

Establishing Carbon-Carbon Double Bond Position and Configuration in Unsaturated Fatty Acids by Gas-Phase Infrared Spectroscopy

Supplementary Information

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List of samples

Table S1. Structures and exact masses of investigated 3-pyridylcarbinol esters and 3-picolylamides. Two alternative nomenclatures to describe the double bond position are shown.

FA 18:1 3-pyridylcarbinol esters; exact mass: 373.3 u (C₂₄H₃₉NO₂)

6Z	<i>n</i> -12(Z)	
6E	<i>n</i> -12(E)	
8Z	<i>n</i> -10(Z)	
9Z	<i>n</i> -9(Z)	
9E	<i>n</i> -9(E)	
11Z	<i>n</i> -7(Z)	
11E	<i>n</i> -7(E)	

FA 18:0 3-pyridylcarbinol ester; exact mass: 375.3 u (C₂₄H₄₁NO₂)

18:0		
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FA 18:1 3-picolylamides; exact mass: 372.3 u (C₂₄H₄₀N₂O)

8Z	<i>n</i> -10(Z)	
9Z	<i>n</i> -9(Z)	
9E	<i>n</i> -9(E)	
11Z	<i>n</i> -7(Z)	
11E	<i>n</i> -7(E)	

Infrared spectra of protonated 3-picolylamides

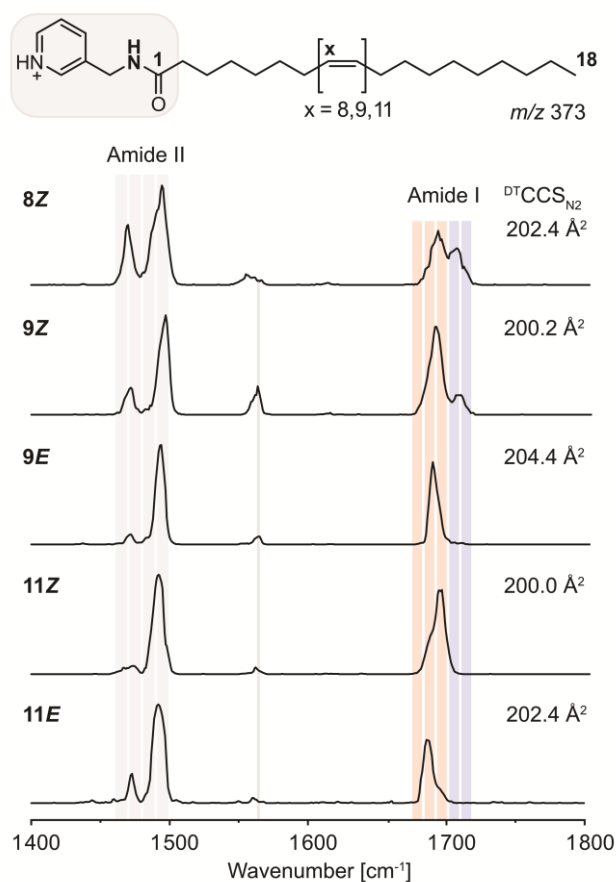


Figure S1. Gas-phase infrared spectra and experimental collision cross sections (^{DT}CCS_{N₂}) of protonated FA 18:1 double bond isomers derivatized with 3-picolylamine. The position of the amide I vibration is dependent on the double bond position and configuration.

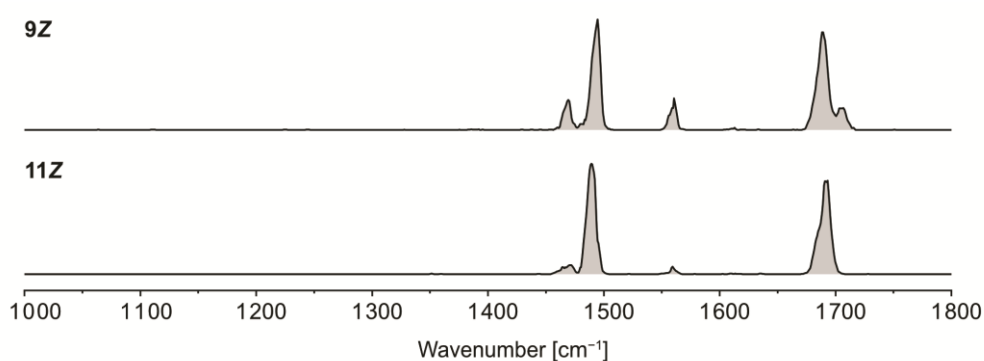


Figure S2. Infrared spectra of protonated 3-picolylamides are dominated by the characteristic amide vibrations but do not yield diagnostic vibrations in the spectral region below 1400 cm⁻¹. Full-range spectra were recorded for C18:1 9Z and 11Z fatty acids derivatized with 3-picolylamine.

Computed structures of 3-pyridylcarbinol esters

In the following, an overview of computed protonated C18:1 3-pyridylcarbinol ester structures is shown. Each conformer is uniquely identifiable by its name *conf_x*, where x is the position of the conformer in the output file from the initial conformer search in CREST. The conformers are ordered by ascending free energy. Computed conformers that exhibit a C=O stretching frequency higher than 1760 cm^{-1} according to the group separation in Figure S3 are highlighted in blue in Table S2–Table S9. Computed conformers that do not exhibit charge-olefin interactions (NH--C=C distances longer than 2.5 Å) are marked by asterisks. XYZ coordinates of all computed conformers are provided in a separate document.

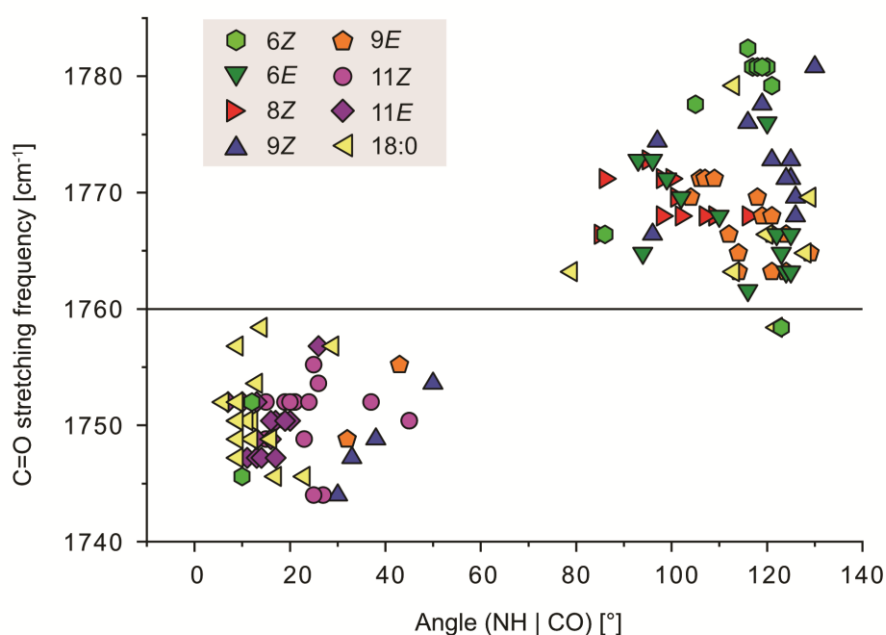


Figure S3. Graphical representation of all computed 3-pyridylcarbinol ester structures in a 2D plot featuring the computed harmonic C=O stretching frequency as a function of the angle between the N-H and C=O bond. Two groups of conformers are discernible, which feature low angles ($< 60^\circ$) and low C=O stretching frequencies ($< 1760\text{ cm}^{-1}$) or large angles ($> 80^\circ$) and high C=O stretching frequencies ($> 1760\text{ cm}^{-1}$), respectively.

Table S2. Overview of computed conformers of protonated C18:1 **6Z** 3-pyridylcarbinol esters. The corresponding harmonic infrared spectra are depicted in Figure S4.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_33	0	2.27	118	197.5
conf_25	0.8	2.19	105	188.1
conf_0	0.9	2.22	120	196.7
conf_6	3.6	2.22	121	195.6
conf_103	4.5	2.27	117	188.9
conf_57	5.2	2.20	116	189.0
conf_84	8.2	2.20	118	205.9
conf_90	8.7	2.46	86	189.4
conf_75	9.2	3.48*	123	194.6
conf_94	10.1	2.26	119	198.3
conf_153	17.0	9.99*	12	203.2
conf_189	24.8	6.69*	10	204.8
average				194.0

Table S3. Overview of computed conformers of protonated C18:1 **6E** 3-pyridylcarbinol esters. The corresponding harmonic infrared spectra are depicted in Figure S5.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_14	0	2.45	120	193.6
conf_0	0.7	2.77*	122	193.3
conf_21	3.4	2.7*	125	195.0
conf_18	3.5	3.25*	124	193.9
conf_2	3.8	2.41	110	193.9
conf_3	4.6	2.27	93	193.2
conf_57	4.7	2.94*	125	201.6
conf_83	4.8	2.41	102	190.9
conf_10	5.7	2.19	99	199.0
conf_47	5.7	2.95*	123	193.9
conf_79	10.1	2.24	96	193.1
conf_93	13.1	3.91*	116	197.2
conf_11	18.1	2.91*	94	191.5
average				194.8

Table S4. Overview of computed conformers of protonated C18:1 **8Z** 3-pyridylcarbinol esters. The corresponding harmonic infrared spectra are depicted in Figure S6.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_0	0	2.09	107	195.5
conf_26	1.1	2.10	86	194.7
conf_20	3.0	2.09	98	197.4
conf_2	3.3	2.07	98	194.2
conf_4	3.3	2.08	109	194.5
conf_34	3.3	2.12	95	190.1
conf_41	3.9	2.09	116	196.5
conf_23	4.5	2.07	101	193.5
conf_7	5.0	2.02	109	194.9
conf_12	5.0	2.12	109	193.5
conf_13	7.9	2.09	102	193.8
conf_29	10	2.10	107	203.2
conf_83	10.2	2.12	100	194.8
conf_87	11.2	2.09	85	194.8
average				194.4

Table S5. Overview of computed conformers of protonated C18:1 **9Z** 3-pyridylcarbinol esters. The corresponding harmonic infrared spectra are depicted in Figure S7.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_1	0	2.05	33	195.0
conf_0	3.8	2.06	121	196.4
conf_2	4.2	2.11	125	195.6
conf_3	6.5	2.08	124	195.3
conf_21	7.4	2.07	116	192.3
conf_39	7.5	2.07	116	192.3
conf_92	7.6	2.20	50	185.7
conf_68	7.7	2.05	126	199.2
conf_34	8.1	2.10	30	193.8
conf_57	8.7	2.19	130	199.4
conf_27	10.5	2.13	125	202.8
conf_12	10.8	2.12	119	197.5
conf_81	11.9	2.16	126	190.5
conf_56	12.4	2.02	38	193.7
conf_61	13.1	2.14	96	190.5
conf_79	15.7	2.05	97	194.4
average				194.5

Table S6. Overview of computed conformers of protonated C18:1 **9E** 3-pyridylcarbinol esters. The corresponding harmonic infrared spectra are depicted in Figure S8.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_2	0	2.09	32	191.8
conf_17	0.5	2.04	121	193.9
conf_8	1.4	2.08	106	192.8
conf_0	1.5	2.05	114	197.1
conf_14	2.7	2.15	124	197.7
conf_4	3.8	2.05	124	198.3
conf_34	4.8	2.03	119	195.7
conf_72	4.8	2.14	118	197.6
conf_11	5.8	2.04	112	196.8
conf_79	6.1	2.09	43	198.4
conf_28	6.2	2.06	121	192.7
conf_77	6.6	2.03	107	198.4
conf_87	7.0	2.05	109	195.2
conf_78	7.6	2.06	32	192.6
conf_46	8.5	2.07	121	193.3
conf_21	9.2	2.14	129	190.7
conf_12	11.8	2.07	104	196.7
conf_85	15.6	2.09	114	197.4
average				195.2

Table S7. Overview of computed conformers of protonated C18:1 **11Z** 3-pyridylcarbinol esters. The corresponding harmonic infrared spectra are depicted in Figure S9.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_5	0	2.11	26	192.1
conf_89	3.1	2.08	37	190.5
conf_0	4.5	2.08	21	192.0
conf_21	5.2	2.1	15	192.8
conf_8	7.3	2.09	21	193.2
conf_3	7.5	2.06	23	192.4
conf_20	9.3	2.09	19	189.9
conf_23	9.4	2.07	19	191.2
conf_72	9.9	2.09	45	192.5
conf_77	10.9	2.07	15	208.2
conf_91	12.6	2.12	20	190.6
conf_56	13.5	2.1	27	193.8
conf_59	13.6	2.09	25	195.1
conf_112	18.7	2.08	24	190.4
conf_106	32.1	2.27	25	198.7
average				191.8

Table S8. Overview of computed conformers of protonated C18:1 **11E** 3-pyridylcarbinol esters. The corresponding harmonic infrared spectra are depicted in Figure S10.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_0	0	2.07	11	190.2
conf_7	3.5	2.07	13	196.9
conf_2	3.6	2.06	17	193.8
conf_32	4.5	2.02	13	207.6
conf_50	7	2.06	20	200.8
conf_11	7.3	2.07	13	194.8
conf_63	7.5	2.01	13	208.3
conf_15	7.9	2.07	16	196.0
conf_61	7.9	2.07	19	196.7
conf_6	8	2.07	7	190.6
conf_45	9.6	2.11	10	196.2
conf_102	11.2	2.06	26	194.8
conf_38	11.3	2.06	14	193.5
conf_59	12.2	2.12	16	194.7
conf_107	12.2	2.05	17	204.9
conf_70	12.9	2.11	19	194.3
average				197.4

Table S9. Overview of computed conformers of protonated C18:0 3-pyridylcarbinol esters. The corresponding harmonic infrared spectra are depicted in Figure S11.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_53	0	29	206.0
conf_55	0.5	120	189.4
conf_51	1.0	13	195.4
conf_36	1.9	12	192.8
conf_14	2.6	129	195.8
conf_6	3.7	122	199.2
conf_0	5.0	9	204.6
conf_24	5.1	113	197.6
conf_19	6.3	17	193.7
conf_18	6.4	113	196.3
conf_21	7.3	12	203.0
conf_22	7.4	11	205.6
conf_156	7.4	128	195.4
conf_139	7.7	23	197.0
conf_67	8.0	9	202.2
conf_43	8.1	79	196.9
conf_3	8.4	9	205.7
conf_52	9.0	6	200.0
conf_120	10.3	16	209.1
conf_26	10.8	9	203.1
conf_32	13.3	9	199.7
conf_33	13.5	14	198.6
conf_174	16.2	9	203.2
average			198.7

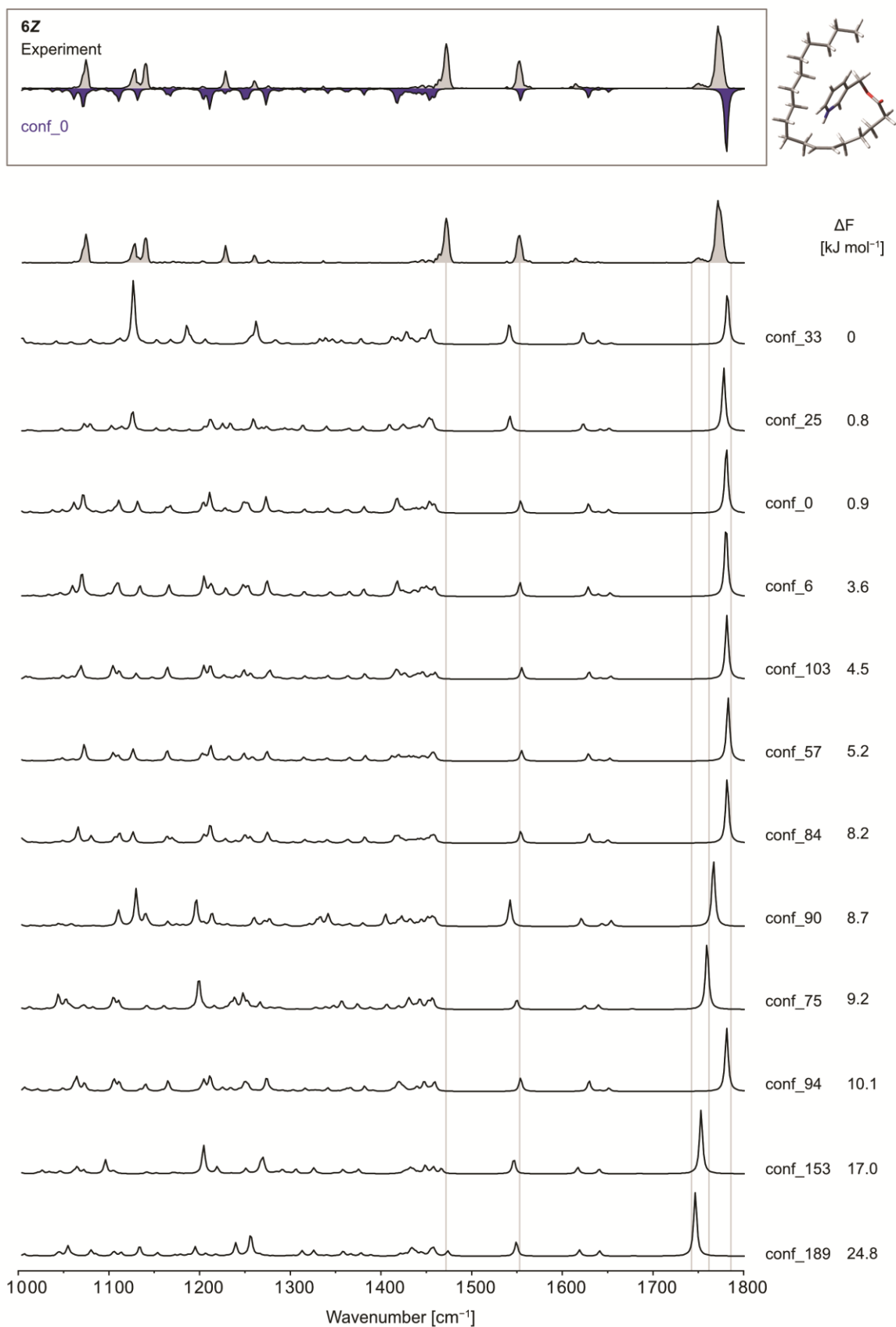


Figure S4. Experimental infrared spectrum of protonated C18:1 **6Z** 3-pyridylcarbinol ester and harmonic spectra of computed conformers. The majority of the computed infrared spectra exhibit a blueshifted C=O stretching vibration ($>1760\text{ cm}^{-1}$). The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S2.

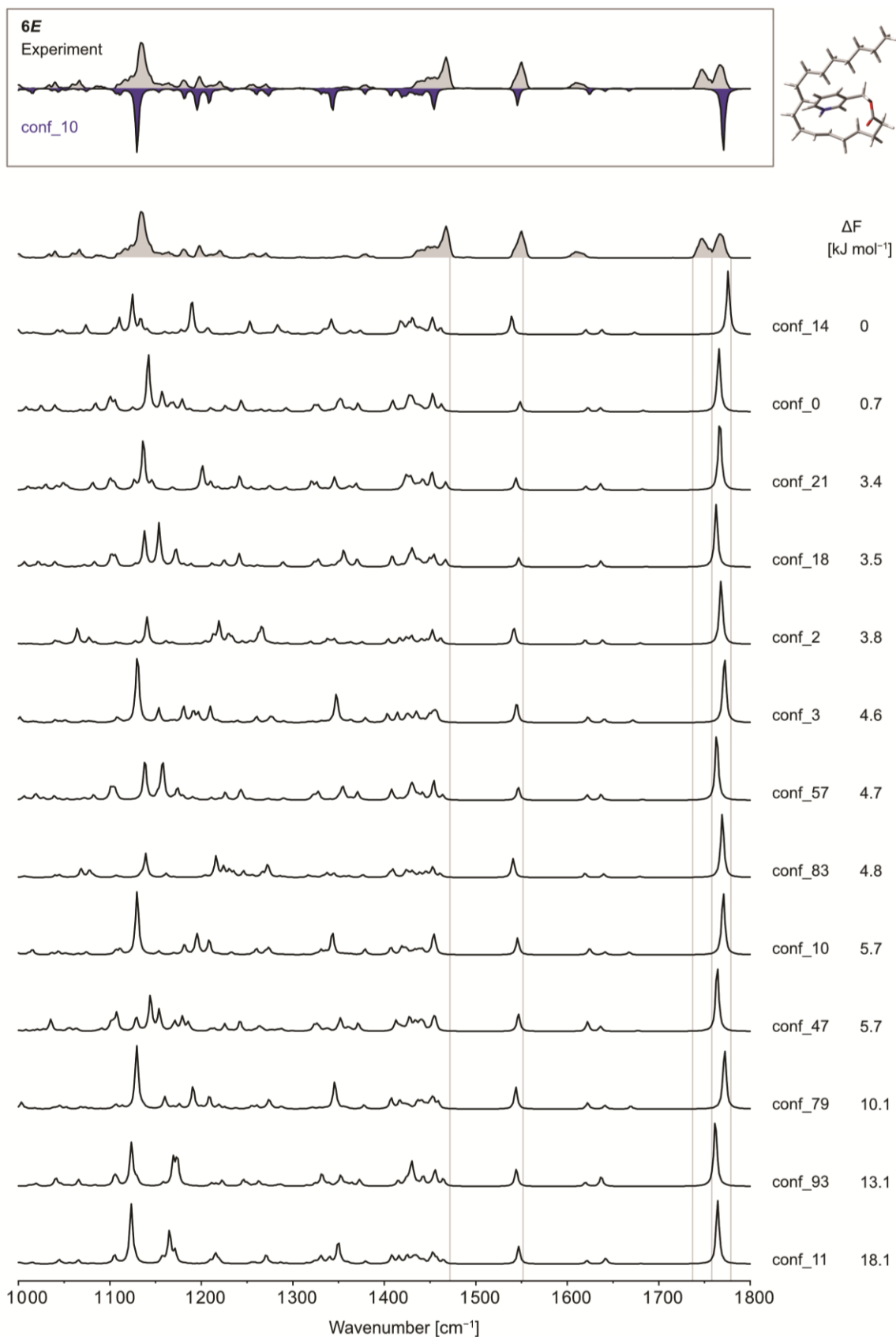


Figure S5. Experimental infrared spectrum of protonated C18:1 **6E** 3-pyridylcarbinol ester and harmonic spectra of computed conformers. All computed infrared spectra exhibit a blueshifted C=O stretching vibration (>1760 cm⁻¹). The best match between experiment and theory is shown on top. Low-energy structures modelling the redshifted carbonyl band were not found in the conformational search. An overview of all computed conformers is given in Table S3.

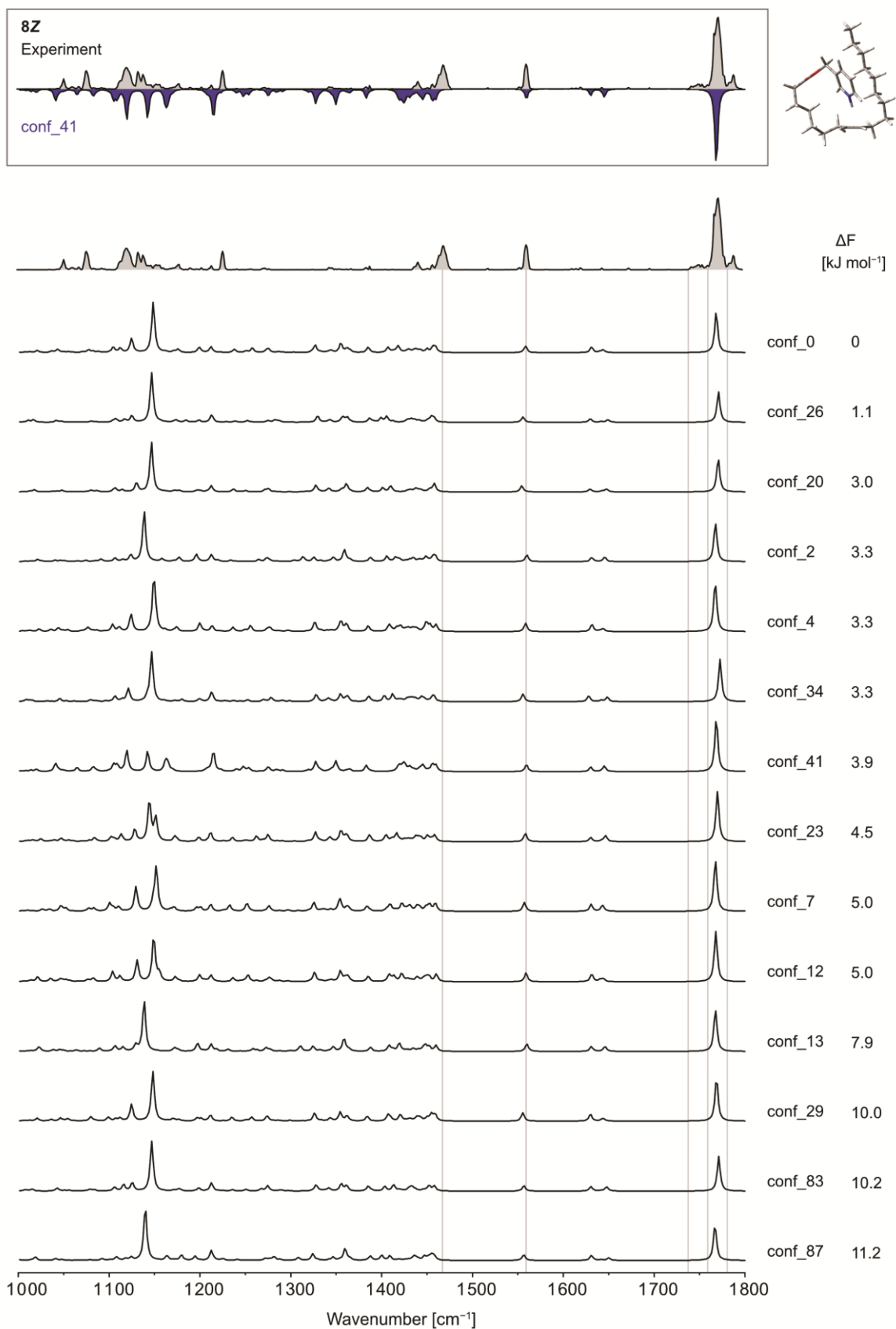


Figure S6. Experimental infrared spectrum of protonated C18:1 **8Z** 3-pyridylcarbinol ester and harmonic spectra of computed conformers. All computed infrared spectra exhibit a blueshifted C=O stretching vibration ($>1760\text{ cm}^{-1}$). The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S4.

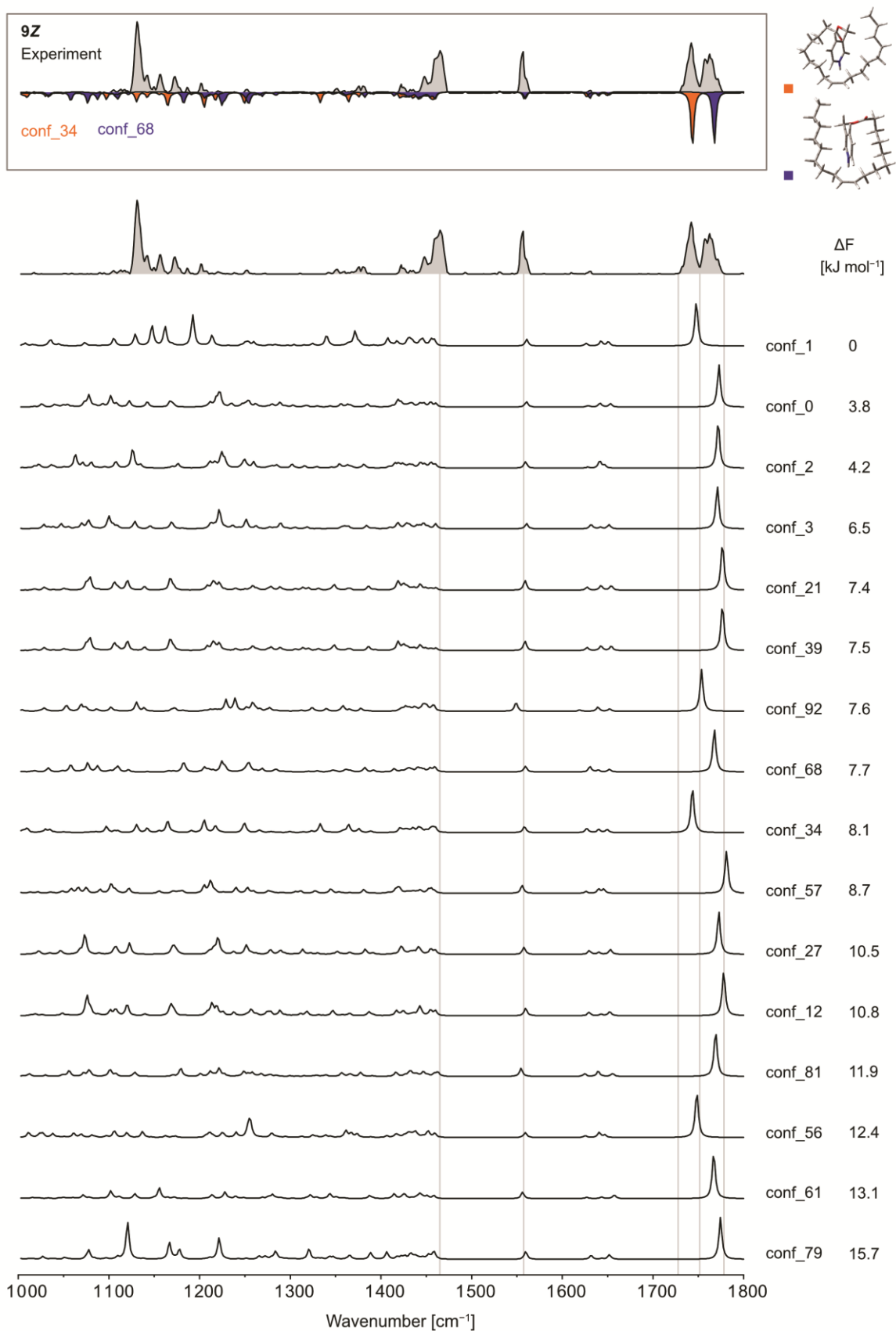


Figure S7. Experimental infrared spectrum of protonated C18:1 **9Z** 3-pyridylcarbinol ester and harmonic spectra of computed conformers. Several computed infrared spectra exhibit a blueshifted C=O stretching vibration ($>1760\text{ cm}^{-1}$). The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S5.



Figure S8. Experimental infrared spectrum of protonated C18:1 **9E** 3-pyridylcarbinol ester and harmonic spectra of computed conformers. Several spectra exhibit a blueshifted C=O stretching vibration ($>1760\text{ cm}^{-1}$), which is not observed in the experiment. The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S6.

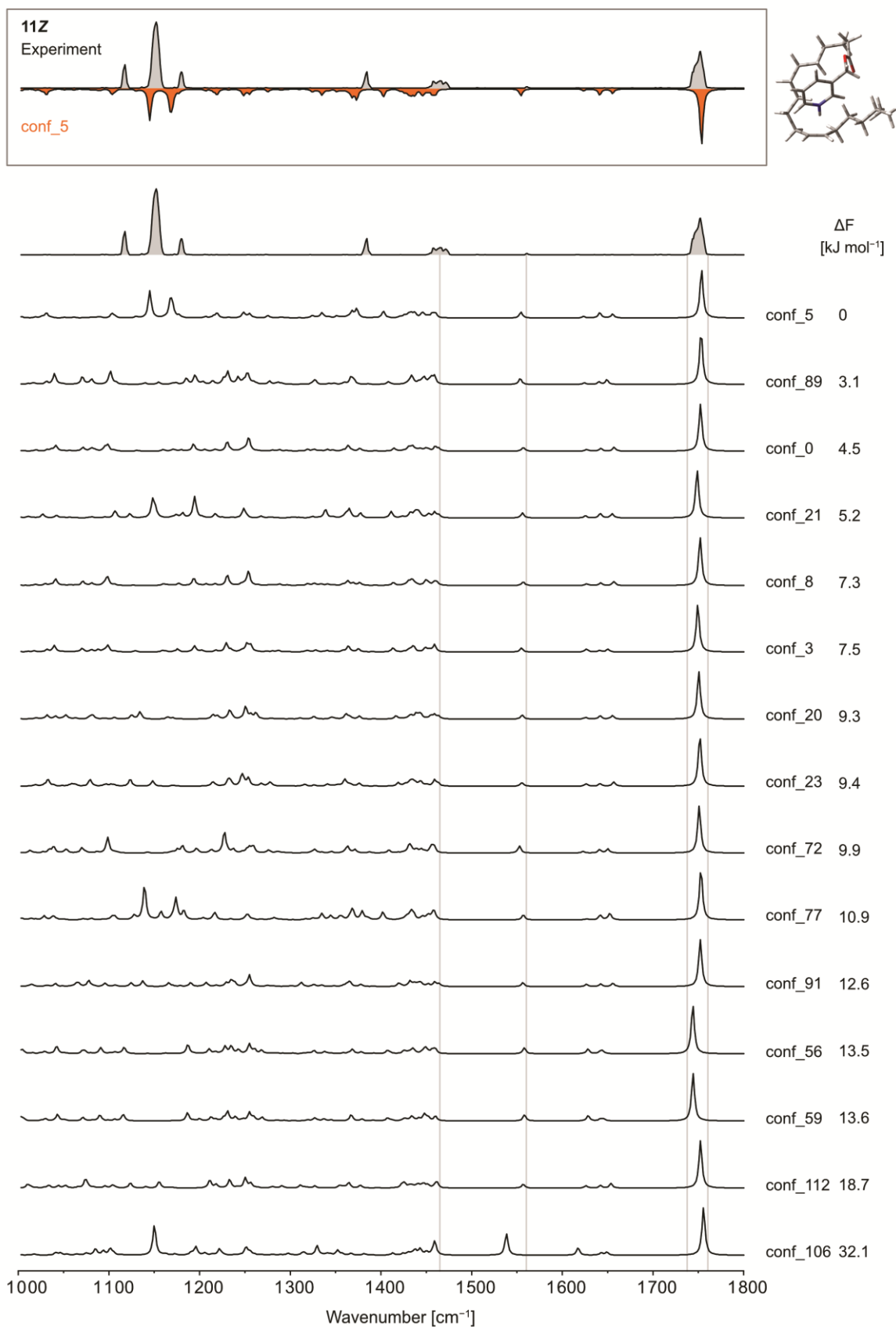


Figure S9. Experimental infrared spectrum of protonated C18:1 **11Z** 3-pyridylcarbinol ester and harmonic spectra of computed conformers. The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S7.

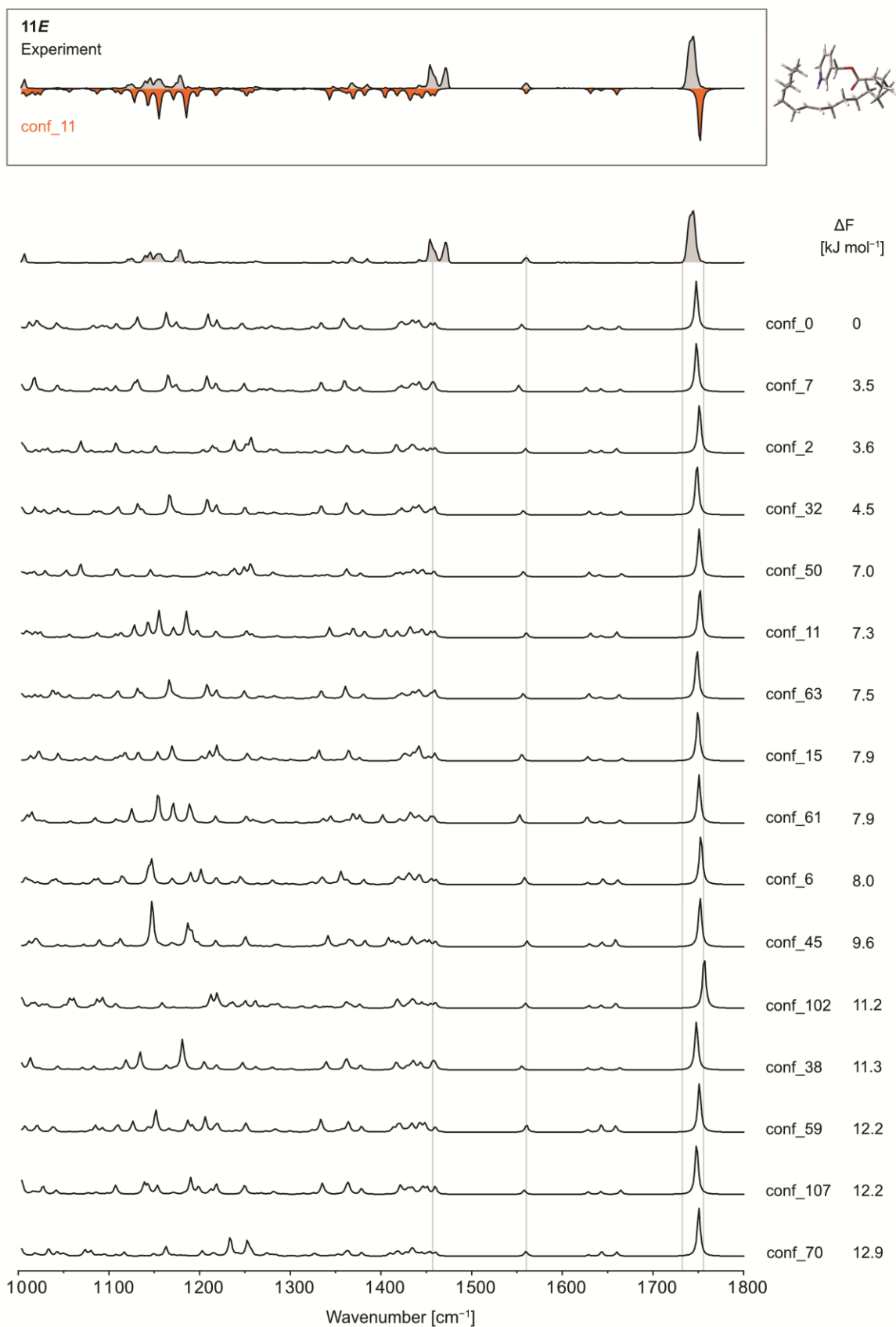


Figure S10. Experimental infrared spectrum of protonated C18:1 **11E** 3-pyridylcarbinol ester and harmonic spectra of computed conformers. The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S8.

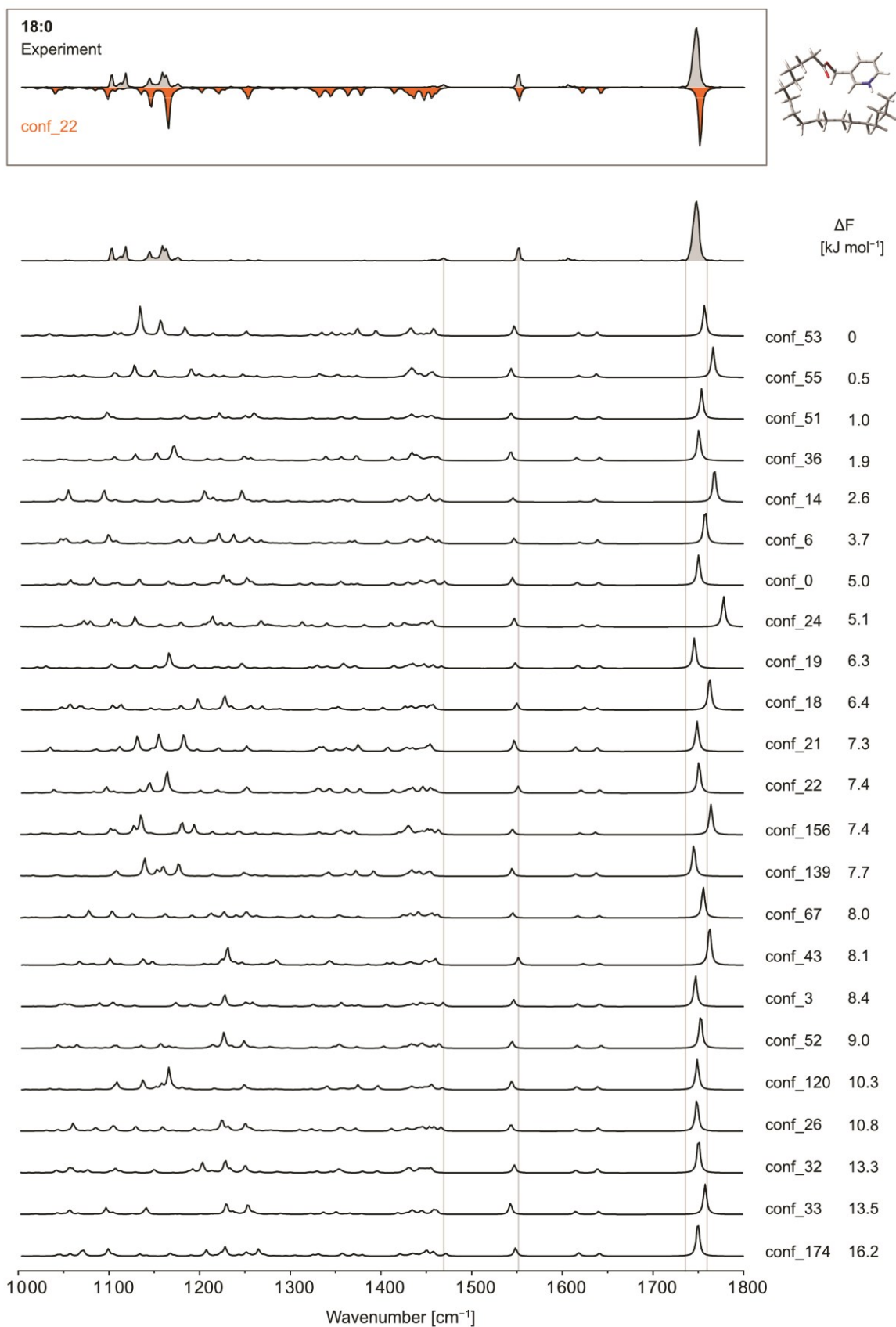


Figure S11. Experimental infrared spectrum of protonated **C18:0** 3-pyridylcarbinol ester and harmonic spectra of computed conformers. A few computed spectra exhibit a blueshifted C=O stretching vibration (>1760 cm⁻¹) that is not observed in the experimental spectrum. The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S9.

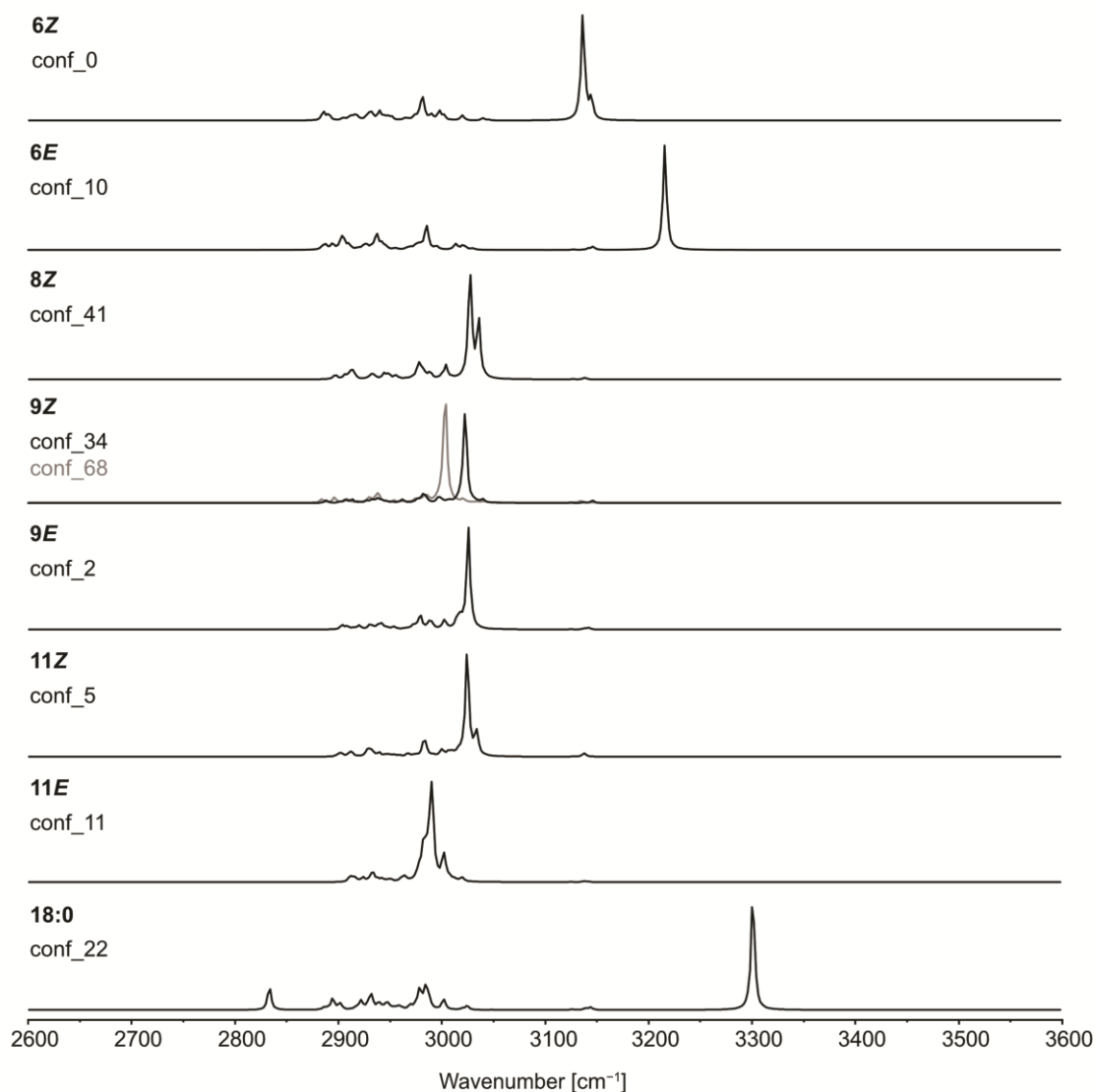


Figure S12. Computed IR spectra of protonated C18:1 and C18:0 3-pyridylcarbinol esters in the 3000 cm^{-1} region. The N-H stretching vibrations in that region are predicted to be indicative of the double bond position and configuration. The absence or weakness of charge-olefin interactions induce a significant blueshift of the N-H stretching vibration, as shown in the computed spectrum of the C18:0 3-pyridylcarbinol ester. The computed spectra of conformers that yielded the best match with the experimental IR spectra in the 1000–1800 cm^{-1} region are shown here.

Computed structures of 3-picolylamides

In the following, an overview of computed protonated C18:1 3-picolylamide structures is shown. Each conformer is uniquely identifiable by its name *conf_x*, where x is the position of the conformer in the output file from the initial conformer search in CREST. The conformers are ordered by ascending free energy. Computed conformers that exhibit a C=O stretching frequency higher than 1700 cm⁻¹ are highlighted in blue in Table S10–Table S14. XYZ coordinates of all computed conformers are provided in a separate file.

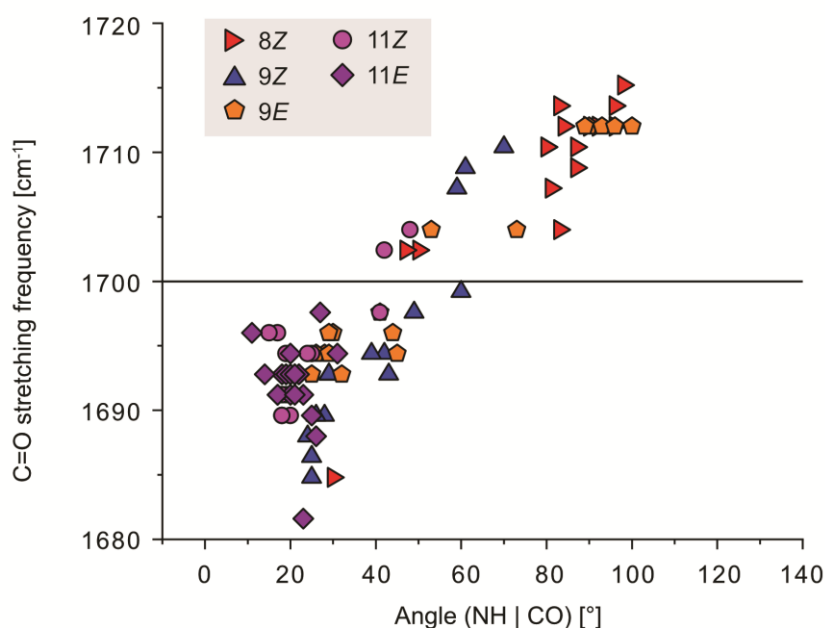


Figure S13. Graphical representation of all computed 3-picolylamide structures in a 2D plot featuring the computed harmonic C=O stretching frequency in dependence of the angle between the aromatic N-H and the C=O bond. The C=O stretching frequency increases with increasing angle. The computed conformers were assigned to two groups with stretching frequencies higher or lower than 1700 cm⁻¹.

Table S10. Overview of computed conformers of protonated C18:1 **8Z** 3-picolylamides. Each conformer is characterized by its free energy at 90 K (ΔF), distance of the charge-olefin interaction, angle between the N-H and C=O bonds and computed collision cross section (CCS). Conformers with blueshifted C=O stretching frequencies are highlighted in blue. The corresponding harmonic infrared spectra are depicted in Figure S14.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_2	0	2.12	96	195.6
conf_17	1.4	2.08	87	194.7
conf_0	1.5	2.08	87	194.6
conf_16	3.4	2.09	83	195.7
conf_109	4.8	2.12	80	195.7
conf_21	6.4	2.07	84	195.6
conf_29	7.2	2.09	81	196.9
conf_18	7.3	2.09	98	196.9
conf_27	7.4	2.16	92	190.2
conf_7	7.9	2.12	96	195.9
conf_22	8.2	2.10	50	195.3
conf_6	8.5	2.11	80	191.1
conf_13	9.1	2.10	47	195.8
conf_28	10.4	2.06	90	198.7
conf_4	10.6	2.15	30	189.6
conf_55	11.2	2.17	83	190.9
average				194.9

Table S11. Overview of computed conformers of protonated C18:1 **9Z** 3-picolylamides. The corresponding harmonic infrared spectra are depicted in Figure S15.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_11	0	2.11	42	192.5
conf_0	0.5	2.09	25	190.6
conf_36	1.6	2.09	39	198.7
conf_4	1.8	2.06	28	193.3
conf_76	2.1	2.17	49	192.9
conf_10	3.1	2.07	26	192.9
conf_6	3.4	2.09	25	192.6
conf_22	4.1	2.10	29	193.6
conf_1	4.5	2.09	70	194.0
conf_40	6.1	2.11	25	195.1
conf_39	6.6	2.08	24	192.7
conf_49	7.3	2.10	43	193.6
conf_42	7.5	2.06	29	192.2
conf_87	10.0	2.08	60	195.5
conf_75	14.6	2.14	61	202.3
conf_77	15.0	2.11	59	208.8
conf_38	25.8	2.14	29	191.1
average				193.4

Table S12. Overview of computed conformers of protonated C18:1 **9E** 3-picolylamides. The corresponding harmonic infrared spectra are depicted in Figure S16.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_61	0	2.06	41	199.8
conf_105	1.8	2.1}	45	196.9
conf_0	2.0	2.07	28	198.0
conf_3	2.4	2.07	30	194.0
conf_42	2.8	2.08	90	196.2
conf_116	3.3	2.03	73	190.9
conf_4	4.0	2.06	93	200.2
conf_2	4.7	2.10	53	197.2
conf_6	5.2	2.09	96	197.4
conf_33	5.7	2.07	89	196.7
conf_1	6.0	2.06	100	200.0
conf_48	6.4	2.09	26	195.5
conf_43	6.6	2.17	29	195.8
conf_44	7.2	2.08	44	199.9
conf_82	7.3	2.04	32	196.5
conf_23	7.8	2.07	119	200.5
conf_7	7.9	2.07	119	200.5
conf_56	8.9	2.10	25	197.6
conf_104	9.1	2.11	29	205.6
average				197.8

Table S13. Overview of computed conformers of protonated C18:1 **11Z** 3-picolylamides. The corresponding harmonic infrared spectra are depicted in Figure S17.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_0	0	2.08	18	192.7
conf_58	1.5	2.08	19	194.6
conf_7	2.1	2.08	25	198.7
conf_1	2.3	2.07	20	193.2
conf_109	3.0	2.06	17	202.4
conf_4	4.0	2.09	19	193.4
conf_50	4.1	2.09	24	196.6
conf_5	4.4	2.08	18	194.3
conf_14	4.6	2.07	48	192.4
conf_40	7.1	2.19	18	194.3
conf_57	7.3	2.05	42	192.0
conf_18	8.2	2.07	18	192.7
conf_116	8.5	2.07	41	189.0
conf_122	9.7	2.17	15	195.7
average				194.4

Table S14. Overview of computed conformers of protonated C18:1 **11E** 3-picolylamides. The corresponding harmonic infrared spectra are depicted in Figure S18.

conformer	$\Delta F_{90\text{ K}}$ [kJ mol ⁻¹]	d(NH--C=C) [Å]	angle (NH CO) [°]	CCS _{N2} [Å ²]
conf_17	0	2.04	20	193.1
conf_0	0.3	2.09	18	194.5
conf_35	1.8	2.09	20	195.4
conf_15	2.6	2.06	19	209.4
conf_2	2.8	2.07	14	195.6
conf_14	4.0	2.07	19	195.2
conf_26	4.2	2.11	11	198.7
conf_41	4.3	2.03	20	212.4
conf_3	5.8	2.16	17	193.0
conf_28	5.9	2.09	22	195.5
conf_18	7.1	2.09	23	196.7
conf_119	7.5	2.15	17	200.5
conf_51	8.0	2.09	17	207.0
conf_153	8.4	2.06	27	197.4
conf_52	8.8	2.04	22	212.4
conf_117	9.2	2.19	21	193.9
conf_61	9.5	2.12	23	191.4
conf_130	10.0	2.04	31	200.9
conf_120	10.4	2.12	21	195.9
conf_64	13.3	2.12	21	191.9
conf_102	14.3	2.08	25	193.5
conf_158	19.6	2.21	26	198.4
average				198.9

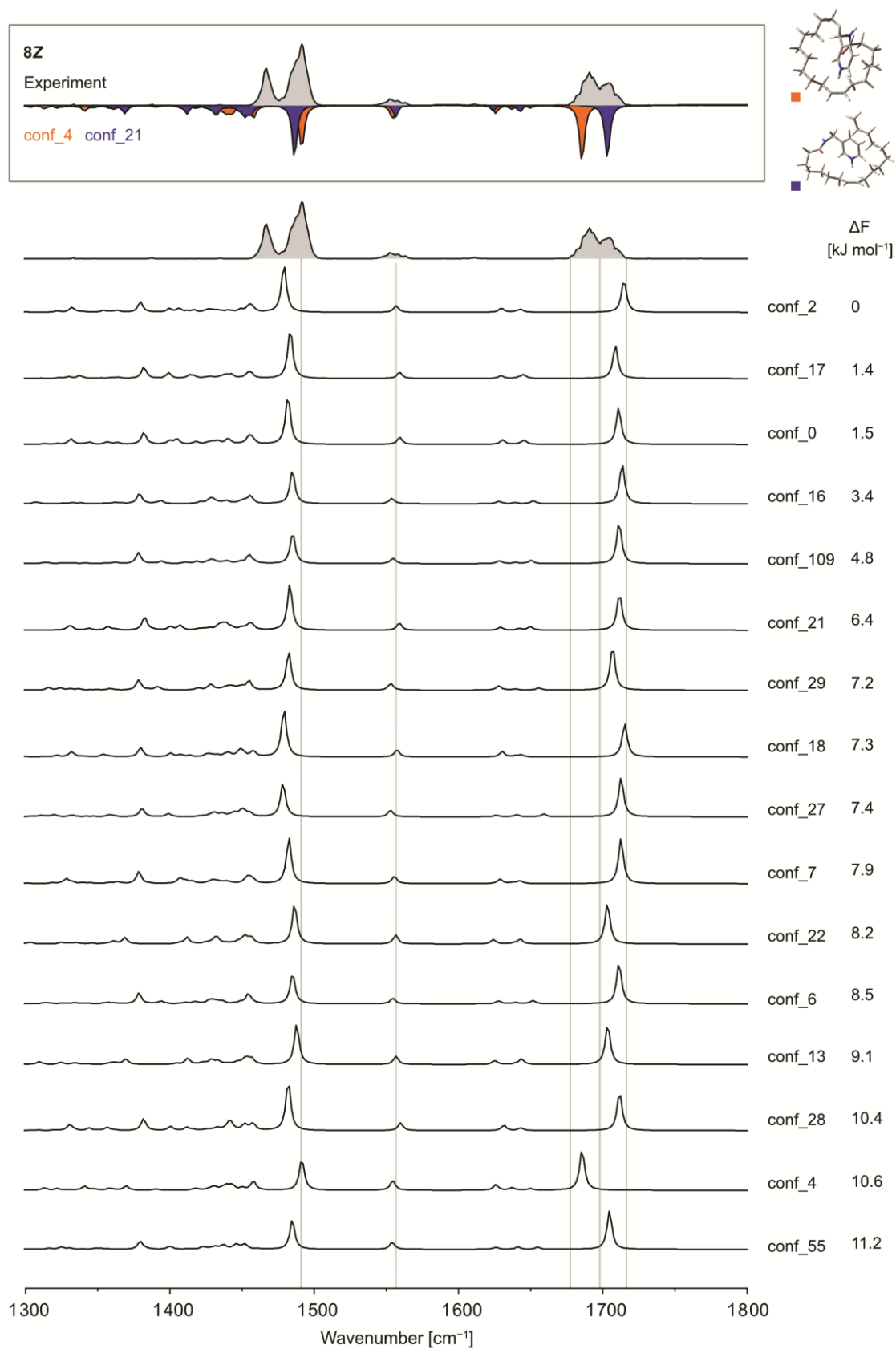


Figure S14. Experimental infrared spectrum of protonated C18:1 **8Z** 3-picolylamide and harmonic spectra of computed conformers. The majority of the computed infrared spectra exhibit a blueshifted C=O stretching vibration (>1700 cm⁻¹). The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S10.

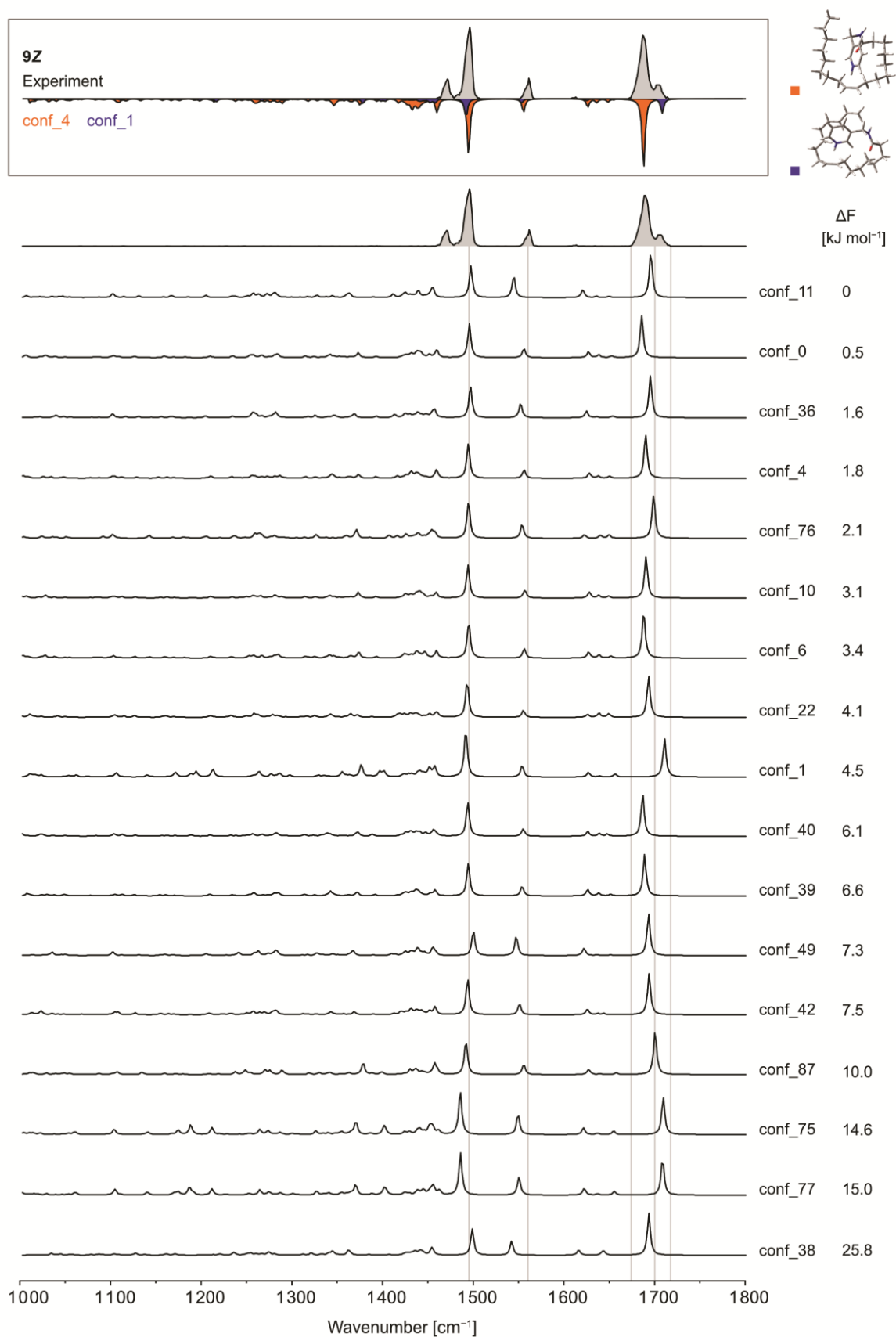


Figure S15. Experimental infrared spectrum of protonated C18:1 **9Z** 3-picolylamide and harmonic spectra of computed conformers. A few computed infrared spectra exhibit a blueshifted C=O stretching vibration (>1700 cm⁻¹) observed in the experimental spectrum. The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S11.

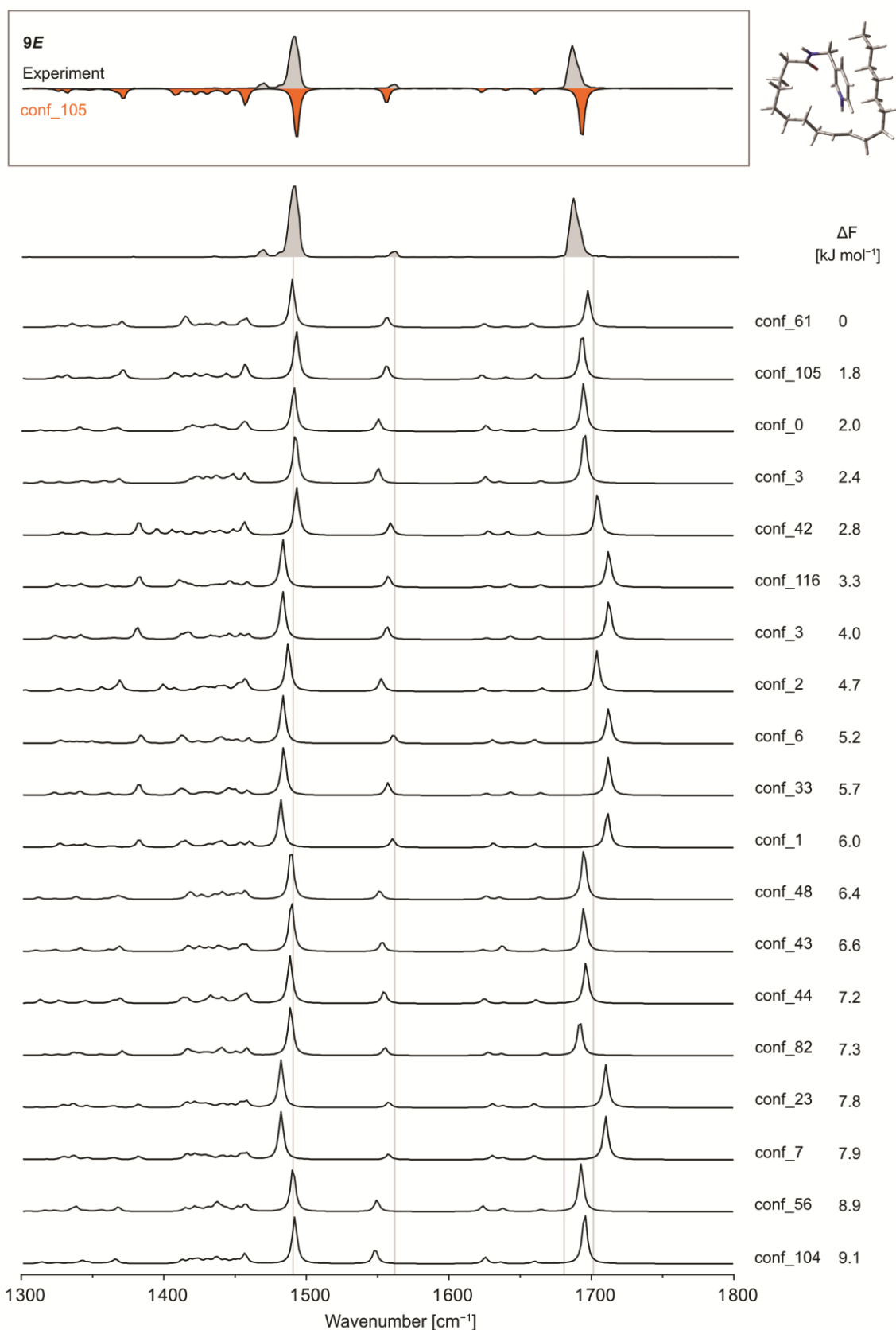


Figure S16. Experimental infrared spectrum of protonated C18:1 **9E** 3-picolylamide and harmonic spectra of computed conformers. Several computed spectra exhibit a blueshifted C=O stretching vibration ($>1700\text{ cm}^{-1}$), which is not observed in the experimental spectrum. The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S12.

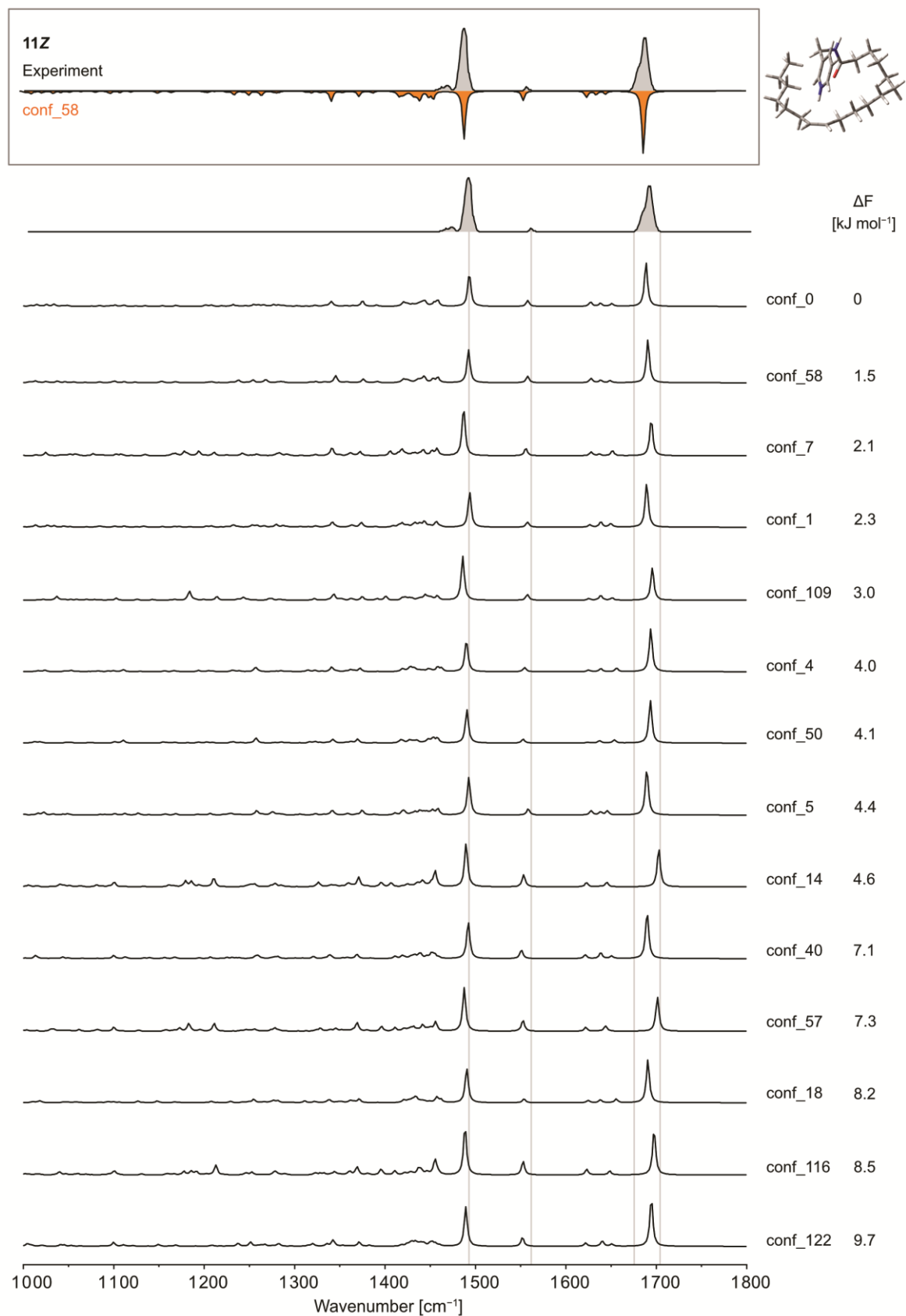


Figure S17. Experimental infrared spectrum of protonated C18:1 **11Z** 3-picolylamide and harmonic spectra of computed conformers. The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S13.

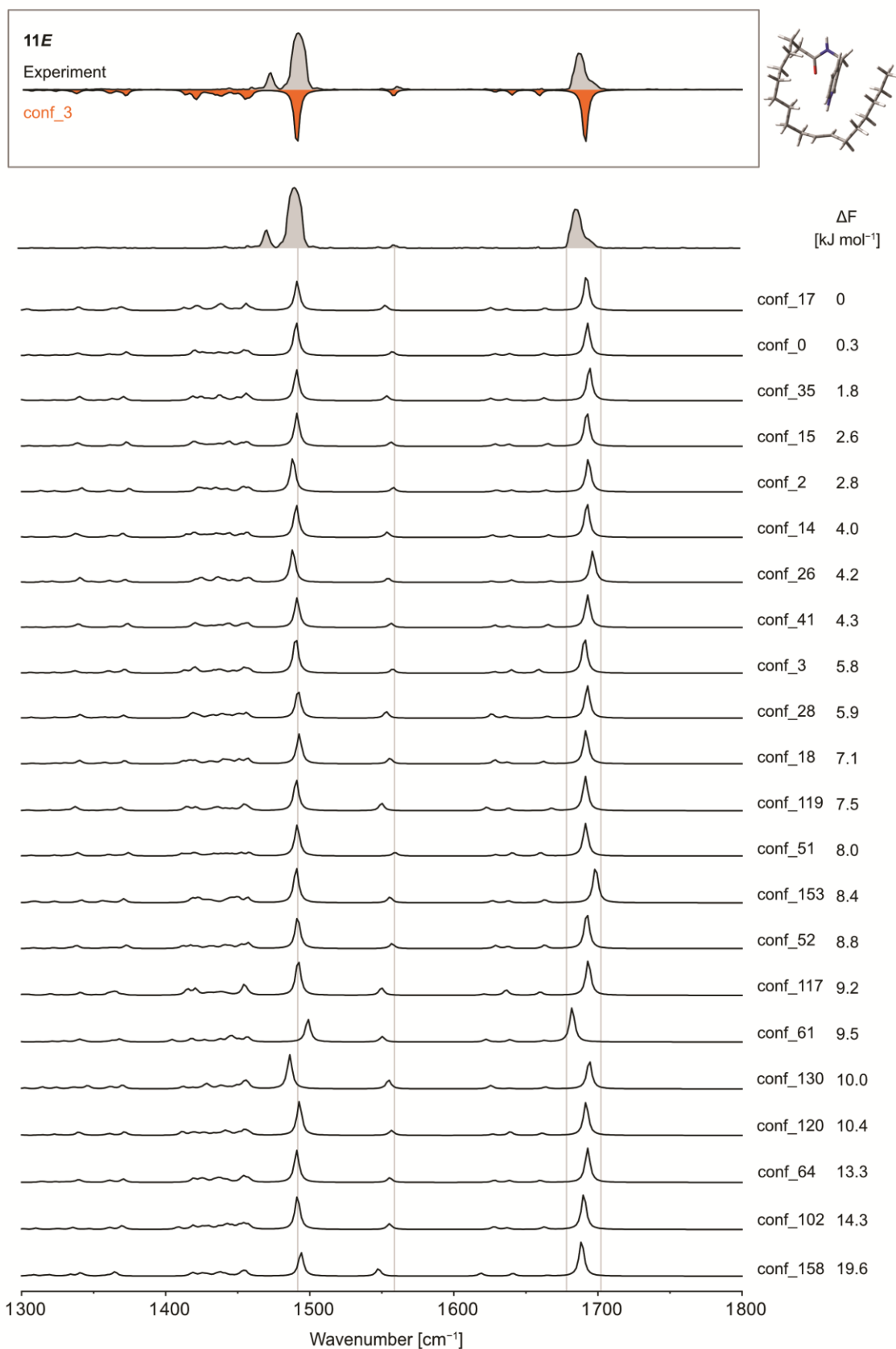


Figure S18. Experimental infrared spectrum of protonated C18:1 **11E** 3-picolylamide and harmonic spectra of computed conformers. The best match between experiment and theory is shown on top. An overview of all computed conformers is given in Table S14.

Collision cross sections

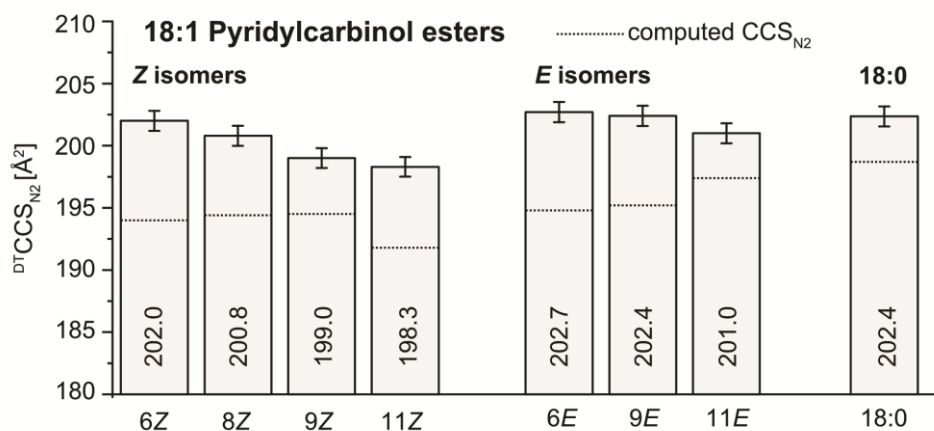


Figure S19. Experimental $^{DT}CCS_{N_2}$ values of 3-pyridylcarbinol esters. The CCS decrease with increasing distance of the double bond from the ester and are larger for *E* than for *Z* isomers. The computed CCS_{N_2} values are systematically underestimated but reflect the experimentally observed trends reasonably well, regarding the small relative CCS differences between double bond isomers. The error bars correspond to an estimated rsd deviation of 0.4 %. Computed CCS_{N_2} values are taken from Table S2–Table S9.

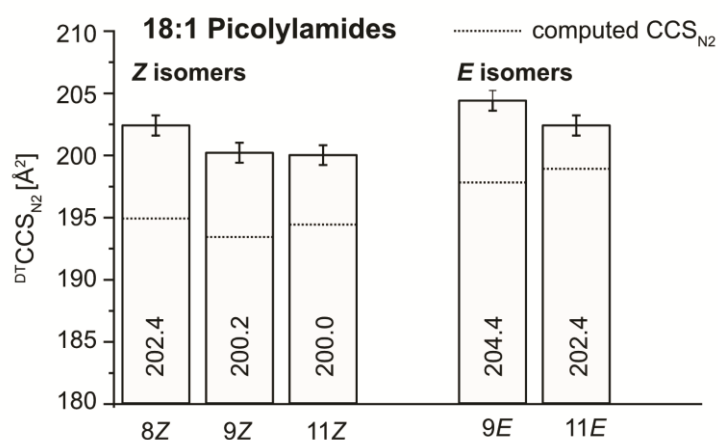


Figure S20. Experimental $^{DT}CCS_{N_2}$ values of 18:1 picolylamides. The CCS decrease with increasing distance of the double bond from the ester and are larger for *E* than for *Z* isomers. The CCS are slightly larger than the corresponding CCS of 3-pyridylcarbinol esters but follow the same trends. The error bars correspond to an estimated rsd deviation of 0.4 %. Computed CCS_{N_2} values are taken from Table S10–Table S14.

Linear regression analysis of mixtures

Table S15. Data matrix of binned component and composite infrared spectra of synthetic 3-pyridylcarbinol esters and isomeric mixtures. The R^2 values of the linear regression are given below.

wavenumber	8Z	9Z	11Z	8Z/9Z 2:1	8Z/11Z 1:1	9Z/11Z 1:2	8Z/9Z/11Z 2:1:2
	Component Spectra			Composite Spectra			
1050	0.146	0.002	0	0.176	0.152	0.032	0.097
1052	0.490	0.004	0	0.662	0.471	0.074	0.224
1054	0.681	0.032	0.001	0.929	0.482	0.130	0.391
1056	0.209	0.036	0.004	0.630	0.099	0.097	0.235
1058	0.059	0.006	0	0.373	0.108	0.034	0.270
1060	0.064	0	0.003	0.131	0.095	0.004	0.160
1062	0.145	0.046	0.018	0.191	0.171	0.017	0.204
1064	0.140	0.034	0	0.224	0.192	0.054	0.249
1066	0.069	0.001	0	0.274	0.085	0.014	0.306
1068	0.064	0	0	0.251	0.128	0.033	0.297
1070	0.175	0.007	0	0.328	0.217	0.006	0.242
1072	0.069	0.026	0	0.431	0.287	0.037	0.202
1074	0.105	0.023	0.002	0.589	0.407	0.039	0.259
1076	0.708	0.004	0.005	1.131	0.909	0.132	0.808
1078	1.364	0.002	0	1.573	0.930	0.080	1.319
1080	1.071	0.013	0	1.114	0.752	0.104	0.819
1082	0.286	0.003	0	0.393	0.422	0.132	0.239
1084	0.067	0.011	0	0.150	0.088	0.065	0.135
1086	0.089	0.008	0	0.154	0.179	0.011	0.108
1088	0.053	0	0	0.196	0.302	0.019	0.111
1090	0.044	0	0.007	0.087	0.265	0.005	0.105
1092	0.034	0.049	0.089	0.130	0.119	0.012	0.075
1094	0.072	0.110	0.050	0.183	0.136	0.113	0.091
1096	0.071	0.026	0.041	0.328	0.182	0.160	0.156
1098	0.058	0.082	0.059	0.351	0.234	0.193	0.081
1100	0.012	0.023	0.003	0.155	0.023	0.128	0.069
1102	0.007	0	0	0.021	0.035	0.103	0.034
1104	0.010	0.018	0	0.058	0.007	0.026	0.045
1106	0	0.116	0.015	0.148	0.041	0.151	0.190
1108	0.001	0.294	0.043	0.501	0.090	0.557	0.378
1110	0.027	0.241	0.035	0.545	0.110	0.549	0.513
1112	0.198	0.123	0.111	0.607	0.484	0.779	0.642
1114	0.513	0.193	1.364	1.069	2.006	3.548	1.313
1116	0.635	0.353	4.702	1.901	4.301	8.795	4.399
1118	0.914	0.271	5.278	2.110	4.726	8.592	5.168
1120	1.474	0.336	1.553	2.079	2.740	2.420	3.463
1122	1.639	0.311	0.103	2.106	1.133	1.004	1.731
1124	1.506	0.228	0.003	2.200	1.303	0.955	1.539
1126	1.185	0.082	0	2.067	1.697	1.482	1.799
1128	0.636	0.464	0	2.304	1.329	1.570	1.533
1130	0.331	1.575	0	2.380	0.523	2.265	1.852
1132	0.372	4.662	0	3.234	0.833	4.431	2.170
1134	1.210	7.455	0.027	4.359	0.953	6.674	2.762
1136	1.053	6.982	0.182	5.048	1.286	7.079	3.362
1138	0.649	5.223	0.103	4.728	1.422	5.051	3.213
1140	0.972	2.938	0.173	4.119	1.550	4.568	2.825
1142	0.718	1.508	0.332	2.272	1.781	5.287	2.574
1144	0.335	1.656	1.655	1.886	3.780	7.282	3.521
1146	0.318	1.926	5.486	1.629	6.922	11.725	5.703
1148	0.311	1.112	11.272	1.496	9.412	16.129	7.916
1150	0.214	0.457	15.210	1.092	11.083	19.599	8.564
1152	0.200	0.510	16.160	0.952	10.553	18.769	7.742
1154	0.339	0.604	12.622	1.117	8.047	16.308	7.425
1156	0.341	0.561	7.280	1.257	5.516	12.145	6.409
1158	0.344	1.436	2.167	1.287	2.819	5.728	2.833
1160	0.173	2.014	0.194	1.649	0.520	2.467	1.376
1162	0.112	1.445	0.044	1.382	0.352	1.444	1.276
1164	0.040	0.561	0.004	0.882	0.228	0.660	0.868
1166	0.034	0.241	0.008	0.456	0.095	0.217	0.341
1168	0.038	0.084	0.018	0.303	0.062	0.199	0.173
1170	0.081	0.127	0.026	0.284	0.181	0.433	0.190
1172	0.104	0.359	0.148	0.542	0.310	0.895	0.492
1174	0.133	1.277	0.085	1.063	0.488	1.639	1.103
1176	0.176	1.781	0.591	1.528	1.504	3.065	1.752
1178	0.324	1.360	2.906	1.269	3.427	6.463	3.018
1180	0.274	0.734	3.980	1.085	4.086	6.789	5.042
1182	0.084	0.483	1.780	0.420	2.717	3.858	1.996
1184	0.025	0.148	0.262	0.251	1.004	0.974	0.987
1186	0.017	0.077	0.080	0.157	0.297	0.412	0.235
1188	0.016	0.326	0.069	0.237	0.129	0.352	0.232
1190	0.040	0.576	0.031	0.479	0.175	0.380	0.305
1192	0.105	0.255	0.009	0.421	0.199	0.320	0.258
1194	0.041	0.060	0.001	0.187	0.144	0.331	0.197
1196	0.021	0.036	0.001	0.338	0.133	0.065	0.145
1198	0.036	0	0.003	0.295	0.188	0.127	0.105

1200	0.040	0.010	0.001	0.106	0.105	0.222	0.082
1202	0.029	0.208	0	0.252	0.238	0.357	0.063
1204	0.127	0.875	0.035	0.641	0.310	0.693	0.367
1206	0.031	0.866	0.077	0.720	0.179	0.824	0.549
1208	0.018	0.301	0.027	0.436	0.099	0.411	0.291
1210	0	0.302	0.006	0.495	0.072	0.310	0.231
1212	0.072	0.177	0.020	0.413	0.133	0.304	0.299
1214	0.207	0.028	0.006	0.411	0.094	0.222	0.254
1216	0.123	0.068	0	0.317	0.109	0.056	0.119
1218	0.003	0.048	0.034	0.226	0.083	0.083	0.112
1220	0	0.040	0.008	0.204	0.021	0.144	0.147
1222	0	0.145	0	0.232	0.042	0.295	0.176
1224	0.173	0.215	0	0.401	0.157	0.243	0.425
1226	0.988	0.134	0.002	1.004	0.706	0.135	0.826
1228	1.276	0.062	0	1.706	1.541	0.166	1.029
1230	0.344	0.044	0.006	1.086	1.541	0.092	0.653
1232	0.023	0.026	0.044	0.319	0.370	0.160	0.151
1234	0.003	0.036	0.006	0.049	0.039	0.120	0.095
1236	0.001	0.013	0	0.002	0.045	0.021	0.029
1238	0.005	0.001	0	0.025	0.002	0.011	0.016
1240	0.007	0.040	0.007	0.101	0.006	0.073	0.091
1242	0.032	0.104	0.002	0.134	0.025	0.165	0.078
1244	0.016	0.050	0	0.055	0.049	0.123	0.080
1246	0.001	0.003	0	0.058	0.032	0.032	0.048
1248	0.009	0	0.004	0	0	0.131	0.156
1250	0.008	0.004	0.002	0	0	0.184	0.180

1700	0	0	0.058	0	0	0.002	0.001
1702	0	0	0.012	0.007	0.008	0.003	0.019
1704	0	0	0.033	0.064	0.006	0.021	0.014
1706	0	0.019	0.074	0.032	0.034	0.012	0
1708	0	0.036	0.025	0.001	0.020	0.051	0.008
1710	0.001	0.011	0	0	0.009	0.013	0.016
1712	0.005	0.001	0.002	0.006	0	0	0.012
1714	0.006	0.004	0.046	0.036	0	0	0.017
1716	0.011	0.007	0.033	0.017	0	0	0.006
1718	0	0.004	0.002	0.026	0.001	0.001	0.009
1720	0	0	0.004	0.010	0	0.002	0.002
1722	0.002	0	0.014	0.010	0.015	0.002	0.005
1724	0	0	0	0.030	0.020	0.044	0.004
1726	0	0.030	0.001	0.006	0.009	0.097	0.015
1728	0	0.057	0.004	0.017	0.030	0.175	0.108
1730	0.001	0.117	0.001	0.159	0.078	0.272	0.121
1732	0.010	0.495	0.010	0.313	0.200	0.484	0.221
1734	0.002	0.872	0.059	0.696	0.286	1.087	0.593
1736	0.014	1.785	0.202	0.993	0.717	2.175	1.105
1738	0.106	2.856	0.412	1.377	1.815	3.165	2.024
1740	0.196	3.662	2.839	1.984	2.875	6.165	2.970
1742	0.183	5.002	4.476	2.524	4.154	8.945	4.594
1744	0.233	4.957	5.732	2.318	4.651	9.974	5.055
1746	0.326	3.227	6.303	2.248	5.536	11.638	4.771
1748	0.359	2.257	8.009	1.841	5.212	11.117	4.909
1750	0.233	1.288	8.562	1.307	5.799	8.654	4.920
1752	0.279	0.745	5.964	1.353	4.218	6.079	3.728
1754	0.165	1.283	3.538	1.334	1.859	3.980	1.685
1756	0.242	2.434	0.806	1.606	0.687	2.273	1.227
1758	0.291	3.616	0.128	2.201	0.656	1.712	1.121
1760	0.510	3.371	0.091	3.055	0.766	2.246	1.322
1762	1.418	3.809	0.019	3.823	1.455	2.082	2.110
1764	3.541	4.034	0.027	5.269	2.070	2.269	3.455
1766	4.305	3.548	0.009	5.388	2.721	1.472	3.469
1768	5.289	2.418	0.002	5.780	4.319	1.114	3.825
1770	4.773	1.621	0.005	6.519	4.912	0.948	3.462
1772	3.423	1.540	0	4.545	2.918	0.837	2.733
1774	1.528	1.055	0.007	2.977	2.076	0.622	1.815
1776	0.837	0.407	0.005	1.821	1.260	0.602	0.956
1778	0.241	0.118	0	0.801	0.483	0.178	0.477
1780	0.381	0.036	0.006	0.649	0.678	0.062	0.737
1782	0.496	0.002	0.005	1.092	0.793	0.013	0.693
1784	0.781	0.002	0	0.948	0.832	0.007	0.619
1786	1.034	0	0.005	0.611	0.737	0	0.918
1788	0.403	0	0.015	0.582	0.506	0	0.537
1790	0.117	0	0	0.284	0.257	0.001	0.311
1792	0.042	0.003	0	0.174	0.171	0.005	0.177
1794	0.032	0.001	0	0	0.049	0.003	0.154
1796	0	0	0	0	0.003	0.001	0.202
1798	0	0.042	0	0	0	0.002	0
1800	0	0.038	0	0	0	0	0
			R ²	0.91221	0.94221	0.94724	0.91647

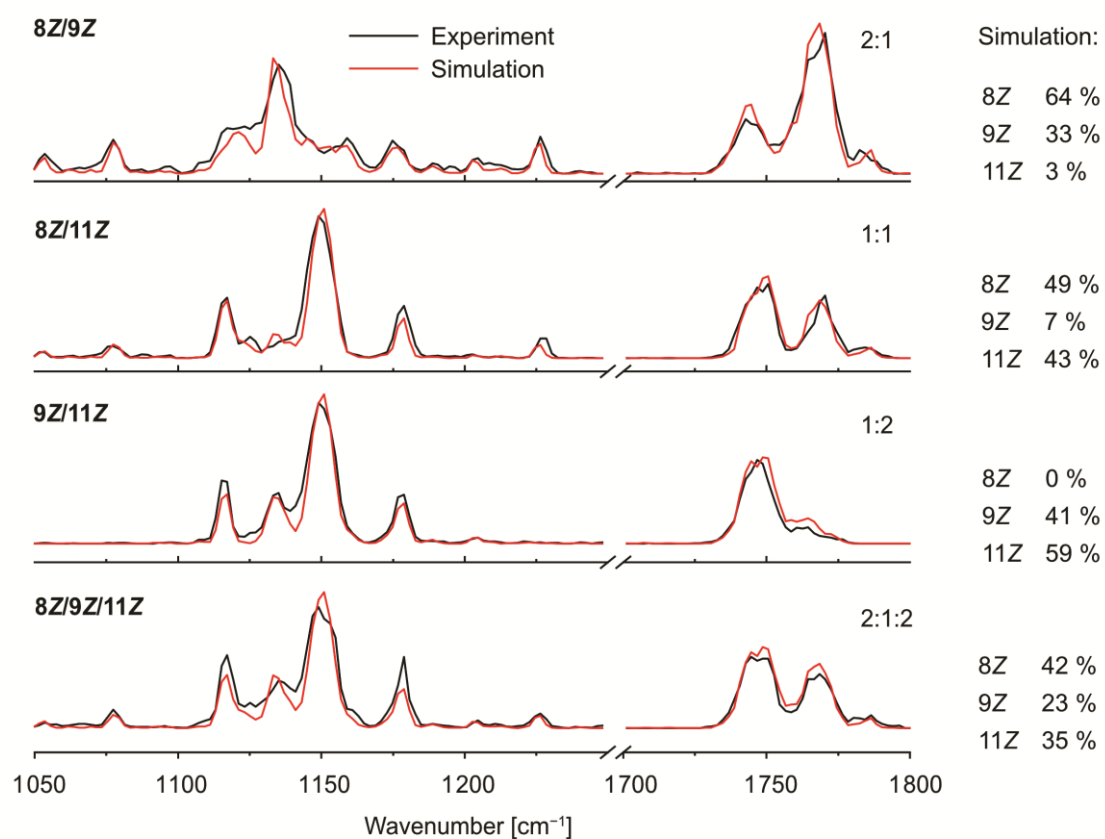


Figure S21. Experimental and simulated infrared spectra of synthetic binary and ternary mixtures of protonated 8Z, 9Z and 11Z C18:1 3-pyridylcarbinol esters. The simulated spectra were created based on the percentages obtained from a linear regression analysis of the experimental mixture spectra. The spectra are binned (resolution: 1 datapoint per 2 cm^{-1}).

