	CB4	CG9	HG31	1.09	106.56	-59.34	109.88	1.09
IC HB6	CB5	CG5	HG4	1.09	108.40	-59.74	110.88	1.09
IC HB6	CB5	CG5	HG7	1.09	108.40	59.69	109.62	1.09
IC HB6	CB5	CG5	HG10	1.09	108.40	179.35	109.89	1.09
IC HB6	CB5	CG10	HG19	1.09	108.25	177.10	110.17	1.09
IC HB6	CB5	CG10	HG27	1.09	108.25	-63.18	109.61	1.09
IC HB6	CB5	CG10	HG32	1.09	108.25	56.08	111.21	1.09
IC HB7	CB7	CG6	HG5	1.09	108.73	63.46	111.30	1.09
IC HB7	CB7	CG6	HG8	1.09	108.73	-56.23	109.51	1.09

IC	HB7	CB7	CG6	HG14	1.09	108.73	-175.70	110.19	1.09
IC	HB7	CB7	CG11	HG20	1.09	108.01	-55.62	111.16	1.09
IC	HB7	CB7	CG11	HG28	1.09	108.01	-176.76	109.98	1.09
IC	HB7	CB7	CG11	HG33	1.09	108.01	63.63	109.68	1.09
IC	HB2	CB2	CG	HG2	1.09	112.00	-41.12	109.38	1.09
IC	HB2	CB2	CG	HG3	1.09	112.00	81.88	112.56	1.09
IC	HB8	CB6	CG3	HG15	1.09	112.65	-44.50	110.19	1.09
IC	HB8	CB6	CG3	HG34	1.09	112.65	78.47	112.06	1.08
IC	HB3	CB2	CG	HG2	1.09	109.30	-163.40	109.38	1.09
IC	HB3	CB2	CG	HG3	1.09	109.30	-40.40	112.56	1.09
IC	HB9	CB6	CG3	HG15	1.09	109.30	-167.16	110.19	1.09
IC	HB9	CB6	CG3	HG34	1.09	109.30	-44.19	112.06	1.08
IC	HG2	CG	CD	HD2	1.09	109.44	35.14	110.38	1.09
IC	HG2	CG	CD	HD3	1.09	109.44	156.31	109.55	1.09
IC	HG15	CG3	CD1	HD1	1.09	109.17	33.93	110.64	1.09
IC	HG15	CG3	CD1	HD4	1.09	109.17	155.46	109.50	1.09
IC	HG3	CG	CD	HD2	1.09	112.29	-87.71	110.38	1.09
IC	HG3	CG	CD	HD3	1.09	112.29	33.46	109.55	1.09
IC	HG34	CG3	CD1	HD1	1.08	112.84	-88.84	110.64	1.09
IC	HG34	CG3	CD1	HD4	1.08	112.84	32.69	109.50	1.09
IC	C2	C11	*C1	C19	0.00	0.00	180.00	0.00	0.00
IC	C3	C1	*C2	N2	0.00	0.00	180.00	0.00	0.00
IC	C4	C2	*C3	O3	0.00	0.00	180.00	0.00	0.00
IC	N10	C1	*C11	C12	0.00	0.00	180.00	0.00	0.00
IC	C9	N10	*C14	C13	0.00	0.00	180.00	0.00	0.00
IC	C6	C14	*C13	O5	0.00	0.00	180.00	0.00	0.00
IC	C7	C13	*C6	C16	0.00	0.00	180.00	0.00	0.00
IC	N01	C6	*C7	C8	0.00	0.00	180.00	0.00	0.00
IC	N	C1	*C19	O7	0.00	0.00	180.00	0.00	0.00
IC	CA	C19	*N	H	0.00	0.00	180.00	0.00	0.00
IC	C	N	*CA	CB	0.00	0.00	120.00	0.00	0.00
IC	C	N	*CA	HA	0.00	0.00	-120.00	0.00	0.00
IC	N1	CA	*C	O	0.00	0.00	180.00	0.00	0.00
IC	CA1	C	*N1	H1	0.00	0.00	180.00	0.00	0.00
IC	C5	N1	*CA1	CB1	0.00	0.00	120.00	0.00	0.00
IC	C5	N1	*CA1	HA1	0.00	0.00	-120.00	0.00	0.00
IC	N3	CA1	*C5	O1	0.00	0.00	180.00	0.00	0.00
IC	CA2	C5	*N3	CD	0.00	0.00	180.00	0.00	0.00
IC	C10	N3	*CA2	CB2	0.00	0.00	120.00	0.00	0.00
IC	C10	N3	*CA2	HA4	0.00	0.00	-120.00	0.00	0.00
IC	N4	CA2	*C10	O2	0.00	0.00	180.00	0.00	0.00
IC	CA3	C10	*N4	CN	0.00	0.00	180.00	0.00	0.00
IC	C17	N4	*CA3	HA2	0.00	0.00	120.00	0.00	0.00
IC	C17	N4	*CA3	HA3	0.00	0.00	-120.00	0.00	0.00

