

Supporting Information

Unraveling the mechanism of enantio-controlling switches of an alcohol dehydrogenase toward sterically small ketone

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Supplementary tables

Table S1 Results of partial deconvolution of two best mutants SZ2172, SZ2074 and other combination of mutants as catalysts in the asymmetric reduction of substrate **1**.

Enzymes	ee (%)	Favored enantiomer	$\Delta\Delta G^{\ddagger}_{\text{expt}}^a$ (kcal/mol)
WT	25	(<i>R</i>)	-0.3
I86V/W110L/L294Q (SZ2172)	95	(<i>S</i>)	-2.2
I86V	59	(<i>S</i>)	-0.8
W110L	36	(<i>S</i>)	-0.5
L294Q	41	(<i>S</i>)	-0.5
I86V/W110L	72	(<i>S</i>)	-1.1
I86V/L294Q	82	(<i>S</i>)	-1.4
W110L/L294Q	82	(<i>S</i>)	-1.4
I86N/C295N (SZ2074)	99	(<i>R</i>)	-3.2
I86N	89	(<i>R</i>)	-1.7
C295N	95	(<i>R</i>)	-2.2
I86N/C295Q	>99	(<i>R</i>)	-3.2
I86N/L294Q	11	(<i>S</i>)	-0.1
L294Q/C295N	94	(<i>R</i>)	-2.1
I86V/W110L/L294M	90	(<i>S</i>)	-1.8
I86N/L294Q/C295N	70	(<i>R</i>)	-1.0
I86V/W110L/C295N	94	(<i>R</i>)	-2.1
I86V/W110L/L294Q/C295N	62	(<i>R</i>)	-0.9

^a The experimental $\Delta\Delta G^{\ddagger}_{\text{expt}}$ was calculated by $-\text{LN}[(100+\text{ee})/(100-\text{ee})]*T*R$, where $T = 303.15\text{K}$, $R = 8.314472 \text{ kJ/mol}\cdot\text{K}^1$.

Table S2 The calculations of the ee values of *pro*-(*R*) and *pro*-(*S*) conformations.

Variants	Substrate	R ^a	S ^a	ee (%) (<i>R</i>)	ee (%) (<i>S</i>)
I86N/C295N	<i>Pro</i> -(<i>R</i>)- 1	0.95	0	97.7 ± 1.8	-
		0.95	0		
		0.73	0.02		
	<i>Pro</i> -(<i>S</i>)- 1	0.87	0.01	87.7 ± 9.8	-
		0.90	0.02		
		0.85	0.13		
I86V/W110L/L294Q	<i>Pro</i> -(<i>R</i>)- 1	0.1	0	-	-
		0.03	0		
		0.02	0		
	<i>Pro</i> -(<i>S</i>)- 1	0	0.99	-	98.6 ± 0.4
		0	0.99		
		0.01	0.91		

^a Calculation of the conformations taking into account distances lower than 4.5 Å which is closer the catalytic distance and their corresponding dihedral are used to classify the *pro*-(*R*) (-100° ~ -60°) and *pro*-(*S*) (60° ~ 100°) conformations. The method of calculation is based on ref 2.

Table S3 Calculated absolute and relative activation barriers for WT and other important mutants.

Enzymes	TS- <i>pro</i> -(<i>R</i>) (kcal/mol)	TS- <i>pro</i> -(<i>S</i>) (kcal/mol)	$\Delta\Delta E^\ddagger_{\text{calc.}}$ ^a (kcal/mol)	$\Delta\Delta G^\ddagger_{\text{expt}}$ ^b (kcal/mol)
WT	9.3	11.5	-2.2	-0.3
I86N	9.9	12.0	-2.1	-1.7
C295N	9.6	13.2	-3.6	-2.2
L294Q/C295N	10.1	10.5	-0.4	-2.1
I86N/C295N	10.5	12.7	-2.2	-3.2
I86N/C295Q	9.4	12.5	-3.1	-3.2
L294Q	12.7	9.1	+3.6	+0.5
I86N/L294Q	14.5	9.4	+3.9	+0.1
I86V/W110L/L294Q	13.8	9.1	+4.7	+2.2
I86V/W110L/L294M	11.4	9.6	+1.8	+1.8

^a The calculated $\Delta\Delta E^\ddagger_{\text{calc.}}$ was calculated by [TS-*pro*-(*R*)] – [TS-*pro*-(*S*)].

^b The experimental $\Delta\Delta G^\ddagger_{\text{expt}}$ was calculated by $-\text{LN}[(100+\text{ee})/(100-\text{ee})]*T*R$, where T = 303.15K, R = 8.314472 kJ/mol·K¹.

Table S4 Results of site-directed saturation mutagenesis of C295 and L294 based on the mutant I86N and I86V/W110L, respectively.

Library	Enzymes	ee (%)	c ^a (%)	Favored enantiomer
A	I86N/C295G	94	80	(R)
	I86N/C295A	89	97	(R)
	I86N/C295V	90	95	(R)
	I86N/C295L	86	95	(R)
	I86N/C295M	>99	57	(R)
	I86N/C295I	>99	84	(R)
	I86N/C295S	94	80	(R)
	I86N/C295T	89	96	(R)
	I86N/C295P	>99	14	(R)
	I86N/C295N	99	96	(R)
	I86N/C295Q	>99	93	(R)
	I86N/C295K	72	62	(R)
	I86N/C295R	94	42	(R)
	I86N/C295H	>99	72	(R)
	I86N/C295D	>99	89	(R)
	I86N/C295E	>99	88	(R)
	I86N/C295F	83	41	(R)
	I86N/C295Y	87	39	(R)
	I86N/C295W	87	15	(R)
B	I86V/W110L/L294G	39	30	(S)
	I86V/W110L/L294A	20	85	(S)
	I86V/W110L/L294V	62	96	(S)
	I86V/W110L/L294M	90	95	(S)
	I86V/W110L/L294I	59	95	(S)
	I86V/W110L/L294S	20	87	(S)
	I86V/W110L/L294T	46	95	(S)
	I86V/W110L/L294C	11	93	(R)
	I86V/W110L/L294P	21	80	(S)
	I86V/W110L/L294N	57	50	(S)
	I86V/W110L/L294Q	95	96	(S)
	I86V/W110L/L294K	.. ^b	<5	.. ^b
	I86V/W110L/L294R	.. ^b	<5	.. ^b
	I86V/W110L/L294H	42	46	(S)
	I86V/W110L/L294D	.. ^b	<5	.. ^b
	I86V/W110L/L294E	50	94	(S)
	I86V/W110L/L294F	41	63	(S)
	I86V/W110L/L294Y	33	53	(S)
	I86V/W110L/L294W	.. ^b	<5	.. ^b

^a Conversion.

^b ee value was not determined if conversion is lower than 5%.

Table S5 Primers used for construction of mutants.

Enzymes	Name	Sequence (5' to 3')
I86V/W110L/L294Q (SZ2172)	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-Q-R2	ACGTCCACCGGGGCATTGCCCCGCTTTTATAG
I86V	ADH-I86-V-F	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-I86-wt-R	AGCTGGCACAACAACGCGATCACCAGGTTTAAAATC
W110L	ADH-W110-L-F	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-W110-wt-R	GCCTGCCAGCATTCCACCGGAGTGCTGGTGATATC
L294Q	ADH-L294-Q-F	ACTATAAAAGGCGGGCAATGCCCGGTGGACGTCTAAG
	ADH-L294-wt-R	CCCCGCTTTTATAGTTTTATGAGCCATGCC
I86V/W110L	ADH-I86-V-F	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
I86V/L294Q	ADH-I86-V-F	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-L294-Q-R	ACGTCCACCGGGGCATTGCCCCGCTTTTATAG
W110L/L294Q	ADH-W110-L-F	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-Q-R	ACGTCCACCGGGGCATTGCCCCGCTTTTATAG
I86N/C295N (SZ2074)	ADH-I86-N-F	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG
	ADH-C295-N-R	TAGACGTCCACCGGGATTAGCCCGCCTTTTATAG
I86N	ADH-I86-N-F	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG
	ADH-I86-wt-R	AGCTGGCACAACAACGCGATCACCAGGTTTAAAATC
C295N	ADH-C295-N-F	ATAAAAGGCGGGCTAATCCCGGTGGACGTCTAAG
	ADH-C295-wt-R	TAGCCCGCCTTTTATAGTTTTATGAGCCATG
I86N/L294Q	ADH-I86-N-F	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG
	ADH-L294-Q-R	ACGTCCACCGGGGCATTGCCCCGCTTTTATAG
L294Q/C295N	ADH-L294-Q-C295-N-F	ACTATAAAAGGCGGGCAAAATCCCGGTGGACGTCTAAG
	ADH-L294-wt-R	CCCCGCTTTTATAGTTTTATGAGCCATGCC
I86N/L294Q/C295N	ADH-I86-N-F	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG
	ADH-L294-Q-C295-N-R	TAGACGTCCACCGGGATTTTGCCCCGCTTTTATAGTTTTATG
I86V/W110L/C295N	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-C295-N-R2	TAGACGTCCACCGGGATTAGCCCGCCTTTTATAG
I86V/W110L/L294Q/C295N	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-Q-C295-N-R2	TAGACGTCCACCGGGATTTTGCCCCGCTTTTATAGTTTTATG
I86N/C295G	ADH-I86-N-F	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG
	ADH-C295-G-R	CTTAGACGTCCACCGGGACCTAGCCCGCCTTTTATAG

I86N/C295A	ADH-I86-N-F ADH-C295-A-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGCGCTAGCCCGCCTTTTATAG
I86N/C295V	ADH-I86-N-F ADH-C295-V-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGCACTAGCCCGCCTTTTATAG
I86N/C295L	ADH-I86-N-F ADH-C295-L-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGCAGTAGCCCGCCTTTTATAG
I86N/C295M	ADH-I86-N-F ADH-C295-M-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGCATTAGCCCGCCTTTTATAG
I86N/C295I	ADH-I86-N-F ADH-C295-I-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGAATTAGCCCGCCTTTTATAG
I86N/C295S	ADH-I86-N-F ADH-C295-S-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGGCTTAGCCCGCCTTTTATAG
I86N/C295T	ADH-I86-N-F ADH-C295-T-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGGGTTAGCCCGCCTTTTATAG
I86N/C295P	ADH-I86-N-F ADH-C295-P-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGCGGTAGCCCGCCTTTTATAG
I86N/C295Q	ADH-I86-N-F ADH-C295-Q-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGCTGTAGCCCGCCTTTTATAG
I86N/C295K	ADH-I86-N-F ADH-C295-K-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGTTTAGCCCGCCTTTTATAG
I86N/C295R	ADH-I86-N-F ADH-C295-R-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGACGTAGCCCGCCTTTTATAG
I86N/C295H	ADH-I86-N-F ADH-C295-H-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGATGTAGCCCGCCTTTTATAG
I86N/C295D	ADH-I86-N-F ADH-C295-D-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGATCTAGCCCGCCTTTTATAG
I86N/C295E	ADH-I86-N-F ADH-C295-E-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGTTCTAGCCCGCCTTTTATAG
I86N/C295F	ADH-I86-N-F ADH-C295-F-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGAAATAGCCCGCCTTTTATAG
I86N/C295Y	ADH-I86-N-F ADH-C295-Y-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGATATAGCCCGCCTTTTATAG
I86N/C295W	ADH-I86-N-F ADH-C295-W-R	GTTGTTGTGCCAGCTAATACCCCTGATTGGCGG CTTAGACGTCCACCGGGCCATAGCCCGCCTTTTATAG
I86V/W110L/L294G	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-G-R2	GACGTCCACCGGGGCAACCCCGCCTTTTATAGT
I86V/W110L/L294A	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-A-R2	GACGTCCACCGGGGCAACCCCGCCTTTTATAGT
I86V/W110L/L294V	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG

	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-V-R2	GACGTCCACCGGGGCACCCCCGCTTTTATAGT
I86V/W110L/L294M	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-M-R2	GACGTCCACCGGGGCACATCCCGCCTTTTATAGT
I86V/W110L/L294I	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-I-R2	GACGTCCACCGGGGCAATCCCGCCTTTTATAGT
I86V/W110L/L294S	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-S-R2	GACGTCCACCGGGGCAGCTCCCGCCTTTTATAGT
I86V/W110L/L294T	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-T-R2	GACGTCCACCGGGGCAGTCCCGCCTTTTATAGT
I86V/W110L/L294C	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-C-R2	GACGTCCACCGGGGCAGCACCCGCCTTTTATAGT
I86V/W110L/L294P	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-P-R2	GACGTCCACCGGGGCACGGCCCGCCTTTTATAGT
I86V/W110L/L294N	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-N-R2	GACGTCCACCGGGGCAATTCCCGCCTTTTATAGT
I86V/W110L/L294K	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-K-R2	GACGTCCACCGGGGCATTTCCCGCCTTTTATAGT
I86V/W110L/L294R	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-R-R2	GACGTCCACCGGGGCACGCCCCGCCTTTTATAGT
I86V/W110L/L294H	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-H-R2	GACGTCCACCGGGGCAATGCCCCGCCTTTTATAGT
I86V/W110L/L294D	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG

	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-D-R2	GACGTCCACCGGGGCAATCCCCGCCTTTTATAGT
I86V/W110L/L294E	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-E-R2	GACGTCCACCGGGGCAATCCCCGCCTTTTATAGT
I86V/W110L/L294F	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-F-R2	GACGTCCACCGGGGCAAAACCCGCCTTTTATAGT
I86V/W110L/L294Y	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-Y-R2	GACGTCCACCGGGGCAATACCCGCCTTTTATAGT
I86V/W110L/L294W	ADH-I86-V-F1	GTTGTTGTGCCAGCTGTTACCCCTGATTGGCGG
	ADH-W110-L-R1	TACATTCGAAAATTTCAAGCCTGCCAGCATTCC
	ADH-W110-L-F2	GGAATGCTGGCAGGCTTGAAATTTTCGAATGTAAAAAG
	ADH-L294-W-R2	GACGTCCACCGGGGCAACCAACCCGCCTTTTATAGT

Table S6 Tables with calculated energies and energy corrections.

	E_{el}^a (a.u.)	E_{bb}^b (a.u.)	E_{solv}^c (a.u.)	E_{ZPE}^d (a.u.)	E_{tot}^e (a.u.)	E_{rel}^f (kcal/mol)
I86N/C295N-pro-(R)						
ES	-6425.521170	-6427.256195	-6425.628486	2.1596322	-6425.203878	0
TS	-6425.504038	-6427.236679	-6425.610316	2.1558427	-6425.187115	10.5
EP	-6425.518984	-6427.253659	-6425.622867	2.1599284	-6425.197613	3.9
I86N/C295N-pro-(S)						
ES	-6425.519735	-6427.253023	-6425.628241	2.1596138	-6425.201915	1.2
TS	-6425.500858	-6427.231602	-6425.609529	2.1566587	-6425.183614	12.7
EP	-6425.516163	-6427.248064	-6425.620167	2.1607442	-6425.191323	7.9
I86V/W110L/L294Q-pro-(R)						
ES	-6410.253874	-6411.903196	-6410.359651	2.1028652	-6409.906108	2.6
TS	-6410.239595	-6411.886165	-6410.341618	2.0998411	-6409.888347	13.8
EP	-6410.253058	-6411.902321	-6410.35459	2.1026271	-6409.901225	5.7
I86V/W110L/L294Q-pro-(S)						
ES	-6410.260582	-6411.909007	-6410.365409	2.1035089	-6409.910326	0
TS	-6410.247813	-6411.893989	-6410.349822	2.1002138	-6409.895784	9.1
EP	-6410.259830	-6411.907869	-6410.361809	2.1036084	-6409.906240	2.6
WT-pro-(R)						
ES	-6604.225953	-6605.911278	-6604.326291	2.1871848	-6603.824431	0
TS	-6604.210619	-6605.893942	-6604.309965	2.1836143	-6603.809675	9.3
EP	-6604.227630	-6605.911000	-6604.319907	2.1885353	-6603.814741	6.1
WT-pro-(S)						
ES	-6604.227177	-6605.910784	-6604.325942	2.1877158	-6603.821834	1.6
TS	-6604.209231	-6605.890842	-6604.308911	2.1844871	-6603.806035	11.5
EP	-6604.225282	-6605.908024	-6604.318879	2.1893084	-6603.812312	7.6
I86N-pro-(R)						
ES	-6654.982987	-6656.691306	-6655.087918	2.1315635	-6654.664673	0
TS	-6654.966695	-6656.672928	-6655.070463	2.1277549	-6654.648941	9.9
I86N-pro-(S)						
ES	-6654.980330	-6656.689300	-6655.082105	2.1300548	-6654.661021	2.3
TS	-6654.959802	-6656.667584	-6655.064111	2.1263375	-6654.645555	12.0
I86N/L294Q-pro-(R)						
ES	-6745.055795	-6746.806713	-6745.166458	2.1016163	-6744.815760	2.9
TS	-6745.036884	-6746.784472	-6745.150241	2.0985917	-6744.799237	13.3
I86N/L294Q-pro-(S)						
ES	-6745.057788	-6746.809487	-6745.170408	2.1017360	-6744.820370	0

TS	-6745.044663	-6746.792849	-6745.155744	2.0985852	-6744.805344	9.4
L294Q/C295N-pro-(R)						
ES	-6464.829363	-6466.576808	-6464.943201	2.1985034	-6464.492143	0.3
TS	-6464.811259	-6466.556539	-6464.926560	2.1953188	-6464.476522	10.1
L294Q/C295N-pro-(S)						
ES	-6464.835953	-6466.579654	-6464.949838	2.2008919	-6464.492647	0
TS	-6464.819559	-6466.560278	-6464.933091	2.1978350	-6464.475975	10.5
L294Q-pro-(R)						
ES	-6694.291162	-6696.016255	-6694.399963	2.1578284	-6693.967228	3.8
TS	-6694.275683	-6695.997907	-6694.385602	2.1547267	-6693.953099	12.7
L294Q-pro-(S)						
ES	-6694.297046	-6696.022382	-6694.406887	2.1589355	-6693.973288	0
TS	-6694.283812	-6696.005940	-6694.392086	2.1554827	-6693.958732	9.1
C295N-pro-(R)						
ES	-6374.760281	-6376.470364	-6374.865573	2.216095	-6374.359560	0
TS	-6374.743903	-6376.451900	-6374.849111	2.212778	-6374.344330	9.6
C295N-pro-(S)						
ES	-6374.761491	-6376.469236	-6374.865736	2.216522	-6374.356958	1.6
TS	-6374.744115	-6376.448600	-6374.847373	2.213376	-6374.338481	13.2
I86N/C295Q-pro-(R)						
ES	-6464.835854	-6466.582060	-6464.945092	2.187135	-6464.504164	0
TS	-6464.820923	-6466.564788	-6464.929026	2.183755	-6464.489135	9.4
EP	-6464.835616	-6466.581285	-6464.942626	2.186933	-6464.501362	1.8
I86N/C295Q-pro-(S)						
ES	-6464.845250	-6466.583336	-6464.948114	2.188625	-6464.497575	4.1
TS	-6464.829981	-6466.566398	-6464.932791	2.185021	-6464.484186	12.5
EP	-6464.845048	-6466.582837	-6464.945274	2.189584	-6464.493479	6.7
I86V/W110L/L294M-pro-(R)						
ES	-6679.051829	-6680.685435	-6679.148313	2.104706	-6678.677212	2.7
TS	-6679.038994	-6680.670233	-6679.133791	2.101642	-6678.663388	11.4
EP	-6679.050943	-6680.685620	-6679.147055	2.104239	-6678.677493	2.6
I86V/W110L/L294M-pro-(S)						
ES	-6679.057262	-6680.690306	-6679.153010	2.1044736	-6678.681580	0
TS	-6679.042946	-6680.673745	-6679.136637	2.1011261	-6678.666310	9.6
EP	-6679.055855	-6680.688581	-6679.150331	2.1044614	-6678.678596	1.9

^a E_{el} = Energy of the optimized geometry at B3LYP-D3(BJ)/6-31G(d,p) level.

^b E_{bb} = Single-point energy of the optimized geometry at B3LYP-D3(BJ)/6-311+G(2d,2p) level.

^c E_{solv} = Single-point energy of the optimized geometry at B3LYP-D3(BJ)/6-31G(d,p) and SMD solvation method with $\epsilon = 4$.

^d E_{zpe} = Zero-point energy of the optimized geometry at B3LYP-D3(BJ)/6-31G(d,p).

^e $E_{\text{tot}} = E_{\text{bb}} + (E_{\text{solv}} - E_{\text{el}}) + E_{\text{ZPE}}$

^f E_{rel} = Energy relative to the lowest-energy binding mode.

Supplementary figures

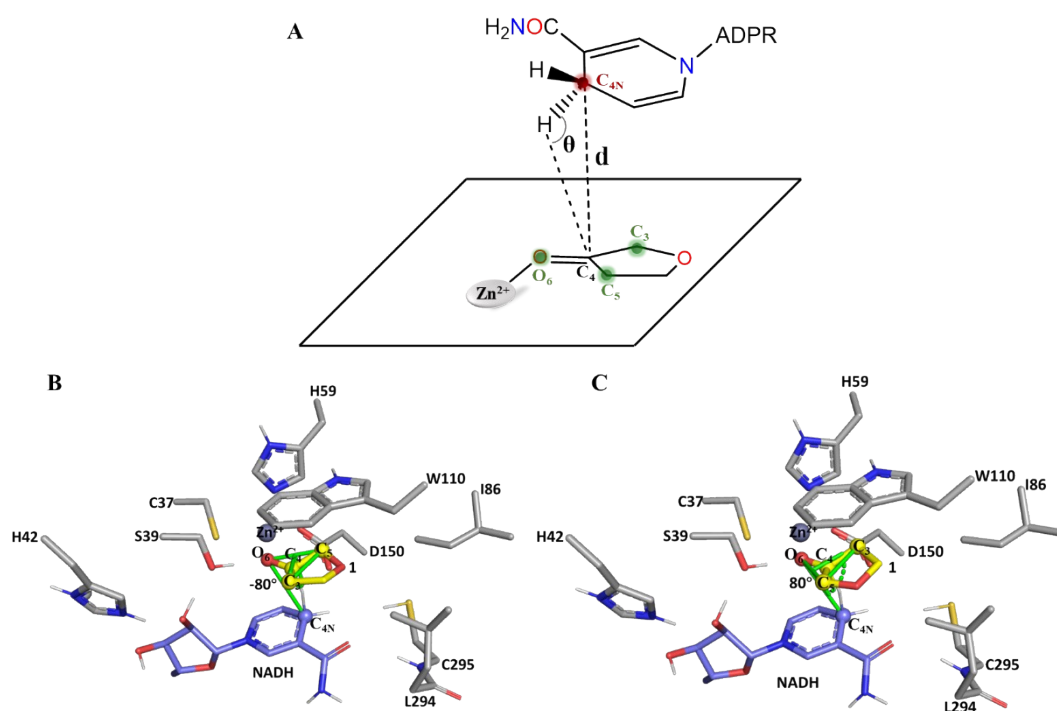


Fig. S1 (A) Representation of selected dihedral angle $\angle\text{C4N-O6-C5-C3}$ between the cofactor NADH (C4N) and substrate **1** (O6, C5, C3). The dihedral angle was selected to distinguish the (C) *pro-R* and (D) *pro-S* orientations. The bond angle (θ) is between NADH (C4N, H) and substrate **1** (C4). The hydride transfer is influenced by the distance d (C4N-C4) between NADH (C4N) and substrate **1** (C4). The angle is obtained based on transition state of wild type through quantum mechanical calculations. Atoms used to calculate the dihedral and bond angle are shown in spheres. ADPR = adenosine diphosphoribose.

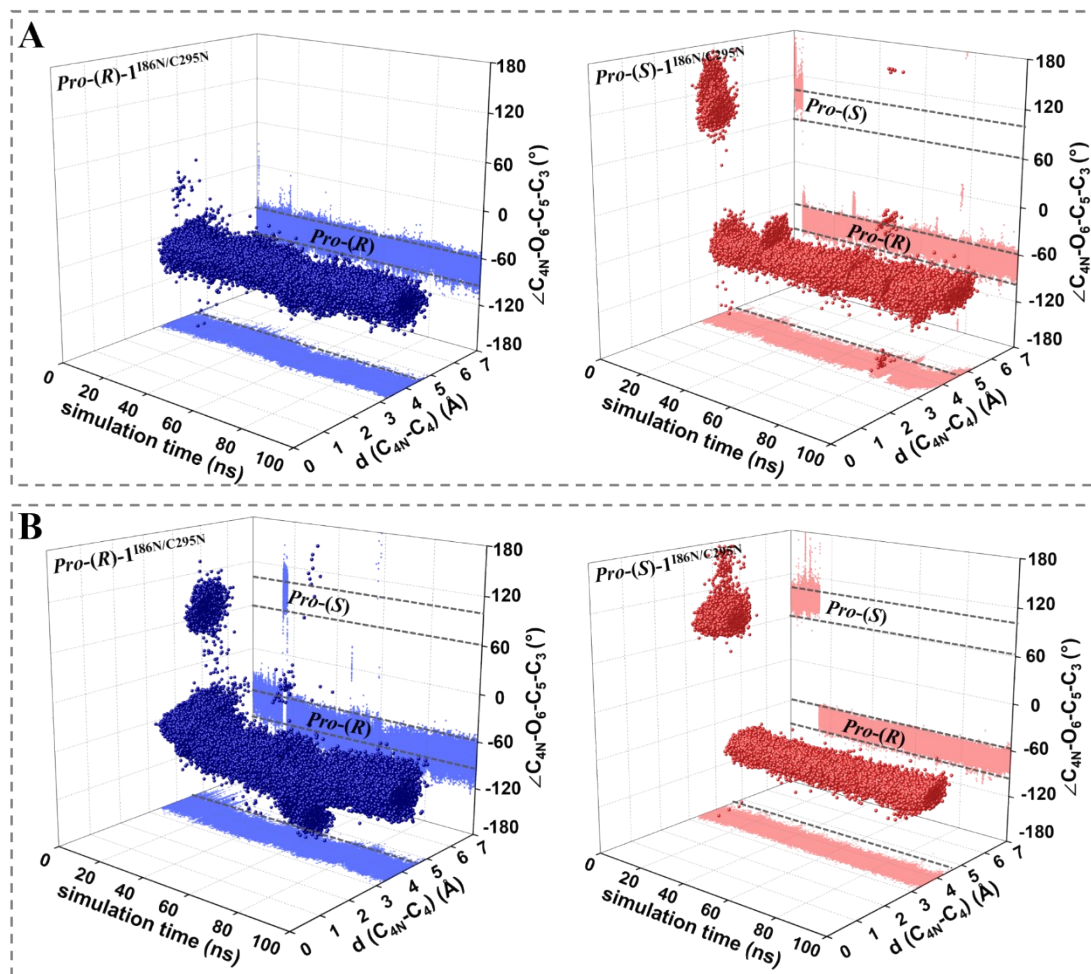


Fig. S2 3D plots of the divergence of the $\angle C4N-O6-C5-C3$ and $d(C4N-C4)$ (detailed in Fig. S1) during the 100 ns MD simulations for *pro-(R)* and *pro-(S)* orientations of prochiral substrate 1 in (A) repeat2 and (B) repeat3 for the I86N/C295N mutant. The dashed lines shown in panels A and B indicate the preference regions of *pro-(R)* ($\angle C4N-O6-C5-C3$ from -60° to -100°) and *pro-(S)* ($\angle C4N-O6-C5-C3$ from 60° to 100°), and the distance $d(C4N-C4)$ shorter than 4.5 Å has been defined as catalytically competent pose.

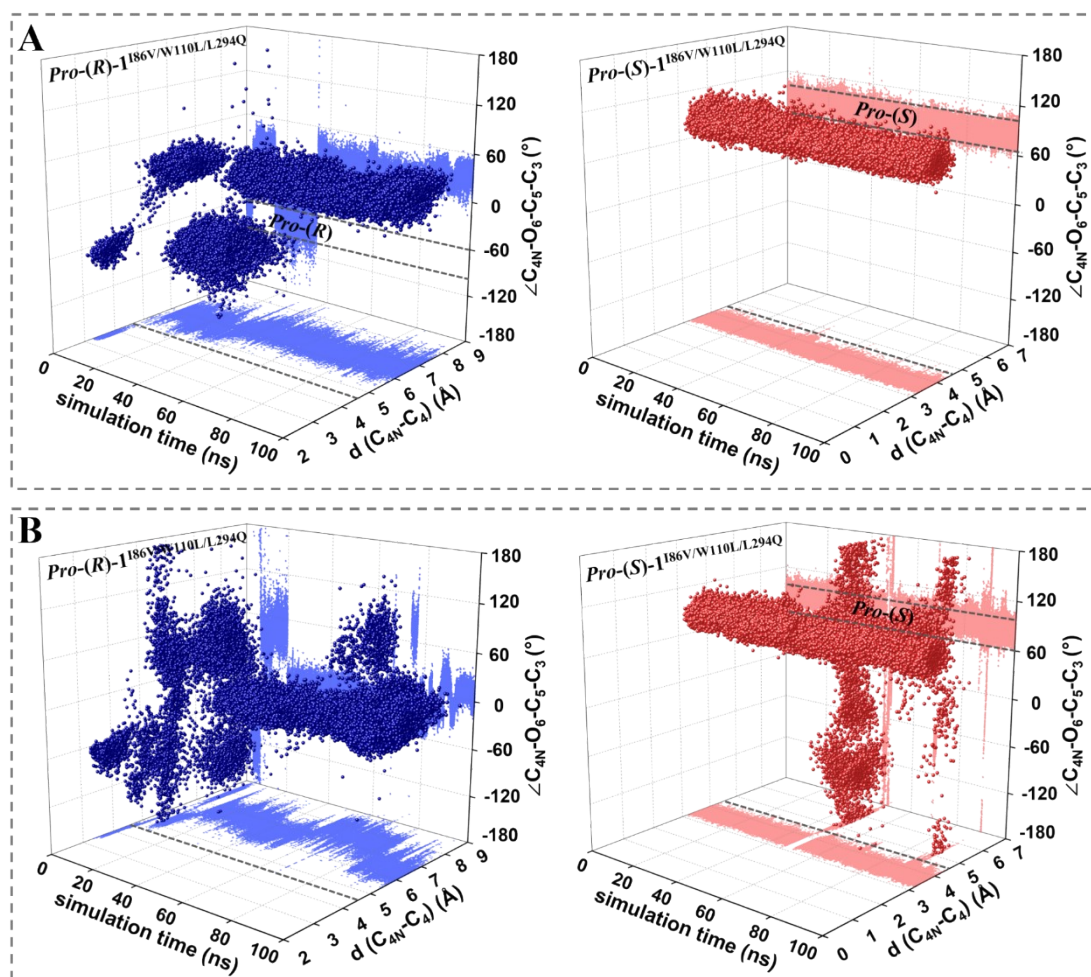


Fig. S3 3D plots of the divergence of the $\angle C4N-O6-C5-C3$ and $d(C4N-C4)$ (detailed in Fig. S1) during the 100 ns MD simulations for *pro*-(R) and *pro*-(S) orientations of prochiral substrate **1** in (A) repeat2 and (B) repeat3 for the I86V/W110L/L294Q mutant. The dashed lines shown in panels A and B indicate the preference regions of *pro*-(R) ($\angle C4N-O6-C5-C3$ from -60° to -100°) and *pro*-(S) ($\angle C4N-O6-C5-C3$ from 60° to 100°), and the distance $d(C4N-C4)$ shorter than 4.5 Å has been defined as catalytically competent pose.

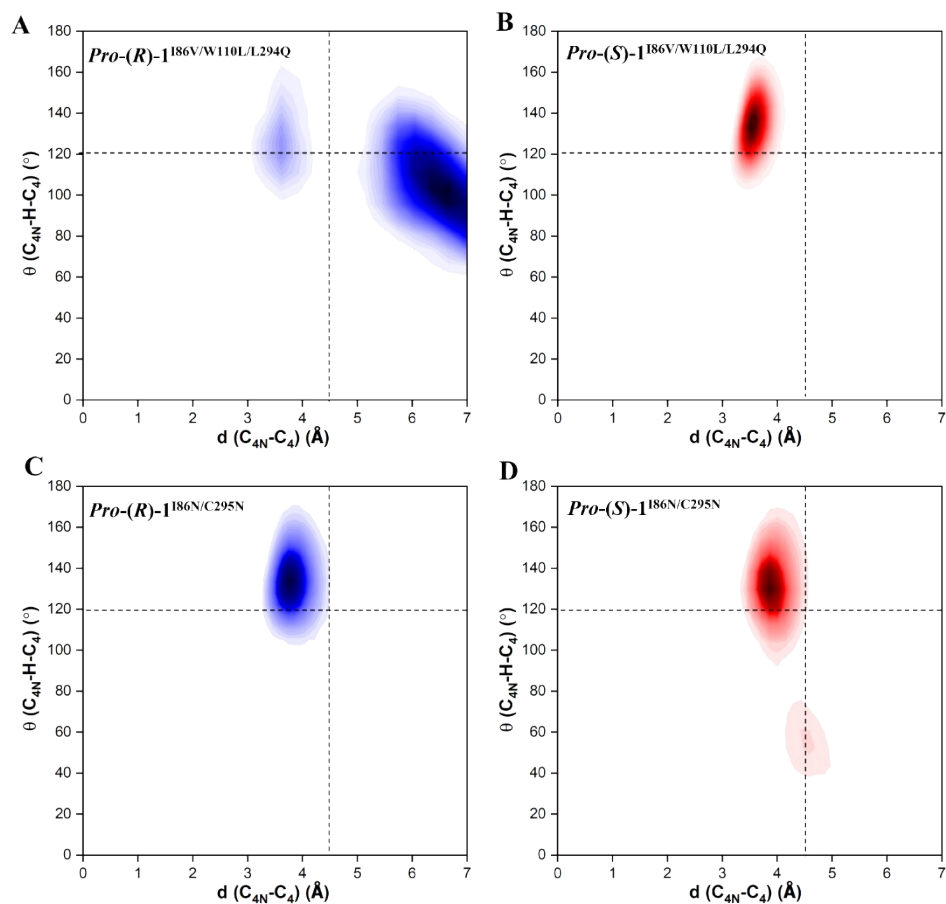


Fig. S4 Representation of the *pro*-(*R*)/*pro*-(*S*) conformations sampled along the MD simulations for (A) the I86V/W110L/L294Q mutant, (C) the I86N/C295N mutant starting from the *pro*-(*R*) orientation of **1**, and (B) the I86V/W110L/L294Q mutant, (D) the I86N/C295N mutant starting from the *pro*-(*S*) orientation of **1**. The histogram of the $d(C_{4N}-C_4)$ together with the *pro*-(*R*)/*pro*-(*S*) bond angle $\theta(C_{4N}-H-C_4)$ (detailed in Fig. S1) is displayed. The conformations with $\theta(C_{4N}-H-C_4) \geq 120^\circ$ and $d(C_{4N}-C_4) \leq 4.5$ Å are considered as reactive (dashes lines).

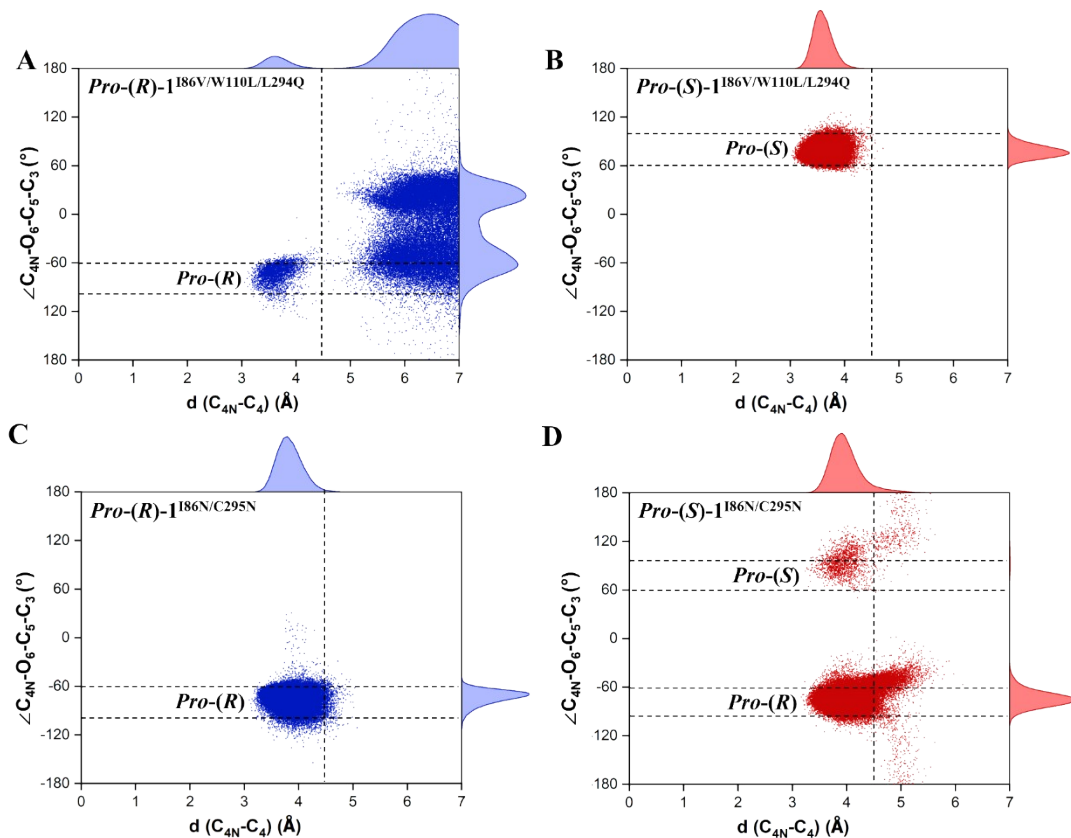


Fig. S5 Representation of the *pro*-(*R*)/*pro*-(*S*) conformations sampled along the MD simulations for (A) the I86V/W110L/L294Q mutant, (C) the I86N/C295N mutant starting from the *pro*-(*R*) orientation of **1**, and (B) the I86V/W110L/L294Q mutant, (D) the I86N/C295N mutant starting from the *pro*-(*S*) orientation of **1**. The histogram of the $d(C_{4N}-C_4)$ together with the $\angle C_{4N}-O_6-C_5-C_3$ (detailed in Fig. S1) of *pro*-(*R*)/*pro*-(*S*) is displayed. The dashed lines shown in panels indicate the preference regions of *pro*-(*R*) ($\angle C_{4N}-O_6-C_5-C_3$ from -60° to -100°) and *pro*-(*S*) ($\angle C_{4N}-O_6-C_5-C_3$ from 60° to 100°), and the distance $d(C_{4N}-C_4)$ shorter than $4.5 \text{ \AA}$ has been defined as catalytically competent pose.

