

CO2-2[dMA][Ala]

0 1

N	-4.20342400	-3.72343000	-0.14275700
C	-5.48616000	-4.08669800	-0.05384200
N	-6.55823600	-3.30111400	0.07151000
C	-6.22631800	-2.01519100	0.10173200
C	-4.93531200	-1.49455600	0.01485100
C	-3.88035400	-2.42967400	-0.11524000
N	-7.08513300	-0.93192200	0.21817100
C	-6.35961900	0.19857500	0.20311900
N	-5.06158700	-0.10175600	0.08158700
N	-2.57614500	-2.01826300	-0.19847000
C	-8.54397700	-0.98585000	0.33845500
C	-4.00538900	0.92183900	0.02883900
H	-5.67401700	-5.15503000	-0.08508800
H	-6.82281700	1.23513200	0.27803100
H	-2.39237900	-1.03277200	-0.09182800
H	-8.81591100	-1.53861500	1.23757900
H	-8.96282800	-1.48943000	-0.53253100
H	-8.91118800	0.03750300	0.39771800
H	-3.46058600	0.83661300	-0.91300500
H	-3.32790100	0.79384700	0.87561200
H	-4.49392000	1.90427700	0.08915800
N	-6.67949400	6.06718100	0.73699300
C	-7.56980400	4.98736300	0.29084200
C	-6.92032400	3.58193000	0.29805600
O	-5.67227800	3.50508100	0.19564200
O	-7.71502200	2.59193800	0.37720300
H	-5.77591400	5.91960200	0.29068900
H	-6.49884900	5.95944700	1.73139000
H	-8.42793000	4.95015200	0.96810100

C	-1.39176900	-2.77175700	-0.44825200
O	-1.37232100	-3.95594900	-0.68247100
O	-0.36771300	-1.94862600	-0.38906000
H	0.56518000	-2.48947200	-0.60002000
N	9.23434800	3.36128400	-0.48384100
C	9.44203200	3.14063800	0.81811700
N	8.84116600	2.24345700	1.60215900
C	7.94557100	1.52310900	0.93602000
C	7.62751900	1.64289900	-0.41665400
C	8.32764900	2.62731500	-1.14559400
N	7.14807200	0.50661800	1.44083800
C	6.38205300	0.02701500	0.44695700
N	6.64303300	0.68717400	-0.68566100
N	8.16754700	2.87318300	-2.46783700
C	7.12897900	0.02254900	2.82468100
C	5.97078700	0.40852900	-1.96363200
H	10.18929400	3.77041600	1.28917600
H	5.63923800	-0.80623600	0.58567700
H	8.67800800	3.64968200	-2.85900400
H	7.43256500	2.45418400	-3.00966100
H	6.87626100	0.84521700	3.49284200
H	8.11241000	-0.36598800	3.08797800
H	6.37990400	-0.76440100	2.89352600
H	6.71205800	0.10981700	-2.70695900
H	5.43256000	1.29945800	-2.29325800
H	5.25779100	-0.40798100	-1.79556600
N	1.76860500	-3.25115400	-0.85566700
C	2.71402200	-3.30413700	0.28500500
C	3.85649600	-2.28856600	0.04508200
O	4.00169500	-1.84032600	-1.11885600
O	4.56704300	-2.00920500	1.05018600

H	1.42124400	-4.17544200	-1.09981100
H	2.29146500	-2.86838600	-1.64734400
H	2.18769600	-2.98842800	1.19015000
C	3.28843900	-4.70734300	0.51186000
H	3.96824900	-4.69814700	1.36529300
H	2.48813000	-5.42525800	0.71562600
H	3.84248600	-5.04703600	-0.36887600
C	-8.08202800	5.29316200	-1.12368600
H	-8.76759700	4.51402300	-1.46472800
H	-8.59608500	6.25714600	-1.13483100
H	-7.24408400	5.34709200	-1.82667300

CO2-2[dMA][Gly]

0 1

N	4.55039000	-3.44097800	0.27502300
C	5.82004000	-3.84705600	0.36708900
N	6.92735400	-3.10236700	0.32970800
C	6.64949000	-1.81168800	0.18366700
C	5.37732600	-1.24860600	0.08059800
C	4.28143700	-2.14238200	0.13417600
N	7.55520600	-0.76337600	0.11393700
C	6.87556000	0.38714900	-0.02440600
N	5.56212600	0.13319200	-0.04795100
N	2.99120400	-1.69051700	0.03153600
C	9.01475200	-0.86714700	0.18229800
C	4.54563900	1.18898600	-0.18363100
H	5.96327600	-4.91646600	0.48280100
H	7.38383500	1.40441500	-0.09920600
H	2.85508600	-0.71445200	-0.18122300
H	9.37607600	-1.48230600	-0.64164400
H	9.30290500	-1.32773300	1.12704300
H	9.42381000	0.13946700	0.11120300