Table S16. Data matrix of binned component and composite infrared spectra of synthetic 3-pyridylcarbinol ester standards and three isomeric mixtures. The R² values of the linear regression are given below.

wavenumber	6Z	6E	8Z	9Z	9E	11Z	11E	37 mix Restek	LNCaP TOFA	PC-3
Component Spectra								Composite Spectra		
1010	0.014	0.062	0	0	0.002	0.006	0.041	0.007	0	0
1012	0	0.030	0.006	0	0.003	0.012	0.044	0	0	0
1014	0	0.073	0.004	0	0	0.002	0.025	0	0	0
1016	0	0.075	0.003	0	0.001	0	0.001	0	0	0
1018	0	0.031	0.001	0.004	0.009	0	0.001	0	0	0.044
1020	0.001	0.023	0	0.060	0.138	0	0.003	0.013	0.004	0.044
1022	0.010	0.028	0	0.102	0.497	0	0.001	0.169	0.006	0.019
1024	0.003	0.026	0	0.021	0.442	0	0	0.183	0	0.060
1026	0	0.064	0	0	0.264	0	0	0.070	0.025	0.050
1028	0	0.104	0	0.002	0.122	0.018	0	0.017	0.017	0
1030	0	0.298	0	0.009	0.014	0.045	0.002	0.027	0	0
1032	0.016	0.549	0	0.002	0	0.014	0.007	0.040	0	0
1034	0.012	0.583	0	0	0.007	0.030	0.019	0.036	0.015	0
1036	0.007	0.392	0.003	0	0.017	0.026	0.046	0.023	0.028	0
1038	0.043	0.816	0.017	0	0.005	0.002	0.064	0.026	0.001	0
1040	0.013	1.069	0.003	0	0.010	0.003	0.115	0.005	0	0
1042	0.019	0.584	0	0.005	0.005	0	0.095	0	0.002	0
1044	0.002	0.235	0.007	0.006	0	0	0.041	0	0.011	0
1046	0	0.232	0.034	0	0	0.001	0.009	0	0.004	0.060
1048	0.001	0.158	0.038	0	0.024	0.004	0.009	0.011	0.007	0.049
1050	0.006	0.162	0.146	0.002	0.025	0	0.011	0.016	0.005	0.006
1052	0.029	0.181	0.490	0.004	0.002	0	0.021	0.034	0.034	0.012
1054	0.008	0.201	0.681	0.032	0	0.001	0.025	0.123	0.004	0.055
1056	0.110	0.335	0.209	0.036	0	0.004	0	0.145	0.001	0.065
1058	0.181	0.731	0.059	0.006	0	0	0	0.081	0.007	0.044
1060	0.160	0.753	0.064	0	0.001	0.003	0	0.018	0.008	0.013
1062	0.234	0.693	0.145	0.046	0.007	0.018	0	0.013	0.021	0
1064	0.570	0.947	0.140	0.034	0.005	0	0	0.005	0.009	0.024
1066	1.676	1.364	0.069	0.001	0.002	0	0.003	0.005	0	0.028
1068	2.545	0.969	0.064	0	0.002	0	0.016	0.009	0.024	0.058
1070	4.084	0.501	0.175	0.007	0.006	0	0.020	0.023	0.086	0.123
1072	3.281	0.217	0.069	0.026	0.007	0	0.052	0.041	0.038	0.073
1074	1.020	0.079	0.105	0.023	0.005	0.002	0.007	0.046	0.003	0.041
1076	0.093	0.086	0.708	0.004	0.029	0.005	0	0.020	0.035	0.050
1078	0.080	0.077	1.364	0.002	0.073	0	0	0.190	0.047	0.128
1080	0.045	0.053	1.071	0.013	0.514	0	0.003	0.233	0.037	0.205
1082	0.030	0.173	0.286	0.003	0.565	0	0.001	0.211	0.021	0.031
1084	0.001	0.413	0.067	0.011	0.083	0	0	0.036	0.003	0.004
1086	0	0.435	0.089	0.008	0.037	0	0.003	0.005	0.007	0
1088	0	0.377	0.053	0	0.002	0	0.006	0.023	0.003	0.046
1090	0.003	0.395	0.044	0	0	0.007	0	0.028	0.001	0.078
1092	0.035	0.249	0.034	0.049	0.019	0.089	0	0.006	0	0.010
1094	0.033	0.255	0.072	0.110	0.103	0.050	0	0.050	0	0
1096	0	0.089	0.071	0.026	0.087	0.041	0.002	0.052	0	0
1098	0	0.015	0.058	0.082	0.021	0.059	0.006	0.019	0	0
1100	0	0.005	0.012	0.023	0.053	0.003	0.027	0.009	0.001	0
1102	0.001	0.010	0.007	0	0.026	0	0.075	0.003	0.004	0.021
1104	0.002	0.033	0.010	0.018	0.016	0	0.070	0.023	0	0.017
1106	0	0.309	0	0.116	0.093	0.015	0.027	0.033	0.021	0.023
1108	0	0.723	0.001	0.294	0.105	0.043	0.016	0.110	0.086	0.112
1110	0.019	0.731	0.027	0.241	0.034	0.035	0.028	0.122	0.050	0.074
1112	0.087	0.921	0.198	0.123	0.015	0.111	0.050	0.182	0.064	0.069
1114	0.179	1.252	0.513	0.193	0.212	1.364	0.128	0.165	0.110	0.353
1116	0.292	1.575	0.635	0.353	0.643	4.702	0.237	0.385	0.280	0.468
1118	0.524	1.450	0.914	0.271	1.143	5.278	0.562	0.729	0.336	0.544
1120	1.114	1.448	1.474	0.336	0.947	1.553	0.592	0.731	0.183	0.436
1122	2.119	2.014	1.639	0.311	0.407	0.103	0.731	0.423	0.118	0.241
1124	2.906	2.089	1.506	0.228	0.282	0.003	0.542	0.378	0.050	0.243
1126	1.547	2.198	1.185	0.082	0.152	0	0.229	0.347	0.050	0.386
1128	0.861	2.805	0.636	0.464	0.963	0	0.091	0.788	0.097	0.350
1130	0.621	4.629	0.331	1.575	1.568	0	0.076	1.642	0.252	0.388
1132	0.857	6.927	0.372	4.662	1.430	0	0.126	2.574	1.109	1.085
1134	2.288	7.834	1.210	7.455	1.324	0.027	0.363	3.658	1.107	1.730
1136	3.792	7.265	1.053	6.982	1.190	0.182	0.936	3.698	0.862	1.188
1138	2.887	5.461	0.649	5.223	0.844	0.103	1.141	2.696	0.510	0.942
1140	0.553	3.825	0.972	2.938	0.927	0.173	1.046	1.508	0.272	0.590
1142	0.082	2.748	0.718	1.508	1.392	0.332	1.565	1.202	0.243	0.551
1144	0.111	2.231	0.335	1.656	2.904	1.655	1.404	1.514	0.382	0.703
1146	0.099	1.522	0.318	1.926	4.312	5.486	0.661	1.439	0.421	0.679
1148	0.024	0.983	0.311	1.112	3.403	11.272	1.034	0.953	0.659	0.747
1150	0.033	0.907	0.214	0.457	1.763	15.210	1.374	0.760	0.680	0.875
1152	0.088	0.878	0.200	0.510	1.193	16.160	1.541	0.616	0.593	0.667
1154	0.032	0.833	0.339	0.604	1.084	12.622	1.515	0.569	0.480	0.690
1156	0.056	0.704	0.341	0.561	1.265	7.280	1.018	0.479	0.319	0.544
1158	0.125	0.684	0.344	1.436	0.583	2.167	0.600	0.535	0.278	0.533
1160	0.041	0.789	0.173	2.014	0.475	0.194	0.317	0.604	0.182	0.505
1162	0.033	0.891	0.112	1.445	1.082	0.044	0.300	0.967	0.180	0.382

1164	0.066	0.961	0.040	0.561	0.661	0.004	0.227	0.891	0.097	0.234
1166	0.193	0.716	0.034	0.241	0.579	0.008	0.217	0.369	0.012	0.036
1168	0.167	0.627	0.038	0.084	0.768	0.018	0.249	0.124	0	0.010
1170	0.070	0.418	0.081	0.127	0.590	0.026	0.572	0.147	0.003	0.029
1172	0.121	0.335	0.104	0.359	0.786	0.148	0.930	0.373	0.035	0.155
1174	0.111	0.337	0.133	1.277	2.637	0.085	1.399	1.213	0.094	0.318
1176	0.025	0.535	0.176	1.781	3.667	0.591	2.175	1.849	0.321	0.434
1178	0.071	1.052	0.324	1.360	3.066	2.906	1.608	1.507	0.261	0.416
1180	0.032	1.410	0.274	0.734	1.480	3.980	0.443	0.818	0.174	0.250
1182	0.011	1.276	0.084	0.483	0.631	1.780	0.056	0.399	0.097	0.138
1184	0.029	0.842	0.025	0.148	0.210	0.262	0.185	0.214	0.017	0.075
1186	0	0.433	0.017	0.077	0.040	0.080	0.213	0.107	0.026	0.057
1188	0.042	0.280	0.016	0.326	0.003	0.069	0.067	0.133	0.008	0.087
1190	0.019	0.181	0.040	0.576	0.013	0.031	0.015	0.158	0.012	0.109
1192	0	0.238	0.105	0.255	0.003	0.009	0.056	0.077	0.041	0.104
1194	0.002	0.784	0.041	0.060	0.018	0.001	0.065	0.055	0.014	0.032
1196	0.032	1.639	0.021	0.036	0.079	0.001	0.132	0.079	0.004	0.036
1198	0.227	2.022	0.036	0	0.007	0.003	0.208	0.053	0.002	0.017
1200	0.242	1.375	0.040	0.010	0.177	0.001	0.106	0.059	0.001	0.046
1202	0.122	0.669	0.029	0.208	0.707	0	0.112	0.129	0.013	0.199
1204	0	0.398	0.127	0.875	0.847	0.035	0.015	0.315	0.076	0.142
1206	0	0.368	0.031	0.866	0.404	0.077	0	0.387	0.107	0.082
1208	0	0.511	0.018	0.301	0.584	0.027	0	0.216	0.045	0.081
1210	0.001	0.559	0	0.302	0.436	0.006	0.001	0.160	0.015	0.045
1212	0.002	0.526	0.072	0.177	0.723	0.020	0.005	0.169	0.017	0.079
1214	0	0.581	0.207	0.028	0.830	0.006	0.008	0.076	0.014	0.077
1216	0.024	0.708	0.123	0.068	0.330	0	0.044	0.002	0.033	0.021
1218	0.126	0.945	0.003	0.048	0.070	0.034	0.094	0.006	0	0.001
1220	0.302	1.210	0	0.040	0.001	0.008	0.119	0.008	0	0.007
1222	0.770	0.905	0	0.145	0	0	0.099	0.043	0.003	0.031
1224	2.296	0.432	0.173	0.215	0	0	0.031	0.010	0.021	0.065
1226	1.635	0.305	0.988	0.134	0.015	0.002	0.049	0.030	0.049	0.170
1228	0.480	0.229	1.276	0.062	0.076	0	0.101	0.035	0.006	0.180
1230	0.061	0.079	0.344	0.044	0.063	0.006	0.036	0.119	0	0.061
1232	0	0.025	0.023	0.026	0.042	0.044	0	0.048	0.003	0.005
1234	0	0.008	0.003	0.036	0.002	0.006	0.036	0.014	0.005	0
1236	0	0.017	0.001	0.013	0.005	0	0.042	0.002	0.001	0
1238	0.016	0.004	0.005	0.001	0.021	0	0	0.002	0.003	0
1240	0.037	0.001	0.007	0.040	0.018	0.007	0	0.023	0.006	0
1242	0.027	0.031	0.032	0.104	0.015	0.002	0.005	0.012	0.001	0
1244	0.015	0.078	0.016	0.050	0.022	0	0.040	0.001	0.003	0
1246	0.044	0.088	0.001	0.003	0.003	0	0.011	0	0.013	0
1248	0.102	0.174	0.009	0	0.015	0.004	0.004	0.008	0.008	0
1250	0.057	0.361	0.008	0.004	0.297	0.002	0.060	0.043	0.002	0.008
1252	0.147	0.595	0.005	0.119	1.646	0.036	0.126	0.187	0.046	0.023
1254	0.405	0.644	0.017	0.349	2.215	0.043	0.152	0.279	0.044	0.078
1256	1.120	0.707	0.029	0.384	1.426	0.002	0.115	0.313	0.024	0.103
1258	0.854	0.562	0.040	0.121	0.428	0	0.173	0.137	0.005	0.059
1260	0.153	0.337	0.015	0.051	0.272	0.001	0.281	0.063	0.005	0.001
1262	0	0.248	0	0.018	0.267	0.019	0.217	0.023	0.013	0.039
1264	0	0.221	0	0.030	0.084	0.017	0.149	0.013	0.065	0.043
1266	0.004	0.340	0	0.002	0.004	0.017	0.072	0.007	0.031	0.063
1268	0.069	0.537	0.004	0	0	0.011	0.014	0.006	0	0.021
1270	0.193	0.749	0.062	0	0	0.004	0.002	0.011	0	0.005
1272	0.361	0.528	0.099	0.019	0	0.066	0	0.008	0.012	0.101
1274	0.140	0.253	0.090	0.052	0	0.036	0	0	0.019	0.033
1276	0.046	0.097	0.031	0.035	0	0.002	0	0.009	0	0.012
1278	0.074	0.092	0.051	0	0.004	0.002	0.001	0.031	0	0.003
1280	0.035	0.076	0.009	0	0.043	0	0.004	0.006	0.006	0
1282	0.041	0.041	0	0	0.138	0	0.004	0.002	0.011	0
1284	0.022	0.022	0	0	0.033	0	0.002	0.004	0.013	0.007
1286	0.004	0.008	0	0	0	0.003	0	0.001	0.062	0.021
1288	0.025	0.023	0	0	0.002	0.009	0	0	0.014	0
1290	0.020	0.013	0.002	0	0.002	0.011	0	0	0.002	0
1292	0	0.006	0.003	0	0.003	0.004	0.001	0	0.008	0
1294	0	0.007	0	0	0.001	0.012	0.003	0	0.015	0
1296	0	0.002	0	0	0	0.001	0.001	0	0.003	0
1298	0.027	0	0	0	0	0	0	0	0	0
1300	0.010	0	0.001	0	0	0	0	0	0.012	0
1302	0.001	0.011	0.004	0	0	0	0	0	0.002	0
1304	0.036	0.086	0.001	0	0	0	0	0	0	0
1306	0.084	0.107	0.003	0	0.044	0	0	0	0	0.008
1308	0.060	0.138	0.002	0	0.100	0.001	0	0	0	0.006
1310	0.003	0.066	0.003	0.006	0	0.002	0	0	0	0
1312	0.008	0.103	0	0.033	0	0.006	0.022	0.001	0	0
1314	0.020	0.042	0	0.046	0.011	0.003	0.067	0.013	0	0
1316	0	0.018	0	0.004	0.045	0.007	0.025	0.004	0	0
1318	0.001	0.016	0	0	0.011	0.001	0.013	0	0.009	0
1320	0.004	0.011	0	0	0	0.018	0	0	0.026	0
1322	0.001	0.002	0	0	0.004	0.024	0	0.020	0.022	0
1324	0.002	0.004	0.003	0	0.016	0.002	0	0.016	0.009	0
1326	0	0.007	0.010	0	0.063	0	0	0	0.001	0
1328	0.001	0.008	0	0	0	0	0	0	0	0
1330	0.100	0.029	0	0	0	0	0	0.032	0	0
1332	0.257	0.062	0	0	0	0.001	0.004	0.020	0	0
1334	0.025	0.039	0	0	0	0.003	0.007	0.002	0	0
1336	0	0.009	0.002	0.005	0	0	0.001	0	0	0

1338	0	0.018	0.003	0.001	0	0	0	0	0	0
1340	0.001	0.022	0.003	0.003	0	0.006	0	0.001	0	0
1342	0.002	0.013	0.058	0.012	0	0.001	0	0.018	0	0
1344	0	0.029	0.148	0.111	0	0	0.115	0.099	0.023	0.056
1346	0.029	0.080	0.123	0.112	0.111	0.001	0.258	0.108	0.016	0.056
1348	0.068	0.163	0.101	0.065	0.099	0.001	0.088	0.060	0.002	0.014
1350	0.060	0.179	0.036	0.088	0.122	0	0.005	0.079	0.002	0.034
1352	0.031	0.183	0.029	0.342	0.103	0	0	0.088	0	0.032
1354	0	0.262	0.046	0.486	0.043	0.001	0.081	0.046	0.004	0.032
1356	0.004	0.309	0.035	0.284	0.023	0.024	0.097	0.062	0.011	0.020
1358	0.002	0.292	0.018	0.094	0.016	0.028	0.033	0.154	0.003	0.004
1360	0.012	0.285	0.019	0.172	0.075	0.013	0.018	0.046	0.009	0.035
1362	0.001	0.184	0.025	0.258	0.157	0.019	0.094	0.003	0.004	0.087
1364	0	0.107	0.018	0.099	0.073	0.001	0.631	0	0.014	0.028
1366	0.007	0.053	0.030	0.123	0.064	0.001	0.874	0.007	0.046	0.002
1368	0.034	0.018	0.046	0.120	0.172	0.007	0.738	0.053	0.011	0
1370	0.004	0.038	0	0.203	0.777	0.002	0.427	0.046	0	0.010
1372	0	0.070	0.002	0.185	1.991	0.051	0.220	0.051	0.017	0.006
1374	0	0.273	0	0.263	1.941	0	0.114	0.084	0.015	0
1376	0	0.482	0	0.520	1.486	0	0.060	0.053	0.042	0.014
1378	0	0.573	0	0.734	1.618	0.395	0.021	0.104	0.088	0.118
1380	0.003	0.619	0.006	0.388	1.732	1.692	0.190	0.084	0.095	0.130
1382	0.038	0.397	0.065	0.648	1.426	3.234	0.470	0.089	0.080	0.169
1384	0.016	0.247	0.143	0.671	0.630	3.413	0.583	0.062	0.120	0.180
1386	0.002	0.206	0.056	0.301	0.105	0.766	0.244	0.012	0.065	0.068
1388	0	0.226	0.186	0.059	0.024	0.085	0.102	0.003	0.014	0.012
1390	0	0.081	0	0.063	0.009	0.002	0.021	0.003	0.025	0
1392	0	0.005	0	0.001	0	0	0.010	0	0.021	0
1394	0.022	0	0.001	0	0	0	0	0	0	0.013
1396	0.009	0.001	0.005	0	0	0	0	0	0.017	0.017
1398	0.010	0.008	0.003	0.002	0	0	0	0	0.016	0.003
1400	0.007	0.006	0.002	0.002	0	0	0	0.005	0.002	0
1402	0.001	0.002	0.003	0.003	0	0	0.014	0.006	0.007	0
1404	0.002	0.001	0.011	0.001	0	0	0.121	0.005	0.003	0
1406	0.002	0.005	0.007	0.007	0	0	0.005	0.034	0.043	0
1408	0	0	0.001	0.005	0	0	0.018	0.020	0.035	0
1410	0	0.003	0	0	0	0	0.006	0.023	0.007	0
1412	0.001	0.010	0.016	0	0	0	0.011	0.043	0.001	0
1414	0.022	0.003	0.010	0	0.024	0.006	0.032	0.012	0.002	0
1416	0.008	0.009	0.003	0	0.034	0.008	0.005	0.005	0.020	0
1418	0.023	0.004	0.001	0	0	0.002	0.012	0.043	0.032	0.016
1420	0.005	0.018	0.003	0.031	0	0.018	0.059	0.014	0.071	0.012
1422	0	0.061	0.001	0.239	0.005	0.004	0.011	0.003	0.021	0
1424	0.002	0.099	0	0.869	0.032	0.003	0.001	0.046	0.002	0
1426	0.013	0.106	0	0.613	0.065	0.003	0	0.116	0.017	0
1428	0.110	0.142	0	0.587	0.116	0.003	0.062	0.009	0.037	0
1430	0.157	0.214	0	0.300	0.162	0	0.048	0	0.016	0.003
1432	0.201	0.455	0	0.116	0.363	0	0.057	0.090	0.003	0.032
1434	0.202	0.917	0.017	0.322	0.962	0.003	0.037	0.134	0.015	0.128
1436	0.118	1.213	0.165	0.293	0.872	0.001	0.072	0.053	0.021	0.096
1438	0.227	1.246	0.260	0.321	0.449	0	0.132	0.091	0.028	0.058
1440	0.417	1.339	0.535	0.130	0.254	0.001	0.453	0.057	0.012	0.044
1442	0.422	1.370	0.342	0.145	0.268	0.007	0.495	0.084	0.022	0.073
1444	0.154	1.306	0.144	0.187	0.295	0.003	0.313	0.108	0.048	0.042
1446	0.217	1.738	0.010	0.515	0.507	0	0.338	0.023	0.080	0.067
1448	0.399	1.906	0.029	1.259	0.592	0.022	0.337	0.118	0.067	0.095
1450	0.328	1.752	0.062	1.778	0.742	0.107	0.817	0.191	0.122	0.108
1452	0.226	1.814	0.080	1.407	1.589	0.296	3.066	0.249	0.069	0.259
1454	0.200	1.920	0.073	1.038	2.441	0.619	3.433	0.361	0.075	0.326
1456	0.573	1.889	0.330	1.125	2.918	1.665	2.617	0.469	0.166	0.426
1458	0.905	1.747	0.205	1.401	2.987	1.407	2.124	0.528	0.194	0.577
1460	1.335	2.091	0.202	3.021	2.688	1.309	1.341	0.415	0.191	0.570
1462	1.449	2.721	0.641	3.777	2.020	1.644	0.501	0.690	0.185	0.655
1464	2.921	3.386	1.099	3.905	2.147	1.807	0.471	0.875	0.313	0.675
1466	5.427	4.613	1.225	4.200	2.937	1.436	1.026	0.816	0.369	0.969
1468	6.643	5.162	1.766	4.471	4.313	1.146	2.342	1.145	0.376	1.003
1470	4.329	4.106	1.461	3.618	5.299	1.388	3.477	1.344	0.285	0.834
1472	1.345	2.265	0.980	2.227	2.704	0.969	2.766	0.703	0.111	0.541
1474	0.385	0.802	0.415	1.025	0.106	0.263	0.799	0.146	0.010	0.177
1476	0.051	0.264	0.107	0.130	0.018	0.007	0.059	0.039	0.002	0.023
1478	0.040	0.118	0.003	0	0.050	0	0	0.002	0	0.011
1480	0.038	0.142	0.003	0	0.073	0	0	0	0	0.012
1482	0.003	0.101	0.001	0	0.012	0	0	0	0	0.003
1484	0.043	0.090	0	0	0.011	0	0	0.017	0.001	0
1486	0.023	0.055	0	0	0.002	0	0	0.040	0.011	0
1488	0.016	0.079	0	0	0	0	0	0.030	0.002	0
1490	0.022	0.126	0	0	0	0	0	0.013	0	0
1492	0.008	0.130	0.001	0.014	0.006	0	0	0.030	0	0.015
1494	0.008	0.100	0.003	0.123	0.014	0.004	0	0.017	0	0.016
1496	0	0.043	0.001	0.097	0.003	0.007	0	0	0	0
1498	0.001	0.020	0	0.011	0.003	0.001	0	0	0	0
1500	0.002	0.007	0	0	0.001	0	0	0.011	0	0
1502	0	0	0	0.002	0	0	0	0	0	0
1504	0	0	0	0.002	0	0.056	0	0	0	0
1506	0	0	0	0	0.001	0.027	0	0	0	0.003
1508	0	0	0	0	0.005	0	0	0	0.008	0.006
1510	0	0	0	0	0.001	0.003	0	0	0.006	0

1512	0	0	0	0	0	0.012	0.002	0	0.001	0
1514	0	0	0.001	0.005	0	0.015	0.003	0.002	0.004	0
1516	0	0	0.057	0.004	0	0	0.002	0.002	0.026	0
1518	0	0.006	0.040	0	0	0	0.004	0.001	0	0
1520	0	0.007	0.007	0	0	0	0	0.009	0.003	0
1522	0	0	0.003	0	0	0.003	0	0.018	0.001	0
1524	0	0	0	0.012	0	0.007	0.002	0.003	0	0
1526	0	0	0	0.038	0	0.009	0.001	0.010	0	0
1528	0	0	0	0.042	0	0.003	0	0.001	0	0
1530	0.002	0	0	0.006	0	0	0	0	0.002	0
1532	0.020	0	0	0.158	0	0	0	0	0.004	0
1534	0.197	0	0.001	0.143	0	0	0	0	0.001	0
1536	0.057	0.017	0.007	0.025	0	0	0	0	0	0.003
1538	0	0.180	0.005	0	0	0	0	0	0.025	0.009
1540	0.074	0.777	0.001	0	0	0	0	0	0.021	0.024
1542	0.443	1.458	0.013	0	0	0.002	0	0.022	0.010	0.061
1544	1.177	2.016	0.008	0	0	0.010	0	0.045	0	0.022
1546	3.273	2.877	0.012	0.043	0	0.017	0	0.047	0.008	0.067
1548	4.236	3.733	0.008	0.014	0.008	0	0.002	0.047	0.012	0.080
1550	3.217	4.453	0.082	0.038	0.014	0	0.003	0.102	0.012	0.114
1552	1.597	3.549	0.120	0.093	0.023	0	0	0.060	0.019	0.029
1554	0.454	2.439	0.101	1.328	0.214	0	0	0.131	0.050	0.021
1556	0.370	1.215	0.444	3.669	0.589	0	0.386	0.529	0.124	0.451
1558	0.254	0.318	1.641	4.426	1.122	0.231	0.738	0.868	0.161	0.490
1560	0.275	0.055	1.550	2.349	1.716	0.183	0.838	0.642	0.287	0.367
1562	0.055	0.014	0.582	1.481	1.602	0.069	0.548	0.405	0.170	0.164
1564	0.003	0.012	0.051	0.715	0.564	0.013	0.151	0.061	0.025	0.044
1566	0.002	0	0.020	0.135	0.093	0.004	0.035	0.029	0.013	0.040
1568	0	0	0.001	0.002	0	0	0	0.001	0	0.005
1570	0	0	0	0.003	0	0	0	0	0	0
1572	0	0	0	0	0.013	0.001	0	0	0	0
1574	0	0	0	0	0.003	0.001	0	0	0	0
1576	0	0	0	0	0	0	0	0	0.001	0
1578	0	0	0.001	0.004	0	0	0	0	0.006	0
1580	0	0	0.010	0.023	0	0	0	0	0.004	0
1582	0	0	0.010	0.024	0.004	0.003	0	0	0.002	0.018
1584	0	0	0.002	0	0.001	0.005	0	0.005	0	0.017
1586	0	0	0	0	0	0.001	0	0.021	0	0
1588	0	0	0	0	0	0	0	0.004	0	0
1590	0	0	0	0	0	0	0.003	0	0	0
1592	0	0	0	0	0.003	0	0.016	0	0.005	0
1594	0.021	0.011	0	0	0.004	0	0.095	0	0.039	0.002
1596	0.066	0.028	0	0	0.003	0.003	0.084	0.013	0.014	0.040
1598	0.007	0.059	0	0	0.007	0	0.022	0.039	0.013	0.023
1600	0.001	0.134	0.002	0	0.041	0	0.037	0.010	0.019	0
1602	0.042	0.261	0.008	0.003	0.021	0	0.096	0.008	0.003	0
1604	0.241	0.423	0.006	0.012	0.024	0	0.004	0.003	0.002	0
1606	0.199	0.714	0.005	0.008	0.013	0	0.032	0	0.001	0
1608	0.528	0.893	0.037	0.001	0.054	0	0.023	0	0.022	0
1610	0.655	1.006	0.039	0.051	0.040	0	0.032	0.045	0.033	0
1612	0.346	0.940	0.043	0.101	0.042	0.015	0.050	0.076	0.004	0
1614	0.231	0.876	0.059	0.041	0.038	0.051	0.026	0.030	0	0.012
1616	0.153	0.785	0.014	0.032	0.060	0.041	0.032	0.041	0.006	0.050
1618	0.104	0.676	0.098	0.023	0.017	0.003	0.038	0.021	0.036	0.033
1620	0.137	0.460	0.038	0.023	0	0	0.006	0.002	0.038	0.023
1622	0.140	0.236	0	0.024	0	0	0	0	0.050	0.007
1624	0.092	0.118	0	0.023	0.003	0	0	0	0.058	0
1626	0.047	0.062	0.001	0.011	0.013	0	0	0	0.049	0
1628	0.080	0.068	0.003	0.096	0.007	0.013	0	0	0.030	0
1630	0.020	0.042	0.002	0.175	0.019	0.003	0.014	0	0.018	0
1632	0.042	0.028	0	0.271	0.003	0.001	0.030	0.038	0.027	0
1634	0.136	0.013	0.006	0.041	0.001	0.013	0.017	0.040	0.027	0
1636	0.046	0.003	0.003	0.002	0.004	0	0.004	0.012	0.003	0
1638	0.043	0	0.008	0.001	0.002	0	0	0.012	0.010	0.003
1640	0.021	0	0.029	0.006	0	0.001	0.001	0.001	0.025	0.001
1642	0	0	0.084	0	0	0.003	0.002	0	0.030	0
1644	0	0	0	0	0.003	0.043	0.003	0	0.008	0
1646	0	0	0	0	0.023	0.009	0.001	0	0.002	0.003
1648	0	0	0	0	0.056	0.003	0	0.008	0.006	0.001
1650	0	0	0	0.011	0.071	0.004	0	0.070	0.001	0
1652	0	0	0.001	0.003	0.054	0.028	0	0.051	0	0.011
1654	0	0	0.002	0.002	0	0.014	0	0.051	0.001	0.020
1656	0	0	0.005	0	0	0	0	0.046	0.003	0.026
1658	0	0	0.004	0	0	0	0	0.060	0	0.037
1660	0	0	0	0	0.004	0	0.008	0.128	0.006	0.014
1662	0.004	0	0	0	0.001	0	0.015	0.112	0.025	0.003
1664	0.002	0	0.001	0	0	0	0.001	0.013	0.007	0
1666	0.003	0	0	0	0	0	0	0.002	0	0
1668	0	0	0	0	0.017	0	0	0.038	0	0
1670	0	0	0.074	0	0.009	0.009	0	0.060	0.013	0
1672	0.001	0	0.049	0.003	0.002	0.003	0	0.021	0.018	0
1674	0.002	0	0	0.002	0.001	0.036	0	0.017	0.027	0
1676	0.001	0	0	0	0	0.020	0.003	0.020	0.063	0
1678	0	0	0	0	0.052	0.002	0.007	0.060	0.031	0
1680	0	0	0	0	0.003	0	0.033	0.044	0.012	0
1682	0	0	0	0	0	0	0.055	0.021	0.034	0.003
1684	0	0	0	0.002	0	0	0.005	0.046	0.039	0.015

1686	0	0	0	0.011	0	0	0	0.037	0.039	0.064
1688	0.002	0	0	0.009	0	0	0	0.005	0.068	0.063
1690	0.002	0	0.001	0.003	0	0	0	0	0.018	0.028
1692	0.001	0.005	0.018	0	0	0.002	0.002	0.014	0.002	0.022
1694	0	0.006	0.062	0.003	0	0.003	0.002	0.020	0.004	0.019
1696	0	0.003	0.001	0.010	0	0	0.003	0.002	0.001	0.018
1698	0	0	0	0.003	0	0.001	0.065	0.011	0.002	0.011
1700	0	0.001	0	0	0	0.058	0.063	0.061	0.021	0.043
1702	0	0.005	0	0	0	0.012	0.017	0.012	0.026	0.009
1704	0.001	0.001	0	0	0	0.033	0	0.017	0.024	0.003
1706	0.004	0	0	0.019	0	0.074	0	0.030	0.013	0
1708	0.008	0	0	0.036	0.002	0.025	0	0.017	0.022	0
1710	0.051	0	0.001	0.011	0.018	0	0	0.005	0.037	0
1712	0.003	0.008	0.005	0.001	0.004	0.002	0	0.003	0	0
1714	0	0.004	0.006	0.004	0	0.046	0	0.025	0	0
1716	0	0.024	0.011	0.007	0	0.033	0	0.030	0.006	0
1718	0	0.008	0	0.004	0.003	0.002	0	0.015	0.026	0
1720	0	0.003	0	0	0.001	0.004	0	0.017	0.016	0
1722	0	0.009	0.002	0	0	0.014	0.002	0.029	0.007	0
1724	0	0.002	0	0	0	0	0.014	0.011	0.001	0.009
1726	0	0	0	0.030	0	0.001	0.022	0.014	0.007	0.021
1728	0	0	0	0.057	0.003	0.004	0.010	0.036	0.015	0.002
1730	0.001	0	0.001	0.117	0.052	0.001	0.045	0.049	0.021	0.001
1732	0.029	0	0.010	0.495	0.172	0.010	0.047	0.089	0.016	0.050
1734	0.070	0.018	0.002	0.872	0.764	0.059	0.488	0.381	0.040	0.289
1736	0.036	0.042	0.014	1.785	3.117	0.202	1.992	1.037	0.194	0.359
1738	0.073	0.239	0.106	2.856	6.445	0.412	4.575	1.875	0.437	0.726
1740	0.266	0.786	0.196	3.662	8.845	2.839	7.241	2.976	0.641	1.216
1742	0.530	1.481	0.183	5.002	10.435	4.476	8.193	3.754	0.962	1.640
1744	0.702	2.286	0.233	4.957	10.905	5.732	8.771	4.088	1.096	1.743
1746	0.712	3.081	0.326	3.227	8.380	6.303	7.262	3.698	1.240	1.767
1748	0.507	3.267	0.359	2.257	6.485	8.009	3.872	2.033	0.849	1.367
1750	0.506	2.880	0.233	1.288	2.530	8.562	1.744	1.168	0.736	0.964
1752	0.378	2.368	0.279	0.745	0.581	5.964	0.577	1.016	0.336	0.503
1754	0.291	1.792	0.165	1.283	0.606	3.538	0.286	1.108	0.122	0.705
1756	0.243	1.505	0.242	2.434	0.460	0.806	0.208	1.592	0.258	0.740
1758	0.428	1.241	0.291	3.616	0.405	0.128	0.046	1.925	0.300	0.560
1760	1.260	1.404	0.510	3.371	0.316	0.091	0	2.073	0.474	1.378
1762	2.384	2.227	1.418	3.809	0.223	0.019	0.025	2.091	0.575	1.549
1764	5.921	3.278	3.541	4.034	0.152	0.027	0.018	2.477	0.676	2.130
1766	9.155	3.867	4.305	3.548	0.036	0.009	0.001	2.166	0.777	2.361
1768	8.708	4.040	5.289	2.418	0.045	0.002	0.003	1.630	0.485	2.032
1770	7.594	3.717	4.773	1.621	0.022	0.005	0.001	1.058	0.320	1.682
1772	4.957	2.720	3.423	1.540	0.016	0	0	0.815	0.208	1.134
1774	2.235	1.523	1.528	1.055	0.058	0.007	0	0.405	0.094	0.577
1776	0.775	0.706	0.837	0.407	0.068	0.005	0	0.101	0.036	0.178
1778	0.170	0.171	0.241	0.118	0.019	0	0.001	0.055	0.031	0.106
1780	0.021	0.031	0.381	0.036	0	0.006	0.006	0.190	0.031	0.173
1782	0.007	0.001	0.496	0.002	0	0.005	0.003	0.112	0.067	0.169
1784	0.029	0	0.781	0.002	0	0	0.004	0.076	0.038	0.104
1786	0.008	0	1.034	0	0	0.005	0.003	0.026	0.020	0.157
1788	0.002	0.003	0.403	0	0	0.015	0	0.020	0.012	0.101
1790	0.003	0.003	0.117	0	0	0	0.001	0.041	0.002	0.007
1792	0.001	0	0.042	0.003	0	0	0.004	0.043	0	0.003
1794	0	0	0.032	0.001	0.008	0	0	0.004	0	0
1796	0	0	0	0	0.003	0	0	0	0	0
1798	0	0	0	0.042	0	0	0	0	0	0
1800	0	0	0	0.038	0	0	0.030	0	0	0
R ²								0.83317	0.83421	0.88664

UPLC-OzID-MS reference data

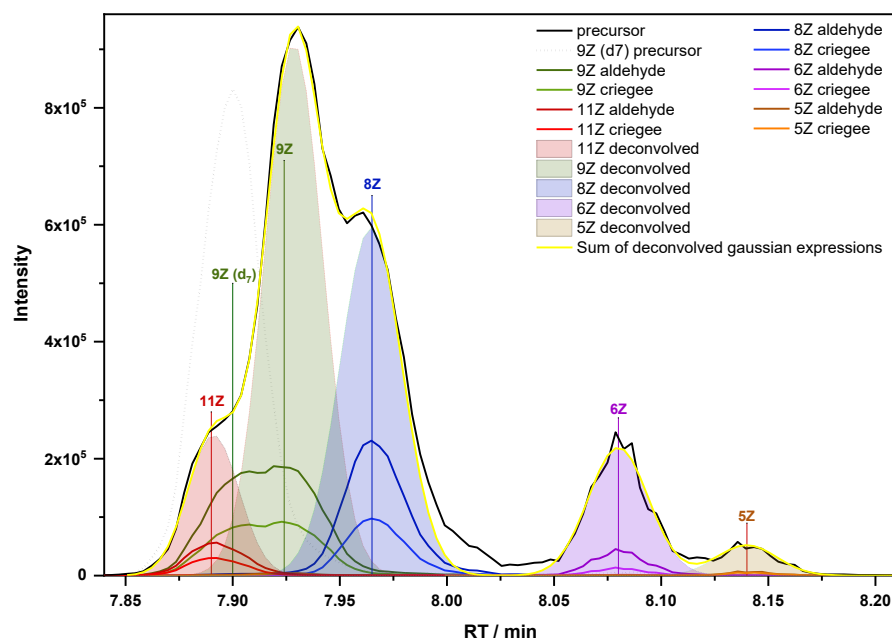


Figure S22: Deconvolution of the precursor chromatogram of octadecenoic acids in PC-3. The chromatograms of the OzID fragments of FA 18:1(9Z) (Oleic acid) were deconvolved separately, refer to Figure S23.

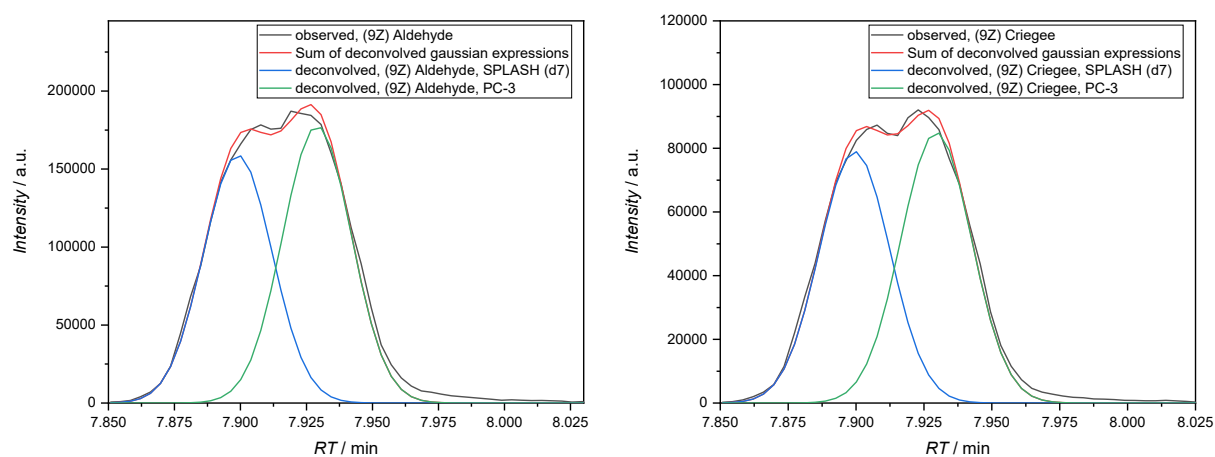


Figure S23: Deconvolution of OzID fragment chromatograms of FA 18:1(9Z) in PC-3.

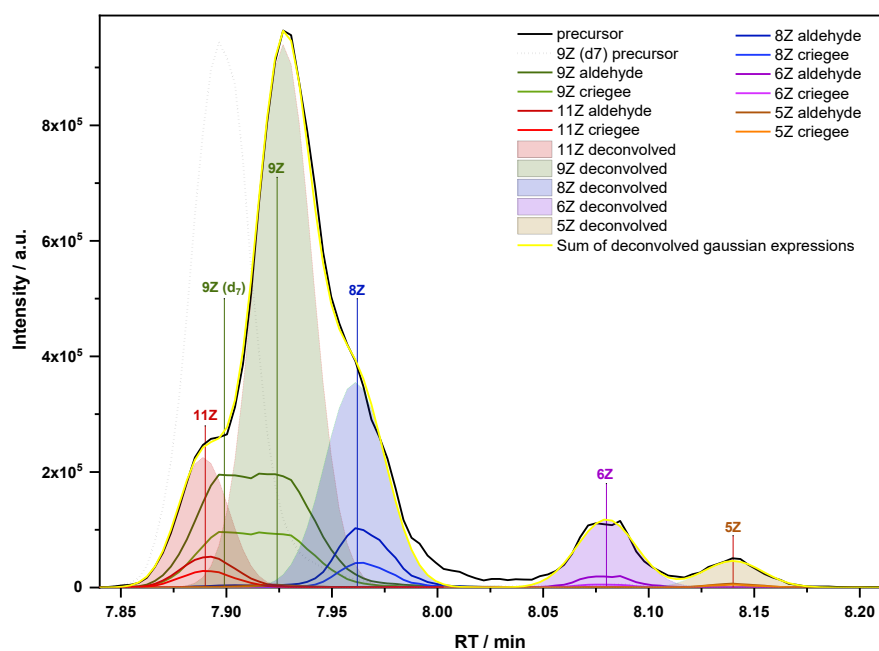


Figure S24: Deconvolution of the precursor chromatogram of octadecenoic acids in LNCaP TOFA. The chromatograms of the OzID fragments of FA 18:1 (9Z) were deconvolved separately, refer to Figure S25.

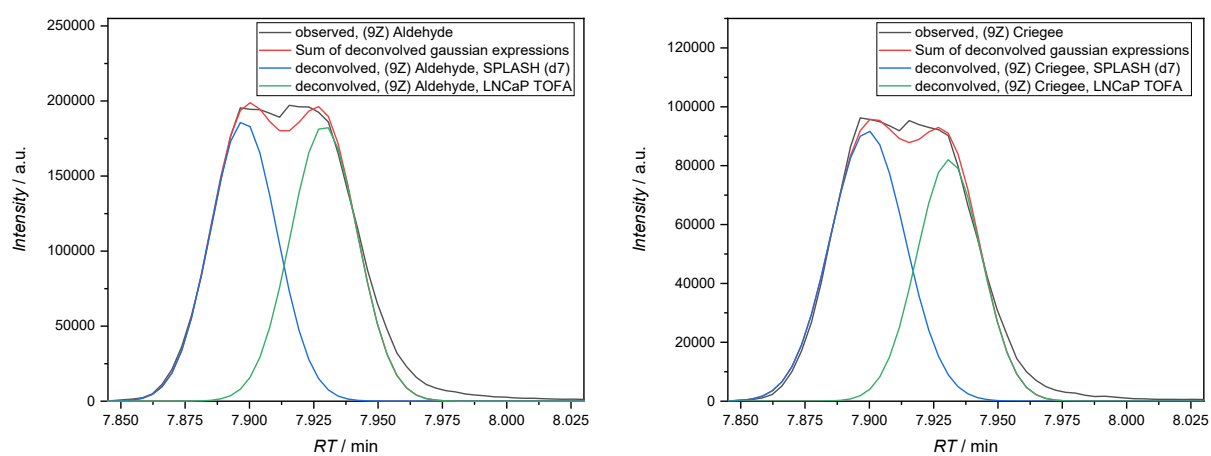


Figure S25: Deconvolution of OzID fragment chromatograms of FA 18:1 (9Z) in LNCaP TOFA.

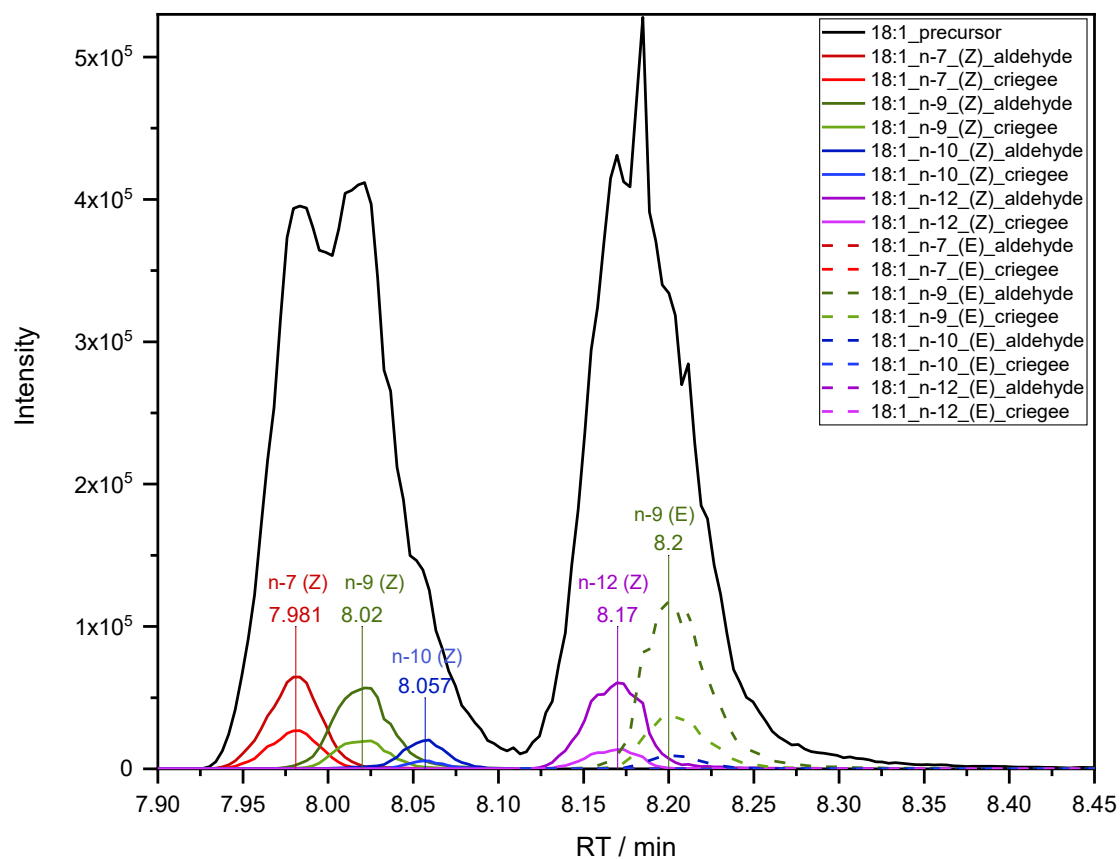


Figure S26: Extracted ion chromatograms for (AMPP-derivatized) octadecenoic acids (18:1 mix) prior to irradiation.

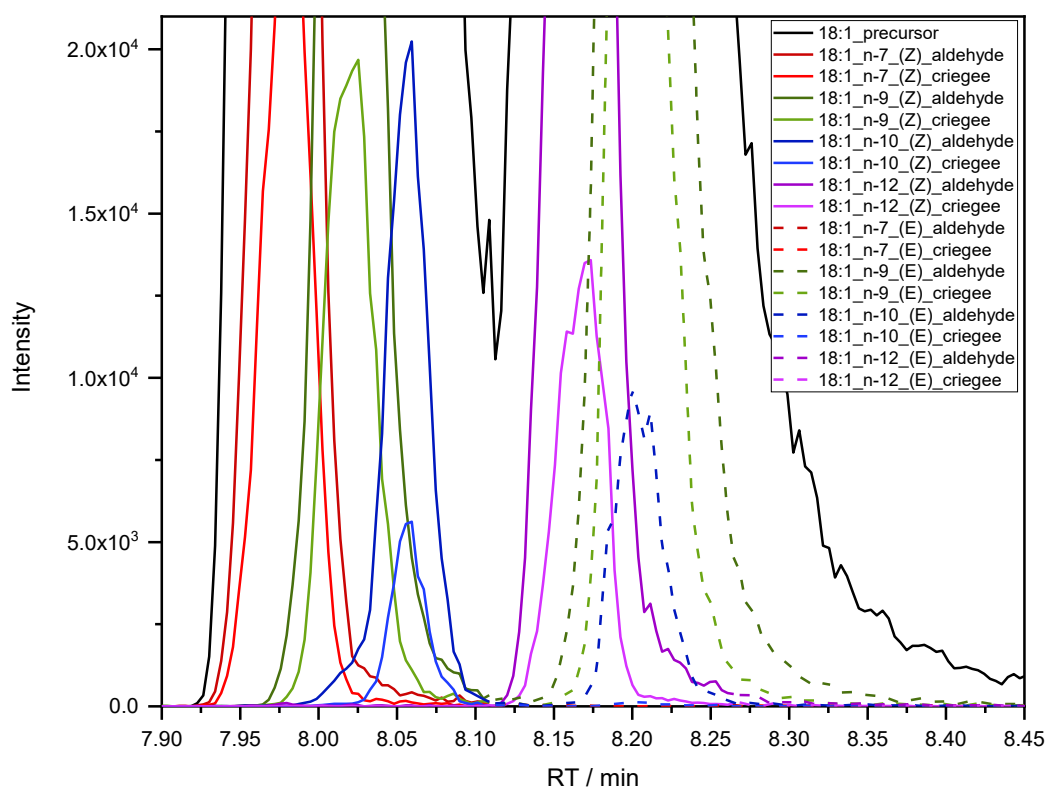


Figure S27: Expansion of the extracted ion chromatograms shown in Figure S26.

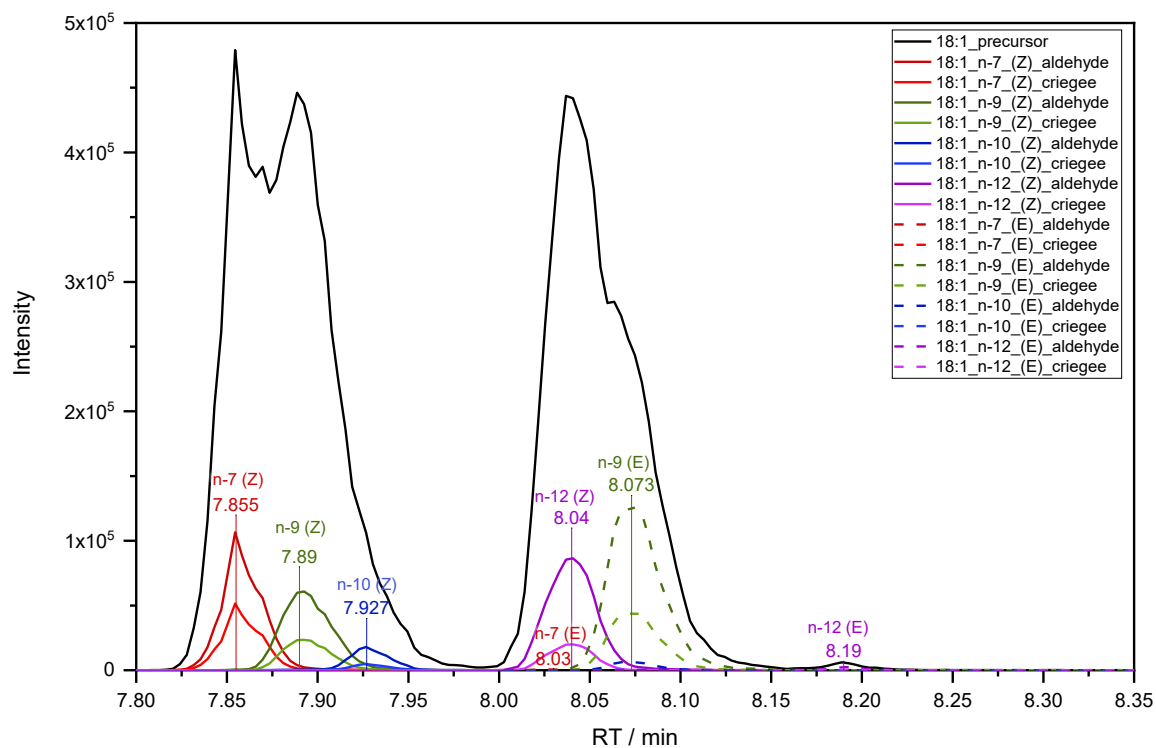


Figure S28: Extracted ion chromatograms for (AMPP-derivatized) octadecenoic acids (18:1 mix) after irradiation.

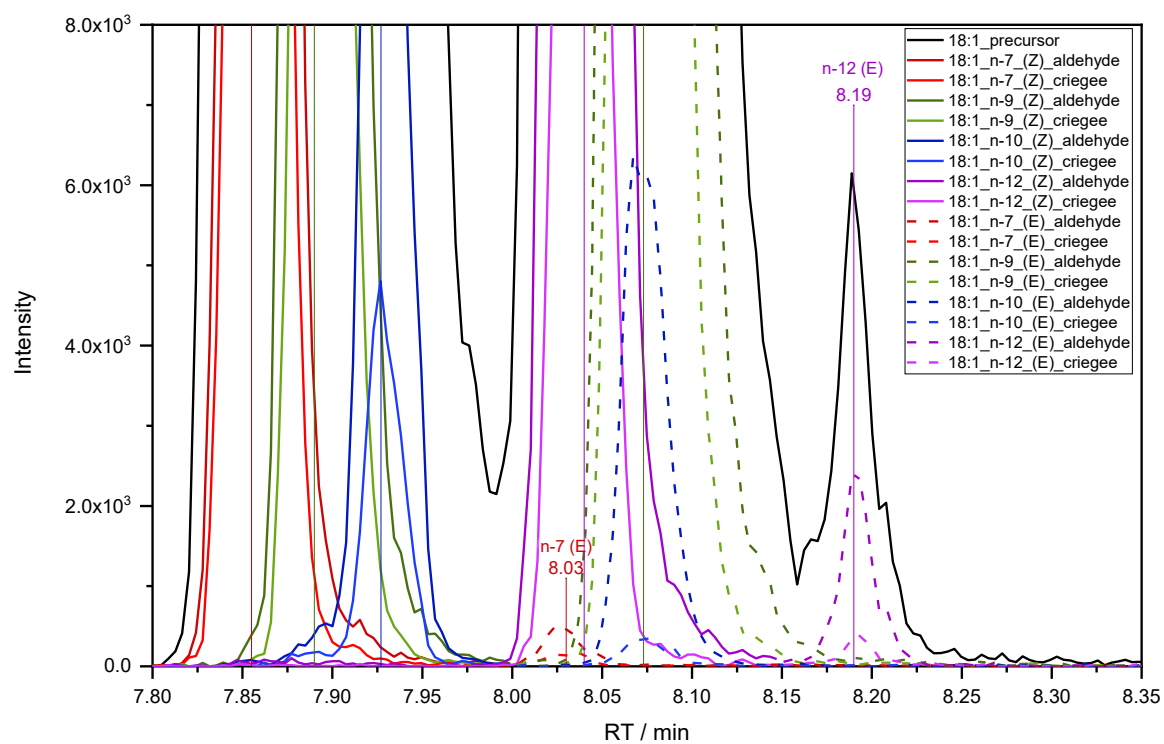


Figure S29: Expansion of the extracted ion chromatograms shown in Figure S28.

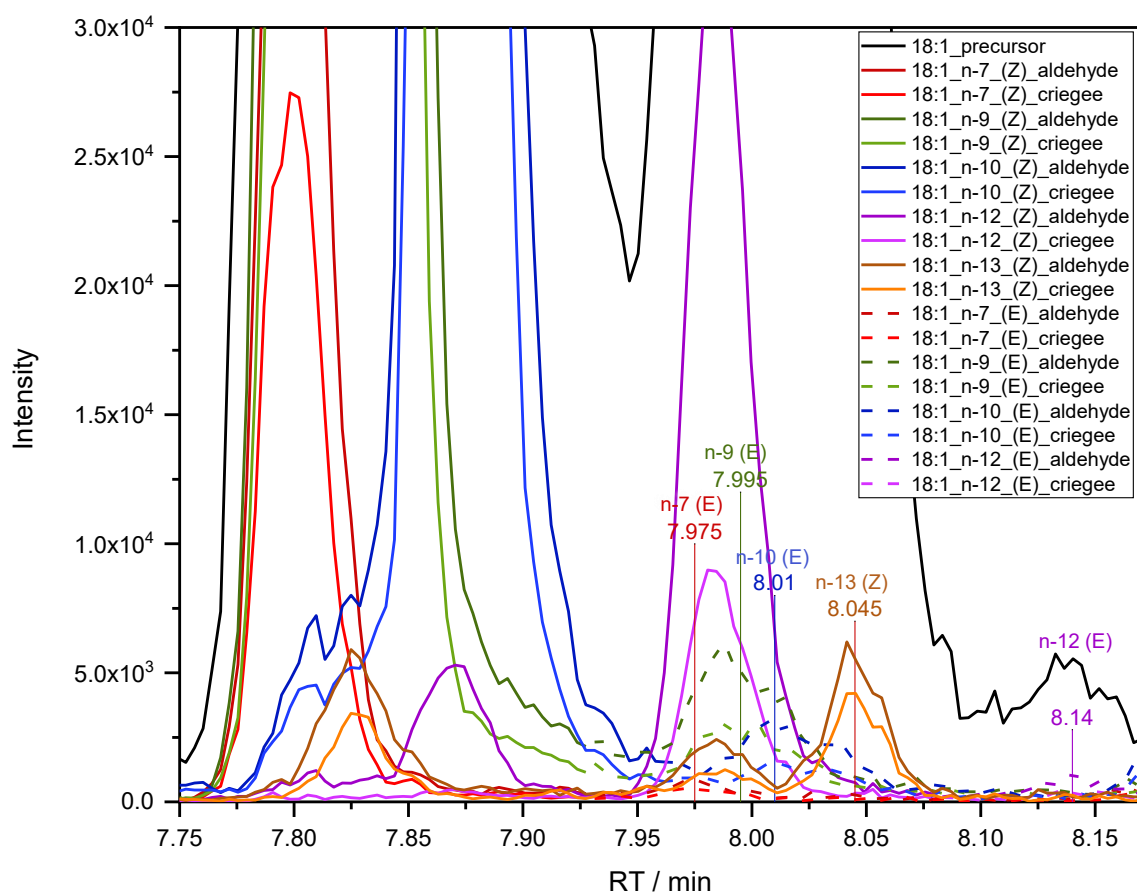


Figure S30: Expansion of extracted ion chromatograms with highlighted retention times for AMPP-derivatized octadecenoic acids that were identified in PC-3 as shown in Figure S22.

Note: The chromatogram of 18:1_n-13 shows features at 7.82 min and 7.98 min, which are not associated to this fatty acid species, but are artifacts partly due to isotopologue distributions of other features (e.g., +2 ^{13}C of another species).

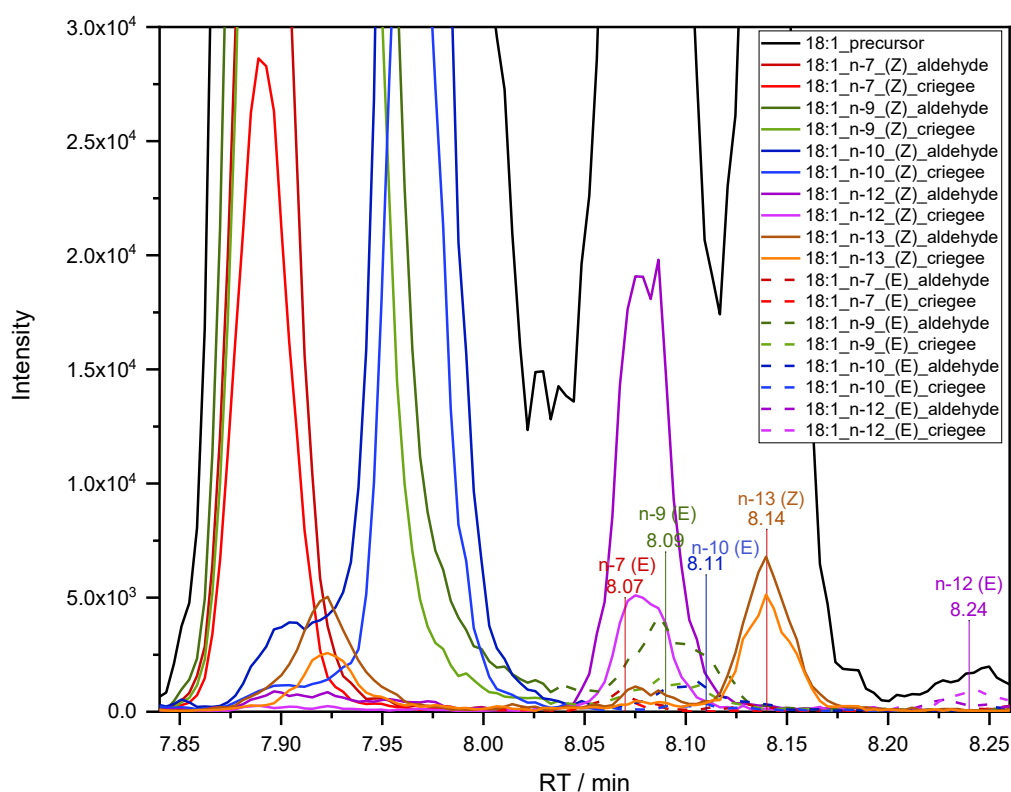


Figure S31: Expansion of extracted ion chromatograms with highlighted retention times for AMPP-derivatized octadecenoic acids that were identified in LNCaP TOFA as shown in Figure S24.

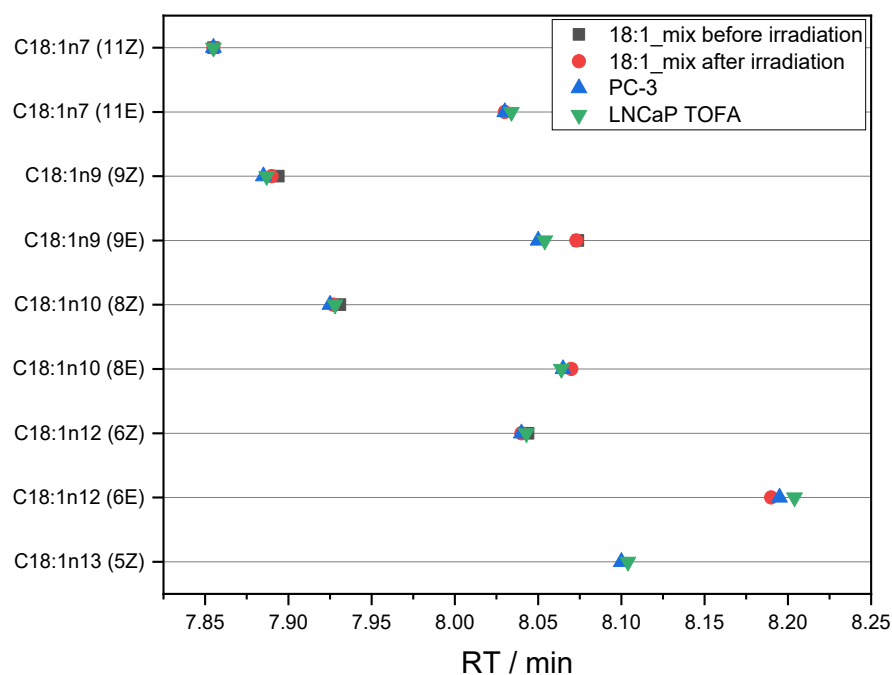


Figure S32: Comparison of relative retention times for fatty acid standards before and after photoinduced isomerization with fatty acids found in cancer cell lines PC-3 and LNCaP TOFA. Retention times of the datasets were shifted by addition or subtraction of a small value (0.055 min, -0.126 min and -0.026 min) to match the retention time for each. By comparison with the standards, the configuration of the fatty acids in the cancer cell lines are determined with high confidence.

Table S17. Relative amounts of octadecenoic acid (FA 18:1) isomers in PC-3 and LNCaP TOFA.

Isomer (<i>n</i> -nomenclature)	<i>n</i> -7 <i>Z</i>	<i>n</i> -7 <i>E</i>	<i>n</i> -9 <i>Z</i>	<i>n</i> -9 <i>E</i>	<i>n</i> -10 <i>Z</i>	<i>n</i> -10 <i>E</i>	<i>n</i> -12 <i>Z</i>	<i>n</i> -12 <i>E</i>	<i>n</i> -13 <i>Z</i>
Isomer (Δ -nomenclature)	11 <i>Z</i>	11 <i>E</i>	9 <i>Z</i>	9 <i>E</i>	8 <i>Z</i>	8 <i>E</i>	6 <i>Z</i>	6 <i>E</i>	5 <i>Z</i>
Relative quantity PC-3 / %	10.2	0.2	40.2	1.9	33.9	1.2	9.7	0.2	2.6
Relative quantity LNCaP TOFA / %	12.0	0.2	51.9	2.4	22.6	1.2	6.5	0.2	3.0

*Shaded columns - isomers also identified in cryogenic IR

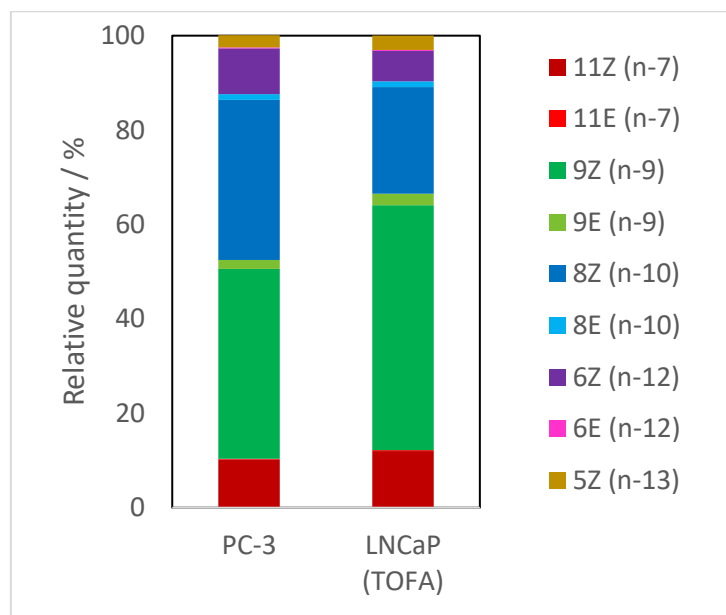


Figure S33: Relative quantification of octadecenoic acid isomers identified in PC-3 and LNCaP TOFA by LC-OzID-MS.

Establishing Carbon-Carbon Double Bond Position and Configuration in Unsaturated Fatty Acids by Gas-Phase Infrared Spectroscopy

Supplementary Information – xyz files

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Pyridylcarbinol esters

C18:1 6Z pyridylcarbinol ester

conf_33

C	-4.122687	-0.198372	0.118373
C	-3.821525	0.793615	1.203660
C	-3.395955	2.054650	1.041194
C	-3.169339	2.763004	-0.260975
C	-2.207600	3.946055	-0.162840
C	-0.757449	3.574681	0.130393
C	-0.062725	2.827963	-1.000941
C	1.388894	2.479767	-0.702192
C	2.103117	1.837466	-1.885633
C	3.566387	1.488842	-1.630038
C	3.769201	0.377023	-0.609893
C	5.224115	0.001073	-0.374975
C	5.393148	-1.124955	0.636950
C	6.846873	-1.498436	0.884822
H	7.412104	-0.643216	1.267293
H	6.937284	-2.309311	1.612162
H	7.330636	-1.826282	-0.040104
H	4.845121	-2.010314	0.284010
H	4.925226	-0.827504	1.586453
H	5.684919	-0.293188	-1.326377
H	5.776820	0.884568	-0.031102
H	3.224228	-0.516835	-0.950209
H	3.322097	0.667862	0.349728
H	4.033882	1.190496	-2.575419
H	4.101552	2.388024	-1.299102
H	2.041895	2.521815	-2.739595
H	1.559377	0.932388	-2.194624
H	1.927237	3.391322	-0.412260
H	1.433617	1.818245	0.174193
H	-0.105432	3.446021	-1.906704
H	-0.610041	1.908761	-1.253073
H	-0.194307	4.491096	0.339875
H	-0.702515	2.987729	1.059470
H	-2.572125	4.627574	0.614563
H	-2.245723	4.511162	-1.100393
H	-2.846705	2.061297	-1.039028
H	-4.143536	3.136926	-0.603805
H	-3.305680	2.674072	1.935844
H	-4.044219	0.459324	2.217994
C	-3.967807	-1.645928	0.583347
C	-4.151384	-2.699968	-0.505540
C	-3.089603	-2.666034	-1.608043
C	-1.709852	-2.807760	-1.038456
O	-1.381698	-3.537906	-0.144613
O	-0.827359	-1.947257	-1.623770
C	0.462175	-1.931122	-1.033466

C	0.436875	-1.179418	0.269767
C	1.427854	-1.309627	1.240844
C	1.349598	-0.592608	2.430397
C	0.271356	0.238412	2.648809
N	-0.667352	0.341769	1.698695
C	-0.608610	-0.318469	0.538186
H	-1.426703	-0.146484	-0.146364
H	-1.504778	0.925753	1.827514
H	0.125360	0.817710	3.551216
H	2.114133	-0.687477	3.190969
H	2.266448	-1.977869	1.073808
H	1.111219	-1.422970	-1.750181
H	0.829023	-2.946892	-0.869842
H	-3.244651	-3.507652	-2.292332
H	-3.138285	-1.759148	-2.214354
H	-5.134778	-2.588258	-0.973759
H	-4.134223	-3.688345	-0.039245
H	-2.987538	-1.789762	1.056500
H	-4.699336	-1.834081	1.376595
H	-3.510354	0.007195	-0.768971
H	-5.157679	-0.043961	-0.217642

conf_25

C	4.052358	0.698323	-0.675999
C	3.847181	0.414663	0.780128
C	3.892741	-0.783347	1.384018
C	4.133182	-2.125387	0.755191
C	2.836914	-2.898260	0.470254
C	2.045723	-2.303151	-0.685645
C	0.636697	-2.846538	-0.863031
C	-0.064146	-2.229995	-2.070313
C	-1.568373	-2.475412	-2.123961
C	-2.342924	-1.684252	-1.076767
C	-3.853345	-1.850484	-1.185566
C	-4.642380	-1.061484	-0.145099
C	-4.554857	0.451463	-0.309030
C	-5.355992	1.213500	0.736434
H	-6.419332	0.965630	0.672240
H	-5.040942	0.962767	1.757560
H	-5.265080	2.296575	0.613275
H	-4.911368	0.722555	-1.309723
H	-3.503469	0.766035	-0.285132
H	-5.697115	-1.356848	-0.189102
H	-4.299782	-1.343349	0.862637
H	-4.101752	-2.914484	-1.094843
H	-4.179177	-1.548972	-2.189353
H	-2.031101	-1.993518	-0.069360
H	-2.069642	-0.625797	-1.176606
H	-1.778487	-3.547334	-2.013838
H	-1.938657	-2.194315	-3.116361
H	0.110604	-1.144846	-2.076775
H	0.406605	-2.616082	-2.981487

H	0.055212	-2.647330	0.047683
H	0.660870	-3.938295	-0.966223
H	1.980681	-1.214667	-0.562804
H	2.612999	-2.452129	-1.613204
H	2.220813	-2.932677	1.383279
H	3.079905	-3.943270	0.252833
H	4.694903	-2.022510	-0.177900
H	4.763281	-2.710964	1.431496
H	3.795957	-0.791036	2.472892
H	3.709904	1.286061	1.422347
C	2.872702	1.392984	-1.368371
C	2.636897	2.836869	-0.937260
C	1.366539	3.445791	-1.553041
C	0.139597	2.771295	-1.020760
O	-0.496904	1.900018	-1.547942
O	-0.156300	3.221664	0.232383
C	-1.254319	2.591369	0.864246
C	-0.882408	1.249830	1.433016
C	-1.825755	0.415939	2.033390
C	-1.453459	-0.823176	2.540786
C	-0.139139	-1.227504	2.435350
N	0.745017	-0.404910	1.857771
C	0.419891	0.796887	1.371983
H	1.232018	1.362778	0.937154
H	1.729675	-0.684192	1.741858
H	0.232929	-2.180788	2.787144
H	-2.179441	-1.479829	3.002929
H	-2.862519	0.731485	2.095901
H	-2.083276	2.467991	0.161295
H	-1.564325	3.266003	1.665166
H	1.315736	4.511415	-1.318457
H	1.369751	3.319775	-2.637357
H	3.490709	3.449965	-1.242165
H	2.582525	2.932180	0.154419
H	3.051749	1.380976	-2.448858
H	1.963061	0.797008	-1.225519
H	4.273582	-0.228214	-1.209567
H	4.942563	1.333634	-0.777112

conf_0

C	-3.594100	-1.088716	-0.837327
C	-3.961727	-0.103492	0.232104
C	-4.002824	1.230900	0.102235
C	-3.739662	2.019047	-1.146273
C	-3.320111	3.464888	-0.883784
C	-2.014120	3.621180	-0.112280
C	-0.785794	3.072276	-0.825851
C	0.503164	3.277893	-0.042088
C	1.711964	2.584680	-0.653856
C	2.968024	2.717636	0.198199
C	4.209997	2.061948	-0.396404

C	4.098620	0.551573	-0.557930
C	5.385467	-0.115580	-1.022829
C	5.248483	-1.622315	-1.182315
H	4.482976	-1.876027	-1.924312
H	6.184367	-2.079127	-1.512739
H	4.970860	-2.098493	-0.234848
H	6.186342	0.109515	-0.308632
H	5.695645	0.329282	-1.975639
H	3.794655	0.111884	0.405352
H	3.300988	0.315848	-1.275629
H	5.071360	2.286937	0.243250
H	4.431551	2.514136	-1.371412
H	3.169550	3.782072	0.366293
H	2.775613	2.288657	1.192895
H	1.903634	2.993820	-1.654135
H	1.474137	1.523212	-0.806808
H	0.703017	4.352269	0.051207
H	0.368095	2.918775	0.988344
H	-0.695862	3.548484	-1.810103
H	-0.914649	2.001056	-1.036977
H	-1.854242	4.683837	0.101697
H	-2.111253	3.144247	0.876088
H	-4.123216	3.969479	-0.334438
H	-3.235703	3.986690	-1.843104
H	-3.005128	1.510873	-1.781366
H	-4.666181	2.029023	-1.735695
H	-4.357542	1.806153	0.958942
H	-4.276667	-0.531713	1.184278
C	-2.978641	-2.377423	-0.290526
C	-2.275858	-3.205322	-1.363610
C	-1.322516	-4.255317	-0.783942
C	-0.245753	-3.615947	0.042033
O	-0.042872	-3.776164	1.214232
O	0.492309	-2.739569	-0.698579
C	1.471084	-2.017490	0.035318
C	0.819688	-0.992029	0.923183
C	1.330265	-0.628765	2.167315
C	0.653345	0.282736	2.970397
C	-0.546615	0.802400	2.533229
N	-1.011090	0.445126	1.329092
C	-0.362574	-0.400311	0.520613
H	-0.830509	-0.614595	-0.430298
H	-1.937875	0.774908	1.013609
H	-1.155702	1.487228	3.108930
H	1.036148	0.567118	3.942197
H	2.251116	-1.079957	2.522684
H	2.105404	-1.537032	-0.711229
H	2.080619	-2.694256	0.637549
H	-1.845812	-4.962578	-0.138221
H	-0.850461	-4.816030	-1.596438
H	-1.704093	-2.547211	-2.027567
H	-3.014124	-3.707720	-1.995501

H	-2.267393	-2.132064	0.508926
H	-3.751046	-2.978466	0.201889
H	-2.913077	-0.622590	-1.561810
H	-4.492245	-1.334379	-1.419768

conf_6

C	-3.472216	-1.276245	-0.853961
C	-3.877239	-0.327545	0.232014
C	-3.901792	1.010223	0.147602
C	-3.572596	1.841195	-1.060059
C	-3.335498	3.313012	-0.729279
C	-2.117044	3.587963	0.146003
C	-0.776532	3.314608	-0.525473
C	0.410868	3.727242	0.336721
C	1.767888	3.594576	-0.345688
C	2.244000	2.163385	-0.562724
C	3.597480	2.104588	-1.262562
C	4.166800	0.702656	-1.450013
C	4.583514	0.011641	-0.156395
C	5.231289	-1.345961	-0.387687
H	4.568217	-2.023968	-0.936209
H	6.144109	-1.244540	-0.981504
H	5.505166	-1.832260	0.552808
H	3.715694	-0.096130	0.508250
H	5.282264	0.662482	0.383197
H	3.439581	0.078614	-1.991510
H	5.042791	0.760157	-2.106413
H	4.318271	2.709716	-0.697261
H	3.503295	2.587786	-2.241909
H	2.302493	1.662340	0.413059
H	1.510288	1.603233	-1.160178
H	2.520162	4.119717	0.254233
H	1.736582	4.117123	-1.310375
H	0.266935	4.771131	0.638803
H	0.414536	3.147723	1.272230
H	-0.737631	3.871115	-1.470754
H	-0.692292	2.256856	-0.807834
H	-2.139810	4.638638	0.456233
H	-2.194357	3.016524	1.085011
H	-4.230833	3.704916	-0.233162
H	-3.236515	3.876777	-1.663083
H	-2.715314	1.424249	-1.603843
H	-4.413467	1.770675	-1.762090
H	-4.292561	1.557476	1.006846
H	-4.228623	-0.785956	1.156667
C	-2.791390	-2.540232	-0.328955
C	-2.097396	-3.345393	-1.424280
C	-1.085574	-4.353300	-0.871488
C	-0.017454	-3.670104	-0.069636
O	0.247880	-3.853654	1.086617
O	0.630150	-2.725780	-0.810377
C	1.592278	-1.965795	-0.092197

C	0.916470	-1.016205	0.857793
C	1.412698	-0.727114	2.126857
C	0.729680	0.141156	2.971494
C	-0.466515	0.683931	2.552089
N	-0.925628	0.383659	1.330311
C	-0.269699	-0.415514	0.481748
H	-0.735192	-0.585722	-0.479625
H	-1.860477	0.707696	1.036948
H	-1.080758	1.337534	3.157834
H	1.104175	0.373366	3.960263
H	2.330389	-1.198364	2.463700
H	2.153156	-1.414188	-0.848848
H	2.275052	-2.619039	0.454198
H	-1.559916	-5.085353	-0.215596
H	-0.608210	-4.891971	-1.696006
H	-1.574788	-2.668576	-2.108953
H	-2.837818	-3.879354	-2.027083
H	-2.060579	-2.264223	0.442579
H	-3.523071	-3.166958	0.193017
H	-2.822581	-0.768400	-1.578765
H	-4.365318	-1.557598	-1.428520

conf_103

C	-1.744965	2.727184	-0.752883
C	-0.906316	3.282585	0.361968
C	0.408329	3.544782	0.322814
C	1.327302	3.379809	-0.848803
C	2.743674	2.952503	-0.465183
C	2.766424	1.628082	0.281821
C	4.146325	1.021110	0.481812
C	4.115270	-0.314145	1.225691
C	3.259424	-1.399292	0.570816
C	3.689777	-1.750233	-0.848020
C	2.846160	-2.836295	-1.510386
C	1.380987	-2.470329	-1.745085
C	1.172862	-1.209100	-2.577481
C	-0.264253	-1.027484	-3.044465
H	-0.394059	-0.093829	-3.599559
H	-0.567598	-1.845055	-3.705338
H	-0.973227	-1.021988	-2.209195
H	1.833232	-1.244926	-3.452312
H	1.491745	-0.328308	-2.005236
H	0.891512	-3.312428	-2.250198
H	0.865460	-2.358604	-0.780676
H	2.895010	-3.751836	-0.908180
H	3.297072	-3.087268	-2.477544
H	3.677022	-0.851654	-1.475447
H	4.735448	-2.079084	-0.825459
H	2.205339	-1.091441	0.568935
H	3.301364	-2.304210	1.190070
H	5.141260	-0.685365	1.327510
H	3.757722	-0.144248	2.250853

H	4.776695	1.725532	1.036333
H	4.627621	0.895292	-0.494608
H	2.307354	1.769134	1.272200
H	2.134134	0.913423	-0.262650
H	3.216555	3.732253	0.143940
H	3.345681	2.869097	-1.376274
H	0.909496	2.666585	-1.569534
H	1.372958	4.341301	-1.377215
H	0.852405	4.005613	1.206610
H	-1.446913	3.547430	1.271268
C	-2.978897	1.971322	-0.257771
C	-3.630928	1.116107	-1.341734
C	-4.586203	0.056058	-0.781781
C	-3.865871	-0.901189	0.120679
O	-4.042853	-1.060847	1.296975
O	-2.887889	-1.573589	-0.553427
C	-2.080381	-2.420950	0.249222
C	-1.176421	-1.613317	1.141289
C	-0.755029	-2.055786	2.392926
C	0.044377	-1.249163	3.195583
C	0.386768	0.010472	2.752524
N	-0.028713	0.410330	1.543996
C	-0.760411	-0.359787	0.732649
H	-1.022721	0.061840	-0.227375
H	0.177069	1.369020	1.222589
H	0.975125	0.715392	3.325220
H	0.375573	-1.580807	4.171343
H	-1.068832	-3.030462	2.753120
H	-1.494319	-3.015353	-0.455538
H	-2.699899	-3.084809	0.856096
H	-5.389880	0.507370	-0.197500
H	-5.033041	-0.510204	-1.604405
H	-2.859935	0.610898	-1.934451
H	-4.181440	1.752025	-2.041233
H	-2.702277	1.338598	0.595669
H	-3.708179	2.679854	0.150190
H	-1.138489	2.077353	-1.398089
H	-2.063162	3.549377	-1.407488

conf_57

C	-0.647099	2.580097	-1.457998
C	0.145060	3.295301	-0.402193
C	1.479614	3.297761	-0.270184
C	2.473048	2.648936	-1.184323
C	3.783053	2.262833	-0.499089
C	3.664588	1.157530	0.546023
C	3.160346	-0.165982	-0.013994
C	3.286052	-1.343056	0.946727
C	2.760664	-2.645775	0.347219
C	1.234498	-2.735164	0.335753
C	0.658030	-3.623810	-0.763563
C	0.779390	-3.039650	-2.170400

C	0.041506	-1.719614	-2.370707
C	0.077601	-1.235880	-3.812978
H	1.107560	-1.095236	-4.155355
H	-0.394094	-1.960987	-4.482457
H	-0.446150	-0.283140	-3.937542
H	0.488721	-0.948262	-1.728281
H	-0.999532	-1.833494	-2.039661
H	1.835223	-2.903779	-2.435388
H	0.388150	-3.771179	-2.886698
H	-0.403454	-3.819043	-0.560322
H	1.151088	-4.602364	-0.732287
H	0.893430	-3.088238	1.317528
H	0.819213	-1.727602	0.222670
H	3.164769	-3.503235	0.894701
H	3.148059	-2.734646	-0.674609
H	4.340942	-1.458601	1.219315
H	2.755726	-1.125947	1.886341
H	3.728345	-0.400279	-0.923945
H	2.117772	-0.065396	-0.345632
H	4.650076	0.999238	0.998440
H	3.021118	1.490282	1.375059
H	4.216258	3.156867	-0.035621
H	4.497347	1.943878	-1.265814
H	2.030934	1.786972	-1.696352
H	2.701197	3.369686	-1.981218
H	1.903022	3.917514	0.522161
H	-0.433507	3.907606	0.290410
C	-2.084931	2.285773	-1.025368
C	-2.757423	1.202608	-1.865029
C	-4.005848	0.613438	-1.198113
C	-3.663689	-0.023543	0.116092
O	-4.023618	0.326204	1.205995
O	-2.800297	-1.067817	-0.052481
C	-2.339676	-1.663910	1.148925
C	-1.342962	-0.782189	1.849872
C	-1.113434	-0.843727	3.221588
C	-0.175596	-0.007641	3.819287
C	0.502070	0.907073	3.041938
N	0.259548	0.948613	1.725018
C	-0.608199	0.132376	1.118783
H	-0.712008	0.241580	0.048402
H	0.705155	1.675799	1.140166
H	1.223202	1.615223	3.429071
H	0.011141	-0.045547	4.884919
H	-1.678565	-1.540760	3.832499
H	-1.863658	-2.599371	0.845411
H	-3.175137	-1.882654	1.817751
H	-4.755639	1.381077	-0.999501
H	-4.450365	-0.144828	-1.849449
H	-2.051056	0.387783	-2.058979
H	-3.035441	1.602283	-2.844736
H	-2.092304	1.989158	0.031585

H	-2.677507	3.206602	-1.055487
H	-0.139229	1.649030	-1.745010
H	-0.656308	3.183911	-2.374935

conf_84

C	-2.380127	0.304055	-2.497221
C	-3.254418	1.221198	-1.690192
C	-2.990150	2.498359	-1.374534
C	-1.809820	3.303633	-1.819726
C	-1.265033	4.270674	-0.767551
C	-0.732203	3.607859	0.499034
C	0.364283	2.579430	0.255588
C	0.940162	1.989297	1.537610
C	1.895924	0.822262	1.309817
C	3.184666	1.184327	0.583688
C	4.118846	-0.005267	0.410125
C	5.411941	0.339741	-0.314678
C	6.344867	-0.851182	-0.489501
C	7.634037	-0.494296	-1.214176
H	8.285397	-1.364852	-1.326465
H	7.429076	-0.101642	-2.215297
H	8.194664	0.271044	-0.668247
H	5.819807	-1.642859	-1.039388
H	6.580727	-1.271500	0.496311
H	5.175123	0.762444	-1.300453
H	5.935567	1.132424	0.235881
H	3.596285	-0.799728	-0.141904
H	4.357619	-0.426455	1.396212
H	2.954851	1.604891	-0.402972
H	3.700546	1.977377	1.140471
H	1.382329	0.037853	0.733138
H	2.150030	0.372235	2.278170
H	1.456148	2.778243	2.098436
H	0.116825	1.662305	2.188398
H	1.163996	3.046166	-0.330672
H	-0.016407	1.764081	-0.377404
H	-0.349360	4.385888	1.169151
H	-1.562741	3.142603	1.050959
H	-2.050014	4.986065	-0.496275
H	-0.464018	4.860625	-1.225938
H	-1.014145	2.652738	-2.194098
H	-2.133507	3.893061	-2.688276
H	-3.753568	3.048448	-0.821189
H	-4.217203	0.810249	-1.383103
C	-2.610378	-1.178776	-2.194215
C	-1.439624	-2.061637	-2.621299
C	-1.463947	-3.454462	-1.981617
C	-1.385343	-3.367757	-0.486259
O	-2.227426	-3.699117	0.302037
O	-0.217383	-2.786318	-0.083436
C	-0.110033	-2.573018	1.315881
C	-1.019032	-1.458934	1.759628

C	-1.557556	-1.379239	3.041220
C	-2.419668	-0.341519	3.381940
C	-2.757880	0.593690	2.427054
N	-2.222024	0.496099	1.203291
C	-1.365114	-0.469473	0.859247
H	-0.988071	-0.442350	-0.152726
H	-2.496900	1.158255	0.457917
H	-3.443508	1.413526	2.598048
H	-2.849065	-0.272179	4.373258
H	-1.318696	-2.142270	3.775432
H	0.935153	-2.306821	1.490556
H	-0.348480	-3.486066	1.865773
H	-2.381683	-3.992337	-2.225301
H	-0.613506	-4.040767	-2.342010
H	-0.491547	-1.577238	-2.359469
H	-1.430564	-2.173564	-3.709485
H	-2.797203	-1.309585	-1.120607
H	-3.532710	-1.519788	-2.676708
H	-1.324276	0.558360	-2.335332
H	-2.550741	0.488114	-3.565823

conf_90

C	-1.252380	-2.598865	-1.451802
C	-1.529739	-2.520501	0.021880
C	-2.688622	-2.168799	0.597670
C	-3.962622	-1.823112	-0.107300
C	-4.770902	-0.704435	0.550781
C	-4.016695	0.613233	0.708917
C	-3.328143	1.092781	-0.562446
C	-2.758832	2.502947	-0.473019
C	-2.078142	2.957891	-1.762444
C	-0.745306	2.277538	-2.070725
C	0.410798	2.745858	-1.194821
C	1.747725	2.132823	-1.588589
C	2.937224	2.725942	-0.846155
C	4.268879	2.133243	-1.284476
H	4.280317	1.043758	-1.173690
H	4.459488	2.348760	-2.339866
H	5.105017	2.545094	-0.712499
H	2.796822	2.591125	0.236081
H	2.950821	3.811233	-1.001132
H	1.724204	1.044169	-1.436070
H	1.899916	2.274079	-2.666347
H	0.205401	2.533580	-0.135585
H	0.484162	3.838868	-1.265598
H	-0.845809	1.185170	-2.003270
H	-0.483195	2.480364	-3.115388
H	-1.914591	4.041098	-1.723701
H	-2.771677	2.789066	-2.594580
H	-3.574000	3.195172	-0.233177
H	-2.052791	2.578357	0.366095
H	-4.052415	1.061460	-1.386793

H	-2.536819	0.385700	-0.845586
H	-4.713994	1.382906	1.058889
H	-3.284949	0.510556	1.526960
H	-5.127761	-1.036855	1.532297
H	-5.666948	-0.529613	-0.054153
H	-3.765076	-1.578971	-1.154812
H	-4.585652	-2.727032	-0.130475
H	-2.752900	-2.239736	1.685654
H	-0.730687	-2.864807	0.680750
C	0.215228	-2.372232	-1.818223
C	1.148657	-3.503866	-1.373383
C	2.573048	-3.026598	-1.072944
C	2.594932	-2.281090	0.228136
O	2.234768	-2.718305	1.289403
O	3.014387	-0.996663	0.090304
C	3.094721	-0.239781	1.287731
C	1.769596	0.331607	1.709950
C	1.685488	1.369060	2.637437
C	0.449378	1.860852	3.044005
C	-0.700257	1.307658	2.522434
N	-0.590108	0.315366	1.628957
C	0.582719	-0.171312	1.214930
H	0.518077	-0.969582	0.493379
H	-1.429602	-0.129399	1.238134
H	-1.701454	1.623904	2.783992
H	0.375724	2.667730	3.761790
H	2.593593	1.799806	3.048713
H	3.799613	0.566496	1.081254
H	3.484202	-0.864328	2.098214
H	3.236733	-3.888017	-0.950079
H	2.970378	-2.400301	-1.874092
H	1.186329	-4.271358	-2.150816
H	0.765079	-3.999985	-0.476175
H	0.298000	-2.243181	-2.901812
H	0.549663	-1.410947	-1.404958
H	-1.880995	-1.885563	-1.993772
H	-1.555228	-3.591629	-1.813414

conf_75

C	-2.775077	1.219575	0.090204
C	-2.391022	2.429291	0.882981
C	-1.726492	3.502967	0.446975
C	-1.190212	3.763186	-0.926558
C	0.274566	4.206825	-0.918487
C	1.206375	3.152644	-0.339080
C	2.679622	3.535834	-0.305917
C	3.556691	2.496448	0.387246
C	3.712254	1.183738	-0.373396
C	4.438024	0.112259	0.430626
C	4.586028	-1.226111	-0.285411
C	3.267582	-1.943758	-0.548564
C	3.440975	-3.330365	-1.153098

C	2.119031	-4.026436	-1.437809
H	1.528634	-4.143724	-0.521323
H	1.522108	-3.455428	-2.158178
H	2.269496	-5.023405	-1.858595
H	4.043513	-3.945898	-0.474961
H	4.018784	-3.248761	-2.081027
H	2.713403	-2.033372	0.398549
H	2.640541	-1.343011	-1.222052
H	5.227892	-1.880712	0.315445
H	5.113328	-1.076417	-1.235951
H	5.430239	0.488698	0.704269
H	3.910981	-0.048288	1.383683
H	4.257946	1.371280	-1.306670
H	2.731625	0.804429	-0.687860
H	4.551548	2.917960	0.566205
H	3.146242	2.295880	1.390433
H	2.777582	4.495574	0.213171
H	3.038776	3.702969	-1.328562
H	0.874204	2.954836	0.695100
H	1.076053	2.230347	-0.928727
H	0.373996	5.131196	-0.336961
H	0.587405	4.448998	-1.939655
H	-1.308155	2.884914	-1.571434
H	-1.790615	4.557188	-1.387853
H	-1.569091	4.314201	1.158471
H	-2.743454	2.441177	1.913640
C	-4.258040	1.198835	-0.290070
C	-4.669974	-0.004783	-1.133427
C	-4.714893	-1.338902	-0.385414
C	-3.404874	-1.948055	0.011373
O	-3.148987	-2.446092	1.077624
O	-2.495637	-1.933609	-0.996735
C	-1.265002	-2.586161	-0.694396
C	-0.478416	-1.817162	0.333002
C	-0.241686	-2.307805	1.615787
C	0.447223	-1.543429	2.551417
C	0.864886	-0.278065	2.202704
N	0.615013	0.174303	0.966114
C	-0.018527	-0.549903	0.035126
H	-0.160627	-0.077235	-0.928227
H	0.900332	1.123041	0.717311
H	1.384849	0.395727	2.871278
H	0.638395	-1.913884	3.550319
H	-0.621122	-3.287236	1.885198
H	-0.726334	-2.632989	-1.640895
H	-1.451517	-3.600965	-0.338011
H	-5.310923	-1.262986	0.526754
H	-5.202270	-2.087331	-1.022735
H	-4.016478	-0.094602	-2.007775
H	-5.676543	0.174931	-1.522021
H	-4.870810	1.243313	0.618569
H	-4.478865	2.113358	-0.850073

H	-2.545974	0.327973	0.688165
H	-2.187446	1.151748	-0.831811

conf_94

C	-4.064790	0.928569	-0.294812
C	-3.537939	1.817040	0.794511
C	-2.832386	2.946755	0.632541
C	-2.445412	3.590107	-0.664564
C	-1.074693	4.266679	-0.639352
C	0.041719	3.301788	-0.271153
C	1.453463	3.841149	-0.453579
C	2.528418	2.903391	0.090517
C	2.592787	1.545437	-0.598622
C	3.629734	0.607387	0.002188
C	3.673745	-0.751248	-0.685050
C	4.516296	-1.794884	0.043632
C	5.984589	-1.418670	0.236414
C	6.728423	-1.162051	-1.066769
H	6.657183	-2.023476	-1.739038
H	6.332814	-0.292426	-1.600463
H	7.788942	-0.973970	-0.882501
H	6.479069	-2.229504	0.782091
H	6.059244	-0.536690	0.883574
H	4.072118	-1.987578	1.031110
H	4.463039	-2.742653	-0.507112
H	4.038476	-0.626563	-1.711351
H	2.647508	-1.131954	-0.787591
H	4.617549	1.080185	-0.042217
H	3.417220	0.469708	1.072840
H	2.803433	1.690020	-1.666428
H	1.612201	1.051705	-0.555699
H	3.506944	3.389249	0.007018
H	2.362477	2.755590	1.168202
H	1.534168	4.811455	0.049814
H	1.633376	4.033906	-1.518563
H	-0.075770	3.015432	0.785005
H	-0.078298	2.385573	-0.865420
H	-1.085332	5.105121	0.067495
H	-0.878237	4.700617	-1.625456
H	-2.479606	2.860149	-1.481627
H	-3.210286	4.339713	-0.907099
H	-2.580473	3.512437	1.531174
H	-3.816810	1.535495	1.810604
C	-4.198092	-0.538401	0.119251
C	-4.359539	-1.476675	-1.075339
C	-4.075888	-2.944450	-0.738954
C	-2.667321	-3.136317	-0.260175
O	-2.318112	-3.529782	0.818640
O	-1.762729	-2.746529	-1.205594
C	-0.406339	-2.801518	-0.788024
C	-0.116693	-1.724609	0.222642
C	0.817517	-1.872625	1.245562

C	1.006100	-0.860849	2.180054
C	0.235868	0.280139	2.100645
N	-0.650286	0.398974	1.104275
C	-0.823904	-0.539374	0.167868
H	-1.558514	-0.328353	-0.596759
H	-1.264438	1.226368	1.051967
H	0.295410	1.100961	2.803380
H	1.726180	-0.964961	2.981487
H	1.391106	-2.790705	1.323290
H	0.184307	-2.652669	-1.694749
H	-0.171570	-3.779542	-0.362569
H	-4.735450	-3.312589	0.048751
H	-4.225992	-3.562598	-1.629377
H	-3.685402	-1.170868	-1.883490
H	-5.372628	-1.397298	-1.480387
H	-3.320182	-0.836557	0.706843
H	-5.042982	-0.656437	0.806522
H	-3.430258	1.008649	-1.186937
H	-5.045791	1.302091	-0.617233

conf_153

C	5.282474	-1.854672	0.832360
C	5.381660	-0.505658	1.474395
C	5.449829	0.684346	0.875199
C	5.445394	0.987344	-0.590932
C	4.452451	2.092960	-0.957336
C	2.999553	1.704042	-0.724381
C	2.015611	2.832841	-0.993041
C	0.563184	2.420659	-0.794212
C	-0.415476	3.579302	-0.936594
C	-1.882973	3.187897	-0.799014
C	-2.266107	2.661213	0.579215
C	-3.756868	2.373880	0.712284
C	-4.130562	1.657573	2.005149
C	-5.617332	1.342684	2.118881
H	-5.999657	0.755574	1.268079
H	-5.850500	0.791835	3.033220
H	-6.211017	2.260623	2.122514
H	-3.832619	2.277228	2.857372
H	-3.527266	0.742326	2.114820
H	-4.318047	3.313276	0.644216
H	-4.097820	1.790172	-0.159640
H	-1.973211	3.392871	1.342340
H	-1.686007	1.758202	0.816849
H	-2.510436	4.056646	-1.031184
H	-2.130109	2.432707	-1.561663
H	-0.264944	4.055613	-1.912493
H	-0.176808	4.345553	-0.187772
H	0.309189	1.643574	-1.531832
H	0.458263	1.951489	0.191612
H	2.152413	3.212682	-2.013931
H	2.244362	3.673399	-0.325046

H	2.752372	0.839649	-1.357625
H	2.879751	1.365713	0.312622
H	4.593710	2.371443	-2.008127
H	4.684849	2.990987	-0.370010
H	6.451964	1.313501	-0.883477
H	5.231661	0.088955	-1.179507
H	5.532527	1.560888	1.518858
H	5.404632	-0.519160	2.564248
C	3.973010	-2.572633	1.172981
C	2.769141	-1.874281	0.559892
C	1.439744	-2.532192	0.951061
C	0.311396	-1.809355	0.295669
O	-0.333523	-0.901252	0.758921
O	0.096868	-2.257224	-0.968055
C	-0.852316	-1.511237	-1.721541
C	-2.255317	-1.763328	-1.238718
C	-2.931957	-2.950580	-1.506030
C	-4.216009	-3.164176	-1.008532
C	-4.807516	-2.183897	-0.245806
N	-4.131557	-1.047027	-0.004571
C	-2.896347	-0.812951	-0.464261
H	-2.436375	0.125360	-0.183517
H	-4.569415	-0.325010	0.566616
H	-5.797934	-2.263570	0.183599
H	-4.753568	-4.081974	-1.209894
H	-2.450711	-3.718805	-2.103496
H	-0.735485	-1.854650	-2.749677
H	-0.618939	-0.445335	-1.666935
H	1.431787	-3.580486	0.640230
H	1.292770	-2.476461	2.031601
H	2.865627	-1.875297	-0.532174
H	2.757682	-0.826827	0.875129
H	4.020620	-3.609029	0.818777
H	3.856310	-2.619352	2.263292
H	6.118776	-2.471893	1.181771
H	5.387745	-1.784096	-0.254818

conf_189

C	-4.408347	0.616049	1.497084
C	-5.054809	0.834061	0.163791
C	-4.479023	1.275546	-0.956375
C	-3.033985	1.631757	-1.122055
C	-2.728934	3.118388	-0.910727
C	-1.248187	3.438293	-1.099310
C	-0.352163	2.869121	-0.002722
C	1.127713	2.878124	-0.362553
C	2.001357	2.180512	0.673083
C	3.439482	1.957627	0.216080
C	4.236387	1.015280	1.110687
C	5.599740	0.642379	0.545377
C	6.373327	-0.336246	1.418854
C	7.725908	-0.714696	0.834795

H	7.619076	-1.184893	-0.148635
H	8.361258	0.167105	0.709223
H	8.258573	-1.416121	1.481406
H	5.769680	-1.241131	1.574764
H	6.510542	0.103905	2.413539
H	5.478751	0.212325	-0.462110
H	6.195735	1.551818	0.399693
H	3.655452	0.098114	1.300139
H	4.359145	1.475439	2.097869
H	3.453783	1.586276	-0.828324
H	3.958392	2.919536	0.136730
H	1.541829	1.216651	0.943481
H	2.002984	2.753264	1.606971
H	1.258836	2.388457	-1.341991
H	1.475654	3.906571	-0.515062
H	-0.651682	1.838996	0.232895
H	-0.509397	3.430249	0.926371
H	-0.925458	3.045809	-2.075041
H	-1.106519	4.523173	-1.154212
H	-3.052974	3.410800	0.095135
H	-3.327022	3.712321	-1.609759
H	-2.429978	1.043927	-0.425892
H	-2.712409	1.364086	-2.139323
H	-5.116332	1.434209	-1.824421
H	-6.128733	0.648278	0.137138
C	-4.866271	-0.673782	2.181639
C	-4.454323	-1.978667	1.505905
C	-2.962731	-2.344656	1.655790
C	-2.082415	-1.722771	0.622281
O	-1.353734	-0.769793	0.759710
O	-2.180382	-2.370906	-0.563261
C	-1.482376	-1.770588	-1.649481
C	0.010471	-1.851902	-1.472174
C	0.705408	-3.055537	-1.554053
C	2.082628	-3.097001	-1.344525
C	2.749303	-1.928961	-1.054639
N	2.053828	-0.780596	-0.986455
C	0.731684	-0.708565	-1.176834
H	0.273088	0.265186	-1.061160
H	2.553153	0.080628	-0.757357
H	3.813960	-1.863212	-0.868631
H	2.633885	-4.026792	-1.403492
H	0.165415	-3.971480	-1.773501
H	-1.795419	-0.731086	-1.762904
H	-1.792537	-2.334456	-2.529735
H	-2.590932	-2.039578	2.636196
H	-2.851659	-3.428558	1.563395
H	-4.728159	-1.966610	0.445156
H	-5.025845	-2.793820	1.958090
H	-4.506011	-0.680371	3.217020
H	-5.960645	-0.659134	2.245016
H	-4.692616	1.452367	2.149812

H -3.317802 0.654931 1.425608

C18:1 6*E*pyridylcarbinol ester

conf_14

C -3.590861 1.240182 -0.940060
C -2.694809 2.424697 -0.739707
C -2.229799 2.904176 0.417591
C -1.430093 4.166092 0.558313
C 0.053825 3.930670 0.863498
H 0.147910 3.230997 1.712802
C 0.841316 3.435365 -0.344940
C 2.258663 2.980214 -0.028853
C 3.011837 2.490122 -1.258245
C 4.405763 1.944573 -0.960217
C 4.444621 0.679641 -0.104259
C 3.723239 -0.514213 -0.718567
C 3.951747 -1.813673 0.040297
C 3.281683 -3.020252 -0.602318
C 3.428670 -4.296021 0.212908
H 2.934746 -5.145372 -0.266629
H 4.482320 -4.559463 0.341830
H 3.004329 -4.182845 1.217575
H 2.217124 -2.799360 -0.764271
H 3.701178 -3.172544 -1.603644
H 3.597828 -1.702034 1.075429
H 5.029346 -2.003322 0.119859
H 2.642550 -0.316823 -0.776698
H 4.056730 -0.640152 -1.757229
H 4.038176 0.880051 0.896656
H 5.494081 0.408242 0.058396
H 4.998140 2.726262 -0.469933
H 4.910581 1.735842 -1.910681
H 2.414035 1.724215 -1.770304
H 3.099830 3.318891 -1.970000
H 2.231828 2.183703 0.727693
H 2.813503 3.803917 0.437237
H 0.297865 2.621366 -0.851056
H 0.874703 4.239699 -1.089339
H 0.505549 4.859430 1.226488
H -1.512810 4.759012 -0.358937
H -1.870177 4.768642 1.360009
H -2.488877 2.394356 1.347777
H -2.454767 2.977330 -1.649185
C -4.006298 0.487067 0.314988
C -4.969103 -0.670625 0.058895
C -4.425604 -1.755048 -0.877705
C -3.132434 -2.307584 -0.363177
O -2.928977 -2.728482 0.743297
O -2.140291 -2.242550 -1.295352
C -0.877524 -2.703191 -0.836094

C -0.287950 -1.741605 0.158980
C -0.497400 -0.384621 0.002532
N -0.004403 0.477758 0.897979
C 0.719854 0.104091 1.961510
C 0.972854 -1.235806 2.159089
C 0.458386 -2.160720 1.258010
H 0.626940 -3.220512 1.418539
H 1.549809 -1.549994 3.019305
H 1.064514 0.891494 2.618938
H -0.219982 1.466264 0.756038
H -1.076315 0.044341 -0.805354
H -0.249019 -2.768914 -1.726994
H -0.967560 -3.693868 -0.385969
H -5.136650 -2.586402 -0.920367
H -4.288067 -1.392262 -1.897432
H -5.226575 -1.133414 1.015251
H -5.901884 -0.290088 -0.369480
H -3.122054 0.105830 0.844407
H -4.485036 1.185445 1.009535
H -4.491722 1.595731 -1.459857
H -3.120647 0.559070 -1.664638

conf_0

C -2.675046 1.454937 -0.076295
C -1.792678 2.655406 -0.179278
C -1.093694 3.180269 0.828192
C -0.196242 4.373346 0.747843
C 1.283406 4.014202 0.928313
H 1.399034 3.383009 1.823694
C 1.902234 3.328611 -0.283835
C 3.336115 2.867760 -0.051392
C 3.997599 2.218982 -1.265784
C 3.414720 0.871236 -1.686668
C 3.597069 -0.233375 -0.653754
C 3.039597 -1.581121 -1.091199
C 2.997865 -2.606609 0.032190
C 2.391584 -3.942924 -0.372109
C 2.269166 -4.917489 0.789249
H 1.641251 -4.507144 1.588830
H 1.830423 -5.867951 0.475513
H 3.248326 -5.134294 1.226233
H 1.401740 -3.772429 -0.817564
H 2.997772 -4.389993 -1.168323
H 2.427880 -2.193736 0.877808
H 4.012500 -2.769705 0.416616
H 2.024993 -1.445994 -1.496223
H 3.632187 -1.969639 -1.928141
H 3.126985 0.054824 0.296245
H 4.664179 -0.339371 -0.422028
H 3.889018 0.560258 -2.624369
H 2.346780 0.979527 -1.928314
H 3.940404 2.914852 -2.110894

H	5.065330	2.086419	-1.056847
H	3.375268	2.185896	0.809944
H	3.929363	3.738926	0.248160
H	1.266125	2.491722	-0.619431
H	1.880011	4.022961	-1.133217
H	1.854612	4.923263	1.143186
H	-0.334752	4.882581	-0.212133
H	-0.485524	5.087090	1.527196
H	-1.183648	2.717238	1.814915
H	-1.736125	3.132517	-1.159269
C	-4.115045	1.692963	-0.529121
C	-4.993755	0.447319	-0.446969
C	-4.478322	-0.739086	-1.268821
C	-3.398447	-1.510000	-0.569630
O	-3.411733	-1.864413	0.579693
O	-2.349546	-1.793427	-1.387362
C	-1.300362	-2.533998	-0.769381
C	-0.603254	-1.710045	0.280057
C	-0.057538	-0.486073	-0.061045
N	0.497844	0.288037	0.879291
C	0.581256	-0.068029	2.169703
C	0.072361	-1.284921	2.563388
C	-0.535294	-2.100996	1.614574
H	-0.983366	-3.041860	1.915170
H	0.130488	-1.577973	3.603743
H	1.047922	0.641205	2.840834
H	0.831566	1.209539	0.597090
H	-0.071632	-0.085924	-1.066661
H	-0.618425	-2.790863	-1.581251
H	-1.690992	-3.450614	-0.323463
H	-5.293302	-1.455855	-1.422224
H	-4.131658	-0.431504	-2.258475
H	-5.106801	0.127616	0.594203
H	-5.994919	0.701513	-0.804658
H	-4.559289	2.485087	0.082129
H	-4.107689	2.067256	-1.560661
H	-2.254607	0.669863	-0.719751
H	-2.665857	1.065967	0.949327

conf_21

C	-4.212937	0.565905	0.248602
C	-3.592689	1.911426	0.044846
C	-2.930751	2.610275	0.968511
C	-2.365581	3.984646	0.780194
C	-0.833968	4.022232	0.791174
H	-0.462801	3.468691	1.671291
C	-0.203810	3.481959	-0.488475
C	1.309011	3.325245	-0.409219
C	1.929462	2.719089	-1.661408
C	3.449551	2.583263	-1.591820
C	3.967465	1.606956	-0.537369
C	3.674164	0.142008	-0.837756