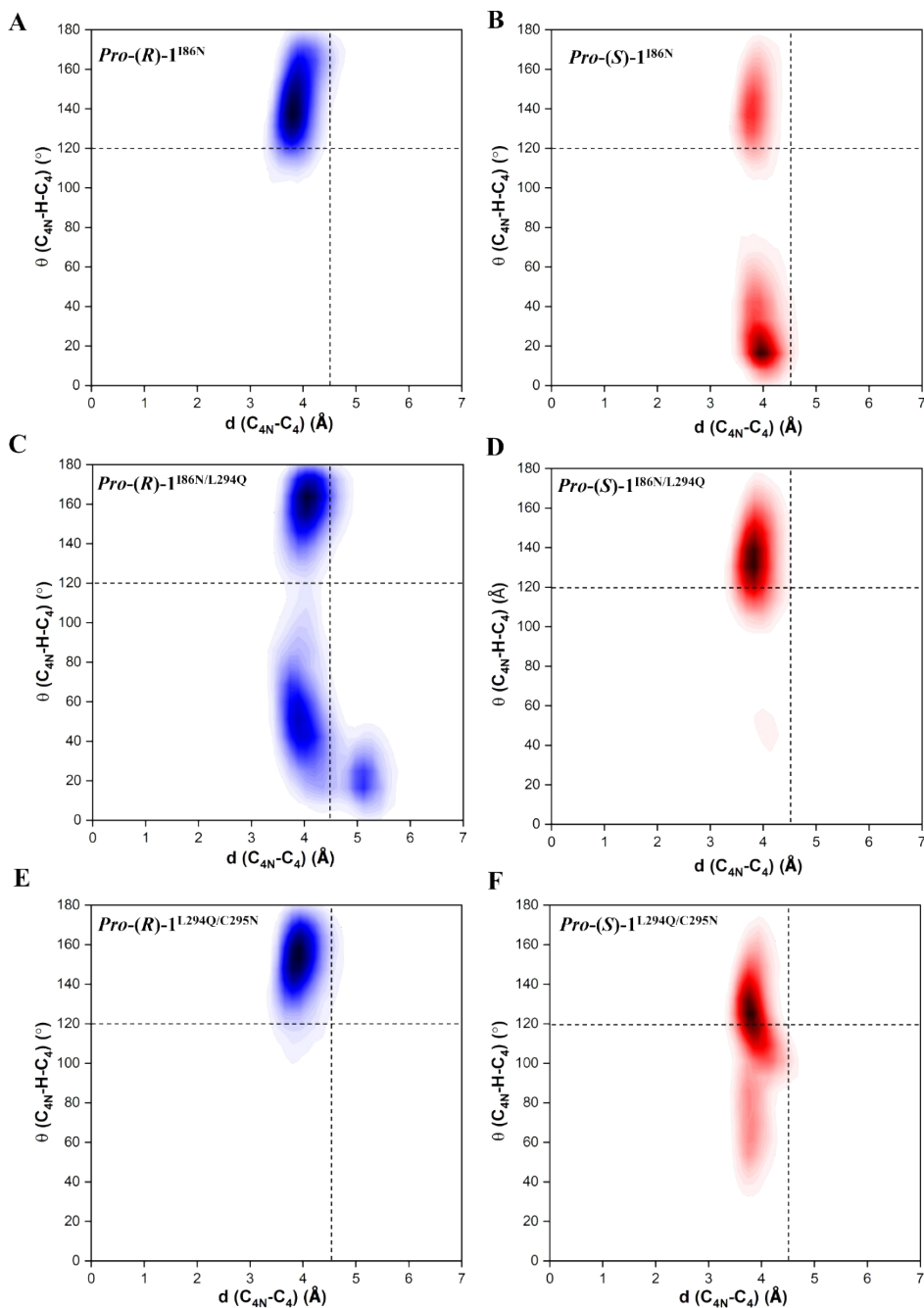


Fig. S6 Representation of the *pro-(R)/pro-(S)* conformations sampled along the MD simulations for (A) the I86N mutant, (C) the I86N/L294Q mutant, (E) the L294Q/C295N mutant starting from the *pro-(R)* orientation of **1**, and (B) the I86N mutant, (D) the I86N/L294Q mutant, (F) the L294Q/C295N mutant starting from the *pro-(S)* orientation of **1**. The histogram of the d ($C_{4N}-C_4$) together with the *pro-(R)/pro-(S)* bond angle θ ($C_{4N}-H-C_4$) (detailed in Fig. S1) is displayed. The conformations with θ ($C_{4N}-H-C_4$) $\geq 120^\circ$ and d ($C_{4N}-C_4$) ≤ 4.5 Å are considered as reactive (dashes lines).

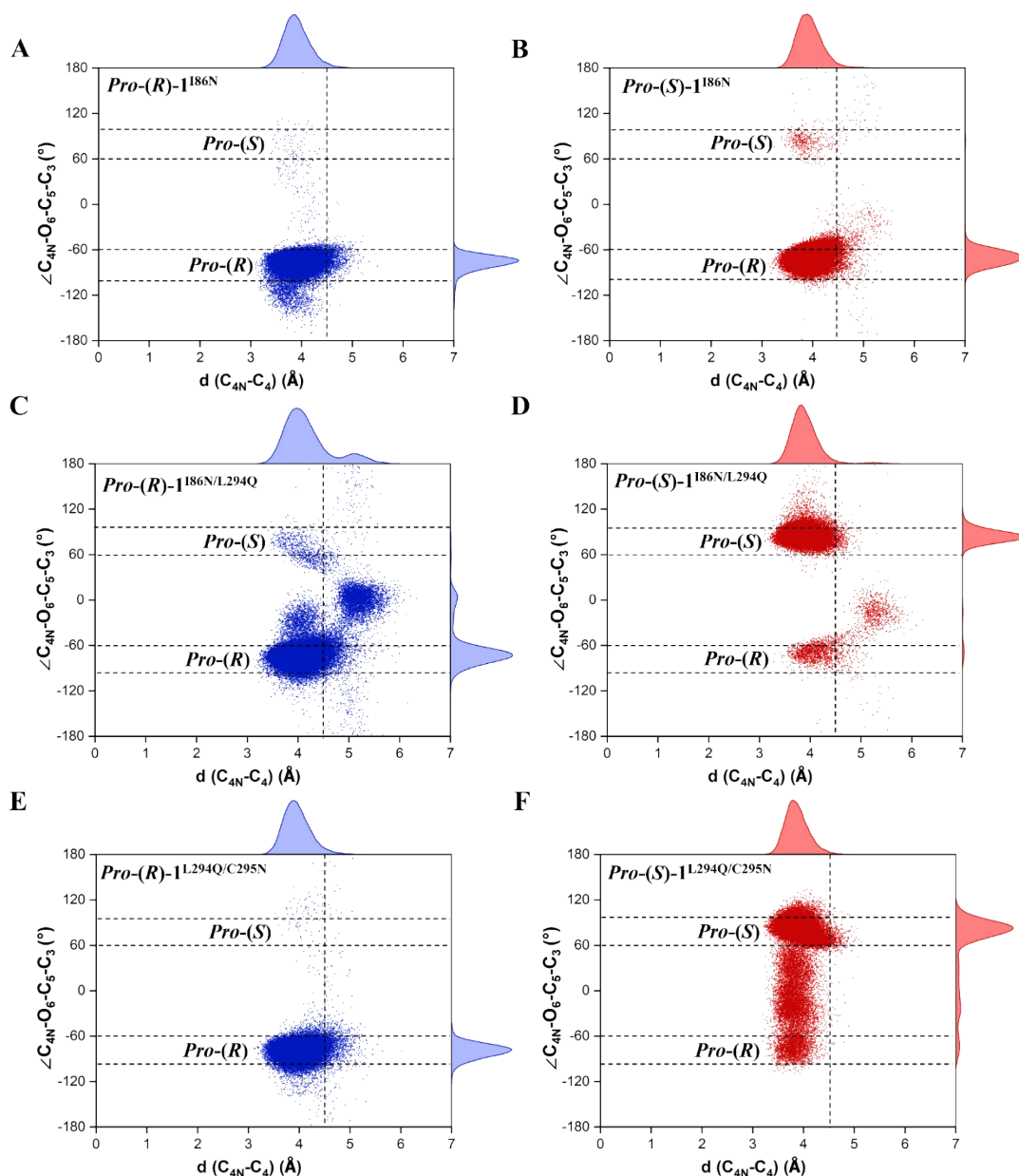


Fig. S7 Representation of the *pro*-(*R*)/*pro*-(*S*) conformations sampled along the MD simulations for (A) the I86N mutant, (C) the I86N/L294Q mutant, (E) the L294Q/C295N mutant starting from the *pro*-(*R*) orientation of **1**, and (B) the I86N mutant, (D) the I86N/L294Q mutant, (F) the L294Q/C295N mutant starting from the *pro*-(*S*) orientation of **1**. The histogram of the $d(C_{4N}-C_4)$ together with the $\angle C_{4N}-O_6-C_5-C_3$ (detailed in Fig. S1) of *pro*-(*R*)/*pro*-(*S*) is displayed. The dashed lines shown in panels indicate the preference regions of *pro*-(*R*) ($\angle C_{4N}-O_6-C_5-C_3$ from -60° to -100°) and *pro*-(*S*) ($\angle C_{4N}-O_6-C_5-C_3$ from 60° to 100°), and the distance $d(C_{4N}-C_4)$ shorter than 4.5 Å has been defined as catalytically competent pose.

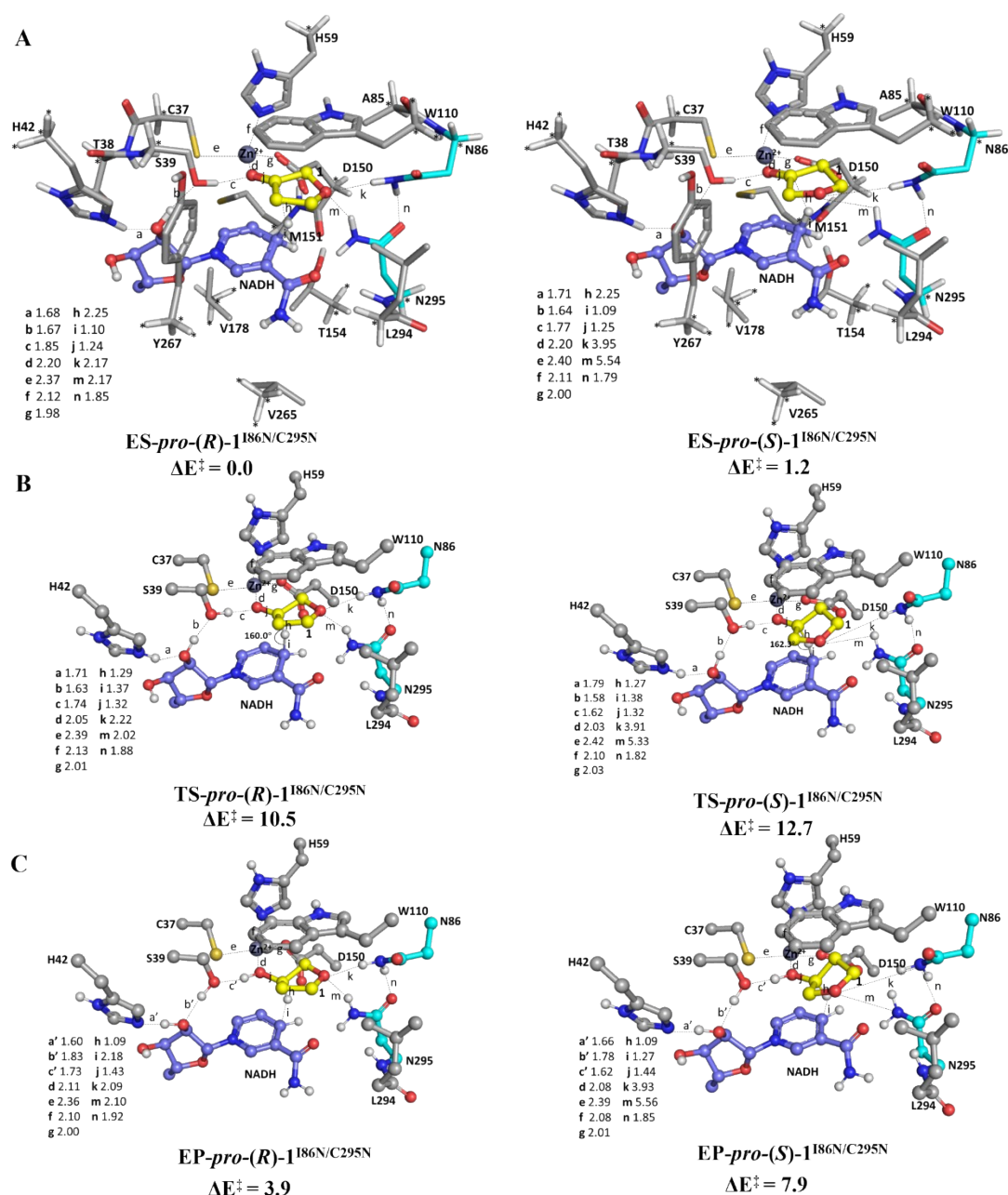


Fig. S8 Optimized structures of stationary point along the reaction pathways for the *pro-(R)* and *pro-(S)* orientations of prochiral substrate **1** reactions in the I86N/L294Q mutant. Note that for clarity only a small part of the model is shown in TS and EP. Asterisks mark the atoms fixed in the geometry optimizations. The numbers represent the distances between atoms in Å. Calculated relative energies are indicated in kcal/mol.

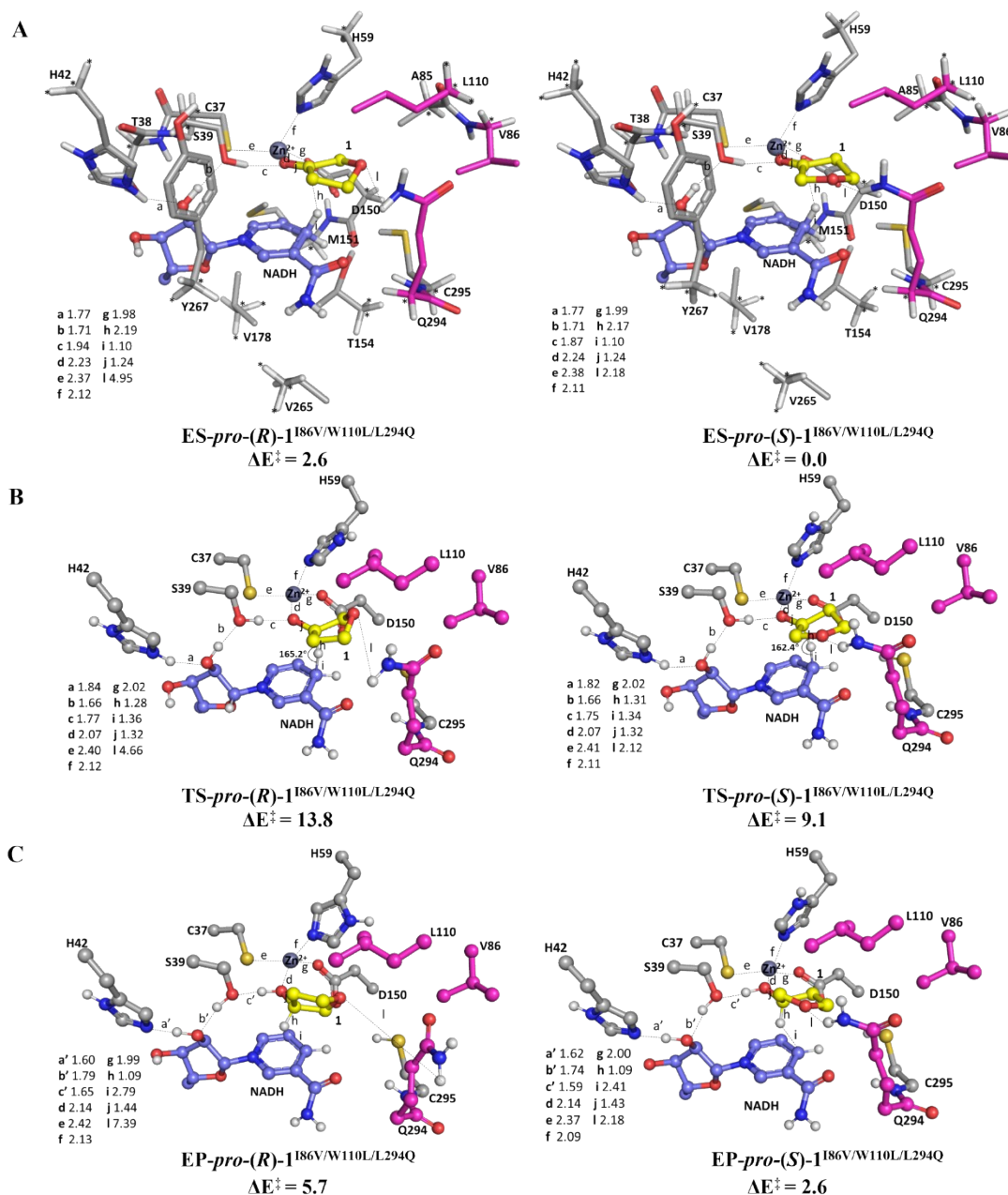


Fig. S9 Optimized structures of stationary point along the reaction pathways for *pro*-(*R*) and *pro*-(*S*) orientations of prochiral substrate **1** reactions in the I86V/W110L/L294Q mutant. Note that for clarity only a small part of the model is shown in **TS** and **EP**. Asterisks mark the atoms fixed in the geometry optimizations. The numbers represent the distances between atoms in Å. Calculated relative energies are indicated in kcal/mol.

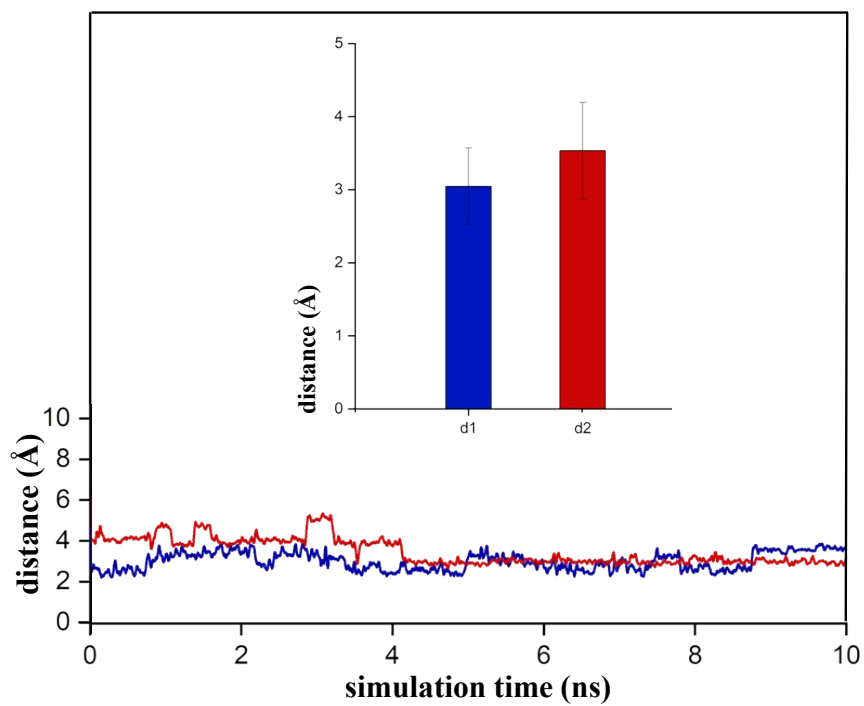


Fig. S10 The distances **d1**, **d2** of the I86N/C295N mutant along 10 ns in front of the 100 ns MD simulations.

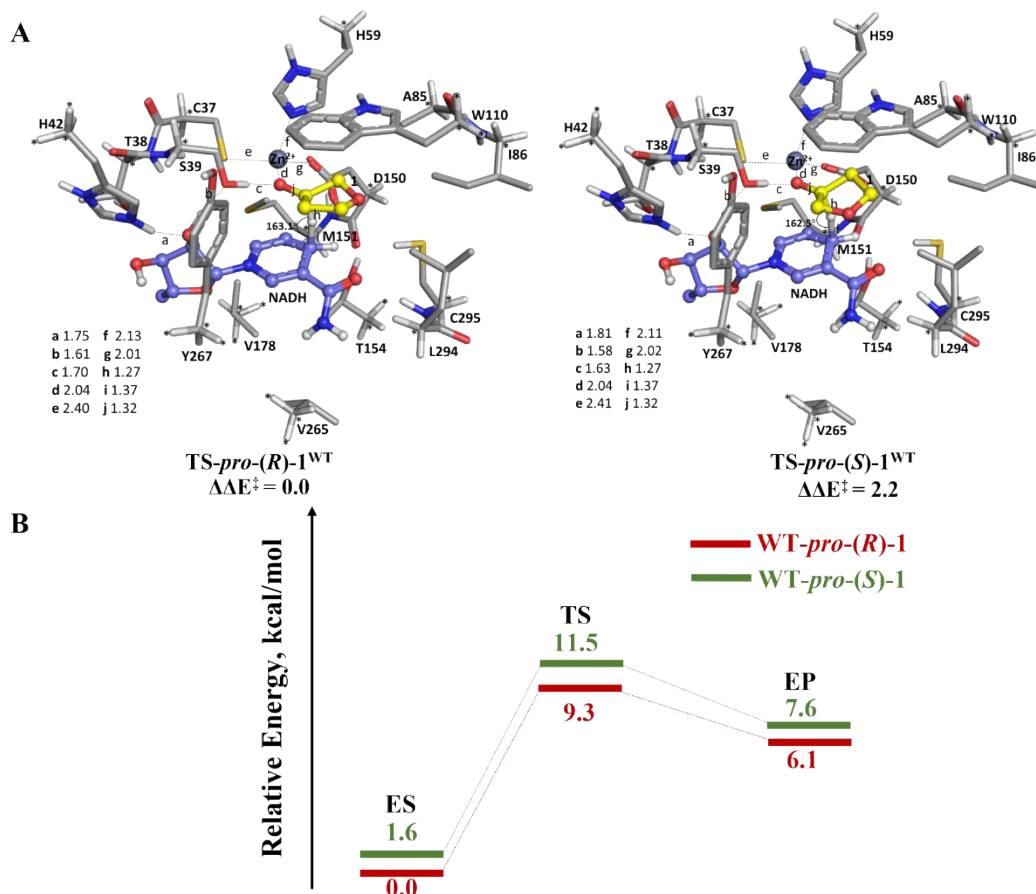


Fig. S11 (A) Optimized structures of TSs for the *pro-(R)* and *pro-(S)* orientations of prochiral substrate **1** reactions in the WT enzyme. Asterisks mark the atoms fixed in the geometry optimizations. The numbers represent the distances between atoms in Å. (B) Calculated energy profile for the reduction of substrate **1** of the WT enzyme. Calculated relative energies are indicated in kcal/mol.

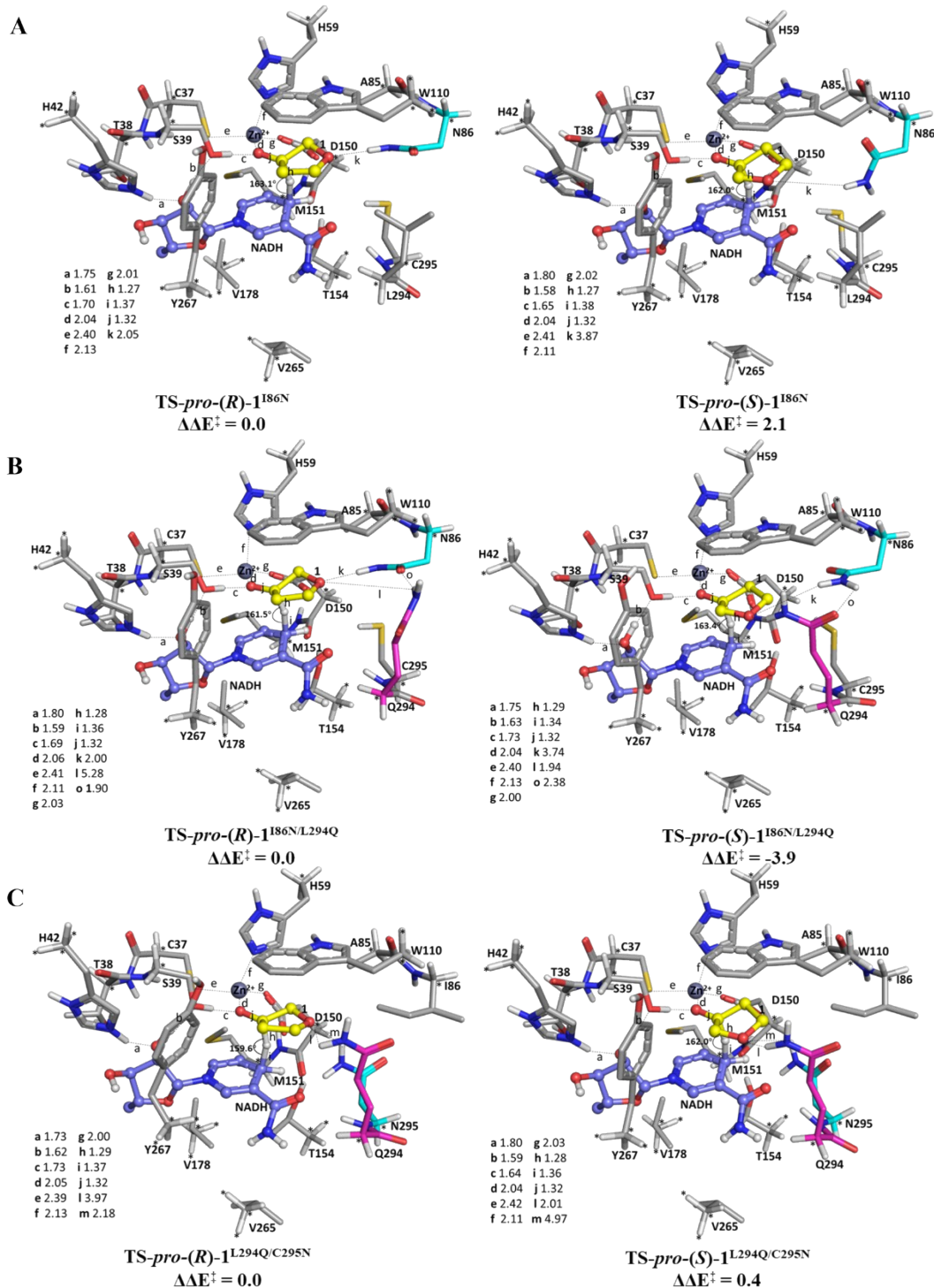


Fig. S12 Optimized structures of TSs for the *pro*-(*R*) and *pro*-(*S*) orientations of prochiral substrate **1** reactions in (A) the I86N mutant, (B) the I86N/L294Q mutant, (C) the L294Q/C295N mutant. Asterisks mark the atoms fixed in the geometry optimizations. The numbers represent the distances between atoms in Å. Calculated relative energies are indicated in kcal/mol.

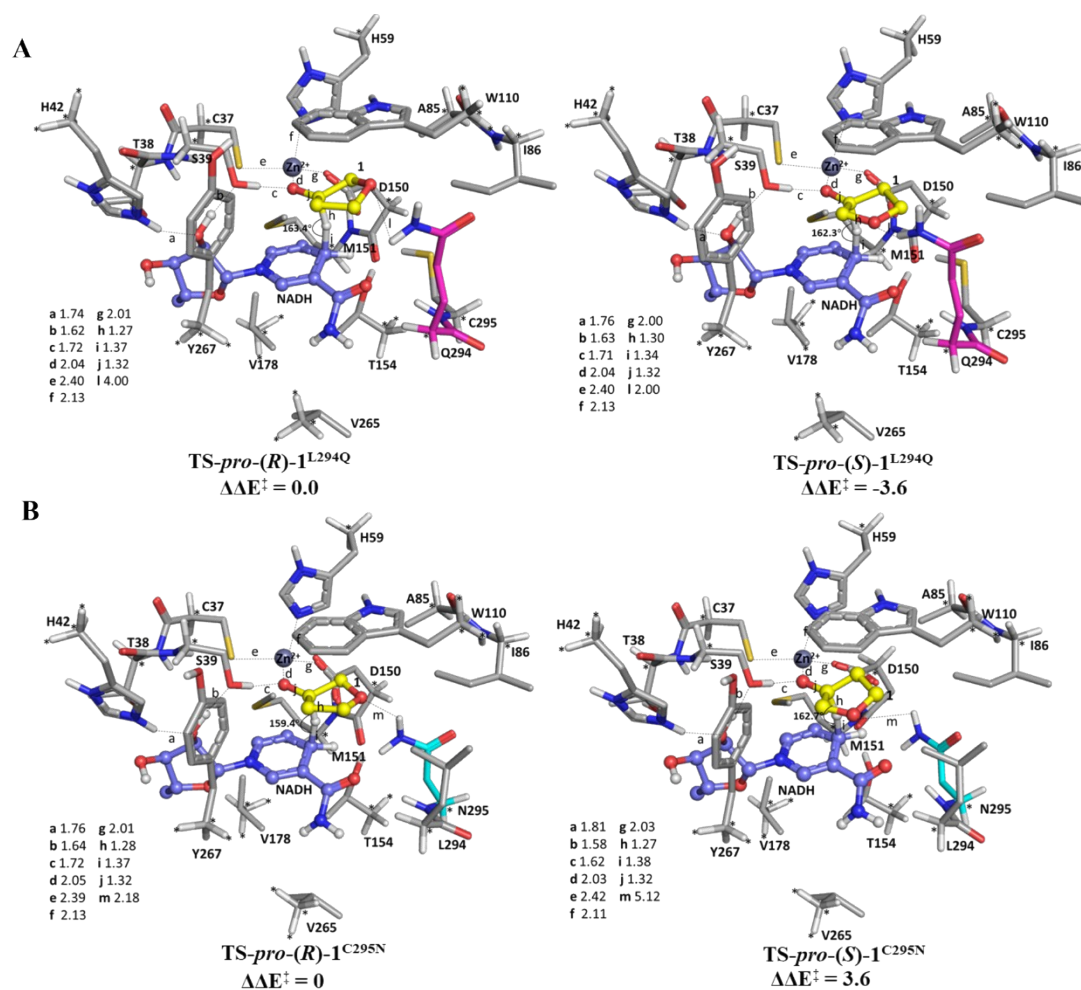


Fig. S13 Optimized structures of TSs for the *pro*-(*R*) and *pro*-(*S*) orientations of prochiral substrate **1** reactions in (A) the L294Q mutant, (B) the C295N mutant. Asterisks mark the atoms fixed in the geometry optimizations. The numbers represent the distances between atoms in Å. Calculated relative energies are indicated in kcal/mol.

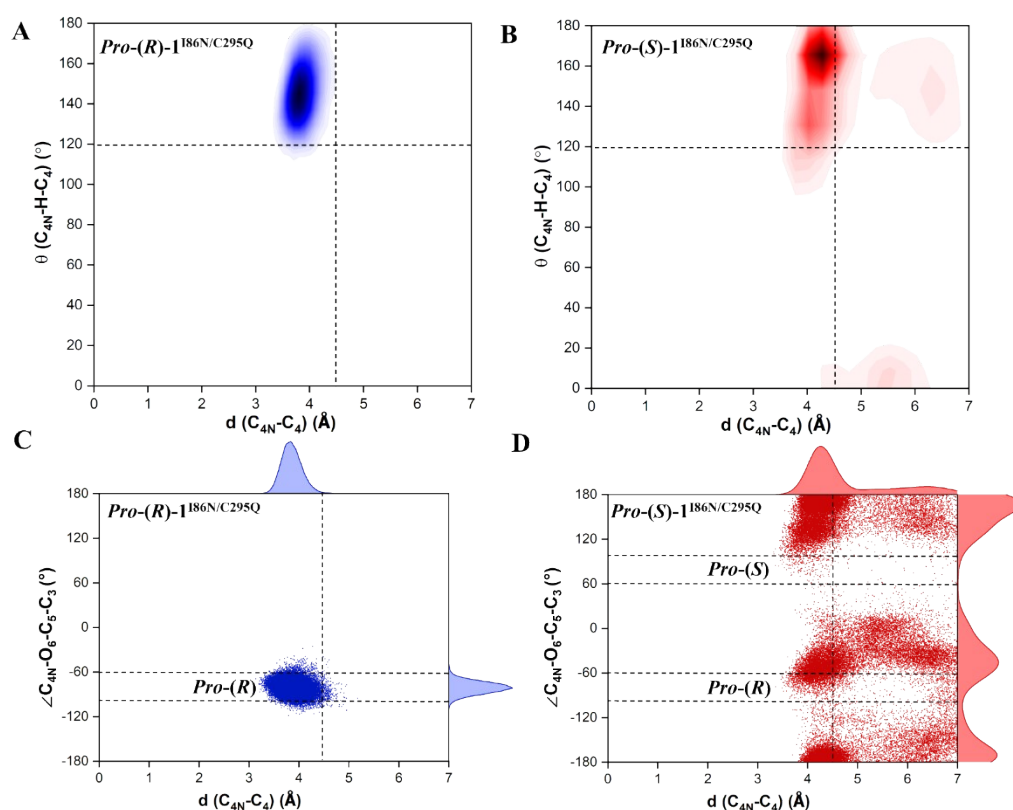


Fig. S14 Representation of the *pro-(R)/pro-(S)* conformations sampled along the MD simulations for the I86N/C295Q mutant. The histogram of the $d(C4N-C4)$ together with the *pro-(R)* (A) and *pro-(S)* (B) bond angle $\theta(C4N-H-C4)$ (detailed in Fig. S1) is displayed. The conformations with $\theta(C4N-H-C4) \geq 120^\circ$ and $d(C4N-C4) \leq 4.5 \text{ \AA}$ are considered as reactive (dashes lines). The histogram of the $d(C4N-C4)$ together with the $\angle C4N-O6-C5-C3$ (detailed in Fig. S1) of *pro-(R)* (C) and *pro-(S)* (D) is displayed. The dashed lines shown in panels indicate the preference regions of *pro-(R)* ($\angle C4N-O6-C5-C3$ from -60° to -100°) and *pro-(S)* ($\angle C4N-O6-C5-C3$ from 60° to 100°), and the distance $d(C4N-C4)$ shorter than $4.5 \text{ \AA}$ has been defined as catalytically competent pose.

