

Electronic Supplementary Information for

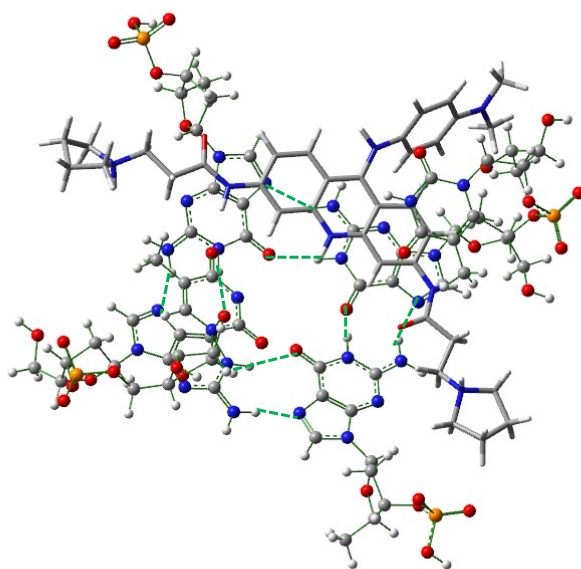
**Exploiting hydrogen bonding interactions to probe smaller linear
and cyclic diamines binding with G-quadruplexes: A DFT and
Molecular Dynamics Study**

Mrinal Kanti Si^{1,2}, Anik Sen¹ and Bishwajit Ganguly^{1,2*}

¹*Computation and Simulation Unit (Analytical Discipline and Centralized Instrument Facility),
CSIR-Central Salt & Marine Chemicals Research Institute, Bhavnagar, Gujarat, India-364 002*

²*Academy of Scientific and Innovative Research, CSIR-CSMCRI, Bhavnagar, Gujarat, India-364
002.*

**Corresponding Author. Fax: (+91)-278-2567562, E-mail: ganguly@csmcri.org*

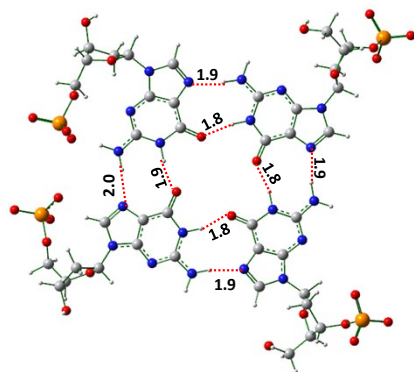


BRACO-DNA complex: B.E = -46.72

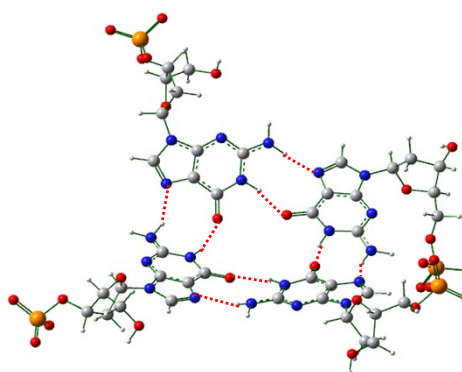
Figure S1. Modeled crystal structure of BRACO-19-Quadruplex-DNA complex and single point energy calculated at RHF/3-21G* level of theory is given in Kcal/mol.

Table S1. Calculated binding free energies (ΔG) and enthalpies (ΔH) of diamine-G-tetrad complexes optimized at B3LYP/6-31G(d) level of theory in aqueous phase. ΔE_1 is the binding energies, calculated with MPW1PW916-31+G(d)//B3LYP/6-31G(d) level of theory in aqueous phase. (All energies are given in Kcal/mol)

Complexes	ΔG	ΔH	ΔE_1
L-1	-8.30	-24.87	-16.36
L-2	-41.38	-58.90	-41.82
L-3	-50.30	-61.83	-44.33
1,2-CBDA-1	-15.52	-31.69	-24.51
1,2-CBDA-2	-45.19	-62.00	-47.01
1,3-CBDA-1	-15.63	-30.14	-22.93
1,3-CBDA-2	-41.43	-58.76	-23.62
1,2-CPDA-1	-19.36	-34.17	-25.90
1,2-CPDA-2	-50.57	-65.05	-47.01
1,3-CPDA-1	-15.49	-25.98	-23.62
1,2-CHDA-1	-18.89	-34.64	-25.96
1,2-CHDA-2	-78.31	-89.44	-62.27
1,3-CHDA-1	-8.19	-23.69	-19.09
1,3-CHDA-2	-16.73	-34.32	-25.02
1,4-CHDA-1	-66.21	-77.10	-50.26

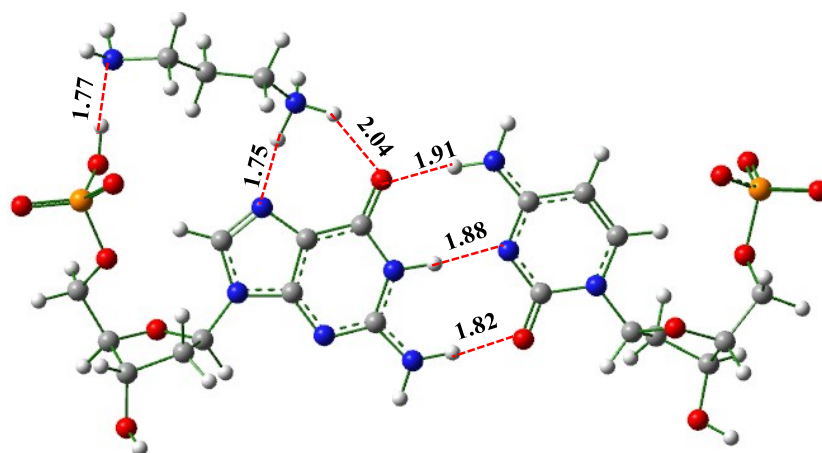


Planar structure G-tetrad



concave structure G-tetrad

Figure S2. The optimized structure of planar G-tetrad and concave G-tetrad complex at B3LYP/6-31G(d) level of theory in aqueous phase.



B.E = -42.3 Kcal/mol

Figure S3. The Diprotonated Linear Diamine Interactions with major groove of Cytosine-Guanine base pair at M06-2X/6-31+G(d)//B3LYP/6-31G(d) level of theory. (B.E = binding energy).

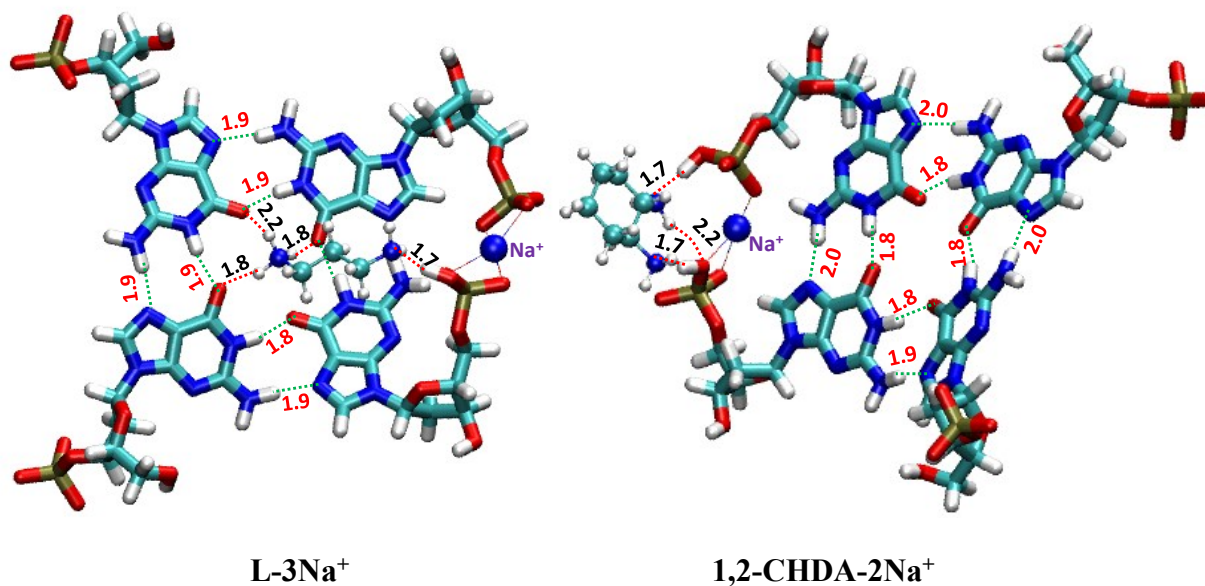


Figure S4. The optimized structure of Diprotonated Linear Diamine and 1,2-CHDA ligand interacted with G-tetrad in presence of sodium metal ion.

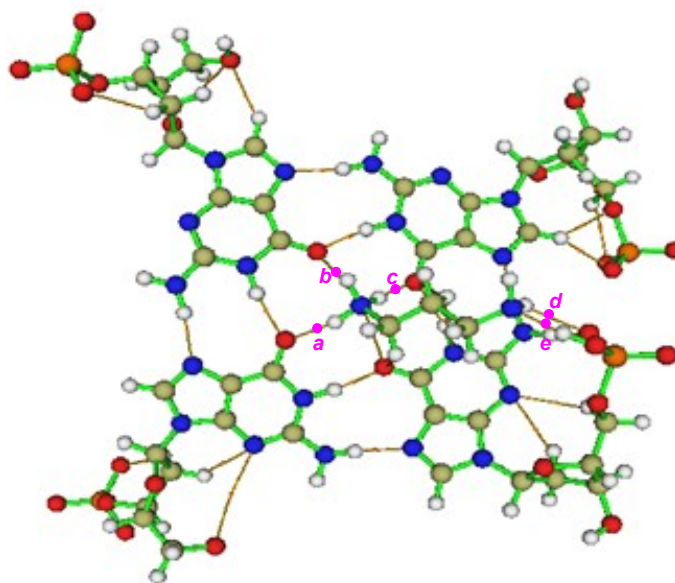
Table S2. Calculated binding free energies (ΔG) and enthalpies (ΔH) of linear diamine in **L-3Na⁺** and 1,2-CHDA in **1,2-CHDA-2Na⁺** complexes at B3LYP/6-31G(d) level of theory in aqueous phase. ΔE_1 and ΔE_2 are the binding energies calculated at MPW1PW91-31+G(d)//B3LYP/6-31G(d) and M06-2X/6-31+G(d)//B3LYP/6-31G(d) level of theory in aqueous phase respectively. (All energies are given in Kcal/mol)

Complex	ΔG	ΔH	ΔE_1	ΔE_2
L-3Na ⁺	-38.38	-55.06	-39.09	-49.92
1,2-CHDA-2Na ⁺	-53.49	-64.79	-50.90	-56.51

Table S3. Table for binding energy for linear diamine, 1,2-CHDA-1, 1,2-CHDA-2 and BRACO-19 (Single point energy calculated at RHF/3-21G* level of theory in water)

	Binding Energy (B.E)
Linear-Diamine (L-1)	-41.90
1,2-CHDA-1	-50.42
1,2-CHDA-2	-66.49
BRACO-19	-46.72

We have taken the optimized complex structures of linear diamine (Table 1), 1,2-CHDA-1 (Table 2), 1,2-CHDA-2 (Table 2) at B3LYP/6-31G(d) level of theory in aqueous solvent.



L-3

Figure S5. Results of the QTAIM analysis for a critical point (3,-1) of the non-covalent interaction between lineardiamine and G-tetrad at M06-2X/aug-cc-pVQZ//B3LYP/6-31G(d) method.

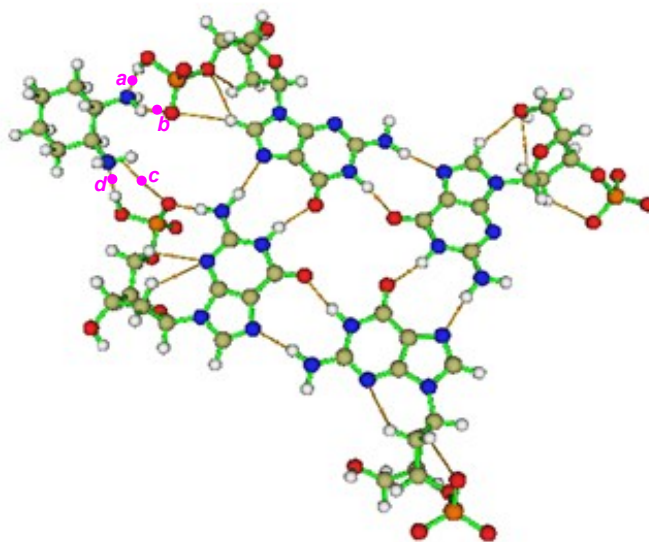


Figure S6. The QTAIM analysis for a critical point (3,-1) of the non-covalent interaction between 1,2-CHDA and G-tetrad at M06-2X/aug-cc-pVQZ//B3LYP/6-31G(d).

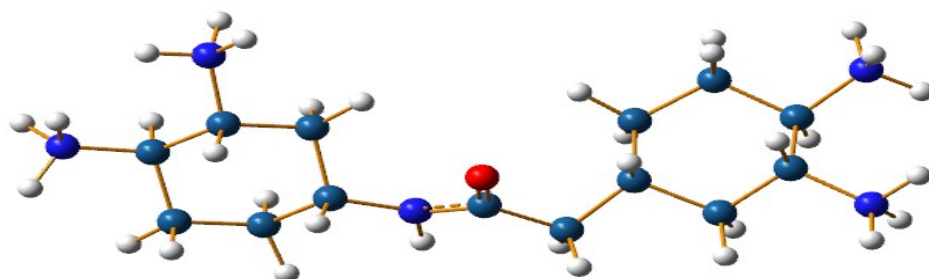


Figure S7. The optimized structure of N,2-bis (3,4-diaminocyclohexyl)acetamide at B3LYP/6-31G(d) level of theory. (carbon = grey, hydrogen = white, nitrogen = blue, and oxygen = red)

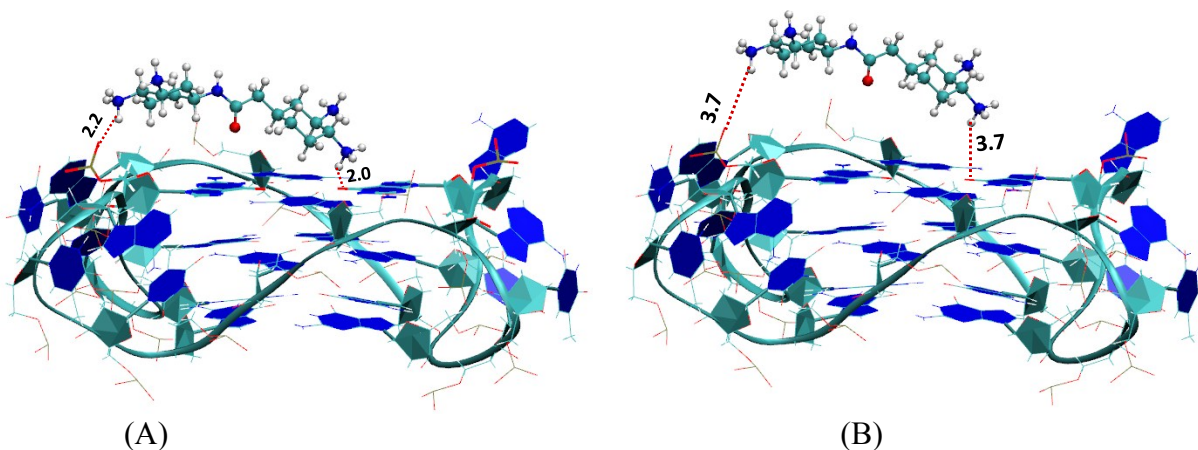
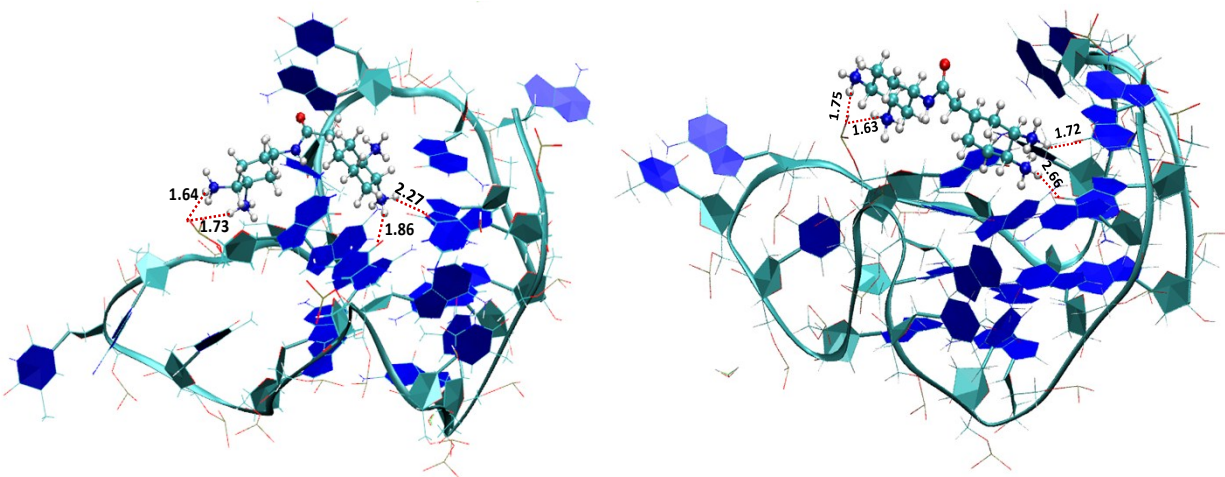


Figure S8. The initial geometry taken for molecular dynamics simulations (A) N,2-bis (3,4-diaminocyclohexyl)acetamide interacted with phosphate backbone and base pair. (B) N,2-bis (3,4-diaminocyclohexyl)acetamide is placed at the longer distance from the G-quadruplex-DNA.

Table S4. Average Binding Energy and its Components Obtained from the MM-PBSA Calculations for the complex of ligand 9 with G-quadruplex-DNA.