C	4.099097	-0.793902	0.285550
C	3.958818	-2.270946	-0.055523
C	4.287342	-3.189253	1.111660
H	3.639240	-2.989583	1.973173
H	4.175303	-4.243257	0.844302
H	5.317997	-3.042833	1.447380
H	2.937533	-2.469319	-0.408385
H	4.609846	-2.507361	-0.905126
H	3.513019	-0.567898	1.188649
H	5.142600	-0.588040	0.555145
H	2.601929	0.001450	-1.035684
H	4.186028	-0.142533	-1.766081
H	3.564029	1.866904	0.450370
H	5.052544	1.730046	-0.447231
H	3.877733	3.574512	-1.402338
H	3.826028	2.276150	-2.574538
H	1.473915	1.738850	-1.862719
H	1.667832	3.343944	-2.522995
H	1.573729	2.718955	0.468710
H	1.759875	4.307403	-0.221334
H	-0.677470	2.526230	-0.772983
H	-0.459307	4.152684	-1.317028
H	-0.489974	5.049870	0.946430
H	-2.730615	4.410028	-0.161000
H	-2.742695	4.630685	1.580733
H	-2.829063	2.180808	1.969389
H	-3.723611	2.355004	-0.943924
C	-3.583328	-0.501640	-0.642566
C	-4.212976	-1.881400	-0.508223
C	-3.436379	-2.953103	-1.285420
C	-2.056179	-3.084400	-0.717833
O	-1.777678	-3.524123	0.366748
O	-1.104036	-2.574178	-1.543098
C	0.211640	-2.579241	-0.996161
C	0.305352	-1.615520	0.156888
C	-0.064197	-0.297061	-0.030024
N	-0.070354	0.553334	1.004266
C	0.299160	0.203750	2.244743
C	0.701996	-1.091382	2.484156
C	0.688439	-2.007051	1.437559
H	0.959203	-3.041674	1.617704
H	0.997198	-1.383707	3.483708
H	0.251572	0.974944	3.002674
H	-0.402988	1.502330	0.832334
H	-0.386321	0.101902	-0.983761
H	0.865005	-2.275273	-1.815446
H	0.487308	-3.583050	-0.667824
H	-3.928507	-3.922632	-1.176057
H	-3.380094	-2.705493	-2.347362
H	-4.255082	-2.174410	0.546368
H	-5.244470	-1.862221	-0.872900
H	-3.617841	-0.180876	-1.691491

H	-2.520689	-0.568845	-0.383326
H	-4.127397	0.269013	1.300316
H	-5.286559	0.630554	0.029294

conf_18

C	-2.818805	1.269887	-0.373575
C	-1.988633	2.497547	-0.564309
C	-1.448464	3.220099	0.416844
C	-0.595835	4.436318	0.238868
C	0.867017	4.166651	0.614647
H	0.897510	3.711335	1.615581
C	1.573345	3.262571	-0.388700
C	2.840368	2.598200	0.138096
C	3.401496	1.536122	-0.798128
C	4.592617	0.784130	-0.221566
C	5.108358	-0.341642	-1.115247
C	4.091667	-1.437571	-1.431634
C	3.526250	-2.145799	-0.207215
C	2.560670	-3.270482	-0.555638
C	2.044348	-4.017991	0.664525
H	2.865037	-4.505306	1.198551
H	1.559277	-3.339754	1.375856
H	1.326033	-4.797454	0.393438
H	1.721702	-2.856573	-1.134806
H	3.056533	-3.976071	-1.231989
H	3.015076	-1.425668	0.448480
H	4.352703	-2.550957	0.391154
H	3.267487	-1.027513	-2.031273
H	4.573841	-2.181531	-2.076023
H	5.981873	-0.797020	-0.634568
H	5.471184	0.086207	-2.057162
H	4.324399	0.382307	0.764617
H	5.407067	1.493987	-0.038232
H	2.606200	0.817971	-1.053609
H	3.680021	1.998620	-1.752949
H	2.646256	2.145390	1.125945
H	3.602295	3.360083	0.336761
H	0.858143	2.498416	-0.739596
H	1.811284	3.831680	-1.294612
H	1.408997	5.113197	0.704673
H	-0.651866	4.785487	-0.798142
H	-0.983486	5.246159	0.866316
H	-1.622532	2.905786	1.449286
H	-1.839297	2.822783	-1.595619
C	-4.204405	1.368262	-1.012926
C	-5.074701	0.130468	-0.814451
C	-4.461701	-1.161933	-1.360707
C	-3.453690	-1.764325	-0.429622
O	-3.571235	-1.879865	0.762518
O	-2.341096	-2.197850	-1.077457
C	-1.353710	-2.779173	-0.228882
C	-0.727411	-1.730554	0.650378
C	-0.015755	-0.691616	0.081411

N	0.490873	0.277763	0.855348
C	0.355666	0.299865	2.188733
C	-0.336887	-0.714497	2.810984
C	-0.891427	-1.725885	2.034335
H	-1.475558	-2.512369	2.499067
H	-0.456690	-0.699987	3.886661
H	0.804186	1.137380	2.706986
H	0.978336	1.051507	0.405027
H	0.153336	-0.597520	-0.984249
H	-0.615848	-3.215599	-0.902669
H	-1.793913	-3.566989	0.384809
H	-5.245698	-1.920343	-1.471037
H	-4.014405	-1.019717	-2.347617
H	-5.298705	-0.011958	0.247785
H	-6.032482	0.293436	-1.315601
H	-4.725580	2.237743	-0.599299
H	-4.087514	1.563484	-2.086610
H	-2.290622	0.423070	-0.835569
H	-2.914321	1.041765	0.694978

conf_2

C	-3.784376	-0.705338	-0.336330
C	-3.691675	0.784503	-0.252872
C	-3.316541	1.483478	0.820266
C	-3.310852	2.978565	0.915286
C	-1.909721	3.589849	1.015706
H	-1.373385	3.146006	1.874124
C	-1.096647	3.460471	-0.267389
C	0.316907	4.018902	-0.161080
C	1.118771	3.908626	-1.456887
C	1.556293	2.493802	-1.832735
C	2.646137	1.926213	-0.932262
C	3.098103	0.527315	-1.327093
C	4.189852	-0.029037	-0.423908
C	4.547867	-1.481136	-0.707858
C	5.628053	-2.021934	0.216525
H	6.553416	-1.447213	0.116860
H	5.321255	-1.962799	1.267072
H	5.862873	-3.066345	-0.003264
H	3.645177	-2.102841	-0.620390
H	4.870645	-1.577742	-1.751126
H	3.881612	0.069044	0.626784
H	5.089947	0.590588	-0.521444
H	2.230776	-0.148858	-1.319757
H	3.452556	0.536470	-2.365190
H	2.307476	1.909606	0.112856
H	3.510034	2.602821	-0.948381
H	1.926706	2.502370	-2.864097
H	0.690739	1.815761	-1.841071
H	0.520202	4.331933	-2.271880
H	2.011619	4.539761	-1.381147
H	0.859089	3.524833	0.658419

H	0.252511	5.073054	0.130987
H	-1.076447	2.413909	-0.605522
H	-1.629604	3.990768	-1.066216
H	-1.995592	4.650306	1.275063
H	-3.820614	3.402288	0.043366
H	-3.893463	3.278265	1.793707
H	-3.050987	0.935847	1.729803
H	-4.001936	1.333818	-1.143394
C	-3.140391	-1.269742	-1.602951
C	-3.229060	-2.788049	-1.746065
C	-2.844189	-3.590036	-0.502449
C	-1.533430	-3.259541	0.144085
O	-1.293139	-3.321558	1.320439
O	-0.584130	-2.873792	-0.751452
C	0.699406	-2.654863	-0.190238
C	0.743521	-1.452998	0.713334
C	-0.124460	-0.394176	0.522625
N	-0.074896	0.669568	1.331254
C	0.795805	0.790682	2.342856
C	1.692564	-0.229202	2.572786
C	1.662663	-1.353719	1.755926
H	2.355286	-2.169002	1.939879
H	2.399656	-0.146031	3.388155
H	0.740923	1.698094	2.930082
H	-0.746244	1.418623	1.159004
H	-0.885310	-0.371075	-0.246913
H	1.364000	-2.504347	-1.044385
H	1.029024	-3.536581	0.364755
H	-3.595296	-3.509783	0.286005
H	-2.792746	-4.655061	-0.760675
H	-4.256377	-3.070028	-1.999085
H	-2.608575	-3.097585	-2.591296
H	-3.613698	-0.810744	-2.477682
H	-2.088024	-0.966428	-1.659257
H	-3.347396	-1.148297	0.567076
H	-4.845010	-0.993386	-0.328159

conf_3

C	-1.520075	-3.245162	-0.452766
C	-2.667120	-2.287992	-0.537966
C	-3.284886	-1.695838	0.488951
C	-4.507246	-0.834747	0.373914
C	-4.236023	0.656875	0.602246
H	-3.711030	0.791482	1.562170
C	-3.458981	1.305336	-0.537127
C	-3.029471	2.740462	-0.262186
C	-2.373356	3.422057	-1.461258
C	-1.060090	2.799385	-1.930537
C	0.102943	2.972249	-0.961337
C	1.394682	2.340626	-1.462386
C	2.602720	2.632320	-0.584941
C	3.891102	1.999109	-1.094124

C	5.081401	2.247191	-0.179393
H	4.908354	1.850433	0.828978
H	5.991406	1.780592	-0.564435
H	5.278459	3.317790	-0.070302
H	3.739052	0.920366	-1.234348
H	4.111167	2.393793	-2.092746
H	2.403403	2.291001	0.442118
H	2.740118	3.718294	-0.506516
H	1.262973	1.252392	-1.557581
H	1.597934	2.699678	-2.479170
H	-0.149092	2.552694	0.022895
H	0.266530	4.044056	-0.789749
H	-0.780357	3.257579	-2.885977
H	-1.202264	1.733008	-2.151864
H	-3.087059	3.416876	-2.293456
H	-2.198811	4.477438	-1.221269
H	-2.351287	2.770949	0.602597
H	-3.909260	3.321936	0.036698
H	-2.585302	0.691248	-0.798975
H	-4.085782	1.285188	-1.437641
H	-5.187505	1.182936	0.730969
H	-4.954902	-0.965670	-0.617101
H	-5.249864	-1.180873	1.100901
H	-2.926351	-1.902187	1.501934
H	-3.071494	-2.120645	-1.538297
C	-0.548821	-3.132843	-1.629665
C	0.628163	-4.120905	-1.554736
C	1.977323	-3.442037	-1.331521
C	2.027289	-2.717119	-0.021356
O	1.621013	-3.123321	1.034449
O	2.579661	-1.480056	-0.147040
C	2.741397	-0.759512	1.060321
C	1.465214	-0.134379	1.547731
C	0.260627	-0.348521	0.907165
N	-0.864898	0.186976	1.393036
C	-0.903598	0.960205	2.485308
C	0.271744	1.229226	3.153114
C	1.455664	0.673630	2.684532
H	2.384337	0.867914	3.212983
H	0.255426	1.858314	4.033808
H	-1.873070	1.335003	2.785505
H	-1.736217	-0.050825	0.907219
H	0.151223	-0.945263	0.012844
H	3.475920	0.018418	0.844606
H	3.132152	-1.417401	1.842770
H	2.777797	-4.190726	-1.303093
H	2.216878	-2.745693	-2.138313
H	0.458142	-4.841864	-0.749587
H	0.696709	-4.699346	-2.478849
H	-1.111957	-3.291547	-2.554961
H	-0.168513	-2.103467	-1.714048
H	-0.993463	-3.148377	0.504075

H -1.929112 -4.265001 -0.457224

conf_57

C -2.645437 -0.754277 -0.992871
C -2.752046 0.692915 -1.349114
C -3.244032 1.648512 -0.559421
C -3.325364 3.104416 -0.896813
C -2.270718 3.935691 -0.152633
H -2.320370 3.705478 0.923337
C -0.860189 3.697203 -0.675718
C 0.246522 4.298229 0.184961
C 1.658173 3.933348 -0.272656
C 1.955261 2.446783 -0.132330
C 3.365086 2.008057 -0.497071
C 3.542396 0.502512 -0.343863
C 4.939415 -0.007793 -0.662391
C 5.075481 -1.515393 -0.492210
C 6.470015 -2.030504 -0.815090
H 6.539112 -3.113377 -0.683724
H 6.743282 -1.803527 -1.850085
H 7.220647 -1.568375 -0.166661
H 4.816020 -1.784413 0.541061
H 4.340403 -2.017755 -1.135500
H 5.667923 0.499182 -0.016957
H 5.201566 0.267753 -1.691782
H 3.285426 0.215376 0.687630
H 2.822023 -0.012185 -0.998936
H 4.090135 2.531915 0.137382
H 3.589119 2.303101 -1.529267
H 1.255990 1.879878 -0.764303
H 1.764070 2.151024 0.910921
H 1.799383 4.241272 -1.315868
H 2.386500 4.501895 0.315826
H 0.119511 3.981378 1.233159
H 0.131896 5.387271 0.199276
H -0.709613 2.614692 -0.809540
H -0.782304 4.099692 -1.693296
H -2.516254 4.999481 -0.233227
H -3.200200 3.244836 -1.976065
H -4.322850 3.478668 -0.643562
H -3.619706 1.362754 0.426693
H -2.403864 0.969214 -2.346137
C -3.312445 -1.685794 -2.005032
C -3.204500 -3.167648 -1.655011
C -1.767617 -3.675104 -1.500361
C -1.186530 -3.372772 -0.151864
O -1.750627 -3.493157 0.904179
O 0.097229 -2.933656 -0.224263
C 0.686144 -2.623165 1.037639
C 0.016300 -1.417927 1.641517
C 0.021427 -0.225836 0.942949
N -0.645120 0.834785 1.416283

C -1.326040 0.817892 2.571263
C -1.349449 -0.337982 3.319460
C -0.686946 -1.465016 2.843014
H -0.735735 -2.397918 3.393924
H -1.901236 -0.361140 4.250413
H -1.834130 1.731922 2.849724
H -0.659410 1.679821 0.846633
H 0.538017 -0.091825 0.001592
H 1.736433 -2.422471 0.819961
H 0.610158 -3.475804 1.714726
H -1.755819 -4.768267 -1.583183
H -1.107998 -3.290052 -2.282078
H -3.750659 -3.382247 -0.730684
H -3.689602 -3.747487 -2.444572
H -4.370387 -1.418409 -2.093877
H -2.868115 -1.511622 -2.993335
H -1.578148 -1.017341 -0.949483
H -3.057628 -0.929473 0.008433

conf_83

C -2.293311 2.288267 -1.214135
C -0.943524 2.904741 -1.395591
C -0.205269 3.466798 -0.436086
C 1.101993 4.165338 -0.655954
C 2.304071 3.445278 -0.038100
H 2.118692 3.278942 1.038564
C 2.654340 2.137002 -0.736746
C 3.811296 1.386604 -0.087574
C 4.074698 0.008297 -0.685844
C 3.010982 -1.030157 -0.349341
C 3.290885 -2.392377 -0.970098
C 2.338003 -3.493915 -0.513305
C 0.859095 -3.221160 -0.774904
C 0.498836 -2.991043 -2.237065
C -1.001929 -2.868257 -2.456712
H -1.241045 -2.670021 -3.504786
H -1.518584 -3.790015 -2.169925
H -1.427762 -2.056054 -1.857913
H 0.998906 -2.086662 -2.604376
H 0.893627 -3.818371 -2.838834
H 0.538056 -2.347326 -0.190475
H 0.275698 -4.071164 -0.396342
H 2.617439 -4.431017 -1.008397
H 2.483527 -3.666819 0.561189
H 4.315857 -2.692367 -0.722804
H 3.263599 -2.301000 -2.062423
H 2.026543 -0.677183 -0.682857
H 2.949364 -1.139670 0.744726
H 4.165400 0.097264 -1.775980
H 5.045223 -0.357532 -0.332514
H 3.630468 1.277176 0.992810
H 4.714674 2.001250 -0.167438

H	1.765701	1.493917	-0.806788
H	2.912893	2.357180	-1.779664
H	3.175399	4.108307	-0.062081
H	1.274199	4.288241	-1.730623
H	1.035820	5.174217	-0.233238
H	-0.606222	3.490853	0.582338
H	-0.562116	2.926525	-2.417868
C	-2.408279	0.911723	-1.870465
C	-3.772923	0.241550	-1.724298
C	-4.361079	0.252527	-0.312282
C	-3.473992	-0.240008	0.790296
O	-3.428756	0.194018	1.910292
O	-2.686773	-1.279954	0.400953
C	-1.921311	-1.871885	1.433814
C	-0.778160	-1.011946	1.898296
C	-0.379779	0.104901	1.189125
N	0.637175	0.854036	1.629471
C	1.330155	0.581860	2.742848
C	0.986210	-0.527781	3.484028
C	-0.072178	-1.322240	3.059990
H	-0.358431	-2.189807	3.646855
H	1.536026	-0.759047	4.387324
H	2.132125	1.261176	2.999590
H	0.891509	1.668714	1.069818
H	-0.850616	0.437829	0.274177
H	-1.531830	-2.799295	1.007401
H	-2.558659	-2.109208	2.290131
H	-4.690005	1.249326	-0.012554
H	-5.255276	-0.382493	-0.289391
H	-4.496939	0.743797	-2.374102
H	-3.698279	-0.788035	-2.084894
H	-2.179992	1.005662	-2.937673
H	-1.633645	0.240611	-1.479265
H	-2.533974	2.245537	-0.144649
H	-3.046339	2.951104	-1.662707

conf_10

C	-2.838768	-2.389438	-0.837482
C	-3.380867	-1.034475	-1.176177
C	-4.000042	-0.194039	-0.339801
C	-4.633820	1.105676	-0.736773
C	-3.895740	2.340643	-0.207380
H	-3.736190	2.233740	0.877857
C	-2.569568	2.596022	-0.912137
C	-1.739737	3.708041	-0.280830
C	-0.326058	3.827394	-0.845049
C	0.564013	2.644639	-0.485925
C	2.001602	2.751193	-0.970976
C	2.834758	1.549070	-0.549529
C	4.276618	1.574530	-1.032227
C	5.078108	0.361445	-0.577628
C	6.517787	0.374620	-1.069060

H	7.068453	-0.505126	-0.726315
H	6.559148	0.387480	-2.162422
H	7.048646	1.260866	-0.708351
H	5.069229	0.316325	0.520798
H	4.579136	-0.551919	-0.929871
H	4.766187	2.489547	-0.675188
H	4.292257	1.629964	-2.128119
H	2.826645	1.484026	0.549499
H	2.350750	0.631852	-0.917609
H	2.457141	3.669900	-0.581262
H	2.014903	2.842946	-2.064050
H	0.135196	1.720382	-0.895496
H	0.568921	2.528123	0.608755
H	-0.371675	3.936593	-1.935909
H	0.135202	4.746692	-0.466978
H	-1.672531	3.547084	0.805877
H	-2.268892	4.659407	-0.403455
H	-1.987121	1.666301	-0.952193
H	-2.767835	2.844865	-1.961968
H	-4.539195	3.220144	-0.313036
H	-4.695139	1.163989	-1.828812
H	-5.664341	1.116082	-0.365002
H	-4.135282	-0.501488	0.702835
H	-3.313601	-0.744929	-2.226599
C	-1.626307	-2.785612	-1.680436
C	-1.026773	-4.148610	-1.293605
C	0.464886	-4.074610	-0.964824
C	0.695360	-3.281165	0.286916
O	0.151829	-3.459071	1.344210
O	1.587264	-2.270629	0.103164
C	1.903522	-1.522899	1.265293
C	0.794127	-0.602866	1.692808
C	-0.345223	-0.449437	0.928139
N	-1.341781	0.336960	1.345060
C	-1.298411	1.038262	2.484359
C	-0.174392	0.948868	3.277695
C	0.869396	0.120180	2.882257
H	1.748763	0.029514	3.512937
H	-0.124696	1.512876	4.200295
H	-2.163788	1.642809	2.721716
H	-2.175004	0.379111	0.743679
H	-0.500668	-0.947722	-0.018079
H	2.790486	-0.941872	1.003899
H	2.143997	-2.196518	2.092860
H	0.856773	-5.079388	-0.773495
H	1.039841	-3.644023	-1.787190
H	-1.549592	-4.556922	-0.423335
H	-1.164675	-4.868959	-2.102981
H	-1.918882	-2.787344	-2.735387
H	-0.852715	-2.006846	-1.617868
H	-2.606631	-2.462568	0.232870
H	-3.630312	-3.130718	-1.013079

conf_47

C	-2.421804	1.758969	0.346156
C	-1.399057	2.793925	0.691848
C	-0.419223	3.186920	-0.125314
C	0.569201	4.275196	0.149951
C	2.015326	3.879254	-0.152624
H	2.668288	4.737450	0.039627
C	2.495732	2.691301	0.668457
C	3.964807	2.326609	0.481503
C	4.329328	1.849892	-0.925373
C	3.497287	0.677737	-1.442962
C	3.500375	-0.545186	-0.534729
C	2.753076	-1.738321	-1.114924
C	2.562373	-2.872061	-0.117704
C	1.801679	-4.066669	-0.675621
C	1.555760	-5.153356	0.359796
H	0.979575	-4.770428	1.210270
H	1.006077	-5.998257	-0.062564
H	2.499320	-5.538963	0.756899
H	0.842639	-3.727019	-1.090591
H	2.355951	-4.483705	-1.524249
H	2.035993	-2.491147	0.770541
H	3.542331	-3.205553	0.246174
H	1.770350	-1.410656	-1.487584
H	3.285939	-2.109183	-1.998787
H	3.062879	-0.288504	0.440630
H	4.535497	-0.836931	-0.316748
H	3.872929	0.390809	-2.431794
H	2.459138	1.001241	-1.612039
H	4.247674	2.682066	-1.632986
H	5.386933	1.562771	-0.926355
H	4.235588	1.553049	1.209313
H	4.580698	3.197258	0.733347
H	2.300096	2.888040	1.731676
H	1.886097	1.820951	0.379758
H	2.113091	3.654577	-1.221575
H	0.311249	5.144402	-0.468172
H	0.476744	4.599877	1.192901
H	-0.348562	2.719100	-1.112430
H	-1.503655	3.285922	1.660033
C	-3.806639	2.321383	0.021154
C	-4.847046	1.236355	-0.249160
C	-4.440795	0.233880	-1.337240
C	-3.542636	-0.850539	-0.819098
O	-3.721744	-1.497043	0.179602
O	-2.455168	-1.053973	-1.608681
C	-1.570361	-2.072770	-1.147679
C	-0.911098	-1.668586	0.144184
C	-0.193144	-0.489527	0.205573
N	0.317329	-0.071882	1.370782
C	0.200781	-0.762508	2.514628
C	-0.480123	-1.959446	2.506846

C	-1.051922	-2.403136	1.319085
H	-1.634932	-3.317604	1.306416
H	-0.584087	-2.521612	3.425962
H	0.652686	-0.327409	3.396524
H	0.787153	0.834215	1.374692
H	-0.034371	0.161481	-0.644061
H	-0.833799	-2.189743	-1.943927
H	-2.108146	-3.013166	-1.013042
H	-5.334715	-0.281674	-1.705962
H	-3.974990	0.725598	-2.194648
H	-5.066723	0.680376	0.668317
H	-5.781561	1.714332	-0.554138
H	-4.155790	2.951415	0.846278
H	-3.717693	2.978420	-0.851936
H	-2.069225	1.204921	-0.529844
H	-2.523947	1.038715	1.170716

conf_79

C	1.687989	-3.089251	-0.273364
C	0.203244	-3.064177	-0.474506
C	-0.723007	-3.014531	0.488876
C	-2.199576	-3.100557	0.256277
C	-2.944825	-1.826693	0.649693
H	-2.551530	-0.990685	0.056346
C	-4.454384	-1.908135	0.446721
C	-5.175595	-0.564938	0.599012
C	-5.362435	0.205130	-0.710571
C	-4.091720	0.552038	-1.482502
C	-3.183383	1.558638	-0.787356
C	-1.868160	1.788826	-1.519906
C	-1.028667	2.908033	-0.921298
C	0.306950	3.127434	-1.618884
C	1.086382	4.299417	-1.041478
H	1.245769	4.181394	0.037475
H	2.062082	4.416142	-1.521257
H	0.540717	5.237626	-1.176841
H	0.909255	2.209727	-1.563666
H	0.133261	3.297749	-2.687665
H	-0.854685	2.712902	0.147072
H	-1.605989	3.840706	-0.953386
H	-1.288578	0.852563	-1.538778
H	-2.076166	2.020347	-2.572007
H	-2.974665	1.236616	0.242785
H	-3.716987	2.512639	-0.690303
H	-4.377117	0.962632	-2.457949
H	-3.530450	-0.364185	-1.710365
H	-6.011491	-0.390979	-1.362796
H	-5.915536	1.128866	-0.501213
H	-4.647415	0.054367	1.336909
H	-6.168995	-0.735451	1.024901
H	-4.660246	-2.319216	-0.549991
H	-4.856722	-2.636404	1.159040

H	-2.747342	-1.597843	1.708316
H	-2.391140	-3.317913	-0.800041
H	-2.606598	-3.943878	0.828240
H	-0.392435	-2.966649	1.530739
H	-0.141111	-3.168732	-1.505463
C	2.470151	-2.512886	-1.453897
C	3.992803	-2.499111	-1.234384
C	4.579877	-1.090351	-1.172383
C	4.040018	-0.316559	-0.008008
O	3.948129	-0.706315	1.125283
O	3.616098	0.923643	-0.373930
C	3.179361	1.754899	0.685849
C	1.821007	1.381682	1.210048
C	1.083879	0.362776	0.639366
N	-0.109053	0.029641	1.141711
C	-0.669979	0.651782	2.186081
C	0.010875	1.688664	2.787235
C	1.262428	2.047064	2.300541
H	1.813255	2.850673	2.780243
H	-0.431706	2.201610	3.631415
H	-1.641050	0.294255	2.501809
H	-0.579237	-0.779903	0.718385
H	1.418642	-0.216516	-0.209704
H	3.150110	2.764483	0.271067
H	3.897825	1.725025	1.510372
H	5.666251	-1.139890	-1.035700
H	4.392583	-0.535995	-2.094497
H	4.241425	-3.024713	-0.307521
H	4.498447	-3.036354	-2.039886
H	2.223997	-3.095257	-2.347533
H	2.117727	-1.496415	-1.684723
H	1.967693	-2.589285	0.662124
H	1.998306	-4.135337	-0.145706

conf_93

C	1.689212	-0.660178	-1.957709
C	1.146151	-1.925997	-1.376967
C	1.046211	-2.223102	-0.082220
C	0.495741	-3.508955	0.452011
C	-0.885761	-3.361886	1.103110
H	-0.815917	-2.682304	1.964468
C	-1.946665	-2.869632	0.129948
C	-3.333644	-2.696894	0.733907
C	-4.407552	-2.327877	-0.292148
C	-4.082993	-1.113374	-1.159868
C	-3.952935	0.195769	-0.390343
C	-3.308132	1.311764	-1.203526
C	-3.233181	2.652809	-0.482621
C	-2.411980	3.699684	-1.223962
C	-2.313938	5.021257	-0.477825
H	-3.305124	5.454446	-0.315782
H	-1.849863	4.891064	0.506093

H	-1.721408	5.752740	-1.032587
H	-1.401892	3.306265	-1.415032
H	-2.849553	3.863614	-2.215391
H	-2.825674	2.522571	0.532500
H	-4.250610	3.029974	-0.327027
H	-2.299783	0.993892	-1.533160
H	-3.854148	1.438112	-2.145642
H	-3.375220	0.029459	0.531659
H	-4.939706	0.521808	-0.041060
H	-4.863848	-0.997519	-1.919281
H	-3.157212	-1.300804	-1.718111
H	-4.565901	-3.188760	-0.951563
H	-5.360061	-2.165504	0.225762
H	-3.304081	-1.945299	1.537308
H	-3.632370	-3.626165	1.231994
H	-1.606311	-1.926838	-0.316807
H	-2.009113	-3.573538	-0.711023
H	-1.186723	-4.330522	1.517340
H	0.425100	-4.236953	-0.363915
H	1.193581	-3.927378	1.186226
H	1.393501	-1.493969	0.652419
H	0.834331	-2.677695	-2.104152
C	3.023561	-0.863426	-2.685877
C	4.215018	-1.107322	-1.765397
C	4.711446	0.152307	-1.043858
C	3.905832	0.534636	0.158718
O	3.706504	-0.148735	1.129399
O	3.411040	1.799047	0.071518
C	2.756088	2.263024	1.246639
C	1.475597	1.518970	1.518269
C	0.455670	1.520140	0.586355
N	-0.668006	0.825705	0.821542
C	-0.875466	0.121347	1.941678
C	0.101600	0.097398	2.912685
C	1.284383	0.789749	2.692099
H	2.082825	0.749687	3.425118
H	-0.057091	-0.477004	3.816311
H	-1.816241	-0.407917	2.014154
H	-1.399127	0.829558	0.110836
H	0.508394	2.051265	-0.355926
H	2.558176	3.319922	1.061487
H	3.421090	2.170131	2.107889
H	5.719646	-0.033382	-0.657527
H	4.772031	1.000203	-1.729461
H	3.981836	-1.883293	-1.028621
H	5.048163	-1.486445	-2.363181
H	2.919902	-1.715313	-3.366966
H	3.229021	0.008007	-3.318520
H	0.963875	-0.254351	-2.674981
H	1.805626	0.094521	-1.172574

conf_11

C	-1.896746	1.700281	-1.821437
C	-1.087676	2.647141	-0.989037
C	-0.849715	2.581711	0.322038
C	-0.033492	3.590602	1.072220
C	1.345451	3.066112	1.496718
H	1.216651	2.213306	2.180432
C	2.224709	2.681877	0.312794
C	3.580023	2.091174	0.682991
C	4.463014	1.755165	-0.521381
C	3.833643	0.802844	-1.537817
C	3.559690	-0.602379	-1.002473
C	2.441230	-1.325535	-1.741628
C	2.093286	-2.687199	-1.156337
C	0.852013	-3.318486	-1.773147
C	0.470265	-4.638937	-1.121994
H	1.271717	-5.376121	-1.225091
H	0.287871	-4.515178	-0.047260
H	-0.428921	-5.068605	-1.571882
H	0.012212	-2.611646	-1.704386
H	1.015950	-3.470349	-2.846070
H	1.947198	-2.595319	-0.069372
H	2.946136	-3.366595	-1.275237
H	1.543052	-0.687727	-1.742744
H	2.708985	-1.436532	-2.799325
H	3.303338	-0.555265	0.064531
H	4.477923	-1.199913	-1.039642
H	4.487025	0.733962	-2.413361
H	2.898367	1.237719	-1.912072
H	4.721878	2.690533	-1.030496
H	5.409748	1.335490	-0.161921
H	3.443089	1.194270	1.307010
H	4.114534	2.797622	1.327480
H	1.670572	1.997603	-0.349412
H	2.381435	3.569185	-0.314158
H	1.852145	3.834433	2.090170
H	0.104524	4.479977	0.447486
H	-0.579460	3.914231	1.965107
H	-1.273981	1.763461	0.907361
H	-0.692012	3.508930	-1.528585
C	-3.364638	2.127002	-1.958961
C	-4.225131	1.778230	-0.749591
C	-4.421297	0.265964	-0.571618
C	-3.422779	-0.406306	0.319554
O	-3.104830	-0.057291	1.425942
O	-2.907296	-1.536563	-0.243228
C	-2.220965	-2.407023	0.639494
C	-0.932993	-1.865028	1.193344
C	-0.271153	-0.808675	0.598197
N	0.854899	-0.333015	1.139722
C	1.422070	-0.845599	2.240663
C	0.823214	-1.920563	2.858345

C	-0.361546	-2.424086	2.334643
H	-0.856197	-3.253204	2.831528
H	1.270868	-2.344889	3.747784
H	2.331541	-0.372627	2.586647
H	1.293955	0.471122	0.690981
H	-0.625325	-0.303300	-0.289074
H	-2.017089	-3.305152	0.050803
H	-2.874005	-2.676982	1.474694
H	-5.381755	0.081246	-0.075283
H	-4.458695	-0.250188	-1.533505
H	-3.806553	2.205369	0.167762
H	-5.209178	2.235532	-0.879078
H	-3.408305	3.206666	-2.136686
H	-3.794296	1.651282	-2.847945
H	-1.448663	1.640289	-2.818440
H	-1.866427	0.679564	-1.422014

C18:1 8Z pyridylcarbinol ester**conf_0**

C	3.214228	0.604563	-0.673692
C	4.537213	-0.121192	-0.889797
C	4.635462	-1.506791	-0.258809
C	3.515784	-2.462140	-0.678906
C	2.332307	-2.424349	0.238746
O	2.366178	-2.309411	1.435083
O	1.153452	-2.573491	-0.425730
C	0.019784	-2.740944	0.413533
C	-0.296214	-1.511970	1.218580
C	-0.913673	-1.585642	2.464801
C	-1.177902	-0.432349	3.194260
C	-0.810322	0.788437	2.670946
N	-0.227006	0.832756	1.466609
C	0.022905	-0.256870	0.735651
H	0.507400	-0.097021	-0.217785
H	0.051558	1.750691	1.068215
H	-0.961681	1.734093	3.175092
H	-1.649033	-0.478741	4.167715
H	-1.172580	-2.554720	2.879654
H	0.172856	-3.585949	1.089515
H	-0.805671	-2.972483	-0.263226
H	3.191609	-2.302164	-1.710416
H	3.871169	-3.498828	-0.625376
H	4.637349	-1.433669	0.833458
H	5.595768	-1.946581	-0.539648
H	4.712815	-0.204487	-1.970094
H	5.353487	0.497153	-0.499305
C	3.225360	2.007357	-1.269137
C	1.882219	2.729344	-1.244412
C	1.417642	3.147795	0.125411
C	0.298719	3.844699	0.376393

C	-0.667333	4.324492	-0.661932
C	-2.129887	4.355262	-0.218536
C	-2.694866	3.005844	0.214966
C	-2.531706	1.889603	-0.808121
C	-3.174621	0.577877	-0.378988
C	-2.900483	-0.574142	-1.335123
C	-3.459978	-1.905908	-0.857857
C	-3.190617	-3.059685	-1.815091
C	-3.658744	-4.403247	-1.277227
H	-4.733700	-4.393137	-1.073643
H	-3.464076	-5.210605	-1.987257
H	-3.151641	-4.657381	-0.339375
H	-2.116687	-3.104528	-2.046315
H	-3.683351	-2.852317	-2.772071
H	-3.041994	-2.142923	0.132858
H	-4.541710	-1.812931	-0.699099
H	-1.815020	-0.671414	-1.491340
H	-3.314988	-0.336095	-2.322567
H	-2.824207	0.305581	0.627317
H	-4.257539	0.719732	-0.278608
H	-1.464424	1.718711	-1.011400
H	-2.959603	2.208472	-1.767036
H	-2.228774	2.701428	1.162758
H	-3.758864	3.127392	0.447543
H	-2.729103	4.747359	-1.047285
H	-2.244779	5.072013	0.602851
H	-0.559959	3.735312	-1.577412
H	-0.370633	5.346515	-0.936091
H	0.115348	4.178219	1.399879
H	2.097016	2.945614	0.954990
H	1.119601	2.106601	-1.735498
H	1.953627	3.627872	-1.869029
H	3.560330	1.939926	-2.309966
H	3.975483	2.617859	-0.751642
H	2.410477	0.028545	-1.156035
H	2.984457	0.640546	0.400639

conf_26

C	2.254909	2.154499	-0.836582
C	3.700911	2.263919	-1.304202
C	4.678287	1.353057	-0.566242
C	4.284526	-0.122345	-0.578574
C	3.368688	-0.512295	0.541698
O	3.314345	-0.013023	1.633723
O	2.583501	-1.572728	0.204846
C	1.902196	-2.199222	1.277074
C	0.618258	-1.525749	1.671935
C	-0.271368	-2.156475	2.541746
C	-1.447705	-1.531056	2.935975
C	-1.726858	-0.270049	2.453864
N	-0.858067	0.313075	1.620265
C	0.279796	-0.265392	1.218919

H	0.892678	0.312410	0.541521
H	-1.060083	1.264465	1.258364
H	-2.615718	0.294186	2.704595
H	-2.143715	-2.015013	3.609112
H	-0.042514	-3.149867	2.916442
H	2.554721	-2.245370	2.155221
H	1.689830	-3.213563	0.934924
H	3.847396	-0.434894	-1.531291
H	5.173254	-0.751175	-0.437215
H	4.782900	1.674968	0.474824
H	5.665541	1.455059	-1.024072
H	3.740969	2.049746	-2.379845
H	4.038118	3.300193	-1.189188
C	1.342586	3.201718	-1.463667
C	-0.139819	2.986562	-1.168815
C	-0.499336	3.140363	0.282957
C	-1.728541	3.334197	0.784238
C	-3.009665	3.441993	0.016212
C	-3.867694	2.171809	0.076625
C	-3.317408	1.037477	-0.776925
C	-4.073033	-0.274419	-0.615157
C	-3.514198	-1.419969	-1.453661
C	-2.121191	-1.872407	-1.033710
C	-1.592909	-3.056702	-1.829701
C	-0.228884	-3.536361	-1.352636
C	0.323148	-4.694748	-2.169408
H	0.441138	-4.411847	-3.219643
H	1.301098	-5.019550	-1.803353
H	-0.348632	-5.557610	-2.134443
H	-0.313687	-3.838894	-0.298551
H	0.479665	-2.697248	-1.379344
H	-2.309760	-3.885560	-1.771742
H	-1.531648	-2.783770	-2.890823
H	-2.142526	-2.139006	0.033574
H	-1.409681	-1.041411	-1.132986
H	-4.196006	-2.275593	-1.388988
H	-3.499183	-1.124996	-2.510631
H	-5.124893	-0.111536	-0.876165
H	-4.073356	-0.571122	0.444542
H	-3.343059	1.341069	-1.831396
H	-2.255833	0.885262	-0.548485
H	-4.884260	2.411092	-0.252667
H	-3.967386	1.845896	1.122546
H	-2.809304	3.685591	-1.031970
H	-3.581255	4.278913	0.430663
H	-1.813501	3.475974	1.863433
H	0.332616	3.148444	0.988964
H	-0.429178	1.986019	-1.523193
H	-0.738194	3.682941	-1.765625
H	1.484780	3.192649	-2.549831
H	1.645347	4.199636	-1.124872
H	1.869441	1.157486	-1.103105

H 2.229398 2.230081 0.258497

conf_20

C 2.565703 -1.983995 -0.740756
C 2.568797 -3.485714 -1.011444
C 1.548619 -4.310420 -0.232633
C 0.102094 -3.844489 -0.397130
C -0.336565 -2.879413 0.660711
O 0.059933 -2.829937 1.794256
O -1.305766 -2.034742 0.210794
C -1.930084 -1.248894 1.210694
C -1.065901 -0.133788 1.727567
C -1.485411 0.671246 2.785058
C -0.676632 1.696394 3.262087
C 0.551063 1.908769 2.672509
N 0.927238 1.124080 1.655513
C 0.169873 0.135064 1.172961
H 0.586105 -0.422239 0.345549
H 1.833284 1.297744 1.181660
H 1.244930 2.681609 2.976994
H -0.992730 2.324498 4.085073
H -2.451782 0.492717 3.247236
H -2.232563 -1.881100 2.050826
H -2.823114 -0.834221 0.737616
H -0.098958 -3.421631 -1.385442
H -0.583454 -4.695299 -0.292008
H 1.792803 -4.309590 0.834380
H 1.623040 -5.349018 -0.564752
H 2.417139 -3.642474 -2.087107
H 3.566771 -3.881043 -0.789624
C 3.755082 -1.295293 -1.402986
C 3.703767 0.228664 -1.415514
C 3.751587 0.870503 -0.058152
C 3.510544 2.162821 0.209393
C 3.117121 3.226346 -0.773088
C 1.635578 3.617651 -0.686828
C 0.713267 2.575591 -1.308185
C -0.752224 2.722316 -0.927269
C -1.631210 1.627367 -1.516521
C -3.049878 1.620486 -0.967728
C -3.912172 0.502199 -1.537021
C -5.277328 0.387168 -0.872086
C -6.128545 -0.733633 -1.449134
H -7.099928 -0.796919 -0.952463
H -6.312077 -0.577568 -2.516459
H -5.634171 -1.704610 -1.339384
H -5.807336 1.342432 -0.968155
H -5.143806 0.229751 0.208084
H -4.045009 0.659987 -2.614670
H -3.379670 -0.456244 -1.447361
H -3.527726 2.588423 -1.163656
H -3.010445 1.532908 0.129195

H -1.659179 1.727412 -2.608522
H -1.170705 0.646382 -1.325921
H -1.122473 3.705456 -1.241804
H -0.847197 2.712530 0.168873
H 0.815883 2.613078 -2.399633
H 1.053329 1.569434 -1.027217
H 1.484928 4.581239 -1.183645
H 1.361674 3.785597 0.364958
H 3.347370 2.907363 -1.794306
H 3.734960 4.109037 -0.577396
H 3.681605 2.506654 1.232711
H 4.094367 0.237277 0.761915
H 2.817606 0.564809 -1.966205
H 4.561242 0.600268 -1.992164
H 3.827728 -1.642298 -2.439604
H 4.677994 -1.626001 -0.910863
H 1.636123 -1.544849 -1.136059
H 2.576567 -1.804292 0.343334

conf_2

C 3.382297 0.771748 -1.545190
C 4.675307 -0.010270 -1.342802
C 4.640584 -1.096976 -0.270486
C 3.578611 -2.174581 -0.529856
C 2.417817 -2.119420 0.412362
O 2.461088 -1.840594 1.581303
O 1.246633 -2.463921 -0.191685
C 0.158802 -2.684093 0.690784
C -0.324283 -1.440604 1.382251
C -1.099645 -1.514964 2.537392
C -1.527914 -0.360294 3.181056
C -1.166520 0.864666 2.663542
N -0.430616 0.909255 1.546130
C -0.016928 -0.183724 0.897724
H 0.575242 -0.023475 0.006984
H -0.155698 1.836209 1.164993
H -1.439751 1.814392 3.104866
H -2.123897 -0.407582 4.083421
H -1.358078 -2.485665 2.949463
H 0.434768 -3.424845 1.446535
H -0.637463 -3.096333 0.066700
H 3.213233 -2.166173 -1.559522
H 4.004495 -3.173462 -0.372076
H 4.476170 -0.667771 0.722576
H 5.625876 -1.566992 -0.229669
H 4.954846 -0.469364 -2.298351
H 5.481497 0.691821 -1.100484
C 2.933402 1.610114 -0.354111
C 1.791025 2.547798 -0.736387
C 1.164327 3.273585 0.422422
C 0.031446 3.990876 0.372946
C -0.787985 4.251680 -0.850588

C	-2.300983	4.206133	-0.631988
C	-2.837231	2.858457	-0.159309
C	-2.484473	1.685792	-1.064806
C	-3.107444	0.367856	-0.626149
C	-2.657821	-0.821370	-1.463050
C	-3.204122	-2.153035	-0.970739
C	-2.754014	-3.343527	-1.807649
C	-3.213209	-4.678774	-1.241903
H	-4.304204	-4.723196	-1.172431
H	-2.887170	-5.513858	-1.866577
H	-2.815889	-4.844618	-0.233799
H	-1.658784	-3.334680	-1.901975
H	-3.132872	-3.225269	-2.829428
H	-2.904597	-2.304342	0.078042
H	-4.300642	-2.116083	-0.954113
H	-1.558010	-0.864565	-1.479636
H	-2.957617	-0.667046	-2.507022
H	-2.870455	0.178900	0.430976
H	-4.200311	0.451188	-0.666562
H	-1.392765	1.566802	-1.118746
H	-2.799578	1.912465	-2.091334
H	-2.475670	2.656989	0.859189
H	-3.927266	2.925645	-0.068185
H	-2.790864	4.477564	-1.573333
H	-2.584799	4.979529	0.091078
H	-0.495756	3.576027	-1.659566
H	-0.524401	5.258794	-1.202013
H	-0.285911	4.508313	1.279746
H	1.723800	3.261775	1.358997
H	1.023857	1.991773	-1.295629
H	2.171752	3.283564	-1.456700
H	3.775965	2.204313	0.019724
H	2.639963	0.962549	0.483359
H	3.517357	1.436779	-2.406506
H	2.569889	0.088819	-1.835640

conf_4

C	3.206659	0.842570	-0.696930
C	4.589177	0.229243	-0.886597
C	4.797292	-1.135064	-0.236457
C	3.774634	-2.190293	-0.667193
C	2.576250	-2.249981	0.229709
O	2.584856	-2.157098	1.428647
O	1.420518	-2.461222	-0.456565
C	0.284573	-2.708131	0.361754
C	-0.098686	-1.516210	1.191933
C	-0.637731	-1.642847	2.469899
C	-0.956474	-0.516426	3.218972
C	-0.719774	0.731313	2.683363
N	-0.211110	0.825554	1.448586
C	0.084944	-0.238706	0.697895
H	0.500126	-0.038492	-0.280542

H	-0.026228	1.763115	1.040571
H	-0.919009	1.660457	3.201434
H	-1.366648	-0.602618	4.216997
H	-0.787886	-2.630722	2.893573
H	0.470989	-3.562594	1.016965
H	-0.517783	-2.961682	-0.333866
H	3.456963	-2.066298	-1.705512
H	4.220611	-3.190083	-0.596617
H	4.771802	-1.051389	0.854808
H	5.797980	-1.490840	-0.494361
H	4.785372	0.146940	-1.963447
H	5.344762	0.920055	-0.495363
C	3.103235	2.225515	-1.328784
C	1.705549	2.835238	-1.322228
C	1.206784	3.254006	0.034355
C	0.009482	3.810715	0.273103
C	-1.026085	4.105797	-0.767908
C	-2.467984	4.067949	-0.264364
C	-2.916348	2.721939	0.296499
C	-2.780378	1.551510	-0.669102
C	-3.328498	0.244730	-0.112137
C	-3.196368	-0.933215	-1.067774
C	-3.775344	-2.226858	-0.505150
C	-3.884954	-3.362990	-1.518598
C	-2.550416	-3.905364	-2.010511
H	-1.980474	-4.351494	-1.187005
H	-2.693965	-4.690284	-2.757109
H	-1.934844	-3.128509	-2.475753
H	-4.474665	-3.013508	-2.374643
H	-4.459449	-4.181818	-1.072737
H	-3.177612	-2.555883	0.358880
H	-4.775108	-2.013859	-0.108100
H	-2.139903	-1.069831	-1.338984
H	-3.711747	-0.690490	-2.006105
H	-2.831687	0.004516	0.839094
H	-4.387048	0.381976	0.141503
H	-1.728296	1.414285	-0.957735
H	-3.305456	1.792869	-1.602172
H	-2.360932	2.504933	1.219863
H	-3.963717	2.803924	0.608454
H	-3.128727	4.350189	-1.091080
H	-2.600475	4.837959	0.504591
H	-0.901853	3.437070	-1.625538
H	-0.822705	5.113763	-1.155808
H	-0.200587	4.171603	1.282044
H	1.917220	3.183055	0.859323
H	0.995772	2.141745	-1.796815
H	1.703782	3.720583	-1.970227
H	3.444984	2.158816	-2.367437
H	3.799384	2.909286	-0.827657
H	2.458698	0.187725	-1.167594
H	2.965916	0.886582	0.374848

conf_34

C	2.065203	2.133372	-0.025023
C	3.471509	2.647921	-0.300773
C	4.581907	1.664170	0.056901
C	4.428142	0.296525	-0.608225
C	3.593986	-0.667482	0.179634
O	3.548534	-0.766755	1.376139
O	2.880774	-1.501951	-0.629161
C	2.297861	-2.620060	0.014123
C	1.086679	-2.302249	0.846531
C	0.498415	-3.283021	1.643311
C	-0.621414	-2.996020	2.414593
C	-1.147769	-1.723282	2.379297
N	-0.569139	-0.800401	1.600017
C	0.511088	-1.046438	0.849888
H	0.895677	-0.216087	0.274950
H	-0.964243	0.157833	1.566632
H	-2.014244	-1.410205	2.946687
H	-1.080345	-3.749322	3.041973
H	0.925095	-4.281348	1.670797
H	3.039762	-3.114826	0.648338
H	2.016403	-3.299995	-0.793679
H	4.041441	0.368880	-1.628431
H	5.407260	-0.193169	-0.687723
H	4.630267	1.520136	1.141165
H	5.541559	2.093082	-0.242391
H	3.547449	2.912680	-1.363214
H	3.633389	3.577505	0.256287
C	0.981073	3.168561	-0.292731
C	-0.440244	2.626385	-0.151633
C	-0.816813	2.284684	1.265406
C	-2.060671	2.232573	1.764943
C	-3.329269	2.521857	1.027972
C	-4.427104	1.472052	1.218374
C	-4.058667	0.072653	0.737632
C	-3.638982	-0.012819	-0.723581
C	-3.308127	-1.431665	-1.168392
C	-3.025531	-1.568156	-2.663828
C	-1.897900	-0.689195	-3.200588
C	-0.553508	-0.916848	-2.523291
C	0.572881	-0.091244	-3.126922
H	0.361576	0.981145	-3.054472
H	1.527382	-0.286032	-2.629202
H	0.701628	-0.323928	-4.187962
H	-0.299658	-1.984438	-2.573384
H	-0.650537	-0.680618	-1.455740
H	-1.789556	-0.875802	-4.275235
H	-2.169985	0.370429	-3.111839
H	-3.943759	-1.337888	-3.216556
H	-2.796546	-2.617768	-2.885199
H	-2.449449	-1.803251	-0.590243
H	-4.144119	-2.092593	-0.910035

H	-2.773072	0.636846	-0.899648
H	-4.444923	0.386902	-1.353173
H	-3.249920	-0.324224	1.366106
H	-4.911252	-0.595072	0.907228
H	-5.320924	1.812326	0.684497
H	-4.706134	1.428149	2.277879
H	-3.130916	2.667613	-0.036192
H	-3.710383	3.481655	1.401450
H	-2.171161	2.035452	2.833368
H	0.010360	2.145263	1.963937
H	-0.546019	1.742652	-0.799656
H	-1.147412	3.360657	-0.547755
H	1.106257	3.554592	-1.310391
H	1.114764	4.026099	0.377404
H	1.874477	1.267796	-0.677197
H	2.012837	1.777682	1.012967

conf_41

C	4.009619	-1.446104	-0.546897
C	2.734926	-2.169110	-0.962201
C	2.616204	-3.576999	-0.393080
C	1.248261	-4.212676	-0.667841
C	0.185510	-3.557620	0.160767
O	0.108799	-3.593919	1.360375
O	-0.705035	-2.849411	-0.585532
C	-1.738089	-2.227084	0.169823
C	-1.197352	-1.139017	1.055942
C	-1.632589	-0.951619	2.365562
C	-1.080454	0.047092	3.159048
C	-0.078352	0.837200	2.638027
N	0.318948	0.642085	1.374333
C	-0.214217	-0.291747	0.580003
H	0.180723	-0.356432	-0.424827
H	1.085798	1.229044	0.991940
H	0.424393	1.620521	3.190594
H	-1.405311	0.197507	4.180616
H	-2.393899	-1.607307	2.775489
H	-2.264257	-2.967411	0.776211
H	-2.426861	-1.814770	-0.570099
H	0.989501	-4.150818	-1.726915
H	1.264524	-5.266452	-0.376123
H	2.789957	-3.568677	0.688597
H	3.391169	-4.214692	-0.829027
H	1.865101	-1.583123	-0.642564
H	2.675162	-2.216015	-2.057616
C	4.263009	-0.149711	-1.314186
C	3.167482	0.913884	-1.204037
C	3.055252	1.523577	0.166327
C	2.624066	2.764260	0.441015
C	2.161227	3.780616	-0.557428
C	1.049166	4.700180	-0.050552
C	-0.227279	3.985165	0.382296

C	-0.847526	3.088323	-0.680962
C	-2.157614	2.448689	-0.241131
C	-2.721107	1.458573	-1.250681
C	-3.959112	0.725581	-0.756304
C	-4.536898	-0.252701	-1.770697
C	-5.702566	-1.061308	-1.222297
H	-6.517865	-0.407348	-0.898666
H	-6.105523	-1.745775	-1.972606
H	-5.400538	-1.660130	-0.355507
H	-3.746116	-0.931180	-2.121631
H	-4.856980	0.301955	-2.660341
H	-3.717896	0.190508	0.175220
H	-4.730111	1.455235	-0.478426
H	-1.946094	0.723183	-1.516936
H	-2.954173	1.982827	-2.185660
H	-2.016814	1.942036	0.724972
H	-2.898263	3.234188	-0.048237
H	-0.137862	2.299324	-0.970466
H	-1.015714	3.670988	-1.595482
H	-0.027108	3.393512	1.287379
H	-0.963491	4.735918	0.690972
H	0.809550	5.417102	-0.843148
H	1.427755	5.293831	0.789615
H	1.854077	3.291552	-1.485903
H	3.026097	4.404566	-0.821403
H	2.682552	3.106815	1.476308
H	3.432602	0.923092	0.995237
H	2.207536	0.477290	-1.516376
H	3.369567	1.703462	-1.933198
H	4.392224	-0.392591	-2.374820
H	5.212781	0.286498	-0.985667
H	3.984921	-1.261293	0.535128
H	4.866749	-2.109566	-0.708800

conf_23

C	3.169914	1.678443	-0.478557
C	4.672729	1.507556	-0.664887
C	5.241543	0.174255	-0.188524
C	4.570041	-1.048366	-0.817064
C	3.410772	-1.566269	-0.021897
O	3.324013	-1.591737	1.176760
O	2.423623	-2.067686	-0.815341
C	1.404184	-2.773527	-0.125563
C	0.546372	-1.889777	0.736051
C	-0.190348	-2.401701	1.802065
C	-0.967660	-1.564754	2.594321
C	-0.985484	-0.213797	2.323425
N	-0.269076	0.252972	1.292569
C	0.467702	-0.530625	0.499661
H	1.010591	-0.036988	-0.294716
H	-0.253463	1.276851	1.111127
H	-1.545863	0.514178	2.895782

H	-1.541430	-1.952750	3.426221
H	-0.144398	-3.462551	2.027571
H	1.844131	-3.558601	0.495302
H	0.797407	-3.239218	-0.905208
H	4.260802	-0.873452	-1.850908
H	5.276370	-1.887687	-0.847858
H	5.165218	0.091012	0.900380
H	6.308087	0.149166	-0.425785
H	4.908391	1.641161	-1.728566
H	5.192914	2.315218	-0.137519
C	2.686524	3.060297	-0.899940
C	1.174489	3.252560	-0.841152
C	0.607217	3.279810	0.552277
C	-0.695018	3.340802	0.869366
C	-1.838392	3.335650	-0.095609
C	-2.961337	2.383330	0.312989
C	-4.041157	2.241590	-0.749696
C	-5.129841	1.231487	-0.391701
C	-4.618607	-0.160808	-0.021042
C	-3.689385	-0.792978	-1.049599
C	-3.262856	-2.205606	-0.676362
C	-2.237014	-2.806529	-1.627376
C	-1.839879	-4.227013	-1.254633
H	-2.705603	-4.894979	-1.278293
H	-1.094409	-4.637977	-1.941672
H	-1.430835	-4.276662	-0.238053
H	-1.348755	-2.158544	-1.655395
H	-2.637971	-2.796590	-2.647513
H	-2.853925	-2.203894	0.344529
H	-4.146458	-2.855036	-0.638583
H	-2.791908	-0.171308	-1.177600
H	-4.181571	-0.806662	-2.030510
H	-4.104188	-0.123341	0.949822
H	-5.481073	-0.819134	0.134663
H	-5.816270	1.146301	-1.241721
H	-5.727991	1.620106	0.440959
H	-4.502243	3.218412	-0.934325
H	-3.567411	1.951442	-1.695936
H	-3.405800	2.717090	1.259947
H	-2.537241	1.390999	0.506654
H	-1.487249	3.080721	-1.101126
H	-2.241293	4.354882	-0.168036
H	-0.957620	3.458213	1.922601
H	1.330851	3.341867	1.365866
H	0.677543	2.483503	-1.449202
H	0.920372	4.202566	-1.327620
H	3.022816	3.252408	-1.924557
H	3.171707	3.821284	-0.276387
H	2.649168	0.927914	-1.092498
H	2.903986	1.480481	0.569507

conf_7

C	3.638092	0.337838	-0.260399
C	4.875534	-0.546933	-0.354929
C	4.655996	-2.022176	-0.034692
C	3.585524	-2.692757	-0.902775
C	2.221678	-2.663155	-0.284198
O	1.965934	-2.876418	0.871305
O	1.242047	-2.388271	-1.187869
C	-0.081116	-2.512907	-0.681871
C	-0.379041	-1.508719	0.396972
C	-1.175954	-1.812234	1.498081
C	-1.394758	-0.868966	2.495253
C	-0.798390	0.368737	2.388231
N	-0.045905	0.639094	1.313958
C	0.161000	-0.238566	0.328149
H	0.797707	0.089569	-0.482470
H	0.427179	1.561950	1.237955
H	-0.893876	1.154302	3.126830
H	-2.005609	-1.096975	3.359378
H	-1.612003	-2.802017	1.587692
H	-0.244332	-3.521526	-0.294570
H	-0.731462	-2.356170	-1.545111
H	3.546844	-2.276047	-1.912190
H	3.814150	-3.759694	-1.013442
H	4.386385	-2.155660	1.017999
H	5.602573	-2.549357	-0.177727
H	5.285793	-0.459523	-1.369357
H	5.648422	-0.155582	0.316377
C	3.948145	1.792293	-0.592478
C	2.734377	2.714932	-0.647753
C	2.118473	3.040185	0.679946
C	0.879494	3.518319	0.872976
C	-0.151939	3.741758	-0.193852
C	-1.583462	3.778015	0.338912
C	-2.636693	3.720828	-0.765354
C	-2.780051	2.350997	-1.428768
C	-3.431765	1.299767	-0.538783
C	-3.484376	-0.085217	-1.168292
C	-4.191105	-1.113620	-0.296514
C	-4.101739	-2.538374	-0.825010
C	-4.797010	-3.552515	0.070542
H	-4.371098	-3.552579	1.080551
H	-5.862135	-3.323755	0.169346
H	-4.712772	-4.567406	-0.325951
H	-3.044877	-2.816633	-0.944874
H	-4.531334	-2.578927	-1.832850
H	-3.775638	-1.077636	0.720633
H	-5.246320	-0.833054	-0.189411
H	-2.459043	-0.422834	-1.380686
H	-3.983208	-0.028667	-2.143705
H	-2.900174	1.229860	0.420359
H	-4.449459	1.624715	-0.287703

H	-1.799062	1.987474	-1.766310
H	-3.378084	2.457810	-2.340469
H	-3.608389	4.015240	-0.353237
H	-2.391508	4.472303	-1.524917
H	-1.715965	4.690286	0.930405
H	-1.744826	2.947687	1.039392
H	-0.054328	2.977087	-0.974546
H	0.059093	4.691806	-0.703371
H	0.608639	3.836411	1.881329
H	2.778717	2.969438	1.544738
H	1.982727	2.315296	-1.341776
H	3.044076	3.669536	-1.095355
H	4.452126	1.826136	-1.564471
H	4.669785	2.187345	0.133189
H	2.883692	-0.028067	-0.971970
H	3.199591	0.256537	0.744746

conf_12

C	3.585986	0.901743	-0.152434
C	4.997084	0.326380	-0.115275
C	5.094417	-1.156892	0.228433
C	4.270580	-2.063932	-0.690771
C	2.888652	-2.325166	-0.175261
O	2.587734	-2.525199	0.971607
O	1.956076	-2.348777	-1.166564
C	0.661160	-2.758495	-0.746907
C	0.035134	-1.786366	0.214297
C	-0.795673	-2.201365	1.252417
C	-1.333333	-1.277632	2.139794
C	-1.022439	0.056151	1.986490
N	-0.230998	0.430775	0.973819
C	0.282422	-0.432264	0.092215
H	0.916081	-0.014788	-0.678554
H	0.008920	1.434356	0.859067
H	-1.379762	0.839419	2.642031
H	-1.972549	-1.588527	2.956111
H	-1.008744	-3.257851	1.379772
H	0.709420	-3.746662	-0.283091
H	0.071622	-2.826680	-1.664034
H	4.221272	-1.687756	-1.715678
H	4.735384	-3.056026	-0.746574
H	4.783870	-1.335872	1.262852
H	6.143709	-1.456230	0.166598
H	5.465474	0.498777	-1.092932
H	5.595849	0.891107	0.608421
C	3.584650	2.393631	-0.464379
C	2.205669	3.010060	-0.676090
C	1.374413	3.144097	0.571896
C	0.132228	3.649494	0.618292
C	-0.644732	4.145325	-0.563740
C	-2.157714	3.972071	-0.445016
C	-2.561823	2.522949	-0.220238
C	-4.054098	2.246666	-0.337121

C	-4.443355	0.839033	0.106918
C	-3.790290	-0.281028	-0.694125
C	-4.206130	-1.672245	-0.238819
C	-3.550886	-2.791322	-1.036855
C	-3.870677	-4.178762	-0.501771
H	-4.948088	-4.366841	-0.516599
H	-3.392379	-4.962995	-1.094533
H	-3.538743	-4.292973	0.536593
H	-2.462386	-2.637280	-1.043535
H	-3.863589	-2.717367	-2.085105
H	-3.964213	-1.793162	0.827111
H	-5.296657	-1.771140	-0.305112
H	-2.695909	-0.203939	-0.628447
H	-4.033252	-0.155656	-1.757599
H	-4.193461	0.715732	1.171198
H	-5.532026	0.730992	0.044293
H	-4.372518	2.409236	-1.374367
H	-4.603307	2.977681	0.267720
H	-2.012939	1.888181	-0.929126
H	-2.238128	2.221143	0.785425
H	-2.626877	4.349951	-1.359611
H	-2.542174	4.592338	0.373883
H	-0.290097	3.653616	-1.477051
H	-0.412759	5.211510	-0.693488
H	-0.326671	3.799193	1.597415
H	1.868775	2.905424	1.514691
H	1.660911	2.444986	-1.446447
H	2.330881	4.012149	-1.104986
H	4.177567	2.557678	-1.370815
H	4.104741	2.934964	0.335481
H	3.011354	0.382645	-0.933454
H	3.080452	0.704260	0.803674

conf_13

C	4.058401	1.096962	-0.985340
C	5.312028	0.302487	-0.635358
C	5.086822	-1.012579	0.107236
C	4.221074	-2.011796	-0.675972
C	2.863997	-2.224113	-0.083665
O	2.604792	-2.305585	1.087789
O	1.896947	-2.351886	-1.034209
C	0.633665	-2.775540	-0.545822
C	-0.023146	-1.771827	0.360405
C	-0.944178	-2.162518	1.330221
C	-1.528260	-1.223935	2.170909
C	-1.176021	0.101697	2.038377
N	-0.297568	0.453185	1.091557
C	0.267693	-0.425134	0.256856
H	0.969012	-0.026985	-0.464624
H	-0.030934	1.453077	1.003899
H	-1.566283	0.897028	2.659712
H	-2.237939	-1.516795	2.933898

H	-1.195234	-3.212782	1.440540
H	0.736438	-3.724277	-0.012423
H	0.022111	-2.938285	-1.436757
H	4.122312	-1.743386	-1.730192
H	4.682428	-3.006828	-0.658891
H	4.634523	-0.840756	1.088736
H	6.061799	-1.462767	0.307264
H	5.858123	0.091726	-1.562317
H	5.976309	0.933269	-0.033269
C	3.274509	1.635751	0.205765
C	2.198208	2.623275	-0.238932
C	1.296548	3.104595	0.863327
C	0.124884	3.737671	0.699289
C	-0.503118	4.111639	-0.607127
C	-2.024565	3.972244	-0.635051
C	-2.483673	2.553325	-0.336702
C	-3.967147	2.300057	-0.563932
C	-4.425161	0.921944	-0.093998
C	-3.754856	-0.244859	-0.809522
C	-4.244921	-1.606130	-0.337991
C	-3.576060	-2.771383	-1.054387
C	-3.973977	-4.129329	-0.496618
H	-3.484324	-4.947578	-1.031269
H	-3.713390	-4.217875	0.564391
H	-5.053725	-4.285198	-0.575566
H	-2.484954	-2.650069	-0.995088
H	-3.817833	-2.724221	-2.122729
H	-4.078006	-1.697935	0.745077
H	-5.331385	-1.673758	-0.473713
H	-2.665434	-0.197635	-0.672179
H	-3.921760	-0.150423	-1.890680
H	-4.249865	0.833095	0.988425
H	-5.510011	0.840789	-0.225563
H	-4.195920	2.420745	-1.630239
H	-4.546592	3.068960	-0.039744
H	-1.893589	1.856280	-0.947208
H	-2.253373	2.323348	0.713225
H	-2.387170	4.278743	-1.621974
H	-2.476061	4.665072	0.085493
H	-0.063745	3.527137	-1.423389
H	-0.234546	5.156567	-0.813933
H	-0.393554	4.086459	1.593684
H	1.676976	2.989340	1.879072
H	1.606144	2.191121	-1.058562
H	2.694164	3.491588	-0.693098
H	3.957895	2.140024	0.899747
H	2.831681	0.810725	0.780580
H	4.356355	1.943945	-1.614721
H	3.391961	0.490952	-1.616958

conf_29

C	4.059468	0.256930	0.139756
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C	5.303993	-0.618938	0.228602
C	5.048055	-2.114442	0.388420
C	4.160636	-2.714828	-0.705750
C	2.707279	-2.732455	-0.344221
O	2.249560	-2.970513	0.741745
O	1.901567	-2.474519	-1.411402
C	0.515826	-2.666221	-1.166338
C	-0.040782	-1.684861	-0.171867
C	-1.128189	-1.994415	0.642630
C	-1.599410	-1.077133	1.573605
C	-0.967139	0.142024	1.690832
N	0.065180	0.420584	0.885871
C	0.526051	-0.432666	-0.033338
H	1.371094	-0.097544	-0.619613
H	0.535278	1.343615	0.950116
H	-1.254697	0.906802	2.400189
H	-2.440077	-1.308989	2.214952
H	-1.599474	-2.969098	0.563684
H	0.333381	-3.683000	-0.809271
H	0.034475	-2.541509	-2.138977
H	4.297562	-2.225316	-1.673290
H	4.417957	-3.770779	-0.855802
H	4.592485	-2.326770	1.360950
H	6.011245	-2.630751	0.381354
H	5.907764	-0.452439	-0.672810
H	5.920227	-0.280662	1.069446
C	4.408243	1.738076	0.051462
C	3.227748	2.664008	-0.222300
C	2.254152	2.798879	0.916131
C	1.074117	3.434777	0.855194
C	0.509263	4.078420	-0.379246
C	-0.466426	3.180888	-1.150375
C	-1.765690	2.892593	-0.406773
C	-2.557525	1.736067	-1.000189
C	-3.810158	1.382421	-0.211131
C	-4.485174	0.106406	-0.692337
C	-5.697198	-0.291920	0.137042
C	-6.352042	-1.586000	-0.327276
C	-7.561039	-1.975578	0.509819
H	-8.011474	-2.906116	0.155363
H	-7.287487	-2.117942	1.560453
H	-8.331855	-1.199695	0.472900
H	-5.610136	-2.395703	-0.303456
H	-6.649178	-1.481149	-1.377919
H	-5.401955	-0.393113	1.191610
H	-6.437020	0.518433	0.112389
H	-3.753216	-0.715334	-0.681598
H	-4.782537	0.224174	-1.742176
H	-3.552167	1.273439	0.852810
H	-4.521739	2.215861	-0.255080
H	-1.910058	0.848333	-1.060728
H	-2.827604	1.968503	-2.037610

H	-1.555387	2.676951	0.650051
H	-2.383568	3.798217	-0.391572
H	0.039067	2.235830	-1.396249
H	-0.696954	3.646869	-2.114106
H	1.326924	4.371242	-1.043883
H	-0.004486	5.002897	-0.093517
H	0.507567	3.545333	1.780323
H	2.586521	2.421696	1.884626
H	2.710849	2.347626	-1.137816
H	3.615489	3.666437	-0.447409
H	5.145052	1.874220	-0.747653
H	4.908081	2.050460	0.976671
H	3.491302	-0.021587	-0.760396
H	3.409122	0.064529	1.005082

conf_83

C	2.293812	2.244478	-0.684803
C	3.751670	2.486349	-1.056338
C	4.731705	1.447799	-0.518256
C	4.374807	0.008192	-0.889018
C	3.480826	-0.663178	0.108687
O	3.488352	-0.500021	1.299316
O	2.638132	-1.558253	-0.479254
C	1.953907	-2.416261	0.417425
C	0.878495	-1.734471	1.214787
C	0.302331	-2.355036	2.321375
C	-0.705437	-1.726495	3.043831
C	-1.124443	-0.472835	2.654178
N	-0.553483	0.101218	1.588250
C	0.408144	-0.482804	0.867741
H	0.790543	0.082437	0.029102
H	-0.869824	1.040458	1.287354
H	-1.896747	0.093497	3.158429
H	-1.156965	-2.199540	3.906453
H	0.648912	-3.337181	2.628319
H	2.664068	-2.884234	1.105078
H	1.506101	-3.191012	-0.209692
H	3.938934	-0.074041	-1.888330
H	5.281144	-0.610810	-0.901747
H	4.801423	1.517446	0.572048
H	5.727697	1.673948	-0.907293
H	3.831106	2.529431	-2.150132
H	4.056480	3.473948	-0.692161
C	1.377159	3.376546	-1.131855
C	-0.111564	3.097960	-0.938850
C	-0.538483	3.025804	0.502110
C	-1.794498	3.137017	0.959426
C	-3.022290	3.425235	0.153313
C	-4.231931	2.508316	0.401576
C	-4.319597	1.310571	-0.539749
C	-3.166707	0.328560	-0.413055

C	-3.261912	-0.877579	-1.335667
C	-2.084745	-1.830437	-1.179258
C	-2.153853	-3.052228	-2.085641
C	-0.962400	-3.995798	-1.945771
C	-0.897998	-4.716734	-0.604800
H	-1.796452	-5.320358	-0.443665
H	-0.039347	-5.392951	-0.553945
H	-0.827407	-4.018390	0.236321
H	-0.035753	-3.430117	-2.118014
H	-1.003878	-4.743460	-2.744333
H	-3.080307	-3.604440	-1.881560
H	-2.224517	-2.714282	-3.125996
H	-2.024751	-2.148949	-0.129046
H	-1.151680	-1.287907	-1.394341
H	-4.197146	-1.416008	-1.138111
H	-3.321478	-0.537010	-2.376917
H	-3.121041	-0.024444	0.627469
H	-2.221437	0.851962	-0.613076
H	-5.262162	0.781723	-0.355867
H	-4.374258	1.673904	-1.573962
H	-5.144042	3.100572	0.286188
H	-4.230815	2.165735	1.445383
H	-2.789861	3.439390	-0.915704
H	-3.311935	4.452101	0.413021
H	-1.944345	3.123448	2.041371
H	0.261664	2.942041	1.239791
H	-0.370281	2.160837	-1.456936
H	-0.690108	3.874577	-1.448328
H	1.556679	3.574492	-2.194260
H	1.648244	4.297422	-0.601706
H	1.955225	1.314826	-1.168069
H	2.218822	2.090772	0.400280

conf_87

C	3.575188	0.100435	-1.625785
C	4.661132	-0.964933	-1.524678
C	4.467010	-2.015733	-0.432679
C	3.158992	-2.803930	-0.563030
C	2.127308	-2.456224	0.463811
O	2.330123	-2.077056	1.587048
O	0.862753	-2.656699	0.001048
C	-0.156426	-2.672540	0.984707
C	-0.597161	-1.315783	1.456382
C	-1.717021	-1.189444	2.279191
C	-2.115562	0.052613	2.755984
C	-1.383352	1.167268	2.406397
N	-0.318615	1.021229	1.610302
C	0.083452	-0.160637	1.127223
H	0.953636	-0.140156	0.487114
H	0.233123	1.856715	1.334946
H	-1.612706	2.172513	2.735518
H	-2.983167	0.158053	3.394614

H	-2.282138	-2.074627	2.555139
H	0.178599	-3.246800	1.855057
H	-1.000607	-3.187651	0.522329
H	2.715607	-2.727688	-1.559263
H	3.339740	-3.875139	-0.405127
H	4.508232	-1.561726	0.562048
H	5.308719	-2.710854	-0.476514
H	4.739977	-1.472943	-2.493055
H	5.627958	-0.474226	-1.363722
C	3.413134	0.977077	-0.390705
C	2.459665	2.142294	-0.646074
C	2.013393	2.846862	0.605258
C	1.101396	3.827264	0.682082
C	0.360802	4.462716	-0.454897
C	-1.126437	4.086634	-0.493120
C	-1.364510	2.709751	-1.101667
C	-2.741265	2.125170	-0.824710
C	-2.882742	0.690912	-1.315176
C	-4.211619	0.047243	-0.941817
C	-4.386769	-1.374192	-1.466812
C	-3.395975	-2.382578	-0.896357
C	-3.646270	-3.802254	-1.383214
H	-2.925082	-4.512569	-0.967345
H	-4.646779	-4.144520	-1.102838
H	-3.572185	-3.859923	-2.473137
H	-3.459731	-2.351721	0.201765
H	-2.373515	-2.083514	-1.159879
H	-5.404126	-1.715631	-1.242909
H	-4.304130	-1.370776	-2.561389
H	-5.027725	0.672357	-1.322412
H	-4.319849	0.046447	0.152778
H	-2.759558	0.663708	-2.405660
H	-2.054098	0.095946	-0.907934
H	-3.512708	2.755050	-1.283852
H	-2.941733	2.158331	0.256306
H	-1.197041	2.761748	-2.184408
H	-0.603226	2.009981	-0.733466
H	-1.681361	4.838955	-1.062171
H	-1.536521	4.125350	0.526253
H	0.826737	4.206357	-1.411619
H	0.456466	5.548212	-0.342257
H	0.906119	4.257178	1.666109
H	2.518217	2.551928	1.526891
H	1.585443	1.786178	-1.208669
H	2.946495	2.861228	-1.317181
H	4.389296	1.368212	-0.079733
H	3.062208	0.375407	0.458672
H	3.802204	0.741698	-2.485774
H	2.608334	-0.367592	-1.863988

C18:1 9Z pyridylcarbinol ester**conf_1**

C	4.940503	0.671079	0.100070
C	3.936505	1.590871	-0.594443
C	2.787047	2.022258	0.307652
C	1.781849	2.932062	-0.394308
C	0.733457	3.478533	0.525615
C	-0.535767	3.785916	0.217499
C	-1.194301	3.669962	-1.125358
C	-2.720474	3.666812	-1.047884
C	-3.317211	2.464633	-0.322579
C	-3.161665	1.146735	-1.068881
C	-3.704926	-0.052242	-0.304915
C	-3.555796	-1.364845	-1.060413
C	-3.955355	-2.588677	-0.248059
C	-3.810013	-3.893064	-1.017482
H	-2.780430	-4.046659	-1.359150
H	-4.447760	-3.896657	-1.906118
H	-4.091085	-4.755290	-0.407428
H	-4.992557	-2.473974	0.088419
H	-3.352442	-2.626332	0.670927
H	-2.516092	-1.472979	-1.402564
H	-4.156999	-1.326086	-1.977163
H	-4.763022	0.114505	-0.068310
H	-3.198420	-0.130345	0.668760
H	-2.105616	0.968559	-1.315925
H	-3.672784	1.222617	-2.036662
H	-4.383515	2.646033	-0.147773
H	-2.871354	2.379203	0.680192
H	-3.043162	4.587328	-0.547978
H	-3.129665	3.714906	-2.062730
H	-0.825438	2.791785	-1.668573
H	-0.875683	4.529552	-1.729675
H	-1.139307	4.252272	0.997880
H	1.076261	3.715922	1.534139
H	1.329277	2.417309	-1.250545
H	2.325219	3.784756	-0.826149
H	2.271062	1.136494	0.700458
H	3.193392	2.546500	1.182491
H	4.456341	2.488156	-0.949338
H	3.531522	1.101182	-1.488775
C	4.412870	-0.739218	0.355470
C	4.362034	-1.601090	-0.905328
C	3.402467	-2.775912	-0.767389
C	1.980248	-2.305305	-0.757135
O	1.545611	-1.371885	-1.387032
O	1.193231	-3.052036	0.047979
C	-0.194624	-2.715584	0.036679
C	-0.488570	-1.554418	0.949127
C	-0.936284	-1.747776	2.254344
C	-1.196994	-0.663933	3.087835

C	-0.996166	0.608605	2.601902
N	-0.563466	0.772134	1.344071
C	-0.312794	-0.247986	0.517058
H	0.047573	-0.010453	-0.475358
H	-0.397902	1.742820	1.002567
H	-1.166247	1.510529	3.176458
H	-1.549864	-0.803642	4.101620
H	-1.086056	-2.757866	2.622941
H	-0.711200	-3.607745	0.388714
H	-0.512612	-2.491832	-0.982869
H	3.594042	-3.369913	0.129805
H	3.492697	-3.457011	-1.622771
H	5.362801	-1.977671	-1.135428
H	4.046749	-1.003012	-1.765156
H	3.410316	-0.674849	0.800531
H	5.034232	-1.239059	1.106453
H	5.243497	1.128615	1.049227
H	5.851509	0.604261	-0.505670

conf_0

C	4.335094	2.086148	-0.493970
C	3.013432	2.609930	-1.053034
C	1.945957	2.804956	0.014761
C	0.639484	3.378217	-0.527479
C	-0.385561	3.607393	0.543054
C	-1.719700	3.595105	0.404354
C	-2.496961	3.382596	-0.858250
C	-3.909060	2.849885	-0.617936
C	-3.965585	1.456640	0.000190
C	-3.447918	0.351304	-0.909677
C	-3.502334	-1.033087	-0.280213
C	-3.004551	-2.133281	-1.206532
C	-2.914670	-3.500337	-0.542784
C	-2.461932	-4.600619	-1.490904
H	-1.479480	-4.383424	-1.924946
H	-3.163118	-4.712995	-2.322829
H	-2.393709	-5.566430	-0.984145
H	-3.893668	-3.759025	-0.122352
H	-2.233435	-3.443064	0.318666
H	-2.020352	-1.852426	-1.611860
H	-3.665228	-2.197598	-2.079914
H	-4.532435	-1.253825	0.025301
H	-2.914757	-1.041433	0.649572
H	-2.415356	0.564991	-1.221441
H	-4.033354	0.350391	-1.837712
H	-5.002302	1.230866	0.273576
H	-3.408220	1.450101	0.949074
H	-4.440884	3.554922	0.031290
H	-4.453484	2.844367	-1.568325
H	-1.946168	2.741383	-1.555682
H	-2.572526	4.354098	-1.365063
H	-2.314685	3.849092	1.282968

H	0.014973	3.880421	1.520592
H	0.237999	2.742337	-1.327678
H	0.853779	4.340472	-1.012920
H	1.753695	1.852891	0.526287
H	2.333304	3.479822	0.788654
H	3.192468	3.571369	-1.547932
H	2.637407	1.938751	-1.836511
C	4.302775	0.639031	-0.005761
C	4.244677	-0.378671	-1.138445
C	4.217315	-1.826809	-0.641867
C	2.947347	-2.179208	0.067448
O	2.818015	-2.496447	1.219630
O	1.876450	-2.109751	-0.772453
C	0.653607	-2.553884	-0.203058
C	0.092637	-1.565303	0.781437
C	-0.207397	-1.919015	2.095784
C	-0.752136	-0.989363	2.973465
C	-0.974494	0.295401	2.526912
N	-0.662289	0.617713	1.265403
C	-0.146362	-0.259447	0.395178
H	0.075830	0.113684	-0.596934
H	-0.825199	1.599794	0.962896
H	-1.388451	1.087061	3.138713
H	-0.990748	-1.251758	3.996193
H	0.001561	-2.928656	2.433211
H	0.791696	-3.520269	0.285901
H	-0.028569	-2.675960	-1.045345
H	5.037911	-2.017724	0.052186
H	4.318150	-2.510135	-1.491007
H	5.127904	-0.256364	-1.773870
H	3.376841	-0.204660	-1.782870
H	3.459919	0.487796	0.682382
H	5.200942	0.443844	0.590962
H	4.647432	2.737722	0.330465
H	5.112639	2.179676	-1.260809

conf_2

C	-3.411134	-2.653049	-0.200614
C	-1.906089	-2.586095	-0.427233
C	-1.275604	-3.909962	-0.830684
C	0.241350	-3.836019	-0.976308
C	0.960294	-3.579049	0.315767
C	2.227546	-3.157614	0.442865
C	3.172376	-2.854304	-0.682256
C	4.402539	-2.056507	-0.254481
C	4.103030	-0.666946	0.298846
C	3.477348	0.290019	-0.706451
C	3.198154	1.671334	-0.131489
C	2.558793	2.625377	-1.129939
C	2.179733	3.972676	-0.530845
C	1.589949	4.938802	-1.547291
H	2.307803	5.154614	-2.343864

H	1.313301	5.889936	-1.085761
H	0.693157	4.528755	-2.025336
H	3.068103	4.422296	-0.071844
H	1.471717	3.817656	0.296290
H	1.667432	2.152852	-1.571096
H	3.245074	2.783355	-1.971137
H	4.135251	2.106744	0.236562
H	2.552739	1.580302	0.754661
H	2.543278	-0.131638	-1.105004
H	4.142329	0.385241	-1.574012
H	5.034703	-0.227041	0.671858
H	3.451898	-0.751618	1.181550
H	4.948705	-2.633365	0.500842
H	5.078992	-1.964263	-1.110977
H	2.645712	-2.350647	-1.501735
H	3.505312	-3.810251	-1.108369
H	2.653023	-3.125927	1.447569
H	0.423258	-3.859003	1.223633
H	0.514997	-3.083064	-1.727592
H	0.611223	-4.788126	-1.380040
H	-1.528789	-4.677624	-0.088505
H	-1.712152	-4.247031	-1.776536
H	-1.677971	-1.836833	-1.198848
H	-1.441858	-2.229418	0.503350
C	-4.020389	-1.295220	0.139392
C	-4.197088	-0.391106	-1.077046
C	-4.533565	1.057388	-0.707184
C	-3.387928	1.727349	-0.014658
O	-3.339600	2.094449	1.129174
O	-2.322156	1.864538	-0.850633
C	-1.186474	2.488169	-0.265288
C	-0.497956	1.563075	0.700188
C	-0.360956	1.864804	2.053568
C	0.276659	0.978556	2.914595
C	0.749877	-0.213506	2.411054
N	0.591271	-0.490101	1.110041
C	-0.002956	0.350942	0.255563
H	-0.083712	0.021042	-0.772212
H	0.939760	-1.407193	0.766169
H	1.248405	-0.967647	3.006942
H	0.392392	1.200517	3.967728
H	-0.772091	2.794145	2.432880
H	-1.476005	3.409608	0.243248
H	-0.528023	2.731270	-1.099787
H	-5.393407	1.104243	-0.036456
H	-4.765500	1.627973	-1.611341
H	-5.003816	-0.783168	-1.704058
H	-3.296690	-0.393529	-1.700160
H	-3.389580	-0.800101	0.891499
H	-4.995196	-1.432171	0.619332
H	-3.611778	-3.359945	0.612092
H	-3.901907	-3.066824	-1.090587

conf_3

C	4.806225	1.299789	0.300567
C	3.769575	2.220627	-0.340490
C	2.532942	2.430381	0.523155
C	1.478387	3.313129	-0.140853
C	0.290834	3.583480	0.732328
C	-0.989646	3.704641	0.349472
C	-1.536228	3.612343	-1.043221
C	-2.976320	3.106330	-1.102976
C	-3.135982	1.696750	-0.555140
C	-4.548538	1.138144	-0.655469
C	-4.718767	-0.210468	0.038086
C	-3.915939	-1.347231	-0.582646
C	-4.087774	-2.674064	0.144516
C	-3.334865	-3.819637	-0.514642
H	-3.458313	-4.756352	0.034869
H	-2.260573	-3.609991	-0.575383
H	-3.687775	-3.987271	-1.536560
H	-5.154228	-2.922058	0.195636
H	-3.760221	-2.560324	1.186994
H	-2.847709	-1.090076	-0.601194
H	-4.212711	-1.466872	-1.633164
H	-5.779362	-0.485801	0.031147
H	-4.444343	-0.107332	1.098118
H	-4.832564	1.049561	-1.711682
H	-5.246123	1.858823	-0.213052
H	-2.839262	1.687312	0.503694
H	-2.437066	1.032093	-1.081428
H	-3.625478	3.791422	-0.543614
H	-3.322673	3.138971	-2.141368
H	-0.891719	2.989724	-1.675885
H	-1.492639	4.617083	-1.484382
H	-1.715887	3.976890	1.117009
H	0.520221	3.773505	1.782165
H	1.171178	2.885874	-1.103152
H	1.941249	4.277851	-0.391540
H	2.098048	1.457146	0.783030
H	2.832496	2.883902	1.476560
H	4.229257	3.196072	-0.535906
H	3.472087	1.831214	-1.322748
C	4.407705	-0.173477	0.372262
C	4.401401	-0.866138	-0.985307
C	4.057471	-2.355668	-0.898615
C	2.655469	-2.606396	-0.438921
O	2.308069	-3.168825	0.565423
O	1.746123	-2.106274	-1.320917
C	0.391819	-2.381479	-0.987376
C	-0.070944	-1.553116	0.179939
C	-0.507227	-2.122795	1.375332
C	-0.937976	-1.319504	2.424533
C	-0.908206	0.050303	2.272026
N	-0.467427	0.574172	1.121843

C	-0.059742	-0.174517	0.090066
H	0.277573	0.359865	-0.789728
H	-0.455692	1.607600	1.008009
H	-1.220651	0.750877	3.036084
H	-1.282231	-1.748206	3.357007
H	-0.496470	-3.201906	1.482829
H	0.264902	-3.442058	-0.762085
H	-0.181393	-2.135152	-1.882792
H	4.720488	-2.870789	-0.201082
H	4.169011	-2.818130	-1.884495
H	5.394503	-0.776237	-1.437737
H	3.704307	-0.378285	-1.674035
H	3.425640	-0.279536	0.853865
H	5.109779	-0.699364	1.029252
H	5.022368	1.663871	1.311880
H	5.748374	1.379112	-0.253843

conf_21

C	-2.340249	3.110605	-1.721712
C	-0.881812	3.233440	-1.284995
C	0.016235	2.141990	-1.849541
C	1.498703	2.371836	-1.565205
C	2.372575	1.301683	-2.145168
C	3.499667	0.791712	-1.625122
C	4.194241	1.217653	-0.372819
C	4.681192	0.068630	0.511331
C	3.575092	-0.771723	1.144287
C	2.560092	0.046138	1.934081
C	1.643933	-0.791054	2.817992
C	0.667320	0.032055	3.653354
C	-0.345062	0.834198	2.843318
C	-1.333595	1.592295	3.717283
H	-1.903307	0.906425	4.351741
H	-2.047597	2.163713	3.117388
H	-0.817295	2.297453	4.375406
H	-0.902743	0.149919	2.190998
H	0.176323	1.546479	2.191005
H	1.236127	0.714402	4.297971
H	0.123928	-0.636782	4.331462
H	2.264416	-1.398557	3.486947
H	1.086682	-1.514500	2.202617
H	1.963046	0.659519	1.245942
H	3.095738	0.763836	2.570012
H	4.039028	-1.508685	1.809823
H	3.060704	-1.363119	0.373470
H	5.347486	-0.579989	-0.069638
H	5.296766	0.494898	1.310923
H	3.573460	1.909172	0.202542
H	5.071370	1.800357	-0.685214
H	4.033317	0.044465	-2.216401
H	2.077188	0.956859	-3.139043
H	1.666013	2.472981	-0.487417

H	1.791604	3.335542	-2.003824
H	-0.294389	1.171307	-1.441489
H	-0.135449	2.070900	-2.934911
H	-0.501768	4.208999	-1.609754
H	-0.808653	3.235969	-0.189858
C	-3.029854	1.799619	-1.350523
C	-3.107992	1.560588	0.151345
C	-3.937445	0.328386	0.540679
C	-3.290382	-0.946406	0.100063
O	-3.454080	-1.527470	-0.938378
O	-2.410889	-1.405066	1.038669
C	-1.803388	-2.646400	0.725398
C	-0.777381	-2.528142	-0.367248
C	-0.617356	-3.518867	-1.334509
C	0.365588	-3.406499	-2.310311
C	1.175087	-2.291042	-2.312891
N	0.996073	-1.348415	-1.379310
C	0.063063	-1.430592	-0.423578
H	0.005369	-0.604436	0.274707
H	1.614160	-0.512859	-1.414212
H	1.961572	-2.113305	-3.035439
H	0.496074	-4.167614	-3.068933
H	-1.277701	-4.380152	-1.330938
H	-2.560953	-3.378817	0.437863
H	-1.325427	-2.972913	1.652355
H	-4.919285	0.375157	0.064382
H	-4.069714	0.297445	1.624360
H	-3.570254	2.430272	0.631303
H	-2.106369	1.474143	0.587468
H	-2.533424	0.954597	-1.842899
H	-4.046896	1.813385	-1.758431
H	-2.393664	3.237307	-2.809422
H	-2.907861	3.944799	-1.293079

conf_39

C	-2.338598	3.102697	-1.736184
C	-0.880160	3.226941	-1.299877
C	0.017354	2.132293	-1.859079
C	1.500020	2.363135	-1.576614
C	2.373283	1.289855	-2.151681
C	3.500321	0.781872	-1.629596
C	4.195501	1.213374	-0.379539
C	4.681583	0.068308	0.510226
C	3.574891	-0.767885	1.147579
C	2.560909	0.054714	1.933752
C	1.644601	-0.777359	2.822334
C	0.668486	0.050621	3.653462
C	-0.344164	0.848379	2.839420
C	-1.331870	1.611849	3.709637
H	-2.046207	2.179867	3.106922
H	-0.814904	2.320761	4.363190
H	-1.901261	0.929880	4.348572

H	-0.902488	0.160532	2.191398
H	0.176994	1.556736	2.182648
H	1.237691	0.736489	4.293983
H	0.125272	-0.614285	4.335563
H	2.264978	-1.381482	3.494434
H	1.086934	-1.503913	2.211010
H	1.963894	0.665051	1.242902
H	3.097385	0.775204	2.565808
H	4.038343	-1.502080	1.816507
H	3.059694	-1.362490	0.379780
H	5.347168	-0.583796	-0.067647
H	5.297720	0.498009	1.307546
H	3.575491	1.908353	0.192478
H	5.073129	1.793673	-0.694999
H	4.033445	0.031605	-2.217513
H	2.077513	0.940508	-3.143870
H	1.667922	2.469607	-0.499435
H	1.792966	3.324550	-2.020206
H	-0.293410	1.163883	-1.445786
H	-0.134825	2.055578	-2.944003
H	-0.499600	4.200730	-1.629309
H	-0.807121	3.234707	-0.204761
C	-3.028869	1.793861	-1.358683
C	-3.107507	1.562301	0.144328
C	-3.937635	0.332418	0.539507
C	-3.291109	-0.944837	0.105288
O	-3.455438	-1.531295	-0.930022
O	-2.411402	-1.398861	1.045928
C	-1.804244	-2.641936	0.738790
C	-0.778924	-2.529331	-0.355103
C	-0.621068	-3.523772	-1.318909
C	0.361198	-3.416256	-2.295938
C	1.172137	-2.301861	-2.303298
N	0.995172	-1.355606	-1.373009
C	0.062897	-1.433100	-0.416162
H	0.006865	-0.604299	0.279118
H	1.614078	-0.520851	-1.411633
H	1.958180	-2.127771	-3.027214
H	0.490037	-4.180298	-3.051895
H	-1.282596	-4.384121	-1.311654
H	-2.562058	-3.375760	0.455549
H	-1.325780	-2.963611	1.667168
H	-4.919364	0.377310	0.062808
H	-4.070111	0.306855	1.623305
H	-3.569509	2.434559	0.619845
H	-2.106052	1.477537	0.581158
H	-2.532640	0.946214	-1.846747
H	-4.045795	1.806035	-1.766935
H	-2.391786	3.224088	-2.824512
H	-2.905879	3.939245	-1.311722

conf_92

C	-1.249559	-2.914450	-1.553515
C	0.262429	-3.125878	-1.561030
C	0.947649	-2.554844	-0.326136
C	2.462376	-2.760529	-0.306855
C	3.104917	-2.089234	0.866460
C	4.022780	-1.110734	0.835429
C	4.657622	-0.497256	-0.377842
C	4.090886	0.881244	-0.741815
C	2.659284	0.807418	-1.253613
C	1.939702	2.145442	-1.362734
C	0.432894	1.978322	-1.505250
C	-0.344570	3.286365	-1.475368
C	-1.859797	3.100959	-1.485655
C	-2.399040	2.506709	-2.780080
H	-2.006027	1.503030	-2.965846
H	-2.128789	3.130511	-3.637802
H	-3.489587	2.433747	-2.757816
H	-2.337888	4.071259	-1.312308
H	-2.151431	2.460317	-0.640848
H	-0.047254	3.910887	-2.327217
H	-0.054820	3.850093	-0.577810
H	0.065893	1.333468	-0.691771
H	0.217457	1.430455	-2.429655
H	2.336027	2.722385	-2.206268
H	2.152400	2.753481	-0.471668
H	2.079822	0.153657	-0.590709
H	2.647213	0.301380	-2.226797
H	4.145331	1.540120	0.137174
H	4.735180	1.346895	-1.494589
H	4.560396	-1.161898	-1.240962
H	5.730649	-0.401526	-0.182190
H	4.397663	-0.745268	1.793536
H	2.809551	-2.474445	1.845920
H	2.887456	-2.389905	-1.243295
H	2.678277	-3.835353	-0.267270
H	0.746353	-1.477962	-0.283352
H	0.500341	-3.000560	0.573370
H	0.477944	-4.198148	-1.627235
H	0.697633	-2.668547	-2.459303
C	-1.662058	-1.447558	-1.629960
C	-3.163607	-1.199498	-1.533044
C	-3.800256	-1.732753	-0.240039
C	-3.041522	-1.305904	0.976471
O	-2.375715	-2.018162	1.686518
O	-3.150493	0.025946	1.200304
C	-2.563497	0.509423	2.405909
C	-1.117366	0.894078	2.235874
C	-0.708382	2.224983	2.309931
C	0.633415	2.568467	2.185540
C	1.554105	1.571190	1.957571
N	1.138298	0.300014	1.872614

C	-0.141556	-0.067159	2.014041
H	-0.371964	-1.122951	1.936493
H	1.843503	-0.417641	1.632309
H	2.614468	1.739854	1.822715
H	0.961125	3.598158	2.249023
H	-1.448814	3.002459	2.470387
H	-2.660435	-0.246603	3.189046
H	-3.146795	1.388490	2.678847
H	-3.823186	-2.822729	-0.229455
H	-4.827422	-1.366547	-0.160374
H	-3.680094	-1.671612	-2.374950
H	-3.357040	-0.125739	-1.608667
H	-1.293869	-1.018292	-2.569498
H	-1.165516	-0.874622	-0.835731
H	-1.658139	-3.373303	-0.645738
H	-1.695133	-3.452174	-2.398308

conf_68

C	-2.563650	-1.415132	-2.630632
C	-3.880319	-0.742751	-2.248367
C	-3.779012	0.328955	-1.165334
C	-2.926168	1.529213	-1.576375
C	-2.964208	2.657467	-0.592935
C	-1.950058	3.462736	-0.240540
C	-0.538303	3.410028	-0.737793
C	0.492496	3.792092	0.326424
C	1.935388	3.554735	-0.110667
C	2.337112	2.084716	-0.113534
C	3.763355	1.826153	-0.576705
C	4.162112	0.360474	-0.473822
C	5.554653	0.061718	-1.012272
C	5.936606	-1.404867	-0.881064
H	5.932190	-1.722888	0.166820
H	6.936414	-1.595728	-1.278570
H	5.235875	-2.046250	-1.425836
H	6.286590	0.683831	-0.483143
H	5.603851	0.364280	-2.065269
H	3.428504	-0.258316	-1.010713
H	4.116691	0.047431	0.580038
H	4.455857	2.436637	0.016165
H	3.872535	2.163775	-1.614930
H	1.659814	1.506501	-0.759768
H	2.215580	1.689663	0.906868
H	2.608976	4.098954	0.559977
H	2.090842	3.982780	-1.108991
H	0.349658	4.847018	0.583996
H	0.304840	3.234041	1.255467
H	-0.442000	4.111719	-1.577597
H	-0.315534	2.426749	-1.167286
H	-2.173572	4.281593	0.444214
H	-3.946573	2.876412	-0.172122
H	-3.307833	1.909013	-2.534995

H	-1.894454	1.223107	-1.778156
H	-4.788850	0.681465	-0.924907
H	-3.388368	-0.112499	-0.238895
H	-4.321540	-0.289683	-3.143911
H	-4.588718	-1.511539	-1.918660
C	-1.939674	-2.245048	-1.516248
C	-0.633942	-2.907415	-1.936627
C	-0.074249	-3.864015	-0.882152
C	0.155789	-3.207258	0.443059
O	-0.302801	-3.543672	1.503177
O	0.968973	-2.124114	0.333299
C	1.226589	-1.452619	1.562014
C	-0.000398	-0.723784	2.039032
C	-0.693342	-1.089579	3.192222
C	-1.840042	-0.401696	3.575623
C	-2.291304	0.636009	2.788798
N	-1.614711	0.961952	1.679156
C	-0.503644	0.323361	1.290665
H	-0.041560	0.670744	0.375708
H	-1.965822	1.733645	1.076612
H	-3.178688	1.217638	3.004648
H	-2.388510	-0.676035	4.467708
H	-0.339892	-1.931532	3.777239
H	2.032333	-0.752776	1.337950
H	1.560345	-2.162451	2.321090
H	0.883005	-4.274092	-1.221493
H	-0.753848	-4.699585	-0.704985
H	0.114376	-2.142741	-2.170564
H	-0.792896	-3.478081	-2.857369
H	-2.654725	-3.012899	-1.193178
H	-1.758186	-1.615715	-0.633209
H	-1.841043	-0.667309	-2.981879
H	-2.746794	-2.069219	-3.490589

conf_34

C	4.029694	-1.813799	-1.190428
C	3.870514	-0.398545	-1.744456
C	3.257688	0.586162	-0.756744
C	3.134299	2.000811	-1.328385
C	2.681781	3.028129	-0.334220
C	1.454066	3.561939	-0.244712
C	0.265985	3.189808	-1.080230
C	-1.055434	3.280301	-0.312454
C	-2.163400	2.457042	-0.952448
C	-3.473049	2.493498	-0.173133
C	-4.489835	1.452957	-0.635290
C	-4.100501	0.026734	-0.265720
C	-5.094685	-1.031425	-0.722577
C	-4.666381	-2.440129	-0.337819
H	-3.696433	-2.692362	-0.781697
H	-5.386277	-3.189105	-0.676850
H	-4.575412	-2.543148	0.749452