H	3.88347400	1.17235200	0.68369000
H	3.97637700	1.03432300	-1.10258700
H	5.07294600	2.15178900	-0.23157800
N	7.45878800	6.27773800	-0.54124500
C	8.28236500	5.10325000	-0.25492200
C	7.56780800	3.73751800	-0.23863700
O	6.31534500	3.71365200	-0.27064200
O	8.32562500	2.71796400	-0.16556800
H	6.59666800	6.19440500	-0.00827800
H	7.16268900	6.24506400	-1.51260800
H	9.10670600	5.04941200	-0.97083200
H	8.75093700	5.22413900	0.72883600
C	1.76426400	-2.38692800	0.22565900
O	1.67880800	-3.53595800	0.58511700
O	0.77836400	-1.55395200	-0.03577300
H	-0.17730800	-2.04443100	0.14293900
N	-10.03378500	2.43222300	0.78759400
C	-10.38085800	2.07874200	-0.45400500
N	-9.70760700	1.29785700	-1.30107200
C	-8.57077200	0.85717700	-0.77323900
C	-8.08702000	1.14056500	0.50373300
C	-8.88400600	1.98058900	1.30971900
N	-7.63597300	0.02703700	-1.37444600
C	-6.63169900	-0.18835000	-0.50838500
N	-6.86948500	0.46573600	0.63295400
N	-8.58457900	2.34953800	2.57811800
C	-7.71282200	-0.53078800	-2.72818300
C	-5.96382500	0.43903900	1.79126000
H	-11.32347200	2.47943000	-0.81161100
H	-5.73747200	-0.83053500	-0.74248800
H	-9.20162900	3.00965700	3.02537200

H	-7.69271800	2.15797200	2.99901900
H	-7.74838400	0.28098700	-3.45418500
H	-8.61406100	-1.13610900	-2.82069600
H	-6.82702200	-1.14282000	-2.88903500
H	-6.50061900	0.05917700	2.66221900
H	-5.58470300	1.44518100	1.98151600
H	-5.12999000	-0.23134200	1.54934500
N	-1.43474500	-2.75747200	0.38628800
C	-2.40432200	-2.76452600	-0.72954200
C	-3.66396800	-1.94824500	-0.38278200
O	-3.76370700	-1.50738600	0.78814400
O	-4.49762000	-1.79825600	-1.31773400
H	-1.12703300	-3.69470800	0.62968600
H	-1.93388800	-2.36288800	1.18859500
H	-1.95558400	-2.33718500	-1.62962600
H	-2.72400200	-3.77936700	-0.98094100

CO2-2[dMA][Val

0 1

N	-3.49247500	-4.24059300	-0.62813400
C	-4.75537700	-4.67507900	-0.66832700
N	-5.87577300	-3.96974900	-0.49625000
C	-5.61932800	-2.68772500	-0.26020200
C	-4.35742300	-2.09871100	-0.18967400
C	-3.24473400	-2.95164500	-0.39040700
N	-6.54341500	-1.67716000	-0.03639100
C	-5.88305500	-0.52442700	0.16194300
N	-4.56563800	-0.73999000	0.07671400
N	-1.96550500	-2.46605200	-0.34283200
C	-8.00116600	-1.81929800	-0.01605900
C	-3.56726700	0.32761600	0.24859400

H	-4.88030300	-5.73471400	-0.86638200
H	-6.40466500	0.46374600	0.36186800
H	-1.85038700	-1.47961300	-0.16979800
H	-8.28733700	-2.52733500	0.76144400
H	-8.34484900	-2.18912100	-0.98189700
H	-8.42894100	-0.83903000	0.18799200
H	-2.97860500	0.42872600	-0.66524000
H	-2.92077900	0.09072600	1.09574300
H	-4.11210000	1.26129400	0.44449700
N	-6.50413700	5.06560700	1.81969400
C	-7.35072900	4.11725000	1.07496000
C	-6.64044000	2.76715600	0.80266200
O	-5.38529500	2.75933100	0.76399200
O	-7.38380200	1.75175400	0.62362000
H	-5.54106200	4.89722000	1.53459100
H	-6.53278800	4.83054300	2.80720000
H	-8.23409200	3.89704200	1.68151400
C	-0.71639700	-3.13820500	-0.50589100
O	-0.60226900	-4.32266100	-0.71361300
O	0.24155000	-2.24802000	-0.38858600
H	1.23552000	-2.73566700	-0.51871800
N	7.94339600	4.80227200	-0.83509700
C	8.09254100	4.79603100	0.49329600
N	7.72520000	3.84431600	1.35347800
C	7.15309200	2.81453500	0.73956400
C	6.93541500	2.68536500	-0.63199400
C	7.36449200	3.75681300	-1.44357300
N	6.65820200	1.66015400	1.32857800
C	6.16501700	0.86394300	0.36569200
N	6.31396000	1.44823900	-0.82721000
N	7.25491600	3.79972700	-2.79303500

C	6.65793600	1.34705900	2.76102500
C	5.86995700	0.84258400	-2.09157700
H	8.56864500	5.67346000	0.91795900
H	5.69699100	-0.13608100	0.57048200
H	7.53300600	4.65356100	-3.25165700
H	6.72507200	3.12241000	-3.31254400
H	6.12333600	2.12774800	3.30112900
H	7.68433400	1.29642400	3.12360100
H	6.16115100	0.38758600	2.89397700
H	6.72968700	0.69882800	-2.74831800
H	5.12889700	1.49068300	-2.56357500
H	5.40783600	-0.12347600	-1.85508100
N	2.47719400	-3.40320200	-0.66585400
C	3.39685700	-3.23343300	0.48534400
C	4.36100800	-2.06352800	0.16363800
O	4.48459200	-1.73145900	-1.04119600
O	4.95466800	-1.53764400	1.14587200
H	2.21628600	-4.37657600	-0.80724100
H	2.97002100	-3.05883800	-1.49280500
H	2.80489500	-2.93382300	1.35484000
C	4.13828900	-4.54938100	0.85011000
H	3.35490800	-5.32018400	0.88422500
C	-7.86064000	4.78571500	-0.23438000
H	-8.26466700	5.74883300	0.09943800
C	4.77059000	-4.48624200	2.24641100
H	5.21188500	-5.45314800	2.50603600
H	5.54848600	-3.72197300	2.28966100
H	4.02381000	-4.24172800	3.00753700
C	5.16626700	-4.97128200	-0.20932100
H	5.57488800	-5.95715500	0.02968600
H	4.72845400	-5.02800700	-1.20969200