Energy component	Energy (kJ/mol)
van der Waal energy	-70.801 +/- 18.387
Electrostatic energy	-8562.656 +/- 422.879
Polar solvation energy	824.980 +/- 153.081
SASA energy	-9.815 +/- 1.764
SAV energy	0.000 +/- 0.000
WCA energy	0.000 +/- 0.000
Binding energy	-7818.291 +/- 291.693



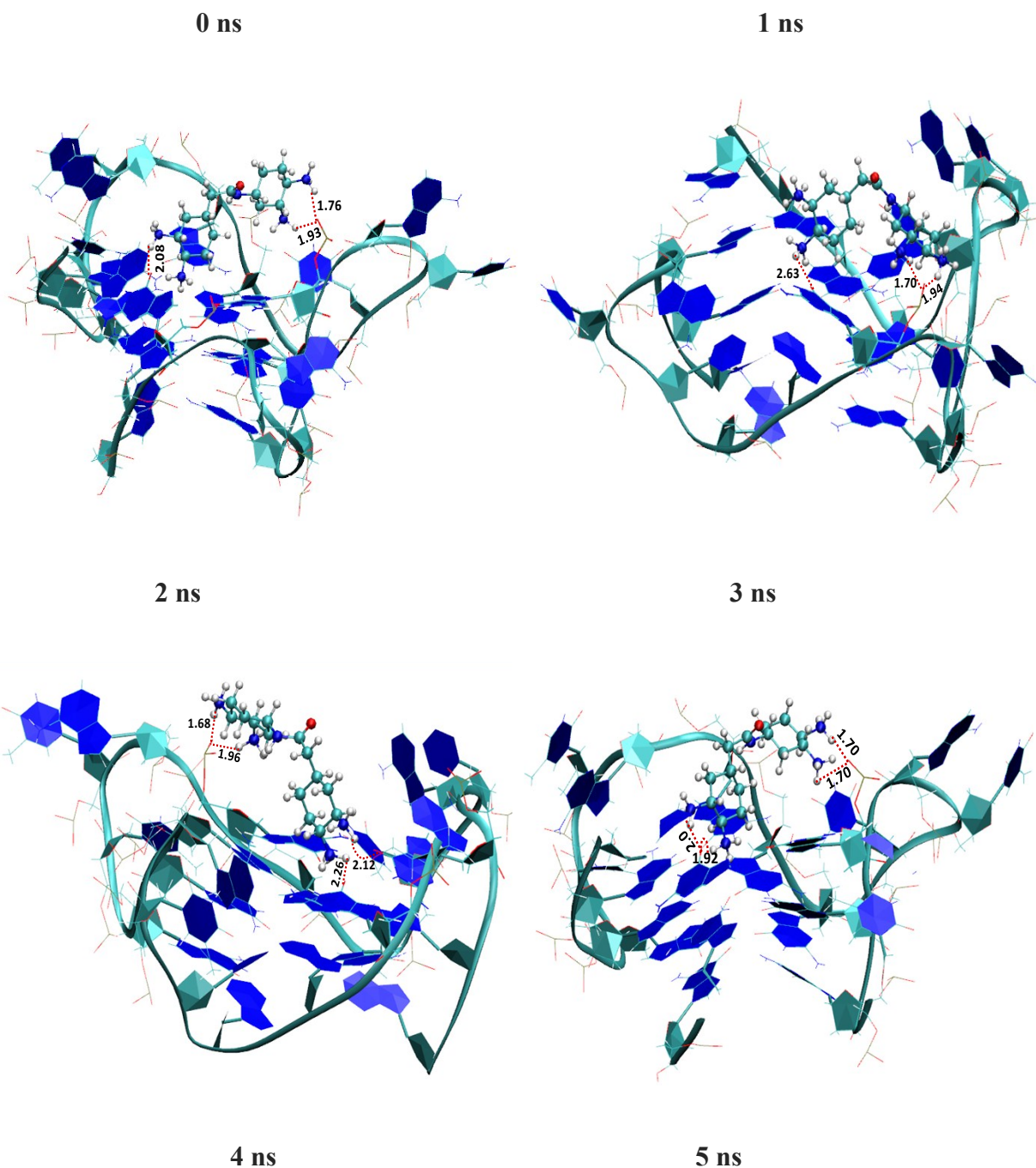


Figure S9. The complexes of G-quadruplex-DNA and modelled compound of two 1,2-CHDA are shown at different time intervals when the ligand is placed at the longer distance from the top of the stack of propeller polymorph of G-quadruplex-DNA.

Table S5. B3LYP/6-31G(d) optimized Cartesian co-ordinate of complex of linear diamine, CBDA, CPDA and CHDA in solvent phase and corresponding electronic energies (E) are given in atomic unit.

L-1				L-2			
E = 6350.58058				E = 6350.61858			
O	-5.39648300	7.96065900	-1.10941900	O	3.65288800	9.39765800	0.86558000
C	-6.56311300	7.66371300	-1.88159100	C	4.44725400	9.52910500	2.04774400
C	-7.48798500	6.61594500	-1.26224900	C	5.66923500	8.61269800	2.10088200
O	-6.82343200	5.33083000	-1.23755800	O	5.24357700	7.23482200	2.20391900
C	-7.94887100	6.88779000	0.18388800	C	6.61708100	8.68385600	0.88664400
O	-9.25411200	6.38500600	0.34439200	O	7.93893500	8.49194400	1.33382000
C	-6.92417700	6.09008900	1.00941200	C	6.12698800	7.51331900	0.01676600
C	-6.62529800	4.89362000	0.10055300	C	5.65065400	6.49473300	1.05737100
N	-5.25724800	4.38118700	0.21817200	N	4.52686200	5.66868300	0.61573800
C	-4.09565500	5.05911700	-0.10425900	C	3.26686000	6.11586500	0.26537500
N	-3.01207100	4.34019100	0.07708800	N	2.45084200	5.13994500	-0.06114800
C	-3.47978600	3.11768000	0.53363400	C	3.20552400	3.98686500	0.08489600
C	-2.78623300	1.94948800	0.92427300	C	2.85935200	2.62004300	-0.12233800
O	-1.53875600	1.78555400	0.99679900	O	1.77740200	2.14629600	-0.50769700
N	-3.64526300	0.90790300	1.28431100	N	3.93496000	1.76322700	0.17107800
C	-5.02472900	1.00813500	1.32351200	C	5.18078300	2.17156100	0.59600700
N	-5.71527800	-0.06729700	1.76368800	N	6.08351500	1.20480900	0.87861200
N	-5.67931200	2.11856800	1.00384300	N	5.51134000	3.44658700	0.77265100
C	-4.87534400	3.12309000	0.61662000	C	4.49600700	4.29538600	0.51469500
O	-9.45372600	6.19806100	2.93627900	O	9.20709400	7.58575100	-0.75562500
P	-10.13800300	6.90927200	1.75637000	P	9.22241700	8.79984200	0.19029900
O	-11.53614700	6.39004600	1.40912000	O	10.42267700	8.86595000	1.13900100
O	-9.97137000	8.43596100	1.74467000	O	8.81806200	10.12842000	-0.46600000
O	7.98232500	-0.36893600	1.33025700	O	-6.96826000	-2.04018700	-0.22884300
P	8.70879000	-1.05739000	2.51715800	P	-8.04824500	-3.07084500	-0.62581600
O	8.16974200	-0.68907000	3.89971100	O	-8.38320200	-3.13880600	-2.10558300
O	10.23256000	-1.05673000	2.36441800	O	-9.26957600	-3.00627200	0.33191600
O	8.25003900	-2.71391600	2.40390900	O	-7.35642800	-4.59586600	-0.32977100
C	8.37356400	-3.28965100	1.12654600	C	-6.93689200	-4.85514100	0.99537900
C	8.07677200	-4.78550100	1.17531600	C	-6.27683800	-6.22740300	1.08142500
O	6.75119800	-5.07835400	1.70157900	O	-5.05838600	-6.30015000	0.28994300
C	8.10589800	-5.43648700	-0.22054100	C	-5.86255500	-6.60177000	2.52086000
O	8.59286600	-6.77898600	-0.20247000	O	-6.06261400	-7.98263600	2.82044800
C	6.63531800	-5.33700100	-0.64904300	C	-4.38794900	-6.18155700	2.55423000
C	5.89339800	-5.55297000	0.67684000	C	-3.92598100	-6.48787800	1.12416800
N	4.58555500	-4.90152700	0.76156000	N	-2.80901200	-5.66534000	0.65971400
C	3.37610700	-5.56557600	0.86156100	C	-1.53748800	-6.13138100	0.38590500
N	2.34107100	-4.76556900	0.92144800	N	-0.69904400	-5.18425000	0.03870900
C	2.88887000	-3.49158700	0.86199900	C	-1.45466500	-4.02477600	0.07497800
C	2.27973100	-2.21852400	0.94105000	C	-1.09397100	-2.67443500	-0.21900100
O	1.05236800	-1.96719900	1.11802400	O	0.01434600	-2.22956400	-0.55797600
N	3.19023400	-1.17209900	0.84257500	N	-2.19193600	-1.80661700	-0.09435800
C	4.57140900	-1.32477100	0.74334800	C	-3.46370600	-2.18795900	0.26207800
N	5.33876000	-0.23585900	0.72797700	N	-4.43864000	-1.22093400	0.31619100
N	5.14370100	-2.53374000	0.68406800	N	-3.78791300	-3.43083100	0.57630200
C	4.28416700	-3.55093500	0.75922100	C	-2.76651700	-4.29957200	0.45607400
				O	5.80237400	-7.57156100	-2.95949900

O	-3.32526100	-9.03124700	-0.43156200	C	7.10333400	-7.23805800	-3.43704800
C	-4.63543900	-9.35700300	0.02572800	C	7.98188800	-6.49618200	-2.43373700
C	-5.71387200	-8.34217300	-0.34350800	O	7.46356700	-5.16053300	-2.23551000
O	-5.50990600	-7.12372700	0.41122400	C	8.09928400	-7.14832100	-1.02741600
C	-5.77574800	-7.93562100	-1.84169200	O	9.45738600	-7.17529500	-0.65436800
O	-7.12103000	-7.95394700	-2.25910100	C	7.26752600	-6.19725500	-0.14531700
C	-5.19528400	-6.50867500	-1.82588900	C	7.52676900	-4.86616300	-0.84233400
C	-5.69968400	-6.02249100	-0.47256000	N	6.61638700	-3.76872600	-0.54621900
N	-5.06081800	-4.84202700	0.09632600	C	7.03008800	-2.47791900	-0.27158600
C	-5.75722800	-3.79877200	0.67905400	N	6.04147700	-1.64171700	-0.07441900
N	-4.98600700	-2.86635300	1.17803500	C	4.90275900	-2.41299000	-0.23638400
C	-3.70092000	-3.30948200	0.91841300	C	3.52713300	-2.04542000	-0.14579400
C	-2.45074900	-2.72344500	1.24433500	O	3.04175100	-0.93025900	0.10632900
O	-2.24472400	-1.66059800	1.88058300	N	2.68167300	-3.13867300	-0.38759000
N	-1.37552000	-3.49003500	0.78373000	C	3.10677900	-4.41712800	-0.67188400
C	-1.49501200	-4.70921300	0.14503100	N	2.15060300	-5.34243000	-0.91938200
N	-0.34972800	-5.31878400	-0.22691800	N	4.38665600	-4.76229500	-0.75162800
N	-2.66357800	-5.27229700	-0.13640400	C	5.23290800	-3.73569300	-0.53454900
C	-3.72167100	-4.53836100	0.25069900	P	9.89521600	-8.18286600	0.70256500
P	-7.42503100	-7.91165400	-3.97842800	O	11.41769700	-8.21312200	0.54069900
O	-8.92828900	-8.20348600	-3.99481800	O	9.16776300	-9.50671000	0.42219300
O	-6.52434500	-9.02453600	-4.53452800	O	9.39020700	-7.42032800	1.93900100
O	-7.03389100	-6.48914300	-4.41442700	O	-9.72589500	1.60162900	0.62216900
O	8.75650400	2.36822300	-3.19317800	P	-9.63801600	1.91382300	-0.90575400
P	8.90885800	3.27826000	-1.96809800	O	-10.92311800	2.51152400	-1.47531800
O	10.33414800	3.77869500	-1.70010200	O	-8.95014900	0.83681500	-1.73783200
O	8.14274100	2.82880900	-0.71045500	O	-8.47188400	3.17943300	-0.97010600
O	8.01644000	4.71452900	-2.36870000	C	-8.73529900	4.34166700	-0.21834200
C	7.77973400	5.04678400	-3.71062800	C	-7.77834700	5.46216200	-0.60606200
C	6.47957300	5.83419100	-3.83743700	O	-6.42017000	5.13443300	-0.22715000
O	5.34832800	4.99076500	-3.50757600	C	-7.72462600	5.77320200	-2.10860200
C	6.37409800	7.05230900	-2.90742600	O	-7.46376800	7.17489000	-2.23526300
O	5.59209800	8.03874400	-3.59207200	C	-6.54548700	4.92316000	-2.58731900
C	5.64028200	6.48081500	-1.69327000	C	-5.60215600	4.95007000	-1.37594700
C	4.68618400	5.47454300	-2.34663800	N	-4.80288100	3.73990300	-1.21082000
N	4.30496400	4.35645900	-1.49066500	C	-5.26357400	2.44379600	-1.04012700
C	5.12767000	3.42600500	-0.86542200	N	-4.29241400	1.58485700	-0.82885100
N	4.44135300	2.54620800	-0.16784100	C	-3.13366800	2.34592000	-0.85325200
C	3.11329000	2.90010900	-0.34301600	C	-1.77119900	1.96906100	-0.67393100
C	1.92280600	2.33086100	0.18501600	O	-1.30215900	0.83919300	-0.45623500
O	1.79973400	1.36059100	0.96006700	N	-0.90780600	3.07475300	-0.76906600
N	0.77704100	3.01614700	-0.26011700	C	-1.30712200	4.37351100	-0.99956000
C	0.78133500	4.12934900	-1.07434300	N	-0.33807600	5.31033200	-1.10152300
N	-0.42220100	4.64797400	-1.41790200	N	-2.57824200	4.72824900	-1.16080800
N	1.89274800	4.67083700	-1.55276900	C	-3.43154000	3.68805500	-1.08091200
C	3.01006400	4.01997800	-1.16764200	H	4.77515500	10.56988700	2.18308500
H	-7.14128700	8.57710400	-2.08188900	H	3.78251800	9.27695600	2.87997800
H	-6.19471800	7.28416600	-2.83985400	H	6.23242700	8.85753000	3.01003300
H	-8.36935000	6.52245200	-1.90819300	H	6.53891000	9.64302300	0.35536700
H	-7.92821500	7.95899700	0.43014200	H	6.94933200	7.14365200	-0.59919200
H	-7.36230600	5.80812900	1.96860700	H	5.28846000	7.81445900	-0.61913000

H	-6.00835200	6.66766300	1.17160000	H	6.43922100	5.78711400	1.33092500
H	-7.27288300	4.03839000	0.31620600	H	3.02618100	7.17055400	0.29441100
H	-4.13673600	6.07367600	-0.47983700	H	7.02251700	1.53479300	1.05598300
H	-6.71767800	0.01721400	1.65082200	H	-7.80348200	-4.85806800	1.67550500
H	9.40584600	-3.18273600	0.74883200	H	-6.23413100	-4.08470000	1.33304400
H	7.69917900	-2.79698600	0.41808000	H	-6.96418100	-6.98154200	0.67974000
H	8.79025900	-5.27924800	1.84562500	H	-6.45475500	-6.06439700	3.26537400
H	8.76803600	-4.90179400	-0.90596200	H	-4.30608400	-5.10743700	2.74387500
H	6.42014600	-4.33750500	-1.03632700	H	-3.81420500	-6.72274100	3.30980700
H	6.36887700	-6.07823900	-1.40579400	H	-3.56339300	-7.52050900	1.03500300
H	5.67849500	-6.61706400	0.84008400	H	-1.29856300	-7.18342800	0.46509900
H	3.33395400	-6.64656400	0.87597100	H	-4.26096600	-0.35100100	-0.20543800
H	4.94450100	0.70170800	0.61919000	H	6.94609000	-6.60169500	-4.31427200
H	-4.56416600	-9.42140100	1.11662400	H	7.64499000	-8.13636200	-3.77055700
H	-4.95039500	-10.34410700	-0.34562100	H	8.99291500	-6.42331400	-2.85763900
H	-6.68819100	-8.76728900	-0.06680000	H	7.69696700	-8.17102700	-1.00635800
H	-5.18494100	-8.60770000	-2.48062500	H	6.20204400	-6.43450300	-0.20264700
H	-4.10230800	-6.52383100	-1.82173000	H	7.62290000	-6.23432100	0.88582900
H	-5.57913900	-5.94180800	-2.67553600	H	8.52588300	-4.49246600	-0.58141100
H	-6.76609200	-5.76996800	-0.53654200	H	8.08199900	-2.22982800	-0.22613300
H	-6.83889200	-3.79141600	0.68990000	H	1.18704400	-5.22739000	-0.58225400
H	0.54526700	-5.10636900	0.23292100	H	-9.76451200	4.69407100	-0.39081400
H	8.58984600	5.67539900	-4.12982700	H	-8.63007200	4.14682700	0.86011100
H	7.71616700	4.14235000	-4.32849300	H	-8.06130700	6.36907900	-0.05791000
H	6.35920700	6.16274300	-4.87775000	H	-8.66101900	5.50391300	-2.61206900
H	7.36187800	7.45261200	-2.64853300	H	-6.06967500	5.31954600	-3.48914500
H	5.10875400	7.23990700	-1.11124600	H	-6.88544200	3.90388100	-2.78001600
H	6.35365300	5.95935600	-1.05242400	H	-4.87399900	5.76374200	-1.44491500
H	3.74065600	5.94848800	-2.62885800	H	-6.32301800	2.21970800	-1.07661800
H	6.21915400	3.42544100	-0.95844400	H	-0.66929100	6.26489600	-1.13576800
H	-0.37370100	5.53761100	-1.89682300	H	-5.39293600	-1.61451300	0.10901800
H	6.37479100	-0.34499600	0.92063700	H	2.48845200	-6.29256600	-0.99352900
H	-0.46266500	-6.25891200	-0.58218500	H	5.99677100	0.24810000	0.51417100
H	-5.34983000	-1.02341500	1.65747100	H	0.61035800	5.16846000	-0.72880700
H	-1.25495500	4.50261500	-0.83470200	H	5.90869000	-8.25893800	-2.28295200
H	-3.31967000	-9.13196900	-1.39656400	H	4.12505900	9.83355000	0.13866500
H	-5.66552800	8.51885300	-0.36284000	H	-5.66894400	-8.51462400	2.10975900
H	8.14808500	-7.25637600	0.51693300	H	-7.36986500	7.36807000	-3.18216900
H	5.46536900	8.78336000	-2.98183300	H	3.72606200	0.75303000	0.10556500
H	-3.19727000	0.01856700	1.54927300	H	0.09815100	2.85764000	-0.66925100
H	-0.12024700	2.62419600	0.05231700	H	-1.98932200	-0.80843900	-0.28146500
H	2.78845700	-0.22306500	0.90864600	H	1.67069300	-2.92081600	-0.40359200
H	-0.43902100	-3.06639000	0.87735600	N	-5.07175500	0.10179400	2.80155600
N	-0.01972500	-1.93129500	3.66051100	H	-5.10734600	1.09012000	2.53228000
H	0.51501200	-2.03125800	2.76417700	H	-4.79810900	-0.44635700	1.93387200
H	-1.01183200	-1.91023100	3.35722400	H	-4.31704400	0.00474800	3.48738600
H	0.14199400	-2.75829000	4.24093400	C	-6.39239100	-0.35537900	3.36706700
C	0.37725800	-0.66103600	4.35582700	H	-6.25267400	-1.39801900	3.66218500
H	0.05522500	-0.72795100	5.39591300	H	-6.57642100	0.24008500	4.26466700
H	1.46818100	-0.61589200	4.32965800	C	-7.48642300	-0.20607600	2.31766900
C	-0.27494400	0.51007700	3.62404100	H	-7.59874600	0.84235000	2.01982900