IC N5	CA3	*C17	O4	0.00	0.00	180.00	0.00	0.00
IC CA4	C17	*N5	CN1	0.00	0.00	180.00	0.00	0.00
IC C18	N5	*CA4	CB3	0.00	0.00	120.00	0.00	0.00
IC C18	N5	*CA4	HA5	0.00	0.00	-120.00	0.00	0.00
IC O6	CA4	*C18	OG1	0.00	0.00	180.00	0.00	0.00
IC CG	CA2	*CB2	HB2	0.00	0.00	120.00	0.00	0.00
IC CG	CA2	*CB2	HB3	0.00	0.00	-120.00	0.00	0.00
IC CG1	CA1	*CB1	CG7	0.00	0.00	120.00	0.00	0.00
IC CG1	CA1	*CB1	HB1	0.00	0.00	-120.00	0.00	0.00
IC CG4	CA4	*CB3	CG8	0.00	0.00	120.00	0.00	0.00
IC CG4	CA4	*CB3	HB4	0.00	0.00	-120.00	0.00	0.00
IC OG1	CA	*CB	CG2	0.00	0.00	120.00	0.00	0.00
IC CG2	CA	*CB	HB	0.00	0.00	-120.00	0.00	0.00
IC C12	C3	*C4	C15	0.00	0.00	180.00	0.00	0.00
IC C8	C14	*C9	C'	0.00	0.00	180.00	0.00	0.00
IC N6	C9	*C'	O'	0.00	0.00	180.00	0.00	0.00
IC CA5	C'	*N6	H2	0.00	0.00	180.00	0.00	0.00
IC C20	N6	*CA5	CB4	0.00	0.00	120.00	0.00	0.00
IC C20	N6	*CA5	HA6	0.00	0.00	-120.00	0.00	0.00
IC N7	CA5	*C20	O8	0.00	0.00	180.00	0.00	0.00
IC CA6	C20	*N7	H3	0.00	0.00	180.00	0.00	0.00
IC C21	N7	*CA6	CB5	0.00	0.00	120.00	0.00	0.00
IC C21	N7	*CA6	HA7	0.00	0.00	-120.00	0.00	0.00
IC N8	CA6	*C21	O9	0.00	0.00	180.00	0.00	0.00
IC CA7	C21	*N8	CD1	0.00	0.00	180.00	0.00	0.00
IC C22	N8	*CA7	CB6	0.00	0.00	120.00	0.00	0.00
IC C22	N8	*CA7	HA8	0.00	0.00	-120.00	0.00	0.00
IC N9	CA7	*C22	O10	0.00	0.00	180.00	0.00	0.00
IC CA8	C22	*N9	CN2	0.00	0.00	180.00	0.00	0.00
IC C23	N9	*CA8	HA10	0.00	0.00	120.00	0.00	0.00
IC C23	N9	*CA8	HA11	0.00	0.00	-120.00	0.00	0.00
IC N11	CA8	*C23	O11	0.00	0.00	180.00	0.00	0.00
IC CA9	C23	*N11	CN3	0.00	0.00	180.00	0.00	0.00
IC C24	N11	*CA9	CB7	0.00	0.00	120.00	0.00	0.00
IC C24	N11	*CA9	HA9	0.00	0.00	-120.00	0.00	0.00
IC O12	CA9	*C24	OG2	0.00	0.00	180.00	0.00	0.00
IC CG3	CA7	*CB6	HB8	0.00	0.00	120.00	0.00	0.00
IC CG3	CA7	*CB6	HB9	0.00	0.00	-120.00	0.00	0.00
IC CG5	CA6	*CB5	CG10	0.00	0.00	120.00	0.00	0.00
IC CG5	CA6	*CB5	HB6	0.00	0.00	-120.00	0.00	0.00
IC CG6	CA9	*CB7	CG11	0.00	0.00	120.00	0.00	0.00
IC CG6	CA9	*CB7	HB7	0.00	0.00	-120.00	0.00	0.00
IC OG2	CA5	*CB4	CG9	0.00	0.00	120.00	0.00	0.00
IC CG9	CA5	*CB4	HB5	0.00	0.00	-120.00	0.00	0.00