H	5.99913100	-4.26355500	-0.25283200
C	-8.99609800	3.99974600	-0.90321700
H	-9.38401300	4.55324400	-1.76493400
H	-8.65755600	3.01914300	-1.24517900
H	-9.82526600	3.83332800	-0.20859900
C	-6.72971000	5.08258000	-1.22836500
H	-7.11609600	5.63822000	-2.08912600
H	-5.94396200	5.68630000	-0.76780500
H	-6.27137500	4.16094000	-1.59984800

CO2-2[dMA][Ile]

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N	-3.11772000	-4.47757000	-0.68413200
C	-4.35036000	-4.99020400	-0.74142200
N	-5.51239200	-4.36879900	-0.52673100
C	-5.33720500	-3.08723800	-0.22387800
C	-4.11528400	-2.42229000	-0.12819700
C	-2.95203400	-3.18891900	-0.38233300
N	-6.32285200	-2.15039800	0.05204500
C	-5.73656500	-0.96875500	0.30534400
N	-4.40857500	-1.09457400	0.20585800
N	-1.70622800	-2.62482400	-0.31492700
C	-7.76857000	-2.38586400	0.06686900
C	-3.48011500	0.02564200	0.42741900
H	-4.40840400	-6.04414300	-0.99333500
H	-6.31926200	-0.02587900	0.54974600
H	-1.65017400	-1.65702700	-0.03844800
H	-8.00782300	-3.14021800	0.81621000
H	-8.08994700	-2.73896700	-0.91276900
H	-8.25726300	-1.44340400	0.30870400
H	-2.90792500	0.21273100	-0.48312500

H	-2.81161100	-0.21224100	1.25720100
H	-4.08243900	0.90961800	0.67779900
N	-6.71727600	4.49770100	2.19411600
C	-7.49587400	3.53055000	1.40015600
C	-6.70131300	2.23556600	1.09366900
O	-5.44729300	2.30083100	1.09312000
O	-7.37886400	1.18823600	0.85007200
H	-5.73831500	4.37571900	1.94113300
H	-6.77179800	4.24161700	3.17517100
H	-8.37410700	3.23645600	1.98235600
C	-0.42585000	-3.17931000	-0.61652900
O	-0.24611700	-4.30542100	-1.01276800
O	0.47754400	-2.25152100	-0.39395800
H	1.48703800	-2.62682000	-0.64529700
N	7.61527500	5.51080700	-0.67226300
C	7.89300000	5.38062400	0.62877400
N	7.65409500	4.32955300	1.41538500
C	7.07180100	3.33622600	0.75282000
C	6.72767300	3.33244700	-0.59872500
C	7.02730400	4.50103700	-1.33041300
N	6.68939500	2.10348800	1.26123100
C	6.14070800	1.38124900	0.27032400
N	6.14643700	2.08884300	-0.86367500
N	6.78574600	4.67225000	-2.65228800
C	6.84556300	1.64922800	2.64646500
C	5.61307100	1.58812000	-2.13940900
H	8.36833300	6.23616200	1.09677900
H	5.74597000	0.33918500	0.41105800
H	6.97834800	5.58214500	-3.04180300
H	6.23637300	4.02385200	-3.18826200
H	6.31096400	2.32618700	3.31211100

H	7.90264300	1.64467900	2.91090500
H	6.43256000	0.64456100	2.71799100
H	6.41155100	1.56365000	-2.88301900
H	4.79808800	2.23458200	-2.47102600
H	5.22840100	0.57581000	-1.96579900
N	2.79050800	-3.13573000	-0.95472900
C	3.77423500	-2.97500700	0.14286600
C	4.55771300	-1.66005600	-0.10282900
O	4.53539700	-1.18391500	-1.26483500
O	5.16819400	-1.17372300	0.88932000
H	2.63729000	-4.11303100	-1.19216300
H	3.16886600	-2.64397900	-1.76718800
H	3.22377200	-2.85271700	1.07995800
C	4.70298500	-4.21307300	0.29677300
H	4.03029000	-5.08375400	0.26133000
C	-8.02503500	4.21613500	0.10593000
H	-8.47859300	5.14790800	0.46783700
C	5.38872600	-4.23910500	1.67603600
H	6.06571400	-3.38423200	1.75521900
H	4.62126800	-4.08505900	2.44339500
C	5.70112500	-4.34142000	-0.86381000
H	6.22091700	-5.30130100	-0.83190700
H	5.20393100	-4.27241500	-1.83493500
H	6.45252100	-3.54733800	-0.82195600
C	-9.13080800	3.39520100	-0.58430500
H	-8.70647600	2.46837100	-0.98210100
H	-9.85511700	3.08372000	0.17731500
C	-6.88762600	4.59985300	-0.85139600
H	-7.25773300	5.20626100	-1.68237500
H	-6.12568100	5.18699800	-0.33361600
H	-6.40076700	3.71274300	-1.26880700