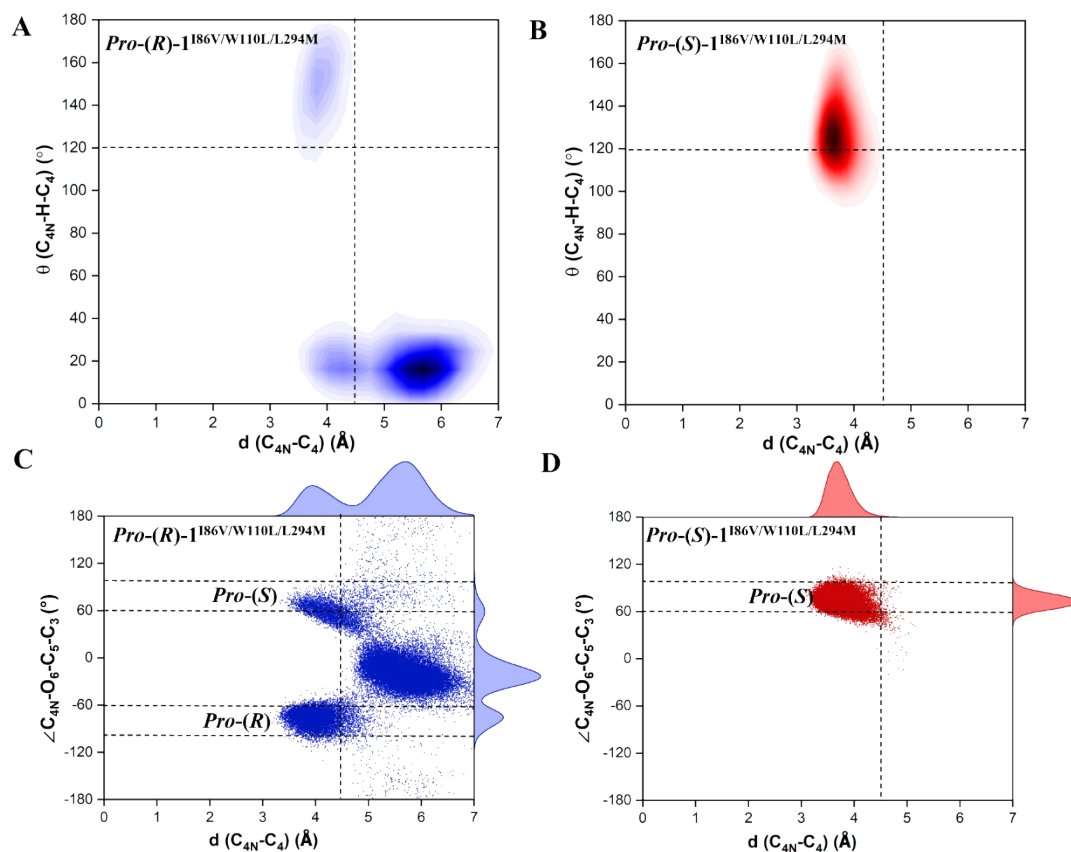


Fig. S15 Representation of the *pro*-(*R*)/*pro*-(*S*) conformations sampled along the MD simulations for the I86V/W110L/L294M mutant. The histogram of the d ($C_{4N}-C_4$) together with the *pro*-(*R*) (A) and *pro*-(*S*) (B) bond angle θ ($C_{4N}-H-C_4$) (detailed in Fig. S1) is displayed. The conformations with θ ($C_{4N}-H-C_4$) $\geq 120^{\circ}$ and d ($C_{4N}-C_4$) ≤ 4.5 Å are considered as reactive (dashes lines). The histogram of the d ($C_{4N}-C_4$) together with the $\angle C_{4N}-O_6-C_5-C_3$ (detailed in Fig. S1) of *pro*-(*R*) (C) and *pro*-(*S*) (D) is displayed. The dashed lines shown in panels indicate the preference regions of *pro*-(*R*) ($\angle C_{4N}-O_6-C_5-C_3$ from -60° to -100°) and *pro*-(*S*) ($\angle C_{4N}-O_6-C_5-C_3$ from 60° to 100°), and the distance d ($C_{4N}-C_4$) shorter than 4.5 Å has been defined as catalytically competent pose.

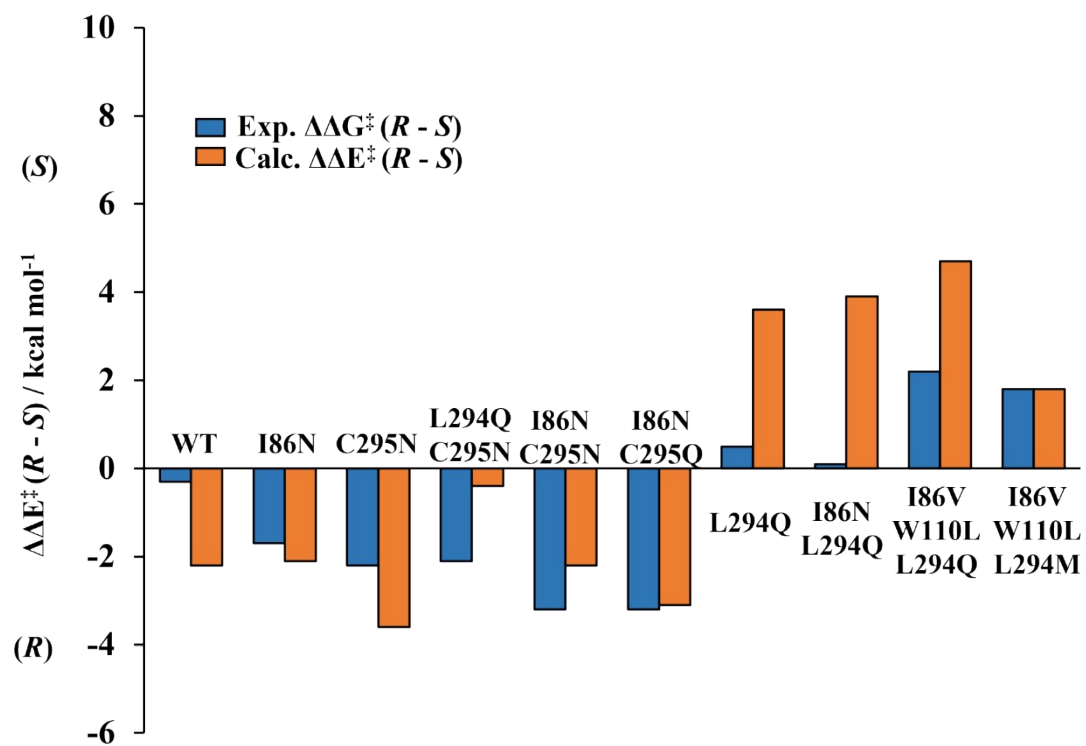


Fig. S16 Comparison between experimental and calculated differences in activation barriers for the WT and other key mutants.

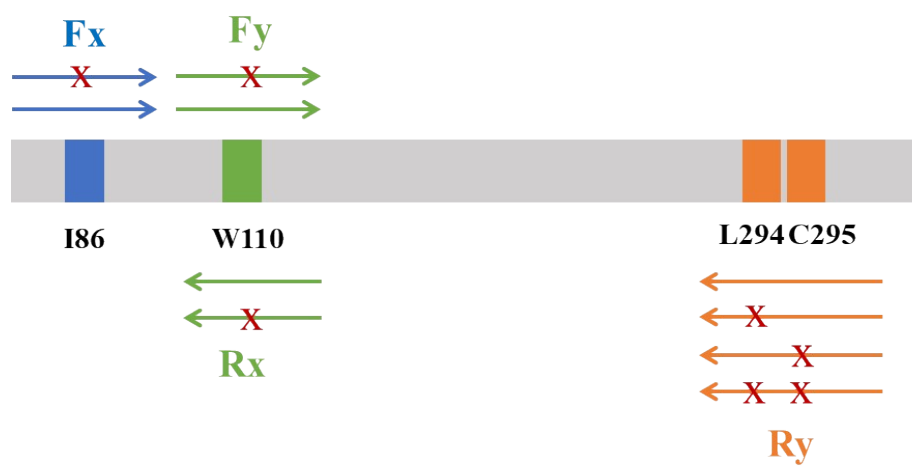


Fig. S17 Primer design for construction of ADH mutants.

Table S7 Cartesian coordinates of stationary points

186N/C29S-N-pro-(R) atoms: 271 charge: +1 ES							
C	4.90618800	-1.00038400	-5.07467300	C	0.15026500	-5.16143400	0.96990900
C	5.87068600	-1.49520500	-4.01368800	H	-7.25638500	-6.01209900	2.16862800
O	6.26906800	-2.65589600	-3.96133100	H	-6.23819700	-7.13569400	1.26467600
C	3.43316600	-1.23807200	-4.65493700	H	-6.74557000	-5.58779700	0.54614000
S	2.97278100	-0.42333800	-3.03743700	H	-5.42469900	-4.46002100	2.48003400
H	5.10185500	-1.56584700	-5.98908500	H	-4.75062200	-6.04648900	2.84149100
H	5.05570100	0.06479700	-5.27828700	H	-5.15791400	-4.77731600	-0.89831000
H	2.77943700	-0.85635300	-5.44200400	H	-2.88954200	-4.65461700	-1.93700500
H	3.26640900	-2.31486900	-4.56629800	H	-2.29017200	-5.62241600	3.32351100
N	6.24565200	-0.56782700	-3.07693800	H	-0.15700900	-4.72697600	-1.12976600
C	7.15997100	-0.91704100	-2.01716600	H	0.18484500	-5.58590500	3.08399200
C	6.62637300	-1.99888400	-1.04821000	H	1.23192100	-5.20283800	0.88500500
O	7.41726600	-2.62023300	-0.33023500	C	-3.64707300	2.61424200	-4.52904300
C	7.51899300	0.32786500	-1.15065800	C	-2.87115700	3.83844600	-4.05537700
C	8.98393400	0.30390400	-0.73809300	O	-3.01069700	4.34761000	-2.94182100
O	7.15803100	1.55779200	-1.77564100	C	-2.70166600	1.42931100	-4.84056000
H	5.87164200	0.37103700	-3.08976600	C	-1.84277300	0.94848100	-3.65710200
H	8.06438400	-1.35546400	-2.45276400	O	-2.17652200	1.19570300	-2.49523300
H	6.89123200	0.29638700	-0.25752500	O	-0.80140600	0.24385200	-4.00500900
H	7.83340600	1.78418400	-2.43030100	H	-4.22674200	2.86265600	-5.42483600
H	9.19534700	1.08898200	-0.00586800	H	-4.33583900	2.34469800	-3.72779200
H	9.23156300	-0.67663000	-0.32327300	H	-3.30018000	0.56797700	-5.16322700
H	9.63079300	0.45769800	-1.61021600	H	-2.03273800	1.65242600	-5.67714600
N	5.28492900	-2.12294900	-0.96024700	N	-1.96969400	4.33298100	-4.94135800
C	4.64243000	-3.14703200	-0.13980600	C	-1.13135700	5.48608900	-4.63517800
C	3.13585100	-2.95044600	-0.16358800	C	-0.20670300	5.81940300	-5.80314500
O	2.78237500	-1.70342900	0.43987400	C	0.75510900	4.70399700	-6.23211700
H	4.88026900	-4.14899000	-0.51928100	S	2.03080900	4.22439300	-5.00537800
H	4.69768300	-1.60889700	-1.61622100	C	1.15489700	2.97005900	-4.01057800
H	5.02240700	-3.09324000	0.88207900	H	-1.76592200	6.34845700	-4.40184000
H	2.78226200	-2.95762900	-1.20082000	H	-1.95738400	3.96442800	-5.88022700
H	2.65613100	-3.77483000	0.37373900	H	-0.55056000	5.27438500	-3.73228300
H	1.95728900	-1.37658500	0.02780900	H	-0.81509500	6.10247100	-6.67439900
C	8.67340800	-5.59016500	2.28728900	H	0.37606600	6.70388200	-5.52874100
C	7.60339200	-4.87824400	3.13347400	H	0.22287300	3.79506500	-6.53427600
C	7.37162500	-3.42608600	2.86109300	H	1.32046500	5.03883200	-7.10636800
C	6.22888700	-2.67796900	2.96766300	H	1.92434800	2.41934700	-3.46478800
N	8.34944300	-2.54637100	2.42304200	H	0.45394700	3.41362500	-3.30144000
C	7.81731500	-1.33290800	2.21819200	H	0.62921600	2.25998000	-4.65144300
N	6.53795500	-1.39136100	2.56652000	C	-3.69960500	6.12467000	0.10806600
H	8.64549100	-5.39691200	1.21546000	C	-2.48750600	5.20549900	0.03271800
H	8.49946200	-6.66684500	2.39061200	C	-1.69951900	5.19208300	1.33503300
H	9.28014100	-2.81608100	2.13826600	O	-2.91212300	3.86962300	-0.23383600
H	9.69019000	-5.45472100	2.65989400	H	-4.22936000	6.11452800	-0.84463300
H	6.63705700	-5.37220800	2.99234600	H	-3.39911500	7.15851900	0.31421700
H	7.85289800	-5.01082700	4.19413000	H	-4.38295600	5.80418000	0.89938300
H	5.23613200	-2.94903700	3.29279000	H	-1.83112300	5.54416900	-0.78223200
H	8.31813300	-0.46237500	1.83259300	H	-3.11942300	3.80945300	-1.18656200
H	5.83622200	-0.65787300	2.32558500	H	-0.80221800	4.57412000	1.24590500
C	-2.14346600	-5.09499400	-6.29294300	H	-1.39184700	6.20467800	1.60838200
C	-2.31534300	-5.12590900	-4.76468600	H	-2.32366500	4.79096500	2.14087200
C	-1.26299200	-4.29050800	-4.11362100	C	3.23630800	8.05962700	-1.84035900
C	-1.19933200	-2.94621800	-3.86076000	C	2.24257500	6.94322200	-0.78805900
N	0.01204000	-4.76250500	-3.83430900	C	1.35249000	7.10048900	0.29710200
C	0.78433800	-3.78457000	-3.42678500	C	2.33592500	5.55288100	-1.42897800
N	0.07233600	-2.60911900	-3.43605200	H	3.13552800	7.97198900	-2.57389900
H	-1.16251500	-5.48045200	-6.58721600	H	2.40557300	9.04261800	-1.37500000
H	-2.22792300	-4.07093300	-6.66625500	H	1.38670600	7.98403900	-2.39051000
H	-2.90768300	-5.70509600	-6.78247600	H	3.40854600	7.02870900	-3.02879000
H	-3.30291200	-4.74116800	-4.48984900	H	1.44049200	6.31436600	1.05499600
H	-2.26947300	-6.15597700	-4.39259800	H	1.42612600	8.06917700	0.80281300
H	0.31046200	-5.72436600	-3.91389200	H	0.34901500	7.02709800	-0.13944400
H	-1.95911100	-2.18869400	-3.98569900	H	2.48062500	4.76700400	-0.68127800
H	1.82088200	-3.81193000	-3.14035700	H	1.35149600	5.40373900	-1.88930000
C	-6.18367800	-2.64294800	-4.21305300	H	3.08201200	5.42443700	-2.21986300
C	-6.86703900	-3.32359100	-3.03898700	C	-0.41806000	6.13328100	5.88827500
O	-6.37939200	-4.32791100	-2.52157800	C	-0.98367100	6.85761500	4.66390200
C	-4.85329100	-2.02177800	-3.75793200	C	-2.23913100	7.65747600	5.02752200
H	-6.82283300	-1.88034500	-4.67080000	C	0.07104100	7.74924500	3.99855700
H	-5.99751600	-3.41188500	-4.97004600	H	-0.15826100	6.82295300	6.69350000
H	-4.24599300	-2.77980800	-3.25512400	H	0.47888400	5.56301300	5.61963800
H	-4.29398700	-1.62557900	-4.61223000	H	-1.14444900	5.42890400	6.29989900
H	-5.02005000	-1.21303300	-3.04128700	H	-1.27812700	6.08943200	3.93583400
N	-8.01771100	-2.73719000	-2.62319000	H	-2.67661100	8.13165100	4.14291900
C	-8.69500200	-3.08930100	-1.38774300	H	-3.00480300	7.01750000	5.47857900
C	-8.39908200	-2.08440700	-0.25145200	H	-2.00020500	8.44954700	5.74703000
C	-6.98554500	-2.28730600	0.27201900	H	-0.32880200	8.23689200	3.10323200
N	-6.01301200	-1.53917300	-0.31958000	H	0.40457700	8.53635100	4.68515600
O	-6.75270800	-3.15556300	1.10987400	H	0.95261800	7.17241500	3.69745400
H	-9.77302300	-3.12891600	-1.57378200	C	3.48937300	0.83331000	6.36054200
H	-8.27749200	-1.86291200	-3.05585500	C	3.26843500	0.11446000	5.01525300
H	-8.35908200	-4.08811100	-1.10494100	C	3.20180900	-1.39352200	4.92778800
H	-8.55604100	-1.05788900	-0.60143200	C	3.66492800	-2.25956400	5.91970200
H	-9.08514200	-2.27735000	0.57681700	C	2.68057500	-1.96010800	3.75217700
H	-5.08482000	-1.68799500	0.06409100	C	3.60618900	-3.64764100	5.75238900
H	-6.24403600	-0.56864300	-0.56393600	C	2.61282400	-3.33569900	3.56961500
C	-6.42559300	-6.07966500	1.46452500	C	3.07121500	-4.19010700	4.58070800
C	-5.15486700	-5.42130600	2.03494200	O	2.96711500	-5.53448600	4.35511900
C	-4.07539000	-5.19401000	1.00844600	H	3.51619600	1.87748100	6.04994600
C	-4.25392900	-4.89648000	-0.31965100	H	4.44367100	0.57636300	6.82876400
C	-2.64561000	-5.10264300	1.22791000	H	2.68457800	0.67419500	7.07962300
C	-2.01063900	-4.94088300	-0.02383600	H	2.34159800	0.50673000	4.57693500
C	-1.83633700	-5.42821800	2.35639600	H	4.06121000	0.44516700	4.32717200

O	6.63978600	-4.10300800	2.64164700	H	-3.25559200	5.32569200	2.20180200	H	3.76644100	1.51816400	-1.33676000
C	4.91993100	-1.79868000	3.73945000	C	0.07505100	6.12379900	-5.91605700	H	4.46110500	0.14008700	-0.54169900
H	6.88269100	-1.50345200	4.62862100	C	0.62849600	6.88015900	-4.70098300	C	4.84584000	-0.58191900	-4.12945900
H	6.15676800	-3.07316300	4.98917900	C	1.85424000	7.71853000	-5.07890600	H	5.32836000	-0.11029500	-3.26995600
H	4.36077700	-2.60444000	3.25385900	C	-0.45397200	7.74248900	-4.04159100	H	3.77507300	-0.35671300	-4.06785400
H	4.33529300	-1.41981300	4.58490800	H	-0.21229800	6.79537500	-6.72482000	C	5.11087300	-2.06989600	-4.04211700
H	5.03185700	-0.99198600	3.00845700	H	-0.78825700	5.52062100	-5.63390500	H	4.28748100	-3.86050500	-4.55920800
N	8.00399400	-2.27026800	2.51141500	H	0.83255200	5.44593000	-6.32962800	O	6.18375000	-2.52908800	-3.67776100
C	8.79721800	-2.67729800	1.36808000	H	0.95180400	6.13150500	-3.96368600	N	4.06458000	-2.88572400	-4.41623600
C	8.75297400	-1.67551800	0.19133000	H	2.27820700	8.21742000	-4.20151700	H	3.29373300	-2.50703500	-4.94445400
C	7.58101600	-1.92844400	-0.76943200	H	2.64011000	7.10022400	-5.52575500	TS			
C	10.08154300	-1.71698900	-0.57402600	H	1.58560000	8.49340200	-5.80658800				
C	6.20309300	-1.93087700	-0.11345600	H	-0.06810800	8.25158300	-3.15233300	C	-4.84186300	-0.81972000	5.20984800
H	9.83563300	-2.86697800	1.70033300	H	-0.81575100	8.51086900	-4.73507500	C	-5.82335200	-1.40840300	4.20866200
H	8.17570100	-1.34837400	2.88431800	H	-1.31458400	7.13927800	-3.73184700	O	-6.21831200	-2.56795700	4.26212100
H	8.43044300	-3.66073400	1.06432900	C	-3.61249300	0.66702800	-6.30434300	C	-3.37100400	-1.03101900	4.77810200
H	8.62589000	-0.66615500	0.60882100	C	-4.45541800	-0.17212700	-5.30507400	S	-2.96719600	-0.29441300	3.11660500
H	7.74565900	-2.88176100	-1.28844400	C	-3.89669700	-1.53520500	-4.96144500	H	-5.00474400	-1.33016100	6.16245500
H	7.60458200	-1.15943500	-1.54828500	C	-4.21545200	-2.67735400	-5.70410500	H	-5.02492500	0.25091300	5.34795700
H	10.92870900	-1.45298600	0.06865400	C	-3.04807000	-1.69246800	-3.85385900	H	-2.71906600	-0.58465800	5.53227300
H	10.26749200	-2.71906900	-0.97916000	C	-3.71722600	-3.93434400	-5.35461700	H	-3.16478500	-2.10453600	4.74669400
H	10.06428700	-1.01947800	-1.41622300	C	-2.54495900	-2.93755700	-3.48676900	N	-6.21950700	-0.56088300	3.20618300
H	6.07881100	-2.76490100	0.57782100	C	-2.87949200	-4.06735800	-4.24158600	C	-7.12151200	-1.01864600	2.17722600
H	6.05175600	-0.99501700	0.43135200	O	-2.37132500	-5.26811600	-3.83138900	C	-6.56032800	-2.14802000	1.28223500
H	5.41898700	-2.02729000	-0.86714000	H	-3.67855800	1.71231200	-6.00291200	O	-7.33798600	-2.83301300	0.60772400
C	6.61845000	-5.79816300	-1.44556700	H	-3.95403800	0.55694200	-7.33533300	C	-7.53675200	0.14543800	1.22726100
C	5.30913400	-5.13086900	-1.89049100	H	-2.55872300	0.37697700	-6.26025800	C	-9.01520700	0.06431200	0.87305800
C	4.23818300	-5.03085200	-0.83876400	H	-4.54179500	0.38593200	-4.36408400	O	-7.17624300	1.43007800	1.73132300
C	4.39584700	-4.89158200	0.51804700	H	-5.47621700	-0.27928900	-5.69002800	H	-5.78883500	0.34727300	3.09881300
C	2.81571000	-5.00877600	-1.08379600	H	-4.87442000	-2.59178900	-6.56390900	H	-8.00451500	-1.45649800	2.65391000
C	2.15976100	-4.86492400	0.17856900	H	-2.80182900	-0.83115300	-3.24291900	H	-6.94219600	-0.05238900	0.31560700
C	2.02751800	-5.12482900	-2.23893700	H	-3.98187800	-4.80873500	-5.94473500	H	-7.78898000	1.66842900	2.44113700
N	3.15058500	-4.76688500	1.12825600	H	-1.90184300	-3.04552600	-2.62149200	H	-9.27174500	0.07928100	0.79787200
C	0.76750500	-4.89382200	0.30168100	H	-2.58666600	-5.95303600	-4.47796000	H	-9.25536500	-0.94710400	0.53451100
C	0.63960200	-5.15156700	-2.12559100	C	5.25747400	1.50145700	-5.53001300	H	-9.63314400	0.26515200	1.75624300
C	0.01795900	-5.05733400	-0.86383200	C	6.18985400	2.19309100	-4.53142400	N	-5.21750800	-2.24309600	1.20049900
H	7.37061200	-5.70683000	-2.23422600	O	7.40546800	2.17673500	-4.69402800	C	-4.54325100	-3.28313600	0.42731200
H	6.47401600	-6.85749800	-1.23255900	C	5.42383400	-0.01935700	-5.44007400	C	-3.04547300	-2.99334800	0.39104900
H	7.02155700	-5.31992900	-0.54739600	H	5.54819500	1.84698200	-6.52624800	O	-2.76168300	-1.75005900	-0.25466900
H	5.54631000	-4.13219600	-2.26922800	H	4.20920000	1.77824800	-5.36118000	H	-4.70386700	-4.26999800	0.87989200
H	4.90384400	-5.68764700	-2.74719800	H	4.93061100	-0.49676700	-6.29595000	H	-4.63960700	-1.66546200	1.81247400
H	5.29080400	-4.78377500	1.12271500	H	6.48903500	-0.26084200	-5.49916000	H	-4.96035800	-3.31898800	-0.57964300
H	3.00328000	-4.42054300	1.12219000	N	5.59003000	2.78098600	-3.45740400	H	-2.66296700	-2.95203200	1.41691100
H	2.49899600	-5.21588700	-3.21231300	C	6.36973300	3.40593500	-2.38963600	H	-2.53956600	-3.80984200	-0.13513800
H	4.28705700	-4.82536400	1.27239000	C	5.67690700	3.25474500	-1.02663600	H	-1.95925400	-1.33307300	0.15973200
H	0.01747700	-5.26816100	-3.00706600	H	7.35486000	2.93415100	-2.38564200	C	-8.50644500	-6.01949500	-1.78930600
H	-1.06235700	-5.14034500	-0.80502600	H	4.58585700	2.70179800	-3.35117200	C	-7.47656000	-5.31328800	-2.68650100
C	3.54709600	-2.83235900	4.49984300	H	6.51698600	4.47299900	-2.60184200	C	-7.29994000	-3.84148100	-2.49278000
C	2.73700300	4.03821700	4.04083100	H	4.66016200	3.65788800	-1.05424800	C	-6.17907900	-3.06866800	-2.63033600
O	2.90962500	4.60003000	2.95792100	H	6.23961600	3.83751200	-0.29285500	N	-8.30966600	-2.96570500	-2.12291200
C	2.65387700	1.61092000	4.81652300	Z	-0.59896000	-0.58133400	2.97240700	C	-7.81582800	-1.72673100	-1.98761600
C	1.77284900	1.11575400	3.65545700	C	-3.37355100	2.00514800	-1.64748100	N	-6.52979200	-1.76928800	-2.31668500
O	2.01482900	1.43737000	2.49017600	N	-2.00493900	1.80203600	-1.27609200	H	-8.47718400	-5.75362000	-0.73306700
O	0.80784400	0.32020500	4.03084800	C	-4.41368300	1.14135100	-0.91345600	H	-8.29030200	-7.09252900	-1.82764900
H	4.12897500	3.09633000	5.39005900	C	-1.02025900	1.98887400	-2.23431200	H	-9.23653400	-3.24364800	-1.83346300
H	4.23911600	2.59328100	3.69161200	O	-4.53395000	-0.14384900	-1.48049500	H	-9.53052700	-5.94362600	-2.15954400
H	3.29101100	0.767256700	5.11002800	C	-5.71548100	1.97331900	-1.06347600	H	-6.48933600	-5.75862900	-2.52999300
H	2.00219000	1.79379500	5.67692300	C	0.29949900	2.02709700	-1.93934200	H	-7.73013100	-5.51201400	-3.73586900
N	1.78165300	4.46535300	4.90482900	O	-6.64702000	1.39545700	-1.97696800	H	-5.17733000	-3.33211300	-2.92533300
C	0.91888300	5.60169600	4.60522000	C	-5.20866700	3.37701000	-1.49811600	H	-8.34873500	-0.84922600	-1.66634700
C	-0.01908600	5.90238600	5.77151500	C	0.79032900	1.79051500	-0.53146800	H	-5.85736100	-0.99596300	-2.14379300
C	-0.94767800	4.75633500	6.19433500	O	-3.78104700	3.34093600	-1.38045300	C	2.35437600	-4.58163900	6.62739300
S	-2.18669600	4.22233100	4.95257100	C	-5.74121600	4.53388600	-0.67664300	C	2.54794700	-4.64264100	5.10093500
C	-1.25175700	2.99178700	3.98156600	C	-0.33721800	1.94569500	0.44751100	C	1.45739300	-3.90905900	4.38814800
H	1.53687900	6.47850800	4.38374500	C	-1.62218400	1.94186300	0.08071900	C	1.32744900	-2.59315500	4.01587800
H	1.73246100	4.04991700	5.82234200	C	1.30936100	2.30156500	-2.98212700	N	0.21487600	-4.47244300	4.12507700
H	0.34467800	5.38827300	3.69773000	N	0.89554900	2.97137200	-4.10573100	C	-0.60107000	-3.51531300	3.61665800
H	0.57689200	6.20071900	6.64597700	O	2.48752500	1.92897500	-2.86642600	N	0.04897300	-2.36540700	3.54094300
H	-0.62872400	6.76874600	5.49755900	H	-5.49119200	4.39220300	0.37839600	H	1.40196100	-5.03194800	6.92394000
H	-0.38970100	3.86855600	6.51307700	H	-3.89126200	-0.75872300	-1.04046500	H	2.35741800	-3.54418500	6.97247400
H	-1.53745400	5.07720800	7.05763000	H	-6.31347600	1.52351400	-2.87623600	H	3.15721500	-5.11888000	7.13965000
H	-1.99216600	2.42886500	3.40885100	H	-3.45216200	1.78352200	-2.72422100	H	3.51068900	-4.19978100	4.82692800
H	-0.53550400	3.45225600	3.29926900	H	-4.15746200	1.06340300	0.14800600	H	2.58374700	-5.68513800	4.76290000
H	-0.73413900	2.28921100	4.63725100	H	-1.38790300	2.09599700	-3.24958700	H	-0.03509800	-5.43818600	4.28311700
C	3.41498600	6.29984500	-0.16797400	H	-6.24655700	2.03822000	-0.11411700	H	2.04151000	-1.78904000	4.08213200
C	2.23561900	5.35337700	0.01854000	H	-5.47486100	3.51560400	-2.56201300	H	-1.62658800	-3.68320900	3.32654700
C	1.36389600	5.29772200	-1.23031900	H	-0.07080600	2.09463800	1.48552300	C	6.29083800	-2.13938800	4.34676400
O	2.70435600	4.03291000	0.27910000	H	-2.43289300	2.09001800	0.78093500	C	6.98825000	-2.87860900	3.22228400
H	4.07760600	6.27592100	0.70230100	H	1.59505100	2.48572500	-0.27335300	O	6.58350400	-3.98054600	2.84021400
H	3.07713300	7.33275900	-0.31095000	H	-6.82870300	4.59702900	-0.77673600	C	4.94973100		

H	9.97649400	-1.24515700	-1.40342800	C	-2.54110500	-3.18165600	-3.35044400	H	2.83286700	-0.60734100	-5.51193800
H	6.00112000	-2.70691100	0.83772500	C	-2.89456500	-4.34238200	-4.04822000	H	3.26057000	-2.13520400	-4.72803300
H	6.06069300	-0.95255000	0.57010700	O	-2.39570800	-5.52681100	-3.58619000	N	6.29555000	-0.51774800	-3.10106000
H	5.33224700	-2.03500800	-0.63579500	H	-3.64044200	1.34897100	-6.09597100	C	7.20997500	-0.92385600	-2.06093500
C	6.60692600	-5.94122100	-1.09120800	H	-3.92104100	0.11899400	-7.35905100	C	6.64730300	-0.122419300	-1.12994900
C	5.32024000	-5.31020200	-1.63085300	H	-2.52795300	-0.00536700	-6.27322700	O	7.42327900	-0.271496800	-0.46515300
C	4.20562800	-5.13153500	-0.63611700	H	-4.49761800	0.12291600	-4.37692600	C	7.60089800	0.28777600	-1.16007300
C	4.29789500	-4.83855900	0.70397700	H	-5.45471800	-0.59185400	-5.66118700	C	9.06026300	0.20264400	-0.73530300
C	2.79794400	-5.14099200	-0.95134100	H	-4.89248900	-2.95739400	-6.42383300	O	7.29045200	1.54309000	-1.76094300
C	2.08322000	-4.82991800	0.24654200	H	-2.77504400	-1.06490800	-3.20490200	H	5.98608300	0.44434900	-3.10587600
C	2.06707500	-5.38991800	-2.12528000	H	-4.02057200	-5.15195100	-5.70414400	H	8.10155600	-1.37136400	-2.51379400
N	3.02547900	-4.65454400	1.23464800	H	-1.88483500	-3.25403700	-2.49154000	H	6.96270300	0.25970700	-0.27473200
C	0.68666800	-4.77563800	0.28543700	H	-2.62044500	-6.23990000	-4.19820000	H	7.98419500	1.76352700	-2.39822300
C	0.67738600	-5.33341500	-2.09394600	C	5.29357100	1.11567700	-5.59632600	H	9.29069700	0.96013000	0.01961200
C	-0.00450600	-5.03701500	-0.89731200	C	6.20082100	1.94079600	-4.68080900	H	9.27365900	-0.79649300	-0.34614200
H	7.39249000	-5.89690000	-1.85077700	O	7.38965200	2.09277000	-4.93878500	H	9.72033500	0.35793800	-1.59722200
H	6.45621900	-6.98554600	-0.81720500	C	5.49529100	-0.38657100	-5.35846500	N	5.30184300	-2.09403100	-1.10116700
H	6.96916700	-5.40603800	-0.20767400	H	5.57303100	1.36949800	-6.62205400	C	4.64615400	-1.16686900	-0.26274100
H	5.58366100	-4.33960400	-2.06332700	H	4.23629000	1.37756100	-5.45351500	C	3.13881200	-3.00353100	-0.32354900
H	4.95238000	-5.92498600	-2.46475800	H	5.01519100	-0.95086400	-6.16672700	O	2.73623300	-1.81857900	0.36655700
H	5.16414400	-4.72798800	1.34202000	H	6.56384300	-0.61760200	-5.39155900	H	4.92075000	-4.14240200	-0.68366800
H	2.83002200	-4.38258300	2.18457800	N	5.62237600	2.45452800	-3.55582200	H	4.72501000	-1.55099000	-1.65261000
H	2.58008200	-5.65287600	-3.04622200	C	6.41231000	3.19352100	-2.57016800	H	4.98788800	-3.16110300	0.77313400
H	0.15797700	-4.45307500	1.20786800	C	5.74189200	3.18158600	-1.19138800	H	2.81611600	-2.93736600	-1.36831300
H	0.09788800	-5.53804800	-2.98769300	H	7.40309600	2.73532700	-2.52013800	H	2.66465900	-3.87773800	0.13482600
H	-1.08965900	-5.05408000	-0.90099500	H	4.64759500	2.26222500	-3.36459500	H	1.95184500	-1.43689300	-0.08128100
C	3.57682700	3.03811500	4.33611700	H	6.55130100	4.23068200	-2.90164800	C	8.62567100	-5.78985500	2.05938000
C	2.79478400	4.23764900	3.81089400	H	4.72259400	3.57624000	-1.24112800	C	7.57304600	-5.08575600	2.93905600
O	3.00496800	4.76094600	2.71494500	H	6.31570400	3.83539600	-0.52934800	C	7.32503700	-3.62788300	2.70316700
C	2.65761800	1.84420600	4.68983600	Z	-0.59341300	-0.43967400	2.88671800	C	6.17378200	-2.89675700	2.84126000
C	1.71219800	1.37536000	3.56728900	C	-3.41193800	2.00452100	-1.71871900	N	8.28678000	-2.72320000	2.28025400
O	1.83014500	1.81813000	2.41931900	N	-2.02708500	1.92904400	-1.29058800	C	7.73630900	-1.51277900	2.10874000
O	0.83278400	0.949485100	3.94442000	C	-4.41062900	1.10399100	-0.96779400	N	6.46041600	-1.59557400	2.46074000
H	4.15010200	3.33023300	5.22295500	C	-1.03332400	1.91373100	-2.23013200	H	8.60034300	-5.55535200	0.99569700
H	4.27824000	2.75607300	3.54991600	O	-4.46026400	-0.19444600	-1.50366600	H	8.42608200	-6.86501800	2.12295600
H	3.27423300	0.98366400	4.97485700	C	-5.74746200	1.88144800	-1.15409200	H	9.21499800	-2.97349000	1.97051400
H	2.04024900	2.05373800	5.57079000	C	0.28851500	1.92456400	-1.88181300	H	9.64598400	-5.69122400	2.43414100
N	1.82864300	4.70852100	4.64105700	O	-6.65313100	1.23498500	-2.04247100	H	6.60436100	-5.57833300	2.81017300
C	0.96440900	5.82366600	4.27552400	C	-5.30810600	3.28965400	-1.63628200	H	7.84411800	-5.23716900	3.99183500
C	0.07666300	6.25156500	5.44042200	C	0.65660400	1.81851900	-0.47895500	H	5.18853200	-3.18783700	3.17184300
C	-0.87374200	5.18714700	5.98859800	O	-3.87403600	3.19277000	-1.52255800	H	8.22194900	-0.62742700	1.73797600
S	-2.10793200	4.50222500	4.80009900	C	-5.88065100	4.44789500	-0.84511500	H	5.74853400	-0.86088300	2.25926100
C	-1.20117600	3.11165100	4.07654800	C	-0.40870000	2.13386700	0.44527800	C	-2.19238200	-4.72771700	-6.46772900
H	1.58800300	6.66205900	3.94965600	C	-1.70021900	2.12727700	0.03939800	C	-2.31635500	-4.89179200	-4.94337400
H	1.72062000	4.28941200	5.55149900	C	1.35400900	2.03015600	-2.91788500	C	-1.27719300	-4.06763000	-4.25731900
H	0.34596400	5.54131000	3.41527200	N	1.00742500	2.65683000	-4.08381200	C	-1.26403500	-2.74884900	-3.87502000
H	0.70707300	6.60710700	6.26736100	O	2.47786300	1.55501800	-2.74427400	N	0.03463900	-4.49513700	-4.09727300
H	-0.51729600	7.10833800	5.10740200	C	5.62947000	4.34161000	0.21377600	C	0.78024000	-3.45927100	-3.69111100
H	-0.33464200	4.32310300	6.41242500	H	-3.84530300	-0.79729600	-0.99298400	N	0.01473200	-2.38901100	-3.49974700
H	-1.46016800	5.60627100	6.80617600	H	-6.30604200	1.30057100	-2.94339300	H	-1.20577500	-5.04387800	-6.82012000
H	-1.92874400	2.53001600	3.50551700	H	-3.42863100	1.71848100	-2.78186400	H	-2.33088400	-3.68077000	-6.75031100
H	-0.38591100	3.43198900	3.42652200	H	-4.16118000	1.06866200	0.09829200	H	-2.94533500	-5.32782100	-6.98622300
H	-0.80425600	2.45913000	4.85696000	H	-1.36269300	1.90758100	-3.26225500	H	-3.30965700	-4.57109600	-4.61365000
C	3.47113200	6.22852300	-0.52592500	H	-6.27792800	1.96205600	-0.20683200	H	-2.21763800	-5.94670000	-4.66118100
C	2.26514700	5.32356100	-0.28528800	H	-5.57649400	3.38651600	-2.70236700	H	0.37635700	-5.42393600	-4.29557800
C	1.39949000	5.22929100	-1.53578700	H	-0.14742100	2.32357900	1.47561200	H	-2.07199200	-2.03687600	-3.85432800
O	2.67533800	3.99898000	0.05358300	H	-2.52659800	2.31850600	0.70908900	H	1.83662000	-3.51155500	-3.62663900
H	4.13235800	6.25160700	0.34541400	H	1.65441400	2.14626500	-0.19566300	C	-6.17290400	-2.26675800	-4.28572300
H	3.15173700	7.25561700	-0.73588800	H	-6.96926400	4.46801100	-0.94801900	C	-6.84832000	-2.96024500	-3.12088100
H	4.05099900	5.86984600	-1.38305000	H	0.84371300	0.48251800	-0.22780100	O	-6.43750500	-4.04926900	-3.71046000
H	1.66780800	5.73600500	0.54098000	H	-5.47584100	5.39700500	-1.20413600	H	-4.73728200	-1.87135000	-3.91594200
H	2.95156500	4.01475800	0.99059400	H	1.76242900	2.79473100	-4.74271100	H	-6.73680600	-1.39092900	-4.62429800
H	0.49411700	4.64674200	-1.34752400	H	0.30090000	3.37788200	-4.07435500	H	-6.15722700	-2.98312600	-5.11420000
H	1.10153400	6.22296100	-1.87989500	O	2.79954000	-1.21098300	-0.39164600	H	-4.23811000	-2.72553800	-3.44977800
H	1.97153600	4.74765100	-2.33606600	C	2.05048600	-1.61252900	-1.55968900	H	-4.17124600	-1.57335300	-4.80506600
C	-2.60216500	8.08454600	1.35012300	C	0.55944500	-1.40950400	-1.23946900	H	-4.70610600	-1.04235200	-3.20390900
C	-2.69787700	6.90236100	0.37569800	C	0.58153700	-0.72713700	0.12386700	N	-7.88292300	-2.28094600	-2.58527400
C	-1.65704500	7.01482800	-0.74346900	C	1.93689100	-1.11169000	0.72124600	C	-8.69493800	-2.74903200	-1.48080000
C	-2.56750300	5.55712500	1.09904900	O	-0.51296500	-0.69479800	0.85700600	C	-8.69629100	-1.85055700	-0.25455300
H	-3.39868300	8.02777500	2.10079400	H	2.27104100	-2.65692200	-1.78989000	C	-7.57317200	-2.12227400	0.74489300
H	-2.71908600	9.03077000	0.82095700	H	2.38614100	-0.96960300	-2.37492200	C	-10.05952100	-1.86495800	0.44642500
H	-1.65623400	8.07803100	1.89461100	H	0.03880500	-2.36472700	-1.13280600	C	-6.16195400	-2.10437500	0.16455500
H	-3.69522300	6.93766100	-0.08820800	H	0.03481100	-0.41433500	-1.99382800	H	-9.72260800	-2.87834600	-1.84465100
H	-1.74062100	6.17933500	-1.44753600	H	2.32868300	-0.35874400	1.40843100	H	-8.11227500	-1.38097200	-2.97887200
H	-1.77002800	7.94586900	-1.30885400	H	1.82519100	-2.07669900	1.24024700	H	-8.32016500	-3.73938600	-1.21226800
H	-0.64320400	6.99748300	-0.32750700	C	5.74353800	1.79291900	-0.55585200	H	-8.54412900	-0.77908600	-0.62325000
H	-2.73069500	4.73119000	0.40027900	O	6.74325400	1.33856700	-0.00241500	H	-7.77302000	-3.10562400	1.19115800
H	-1.56720800	5.44302100	1.53402800	N	4.56986100	1.11734700	-0.65763000	H	-7.62419200	-1.40402400	1.56938900
H	-3.28619900	5.46703200	1.91989300	H	3.79339300	1.47842000	-1.19108100	H	-10.87366400	-1.56127900	-0.22101500
C	0.13823100	5.73677500	-6.25973800	H	4.50534100	0.14918900	-0.37634500	H	-10.27315000	-2.88280100	0.79375000
C	0.69342900	6.56179									