IC H01	C7	*N01	H02	0.00	0.00	180.00	0.00	0.00
IC HN1	N4	*CN	HN2	0.00	0.00	120.00	0.00	0.00
IC HN1	N4	*CN	HN3	0.00	0.00	-120.00	0.00	0.00
IC HN4	N5	*CN1	HN7	0.00	0.00	120.00	0.00	0.00
IC HN4	N5	*CN1	HN10	0.00	0.00	-120.00	0.00	0.00
IC HN5	N9	*CN2	HN8	0.00	0.00	120.00	0.00	0.00
IC HN5	N9	*CN2	HN11	0.00	0.00	-120.00	0.00	0.00
IC HN6	N11	*CN3	HN9	0.00	0.00	120.00	0.00	0.00
IC HN6	N11	*CN3	HN12	0.00	0.00	-120.00	0.00	0.00
IC HN21	C2	*N2	HN22	0.00	0.00	180.00	0.00	0.00
IC HG11	CB1	*CG1	HG12	0.00	0.00	120.00	0.00	0.00
IC HG11	CB1	*CG1	HG13	0.00	0.00	-120.00	0.00	0.00
IC HG1	CB3	*CG4	HG6	0.00	0.00	120.00	0.00	0.00
IC HG1	CB3	*CG4	HG9	0.00	0.00	-120.00	0.00	0.00
IC HG4	CB5	*CG5	HG7	0.00	0.00	120.00	0.00	0.00
IC HG4	CB5	*CG5	HG10	0.00	0.00	-120.00	0.00	0.00
IC HG5	CB7	*CG6	HG8	0.00	0.00	120.00	0.00	0.00
IC HG5	CB7	*CG6	HG14	0.00	0.00	-120.00	0.00	0.00
IC CD	CB2	*CG	HG2	0.00	0.00	120.00	0.00	0.00
IC CD	CB2	*CG	HG3	0.00	0.00	-120.00	0.00	0.00
IC CD1	CB6	*CG3	HG15	0.00	0.00	120.00	0.00	0.00
IC CD1	CB6	*CG3	HG34	0.00	0.00	-120.00	0.00	0.00
IC HG21	CB	*CG2	HG22	0.00	0.00	120.00	0.00	0.00
IC HG21	CB	*CG2	HG23	0.00	0.00	-120.00	0.00	0.00
IC HG16	CB1	*CG7	HG24	0.00	0.00	120.00	0.00	0.00
IC HG16	CB1	*CG7	HG29	0.00	0.00	-120.00	0.00	0.00
IC HG17	CB3	*CG8	HG25	0.00	0.00	120.00	0.00	0.00
IC HG17	CB3	*CG8	HG30	0.00	0.00	-120.00	0.00	0.00
IC HG18	CB4	*CG9	HG26	0.00	0.00	120.00	0.00	0.00
IC HG18	CB4	*CG9	HG31	0.00	0.00	-120.00	0.00	0.00
IC HG19	CB5	*CG1	HG27	0.00	0.00	120.00	0.00	0.00
IC HG19	CB5	*CG1	HG32	0.00	0.00	-120.00	0.00	0.00
IC HG20	CB7	*CG1	HG28	0.00	0.00	120.00	0.00	0.00
IC HG20	CB7	*CG1	HG33	0.00	0.00	-120.00	0.00	0.00
IC CG	N3	*CD	HD2	0.00	0.00	120.00	0.00	0.00
IC CG	N3	*CD	HD3	0.00	0.00	-120.00	0.00	0.00
IC CG3	N8	*CD1	HD1	0.00	0.00	120.00	0.00	0.00
IC CG3	N8	*CD1	HD4	0.00	0.00	-120.00	0.00	0.00
IC C9	C7	*C8	H8	0.00	0.00	180.00	0.00	0.00
IC H151	C4	*C15	H152	0.00	0.00	120.00	0.00	0.00
IC H151	C4	*C15	H153	0.00	0.00	-120.00	0.00	0.00
IC H161	C6	*C16	H162	0.00	0.00	120.00	0.00	0.00
IC H161	C6	*C16	H163	0.00	0.00	-120.00	0.00	0.00