C	-9.87475800	4.15013500	-1.69250300
H	-9.22149600	4.39485800	-2.53457000
H	-10.70073800	3.54950100	-2.08607700
H	-10.29824300	5.08892200	-1.31893200
C	6.13737500	-5.54169100	1.98041400
H	6.99099800	-5.69151900	1.31429200
H	6.52211300	-5.53487700	3.00419000
H	5.48090400	-6.41292800	1.88131300

CO2-2[dMA][Leu]

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N	-3.05245100	-4.50884000	-0.60155100
C	-4.28141200	-5.03313200	-0.62332800
N	-5.44326300	-4.41956000	-0.38635400
C	-5.27269700	-3.13291800	-0.10357700
C	-4.05507300	-2.45535600	-0.04869000
C	-2.89177600	-3.21507700	-0.32048000
N	-6.25974600	-2.20140200	0.18478100
C	-5.67842200	-1.01073800	0.40528600
N	-4.35226700	-1.12559600	0.27281000
N	-1.64843000	-2.64123300	-0.28552200
C	-7.70224600	-2.45025500	0.24118700
C	-3.42859800	0.00661500	0.44931600
H	-4.33592900	-6.09043900	-0.86139300
H	-6.26370000	-0.07080300	0.65341400
H	-1.58954500	-1.67899400	0.00923500
H	-7.91448400	-3.19470100	1.00836300
H	-8.04551300	-2.82194900	-0.72403300
H	-8.19367400	-1.50872300	0.48093100
H	-2.87163100	0.17113000	-0.47476200
H	-2.74602800	-0.20338100	1.27533600

H	-4.03379000	0.89351700	0.68313700
N	-6.79121100	4.36319100	2.41729900
C	-7.43506900	3.50692800	1.40620500
C	-6.65021900	2.20362800	1.12907600
O	-5.39864400	2.28254400	1.06318200
O	-7.32825200	1.13941900	0.97069500
H	-5.79915300	4.40567900	2.19067700
H	-6.84310300	3.90788100	3.32463500
H	-8.42168400	3.22845900	1.78330400
C	-0.37979100	-3.17854800	-0.65376600
O	-0.21204700	-4.28359100	-1.10913500
O	0.53104800	-2.25845400	-0.42096100
H	1.51974400	-2.61644100	-0.72921700
N	7.31784700	5.66773000	-0.52887300
C	7.57019200	5.50517300	0.77372700
N	7.35080400	4.42149500	1.52076700
C	6.82002100	3.43025100	0.81327300
C	6.50786000	3.45816500	-0.54574800
C	6.78162700	4.65982600	-1.23244500
N	6.47051200	2.16898300	1.27301200
C	5.97162000	1.46025800	0.24657600
N	5.97840000	2.20399500	-0.86402200
N	6.56403100	4.86492000	-2.55375100
C	6.60921700	1.67622400	2.64688000
C	5.49366200	1.72607000	-2.16771200
H	8.00383500	6.36114300	1.27987400
H	5.61319500	0.39989300	0.34384600
H	6.73091800	5.79360600	-2.90934100
H	6.04746200	4.21632700	-3.12124100
H	6.02537400	2.30517400	3.31830800
H	7.65764700	1.71126200	2.94157900

H	6.24166300	0.65193200	2.67389900
H	6.30619200	1.76725600	-2.89520700
H	4.65473500	2.34483300	-2.49254500
H	5.15660800	0.69007700	-2.03937500
N	2.81526000	-3.13159800	-1.14141400
C	3.89002600	-3.02875600	-0.12442100
C	4.56630300	-1.64684600	-0.28316600
O	4.55686400	-1.13478800	-1.42982800
O	5.09605700	-1.15353200	0.75155300
H	2.63089800	-4.09910200	-1.39829400
H	3.14621300	-2.62823400	-1.96707300
H	3.43211600	-3.06830400	0.86549000
C	4.91423900	-4.17367500	-0.27666900
H	4.35842400	-5.12230200	-0.26152300
C	-7.59141000	4.32667300	0.11062400
H	-8.14216700	5.23901900	0.36989400
C	6.03613400	-4.25265100	0.77558000
H	6.56379100	-3.29323900	0.77709500
C	-8.28071800	3.63161900	-1.07719000
H	-7.71646800	2.72195500	-1.31584600
C	-8.24505500	4.54429000	-2.31212200
H	-7.21880900	4.81858200	-2.57573000
H	-8.69585500	4.05392100	-3.18111300
H	-8.79999400	5.47170100	-2.12992300
C	7.03668200	-5.35077100	0.38555100
H	7.45943800	-5.17295200	-0.60806700
H	7.86569500	-5.39859000	1.09805700
H	6.55640100	-6.33581700	0.37148800
H	-6.58799400	4.64510700	-0.19818700
C	-9.72213400	3.21215600	-0.75446400
H	-9.75025100	2.47348100	0.04893400

H	-10.32125800	4.07827200	-0.44920500
H	-10.20471900	2.76881500	-1.63188500
C	5.49504200	-4.49020400	2.19242800
H	4.90354000	-5.41208500	2.23860000
H	6.31744800	-4.59072800	2.90734200
H	4.86770300	-3.66255600	2.52920800
H	5.36207400	-4.09076800	-1.27459700