H	-5.213570	-0.966914	-1.810696
H	-6.080920	-0.814637	-0.295484
H	-3.995029	-0.032468	0.829012
H	-3.117421	-0.214678	-0.690866
H	-4.623084	1.526874	-1.722314
H	-5.466720	1.679995	-0.193725
H	-3.906659	3.496937	-0.248405
H	-3.266321	2.335949	0.895869
H	-1.817084	1.419836	-1.057940
H	-2.337047	2.808405	-1.977183
H	-0.914814	2.938404	0.724115
H	-1.361556	4.328813	-0.221940
H	0.389811	2.176609	-1.480949
H	0.215735	3.847904	-1.957290
H	1.296783	4.362877	0.479540
H	3.448492	3.406973	0.342706
H	2.462434	1.981003	-2.191311
H	4.113471	2.312815	-1.710460
H	2.259289	0.235257	-0.471339
H	3.863808	0.604894	0.160603
H	4.856276	-0.029687	-2.049812
H	3.263433	-0.413449	-2.657529
C	2.733917	-2.489490	-0.746670
C	1.737500	-2.729130	-1.875632
C	0.402532	-3.281933	-1.371313
C	-0.284533	-2.252488	-0.528889
O	-0.525908	-1.121014	-0.875499
O	-0.581287	-2.700843	0.708703
C	-1.170823	-1.737589	1.587513
C	-0.110400	-0.797013	2.093454
C	0.699188	-1.115388	3.182243
C	1.729737	-0.265651	3.574667
C	1.950590	0.887240	2.854357
N	1.152927	1.177575	1.816889
C	0.144149	0.390539	1.426463
H	-0.422145	0.705721	0.560574
H	1.379531	2.005808	1.231223
H	2.745820	1.590763	3.066411
H	2.364057	-0.501086	4.419706
H	0.528278	-2.040786	3.723640
H	-1.594149	-2.319804	2.405153
H	-1.966617	-1.196361	1.074420
H	0.533860	-4.202280	-0.798938
H	-0.258968	-3.497979	-2.216489
H	2.161459	-3.433024	-2.598581
H	1.537109	-1.800685	-2.418635
H	2.259905	-1.887745	0.041903
H	2.976187	-3.449530	-0.276052
H	4.721170	-1.785866	-0.339349
H	4.514792	-2.437885	-1.949801

conf_57

C	2.806363	-1.093621	-1.399273
C	3.837485	-1.008033	-0.280610
C	4.854852	0.117118	-0.437306
C	4.254721	1.513812	-0.582294
C	3.446288	1.973984	0.593014
C	2.450911	2.874051	0.564974
C	1.945725	3.593189	-0.649294
C	0.463082	3.954320	-0.600385
C	-0.429373	2.732769	-0.450740
C	-1.919402	2.993498	-0.607015
C	-2.753686	1.744671	-0.354718
C	-4.251085	1.943859	-0.535046
C	-5.061252	0.685241	-0.253043
C	-6.557234	0.878947	-0.450306
H	-6.782252	1.173987	-1.479601
H	-6.943158	1.661817	0.209617
H	-7.113034	-0.038087	-0.238974
H	-4.870048	0.358984	0.779272
H	-4.707942	-0.124091	-0.906768
H	-4.450763	2.281613	-1.559787
H	-4.593473	2.752299	0.123432
H	-2.561643	1.391237	0.670400
H	-2.417794	0.942739	-1.029707
H	-2.120609	3.373678	-1.615820
H	-2.228227	3.786083	0.085797
H	-0.259423	2.296835	0.542892
H	-0.119069	1.975955	-1.188633
H	0.274815	4.649773	0.226811
H	0.201906	4.492687	-1.517497
H	2.150239	3.004901	-1.550658
H	2.534895	4.513681	-0.758546
H	2.027745	3.200297	1.517553
H	3.790850	1.623062	1.568844
H	3.664821	1.581432	-1.501537
H	5.077622	2.228959	-0.715913
H	5.537140	0.104863	0.420840
H	5.475539	-0.082595	-1.317491
H	3.318442	-0.909474	0.683850
H	4.375763	-1.960618	-0.218429
C	1.903698	-2.311832	-1.267485
C	0.786506	-2.360454	-2.302696
C	-0.226511	-3.484435	-2.044776
C	-0.830323	-3.327963	-0.684179
O	-0.622773	-4.007367	0.283395
O	-1.624323	-2.219714	-0.624407
C	-2.074337	-1.893349	0.682380
C	-0.945118	-1.302389	1.482309
C	-0.703101	-1.628521	2.813935
C	0.363302	-1.054493	3.499559
C	1.180368	-0.162685	2.839940
N	0.931063	0.131357	1.555947

C	-0.086485	-0.403837	0.872472
H	-0.190096	-0.104142	-0.161370
H	1.551950	0.812633	1.081168
H	2.033562	0.326346	3.292495
H	0.567428	-1.304738	4.532802
H	-1.342270	-2.349172	3.313761
H	-2.473661	-2.774405	1.187610
H	-2.870879	-1.159541	0.543389
H	0.254584	-4.463276	-2.078371
H	-1.018661	-3.454379	-2.797630
H	1.210206	-2.498172	-3.302247
H	0.252714	-1.402665	-2.327364
H	1.477207	-2.331169	-0.254707
H	2.505892	-3.225669	-1.335832
H	3.318193	-1.114464	-2.369692
H	2.188448	-0.183145	-1.413986

conf_27

C	4.737636	-0.704138	-0.908020
C	4.168163	0.677052	-1.224178
C	3.254748	1.228963	-0.138589
C	2.800588	2.662383	-0.410525
C	1.931772	3.226221	0.671404
C	0.777564	3.897127	0.532062
C	0.096059	4.280408	-0.743647
C	-1.405343	3.988703	-0.766648
C	-1.706333	2.508641	-0.595431
C	-3.152085	2.098398	-0.827003
C	-3.362921	0.607124	-0.599674
C	-4.787272	0.125834	-0.830233
C	-4.955794	-1.369882	-0.596368
C	-6.379793	-1.855522	-0.821585
H	-6.704913	-1.656114	-1.847080
H	-7.079154	-1.349465	-0.149167
H	-6.470583	-2.930789	-0.648013
H	-4.645767	-1.610441	0.430424
H	-4.274399	-1.916449	-1.263033
H	-5.092166	0.369494	-1.855721
H	-5.469957	0.676950	-0.171004
H	-3.066203	0.357796	0.430982
H	-2.686190	0.046845	-1.262960
H	-3.449121	2.360348	-1.849654
H	-3.810081	2.669713	-0.160604
H	-1.425152	2.212167	0.423657
H	-1.061066	1.937860	-1.281493
H	-1.912014	4.563330	0.018302
H	-1.814971	4.342458	-1.718597
H	0.574448	3.794809	-1.599488
H	0.250202	5.358499	-0.882487
H	0.306843	4.281217	1.439331

H	2.341373	3.138893	1.681266
H	2.298788	2.713041	-1.381217
H	3.692315	3.297576	-0.498945
H	2.377140	0.576781	-0.049180
H	3.769158	1.183901	0.831316
H	5.001591	1.372385	-1.376730
H	3.622774	0.653710	-2.176091
C	3.706811	-1.800244	-0.645412
C	2.758035	-2.047194	-1.812263
C	1.895782	-3.308040	-1.648487
C	1.004139	-3.218580	-0.450886
O	1.244097	-3.612400	0.659171
O	-0.160836	-2.571485	-0.737988
C	-1.042394	-2.442217	0.370290
C	-0.527609	-1.423413	1.348374
C	-0.416702	-1.669464	2.715031
C	0.066039	-0.686977	3.573060
C	0.445960	0.530365	3.049525
N	0.338150	0.739263	1.730691
C	-0.128132	-0.184905	0.882768
H	-0.165927	0.091448	-0.162755
H	0.637304	1.653239	1.340913
H	0.839997	1.347168	3.640767
H	0.161857	-0.866314	4.636330
H	-0.694212	-2.642704	3.106222
H	-1.175442	-3.404716	0.867569
H	-1.995397	-2.117348	-0.052000
H	2.537504	-4.180328	-1.507381
H	1.282349	-3.458700	-2.539461
H	3.338051	-2.167026	-2.733859
H	2.105095	-1.181555	-1.976792
H	3.134517	-1.572889	0.262802
H	4.240150	-2.730874	-0.420810
H	5.392947	-0.626183	-0.032368
H	5.381667	-1.015354	-1.738684

conf_12

C	5.009598	-0.719073	0.145440
C	4.533546	0.650321	-0.333921
C	3.391712	1.223548	0.493141
C	2.992734	2.637484	0.071996
C	1.890808	3.201549	0.912951
C	0.776610	3.815407	0.486392
C	0.400472	4.087117	-0.942509
C	-0.473777	2.996402	-1.570149
C	-1.805664	2.779073	-0.864374
C	-2.577432	1.571088	-1.381253
C	-3.687680	1.121877	-0.441918
C	-4.397574	-0.145539	-0.893387
C	-5.413288	-0.665919	0.114487
C	-6.089939	-1.953269	-0.331083
H	-6.626392	-1.810132	-1.273791

H	-6.812350	-2.305221	0.409488
H	-5.358880	-2.753868	-0.488833
H	-6.170230	0.106633	0.294644
H	-4.913331	-0.824743	1.080476
H	-3.651979	-0.930288	-1.089089
H	-4.894195	0.032839	-1.855237
H	-4.419747	1.929906	-0.320724
H	-3.262538	0.956219	0.559246
H	-1.880863	0.733138	-1.533937
H	-2.989117	1.787575	-2.374017
H	-2.421185	3.681830	-0.956258
H	-1.638374	2.656824	0.213987
H	-0.651497	3.241769	-2.622799
H	0.095815	2.055333	-1.580280
H	1.301461	4.215212	-1.548221
H	-0.135277	5.041586	-0.982570
H	0.095279	4.196964	1.246667
H	2.054264	3.141410	1.991259
H	2.720778	2.648154	-0.987979
H	3.871352	3.289144	0.170779
H	2.522258	0.557958	0.415334
H	3.673740	1.224555	1.554453
H	5.379293	1.346680	-0.301483
H	4.230235	0.600787	-1.387394
C	3.950322	-1.819382	0.151895
C	3.363626	-2.111963	-1.223427
C	2.460023	-3.352905	-1.255830
C	1.226602	-3.174714	-0.428354
O	1.068229	-3.492901	0.718753
O	0.238996	-2.547269	-1.134020
C	-0.986306	-2.412933	-0.434092
C	-0.927330	-1.338162	0.614749
C	-1.625328	-1.430749	1.816743
C	-1.568203	-0.401271	2.749197
C	-0.810511	0.714912	2.466923
N	-0.146515	0.779315	1.305494
C	-0.182755	-0.195050	0.390218
H	0.399916	-0.041993	-0.509099
H	0.397891	1.637834	1.092820
H	-0.711179	1.564022	3.131043
H	-2.100629	-0.464046	3.689626
H	-2.208484	-2.320748	2.030676
H	-1.269670	-3.361472	0.027175
H	-1.725735	-2.150168	-1.194452
H	2.997224	-4.213516	-0.851459
H	2.164316	-3.570775	-2.284396
H	4.178582	-2.282749	-1.935260
H	2.806711	-1.248516	-1.607255
H	3.149614	-1.574506	0.860821
H	4.405800	-2.736811	0.541532
H	5.415144	-0.618786	1.159102
H	5.848186	-1.038971	-0.483921

conf_81

C	-0.349493	-0.280757	3.103983
C	-1.711526	-0.925907	3.361286
C	-2.574378	-1.096937	2.112493
C	-3.291507	0.187318	1.690808
C	-3.934298	0.065092	0.343253
C	-4.104052	1.032302	-0.569830
C	-3.765474	2.485244	-0.423029
C	-2.493474	2.913623	-1.164355
C	-1.222940	2.568004	-0.400937
C	0.059795	2.863035	-1.165410
C	1.318197	2.500858	-0.388569
C	2.607455	2.813951	-1.136621
C	3.872064	2.337661	-0.426104
C	4.092108	2.970597	0.941670
H	4.102498	4.063337	0.874171
H	5.048777	2.659470	1.369430
H	3.310901	2.691648	1.655487
H	4.734422	2.556352	-1.065172
H	3.834396	1.245974	-0.326693
H	2.669240	3.896411	-1.307851
H	2.563424	2.356848	-2.134872
H	1.307322	1.431130	-0.132814
H	1.304258	3.032089	0.570162
H	0.085609	3.928073	-1.425480
H	0.050426	2.336172	-2.132671
H	-1.245305	1.510077	-0.095967
H	-1.212983	3.126143	0.543865
H	-2.473923	2.456589	-2.163519
H	-2.521609	3.995158	-1.332081
H	-3.675675	2.753545	0.634228
H	-4.615734	3.054621	-0.812605
H	-4.608403	0.763527	-1.499320
H	-4.346724	-0.920694	0.114456
H	-2.600969	1.035547	1.706928
H	-4.064051	0.413235	2.438245
H	-1.948934	-1.465101	1.288412
H	-3.326403	-1.875410	2.283769
H	-1.548708	-1.904203	3.827303
H	-2.267254	-0.331804	4.095792
C	0.627140	-1.198719	2.376776
C	2.018880	-0.599136	2.226351
C	3.018028	-1.554011	1.565513
C	2.574753	-1.999220	0.206597
O	2.318920	-3.121540	-0.141701
O	2.458736	-0.947194	-0.647118
C	2.019164	-1.284645	-1.958450
C	0.565583	-1.674430	-1.941601
C	0.130662	-2.970444	-2.212517
C	-1.220523	-3.291403	-2.130946
C	-2.115778	-2.317183	-1.747516
N	-1.672379	-1.079872	-1.482442

C	-0.381388	-0.736520	-1.575213
H	-0.133044	0.287698	-1.327644
H	-2.359438	-0.384178	-1.136839
H	-3.178753	-2.484852	-1.629910
H	-1.574575	-4.293239	-2.337880
H	0.859388	-3.732943	-2.464774
H	2.623104	-2.096947	-2.366878
H	2.175810	-0.382506	-2.551447
H	3.155780	-2.455515	2.165137
H	3.989254	-1.059564	1.461207
H	2.411695	-0.333489	3.213139
H	1.970624	0.331922	1.653095
H	0.232401	-1.458364	1.384060
H	0.700192	-2.148826	2.921650
H	0.091907	0.005711	4.065196
H	-0.467527	0.655087	2.540534

conf_56

C	-3.627252	-0.028965	-0.726382
C	-3.789819	1.162197	0.211758
C	-3.658907	2.510151	-0.493305
C	-2.216256	2.926414	-0.774608
C	-1.479583	3.383213	0.449999
C	-0.154602	3.562086	0.558728
C	0.864203	3.298417	-0.510921
C	2.282752	3.176915	0.039761
C	3.324340	2.837355	-1.022172
C	3.265458	1.402900	-1.542834
C	3.663063	0.356223	-0.509219
C	3.662257	-1.061228	-1.065832
C	3.972425	-2.138689	-0.029677
C	5.391266	-2.076439	0.520180
H	5.584609	-2.899779	1.212546
H	5.580115	-1.144036	1.059110
H	6.124637	-2.145953	-0.289094
H	3.806690	-3.124930	-0.479343
H	3.260823	-2.056705	0.805856
H	4.392156	-1.129368	-1.882305
H	2.687131	-1.256530	-1.533804
H	2.988951	0.397308	0.359390
H	4.657110	0.604871	-0.119568
H	3.938597	1.314876	-2.403081
H	2.264758	1.174986	-1.936061
H	4.324026	3.018504	-0.611263
H	3.211997	3.535148	-1.860448
H	2.547986	4.127087	0.516854
H	2.310615	2.427647	0.842962
H	0.836647	4.124161	-1.235644
H	0.587953	2.409894	-1.094122
H	0.223690	4.010231	1.478897

H	-2.100337	3.677948	1.297208
H	-2.215013	3.761978	-1.487494
H	-1.669182	2.122539	-1.284576
H	-4.216283	2.475006	-1.435352
H	-4.134051	3.293961	0.107340
H	-4.767758	1.095402	0.700983
H	-3.049353	1.098044	1.024050
C	-3.571585	-1.357977	0.016010
C	-3.582753	-2.600883	-0.871424
C	-2.505752	-2.615851	-1.966156
C	-1.155335	-2.251665	-1.437825
O	-0.490111	-1.306762	-1.786527
O	-0.752964	-3.084837	-0.452353
C	0.464419	-2.718048	0.201288
C	0.184382	-1.617650	1.189879
C	-0.178825	-1.895103	2.506123
C	-0.545095	-0.872245	3.376201
C	-0.565588	0.421315	2.905403
N	-0.199355	0.667697	1.639312
C	0.183606	-0.289464	0.787246
H	0.448469	0.015623	-0.216159
H	-0.281926	1.645670	1.289323
H	-0.868124	1.276868	3.496246
H	-0.829073	-1.076855	4.400576
H	-0.186652	-2.924228	2.851716
H	1.209515	-2.412050	-0.532058
H	0.803115	-3.618177	0.712199
H	-2.730695	-1.905338	-2.762462
H	-2.450327	-3.614077	-2.411376
H	-4.554832	-2.691158	-1.366637
H	-3.468964	-3.489319	-0.244019
H	-4.420244	-1.422910	0.706942
H	-2.675026	-1.374283	0.652584
H	-2.724316	0.095924	-1.335853
H	-4.468251	-0.036927	-1.431526

conf_61

C	4.827679	0.091868	-0.466164
C	4.081406	1.401622	-0.718814
C	2.922162	1.632756	0.240715
C	2.347510	3.046059	0.193990
C	1.238193	3.239261	1.178718
C	0.010551	3.725684	0.943078
C	-0.537744	4.249026	-0.345779
C	-1.945661	3.757512	-0.680874
C	-2.011637	2.306307	-1.137241
C	-3.427930	1.872671	-1.493930
C	-3.553205	0.442360	-2.006297
C	-3.264389	-0.635807	-0.968621
C	-3.589433	-2.037225	-1.469077
C	-3.352946	-3.118891	-0.426936
H	-2.295433	-3.147213	-0.147752

H	-3.621461	-4.108342	-0.805929
H	-3.952096	-2.938613	0.473474
H	-2.983396	-2.249904	-2.357062
H	-4.635543	-2.065155	-1.796597
H	-3.858921	-0.429489	-0.065690
H	-2.208090	-0.605235	-0.668972
H	-2.891340	0.301868	-2.870675
H	-4.572751	0.296357	-2.381887
H	-3.816132	2.559221	-2.255512
H	-4.079200	2.001341	-0.617759
H	-1.605176	1.647786	-0.360228
H	-1.360166	2.171330	-2.011138
H	-2.601963	3.905331	0.187948
H	-2.356881	4.392576	-1.472773
H	0.137820	4.032434	-1.178292
H	-0.563460	5.343103	-0.253849
H	-0.650839	3.851610	1.804152
H	1.497995	3.008981	2.214876
H	2.019327	3.280473	-0.822150
H	3.147803	3.759354	0.431275
H	2.117676	0.928568	-0.009399
H	3.240959	1.403379	1.267406
H	4.793178	2.230162	-0.631099
H	3.707231	1.437603	-1.749082
C	3.953480	-1.157473	-0.384863
C	3.145666	-1.436018	-1.645627
C	2.356952	-2.754096	-1.605500
C	1.151537	-2.689783	-0.719401
O	0.035507	-2.396603	-1.058863
O	1.442654	-2.983194	0.578944
C	0.325397	-3.107403	1.441306
C	-0.359100	-1.806221	1.758320
C	-1.611016	-1.788001	2.372502
C	-2.248258	-0.584943	2.647717
C	-1.631576	0.594424	2.291175
N	-0.424483	0.551483	1.713200
C	0.220075	-0.591401	1.450628
H	1.190085	-0.502521	0.980794
H	0.010369	1.449921	1.429571
H	-2.064994	1.575705	2.435730
H	-3.225087	-0.560391	3.113299
H	-2.101458	-2.723542	2.622201
H	0.720268	-3.552643	2.357572
H	-0.408365	-3.793273	1.007333
H	3.008023	-3.566246	-1.271700
H	1.983670	-2.989454	-2.603752
H	3.828802	-1.491283	-2.499808
H	2.456016	-0.612499	-1.866626
H	3.290511	-1.090718	0.486885
H	4.597353	-2.021193	-0.182976
H	5.386337	0.179967	0.473061
H	5.579136	-0.045094	-1.252055

conf_79

C	4.835375	-0.844369	-0.421869
C	4.468932	0.518996	-1.011691
C	3.834347	1.533335	-0.060845
C	2.335323	1.328888	0.191599
C	1.762896	2.404007	1.065448
C	1.063178	3.477521	0.665801
C	0.709877	3.861640	-0.735290
C	-0.715719	4.393532	-0.894455
C	-1.812427	3.394759	-0.540279
C	-1.782320	2.110142	-1.357769
C	-2.951249	1.178572	-1.068812
C	-2.882597	-0.135143	-1.834034
C	-4.025865	-1.087822	-1.513453
C	-3.946346	-2.394934	-2.288617
H	-2.995706	-2.911130	-2.112544
H	-4.015470	-2.214289	-3.365246
H	-4.756645	-3.076594	-2.017515
H	-4.980296	-0.592099	-1.725940
H	-4.037828	-1.288035	-0.431769
H	-1.924444	-0.635976	-1.630562
H	-2.878109	0.073068	-2.911404
H	-3.889650	1.692279	-1.311175
H	-3.005216	0.971989	0.010449
H	-0.838266	1.572910	-1.186286
H	-1.778277	2.362769	-2.425759
H	-2.786110	3.879247	-0.675214
H	-1.757209	3.152870	0.531336
H	-0.833486	5.290770	-0.275870
H	-0.848685	4.720758	-1.931323
H	0.894588	3.036283	-1.428337
H	1.405015	4.657760	-1.033972
H	0.773619	4.199642	1.431089
H	2.024021	2.339437	2.122892
H	2.189840	0.355383	0.672618
H	1.819010	1.296806	-0.775147
H	4.368653	1.527502	0.897351
H	3.964409	2.539433	-0.473986
H	5.396469	0.961274	-1.389812
H	3.828249	0.395662	-1.894767
C	3.700975	-1.792986	-0.031566
C	2.744362	-2.100822	-1.177371
C	1.809348	-3.292828	-0.926511
C	0.827711	-3.048174	0.176804
O	1.056763	-3.018876	1.355935
O	-0.429243	-2.823961	-0.308790
C	-1.450069	-2.739053	0.666921
C	-1.510689	-1.409689	1.363018
C	-2.422666	-1.183425	2.393437
C	-2.475304	0.045676	3.038577
C	-1.604528	1.041115	2.648747
N	-0.742054	0.800565	1.654678

C	-0.675154	-0.369165	1.008746
H	0.055321	-0.441107	0.215566
H	-0.084604	1.554820	1.372789
H	-1.567730	2.025346	3.097858
H	-3.178908	0.230815	3.840074
H	-3.096419	-1.978451	2.699036
H	-1.318518	-3.524644	1.416991
H	-2.384182	-2.912287	0.128027
H	2.404948	-4.161300	-0.629610
H	1.263311	-3.542789	-1.837406
H	3.326824	-2.339123	-2.074468
H	2.148241	-1.218193	-1.440669
H	3.151536	-1.419445	0.838660
H	4.152679	-2.733081	0.306282
H	5.474550	-0.685933	0.454896
H	5.464347	-1.362266	-1.156266

C18:1 9E pyridylcarbinol ester**conf_2**

C	-3.968422	0.337344	0.838983
C	-5.110883	-0.198045	-0.019682
C	-4.723104	-0.823658	-1.357248
C	-3.882299	-2.092177	-1.222095
C	-2.412058	-1.839793	-1.113313
O	-1.801890	-0.960398	-1.671031
O	-1.793999	-2.758905	-0.337658
C	-0.368333	-2.690068	-0.304692
C	0.117925	-1.631657	0.648532
C	0.446119	-1.921095	1.970800
C	0.889716	-0.919269	2.830394
C	0.989212	0.368992	2.354903
N	0.662590	0.622564	1.080223
C	0.244146	-0.317043	0.229833
H	-0.013982	0.001179	-0.771484
H	0.678020	1.597168	0.719718
H	1.315495	1.211181	2.951774
H	1.153423	-1.134843	3.857909
H	0.360728	-2.940827	2.332734
H	0.017480	-2.504130	-1.309339
H	-0.043999	-3.674822	0.030165
H	-4.207162	-2.715819	-0.385219
H	-3.988868	-2.709042	-2.123912
H	-5.640895	-1.080662	-1.892885
H	-4.189262	-0.107893	-1.990208
H	-5.669874	-0.941224	0.561794
H	-5.813429	0.621327	-0.211581
C	-3.229119	1.532830	0.246059
C	-2.348109	2.226557	1.278800
C	-1.546028	3.419287	0.750209
C	-0.504299	3.112738	-0.282708

C	0.750398	3.584108	-0.268226	H	0.141470	-0.015015	-0.911549
C	1.735169	3.476485	-1.392708	H	-0.347477	1.415015	0.847527
C	3.193795	3.340994	-0.955535	H	-0.975868	0.766744	2.983525
C	3.539842	2.053024	-0.215921	H	-1.163848	-1.691973	3.511535
C	3.368071	0.787909	-1.046671	H	-0.620032	-3.331851	1.708729
C	3.797098	-0.482027	-0.324071	H	0.051992	-3.796724	-0.528859
C	3.655330	-1.734516	-1.180892	H	-0.497625	-2.611481	-1.737201
C	4.214895	-3.002935	-0.543370	H	3.772650	-2.375100	-2.057645
C	3.464862	-3.466886	0.697629	H	4.426703	-3.405307	-0.768756
H	3.481738	-2.714111	1.492169	H	5.476518	-1.230655	-0.580587
H	2.417572	-3.686076	0.458852	H	4.419064	-1.463377	0.800952
H	3.902357	-4.381248	1.106015	H	2.662359	-0.061960	-0.339456
H	5.269368	-2.838783	-0.291305	H	3.729366	0.142578	-1.716429
H	4.205653	-3.807304	-1.286421	C	3.892710	2.558253	-0.526224
H	2.596279	-1.887610	-1.437698	C	2.393825	2.836951	-0.440487
H	4.168222	-1.562905	-2.134425	C	1.870422	2.944988	0.983698
H	3.223166	-0.591101	0.606677	C	0.421004	3.308744	1.121902
H	4.844523	-0.378789	-0.012481	C	-0.429450	3.598599	0.128417
H	2.327143	0.684529	-1.383027	C	-1.842829	4.060661	0.304179
H	3.955873	0.890224	-1.967687	C	-2.820777	3.442174	-0.695868
H	2.947690	1.983677	0.708709	C	-2.818547	1.922028	-0.664082
H	4.581280	2.111746	0.120468	C	-3.855947	1.266556	-1.564337
H	3.450808	4.198866	-0.323088	C	-3.716292	-0.250979	-1.649354
H	3.830787	3.421162	-1.843160	C	-3.936373	-0.983299	-0.331198
H	1.444722	2.668388	-2.073508	C	-3.855673	-2.498430	-0.460399
H	1.648394	4.399295	-1.981657	C	-4.121544	-3.226034	0.848620
H	1.058338	4.201402	0.580258	H	-4.033408	-4.309688	0.735419
H	-0.829294	2.542403	-1.155916	H	-3.421443	-2.911734	1.631014
H	-2.255222	4.127957	0.300023	H	-5.129792	-3.014404	1.216500
H	-1.078453	3.954625	1.584209	H	-2.866965	-2.778100	-0.850283
H	-1.678316	1.490945	1.742800	H	-4.573733	-2.834356	-1.217390
H	-2.986313	2.586699	2.093646	H	-3.204533	-0.650964	0.418396
H	-2.640136	1.211468	-0.619950	H	-4.919468	-0.708273	0.073128
H	-3.960602	2.257278	-0.135026	H	-2.719563	-0.499665	-2.044966
H	-3.250683	-0.465230	1.066542	H	-4.430466	-0.634192	-2.386980
H	-4.387142	0.630779	1.809412	H	-4.861659	1.523429	-1.209001
conf_17				H	-3.772017	1.691072	-2.571587
C	4.358270	1.219183	0.041391	H	-2.961918	1.586811	0.372244
C	3.720717	0.006405	-0.626482	H	-1.825252	1.567963	-0.975907
C	4.425565	-1.299275	-0.282263	H	-2.573468	3.784421	-1.708410
C	3.816036	-2.522755	-0.976577	H	-3.827805	3.817417	-0.485274
C	2.446887	-2.812143	-0.446729	H	-2.172759	3.865483	1.331975
O	2.187765	-3.224371	0.653804	H	-1.858849	5.151422	0.182446
O	1.468454	-2.517615	-1.342271	H	-0.068505	3.559194	-0.900295
C	0.147520	-2.764185	-0.870611	H	0.055244	3.404935	2.147781
C	-0.215936	-1.820331	0.243189	H	2.060192	2.009498	1.531090
C	-0.583943	-2.266133	1.511003	H	2.456415	3.698203	1.528229
C	-0.878130	-1.359177	2.521894	H	1.840181	2.061459	-0.988661
C	-0.779368	-0.010451	2.255798	H	2.188126	3.775298	-0.967003
N	-0.416447	0.393504	1.032486	H	4.431167	3.367338	-0.019020
C	-0.145485	-0.456192	0.035291	H	4.192153	2.612332	-1.579343
				H	5.445499	1.159471	-0.084458

H 4.186745 1.175169 1.124279

conf_8

C 3.517338 1.299289 -0.316664
C 4.994059 0.975592 -0.495307
C 5.387425 -0.430007 -0.052676
C 4.600368 -1.531460 -0.762782
C 3.308003 -1.882025 -0.091035
O 3.109873 -1.947995 1.092454
O 2.331820 -2.190239 -0.991150
C 1.180071 -2.796744 -0.428790
C 0.353702 -1.868343 0.418089
C -0.333706 -2.335761 1.537535
C -1.130444 -1.483423 2.290172
C -1.221418 -0.159146 1.920374
N -0.549907 0.268247 0.844393
C 0.212870 -0.532532 0.089765
H 0.711777 -0.075256 -0.755007
H -0.644554 1.271407 0.593867
H -1.809493 0.581072 2.446823
H -1.667116 -1.836479 3.161368
H -0.235576 -3.376823 1.827941
H 1.467067 -3.665306 0.169209
H 0.592859 -3.138899 -1.284490
H 4.415704 -1.296703 -1.814371
H 5.174205 -2.466957 -0.752190
H 6.451807 -0.577851 -0.252578
H 5.254418 -0.544840 1.028088
H 5.261930 1.109520 -1.551503
H 5.593735 1.702487 0.064051
C 3.158471 2.713925 -0.754391
C 1.666797 3.023132 -0.676392
C 1.145557 3.140104 0.748745
C -0.334799 3.330528 0.894607
C -1.235895 3.418941 -0.092667
C -2.679858 3.760961 0.098486
C -3.660129 2.880121 -0.675128
C -3.624846 1.417554 -0.257154
C -4.755982 0.582654 -0.842345
C -4.778185 -0.861933 -0.352854
C -3.617859 -1.722405 -0.838469
C -3.703402 -3.162547 -0.349370
C -2.612184 -4.059375 -0.912906
H -2.699317 -5.084437 -0.543662
H -2.656483 -4.096170 -2.005670
H -1.617189 -3.691902 -0.638951
H -4.683055 -3.573142 -0.619744
H -3.669391 -3.175544 0.748306
H -3.597904 -1.712541 -1.936518
H -2.659064 -1.290553 -0.517209
H -5.713581 -1.331476 -0.677779
H -4.806655 -0.871523 0.746119

H -5.708828 1.059769 -0.585851
H -4.694502 0.599231 -1.938177
H -3.676590 1.358092 0.840993
H -2.661938 0.982373 -0.552050
H -3.461124 2.960865 -1.751039
H -4.670644 3.275053 -0.524328
H -2.924189 3.746175 1.167579
H -2.814862 4.799965 -0.229780
H -0.902806 3.322744 -1.127281
H -0.688798 3.474870 1.917852
H 1.457811 2.270772 1.345979
H 1.639497 3.989276 1.239766
H 1.115286 2.244209 -1.225102
H 1.455747 3.957794 -1.206826
H 3.715959 3.439938 -0.149654
H 3.496353 2.858109 -1.786696
H 3.237991 1.132014 0.731401
H 2.921597 0.596195 -0.917125

conf_0

C 3.550825 1.016870 0.327880
C 5.018606 0.608438 0.337900
C 5.273778 -0.894464 0.379822
C 4.657618 -1.653051 -0.798827
C 3.252840 -2.106489 -0.546380
O 2.836726 -2.591353 0.473160
O 2.453558 -1.953625 -1.635170
C 1.154890 -2.520226 -1.496910
C 0.331767 -1.810141 -0.456303
C -0.237961 -2.486554 0.621704
C -0.976300 -1.803017 1.578031
C -1.119323 -0.437970 1.454793
N -0.564648 0.190308 0.412282
C 0.136859 -0.444357 -0.534800
H 0.544168 0.169249 -1.328822
H -0.684525 1.221123 0.351241
H -1.660876 0.180999 2.158405
H -1.422969 -2.317067 2.419347
H -0.080917 -3.555326 0.720295
H 1.232824 -3.579169 -1.241162
H 0.698839 -2.425066 -2.483754
H 4.700064 -1.077727 -1.726982
H 5.218168 -2.578901 -0.977296
H 6.353572 -1.064185 0.374781
H 4.896648 -1.327265 1.312240
H 5.505486 1.027281 -0.552603
H 5.514260 1.072591 1.198183
C 3.372243 2.529617 0.244504
C 1.924400 2.981738 0.083028
C 1.090426 2.842550 1.348831
C -0.380558 3.092633 1.191352
C -1.009291 3.472604 0.071246

C	-2.463128	3.810802	-0.033916
C	-3.114836	3.335920	-1.334311
C	-3.059041	1.830519	-1.571809
C	-3.779232	0.995983	-0.521447
C	-3.756956	-0.497209	-0.818887
C	-4.403883	-1.348332	0.264216
C	-4.280897	-2.844833	0.013885
C	-4.884557	-3.688934	1.125900
H	-5.950434	-3.475136	1.248227
H	-4.784154	-4.757689	0.920798
H	-4.400024	-3.487213	2.087777
H	-3.219767	-3.102440	-0.113194
H	-4.761718	-3.090848	-0.940356
H	-3.955731	-1.106499	1.239534
H	-5.463474	-1.079456	0.356796
H	-2.718875	-0.829339	-0.968473
H	-4.259211	-0.682159	-1.776430
H	-3.342976	1.177480	0.471366
H	-4.819646	1.335367	-0.442784
H	-2.008526	1.509165	-1.643418
H	-3.491609	1.612770	-2.554940
H	-2.632707	3.846943	-2.175879
H	-4.159819	3.664229	-1.340943
H	-3.001298	3.432882	0.842109
H	-2.553693	4.904062	0.009526
H	-0.422796	3.622807	-0.836379
H	-0.976314	2.998949	2.102648
H	1.238367	1.847877	1.794545
H	1.472587	3.535862	2.109862
H	1.469646	2.406825	-0.737634
H	1.898868	4.026982	-0.242995
H	3.811212	3.003253	1.131407
H	3.950789	2.898074	-0.610019
H	3.054883	0.611399	1.219628
H	3.052205	0.564388	-0.541552

conf_14

C	4.335355	1.473209	0.940512
C	4.038408	0.362231	-0.058705
C	4.901528	-0.877837	0.124054
C	4.549252	-1.988835	-0.872420
C	3.134361	-2.438336	-0.674138
O	2.704916	-3.023826	0.286084
O	2.326124	-2.071084	-1.701692
C	0.960465	-2.449322	-1.550644
C	0.283074	-1.636527	-0.479178
C	-0.109055	-2.195818	0.737594
C	-0.709264	-1.411495	1.714606
C	-0.892808	-0.067702	1.470236
N	-0.504498	0.448636	0.298536
C	0.064394	-0.285234	-0.667111
H	0.343915	0.241018	-1.572211

H	-0.625824	1.467133	0.147827
H	-1.336539	0.620199	2.178327
H	-1.020153	-1.832425	2.662127
H	0.079510	-3.247875	0.919746
H	0.886724	-3.512137	-1.312603
H	0.505167	-2.265996	-2.524503
H	4.686331	-1.648699	-1.900866
H	5.189879	-2.858482	-0.703771
H	5.958427	-0.623551	-0.003092
H	4.789644	-1.265739	1.142275
H	2.984761	0.067469	0.031145
H	4.160239	0.745294	-1.081282
C	3.522834	2.744133	0.699924
C	2.018660	2.513838	0.753633
C	1.184552	3.768111	0.502488
C	-0.290334	3.556468	0.664151
C	-1.205500	3.705806	-0.302402
C	-2.692235	3.699081	-0.117746
C	-3.476428	3.115321	-1.293657
C	-3.285416	1.620500	-1.525755
C	-3.838778	0.739876	-0.412805
C	-3.665799	-0.750077	-0.672214
C	-4.154273	-1.631240	0.468556
C	-3.880754	-3.112664	0.249301
C	-4.321961	-3.981791	1.416872
H	-4.116032	-5.039199	1.232981
H	-3.807525	-3.697992	2.341668
H	-5.396116	-3.881390	1.598209
H	-2.806456	-3.257372	0.065122
H	-4.384727	-3.440267	-0.667804
H	-3.680460	-1.310527	1.407995
H	-5.230419	-1.477101	0.615916
H	-2.606816	-0.970671	-0.869178
H	-4.193958	-1.020576	-1.594958
H	-3.370285	0.997431	0.547427
H	-4.904619	0.963236	-0.279420
H	-2.217421	1.404610	-1.681759
H	-3.772898	1.344058	-2.467493
H	-3.196265	3.660638	-2.202392
H	-4.541714	3.317733	-1.138328
H	-2.958614	3.208689	0.825853
H	-3.000423	4.746299	0.001972
H	-0.852472	3.966408	-1.303174
H	-0.638719	3.347675	1.680351
H	1.497019	4.551261	1.205264
H	1.392745	4.153509	-0.501686
H	1.753689	2.076638	1.727495
H	1.754492	1.769361	-0.004552
H	3.800973	3.499746	1.443134
H	3.786479	3.165671	-0.278798
H	5.402249	1.719772	0.899554
H	4.147714	1.104798	1.957688

conf_4

C	-3.473846	0.710375	-0.961173
C	-4.963221	0.516072	-0.696980
C	-5.354884	-0.828296	-0.091385
C	-4.647164	-1.155360	1.222053
C	-3.306058	-1.793181	1.027369
O	-2.986051	-2.524875	0.127633
O	-2.442466	-1.486851	2.030944
C	-1.182034	-2.144773	1.937914
C	-0.379724	-1.604611	0.785703
C	0.029677	-2.398166	-0.284831
C	0.735712	-1.844559	-1.346079
C	1.003549	-0.492483	-1.335321
N	0.595995	0.248826	-0.298894
C	-0.070321	-0.259085	0.743213
H	-0.357195	0.441060	1.518751
H	0.780269	1.272240	-0.294686
H	1.530836	0.025889	-2.125537
H	1.061873	-2.449402	-2.182475
H	-0.226822	-3.451971	-0.292337
H	-1.321833	-3.221400	1.824266
H	-0.685176	-1.944349	2.888228
H	-4.545858	-0.282185	1.872484
H	-5.230110	-1.892280	1.789092
H	-6.433534	-0.828975	0.086649
H	-5.155769	-1.636286	-0.802614
H	-5.313967	1.325805	-0.043801
H	-5.507965	0.635869	-1.640742
C	-3.194509	1.958207	-1.794279
C	-1.715115	2.322002	-1.887761
C	-1.205379	3.068048	-0.653872
C	0.279396	3.284414	-0.634069
C	1.036638	3.353179	0.468611
C	2.489392	3.717662	0.509492
C	3.261535	3.084649	1.667549
C	3.239500	1.560689	1.708493
C	3.853459	0.877503	0.494337
C	3.855184	-0.641256	0.605222
C	4.380026	-1.350277	-0.634594
C	4.295174	-2.867714	-0.546784
C	4.766731	-3.567446	-1.812289
H	5.809158	-3.320420	-2.033929
H	4.697601	-4.654298	-1.721370
H	4.169661	-3.267138	-2.680652
H	3.258517	-3.158775	-0.325579
H	4.887655	-3.211750	0.309252
H	3.823886	-1.007300	-1.520071
H	5.420621	-1.052413	-0.813686
H	2.836592	-0.996234	0.822811
H	4.454623	-0.937913	1.474704
H	3.322950	1.178294	-0.421061
H	4.881918	1.234602	0.358682

H	2.204376	1.211636	1.840735
H	3.769539	1.226096	2.607502
H	2.856066	3.469658	2.610608
H	4.299867	3.430514	1.623680
H	2.958314	3.489531	-0.453991
H	2.554797	4.808309	0.617086
H	0.547029	3.221131	1.438042
H	0.753804	3.472784	-1.600457
H	-1.697129	4.049690	-0.630573
H	-1.522447	2.565288	0.269006
H	-1.539109	2.951414	-2.766851
H	-1.133703	1.405239	-2.055659
H	-3.597680	1.798931	-2.799895
H	-3.748850	2.810502	-1.380295
H	-3.070928	-0.167801	-1.482442
H	-2.938016	0.774860	-0.002459

conf_34

C	3.567625	0.882584	0.586743
C	5.025578	0.504483	0.355136
C	5.290302	-0.985170	0.160603
C	4.511330	-1.609439	-0.996458
C	3.147820	-2.091562	-0.606865
O	2.828304	-2.549827	0.458138
O	2.260107	-2.001965	-1.633703
C	0.989199	-2.582433	-1.360261
C	0.235495	-1.797163	-0.322066
C	-0.283555	-2.384110	0.830605
C	-0.949215	-1.616178	1.777377
C	-1.070425	-0.258941	1.568797
N	-0.564897	0.281901	0.454599
C	0.063219	-0.436066	-0.483422
H	0.430388	0.109545	-1.343587
H	-0.659923	1.307423	0.301815
H	-1.555794	0.418202	2.259716
H	-1.354871	-2.059617	2.677628
H	-0.144983	-3.447329	0.995442
H	1.107951	-3.615776	-1.027961
H	0.460571	-2.572051	-2.315048
H	4.430989	-0.939117	-1.856657
H	5.030337	-2.506704	-1.357145
H	6.358400	-1.127697	-0.023380
H	5.055583	-1.537337	1.076279
H	5.397359	1.054693	-0.519282
H	5.623271	0.852903	1.205363
C	3.397144	2.362931	0.916317
C	1.942261	2.826053	0.950502
C	1.351145	2.996588	-0.443219
C	-0.129637	3.211664	-0.534354
C	-0.970083	3.410168	0.489254
C	-2.438743	3.706009	0.393770
C	-3.126344	3.418472	-0.939038

C	-3.162049	1.950128	-1.363450
C	-3.846259	1.015501	-0.374290
C	-3.788986	-0.447245	-0.793171
C	-4.378808	-1.402663	0.234325
C	-4.181732	-2.870061	-0.119959
C	-4.731275	-3.818788	0.934258
H	-4.577050	-4.864365	0.655922
H	-4.249584	-3.657534	1.905107
H	-5.805825	-3.670246	1.075863
H	-3.109357	-3.062344	-0.268492
H	-4.656902	-3.075142	-1.086672
H	-3.927523	-1.205652	1.218053
H	-5.449357	-1.196444	0.356343
H	-2.743231	-0.729582	-0.986325
H	-4.305492	-0.574292	-1.752518
H	-3.391217	1.116416	0.620601
H	-4.891580	1.321985	-0.244072
H	-2.143732	1.586394	-1.556220
H	-3.675789	1.881175	-2.328943
H	-2.657385	4.013267	-1.730995
H	-4.155284	3.787307	-0.867133
H	-2.958605	3.182087	1.205347
H	-2.568441	4.769205	0.636929
H	-0.556476	3.435226	1.498827
H	-0.531025	3.241241	-1.547117
H	1.842258	3.845821	-0.937990
H	1.621527	2.137336	-1.073511
H	1.865167	3.775266	1.490868
H	1.356346	2.100319	1.532566
H	3.864662	2.559859	1.886741
H	3.951579	2.967734	0.187202
H	3.151843	0.277266	1.403239
H	2.984149	0.633009	-0.311278

conf_72

C	4.871477	0.715293	0.055642
C	4.069065	-0.434375	-0.540384
C	4.641743	-1.811824	-0.240259
C	3.766187	-2.933869	-0.804115
C	2.412187	-2.930084	-0.161239
O	2.182117	-3.058003	1.011901
O	1.410847	-2.733353	-1.062574
C	0.103614	-2.777829	-0.506552
C	-0.184423	-1.581331	0.359907
C	-0.763230	-1.703298	1.622020
C	-1.028763	-0.578078	2.391700
C	-0.697636	0.663721	1.894015
N	-0.134030	0.756112	0.683429
C	0.120484	-0.309246	-0.087265
H	0.581730	-0.115585	-1.048178
H	0.108029	1.698663	0.327432
H	-0.860462	1.593075	2.424368

H	-1.476843	-0.660255	3.373652
H	-0.994233	-2.690389	2.008201
H	-0.031771	-3.691855	0.075183
H	-0.571620	-2.798232	-1.364384
H	3.657742	-2.845607	-1.887055
H	4.216202	-3.907054	-0.584906
H	5.645348	-1.905619	-0.666385
H	4.741436	-1.948048	0.841707
H	3.044918	-0.397535	-0.145998
H	3.985132	-0.301004	-1.628088
C	4.327554	2.095641	-0.310301
C	2.867575	2.278629	0.079537
C	2.288815	3.663615	-0.208426
C	0.862564	3.758483	0.237096
C	-0.203523	3.804593	-0.570696
C	-1.629739	3.866255	-0.123957
C	-2.496029	2.785865	-0.777610
C	-3.845570	2.589911	-0.097593
C	-4.591183	1.344958	-0.571701
C	-3.931704	0.037999	-0.144323
C	-4.696390	-1.207173	-0.569111
C	-4.006078	-2.502679	-0.162931
C	-4.772841	-3.749554	-0.576720
H	-4.908873	-3.785909	-1.661830
H	-4.254484	-4.663819	-0.275231
H	-5.766795	-3.767264	-0.120226
H	-3.858136	-2.505031	0.925871
H	-3.001688	-2.524512	-0.610075
H	-5.703879	-1.182374	-0.135473
H	-4.835772	-1.197088	-1.657745
H	-3.821884	0.036621	0.949845
H	-2.914531	-0.023080	-0.556639
H	-5.612757	1.368137	-0.176317
H	-4.689439	1.366611	-1.664637
H	-4.464341	3.479342	-0.259164
H	-3.697718	2.521010	0.989829
H	-1.952493	1.834610	-0.773408
H	-2.646698	3.028108	-1.836249
H	-1.676296	3.779646	0.969692
H	-2.044710	4.853531	-0.362137
H	-0.034985	3.806241	-1.649535
H	0.697729	3.802121	1.317899
H	2.884797	4.424625	0.308794
H	2.360170	3.878285	-1.280009
H	2.745876	2.041130	1.146733
H	2.266200	1.547034	-0.473743
H	4.934712	2.865660	0.178406
H	4.434435	2.259527	-1.390240
H	5.912836	0.641342	-0.277095
H	4.892697	0.609269	1.148108

conf_11

C	3.501223	0.123775	-0.547637
C	4.670569	-0.829840	-0.755345
C	4.487552	-2.217867	-0.149672
C	3.251289	-2.955829	-0.670220
C	2.020410	-2.712323	0.147773
O	1.969306	-2.630444	1.346629
O	0.897215	-2.628790	-0.616001
C	-0.315957	-2.588087	0.125791
C	-0.442866	-1.336316	0.948694
C	-0.849848	-1.364461	2.280940
C	-0.947573	-0.191248	3.018117
C	-0.625602	1.003633	2.411622
N	-0.240777	1.005909	1.129704
C	-0.150538	-0.105410	0.391582
H	0.177925	0.017609	-0.632474
H	-0.028152	1.922204	0.686556
H	-0.661881	1.965289	2.907507
H	-1.254551	-0.201813	4.056065
H	-1.070883	-2.317366	2.750453
H	-0.388618	-3.461973	0.777212
H	-1.110536	-2.635960	-0.621846
H	3.046922	-2.734276	-1.720885
H	3.411184	-4.039540	-0.607845
H	5.372714	-2.816554	-0.379248
H	4.427480	-2.160251	0.942014
H	4.850593	-0.932820	-1.833514
H	5.580105	-0.381829	-0.339429
C	3.717670	1.473608	-1.225043
C	2.500854	2.392644	-1.168949
C	2.286759	3.054682	0.186063
C	0.965816	3.741021	0.376833
C	-0.037156	3.785519	-0.509652
C	-1.369168	4.436245	-0.284395
C	-2.460900	3.428305	0.104330
C	-2.632225	2.268136	-0.871034
C	-3.433736	1.104855	-0.302135
C	-3.446528	-0.116810	-1.211356
C	-4.024489	-1.360174	-0.552168
C	-4.042692	-2.581024	-1.462381
C	-4.514818	-3.843465	-0.757587
H	-4.527398	-4.701272	-1.434314
H	-3.863248	-4.096250	0.086578
H	-5.527448	-3.718846	-0.362352
H	-3.038659	-2.742571	-1.879977
H	-4.686700	-2.375873	-2.325381
H	-3.445700	-1.589710	0.355881
H	-5.044031	-1.152624	-0.203405
H	-2.418535	-0.331937	-1.542289
H	-4.005005	0.109699	-2.127727
H	-3.011706	0.819259	0.672943
H	-4.461712	1.423308	-0.092056

H	-1.647609	1.888720	-1.177216
H	-3.097283	2.628049	-1.796542
H	-3.412581	3.956822	0.221865
H	-2.225313	3.030514	1.101550
H	-1.285933	5.194506	0.500340
H	-1.667220	4.959326	-1.199866
H	0.109282	3.314347	-1.480095
H	0.834756	4.260007	1.329149
H	2.418156	2.318868	0.994358
H	3.084870	3.787650	0.360407
H	1.616134	1.802948	-1.450901
H	2.585115	3.173728	-1.931767
H	4.587200	1.976469	-0.784135
H	3.974236	1.294234	-2.275010
H	3.318064	0.248896	0.527965
H	2.590967	-0.325879	-0.970564

conf_79

C	3.436772	0.850498	0.527451
C	4.799996	0.204173	0.733639
C	4.839665	-1.304331	0.503176
C	4.578873	-1.746019	-0.948530
C	3.133519	-1.776218	-1.338466
O	2.579891	-1.055381	-2.130492
O	2.466670	-2.749817	-0.670565
C	1.078053	-2.874034	-0.971052
C	0.267838	-1.974480	-0.078285
C	-0.376454	-2.463453	1.056772
C	-1.086742	-1.612492	1.896399
C	-1.133675	-0.271605	1.589894
N	-0.512155	0.176717	0.491300
C	0.169575	-0.615882	-0.342305
H	0.639173	-0.154138	-1.202741
H	-0.570335	1.196517	0.303103
H	-1.651435	0.469953	2.184576
H	-1.596265	-1.982361	2.776887
H	-0.321930	-3.523183	1.285792
H	0.828254	-3.917315	-0.780525
H	0.902364	-2.641149	-2.023034
H	5.092838	-1.088474	-1.652571
H	4.964708	-2.760816	-1.085054
H	5.833538	-1.669528	0.776410
H	4.136287	-1.814637	1.170956
H	5.526878	0.684963	0.066596
H	5.146839	0.407603	1.753476
C	3.442245	2.364931	0.704368
C	2.087269	2.994511	0.387542
C	1.074503	2.849911	1.516442
C	-0.357136	3.121327	1.158951
C	-0.832861	3.477785	-0.041412

C	-2.254966	3.841709	-0.330480
C	-2.783588	3.286286	-1.654816
C	-2.764371	1.765664	-1.770337
C	-3.597093	1.041632	-0.720944
C	-3.621548	-0.469790	-0.904204
C	-4.368957	-1.208158	0.196954
C	-4.285148	-2.723336	0.076512
C	-4.986353	-3.453269	1.211837
H	-4.912939	-4.538031	1.100672
H	-4.555035	-3.187401	2.183517
H	-6.049182	-3.196733	1.247756
H	-3.227999	-3.023282	0.039181
H	-4.714216	-3.032811	-0.883829
H	-3.975637	-0.901105	1.177615
H	-5.421668	-0.899416	0.196213
H	-2.592066	-0.852686	-0.961448
H	-4.071105	-0.709351	-1.875592
H	-3.226923	1.280730	0.286430
H	-4.624014	1.427248	-0.746548
H	-1.724087	1.407849	-1.731706
H	-3.124133	1.483655	-2.766330
H	-2.197084	3.713199	-2.476603
H	-3.808558	3.645643	-1.797019
H	-2.895398	3.545076	0.507187
H	-2.312819	4.937012	-0.377598
H	-0.136960	3.591407	-0.873626
H	-1.067421	3.070646	1.988276
H	1.147731	1.845797	1.961670
H	1.351088	3.523476	2.338048
H	1.705095	2.528802	-0.531752
H	2.205008	4.057456	0.153749
H	3.755231	2.631563	1.721651
H	4.197775	2.787367	0.033225
H	2.714422	0.386910	1.216149
H	3.086064	0.641954	-0.488452

conf_28

C	3.726357	0.610727	0.275635
C	5.054385	0.017656	-0.181990
C	5.085126	-1.502547	-0.304391
C	4.016043	-2.076402	-1.231519
C	2.702685	-2.310427	-0.550707
O	2.535792	-2.612614	0.601346
O	1.654230	-2.185805	-1.407765
C	0.394963	-2.531305	-0.841820
C	-0.043753	-1.521208	0.182891
C	-0.391960	-1.874695	1.485177
C	-0.783959	-0.906089	2.401079
C	-0.802154	0.415355	2.008398
N	-0.451255	0.731079	0.756077
C	-0.087145	-0.181931	-0.151475
H	0.179561	0.192341	-1.132307

H	-0.455385	1.725806	0.458267
H	-1.081383	1.236096	2.656715
H	-1.057492	-1.168255	3.415084
H	-0.338405	-2.915438	1.785154
H	0.438768	-3.523604	-0.388960
H	-0.298976	-2.554536	-1.683610
H	3.860889	-1.462840	-2.123366
H	4.323509	-3.065885	-1.593542
H	6.067300	-1.802721	-0.679035
H	4.972919	-1.964240	0.681814
H	5.327889	0.466299	-1.145947
H	5.838342	0.319672	0.522194
C	3.841433	2.094892	0.609318
C	2.501142	2.777580	0.867535
C	1.758424	3.152026	-0.417581
C	0.380262	3.681471	-0.173808
C	-0.713803	3.368353	-0.878733
C	-2.084265	3.921306	-0.633073
C	-3.049900	2.902589	-0.016882
C	-3.338770	1.685303	-0.887370
C	-4.090613	0.588006	-0.147496
C	-4.475637	-0.587307	-1.036888
C	-5.152361	-1.732557	-0.286023
C	-4.231732	-2.538134	0.630398
C	-3.203545	-3.368815	-0.125765
H	-2.571786	-3.947078	0.556008
H	-3.694057	-4.080877	-0.796199
H	-2.551818	-2.741931	-0.742873
H	-4.844034	-3.206501	1.244540
H	-3.725644	-1.867915	1.337862
H	-5.981866	-1.324474	0.303547
H	-5.606766	-2.418380	-1.010567
H	-3.585350	-0.955810	-1.564799
H	-5.151514	-0.225838	-1.820117
H	-3.475044	0.237661	0.693113
H	-4.997713	1.007901	0.305687
H	-2.406069	1.265416	-1.288567
H	-3.914171	2.001181	-1.766216
H	-3.994219	3.406069	0.215996
H	-2.649449	2.578618	0.955301
H	-2.009000	4.792071	0.025391
H	-2.499630	4.279437	-1.582767
H	-0.603147	2.680047	-1.720351
H	0.283247	4.410833	0.633321
H	2.343537	3.925953	-0.931820
H	1.718079	2.303869	-1.112943
H	2.653178	3.690107	1.454037
H	1.880000	2.120867	1.492892
H	4.481417	2.201215	1.491598
H	4.361297	2.617854	-0.203832
H	3.363034	0.070126	1.159364
H	2.971209	0.463595	-0.510727

conf_77

C	4.924278	0.529217	-0.244362
C	3.987194	-0.565624	-0.739050
C	4.415062	-1.965186	-0.318989
C	3.444711	-3.045425	-0.796235
C	2.143894	-2.990322	-0.055345
O	2.008034	-2.989118	1.138971
O	1.070396	-2.930408	-0.892175
C	-0.189641	-3.005767	-0.244758
C	-0.495960	-1.787077	0.581034
C	-1.346327	-1.848235	1.683944
C	-1.611974	-0.713273	2.438330
C	-1.014025	0.477413	2.085310
N	-0.206804	0.512120	1.018735
C	0.053934	-0.559954	0.262596
H	0.721538	-0.411591	-0.577245
H	0.230864	1.419890	0.756402
H	-1.153849	1.408550	2.619141
H	-2.267477	-0.750604	3.298949
H	-1.793729	-2.796617	1.963859
H	-0.235100	-3.892515	0.392362
H	-0.921056	-3.110510	-1.049850
H	3.261038	-2.974749	-1.870511
H	3.863155	-4.038019	-0.596249
H	5.405030	-2.181562	-0.732236
H	4.507869	-2.024819	0.770462
H	2.973157	-0.371843	-0.361187
H	3.918015	-0.522782	-1.834674
C	4.676081	1.892694	-0.888584
C	3.249203	2.423770	-0.772451
C	2.801531	2.677992	0.658530
C	1.388210	3.149007	0.822866
C	0.509430	3.398089	-0.156877
C	-0.906486	3.838600	0.043480
C	-1.889163	2.955257	-0.732936
C	-3.331875	3.058414	-0.254135
C	-4.239697	1.980718	-0.842882
C	-3.930109	0.577139	-0.332885
C	-4.835473	-0.504009	-0.904445
C	-4.477275	-1.902383	-0.418054
C	-5.383407	-2.986536	-0.981535
H	-5.103515	-3.979297	-0.618678
H	-6.425321	-2.812640	-0.697181
H	-5.340221	-3.006751	-2.074737
H	-4.517140	-1.922208	0.679814
H	-3.433530	-2.115973	-0.691785
H	-5.878179	-0.284928	-0.642813
H	-4.787113	-0.478876	-2.000685
H	-4.010955	0.571767	0.763723
H	-2.889018	0.312460	-0.566358
H	-5.282068	2.219689	-0.604757
H	-4.168125	1.997096	-1.938035

H	-3.725415	4.051726	-0.495863
H	-3.357758	2.984090	0.842611
H	-1.566503	1.910735	-0.661000
H	-1.835423	3.199806	-1.800318
H	-1.148457	3.829412	1.114249
H	-1.018862	4.880517	-0.280221
H	0.822433	3.264255	-1.192500
H	1.071831	3.335756	1.852833
H	2.938101	1.772045	1.267195
H	3.465057	3.419188	1.124516
H	2.558624	1.722254	-1.260151
H	3.174402	3.356443	-1.342431
H	5.369333	2.623964	-0.457185
H	4.930375	1.827994	-1.952857
H	5.958540	0.234684	-0.455969
H	4.856966	0.598225	0.848441

conf_87

C	4.092795	1.780554	-0.736545
C	3.586214	0.359875	-0.937866
C	4.540871	-0.700353	-0.408253
C	4.013609	-2.121512	-0.610799
C	2.804029	-2.380524	0.233602
O	2.754268	-2.338598	1.433957
O	1.702239	-2.667943	-0.513087
C	0.565408	-3.058059	0.239930
C	-0.035044	-1.931411	1.033684
C	-0.666563	-2.160197	2.254811
C	-1.240775	-1.113722	2.965229
C	-1.168142	0.161195	2.446712
N	-0.556974	0.356883	1.272170
C	-0.006144	-0.632226	0.560009
H	0.462803	-0.355988	-0.375970
H	-0.522496	1.328998	0.902292
H	-1.575679	1.038494	2.932195
H	-1.728751	-1.280035	3.917046
H	-0.696250	-3.166286	2.661003
H	0.823745	-3.876779	0.915852
H	-0.156022	-3.418599	-0.496522
H	3.777727	-2.309736	-1.660184
H	4.769669	-2.847503	-0.295859
H	5.504468	-0.613711	-0.919909
H	4.734228	-0.539036	0.657638
H	2.614424	0.248069	-0.437013
H	3.400814	0.182213	-2.005888
C	3.247076	2.842303	-1.434800
C	1.766756	2.863876	-1.057703
C	1.520879	3.068290	0.429397
C	0.095495	3.297019	0.836922
C	-0.967557	3.405203	0.028395

C	-2.330336	3.838530	0.473724
C	-3.524967	3.206826	-0.240596
C	-3.719510	1.706985	-0.016805
C	-2.985979	0.803796	-1.002001
C	-3.231101	-0.675015	-0.737622
C	-2.541743	-1.604246	-1.727549
C	-2.776803	-3.087199	-1.450831
C	-4.217368	-3.535650	-1.659299
H	-4.320754	-4.612542	-1.505361
H	-4.905242	-3.040093	-0.968945
H	-4.550357	-3.313742	-2.677825
H	-2.476878	-3.315297	-0.417416
H	-2.122805	-3.678526	-2.102583
H	-2.883310	-1.370224	-2.743794
H	-1.461765	-1.398020	-1.729060
H	-4.311917	-0.854790	-0.755145
H	-2.911452	-0.929785	0.284193
H	-3.320393	1.047295	-2.018124
H	-1.907886	1.016621	-0.998805
H	-4.787646	1.472472	-0.083839
H	-3.434949	1.449245	1.014383
H	-3.454350	3.408647	-1.316771
H	-4.418827	3.737081	0.101050
H	-2.427094	3.707309	1.559186
H	-2.381975	4.923041	0.304977
H	-0.830963	3.280423	-1.045843
H	-0.059601	3.477683	1.903993
H	1.933962	2.227354	1.005922
H	2.099044	3.937092	0.774504
H	1.278963	1.939048	-1.397511
H	1.285586	3.673448	-1.616916
H	3.676243	3.829457	-1.227634
H	3.324316	2.701778	-2.519166
H	5.117631	1.850982	-1.118471
H	4.163898	1.992081	0.337695

conf_78

C	-4.709744	1.138630	0.731295
C	-4.307112	-0.309809	0.417430
C	-4.419025	-0.656160	-1.064512
C	-3.845086	-2.032861	-1.406927
C	-2.353040	-2.003452	-1.299752
O	-1.628944	-1.259105	-1.914939
O	-1.870961	-2.885246	-0.397256
C	-0.452037	-2.875010	-0.225850
C	-0.034571	-1.722620	0.647854
C	0.058457	-1.846722	2.032055
C	0.395683	-0.752766	2.824230
C	0.624315	0.461474	2.216335
N	0.533602	0.555193	0.882887
C	0.226720	-0.478613	0.094937
H	0.164346	-0.288504	-0.968507

H	0.669641	1.479896	0.425490
H	0.879550	1.367517	2.751227
H	0.474254	-0.838720	3.900452
H	-0.134388	-2.808675	2.496670
H	0.042618	-2.825991	-1.197813
H	-0.216306	-3.823006	0.255922
H	-4.253114	-2.812605	-0.760805
H	-4.080801	-2.288355	-2.444731
H	-5.472364	-0.631694	-1.360052
H	-3.906792	0.095285	-1.674154
H	-3.279536	-0.487497	0.767582
H	-4.931242	-1.008111	0.985180
C	-3.537461	2.071540	1.023774
C	-2.489462	2.160475	-0.078102
C	-1.421495	3.209686	0.230881
C	-0.206953	3.133167	-0.646891
C	1.027618	3.512453	-0.291694
C	2.212881	3.579523	-1.205668
C	3.551223	3.306923	-0.519544
C	3.675271	1.941470	0.147551
C	3.522252	0.754675	-0.794464
C	3.781675	-0.583864	-0.115784
C	3.632225	-1.778692	-1.049724
C	4.075214	-3.106849	-0.442305
C	3.235317	-3.570153	0.740101
H	3.594940	-4.525634	1.129937
H	3.256868	-2.852204	1.565963
H	2.190594	-3.713677	0.442311
H	5.123413	-3.021727	-0.131779
H	4.054081	-3.877900	-1.219688
H	2.587919	-1.856981	-1.388224
H	4.221719	-1.590744	-1.954686
H	3.115518	-0.693343	0.751509
H	4.798832	-0.579156	0.296914
H	2.522866	0.752268	-1.253003
H	4.220226	0.872339	-1.632971
H	2.946059	1.862652	0.967822
H	4.654952	1.878809	0.634964
H	3.727285	4.086214	0.231359
H	4.350199	3.417887	-1.260592
H	2.061221	2.911112	-2.060183
H	2.250494	4.592914	-1.626332
H	1.177274	3.901611	0.720251
H	-0.370557	2.795498	-1.672820
H	-1.872055	4.204491	0.117890
H	-1.123300	3.151033	1.286882
H	-2.967618	2.408545	-1.033451
H	-2.025721	1.177836	-0.229692
H	-3.926160	3.076032	1.230160
H	-3.045262	1.744668	1.951413
H	-5.382627	1.159771	1.593404
H	-5.290189	1.541927	-0.107804

conf_46

C	3.641908	2.411171	-0.101037
C	3.580002	0.953988	-0.545151
C	4.582312	0.057193	0.169205
C	4.580303	-1.391220	-0.341899
C	3.296664	-2.079816	-0.001153
O	3.009129	-2.552417	1.068152
O	2.418339	-2.080212	-1.036888
C	1.152330	-2.666009	-0.743387
C	0.394020	-1.829994	0.252379
C	0.126509	-2.279322	1.544390
C	-0.517364	-1.455991	2.460544
C	-0.866658	-0.180740	2.075174
N	-0.595982	0.232287	0.830010
C	0.004968	-0.545375	-0.078792
H	0.179211	-0.104753	-1.052971
H	-0.865460	1.204666	0.579488
H	-1.356073	0.535518	2.722820
H	-0.729365	-1.790540	3.467880
H	0.450279	-3.272253	1.835617
H	1.282101	-3.679117	-0.357870
H	0.630360	-2.709594	-1.699821
H	4.735786	-1.412587	-1.422899
H	5.380855	-1.954133	0.142665
H	5.591176	0.457763	0.026991
H	4.398455	0.057771	1.249604
H	2.567273	0.560787	-0.393024
H	3.760981	0.899083	-1.626993
C	2.864387	3.355838	-1.016235
C	1.354839	3.133948	-1.063655
C	0.614481	3.612019	0.184668
C	-0.865296	3.396880	0.097350
C	-1.673503	3.099181	1.121831
C	-3.169534	2.979928	1.087727
C	-3.828641	2.867243	-0.285348
C	-3.471088	1.619259	-1.092086
C	-3.793120	0.297423	-0.407563
C	-3.335942	-0.912799	-1.212584
C	-3.330763	-2.209583	-0.416957
C	-2.767321	-3.395063	-1.188211
C	-2.642086	-4.653056	-0.342667
H	-2.235393	-5.488671	-0.917826
H	-1.985051	-4.489090	0.519659
H	-3.615372	-4.964429	0.047800
H	-1.783773	-3.122313	-1.596173
H	-3.400209	-3.596038	-2.060150
H	-2.741561	-2.066306	0.500836
H	-4.348200	-2.442261	-0.078847
H	-2.320973	-0.727542	-1.595889
H	-3.963439	-1.023813	-2.104865
H	-3.318386	0.260191	0.581632
H	-4.870493	0.231364	-0.212928

H	-2.403944	1.631036	-1.352305
H	-3.999370	1.662897	-2.051144
H	-3.594694	3.759357	-0.877086
H	-4.913418	2.891131	-0.135060
H	-3.476565	2.136357	1.719702
H	-3.575070	3.860717	1.603470
H	-1.218337	3.013987	2.113127
H	-1.305098	3.549862	-0.888311
H	1.014055	3.145453	1.093508
H	0.801292	4.688860	0.297218
H	1.140317	2.072106	-1.247177
H	0.943594	3.667465	-1.928139
H	3.057305	4.392787	-0.717139
H	3.265735	3.256316	-2.031323
H	4.689651	2.732636	-0.090284
H	3.295516	2.499729	0.936763

conf_21

C	2.962271	1.250376	0.750485
C	4.253387	1.454890	-0.034304
C	5.097784	0.192830	-0.200397
C	4.516497	-0.837184	-1.172624
C	3.363003	-1.612083	-0.612855
O	3.302904	-2.114626	0.478653
O	2.337789	-1.709893	-1.500383
C	1.195090	-2.416795	-1.019631
C	0.479011	-1.578791	0.003508
C	0.462231	-1.901796	1.357926
C	-0.121646	-1.039439	2.280645
C	-0.660692	0.146550	1.835792
N	-0.630853	0.437438	0.527518
C	-0.090029	-0.378727	-0.382996
H	-0.097655	-0.031504	-1.409067
H	-0.985530	1.360949	0.221281
H	-1.114243	0.884688	2.484824
H	-0.139829	-1.273666	3.337279
H	0.935689	-2.819149	1.689246
H	1.488550	-3.375485	-0.588901
H	0.572997	-2.587996	-1.898702
H	4.220339	-0.374671	-2.117130
H	5.283153	-1.584789	-1.408278
H	6.083565	0.477226	-0.578558
H	5.262386	-0.285944	0.770752
H	4.032697	1.867178	-1.026836
H	4.855922	2.212012	0.480982
C	2.103831	2.502814	0.903660
C	1.522886	3.008235	-0.414156
C	0.396155	4.036125	-0.270372
C	-0.859432	3.521585	0.369741
C	-2.031617	3.392493	-0.264150

C	-3.351032	3.026710	0.350397
C	-4.326253	2.390588	-0.641384
C	-3.871728	1.057291	-1.225696
C	-3.898146	-0.104629	-0.241707
C	-3.387194	-1.407219	-0.843106
C	-3.169570	-2.511908	0.179955
C	-2.552734	-3.773993	-0.406987
C	-2.239375	-4.828886	0.642805
H	-1.796216	-5.723405	0.198041
H	-1.538465	-4.446777	1.394193
H	-3.144701	-5.138172	1.173283
H	-1.634698	-3.507131	-0.949486
H	-3.228567	-4.191660	-1.162130
H	-2.522110	-2.137106	0.985579
H	-4.122763	-2.761484	0.662415
H	-2.440803	-1.217175	-1.371441
H	-4.083445	-1.749975	-1.618014
H	-3.305334	0.138946	0.650228
H	-4.922156	-0.246035	0.124768
H	-2.857342	1.166593	-1.640938
H	-4.506858	0.807388	-2.082708
H	-4.491393	3.102722	-1.457920
H	-5.298358	2.261514	-0.153463
H	-3.208384	2.391820	1.234447
H	-3.806591	3.950199	0.730386
H	-2.064361	3.659692	-1.322734
H	-0.823697	3.320924	1.443978
H	0.764943	4.884886	0.319646
H	0.147427	4.433047	-1.259495
H	1.155413	2.158078	-1.007425
H	2.319077	3.456566	-1.016331
H	1.293024	2.283121	1.609492
H	2.688666	3.303290	1.372984
H	3.211096	0.849325	1.739698
H	2.352797	0.481816	0.259964

conf_12

C	3.991920	1.166077	-0.221352
C	5.324594	0.468910	-0.477649
C	5.335914	-1.030174	-0.186972
C	4.388844	-1.822867	-1.087744
C	3.028085	-2.069329	-0.514069
O	2.741968	-2.186743	0.647516
O	2.094331	-2.226765	-1.496024
C	0.864078	-2.790687	-1.068595
C	0.063864	-1.886470	-0.172528
C	-0.677293	-2.395069	0.894121
C	-1.403586	-1.550531	1.721361
C	-1.368750	-0.193553	1.480789
N	-0.665675	0.269125	0.442310
C	0.032394	-0.521250	-0.382093
H	0.582543	-0.030622	-1.175827

H	-0.605499	1.298383	0.308142
H	-1.877159	0.542231	2.089611
H	-1.974976	-1.934338	2.556704
H	-0.665542	-3.462153	1.092049
H	1.046183	-3.735970	-0.550927
H	0.312234	-2.995784	-1.988868
H	4.285789	-1.373787	-2.079731
H	4.786875	-2.831665	-1.260829
H	6.351985	-1.403356	-0.338448
H	5.087888	-1.236337	0.858870
H	5.614168	0.618917	-1.524472
H	6.102952	0.954843	0.121895
C	3.687559	1.395254	1.257319
C	2.224078	1.726160	1.532288
C	1.704850	2.940048	0.758557
C	0.232203	3.185257	0.886489
C	-0.578968	3.470988	-0.141159
C	-2.017797	3.886122	-0.054513
C	-2.831327	3.547537	-1.304569
C	-2.957457	2.059487	-1.614307
C	-3.794187	1.276997	-0.611145
C	-3.865730	-0.213266	-0.914477
C	-4.650234	-1.011375	0.116866
C	-4.612870	-2.514236	-0.122627
C	-5.360025	-3.307825	0.938289
H	-5.318447	-4.382220	0.742357
H	-4.940454	-3.134338	1.935520
H	-6.414754	-3.019861	0.975252
H	-3.565424	-2.845775	-0.164892
H	-5.032624	-2.731892	-1.111950
H	-4.260913	-0.795331	1.122932
H	-5.692554	-0.669419	0.128848
H	-2.847773	-0.623324	-0.991619
H	-4.311556	-0.359905	-1.906020
H	-3.404739	1.423279	0.406164
H	-4.808770	1.693533	-0.589459
H	-1.954377	1.612598	-1.692848
H	-3.400288	1.940425	-2.609484
H	-2.370394	4.053312	-2.160965
H	-3.832283	3.980657	-1.203009
H	-2.481833	3.477107	0.850770
H	-2.038671	4.975814	0.076657
H	-0.137152	3.501925	-1.140742
H	-0.178324	3.199141	1.899956
H	2.235865	3.831107	1.121026
H	1.953490	2.856252	-0.304606
H	2.077550	1.891386	2.606057
H	1.635961	0.836195	1.282932
H	3.944899	0.498850	1.831316
H	4.332919	2.197942	1.634223
H	3.177274	0.583506	-0.679795
H	3.994328	2.125617	-0.748588

conf_85

C	3.430405	1.247949	-0.150150
C	4.923864	0.954379	-0.084903
C	5.290436	-0.465426	0.333817
C	4.731751	-1.543176	-0.603914
C	3.383868	-2.048455	-0.191258
O	3.070269	-2.393677	0.918199
O	2.508535	-2.118837	-1.228186
C	1.259765	-2.724292	-0.907628
C	0.469929	-1.910005	0.081381
C	0.072114	-2.430229	1.311621
C	-0.636996	-1.650023	2.215409
C	-0.917820	-0.342742	1.884210
N	-0.518892	0.139335	0.700661
C	0.144607	-0.596243	-0.199518
H	0.421303	-0.100307	-1.121290
H	-0.737745	1.133680	0.496014
H	-1.449308	0.345498	2.528769
H	-0.951086	-2.041376	3.174436
H	0.340982	-3.449234	1.567843
H	1.421918	-3.727778	-0.508248
H	0.730479	-2.800687	-1.858768
H	4.701269	-1.204972	-1.642323
H	5.379169	-2.427388	-0.574265
H	6.379912	-0.551912	0.348758
H	4.951476	-0.673897	1.354043
H	5.362840	1.154984	-1.071100
H	5.400285	1.660038	0.605110
C	3.135953	2.638095	-0.705014
C	1.650473	2.939883	-0.867048
C	0.934032	3.313461	0.431588
C	-0.555004	3.342067	0.264684
C	-1.454013	3.037833	1.207719
C	-2.947777	3.104142	1.078816
C	-3.515321	3.145007	-0.338975
C	-3.208574	1.925709	-1.208214
C	-3.664635	0.592738	-0.630210
C	-3.296460	-0.590046	-1.520459
C	-3.419899	-1.949460	-0.841393
C	-4.829962	-2.306229	-0.387479
C	-4.910237	-3.690085	0.239074
H	-5.927965	-3.928609	0.557216
H	-4.594887	-4.463732	-0.468167
H	-4.263595	-3.763860	1.120558
H	-5.506521	-2.249640	-1.249017
H	-5.189330	-1.559604	0.330161
H	-3.061839	-2.727898	-1.527170
H	-2.748862	-1.982149	0.030664
H	-2.263839	-0.459864	-1.875447
H	-3.917659	-0.572262	-2.424244
H	-3.223040	0.438644	0.363912
H	-4.747554	0.618745	-0.463863

H	-2.131742	1.871848	-1.418104
H	-3.682955	2.069583	-2.185609
H	-3.165415	4.049401	-0.849254
H	-4.601960	3.256579	-0.257354
H	-3.389916	2.265168	1.631169
H	-3.287474	3.994885	1.624024
H	-1.075425	2.781443	2.201588
H	-0.912560	3.664171	-0.713274
H	1.210737	2.635710	1.249240
H	1.281438	4.307224	0.742837
H	1.159159	2.071325	-1.330598
H	1.513115	3.760193	-1.579855
H	3.599542	3.400698	-0.066690
H	3.624609	2.726369	-1.681692
H	2.988079	1.122074	0.847609
H	2.943189	0.512550	-0.805292

C18:1 11Z pyridylcarbinol ester**conf_5**

C	-0.214502	-2.619706	-1.165320
C	-1.256329	-3.303920	-2.044652
C	-2.526862	-2.505422	-2.317050
C	-3.365794	-2.220930	-1.074720
C	-2.858153	-1.072026	-0.262527
O	-2.293674	-0.094521	-0.686463
O	-3.133741	-1.221744	1.053858
C	-2.742040	-0.130903	1.886674
C	-1.268641	-0.197164	2.182708
C	-0.770899	-0.982457	3.220789
C	0.597400	-1.063427	3.458069
C	1.452609	-0.360278	2.639964
N	0.951854	0.386628	1.645777
C	-0.358326	0.491132	1.396104
H	-0.656671	1.106447	0.556979
H	1.626485	0.883376	1.030757
H	2.530172	-0.367756	2.739693
H	0.997372	-1.665750	4.263697
H	-1.461304	-1.536075	3.849718
H	-3.320075	-0.247111	2.803013
H	-2.998770	0.816722	1.410866
H	-4.385577	-1.937629	-1.365607
H	-3.464802	-3.100595	-0.432851
H	-3.146663	-3.066579	-3.021858
H	-2.281902	-1.555484	-2.803459
H	-0.791045	-3.541676	-3.008359
H	-1.525283	-4.269774	-1.596657
C	1.058151	-3.449893	-1.051264
C	2.152687	-2.841089	-0.182678
C	2.714254	-1.523516	-0.705110
C	4.005734	-1.112427	-0.009003

C	4.474345	0.301904	-0.368384
C	3.698613	1.382453	0.319236
C	2.800995	2.224245	-0.215983
C	2.346958	2.278318	-1.639724
C	0.827848	2.187425	-1.817293
C	0.041837	3.283169	-1.107025
C	-1.438531	3.283604	-1.471483
C	-2.265603	4.307120	-0.698341
C	-2.433040	3.976128	0.779161
H	-1.473827	3.933805	1.306011
H	-2.932807	3.008179	0.901976
H	-3.045174	4.724320	1.288889
H	-1.809863	5.299268	-0.803147
H	-3.256701	4.380839	-1.157803
H	-1.527889	3.484027	-2.545467
H	-1.859845	2.281298	-1.319510
H	0.157265	3.190030	-0.018312
H	0.474940	4.260197	-1.359253
H	0.607611	2.233883	-2.889542
H	0.472910	1.197551	-1.495059
H	2.828354	1.492522	-2.226299
H	2.684882	3.234184	-2.062270
H	2.398748	3.000367	0.436788
H	3.947417	1.526783	1.373489
H	4.442078	0.426828	-1.454176
H	5.524171	0.414684	-0.076411
H	3.895612	-1.198878	1.081665
H	4.791267	-1.827525	-0.274743
H	1.963639	-0.727435	-0.618842
H	2.911654	-1.615973	-1.780935
H	1.776137	-2.701448	0.841933
H	2.974449	-3.562319	-0.099100
H	1.461315	-3.622600	-2.057516
H	0.800743	-4.440530	-0.657962
H	0.008182	-1.628077	-1.577907
H	-0.617112	-2.452423	-0.154905

conf_89

C	-0.627350	0.890989	1.920522
C	-2.084539	1.139360	2.307012
C	-2.853441	2.162631	1.477128
C	-3.132653	1.759786	0.026787
C	-1.970621	1.845822	-0.910406
O	-1.619292	0.998839	-1.694006
O	-1.340208	3.041638	-0.823486
C	-0.276275	3.249879	-1.748708
C	1.005996	2.654541	-1.233554
C	1.952096	3.425617	-0.561403
C	3.120937	2.851851	-0.071018
C	3.321558	1.501657	-0.249967
N	2.394965	0.778114	-0.893886
C	1.267970	1.301115	-1.386923

H	0.577362	0.624027	-1.875681
H	2.538232	-0.246773	-0.994493
H	4.194692	0.968295	0.102216
H	3.866034	3.442044	0.447050
H	1.774084	4.487452	-0.421864
H	-0.178981	4.331323	-1.839557
H	-0.537642	2.824271	-2.719598
H	-3.524511	0.743414	-0.039260
H	-3.895580	2.429880	-0.387938
H	-2.337837	3.128247	1.494857
H	-3.823297	2.326736	1.955844
H	-2.624804	0.183841	2.298145
H	-2.105290	1.480896	3.348750
C	0.106143	0.129575	3.022796
C	1.570991	-0.199487	2.749359
C	1.787286	-1.320630	1.741493
C	3.247852	-1.724178	1.585598
C	3.490575	-2.762714	0.482653
C	3.307266	-2.227432	-0.907203
C	2.235213	-2.378258	-1.701491
C	0.978137	-3.116127	-1.374745
C	-0.266247	-2.227731	-1.327786
C	-1.517981	-2.997547	-0.925791
C	-2.696676	-2.090087	-0.607478
C	-3.965031	-2.843109	-0.232743
C	-5.111536	-1.914431	0.139305
H	-5.360074	-1.241923	-0.688673
H	-4.854335	-1.296563	1.007206
H	-6.016493	-2.472151	0.392733
H	-4.266655	-3.482800	-1.070832
H	-3.753255	-3.520082	0.604282
H	-2.413070	-1.427182	0.222733
H	-2.894442	-1.430648	-1.461254
H	-1.789975	-3.698095	-1.725115
H	-1.292293	-3.614565	-0.045792
H	-0.108141	-1.421078	-0.600600
H	-0.426187	-1.741236	-2.298365
H	1.077832	-3.634275	-0.417415
H	0.827864	-3.893612	-2.134685
H	2.287716	-1.957549	-2.708005
H	4.171504	-1.705385	-1.325909
H	2.833603	-3.619983	0.654094
H	4.515076	-3.138659	0.568981
H	3.869805	-0.836329	1.401020
H	3.608479	-2.131218	2.536300
H	1.368605	-1.036068	0.770106
H	1.210641	-2.200434	2.054869
H	2.094804	0.708936	2.415422
H	2.049320	-0.484525	3.693671
H	-0.434443	-0.801376	3.238275
H	0.045158	0.727088	3.939601
H	-0.577805	0.335933	0.974054

H -0.122469 1.852959 1.751338

conf_0

C -2.543975 1.653521 -0.686992
C -2.697442 2.992252 -1.404237
C -1.640953 4.050838 -1.107481
C -0.227218 3.714478 -1.599329
C 0.513109 2.733890 -0.747408
O 0.954475 1.665989 -1.093322
O 0.665225 3.190646 0.518114
C 1.384915 2.332339 1.400462
C 0.518848 1.184903 1.841946
C -0.431412 1.322297 2.851221
C -1.253921 0.255141 3.200219
C -1.117036 -0.937136 2.524973
N -0.192420 -1.045732 1.560196
C 0.612711 -0.039901 1.204024
H 1.304342 -0.225340 0.393501
H -0.117701 -1.945065 1.042877
H -1.719540 -1.815491 2.717907
H -1.996335 0.346816 3.982695
H -0.532787 2.272837 3.365958
H 1.655862 2.958461 2.250312
H 2.292518 1.966758 0.915523
H -0.247183 3.312216 -2.614147
H 0.374025 4.630052 -1.611689
H -1.609431 4.270350 -0.034795
H -1.941072 4.981067 -1.598311
H -2.732547 2.813472 -2.486540
H -3.674863 3.413956 -1.141098
C -3.766473 0.769150 -0.909525
C -3.739174 -0.584679 -0.210241
C -2.724282 -1.582563 -0.757339
C -2.945686 -2.985364 -0.201178
C -1.853349 -3.994723 -0.569348
C -0.649454 -3.921136 0.315845
C 0.633202 -3.730365 -0.029069
C 1.185771 -3.524904 -1.403558
C 1.875000 -2.171510 -1.605338
C 3.038649 -1.899077 -0.659492
C 3.714697 -0.558895 -0.926010
C 4.683616 -0.137813 0.170668
C 5.350022 1.200850 -0.109690
H 5.936826 1.161494 -1.032065
H 6.024265 1.493993 0.698985
H 4.608241 1.998022 -0.234229
H 4.146282 -0.090990 1.129831
H 5.449525 -0.911485 0.301604
H 4.245221 -0.607525 -1.884839
H 2.952661 0.220860 -1.059349
H 2.698989 -1.928015 0.386709
H 3.774822 -2.708624 -0.739307

H 2.238694 -2.120112 -2.637434
H 1.128850 -1.367750 -1.524804
H 0.402951 -3.646075 -2.155528
H 1.918270 -4.321544 -1.588326
H 1.372406 -3.788021 0.770888
H -0.853375 -4.127866 1.370304
H -1.581461 -3.875715 -1.621556
H -2.261991 -5.007742 -0.469714
H -3.051299 -2.945995 0.893155
H -3.910089 -3.351392 -0.568175
H -1.700289 -1.241562 -0.559331
H -2.807557 -1.620897 -1.850846
H -3.568996 -0.437669 0.866916
H -4.735898 -1.035014 -0.289359
H -3.903087 0.611457 -1.987231
H -4.654154 1.318096 -0.573847
H -1.640685 1.139099 -1.035057
H -2.416060 1.828359 0.391960

conf_21

C -1.007730 -3.995343 -1.438848
C -2.113551 -3.244844 -0.698686
C -2.964183 -2.391069 -1.636008
C -3.818968 -1.369267 -0.895276
C -2.960556 -0.305166 -0.285214
O -1.983188 0.187355 -0.793199
O -3.386006 0.068291 0.942166
C -2.595990 1.077856 1.570225
C -1.286588 0.502515 2.037502
C -1.203723 -0.305116 3.169317
C 0.012626 -0.861144 3.555727
C 1.132344 -0.599027 2.798819
N 1.027002 0.179087 1.711429
C -0.127414 0.722785 1.312685
H -0.106928 1.311678 0.405635
H 1.885224 0.369229 1.156523
H 2.118296 -0.985669 3.022243
H 0.092965 -1.488386 4.434327
H -2.098063 -0.504334 3.751720
H -3.190423 1.419069 2.417566
H -2.429916 1.911031 0.884515
H -4.499247 -0.860147 -1.588611
H -4.436610 -1.827700 -0.119302
H -3.616042 -3.039677 -2.228764
H -2.325477 -1.855208 -2.344751
H -2.762880 -3.948541 -0.166035
H -1.658905 -2.608960 0.075239
C 0.198474 -3.112733 -1.762123
C 1.169159 -2.969131 -0.594680
C 2.271891 -1.951612 -0.856925
C 3.452116 -2.061240 0.099349
C 4.454478 -0.907281 -0.038775

C	4.006103	0.349825	0.641080
C	3.506173	1.464813	0.085971
C	3.271789	1.732323	-1.366731
C	1.802658	1.984815	-1.724283
C	1.155343	3.163218	-1.007370
C	-0.307274	3.351714	-1.393926
C	-1.047778	4.347501	-0.511294
C	-2.507163	4.517456	-0.906550
H	-2.594484	4.902544	-1.926669
H	-3.026964	5.214702	-0.244602
H	-3.042891	3.561693	-0.877852
H	-0.981643	4.021054	0.537704
H	-0.539846	5.318491	-0.546231
H	-0.365155	3.676552	-2.439994
H	-0.828377	2.384117	-1.365928
H	1.225528	3.035204	0.083033
H	1.717606	4.080510	-1.221140
H	1.733556	2.146018	-2.805644
H	1.220672	1.071882	-1.532793
H	3.650299	0.906608	-1.973744
H	3.856775	2.618855	-1.644221
H	3.290213	2.295681	0.758711
H	4.156113	0.363257	1.723715
H	4.651549	-0.730140	-1.099916
H	5.409136	-1.204033	0.407910
H	3.098455	-2.124075	1.138991
H	3.968237	-3.008952	-0.085869
H	1.846748	-0.939132	-0.831237
H	2.646080	-2.078362	-1.880716
H	0.623906	-2.692053	0.319668
H	1.618257	-3.948873	-0.386886
H	-0.143086	-2.118338	-2.079014
H	0.746573	-3.528483	-2.614770
H	-0.673904	-4.854533	-0.845771
H	-1.424219	-4.412440	-2.362691

conf_8

C	3.117715	-0.146802	-0.649382
C	3.957754	-1.196865	-1.371611
C	3.602574	-2.655303	-1.104535
C	2.226337	-3.093508	-1.621233
C	1.072340	-2.655772	-0.777176
O	0.138187	-1.977872	-1.127638
O	1.170226	-3.134950	0.485333
C	0.094813	-2.796353	1.358288
C	0.220750	-1.370699	1.820090
C	1.083811	-1.001172	2.849260
C	1.217757	0.334555	3.216602
C	0.488173	1.285838	2.539055
N	-0.338823	0.904740	1.555069
C	-0.491034	-0.369759	1.181831
H	-1.163412	-0.565261	0.357543

H	-0.863168	1.637315	1.034902
H	0.537513	2.347416	2.744854
H	1.883888	0.636677	4.014629
H	1.659837	-1.763286	3.365140
H	0.183551	-3.482268	2.200506
H	-0.862550	-2.957084	0.858123
H	2.047045	-2.723083	-2.632545
H	2.188240	-4.187904	-1.652502
H	3.676195	-2.877609	-0.034543
H	4.348734	-3.285389	-1.597027
H	3.911010	-1.007724	-2.451708
H	5.007540	-1.052059	-1.089842
C	3.701727	1.249108	-0.840072
C	2.958685	2.377983	-0.135813
C	1.583572	2.709803	-0.705072
C	1.030034	4.013180	-0.138786
C	-0.418723	4.313399	-0.536981
C	-1.430151	3.605048	0.307792
C	-2.403030	2.765554	-0.078717
C	-2.712945	2.308491	-1.468439
C	-2.602664	0.793540	-1.668564
C	-3.502385	-0.037056	-0.761004
C	-3.398249	-1.533437	-1.041900
C	-4.036185	-2.412411	0.029669
C	-5.534804	-2.200935	0.195689
H	-5.954175	-2.892183	0.930947
H	-6.058269	-2.367296	-0.751163
H	-5.769555	-1.186187	0.529926
H	-3.844852	-3.463159	-0.216006
H	-3.536107	-2.229121	0.993041
H	-3.862430	-1.747428	-2.012724
H	-2.342091	-1.807630	-1.158344
H	-3.260179	0.145925	0.297254
H	-4.539379	0.298833	-0.876450
H	-2.848037	0.565485	-2.711668
H	-1.554267	0.484613	-1.548544
H	-2.071895	2.815656	-2.192883
H	-3.741894	2.616542	-1.696359
H	-3.088551	2.416209	0.694435
H	-1.403580	3.878934	1.366277
H	-0.561727	4.092357	-1.598071
H	-0.600665	5.388593	-0.419517
H	1.114737	4.015602	0.958060
H	1.671502	4.833694	-0.476533
H	0.883384	1.882184	-0.534945
H	1.656812	2.804069	-1.795913
H	2.868814	2.145192	0.935880
H	3.575534	3.283174	-0.187162
H	3.754458	1.471944	-1.913643
H	4.739427	1.239280	-0.486442
H	2.083963	-0.173676	-1.013407
H	3.083823	-0.380497	0.425434

conf_3

C	2.715704	-1.118337	-0.967246
C	2.984660	-2.392371	-1.762674
C	2.150719	-3.612091	-1.386104
C	0.644833	-3.469586	-1.642079
C	-0.091415	-2.658266	-0.623904
O	-0.760168	-1.675352	-0.830884
O	0.054559	-3.170974	0.619814
C	-0.635339	-2.479578	1.659450
C	0.097758	-1.219029	2.027273
C	1.195774	-1.227461	2.884890
C	1.887065	-0.052352	3.164704
C	1.474454	1.119081	2.569240
N	0.413645	1.101284	1.750209
C	-0.274601	-0.009018	1.467066
H	-1.100882	0.089608	0.774299
H	0.116195	1.976005	1.271511
H	1.958174	2.076095	2.716786
H	2.740097	-0.044394	3.831146
H	1.515796	-2.161846	3.335738
H	-0.652917	-3.172879	2.500027
H	-1.658706	-2.258325	1.350005
H	0.448685	-3.020705	-2.617920
H	0.184563	-4.463851	-1.632619
H	2.315951	-3.879835	-0.337096
H	2.501873	-4.463831	-1.975551
H	2.846647	-2.178871	-2.830373
H	4.041879	-2.659171	-1.646701
C	3.728299	-0.028589	-1.302628
C	3.533191	1.292805	-0.568153
C	2.277521	2.064000	-0.958328
C	2.258515	3.478343	-0.389169
C	0.946783	4.232725	-0.639613
C	-0.151052	3.868683	0.311265
C	-1.257940	3.164341	0.032260
C	-1.638494	2.586728	-1.303109
C	-3.083969	2.097833	-1.357931
C	-3.342675	0.861239	-0.507489
C	-4.788173	0.381589	-0.557369
C	-5.053389	-0.861893	0.286996
C	-4.392113	-2.124970	-0.250844
H	-3.305888	-2.020117	-0.332937
H	-4.765818	-2.362412	-1.251932
H	-4.602718	-2.986532	0.389377
H	-4.721252	-0.673787	1.317535
H	-6.134252	-1.025261	0.349229
H	-5.442071	1.195041	-0.221324
H	-5.065242	0.178428	-1.599909
H	-2.671639	0.059759	-0.842029
H	-3.094354	1.073072	0.544568
H	-3.754965	2.909831	-1.050760
H	-3.339045	1.870423	-2.398312

H	-0.967086	1.756149	-1.564260
H	-1.475693	3.344854	-2.077177
H	-1.990255	3.046303	0.832944
H	-0.054751	4.280241	1.318688
H	0.629663	4.067834	-1.673827
H	1.130775	5.307696	-0.535542
H	2.471276	3.459014	0.690141
H	3.085373	4.042153	-0.833608
H	1.378158	1.513427	-0.655386
H	2.219629	2.127714	-2.052395
H	3.535948	1.112499	0.517305
H	4.403332	1.931475	-0.761171
H	3.706418	0.159288	-2.383942
H	4.733396	-0.408787	-1.085827
H	1.700664	-0.757801	-1.170132
H	2.765697	-1.339854	0.109491

conf_20

C	-3.281874	-2.206807	-1.445536
C	-3.754462	-1.333777	-0.272032
C	-4.446313	-0.036229	-0.686140
C	-3.564865	0.934971	-1.476152
C	-2.350053	1.371810	-0.720768
O	-1.206659	1.297799	-1.098736
O	-2.662799	1.869026	0.497938
C	-1.549083	2.251700	1.302866
C	-0.853281	1.029416	1.836998
C	-1.366524	0.300511	2.907494
C	-0.731168	-0.857933	3.345548
C	0.410190	-1.274526	2.697463
N	0.883937	-0.557091	1.668580
C	0.296072	0.558643	1.225134
H	0.744715	1.045437	0.369934
H	1.736405	-0.896159	1.179162
H	0.966614	-2.164039	2.963560
H	-1.116613	-1.433173	4.177609
H	-2.272919	0.638654	3.400234
H	-1.972503	2.840677	2.116137
H	-0.858282	2.871082	0.727448
H	-3.216411	0.500529	-2.414553
H	-4.141211	1.833804	-1.721966
H	-4.831191	0.476430	0.200220
H	-5.315183	-0.276944	-1.307439
H	-4.458483	-1.896028	0.349052
H	-2.904996	-1.103067	0.387228
C	-1.784083	-2.138012	-1.742621
C	-0.932178	-2.873342	-0.714410
C	0.563274	-2.755685	-0.974826
C	1.405739	-3.683684	-0.108844
C	2.912500	-3.409433	-0.203655
C	3.350212	-2.233496	0.613696
C	3.733061	-1.019140	0.189473

C	3.824860	-0.536767	-1.223534
C	2.861654	0.607530	-1.558435
C	3.016790	1.855199	-0.697815
C	2.035625	2.957305	-1.081628
C	1.977127	4.099013	-0.075677
C	1.000132	5.193779	-0.477878
H	1.291162	5.648734	-1.429127
H	0.955248	5.990081	0.269363
H	-0.013439	4.797728	-0.608778
H	1.701205	3.698356	0.911494
H	2.978470	4.526820	0.052516
H	2.305703	3.352415	-2.068543
H	1.029843	2.532556	-1.210390
H	2.882259	1.607327	0.365696
H	4.044694	2.230994	-0.772327
H	3.004145	0.881624	-2.609484
H	1.827435	0.240195	-1.496167
H	3.655834	-1.360304	-1.921113
H	4.852593	-0.190303	-1.392314
H	4.067604	-0.313407	0.950784
H	3.407252	-2.421525	1.689225
H	3.189352	-3.283125	-1.253994
H	3.460062	-4.286370	0.158044
H	1.084323	-3.620908	0.941299
H	1.209916	-4.718633	-0.407591
H	0.877356	-1.711632	-0.842309
H	0.767605	-2.981575	-2.028857
H	-1.155757	-2.504129	0.297594
H	-1.216904	-3.933609	-0.709555
H	-1.454462	-1.094810	-1.814465
H	-1.595014	-2.583559	-2.726281
H	-3.544739	-3.252841	-1.252479
H	-3.843702	-1.928538	-2.344864

conf_23

C	2.593987	-1.825128	-1.727529
C	2.231709	-2.681700	-0.515237
C	1.372370	-3.900375	-0.844151
C	0.049959	-3.575563	-1.553309
C	-0.745230	-2.581204	-0.773962
O	-0.958183	-1.435349	-1.085570
O	-1.176510	-3.092191	0.402776
C	-1.827482	-2.163706	1.269983
C	-0.812793	-1.209280	1.836685
C	0.072896	-1.585450	2.843437
C	1.067150	-0.711195	3.274986
C	1.166847	0.527348	2.681551
N	0.297499	0.868006	1.718721
C	-0.670301	0.053713	1.288472
H	-1.297565	0.420008	0.487421
H	0.387852	1.796835	1.258401
H	1.917050	1.263667	2.939799

H	1.763059	-0.989688	4.055997
H	-0.006717	-2.573574	3.286074
H	-2.276216	-2.771215	2.055389
H	-2.611883	-1.626060	0.733379
H	0.222893	-3.145806	-2.540603
H	-0.537769	-4.490408	-1.669822
H	1.156654	-4.459991	0.071086
H	1.938037	-4.574023	-1.496022
H	3.152759	-3.040805	-0.040090
H	1.728591	-2.065572	0.243487
C	3.844210	-0.974676	-1.520663
C	3.768408	0.098819	-0.437809
C	2.842736	1.272815	-0.753081
C	3.206492	2.514498	0.055632
C	2.296983	3.725794	-0.181903
C	1.039505	3.712075	0.628471
C	-0.230618	3.667228	0.197745
C	-0.709208	3.601114	-1.217055
C	-1.539369	2.354271	-1.539700
C	-2.804914	2.195057	-0.705241
C	-3.601902	0.948933	-1.073321
C	-4.723197	0.632723	-0.092807
C	-5.507783	-0.614704	-0.471261
H	-5.982092	-0.498177	-1.450113
H	-6.295618	-0.831996	0.254355
H	-4.856647	-1.494357	-0.531726
H	-4.299871	0.513004	0.915702
H	-5.403527	1.489901	-0.024765
H	-4.019740	1.072240	-2.080049
H	-2.924076	0.087654	-1.146659
H	-2.558966	2.159086	0.366651
H	-3.434906	3.085980	-0.819696
H	-1.817909	2.391249	-2.598559
H	-0.908220	1.459747	-1.441017
H	0.132457	3.661558	-1.910472
H	-1.327248	4.490112	-1.400152
H	-1.011447	3.740759	0.955726
H	1.194041	3.830195	1.704931
H	2.078447	3.811450	-1.249593
H	2.844688	4.634906	0.092874
H	3.235145	2.276995	1.129602
H	4.234398	2.791751	-0.200696
H	1.791068	0.993722	-0.603254
H	2.926862	1.521617	-1.818677
H	3.490161	-0.350078	0.526143
H	4.780581	0.495147	-0.292432
H	4.106774	-0.489409	-2.468312
H	4.679247	-1.646105	-1.286374
H	2.779189	-2.488264	-2.581784
H	1.742787	-1.196233	-2.014442

conf_72

C	-0.663459	0.505909	1.840936
C	-2.034753	0.430423	2.499998
C	-3.063297	1.430030	1.978983
C	-3.492708	1.215972	0.523658
C	-2.500354	1.617061	-0.523003
O	-2.158754	0.956602	-1.472978
O	-2.024020	2.868404	-0.316722
C	-1.145526	3.374224	-1.319593
C	0.277627	2.967389	-1.046362
C	1.195203	3.850233	-0.480933
C	2.499271	3.447684	-0.207814
C	2.863542	2.150670	-0.489617
N	1.965375	1.319416	-1.035813
C	0.710763	1.678225	-1.323682
H	0.060282	0.922952	-1.749263
H	2.246425	0.331778	-1.183431
H	3.844165	1.737898	-0.289829
H	3.220175	4.126797	0.229188
H	0.886582	4.865079	-0.249719
H	-1.241022	4.458481	-1.269676
H	-1.464598	3.024432	-2.303559
H	-3.751767	0.172671	0.332967
H	-4.389742	1.815122	0.325604
H	-2.694443	2.453299	2.103677
H	-3.964112	1.352448	2.594540
H	-2.430966	-0.587576	2.390752
H	-1.916456	0.592294	3.577749
C	0.361975	-0.426346	2.475251
C	1.707729	-0.390370	1.765864
C	2.779110	-1.269694	2.391457
C	4.073852	-1.365533	1.585238
C	3.971881	-2.194382	0.291365
C	3.611014	-1.461642	-0.964555
C	2.585607	-1.706102	-1.796076
C	1.490871	-2.707512	-1.608907
C	0.111703	-2.066840	-1.439630
C	-0.990507	-3.083525	-1.170830
C	-2.295829	-2.435374	-0.733226
C	-3.421979	-3.430297	-0.491788
C	-4.697386	-2.764577	0.003446
H	-5.059486	-2.021474	-0.715006
H	-4.531235	-2.254465	0.959128
H	-5.498516	-3.491773	0.157029
H	-3.628042	-3.975044	-1.420966
H	-3.093723	-4.183731	0.235053
H	-2.113148	-1.868777	0.191460
H	-2.609467	-1.694575	-1.478625
H	-1.156087	-3.691575	-2.068779
H	-0.654026	-3.779072	-0.390689
H	0.144462	-1.364682	-0.596394
H	-0.143415	-1.477072	-2.330516

