Supporting Information

Sequential Norrish-Yang Cyclization and C–C Cleavage/Cross-Coupling of a [4.1.0] Fused Saturated Azacycle

Charis Amber Roberts,[a, b] Bohyun Park,[a, c] Li-Ping Xu,[d] Jose B. Roque,[a] Charles S. Yeung,[e] Djamaladdin G. Musaev,[d]* Richmond Sarpong,[a]* Rebecca Lyn LaLonde [b]*

[a] Department of Chemistry, University of California, Berkeley, California 94720, United States.

[b] Chemistry Department, Reed College, Portland, Oregon 97202, United States.

[c] Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.

[d] Cherry L. Emerson Center for Scientific Computation, and Department of Chemistry, Emory University, Atlanta, Georgia 30322, United States.

[e] Disruptive Chemistry Fellow, Department of Discovery Chemistry, Merck & Co., Inc., 33 Avenue Louis Pasteur, Boston, Massachusetts 02115, United States.

*dmusaev@emory.edu

*rsarpong@berkeley.edu

*rlalonde@reed.edu

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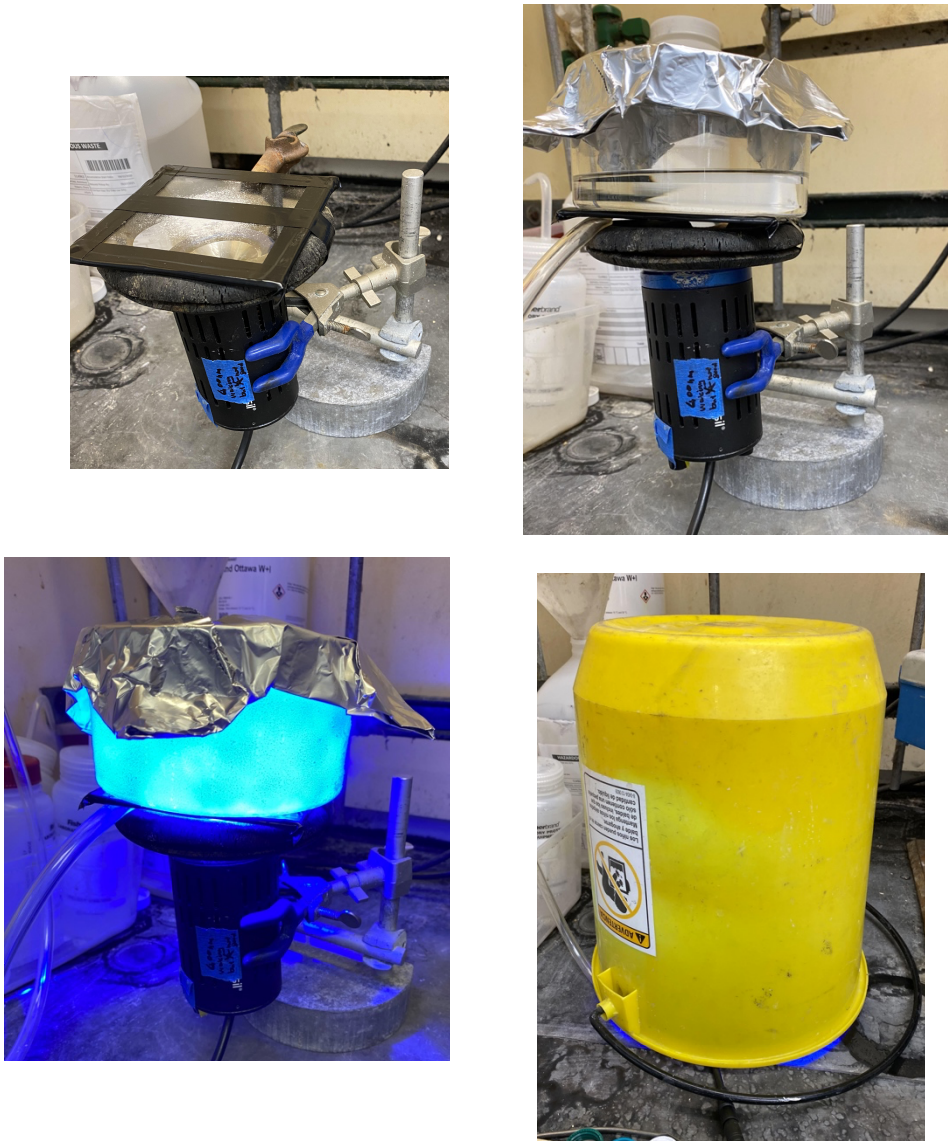


Figure S1. Low-temperature solid-state photoreaction set up for the conversion of **1** to **2a**.

High-Throughput Experimentation (HTE) Catalyst Screening Protocol

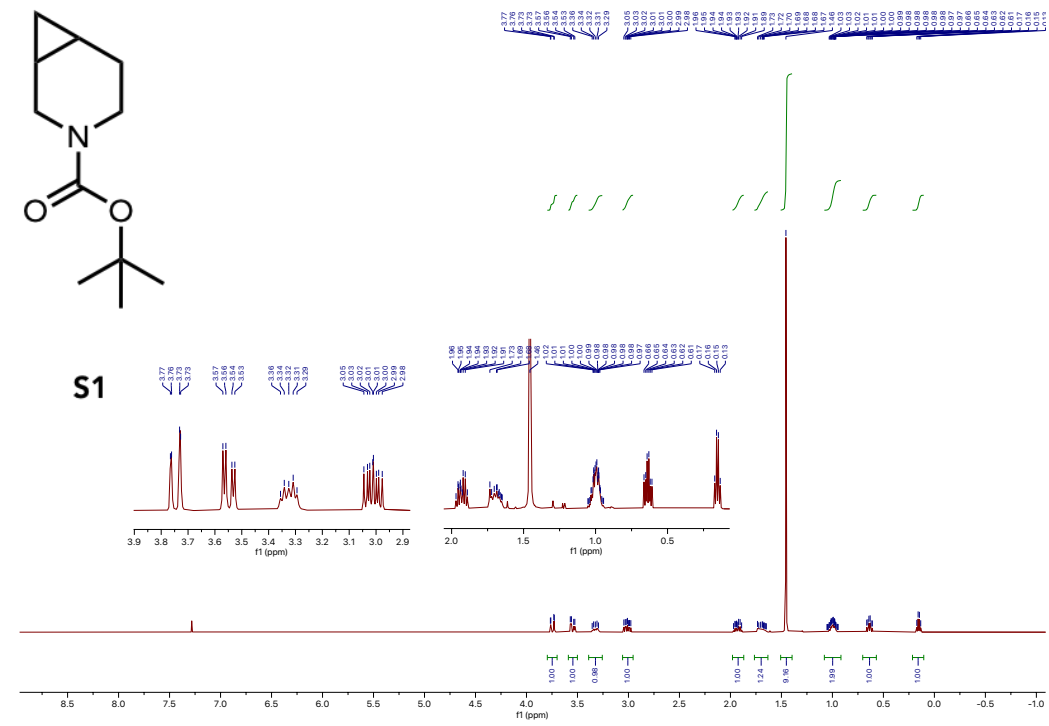
To a 1 dram vial charged with a stir bar was added lactam **2a** (22.3 mg) and Cs_2CO_3 (63.5 mg). The vial was brought into a glove box and toluene (859 μL) and PhBr (23.0 mg) were added. The resulting suspension was vigorously stirred for 5–10 min until a milky suspension was formed. To each reaction well of a custom plated catalysis kit containing a 0.25 μmol of commercially available palladium pre-catalysts (see below) was added 25 μL of the suspension containing lactam **2a** (2.5 mg, 2.5 μmol), Cs_2CO_3 (1.6 mg, 5 μmol), and PhBr (0.6 mg, 3.8 μmol). The reaction block was sealed, and the catalysis kit was stirred (by action of a tumble stirrer) at 40 °C for 24 h. After cooling to rt, each reaction vial was analyzed by LCMS.

XPhos-Pd-G2	RuPhos-Pd-G2	SPhos-Pd-G2	water soluble SPhos-Pd-G2	tBuXPhos-Pd-G3	RockPhos-Pd-G3
BrettPhos-Pd-G3	tBuBrettPhos-Pd-G3	AdBrettPhos-Pd-G3	QPhos-Pd-G3	MorDalPhos-Pd-G3	APhos-Pd-G2
Catacxium A-Pd-G2	tBu3P-Pd-G2	Cy3P-Pd-G2	meCgPPh-Pd-G3	P(oTol)3-Pd-G2	PPh3-Pd-G2
BINAP-Pd-G3	DPPF-Pd-G3	DTBPF-Pd-G3	J009-Pd-G3	XantPhos-Pd-G2	N-XantPhos-Pd-G3

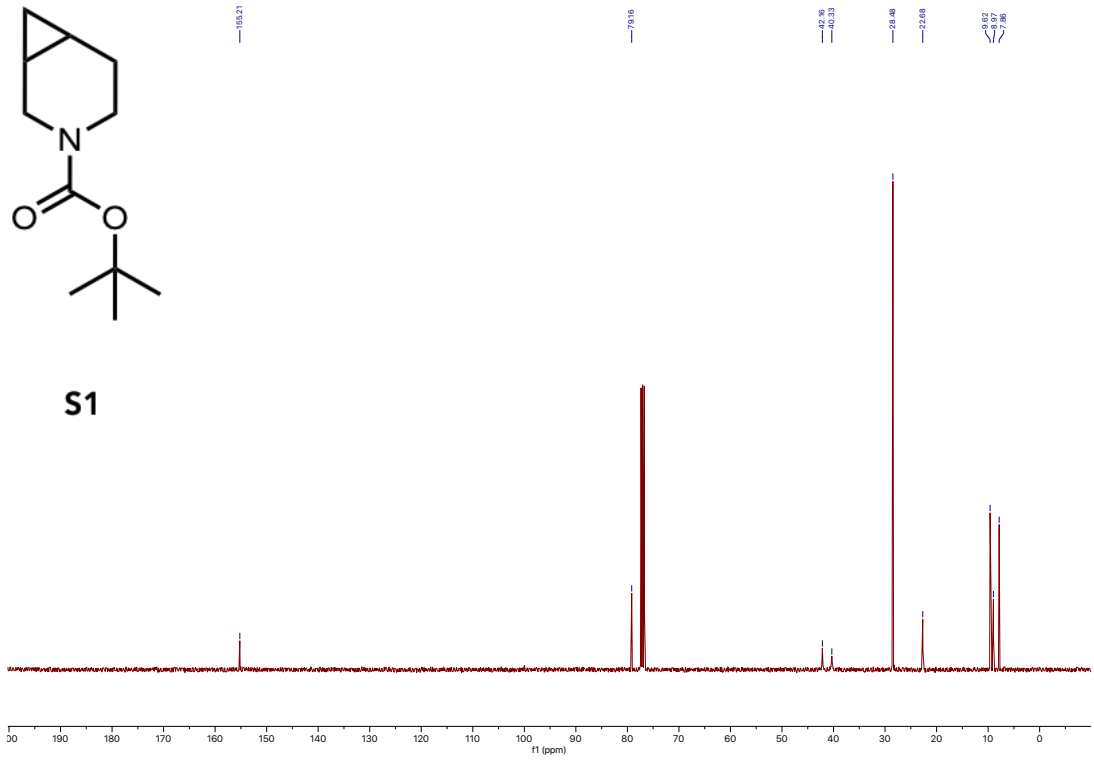
The HTE screen afforded several hits as depicted in the following table showing conversion to what was later identified as compound **3b**.

0	0	0	0	0	0
0	0	0	80	0	76
79	60	0	0	0	0
0	0	67	0	0	0

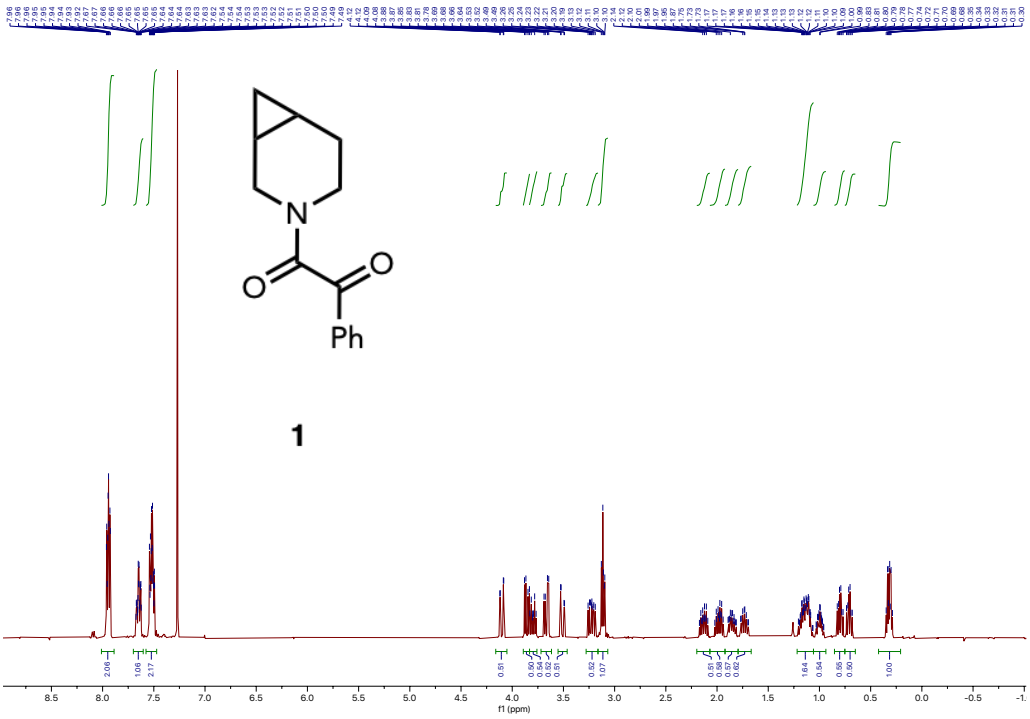
Experimental Spectra



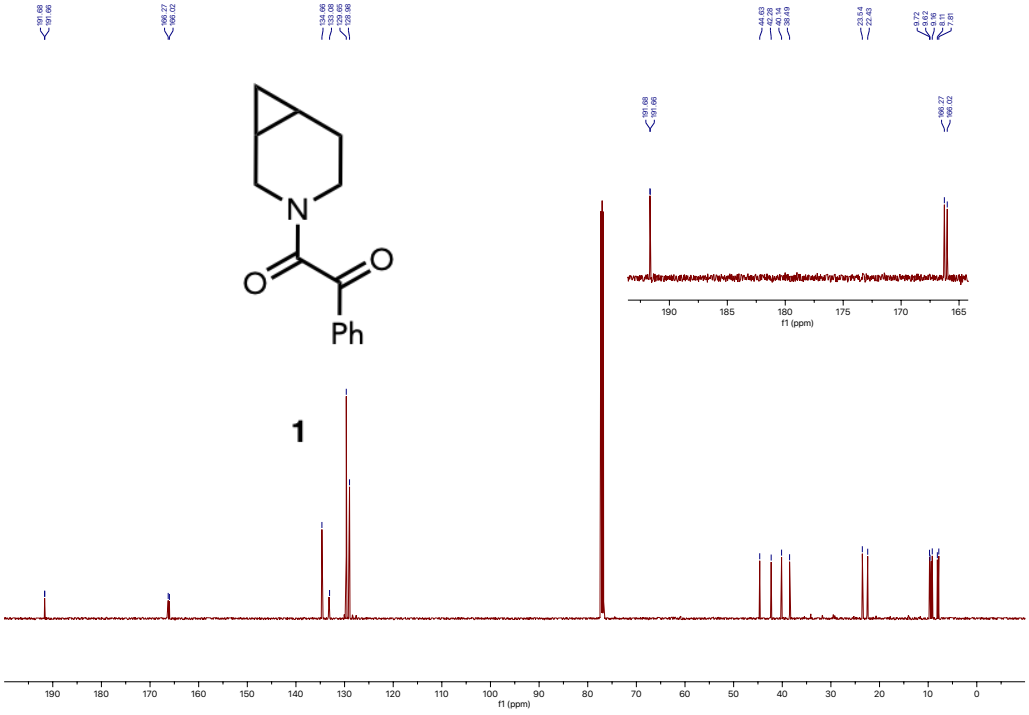
^{1}H NMR of **S1** in $CDCl_3$ @ 400 MHz.