2[dMA][Gly]-CO2

O 1

N	11.50396800	-0.54540100	-0.08519700
C	11.60211800	0.78774700	-0.09509500
N	10.61207800	1.68195000	-0.07162900
C	9.41808300	1.09986000	-0.03622800
C	9.16700900	-0.27199600	-0.02354200
C	10.29302100	-1.12117700	-0.05019900
N	8.18149400	1.72745300	-0.00728500
C	7.22142600	0.78766000	0.02099800
N	7.77815800	-0.42778700	0.01209700
N	10.24252900	-2.47440500	-0.05906000
C	7.93998300	3.17358900	-0.00900100
C	7.00330200	-1.67758200	0.03545500
H	12.61115500	1.18521900	-0.12450600
H	6.11838600	1.02595800	0.04549900
H	11.11817500	-2.97251000	-0.02362500
H	9.38581200	-2.98494200	0.06112600
H	8.36605100	3.61221300	-0.91088900
H	8.41019200	3.62181800	0.86582500
H	6.86336000	3.33289300	0.01677700
H	7.24728600	-2.24081200	0.93855300
H	7.23161200	-2.26333700	-0.85679300

H	5.93855900	-1.41095300	0.04262600
N	1.49075200	-0.25373600	0.06596400
C	2.28086200	0.96170800	0.07609600
C	3.77939800	0.61650800	0.06481800
O	4.10641400	-0.59452600	0.05130500
O	4.56415900	1.60652600	0.07036400
H	2.02350600	-1.11519800	0.05547100
H	2.05882300	1.58580900	-0.79419200
H	2.06794700	1.56585800	0.96269600
C	0.15237600	-0.27592700	0.05831600
O	-0.35016600	-1.52332000	0.04355600
H	-1.34017400	-1.47785600	0.03771400
O	-0.55466900	0.73937000	0.06434600
N	-3.17188500	-1.54689300	0.02252900
C	-3.74634700	-2.75611900	0.00581700
N	-5.04464400	-3.04544600	-0.00867000
C	-5.79604800	-1.94388300	-0.00513900
C	-5.33840100	-0.62993100	0.01128300
C	-3.93669900	-0.42784400	0.02616500
N	-7.18001700	-1.87997200	-0.01695200
C	-7.55597800	-0.58798600	-0.00813700
N	-6.47014200	0.19127400	0.00868300
N	-3.32193700	0.75958700	0.04344300
C	-8.10495300	-3.01591900	-0.03632100
C	-6.53122600	1.66109400	0.02125000
H	-3.06151900	-3.59824400	0.00405200
H	-8.64747500	-0.25690800	-0.01541300
H	-2.28633500	0.79677500	0.05223800
H	-3.85021700	1.61441700	0.04633700
H	-7.94537900	-3.63131900	0.84885200
H	-7.92633000	-3.61629400	-0.92813600

H	-9.11895300	-2.61922800	-0.04392100
H	-6.02831100	2.05340200	-0.86463100
H	-6.05542300	2.03733900	0.92884100
H	-7.59146800	1.94856600	0.00651600
N	-12.23808000	3.06141100	0.00571000
C	-11.94352000	1.63610600	-0.13569400
C	-10.46245900	1.21630500	-0.05717800
O	-9.58272800	2.10838700	-0.04570900
O	-10.24473200	-0.03757700	-0.03362600
H	-11.58137000	3.57909400	-0.57274900
H	-12.02423100	3.35099200	0.95581900
H	-12.49794700	1.07106300	0.61847600
H	-12.31956200	1.28579300	-1.10389200

2[dMA][Ala]-CO2

0 1

N	11.53676700	0.58490000	1.15313300
C	11.62723400	-0.74811200	1.19613200
N	10.66868800	-1.64223100	0.94705800
C	9.51779500	-1.06020600	0.62680800
C	9.27918300	0.31149900	0.54529600
C	10.36922900	1.16057300	0.82964900
N	8.32211000	-1.68811700	0.31074200
C	7.39756500	-0.74861200	0.04942400
N	7.93826700	0.46689500	0.18162300
N	10.32199300	2.51360300	0.81332100
C	8.08496300	-3.13422700	0.26489800
C	7.19287500	1.71654600	-0.03239600
H	12.60013700	-1.14549800	1.46548400
H	6.33226500	-0.98885600	-0.23479000
H	11.18009000	3.01207800	0.98984800

H	9.51361100	3.02468900	0.50655100
H	8.29755600	-3.56778500	1.24164400
H	8.73922600	-3.58684600	-0.47976100
H	7.04144500	-3.29364100	-0.00126700
H	7.63582200	2.26735600	-0.86464600
H	7.21651300	2.31418800	0.88066500
H	6.15584100	1.44923500	-0.27256200
N	1.80313000	0.29314700	-1.03027500
C	2.58368300	-0.93706600	-1.08942000
C	4.05318200	-0.59603200	-0.74876400
O	4.37114100	0.61401000	-0.64292400
O	4.82874800	-1.58471800	-0.61569700
H	2.35080400	1.14062400	-0.93398800
C	0.47600700	0.33035200	-0.85242800
O	0.00233200	1.58226300	-0.71757700
H	-0.98128700	1.55017700	-0.60422100
O	-0.24931500	-0.67205500	-0.81772600
N	-2.80412000	1.64774400	-0.38475800
C	-3.35374100	2.86225500	-0.26144900
N	-4.63719500	3.16613500	-0.08743800
C	-5.40127000	2.07433200	-0.04143100
C	-4.96941400	0.75652500	-0.15510000
C	-3.58200100	0.53880200	-0.33816800
N	-6.77561300	2.02627500	0.12798000
C	-7.17014600	0.73985400	0.11878800
N	-6.10597000	-0.05097300	-0.04999600
N	-2.99238500	-0.65459000	-0.46587100
C	-7.67449200	3.17131100	0.29242700
C	-6.19114000	-1.51851400	-0.10685200
H	-2.66021000	3.69576600	-0.31054700
H	-8.25737000	0.42191300	0.23943400