END

**7ACTD.prm**

\* ----  
\* Built parameters for 7actd.mol2  
\* by user Fri Nov 2 04:37:37 CET 2018  
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**ATOMS**

MASS	-1 C7C	12.011000
MASS	-1 C7O	12.011000
MASS	-1 C7B	12.011000
MASS	-1 N7C	14.006700
MASS	-1 NC7O	14.006700
MASS	-1 C7R	12.011000
MASS	-1 O7C	15.999400
MASS	-1 O7R	15.999400
MASS	-1 NC7C	14.006700
MASS	-1 HNCO	1.007940
MASS	-1 HCMM	1.007940

**BONDS**

NC7O	C7R	335.651	1.4360
NC7O	C7O	419.491	1.3690
NC7O	HNCO	479.511	1.0150
C7R	C7O	301.539	1.4920
C7R	C7R	306.432	1.5080
C7R	HCMM	342.991	1.0930
C7O	O7C	931.963	1.2220
C7O	C7C	328.526	1.4680
C7R	O7R	363.214	1.4180
C7O	O7R	417.476	1.3550
C7C	C7C	684.039	1.3330
C7C	NC7C	439.714	1.3700
NC7C	HNCO	473.250	1.0180
C7C	C7R	326.655	1.4820
O7R	C7C	397.254	1.3730
O7R	C7B	404.019	1.3760
C7B	C7B	401.068	1.3740
C7B	C7R	356.737	1.4860
C7B	NC7C	443.888	1.3980
C7B	HCMM	381.853	1.0840

C7B	C7O	322.985	1.4570
N7C	C7O	725.204	1.2900
N7C	C7B	397.901	1.3930

#### ANGLES

C7C	C7C	C7O	39.221	111.2970
C7O	C7C	C7O	61.387	120.3700
C7C	C7C	NC7C	55.629	126.8300
C7O	C7C	NC7C	73.693	116.4080
C7C	C7O	C7C	70.239	112.5620
C7C	C7O	O7C	67.360	122.6230
C7O	C7C	C7R	50.232	116.1040
C7C	C7C	C7R	48.361	122.1410
C7B	C7B	C7B	48.145	119.9770
C7B	C7B	C7R	57.788	120.4190
C7B	C7B	NC7C	75.204	121.6330
C7B	C7B	HCMM	40.517	120.5710
C7B	C7B	C7O	57.429	114.4750
C7O	N7C	C7B	85.279	111.6630
C7C	C7O	N7C	59.803	122.2530
C7C	C7C	O7R	80.386	121.2670
C7O	C7C	O7R	82.185	116.7380
C7B	C7B	O7R	69.663	116.4950
C7B	C7B	N7C	70.095	121.0030
C7R	NC7O	C7O	59.084	119.6000
C7R	NC7O	HNCO	39.725	120.0660
C7O	NC7O	HNCO	41.380	120.2770
C7R	NC7O	C7R	80.386	117.9090
NC7O	C7R	C7O	45.626	102.6550
NC7O	C7R	C7R	75.564	109.9600
NC7O	C7R	HCMM	53.255	107.6460
C7O	C7R	C7R	55.917	107.5170
C7O	C7R	HCMM	46.778	108.3850
C7R	C7R	HCMM	45.770	110.5490
HCMM	C7R	HCMM	37.134	108.8360
NC7O	C7O	C7R	70.814	112.7350
NC7O	C7O	O7C	65.273	127.1520
C7R	C7O	O7C	67.504	124.4100
C7R	C7O	O7R	75.060	109.7160
O7C	C7O	O7R	83.120	124.4250
C7C	C7O	NC7O	74.988	111.7210
C7R	C7R	C7R	61.243	109.6080
C7R	C7R	O7R	71.390	108.1330
O7R	C7R	HCMM	56.205	108.5770

C7O	O7R	C7R	66.424	108.0550
C7C	NC7C	HNCO	55.198	111.0530
HNCO	NC7C	HNCO	40.301	109.1600
C7C	O7R	C7B	102.047	110.6940
C7C	C7R	HCMM	45.482	110.2920
C7B	C7R	HCMM	45.122	109.4910
C7B	C7O	NC7O	79.234	112.4950
C7B	C7O	O7C	52.823	119.9680
C7B	NC7C	HNCO	47.641	110.2880