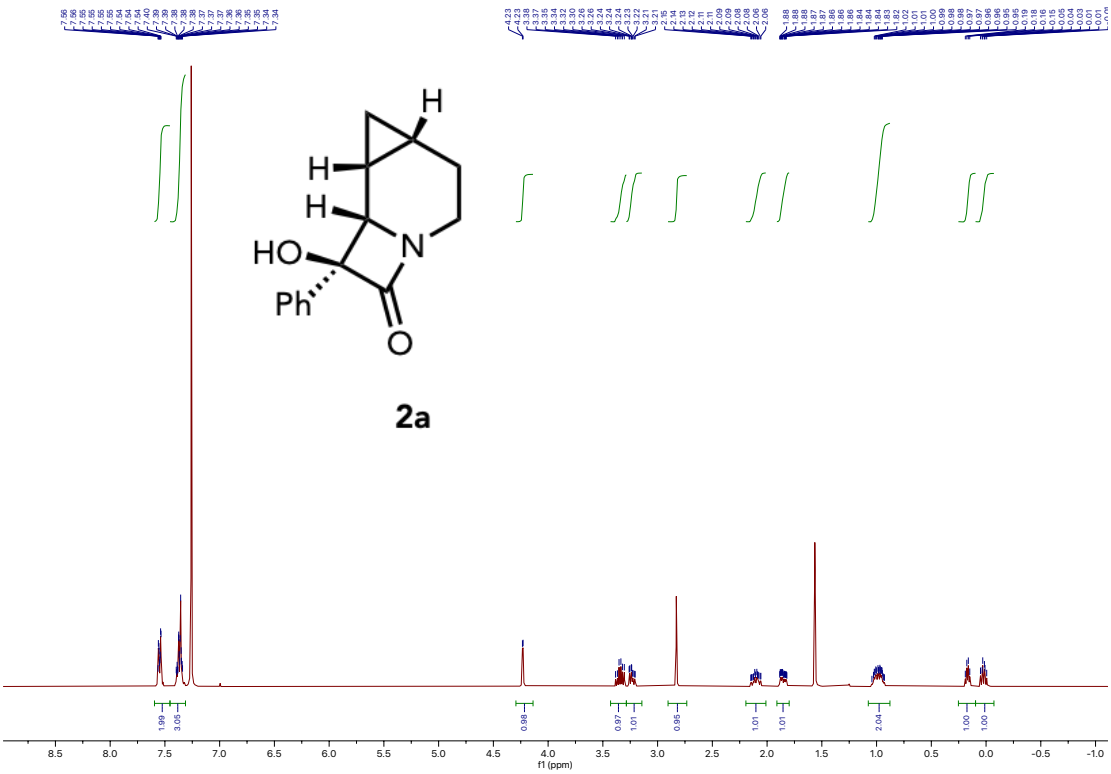
^{13}C{^{1}H} NMR of **S1** in $CDCl_3$ @ 100 MHz.



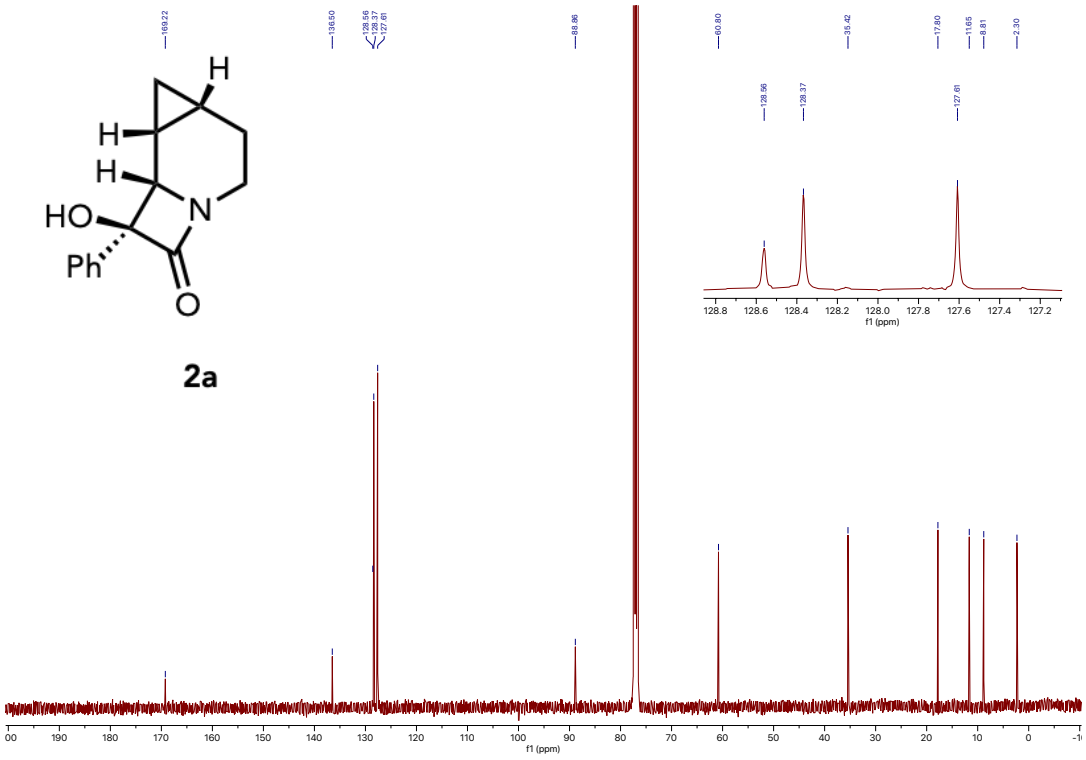
^{1}H NMR of **1** (1: 0.5 mixture of rotamers) in $CDCl_3$ @ 400 MHz.



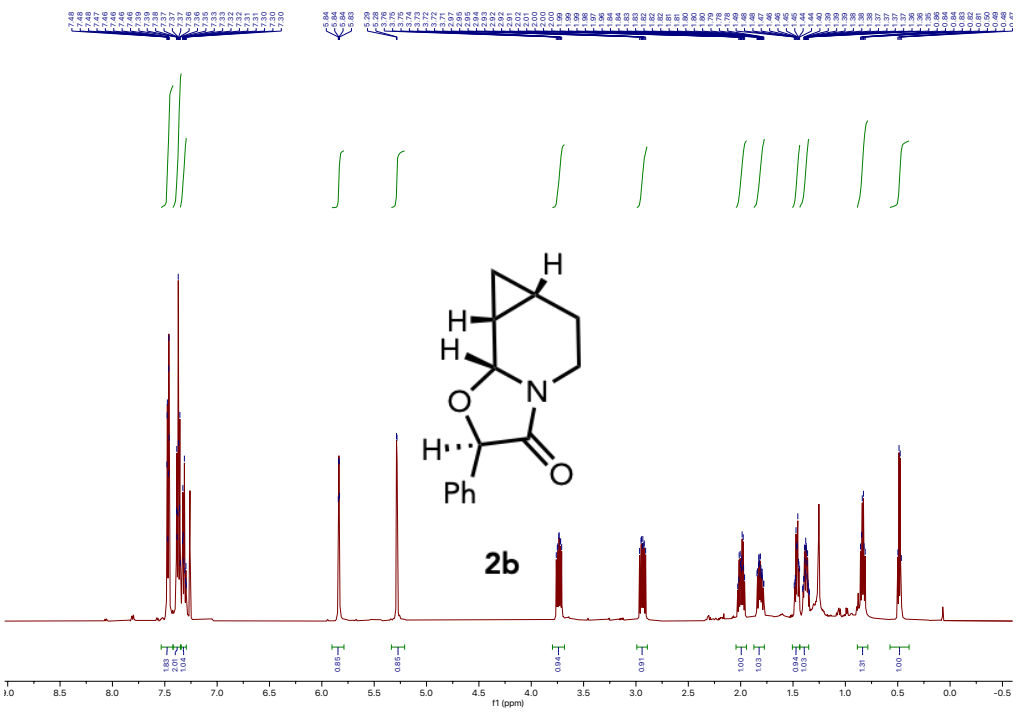
$^{13}C\{^{1}H\}$ NMR of **1** in $CDCl_3$ @ 100 MHz.



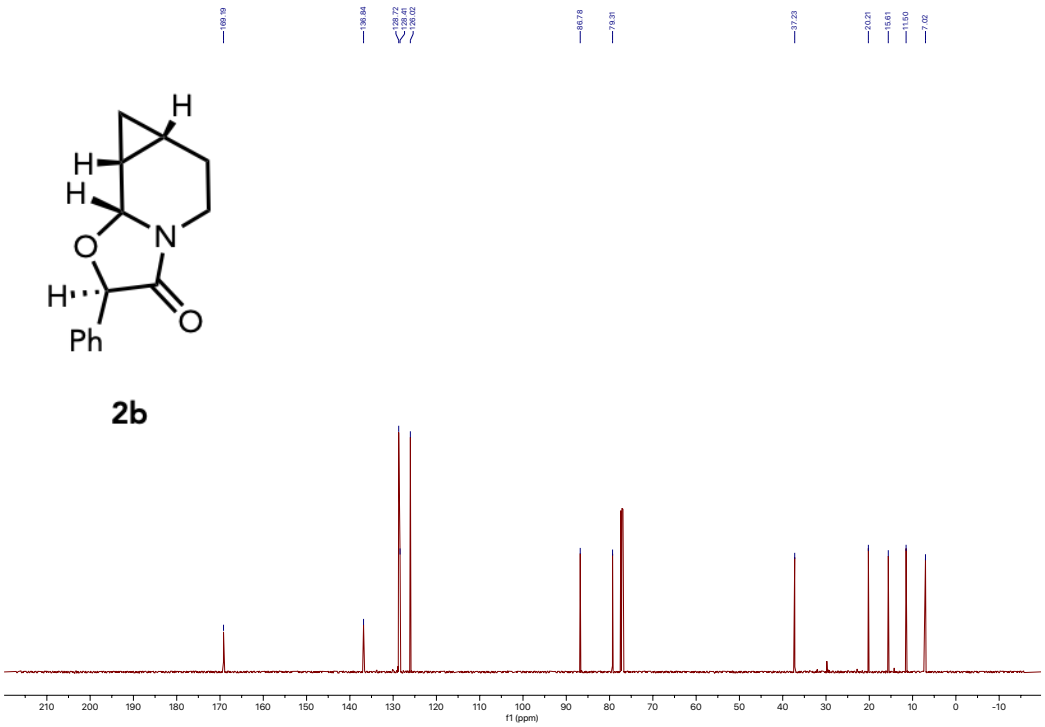
^{1}H NMR of **2a** in $CDCl_3$ @ 400 MHz.



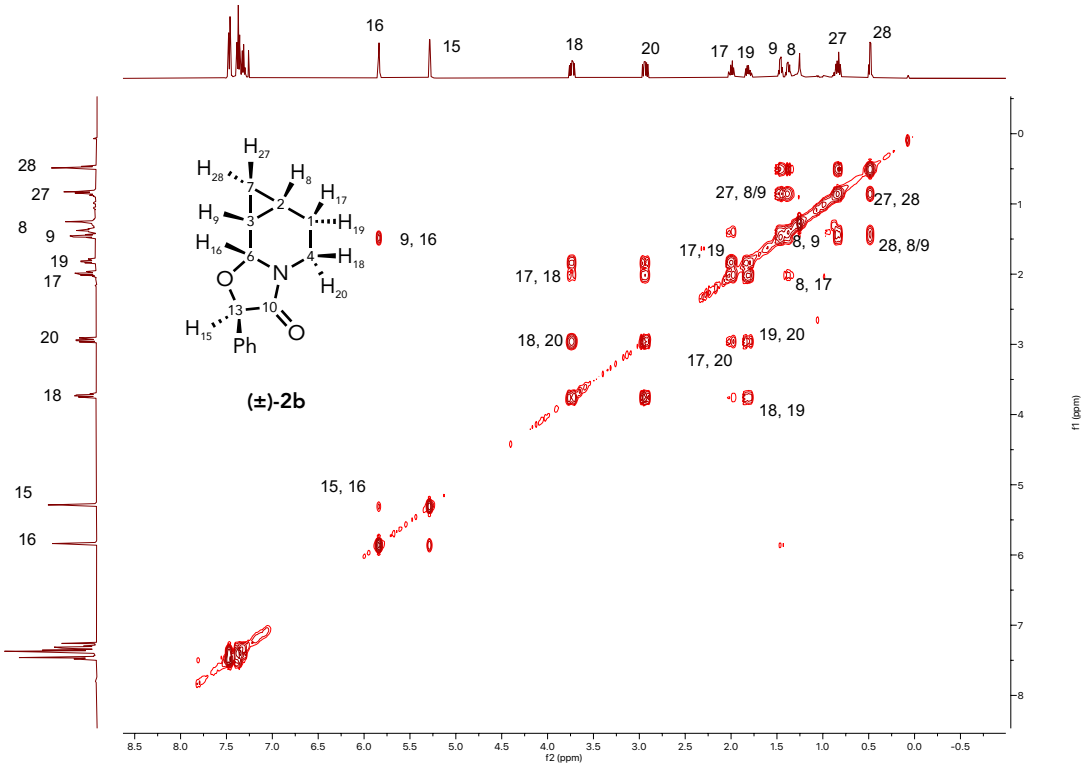
^{13}C{^{1}H} NMR of **2a** in $CDCl_3$ @ 100 MHz.



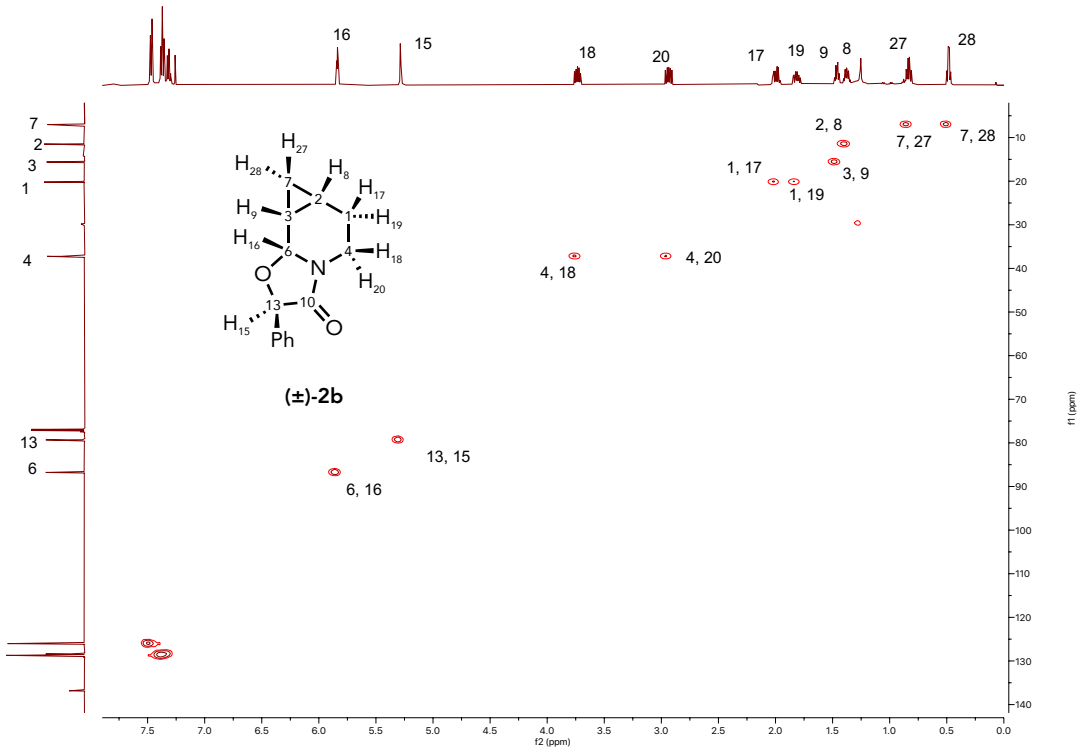
^{1}H NMR of **2b** in $CDCl_3$ @ 400 MHz.