H	-1.96559100	-0.70383300	-0.59830300
H	-3.53143800	-1.50224400	-0.43838400
H	-7.60718800	3.81675700	-0.58315300
H	-7.38646000	3.73696400	1.17835100
H	-8.68715800	2.78637100	0.40184500
H	-5.60412200	-1.94883500	0.70673600
H	-5.81954200	-1.86710400	-1.07229500
H	-7.24881700	-1.79286300	0.00779900
N	-11.89384500	-2.77691200	0.08784100
C	-11.55561100	-1.45772900	0.63707900
C	-10.08703200	-1.02663300	0.40429500
O	-9.22442400	-1.92181000	0.23657300
O	-9.85382700	0.22402900	0.43084400
H	-11.13747700	-3.41291600	0.33408400
H	-11.87410400	-2.73002300	-0.92724800
H	-12.19142600	-0.71211500	0.15094300
C	-11.84958400	-1.43585400	2.14371800
H	-11.62746300	-0.45392900	2.56767400
H	-12.89970300	-1.67813400	2.32288800
H	-11.23625200	-2.18147700	2.66055800
H	2.21930100	-1.62634400	-0.32244500
C	2.48341700	-1.62728600	-2.45732100
H	1.44460700	-1.88596300	-2.67031800
H	2.84907800	-0.96574300	-3.24796400
H	3.08509900	-2.53752500	-2.45517100

2[dMA][Val]-CO2

0 1

N	-11.84604000	1.00972000	-1.53192400
C	-11.95483200	-0.29953300	-1.77908200
N	-11.02005400	-1.24060600	-1.63439000

C	-9.87454800	-0.73776400	-1.18631000
C	-9.62003000	0.60013600	-0.88593300
C	-10.68473400	1.50520200	-1.07915900
N	-8.70233500	-1.43105600	-0.92307900
C	-7.77697600	-0.56175400	-0.48281200
N	-8.29441800	0.67037000	-0.44765500
N	-10.62618700	2.83460800	-0.82946900
C	-8.48784600	-2.87157200	-1.09152400
C	-7.54265500	1.85694300	-0.01208500
H	-12.92190600	-0.63124200	-2.14205500
H	-6.73123100	-0.86466200	-0.19076600
H	-11.44038400	3.38658900	-1.04939500
H	-9.77658300	3.30007200	-0.56423400
H	-8.64964400	-3.14335000	-2.13426700
H	-9.18997400	-3.41934400	-0.46363500
H	-7.46357700	-3.09382200	-0.79739600
H	-8.03961000	2.30620600	0.84968600
H	-7.48025300	2.57061000	-0.83605000
H	-6.53448400	1.52720800	0.26935300
N	-2.27973600	0.20231400	1.11031700
C	-3.05064400	-1.02616200	0.94764100
C	-4.49707500	-0.62298700	0.56764100
O	-4.81842100	0.58601900	0.68045100
O	-5.25469500	-1.55561600	0.17577200
H	-2.83327100	1.05121200	1.13285600
C	-0.95294700	0.28227500	0.93962400
O	-0.49561500	1.54577200	1.00707300
H	0.48799900	1.54593900	0.88796600
O	-0.21444500	-0.69198000	0.74588700
N	2.30419400	1.70614400	0.68802300
C	2.83005500	2.93651800	0.73154600

N	4.10892800	3.28466000	0.61773100
C	4.89589300	2.22250200	0.44381000
C	4.49017700	0.89298300	0.38072500
C	3.10481200	0.62720400	0.50973000
N	6.27307900	2.22304100	0.29180800
C	6.69396300	0.95379300	0.14331600
N	5.64481000	0.12739800	0.19231600
N	2.53735800	-0.58295400	0.47063400
C	7.14993700	3.39678400	0.29308800
C	5.76039900	-1.33361600	0.06512200
H	2.11885500	3.74335000	0.87771500
H	7.78671900	0.67534400	0.00285600
H	1.50882000	-0.66656700	0.56812600
H	3.09230200	-1.40948900	0.33346500
H	7.04727300	3.92677900	1.23976300
H	6.87022200	4.06242800	-0.52326100
H	8.17322200	3.04791200	0.16358000
H	5.21729000	-1.66638700	-0.82146800
H	5.35767600	-1.80860200	0.96157400
H	6.82790900	-1.57250400	-0.03357300
N	11.43954300	-2.44677900	0.23467600
C	11.16372600	-1.10224100	-0.29929600
C	9.67090400	-0.70455200	-0.18111700
O	8.81831600	-1.62451800	-0.12476900
O	9.40548500	0.53903400	-0.16032500
H	10.61584700	-3.01775200	0.05436600
H	11.50837700	-2.39447200	1.24648100
H	11.73513200	-0.37661200	0.28706400
C	11.68135200	-1.00321300	-1.76356700
H	12.70699100	-1.38668500	-1.70870300
H	-2.63311400	-1.59487900	0.11244500