H	-0.25486300	0.32638400	2.54685600	H	-7.22528700	-0.78814100	1.42269000
H	-1.32650300	0.57940100	3.92639500	C	-8.83662000	-0.71600000	2.82549300
C	0.44489400	1.82787200	3.88643700	H	-9.25633900	-0.05576100	3.59020500
H	1.41619600	1.83794100	3.39133400	H	-8.74516800	-1.71969100	3.25348900
H	0.56700000	2.05583400	4.94673000	N	-9.78701500	-0.79130600	1.68144200
N	-0.35821600	2.95085100	3.27760900	H	-9.52905600	-1.63580300	1.04338100
H	-1.15043200	3.20996500	3.87367900	H	-10.73577400	-0.95826600	2.02248900
H	0.20756700	3.79482800	3.14793100	H	-9.78638500	0.16015800	1.13502400
H	-0.75307100	2.65750900	2.35213100			L-3	
CBDA-T1				E = -6350.63092			
E = -6388.64854				O	-4.21679000	8.94068300	-0.54300000
O	-4.15274800	9.08983600	0.14288600	C	-5.47770600	8.97885500	-1.21704100
C	-4.93911600	9.23955200	-1.04263600	C	-6.52610200	8.01442200	-0.66336700
C	-6.03644400	8.19014500	-1.21517300	O	-6.11453400	6.64981100	-0.91039600
O	-5.43990500	6.88852800	-1.42324200	C	-6.80470900	8.11424500	0.84992800
C	-7.01424900	8.03494300	-0.03284100	O	-8.16749200	7.84220700	1.07735000
O	-8.29405100	7.73238200	-0.53655600	C	-5.89208100	7.01696500	1.42495200
C	-6.40706400	6.85507500	0.74526100	C	-5.88966500	5.96169300	0.31421500
C	-5.77594200	6.00421300	-0.36218600	N	-4.63301300	5.21730300	0.20224600
N	-4.56105700	5.29735400	0.05391300	C	-3.39737000	5.74043000	-0.12930300
C	-3.37558800	5.87679300	0.46729900	N	-2.45139600	4.83069900	-0.17155800
N	-2.45788500	4.99469600	0.78638000	C	-3.09208600	3.64297700	0.14184700
C	-3.05922000	3.76630100	0.56427600	C	-2.58524600	2.32182800	0.26676400
C	-2.57743300	2.45101800	0.76191500	O	-1.40724000	1.92984500	0.13656900
O	-1.45786700	2.10704600	1.22260400	N	-3.59471000	1.40230700	0.58928800
N	-3.51571000	1.47906200	0.39463600	C	-4.92282600	1.72127200	0.78997600
C	-4.79072400	1.75127900	-0.07144700	N	-5.75131200	0.71459700	1.14495100
N	-5.56493900	0.70452400	-0.40461400	N	-5.39561400	2.95864100	0.69270500
N	-5.26069900	2.98622900	-0.21895000	C	-4.45181700	3.86371100	0.37037700
C	-4.36727400	3.93744700	0.09893900	O	-8.21863200	7.14714500	3.58615600
O	-9.47967500	6.70161100	1.54257300	P	-8.80372800	8.22558400	2.65784400
P	-9.63538600	7.88496100	0.57215100	O	-10.30521000	8.10000400	2.38480600
O	-10.81001400	7.77095400	0.40308300	O	-8.29316700	9.64964700	2.92532500
O	-9.42947500	9.26747800	1.20902800	O	6.88626500	-0.95444300	2.26928000
O	7.87459500	-1.18715000	0.68782100	P	7.48484900	-1.70518300	3.45076100
P	8.52500600	-1.88301400	1.91251200	O	6.71365400	-1.29822700	4.81950600
O	7.95956000	-1.45544000	3.26796500	O	8.97294400	-1.66091500	3.67899300
O	10.05175700	-1.96314400	1.81525500	O	6.99150900	-3.29888400	3.37605300
O	7.98596500	-3.51869700	1.81721400	C	7.41668300	-4.03582800	2.23213400
C	8.04589000	-4.11226900	0.54313500	C	6.94915300	-5.48051800	2.35599500
C	7.59913400	-5.57037000	0.60316200	O	5.50504600	-5.57134400	2.44522200
O	6.24374500	-5.71924700	1.11287600	C	7.34799300	-6.33808800	1.13568800
C	7.58276000	-6.23623900	-0.78666600	O	7.69263600	-7.67674000	1.48510400
O	7.94285300	-7.61780900	-0.75111000	C	6.09752100	-6.23999900	0.25094400
C	6.13276000	-6.00429300	-1.23444800	C	4.96071000	-6.17744500	1.27967700
C	5.35943800	-6.13763400	0.08367500	N	3.77642100	-5.44697500	0.83707200
N	4.10969200	-5.38157400	0.14523700	C	2.50344200	-5.97990700	0.74248700
C	2.85550800	-5.93868200	0.31674000	N	1.60911500	-5.11817500	0.32668400
N	1.89426300	-5.05080200	0.36631700	C	2.32110200	-3.94445600	0.13621800
C	2.53905000	-3.83100200	0.22763500	C	1.87879100	-2.64772100	-0.24986800
C	2.02908500	-2.50526700	0.27580700	O	0.71370600	-2.26391700	-0.47776800

O	0.84683000	-2.13983400	0.45747600	N	2.93840000	-1.73202100	-0.31679100
N	3.04231900	-1.54541700	0.13691400	C	4.24957500	-1.99965800	0.03720000
C	4.40195600	-1.82161000	0.01576300	N	5.13406000	-0.98703500	0.00249300
N	5.26224200	-0.80243700	-0.03587500	N	4.65539100	-3.21318600	0.40858300
N	4.86242800	-3.07493700	-0.04395400	C	3.66918000	-4.12300900	0.45183300
C	3.91805500	-4.01145500	0.09074800	O	-4.64419800	-8.70810700	-0.01699000
O	-4.51727500	-8.64630800	1.03666600	C	-5.94488200	-8.75395600	0.56458900
C	-5.89049100	-8.59650100	1.41613000	C	-6.89861400	-7.66380700	0.08461100
C	-6.75546100	-7.66914500	0.56727800	O	-6.46661600	-6.38254900	0.60226400
O	-6.39779500	-6.29286200	0.83802500	C	-7.02253500	-7.50590000	-1.45586500
C	-6.64944500	-7.86559300	-0.97001200	O	-8.38652200	-7.39053300	-1.78920400
O	-7.94807600	-7.86744800	-1.51459700	C	-6.24892400	-6.20073500	-1.72188400
C	-5.83595200	-6.63310500	-1.40954600	C	-6.57112200	-5.42676700	-0.44929500
C	-6.33413100	-5.60039000	-0.40552000	N	-5.73241600	-4.27648200	-0.13534300
N	-5.53795800	-4.39155600	-0.23266000	C	-6.23204600	-3.05252100	0.26970400
C	-6.08159500	-3.12185400	-0.15083900	N	-5.30480100	-2.16439500	0.52523100
N	-5.19726800	-2.18404500	0.07428100	C	-4.11617000	-2.83264300	0.28419900
C	-3.99215900	-2.86254400	0.15383100	C	-2.77370200	-2.37919800	0.38129700
C	-2.68537100	-2.38043900	0.40992400	O	-2.38709700	-1.23996900	0.73330700
O	-2.33896900	-1.19401000	0.64358000	N	-1.85257100	-3.36424100	0.02784900
N	-1.72646900	-3.39231600	0.39964300	C	-2.18846800	-4.65082900	-0.34608100
C	-2.00784500	-4.73174500	0.20602200	N	-1.16992600	-5.47534500	-0.67419400
N	-0.98247300	-5.59592600	0.26280000	N	-3.44015900	-5.08522300	-0.42750400
N	-3.23825800	-5.19403100	-0.00602900	C	-4.35612600	-4.14787400	-0.12346500
C	-4.17893500	-4.23710100	-0.02972300	P	-8.81093400	-7.56346200	-3.47472600
P	-8.13458900	-8.48503900	-3.13746000	O	-10.33485800	-7.66111100	-3.36268700
O	-9.66091500	-8.58068400	-3.21538600	O	-8.08877500	-8.85068900	-3.90003700
O	-7.38368500	-9.82506200	-3.10751800	O	-8.28911600	-6.28148000	-4.14590800
O	-7.50110100	-7.41561000	-4.04300200	O	8.44946400	1.62818900	-4.36165100
O	7.96995900	2.50047700	-4.19520300	P	8.95181200	2.00629400	-2.96200700
P	8.56461000	2.60239500	-2.78493900	O	10.47723400	2.08655500	-2.81773800
O	10.09661900	2.57391300	2.71812200	O	8.22900600	1.31716200	-1.79126700
O	7.86455400	1.75201600	-1.70844300	O	8.40309200	3.63665000	-2.72379700
O	8.13658000	4.19717600	-2.23930400	C	8.29888000	4.50094500	-3.82334000
C	7.84532000	5.20500600	-3.17077200	C	7.29850000	5.61272400	-3.52417200
C	6.91512600	6.24395100	-2.55293600	O	5.96359900	5.06746500	-3.38763300
O	5.61565100	5.66129900	-2.28452200	C	7.56181000	6.38270700	-2.22195300
C	7.39245800	6.82088900	-1.21215800	O	7.09055100	7.72057700	-2.42207400
O	6.91339200	8.16916300	-1.13912000	C	6.71024800	5.61955600	-1.20529200
C	6.70219500	5.91107500	-0.19445300	C	5.50144900	5.19692200	-2.04946600
C	5.36617300	5.61547000	-0.88635500	N	4.86701700	3.95440200	-1.61714200
N	4.77483300	4.32912200	-0.52909600	C	5.44362300	2.69983500	-1.44357000
C	5.34243000	3.06274700	-0.62472600	N	4.56278300	1.79156600	-1.08578100
N	4.51740900	2.11676600	-0.23395500	C	3.35312300	2.46539900	-1.02643500
C	3.35140900	2.77501000	0.12229300	C	2.05464100	2.01142700	-0.69792100
C	2.11832500	2.28601100	0.60707900	O	1.71575700	0.83859100	-0.39866500
O	1.80992800	1.08872100	0.86169900	N	1.10008400	3.03064700	-0.73240900
N	1.17835200	3.30035700	0.81129400	C	1.36955500	4.34333700	-1.07216300
C	1.41962300	4.64623500	0.61060900	N	0.33457700	5.20246100	-1.09197400
N	0.43313600	5.51340800	0.92692000	N	2.58533000	4.77436900	-1.39617800
N	2.58346700	5.11361900	0.17327700	C	3.52267400	3.81000800	-1.35641800

C	3.49333300	4.15292000	-0.06254500	H	-5.89151300	9.99747200	-1.21208500
H	-5.39224200	10.24026600	1.08582900	H	-5.26540700	8.70876400	-2.25623800
H	-4.23556400	9.15461400	-1.87680000	H	-7.46091000	8.18440200	-1.21125400
H	-6.60488400	8.44353400	-2.11829400	H	-6.54979400	9.10438500	1.25374900
H	-7.06293500	8.94311200	0.58458200	H	-6.30337300	6.65122900	2.36787700
H	-7.19226100	6.33615800	1.29809800	H	-4.87463800	7.39031700	1.57955000
H	-5.62904900	7.19439500	1.43680400	H	-6.66247200	5.20163200	0.46405200
H	-6.45306600	5.22427100	-0.72362200	H	-3.28194200	6.79649500	-0.33619100
H	-3.26701600	6.95362100	0.49110200	H	-6.73407100	0.95313300	1.14457900
H	-6.51425500	0.92475300	-0.67153600	H	8.51456900	-4.03605600	2.16987000
H	9.08149100	-4.11327100	0.15803600	H	7.00574400	-3.58454200	1.32369500
H	7.42105400	-3.56118400	-0.16750000	H	7.35573100	-5.91585400	3.27599700
H	8.25124600	-6.12639400	1.28735700	H	8.23331800	-5.94139900	0.63290100
H	8.29999400	-5.77262800	-1.46843300	H	6.11912500	-5.31509600	-0.33122900
H	6.01638300	-4.99218400	-1.63106600	H	6.00240600	-7.08833300	-0.43030500
H	5.80728200	-6.72464500	-1.98832900	H	4.58980600	-7.17951900	1.52826200
H	5.05708500	-7.17823700	0.25976100	H	2.31169000	-7.01546200	0.98969100
H	2.72499900	-7.01005600	0.39105000	H	4.85878100	-0.05071600	-0.31332100
H	4.93521800	0.16854700	-0.02522400	H	-5.79396100	-8.64685100	1.64393100
H	-5.90184700	-8.24577100	2.45348300	H	-6.42206200	-9.73049500	0.39090800
H	-6.34214100	-9.60008700	1.39926600	H	-7.89731700	-7.88573800	0.48474200
H	-7.80362300	-7.82307400	0.85737600	H	-6.58429000	-8.35438200	-2.00089500
H	-6.13989600	-8.80268400	-1.23627200	H	-5.17197400	-6.38097300	-1.77442800
H	-4.76475800	-6.79394200	-1.26422300	H	-6.61730700	-5.73125300	-2.63539700
H	-6.05976300	-6.38740400	-2.44872500	H	-7.59399500	-5.03113100	-0.49845500
H	-7.33354100	-5.24845500	-0.69301200	H	-7.29820700	-2.88671600	0.34638100
H	-7.14456200	-2.96500300	-0.27633300	H	-0.21863600	-5.31690400	-0.31522000
H	0.00839900	-5.32294800	0.32993200	H	9.26792500	4.97791100	-4.06779500
H	8.75845300	5.73502900	-3.50563100	H	7.97129000	3.95257900	-4.71613500
H	7.37017100	4.78146200	-4.06447100	H	7.28375200	6.31710100	-4.36531100
H	6.76966500	7.06326500	-3.26823900	H	8.62637800	6.38274900	-1.95765600
H	8.48528800	6.79267000	-1.12306600	H	6.41955600	6.22714400	-0.34296800
H	6.56758100	6.38020000	0.78486800	H	7.25815200	4.74009400	-0.86383500
H	7.28000500	4.99178800	-0.08418100	H	4.70372100	5.94491400	-2.01010100
H	4.60564300	6.35720200	-0.62342200	H	6.50476900	2.49623100	-1.60682400
H	6.34901200	2.87459000	-1.01423300	H	0.56395200	6.17091900	-1.26397900
H	0.60348300	6.46392400	0.62500000	H	5.92201500	-1.05809400	0.65978300
H	6.27245900	-1.00034800	0.19543100	H	-1.43768200	-6.43922600	-0.82344500
H	-1.19812100	-6.55907200	0.04812700	H	-5.52276000	-0.26961700	0.95324500
H	-5.35412300	-0.27278700	-0.16428800	H	-0.60728000	4.98763800	-0.73798900
H	-0.55674500	5.23230800	0.96136100	H	-4.73166700	-8.96498000	-0.94850200
H	-4.46658400	-9.11002000	0.18591800	H	-4.31791300	9.39702200	0.30724500
H	-4.68241200	9.39861400	0.89476600	H	6.97767200	-8.05119000	2.02537100
H	7.43962000	-8.04700900	-0.04003800	H	7.19686800	8.19431300	-1.58119600
H	7.15543000	8.51587600	-0.26501200	H	-3.28936800	0.42231700	0.67623200
H	-3.20334200	0.49815100	0.43881500	H	0.13775500	2.75717800	-0.47622400
H	0.23354500	2.98731800	1.07658900	H	2.65470200	-0.75642900	-0.49033700
H	2.73491900	-0.57051800	0.23723800	H	-0.86528700	-3.06354900	-0.05346100
H	-0.74433700	-3.07819900	0.48989600	N	-0.02495200	-0.00686500	1.62381300
C	0.76056500	-1.87214400	4.75107300	H	0.53301600	0.25996100	0.78317300
C	-0.78204500	-1.68378800	4.81188900	H	-0.42945000	0.86921100	1.96520200

