

Predicting the interactions of organometallic ruthenium ethylenediamine complexes with mononucleotides: insights from density functional theory

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Table S1

The relative energies (kcal mol⁻¹) for the reaction of **1** with 5'-GMP under neutral and acidic conditions

Neutral	$\Delta E_{\text{ZPE(aq)}}^{298}$	$\Delta H_{\text{(aq)}}^{298}$	$\Delta G_{\text{(aq)}}^{298}$		$\Delta E_{\text{ZPE(aq)}}^{298}$	$\Delta H_{\text{(aq)}}^{298}$	$\Delta G_{\text{(aq)}}^{298}$
SM	0.0	0.0	0.0	SM	0.0	0.0	0.0
GMP-RCa	-19.2	-19.4	-4.2	GMP-RCb	-16.4	-16.5	-2.0
GMP-TS1a	-4.5	-5.0	11.4	GMP-TS1b	5.8	5.3	21.3
GMP-IM1a	-22.5	-22.4	-7.1	GMP-IM1b	-17.2	-17.2	-1.9
GMP-IM2a	-19.2	-19.1	-4.0				
GMP-TS2a	2.2	1.7	18.7				
GMP-PCa	-22.2	-22.3	-6.6				
SM				SM	0.0	0.0	0.0
GMP-RCc	-18.3	-18.6	-3.3	GMP-RCd	-16.7	-17.1	-1.1
GMP-TSc	1.2	0.8	17.4	GMP-TSd	2.2	1.8	18.0
GMP-PCc	-23.5	-23.5	-8.1	GMP-PCd	-22.0	-22.0	-6.8
Acidic							
SM	0.0	0.0	0.0	SM	0.0	0.0	0.0
GMPH-RCa	-11.0	-11.3	3.8	GMPH-RCb	-8.0	-8.1	5.8
GMPH-TS1a	0.1	-0.3	15.5	GMPH-TS1b	10.9	10.5	25.8
GMPH-IM1a	-14.4	-14.3	0.5	GMPH-IM1b	-9.4	-9.6	5.0
GMPH-IM2a	-7.4	-7.0	6.3				
GMPH-TS2a	6.7	6.5	21.7				
GMPH-PCa	-18.2	-18.1	-3.4				
SM				SM	0.0	0.0	0.0
GMPH-RCc	-18.2	-18.7	-3.4	GMPH-RCd	-14.1	-14.8	1.7
GMPH-TSc	4.7	4.0	21.5	GMPH-TSd	5.0	4.8	20.0
GMPH-PCc	-17.5	-17.5	-3.1	GMPH-PCd	-17.4	-17.3	-2.4

Table S2

The relative energies (kcal mol⁻¹) for the reaction of **1** with 5'-AMP under neutral and acid conditions

Neutral	$\Delta E_{\text{ZPE(aq)}}^{298}$	$\Delta H_{\text{(aq)}}^{298}$	$\Delta G_{\text{(aq)}}^{298}$		$\Delta E_{\text{ZPE(aq)}}^{298}$	$\Delta H_{\text{(aq)}}^{298}$	$\Delta G_{\text{(aq)}}^{298}$
SM	0.0	0.0	0.0	SM	0.0	0.0	0.0
AMP-RCa	-15.1	-15.1	-0.7	AMP-RCb	-10.4	-10.1	3.3
AMP-TS1a	-0.9	-1.0	13.8	AMP-TS1b	6.2	6.4	19.5
AMP-IM1a	-20.6	-20.2	-6.5	AMP-IM1b	-14.6	-13.9	-1.3
AMP-IM2a	-24.2	-23.9	-11.0	AMP-IM2b	-19.6	-18.9	-6.6
AMP-TS2a	8.3	8.3	22.8	AMP-TS2b	11.0	11.1	25.6
AMP-PCa	-12.1	-12.1	3.8	AMP-PCb	-16.7	-16.7	-0.9
SM				SM	0.0	0.0	0.0
AMP-RCc	-6.8	-6.7	7.6	AMP-RCd			
AMP-TSc	15.5	15.5	31.0	AMP-TSd	10.5	10.2	26.9
AMP-PCc	-10.7	-10.5	5.1	AMP-PCd	-12.1	-11.9	3.3
Acidic							
SM	0.0	0.0	0.0	SM	0.0	0.0	0.0
AMPH-RCa	-5.1	-5.2	9.7	AMPH-RCb	-1.3	-1.8	13.6
AMPH-TS1a	6.3	6.1	21.5	AMPH-TS1b	11.3	11.3	24.8
AMPH-IM1a	-9.7	-9.4	4.8	AMPH-IM1b	-9.9	-9.7	4.5
AMPH-IM2a	-13.1	-13.1	1.1	AMPH-IM2b	-11.5	-11.5	3.4
AMPH-TS2a	15.0	14.8	29.5	AMPH-TS2b	7.2	6.6	23.1
AMPH-PCa	-7.5	-7.7	7.8	AMPH-PCb	-2.7	-2.8	12.7
SM	0.0	0.0	0.0	SM	0.0	0.0	0.0
AMPH-RCc	-6.6	-7.0	8.3	AMPH-RCd			
AMPH-TSc	15.2	14.7	31.1	AMPH-TSd	21.2	21.1	36.1
AMPH-PCc	-5.1	-5.1	10.6	AMPH-PCd	-6.0	-5.8	9.7

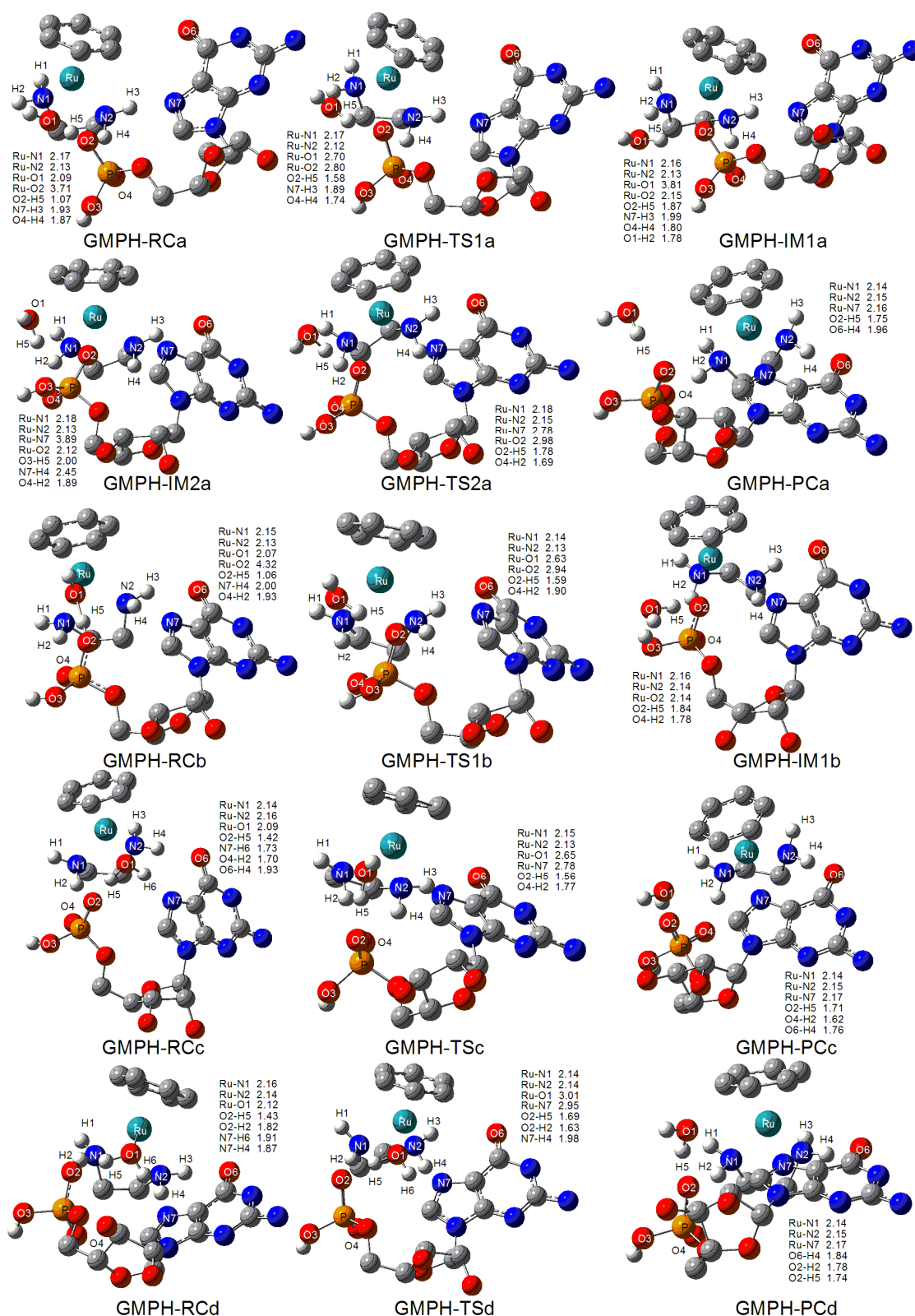


Fig. S1. Optimized structures and selected structural parameters of reaction of **1** with 5'-GMP under acid conditions. Some hydrogen atoms are omitted for clarity. The distances reported are in angstroms.

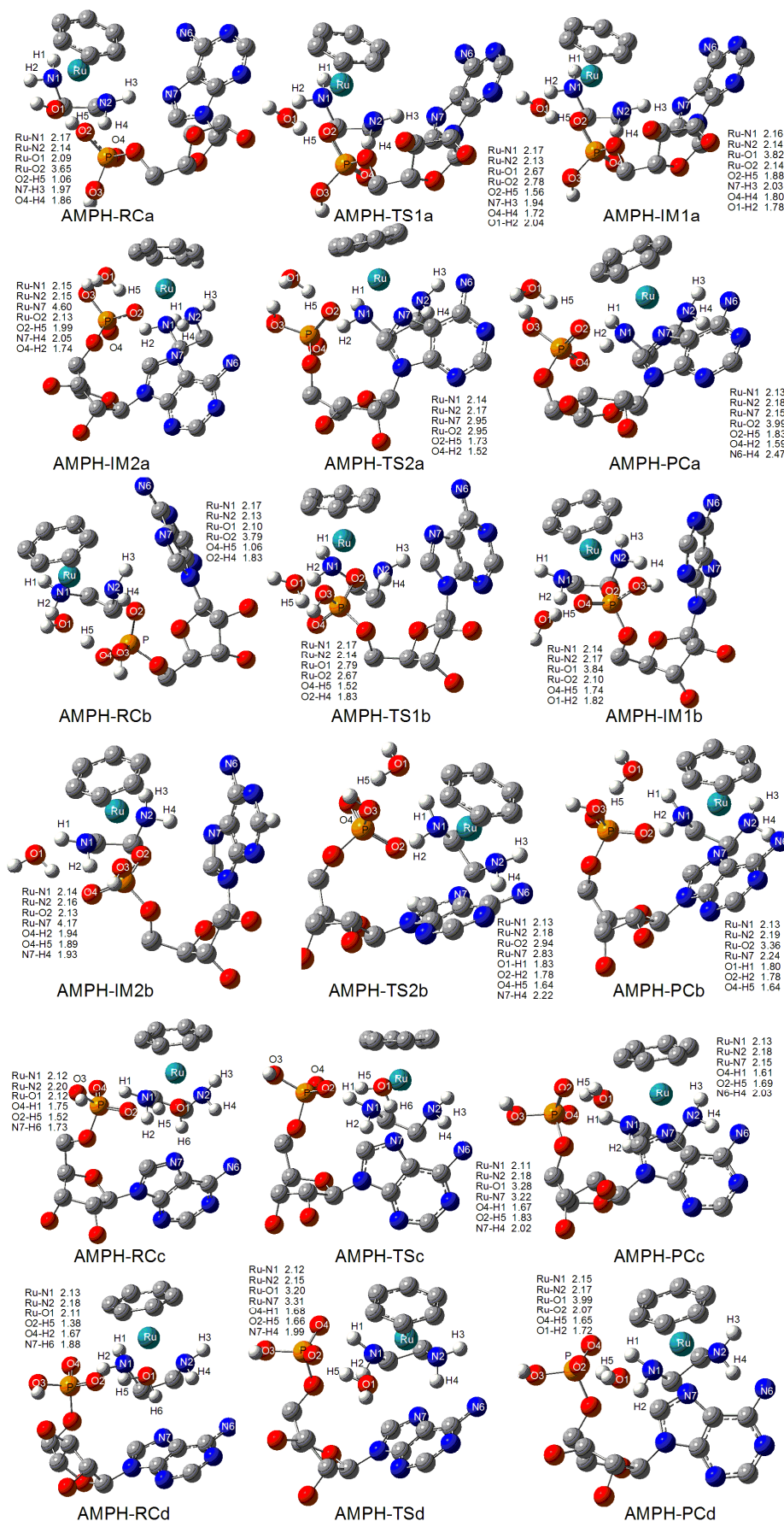


Fig. S2. Optimized structures and selected structural parameters of reaction of **1** with 5'-AMP under acid conditions. Some hydrogen atoms are omitted for clarity. The distances reported are in angstroms.

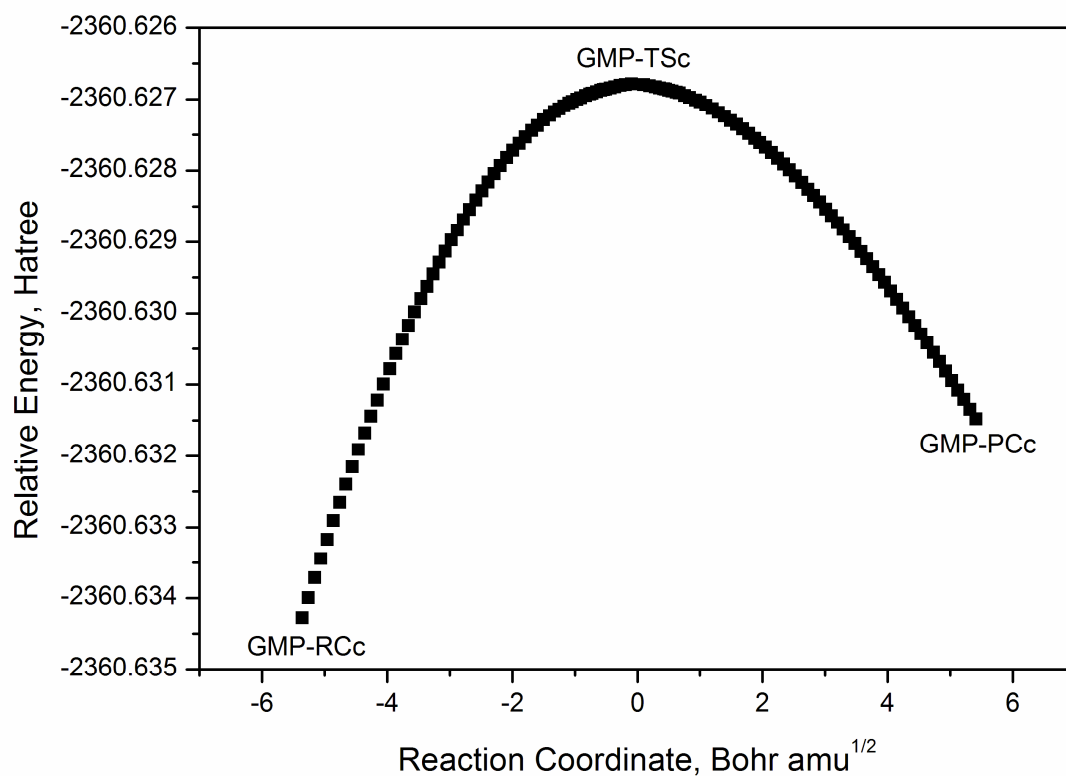


Fig. S3. IRC along the reaction coordinate for the GMP-TSc at the B3LYP/6-31G(d,p) (LanL2DZ for Ru) level of theory. IRC calculations (examined by 120 points) were performed with a step size of 0.1 bohr amu^{1/2}.

Cartesian coordinates for the species involved in Fig. 1:

GMP-RCa

C	-1.92200400	2.49257800	0.99277000
C	-1.37580800	1.32658300	1.62686200
C	-2.17843100	0.51451900	2.45072900
C	-3.55444100	0.86044100	2.66884600
C	-4.10207300	1.98683400	2.03187100
C	-3.28094900	2.80402000	1.18076700
H	-0.35929000	1.02662600	1.40510300
H	-1.77508800	-0.40935500	2.84885700
H	-5.15360500	2.22221900	2.15740200
H	-3.71459900	3.65644500	0.66896600
H	-1.72853400	-0.82060300	-1.27548800
N	-2.00413400	0.17967300	-1.30855900
H	-1.10916800	0.70012100	-1.30298700
C	-2.76131800	0.45421100	-2.54916500
H	-2.70902400	1.52717200	-2.76474900
H	-2.32374800	-0.07733900	-3.40239200
C	-4.20041300	0.01776700	-2.33160000
H	-4.83404600	0.24550300	-3.19544200
H	-4.23462400	-1.05338900	-2.12614700
N	-4.70386800	0.69295000	-1.09855300
H	-5.00582500	1.64332600	-1.30671100
H	-5.51300400	0.18772100	-0.74330200
O	-3.57335500	-1.39180300	0.27398700
H	-2.27167500	-2.05966900	0.75165700
H	-4.17413900	-1.63198500	0.99257000
H	-4.18303500	0.22269500	3.28069900
H	-1.30426500	3.08767700	0.32305100
Ru	-3.15220400	0.64419900	0.42639300
P	-0.45647400	-3.06758600	0.02371000
O	-0.74322300	-2.40362800	-1.34930700
O	-1.38909100	-2.41508600	1.13730600
O	1.00849900	-2.59487100	0.58137600
C	2.14011800	-3.46737500	0.46720800
H	2.03230100	-4.13934800	-0.38913000
H	2.22019800	-4.08323500	1.37033300
C	3.41225600	-2.65281600	0.33297200
H	4.25765600	-3.35389500	0.31053800
O	3.40665300	-1.90091300	-0.90690400
C	3.92744700	-0.61053500	-0.71197200
H	4.67712800	-0.38839000	-1.47879500
N	2.82830700	0.37258700	-0.85028800
C	1.49908800	0.08556900	-1.07593900
H	1.14457800	-0.92476700	-1.20916800

N	0.74418000	1.16410700	-1.08654500
C	1.61562700	2.21352900	-0.86841800
C	1.36040000	3.61439900	-0.72024500
O	0.29695200	4.22910000	-0.72229400
N	2.58557200	4.31735800	-0.52910600
H	2.47641200	5.32359800	-0.47714300
C	3.83659400	3.75127500	-0.43052900
N	4.89267000	4.60216100	-0.28636300
H	4.75523700	5.52181100	0.10360900
H	5.77851000	4.16112400	-0.08976600
N	4.05215800	2.45384200	-0.50573900
C	2.91985700	1.74151800	-0.73122500
C	3.66156500	-1.61184800	1.44430200
H	2.70897300	-1.16177500	1.73767100
C	4.52996600	-0.57708500	0.70699500
H	4.49939600	0.42179900	1.15052600
O	5.84689400	-1.11154400	0.70388300
H	6.47684600	-0.41164600	0.49323300
O	4.25677300	-2.13505900	2.60013700
O	-0.50621000	-4.58418600	-0.09012500
H	5.20228300	-2.22468000	2.40032900
Na	-1.00472400	-4.47409700	-2.22036800

GMP-TS1a

C	1.47282900	-2.59694700	0.85527200
C	0.90706900	-1.48667700	1.56126600
C	1.70562900	-0.74984400	2.45054300
C	3.04724900	-1.16952200	2.75109500
C	3.59533700	-2.28501600	2.10564500
C	2.82224800	-2.97551900	1.11131300
H	-0.07947300	-1.13014700	1.29679300
H	1.34183700	0.19365700	2.83822100
H	4.62583600	-2.57067000	2.28792700
H	3.26093800	-3.79982300	0.55900900
H	1.65353700	0.56713200	-1.44556700
N	1.86342400	-0.46649700	-1.39080700
H	0.92879400	-0.91477300	-1.43042400
C	2.69794000	-0.87041800	-2.54109300
H	2.64470900	-1.95793000	-2.66246400
H	2.33164500	-0.41068400	-3.46648200
C	4.11837900	-0.42734900	-2.24015700
H	4.83054000	-0.75896500	-3.00246400
H	4.16028900	0.66300500	-2.17432400
N	4.48671300	-0.95153200	-0.89297700
H	4.92512100	-1.86738700	-0.96027700
H	5.12160500	-0.29444400	-0.43711400

O	4.34490800	1.25758700	0.62423800	C	0.13897300	-1.48873500	1.56858200
H	3.40245700	1.66475100	0.67285600	C	0.95652000	-0.74900100	2.44784100
H	4.73798000	1.44188700	1.48700000	C	2.21646700	-1.26173800	2.88444700
H	3.65588600	-0.57521900	3.42260900	C	2.66300500	-2.49809400	2.37376900
H	0.88191500	-3.12386100	0.10798300	C	1.85436000	-3.25751800	1.46770600
Ru	2.79005100	-0.88076800	0.47149900	H	-0.79458000	-1.07630700	1.21280600
P	1.06222100	2.66551900	-0.09176100	H	0.66077200	0.25409000	2.73305900
O	1.03886300	2.14447700	-1.57482200	H	3.64858100	-2.86339500	2.64537400
O	1.91956300	1.72855200	0.79649000	H	2.21162400	-4.20129000	1.07212400
O	-0.46423900	2.45863900	0.52432500	H	1.60173700	-0.11723700	-1.72662100
C	-1.40346100	3.53205900	0.46632300	N	1.63626300	-1.12779000	-1.47192300
H	-1.21425400	4.18230100	-0.39431800	H	0.67728800	-1.47796200	-1.62339700
H	-1.32057200	4.14856700	1.36984600	C	2.65804500	-1.81550500	-2.28734100
C	-2.82282300	2.99807000	0.39052300	H	2.58099100	-2.89550000	-2.12239300
H	-3.50812400	3.85444200	0.44744200	H	2.50417100	-1.62698600	-3.35689000
O	-3.05127400	2.32219300	-0.87505900	C	4.01006900	-1.28727700	-1.83489600
C	-3.77432000	1.13429000	-0.68706100	H	4.83898900	-1.80453800	-2.32858000
H	-4.58575900	1.07056400	-1.41954200	H	4.08750800	-0.22195100	-2.06466800
N	-2.86366100	-0.01613300	-0.90648400	N	4.10562600	-1.41452500	-0.35114700
C	-1.52412800	0.06751700	-1.21977900	H	4.51980400	-2.31069200	-0.10340200
H	-1.02892700	1.01258500	-1.38614400	H	4.72447800	-0.66136200	0.00175100
N	-0.94070900	-1.11227000	-1.25735900	O	5.28005500	1.03789500	0.21674600
C	-1.94239000	-2.01766400	-0.96946500	H	4.35331100	1.29181300	0.42024000
C	-1.87810000	-3.43551100	-0.78983700	H	5.83660500	1.47272100	0.87322700
O	-0.90705700	-4.18821400	-0.81257800	H	2.85149300	-0.67131400	3.53315800
N	-3.17863400	-3.95396500	-0.52528400	H	0.00141000	-3.27462700	0.32456000
H	-3.21173900	-4.96416100	-0.45103100	Ru	2.16569700	-1.18326300	0.58758300
C	-4.32855000	-3.21060800	-0.37556600	P	1.81973600	2.03860200	-0.32785000
N	-5.48756300	-3.89690800	-0.16475800	O	1.49552200	1.63246800	-1.79550700
H	-5.46829500	-4.82727300	0.22309300	O	2.58751600	0.89216400	0.42389600
H	-6.29054800	-3.33076000	0.06412000	O	0.39904900	2.16812200	0.50360900
N	-4.35898200	-1.89619700	-0.46129700	C	-0.25840700	3.44392100	0.54428100
C	-3.15159100	-1.35615600	-0.76306000	H	0.09271800	4.08982000	-0.26541600
C	-3.21205800	1.97595700	1.47838100	H	-0.01678000	3.93997500	1.49163100
H	-2.34862100	1.34232000	1.69934500	C	-1.76689600	3.30396300	0.46591900
C	-4.29927700	1.15429400	0.76213600	H	-2.19207500	4.30838900	0.60076800
H	-4.43664800	0.15005000	1.17219200	O	-2.18293600	2.80460300	-0.82914000
O	-5.48871200	1.92677500	0.85325100	C	-3.24455600	1.88950500	-0.69340300
H	-6.25070700	1.36806500	0.65773400	H	-4.04073300	2.13786200	-1.40276400
O	-3.63661200	2.54815700	2.68576300	N	-2.73991800	0.53223100	-1.00480700
O	1.40188000	4.15563500	-0.09131300	C	-1.45647400	0.22504800	-1.41188600
H	-4.55584800	2.82512100	2.54382500	H	-0.71956600	0.99015600	-1.60875600
Na	1.54711700	4.21373000	-2.26525800	N	-1.24941000	-1.07142700	-1.49362700
				C	-2.45134100	-1.64877300	-1.13989400
GMP-IM1a				C	-2.78364500	-3.02827600	-0.93706000
C	0.60346400	-2.74148000	1.05691800	O	-2.06961200	-4.02309500	-0.98139600

N	-4.16736800	-3.15051900	-0.60489500	H	-1.80055900	-4.25379600	0.74725900
H	-4.48395700	-4.10896300	-0.51363400	Ru	-2.12568000	-1.28298600	0.12001500
C	-5.04223300	-2.10897800	-0.39491100	P	-1.57255400	2.04866800	0.19459100
N	-6.33767800	-2.43067600	-0.12093800	O	-2.78507200	2.22153600	1.13654300
H	-6.57675600	-3.33821200	0.24651500	O	-1.67008600	0.66614100	-0.57050500
H	-6.93229900	-1.66137300	0.14687100	O	-0.18399400	1.83031500	1.06794600
N	-4.69358500	-0.84027700	-0.47784900	C	0.52255200	2.95226300	1.63273500
C	-3.40031300	-0.66950200	-0.85274700	H	0.60385800	2.77678000	2.70989200
C	-2.41623300	2.35756100	1.49400100	H	-0.02489800	3.88473500	1.46449100
H	-1.78573900	1.47207700	1.61678800	C	1.90844200	3.09095100	1.01709200
C	-3.71894300	1.97406700	0.77178000	H	2.44914100	3.86540700	1.58064100
H	-4.16314200	1.03951800	1.12268800	O	2.61104200	1.84081800	1.12780100
O	-4.59621400	3.07638700	0.95761200	C	3.34495700	1.55503100	-0.05288900
H	-5.50019600	2.80562400	0.75574000	H	4.38701900	1.34985000	0.20586400
O	-2.60705200	2.92229900	2.76226000	N	2.83932300	0.31817200	-0.65323800
O	2.57095600	3.36405200	-0.29559300	C	1.59772300	0.10554500	-1.23980500
H	-3.40019800	3.47758700	2.69268500	H	0.94238800	0.92009600	-1.50746000
Na	2.59644200	3.47301800	-2.49742000	N	1.30803100	-1.16186400	-1.39503900
GMP-IM2a				C	2.40001800	-1.83326000	-0.87544700
C	-2.19468500	-3.55411300	0.01872000	C	2.59305800	-3.23576200	-0.65550400
C	-1.36232300	-3.08974300	-1.05183600	O	1.82137200	-4.17330200	-0.84199300
C	-1.86345000	-2.15162400	-1.97246300	N	3.87816900	-3.47067400	-0.08660400
C	-3.21084600	-1.67750400	-1.85026800	H	4.06236000	-4.44408200	0.12774100
C	-4.03782500	-2.13139000	-0.80883400	C	4.78113700	-2.49997100	0.29106200
C	-3.51019700	-3.05979500	0.15030800	N	5.93428100	-2.92526300	0.88491700
H	-0.32347700	-3.40827900	-1.11326000	H	6.29844500	-3.84090100	0.66775700
H	-1.19392100	-1.73123300	-2.71170000	H	6.62379300	-2.20206900	1.03111000
H	-5.04170000	-1.73844000	-0.69708000	N	4.55734600	-1.21017100	0.15551400
H	-4.12463600	-3.37810200	0.98615900	C	3.35998100	-0.93627200	-0.41155400
H	0.00308500	-0.14114200	1.17265400	C	1.93058400	3.47469900	-0.48002100
N	-0.37059100	-1.08604100	1.33306000	H	1.05537000	3.05553300	-0.98320000
H	0.34968400	-1.74798000	1.05103300	C	3.23085800	2.79506100	-0.96400400
C	-0.74671500	-1.24712300	2.75925800	H	3.21404400	2.53314200	-2.02736300
H	-1.03785200	-2.29015700	2.91473900	O	4.27612600	3.71496400	-0.66831800
H	0.09645800	-1.02337700	3.42361900	H	5.04509900	3.52470200	-1.21882100
C	-1.91062600	-0.30269800	3.03624100	O	1.90101100	4.85720700	-0.70867900
H	-2.37412100	-0.53070300	4.00014000	O	-1.41506500	3.20621800	-0.77302300
H	-1.55377700	0.72856400	3.06773200	H	2.81498800	5.16642000	-0.60129000
N	-2.91481700	-0.37962200	1.92857200	Na	-3.67151300	3.54087200	-0.59240500
H	-3.75910400	-0.85220500	2.23983600	GMP-TS2a			
H	-3.14690500	0.60541100	1.66123100	C	-3.36463300	-2.79111100	-0.85781600
O	-3.76819200	1.75447600	-2.15622700	C	-2.19219000	-2.90885400	-1.67531200
H	-3.01430800	1.29410400	-1.71786800	C	-1.75459500	-1.79203600	-2.39658400
H	-3.38786400	2.08095600	-2.98347300	C	-2.49851700	-0.56256300	-2.36838100
H	-3.57292400	-0.89597400	-2.50878800	C	-3.70208000	-0.46478900	-1.65642900