H	-4.80967300	-5.89001600	2.61551000	H	-4.84672000	-0.76645800	6.03918900	H	4.75208000	-1.47593300	-1.66878300
H	-5.10307300	-4.86727200	-1.21464500	H	-6.44423900	-0.52144800	5.33886400	H	5.02891900	-3.14737700	-0.91266500
H	-2.79853200	-4.74554600	-2.18133600	N	-5.59608800	2.64280300	3.52557000	H	2.85930800	-2.91739200	-1.43217000
H	-2.35468200	-5.55621400	3.12727200	C	-6.40493700	3.26403300	2.47090800	H	2.71029100	-3.85831500	0.06876600
H	-0.09968100	-4.86439500	-1.30277200	C	-5.58865300	3.37904500	1.18982800	H	1.93449200	-1.42092600	-0.15218600
H	0.11828800	-5.55455600	2.95109800	H	-7.30211500	2.65954500	2.30762300	C	8.68088900	-5.77611800	1.95051400
H	1.22860600	-5.26166000	0.77074000	H	-4.65799200	2.34124700	3.27951300	C	7.61174400	-5.11205300	2.84603800
C	-3.51984200	2.94061500	-4.40874200	H	-6.73276500	4.25834600	2.79457000	C	7.30183300	-3.66018800	2.63675000
C	-2.39911000	3.84355400	-3.93375600	H	-4.61015600	3.82057300	1.40412300	C	6.12330900	-2.97946100	2.80696900
O	-1.72510000	3.54186200	-2.93584600	H	-6.08503700	4.06466100	0.49371600	N	8.21942800	-2.70795500	2.22045800
C	-2.85040500	1.58066400	-4.77145500	Z	0.56774000	-0.44255500	-2.90778500	C	7.61941500	-1.51825800	2.07999600
C	-2.10709600	0.89034600	-3.60477200	C	3.10743700	1.96777000	1.59146500	N	6.35192800	-1.65934800	2.45487300
O	-2.74017100	0.59062000	-2.58380700	N	1.75588600	1.74632200	1.17177200	H	8.65766400	-5.51579600	0.89278800
O	-0.85911800	0.60412000	-3.83153000	C	4.19013800	1.08498500	0.94072500	H	8.49251800	-6.85467900	1.98368700
H	-4.05308900	3.34413800	-5.27335200	C	0.73981800	1.91025600	2.11256300	H	9.14634800	-2.91590700	1.87682800
H	-4.22301300	2.79375300	-3.58368100	O	4.33401000	-0.14507200	1.62338500	H	9.69890600	-5.67839800	2.33165100
H	-3.63060900	2.88609300	-5.10073700	C	5.46603300	1.96989300	1.04309100	H	6.66024000	-5.63775000	2.72040800
H	-2.15475200	1.72289900	-5.60246600	C	-0.56698500	1.93733700	1.78356700	H	7.89674200	-5.26571900	3.89477800
N	-2.09550600	4.91591200	-4.68866500	O	6.47283600	1.42671100	1.89361200	H	5.15507300	-3.31643700	3.14357000
C	-0.94041100	5.57560100	-4.41225900	C	4.93076700	3.34331400	1.52627400	H	8.06393200	-0.60688500	1.72143200
C	-0.04068300	5.91367900	-5.64108500	C	-1.01414400	1.70930000	0.36224300	H	5.62009300	-0.93937900	2.95513300
C	0.66076600	4.62937400	-6.09583700	O	3.51896400	3.30320300	1.30955800	C	-2.11293700	-4.59323600	-6.59142300
S	2.13233100	4.12720900	-5.11998600	C	5.51769500	4.54777300	0.82079200	C	-2.26701900	-4.77496900	-5.07153200
C	1.41688200	3.11145200	-3.78282700	C	0.13014500	1.92696900	-0.59195000	C	-1.22959200	-3.97602400	-4.35353800
H	-1.28027300	6.74506700	-4.07643700	C	1.40785400	1.91985000	-0.18757000	C	-1.20493000	-2.66366300	-3.95088700
H	-2.66960600	5.12887900	-5.49178200	C	-1.63437400	2.15710600	2.78598500	N	0.07225200	-4.42531000	-4.17142600
H	-0.40523400	5.29561900	-3.58420200	N	-1.27498000	2.72229200	3.98964200	C	0.82164400	-3.40720900	-3.68051000
H	-0.64575900	6.29886900	-6.47526500	O	-2.80102800	1.83599100	2.54797100	N	0.06971300	-2.32758000	-3.54218200
H	0.71029200	6.68003900	-5.42504600	H	5.31663100	4.48914900	-0.25248500	H	-1.12460600	-4.91920300	-6.92994000
H	-0.03721700	3.78588100	-6.13002800	H	3.76240000	-0.81385100	1.16374500	H	-2.23071000	-3.54079500	-6.86310900
H	1.04498200	4.76757000	-7.11029500	H	6.17316200	1.52040400	2.80881300	H	-2.86476400	-5.17557400	-7.13154200
H	2.22472500	2.46907900	-3.42440800	H	3.14363700	1.77825600	2.67388000	H	-3.26114600	-4.44562200	-4.75314600
H	1.03328700	3.71418200	-2.96020900	H	3.95207800	0.90109600	-0.11216700	H	-2.18910800	-5.83466000	-4.80125800
H	0.61826000	2.47314200	-4.16516500	H	1.08286000	2.00363300	3.13712600	H	0.40375700	-5.35729600	-4.37533500
C	-3.48509700	6.27310800	0.35804300	H	5.93956700	2.07769900	0.06712000	H	-2.00440400	-1.94231500	-3.93484900
C	-2.20156200	5.53655900	0.00956500	H	5.12230800	3.41317600	2.61422400	H	1.87164600	-3.48017600	-3.44060900
C	-1.29981200	5.33189300	1.22367500	H	-0.10214300	2.12713500	-1.63057500	C	-6.12180000	-2.21877900	-4.36589500
O	-2.57773300	4.27319500	-0.53939200	H	2.23727100	2.09998800	-0.85912200	C	-6.79357600	-2.94445100	-3.21821500
H	-4.13179700	6.29744300	-0.52389000	H	-1.83946300	2.37997100	0.12405900	O	-6.36862200	-4.03324600	-2.82264400
H	-3.28201100	7.30026500	0.67818200	H	6.60019900	4.57904400	0.97493100	C	-4.71098900	-1.76699800	-3.96126500
H	-4.01757900	5.76554200	1.16496800	H	-1.44004800	0.70412000	0.27222200	H	-6.71319700	-1.36454300	-4.71288400
H	-1.65349400	6.10882800	-0.75450200	H	5.08069400	5.47221900	1.20517300	H	-6.05802700	-2.92973700	-5.19644100
H	-2.08643700	4.08302900	-1.36136000	H	-2.04852200	2.94808400	4.60037400	H	-4.18159800	-2.60375400	-3.49711700
H	-0.39324000	4.78529600	0.95111300	H	-0.49923200	3.36685700	4.01722900	H	-4.14186500	-1.42992400	-4.83435600
H	-1.00867100	6.29012200	1.66392100	O	-1.79877600	-1.30013600	1.86623300	H	-4.73130300	-0.94979400	-3.42922200
H	-1.83831700	4.75517000	1.98148300	C	-2.78478800	-1.56568700	0.82701200	N	-7.84162600	-2.28963100	-2.67628300
C	2.57883300	8.14532200	-1.53100600	C	-2.02606900	-1.54304300	-0.50903000	C	-8.65049200	-2.79000300	-1.58375000
C	2.66591700	6.97396500	-0.54123200	C	-0.59997700	-1.40144600	-0.10276300	C	-8.65023100	-1.88445400	-0.32815200
C	1.77515500	7.20598100	0.68390100	C	-0.50824200	-1.61223700	1.38882000	C	-7.52127800	-2.22224700	0.65890900
C	2.31116000	5.64684900	-1.22456500	O	0.37156300	-1.13593000	-0.83017700	C	-10.01009100	-1.97901200	0.37610900
H	3.37623600	8.07552300	-2.7962000	H	-3.53867500	-0.78177000	0.90627800	C	-6.10652900	-2.13165700	0.09208800
H	2.68104300	9.10783800	-1.02895400	H	-3.24580200	-2.53717100	1.00765400	H	-9.67891800	-2.90882800	-1.94877900
H	1.63694300	8.11157000	-2.08129500	H	-2.31695400	-0.73725800	-1.19400500	H	-8.08098900	-1.38518000	-3.05317700
H	3.70607800	6.90779400	-0.19112800	H	-2.12881300	-2.48567600	-1.05858500	H	-8.27369300	-3.78743800	-1.34555600
H	1.82240900	6.35692100	1.37435400	H	-0.22042400	-2.66074500	1.57950000	H	-8.50704700	-0.84590200	-0.66283700
H	2.07015900	8.10752200	1.23111700	H	0.22326100	-0.94468900	1.85160500	H	-7.69547600	-3.23151500	1.05510000
H	0.72876300	7.32894600	0.38165100	C	-5.33725200	2.05983400	0.45325700	H	-7.59956000	-1.54752500	1.51775600
H	2.46763000	4.79947100	-0.55039600	O	-5.80206200	0.98464300	0.82424800	H	-10.83007600	-1.66576000	-0.27970700
H	1.25365000	5.64598800	-1.52070400	H	-4.23990900	1.38421300	-1.14617800	H	-10.21170600	-3.00838800	0.69569100
H	2.90330500	5.48629100	-2.13223400	N	-4.59223500	2.21104200	-0.67886400	H	-10.02918700	-1.34821800	1.26929600
C	-0.18692900	5.98852100	6.12600800	H	-4.00807300	3.04028900	-0.74998300	H	-5.93810600	-2.85107500	-0.71049800
C	-0.74471900	6.76534700	4.92560600	C	-4.85195500	-0.59558600	3.88231900	H	-5.90146900	-1.12098700	-0.26933800
C	-1.98728300	7.57376200	5.31421600	H	-5.47027400	-0.16127700	3.09038400	H	-5.38901600	-2.35283300	0.88372300
C	0.32712600	7.66164700	4.29435300	H	-8.33777900	-0.20497900	3.74905800	C	-6.42281500	-6.00841100	1.08664300
H	0.08222700	6.64115700	6.95624500	C	-4.88174800	-2.10319200	3.73842300	C	-5.13241300	-5.37650700	1.63239300
H	0.68910200	5.40895500	5.83364800	O	-5.93214100	-2.73969300	3.71910300	C	-4.01632800	-5.24705400	0.62974500
H	-0.93464200	5.28471400	6.51197100	H	-2.83404700	-2.19467600	3.43008300	C	-4.12637800	-5.00375200	-0.71932900
H	-1.05004400	6.02742800	4.16828500	N	-3.65570000	-2.71467900	3.71243800	C	-2.59938100	-5.29382600	0.91716500
H	-2.41279700	8.08928800	4.44692100	H	-3.65194800	-3.70700900	3.53123000	C	-1.90328800	-5.06914100	-0.31021400
H	-2.76604100	6.93148000	5.73867100					C	-1.84529200	-5.50840600	2.08375500
H	-1.73661200	8.33360400	6.06380000	TS				N	-2.86066600	-4.89721400	-1.28468200
H	-0.06091800	8.18748400	3.41543300	C	4.99154700	-0.68283200	-5.11378300	C	-0.50736200	-5.05657000	-0.38662100
H	0.67134700	8.41845500	5.00914400	C	5.93485400	-1.26290800	-4.07326300	C	-0.45557300	-5.49903700	2.01530800
H	1.19991200	7.08063800	3.97651700	O	6.29043800	-2.43694400	-4.07516900	C	0.20551800	-5.27870500	0.79018700
C	3.59427500	0.58850500	6.38683700	C	3.50321100	-0.91477600	-4.73811200	H	-7.21211400	-5.96228300	1.84311700
C	3.34725800	-0.07322500	5.01763600	S	3.01586800	-0.22234500	-3.07485100	H	-6.24838600	-7.04308800	0.81961500
C	3.22784100	-1.57411600	4.87814400	H	5.19277600	-1.19123600	-6.06013000	H	-6.78031500	-5.47032900	0.19891900
C	3.66513800	-2.49259200	5.83392100	H	5.16651900	0.38977500	-5.24536900	H	-5.38109500	-4.39966300	2.05880100
C	2.67946000	-2.0786500	3.68740400	H	2.87570800	-0.45937200	-5.50718600	H	-4.77950900	-5.98325200	2.47721700
C	3.55377100	-3.87058200	5.61568200	C	3.31251300	-1.99133000	-4.73871100	H	-5.00132200	-4.87988400	-1.34207300
C	2.56369500										

C	0.707978100	4.88584500	-5.99871400	O	3.46486000	3.34660200	1.38412700	H	-8.36940400	-0.68408700	-1.69018200
S	2.14547900	4.34238600	-4.99165900	C	5.51384400	4.49388900	0.86688200	H	-5.87053300	-0.82894300	-2.19827100
C	1.38234500	3.21718000	-3.77441300	C	0.10200300	1.96764100	-0.68325600	C	2.25625300	-4.66921100	6.55903400
H	-1.34707300	6.80018400	-3.89446700	C	1.36607500	2.07154300	-0.19952400	C	2.42906400	-4.79590600	5.03543600
H	-2.54999500	5.11828600	-5.48947500	C	-1.91089400	1.93680600	2.50905300	C	1.36457300	-4.01919500	4.33202000
H	-0.40953300	5.37429500	-3.46082500	N	-1.74986200	2.57891800	3.70867200	C	1.28062300	-2.69060300	3.99551300
H	-0.65491100	6.52406200	-6.29819800	O	-2.97695200	1.43080000	2.17042600	N	0.09363500	-4.52475900	4.09128000
H	0.66941300	6.89187800	-5.20490700	H	5.30053400	4.43909800	-0.20415500	C	-0.69589400	-3.52243300	3.62955400
H	0.03898900	4.03026300	-6.13142400	H	3.62283700	-0.82456900	1.18954500	N	0.00142600	-2.40009400	3.56408700
H	1.13657900	5.11387600	-6.97931300	H	6.03848300	1.39755400	2.84428200	H	1.28083700	-5.04893400	6.87809600
H	2.18286800	2.56664000	-3.41279400	H	2.94647000	1.83769500	2.72672700	H	2.32581200	-3.62199300	6.86490800
H	0.93397300	3.75590600	-2.93885300	H	3.77728500	0.89664100	-0.03242900	H	3.02923600	-5.23527600	7.08624000
H	0.62826500	2.58099000	-4.24206300	H	0.83842000	2.04504400	3.08584400	H	3.41127800	-4.41549300	4.73611800
C	-3.52188500	6.22626700	0.49599500	H	5.79849400	2.00742800	0.10974300	H	2.39804200	-5.84912200	4.73215600
C	-2.20934500	5.49328200	0.23950900	H	5.08742600	3.38326100	2.66910900	H	-0.19540400	-5.48015800	4.24648500
C	-1.34233400	5.46410100	1.49443100	H	-0.10350300	2.12440700	-1.73294400	H	2.03153800	-1.92104500	4.06616300
O	-2.45991900	4.14154600	-0.15546800	H	2.21986800	2.29150300	-0.82578300	H	-1.73508800	-3.63804000	3.36334300
H	-4.16533300	6.26709900	-0.38765500	H	-1.99064200	1.69058800	-0.13874500	C	6.23151600	-2.22162500	4.35238700
H	-3.32428100	7.25869300	0.80596100	H	6.59796700	4.47542300	1.00932700	C	6.92266500	-2.95520200	3.20975500
H	-4.07833900	5.74063100	1.30088400	H	-0.93292600	0.22707200	0.12777800	O	6.50053000	-4.04247400	2.81732600
H	-1.65942100	6.00229300	-0.56569000	H	5.12375500	5.43849200	1.25254000	C	4.87363600	-1.67789700	3.87613900
H	-2.19859200	4.02955600	-1.09132700	H	-2.60611300	2.73341700	4.22691600	H	6.84805000	-1.40791200	4.74884100
H	-0.40136400	4.94212400	1.30161500	H	-1.04814000	3.29865200	3.80013400	H	6.07962900	-2.94240100	5.16223900
H	-1.11532400	6.47263400	1.84924700	O	-1.73934100	-1.49707900	1.83123900	H	4.29422700	-2.48426400	3.41689000
H	-1.88089500	4.93584400	2.28707700	C	-2.66911500	-1.64562000	0.71345600	H	4.30243100	-1.26245600	4.71322900
C	2.53374500	8.19335600	-1.32240200	C	-1.83699000	-1.58152500	-0.57000900	H	4.99796500	-0.89445100	3.12241500
C	2.63506500	6.99549000	-0.36730600	C	-0.53237400	-0.96764200	-0.08315400	N	7.97261000	-2.29425500	2.68943700
C	1.76569900	7.19310300	0.87852300	C	-0.41075100	-1.46869600	1.35213000	C	8.74858300	-2.74293800	1.55026800
C	2.26786700	5.68903100	-1.08373500	O	0.54938200	-0.87394500	-0.83330700	C	8.69991700	-1.77648400	0.34578200
H	3.33211900	8.15264400	-2.07216500	H	-3.38597000	-0.82566900	0.79053900	C	9.99596600	-1.89841900	-0.46611100
H	2.62605500	9.14407200	-0.79649400	H	-3.19202100	-2.59628200	0.81609700	C	7.48477300	-1.99577300	-0.57060100
H	1.59418300	8.16543300	-1.87703200	H	-2.30639600	-0.98925600	-1.35513400	H	9.78920300	-2.87394900	1.87349000
H	3.68082700	6.91785700	-0.03669500	H	-1.60421800	-2.58049000	-0.94701100	H	8.20119900	-1.38935100	3.70621400
H	1.82434000	6.32529300	1.54475100	H	0.05153200	-2.46857000	1.34062700	H	8.36681600	-3.72969900	1.27691200
H	2.07154900	8.07824100	1.44593900	H	0.18428800	-0.81088400	1.99432900	H	8.64425400	-0.75291300	0.74893800
H	0.71497600	7.52598800	0.59767600	C	-5.48323700	2.08312300	0.38103600	H	10.87760300	-1.65332900	0.13619100
H	2.44216700	4.82594500	-0.43466400	O	-6.08960100	1.04204800	0.61421500	H	10.12105600	-2.91957900	-0.84498100
H	1.20464800	5.69280900	-1.35856900	H	-4.34015400	1.44710200	-1.21125200	H	9.97676500	-1.22870000	-1.33046300
H	2.84195500	5.55527800	-2.00699200	N	-4.64533600	2.25571400	-0.68202700	H	7.51190900	-1.23431600	-1.35666000
C	-0.24348100	5.82736400	6.26858900	H	-3.99024100	3.02969300	-0.63426400	H	7.60492000	-2.95487200	-1.08938900
C	-0.79657500	6.64049700	5.09110400	C	-4.87026500	-0.76006300	3.84008500	C	6.55275900	-5.93854500	-1.15573600
C	-2.04887700	7.72614600	5.49471600	H	-5.46261900	-0.32746800	3.02688200	C	5.27609400	-5.29099400	-1.70218500
C	0.27401400	7.45640300	4.50034900	H	-3.85126300	-0.37272300	3.74166700	H	7.37877200	-5.90385800	-1.86691000
H	0.01716000	6.46167000	7.11550500	C	-4.89124000	-2.26898600	3.67934300	H	6.38298600	-6.98412800	-0.89915300
H	0.63839600	5.26229100	5.96555800	O	-5.94050900	-2.90739800	3.70086400	H	6.89197000	-5.42428400	-0.25025200
H	-0.98966300	5.10960500	6.63003200	H	-2.85091700	-2.34419900	3.27963900	H	5.53167800	-4.30920200	-2.11158000
H	-1.08975700	5.92864700	4.30520300	N	-3.66578300	-2.86670200	3.58139800	H	4.90476600	-5.88456900	-2.54883000
H	-2.47096400	7.96680900	4.64113300	H	-3.66410500	-3.85539500	3.38149300	C	3.56613300	2.98059600	4.42150700
H	-2.82604600	6.76467200	5.89164600	L294Q-pro-(R)							
H	-1.81050500	8.16282200	6.27081500	atoms: 271 charge: +1							
H	-0.11088200	8.12169300	3.63898600	ES							
H	0.60838300	8.29716100	5.24513300	C	-4.89418000	-0.81303900	5.16395700	C	-4.89418000	-0.81303900	5.16395700
H	1.15281400	7.00176000	4.16797700	C	-5.84497900	-1.38453100	4.12446200	O	0.78538200	0.49837300	4.06957500
C	3.58090300	0.45344600	6.41239700	O	-6.19710800	-2.55974700	4.12023000	H	4.15836700	3.28798900	5.29072000
C	3.34835500	-0.18894800	5.03124900	C	-3.41296400	-1.04141000	4.76277700	H	4.244442800	2.68061300	3.62204000
C	3.24532400	-1.69039600	4.87719800	S	-2.96038900	-0.31383100	3.10100200	H	3.27769400	0.96839700	5.17986700
C	3.73950900	-2.60739000	5.80707700	H	-5.08223400	-1.33422500	6.10588600	H	1.98923000	2.04685700	5.64685300
C	2.65626900	-2.19834700	3.70704400	H	-5.06752600	0.25780500	5.31024400	N	1.83402600	4.66407800	4.75040200
C	3.64512300	-3.98543200	5.58378200	H	-2.77119700	-0.59950600	5.52785700	C	0.98045300	5.79141600	4.39586800
C	2.55577000	-3.56258700	3.46586200	H	-3.22281000	-0.11776200	4.73841000	C	0.03207200	6.14150000	5.53997000
C	3.04490100	-4.46778400	4.41669500	N	-6.24729200	-2.50996800	3.15169400	C	-0.90554300	5.01659200	5.99788700
O	2.90569000	-5.79859700	4.14000100	C	-7.15432000	-0.93247100	2.11202400	S	-2.15170100	4.45608900	4.77541800
H	3.62269300	1.51451700	6.16754600	C	-6.59203900	-2.04324400	1.19368900	C	-1.22972900	3.19288000	3.83419300
H	0.53039800	0.15562800	6.86567300	O	-7.36862800	-2.73699800	0.52966800	H	1.60298300	6.65763000	4.14560800
H	2.77253800	0.26121800	7.11937800	C	-7.55566300	0.26622000	1.19697000	H	1.80079600	4.31269900	5.69510600
H	2.43158800	0.24564100	4.61060800	C	-9.02090900	0.19526100	0.82094000	H	0.41659400	5.54199900	3.49161100
H	4.14810900	0.16000000	4.36055300	O	-7.20700400	1.52951500	1.75828300	H	0.62153600	6.47075200	6.40796500
H	4.19794700	-2.25576800	6.72634600	H	-5.89831400	0.38310100	3.11856400	H	-0.57028300	6.99988200	5.27463000
H	2.27050400	-1.51107600	2.96352900	H	-8.04301600	-1.37884300	2.57090700	H	-0.35380000	4.13458600	6.34205900
H	4.02452300	-4.68231800	6.32755700	H	-6.94766300	0.20899500	0.29179500	H	-1.49169900	5.36861100	6.85149200
H	2.06891800	-9.33643700	2.57283800	H	-7.87275300	1.77237000	2.41687100	H	-1.97795900	2.60770000	3.29486500
H	3.14272100	-6.31821200	4.91944600	H	-9.27356700	0.94386500	0.06143100	H	-0.52836800	3.63053300	3.12197200
C	-5.29875500	1.10189600	5.57156600	H	-9.26822200	-0.80665500	0.45460300	H	-0.69896000	2.51587100	4.50589400
C	-6.14084900	2.03837200	4.69588600	H	-9.65862600	0.37368400	1.70103300	C	3.52479300	6.26360400	-0.37966400
O	-7.24447500	2.43095700	5.05812700	N	-5.24643000	-2.11888800	1.08377500	C	2.34899500	5.30769500	-0.23672500
C	-5.46482800	-0.38265200	5.20788800	C	-4.58482200	-3.18835200	0.33781800	C	1.55000300	5.18551000	-1.52688000
H	-5.63075300	1.27120800	6.59813900	C	-3.07912200	-2.97977100	0.35678600	O	2.83538600	4.01348900	0.10809200
H	-4.23411300	1.36952500	5.51078900	O	-2.71513900	-1.79527600	-0.35505200	H	4.05718800	6.31757700	0.56967600
H	-4.97206300	-0.97927800	5.98492600	H	-4.81659500	-4.16409400	0.78421800	H	3.19463600	7.27461000	-0.64475100
H	-6.52306900	-0.65778400	5.22580700	H	-4.67009300	-1.56310900	1.71545400	H	4.21444200	5.91044400	-1.15274900
N											

H	-1.96268700	2.82358900	4.60085700	C	-7.07967300	-2.06498500	0.46445800	H	-2.95517400	6.98970600	5.59080800
H	-0.50188100	3.45302400	3.97360000	C	-9.55215200	-2.33784700	0.82139200	H	-1.95973100	8.42237200	5.88704800
O	-2.74967300	-1.28696400	0.49838200	C	-5.86778900	-1.74575400	-0.41813500	H	-0.27578900	8.25875300	3.24516700
C	-1.98423600	-1.64085800	1.67496600	H	-9.67598400	-3.12909500	-1.65127400	H	0.44732800	8.54178900	4.83471400
C	-0.50368100	-1.37297500	1.34618900	H	-8.11746900	-2.97814600	-1.71798500	H	1.00993800	7.19462300	3.83261900
C	-0.55167100	-0.77997100	-0.05854600	H	-8.24243000	-0.40191700	-1.12920100	C	3.56829000	0.82796200	6.39985600
C	-1.89635200	-1.24291500	-0.62477400	H	-8.61728400	-1.02902900	-0.60336200	C	3.34426800	0.07176600	5.05617900
O	0.54056200	-0.75402700	-0.79757700	H	-6.93673700	-3.04354200	0.94400400	C	3.33307100	-1.40310100	4.97463200
H	-2.15227500	-2.69201000	1.91793200	H	-7.11719600	-1.32039100	1.26408200	C	3.90871900	-2.24164200	5.93148300
H	-2.35402200	-1.01356900	2.48458400	H	-10.55572400	-2.24528700	0.39270700	C	2.76237400	-2.00208500	3.83877700
H	0.07831200	-2.29798800	1.31133600	H	-9.45049900	-3.35529400	1.21810500	C	3.91793600	-3.63069200	5.76557700
H	0.02472500	-0.69616000	2.06157400	H	-9.47860200	-1.64535700	1.66462300	C	2.76439800	-3.37988000	3.65521400
H	-2.31186400	-0.54895300	-1.35883400	H	-5.51567800	-2.62152200	-0.96376400	C	3.34201500	-4.20517700	4.62888600
H	-1.75872500	-2.23759200	-1.07807800	H	-6.09989900	-0.94430400	-1.12225700	O	3.31703800	-5.55281400	4.40095600
C	-5.85424800	1.54566500	0.55649200	H	-5.05382900	-1.37350100	0.20349800	H	3.59023200	1.87636600	6.10347300
O	-6.88195300	0.94218600	0.25146700	C	-6.32275900	-0.06175500	1.42085400	H	4.52494200	0.57360100	6.86482300
N	-4.61064200	1.00505100	0.48853400	C	-5.05358900	-5.36517100	1.93408900	H	2.76488300	0.65564200	7.11751500
H	-3.82429100	1.48485200	0.90005400	C	-3.95799100	-5.28630200	0.90045500	H	2.39554400	0.46726700	4.63676000
H	-4.49147300	0.01011000	0.35549800	C	-4.11664800	-5.13800300	-0.45727400	H	4.10899400	0.46478500	4.35058000
C295N-pro-[5]				C	-2.53189600	-5.32188800	1.14385900	H	4.35508100	-1.81825900	6.82598000
atoms: 276 charge: +1				C	-1.87920400	-5.19875400	-0.11826400	H	2.31267800	-1.37461400	3.07746700
ES				C	-1.74224200	-5.43370100	2.29899000	H	4.36430100	-4.26496900	6.52802500
C	4.98145800	-0.84420300	-5.06046300	N	-2.86982600	-5.06993300	-1.06980900	H	2.29996500	-3.83231100	2.78603100
C	5.92997400	-1.35918700	-3.99109500	C	-0.48635200	-5.19248700	-0.24457900	H	3.60811300	-6.01902700	5.19561800
O	6.29404300	-2.52932800	-3.93158100	C	-0.35624000	-5.44189000	2.18161600	C	-5.32308600	1.27114200	5.55047000
C	3.49404200	-1.09228200	-4.67713200	C	0.26457700	-5.32830300	0.92172200	C	-6.13663800	2.21835500	4.66011000
S	2.98013800	-0.34328700	-3.03999400	H	-7.15223200	-6.00502600	2.12556600	O	-7.18468300	2.71802600	5.06057300
H	5.19225200	-1.39178400	-5.98238600	H	-6.12951400	-7.11240500	1.20432800	C	-6.04045600	-0.09053700	5.64100200
H	5.13380500	0.22458300	-5.24075400	H	-6.66885500	-5.59584700	0.49181600	C	-6.17799900	-0.84702700	4.30504100
H	2.85939500	-0.68071000	-5.46453800	H	-5.30540700	-4.35440900	2.28436100	C	-4.82394800	-1.29504500	3.73977000
H	3.32905300	-2.17202700	-4.63682200	H	-4.67453200	-5.89496100	2.81613600	C	-7.10804400	-2.05455200	4.47706700
N	6.31927900	-0.43634200	-3.05886800	H	-5.01010900	-5.05261300	-1.06023900	H	-5.26713300	1.72459000	6.54375100
C	7.23798400	-0.79264000	-2.00439600	H	-2.72259600	-5.01955500	-2.06384900	H	-4.30196700	1.14212000	5.17099300
C	6.70072200	-1.88571600	-1.05021900	H	-2.20958000	-5.50969300	3.27576700	H	-5.51271400	-0.72905800	6.36235700
O	7.49318200	-2.54164800	-0.36622100	H	-0.00907900	-5.11118800	-1.21728200	H	-7.03936500	0.09573900	6.05093000
C	7.58602200	0.45266800	-1.12943300	H	0.26221200	-5.54472800	3.06826200	H	-6.63777100	-0.16995100	3.57252200
C	9.04823500	0.42730400	-0.70625500	H	1.34807700	-5.37947300	0.85708400	H	-4.96740300	-1.83939900	2.80108800
O	7.23105800	1.68360500	-1.75498600	C	-3.58677500	2.72592900	-4.45779000	H	-4.15519700	-0.45714300	3.52686200
H	5.96891300	0.51153500	-3.07736000	C	-2.49656500	3.67326500	-4.00198000	H	-4.31138200	-1.96806500	4.43861300
H	8.14522400	-1.22407200	-2.44093200	O	-1.84439800	3.44052300	-2.97122500	H	-7.24425900	-2.58439000	3.52857900
H	6.94981200	0.42239700	-0.24239800	C	-2.89138600	1.36491800	-4.76977900	H	-6.69368400	-2.76711700	5.20127400
H	7.91035900	1.90923900	-2.40593400	C	-2.12422300	0.71640500	-3.59128300	H	-8.09603400	-1.74928000	4.83737600
H	9.25422500	1.20867700	0.03122300	O	-2.74432300	0.37625700	-2.57493400	N	-5.66342500	2.43872600	3.97911400
H	9.29689300	-0.55524400	-0.29616600	O	-0.85945600	0.50374600	-3.81098000	C	-6.49168600	3.13967800	2.40879100
H	9.70092900	0.58645100	-1.57306100	H	-4.12049400	3.08670000	-5.34088800	C	-5.73844800	3.28020000	1.09531700
N	5.35682700	-1.98549400	-0.92866600	H	-4.29540700	2.59554600	-3.63429200	H	-7.42329100	2.58833800	2.24623900
C	4.73171700	-3.05882900	-0.15494400	H	-3.66164700	0.64746700	-5.07238200	H	-4.86932800	1.90478600	3.05940200
C	3.21991400	-2.93799300	-0.20447400	H	-2.20293300	1.49299700	-5.60900700	H	-6.75392400	4.12173100	2.81241700
O	2.78948700	-1.74807500	0.46043100	N	-2.19617900	4.71265700	-4.80262200	H	-4.72463300	3.65156300	1.26821600
H	5.02801100	-4.03560300	-0.55818900	C	-1.08329200	5.60981600	-4.52710600	H	-6.23854100	4.02365200	0.46319600
H	4.75457700	-1.47389600	-1.58306900	C	-0.19315500	5.80519400	-5.75675200	Z	0.58159700	-0.49362200	-2.85078000
H	5.08216900	-3.02408600	0.87745000	C	0.55940500	4.55160400	-6.21530100	C	2.98033700	2.05350400	1.57730300
H	2.88424700	-2.90609800	-1.24659800	S	2.04127000	4.09663500	-5.23133500	N	1.65227200	1.79129500	1.10680600
H	2.77238400	-3.81331600	0.27946400	C	1.34680700	3.05993400	-3.89867000	C	4.10891200	1.18152200	0.98373300
H	2.01000600	-1.38273800	-0.01043700	H	-1.46939300	6.58109500	-4.19322100	C	0.58762900	1.87552900	2.00114700
C	8.77555000	-5.51750000	2.23493900	H	-2.75684300	4.87480400	-5.62683800	O	4.29208400	-0.00735200	1.72833500
C	7.70674200	-4.81234700	3.09460400	H	-0.52687100	5.17634600	-3.69763500	C	5.35196200	2.11531000	1.05652500
C	7.42531000	-3.36772800	2.81701200	H	-0.81452100	6.16717400	-6.58952900	C	-0.70281500	1.81044500	1.61189700
C	6.25596500	-2.66296400	2.93532400	H	0.52582100	6.60136900	-5.53994100	O	6.38988400	1.62633800	1.90178700
N	8.36419000	-2.44953500	2.37168300	H	-0.10660500	3.68314600	-6.26037000	C	4.77180800	3.47472700	1.52300900
C	7.78284600	-1.25812600	2.16936200	H	0.94568100	4.71163000	-7.22577100	C	-1.07423000	1.59132900	0.16643700
N	6.50890100	-1.36527400	2.52843900	H	2.16913600	2.44057100	-3.53233800	O	3.36658500	3.39310800	1.27945700
H	8.74586200	-5.30957200	1.16581100	H	0.94123900	3.65254800	-3.07895700	C	5.33818400	4.69235000	0.82359900
H	8.60100200	-6.59484900	2.32672200	H	0.56950000	2.39704700	-4.28383400	C	0.10283300	1.85897200	-0.73091100
H	9.29878200	-2.68327000	2.06832300	C	-3.64928200	6.17315500	0.22635500	C	1.35789000	1.93368600	-0.26718500
H	9.79219900	-5.38251000	2.60827700	C	-2.37138000	5.40656600	-0.08075300	C	-1.83341900	1.90043900	2.56705000
H	6.74862100	-5.32948900	2.98288000	H	-1.47517900	5.24879800	1.14435700	N	-1.62107300	2.56215100	3.75112800
H	7.98215700	-4.92595700	4.15109900	O	-2.74536000	4.11906800	-0.57576300	O	-2.92390900	1.38344000	2.30208700
H	5.27881500	-2.97129600	3.27236600	H	-4.29480600	6.15885300	-0.65661000	H	5.15786300	4.62484200	-0.25821200
H	8.24722800	-0.37049200	1.77766200	H	-3.43659100	7.21299400	0.49524500	H	3.75411700	-0.71614400	1.28783600
H	5.77562900	-0.65441000	2.31455900	H	-4.18953800	5.71091000	1.05585900	H	6.09374300	1.71632300	2.81858100
C	-2.05185500	-4.95208800	-6.32763400	H	-1.81325700	5.93773200	-0.86642900	H	2.97826700	1.88775500	2.66394600
C	-2.15055700	-5.08747000	-4.79857300	H	-2.29791300	3.93551800	-1.42535300	H	3.89057000	0.93541300	-0.06063400
C	-1.14150400	-4.20753900	-4.13668300	H	-0.56595800	4.69591400	0.89369700	H	0.87402100	1.97752000	3.04253500
C	-1.17869300	-2.88434700	-3.77195800	H	-1.18937600	6.22299700	1.55175700	H	5.80868600	2.22285200	0.07191400
N	0.18679700	-4.58140700	-3.97624600	H	-2.01471500	4.69638900	1.92012400	H	4.94055600	3.55376100	2.61428600
C	0.89250100	-3.51136800	-3.53407700	C	2.36603400	8.15999000	-1.70100200	H	-0.09311900	2.05525700	-1.77832400
N	0.08659100	-2.46983300	-3.40657300	C	2.47770600	7.01355900	-0.68490800	H	2.20570100	2.15718300	-0.90169200
H	-1.05684600	-5.23353600	-6.68581800	C	1.54684300	7.23052400	0.51309400	H	-1.90347100	2.24778800	-0.09219200
H	-2.23814900	-3.91829600	-6.63052100	C	2.19431300	5.65940100	-1.34873300	H	6.41657500		