#### DIHEDRALS

C7C	C7C	C7O	C7C	1.250	2	180.00
C7C	C7C	C7O	O7C	0.181	1	0.00
C7C	C7C	C7O	O7C	0.989	2	180.00
C7C	C7C	NC7C	HNCO	1.878	2	180.00
C7C	C7C	NC7C	HNCO	-0.265	3	0.00
C7C	C7O	N7C	C7B	0.900	2	180.00
C7C	C7O	C7C	O7R	1.250	2	180.00
C7C	C7O	NC7O	C7R	3.000	2	180.00
C7C	C7O	NC7O	HNCO	-0.143	1	0.00
C7C	C7O	NC7O	HNCO	3.571	2	180.00
C7C	C7O	NC7O	HNCO	0.060	3	0.00
C7C	C7C	C7O	N7C	0.148	1	0.00
C7C	C7C	C7O	N7C	0.757	2	180.00
C7C	C7C	C7O	N7C	0.240	3	0.00
C7C	C7C	C7O	NC7O	1.250	2	180.00
C7C	C7O	C7C	C7R	1.250	2	180.00
C7O	C7C	C7C	C7O	0.900	2	180.00
C7O	C7C	NC7C	HNCO	1.800	2	180.00
C7O	C7C	C7C	O7R	0.900	2	180.00
C7O	C7C	C7R	HCMM	-0.054	3	0.00
C7C	C7O	C7C	NC7C	1.250	2	180.00
C7C	C7C	O7R	C7B	1.550	2	180.00
C7B	C7B	C7B	C7B	3.500	2	180.00
C7B	C7B	C7B	HCMM	3.500	2	180.00
C7B	C7B	NC7C	HNCO	0.357	1	0.00
C7B	C7B	NC7C	HNCO	1.314	2	180.00
C7B	C7B	NC7C	HNCO	1.677	3	0.00
C7B	C7B	C7B	N7C	3.500	2	180.00
C7B	C7B	O7R	C7C	1.600	2	180.00
C7B	C7B	C7B	O7R	3.500	2	180.00
C7B	C7B	C7R	HCMM	-0.210	2	180.00
C7B	C7B	C7R	HCMM	0.196	3	0.00
C7B	C7B	C7B	C7O	3.500	2	180.00

C7B	C7B	C7B	C7R	3.500	2	180.00
C7B	C7B	C7O	NC7O	1.250	2	180.00
C7B	C7B	C7O	O7C	1.128	2	180.00
C7B	C7B	C7B	NC7C	3.500	2	180.00
C7B	C7B	N7C	C7O	0.900	2	180.00
C7B	C7O	NC7O	C7R	3.000	2	180.00
C7B	C7O	NC7O	HNCO	3.000	2	180.00
N7C	C7O	C7C	C7O	1.250	2	180.00
N7C	C7O	C7C	O7R	1.250	2	180.00
N7C	C7B	C7B	C7O	1.000	2	180.00
N7C	C7B	C7B	O7R	1.000	2	180.00
C7O	C7C	C7C	NC7C	0.900	2	180.00
C7O	C7C	C7O	NC7O	1.250	2	180.00
C7O	C7C	C7O	O7C	1.250	2	180.00
C7O	C7C	C7C	C7R	0.900	2	180.00
C7O	C7C	O7R	C7B	1.800	2	180.00
C7C	C7C	C7R	HCMM	0.251	1	0.00
C7C	C7C	C7R	HCMM	-0.205	2	180.00
C7C	C7C	C7R	HCMM	-0.268	3	0.00
C7C	C7O	C7C	C7O	1.250	2	180.00
NC7O	C7R	C7O	NC7O	0.274	1	0.00
NC7O	C7R	C7O	NC7O	0.897	3	0.00
NC7O	C7R	C7O	O7C	0.169	1	0.00
NC7O	C7R	C7O	O7C	1.386	2	180.00
NC7O	C7R	C7O	O7C	1.073	3	0.00
NC7O	C7R	C7R	C7R	0.150	3	0.00
NC7O	C7R	C7R	O7R	0.150	3	0.00
NC7O	C7R	C7R	HCMM	0.213	3	0.00
NC7O	C7O	C7R	C7R	-0.464	1	0.00
NC7O	C7O	C7R	C7R	0.556	2	180.00
NC7O	C7O	C7R	C7R	0.694	3	0.00
NC7O	C7O	C7R	HCMM	-0.206	1	0.00
NC7O	C7O	C7R	HCMM	0.346	2	180.00
NC7O	C7O	C7R	HCMM	0.043	3	0.00
NC7O	C7R	C7O	O7R	0.200	2	180.00
NC7O	C7R	C7O	O7R	0.150	3	0.00
C7R	NC7O	C7O	O7C	-0.160	1	0.00
C7R	NC7O	C7O	O7C	3.147	2	180.00
C7R	NC7O	C7O	O7C	-0.073	3	0.00
C7R	C7O	NC7O	C7R	0.324	1	0.00
C7R	C7O	NC7O	C7R	3.079	2	180.00
C7R	C7O	NC7O	C7R	0.254	3	0.00
C7R	C7O	NC7O	HNCO	-0.147	1	0.00
C7R	C7O	NC7O	HNCO	2.902	2	180.00