H	1.694756	-3.341206	-0.741963
H	1.470752	-3.374240	-2.479841
H	2.551606	-1.146315	-2.734486
H	4.343401	-0.713348	-1.279777
H	3.291449	-3.033467	0.459240
H	4.954693	-2.642621	0.098698
H	4.455434	-0.359084	1.361295
H	4.834236	-1.830189	2.219447
H	2.380486	-2.282239	2.535400
H	3.009331	-0.893694	3.395018
H	1.559149	-0.698813	0.725589
H	2.071318	0.647289	1.739547
H	-0.024650	-1.453677	2.462522
H	0.491860	-0.164040	3.532548
H	-0.753198	0.252252	0.776164
H	-0.293994	1.540225	1.887115

conf_77

C	3.300237	1.125958	2.054435
C	3.683491	2.601682	2.108977
C	3.149432	3.474209	0.974994
C	3.691050	3.095708	-0.401743
C	2.921140	2.019165	-1.099630
O	1.732001	1.828312	-1.036527
O	3.716352	1.271831	-1.902622
C	3.030754	0.336812	-2.729924
C	2.594236	-0.878541	-1.956755
C	3.488915	-1.896606	-1.632006
C	3.063451	-3.017860	-0.926720
C	1.740414	-3.103538	-0.554414
N	0.899986	-2.107913	-0.868828
C	1.281132	-1.014742	-1.538033
H	0.530294	-0.254319	-1.711236
H	-0.091182	-2.184264	-0.558925
H	1.318142	-3.937139	-0.008112
H	3.746448	-3.818304	-0.672515
H	4.527433	-1.812662	-1.937267
H	3.751956	0.053481	-3.496731
H	2.171448	0.816484	-3.203009
H	3.626737	3.957799	-1.078696
H	4.747624	2.817011	-0.366176
H	3.434067	4.510443	1.176555
H	2.055540	3.457722	0.945588
H	3.332021	3.018837	3.059844
H	4.776834	2.686087	2.129937
C	1.805171	0.862645	2.173927
C	1.470650	-0.615279	2.326691
C	-0.012986	-0.904213	2.154819
C	-0.412100	-2.341534	2.464873
C	-1.813947	-2.698362	1.951621

C	-1.851177	-2.946488	0.473655
C	-2.263068	-2.107651	-0.490078
C	-2.821914	-0.732359	-0.316031
C	-4.305605	-0.671540	-0.689265
C	-4.881546	0.732700	-0.576095
C	-6.362410	0.793294	-0.929059
C	-6.954738	2.199562	-0.898485
C	-6.946970	2.847538	0.479810
H	-7.446712	3.819492	0.460596
H	-5.931027	3.013064	0.850571
H	-7.470067	2.221649	1.210742
H	-6.410672	2.835666	-1.608443
H	-7.985421	2.151181	-1.266213
H	-6.505894	0.366269	-1.929507
H	-6.924302	0.149137	-0.239319
H	-4.724373	1.102769	0.444242
H	-4.323387	1.410272	-1.237042
H	-4.441157	-1.044868	-1.712317
H	-4.863210	-1.355964	-0.038715
H	-2.275220	-0.028645	-0.959881
H	-2.684802	-0.379927	0.709979
H	-2.273444	-2.488312	-1.513779
H	-1.539838	-3.946478	0.162916
H	-2.512211	-1.903344	2.229798
H	-2.162614	-3.607018	2.452591
H	0.322880	-3.041562	2.041348
H	-0.370305	-2.500984	3.547086
H	-0.310593	-0.637107	1.131571
H	-0.592598	-0.232007	2.799656
H	2.044315	-1.198028	1.589898
H	1.808676	-0.971998	3.307688
H	1.286279	1.263155	1.296073
H	1.408634	1.409407	3.038927
H	3.678733	0.668442	1.127379
H	3.822565	0.605440	2.866502

conf_91

C	-3.214674	-0.751491	-1.496700
C	-4.291492	0.314877	-1.674225
C	-4.047387	1.651351	-0.978803
C	-2.802814	2.407699	-1.482128
C	-1.560285	2.151632	-0.690304
O	-0.560942	1.589131	-1.064117
O	-1.661550	2.665585	0.560149
C	-0.486744	2.583135	1.363756
C	-0.269379	1.188622	1.883306
C	-0.972853	0.682042	2.973544
C	-0.774813	-0.629677	3.396345
C	0.120187	-1.421425	2.711917
N	0.788536	-0.908359	1.668717
C	0.621577	0.346961	1.241533
H	1.181836	0.647588	0.367248

H	1.413568	-1.529430	1.119464
H	0.323410	-2.456215	2.956356
H	-1.314529	-1.037462	4.241453
H	-1.686005	1.314696	3.493036
H	-0.658877	3.275231	2.188006
H	0.382211	2.914697	0.791094
H	-2.585213	2.156615	-2.522001
H	-2.986033	3.484867	-1.425375
H	-3.987515	1.523541	0.107017
H	-4.918974	2.287670	-1.152864
H	-4.433518	0.500897	-2.745386
H	-5.245145	-0.085543	-1.309473
C	-2.969441	-1.147005	-0.042883
C	-2.312913	-2.513632	0.126274
C	-0.979512	-2.688006	-0.591042
C	-0.298280	-4.005280	-0.237621
C	1.149930	-4.112076	-0.725710
C	2.120565	-3.368363	0.137986
C	2.989438	-2.409949	-0.218245
C	3.197834	-1.843486	-1.588043
C	2.769125	-0.380580	-1.737577
C	3.488882	0.593998	-0.813339
C	3.042216	2.037509	-1.018278
C	3.517882	2.985001	0.074678
C	3.084406	4.424778	-0.157354
H	1.993862	4.509113	-0.228559
H	3.497597	4.812787	-1.092920
H	3.417890	5.082210	0.649460
H	3.140556	2.635332	1.047460
H	4.610634	2.937017	0.150548
H	3.403686	2.390326	-1.991860
H	1.946094	2.079734	-1.090846
H	3.333625	0.312167	0.239091
H	4.572197	0.516794	-0.967539
H	2.940608	-0.074740	-2.775553
H	1.682091	-0.305083	-1.591635
H	2.674793	-2.446378	-2.333527
H	4.267085	-1.922488	-1.822005
H	3.664373	-2.039594	0.554688
H	2.159800	-3.716496	1.174262
H	1.212952	-3.783951	-1.766613
H	1.448983	-5.167338	-0.714814
H	-0.322980	-4.157728	0.851418
H	-0.882189	-4.830274	-0.658569
H	-0.320553	-1.841726	-0.362733
H	-1.128760	-2.643133	-1.675702
H	-2.172592	-2.711303	1.198228
H	-3.006516	-3.288190	-0.224737
H	-3.926185	-1.155593	0.494569
H	-2.354873	-0.383003	0.452653
H	-3.530174	-1.640621	-2.056428
H	-2.275776	-0.424012	-1.958699

conf_56

C	3.425209	-0.728412	-0.286984
C	3.991577	-1.934719	-1.022318
C	3.124151	-3.187711	-0.959228
C	1.753187	-3.039646	-1.628689
C	0.685621	-2.350169	-0.835587
O	-0.065726	-1.496026	-1.240818
O	0.592515	-2.840074	0.421861
C	-0.511697	-2.368522	1.191609
C	-0.258171	-0.995009	1.752408
C	0.418994	-0.797843	2.953929
C	0.643181	0.487110	3.440773
C	0.198548	1.563566	2.706110
N	-0.447973	1.349066	1.551885
C	-0.685655	0.127346	1.063459
H	-1.191702	0.065046	0.109911
H	-0.694469	2.160544	0.952085
H	0.345674	2.595856	2.996507
H	1.162335	0.653105	4.376055
H	0.773095	-1.656367	3.516394
H	-0.620552	-3.090664	2.000696
H	-1.418218	-2.369857	0.582919
H	1.829175	-2.515695	-2.584150
H	1.348475	-4.037140	-1.840454
H	2.990750	-3.509866	0.078527
H	3.650378	-4.001442	-1.466144
H	4.158134	-1.667048	-2.074006
H	4.979601	-2.174852	-0.613123
C	4.322513	0.500751	-0.381708
C	3.835308	1.690158	0.445369
C	2.411204	2.134756	0.124142
C	2.222642	2.753846	-1.255887
C	0.761655	2.801764	-1.699024
C	-0.149030	3.578233	-0.795128
C	-1.467225	3.379390	-0.633077
C	-2.287850	2.316539	-1.299192
C	-3.392321	1.737369	-0.412279
C	-3.927174	0.412341	-0.937061
C	-4.957567	-0.229707	-0.017696
C	-5.403927	-1.620156	-0.461483
C	-4.310797	-2.677214	-0.364010
H	-4.687603	-3.663731	-0.645329
H	-3.936694	-2.752086	0.664476
H	-3.464350	-2.456339	-1.022542
H	-6.255089	-1.930797	0.153210
H	-5.777082	-1.570324	-1.491482
H	-4.545758	-0.294795	1.000566
H	-5.831270	0.428385	0.053413
H	-4.364854	0.561748	-1.932094
H	-3.084174	-0.275374	-1.091987
H	-3.022046	1.587195	0.612152
H	-4.207989	2.462756	-0.314102

H	-1.641023	1.509890	-1.665638
H	-2.745429	2.739389	-2.203375
H	-2.016672	4.086974	-0.010682
H	0.298227	4.433045	-0.286205
H	0.391043	1.778210	-1.832770
H	0.708283	3.260958	-2.695452
H	2.653172	3.762307	-1.267695
H	2.780110	2.178527	-2.001640
H	2.079803	2.852617	0.885917
H	1.750130	1.264823	0.209144
H	3.888600	1.421367	1.508382
H	4.522996	2.533160	0.311805
H	4.425270	0.787257	-1.435321
H	5.332527	0.235626	-0.049047
H	2.439655	-0.485511	-0.701661
H	3.264787	-0.985915	0.770503

conf_59

C	-3.450461	0.536270	-0.549297
C	-4.017428	1.813676	-1.150690
C	-3.277172	3.085296	-0.749037
C	-1.815638	3.130800	-1.210046
C	-0.821394	2.379550	-0.378302
O	0.046885	1.647663	-0.788623
O	-0.948711	2.660705	0.939133
C	0.074854	2.141142	1.784971
C	-0.122360	0.678444	2.079639
C	-0.970184	0.231019	3.090326
C	-1.128824	-1.131012	3.332809
C	-0.444226	-2.031011	2.546996
N	0.363953	-1.576155	1.579284
C	0.539734	-0.275587	1.325903
H	1.193234	-0.015611	0.504994
H	0.795532	-2.250477	0.917490
H	-0.522121	-3.105633	2.650909
H	-1.780427	-1.491465	4.118506
H	-1.510769	0.952537	3.695338
H	0.003804	2.723027	2.703904
H	1.052992	2.304741	1.327308
H	-1.709227	2.771623	-2.236168
H	-1.467487	4.171081	-1.195549
H	-3.322655	3.229775	0.335197
H	-3.789071	3.943496	-1.193345
H	-4.011371	1.727051	-2.245195
H	-5.069935	1.915182	-0.862459
C	-4.187094	-0.718886	-1.001446
C	-3.687925	-2.000930	-0.334665
C	-2.180538	-2.215325	-0.440598
C	-1.657589	-2.423775	-1.856889
C	-0.141301	-2.282381	-1.971672

C	0.645709	-3.243703	-1.130451
C	1.911354	-3.081276	-0.713168
C	2.792759	-1.902453	-0.996416
C	3.768455	-1.576432	0.135651
C	4.570474	-0.300473	-0.103962
C	3.756326	0.979160	0.063769
C	4.550196	2.262876	-0.166372
C	5.018888	2.446214	-1.603463
H	5.726290	1.669568	-1.906345
H	5.520977	3.408179	-1.732376
H	4.173391	2.417385	-2.299035
H	3.926114	3.118312	0.117727
H	5.412736	2.279135	0.511147
H	2.895948	0.980241	-0.620382
H	3.351387	0.993689	1.086860
H	5.414973	-0.269669	0.593820
H	5.007296	-0.339965	-1.108339
H	3.232467	-1.488132	1.092578
H	4.450439	-2.424697	0.260797
H	2.190009	-1.027473	-1.264864
H	3.379952	-2.123200	-1.898778
H	2.381852	-3.908895	-0.180600
H	0.159088	-4.193421	-0.905236
H	0.144429	-1.246503	-1.748339
H	0.150866	-2.439431	-3.018769
H	-1.970711	-3.409633	-2.221418
H	-2.113802	-1.693243	-2.532209
H	-1.898833	-3.077201	0.178644
H	-1.676808	-1.343907	-0.006601
H	-3.962569	-1.974758	0.727731
H	-4.214440	-2.861929	-0.762127
H	-4.108636	-0.803970	-2.091941
H	-5.256948	-0.608468	-0.791258
H	-2.394661	0.447245	-0.830707
H	-3.476049	0.604342	0.548472

conf_112

C	3.828376	-0.980099	-1.533781
C	2.484331	-1.542106	-1.994530
C	2.248143	-2.955576	-1.472021
C	0.816712	-3.470993	-1.689059
C	-0.129991	-2.756786	-0.780709
O	-0.774803	-1.771268	-1.042032
O	-0.147169	-3.315190	0.453426
C	-0.966202	-2.655142	1.418072
C	-0.298474	-1.392986	1.891231
C	0.739831	-1.409696	2.819785
C	1.386816	-0.231084	3.182367
C	0.995180	0.949600	2.592979
N	-0.009800	0.940058	1.704840
C	-0.657919	-0.171973	1.345993
H	-1.437008	-0.069191	0.602535

H	-0.243367	1.822199	1.206102
H	1.459454	1.907952	2.788074
H	2.195137	-0.229856	3.902359
H	1.051856	-2.352924	3.257642
H	-1.072653	-3.366636	2.236562
H	-1.947704	-2.437220	0.993407
H	0.496039	-3.291436	-2.717278
H	0.769090	-4.541924	-1.480940
H	2.488720	-3.017058	-0.403863
H	2.936204	-3.642651	-1.974534
H	1.675935	-0.876391	-1.668387
H	2.436921	-1.560035	-3.089142
C	3.825033	-0.506984	-0.071315
C	3.773400	1.009551	0.093470
C	2.564510	1.693448	-0.532591
C	2.550036	3.196096	-0.277439
C	1.266107	3.896780	-0.728793
C	0.126408	3.753652	0.230960
C	-1.138956	3.386609	-0.026570
C	-1.722579	3.011511	-1.351857
C	-2.552597	1.723864	-1.355928
C	-3.736278	1.736828	-0.392602
C	-4.675053	0.543243	-0.541663
C	-4.071354	-0.785762	-0.103612
C	-5.038894	-1.952203	-0.242090
H	-5.942105	-1.790763	0.353873
H	-4.590203	-2.895252	0.084449
H	-5.348460	-2.079989	-1.283495
H	-3.168388	-0.997529	-0.688366
H	-3.761416	-0.695150	0.949379
H	-5.583305	0.728176	0.043469
H	-4.999022	0.465840	-1.587402
H	-3.390022	1.783604	0.650275
H	-4.304170	2.660935	-0.556114
H	-2.934654	1.575355	-2.372381
H	-1.895235	0.864024	-1.175070
H	-0.939645	2.941636	-2.110640
H	-2.375355	3.839520	-1.662404
H	-1.849017	3.448671	0.799474
H	0.350974	4.083850	1.249191
H	0.987863	3.555210	-1.729574
H	1.466584	4.972090	-0.819749
H	2.715168	3.396468	0.791169
H	3.404625	3.646717	-0.792662
H	1.642536	1.231535	-0.158437
H	2.551593	1.518384	-1.614874
H	3.808552	1.254291	1.164524
H	4.685308	1.444875	-0.334758
H	4.715963	-0.874679	0.447204
H	2.969284	-0.955992	0.454370
H	4.597160	-1.746984	-1.678508
H	4.121621	-0.147166	-2.182285

conf_106

C	4.516282	0.687677	0.519415
C	5.393374	-0.555711	0.364968
C	5.115310	-1.618586	1.437118
C	4.103393	-2.701384	1.015575
C	2.850156	-2.088212	0.475822
O	2.043981	-1.442467	1.096857
O	2.728041	-2.291910	-0.860308
C	1.777320	-1.477750	-1.536114
C	0.369042	-1.614690	-1.027318
C	-0.345171	-2.808961	-1.059574
C	-1.642563	-2.866222	-0.556228
C	-2.214268	-1.727785	-0.031900
N	-1.504357	-0.588048	-0.026675
C	-0.258689	-0.504172	-0.495269
H	0.221104	0.461855	-0.403306
H	-1.895600	0.277938	0.369084
H	-3.213163	-1.684415	0.382056
H	-2.209186	-3.788665	-0.567045
H	0.118354	-3.703199	-1.464434
H	1.836168	-1.790932	-2.579708
H	2.089826	-0.432238	-1.467897
H	4.538616	-3.349408	0.252723
H	3.834955	-3.310356	1.883120
H	4.756492	-1.132269	2.350078
H	6.035988	-2.142519	1.706549
H	5.254015	-0.992189	-0.633133
H	6.445231	-0.256372	0.408683
C	4.530732	1.622990	-0.682129
C	3.595143	2.821176	-0.530107
C	2.112569	2.458823	-0.526747
C	1.195251	3.664408	-0.363771
C	-0.294808	3.330467	-0.424188
C	-0.796928	2.564031	0.770446
C	-2.079469	2.404230	1.128762
C	-3.270862	2.941290	0.394166
C	-4.090538	1.869642	-0.334095
C	-4.721139	0.827914	0.581236
C	-5.507319	-0.236360	-0.172247
C	-6.068869	-1.331955	0.724705
C	-6.826609	-2.403103	-0.044725
H	-7.674616	-1.971982	-0.584698
H	-7.217493	-3.175379	0.622049
H	-6.184329	-2.893802	-0.784163
H	-5.254014	-1.797099	1.300511
H	-6.726632	-0.878629	1.475323
H	-6.330285	0.242396	-0.716572
H	-4.873053	-0.685523	-0.951942
H	-3.953790	0.343560	1.206535
H	-5.381366	1.329828	1.299179
H	-4.884647	2.363231	-0.904709
H	-3.456565	1.375478	-1.085216

H	-2.953438	3.694806	-0.331237
H	-3.922802	3.452505	1.112902
H	-2.275449	1.893184	2.072157
H	-0.036732	2.156456	1.438457
H	-0.500864	2.775047	-1.351676
H	-0.868783	4.258623	-0.517150
H	1.415795	4.166985	0.585893
H	1.422420	4.391181	-1.151079
H	1.919057	1.734613	0.276064
H	1.870815	1.957144	-1.477431
H	3.836522	3.353828	0.398645
H	3.778893	3.531844	-1.343991
H	4.259045	1.062518	-1.589007
H	5.551778	1.982499	-0.852857
H	3.488953	0.383896	0.735798
H	4.845062	1.240360	1.408963

C18:1 11*E* pyridylcarbinol ester**conf_0**

C	4.369176	1.206343	1.402142
C	3.645910	2.400741	0.782223
C	2.136279	2.228799	0.674425
C	1.427087	3.482851	0.175389
C	-0.065085	3.280525	-0.074924
C	-0.346860	2.469057	-1.332834
C	-1.757372	2.003973	-1.528860
C	-2.824686	2.303864	-0.776179
C	-4.228051	1.900833	-1.107491
C	-5.047582	1.379847	0.074459
C	-4.458217	0.165405	0.785440
C	-4.169600	-1.024992	-0.119623
C	-3.699395	-2.262520	0.634691
C	-3.325229	-3.415933	-0.284130
H	-2.984529	-4.288504	0.279742
H	-4.179550	-3.729514	-0.890781
H	-2.526247	-3.131387	-0.979232
H	-4.488995	-2.583161	1.323844
H	-2.843775	-2.003887	1.274124
H	-5.074071	-1.273599	-0.689385
H	-3.419997	-0.751951	-0.876422
H	-5.147777	-0.146867	1.578115
H	-3.538269	0.461351	1.310393
H	-5.183541	2.187587	0.803085
H	-6.050399	1.131465	-0.289693
H	-4.214450	1.169316	-1.922326
H	-4.740484	2.785075	-1.508300
H	-2.700180	2.955898	0.090655
H	-1.926518	1.393353	-2.418697
H	0.324116	1.600094	-1.387274
H	-0.069896	3.066934	-2.211756

H	-0.504638	2.791413	0.807396
H	-0.568496	4.249809	-0.153181
H	1.905013	3.829309	-0.749827
H	1.568372	4.286130	0.906445
H	1.916464	1.387334	0.004881
H	1.730817	1.954797	1.660270
H	4.051052	2.610164	-0.215181
H	3.865424	3.291612	1.381924
C	4.094524	-0.134067	0.725086
C	4.466367	-0.174491	-0.752155
C	4.129137	-1.517082	-1.406548
C	2.649448	-1.741430	-1.379010
O	1.819561	-1.027618	-1.887612
O	2.304296	-2.837379	-0.665787
C	0.900792	-3.066308	-0.548619
C	0.274414	-2.030963	0.344013
C	0.486537	-2.020451	1.720030
C	-0.050618	-1.008969	2.511618
C	-0.794034	-0.018276	1.910388
N	-0.986563	-0.053994	0.584727
C	-0.481637	-1.007928	-0.199552
H	-0.675401	-0.918858	-1.260530
H	-1.546756	0.689598	0.121388
H	-1.246439	0.806896	2.445074
H	0.105939	-0.987707	3.582471
H	1.085053	-2.803271	2.175555
H	0.808972	-4.061132	-0.113055
H	0.433729	-3.059198	-1.535588
H	4.434576	-1.509708	-2.457206
H	4.636268	-2.344446	-0.906477
H	5.538201	0.013368	-0.871494
H	3.944979	0.615394	-1.301651
H	4.642743	-0.922188	1.255066
H	3.030269	-0.383404	0.839798
H	4.087699	1.126714	2.459480
H	5.447979	1.400143	1.392578

conf_7

C	3.975436	0.421786	2.395533
C	3.423842	1.800259	2.035525
C	2.010631	1.776182	1.468061
C	1.426064	3.168104	1.257168
C	0.061587	3.150252	0.573565
C	0.149386	2.855420	-0.918603
C	-1.140176	2.542096	-1.611884
C	-2.362883	2.528903	-1.065362
C	-3.619507	2.180848	-1.806212
C	-4.110875	0.758438	-1.511716
C	-4.439269	0.492873	-0.047555
C	-4.669812	-0.979703	0.259863
C	-4.950780	-1.261561	1.729621
C	-5.097808	-2.744610	2.033807

H	-4.187862	-3.296251	1.771802
H	-5.301174	-2.920213	3.093006
H	-5.920812	-3.183631	1.462235
H	-5.859732	-0.728881	2.032045
H	-4.144394	-0.836990	2.345394
H	-5.502332	-1.354695	-0.348248
H	-3.791184	-1.560893	-0.059837
H	-5.322737	1.075592	0.240054
H	-3.631558	0.870779	0.596631
H	-4.995600	0.551188	-2.123074
H	-3.346037	0.045002	-1.852120
H	-3.449343	2.285462	-2.882202
H	-4.404817	2.897382	-1.539200
H	-2.470332	2.806532	-0.016926
H	-1.057610	2.319612	-2.678054
H	0.853697	2.031593	-1.106027
H	0.608110	3.713450	-1.427952
H	-0.566213	2.400625	1.078254
H	-0.448560	4.108063	0.719816
H	2.123292	3.773756	0.664341
H	1.341151	3.668885	2.227567
H	2.011538	1.227972	0.517160
H	1.355220	1.212885	2.149882
H	4.087172	2.296024	1.316506
H	3.441169	2.428592	2.933519
C	3.927018	-0.603224	1.265433
C	4.687655	-0.185044	0.013150
C	4.563259	-1.209287	-1.116918
C	3.137555	-1.315598	-1.560657
O	2.458473	-0.408058	-1.975461
O	2.641845	-2.565556	-1.415854
C	1.274385	-2.722201	-1.789994
C	0.371358	-2.051615	-0.790948
C	0.161066	-2.579352	0.481297
C	-0.634279	-1.907250	1.404793
C	-1.205522	-0.707717	1.042561
N	-0.990044	-0.222753	-0.187991
C	-0.231560	-0.844121	-1.094881
H	-0.102248	-0.343066	-2.045717
H	-1.403849	0.688313	-0.469851
H	-1.835440	-0.117105	1.694645
H	-0.809720	-2.306823	2.395454
H	0.629520	-3.519823	0.754650
H	1.104531	-3.798733	-1.802649
H	1.109780	-2.317936	-2.790874
H	5.145399	-0.884534	-1.984980
H	4.926362	-2.191932	-0.809670
H	5.748043	-0.050218	0.249092
H	4.321856	0.778331	-0.355065
H	4.328588	-1.556941	1.628354
H	2.877664	-0.801699	1.004846
H	3.415029	0.024205	3.250675

H 5.010571 0.531022 2.739110

conf_2

C 3.885868 0.831365 0.523962
C 3.304802 1.644612 1.673618
C 3.095930 3.123624 1.355643
C 2.107436 3.413550 0.227270
C 0.709463 2.866161 0.482927
C -0.285147 3.230902 -0.617542
C -1.707018 2.868065 -0.315031
C -2.578143 2.324573 -1.176434
C -4.050574 2.176583 -0.939683
C -4.694214 0.966836 -1.616474
C -4.183733 -0.391741 -1.149655
C -4.409063 -0.679518 0.328515
C -3.968562 -2.075965 0.748074
C -4.168157 -2.346796 2.231527
H -5.223438 -2.264718 2.506946
H -3.833088 -3.349825 2.508713
H -3.617515 -1.627679 2.848851
H -2.913316 -2.226039 0.479635
H -4.525225 -2.816353 0.161943
H -3.891812 0.067293 0.948144
H -5.474462 -0.554100 0.560048
H -3.114579 -0.484754 -1.388812
H -4.676670 -1.172819 -1.739766
H -5.776681 1.016481 -1.455790
H -4.547040 1.050519 -2.699631
H -4.531228 3.078167 -1.342409
H -4.260844 2.190388 0.135608
H -2.221286 2.068175 -2.177646
H -2.079713 3.173887 0.666916
H 0.022855 2.791580 -1.573809
H -0.249365 4.319749 -0.761965
H 0.766316 1.776304 0.583568
H 0.342113 3.247844 1.445878
H 2.483475 3.012362 -0.721694
H 2.043390 4.498862 0.087253
H 2.755750 3.635734 2.263994
H 4.062579 3.573494 1.101069
H 3.969811 1.561076 2.541067
H 2.354034 1.192962 1.990457
C 3.963918 -0.655207 0.847654
C 4.661114 -1.508814 -0.207853
C 4.086942 -1.357405 -1.621252
C 2.602451 -1.531109 -1.677855
O 1.807733 -0.743986 -2.130051
O 2.206335 -2.705019 -1.132232
C 0.798003 -2.926905 -1.125064
C 0.125688 -2.047725 -0.105362
C 0.159947 -2.340922 1.256033
C -0.425853 -1.482532 2.182003

C -1.036119 -0.334193 1.729361
N -1.059807 -0.076449 0.414785
C -0.506158 -0.879641 -0.497131
H -0.554663 -0.557493 -1.529029
H -1.505630 0.802057 0.076860
H -1.508262 0.395250 2.374868
H -0.409200 -1.700019 3.242204
H 0.653435 -3.246169 1.596153
H 0.676144 -3.978202 -0.865018
H 0.384324 -2.749395 -2.119875
H 4.301832 -0.374704 -2.042673
H 4.536825 -2.106630 -2.281552
H 4.616672 -2.560745 0.088205
H 5.722054 -1.242707 -0.254948
H 4.484352 -0.793425 1.802460
H 2.944696 -1.035917 1.009862
H 4.887379 1.211065 0.282210
H 3.279177 0.978842 -0.377020

conf_32

C 4.810153 0.803808 1.822777
C 4.199082 2.072411 1.230489
C 2.706770 1.968598 0.943515
C 2.086465 3.294032 0.517120
C 0.615813 3.173169 0.127758
C 0.412576 2.542079 -1.243728
C -0.989700 2.144803 -1.589646
C -2.081046 2.316809 -0.831793
C -3.468467 1.910357 -1.210567
C -4.069281 0.887455 -0.244942
C -5.522099 0.550669 -0.549119
C -6.106439 -0.489471 0.395910
C -7.562369 -0.825470 0.100852
C -8.134052 -1.868846 1.048750
H -9.178592 -2.090675 0.816367
H -7.574857 -2.808259 0.987545
H -8.092042 -1.525199 2.087339
H -7.647468 -1.179990 -0.933827
H -8.161079 0.091818 0.157160
H -5.506698 -1.409165 0.342334
H -6.021502 -0.130531 1.430877
H -5.602319 0.191501 -1.583248
H -6.121127 1.468694 -0.499214
H -3.476233 -0.038473 -0.277588
H -3.994220 1.268694 0.783249
H -3.478494 1.513345 -2.231595
H -4.106846 2.803081 -1.216062
H -1.979823 2.815681 0.133864
H -1.121903 1.690636 -2.574003
H 1.065528 1.664921 -1.362742
H 0.765466 3.238770 -2.015805
H 0.102711 2.583539 0.901940

H	0.138012	4.158418	0.141388
H	2.654334	3.713276	-0.323210
H	2.187369	4.012522	1.337665
H	2.538159	1.213097	0.165124
H	2.188499	1.606031	1.844400
H	4.721334	2.347592	0.306191
H	4.374913	2.901386	1.925766
C	4.563217	-0.465326	1.011853
C	5.091739	-0.403482	-0.415756
C	4.777427	-1.672195	-1.211520
C	3.297218	-1.828809	-1.368805
O	2.556017	-1.035866	-1.896668
O	2.835000	-2.971596	-0.812318
C	1.426325	-3.167541	-0.913290
C	0.685465	-2.220774	-0.008407
C	0.668787	-2.384816	1.374933
C	0.007699	-1.469825	2.189936
C	-0.625821	-0.395402	1.605890
N	-0.592118	-0.258068	0.273260
C	0.035730	-1.117411	-0.533468
H	0.027062	-0.888823	-1.591592
H	-1.042961	0.571681	-0.169676
H	-1.161835	0.366365	2.157817
H	-0.015895	-1.587727	3.265756
H	1.182170	-3.231762	1.819660
H	1.260392	-4.200435	-0.607286
H	1.103210	-3.041156	-1.948694
H	5.199734	-1.599078	-2.218501
H	5.191673	-2.559881	-0.729604
H	6.176461	-0.256588	-0.405069
H	4.663298	0.451365	-0.948027
H	5.022506	-1.316606	1.528477
H	3.484355	-0.675512	0.992404
H	4.412521	0.654034	2.834124
H	5.889745	0.950659	1.942919

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C	4.185603	0.212653	0.251415
C	3.918499	1.215636	1.366978
C	4.012306	2.679311	0.941076
C	3.015251	3.111833	-0.132771
C	1.560819	2.885992	0.257675
C	0.572116	3.385194	-0.795583
C	-0.862018	3.249843	-0.389599
C	-1.814287	2.630754	-1.099989
C	-3.266725	2.558096	-0.750933
C	-3.806905	1.128368	-0.712877
C	-5.303841	1.053693	-0.443887
C	-5.855996	-0.368312	-0.441314
C	-5.283730	-1.270264	0.647476
C	-5.946831	-2.639520	0.683757
H	-5.524578	-3.273656	1.468176

H	-7.020516	-2.550213	0.873665
H	-5.825776	-3.162283	-0.270421
H	-5.402472	-0.776397	1.621174
H	-4.202987	-1.398603	0.498750
H	-6.944450	-0.322253	-0.320621
H	-5.682755	-0.829515	-1.423036
H	-5.830495	1.644964	-1.201979
H	-5.521928	1.531319	0.520584
H	-3.585232	0.630235	-1.667162
H	-3.279099	0.560077	0.062172
H	-3.829724	3.123490	-1.505325
H	-3.449346	3.059203	0.206805
H	-1.526659	2.170126	-2.048969
H	-1.151956	3.752384	0.537249
H	0.741098	2.865074	-1.745430
H	0.773512	4.447744	-0.986157
H	1.402026	1.814003	0.424184
H	1.358911	3.383788	1.216553
H	3.218981	2.587538	-1.074304
H	3.166943	4.176349	-0.345277
H	3.876273	3.312485	1.826298
H	5.027489	2.881428	0.580376
H	4.632865	1.040602	2.179918
H	2.928511	1.015882	1.801392
C	3.991667	-1.226445	0.713359
C	4.388525	-2.293086	-0.303234
C	3.699557	-2.156704	-1.665833
C	2.211900	-2.040231	-1.565440
O	1.533697	-1.152012	-2.020170
O	1.666410	-3.063064	-0.865992
C	0.252209	-2.996477	-0.690921
C	-0.100386	-1.921316	0.301410
C	0.038963	-2.112069	1.674242
C	-0.216666	-1.073298	2.565872
C	-0.597712	0.152214	2.066825
N	-0.731794	0.307672	0.742036
C	-0.502324	-0.670875	-0.137216
H	-0.615819	-0.422084	-1.184158
H	-0.988799	1.238247	0.351618
H	-0.797276	1.021261	2.680851
H	-0.111742	-1.209352	3.634650
H	0.359413	-3.078760	2.050422
H	-0.035883	-3.978188	-0.315901
H	-0.238056	-2.815511	-1.649561
H	4.044833	-1.275802	-2.208391
H	3.926518	-3.034580	-2.280237
H	4.176387	-3.283666	0.109057
H	5.468829	-2.252402	-0.476196
H	4.569420	-1.393678	1.629849
H	2.938887	-1.368140	0.999424
H	5.210674	0.347521	-0.118234
H	3.525698	0.418312	-0.599697

conf_11

C	5.253883	0.933221	0.192380
C	4.228081	2.004173	-0.178814
C	3.401327	2.456437	1.021782
C	2.201327	3.329255	0.670039
C	1.052741	2.549724	0.041798
C	-0.175282	3.418816	-0.222974
C	-1.298646	2.724751	-0.929091
C	-2.594190	2.799365	-0.593787
C	-3.737276	2.300211	-1.424459
C	-4.939116	1.792330	-0.628097
C	-4.684698	0.550531	0.219183
C	-4.304641	-0.688631	-0.580177
C	-4.121610	-1.934013	0.277059
C	-3.715278	-3.158273	-0.529219
H	-2.790715	-2.978743	-1.090272
H	-3.558256	-4.031426	0.110065
H	-4.484943	-3.421099	-1.260388
H	-5.055235	-2.141231	0.812552
H	-3.375353	-1.737085	1.059129
H	-5.080740	-0.880258	-1.332071
H	-3.386357	-0.506465	-1.156368
H	-5.587443	0.331224	0.800691
H	-3.908165	0.766386	0.967618
H	-5.297591	2.601099	0.019456
H	-5.755722	1.584239	-1.328041
H	-3.383867	1.547901	-2.138520
H	-4.077486	3.145876	-2.037000
H	-2.862765	3.372328	0.297893
H	-1.032662	2.195913	-1.848740
H	0.136239	4.263680	-0.852884
H	-0.539148	3.862590	0.711749
H	1.376093	2.080745	-0.895179
H	0.794857	1.724868	0.718661
H	2.513586	4.133418	-0.008449
H	1.834170	3.824229	1.577568
H	3.048263	1.579658	1.583133
H	4.059268	3.002372	1.707287
H	3.573101	1.619458	-0.970719
H	4.733973	2.878107	-0.603859
C	4.647491	-0.467512	0.275418
C	4.510754	-1.126035	-1.093457
C	3.707607	-2.418724	-1.052327
C	2.232064	-2.181413	-0.961679
O	1.626327	-1.257447	-1.445613
O	1.598162	-3.171263	-0.289975
C	0.174744	-3.103614	-0.312163
C	-0.352113	-2.006162	0.572064
C	-0.403028	-2.133911	1.957168
C	-0.891697	-1.096407	2.747866
C	-1.327768	0.056947	2.135810
N	-1.265477	0.156129	0.800014

C	-0.792116	-0.815987	0.018040
H	-0.751246	-0.614728	-1.044246
H	-1.575549	1.035923	0.337658
H	-1.726184	0.911356	2.668028
H	-0.939436	-1.183475	3.825807
H	-0.058087	-3.051592	2.423595
H	-0.162205	-4.074849	0.050244
H	-0.174082	-2.963440	-1.337679
H	3.849418	-2.992117	-1.977774
H	4.018326	-3.074803	-0.234860
H	5.508533	-1.343013	-1.487063
H	4.036331	-0.441431	-1.803629
H	5.262186	-1.110002	0.916193
H	3.662373	-0.409862	0.760272
H	5.714489	1.199257	1.150620
H	6.069110	0.921299	-0.540051

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C	4.847082	2.181527	0.977032
C	3.680241	3.012364	0.446109
C	2.326093	2.323425	0.553426
C	1.162629	3.227047	0.161722
C	-0.183088	2.507271	0.152694
C	-0.360315	1.594256	-1.053662
C	-1.523839	0.652531	-1.008370
C	-2.441182	0.553095	-0.036270
C	-3.619726	-0.366110	-0.061449
C	-4.942714	0.399603	-0.135536
C	-6.157303	-0.517588	-0.121654
C	-7.476867	0.236883	-0.203184
C	-8.695588	-0.676423	-0.191281
C	-10.009048	0.086800	-0.273455
H	-10.867111	-0.590224	-0.263398
H	-10.119628	0.775184	0.570513
H	-10.064784	0.679365	-1.192176
H	-8.679944	-1.286547	0.720674
H	-8.625592	-1.381270	-1.029303
H	-7.545171	0.943195	0.635092
H	-7.490873	0.847694	-1.115659
H	-6.142770	-1.127760	0.791557
H	-6.090017	-1.223192	-0.960381
H	-5.003906	1.102317	0.705445
H	-4.948465	1.010820	-1.045920
H	-3.629832	-0.986761	0.845798
H	-3.540737	-1.051514	-0.913259
H	-2.388588	1.238737	0.811608
H	-1.634375	-0.000647	-1.876736
H	0.555560	1.011944	-1.232149
H	-0.460636	2.209149	-1.958087
H	-0.272469	1.932133	1.086280
H	-1.001878	3.234056	0.174379
H	1.351254	3.660875	-0.828545

H	1.119099	4.071639	0.857730
H	2.325477	1.424985	-0.077213
H	2.176532	1.976260	1.587227
H	3.857848	3.286657	-0.600788
H	3.647137	3.959491	0.996872
C	4.969413	0.786556	0.369575
C	5.135333	0.779981	-1.145017
C	5.199072	-0.636461	-1.721040
C	3.904303	-1.348470	-1.482154
O	2.818995	-0.988335	-1.868222
O	4.056872	-2.462765	-0.730489
C	2.851712	-3.169288	-0.445502
C	1.997772	-2.398073	0.523875
C	2.348360	-2.259948	1.865021
C	1.565900	-1.496642	2.727183
C	0.441839	-0.874692	2.230623
N	0.125320	-1.023582	0.936658
C	0.858741	-1.746037	0.085678
H	0.530488	-1.764174	-0.945853
H	-0.700129	-0.519164	0.543539
H	-0.218832	-0.255119	2.823818
H	1.826292	-1.381651	3.771615
H	3.245635	-2.745294	2.236479
H	3.172790	-4.115028	-0.008909
H	2.303500	-3.365370	-1.369318
H	5.346568	-0.595506	-2.804666
H	6.019340	-1.209740	-1.284781
H	6.051181	1.312015	-1.421513
H	4.306450	1.309047	-1.625270
H	5.821586	0.269463	0.826687
H	4.082352	0.196834	0.641243
H	4.748794	2.080612	2.064939
H	5.780757	2.730714	0.809329

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C	4.695617	0.117421	1.273347
C	4.278145	1.518757	0.832861
C	2.772383	1.755616	0.844797
C	2.406915	3.227250	0.690938
C	0.904789	3.483024	0.638052
C	0.269931	3.185857	-0.722642
C	-1.224997	3.249206	-0.674482
C	-2.078240	2.447893	-1.324083
C	-3.569496	2.562815	-1.252813
C	-4.248426	1.403984	-0.514307
C	-4.147051	0.055829	-1.218318
C	-4.820896	-1.088599	-0.466524
C	-4.148845	-1.466122	0.849444
C	-4.819072	-2.645260	1.539076
H	-4.809678	-3.533893	0.900354
H	-4.321330	-2.902916	2.478227
H	-5.864079	-2.420504	1.771328

H	-4.145821	-0.605555	1.529477
H	-3.095430	-1.711377	0.652458
H	-5.868915	-0.826775	-0.273173
H	-4.847980	-1.973777	-1.113089
H	-3.094932	-0.207147	-1.397053
H	-4.597689	0.149016	-2.213329
H	-3.833798	1.342215	0.500648
H	-5.308792	1.648753	-0.384633
H	-3.972089	2.620488	-2.271826
H	-3.828657	3.504852	-0.759775
H	-1.669340	1.682123	-1.988366
H	-1.645351	4.050263	-0.062635
H	0.601857	2.217129	-1.117251
H	0.632914	3.934065	-1.439384
H	0.415997	2.885404	1.421952
H	0.693008	4.527161	0.892628
H	2.878475	3.633740	-0.212930
H	2.838591	3.782243	1.530988
H	2.299310	1.165540	0.048372
H	2.355721	1.386025	1.794209
H	4.667261	1.734956	-0.169335
H	4.757853	2.246305	1.497890
C	4.036227	-1.021366	0.502360
C	4.321164	-1.004276	-0.993836
C	3.631397	-2.153111	-1.736139
C	2.146634	-2.019586	-1.611831
O	1.478987	-1.123561	-2.068042
O	1.598330	-3.010774	-0.873112
C	0.186381	-2.927532	-0.695589
C	-0.186433	-1.841865	0.278320
C	-0.122566	-2.028606	1.657027
C	-0.483551	-1.004748	2.528790
C	-0.902452	0.198583	2.006173
N	-0.945749	0.357440	0.676277
C	-0.603673	-0.605357	-0.183874
H	-0.652539	-0.365609	-1.237427
H	-1.270153	1.259480	0.275065
H	-1.206746	1.046019	2.607190
H	-0.446581	-1.139483	3.602224
H	0.206658	-2.984046	2.053790
H	-0.109272	-3.901919	-0.307148
H	-0.301307	-2.759365	-1.658146
H	3.871511	-2.109536	-2.802157
H	3.948367	-3.122228	-1.346184
H	5.399592	-1.076238	-1.167925
H	3.992702	-0.059325	-1.438091
H	4.369982	-1.978745	0.920139
H	2.950395	-0.986896	0.668832
H	4.463840	-0.003107	2.338778
H	5.784846	0.026403	1.190120

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C	5.164906	0.575263	0.236690
C	4.349494	1.787558	-0.215066
C	3.548269	2.411469	0.923099
C	2.737833	3.641925	0.524151
C	1.550764	3.382398	-0.400341
C	0.479991	2.495804	0.242437
C	-0.745960	2.377398	-0.606109
C	-1.954844	2.864125	-0.294847
C	-3.144148	2.872792	-1.203034
C	-4.469506	2.526346	-0.521886
C	-4.525078	1.146337	0.125817
C	-4.251244	-0.010860	-0.825183
C	-4.407527	-1.381316	-0.178474
C	-4.076466	-2.527009	-1.123058
H	-4.745330	-2.529451	-1.988352
H	-3.054185	-2.443186	-1.510368
H	-4.171776	-3.498780	-0.631064
H	-5.435546	-1.491122	0.185280
H	-3.774429	-1.442141	0.718010
H	-4.931003	0.060801	-1.683836
H	-3.241537	0.078371	-1.250939
H	-5.514710	1.010017	0.576733
H	-3.820745	1.107643	0.970245
H	-4.689167	3.285582	0.237827
H	-5.269270	2.605426	-1.266241
H	-2.958769	2.215923	-2.059470
H	-3.234633	3.885185	-1.617991
H	-2.074650	3.377077	0.663832
H	-0.611780	1.914336	-1.586885
H	0.213207	2.907797	1.224740
H	0.912855	1.500942	0.415436
H	1.093915	4.339944	-0.671699
H	1.883885	2.924805	-1.339112
H	3.406598	4.362556	0.039098
H	2.369323	4.137961	1.430812
H	2.893680	1.657301	1.380390
H	4.249902	2.703572	1.713430
H	3.686119	1.499681	-1.040794
H	5.021849	2.551611	-0.621945
C	4.362287	-0.724478	0.302643
C	4.234629	-1.400476	-1.058098
C	3.389608	-2.665814	-1.021910
C	1.921079	-2.389739	-0.945061
O	1.354130	-1.419335	-1.383784
O	1.247410	-3.398496	-0.345402
C	-0.174865	-3.291327	-0.373202
C	-0.675346	-2.269217	0.611100
C	-0.860647	-2.563339	1.959160
C	-1.303366	-1.583885	2.845761
C	-1.553151	-0.316913	2.367986
N	-1.368073	-0.060971	1.065172

C	-0.946394	-0.977516	0.192559
H	-0.807454	-0.650673	-0.829236
H	-1.540068	0.889486	0.681475
H	-1.897557	0.504876	2.982745
H	-1.453558	-1.800960	3.895604
H	-0.657101	-3.566052	2.322266
H	-0.539762	-4.283555	-0.108903
H	-0.508929	-3.042384	-1.382742
H	3.524895	-3.247559	-1.943236
H	3.672988	-3.329887	-0.200552
H	5.234809	-1.662484	-1.417517
H	3.808517	-0.709759	-1.792523
H	4.843488	-1.423807	0.996580
H	3.363800	-0.523015	0.716021
H	5.600150	0.791994	1.218888
H	6.014264	0.424223	-0.439520

conf_6

C	4.148703	1.495823	1.558336
C	3.561650	2.520338	0.587477
C	2.125322	2.235905	0.166182
C	1.619523	3.187932	-0.911708
C	0.232554	2.825603	-1.430150
C	-0.907693	3.217497	-0.489667
C	-2.216934	2.589876	-0.871129
C	-3.236761	2.319523	-0.046289
C	-4.582581	1.829509	-0.485032
C	-5.282625	0.892797	0.499452
C	-4.510635	-0.371275	0.861625
C	-4.116726	-1.246351	-0.320256
C	-3.453972	-2.551680	0.101819
C	-2.971403	-3.390266	-1.071882
H	-2.253313	-2.840713	-1.692121
H	-2.490913	-4.314600	-0.739081
H	-3.803486	-3.670725	-1.723854
H	-4.163223	-3.134262	0.700793
H	-2.614812	-2.334326	0.777720
H	-5.007198	-1.470917	-0.921064
H	-3.445449	-0.695002	-0.994989
H	-5.117215	-0.964117	1.555950
H	-3.609363	-0.100720	1.429839
H	-5.506614	1.445990	1.419207
H	-6.252767	0.613228	0.074579
H	-4.497847	1.367985	-1.474695
H	-5.224393	2.709623	-0.623748
H	-3.129103	2.560536	1.015728
H	-2.360310	2.399050	-1.937256
H	-1.017333	4.309331	-0.516103
H	-0.660191	2.979798	0.553249
H	0.055931	3.305134	-2.398995

H	0.209766	1.744766	-1.629839
H	2.326444	3.163063	-1.748310
H	1.622830	4.221131	-0.541726
H	2.056102	1.217030	-0.234689
H	1.475669	2.271890	1.053020
H	4.186040	2.575758	-0.312288
H	3.619222	3.514750	1.044496
C	4.058781	0.045722	1.084809
C	4.705138	-0.212603	-0.272598
C	4.401407	-1.612523	-0.807033
C	2.931145	-1.751133	-1.059290
O	2.245627	-0.979620	-1.682831
O	2.401664	-2.846064	-0.463526
C	0.987622	-2.964105	-0.597220
C	0.305264	-1.923881	0.247651
C	0.432215	-1.929166	1.635002
C	-0.167828	-0.938766	2.405205
C	-0.896520	0.042128	1.770580
N	-1.002232	0.027637	0.435201
C	-0.422577	-0.900434	-0.331722
H	-0.543671	-0.797515	-1.402382
H	-1.580860	0.768486	-0.008890
H	-1.406141	0.846655	2.285188
H	-0.077312	-0.928783	3.483803
H	1.014066	-2.710655	2.113683
H	0.747108	-3.966509	-0.241960
H	0.692650	-2.870384	-1.643911
H	4.909651	-1.771351	-1.764029
H	4.729995	-2.394601	-0.119468
H	5.789658	-0.084008	-0.202424
H	4.348222	0.512614	-1.009166
H	4.518619	-0.608365	1.835174
H	3.000848	-0.248627	1.042601
H	3.639892	1.578149	2.526904
H	5.197677	1.750407	1.748537

conf_45

C	5.073965	1.012349	0.352149
C	4.020095	1.961702	-0.216745
C	2.865419	2.223646	0.743548
C	1.685011	2.922993	0.084920
C	0.592428	3.299404	1.076546
C	-0.669053	3.901842	0.451633
C	-1.349936	3.066057	-0.590472
C	-2.655675	2.764184	-0.611809
C	-3.379708	2.160114	-1.776277
C	-4.499859	1.184213	-1.424799
C	-4.022444	-0.097347	-0.759494
C	-5.130001	-1.121563	-0.548937
C	-4.644785	-2.459357	0.001401
C	-4.024669	-2.372469	1.389473
H	-3.120595	-1.755348	1.392655

H	-4.725150	-1.932618	2.106852
H	-3.747553	-3.361710	1.764505
H	-3.921444	-2.895967	-0.700514
H	-5.489104	-3.155510	0.031514
H	-5.887686	-0.701830	0.125449
H	-5.637173	-1.292685	-1.505513
H	-3.564694	0.147633	0.207126
H	-3.232476	-0.550767	-1.378265
H	-5.229417	1.684115	-0.775260
H	-5.039170	0.931844	-2.344183
H	-2.661302	1.689193	-2.459242
H	-3.819309	2.994586	-2.339264
H	-3.277530	3.085190	0.227926
H	-0.751607	2.789077	-1.460913
H	-0.390046	4.849882	-0.028407
H	-1.387435	4.162910	1.236619
H	0.331654	2.417023	1.675805
H	0.996471	4.021184	1.794927
H	1.288696	2.263576	-0.698319
H	2.029143	3.827608	-0.432651
H	2.514694	1.275488	1.175192
H	3.227248	2.822016	1.589576
H	3.623404	1.554327	-1.155546
H	4.486007	2.918237	-0.477645
C	4.632575	-0.450108	0.340598
C	4.700839	-1.081838	-1.047296
C	3.928414	-2.391554	-1.131936
C	2.448235	-2.163534	-1.099484
O	1.859607	-1.235337	-1.596097
O	1.791176	-3.150696	-0.446588
C	0.370558	-3.038925	-0.462063
C	-0.105892	-1.938059	0.446186
C	-0.100499	-2.077710	1.831654
C	-0.544966	-1.043146	2.649785
C	-0.989725	0.121064	2.065110
N	-0.972589	0.237176	0.728941
C	-0.545599	-0.735513	-0.080830
H	-0.546726	-0.527331	-1.142594
H	-1.310159	1.122617	0.300092
H	-1.363408	0.971719	2.620400
H	-0.556462	-1.140782	3.727740
H	0.249954	-3.004753	2.274730
H	0.005413	-4.004003	-0.110331
H	0.019176	-2.870615	-1.482323
H	4.132432	-2.902052	-2.081601
H	4.203346	-3.088577	-0.336203
H	5.745679	-1.265796	-1.314682
H	4.300214	-0.396850	-1.800332
H	5.250998	-1.035770	1.030055
H	3.605872	-0.520092	0.726952
H	5.316692	1.318711	1.376347
H	6.004856	1.105492	-0.218946

conf_102

C	4.188614	0.627981	1.270710
C	3.352520	1.695785	1.974842
C	3.254286	3.064103	1.295070
C	2.350996	3.189475	0.067589
C	0.899829	2.807056	0.324333
C	0.003239	3.022037	-0.893714
C	-1.458084	2.818679	-0.630881
C	-2.331370	2.227879	-1.458444
C	-3.819660	2.231859	-1.283443
C	-4.536397	0.983247	-1.796578
C	-4.143699	-0.322531	-1.114531
C	-4.391056	-0.354565	0.387558
C	-4.074736	-1.701488	1.024826
C	-4.283850	-1.715275	2.531451
H	-5.324001	-1.492123	2.785456
H	-4.041041	-2.688984	2.965065
H	-3.662244	-0.962688	3.030257
H	-3.039921	-1.987432	0.788729
H	-4.701360	-2.471557	0.560239
H	-3.808072	0.431750	0.888914
H	-5.440480	-0.101167	0.584894
H	-3.086656	-0.541601	-1.322299
H	-4.700529	-1.142803	-1.581830
H	-5.615327	1.135688	-1.684064
H	-4.356632	0.890315	-2.874014
H	-4.206118	3.092334	-1.845837
H	-4.070737	2.431328	-0.235821
H	-1.953516	1.804461	-2.393207
H	-1.849743	3.287755	0.276123
H	0.330617	2.392051	-1.729802
H	0.133844	4.059180	-1.232878
H	0.855898	1.758130	0.637749
H	0.513566	3.397078	1.166958
H	2.737722	2.595919	-0.767010
H	2.382340	4.231640	-0.272319
H	2.901356	3.785512	2.042605
H	4.264802	3.392142	1.023807
H	3.796410	1.858695	2.962935
H	2.347867	1.296047	2.173224
C	3.587362	0.027190	0.005247
C	4.331104	-1.218610	-0.459306
C	3.818236	-1.764832	-1.797349
C	2.343501	-2.006387	-1.752807
O	1.498397	-1.401203	-2.363759
O	2.025989	-2.988873	-0.875756
C	0.630504	-3.223493	-0.697004
C	0.034337	-2.160547	0.185593
C	0.082872	-2.247383	1.575569
C	-0.426880	-1.224982	2.370148
C	-0.973887	-0.119479	1.757784
N	-1.012028	-0.059860	0.420317

C	-0.536004	-1.026129	-0.369544
H	-0.592432	-0.864385	-1.438302
H	-1.408367	0.789749	-0.034450
H	-1.382922	0.728498	2.292076
H	-0.399854	-1.282713	3.450706
H	0.525939	-3.122289	2.041260
H	0.561304	-4.200583	-0.219894
H	0.126807	-3.253814	-1.664978
H	4.001112	-1.055592	-2.606395
H	4.323645	-2.704931	-2.036698
H	4.260109	-2.000524	0.304099
H	5.395879	-0.991402	-0.574225
H	2.532672	-0.224065	0.194266
H	3.581411	0.760686	-0.807251
H	4.365781	-0.187639	1.983716
H	5.179330	1.039407	1.039378

conf_38

C	4.798679	0.535439	1.407239
C	4.645417	1.926536	0.791236
C	3.229944	2.510668	0.868979
C	2.389990	2.286284	-0.382343
C	0.948536	2.751848	-0.231228
C	0.134206	2.496681	-1.491337
C	-1.352014	2.647840	-1.389799
C	-2.060316	3.034014	-0.320489
C	-3.553698	3.164780	-0.279911
C	-4.230751	1.975302	0.417447
C	-4.265815	0.720966	-0.449471
C	-4.531903	-0.564808	0.320400
C	-4.439643	-1.816346	-0.542779
C	-4.557016	-3.104043	0.257946
H	-5.509228	-3.150465	0.794420
H	-4.498622	-3.985929	-0.385115
H	-3.758294	-3.179974	1.005104
H	-3.485020	-1.807845	-1.088855
H	-5.218747	-1.784584	-1.312985
H	-3.816664	-0.649567	1.151856
H	-5.520315	-0.516525	0.793371
H	-3.318072	0.621145	-0.998068
H	-5.025158	0.847447	-1.230246
H	-3.711650	1.766297	1.365154
H	-5.250697	2.250622	0.703248
H	-3.947352	3.257300	-1.297823
H	-3.812902	4.090191	0.243911
H	-1.529371	3.302439	0.596014
H	-1.902896	2.437553	-2.308205
H	0.363562	1.490643	-1.873603
H	0.483250	3.163805	-2.290960
H	0.507876	2.226143	0.627633

H	0.916269	3.816869	0.027542
H	2.385561	1.225380	-0.656843
H	2.856638	2.810569	-1.225922
H	2.711317	2.085094	1.740610
H	3.286522	3.588622	1.057611
H	4.982108	1.921068	-0.252857
H	5.338639	2.590541	1.316635
C	3.983236	-0.590169	0.775372
C	4.369023	-0.906531	-0.665171
C	3.703608	-2.177903	-1.190545
C	2.212706	-2.052029	-1.242117
O	1.594040	-1.137089	-1.728913
O	1.589377	-3.103295	-0.661946
C	0.163215	-3.061363	-0.691069
C	-0.351624	-2.011736	0.254406
C	-0.321430	-2.183988	1.635643
C	-0.735173	-1.161892	2.486241
C	-1.167202	0.024791	1.938045
N	-1.192667	0.162089	0.604818
C	-0.807573	-0.800442	-0.235071
H	-0.846864	-0.570682	-1.291422
H	-1.503643	1.062428	0.188977
H	-1.496074	0.876665	2.519473
H	-0.718550	-1.282037	3.561906
H	0.037786	-3.120445	2.051094
H	-0.157343	-4.055330	-0.379584
H	-0.186779	-2.870063	-1.707628
H	4.031736	-2.377461	-2.217062
H	3.970205	-3.047217	-0.585800
H	5.453642	-1.042524	-0.730219
H	4.119051	-0.072351	-1.327237
H	4.119717	-1.494773	1.381828
H	2.911427	-0.350433	0.828604
H	4.535848	0.600033	2.470377
H	5.857994	0.252401	1.378462

conf_59

C	4.344308	0.892996	0.561739
C	3.019934	1.541950	0.177955
C	3.038776	3.064841	0.214226
C	1.699511	3.691970	-0.164108
C	0.628670	3.526077	0.909950
C	-0.778622	3.933912	0.467977
C	-1.388715	3.081962	-0.605521
C	-2.660789	2.660507	-0.624148
C	-3.345067	2.027196	-1.797639
C	-4.390141	0.969879	-1.449264
C	-3.813549	-0.254874	-0.757313
C	-4.822672	-1.371863	-0.529664
C	-4.223788	-2.621334	0.110613
C	-3.723798	-2.411786	1.534103
H	-3.338153	-3.341636	1.961915

H	-2.920453	-1.669524	1.582303
H	-4.530732	-2.060937	2.185112
H	-3.404444	-2.991185	-0.521561
H	-4.978307	-3.414437	0.113665
H	-5.643830	-0.998901	0.096029
H	-5.272458	-1.642066	-1.491948
H	-3.385669	0.049570	0.206081
H	-2.983901	-0.649252	-1.363813
H	-5.164724	1.417793	-0.814165
H	-4.895765	0.662333	-2.370904
H	-2.598491	1.616165	-2.488855
H	-3.845251	2.835169	-2.348323
H	-3.296800	2.893394	0.234095
H	-0.776387	2.892176	-1.489396
H	-0.730008	4.963085	0.085573
H	-1.455409	3.971365	1.329748
H	0.623449	2.487933	1.261513
H	0.909244	4.129099	1.780899
H	1.365223	3.248892	-1.110937
H	1.831048	4.761520	-0.362416
H	3.341587	3.411080	1.211170
H	3.810314	3.421691	-0.477004
H	2.246241	1.156422	0.857758
H	2.723921	1.217643	-0.828671
C	4.319596	-0.620805	0.369327
C	4.455829	-1.041179	-1.095422
C	3.839045	-2.410954	-1.380337
C	2.348789	-2.325666	-1.259064
O	1.641158	-1.548714	-1.851512
O	1.842875	-3.207404	-0.367004
C	0.427523	-3.147073	-0.199717
C	0.028855	-1.943759	0.611681
C	0.133970	-1.932418	2.000324
C	-0.241359	-0.809306	2.731696
C	-0.719801	0.291289	2.057408
N	-0.799935	0.262218	0.718778
C	-0.439910	-0.798217	-0.010624
H	-0.519066	-0.709651	-1.085664
H	-1.172376	1.101564	0.231662
H	-1.044617	1.203607	2.541075
H	-0.173933	-0.790122	3.811849
H	0.506890	-2.812236	2.515552
H	0.162703	-4.063201	0.327843
H	-0.065108	-3.134265	-1.173950
H	4.056607	-2.718506	-2.408390
H	4.223281	-3.180047	-0.707288
H	5.511981	-1.059306	-1.378372
H	3.970896	-0.311059	-1.750772
H	5.113601	-1.095285	0.955273
H	3.375844	-1.005212	0.784166
H	4.573578	1.133820	1.605897
H	5.157188	1.325869	-0.035129

conf_107

C	4.438444	2.376917	1.011813
C	2.965803	2.779630	0.946207
C	2.015377	1.709069	1.470959
C	0.542835	2.096298	1.396466
C	0.019847	2.279800	-0.026593
C	-1.511211	2.200044	-0.106994
C	-2.027808	0.796234	-0.089538
C	-2.680928	0.204595	0.918889
C	-3.269405	-1.171953	0.885582
C	-4.801178	-1.149876	0.960921
C	-5.456168	-0.485911	-0.241259
C	-6.977340	-0.484368	-0.156840
C	-7.668075	0.116330	-1.378000
C	-7.371764	1.594499	-1.595116
H	-7.633396	2.181686	-0.708279
H	-6.314530	1.774078	-1.812609
H	-7.947026	1.992169	-2.435178
H	-8.749362	-0.020207	-1.269006
H	-7.380981	-0.452807	-2.271449
H	-7.327494	-1.514687	-0.017670
H	-7.287692	0.066694	0.741329
H	-5.144881	-1.007336	-1.157714
H	-5.086991	0.541447	-0.335010
H	-5.158870	-2.181435	1.054079
H	-5.108882	-0.635836	1.880403
H	-2.892006	-1.761439	1.733127
H	-2.959215	-1.689054	-0.031917
H	-2.873481	0.788644	1.821342
H	-1.884875	0.226529	-1.012823
H	-1.850362	2.673103	-1.034892
H	-1.952722	2.770975	0.717106
H	0.346973	3.247558	-0.416741
H	0.465974	1.528133	-0.693623
H	0.372462	3.019378	1.963807
H	-0.060649	1.335037	1.910302
H	2.161826	0.784325	0.896814
H	2.283952	1.476989	2.510095
H	2.696121	3.038855	-0.083502
H	2.822778	3.695529	1.531474
C	4.805463	1.166081	0.156611
C	4.681606	1.409504	-1.344433
C	4.758023	0.114235	-2.153287
C	3.527189	-0.708442	-1.928074
O	2.391811	-0.328734	-2.080868
O	3.804024	-1.960580	-1.499073
C	2.663562	-2.788919	-1.277565
C	1.928026	-2.371315	-0.032522
C	2.407480	-2.674984	1.239567
C	1.729924	-2.241043	2.375731
C	0.579641	-1.500560	2.220866
N	0.137477	-1.221577	0.986596

C	0.767364	-1.620954	-0.121524
H	0.345239	-1.305845	-1.066831
H	-0.704207	-0.618818	0.876901
H	-0.004252	-1.109472	3.044426
H	2.091623	-2.470151	3.369954
H	3.322247	-3.250402	1.343486
H	3.062120	-3.797170	-1.166401
H	2.001860	-2.754739	-2.145384
H	4.791767	0.338789	-3.224598
H	5.645365	-0.470580	-1.902655
H	5.476725	2.084118	-1.675901
H	3.733619	1.900559	-1.582866
H	5.833277	0.860773	0.383547
H	4.177500	0.312175	0.446002
H	4.704539	2.168927	2.055257
H	5.056647	3.229601	0.707764

conf_70

C	4.341316	0.737610	1.215941
C	3.053570	1.374740	0.705755
C	2.921062	2.857290	1.037641
C	1.758846	3.533147	0.313138
C	0.409927	2.886807	0.598334
C	-0.734895	3.475302	-0.223064
C	-2.075848	2.880181	0.078764
C	-2.935676	2.396612	-0.828460
C	-4.358488	2.009399	-0.560173
C	-4.887816	0.863245	-1.421980
C	-4.217130	-0.487769	-1.198583
C	-4.392605	-1.051847	0.205040
C	-3.788452	-2.438207	0.386836
C	-3.958501	-2.983924	1.796573
H	-5.016845	-3.076615	2.056418
H	-3.505543	-3.972975	1.905251
H	-3.500268	-2.322453	2.540643
H	-2.721970	-2.414325	0.122564
H	-4.250598	-3.125603	-0.331182
H	-3.963298	-0.367408	0.950665
H	-5.463708	-1.094204	0.440302
H	-3.147663	-0.414317	-1.444400
H	-4.625735	-1.205262	-1.919332
H	-5.963074	0.760711	-1.239290
H	-4.787643	1.143192	-2.477151
H	-4.972928	2.894810	-0.771275
H	-4.500276	1.805287	0.507162
H	-2.625698	2.390298	-1.876710
H	-2.403736	2.936083	1.121021
H	-0.517094	3.373887	-1.292533
H	-0.793316	4.554123	-0.024469
H	0.490893	1.818625	0.379163

H	0.180135	2.969889	1.670039
H	1.945613	3.496705	-0.768231
H	1.720649	4.594695	0.582537
H	2.812291	2.983827	2.122678
H	3.850407	3.370744	0.765540
H	2.210345	0.822085	1.143425
H	2.960501	1.253726	-0.378909
C	4.404381	-0.782921	1.040732
C	4.956204	-1.295441	-0.289575
C	4.242319	-0.823754	-1.556174
C	2.777470	-1.123397	-1.637794
O	1.935097	-0.407868	-2.121243
O	2.464291	-2.332220	-1.116656
C	1.083919	-2.681647	-1.190975
C	0.282540	-1.910597	-0.176621
C	0.280254	-2.262887	1.171495
C	-0.435704	-1.513964	2.099926
C	-1.139476	-0.413984	1.663105
N	-1.125373	-0.096745	0.361783
C	-0.445261	-0.794344	-0.553509
H	-0.472581	-0.430342	-1.572429
H	-1.640570	0.754271	0.059012
H	-1.715910	0.233066	2.311676
H	-0.448551	-1.778282	3.149492
H	0.846950	-3.129323	1.498331
H	1.047714	-3.748881	-0.972828
H	0.704555	-2.504046	-2.199119
H	4.350152	0.250128	-1.717712
H	4.698233	-1.311353	-2.427426
H	4.959074	-2.389266	-0.270488
H	6.003689	-0.988596	-0.380382
H	5.037486	-1.207063	1.826727
H	3.403815	-1.204408	1.210512
H	4.437673	0.972697	2.282381
H	5.207589	1.205896	0.730792

C18:0 pyridylcarbinol ester

conf_53

C	3.534491	0.337770	1.944466
C	4.935364	-0.236242	2.140496
C	5.646725	-0.724390	0.879026
C	5.025625	-1.964037	0.244270
C	3.869554	-1.703519	-0.668938
O	3.610322	-0.674878	-1.241195
O	3.123338	-2.823108	-0.843707
C	2.084453	-2.725620	-1.813994
C	0.845870	-2.113719	-1.216231
C	-0.131546	-2.898009	-0.603543
C	-1.260077	-2.316849	-0.035195
C	-1.396913	-0.947720	-0.080727

N	-0.442239	-0.214333	-0.674489
C	0.656593	-0.741780	-1.232483
H	1.379022	-0.056713	-1.659609
H	-0.544072	0.803780	-0.685717
H	-2.238609	-0.409137	0.334998
H	-2.028464	-2.913974	0.439395
H	-0.007087	-3.976114	-0.572994
H	1.882722	-3.750175	-2.125930
H	2.426477	-2.144403	-2.672413
H	5.764175	-2.477895	-0.385317
H	4.720013	-2.700533	0.993976
H	6.678160	-0.972442	1.144728
H	5.708443	0.071281	0.130559
H	5.560746	0.531922	2.609926
H	4.889063	-1.064109	2.858819
C	3.501141	1.610146	1.108773
C	2.108597	2.211386	0.981427
C	2.053020	3.367504	-0.010018
C	0.698378	4.059619	-0.117080
H	0.770570	4.877830	-0.842405
C	-0.436591	3.133180	-0.536614
C	-1.742162	3.840272	-0.878070
C	-2.870303	2.879508	-1.244523
C	-3.444128	2.111880	-0.058107
C	-4.374461	0.975835	-0.460498
C	-4.907817	0.173329	0.719043
C	-5.705011	-1.056105	0.307617
C	-6.222574	-1.869010	1.486682
C	-7.008668	-3.099909	1.061130
H	-7.880780	-2.822444	0.461282
H	-7.367935	-3.664460	1.925089
H	-6.394529	-3.774621	0.455231
H	-5.376720	-2.170273	2.119451
H	-6.852683	-1.228331	2.115173
H	-5.082396	-1.699133	-0.332512
H	-6.550207	-0.746176	-0.319946
H	-4.075940	-0.137744	1.372486
H	-5.529113	0.822389	1.348053
H	-3.852702	0.302871	-1.159141
H	-5.216080	1.379725	-1.035548
H	-3.977893	2.808586	0.599243
H	-2.630304	1.712769	0.567964
H	-3.681374	3.431295	-1.730982
H	-2.506277	2.169879	-2.003998
H	-1.558234	4.526529	-1.711494
H	-2.048926	4.464853	-0.030064
H	-0.615387	2.422037	0.284545
H	-0.107849	2.566623	-1.427658
H	0.440130	4.523691	0.842679
H	2.353322	3.002674	-1.002457
H	2.808093	4.109769	0.272227
H	1.415713	1.414555	0.674397

H	1.753694	2.547679	1.964915
H	3.888745	1.401661	0.106283
H	4.174630	2.352871	1.554892
H	2.874929	-0.416214	1.488715
H	3.103950	0.542731	2.932347

conf_55

C	0.838015	-2.400492	1.318169
C	1.436651	-1.132947	1.913448
C	2.909170	-1.235089	2.299160
C	3.823971	-1.734813	1.173820
C	3.712491	-0.867973	-0.040090
O	4.000877	0.297687	-0.117708
O	3.191043	-1.541122	-1.100735
C	3.050549	-0.764459	-2.282782
C	1.988739	0.290186	-2.120188
C	2.277913	1.649712	-2.234930
C	1.283936	2.604480	-2.061331
C	0.009021	2.187786	-1.751135
N	-0.241436	0.875609	-1.633988
C	0.692221	-0.072095	-1.806767
H	0.374432	-1.098484	-1.663204
H	-1.185603	0.596158	-1.365715
H	-0.822660	2.855937	-1.570281
H	1.496491	3.662680	-2.142235
H	3.297712	1.957045	-2.439742
H	2.776706	-1.476513	-3.062719
H	4.000466	-0.293785	-2.544137
H	4.865247	-1.690070	1.505617
H	3.597967	-2.767317	0.904212
H	3.022268	-1.921654	3.144320
H	3.265602	-0.257393	2.636630
H	1.302712	-0.304521	1.202782
H	0.866334	-0.842301	2.803532
C	-0.676080	-2.328145	1.161933
C	-1.227921	-3.411292	0.242035
C	-2.739821	-3.606175	0.322315
C	-3.569693	-2.338580	0.145918
H	-3.372536	-1.656371	0.981719
C	-3.347366	-1.610868	-1.173595
C	-4.345423	-0.479972	-1.423207
C	-4.445556	0.557047	-0.306828
C	-3.142948	1.291514	-0.024802
C	-3.243165	2.326635	1.090347
C	-2.009156	3.209714	1.243235
C	-0.731004	2.482125	1.643717
C	0.480331	3.403621	1.714801
C	1.783447	2.676059	2.007991
H	2.042750	1.968401	1.213044
H	1.715960	2.110092	2.942426
H	2.618799	3.373792	2.105905
H	0.571526	3.955929	0.768576

H	0.301652	4.167578	2.480146
H	-0.514919	1.661339	0.946484
H	-0.879056	1.996752	2.616970
H	-1.841806	3.757120	0.302412
H	-2.216380	3.985870	1.988347
H	-3.448057	1.810112	2.036080
H	-4.113926	2.963412	0.897882
H	-2.831656	1.802486	-0.953765
H	-2.367488	0.558689	0.243669
H	-5.213665	1.291665	-0.572654
H	-4.794239	0.081184	0.616422
H	-5.335553	-0.923759	-1.574930
H	-4.098881	0.024511	-2.367349
H	-3.410022	-2.326046	-2.002532
H	-2.313582	-1.228412	-1.204284
H	-4.631608	-2.601230	0.223935
H	-2.984269	-4.045738	1.296384
H	-3.042892	-4.345995	-0.427893
H	-0.931253	-3.191786	-0.794108
H	-0.742473	-4.364072	0.483732
H	-0.957871	-1.333400	0.783646
H	-1.146504	-2.401690	2.150491
H	1.294748	-2.604169	0.341244
H	1.090292	-3.263718	1.946995

conf_51

C	4.179788	1.101514	-1.061968
C	3.203547	-0.046898	-1.286917
C	3.903928	-1.382630	-1.495826
C	2.943135	-2.520383	-1.841161
C	1.898376	-2.759403	-0.797648
O	0.708545	-2.840831	-0.976071
O	2.438249	-2.887581	0.438915
C	1.504868	-3.150720	1.480908
C	0.680754	-1.929192	1.787277
C	1.213116	-0.834455	2.465801
C	0.440777	0.299004	2.701853
C	-0.858496	0.326120	2.249488
N	-1.344975	-0.741023	1.593752
C	-0.628155	-1.845514	1.348191
H	-1.112095	-2.628602	0.779212
H	-2.300398	-0.701503	1.238785
H	-1.525891	1.168845	2.369147
H	0.842952	1.159248	3.221311
H	2.243894	-0.864854	2.805304
H	2.110318	-3.428760	2.343739
H	0.860396	-3.988822	1.207157
H	2.414526	-2.328117	-2.776858
H	3.499926	-3.456895	-1.960875
H	4.479037	-1.647197	-0.602806
H	4.625435	-1.293051	-2.314403
H	2.514003	-0.125274	-0.434387

H	2.579025	0.179191	-2.161570
C	3.505018	2.454289	-0.857591
C	2.830272	2.615326	0.500758
C	2.082114	3.938583	0.661898
C	0.833121	4.081827	-0.206825
H	1.088873	3.943531	-1.263964
C	-0.279898	3.115891	0.173523
C	-1.509133	3.178427	-0.721583
C	-2.617137	2.251941	-0.240343
C	-3.771384	2.082709	-1.216717
C	-4.963535	1.321812	-0.639399
C	-4.640312	-0.035617	-0.017597
C	-3.909965	-1.008152	-0.936057
C	-3.815643	-2.420045	-0.367961
C	-2.986632	-3.364343	-1.226616
H	-1.959430	-3.008166	-1.362298
H	-3.424118	-3.458077	-2.224570
H	-2.943974	-4.368526	-0.795789
H	-3.414431	-2.391875	0.660238
H	-4.827589	-2.821915	-0.245351
H	-2.903549	-0.633809	-1.175125
H	-4.432037	-1.052162	-1.899493
H	-4.063031	0.122222	0.911779
H	-5.575284	-0.498072	0.318995
H	-5.706048	1.173154	-1.431605
H	-5.453270	1.943424	0.119532
H	-3.401962	1.578628	-2.118216
H	-4.114439	3.069578	-1.546797
H	-2.172319	1.264865	-0.051965
H	-3.000942	2.615686	0.724737
H	-1.224476	2.906780	-1.745999
H	-1.886450	4.206721	-0.772159
H	-0.576409	3.316856	1.214765
H	0.105970	2.087087	0.152737
H	0.456496	5.107546	-0.123689
H	2.772513	4.759891	0.437602
H	1.795384	4.069264	1.713817
H	2.143625	1.776673	0.676895
H	3.599006	2.543539	1.280658
H	2.776275	2.609026	-1.662765
H	4.249247	3.251208	-0.968467
H	4.822618	0.875958	-0.200365
H	4.847962	1.160673	-1.928827

conf_36

C	-2.431450	2.114672	0.654922
C	-3.491072	2.641418	-0.312429
C	-3.767368	1.776997	-1.540192
C	-4.417349	0.428229	-1.223006
C	-3.450715	-0.614699	-0.759389
O	-2.384767	-0.871105	-1.262094
O	-3.910314	-1.303730	0.313156

C	-3.051711	-2.346990	0.765569
C	-1.837739	-1.775736	1.446219
C	-1.925493	-1.143143	2.684543
C	-0.799181	-0.577751	3.275700
C	0.405759	-0.653239	2.615813
N	0.462429	-1.272032	1.425544
C	-0.603197	-1.813219	0.823400
H	-0.446426	-2.246404	-0.156061
H	1.360668	-1.288825	0.941514
H	1.333513	-0.237179	2.987375
H	-0.854611	-0.079831	4.235183
H	-2.885999	-1.084423	3.187193
H	-2.759524	-2.985309	-0.070746
H	-3.650184	-2.924701	1.470219
H	-5.222501	0.530647	-0.491826
H	-4.863466	0.015275	-2.135907
H	-2.852876	1.605983	-2.117608
H	-4.447098	2.323222	-2.199905
H	-4.429083	2.779745	0.238766
H	-3.201980	3.640948	-0.652437
C	-1.036077	1.926055	0.061278
C	-0.430629	3.189701	-0.541877
C	0.953400	2.967864	-1.145292
C	2.070348	2.753726	-0.129687
H	1.749250	2.021681	0.622934
C	3.360152	2.281497	-0.789601
C	4.533304	2.042248	0.157727
C	4.246633	1.071965	1.306092
C	3.564908	-0.224723	0.878084
C	4.341169	-1.104241	-0.093515
C	3.532515	-2.310527	-0.565781
C	2.398986	-1.969816	-1.530082
C	1.544675	-3.171384	-1.914601
C	0.404594	-2.820321	-2.860378
H	-0.187604	-3.702242	-3.117941
H	0.790875	-2.401540	-3.794178
H	-0.276015	-2.073935	-2.434348
H	2.186266	-3.930223	-2.376400
H	1.152363	-3.650461	-1.004389
H	2.825383	-1.525206	-2.437744
H	1.747897	-1.178050	-1.124118
H	4.196887	-3.028486	-1.058114
H	3.132901	-2.846766	0.310832
H	5.262732	-1.442712	0.392053
H	4.651617	-0.515318	-0.963842
H	2.606189	0.051571	0.414947
H	3.350402	-0.822354	1.779199
H	5.184293	0.837009	1.822095
H	3.612274	1.570034	2.049741
H	4.857451	2.996385	0.588233
H	5.384925	1.677522	-0.426964
H	3.663803	3.017035	-1.543326

H	3.147706	1.362735	-1.353704
H	2.251061	3.685542	0.421558
H	1.215883	3.821829	-1.779544
H	0.907683	2.099714	-1.818154
H	-1.094444	3.562994	-1.328611
H	-0.386081	3.980864	0.218557
H	-1.059740	1.144604	-0.707683
H	-0.376407	1.554894	0.857075
H	-2.368095	2.811313	1.500061
H	-2.773011	1.163829	1.087605

conf_14

C	-3.535340	1.265365	-0.681426
C	-3.704563	-0.176122	-0.223540
C	-3.911998	-1.144889	-1.381903
C	-3.909905	-2.616181	-0.953554
C	-2.629313	-2.976441	-0.268454
O	-2.494122	-3.345049	0.868458
O	-1.558297	-2.782408	-1.084885
C	-0.292472	-2.953860	-0.455419
C	-0.048238	-1.810588	0.492276
C	-0.088623	-1.966000	1.877471
C	0.063212	-0.867074	2.716733
C	0.238734	0.379793	2.159584
N	0.269281	0.502203	0.824187
C	0.137516	-0.537204	-0.010715
H	0.174529	-0.315594	-1.070335
H	0.416042	1.428618	0.424447
H	0.356379	1.290808	2.732201
H	0.030933	-0.972014	3.793605
H	-0.262439	-2.952458	2.292499
H	0.438839	-2.958992	-1.263960
H	-0.250043	-3.905072	0.077415
H	-4.719850	-2.831867	-0.254658
H	-4.030227	-3.260141	-1.830197
H	-3.132030	-0.994470	-2.136129
H	-4.864874	-0.930745	-1.875594
H	-2.816942	-0.471531	0.356055
H	-4.546082	-0.251491	0.476087
C	-3.332887	2.247975	0.466239
C	-3.071787	3.685138	0.014194
C	-1.719862	3.895733	-0.666000
C	-0.534088	3.871677	0.294823
H	-0.700010	3.102655	1.066329
C	0.797511	3.625339	-0.404072
C	2.009819	3.623736	0.524189
C	3.285570	3.071288	-0.109088
C	3.217863	1.572322	-0.371459
C	4.494729	0.957735	-0.928918
C	4.319449	-0.498082	-1.353109
C	3.928038	-1.445921	-0.225545
C	3.719328	-2.881486	-0.689106

C	3.323718	-3.822166	0.439229
H	3.152333	-4.839734	0.078694
H	2.407341	-3.484254	0.938294
H	4.104721	-3.870379	1.203823
H	2.955035	-2.898032	-1.478673
H	4.636988	-3.246467	-1.164257
H	3.005078	-1.097504	0.259625
H	4.700077	-1.422690	0.554985
H	3.561252	-0.548629	-2.148195
H	5.250167	-0.855658	-1.807591
H	5.293736	1.035214	-0.181046
H	4.827266	1.544177	-1.792999
H	2.406198	1.354403	-1.082100
H	2.960841	1.068682	0.570191
H	3.492984	3.603413	-1.045554
H	4.133814	3.277725	0.552780
H	1.788715	3.042645	1.435114
H	2.178905	4.646167	0.877228
H	0.944611	4.381085	-1.184422
H	0.737412	2.679712	-0.971672
H	-0.488200	4.814690	0.851588
H	-1.721052	4.852378	-1.198549
H	-1.575657	3.132405	-1.441993
H	-3.871806	3.985270	-0.671764
H	-3.147138	4.358120	0.876418
H	-2.508581	1.896897	1.104977
H	-4.221343	2.230550	1.107372
H	-2.688296	1.314890	-1.379007
H	-4.413709	1.570937	-1.263504

conf_6

C	2.328326	1.767830	-0.852535
C	3.662465	2.054032	-1.529661
C	4.520875	0.826286	-1.817069
C	5.116778	0.158728	-0.576265
C	4.174863	-0.609925	0.296901
O	4.133585	-0.578297	1.500553
O	3.363946	-1.431853	-0.416369
C	2.540918	-2.290553	0.365710
C	1.396496	-1.546463	1.003125
C	1.411737	-1.160631	2.344632
C	0.336776	-0.469568	2.894698
C	-0.743225	-0.168185	2.095866
N	-0.733427	-0.552028	0.811036
C	0.286551	-1.215563	0.250417
H	0.179935	-1.472351	-0.795837
H	-1.542304	-0.325843	0.233450
H	-1.621337	0.366202	2.434787
H	0.337175	-0.162140	3.932605
H	2.282793	-1.391869	2.946981
H	3.136789	-2.782816	1.136916
H	2.166223	-3.038948	-0.333566

H	5.878043	-0.566672	-0.889694
H	5.616227	0.886956	0.066582
H	5.359387	1.127853	-2.451457
H	3.950273	0.090085	-2.392972
H	3.466405	2.565772	-2.478929
H	4.235571	2.763070	-0.918422
C	1.478922	3.015673	-0.652755
C	0.107418	2.709103	-0.072080
C	-0.741223	3.937326	0.233201
C	-2.184335	3.586990	0.591428
H	-2.644807	4.409614	1.149383
C	-3.047640	3.283032	-0.630106
C	-4.421282	2.699455	-0.307210
C	-4.406659	1.293501	0.290391
C	-3.797537	0.237566	-0.622933
C	-3.844999	-1.174730	-0.052216
C	-3.153232	-2.214667	-0.926808
C	-2.991331	-3.565594	-0.242366
C	-2.300301	-4.628424	-1.091383
C	-0.840601	-4.323358	-1.403556
H	-0.271041	-4.171645	-0.477823
H	-0.732353	-3.431057	-2.029899
H	-0.370624	-5.148306	-1.944427
H	-2.357232	-5.587616	-0.566878
H	-2.854313	-4.763058	-2.027787
H	-3.982294	-3.928863	0.052841
H	-2.431033	-3.433313	0.695666
H	-3.717959	-2.337940	-1.858710
H	-2.169826	-1.836996	-1.247889
H	-4.890186	-1.465546	0.100454
H	-3.407757	-1.190608	0.959273
H	-2.757651	0.519000	-0.870756
H	-4.308932	0.251566	-1.593382
H	-3.876964	1.297704	1.253690
H	-5.435176	0.998904	0.527428
H	-5.023796	2.680596	-1.222961
H	-4.943567	3.371986	0.383098
H	-2.510722	2.613964	-1.314433
H	-3.184932	4.214385	-1.190612
H	-2.179318	2.730620	1.281880
H	-0.737524	4.611413	-0.632563
H	-0.273302	4.494186	1.052516
H	-0.431171	2.053683	-0.772810
H	0.235790	2.135344	0.857535
H	1.357216	3.533092	-1.612425
H	2.008153	3.716048	0.005421
H	1.770682	1.040331	-1.460281
H	2.490623	1.297444	0.126731

conf_0

C	4.393686	-0.158542	1.788615
C	5.185172	-1.452887	1.628963

C	4.633134	-2.445769	0.606328
C	3.172672	-2.864098	0.848387
C	2.149227	-1.912632	0.311992
O	1.297572	-1.327093	0.933677
O	2.251661	-1.778247	-1.035479
C	1.377590	-0.814352	-1.611093
C	-0.049284	-1.292843	-1.603482
C	-0.487940	-2.322673	-2.431840
C	-1.806126	-2.770117	-2.373368
C	-2.672213	-2.177502	-1.483803
N	-2.222926	-1.184211	-0.697862
C	-0.961869	-0.737144	-0.724667
H	-0.703865	0.050301	-0.029026
H	-2.870302	-0.746903	-0.041497
H	-3.711590	-2.456708	-1.367204
H	-2.159402	-3.569641	-3.011954
H	0.208368	-2.784726	-3.124922
H	1.729416	-0.685313	-2.635193
H	1.463926	0.136203	-1.080371
H	2.989822	-3.822248	0.349075
H	2.967917	-2.995785	1.912822
H	5.245608	-3.351109	0.641417
H	4.730931	-2.058658	-0.412251
H	6.220004	-1.220460	1.351042
H	5.239872	-1.951699	2.603935
C	4.301031	0.695273	0.528864
C	3.293209	1.827848	0.666281
C	3.176228	2.698268	-0.579276
C	2.046935	3.723265	-0.518181
H	2.154890	4.433929	-1.345740
C	0.655160	3.105348	-0.583365
C	-0.472470	4.129027	-0.519988
C	-1.861389	3.520910	-0.690980
C	-2.307341	2.640641	0.470809
C	-3.579668	1.858746	0.174961
C	-3.942385	0.845070	1.253837
C	-5.104457	-0.069171	0.879791
C	-5.363855	-1.182502	1.886186
C	-6.518783	-2.088164	1.487148
H	-7.450121	-1.521896	1.395150
H	-6.682393	-2.876587	2.225351
H	-6.334222	-2.572512	0.521499
H	-4.450833	-1.780908	2.017675
H	-5.565248	-0.736136	2.866570
H	-4.938873	-0.510154	-0.119581
H	-6.010144	0.536051	0.756690
H	-3.053008	0.242838	1.520785
H	-4.180042	1.366899	2.187541
H	-3.466970	1.349088	-0.795232
H	-4.418135	2.549919	0.031177
H	-2.449925	3.256758	1.366760
H	-1.506137	1.936167	0.733891

H	-2.598172	4.319296	-0.833930
H	-1.876362	2.930433	-1.618917
H	-0.312739	4.877661	-1.304267
H	-0.420096	4.672118	0.432203
H	0.543219	2.382423	0.234444
H	0.563318	2.537458	-1.522793
H	2.139503	4.313181	0.402762
H	3.034273	2.060108	-1.464627
H	4.128761	3.215172	-0.741230
H	2.319167	1.389584	0.921137
H	3.563659	2.460084	1.521650
H	4.018983	0.074896	-0.332302
H	5.291018	1.099916	0.283094
H	3.381966	-0.388469	2.144516
H	4.853004	0.435628	2.586594

conf_24

C	-2.900011	-3.390277	0.062910
C	-4.007441	-2.338213	0.084862
C	-4.126046	-1.539631	-1.211684
C	-4.945250	-0.247230	-1.062701
C	-4.193104	0.770080	-0.263534
O	-4.236797	0.941892	0.923940
O	-3.350385	1.499288	-1.057314
C	-2.617168	2.503846	-0.381462
C	-1.461748	1.942334	0.400529
C	-0.886079	2.632475	1.467479
C	0.196626	2.099516	2.155369
C	0.690798	0.869092	1.778312
N	0.115471	0.225387	0.754402
C	-0.920498	0.718374	0.062401
H	-1.307576	0.106509	-0.740909
H	0.470024	-0.698328	0.499903
H	1.522783	0.373059	2.260935
H	0.649591	2.625445	2.985893
H	-1.293384	3.592608	1.768498
H	-3.269216	3.068900	0.288943
H	-2.244467	3.170568	-1.163520
H	-5.170298	0.170484	-2.046013
H	-5.881898	-0.452074	-0.539757
H	-4.602817	-2.157361	-1.978756
H	-3.137882	-1.285484	-1.614090
H	-4.971020	-2.817987	0.285360
H	-3.833005	-1.659874	0.929594
C	-1.513569	-2.768259	0.160879
C	-0.346758	-3.742730	0.221459
C	0.981097	-3.011510	0.365162
C	2.224384	-3.890769	0.408427
H	2.230651	-4.554310	-0.464933
C	3.516135	-3.077358	0.445743
C	3.895395	-2.473000	-0.903630
C	5.045667	-1.470996	-0.838528

C	4.729023	-0.161149	-0.118203
C	3.617383	0.655104	-0.766986
C	3.433577	2.032707	-0.145675
C	2.312201	2.843737	-0.779610
C	2.118692	4.218675	-0.155171
C	0.965631	4.996614	-0.770519
H	0.017480	4.456165	-0.660883
H	1.123522	5.154938	-1.841458
H	0.844078	5.978248	-0.305741
H	1.961192	4.109624	0.926535
H	3.045276	4.794455	-0.259792
H	1.368013	2.281810	-0.719014
H	2.511391	2.959077	-1.852616
H	3.252009	1.931942	0.934883
H	4.373621	2.591820	-0.228394
H	2.666730	0.103665	-0.718016
H	3.830510	0.769642	-1.837889
H	5.639737	0.448391	-0.091910
H	4.477363	-0.354699	0.933331
H	5.906300	-1.945921	-0.352866
H	5.367938	-1.235642	-1.859775
H	3.023418	-1.995607	-1.368522
H	4.173335	-3.289100	-1.580212
H	4.341322	-3.710021	0.789816
H	3.414575	-2.287783	1.203853
H	2.162464	-4.540255	1.288297
H	0.960339	-2.426910	1.301847
H	1.083616	-2.304370	-0.476490
H	-0.479298	-4.432133	1.063344
H	-0.328428	-4.359325	-0.684602
H	-1.495443	-2.132976	1.059526
H	-1.355207	-2.105617	-0.703316
H	-3.038820	-4.076203	0.905525
H	-2.972997	-4.001116	-0.845469

conf_19

C	0.713480	-2.512582	-0.575625
C	1.192489	-2.819257	-1.990708
C	2.207439	-1.834471	-2.562503
C	3.472878	-1.677631	-1.709656
C	3.295747	-0.680845	-0.607923
O	2.837902	0.428158	-0.738540
O	3.712226	-1.136735	0.595702
C	3.545204	-0.221586	1.678887
C	2.083509	-0.043439	1.992343
C	1.338820	-1.033431	2.628656
C	-0.031420	-0.877487	2.821205
C	-0.644408	0.265259	2.362445
N	0.099090	1.207670	1.757132
C	1.418893	1.091297	1.563596
H	1.909574	1.898710	1.037435
H	-0.364558	2.035902	1.382649

H	-1.706205	0.459065	2.444340
H	-0.623579	-1.640665	3.309172
H	1.830303	-1.941312	2.964479
H	4.008428	0.737152	1.436896
H	4.070953	-0.675861	2.518360
H	3.811580	-2.631985	-1.300168
H	4.284942	-1.281484	-2.329933
H	1.755100	-0.846288	-2.698375
H	2.505824	-2.177090	-3.556836
H	1.630469	-3.825888	-1.995318
H	0.334672	-2.862143	-2.670731
C	-0.318744	-3.519467	-0.066515
C	-1.732059	-3.326352	-0.612622
C	-2.479998	-2.172639	0.042978
C	-3.897186	-1.984301	-0.487344
H	-4.387369	-2.963455	-0.537486
C	-4.757543	-1.059631	0.371937
C	-4.225124	0.363240	0.510550
C	-4.330406	1.211247	-0.753515
C	-3.493133	2.485031	-0.667755
C	-2.019464	2.241042	-0.976522
C	-1.101702	3.377876	-0.550001
C	0.332452	3.228906	-1.043461
C	1.310257	4.201865	-0.396504
C	2.731074	4.058475	-0.922985
H	3.417303	4.741786	-0.416564
H	2.771297	4.283400	-1.992643
H	3.105631	3.036886	-0.798914
H	0.956924	5.227450	-0.553667
H	1.300566	4.066930	0.697544
H	0.345658	3.374895	-2.129929
H	0.683292	2.196008	-0.902776
H	-1.509694	4.332566	-0.902797
H	-1.127501	3.487270	0.552862
H	-1.902441	2.072337	-2.053807
H	-1.688121	1.301530	-0.507451
H	-3.598841	2.917937	0.337353
H	-3.875572	3.242482	-1.359848
H	-4.011765	0.632535	-1.629346
H	-5.383368	1.459455	-0.922253
H	-3.173358	0.319876	0.826796
H	-4.761508	0.876542	1.317710
H	-4.853525	-1.505238	1.370149
H	-5.773198	-1.021945	-0.038763
H	-3.854163	-1.621103	-1.521224
H	-1.907820	-1.244014	-0.085977
H	-2.528236	-2.359244	1.127037
H	-1.701793	-3.177160	-1.699057
H	-2.306176	-4.246198	-0.455000
H	-0.365452	-3.481680	1.030325
H	0.036507	-4.527041	-0.311522
H	1.576812	-2.531162	0.100311

H	0.307423	-1.491543	-0.533995
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conf_18

C	-3.629405	0.503202	0.116677
C	-4.897162	-0.272002	0.451036
C	-4.686907	-1.634642	1.102744
C	-4.142227	-2.714163	0.166990
C	-2.674081	-2.726430	-0.124918
O	-2.163062	-3.020885	-1.173955
O	-1.916659	-2.443682	0.970104
C	-0.530829	-2.706621	0.802292
C	0.123288	-1.784970	-0.190446
C	0.931008	-2.263797	-1.221467
C	1.541117	-1.390420	-2.111967
C	1.324846	-0.036975	-1.972032
N	0.538128	0.396699	-0.978455
C	-0.052686	-0.419108	-0.093781
H	-0.672629	0.050869	0.659912
H	0.398768	1.402504	-0.861509
H	1.750447	0.716871	-2.621162
H	2.168933	-1.752299	-2.915942
H	1.068514	-3.333695	-1.333826
H	-0.379191	-3.742092	0.489087
H	-0.093348	-2.569504	1.793314
H	-4.334029	-3.700869	0.609355
H	-4.654585	-2.705154	-0.797985
H	-5.653574	-1.989779	1.471228
H	-4.040914	-1.544062	1.982137
H	-5.503329	0.341663	1.127213
H	-5.497559	-0.395784	-0.459650
C	-3.930206	1.855182	-0.524155
C	-2.712332	2.762621	-0.679332
C	-2.256208	3.397289	0.631835
C	-1.004429	4.263676	0.524906
H	-0.810009	4.730382	1.496985
C	0.229899	3.473593	0.109895
C	1.562943	4.196105	0.256376
C	2.748964	3.353272	-0.208683
C	3.028607	2.131273	0.661057
C	4.030236	1.154154	0.058594
C	4.049538	-0.190850	0.771687
C	5.031845	-1.186304	0.168987
C	5.066673	-2.538584	0.875676
C	3.781665	-3.345441	0.740468
H	3.550915	-3.530834	-0.315184
H	2.927005	-2.829209	1.191061
H	3.870319	-4.317661	1.231866
H	5.897402	-3.127369	0.473196
H	5.292682	-2.384842	1.937738
H	6.035513	-0.746268	0.189574
H	4.792448	-1.337801	-0.893917
H	4.291680	-0.039749	1.831726

H	3.033700	-0.611722	0.755222
H	5.033707	1.595848	0.066343
H	3.793182	0.992409	-1.003484
H	2.096468	1.587479	0.863544
H	3.381273	2.460167	1.645907
H	2.569365	3.032099	-1.247390
H	3.648735	3.975758	-0.253195
H	1.702251	4.487577	1.304421
H	1.527288	5.127372	-0.319121
H	0.117931	3.185585	-0.950648
H	0.249624	2.558729	0.723006
H	-1.171082	5.084850	-0.182311
H	-2.078079	2.618815	1.386986
H	-3.080086	4.004293	1.023304
H	-1.899181	2.180968	-1.138209
H	-2.939285	3.562374	-1.393903
H	-4.688117	2.376917	0.073866
H	-4.387445	1.682431	-1.504760
H	-3.052081	0.640370	1.041409
H	-2.997694	-0.078350	-0.570842

conf_21

C	-4.415280	-0.830053	-1.408675
C	-5.080360	-2.099031	-0.881932
C	-4.422401	-2.727176	0.346701
C	-2.974751	-3.168356	0.120826
C	-1.989377	-2.044431	0.201311
O	-2.017291	-1.124016	0.980692
O	-0.985471	-2.172982	-0.701383
C	-0.069567	-1.083969	-0.743439
C	0.814890	-1.029423	0.473031
C	1.891087	-1.894067	0.644829
C	2.686656	-1.822583	1.787174
C	2.393481	-0.883089	2.745958
N	1.348011	-0.056676	2.551453
C	0.562884	-0.100391	1.467648
H	-0.257190	0.603962	1.417999
H	1.141829	0.638647	3.260256
H	2.956092	-0.754019	3.661360
H	3.528876	-2.487418	1.929897
H	2.114530	-2.630325	-0.120989
H	-0.617820	-0.145171	-0.851690
H	0.531777	-1.251245	-1.637425
H	-2.677827	-3.872787	0.908321
H	-2.850934	-3.688740	-0.832095
H	-4.999221	-3.609769	0.636905
H	-4.454081	-2.045725	1.202180
H	-6.126578	-1.881583	-0.637482
H	-5.107393	-2.846890	-1.683744
C	-4.488163	0.362981	-0.462562
C	-3.551662	1.493252	-0.863758
C	-3.546328	2.657441	0.120543

C	-2.406086	3.649950	-0.095245
H	-2.585610	4.550098	0.503842
C	-1.039289	3.082593	0.269120
C	0.118661	4.051659	0.069399
C	1.484700	3.444603	0.380388
C	1.952821	2.408474	-0.635074
C	3.244311	1.705515	-0.243216
C	3.678356	0.632759	-1.231474
C	4.910928	-0.142179	-0.789776
C	5.257958	-1.309432	-1.703615
C	6.482922	-2.084967	-1.243656
H	7.366460	-1.440645	-1.209494
H	6.707248	-2.917879	-1.914479
H	6.339962	-2.497496	-0.238675
H	4.394440	-1.986780	-1.770155
H	5.418591	-0.935026	-2.721502
H	4.759656	-0.516831	0.233697
H	5.767900	0.540106	-0.727187
H	2.847025	-0.070082	-1.391814
H	3.864027	1.090141	-2.210923
H	3.124670	1.249895	0.751689
H	4.046220	2.445114	-0.128079
H	2.083557	2.896340	-1.608834
H	1.170729	1.653288	-0.792167
H	2.235720	4.240124	0.441977
H	1.456445	2.990870	1.384381
H	-0.041804	4.932021	0.701715
H	0.113066	4.417480	-0.965176
H	-0.860956	2.176866	-0.323559
H	-1.064573	2.769685	1.325605
H	-2.394233	3.978382	-1.142554
H	-3.485876	2.262036	1.144160
H	-4.505550	3.182978	0.058459
H	-2.539553	1.075224	-0.946168
H	-3.805417	1.860476	-1.866538
H	-4.226185	0.049673	0.553608
H	-5.521418	0.728777	-0.416151
H	-3.363308	-1.039467	-1.654376
H	-4.875622	-0.562064	-2.366481

conf_22

C	3.913553	-0.448165	0.882424
C	4.346604	-1.597392	1.781783
C	3.196281	-2.464344	2.285900
C	2.416869	-3.175352	1.175087
C	1.510004	-2.253508	0.421309
O	0.748112	-1.451597	0.901823
O	1.609504	-2.417945	-0.922312
C	0.858849	-1.489906	-1.698042
C	-0.615114	-1.781125	-1.630418
C	-1.187388	-2.861293	-2.296710
C	-2.550546	-3.126296	-2.181262