C	-0.59022600	-0.37315600	4.01475400	H	-0.82425900	-0.58999300	1.29421200
C	0.76115000	-0.92300000	3.53319500	C	0.81515900	-0.70040000	2.65148100
H	1.25679900	-1.43171100	5.62027700	H	0.20352600	-0.82270000	3.54861700
H	1.14581800	-2.87776500	4.57926100	H	1.03074400	-1.69284100	2.25026400
H	-1.24690500	-1.59047600	5.79384600	C	2.10374400	0.07273200	2.93316800
H	-1.30694600	-2.44292400	4.22557400	H	2.60154500	0.29293100	1.98179900
H	0.67882300	-1.46181800	2.58534100	H	1.86687900	1.03688400	3.40215600
N	1.89206100	0.04560200	3.37548200	C	3.07411200	-0.71460100	3.82931700
H	2.79060700	-0.44917900	3.38257100	H	3.23771100	-1.71338800	3.40779600
H	1.82765600	0.55912900	2.45114500	H	2.64028000	-0.85580000	4.82585600
H	1.92615500	0.73112800	4.13708800	N	4.39331700	-0.08405000	3.98663400
H	-0.47310100	0.48575200	4.67906300	H	4.29324400	0.86090200	4.35717500
N	-1.61181000	-0.00970800	2.99600600	H	5.80308500	-0.91694300	4.61916700
H	-2.52093000	0.12326800	3.45114900	H	4.85792200	-0.00087900	3.07931800
H	-1.40716600	0.87278300	2.46294600	CBDA-T2			
H	-1.75020500	-0.72226500	2.24255500	E = -6388.68814			
CBDA-C1				O	4.26739900	9.44035100	0.08006100
E = -6388.65324				C	5.27277400	9.68134800	1.06769700
O	-3.87236300	9.30687900	-0.35086200	C	6.43491200	8.68830700	1.05217100
C	-4.90022400	9.46254000	-1.33221700	O	5.95841400	7.37328300	1.41987900
C	-6.05092000	8.46329600	-1.21565700	C	7.16527100	8.51883000	-0.29576000
O	-5.56704800	7.12563100	-1.48152100	O	8.52539500	8.26020400	0.03688700
C	-6.76198300	8.39824700	0.15108300	C	6.45363500	7.29625200	-0.89971200
O	-8.12297500	8.11392400	-0.06991100	C	6.12645000	6.45970100	0.34052200
C	-6.03334300	7.23301300	0.84381400	N	4.90946400	5.65722500	0.21935500
C	-5.69925000	6.30521200	-0.32812100	C	3.61971000	6.13240800	0.07649600
N	-4.45425800	5.55036400	-0.15523300	N	2.72774400	5.17098000	0.00558200
C	-3.17380700	6.07370800	-0.13739700	C	3.46084900	3.99987000	0.10728500
N	-2.24856600	5.15940800	0.03951000	C	3.04125400	2.63794200	0.08081300
C	-2.95049400	3.96976900	0.14295200	O	1.89164300	2.18461300	0.04611600
C	-2.49572900	2.64964100	0.37099000	N	4.13145000	1.75876100	0.22069600
O	-1.31251800	2.27256700	0.54170900	C	5.44729500	2.14452400	0.37017200
N	-3.54311700	1.72134000	0.40635300	N	6.36464900	1.17130100	0.54669800
C	-4.88255800	2.04289200	0.27004500	N	5.84011200	3.41491900	0.38069600
N	-5.77371500	1.04088700	0.37618900	C	4.81901300	4.28354300	0.24909800
N	-5.31492700	3.28543200	0.07676700	O	9.32625700	7.06099800	2.20885800
C	-4.32419900	4.19304700	0.01931100	P	9.62856800	8.32707100	-1.38859900
O	-8.89335200	6.99708200	2.15420300	O	10.96824900	8.31254500	0.64706400
P	-9.20553800	8.23469800	1.29505600	O	9.26927800	9.64600000	2.08872300
O	-10.55571600	8.19897700	0.57362000	O	-6.74854100	-1.43605400	1.54984000
O	-8.82996600	9.57596600	1.94206500	P	-7.67536200	-2.33353200	2.43755600
O	7.79905600	-1.67026300	0.64655300	O	-7.70109200	-1.94143700	3.90366100
P	8.42095000	-2.31993700	1.91019700	O	-9.04428600	-2.54710600	1.75500100
O	7.89568200	-1.77232900	3.23733400	O	-6.93543600	-3.85842400	2.46382200
O	9.93888900	-2.49648200	1.80608300	C	-6.93694900	-4.59551900	1.25560300
O	7.77934800	-3.92096500	1.93351900	C	-6.36118700	-5.98745500	1.48857200
C	7.81738900	-4.62235500	0.71452200	O	-4.96657600	-5.94329900	1.89793900
C	7.21227100	-6.01467200	0.87024700	C	-6.38617400	-6.86328500	0.21919600
O	5.82591800	-5.97308100	1.31211400	O	-6.62501900	-8.24171500	0.49918900
C	7.19343100	-6.79808400	-0.45796700	C	-4.99725300	-6.60104100	0.37662700

O	7.42077600	-8.19802400	-0.28768200	C	-4.12475400	-6.45763200	0.87753000
C	5.79308000	-6.47772000	-0.99692600	N	-2.94845200	-5.60488600	0.70385200
C	4.95720200	-6.43217900	0.28724800	C	-1.64028500	-6.04486100	0.74805100
N	3.76441700	-5.59117600	0.21681100	N	-0.76495800	-5.09741700	0.51244900
C	2.46346100	-6.04958200	0.31684400	C	-1.52910500	-3.96212000	0.30895500
N	1.56798500	-5.09756600	0.22955300	C	-1.13068400	-2.61806000	0.03305800
C	2.30976400	-3.93649900	0.06953100	O	0.01709800	-2.17442700	0.11768200
C	1.89641700	-2.57939000	-0.01718300	N	-2.24357100	-1.75613100	0.05045600
O	0.72956100	-2.12755500	0.01880400	C	-3.55482300	-2.14771600	0.08618100
N	2.98249800	-1.70296700	-0.12043700	N	-4.54516100	-1.20060500	0.03503900
C	4.32117600	-2.07714200	-0.11256600	N	-3.92054300	-3.40101500	0.29769300
N	5.25347200	-1.12237200	-0.15944500	C	-2.88602400	-4.25304000	0.42397700
N	4.69678600	-3.35976900	-0.05779900	O	5.74689300	-8.06441300	1.75893800
C	3.67874100	-4.21840600	0.05835500	C	7.07173600	-7.86474200	2.24486600
O	-4.76275100	-8.39489600	0.62607500	C	7.95071100	-6.98801600	1.35794500
C	-6.07856500	-8.34898700	1.17199200	O	7.47290100	-5.62412000	1.40583900
C	-7.01216100	-7.34133100	0.50711700	C	8.01310400	-7.39265300	0.14150700
O	-6.57999500	-5.99887200	0.82884900	O	9.36177400	-7.41165800	0.54714800
C	-7.10511700	-7.42667800	-1.04133600	C	7.21089900	-6.27145800	0.82947800
O	-8.46289500	-7.39823400	-1.41336400	C	7.52352200	-5.09220900	0.08499900
C	-6.34425400	-6.16561700	-1.49699900	N	6.64107000	-3.93634500	0.00305300
C	-6.66590800	-5.20927900	-0.35401100	C	7.09101500	-2.63042100	0.05719000
N	-5.81012000	-4.03908800	-0.19763500	N	6.12614500	-1.74629900	0.09889400
C	-6.28742100	-2.76896200	0.06917300	C	4.96577900	-2.50028800	0.05451200
N	-5.34350000	-1.88266700	0.26221600	C	3.60207200	-2.08132000	0.07728200
C	-4.16675200	-2.59992100	0.12514900	O	3.15280300	-0.92601400	0.14345800
C	-2.81658500	-2.18098300	0.25792600	N	2.72233800	-3.17528200	0.01573400
O	-2.40164100	-1.03452000	0.55019500	C	3.11224300	-4.49647900	0.05026500
N	-1.91179900	-3.22124000	0.03566100	N	2.14078300	-5.43173700	0.05786800
C	-2.27249400	-4.52371200	-0.25220800	N	4.38314200	-4.88504800	0.07329200
N	-1.27749900	-5.40457800	-0.47130700	C	5.25853300	-3.86281100	0.01416700
N	-3.53510300	-4.92685300	-0.34599900	P	9.73436400	-8.19568400	2.06077300
C	-4.43132400	-3.94282400	-0.15844300	O	11.25849700	-8.29565300	1.94651400
P	-8.85435600	-7.89266100	-3.04189700	O	8.97164800	-9.52731900	1.98257100
O	-10.37462300	-8.03897600	-2.92466900	O	9.22607300	-7.22968500	3.14493000
O	-8.07235700	-9.20224600	-3.22515800	O	-9.34134600	1.93118200	2.34540600
O	-8.38043700	-6.72964900	-3.92949000	P	-9.77754300	2.67856600	1.07908200
O	9.08755900	2.24251400	-3.45101700	O	-11.05478600	3.50508000	1.19320900
P	9.44751700	2.43108500	-1.97151700	O	-9.68192400	1.82620100	-0.21566600
O	10.94532300	2.36110100	-1.64905500	O	-8.51700400	3.81395700	0.77240400
O	8.54526800	1.68008000	-0.97365000	C	-8.42066400	4.88779900	1.68406500
O	9.00886700	4.07126400	-1.60869700	C	-7.39452700	5.91264300	1.21994700
C	8.84418500	5.01309900	-2.63414500	O	-6.05144300	5.38723700	1.34774800
C	7.73960300	6.00133100	-2.27236000	C	-7.53513700	6.34539500	-0.24763000
O	6.45186600	5.33636100	-2.27208900	O	-7.12719500	7.71567500	-0.32039600
C	7.88265600	6.63435900	-0.87869500	C	-6.55215200	5.41589900	-0.96369300
O	7.35920000	7.96565100	-0.96438700	C	-5.42989100	5.28052200	0.07230300
C	7.00618500	5.73054300	-0.00952900	N	-4.68910100	4.02735400	0.01151800
C	5.87015000	5.37966000	-0.97550100	C	-5.19146400	2.74373400	0.14508700
N	5.19564500	4.11679900	-0.69877500	N	-4.25203300	1.82686700	0.15571300
C	5.73865900	2.83626800	-0.65728300	C	-3.06585200	2.53532300	0.03270300

N	4.82889000	1.91825200	-0.41227000	C	-1.71204500	2.08801200	0.01947000
C	3.63549500	2.61425800	-0.28956200	O	-1.28011400	0.92668800	0.10861400
C	2.31964600	2.16422700	-0.01956700	N	-0.81054900	3.16255100	-0.10681900
O	1.94226700	0.98164300	0.16291000	C	-1.16942900	4.49095800	-0.20305000
N	1.39423800	3.21620500	0.03258600	N	-0.18499100	5.39619000	-0.36925200
C	1.70772400	4.54980700	-0.15079200	N	-2.43196600	4.90903600	-0.17126000
N	0.71278800	5.44972100	-0.02195200	C	-3.31802700	3.90333600	-0.05100300
N	2.93899900	4.97475700	-0.41157100	H	5.67329700	10.70138900	0.97706600
C	3.84600700	3.98217500	-0.46855300	H	4.76162000	9.60772500	2.03282800
H	-5.30996500	10.48261500	-1.31126000	H	7.15796400	9.00770300	1.81288800
H	-4.40792700	9.31985900	-2.29936200	H	7.06759000	9.40674800	-0.93699800
H	-6.78776500	8.71029500	-1.98954100	H	7.11987200	6.78757900	-1.59917200
H	-6.66112500	9.33422700	0.71928000	H	5.52592700	7.58559600	-1.40405600
H	-6.69196300	6.77118600	1.58230200	H	6.92220200	5.74558400	0.57387500
H	-5.10733500	7.57088400	1.32048600	H	3.42194200	7.19577800	0.04418300
H	-6.47572000	5.55081800	-0.48918000	H	7.32838100	1.47480600	0.53258800
H	-3.01170700	7.13641600	-0.26200700	H	-7.96563200	-4.71118400	-0.88465300
H	-6.73334600	1.28163500	0.17090700	H	-6.33966800	-4.07932900	-0.49428500
H	8.85892400	-4.76718400	0.37521200	H	-6.91427200	-6.47523400	-2.29947400
H	7.28245200	-4.06915400	-0.06531700	H	-7.18660800	-6.56953200	0.46402100
H	7.76845400	-6.57121800	1.63439400	H	-4.99717800	-5.66207800	0.93756300
H	7.98007900	-6.46377100	-1.13885000	H	-4.66284100	-7.40778500	1.03260700
H	5.78740200	-5.49390800	-1.47422100	H	-3.71740500	-7.42757600	-1.19037100
H	5.43524100	-7.22522500	-1.70859500	H	-1.40420800	-7.07980700	-0.95569200
H	4.57552200	-7.42984400	0.54293300	H	-4.26779100	-0.21013200	0.05506500
H	2.24994500	-7.10203900	0.44734700	H	6.96228800	-7.38746500	-3.22438800
H	5.00330500	-0.13005600	-0.19228500	H	7.58663100	-8.82544500	-2.39836900
H	-5.95557100	-8.08109700	2.22672800	H	8.97367900	-7.01852900	-1.75794200
H	-6.55795000	-9.33907300	1.13423600	H	7.56449800	-8.37907300	0.32648800
H	-8.02121200	-7.49363900	0.91409900	H	6.13716200	-6.47370900	0.80080100
H	-6.63904300	-8.34010300	-1.43627500	H	7.55816800	-6.14286100	1.85599200
H	-5.26641500	-6.34399600	-1.52848800	H	8.52909400	-4.70458000	0.12658600
H	-6.71422400	-5.83578300	-2.46946400	H	8.14945900	-2.40792900	0.07415900
H	-7.68221600	-4.80981200	-0.46872500	H	1.15258100	-5.22016400	-0.24316700
H	-7.35038500	-2.57039900	0.09777100	H	-9.39327900	5.39161300	1.78734300
H	-0.30433900	-5.23356600	-0.18142000	H	-8.12834200	4.53139900	2.68471200
H	9.76785600	5.60035500	-2.80408400	H	-7.46646500	6.79554500	1.86700900
H	8.59337900	4.51611200	-3.57919500	H	-8.56245500	6.22403300	-0.61064100
H	7.70662600	6.79719800	-3.02779800	H	-6.19315100	5.81690700	-1.91601900
H	8.92705700	6.64995300	-0.54479200	H	-7.02871900	4.44856800	-1.13546800
H	6.64388400	6.22275000	0.89820900	H	-4.67635300	6.06523700	-0.04550000
H	7.56453400	4.83152300	0.25799900	H	-6.25506600	2.57175200	0.24503600
H	5.07844900	6.13533800	-0.94492900	H	-0.47412200	6.36353900	-0.32767500
H	6.80376500	2.62642200	-0.81690600	H	-5.35083800	-1.37489800	-0.61957400
H	0.95263700	6.40106400	-0.26358600	H	2.45045200	-6.37831800	-0.22864100
H	6.23463300	-1.38343100	0.12972700	H	6.18470500	0.17766000	0.35475300
H	-1.56654500	-6.36818500	-0.56981500	H	0.81426500	5.20153800	-0.21922100
H	-5.52321800	0.04371900	0.36440700	H	5.80778800	-8.62602900	-0.97007500
H	-0.28739700	5.21677800	0.00858200	H	4.61744500	9.72379400	-0.77919500
H	-4.82612700	-8.79194900	-0.25697800	H	-6.02548100	-8.52052500	-1.21066100
H	-4.20669300	9.65066000	0.49252300	H	-7.16340700	7.98062800	-1.25389700

H	6.85774200	-8.51576800	0.43701500	H	3.89224000	0.75416500	0.20799700
H	7.38584600	8.34565900	-0.07120100	H	0.18969100	2.90507900	-0.11305300
H	-3.26948500	0.73484400	0.51018400	H	-2.01590800	-0.75171500	0.14605600
H	0.41242700	2.95893800	0.20465300	H	1.71842100	-2.93600100	0.03543200
H	2.74419200	-0.70190600	-0.10772400	C	-9.69890800	-1.73503700	2.21512000
H	-0.91035800	-2.96046000	0.04350000	C	-8.60722700	-2.49950100	3.01594200
C	-1.16998200	-0.69001300	4.00978500	C	-7.61206300	-2.08765400	1.91161600
C	-0.30823100	-1.83752000	4.57838800	C	-8.56289500	-0.94010900	1.52439900
C	0.67618600	-1.68571100	3.40054500	H	-10.21872700	-2.39315700	1.51221300
C	0.06844100	-0.27894500	3.17392500	H	-10.42611900	-1.14774000	2.77823500
H	-1.97627100	-1.05783800	3.36685800	H	-8.74000800	-3.57007900	3.18259600
H	-1.57121100	0.03406900	4.71999700	H	-8.38737600	-2.00790900	3.96854800
H	0.13447800	-1.60856200	5.54718000	H	-8.37204000	-0.01290000	2.07584600
H	0.65112900	0.51093300	3.64865000	N	-8.70547100	-0.59098200	0.10254600
N	-0.18318700	0.12369900	1.77268300	H	-9.16609600	0.39534800	-0.01403500
H	-0.71949200	1.00819400	1.68266000	H	-7.78589200	-0.61403500	-0.40812900
H	0.68884200	0.30303200	1.23041600	H	-9.17884900	-1.34127300	-0.46210900
H	-0.75203700	-0.56842300	1.24730600	H	-7.52914800	-2.83855800	1.12495600
H	0.44060700	-2.35615900	2.56887200	N	-6.20911900	-1.73802400	2.32240200
H	1.74105800	-1.74917100	3.62815000	H	-5.76794600	-2.52725400	2.80630000
N	-0.97951000	-3.17621700	4.73042200	H	-5.58382400	-1.49674600	1.49520500
H	-0.30517600	-3.90704100	4.98652100	H	-6.19546600	-0.94538000	2.972308002b
H	-1.69627800	-3.15585900	5.46544800	CBDA-C2			
H	-1.44042600	-3.47710500	3.86416900	E = -6388.68789			
CPDA-T1				O	-3.32442000	9.65978400	-0.35256700
E = -6427.97621				C	-4.29031600	9.95687800	-1.36437800
O	-1.24513300	9.40127300	-0.26159300	C	-5.51649200	9.04449600	-1.36644600
C	-0.17391600	10.32440500	-0.04846400	O	-5.11842100	7.69667800	-1.70888400
C	1.17542900	9.87977100	-0.61228000	C	-6.28940700	8.93929100	-0.03541600
O	1.64092300	8.70788000	0.09788100	O	-7.65706700	8.76238600	-0.32542900
C	1.20207400	9.50918900	-2.10866900	C	-5.67220800	7.68060100	0.59695000
O	2.46321300	9.85345800	-2.63188200	C	-5.39123100	6.80896400	-0.62932600
C	1.00008600	7.98477400	-2.07091900	N	-4.25501600	5.90247000	-0.47449400
C	1.72149000	7.59029100	-0.77811900	C	-2.93415700	6.25741400	-0.27876000
N	1.14023800	6.43167800	-0.09454400	N	-2.13773400	5.21852700	-0.16927900
C	-0.11210400	6.36825600	0.48943700	C	-2.97165000	4.11934400	-0.29905400
N	-0.34700400	5.21800000	1.07596500	C	-2.68372500	2.72381500	-0.25084800
C	0.80571000	4.47832400	0.86789800	O	-1.58816000	2.16460000	-0.07618100
C	1.15156700	3.17105300	1.27990200	N	-3.84481300	1.94990400	-0.43121500
O	0.45479700	2.37834600	1.96612200	C	-5.11158500	2.45500800	-0.63310800
N	2.42459100	2.79271800	0.84686800	N	-6.10715700	1.56597600	-0.84660100
C	3.28927800	3.60905100	0.13939500	N	-5.38310000	3.75549000	-0.66511700
N	4.47998700	3.08293000	-0.20380500	C	-4.29069800	4.52636100	-0.49746200
N	2.98198700	4.84870100	-0.22640200	O	-8.54862500	7.60727900	1.83651900
C	1.74509400	5.22163300	0.14600900	P	-8.78335800	8.88000600	1.00442800
O	2.60726500	8.41884500	-4.80331600	O	-10.10770600	8.91229700	0.23640600
P	2.62360900	9.89474700	-4.37043300	O	-8.38578200	10.18770300	1.70459100
O	3.98001400	10.59388000	-4.49827400	O	6.56590300	-2.17394600	1.08363500
O	1.40668000	10.71255300	-4.82841400	P	7.43016200	-3.08261700	2.03041400
O	-5.65791700	-3.36155900	-2.65377500	O	7.29354100	-2.73880400	3.50366700