C	-2.97215300	-1.92238800	2.21870600
H	-1.90620100	-1.94865800	2.46971500
C	-3.41552500	-3.36434200	1.94291600
H	-3.25827700	-3.98326800	2.83196400
H	-4.47068200	-3.40741500	1.66738700
H	-2.83876900	-3.80349000	1.12312900
C	-3.72574800	-1.31659700	3.40960600
H	-4.80603800	-1.30946500	3.23275800
H	-3.54040500	-1.90081100	4.31592100
H	-3.40849700	-0.28857500	3.60271400
C	11.73914400	0.44068800	-2.27954500
H	12.19082300	0.46968300	-3.27685300
H	10.74307900	0.88528600	-2.33663400
H	12.34034600	1.07363700	-1.61936500
C	10.90365300	-1.90770900	-2.72934600
H	11.35819600	-1.88178000	-3.72506300
H	10.90533000	-2.94634500	-2.38995100
H	9.86167500	-1.58737100	-2.82599800

2[dMA][Ile]-CO2

0 1

N	-11.98919100	-1.64494200	1.54564400
C	-12.07619000	-0.45867200	2.15568200
N	-11.15299400	0.50308800	2.21115800
C	-10.04475500	0.16567100	1.56022000
C	-9.81521900	-1.03193800	0.88336100
C	-10.86480700	-1.97444000	0.89267100
N	-8.89278800	0.92536900	1.41957600
C	-8.00250800	0.22811700	0.69358500
N	-8.52363000	-0.95515800	0.35396100
N	-10.81792900	-3.19224900	0.30280200

C	-8.66321800	2.26585400	1.96710800
C	-7.80465500	-1.96254500	-0.44047200
H	-13.01313500	-0.25866600	2.66473700
H	-6.97688800	0.61672400	0.43034500
H	-11.64984000	-3.76015800	0.33989000
H	-10.04871400	-3.48834200	-0.27117700
H	-8.76619200	2.23713400	3.05144800
H	-9.39626500	2.95823400	1.55398600
H	-7.65568300	2.57201300	1.69089500
H	-8.33898700	-2.13861400	-1.37629500
H	-7.72161600	-2.88630900	0.13492700
H	-6.80314200	-1.56697500	-0.65204700
N	-2.53655900	-0.06548000	-1.13643700
C	-3.31353500	1.07746100	-0.66770400
C	-4.75858600	0.58602500	-0.40467300
O	-5.07220800	-0.56185400	-0.80603700
O	-5.52176400	1.39266500	0.19926400
H	-3.08305300	-0.88815600	-1.36453000
C	-1.20666800	-0.16624900	-1.00588100
O	-0.73343400	-1.36482700	-1.39256900
H	0.25212400	-1.37506100	-1.29392900
O	-0.47824700	0.74034300	-0.58208200
N	2.08362200	-1.53444500	-1.18295900
C	2.63424700	-2.69444100	-1.56177800
N	3.92380200	-3.02078100	-1.58178300
C	4.69363100	-2.01708100	-1.16006500
C	4.26157300	-0.76346300	-0.73835700
C	2.86724200	-0.51546900	-0.75327500
N	6.07535500	-2.01432600	-1.05589400
C	6.47354200	-0.81544200	-0.59287000
N	5.40527000	-0.03816600	-0.39104500

N	2.27623100	0.62512800	-0.38220600
C	6.97696800	-3.11999600	-1.38916200
C	5.49237800	1.34051700	0.11494100
H	1.93586400	-3.45689700	-1.89201000
H	7.56422400	-0.55095500	-0.41350000
H	1.24433100	0.70537600	-0.43783800
H	2.81901400	1.40830300	-0.06298500
H	6.85852600	-3.38276900	-2.44016600
H	6.73548300	-3.98589700	-0.77303300
H	7.99583300	-2.78914800	-1.19417700
H	4.95502800	1.41469800	1.06221400
H	5.06643600	2.02515900	-0.62091900
H	6.55566700	1.56982200	0.26689300
N	11.14151200	2.58056100	0.36395500
C	10.90276600	1.12782600	0.41971500
C	9.41902200	0.75700700	0.16860300
O	8.54594400	1.63019600	0.39494300
O	9.18208900	-0.42267500	-0.24260400
H	10.29108200	3.03902500	0.68586000
H	11.24469900	2.86369800	-0.60564700
H	11.48878800	0.65299900	-0.37271100
C	11.43045500	0.55929000	1.77012400
H	12.43932700	0.98251100	1.85745400
H	-2.90033700	1.41414100	0.28714900
C	-3.23596500	2.27143000	-1.66545100
H	-2.17150000	2.34962300	-1.91668400
C	-4.01120400	1.98757700	-2.95926900
H	-5.09115000	1.97981500	-2.77919800
H	-3.80339300	2.74510900	-3.71859900
H	-3.73214400	1.01733200	-3.37813100
C	-3.64065800	3.59981700	-1.00012300