N	-4.75741400	2.00894800	-0.71971200	C	-2.51132100	-5.32131700	1.09161600	H	4.27926400	-1.95307600	6.82820000
H	-4.07597400	2.76173000	-0.73057100	C	-1.81143900	-5.18786100	-0.14538200	H	2.26405000	-1.44445700	3.07183700
TS				C	-1.76626900	-5.41272500	2.27884300	H	4.20650500	-4.39839800	6.52923100
				N	-2.76503700	-5.09906900	-1.13590800	H	2.16598600	-3.88953400	2.77974400
C	5.04845700	-0.77654700	-5.05226200	C	-0.41509200	-5.16891600	-0.21604300	H	3.38413400	-6.12537500	5.20020400
C	5.99820100	-1.30423300	-3.98993800	C	-0.37691000	-5.39931400	2.21559400	C	-5.35203200	1.15800700	5.49941100
O	6.38115600	-2.46913900	-3.95547300	C	0.29096600	-5.28541600	0.97934100	C	-6.15383400	2.11539500	4.61202700
C	3.56305100	-1.03088000	-4.68075900	H	-7.14402100	-6.06283600	1.94045200	O	-7.18549900	2.64092600	5.01865400
S	3.04717100	-0.29483000	-3.04617500	H	-6.11218000	-7.15432200	1.01046200	C	-6.03438700	-0.22108300	5.56618400
H	5.26852500	-1.30718700	-5.98216600	H	-6.64185300	-5.62480300	0.31735100	C	-6.00014300	-1.03754600	4.25999200
H	5.20005500	0.29553800	-5.21382500	H	-5.31733300	-4.40785100	2.13860200	C	-4.57354900	-1.44163200	3.86366900
H	2.93209100	-0.61644700	-5.47000100	H	-4.69624400	-5.95050300	2.67807900	C	-6.88465700	-2.28225000	4.40639800
H	3.39773300	-2.11120300	-4.64735800	H	-4.90363900	-5.10506800	-1.20727600	H	-5.32893200	1.60303000	6.49782900
N	6.37668000	-0.39560900	-3.03807000	H	-2.57811000	-4.92991000	-2.11024000	H	-4.31832800	1.05243800	5.14814100
C	7.27765600	-0.77301600	-1.97575100	H	-2.27089500	-5.49706200	3.23642000	H	-5.56180600	-0.81232500	6.36208700
C	6.73244400	-1.89010800	-1.05514900	H	0.09933700	-5.08034300	-1.16894100	H	-7.07515000	-0.05876600	5.86890400
O	7.52083700	-2.56220800	-0.38027600	H	0.20794200	-5.49017300	3.12577600	H	-6.41494500	-0.41937400	3.45124500
C	7.60270900	0.45107600	-1.06325100	H	1.37659200	-5.32064000	0.95788500	H	-4.58787300	-2.08692700	2.98052700
C	9.05666900	0.42202600	-0.61183300	C	-3.52804200	2.77677100	-4.46800000	H	-3.93750900	-0.58749000	3.61879500
O	7.25009200	1.69848700	-1.65671200	C	-2.49540400	3.76172500	-3.95482300	H	-4.08995800	-2.00378900	4.67242300
H	5.97976500	0.53352200	-3.01720100	O	-1.94558100	3.60510300	-2.85319500	H	-6.89597100	-2.87014800	3.48360900
H	8.19464100	-1.18784400	-2.40740100	C	-2.76397300	1.45150700	-4.77221200	H	-6.51337100	-2.92983700	5.21042000
H	6.94944800	0.39325100	-0.19010900	C	-2.03541200	0.81483000	-3.56335500	H	-7.91854800	-2.01219300	4.64598600
H	7.91013300	1.92086400	-2.32839100	O	-2.67791900	0.56020100	-2.53528500	N	-5.67111300	2.34585500	3.35100400
H	9.24600500	1.18823100	0.14579000	O	-0.78073000	0.54044800	-3.76057400	C	-6.49430900	3.07652200	2.37826400
H	9.30081400	-0.56819800	-0.21716200	H	-4.03653200	3.13269600	-5.36788200	C	-5.73609800	3.25814300	1.07224100
H	9.72566600	0.60163000	-1.46181000	H	-4.26353400	2.60450300	-3.67776200	H	-7.42804800	2.53381100	2.19556800
N	5.38925300	-1.98862400	-0.94177700	H	-3.48933300	0.71091300	-5.12679400	H	-4.94846500	1.73779300	2.97797400
C	4.75705500	-3.07708600	-0.18584600	H	-2.04099600	1.61863500	-5.57473600	H	-6.75554100	0.04490600	2.81232200
C	3.24164000	-2.95263200	-0.26550200	N	-2.10929100	4.74435300	-4.79173500	H	-4.73358500	3.65076100	1.26170300
O	2.78368500	-1.75714700	0.35893600	C	-1.02664300	5.66332800	-4.46805100	H	-6.25057400	4.00420700	0.45459500
H	5.06437800	-4.04294500	-0.59150100	C	-0.10839200	5.89738300	-5.66882600	Z	0.65181900	-0.53131500	-2.80240200
H	4.79721000	-1.46054400	-1.58421100	C	0.67863300	4.66688300	-6.13120400	C	2.88243800	2.11990100	1.64016800
H	5.08697600	-3.04275000	0.85259500	S	2.10913300	4.18963500	-5.08416700	N	1.52484500	1.98608500	1.13413700
H	2.93182900	-2.94553600	-1.31664700	C	1.35095400	3.09131400	-3.83943400	C	3.94591300	1.15885900	1.04443600
H	2.79114700	-3.82566700	0.22132300	H	-1.44277700	6.62103600	-4.13004000	C	0.45810600	1.97622600	2.00642800
H	1.96642000	-1.41435700	-0.10870400	H	-2.59174200	4.85602600	-5.67188700	O	4.06906100	-0.03343700	1.78320000
C	8.78169600	-5.65015000	2.19967400	H	-0.48320200	5.23219700	-3.62873600	C	5.24457500	2.02401300	1.09145700
C	7.69445500	-4.89068200	3.06616100	H	-0.71212000	6.26610200	-6.51171700	C	-0.82224300	1.82504500	1.55919400
C	7.35133500	-3.45444800	2.80441500	H	0.59038800	6.70102200	-5.41661800	O	6.25791900	1.40908400	1.93596600
C	6.15559200	-2.79845600	2.94945000	H	0.02543400	3.79446200	-6.23966700	C	4.76214000	3.42384100	1.53963300
N	8.24589100	-2.49323600	2.35923500	H	1.11489900	4.86518200	-7.11411600	C	-1.03141800	1.51453100	0.15946400
C	7.61622000	-1.32432100	2.17847900	H	2.15867900	2.46835100	-3.44661900	O	3.34194900	3.42060700	1.33836400
N	6.35145600	-1.48530000	2.55478700	H	0.88127900	3.64888000	-3.02829000	C	5.37080900	4.58934900	0.78976600
H	8.76131100	-5.33981200	1.13385800	H	0.61512800	2.42576500	-4.29504500	C	0.03616300	1.91141300	-0.72521300
H	8.61239000	-6.64509200	2.26740800	C	-3.63536100	6.14726000	0.27088300	C	1.28768800	2.07003900	-0.22440700
H	9.17737500	-2.68892900	2.02082800	C	-2.31836600	5.40700600	0.05443400	C	-2.03509900	1.87207400	2.42974000
H	9.79485100	-5.43539000	2.58424000	C	-1.46446300	5.42160700	1.31885400	N	-1.93389600	2.55985900	3.60902900
H	6.75500200	-5.44135700	2.95763300	O	-2.55815400	4.01443700	-0.29951000	O	-3.06871600	1.30760700	2.08181400
H	7.97863000	-4.99928800	4.12078300	H	-4.27295700	6.14688500	-0.61793600	H	5.15943400	4.50143600	-0.27942300
H	5.19521900	-3.14878600	3.29405000	H	-3.44208400	7.19220600	0.53827400	H	3.60007800	-0.75494300	1.26756300
H	8.03873400	-0.44142700	1.79136400	H	-4.19648400	5.69378500	1.09162000	H	5.95374000	1.56168400	2.85184900
H	5.60220500	-0.78866200	2.37462400	H	-1.76059500	5.89031000	-0.76106900	H	2.83620200	1.94575800	2.72427800
C	-1.96958400	-4.86863100	-6.44876700	H	-2.28730700	3.90344700	-1.22923500	H	3.69892500	0.92760400	0.00272900
C	-2.13543800	-5.00641100	-4.92534400	H	-0.51732100	4.90221500	1.15094800	H	0.70822600	2.09667600	3.05367300
C	-1.11939900	-4.16623200	-4.22420900	H	-1.24939100	6.44198200	1.64636100	H	5.69682200	2.08477000	0.10108100
C	-1.12435500	-2.84208500	-3.86227200	H	-2.00672800	4.91133400	2.12104200	H	4.96282800	3.52204900	2.98189700
N	0.19194900	-4.58114600	-4.02731700	C	2.39509600	8.16979600	-1.57022700	H	-0.15828800	2.03500800	-1.78132100
C	0.91779100	-3.53144300	-3.56811500	C	2.50688400	7.00753400	-0.57313600	H	2.14392800	2.30589500	-0.84138100
N	0.14201800	-2.46527100	-3.46479000	C	1.60514700	7.22281500	0.64666800	H	-2.05008900	1.55023800	-0.20725100
H	-0.97218200	-5.18684300	-6.76741800	C	2.18839600	5.66858300	-1.25159800	H	6.45498100	4.59335100	0.93306800
H	-2.10279300	-3.82708600	-6.75323400	H	3.20101400	8.11764900	-2.31106000	H	-0.92705700	0.14411300	0.12710700
H	-2.70534700	-5.48044500	-6.97846500	H	2.46550300	9.13875700	-1.07511900	H	4.96420400	5.53743400	1.14890600
H	-3.13817090	-4.68470900	-4.62643500	H	1.46032800	8.10577200	-2.12993900	H	-2.81008500	2.69662300	4.09867700
H	-2.04139900	-6.05617300	-4.62268400	H	3.54687300	9.68993300	-0.21829600	H	-1.25866300	3.30467500	3.69724900
H	0.54538500	-5.51041800	-4.20464200	H	1.67507000	6.38126500	1.34465800	O	-1.62346500	-1.53397100	1.92798900
H	-1.93993200	-2.13878800	-3.86619000	H	1.87171300	8.13646000	1.18815800	C	-2.56682400	-1.75860000	0.84642000
H	1.96863200	-3.57336200	-3.32789400	H	0.55707500	7.31299700	0.33944800	C	-1.77646000	-1.71391600	-0.47012000
C	-6.03898300	-2.50018500	-4.32921100	H	2.36486400	4.83311800	-0.56781900	C	-0.48503000	-1.03146200	-0.03811300
C	-6.71566400	-3.21124500	-3.17517400	H	1.13281600	5.63773400	-1.55263500	C	-0.31688100	-1.47295200	1.41166600
O	-6.27314800	-4.27608100	-2.73651800	H	2.78830100	5.51594300	-2.15519800	O	0.58530500	-0.92895900	-0.80870200
C	-4.64863400	-2.00169200	-3.90907500	C	-0.39246300	5.99800500	6.07534800	H	-3.31196100	-0.96283800	0.90440100
H	-6.64516800	-1.67154600	-4.71094000	C	-0.95242300	6.76359700	4.86845400	H	-3.05168400	-2.72487800	0.99393600
H	-5.93993000	-3.23099600	-5.13891600	C	-2.22106700	7.53938500	5.23888100	H	-2.28893400	-1.17038600	-1.26425100
H	-4.10601100	-2.81135800	-3.41336700	C	0.10515900	7.68795900	4.25388200	H	-1.51558300	-2.71671500	-0.81842100
H	-4.07251200	-1.67215100	-4.78019100	H	-0.15012400	6.66627900	6.90276900	H	0.18929600	-2.45289500	1.42217100
H	-4.70299200	-1.16654200	-3.20565300	H	0.50216400	5.44217000	5.79691500	H	0.27341100	-0.77058300	2.01095300
N	-7.78980400	-2.56633900	-2.67160000	H	-1.12758400	5.27999400	6.45485900	C	-5.60554200	1.98195600	0.23282900
C	-8.57670500	-3.02876900	-1.54688200	H	-1.22747100	6.02104900	4.10492800	O	-6.28963800	0.98328400	0.43562000
C	-8.58334600	-2.05042100	-0.34940800	H	-2.64724100	8.044343					

C	7.51801200	0.37568600	-1.15733400	C	-1.85847000	0.93531300	-3.63914500	H	-7.69595000	-2.25408500	5.22331500
C	8.98001900	0.36233800	-0.73368300	O	-2.22661400	1.13785800	-2.47934200	N	-5.75152400	2.50714500	3.42646000
O	7.15370700	1.60346800	-1.78371800	O	-0.78968200	0.27362500	-3.98816000	C	-6.56490200	3.06710600	2.34557000
H	5.88680800	0.41427100	-3.10160200	H	-4.24536800	2.82972000	-5.41977700	C	-5.82955400	3.02365500	0.99911000
H	8.08686900	-1.29883800	-2.46339400	H	-4.33518600	2.32985600	-3.71907900	H	-7.48765700	2.48458200	2.30069700
H	6.88261200	0.33965500	-0.26984000	H	-3.29517100	0.56176400	-5.16392900	H	-4.75525000	2.38581000	3.28760100
H	7.83194800	1.83505700	-2.43356500	H	-2.02277900	1.64654800	-5.65931100	H	-6.84572000	4.10307800	2.57481400
H	9.17814100	1.14563600	0.00398600	N	-1.95906700	4.30968400	-4.92219300	H	-6.54239200	3.33053100	0.22708100
H	9.23505200	-0.61803700	-0.32276100	C	-1.15754400	5.48882900	-4.61706100	H	-5.02032700	3.75644400	0.99273400
H	9.63183800	0.52675300	-1.60016600	C	-0.20630200	5.81711100	-5.76528500	Z	0.62771200	-0.60911200	-2.93209300
N	5.30618200	-2.08497900	-0.96946000	C	0.77761500	4.70669000	-6.15723800	C	3.16070800	2.13781100	1.68737600
C	4.67345900	-3.12802900	-0.16454300	S	2.02885000	4.24837800	-4.89817100	N	1.79980900	1.88858700	1.32767100
C	3.16561700	-2.95106000	-0.18247800	C	1.13668700	3.01641000	-3.88862500	C	4.21982400	1.25434600	1.00223100
O	2.79363500	-1.72028300	0.44158700	H	-1.82143300	6.33795000	-4.42308300	C	0.81184100	2.00162100	2.29568600
H	4.92397000	-4.12126900	-0.55895900	H	-1.85847100	3.87661300	-5.82715100	O	4.37835800	0.01502100	1.66455000
H	4.71506000	-1.57123300	-1.62245900	H	-0.59790100	5.31336200	-3.69268800	C	5.49854400	2.13563500	1.06582800
H	5.05327500	-3.08624100	0.85776700	H	-0.79500400	6.08210300	-6.65528900	C	-0.50815300	1.93609800	2.01239800
H	2.80839500	-2.94719600	-1.21824100	H	0.36102900	6.71037600	-5.48712700	O	6.49975300	1.62095900	1.94195100
H	2.69903900	-3.79009800	0.34427500	H	0.26402100	3.78997900	-6.46897600	C	4.96619900	3.53213700	1.48815800
H	2.00958500	-1.35626300	-0.01909700	H	1.36269000	5.04032900	-7.01897900	C	-0.99811800	1.68797100	0.60710600
C	8.72028900	-5.56275000	2.25108100	H	1.90050500	2.46591700	-3.33474700	O	3.54462200	3.46744400	1.35049100
C	7.64557200	-4.85100500	3.10012300	H	0.43919800	3.47555000	-3.18594200	C	5.49429400	4.69446300	0.67242800
C	7.38507500	-3.40273600	2.82533400	H	0.60632900	2.30301600	-4.52162700	C	0.11260600	1.90218200	-0.38222400
C	6.22860300	-2.67669600	2.94301300	C	-3.73142900	6.08527600	0.12877500	C	1.39891800	1.98585100	-0.02620900
N	8.34100700	-2.50309100	2.37954000	C	-2.48380400	5.21770100	0.01286600	C	-1.53044300	2.09639400	3.37030890
C	7.78281400	-1.30049600	2.17907600	C	-1.70676000	5.15298400	1.32049200	N	-1.17319700	8.29057000	4.18015000
N	6.50755100	-1.38365800	2.53820900	O	-2.84742400	3.88958400	-0.34742200	O	-2.64876000	1.57823000	2.97854700
H	8.69132900	-5.35771100	1.18025200	H	-4.26052900	6.07699700	-0.82428400	H	5.25130100	4.55235600	-0.38414900
H	8.55060600	-6.63385000	2.35054200	H	-3.47279500	7.12399400	0.36558800	H	3.81575500	-0.66009200	1.20585000
H	9.27204800	-2.75473100	2.07963900	H	-4.39815700	5.71056000	0.90956300	H	6.20876700	1.77065200	2.85242400
H	9.73603800	-5.41588000	2.62466500	H	-1.83073900	5.63977300	-0.76758300	H	3.24466400	1.97676600	2.77175400
H	6.68570100	-5.36021700	2.96931200	H	-3.08536100	3.89467400	-1.29364800	H	3.94810300	1.08456500	-0.04457500
H	7.90411100	-4.937390800	4.15978200	H	-0.78948400	4.57014700	1.20426500	H	1.17692800	2.13825200	3.30783100
H	5.24473000	-2.96689900	3.27826800	H	-1.43628200	6.15793900	1.65535500	H	5.97526600	2.19862500	0.08806700
H	8.26266600	-0.42038800	1.78876900	H	-2.32500200	4.68419300	2.09377800	H	5.21502400	3.67681600	2.55660900
H	5.79104600	-0.65686000	2.31703900	C	2.28193300	8.07128600	-1.80806000	H	-0.16820900	2.02639200	-1.42048200
C	-2.09756800	-5.09018300	-6.32954000	C	2.38105600	6.96115100	-0.74867200	H	2.19501800	2.18338600	-0.73184100
C	-2.29507900	-5.10844400	-4.80340500	C	1.31643000	7.13264900	0.34174400	H	-1.82705900	2.35789600	0.36159900
C	-1.25249500	-4.27361600	-4.13483100	C	2.28165800	5.56591100	-1.37546400	H	6.58085000	4.76378100	0.77846000
C	-1.20327600	-2.93188900	-3.84587300	H	3.09379700	7.98646700	-2.53873700	H	-1.43760300	0.68538600	0.52902600
N	0.02815700	-4.73882900	-3.86771000	H	2.35443400	9.05239400	-1.33763200	H	5.04701600	5.63383500	1.00569600
C	0.78989700	-3.70262400	-3.43646800	H	1.34301000	7.99219200	-2.35887600	H	-1.91801300	2.99462900	4.84361300
N	0.06581800	-2.59505700	-3.15647700	H	3.36826000	7.04662600	-0.27013300	H	-0.50835000	3.58095300	4.07542300
H	-1.11469000	-5.84454200	-6.60527400	H	1.40487000	6.35170800	1.10475000	O	-2.74326100	-1.31313800	0.64583700
H	-2.16931600	-0.68661100	-6.71227900	H	1.39873100	8.10481300	0.83947000	C	-1.96444600	-1.74401600	1.78770100
H	-2.85774700	-5.69952800	-6.82607700	H	0.30976000	7.06109900	-0.08745400	C	-0.49059200	-1.57793100	1.38508600
H	-3.28540500	-4.71828800	-4.54736000	H	2.42300900	4.78711100	-0.61994300	C	-0.55676900	-1.34067300	-0.09554900
H	-2.26075800	-6.13646700	-4.42416700	H	1.29409800	5.19353500	-1.82946900	C	-1.98728300	-1.43659300	-0.54234500
H	0.33771000	-5.69429700	-3.97372100	H	3.02346000	5.42524400	-2.16816200	O	0.42043700	-1.10046500	-0.82179700
H	-1.97214700	-2.18385600	-3.94857300	C	-0.44399500	6.08673900	5.90977600	H	-2.20020300	-2.78382700	2.02140500
H	1.82929800	-3.78443100	-3.15858300	C	-1.02389300	6.81267200	4.68955600	H	-2.24837200	-1.09704500	2.65131200
C	-6.15481000	-2.67628800	-4.23819900	C	-2.28442100	7.60173800	5.05918100	H	0.11583700	-2.46462000	1.59171400
C	-6.82918000	-3.34649400	-3.05744400	C	0.02365000	7.71487100	4.02730100	H	-0.01119800	-0.71522800	1.86190900
O	-6.36140800	-4.37529500	-2.56638300	H	-0.19630400	6.77390800	6.71862400	H	-2.24978400	-0.63332700	-1.24068800
C	-4.84480100	-2.01889600	-3.76887600	H	0.44961100	5.62386500	5.63846500	H	-2.13522400	-2.41678300	-1.02430600
H	-6.80370500	-1.93121700	-4.71121300	H	-1.17198400	5.37512100	6.31931100	C	-6.15674300	0.54514600	0.33230000
H	-5.94420400	-3.45155400	-4.98112900	H	-1.31477400	6.04667300	3.95756100	N	-5.55149900	-0.66569900	0.16547300
H	-4.21158500	-2.76619100	-3.28167000	H	-2.72661900	8.07691800	4.17754400	H	-4.58197200	-0.78738700	0.43675300
H	-4.29629400	-1.58594600	-4.61195700	H	-3.04487300	6.95386600	5.50790800	H	-6.11945900	-1.50364300	0.18151800
H	-5.03650700	-1.22928700	-3.03514700	H	-2.05008200	8.39183100	5.78242300	O	-7.37591900	0.70561300	0.22191100
N	-7.91593900	-2.69981500	-2.57455400	H	-0.38052000	8.20313200	3.13435800	C	-5.19053800	1.69089900	0.59673200
C	-8.66372900	-3.15415500	-1.41593000	H	0.35204500	8.50133000	4.71717200	H	-4.61141800	1.85195300	-0.32139900
C	-8.97870400	-2.02199000	-0.42533100	H	0.90888200	7.14562100	3.72282400	H	-4.44815700	1.36980600	1.33415600
C	-8.32253400	-2.22135000	0.94055100	C	3.49186300	0.81090900	6.35585200	TS			
N	-8.80763800	-1.42493400	1.92741200	C	3.27578900	0.08639100	5.01420100	C	-5.13350800	-0.76483500	5.05326600
O	-7.41582200	-3.03705800	1.12431800	C	3.22571000	-1.42290800	4.93719600	C	-6.08789100	-1.32690500	4.01127000
H	-5.58984100	-3.64009000	-1.74389800	C	3.70406200	-2.27736700	5.93203600	O	-6.50333000	-2.48032600	4.03968600
H	-8.23763100	-1.87501600	-3.05855400	C	2.70614200	-2.00351300	3.76775600	C	-3.65049200	-0.99940900	4.66755700
H	-8.04467400	-3.90629700	-0.92506900	C	3.66261500	-3.66706200	5.77331300	S	-3.17579400	-0.26942500	3.01939800
H	-8.59547800	-1.05523300	-0.77730800	C	2.65721500	-3.38103600	3.59291800	H	-5.33617800	-1.28225400	5.99422900
H	-10.05732900	-1.90062900	-0.28645300	C	3.13098400	-4.22366100	4.60683300	H	-5.30204300	0.30756600	5.19567200
H	-8.26595000	-1.39495700	2.78036400	O	3.04494300	-5.70614400	4.38895000	H	-3.01589200	-0.56506200	5.44311700
H	-9.23705600	-0.54982500	1.66037100	H	3.51170500	1.85681500	6.05066600	H	-3.46265300	-2.07636800	4.64127700
C	-6.37485700	-6.14372900	1.42151900	H	4.44765800	0.56077800	6.82507600	N	-6.43277700	-0.46460700	3.00275400
C	-5.14708900	-5.39764200	1.96663200	H	2.68800200	0.64263500	7.07390300	C	-7.30458600	-0.90037000	1.93840700
C	-4.04770700	-5.18965500	0.95697400	H	2.34877000	0.46542500	4.57576000	C	-6.72951400	-2.03443500	1.05892400
C	-4.20207800	-4.89201000	-0.37448300	H	4.06199900	0.42073700	4.32156500	O	-7.49513200	-2.71351900	0.36446200
C	-2.62364200	-5.22042300	1.20353300	H	4.11020300	-1.86625400	6.85116900	C	-7.67128400	0.27665000	0.98512900
C	-1.96584400	-4.93959500	-0.03408200	H	2.33931700	-1.36361300	2.97297900	C	-9.13422500	0.21101600	0.56843200
C	-1.83619700	-5.44589300	2.34518100	H	4.03053200	-3.14648800	6.56582600	O	-7.321		

C	-7.55627800	-5.17954400	-2.96842300	H	-0.57620600	3.49733500	3.28005800	C	-5.78802600	4.48910600	-0.92786800
C	-7.31263500	-3.71649000	-2.76588200	H	-0.95888400	2.46050900	4.67607800	C	-0.32741000	2.10786700	0.40186400
C	-6.16093900	-2.98561400	-2.90051400	C	3.52321200	6.14509400	-0.33205600	C	-1.60859800	2.16346000	-0.03257700
N	-8.28522000	-2.80569100	-2.38376200	C	2.26584700	5.28373300	-0.21181100	C	1.51113800	1.90208700	-2.91280400
C	-7.74348500	-1.58950800	-2.23229900	C	1.53148300	5.18144700	-1.54151900	N	1.24077400	2.58562700	-4.06994800
H	-6.46062100	-1.67648800	-2.56614200	O	2.58149200	3.95803000	0.20630800	O	2.58685000	1.33891800	-2.71811000
N	-8.64816800	-5.59020700	-1.04921400	H	4.02676100	6.20117600	0.63318200	H	-5.55337300	4.38030800	0.13444700
H	-8.45554700	-6.92778400	-2.13811800	H	3.26567600	7.16580900	-0.63759100	H	-3.80989300	-0.78131500	-1.20661200
H	-9.21532300	-3.05353200	-2.07761600	H	4.21344800	5.73016300	-1.07099400	H	-6.25271500	1.41855500	-3.04398100
H	-9.65264900	-5.75092500	-2.51425900	H	1.59564400	5.74589500	0.53030700	H	-3.28811200	1.83676800	-2.89451900
H	-6.59600200	-5.67267400	-2.78855100	H	2.81106200	3.99713100	1.15452800	H	-4.04438300	1.01904600	-0.06935200
H	-7.78902600	-5.36091400	-4.02563300	H	0.60718000	4.60752000	-1.43419800	H	-1.20593300	1.94148900	-3.32789000
H	-5.16788200	-3.28193600	-3.20141200	H	1.27721200	6.17475800	-1.91982600	H	-6.13170800	1.99284800	-0.29376600
H	-8.23948100	-0.69676300	-1.89466100	H	2.17331900	4.68452900	-2.27697500	H	-5.43172100	3.44749500	-2.78673100
H	-5.76177900	-0.92793600	-2.38065500	C	-2.57624500	8.11372500	1.33434900	H	-0.07681200	2.29572700	1.43523300
C	1.92935900	-4.68013200	6.70685300	C	-2.64765800	6.93844100	0.34853200	H	-2.44176200	2.40407600	0.61271600
C	2.19321100	-4.69654000	5.18976500	C	-1.54877000	7.03013300	-0.71658900	H	1.74623500	1.95462000	-0.19559800
C	1.14067300	-3.93915800	4.44624100	C	-2.58157100	5.58849800	1.07158600	H	-6.87498500	4.49425100	-1.04835000
C	1.05323900	-2.62459300	4.05711400	H	-3.40258800	8.06456700	2.05235300	H	0.79697400	0.37797200	-0.25884400
N	-0.10609800	-4.47571600	4.15185300	H	-2.65469700	9.06515300	0.80722100	H	-5.39017200	5.44589500	-1.27544200
C	-0.88324400	-3.50579300	3.60838600	H	-1.65100300	8.08502100	1.91257700	H	2.02196500	2.68150300	-0.70559600
N	-0.20441400	-2.37239500	3.54058200	H	-3.61904600	6.99635700	-0.16541600	H	0.59852000	3.36455100	-4.04935000
H	0.96424900	-5.13745100	6.94620000	H	-1.62172200	6.20257600	-1.43101900	O	2.68547400	-1.33277600	-0.37861500
H	1.91659000	-3.65352800	7.08296100	H	-1.60695100	7.96808000	-1.27884100	C	1.95181400	-1.74648200	-1.55951600
H	2.70701700	-5.23431400	7.23950100	H	-0.55675900	6.97965900	-0.25240100	C	0.46078800	-1.50368100	-1.26420600
H	3.16806100	-4.24884800	4.97313900	H	-2.72006500	4.78619000	0.36145700	C	0.47541500	-0.81848800	0.09829900
H	2.24366200	-5.72857700	4.82290200	H	-1.60873600	5.45660100	1.56039500	C	1.80684800	-1.22829300	0.72324100
H	-0.38121800	-5.43543200	4.30469300	H	-3.34562300	5.50865500	1.85141600	O	-0.63157600	-0.73598400	0.80873100
H	1.78441700	-1.83737900	4.13775200	C	0.39185500	5.75392500	-6.18595900	H	2.15505200	-2.79909500	-1.76078300
H	-1.90278700	-3.65296200	3.28753000	C	0.92333900	6.56249600	-4.99614100	H	2.31899700	-1.13379400	-2.38074400
C	5.99457600	-2.30549400	4.58624900	C	2.17696400	7.35653200	-5.37829500	H	-0.09299600	-2.44232400	-1.17272200
C	6.71672500	-3.02550600	3.46401500	C	-0.16004100	7.47779400	-4.41457200	H	-0.02799600	-0.89086000	-2.02845000
O	6.27133000	-4.07582300	3.00041500	H	0.15295500	6.38925900	-7.03866800	H	2.19582300	-0.48467500	1.42190200
C	4.70689300	-1.67025600	4.03293000	H	-0.49782500	5.18908300	-5.90611800	H	1.67160300	-2.19425700	1.23199100
H	6.62444200	-1.54011500	5.05293300	H	1.14473900	5.03585900	-6.53456100	C	6.06398800	0.63864300	-0.18205000
H	5.75201900	-3.04765200	5.35284200	H	1.21088500	5.84802900	-4.21215100	N	5.46509200	-0.56084200	0.05788700
H	4.08847200	-2.43785800	3.55925300	H	2.58555600	7.89124700	-4.51477900	H	4.48725600	-0.70635900	-0.17725700
H	4.12806300	-1.19339400	4.83060500	H	2.96222400	6.70113000	-5.76951200	H	6.04165500	-1.39474600	0.06460000
H	4.93284100	-0.92086000	3.26741900	H	1.94556800	8.09834600	-6.15170500	O	7.28565200	0.80589600	-0.11318800
N	7.82045600	-2.39726200	2.99164600	H	0.21030300	8.02749700	-3.54281500	C	5.09443000	1.77564400	-0.47650400
C	8.58653000	-2.89017200	1.86078500	H	-0.48676200	8.21461700	-5.15792800	H	4.54120600	1.98509400	0.44831900
C	8.91693200	-1.79263600	0.83585100	H	-1.04114600	6.90803900	-4.09909600	H	4.33279800	1.41625800	-1.17445100
C	8.34654200	-2.08277700	-0.55076700	C	-3.43006700	0.38209400	-6.43213900				
N	8.93787500	-1.40799000	-1.57028300	C	-3.23901900	-0.26139300	-5.04495800	EP			
O	7.40800300	-2.86388300	-0.72430300	C	-3.16146700	-1.76330500	-4.88431500	C	-5.13347800	-0.76480300	5.05324100
H	9.50710200	-3.36709700	2.21653900	C	-3.62663900	-2.67511400	-5.83371900	C	-6.05302700	-1.34002100	3.98867400
H	8.12461800	-1.55016200	3.44738000	C	-2.62967800	-2.27502600	-3.68832800	O	-6.39763400	-2.51742800	3.98176600
H	7.97186100	-3.65723500	1.38784900	C	-3.56019600	-4.05378200	-5.60523200	C	-3.64413300	-0.97326200	4.69609000
H	8.46583500	-0.83121300	1.11370000	C	-2.55194400	-3.64088500	-3.44577900	S	-3.15729500	-0.20209000	3.07272600
H	9.99556600	-1.62538500	0.75873200	C	-3.01385100	-4.54148700	-4.41446700	H	-5.34637700	-1.29073700	5.98755200
H	8.44252100	-1.41362400	-2.45141000	O	-2.90253500	-5.87343000	-4.13115700	H	-5.32304600	0.30356000	5.20078600
H	9.42375000	-0.54956800	-1.35281900	H	-3.47784700	1.44291800	-6.18754400	H	-3.02919100	-0.54555100	5.49468300
C	6.43126600	-6.08084200	-0.85980700	H	-4.36788200	0.08719600	-6.91104800	H	-3.44110100	-2.04631500	4.65177200
C	5.20999200	-5.39315400	-1.49203500	H	-2.60427900	0.19012700	-7.11870900	N	-6.43365000	-0.46884000	3.00687300
C	4.07101600	-5.12851200	-0.54141100	H	-2.32605400	0.16036100	-4.60364600	C	-7.30455900	-0.90035200	1.93842900
C	4.16851900	-4.70645600	0.76283200	H	-4.05068600	0.09272300	-4.39452000	C	-6.72333700	-2.06115700	1.09351300
C	2.65950300	-5.21933800	-0.83341600	H	-4.04115200	-3.81872800	-6.77179900	O	-7.48254100	-2.80428600	0.47405000
C	1.95092000	-4.84320200	0.34994300	H	-2.27197900	-1.59302500	-2.92477600	C	-7.63304100	0.27148700	0.97031000
C	1.91901400	-5.57235700	-1.97478000	H	-3.91832900	-4.74689400	-6.36297000	C	-9.08433700	0.21741700	0.51986600
N	2.89829000	-4.53420300	1.29948400	H	-2.10082800	-4.02259600	-2.53747200	O	-7.28960100	1.54890500	1.51770200
C	0.55485900	-4.83810900	0.41333400	H	-3.12301100	-6.39066900	-4.91693200	H	-6.09131400	0.48149900	2.98225400
C	0.52803000	-5.56847600	-1.91813300	C	5.42438500	1.02509600	-5.36554700	H	-8.22445800	-1.31026000	2.36912600
C	-0.14547900	-5.21460600	-0.73178000	C	6.30080600	1.87225200	-4.44229100	H	-6.98741000	0.17329700	0.09770800
H	7.27990500	-6.04536000	-1.54476400	O	7.50156800	2.01436200	-4.66068300	H	-8.00451000	1.83182600	2.10476500
H	6.25124500	-7.12510300	-0.60019800	C	6.01882200	-0.39066700	-5.48073600	H	-9.26907400	0.94210100	-0.27763400
H	6.74052600	-5.55360500	0.04659100	C	6.18374900	-1.13370000	-4.14219800	H	-9.31899200	-0.78989500	0.16708200
H	5.54456800	-4.44038300	-1.92031600	C	4.85382500	-1.36687600	-3.41852500	H	-9.75601400	0.43332300	1.36006900
H	4.84194400	-5.99441500	-2.33239600	C	6.91400900	-2.46675000	-4.35325900	N	-5.36946600	-2.12073200	0.99394600
H	5.03890000	-4.51445000	1.37410400	H	5.42062100	1.49745300	-6.35374100	C	-4.71057600	-3.20667900	0.26904300
H	2.70380100	-4.24988300	2.24573500	H	4.38958700	0.98911800	-5.00568800	C	-3.20081600	-2.99608000	0.24016900
H	2.42954700	-5.85152900	-2.89173000	H	5.39488300	-0.99267400	-6.15484700	O	-2.77748200	-1.72989700	-0.27700700
H	0.03413200	-4.56302400	1.32557000	H	7.00333300	-0.29443800	-5.94982100	H	-4.91708700	-4.17548000	0.74300700
H	-0.05363300	-5.85396200	-2.78969500	H	6.80562800	-0.49818600	-3.49483600	H	-4.80330600	-1.55848000	1.62650200
H	-1.23000000	-5.26827600	-0.70251200	H	5.01855500	-1.89555800	-2.47523700	H	-5.12029700	-3.25382600	-0.74303800
C	3.38727400	2.92601500	4.51017000	H	4.34310100	-0.42931500	-3.18770900	H	-2.79906600	-3.05008100	1.25799200
C	2.64597900	4.14240800	3.96421200	H	4.18135900	-1.97716900	-4.03539200	H	-2.74677900	-3.80267300	-0.34625200
O	2.89680600	4.66245000	2.87504400	H	7.06833300	-2.98438800	-3.40060100	H	-1.41518100	-1.09080800	0.41278700
C	2.43150400	1.74338800	4.79244700	H	6.32704800	-3.13022300	-4.99987500	C	-8.64471300	-5.84915300	-2.10741200
C	1.58614700	1.27684000	3.59117100	H	7.88859700	-2.32043100	-4.83314200	C	-7.54729000	-5.17908200	-2.95588700
O	1.89016600	1.61670400	2.44201100	N	5.68699300	2.41331000	-3.35224700	C	-7.32419200	-3.70985900	-2.76791900
O	0.59106200										