C	-4.12145700	-1.58026600	-0.85920800	H	5.02239600	-5.20271600	0.40169000
H	-1.57344900	-3.79670000	-1.61206100	H	5.89453800	-3.72316700	0.43991200
H	-0.79592800	-1.81850800	-2.89819500	N	4.01752700	-2.17227600	0.06990800
H	-4.20866900	0.49307500	-1.59875400	C	2.83476600	-1.55682300	-0.13751500
H	-5.01063400	-1.50344600	-0.24192100	C	2.73588600	3.02649600	-0.72323100
H	-0.32084000	-1.77317500	1.56706000	H	1.71324600	2.81985200	-1.04936200
N	-1.23513700	-2.21553600	1.46865900	C	3.69701600	1.92612300	-1.23406400
H	-1.03413400	-3.19217500	1.23246700	H	3.41835900	1.53049700	-2.21702400
C	-2.01545500	-2.00960200	2.70977500	O	4.98956600	2.51982200	-1.25376200
H	-2.95729500	-2.56012600	2.62076000	H	5.56027200	2.04199500	-1.86702100
H	-1.47986000	-2.38735100	3.58840500	O	3.05453500	4.30477200	-1.20008400
C	-2.25372400	-0.51058900	2.79901000	O	-0.81153500	4.06496700	0.03354900
H	-2.93159500	-0.25758100	3.62029000	H	4.02351700	4.34413500	-1.23851600
H	-1.31105300	0.01648900	2.97964400	Na	-3.01512500	4.24061100	0.43775400
N	-2.78049300	-0.02143600	1.49841600				
H	-3.79784300	-0.06782600	1.51137800	GMP-PCa			
H	-2.51092500	1.03568900	1.43676900	C	-1.86649800	-3.73679100	1.67922000
O	-3.39867300	2.77743800	-1.40617000	C	-2.18783300	-2.52256700	2.35845300
H	-2.54718800	2.28688000	-1.20053700	C	-1.15671700	-1.59175000	2.59788300
H	-3.21057300	3.24664300	-2.23016800	C	0.19208600	-1.86249200	2.21402200
H	-2.07773800	0.32208900	-2.82872600	C	0.49650700	-3.07972400	1.56913500
H	-3.67921800	-3.62313800	-0.23692800	C	-0.53380500	-4.03684000	1.31083100
Ru	-2.09107700	-1.15286500	-0.20382000	H	-3.21190300	-2.29920500	2.63194400
P	-0.88602600	2.62495500	0.52573600	H	-1.40264800	-0.62966200	3.03403100
O	-2.03447700	2.46471800	1.58093900	H	1.51867200	-3.25280900	1.24124300
O	-1.10831400	1.55585100	-0.59137000	H	-0.30553900	-4.96813200	0.80498400
O	0.54335400	2.18431600	1.22316200	H	-3.32454400	-1.61481200	-1.05215400
C	1.54811300	3.13799800	1.58180300	N	-2.65095500	-2.39603000	-1.15098800
H	1.73500800	3.04151200	2.65660100	H	-3.18273100	-3.23491400	-0.93092000
H	1.21028900	4.15593000	1.36183600	C	-2.10800600	-2.50074700	-2.54009300
C	2.84048100	2.87815200	0.81431000	H	-1.97088600	-3.56221900	-2.77271700
H	3.60371700	3.57750400	1.18131100	H	-2.82162600	-2.09195500	-3.26252700
O	3.30246900	1.52884100	1.06684200	C	-0.76618200	-1.78328200	-2.59668600
C	3.63278900	0.85977100	-0.12288900	H	-0.24016100	-2.00154900	-3.53299600
H	4.58934400	0.34327000	-0.00763500	H	-0.89326000	-0.70077200	-2.53169600
N	2.64590000	-0.21298100	-0.38392800	N	0.02983700	-2.21891800	-1.43163900
C	1.29050900	-0.03612800	-0.54631400	H	0.22603700	-3.21472000	-1.54397500
H	0.80715100	0.91089800	-0.72404500	H	1.04892700	-1.78296800	-1.44659400
N	0.60752600	-1.15027500	-0.42402800	O	3.70452700	-2.76033200	1.08658800
C	1.56265700	-2.13171000	-0.17344800	H	3.27310200	-1.84833000	1.06345800
C	1.42535100	-3.53074200	0.06989400	H	4.31753000	-2.72999800	1.83239100
O	0.40250500	-4.22501900	0.14851300	H	0.97438200	-1.11903600	2.31331200
N	2.69397800	-4.12964400	0.26979000	H	-2.65960500	-4.43780500	1.43702800
H	2.65298200	-5.11827500	0.49004500	Ru	-1.12717300	-2.05881500	0.34718000
C	3.90476100	-3.46836800	0.27434000	P	3.05113300	-0.32150400	-0.77881600
N	5.01452400	-4.20537600	0.54816200	O	2.48547600	-1.50728400	-1.63694900

O	2.46235000	-0.41852000	0.66275000	H	5.92556900	0.04209300	1.47242000
O	2.39359700	1.03316800	-1.45356000	H	0.97038900	0.92072600	-0.27213600
C	3.12368700	2.25996200	-1.50085000	N	1.67542500	0.99822300	0.48201700
H	3.07551000	2.63114500	-2.53015700	H	1.78585700	2.00914100	0.59588100
H	4.17374100	2.10128400	-1.23343800	C	1.10132400	0.38324100	1.71851800
C	2.50547800	3.28701100	-0.56431600	H	0.72836300	1.16106700	2.39117200
H	3.02000300	4.24813500	-0.69671500	H	0.25558200	-0.24446800	1.43063700
O	1.11096000	3.46689000	-0.92618800	C	2.15686700	-0.46720600	2.40919700
C	0.27933700	3.41911500	0.18937200	H	2.91543500	0.15556400	2.89379300
H	-0.43254500	4.24818800	0.16531300	H	1.69297000	-1.11344800	3.16200400
N	-0.59570500	2.20755500	0.14504900	N	2.82038600	-1.27820800	1.35457200
C	-0.24320600	0.88379700	0.16832900	H	3.59218500	-1.80897000	1.75297700
H	0.77292000	0.52240600	0.34246800	H	2.12114900	-1.96690500	1.01009400
N	-1.28987200	0.08776500	-0.01926700	O	2.05719000	-1.12591800	-1.26261300
C	-2.38835300	0.93871200	-0.18308900	H	0.67604300	-1.73987900	-1.12040000
C	-3.77652200	0.70682300	-0.42001800	H	2.11096100	-0.91211300	-2.20214000
O	-4.39579000	-0.35605500	-0.56945600	H	5.03795700	-0.93864300	-2.64702500
N	-4.49638800	1.91820300	-0.49823300	H	4.90962400	2.30363200	1.17482600
H	-5.48180100	1.79039300	-0.69959800	Ru	3.42177600	0.02972100	-0.23973900
C	-3.96118300	3.18258000	-0.38585700	P	-0.64780400	-2.92208700	0.20990600
N	-4.79820700	4.23497700	-0.53019800	O	0.59156200	-3.04216100	1.12801100
H	-5.79985500	4.13670100	-0.54397500	O	-0.26378900	-2.14704100	-1.12901000
H	-4.40708200	5.15508100	-0.39987600	O	-1.73166300	-1.87815300	0.86542800
N	-2.67958700	3.39066300	-0.16757200	C	-3.01696800	-2.30127600	1.34512500
C	-1.95106900	2.26063100	-0.08210800	H	-3.05991900	-2.09211500	2.41937400
C	2.51635400	2.90730900	0.93667900	H	-3.15126700	-3.37388400	1.17417500
H	2.51206500	1.81863000	1.04692400	C	-4.13800100	-1.55138200	0.63737300
C	1.17929100	3.49525800	1.43889100	H	-5.09124600	-1.89840500	1.06107900
H	0.76406100	2.95660900	2.29871300	O	-4.01012000	-0.13687400	0.87927500
O	1.43737800	4.85879600	1.74995800	C	-4.18083800	0.61352500	-0.30449700
H	0.76686800	5.19019400	2.35874700	H	-4.88801700	1.42637100	-0.12073600
O	3.63181900	3.38191600	1.64245800	N	-2.91455400	1.27031300	-0.66307400
O	4.57110000	-0.28351800	-0.85371700	C	-1.75682400	0.65816900	-1.11155800
H	3.46746800	4.32217800	1.81458200	H	-1.73021300	-0.35652600	-1.47885700
Na	4.55328600	-2.49760500	-1.08958000	N	-0.69652000	1.41876400	-0.99776300
GMP-RCb				C	-1.15828800	2.59029400	-0.42359900
C	4.96036200	1.61332500	0.34106700	C	-0.43091900	3.70628800	0.09549500
C	4.37638900	1.95893700	-0.91886200	O	0.78716600	3.88806600	0.17990400
C	4.42172300	1.05609200	-2.00231700	N	-1.32757900	4.67462900	0.62191300
C	5.05115100	-0.22207900	-1.83318400	H	-0.87081100	5.47100500	1.05119100
C	5.61468200	-0.58216600	-0.59962700	C	-2.69566000	4.53070900	0.72536000
C	5.53567500	0.33502500	0.50308900	N	-3.37906000	5.54903500	1.32662200
H	3.85050500	2.90206700	-1.02696200	H	-3.01775400	6.48963300	1.27215600
H	3.95198600	1.31390800	-2.94409300	H	-4.38422500	5.46326000	1.27924300
H	6.05520300	-1.56314500	-0.46508700	N	-3.34209300	3.45659200	0.32840800
				C	-2.53217200	2.51690500	-0.20914600

C	-4.18910600	-1.73444800	-0.89791400	H	-2.35193300	-3.34383400	1.38922700
H	-3.18163000	-1.91261500	-1.28301300	C	-3.67158000	-1.82657600	0.68197900
C	-4.70781800	-0.35840500	-1.37838100	H	-4.54438000	-2.31377400	1.13902000
H	-4.36935100	-0.09790000	-2.38708600	O	-3.84417800	-0.39853300	0.77539500
O	-6.12692700	-0.43771500	-1.30709100	C	-4.06671500	0.18467300	-0.48867900
H	-6.52037800	0.22447000	-1.88767000	H	-4.90432100	0.88244700	-0.41332900
O	-4.98193700	-2.80916000	-1.32089500	N	-2.90252400	1.00074900	-0.87596200
O	-1.30925800	-4.26897100	-0.02980400	C	-1.69614700	0.57200100	-1.41523400
H	-5.89580600	-2.48180000	-1.32634800	H	-1.58011900	-0.39699100	-1.87542100
Na	0.21095100	-5.29943900	1.14992000	N	-0.72427100	1.43766300	-1.27654300
GMP-TS1b				C	-1.29866600	2.48991200	-0.58840800
C	3.73837000	2.23901300	-0.14339700	C	-0.66993500	3.58481700	0.06956200
C	2.90669400	2.19183300	-1.30899900	O	0.54124200	3.82353500	0.19837900
C	3.13850100	1.20320200	-2.27788000	N	-1.62770300	4.40912900	0.70535400
C	4.27002900	0.32548600	-2.15487600	H	-1.23517800	5.17819800	1.23620200
C	5.13105700	0.39907000	-1.05426400	C	-2.97665000	4.12463800	0.80813500
C	4.81951000	1.31998900	-0.00222600	N	-3.73675900	5.01056200	1.51831400
H	2.02095400	2.81826000	-1.34631000	H	-3.47569800	5.98545500	1.53091500
H	2.43754700	1.07398600	-3.09368100	H	-4.72951000	4.82698800	1.48332300
H	5.95454100	-0.29750100	-0.95102200	N	-3.52503600	3.03652900	0.31699800
H	5.42497900	1.33913700	0.89803600	C	-2.64611800	2.24239200	-0.33485300
H	0.49002800	0.28682800	0.32748200	C	-3.64479000	-2.17545700	-0.82559700
N	1.21540400	0.76819000	0.87360800	H	-2.60902900	-2.22744600	-1.16930400
H	1.06477100	1.77473500	0.77193900	C	-4.37384800	-0.96761300	-1.46305300
C	1.18965700	0.33437100	2.30443500	H	-4.04929600	-0.75847700	-2.48845000
H	0.88865600	1.17011100	2.94167000	O	-5.76044500	-1.28335000	-1.41153300
H	0.45349300	-0.46376600	2.39846700	H	-6.23977200	-0.75707800	-2.06238300
C	2.56913200	-0.18407900	2.70217200	O	-4.23587000	-3.40786300	-1.13786000
H	3.26544800	0.63585800	2.90426300	O	-0.52763500	-3.81943600	-0.22185400
H	2.49883800	-0.80763400	3.60045600	H	-5.19138000	-3.24309800	-1.18214600
N	3.07880300	-0.97120100	1.54988400	Na	0.81669100	-4.99733200	1.03134200
H	4.00839500	-1.34171100	1.73640200	GMP-IM1b			
H	2.41402000	-1.78388700	1.41978300	C	-2.92946700	-3.00443600	-0.59371900
O	2.98089400	-2.29446200	-1.08145000	C	-2.00855000	-2.52318400	-1.58314200
H	1.98244500	-2.11865400	-1.04356400	C	-2.31191400	-1.36669700	-2.32121300
H	3.18005500	-2.45163300	-2.01311600	C	-3.54740100	-0.67486700	-2.08944100
H	4.42124900	-0.44694300	-2.89977300	C	-4.45970000	-1.14278800	-1.12854400
H	3.51663800	2.95308300	0.64164500	C	-4.13520200	-2.31070100	-0.35862500
Ru	2.95024400	0.20823800	-0.22307500	H	-1.03517400	-2.99257800	-1.67160500
P	0.00936400	-2.50632100	0.34746800	H	-1.56879200	-0.95090200	-2.98943900
O	1.01556700	-2.81052600	1.51106000	H	-5.37248700	-0.59242100	-0.93098200
O	0.62998200	-1.49744600	-0.65973100	H	-4.81077900	-2.64886800	0.42001800
O	-1.25694200	-1.62009100	0.94796700	H	0.03381800	-0.66236200	0.69966700
C	-2.43308100	-2.25407500	1.46133800	N	-0.69476100	-1.26860800	1.08253000
H	-2.54508500	-1.96721100	2.51271900	H	-0.40680600	-2.23388800	0.91118800

C	-0.88067500	-0.97092000	2.53473100	O	4.99050200	2.93786500	-1.03488100
H	-0.34325300	-1.69628100	3.15262900	H	5.65677600	2.67514500	-1.68114200
H	-0.45952600	0.01873800	2.71734900	O	2.82410000	4.39215900	-0.71409800
C	-2.36680400	-0.96455300	2.86685700	O	-0.76926700	3.46211900	-0.25946300
H	-2.77958900	-1.97825000	2.83901400	H	3.77997300	4.56076600	-0.69651800
H	-2.53083200	-0.55341600	3.87005900	Na	-2.78272600	4.14816400	0.51750000
N	-3.04868700	-0.14890900	1.83063100	GMP-RCc			
H	-4.05701700	-0.17317900	1.96539800	C	4.34498300	2.31331800	0.11989200
H	-2.72472300	0.85189700	1.88976200	C	3.20579000	2.68067600	-0.66995500
O	-3.58250600	2.83838200	-1.30151700	C	2.93621700	1.95368600	-1.84718700
H	-2.89288800	2.15404300	-1.13922400	C	3.78133000	0.87953500	-2.26290400
H	-3.26068500	3.29694700	-2.09024100	C	4.89039700	0.52999700	-1.46027300
H	-3.74657100	0.26198500	-2.59676700	C	5.21021000	1.27356600	-0.28097900
H	-2.66920500	-3.87123000	0.00317200	H	2.50948100	3.43974700	-0.32627200
Ru	-2.43363100	-0.85268100	-0.10477400	H	2.02921800	2.15886600	-2.40377300
P	-0.96926600	2.15723100	0.49044500	H	5.50420100	-0.32056400	-1.73937700
O	-1.91128500	2.32159800	1.71021000	H	6.06841400	1.00539200	0.32379100
O	-1.51881400	1.02240200	-0.46368800	H	1.23568100	1.05272300	1.70464300
O	0.49146300	1.55340500	0.97471700	N	2.16936100	0.61416400	1.82053800
C	1.41045000	2.45056700	1.63620900	H	2.72564800	1.22059100	2.41979700
H	1.56517000	2.07970900	2.65430300	C	2.01862900	-0.73191900	2.43922400
H	0.99408000	3.46125300	1.68351700	H	1.93682100	-0.65900100	3.52869900
C	2.74439400	2.52360700	0.90682000	H	1.10368700	-1.17940900	2.04720700
H	3.39038500	3.21260800	1.46927500	C	3.19444200	-1.59920800	2.02474900
O	3.36375300	1.22394900	0.88702000	H	4.13645300	-1.21563100	2.43102400
C	3.84773200	0.89650400	-0.39971100	H	3.04920900	-2.62647900	2.37500000
H	4.86593200	0.51132200	-0.30782500	N	3.25559900	-1.55552600	0.53991600
N	3.04601700	-0.20711900	-0.95117500	H	4.10315800	-2.01391000	0.21230400
C	1.78237400	-0.12972300	-1.52399400	H	2.44522900	-2.11298700	0.20033700
H	1.40942200	0.78464300	-1.96040400	O	1.17365600	-0.20811000	-0.64601700
N	1.11593600	-1.25461600	-1.47914800	H	0.44088300	-1.37503900	-1.25197700
C	1.96472400	-2.12977600	-0.82356400	H	0.53492600	0.42005600	-0.27842800
C	1.68561000	-3.41018500	-0.25727100	H	3.53263000	0.29785300	-3.14183700
O	0.60835900	-4.01334800	-0.18811600	H	4.53500100	2.83683100	1.05182600
N	2.84160300	-3.94432000	0.36669600	P	-0.23113100	-3.27214000	-0.40093200
H	2.69407600	-4.83705900	0.82370400	O	1.11578700	-3.42603900	0.34506400
C	4.03150500	-3.26787700	0.55187000	O	-0.12074200	-2.17842400	-1.54987500
N	5.01044800	-3.92257700	1.24130600	O	-1.31599900	-2.63245300	0.67150900
H	5.05531900	-4.93008000	1.20626200	C	-2.63925700	-3.18374800	0.79517100
H	5.89989000	-3.44447400	1.26309200	H	-2.76020400	-3.52319500	1.82986700
N	4.22739100	-2.03016800	0.15399700	H	-2.75086500	-4.04013000	0.12386800
C	3.16502000	-1.50417700	-0.49499500	C	-3.72554100	-2.17164600	0.47254500
C	2.67106400	3.00771300	-0.56181700	H	-4.69099000	-2.68838300	0.56492000
H	1.69574200	2.75182800	-0.98224300	O	-3.70223600	-1.08246100	1.43234400
C	3.79867400	2.18815100	-1.23638700	C	-3.96007300	0.14615700	0.80601200
H	3.61940100	1.99981300	-2.30084300				

H	-4.74485400	0.69297000	1.33924000	H	1.54676600	-2.93047800	2.76781100
N	-2.72683700	0.96448100	0.87041800	H	-0.20408600	-3.07798400	2.43760500
C	-1.49211800	0.51545100	1.26487400	N	0.98350100	-2.67920600	0.73351200
H	-1.34507800	-0.50949000	1.56755500	H	1.38832100	-3.60018600	0.57289600
N	-0.55995600	1.44417600	1.17122800	H	0.02259100	-2.76829000	0.27715200
C	-1.21830400	2.56379200	0.69692900	O	0.53433800	-1.57715200	-2.10574100
C	-0.71232900	3.85602400	0.34002800	H	-0.44624300	-1.68076700	-1.88900600
O	0.43427300	4.29268900	0.35828900	H	0.56932300	-0.68103000	-2.46350500
N	-1.78300000	4.68943100	-0.10052000	H	2.94948200	-1.38534800	-2.97245800
H	-1.50055500	5.63979400	-0.31083700	H	4.80462000	-1.47635300	1.65874300
C	-3.10274200	4.31713200	-0.22878800	P	-2.52050600	-2.31109600	-0.26073100
N	-3.98250800	5.27662600	-0.62975900	O	-1.49174100	-3.39989700	0.21418600
H	-3.66375800	6.08301000	-1.14388500	O	-1.94855500	-1.45922300	-1.40640100
H	-4.91685900	4.95338500	-0.83044800	O	-2.60307100	-1.26785200	1.05012200
N	-3.54417100	3.10662400	0.04878000	C	-3.82838100	-0.62353300	1.39525900
C	-2.57123400	2.28477000	0.50987900	H	-3.86701400	-0.58076900	2.48979100
C	-3.65137200	-1.50055000	-0.91561900	H	-4.68356000	-1.20576200	1.03442500
H	-2.60563100	-1.32695200	-1.18666200	C	-3.94361800	0.79391000	0.84469700
C	-4.36558700	-0.15945800	-0.65027700	H	-4.84178000	1.25265400	1.28447100
H	-4.07234600	0.63666500	-1.34157900	O	-2.78209400	1.55864500	1.24949600
O	-5.75689000	-0.43807800	-0.72712300	C	-2.39222600	2.45941800	0.24442800
H	-6.24503800	0.38678600	-0.83755300	H	-2.37318700	3.48620900	0.62207700
O	-4.23126500	-2.25224400	-1.94587600	N	-0.98769900	2.17206300	-0.12734300
O	-0.75507600	-4.59848100	-0.92369200	C	-0.43374000	0.94522800	-0.41183100
H	-5.18942500	-2.11664200	-1.87415600	H	-1.04121000	0.05612300	-0.58769800
Na	0.98227600	-5.66303900	-0.15536500	N	0.88740200	0.98890700	-0.47891900
Ru	3.04238100	0.47414200	-0.14571400	C	1.21899200	2.32280700	-0.22432600
GMP-TSc				C	2.47596600	3.01270800	-0.18989700
C	4.45342400	-1.45595700	0.63196800	O	3.62408400	2.59968900	-0.35179900
C	4.45414300	-0.22875400	-0.10578400	N	2.28194900	4.39334700	0.09225500
C	3.91376000	-0.20971900	-1.39755300	H	3.14794600	4.91656700	0.15357700
C	3.44806100	-1.42104500	-2.01255100	C	1.07498800	5.01860900	0.30224500
C	3.52143800	-2.64135200	-1.33029600	N	1.09827900	6.34227700	0.61095700
C	3.99116900	-2.65833700	0.02367900	H	1.89119400	6.91634900	0.37032300
H	4.73824200	0.70866900	0.35472300	H	0.19884700	6.79902400	0.64295700
H	3.78294300	0.74675800	-1.88620800	N	-0.07537100	4.38074300	0.25368300
H	3.11054600	-3.53678300	-1.78151200	C	0.05285400	3.06179900	-0.00585800
H	3.99266000	-3.58329600	0.59072100	C	-4.02554100	0.94021700	-0.69156300
H	1.53830800	0.63846700	1.76155500	H	-3.40730600	0.18088300	-1.17875100
N	1.73516400	-0.34848700	1.91953100	C	-3.40628500	2.33672300	-0.91375300
H	2.49348700	-0.39738100	2.59837400	H	-2.93616400	2.44793900	-1.89641700
C	0.52506500	-1.04748800	2.45392700	O	-4.45711700	3.28065600	-0.72483200
H	0.39515500	-0.83670700	3.52043400	H	-4.27133900	4.07942100	-1.23183900
H	-0.35707400	-0.68345400	1.92069100	O	-5.32560700	0.82121700	-1.20332500
C	0.70759400	-2.52804300	2.18800700	O	-3.89613300	-2.94740500	-0.45331000
				H	-5.75579600	1.67715400	-1.04918000

Na	-3.12987500	-4.93046700	-0.06529100	N	-1.07678200	0.52551400	-0.06929500
Ru	2.37066300	-1.19682100	0.01204000	C	-1.67885300	1.72865500	-0.43731600
GMP-PCc				C	-2.95678400	2.03009400	-0.99832700
C	-3.95252900	-2.44986300	1.01018100	O	-3.87829000	1.27077100	-1.32378000
C	-4.14842900	-1.06705700	1.33838700	N	-3.10176500	3.42087600	-1.20663300
C	-3.18724600	-0.41083000	2.12223200	H	-3.97694800	3.67764200	-1.64950000
C	-2.02902500	-1.11191400	2.59869800	C	-2.13712600	4.37620600	-0.96184700
C	-1.84725300	-2.47086300	2.28765300	N	-2.43643300	5.66020300	-1.26936300
C	-2.82907200	-3.15040000	1.49201400	H	-3.37903300	5.96673600	-1.44629900
H	-4.99130000	-0.52057100	0.93267600	H	-1.74568800	6.35662300	-1.03477800
H	-3.29020600	0.65008100	2.32052500	N	-0.94826800	4.08124200	-0.47801500
H	-0.91954400	-2.98030700	2.54212600	C	-0.76526700	2.76527400	-0.25373700
H	-2.67719600	-4.18945000	1.22255300	C	3.39827600	1.52066100	1.35693600
H	-3.09765900	-0.35014400	-1.89187700	H	2.94847600	0.52362200	1.34845000
N	-2.64015400	-1.26198900	-1.75194700	C	2.35071000	2.57399300	1.78308600
H	-3.33730100	-1.97639800	-1.95504800	H	1.65076200	2.20904800	2.54388100
C	-1.43977600	-1.46985800	-2.61335800	O	3.08933700	3.69666900	2.24862900
H	-1.73156100	-1.65639600	-3.65229900	H	2.53468200	4.24229700	2.81842200
H	-0.84521600	-0.55445700	-2.58155900	O	4.50461600	1.46122000	2.21566500
C	-0.65112300	-2.63052400	-2.03231600	O	4.37507000	-1.96600100	-0.22560200
H	-1.21083000	-3.56545000	-2.15683400	H	4.70299200	2.37626200	2.46890100
H	0.33857800	-2.72921100	-2.49096100	Na	4.45066700	-3.45098100	-1.83350900
N	-0.46684500	-2.37653200	-0.57962600	Ru	-2.08838700	-1.34577200	0.31991700
H	-0.27702900	-3.24878600	-0.07404700	GMP-RCd			
H	0.42494700	-1.86654400	-0.39658500	C	-4.80515900	1.57445700	0.35539400
O	0.83909400	-3.70546700	1.60354500	C	-3.67026000	2.20747100	0.96840200
H	1.37892400	-2.91453100	1.31515900	C	-3.06584400	1.61000300	2.08974200
H	1.47765900	-4.36998100	1.88680300	C	-3.57190900	0.37885500	2.62148300
H	-1.26589600	-0.58052900	3.15497600	C	-4.66609600	-0.24706400	1.99900400
H	-4.66852600	-2.95503300	0.36971800	C	-5.30451500	0.36228600	0.86483100
P	2.94289000	-1.59941200	-0.62963000	H	-3.23229500	3.09340500	0.52212300
O	2.44481900	-2.49474000	-1.78971800	H	-2.16280700	2.03743000	2.50831100
O	1.89565700	-1.52144300	0.53242700	H	-5.01442500	-1.20800600	2.36252000
O	2.93587000	-0.03846700	-1.21355300	H	-6.14429000	-0.12676300	0.38395200
C	4.05377400	0.82480000	-1.05373200	H	-1.35497200	0.52057600	-1.59166100
H	4.29580300	1.25104800	-2.03476900	N	-2.39392200	0.53309900	-1.57228400
H	4.92344300	0.27331700	-0.67922700	H	-2.63459600	1.48216300	-1.85879400
C	3.73569800	1.95711000	-0.08805900	C	-2.92291100	-0.49168400	-2.50324300
H	4.58472000	2.65372400	-0.06147900	H	-4.00275900	-0.34399100	-2.61053000
O	2.57249200	2.67834300	-0.57206700	H	-2.46523500	-0.39860300	-3.49556800
C	1.66063600	2.93033100	0.45082600	C	-2.60713500	-1.85178100	-1.89873700
H	1.35271600	3.97931400	0.43060700	H	-3.08176600	-2.65395300	-2.47384300
N	0.38905600	2.18409200	0.22119500	H	-1.52626900	-2.03209100	-1.89123300
C	0.15948000	0.83582900	0.30333900	N	-3.07089000	-1.88028700	-0.47471300
H	0.91105200	0.09321600	0.59064300	H	-3.99307300	-2.30430900	-0.40489300