P	-5.64022400	-3.20790200	-4.19911800	O	8.85588100	-3.23450300	1.47715900
O	-5.28642800	-1.80809500	-4.69929800	O	6.69716900	-4.60876900	1.93919900
O	-6.83265100	-3.88855800	-4.87744600	C	6.66777600	-5.25369900	0.68080500
O	-4.25894200	-4.10556100	-4.70617800	C	5.97585700	-6.60761100	0.80589800
C	-4.18551200	-5.42984300	-4.23635700	O	4.59004900	-6.47263800	1.22331100
C	-2.98434100	-6.15805500	-4.83274500	C	5.93302900	-7.38758100	-0.52556900
O	-1.71369000	-5.53662800	-4.48355800	O	6.10183000	-8.79394100	-0.35300300
C	-2.87126400	-7.61077800	-4.33058100	C	4.55351900	-7.00814600	-1.08061500
O	-2.35824100	-8.50653300	-5.31742200	C	3.70734000	-6.89277200	0.19358500
C	-1.94058500	-7.45632300	-3.12032900	N	2.57544300	-5.97202500	0.09425800
C	-0.97853700	-6.35896100	-3.59376300	C	1.24538100	-6.32021300	0.22539500
N	-0.38746500	-5.55542000	-2.52075200	N	0.42623200	-5.30472000	0.08965400
C	0.93488000	-5.62567800	-2.11890100	C	1.25451800	-4.21807200	-0.13258100
N	1.21781400	-4.84023600	-1.11068500	C	0.94157400	-2.83579200	-0.32030600
C	0.02266100	-4.19517500	-0.82955500	O	-0.17403700	-2.29657400	-0.35950900
C	-0.29527600	-3.21287200	0.13523000	N	2.10763800	-2.05704900	-0.45621500
O	0.48040400	-2.71647000	1.00220100	C	3.38963100	-2.54836300	-0.42648500
N	-1.62214000	-2.79553100	0.06541900	N	4.43794900	-1.66602100	-0.56789400
C	-2.57509900	-3.30187400	-0.81769000	N	3.67621500	-3.83140400	-0.29718200
N	-3.80939200	-2.80721800	-0.76911300	C	2.59076000	-4.61011300	-0.13128900
N	-2.27383100	-4.25529200	-1.70544500	O	-6.30165500	-7.57577500	2.12154700
C	-0.99385300	-4.63063500	-1.69091100	C	-7.53542700	-7.18166600	2.71725300
O	8.08138800	-5.21467700	-1.35760500	C	-8.38558200	-6.24453200	1.86457900
C	9.09275200	-4.40193900	-1.94765000	O	-7.75058000	-4.94676000	1.79632000
C	9.55195200	-3.22346900	-1.09383000	C	-8.63336000	-6.70331500	0.40010500
O	8.50091600	-2.23056200	-1.03296900	O	-10.00404400	-6.56305100	0.10547500
C	9.94271900	-3.55788500	0.37281300	C	-7.76431900	-5.72392200	-0.41140400
O	11.18058200	-2.95015200	0.65729500	C	-7.86527600	-4.47456800	0.45720500
C	8.78626800	-2.93778000	1.18128600	N	-6.88247500	-3.42439100	0.23271900
C	8.43271600	-1.74337700	0.30152700	C	-7.21000100	-2.09143200	0.06373600
N	7.12809700	-1.12631200	0.51448000	N	-6.17088400	-1.31774900	-0.12487700
C	6.93204200	0.23148900	0.67995000	C	-5.08730100	-2.17793600	-0.07040700
N	5.67494900	0.56750900	0.83149400	C	-3.69592800	-1.90455400	-0.22091900
C	4.98870500	-0.63269900	0.74573900	O	-3.14501400	-0.81297200	-0.43711400
C	3.60187200	-0.90953100	0.86877300	N	-2.92141400	-3.06981000	-0.09981600
O	2.67550600	-0.10066700	1.12183100	C	-3.42754500	-4.33198600	0.13077000
N	3.31301300	-2.26208300	0.69261500	N	-2.54897000	-5.34855900	0.20416800
C	4.25506400	-3.24076800	0.44787600	N	-4.72604000	-4.58650900	0.26913000
N	3.79647000	-4.50881600	0.31011700	C	-5.50179200	-3.49129200	0.15544400
N	5.55701000	-2.99680900	0.38573000	P	-10.60548900	-7.44733200	-1.27456200
C	5.87069500	-1.69825900	0.54069300	O	-12.10990100	-7.20629200	-1.11847500
P	12.02939100	-3.47962700	2.08812200	O	-10.13042200	-8.88581600	-1.01836000
O	13.42460000	-2.91653600	1.79973400	O	-9.95867500	-6.76778300	-2.49344000
O	11.90826800	-5.01023400	2.04255200	O	8.99002300	2.78673300	-2.25584400
O	11.28748000	-2.80811400	3.25656000	P	9.55788400	2.50853800	-0.86363200
O	-9.06108700	-3.02584600	3.46882900	O	10.99978300	2.01151700	-0.79980500
P	-9.20241200	-2.83508400	1.95259500	O	8.60232300	1.67777000	0.06197100
O	-10.48185400	-3.42153500	1.34053900	O	9.59596400	4.01684500	-0.05243700
O	-7.92276800	-3.07893100	1.13445800	C	9.03586500	5.18549600	-0.60911500
O	-9.36092500	-1.11757900	1.73691300	C	7.80666500	5.68995200	0.15101600
C	-10.00611600	-0.35023300	2.71671300	O	6.61561100	4.97597700	-0.26433400

C	-9.63547000	1.12011100	2.55480800	C	7.89488100	5.52657400	1.68283000
O	-8.22614500	1.32022600	2.82289100	O	7.36076300	6.72099400	2.26867000
C	-9.86822900	1.69320600	1.14972100	C	7.00078900	4.30943100	1.93918500
O	-10.17437200	3.08325100	1.30999300	C	5.90788900	4.54081600	0.89611000
C	-8.51347500	1.47731400	0.47120900	N	5.09029500	3.39243600	0.55516200
C	-7.53150300	1.67259400	1.63409300	C	5.51383500	2.12013600	0.19903600
N	-6.30264400	0.88844000	1.52235600	N	4.51194900	1.32937300	-0.11746500
C	-6.16316200	-0.48391800	1.34538600	C	3.37474500	2.11057700	0.02949800
N	-4.90383500	-0.86388400	1.34399900	C	1.99863400	1.79980300	-0.17668300
C	-4.17731500	0.30158000	1.53052300	O	1.49220600	0.72592100	-0.54665900
C	-2.78452800	0.51285200	1.65801400	N	1.17092200	2.90684100	0.08994900
O	-1.86941200	-0.35115000	1.66932100	C	1.61355500	4.14687300	0.49802600
N	-2.46137300	1.86696000	1.81563400	N	0.67817000	5.08774900	0.75774900
C	-3.38588100	2.89145100	1.89784200	N	2.89690600	4.43905200	0.68189100
N	-2.91234200	4.14111100	2.11364300	C	3.71585400	3.39744100	0.43959300
N	-4.69554300	2.69017200	1.82762200	H	-4.62301600	11.00251100	-1.29273300
C	-5.03110700	1.39964200	1.64558500	H	-3.76491200	9.83828200	-2.31737800
H	-0.42346100	11.31345100	-0.45855400	H	-6.19856200	9.40210300	-2.14786500
H	-0.08375500	10.42593800	1.03765300	H	-6.15041700	9.82752300	0.59801900
H	1.89555000	10.68696600	-0.43118500	H	-6.38020800	7.22762400	1.29342700
H	0.40938800	10.01567900	-2.67735400	H	-4.73206100	7.91296100	1.10737900
H	1.43430400	7.53151800	-2.96384900	H	-6.24260900	6.16719800	-0.87612100
H	-0.06044400	7.72314600	-1.99672300	H	-2.64033500	7.29813600	-0.24159700
H	2.76846500	7.32639900	-0.95589600	H	-7.03730900	1.96220200	-0.85322600
H	-0.78418800	7.21550500	0.44403400	H	7.69149400	-5.42950400	0.31567000
H	5.13551900	3.71791500	-0.63776700	H	6.13481500	-4.63899000	-0.05409000
H	-5.08194000	-5.99882000	-4.53818000	H	6.48449400	-7.20139400	1.57456000
H	-4.12369600	-5.44920900	-3.14242700	H	6.73947800	-7.08742800	-1.19899100
H	-3.05081400	-6.13404500	-5.92696200	H	4.60155300	-6.03717500	-1.58122500
H	-3.84357600	-8.02243900	-4.04940800	H	4.16501700	-7.75205900	-1.77966000
H	-2.50406800	-7.10662200	-2.25035500	H	3.25587300	-7.85715500	0.46021500
H	-1.42743700	-8.38580300	-2.86364300	H	0.95114800	-7.34326300	0.41731600
H	-0.11554700	-6.79241200	-4.11649400	H	4.23668500	-0.66540500	-0.43535200
H	1.63517900	-6.28428400	-2.61499300	H	-7.26886700	-6.67315300	3.64980200
H	-4.09841500	-2.16945600	-0.02421400	H	-8.14606800	-8.05892500	2.97964100
H	8.66402000	-4.02067100	-2.88040900	H	-9.36363900	-6.13341600	2.35268100
H	9.97821300	-5.00107600	-2.20938500	H	-8.33216200	-7.74787000	0.23812000
H	10.42889600	-2.77560500	-1.58077800	H	-6.72222300	-6.05231400	-0.45291900
H	10.01895600	-4.63961100	0.54974900	H	-8.17489600	-5.60745600	-1.41547100
H	7.93011400	-3.61567800	1.23443500	H	-8.84093700	-3.99226500	0.31017800
H	9.12977800	-2.66453800	2.18016700	H	-8.24130900	-1.76574200	0.08557600
H	9.16126100	-0.93530400	0.44953100	H	-1.52861900	-5.24129800	0.16975000
H	7.76848700	0.91741000	0.67883800	H	9.78885000	5.98972000	-0.56674500
H	2.86290800	-4.65419700	-0.10183100	H	8.76621500	5.02321800	-1.65853500
H	-11.10828000	-0.42888000	2.64642200	H	7.66356400	6.75420500	-0.08210700
H	-9.72224500	-0.68274900	3.72409300	H	8.92584200	5.36059600	2.01177700
H	-10.19680600	1.71399900	3.28680800	H	6.61692300	4.26102600	2.96265500
H	-10.68219700	1.17523700	0.62773100	H	7.55371100	3.39594700	1.69904700
H	-8.32641100	2.17821300	-0.34786400	H	5.20517100	5.31285900	1.22798100
H	-8.45640200	0.45494000	0.09460600	H	6.57610400	1.86827400	0.17350000
H	-7.19329300	2.71060400	1.70596900	H	1.04519500	6.01435800	0.92790100

H	-7.01024200	-1.16562900	1.24488300	H	5.24749300	-1.95493500	0.03507900
H	-3.61595100	4.86391400	2.03067400	H	-2.92916200	-6.25708700	0.42642700
H	-4.49661400	-3.05539100	-1.54042400	H	-6.03554100	0.57727100	-0.57373700
H	4.50527300	-5.15933300	-0.00636600	H	-0.27924100	5.04078700	0.38457500
H	4.86077900	2.23934800	0.24160700	H	-6.50956200	-8.18179300	1.39300700
H	-1.96896100	4.42158700	1.81249800	H	-3.66955200	9.98309700	0.49454400
H	8.48792500	-5.69792700	-0.62093900	H	5.48996500	-9.09689700	0.33782300
H	-1.51821000	9.46688900	-1.19023400	H	7.38956100	6.60729700	3.23263600
H	-1.58456300	-8.09393900	-5.73508200	H	-3.70011700	0.92683500	-0.42642300
H	-10.25530800	3.46706400	0.42178300	H	0.15565000	2.73593400	0.00275200
H	2.68048200	1.80503500	0.99450500	H	1.95918000	-1.03546600	-0.52103800
H	-1.45935900	2.09492500	1.87539500	H	-1.90228000	-2.92951500	-0.18745900
H	-1.86490000	-1.97131900	0.63134000	C	7.52703200	-0.32779700	-2.37827200
H	2.31590600	-2.52180700	0.76906300	C	8.58586500	-1.15562600	-1.60730400
C	-0.10716400	0.64355800	5.51217000	C	7.92037200	-2.46484800	-2.10781400
C	-1.14242200	-0.26117800	6.19595000	C	7.12891700	-1.61678300	-3.13067300
C	-0.63228000	-1.68307700	5.88703800	H	6.73114100	0.02427700	-1.71506700
C	0.05299400	-1.59357800	4.49860100	H	7.89356500	0.52327700	-2.95295400
C	0.13913200	-0.07970200	4.18090200	H	9.59639000	-1.00612700	-1.99200500
H	-0.44672600	1.67154500	5.36073800	H	7.50760900	-1.67972700	-4.15087700
H	0.81768800	0.67483700	6.10298400	N	5.65144600	-1.89009900	-3.18926800
H	-2.13396500	-0.09945900	5.75744600	H	5.17614300	-1.23059000	-3.81416300
H	-1.22127200	-0.07230200	7.26938400	H	5.45843900	-2.83297500	-3.54283700
H	0.12305600	-1.97978200	6.62057700	H	5.20517200	-1.80301500	-2.22901500
H	-1.42049500	-2.44151600	5.91263300	H	7.28385100	-2.89474000	-1.32921200
H	-0.64662600	0.17091300	3.46567100	H	8.57086900	-3.24007600	-2.51753200
N	1.40271100	0.35712200	3.51003000	N	8.59520200	-0.93783400	-0.14974600
H	1.70158300	-0.20847500	2.68910600	H	9.23899700	-1.57873200	0.34316600
H	1.22509400	1.29699900	3.07646300	H	8.74882400	0.12120300	0.03694500
H	2.19505400	0.41098600	4.15655900	H	7.67532000	-1.25351500	0.28774500
H	1.03209300	-2.07656900	4.50484100	CPDA-T2			
N	-0.73915000	-2.29497600	3.42189400	E = -6428.01255			
H	-1.55394300	-1.73769800	3.11746000	O	-4.51048000	9.35830500	0.26260400
H	-0.18442400	-2.45276200	2.53419700	C	-5.54869200	9.63388100	-0.68089500
H	-1.06794400	-3.20933600	3.74506200	C	-6.69453800	8.62193800	-0.68662400
CPDA-S1				O	-6.21158900	7.33648900	-1.13976300
E = -6427.98332				C	-7.38484600	8.36503200	0.66814700
O	2.55394900	9.32320800	-1.16440600	O	-8.74480600	8.09116000	0.42670400
C	3.20489200	9.72998800	0.04221100	C	-6.63456300	7.12636400	1.18604200
C	4.41652100	8.88436500	0.43201700	C	-6.32925300	6.36330800	-0.10654700
O	3.99121200	7.53879000	0.75401700	N	-5.09322800	5.58156300	-0.07040100
C	5.52174800	8.73649100	-0.63286200	C	-3.80759200	6.08031700	0.02085700
O	6.76072600	8.63856400	0.02931900	N	-2.89201000	5.13942900	-0.01749500
C	5.13520800	7.41633500	-1.32203500	C	-3.60474200	3.95767000	-0.14294100
C	4.54901200	6.60652200	-0.16305700	C	-3.15475900	2.60829200	-0.23169100
N	3.49564300	5.66556000	-0.55693100	O	-1.98919300	2.17862200	-0.21704000
C	2.25142900	5.98813300	-1.06101100	N	-4.23223300	1.71018100	-0.34808800
N	1.49453800	4.93359000	-1.27041100	C	-5.56302200	2.07023600	-0.39477900
C	2.27699400	3.86019300	-0.88703000	N	-6.46816800	1.08603700	-0.57005500
C	1.98469300	2.46524000	-0.85955100	N	-5.98291100	3.32923400	-0.30873900