C7R	C7O	NC7O HNCO	0.671	3	0.00
C7R	C7R	C7R HCMM	0.320	1	0.00
C7R	C7R	C7R HCMM	-0.315	2	180.00
C7R	C7R	C7R HCMM	0.132	3	0.00
C7R	C7R	O7R C7O	-0.274	1	0.00
C7R	C7R	O7R C7O	0.160	3	0.00
C7R	NC7O C7R	C7R	0.150	3	0.00
C7R	NC7O C7R	HCMM	0.390	3	0.00
C7R	C7R	C7R C7R	0.051	1	0.00
C7R	C7R	C7R C7R	0.341	2	180.00
C7R	C7R	C7R C7R	0.166	3	0.00
C7R	C7O	O7R C7R	-0.622	1	0.00
C7R	C7O	O7R C7R	2.741	2	180.00
C7R	C7O	O7R C7R	0.182	3	0.00
C7O	NC7O C7R	C7O	1.550	1	0.00
C7O	NC7O C7R	C7O	-1.264	2	180.00
C7O	NC7O C7R	C7O	0.747	3	0.00
C7O	NC7O C7R	C7R	-0.513	1	0.00
C7O	NC7O C7R	C7R	0.347	2	180.00
C7O	NC7O C7R	C7R	0.474	3	0.00
C7O	NC7O C7R	HCMM	-1.050	1	0.00
C7O	NC7O C7R	HCMM	0.681	2	180.00
C7O	NC7O C7R	HCMM	0.011	3	0.00
C7O	C7R	NC7O HNCO	0.040	1	0.00
C7O	C7R	NC7O HNCO	0.140	2	180.00
C7O	C7R	NC7O HNCO	0.201	3	0.00
C7O	C7R	C7R C7R	0.033	1	0.00
C7O	C7R	C7R C7R	-0.078	2	180.00
C7O	C7R	C7R C7R	0.071	3	0.00
C7O	C7R	C7R O7R	-0.340	1	0.00
C7O	C7R	C7R O7R	-0.015	2	180.00
C7O	C7R	C7R HCMM	-0.128	1	0.00
C7O	C7R	C7R HCMM	0.029	2	180.00
C7O	C7R	NC7O C7R	0.150	3	0.00
C7O	O7R	C7R HCMM	0.286	1	0.00
C7O	O7R	C7R HCMM	-0.152	3	0.00
O7C	C7O	NC7O HNCO	0.718	1	0.00
O7C	C7O	NC7O HNCO	2.487	2	180.00
O7C	C7O	NC7O HNCO	-0.227	3	0.00
O7C	C7O	C7R C7R	0.412	1	0.00
O7C	C7O	C7R C7R	0.070	2	180.00
O7C	C7O	C7R C7R	0.163	3	0.00
O7C	C7O	C7R HCMM	0.330	1	0.00
O7C	C7O	C7R HCMM	-0.704	2	180.00