H	-2.41224700	-2.46069800	0.06237900	C	-4.76147400	0.41656200	0.67013500
O	-1.10255600	-0.36297500	0.87098100	C	-3.98757800	1.61252700	0.81850200
H	-0.51035600	0.07136900	0.23863400	C	-2.91130800	1.61626100	1.71680600
H	-0.75164600	-1.73243400	0.90642900	C	-2.64840300	0.48132000	2.55487200
H	-3.05872200	-0.10624400	3.44292000	C	-3.44187500	-0.66798700	2.46819100
H	-5.25306400	2.01329500	-0.52986400	C	-4.47882200	-0.72120200	1.48180800
Ru	-3.06087700	0.10351600	0.41446500	H	-4.12770400	2.45610500	0.15395100
P	0.65961800	-3.24806400	0.01884000	H	-2.24298700	2.46756200	1.74178200
O	0.53405100	-2.86965600	-1.47456700	H	-3.20076100	-1.54297000	3.06050400
O	-0.62437400	-2.78616400	0.84560800	H	-5.05909500	-1.62861400	1.35009000
O	1.82198800	-2.29921200	0.69843800	H	-1.82205200	0.32746400	-1.95402300
C	3.18441000	-2.73289300	0.69793800	N	-2.79253900	0.01769300	-1.79976800
H	3.38805700	-3.40747000	-0.14086400	H	-3.40718500	0.76951800	-2.10587200
H	3.39573100	-3.27547200	1.62657000	C	-3.07796800	-1.27009000	-2.48051300
C	4.11763300	-1.53836100	0.61722200	H	-4.14437500	-1.48899100	-2.35865000
H	5.14586000	-1.90318000	0.74185900	H	-2.86481500	-1.20333300	-3.55372900
O	4.01983100	-0.90447600	-0.68606000	C	-2.21094300	-2.32269000	-1.80853100
C	4.00131100	0.49262300	-0.56651900	H	-2.49557400	-3.32772600	-2.13795500
H	4.70304300	0.93831100	-1.27922400	H	-1.14731400	-2.19058600	-2.03644600
N	2.63739100	0.97685400	-0.90236800	N	-2.34652400	-2.20394800	-0.32828300
C	1.57890700	0.18431400	-1.28629700	H	-3.10447800	-2.80260500	-0.00391700
H	1.66053900	-0.88525700	-1.41641200	H	-1.43263400	-2.60111200	0.13823600
N	0.46645100	0.87541200	-1.43544100	O	-0.21771000	-0.77486100	1.96948900
C	0.80917100	2.18259500	-1.15325700	H	0.68823700	-0.57346400	1.70033300
C	-0.01503400	3.34837700	-1.07624800	H	-0.24564500	-1.74355100	1.75434700
O	-1.23163100	3.46562200	-1.23129100	H	-1.75583300	0.45893800	3.16514000
N	0.77706200	4.48175800	-0.74361500	H	-5.55199400	0.36587400	-0.07099900
H	0.24955300	5.34096300	-0.64014800	Ru	-2.70148100	-0.21000100	0.32475400
C	2.13076200	4.47109100	-0.48026600	P	1.07874500	-3.26516400	-0.02273300
N	2.69928000	5.66088300	-0.12693100	O	0.88160900	-2.72658000	-1.47496300
H	2.28748800	6.52530900	-0.44519400	O	-0.22189700	-3.16173900	0.81800000
H	3.70764800	5.64962000	-0.07796500	O	2.07476700	-2.15790400	0.75847700
N	2.86743200	3.37988900	-0.50545500	C	3.48523500	-2.27188600	0.60749400
C	2.16048500	2.26894000	-0.82929500	H	3.74180200	-2.93659000	-0.22321500
C	3.85473700	-0.41646900	1.64424400	H	3.92171900	-2.70382000	1.51732500
H	2.77819300	-0.32929900	1.81487900	C	4.12297300	-0.91094600	0.38800300
C	4.37269200	0.82416600	0.89297600	H	5.20846800	-1.05128800	0.29483100
H	3.93165500	1.76284200	1.23795000	O	3.63399800	-0.31492800	-0.84353900
O	5.78504400	0.81520100	1.05468600	C	3.38800700	1.05101200	-0.67952500
H	6.13459300	1.69721200	0.87972900	H	3.84965300	1.62285600	-1.49173000
O	4.46676500	-0.62005700	2.88830900	N	1.92245000	1.29426800	-0.75195900
O	0.98349300	-4.72251300	0.19371500	C	0.93196400	0.35094200	-0.89392600
H	5.39755400	-0.36968200	2.77490800	H	1.14201300	-0.70906200	-1.00395300
Na	1.00135900	-5.00998100	-1.98756300	N	-0.27255100	0.89763700	-0.92696400
				C	-0.05673600	2.26288000	-0.83107200
GMP-TSd				C	-0.97509000	3.35680700	-0.88481100

O	-2.20226300	3.35352200	-0.99143300	H	-1.08225500	-0.30745600	2.97949400
N	-0.27582500	4.59254700	-0.79417900	H	-4.43110300	-3.30720800	0.78949000
H	-0.87879100	5.40728700	-0.79953300	Ru	-2.02753700	-1.47582600	0.35632800
C	1.08947800	4.74401600	-0.68507600	P	2.93438800	-1.65933700	-0.70550100
N	1.56625200	6.01476900	-0.56374400	O	2.55288900	-2.57064300	-1.89333300
H	1.02674400	6.79550200	-0.90516400	O	1.81708300	-1.67293200	0.39308000
H	2.56934600	6.10599900	-0.62822100	O	2.86449300	-0.08557300	-1.25590100
N	1.92686800	3.72762800	-0.65085300	C	3.97680400	0.79598600	-1.16340100
C	1.30677900	2.52574100	-0.72841300	H	4.18330200	1.19704800	-2.16301100
C	3.85880000	0.13982400	1.48598500	H	4.86295600	0.26630900	-0.79697000
H	2.84489000	0.01426500	1.87710000	C	3.66553400	1.94770200	-0.21764300
C	3.95670600	1.45851600	0.69581500	H	4.51327200	2.64565500	-0.20610000
H	3.40542600	2.28641200	1.15104300	O	2.49991900	2.66058300	-0.70807200
O	5.34380300	1.74550100	0.59103500	C	1.56301500	2.87984700	0.30043500
H	5.46342200	2.67543600	0.36348500	H	1.23002900	3.92096500	0.28445000
O	4.73266700	0.06659700	2.57805300	N	0.31806700	2.10061900	0.04536300
O	1.80099400	-4.61135900	-0.06220600	C	0.13642300	0.74861500	0.13063400
H	5.55573400	0.49681000	2.2967210	H	0.91143500	0.03667600	0.40534100
Na	1.86405800	-4.57896400	-2.24065200	N	-1.09551400	0.39291400	-0.20725100
GMP-PCd				C	-1.74844700	1.57419400	-0.56248600
C	-3.73029300	-2.65754000	1.30310000	C	-3.04915800	1.83006300	-1.09041000
C	-4.03443200	-1.26319400	1.46558900	O	-3.95821300	1.04064000	-1.37991100
C	-3.10732600	-0.42341900	2.10334600	N	-3.24508900	3.21421800	-1.30027700
C	-1.85900000	-0.94785100	2.57727500	H	-4.16560700	3.44800200	-1.65517800
C	-1.56394400	-2.31228100	2.42511600	C	-2.30804900	4.20221400	-1.08302600
C	-2.51535900	-3.17834200	1.78917100	N	-2.68567800	5.48576300	-1.31119500
H	-4.95046500	-0.85343800	1.05626900	H	-3.47623900	5.70080500	-1.89846300
H	-3.30750700	0.63929700	2.17631200	H	-1.94716600	6.17286100	-1.27013800
H	-0.58529000	-2.66053200	2.73566400	N	-1.09562700	3.94892900	-0.63674200
H	-2.28271100	-4.22773700	1.64193300	C	-0.86624600	2.64219600	-0.40204800
H	-3.23168200	-0.61200800	-1.81054400	C	3.33387200	1.52465300	1.23148400
N	-2.70732900	-1.49077500	-1.67883800	H	2.92105600	0.51448400	1.23718100
H	-3.35393900	-2.26050600	-1.84369900	C	2.23430000	2.52771700	1.64502700
C	-1.53243200	-1.60164300	-2.59196700	H	1.54017600	2.10108000	2.37678600
H	-1.85443100	-1.79221100	-3.62147600	O	2.90509600	3.67619700	2.15187000
H	-1.00965300	-0.64452900	-2.56731900	H	2.33601600	4.13575800	2.77995600
C	-0.63255300	-2.71465100	-2.07875200	O	4.43133900	1.51969100	2.10499400
H	-1.09826800	-3.68726200	-2.27715000	O	4.35859900	-1.93756300	-0.21570800
H	0.36017700	-2.69365400	-2.54238000	H	4.56629200	2.44269700	2.3722890
N	-0.46588200	-2.55881500	-0.60308900	Na	4.58994200	-3.46270900	-1.77443700
H	-0.40724600	-3.48639200	-0.18859200	Cartesian coordinates for the species involved in Fig. 3:			
H	0.47601100	-2.13126700	-0.33624000	AMP-RCa			
O	1.21813600	-0.83834600	2.85818300	C	-2.05263300	2.23970900	1.2453200
H	1.96900200	-0.84994700	3.46437600	C	-1.28199100	1.11304500	1.68329700
H	1.56866700	-1.22327700	2.01454200				

C	-1.87354700	0.09086900	2.45044000	N	3.75985100	3.13191600	-0.40093000
C	-3.26358400	0.17995000	2.79341400	C	2.77138400	2.29119100	-0.72728600
C	-4.03450800	1.26687200	2.34836800	C	3.79833300	-0.95772100	1.53531600
C	-3.42426900	2.29676800	1.55311000	H	2.77530200	-0.65385000	1.77682600
H	-0.25042800	1.01865000	1.36692200	C	4.53785400	0.19685400	0.83706700
H	-1.30245200	-0.79506500	2.70237300	H	4.33234300	1.18009700	1.26726000
H	-5.09384700	1.31280000	2.57567400	O	5.91906000	-0.12729500	0.90536000
H	-4.02739800	3.12073500	1.18649700	H	6.44073600	0.67307300	0.76669300
H	-1.51364000	-0.84194600	-1.33563800	O	4.40583700	-1.39047000	2.72100200
N	-1.92577500	0.11211100	-1.29708900	O	0.30107200	-4.46461600	-0.50355700
H	-1.10821000	0.74527700	-1.31106600	H	5.36266700	-1.31216900	2.57589100
C	-2.77577100	0.35926500	-2.48352400	Na	-0.06162800	-4.14925300	-2.6379060
H	-2.84576200	1.44127800	-2.64579200	N	-0.13258000	4.49293000	-1.16137000
H	-2.33216500	-0.08092600	-3.38400700	H	-0.68921700	3.97834800	-1.82994200
C	-4.15276900	-0.22845900	-2.22630800	H	-0.16350700	5.49905700	-1.27417800
H	-4.84873800	-0.01247000	-3.04384900	H	4.08273800	5.14827500	-0.10534100
H	-4.07537600	-1.30730900	-2.08552200				
N	-4.65168400	0.32397800	-0.93191000	AMP-TS1a			
H	-5.03862700	1.25723300	-1.06420300	C	-1.62429800	2.37887600	1.06256900
H	-5.40346800	-0.26688600	-0.58236200	C	-0.84324900	1.30643000	1.60217800
O	-3.28281500	-1.74493400	0.17360900	C	-1.44838500	0.36850400	2.45151600
H	-1.93392800	-2.37661600	0.56494200	C	-2.81197500	0.54167500	2.87323600
H	-3.84357500	-2.10769200	0.87303500	C	-3.56859100	1.62393300	2.40717700
H	-3.73128700	-0.62143500	3.35508100	C	-2.98854400	2.52115800	1.44826400
H	-1.59172800	3.00784800	0.63203700	H	0.16680500	1.14609700	1.24793800
Ru	-3.03171100	0.29181000	0.51999200	H	-0.91934000	-0.53958000	2.71150700
P	0.04942100	-2.99885100	-0.18735800	H	-4.60954100	1.72957000	2.69225400
O	-0.30641400	-2.20978900	-1.47729800	H	-3.58516800	3.32351400	1.02706800
O	-1.03900100	-2.70600500	0.93754200	H	-1.44691100	-0.61703900	-1.48169700
O	1.36758800	-2.33737100	0.51742900	N	-1.80130700	0.37487800	-1.35757700
C	2.62824900	-3.02381200	0.50848100	H	-0.94171700	0.94767500	-1.41979700
H	2.67326300	-3.73547000	-0.31968900	C	-2.72631700	0.72104300	-2.45773800
H	2.74310400	-3.58471400	1.44331200	H	-2.79601500	1.81176000	-2.54288400
C	3.76080600	-2.02126200	0.41923000	H	-2.35457600	0.33321000	-3.41318500
H	4.70689600	-2.57951200	0.43253900	C	-4.08033300	0.12612000	-2.11935900
O	3.67884800	-1.27482300	-0.81962800	H	-4.85023600	0.40205600	-2.84719000
C	4.02244000	0.07206800	-0.61189500	H	-4.01130300	-0.96371700	-2.07907200
H	4.78075700	0.38537900	-1.33720900	N	-4.44706400	0.57943800	-0.74742900
N	2.82294500	0.91312300	-0.82628400	H	-4.93280600	1.47361800	-0.77270400
C	1.55918200	0.49848500	-1.16430600	H	-5.04461300	-0.12525100	-0.31522200
H	1.31308800	-0.54633900	-1.29345300	O	-4.04385100	-1.70781900	0.55423800
N	0.69728900	1.49612100	-1.27926700	H	-3.07283100	-2.05006200	0.54261500
C	1.44301500	2.63341100	-1.01088400	H	-4.39304700	-1.98618900	1.41078800
C	1.13865900	4.00603700	-0.94730300	H	-3.27086000	-0.20954600	3.50575800
N	2.10525900	4.87261700	-0.61922800	H	-1.18127600	3.06849400	0.35009000
C	3.33811200	4.40042100	-0.36624400	Ru	-2.70527300	0.53981200	0.56437300

P	-0.57430000	-2.68404100	-0.27447800	H	-3.65958200	2.28494300	2.93169900
O	-0.60317600	-2.03875600	-1.70925700	H	-2.36385500	3.91941600	1.52195300
O	-1.60296800	-1.98320500	0.64821100	H	-1.42861700	0.17335600	-1.72827500
O	0.86759800	-2.26443700	0.42248900	N	-1.53753800	1.15633100	-1.39247900
C	1.95539100	-3.19146000	0.43046100	H	-0.61341200	1.59056300	-1.52935400
H	1.89855600	-3.87416700	-0.42291700	C	-2.61096800	1.83303700	-2.15160100
H	1.91991100	-3.79939500	1.34290800	H	-2.60688100	2.89982400	-1.90169900
C	3.27612900	-2.44705200	0.40964600	H	-2.45228000	1.73868200	-3.23284500
H	4.08580700	-3.18572900	0.48044900	C	-3.92402400	1.18672500	-1.74054300
O	3.42636100	-1.72245700	-0.83853300	H	-4.78479100	1.68449500	-2.19836400
C	3.96954300	-0.44856600	-0.61427800	H	-3.93506500	0.13801500	-2.04581900
H	4.79488300	-0.26447500	-1.30994900	N	-4.02420800	1.20199300	-0.25253600
N	2.92323100	0.57130000	-0.87269900	H	-4.48534800	2.05430100	0.05940400
C	1.64752300	0.34739800	-1.32781200	H	-4.60342600	0.39247900	0.03964700
H	1.27143900	-0.64860000	-1.51972600	O	-5.08981500	-1.33652400	0.07777000
N	0.93832300	1.45759300	-1.45627400	H	-4.15402400	-1.57442400	0.25284300
C	1.80498500	2.47014700	-1.07733700	H	-5.62905000	-1.86189300	0.68029300
C	1.67696500	3.86683300	-0.96791100	H	-2.66950100	0.07605800	3.53089300
N	2.71643700	4.58333600	-0.52292900	H	-0.10057900	3.28085300	0.66104800
C	3.85310700	3.94007000	-0.20309800	Ru	-2.07474500	0.99496200	0.66795700
N	4.10788800	2.62920300	-0.27101800	P	-1.51990300	-2.08475900	-0.49333800
C	3.04899400	1.93950300	-0.71156700	O	-1.15432800	-1.54009800	-1.90610100
C	3.46494300	-1.39427500	1.52118700	O	-2.41293500	-1.05738000	0.29454600
H	2.50649900	-0.90366200	1.71421100	O	-0.14739800	-2.16213900	0.41528900
C	4.43658200	-0.40484400	0.85452600	C	0.62358400	-3.37486500	0.41011400
H	4.40291000	0.60346500	1.27382000	H	0.34836300	-4.00697800	-0.43863000
O	5.72847800	-0.98272700	0.98203700	H	0.40756100	-3.93639700	1.32630300
H	6.39692500	-0.29428000	0.87760500	C	2.11078100	-3.08421300	0.37909800
O	3.92825000	-1.91497200	2.73688500	H	2.63500900	-4.04699400	0.45871800
O	-0.64766500	-4.20311400	-0.40788600	O	2.48682300	-2.45321500	-0.86687800
H	4.88671000	-2.02765600	2.63068200	C	3.47961300	-1.47777400	-0.64962000
Na	-0.70174700	-4.10418500	-2.58750000	H	4.31909300	-1.63944800	-1.33388800
N	0.49723200	4.52302100	-1.25300600	N	2.90251000	-0.14483000	-0.93185600
H	-0.04762000	4.12148300	-2.00453200	C	1.65404900	0.12207900	-1.44295900
H	0.60566200	5.52874300	-1.31129200	H	0.95374500	-0.67080000	-1.67215200
H	4.66523500	4.57014100	0.15082200	N	1.41132100	1.41457500	-1.57669400
				C	2.57410700	2.03240000	-1.14467300
				C	2.96329000	3.38032700	-1.00763200
AMP-IM1a				N	4.18164100	3.65733600	-0.52141100
C	-0.64278000	2.61026400	1.32019900	C	4.98810100	2.63859900	-0.18091200
C	-0.06441000	1.34846700	1.66948200	N	4.74279300	1.32568900	-0.25813900
C	-0.80242700	0.44343100	2.45768800	C	3.51989000	1.08019400	-0.74512500
C	-2.09594200	0.79374500	2.95736000	C	2.63857200	-2.14685700	1.48191900
C	-2.65246800	2.03972500	2.60970600	H	1.92056800	-1.33532500	1.63443800
C	-1.92422000	2.96716500	1.79551400	C	3.91426100	-1.59239200	0.82670000
H	0.89808200	1.06607200	1.26528400	H	4.24780700	-0.63645500	1.23637600
H	-0.42139200	-0.55836400	2.61727900				

O	4.89979900	-2.60312100	0.98447400	O	3.01211500	1.98585100	1.30290900
H	5.77636300	-2.21081700	0.88564600	C	3.87663400	1.33845400	0.39345000
O	2.84869000	-2.76915600	2.71898100	H	4.87630300	1.22364500	0.82375900
O	-2.16539800	-3.45932300	-0.60309500	N	3.39356000	-0.02635900	0.13879800
H	3.70793200	-3.21650300	2.65095900	C	2.09311400	-0.45000500	0.02296900
Na	-2.03549800	-3.41785400	-2.80543300	H	1.26359400	0.23285700	0.12510600
N	2.12259800	4.42190700	-1.30178400	N	1.97940300	-1.74819700	-0.18560600
H	1.42167100	4.25214100	-2.00872700	C	3.29064000	-2.21065900	-0.21121300
H	2.57372100	5.32673100	-1.34187000	C	3.88333300	-3.47657500	-0.40215600
H	5.96433600	2.92223800	0.20467500	N	5.22108700	-3.57970300	-0.35477500
AMP-IM2a				C	5.94940800	-2.47380000	-0.13685900
C	-3.80549400	-2.93328700	-0.92145700	N	5.51833000	-1.21929900	0.03409100
C	-3.13374800	-2.28380000	-2.01185900	C	4.18458600	-1.15121600	-0.00880300
C	-3.29170400	-0.90206200	-2.20422500	C	2.54940800	2.92068100	-0.83657300
C	-4.13915500	-0.13987400	-1.33222500	H	1.76613100	2.26544600	-1.22970100
C	-4.80170400	-0.78054600	-0.27080900	C	3.91259600	2.20489000	-0.88380900
C	-4.63305400	-2.18996700	-0.05675700	H	4.06162000	1.60366200	-1.78740800
H	-2.46456400	-2.84784900	-2.65181100	O	4.88214200	3.23740800	-0.77044300
H	-2.71836600	-0.39355600	-2.97039600	H	5.75484700	2.88896800	-0.99165400
H	-5.40530800	-0.19873500	0.41696200	O	2.50444400	4.11474100	-1.56965900
H	-5.12322500	-2.67884000	0.77790100	O	-1.52916000	2.82786800	-0.69783500
H	0.00938400	-2.04300100	0.07074100	H	3.38676100	4.51172800	-1.48820200
N	-0.87034800	-2.44722000	0.44253000	Na	-3.28913000	3.64908500	0.68943500
H	-0.93468600	-3.37245300	0.02202900	N	3.15850700	-4.61679400	-0.60189800
C	-0.73549300	-2.59366800	1.92075300	H	2.22704100	-4.52204800	-0.97450300
H	-1.42748500	-3.37464000	2.25332900	H	3.69160400	-5.41843700	-0.90893800
H	0.28324100	-2.89870700	2.18110200	H	7.02647600	-2.62019900	-0.10555100
C	-1.08747000	-1.25989500	2.55710000	O	-3.98813800	3.19588600	-1.42746700
H	-1.10436400	-1.33583600	3.64929500	H	-4.21762400	3.71568700	-2.20692800
H	-0.35299700	-0.50178000	2.27854700	H	-3.00431100	3.01733800	-1.45943900
N	-2.40667800	-0.81201600	2.03360100	AMP-TS2a			
H	-3.16653300	-1.21369000	2.57888100	C	4.45034400	0.79098200	-0.63127200
H	-2.46553700	0.23440500	2.06704600	C	3.64238500	1.54920100	-1.54308800
H	-4.21835900	0.93672600	-1.45626800	C	2.66599000	0.89953400	-2.30553300
H	-3.65643600	-3.99344400	-0.74644400	C	2.50675600	-0.52225200	-2.20253500
Ru	-2.57981500	-1.23282800	-0.05934000	C	3.38319400	-1.29969500	-1.42378000
P	-1.25285600	1.73858400	0.34669400	C	4.33705700	-0.63071900	-0.59756400
O	-2.26466600	1.84820000	1.51895800	H	3.73966700	2.62875600	-1.57187800
O	-1.13108600	0.27001100	-0.19345300	H	1.96139700	1.47134700	-2.89624400
O	0.27437400	1.91344800	0.90455400	H	3.22184300	-2.37066200	-1.35581100
C	0.90645400	3.17494700	1.14513800	H	4.96342700	-1.20106300	0.08058500
H	0.85729600	3.38973600	2.21825400	H	1.05102500	1.94465100	1.31087800
H	0.40848700	3.97501600	0.58559700	N	2.03661900	1.72985400	1.47049400
C	2.35506500	3.10733500	0.68383600	H	2.52240800	2.61825500	1.34793300
H	2.85441700	4.03785500	0.98870900	C	2.20454000	1.16775500	2.83744600

H	3.27508300	1.13765400	3.06414000	H	-2.63310000	5.90948200	0.6899820
H	1.71191700	1.79819900	3.58572400	O	1.59691200	-3.95033000	-1.56661300
C	1.61617800	-0.23203300	2.79201000	H	1.28068600	-4.29636600	-2.41167900
H	1.79230300	-0.77236100	3.72808700	H	1.03820300	-3.13730300	-1.39424200
H	0.53291000	-0.19702500	2.63456100				
N	2.20677300	-0.96107700	1.64402800	AMP-PCa			
H	3.13127300	-1.29802300	1.91234300	C	3.78660800	-1.94962900	-1.38035600
H	1.55534200	-1.90107400	1.47223600	C	3.44585700	-0.79727900	-2.15447200
H	1.65900300	-0.99909000	-2.67757400	C	2.09566200	-0.58519100	-2.49950500
H	5.16742700	1.29290000	0.00920100	C	1.08237300	-1.51832400	-2.12232800
Ru	2.40592200	0.24952800	-0.07832300	C	1.44309500	-2.67551700	-1.40002800
P	-0.46779400	-2.62316900	0.41613100	C	2.80506300	-2.90538100	-1.03264700
O	0.70601600	-2.97065500	1.41623700	H	4.21192100	-0.09130500	-2.45521900
O	0.13339700	-1.78654700	-0.74887200	H	1.81357400	0.32647000	-3.01534200
O	-1.49097400	-1.59207200	1.18923300	H	0.65547100	-3.35812600	-1.09422400
C	-2.81776000	-1.99046000	1.56628400	H	3.07998400	-3.78580600	-0.46283800
H	-2.92145700	-1.82127700	2.64281300	H	3.59259300	0.79433000	1.33421000
H	-2.97609400	-3.05032200	1.34572100	N	3.43131100	-0.21449000	1.43907500
C	-3.85372200	-1.16505800	0.81729900	H	4.35552400	-0.63194400	1.35150200
H	-4.85122400	-1.44923900	1.17907400	C	2.86977700	-0.54316900	2.79251200
O	-3.64220200	0.23594100	1.10198500	H	3.34461600	-1.46818700	3.13522600
C	-3.67734900	1.01271700	-0.06705900	H	3.11957800	0.24403100	3.50995800
H	-4.30767700	1.89245800	0.08954100	C	1.36660700	-0.75086000	2.66627600
N	-2.33458200	1.56654900	-0.34945700	H	0.95784700	-1.20684700	3.57530700
C	-1.17585300	0.88213800	-0.61126400	H	0.84445800	0.19457500	2.50910100
H	-1.11946500	-0.18473700	-0.78746200	N	1.13031300	-1.61687400	1.49587900
N	-0.09467400	1.64360200	-0.58403700	H	1.58054500	-2.51350400	1.68927400
C	-0.57256600	2.91766500	-0.27539800	H	0.04698600	-1.94461400	1.39701400
C	0.02433200	4.17818700	-0.09522800	H	0.02914000	-1.32053000	-2.28943200
N	-0.73669700	5.21878300	0.25682500	H	4.81485600	-2.09744900	-1.06422300
C	-2.06095600	5.03168200	0.40175100	Ru	2.15014700	-0.87356200	-0.21098500
N	-2.75207000	3.90303500	0.22072900	P	-2.31157300	-1.89998200	0.5802180
C	-1.96572000	2.87919400	-0.10990200	O	-1.18827000	-2.63200800	1.40716800
C	-3.82841300	-1.30643700	-0.72419200	O	-1.73325500	-1.52982300	-0.81641600
H	-2.81534100	-1.54142800	-1.06176400	O	-2.53646700	-0.47887700	1.38366500
C	-4.22666600	0.11257600	-1.19064400	C	-3.83073200	0.12484700	1.46412800
H	-3.82631200	0.37408000	-2.17689500	H	-4.01178500	0.36715100	2.51643600
O	-5.64717600	0.13196600	-1.17748300	H	-4.60641500	-0.56894000	1.12386500
H	-5.97151800	0.88204700	-1.69051000	C	-3.88062400	1.39843100	0.63556300
O	-4.66343100	-2.31354600	-1.22408000	H	-4.84093100	1.90136000	0.81148600
O	-1.18752500	-3.90160500	0.01918800	O	-2.81567400	2.27900500	1.07855000
H	-5.55761600	-1.93698800	-1.24760700	C	-2.13586300	2.84025100	0.00114800
Na	0.70087400	-5.05180200	0.32826300	H	-2.01718600	3.91840300	0.14099800
N	1.39559800	4.38475300	-0.21682300	N	-0.72478600	2.34183800	-0.04554300
H	1.80782500	3.89620500	-1.00182300	C	-0.26054200	1.06405800	-0.11340800
H	1.61726400	5.37546700	-0.21906000	H	-0.89513900	0.18904500	-0.26198800

N	1.06930600	1.00087300	-0.02126000	H	3.89585300	-0.48050000	2.72381700
C	1.50340200	2.32584600	0.09780700	H	2.71529500	-1.65162700	2.66567200
C	2.73919200	2.99798400	0.16407700	H	3.76490800	1.67957500	-0.86553600
N	2.75995500	4.32151000	0.32865500	H	3.71597900	-3.29646500	-1.46392300
C	1.59680300	4.99249700	0.38085200	Ru	2.72745700	-0.99059200	0.24872700
N	0.37063600	4.48771000	0.24695300	P	-1.49726100	-2.57003900	-0.44943200
C	0.37551100	3.16309100	0.10841000	O	-0.77876000	-3.07702500	0.88751800
C	-3.67733800	1.21743000	-0.88787400	O	-0.87477400	-1.28323200	-0.94736200
H	-3.03614700	0.35177500	-1.08153500	O	-3.06341000	-2.28165800	0.15619700
C	-2.94277400	2.51949800	-1.27322400	C	-3.28686500	-1.64785900	1.42693800
H	-2.31097400	2.41755400	-2.16363500	H	-2.41546900	-1.80046700	2.06895400
O	-3.95580700	3.49769800	-1.45540100	H	-4.13663600	-2.16441500	1.89026400
H	-3.60155200	4.25703800	-1.93385100	C	-3.62779800	-0.16443000	1.34982500
O	-4.86423700	1.01216800	-1.60527500	H	-4.01505600	0.12327600	2.33904500
O	-3.58624700	-2.72890800	0.56883100	O	-2.44500500	0.61555400	1.07628000
H	-5.28584200	1.88126100	-1.69422000	C	-2.78934800	1.62797500	0.12682600
Na	-2.36816600	-4.57543800	0.70744900	H	-3.24518100	2.49139200	0.62276100
N	3.97217900	2.34675100	0.11137000	N	-1.59324000	2.10792200	-0.52974300
H	4.04306800	1.66441200	-0.63625800	C	-0.91366800	1.56980500	-1.61044200
H	4.73056300	3.02260800	0.08652000	H	-1.26743300	0.68353500	-2.11463800
H	1.67179500	6.06623700	0.52831100	N	0.22068500	2.17741300	-1.87561800
O	-1.44556600	-4.15870000	-1.40851300	C	0.31062700	3.17233500	-0.91120500
H	-1.91234100	-4.44054400	-2.20559100	C	1.28600100	4.14896300	-0.62348100
H	-1.60790900	-3.16932700	-1.34108600	N	2.45170600	4.25347500	-1.33760100
AMP-RCb				H	2.96334900	5.11290400	-1.18404700
C	3.77954000	0.60567300	-1.0190670	H	2.42290400	3.92826500	-2.29425000
C	2.75398200	-0.01826200	-1.78640800	N	1.09325800	4.96711700	0.42129500
C	2.73430800	-1.42371300	-1.97350400	C	-0.02950600	4.82879700	1.14865800
C	3.75405400	-2.21593500	-1.36793500	H	-0.13782500	5.52326600	1.97833100
C	4.77174500	-1.62341300	-0.58763400	N	-1.02358200	3.94941800	0.98295300
C	4.74859200	-0.20764200	-0.38307900	C	-0.80146800	3.14768600	-0.06205500
H	1.94141300	0.59215100	-2.17393100	C	-4.68505200	0.24548000	0.28572800
H	1.91675000	-1.88878400	-2.51008200	H	-5.21466400	-0.62492100	-0.12441800
H	5.52582400	-2.23618400	-0.10834000	C	-3.81452300	0.92486500	-0.78005100
H	5.48889300	0.24933300	0.26592300	H	-3.28865900	0.12909800	-1.32645000
H	0.13723200	-0.47789000	0.19666200	O	-5.58447400	1.21599200	0.78254600
N	0.89900800	-0.00581400	0.73745700	O	-1.79376100	-3.68038000	-1.43957400
H	0.94114200	0.95404600	0.39748500	Na	-3.87029000	-4.01838500	-1.17813700
C	0.64125200	-0.01041200	2.19664100	O	1.74251400	-2.62413700	1.08782000
H	-0.12571600	0.72450900	2.45726100	H	2.12159600	-3.43812600	0.73156000
H	0.26658800	-1.00175100	2.45992900	H	0.22188100	-2.87240100	0.92967400
C	1.95545600	0.26487300	2.91212300	O	-4.56838400	1.75772400	-1.61572200
H	2.31234000	1.27671200	2.69518600	H	-3.99482100	2.09105300	-2.31791300
H	1.84576900	0.16665700	3.99781800	H	-6.19764600	0.79214400	1.39589700
N	2.96214200	-0.69767200	2.38288800	AMP-TS1b			