N	-0.27717200	-2.447798000	3.61261600	H	-3.64117800	7.01098600	-0.15876500	H	0.43796100	3.41883600	-4.20037800
H	0.94866900	-5.04782800	7.02377500	H	-1.66226300	6.22122800	-1.45764900	O	2.68003300	-1.77476400	-0.17367800
H	2.00638200	-3.63052000	7.00315300	H	-1.64349400	7.98344600	-1.28991800	C	1.98191800	-1.90038700	-1.44236500
H	2.69434000	-5.24776600	7.24400200	H	-0.58116300	6.98818600	-0.28411300	C	0.49866500	-1.64058800	-1.14444300
H	3.09933700	-4.45830100	4.89033400	H	-2.77894800	4.77455700	0.33404100	C	0.59326300	-0.84392800	-0.15099700
H	2.07749600	-5.88028400	4.89244500	H	-1.61644400	5.42736400	1.50947000	C	1.73806300	-1.55507600	0.86676200
H	-0.46396500	-5.53702600	4.25371200	H	-3.34361700	5.50713400	1.84960000	O	-0.61742900	-0.74783600	0.90607700
H	1.71188500	-1.93953200	4.22648000	C	0.39185400	5.75392800	-6.18595200	H	2.15679600	-2.89742100	-1.84794700
H	-1.97971900	-3.71430800	3.30338100	C	0.92265200	6.56308000	-4.99583900	H	2.39363400	-1.14735900	-2.11649800
C	5.99459200	-2.30550000	4.58626600	C	2.17525200	7.35842500	-5.37843200	H	-0.03676700	-2.57675100	-0.96665900
C	6.71455000	-3.02387100	3.46122700	C	-0.16239900	7.47711600	-4.41501700	H	-0.00095700	-1.09980400	-1.95299700
O	6.28169300	-4.08458300	3.01116500	H	0.15295400	6.38925600	-7.03867000	H	2.21015200	-0.94409800	1.64085400
C	4.66277400	-1.74376200	4.05917500	H	-0.49782700	5.18908600	-5.90611700	H	1.39018100	-2.49925900	1.30061100
H	6.60327600	-1.50111600	5.01366500	H	1.14595900	5.03763300	-6.53630600	C	5.97932000	0.59973800	-0.19047900
H	5.80835200	-3.03668500	5.37883500	H	1.21152300	5.84837000	-4.21186300	N	5.36596500	-0.57036500	0.14697200
H	4.06791900	-2.55039000	3.62135000	H	2.58299500	7.89460400	-4.51544500	H	4.38309200	-0.72950900	-0.05455800
H	4.08572100	-1.27582300	4.86354000	H	2.96151700	6.70420600	-5.76954400	H	5.93762300	-1.41057600	-0.15091500
H	4.83401600	-1.00309100	3.27086600	H	1.94251100	8.09938100	-6.15198900	O	7.20490100	0.74006200	-0.17171800
N	7.80684300	-2.38453700	2.97554200	H	0.20648900	8.02811600	-3.54357800	C	5.03257400	1.74232300	-0.53866300
C	8.58644100	-2.89015100	1.86077300	H	-0.48948900	8.21280400	-5.15881700	H	4.41640600	1.94996900	0.34592400
C	8.91225400	-1.80953000	0.81394800	H	-1.04368100	6.90695000	-4.10021900	H	4.32276300	1.38455200	-1.29096200
C	8.28598100	-2.09259300	-0.54818000	C	-3.43003700	0.38197400	-6.43209800				
N	8.92469800	-1.53761000	-1.60887700	C	-3.24188600	-0.27052500	-5.04992500				
O	7.26519900	-2.77455700	-0.66957800	C	-3.02031300	-1.75916200	-4.91279200				
H	9.51188400	-3.34501700	2.23263700	C	-3.35324800	-2.69122500	-5.89590300				
H	8.10665000	-1.53320500	3.42610100	C	-2.48548300	-2.23908300	-3.70582100	C	4.98647400	-0.62415500	-5.03560900
H	7.98416100	-3.67672100	1.40438800	C	-3.15556000	-4.06016500	-5.68766300	C	5.94926300	-1.15631900	-3.98679100
H	8.49466800	-0.83567700	1.09929900	C	-2.27747900	-3.59329000	-3.48276900	O	6.34922000	-2.31600600	-3.97799100
H	9.99267100	-1.67506700	0.70482300	C	-2.61159300	-4.51411500	-4.48362200	C	3.50494900	-0.89519800	-4.64916700
H	8.41798400	-1.52104500	-2.48285600	O	-2.37434900	-5.83391700	-4.21950200	S	3.00211100	-0.20096500	-2.98574500
H	9.57761800	-0.76777000	-1.45030300	H	-3.47786300	1.44291400	-6.18753100	H	5.19744500	-1.14509500	-5.97274500
C	6.43128700	-6.08080500	-0.85979900	H	-4.36533500	0.08441900	-6.91329200	H	5.12738300	0.45063400	-5.18786700
C	5.20014800	-5.98101000	-1.47438400	H	-2.60427100	0.19016800	-7.11871100	H	2.86024300	-0.46585600	-5.41877100
C	4.05565800	-5.20332400	-0.51403300	H	-2.38608500	0.22249000	-4.56598300	H	3.34879000	-1.97710400	-4.63935000
C	4.14304700	-4.84177800	0.80880100	H	-4.10866500	-0.00620100	-4.42855100	N	6.30892600	-0.26296600	-3.01426100
C	2.64747900	-5.31747900	-0.81123100	H	-3.76990700	-2.35845600	-6.84172000	C	7.22364400	-0.64411400	-1.96488600
C	1.93007700	-5.01787200	0.38803300	H	-2.23423300	-1.53762300	-2.91703300	C	6.69580500	-1.77426400	-1.04961300
C	1.91602000	-5.63445400	-1.96862800	H	-3.41565100	-7.77068900	-6.46885600	O	7.49317400	-2.43488900	-0.37541000
N	2.86966500	-4.73967900	1.35440100	H	-1.82596300	-3.94911400	-2.56417900	C	7.56532000	0.57375900	-1.05133900
C	0.53390800	-5.04787000	0.44795300	H	-2.56946700	-6.36112000	-5.00513900	C	9.03142800	0.55121400	-0.64124100
C	0.52479900	-5.66132900	-1.91685400	C	5.42437600	1.02513200	-5.36557300	O	7.19177100	1.82138100	-1.63132900
C	-0.15819700	-5.37783000	-0.71682100	C	6.31728700	1.84785400	-4.43624100	H	5.91761500	0.66852300	-2.98605200
H	7.27989700	-6.04538300	-1.54477600	O	7.52937200	1.92104100	-4.61701000	H	8.13412400	-1.05487400	-2.41422400
H	6.25123200	-7.12510000	-0.60019400	C	5.97095500	-0.41072500	-5.46590700	H	6.93810300	0.50640300	-0.16028800
H	6.74174900	-5.56699100	0.04872700	C	6.11802800	-1.14184200	-4.11909500	H	7.85233700	2.06647300	-2.39433900
H	5.51225200	-4.42143100	-1.86399100	C	4.78717300	-1.31409800	-3.38068400	H	9.23485300	1.31110500	0.11909400
H	4.84890100	-5.97683300	-2.33745800	C	6.79174000	-2.50598300	-4.31878600	H	9.29385700	-0.44113900	-0.26473600
H	5.00837200	-4.64529300	1.42578600	H	5.44635500	1.49098900	-6.35670700	H	9.67474400	0.74588400	-1.50789300
H	2.66779200	-4.54343900	2.29796000	H	4.38388800	1.02739700	-5.01888000	N	5.35417300	-1.90313400	-0.95240400
H	2.43373600	-5.86147400	-2.89611400	H	5.32453100	-0.99864600	-6.13090500	C	4.72993200	-2.99292100	-0.20309700
H	0.00620800	-4.83601900	1.37333700	H	6.95609600	-0.35290500	-5.93960500	C	3.21881000	-2.86134800	-0.25061500
H	-0.04977800	-5.91601700	-2.80203600	H	6.77081300	-0.52399500	-3.48569500	O	2.80723700	-2.86724700	0.14793600
H	-1.24209300	-5.44726300	-0.69512000	H	4.94565700	-1.81821000	-2.42325000	H	5.02320200	-3.96161900	-0.62719400
C	3.38726500	2.92596900	4.51019000	H	4.30513800	-0.35422800	-3.17642200	H	4.75984100	-1.36918900	-1.58613400
C	2.65984400	4.15919600	3.98302100	H	4.09131100	-1.92130000	-3.97369400	H	5.08097300	-2.98045300	0.83003100
O	2.95330000	4.71615100	2.92132300	H	6.93216900	-3.01711100	-3.36071600	H	2.88176600	-2.82236200	-1.29229800
C	2.43882000	1.73488200	4.77618300	H	6.17369100	-3.15358400	-4.95214300	H	2.76070700	-3.73334300	0.23092600
C	1.49935500	1.32667400	3.62357100	H	7.76745700	-2.40526400	-4.80811700	H	2.02885500	-1.28925100	-0.04568500
O	1.54572400	1.89017700	2.52398600	N	5.69719100	2.44990100	-3.38058700	C	8.78527700	-5.48176500	2.13551400
O	0.68588300	0.36510900	3.94316600	C	6.47146900	3.06523400	-2.30049900	C	7.70850200	-4.80576000	3.00773300
H	3.91650700	3.17904600	5.43544900	C	5.69152600	3.05822000	-0.97483700	C	7.43438500	-3.35269000	2.77166200
H	4.12938200	2.66163500	3.75538500	H	7.39978000	2.49917100	-2.20168500	C	6.26675500	-2.64772500	2.89997700
H	3.02825400	0.85148600	5.04416800	H	4.71362700	2.27130900	-3.23145300	N	8.38052900	-2.42502100	2.36219900
H	1.80015300	1.91882600	5.64890500	H	6.73883600	4.09692700	-2.56011900	C	7.80436500	-1.22637200	2.18916300
N	1.66110000	4.63008000	4.76910400	H	6.37833000	3.39237900	-0.19100700	N	6.52722800	-1.33991800	2.53397100
C	0.83530000	5.76428400	4.37259300	H	4.88516500	3.79429000	-1.02021400	H	8.75978900	-5.24164200	1.07325300
C	-0.07338000	6.22779000	5.50669000	Z	-0.82152200	-0.50989500	2.98314200	H	8.61767200	-6.56239200	2.19537900
C	-1.07400600	5.18811400	6.03022300	C	-3.46745500	2.00664200	-1.90918800	H	9.31713600	-2.65287200	2.06086400
S	-2.26589700	4.53390000	4.79685400	N	-2.07539300	1.99417600	-1.42127900	H	9.79797000	-5.34846700	2.51966900
C	-1.36678000	3.07935100	4.15999000	C	-4.47677300	1.07366400	-1.20786700	H	6.75040100	-5.31726300	2.87180400
H	1.49431700	6.57894600	0.405896700	C	-1.07665600	1.96834800	-2.33792600	H	7.97471000	-4.95274300	4.06253500
H	1.46155400	4.16435700	5.64065100	O	-4.42911300	-0.18589900	-1.82484800	H	5.28581800	-2.96316500	3.21804200
H	0.23235800	5.49279800	3.49728700	C	-5.79797100	1.91174100	-1.35349200	H	8.27505100	-0.32950000	1.82723400
H	0.54053800	6.57117000	6.35053000	C	0.24239400	2.08691000	-1.94895100	H	5.79510200	-0.62363800	2.33352800
H	-0.63042800	7.09870500	5.14745900	O	-6.83280700	1.28311200	-2.07641500	C	-1.99447000	-4.76416000	-6.47574900
H	-0.57678400	4.32983000	6.49731700	C	-5.35068700	3.25226900	-1.98757300	C	-2.23753700	-4.77017200	-4.95670900
H	-1.68693300	5.64616300	6.81119200	C	0.53217300	2.21975400	-0.58223700	C	-1.21569300	-3.92810300	-4.26818100
H	-2.08293100	2.49850100	3.57375200	O	-3.92739900	3.31748700	-1.75129800	C	-1.23935400	-2.62981600	-3.82340900
H	-0.50920900	3.35211400	3.54366600	C	-6.00213900	4.48817500	-1.40936400	N	0.11045500	-4.32297400	-4.14317100
H	-1.03101700	2.44118300	4.98129500	C	-0.51510800	2.28823000	0.33873200	C	0.82964400	-3.28896600	-3.64365400
C	3.52318800	6.14513600	-0.33208400	C	-1.81587700	2.16929400	-				

C	-8.59966600	-3.07666600	-1.52382700	H	0.28835600	8.40424800	5.11935700	H	-6.49502000	0.71273700	1.43163400
C	-8.21035500	-2.25723100	-0.28413500	H	0.86960800	7.09569900	4.07732500	H	-7.22878500	1.32456100	-0.05450300
C	-6.70938400	-2.17729900	0.00413500	C	3.48450700	0.67565100	6.46141000	TS			
N	-6.37591500	-1.97048600	1.30875600	C	3.29001300	-0.01353900	5.09702800				
O	-5.85421400	-2.24938900	-0.86956300	C	3.32940600	-1.52147500	4.97575100	C	5.17877300	-0.15710100	-4.89571800
H	-9.68726200	-3.04475800	-1.64490300	C	3.94395200	-2.36284100	5.90567600	C	6.05981400	-0.75004800	-3.81143100
H	-8.09337100	-1.66857200	-3.01785400	C	2.77343900	-2.11077700	3.82743000	O	6.40762600	-1.92707100	-3.81267300
H	-8.30569800	-4.12024300	-1.39370200	C	4.00864500	-3.74481100	5.70016200	C	3.67350300	-0.44915400	-4.63171400
H	-8.56013200	-1.22138100	-0.39995000	C	2.82529700	-3.48287700	3.60760200	S	3.06824100	0.04699800	-2.93675300
H	-8.74228500	-2.65842100	0.58626900	C	3.44788300	-4.31021100	4.55144500	H	5.46217100	-0.61981700	-5.84424800
H	-5.46569200	-1.54489900	1.45682600	O	3.48556600	-5.65017500	4.28259600	H	5.32630700	0.92514300	-4.97157800
H	-7.08613100	-1.77372500	1.99640200	H	3.49761300	1.73297400	6.19799000	H	3.08116900	0.07478200	-5.38471700
C	-6.30118500	-6.15880900	1.20626700	H	4.44008300	0.42306700	6.92996700	H	3.50982700	-1.52192800	-4.76172000
C	-5.03714100	-5.46361800	1.73174800	H	2.67887200	0.47274200	7.16825000	N	6.41201700	0.09404100	-2.78657300
C	-3.96529500	-5.31806500	0.68048400	H	2.33519600	0.32753700	4.67767800	C	7.33947900	-0.36594500	-1.77762700
C	-4.15876700	-4.99105600	-0.64146200	H	4.05045200	0.38422700	4.40889100	C	6.76646300	-1.47037700	-0.85941300
C	-2.53567000	-5.42730500	0.807174100	H	4.38001100	-1.94707400	6.80876100	O	7.54909000	-2.14114200	-0.17568400
C	-1.91550200	-5.15416000	-0.38353800	H	2.29765900	-1.47893800	3.08554400	C	7.97288500	0.80076300	-0.95806300
C	-1.71501400	-5.70506300	1.97594100	H	4.48850900	-4.38137200	6.44008700	C	9.43317900	0.04936600	-0.64334700
N	-2.92970500	-4.88610400	-1.27947000	H	2.36677200	-3.93243700	2.73323900	O	7.80988300	2.05649300	-1.61193500
C	-0.52750900	-5.14753500	-0.54841100	H	3.80286700	-6.12491700	5.06196900	H	6.15297200	1.06952100	-2.79851700
C	-0.33297400	-5.71216300	1.81800100	C	-5.40489100	1.05148700	5.56830500	H	8.14548800	-0.90020700	-2.29642900
C	0.25513600	-5.43855700	0.56762100	C	-6.35691200	1.72206800	4.57809600	H	7.43661300	0.92369500	-0.01631500
H	-7.13540000	-6.13306000	1.90747500	O	-7.56553700	1.77588800	4.79661200	H	8.41485700	2.08859200	-2.36653500
H	-6.09538500	-7.20036800	0.95896100	C	-5.84380000	-0.39079700	5.85549400	H	9.85689900	1.26887400	0.00761300
H	-6.64925100	-5.67322200	0.28791100	C	-5.76329700	-1.32299000	4.63530800	H	9.50764300	-0.48032800	-0.16383400
H	-5.30485300	-4.47094600	2.11802100	C	-4.32403700	-1.51675400	4.13902700	H	10.02497700	0.45716100	-1.56572300
H	-4.63505100	-6.02264500	2.58476300	C	-6.41944600	-2.67440300	4.94132500	N	5.42672900	-1.65514100	-0.83152500
H	-5.06503700	-4.80061200	-1.20037300	H	-5.45006000	1.63740200	6.49343900	C	4.84461600	-2.87589600	-0.25604600
H	-2.80953200	-4.67509300	-2.25559300	H	-4.37385500	1.08510000	5.20132400	C	3.34580800	-2.93516200	-0.52536100
H	-2.15499200	-5.90265800	2.94866500	H	-5.23151800	-0.80569700	6.66698300	O	2.64128700	-1.97106500	0.20325200
H	-0.07684600	-4.94440600	-1.51537100	H	-6.87802700	-0.35549500	6.21334200	H	5.32815800	-3.75275900	-0.70303500
H	0.30688400	-5.93211000	2.66772000	H	-6.34294300	-0.84024000	3.83483900	H	4.85060700	-1.13776500	-1.49737800
H	1.33650000	-5.48117700	0.46558400	H	-4.28190600	-2.26730700	3.34357200	H	5.03404800	-2.91848800	0.81542700
C	-3.62256700	2.83520100	-4.37847400	H	-3.88709500	-0.59387600	3.74966500	H	3.16266000	-2.75310200	-1.58883100
C	-2.67704500	3.87980500	-3.80690800	H	-3.68438000	-1.87968800	4.95289400	H	2.98730300	-3.94086900	-0.27691100
O	-2.30251800	3.84783100	-2.62919100	H	-6.42181900	-3.32140700	4.05609000	H	1.88006700	-1.56263400	-0.24492500
C	-2.75471200	1.60920400	-4.79968500	H	-5.87339900	-0.20117400	5.73284400	C	8.88402300	-5.46478500	2.00080500
C	-1.94360500	0.92750400	-3.67564900	H	-7.45431300	-2.54954400	5.27713000	C	7.75336900	-4.92351700	2.91022800
O	-2.52820000	0.46750500	-2.68331600	N	-5.78366400	2.25216500	3.45951500	C	7.31306100	-3.49349700	2.78789200
O	-0.67227700	0.81165800	-3.88936800	C	-6.57052200	3.00777100	2.49145400	C	6.06304700	-2.94940700	2.94166900
H	-4.17229500	3.20453300	-5.24897100	C	-6.07235300	2.80111900	1.06796300	N	8.14848900	-2.41968800	2.51723000
H	-4.33384000	2.55256900	-3.60374700	H	-7.61048600	2.69310800	2.61134600	C	7.43467100	-1.28863300	2.43155100
H	-3.41962700	0.83940300	-5.20713600	H	-4.79057500	2.11348900	3.29119000	N	6.17090800	-1.58639400	2.71671900
H	-2.06745500	1.90862500	-5.59407300	H	-6.53275200	4.07913900	2.73663900	H	8.88055600	-5.14822100	0.95737600
N	-2.16996300	4.76495000	-4.69305100	H	-6.56970200	3.52667700	0.41496800	H	8.75173500	-6.55195900	1.96326600
C	-1.14989300	5.74616200	-4.34196500	H	-5.00447200	3.03346700	1.01254800	H	9.10555900	-2.50171100	2.20539000
C	-0.20356400	6.00934200	-5.51307500	Z	0.60710100	-0.32075600	-2.82917600	H	9.88443000	-5.34399200	2.41901500
C	0.67590600	4.82274000	-5.92071200	C	3.01266800	2.08520500	1.75159200	H	6.84946900	-5.51728300	2.74354300
S	2.07919500	4.44933400	-4.79808300	N	1.66243600	1.81461500	1.35864800	H	8.03958200	-5.11394000	3.95274100
C	1.32589900	3.31153400	-3.58494900	C	4.11257100	1.24175200	1.07741300	H	5.12003200	-3.40627700	3.19836400
H	-1.62726600	6.68546600	-0.34982000	C	0.66558000	1.86601600	2.32743500	H	7.79402400	-0.31206500	2.15871500
H	-2.54466300	4.78264400	-5.63062600	O	4.31420900	0.01611100	1.75332300	H	5.37978800	-0.93192300	2.58535500
H	-0.61510900	5.36072000	-3.47377100	C	3.55879000	2.16877900	1.15190600	C	-1.69079800	-4.29005900	-6.81269400
H	-0.79679400	6.32503400	-6.38501800	C	-0.64950100	1.79907900	2.03208600	C	-1.55544500	-4.79581400	-5.36752300
H	0.43545100	6.85883700	-5.25348000	O	6.39515800	1.66682000	1.99342300	C	-0.69146000	-3.86985400	-4.57465600
H	0.08320900	3.91022200	-6.04529200	C	4.78521500	3.52765500	1.63187000	C	-0.89982500	-2.59860000	-4.09342900
H	1.14490000	5.03621400	-6.88531500	C	-1.11940400	1.58428100	0.61308500	N	0.66027900	-4.10904000	-4.37271400
H	2.14513400	2.72584700	-3.16140200	O	3.36978600	3.43389600	1.45776100	C	1.21783500	-3.01559800	-3.79750500
H	0.80249100	3.83711500	-2.78543600	C	5.30741200	4.74154200	0.89208700	N	0.29292300	-2.08628800	-3.62227300
H	0.64240300	2.62137300	-4.08013100	C	-0.01895800	1.93380400	-0.35518200	H	-0.71043200	-4.20400400	-7.29074400
C	-3.75114100	6.13432700	0.41014300	C	1.266611000	0.16409000	0.01538400	H	-2.16087600	-3.30346100	-6.82793300
C	-2.58850900	5.15422500	0.30373000	C	-1.68723100	1.93267100	3.08114300	H	-2.30417800	-4.97165300	-7.40922400
C	-1.78915600	5.06911500	1.59768000	N	-1.32348100	2.57383400	4.24572100	H	-2.54430200	-0.87431500	-4.79071800
O	-3.10940700	3.86105800	-0.00729000	O	-2.82349900	1.47791300	2.92432100	H	-1.13024500	-5.80573800	-5.35127300
H	-4.27612500	6.15859900	-0.54490000	H	5.08621600	4.65515500	-0.17523500	H	1.14508000	-4.96005600	-4.61813900
H	-3.41233300	7.14864200	0.64768200	H	3.77336700	-0.67241700	1.28561600	H	-1.80002100	-2.00561400	-4.05895800
H	-4.45192600	5.80772600	1.18518500	H	6.09961900	1.74821300	2.91116200	H	2.25876100	-2.92296900	-3.53326700
H	-1.91813900	5.40730700	-0.50679300	H	-3.07520900	1.89953300	2.83334400	C	-5.86987900	-2.22180200	-4.59414400
H	-3.00810600	3.71597600	-0.96425700	H	3.85509300	1.05287300	0.02968700	C	-6.58817500	-3.05237300	-3.53887600
H	-0.92136700	4.41642700	1.47814600	H	1.02465300	1.96163000	3.34630700	O	-6.21399800	-4.18321000	-3.23581300
H	-1.43777400	6.06027200	1.89893800	H	5.81617900	2.28275700	0.16916300	C	-4.36072100	-2.43061700	-4.51075100
C	-2.42097200	4.66701000	2.39672300	H	5.00567900	3.62120800	2.71234400	H	-6.11790800	-1.15990100	-4.48577700
C	2.25462300	8.24308100	-1.41550400	H	-0.29202000	2.17339600	-1.37743500	H	-6.24507700	-2.54122000	-5.57447900
C	2.34564100	7.08562300	-0.40834700	H	2.06153900	2.29913900	-0.66191300	H	-4.14548600	-3.49979600	-4.56779900
C	1.32033700	7.24142100	0.72196200	H	-2.00055800	2.19952400	0.42394600	H	-3.84667500	-1.91383600	-5.32590200
C	2.16775200	5.73103900	-1.10176000	H	6.39086400	4.81882700	1.02162100	H	-3.97097700	-2.04336400	-3.56671200
H	3.06967000	8.19096100	-2.14543300	H	-1.46919900	0.55538900	0.47739600	N	-7.69546700	-2.46709500	-3.00357200
H	2.31668600	9.20543000	-0.90631400	H	4.84132800	5.65476700	1.26862600	C	-8.44479200	-3.07229800	-1.92418200
H	1.31898700	8.17835500	-1.97378200	H	-2.07899100	2.72788300	4.89945300	C	-8.31908700	-2.32242300	-0.58587400
H											

C	-0.26249700	-5.59591600	1.64614600	C	-5.49894400	0.57706500	5.52916400	H	8.17251600	-0.88412300	-2.27267300
C	0.38504600	-5.24318700	0.44500400	C	-6.43894600	1.30469400	4.56956900	H	7.22081900	1.12173500	-0.20332300
H	-7.01230100	-6.34753100	1.31318300	O	-7.65456000	1.30854200	4.75181500	H	8.76595500	1.88278700	-2.40378000
H	-5.93062900	-7.32631400	0.31699000	C	-5.91445400	-0.88490600	5.72859800	H	9.60589300	1.28148900	0.29975900
H	-6.48527500	-5.75452700	-0.25332300	C	-5.80462800	-1.75978300	4.46762900	H	9.14641200	-0.45045200	0.24677700
H	-5.24753900	-4.71839200	1.77536700	C	-4.36452800	-1.86857400	3.94436900	H	10.01027000	0.27270500	-1.10830900
H	-4.54125400	-6.28822900	2.06744400	C	-6.38720200	-3.15135000	4.75139800	N	5.40528100	-1.63573200	-0.81791700
H	-4.83990400	-4.79099500	-1.62415300	H	-5.56235000	1.10339900	6.48835000	C	4.84463300	-2.87589400	-0.25605400
H	-2.53338500	-4.40546900	-2.50178700	H	-4.45943300	0.64365600	5.18804600	C	3.35343800	-2.99849600	-0.53014100
H	-2.13942500	-5.91934100	2.65081300	H	-5.30519700	-1.32945700	6.52642400	O	2.56761400	-1.93697700	0.00556600
H	0.16082000	-4.66289700	-1.63059800	H	-6.95360200	-0.88733600	6.07381300	H	5.35522400	-3.73922900	-0.70055000
H	0.33570300	-5.83790000	2.51952100	H	-6.42097700	-1.27757500	3.69464400	H	4.83425700	-1.12568600	-1.48892900
H	1.47048600	-5.23399300	0.41354400	H	-4.28238400	-2.57340600	3.10753200	H	5.04636800	-2.98090000	0.81321000
C	-3.50321100	3.10950800	-4.21251600	H	-3.96298000	-0.91480300	3.59551000	H	3.17262400	-2.98923700	-1.60867700
C	-2.49590100	4.04314800	-3.55509800	H	-3.69798500	-2.25012800	4.72706000	H	3.00618300	-3.96139200	-0.13338700
O	-1.96424300	3.77939200	-2.47566600	H	-6.34577700	-3.80180600	3.86971500	H	1.19099200	-1.29180600	-0.62657300
C	-2.67317300	1.93861900	-4.83510200	H	-5.81795800	-3.65245300	5.54293900	C	8.88401400	-5.46478400	2.00009400
C	-1.95913800	0.99812900	-3.84089500	H	-7.42943000	-3.08924300	5.08231900	C	7.73106800	-4.98026100	2.91716200
O	-2.65049100	0.17822200	-3.20947100	N	-5.84209100	1.95820100	3.53383000	C	7.17319200	-3.58978900	2.81394900
O	-0.66633000	1.06165900	-3.78035700	C	-6.62241900	2.73408300	2.57319400	C	5.87462100	-3.14967400	2.95426200
H	-4.07427500	3.60310500	-5.00434000	C	-5.94238400	2.77563900	1.20555900	N	7.91339700	-2.43339000	2.65893500
H	-4.17438200	2.74383200	-3.43324500	H	-7.62022000	2.28654900	2.52456700	C	7.06269100	-1.37187800	2.65579300
H	-3.35483400	1.30075700	-5.40725300	H	-4.86143200	1.78795800	3.33231300	N	5.81518400	-1.76809100	2.84408200
H	-1.93399800	2.35119200	-5.52768900	H	-6.75575100	3.76006700	2.94198500	H	8.88056000	-5.14821600	0.95773700
N	-2.13138700	5.12370400	-4.30002200	H	-6.50732900	3.45161100	0.55496900	H	8.78010900	-6.55638600	1.94543900
C	-1.08361400	6.04851000	-3.90088900	H	-4.94695400	3.21365800	1.30864100	H	8.88721500	-2.39904400	2.39894900
C	-0.15456500	6.40393500	-5.06343100	Z	0.62959900	-0.17107000	-2.80682100	H	9.88442700	-5.34399000	2.41902100
C	0.69275300	5.24545600	-5.9640400	C	2.85288800	2.01380500	1.64827100	H	6.87230900	-5.64178700	2.76391900
S	2.12158000	4.75165700	-4.55248100	N	1.44073000	2.01851000	1.24415500	H	8.04666900	-5.15691500	3.95476900
C	1.37668200	3.53367900	-3.41558300	C	3.66234100	0.83975900	1.05353700	H	4.98582700	-3.73287300	3.14726300
H	-1.52703400	6.96884700	-3.49724600	C	0.44442700	1.87572300	2.17199900	H	7.37991500	-0.34946500	2.52636600
H	-2.64778300	5.32438800	-5.14373700	O	3.70403200	-0.28503100	1.89631600	H	4.39829600	-0.85193800	2.40292800
H	-0.53945300	5.537383600	-3.08449700	C	5.04211700	1.46056400	0.80676000	C	-1.69079600	-4.29005200	-6.81268600
H	-0.75960800	6.80310100	-5.89160100	C	-0.86274800	1.73246000	1.79598800	C	-1.56649000	-4.79530400	-5.36706500
H	0.50467400	7.21770800	-4.74436200	O	5.92518300	1.28478900	1.91835500	C	-0.68106700	-3.87547800	-4.59194600
H	0.07863900	4.35701000	-5.77604300	C	4.72133000	2.92385900	0.49953600	C	-0.85936200	-2.57380700	-4.19377100
H	1.13922500	5.52991600	-6.55341200	C	-1.16299900	1.54958000	0.38707000	N	0.65921000	-4.14141200	-4.34817300
H	2.18685600	2.87716700	-3.09037200	O	3.47459000	3.19594800	1.20683100	C	1.23821500	-3.03185300	-3.82854700
H	0.90773800	4.00879700	-2.55348600	C	4.59980000	3.21885300	-0.98842400	N	0.33643600	-2.06763000	-3.72980400
H	0.63836400	2.91789300	-3.93085400	C	-0.16691900	2.07816100	-0.51781600	H	-0.70834200	-4.22559100	-7.28940300
C	-3.80780300	6.04802700	0.79786200	C	1.10936600	2.22315000	-0.08200200	H	-2.13923200	-3.29342200	-6.82969200
C	-2.54522400	5.18747700	0.69990200	C	-1.98243200	1.71380200	2.77469000	H	-2.31789800	-4.95859100	-7.40988100
C	-1.67898700	5.33312200	1.94403300	N	-1.74829800	2.34870200	3.96797700	H	-2.55912700	-4.84420700	-4.19377100
H	-2.86381200	3.80803100	0.61049800	O	-3.04427300	1.13951300	2.53347100	H	-1.16463000	-5.81436400	-5.34542900
H	-4.309370300	6.13370300	-0.16616500	H	3.99643000	2.46645300	-1.50754000	H	1.12733700	-5.01557200	-6.83822200
H	-3.55838400	7.06718700	1.11553200	H	3.31081700	-1.03203500	1.36565300	H	-1.74941200	-1.96711900	-4.20890600
H	-4.50118000	5.62130200	1.52836500	H	5.66669600	1.89598700	2.62152300	H	2.27519700	-2.95498400	-3.54328500
H	-1.96406900	5.49115800	-0.18477100	H	2.85226900	1.94714000	2.74380700	C	-5.86985100	-2.22179100	-4.59411100
H	-3.39368800	3.61310300	-0.18888700	H	3.23020800	0.56832400	0.08410300	C	-6.52800500	-3.01295700	-3.47127600
H	-0.76843800	4.73328400	1.85137100	H	0.75724800	1.89599800	3.20947500	O	-6.06531700	-4.07456800	-3.06253900
H	-1.39175500	6.37241900	2.11590100	H	5.52230800	0.96629700	-0.03121000	C	-4.34791400	-2.21843300	-4.46057400
H	-2.24651400	4.98198900	2.81167100	H	5.47742500	3.57882300	0.94544100	H	-6.25788100	-1.19781000	-4.63031900
C	2.20330100	8.37839300	-0.71384700	H	-0.44750800	2.33690700	-1.53102500	H	-6.16219300	-2.70628800	-5.53418300
C	2.27479200	7.14477000	0.20108900	H	1.91568400	2.55904800	-0.71660900	H	-4.00150000	-3.23961200	-4.28597800
C	1.40080300	7.33072100	1.44650000	H	-2.20228800	1.63351600	0.09431200	H	-3.87820400	-1.83238000	-5.37069600
C	1.86443200	5.87864900	-0.56148200	H	5.60025500	3.20896100	-1.43097500	H	4.02247300	-1.59799600	-3.62195800
C	3.03329200	8.38936700	-1.42809600	H	-1.02926400	0.21497000	0.19327500	N	-7.69666000	-2.48451900	-3.01225100
H	2.23588700	9.30186200	-0.13473600	H	4.15465800	4.20266400	-1.14568600	C	-8.44484400	-3.07231600	-1.92418400
H	1.28300900	8.33987700	-1.29938300	H	-2.54675500	2.41292900	4.58535100	C	-8.35446400	-2.27784600	-0.60586400
H	3.31486400	7.02112200	0.53585800	H	-1.12964700	3.14642500	3.98066300	C	-6.95849100	-2.26399100	-0.00322500
H	1.41214100	6.43758500	2.08065000	O	-1.78876100	-1.90939500	1.66110000	N	-6.85181200	-2.71746900	1.26480100
H	1.73786100	8.17949100	2.05080000	C	-2.71158700	-1.72959500	0.56014100	O	-5.97462300	-1.85151300	-0.62039800
H	0.35980500	7.51892000	1.15974600	C	-1.86515100	-1.54223300	-0.69596200	H	-9.50011900	-3.15373200	-2.20672600
H	2.03375100	4.98361000	0.04327100	C	-0.58692800	-0.95018600	-0.12400900	H	-7.95851300	-1.56340500	-3.32961700
H	0.79735000	5.91554400	-0.81666800	C	-0.47250900	-1.58611600	1.26079600	H	-8.05399200	-4.08277000	-1.78943900
H	2.41864700	5.77671900	-1.50125000	C	0.50682000	-0.74937400	-0.83936400	H	-8.63864500	-1.23428600	-0.78819100
C	-0.68984100	5.47590300	6.64421400	H	-3.32123000	-0.84169300	0.76219600	H	-9.08394000	-2.68670000	0.00639000
C	-1.23588200	6.34042700	5.50172100	H	-3.36388000	-2.60182500	0.50100600	H	-5.94487500	-2.68759700	1.70733500
C	-2.54376300	7.03297000	5.90032900	H	-2.32248700	-0.91266700	-1.45790400	H	-7.63337400	-3.06768900	1.79378100
C	-0.19251200	7.35702800	5.02436900	H	-1.60001400	-2.50288100	-1.14328900	C	-6.16071400	-6.30892500	0.63380100
H	-0.48403800	6.07337600	7.53206600	H	0.15278000	-2.48756700	1.18221200	C	-4.89355300	-5.72534800	1.27170100
H	0.22590200	4.96810300	6.34001100	H	-0.01276000	-0.90810300	1.99328200	C	-3.75771700	-5.59861700	0.29197400
H	-1.41598900	4.70797200	6.93700800	N	-5.03370600	0.40224000	-1.57910900	C	-3.85272000	-5.31576800	-1.05100200
H	-1.45732800	5.67367400	4.65789500	H	-5.36349400	-0.49217600	-1.22369800	C	-2.34733500	-5.68732800	0.59499900
H	-2.95734500	7.60889400	5.06644000	H	-4.34712400	0.38784700	-2.33435000	C	-1.63758300	-5.45336700	-0.61813100
H	-3.30091900	6.30634800	6.21566900	C	-5.06294500	1.51337100	-0.81424000	C	-1.61542300	-5.91959100	1.77005900
H	-2.37835100	7.72402600	6.73475200	O	-4.52175400	2.56713200	-1.18693000	N	-2.58119600	-5.24408300	-1.60211200
H	-0.56840100	7.94655900	4.18170600	C	-5.79575300	1.41335700	0.52235100	C	-0.24008400	-5.43847200	-0.67527100
H	0.06729400	8.05451800	5.82952600	H	-5.22565800	0.72906100	1.16141000	C	-0.22568300	-5.91975500	1.71930700
H	0.73002700	6.86317300	4.70007400	H	-6.77261700	0.93839400	0.36089800	C			