C	-3.324708	-2.301829	-1.398219
N	-2.746364	-1.265292	-0.767751
C	-1.440690	-0.988538	-0.852779
H	-1.078324	-0.144593	-0.281226
H	-3.329977	-0.653599	-0.190928
H	-4.389299	-2.429658	-1.249028
H	-3.008152	-3.962466	-2.694335
H	-0.562511	-3.505877	-2.907252
H	1.224495	-1.609455	-2.718181
H	1.062510	-0.470835	-1.358795
H	3.086283	-3.679571	0.474348
H	1.767500	-3.940297	1.617466
H	2.496708	-1.859443	2.872808
H	3.589791	-3.231216	2.959080
H	5.072463	-2.226119	1.249505
H	4.877660	-1.192030	2.650659
C	5.046470	0.473027	0.450523
C	4.559968	1.608733	-0.446082
C	3.804966	2.702014	0.305031
C	3.083690	3.688442	-0.610296
H	3.773405	4.014527	-1.398183
C	1.802886	3.156981	-1.253330
C	0.686832	2.869317	-0.252542
C	-0.679306	2.688475	-0.902218
C	-1.813559	2.528627	0.102607
C	-3.197731	2.508620	-0.538019
C	-4.343914	2.336859	0.456950
C	-4.521263	0.910235	0.961234
C	-5.551045	0.746072	2.070982
C	-5.736551	-0.702995	2.493560
H	-4.797767	-1.135136	2.857242
H	-6.092409	-1.318046	1.658773
H	-6.470292	-0.795317	3.297330
H	-5.240167	1.348709	2.931504
H	-6.506790	1.163250	1.734276
H	-3.557284	0.524774	1.334232
H	-4.848232	0.285554	0.108957
H	-4.179344	3.001255	1.313875
H	-5.284529	2.660489	-0.001231
H	-3.250720	1.721918	-1.307395
H	-3.333220	3.448419	-1.083984
H	-1.773041	3.363238	0.813401
H	-1.648943	1.632109	0.719678
H	-0.891550	3.560453	-1.533703
H	-0.659147	1.832320	-1.594995
H	0.625021	3.705950	0.455898
H	0.929766	1.985587	0.352544
H	2.017068	2.255955	-1.844488
H	1.443018	3.903173	-1.972109
H	2.828596	4.590513	-0.041140
H	4.521082	3.248167	0.929541
H	3.085469	2.257939	1.002996

H	5.411081	2.066186	-0.963067
H	3.924449	1.184273	-1.236056
H	5.803588	-0.117787	-0.078424
H	5.545681	0.888941	1.335181
H	3.456745	-0.846806	-0.033537
H	3.131999	0.127973	1.392108

conf_156

C	3.948154	1.195889	-0.205071
C	4.141778	0.062908	0.796129
C	4.962315	-1.120441	0.292087
C	4.304443	-1.883602	-0.861606
C	2.951745	-2.389234	-0.465803
O	2.686110	-3.010015	0.530276
O	1.989710	-2.041150	-1.361035
C	0.676935	-2.470778	-1.011923
C	0.144523	-1.643733	0.127162
C	-0.067392	-2.166587	1.402425
C	-0.528659	-1.352501	2.431545
C	-0.755331	-0.017290	2.179436
N	-0.528376	0.463278	0.948472
C	-0.098398	-0.298431	-0.067171
H	0.050888	0.201447	-1.016534
H	-0.706022	1.450526	0.766545
H	-1.108336	0.688443	2.920180
H	-0.699323	-1.744624	3.425972
H	0.150079	-3.212789	1.586621
H	0.677176	-3.527697	-0.741364
H	0.075812	-2.327086	-1.910427
H	4.215183	-1.276948	-1.763870
H	4.910347	-2.759843	-1.115816
H	5.130964	-1.818515	1.116697
H	5.947823	-0.779991	-0.041640
H	4.620769	0.462778	1.696821
H	3.157850	-0.301305	1.128291
C	2.957651	2.237150	0.294903
C	2.778848	3.448927	-0.615141
C	1.493519	4.212631	-0.297505
C	0.256284	3.514403	-0.865412
H	0.469893	2.437330	-0.952961
C	-1.015313	3.695344	-0.047597
C	-2.214535	2.945073	-0.619682
C	-3.398620	2.831886	0.336815
C	-4.429895	1.783551	-0.075414
C	-3.922177	0.354873	0.079152
C	-4.934981	-0.720094	-0.291219
C	-4.411405	-2.139128	-0.085650
C	-3.298734	-2.547041	-1.045619
C	-2.752115	-3.937706	-0.759367
H	-2.325476	-3.998153	0.248803
H	-1.978123	-4.229987	-1.475494
H	-3.543732	-4.690398	-0.814982

H	-3.678452	-2.503435	-2.073536
H	-2.480931	-1.815782	-0.998729
H	-5.238998	-2.849701	-0.190587
H	-4.056054	-2.245809	0.949689
H	-5.839428	-0.578379	0.311171
H	-5.242440	-0.589243	-1.336646
H	-3.615579	0.199625	1.125308
H	-3.021747	0.218483	-0.532044
H	-4.737259	1.955748	-1.114610
H	-5.332958	1.907286	0.532278
H	-3.034945	2.586319	1.347237
H	-3.876693	3.812301	0.432079
H	-1.897041	1.939561	-0.935324
H	-2.536867	3.429397	-1.548081
H	-1.252976	4.760283	0.053687
H	-0.823171	3.370158	0.992644
H	0.081267	3.846614	-1.894874
H	1.545864	5.234642	-0.683986
H	1.399594	4.307759	0.792792
H	3.648318	4.106144	-0.514887
H	2.759831	3.129633	-1.665784
H	3.254776	2.582294	1.293599
H	1.986622	1.738798	0.435907
H	4.914965	1.669733	-0.414786
H	3.588762	0.804353	-1.165452

conf_139

C	-3.177473	3.220768	0.703350
C	-1.953739	2.844679	1.535801
C	-0.719715	2.522730	0.700335
C	0.443427	1.981566	1.518940
C	0.239447	0.565122	1.950126
O	-0.765427	-0.090546	1.818249
O	1.350385	0.037355	2.515323
C	1.213062	-1.306896	2.972514
C	1.186545	-2.272843	1.816147
C	2.356020	-2.707958	1.197246
C	2.306775	-3.567826	0.102960
C	1.081240	-3.965765	-0.376397
N	-0.032564	-3.529178	0.236920
C	-0.020376	-2.713940	1.299059
H	-0.977566	-2.400925	1.693374
H	-0.935152	-3.783007	-0.152760
H	0.946102	-4.610941	-1.234730
H	3.209393	-3.913781	-0.384174
H	3.316917	-2.367353	1.570266
H	0.310358	-1.406732	3.578565
H	2.088272	-1.486254	3.596337
H	1.386545	2.017599	0.965145
H	0.614499	2.578459	2.423963
H	-0.385605	3.424756	0.176398
H	-0.968594	1.789460	-0.074007

H	-1.715353	3.672280	2.214820
H	-2.196418	1.986728	2.170710
C	-3.650169	2.137437	-0.265646
C	-3.957399	0.800687	0.401814
C	-4.573090	-0.231963	-0.540727
C	-3.676691	-0.668990	-1.695845
H	-3.331481	0.212394	-2.248690
C	-2.467643	-1.510775	-1.289993
C	-1.521618	-1.749574	-2.470930
C	-0.538106	-0.603272	-2.706622
C	0.650278	-0.634939	-1.754165
C	1.635904	0.509678	-1.939132
C	2.911627	0.331635	-1.122718
C	3.959077	1.419128	-1.344078
C	3.571536	2.794088	-0.812266
C	4.637917	3.846692	-1.077018
H	4.347787	4.821996	-0.678071
H	4.813690	3.966045	-2.150508
H	5.590531	3.568229	-0.615608
H	2.624829	3.117682	-1.261222
H	3.394564	2.721758	0.269510
H	4.174047	1.494403	-2.418116
H	4.900480	1.114581	-0.870540
H	2.663818	0.275698	-0.052345
H	3.352237	-0.640860	-1.383158
H	1.144111	1.455532	-1.683756
H	1.904170	0.586672	-3.000586
H	1.187114	-1.582892	-1.905870
H	0.292964	-0.638521	-0.715421
H	-0.163360	-0.642976	-3.735312
H	-1.062252	0.356231	-2.614337
H	-2.124744	-1.915560	-3.370224
H	-0.942461	-2.676418	-2.340628
H	-2.844854	-2.467360	-0.894151
H	-1.929574	-1.018895	-0.469080
H	-4.269905	-1.250523	-2.411195
H	-5.500536	0.178865	-0.956868
H	-4.870614	-1.117403	0.036306
H	-3.047034	0.396538	0.857962
H	-4.655123	0.974390	1.230836
H	-2.900358	1.999439	-1.054152
H	-4.550240	2.497864	-0.778664
H	-3.997423	3.468471	1.387584
H	-2.966526	4.137293	0.138848

conf_67

C	4.544986	-0.023879	-1.863634
C	3.360231	-0.976321	-2.008099
C	3.542479	-2.283656	-1.247334
C	2.320424	-3.212049	-1.328622
C	1.216738	-2.750220	-0.432799
O	0.246871	-2.101548	-0.735661

O	1.437692	-3.136294	0.851023
C	0.410110	-2.794000	1.771555
C	0.400899	-1.319520	2.067844
C	1.414965	-0.710542	2.804008
C	1.391142	0.659720	3.045451
C	0.350427	1.406612	2.543206
N	-0.612017	0.794271	1.834583
C	-0.614786	-0.519414	1.578111
H	-1.423614	-0.895352	0.964772
H	-1.361373	1.359753	1.435945
H	0.254155	2.476490	2.672218
H	2.172770	1.146849	3.613935
H	2.233914	-1.312450	3.185655
H	0.635851	-3.360858	2.675367
H	-0.561229	-3.109023	1.383576
H	1.931223	-3.241992	-2.348386
H	2.601014	-4.223750	-1.026710
H	3.782852	-2.098551	-0.194449
H	4.401460	-2.820831	-1.662058
H	2.433047	-0.480815	-1.694598
H	3.220283	-1.211924	-3.069303
C	4.709392	0.599854	-0.476154
C	3.506880	1.411358	0.001865
C	3.196699	2.632618	-0.859360
C	1.879309	3.316229	-0.504732
H	1.847026	4.313998	-0.956125
C	0.659705	2.525066	-0.959613
C	-0.668948	3.109744	-0.503899
C	-1.860863	2.222572	-0.851859
C	-3.120289	2.539458	-0.052353
C	-4.283948	1.588213	-0.307350
C	-4.025670	0.159606	0.163234
C	-5.238815	-0.761558	0.070521
C	-5.724046	-1.012244	-1.352669
C	-6.870965	-2.010237	-1.410189
H	-7.730982	-1.656457	-0.833035
H	-6.573274	-2.979958	-0.998577
H	-7.206680	-2.174462	-2.437073
H	-6.043017	-0.068526	-1.809109
H	-4.884756	-1.377123	-1.959457
H	-6.058432	-0.340549	0.667290
H	-4.992561	-1.725430	0.533794
H	-3.207406	-0.284004	-0.421914
H	-3.695234	0.195641	1.214463
H	-4.518241	1.591434	-1.377488
H	-5.176661	1.969162	0.201911
H	-3.427073	3.569492	-0.265049
H	-2.896694	2.539625	1.032095
H	-2.083963	2.308400	-1.921159
H	-1.576423	1.168719	-0.719563
H	-0.810179	4.109183	-0.930332
H	-0.635638	3.282891	0.584732

H	0.733021	1.489172	-0.600493
H	0.666508	2.449636	-2.053924
H	1.833646	3.479232	0.582830
H	3.163474	2.347819	-1.917251
H	4.023087	3.345927	-0.765411
H	2.626992	0.756705	0.053214
H	3.692324	1.748083	1.030776
H	5.594727	1.246263	-0.487453
H	4.927064	-0.184431	0.258908
H	5.467005	-0.559715	-2.118730
H	4.453270	0.770107	-2.611577

conf_43

C	4.309741	-1.278585	-1.180927
C	4.043416	-1.964719	0.153267
C	3.199044	-3.232852	0.072025
C	1.821206	-3.028113	-0.572953
C	1.099803	-1.836015	-0.032142
O	0.642809	-0.921377	-0.667202
O	1.003241	-1.866426	1.326424
C	0.663903	-0.639575	1.943930
C	-0.811686	-0.382425	2.042385
C	-1.299839	0.595550	2.909430
C	-2.660113	0.866843	2.988198
C	-3.528091	0.155802	2.190030
N	-3.034424	-0.780982	1.368093
C	-1.729058	-1.066878	1.268523
H	-1.455222	-1.834645	0.559305
H	-3.683613	-1.275984	0.755156
H	-4.599963	0.304821	2.173994
H	-3.045968	1.625127	3.657325
H	-0.605985	1.154059	3.530766
H	1.120886	0.193549	1.397348
H	1.094269	-0.683365	2.946352
H	1.892641	-2.880710	-1.651242
H	1.199739	-3.914290	-0.4000
H	3.065233	-3.641237	1.077755
H	3.723570	-3.997093	-0.510648
H	5.000179	-2.215672	0.625924
H	3.558286	-1.259134	0.840250
C	5.203517	-0.045139	-1.054259
C	4.663812	1.059661	-0.146677
C	3.328993	1.644096	-0.592351
C	2.840347	2.769675	0.313427
H	3.647706	3.502365	0.429289
C	1.594981	3.488485	-0.196654
C	0.325355	2.645350	-0.196064
C	-0.859368	3.371240	-0.822134
C	-2.171025	2.594000	-0.794642
C	-2.131538	1.271702	-1.551534
C	-3.496293	0.604327	-1.663216
C	-3.429389	-0.813849	-2.218465

C	-4.763074	-1.555124	-2.240352
C	-5.290282	-1.923554	-0.859261
H	-6.236997	-2.466007	-0.914157
H	-5.484997	-1.034575	-0.244665
H	-4.589996	-2.597093	-0.339985
H	-5.510090	-0.944548	-2.759940
H	-4.657299	-2.471601	-2.829230
H	-2.693393	-1.402798	-1.647287
H	-3.023077	-0.770653	-3.234716
H	-3.982304	0.612889	-0.677302
H	-4.151622	1.209161	-2.301877
H	-1.422381	0.585326	-1.073276
H	-1.731586	1.441006	-2.559371
H	-2.965706	3.223333	-1.213597
H	-2.460038	2.405014	0.250853
H	-1.001243	4.333293	-0.314964
H	-0.612898	3.614745	-1.863593
H	0.073558	2.377892	0.843611
H	0.502469	1.702726	-0.723837
H	1.785747	3.840151	-1.219052
H	1.423184	4.390505	0.403140
H	2.654476	2.376434	1.324956
H	2.571772	0.853796	-0.650801
H	3.431757	2.030260	-1.615682
H	4.577354	0.691388	0.884215
H	5.405509	1.866041	-0.104920
H	5.374049	0.369692	-2.054769
H	6.187623	-0.356618	-0.683647
H	4.787163	-1.993053	-1.862703
H	3.363623	-0.994604	-1.656920

conf_3

C	4.001558	-0.585861	0.807167
C	4.530173	-1.902750	1.359726
C	3.799291	-3.141661	0.850279
C	2.314685	-3.205218	1.227704
C	1.423033	-2.239395	0.511553
O	0.590920	-1.520746	1.008861
O	1.616825	-2.267776	-0.830556
C	0.887889	-1.291094	-1.563047
C	-0.586669	-1.592250	-1.574482
C	-1.117876	-2.677983	-2.265181
C	-2.483629	-2.951074	-2.216887
C	-3.302502	-2.130573	-1.476095
N	-2.762641	-1.087908	-0.821514
C	-1.455917	-0.803114	-0.843421
H	-1.130129	0.046035	-0.257228
H	-3.374754	-0.480608	-0.275330
H	-4.372077	-2.265808	-1.378900
H	-2.909537	-3.792138	-2.748922
H	-0.458862	-3.322047	-2.839248
H	1.293126	-1.332214	-2.574727

H	1.070202	-0.297816	-1.144976
H	1.927596	-4.205434	0.996290
H	2.165252	-3.038996	2.296882
H	4.277939	-4.033721	1.265011
H	3.897302	-3.215668	-0.237701
H	5.591497	-2.001343	1.103795
H	4.484712	-1.878589	2.456272
C	4.811087	0.631649	1.240181
C	4.108731	1.949667	0.928919
C	3.972802	2.263732	-0.559513
C	2.964915	3.373822	-0.848635
H	3.141271	3.790152	-1.847069
C	1.517833	2.900110	-0.764217
C	0.499478	4.025160	-0.900125
C	-0.944780	3.547279	-1.008527
C	-1.471709	2.834637	0.231090
C	-2.900029	2.333902	0.060856
C	-3.393311	1.467549	1.213244
C	-4.800570	0.913354	1.010294
C	-5.213933	-0.122752	2.047539
C	-6.615362	-0.668513	1.821025
H	-7.360811	0.130925	1.860894
H	-6.883568	-1.408902	2.578139
H	-6.705860	-1.149697	0.840393
H	-4.488166	-0.949065	2.054372
H	-5.148100	0.328989	3.043667
H	-4.911337	0.483064	-0.004287
H	-5.517616	1.742587	1.009917
H	-2.684156	0.642542	1.396683
H	-3.370796	2.045899	2.143520
H	-2.973340	1.776976	-0.887525
H	-3.575345	3.188209	-0.066224
H	-1.420965	3.510132	1.093951
H	-0.812890	1.993142	0.489235
H	-1.595113	4.402562	-1.226406
H	-1.033733	2.875745	-1.875656
H	0.741898	4.616984	-1.790540
H	0.598023	4.708949	-0.047421
H	1.363423	2.369089	0.183238
H	1.344699	2.164032	-1.565261
H	3.120534	4.200625	-0.143340
H	3.670632	1.364999	-1.113507
H	4.957278	2.539491	-0.953608
H	3.115164	1.925541	1.396647
H	4.644815	2.775094	1.410898
H	5.800894	0.607940	0.766829
H	4.988136	0.571087	2.320670
H	3.969182	-0.645981	-0.287858
H	2.968969	-0.430972	1.145904

conf_52

C	4.005768	0.525977	-1.352489
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C	4.196094	-0.477985	-0.214912
C	4.423921	-1.911526	-0.685973
C	3.267464	-2.514574	-1.477172
C	2.002407	-2.749382	-0.712402
O	0.884474	-2.730494	-1.163962
O	2.230519	-3.040257	0.592325
C	1.071279	-3.375609	1.343600
C	0.168976	-2.184455	1.515078
C	0.559158	-1.064772	2.247035
C	-0.277676	0.042439	2.346984
C	-1.501621	0.012423	1.718174
N	-1.851665	-1.079927	1.020033
C	-1.063546	-2.153411	0.891252
H	-1.427916	-2.957354	0.265360
H	-2.751360	-1.078937	0.540461
H	-2.211773	0.828569	1.730206
H	0.015034	0.925127	2.900998
H	1.531384	-1.054154	2.730067
H	1.445934	-3.714636	2.310107
H	0.532729	-4.194422	0.860811
H	3.000729	-1.914220	-2.349698
H	3.557670	-3.500365	-1.863680
H	4.649592	-2.554650	0.168971
H	5.309552	-1.931173	-1.330083
H	5.068847	-0.179373	0.378098
H	3.342486	-0.441344	0.475376
C	4.388415	1.954571	-0.974188
C	3.553032	2.606024	0.124359
C	2.109066	2.896862	-0.271649
C	1.414041	3.849833	0.696453
H	2.054105	4.730261	0.825005
C	0.032596	4.313939	0.245616
C	-1.044475	3.240401	0.318147
C	-2.393854	3.703423	-0.218219
C	-3.505563	2.666218	-0.094064
C	-3.325326	1.445565	-0.989450
C	-4.352574	0.350305	-0.736843
C	-4.187956	-0.862581	-1.648501
C	-5.136854	-2.017787	-1.341563
C	-4.832654	-2.735382	-0.032984
H	-4.910148	-2.072320	0.836582
H	-3.827866	-3.178602	-0.053536
H	-5.528685	-3.558450	0.144170
H	-6.166545	-1.643065	-1.322327
H	-5.093145	-2.742190	-2.160694
H	-3.146598	-1.225768	-1.620786
H	-4.336641	-0.533317	-2.682313
H	-4.325648	0.058034	0.328136
H	-5.362691	0.756627	-0.867216
H	-2.312892	1.033349	-0.876709
H	-3.386274	1.759392	-2.038423
H	-4.468853	3.132741	-0.328343

H	-3.590398	2.352683	0.958995
H	-2.691981	4.612749	0.315819
H	-2.284158	3.993812	-1.270714
H	-1.162471	2.942200	1.371671
H	-0.708174	2.349934	-0.227580
H	0.100089	4.688704	-0.783895
H	-0.282531	5.167432	0.857147
H	1.344188	3.388686	1.692807
H	1.544718	1.959393	-0.363916
H	2.101594	3.351216	-1.271746
H	3.576603	1.993666	1.035959
H	4.032296	3.554220	0.395577
H	4.338575	2.586274	-1.869308
H	5.440546	1.954098	-0.664080
H	4.636864	0.221921	-2.197126
H	2.974219	0.495659	-1.725033

conf_120

C	4.517779	-0.304054	1.297385
C	3.878450	-1.655729	1.015738
C	2.715305	-1.963364	1.954312
C	1.784111	-3.037740	1.413164
C	0.970606	-2.549022	0.254252
O	0.793477	-1.399998	-0.067463
O	0.394135	-3.567871	-0.428337
C	-0.365724	-3.175853	-1.568128
C	-1.670969	-2.540870	-1.167289
C	-2.756199	-3.302767	-0.739376
C	-3.942852	-2.692660	-0.339959
C	-4.028194	-1.319719	-0.369784
N	-2.967216	-0.609213	-0.787521
C	-1.812420	-1.163329	-1.176443
H	-1.013674	-0.490094	-1.460208
H	-3.031019	0.409713	-0.783770
H	-4.901808	-0.754335	-0.070373
H	-4.792687	-3.274823	-0.007214
H	-2.671908	-4.384928	-0.714013
H	-0.547157	-4.097902	-2.120319
H	0.217115	-2.492301	-2.189112
H	2.323783	-3.937682	1.101231
H	1.066402	-3.370197	2.174451
H	2.133805	-1.050691	2.123153
H	3.092597	-2.279818	2.931312
H	3.518035	-1.646226	-0.021517
H	4.625516	-2.457320	1.072464
C	5.649221	0.041071	0.333999
C	5.991520	1.531278	0.272577
C	4.805950	2.442098	-0.054511
C	4.076356	2.080332	-1.345327
H	3.903631	0.997690	-1.383282
C	2.724889	2.766888	-1.5215
C	1.684637	2.308838	-0.503125

C	0.263193	2.725385	-0.853560
C	-0.750054	2.315846	0.206711
C	-2.194642	2.589950	-0.186879
C	-3.209109	2.195046	0.882020
C	-4.656389	2.231634	0.407226
C	-5.657480	1.765111	1.455950
C	-7.090372	1.740142	0.945942
H	-7.201452	1.067482	0.087507
H	-7.409530	2.734509	0.620754
H	-7.785640	1.406854	1.719914
H	-5.371002	0.767387	1.819586
H	-5.587023	2.421454	2.330616
H	-4.777699	1.621419	-0.506279
H	-4.909325	3.248900	0.085352
H	-2.970087	1.195134	1.277990
H	-3.094065	2.862953	1.742723
H	-2.412896	2.083405	-1.148007
H	-2.321311	3.651319	-0.430251
H	-0.529856	2.841884	1.143691
H	-0.621670	1.247693	0.437632
H	0.216954	3.811630	-1.002278
H	-0.013689	2.281418	-1.821718
H	1.933376	2.700534	0.490432
H	1.721981	1.214315	-0.414803
H	2.350522	2.551732	-2.530756
H	2.841496	3.856935	-1.467495
H	4.723875	2.311013	-2.199612
H	5.160101	3.477595	-0.120366
H	4.102411	2.428855	0.784937
H	6.422149	1.847535	1.230230
H	6.779879	1.675983	-0.475770
H	5.378388	-0.308053	-0.670043
H	6.549028	-0.522755	0.604804
H	3.726164	0.450195	1.224577
H	4.880222	-0.262034	2.332489

conf_26

C	4.329927	0.385385	1.630204
C	5.355909	-0.719538	1.395042
C	4.974760	-1.771427	0.353863
C	3.650352	-2.499363	0.636112
C	2.421772	-1.745694	0.233580
O	1.507800	-1.406970	0.944296
O	2.411944	-1.479723	-1.097353
C	1.333351	-0.663606	-1.540324
C	0.030041	-1.414086	-1.511236
C	-0.262584	-2.416659	-2.431651
C	-1.459597	-3.125432	-2.355326
C	-2.351859	-2.817277	-1.355234
N	-2.045149	-1.843009	-0.481648
C	-0.902421	-1.149071	-0.523436
H	-0.748718	-0.404547	0.246303

H	-2.721652	-1.611779	0.245769
H	-3.305664	-3.310108	-1.217574
H	-1.699521	-3.906991	-3.064821
H	0.454478	-2.651006	-3.212406
H	1.588207	-0.384401	-2.563055
H	1.269624	0.239395	-0.929532
H	3.633332	-3.438251	0.071060
H	3.548318	-2.743341	1.695554
H	5.764627	-2.527349	0.324185
H	4.938191	-1.337618	-0.649830
H	6.310980	-0.274548	1.091737
H	5.549031	-1.226327	2.348069
C	4.017975	1.238988	0.405907
C	2.832480	2.168721	0.624333
C	2.523481	3.057989	-0.573947
C	1.283300	3.927101	-0.387562
H	1.301483	4.755608	-1.104570
C	-0.042575	3.188690	-0.547371
C	-1.228694	4.045681	-0.118048
C	-2.600292	3.516889	-0.519450
C	-2.911782	2.102362	-0.041437
C	-4.395853	1.770158	-0.157078
C	-4.744460	0.299482	0.043085
C	-4.292142	-0.285385	1.376282
C	-4.752589	-1.722367	1.607437
C	-4.177790	-2.348368	2.869241
H	-4.544491	-3.366809	3.016617
H	-4.455336	-1.765614	3.751829
H	-3.082586	-2.389380	2.841364
H	-5.846971	-1.737050	1.646708
H	-4.510400	-2.352097	0.733307
H	-4.668301	0.339601	2.195077
H	-3.195131	-0.214822	1.480390
H	-5.829520	0.171608	-0.043311
H	-4.318236	-0.283395	-0.788681
H	-4.755651	2.083157	-1.144264
H	-4.950688	2.376045	0.569777
H	-2.581651	1.990665	1.000121
H	-2.327822	1.382737	-0.634852
H	-3.364302	4.196901	-0.123886
H	-2.704675	3.552737	-1.611774
H	-1.107370	5.050309	-0.540224
H	-1.192986	4.173674	0.971775
H	-0.027915	2.262639	0.044485
H	-0.161765	2.887378	-1.598623
H	1.319751	4.390845	0.606999
H	2.408139	2.442945	-1.479063
H	3.391721	3.698813	-0.764616
H	1.953969	1.564877	0.892952
H	3.024626	2.805631	1.497211
H	3.815681	0.601133	-0.464039
H	4.903824	1.826976	0.134004

H	3.400919	-0.049964	2.017530
H	4.698284	1.037289	2.430381

conf_32

C	-3.509154	-0.113997	-0.108545
C	-4.579204	-1.141931	-0.454785
C	-4.098199	-2.374009	-1.215387
C	-3.294949	-3.377227	-0.390049
C	-1.853847	-3.087586	-0.106523
O	-1.235288	-3.483132	0.849870
O	-1.246998	-2.374182	-1.087729
C	0.159170	-2.241272	-0.934813
C	0.524203	-1.445392	0.287887
C	0.043549	-0.155067	0.491567
C	0.389079	0.559376	1.634907
C	1.219525	-0.022991	2.561694
N	1.663801	-1.274726	2.342124
C	1.341376	-1.991809	1.257967
H	1.734555	-2.998313	1.200786
H	2.264769	-1.702735	3.037194
H	1.544638	0.458849	3.474414
H	0.020047	1.563260	1.798989
H	-0.620673	0.289924	-0.240837
H	0.495659	-1.723573	-1.834950
H	0.627947	-3.227677	-0.895919
H	-3.767943	-3.578547	0.574808
H	-3.270220	-4.340765	-0.917204
H	-3.524047	-2.074935	-2.098208
H	-4.976921	-2.906794	-1.590611
H	-5.094152	-1.457953	0.462063
H	-5.339972	-0.643510	-1.066415
C	-4.090651	1.116690	0.581097
C	-3.130600	2.297056	0.713287
C	-2.829008	2.998257	-0.608877
C	-2.067155	4.315412	-0.466340
H	-2.660566	4.997322	0.154196
C	-0.663511	4.207459	0.124915
C	0.297981	3.371688	-0.708736
C	1.699932	3.276832	-0.121731
C	2.571346	2.236366	-0.810472
C	3.926070	2.036737	-0.143121
C	4.744645	0.887003	-0.723068
C	4.162875	-0.490296	-0.428584
C	4.988888	-1.642732	-0.981928
C	4.390288	-3.006568	-0.671920
H	4.323363	-3.173220	0.410181
H	4.993369	-3.818390	-1.085179
H	3.383514	-3.102358	-1.096488
H	5.088846	-1.524640	-2.067105
H	6.005987	-1.587480	-0.577140
H	3.144748	-0.559398	-0.835466
H	4.068498	-0.605894	0.662771

H	4.840521	1.016110	-1.808683
H	5.763862	0.930210	-0.322364
H	3.777892	1.863773	0.933602
H	4.499936	2.967193	-0.217083
H	2.719395	2.514436	-1.861593
H	2.025696	1.282928	-0.832591
H	2.186261	4.258802	-0.164077
H	1.633933	3.035620	0.949489
H	0.352072	3.782345	-1.724824
H	-0.106346	2.357891	-0.831540
H	-0.719065	3.797996	1.143991
H	-0.250718	5.216248	0.240876
H	-1.996409	4.789612	-1.452499
H	-3.782772	3.208745	-1.107359
H	-2.289886	2.325603	-1.287647
H	-3.565478	3.030855	1.402625
H	-2.201002	1.959402	1.193008
H	-4.453466	0.825185	1.573673
H	-4.975954	1.450633	0.024905
H	-2.750837	-0.563346	0.548834
H	-2.993293	0.176195	-1.033260

conf_33

C	5.197771	0.567709	-0.859591
C	5.272970	-0.545105	0.184856
C	5.280108	-1.966888	-0.370719
C	4.025150	-2.327314	-1.188930
C	2.781927	-1.831738	-0.523481
O	2.046781	-0.968434	-0.929828
O	2.565057	-2.435982	0.674889
C	1.590262	-1.803101	1.492994
C	0.208259	-1.850916	0.901378
C	-0.430383	-3.054325	0.612859
C	-1.696717	-3.061576	0.036271
C	-2.314736	-1.862858	-0.237694
N	-1.680288	-0.716824	0.063973
C	-0.457295	-0.675375	0.606029
H	-0.027506	0.306068	0.764228
H	-2.147238	0.163997	-0.147602
H	-3.295933	-1.772420	-0.684604
H	-2.204293	-3.987862	-0.201051
H	0.074589	-3.991517	0.825291
H	1.880245	-0.764552	1.674724
H	1.617493	-2.347696	2.438124
H	4.047752	-1.879036	-2.182477
H	3.962607	-3.413385	-1.306011
H	5.373713	-2.672427	0.459725
H	6.151318	-2.122206	-1.015138
H	6.169809	-0.403781	0.797550
H	4.432681	-0.452200	0.885349
C	4.736187	1.905563	-0.281717
C	3.256579	1.906027	0.085523

C	2.736408	3.232416	0.618040
C	1.268587	3.181601	1.034360
H	1.000802	4.121414	1.531261
C	0.294185	2.951239	-0.116742
C	-1.165681	3.006302	0.316247
C	-2.157986	2.906795	-0.838728
C	-3.609545	3.143103	-0.424477
C	-4.264255	1.990539	0.335774
C	-4.748355	0.858885	-0.564781
C	-5.384794	-0.296383	0.195952
C	-5.949919	-1.389805	-0.702647
C	-6.464219	-2.593272	0.072395
H	-6.876995	-3.354665	-0.593653
H	-7.253904	-2.301085	0.770536
H	-5.667224	-3.060497	0.662211
H	-6.757043	-0.966765	-1.311212
H	-5.191890	-1.713349	-1.433092
H	-6.190532	0.095334	0.828292
H	-4.660390	-0.729297	0.903369
H	-5.477047	1.265507	-1.276439
H	-3.930734	0.486439	-1.206732
H	-5.127151	2.367979	0.894716
H	-3.579891	1.602648	1.106308
H	-4.212920	3.360344	-1.313104
H	-3.642914	4.049790	0.189495
H	-1.878558	3.651747	-1.591835
H	-2.054328	1.940946	-1.361570
H	-1.342039	3.954426	0.839286
H	-1.364413	2.232297	1.075099
H	0.507450	1.997389	-0.619508
H	0.462886	3.720075	-0.881397
H	1.137223	2.398250	1.797718
H	2.870663	4.014041	-0.140819
H	3.340903	3.539414	1.479583
H	2.683458	1.600239	-0.796664
H	3.065146	1.136338	0.846226
H	4.916979	2.697265	-1.017819
H	5.341220	2.162696	0.597730
H	6.180539	0.681656	-1.329788
H	4.505724	0.290383	-1.663622

conf_174

C	5.429866	-0.103020	-0.857481
C	4.115983	-0.612451	-1.432662
C	3.966866	-2.126278	-1.379746
C	2.537761	-2.589773	-1.709342
C	1.567379	-2.009289	-0.731145
O	0.815688	-1.084024	-0.916297
O	1.649994	-2.619790	0.478009
C	0.907193	-1.999019	1.521663
C	-0.577146	-2.144583	1.319143
C	-1.228149	-3.369349	1.439056

C	-2.598346	-3.471045	1.206100
C	-3.301452	-2.341666	0.855179
N	-2.647613	-1.171908	0.750417
C	-1.333103	-1.042632	0.961802
H	-0.908275	-0.058037	0.814458
H	-3.173462	-0.338831	0.480128
H	-4.364100	-2.324358	0.648751
H	-3.116334	-4.417493	1.294330
H	-0.659402	-4.254349	1.707350
H	1.177042	-0.942456	1.593573
H	1.218556	-2.510004	2.433330
H	2.240400	-2.253566	-2.704425
H	2.478087	-3.680763	-1.667799
H	4.236689	-2.494227	-0.383454
H	4.652466	-2.606356	-2.084707
H	3.291004	-0.156622	-0.874515
H	3.995914	-0.264453	-2.466980
C	5.541989	1.424602	-0.854885
C	4.307145	2.152327	-0.320576
C	3.897653	1.760487	1.103100
C	2.393261	1.847578	1.343158
H	2.161792	1.476784	2.351951
C	1.798912	3.243558	1.194347
C	0.278997	3.264930	1.338131
C	-0.457579	2.662431	0.146236
C	-1.953224	2.497696	0.380545
C	-2.676728	1.822001	-0.777933
C	-4.141748	1.508669	-0.489212
C	-4.796769	0.609292	-1.532029
C	-6.201360	0.139211	-1.163907
C	-7.217865	1.265287	-1.034936
H	-6.973048	1.949437	-0.217714
H	-8.218306	0.871493	-0.840917
H	-7.266988	1.852164	-1.957499
H	-6.543801	-0.571754	-1.923402
H	-6.163482	-0.422829	-0.217972
H	-4.155895	-0.266705	-1.714981
H	-4.829297	1.142024	-2.489976
H	-4.250580	1.055455	0.517045
H	-4.698726	2.446392	-0.394940
H	-2.140490	0.902350	-1.061777
H	-2.616084	2.454766	-1.670304
H	-2.409091	3.474621	0.580837
H	-2.111760	1.919223	1.306012
H	-0.294566	3.292403	-0.736907
H	-0.020814	1.688453	-0.116292
H	-0.065396	4.295163	1.482353
H	-0.001447	2.724717	2.254438
H	2.074652	3.665401	0.220326
H	2.247504	3.900056	1.948702
H	1.901054	1.165476	0.635080
H	4.429926	2.383863	1.831322

H	4.213352	0.731659	1.309622
H	4.484882	3.231171	-0.374605
H	3.465199	1.964395	-0.999252
H	5.727883	1.772484	-1.877818
H	6.425159	1.712703	-0.273010
H	5.537635	-0.487917	0.164468
H	6.272779	-0.521857	-1.419090

Picolylamides

C18:1 8Z picolylamide

conf_2

C	2.813481	1.590318	-0.706196
C	4.297964	1.339884	-0.947018
C	4.879676	0.120905	-0.238062
C	4.166893	-1.192778	-0.553365
C	2.977520	-1.451064	0.339264
O	2.917761	-1.093679	1.501505
N	1.930491	-2.140887	-0.217050
H	2.037651	-2.543734	-1.134193
C	0.894100	-2.655597	0.644079
C	0.137802	-1.571553	1.365903
C	-0.534092	-1.821792	2.559115
C	-1.203343	-0.801734	3.226970
C	-1.190429	0.467600	2.693192
N	-0.545979	0.680729	1.537598
C	0.098491	-0.280398	0.872418
H	0.601297	0.014290	-0.038302
H	-0.544112	1.631219	1.123886
H	-1.672198	1.322516	3.149114
H	-1.719799	-0.985783	4.160288
H	-0.518260	-2.820478	2.984711
H	1.313078	-3.331841	1.398160
H	0.195542	-3.233392	0.032259
H	3.880615	-1.251751	-1.610131
H	4.848643	-2.032999	-0.371069
H	4.856853	0.264689	0.846746
H	5.931784	0.025535	-0.519481
H	4.465366	1.246720	-2.028220
H	4.863152	2.224465	-0.631581
C	2.338835	2.893595	-1.335628
C	0.831570	3.118916	-1.280069
C	0.285219	3.378282	0.099512
C	-0.986578	3.710266	0.368648
C	-2.062371	3.886021	-0.657667
C	-3.453261	3.412877	-0.234198
C	-3.537571	1.938717	0.151229
C	-2.955037	0.977498	-0.876296
C	-3.133565	-0.487526	-0.502210
C	-2.404110	-1.442798	-1.435770
C	-2.515829	-2.902093	-1.021188
C	-1.751223	-3.854230	-1.931361
C	-1.780038	-5.296760	-1.449559
H	-1.333973	-5.395976	-0.453211
H	-2.806994	-5.667658	-1.382679
H	-1.233268	-5.959151	-2.125144
H	-0.709582	-3.512280	-2.024859
H	-2.165909	-3.793759	-2.944195
H	-2.159280	-3.014189	0.014065

H	-3.572284	-3.196908	-0.996246
H	-1.340893	-1.161253	-1.485714
H	-2.786483	-1.321384	-2.456950
H	-2.784138	-0.651360	0.527455
H	-4.202465	-0.732796	-0.488085
H	-1.884250	1.184838	-1.015716
H	-3.415903	1.163188	-1.854855
H	-3.034012	1.783857	1.115214
H	-4.587090	1.680850	0.333274
H	-4.143351	3.609446	-1.061762
H	-3.806885	4.023134	0.604914
H	-1.769648	3.402407	-1.593783
H	-2.122280	4.959037	-0.887089
H	-1.249321	3.968743	1.396547
H	1.005560	3.382821	0.919054
H	0.316301	2.262070	-1.739866
H	0.578516	3.974687	-1.916708
H	2.651075	2.910845	-2.385723
H	2.850541	3.737235	-0.856348
H	2.235320	0.761804	-1.143393
H	2.612776	1.583484	0.373290

conf_17

C	2.486284	-3.363163	-1.378071
C	0.963227	-3.331415	-1.507483
C	0.276191	-4.324797	-0.574596
C	-1.213065	-4.042784	-0.395124
C	-1.431151	-2.887279	0.548544
O	-0.914661	-2.826788	1.651042
N	-2.226796	-1.863847	0.110561
H	-2.718905	-1.960042	-0.762921
C	-2.670602	-0.857660	1.040870
C	-1.570356	0.016401	1.583934
C	-1.819897	0.899643	2.631481
C	-0.803112	1.686602	3.160934
C	0.464312	1.578144	2.634266
N	0.679005	0.727496	1.621505
C	-0.278946	-0.039490	1.092041
H	0.015063	-0.696112	0.285536
H	1.636672	0.663328	1.227301
H	1.318822	2.141588	2.985712
H	-0.989056	2.371514	3.978207
H	-2.819976	0.965475	3.049793
H	-3.166928	-1.327320	1.898765
H	-3.408035	-0.227510	0.536858
H	-1.700955	-3.869279	-1.360506
H	-1.705901	-4.904847	0.067201
H	0.741673	-4.311036	0.416333
H	0.410011	-5.336526	-0.968657
H	0.600562	-2.312026	-1.303593

H	0.662238	-3.543327	-2.539304
C	3.001326	-2.501298	-0.225752
C	3.070692	-1.024498	-0.602744
C	3.453072	-0.121384	0.539792
C	3.770960	1.176915	0.430158
C	3.832711	1.950708	-0.848476
C	3.290297	3.378096	-0.761250
C	1.824154	3.479179	-0.352268
C	0.867390	2.666007	-1.214076
C	-0.596376	2.875366	-0.852336
C	-1.545041	1.958551	-1.610956
C	-3.002704	2.129798	-1.210904
C	-3.947703	1.174002	-1.926752
C	-5.388093	1.283810	-1.450363
H	-5.475712	1.063700	-0.380009
H	-5.775781	2.294970	-1.604621
H	-6.044750	0.593453	-1.985478
H	-3.588239	0.142412	-1.796004
H	-3.899344	1.361115	-3.005644
H	-3.098887	1.998620	-0.122425
H	-3.318043	3.162287	-1.406159
H	-1.246128	0.911368	-1.451311
H	-1.438530	2.132389	-2.689029
H	-0.735333	2.726441	0.228299
H	-0.870585	3.920957	-1.038484
H	1.108664	1.596273	-1.136077
H	1.021213	2.920821	-2.270480
H	1.715253	3.173308	0.697582
H	1.523460	4.532820	-0.377657
H	3.425504	3.854500	-1.738303
H	3.899804	3.955113	-0.056203
H	3.329000	1.401629	-1.648789
H	4.889391	2.005349	-1.144816
H	4.089602	1.707233	1.329215
H	3.543144	-0.592938	1.519868
H	2.110278	-0.704431	-1.035676
H	3.793570	-0.903724	-1.418136
H	4.000267	-2.831925	0.077186
H	2.357302	-2.635662	0.654437
H	2.806527	-4.401344	-1.239583
H	2.953468	-3.026577	-2.310443

conf_0

C	2.986109	1.530084	-1.542149
C	4.461086	1.179601	-1.382103
C	4.807237	0.216432	-0.249463
C	4.128364	-1.150146	-0.369707
C	2.892262	-1.296050	0.481534
O	2.772892	-0.791140	1.583869
N	1.881675	-2.069712	-0.030164
H	2.041113	-2.563322	-0.894002
C	0.849249	-2.567330	0.846481

C	0.002434	-1.491059	1.470925
C	-0.797983	-1.761883	2.577212
C	-1.552484	-0.757958	3.175033
C	-1.491708	0.517188	2.659821
N	-0.722146	0.750431	1.587585
C	0.006287	-0.195271	0.988952
H	0.598871	0.111092	0.138574
H	-0.678551	1.713158	1.202830
H	-2.030610	1.363107	3.066095
H	-2.171729	-0.959241	4.039687
H	-0.820214	-2.765889	2.990323
H	1.286272	-3.156828	1.661754
H	0.204077	-3.234373	0.267760
H	3.914455	-1.400777	-1.415027
H	4.804215	-1.932163	-0.001244
H	4.554195	0.641329	0.726827
H	5.890750	0.073587	-0.245640
H	4.820717	0.752994	-2.326383
H	5.029498	2.105712	-1.237348
C	2.369026	2.297098	-0.378039
C	1.000495	2.860346	-0.752361
C	0.219898	3.426202	0.403024
C	-1.053072	3.846243	0.349971
C	-1.907048	3.889866	-0.877036
C	-3.351884	3.428389	-0.677946
C	-3.503697	1.978856	-0.226549
C	-2.804984	0.963486	-1.121042
C	-3.050413	-0.482427	-0.713001
C	-2.231506	-1.480656	-1.519148
C	-2.403934	-2.921244	-1.062432
C	-1.564072	-3.915010	-1.854145
C	-1.652948	-5.336010	-1.318769
H	-2.685191	-5.697761	-1.335521
H	-1.050702	-6.029314	-1.911029
H	-1.305218	-5.396385	-0.280936
H	-0.515175	-3.582774	-1.860158
H	-1.878270	-3.894500	-2.904023
H	-2.154487	-2.995981	0.006965
H	-3.461221	-3.205510	-1.133073
H	-1.166433	-1.208278	-1.461391
H	-2.496741	-1.398746	-2.580633
H	-2.826564	-0.609122	0.355901
H	-4.117329	-0.714887	-0.815789
H	-1.722458	1.153531	-1.127786
H	-3.129949	1.108561	-2.159319
H	-3.132306	1.874877	0.802476
H	-4.571264	1.736877	-0.172604
H	-3.886675	3.567832	-1.623740
H	-3.845341	4.084539	0.048323
H	-1.436031	3.330632	-1.690258
H	-1.928191	4.935483	-1.213776
H	-1.489190	4.276741	1.252784

H	0.765924	3.555614	1.338629
H	0.408838	2.085825	-1.263488
H	1.138692	3.640666	-1.511771
H	3.029563	3.123221	-0.088415
H	2.297839	1.653451	0.508075
H	2.876176	2.130864	-2.453173
H	2.398528	0.617765	-1.727738

conf_16

C	-0.965750	4.111503	-0.599179
C	-1.861063	2.962273	-1.041385
C	-3.190991	2.919122	-0.300994
C	-4.030041	1.674340	-0.624806
C	-3.305659	0.415238	-0.225916
O	-2.586490	-0.220707	-0.976334
N	-3.416946	0.050189	1.090316
H	-4.082561	0.522828	1.680027
C	-2.834765	-1.183551	1.549210
C	-1.356846	-1.111621	1.843470
C	-0.710132	-2.141975	2.526162
C	0.656928	-2.091119	2.768744
C	1.374997	-1.007630	2.311231
N	0.733853	-0.030934	1.658928
C	-0.582876	-0.048681	1.416786
H	-0.985475	0.796568	0.875453
H	1.282024	0.776256	1.305635
H	2.443354	-0.887751	2.436212
H	1.164688	-2.886458	3.299233
H	-1.283094	-2.997619	2.871223
H	-2.973009	-1.953890	0.780584
H	-3.363095	-1.513277	2.446547
H	-4.999780	1.735708	-0.120706
H	-4.211763	1.610353	-1.699633
H	-3.782000	3.807062	-0.547468
H	-3.012967	2.967500	0.781848
H	-2.046544	3.031470	-2.120393
H	-1.341209	2.006338	-0.909433
C	0.408799	4.112509	-1.265768
C	1.268280	2.874660	-0.984394
C	1.645696	2.730717	0.458008
C	2.836166	2.355070	0.950189
C	4.065631	1.987419	0.179220
C	4.319177	0.476352	0.116190
C	3.344257	-0.271941	-0.782947
C	3.567307	-1.779181	-0.784994
C	2.551107	-2.565399	-1.608044
C	1.151388	-2.589033	-1.006119
C	0.166472	-3.460575	-1.771622
C	-1.213294	-3.504368	-1.128417
C	-2.199760	-4.380038	-1.886393
H	-3.181362	-4.397167	-1.403872
H	-2.342207	-4.012627	-2.907067

H	-1.845192	-5.413259	-1.953375
H	-1.604712	-2.482261	-1.062343
H	-1.110438	-3.877008	-0.097660
H	0.073209	-3.088995	-2.799902
H	0.567973	-4.479162	-1.851224
H	0.743903	-1.570620	-0.948585
H	1.221325	-2.959190	0.027110
H	2.507235	-2.156659	-2.625616
H	2.902974	-3.598083	-1.713102
H	3.556164	-2.154597	0.249493
H	4.576997	-1.982217	-1.159834
H	2.311754	-0.045747	-0.490225
H	3.440119	0.106961	-1.808454
H	4.292930	0.058334	1.133598
H	5.340188	0.304956	-0.241311
H	4.921976	2.470755	0.661102
H	4.016245	2.382204	-0.839820
H	2.948049	2.346064	2.036564
H	0.879913	3.015759	1.182208
H	2.168267	2.912026	-1.603236
H	0.729801	1.976069	-1.316771
H	0.960938	5.005494	-0.953791
H	0.278004	4.196440	-2.350339
H	-1.461180	5.063474	-0.819956
H	-0.858040	4.090287	0.493862

conf_109

C	2.518222	-2.086222	-0.570020
C	4.025270	-2.010353	-0.774453
C	4.697911	-0.788708	-0.155166
C	4.277062	0.557108	-0.766064
C	2.954463	1.116693	-0.300839
O	1.991593	1.292595	-1.027190
N	2.873835	1.436374	1.029804
H	3.702936	1.370282	1.598159
C	1.769422	2.222440	1.521856
C	0.528625	1.432756	1.851100
C	-0.479639	1.962391	2.654941
C	-1.632903	1.234130	2.926078
C	-1.769516	-0.025532	2.384994
N	-0.787526	-0.512513	1.616073
C	0.330299	0.166076	1.333411
H	1.043105	-0.327204	0.688303
H	-0.887394	-1.461699	1.210448
H	-2.630826	-0.663095	2.536494
H	-2.419619	1.638162	3.550293
H	-0.364497	2.957095	3.075387
H	1.490024	2.963207	0.762969
H	2.093307	2.767107	2.411399
H	5.043008	1.308838	-0.542024
H	4.214725	0.477094	-1.853371
H	5.779185	-0.886981	-0.288015

H	4.530119	-0.785164	0.929940
H	4.489324	-2.910508	-0.354591
H	4.242799	-2.030372	-1.849589
C	1.900816	-3.367975	-1.113692
C	0.377034	-3.393547	-1.035916
C	-0.159725	-3.409640	0.369555
C	-1.447483	-3.538354	0.719782
C	-2.613537	-3.698327	-0.204665
C	-3.588062	-2.516393	-0.177179
C	-3.084659	-1.291656	-0.930041
C	-3.995499	-0.081436	-0.770265
C	-3.527541	1.168670	-1.507314
C	-2.248362	1.781997	-0.950791
C	-1.881099	3.107572	-1.602461
C	-0.626444	3.738258	-1.014371
C	-0.261102	5.064022	-1.664994
H	0.640782	5.498071	-1.223629
H	-0.073441	4.934350	-2.735084
H	-1.068052	5.795556	-1.557914
H	0.205211	3.031408	-1.118571
H	-0.782399	3.891767	0.064717
H	-1.736118	2.954669	-2.679409
H	-2.723064	3.805456	-1.505689
H	-1.406475	1.087274	-1.069591
H	-2.375301	1.941442	0.130544
H	-3.389675	0.937181	-2.571154
H	-4.323403	1.921274	-1.464005
H	-4.107248	0.154306	0.298992
H	-4.999254	-0.353039	-1.117412
H	-2.065440	-1.041576	-0.609866
H	-2.996921	-1.539509	-1.995538
H	-3.812874	-2.252748	0.867019
H	-4.544003	-2.830410	-0.609168
H	-3.148597	-4.606951	0.095259
H	-2.271348	-3.861741	-1.230958
H	-1.680382	-3.603892	1.785119
H	0.579823	-3.383787	1.171769
H	0.003708	-4.276984	-1.566416
H	-0.028576	-2.531643	-1.583474
H	2.311307	-4.234054	-0.579781
H	2.198244	-3.487111	-2.161059
H	2.312260	-2.005570	0.507900
H	2.036811	-1.232117	-1.062929

conf_21

C	3.295451	1.715479	-1.423952
C	4.788485	1.417525	-1.339023
C	5.204846	0.322562	-0.360188
C	4.605883	-1.049622	-0.676187
C	3.363459	-1.374108	0.114139
O	3.201225	-1.045036	1.275946
N	2.399620	-2.105275	-0.532262

H	2.598920	-2.451774	-1.457033
C	1.375858	-2.778405	0.229712
C	0.441630	-1.856261	0.966848
C	-0.419213	-2.346357	1.945568
C	-1.253630	-1.490251	2.656431
C	-1.203668	-0.140354	2.392138
N	-0.368774	0.307400	1.443551
C	0.431360	-0.493635	0.733546
H	1.069429	-0.019899	0.001361
H	-0.311792	1.331690	1.280499
H	-1.798845	0.603918	2.905233
H	-1.924621	-1.864312	3.419020
H	-0.428607	-3.409023	2.168539
H	1.828006	-3.446131	0.973662
H	0.791821	-3.399971	-0.454417
H	4.427892	-1.168688	-1.751114
H	5.317936	-1.835889	-0.395471
H	4.941411	0.585138	0.669138
H	6.294713	0.244079	-0.383604
H	5.146662	1.146420	-2.339629
H	5.315946	2.341093	-1.073472
C	2.678349	2.288992	-0.153490
C	1.279886	2.845795	-0.412402
C	0.539589	3.244884	0.833376
C	-0.779771	3.465112	0.933879
C	-1.782490	3.359782	-0.170058
C	-2.959104	2.444324	0.168008
C	-3.915769	2.255684	-1.000612
C	-5.036072	1.254170	-0.728595
C	-4.567051	-0.132163	-0.286533
C	-3.538550	-0.777466	-1.207013
C	-3.185815	-2.200928	-0.799943
C	-2.069431	-2.815886	-1.632706
C	-1.751180	-4.249199	-1.233929
H	-0.939729	-4.672302	-1.833879
H	-1.467088	-4.318791	-0.176873
H	-2.622663	-4.896214	-1.368341
H	-1.170023	-2.188653	-1.546743
H	-2.348485	-2.785806	-2.692452
H	-2.897167	-2.215382	0.260762
H	-4.080557	-2.832019	-0.871349
H	-2.620573	-0.172994	-1.226159
H	-3.915852	-0.775662	-2.237844
H	-4.154659	-0.082210	0.731082
H	-5.442108	-0.788175	-0.211909
H	-5.637635	1.153062	-1.639144
H	-5.710767	1.659111	0.034920
H	-4.354748	3.222793	-1.270574
H	-3.341530	1.933648	-1.878416
H	-3.500346	2.837852	1.038242
H	-2.574220	1.461814	0.465365
H	-1.304927	3.017384	-1.093897

H	-2.164882	4.366305	-0.385715
H	-1.167409	3.789164	1.900441
H	1.152304	3.412417	1.719294
H	0.690103	2.124095	-0.995869
H	1.368214	3.720304	-1.070600
H	3.315022	3.094106	0.232813
H	2.655000	1.528668	0.637691
H	3.136595	2.428554	-2.242011
H	2.745230	0.809652	-1.722230

conf_29

C	0.774544	-3.999405	-1.553417
C	1.880085	-2.964395	-1.349754
C	2.563928	-3.053775	0.010141
C	3.558696	-1.914564	0.280608
C	2.843982	-0.625157	0.586028
O	2.214084	0.016017	-0.238689
N	2.863557	-0.215910	1.893745
H	3.457709	-0.695679	2.549972
C	2.349988	1.082179	2.250693
C	0.847503	1.169671	2.346312
C	0.224954	2.299737	2.875204
C	-1.160792	2.406916	2.897484
C	-1.918386	1.380639	2.375539
N	-1.298640	0.299900	1.886135
C	0.032592	0.165150	1.860218
H	0.415482	-0.749615	1.431943
H	-1.860348	-0.467834	1.471912
H	-2.999678	1.385376	2.329840
H	-1.650708	3.282712	3.303366
H	0.830077	3.112671	3.265818
H	2.663148	1.812220	1.493624
H	2.790537	1.384365	3.203374
H	4.226347	-2.186187	1.103580
H	4.178665	-1.743022	-0.604380
H	3.101250	-4.005234	0.085462
H	1.821572	-3.070291	0.818784
H	2.638272	-3.101372	-2.129290
H	1.491699	-1.952355	-1.499473
C	-0.375966	-3.918931	-0.550954
C	-1.074265	-2.559318	-0.528591
C	-2.033672	-2.429699	0.612335
C	-3.298881	-1.985468	0.575819
C	-4.069477	-1.525959	-0.624007
C	-4.085093	-0.001084	-0.795210
C	-2.767579	0.559294	-1.312374
C	-2.737536	2.080162	-1.384627
C	-1.413675	2.648731	-1.886857
C	-0.251146	2.419474	-0.927286
C	1.056217	3.085531	-1.340853
C	1.670110	2.512424	-2.612160
C	3.034049	3.110281	-2.922075

H	3.455487	2.694585	-3.841038
H	2.973515	4.196170	-3.047813
H	3.743458	2.909853	-2.112000
H	0.997398	2.684862	-3.460009
H	1.760993	1.426030	-2.496334
H	0.898768	4.166102	-1.460315
H	1.784514	2.969705	-0.527281
H	-0.058784	1.346151	-0.810505
H	-0.548871	2.800641	0.060009
H	-1.184403	2.212385	-2.865929
H	-1.526958	3.726651	-2.053399
H	-2.956538	2.499963	-0.390848
H	-3.552307	2.419144	-2.034865
H	-1.938630	0.200021	-0.691857
H	-2.574411	0.149651	-2.312335
H	-4.349780	0.472901	0.161672
H	-4.888498	0.270838	-1.488071
H	-5.097938	-1.885521	-0.520157
H	-3.670211	-1.981846	-1.535518
H	-3.852845	-1.984933	1.516164
H	-1.656747	-2.782904	1.575966
H	-1.573457	-2.373245	-1.483980
H	-0.311312	-1.771576	-0.448533
H	-0.011085	-4.152391	0.457252
H	-1.113025	-4.695027	-0.781576
H	0.375825	-3.887487	-2.568287
H	1.203654	-5.007155	-1.507883

conf_18

C	3.789066	0.265510	-0.220509
C	5.021108	-0.629677	-0.302528
C	4.803157	-2.095316	0.059595
C	3.729685	-2.800520	-0.768128
C	2.344014	-2.651166	-0.189285
O	2.118654	-2.583165	1.005020
N	1.305484	-2.604551	-1.084703
H	1.484270	-2.801316	-2.056362
C	-0.047931	-2.712803	-0.593287
C	-0.397915	-1.605223	0.366193
C	-1.315448	-1.787851	1.396746
C	-1.594450	-0.759808	2.289858
C	-0.946116	0.446160	2.146069
N	-0.075632	0.600548	1.139299
C	0.203345	-0.364975	0.260901
H	0.942018	-0.133020	-0.494591
H	0.418850	1.504580	1.025991
H	-1.090484	1.294881	2.801670
H	-2.300274	-0.895529	3.099186
H	-1.805692	-2.749014	1.513609
H	-0.207322	-3.668442	-0.081196
H	-0.728734	-2.681155	-1.449379
H	3.751995	-2.477342	-1.815526

H	3.922076	-3.880730	-0.774025
H	4.531911	-2.191368	1.115609
H	5.750097	-2.626223	-0.069520
H	5.430764	-0.564332	-1.319251
H	5.796465	-0.224878	0.358203
C	4.133673	1.728963	-0.470436
C	2.933774	2.660623	-0.599326
C	2.159653	2.877563	0.671931
C	1.013533	3.569347	0.762877
C	0.309859	4.195951	-0.407620
C	-0.718511	3.275015	-1.075399
C	-1.977025	3.035523	-0.249695
C	-2.830974	1.900115	-0.794959
C	-4.129903	1.680657	-0.029745
C	-4.957383	0.504616	-0.542547
C	-4.326492	-0.855721	-0.275465
C	-5.140570	-2.031833	-0.794873
C	-4.483992	-3.373568	-0.505150
H	-4.365390	-3.531467	0.572811
H	-5.074925	-4.206934	-0.892640
H	-3.490887	-3.435462	-0.966634
H	-5.289898	-1.919361	-1.875351
H	-6.140856	-2.007605	-0.346998
H	-3.324098	-0.898687	-0.723462
H	-4.181820	-0.971087	0.808420
H	-5.128483	0.623807	-1.620330
H	-5.948337	0.530703	-0.075214
H	-3.907946	1.529383	1.036783
H	-4.729107	2.596677	-0.083915
H	-2.234776	0.977367	-0.794507
H	-3.065374	2.098958	-1.848880
H	-1.714937	2.824286	0.796317
H	-2.565450	3.960368	-0.215595
H	-0.238560	2.313687	-1.309704
H	-1.005494	3.701040	-2.042744
H	1.052845	4.497665	-1.152044
H	-0.190284	5.113285	-0.079602
H	0.593361	3.738244	1.754735
H	2.617941	2.509693	1.591057
H	2.269567	2.300635	-1.396277
H	3.285930	3.641187	-0.946592
H	4.722884	1.797811	-1.391638
H	4.789226	2.089333	0.332018
H	3.057733	-0.057458	-0.977045
H	3.308062	0.141685	0.758971

conf_27

C	-0.884621	3.452646	1.334256
C	0.559817	3.246369	1.786007
C	1.598409	3.792426	0.802170
C	2.949561	3.062337	0.861109
C	2.835707	1.667255	0.303406

O	2.407662	0.714835	0.930892
N	3.169439	1.514507	-1.020244
H	3.651387	2.261174	-1.493781
C	3.231587	0.190512	-1.585117
C	1.886977	-0.460524	-1.794826
C	1.790490	-1.807828	-2.141492
C	0.551102	-2.415669	-2.299592
C	-0.589340	-1.668604	-2.099866
N	-0.471571	-0.375803	-1.772169
C	0.708998	0.237003	-1.618510
H	0.682377	1.279344	-1.335159
H	-1.338960	0.169677	-1.619815
H	-1.596050	-2.058130	-2.179728
H	0.467900	-3.463197	-2.559346
H	2.694491	-2.395047	-2.270920
H	3.813728	-0.470220	-0.931140
H	3.753966	0.247176	-2.543972
H	3.706751	3.632447	0.314055
H	3.283472	2.972097	1.897818
H	1.771457	4.854731	0.998996
H	1.223439	3.743760	-0.227586
H	0.715505	3.718256	2.761320
H	0.725846	2.174129	1.938931
C	-1.228038	2.567510	0.144209
C	-2.687663	2.596022	-0.306092
C	-2.868992	1.763938	-1.536399
C	-3.608564	0.654402	-1.675586
C	-4.506361	0.021058	-0.658998
C	-3.959985	-1.273462	-0.047115
C	-2.829030	-1.055802	0.949006
C	-2.386494	-2.338213	1.642229
C	-1.312286	-2.124854	2.706836
C	0.090837	-1.832488	2.180456
C	0.740054	-3.018454	1.475507
C	2.217811	-2.808265	1.175693
C	2.852500	-3.987665	0.454054
H	3.907097	-3.807378	0.224478
H	2.803446	-4.895080	1.063256
H	2.335386	-4.213129	-0.486503
H	2.749359	-2.629278	2.117532
H	2.342658	-1.881957	0.602823
H	0.625563	-3.914131	2.100750
H	0.208498	-3.244517	0.540068
H	0.725858	-1.541609	3.025069
H	0.088681	-0.959599	1.514009
H	-1.631762	-1.307312	3.364875
H	-1.260333	-3.016808	3.342140
H	-2.042137	-3.067076	0.896246
H	-3.266215	-2.792945	2.112364
H	-1.971176	-0.576455	0.460620
H	-3.165164	-0.341191	1.712090
H	-3.641796	-1.959929	-0.845319

H	-4.781627	-1.786105	0.464818
H	-5.458272	-0.197560	-1.155351
H	-4.734940	0.724952	0.146361
H	-3.614197	0.180431	-2.659488
H	-2.335433	2.125249	-2.418978
H	-2.979132	3.630611	-0.525451
H	-3.331584	2.249266	0.505910
H	-0.960537	1.534258	0.405441
H	-0.604003	2.856006	-0.713197
H	-1.558392	3.212325	2.164108
H	-1.066359	4.505247	1.083335

conf_7

C	0.800030	2.773934	-0.922146
C	2.093850	3.484286	-1.304318
C	3.367839	2.652077	-1.199656
C	3.796628	2.300359	0.227664
C	3.059956	1.187292	0.929528
O	2.613348	1.283397	2.058704
N	2.930551	0.005479	0.242161
H	3.421100	-0.108825	-0.630316
C	2.541254	-1.184685	0.958887
C	1.166931	-1.082770	1.563789
C	0.799957	-1.833093	2.677129
C	-0.462964	-1.694842	3.243286
C	-1.348594	-0.797266	2.690339
N	-0.976106	-0.098224	1.609059
C	0.224371	-0.217859	1.039350
H	0.420286	0.410946	0.181737
H	-1.640259	0.571349	1.180842
H	-2.343111	-0.611776	3.074058
H	-0.752761	-2.265536	4.116224
H	1.515340	-2.516943	3.123487
H	3.248434	-1.403833	1.767524
H	2.565267	-2.026312	0.260644
H	4.853986	2.006315	0.224800
H	3.718806	3.175062	0.877075
H	4.183838	3.222460	-1.653099
H	3.267507	1.747773	-1.814638
H	2.000519	3.831788	-2.339752
H	2.205633	4.388181	-0.692445
C	-0.429097	3.625787	-1.221021
C	-1.761030	2.887309	-1.146863
C	-2.226091	2.512226	0.233909
C	-3.338420	1.807157	0.493934
C	-4.281724	1.287560	-0.546938
C	-4.887142	-0.089022	-0.267606
C	-3.869283	-1.204411	-0.041654
C	-2.754800	-1.276850	-1.076894
C	-1.786054	-2.428382	-0.840463
C	-0.538267	-2.352722	-1.708671
C	0.486956	-3.432952	-1.398602

C	1.778881	-3.288895	-2.191942
C	2.829618	-4.324712	-1.821359
H	2.460020	-5.338918	-1.998255
H	3.744259	-4.200338	-2.406430
H	3.101465	-4.261429	-0.761092
H	2.182122	-2.275681	-2.044873
H	1.554297	-3.357943	-3.262600
H	0.712781	-3.418660	-0.321587
H	0.051223	-4.421232	-1.590751
H	-0.069005	-1.365228	-1.580766
H	-0.821191	-2.406071	-2.767310
H	-1.486206	-2.444433	0.217533
H	-2.298853	-3.382627	-1.010672
H	-2.191185	-0.332805	-1.079287
H	-3.187224	-1.359692	-2.081970
H	-3.421339	-1.091086	0.954547
H	-4.396992	-2.164265	-0.006596
H	-5.528475	-0.349873	-1.116237
H	-5.550400	-0.029671	0.603090
H	-3.790744	1.286359	-1.523893
H	-5.104194	2.010809	-0.634661
H	-3.646404	1.685470	1.535057
H	-1.667694	2.933377	1.071764
H	-1.717029	1.994966	-1.786763
H	-2.534718	3.521474	-1.597736
H	-0.327763	4.032335	-2.233272
H	-0.448759	4.493512	-0.550317
H	0.730556	1.834679	-1.492794
H	0.822139	2.511183	0.143481

conf_22

C	-3.867977	-0.840732	1.081154
C	-3.563285	-1.388887	-0.309084
C	-3.079872	-2.836352	-0.276390
C	-2.409156	-3.304225	-1.580917
C	-1.091752	-2.592904	-1.722944
O	-0.968398	-1.507597	-2.269397
N	-0.038660	-3.178998	-1.078334
H	-0.194500	-4.036509	-0.572493
C	1.174004	-2.432511	-0.823240
C	0.996186	-1.514796	0.364258
C	1.621665	-1.719840	1.590746
C	1.348812	-0.891897	2.677599
C	0.441580	0.132329	2.525409
N	-0.140500	0.317948	1.331633
C	0.114167	-0.446238	0.266837
H	-0.400791	-0.205962	-0.655500
H	-0.824608	1.092533	1.213870
H	0.161733	0.816221	3.316577
H	1.832542	-1.042567	3.634347
H	2.332806	-2.532645	1.702738
H	1.407087	-1.848055	-1.716356

H	1.998151	-3.125310	-0.647013
H	-2.267127	-4.389083	-1.563196
H	-3.028404	-3.054628	-2.444594
H	-3.924255	-3.498073	-0.059363
H	-2.374445	-2.970450	0.555735
H	-4.464922	-1.329187	-0.931129
H	-2.820769	-0.761369	-0.812836
C	-4.614223	0.490189	1.073657
C	-3.863827	1.662229	0.444888
C	-2.723128	2.190549	1.267239
C	-1.780166	3.044466	0.838378
C	-1.682298	3.615663	-0.543468
C	-0.262532	3.947253	-0.996166
C	0.638962	2.723765	-1.055697
C	1.999110	2.970417	-1.693385
C	2.890503	1.731395	-1.711242
C	3.427602	1.322728	-0.344386
C	4.251896	0.044095	-0.379663
C	4.864548	-0.327263	0.963696
C	5.562986	-1.678493	0.949426
H	6.000310	-1.920526	1.921553
H	4.868672	-2.485091	0.684555
H	6.370074	-1.696927	0.211268
H	4.082197	-0.319625	1.735065
H	5.575390	0.452169	1.261662
H	3.623362	-0.784443	-0.738049
H	5.050801	0.144335	-1.125009
H	2.601187	1.192507	0.369013
H	4.039856	2.139522	0.059184
H	2.332182	0.894084	-2.154867
H	3.741266	1.907658	-2.378824
H	2.512383	3.784855	-1.165843
H	1.846146	3.321729	-2.719938
H	0.785019	2.345876	-0.036355
H	0.127025	1.930104	-1.620053
H	0.175942	4.696838	-0.325429
H	-0.311134	4.414942	-1.985264
H	-2.287514	4.532598	-0.562953
H	-2.151801	2.939012	-1.266540
H	-1.077398	3.446638	1.571564
H	-2.746628	1.944192	2.331144
H	-4.572566	2.489142	0.303755
H	-3.525605	1.406173	-0.565666
H	-4.892144	0.757294	2.100150
H	-5.557987	0.353866	0.534424
H	-4.472550	-1.571218	1.631764
H	-2.930515	-0.748141	1.650760

conf_6

C	-2.547007	2.026769	-0.449114
C	-4.041313	1.983441	-0.739623
C	-4.737575	0.688374	-0.332347

C	-4.259748	-0.562420	-1.085128
C	-2.964554	-1.176558	-0.611856
O	-1.967470	-1.287025	-1.304173
N	-2.951948	-1.633859	0.680499
H	-3.808340	-1.617841	1.210761
C	-1.884891	-2.490524	1.136748
C	-0.646637	-1.768880	1.602260
C	0.293392	-2.393108	2.421027
C	1.456300	-1.734288	2.805846
C	1.662937	-0.441941	2.376570
N	0.740250	0.140413	1.599958
C	-0.380126	-0.472566	1.201026
H	-1.040700	0.097603	0.563379
H	0.869719	1.129010	1.315696
H	2.531617	0.152087	2.629324
H	2.192312	-2.214866	3.437543
H	0.115887	-3.407723	2.764498
H	-1.583395	-3.156253	0.318535
H	-2.259370	-3.118032	1.948310
H	-5.028082	-1.341414	-1.013693
H	-4.127343	-0.340353	-2.146110
H	-5.809204	0.798998	-0.521577
H	-4.640129	0.543878	0.751735
H	-4.530863	2.815953	-0.220767
H	-4.204405	2.155701	-1.810709
C	-1.918925	3.385131	-0.734087
C	-0.402974	3.406666	-0.558313
C	0.041735	3.173495	0.859345
C	1.294695	3.270731	1.326184
C	2.518947	3.629076	0.544225
C	3.461477	2.444582	0.300323
C	2.986595	1.501183	-0.797205
C	3.902526	0.299217	-0.990596
C	3.594881	-0.516595	-2.243440
C	2.266658	-1.268652	-2.236518
C	2.206301	-2.417227	-1.236404
C	0.968772	-3.288441	-1.408199
C	0.951800	-4.494442	-0.480897
H	0.044463	-5.092999	-0.606805
H	1.804333	-5.153065	-0.672545
H	1.016648	-4.195392	0.572014
H	0.925445	-3.638022	-2.446522
H	0.069880	-2.675954	-1.270905
H	3.105434	-3.037867	-1.350868
H	2.242171	-2.032253	-0.206544
H	2.100169	-1.679170	-3.239189
H	1.428842	-0.580263	-2.062779
H	3.621940	0.157352	-3.108274
H	4.402615	-1.240897	-2.402203
H	3.869011	-0.343651	-0.099818
H	4.936200	0.659544	-1.054069
H	1.958568	1.166886	-0.603602

H	2.932161	2.063865	-1.738237
H	3.615622	1.894172	1.240607
H	4.449803	2.828448	0.026221
H	3.056623	4.403173	1.102732
H	2.243750	4.070647	-0.418627
H	1.445427	3.132262	2.399088
H	-0.746263	2.964803	1.584684
H	-0.010728	4.371290	-0.900283
H	0.048958	2.657474	-1.222813
H	-2.374574	4.146150	-0.088443
H	-2.155891	3.676894	-1.762832
H	-2.394197	1.763062	0.607961
H	-2.032052	1.268937	-1.053653

conf_13

C	-3.449827	-0.261821	0.194672
C	-4.358075	-1.486871	0.167825
C	-3.674638	-2.839426	-0.020417
C	-2.998641	-3.068741	-1.386739
C	-1.617572	-2.473176	-1.480653
O	-1.360484	-1.424621	-2.051722
N	-0.639275	-3.170480	-0.831342
H	-0.879535	-4.012290	-0.332926
C	0.692498	-2.623879	-0.689880
C	0.743949	-1.618487	0.435862
C	1.339740	-1.881453	1.666197
C	1.268560	-0.956315	2.705188
C	0.584751	0.221148	2.502446
N	0.029901	0.457293	1.305107
C	0.102008	-0.397173	0.281671
H	-0.380976	-0.112358	-0.645559
H	-0.507371	1.334845	1.159846
H	0.462761	0.988349	3.256467
H	1.732048	-1.150085	3.664166
H	1.866941	-2.818323	1.818787
H	0.967826	-2.144324	-1.632271
H	1.397365	-3.435626	-0.504105
H	-2.929352	-4.145050	-1.577026
H	-3.597828	-2.632319	-2.188417
H	-4.433596	-3.617723	0.102416
H	-2.947741	-3.003156	0.786614
H	-4.927441	-1.526288	1.104555
H	-5.101933	-1.354974	-0.627999
C	-4.224274	1.017045	0.494511
C	-3.448485	2.306822	0.239480
C	-2.327964	2.592286	1.195358
C	-1.265022	3.377746	0.956678
C	-0.976943	4.115126	-0.315267
C	0.502171	4.199871	-0.687691
C	1.142144	2.834528	-0.893155
C	2.514512	2.871295	-1.551541
C	3.140568	1.488549	-1.714009

C	3.620717	0.857697	-0.411900
C	4.128477	-0.566303	-0.585973
C	4.703111	-1.171359	0.687429
C	5.049811	-2.645632	0.545726
H	5.467746	-3.056084	1.468715
H	4.166023	-3.240332	0.284326
H	5.786080	-2.803128	-0.247799
H	3.987969	-1.033815	1.509899
H	5.596870	-0.608804	0.981125
H	3.308992	-1.199428	-0.956611
H	4.892190	-0.589886	-1.373392
H	2.812835	0.856092	0.333839
H	4.416822	1.480097	0.016626
H	2.414676	0.821197	-2.200936
H	3.991351	1.553853	-2.401266
H	3.187062	3.514695	-0.969447
H	2.417900	3.343855	-2.535430
H	1.228946	2.337004	0.079712
H	0.474633	2.212634	-1.508561
H	1.052115	4.753666	0.083478
H	0.592874	4.788717	-1.606770
H	-1.373702	5.133139	-0.201216
H	-1.536321	3.670743	-1.144949
H	-0.590319	3.593346	1.789040
H	-2.463682	2.209648	2.209580
H	-4.149457	3.150083	0.308187
H	-3.084005	2.315857	-0.793731
H	-4.589213	1.000960	1.529516
H	-5.119473	1.035272	-0.137047
H	-2.666182	-0.412260	0.952064
H	-2.943864	-0.157377	-0.770981

conf_28

C	3.816687	0.074132	-1.477106
C	4.898808	-0.982926	-1.288496
C	4.596004	-2.091215	-0.283044
C	3.348290	-2.912932	-0.619988
C	2.130408	-2.527985	0.182092
O	2.181402	-2.156600	1.341117
N	0.917604	-2.640117	-0.449896
H	0.887541	-3.060773	-1.364961
C	-0.296723	-2.637901	0.331938
C	-0.496098	-1.372990	1.122490
C	-1.285640	-1.354615	2.268675
C	-1.440531	-0.187756	3.009226
C	-0.791374	0.954516	2.597130
N	-0.044657	0.913187	1.485299
C	0.111562	-0.188805	0.748884
H	0.750700	-0.108051	-0.120186
H	0.453386	1.771896	1.181671
H	-0.839051	1.902284	3.117419
H	-2.046406	-0.167472	3.906002

H -1.770136 -2.267839 2.600356
 H -0.309253 -3.477864 1.036745
 H -1.144825 -2.768224 -0.347360
 H 3.130870 -2.891787 -1.693966
 H 3.519102 -3.966494 -0.365340
 H 4.480295 -1.690314 0.728628
 H 5.460435 -2.758787 -0.245743
 H 5.108010 -1.441259 -2.262736
 H 5.828188 -0.485730 -0.987099
 C 3.517987 0.930930 -0.251589
 C 2.670035 2.145834 -0.624441
 C 2.117170 2.909358 0.545501
 C 1.106571 3.789507 0.482211
 C 0.395015 4.177649 -0.783344
 C -0.807142 3.297138 -1.145627
 C -2.000294 3.432761 -0.207107
 C -3.196852 2.573788 -0.611389
 C -2.949025 1.074720 -0.504455
 C -4.131414 0.210430 -0.916708
 C -3.826741 -1.277433 -0.812196
 C -4.977871 -2.185973 -1.218561
 C -4.629730 -3.662585 -1.105339
 H -4.359947 -3.928894 -0.077204
 H -5.468610 -4.298560 -1.397858
 H -3.783267 -3.920461 -1.751616
 H -5.273941 -1.953778 -2.248339
 H -5.851144 -1.962638 -0.594241
 H -2.952021 -1.505699 -1.440192
 H -3.533453 -1.512882 0.221988
 H -4.419920 0.451823 -1.947275
 H -5.000935 0.452270 -0.292597
 H -2.085051 0.793962 -1.121099
 H -2.683436 0.831966 0.533820
 H -3.484276 2.822275 -1.640945
 H -4.057447 2.837960 0.013943
 H -1.707081 3.186478 0.823573
 H -2.304742 4.485461 -0.181712
 H -0.479060 2.251280 -1.200971
 H -1.131729 3.557202 -2.159782
 H 1.107904 4.153917 -1.613438
 H 0.059593 5.216306 -0.695355
 H 0.819322 4.305017 1.397946
 H 2.617368 2.759820 1.503317
 H 1.853745 1.838301 -1.291683
 H 3.282845 2.825436 -1.232953
 H 4.457128 1.272698 0.200042
 H 3.021871 0.329817 0.520921
 H 4.126432 0.733847 -2.296762
 H 2.884543 -0.397070 -1.824245

conf_4

C -2.738511 -1.975461 -0.606455

C -2.083217 -2.729233 -1.760650
 C -1.051151 -3.761223 -1.296640
 C 0.393027 -3.236271 -1.219039
 C 0.546524 -1.999592 -0.375253
 O 0.421749 -0.866969 -0.824399
 N 0.801160 -2.189620 0.947727
 H 0.953128 -3.121302 1.297801
 C 0.953353 -1.058621 1.840212
 C -0.377488 -0.399482 2.116050
 C -1.215275 -0.784150 3.158472
 C -2.475999 -0.209556 3.308386
 C -2.893640 0.730445 2.393447
 N -2.063355 1.095730 1.405233
 C -0.840177 0.579312 1.250102
 H -0.257521 0.927672 0.410399
 H -2.401379 1.735320 0.663069
 H -3.867159 1.203471 2.412598
 H -3.134257 -0.499374 4.117444
 H -0.888510 -1.545879 3.860018
 H 1.636935 -0.333030 1.391278
 H 1.399200 -1.410595 2.771548
 H 1.050357 -4.030570 -0.850512
 H 0.733196 -2.963225 -2.220755
 H -1.034479 -4.609498 -1.986379
 H -1.350983 -4.171061 -0.324053
 H -2.866778 -3.230466 -2.338628
 H -1.600488 -2.023740 -2.445682
 C -3.574396 -0.772125 -1.029478
 C -2.753968 0.311586 -1.752079
 C -3.199465 1.706434 -1.433954
 C -2.421547 2.794265 -1.320141
 C -0.938078 2.871070 -1.512514
 C -0.249796 3.783114 -0.493691
 C 1.272767 3.789861 -0.595536
 C 1.928931 2.507076 -0.098197
 C 3.451944 2.547295 -0.135075
 C 4.110271 1.290899 0.427779
 C 3.939043 0.049768 -0.440489
 C 4.518197 -1.209963 0.190330
 C 4.387988 -2.436585 -0.700246
 H 4.792012 -3.331633 -0.219261
 H 3.340690 -2.633595 -0.953388
 H 4.926454 -2.296669 -1.642314
 H 4.020855 -1.395842 1.152955
 H 5.574651 -1.043280 0.432415
 H 2.879188 -0.117492 -0.668892
 H 4.425637 0.224209 -1.409104
 H 3.709791 1.097230 1.434808
 H 5.181046 1.476420 0.570039
 H 3.787687 2.704437 -1.168085
 H 3.794151 3.420884 0.432230
 H 1.574190 1.649200 -0.682769

H	1.615120	2.335496	0.943909
H	1.567892	3.974944	-1.636107
H	1.663812	4.633325	-0.015477
H	-0.534904	3.494554	0.529431
H	-0.633716	4.800732	-0.626072
H	-0.746205	3.276049	-2.515763
H	-0.491805	1.870893	-1.523788
H	-2.915909	3.745716	-1.121625
H	-4.275458	1.846689	-1.323877
H	-2.831253	0.166678	-2.836795
H	-1.689795	0.183252	-1.528481
H	-4.045518	-0.345102	-0.134862
H	-4.405483	-1.097911	-1.664595
H	-3.365849	-2.674151	-0.039630
H	-1.963187	-1.632950	0.089389

conf_55

C	4.161608	-0.410619	-0.672502
C	3.940573	1.062538	-1.014700
C	2.936384	1.285676	-2.148851
C	2.208638	2.632175	-2.057836
C	1.063204	2.544333	-1.081197
O	0.097758	1.823792	-1.272409
N	1.162907	3.257321	0.081600
H	1.917180	3.915234	0.192083
C	0.031772	3.346247	0.973223
C	-0.300189	2.068404	1.703116
C	-1.369111	2.005710	2.594963
C	-1.721722	0.804138	3.199933
C	-0.998949	-0.330714	2.905304
N	0.039683	-0.241217	2.062838
C	0.402136	0.901905	1.470087
H	1.251246	0.850517	0.807581
H	0.574332	-1.104134	1.851884
H	-1.212159	-1.311243	3.311035
H	-2.557419	0.744884	3.885317
H	-1.944856	2.900646	2.810162
H	-0.864407	3.629260	0.407049
H	0.224945	4.138930	1.700006
H	2.906953	3.434924	-1.798968
H	1.760115	2.881224	-3.023505
H	2.176325	0.496606	-2.164100
H	3.455869	1.222407	-3.108789
H	3.601895	1.578920	-0.104228
H	4.890435	1.536194	-1.281833
C	3.049023	-0.938939	0.222451
C	3.119844	-2.427838	0.560482
C	2.153414	-2.793823	1.648475
C	0.916213	-3.280346	1.477439
C	0.241911	-3.563474	0.171061
C	-1.269189	-3.344891	0.217177
C	-1.960337	-3.629687	-1.112784

C	-1.590160	-2.668608	-2.243547
C	-1.899137	-1.199077	-1.965548
C	-3.380259	-0.926532	-1.723950
C	-3.734863	0.550336	-1.592166
C	-3.188127	1.210811	-0.332544
C	-3.609830	2.668111	-0.214443
H	-3.252348	3.131826	0.712188
H	-3.221436	3.255805	-1.052320
H	-4.699343	2.769630	-0.220892
H	-2.095083	1.149147	-0.339367
H	-3.542995	0.649200	0.543612
H	-3.364970	1.094133	-2.471156
H	-4.826228	0.658821	-1.602660
H	-3.720962	-1.453745	-0.822726
H	-3.951337	-1.357631	-2.555537
H	-1.302966	-0.839709	-1.116983
H	-1.564024	-0.599401	-2.819876
H	-2.130518	-2.978240	-3.145792
H	-0.526636	-2.774115	-2.489359
H	-1.721987	-4.654391	-1.422301
H	-3.044033	-3.610557	-0.958694
H	-1.488411	-2.313963	0.527749
H	-1.695094	-3.994124	0.991853
H	0.429827	-4.611951	-0.100456
H	0.689569	-2.961640	-0.625457
H	0.353376	-3.557622	2.371487
H	2.514227	-2.668061	2.669506
H	4.133520	-2.673731	0.894596
H	2.935657	-3.019899	-0.340480
H	2.076946	-0.744002	-0.253487
H	3.074600	-0.365605	1.160877
H	4.222547	-1.004337	-1.592757
H	5.120373	-0.538288	-0.158909

C18:1 9Z picolylamide

conf_11

C	-4.464300	-0.158818	0.031402
C	-3.783973	-1.496010	0.301944
C	-3.816467	-2.463873	-0.877612
C	-3.049185	-1.974195	-2.112234
C	-1.631936	-1.568800	-1.797415
O	-1.199233	-0.439048	-1.980195
N	-0.846272	-2.539582	-1.252496
H	-1.237411	-3.452988	-1.088349
C	0.538393	-2.300002	-0.914732
C	0.718632	-1.597445	0.410307
C	0.240792	-0.303169	0.560272
N	0.411357	0.350874	1.710625
C	1.030172	-0.178851	2.776346
C	1.517521	-1.463504	2.692617

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H -3.972217  0.355308 -0.802051
H -5.491636 -0.351563 -0.299585
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C	-3.043892	-1.492049	-1.915815
C	-2.814097	-2.226641	-0.600214
C	-1.917274	-3.455668	-0.722158
C	-0.491718	-3.154341	-1.212806
C	0.140820	-2.068140	-0.388089
O	0.215595	-0.901790	-0.755105
N	0.571153	-2.429056	0.850315
H	0.543469	-3.396730	1.126936
C	1.088353	-1.438075	1.769702
C	-0.007360	-0.487797	2.189599
C	-0.205684	0.675693	1.463447
N	-1.244592	1.471470	1.733187
C	-2.130411	1.216198	2.708435
C	-1.965587	0.094094	3.488194
C	-0.904082	-0.767511	3.215440
H	-0.783585	-1.670770	3.806026
H	-2.667073	-0.112031	4.286482
H	-2.944127	1.920621	2.824526
H	-1.400811	2.269195	1.086967
H	0.437106	0.966081	0.646256
H	1.899840	-0.880004	1.294840
H	1.498327	-1.953642	2.639372
H	-0.499715	-2.804408	-2.245653
H	0.114500	-4.065286	-1.174764
H	-2.367878	-4.172836	-1.416243
H	-1.866961	-3.962706	0.248503
H	-3.781871	-2.545874	-0.194766
H	-2.388083	-1.538942	0.143052
C	-4.056301	-0.353940	-1.811633
C	-3.623247	0.834787	-0.956638
C	-2.413154	1.584930	-1.513614
C	-2.179733	2.907543	-0.847426
C	-1.008714	3.543318	-0.689803
C	0.342653	3.072744	-1.132386
C	1.465147	3.540318	-0.203710
C	2.841271	2.989755	-0.564497
C	3.019105	1.513165	-0.231721
C	4.409819	0.981034	-0.557815
C	4.622719	-0.474788	-0.154044
C	3.819065	-1.477466	-0.974821
C	3.995206	-2.910662	-0.494561
H	3.671851	-3.023202	0.546971
H	5.043857	-3.219489	-0.541234
H	3.418257	-3.614052	-1.102234
H	4.127221	-1.402135	-2.024798
H	2.756426	-1.211943	-0.959949
H	4.379286	-0.591946	0.913109
H	5.687292	-0.721639	-0.239547

H	5.153578	1.608537	-0.052701
H	4.598064	1.092611	-1.633365
H	2.840179	1.375958	0.846875
H	2.265593	0.913859	-0.757515
H	3.606616	3.565536	-0.032165
H	3.029708	3.151216	-1.633493
H	1.489931	4.635614	-0.219851
H	1.233654	3.269624	0.837692
H	0.535345	3.481892	-2.134113
H	0.352751	1.985078	-1.267416
H	-1.035007	4.539668	-0.246753
H	-3.079082	3.434766	-0.524636
H	-1.515437	0.958238	-1.479849
H	-2.594131	1.781014	-2.580747
H	-4.466153	1.532548	-0.883863
H	-3.419642	0.502894	0.070538
H	-4.283375	0.013259	-2.819494
H	-4.998772	-0.750637	-1.415467
H	-2.092314	-1.109443	-2.300449
H	-3.406946	-2.212065	-2.659134

conf_36

C	-4.315906	-0.713134	-0.789083
C	-3.609802	-1.844717	-0.050626
C	-3.215330	-3.019353	-0.941395
C	-2.201911	-2.663659	-2.037178
C	-0.981920	-1.970903	-1.487335
O	-0.674427	-0.821777	-1.773993
N	-0.242096	-2.692892	-0.600359
H	-0.533582	-3.626715	-0.361384
C	0.944491	-2.145229	0.018429
C	0.626042	-1.210742	1.162099
C	0.067703	0.030327	0.888429
N	-0.248317	0.863837	1.883472
C	-0.044261	0.576403	3.177211
C	0.521047	-0.633839	3.512549
C	0.855327	-1.528906	2.497840
H	1.302610	-2.484592	2.754165
H	0.697265	-0.872989	4.553624
H	-0.338795	1.328230	3.898229
H	-0.669940	1.772614	1.604616
H	-0.142406	0.350235	-0.125429
H	1.514486	-1.599087	-0.737040
H	1.567838	-2.966484	0.374786
H	-2.637631	-1.985270	-2.771219
H	-1.896168	-3.570187	-2.570603
H	-4.107788	-3.429682	-1.425401
H	-2.820049	-3.829221	-0.316057
H	-4.269346	-2.217111	0.742407
H	-2.715113	-1.462051	0.460300
C	-4.852832	0.375670	0.137489
C	-3.793929	1.212001	0.852306

C	-2.969057	2.088645	-0.089947
C	-2.095273	3.069946	0.631884
C	-0.891679	3.526421	0.252039
C	-0.122841	3.145432	-0.973153
C	1.363312	2.915922	-0.702453
C	2.129736	2.446319	-1.934004
C	3.521030	1.907768	-1.609059
C	3.486782	0.537667	-0.942658
C	4.850923	-0.004860	-0.545465
C	4.776351	-1.370183	0.126569
C	6.136023	-1.910125	0.543806
H	6.054503	-2.890607	1.020841
H	6.627830	-1.235074	1.250908
H	6.796623	-2.017413	-0.321632
H	4.293832	-2.080859	-0.558024
H	4.122874	-1.298203	1.008779
H	5.343914	0.705789	0.130551
H	5.491904	-0.072033	-1.433444
H	3.000898	-0.168328	-1.631045
H	2.855351	0.576929	-0.043177
H	4.108052	1.835355	-2.531161
H	4.053749	2.619960	-0.965283
H	2.205280	3.277396	-2.643675
H	1.553964	1.662177	-2.443839
H	1.814072	3.838630	-0.316903
H	1.478685	2.177697	0.100856
H	-0.225678	3.956953	-1.706819
H	-0.558032	2.262768	-1.455110
H	-0.429331	4.295317	0.872684
H	-2.534759	3.509801	1.528882
H	-2.386803	1.475914	-0.785925
H	-3.665403	2.662519	-0.718261
H	-4.295903	1.859327	1.581167
H	-3.131905	0.560144	1.438795
H	-5.493217	1.052679	-0.440103
H	-5.503826	-0.088734	0.887643
H	-3.646164	-0.273522	-1.536943
H	-5.157739	-1.135880	-1.350357

conf_4

C	-3.360613	-1.102716	-1.874564
C	-2.942550	-2.116055	-0.815401
C	-2.093560	-3.263700	-1.355181
C	-0.740967	-2.827049	-1.937799
C	0.030185	-1.980182	-0.961337
O	0.193036	-0.774170	-1.094145
N	0.500888	-2.623708	0.141835
H	0.354899	-3.615120	0.240500
C	1.155240	-1.891416	1.204528
C	0.178023	-0.999431	1.930693
C	-0.035553	0.289305	1.465875
N	-0.971872	1.060226	2.026261

C	-1.732331	0.662062	3.056933
C	-1.542475	-0.594504	3.585899
C	-0.589493	-1.431195	3.008156
H	-0.449690	-2.433763	3.401280
H	-2.141420	-0.919096	4.427204
H	-2.471840	1.365832	3.417192
H	-1.166052	1.970043	1.561792
H	0.503550	0.700580	0.623946
H	1.960459	-1.285018	0.785833
H	1.601698	-2.607790	1.895560
H	-0.875854	-2.225745	-2.837404
H	-0.153433	-3.708711	-2.214755
H	-2.645453	-3.793000	-2.139010
H	-1.929171	-3.996860	-0.556504
H	-3.842439	-2.539079	-0.352821
H	-2.397299	-1.611243	-0.005762
C	-4.321044	-0.035429	-1.354446
C	-3.729070	0.942612	-0.342261
C	-2.617109	1.817861	-0.918682
C	-2.225495	2.953962	-0.022395
C	-1.025744	3.551961	0.040787
C	0.181861	3.225660	-0.781976
C	1.504543	3.486832	-0.062405
C	2.722482	3.334472	-0.970786
C	3.037516	1.904651	-1.406544
C	3.642078	1.042484	-0.305418
C	3.952920	-0.376169	-0.760961
C	4.657419	-1.217486	0.296498
C	4.793579	-2.679809	-0.100532
H	3.811581	-3.139582	-0.263285
H	5.314298	-3.261456	0.664725
H	5.355795	-2.782940	-1.033463
H	4.118759	-1.141117	1.251904
H	5.648781	-0.792420	0.491337
H	4.578545	-0.338564	-1.661603
H	3.020505	-0.865723	-1.075832
H	2.968743	1.003155	0.564542
H	4.560974	1.518885	0.060707
H	2.140470	1.413804	-1.805358
H	3.747798	1.942097	-2.240281
H	3.600859	3.749908	-0.463323
H	2.564981	3.958576	-1.858559
H	1.485843	4.506895	0.338718
H	1.600641	2.829799	0.813715
H	0.151893	3.865827	-1.675968
H	0.130453	2.200690	-1.165604
H	-0.928266	4.417485	0.697536
H	-3.029151	3.376378	0.583537
H	-1.744819	1.212337	-1.187685
H	-2.976609	2.249793	-1.864244
H	-4.533858	1.591076	0.024403
H	-3.360356	0.395568	0.536027

H	-4.705697	0.541220	-2.203917
H	-5.191452	-0.528584	-0.905436
H	-2.474591	-0.627103	-2.309599
H	-3.850526	-1.639625	-2.695633

conf_76

C	-4.136551	-0.051090	-0.514319
C	-3.785430	-1.227985	0.389101
C	-3.912034	-2.593210	-0.280792
C	-3.017424	-2.768749	-1.516795
C	-1.585658	-2.369313	-1.265333
O	-1.045795	-1.419659	-1.814362
N	-0.911002	-3.111505	-0.340806
H	-1.371776	-3.891952	0.098492
C	0.491381	-2.883927	-0.077766
C	0.752858	-1.782368	0.922538
C	0.295132	-0.497824	0.662482
N	0.527530	0.488545	1.533218
C	1.206958	0.315834	2.676516
C	1.693050	-0.933962	2.986588
C	1.462084	-1.985692	2.102656
H	1.847158	-2.973775	2.335446
H	2.245625	-1.082224	3.905634
H	1.339158	1.190458	3.300588
H	0.178853	1.438472	1.306874
H	-0.245873	-0.256815	-0.245294
H	0.976618	-2.618174	-1.022406
H	0.940752	-3.812775	0.277489
H	-3.365761	-2.148803	-2.343218
H	-3.051086	-3.810296	-1.854058
H	-4.948604	-2.763690	-0.589726
H	-3.688894	-3.374632	0.455602
H	-4.430486	-1.209355	1.275692
H	-2.759488	-1.116904	0.765055
C	-3.991833	1.309743	0.161359
C	-2.562513	1.614266	0.593486
C	-2.346999	3.061812	1.038652
C	-0.940884	3.330009	1.496413
C	0.076994	3.712168	0.711062
C	0.007942	3.973823	-0.762359
C	1.253509	3.528973	-1.528217
C	1.547293	2.044253	-1.375912
C	2.666696	1.534283	-2.272859
C	3.038049	0.075012	-2.020791
C	3.755195	-0.166241	-0.696885
C	4.200139	-1.608810	-0.497718
C	4.958512	-1.826870	0.802830
H	4.356372	-1.534975	1.670873
H	5.871833	-1.225259	0.829022
H	5.250122	-2.872551	0.932645
H	4.830617	-1.909133	-1.342604
H	3.324958	-2.271521	-0.536670

H	3.116919	0.130149	0.147922
H	4.635115	0.488309	-0.643469
H	3.687284	-0.272547	-2.832464
H	2.130979	-0.544101	-2.077447
H	2.362251	1.656818	-3.318189
H	3.557186	2.162356	-2.139173
H	0.633830	1.470432	-1.591665
H	1.810082	1.848019	-0.328890
H	1.119243	3.771902	-2.587681
H	2.121502	4.108399	-1.189503
H	-0.128387	5.054296	-0.905321
H	-0.877611	3.495516	-1.193031
H	1.039045	3.921188	1.183051
H	-0.755601	3.250447	2.568854
H	-2.608974	3.731558	0.213735
H	-3.038942	3.294965	1.854521
H	-2.276069	0.941297	1.411781
H	-1.887827	1.401377	-0.248539
H	-4.324297	2.087719	-0.535515
H	-4.657922	1.372787	1.031099
H	-3.498850	-0.064117	-1.406245
H	-5.167182	-0.169665	-0.868884

conf_10

C	-2.693666	-1.466415	-2.240186
C	-2.652490	-2.242253	-0.928407
C	-1.731915	-3.459750	-0.952763
C	-0.250252	-3.131262	-1.196722
C	0.231893	-2.076458	-0.239460
O	0.391952	-0.904555	-0.554483
N	0.417032	-2.476176	1.048536
H	0.296984	-3.445869	1.291709
C	0.744168	-1.518814	2.083564
C	-0.404457	-0.567052	2.316203
C	-0.471726	0.605087	1.578952
N	-1.533044	1.409221	1.687604
C	-2.567359	1.154632	2.503395
C	-2.543283	0.022436	3.285523
C	-1.459082	-0.847157	3.179093
H	-1.442960	-1.756400	3.772553
H	-3.366923	-0.183821	3.957021
H	-3.381468	1.868124	2.494821
H	-1.577742	2.217234	1.034868
H	0.295101	0.893174	0.874152
H	1.637323	-0.956711	1.797597
H	0.973612	-2.065805	2.999139
H	-0.096665	-2.738614	-2.202491
H	0.353352	-4.039487	-1.098707
H	-2.057926	-4.151554	-1.736507
H	-1.832281	-4.005341	-0.007059
H	-3.665884	-2.582808	-0.683520
H	-2.352174	-1.576194	-0.107795