C	2.50129300	2.90025000	-0.43925200	N	-4.21420000	4.43209300	0.25626100
C	1.71786300	2.17556700	-1.39665300	C	-4.92882800	3.41994100	0.77316800
C	2.32719800	1.14823200	-2.13058300	H	-5.86462800	3.70240500	1.24955400
C	3.73730900	0.89587100	-2.00718500	N	-4.64114200	2.11346300	0.76901800
C	4.53182300	1.67308600	-1.15114700	C	-3.47250200	1.87333600	0.17067100
C	3.90126700	2.65385700	-0.31735700	C	-3.53328400	-2.96844800	0.24695800
H	0.63808000	2.32622900	-1.43289000	H	-3.27955600	-3.86839100	-0.33351600
H	1.71832400	0.47053900	-2.71527000	C	-3.52215700	-1.70518300	-0.61936500
H	5.58786600	1.45644600	-1.03618500	H	-2.60861700	-1.73136300	-1.23455200
H	4.48640000	3.20762200	0.40919700	O	-4.81705200	-3.07411300	0.82641100
H	0.64450900	-0.00970000	0.91819400	O	1.28165800	-3.10389900	-1.88893100
N	1.24267100	0.59825900	1.51746300	Na	-0.38787000	-4.37473000	-2.19451200
H	0.75615300	1.45715000	1.76561100	O	3.95891300	-1.75065500	0.31682400
C	1.70256700	-0.16223400	2.70762000	H	4.45020600	-2.19082700	-0.38719400
H	0.98380900	-0.08100300	3.52930700	H	3.13547400	-2.34740400	0.50306400
H	1.76837900	-1.21242600	2.40236700	O	-4.68394800	-1.58245200	-1.38934400
C	3.06977900	0.36403800	3.11075400	H	-4.67701600	-0.71814300	-1.82208500
H	3.00015900	1.39639900	3.46918500	H	-4.84494800	-3.86104600	1.38549400
H	3.51254700	-0.24466600	3.90648200				
N	3.92053500	0.35086400	1.89108100	AMP-IM1b			
H	4.75222600	0.92111300	2.02629500	C	-2.66429900	2.67560300	-1.22571200
H	4.22381300	-0.60495600	1.63358600	C	-1.34812900	2.61839800	-0.65294000
H	2.02781600	3.63755100	0.20038000	C	-1.18501600	2.23361900	0.68768800
H	4.17287900	0.05561700	-2.53517800	C	-2.33152900	1.90777800	1.48887000
Ru	2.81633700	0.80665000	0.07801000	C	-3.62270700	1.99175900	0.93943300
P	0.98486100	-2.50539600	-0.51465800	C	-3.79144900	2.37180400	-0.43489700
O	1.80901400	-3.00448900	0.68133500	H	-0.47842500	2.80660800	-1.27463800
O	0.85484000	-0.95694900	-0.51646900	H	-0.20300100	2.07369800	1.11110700
O	-0.59923500	-3.12978700	-0.25580000	H	-4.48267900	1.70141900	1.53274300
C	-1.08674400	-3.29332200	1.08213300	H	-4.78222000	2.39073900	-0.87569300
H	-0.35855300	-2.89783100	1.79416500	H	-0.63062400	-0.67910300	-1.80952400
H	-1.18854900	-4.36736900	1.29094700	N	-1.58605600	-0.43686200	-2.08863600
C	-2.44146100	-2.63389800	1.29845500	H	-1.54786000	0.12841000	-2.93440800
H	-2.80387500	-2.95199400	2.28726300	C	-2.34424200	-1.70202700	-2.32210100
O	-2.30383600	-1.19640400	1.30316200	H	-2.20714300	-2.06185200	-3.34697400
C	-3.31069600	-0.63282700	0.46653400	H	-1.93633000	-2.43963100	-1.63063100
H	-4.24670400	-0.44604900	1.00454500	C	-3.81281200	-1.47052700	-2.00883800
N	-2.85186400	0.64783000	-0.02488400	H	-4.25453300	-0.76903700	-2.72522500
C	-1.66063700	0.91547900	-0.67022500	H	-4.36959100	-2.41290000	-2.07375200
H	-0.94410700	0.13013300	-0.88963600	N	-3.90772200	-0.88402500	-0.65012100
N	-1.47649100	2.19689800	-0.91218200	H	-4.84283700	-0.50755000	-0.50697200
C	-2.60961700	2.81524500	-0.39927600	H	-3.78592500	-1.60930400	0.10068500
C	-3.04458500	4.15725000	-0.34365800	H	-2.79140500	2.93074700	-2.27207800
N	-2.31263200	5.19310000	-0.84170800	H	-2.16985900	1.51875500	2.48671700
H	-2.79487700	6.07773900	-0.91420200	Ru	-2.38616300	0.60407800	-0.35840900
H	-1.61488600	4.98959900	-1.54025500	P	-0.73156000	-1.27284900	1.82846000

O	-1.56220000	-2.23992500	2.63763700	H	3.81717900	-2.49650000	2.11584900
O	-1.37194300	-1.03082400	0.40231300	H	3.79555400	-0.02840400	2.41988700
O	0.73396800	-2.06050300	1.40217200	H	4.88614100	0.52022500	-1.73243200
C	0.63678900	-3.17512600	0.52177200	H	4.92357600	-1.98435100	-2.05047300
H	-0.39813800	-3.28798000	0.18967100	H	0.43886500	-1.91250700	0.76357500
H	0.91178800	-4.09629700	1.05284900	N	0.97991700	-2.23927000	-0.04834900
C	1.53943800	-3.03000500	-0.71179800	H	1.24940200	-3.20414700	0.13240900
H	1.21448500	-3.77112800	-1.45324500	C	0.08302600	-2.16846900	-1.24451300
O	1.38827800	-1.70551300	-1.30095600	H	-0.46759800	-3.10380100	-1.37642600
C	2.66225000	-1.07123400	-1.36628200	H	-0.63764500	-1.36830700	-1.06797300
H	3.12155200	-1.23778400	-2.34788900	C	0.90788400	-1.82928500	-2.47242700
N	2.51560700	0.37149300	-1.21273900	H	1.60305000	-2.63584200	-2.72643100
C	2.10640800	1.18944600	-2.25347500	H	0.25669100	-1.64930100	-3.33534300
H	1.86053400	0.76459400	-3.21831900	N	1.69968400	-0.61771800	-2.13250000
N	2.07403000	2.46459000	-1.95864100	H	2.33967300	-0.37984400	-2.88733600
C	2.51050500	2.50809600	-0.64837100	H	1.06282500	0.18559400	-1.99676200
C	2.76737800	3.60242600	0.20966400	H	4.26378900	1.48387800	0.46607400
N	2.55083500	4.87701400	-0.15883800	H	4.36160600	-3.48267100	-0.13983400
H	2.84715900	5.61558000	0.46177100	Ru	2.68704200	-0.91122300	-0.24841400
H	2.32627600	5.09270400	-1.11771700	P	0.94704000	1.83348900	0.15406000
N	3.24208200	3.35375000	1.44816900	O	2.14825300	2.69636600	-0.23478700
C	3.44189700	2.08857300	1.80612400	O	1.26742900	0.35402900	0.56272800
H	3.83098900	1.94594100	2.81352500	O	0.02928500	1.51899200	-1.20803000
N	3.23307700	0.96052800	1.09554200	C	-0.77497100	2.49197000	-1.88641200
C	2.77894200	1.22700000	-0.15208500	H	-0.61173000	2.33334200	-2.95697600
C	3.06260700	-3.21363100	-0.49920700	H	-0.46242100	3.51577700	-1.64931500
H	3.28695800	-3.84028000	0.37264900	C	-2.26310600	2.34559200	-1.56799500
C	3.51430000	-1.76908300	-0.29319700	H	-2.81736100	2.92176300	-2.32462500
H	3.14175100	-1.45835500	0.68402300	O	-2.63934600	0.96189400	-1.64338600
O	3.69103900	-3.69392900	-1.67242800	C	-3.60779000	0.64599800	-0.65025100
O	-0.17156200	-0.01189300	2.48597100	H	-4.48657500	0.19609300	-1.12145200
Na	1.93304600	-0.46287800	2.59719500	N	-3.08795400	-0.39277900	0.24193100
O	-3.95668200	-2.52245100	1.55021900	C	-1.96027700	-0.37352000	1.04456700
H	-4.17196700	-3.46096700	1.59659700	H	-1.38160800	0.52584400	1.20780400
H	-3.08895800	-2.42738000	2.03835900	N	-1.66252000	-1.54821100	1.56153000
O	4.89226800	-1.57539000	-0.41653400	C	-2.65062200	-2.39573200	1.08005900
H	5.11929000	-0.76562300	0.06086200	C	-2.91446900	-3.77032400	1.25333700
H	3.66150200	-4.65825500	-1.67872300	N	-3.95995200	-4.31431400	0.61059700
				C	-4.72087600	-3.52473900	-0.16553300
AMP-IM2b				N	-4.58926300	-2.21398800	-0.39789600
C	4.39603800	-2.40835800	0.00509800	C	-3.53868400	-1.70419100	0.25104800
C	4.09645900	-1.84660500	1.29395100	C	-2.71501300	2.82842900	-0.17315400
C	4.10541900	-0.45402600	1.47287700	H	-1.94680900	2.59524100	0.56583000
C	4.39791000	0.41308000	0.36764700	C	-3.97027900	1.97064200	0.05538400
C	4.70811900	-0.13815400	-0.88946200	H	-4.21356600	1.82313000	1.11344500
C	4.71378100	-1.56219900	-1.07374000	O	-5.01881200	2.63801300	-0.63685400

H	-5.87238400	2.28177800	-0.36104000	C	1.61693600	3.31023300	1.00838200
O	-2.94203500	4.21479000	-0.10315100	H	2.07251300	4.17942800	1.50396900
O	0.05130200	2.50263500	1.20345200	O	2.45390500	2.15511700	1.21804200
H	-3.82636200	4.36344800	-0.47505600	C	3.19951300	1.84013100	0.06112000
Na	1.57171600	4.38875100	1.12226400	H	4.25902000	1.74118200	0.31472700
N	-2.12011100	-4.58009500	2.01607800	N	2.80516100	0.51152100	-0.43534400
H	-1.58616100	-4.13688000	2.74959100	C	1.55515000	0.10899600	-0.84852200
H	-2.51584900	-5.48435100	2.23505500	H	0.71802200	0.77901100	-0.99791400
H	-5.55321900	-4.01810900	-0.66187300	N	1.43447100	-1.19917000	-0.98223000
O	1.09927300	3.89047700	3.24198600	C	2.68659900	-1.69046100	-0.63758000
H	0.56295800	4.26491000	3.94959800	C	3.22267400	-2.98102100	-0.53505700
H	0.55699200	3.19559300	2.80034200	N	4.47371700	-3.14608600	-0.09980800
AMP-TS2b				C	5.19109700	-2.04910700	0.21304300
C	-2.88965300	-3.57652700	-0.12709000	N	4.80770100	-0.77097800	0.14470300
C	-2.19095700	-3.64162700	-1.37822500	C	3.54945400	-0.64452800	-0.27930900
C	-2.14333200	-2.50794400	-2.20096100	C	1.60811000	3.56796700	-0.51583300
C	-2.83523100	-1.31070900	-1.81541500	H	0.78735500	3.01775900	-0.98275200
C	-3.58739900	-1.25377600	-0.62989300	C	2.96987800	2.98142500	-0.95083100
C	-3.58524900	-2.38733900	0.24058600	H	2.98053700	2.62903800	-1.98822600
H	-1.63103000	-4.53309600	-1.63850900	O	3.91818000	4.02011100	-0.73963900
H	-1.52452900	-2.50330200	-3.09036500	H	4.72170700	3.83692600	-1.24136600
H	-3.98219700	-0.30479500	-0.28421900	O	1.44178400	4.91597400	-0.86288800
H	-4.08754700	-2.33654200	1.20090900	O	-1.88639700	3.20615100	-0.43125700
H	0.83983800	-3.31499600	0.45183400	H	2.32002500	5.32265700	-0.78713000
N	0.03274000	-3.05950200	1.03190600	Na	-3.95590200	3.33551800	0.66717700
H	-0.40900200	-3.94285300	1.28373700	N	2.44604000	-4.11097700	-0.80046700
C	0.46841900	-2.37115800	2.28093700	H	1.90279700	-4.03131700	-1.65367600
H	0.88070700	-3.08207100	3.00411200	H	3.00783400	-4.95687100	-0.78768700
H	1.25730400	-1.66487500	2.01030500	H	6.20529400	-2.23238100	0.55758400
C	-0.73205400	-1.62157400	2.84256500	O	-4.18537100	4.10652200	-1.41326500
H	-1.51096600	-2.31489400	3.17678400	H	-4.27577300	4.94916100	-1.87140300
H	-0.44192300	-0.99872600	3.69595800	H	-3.22541200	3.87285800	-1.41751200
N	-1.25690100	-0.79706500	1.73486400	AMP-PCb			
H	-2.11020600	-0.25240100	1.93396900	C	2.35167300	-3.67756900	-0.92674300
H	-0.57481100	-0.05237400	1.52543200	C	2.73700200	-2.71822700	-1.91658700
H	-2.67042900	-0.40059500	-2.37586800	C	1.74488900	-1.90445100	-2.49902500
H	-2.88833300	-4.43156200	0.54119700	C	0.37428300	-2.03508100	-2.12134400
Ru	-1.48321500	-1.89432300	-0.07708900	C	0.00754900	-2.99501200	-1.15452800
P	-1.68486400	1.80258800	0.14789700	C	0.99766700	-3.84372100	-0.56692000
O	-2.88529500	1.39689600	1.05701900	H	3.77746600	-2.61673600	-2.20371800
O	-1.25545500	0.68015700	-0.82030900	H	2.03236900	-1.13045600	-3.20295700
O	-0.33373200	1.85836000	1.15054900	H	-1.01255100	-2.99407400	-0.77360800
C	0.24937600	3.06639100	1.63796200	H	0.71740500	-4.57123600	0.18596200
H	0.35611800	2.97556400	2.72470100	H	3.76583600	-0.87567200	1.19839300
H	-0.38901100	3.92604300	1.40924400	N	2.98520400	-1.49654600	1.45134700

H	3.39204900	-2.41603900	1.61402800	H	4.47961600	-0.29744200	-0.86745500
C	2.30904300	-1.03211100	2.69950100	H	5.73247600	0.57218600	-0.14503100
H	2.89787200	-1.29050200	3.58524000	H	4.39343100	4.66949900	0.52835200
H	2.23531200	0.05795500	2.64844200	O	-5.61523700	-2.87237300	-0.84603900
C	0.92060400	-1.65086300	2.73727900	H	-6.53174900	-2.82186500	-1.13785100
H	0.98628900	-2.73885700	2.84453800	H	-5.25675500	-1.95038000	-0.85095800
H	0.34113300	-1.26499000	3.58342100				
N	0.25283700	-1.34355600	1.45419000	AMP-RCc			
H	-0.66227600	-1.86441400	1.32015900	C	4.52541700	-0.56898200	1.28580300
H	-0.07195400	-0.37227900	1.47412200	C	5.16298500	0.35500500	0.42521100
H	-0.39457800	-1.35523300	-2.47046700	C	5.07049500	0.22581100	-0.99838600
H	3.11471000	-4.28158900	-0.44485000	C	4.27289300	-0.80162500	-1.53405100
Ru	1.56799300	-1.65813100	-0.20066900	C	3.58895100	-1.72458900	-0.68165000
P	-2.71622100	-0.82939900	0.14499300	C	3.72072700	-1.60625100	0.71989100
O	-2.24202400	-2.16713000	0.83227300	H	5.72906300	1.17877600	0.84973200
O	-1.91756700	-0.50007300	-1.11701600	H	5.56175900	0.94001000	-1.64838100
O	-2.23501200	0.33748000	1.26463900	H	2.91759700	-2.47618300	-1.08903800
C	-3.05191800	1.47344900	1.55182600	H	3.10930600	-2.24511400	1.35073600
H	-2.99678400	1.64422900	2.63270000	H	2.51720300	3.03527600	-0.45347100
H	-4.09366400	1.27161000	1.27912400	N	2.66697900	2.49465900	0.39740900
C	-2.60085600	2.73894700	0.83116700	H	3.52533300	2.85536400	0.80901200
H	-3.21450600	3.57366900	1.19858100	C	1.51395600	2.71954400	1.33661900
O	-1.21413700	3.01134700	1.15975100	H	1.69330600	3.59511000	1.96692000
C	-0.50308700	3.46385600	0.04005800	H	0.63349700	2.92293100	0.72483300
H	0.03446700	4.38895700	0.26625200	C	1.29379600	1.45684800	2.15982400
N	0.57495700	2.48173900	-0.26491800	H	2.10559700	1.30179800	2.87723900
C	0.41894100	1.13976800	-0.42788900	H	0.35549400	1.52826200	2.72229500
H	-0.54242100	0.63691100	-0.61726600	N	1.27234700	0.32228800	1.21835500
N	1.57641500	0.48360500	-0.34820600	H	1.16199700	-0.64446500	1.61829600
C	2.55479700	1.45867200	-0.14629300	H	0.45134500	0.37694600	0.61030100
C	3.95661200	1.47976200	-0.03463000	H	4.60824200	-0.46328900	2.36131900
N	4.57434600	2.63628200	0.21412500	H	4.10565400	-0.84568800	-2.60469000
C	3.84060400	3.75848200	0.31637400	Ru	2.95705400	0.37117200	-0.06518600
N	2.52038600	3.87992000	0.16498300	P	0.22654400	-2.59434900	0.00673000
C	1.92531700	2.71177700	-0.06783900	O	0.79347500	-2.28986300	1.39454200
C	-2.67379300	2.72004700	-0.71365300	O	0.01776800	-1.33624000	-0.88068500
H	-2.47451000	1.71254400	-1.09136100	O	-1.36669300	-3.20508800	0.25767300
C	-1.51826900	3.66989400	-1.10247000	C	-2.05972400	-2.90332800	1.47867500
H	-1.09446000	3.45617500	-2.08984800	H	-1.34492500	-2.50554200	2.20406900
O	-2.04977000	4.98646300	-1.02976500	H	-2.45931000	-3.84662900	1.87578200
H	-1.51204700	5.58939400	-1.55720300	C	-3.23021200	-1.93808000	1.32498100
O	-3.91600700	3.11627600	-1.22769400	H	-3.78087300	-1.96090400	2.27779700
O	-4.24782000	-0.79561700	0.07860100	O	-2.75332300	-0.59215500	1.10831500
H	-3.93179300	4.08582800	-1.18535800	C	-3.55455100	0.01736700	0.09986700
Na	-4.38280800	-2.88360600	1.01442100	H	-4.46772900	0.46069700	0.51073000
N	4.74533400	0.33349200	-0.11911600	N	-2.79197200	1.09822100	-0.49764000

C	-1.66393100	0.94886900	-1.26814000	H	-0.21281300	0.50375800	-3.20879800
H	-1.35804200	-0.02254700	-1.62686800	N	-0.75246000	-0.48673900	-1.40196700
N	-0.96999700	2.05919600	-1.42258700	H	-0.28400800	-1.45076600	-1.53954300
C	-1.69505900	3.01307000	-0.71373900	H	-0.02372500	0.02122400	-0.89406300
C	-1.50959500	4.38810000	-0.47844100	H	-3.35276200	-2.48626100	-2.23798300
N	-0.43050200	5.08097800	-0.97990400	H	-3.30780700	-1.56142700	2.66028100
H	-0.52849000	6.08632000	-0.90548000	Ru	-2.41440000	-0.67359500	-0.12839300
H	-0.08615100	4.76053900	-1.87541300	P	1.25401200	-2.70849100	0.08718600
N	-2.38161400	5.03352800	0.30741700	O	0.55402900	-2.74140700	-1.28743600
C	-3.41101500	4.34340700	0.83014600	O	0.67263800	-1.64497700	1.03320500
H	-4.08783700	4.91548100	1.45976600	O	2.88919800	-2.17921500	-0.25471000
N	-3.70758300	3.04966800	0.66725900	C	3.19717800	-1.52012700	-1.48295400
C	-2.81999600	2.43355900	-0.11324800	H	2.35919800	-1.63168900	-2.17760000
C	-4.24469900	-2.23437600	0.18494200	H	4.06701000	-2.02172300	-1.93239900
H	-4.11345200	-3.24209000	-0.23233400	C	3.56677300	-0.04564400	-1.34190900
C	-3.89243500	-1.15298600	-0.84366800	H	4.00147700	0.27094200	-2.30065000
H	-2.96149900	-1.47291800	-1.33424600	O	2.38713500	0.76971500	-1.10060100
O	-5.57963100	-2.01111700	0.59528600	C	2.68452800	1.70793600	-0.06406100
O	0.86467400	-3.76238100	-0.75567200	H	3.15161600	2.62071100	-0.44759300
Na	-0.75427100	-5.12717200	-0.87344700	N	1.42436500	2.09411100	0.54617400
O	1.48706000	0.50725000	-1.59511600	C	0.55891500	1.20596700	1.13487600
H	0.89059800	-0.35121900	-1.37426000	H	0.84825800	0.17334000	1.32475000
H	0.85359200	1.25911500	-1.60323900	N	-0.66123000	1.68501300	1.30557400
O	-4.93614200	-0.92810100	-1.74971300	C	-0.58810000	2.98049200	0.80760200
H	-4.63197700	-0.30177300	-2.41923100	C	-1.54674600	3.98705200	0.61179300
H	-5.83998500	-2.71207400	1.20594900	N	-2.88465500	3.78276500	0.92154100
AMP-TSc				H	-3.42841100	4.63829500	0.87582600
C	-3.37722000	-2.33712700	-1.16403000	H	-3.04291000	3.25659200	1.77356300
C	-4.39598700	-1.52348000	-0.58085100	N	-1.18735200	5.12660800	0.01386800
C	-4.44330000	-1.30876500	0.82805600	C	0.09058200	5.26345800	-0.39031200
C	-3.40905800	-1.83820800	1.61896400	H	0.33546600	6.21074800	-0.86319600
C	-2.38658100	-2.66274700	1.04507300	N	1.08553900	4.37584200	-0.29010200
C	-2.38712500	-2.94588600	-0.32919300	C	0.69523800	3.25272400	0.31157700
H	-5.13622400	-1.05556800	-1.22339200	C	4.57269300	0.31277900	-0.21531100
H	-5.20743400	-0.67578100	1.26343700	H	5.08768000	-0.57503000	0.17288100
H	-1.55884900	-2.99271100	1.65770300	C	3.65894900	0.93641900	0.84702500
H	-1.54306500	-3.46824800	-0.77311200	H	3.10528600	0.11373500	1.32163900
H	-2.94940200	1.98350800	-0.48597600	O	5.48513400	1.31346700	-0.62471000
N	-2.85065300	1.20619700	-1.15069800	O	1.53933100	-4.06270800	0.73182700
H	-3.75831500	1.11556900	-1.60325100	Na	3.64347400	-4.15043400	0.72068500
C	-1.81022800	1.54559200	-2.18326600	O	-1.12719300	-0.78941100	2.97132800
H	-2.26342900	2.07460900	-3.02675500	H	-0.40453600	-1.19407100	2.44465500
H	-1.09241000	2.21971700	-1.71308400	H	-1.06979600	0.15811500	2.78328800
C	-1.10666500	0.26657800	-2.62064100	O	4.37133200	1.71741600	1.76467500
H	-1.76118700	-0.35689500	-3.23783800	H	3.80004100	1.90272000	2.52074800
				H	6.15547000	0.91521400	-1.19354400

				H	-4.82011600	3.07700700	-0.09577900
AMP-PCc				H	-4.21937100	1.76563200	0.76054300
C	-3.38540000	-2.95874400	0.55531100	N	-2.76256000	4.27057900	-0.36040200
C	-3.92151500	-1.93498700	1.40431500	C	-1.55478500	4.85976700	-0.42424500
C	-3.08028600	-1.21201600	2.26918100	H	-1.55677900	5.92198600	-0.65210500
C	-1.67351500	-1.47890500	2.27234400	N	-0.36207900	4.29319900	-0.22482400
C	-1.13445400	-2.48553800	1.44651500	C	-0.45336900	2.98965500	0.02056600
C	-2.00126200	-3.22414200	0.58014100	C	4.22187500	1.51813900	0.18098400
H	-4.98237100	-1.70768300	1.36573600	H	4.90282300	0.73840300	0.53612000
H	-3.48593200	-0.42905800	2.89955800	C	2.93429800	1.57645800	1.01087100
H	-0.05447800	-2.60516300	1.40061100	H	2.57907600	0.55430700	1.15570300
H	-1.57796100	-3.96042100	-0.09524800	O	4.79961700	2.81754100	0.30242400
H	-3.90952500	0.69176300	-1.22991900	O	2.94065000	-3.49903200	0.00552200
N	-3.58259800	-0.25562000	-1.46633400	Na	4.98620000	-3.10620800	-0.23914200
H	-4.40953100	-0.84916400	-1.48619100	O	0.95102500	-0.05924700	3.15572700
C	-2.92562400	-0.26765700	-2.81250500	H	1.41770600	-0.66378300	2.54386600
H	-3.66405900	-0.41818300	-3.60586900	H	1.58704900	0.63372600	3.37872500
H	-2.47029200	0.71580600	-2.96420400	O	3.05170900	2.19081800	2.26417500
C	-1.84521800	-1.34138000	-2.82361600	H	3.69228400	2.91331700	2.16441400
H	-2.28094200	-2.34401400	-2.77741500	H	5.70907900	2.80515400	-0.01909500
H	-1.24204600	-1.27987600	-3.73696000	AMP-RCd			
N	-1.01299100	-1.12670900	-1.62145300	C	-5.00843400	-1.27266400	-0.54756600
H	-0.13743900	-1.74591300	-1.56129300	C	-4.38858000	-2.51085000	-0.79083300
H	-0.57181500	-0.21086400	-1.71909100	C	-3.32013200	-2.60971300	-1.74570700
H	-4.03771100	-3.50925300	-0.11367800	C	-2.88302200	-1.45899100	-2.42677300
H	-0.99045400	-0.86222200	2.85552200	C	-3.49255000	-0.18783100	-2.16943200
Ru	-2.26318000	-1.00980900	0.10477400	C	-4.53539400	-0.10027800	-1.22720600
P	2.29109600	-2.15242400	-0.30872400	H	-4.70888100	-3.39216400	-0.24526900
O	1.42582700	-2.06653600	-1.56948300	H	-2.82978500	-3.56130200	-1.91724800
O	1.66634200	-1.44968700	0.91497200	H	-3.09541600	0.70968600	-2.62898300
O	3.73207700	-1.21207900	-0.66715300	H	-4.96023700	0.86879800	-0.98956200
C	3.77340800	-0.23436500	-1.70662200	H	-0.68703900	-2.16066200	1.04991600
H	2.97177700	-0.42440100	-2.42786300	N	-1.70304700	-2.22726100	1.25663600
H	4.73594800	-0.35236100	-2.22360200	H	-1.95455900	-3.21287500	1.21594900
C	3.68456900	1.22853600	-1.23781500	C	-1.94831800	-1.69940100	2.62833100
H	4.22349400	1.84984800	-1.96591800	H	-2.94055200	-2.03273300	2.95070700
O	2.30188800	1.67364600	-1.23297800	H	-1.20854900	-2.09176400	3.33517400
C	2.00093600	2.28883900	0.00913900	C	-1.88462600	-0.18294800	2.56365200
H	2.16407600	3.37213700	-0.00756900	H	-2.14631400	0.26153400	3.52984300
N	0.57551000	2.08922800	0.24771900	H	-0.88024800	0.14862200	2.29883500
C	0.01132300	0.86353300	0.39040500	N	-2.79266600	0.29814800	1.49055600
H	0.60724200	-0.04863600	0.53452300	H	-3.74253900	0.37458200	1.85030600
N	-1.31222500	0.89819500	0.28273500	H	-2.48417100	1.26503900	1.21191500
C	-1.64117400	2.23768700	0.07325800	H	-2.04194400	-1.52130600	-3.10797000
C	-2.82889000	2.96482900	-0.09464100	H	-5.80617100	-1.19642700	0.18275000
N	-4.09348700	2.36777200	-0.04734600				