H	-4.18171900	2.80178000	-3.41478100	H	-7.62977000	2.30873700	2.49549700	C	6.29323100	-3.15950200	2.28409600
H	-3.45236200	1.17776900	-5.20773900	H	-4.97258000	1.49205200	3.12157100	N	8.41383500	-3.00858800	1.75572100
H	-2.07107800	2.21524600	-5.59425500	H	-6.74244300	3.72769200	3.02094200	C	7.92052500	-1.76124400	1.75183700
N	-2.15353100	5.14575800	-4.29196500	H	-6.46700800	3.62691100	0.62976100	N	6.63978100	-1.83743500	2.09220300
C	1.08361400	6.04851900	-3.90088800	H	-4.93002700	3.21819200	1.35568400	H	9.33832200	-3.25645900	1.43344100
C	-0.23012100	6.47422700	-5.09828900	O	0.67645600	-0.14184700	-2.98630300	H	8.58473800	-5.61107300	0.10304000
C	0.58473000	5.35110100	-5.74808700	C	2.80300500	1.84911300	1.72300800	H	8.43888000	-0.77239700	1.04918300
S	2.13299600	4.87212800	-4.88425000	N	1.44115900	1.90625900	1.10543200	H	9.64787800	-5.92138800	1.50278100
C	1.54445000	3.66276900	-3.65105800	C	3.68895000	0.66519500	1.26167900	H	6.60789400	-5.84282500	1.92759400
H	-1.50269400	6.94088400	-3.41696500	C	0.34128800	1.75615800	1.88931300	H	7.86698600	-5.69886200	3.11978200
H	-2.70875500	5.38122900	-5.10138200	O	3.52100900	-0.48840200	2.03645200	H	5.29653400	-3.44676800	2.57231700
H	-0.49228100	5.52581600	-3.14975800	C	5.07988800	1.31189500	1.32311500	H	8.45281000	-0.85886000	1.50824600
H	-0.89017300	6.91386000	-5.86115300	C	-0.92911600	1.83656200	1.35515800	H	5.95344000	-1.06206000	2.02340500
H	0.44507200	7.27449400	-4.77922400	O	5.64419800	1.29652100	2.62264000	C	-2.29395900	-4.05894300	-7.11476900
H	-0.02416100	4.45195300	-5.88997700	C	4.80437900	2.72878300	0.81993600	C	-3.01937400	-3.59013900	-5.84372900
H	0.92215100	5.67136300	-6.73781700	C	-1.07271600	2.05622600	-0.02623800	C	-2.03714800	-3.07271400	-4.85018300
H	2.39583100	3.02695000	-3.39522000	O	3.47549500	3.02420300	1.37308800	C	-1.46691500	-1.83490800	-4.58306300
H	1.16910500	4.15375700	-2.75210300	C	4.83898800	2.91435300	-0.69020500	N	-1.36517700	-3.87955100	-3.94493600
H	0.76560900	3.02451300	-4.07357700	C	0.06903900	2.27185600	-0.79633700	C	-0.43970800	-3.13127000	-3.29503300
C	-3.80781300	6.04803700	0.97986000	C	1.31679600	2.18701300	-0.21322800	N	-0.48062900	-1.88451400	-3.74171600
C	-2.53409800	5.21802300	0.74012500	C	-2.14760500	1.65485800	2.22470800	H	-1.58601800	-4.86381200	-6.89327000
C	-1.69413900	5.42470300	1.99268000	N	-2.07271900	2.25002300	3.45088500	H	-1.73331700	-3.23391400	-7.56248500
O	-2.84822400	3.83710700	0.70363500	O	-3.09124300	0.96321800	1.86070300	H	-3.00662400	-4.43284100	-7.85550400
H	-4.30937300	6.13371200	-0.16616700	H	4.34326700	2.10167700	-1.23192000	H	-3.71655200	-2.78476700	-6.08896400
H	-3.58554100	7.07337900	1.11724100	H	2.90613200	-1.62851600	0.87939400	H	-3.62187800	-4.39388300	-5.40562500
H	-4.50203900	5.61546100	1.52390100	H	5.12634700	1.86161300	3.21144200	H	-1.56747900	-8.54017700	-3.77094900
H	-1.94511200	5.49102000	-0.14969900	H	2.62233400	1.78446700	2.80180200	H	-1.68808600	-0.91243600	-5.21999500
H	-3.45034100	3.62059600	-0.04662900	H	3.46026200	0.44242000	0.21053500	H	0.20823100	-3.50673200	-2.51898300
H	-0.77899200	4.82407300	1.95722700	H	0.52216800	1.56218200	2.93917900	C	-6.32843200	-2.06554100	-4.58306400
H	-1.40555100	6.46917100	2.21982800	H	5.76307400	0.74860000	0.69503600	C	-6.98583200	-2.95622700	-3.54212500
H	-2.28604800	5.12808100	2.86374300	H	5.48406400	3.43625900	1.30171500	O	-6.48896700	-4.03331200	-3.21464200
C	2.20329400	8.37838800	-0.71384500	H	-0.03987200	2.50355000	-1.84657700	C	-5.11279400	-1.35200000	-3.96777300
C	2.31306500	7.14891300	0.19948600	H	2.23319800	2.33287000	-0.76654100	H	-7.03436600	-1.33324200	-4.99060400
C	1.35701000	7.26559600	1.39069300	H	-2.04337900	2.06648500	-0.49931600	H	-6.01068300	-2.71131600	-5.40670200
C	2.05335900	5.85332700	-0.58091500	H	5.87705400	2.95488700	-1.03374200	H	-4.42252300	-2.08426900	-3.54162400
H	3.03019300	4.80384000	-1.43204400	H	-1.33591500	-0.10536400	-0.20662600	H	-4.57324400	-0.76914200	-3.21367700
H	2.23588800	9.30186400	-0.13473900	H	4.36056000	3.85998100	-0.95713600	H	-5.41459700	-0.67089600	-3.16588600
H	1.28301000	8.33987500	-1.29938400	H	-2.93382300	2.25441600	3.98407900	N	-8.11821700	-2.44192100	-2.99554100
H	3.33881800	7.10742000	0.59258500	H	-1.51300900	3.08615900	3.54276000	C	-8.80304000	-3.04281100	-1.86549100
H	1.40210900	6.37902700	2.03274900	O	-1.85162400	-2.20707200	1.47099500	C	-8.45621200	-2.39390600	-0.51135800
H	1.58937900	8.13971900	2.00746500	C	-2.70105000	-2.23854700	0.29942900	C	-9.30879500	-3.02794900	0.59376700
H	0.32423100	7.37122700	1.04035300	C	-1.76521900	-2.05101600	-0.89369700	C	-6.96521000	-2.50758100	-0.18226200
H	2.23935900	4.97484100	0.04571200	C	-0.80077300	-1.05040800	-0.27710200	H	-9.88340400	-2.98651100	-2.04161000
H	1.00961300	5.81178500	-0.91939400	C	-0.60096100	-1.63775800	1.12462000	H	-8.39875200	-1.51413700	-3.27573400
H	2.68879800	5.78517500	-1.47113500	O	0.42065400	-0.76193100	-0.97334500	H	-8.51992700	-4.09888500	-1.85560700
C	-0.68984000	5.47590300	6.64421300	H	-3.42473400	-1.41692000	0.35502400	H	-8.71432300	-1.32599200	-0.57646800
C	-1.23200600	6.34644400	5.50571900	H	-3.23844000	-3.18391500	0.28777800	H	-10.38042600	-2.93089800	0.38780100
C	-2.53878500	7.04047700	5.90431800	H	-2.26692300	-1.65045000	-1.77192200	H	-9.07959600	-4.09565700	0.69245300
C	-0.18578500	7.36215300	5.03242400	H	-1.24400100	-2.97743800	-1.13744100	H	-9.10593000	-2.55586400	1.55934600
H	-0.48403900	6.07337500	7.53206700	H	0.18795700	-2.40458100	1.10209700	H	-6.74086200	-2.00356800	0.76052400
H	0.22590200	4.96810200	6.34001200	H	-0.32061900	-0.88182900	1.86921100	H	-6.66947000	-3.55568600	-0.08995800
H	-1.41777600	7.47090900	6.93385500	N	-4.97646400	0.58430900	-1.63156200	H	-6.33817900	-2.04875200	-0.95111400
H	-1.45249100	5.68111500	4.66138000	H	-5.38849700	-0.29525600	-1.32639100	C	-6.47927700	-6.49840100	0.38382200
H	-2.95046500	7.62111700	5.07198800	H	-4.18826600	0.54777100	-2.28207500	C	-5.18619200	-5.98906900	1.02145800
H	-3.29780900	6.21790200	6.21790200	C	-5.03721400	1.66523400	-0.83741300	C	-3.98094500	-5.96407800	0.05715500
H	-2.37241500	7.72966400	6.74047700	O	-4.41594900	2.70935000	-1.11760100	C	-4.04124300	-4.77061200	-0.90894600
H	-0.56053400	7.89881500	4.19392300	C	-5.90654000	1.55489500	0.40985000	C	-2.66514100	-5.96648600	0.84753500
H	0.07705600	8.05425500	5.84104200	H	-5.49890100	0.73504100	1.01051100	H	-7.29924400	-6.58632700	1.09655600
H	0.73519600	6.86703900	4.70548900	H	-6.91544800	1.24114000	0.11191800	H	-6.27609800	-7.49368800	-0.01094400
C	3.37090800	0.27660000	6.62250700	I86V/W110L/L294M-pro(R)							
C	3.21382900	-0.33352400	5.21535400	atoms: 263 charge: +1							
C	2.96306800	-1.81692800	5.07077100	ES							
C	3.63234900	-2.77878700	5.83203700	C	4.73695300	-0.18375500	-5.24474800	H	-4.93783800	-4.77480100	-1.53382700
C	2.07964300	-2.27064800	4.07992500	C	5.73852300	-0.84072900	-4.30831100	H	-4.03004800	-3.82230900	-0.35921200
C	3.43248600	-4.14345700	5.61062500	O	6.17645000	-1.97194300	-4.48710000	H	-3.17324100	-4.77783400	-1.58487700
C	1.87363000	-3.62305800	3.83549500	C	3.27650300	-0.52405300	-4.85030400	H	-1.79399500	-5.88124700	0.08500700
C	2.55557000	-4.56880600	4.60817600	S	2.81625400	0.00500500	-3.11609500	H	-2.63359400	-5.12792500	1.55191000
O	2.32084400	-5.89014900	4.33546900	H	4.92333500	-0.57368800	-6.24836200	H	-2.55292100	-6.88632700	1.43152800
H	3.37193900	1.35041100	6.43693000	H	4.86487100	0.90346800	-5.25638900	C	-3.83764000	3.18640900	-3.96425800
H	4.31437700	-0.00370200	7.09839200	H	2.60349800	-0.03270300	-5.55614400	C	-3.08374400	4.32952100	-3.29453300
H	2.55175100	0.10042000	7.29170300	H	3.13119600	-1.60410900	-4.93140900	O	-3.28794700	4.68692900	-2.13217000
H	2.38515200	0.18454800	4.71455300	N	6.09313300	-0.10171200	-3.20988000	C	-2.87670000	2.14235700	-4.57863300
H	4.10975800	-0.07894100	4.63289100	C	7.02611800	-0.63446400	-2.24633300	C	-1.88208500	1.51188700	-3.58955800
H	4.32789400	-2.46889400	6.60634300	C	6.50825300	-1.87176500	-1.47708300	O	-2.16615300	1.40297400	-2.39129100
H	1.55099300	-1.54375000	3.47213700	O	7.31298000	-2.61346500	-0.90493000	O	-0.77866800	1.07520500	-4.12534400
H	3.96217500	-4.87568700	6.21619000	C	7.42954600	0.44375000	-1.19232000	H	-4.49619100	3.58480500	-4.74390400
H	1.17681300	-3.95734600	3.07462300	C	8.92255500	0.38697900	-0.89921000	H	-4.45098600	2.72062300	-3.19216000
H	2.78822300	-6.43847200	4.97863700	O	7.00631000	1.75557000	-1.55601300	H	-3.47038900	1.31481800	-4.98798700
C	-5.49894700	0.57707300	5.52916200	H	5.66699000	0.79485300	-3.01976500	H	-2.31267500	2.54637200	-5.42501000
C	-6.39696100	1.41123500	4.62436200	H	7.91106900	-0.99734200	-2.77909800	N	-2.14764800	4.94030000	-4.06173400

O	-3.09018700	3.67503900	0.42146600	H	3.88405800	0.86922600	0.07119200	H	-6.99644300	-1.34865700	-5.02407100
H	-4.40515100	5.95873900	0.30256200	H	1.06234400	1.30498300	3.48659400	H	-5.97398800	-2.72675900	-5.44502200
H	-3.57555600	6.77304900	1.63837300	H	5.86933800	2.01836500	0.36697000	H	-4.39203100	-2.11586800	-3.56720900
H	-4.52900300	5.30546200	1.95076500	H	5.12302900	3.00271900	3.08246300	H	-4.53378900	-0.79607000	-4.74231000
H	-2.01052500	5.42644500	0.20958000	H	-0.16916100	2.17377100	-1.19579400	H	-5.38258000	-0.70176700	-3.91218800
H	-3.33070200	3.82314200	-0.51335900	H	2.17722100	2.13197500	-0.44373300	N	-8.08798300	-2.46264300	-3.03407500
H	-0.93277900	4.08131500	1.98089800	H	-1.87558300	2.18665200	0.59381800	C	-8.76890100	-3.06312400	-1.90106200
H	-1.53531400	5.59396300	2.67616300	H	6.47893600	4.41517300	1.53818400	C	-8.40252300	-2.42436100	-0.54722400
H	-2.44089700	4.08792000	2.92439800	H	-1.51463900	0.51733400	0.41181700	C	-9.24189000	-3.06347800	0.56505900
C	2.12382000	8.11232200	-0.39209300	H	4.94083100	5.21556000	1.93158300	C	-6.90798300	-2.54587900	-0.23958000
C	2.23972400	6.83262200	0.45182800	H	-2.04476500	1.88658900	5.11086100	H	-9.85029100	-2.99583000	-2.06685600
C	1.18448900	6.79927600	1.56421500	H	-0.60475600	2.57812400	4.50821000	H	-8.35709400	-1.52772100	-3.30165500
C	2.14066700	5.57184700	-0.41381300	C	-0.76831800	-1.82958800	1.03055200	H	-8.49528600	-4.12172500	-1.89926900
H	2.92467400	8.16078900	-1.13790900	C	-0.76894700	-1.34492300	-0.39516200	H	-8.65731700	-1.35503200	-0.61000700
H	2.20164400	8.99516600	0.24216800	C	-2.19392800	-1.39073800	-0.89914100	H	-10.31600900	-2.96299800	0.37399300
H	1.17674100	8.12785900	-0.93587500	O	0.24523500	-1.01745300	-1.03092600	H	-9.01358700	-4.13215100	0.65439200
H	3.23099800	6.83760700	0.92953800	H	-0.14232700	-2.72424300	1.12179100	H	-9.02515800	-2.59781200	1.53084900
H	1.28409100	5.89542700	2.17518900	H	-0.32649900	-1.05662100	1.67054700	H	-6.67094800	-2.05987100	0.70925800
H	1.26605000	7.66762400	2.22666600	H	-2.45038600	-0.52799700	-1.51978100	H	-6.61214700	-3.59515600	-0.16835500
H	0.17437500	6.79882300	1.13688300	H	-2.31318400	-2.31828000	-1.48921500	H	-6.28943100	-2.07558700	-1.00828900
H	2.87546900	5.58114100	-1.22537000	O	-2.98731500	-1.40354900	0.26800000	C	-6.44513800	-6.51871400	0.34825100
H	2.29234800	4.67041200	0.18739400	C	-2.26221200	-2.06461000	1.32064000	C	-5.15079100	-6.00803400	0.98349800
H	1.14923400	5.50419000	-0.87756800	H	-2.58598400	-1.61139100	2.25436100	C	-3.94389600	-5.98724400	0.02109400
C	-0.50613500	4.78738800	6.88545000	H	-2.50973500	-3.12879400	1.32811900	C	-4.00028800	-4.79854500	-0.95098300
C	-1.09973600	5.71552300	5.81821200	S	-5.11167000	-3.25979100	3.17495800	C	-2.62913200	-5.98189500	0.81306400
C	-2.36005400	6.41975300	6.33195100	C	-3.83466800	-4.03877400	4.21632200	H	-7.26510500	-6.60664000	1.06098500
C	-0.06173100	6.72675800	5.31819100	H	-4.11777400	-4.05074600	5.27097800	H	-6.24195900	-7.51400100	-0.04651500
H	-0.24970600	5.32181200	7.79996100	H	-3.73110600	-5.07002600	3.87230000	H	-6.77370200	-5.88827700	-0.48398800
H	0.38468800	4.48240300	6.50856900	H	-2.87107600	-3.52988100	4.10523100	H	-5.29212900	-5.00117500	1.38179600
H	-1.22880800	4.01225200	7.17000100	TS				H	-4.98004000	-6.65338300	1.83905000
H	-1.39357800	5.09003200	4.96362900					H	-3.96799800	-6.91412000	-0.57190500
H	-2.81170400	7.04193300	5.55247800	C	4.77109200	-0.20406800	-5.28031900	H	-4.89794300	-4.80140700	-1.57452100
H	-3.11410300	5.69858000	6.66480300	C	5.80288300	-0.83994200	-4.36136400	H	-3.97782200	-3.84623800	-0.40855300
H	-2.12239100	7.06994600	7.18218100	O	6.29358100	-1.94341700	-4.56924400	H	-3.13314700	-4.81376400	-1.62708100
H	-0.47576300	7.36377500	4.52956200	C	3.31826700	-0.53168500	-4.84308200	H	-1.75777300	-5.91407100	0.14923600
H	0.26977800	7.37997300	6.13404800	S	2.88740500	0.02255500	-3.11122700	H	-2.59225800	-5.12796500	1.49861500
H	0.82307100	6.22548200	4.91046100	H	4.93243200	-0.61237900	-6.28072200	H	-2.52219100	-6.89058300	1.41550400
C	3.44131700	-0.47132100	6.34712900	H	4.90096600	0.88263900	-5.31402000	C	-3.80350100	3.16609600	-3.99982900
C	3.23546800	-0.99733500	4.91255700	H	2.63147000	-0.04996600	-5.54223900	C	-3.06733300	4.32233100	-3.32897300
C	3.41686600	-2.46986000	4.60505000	H	3.16524400	-1.61206400	-4.90469300	O	-3.28392700	4.69232200	-2.17265800
C	4.22785700	-3.32200400	5.36528900	N	6.14032100	-0.10447000	-3.25018700	C	-2.81343700	2.09235700	-4.51283400
C	2.82984500	-2.99522000	3.44479100	C	7.06025700	-0.65477700	-2.28190400	C	-1.84475500	1.54976700	-3.44581300
C	4.45625300	-4.64387300	4.98420400	C	6.53446900	-1.88650300	-1.51240200	O	-2.14273900	1.62279700	-2.24725800
C	3.04694700	-4.31549500	3.04926200	O	7.33923400	-2.62743600	-0.93663500	O	-0.75967700	1.01115600	-3.91447200
C	3.86973100	-5.14597100	3.81922100	C	7.50954700	0.41277100	-1.23704600	H	-4.40866100	3.54069800	-4.83261000
O	4.16645000	-6.43359700	3.46302300	C	9.01432400	0.35505900	-1.00806600	H	-4.46624400	2.73748100	-3.24766500
C	3.45455700	0.61252100	6.23099300	O	7.06674400	1.72739200	-1.56354800	H	-3.38110800	1.23227500	-4.88957200
H	4.40328000	-0.77350800	6.77087900	H	5.60409700	0.71608700	-3.00152500	H	-2.22348700	2.44976100	-5.36287800
H	2.64666000	-0.76694800	7.03375100	H	7.92868000	-1.03611600	-2.82724800	N	-2.12167600	4.92487600	-4.09395700
H	2.23471000	-0.69976100	4.57442300	H	6.99825400	0.19839700	-0.29660200	C	-1.31198200	6.03442700	-3.60815500
H	3.92595200	-0.45554300	4.25040800	H	7.55263000	3.02325900	-2.34224600	C	-0.44783400	6.62112300	-4.72123200
H	4.69455800	-2.95465200	6.27363300	H	9.31097000	1.20369500	-0.19434800	C	0.57095200	5.66371100	-5.35332000
H	2.21687100	-2.35664800	2.81594900	H	9.31163900	-0.67196800	-0.77702400	S	1.91438600	5.07545400	-4.25098800
H	5.08319900	-5.29951700	5.57874500	H	9.55375600	0.65180700	-1.91508300	C	1.15945900	3.59974000	-3.48751200
H	2.58342400	-4.69510300	2.14121600	N	5.50502600	-2.03672600	-1.42883900	H	-1.97453400	6.80526100	-3.20107000
H	3.58212600	-6.71129900	2.74561200	C	4.58271300	-3.21371000	-0.81519800	H	-2.01603200	4.63607400	-5.05414300
C	-5.48419300	0.07985000	5.67546800	C	3.06345900	-3.04914100	-0.79188200	H	-0.68369600	5.69445700	-2.77746300
C	-6.42217100	0.95610200	4.85879100	O	2.66170300	-1.96252500	0.04655800	H	-1.10071400	7.00546500	-5.51781000
O	-7.63423700	0.94164600	5.04896400	H	4.83386900	-4.11757400	-1.38435000	H	0.08772000	7.48285600	-4.31142000
C	-5.59496500	-1.38504800	5.23026500	H	4.58720500	-1.42111100	-1.97236500	H	0.09340000	5.78186600	-4.78186600
C	-5.07741000	-1.55335800	3.80488400	H	4.97353400	-3.34873500	0.19498500	H	1.08400000	6.17956800	-6.16979500
H	-5.78163700	0.17416800	6.72361100	H	2.70688400	-2.86879000	-1.81316700	H	1.97686700	2.99875700	-3.08216700
H	-4.44389200	0.41726000	5.58357300	H	2.61809300	-3.98582700	-0.42746100	H	0.46331900	3.86072200	-2.68805800
H	-5.02170900	-2.01292000	5.92120600	H	1.84557800	-1.53560300	-0.32266400	H	0.64434300	2.98969000	-4.23041300
H	-6.64017300	-1.70204300	5.29026700	C	8.66138500	-6.01700000	1.08631600	C	-3.82898000	5.77562500	1.19817300
H	-5.68978000	-0.98933900	3.09544500	C	7.62299700	-5.43529900	2.06569500	C	-2.58170500	4.94185700	0.91958200
H	-4.06190100	-1.15238500	3.71727400	C	7.40381000	-3.95596600	2.01484600	C	-1.76663800	4.71668700	2.18503000
N	-5.83252500	1.71003100	3.88670900	C	6.27048700	-3.22357700	2.24579400	O	-2.94222800	3.66395100	0.39688400
C	-6.65400400	2.41518800	2.91578700	N	8.38472500	-3.02475100	1.70609400	H	-4.37101200	5.93842600	0.26699100
C	-5.99266600	2.47093600	1.53719000	C	7.86169800	-1.79052400	1.69240900	H	-3.56827900	6.75416100	1.61663500
S	-5.67333600	0.83273600	0.75113400	N	6.58432700	-1.89444600	2.04202400	H	-4.48530900	5.25854200	1.90544000
H	-7.62146700	1.90902600	2.87438200	H	9.30926400	-3.25291900	1.36952500	H	-1.95910000	5.47001600	0.18151700
H	-4.84982600	1.56676600	3.68088500	H	8.61887700	-5.63138600	0.06746900	H	-3.21496800	3.79706200	-0.53197500
H	-6.84255700	3.44680300	3.24809100	H	8.47784600	-7.09337900	1.00903200	H	-0.84922500	4.16312100	1.96867400
H	-6.65359100	3.00886400	0.85256800	H	9.68201700	-5.94170100	1.46721000	H	-1.49044800	5.67130700	2.63976500
H	-5.04066800	3.00592300	1.54493900	H	6.64460500	-5.89695700	1.90195200	H	-2.36160300	4.14985700	2.90884900
H	-4.42074600	0.65451400	1.21206800	H	7.90759900	-5.72022400	3.08669700	C	2.15795900	8.09200900	-0.42766400
Z	0.45035700	-0.10766100	-3.06890500	H	5.82854000	-3.53288500	2.54102000	C	2.28092900	6.80997100	0.40912900
C	3.07983200	1.63796200	1.94258400	H	8.37094400	-0.87814500	1.43704500	C	1.24290600	6.77566500	1.53695500
N	1.72473400	1.46337500	1.51297400	H	5.88809500	-1.13151800	1.97805700	C	2.16415300	5.55486300	-0.46282200
C											

H	-3.07924600	5.68105700	6.62921100	C	5.73963300	-0.87661600	-4.32124200	H	-4.10758100	-4.13787400	-0.94590900
H	-2.08678700	7.05007600	7.15054700	O	6.10888600	-2.03791900	-4.46229300	H	-3.22921000	-5.31605700	-1.93132600
H	-0.43744400	7.35071000	4.50184700	C	3.30480700	-0.52081900	-4.91210700	H	-1.76644900	-5.88937800	0.05616000
H	0.30684500	7.36019100	6.10661300	S	2.83742100	0.02901600	-3.18955400	H	-2.65336500	-4.73634600	1.06334700
H	0.86044900	6.20982900	4.87974400	H	4.97172500	-0.59924400	-6.27948500	H	-2.48970100	-6.47205100	1.58226400
C	3.47545600	-0.49163400	6.31155800	H	4.91686100	0.88102200	-5.29405600	C	-3.80350600	3.16609200	-3.99982900
C	3.26397100	-1.01248500	4.87528700	H	2.64574100	-0.02757000	-5.62993300	C	-3.06805400	4.32953100	-3.34185500
C	3.13490100	-2.48778200	4.56701900	H	3.14626900	-1.59971600	-4.98277800	O	-3.31183200	4.72926300	-2.19928900
C	4.22038800	-3.35046000	5.32602100	N	6.13382400	-0.12068800	-3.25265700	C	-2.84663600	2.06182500	-4.50564300
C	2.81517700	-3.00720000	3.41294000	C	7.06024700	-0.65478600	-2.28192400	C	-1.82677400	1.52307700	-3.48460700
C	4.42197700	-4.67787300	4.94988200	C	6.53506500	-1.91751400	-1.55453200	O	-1.87031800	1.86596900	-2.29644900
C	3.00563200	-4.33281200	3.02231000	O	7.32905500	-2.72792700	-1.08337200	O	-0.95709900	0.70731000	-3.99783500
C	3.81831800	-5.17466800	3.79095700	C	7.42014800	0.40822300	-1.20349900	H	-4.40369800	3.53763700	-4.83767800
O	4.08788600	-6.46884500	3.44083200	C	8.89642500	0.34054000	-0.84439600	H	-4.48035800	2.76408800	-3.24455600
H	3.48869600	0.59220800	6.19542200	O	7.02165100	1.73041900	-1.58055200	H	-3.43475000	1.20595900	-4.85643000
H	4.43764400	-0.79677400	6.73195400	H	5.78425000	0.81599500	-3.10694200	H	-2.27736600	2.39056800	-5.38294800
H	2.68079900	-0.78726100	6.99818000	H	7.96299200	-0.99729400	-2.79893700	N	-2.11735000	4.92451400	-4.10219100
H	2.26713200	-0.69937900	4.53765200	H	6.82938200	0.19766400	-0.31278900	C	-1.31198000	6.03442600	-3.60815400
H	3.96265800	-0.47837300	4.21487600	H	7.69429700	2.09605900	-2.17189900	C	-0.43251600	6.62099800	-4.70826500
H	4.69954900	-2.98762700	6.22974100	H	9.11527100	0.97924000	0.01566900	C	0.58009900	5.65553200	-5.33870000
H	2.20736200	-2.36339300	2.78434600	H	9.17146100	-0.69261800	-0.61724100	S	1.83635800	4.95872100	-4.95724300
H	5.04064800	-5.34218700	5.54341600	H	9.51438600	0.66234100	-1.69189100	C	1.00059600	3.44802500	-3.60570900
H	2.52735700	-4.70684600	2.11988500	N	5.18653600	-2.00355900	-1.37898200	H	-1.98007100	6.80364900	-3.20846100
H	3.49942600	-6.73738700	2.72318800	C	4.58272000	-3.21369900	-0.81519400	H	-1.97844500	4.60823600	-5.04939800
C	-5.45005400	0.05953700	5.63989700	C	3.06539100	-3.09746800	-0.81223900	H	-0.69113700	5.69285700	-2.77175900
C	-6.37582300	0.97426300	4.85176000	O	2.53063400	-2.04079600	0.00486200	H	-1.06976700	7.02402300	-5.50770900
O	-7.57420600	1.04245400	5.10322300	H	4.86161200	-4.09258400	-1.41106700	H	0.11080700	7.46983200	-4.28185600
C	-5.62790000	-1.40038200	5.19979600	H	4.58883600	-1.39939700	-1.94105200	H	0.09314300	4.81595000	-5.84815600
C	-5.17083300	-1.58943100	3.75638200	H	4.97036700	-3.77499200	0.19389500	H	1.15133400	6.18834700	-6.10376300
H	-5.71101300	0.16571700	6.69641600	H	2.72607600	-2.91717300	-1.83987000	H	1.76556800	2.83816600	-3.11958900
H	-4.39982700	0.35591700	5.51685900	H	2.64443500	-4.05041400	-0.46594300	H	0.18868800	3.65987400	-2.90849900
H	-5.05059100	-2.04666700	5.86988800	H	1.16415900	-1.30714700	-0.65352200	H	0.61246200	2.86609900	-4.44424100
H	-6.67978800	-1.68320200	5.30058300	C	8.66137600	-6.01698100	1.08632200	C	-3.82898500	5.77562100	1.19817300
H	-5.80632300	-1.02843400	3.06532000	C	7.60039500	-5.45842800	2.05777000	C	-2.52087400	5.05919400	0.90422700
H	-4.15534200	-1.20147100	3.62266000	C	7.32781500	-3.98458400	2.02596100	C	-1.71156600	4.85490900	2.17746100
N	-5.79361100	1.66687300	3.83035300	C	6.18439100	-3.27516600	2.31147700	O	-2.78480500	3.78278400	0.32736500
C	-6.61986500	2.39487500	2.88021600	N	8.26442100	-3.02211400	1.70173000	H	-4.37101000	5.93843000	0.26699000
C	-5.97725300	2.43966000	1.49188400	C	7.66916600	-1.80487400	1.74545900	H	-3.65423900	6.75271700	1.66241200
S	-5.79747800	0.80067600	0.66296500	N	6.40546200	-1.91819600	2.12513400	H	-4.45070900	5.17880200	1.87252400
H	-7.60110400	1.91468400	2.84924900	H	9.17653300	-3.20962900	1.31352200	H	-1.93083900	5.66155900	0.19690600
H	-4.83572900	1.45649800	3.57400400	H	8.61888000	-5.63139800	0.06746400	H	-3.07323800	3.92491800	-0.59826100
H	-6.77672300	3.42830900	3.22252000	H	8.49000300	-7.09585700	0.99933500	H	-0.73587700	4.41009400	1.96905600
H	-6.61006700	3.03737400	0.83102000	H	9.68201700	-5.94717000	1.46720900	H	-1.54151900	5.81076000	2.67833600
H	-4.99130200	2.91150300	1.49795000	H	6.64140200	-5.95312700	1.87204900	H	-2.26603600	4.20570200	2.86360900
H	-4.54724900	0.50932700	1.07012800	H	7.88326400	-5.75291100	3.07726200	C	2.15794700	8.09195300	-0.42766900
Z	0.50710900	-0.20147200	-2.90691100	H	5.22945900	-3.64868100	2.64515700	C	2.29630400	6.81706400	0.42086900
C	3.08289300	1.67938000	1.89249400	H	8.16818100	-0.88336900	1.49788700	C	1.27893100	6.80123500	1.56720200
N	1.69691100	1.60534500	1.46308500	H	5.11920100	-0.94519300	1.73044200	C	2.17221800	5.54422000	-0.42634200
C	4.09454800	0.84633900	1.07610800	C	-2.25981900	-4.07925300	-7.15033300	H	2.95598200	8.14628600	-1.17604900
C	0.70367500	1.43448500	2.38802300	C	-2.63619400	-4.27753500	-5.67243400	H	2.23580000	8.97485300	0.20659400
O	4.23511800	-0.46403700	1.57267700	C	-1.62782800	-3.61633200	-4.79202200	H	1.21087200	8.10757700	-0.97143200
C	5.40151800	1.68391000	1.21796000	C	-1.31551800	-2.29340500	-4.60549900	H	3.30225500	6.82460900	0.86596800
C	-0.61644300	1.42098700	2.03098800	N	-0.65311500	-4.31129200	-4.09430200	H	1.39079900	5.90256400	2.18472900
O	6.41040000	1.03307900	1.98452700	C	0.19483600	-3.34251700	-3.51937500	H	1.39197400	7.67304200	2.21994100
C	4.94123800	3.02568800	1.83937300	N	-0.18346100	-2.19096900	-3.81793200	H	0.25571600	6.80986700	1.17376300
O	-0.96832000	1.46059000	0.62205500	H	-1.27146300	-4.49738700	-7.36300900	H	2.86907300	5.54850500	-1.26980200
C	3.50724400	3.01740500	1.76939000	H	-2.23468400	-3.01544300	-7.40223800	H	2.37245000	4.65536800	0.18303000
C	5.46069300	4.26844400	1.14645600	H	-2.98599800	-4.56822800	-7.80612300	H	1.16232800	5.45179700	-0.84522400
C	0.07625200	1.94995800	-0.24778800	H	-3.62941000	-3.86516700	-5.46986500	C	-0.47199600	4.76707400	6.84987400
C	1.36599500	1.95099800	0.16452900	H	-2.69816700	-5.34422000	-5.43079500	C	-1.06294700	5.70306900	5.78752900
C	-1.70320400	1.35642500	3.05119300	H	-0.59904500	-5.31691400	-4.01848500	C	-2.32078100	6.40783400	6.30633300
N	-1.39249100	1.84659000	4.29410000	H	-1.80831200	-1.40702400	-4.97015300	C	-0.02023400	6.71335100	5.29544900
O	-2.80340700	0.86858800	2.79519400	H	1.03705500	-3.70225400	-2.90646100	H	-0.21556800	5.30149900	7.76439000
H	5.16896900	4.26236600	0.09286500	C	-6.29428100	-2.08584800	-4.61863700	H	0.41882900	4.26389200	6.47300100
H	3.67747000	-1.06939500	1.01330700	C	-6.98746100	-2.98200700	-3.60538500	H	-1.19741700	3.99508500	7.13762400
H	6.15353100	1.06253400	2.91694800	O	-6.54296700	-4.09396500	-3.33069400	H	-1.36034900	5.08570100	4.92780900
H	3.11270200	1.33238700	2.93512200	C	-4.95466800	-1.58458600	-0.05411300	H	-2.76999800	7.03721600	5.53144700
H	3.79545700	0.82139600	0.02246600	H	-6.92536700	-1.23989400	-4.91342100	H	-3.07765900	5.68766000	6.63495700
H	1.03151400	1.32638300	3.41494500	H	-6.11725500	-2.68942200	-5.51473000	H	-2.08034700	7.05118300	7.16054800
H	5.84672700	1.86162700	0.24062800	H	-4.35514400	-2.42941800	-3.70484500	H	-0.43118900	7.35946100	4.51283500
H	5.23931400	3.03184400	2.90303800	H	-4.38577100	-1.04230600	-4.81690800	H	0.31383000	7.35781700	6.11667700
H	-0.19302500	2.25513600	-1.24808600	H	-5.10923800	-0.91281300	-3.20324100	H	0.86330500	6.21264400	4.88396300
H	2.18643200	2.26526500	-0.46530300	N	-8.09482800	-2.44261500	-3.02735500	C	3.47543900	-0.49161800	6.31153100
H	-1.98858800	1.73594200	0.37333200	C	-8.76891100	-3.06312700	-1.90105700	C	3.27022000	-1.01968600	4.87932900
H	6.55218000	4.29752700	1.20689500	C	-8.36090800	-2.47690900	-0.53432800	C	3.28998800	-2.50840500	4.60885100
H	-1.05447200	0.16182000	0.21898100	C	-9.12779600	-3.19943500	0.57932600	C	3.97694600	-3.42222200	5.41644200
H	5.05664800	5.16938400	1.61383800	C	-6.84915600	-2.55769800	-0.30004300	C	2.67603900	-2.99521600	3.44732200
H	-2.16455100	1.88179800	4.94691200	H	-9.85197100	-2.96998200	-2.04058700	C	4.05539700	-4.77197900	5.08045300
H	-0.72533000	2.60023600	4.37657300	H	-8.32938900	-1.48732200	-3.25150100	C	2.74412300	-4.34228400	3.09605900
C	-0.75989100	-1.79465600	1.04749700	H	-8.51523100	-4.12578900	-1.93855300	C	3		