O	0.93315400	1.88025200	-1.16846000	C	-4.97500800	4.21436900	-0.18553800
N	3.07975500	1.72426400	-0.37669200	O	-9.48939400	6.80388700	2.56644900
C	4.25130100	2.26270700	0.09084000	P	-9.82675900	8.09199700	1.79575700
N	5.12279800	1.37807400	0.70420400	O	-11.17671800	8.07952600	1.07268900
N	4.53102500	3.54851900	0.06919000	O	-9.48028800	9.39196000	2.53696000
C	3.51933300	4.29839000	-0.42803000	O	6.50481300	-1.28637700	2.16127600
O	8.26061500	7.35821500	-1.67267500	P	7.42428600	-2.12981300	3.10534300
P	8.21077800	8.71084400	-0.94101600	O	7.29344700	-1.78043200	4.57566600
O	9.26152400	8.89047100	0.15852100	O	8.85960700	-2.21485200	2.53966000
O	7.98286100	9.92616700	-1.85103100	O	6.81317400	-3.71031700	3.03431800
O	-7.63810800	-2.24418800	-0.61908100	C	6.94435300	-4.39573200	1.80311700
P	-8.10076100	-2.83029700	-1.98032400	C	6.34621800	-5.79361300	1.91527200
O	-7.51949800	-2.13141700	-3.20915700	O	4.91869600	-5.75757900	2.18750000
O	-9.60115200	-3.13505700	-2.02204000	C	6.50146200	-6.61421900	0.61728000
O	-7.32852400	-4.36832300	-2.07348000	O	6.76089900	-7.99633900	0.85758400
C	-7.42617600	-5.18297700	-0.93047100	C	5.16090400	-6.36312900	-0.08570800
C	-6.75752600	-6.53446500	-1.17138700	C	4.18364200	-6.28418700	1.09358500
O	-5.34178400	-6.41263200	-1.49124200	N	2.99204900	-5.47337200	0.84412000
C	-6.81380200	-7.45037100	0.06708500	C	1.70073300	-5.95914900	0.78014600
O	-6.96307400	-8.83170400	-0.26426900	N	0.81184100	-5.03712300	0.49835500
C	-5.47767300	-7.13929400	0.75492900	C	1.54751300	-3.87145200	0.37677500
C	-4.53943200	-6.92692800	-0.43967900	C	1.12338700	-2.53437900	0.10346400
N	-3.40585900	-6.03950900	-0.17844600	O	-0.02452500	-2.12334900	-0.12104900
C	-2.07670300	-6.42488700	-0.16980300	N	2.20837500	-1.63432900	0.12452700
N	-1.25136900	-5.44739000	0.11084200	C	3.51812900	-1.98561000	0.34931700
C	-2.07170100	-4.34199200	0.28542200	N	4.48241600	-1.00509700	0.32561300
C	-1.75804000	-2.99300700	0.58700600	N	3.91209900	-3.23030900	0.55785000
O	-0.62199800	-2.51196400	0.81995700	C	2.90163600	-4.11861500	0.58843900
N	-2.88779400	-2.17003900	0.60368900	O	-5.65472200	-8.16749300	1.55580600
C	-4.19525700	-2.60279700	0.39670100	C	-6.97969600	-7.97939200	2.04625300
N	-5.17919300	-1.70310100	0.41227500	C	-7.87306100	-7.11936100	1.15725900
N	-4.48505200	-3.89198000	0.19118600	O	-7.42090500	-5.74619500	1.20276800
C	-3.41538500	-4.68645700	0.10884900	C	-7.92475800	-7.52721500	-0.34143900
O	5.28993900	-7.93982700	-1.79898000	O	-9.27103600	-7.55070600	-0.75465800
C	6.43305400	-7.61116300	-2.58474900	C	-7.12430400	-6.40227100	-1.02524200
C	7.36608700	-6.57719100	-1.95939100	C	-7.46705600	-5.22308900	-0.12201200
O	6.73357500	-5.27458300	-1.98289700	N	-6.60801100	-4.04981300	-0.20295600
C	7.78149400	-6.84698000	-0.48683300	C	-7.08731300	-2.75536600	-0.28338000
O	9.17016800	-6.64803600	-0.36618600	N	-6.14293700	-1.84937000	-0.32293200
C	6.97537300	-5.78700400	0.28850600	C	-4.96632200	-2.57562400	-0.25478300
C	6.96958300	-4.64936300	-0.72623500	C	-3.61314800	-2.12403600	-0.26240100
N	5.99072800	-3.58610700	-0.53043500	O	-3.19207100	-0.95926100	-0.34193000
C	6.30567800	-2.23880100	-0.53773600	N	-2.70818700	-3.19500100	-0.16668000
N	5.27281000	-1.45429600	-0.35747300	C	-3.06730800	-4.52453800	-0.09335400
C	4.20389800	-2.32757400	-0.23410900	N	-2.07355600	-5.43626400	-0.05847800
C	2.83091800	-2.06431500	-0.01446400	N	-4.32859700	-4.94369800	-0.09040700
O	2.29317000	-0.93269600	0.09385900	C	-5.22768800	-3.94378400	-0.17406200
N	2.06530600	-3.22133300	0.09285700	P	-9.63508700	-8.33660500	-2.26940100
C	2.57454800	-4.50275300	-0.01382300	O	-11.15951300	-8.43921600	-2.16180300
N	1.71530700	-5.52385500	0.15277100	O	-8.87032300	-9.66671400	-2.18644800
N	3.85981100	-4.75797600	-0.24178400	O	-9.12363200	-7.37060600	-3.35204400

C	4.62425100	-3.65706800	-0.33415500	O	9.14462400	1.70182900	-2.18251000
P	9.95094900	-7.27900000	1.06310500	P	9.40994500	2.55136600	-0.93189000
O	11.41982800	-7.11350700	0.66238100	O	10.74982700	3.28140100	-0.89442200
O	9.44067200	-8.72557700	1.14683200	O	9.01530700	1.84455700	0.39087200
O	9.48156700	-6.36535800	2.20849100	O	8.20910900	3.78419400	-0.95673700
O	-8.78314300	2.45665600	3.56070500	C	8.23432900	4.67283700	-2.05153400
P	-9.35461700	1.85427300	2.26952800	C	7.23706700	5.80562000	-1.84653000
O	-10.86877200	1.60798400	2.28155500	O	5.87917300	5.30898000	-1.90275800
O	-8.52135200	0.72219200	1.64422100	C	7.35412900	6.53337100	-0.49959200
O	-9.11754200	3.08434900	1.06422300	O	6.96485800	7.89219600	-0.72578800
C	-9.20375300	4.43665200	1.42479500	C	6.34441900	5.78508100	0.37442900
C	-8.43641400	5.29718600	0.42651000	C	5.24617300	5.41945500	-0.63305100
O	-7.01696100	5.02273700	0.50827800	N	4.53895100	4.17898600	-0.33528700
C	-8.81274300	5.06978700	-1.04467300	C	5.07528000	2.91284100	-0.15649900
O	-8.61986700	6.31611700	-1.72399100	N	4.15411400	1.98779700	-0.01351000
C	-7.80155300	4.01066900	-1.48980700	C	2.94922800	2.66683400	-0.11189300
C	-6.55563800	4.38901000	-0.67814500	C	1.60627000	2.19132300	-0.05780300
N	-5.69240700	3.26158700	-0.33593500	O	1.20316800	1.02582500	0.09435100
C	-6.02905100	2.08389300	0.32266200	N	0.67759300	3.23829300	-0.20875900
N	-4.98502200	1.31209200	0.52996600	C	1.00360700	4.56375300	-0.40536300
C	-3.91143400	2.00327400	-0.00762800	N	-0.01049200	5.43640300	-0.58117400
C	-2.53263800	1.68099700	-0.05568100	N	2.25623500	5.00561300	-0.46539900
O	-1.97387900	0.65304200	0.39821100	C	3.16915300	4.02680700	-0.31876700
N	-1.77742200	2.67091400	-0.69625400	H	-5.96279500	10.64031700	-0.52333200
C	-2.29313400	3.84341800	-1.21161800	H	-5.06533200	9.62139500	-1.66291900
N	-1.43354300	4.67128100	-1.85055500	H	-7.44372200	8.97050000	-1.40793900
N	-3.57985900	4.16278300	-1.14394200	H	-7.28950200	9.21876000	1.35452800
C	-4.33240500	3.21939900	-0.54627200	H	-7.27063700	6.56873000	1.87606200
H	3.50892400	10.78504300	-0.01438800	H	-5.69739300	7.40553900	1.67873900
H	2.44913700	9.64190400	0.82910200	H	-7.11847200	5.64671900	-0.35404100
H	4.85139600	9.32157100	1.33900100	H	-3.63154600	7.14491800	0.10207500
H	5.53500200	9.57743800	-1.34118700	H	-7.43607500	1.36203200	-0.48139900
H	6.02151300	6.95552500	-1.76272900	H	8.00705900	-4.50263700	1.53877900
H	4.36932500	7.57578700	-2.08776800	H	6.43843000	-3.84519600	0.99987600
H	5.30884700	5.99702800	0.33517700	H	6.81825000	-6.31919300	2.75373800
H	1.97594500	7.02034300	-1.23420900	H	7.34659300	-6.26903100	0.01694800
H	6.04527600	1.79013100	0.81845700	H	5.18358200	-5.40378500	-0.61070100
H	-8.48319200	-5.39151400	-0.68600200	H	4.90507400	-7.15312400	-0.79519800
H	-6.96911000	-4.69153900	-0.06450300	H	3.79259600	-7.27715200	1.35161200
H	-7.22940600	-7.02487200	-2.03131200	H	1.48729700	-7.00614600	0.94828100
H	-7.66765300	-7.21723700	0.70787100	H	4.18037200	-0.02252500	0.28970400
H	-5.55609100	-6.21286900	1.33067400	H	-6.87171400	-7.49417100	3.02202400
H	-5.14708300	-7.94506800	1.41428600	H	-7.48248200	-8.94504300	2.20855800
H	-4.07948700	-7.87344400	-0.75366300	H	-8.89567500	-7.16728000	1.55609700
H	-1.79005200	-7.44681700	-0.37900700	H	-7.47147400	-8.51222500	-0.52239000
H	-4.99012900	-0.70396000	0.53202400	H	-6.04873800	-6.59159600	-0.97823600
H	6.04448200	-7.21635300	-3.52936600	H	-7.45803800	-6.28315200	-2.05736000
H	7.02353900	-8.51027800	-2.81767400	H	-8.47775600	-4.85723600	-0.34708600
H	8.28017800	-6.53291700	-2.56686500	H	-8.15040800	-2.55802000	-0.31521000
H	7.52864200	-7.86630400	-0.16220000	H	-1.09596000	-5.19949000	0.15077900
H	5.94920900	-6.11877200	0.46887500	H	9.23663700	5.11215400	-2.17589700

H	7.48069300	-5.54512400	1.22476800	H	7.98509300	4.15091400	-2.98838200
H	7.94445300	-4.14430300	-0.73067800	H	7.35615300	6.52895100	-2.66235800
H	7.32716900	-1.90940400	-0.67271100	H	8.37236900	6.48180700	-0.09547000
H	0.69134600	-5.41801500	0.14674800	H	5.96081300	6.39047800	1.20093100
H	-10.25157600	4.79436300	1.44159300	H	6.81021000	4.88320300	0.77543000
H	-8.78845200	4.59801000	2.42822800	H	4.46646400	6.18534800	-0.67793600
H	-8.58275900	6.35493900	0.67910200	H	6.14676400	2.75419300	-0.15468200
H	-9.84907400	4.72658300	-1.15157800	H	0.25913900	6.41023200	-0.60386300
H	-7.61096700	4.02398800	-2.56715900	H	5.22755300	-1.17704600	1.04239400
H	-8.15930800	3.02230700	-1.19751200	H	-2.36472400	-6.38681900	0.12304000
H	-5.90959500	5.07801600	-1.23051100	H	-6.25355300	0.08636400	-0.46577700
H	-7.04393500	1.84376800	0.64757900	H	-0.98643200	5.23314900	-0.32648900
H	-1.82650500	5.57043600	-2.09627300	H	-5.71266700	-8.73551200	0.77135900
H	-6.11786800	-1.98070900	0.01040900	H	-4.83975200	9.58664600	1.14616500
H	2.09010400	-6.44542300	-0.02477300	H	6.10706600	-8.32827500	1.49442900
H	5.17526200	0.43015200	0.29419200	H	6.97446400	8.34367100	0.13371100
H	-0.42481700	4.66848000	-1.65455200	H	-3.97127300	0.71199500	-0.38797800
H	5.59968000	-8.44836200	-1.03293600	H	-0.31607000	2.95575700	-0.19628300
H	3.10023800	9.61255700	-1.91212100	H	1.95506700	-0.63460400	0.04427800
H	-6.33036500	-9.04771900	-0.96861000	H	-1.71062900	-2.93046600	-0.15416200
H	-8.79105600	6.16184300	-2.66724100	C	9.77847600	-1.64193600	-1.55972800
H	2.92220000	0.70674500	-0.28969700	C	9.45168200	-2.08501000	-2.99166800
H	-0.77773500	2.45938300	-0.84319100	C	8.25915000	-1.18247700	-3.37548200
H	-2.70342200	-1.16026900	0.66252400	C	7.53256400	-0.86150600	-2.04373700
H	1.06075200	-3.08668100	0.29768500	C	8.38835800	-1.49676300	-0.92183300
C	2.29535300	2.21742100	3.95054200	H	10.41370100	-2.34200200	-1.00816800
C	1.24619800	1.95960600	2.85533800	H	10.25459700	-0.65562800	-1.57541200
C	0.88219000	0.48114400	3.05051900	H	9.15807900	-3.14222800	-3.00352500
C	2.21751300	-0.20793500	3.40850500	H	10.29670300	-1.97129600	-3.67701300
C	3.03808200	0.87176800	4.15084500	H	8.61914700	-0.23331200	-3.77738000
H	2.96873300	3.04332100	3.70383200	H	7.59717500	-1.64035300	-4.11849100
H	1.80529700	2.47755400	4.89317300	H	7.99940500	-2.49438000	-0.68011200
H	1.68222900	2.10459100	1.86259700	N	8.40161400	-0.72393200	0.33768300
H	0.37950800	2.62042200	2.93789600	H	7.48091800	-0.76078500	0.85039900
H	2.08287700	-1.11097600	4.00774000	H	8.94834900	-1.23848800	1.07738400
H	2.72708000	-0.49629800	2.48301600	H	8.71632300	0.31275900	0.24404000
H	3.15493700	0.63923800	5.20927400	H	7.47440600	0.21942300	-1.90644300
N	4.46040800	0.91482800	3.61954800	N	6.11401100	-1.39284400	-2.04590600
H	5.00398600	1.64268200	4.09548700	H	5.56633800	-1.20059700	-1.15874400
H	4.94095000	0.02715300	3.80366600	H	5.58076400	-0.96878300	-2.81151900
H	4.54732000	1.09306400	2.58838700	H	6.09008900	-2.40647000	-2.19885800
H	0.15837400	0.37238500	3.86198800	1,2-CHDA-1			
N	0.26109800	-0.12387400	1.83367700	E = -6467.27850			
H	-0.15350000	-1.05920200	1.98104800	O	-4.05373600	9.06678700	-0.06279200
H	-0.50774200	0.43906800	1.41105400	C	-4.83077800	9.22062600	-1.25403500
H	0.96128500	-0.30349800	1.08443300	C	-5.93114000	8.17584700	-1.43511800
1,2-CHDA-2				O	-5.33819600	6.87172700	-1.63947500
E = -6467.33863				C	-6.91785100	8.02354500	-0.25985900
O	-4.51431200	-9.45234400	-0.33965400	O	-8.19480700	7.72377100	-0.77250800
C	-5.50814500	-9.74236800	0.64696700	C	-6.31936100	6.84235400	0.52296200

C	-6.68327400	-8.76531400	0.67764700	C	-5.68306200	5.98956600	-0.57987000
O	-6.22050300	-7.45965900	1.09287600	N	-4.47234100	5.28020900	-0.15446300
C	-7.42562600	-8.55358600	-0.65773200	C	-3.28869100	5.85674700	0.26805900
O	-8.78791200	-8.32492600	-0.38123700	N	-2.37207500	4.97419900	0.58982900
C	-6.73680300	-7.29788000	-1.21695400	C	-2.97406200	3.74629700	0.36113100
C	-6.41770400	-6.50553100	0.05391200	C	-2.49571600	2.43107100	0.54197000
N	-5.22082000	-5.67159000	-0.04335100	O	-1.37122400	2.07903400	1.00635700
C	-3.92604800	-6.10809900	-0.24959600	N	-3.41668500	1.46033000	0.15423500
N	-3.05526600	-5.12534300	-0.27890900	C	-4.68660400	1.73392200	-0.32418700
C	-3.80862600	-3.97977900	-0.07833800	N	-5.45235100	0.69207900	-0.68721800
C	-3.41776600	-2.61005400	-0.02098800	N	-5.16173800	2.97042900	-0.45632100
O	-2.28327700	-2.12281900	-0.15667300	C	-4.27877700	3.92039100	-0.11609200
N	-4.51818800	-1.76757600	0.22207800	O	-9.39127400	6.69385900	1.30084900
C	-5.82109000	-2.19112000	0.37972400	P	-9.54202700	7.87699100	0.32931400
N	-6.74842100	-1.25150000	0.66338400	O	-10.71217600	7.76288100	-0.65118900
N	-6.18977000	-3.46599300	0.30183400	O	-9.33865000	9.25967500	0.96650700
C	-5.15623300	-4.30158400	0.08053800	O	7.99810300	-1.28908000	0.91158800
O	-9.61031200	-7.07242500	-2.51505900	P	8.66965800	-2.08122300	2.06486900
P	-9.89778800	-8.36320700	-1.72859200	O	8.14966200	-1.74546900	3.46286800
O	-11.23355500	-8.37865900	-0.98009100	O	10.19094600	-2.17921200	1.91675200
O	-9.53271800	-9.65937100	-2.46726900	O	8.09312600	-3.69351800	1.86753200
O	6.52988400	1.74592100	-1.19347600	C	8.14836600	-4.20875400	0.55992500
P	6.80725700	2.47760200	-2.50024500	C	7.69092600	-5.66427000	0.53413500
O	6.34632600	1.90048700	-3.81074000	O	6.33264800	-5.83188200	1.03148200
O	8.39309300	2.84774200	-2.55790800	C	7.67345300	-6.25064500	-0.89049500
O	6.13128500	3.99413000	-2.43837700	O	8.02229500	-7.63479600	-0.93306600
C	6.33829100	4.74903200	-1.24838100	C	6.22654400	-5.98166200	-1.32808100
C	5.74779400	6.14327800	-1.41531800	C	5.44843300	-6.18145000	-0.02095700
O	4.32466400	6.10827100	-1.69193100	N	4.20593900	-5.41452900	0.07817900
C	5.89599400	6.99430000	-0.13800400	C	2.93941100	-5.96663100	0.15467300
O	6.09644400	8.37891200	-0.41449900	N	1.98397700	-5.07557800	0.23434800
C	4.57360500	6.70631200	0.58638500	C	2.64598300	-3.85699300	0.21432800
C	3.58055300	6.58467300	-0.57723000	C	2.15480700	-2.53703900	0.33680600
N	2.43294400	5.72011100	-0.31899800	O	0.95316000	-2.18463600	0.49498500
C	1.12131700	6.15487300	-0.25425000	N	3.16480100	-1.57671200	0.30011300
N	0.27147200	5.19797700	0.02239300	C	4.52886800	-1.85577900	0.21181200
C	1.05323500	4.06019500	0.14016800	N	5.39358500	-0.84468700	0.25780600
C	0.68030400	2.70908700	0.40508500	N	4.98284100	-3.10904400	0.09718000
O	-0.45650000	2.25406400	0.61788900	C	4.03045100	-4.04289000	0.12077000
N	1.79318300	1.85118200	0.39436700	O	-4.44704200	-8.63013400	0.93956500
C	3.10172300	2.24281200	0.16515300	C	-5.81570500	-8.56465000	1.33280900
N	4.05625000	1.30064500	0.16864900	C	-6.68346600	-7.64593300	0.47742500
N	3.44432600	3.51565600	-0.04669600	O	-6.31624000	-6.26780300	0.72367200
C	2.39993200	4.35776800	-0.07021100	C	-6.59145600	-7.86803400	-1.05758300
O	-6.09552000	7.94647500	-1.62436700	O	-7.89486400	-7.88056600	-1.59097100
C	-7.39419100	7.74017300	-2.17455500	C	-5.78269000	-6.64295900	-1.52466800
C	-8.32134000	6.87659300	-1.32399800	C	-6.26768000	-5.59392500	-0.53088400
O	-7.83239500	5.51691800	-1.31130900	N	-5.46903200	-4.38323700	-0.39120400
C	-8.48791200	7.31334200	0.15856600	C	-6.00754200	-3.11031100	-0.35795900
O	-9.86295600	7.35985800	0.46132300	N	-5.11460600	-2.16929600	-0.18266900
C	-7.75041000	6.20061600	0.92830900	C	-3.91162500	-2.84777200	-0.08625100