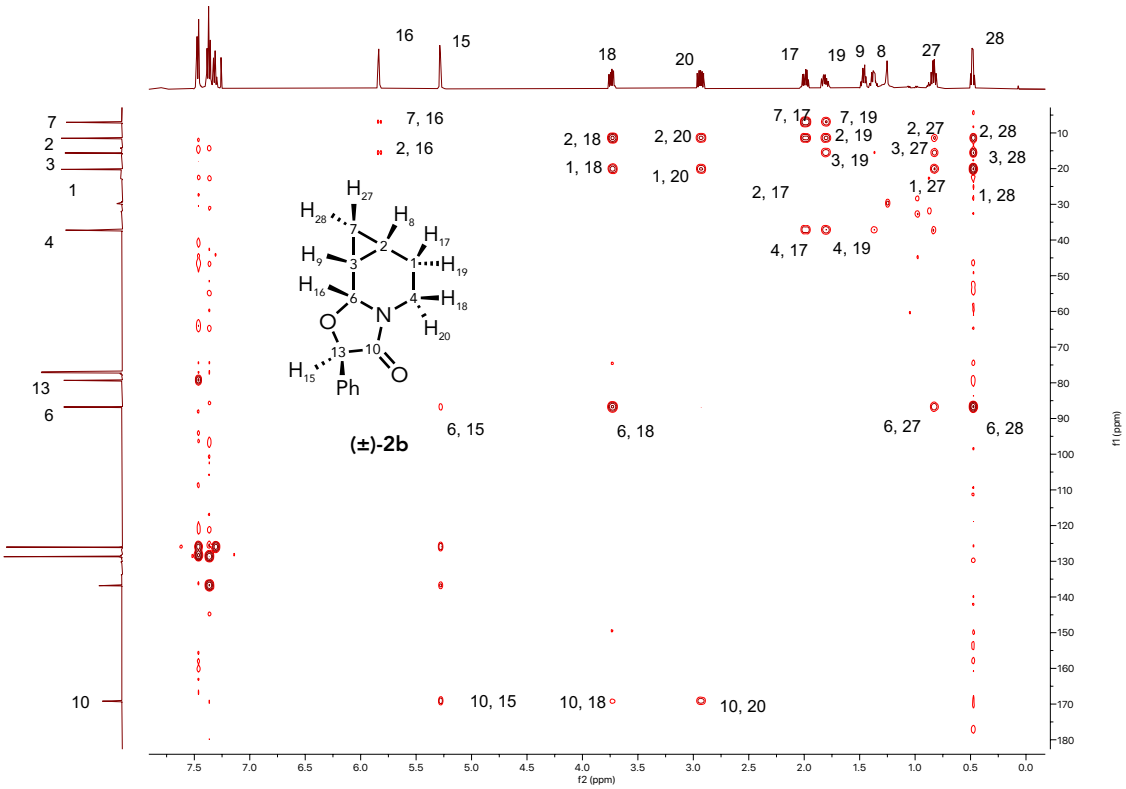
^{13}C{^{1}H} NMR of **2b** in $CDCl_3$ @ 100 MHz.



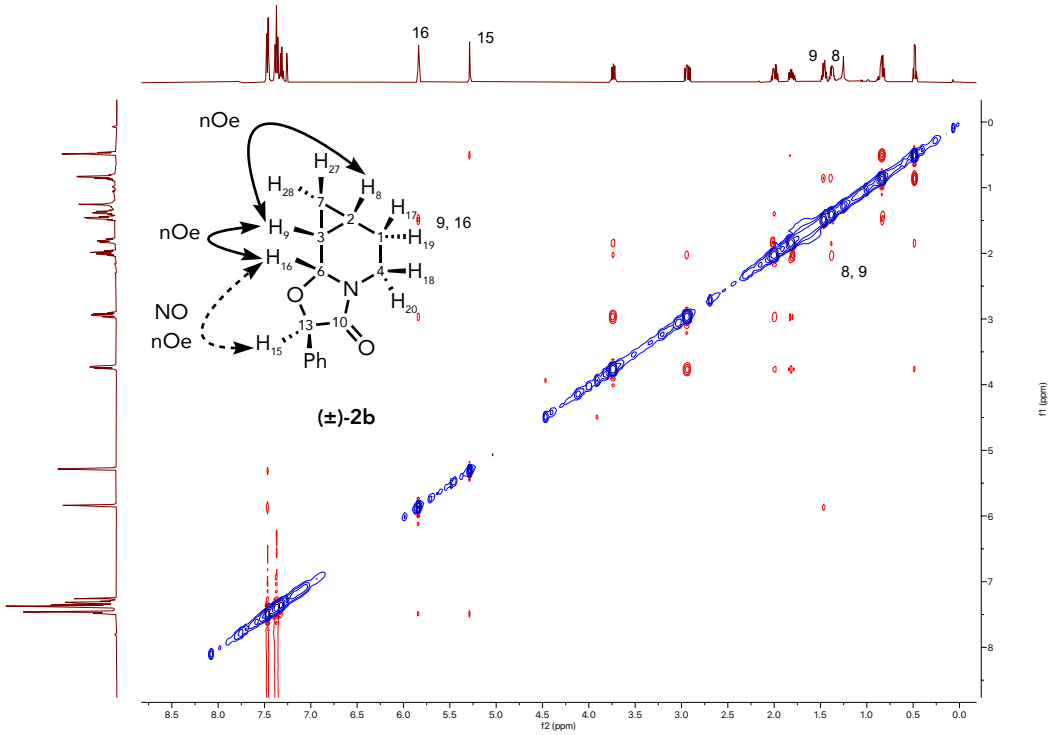
COSY of **2b** in $CDCl_3$ @ 400 MHz.



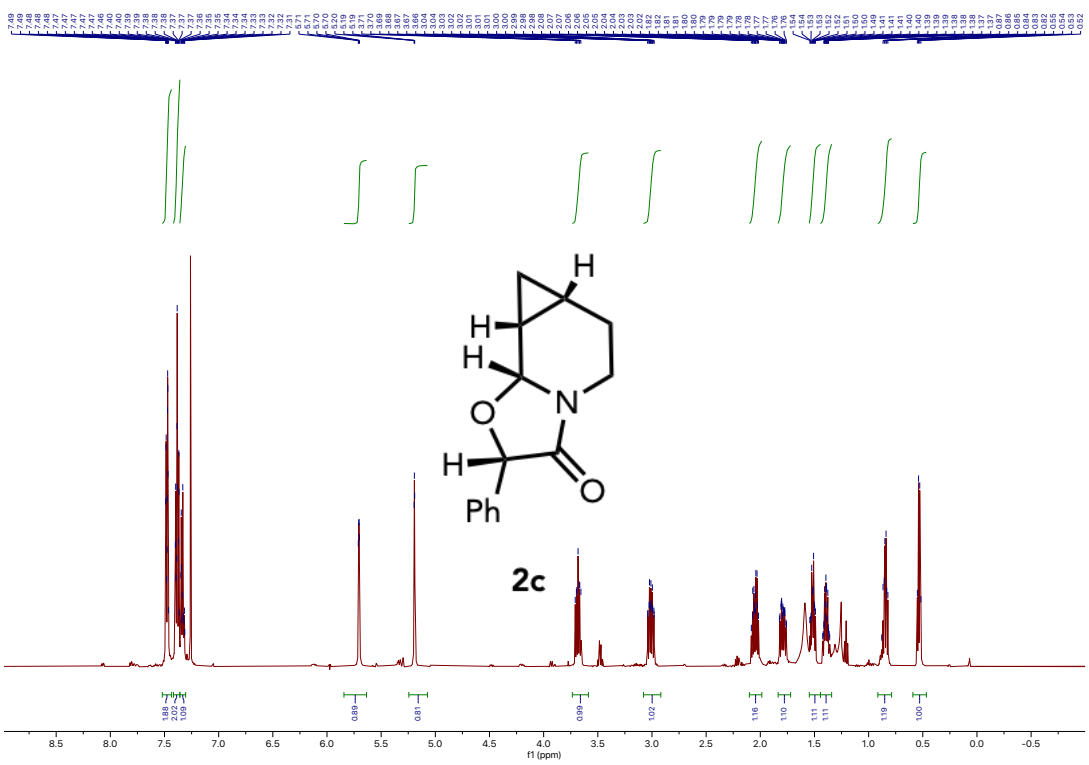
HSQC of **2b** in $CDCl_3$ @ 400 MHz.



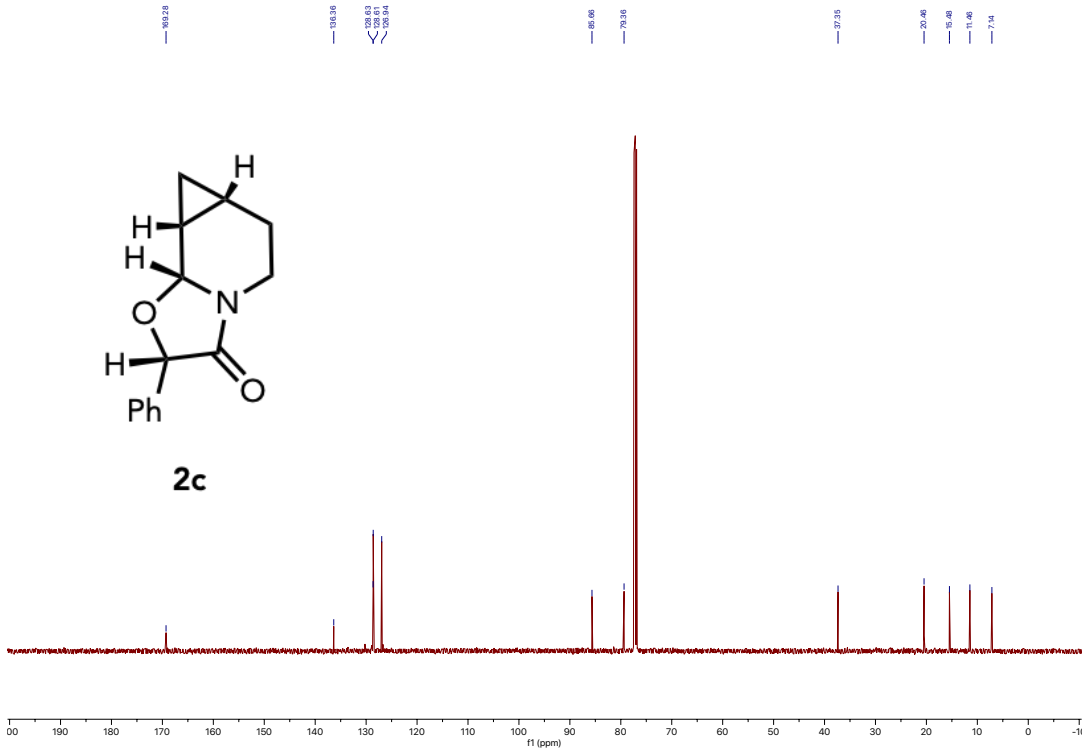
HMBC of **2b** in $CDCl_3$ @400 MHz.



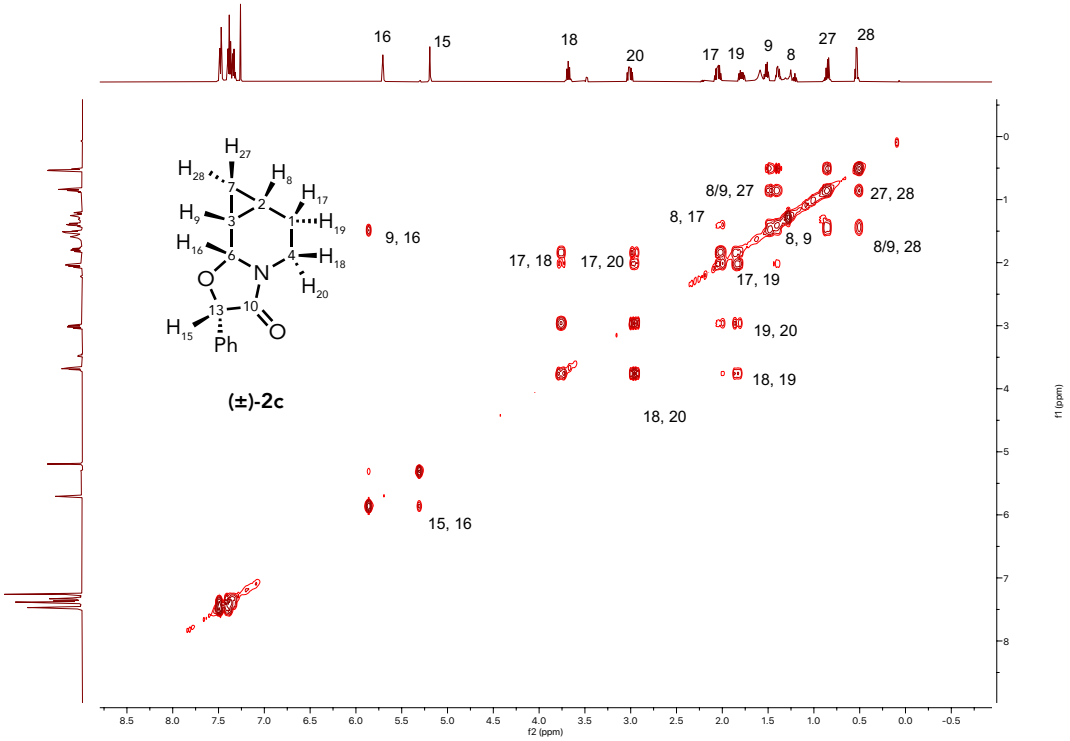
NOESY of **2b** in $CDCl_3$ @ 400 MHz.