Ru	-2.74354900	-1.02231400	-0.20404300	C	2.03840400	-1.46157800	-1.98452300
P	-0.72508000	3.11922800	-0.00167100	C	2.82740200	-2.28720200	-1.15394800
O	-1.90257600	2.85162100	0.97297100	H	5.42162800	-0.09221200	-0.51413600
O	-0.84456600	2.18809500	-1.29045600	H	4.02793900	1.37033100	-2.00637900
O	0.64594000	2.59009200	0.73617400	H	1.04034500	-1.79139100	-2.26196100
C	1.80008300	3.44128800	0.84576900	H	2.40135700	-3.23252800	-0.82831100
H	1.91428000	3.72376900	1.89848800	H	2.33019800	1.23448100	1.95495400
H	1.66268500	4.34617800	0.24698200	N	3.07435400	0.52176400	1.84264700
C	3.05506700	2.73259100	0.37606800	H	3.97552000	0.99462600	1.82532800
H	3.89280900	3.43743900	0.47972800	C	3.04323500	-0.50063300	2.92752100
O	3.30603200	1.57531900	1.20443400	H	3.87405300	-1.18893500	2.75066500
C	3.93801700	0.56280300	0.45929200	H	3.18583500	-0.04010800	3.91157000
H	4.90965700	0.29928500	0.89127800	C	1.70513800	-1.23240300	2.84835700
N	3.10501300	-0.65007900	0.52334700	H	1.76987900	-2.20394300	3.34527100
C	1.78271000	-0.74207300	0.86186800	H	0.93519300	-0.65402900	3.36823700
H	1.21328000	0.14231200	1.10663900	N	1.30248600	-1.40675000	1.42519500
N	1.31413900	-1.98063100	0.81443500	H	1.15050200	-2.40112600	1.09372000
C	2.40713900	-2.74726000	0.42576500	H	0.32984700	-1.08341300	1.31138700
C	2.61270500	-4.12362400	0.19257400	H	1.79064600	0.53431000	-2.75799600
N	3.81993300	-4.53645900	-0.22200400	H	4.62705400	-2.39563900	0.08172800
C	4.79589700	-3.63033200	-0.39089400	Ru	2.47256300	-0.39063800	-0.00508600
N	4.74213100	-2.31010600	-0.18340900	P	-1.05062800	-2.93125800	-0.30685800
C	3.52810200	-1.93101600	0.22843000	O	0.35616900	-3.42101100	0.04000200
C	3.03712000	2.19217700	-1.06722800	O	-1.09601900	-1.99778100	-1.57438400
H	2.05360800	1.75928400	-1.27614500	O	-1.39019500	-1.84483700	0.99470000
C	4.10457600	1.08235800	-0.98750900	C	-2.67496300	-1.85524300	1.60959900
H	3.96843400	0.28687300	-1.72748100	H	-2.54579500	-1.87958900	2.69871400
O	5.35435400	1.73686500	-1.14663600	H	-3.21184800	-2.75973700	1.30795000
H	6.03727300	1.08102700	-1.33599000	C	-3.51323400	-0.63291700	1.24888800
O	3.29322000	3.15706900	-2.04915200	H	-4.55627000	-0.81974800	1.53707100
O	-0.61783500	4.58972800	-0.35659400	O	-3.05517300	0.53535700	1.98865900
H	4.25770500	3.26179100	-2.08020200	C	-3.03385500	1.67743500	1.17356600
Na	-2.31857900	5.09790000	0.91491200	H	-3.54367800	2.50820200	1.67317800
N	1.62640600	-5.06226600	0.33365600	N	-1.61442300	2.06823800	0.97164200
H	0.89053700	-4.86069800	0.99300700	C	-0.54238100	1.51151200	1.60404900
H	1.95342700	-6.01921600	0.31774400	H	-0.69243700	0.72238700	2.32334200
H	5.74912000	-4.02555100	-0.73348500	N	0.62130800	2.04110100	1.25978200
O	-0.88589000	-0.16189200	-0.35998500	C	0.28277500	3.02008200	0.33414600
H	-0.83776400	1.20450200	-1.00649600	C	1.02534800	3.93815700	-0.43362200
H	-0.25684900	-0.79953700	-0.72167200	N	0.37752800	4.73672900	-1.29391600
				C	-0.95765800	4.64294200	-1.38795100
				N	-1.77705600	3.83313500	-0.70749100
AMP-TSd				C	-1.10428100	3.04517000	0.13682300
C	4.04646300	-1.78511100	-0.60099500	C	-3.43035200	-0.19754900	-0.22308600
C	4.50438600	-0.47280500	-0.95244600	H	-2.41578200	-0.35219800	-0.58334600
C	3.72974500	0.34972800	-1.79904600	C	-3.72813000	1.30064600	-0.15410600
C	2.47731800	-0.13915800	-2.26267000				

H	-3.34158000	1.87300600	-1.00068600
O	-5.13951700	1.41711700	-0.03666100
H	-5.41152500	2.31334000	-0.27151500
O	-4.29972800	-0.90868400	-1.09856500
O	-2.22342100	-3.90173300	-0.35990200
H	-5.18214400	-0.51955100	-0.98346900
N	2.39592300	4.02995300	-0.37989200
H	2.82296200	3.81237700	0.50897600
H	2.76022900	4.86200500	-0.82796500
H	-1.42781800	5.31424700	-2.10232400
O	-0.30312000	0.48269100	-1.50218300
H	-0.61785900	-0.47332200	-1.55739800
H	-0.76913500	0.95970900	-2.19939900
Na	-3.21687500	-2.78538200	-1.99936300

AMP-PCd

C	-3.46990100	-2.54742000	0.99203800
C	-3.72458800	-1.38401600	1.79427100
C	-2.66536100	-0.77190600	2.48464800
C	-1.33636800	-1.30087300	2.38981900
C	-1.09063200	-2.44533800	1.60938900
C	-2.16916300	-3.07620700	0.90687600
H	-4.72751900	-0.97418200	1.85124700
H	-2.84250200	0.13190300	3.05756400
H	-0.06166500	-2.75803400	1.45723500
H	-1.96554200	-3.93076300	0.27141600
H	-3.36015000	0.60964000	-1.61427000
N	-3.33975900	-0.40086000	-1.45026300
H	-4.30941500	-0.64879300	-1.26189400
C	-2.85557900	-1.15238600	-2.64452100
H	-3.11694300	-2.20397300	-2.49519300
H	-3.34465600	-0.80208800	-3.56018400
C	-1.34952200	-0.98008700	-2.72112100
H	-0.91994500	-1.63123200	-3.48889400
H	-1.11132000	0.05277200	-2.99543400
N	-0.74668300	-1.26480700	-1.39247400
H	-0.30975600	-2.21499200	-1.31560600
H	0.09925300	-0.69016500	-1.31723400
H	-0.49866200	-0.78050500	2.85507000
H	-4.28044800	-3.00446500	0.43332400
Ru	-2.07723300	-0.89293600	0.24797900
P	2.16699200	-2.20237900	-0.21156600
O	1.10956100	-3.17620400	-0.84548000
O	1.66515600	-1.60003900	1.10970000
O	2.16754800	-0.88334100	-1.27198600
C	3.38911300	-0.25000000	-1.67076900

H	3.33611200	-0.09256200	-2.75403800
H	4.23783500	-0.90450500	-1.44703400
C	3.61201600	1.09375400	-0.98484300
H	4.53535300	1.53243700	-1.38845300
O	2.50721600	1.97771200	-1.29581300
C	2.08639500	2.70068200	-0.16850400
H	2.06178200	3.77278600	-0.38134000
N	0.66853300	2.34759400	0.10474400
C	0.18300500	1.09997000	0.32483500
H	0.81028500	0.24363000	0.56043700
N	-1.14148000	1.03615500	0.20180900
C	-1.55316100	2.33523700	-0.10217100
C	-2.78230100	2.97852500	-0.33584600
N	-2.78784500	4.27208200	-0.66574400
C	-1.61838500	4.93108000	-0.74189400
N	-0.39817700	4.44938100	-0.49955400
C	-0.41690600	3.15599200	-0.18449200
C	3.71030600	1.05324200	0.55656800
H	3.11758900	0.22219100	0.94295500
C	3.05990000	2.38869200	0.98773500
H	2.55562800	2.30266200	1.95493900
O	4.09754800	3.36349800	0.99976100
H	3.89654000	4.04500900	1.65164600
O	5.01596200	0.89248200	1.04138900
O	3.55443700	-2.83947400	-0.24829400
H	5.41148000	1.77906700	1.04310600
Na	2.78263700	-4.66141400	-1.14179900
N	-4.00442600	2.31742200	-0.30211100
H	-4.10408200	1.66029900	0.46296000
H	-4.77788600	2.97256800	-0.36072000
H	-1.68194200	5.97901800	-1.02170200
O	1.40506800	0.16089600	3.07062100
H	1.67493200	-0.54789000	2.43610800
H	1.97568100	0.04395600	3.84004400

Cartesian coordinates for the species involved in Fig. S1:

GMPH-RCa

C	2.36742600	2.31473500	-0.82179200
C	1.74907300	1.29340900	-1.61677800
C	2.53449900	0.44416100	-2.41792500
C	3.95973700	0.60669900	-2.45855900
C	4.56752300	1.59236400	-1.66161200
C	3.76739300	2.45390600	-0.83644100
H	0.68067200	1.13438300	-1.54119100
H	2.06535300	-0.37091200	-2.95757100

H	5.64847200	1.68597300	-1.65105500	C	-2.77616200	1.85923100	0.55990000
H	4.24396200	3.20108000	-0.21134200	C	-3.88415800	-1.72288100	-1.17906600
H	1.57656000	-0.99653400	1.30701000	H	-2.92368800	-1.40429500	-1.59347300
N	1.97887000	-0.04446200	1.35770600	C	-4.61251800	-0.51698000	-0.55536800
H	1.16232900	0.59066200	1.31076000	H	-4.51825700	0.40291900	-1.13926300
C	2.69946000	0.08781800	2.64443600	O	-5.96807200	-0.91808700	-0.41604400
H	2.84950300	1.15108200	2.86044200	H	-6.52280500	-0.14033400	-0.27978200
H	2.11544200	-0.34654100	3.46335400	O	-4.60031200	-2.35433000	-2.20356500
C	4.02746200	-0.63218600	2.49574300	O	0.22940200	-4.73616000	0.20868200
H	4.65182800	-0.53831800	3.38993900	H	-5.53526000	-2.31359900	-1.94572700
H	3.85039700	-1.68963800	2.29053800	H	0.61087800	-5.01764300	1.05203400
N	4.72123500	-0.07274300	1.29423100				
H	5.23177000	0.77380500	1.54010700	GMPH-TS1a			
H	5.40274800	-0.74904900	0.95497100	C	1.94165900	2.39826100	-0.74001900
O	3.31285500	-1.81678500	-0.28985600	C	1.26569500	1.42041100	-1.53500200
H	2.06737900	-2.29765600	-0.70365300	C	2.00922300	0.59703400	-2.39594400
H	3.91511700	-2.12105200	-0.98211000	C	3.41713400	0.81190700	-2.58698500
H	4.56741700	-0.05855600	-3.06157200	C	4.07923400	1.80231000	-1.85100400
H	1.74575000	2.94170900	-0.18515600	C	3.34962700	2.56819100	-0.87932300
Ru	3.27994200	0.27688800	-0.29503200	H	0.21562500	1.22499900	-1.36317200
P	0.18613600	-3.12060400	0.12237100	H	1.53226300	-0.25782900	-2.86013300
O	0.46579500	-2.49624800	1.46018000	H	5.15205800	1.93029500	-1.94965700
O	1.10742300	-2.63673400	-1.04416900	H	3.86536100	3.29587000	-0.26197000
O	-1.27684000	-2.83672900	-0.48255000	H	1.56182400	-0.74559200	1.55904400
C	-2.44595400	-3.54490200	-0.01653800	N	1.89383100	0.24592300	1.48686200
H	-2.26676900	-3.99318500	0.96465100	H	1.02207800	0.80922000	1.46969500
H	-2.66774400	-4.34100200	-0.73350000	C	2.73687800	0.56074600	2.66041900
C	-3.63714500	-2.60882600	0.06119900	H	2.88007700	1.64491500	2.71993600
H	-4.52769800	-3.22638100	0.24141200	H	2.25263700	0.22879000	3.58560000
O	-3.48024000	-1.69236500	1.16811200	C	4.05934900	-0.15532000	2.45249600
C	-3.93712900	-0.40704800	0.82748100	H	4.79647200	0.09798100	3.22012700
H	-4.63598300	-0.04222300	1.58783100	H	3.90000500	-1.23678800	2.47082800
N	-2.77305000	0.50442200	0.80424700	N	4.56303500	0.19713300	1.08887400
C	-1.46457200	0.15266900	1.05281200	H	5.20766900	0.98334900	1.12832400
H	-1.18311200	-0.85942600	1.30009000	H	5.03509600	-0.60866700	0.67201800
N	-0.63886700	1.17352900	0.95907400	O	4.16672100	-1.91167800	-0.57724700
C	-1.44196800	2.25386700	0.64813500	H	3.19421200	-2.16217900	-0.65686200
C	-1.10029300	3.62178400	0.40016300	H	4.56826500	-2.15524800	-1.42077400
O	-0.00112800	4.16975800	0.37273700	H	3.97546100	0.15798400	-3.24648800
N	-2.27840800	4.38261900	0.14911300	H	1.37206400	2.98805400	-0.02426600
H	-2.10695100	5.37384200	0.02536100	Ru	2.94972200	0.48616200	-0.33796900
C	-3.56427600	3.89215000	0.09911900	P	0.76002700	-2.74019900	0.22765800
N	-4.56402400	4.79299700	-0.11240500	O	0.78774800	-2.30018600	1.67701600
H	-4.37345700	5.67649100	-0.55891700	O	1.63621400	-1.94850600	-0.74659700
H	-5.48044900	4.39940600	-0.26344600	O	-0.73710400	-2.67204600	-0.40618500
N	-3.86208800	2.62115600	0.28052400	C	-1.75110300	-3.60363500	0.01363200

H	-1.52833700	-4.00413400	1.00779800	H	0.85431500	-1.41745300	-1.70476500
H	-1.77958800	-4.43075300	-0.70297600	C	2.85826500	-1.53084800	-2.39707600
C	-3.11617500	-2.93759300	0.04661100	H	2.91699800	-2.60677000	-2.20195400
H	-3.86930500	-3.72964300	0.15289500	H	2.66934700	-1.38886100	-3.46735000
O	-3.21989000	-2.06277900	1.19709600	C	4.13560500	-0.82402900	-1.97280700
C	-3.84701500	-0.85360500	0.86002200	H	5.01975700	-1.24443300	-2.46195200
H	-4.62241900	-0.61731800	1.59632300	H	4.07608800	0.23642900	-2.22913800
N	-2.82743600	0.22221200	0.90418900	N	4.25519600	-0.91074900	-0.48695700
C	-1.50772700	0.05153200	1.26002600	H	4.75602500	-1.75823400	-0.22777000
H	-1.11608700	-0.90775200	1.56323000	H	4.79871100	-0.09786600	-0.14091800
N	-0.81210400	1.16571500	1.17513800	O	5.19595700	1.59963700	0.21550200
C	-1.71824300	2.12116100	0.75886400	H	4.26497300	1.81428500	0.41925600
C	-1.52098700	3.50308100	0.44613100	H	5.74631200	2.07110200	0.85107500
O	-0.48712100	4.16774700	0.43739300	H	3.09550200	-0.33091500	3.40041100
N	-2.76026900	4.10491300	0.08615400	H	0.31109900	-3.13548700	0.30335100
H	-2.69890300	5.10171300	-0.08673800	Ru	2.32058400	-0.87901400	0.47466500
C	-3.97251900	3.45801200	-0.01643300	P	1.64146500	2.22399200	-0.57443000
N	-5.05590200	4.21858600	-0.33601400	O	1.37618100	1.80802200	-1.99572700
H	-4.94507500	5.10363500	-0.80536400	O	2.48611000	1.25426900	0.29309900
H	-5.90786400	3.71094400	-0.52007400	O	0.29082700	2.49287900	0.28256200
N	-4.12835000	2.16889600	0.21021200	C	-0.51751200	3.65888400	-0.01019400
C	-2.98299100	1.55653100	0.59902200	H	-0.25610600	4.07462400	-0.98721400
C	-3.47262600	-2.06310000	-1.17586200	H	-0.30874800	4.40734600	0.75984000
H	-2.56950800	-1.56258800	-1.53488600	C	-2.00231300	3.34587200	0.01119800
C	-4.43323600	-1.03064600	-0.55468200	H	-2.52833100	4.31064700	0.01143600
H	-4.48468300	-0.08930500	-1.10867800	O	-2.39211500	2.61647100	-1.17452900
O	-5.69806400	-1.67424700	-0.48859700	C	-3.35709200	1.63783100	-0.86821500
H	-6.39104000	-1.01454900	-0.36331200	H	-4.20089000	1.71827300	-1.56134700
O	-4.02101100	-2.77166000	-2.25285700	N	-2.72984100	0.30837300	-1.03964100
O	1.13317400	-4.32143600	0.12949000	C	-1.44943100	0.08520900	-1.50609000
H	-4.95484900	-2.91776800	-2.03200900	H	-0.82064600	0.89675400	-1.84185000
H	1.33629200	-4.66278600	1.01150100	N	-1.11206000	-1.18537900	-1.47291800
GMPH-IM1a				C	-2.22515400	-1.83548000	-0.97913200
C	0.90434200	-2.55418200	1.00677700	C	-2.40532400	-3.21209900	-0.62541900
C	0.36562400	-1.35004000	1.55413200	O	-1.59604200	-4.13389400	-0.62492200
C	1.16667600	-0.55219600	2.39892000	N	-3.74437800	-3.43291200	-0.18688100
C	2.48197900	-0.96234600	2.76980100	H	-3.95346200	-4.40289600	0.01992700
C	3.00042100	-2.15718400	2.22619500	C	-4.70767300	-2.46384200	-0.01614400
C	2.21453600	-2.96905300	1.34936800	N	-5.94050000	-2.87628600	0.38278800
H	-0.61788600	-1.01518400	1.25429800	H	-6.07939400	-3.77708900	0.81176300
H	0.80458400	0.41920600	2.71680100	H	-6.60432600	-2.15065800	0.60448100
H	4.02356400	-2.44452500	2.44848600	N	-4.49515600	-1.18203900	-0.24399700
H	2.62525000	-3.87970000	0.92898200	C	-3.25210500	-0.92763800	-0.72311100
H	1.61159800	0.03090500	-1.88178900	C	-2.51370800	2.50308000	1.19703200
N	1.76640400	-0.95093000	-1.58405300	H	-1.78314600	1.72076800	1.42240500
				C	-3.78399300	1.87483500	0.59514300

H	-4.10120700	0.95479600	1.09245500	O	-3.53291500	-0.90952900	1.01477700
O	-4.77860800	2.88578200	0.67150700	C	-3.93584100	-0.40293500	-0.24423600
H	-5.65125300	2.49177300	0.55036600	H	-4.81641900	0.22888100	-0.10560200
O	-2.73514100	3.22900900	2.37387900	N	-2.89931100	0.48365800	-0.79245400
O	2.40168100	3.65445400	-0.50186200	C	-1.65969900	0.13058100	-1.31524400
H	-3.59320100	3.66933800	2.26232900	H	-1.43531000	-0.88064500	-1.61361400
H	2.72946900	3.90633800	-1.37716000	N	-0.81603800	1.12627300	-1.38626200
GMPH-IM2a				C	-1.51598000	2.20261800	-0.87273900
C	4.01976300	1.93344500	-0.89818400	C	-1.04373300	3.49692400	-0.50646000
C	2.93278000	1.67883400	-1.79796700	O	0.11572000	3.93110900	-0.51158900
C	2.71981900	0.38036000	-2.29874700	N	-2.10135000	4.29226500	-0.00073900
C	3.59263100	-0.69301400	-1.91995700	H	-1.81885100	5.21293400	0.31577300
C	4.66463200	-0.45421300	-1.04188500	C	-3.38582600	3.84646300	0.24483300
C	4.85705900	0.86352900	-0.50618600	N	-4.25182200	4.74206700	0.80017300
H	2.21238400	2.46232200	-2.01053300	H	-4.12871600	5.72900200	0.63025100
H	1.83546700	0.17761800	-2.88946400	H	-5.20751100	4.42202000	0.86412900
H	5.29541100	-1.27447600	-0.71932100	N	-3.77614800	2.60923800	0.02551800
H	5.64587700	1.04037900	0.21820500	C	-2.80728800	1.83010600	-0.50434200
H	0.43712000	0.94838600	0.90580500	C	-3.34583500	-2.72941900	-0.53242600
N	1.27747100	1.52992900	0.88995800	H	-2.34734000	-2.68099900	-0.97581800
H	1.04408100	2.36214300	0.33127200	C	-4.24778500	-1.62523200	-1.12961800
C	1.71660800	1.90467700	2.25483000	H	-4.05772600	-1.43791300	-2.19219200
H	2.53754900	2.61971500	2.14789400	O	-5.57965200	-2.06701200	-0.90423700
H	0.91163400	2.39472900	2.81528000	H	-6.18388500	-1.61058600	-1.50211200
C	2.17578000	0.64222200	2.96838700	O	-3.82197700	-4.02831000	-0.74773400
H	2.69505300	0.88501100	3.89996900	O	0.72388600	-3.66400100	0.19608200
H	1.32165700	0.00733300	3.21551500	H	-4.79062800	-3.97049400	-0.71043900
N	3.05286100	-0.16833400	2.06359200	H	1.11535700	-4.31731100	0.79477600
H	4.03104800	-0.07734900	2.32574900	GMPH-TS2a			
H	2.76203500	-1.15113500	2.19307800	C	4.09184900	1.37164600	-1.02431000
O	2.74081500	-3.66165000	-1.95684100	C	2.95448300	1.75400100	-1.80781600
H	1.97386900	-3.62130600	-1.36186700	C	2.21014500	0.75447300	-2.44904500
H	2.49237100	-4.28312900	-2.65125700	C	2.62176200	-0.62105700	-2.39821600
H	3.35156800	-1.71711600	-2.20616900	C	3.78446800	-0.99254800	-1.71137500
H	4.16537600	2.92429400	-0.48326200	C	4.50533400	0.00585700	-0.97879600
Ru	2.73767700	0.29164100	-0.04128600	H	2.59445000	2.77586300	-1.77515300
P	0.66006200	-2.20570300	0.95477500	H	1.26852500	1.00866200	-2.91895500
O	1.27718200	-2.31522900	2.31952000	H	4.01637600	-2.04965700	-1.63664300
O	1.20288100	-1.17044300	-0.03748800	H	5.36534800	-0.27239200	-0.37841500
O	-0.91929900	-1.85679400	0.93560500	H	1.09214700	1.26111900	1.66410800
C	-1.92687900	-2.62059000	1.61899200	N	2.05872300	1.47304400	1.41108500
H	-1.93752000	-2.33620300	2.67537800	H	2.04785200	2.45689700	1.11018500
H	-1.72753300	-3.69544900	1.53553300	C	2.95365900	1.17181400	2.55164200
C	-3.26672700	-2.32119900	0.95940400	H	3.97194100	1.45245200	2.26685300
H	-4.04877100	-2.85706800	1.51403100	H	2.67850200	1.74777100	3.44279800

C	2.83425500	-0.32440200	2.80435500	O	-0.39586400	-4.31028900	0.53996600
H	3.61154700	-0.67681200	3.48809400	H	-5.31920800	-2.86124100	-1.36168600
H	1.86601300	-0.56274900	3.25480000	H	-0.05275500	-4.91427700	1.21353700
N	2.88579500	-1.05988800	1.50452500	GMPH-PCa			
H	3.79464900	-1.50073300	1.38262400	C	3.74893700	-1.75854900	-1.73393000
H	2.17597100	-1.83123700	1.59260000	C	3.13206600	-0.66628800	-2.41573400
O	2.35267900	-3.56163200	-1.82931100	C	1.72978400	-0.66903200	-2.56003900
H	1.64584000	-3.15014200	-1.28512000	C	0.93844700	-1.75573600	-2.07812400
H	1.99207100	-4.40445700	-2.12742200	C	1.56294700	-2.84002000	-1.42735600
H	2.00343100	-1.40989900	-2.80881100	C	2.98198700	-2.84643700	-1.25637800
H	4.63510500	2.11995900	-0.45696100	H	3.72484200	0.16798500	-2.77070000
Ru	2.46334500	0.16650300	-0.24151000	H	1.24164300	0.19126100	-3.00523700
P	0.01813800	-2.77924300	0.91440800	H	0.92752400	-3.64291200	-1.04749900
O	0.87710400	-2.75852400	2.15918600	H	3.46784400	-3.67009800	-0.74522800
O	0.58938100	-2.09066200	-0.32348600	H	3.59096400	0.93816700	0.92651300
O	-1.41825900	-2.04795000	1.14350800	N	3.66448600	-0.09144800	1.00941100
C	-2.66323400	-2.61336700	1.55252300	H	4.60109400	-0.31693200	0.68150500
H	-2.79606000	-2.45076900	2.62729800	C	3.50692800	-0.55293400	2.42052000
H	-2.69572700	-3.68748600	1.34061700	H	4.10196700	-1.46306900	2.55108700
C	-3.77076000	-1.91681100	0.76838500	H	3.88825600	0.19904100	3.11883700
H	-4.74080900	-2.29941300	1.11090500	C	2.03736900	-0.85666700	2.66424400
O	-3.72034100	-0.49528800	1.02017600	H	1.88654400	-1.34769100	3.63174800
C	-3.72701000	0.24844900	-0.17360900	H	1.44115600	0.05889500	2.65720400
H	-4.43211400	1.07874600	-0.08451900	N	1.56321500	-1.71477500	1.55647500
N	-2.40970400	0.89139700	-0.38301100	H	1.99570600	-2.63437900	1.64989800
C	-1.19233800	0.25874400	-0.52535500	H	0.52092700	-1.93151400	1.66378200
H	-1.07786900	-0.79539500	-0.70878500	O	-0.85535400	-4.54731900	-1.28387500
N	-0.16892100	1.06559800	-0.37262700	H	-1.36335600	-3.73871500	-1.06115900
C	-0.73244700	2.31378500	-0.12651200	H	-1.36296500	-5.26711900	-0.89114600
C	-0.12822100	3.58154900	0.12001000	H	-0.14328200	-1.73849300	-2.13703600
O	1.07111200	3.88510100	0.20722600	H	4.82189800	-1.74588800	-1.56747100
N	-1.11306800	4.58097900	0.30392600	Ru	2.17980200	-0.92354700	-0.32336000
H	-0.73577700	5.49610900	0.52284700	P	-2.05045300	-2.36409700	1.11135900
C	-2.47784600	4.37909100	0.28421500	O	-0.86479700	-2.57132100	2.02805600
N	-3.26952600	5.45239700	0.54101900	O	-1.80486500	-2.11160100	-0.36960200
H	-2.92750500	6.39374700	0.42906100	O	-2.85999800	-1.10224100	1.75227900
H	-4.26111100	5.30667600	0.42369800	C	-4.17735300	-0.69847500	1.37878400
N	-3.02644600	3.20089100	0.06835400	H	-4.68927700	-0.44894500	2.31295100
C	-2.12517300	2.21602400	-0.12238600	H	-4.73318900	-1.50655300	0.88882500
C	-3.66952400	-2.09523500	-0.76746900	C	-4.17914300	0.52240100	0.46008800
H	-2.62630600	-2.26598900	-1.04733700	H	-5.18366800	0.96766800	0.49447100
C	-4.13913700	-0.72107700	-1.29906600	O	-3.22125000	1.49063500	0.94540500
H	-3.69792600	-0.45875400	-2.26690000	C	-2.56431400	2.12530200	-0.11207500
O	-5.55637300	-0.80300300	-1.37060300	H	-2.63418100	3.21227900	-0.01530900
H	-5.89359200	-0.14761200	-1.99285900	N	-1.09921100	1.85405800	-0.04687200
O	-4.40466800	-3.17438100	-1.27242100				

C	-0.45285200	0.64746400	-0.04555300	H	3.62468300	-1.63490500	2.11913400
H	-0.96657800	-0.30652600	-0.15658000	H	2.17355200	-1.88112500	1.36947700
N	0.86302800	0.78386900	0.07233400	O	2.23006100	-1.56045200	-1.03251900
C	1.08844500	2.16048800	0.16487500	H	0.90506900	-2.05176200	-0.93254600
C	2.27250800	2.94566100	0.31602400	H	2.53731100	-1.81280300	-1.91106700
O	3.45367400	2.59425300	0.42872200	H	5.34099900	-1.61342100	-2.22359800
N	1.97454400	4.32515600	0.33921400	H	4.86263700	2.37534800	0.77021400
H	2.79502900	4.91563300	0.41958300	Ru	3.53713600	-0.19853300	-0.19120400
C	0.71706600	4.88144400	0.25616500	P	-0.55229100	-2.90450000	0.50762600
N	0.62489500	6.23264600	0.27065800	O	0.42979300	-2.67550700	1.61654800
H	1.38226600	6.81127400	0.59797600	O	-0.06674900	-2.46212200	-0.91510100
H	-0.30721100	6.61585500	0.32403200	O	-1.93997400	-2.10340400	0.60509700
N	-0.37228600	4.15209500	0.13063600	C	-3.12696600	-2.50127000	1.31365900
C	-0.13628300	2.82663000	0.08807900	H	-3.01025500	-2.26567200	2.37605000
C	-3.81212900	0.27422300	-1.01946700	H	-3.29843200	-3.57477900	1.19036100
H	-3.05670500	-0.51342900	-1.08447700	C	-4.29362900	-1.72428500	0.71996000
C	-3.21983700	1.63991700	-1.42475900	H	-5.21339200	-2.04579500	1.22642800
H	-2.50849800	1.58006200	-2.25668100	O	-4.09878400	-0.31742900	0.94930400
O	-4.32930900	2.46956500	-1.74139500	C	-4.28345100	0.43858700	-0.23060700
H	-4.04381700	3.20798500	-2.29241500	H	-4.93042900	1.29168400	-0.01247000
O	-4.89436000	-0.12838300	-1.81421600	N	-3.00375300	1.02766700	-0.65715500
O	-3.07928900	-3.62236700	1.20418700	C	-1.87362600	0.36933300	-1.11827200
H	-5.41528900	0.66971400	-1.99557700	H	-1.89309700	-0.65550100	-1.45270100
H	-3.06789900	-4.00333500	2.09388700	N	-0.79198200	1.10531700	-1.07137000
GMPH-RCb				C	-1.20846900	2.31406000	-0.53878600
C	4.99316200	1.52321400	0.11360900	C	-0.44853700	3.45141600	-0.12316000
C	4.50290500	1.56838000	-1.23041400	O	0.77437300	3.62852800	-0.10729300
C	4.63892600	0.45157300	-2.07875400	N	-1.30762100	4.46289200	0.38078400
C	5.27592500	-0.73716000	-1.58747200	H	-0.82128100	5.27956200	0.73257700
C	5.75789200	-0.79839000	-0.27111700	C	-2.67213700	4.35041900	0.54728400
C	5.58330200	0.33462200	0.59423000	N	-3.31565300	5.41109100	1.11396300
H	3.97798200	2.45045100	-1.58167500	H	-2.93522700	6.34031400	1.01648800
H	4.23151600	0.47813800	-3.08233800	H	-4.32316100	5.34391400	1.11483900
H	6.20650600	-1.71049700	0.10493100	N	-3.34943900	3.26622900	0.23688000
H	5.90976000	0.27657200	1.62720400	C	-2.57639800	2.28425000	-0.27677500
H	1.03987400	0.60943500	-0.44735700	C	-4.46848000	-1.90607000	-0.80966100
N	1.74511600	0.86062900	0.26219700	H	-3.49997200	-2.13959300	-1.25979100
H	1.82129800	1.87776000	0.15430400	C	-4.93335900	-0.50310700	-1.26339000
C	1.17350500	0.54772000	1.61153900	H	-4.64358100	-0.26619200	-2.29274600
H	0.82605400	1.46662600	2.09104700	O	-6.34622600	-0.49876900	-1.10075100
H	0.31867500	-0.11636200	1.48005700	H	-6.73947300	0.17815500	-1.66438300
C	2.21532300	-0.15264200	2.47158400	O	-5.34665000	-2.93518600	-1.16900300
H	2.97656900	0.54659800	2.83092300	O	-1.05797700	-4.43532600	0.42634700
H	1.73796800	-0.63112700	3.33317000	H	-6.23950700	-2.55634100	-1.12204400
N	2.88036900	-1.16423800	1.60829200	H	-0.44979200	-5.02940300	0.88722000