C	-7.98069100	5.00458800	0.01033300	C	-2.59375300	-2.34858800	0.11529800
N	-7.09233200	3.86183000	0.17382800	O	-2.22945200	-1.16594500	0.27002800
C	-7.52020900	2.54722700	0.17684600	N	-1.64476300	-3.38194300	0.14094900
N	-6.54421700	1.68003800	0.27847800	C	-1.93752200	-4.72664100	0.01836800
C	-5.39793700	2.45529300	0.33521800	N	-0.91532700	-5.59444600	0.10307700
C	-4.02993200	2.06243600	0.44476100	N	-3.17118700	-5.19080800	-0.15793000
O	-3.56290000	0.91442300	0.52045300	C	-4.10646600	-4.22585200	-0.20851400
N	-3.17060300	3.17396800	0.46400100	P	-8.09336100	-8.52080900	-3.20364900
C	-3.58234500	4.48801000	0.39698200	O	-9.62012600	-8.61850300	-3.26869300
N	-2.63272000	5.44356200	0.48092800	O	-7.34124800	-9.85977400	-3.16126600
N	-4.85622400	4.85222100	0.29205500	O	-7.46796700	-7.46418900	-4.12983200
C	-5.71205100	3.81283400	0.26748500	O	8.35242500	2.28754400	-3.83095600
P	-10.33176400	8.18934400	1.92194200	P	8.96310500	2.50644900	-2.44090400
O	-11.84693900	8.27123200	1.71382000	O	10.49342100	2.42626600	-2.37999500
O	-9.57661000	9.52527900	1.84551700	O	8.24248700	1.78661600	-1.28485000
O	-9.88114100	7.26367200	3.06521700	O	8.60290100	4.16046800	-2.04818300
O	7.77977700	-2.25980200	4.08415300	C	8.30754600	5.07929100	-3.06705200
P	8.23028200	-2.25741900	2.64889400	C	7.26126000	6.08228500	-2.59264900
O	9.83977900	-2.54094800	2.61388500	O	5.98719900	5.42056000	-2.39575100
O	7.87992900	-1.12303700	1.70560500	C	7.58956100	6.76434200	-1.25461100
O	7.62273800	-3.60332700	1.87252500	O	7.05949000	8.09399400	-1.31739000
C	7.60213000	-4.85481400	2.54673900	C	6.83954700	5.89566500	-0.24325300
C	6.79662700	-5.85602900	1.73007100	C	5.58645000	5.50711400	-1.03454600
O	5.41496000	-5.44658900	1.66254200	N	4.97166900	4.25061400	-0.62288800
C	7.25303200	-6.03230100	0.27297200	C	5.55444100	2.99020300	-0.54643600
O	6.98324200	-7.39175000	-0.07924000	N	4.69934200	2.07093600	-0.15481000
C	6.35366900	-5.05102100	-0.48365100	C	3.49932900	2.74159100	0.02334000
C	5.05200300	-5.09852300	0.32790800	C	2.22248000	2.27726700	0.42147400
N	4.29603400	-3.85273100	0.32944700	O	1.89303700	1.10581600	0.73178800
C	4.74437600	-2.56814000	0.60422600	N	1.26610600	3.30080600	0.44463600
N	3.77646400	-1.68167500	0.59342400	C	1.52630600	4.63118400	0.17092200
C	2.62983800	-2.40682100	0.31061600	N	0.51681000	5.50770600	0.32488700
C	1.27063900	-1.98895700	0.20419600	N	2.72344000	5.07046900	-0.19974600
O	0.80158800	-0.84724300	0.33673500	C	3.65120700	4.09872300	-0.26874400
N	0.41668700	-3.07175400	-0.08222800	H	-5.27925100	10.22326000	-1.29983700
C	0.82315800	-4.37894800	-0.24612600	H	-4.12157800	9.13312500	-2.08312700
N	-0.11721900	-5.28876100	-0.57863500	H	-6.49185300	8.43154800	-2.34235900
N	2.08898400	-4.76981700	-0.12888400	H	-6.96854000	8.93198400	0.35700000
C	2.93112900	-3.75635800	0.14953200	H	-7.11005000	6.32596700	1.07033100
H	-5.89593400	-10.76374700	0.52225400	H	-5.54532400	7.17991600	1.21977500
H	-4.98972100	-9.69713100	1.61000000	H	-6.35893700	5.21029300	-0.94502700
H	-7.39685200	-9.12367400	1.43002900	H	-3.17930200	6.93358300	0.29383200
H	-7.31938200	-9.41432000	-1.33375100	H	-6.40010400	0.91738700	-0.95620300
H	-7.41376300	-6.77401600	-1.89445500	H	9.18390300	-4.19322000	0.17584700
H	-5.80684100	-7.55328500	-1.73499000	H	7.52717300	-3.61154600	-0.11586000
H	-7.22710000	-5.82001500	0.32310700	H	8.33644300	-6.26236300	1.18825800
H	-3.70694100	-7.16282200	-0.35218500	H	8.39611100	-5.75512000	-1.54336100
H	-7.70647200	-1.57325000	0.64571700	H	6.11966700	-4.94801200	-1.66826200
H	7.41576100	4.85951100	-1.05615200	H	5.89673800	-6.65545500	-2.12199300
H	5.87430500	4.23765300	-0.40116300	H	5.13262200	-7.22642500	0.09482300
H	6.22454400	6.64174000	-2.26690500	H	2.79663600	-7.03894300	0.14065200

H	6.76211400	6.69445700	0.45704400	H	5.08199600	0.13137900	0.23337300
H	4.63404200	5.75563500	1.12356400	H	-5.81351600	-8.19644500	2.36413100
H	4.30240200	7.49647600	1.28993400	H	-6.27400600	-9.56539900	1.33768700
H	3.14091900	7.55945700	-0.82387100	H	-7.72993200	-7.79017500	0.77880400
H	0.86758900	7.19356500	-0.41821300	H	-6.08355100	-8.80931800	-1.31221900
H	3.84495300	0.31018900	0.32017600	H	-4.70981500	-6.80167300	-1.38925300
H	-7.23410900	7.24871600	-3.14000700	H	-6.01815100	-6.41285400	-2.56479900
H	-7.89960100	8.69854000	-2.36888000	H	-7.27104100	-5.24669800	-0.81079300
H	-9.31682200	6.89064700	-1.78931700	H	-7.07093300	-2.95320600	-0.47860300
H	-8.03959300	8.29798500	0.35443000	H	0.07564200	-5.32762400	0.16673500
H	-6.67850400	6.40513900	0.98826300	H	9.20302700	5.65595600	-3.37057000
H	-8.18140900	6.08938900	1.92481400	H	7.93340500	4.55889300	-3.95706200
H	-8.99497000	4.60638800	0.14848400	H	7.12496400	6.85178200	-3.36367900
H	-8.57219400	2.30506400	0.10739100	H	8.66943900	6.78712400	-1.06486400
H	-1.63393500	5.25857600	0.31743500	H	6.59924900	6.42162400	0.68572700
H	8.62384500	-5.23876300	2.68345300	H	7.43251600	5.00689900	-0.01917500
H	7.14361500	-4.74477200	3.53645600	H	4.79738100	6.25794700	-0.92410600
H	6.83687500	-6.82617900	2.23968600	H	6.59860700	2.78652700	-0.81561000
H	8.31797900	-5.80134700	0.14679600	H	0.69708300	6.45036200	0.00953200
H	6.19638800	-5.33461500	-1.52812600	H	6.40715600	-1.06361800	0.46751700
H	6.79203000	-4.05215600	-0.45113600	H	-1.14052400	-6.56814300	-0.04159700
H	4.35894800	-5.84911600	-0.06192100	H	-5.24966800	-0.28837500	-0.44593500
H	5.78339800	-2.35695200	0.82359500	H	-0.46201000	5.23879100	0.48345100
H	0.19264400	-6.25076800	-0.56185000	H	-4.40926200	-9.10439300	0.09396400
H	4.96355500	1.53871400	-0.26323100	H	-4.58631400	9.38023400	0.68507600
H	-2.95565900	6.38287700	0.29305500	H	7.51227000	-8.10130100	-0.25084000
H	-6.59414900	-0.24783900	0.50128800	H	7.21494400	8.50930900	-0.45348600
H	-1.12713200	-5.12898800	-0.46259600	H	-3.09431100	0.47872200	0.20239000
H	-6.19546700	8.51852400	-0.84701900	H	0.30194100	3.00478100	0.64232300
H	-4.86655700	-9.71354900	-1.20504300	H	2.86105000	-0.59934500	0.40131600
H	5.42225500	8.66710600	-1.05152000	H	-0.66438700	-3.08129500	0.24864700
H	7.21540400	-7.50244500	-1.01554800	C	-0.87985100	-0.35124100	3.12896200
H	-4.29220000	-0.76354600	0.31277200	C	-1.21682100	-1.73139100	3.71362300
H	-0.58616200	-2.83491800	-0.15741000	C	-1.02841800	0.72935700	4.21176700
H	1.56950100	0.84637900	0.46701800	H	-1.54425800	-0.13660200	2.28971800
H	-2.16245900	2.95486600	0.53001400	C	-2.64029700	-1.75381900	4.28751600
C	10.93312600	0.89559700	-0.86862300	H	-0.49243300	-1.98258100	4.50027300
C	12.01336800	1.98282000	-0.98080800	C	-2.45816300	0.72529000	4.77440200
C	11.35693700	-0.22471400	0.11577500	H	-0.31123900	0.56251500	5.02120400
H	10.79707600	0.43303300	-1.85766600	C	-2.82729500	-0.65412000	5.33943300
C	13.38855600	1.40499400	-1.34038200	H	-2.83883600	-2.73795300	4.72461000
H	12.08312800	2.51044000	-0.01687400	H	-3.36234900	-1.61507200	3.47214100
C	12.74330100	-0.78216400	-0.24330600	H	-2.53478100	1.48881800	5.55688300
H	11.40937000	0.22216500	1.12029000	H	-3.15981600	1.00201500	3.97654200
C	13.80884400	0.31655600	-0.34310700	H	-3.86424100	-0.62953200	5.69019500
H	14.13455300	2.20876500	-1.36813500	H	-2.20033800	-0.86879800	6.21490500
H	13.35094000	0.97621100	-2.35224700	N	-0.71756900	2.11116100	3.66414800
H	13.02699000	-1.53545400	0.50140000	H	-1.15641800	2.83361400	4.24512400
H	12.67130000	-1.30686400	-1.20878900	H	0.28654900	2.31558800	3.67334900
H	14.77086400	-0.12079300	-0.63749600	H	-1.06201200	2.23202600	2.67317900
H	13.95978400	0.76949000	0.64749200	H	-1.10952400	-2.48344300	2.92560200

N	10.39458100	-1.33431400	0.20152200	N	0.49671800	-0.39012700	2.52691600
H	10.21106700	-2.24374200	1.72952800	H	0.57588800	-1.15755100	1.80676600
H	9.45004000	-1.00569200	0.43411900	H	0.78565600	0.44767800	1.97223800
H	10.33700000	-1.81898300	-0.69513100	H	1.22239300	-0.56389600	3.23002300
H	11.69536200	2.72574100	-1.72220800	1,3-CHDA-1			
N	9.64943100	1.53888600	-0.52856100	E = -6467.27384			
H	8.88817500	2.43190100	-1.77946200	O	-2.89891600	9.36933800	-0.73829100
H	8.89383700	0.86252600	-0.41296900	C	-3.88274800	9.63308400	-1.74202400
H	9.72938100	2.03021200	0.36279900	C	-5.10779800	8.72055200	-1.69188800
1,3-CHDA-2				O	-4.71445800	7.36150800	-1.99625600
E = -6467.29899				C	-5.85801100	8.65759300	-0.34552600
O	-3.40032600	9.32580900	0.46043900	O	-7.22851500	8.46520700	-0.60819700
C	-4.02527100	9.82019400	-0.72709900	C	-5.22546000	7.42304900	0.31912800
C	-5.14179800	8.93316900	-1.27731800	C	-4.95988600	6.51215400	-0.88186300
O	-4.58871200	7.67781700	-1.73861300	N	-3.80881400	5.62315400	-0.71632000
C	-6.26705600	8.56789200	-0.28868100	C	-2.48630100	6.00335100	-0.59043900
O	-7.47841800	8.46674500	-0.99945700	N	-1.67050700	4.98302600	-0.45215000
C	-5.80279900	7.20217000	0.24563300	C	-2.49612500	3.86902700	-0.48885800
C	-5.08872300	6.59420800	-0.96550100	C	-2.19723000	2.48711500	-0.36877700
N	-3.96739400	5.71701900	-0.61675300	O	-1.08128200	1.94681600	-0.21459200
C	-2.79883400	6.09002100	0.02009000	N	-3.34683800	1.68832100	-0.42038800
N	-1.97256700	5.08636500	0.20463800	C	-4.63284300	2.16392500	-0.59173900
C	-2.62350200	3.99195200	-0.34137300	N	-5.62254900	1.25505500	-0.65432100
C	-2.23852900	2.62991600	-0.42372300	N	-4.91630000	3.45724000	-0.71582200
O	-1.18091700	2.11514700	0.01245900	C	-3.82982400	4.24917400	-0.65341700
N	-3.19406700	1.84730400	-1.07857400	O	-8.08865400	7.34075400	1.58147400
C	-4.39802300	2.31935400	-1.56750100	P	-8.33510100	8.60271200	0.73620300
N	-5.19018100	1.43147500	-2.21121000	O	-9.66974100	8.62539700	-0.01377900
N	-4.77763000	3.58700500	-1.46690500	O	-7.92536700	9.91893600	1.41280400
C	-3.86262100	4.36930600	-0.86554300	O	7.60008900	-2.41510500	0.21418700
O	-8.94051600	7.05184800	0.63138700	P	8.13427000	-2.94847300	1.56946600
P	-8.95074500	8.42563400	-0.06120600	O	7.54396500	-2.26771900	2.80495800
O	-9.98611600	8.58171700	-1.17859200	O	9.65215600	-3.15238800	1.57490600
O	-8.81152800	9.62248500	0.89156800	O	7.46436500	-4.53265800	1.70438200
O	7.67266000	-2.06788400	0.55866900	C	7.42936000	-5.30829500	0.53141500
P	8.18549300	-3.15217600	1.54298800	C	6.77644100	-6.66188900	0.80257800
O	7.62896300	-3.04670400	2.96258400	O	5.41903800	-6.53268400	1.31179400
O	9.69185100	-3.40293300	1.42414300	C	6.65179100	-7.52384500	-0.46919200
O	7.44396800	-4.61242300	1.00541900	O	6.82303900	-8.91968100	-0.21834200
C	7.60840300	-4.91143600	-0.35990700	C	5.24046000	-7.17115700	-0.95872200
C	6.97521900	-6.25506200	-0.71176300	C	4.47477700	-6.99740200	0.35854400
O	5.55208900	-6.30371100	-0.41002000	N	3.33192000	-6.08917200	0.29242200
C	7.08170300	-6.57162700	-2.21715800	C	2.01701700	-6.44706400	0.52928600
O	7.27800000	-7.95992200	-2.48792900	N	1.17858400	-5.44570800	0.42973600
C	5.74574400	-6.03699000	-2.75204800	C	1.97659700	-4.35513600	0.11657500
C	4.78397800	-6.35862100	-1.60185700	C	1.64468600	-2.98435800	-0.05732300
N	3.62437100	-5.47260000	-1.50055000	O	0.51684800	-2.45059000	0.02740200
C	2.30758900	-5.87376000	-1.63526100	N	2.77066900	-2.19679900	-0.32790200
N	1.44532800	-4.89945200	-1.48543700	C	4.07998800	-2.66080900	-0.38455000
C	2.22854200	-3.78360700	-1.22490800	N	5.06729000	-1.78439600	-0.59507400
C	1.86690400	-2.44899800	-0.92209200				

O	0.69685700	-1.98055700	-0.86326900	N	4.37651000	-3.95603000	-0.23800000
N	2.96322000	-1.63618100	-0.65312800	C	3.31938500	-4.73064900	0.02701200
C	4.28850800	-2.06355400	-0.65061300	O	-5.58482100	-8.07061600	1.50219500
N	5.24018500	-1.19569000	-0.30591800	C	-6.91014100	-7.79216600	1.94642000
N	4.62663200	-3.31606900	-0.97870400	C	-7.69056400	-6.82580700	1.06007300
C	3.58713500	-4.11708800	-1.22227500	O	-7.12875000	-5.49879200	1.18365600
O	-4.37349900	-6.11070800	2.32379600	C	-7.71197200	-7.16969200	-0.45560900
C	-5.66043700	-5.88322300	2.91638800	O	-9.04073100	-7.10338900	-0.91642100
C	-6.77227700	-5.59867800	1.91152700	C	-6.82010500	-6.07089200	-1.06656400
O	-6.49489900	-4.35497900	1.23365600	C	-7.09335000	-4.91284900	-0.11332400
C	-7.01119500	-6.66619000	0.81132900	N	-6.13483400	-3.81400700	-0.10954300
O	-8.39866200	-6.86553600	0.68248400	C	-6.49227000	-2.47897000	-0.15914200
C	-6.40098100	-6.00892300	-0.44115700	N	-5.47410900	-1.65901600	-0.09343200
C	-6.67766200	-4.53375600	-0.17127300	C	-4.37103900	-2.49109700	0.01222600
N	-5.82747600	-3.55996500	-0.85404700	C	-2.99341200	-2.17890900	0.14124400
C	-6.24986700	-2.28534500	-1.18513400	O	-2.47651700	-1.03570600	0.20012000
N	-5.27627800	-1.48449100	-1.54166500	N	-2.18942600	-3.31659000	0.21060000
C	-4.13669600	-2.26145400	-1.43407800	C	-2.66686800	-4.61356300	0.19589900
C	-2.76498200	-1.89564600	-1.57701900	N	-1.76608700	-5.60425300	0.28733500
O	-2.28402200	-0.77756700	-1.82561200	N	-3.96007100	-4.91226700	0.10324900
N	-1.90966000	-2.98949700	-1.34023000	C	-4.75724300	-3.83543700	0.00779800
C	-2.32744700	-4.23321800	-0.92964800	P	-9.38190400	-7.81128400	-2.47626600
N	-1.35661200	-5.13663400	-0.57226900	O	-10.91049700	-7.88080100	-2.41614500
N	-3.59353800	-4.56023000	-0.75602100	O	-8.65191200	-9.16275200	-2.43440000
C	-4.45438100	-3.54969200	-1.00434400	O	-8.81421500	-6.80783400	-3.49459300
P	-8.92684300	-8.29346100	-0.17385800	O	8.70997300	2.11191800	-3.99533200
O	-10.42648700	-8.25218000	0.13370400	P	9.24850600	1.67916800	-2.62517200
O	-8.14024300	-9.43066400	0.49489000	O	10.74793200	1.35733600	-2.58751600
O	-8.55420700	-8.03331300	-1.64330600	O	8.35941700	0.69070400	-1.84842300
O	9.58171800	2.82571500	-2.25343200	O	9.07793400	3.08693400	-1.61919400
P	9.72365600	2.49614600	-0.76153800	C	9.12016400	4.36333400	-2.20052200
O	11.15734700	2.22762100	-0.28583400	C	8.23697500	5.33249800	-1.42143400
O	8.67458500	1.51656800	-0.20231500	O	6.84350200	4.95326700	-1.54586900
O	9.26777000	3.95680500	0.06345500	C	8.51688400	5.38786400	0.08815800
C	9.25291400	5.18061200	-0.62229600	O	8.23121800	6.72298800	0.52177900
C	8.14359700	6.07950800	-0.08630600	C	7.51592000	4.37668000	0.65023800
O	6.84625500	5.52585100	-0.41862300	C	6.31642100	4.56761300	-0.28449300
C	8.14357700	6.25833800	1.44041300	N	5.47627300	3.38182600	-0.43734800
O	7.67185900	7.58453500	1.70957800	C	5.85802900	2.08921800	-0.77291200
C	7.14832700	5.19219300	1.90092400	N	4.83357800	1.26367100	-0.82176000
C	6.12109200	5.21491200	0.76439800	C	3.72798100	2.04163000	-0.53182700
N	5.38655700	3.96950300	0.58057900	C	2.35040600	1.70718800	-0.43194200
C	5.88977200	2.69722800	0.33255500	O	1.80730600	0.58245400	-0.49374200
N	4.93450000	1.80017600	0.21461800	N	1.55632700	2.84405100	-0.20886600
C	3.75175300	2.50413000	0.38150900	C	2.04357300	4.08614100	0.11685500
C	2.39870700	2.07295800	0.35131500	N	1.12490500	4.98697600	0.62605900
O	1.95526400	0.91681300	0.18887600	N	3.32091600	4.40047200	0.07259200
N	1.50238600	3.13870000	0.53971700	C	4.10964400	3.36205100	-0.29082200
C	1.86717500	4.44996100	0.76658900	H	-4.21508000	10.68025400	-1.69842300
N	0.87657600	5.33921900	0.99926700	H	-3.37434500	9.48361800	-2.69983500
N	3.13140900	4.85255700	0.80784100	H	-5.80326500	9.05037500	-2.47337200