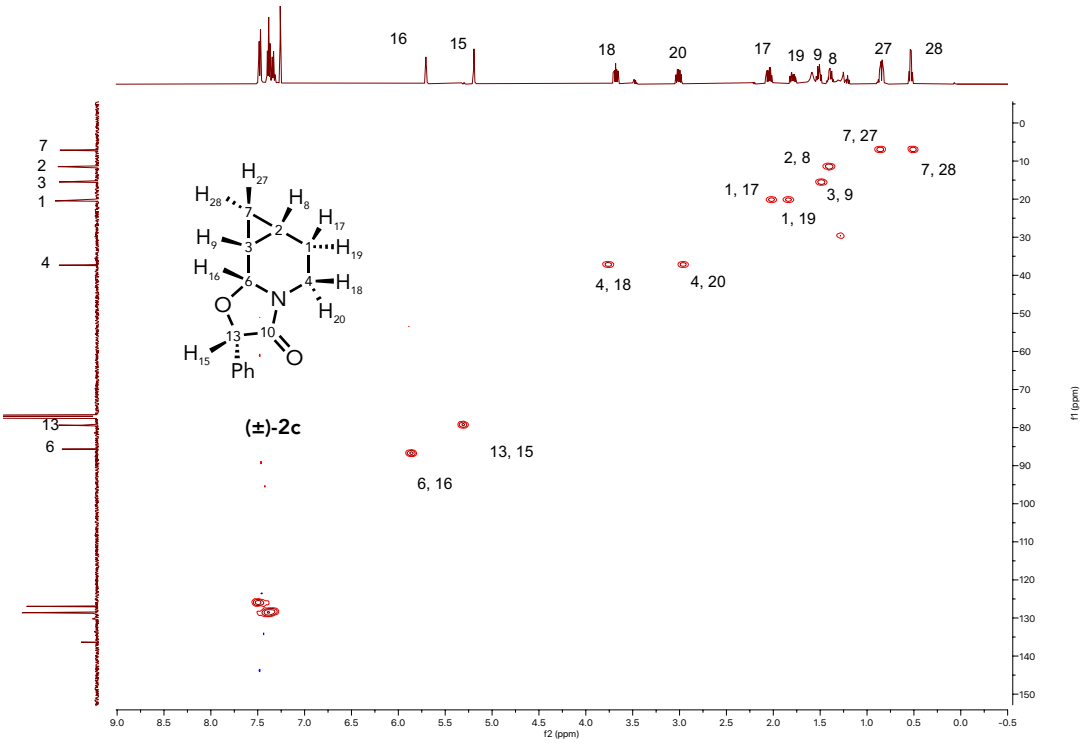
^{1}H NMR of **2c** in $CDCl_3$ @ 400 MHz.



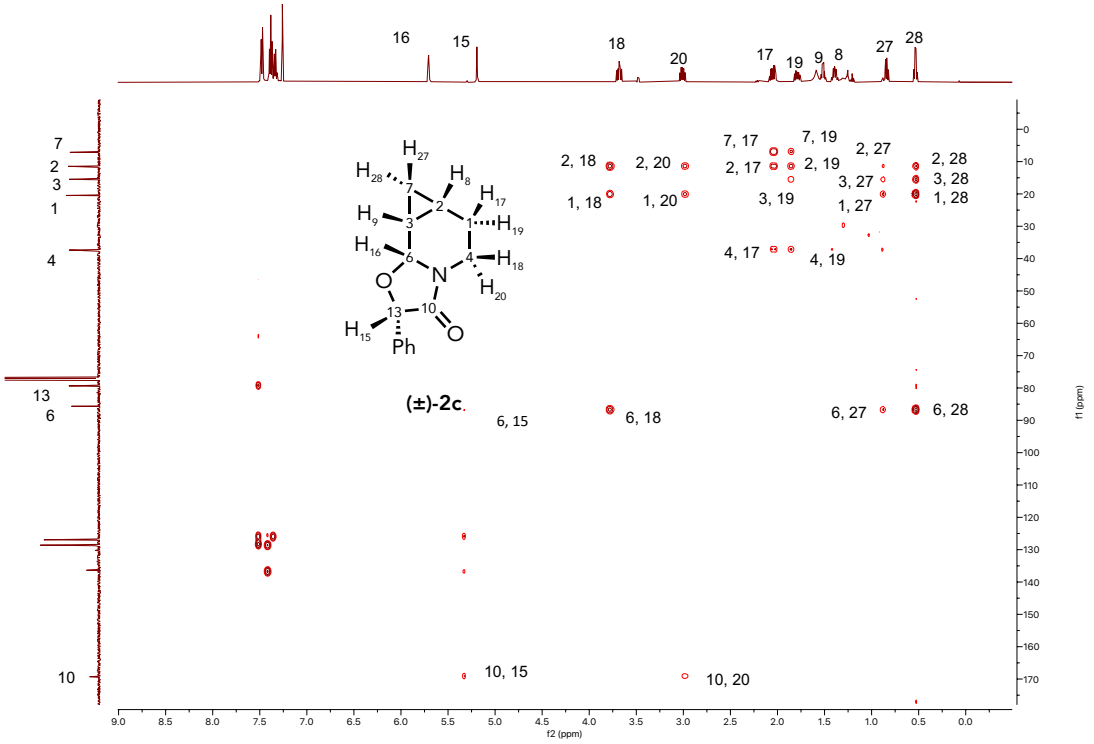
^{13}C{^{1}H} NMR of **2c** in $CDCl_3$ @ 400 MHz.



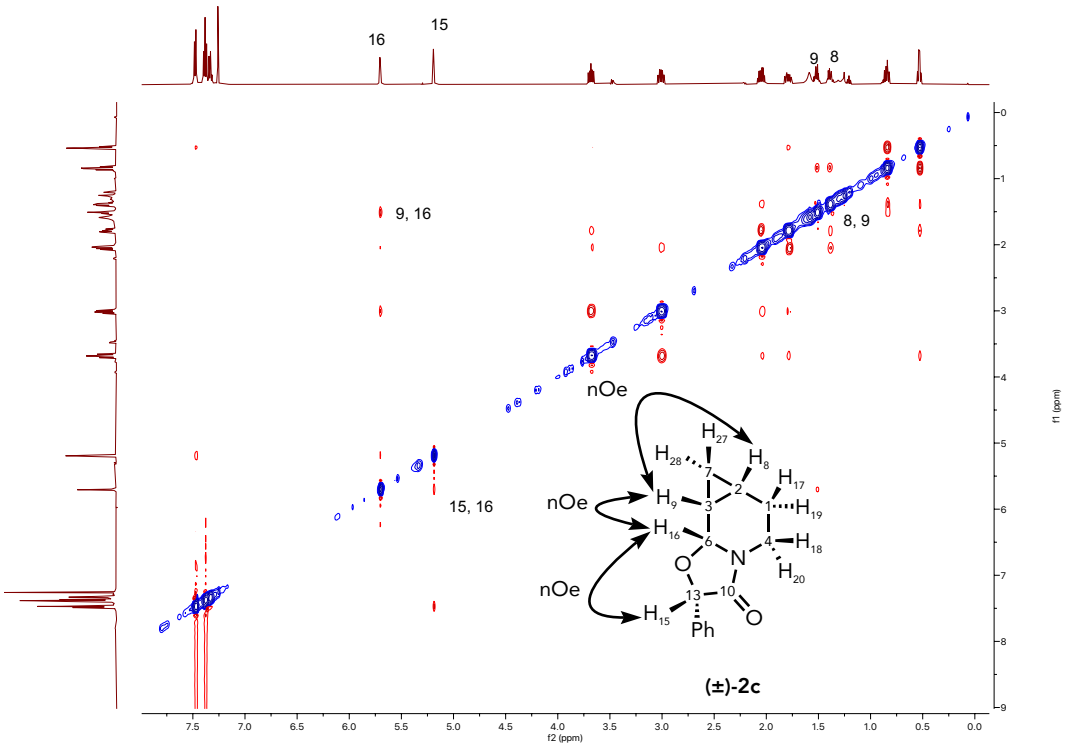
COSY of **2c** in $CDCl_3$ @ 400 MHz.



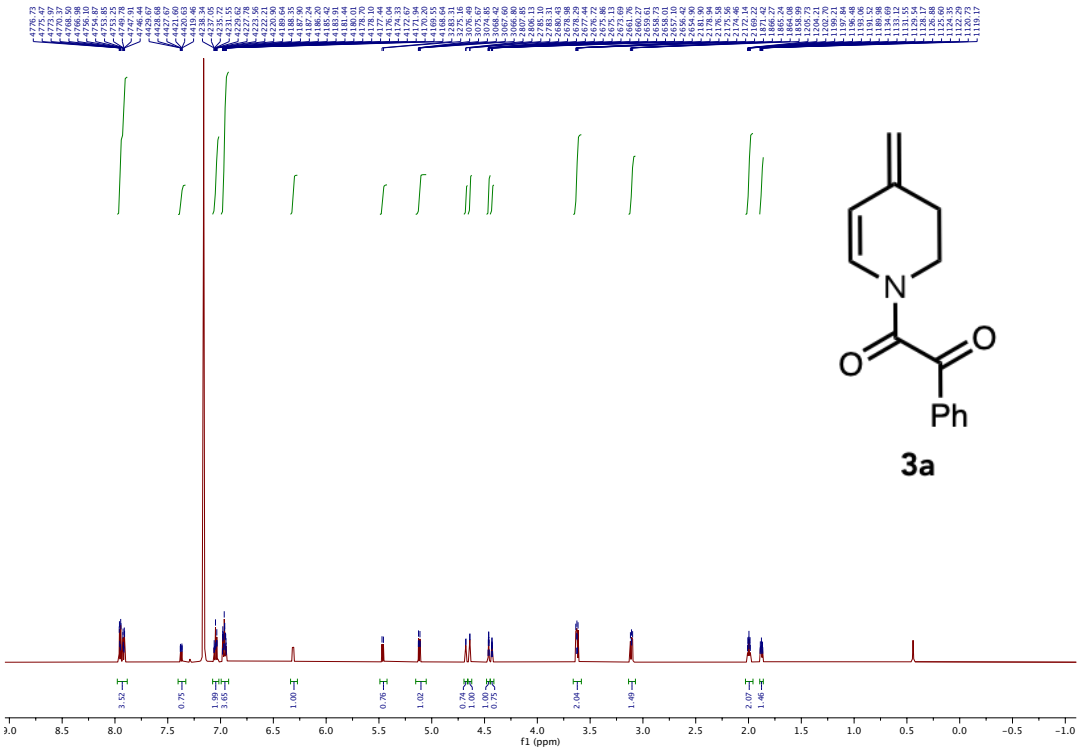
HSQC of **2c** in $CDCl_3$ @ 400 MHz.



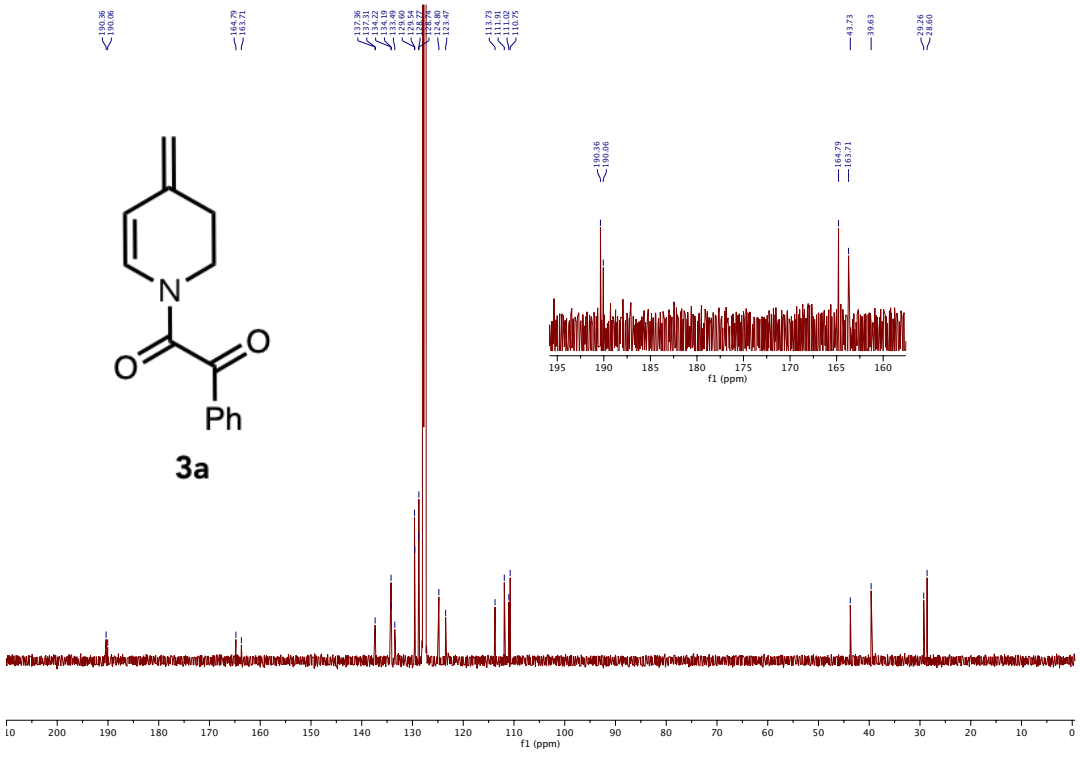
HMBC of **2c** in $CDCl_3$ @ 400 MHz.



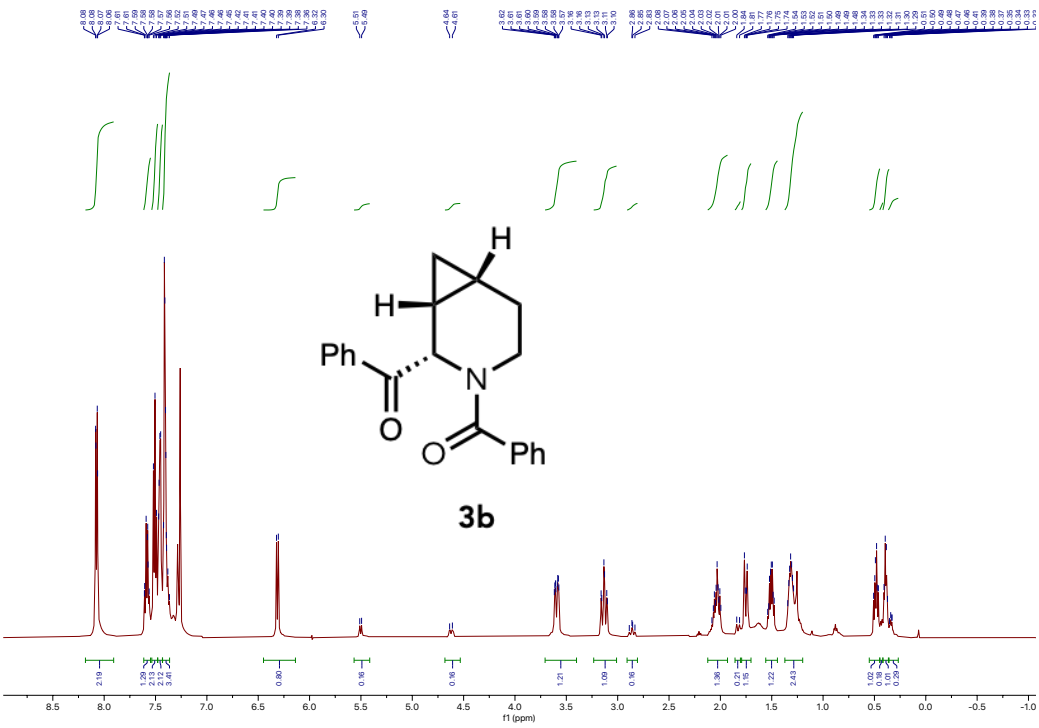
NOESY of **2c** in $CDCl_3$ @ 400 MHz.