GMPH-TS1b

C	3.87266500	1.92925100	-0.41497900
C	2.95946000	1.77966800	-1.50788400
C	3.08764300	0.67912200	-2.37096900
C	4.18661300	-0.23002100	-2.21049800
C	5.13116800	-0.06296600	-1.18793000
C	4.93115100	0.98924400	-0.24003800
H	2.09544100	2.43396100	-1.56417100
H	2.32754100	0.48812200	-3.11849900
H	5.93139000	-0.78065200	-1.05300200
H	5.59935500	1.08712500	0.60943300
H	0.54563400	0.19535700	0.41022800
N	1.32713400	0.67577100	0.86628000
H	1.22266500	1.67214500	0.64649100
C	1.34581600	0.43918300	2.34452200
H	1.07078700	1.35701800	2.87067300
H	0.62240300	-0.34226500	2.57395000
C	2.73598600	-0.03385700	2.76184100
H	3.44759100	0.79586200	2.81338800
H	2.69708900	-0.52004900	3.74266100
N	3.19530000	-0.98387800	1.71567700
H	4.12307400	-1.35030100	1.91798300
H	2.52725200	-1.78417700	1.70726200
O	3.08641500	-2.66830700	-0.59589700
H	2.09946100	-2.54909200	-0.71623600
H	3.41726700	-3.07734700	-1.40499300
H	4.24805800	-1.09701100	-2.85797700
H	3.73140700	2.73808100	0.29319000
Ru	3.01109500	-0.06853600	-0.20952000
P	0.04144400	-2.55948600	0.67523500
O	0.82326200	-2.58701600	1.96830800
O	0.68883400	-1.83876200	-0.51345900
O	-1.39748500	-1.80421100	0.80058600
C	-2.54471700	-2.36034400	1.45922000
H	-2.55309400	-2.03655900	2.50507300
H	-2.51943000	-3.45450100	1.41851700
C	-3.79923400	-1.87573200	0.74419500
H	-4.67208000	-2.31284200	1.24698300
O	-3.88841900	-0.44050800	0.83156700
C	-4.10471800	0.14851700	-0.43198900
H	-4.88618200	0.90614900	-0.33787700
N	-2.89732700	0.87812800	-0.85993400
C	-1.71584300	0.35583500	-1.37272700
H	-1.65864900	-0.63589700	-1.79314100
N	-0.69588000	1.16950900	-1.27215400
C	-1.21114600	2.28711100	-0.64075800

C	-0.52592300	3.38847200	-0.05628800
O	0.69815200	3.57570900	0.04736000
N	-1.43530300	4.29654600	0.53148000
H	-1.00113900	5.07919100	1.00739700
C	-2.79704700	4.08929700	0.65350000
N	-3.50781600	5.05040400	1.30998400
H	-3.18813400	6.00728200	1.29700300
H	-4.50917700	4.91988300	1.29336800
N	-3.40319400	3.00366900	0.22562200
C	-2.57058800	2.12946700	-0.38027600
C	-3.85445700	-2.23542600	-0.76203000
H	-2.83598500	-2.34544200	-1.14345100
C	-4.52445600	-0.98671100	-1.38415800
H	-4.22222400	-0.80672500	-2.42182100
O	-5.92408300	-1.21267000	-1.27935400
H	-6.39417000	-0.66864700	-1.92248800
O	-4.52637300	-3.43105100	-1.04421800
O	-0.38252100	-4.06863600	0.23869300
H	-5.47195400	-3.21161600	-1.06239300
H	-0.02090100	-4.70726700	0.86889400

GMPH-IM1b

C	3.98058600	1.89887100	-0.71571200
C	2.92041800	1.69659000	-1.65904300
C	2.77402000	0.45014300	-2.29811100
C	3.68684800	-0.61622200	-2.00524100
C	4.73154900	-0.43253400	-1.08232700
C	4.85594000	0.83002300	-0.41322400
H	2.17293900	2.47164100	-1.80071500
H	1.91803200	0.27817700	-2.93836700
H	5.39189600	-1.25463000	-0.83267300
H	5.62185100	0.96368200	0.34389500
H	0.36584100	0.81672000	0.55008700
N	1.21267100	1.22919700	0.94362000
H	1.20959700	2.20399300	0.62932400
C	1.23843400	1.11020700	2.43292000
H	0.90412100	2.04141300	2.89912700
H	0.56338100	0.30179400	2.71867600
C	2.65160100	0.75230600	2.87237600
H	3.34081500	1.58912800	2.72114700
H	2.66545500	0.47839300	3.93332100
N	3.09099300	-0.38660300	2.02110100
H	4.05041600	-0.64994700	2.23574400
H	2.46616500	-1.19247000	2.23308900
O	1.73989800	-3.26590900	-2.13603800
H	1.43986200	-2.42496800	-1.73164900

H	1.07444500	-3.52035900	-2.78818100	C	4.43498000	-1.07866600	-1.79926100
H	3.50556100	-1.60186900	-2.42243200	C	5.05296000	-1.39733600	-0.57754400
H	4.07777100	2.84778800	-0.20086300	C	5.55136700	-0.34834100	0.26824600
Ru	2.75661400	0.13461300	-0.04674000	H	4.66779300	2.35448600	-1.67720100
P	0.66405500	-2.37644300	0.85270900	H	3.77953700	0.52981300	-3.12106800
O	0.91016000	-2.05542300	2.29763900	H	5.10809300	-2.43098800	-0.25461400
O	1.26888400	-1.39862500	-0.20855300	H	6.00331500	-0.58782300	1.22454600
O	-0.91296000	-2.31743600	0.45525900	H	1.74031900	2.26149000	0.24676700
C	-1.93701100	-2.83853400	1.32453300	N	2.31443200	1.65656500	0.85796600
H	-1.72786600	-2.54095900	2.35598800	H	3.01135400	2.28252400	1.26003400
H	-1.95820000	-3.93270000	1.26141300	C	1.45937100	1.11648900	1.95601300
C	-3.28178600	-2.29109700	0.87087100	H	1.18160600	1.90924900	2.65815300
H	-4.06021400	-2.74570700	1.49872900	H	0.55079700	0.71779600	1.50134700
O	-3.30935900	-0.86141400	1.04418600	C	2.21370000	-0.00589300	2.64166800
C	-3.88166600	-0.20902700	-0.07361600	H	3.11440400	0.37004300	3.13985800
H	-4.65957300	0.48278800	0.25988200	H	1.57913500	-0.50168000	3.38275100
N	-2.85969200	0.63350400	-0.71536900	N	2.60291700	-0.97476100	1.58127000
C	-1.65860200	0.19847500	-1.25867000	H	3.29195600	-1.62612700	1.95309000
H	-1.49682100	-0.83381700	-1.52222800	H	1.74176200	-1.55447700	1.40071600
N	-0.75622300	1.14056900	-1.36318600	O	1.53168800	-0.36951200	-1.09374100
C	-1.37827700	2.26808200	-0.85404500	H	1.12317900	-1.33797800	-0.99028800
C	-0.80916900	3.52372900	-0.48581800	H	0.78390600	0.28523900	-1.01632200
O	0.37517800	3.87933300	-0.50578000	H	3.98697300	-1.86131600	-2.40036000
N	-1.80317600	4.38469600	0.04540600	H	5.76481400	1.78897100	0.52207400
H	-1.45287100	5.28359600	0.35702200	P	-0.20510300	-2.99581700	0.40620700
C	-3.10659300	4.02231200	0.32331500	O	0.28425900	-2.37913100	1.70377700
N	-3.89953700	4.96742600	0.90047000	O	0.53332600	-2.61879400	-0.86736200
H	-3.70860800	5.94687700	0.75305400	O	-1.76310900	-2.61589800	0.09308100
H	-4.87223400	4.71240100	0.99167100	C	-2.83801400	-2.93292200	0.98573300
N	-3.58145600	2.81254900	0.11073900	H	-2.54257500	-2.73683800	2.02225000
C	-2.67945800	1.97679300	-0.44783300	H	-3.10196000	-3.99076200	0.87637700
C	-3.62520400	-2.55234500	-0.61589500	C	-4.04540400	-2.07585400	0.62759500
H	-2.70242700	-2.56440400	-1.20212800	H	-4.91208000	-2.44998900	1.18807000
C	-4.46654800	-1.30941100	-0.98221800	O	-3.79883900	-0.70702100	1.02030900
H	-4.41386900	-1.04827100	-2.04481900	C	-4.16199500	0.20450100	0.01053600
O	-5.79387400	-1.62180700	-0.58153700	H	-4.79313400	0.99816000	0.42006400
H	-6.42141100	-1.06081600	-1.05304000	N	-2.94209200	0.89092200	-0.46622700
O	-4.27448400	-3.76847000	-0.85454100	C	-1.76324300	0.26886400	-0.82086600
O	1.16431300	-3.85480800	0.48825100	H	-1.70420500	-0.79262600	-1.00746600
H	-5.21349500	-3.61791100	-0.65853400	N	-0.73642200	1.08679500	-0.83217800
H	1.40998100	-3.92894400	-0.46473700	C	-1.25277600	2.31549100	-0.46687900
				C	-0.58479000	3.53933200	-0.18041800
				O	0.62802900	3.78529600	-0.17332700
GMPH-RCc				N	-1.51572100	4.54210600	0.18211100
C	5.41716800	0.99500000	-0.13032800	H	-1.09696100	5.43040500	0.43312800
C	4.80100400	1.31805400	-1.38791900	C	-2.87476100	4.35165800	0.33982200
C	4.31730800	0.29041300	-2.21152400				

N	-3.60251700	5.42196000	0.76231000	O	-0.19707800	-1.90089000	-1.86052800
H	-3.27629000	6.36047600	0.58940900	O	1.05214400	-2.86566100	0.20995600
H	-4.60324700	5.28872600	0.76011200	O	2.24241500	-1.38565200	-1.54685100
N	-3.46985300	3.19229800	0.15039600	C	3.64300500	-1.70232400	-1.47257300
C	-2.62215800	2.21297700	-0.23202000	H	4.08697200	-1.36367500	-2.41384700
C	-4.39553100	-2.03703200	-0.88158300	H	3.80811000	-2.78125200	-1.38070700
H	-3.48412900	-2.17818900	-1.46812000	C	4.32566600	-0.99322700	-0.30890800
C	-4.92294000	-0.59543500	-1.06702500	H	5.40778000	-1.15189900	-0.40911100
H	-4.75758700	-0.20420000	-2.07633400	O	4.07028400	0.42581000	-0.38551600
O	-6.30657300	-0.64160300	-0.73881800	C	3.54604500	0.91633100	0.81819300
H	-6.77449600	0.07014400	-1.19121600	H	4.00038500	1.88752800	1.02703000
O	-5.30287500	-3.02242500	-1.28793400	N	2.09459700	1.18910600	0.68447000
O	-0.28016200	-4.61205100	0.56068200	C	1.02537100	0.33156200	0.84003000
H	-6.18568500	-2.68295600	-1.06901200	H	1.12646000	-0.65833500	1.25299000
Ru	3.34760000	0.04530200	-0.15076500	N	-0.10673400	0.82457700	0.39309800
H	0.10689400	-4.87748800	1.40544900	C	0.23012800	2.07512000	-0.11322400
GMPH-TSc				C	-0.53739100	3.04003200	-0.82993400
C	-4.51025500	0.81395100	0.39530500	O	-1.72419800	2.99963300	-1.19373200
C	-3.58680200	1.73101900	0.99431600	N	0.24491400	4.16882800	-1.16093700
C	-2.86286400	1.32403400	2.12104800	H	-0.26550600	4.89349400	-1.65276800
C	-3.12465500	0.05264800	2.74299600	C	1.59090600	4.31974700	-0.89805000
C	-4.09416300	-0.81064000	2.22770200	N	2.17079600	5.49536500	-1.25856200
C	-4.75111600	-0.45746100	1.00187700	H	1.75737800	6.07853600	-1.96955400
H	-3.33297300	2.65171600	0.48262500	H	3.17736400	5.52058800	-1.18334500
H	-2.06007600	1.94453600	2.49885100	N	2.30729200	3.39876500	-0.29024200
H	-4.26003800	-1.78319100	2.67618500	C	1.59481500	2.31129900	0.06496400
H	-5.45283300	-1.14815900	0.54719200	C	3.88787300	-1.45409900	1.10529700
H	-1.15463400	-0.27034000	-1.62139200	H	2.88649700	-1.88922200	1.05718700
N	-2.10669900	0.12352900	-1.53112500	C	3.87698200	-0.12659000	1.90045800
H	-2.07868700	1.14197600	-1.66675500	H	3.16519100	-0.12510700	2.73445500
C	-2.98025800	-0.58240700	-2.50166900	O	5.20945700	0.06528100	2.35379700
H	-3.86998000	0.02497800	-2.68210300	H	5.22263300	0.69269500	3.08633900
H	-2.44686600	-0.69750900	-3.44900300	O	4.71868000	-2.43314300	1.66914000
C	-3.36670200	-1.96069700	-1.91106000	O	1.54402400	-3.80654200	-2.08297700
H	-4.43976100	-2.01221800	-1.71115200	H	5.49910000	-1.96782700	2.00955700
H	-3.10957800	-2.77137600	-2.59933300	Ru	-2.65304100	-0.29630300	0.48854400
N	-2.63209300	-2.13056800	-0.63347000	H	1.38153200	-3.69888700	-3.03058700
H	-2.95518700	-2.93391600	-0.09959100	GMPH-PCc			
H	-1.63064700	-2.27674500	-0.88428600	C	-4.14749700	-1.46365300	1.53726300
O	-0.99203300	-2.06956000	1.54814900	C	-3.89360900	-0.09783000	1.90043000
H	-0.20220400	-2.44436900	1.03691200	C	-2.63917000	0.26337200	2.41732300
H	-0.71010300	-2.03897000	2.46976300	C	-1.61609600	-0.72810800	2.57746800
H	-2.52376800	-0.25584400	3.59051200	C	-1.85991200	-2.06579100	2.23016400
H	-5.02584500	1.08494600	-0.51908000	C	-3.14004500	-2.43431400	1.69979500
P	1.07330000	-2.48706900	-1.25784400	H	-4.65532900	0.65741300	1.74122400

H	-2.42989700	1.30128300	2.64857900	C	0.40552700	2.59520100	-0.23206400
H	-1.04799700	-2.77747200	2.32684700	C	3.79689900	-0.26981800	1.06910400
H	-3.32772500	-3.45909000	1.39621400	H	3.01074300	-1.01485500	0.95052600
H	-3.36151000	0.90311400	-1.37991500	C	3.20228000	1.02928800	1.64453400
N	-3.36765800	-0.13245200	-1.38005500	H	2.40504500	0.83360700	2.36936400
H	-4.34188600	-0.42375100	-1.31688800	O	4.28810800	1.74244000	2.22323400
C	-2.75316200	-0.70773100	-2.60797200	H	3.96067200	2.35528100	2.89203000
H	-3.42563600	-0.61132500	-3.46663400	O	4.77826400	-0.84647100	1.89028500
H	-1.83821700	-0.14859800	-2.81926300	O	2.87649100	-3.66957100	-1.77320000
C	-2.41339500	-2.15585800	-2.31033000	H	5.29540300	-0.11031200	2.25403200
H	-3.32579600	-2.73991800	-2.14363300	Ru	-2.31355800	-0.77239700	0.37583600
H	-1.84567400	-2.60952100	-3.12821400	H	2.83564400	-3.86215400	-2.72058300
N	-1.58310900	-2.15761500	-1.07592800				
H	-1.56514300	-3.09785400	-0.68374800	GMPH-RCd			
H	-0.58709100	-2.03138300	-1.41858400	C	-4.90677400	1.37622200	0.20689800
O	1.22760100	-1.80761200	2.64067700	C	-3.87966200	2.06429800	0.93721300
H	1.40917900	-2.18484000	1.74883700	C	-3.30732500	1.44867200	2.06318100
H	1.97394000	-2.09300500	3.18226000	C	-3.75726000	0.15857000	2.50081500
H	-0.61493300	-0.47346300	2.90655200	C	-4.76418300	-0.50921900	1.78537700
H	-5.10805600	-1.74417700	1.11823800	C	-5.34589000	0.10249200	0.62259200
P	1.89775300	-2.42568500	-1.40449500	H	-3.48229700	3.00610100	0.57593100
O	0.71009800	-2.34487000	-2.34117300	H	-2.46983700	1.91808000	2.56553600
O	1.60621900	-2.49664800	0.08225600	H	-5.06987500	-1.50598100	2.08445400
O	2.77851200	-1.09197300	-1.74717400	H	-6.10437500	-0.42260400	0.05270500
C	4.15195100	-0.89032300	-1.41338500	H	-1.32579000	0.60286400	-1.58872200
H	4.64968900	-0.54981400	-2.32693900	N	-2.36544300	0.60089200	-1.61405900
H	4.63618100	-1.81604700	-1.08158200	H	-2.61935500	1.56159800	-1.84228700
C	4.29470300	0.16820000	-0.32447400	C	-2.85055700	-0.36749500	-2.63146800
H	5.34893300	0.46872000	-0.25765000	H	-3.92980600	-0.22782000	-2.75233700
O	3.50761800	1.32758000	-0.68581800	H	-2.37101200	-0.19129000	-3.60127600
C	2.71882800	1.76668500	0.37831300	C	-2.52261800	-1.76162500	-2.11873400
H	2.81514400	2.84994300	0.48433400	H	-3.00551800	-2.52671300	-2.73375200
N	1.26265300	1.57093000	0.10213100	H	-1.44355800	-1.95025000	-2.14220600
C	0.51995300	0.42161000	0.11770000	N	-2.96567500	-1.88532300	-0.68916000
H	0.93190100	-0.56010100	0.32732500	H	-3.84973600	-2.38512500	-0.62955200
N	-0.75751500	0.64549300	-0.16135900	H	-2.24765900	-2.43795200	-0.17705900
C	-0.85483600	2.01900700	-0.39667300	O	-1.08460400	-0.31936600	0.87241100
C	-1.94820200	2.86781400	-0.74845100	H	-0.47966700	0.09701500	0.22497300
O	-3.13842300	2.59330400	-0.95405200	H	-0.84106000	-1.34489900	0.86491200
N	-1.53397300	4.21203800	-0.86441600	H	-3.26792200	-0.32810300	3.33632700
H	-2.28647800	4.85092600	-1.09628000	H	-5.32177200	1.82161000	-0.69099700
C	-0.25120400	4.68006900	-0.67845900	Ru	-3.09904100	0.02467500	0.30668300
N	-0.04538500	6.01447300	-0.79880900	P	0.51506400	-3.21895400	-0.20081400
H	-0.70143800	6.60526000	-1.28520300	O	0.50103100	-2.87616300	-1.66552200
H	0.91799300	6.31568100	-0.78088100	O	-0.67009600	-2.74939600	0.66534700
N	0.75193200	3.89010900	-0.35752900	O	1.82184700	-2.58430400	0.55009700

C	3.13456000	-3.07048400	0.22570600	N	-2.71922100	0.22510100	-1.87857900
H	3.13819800	-3.57438000	-0.74645200	H	-3.27815600	1.02821500	-2.16081700
H	3.43982000	-3.78630800	0.99616900	C	-3.07804100	-1.00197500	-2.63730400
C	4.14703500	-1.93721000	0.19063400	H	-4.15998100	-1.14697100	-2.54833500
H	5.14876800	-2.38535300	0.16642200	H	-2.83455500	-0.89211700	-3.69987100
O	3.98514700	-1.15045900	-1.02012400	C	-2.30742200	-2.15294400	-2.01350600
C	4.06784300	0.21978000	-0.74902700	H	-2.65627400	-3.11349600	-2.40530400
H	4.72154500	0.70882400	-1.47844600	H	-1.23361300	-2.09278400	-2.21637700
N	2.70510100	0.80112300	-0.89498000	N	-2.47534000	-2.10379200	-0.52909700
C	1.59012300	0.09342100	-1.26791200	H	-3.28019500	-2.66466800	-0.25447600
H	1.61526300	-0.95426200	-1.53649400	H	-1.63109600	-2.56305500	-0.06613100
N	0.49568700	0.83374300	-1.23681500	O	-0.31122400	-0.87413700	1.87087900
C	0.91873300	2.09185800	-0.85173700	H	0.58066100	-0.56298800	1.67578900
C	0.15526900	3.27635000	-0.61450400	H	-0.27937200	-1.82809900	1.59823500
O	-1.06151400	3.45076900	-0.68803100	H	-1.89750500	0.21936500	3.18523700
N	1.01853900	4.33895600	-0.23225100	H	-5.46942500	0.76815700	-0.25900000
H	0.54155600	5.20739100	-0.01865000	Ru	-2.71469800	-0.11849900	0.23090800
C	2.38688200	4.24958300	-0.07522100	P	0.84019400	-3.39724200	-0.27117700
N	3.03392500	5.37198700	0.34679100	O	0.70864700	-2.85763900	-1.67255400
H	2.63315500	6.28221400	0.17875700	O	-0.35268200	-3.23991600	0.67602900
H	4.04179500	5.32048100	0.32337100	O	2.07158300	-2.66206600	0.52811500
N	3.07064600	3.13909600	-0.26651200	C	3.41386300	-2.82419100	0.04939200
C	2.29368000	2.09483300	-0.64110100	H	3.42613500	-3.29760800	-0.93692800
C	4.07269900	-0.92657400	1.35635000	H	3.95913500	-3.46293200	0.75238700
H	3.02867600	-0.79697700	1.65384400	C	4.12657300	-1.48724300	-0.03927100
C	4.59597800	0.36286200	0.69263000	H	5.18468000	-1.68038800	-0.26188200
H	4.25163800	1.27846200	1.18118600	O	3.56636700	-0.70128800	-1.12058300
O	6.01248800	0.25795800	0.70530500	C	3.49204500	0.65127200	-0.77671500
H	6.40383300	1.13196400	0.58770600	H	3.97125200	1.27248100	-1.54144100
O	4.79221600	-1.30567800	2.49664800	N	2.06047400	1.04685200	-0.73163400
O	0.69325700	-4.81844700	0.02244000	C	0.97324200	0.22885500	-0.92392500
H	5.72249200	-1.10033300	2.31111800	H	1.07735200	-0.82866000	-1.14575700
H	0.73552600	-5.26027900	-0.83684300	N	-0.16961800	0.89401900	-0.85831300
GMPH-TSd				C	0.19198800	2.21517100	-0.64248700
C	-4.72467500	0.67872000	0.52493800	C	-0.60281100	3.40130700	-0.55556200
C	-3.85178000	1.77427100	0.81864300	O	-1.82469500	3.53994100	-0.61147400
C	-2.83313100	1.58913700	1.76451500	N	0.22896700	4.54156300	-0.37834100
C	-2.73887700	0.37398800	2.52382700	H	-0.28330300	5.41150200	-0.28671900
C	-3.62897100	-0.67756800	2.28859000	C	1.60512900	4.53915900	-0.31007200
C	-4.60009800	-0.54679200	1.24226400	N	2.22009400	5.73355900	-0.09446600
H	-3.86960400	2.68212400	0.22911900	H	1.75424500	6.59933500	-0.31845200
H	-2.08678000	2.36250600	1.89309100	H	3.22518200	5.72839000	-0.18505700
H	-3.51627400	-1.61685700	2.81803300	N	2.32783600	3.44078500	-0.40243000
H	-5.25513400	-1.37707800	0.99939500	C	1.57888000	2.32579700	-0.56891700
H	-1.72904800	0.47909800	-2.00039100	C	4.03285700	-0.58624900	1.20933800
				H	3.04040400	-0.69824500	1.65612000

C	4.18018400	0.82017500	0.59533900
H	3.72600300	1.61228600	1.19846800
O	5.57493100	1.02264600	0.42608500
H	5.75286600	1.96327200	0.30520700
O	4.97316800	-0.87234200	2.20550000
O	1.31586900	-4.95259700	-0.30262600
H	5.80462500	-0.45943400	1.92262400
H	1.33978300	-5.26154600	-1.21854100
GMPH-PCd			
C	-4.12156700	-1.89703100	1.29806600
C	-3.90507500	-0.62942800	1.93474800
C	-2.64417300	-0.34705300	2.48652900
C	-1.58202000	-1.30881400	2.42311300
C	-1.80368900	-2.54866700	1.79738000
C	-3.09060200	-2.85493500	1.24173700
H	-4.69181600	0.11565600	1.95114300
H	-2.45446900	0.63022000	2.91622500
H	-0.97046700	-3.23155100	1.66921400
H	-3.25874100	-3.80392200	0.74417600
H	-3.34926700	0.79902000	-1.40484400
N	-3.38414200	-0.22946900	-1.46148300
H	-4.37416200	-0.45500600	-1.39330500
C	-2.83466500	-0.78230700	-2.74130800
H	-3.40748100	-1.68333700	-2.98411600
H	-2.97325700	-0.07136400	-3.56170900
C	-1.36451200	-1.13676200	-2.55139100
H	-0.97416700	-1.72444300	-3.38735700
H	-0.74661200	-0.24232200	-2.46868200
N	-1.24936100	-1.89100600	-1.28261400
H	-1.61477600	-2.83336900	-1.41640500
H	-0.26277900	-2.03418700	-0.95577600
O	1.49409700	-1.32846900	2.49036400
H	2.13692600	-1.77174600	3.05753200
H	1.45547200	-1.86872400	1.66292500
H	-0.57578800	-1.07907200	2.77054200
H	-5.08109200	-2.11160300	0.83859700
Ru	-2.31920600	-0.93638200	0.28182500
P	2.13910900	-2.71334900	-0.97410200
O	1.87716500	-2.26332800	-2.37650900
O	1.04272000	-2.44786300	0.07964400
O	3.50315000	-2.05800500	-0.34338600
C	4.32151300	-1.12958200	-1.05477800
H	4.08106600	-1.14514800	-2.12227300
H	5.36218600	-1.43650400	-0.90867500
C	4.17266900	0.28744500	-0.51809400

H	5.01055100	0.89021100	-0.89982700
O	2.92756400	0.84959800	-0.98989100
C	2.50243300	1.87239400	-0.12483200
H	2.64756700	2.87014300	-0.55483200
N	1.04064800	1.71848600	0.01932400
C	0.37139100	0.53044000	0.08910500
H	0.86261400	-0.43077800	0.19132300
N	-0.93903800	0.69318100	-0.02020900
C	-1.13807600	2.06570000	-0.17159800
C	-2.30473000	2.84135000	-0.43925300
O	-3.47012100	2.47040900	-0.62270200
N	-1.99073400	4.21697300	-0.52267700
H	-2.79600300	4.81099800	-0.68699000
C	-0.72442400	4.75867500	-0.45311100
N	-0.61162300	6.10451400	-0.54675200
H	-1.36234600	6.68040100	-0.89280100
H	0.32544300	6.47449200	-0.60238500
N	0.35643700	4.02470300	-0.27451900
C	0.09969400	2.70910000	-0.14465100
C	4.08607300	0.42600600	1.01496800
H	3.46435500	-0.38300800	1.40470200
C	3.32827400	1.76354700	1.18651500
H	2.69416300	1.77134100	2.07821100
O	4.30535200	2.79860600	1.22335900
H	4.01254300	3.50437000	1.81091900
O	5.31889400	0.39163500	1.67852800
O	2.42642500	-4.31168600	-0.85034600
H	5.67850700	1.29180500	1.62816200
H	2.95189300	-4.62082900	-1.60133700

Cartesian coordinates for the species involved in Fig. S2:

AMPH-RCa			
C	-2.20131600	2.01361000	1.19139600
C	-1.37617900	0.93115900	1.64395200
C	-1.93419000	-0.13148200	2.37846300
C	-3.33703800	-0.13022600	2.68050200
C	-4.15465500	0.91444300	2.21915100
C	-3.58163200	1.99150600	1.46015200
H	-0.32996500	0.90566100	1.36541200
H	-1.31949200	-0.98248700	2.64814300
H	-5.22193200	0.89450000	2.41123000
H	-4.21874900	2.78621100	1.08696000
H	-1.46267000	-0.90978600	-1.50524500
N	-1.93345800	0.00832300	-1.41236400
H	-1.15852700	0.69362200	-1.39652800