O7C	C7O	C7R	HCMM	0.154	3	0.00
O7C	C7O	O7R	C7R	0.341	1	0.00
O7C	C7O	O7R	C7R	3.592	2	180.00
O7C	C7O	O7R	C7R	-0.468	3	0.00
C7R	C7R	NC7O	HNCO	0.276	1	0.00
C7R	C7R	NC7O	HNCO	-0.190	2	180.00
C7R	C7R	NC7O	HNCO	0.163	3	0.00
C7R	C7R	C7O	O7R	-0.059	1	0.00
C7R	C7R	C7O	O7R	-0.167	2	180.00
C7R	C7R	C7O	O7R	0.101	3	0.00
O7R	C7O	C7R	HCMM	-0.312	2	180.00
O7R	C7O	C7R	HCMM	0.165	3	0.00
O7R	C7R	C7R	HCMM	-0.327	1	0.00
O7R	C7R	C7R	HCMM	0.536	2	180.00
O7R	C7R	C7R	HCMM	0.140	3	0.00
NC7C	C7C	C7O	O7C	1.250	2	180.00
O7C	C7O	C7C	C7R	-0.201	1	0.00
O7C	C7O	C7C	C7R	1.014	2	180.00
O7C	C7O	C7C	C7R	-0.159	3	0.00
O7R	C7C	C7C	C7R	6.000	2	180.00
O7R	C7B	C7B	C7R	3.500	2	180.00
C7R	C7B	C7B	NC7C	3.500	2	180.00
C7O	C7B	C7B	HCMM	1.000	2	180.00
NC7C	C7B	C7B	HCMM	3.500	2	180.00
HNCO	NC7O	C7R	HCMM	-0.308	1	0.00
HNCO	NC7O	C7R	HCMM	0.137	3	0.00
HCMM	C7R	C7R	HCMM	0.142	1	0.00
HCMM	C7R	C7R	HCMM	-0.693	2	180.00
HCMM	C7R	C7R	HCMM	0.157	3	0.00

#### IMPROPER

C7C	C7C	C7O	C7O	1.439	0	0.00
C7C	C7O	C7C	NC7C	1.439	0	0.00
C7O	C7C	C7C	O7C	9.356	0	0.00
C7O	N7C	C7C	C7C	9.356	0	0.00
C7B	C7B	N7C	C7B	2.519	0	0.00
C7B	C7B	C7B	O7R	3.454	0	0.00
C7B	C7B	C7B	C7R	2.879	0	0.00
C7B	NC7C	C7B	C7B	3.310	0	0.00
C7O	NC7O	C7C	O7C	8.348	0	0.00
NC7O	C7R	C7O	HNCO	-1.439	0	0.00
C7R	C7O	NC7O	C7R	0.000	0	0.00
C7R	C7O	NC7O	HCMM	0.000	0	0.00
C7O	NC7O	C7R	O7C	9.284	0	0.00

NC7O	C7R	C7O	C7R	-1.439	0	0.00
C7O	O7C	C7R	O7R	10.147	0	0.00
C7R	C7R	C7R	HCMM	0.000	0	0.00
C7R	C7R	C7R	C7R	0.000	0	0.00
C7R	O7R	C7R	C7R	0.000	0	0.00
C7C	C7C	C7O	C7R	1.871	0	0.00
C7B	C7B	C7B	C7O	1.943	0	0.00
C7O	NC7O	C7B	O7C	9.356	0	0.00
NC7C	HNCO	C7B	HNCO	0.288	0	0.00
C7R	HCMM	NC7O	HCMM	0.000	0	0.00
NC7C	HNCO	C7C	HNCO	-0.504	0	0.00
C7R	HCMM	C7R	HCMM	0.000	0	0.00
C7R	C7R	NC7O	HCMM	0.000	0	0.00
C7B	C7B	C7B	HCMM	1.079	0	0.00
C7R	HCMM	C7C	HCMM	0.000	0	0.00
C7R	HCMM	C7B	HCMM	0.000	0	0.00

NONBONDED nbxmod 5 atom cdiel shift vatom vdistance vswitch -  
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5

C7C	0.000000	-0.068000	2.090000			
C7O	0.000000	-0.110000	2.000000			
C7B	0.000000	-0.070000	1.992400			
N7C	0.000000	-0.200000	1.850000			
NC7O	0.000000	-0.200000	1.850000			
C7R	0.000000	-0.055000	2.175000	0.000000	-0.010000	1.900000
O7C	0.000000	-0.120000	1.700000	0.000000	-0.120000	1.400000
O7R	0.000000	-0.152100	1.770000			
NC7C	0.000000	-0.200000	1.850000			
HNCO	0.000000	-0.046000	0.224500			
HCMM	0.000000	-0.022000	1.320000			