C	-3.738718	-0.352657	-2.260500
C	-3.470309	0.820787	-1.320804
C	-2.218130	1.619108	-1.682087
C	-2.096642	2.913183	-0.933547
C	-0.962769	3.554765	-0.609996
C	0.431799	3.113461	-0.926918
C	1.450231	3.469678	0.156235
C	2.872766	3.029690	-0.175733
C	3.039175	1.521425	-0.313533
C	4.487413	1.089998	-0.517374
C	4.642609	-0.369817	-0.933131
C	4.036880	-1.369484	0.044349
C	4.260106	-2.816284	-0.370544
H	5.326790	-3.050477	-0.436995
H	3.820459	-3.013947	-1.353904
H	3.813783	-3.516451	0.342574
H	2.960158	-1.181535	0.116459
H	4.458815	-1.199726	1.044503
H	5.707824	-0.594566	-1.063574
H	4.178867	-0.513681	-1.918403
H	5.055841	1.276794	0.403214
H	4.941855	1.725967	-1.286550
H	2.638791	1.036457	0.588300
H	2.437381	1.144089	-1.149095
H	3.548159	3.397325	0.605593
H	3.193611	3.516203	-1.105737
H	1.429863	4.553632	0.317596
H	1.151987	3.024573	1.117405
H	0.738479	3.608479	-1.859762
H	0.453515	2.042305	-1.152401
H	-1.053832	4.527399	-0.124869
H	-3.038811	3.410635	-0.696856
H	-1.318940	1.006060	-1.558484
H	-2.263664	1.859421	-2.754411
H	-4.336706	1.492465	-1.349378
H	-3.402721	0.462030	-0.284822
H	-3.821930	0.037907	-3.281622
H	-4.719077	-0.781551	-2.020891
H	-1.703187	-1.054198	-2.462064
H	-2.920639	-2.167499	-3.052374

conf_6

C	-2.974506	-1.373364	-2.040146
C	-2.969649	-2.023717	-0.661651
C	-2.196884	-3.338353	-0.597576
C	-0.701042	-3.210860	-0.928380
C	-0.055578	-2.138240	-0.095636
O	0.194426	-1.016560	-0.518593
N	0.179982	-2.451768	1.207279
H	-0.007084	-3.384232	1.537938
C	0.679152	-1.455127	2.130941
C	-0.344860	-0.364958	2.335531

C	-0.308741	0.753985	1.518812
N	-1.275912	1.672893	1.590436
C	-2.306820	1.588108	2.445498
C	-2.377221	0.518636	3.308826
C	-1.395653	-0.469030	3.240698
H	-1.459594	-1.332391	3.896204
H	-3.197245	0.449990	4.012152
H	-3.042569	2.380939	2.401607
H	-1.256796	2.427946	0.877379
H	0.466007	0.910831	0.783179
H	1.606195	-1.022531	1.744239
H	0.907288	-1.945805	3.078215
H	-0.553761	-2.932779	-1.972543
H	-0.201688	-4.171709	-0.766680
H	-2.636384	-4.058101	-1.296095
H	-2.311870	-3.775902	0.401075
H	-4.004403	-2.217176	-0.353902
H	-2.560022	-1.325295	0.080845
C	-3.865477	-0.136704	-2.130531
C	-3.402786	1.067230	-1.313209
C	-2.063534	1.642710	-1.773553
C	-1.754323	2.980622	-1.172643
C	-0.540820	3.494085	-0.919010
C	0.784606	2.843484	-1.171042
C	1.850853	3.250105	-0.152674
C	3.196678	2.563123	-0.358724
C	3.216541	1.089060	0.030313
C	4.575962	0.439711	-0.199369
C	4.678061	-0.999803	0.297508
C	3.705706	-1.983535	-0.351736
C	3.854056	-2.096396	-1.862614
H	4.879762	-2.358909	-2.140680
H	3.604416	-1.157643	-2.365713
H	3.193459	-2.867420	-2.268999
H	2.674405	-1.694665	-0.120800
H	3.857328	-2.969753	0.102584
H	4.528789	-1.011525	1.386056
H	5.702213	-1.355432	0.133555
H	5.344203	1.039465	0.303130
H	4.816990	0.483796	-1.268175
H	2.959398	1.002931	1.098504
H	2.447796	0.536499	-0.524404
H	3.959113	3.090154	0.225717
H	3.497425	2.666851	-1.409253
H	1.981550	4.336726	-0.207821
H	1.497544	3.051246	0.870557
H	1.130631	3.153336	-2.167320
H	0.680255	1.754395	-1.236021
H	-0.496779	4.518947	-0.548276
H	-2.616090	3.625798	-0.993666
H	-1.250832	0.930579	-1.594722
H	-2.104717	1.773262	-2.865022

H	-4.167054	1.850113	-1.388359
H	-3.351105	0.799964	-0.248980
H	-3.941375	0.170364	-3.180341
H	-4.882233	-0.406386	-1.820674
H	-1.951316	-1.116873	-2.335549
H	-3.328068	-2.109626	-2.772005

conf_22

C	-3.650826	-0.332741	-1.558958
C	-3.454916	-1.433413	-0.521332
C	-3.088979	-2.791586	-1.114282
C	-1.756359	-2.813911	-1.876735
C	-0.630473	-2.267627	-1.040176
O	-0.092742	-1.189928	-1.254832
N	-0.266173	-3.020139	0.035080
H	-0.728401	-3.897670	0.208984
C	0.703563	-2.525243	0.988545
C	0.144910	-1.355565	1.762532
C	0.286636	-0.075800	1.247197
N	-0.300581	0.960886	1.851781
C	-1.026764	0.842455	2.973950
C	-1.169980	-0.396744	3.554941
C	-0.589212	-1.501800	2.935278
H	-0.718590	-2.488154	3.370733
H	-1.740338	-0.498199	4.469381
H	-1.471912	1.749357	3.362715
H	-0.264567	1.883281	1.377937
H	0.832688	0.128796	0.338194
H	1.609538	-2.218009	0.462131
H	0.970062	-3.337335	1.666436
H	-1.806888	-2.196779	-2.774413
H	-1.525874	-3.837164	-2.191666
H	-3.877689	-3.114602	-1.801898
H	-3.066512	-3.539489	-0.312523
H	-4.382291	-1.549515	0.052724
H	-2.686965	-1.134362	0.205655
C	-4.264831	0.943209	-0.985567
C	-3.382192	1.723541	-0.014529
C	-2.165699	2.366828	-0.674318
C	-1.396401	3.268893	0.253070
C	-0.204842	3.831429	0.004468
C	0.571676	3.720455	-1.268355
C	2.074660	3.525144	-1.078597
C	2.420050	2.178930	-0.462027
C	3.913951	1.902797	-0.364211
C	4.250113	0.527995	0.206899
C	3.875282	-0.636851	-0.702439
C	4.289590	-1.992915	-0.145683
C	3.905968	-3.152350	-1.054160
H	4.197434	-4.115150	-0.626029
H	4.395099	-3.062614	-2.028560
H	2.826117	-3.179262	-1.241385

H	3.845760	-2.130945	0.850992
H	5.373450	-1.999268	0.018336
H	4.349986	-0.492830	-1.681817
H	2.794972	-0.644870	-0.903911
H	3.759545	0.407497	1.184789
H	5.326175	0.480245	0.409651
H	4.363556	1.998792	-1.360673
H	4.378806	2.679095	0.254695
H	1.935036	1.393694	-1.058167
H	1.993339	2.128385	0.551266
H	2.565274	3.609837	-2.054024
H	2.480670	4.335369	-0.460032
H	0.403354	4.652950	-1.824600
H	0.169134	2.918573	-1.896454
H	0.208780	4.506857	0.754771
H	-1.904794	3.551025	1.177949
H	-1.506209	1.598203	-1.096284
H	-2.509534	2.957393	-1.534435
H	-3.985929	2.513949	0.447117
H	-3.062916	1.070403	0.809538
H	-4.540877	1.609488	-1.811417
H	-5.203553	0.684325	-0.481527
H	-2.698534	-0.107528	-2.052273
H	-4.316727	-0.710342	-2.344343

conf_1

C	3.231948	1.671350	1.409051
C	3.995388	1.213498	0.171685
C	4.684954	-0.140515	0.309600
C	3.757810	-1.316753	0.587761
C	2.796842	-1.621570	-0.536802
O	2.856318	-1.127858	-1.650043
N	1.812399	-2.522280	-0.233927
H	1.770448	-2.922511	0.689551
C	0.974008	-3.077681	-1.265407
C	-0.271372	-2.274586	-1.544662
C	-0.231963	-0.890983	-1.489176
N	-1.329441	-0.173824	-1.750682
C	-2.505824	-0.723161	-2.082561
C	-2.604561	-2.094091	-2.168357
C	-1.480949	-2.868976	-1.896098
H	-1.550655	-3.951158	-1.952985
H	-3.550171	-2.548194	-2.435865
H	-3.326298	-0.042020	-2.266452
H	-1.252134	0.858671	-1.669406
H	0.671046	-0.340601	-1.258780
H	0.695058	-4.097671	-0.993196
H	1.558613	-3.127218	-2.191615
H	3.187316	-1.169002	1.512781
H	4.352384	-2.224718	0.749147
H	5.419206	-0.094869	1.121557
H	5.243466	-0.349172	-0.607230

H	4.761762	1.961711	-0.064127
H	3.332873	1.181224	-0.699329
C	2.712511	3.106037	1.306636
C	1.840876	3.387409	0.084625
C	0.575333	2.529527	0.031136
C	-0.135413	2.650959	-1.278481
C	-1.383128	3.093694	-1.495267
C	-2.364823	3.591122	-0.477316
C	-3.401057	2.540796	-0.056520
C	-2.842641	1.504598	0.909580
C	-3.811183	0.371359	1.218369
C	-3.305622	-0.608524	2.271805
C	-2.034479	-1.354918	1.884803
C	-1.617516	-2.392064	2.919125
C	-0.322650	-3.107270	2.565060
H	-0.413397	-3.625419	1.602477
H	-0.054263	-3.853318	3.316942
H	0.504661	-2.391229	2.496236
H	-2.422357	-3.126500	3.040188
H	-1.506828	-1.902651	3.893714
H	-1.208579	-0.645251	1.740668
H	-2.187470	-1.853008	0.915578
H	-4.094064	-1.339670	2.485410
H	-3.132571	-0.069315	3.211865
H	-4.763247	0.798607	1.553849
H	-4.043388	-0.178421	0.294217
H	-2.569434	2.008123	1.846279
H	-1.902912	1.097367	0.518370
H	-4.252926	3.044384	0.412385
H	-3.809127	2.048935	-0.951979
H	-2.883201	4.453072	-0.908708
H	-1.844940	3.956775	0.413739
H	-1.720925	3.141370	-2.531924
H	0.465158	2.394369	-2.154547
H	0.862923	1.479105	0.180673
H	-0.085230	2.780400	0.865946
H	1.551172	4.443323	0.076694
H	2.422989	3.229515	-0.830440
H	2.154679	3.353854	2.217786
H	3.568692	3.789704	1.280200
H	2.395425	0.989581	1.614576
H	3.886076	1.601878	2.286812

conf_40

C	1.597057	-0.659151	2.968228
C	2.129686	-1.695125	1.985004
C	1.289366	-2.967052	1.904412
C	-0.144914	-2.751713	1.394964
C	-0.145790	-2.008942	0.088297
O	-0.395229	-0.813778	-0.007177
N	0.227084	-2.721631	-1.009421
H	0.408705	-3.708698	-0.927922

C	0.395474	-2.067410	-2.289408
C	1.533654	-1.076525	-2.224327
C	1.258513	0.242909	-1.904096
N	2.253427	1.109256	-1.691221
C	3.549454	0.775927	-1.796709
C	3.885312	-0.509423	-2.156110
C	2.868912	-1.443167	-2.353611
H	3.126012	-2.469143	-2.599383
H	4.927840	-0.782331	-2.258412
H	4.271513	1.552930	-1.580768
H	1.988678	2.043864	-1.325336
H	0.253279	0.614184	-1.773297
H	-0.528215	-1.551308	-2.566916
H	0.594517	-2.829198	-3.044490
H	-0.725801	-2.154197	2.098552
H	-0.649363	-3.716889	1.283926
H	1.229379	-3.431416	2.894320
H	1.797113	-3.693990	1.259556
H	3.148678	-1.974190	2.279358
H	2.215832	-1.252069	0.983487
C	2.510642	0.553377	3.136502
C	2.628350	1.461045	1.913593
C	1.311674	2.137088	1.531382
C	1.461375	3.215271	0.501807
C	0.591934	3.516726	-0.476192
C	-0.714425	2.828472	-0.726945
C	-1.899995	3.557167	-0.080727
C	-3.233228	2.867159	-0.356061
C	-3.315493	1.445409	0.185829
C	-4.667872	0.782064	-0.046128
C	-4.704368	-0.682266	0.384509
C	-3.898870	-1.612053	-0.517571
C	-3.860334	-3.045716	-0.007899
H	-4.867304	-3.465907	0.075269
H	-3.405388	-3.096631	0.987515
H	-3.287512	-3.698388	-0.674727
H	-2.874900	-1.234713	-0.611997
H	-4.331794	-1.590701	-1.525994
H	-5.743773	-1.029973	0.411123
H	-4.332030	-0.764221	1.415133
H	-4.932605	0.852869	-1.110108
H	-5.439555	1.342333	0.494493
H	-2.531695	0.827996	-0.265102
H	-3.101630	1.455879	1.263839
H	-3.420000	2.856422	-1.438645
H	-4.037410	3.470034	0.081517
H	-1.727272	3.614267	1.000784
H	-1.932872	4.590155	-0.444096
H	-0.688804	1.808409	-0.333585
H	-0.902117	2.766183	-1.807960
H	0.806578	4.389482	-1.092753
H	2.336669	3.856873	0.614849

H	0.573085	1.393256	1.217317
H	0.896844	2.605026	2.436298
H	3.376889	2.234244	2.124483
H	3.018146	0.888696	1.061213
H	2.148764	1.156485	3.977544
H	3.511746	0.208187	3.421394
H	0.597174	-0.332377	2.662395
H	1.474151	-1.139009	3.946572

conf_39

C	2.555759	1.106309	-2.350909
C	3.066462	1.536160	-0.980354
C	2.667651	2.954207	-0.580074
C	1.150284	3.192396	-0.497515
C	0.490526	2.139937	0.347640
O	-0.039339	1.141132	-0.121849
N	0.573655	2.299797	1.696170
H	0.989481	3.132739	2.079698
C	0.064896	1.276979	2.585635
C	0.865847	0.003826	2.448682
C	0.448692	-0.967046	1.551881
N	1.197600	-2.049942	1.331116
C	2.366274	-2.273973	1.951529
C	2.819824	-1.360801	2.875837
C	2.067904	-0.211030	3.114493
H	2.431712	0.527609	3.822462
H	3.754771	-1.538771	3.391629
H	2.898130	-3.176809	1.679849
H	0.872724	-2.684870	0.575723
H	-0.462590	-0.879954	0.978257
H	-0.985509	1.076220	2.356048
H	0.120475	1.650142	3.609311
H	0.693377	3.135324	-1.486423
H	0.952596	4.191742	-0.097052
H	3.079823	3.669721	-1.299285
H	3.124450	3.196897	0.386494
H	4.161386	1.472965	-0.969958
H	2.716625	0.831422	-0.214045
C	3.087361	-0.252671	-2.801095
C	2.603725	-1.451939	-1.989006
C	1.105005	-1.723575	-2.116134
C	0.697386	-3.039376	-1.519604
C	-0.517514	-3.388723	-1.068860
C	-1.761218	-2.556643	-1.077197
C	-2.635836	-2.754440	0.161152
C	-4.039695	-2.165132	0.034044
C	-4.099500	-0.679893	-0.315515
C	-3.337577	0.214633	0.653774
C	-3.535770	1.709802	0.424806
C	-3.147402	2.184018	-0.972174
C	-3.076717	3.700348	-1.074861
H	-2.321010	4.106407	-0.392329

H	-4.033387	4.162957	-0.812411
H	-2.820310	4.025034	-2.086969
H	-3.868799	1.804426	-1.704164
H	-2.176510	1.750185	-1.238624
H	-2.938933	2.263333	1.163595
H	-4.580645	1.978747	0.626629
H	-2.263972	0.006339	0.564041
H	-3.627665	-0.039618	1.682630
H	-3.720847	-0.523239	-1.332022
H	-5.151470	-0.371413	-0.339794
H	-4.571446	-2.335067	0.977785
H	-4.588100	-2.730852	-0.728561
H	-2.726567	-3.828340	0.363207
H	-2.136560	-2.332673	1.044143
H	-2.344820	-2.856198	-1.960423
H	-1.524804	-1.498139	-1.231125
H	-0.648052	-4.416523	-0.727035
H	1.465485	-3.815529	-1.527416
H	0.522990	-0.898887	-1.690407
H	0.849118	-1.744519	-3.185373
H	3.149309	-2.340721	-2.328380
H	2.873146	-1.321127	-0.931956
H	2.810699	-0.413844	-3.849778
H	4.183519	-0.230071	-2.778697
H	1.460623	1.098092	-2.353463
H	2.859267	1.858583	-3.089065

conf_49

C	3.895030	0.789795	-1.208940
C	3.615975	1.488341	0.116889
C	3.176766	2.942737	-0.023339
C	1.864265	3.125869	-0.796509
C	0.751839	2.259508	-0.265866
O	0.207686	1.385718	-0.928762
N	0.400646	2.475979	1.031663
H	0.877036	3.195578	1.550859
C	-0.710160	1.791396	1.653377
C	-0.385638	0.403398	2.151684
C	0.058488	-0.557627	1.253519
N	0.280434	-1.809787	1.656998
C	0.106501	-2.218791	2.922921
C	-0.318123	-1.308903	3.864301
C	-0.570232	0.005529	3.471878
H	-0.923444	0.722955	4.206459
H	-0.459778	-1.625375	4.889885
H	0.308849	-3.260821	3.134604
H	0.553083	-2.475678	0.909369
H	0.218308	-0.333010	0.205516
H	-1.522709	1.710144	0.923647
H	-1.073572	2.400452	2.482627
H	1.986112	2.859474	-1.846724
H	1.552072	4.175274	-0.759897

H	3.954626	3.516570	-0.537774
H	3.090071	3.391278	0.973910
H	4.521789	1.455447	0.733771
H	2.852188	0.935568	0.681181
C	4.426599	-0.631950	-1.042900
C	3.428822	-1.640380	-0.478317
C	2.256995	-1.936180	-1.413268
C	1.414431	-3.089061	-0.956657
C	0.108924	-3.274542	-1.203218
C	-0.793833	-2.377594	-1.999327
C	-2.278409	-2.661620	-1.774716
C	-2.775060	-2.321876	-0.370880
C	-2.909681	-0.824778	-0.098925
C	-4.140209	-0.185211	-0.735411
C	-4.194381	1.327714	-0.541248
C	-3.219618	2.098797	-1.426003
C	-3.165510	3.583407	-1.096874
H	-4.150200	4.050616	-1.195400
H	-2.478437	4.116585	-1.759593
H	-2.831225	3.751392	-0.065863
H	-3.517699	1.966561	-2.473103
H	-2.212249	1.674279	-1.349879
H	-4.001085	1.561554	0.517230
H	-5.210681	1.687415	-0.737802
H	-5.035188	-0.648445	-0.304002
H	-4.168800	-0.408989	-1.808880
H	-2.965193	-0.657754	0.985809
H	-2.012147	-0.299721	-0.449575
H	-2.097951	-2.778256	0.365197
H	-3.747684	-2.798629	-0.204155
H	-2.863507	-2.109811	-2.516969
H	-2.462642	-3.722839	-1.977873
H	-0.562862	-2.536982	-3.061226
H	-0.563336	-1.319927	-1.821585
H	-0.334444	-4.214458	-0.870538
H	1.952670	-3.896346	-0.455820
H	1.642968	-1.043446	-1.578043
H	2.664198	-2.191639	-2.402676
H	3.959038	-2.579288	-0.279212
H	3.056810	-1.297545	0.497153
H	4.774883	-1.000036	-2.015125
H	5.310910	-0.606326	-0.395246
H	2.991735	0.779915	-1.829553
H	4.635759	1.377322	-1.764255

conf_42

C	-4.337176	0.418220	0.115949
C	-3.830943	-0.972540	0.480933
C	-4.113914	-2.034926	-0.577768
C	-3.434022	-1.775488	-1.930914
C	-1.958060	-1.531648	-1.764976
O	-1.437907	-0.431273	-1.890701

N	-1.214831	-2.611425	-1.395469
H	-1.661671	-3.506173	-1.278036
C	0.189627	-2.472182	-1.077869
C	0.390476	-1.755179	0.235771
C	0.377602	-0.369159	0.261696
N	0.488071	0.285917	1.419025
C	0.634664	-0.328837	2.601543
C	0.680540	-1.704319	2.638732
C	0.549748	-2.417535	1.448293
H	0.577593	-3.502747	1.470198
H	0.811761	-2.210980	3.586376
H	0.709567	0.304080	3.476476
H	0.414726	1.320604	1.361992
H	0.252570	0.226184	-0.631192
H	0.684853	-1.914514	-1.877498
H	0.638444	-3.465513	-1.034015
H	-3.846482	-0.889115	-2.413816
H	-3.602285	-2.625612	-2.600226
H	-5.193178	-2.104841	-0.749303
H	-3.806735	-3.015434	-0.194698
H	-4.300085	-1.287922	1.420779
H	-2.750855	-0.938721	0.681115
C	-4.198641	1.436214	1.245822
C	-2.766436	1.792943	1.636846
C	-1.983084	2.484254	0.522837
C	-0.671539	3.057429	0.975503
C	0.386819	3.324207	0.194161
C	0.451414	3.122069	-1.290922
C	1.846926	3.115715	-1.913593
C	2.728290	1.905012	-1.608214
C	3.400933	1.908873	-0.237395
C	4.418915	0.786962	-0.045824
C	3.807865	-0.604318	0.052793
C	4.832724	-1.721969	0.183796
C	4.192481	-3.096176	0.313657
H	3.564995	-3.322300	-0.556305
H	3.562813	-3.154577	1.209009
H	4.942988	-3.886635	0.389534
H	5.471727	-1.528734	1.053677
H	5.496050	-1.705839	-0.688680
H	3.183618	-0.802057	-0.829095
H	3.137660	-0.637416	0.924384
H	5.003700	0.979641	0.861316
H	5.135189	0.810195	-0.877007
H	3.907246	2.872869	-0.108355
H	2.653643	1.860413	0.566061
H	3.522394	1.862614	-2.363304
H	2.143148	0.987067	-1.755084
H	1.716271	3.179296	-2.998253
H	2.376772	4.031930	-1.623123
H	-0.111849	3.950799	-1.743361
H	-0.102712	2.223269	-1.591889

H	1.240002	3.824985	0.650332
H	-0.621795	3.372543	2.019637
H	-1.841690	1.810295	-0.330068
H	-2.594613	3.312643	0.135435
H	-2.800492	2.458420	2.507788
H	-2.234226	0.891393	1.969755
H	-4.716332	2.358763	0.957655
H	-4.724413	1.058777	2.130989
H	-3.821488	0.781641	-0.779825
H	-5.397511	0.343724	-0.153805

conf_87

C	-3.673429	-1.634824	-1.022607
C	-3.317074	-2.126613	0.377774
C	-2.676730	-3.511415	0.413880
C	-1.448896	-3.677967	-0.491364
C	-0.361176	-2.668092	-0.234992
O	-0.124913	-1.731888	-0.984227
N	0.357551	-2.823883	0.917522
H	0.179909	-3.632562	1.491582
C	1.588624	-2.096283	1.129329
C	1.428823	-0.709316	1.697099
C	0.379207	0.099260	1.292882
N	0.284258	1.356106	1.737760
C	1.166833	1.907048	2.581864
C	2.227722	1.150842	3.028331
C	2.358454	-0.159636	2.577058
H	3.199490	-0.758702	2.913160
H	2.945416	1.583736	3.713391
H	0.993952	2.937286	2.865433
H	-0.494249	1.931598	1.361784
H	-0.366521	-0.230039	0.582231
H	2.106650	-1.994553	0.167482
H	2.232975	-2.682875	1.786554
H	-1.729807	-3.559666	-1.538702
H	-1.042840	-4.688172	-0.371658
H	-3.413593	-4.258122	0.099469
H	-2.415311	-3.762714	1.448616
H	-4.221010	-2.156258	0.998157
H	-2.649046	-1.404142	0.868010
C	-4.635817	-0.445870	-1.035566
C	-4.231539	0.723568	-0.143178
C	-2.865184	1.324527	-0.467223
C	-2.449700	2.325652	0.568945
C	-1.771713	3.469669	0.395102
C	-1.216241	4.033203	-0.875657
C	0.298916	3.808357	-0.994769
C	0.652413	2.401930	-1.465105
C	2.096115	2.001956	-1.198262
C	2.442783	0.622042	-1.741946
C	3.776598	0.089405	-1.239517
C	4.152994	-1.261772	-1.833640

C	5.411001	-1.855589	-1.218821
H	6.267920	-1.187980	-1.351063
H	5.667680	-2.816155	-1.672550
H	5.288747	-2.019756	-0.141777
H	4.286820	-1.150890	-2.915918
H	3.312967	-1.960269	-1.715909
H	3.743506	0.007937	-0.141316
H	4.573884	0.813370	-1.452547
H	2.454743	0.659431	-2.838367
H	1.645990	-0.087374	-1.483250
H	2.774016	2.751862	-1.624689
H	2.284294	2.025734	-0.113824
H	0.441288	2.320906	-2.538224
H	-0.015690	1.668733	-0.994810
H	0.725043	4.541330	-1.687025
H	0.773000	4.012831	-0.023425
H	-1.427680	5.107142	-0.890607
H	-1.715594	3.600021	-1.747731
H	-1.606957	4.086490	1.281302
H	-2.794612	2.103611	1.581908
H	-2.126657	0.512338	-0.523536
H	-2.868619	1.774552	-1.465000
H	-4.992329	1.508767	-0.208608
H	-4.231955	0.396574	0.904576
H	-4.755256	-0.097526	-2.067985
H	-5.627060	-0.787098	-0.715151
H	-2.756046	-1.385250	-1.567695
H	-4.138706	-2.455099	-1.583157

conf_75

C	4.557511	1.286906	1.234395
C	5.111955	0.676231	-0.046773
C	5.733837	-0.707492	0.119741
C	4.816080	-1.771494	0.709857
C	3.599540	-2.082041	-0.128142
O	3.413770	-1.666026	-1.259658
N	2.671385	-2.893135	0.468870
H	2.863783	-3.263400	1.385914
C	1.595230	-3.474028	-0.300620
C	0.350057	-2.622716	-0.341771
C	0.448271	-1.275136	-0.654627
N	-0.647982	-0.509588	-0.690870
C	-1.882053	-0.981080	-0.455834
C	-2.044476	-2.314538	-0.154175
C	-0.921099	-3.134561	-0.092789
H	-1.037890	-4.185648	0.153559
H	-3.038945	-2.697215	0.038058
H	-2.697348	-0.272642	-0.514020
H	-0.510965	0.499197	-0.890091
H	1.395347	-0.805445	-0.894647
H	1.350754	-4.455473	0.109840
H	1.948982	-3.618769	-1.327480

H	4.486114	-1.498005	1.719197
H	5.371156	-2.711144	0.824604
H	6.614063	-0.637372	0.768508
H	6.090845	-1.054578	-0.854164
H	5.879028	1.345755	-0.454195
H	4.329711	0.615938	-0.809211
C	4.070123	2.725632	1.061106
C	3.045780	2.925994	-0.054009
C	1.781920	2.078293	0.117064
C	0.883622	2.172311	-1.075885
C	-0.303656	2.793062	-1.145988
C	-0.982840	3.533713	-0.032602
C	-2.107429	2.746366	0.647328
C	-3.250671	2.357910	-0.279822
C	-4.331954	1.539128	0.413806
C	-5.379025	0.984967	-0.545933
C	-6.372992	0.024370	0.099021
C	-5.771776	-1.321270	0.492112
C	-6.792996	-2.273908	1.096524
H	-6.345233	-3.235117	1.364069
H	-7.608855	-2.471258	0.394951
H	-7.233921	-1.850381	2.003752
H	-4.953595	-1.170278	1.208922
H	-5.329190	-1.779629	-0.405004
H	-7.201006	-0.155022	-0.596129
H	-6.818612	0.496006	0.984236
H	-4.879939	0.471702	-1.382762
H	-5.919034	1.823293	-1.000035
H	-3.861679	0.720812	0.977439
H	-4.825510	2.156318	1.174028
H	-2.862169	1.794808	-1.142591
H	-3.695032	3.261672	-0.714463
H	-1.682860	1.843134	1.110045
H	-2.503782	3.343114	1.476212
H	-1.399142	4.460658	-0.443823
H	-0.250370	3.833839	0.721144
H	-0.804478	2.805741	-2.113514
H	1.285496	1.746633	-1.997920
H	2.085798	1.032806	0.256026
H	1.258903	2.368915	1.033653
H	2.757792	3.981493	-0.100413
H	3.501048	2.696882	-1.024106
H	3.649543	3.079262	2.010218
H	4.931616	3.370213	0.852353
H	3.737549	0.668747	1.624393
H	5.330300	1.271989	2.012797

conf_77

C	4.755772	-1.473784	-1.012949
C	5.253222	-0.854182	0.287221
C	5.968228	0.484815	0.127815
C	5.164286	1.580231	-0.562664

C	3.906211	1.987519	0.165393
O	3.601148	1.610472	1.284856
N	3.085628	2.841072	-0.522305
H	3.374931	3.174557	-1.427919
C	1.979465	3.496346	0.137560
C	0.691827	2.711516	0.076520
C	0.681038	1.380254	0.466858
N	-0.448925	0.668338	0.404145
C	-1.619141	1.179715	-0.007126
C	-1.675191	2.501305	-0.388913
C	-0.512007	3.266018	-0.350501
H	-0.544540	4.306425	-0.659630
H	-2.616186	2.922321	-0.719802
H	-2.468323	0.509153	-0.017917
H	-0.388178	-0.334069	0.669378
H	1.568373	0.882672	0.842762
H	1.827575	4.480133	-0.310143
H	2.247808	3.644024	1.189317
H	4.897564	1.292421	-1.586671
H	5.782343	2.481645	-0.660424
H	6.888733	0.341642	-0.449075
H	6.271984	0.843264	1.115602
H	5.947266	-1.553449	0.768888
H	4.423381	-0.723121	0.987748
C	4.169418	-2.874557	-0.833692
C	3.057862	-2.975996	0.209193
C	1.862359	-2.063714	-0.079986
C	0.888312	-2.047898	1.055414
C	-0.346034	-2.573504	1.076093
C	-1.021898	-3.309388	-0.041090
C	-2.115533	-2.506628	-0.753377
C	-3.244324	-2.034656	0.153401
C	-4.341408	-1.286028	-0.593484
C	-5.375681	-0.647742	0.323179
C	-6.468373	0.102769	-0.424620
C	-7.497261	0.749231	0.493386
C	-8.583232	1.497291	-0.265079
H	-9.131156	0.826186	-0.933793
H	-8.158621	2.298965	-0.878290
H	-9.308279	1.949809	0.416055
H	-6.987608	1.435691	1.182019
H	-7.953461	-0.025072	1.122195
H	-6.976960	-0.586794	-1.110767
H	-6.013241	0.875642	-1.060707
H	-4.875546	0.040234	1.021760
H	-5.830116	-1.424187	0.951480
H	-3.896540	-0.512353	-1.239244
H	-4.839162	-1.975262	-1.286148
H	-2.846979	-1.398453	0.959356
H	-3.682497	-2.897400	0.670157
H	-1.657589	-1.643874	-1.259756
H	-2.535715	-3.124683	-1.554488

H	-1.471647	-4.217397	0.378134
H	-0.285426	-3.642848	-0.776480
H	-0.899374	-2.507330	2.012439
H	1.264952	-1.614224	1.984315
H	2.239322	-1.045363	-0.240762
H	1.381287	-2.363858	-1.016218
H	2.704928	-4.010909	0.267978
H	3.456343	-2.738572	1.202007
H	3.796845	-3.234646	-1.800265
H	4.972462	-3.561584	-0.543323
H	4.005645	-0.821471	-1.480310
H	5.581786	-1.531130	-1.732490

conf_38

C	-3.974698	0.565923	-1.274766
C	-4.227398	-0.725460	-0.502199
C	-3.763741	-2.002454	-1.200587
C	-2.243947	-2.077844	-1.455727
C	-1.501302	-1.600591	-0.240910
O	-1.089296	-0.453968	-0.132582
N	-1.371582	-2.483464	0.789540
H	-1.794719	-3.393703	0.701458
C	-1.025798	-2.023811	2.120613
C	0.290272	-1.287759	2.152953
C	0.285537	0.094698	2.053848
N	1.431947	0.769564	2.003253
C	2.640226	0.177857	2.051198
C	2.706766	-1.188703	2.167848
C	1.521270	-1.926169	2.205607
H	1.565948	-3.009426	2.260974
H	3.672476	-1.675513	2.210014
H	3.504909	0.824249	1.982831
H	1.345686	1.779470	1.835794
H	-0.616207	0.686646	1.970673
H	-0.975535	-2.895127	2.775920
H	-1.808662	-1.362496	2.510859
H	-1.952959	-1.423658	-2.278355
H	-1.957549	-3.100300	-1.721316
H	-4.272177	-2.112082	-2.163977
H	-4.069098	-2.864738	-0.596818
H	-5.300843	-0.813639	-0.300173
H	-3.749124	-0.662141	0.484332
C	-4.246388	1.818046	-0.438388
C	-3.155329	2.172439	0.574154
C	-1.874690	2.686787	-0.078046
C	-0.865743	3.246514	0.876941
C	0.444297	3.374778	0.620756
C	1.121834	2.924559	-0.643417
C	2.645912	2.983204	-0.569723
C	3.371056	2.380671	-1.776109
C	3.716044	0.897367	-1.653323
C	2.537010	-0.064701	-1.579969

C	2.966901	-1.523170	-1.507454
C	1.798965	-2.493705	-1.404840
C	2.232441	-3.942119	-1.240142
H	1.374615	-4.617293	-1.169933
H	2.837177	-4.075893	-0.335823
H	2.842011	-4.272962	-2.086066
H	1.169840	-2.393389	-2.298055
H	1.164036	-2.199038	-0.560759
H	3.632205	-1.662999	-0.642654
H	3.573923	-1.772139	-2.386926
H	1.889264	0.083109	-2.453990
H	1.907686	0.157798	-0.709486
H	4.340599	0.614723	-2.509035
H	4.353949	0.755266	-0.767957
H	4.305152	2.927906	-1.936256
H	2.769958	2.546045	-2.679232
H	2.938949	4.031689	-0.447617
H	3.004231	2.479680	0.341864
H	0.793183	3.562926	-1.474615
H	0.780277	1.917648	-0.908623
H	1.054525	3.931308	1.337027
H	-1.250582	3.662361	1.808733
H	-1.419524	1.903027	-0.689906
H	-2.143798	3.496335	-0.774092
H	-3.542562	2.941484	1.253050
H	-2.924855	1.300181	1.200480
H	-4.384257	2.677122	-1.105525
H	-5.199727	1.692678	0.088785
H	-2.944385	0.590227	-1.643314
H	-4.619206	0.575558	-2.161102

C18:1 9E picolylamide

conf_61

C	4.555727	0.924774	1.090886
C	4.046236	-0.430022	0.618488
C	4.748303	-0.925562	-0.639281
C	4.190828	-2.253478	-1.149345
C	2.721262	-2.122251	-1.457804
O	2.264586	-1.206152	-2.125708
N	1.901409	-3.066745	-0.918448
H	2.291411	-3.791301	-0.338419
C	0.469504	-3.000273	-1.110331
C	-0.175172	-2.018449	-0.159651
C	-0.912847	-2.417976	0.952238
C	-1.439249	-1.479514	1.835292
C	-1.213091	-0.142663	1.596518
N	-0.512000	0.219396	0.514214
C	-0.003499	-0.654697	-0.358770
H	0.560849	-0.262859	-1.198457
H	-0.334490	1.230538	0.342088

H	-1.572274	0.655544	2.233034
H	-2.019131	-1.780895	2.698308
H	-1.081222	-3.475331	1.133286
H	0.044759	-3.994441	-0.963181
H	0.273642	-2.696789	-2.141870
H	4.694086	-2.540348	-2.078595
H	4.366745	-3.055518	-0.424303
H	4.639025	-0.179500	-1.432719
H	5.821222	-1.038896	-0.454173
H	4.155526	-1.166285	1.426762
H	2.970339	-0.360119	0.411425
C	3.766358	1.517463	2.256762
C	2.284236	1.765365	1.974512
C	2.038440	2.684915	0.778475
C	0.612805	3.108951	0.593692
C	-0.008400	3.230848	-0.587472
C	-1.352267	3.858104	-0.805893
C	-2.117591	3.314243	-2.012057
C	-2.470240	1.832676	-1.945886
C	-3.401634	1.454411	-0.802214
C	-3.768052	-0.023172	-0.789977
C	-4.637558	-0.430187	0.390606
C	-4.931575	-1.922970	0.441335
C	-5.753537	-2.330229	1.654635
H	-5.952639	-3.404821	1.665130
H	-5.239023	-2.077185	2.588422
H	-6.718952	-1.815817	1.666561
H	-3.982651	-2.477976	0.432285
H	-5.454575	-2.217689	-0.476186
H	-4.150818	-0.124255	1.328747
H	-5.582619	0.126163	0.358224
H	-2.851102	-0.630630	-0.791919
H	-4.282452	-0.275062	-1.725615
H	-2.950721	1.725758	0.163130
H	-4.317068	2.055588	-0.869263
H	-1.547592	1.237055	-1.887369
H	-2.937849	1.540109	-2.892875
H	-1.522889	3.498674	-2.914290
H	-3.036720	3.897916	-2.132870
H	-1.951460	3.796360	0.109636
H	-1.184513	4.930560	-0.971946
H	0.543200	2.948786	-1.488384
H	0.085157	3.438847	1.493087
H	2.637897	3.594993	0.924963
H	2.407856	2.231612	-0.148300
H	1.828453	2.211821	2.866755
H	1.773881	0.805811	1.824079
H	3.852784	0.856842	3.127601
H	4.230078	2.466569	2.549793
H	4.551392	1.623624	0.245412
H	5.606003	0.831342	1.388769

conf_105

C	-4.376677	-2.113088	0.151910
C	-4.228279	-0.605097	0.339274
C	-4.358293	0.196332	-0.950975
C	-4.018381	1.674174	-0.759069
C	-2.543577	1.840743	-0.501331
O	-1.692735	1.446668	-1.287145
N	-2.186599	2.426800	0.674168
H	-2.902932	2.732492	1.312040
C	-0.801419	2.714126	0.973254
C	-0.041248	1.531467	1.526033
C	0.518410	1.525843	2.800475
C	1.222557	0.418102	3.267037
C	1.355404	-0.679400	2.447055
N	0.810597	-0.651485	1.222304
C	0.137963	0.397986	0.742835
H	-0.257139	0.335007	-0.266005
H	0.918043	-1.482632	0.608323
H	1.880535	-1.583707	2.725673
H	1.662225	0.405858	4.256191
H	0.408879	2.397134	3.439111
H	-0.759694	3.539267	1.686002
H	-0.313341	3.044504	0.052197
H	-4.239856	2.233043	-1.673563
H	-4.616893	2.111145	0.047525
H	-3.694260	-0.199693	-1.724992
H	-5.379149	0.109545	-1.336233
H	-4.988447	-0.259215	1.050342
H	-3.261444	-0.388145	0.814188
C	-3.275567	-2.772717	-0.676492
C	-1.882695	-2.627664	-0.076650
C	-0.808327	-3.346610	-0.889358
C	0.536049	-3.402525	-0.232685
C	1.704437	-3.121290	-0.824238
C	3.056445	-3.402772	-0.240602
C	4.198632	-2.475707	-0.656776
C	4.104722	-1.029411	-0.174627
C	3.238838	-0.113707	-1.031826
C	3.189455	1.315951	-0.512306
C	2.337518	2.247851	-1.361762
C	2.298863	3.677126	-0.837938
C	1.431946	4.597777	-1.684252
H	1.396884	5.610298	-1.273993
H	1.819060	4.668085	-2.704937
H	0.403246	4.227220	-1.759591
H	3.320421	4.072659	-0.792810
H	1.942954	3.674460	0.202835
H	2.722011	2.252352	-2.389467
H	1.311967	1.858150	-1.439384
H	4.211868	1.710484	-0.455805
H	2.821060	1.321423	0.524916
H	3.635083	-0.110739	-2.054889

H	2.219362	-0.511253	-1.124383
H	5.113514	-0.602510	-0.142713
H	3.755116	-1.011634	0.868664
H	4.292778	-2.487932	-1.749887
H	5.124953	-2.916154	-0.275404
H	2.989948	-3.456231	0.854616
H	3.327311	-4.418308	-0.560681
H	1.686829	-2.767095	-1.856393
H	0.555078	-3.814012	0.781499
H	-1.137926	-4.382021	-1.053760
H	-0.719560	-2.895104	-1.883841
H	-1.889046	-3.017529	0.951044
H	-1.630563	-1.563521	-0.004090
H	-3.506545	-3.839412	-0.778023
H	-3.272583	-2.370581	-1.696649
H	-5.345850	-2.320537	-0.316402
H	-4.410668	-2.590638	1.138683

conf_0

C	4.221514	0.724157	1.173314
C	3.779545	-0.734526	1.216653
C	4.584404	-1.658751	0.306691
C	4.497050	-1.312645	-1.187921
C	3.066106	-1.181522	-1.634216
O	2.526284	-0.106772	-1.856542
N	2.355690	-2.341361	-1.716586
H	2.807307	-3.219226	-1.518064
C	0.935529	-2.316680	-1.992686
C	0.167874	-1.767525	-0.813272
C	-0.326612	-2.571089	0.210651
C	-0.943277	-2.008177	1.325510
C	-1.041987	-0.637370	1.410276
N	-0.572183	0.113192	0.405392
C	0.005792	-0.396511	-0.684399
H	0.370439	0.305093	-1.422489
H	-0.613242	1.150365	0.455024
H	-1.482994	-0.112450	2.247454
H	-1.337559	-2.624726	2.123155
H	-0.228760	-3.650483	0.142862
H	0.606110	-3.331880	-2.218297
H	0.750077	-1.697816	-2.874468
H	4.979874	-0.357544	-1.397324
H	5.009885	-2.079872	-1.777141
H	5.639719	-1.633064	0.597878
H	4.254095	-2.692644	0.462871
H	3.867626	-1.103898	2.245650
H	2.713829	-0.811828	0.960040
C	3.539022	1.599283	2.222779
C	2.040365	1.815764	2.023456
C	1.701324	2.647552	0.786282
C	0.258493	3.051696	0.701108
C	-0.438994	3.223787	-0.429723

C	-1.816320	3.809244	-0.516622
C	-2.651866	3.297616	-1.690340
C	-2.882844	1.790992	-1.719567
C	-3.624168	1.231168	-0.513268
C	-3.868111	-0.268902	-0.609943
C	-4.514010	-0.869898	0.629705
C	-4.672368	-2.382264	0.558695
C	-5.266488	-2.981732	1.824129
H	-6.258398	-2.567705	2.027852
H	-5.372123	-4.066694	1.745441
H	-4.640150	-2.770145	2.697998
H	-3.692596	-2.837723	0.356166
H	-5.300991	-2.637787	-0.302561
H	-3.919323	-0.609805	1.518356
H	-5.495389	-0.407220	0.792595
H	-2.916808	-0.784444	-0.809557
H	-4.496521	-0.476184	-1.484882
H	-3.071103	1.452819	0.411204
H	-4.584064	1.750991	-0.402978
H	-1.917986	1.275147	-1.828573
H	-3.444352	1.539554	-2.626638
H	-2.163703	3.597711	-2.624931
H	-3.619065	3.811838	-1.677717
H	-2.341018	3.670693	0.435356
H	-1.705009	4.895323	-0.633655
H	0.060017	3.015193	-1.380116
H	-0.223236	3.316931	1.646542
H	2.299984	3.568554	0.830732
H	2.008733	2.137637	-0.134199
H	1.642958	2.329737	2.907068
H	1.528158	0.845513	1.985670
H	3.704472	1.157793	3.212803
H	4.029096	2.579790	2.244073
H	4.052852	1.136599	0.172517
H	5.304483	0.765212	1.341214

conf_3

C	4.495800	0.486759	0.120773
C	3.938884	-0.790985	0.739048
C	4.303690	-2.062624	-0.022227
C	3.773922	-2.112201	-1.463479
C	2.296395	-1.830767	-1.513449
O	1.825350	-0.776233	-1.916033
N	1.485858	-2.806027	-1.015317
H	1.888726	-3.663972	-0.675300
C	0.058850	-2.597765	-0.903038
C	-0.272348	-1.638851	0.216597
C	-0.612031	-2.058101	1.499283
C	-0.844650	-1.132594	2.514524
C	-0.716455	0.209453	2.235617
N	-0.398024	0.588271	0.990002
C	-0.192670	-0.272722	-0.008982

H	0.073805	0.140193	-0.972787
H	-0.275903	1.592653	0.755889
H	-0.858826	0.996599	2.964995
H	-1.115593	-1.449683	3.513489
H	-0.701920	-3.118826	1.712470
H	-0.422655	-3.560222	-0.724705
H	-0.320499	-2.201833	-1.849085
H	4.257829	-1.357659	-2.084472
H	3.987712	-3.091384	-1.904355
H	5.392963	-2.168781	-0.059098
H	3.935273	-2.932638	0.534319
H	4.314966	-0.884685	1.765077
H	2.845521	-0.721450	0.825319
C	4.293988	1.724057	0.992985
C	2.845838	2.176340	1.167877
C	2.207830	2.704061	-0.118601
C	0.871765	3.344215	0.099825
C	-0.203192	3.204324	-0.686595
C	-1.505277	3.918901	-0.498567
C	-2.705333	2.994836	-0.263989
C	-3.053724	2.096433	-1.446252
C	-4.193837	1.122577	-1.157990
C	-3.785075	-0.060485	-0.288384
C	-4.945254	-0.976555	0.079222
C	-4.532636	-2.203181	0.888811
C	-3.752798	-3.235178	0.084357
H	-4.357362	-3.623806	-0.740654
H	-2.845999	-2.807712	-0.355470
H	-3.458216	-4.088065	0.703562
H	-5.428014	-2.680728	1.299653
H	-3.941886	-1.878621	1.757022
H	-5.681497	-0.397454	0.648494
H	-5.457528	-1.301873	-0.835498
H	-3.320616	0.297834	0.641128
H	-3.013456	-0.630729	-0.823000
H	-5.021432	1.662302	-0.679975
H	-4.591151	0.738368	-2.104020
H	-2.173653	1.524369	-1.771358
H	-3.320671	2.735325	-2.295769
H	-3.577890	3.614790	-0.029726
H	-2.528619	2.390602	0.636312
H	-1.412861	4.620763	0.336674
H	-1.701150	4.524478	-1.393115
H	-0.114895	2.561792	-1.565399
H	0.802612	4.030277	0.947812
H	2.878692	3.467586	-0.537332
H	2.134086	1.918341	-0.879190
H	2.818720	2.972319	1.921711
H	2.245211	1.354162	1.579656
H	4.726833	1.533181	1.982258
H	4.866109	2.557684	0.569026
H	4.053789	0.647598	-0.868666

H 5.571717 0.353370 -0.044623

conf_42

C 4.631328 1.004608 -1.000992
C 3.950145 -0.268710 -1.500250
C 4.434096 -1.526716 -0.786129
C 3.517452 -2.721975 -1.021329
C 2.258751 -2.625728 -0.195288
O 2.256771 -2.321535 0.984231
N 1.076724 -2.897205 -0.834930
H 1.105662 -3.255979 -1.775736
C -0.114393 -3.128842 -0.055474
C -0.549107 -1.941869 0.763629
C -1.364756 -2.109814 1.880089
C -1.757506 -1.020053 2.647680
C -1.319467 0.235946 2.291841
N -0.539193 0.373045 1.212178
C -0.153625 -0.654268 0.450168
H 0.489034 -0.427011 -0.390431
H -0.230880 1.332760 0.963951
H -1.562406 1.142239 2.831318
H -2.388549 -1.143084 3.518532
H -1.685896 -3.107711 2.162275
H 0.029780 -3.970445 0.632399
H -0.923121 -3.401636 -0.740179
H 3.284002 -2.836584 -2.085780
H 4.011694 -3.646600 -0.700846
H 5.444306 -1.770999 -1.127908
H 4.498322 -1.360322 0.293510
H 2.861150 -0.172623 -1.380221
H 4.116114 -0.384668 -2.577295
C 4.063193 1.520201 0.320981
C 2.702226 2.183943 0.152083
C 2.057086 2.588121 1.467472
C 0.682883 3.180233 1.356290
C 0.050170 3.504956 0.221669
C -1.287414 4.171463 0.128966
C -2.155485 3.636326 -1.010520
C -2.389171 2.135873 -0.929786
C -3.313382 1.584707 -2.006320
C -3.388738 0.060689 -2.022507
C -3.991246 -0.557091 -0.766768
C -4.092403 -2.074961 -0.831658
C -4.748373 -2.686388 0.397069
H -4.213224 -2.414544 1.313704
H -5.776922 -2.331070 0.508706
H -4.782527 -3.777588 0.339055
H -3.086503 -2.495809 -0.969488
H -4.656222 -2.361429 -1.727083
H -3.401350 -0.277972 0.116988
H -4.991648 -0.135443 -0.602430
H -2.379248 -0.347783 -2.181721

H -3.979331 -0.258791 -2.888800
H -4.319579 2.001655 -1.873785
H -2.965980 1.935967 -2.985077
H -2.785734 1.888867 0.064385
H -1.420675 1.622641 -1.018129
H -1.682196 3.877045 -1.970729
H -3.115755 4.162922 -1.004617
H -1.815110 4.085047 1.086770
H -1.122703 5.244942 -0.030315
H 0.556076 3.330322 -0.728948
H 0.186780 3.409750 2.302550
H 2.022922 1.719156 2.141814
H 2.699387 3.310392 1.989186
H 2.028000 1.504641 -0.389215
H 2.811919 3.064415 -0.492397
H 3.983613 0.695528 1.040900
H 4.757868 2.243045 0.762562
H 4.544382 1.793994 -1.756637
H 5.704089 0.810257 -0.890917

conf_116

C 2.069502 3.475148 1.164922
C 2.632666 2.060266 1.291744
C 3.849813 1.828933 0.399422
C 4.116096 0.353827 0.135700
C 3.116687 -0.219638 -0.838701
O 2.691649 0.395368 -1.803201
N 2.694920 -1.496560 -0.601931
H 3.060627 -2.001448 0.189398
C 1.983729 -2.226423 -1.618936
C 0.511888 -1.918607 -1.725968
C -0.355310 -2.806769 -2.359550
C -1.700521 -2.498091 -2.526661
C -2.166730 -1.292032 -2.053460
N -1.318063 -0.458094 -1.438487
C -0.019142 -0.726021 -1.263364
H 0.572643 0.033508 -0.772525
H -1.698780 0.440648 -1.080210
H -3.192760 -0.960463 -2.142626
H -2.379666 -3.182841 -3.018178
H 0.026038 -3.752880 -2.732397
H 2.112984 -3.295662 -1.438480
H 2.430393 -1.999377 -2.595260
H 5.100137 0.220078 -0.329959
H 4.127188 -0.223903 1.067079
H 3.712158 2.320371 -0.568316
H 4.731706 2.283054 0.860565
H 2.902312 1.848719 2.332447
H 1.845855 1.333176 1.040960
C 1.208509 3.659684 -0.085399
C -0.183101 3.061488 0.081558
C -0.991121 3.025048 -1.206478

C	-2.342646	2.379749	-1.094614
C	-2.955934	2.041324	0.046829
C	-4.335035	1.470059	0.165047
C	-4.547096	0.485127	1.318341
C	-3.722381	-0.801696	1.273132
C	-2.290114	-0.664508	1.778262
C	-1.482843	-1.952973	1.715083
C	-0.062700	-1.783316	2.237003
C	0.803714	-3.025229	2.086807
C	2.184073	-2.859899	2.706386
H	2.826579	-3.723943	2.515023
H	2.688197	-1.961955	2.328761
H	2.114145	-2.740301	3.791194
H	0.891524	-3.273973	1.019788
H	0.298824	-3.882254	2.547564
H	0.423592	-0.942769	1.719785
H	-0.100858	-1.493707	3.294755
H	-1.454215	-2.325001	0.680321
H	-1.993162	-2.734364	2.291681
H	-1.757406	0.118130	1.223999
H	-2.317490	-0.308457	2.815982
H	-3.726165	-1.206706	0.250737
H	-4.224335	-1.562419	1.881678
H	-5.610024	0.225604	1.333013
H	-4.354133	1.000046	2.267931
H	-5.025778	2.310049	0.319418
H	-4.638067	1.015436	-0.787266
H	-2.452443	2.251596	0.989345
H	-2.879466	2.227866	-2.034626
H	-1.125155	4.044887	-1.591917
H	-0.409704	2.514938	-1.988847
H	-0.723675	3.633360	0.845061
H	-0.098994	2.041423	0.485626
H	1.111884	4.725267	-0.319434
H	1.706295	3.200342	-0.949099
H	2.902649	4.186598	1.152465
H	1.473323	3.724262	2.050474

conf_4

C	-4.861513	1.260825	-0.268931
C	-4.406398	0.006776	-1.013817
C	-4.823773	-1.286317	-0.320749
C	-4.082604	-2.505245	-0.860335
C	-2.670200	-2.567747	-0.334485
O	-2.391645	-2.424278	0.842570
N	-1.675923	-2.789962	-1.252150
H	-1.930533	-3.028353	-2.197138
C	-0.356165	-3.145203	-0.789808
C	0.280445	-2.087975	0.074266
C	1.212696	-2.429153	1.052097
C	1.794117	-1.455760	1.853928
C	1.431509	-0.140032	1.670393

N	0.541808	0.165736	0.717966
C	-0.030334	-0.748296	-0.071477
H	-0.751436	-0.389161	-0.794681
H	0.296375	1.168192	0.598872
H	1.820795	0.685691	2.251429
H	2.514852	-1.713884	2.619082
H	1.473290	-3.472353	1.201461
H	0.276843	-3.319856	-1.665136
H	-0.382421	-4.077018	-0.213019
H	-4.568597	-3.425405	-0.516299
H	-4.099394	-2.522897	-1.955731
H	-4.636355	-1.228860	0.755901
H	-5.900923	-1.432151	-0.445473
H	-4.809564	0.009942	-2.032878
H	-3.313152	0.026225	-1.130863
C	-3.981086	1.610779	0.930478
C	-2.642571	2.210249	0.517691
C	-1.708485	2.469361	1.688108
C	-0.356202	3.011618	1.329345
C	0.049800	3.385721	0.109033
C	1.358855	4.038726	-0.210518
C	1.925397	3.650353	-1.577016
C	2.224604	2.165749	-1.754633
C	3.309247	1.624885	-0.833068
C	3.616133	0.152000	-1.065593
C	4.661886	-0.414368	-0.116312
C	4.901527	-1.906546	-0.299363
C	5.905549	-2.477309	0.690451
H	6.877613	-1.984969	0.592981
H	5.571213	-2.335141	1.724112
H	6.061344	-3.547956	0.535631
H	5.244897	-2.092768	-1.324033
H	3.944362	-2.439073	-0.205299
H	5.607765	0.125235	-0.249964
H	4.358070	-0.220226	0.922724
H	3.950575	0.012205	-2.101246
H	2.690587	-0.435733	-0.976776
H	4.225013	2.213111	-0.972055
H	3.025571	1.776266	0.217823
H	2.524383	1.988698	-2.793949
H	1.299433	1.585490	-1.618350
H	2.840134	4.226389	-1.754343
H	1.215660	3.966029	-2.350778
H	1.194796	5.124385	-0.210163
H	2.081923	3.849471	0.590509
H	-0.644938	3.289231	-0.726716
H	0.331305	3.162113	2.165220
H	-2.179748	3.172924	2.387656
H	-1.587177	1.545931	2.274400
H	-2.822538	3.146415	-0.024395
H	-2.149262	1.542260	-0.202813
H	-4.505390	2.325524	1.574220

H	-3.810950	0.716539	1.543838
H	-5.896106	1.117740	0.062473
H	-4.880948	2.115072	-0.955626

conf_2

C	4.394260	0.986494	0.226087
C	4.224275	0.412830	-1.175774
C	4.657311	-1.044001	-1.326470
C	4.064045	-2.014792	-0.312050
C	2.557435	-2.094654	-0.326032
O	1.853917	-1.665054	-1.226777
N	1.998475	-2.704255	0.762690
H	2.600607	-3.065599	1.484823
C	0.591478	-3.035711	0.795534
C	-0.265035	-1.914567	1.331235
C	-1.092579	-2.050093	2.441985
C	-1.841878	-0.972448	2.908911
C	-1.739844	0.239457	2.263799
N	-0.939486	0.344324	1.193568
C	-0.229424	-0.676211	0.706050
H	0.365945	-0.502666	-0.184328
H	-0.846970	1.263174	0.721177
H	-2.269279	1.134405	2.563943
H	-2.490283	-1.068722	3.770450
H	-1.155001	-3.006390	2.952518
H	0.449283	-3.929664	1.405253
H	0.268441	-3.270036	-0.223046
H	4.435061	-3.027087	-0.516784
H	4.396857	-1.775747	0.704682
H	4.404173	-1.386681	-2.333707
H	5.747374	-1.110913	-1.238627
H	3.181446	0.502453	-1.495972
H	4.810055	1.014139	-1.881346
C	4.175444	2.497969	0.303777
C	2.857453	2.992523	-0.288967
C	1.621876	2.333397	0.327286
C	0.359715	2.775574	-0.343040
C	-0.660071	3.407217	0.251779
C	-1.880848	3.941697	-0.430049
C	-3.157325	3.159304	-0.097075
C	-3.274658	1.853450	-0.872782
C	-4.397074	0.950186	-0.378992
C	-4.532123	-0.359601	-1.148512
C	-3.351139	-1.307668	-0.980139
C	-3.534163	-2.638596	-1.696176
C	-2.352970	-3.578609	-1.510884
H	-1.428663	-3.127381	-1.889470
H	-2.207929	-3.820259	-0.451086
H	-2.499957	-4.521600	-2.042993
H	-3.689916	-2.452081	-2.765065
H	-4.450710	-3.120572	-1.335830
H	-2.431835	-0.835656	-1.352174

H	-3.194785	-1.496286	0.093327
H	-4.673372	-0.142312	-2.214841
H	-5.444219	-0.872469	-0.821961
H	-4.247322	0.726288	0.688177
H	-5.342634	1.501929	-0.433177
H	-2.318602	1.315410	-0.846835
H	-3.437573	2.084918	-1.932912
H	-4.032486	3.781970	-0.308814
H	-3.194186	2.964161	0.985275
H	-2.007302	4.986645	-0.126204
H	-1.728777	3.946675	-1.514797
H	-0.588163	3.603828	1.325702
H	0.309656	2.615434	-1.421991
H	1.738164	1.246775	0.221664
H	1.577050	2.547026	1.402590
H	2.848017	2.815271	-1.370633
H	2.784720	4.077274	-0.159389
H	4.246693	2.816712	1.350671
H	4.993932	3.002447	-0.222217
H	5.403397	0.764358	0.595124
H	3.709851	0.481896	0.922243

conf_6

C	-4.619798	1.478269	-0.901492
C	-4.041421	0.134613	-1.334421
C	-4.702798	-1.063472	-0.663372
C	-3.959503	-2.366640	-0.935192
C	-2.665676	-2.422639	-0.162551
O	-2.580433	-2.129219	1.016618
N	-1.547586	-2.807989	-0.854535
H	-1.648742	-3.167266	-1.789989
C	-0.340830	-3.110733	-0.125644
C	0.191067	-1.935013	0.651205
C	0.929131	-2.116953	1.818960
C	1.419606	-1.028638	2.529597
C	1.155111	0.242226	2.068422
N	0.445630	0.392686	0.943057
C	-0.027741	-0.635477	0.232368
H	-0.603212	-0.394285	-0.652632
H	0.249385	1.357559	0.611431
H	1.482510	1.148416	2.560518
H	1.989071	-1.162103	3.440413
H	1.107607	-3.122351	2.187246
H	0.420496	-3.438310	-0.839932
H	-0.505085	-3.933274	0.579847
H	-4.555595	-3.220102	-0.592520
H	-3.785105	-2.505103	-2.008040
H	-4.748298	-0.924856	0.420504
H	-5.734696	-1.153779	-1.016481
H	-4.137529	0.032181	-2.421956
H	-2.960865	0.119330	-1.129311
C	-4.311478	1.870896	0.544096

C	-2.823877	1.962571	0.881561
C	-2.062474	2.928461	-0.025980
C	-0.678540	3.274281	0.429290
C	0.391786	3.391394	-0.367967
C	1.711894	3.981386	0.027019
C	2.924565	3.400397	-0.694824
C	3.227078	1.949627	-0.352687
C	4.483715	1.424397	-1.035303
C	4.929804	0.046737	-0.559025
C	3.929446	-1.075494	-0.808200
C	4.491296	-2.449012	-0.463596
C	3.504339	-3.584194	-0.687221
H	3.954443	-4.557964	-0.478666
H	2.632637	-3.480123	-0.031834
H	3.147593	-3.599872	-1.722771
H	4.826739	-2.452149	0.581223
H	5.389933	-2.625263	-1.065812
H	3.015075	-0.902505	-0.222886
H	3.622989	-1.063268	-1.863668
H	5.162645	0.091285	0.513770
H	5.871820	-0.208444	-1.058100
H	4.322349	1.403572	-2.120958
H	5.299417	2.136906	-0.865547
H	2.372218	1.321184	-0.633027
H	3.345600	1.852894	0.737362
H	3.799751	4.013292	-0.453636
H	2.779496	3.497455	-1.778423
H	1.660527	5.054124	-0.203065
H	1.843454	3.921219	1.115074
H	0.273299	3.151053	-1.427791
H	-0.576426	3.561810	1.479454
H	-2.027295	2.557944	-1.056858
H	-2.632229	3.868284	-0.069092
H	-2.376458	0.961360	0.845025
H	-2.723123	2.294103	1.922045
H	-4.777221	2.842945	0.744595
H	-4.784021	1.165139	1.235108
H	-5.707519	1.457859	-1.035655
H	-4.256689	2.260040	-1.577815

conf_33

C	-4.703291	0.948029	-1.075130
C	-4.024660	-0.363385	-1.466993
C	-4.504930	-1.559099	-0.651388
C	-3.616446	-2.785586	-0.833224
C	-2.326320	-2.652768	-0.063054
O	-2.280976	-2.313454	1.106069
N	-1.167816	-2.924585	-0.743741
H	-1.230361	-3.308198	-1.672939
C	0.061437	-3.110911	-0.013122
C	0.517375	-1.893007	0.746436
C	1.435163	-2.010718	1.786888

C	1.854930	-0.893133	2.498378
C	1.345610	0.339809	2.159278
N	0.469698	0.429814	1.149589
C	0.050939	-0.625926	0.446399
H	-0.667688	-0.437233	-0.340227
H	0.117931	1.376792	0.909308
H	1.604249	1.264943	2.658135
H	2.563500	-0.978233	3.312157
H	1.819574	-2.990261	2.054256
H	0.842517	-3.394448	-0.725377
H	-0.037355	-3.931745	0.707317
H	-4.113396	-3.674490	-0.428274
H	-3.426747	-2.978883	-1.894897
H	-4.532269	-1.318864	0.415818
H	-5.529320	-1.807932	-0.944534
H	-4.198468	-0.566754	-2.529908
H	-2.934682	-0.259287	-1.364410
C	-4.163917	1.562476	0.216031
C	-2.777930	2.171364	0.044941
C	-2.196689	2.722238	1.336480
C	-0.815095	3.294800	1.234562
C	-0.081639	3.401268	0.118930
C	1.279265	4.020511	0.037387
C	2.394546	3.038150	-0.339680
C	2.186462	2.328581	-1.672866
C	3.297658	1.348191	-2.037115
C	3.361613	0.123388	-1.132141
C	4.371960	-0.920103	-1.590997
C	4.426013	-2.160869	-0.703264
C	5.016456	-1.909341	0.677935
H	4.449807	-1.157944	1.236477
H	5.038598	-2.824299	1.277206
H	6.045517	-1.546083	0.599194
H	5.016286	-2.934689	-1.204978
H	3.411535	-2.575226	-0.605978
H	4.126907	-1.219465	-2.617070
H	5.370150	-0.466422	-1.638795
H	2.366257	-0.344937	-1.100575
H	3.592831	0.431825	-0.105809
H	3.150846	1.015100	-3.071215
H	4.264949	1.865937	-2.021095
H	2.095254	3.085290	-2.461211
H	1.230399	1.785857	-1.669856
H	2.511032	2.301723	0.465099
H	3.342918	3.586314	-0.374509
H	1.248052	4.819171	-0.714737
H	1.521318	4.501095	0.991032
H	-0.510217	3.054145	-0.820716
H	-0.397134	3.689626	2.163003
H	-2.857631	3.504083	1.734071
H	-2.205569	1.940539	2.111063
H	-2.826139	2.969109	-0.706264

H	-2.096821	1.415350	-0.370609
H	-4.851649	2.342039	0.561869
H	-4.137921	0.806493	1.011086
H	-5.779877	0.770084	-0.974230
H	-4.593607	1.677165	-1.886378

conf_1

C	-4.858364	1.140494	0.013569
C	-4.286184	-0.003127	-0.819855
C	-4.702583	-1.385726	-0.330691
C	-3.942877	-2.508095	-1.030817
C	-2.522231	-2.593047	-0.532400
O	-2.229131	-2.555186	0.649352
N	-1.536113	-2.697414	-1.478272
H	-1.788532	-2.864209	-2.438968
C	-0.188522	-2.988825	-1.050524
C	0.349422	-1.940821	-0.110534
C	1.178036	-2.273979	0.959141
C	1.642829	-1.297577	1.830015
C	1.267894	0.012458	1.624969
N	0.484541	0.310829	0.581961
C	0.028260	-0.606526	-0.276169
H	-0.621372	-0.252230	-1.067065
H	0.194667	1.298516	0.440427
H	1.565008	0.834963	2.262075
H	2.277420	-1.549685	2.669813
H	1.440942	-3.313333	1.128002
H	0.449397	-3.045221	-1.937558
H	-0.137154	-3.958909	-0.543895
H	-4.403884	-3.475432	-0.800892
H	-3.973717	-2.386666	-2.119315
H	-4.530004	-1.485744	0.744744
H	-5.776442	-1.518897	-0.494166
H	-4.604451	0.114951	-1.862551
H	-3.188726	0.066824	-0.834964
C	-4.253473	1.281071	1.411821
C	-2.742435	1.508588	1.437250
C	-2.306294	2.739694	0.642909
C	-0.858232	3.100035	0.767684
C	-0.062463	3.424046	-0.260068
C	1.324626	3.987893	-0.169283
C	2.185115	3.711987	-1.402194
C	2.516006	2.243460	-1.645194
C	3.478627	1.642878	-0.629380
C	3.770283	0.169279	-0.873969
C	4.709592	-0.448847	0.151165
C	4.928919	-1.941624	-0.051402
C	5.823382	-2.564722	1.009336
H	6.811733	-2.095739	1.015332
H	5.398487	-2.441418	2.011621
H	5.967170	-3.634602	0.838536
H	5.360391	-2.110233	-1.045369

H	3.954591	-2.450863	-0.060533
H	5.676649	0.068403	0.120210
H	4.315114	-0.273411	1.162561
H	4.195702	0.046995	-1.878066
H	2.826303	-0.394808	-0.886120
H	4.418453	2.208435	-0.651595
H	3.088960	1.771606	0.389926
H	2.952420	2.138226	-2.644901
H	1.586327	1.655071	-1.672458
H	3.117315	4.281113	-1.318502
H	1.665013	4.114585	-2.279233
H	1.226515	5.076136	-0.062257
H	1.818983	3.651556	0.750000
H	-0.487935	3.372996	-1.265558
H	-0.466559	3.195833	1.784712
H	-2.555543	2.625926	-0.417730
H	-2.894351	3.597910	0.998597
H	-2.234780	0.610932	1.063689
H	-2.422117	1.620049	2.480333
H	-4.745620	2.119104	1.919097
H	-4.481854	0.392999	2.010458
H	-5.941068	1.000795	0.112678
H	-4.735394	2.081256	-0.534013

conf_48

C	-4.569426	-0.035454	-0.042289
C	-3.793944	-1.217604	-0.618379
C	-3.942857	-2.523251	0.157807
C	-3.292095	-2.508791	1.550664
C	-1.858848	-2.053230	1.478186
O	-1.486236	-0.944051	1.833122
N	-0.976224	-2.927875	0.917974
H	-1.291004	-3.835679	0.616641
C	0.388149	-2.521354	0.658546
C	0.438943	-1.508269	-0.460122
C	0.529571	-1.871367	-1.800745
C	0.481105	-0.909105	-2.806377
C	0.322248	0.412862	-2.455153
N	0.243277	0.737759	-1.157462
C	0.308826	-0.159512	-0.169775
H	0.215060	0.214834	0.840472
H	0.088052	1.724133	-0.873397
H	0.255607	1.225442	-3.167133
H	0.556937	-1.181519	-3.851280
H	0.637810	-2.918305	-2.067917
H	0.975123	-3.402413	0.395507
H	0.817224	-2.090256	1.566596
H	-3.805798	-1.817220	2.219191
H	-3.351829	-3.506521	1.997696
H	-5.003936	-2.765461	0.279062
H	-3.514133	-3.341363	-0.433099
H	-4.127266	-1.383441	-1.649445

H	-2.727438	-0.960700	-0.688444
C	-4.172386	1.290669	-0.690559
C	-2.882562	1.855189	-0.101641
C	-2.252259	2.945614	-0.953882
C	-0.970338	3.532791	-0.435999
C	-0.391983	3.250366	0.738778
C	0.816235	3.921145	1.312784
C	1.925301	2.935684	1.694972
C	2.738319	2.447883	0.499919
C	3.485903	1.147108	0.755318
C	4.208713	0.614265	-0.475391
C	4.957685	-0.695192	-0.247287
C	4.058666	-1.897660	0.017843
C	4.838290	-3.190374	0.208059
H	4.177427	-4.042580	0.392488
H	5.439944	-3.421673	-0.676135
H	5.521419	-3.114154	1.059083
H	3.362455	-2.006849	-0.825827
H	3.443271	-1.712608	0.907397
H	5.579080	-0.910553	-1.124515
H	5.654391	-0.573228	0.591976
H	4.913933	1.375836	-0.827955
H	3.483615	0.477357	-1.292689
H	4.208489	1.293069	1.568120
H	2.776022	0.395998	1.127611
H	3.446634	3.228921	0.198698
H	2.081223	2.317868	-0.370251
H	1.473600	2.079612	2.215716
H	2.595839	3.401086	2.423827
H	1.199445	4.677383	0.618591
H	0.493611	4.459396	2.212561
H	-0.863804	2.510244	1.388902
H	-0.516505	4.306346	-1.058064
H	-2.093640	2.568169	-1.976462
H	-2.965550	3.770687	-1.086115
H	-2.171794	1.034961	0.052611
H	-3.091419	2.243717	0.901596
H	-4.057626	1.141716	-1.773200
H	-4.975051	2.025720	-0.571310
H	-4.405996	0.038648	1.039220
H	-5.640453	-0.217895	-0.180543

conf_43

C	4.188944	1.349977	-0.280367
C	4.028545	0.162723	0.662361
C	4.726122	-1.110593	0.191162
C	4.245265	-1.628226	-1.175816
C	2.743067	-1.696831	-1.248802
O	2.057246	-0.852245	-1.806994
N	2.150269	-2.735765	-0.595800
H	2.714149	-3.441685	-0.151379
C	0.707892	-2.832406	-0.549995

C	0.118060	-1.805347	0.388121
C	-0.100176	-2.069470	1.736645
C	-0.580782	-1.079473	2.590106
C	-0.825751	0.173614	2.078461
N	-0.614096	0.404850	0.774392
C	-0.164828	-0.526516	-0.072131
H	0.007276	-0.230407	-1.098420
H	-0.752761	1.368394	0.424970
H	-1.183310	1.008594	2.666815
H	-0.759526	-1.275920	3.639459
H	0.108461	-3.059743	2.130073
H	0.432582	-3.835430	-0.220508
H	0.305898	-2.684795	-1.555903
H	4.565025	-0.961877	-1.977628
H	4.682000	-2.612898	-1.371436
H	5.806073	-0.942583	0.123523
H	4.587946	-1.893344	0.946212
H	4.415177	0.427342	1.654082
H	2.961188	-0.053676	0.803731
C	3.453310	2.608052	0.173823
C	1.950986	2.394317	0.330835
C	1.147138	3.693880	0.380972
C	-0.302142	3.491168	0.705403
C	-1.313408	3.635445	-0.158677
C	-2.776887	3.567433	0.160727
C	-3.637959	3.094226	-1.011413
C	-3.354451	1.674064	-1.488009
C	-3.764596	0.584753	-0.506056
C	-3.465962	-0.818659	-1.017485
C	-3.590849	-1.899332	0.045751
C	-3.202546	-3.285984	-0.448633
C	-3.208080	-4.335929	0.651727
H	-2.510615	-4.072930	1.456090
H	-4.199841	-4.428704	1.104016
H	-2.926050	-5.321745	0.272887
H	-2.207046	-3.236946	-0.911507
H	-3.883678	-3.588903	-1.252095
H	-2.959397	-1.634588	0.906331
H	-4.617490	-1.922513	0.432150
H	-2.449513	-0.844789	-1.437020
H	-4.128505	-1.048479	-1.860611
H	-3.260417	0.733827	0.458384
H	-4.835447	0.676222	-0.286717
H	-2.283644	1.573225	-1.724284
H	-3.875188	1.506790	-2.437489
H	-3.488360	3.788170	-1.846497
H	-4.694201	3.180070	-0.733787
H	-2.949384	2.957329	1.056332
H	-3.102841	4.579988	0.432132
H	-1.065445	3.912775	-1.185586
H	-0.537834	3.269760	1.751162
H	1.586384	4.359092	1.134898

H	1.238010	4.210216	-0.580428
H	1.759791	1.811198	1.241210
H	1.594683	1.789076	-0.514090
H	3.871424	2.976398	1.119095
H	3.626057	3.399073	-0.565075
H	3.815900	1.078225	-1.274006
H	5.255807	1.575231	-0.395538

conf_44

C	-4.893695	1.021197	0.743821
C	-4.499024	0.066102	-0.379419
C	-4.479885	-1.401054	0.032121
C	-4.035148	-2.351552	-1.091319
C	-2.569995	-2.183203	-1.388127
O	-2.119178	-1.258463	-2.049042
N	-1.734422	-3.095628	-0.812924
H	-2.118732	-3.853891	-0.273611
C	-0.301881	-3.005156	-0.991801
C	0.327097	-2.005655	-0.049888
C	1.115181	-2.379442	1.036080
C	1.629933	-1.423425	1.907146
C	1.338539	-0.096002	1.685673
N	0.589716	0.240975	0.627897
C	0.094553	-0.649681	-0.235499
H	-0.508590	-0.278219	-1.057563
H	0.342278	1.237774	0.472665
H	1.681994	0.712171	2.318191
H	2.247969	-1.704398	2.750326
H	1.331699	-3.429679	1.206929
H	-0.102367	-2.707817	-2.025068
H	0.137269	-3.991200	-0.832947
H	-4.255048	-3.387192	-0.814795
H	-4.583807	-2.126927	-2.009702
H	-3.829148	-1.549297	0.903393
H	-5.483817	-1.700557	0.352344
H	-5.205748	0.185737	-1.208600
H	-3.523415	0.345593	-0.790791
C	-3.953497	1.034999	1.950560
C	-2.483361	1.279233	1.617491
C	-2.232061	2.587545	0.865530
C	-0.794505	2.999958	0.777884
C	-0.147461	3.309379	-0.353641
C	1.213210	3.930509	-0.449628
C	1.998099	3.539633	-1.702235
C	2.381290	2.066985	-1.796860
C	3.378011	1.609539	-0.739969
C	3.757158	0.140197	-0.860749
C	4.706267	-0.338654	0.228209
C	5.003121	-1.830199	0.161185
C	5.910716	-2.310677	1.283220
H	6.874584	-1.793835	1.258237
H	5.465124	-2.120076	2.265967

H	6.109845	-3.382863	1.210412
H	5.458073	-2.063302	-0.808844
H	4.055703	-2.387441	0.185636
H	5.646722	0.223061	0.167289
H	4.284827	-0.097046	1.215355
H	4.210876	-0.036231	-1.843856
H	2.848136	-0.478511	-0.846983
H	4.283359	2.225126	-0.812320
H	2.982605	1.800982	0.267745
H	2.808650	1.876462	-2.787746
H	1.474186	1.446317	-1.752895
H	2.906229	4.150366	-1.751214
H	1.403647	3.812688	-2.581777
H	1.066496	5.018570	-0.472576
H	1.788634	3.735630	0.463110
H	-0.688339	3.198352	-1.296547
H	-0.278532	3.154172	1.730831
H	-2.657332	2.536934	-0.142005
H	-2.773841	3.390079	1.385575
H	-2.105757	0.437782	1.023376
H	-1.907357	1.280403	2.552281
H	-4.292712	1.810068	2.647678
H	-4.034788	0.089241	2.498277
H	-5.902672	0.775369	1.095006
H	-4.966520	2.032405	0.328031

conf_82

C	4.737704	1.210500	1.135356
C	4.399206	-0.226051	0.741927
C	4.769115	-0.582663	-0.693509
C	4.245450	-1.955732	-1.109641
C	2.739978	-1.936684	-1.178863
O	2.121473	-1.059379	-1.764986
N	2.074895	-2.934042	-0.535162
H	2.590124	-3.643192	-0.040127
C	0.627341	-2.956353	-0.523590
C	0.076822	-1.882505	0.385666
C	-0.221665	-2.113526	1.725837
C	-0.651762	-1.078187	2.551724
C	-0.752659	0.190895	2.027098
N	-0.465677	0.387442	0.733551
C	-0.079575	-0.589575	-0.091508
H	0.146051	-0.315967	-1.114083
H	-0.477627	1.351207	0.346904
H	-1.050575	1.060788	2.598302
H	-0.894242	-1.250695	3.592503
H	-0.118202	-3.114339	2.134400
H	0.293801	-3.938971	-0.187332
H	0.256295	-2.804066	-1.540226
H	4.606595	-2.208905	-2.112099
H	4.600086	-2.737196	-0.428732
H	4.358021	0.152919	-1.390596

H	5.857066	-0.560190	-0.811750
H	4.915728	-0.911218	1.425249
H	3.326112	-0.403695	0.898978
C	3.979618	2.292485	0.366567
C	2.465204	2.194176	0.500043
C	1.724166	3.334208	-0.201688
C	0.249047	3.322820	0.048251
C	-0.697166	3.141725	-0.881151
C	-2.174455	3.156333	-0.643535
C	-2.904332	2.011777	-1.351283
C	-4.381925	1.922418	-0.975411
C	-4.653968	1.336430	0.417798
C	-5.005218	-0.149982	0.421312
C	-3.909104	-1.087106	-0.069543
C	-4.328432	-2.551503	-0.055737
C	-3.224378	-3.499123	-0.500088
H	-2.372226	-3.456451	0.187534
H	-3.570304	-4.535359	-0.529465
H	-2.861094	-3.243216	-1.501463
H	-5.200747	-2.676502	-0.707542
H	-4.665133	-2.823952	0.952014
H	-3.609225	-0.816218	-1.090051
H	-3.015691	-0.960296	0.560622
H	-5.900328	-0.298954	-0.196160
H	-5.291903	-0.446028	1.438117
H	-3.786683	1.507977	1.072490
H	-5.481171	1.878677	0.885772
H	-4.909793	1.319442	-1.722964
H	-4.814055	2.926703	-1.048770
H	-2.414157	1.056351	-1.126943
H	-2.803059	2.153260	-2.433244
H	-2.380694	3.147921	0.434502
H	-2.583760	4.104680	-1.015866
H	-0.378810	2.991636	-1.914883
H	-0.065563	3.516175	1.078807
H	2.129518	4.291059	0.151634
H	1.917024	3.290929	-1.278904
H	2.197163	2.180491	1.566900
H	2.128789	1.241908	0.074027
H	4.308115	3.272824	0.730606
H	4.247856	2.263962	-0.696149
H	5.814100	1.372520	1.005572
H	4.542225	1.336538	2.207398

conf_23

C	4.285463	1.531028	0.623731
C	3.990906	0.041399	0.504811
C	4.693620	-0.610116	-0.679133
C	4.502452	-2.130162	-0.736523
C	3.048519	-2.522143	-0.699204
O	2.515626	-3.076766	0.246127
N	2.297831	-2.157997	-1.784037

H	2.742036	-1.819446	-2.621660
C	0.887441	-2.467867	-1.789975
C	0.182037	-1.734197	-0.674542
C	-0.309646	-2.393756	0.451584
C	-0.895334	-1.681094	1.490904
C	-0.967944	-0.308163	1.400466
N	-0.485299	0.304096	0.312788
C	0.077133	-0.358254	-0.706102
H	0.447459	0.249226	-1.523414
H	-0.531520	1.339743	0.251107
H	-1.394354	0.327413	2.165678
H	-1.278782	-2.182241	2.370341
H	-0.207381	-3.470985	0.517682
H	0.725909	-3.542672	-1.663685
H	0.470768	-2.176421	-2.756640
H	4.972769	-2.535840	-1.639101
H	4.972099	-2.607476	0.125281
H	4.341712	-0.149810	-1.611609
H	5.767899	-0.403455	-0.630521
H	4.291766	-0.465094	1.430710
H	2.908824	-0.124456	0.415955
C	3.595705	2.206766	1.807429
C	2.071537	2.268206	1.727631
C	1.557486	3.153591	0.592570
C	0.070846	3.347487	0.579685
C	-0.689480	3.445513	-0.518874
C	-2.134768	3.841726	-0.546469
C	-2.931410	3.251514	-1.709831
C	-3.005109	1.729197	-1.742249
C	-3.699217	1.100531	-0.541744
C	-3.798297	-0.415905	-0.634398
C	-4.414216	-1.067788	0.594837
C	-4.438132	-2.588384	0.526363
C	-5.003283	-3.234689	1.781899
H	-6.031754	-2.908986	1.963762
H	-5.011056	-4.324832	1.705406
H	-4.415684	-2.967241	2.667157
H	-3.418680	-2.957326	0.345780
H	-5.024561	-2.899639	-0.346347
H	-3.862039	-0.754182	1.493269
H	-5.435738	-0.692806	0.735119
H	-2.798627	-0.841014	-0.807154
H	-4.384513	-0.685405	-1.521752
H	-3.178848	1.375857	0.386710
H	-4.705725	1.526122	-0.443530
H	-1.991031	1.313913	-1.840546
H	-3.529741	1.421851	-2.654156
H	-2.493103	3.607552	-2.649696
H	-3.947165	3.660349	-1.678556
H	-2.605397	3.613065	0.416201
H	-2.170367	4.935523	-0.636393
H	-0.203975	3.331099	-1.492272

H	-0.401275	3.516654	1.551236
H	2.021565	4.143778	0.704772
H	1.890199	2.782660	-0.384116
H	1.686349	2.660964	2.676187
H	1.666056	1.252973	1.636982
H	3.880060	1.682642	2.727172
H	3.980173	3.228314	1.910451
H	4.017403	2.037089	-0.312994
H	5.367682	1.667342	0.729709

conf_7

C	-4.284135	1.532456	0.625395
C	-3.990139	0.042775	0.505584
C	-4.693781	-0.607657	-0.678392
C	-4.503744	-2.127828	-0.736869
C	-3.050057	-2.520699	-0.699789
O	-2.517357	-3.075642	0.245484
N	-2.299322	-2.157188	-1.784749
H	-2.743223	-1.817051	-2.621883
C	-0.889052	-2.467602	-1.790766
C	-0.183176	-1.734231	-0.675413
C	0.307625	-2.394047	0.450966
C	0.893671	-1.681738	1.490317
C	0.967498	-0.308885	1.399663
N	0.485689	0.303623	0.311761
C	-0.077066	-0.358397	-0.707182
H	-0.446590	0.249290	-1.524700
H	0.532814	1.339215	0.250083
H	1.394224	0.326457	2.164892
H	1.276457	-2.183048	2.369949
H	0.204390	-3.471174	0.517167
H	-0.472380	-2.176484	-2.757522
H	-0.728060	-3.542468	-1.664383
H	-4.973731	-2.605434	0.124582
H	-4.974363	-2.532392	-1.639773
H	-5.767898	-0.400273	-0.629216
H	-4.341959	-0.147062	-1.610760
H	-2.908161	-0.123392	0.416026
H	-4.290675	-0.464140	1.431345
C	-3.593440	2.207490	1.808923
C	-2.069289	2.268247	1.728275
C	-1.555400	3.153600	0.593127
C	-0.068670	3.346897	0.579643
C	0.691153	3.445504	-0.519207
C	2.136561	3.841176	-0.547201
C	2.932816	3.250332	-1.710508
C	3.005838	1.727970	-1.742590
C	3.699335	1.099257	-0.541755
C	3.798053	-0.417218	-0.634127
C	4.413327	-1.069024	0.595483
C	4.436816	-2.589649	0.527357
C	5.001266	-3.235850	1.783264

H	6.029731	-2.910350	1.965527
H	4.413335	-2.968112	2.668214
H	5.008828	-4.326010	1.706975
H	5.023513	-2.901264	-0.345042
H	3.417328	-2.958317	0.346447
H	5.434908	-0.694314	0.736048
H	3.860914	-0.755049	1.493644
H	4.384553	-0.687024	-1.521199
H	2.798350	-0.842120	-0.807202
H	4.705918	1.524592	-0.443204
H	3.178682	1.374865	0.386460
H	3.530573	1.420217	-2.654297
H	1.991601	1.313131	-1.841080
H	3.948755	3.658726	-1.679417
H	2.494594	3.606346	-2.650423
H	2.172504	4.934931	-0.637538
H	2.607253	3.612691	0.415474
H	0.205147	3.332021	-1.492467
H	0.404004	3.515101	1.551093
H	-1.888701	2.782959	-0.383466
H	-2.019020	4.143967	0.705668
H	-1.664347	1.252836	1.637220
H	-1.683402	2.660660	2.676689
H	-3.977421	3.229172	1.912482
H	-3.877502	1.683217	2.728667
H	-5.366248	1.669081	0.732064
H	-4.016477	2.038809	-0.311288

conf_56

C	3.690513	1.382930	1.732527
C	3.619582	-0.135705	1.621134
C	4.822235	-0.765251	0.922750
C	5.002202	-0.339035	-0.543250
C	3.736177	-0.554441	-1.326483
O	2.967827	0.347943	-1.629342
N	3.431844	-1.847665	-1.629332
H	4.067264	-2.585512	-1.372832
C	2.153795	-2.178772	-2.221729
C	1.039050	-1.905794	-1.240321
C	0.672057	-2.810608	-0.247751
C	-0.268669	-2.465177	0.718968
C	-0.816632	-1.202366	0.692930
N	-0.461125	-0.355061	-0.282972
C	0.424970	-0.664056	-1.234127
H	0.662222	0.109619	-1.950927
H	-0.805155	0.624562	-0.278037
H	-1.531447	-0.839220	1.418422
H	-0.566178	-3.160275	1.493635
H	1.132944	-3.793487	-0.218444
H	2.163524	-3.232228	-2.505099
H	2.004588	-1.586601	-3.128489
H	5.243592	0.721905	-0.616106

H	5.828518	-0.899261	-0.992821
H	5.738150	-0.506496	1.464365
H	4.738339	-1.857271	0.976001
H	3.543295	-0.564091	2.627990
H	2.699852	-0.430567	1.097473
C	2.558505	1.990931	2.558097
C	1.164158	1.870073	1.946323
C	1.009238	2.632804	0.630180
C	-0.405352	2.741224	0.146475
C	-0.783504	2.650858	-1.134962
C	-2.142286	2.920318	-1.709349
C	-3.290949	3.095613	-0.721676
C	-3.782427	1.811611	-0.054900
C	-4.414621	0.819033	-1.027796
C	-5.158696	-0.331966	-0.357595
C	-4.266551	-1.256094	0.458521
C	-4.988869	-2.459077	1.048043
C	-4.061103	-3.378728	1.828370
H	-3.582142	-2.846969	2.658899
H	-4.598813	-4.229096	2.254459
H	-3.273008	-3.781598	1.181431
H	-5.471574	-3.021652	0.240338
H	-5.797618	-2.110063	1.700427
H	-3.445950	-1.612454	-0.183131
H	-3.805426	-0.689154	1.279794
H	-5.668485	-0.922715	-1.127562
H	-5.948931	0.072788	0.287410
H	-5.115160	1.365399	-1.670706
H	-3.651952	0.405007	-1.701841
H	-4.527401	2.079575	0.704069
H	-2.961963	1.336175	0.499789
H	-4.134218	3.543570	-1.258601
H	-3.007189	3.827856	0.042329
H	-2.046346	3.832858	-2.313207
H	-2.386575	2.139349	-2.441083
H	-0.001831	2.454584	-1.873806
H	-1.152173	2.988278	0.902454
H	1.379090	3.655608	0.792582
H	1.644528	2.204482	-0.153349
H	0.433614	2.257165	2.667006
H	0.913284	0.810948	1.803840
H	2.552509	1.526346	3.551453
H	2.770776	3.053834	2.722933
H	3.704346	1.830654	0.732898
H	4.644530	1.653737	2.200626

conf_104

C	4.745204	0.434456	-0.272816
C	4.315193	-0.790457	0.526694
C	4.633268	-2.121478	-0.148950
C	3.939441	-2.325403	-1.504750

C	2.459564	-2.071444	-1.405253
O	1.916669	-1.070759	-1.852172
N	1.738559	-3.001008	-0.717543
H	2.200561	-3.812851	-0.341400
C	0.330852	-2.797252	-0.454875
C	0.115247	-1.734792	0.597748
C	-0.050148	-2.027051	1.949244
C	-0.178217	-1.007713	2.889864
C	-0.126006	0.301773	2.465749
N	0.026709	0.556524	1.159985
C	0.134281	-0.397367	0.232136
H	0.269539	-0.077651	-0.793022
H	0.073927	1.532420	0.809560
H	-0.202761	1.156159	3.125842
H	-0.312718	-1.226041	3.941586
H	-0.080592	-3.062053	2.276459
H	-0.104079	-3.742598	-0.127378
H	-0.166091	-2.500972	-1.382429
H	4.326717	-1.631068	-2.251072
H	4.125878	-3.341143	-1.868546
H	5.713638	-2.205073	-0.306750
H	4.363912	-2.940971	0.528026
H	4.813814	-0.772530	1.503413
H	3.238083	-0.741086	0.739142
C	4.584781	1.746759	0.491762
C	3.145132	2.165412	0.782513
C	2.348815	2.534213	-0.469612
C	1.022493	3.173067	-0.177465
C	-0.085048	3.060915	-0.922905
C	-1.340324	3.855336	-0.726421
C	-2.632604	3.081239	-0.984186
C	-2.772565	1.840608	-0.116859
C	-4.104675	1.118252	-0.240040
C	-4.146157	-0.159908	0.590169
C	-5.480913	-0.897050	0.557323
C	-5.865626	-1.443878	-0.812542
C	-7.155160	-2.250854	-0.779993
H	-7.414864	-2.633126	-1.770467
H	-7.069161	-3.107677	-0.104020
H	-7.993051	-1.639321	-0.430971
H	-5.046950	-2.070840	-1.191658
H	-5.973534	-0.619987	-1.527033
H	-5.446523	-1.728911	1.272066
H	-6.272771	-0.226375	0.916023
H	-3.901566	0.089689	1.631823
H	-3.352032	-0.838871	0.242545
H	-4.916589	1.785430	0.075830
H	-4.290682	0.888249	-1.295359
H	-2.604355	2.110790	0.937058
H	-1.979013	1.133192	-0.388325
H	-2.680755	2.791136	-2.041212
H	-3.482671	3.750560	-0.814175

H	-1.348234	4.283757	0.283302
H	-1.303070	4.709426	-1.415441
H	-0.055638	2.410725	-1.801711
H	1.002761	3.870363	0.664827
H	2.945289	3.259812	-1.040873
H	2.220969	1.669890	-1.131677
H	3.165251	3.035850	1.449436
H	2.633791	1.371442	1.342783
H	5.130561	1.672628	1.439960
H	5.069710	2.551390	-0.073408
H	4.190767	0.479501	-1.216623
H	5.801332	0.319888	-0.545078

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conf_0

C	-3.403402	-0.757467	-1.112273
C	-3.291759	-1.977115	-0.207159
C	-2.700502	-3.213804	-0.878866
C	-1.320315	-2.988681	-1.509945
C	-0.337632	-2.320505	-0.583609
O	0.208350	-1.254434	-0.834651
N	-0.092209	-2.954559	0.595568
H	-0.535982	-3.836170	0.794261
C	0.802712	-2.367548	1.567705
C	0.264061	-1.050437	2.073184
C	-0.737316	-0.960990	3.033517
C	-1.260829	0.277266	3.403367
C	-0.782835	1.412005	2.789779
N	0.189809	1.300839	1.871151
C	0.715151	0.129275	1.503217
H	1.475156	0.150347	0.735370
H	0.509957	2.149911	1.363587
H	-1.147075	2.410841	2.993166
H	-2.039244	0.358817	4.151160
H	-1.123960	-1.864627	3.495117
H	1.787290	-2.209239	1.118697
H	0.919923	-3.068411	2.395977
H	-0.901405	-3.945805	-1.840687
H	-1.390602	-2.348274	-2.389797
H	-3.374312	-3.563805	-1.667823
H	-2.653005	-4.032482	-0.150054
H	-2.682883	-1.711254	0.669217
H	-4.282565	-2.233803	0.185244
C	-4.058329	0.426801	-0.413453
C	-4.157905	1.684065	-1.275073
C	-2.825103	2.229604	-1.783779
C	-1.845596	2.596514	-0.677176
C	-0.522362	3.140311	-1.215622
C	0.369550	3.714248	-0.161195
C	1.665089	3.431539	0.043288

C	2.502882	2.452417	-0.726056
C	3.714874	1.954529	0.061919
C	4.474942	0.829689	-0.635137
C	3.764664	-0.516744	-0.566212
C	4.476788	-1.633830	-1.316433
C	3.762883	-2.971649	-1.188048
H	4.268378	-3.754247	-1.759116
H	3.729126	-3.302221	-0.143343
H	2.733082	-2.902240	-1.554303
H	5.505374	-1.724039	-0.947475
H	4.555572	-1.358976	-2.374815
H	2.743262	-0.437306	-0.962094
H	3.672458	-0.806227	0.492806
H	4.645559	1.102769	-1.684365
H	5.467937	0.729351	-0.183544
H	4.384374	2.803189	0.239833
H	3.403762	1.613534	1.061044
H	1.889997	1.613533	-1.076850
H	2.864090	2.941403	-1.641002
H	2.190638	4.003068	0.809644
H	-0.079783	4.491303	0.459708
H	-0.742180	3.945715	-1.930235
H	-0.007318	2.362520	-1.787521
H	-2.308736	3.340739	-0.014068
H	-1.646479	1.709782	-0.063898
H	-3.018634	3.118828	-2.394878
H	-2.351314	1.503686	-2.455508
H	-4.801848	1.473743	-2.136939
H	-4.669207	2.467058	-0.701748
H	-3.505024	0.648597	0.510109
H	-5.066440	0.141917	-0.089854
H	-2.404908	-0.471628	-1.460679
H	-3.981298	-1.015354	-2.009811

conf_58

C	-4.366424	-0.544236	-1.327846
C	-3.915813	-1.282384	-0.072202
C	-3.425507	-2.701726	-0.345678
C	-2.084424	-2.755658	-1.083911
C	-0.937290	-2.124519	-0.334502
O	-0.222432	-1.246905	-0.798727
N	-0.713429	-2.595167	0.924412
H	-1.267488	-3.358652	1.275989
C	0.448103	-2.165047	1.669005
C	0.349372	-0.722398	2.103622
C	-0.321405	-0.320871	3.254207
C	-0.398082	1.027120	3.600443
C	0.191250	1.960209	2.778420
N	0.832612	1.548585	1.673815
C	0.924165	0.264009	1.318665
H	1.439554	0.041391	0.395601
H	1.224215	2.254878	1.019380

H	0.169036	3.027371	2.958835
H	-0.912577	1.350150	4.496433
H	-0.790659	-1.064438	3.891371
H	1.346570	-2.291985	1.057703
H	0.547845	-2.805242	2.547344
H	-1.815033	-3.798017	-1.292227
H	-2.141324	-2.244978	-2.045956
H	-4.167477	-3.237813	-0.946992
H	-3.357493	-3.257559	0.597629
H	-3.120308	-0.718238	0.433327
H	-4.752463	-1.322172	0.635215
C	-4.816803	0.893494	-1.078568
C	-3.747753	1.804078	-0.476991
C	-2.456100	1.853194	-1.281131
C	-1.412187	2.778925	-0.675897
C	-0.075675	2.706994	-1.411999
C	1.018601	3.487943	-0.752550
C	2.314916	3.148699	-0.671657
C	2.958882	1.922058	-1.240265
C	4.070302	1.350185	-0.358000
C	4.622695	0.021628	-0.867853
C	3.681343	-1.157036	-0.649607
C	4.198284	-2.474862	-1.209798
C	3.256177	-3.637530	-0.933748
H	3.623707	-4.567110	-1.375064
H	3.147919	-3.810257	0.143422
H	2.260658	-3.443312	-1.347844
H	5.186736	-2.688556	-0.786168
H	4.346309	-2.369533	-2.290885
H	2.700164	-0.956544	-1.102165
H	3.513213	-1.273434	0.432590
H	4.855834	0.112634	-1.936388
H	5.574068	-0.190028	-0.367602
H	4.877366	2.087958	-0.291815
H	3.709125	1.216807	0.672657
H	2.205930	1.160601	-1.470113
H	3.397769	2.187282	-2.212086
H	2.993330	3.857818	-0.196125
H	0.725857	4.454097	-0.338956
H	-0.214640	3.099839	-2.428625
H	0.211711	1.657807	-1.543930
H	-1.777312	3.813367	-0.668916
H	-1.275580	2.502800	0.378520
H	-2.673273	2.167194	-2.310466
H	-2.021067	0.849227	-1.353917
H	-4.159415	2.816183	-0.384349
H	-3.518485	1.482729	0.548373
H	-5.693471	0.890187	-0.419777
H	-5.154502	1.321906	-2.029457
H	-3.563470	-0.546778	-2.073546
H	-5.195458	-1.099884	-1.781750

conf_7

C	-4.459590	1.714868	0.213796
C	-4.135735	0.226904	0.209009
C	-4.627030	-0.469056	-1.053544
C	-4.261105	-1.947408	-1.108828
C	-2.769789	-2.149618	-1.196694
O	-2.034449	-1.429401	-1.855980
N	-2.254609	-3.199126	-0.498094
H	-2.863985	-3.796062	0.036381
C	-0.838990	-3.488780	-0.562687
C	-0.038527	-2.463348	0.205423
C	0.242577	-2.598211	1.562385
C	0.917208	-1.596644	2.254815
C	1.292625	-0.459181	1.577237
N	1.019205	-0.354033	0.269397
C	0.385178	-1.303234	-0.425370
H	0.189097	-1.104350	-1.470968
H	1.274712	0.512233	-0.246655
H	1.808872	0.373490	2.035857
H	1.147726	-1.694837	3.307832
H	-0.069950	-3.494847	2.089213
H	-0.517597	-3.498378	-1.607759
H	-0.667219	-4.482925	-0.147274
H	-4.671229	-2.486235	-0.247174
H	-4.692321	-2.408299	-2.005505
H	-4.202512	0.025016	-1.933207
H	-5.714943	-0.373276	-1.130005
H	-3.050217	0.085649	0.295961
H	-4.582073	-0.248667	1.093454
C	-4.020761	2.455471	1.474536
C	-2.525683	2.392488	1.781376
C	-1.633912	2.877426	0.644791
C	-0.171319	2.983755	1.057180
C	0.791457	3.374357	-0.068891
C	0.866335	2.392762	-1.196772
C	1.977872	1.934276	-1.792504
C	3.399582	2.295554	-1.477357
C	4.406133	1.261454	-1.980711
C	4.261915	-0.126332	-1.363942
C	4.555862	-0.188646	0.128686
C	4.439897	-1.593218	0.706210
C	4.727112	-1.655251	2.198699
H	4.620462	-2.670624	2.589698
H	5.746717	-1.324499	2.416117
H	4.052110	-1.005189	2.767533
H	5.132289	-2.255086	0.173249
H	3.437193	-1.993642	0.499175
H	3.888217	0.490111	0.679418
H	5.567494	0.194658	0.312867
H	3.251095	-0.515286	-1.558095
H	4.938721	-0.814410	-1.883030
H	5.419617	1.633967	-1.796541