C	-2.80777800	0.24534000	-2.58497100	N	-0.35970100	4.45302900	-0.79029300
H	-2.98902200	1.32245300	-2.67428900	H	-0.83675500	4.03102400	-1.57627000
H	-2.32338500	-0.09157000	-3.50792300	H	-0.42419000	5.46417800	-0.76457100
C	-4.11222900	-0.49882200	-2.36386200	H	3.76851900	5.12814200	0.56631500
H	-4.83379000	-0.30658700	-3.16444200	H	0.09161900	-4.75424200	-1.70575600
H	-3.92294900	-1.57127600	-2.29811600				
N	-4.65871200	-0.08053000	-1.03589400	AMPH-TS1a			
H	-5.15456200	0.80575500	-1.11735100	C	-1.90863300	2.14745200	1.0452330
H	-5.33620600	-0.77161500	-0.71898500	C	-1.05055900	1.14678700	1.60305400
O	-3.07074000	-2.03338000	0.04170800	C	-1.60405500	0.12617500	2.38997500
H	-1.79927200	-2.54197000	0.39316500	C	-2.99834100	0.14710500	2.74038900
H	-3.66117000	-2.45799900	0.67899500	C	-3.83614000	1.15715400	2.25370600
H	-3.77321000	-0.96280700	3.22153000	C	-3.30033700	2.13565200	1.34997000
H	-1.76597900	2.81821800	0.60573200	H	-0.00924800	1.10824700	1.31026600
Ru	-3.04199000	0.02377800	0.41360600	H	-0.99847300	-0.72844900	2.66456000
P	0.19812100	-3.00032900	-0.45385000	H	-4.89656700	1.14761900	2.48103000
O	-0.12456800	-2.19165700	-1.67877400	H	-3.95156700	2.88621500	0.91474000
O	-0.83840200	-2.87101400	0.71325300	H	-1.36818500	-0.69128600	-1.62883200
O	1.56490800	-2.61720600	0.29399400	N	-1.80673500	0.24981400	-1.46253600
C	2.85404600	-3.14918500	-0.08484500	H	-1.00059800	0.90028100	-1.46968400
H	2.81259100	-3.59520500	-1.08148900	C	-2.73952000	0.55586100	-2.57106200
H	3.12205500	-3.92478700	0.63859700	H	-2.94089500	1.63290400	-2.58530800
C	3.90429500	-2.05778700	-0.04672200	H	-2.29665600	0.27976700	-3.53422100
H	4.88374700	-2.53736000	-0.18116600	C	-4.01300700	-0.22679400	-2.31393500
O	3.68577700	-1.12801100	-1.12967400	H	-4.80022100	0.00892400	-3.03656900
C	3.98972600	0.18576000	-0.72935000	H	-3.80903800	-1.29957100	-2.36195500
H	4.71549900	0.63343700	-1.41688000	N	-4.45760300	0.07071300	-0.91902000
N	2.74980400	0.98795800	-0.79988300	H	-5.07252000	0.88162000	-0.89462300
C	1.52127800	0.57092100	-1.24713800	H	-4.94905400	-0.74151100	-0.54284500
H	1.33780200	-0.45277600	-1.54309400	O	-3.87599900	-2.20929100	0.39090700
N	0.61280900	1.53231000	-1.25059000	H	-2.89490900	-2.44722500	0.38772300
C	1.29147400	2.65239600	-0.79456400	H	-4.22114100	-2.56234000	1.22089000
C	0.92209000	3.99106500	-0.56784100	H	-3.40967300	-0.66255600	3.33201200
N	1.83000700	4.84283300	-0.07659100	H	-1.49778900	2.90302900	0.38130700
C	3.07331700	4.39356500	0.16799000	Ru	-2.76690000	0.22056100	0.43681200
N	3.55830700	3.16239100	-0.02617000	P	-0.34881000	-2.71056700	-0.52437100
C	2.62562600	2.33334300	-0.50746300	O	-0.39219100	-2.07826300	-1.90122800
C	3.94052800	-1.19665000	1.23366800	O	-1.36573600	-2.18448400	0.49284200
H	2.91691200	-1.01683300	1.57488600	O	1.08570300	-2.51029800	0.20865100
C	4.55386800	0.11422900	0.70604200	C	2.24517300	-3.27467800	-0.17106400
H	4.29084400	0.99377100	1.29888100	H	2.14747200	-3.65751300	-1.19147600
O	5.95754400	-0.09832600	0.67683200	H	2.34034200	-4.12174400	0.51562400
H	6.41005500	0.75442800	0.66362800	C	3.49617400	-2.42076400	-0.07588900
O	4.65011200	-1.77272200	2.29374800	H	4.36436800	-3.08721900	-0.16451600
O	0.40659700	-4.56221900	-0.81132000	O	3.53193400	-1.47660100	-1.17256200
H	5.58731000	-1.58245000	2.12469700	C	3.98688200	-0.22094100	-0.74292600

H	4.78415800	0.13598500	-1.40342800	N	-4.11156700	0.79160600	-0.35082800
N	2.85870200	0.73682400	-0.83836000	H	-4.62400200	1.59856600	-0.00035000
C	1.62510800	0.48414400	-1.38367500	H	-4.63407800	-0.06407500	-0.08295500
H	1.35214000	-0.49816800	-1.74473600	O	-5.01672300	-1.79561100	0.00453800
N	0.82772100	1.53990000	-1.38456100	H	-4.07971600	-2.04086600	0.12600400
C	1.59179400	2.55129100	-0.82407900	H	-5.54421400	-2.38130800	0.55934200
C	1.34948000	3.90792300	-0.54248200	H	-2.66617600	-0.48084100	3.35633500
N	2.30437000	4.62932600	0.05562900	H	-0.41234100	3.13750300	0.72280100
C	3.47445800	4.03431200	0.34907500	Ru	-2.15827900	0.68159300	0.56090800
N	3.84028100	2.77029800	0.11117500	P	-1.33946300	-2.20654900	-0.83147600
C	2.86200800	2.07151300	-0.47551500	O	-0.98029600	-1.61020000	-2.16519300
C	3.63901100	-1.57192700	1.20659100	O	-2.31934900	-1.38680100	0.05147500
H	2.64996600	-1.21993000	1.51236800	O	-0.06567800	-2.48781800	0.12712100
C	4.48452200	-0.38506500	0.70727800	C	0.87024100	-3.54753200	-0.19050100
H	4.35933600	0.52610300	1.29740300	H	0.68269300	-3.94239200	-1.19257500
O	5.83106000	-0.83683800	0.71670200	H	0.71543400	-4.34814100	0.53850700
H	6.42476600	-0.07583300	0.73180300	C	2.30832600	-3.07778200	-0.09467500
O	4.20292700	-2.25441100	2.29148300	H	2.94201900	-3.97472100	-0.13934900
O	-0.48207800	-4.32452000	-0.65372500	O	2.63805700	-2.22039800	-1.20803200
H	5.16335600	-2.23708900	2.14918700	C	3.53304600	-1.20758800	-0.80911000
N	0.13804900	4.51278200	-0.81926300	H	4.41390300	-1.20838500	-1.45989100
H	-0.30928700	4.19481600	-1.66972200	N	2.84583900	0.09369800	-0.95775200
H	0.17592700	5.52220100	-0.73312700	C	1.63545800	0.30870100	-1.57480900
H	4.21413300	4.66661500	0.8334410	H	1.05819700	-0.51104800	-1.98208300
H	-0.61697200	-4.57121400	-1.57936600	N	1.26720100	1.57764000	-1.57470400
AMPH-IM1a				C	2.30765500	2.23923200	-0.94219500
C	-0.88921200	2.37453000	1.3304840	C	2.53312100	3.58843100	-0.60180000
C	-0.18885400	1.15821800	1.61045900	N	3.65795500	3.91367400	0.04983200
C	-0.83933400	0.13694600	2.32905200	C	4.53305000	2.94059000	0.35367200
C	-2.16456400	0.32504700	2.83478500	N	4.44051800	1.63199300	0.09130700
C	-2.83918400	1.52990700	2.56534300	C	3.30677800	1.33624800	-0.55630800
C	-2.20382700	2.57000000	1.81111900	C	2.68516500	-2.26827900	1.16164500
H	0.80284100	1.00235400	1.20736900	H	1.87429800	-1.56991300	1.39014900
H	-0.36040000	-0.82893400	2.44259200	C	3.91316400	-1.48754500	0.66083100
H	-3.86565300	1.65562400	2.89471100	H	4.11684100	-0.57115200	1.21908600
H	-2.73479400	3.48918300	1.59107300	O	5.00034300	-2.39829000	0.73259100
H	-1.42878000	0.10824900	-1.88838000	H	5.83092100	-1.90605500	0.74171500
N	-1.64150600	1.04036300	-1.48342400	O	2.92102800	-3.04111000	2.30406400
H	-0.76686400	1.57642600	-1.58235200	O	-2.01238400	-3.67091900	-0.98836800
C	-2.77911000	1.64329700	-2.21623500	H	3.83248100	-3.36695500	2.22308300
H	-2.87837000	2.69282300	-1.91845800	N	1.61525200	4.57460700	-0.86260600
H	-2.60917000	1.61152700	-3.29851900	H	1.02927800	4.43684400	-1.67438900
C	-4.01999800	0.85136300	-1.83881300	H	1.97158600	5.51472100	-0.74365600
H	-4.92761700	1.28517100	-2.26991500	H	5.42926000	3.26268900	0.8780410
H	-3.93314500	-0.17718200	-2.19624400	H	-2.22557100	-3.85016600	-1.91553300

AMPH-IM2a				N	4.92197900	2.01959900	-0.29620900
C	-4.67135500	1.84438200	0.47466900	C	3.65872200	1.66901200	-0.03930700
C	-4.16402200	1.25452900	1.68115400	C	3.32515400	-2.68075600	0.67366500
C	-4.04853600	-0.14129800	1.77748200	H	2.59070700	-2.24617400	1.35863800
C	-4.45990800	-0.97813300	0.68558400	C	4.41759500	-1.64250900	0.35656900
C	-4.98199900	-0.40016500	-0.48348900	H	4.72214500	-1.04812900	1.22461300
C	-5.08596300	1.02648300	-0.59590900	O	5.49922900	-2.38559300	-0.18324800
H	-3.82119000	1.88632600	2.49289500	H	6.29725400	-1.84207200	-0.18903400
H	-3.56729000	-0.59203300	2.63907100	O	3.80146100	-3.86123800	1.25502500
H	-5.25106900	-1.03228100	-1.32281300	O	-1.98154900	-3.07622400	0.69034900
H	-5.46021900	1.47630900	-1.50901100	H	4.66993500	-4.02967500	0.85471900
H	-0.58326800	1.81608400	0.27157700	N	2.10707300	4.77729400	1.12022700
N	-1.46459800	2.10025000	-0.19347700	H	1.30766100	4.45462100	1.64326200
H	-1.77560200	2.93971000	0.29199100	H	2.52329000	5.64696300	1.42424100
C	-1.13893900	2.44056700	-1.60968800	H	6.12763100	3.69387100	-0.24736700
H	-1.94818000	3.05894800	-2.01129900	O	-1.50388600	-1.65427300	2.96269200
H	-0.20693900	3.01269500	-1.65880900	H	-0.79147100	-1.87409300	3.57696000
C	-1.01891900	1.13748300	-2.38110500	H	-1.12999800	-1.03997800	2.30221400
H	-0.88408800	1.32177900	-3.45156700	H	-1.85032200	-2.83971000	1.64046100
H	-0.15915300	0.56605800	-2.02606100	AMPH-TS2a			
N	-2.23231800	0.31215800	-2.13148000	C	4.58432800	0.23670800	0.0641070
H	-2.96324800	0.53425000	-2.80398200	C	4.08689400	0.74475500	-1.18051500
H	-1.99300500	-0.70091100	-2.21550600	C	3.28389700	-0.08102500	-1.97913900
H	-4.29682900	-2.04821300	0.73631000	C	3.05159600	-1.45181000	-1.61937800
H	-4.72313900	2.92375600	0.37833700	C	3.59708400	-1.97813300	-0.44372400
Ru	-2.93018200	0.52472300	-0.11432500	C	4.33087700	-1.11667000	0.43374600
P	-1.09890500	-2.10436900	-0.23878900	H	4.24956700	1.78326700	-1.44506200
O	-1.44920300	-2.26770600	-1.68570000	H	2.79471600	0.32148800	-2.85832700
O	-1.21117200	-0.64732800	0.35343600	H	3.36947000	-2.99701300	-0.15247700
O	0.44524400	-2.44666800	0.10937100	H	4.70689900	-1.49237800	1.37967100
C	1.23399600	-3.34154800	-0.71068200	H	1.25257400	2.15713400	0.85619800
H	0.82716600	-3.35785900	-1.72486800	N	2.07071800	1.73805000	1.30137700
H	1.18972900	-4.34768000	-0.28122800	H	2.81740200	2.42362300	1.20085500
C	2.67551200	-2.87115400	-0.71459700	C	1.77558500	1.46816100	2.73913000
H	3.26342800	-3.60464000	-1.28394500	H	2.72786700	1.31183600	3.25548300
O	2.76372200	-1.58255800	-1.35418200	H	1.27229400	2.32347400	3.20164900
C	3.74383300	-0.77782600	-0.73132700	C	0.92711700	0.21030500	2.78712100
H	4.47952300	-0.42231400	-1.45987200	H	0.76168800	-0.12119300	3.81735100
N	3.08653000	0.41913400	-0.18653900	H	-0.05608300	0.37424000	2.33577900
C	1.77273500	0.54867600	0.18475100	N	1.61161800	-0.84115900	1.99673600
H	1.09093300	-0.28533600	0.14561500	H	2.35834300	-1.24670800	2.56061800
N	1.44740500	1.77259500	0.55828300	H	0.90120900	-1.64372400	1.82841600
C	2.62856100	2.49544100	0.42859800	H	2.39556200	-2.07109100	-2.22143900
C	2.98989500	3.83862300	0.66890600	H	5.15212200	0.87946100	0.7286310
N	4.24931900	4.22460500	0.41033400	Ru	2.43111000	-0.07834600	0.17623100
C	5.12509100	3.31998100	-0.05416000				

P	-0.45892700	-2.87040100	0.2524910	C	3.02505600	-2.65816800	-0.62022400
O	-0.19783100	-2.69630400	1.73542500	H	4.57470000	0.07267600	-2.01929900
O	0.30129500	-1.92657200	-0.69151100	H	2.25486300	0.45903200	-2.86719000
O	-2.03327600	-2.60412600	-0.08649500	H	0.87975400	-3.09250500	-0.82236500
C	-3.06906400	-2.56722300	0.90435600	H	3.23129000	-3.50778400	0.02232600
H	-2.63793700	-2.65342900	1.90540300	H	3.19333300	1.57655300	1.37986900
H	-3.75070400	-3.40584800	0.72716100	N	3.47968500	0.60123100	1.48524100
C	-3.85481400	-1.27256200	0.77379100	H	4.47878200	0.59325500	1.28819200
H	-4.72726700	-1.32535000	1.43944900	C	3.24306000	0.12592900	2.88604900
O	-3.02146300	-0.15748800	1.17162600	H	3.93046800	-0.70575200	3.06954900
C	-3.31325700	0.99064300	0.40794400	H	3.46905600	0.91562700	3.60948800
H	-3.64149800	1.82123700	1.04223100	C	1.80110800	-0.34615800	3.00367200
N	-2.05511400	1.44976000	-0.21476100	H	1.62554600	-0.82053600	3.97506800
C	-1.01245000	0.65820700	-0.62250600	H	1.11029400	0.49466100	2.91388500
H	-1.06410700	-0.41984900	-0.66123500	N	1.52867700	-1.28876300	1.89365900
N	0.08460200	1.33666700	-0.92133700	H	1.98031500	-2.17922500	2.10138600
C	-0.27124400	2.66920100	-0.70809600	H	0.49204400	-1.53335300	1.79069500
C	0.40049600	3.89950800	-0.85193400	H	0.38567000	-1.12576600	-2.17071400
N	-0.22951800	5.02968800	-0.50737700	H	5.05030500	-1.90066700	-0.53358400
C	-1.49388200	4.95586100	-0.05775700	Ru	2.32962700	-0.56965500	0.04999200
N	-2.25362100	3.86390000	0.08627500	P	-1.73377000	-2.35947200	0.25367700
C	-1.59736500	2.75358800	-0.25198200	O	-1.01819300	-1.94715200	1.53812200
C	-4.32261400	-0.92588600	-0.65637400	O	-1.38348700	-1.58128700	-1.01562900
H	-3.53927600	-1.21689900	-1.36213500	O	-3.34302300	-2.27215200	0.47567200
C	-4.42819600	0.61121800	-0.59354600	C	-3.98950600	-1.39796000	1.40454600
H	-4.29585500	1.09706700	-1.56631600	H	-3.51356000	-1.46916300	2.38800000
O	-5.70405800	0.88628500	-0.03367600	H	-5.01190800	-1.77589900	1.47743600
H	-5.96299300	1.79424000	-0.23382700	C	-4.06244000	0.07593500	0.99646100
O	-5.50487900	-1.56117400	-1.05085100	H	-4.94578000	0.51111600	1.48450000
O	-0.17306800	-4.38889800	-0.19301100	O	-2.88952600	0.78454600	1.48274000
H	-6.23286000	-1.04472800	-0.66937900	C	-2.62322300	1.90324700	0.68174200
N	1.71282500	3.98310700	-1.27563400	H	-2.76539200	2.84239700	1.22957700
H	1.97064200	3.30634700	-1.98226000	N	-1.18268000	1.84336300	0.32847900
H	1.98626700	4.93244600	-1.50460200	C	-0.38044600	0.77483900	0.52739400
H	-1.95454800	5.90300100	0.21056000	H	-0.75245400	-0.15442500	0.94136700
O	0.78298200	-3.57222800	-2.69315900	N	0.88719000	1.01799500	0.19680000
H	0.21272300	-3.66309700	-3.46693700	C	0.90972900	2.34791200	-0.23802700
H	0.46100100	-2.79119300	-2.18059500	C	1.90187200	3.26449800	-0.63497200
H	0.14974200	-4.41826900	-1.12161900	N	1.54753900	4.52324500	-0.91413500
				C	0.25833700	4.88260800	-0.80360900
AMPH-PCa				N	-0.77114300	4.11662900	-0.43049000
C	4.05145800	-1.74925800	-0.9288410	C	-0.39164100	2.87036300	-0.15053800
C	3.77562700	-0.61763400	-1.76824500	C	-4.09998600	0.39804800	-0.51229000
C	2.47517400	-0.41213500	-2.25967900	H	-3.39302700	-0.25711300	-1.02769300
C	1.42124700	-1.31756700	-1.91263800	C	-3.57446900	1.85270200	-0.54054800
C	1.69520000	-2.43613100	-1.10702300	H	-3.06357900	2.10546800	-1.47550600

O	-4.69793600	2.68924400	-0.31316400	H	-3.95956700	-3.12848800	1.47750500
H	-4.50274900	3.58533900	-0.61442200	C	-3.72592600	-1.02640500	1.14720300
O	-5.35592200	0.24541100	-1.11094400	H	-4.18507200	-0.81796200	2.12282700
O	-1.46994000	-3.92528700	-0.00510900	O	-2.65051200	-0.08723400	0.90863600
H	-5.85529100	1.05379900	-0.91375600	C	-3.14712200	0.93736500	0.04747600
N	3.24954000	2.95227900	-0.67587400	H	-3.72073000	1.67804700	0.61539700
H	3.47251000	2.03056900	-1.02810800	N	-2.03608800	1.64299600	-0.55502900
H	3.80233300	3.69624100	-1.08829600	C	-1.30542100	1.32778300	-1.68809200
H	0.03232800	5.91733600	-1.04615500	H	-1.55056100	0.47423900	-2.30088300
O	-1.67073100	-3.71958800	-2.67596600	N	-0.26879800	2.11010300	-1.88544700
H	-2.54030400	-3.88112100	-3.06396100	C	-0.30115000	2.99495900	-0.81549800
H	-1.68083700	-2.78582400	-2.36646300	C	0.53544100	4.05816500	-0.41762700
H	-1.59430800	-4.12616100	-0.96952200	N	1.66167600	4.40823400	-1.11849100
AMPH-RCb				H	2.04786100	5.30902000	-0.86505400
C	3.49405700	1.12104700	-1.02203500	H	1.65219700	4.20511000	-2.10909600
C	2.62449400	0.31598800	-1.81714300	N	0.25512000	4.71132300	0.71956800
C	2.87841100	-1.06429200	-2.00090300	C	-0.82441500	4.33688300	1.42909600
C	4.01434700	-1.65099100	-1.36496600	H	-1.00899400	4.90622100	2.33685900
C	4.87913200	-0.87874900	-0.56044700	N	-1.69387500	3.35613300	1.16098400
C	4.58641600	0.50837700	-0.36460900	C	-1.38636700	2.72178400	0.02636100
H	1.72084400	0.76298200	-2.22501200	C	-4.79586900	-0.76268000	0.06526000
H	2.18069900	-1.67389400	-2.56151000	H	-5.11528400	-1.68639900	-0.43534900
H	5.72306000	-1.33881200	-0.06032400	C	-4.07991800	0.18573400	-0.91586400
H	5.21130300	1.09787700	0.29862900	H	-3.48703200	-0.40879700	-1.62017900
H	0.10112800	-0.50420300	0.12214900	O	-5.87935700	-0.10343900	0.68617200
N	0.76652800	0.05458100	0.68831800	O	-1.06154700	-3.98447700	-1.61646100
H	0.68017000	1.01740600	0.36424100	O	1.99685700	-2.43964800	1.01451700
C	0.47864000	-0.01092500	2.14207500	H	2.53647400	-3.17492100	0.69662600
H	-0.39070900	0.60327500	2.39337500	H	0.65971100	-2.86024500	0.82904800
H	0.24307800	-1.04845000	2.38654600	O	-5.03197100	1.00728900	-1.55460300
C	1.72538600	0.44415700	2.88540700	H	-4.71366300	1.27288700	-2.42486900
H	1.93158300	1.50082400	2.68795100	H	-6.38785400	0.33163200	-0.01557300
H	1.61262000	0.31428400	3.96708400	H	-1.48066800	-4.80284200	-1.31329300
N	2.87632600	-0.34960500	2.36519300	AMPH-TS1b			
H	3.75916400	0.00962500	2.72181300	C	2.94612500	1.84773900	-0.79508000
H	2.77972000	-1.32895600	2.64944600	C	2.34258000	1.06312200	-1.83162200
H	3.27191100	2.17266200	-0.87017400	C	2.87897700	-0.19562500	-2.13176600
H	4.18620800	-2.71839300	-1.46119500	C	4.08766200	-0.64745400	-1.49678900
Ru	2.72877200	-0.64171500	0.22282900	C	4.74079500	0.15857400	-0.55377000
P	-1.13784000	-2.79895700	-0.53496700	C	4.14059400	1.39959600	-0.15701700
O	-0.34688800	-3.20019000	0.76375000	H	1.38882300	1.38074000	-2.24348700
O	-0.68671700	-1.52249600	-1.17451100	H	2.33132100	-0.87288900	-2.77559600
O	-2.68791900	-2.88368600	-0.09614200	H	5.63228600	-0.20022800	-0.05109300
C	-3.16327900	-2.43533600	1.19230100	H	4.59369700	1.99834400	0.62584700
H	-2.35891200	-2.50640800	1.92854900	H	0.07650700	-0.08182800	0.37640300

N	0.69749900	0.43309600	1.02124200	O	2.82879800	-2.73768500	0.99551700
H	0.47692400	1.42727000	0.99366300	H	3.48296700	-3.35171500	0.64081600
C	0.56476800	-0.12721000	2.38921100	H	1.92011000	-3.18620800	0.86187700
H	-0.28817400	0.31268500	2.91369400	O	-5.22507300	-0.01572000	-1.41790600
H	0.37837600	-1.19918800	2.27791700	H	-4.98654200	0.62457300	-2.09921900
C	1.87435900	0.10591400	3.12216800	H	-6.26594600	-1.07996500	0.15138400
H	2.04288200	1.17476900	3.28870600	H	-0.10683200	-4.50675300	-2.05187200
H	1.88336300	-0.39686100	4.09502500				
N	2.96041000	-0.40677700	2.24401100	AMPH-IM1b			
H	3.86769000	-0.06701000	2.55540000	C	3.78058900	1.78670800	-0.02608600
H	2.99270000	-1.44059300	2.22359100	C	2.85518100	1.78251100	-1.12347100
H	2.48432800	2.78377900	-0.49372100	C	2.72379000	0.62416100	-1.90658500
H	4.45847400	-1.64362500	-1.70743500	C	3.51429100	-0.54104300	-1.62850700
Ru	2.57452600	-0.09180700	0.13238900	C	4.44031600	-0.51513300	-0.56954000
P	-0.05401700	-2.88499600	-0.60730100	C	4.58645800	0.65938700	0.23916600
O	0.52110400	-3.69328300	0.54049900	H	2.21547900	2.63974500	-1.30571000
O	0.45782600	-1.45504100	-0.76502700	H	1.95879400	0.56522600	-2.67171600
O	-1.68598900	-2.90890600	-0.50864200	H	5.00562100	-1.40975200	-0.33073100
C	-2.31533600	-3.02653400	0.77857800	H	5.28038900	0.66873100	1.07209800
H	-1.55942100	-3.05295600	1.56711700	H	0.25521500	1.24904000	1.18156900
H	-2.86110200	-3.97634900	0.81146700	N	1.07451600	0.95445400	1.71212100
C	-3.28983600	-1.88485100	1.01232700	H	1.47251300	1.78626200	2.14459700
H	-3.71732000	-2.00068800	2.01624900	C	0.65457700	-0.03901200	2.74648000
O	-2.57203400	-0.62612000	0.93920800	H	0.23361000	0.46526700	3.62246200
C	-3.31382800	0.28445500	0.13410900	H	-0.12003500	-0.65481900	2.28917400
H	-4.02992500	0.85521400	0.73479100	C	1.86651800	-0.87199100	3.13132000
N	-2.40297700	1.25082600	-0.44977300	H	2.60004500	-0.25636300	3.66306900
C	-1.50949000	1.06651300	-1.48981200	H	1.57417000	-1.69165100	3.79682200
H	-1.46747400	0.14067800	-2.04446800	N	2.51109600	-1.39131500	1.89556900
N	-0.70316900	2.08589400	-1.68129800	H	3.46938700	-1.66685000	2.10008900
C	-1.06551200	2.99818800	-0.70039000	H	2.06032900	-2.25298000	1.53434100
C	-0.57206600	4.26750600	-0.33331000	H	3.85295300	2.66010300	0.61371700
N	0.49519100	4.85214700	-0.96788400	H	3.32052100	-1.45830000	-2.17280200
H	0.62098300	5.83300700	-0.75065200	Ru	2.40817700	0.01805000	0.28422000
H	0.62589700	4.60744500	-1.94017900	P	0.22761900	-1.76181000	-1.32823100
N	-1.12212600	4.89607800	0.71482200	O	1.26051400	-2.74755200	-1.78670800
C	-2.13249100	4.29618800	1.36986800	O	0.58081300	-0.96635100	-0.02600800
H	-2.54650700	4.85535300	2.20527300	O	-1.23673100	-2.40032400	-1.04421500
N	-2.68689900	3.10408500	1.12531600	C	-1.59622100	-3.03853900	0.18641400
C	-2.11470600	2.49946300	0.08153000	H	-0.77478700	-2.99577300	0.90727400
C	-4.46576600	-1.78060100	0.02202500	H	-1.82075300	-4.08959800	-0.02665700
H	-4.60225200	-2.70259800	-0.55924500	C	-2.83440500	-2.36380600	0.74969600
C	-4.06438500	-0.60226100	-0.87597500	H	-3.19962000	-2.94073200	1.60814700
H	-3.37546800	-0.96336600	-1.64954700	O	-2.48454600	-1.02567400	1.19111700
O	-5.62145900	-1.45769400	0.76919100	C	-3.44597300	-0.11030100	0.69407100
O	0.17439900	-3.58059800	-2.05272400	H	-4.31581300	-0.05185600	1.36162000