H	-6.55219900	-1.75454900	5.26531000	H	2.60872700	-3.94454200	-0.23895600	H	0.49731400	3.85552700	-2.67896700
H	-5.54083000	-1.01270200	3.09588700	H	1.90934600	-1.47784800	-0.13047200	H	0.46032300	2.93043300	-4.20196100
H	-3.92755500	-1.24457200	3.75505100	C	8.66228400	-5.89868600	1.25408900	C	-3.89949400	5.81666900	1.05528400
N	-5.81576200	1.70480500	3.87259100	C	7.63328400	-5.27547100	2.21599100	C	-2.69067100	4.92688200	0.80339600
C	-6.61986400	2.39486000	2.88023400	C	7.45448700	-3.79281200	2.12704500	C	-1.87932800	4.69626600	2.06939900
C	-5.92469200	2.44851400	1.51680100	C	6.34401200	-3.02061800	2.33814100	O	-3.12789400	3.65979700	0.30707300
S	-5.60012300	0.81130400	0.73337100	N	8.46234700	-2.89952700	1.79288600	H	-4.44811400	5.94548600	0.12263200
H	-7.57786300	1.87422600	2.81765300	C	7.97656800	-1.64992300	1.75211300	H	-3.59900100	6.80753600	1.41408600
H	-4.81579300	1.63890400	3.73092900	N	6.69769900	-1.70773100	2.10251600	H	-4.56412600	5.36825300	1.79961000
H	-6.82778200	3.42723900	3.19862800	H	9.38447500	-3.16344900	1.47671600	H	-2.04823100	5.40225900	0.04759200
H	-6.56505100	2.98417700	0.81140000	H	8.61129600	-5.54700800	0.22338600	H	-3.34452700	3.78629200	-0.63785200
H	-4.97412700	2.98700300	1.55018800	H	8.47914200	-6.97713700	1.21891900	H	-0.97856800	4.11337500	1.86262300
H	-4.46032900	0.53923900	1.39570400	H	9.68470500	-5.80478300	1.62595400	H	-1.57413300	5.65203700	2.50367400
Z	0.51118900	-0.33195400	-3.13123600	H	6.64522000	-5.71838300	2.06050100	H	-2.48514400	4.15939000	2.80668300
C	3.15327100	1.59416400	2.00944900	H	7.90727500	-5.54259800	3.24466700	C	2.06316300	8.11385400	-0.68296600
N	1.72935800	1.60587600	1.60802200	H	5.34682200	-3.29254000	2.63969100	C	2.19319300	6.85684800	0.19201500
C	4.14854100	0.79225500	1.13836500	H	8.51290300	-0.75927600	1.47602200	C	1.15083900	6.84586100	1.31698400
C	0.79190600	1.52517800	2.58374500	H	6.01276200	-0.93369800	2.01035300	C	2.08726900	5.57663400	-0.64445700
O	4.19317300	-0.53645100	1.59419800	C	-2.31988800	-4.29836700	-6.97398600	H	2.85805600	8.14585800	-1.43615400
C	5.44790800	1.66151800	1.30244700	C	-3.03996800	-3.71285500	-5.74854500	H	2.13941100	9.01755300	-0.07863500
C	-0.55264500	1.64715700	2.28365100	C	-2.05708000	-3.20237600	-4.75096300	H	1.11279300	8.10582100	-1.22112000
O	6.54848800	1.00139300	1.88549900	C	-1.45831900	-1.97761300	-4.61141800	H	3.18994700	6.87553900	0.65758900
C	5.00076000	2.89952900	2.11822500	N	-1.43358700	-4.01088800	-3.81285100	H	1.26028500	5.95625200	1.94697000
C	-0.92905200	1.83874600	0.94710400	C	-0.50828700	-3.27659400	-3.14794500	H	1.23730600	7.72903300	1.95880300
O	3.56221000	2.93043900	1.99172200	N	-0.50155400	-2.03687600	-3.61503500	H	0.13572100	6.83317400	0.90147600
C	5.56336900	4.22108700	1.64562800	H	-1.67380200	-5.13573100	-6.69211500	H	2.80722000	5.57190800	-1.46928700
C	0.05561500	1.98688900	-0.02947400	H	-1.69459700	-3.53887300	-7.45121800	H	2.25473800	4.68866300	-0.02758400
C	1.38311400	1.86469500	0.32111100	H	-3.04070400	-4.66398800	-7.71076700	H	1.08773800	5.49476400	-1.08880300
C	-1.62451300	1.56438000	3.33878600	H	-3.67835400	-2.88013900	-6.05577900	C	-0.50251900	5.01486600	6.71618800
N	-1.28141200	2.02662600	4.57118300	H	-3.70285700	-4.45249900	-5.28466600	C	-1.10935200	5.90288200	5.62281600
O	-2.72429200	1.08595000	3.07704600	H	-1.67091300	-4.97468500	-3.62391000	C	-2.36795100	6.61987600	6.12301800
H	5.29679500	4.39360500	0.59894500	H	-1.64798800	-1.05747000	-5.13963000	C	-0.08051300	6.89999700	5.07746500
H	3.22000500	-1.59735400	0.54336500	H	0.10476200	-3.65681400	-2.34625600	H	-0.24389600	5.58063700	7.61101500
H	6.25773100	0.40553100	2.59190400	C	-6.35125200	-2.24673600	-4.48424800	H	0.38909800	4.50484000	6.35055400
H	3.17883600	1.15739500	3.301584100	C	-7.01724600	-3.11289600	-3.42810900	H	-1.21821000	4.24493600	7.03046200
H	3.85264100	0.80894800	0.08198800	O	-6.52652100	-4.18584000	-3.08088900	H	-1.40833400	5.24588500	4.79408400
H	1.16222200	1.33931300	3.58388100	C	-5.13889000	-1.51628000	-3.88207100	H	-2.82957100	7.21240700	5.32637500
H	5.78555900	1.98556900	0.31640300	H	-7.05456400	-1.52503500	-4.91491000	H	-3.11559300	5.90788800	6.48837100
H	5.25473300	2.72024600	3.17450500	H	-6.02729500	-2.91244700	-5.28919000	H	-2.12522800	7.30077300	6.94738300
H	-0.25129100	2.14758000	-1.05734000	H	-4.45515300	-2.23434800	-3.42229000	H	-0.50462700	7.50738500	4.27089600
H	2.19175000	1.96194800	-0.39030400	H	-4.58867300	-0.96541800	-4.65132300	H	0.25589900	7.58298600	5.86648200
H	-1.97343200	1.94422100	0.68613500	H	-5.44228300	-0.80012400	-3.11208800	H	0.80268000	6.38816700	4.67940500
H	6.65331400	4.20322500	1.73100900	N	-8.14920900	-2.88911200	-2.88911200	C	3.47391100	-0.23513700	6.32673600
H	-1.39000700	-0.14663900	-0.40189600	C	-8.80345300	-3.14863700	-1.72067000	C	3.26727000	-0.81367500	4.91294900
H	5.17863100	5.04855900	2.24689000	C	-8.42989200	-2.44212700	-0.40202300	C	3.47662400	-2.29271200	4.65830500
H	-2.01499800	2.04252300	5.26750500	C	-9.17202400	-3.10794000	0.76243800	C	4.31887500	-3.09802000	5.43549600
H	-0.54550800	2.70806900	4.68816800	C	-6.91745800	-2.43998300	-0.15652400	C	2.88208700	-2.87433500	3.52953300
C	-0.69561500	-1.61339800	1.04311100	H	-9.88835800	-3.11323400	-1.87028800	C	4.56858200	-4.42861300	5.10081000
C	-0.85136900	-1.09737600	-0.38374500	H	-8.42245300	-1.65814900	-3.17996600	C	3.12061800	-4.20364200	3.17976100
C	-1.79934000	-2.15786200	-0.95559400	H	-8.50439300	-4.19926400	-1.67692900	C	3.97271100	-4.98709000	3.96668700
O	0.37411700	-0.88201100	-1.08801200	H	-8.76584200	-1.39668800	-0.47447100	O	4.28940600	-6.28163800	3.65468300
H	-0.00869200	-2.46666700	1.04195000	H	-10.25674200	-3.10071400	0.60969800	H	3.47978400	0.84435300	6.17491800
H	-0.31266300	-0.87481300	1.74752800	H	-8.85359400	-4.10573700	0.87561300	H	4.43996800	-0.51500800	6.75659700
H	-2.32045300	-1.84321300	-1.86201500	H	-8.96017800	-2.59425400	1.70465100	H	2.68523100	-0.51270500	7.02763600
H	-1.25466600	-0.89208000	-1.16496000	H	-6.67965600	-1.92411600	0.77714000	H	2.25794100	-0.54865300	4.57316400
O	-2.75401300	-2.32228800	0.08191700	H	-6.53460500	-3.46184800	-0.08839900	H	3.94242700	-0.28237600	4.22653600
C	-2.13488300	-2.04012800	1.35435800	H	-6.37841200	-1.92907100	-0.95954600	H	4.79292600	-2.68714200	6.32107800
H	-2.69417400	-1.23231000	1.83440700	C	-6.44494400	-6.51444900	0.62656000	H	2.24482800	-2.27238200	2.88936500
H	-2.18870100	-2.92488300	1.99358800	C	-5.14356900	-5.93905900	1.18827200	H	5.21864700	-5.04819100	5.70905700
S	-5.04751800	-3.29757500	3.15652700	C	-3.95359700	-6.03947900	0.21046000	H	2.64860800	-4.62779600	2.29620600
C	-3.85342700	-4.15020200	4.23783800	C	-4.12327900	-5.12091500	-1.00765600	H	3.69127200	-6.60152000	2.96676900
H	-4.20497700	-4.12391700	5.26991800	C	-2.62778600	-5.73384400	0.92110700	C	-5.45872100	0.24043500	5.69260900
H	-3.74154200	-5.16180700	3.84256100	H	-7.26015700	-6.58355600	1.34693300	C	-6.37615400	1.13852800	4.87564600
H	-2.87735000	-3.65423100	4.21383300	H	-6.23816300	-7.52092100	0.26367700	O	-7.56709100	1.26026800	5.14698300
I86V/W110L/L294M-pro-(S)				H	-6.80709800	-5.93101200	-0.22676700	C	-5.58925800	-1.22507700	5.24816400
atoms: 263 charge: +1				H	-5.27975300	-4.89210000	1.47031700	C	-5.12352800	-1.42590400	3.80649900
ES				H	-4.88259100	-6.47891800	2.10833500	H	-5.75446600	0.34156100	6.73976900
C	4.69816700	-0.32190400	-5.27615100	H	-3.90998300	-7.07779100	-0.15255600	H	-4.41285000	0.56062500	5.59705900
C	5.71848600	-0.93690100	-4.33131600	H	-5.03095800	-5.31372600	-1.58179800	H	-5.00043000	-1.85511800	5.92400800
O	6.17228100	-2.06564900	-4.48299700	H	-4.16513500	-4.07168200	-0.69274200	H	-6.63320200	-1.53859800	5.34433100
C	3.24291600	-0.66187300	-4.84192600	H	-1.77737300	-5.87096900	0.23942500	H	-5.75206400	-0.86524200	3.10982800
S	2.79565500	-0.08329800	-3.11547300	H	-2.59697100	-4.70119400	1.28400500	N	-5.80795500	1.75786700	3.79991600
H	4.86755700	-0.74876000	-6.26734800	H	-2.47193600	-6.39777500	1.77859500	C	-6.65938300	2.47666200	2.86495400
H	4.81588000	0.76513900	-5.33000700	C	-3.88919900	3.03758500	-4.05410700	C	-5.97999600	2.68859500	1.51712200
H	2.55330800	-0.19974300	-5.55113300	C	-3.12823800	4.20064100	-3.43078600	S	-5.68153100	1.11742600	0.58323100
H	3.10777200	-1.74520800	-4.88569800	O	-3.26329900	4.54742600	-2.25413900	H	-7.60420900	1.93272800	2.76048500
N	6.06964200	-0.16236800	-3.25622500	C	-2.92028800	1.92672100	-4.52490100	H	-4.86347700	1.51937300	3.51459500
C	7.00800200	-0.65994700	-2.78771100	C	-2.06267700	1.28656400	-3.41556000	H	-6.91844200	3.46312500	3.27339900
C	6.49829200	-1.87014600	-1.46272500	O	-2.53617900	1.08983100	-2.29259000	H	-6.60299800	3.34293700	0.90339200
O	7.31049800	-2.58363500	-0.86571700	O	-0.86408100	0.94882100	-3.80093500	H	-5.00		

O	-2.73723300	1.00065300	2.82280000	H	0.00544000	-3.66128000	-2.25628800	H	-0.20883900	5.55750500	7.57942300
H	5.16497100	4.48431900	0.15871000	C	-6.31619500	-2.26986800	-4.51584000	H	0.42415500	4.48170800	6.31896200
H	3.81599700	-0.96034300	1.09965500	C	-6.98922400	-3.13997800	-3.46704600	H	-1.18402300	4.22253000	6.99880700
H	6.21190400	1.29306700	2.92138000	O	-6.50825200	-4.22014000	-3.12987500	H	-1.37007900	5.23039600	4.76046200
H	3.16605900	1.41871000	2.85681200	C	-5.10345400	-1.54825900	-3.90411800	H	-2.79310000	7.19257800	5.29771200
H	3.95053000	0.88735400	-0.02362800	H	-7.01521100	-1.54271800	-4.94448200	H	-3.08108300	5.88360100	6.45419100
H	1.09386400	1.43909500	3.34957300	H	-5.99090100	-2.93143100	-5.32352700	H	-2.09255500	7.27510000	6.92056600
H	5.90558600	2.09240800	0.24893500	H	-4.42514800	-2.27030600	-3.44253900	H	-0.46569000	7.49346600	4.24902800
H	5.10753500	3.15381800	2.92328300	H	-4.54669800	-0.99701300	-4.66824300	H	0.29049000	7.56303700	5.84668000
H	-0.11717300	2.06567100	-1.38015300	H	-5.41075200	-0.83483800	-3.13282600	H	0.84176500	6.37376200	4.65656000
H	2.21756100	2.05876300	-0.62102000	N	-8.11595300	-2.60646500	-2.92107900	C	3.50896800	-0.25826900	6.29514400
H	-1.83444100	2.18897100	0.41908600	C	-8.76839600	-3.17176900	-1.75226200	C	3.29450400	-0.83261800	4.88019500
H	6.47749200	4.53188500	1.35799100	C	-8.38326500	-2.47487500	-0.43164100	C	3.47547200	-2.31539800	4.62609000
H	-1.46800000	0.50752100	0.31098500	C	-9.11610800	-3.14915900	0.73388500	C	4.31436400	-3.13003100	5.39731500
H	4.92459500	5.32670300	1.70068200	C	-6.86887400	-2.47655500	-0.19940600	C	2.85465000	-2.89339000	3.50956400
H	-2.03692000	2.00192700	4.95054500	H	-9.85386100	-3.12895200	-1.89605000	C	4.53546200	-4.46697600	5.06883100
H	-0.59641400	2.69371400	4.35094900	H	-8.38032100	-1.67394400	-3.20226900	C	3.06472000	-4.22898100	3.16603800
C	-2.91055200	-1.71212800	0.74755900	H	-8.47539800	-4.22435800	-1.71573600	C	3.91403900	-5.02220500	3.94643600
O	-1.95167000	-2.37429500	1.60995900	H	-8.71869800	-1.42855200	-0.49303200	O	4.20305300	-6.32372500	3.64032900
C	-0.66719300	-1.91706000	1.25701200	H	-10.20199400	-3.14215000	0.58935200	H	3.51484100	0.82122100	6.14332600
C	-0.76148100	-1.50407600	-0.19694400	H	-8.79568900	-4.19223900	0.83798700	H	4.47537600	-0.54146200	6.72133300
C	-2.19984900	-1.63026300	-0.61219200	H	-8.89787400	-2.64144800	1.67795900	H	2.72028800	-0.53583700	6.99604400
O	0.22343400	-1.16599700	-0.87534600	H	-6.62130200	-1.97954100	0.74183700	H	2.28894500	-0.55108600	4.54100600
H	-3.81327900	-2.32031600	0.75281300	H	-6.48463100	-3.49892200	-0.15421300	H	3.97769600	-0.31062300	4.19437800
H	-3.14295300	-0.71972700	1.14749400	H	-6.33683200	-1.95127600	-0.99781500	H	4.807771800	-2.72184500	6.27363700
H	0.07726300	-2.70915900	1.40111400	C	-6.40988700	-6.53758100	0.59496800	H	2.21461300	-2.28844200	2.74897900
H	-0.34742000	-1.03817200	1.84462700	C	-5.11518700	-5.94622800	1.15625100	H	5.18262800	-5.09409900	5.67238800
H	-2.51098900	-0.81505800	-1.27232600	C	-3.91574800	-6.03899600	0.18964400	H	2.57016200	-4.64932400	2.29331800
H	-2.30077400	-2.58312000	-1.15162400	C	-4.09639200	-5.15958000	-1.05537900	H	3.59602700	-6.63519400	2.95623300
S	-5.21701100	-3.15555900	3.24171900	C	-2.60506000	-5.67530300	0.90238600	C	-5.42366400	0.21730300	5.66101700
C	-3.75369600	-3.85150000	4.07982300	H	-7.22510000	-6.60668800	1.31534100	C	-6.33868700	1.12774100	4.85515300
H	-3.84219500	-3.77781200	5.16618600	H	-6.20310600	-7.54405300	0.23208500	O	-7.51777800	1.29064300	5.15337200
H	-3.70216900	-4.90627500	3.80374300	H	-6.77644100	-5.95821900	-0.25944900	C	-5.58241000	-1.24987500	5.23205300
H	-2.84982000	-3.34722000	3.73107400	H	-5.26516900	-4.89876300	1.42890700	C	-5.15472100	-1.47109200	3.78156100
TS				H	-4.85305500	-6.47443400	2.08288500	H	-5.69804800	0.33167900	6.71267300
C	4.73322400	-0.34503600	-5.30774300	H	-3.83949800	-7.08548500	-0.14364000	H	-4.37432000	0.51933000	5.54417000
C	5.77787500	-0.94056000	-4.37676000	H	-5.00371800	-5.37793300	-1.62084000	H	-4.98380000	-1.88022000	5.89887800
O	6.27914000	-2.04435600	-4.55507500	H	-4.13988000	-4.10042100	-0.77680900	H	-6.62660700	-1.55190700	5.35777200
C	3.28348600	-0.67340900	-4.84376200	H	-3.24265200	-5.28218500	-1.73697700	H	-5.80969900	-0.93018700	3.09381900
S	2.84958200	-0.07278800	-3.12331400	H	-1.74539400	-5.80474700	0.23138700	H	-4.14022200	-1.10071300	3.59965700
H	4.88571500	-0.78726300	-6.29477800	H	-2.60593800	-4.63289800	1.23922000	N	-5.77799900	1.71574800	3.75804500
H	4.85156400	0.74104900	-5.38004400	H	-2.43672100	-6.31066300	1.77904200	C	-6.62432600	2.45353000	2.83336200
H	2.58600800	-0.22152000	-5.55196000	C	-3.85414200	3.01445300	-4.08569900	C	-5.93409300	2.66980000	1.48928500
H	3.14323200	-1.75677700	-4.87020200	C	-3.10905100	4.18888000	-3.46102800	S	-5.72239600	1.09372600	0.54130700
N	6.11359800	-0.16855800	-3.28990500	O	-3.26156600	4.54918300	-2.29062500	H	-7.57672000	1.92449100	2.71821100
C	7.04305900	-0.68307900	-2.31036300	C	-2.86580900	1.88789000	-4.47590700	H	-4.85080300	1.43978900	3.45206000
C	6.52589800	-1.88751000	-1.49363500	C	-2.00237200	1.34386200	-3.31931200	H	-6.87015500	3.43769500	3.25370100
O	7.33845000	-2.60329900	-0.89747900	O	-2.44837400	1.32878900	-2.16520700	H	-6.52701100	3.36386300	0.88973900
C	7.50824200	0.42107800	-1.31231800	O	-0.83649400	0.90336000	-3.68735800	H	-4.93631700	3.09317600	1.61067900
C	9.01622300	0.37038700	-1.10349600	H	-4.40792100	3.34265900	-4.97178600	H	-4.63444300	1.48718400	-0.15028400
O	7.06135100	1.72293900	-1.68188800	H	-4.56156400	2.65144100	-3.33974700	Z	0.47258700	-0.34859300	-2.80164000
H	5.57120000	0.65417000	-3.60306200	H	-3.43672700	1.03568300	-4.86560400	C	3.08854900	1.77459600	1.78269400
H	7.90395400	-1.08551800	-2.85235900	H	-2.19924800	2.20287700	-5.28373600	N	1.69748700	1.65952700	1.37996100
H	7.01167100	0.24222300	-0.35682200	N	-2.21203900	4.80642400	-4.26865300	C	4.10052800	0.90761100	1.00337900
H	7.53136300	1.99535500	-2.48242100	C	-1.37800000	5.90886900	-3.80403400	C	0.72251700	1.53294500	2.33372900
H	9.32510800	1.07059300	-0.32155000	C	-0.49846900	6.44994000	-4.92817800	O	4.25811800	-0.37196900	1.509571800
H	9.31568300	-0.64698400	-0.83544100	C	0.49641100	5.45417600	-5.53806400	C	5.39998900	1.76441900	1.06952000
H	9.54269700	0.62974900	-2.02939900	S	1.85332100	4.88850000	-4.44114200	C	-0.60121600	1.47398900	2.00282500
N	5.18769200	-2.04399400	-1.39869400	C	1.08832800	3.47733200	-3.57205300	O	6.42240200	1.16278200	1.87861600
C	4.59015300	-3.20701200	-0.74489900	H	-2.02090600	6.70549500	-3.41457600	C	4.93114000	3.13162700	1.64604100
C	3.07306300	-3.05205400	-0.68808400	H	-2.15912200	4.53477200	-5.23853200	C	-0.97620300	1.40600300	0.60042100
O	2.68681500	-1.94775800	0.13332200	H	-0.76321000	5.56695800	-2.96516400	H	3.49684100	3.10757700	1.57946200
H	4.83266000	-4.12344200	-1.29781500	H	-1.14213400	6.83195500	-5.73362100	C	5.43958600	4.34166600	0.89031200
H	4.57195200	-1.45296800	-1.96029200	H	0.05648200	7.30832100	-4.53778300	C	0.04255700	1.85386100	-0.32211600
H	5.00606600	-3.31693500	0.25822000	H	-0.00215600	4.56391400	-5.93800200	C	1.33912600	1.91198700	0.06824700
H	2.68848800	-2.89930500	-1.70376200	H	1.00376800	5.93118300	-6.38134000	C	-1.67800600	1.43765800	3.03549000
H	2.64371600	-3.98212100	-0.28954800	H	1.90312600	2.83828400	-3.22307000	N	-1.36064100	1.96381100	4.26273900
H	1.84754800	-1.55160600	-0.22017300	H	0.48314000	3.79720700	-2.72126200	O	-2.77552900	0.94274600	2.79301700
C	8.69734100	-5.92181800	1.22249700	H	0.47512500	2.88027600	-4.24767100	H	5.14304200	4.28149900	-0.16024700
C	7.66211000	-5.31087000	2.18776800	C	-3.86443700	5.79353700	1.02369200	H	3.70014100	-1.01159400	1.04960200
C	7.43870900	-3.83439600	2.08923500	C	-2.61795400	4.94474500	0.77703700	H	6.16445900	1.21942400	2.80950500
C	6.30499500	-3.09675900	2.30158400	C	-1.80636000	4.76089100	2.05099800	H	3.13672300	1.48734200	2.84283200
N	8.41628000	-2.91175500	1.74555900	O	-2.97037300	3.64809700	0.29014500	H	3.79374100	0.82242100	-0.04495700
C	7.89086400	-1.67948000	1.69437000	H	-4.41305700	5.92235400	0.09104000	H	1.07065700	1.49431900	3.35876800
N	6.61544300	-1.77438100	2.05349000	H	-3.59363100	6.78742200	1.39712800	H	5.83421300	1.89763100	0.10159800
H	9.34029900	-3.14906300	1.41400000	H	-4.51941800	5.31672900	1.75887500	H	5.23091000	3.19279600	2.70739100
H	8.64635300	-5.57022000	0.19179400	H	-1.99249000	5.44870300	0.02486200	H	-0.24049500	2.09154000	-1.33727700
H	8.51846600	-7.00096700	1.18304900	H	-3.20853500	3.75528600	-0.65180100	H	2.14237000	2.20111600	-0.59544600
H	9.71976200	-5.82791500	1.59436200	H	-0.88930300	4.20017600	1.85260700	H	-2.00391600	1.65127600	0.35385200
H	6.68425800	-5.78048300	2.04530400	H	-1.53034200	5.72972800	2.47480200	H	6.53		

H	-3.65301800	-4.91205900	3.77863400	H	-6.65965700	-1.92865600	0.75194400	C	3.37195600	-2.33658400	4.66532200
H	-2.84539700	-3.33371600	3.62663200	H	-6.48611800	-3.45098700	-0.13239600	C	4.12144100	-3.19425200	5.47908200
EP				H	-6.36019600	-1.90668700	-0.98586200	C	2.74460100	-2.88707700	3.54018500
C	4.73320400	-0.34502000	-5.30773100	C	-6.40989100	-6.53742300	0.59503100	C	4.24837300	-4.54961500	5.18296200
S	5.73150200	-0.97069600	-4.34690400	C	-5.10696600	-5.97556300	1.16700000	C	2.85961600	-4.24106900	3.22933200
O	6.13386400	-2.12253900	-4.47014900	C	-3.91103200	-6.10302300	0.20032700	C	3.62019200	-5.07995300	4.05211700
C	3.27439100	-0.66796000	-4.89359300	C	-4.03037400	-5.14829100	-0.99556300	O	3.79848400	-6.40910300	3.79536500
S	2.82220800	-0.07396600	-3.17609500	C	-2.58334100	-5.86491600	0.93093300	H	3.51481500	0.82122300	6.14333600
H	4.91211900	-0.77591300	-6.29587000	H	-7.22509700	-6.60680000	1.31533300	H	4.47387800	-0.54232700	6.72328800
H	4.86433000	0.74056000	-5.36448600	H	-6.20311400	-7.54403500	0.23203000	H	2.72031600	-0.53583900	6.99607400
H	2.59394800	-0.20594900	-5.61199900	H	-6.76479700	-5.94970500	-0.25834200	H	2.32948200	-0.49342300	4.50704400
H	3.13098600	-1.75044200	-4.92575300	H	-5.22932500	-4.92441200	1.44021300	H	4.04827600	-0.38748700	4.21793500
N	6.11338600	-0.18263900	-3.29662700	H	-4.86475300	-6.51355200	2.09323700	H	4.62259000	-2.80421600	6.35925400
C	7.04305900	-0.68307200	-2.31036600	H	-3.90678800	-7.13361200	-0.18631300	H	2.17908300	-2.24413000	2.87211700
C	6.52267600	-1.91982800	-1.53663900	H	-4.95150700	-5.27277000	-1.56798800	H	4.83011100	-5.21096700	5.81562800
O	7.32467400	-2.69868200	-1.02664200	H	-3.99531900	-4.10672600	-0.65499000	H	2.35999700	-4.64307400	2.35051200
C	7.41406500	0.41755900	-1.27414400	H	-3.18729300	-5.29214900	-1.68579400	H	3.24334800	-6.66940100	3.04909700
C	8.89824200	0.37754800	-0.94476400	H	-1.73072700	-6.01554500	0.25522000	C	-5.42363200	0.21729400	5.66101700
O	6.99325300	1.72268000	-1.68562700	H	-2.52745500	-4.84114700	1.31408200	C	-6.36260200	1.08731600	4.83853100
H	5.73026400	0.74225700	-3.16094600	C	-2.46054400	-6.55509300	1.77307800	O	-7.56530400	1.14819200	5.06921500
H	7.94086200	-1.04510900	-2.82193000	C	-3.85414900	3.01446000	-4.08575200	C	-5.51186900	-1.25096200	5.21343700
H	6.84563300	0.23087200	-0.36370200	C	-3.14297200	4.22071900	-3.47862800	C	-5.03314100	-1.43358300	3.77377800
H	7.64204200	2.06900900	-2.31406000	O	-3.40647600	4.67405800	-2.36044200	H	-5.72757900	0.30774200	6.70705800
H	9.12842400	1.05069800	-0.11440900	C	-2.85946300	1.90015100	-4.47957000	H	-4.38741000	0.56853700	5.57114500
H	9.18747900	-0.64380300	-0.68436200	H	-1.87186500	1.47715600	-3.37682300	H	-4.91029000	-1.86770200	5.89001200
H	9.49489600	0.67255200	-1.81692000	O	-2.06648100	1.80621700	-2.19796200	H	-6.54762700	-1.59168700	5.30266400
N	5.17389300	-2.01839200	-1.36945300	O	-0.87403100	0.77418600	-3.80865000	H	-5.66762700	-0.87676000	3.07940300
C	4.59014700	-3.20700800	-0.74490200	H	-4.28041000	3.32422900	-4.96590600	H	-4.01654400	-1.04684300	3.64294700
C	3.08327100	-3.07684000	-0.60915300	H	-4.55224200	2.65365600	-3.32945600	N	-5.78660300	1.75549200	3.79554900
O	2.64207200	-1.94756400	0.15434100	H	-3.41665000	1.00233400	-4.77244600	C	-6.62427600	2.45355100	2.83333800
H	4.80501400	-4.10288400	-1.34303000	H	-2.27064100	2.17379500	-5.36177500	C	-5.87100700	2.1863000	1.53263000
H	4.56652100	-1.44459900	-1.95291900	N	-2.17792600	4.77511200	-4.25099300	S	-5.47667800	1.16683300	0.60349300
H	5.06181100	-3.35590900	0.22955000	C	-1.37798800	5.90887500	-3.80399300	H	-7.53568300	1.87069900	2.66266200
H	2.62980900	-2.97990800	-1.60289400	C	-0.51159800	6.46212600	-4.93145800	H	-4.82379200	1.55926900	3.54844400
H	2.69945800	-3.99427800	-0.14414700	C	0.51899500	5.48914500	-5.51949400	H	-6.94767600	3.41974400	3.24232900
H	1.36198500	-1.29711400	-0.54645200	S	1.80710200	4.89231100	-4.35723200	H	-6.47023600	3.37058400	0.89389600
C	8.69732700	-5.92183100	1.22250500	C	0.101572700	3.40478000	-3.65624700	H	-4.91883900	3.21324200	1.72577700
C	7.64665900	-5.32267000	2.18042200	H	-2.05211700	6.68527000	-3.42970100	H	-4.48792000	1.71179800	-0.13377700
C	7.39138400	-3.84786000	2.09830000	H	-2.02028200	4.40713700	-5.17644000	Z	0.49026100	-0.42311700	-2.96902800
C	6.25395100	-3.18120500	2.35258100	H	-0.74893100	5.60578800	-2.95886900	C	3.19758400	1.70086900	1.92904600
N	8.34029800	-2.90543200	1.74954000	H	-1.15881400	6.81611700	-5.74594100	N	1.76703600	1.66322600	1.54684100
C	7.75777400	-1.68086600	1.75077200	H	0.01615600	7.33950900	-4.54530600	C	4.20368400	0.87238300	1.09664600
N	6.49145800	-1.77112000	2.12547800	H	0.04939200	4.60977900	-5.97565700	C	0.84766100	1.59116100	2.54191400
H	9.25516000	-3.11435000	1.37921400	H	1.06786300	5.99310900	-6.31970600	O	4.29681300	-0.41570300	1.64740000
H	8.64635000	-5.57022400	0.19179300	H	1.80703500	2.82104900	-3.18039700	C	5.48220400	1.78152800	1.19061000
H	8.52590500	-7.00300100	1.17729700	H	0.23916800	3.64576000	-2.92746400	C	-0.50210900	1.70516800	2.26750100
H	9.71976100	-5.82788300	1.59435600	H	0.58815900	2.78150200	-4.44288500	O	6.60411300	1.17435600	1.79164100
H	6.68107400	-5.81279800	2.01840800	C	-3.86444900	5.79346400	1.02370300	C	5.01679000	3.05090500	1.94481200
H	7.93251900	-5.58451900	3.20799200	C	-2.56307300	5.05777300	0.74355600	C	-0.90359200	1.87265900	0.93523100
H	5.29245100	-3.47042200	2.68992000	C	-1.75412600	4.87335700	2.02000100	O	3.57631800	3.04293000	1.83323700
H	8.26694500	-7.70214800	1.47701100	O	-2.82954500	3.77247800	0.18022600	C	5.54439000	4.35756800	1.39648100
H	5.23894100	-0.81537700	1.76196500	H	-4.41305500	5.92240300	0.09104600	C	0.05902600	1.99313300	-0.06721300
C	-2.28482800	-4.32151400	-7.00554800	H	-3.67151500	6.78839900	1.44038700	C	1.39575700	1.09608900	0.26092900
C	-3.02586500	-8.82411100	-5.75444100	H	-4.48451900	5.24042300	1.73323600	C	-1.55622300	1.63325300	3.34366900
C	-2.05817800	-3.30865900	-4.74430400	H	-1.96944600	5.64511200	0.02680100	N	-1.19497000	2.12685400	4.56061700
C	-1.42048200	-2.10006200	-4.64564200	H	-3.09247500	3.90779500	-0.75382600	O	-2.65062600	1.13886200	3.10501900
N	-1.48842800	-4.09328600	-3.75378500	H	-0.77277600	4.43885100	1.81782500	H	5.26209300	4.46890300	0.36574700
C	-0.55669600	-3.36252800	-3.09621300	H	-1.59540800	5.83701600	2.50961700	H	3.35815600	-1.52159300	0.68555900
N	-0.49219700	-2.14770200	-3.62216100	H	-2.30087000	4.22578700	2.71400500	H	6.33217200	0.64454400	2.55524400
H	-1.59316800	-5.13284100	-6.75874200	C	2.09816600	8.09056500	-0.71453600	H	3.24207800	1.32164800	2.95777800
H	-1.70374900	-3.51141200	-7.45455100	C	2.24415800	6.84635200	0.17740800	H	3.89287800	0.80875200	0.04559500
H	-2.98965000	-4.69525700	-7.75390700	C	1.22181400	6.85913900	1.31966400	H	1.23765600	1.42684500	3.38253300
H	-3.70738400	-3.01331000	-6.02633400	C	2.13514000	5.54446100	-0.62625800	H	5.80025600	2.05820400	0.18422300
H	-3.64781100	-4.61347500	-5.31770000	H	2.89253900	8.12229900	-1.46791000	H	5.28457400	2.93508700	3.00665200
H	-1.77452700	-5.03302700	-3.51633600	H	2.17449400	8.99441500	-0.11022100	H	-0.27327000	2.13475100	-1.08977500
H	-1.56974200	-1.19576300	-5.21265400	H	1.14785400	8.08276700	-1.25272000	H	2.19275600	1.98163500	-0.46509300
H	0.01617900	-3.72015700	-2.25625800	H	3.24799000	6.87786900	0.62613600	H	-1.95265800	1.97652900	0.69319000
C	-6.31619300	-2.26987100	-4.51584900	H	1.34177600	5.98444100	1.96923400	H	6.63538800	4.36703900	1.46865100
C	-6.97577900	-3.12930000	-3.45006200	H	1.32154100	7.75472200	1.94157300	H	-0.33873300	-0.51497000	0.85601400
O	-6.47280400	-4.19038800	-3.08583300	H	0.19991600	6.84140700	0.92253800	H	5.14887500	5.20732600	1.95837500
C	-5.10072800	-1.53897100	-3.92315300	H	2.83698300	5.52620700	-1.46537800	H	-1.91937500	2.15107500	5.26631400
H	-7.02072400	-1.55027900	-4.94797300	H	2.33895000	4.67877600	0.01461900	H	-0.46954800	2.82374900	4.64790200
H	-5.99640000	-2.94094700	-5.31789600	H	1.12835800	5.43027900	-1.04719900	C	-2.75176500	-1.64517800	0.73713400
H	-4.41970700	-2.25500500	-3.45650000	C	-0.46746700	4.99172500	6.68455800	O	-1.85088300	-2.56676500	1.41444100
H	-4.55011100	-0.99751600	-4.69890500	C	-1.07292400	5.88476000	5.59409700	C	-0.61573600	-2.61716600	0.72135000
H	-5.40753500	-0.81709200	-3.15921400	C	-2.33093400	6.60031300	6.09745500	C	-0.53122700	-1.23946600	0.06126300
N	-8.11553500	-2.60817700	-2.92095200	C	-0.04113100	6.88271300	5.05592300	C	-1.95913500	-1.07454000	-0.44555700
C	-8.76837500	-3.17179200	-1.75225300	H	-0.20884800	5.55750200	7.57942700	O	0.46868600	-1.08547200	-0.94887300
C	-8.40264200	-2.46192100	-0.43282600	H	0.42416400	4.48172200	6.31896400	H	-3.65561100	-2.18115900	0.44115000
C	-9.13324100	-3.14268400	0.73043500	H	-1.18546800	4.22497600	7.00298200	H	-3.03252200	-0.86468300	1.4

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