C	4.01478900	3.85569500	0.60282900	H	-5.71260600	9.56651200	0.25627900
H	-4.42062500	10.83352200	-0.56689400	H	-5.92175100	6.99044300	1.04009900
H	-3.22839300	9.88603700	-1.47452600	H	-4.27843100	7.67587000	0.80687200
H	-5.57812300	9.44259800	-2.14524300	H	-5.80817000	5.85267600	-1.08947500
H	-6.36847600	9.30878200	0.51719600	H	-2.20708300	7.04853200	-0.61703100
H	-6.66837100	6.62456700	0.57478300	H	-6.56378300	1.62083500	-0.68093300
H	-5.09400400	7.31723100	1.07195300	H	8.45034700	-5.51905500	0.16208500
H	-5.75805200	5.97740200	-1.57275400	H	6.88658400	-4.78312000	-0.26145800
H	-2.63102900	7.12052500	0.30568100	H	7.34853900	-7.19607500	1.57088300
H	-6.10897100	1.78675500	-2.44241000	H	7.41579700	-7.27165000	-1.20863100
H	8.68007500	-4.99220600	-0.61443000	H	5.25481500	-6.22415100	-1.50474500
H	7.17132400	-4.12231500	-0.98236000	H	4.81198500	-7.94750200	-1.59665000
H	7.44657200	-7.04827800	-0.11897200	H	4.04814800	-7.95175700	0.69507500
H	7.93552300	-6.06932500	-2.67833200	H	1.74985800	-7.46867800	0.76441300
H	5.80168300	-4.95442600	-2.89543200	H	4.87669900	-0.78148200	-0.66459100
H	5.45228700	-6.50875600	-3.69246400	H	-6.80593600	-7.35702700	2.94592700
H	4.35176700	-7.36150800	-1.71800500	H	-7.49714400	-8.71786900	2.04583100
H	2.05726000	-6.90505300	-1.84512700	H	-8.72994700	-6.80273400	1.41527300
H	5.02434000	-0.22028300	-0.07836200	H	-7.30736400	-8.17039800	-0.66146100
H	-5.53228800	-5.01402100	3.56713500	H	-5.76312500	-6.34408100	-1.01057100
H	-5.94912600	-6.73678100	3.54333400	H	-7.12088600	-5.87643700	-2.09744800
H	-7.70384300	-5.49188200	2.48332300	H	-8.06152700	-4.44981000	-0.34605500
H	-6.52070900	-7.62162600	1.04752500	H	-7.52916500	-2.18537500	-0.25275300
H	-5.32333600	-6.17513900	-0.49079400	H	-0.74883100	-5.46863200	0.36327200
H	-6.89557900	-6.39335600	-1.33485500	H	10.14621700	4.77998900	-2.20606700
H	-7.70536900	-4.27031400	-0.45017200	H	8.77608300	4.32051300	-3.24135800
H	-7.29749500	-2.01933600	-1.14253800	H	8.34761500	6.33846600	-1.84598200
H	-0.40983400	-5.03366400	-0.97529300	H	9.55485500	5.11937800	0.31909100
H	10.20746900	5.72987500	-0.50309700	H	7.25871100	4.55911100	1.69794900
H	9.10051400	5.01854400	-1.69621200	H	7.92266900	3.36971200	0.54283500
H	8.22051600	7.06556000	-0.56284900	H	5.64042500	5.34469800	0.08563500
H	9.14296100	6.10930200	1.86659900	H	6.88661300	1.80354300	-1.01796500
H	6.69800100	5.41090200	2.87393100	H	1.50432900	5.92972200	0.64679800
H	7.64747000	4.22181800	1.93737500	H	6.04163200	-2.07972100	-0.31192100
H	5.35149300	5.97328500	0.94110200	H	-2.12745100	-6.54680300	0.26223000
H	6.95907600	2.48392500	0.21726900	H	-5.49847500	0.26093100	-0.42410600
H	1.16681900	6.30764200	1.01034900	H	0.17368400	4.96588300	0.21570800
H	6.18038100	-1.58215200	-0.02016200	H	-5.65483600	-8.60420800	0.69486200
H	-1.69601000	-6.09363200	-0.58073100	H	-3.22781900	9.72283300	0.10318100
H	-5.14617700	0.42634300	-2.00123600	H	6.27994100	-9.16169400	0.54960700
H	-0.10217900	5.15889800	0.73987500	H	8.35419200	6.74769300	1.48475200
H	-4.36218200	-6.98394800	1.90150700	H	-3.18402200	0.67930200	-0.29325800
H	-4.00528300	9.47795400	1.20348900	H	0.53296400	2.67570800	-0.23549300
H	6.63152600	-8.46859000	-1.97179400	H	2.58480800	-1.19039400	-0.43013100
H	7.61204200	7.68115900	2.67396800	H	-1.16817900	-3.14908100	0.21517400
H	-2.93168400	0.86990600	-1.28079600	C	0.32849400	1.89195200	2.74992600
H	0.50573300	2.89823900	0.45553100	C	-0.31613700	2.98405000	3.59986300
H	2.74581400	-0.66736900	-0.36963900	C	-0.68736800	0.76394500	2.57181700
H	-0.90066900	-2.76398800	-1.35003100	H	1.23599900	1.51500400	3.23951500
C	-1.01372800	-2.55196900	1.98934300	C	-0.65259400	2.46114200	4.99670500
C	-1.43837900	-1.08989800	1.80988000	H	-1.22092900	3.35102700	3.10577000

C	-2.22015000	-3.32986300	2.52301200	C	-1.03995100	0.14114200	3.92483200
H	-0.18233600	-2.61821800	2.70306800	H	-1.58730200	1.17306600	2.10976900
C	-1.85133000	-0.47298800	3.14868200	C	-1.58089600	1.23177000	4.87401300
H	-2.28341100	-1.04544500	1.11590200	H	-1.14427300	3.23609800	5.59467400
C	-2.64406900	-2.80467400	3.89637000	H	0.27454900	2.18182500	5.51361500
H	-3.06014100	-3.24200500	1.82772900	H	-1.79195200	-0.64600800	3.80188400
C	-2.98167300	-1.30311000	3.78837600	H	-0.14361200	-0.32346600	4.35707600
H	-2.18339500	0.56077600	3.00382800	H	-1.73697600	0.80269000	5.86832900
H	-0.97962200	-0.44750100	3.81630800	H	-2.56504100	1.56146000	4.51750800
H	-3.51536100	-3.35358100	4.26951500	N	-0.18500400	-0.24754100	1.57695900
H	-1.82657700	-2.95699300	4.61308000	H	-0.98766600	-0.69739500	1.07702200
H	-3.20262800	-0.91021300	4.78536600	H	0.39989000	0.16934200	0.82505000
H	-3.89649700	-1.18457500	3.19374300	H	0.37506100	-0.99114500	2.00200700
N	-1.91818100	-4.80885000	2.53242500	H	0.61156800	2.29276500	1.78063600
H	-2.79834400	-5.36555600	2.64906800	N	0.60319400	4.18895600	3.62824400
H	-1.51576000	-5.08284600	1.61660400	H	0.79211400	4.53233700	2.65745200
H	-1.24966500	-5.06719000	3.26497900	H	0.18951900	4.96360200	4.15833700
H	-0.66241200	-2.96598400	1.04203200	H	1.50642400	3.97303300	4.06521900
N	-0.35443800	-0.30485700	1.13426800				
H	0.08015300	-0.83714300	0.34428600				
H	-0.72194500	0.58426000	0.72637700				
H	0.41655600	-0.05368200	1.75980700				
1,4-CHDA							
E = -6467.33577							
O	-2.74960100	9.72349500	0.24056200				
C	-3.96186400	10.18138800	-0.36409100				
C	-5.21089100	9.39258700	0.02840300				
O	-5.12301000	8.04487400	-0.48755700				
C	-5.48293600	9.25447700	1.53983900				
O	-6.87664200	9.23212800	1.74094300				
C	-4.83378200	7.89753700	1.86362500				
C	-5.07598500	7.10062300	0.57787800				
N	-4.04073100	6.11352700	0.27100500				
C	-2.71864500	6.37685000	-0.03588100				
N	-2.03604700	5.29317900	-0.32660500				
C	-2.95177300	4.25920900	-0.20982800				
C	-2.79824000	2.85727400	-0.41255600				
O	-1.77893700	2.23042900	-0.74577000				
N	-4.00079500	2.16468000	-0.18849100				
C	-5.19559500	2.74897600	0.17416100				
N	-6.24491200	1.92661200	0.38480000				
N	-5.34399900	4.05807100	0.35392000				
C	-4.20525200	4.75101000	0.15346900				
O	-7.11681200	8.14793200	4.09925000				
P	-7.45877900	9.45867900	3.37053400				
O	-8.94997200	9.67454000	3.09618300				
O	-6.68618400	10.69037000	3.86570600				
O	5.78639500	-2.28741400	2.28617300				
P	5.59391200	-2.71160000	3.73600700				
O	4.85007200	-1.80726800	4.68298400				

O	7.02000600	-3.19935600	4.35854900
O	4.80047800	-4.16592100	3.78676100
C	5.18945900	-5.15968900	2.84228800
C	4.38833800	-6.43327600	3.07978000
O	2.96077800	-6.20903600	2.96288900
C	4.71986800	-7.52707400	2.04367300
O	4.66191700	-8.84408900	2.58740800
C	3.66012300	-7.26896200	0.96358100
C	2.44532500	-6.83036300	1.79196000
N	1.52142200	-5.93436100	1.10382600
C	0.20806200	-6.24427500	0.79940400
N	-0.41528700	-5.28747300	0.15878600
C	0.52750100	-4.27943100	0.03598800
C	0.41413800	-2.97697100	-0.53386800
O	-0.58181700	-2.45721900	-1.06848600
N	1.61213700	-2.25492600	-0.42076300
C	2.77087700	-2.71766600	0.17776100
N	3.82366600	-1.88627100	0.23026500
N	2.87480800	-3.94332100	0.69491100
C	1.73907500	-4.65602000	0.61717500
O	-7.08575200	-7.33199600	0.81460600
C	-8.34142200	-6.97844300	1.38967000
C	-9.11646500	-5.91223100	0.62123000
O	-8.43216600	-4.64423300	0.73985800
C	-9.30955500	-6.17978300	-0.89691600
O	-10.65583900	-5.93329800	-1.22905900
C	-8.35086200	-5.16126700	-1.54412300
C	-8.43307700	-4.01641000	-0.54053500
N	-7.37496700	-3.01588800	-0.57220200
C	-7.60218600	-1.66092900	-0.41697400
N	-6.50551400	-0.94590300	-0.38414600
C	-5.48612500	-1.87466600	-0.51197200
C	-4.07153500	-1.68359100	-0.53695700
O	-3.43736900	-0.62011900	-0.44813900
N	-3.38656400	-2.90023400	-0.68508700
C	-3.98859400	-4.13590500	-0.77885300
N	-3.17384800	-5.20565600	-0.94944000
N	-5.30351900	-4.31450900	-0.75075200
C	-5.99969800	-3.16680800	-0.62469200
P	-11.22855000	-6.54153300	-2.76127100
O	-12.73997000	-6.38366100	-2.56885600
O	-10.70903300	-7.98689000	-2.79839100
O	-10.60673200	-5.60906900	-3.81436400
O	8.48477500	-0.14855200	-5.07010800
P	8.61956400	0.15388400	-3.60016300
O	10.20964500	0.29004100	-3.26319700
O	7.90279700	-0.67805800	-2.56140000
O	8.08258700	1.71022900	-3.30354500
C	8.23002300	2.69963300	-4.31083100
C	7.54165600	3.98056200	-3.85964200
O	6.12923300	3.74534200	-3.67749500

C	8.04737000	4.56110800	-2.52916900
O	7.92377300	5.98263400	-2.62767500
C	7.07200100	3.96878500	-1.51022600
C	5.76349900	3.90111800	-2.30842400
N	4.86714500	2.82694700	-1.90107800
C	5.14718900	1.47796900	-1.72245700
N	4.09352000	0.78704500	-1.35133500
C	3.06347100	1.71339300	-1.29378600
C	1.68329200	1.54870200	-0.97746500
O	1.08085800	0.50979000	-0.66035000
N	0.98072800	2.76350300	-1.06542900
C	1.53544000	3.97661800	-1.40893400
N	0.70286300	5.03802600	-1.48497200
N	2.82326600	4.13338400	-1.69990200
C	3.52186900	2.98239400	-1.63774900
H	-4.12891000	11.24601000	-0.14560700
H	-3.80943000	10.08163800	-1.44342700
H	-6.07347900	9.87600800	-0.44634800
H	-5.03347200	10.07249700	2.12074600
H	-5.30901400	7.45576500	2.74125100
H	-3.75761200	8.00354300	2.03457000
H	-6.01180700	6.53483200	0.61786600
H	-2.34201700	7.39123700	-0.03571600
H	-7.13542200	2.38111900	0.53095000
H	6.25491800	-5.40125200	2.96585600
H	5.02152500	-4.79059200	1.82760100
H	4.57171400	-6.79834600	4.09672400
H	5.73523500	-7.42560700	1.65274700
H	3.97623100	-6.45209900	0.30891400
H	3.45804800	-8.15459000	0.35713800
H	1.82984200	-7.69241000	2.07862100
H	-0.21922100	-7.19871200	1.07642600
H	3.81952500	-0.98246100	-0.24611100
H	-8.11538600	-6.60269400	2.39315200
H	-8.98808300	-7.86188300	1.50296600
H	-10.11174800	-5.82115100	1.07769700
H	-9.04914500	-7.21110800	-1.17471700
H	-7.32800000	-5.54435600	-1.57381100
H	-8.70005600	-4.90052800	-2.54472300
H	-9.36628500	-3.45573800	-0.68354000
H	-8.60890500	-1.27244600	-0.33990700
H	-2.20599300	-5.18439800	-0.59908000
H	9.29262200	2.91295500	-4.50260600
H	7.78182500	2.35474100	-5.24969700
H	7.66227800	4.73392500	-4.64753000
H	9.08712400	4.27464200	-2.32714200
H	6.97282800	4.57952200	-0.60833600
H	7.39994000	2.96706400	-1.22643400
H	5.17550900	4.81627900	-2.19545100
H	6.13068300	1.06640100	-1.91607900
H	1.15438600	5.93262200	-1.61650600

H	4.57152400	-2.09524100	0.90964200
H	-3.64526200	-6.09722100	-0.86579800
H	-6.26170500	0.94924700	0.06863200
H	-0.22827500	5.04879500	-1.04819800
H	-7.26762400	-7.81797600	-0.00527700
H	-2.74785000	10.01520500	1.16583300
H	3.81875700	-8.94798300	3.05827000
H	8.17602200	6.35760700	-1.76821500
H	-3.93907700	1.13813300	-0.28848200
H	-0.03858400	2.69450900	-0.90464800
H	1.54339600	-1.25160000	-0.65551300
H	-2.35792900	-2.82738100	-0.76924300
C	9.05347400	-1.24632400	1.64145300
C	9.24843500	-0.18699800	0.54930600
C	9.62066500	-0.78305300	2.98847000
H	9.56810000	-2.17411100	1.34383300
C	10.72505000	0.19296000	0.39118100
H	8.68304700	0.71954600	0.82100000
C	11.09611100	-0.36589900	2.84724100
H	9.04254400	0.09019600	3.32199800
C	11.29811800	0.67800600	1.73482100
H	11.28169500	-0.70340300	0.08152800
H	11.47018000	0.02283400	3.80354400
H	11.69117200	-1.26285000	2.61706500
H	12.36572600	0.91208800	1.62812300
H	10.79423900	1.61609700	2.01250800
N	9.40104100	-1.83617900	4.00498900
H	9.71120800	-1.50226000	4.91857300
H	7.79705400	-2.59377700	4.14989400
H	10.00177000	-2.63495200	3.79101900
H	7.99228600	-1.49249600	1.75679800
H	8.84256900	-0.53315500	-0.40707600
N	10.87660100	1.16993900	-0.71023100
H	11.85392500	1.45757400	-0.78093900
H	10.38014100	0.58384100	-2.31381000
H	10.35785900	2.01965200	-0.48104200