N	-2.87822400	1.22495900	0.66701700	H	3.81297000	-0.88346700	2.89358600
C	-3.04949500	2.12185600	1.71303600	H	2.77454200	-2.28826100	3.19070000
H	-3.68254500	1.86550300	2.55286700	N	2.85536100	-1.60685100	1.16487100
N	-2.40028800	3.24726300	1.57188700	H	3.68529100	-2.10117600	0.82636600
C	-1.75729400	3.10255300	0.35840500	H	2.08193800	-2.23571200	0.90178200
C	-0.92584500	3.99025400	-0.35954700	H	4.33192700	2.49430100	0.63412000
N	-0.57773400	5.20146200	0.12710600	H	2.37289800	-0.46272200	-2.87931600
H	-0.14296400	5.85596600	-0.50674900	Ru	2.46154400	0.18941100	0.06498800
H	-1.08119400	5.56450500	0.92318700	P	0.15887300	-1.90796400	-0.80288500
N	-0.43875200	3.59750400	-1.55413900	O	0.97487900	-3.12078500	-0.42425400
C	-0.78192000	2.38764500	-2.00749400	O	0.48335000	-0.60571200	-0.03668300
H	-0.37910300	2.12014300	-2.98195900	O	-1.42964600	-2.16892100	-0.68682600
N	-1.54621200	1.45301000	-1.42173600	C	-2.03153700	-3.06444000	0.27189100
C	-2.02645100	1.85642200	-0.22733100	H	-1.39936500	-3.16650800	1.15837900
C	-3.99409300	-2.19841200	-0.25301100	H	-2.13799000	-4.05056500	-0.19209300
H	-3.88027700	-2.85558000	-1.12565400	C	-3.39689800	-2.52526400	0.67560000
C	-3.91491500	-0.70378800	-0.63883300	H	-3.90424300	-3.29109000	1.27223900
H	-3.16539800	-0.53981400	-1.41536200	O	-3.23175900	-1.35249600	1.51126000
O	-5.20393600	-2.44231000	0.43573200	C	-3.73951300	-0.21002300	0.86406300
O	-0.15050500	-0.72693500	-2.49363800	H	-4.67131400	0.12225800	1.33684500
O	2.08409100	-3.79361800	0.57196100	N	-2.73438500	0.85872600	0.99667500
H	1.83713100	-4.71879300	0.68132300	C	-1.72627400	0.90466700	1.92079000
H	1.85839600	-3.55141700	-0.35987000	H	-1.63537700	0.13090600	2.66737700
O	-5.17877600	-0.16428800	-0.98177600	N	-0.91725400	1.93728800	1.78028000
H	-5.25824100	-0.13043600	-1.94312300	C	-1.43474100	2.62180900	0.69150500
H	-5.88798700	-1.92768900	-0.02299500	C	-1.05572000	3.79536400	0.01328900
H	-0.80875600	-0.06693500	-2.15682300	N	0.04947400	4.53511000	0.36683000
AMPH-IM2b				H	0.06264500	5.46156800	-0.04290800
C	3.93432500	1.87797500	-0.16577000	H	0.29964500	4.50577000	1.34640600
C	2.73262400	2.27856200	-0.84374100	N	-1.76941700	4.19289800	-1.05028100
C	2.19554500	1.44063500	-1.83298600	C	-2.83341100	3.46801200	-1.42491300
C	2.84923000	0.21072200	-2.17917200	H	-3.37898300	3.83854700	-2.28872700
C	4.03504100	-0.17037600	-1.52690300	N	-3.30663600	2.35044700	-0.86022900
C	4.58814200	0.67467900	-0.50795900	C	-2.56827000	1.96586100	0.19155800
H	2.19900300	3.17516500	-0.54318400	C	-4.31497800	-2.08963200	-0.47586200
H	1.24014300	1.68104200	-2.28452600	H	-4.09972200	-2.63525800	-1.40568200
H	4.45772200	-1.15132500	-1.71708100	C	-4.00040700	-0.59256100	-0.61274700
H	5.48202300	0.37157900	0.02567500	H	-3.07538700	-0.46311600	-1.18373900
H	0.87457600	1.23828000	1.96075100	O	-5.65047800	-2.27188100	-0.05681000
N	1.79563900	0.76534500	2.03653400	O	0.26448700	-1.52260800	-2.37789000
H	2.44130000	1.44054700	2.44251500	O	3.75473200	-3.29231000	-0.92222200
C	1.69445200	-0.42534800	2.92399400	H	4.11021300	-4.17649700	-1.07249800
H	1.67256500	-0.13485100	3.97946700	H	2.78044400	-3.39538100	-0.91572700
H	0.75354600	-0.92463300	2.68202500	O	-5.08405000	0.08279800	-1.19090700
C	2.86176300	-1.35431400	2.62388900	H	-4.78996200	1.00540700	-1.32135100
				H	-6.18424300	-1.62897000	-0.55015800

H	-0.04567700	-2.24384700	-2.94471800	N	1.41571200	4.24452000	-0.03460200
				H	1.51914700	5.21505900	-0.30908300
AMPH-TS2b				H	1.86370200	4.01966800	0.84309900
C	4.35177400	0.71662400	-0.67681000	N	-0.71728700	4.53981200	-0.90792400
C	3.45151800	1.74557600	-1.10258500	C	-1.98700800	4.14367700	-1.05736100
C	2.27846500	1.37828500	-1.77573800	H	-2.61811400	4.78018900	-1.67129900
C	2.01921400	0.00890300	-2.12111000	N	-2.56986100	3.06462600	-0.52015300
C	2.95046400	-0.98922500	-1.79430200	C	-1.71064700	2.32651800	0.19115400
C	4.11354000	-0.64260900	-1.03466300	C	-4.77839700	-1.02981100	-0.04023900
H	3.60745600	2.77936700	-0.82112500	H	-4.98854900	-1.61698600	-0.94433700
H	1.52872700	2.13198800	-1.98318900	C	-3.95889700	0.23105900	-0.36414900
H	2.73138400	-2.03923700	-1.96389800	H	-3.19203200	-0.00532100	-1.11201900
H	4.79566700	-1.41939200	-0.70815300	O	-5.96112100	-0.67059500	0.64441100
H	2.14455700	1.50616400	2.26993600	O	-0.61089000	-1.75953900	-2.48507200
N	2.78058800	0.71082000	2.18903200	O	2.46208600	-3.82336200	-0.63085200
H	3.73519600	1.02021400	2.35983300	H	2.79520700	-4.72742000	-0.58143400
C	2.37449700	-0.34251400	3.17123800	H	1.46964000	-3.90203900	-0.76245700
H	2.87520400	-0.19620200	4.13301800	O	-4.82151500	1.26141000	-0.76859500
H	1.29954100	-0.23159900	3.33453600	H	-4.28853900	2.07540700	-0.85553300
C	2.67943900	-1.70710800	2.57465800	H	-6.30030200	0.12400700	0.20210000
H	3.76098400	-1.87486800	2.53117900	H	-0.90283600	-2.40049300	-3.14925800
H	2.24375600	-2.50417100	3.18810900				
N	2.14597100	-1.73397300	1.19940600	AMPH-PCb			
H	2.47494200	-2.55716800	0.65622500	C	4.55410500	-0.05881700	-0.65692000
H	1.11064600	-1.79153100	1.12346900	C	3.91086500	1.08942600	-1.20351500
H	5.22601100	0.97022200	-0.08554700	C	2.67116800	0.92930100	-1.86015300
H	1.06574300	-0.27800200	-2.55207900	C	2.08102000	-0.35697700	-2.02456200
Ru	2.41846600	0.08569000	0.13587800	C	2.75561000	-1.49073900	-1.52110300
P	-0.73139400	-2.38903300	-0.97742600	C	4.00065500	-1.34979800	-0.83731800
O	-0.16315200	-3.78558500	-0.91045900	H	4.33955700	2.07613200	-1.08717100
O	-0.15092000	-1.33536000	-0.04373000	H	2.13978500	1.81101900	-2.19711300
O	-2.35967000	-2.40359000	-0.86097500	H	2.28137000	-2.46917500	-1.54933700
C	-3.00132400	-2.87397800	0.33261500	H	4.49216200	-2.22183800	-0.42185800
H	-2.27044400	-3.21398900	1.07360600	H	3.11050500	1.22352800	2.53439200
H	-3.62862400	-3.72995500	0.06109400	N	3.00883900	0.23710500	2.30416500
C	-3.87695500	-1.78914600	0.94360200	H	3.91488700	-0.19476000	2.48212000
H	-4.50127500	-2.24235600	1.72117700	C	1.97079600	-0.37162300	3.19199400
O	-3.04835800	-0.77525200	1.58432100	H	2.33061100	-0.44319000	4.22390900
C	-3.27721300	0.47714100	1.00193900	H	1.11292400	0.30105800	3.17936000
H	-3.92413500	1.10400000	1.62968600	C	1.60722900	-1.74613200	2.64199100
N	-1.97130100	1.16136000	0.88301400	H	2.40899200	-2.45748400	2.86723600
C	-0.79053200	0.75804300	1.41617400	H	0.69999800	-2.12191600	3.12672800
H	-0.74291300	-0.15630200	1.97986900	N	1.45024400	-1.68947500	1.16809100
N	0.23160300	1.56468300	1.14184500	H	1.74339200	-2.59780700	0.76067000
C	-0.34371400	2.58089900	0.37548400	H	0.48400100	-1.61351100	0.78510900
C	0.12061100	3.79065400	-0.17515800	H	5.47825300	0.05718300	-0.09871600

H	1.08577200	-0.47152500	-2.43616300	C	4.58186900	-0.59075000	-1.49979000
Ru	2.44942800	-0.06767400	0.21296700	C	3.79514500	-1.69292300	-1.02251300
P	-1.39452200	-2.52426600	-1.05525400	C	3.68529900	-1.94789400	0.35754300
O	-1.06523300	-3.86106300	-0.42574700	H	5.52706900	0.71706900	1.52979000
O	-0.54008000	-1.33599700	-0.64387600	H	5.76412900	1.13091800	-0.94475200
O	-2.98558200	-2.17749700	-0.84845900	H	3.21855800	-2.28753300	-1.72139000
C	-3.60955700	-2.36086500	0.42515700	H	3.00704300	-2.71926500	0.71029400
H	-2.93488900	-2.86317400	1.12612200	H	2.21568700	2.80246100	-0.19779300
H	-4.47984300	-3.01111000	0.27920300	N	2.56063500	2.23314400	0.57718500
C	-4.09471800	-1.04408400	1.01392200	H	3.44012400	2.65830600	0.86177400
H	-4.74531300	-1.26424300	1.86717700	C	1.55994100	2.32227800	1.70150500
O	-2.96458800	-0.26346400	1.51945000	H	1.88298600	3.05466800	2.44571100
C	-2.96573700	1.00927700	0.93832200	H	0.62090000	2.67764800	1.27395900
H	-3.41340500	1.76591600	1.59607900	C	1.35898200	0.94323300	2.32192300
N	-1.55295800	1.39412000	0.71926200	H	2.20798000	0.65622300	2.94789300
C	-0.47523200	0.65681800	1.04344800	H	0.45826200	0.93321300	2.94688000
H	-0.61678900	-0.28604200	1.53153400	N	1.25587200	-0.02157000	1.20720400
N	0.68485900	1.21667700	0.69700500	H	1.09377700	-1.02320800	1.45813600
C	0.31400200	2.43775000	0.10739900	H	0.44685400	0.22025800	0.63132000
C	0.98295100	3.59643400	-0.34574700	H	4.22468500	-1.24223400	2.35671800
N	2.34143600	3.77577400	-0.29707500	H	4.61563900	-0.37689700	-2.56185400
H	2.63062300	4.73185700	-0.46460500	Ru	2.96412300	0.15294000	-0.03026300
H	2.84768000	3.28565400	0.42441600	P	-0.01957100	-2.81778200	-0.32137400
N	0.26351600	4.59467700	-0.88244100	O	0.68283200	-2.65926600	1.00842000
C	-1.06854200	4.50053200	-0.92639400	O	0.37800400	-1.93778500	-1.50189000
H	-1.59401900	5.32635300	-1.39764000	O	-1.63261300	-2.54406100	-0.14473100
N	-1.82377500	3.51358900	-0.42965900	C	-2.28611700	-2.87468100	1.09388700
C	-1.08672200	2.52912600	0.09047600	H	-1.60060300	-2.69028500	1.92545600
C	-4.84749400	-0.11256200	0.05116400	H	-2.56066100	-3.93676500	1.09874800
H	-5.25135500	-0.65468700	-0.81365200	C	-3.53728700	-2.02314400	1.26036300
C	-3.77377900	0.90555800	-0.37314900	H	-3.99036600	-2.27481600	2.22597000
H	-3.13356600	0.47283000	-1.15252700	O	-3.17184200	-0.62082100	1.28245900
O	-5.86018600	0.54211700	0.78892400	C	-3.77718300	0.07840000	0.21436500
O	-1.34355000	-2.56256400	-2.67852200	H	-4.59555000	0.71793200	0.56013300
O	1.55599700	-4.08878900	-0.22667900	N	-2.78126100	0.97767100	-0.37049400
H	1.82255700	-5.00937200	-0.11992500	C	-1.62726700	0.58156300	-0.99046600
H	0.55271300	-4.09610500	-0.31570600	H	-1.42647500	-0.45166800	-1.24206000
O	-4.39286100	2.10367200	-0.76514700	N	-0.77584700	1.57140600	-1.19754400
H	-3.71371400	2.80159100	-0.81740000	C	-1.40862300	2.69121000	-0.68162300
H	-6.03653100	1.37674300	0.32580400	C	-1.03112700	4.03847100	-0.56027200
H	-1.80952500	-3.33664300	-3.02483700	N	0.19494100	4.49995900	-1.01970600
AMPH-RCc				H	0.24868700	5.51324500	-1.00102700
C	4.33680700	-1.07505400	1.29110700	H	0.47180900	4.11426700	-1.91548000
C	5.07042100	0.03330300	0.82166400	N	-1.84979000	4.88274200	0.07307400
C	5.21134200	0.26825100	-0.58972000	C	-3.01704400	4.40932100	0.55411300
				H	-3.64614300	5.13799000	1.05826200

N	-3.49480500	3.16317500	0.48346300	C	-2.68170300	-2.51534400	1.20133100
C	-2.65306500	2.34035100	-0.14128400	H	-1.96225100	-2.45658900	2.02367800
C	-4.61615300	-2.15855800	0.17597800	H	-3.21425500	-3.47167100	1.27751900
H	-4.56313000	-3.12978300	-0.33829900	C	-3.67538400	-1.36711900	1.29382200
C	-4.30381400	-0.98271800	-0.76950800	H	-4.19300300	-1.42204000	2.25760000
H	-3.52160600	-1.27146300	-1.47839100	O	-2.95570800	-0.10412600	1.23568700
O	-5.87455900	-1.95641200	0.78164300	C	-3.36547600	0.65090800	0.11116500
O	0.09466700	-4.37676200	-0.75080000	H	-4.03427500	1.47057500	0.39286400
H	-0.13050300	-4.49986700	-1.68366300	N	-2.17600800	1.28444000	-0.46073100
O	1.56646600	0.30841500	-1.62049300	C	-1.08084600	0.63291100	-0.96585100
H	1.10871100	-0.61238900	-1.63630500	H	-1.07699200	-0.43246200	-1.17378100
H	0.80705800	0.95284000	-1.54072000	N	-0.02780200	1.42092200	-1.13140600
O	-5.45257900	-0.47545700	-1.42518600	C	-0.46708400	2.67200700	-0.72304600
H	-5.56454400	-0.93149200	-2.26917000	C	0.15965400	3.92151000	-0.59524600
H	-6.43220000	-1.51447900	0.12072600	N	1.51084100	4.09576200	-0.89353600
AMPH-TSc				H	1.76977400	5.07809700	-0.88746600
C	3.96238800	-1.37318600	1.13301700	H	1.80686700	3.62860200	-1.74471600
C	4.70066600	-0.28833500	0.57354800	N	-0.52335900	4.94693400	-0.08509700
C	4.68026800	-0.03778700	-0.83054500	C	-1.80382600	4.74513300	0.28826300
C	3.84781500	-0.82848800	-1.64085100	H	-2.31858900	5.61259100	0.69202500
C	3.09939000	-1.91867500	-1.08820200	N	-2.50752600	3.61187400	0.22496500
C	3.18203900	-2.21689700	0.28027000	C	-1.79758600	2.60621600	-0.28543000
H	5.27491400	0.35898000	1.22994200	C	-4.72557100	-1.29734100	0.17625300
H	5.23049100	0.79716600	-1.24834700	H	-4.91960800	-2.28519100	-0.26674100
H	2.38070300	-2.44892800	-1.69937500	C	-4.09020300	-0.32097900	-0.83369300
H	2.52112600	-2.96819700	0.70469300	H	-3.37369200	-0.85023500	-1.46885000
H	2.24272800	2.65438700	0.49233800	O	-5.89813400	-0.72238100	0.71194700
N	2.44043100	1.88733600	1.15370100	O	-0.69926700	-4.63182700	-0.48729800
H	3.35671000	2.09206500	1.54767500	H	-0.91170800	-4.81038300	-1.41412100
C	1.41034300	1.88964000	2.25106600	O	1.37679800	-0.37885800	-2.91245300
H	1.74589200	2.50046000	3.09372300	H	0.81918900	-1.11157300	-2.57871800
H	0.50461300	2.34781400	1.84856300	H	0.93062200	0.42078700	-2.59505200
C	1.11965700	0.45455300	2.67470900	O	-5.04895100	0.39875400	-1.58784600
H	1.95651600	0.02386500	3.23195400	H	-5.22835000	-0.07680000	-2.40905300
H	0.23068700	0.41335500	3.31414900	H	-6.32244900	-0.23328600	-0.01169100
N	0.92503900	-0.33455700	1.43742000	AMPH-PCc			
H	0.73796300	-1.36797800	1.55052000	C	3.97972000	-1.98666600	-0.54826500
H	0.08327800	0.00313400	0.96622600	C	4.02909200	-0.92361000	-1.51288600
H	3.98541800	-1.54786600	2.20321100	C	2.90503800	-0.64903500	-2.30816600
H	3.68082300	-0.57081400	-2.67841800	C	1.71106300	-1.42859600	-2.15628300
Ru	2.55481500	-0.03235900	0.12462900	C	1.66575500	-2.48358000	-1.22692800
P	-0.47797300	-3.04346400	-0.24565400	C	2.81184500	-2.75916400	-0.41136600
O	0.28454900	-2.90089800	1.06090700	H	4.92757200	-0.32270600	-1.60762800
O	0.02666200	-2.36970500	-1.50347200	H	2.92440800	0.17539900	-3.01249200
O	-1.99644500	-2.43013900	-0.05370900	H	0.72871100	-3.02563700	-1.09665000

H	2.76024200	-3.54124900	0.33858000	O	-5.61404900	1.43476600	0.16733300
H	3.44578100	1.52503500	1.15908000	O	-2.81697100	-4.12149400	0.68627300
N	3.31495900	0.54601500	1.45157400	H	-3.17506600	-4.52389800	-0.11728700
H	4.24768500	0.14393200	1.52836600	O	-1.35735500	-1.01292900	-2.79511600
C	2.63217200	0.46681300	2.78028300	H	-1.43748400	-1.82723900	-2.23064800
H	3.34815400	0.59674200	3.59750300	H	-1.73460400	-1.26190000	-3.64793000
H	1.91326600	1.29014600	2.83085400	O	-4.02717000	1.96310200	-1.91838700
C	1.90230700	-0.86563500	2.86569900	H	-4.11301500	1.50997300	-2.76615900
H	2.60671800	-1.70258900	2.88980500	H	-5.69283700	1.94036800	-0.65817700
H	1.28556100	-0.92098100	3.76972900				
N	1.07194400	-0.98442100	1.64585600	AMPH-RCd			
H	0.51611000	-1.88830400	1.57983800	C	4.93138300	-0.98441600	-0.51712400
H	0.33685600	-0.27760500	1.70218500	C	5.25623500	0.36055400	-0.78824000
H	4.83952800	-2.18335100	0.08385600	C	4.48893500	1.10907100	-1.74619200
H	0.79990300	-1.17643100	-2.69892500	C	3.39788000	0.50582900	-2.38819600
Ru	2.24442400	-0.56918600	-0.08638600	C	3.03935000	-0.85002400	-2.07799800
P	-1.72163700	-2.98975100	0.29973000	C	3.80635600	-1.59745800	-1.16524300
O	-0.67736100	-2.95176700	1.39233900	H	6.08004800	0.83396900	-0.26502400
O	-1.29780700	-3.11803700	-1.14997500	H	4.72758600	2.14930000	-1.93869100
O	-2.58553200	-1.57742000	0.32195200	H	2.11828200	-1.26888600	-2.46818900
C	-3.35302100	-1.20189700	1.47222400	H	3.46626600	-2.58435200	-0.86968300
H	-2.72851300	-1.23223100	2.37293200	H	2.15622100	2.42232100	1.06099800
H	-4.18630000	-1.90149500	1.60841600	N	2.99326900	1.89674600	1.31543500
C	-3.89149700	0.20515900	1.26891300	H	3.77241700	2.54927500	1.25614800
H	-4.56548300	0.44840800	2.09680700	C	2.85718400	1.37587500	2.71256600
O	-2.79252000	1.15760200	1.29938000	H	3.86357300	1.13743200	3.07060400
C	-2.66855000	1.82499800	0.06547500	H	2.43026900	2.13387600	3.37702300
H	-2.99292100	2.86862400	0.12365200	C	1.99568800	0.11989800	2.67322600
N	-1.22998100	1.87316200	-0.25434400	H	1.95256700	-0.35120200	3.66101500
C	-0.44413000	0.77478900	-0.36976500	H	0.97508100	0.36778900	2.37453300
H	-0.86495500	-0.21421400	-0.46466100	N	2.56913700	-0.79549200	1.66190900
N	0.85395800	1.05440500	-0.31601000	H	3.40274000	-1.24087000	2.04382900
C	0.92494000	2.44269500	-0.17485300	H	1.93861400	-1.59257000	1.36862700
C	1.95449900	3.39651300	-0.09070800	H	2.76574100	1.08827100	-3.04828900
N	3.30899800	3.06369400	-0.16461500	H	5.50336300	-1.54091900	0.21748700
H	3.88098000	3.90370700	-0.18746100	Ru	3.08649700	0.25723300	-0.12181900
H	3.53249900	2.43620900	-0.93024700	P	-0.02842100	-2.60366700	-0.06098300
N	1.64173600	4.67446300	0.12248600	O	1.31981800	-2.90769900	0.54547900
C	0.34526200	5.02337000	0.21758200	O	-0.10402400	-1.39610800	-1.00994700
H	0.14895200	6.07552500	0.40316000	O	-1.06713400	-2.29951700	1.18326600
N	-0.71844100	4.22820900	0.09278300	C	-2.29512500	-3.01194300	1.39249800
C	-0.38229600	2.95708400	-0.10466600	H	-2.43921000	-3.08185900	2.47418100
C	-4.61965600	0.45896900	-0.05859500	H	-2.22104300	-4.02378600	0.98481500
H	-5.04036100	-0.46627200	-0.47789700	C	-3.49042300	-2.31120000	0.76513900
C	-3.51334000	1.04902100	-0.96121900	H	-4.35067600	-2.99340700	0.81123900
H	-2.92880600	0.25584800	-1.43689700	O	-3.81852300	-1.11179900	1.50615700

C	-4.19077900	-0.07723200	0.62791100	H	2.94144600	0.17762500	3.96017500
H	-5.11364800	0.40179300	0.96843700	C	1.63355800	-1.12472100	2.80734600
N	-3.11938800	0.94565100	0.64124800	H	1.78546400	-2.09774100	3.28137200
C	-1.88311800	0.83019000	1.21598500	H	0.78655800	-0.64830100	3.30882100
H	-1.59491400	-0.07671700	1.72506600	N	1.30802000	-1.30453600	1.36265900
N	-1.10880500	1.88814700	1.02750200	H	1.31127000	-2.30075200	1.02154000
C	-1.90127600	2.76082400	0.28716900	H	0.32123100	-1.07213600	1.20741200
C	-1.71333500	4.06015400	-0.22557200	H	1.73000700	0.78298400	-2.76221300
N	-2.69233600	4.61592900	-0.95358100	H	4.85591800	-1.75096400	0.15797900
C	-3.82834300	3.92774800	-1.14979600	Ru	2.41521400	-0.10125800	0.01054300
N	-4.14980900	2.71534400	-0.68438200	P	-0.60368100	-3.12615700	-0.58464400
C	-3.15139700	2.18506900	0.02796800	O	0.76747700	-3.48178800	-0.04437900
C	-3.28922500	-1.81820500	-0.67956700	O	-0.69764500	-2.26949600	-1.83695300
H	-2.30462900	-1.35973900	-0.78088700	O	-1.34552400	-2.32011400	0.66925300
C	-4.34202800	-0.71246200	-0.77608900	C	-2.70410300	-2.52609100	1.08240400
H	-4.15346500	0.00895400	-1.57694600	H	-2.68735000	-2.79588000	2.14392400
O	-5.59432200	-1.35857000	-0.92122200	H	-3.14628000	-3.35779800	0.52755100
H	-6.25642000	-0.71935700	-1.21372700	C	-3.58358200	-1.30529300	0.88036700
O	-3.35264700	-2.83348500	-1.65505300	H	-4.60554700	-1.58773800	1.16915500
O	-0.63296100	-3.89418100	-0.80808900	O	-3.15979900	-0.20969200	1.73551200
H	-4.28422200	-3.08183200	-1.76163100	C	-3.33529700	1.02509200	1.08237700
N	-0.55749000	4.77570100	-0.03876500	H	-3.94614200	1.69302500	1.69928800
H	-0.06457400	4.60600900	0.82585200	N	-1.99230600	1.64690100	0.93482300
H	-0.63501000	5.75023800	-0.30128000	C	-0.87806000	1.24862200	1.60802500
H	-4.58200400	4.42697000	-1.75366500	H	-0.93793800	0.42302900	2.29976300
O	1.03179500	0.67238700	-0.35634300	N	0.20245200	1.96737800	1.34234700
H	0.50527000	-0.21456700	-0.64540900	C	-0.24465500	2.91512000	0.43149800
H	0.44569800	1.18189400	0.25177000	C	0.37968600	3.97223400	-0.25942700
H	-1.40928800	-3.68731600	-1.36363100	N	-0.34173500	4.69428100	-1.12701100
AMPH-TSd				C	-1.63930200	4.39580400	-1.29790300
C	4.21717200	-1.21648900	-0.53649000	N	-2.35184900	3.44048700	-0.69088900
C	4.48070600	0.15962000	-0.83780600	C	-1.60774600	2.72884800	0.16186200
C	3.62135500	0.87725300	-1.69626300	C	-3.60526800	-0.71692800	-0.54113500
C	2.48757900	0.21133200	-2.24190500	H	-2.59601500	-0.73914400	-0.95493100
C	2.25431900	-1.17118700	-2.02260800	C	-4.01939800	0.73951800	-0.27245200
C	3.11778100	-1.88375900	-1.16077500	H	-3.71339900	1.44031200	-1.05129600
H	5.30624000	0.66582200	-0.34740500	O	-5.43090300	0.72595100	-0.10256700
H	3.76306900	1.93849700	-1.86207500	H	-5.78922600	1.59616100	-0.31652900
H	1.34383800	-1.64702200	-2.37708600	O	-4.45066600	-1.39783500	-1.42718700
H	2.84415500	-2.89723400	-0.88121000	O	-1.51247200	-4.45405500	-0.77243300
H	1.98415700	1.41225600	2.02196300	H	-5.34980200	-1.08535500	-1.23583600
N	2.82031400	0.80771400	1.91149300	N	1.71363200	4.27629700	-0.11991400
H	3.65372000	1.39099400	1.94698200	H	2.11483300	4.10309500	0.79084900
C	2.87893300	-0.25474900	2.95533300	H	1.96203600	5.17317600	-0.52025100
H	3.78559500	-0.83942200	2.77813700	H	-2.17465000	5.01389000	-2.01420700
				O	-0.36382700	0.33659700	-1.51985400

H	-0.55207700	-0.62679300	-1.69468100	H	-4.07396500	-1.70819400	1.59149600
H	-0.93645800	0.83199000	-2.11795300	C	-3.75603900	0.33787200	1.04312800
H	-1.95373400	-4.43040600	-1.63383200	H	-4.72899700	0.64363500	1.45282700
AMPH-PCd				O	-2.79249400	1.38662800	1.29500300
C	3.50452200	-2.44552800	-0.70740000	C	-2.56204000	2.16146500	0.14327500
C	3.85418100	-1.33740600	-1.54802500	H	-2.72402700	3.22369200	0.34641600
C	2.88966000	-0.73169900	-2.37515600	N	-1.11889800	2.06042600	-0.18854300
C	1.54647200	-1.22715100	-2.36613700	C	-0.42581200	0.90475500	-0.34139500
C	1.19362000	-2.31687500	-1.55063100	H	-0.91273100	-0.04846200	-0.47086300
C	2.17751300	-2.91809000	-0.70367900	N	0.89085800	1.07426200	-0.28528900
H	4.86784700	-0.94869600	-1.52842900	C	1.07686800	2.44632800	-0.10212800
H	3.15549700	0.11660800	-2.99561400	C	2.18312800	3.30713100	0.01854200
H	0.15982500	-2.64869400	-1.50064600	N	1.97481400	4.60253200	0.26211300
H	1.85601300	-3.69922800	-0.02277100	C	0.71245900	5.05558400	0.35740600
H	3.32563400	1.18782600	1.35366800	N	-0.41408800	4.35486800	0.21068000
N	3.40632400	0.16553800	1.33533900	C	-0.18093400	3.06479800	-0.01674400
H	4.38390900	-0.01212400	1.11103400	C	-3.86839600	0.22703700	-0.49158800
C	3.08653500	-0.44552100	2.65965800	H	-3.12586300	-0.47850200	-0.86682200
H	3.48181600	-1.46524900	2.65484800	C	-3.51329000	1.65370500	-0.96368200
H	3.56552900	0.10549500	3.47610400	H	-3.04733500	1.65960600	-1.95392800
C	1.57715300	-0.45949700	2.81228600	O	-4.72405000	2.39628300	-0.92806600
H	1.27813500	-1.02120600	3.70284100	H	-4.67235400	3.14304300	-1.53663600
H	1.20727000	0.56469100	2.92594700	O	-5.11804200	-0.22183300	-0.94082400
N	0.96677100	-1.04265500	1.58988600	O	-2.95944000	-3.73404300	0.94443000
H	0.74961400	-2.05840100	1.64657200	H	-5.70176000	0.55390300	-0.94218000
H	0.01759900	-0.67014700	1.50071300	N	3.49837300	2.86263700	-0.04320000
H	0.75380700	-0.73557000	-2.92626700	H	3.67736600	2.19078600	-0.78109300
H	4.25053400	-2.89555200	-0.06166600	H	4.14955100	3.64192800	-0.05877700
Ru	2.12062900	-0.69144200	-0.19095700	H	0.60320200	6.11633000	0.56504400
P	-1.73169200	-2.77190300	0.49610500	O	-1.46685900	-0.54730200	-2.86148700
O	-0.40455300	-3.27856100	1.00799800	H	-1.68556500	-1.30128500	-2.26500200
O	-1.86501200	-2.44964300	-0.98387400	H	-2.02246700	-0.67377300	-3.64042100
O	-2.02217100	-1.38464300	1.36645300	H	-3.46894700	-4.00105400	0.16643600
C	-3.32596600	-0.93012100	1.76726300				
H	-3.27733400	-0.73852000	2.84377400				