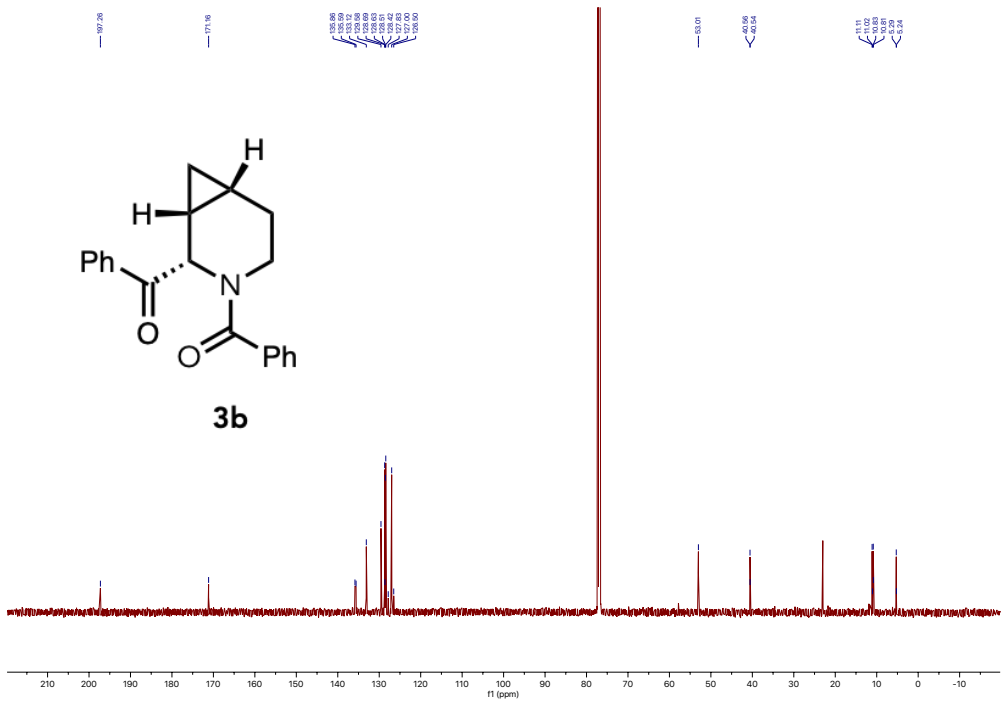
^{1}H NMR spectrum of **3a** in C_6D_6 (mixture of rotamers, 1: ~0.75) @ 600 MHz.



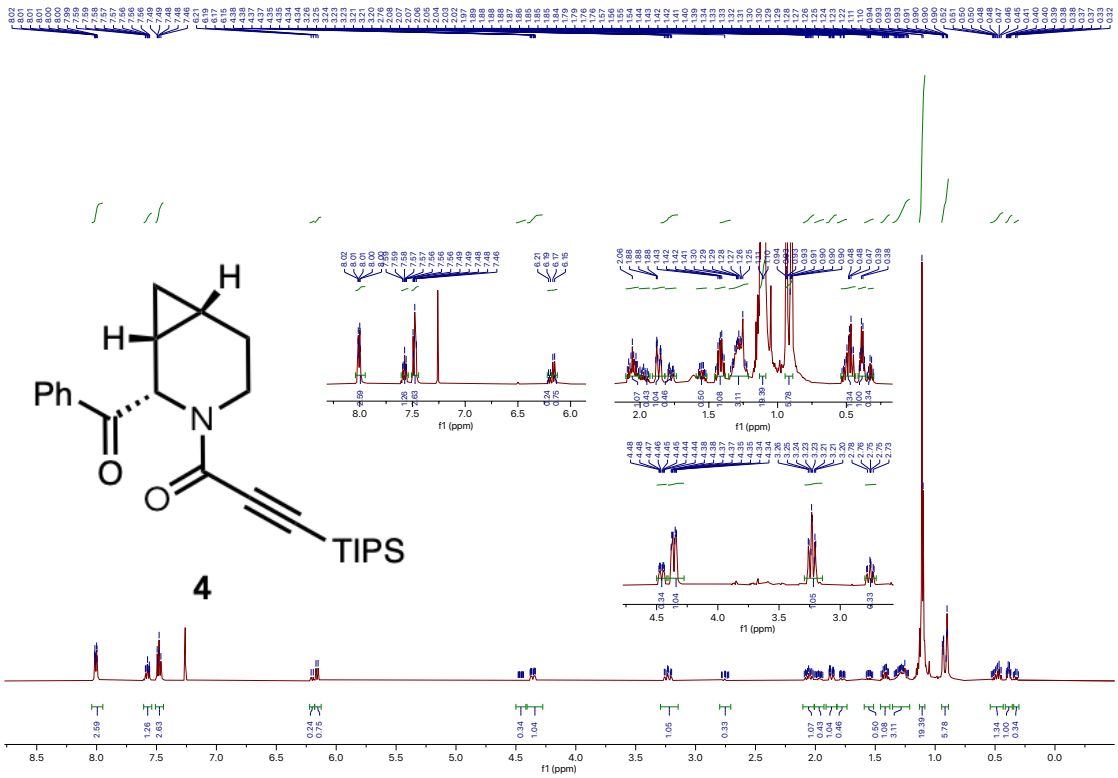
^{13}C{^{1}H} NMR spectrum of **3a** in C_6D_6 @ 151 MHz.



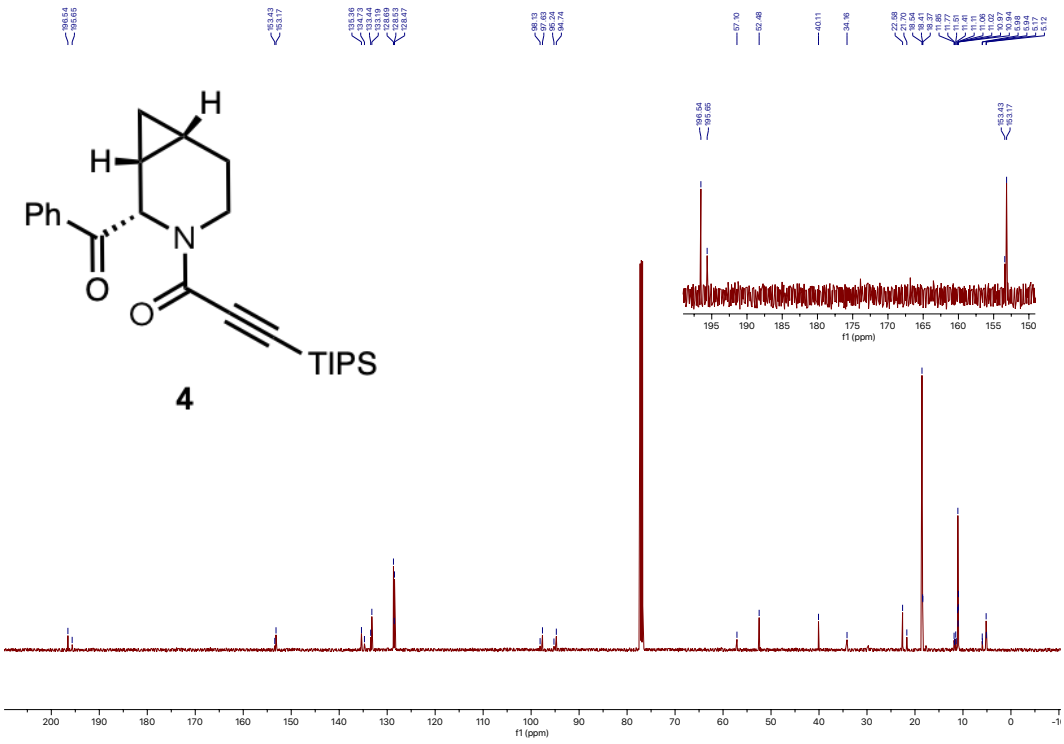
^{1}H NMR of **3b** (1: ~0.2 mixture of rotamers) in $CDCl_3$ @ 500 MHz.



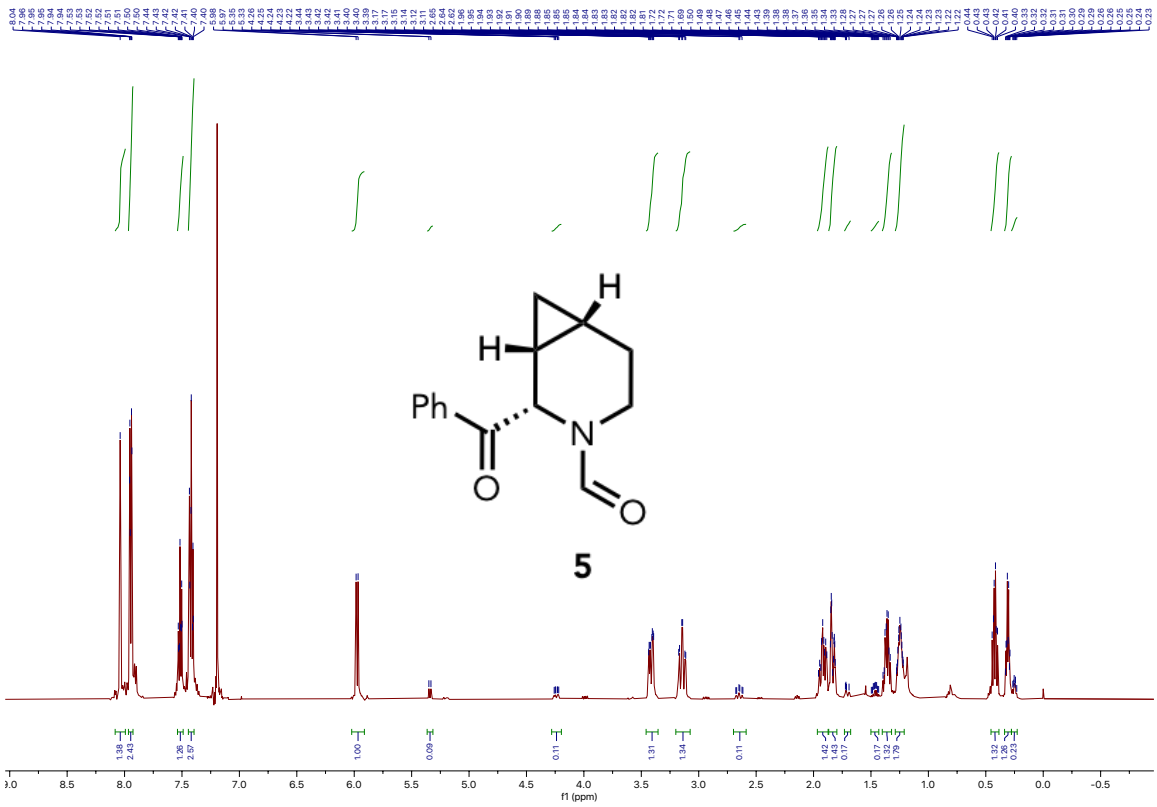
^{13}C{^{1}H} NMR of **3b** (1: ~0.2 mixture of rotamers) in $CDCl_3$ @ 126 MHz.



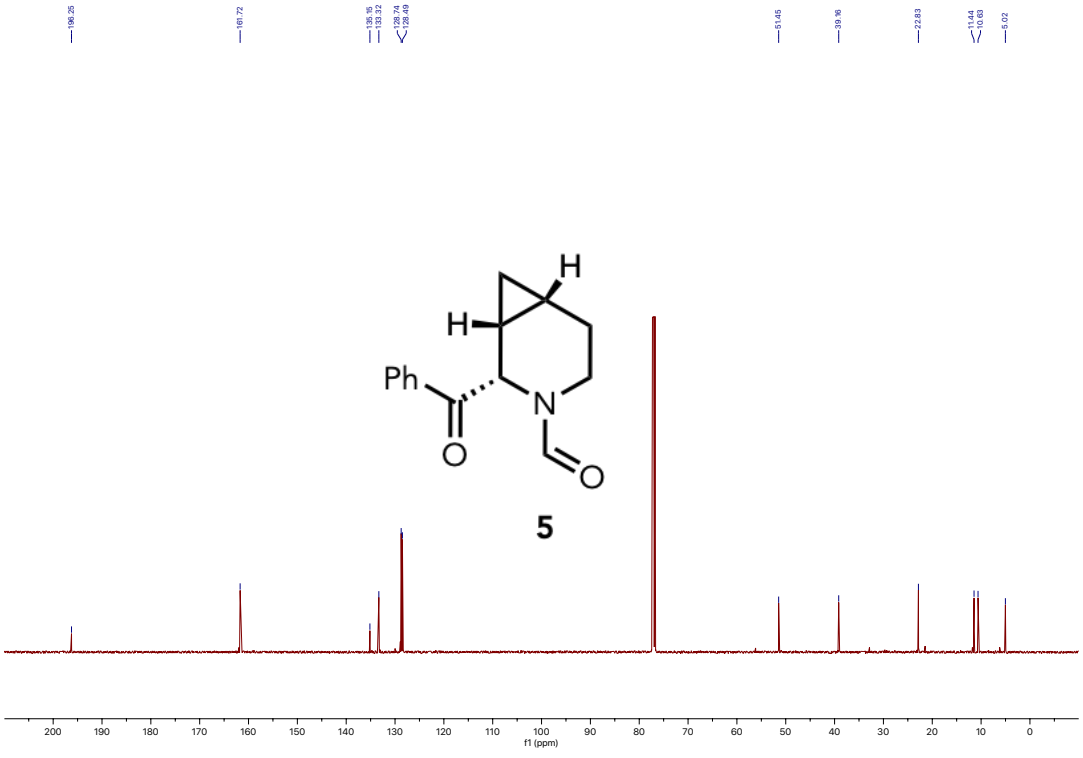
^{1}H NMR of **4** (1: ~0.3 mixture of rotamers) in $CDCl_3$ @ 500 MHz.



^{13}C{^{1}H} NMR of **4** (1: ~0.3 mixture of rotamers) in $CDCl_3$ @ 126 MHz.



^{1}H NMR of **5** (1: ~0.1 mixture of rotamers) in $CDCl_3$ @ 500 MHz.



^{13}C{^{1}H} NMR of **5** (1: ~0.1 mixture of rotamers) in $CDCl_3$ @ 126 MHz.

X-ray Crystallographic data and Methods

Representative Procedure

A colorless block 0.18 x 0.06 x 0.05 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using omega scans. Crystal-to-detector distance was 30.23 mm and exposure time was 0.50 seconds per frame at low angles and 2.00 seconds at high angles, using a scan width of 0.5°. Data collection was 100% complete to 74.000° in ϑ. A total of 14176 reflections were collected covering the indices -12<=h<=12, -14<=k<=14, -12<=l<=14. 2397 reflections were founded to be symmetry independent, with an R_{int} of 0.0447. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P 21/c (No. 14). The data were integrated using the CrysAlis^{Pro} 1.171.40.84a software program and scaled using the SCALE3 ABSPACK scaling algorithm. Solution by intrinsic phasing (SHELXT-2015) produced a heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

ORTEPS

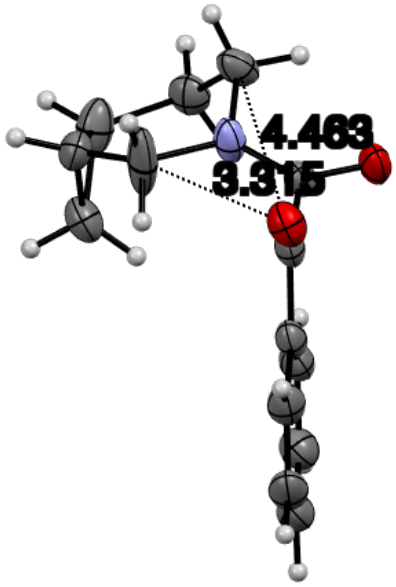


Figure S2. Single crystal XRD structure (major conformer shown, see CIF for more information) of **1**. Reacting methylene position is closer to the ketone carbonyl oxygen by ~1.1 Å. Reactivity at this alpha position leads to the observed major site-isomer **2a**. Ortep drawn at 50% probability level. Minor conformer omitted for clarity.

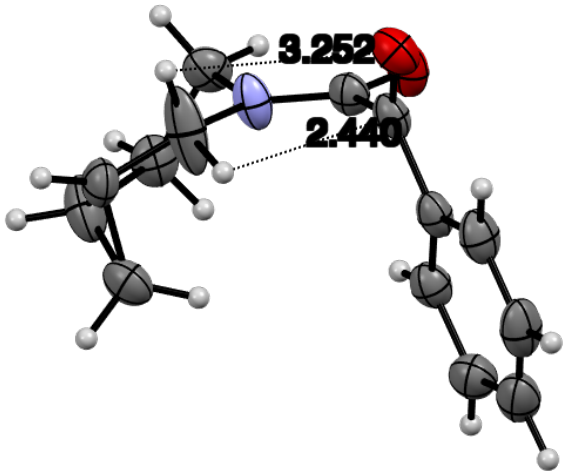


Figure S3. Single crystal XRD structure (major conformer shown) of **1**. Reacting C–H bond is ~0.8 Å closer to the ketone carbonyl oxygen. Hydrogen atom-abstraction from this more proximal methylene C–H bond leads to the observed stereochemistry of the major product **2a**. Ortep drawn at 50% probability level. Minor conformer omitted for clarity.