H	-3.10470300	3.68261400	-0.04728600
H	-4.70355900	3.56873700	-0.74593400
C	-3.33182800	4.83992500	-1.84701900
H	-3.91700500	4.86478500	-2.77044200
H	-3.56166300	5.75490600	-1.29289400
H	-2.27285800	4.87950200	-2.12407000
C	10.61341300	1.06536100	2.96749500
H	9.59791400	0.65650200	2.95779600
H	11.08240300	0.78418700	3.91411900
H	10.53577400	2.15491500	2.95336500
C	11.56638800	-0.97483400	1.75088700
H	12.07581000	-1.26501300	0.82445200
H	10.57348900	-1.43123000	1.69504600
C	12.34298300	-1.55176400	2.94091800
H	11.82905400	-1.37969200	3.89068900
H	12.47382000	-2.63315900	2.83360900
H	13.34029600	-1.10507000	3.01934300

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N	-11.94078700	-1.74182600	1.52669600
C	-12.01074900	-0.57957200	2.18337800
N	-11.07595400	0.36842400	2.27173200
C	-9.97614200	0.04530300	1.59962800
C	-9.76546100	-1.12565400	0.87194600
C	-10.82535600	-2.05640200	0.85139800
N	-8.81730500	0.79812100	1.47987700
C	-7.94162500	0.12288000	0.71632400
N	-8.47861100	-1.03959900	0.33248900
N	-10.80655000	-3.23772100	0.19009900
C	-8.56902200	2.11276100	2.07945600

C	-7.77996000	-2.01832400	-0.51422000
H	-12.94187000	-0.38995200	2.70688600
H	-6.91566600	0.51249900	0.45737200
H	-11.60901200	-3.83961700	0.28897300
H	-9.98658800	-3.58796400	-0.27232300
H	-8.65726500	2.03982600	3.16303900
H	-9.30200900	2.82726000	1.70581000
H	-7.56295200	2.42247800	1.80196000
H	-8.34619100	-2.17286200	-1.43451700
H	-7.66870000	-2.95745100	0.03148200
H	-6.78937700	-1.60851000	-0.74929800
N	-2.52377200	-0.09285300	-1.26492000
C	-3.31165100	1.04224400	-0.79458800
C	-4.73462300	0.52890200	-0.47558200
O	-5.07655800	-0.58385000	-0.94662200
O	-5.45794100	1.28941300	0.23009100
H	-3.06253700	-0.90760900	-1.53390700
C	-1.19061300	-0.17234000	-1.16758300
O	-0.70654400	-1.35633500	-1.58508800
H	0.28030400	-1.35524700	-1.49952700
O	-0.46859300	0.73919400	-0.74306600
N	2.11136900	-1.50195800	-1.39220900
C	2.67100500	-2.64967700	-1.79432000
N	3.96118100	-2.97415400	-1.79844200
C	4.72087800	-1.98300100	-1.33114600
C	4.27879400	-0.74275000	-0.88125400
C	2.88470900	-0.49518500	-0.91741600
N	6.10006500	-1.98289000	-1.19775200
C	6.48706300	-0.79855100	-0.69001200
N	5.41410300	-0.02796200	-0.48763900
N	2.28476200	0.63411900	-0.52692900

C	7.00968500	-3.07750300	-1.54543800
C	5.48878900	1.33460800	0.06226300
H	1.98033700	-3.40275400	-2.16037400
H	7.57342500	-0.53893300	-0.48244200
H	1.25308600	0.71180300	-0.59255300
H	2.81915000	1.40527600	-0.16681700
H	6.91357800	-3.30833400	-2.60618200
H	6.75632600	-3.96185800	-0.96110500
H	8.02382700	-2.75214500	-1.31915900
H	4.93377400	1.37833200	1.00124800
H	5.07472600	2.04073900	-0.65991700
H	6.54881100	1.56083700	0.24094800
N	11.22315800	2.49977700	0.11645300
C	10.87918000	1.11958200	0.49805300
C	9.41134000	0.75119700	0.18181900
O	8.53099300	1.61559800	0.41432200
O	9.19128400	-0.41371200	-0.28036600
H	10.47498800	3.10380200	0.45211600
H	11.20505900	2.58262000	-0.89649100
H	11.52189500	0.44509000	-0.07223800
C	11.16323000	0.95219900	2.00353300
H	12.20864800	1.23930100	2.16897900
H	-2.86739800	1.41497700	0.12958800
C	-3.32791100	2.17195200	-1.85389300
H	-2.28925900	2.33114400	-2.16492600
C	-3.92674300	3.52344000	-1.42247400
C	10.91026000	-0.43866400	2.61276600
H	-3.86587900	1.79803800	-2.73319100
C	-4.02913400	4.45559300	-2.63909600
H	-4.47797800	5.41525900	-2.36414000
H	-3.03934200	4.66272400	-3.06206700

H	-4.64215300	4.01386800	-3.43099000
C	11.12151300	-0.39039800	4.13334400
H	10.47127800	0.35459800	4.60243500
H	10.90942700	-1.36011300	4.59536200
H	12.15712400	-0.12650500	4.37670500
H	10.54908000	1.68890200	2.53598700
H	-4.93587200	3.33977100	-1.04174200
H	9.86332500	-0.70749900	2.42736200
C	11.78785300	-1.52610100	1.97642100
H	12.85109700	-1.27786700	2.07704100
H	11.62602700	-2.49300500	2.46453700
H	11.56203300	-1.64849200	0.91533600
C	-3.11507700	4.18933200	-0.30201400
H	-2.07503700	4.34520500	-0.60991100
H	-3.53725100	5.16660300	-0.04715500
H	-3.10911800	3.58773200	0.60967900