H	4.306729	1.180489	-3.069359
H	3.619798	3.257683	-1.958126
H	3.529719	2.475017	-0.404322
H	1.843289	1.282835	-2.658000
H	-0.087044	2.076139	-1.619448
H	1.788830	3.560934	0.340681
H	0.458432	4.334321	-0.487823
H	-0.081789	3.724568	1.859496
H	0.143018	2.031037	1.505136
H	-1.980204	3.859468	0.296891
H	-1.739832	2.200054	-0.210743
H	-2.328478	2.995304	2.676168
H	-2.240329	1.365036	2.046606
H	-4.573963	2.061558	2.335656
H	-4.316871	3.507063	1.381776
H	-4.006514	2.181005	-0.670146
H	-5.541511	1.843977	0.092681

conf_1

C	-3.587157	0.573747	-0.919768
C	-3.919945	-0.705237	-0.162191
C	-3.937857	-1.966592	-1.021543
C	-2.638354	-2.222144	-1.793533
C	-1.398307	-2.161826	-0.939752
O	-0.450561	-1.425878	-1.179578
N	-1.375895	-2.970537	0.154872
H	-2.158560	-3.572453	0.351871
C	-0.240126	-2.955607	1.049804
C	-0.102992	-1.618326	1.738263
C	-0.840171	-1.277537	2.867092
C	-0.736761	-0.006853	3.430594
C	0.098749	0.913412	2.841734
N	0.805974	0.559687	1.757241
C	0.731947	-0.651232	1.198627
H	1.321644	-0.818567	0.308409
H	1.390604	1.282925	1.291561
H	0.226434	1.929324	3.192919
H	-1.304398	0.267738	4.310436
H	-1.510145	-2.006931	3.312393
H	0.674339	-3.173903	0.492588
H	-0.376019	-3.744026	1.791955
H	-2.680170	-3.203632	-2.279446
H	-2.497596	-1.481913	-2.581972
H	-4.751305	-1.902868	-1.751799
H	-4.180693	-2.831141	-0.390809
H	-3.196440	-0.828911	0.656722
H	-4.899108	-0.598879	0.319007
C	-3.692423	1.810578	-0.037294
C	-3.332751	3.117132	-0.740525
C	-1.904913	3.196846	-1.277440
C	-0.837308	2.989631	-0.211804
C	0.579258	3.223282	-0.731568

C	1.626023	3.154744	0.336328
C	2.860243	2.640220	0.227135
C	3.484605	2.062561	-1.007721
C	4.679700	1.154785	-0.724871
C	4.329608	-0.195950	-0.108889
C	3.593366	-1.135843	-1.056571
C	3.414015	-2.542508	-0.499442
C	2.643804	-3.457274	-1.440910
H	3.177408	-3.575859	-2.388449
H	2.511200	-4.456628	-1.015925
H	1.656493	-3.045090	-1.674835
H	2.911319	-2.491553	0.478220
H	4.400395	-2.971275	-0.288063
H	4.153212	-1.199377	-1.998350
H	2.612805	-0.725014	-1.338785
H	5.255543	-0.683901	0.216189
H	3.743049	-0.048953	0.811728
H	5.222810	0.982629	-1.660373
H	5.375520	1.688185	-0.066611
H	2.737675	1.547234	-1.621631
H	3.826210	2.907124	-1.621262
H	3.523929	2.737744	1.088036
H	1.371101	3.654668	1.273963
H	0.624465	4.224917	-1.182324
H	0.803038	2.522392	-1.542571
H	-1.030388	3.668420	0.631118
H	-0.917690	1.969911	0.184314
H	-1.760152	4.180563	-1.739251
H	-1.758332	2.465160	-2.081129
H	-4.030598	3.279617	-1.570199
H	-3.495067	3.948364	-0.043489
H	-3.055762	1.675826	0.848524
H	-4.716231	1.889452	0.347087
H	-2.575602	0.500225	-1.334993
H	-4.264527	0.681388	-1.777456

conf_109

C	-4.795915	-0.391553	-1.186674
C	-3.823982	-1.409367	-0.603906
C	-3.246545	-2.338851	-1.662094
C	-2.214160	-3.309319	-1.106009
C	-0.966032	-2.616155	-0.616349
O	-0.516283	-1.593016	-1.110510
N	-0.319343	-3.214562	0.423973
H	-0.665241	-4.084507	0.794287
C	0.967343	-2.717330	0.855065
C	0.849039	-1.408054	1.598638
C	0.596344	-1.347118	2.966096
C	0.472228	-0.121787	3.616193
C	0.602906	1.034066	2.880837
N	0.848186	0.951761	1.564818
C	0.968758	-0.209527	0.912248

H	1.138285	-0.167880	-0.155309
H	0.936048	1.841503	1.032981
H	0.518557	2.030970	3.294747
H	0.279583	-0.063876	4.679835
H	0.496050	-2.266676	3.534836
H	1.618956	-2.578137	-0.012199
H	1.427873	-3.464469	1.503714
H	-2.643062	-3.920636	-0.303483
H	-1.889922	-4.005704	-1.889613
H	-2.774196	-1.743445	-2.450085
H	-4.048793	-2.913104	-2.136844
H	-2.995182	-0.885126	-0.112884
H	-4.326317	-1.995821	0.177643
C	-5.285889	0.657147	-0.188761
C	-4.172731	1.419639	0.530048
C	-3.146030	2.047342	-0.403039
C	-1.991542	2.705320	0.337277
C	-0.885937	3.178385	-0.606013
C	0.318836	3.711484	0.103136
C	1.607359	3.481526	-0.195569
C	2.142797	2.634589	-1.308546
C	3.356064	1.798851	-0.901245
C	3.804299	0.839253	-1.996892
C	4.881422	-0.146178	-1.554035
C	4.377572	-1.222294	-0.597631
C	5.456261	-2.218354	-0.198838
H	5.865865	-2.725561	-1.077312
H	6.286220	-1.717115	0.308181
H	5.070697	-2.986956	0.477433
H	3.546144	-1.753189	-1.082448
H	3.966248	-0.756753	0.308411
H	5.713369	0.397938	-1.088291
H	5.301167	-0.638383	-2.438574
H	2.935759	0.276103	-2.367420
H	4.166100	1.423767	-2.850195
H	3.129757	1.235411	0.012750
H	4.185675	2.463814	-0.632230
H	1.360259	1.984196	-1.716534
H	2.431648	3.292844	-2.139050
H	2.360348	3.993893	0.404314
H	0.111722	4.397072	0.926133
H	-1.287584	3.975148	-1.246698
H	-0.612525	2.365004	-1.286819
H	-2.353345	3.548785	0.938299
H	-1.584462	1.977339	1.052574
H	-3.634263	2.780533	-1.057634
H	-2.732020	1.277519	-1.065446
H	-4.621939	2.197628	1.158622
H	-3.653331	0.742710	1.221930
H	-5.923910	0.177526	0.563025
H	-5.928035	1.369846	-0.719198
H	-4.315895	0.107217	-2.037578

H	-5.662738	-0.915981	-1.604936
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conf_4

C	-2.009347	-2.252243	-0.731994
C	-1.765934	-3.544871	-1.506184
C	-0.469536	-4.290151	-1.205663
C	0.819030	-3.566534	-1.623197
C	1.237809	-2.448236	-0.705652
O	1.230333	-1.266043	-1.017157
N	1.634318	-2.821950	0.543493
H	1.677537	-3.797317	0.789103
C	2.035211	-1.822942	1.508039
C	0.856574	-0.981504	1.933860
C	-0.045232	-1.391051	2.911152
C	-1.159847	-0.615751	3.221245
C	-1.363011	0.559431	2.534555
N	-0.477397	0.936020	1.600420
C	0.604485	0.216895	1.286319
H	1.239335	0.599139	0.499412
H	-0.654413	1.813828	1.073691
H	-2.207668	1.217178	2.693487
H	-1.866809	-0.922361	3.981498
H	0.118147	-2.327641	3.435809
H	2.807154	-1.178507	1.077054
H	2.466133	-2.329354	2.373261
H	1.641078	-4.290081	-1.669752
H	0.709206	-3.134647	-2.619978
H	-0.494389	-5.245587	-1.738327
H	-0.430085	-4.545243	-0.138383
H	-2.597810	-4.231126	-1.306330
H	-1.809799	-3.329185	-2.581314
C	-3.425858	-1.735735	-0.959527
C	-3.777689	-0.443557	-0.231865
C	-3.065234	0.803518	-0.744109
C	-3.657786	2.083021	-0.163716
C	-2.885413	3.356791	-0.521968
C	-1.682871	3.589896	0.337118
C	-0.400669	3.718494	-0.036669
C	0.156794	3.640873	-1.422124
C	1.183555	2.521144	-1.621392
C	2.408024	2.608872	-0.717929
C	3.410690	1.489370	-0.974852
C	4.493047	1.386459	0.091150
C	5.480147	0.259523	-0.174723
H	6.235526	0.189054	0.612168
H	4.970952	-0.708926	-0.240304
H	6.003470	0.411929	-1.123252
H	4.020127	1.240388	1.073972
H	5.030954	2.339226	0.164081
H	3.876646	1.641256	-1.956293
H	2.880403	0.530719	-1.052267
H	2.895240	3.583056	-0.850495

H	2.107633	2.584717	0.340323
H	0.692849	1.546112	-1.493311
H	1.514029	2.539351	-2.665777
H	-0.646232	3.527002	-2.153707
H	0.640291	4.602462	-1.639771
H	0.318243	3.963921	0.746088
H	-1.908712	3.745539	1.395803
H	-3.548202	4.220181	-0.387280
H	-2.618346	3.337512	-1.581920
H	-4.688513	2.177796	-0.521027
H	-3.739540	2.001366	0.930357
H	-3.149097	0.843133	-1.837616
H	-1.988590	0.744604	-0.541138
H	-4.858477	-0.279248	-0.318459
H	-3.584184	-0.564479	0.844529
H	-4.133663	-2.515348	-0.653695
H	-3.586291	-1.592530	-2.036128
H	-1.859705	-2.433917	0.343393
H	-1.277171	-1.494385	-1.028893

conf_50

C	-0.372558	-1.650532	-1.977603
C	0.709284	-2.543972	-2.579867
C	1.369439	-3.548184	-1.640961
C	2.213826	-2.938527	-0.514719
C	1.428135	-2.336799	0.620412
O	1.458108	-1.151093	0.917291
N	0.654304	-3.197535	1.338679
H	0.655577	-4.180821	1.122576
C	-0.112161	-2.712825	2.464120
C	-1.281876	-1.872945	2.008789
C	-2.515820	-2.428634	1.682548
C	-3.553761	-1.632035	1.207465
C	-3.333988	-0.282812	1.047752
N	-2.138399	0.231282	1.369886
C	-1.127784	-0.504934	1.843650
H	-0.196597	0.006938	2.049411
H	-1.971907	1.244561	1.208510
H	-4.072879	0.410769	0.668543
H	-4.519300	-2.052376	0.956714
H	-2.671696	-3.496951	1.799251
H	0.533744	-2.118173	3.116215
H	-0.470988	-3.570279	3.035545
H	2.868217	-3.710675	-0.093488
H	2.857001	-2.146880	-0.904972
H	2.029754	-4.187826	-2.234279
H	0.605390	-4.217418	-1.223683
H	0.268775	-3.107765	-3.411021
H	1.485909	-1.911185	-3.027836
C	-1.141217	-0.911763	-3.068562
C	-2.243585	0.021398	-2.580437
C	-1.757463	1.302209	-1.911677

C	-2.894395	2.282688	-1.646858
C	-2.477186	3.538306	-0.874698
C	-2.240423	3.304478	0.586439
C	-1.061239	3.278647	1.225781
C	0.295938	3.452519	0.627020
C	1.284270	2.366085	1.046823
C	2.676790	2.576000	0.467606
C	3.686730	1.554957	0.977170
C	5.061978	1.658548	0.323493
C	5.074475	1.264469	-1.148030
H	4.694564	0.245201	-1.281859
H	4.457241	1.930509	-1.758032
H	6.087113	1.296409	-1.558530
H	5.759704	1.014650	0.870358
H	5.445485	2.680566	0.435018
H	3.283894	0.546365	0.824584
H	3.793223	1.681607	2.062119
H	2.610884	2.529215	-0.626192
H	3.025425	3.588765	0.709586
H	1.345527	2.332369	2.143728
H	0.922184	1.383273	0.719505
H	0.238422	3.493563	-0.464112
H	0.688463	4.425483	0.953151
H	-1.078444	3.166846	2.312572
H	-3.143789	3.211914	1.194678
H	-3.270822	4.288095	-0.964525
H	-1.591505	3.972851	-1.346022
H	-3.322703	2.585928	-2.608258
H	-3.714987	1.779386	-1.114797
H	-1.019939	1.788961	-2.562603
H	-1.216199	1.073230	-0.984904
H	-2.869041	0.300346	-3.436751
H	-2.908954	-0.525510	-1.895654
H	-1.583242	-1.656207	-3.741191
H	-0.433971	-0.338425	-3.682047
H	-1.076351	-2.265342	-1.396177
H	0.076174	-0.937508	-1.277335

conf_5

C	-3.587727	0.005899	-1.025035
C	-3.828049	-1.239163	-0.182374
C	-3.640925	-2.557778	-0.929691
C	-2.290711	-2.690754	-1.648623
C	-1.106782	-2.314459	-0.795067
O	-0.308919	-1.437552	-1.097466
N	-0.966258	-2.988922	0.378880
H	-1.630705	-3.700976	0.634374
C	0.098681	-2.637560	1.290971
C	-0.098404	-1.250108	1.856202
C	-0.930930	-0.990043	2.939664
C	-1.129766	0.313922	3.389744
C	-0.495378	1.345906	2.737504

N	0.305090	1.071218	1.696395
C	0.517121	-0.168213	1.244932
H	1.163528	-0.278117	0.386364
H	0.763377	1.857047	1.193940
H	-0.599982	2.388851	3.008150
H	-1.772788	0.526950	4.234076
H	-1.435376	-1.811006	3.440460
H	1.058310	-2.684637	0.769241
H	0.118547	-3.370455	2.099283
H	-2.158719	-3.718881	-2.003912
H	-2.247413	-2.042379	-2.524384
H	-4.428401	-2.674303	-1.681391
H	-3.780448	-3.390964	-0.229617
H	-3.145821	-1.210871	0.679424
H	-4.839916	-1.213719	0.238419
C	-3.790139	1.300798	-0.242638
C	-3.157140	2.514843	-0.918706
C	-1.638873	2.528022	-0.789761
C	-0.950747	3.640701	-1.565093
C	0.571870	3.526609	-1.541149
C	1.186544	3.686998	-0.186742
C	2.257724	3.027770	0.280443
C	3.025682	1.958485	-0.445356
C	3.931645	1.135727	0.469342
C	4.562933	-0.069282	-0.222717
C	3.591751	-1.221975	-0.447222
C	4.193232	-2.407916	-1.188297
C	3.213461	-3.563085	-1.334367
H	3.645300	-4.386618	-1.908189
H	2.929096	-3.964587	-0.354674
H	2.299408	-3.242191	-1.845215
H	5.093523	-2.747281	-0.662367
H	4.525604	-2.078144	-2.179556
H	2.711112	-0.881416	-1.009901
H	3.226951	-1.564983	0.533488
H	4.989798	0.245492	-1.183519
H	5.404829	-0.431313	0.377438
H	4.715380	1.792453	0.862423
H	3.369187	0.789809	1.349500
H	2.337912	1.308041	-1.000593
H	3.648223	2.429025	-1.218140
H	2.664122	3.336382	1.245151
H	0.765281	4.478990	0.434689
H	0.997393	4.311921	-2.181238
H	0.879319	2.577161	-1.993399
H	-1.285409	3.615657	-2.607662
H	-1.256732	4.617615	-1.169882
H	-1.227786	1.563502	-1.117260
H	-1.389072	2.624069	0.276191
H	-3.434789	2.526378	-1.980384
H	-3.562691	3.437918	-0.489013
H	-3.356969	1.188641	0.762952

H	-4.861298	1.470125	-0.088933
H	-2.568027	-0.021737	-1.422977
H	-4.254781	0.000847	-1.896337

conf_14

C	-4.088963	-1.770962	0.260144
C	-2.597445	-1.991545	0.485186
C	-2.124592	-3.310111	-0.112897
C	-0.636337	-3.577015	0.051354
C	0.238794	-2.726214	-0.838868
O	-0.183190	-1.990271	-1.716997
N	1.581280	-2.841845	-0.614651
H	1.907593	-3.443914	0.124094
C	2.546800	-2.262277	-1.518873
C	2.871142	-0.815947	-1.226941
C	4.155281	-0.381868	-0.907703
C	4.415372	0.964747	-0.665972
C	3.376600	1.865480	-0.737595
N	2.148896	1.425296	-1.046544
C	1.868424	0.141906	-1.292064
H	0.843243	-0.117427	-1.538917
H	1.358550	2.102498	-1.063304
H	3.481132	2.927457	-0.555546
H	5.410815	1.310816	-0.418429
H	4.966104	-1.101789	-0.849582
H	2.147969	-2.331397	-2.536080
H	3.463519	-2.853307	-1.480156
H	-0.323786	-3.433903	1.094141
H	-0.409439	-4.622872	-0.190589
H	-2.369681	-3.333693	-1.179690
H	-2.673643	-4.135505	0.352740
H	-2.026358	-1.171433	0.035732
H	-2.380079	-1.975032	1.562804
C	-4.655120	-0.508817	0.909064
C	-3.944386	0.786558	0.524439
C	-3.968733	1.103286	-0.968844
C	-3.029532	2.242757	-1.356176
C	-1.562884	1.797712	-1.287297
C	-0.581466	2.915420	-1.462507
C	-0.076744	3.676393	-0.477919
C	-0.410111	3.604494	0.984348
C	0.647064	2.889047	1.839751
C	0.468494	1.376048	1.844819
C	1.639422	0.596973	2.421941
C	1.376600	-0.903051	2.454957
C	2.604784	-1.725346	2.810761
H	3.404486	-1.580713	2.074608
H	3.007860	-1.439207	3.786642
H	2.378176	-2.794958	2.856973
H	0.997974	-1.214985	1.473731
H	0.570075	-1.110555	3.167879
H	1.869906	0.956701	3.432268

H	2.541490	0.795421	1.824416
H	-0.444623	1.132523	2.402653
H	0.280386	1.017880	0.825452
H	0.593889	3.258042	2.868982
H	1.653461	3.154916	1.485817
H	-0.525284	4.633535	1.339649
H	-1.379294	3.117657	1.132694
H	0.603662	4.480816	-0.762924
H	-0.300702	3.165462	-2.486418
H	-1.399562	1.033035	-2.056151
H	-1.396594	1.308958	-0.324341
H	-3.254616	2.597493	-2.367239
H	-3.180840	3.098162	-0.686595
H	-4.993587	1.354004	-1.263755
H	-3.695241	0.214316	-1.550270
H	-4.403134	1.620399	1.069287
H	-2.908399	0.735642	0.882338
H	-4.613364	-0.618312	1.999669
H	-5.718579	-0.429582	0.654310
H	-4.284339	-1.758711	-0.819004
H	-4.639649	-2.636438	0.647813

conf_40

C	-3.137449	1.178466	-1.292015
C	-3.994388	0.237674	-0.454834
C	-4.320627	-1.097494	-1.119745
C	-3.095673	-1.859670	-1.643778
C	-1.960514	-1.939520	-0.656660
O	-0.841164	-1.501264	-0.883477
N	-2.235628	-2.507038	0.550022
H	-3.153884	-2.873472	0.740664
C	-1.210810	-2.564344	1.567983
C	-0.811876	-1.176941	2.014365
C	-1.562054	-0.432938	2.918123
C	-1.196033	0.872411	3.242303
C	-0.088386	1.420811	2.639112
N	0.622655	0.682694	1.771864
C	0.301323	-0.573585	1.450266
H	0.929406	-1.072411	0.726397
H	1.429319	1.134160	1.304189
H	0.260029	2.430882	2.812672
H	-1.769331	1.460120	3.947717
H	-2.446149	-0.869383	3.373097
H	-0.331828	-3.088013	1.180267
H	-1.595115	-3.134895	2.415120
H	-3.385918	-2.875277	-1.935335
H	-2.685205	-1.376637	-2.531233
H	-4.995512	-0.935928	-1.966587
H	-4.881516	-1.722449	-0.413799
H	-3.475562	0.052004	0.496592
H	-4.934640	0.734075	-0.187898
C	-2.897335	2.515372	-0.597673

C	-1.778658	3.344983	-1.221498
C	-0.388650	2.789867	-0.934402
C	0.738993	3.638036	-1.503040
C	2.127268	3.058844	-1.243108
C	2.478883	2.960445	0.212246
C	3.360878	2.110798	0.757592
C	4.145886	1.070062	0.014369
C	3.470781	-0.301705	0.045584
C	4.281327	-1.414154	-0.605522
C	3.599807	-2.777833	-0.529947
C	2.345978	-2.907583	-1.388302
C	1.658673	-4.255125	-1.228107
H	0.758295	-4.319378	-1.844510
H	2.320741	-5.077547	-1.515499
H	1.364831	-4.428825	-0.185935
H	2.618668	-2.757849	-2.440159
H	1.623931	-2.115868	-1.158142
H	3.352680	-2.997952	0.519487
H	4.313944	-3.552400	-0.831708
H	4.477139	-1.156497	-1.654102
H	5.260078	-1.467653	-0.115104
H	3.274143	-0.582058	1.091557
H	2.499813	-0.212799	-0.460760
H	4.295513	1.374673	-1.025738
H	5.142650	0.990620	0.461195
H	3.565515	2.200376	1.825396
H	2.020561	3.708827	0.862020
H	2.875255	3.700469	-1.728265
H	2.215824	2.078432	-1.724449
H	0.599955	3.750705	-2.583531
H	0.683176	4.650593	-1.082799
H	-0.299365	1.764909	-1.318125
H	-0.270866	2.720506	0.156105
H	-1.930554	3.413452	-2.306132
H	-1.832073	4.372703	-0.843251
H	-2.654026	2.333792	0.460327
H	-3.829366	3.091366	-0.593962
H	-2.177344	0.698418	-1.507900
H	-3.617148	1.355471	-2.263151

conf_57

C	4.308025	0.912458	0.219999
C	2.952231	1.467658	0.637783
C	2.820895	2.952763	0.329082
C	1.462162	3.542310	0.675244
C	0.353067	3.105791	-0.253648
O	0.520794	2.421082	-1.250925
N	-0.894100	3.549121	0.081506
H	-1.008019	4.128458	0.897387
C	-2.013243	3.376738	-0.817019
C	-2.683927	2.029534	-0.683761
C	-3.960667	1.871143	-0.152985

C	-4.533415	0.606519	-0.033506
C	-3.813165	-0.490923	-0.446206
N	-2.587178	-0.313692	-0.960827
C	-2.012564	0.885147	-1.093532
H	-1.009787	0.927881	-1.505186
H	-2.036084	-1.151348	-1.237723
H	-4.168511	-1.511363	-0.379204
H	-5.525559	0.474028	0.378887
H	-4.518856	2.743372	0.173685
H	-1.654231	3.495023	-1.843851
H	-2.742082	4.165849	-0.624587
H	1.176036	3.287399	1.703951
H	1.501191	4.637935	0.634648
H	3.016455	3.120081	-0.735167
H	3.587135	3.509159	0.879398
H	2.155823	0.928622	0.113758
H	2.797124	1.296529	1.712682
C	4.503925	-0.572289	0.523214
C	3.411589	-1.485020	-0.029916
C	3.223298	-1.397980	-1.541419
C	2.011925	-2.174702	-2.048388
C	0.691550	-1.508995	-1.640547
C	-0.524721	-2.293516	-2.039241
C	-1.052860	-3.310449	-1.339575
C	-0.497200	-3.910805	-0.085868
C	-1.424378	-3.846524	1.132536
C	-1.514673	-2.466716	1.778029
C	-0.222004	-1.999318	2.437894
C	-0.333641	-0.649793	3.141305
C	-0.695614	0.503369	2.213985
H	-1.710799	0.400033	1.816970
H	-0.654510	1.461025	2.740642
H	-0.002580	0.560667	1.366991
H	0.622241	-0.429720	3.628282
H	-1.075150	-0.717735	3.946591
H	0.581650	-1.941108	1.693113
H	0.096469	-2.756350	3.164174
H	-1.820420	-1.732404	1.024741
H	-2.311906	-2.476305	2.532033
H	-1.068823	-4.563576	1.880449
H	-2.425591	-4.188242	0.841510
H	-0.299412	-4.966243	-0.311629
H	0.473287	-3.470157	0.154992
H	-1.922988	-3.819322	-1.757623
H	-0.964523	-2.065924	-3.011753
H	0.664765	-0.511818	-2.095690
H	0.686907	-1.354016	-0.556492
H	2.045830	-2.255159	-3.140083
H	2.034243	-3.201393	-1.663801
H	4.127711	-1.771103	-2.035131
H	3.119784	-0.350615	-1.850409
H	3.642630	-2.522621	0.240296

H	2.469390	-1.249322	0.479834
H	4.559307	-0.713960	1.609431
H	5.476541	-0.887123	0.127190
H	4.447412	1.095373	-0.852427
H	5.100921	1.480430	0.721009

conf_18

C	-2.375833	-2.036797	-1.783571
C	-1.942727	-2.901684	-0.601395
C	-0.933098	-3.988046	-0.964536
C	0.367616	-3.468071	-1.594261
C	1.004313	-2.416854	-0.729674
O	0.940797	-1.218997	-0.969834
N	1.610503	-2.855271	0.408504
H	1.664585	-3.841730	0.602952
C	2.097339	-1.903696	1.383870
C	0.949641	-1.092650	1.934553
C	0.082591	-1.580717	2.905893
C	-1.033312	-0.844078	3.299095
C	-1.273987	0.369737	2.697693
N	-0.417911	0.823327	1.769019
C	0.664764	0.144884	1.380361
H	1.272559	0.595314	0.608504
H	-0.608557	1.730872	1.300686
H	-2.124854	0.999601	2.922395
H	-1.714307	-1.212626	4.055503
H	0.268972	-2.551118	3.356104
H	2.833254	-1.237490	0.924604
H	2.596006	-2.451764	2.184796
H	1.060610	-4.300186	-1.756337
H	0.171543	-3.003923	-2.561652
H	-1.392166	-4.684170	-1.674478
H	-0.697725	-4.578829	-0.071077
H	-1.534739	-2.268622	0.198425
H	-2.824505	-3.394139	-0.173264
C	-3.709119	-1.327939	-1.562953
C	-3.745332	-0.273406	-0.459440
C	-2.944283	0.994404	-0.753427
C	-3.439714	2.182888	0.065061
C	-2.661198	3.484818	-0.157837
C	-1.398191	3.583555	0.638489
C	-0.134214	3.641269	0.191992
C	0.330066	3.604331	-1.228536
C	1.266426	2.435239	-1.551331
C	2.566281	2.417988	-0.755051
C	3.458057	1.234977	-1.113438
C	4.636500	1.050780	-0.166966
C	5.504478	-0.145384	-0.528883
H	6.333469	-0.270844	0.172351
H	4.922796	-1.074584	-0.530890
H	5.931562	-0.031821	-1.529638
H	4.261779	0.939249	0.861581

H	5.247741	1.961038	-0.157870
H	3.828452	1.359906	-2.138502
H	2.854305	0.317847	-1.132674
H	3.109939	3.357431	-0.915953
H	2.357192	2.394399	0.325054
H	0.730788	1.486034	-1.414072
H	1.509522	2.475641	-2.618887
H	-0.523483	3.578487	-1.909544
H	0.860198	4.544834	-1.429998
H	0.647464	3.782238	0.939568
H	-1.549500	3.693972	1.716177
H	-3.295659	4.328225	0.138519
H	-2.464927	3.610084	-1.225972
H	-4.490179	2.354159	-0.193093
H	-3.447082	1.934187	1.136890
H	-3.047473	1.245791	-1.816822
H	-1.870707	0.822701	-0.599557
H	-4.793097	0.013605	-0.308642
H	-3.421315	-0.709066	0.496194
H	-4.470788	-2.086862	-1.345813
H	-4.019208	-0.852254	-2.501126
H	-1.588880	-1.313619	-2.025950
H	-2.480497	-2.679682	-2.666738

conf_116

C	-3.228504	-1.689753	1.642681
C	-1.801504	-2.138685	1.298714
C	-1.734821	-3.269820	0.277517
C	-0.313757	-3.628295	-0.130492
C	0.334808	-2.583554	-1.006208
O	-0.291081	-1.767025	-1.665619
N	1.697912	-2.614719	-1.052706
H	2.194747	-3.293326	-0.498716
C	2.433329	-1.812809	-2.005111
C	2.663426	-0.390668	-1.546665
C	3.920407	0.096556	-1.196841
C	4.085154	1.415574	-0.781669
C	2.979540	2.233150	-0.707609
N	1.780028	1.743218	-1.049846
C	1.591073	0.486366	-1.464052
H	0.579372	0.177359	-1.706657
H	0.935015	2.342561	-0.951533
H	3.009640	3.265030	-0.381623
H	5.058837	1.803281	-0.510362
H	4.784768	-0.558426	-1.251153
H	1.875869	-1.794974	-2.946457
H	3.394816	-2.292498	-2.195445
H	0.314950	-3.812938	0.749485
H	-0.309379	-4.559273	-0.711779
H	-2.300305	-3.008727	-0.620355
H	-2.211001	-4.161018	0.699255
H	-1.231606	-1.277157	0.927648

H	-1.288091	-2.469935	2.209637
C	-3.707589	-0.463548	0.867463
C	-3.725105	-0.637423	-0.646123
C	-4.202891	0.591784	-1.416935
C	-3.397343	1.865514	-1.161651
C	-1.884554	1.649149	-1.284359
C	-1.101133	2.926298	-1.209011
C	-0.726712	3.565213	-0.089413
C	-1.033745	3.179684	1.326670
C	0.178690	2.648059	2.105737
C	0.356759	1.143390	1.944774
C	1.701175	0.616910	2.421325
C	1.840643	-0.891214	2.261552
C	3.239182	-1.401494	2.571437
H	3.982389	-0.953882	1.901365
H	3.535454	-1.153655	3.594939
H	3.307209	-2.488430	2.467977
H	1.567333	-1.167394	1.235503
H	1.110676	-1.390101	2.909459
H	1.856018	0.892709	3.471881
H	2.507359	1.116612	1.864677
H	-0.450174	0.633769	2.485477
H	0.212490	0.861229	0.893936
H	0.067259	2.882585	3.169012
H	1.086929	3.176852	1.782703
H	-1.422712	4.074914	1.823602
H	-1.836882	2.437245	1.359383
H	-0.190126	4.508567	-0.205675
H	-0.870985	3.409979	-2.159233
H	-1.677339	1.146552	-2.236647
H	-1.565759	0.959635	-0.495705
H	-3.713351	2.641676	-1.866880
H	-3.613415	2.262637	-0.163489
H	-5.253692	0.793398	-1.178300
H	-4.173058	0.362193	-2.488798
H	-2.726262	-0.917000	-1.000290
H	-4.377729	-1.481771	-0.899827
H	-3.060291	0.383247	1.135797
H	-4.712412	-0.190410	1.212727
H	-3.921856	-2.523769	1.474966
H	-3.290792	-1.462949	2.711938

conf_122

C	-3.845375	0.487677	-1.777899
C	-3.965220	-0.199177	-0.421721
C	-4.037899	-1.720143	-0.506442
C	-2.766572	-2.377391	-1.059484
C	-1.547481	-2.087757	-0.223540
O	-0.638007	-1.349650	-0.573723
N	-1.509883	-2.686953	1.002506
H	-2.210341	-3.369620	1.242085
C	-0.327478	-2.578512	1.826220

C	-0.081377	-1.158158	2.271988
C	-0.811490	-0.543733	3.282906
C	-0.568140	0.785369	3.625905
C	0.392740	1.486486	2.934970
N	1.083759	0.871437	1.961059
C	0.877227	-0.402629	1.618587
H	1.469419	-0.794041	0.803694
H	1.754508	1.440302	1.412082
H	0.633939	2.526076	3.115635
H	-1.124645	1.274618	4.415040
H	-1.582039	-1.101076	3.806705
H	0.549821	-2.936239	1.276540
H	-0.458267	-3.220765	2.699235
H	-2.909433	-3.462061	-1.120860
H	-2.548893	-2.019360	-2.066319
H	-4.874483	-2.011248	-1.150666
H	-4.261949	-2.131963	0.484825
H	-3.122870	0.089565	0.220736
H	-4.868815	0.164029	0.082916
C	-3.951940	2.009720	-1.706767
C	-2.884023	2.689428	-0.853874
C	-1.460772	2.492391	-1.359825
C	-0.424505	3.077357	-0.413449
C	1.008574	2.957566	-0.928969
C	2.031517	3.238819	0.131464
C	3.268495	2.726271	0.199181
C	3.883380	1.792044	-0.802990
C	3.548015	0.323623	-0.535652
C	4.286837	-0.657388	-1.436130
C	3.902402	-2.112334	-1.180082
C	2.497583	-2.481582	-1.645400
C	2.111577	-3.908357	-1.285262
H	2.153857	-4.070670	-0.201292
H	1.098826	-4.146104	-1.622518
H	2.791968	-4.633501	-1.741768
H	2.438180	-2.350141	-2.732623
H	1.749577	-1.796040	-1.230761
H	4.005281	-2.328069	-0.106034
H	4.622647	-2.768713	-1.681278
H	4.093171	-0.404796	-2.486395
H	5.364520	-0.529633	-1.283831
H	3.780694	0.081856	0.512283
H	2.466930	0.194532	-0.673490
H	3.553562	2.053488	-1.813867
H	4.970155	1.920751	-0.787602
H	3.902107	3.037480	1.029000
H	1.739059	3.963800	0.893642
H	1.147198	3.663071	-1.759372
H	1.166012	1.961586	-1.358227
H	-0.649350	4.131886	-0.209676
H	-0.518372	2.561597	0.551872
H	-1.358683	2.949750	-2.352458

H	-1.247720	1.423988	-1.488960
H	-3.100793	3.763163	-0.805920
H	-2.952290	2.327889	0.181195
H	-4.940602	2.278188	-1.315332
H	-3.908805	2.415756	-2.724333
H	-2.901615	0.205868	-2.257866
H	-4.640988	0.113053	-2.433620

C18:1 11*E* picolylamide

conf_17

C	3.461463	-0.785644	-0.710138
C	3.629214	0.433065	0.188713
C	4.086440	1.697162	-0.533441
C	3.185847	2.146953	-1.683838
C	1.713486	2.338766	-1.328036
C	1.476749	3.383283	-0.246896
C	0.041122	3.669542	0.083339
C	-1.027764	3.134158	-0.521293
C	-2.452508	3.483700	-0.227613
C	-3.311892	2.286197	0.192145
C	-3.458599	1.204975	-0.872360
C	-4.177004	-0.039003	-0.367372
C	-4.210524	-1.171909	-1.384719
C	-4.909537	-2.418972	-0.864308
H	-5.950783	-2.208398	-0.602632
H	-4.910874	-3.219005	-1.608808
H	-4.421932	-2.805808	0.038289
H	-3.183046	-1.414399	-1.689090
H	-4.712689	-0.823013	-2.294594
H	-3.690073	-0.392724	0.555303
H	-5.200451	0.221721	-0.070128
H	-2.477311	0.910390	-1.269943
H	-3.998773	1.616468	-1.733758
H	-2.898297	1.847059	1.111603
H	-4.307075	2.649858	0.470022
H	-2.889975	3.927724	-1.131682
H	-2.489246	4.256688	0.546824
H	-0.860158	2.414571	-1.322224
H	-0.129079	4.426074	0.852637
H	1.944786	4.331804	-0.545125
H	2.007644	3.102945	0.675145
H	1.176466	2.636109	-2.235485
H	1.277661	1.375764	-1.028897
H	3.248683	1.421713	-2.502122
H	3.580782	3.085617	-2.089732
H	4.188837	2.507114	0.198549
H	5.095088	1.533742	-0.930092
H	4.350520	0.201118	0.982142
H	2.673711	0.620968	0.700698
C	3.124832	-2.038038	0.088574

C	2.793208	-3.270490	-0.748605
C	1.585852	-3.090651	-1.681827
C	0.410078	-2.456913	-0.984783
O	-0.045593	-1.363723	-1.290732
N	-0.112118	-3.146458	0.067320
H	0.286462	-4.031876	0.334218
C	-1.137919	-2.546129	0.891976
C	-0.598808	-1.342125	1.628524
C	0.100673	-1.439150	2.827288
C	0.655542	-0.308095	3.423572
C	0.512068	0.911024	2.801103
N	-0.173452	0.980862	1.650181
C	-0.723069	-0.083836	1.060303
H	-1.235158	0.086598	0.123880
H	-0.278120	1.890663	1.155711
H	0.921420	1.837752	3.182308
H	1.200092	-0.373419	4.356786
H	0.222910	-2.407728	3.302889
H	-1.495127	-3.294115	1.601493
H	-1.982926	-2.244958	0.267369
H	1.828881	-2.439165	-2.521682
H	1.288158	-4.059219	-2.097710
H	2.620434	-4.120743	-0.077440
H	3.655968	-3.550828	-1.361606
H	3.962622	-2.279593	0.752888
H	2.276231	-1.814751	0.751141
H	4.382736	-0.951261	-1.283356
H	2.671039	-0.589727	-1.442299

conf_0

C	3.976722	0.107769	0.171754
C	3.789919	1.224812	1.190962
C	3.941405	2.631523	0.614997
C	2.907863	3.017847	-0.441732
C	1.474324	3.006338	0.072144
C	0.454601	3.410798	-0.992579
C	-0.946610	3.508639	-0.476793
C	-2.018299	2.905287	-1.007509
C	-3.431136	3.074557	-0.531936
C	-4.003851	1.848011	0.188193
C	-4.036745	0.574805	-0.649863
C	-4.265013	-0.685075	0.173798
C	-4.179264	-1.967051	-0.643585
C	-4.248143	-3.223822	0.210160
H	-4.182325	-4.129908	-0.397783
H	-3.433280	-3.248986	0.943784
H	-5.186740	-3.270779	0.770069
H	-3.244537	-1.962418	-1.222156
H	-4.983513	-1.979717	-1.387918
H	-3.521926	-0.727098	0.984565
H	-5.239462	-0.631638	0.674717
H	-3.096253	0.463270	-1.205134

H	-4.812558	0.663176	-1.419691
H	-3.420087	1.670612	1.102448
H	-5.016025	2.081566	0.535027
H	-4.062585	3.307749	-1.397934
H	-3.485831	3.940223	0.135553
H	-1.863987	2.281345	-1.890449
H	-1.098559	4.174414	0.376529
H	0.496894	2.715458	-1.839307
H	0.739538	4.394470	-1.389379
H	1.235630	2.002422	0.442709
H	1.390773	3.681609	0.934575
H	2.984258	2.352012	-1.309766
H	3.142545	4.021961	-0.813578
H	3.896967	3.357625	1.435936
H	4.943034	2.730279	0.180475
H	4.519295	1.095615	1.999269
H	2.804941	1.118443	1.666963
C	3.717000	-1.270104	0.767820
C	4.036441	-2.436693	-0.163203
C	3.315209	-2.381679	-1.516739
C	1.833216	-2.149126	-1.385214
O	1.265674	-1.153025	-1.811693
N	1.125559	-3.103600	-0.718939
H	1.589338	-3.926518	-0.370424
C	-0.291060	-2.925964	-0.492833
C	-0.550953	-1.776344	0.451282
C	-0.517486	-1.919863	1.834185
C	-0.694686	-0.819494	2.670876
C	-0.902021	0.417619	2.105756
N	-0.936919	0.529890	0.769529
C	-0.771278	-0.505384	-0.056977
H	-0.791135	-0.298832	-1.117999
H	-1.113546	1.461111	0.345010
H	-1.043849	1.328351	2.673469
H	-0.672624	-0.921176	3.748316
H	-0.347695	-2.900261	2.269069
H	-0.697871	-3.848883	-0.076599
H	-0.795789	-2.737043	-1.444587
H	3.697644	-1.565247	-2.130231
H	3.488047	-3.312133	-2.068635
H	3.804705	-3.379332	0.347727
H	5.112982	-2.465612	-0.361259
H	4.305783	-1.388624	1.685016
H	2.663751	-1.327979	1.080199
H	4.999487	0.150652	-0.225885
H	3.307755	0.265557	-0.681079

conf_35

C	3.385950	-1.354574	-0.820945
C	3.551670	-0.023939	-0.100391
C	4.081870	1.090184	-0.992527
C	4.138524	2.459724	-0.317083

C	2.794806	2.985928	0.184729
C	1.751548	3.151423	-0.919184
C	0.420163	3.633440	-0.433532
C	-0.760051	3.161939	-0.857148
C	-2.103359	3.698836	-0.473408
C	-3.063983	2.650015	0.096590
C	-3.453925	1.548523	-0.882447
C	-4.246153	0.422480	-0.232669
C	-4.546684	-0.731617	-1.179630
C	-5.314036	-1.863921	-0.513710
H	-4.761917	-2.275017	0.339510
H	-6.280330	-1.516968	-0.135767
H	-5.506388	-2.683470	-1.210560
H	-3.604563	-1.111365	-1.599315
H	-5.118020	-0.355174	-2.036095
H	-3.691159	0.042067	0.639313
H	-5.184843	0.819833	0.173378
H	-2.563677	1.122873	-1.365554
H	-4.038453	1.983876	-1.702058
H	-2.624527	2.203899	0.999998
H	-3.971760	3.157857	0.439830
H	-2.561587	4.140786	-1.368479
H	-1.976947	4.516734	0.243304
H	-0.744286	2.359480	-1.598222
H	0.426840	4.472468	0.266306
H	1.615659	2.215670	-1.472567
H	2.137488	3.878165	-1.647475
H	2.411183	2.312865	0.962608
H	2.950100	3.952804	0.677338
H	4.561594	3.186607	-1.020228
H	4.835108	2.416174	0.528485
H	5.089782	0.826423	-1.331835
H	3.472048	1.144228	-1.902817
H	4.215513	-0.145843	0.766500
H	2.570801	0.258875	0.306367
C	2.893104	-2.453021	0.112713
C	2.463370	-3.744966	-0.576780
C	1.300183	-3.568381	-1.566223
C	0.185326	-2.734308	-0.990503
O	-0.122449	-1.630545	-1.417553
N	-0.454963	-3.249034	0.096271
H	-0.188017	-4.149608	0.459057
C	-1.443910	-2.458416	0.794484
C	-0.810833	-1.261358	1.465203
C	-0.223815	-1.326589	2.724970
C	0.406039	-0.213287	3.278031
C	0.448486	0.955726	2.553246
N	-0.126225	0.995853	1.341656
C	-0.742682	-0.052802	0.789001
H	-1.156066	0.085270	-0.200050
H	-0.098738	1.874254	0.786316
H	0.923209	1.865871	2.896887

H	0.861054	-0.253058	4.259414
H	-0.253736	-2.256390	3.285176
H	-1.931477	-3.089725	1.539013
H	-2.207984	-2.119396	0.089906
H	1.626360	-3.058281	-2.472880
H	0.912917	-4.548196	-1.865365
H	2.189902	-4.482147	0.187880
H	3.307612	-4.181932	-1.119919
H	3.675371	-2.686193	0.844159
H	2.047328	-2.063334	0.697753
H	4.336700	-1.656796	-1.277084
H	2.676168	-1.213780	-1.644007

conf_15

C	4.395393	0.308346	0.114661
C	4.121515	1.307501	1.231496
C	4.114841	2.767245	0.781963
C	3.070891	3.117935	-0.276615
C	1.639376	2.826840	0.153229
C	0.608800	3.219483	-0.905073
C	-0.811085	3.083214	-0.453024
C	-1.766474	2.393003	-1.089505
C	-3.211301	2.337146	-0.708105
C	-3.751840	0.916572	-0.541004
C	-5.256852	0.869331	-0.318735
C	-5.788658	-0.543080	-0.121975
C	-7.295719	-0.599054	0.090618
C	-7.814465	-2.015073	0.290299
H	-7.354834	-2.485437	1.165819
H	-8.897052	-2.027275	0.439215
H	-7.592987	-2.643626	-0.578286
H	-7.796959	-0.140504	-0.770479
H	-7.560111	0.017253	0.958824
H	-5.523998	-1.156693	-0.994085
H	-5.286009	-1.005583	0.739426
H	-5.760906	1.334413	-1.175343
H	-5.515156	1.482309	0.554600
H	-3.498676	0.324366	-1.431198
H	-3.255434	0.425986	0.308121
H	-3.788863	2.833517	-1.499483
H	-3.382299	2.918641	0.205108
H	-1.491454	1.863224	-2.005602
H	-1.090609	3.650437	0.438942
H	0.768340	2.633829	-1.817474
H	0.775440	4.269974	-1.179119
H	1.544134	1.756591	0.370159
H	1.425950	3.358700	1.091278
H	3.280936	2.580025	-1.208897
H	3.160218	4.183028	-0.519748
H	3.960233	3.406359	1.659945
H	5.107555	3.024188	0.394405
H	4.878761	1.185590	2.015028

H	3.163108	1.058581	1.709007
C	4.349384	-1.133285	0.604685
C	4.720461	-2.175827	-0.446715
C	3.876022	-2.111620	-1.725928
C	2.393167	-2.081961	-1.462857
O	1.663309	-1.165209	-1.813479
N	1.878384	-3.135301	-0.768719
H	2.476218	-3.893384	-0.482969
C	0.476561	-3.153587	-0.416337
C	0.148948	-2.022356	0.529080
C	0.418419	-2.083552	1.892198
C	0.193170	-0.981081	2.714753
C	-0.285802	0.179780	2.152660
N	-0.546862	0.210909	0.837172
C	-0.351318	-0.831549	0.026559
H	-0.569357	-0.682263	-1.022164
H	-0.867570	1.097150	0.397058
H	-0.465892	1.092828	2.705542
H	0.398559	-1.019185	3.776875
H	0.819384	-2.997192	2.320690
H	0.248757	-4.112821	0.051300
H	-0.136334	-3.065515	-1.318209
H	4.099835	-1.211107	-2.298825
H	4.107210	-2.968742	-2.368205
H	4.654288	-3.176279	-0.001332
H	5.769808	-2.052299	-0.734080
H	5.023962	-1.249186	1.461010
H	3.340469	-1.343561	0.988943
H	5.379687	0.517246	-0.325215
H	3.663916	0.442611	-0.689901

conf_2

C	4.773244	0.295613	-0.159154
C	4.859101	1.642723	0.555942
C	3.515596	2.241387	0.965204
C	2.567469	2.492872	-0.199421
C	1.222482	3.045213	0.248594
C	0.256421	3.274011	-0.916584
C	-1.164383	3.463611	-0.485897
C	-2.213810	2.828194	-1.022782
C	-3.646448	2.995736	-0.617292
C	-4.218147	1.772082	0.111102
C	-4.187232	0.479361	-0.698483
C	-4.395118	-0.772157	0.143111
C	-4.242900	-2.064181	-0.648812
C	-4.290957	-3.308291	0.224668
H	-5.239976	-3.376560	0.764476
H	-4.182807	-4.221593	-0.366250
H	-3.491975	-3.295396	0.975775
H	-3.292566	-2.036196	-1.201044
H	-5.025606	-2.117522	-1.414061
H	-3.672080	-0.774686	0.972592

H	-5.383680	-0.744446	0.617748
H	-3.228510	0.385020	-1.224542
H	-4.943662	0.526232	-1.490927
H	-3.662954	1.631106	1.049454
H	-5.247822	1.987052	0.415590
H	-4.246082	3.191455	-1.514630
H	-3.744287	3.877113	0.024003
H	-2.016744	2.147119	-1.853755
H	-1.342972	4.190193	0.309928
H	0.317235	2.436660	-1.623343
H	0.583727	4.160722	-1.474222
H	0.785905	2.340694	0.970057
H	1.359884	3.982549	0.801135
H	2.394474	1.560910	-0.751872
H	3.033374	3.188212	-0.909728
H	3.023884	1.582265	1.693803
H	3.696750	3.184460	1.494510
H	5.383684	2.353401	-0.093554
H	5.483302	1.532412	1.450901
C	4.092568	-0.794151	0.661781
C	4.189621	-2.184118	0.041074
C	3.487043	-2.323863	-1.317511
C	2.014185	-2.026690	-1.230247
O	1.508455	-0.967844	-1.575212
N	1.238037	-3.009557	-0.689048
H	1.640962	-3.907577	-0.477238
C	-0.193377	-2.834251	-0.600085
C	-0.561565	-1.748550	0.380841
C	-0.616258	-1.962650	1.753698
C	-0.921903	-0.919631	2.625982
C	-1.171123	0.329609	2.106301
N	-1.113892	0.510202	0.778250
C	-0.818132	-0.467819	-0.080049
H	-0.769007	-0.205650	-1.128143
H	-1.322459	1.447454	0.382139
H	-1.417231	1.197538	2.704579
H	-0.970885	-1.075637	3.696022
H	-0.416495	-2.952853	2.151819
H	-0.640753	-3.779261	-0.287005
H	-0.601057	-2.581810	-1.584257
H	3.908447	-1.629183	-2.045143
H	3.636000	-3.337614	-1.704440
H	3.782026	-2.925940	0.738261
H	5.243526	-2.446976	-0.100043
H	4.549674	-0.829826	1.658331
H	3.037122	-0.537112	0.821136
H	5.790617	-0.031828	-0.406646
H	4.254107	0.418995	-1.116010

conf_14

C	3.652982	1.090991	0.804388
C	2.848655	1.727340	1.931182

C	2.529250	3.206608	1.722441
C	1.719164	3.527499	0.467819
C	0.374646	2.815509	0.406206
C	-0.414853	3.144271	-0.860578
C	-1.791941	2.557585	-0.894718
C	-2.245503	1.739699	-1.853449
C	-3.640901	1.224700	-2.042655
C	-4.651248	1.486187	-0.930352
C	-4.437712	0.706080	0.366203
C	-4.414760	-0.808167	0.198126
C	-4.389602	-1.562731	1.521661
C	-4.135778	-3.052713	1.353511
H	-4.896685	-3.513412	0.716547
H	-3.162091	-3.237158	0.883910
H	-4.148193	-3.576086	2.313011
H	-5.339232	-1.402343	2.044574
H	-3.621302	-1.130845	2.177745
H	-5.293129	-1.123267	-0.379642
H	-3.548225	-1.113710	-0.403689
H	-5.242096	0.972047	1.061647
H	-3.513715	1.034578	0.863434
H	-4.684328	2.559348	-0.711135
H	-5.644008	1.233879	-1.318740
H	-3.600380	0.151675	-2.272656
H	-4.013615	1.679987	-2.970123
H	-1.546604	1.474297	-2.650970
H	-2.472059	2.880243	-0.104855
H	0.149341	2.817969	-1.741566
H	-0.509175	4.235510	-0.939665
H	0.546327	1.734170	0.449897
H	-0.219222	3.077370	1.293425
H	2.297383	3.275335	-0.429309
H	1.553249	4.609940	0.421534
H	1.988526	3.578136	2.601553
H	3.468485	3.770753	1.687088
H	3.402357	1.618698	2.871353
H	1.918009	1.159333	2.072406
C	3.920481	-0.388282	1.051850
C	4.814811	-1.059667	0.012772
C	4.305455	-0.947659	-1.429938
C	2.862751	-1.351510	-1.588140
O	1.993985	-0.598946	-2.006311
N	2.541431	-2.619370	-1.206155
H	3.255092	-3.236484	-0.854460
C	1.163863	-3.058741	-1.236465
C	0.332406	-2.251626	-0.268130
C	0.320976	-2.504252	1.099819
C	-0.356598	-1.658726	1.975419
C	-1.005291	-0.557348	1.466298
N	-0.998171	-0.346869	0.142037
C	-0.363405	-1.142685	-0.721727
H	-0.393992	-0.854463	-1.763657

H	-1.455596	0.501054	-0.248598
H	-1.528904	0.171620	2.070221
H	-0.369036	-1.843935	3.041787
H	0.859507	-3.361275	1.493037
H	1.131306	-4.117202	-0.973371
H	0.760290	-2.950759	-2.247313
H	4.373496	0.078864	-1.791773
H	4.923457	-1.564774	-2.091637
H	4.950684	-2.114348	0.282956
H	5.816130	-0.617933	0.047913
H	4.381795	-0.514238	2.038358
H	2.957712	-0.917440	1.103090
H	4.606305	1.624611	0.693297
H	3.120340	1.211321	-0.145576

conf_26

C	4.415138	1.042531	0.476760
C	3.666207	2.180090	1.163413
C	2.164862	2.159666	0.897987
C	1.451695	3.430515	1.344364
C	-0.051795	3.400021	1.088725
C	-0.418277	3.468002	-0.397053
C	-1.841060	3.104114	-0.681875
C	-2.239926	2.293904	-1.669833
C	-3.651963	1.950114	-2.025635
C	-3.988945	0.476788	-1.761792
C	-4.282893	0.186527	-0.294234
C	-4.208787	-1.290324	0.064617
C	-4.534830	-1.584881	1.522494
C	-4.335908	-3.046538	1.892211
H	-4.968567	-3.697064	1.281053
H	-3.297188	-3.358042	1.731039
H	-4.582916	-3.235866	2.939845
H	-5.569722	-1.288118	1.727862
H	-3.913876	-0.951261	2.171328
H	-4.890965	-1.857463	-0.581095
H	-3.203560	-1.673801	-0.167887
H	-5.277468	0.575795	-0.045635
H	-3.591871	0.755929	0.344280
H	-4.851980	0.182376	-2.367001
H	-3.157737	-0.153094	-2.111069
H	-3.797715	2.170639	-3.088950
H	-4.345966	2.593210	-1.473761
H	-1.471730	1.870876	-2.325640
H	-2.601925	3.570101	-0.052916
H	0.244579	2.830718	-0.993551
H	-0.238282	4.492704	-0.747353
H	-0.462636	2.484517	1.537089
H	-0.541154	4.228010	1.612714
H	1.890658	4.296642	0.833112
H	1.631821	3.587345	2.414024
H	2.009801	1.991055	-0.175255

H	1.707613	1.301666	1.410629
H	4.073047	3.132631	0.804349
H	3.853199	2.158438	2.244883
C	4.042158	-0.344582	0.986744
C	4.740923	-1.482157	0.248097
C	4.382221	-1.570968	-1.243839
C	2.892696	-1.618371	-1.458809
O	2.230558	-0.678345	-1.873366
N	2.274960	-2.782393	-1.106375
H	2.819886	-3.580106	-0.823199
C	0.843701	-2.904919	-1.252047
C	0.115906	-2.000006	-0.287390
C	-0.057647	-2.329790	1.053283
C	-0.695868	-1.452897	1.925933
C	-1.151183	-0.248878	1.440384
N	-0.972054	0.048410	0.145434
C	-0.361588	-0.771777	-0.714710
H	-0.245967	-0.423584	-1.732446
H	-1.352101	0.942241	-0.216573
H	-1.662629	0.491497	2.041145
H	-0.845470	-1.702080	2.968592
H	0.308746	-3.282502	1.423528
H	0.562971	-3.943293	-1.067035
H	0.550252	-2.654785	-2.276096
H	4.751104	-0.701585	-1.788577
H	4.850289	-2.457696	-1.684427
H	4.500821	-2.433293	0.737894
H	5.827097	-1.366854	0.327823
H	4.287253	-0.414174	2.053386
H	2.955906	-0.487046	0.915930
H	5.494607	1.186894	0.604490
H	4.217948	1.105964	-0.599794

conf_41

C	4.353987	1.411704	-0.318430
C	3.897699	2.290028	0.839410
C	3.254630	3.608222	0.413861
C	1.993152	3.472930	-0.437192
C	0.886204	2.671184	0.233899
C	-0.400498	2.619257	-0.590094
C	-1.526411	1.931574	0.113413
C	-2.222697	0.888802	-0.357697
C	-3.399570	0.256073	0.313810
C	-4.691305	0.447618	-0.484415
C	-5.891397	-0.227437	0.164105
C	-7.181702	-0.034878	-0.620244
C	-8.386093	-0.707362	0.025314
C	-9.670451	-0.508581	-0.765492
H	-9.913820	0.554210	-0.862847
H	-9.580252	-0.920305	-1.775787
H	-10.518812	-0.999752	-0.281974
H	-8.514960	-0.315974	1.042301

H	-8.183546	-1.780189	0.136209
H	-7.382743	1.038879	-0.731510
H	-7.050880	-0.425419	-1.638325
H	-6.023472	0.163855	1.181714
H	-5.689859	-1.301673	0.274479
H	-4.882548	1.521387	-0.595755
H	-4.552112	0.054463	-1.499490
H	-3.524388	0.673539	1.320339
H	-3.228676	-0.823864	0.435677
H	-1.962469	0.501705	-1.346289
H	-1.819134	2.352125	1.079512
H	-0.209644	2.135205	-1.554388
H	-0.713468	3.647707	-0.814251
H	1.242083	1.648994	0.410410
H	0.671766	3.103828	1.221417
H	2.233453	3.013412	-1.403406
H	1.616703	4.476121	-0.668505
H	3.015392	4.189828	1.312579
H	3.991126	4.201246	-0.140792
H	4.758300	2.510889	1.481881
H	3.199994	1.720485	1.469634
C	4.936820	0.086692	0.156352
C	5.521669	-0.784882	-0.951707
C	4.539077	-1.109082	-2.084276
C	3.217873	-1.639521	-1.592785
O	2.147649	-1.084784	-1.799540
N	3.260289	-2.785217	-0.856454
H	4.138488	-3.250115	-0.694120
C	2.043265	-3.335471	-0.304202
C	1.447107	-2.400699	0.721595
C	1.908823	-2.333861	2.032074
C	1.393082	-1.395097	2.923751
C	0.427189	-0.520187	2.482120
N	-0.007762	-0.609047	1.216218
C	0.461603	-1.502911	0.342204
H	0.063960	-1.459930	-0.662916
H	-0.697940	0.084889	0.858867
H	-0.013168	0.256995	3.093648
H	1.744791	-1.336313	3.945821
H	2.687450	-3.014359	2.363376
H	2.274863	-4.297743	0.155279
H	1.317323	-3.511031	-1.103621
H	4.309375	-0.218935	-2.670818
H	4.985973	-1.840146	-2.767214
H	5.910579	-1.712458	-0.513610
H	6.388367	-0.284322	-1.395843
H	5.721557	0.278039	0.897538
H	4.153815	-0.473555	0.688427
H	5.103816	1.953490	-0.910230
H	3.511508	1.218231	-0.991683

conf_3

C	3.820742	0.670665	0.374403
C	3.275790	1.643056	1.418415
C	2.768451	2.951496	0.815297
C	1.413930	2.789841	0.135644
C	0.934402	4.019194	-0.618727
C	-0.355183	3.785131	-1.403819
C	-1.567290	3.486972	-0.575691
C	-2.523844	2.604676	-0.895326
C	-3.846595	2.465080	-0.199490
C	-4.103797	1.109188	0.465858
C	-4.001795	-0.093313	-0.465561
C	-3.943141	-1.422878	0.273952
C	-3.699105	-2.616312	-0.639760
C	-3.503112	-3.918170	0.121768
H	-4.384138	-4.161281	0.722886
H	-3.323366	-4.758762	-0.553470
H	-2.652084	-3.849631	0.810158
H	-2.817200	-2.416234	-1.264971
H	-4.536746	-2.718419	-1.339074
H	-3.143731	-1.381511	1.029023
H	-4.870418	-1.575480	0.839812
H	-3.109678	-0.007514	-1.099609
H	-4.848119	-0.090303	-1.162876
H	-3.404922	0.982464	1.303496
H	-5.097675	1.127396	0.925702
H	-4.632928	2.645656	-0.943995
H	-3.945948	3.258323	0.548445
H	-2.382174	2.015123	-1.804145
H	-1.721907	4.124813	0.298309
H	-0.206644	2.991250	-2.146354
H	-0.579158	4.694812	-1.977073
H	0.794982	4.854170	0.079484
H	1.712518	4.337816	-1.320667
H	0.677005	2.533943	0.909927
H	1.448436	1.938882	-0.558825
H	2.690547	3.719746	1.592883
H	3.501104	3.326563	0.089539
H	4.051113	1.846201	2.164793
H	2.451554	1.162792	1.967433
C	3.895345	-0.761927	0.885927
C	4.498220	-1.763367	-0.096732
C	3.839074	-1.768183	-1.484021
C	2.334019	-1.805204	-1.432204
O	1.623371	-0.914848	-1.878261
N	1.768481	-2.881173	-0.818022
H	2.348954	-3.610579	-0.437250
C	0.335098	-2.928820	-0.632375
C	-0.117539	-1.835558	0.305915
C	-0.044652	-1.964051	1.688361
C	-0.388250	-0.902416	2.522794
C	-0.798131	0.280957	1.954611

N	-0.868529	0.379150	0.618717
C	-0.547665	-0.620316	-0.205653
H	-0.615231	-0.426731	-1.267146
H	-1.195240	1.270864	0.203830
H	-1.076324	1.160493	2.520779
H	-0.336305	-0.991502	3.600268
H	0.290005	-2.900595	2.124260
H	0.066002	-3.905515	-0.227197
H	-0.166801	-2.816341	-1.597351
H	4.097844	-0.867878	-2.042363
H	4.201375	-2.623905	-2.064271
H	4.455478	-2.767152	0.343641
H	5.562850	-1.550188	-0.237749
H	4.475323	-0.792986	1.815768
H	2.880314	-1.086178	1.157781
H	4.816122	1.004555	0.055293
H	3.188744	0.701308	-0.519416

conf_28

C	3.572028	-0.937884	-0.721599
C	4.070907	0.227386	0.125305
C	4.399033	1.477790	-0.689355
C	3.179168	2.266456	-1.164172
C	2.541405	3.105551	-0.061352
C	1.330215	3.923902	-0.517336
C	0.122882	3.111971	-0.868301
C	-1.126333	3.375693	-0.464097
C	-2.348551	2.631775	-0.903826
C	-3.335012	2.334733	0.227962
C	-4.489143	1.429476	-0.193664
C	-4.089641	-0.029845	-0.377752
C	-5.234158	-0.927494	-0.827620
C	-4.824098	-2.386904	-0.955957
H	-4.001350	-2.505877	-1.669702
H	-4.497489	-2.791703	0.008879
H	-5.652589	-3.008271	-1.304289
H	-5.615226	-0.565711	-1.789715
H	-6.065257	-0.837312	-0.118077
H	-3.275293	-0.113671	-1.111228
H	-3.693208	-0.408328	0.577146
H	-4.929023	1.810431	-1.124035
H	-5.282581	1.483066	0.559990
H	-2.815166	1.874006	1.080143
H	-3.728143	3.286059	0.603147
H	-2.051378	1.716553	-1.429689
H	-2.870975	3.241071	-1.653762
H	-1.291894	4.234339	0.190918
H	0.273864	2.277945	-1.557310
H	1.624267	4.499611	-1.405772
H	1.060450	4.662410	0.245551
H	2.262575	2.463755	0.785822
H	3.296724	3.796716	0.329641

H	2.443366	1.580855	-1.602153
H	3.477996	2.941174	-1.974725
H	5.039186	2.144002	-0.098981
H	4.998019	1.178639	-1.557008
H	4.965947	-0.092788	0.671285
H	3.323213	0.464878	0.896410
C	3.206705	-2.154624	0.118706
C	2.839695	-3.399348	-0.685628
C	1.679141	-3.198689	-1.669540
C	0.484953	-2.533117	-1.037397
O	0.037688	-1.457503	-1.410701
N	-0.070628	-3.174719	0.027608
H	0.327939	-4.039929	0.354092
C	-1.126389	-2.542564	0.788049
C	-0.611900	-1.313978	1.500920
C	0.004044	-1.363241	2.747323
C	0.542775	-0.214031	3.324104
C	0.467711	0.974822	2.635073
N	-0.138686	0.999105	1.438353
C	-0.672850	-0.082971	0.865609
H	-1.121246	0.047440	-0.108154
H	-0.194449	1.881327	0.893866
H	0.872012	1.911610	2.996635
H	1.022326	-0.242627	4.294144
H	0.072688	-2.308717	3.277106
H	-1.514199	-3.263015	1.509867
H	-1.944656	-2.263357	0.119580
H	1.976196	-2.561212	-2.502986
H	1.375704	-4.163401	-2.090677
H	2.608448	-4.218988	0.006123
H	3.709597	-3.737397	-1.258251
H	4.047014	-2.404601	0.777096
H	2.374052	-1.889853	0.786418
H	4.354832	-1.213756	-1.440352
H	2.705863	-0.625249	-1.315835

conf_18

C	3.725090	-0.585600	-0.560763
C	4.129948	0.554292	0.369663
C	3.912462	1.935204	-0.245293
C	2.460811	2.394488	-0.165557
C	2.158427	3.626343	-1.005093
C	0.763449	4.206088	-0.781276
C	-0.356062	3.243525	-1.043573
C	-1.552877	3.261367	-0.442870
C	-2.720644	2.401523	-0.823838
C	-3.576995	1.947710	0.360226
C	-4.633572	0.912175	-0.014624
C	-4.064286	-0.476849	-0.278910
C	-5.114803	-1.507900	-0.667735
C	-4.528961	-2.896091	-0.877746
H	-5.295147	-3.615050	-1.177534

H	-3.761805	-2.888211	-1.659948
H	-4.070203	-3.274281	0.043110
H	-5.618663	-1.177814	-1.583667
H	-5.888780	-1.545992	0.108058
H	-3.309029	-0.434255	-1.076214
H	-3.543679	-0.822179	0.627611
H	-5.185789	1.257646	-0.897775
H	-5.370134	0.840867	0.793384
H	-2.945320	1.534051	1.158693
H	-4.060391	2.829583	0.795001
H	-2.368869	1.547494	-1.414919
H	-3.365276	2.976286	-1.502499
H	-1.734734	4.009003	0.333588
H	-0.196121	2.526107	-1.852852
H	0.632573	5.062239	-1.455978
H	0.674261	4.612953	0.233943
H	2.899686	4.405150	-0.794956
H	2.278713	3.372546	-2.065650
H	2.220660	2.603422	0.888106
H	1.803131	1.572932	-0.480894
H	4.545512	2.677030	0.253634
H	4.234463	1.919161	-1.294400
H	5.180381	0.427731	0.652810
H	3.557713	0.484546	1.307011
C	3.602886	-1.920550	0.162777
C	3.377313	-3.125134	-0.749426
C	2.222994	-2.966358	-1.746833
C	0.938367	-2.471508	-1.134582
O	0.337916	-1.486989	-1.543019
N	0.465194	-3.164724	-0.062801
H	0.984095	-3.949480	0.296373
C	-0.698888	-2.687566	0.651042
C	-0.402877	-1.385872	1.358863
C	0.148004	-1.329862	2.635165
C	0.474429	-0.107458	3.219708
C	0.255431	1.049643	2.507865
N	-0.280523	0.971138	1.281102
C	-0.614587	-0.183974	0.699809
H	-1.023913	-0.132858	-0.298645
H	-0.440291	1.834603	0.726769
H	0.490639	2.040078	2.875087
H	0.899384	-0.054028	4.213860
H	0.328838	-2.249276	3.184094
H	-0.999616	-3.447788	1.373642
H	-1.525748	-2.544255	-0.049285
H	2.476126	-2.247024	-2.526712
H	2.028492	-3.922555	-2.245564
H	3.228265	-4.021126	-0.133530
H	4.285668	-3.321487	-1.328400
H	4.507828	-2.100127	0.754950
H	2.781538	-1.848946	0.889896
H	4.465758	-0.666480	-1.366782

H 2.773417 -0.345019 -1.049366

conf_119

C 2.931314 1.701362 1.567338
C 1.565804 1.865582 2.231789
C 0.676509 2.872912 1.505608
C 0.093316 2.302357 0.217601
C -0.589065 3.326346 -0.674868
C -1.037425 2.748101 -2.016353
C -2.078902 1.679515 -1.912300
C -2.093505 0.542735 -2.618246
C -3.205360 -0.465959 -2.692198
C -4.356869 -0.296054 -1.708024
C -3.983823 -0.599601 -0.262957
C -5.137451 -0.482019 0.721242
C -4.722082 -0.775555 2.157190
C -5.870220 -0.664469 3.149026
H -6.671149 -1.367800 2.902459
H -5.542799 -0.878234 4.169589
H -6.300066 0.341660 3.141389
H -3.920937 -0.081031 2.448606
H -4.292616 -1.785973 2.207544
H -5.563890 0.527564 0.664634
H -5.940677 -1.168160 0.425253
H -3.185831 0.083295 0.063061
H -3.575102 -1.619912 -0.213464
H -4.766494 0.718257 -1.783024
H -5.168360 -0.967555 -2.007845
H -2.787329 -1.479275 -2.592245
H -3.595487 -0.434209 -3.717847
H -1.259617 0.365232 -3.302644
H -2.922733 1.906928 -1.259199
H -0.170734 2.372530 -2.573660
H -1.461853 3.560321 -2.621412
H -1.450873 3.762461 -0.153762
H 0.101292 4.154869 -0.866518
H -0.631806 1.521423 0.489254
H 0.885247 1.805593 -0.359659
H -0.139611 3.201501 2.158827
H 1.262535 3.771929 1.276064
H 1.699003 2.158822 3.278488
H 1.052893 0.892050 2.256099
C 3.622718 0.395641 1.933859
C 4.991395 0.198134 1.286395
C 4.991677 0.338882 -0.244000
C 3.881646 -0.433456 -0.907805
O 2.966185 0.092597 -1.525482
N 3.906845 -1.787014 -0.756206
H 4.661077 -2.228765 -0.256445
C 2.821728 -2.585146 -1.280130
C 1.530815 -2.262364 -0.565346
C 1.239525 -2.763343 0.699316

C 0.084415 -2.372414 1.371272
C -0.765283 -1.473966 0.767971
N -0.469124 -1.011866 -0.456774
C 0.632639 -1.367460 -1.124753
H 0.792007 -0.903354 -2.088619
H -1.091112 -0.317079 -0.908507
H -1.677999 -1.107343 1.218312
H -0.152381 -2.754016 2.356198
H 1.925810 -3.458853 1.173034
H 3.070006 -3.639552 -1.147994
H 2.705869 -2.398351 -2.351520
H 4.856825 1.379372 -0.540916
H 5.955531 0.009018 -0.646714
H 5.384827 -0.784936 1.572231
H 5.702333 0.928298 1.686618
H 3.734788 0.325306 3.022125
H 2.964244 -0.437409 1.647627
H 3.570791 2.550467 1.839220
H 2.809745 1.747733 0.480321

conf_51

C 4.298278 0.481979 0.711236
C 3.604365 1.342015 1.764866
C 3.125108 2.685584 1.219809
C 1.869969 2.551711 0.365596
C 1.437927 3.838309 -0.318602
C 0.237280 3.663075 -1.246061
C -1.032206 3.249459 -0.566290
C -1.969682 2.448942 -1.091470
C -3.333879 2.210125 -0.520634
C -3.771184 0.746328 -0.489600
C -5.229181 0.567836 -0.090418
C -5.656286 -0.891205 -0.018875
C -7.117478 -1.076899 0.368274
C -7.530565 -2.539047 0.442459
H -8.582348 -2.644138 0.719947
H -7.391270 -3.038726 -0.521591
H -6.936649 -3.081258 1.185686
H -7.750390 -0.551189 -0.356986
H -7.298425 -0.592099 1.335679
H -5.475793 -1.371634 -0.990229
H -5.021622 -1.422131 0.705164
H -5.866064 1.100980 -0.807547
H -5.402075 1.047093 0.882243
H -3.608638 0.297383 -1.478943
H -3.145354 0.177510 0.211012
H -4.051335 2.763456 -1.142424
H -3.404044 2.651783 0.480503
H -1.778494 2.009344 -2.074818
H -1.244164 3.731823 0.391599
H 0.477471 2.958148 -2.051580
H 0.038183 4.624396 -1.738484

H	1.208452	4.600924	0.436555	C	-3.956888	-2.450629	-0.583479
H	2.274297	4.234607	-0.904305	H	-3.382459	-2.632739	0.332851
H	1.056516	2.199216	1.015376	H	-4.225090	-3.423447	-1.003491
H	2.019175	1.774983	-0.397039	H	-3.300528	-1.957169	-1.308138
H	2.924095	3.377216	2.045846	H	-5.765912	-1.456063	-1.199409
H	3.925947	3.145103	0.626692	H	-5.851894	-2.191916	0.386030
H	4.280588	1.496542	2.612386	H	-4.289194	-0.437051	1.279040
H	2.738988	0.794677	2.168507	H	-5.829169	0.179877	0.716236
C	4.354594	-0.990860	1.093390	H	-3.235318	0.285699	-0.893213
C	5.074105	-1.883750	0.085178	H	-4.781367	0.890012	-1.435713
C	4.555162	-1.756808	-1.354731	H	-3.355480	1.885969	1.082483
C	3.053470	-1.815314	-1.460197	H	-4.871170	2.486960	0.461881
O	2.371427	-0.899296	-1.898441	H	-3.776754	3.297537	-1.598903
N	2.452687	-2.949236	-1.003603	H	-3.099145	4.027159	-0.152759
H	3.007460	-3.708549	-0.643755	H	-1.743495	1.880745	-1.904883
C	1.010472	-3.044434	-1.001073	H	-0.736771	4.073046	-0.034615
C	0.406728	-2.040714	-0.046873	H	0.686684	2.077883	-1.925290
C	0.342022	-2.264854	1.324287	H	1.043360	3.794111	-1.852332
C	-0.147894	-1.285412	2.185734	H	1.495173	1.785992	0.399236
C	-0.557853	-0.083656	1.657122	H	1.646654	3.523831	0.607593
N	-0.489767	0.108708	0.331623	H	3.246573	1.872854	-1.403317
C	-0.031459	-0.812432	-0.519041	H	3.380027	3.596529	-1.170951
H	0.004187	-0.542683	-1.565836	H	4.172425	3.355693	1.103922
H	-0.797778	1.024671	-0.051872	H	5.208673	2.498546	-0.011491
H	-0.940622	0.739680	2.246656	H	4.788169	1.390640	2.185419
H	-0.205055	-1.450810	3.253947	H	3.112769	1.146646	1.769029
H	0.683234	-3.212296	1.730552	C	3.482463	-0.699920	-0.271198
H	0.729328	-4.056698	-0.706048	C	3.811924	-2.134346	-0.663524
H	0.625274	-2.868830	-2.009571	C	2.871089	-2.696433	-1.736571
H	4.850074	-0.803164	-1.793783	C	1.425842	-2.520520	-1.352708
H	4.989609	-2.546733	-1.977332	O	0.675761	-1.719812	-1.891392
H	5.009561	-2.926732	0.418817	N	0.990357	-3.275298	-0.304892
H	6.142656	-1.645428	0.073289	H	1.616647	-3.925514	0.140999
H	4.839326	-1.103074	2.070232	C	-0.352609	-3.110120	0.203740
H	3.325054	-1.353037	1.228460	C	-0.501278	-1.809322	0.958553
H	5.313697	0.863024	0.544529	C	-0.301694	-1.711099	2.332517
H	3.774222	0.584866	-0.244675	C	-0.387016	-0.481533	2.982303
conf_153				C	-0.665853	0.643349	2.240075
C	4.501648	-0.104229	0.692837	N	-0.861819	0.523734	0.919115
C	4.118568	1.229805	1.333530	C	-0.795267	-0.641140	0.268868
C	4.213990	2.475827	0.449532	H	-0.940662	-0.624477	-0.803125
C	3.163514	2.658516	-0.645625	H	-1.054020	1.379356	0.359685
C	1.731221	2.715818	-0.132014	H	-0.738160	1.641432	2.653201
C	0.709523	2.939620	-1.247691	H	-0.236003	-0.396874	4.050892
C	-0.666267	3.250561	-0.750907	H	-0.075355	-2.604114	2.907475
C	-1.804875	2.669880	-1.151856	H	-0.583831	-3.949633	0.861142
C	-3.174254	3.085852	-0.706545	H	-1.058913	-3.131187	-0.629644
C	-3.914205	2.053968	0.150097	H	3.006886	-2.164103	-2.679536
C	-4.177066	0.719992	-0.535359	H	3.086365	-3.755277	-1.914973
C	-4.891767	-0.272963	0.372893	H	3.793265	-2.771212	0.230480
C	-5.195443	-1.619283	-0.277393	H	4.836426	-2.187834	-1.046483
				H	2.486562	-0.668753	0.194186

H	3.406413	-0.097122	-1.180912
H	4.673643	-0.830683	1.497849
H	5.466315	0.004176	0.180685

conf_52

C	4.157429	0.742017	-0.950696
C	4.133587	1.915468	0.024336
C	3.226297	3.056007	-0.431895
C	1.754461	2.802678	-0.125240
C	0.812629	3.798688	-0.785566
C	-0.628615	3.716765	-0.285589
C	-1.273444	2.378031	-0.463701
C	-2.122601	1.805422	0.399384
C	-2.890653	0.544437	0.148243
C	-4.392081	0.802501	0.002413
C	-5.193662	-0.475269	-0.200436
C	-6.687359	-0.226257	-0.355506
C	-7.494112	-1.502234	-0.556861
C	-8.985049	-1.242499	-0.712117
H	-9.393632	-0.744353	0.172863
H	-9.186111	-0.599639	-1.574941
H	-9.541094	-2.172591	-0.855236
H	-7.323629	-2.174529	0.293651
H	-7.117768	-2.030430	-1.442032
H	-7.062009	0.303599	0.530437
H	-6.856992	0.447679	-1.205592
H	-5.024653	-1.150224	0.649896
H	-4.819751	-1.002876	-1.088238
H	-4.757183	1.328292	0.893693
H	-4.553003	1.482780	-0.841977
H	-2.748439	-0.162145	0.979802
H	-2.516457	0.054972	-0.759820
H	-2.358274	2.337969	1.324713
H	-1.078066	1.869210	-1.411041
H	-1.229297	4.450104	-0.839840
H	-0.685789	4.017337	0.767951
H	1.180824	4.816879	-0.618225
H	0.831756	3.644607	-1.871489
H	1.617035	2.841842	0.966215
H	1.484582	1.785063	-0.439730
H	3.527619	3.994327	0.046565
H	3.354665	3.211968	-1.510678
H	5.156225	2.280693	0.167500
H	3.800718	1.565491	1.013124
C	4.768309	-0.514436	-0.343433
C	4.990832	-1.659395	-1.329794
C	3.758541	-2.032563	-2.163810
C	2.500121	-2.205885	-1.354687
O	1.473192	-1.576643	-1.568149
N	2.551301	-3.095540	-0.324792
H	3.403371	-3.596204	-0.131524
C	1.417311	-3.236408	0.561312

C	1.196824	-1.967548	1.351734
C	1.897644	-1.683738	2.519769
C	1.735029	-0.463373	3.171794
C	0.879870	0.469198	2.630857
N	0.210748	0.171870	1.507444
C	0.334956	-0.994687	0.867785
H	-0.234761	-1.118364	-0.042891
H	-0.410958	0.887012	1.077924
H	0.706484	1.449580	3.055170
H	2.273042	-0.234717	4.082838
H	2.584967	-2.419440	2.926689
H	1.604656	-4.072739	1.236508
H	0.521536	-3.467862	-0.021373
H	3.534939	-1.258417	-2.898872
H	3.951583	-2.956691	-2.720091
H	5.361772	-2.537013	-0.785560
H	5.790818	-1.392178	-2.027959
H	5.729958	-0.266486	0.120906
H	4.121297	-0.855543	0.477355
H	4.723117	1.034919	-1.844595
H	3.139414	0.525435	-1.295238

conf_117

C	3.393908	1.492998	-0.028909
C	2.325840	2.227367	0.774031
C	1.425517	3.086584	-0.101037
C	0.329765	3.815959	0.663126
C	-0.580442	4.656084	-0.225640
C	-1.457590	3.856500	-1.189671
C	-2.537274	3.058756	-0.526464
C	-3.038919	1.891469	-0.951376
C	-4.291257	1.264304	-0.409405
C	-4.128532	-0.110443	0.241727
C	-3.585965	-1.195868	-0.678192
C	-3.223157	-2.474482	0.063103
C	-2.580648	-3.532587	-0.822652
C	-2.124963	-4.758979	-0.047132
H	-1.408858	-4.488691	0.738141
H	-2.969265	-5.250815	0.444613
H	-1.647781	-5.495937	-0.698163
H	-1.727874	-3.088505	-1.355244
H	-3.288063	-3.831599	-1.604467
H	-2.537896	-2.231412	0.889361
H	-4.118949	-2.890150	0.540960
H	-2.700005	-0.833239	-1.216720
H	-4.324013	-1.415079	-1.459260
H	-3.480460	-0.018120	1.123770
H	-5.101311	-0.427582	0.633208
H	-5.005172	1.176076	-1.238976
H	-4.746014	1.951292	0.311573
H	-2.589187	1.428080	-1.833382
H	-3.032579	3.547224	0.316679

H	-0.857229	3.219581	-1.848993
H	-1.961470	4.571024	-1.854501
H	-1.230367	5.277849	0.401195
H	0.034683	5.352794	-0.805452
H	0.789967	4.463691	1.417834
H	-0.276346	3.093323	1.230199
H	2.034042	3.824216	-0.639408
H	0.986976	2.447295	-0.879434
H	2.787231	2.840417	1.557838
H	1.709300	1.485936	1.303596
C	3.998557	0.318587	0.730611
C	4.893232	-0.597072	-0.103705
C	4.253665	-1.092003	-1.412220
C	2.809862	-1.500668	-1.267947
O	1.899560	-0.984901	-1.901211
N	2.534566	-2.468812	-0.351046
H	3.275923	-2.867843	0.201598
C	1.159989	-2.815502	-0.071769
C	0.441288	-1.712728	0.674284
C	0.416480	-1.657826	2.065061
C	-0.230705	-0.620043	2.730253
C	-0.852840	0.356179	1.986965
N	-0.816459	0.286701	0.648256
C	-0.200729	-0.695273	-0.019793
H	-0.210533	-0.651263	-1.100825
H	-1.333216	1.011752	0.121722
H	-1.387477	1.195886	2.411990
H	-0.258993	-0.572329	3.811238
H	0.903842	-2.439034	2.640804
H	1.143062	-3.730633	0.521896
H	0.642083	-3.018095	-1.012169
H	4.265058	-0.311738	-2.173830
H	4.827746	-1.935750	-1.810365
H	5.198790	-1.450985	0.513272
H	5.822059	-0.080696	-0.366026
H	4.568175	0.681605	1.593499
H	3.175599	-0.277227	1.149323
H	4.181740	2.192556	-0.332945
H	2.933050	1.132236	-0.954434

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C	4.173834	-0.684323	-0.980910
C	3.186322	0.437776	-0.677718
C	3.365022	1.664181	-1.563286
C	2.485123	2.842353	-1.157662
C	0.989402	2.567023	-1.260925
C	0.151727	3.744943	-0.785778
C	-1.324967	3.510470	-0.660580
C	-1.988514	2.398380	-1.003777
C	-3.475965	2.252804	-0.937550
C	-3.968583	1.031854	-0.155446
C	-3.659642	-0.311168	-0.809405

C	-4.202828	-1.490702	-0.008501
C	-4.145363	-2.829470	-0.739145
C	-2.738349	-3.346565	-1.005864
H	-2.203328	-3.529723	-0.066400
H	-2.767281	-4.294160	-1.550277
H	-2.144381	-2.640856	-1.592154
H	-4.683709	-2.732518	-1.689861
H	-4.698278	-3.574112	-0.156326
H	-3.664014	-1.569618	0.948805
H	-5.245527	-1.280667	0.258875
H	-2.582160	-0.434198	-0.977329
H	-4.113630	-0.321549	-1.809086
H	-3.566730	1.061772	0.868797
H	-5.054462	1.117633	-0.036703
H	-3.858582	2.177870	-1.964663
H	-3.908889	3.164895	-0.513873
H	-1.429161	1.552899	-1.406815
H	-1.907336	4.362158	-0.303582
H	0.300201	4.599395	-1.459754
H	0.540873	4.107315	0.179361
H	0.729802	2.324713	-2.298496
H	0.740679	1.669897	-0.683027
H	2.734870	3.713227	-1.774590
H	2.728488	3.126760	-0.123347
H	4.414881	1.978710	-1.535946
H	3.157062	1.392586	-2.606375
H	3.306803	0.733832	0.375461
H	2.161082	0.068569	-0.773853
C	3.928347	-1.959256	-0.165438
C	3.080005	-3.021209	-0.868993
C	1.721409	-2.562287	-1.395099
C	0.735219	-2.013577	-0.396958
O	-0.085019	-1.152575	-0.690642
N	0.770350	-2.525544	0.860672
H	1.445027	-3.235734	1.093072
C	-0.167299	-2.072559	1.864377
C	0.034680	-0.610212	2.179734
C	1.016181	-0.148565	3.049235
C	1.211719	1.218650	3.240124
C	0.433985	2.108344	2.535589
N	-0.508739	1.636926	1.703846
C	-0.728871	0.333963	1.513197
H	-1.492516	0.068715	0.795210
H	-1.039397	2.282583	1.091211
H	0.533769	3.183697	2.601722
H	1.969693	1.589667	3.918053
H	1.643910	-0.857950	3.580096
H	-0.026659	-2.674757	2.763428
H	-1.191827	-2.226687	1.512873
H	1.833526	-1.788685	-2.158043
H	1.217235	-3.400439	-1.892492
H	2.960281	-3.891711	-0.209350

H	3.642339	-3.401953	-1.728264
H	4.885023	-2.426574	0.087224
H	3.470877	-1.682805	0.794326
H	5.186841	-0.316169	-0.786678
H	4.147921	-0.920183	-2.053047

conf_130

C	4.888208	-0.717426	0.175191
C	5.420762	0.529456	-0.530631
C	4.400275	1.652913	-0.700925
C	4.033797	2.355521	0.604934
C	2.767204	3.201772	0.507648
C	1.503918	2.337548	0.499475
C	0.239381	3.124727	0.359519
C	-0.623068	2.998959	-0.657279
C	-1.902907	3.759859	-0.820168
C	-3.142868	2.915485	-0.494939
C	-3.295788	1.660584	-1.348211
C	-4.288975	0.655896	-0.781164
C	-4.355736	-0.639196	-1.579764
C	-5.211693	-1.706932	-0.916409
H	-5.245912	-2.624101	-1.510126
H	-4.825282	-1.963360	0.077464
H	-6.241471	-1.362618	-0.783061
H	-3.335619	-1.020133	-1.729623
H	-4.738926	-0.428002	-2.584512
H	-4.012565	0.421692	0.258241
H	-5.287455	1.106476	-0.722958
H	-2.325866	1.159365	-1.461519
H	-3.591026	1.943424	-2.365647
H	-3.104642	2.634018	0.567383
H	-4.037152	3.539258	-0.596366
H	-1.973034	4.121064	-1.852906
H	-1.889102	4.644270	-0.175748
H	-0.373423	2.282340	-1.442351
H	0.038813	3.875124	1.128021
H	1.486804	1.771784	1.444066
H	1.561525	1.597836	-0.307652
H	2.714501	3.899314	1.351240
H	2.792837	3.814479	-0.401220
H	4.874083	2.986575	0.913640
H	3.901499	1.619811	1.408900
H	4.798539	2.399356	-1.397374
H	3.501060	1.253312	-1.184592
H	5.798513	0.236729	-1.517471
H	6.286489	0.913030	0.022597
C	3.794447	-1.442281	-0.600089
C	3.346009	-2.725319	0.085995
C	2.292998	-3.527560	-0.691562
C	0.945749	-2.857344	-0.716197
O	0.713678	-1.826383	-1.332538
N	-0.034567	-3.454553	0.021687

H	0.158748	-4.322336	0.493579
C	-1.392828	-2.958644	-0.013562
C	-1.605262	-1.752942	0.871316
C	-2.261912	-1.822247	2.096897
C	-2.427533	-0.685186	2.884603
C	-1.934454	0.516626	2.429152
N	-1.309169	0.559748	1.244203
C	-1.135644	-0.511241	0.465848
H	-0.602840	-0.379495	-0.469282
H	-0.967521	1.471513	0.877962
H	-2.022725	1.451347	2.968195
H	-2.939333	-0.729569	3.837488
H	-2.654830	-2.773562	2.442929
H	-2.065098	-3.760266	0.296002
H	-1.642341	-2.691239	-1.044772
H	2.612212	-3.635965	-1.732918
H	2.207632	-4.533940	-0.270231
H	2.967754	-2.501169	1.092318
H	4.213767	-3.378297	0.230856
H	2.929119	-0.790562	-0.751788
H	4.164146	-1.685609	-1.604987
H	4.516362	-0.457752	1.175222
H	5.723998	-1.407619	0.342012

conf_120

C	4.425096	0.571718	0.801728
C	3.157181	1.273796	0.327900
C	3.293038	2.791525	0.244744
C	2.149694	3.456915	-0.517501
C	0.777007	3.208576	0.094562
C	-0.371343	3.686447	-0.794529
C	-1.728914	3.424447	-0.221771
C	-2.683112	2.687144	-0.805640
C	-4.076925	2.493590	-0.283742
C	-4.352538	1.099563	0.292232
C	-4.094473	-0.054290	-0.669965
C	-4.061986	-1.413449	0.015635
C	-3.666388	-2.553482	-0.913318
C	-3.487923	-3.877795	-0.187080
H	-4.413258	-4.184828	0.309054
H	-3.200263	-4.679235	-0.872450
H	-2.715624	-3.802906	0.588027
H	-2.735169	-2.287864	-1.433856
H	-4.420605	-2.660914	-1.701110
H	-3.355208	-1.377097	0.858578
H	-5.039368	-1.626907	0.465527
H	-3.141426	0.096485	-1.194595
H	-4.855676	-0.051965	-1.459244
H	-3.742590	0.963893	1.196279
H	-5.390448	1.059159	0.639401
H	-4.779187	2.686213	-1.103770
H	-4.283630	3.244906	0.484970

H	-2.452888	2.238628	-1.774208
H	-1.960907	3.918604	0.725105
H	-0.291861	3.213764	-1.780404
H	-0.266993	4.766561	-0.960494
H	0.667471	2.133583	0.267447
H	0.714782	3.689584	1.080019
H	2.148789	3.077542	-1.547835
H	2.327724	4.535880	-0.587943
H	3.372070	3.214126	1.254752
H	4.234947	3.037609	-0.259227
H	2.345667	1.009149	1.020331
H	2.847246	0.896663	-0.652448
C	4.282855	-0.943435	0.982247
C	4.592741	-1.794381	-0.250996
C	3.747835	-1.526738	-1.497459
C	2.254095	-1.652365	-1.334345
O	1.458564	-0.886638	-1.860307
N	1.802684	-2.684724	-0.570706
H	2.456644	-3.303905	-0.120695
C	0.383570	-2.858005	-0.359130
C	-0.172146	-1.771849	0.531581
C	-0.163186	-1.870699	1.919569
C	-0.625057	-0.824150	2.714011
C	-1.092758	0.315716	2.101433
N	-1.099512	0.385368	0.762602
C	-0.662507	-0.600526	-0.026402
H	-0.682324	-0.430542	-1.094516
H	-1.466894	1.249392	0.320730
H	-1.466047	1.181887	2.632738
H	-0.623897	-0.892315	3.794330
H	0.210533	-2.774813	2.390903
H	0.213926	-3.834683	0.096770
H	-0.133803	-2.842317	-1.322040
H	3.926611	-0.524874	-1.891036
H	4.041407	-2.222442	-2.293196
H	4.532247	-2.856438	0.023617
H	5.640454	-1.639944	-0.530409
H	4.960971	-1.275269	1.775094
H	3.269703	-1.165080	1.346495
H	4.724805	1.014399	1.758616
H	5.248205	0.785268	0.107286

conf_64

C	4.083564	0.758360	-0.044500
C	3.851266	1.907574	0.937846
C	2.431225	2.021361	1.508627
C	1.490739	2.951366	0.744636
C	1.242251	2.568384	-0.709034
C	0.128993	3.369617	-1.395556
C	-1.209321	3.332695	-0.716212
C	-2.285608	2.681264	-1.176832
C	-3.659883	2.732335	-0.574931

C	-4.079744	1.460688	0.172528
C	-3.998456	0.179468	-0.649023
C	-4.094741	-1.085336	0.193145
C	-3.868421	-2.362639	-0.604684
C	-3.806340	-3.606753	0.267866
H	-3.642469	-4.509502	-0.326300
H	-2.995367	-3.534296	1.002589
H	-4.736452	-3.744896	0.826879
H	-2.936290	-2.266648	-1.179614
H	-4.662820	-2.472097	-1.351660
H	-3.354599	-1.036165	1.006191
H	-5.071205	-1.129273	0.690932
H	-3.055969	0.153372	-1.211668
H	-4.785613	0.181329	-1.412457
H	-3.457321	1.356667	1.072214
H	-5.100641	1.591695	0.546657
H	-4.377292	2.924458	-1.381774
H	-3.724791	3.585409	0.107945
H	-2.174827	2.112266	-2.101837
H	-1.326990	3.944658	0.180465
H	0.018686	3.009528	-2.423303
H	0.440411	4.419279	-1.465060
H	2.161613	2.710171	-1.285984
H	1.023802	1.496669	-0.789685
H	1.885927	3.974545	0.782821
H	0.535932	2.994686	1.287279
H	1.979744	1.021734	1.571256
H	2.490793	2.382708	2.540890
H	4.117468	2.855845	0.455794
H	4.559538	1.789851	1.765977
C	3.975352	-0.618593	0.603794
C	4.398574	-1.774647	-0.298615
C	3.609950	-1.876312	-1.610229
C	2.117299	-1.858966	-1.409858
O	1.387735	-0.988215	-1.863340
N	1.592620	-2.864936	-0.655893
H	2.192378	-3.584595	-0.286921
C	0.173520	-2.902641	-0.379961
C	-0.237864	-1.765733	0.525178
C	-0.170516	-1.845231	1.912318
C	-0.491631	-0.746209	2.706404
C	-0.868334	0.427896	2.095461
N	-0.932922	0.477747	0.757412
C	-0.640679	-0.560691	-0.028896
H	-0.702744	-0.404059	-1.096736
H	-1.212647	1.360029	0.289909
H	-1.120971	1.334604	2.629689
H	-0.444149	-0.797931	3.786533
H	0.139256	-2.773102	2.383729
H	-0.065561	-3.858091	0.089438
H	-0.385312	-2.841273	-1.318180
H	3.836755	-1.037808	-2.269559

H	3.889969	-2.792403	-2.142055
H	4.318241	-2.714834	0.260931
H	5.458667	-1.673731	-0.553954
H	4.598339	-0.640218	1.506014
H	2.946158	-0.790421	0.947266
H	5.088561	0.865990	-0.471100
H	3.384840	0.828355	-0.884291

conf_102

C	3.140731	-0.063713	0.932708
C	4.361650	0.798902	0.641390
C	4.085929	2.301730	0.635549
C	3.037564	2.760238	-0.386775
C	1.626108	2.896730	0.176794
C	0.601235	3.274822	-0.892104
C	-0.786706	3.464780	-0.364783
C	-1.894152	2.928225	-0.893940
C	-3.295556	3.169269	-0.417492
C	-3.940723	1.954267	0.261199
C	-4.031645	0.709200	-0.615164
C	-4.309861	-0.566345	0.168276
C	-4.272313	-1.823543	-0.690457
C	-4.393898	-3.103639	0.121646
H	-3.579265	-3.188102	0.850939
H	-5.333162	-3.129251	0.681914
H	-4.366966	-3.990910	-0.516179
H	-3.335434	-1.837643	-1.265544
H	-5.073787	-1.779578	-1.436633
H	-3.569130	-0.663768	0.976417
H	-5.281757	-0.491838	0.671460
H	-3.099044	0.573679	-1.177777
H	-4.805209	0.854636	-1.378477
H	-3.376777	1.719403	1.175133
H	-4.942266	2.231225	0.606694
H	-3.908115	3.464748	-1.278142
H	-3.302968	4.015843	0.276175
H	-1.776204	2.299330	-1.779006
H	-0.892645	4.138792	0.488828
H	0.598777	2.525946	-1.693449
H	0.921049	4.217101	-1.357663
H	1.331789	1.958572	0.661445
H	1.626947	3.658340	0.967228
H	3.022435	2.064990	-1.237023
H	3.329374	3.730837	-0.802773
H	3.779123	2.620864	1.640588
H	5.031539	2.815658	0.438467
H	4.786801	0.519058	-0.331029
H	5.139268	0.581504	1.383995
C	3.428086	-1.559170	1.037263
C	3.998893	-2.217334	-0.224077
C	3.314067	-1.836287	-1.542429
C	1.807816	-1.840925	-1.529503

O	1.140890	-0.933501	-2.007564
N	1.194711	-2.901846	-0.935254
H	1.753255	-3.607697	-0.482923
C	-0.233501	-2.865666	-0.698299
C	-0.562795	-1.803409	0.324389
C	-0.556596	-2.052134	1.693492
C	-0.747101	-1.019126	2.608733
C	-0.935009	0.260128	2.137153
N	-0.952569	0.473120	0.813818
C	-0.785389	-0.497378	-0.087841
H	-0.797252	-0.210694	-1.130099
H	-1.106726	1.434472	0.451018
H	-1.076623	1.125744	2.771606
H	-0.744966	-1.203706	3.675354
H	-0.395178	-3.063180	2.055663
H	-0.557531	-3.845992	-0.346248
H	-0.751691	-2.655344	-1.636722
H	3.592270	-0.827080	-1.851038
H	3.651088	-2.507547	-2.340645
H	3.987792	-3.306356	-0.089384
H	5.057136	-1.959754	-0.328615
H	4.127782	-1.738985	1.861381
H	2.498116	-2.066258	1.323373
H	2.383234	0.107811	0.158680
H	2.691790	0.266493	1.879218

conf_158

C	-3.717821	-1.701863	0.186858
C	-4.811855	-0.704486	-0.192585
C	-4.361068	0.487029	-1.035760
C	-3.292152	1.348679	-0.374373
C	-2.989250	2.630494	-1.143692
C	-1.807870	3.413385	-0.563550
C	-0.494260	2.750352	-0.855875
C	0.649197	3.377574	-1.157543
C	1.944885	2.704390	-1.512474
C	1.909180	1.183781	-1.556428
C	3.280429	0.540309	-1.698155
C	3.214003	-0.979321	-1.630787
C	4.568810	-1.663098	-1.746766
C	4.475599	-3.178732	-1.653437
H	5.458411	-3.648869	-1.739141
H	4.041788	-3.490451	-0.696822
H	3.844482	-3.584780	-2.450400
H	5.234652	-1.284522	-0.960399
H	5.035347	-1.380437	-2.697991
H	2.737760	-1.275702	-0.684284
H	2.551776	-1.347611	-2.425628
H	3.943658	0.907797	-0.901134
H	3.747179	0.849369	-2.641631
H	1.431576	0.780968	-0.656650
H	1.263376	0.862450	-2.382116

H	2.730683	3.039721	-0.815051
H	2.278627	3.095278	-2.482577
H	0.653139	4.468196	-1.195218
H	-0.504702	1.660023	-0.867074
H	-1.958680	3.499163	0.524235
H	-1.793759	4.439139	-0.944797
H	-2.781695	2.393204	-2.194517
H	-3.878322	3.270204	-1.144499
H	-2.377775	0.755044	-0.263734
H	-3.620345	1.615575	0.641746
H	-3.991517	0.143602	-2.009856
H	-5.239204	1.106628	-1.253507
H	-5.274695	-0.327715	0.728085
H	-5.604445	-1.238938	-0.729994
C	-3.086500	-2.419143	-1.004118
C	-2.057025	-3.487380	-0.622201
C	-0.606420	-2.986851	-0.500316
C	-0.476692	-1.826601	0.442504
O	-0.528747	-0.661113	0.071522
N	-0.330524	-2.120151	1.765685
H	-0.386963	-3.081124	2.062791
C	-0.453238	-1.078325	2.764213
C	0.610159	-0.020921	2.595827
C	1.926162	-0.191654	3.007692
C	2.885913	0.785474	2.742869
C	2.519410	1.909857	2.040965
N	1.239369	2.050968	1.656210
C	0.296819	1.141882	1.913347
H	-0.689161	1.342828	1.517299
H	0.967667	2.808899	1.012707
H	3.204024	2.699394	1.761111
H	3.913754	0.664515	3.060071
H	2.215634	-1.100268	3.526583
H	-0.367803	-1.539126	3.749882
H	-1.440307	-0.605846	2.701384
H	0.042670	-3.810305	-0.184268
H	-0.255171	-2.636212	-1.473149
H	-2.046607	-4.278561	-1.377333
H	-2.362022	-3.971104	0.314396
H	-3.890050	-2.897228	-1.575488
H	-2.621853	-1.693718	-1.681865
H	-4.154710	-2.456578	0.852901
H	-2.946846	-1.188705	0.773210