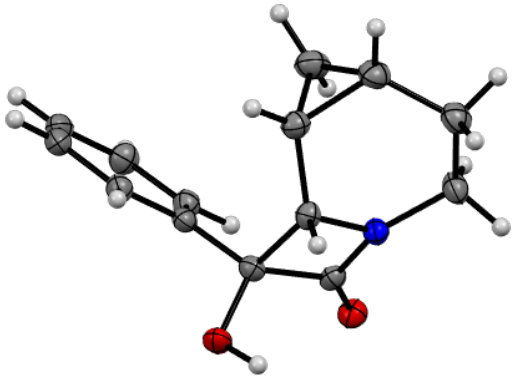


Figure S4. Single crystal XRD structure of compound **2a**. Ortep drawn at 50% probability level.

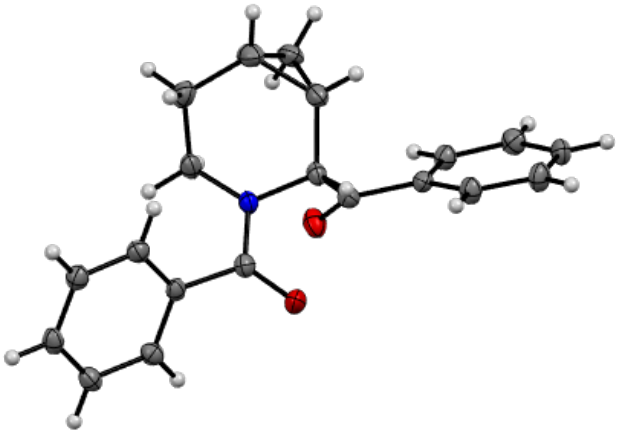


Figure S5. Single crystal XRD structure of compound **3b**. Ortep drawn at 50% probability level.

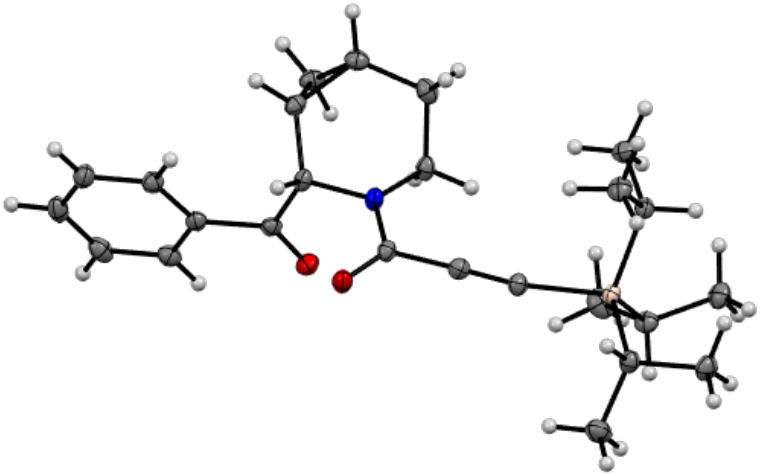


Figure S6. Single crystal XRD structure of compound **4**. Ortep drawn at 50% probability level.

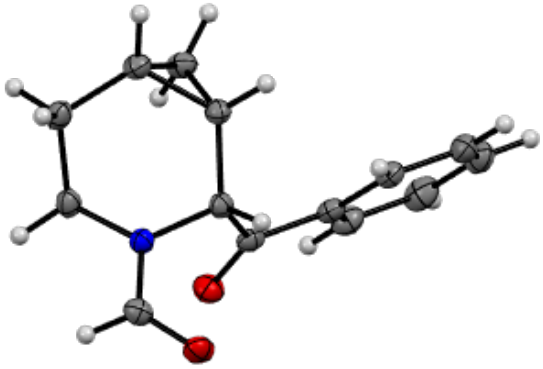
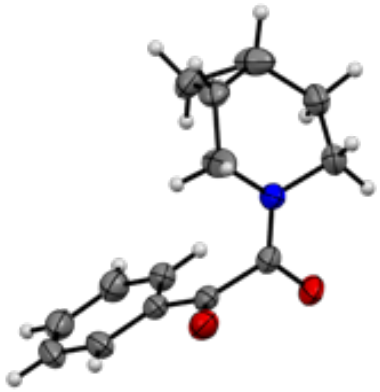


Figure S7. Single crystal XRD structure of compound **5**. Ortep drawn at 50% probability level.

Crystal Data and Structure Refinement



1

Figure S8. Single crystal XRD structure of **1**. Ortep drawn at 50% probability level.

Table S1A. Crystal data and structure refinement for **1**.

Identification code	CRoberts01_Sarpong	
Empirical formula	C14 H15 N O2	
Formula weight	229.27	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 9.8713(2) Å	α= 90°.
	b = 11.2665(2) Å	β= 109.383(3)°.
	c = 11.2229(3) Å	γ = 90°.
Volume	1177.41(5) $Å^3$	
Z	4	
Density (calculated)	1.293 Mg/m^3	
Absorption coefficient	0.696 mm^{-1}	
F(000)	488	
Crystal size	0.180 x 0.060 x 0.050 mm^3	
Theta range for data collection	4.749 to 74.491°.	
Index ranges	-12<=h<=12, -14<=k<=14, -12<=l<=14	
Reflections collected	14176	
Independent reflections	2397 [R(int) = 0.0447]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	1.00000 and 0.76396
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2397 / 12 / 209
Goodness-of-fit on F^2	1.101
Final R indices [I>2sigma(I)]	R1 = 0.0431, wR2 = 0.1158
R indices (all data)	R1 = 0.0490, wR2 = 0.1208
Extinction coefficient	n/a
Largest diff. peak and hole	0.330 and -0.224 e.$Å^{-3}$

Table S1B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6970(1)	6452(1)	9187(1)	43(1)
O(2)	6818(1)	8842(1)	7779(1)	44(1)
N(1)	4909(1)	7679(1)	6727(1)	41(1)
C(1)	8316(1)	6751(1)	6573(1)	38(1)
C(2)	9344(2)	6285(1)	6106(2)	46(1)
C(3)	10224(2)	5369(1)	6742(2)	50(1)
C(4)	10073(2)	4907(1)	7832(2)	50(1)
C(5)	9058(2)	5369(1)	8307(1)	43(1)
C(6)	8179(1)	6305(1)	7681(1)	34(1)
C(7)	7108(1)	6798(1)	8203(1)	34(1)
C(8)	6234(1)	7867(1)	7525(1)	34(1)
C(9)	3974(9)	8690(8)	6170(8)	42(1)
C(10)	3578(5)	8569(5)	4713(6)	44(1)
C(11)	2993(9)	7270(7)	4277(7)	57(3)
C(12)	4030(3)	6360(2)	4258(3)	46(1)
C(13)	3261(3)	6342(3)	5212(4)	40(1)
C(14)	4272(7)	6485(6)	6472(6)	76(2)
C(15)	4113(9)	6555(8)	6563(7)	33(2)
C(16)	3845(9)	6196(5)	5019(8)	70(3)
C(17)	2901(13)	7292(11)	4220(10)	52(4)
C(18)	1837(6)	7586(6)	4727(7)	90(2)
C(19)	3114(9)	8392(8)	4753(10)	50(2)
C(20)	4171(14)	8683(12)	5901(12)	48(3)

Table S1C. Bond lengths [Å] and angles [°] for **1**.

O(1)-C(7)	1.2212(17)
O(2)-C(8)	1.2289(15)
N(1)-C(8)	1.3336(17)
N(1)-C(9)	1.469(9)
N(1)-C(15)	1.470(10)
N(1)-C(14)	1.473(6)
N(1)-C(20)	1.490(14)
C(1)-C(6)	1.389(2)
C(1)-C(2)	1.390(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.385(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.383(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3988(18)
C(5)-H(5)	0.9500
C(6)-C(7)	1.4759(19)
C(7)-C(8)	1.5301(17)
C(9)-C(10)	1.556(9)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.590(8)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(13)	1.442(8)
C(11)-C(12)	1.453(9)
C(11)-H(11)	1.0000
C(12)-C(13)	1.504(4)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.444(7)
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.712(10)
C(15)-H(15A)	0.9900

C(15)-H(15B)	0.9900
C(16)-C(17)	1.626(13)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(19)	1.362(13)
C(17)-C(18)	1.391(13)
C(17)-H(17)	1.0000
C(18)-C(19)	1.546(9)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.402(14)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(8)-N(1)-C(9)	120.0(3)
C(8)-N(1)-C(15)	125.8(4)
C(8)-N(1)-C(14)	122.4(3)
C(9)-N(1)-C(14)	117.3(4)
C(8)-N(1)-C(20)	117.7(5)
C(15)-N(1)-C(20)	116.5(5)
C(6)-C(1)-C(2)	120.08(13)
C(6)-C(1)-H(1)	120.0
C(2)-C(1)-H(1)	120.0
C(3)-C(2)-C(1)	119.93(15)
C(3)-C(2)-H(2)	120.0
C(1)-C(2)-H(2)	120.0
C(4)-C(3)-C(2)	120.19(14)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	120.29(14)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	119.87(15)
C(4)-C(5)-H(5)	120.1
C(6)-C(5)-H(5)	120.1
C(1)-C(6)-C(5)	119.62(13)
C(1)-C(6)-C(7)	121.01(12)
C(5)-C(6)-C(7)	119.36(13)
O(1)-C(7)-C(6)	123.32(12)

O(1)-C(7)-C(8)	119.14(12)
C(6)-C(7)-C(8)	117.30(11)
O(2)-C(8)-N(1)	125.26(12)
O(2)-C(8)-C(7)	116.39(11)
N(1)-C(8)-C(7)	118.34(11)
N(1)-C(9)-C(10)	106.4(5)
N(1)-C(9)-H(9A)	110.5
C(10)-C(9)-H(9A)	110.5
N(1)-C(9)-H(9B)	110.5
C(10)-C(9)-H(9B)	110.5
H(9A)-C(9)-H(9B)	108.6
C(9)-C(10)-C(11)	110.0(5)
C(9)-C(10)-H(10A)	109.7
C(11)-C(10)-H(10A)	109.7
C(9)-C(10)-H(10B)	109.7
C(11)-C(10)-H(10B)	109.7
H(10A)-C(10)-H(10B)	108.2
C(13)-C(11)-C(12)	62.6(4)
C(13)-C(11)-C(10)	118.9(5)
C(12)-C(11)-C(10)	117.9(6)
C(13)-C(11)-H(11)	115.7
C(12)-C(11)-H(11)	115.7
C(10)-C(11)-H(11)	115.7
C(11)-C(12)-C(13)	58.3(3)
C(11)-C(12)-H(12A)	117.9
C(13)-C(12)-H(12A)	117.9
C(11)-C(12)-H(12B)	117.9
C(13)-C(12)-H(12B)	117.9
H(12A)-C(12)-H(12B)	115.1
C(11)-C(13)-C(14)	122.1(4)
C(11)-C(13)-C(12)	59.1(4)
C(14)-C(13)-C(12)	110.3(4)
C(11)-C(13)-H(13)	117.0
C(14)-C(13)-H(13)	117.0
C(12)-C(13)-H(13)	117.0
C(13)-C(14)-N(1)	113.8(5)
C(13)-C(14)-H(14A)	108.8
N(1)-C(14)-H(14A)	108.8
C(13)-C(14)-H(14B)	108.8

N(1)-C(14)-H(14B)	108.8
H(14A)-C(14)-H(14B)	107.7
N(1)-C(15)-C(16)	103.1(5)
N(1)-C(15)-H(15A)	111.1
C(16)-C(15)-H(15A)	111.1
N(1)-C(15)-H(15B)	111.1
C(16)-C(15)-H(15B)	111.1
H(15A)-C(15)-H(15B)	109.1
C(17)-C(16)-C(15)	104.3(6)
C(17)-C(16)-H(16A)	110.9
C(15)-C(16)-H(16A)	110.9
C(17)-C(16)-H(16B)	110.9
C(15)-C(16)-H(16B)	110.9
H(16A)-C(16)-H(16B)	108.9
C(19)-C(17)-C(18)	68.3(6)
C(19)-C(17)-C(16)	118.2(8)
C(18)-C(17)-C(16)	109.1(9)
C(19)-C(17)-H(17)	117.1
C(18)-C(17)-H(17)	117.1
C(16)-C(17)-H(17)	117.1
C(17)-C(18)-C(19)	54.9(6)
C(17)-C(18)-H(18A)	118.3
C(19)-C(18)-H(18A)	118.3
C(17)-C(18)-H(18B)	118.3
C(19)-C(18)-H(18B)	118.3
H(18A)-C(18)-H(18B)	115.5
C(17)-C(19)-C(20)	125.2(10)
C(17)-C(19)-C(18)	56.7(6)
C(20)-C(19)-C(18)	120.5(9)
C(17)-C(19)-H(19)	114.1
C(20)-C(19)-H(19)	114.1
C(18)-C(19)-H(19)	114.1
C(19)-C(20)-N(1)	117.1(10)
C(19)-C(20)-H(20A)	108.0
N(1)-C(20)-H(20A)	108.0
C(19)-C(20)-H(20B)	108.0
N(1)-C(20)-H(20B)	108.0
H(20A)-C(20)-H(20B)	107.3

Symmetry transformations used to generate equivalent atoms:

Table S1D. Anisotropic displacement parameters ($Å^2$x 10^3)for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	53(1)	36(1)	37(1)	-2(1)	10(1)	-3(1)
O(2)	39(1)	24(1)	60(1)	-7(1)	7(1)	-4(1)
N(1)	40(1)	23(1)	47(1)	-1(1)	-3(1)	-1(1)
C(1)	39(1)	30(1)	38(1)	-4(1)	6(1)	2(1)
C(2)	47(1)	44(1)	47(1)	-9(1)	15(1)	1(1)
C(3)	38(1)	45(1)	62(1)	-18(1)	10(1)	2(1)
C(4)	36(1)	36(1)	65(1)	-5(1)	-2(1)	9(1)
C(5)	38(1)	34(1)	44(1)	2(1)	-2(1)	4(1)
C(6)	34(1)	26(1)	34(1)	-5(1)	1(1)	0(1)
C(7)	36(1)	25(1)	34(1)	-5(1)	3(1)	-3(1)
C(8)	35(1)	25(1)	39(1)	-5(1)	9(1)	-1(1)
C(9)	47(2)	32(2)	43(3)	-2(2)	9(2)	12(1)
C(10)	45(2)	31(2)	50(2)	4(1)	8(2)	6(2)
C(11)	52(4)	56(4)	46(4)	10(3)	-5(3)	-16(3)
C(12)	56(2)	37(1)	43(2)	-10(1)	14(1)	-5(1)
C(13)	30(1)	38(2)	49(2)	-7(1)	9(1)	-7(1)
C(14)	68(3)	24(2)	92(5)	7(2)	-31(3)	-14(2)
C(15)	40(3)	37(4)	23(3)	-1(2)	12(3)	-6(2)
C(16)	83(5)	26(2)	71(5)	-10(3)	-16(5)	-2(3)
C(17)	51(6)	59(7)	40(6)	-15(4)	8(4)	18(5)
C(18)	46(3)	82(4)	115(5)	21(4)	-7(3)	-6(3)
C(19)	55(5)	35(3)	45(3)	6(2)	-2(4)	3(3)
C(20)	56(5)	24(3)	48(6)	-2(3)	-6(4)	4(3)

Table S1E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(1)	7708	7376	6134	45
H(2)	9441	6594	5351	56

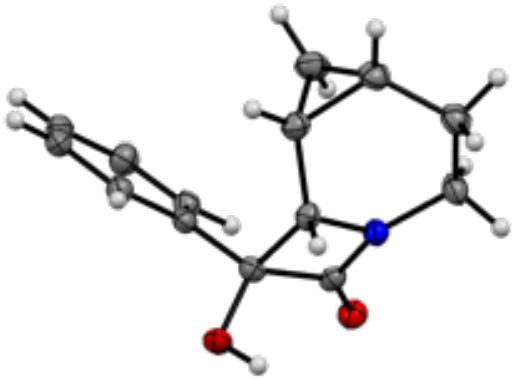
H(3)	10934	5057	6428	60
H(4)	10669	4270	8257	60
H(5)	8959	5051	9058	51
H(9A)	4482	9448	6465	50
H(9B)	3097	8671	6413	50
H(10A)	4437	8726	4468	52
H(10B)	2834	9162	4286	52
H(11)	2049	7228	3580	68
H(12A)	5060	6580	4555	55
H(12B)	3746	5768	3567	55
H(13)	2492	5731	5093	48
H(14A)	5052	5896	6604	91
H(14B)	3777	6312	7089	91
H(15A)	3188	6660	6715	39
H(15B)	4683	5937	7142	39
H(16A)	4772	6126	4863	84
H(16B)	3316	5437	4791	84
H(17)	2614	7250	3279	62
H(18A)	1855	7196	5522	108
H(18B)	872	7792	4139	108
H(19)	2853	9058	4128	60
H(20A)	3722	9189	6388	58
H(20B)	4911	9169	5712	58

Table S1F. Torsion angles [°] for **1**.

C(6)-C(1)-C(2)-C(3)	0.4(2)
C(1)-C(2)-C(3)-C(4)	0.8(2)
C(2)-C(3)-C(4)-C(5)	-1.0(2)
C(3)-C(4)-C(5)-C(6)	0.1(2)
C(2)-C(1)-C(6)-C(5)	-1.3(2)
C(2)-C(1)-C(6)-C(7)	179.19(12)
C(4)-C(5)-C(6)-C(1)	1.0(2)
C(4)-C(5)-C(6)-C(7)	-179.46(12)
C(1)-C(6)-C(7)-O(1)	-178.36(12)
C(5)-C(6)-C(7)-O(1)	2.15(19)
C(1)-C(6)-C(7)-C(8)	-3.97(17)
C(5)-C(6)-C(7)-C(8)	176.55(11)
C(9)-N(1)-C(8)-O(2)	-6.3(4)

C(15)-N(1)-C(8)-O(2)	-169.7(3)
C(14)-N(1)-C(8)-O(2)	-179.6(4)
C(20)-N(1)-C(8)-O(2)	11.7(6)
C(9)-N(1)-C(8)-C(7)	172.9(3)
C(15)-N(1)-C(8)-C(7)	9.4(4)
C(14)-N(1)-C(8)-C(7)	-0.5(4)
C(20)-N(1)-C(8)-C(7)	-169.1(5)
O(1)-C(7)-C(8)-O(2)	93.21(16)
C(6)-C(7)-C(8)-O(2)	-81.43(15)
O(1)-C(7)-C(8)-N(1)	-86.02(16)
C(6)-C(7)-C(8)-N(1)	99.35(15)
C(8)-N(1)-C(9)-C(10)	120.9(4)
C(14)-N(1)-C(9)-C(10)	-65.4(6)
N(1)-C(9)-C(10)-C(11)	51.0(6)
C(9)-C(10)-C(11)-C(13)	-16.6(8)
C(9)-C(10)-C(11)-C(12)	-89.0(6)
C(10)-C(11)-C(12)-C(13)	110.0(6)
C(12)-C(11)-C(13)-C(14)	95.9(5)
C(10)-C(11)-C(13)-C(14)	-12.5(9)
C(10)-C(11)-C(13)-C(12)	-108.4(7)
C(11)-C(12)-C(13)-C(14)	-116.0(5)
C(11)-C(13)-C(14)-N(1)	4.1(9)
C(12)-C(13)-C(14)-N(1)	69.6(6)
C(8)-N(1)-C(14)-C(13)	-149.3(4)
C(9)-N(1)-C(14)-C(13)	37.2(7)
C(8)-N(1)-C(15)-C(16)	-118.1(5)
C(20)-N(1)-C(15)-C(16)	60.4(8)
N(1)-C(15)-C(16)-C(17)	-61.0(8)
C(15)-C(16)-C(17)-C(19)	31.8(12)
C(15)-C(16)-C(17)-C(18)	-43.2(10)
C(16)-C(17)-C(18)-C(19)	113.6(9)
C(18)-C(17)-C(19)-C(20)	106.3(12)
C(16)-C(17)-C(19)-C(20)	5.5(17)
C(16)-C(17)-C(19)-C(18)	-100.8(10)
C(17)-C(18)-C(19)-C(20)	-114.4(12)
C(17)-C(19)-C(20)-N(1)	-13.5(17)
C(18)-C(19)-C(20)-N(1)	55.2(14)
C(8)-N(1)-C(20)-C(19)	153.9(8)
C(15)-N(1)-C(20)-C(19)	-24.8(12)

Symmetry transformations used to generate equivalent atoms:



2a

Figure S9. Single crystal XRD structure of **2a**. Ortep drawn at 50% probability level.

Table S2A. Crystal data and structure refinement for **2a**.

Identification code	JRoque002_Sarpong	
Empirical formula	C14 H15 N O2	
Formula weight	229.27	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	C c	
Unit cell dimensions	a = 11.21720(10) Å	α= 90°.
	b = 11.38930(10) Å	β= 101.0980(10)°.
	c = 18.10010(10) Å	γ = 90°.
Volume	2269.15(3) $Å^3$	
Z	8	
Density (calculated)	1.342 Mg/m^3	
Absorption coefficient	0.723 mm^{-1}	
F(000)	976	
Crystal size	0.520 x 0.250 x 0.230 mm^3	
Theta range for data collection	5.589 to 74.452°.	

Index ranges	-14<=h<=13, -14<=k<=14, -22<=l<=22
Reflections collected	44300
Independent reflections	4472 [R(int) = 0.0560]
Completeness to theta = 74.000°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.60159
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4472 / 2 / 316
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0279, wR2 = 0.0727
R indices (all data)	R1 = 0.0279, wR2 = 0.0728
Absolute structure parameter	-0.01(6)
Extinction coefficient	0.0037(5)
Largest diff. peak and hole	0.213 and -0.153 e.$Å^{-3}$

Table S2B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2031(2)	2775(2)	4750(1)	26(1)
C(2)	1277(2)	2028(2)	5195(1)	28(1)
C(3)	1824(2)	1857(2)	6021(1)	28(1)
C(4)	3190(2)	1816(2)	6300(1)	30(1)
C(5)	2472(2)	2877(2)	6462(1)	23(1)
C(6)	2501(2)	3982(2)	6013(1)	19(1)
C(7)	3684(2)	4762(2)	6066(1)	19(1)
C(8)	3615(2)	4378(2)	5234(1)	19(1)
C(9)	4785(2)	4305(2)	6608(1)	19(1)
C(10)	5792(2)	3853(2)	6362(1)	23(1)
C(11)	6783(2)	3429(2)	6876(1)	26(1)
C(12)	6768(2)	3440(2)	7641(1)	25(1)
C(13)	5758(2)	3873(2)	7888(1)	24(1)
C(14)	4776(2)	4317(2)	7380(1)	23(1)
C(15)	8130(2)	3769(2)	5115(1)	26(1)
C(16)	8732(2)	4571(2)	4612(1)	29(1)
C(17)	8627(2)	4165(2)	3807(1)	28(1)
C(18)	8564(2)	2877(2)	3601(1)	28(1)
C(19)	7434(2)	3629(2)	3407(1)	22(1)

C(20)	6477(2)	3555(2)	3882(1)	20(1)
C(21)	5660(2)	2432(2)	3895(1)	19(1)
C(22)	6395(2)	2275(2)	4709(1)	20(1)
C(23)	5790(2)	1476(2)	3341(1)	19(1)
C(24)	5080(2)	1528(2)	2619(1)	22(1)
C(25)	5157(2)	643(2)	2104(1)	24(1)
C(26)	5958(2)	-293(2)	2292(1)	25(1)
C(27)	6693(2)	-323(2)	3004(1)	25(1)
C(28)	6605(2)	551(2)	3525(1)	23(1)
N(1)	2629(1)	3719(1)	5234(1)	20(1)
N(2)	7021(1)	3272(2)	4671(1)	21(1)
O(1)	4211(1)	4576(1)	4744(1)	23(1)
O(2)	3550(1)	5965(1)	6202(1)	24(1)
O(3)	6430(1)	1548(1)	5213(1)	26(1)
O(4)	4413(1)	2672(1)	3842(1)	24(1)

Table S2C. Bond lengths [Å] and angles [°] for **2a**.

C(1)-N(1)	1.466(2)
C(1)-C(2)	1.533(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.516(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(5)	1.514(3)
C(3)-C(4)	1.519(3)
C(3)-H(3)	1.0000
C(4)-C(5)	1.512(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.502(3)
C(5)-H(5)	1.0000
C(6)-N(1)	1.475(2)
C(6)-C(7)	1.584(3)
C(6)-H(6)	1.0000
C(7)-O(2)	1.405(2)
C(7)-C(9)	1.514(2)
C(7)-C(8)	1.556(2)

C(8)-O(1)	1.230(2)
C(8)-N(1)	1.337(3)
C(9)-C(10)	1.391(3)
C(9)-C(14)	1.398(3)
C(10)-C(11)	1.391(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.388(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.386(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.387(3)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-N(2)	1.459(2)
C(15)-C(16)	1.534(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.512(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.512(3)
C(17)-C(19)	1.522(3)
C(17)-H(17)	1.0000
C(18)-C(19)	1.514(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.502(3)
C(19)-H(19)	1.0000
C(20)-N(2)	1.476(2)
C(20)-C(21)	1.576(3)
C(20)-H(20)	1.0000
C(21)-O(4)	1.411(2)
C(21)-C(23)	1.506(3)
C(21)-C(22)	1.554(2)
C(22)-O(3)	1.226(2)
C(22)-N(2)	1.343(3)
C(23)-C(28)	1.393(3)
C(23)-C(24)	1.396(3)
C(24)-C(25)	1.386(3)

C(24)-H(24)	0.9500
C(25)-C(26)	1.393(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.390(3)
C(26)-H(26)	0.9500
C(27)-C(28)	1.388(3)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
O(2)-H(2)	0.91(4)
O(4)-H(4)	0.90(3)
N(1)-C(1)-C(2)	109.20(16)
N(1)-C(1)-H(1A)	109.8
C(2)-C(1)-H(1A)	109.8
N(1)-C(1)-H(1B)	109.8
C(2)-C(1)-H(1B)	109.8
H(1A)-C(1)-H(1B)	108.3
C(3)-C(2)-C(1)	115.45(17)
C(3)-C(2)-H(2A)	108.4
C(1)-C(2)-H(2A)	108.4
C(3)-C(2)-H(2B)	108.4
C(1)-C(2)-H(2B)	108.4
H(2A)-C(2)-H(2B)	107.5
C(5)-C(3)-C(2)	118.92(17)
C(5)-C(3)-C(4)	59.81(13)
C(2)-C(3)-C(4)	121.51(19)
C(5)-C(3)-H(3)	115.1
C(2)-C(3)-H(3)	115.1
C(4)-C(3)-H(3)	115.1
C(5)-C(4)-C(3)	59.94(14)
C(5)-C(4)-H(4A)	117.8
C(3)-C(4)-H(4A)	117.8
C(5)-C(4)-H(4B)	117.8
C(3)-C(4)-H(4B)	117.8
H(4A)-C(4)-H(4B)	114.9
C(6)-C(5)-C(4)	119.81(17)
C(6)-C(5)-C(3)	114.59(16)
C(4)-C(5)-C(3)	60.25(14)
C(6)-C(5)-H(5)	116.7
C(4)-C(5)-H(5)	116.7

C(3)-C(5)-H(5)	116.7
N(1)-C(6)-C(5)	111.31(15)
N(1)-C(6)-C(7)	86.40(13)
C(5)-C(6)-C(7)	122.82(15)
N(1)-C(6)-H(6)	111.2
C(5)-C(6)-H(6)	111.2
C(7)-C(6)-H(6)	111.2
O(2)-C(7)-C(9)	108.82(15)
O(2)-C(7)-C(8)	117.15(15)
C(9)-C(7)-C(8)	114.40(15)
O(2)-C(7)-C(6)	116.15(15)
C(9)-C(7)-C(6)	114.60(15)
C(8)-C(7)-C(6)	84.21(13)
O(1)-C(8)-N(1)	131.89(17)
O(1)-C(8)-C(7)	135.59(17)
N(1)-C(8)-C(7)	92.53(14)
C(10)-C(9)-C(14)	119.09(17)
C(10)-C(9)-C(7)	122.09(17)
C(14)-C(9)-C(7)	118.80(17)
C(9)-C(10)-C(11)	120.51(18)
C(9)-C(10)-H(10)	119.7
C(11)-C(10)-H(10)	119.7
C(12)-C(11)-C(10)	120.19(19)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(13)-C(12)-C(11)	119.44(18)
C(13)-C(12)-H(12)	120.3
C(11)-C(12)-H(12)	120.3
C(12)-C(13)-C(14)	120.70(19)
C(12)-C(13)-H(13)	119.6
C(14)-C(13)-H(13)	119.6
C(13)-C(14)-C(9)	120.05(19)
C(13)-C(14)-H(14)	120.0
C(9)-C(14)-H(14)	120.0
N(2)-C(15)-C(16)	109.34(16)
N(2)-C(15)-H(15A)	109.8
C(16)-C(15)-H(15A)	109.8
N(2)-C(15)-H(15B)	109.8
C(16)-C(15)-H(15B)	109.8

H(15A)-C(15)-H(15B)	108.3
C(17)-C(16)-C(15)	115.34(17)
C(17)-C(16)-H(16A)	108.4
C(15)-C(16)-H(16A)	108.4
C(17)-C(16)-H(16B)	108.4
C(15)-C(16)-H(16B)	108.4
H(16A)-C(16)-H(16B)	107.5
C(16)-C(17)-C(18)	121.73(19)
C(16)-C(17)-C(19)	118.69(17)
C(18)-C(17)-C(19)	59.87(13)
C(16)-C(17)-H(17)	115.1
C(18)-C(17)-H(17)	115.1
C(19)-C(17)-H(17)	115.1
C(17)-C(18)-C(19)	60.40(13)
C(17)-C(18)-H(18A)	117.7
C(19)-C(18)-H(18A)	117.7
C(17)-C(18)-H(18B)	117.7
C(19)-C(18)-H(18B)	117.7
H(18A)-C(18)-H(18B)	114.9
C(20)-C(19)-C(18)	119.59(16)
C(20)-C(19)-C(17)	114.14(16)
C(18)-C(19)-C(17)	59.73(13)
C(20)-C(19)-H(19)	116.9
C(18)-C(19)-H(19)	116.9
C(17)-C(19)-H(19)	116.9
N(2)-C(20)-C(19)	111.04(15)
N(2)-C(20)-C(21)	86.63(13)
C(19)-C(20)-C(21)	122.37(16)
N(2)-C(20)-H(20)	111.4
C(19)-C(20)-H(20)	111.4
C(21)-C(20)-H(20)	111.4
O(4)-C(21)-C(23)	108.46(14)
O(4)-C(21)-C(22)	115.20(15)
C(23)-C(21)-C(22)	116.49(16)
O(4)-C(21)-C(20)	114.42(15)
C(23)-C(21)-C(20)	116.46(15)
C(22)-C(21)-C(20)	84.47(13)
O(3)-C(22)-N(2)	131.81(18)
O(3)-C(22)-C(21)	135.85(17)

N(2)-C(22)-C(21)	92.33(14)
C(28)-C(23)-C(24)	119.08(17)
C(28)-C(23)-C(21)	122.09(16)
C(24)-C(23)-C(21)	118.83(17)
C(25)-C(24)-C(23)	120.04(18)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	120.86(18)
C(24)-C(25)-H(25)	119.6
C(26)-C(25)-H(25)	119.6
C(27)-C(26)-C(25)	119.00(18)
C(27)-C(26)-H(26)	120.5
C(25)-C(26)-H(26)	120.5
C(28)-C(27)-C(26)	120.35(18)
C(28)-C(27)-H(27)	119.8
C(26)-C(27)-H(27)	119.8
C(27)-C(28)-C(23)	120.62(18)
C(27)-C(28)-H(28)	119.7
C(23)-C(28)-H(28)	119.7
C(8)-N(1)-C(1)	134.06(17)
C(8)-N(1)-C(6)	96.84(14)
C(1)-N(1)-C(6)	127.07(16)
C(22)-N(2)-C(15)	134.29(16)
C(22)-N(2)-C(20)	96.45(14)
C(15)-N(2)-C(20)	126.66(16)
C(7)-O(2)-H(2)	107(2)
C(21)-O(4)-H(4)	107.7(19)

Symmetry transformations used to generate equivalent atoms:

Table S2D. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(1)	27(1)	24(1)	-5(1)	3(1)	-8(1)
C(2)	23(1)	27(1)	32(1)	-2(1)	3(1)	-6(1)
C(3)	26(1)	24(1)	33(1)	4(1)	5(1)	-5(1)
C(4)	28(1)	24(1)	38(1)	5(1)	4(1)	2(1)

C(5)	20(1)	23(1)	24(1)	3(1)	4(1)	0(1)
C(6)	17(1)	22(1)	19(1)	0(1)	3(1)	1(1)
C(7)	20(1)	17(1)	20(1)	-1(1)	4(1)	0(1)
C(8)	19(1)	18(1)	20(1)	2(1)	2(1)	3(1)
C(9)	19(1)	16(1)	22(1)	0(1)	1(1)	-2(1)
C(10)	21(1)	25(1)	23(1)	-1(1)	2(1)	-2(1)
C(11)	20(1)	27(1)	31(1)	0(1)	2(1)	2(1)
C(12)	22(1)	20(1)	30(1)	2(1)	-3(1)	-2(1)
C(13)	28(1)	20(1)	22(1)	0(1)	-1(1)	-4(1)
C(14)	22(1)	22(1)	22(1)	-2(1)	2(1)	-2(1)
C(15)	19(1)	33(1)	24(1)	-5(1)	0(1)	-5(1)
C(16)	23(1)	28(1)	36(1)	-4(1)	4(1)	-9(1)
C(17)	24(1)	27(1)	35(1)	-2(1)	10(1)	-5(1)
C(18)	24(1)	27(1)	32(1)	-3(1)	7(1)	0(1)
C(19)	23(1)	21(1)	23(1)	0(1)	6(1)	-1(1)
C(20)	18(1)	21(1)	20(1)	1(1)	1(1)	0(1)
C(21)	14(1)	22(1)	20(1)	1(1)	1(1)	-1(1)
C(22)	18(1)	22(1)	20(1)	-2(1)	3(1)	1(1)
C(23)	15(1)	19(1)	21(1)	0(1)	3(1)	-5(1)
C(24)	16(1)	26(1)	22(1)	1(1)	2(1)	0(1)
C(25)	22(1)	31(1)	20(1)	-2(1)	2(1)	-2(1)
C(26)	27(1)	23(1)	26(1)	-3(1)	8(1)	-5(1)
C(27)	25(1)	20(1)	29(1)	2(1)	5(1)	2(1)
C(28)	22(1)	22(1)	22(1)	2(1)	1(1)	-1(1)
N(1)	20(1)	20(1)	19(1)	-1(1)	3(1)	-2(1)
N(2)	17(1)	24(1)	19(1)	1(1)	1(1)	-2(1)
O(1)	21(1)	27(1)	22(1)	1(1)	6(1)	-1(1)
O(2)	26(1)	17(1)	27(1)	-1(1)	1(1)	2(1)
O(3)	29(1)	26(1)	21(1)	4(1)	1(1)	0(1)
O(4)	14(1)	31(1)	26(1)	-4(1)	2(1)	1(1)

Table S2E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2a**.

	x	y	z	U(eq)
H(1A)	2649	2279	4577	31
H(1B)	1497	3114	4301	31

H(2A)	469	2398	5156	33
H(2B)	1150	1245	4954	33
H(3)	1340	1351	6305	33
H(4A)	3508	1282	6724	36
H(4B)	3717	1901	5923	36
H(5)	2351	2973	6992	27
H(6)	1769	4479	6022	23
H(10)	5804	3834	5839	28
H(11)	7471	3132	6703	32
H(12)	7445	3152	7993	30
H(13)	5738	3866	8410	29
H(14)	4097	4630	7556	27
H(15A)	8695	3130	5322	31
H(15B)	7933	4226	5541	31
H(16A)	8366	5362	4609	35
H(16B)	9604	4645	4841	35
H(17)	9046	4674	3486	34
H(18A)	8604	2299	4014	33
H(18B)	8959	2623	3183	33
H(19)	7154	3838	2864	27
H(20)	5984	4291	3848	24
H(24)	4542	2169	2479	26
H(25)	4659	676	1617	29
H(26)	6000	-902	1940	30
H(27)	7259	-944	3135	30
H(28)	7106	518	4012	27
H(2)	2830(30)	6190(30)	5911(19)	56(10)
H(4)	4350(30)	3320(30)	4118(17)	37(7)

Table S2F. Torsion angles [°] for **2a**.

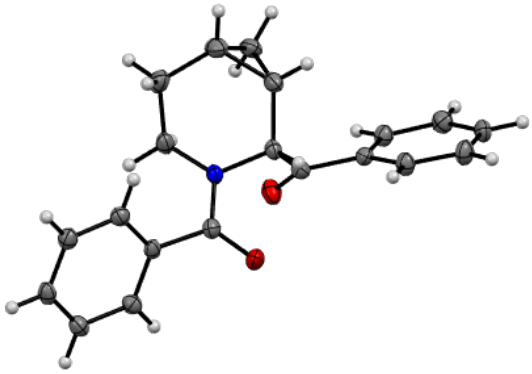
N(1)-C(1)-C(2)-C(3)	-36.1(2)
C(1)-C(2)-C(3)-C(5)	38.9(3)
C(1)-C(2)-C(3)-C(4)	-31.5(3)
C(2)-C(3)-C(4)-C(5)	107.4(2)
C(3)-C(4)-C(5)-C(6)	-103.0(2)
C(2)-C(3)-C(5)-C(6)	-0.1(3)
C(4)-C(3)-C(5)-C(6)	111.60(19)
C(2)-C(3)-C(5)-C(4)	-111.7(2)

C(4)-C(5)-C(6)-N(1)	32.5(2)
C(3)-C(5)-C(6)-N(1)	-36.0(2)
C(4)-C(5)-C(6)-C(7)	-67.4(2)
C(3)-C(5)-C(6)-C(7)	-135.85(18)
N(1)-C(6)-C(7)-O(2)	118.43(16)
C(5)-C(6)-C(7)-O(2)	-128.45(18)
N(1)-C(6)-C(7)-C(9)	-113.25(15)
C(5)-C(6)-C(7)-C(9)	-0.1(2)
N(1)-C(6)-C(7)-C(8)	0.97(12)
C(5)-C(6)-C(7)-C(8)	114.09(18)
O(2)-C(7)-C(8)-O(1)	62.6(3)
C(9)-C(7)-C(8)-O(1)	-66.5(3)
C(6)-C(7)-C(8)-O(1)	179.1(2)
O(2)-C(7)-C(8)-N(1)	-117.55(17)
C(9)-C(7)-C(8)-N(1)	113.35(16)
C(6)-C(7)-C(8)-N(1)	-1.07(14)
O(2)-C(7)-C(9)-C(10)	-117.20(18)
C(8)-C(7)-C(9)-C(10)	16.0(2)
C(6)-C(7)-C(9)-C(10)	110.88(19)
O(2)-C(7)-C(9)-C(14)	64.2(2)
C(8)-C(7)-C(9)-C(14)	-162.70(16)
C(6)-C(7)-C(9)-C(14)	-67.8(2)
C(14)-C(9)-C(10)-C(11)	-0.6(3)
C(7)-C(9)-C(10)-C(11)	-179.28(17)
C(9)-C(10)-C(11)-C(12)	0.9(3)
C(10)-C(11)-C(12)-C(13)	0.1(3)
C(11)-C(12)-C(13)-C(14)	-1.4(3)
C(12)-C(13)-C(14)-C(9)	1.6(3)
C(10)-C(9)-C(14)-C(13)	-0.6(3)
C(7)-C(9)-C(14)-C(13)	178.12(17)
N(2)-C(15)-C(16)-C(17)	-35.9(2)
C(15)-C(16)-C(17)-C(18)	-30.7(3)
C(15)-C(16)-C(17)-C(19)	39.8(3)
C(16)-C(17)-C(18)-C(19)	107.1(2)
C(17)-C(18)-C(19)-C(20)	-102.3(2)
C(16)-C(17)-C(19)-C(20)	-0.7(3)
C(18)-C(17)-C(19)-C(20)	111.41(19)
C(16)-C(17)-C(19)-C(18)	-112.1(2)
C(18)-C(19)-C(20)-N(2)	30.8(2)

C(17)-C(19)-C(20)-N(2)	-36.9(2)
C(18)-C(19)-C(20)-C(21)	-69.0(2)
C(17)-C(19)-C(20)-C(21)	-136.60(18)
N(2)-C(20)-C(21)-O(4)	112.85(15)
C(19)-C(20)-C(21)-O(4)	-134.29(17)
N(2)-C(20)-C(21)-C(23)	-119.25(16)
C(19)-C(20)-C(21)-C(23)	-6.4(2)
N(2)-C(20)-C(21)-C(22)	-2.35(13)
C(19)-C(20)-C(21)-C(22)	110.50(18)
O(4)-C(21)-C(22)-O(3)	68.2(3)
C(23)-C(21)-C(22)-O(3)	-60.5(3)
C(20)-C(21)-C(22)-O(3)	-177.4(2)
O(4)-C(21)-C(22)-N(2)	-111.84(17)
C(23)-C(21)-C(22)-N(2)	119.45(16)
C(20)-C(21)-C(22)-N(2)	2.58(14)
O(4)-C(21)-C(23)-C(28)	-137.44(17)
C(22)-C(21)-C(23)-C(28)	-5.5(2)
C(20)-C(21)-C(23)-C(28)	91.8(2)
O(4)-C(21)-C(23)-C(24)	43.2(2)
C(22)-C(21)-C(23)-C(24)	175.15(16)
C(20)-C(21)-C(23)-C(24)	-87.5(2)
C(28)-C(23)-C(24)-C(25)	2.4(3)
C(21)-C(23)-C(24)-C(25)	-178.27(17)
C(23)-C(24)-C(25)-C(26)	-1.3(3)
C(24)-C(25)-C(26)-C(27)	-0.8(3)
C(25)-C(26)-C(27)-C(28)	1.8(3)
C(26)-C(27)-C(28)-C(23)	-0.7(3)
C(24)-C(23)-C(28)-C(27)	-1.4(3)
C(21)-C(23)-C(28)-C(27)	179.29(18)
O(1)-C(8)-N(1)-C(1)	17.1(4)
C(7)-C(8)-N(1)-C(1)	-162.8(2)
O(1)-C(8)-N(1)-C(6)	-179.0(2)
C(7)-C(8)-N(1)-C(6)	1.15(15)
C(2)-C(1)-N(1)-C(8)	156.8(2)
C(2)-C(1)-N(1)-C(6)	-3.1(3)
C(5)-C(6)-N(1)-C(8)	-125.08(16)
C(7)-C(6)-N(1)-C(8)	-1.14(14)
C(5)-C(6)-N(1)-C(1)	40.5(2)
C(7)-C(6)-N(1)-C(1)	164.45(18)

O(3)-C(22)-N(2)-C(15)	15.5(4)
C(21)-C(22)-N(2)-C(15)	-164.5(2)
O(3)-C(22)-N(2)-C(20)	177.2(2)
C(21)-C(22)-N(2)-C(20)	-2.76(15)
C(16)-C(15)-N(2)-C(22)	152.0(2)
C(16)-C(15)-N(2)-C(20)	-5.1(3)
C(19)-C(20)-N(2)-C(22)	-120.78(16)
C(21)-C(20)-N(2)-C(22)	2.73(15)
C(19)-C(20)-N(2)-C(15)	43.0(2)
C(21)-C(20)-N(2)-C(15)	166.48(18)

Symmetry transformations used to generate equivalent atoms:



3b

Figure S10. Single crystal XRD structure of **3b**. Ortep drawn at 50% probability level.

Table S3A. Crystal data and structure refinement for **3b**.

Identification code	CRoberts04_Sarpong	
Empirical formula	C20 H19 N O2	
Formula weight	305.36	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	I a	
Unit cell dimensions	a = 10.52883(16) Å	α= 90°.
	b = 10.98437(15) Å	β= 95.4721(13)°.

	c = 13.37045(19) Å γ = 90°.
Volume	1539.28(4) $Å^3$
Z	4
Density (calculated)	1.318 Mg/m^3
Absorption coefficient	0.673 mm^{-1}
F(000)	648
Crystal size	0.180 x 0.110 x 0.080 mm^3
Theta range for data collection	5.221 to 66.594°.
Index ranges	-12<=h<=12, -13<=k<=13, -15<=l<=15
Reflections collected	17793
Independent reflections	2715 [R(int) = 0.0380]
Completeness to theta = 66.594°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.78956
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2715 / 2 / 208
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0257, wR2 = 0.0657
R indices (all data)	R1 = 0.0260, wR2 = 0.0660
Absolute structure parameter	0.02(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.102 and -0.163 e.$Å^{-3}$

Table S3B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5104(2)	6578(1)	4536(1)	28(1)
O(2)	3116(1)	4199(1)	5215(1)	28(1)
N(1)	5458(1)	4549(1)	4485(1)	19(1)
C(1)	5391(2)	5672(2)	4068(1)	20(1)
C(2)	5738(2)	5800(2)	3007(1)	19(1)
C(3)	6927(2)	5427(2)	2744(1)	21(1)
C(4)	7262(2)	5641(2)	1782(1)	23(1)
C(5)	6411(2)	6216(2)	1074(1)	23(1)
C(6)	5233(2)	6591(2)	1333(2)	23(1)
C(7)	4899(2)	6396(2)	2302(1)	21(1)
C(8)	5404(2)	3408(2)	3915(1)	23(1)

C(9)	6522(2)	2588(2)	4259(2)	30(1)
C(10)	6619(2)	2399(2)	5387(2)	30(1)
C(11)	5455(2)	2095(2)	5901(2)	29(1)
C(12)	6061(2)	3343(2)	6038(2)	25(1)
C(13)	5377(2)	4469(2)	5566(1)	19(1)
C(14)	4000(2)	4432(2)	5835(1)	19(1)
C(15)	3813(2)	4580(2)	6925(1)	19(1)
C(16)	4482(2)	5451(2)	7521(1)	23(1)
C(17)	4258(2)	5590(2)	8520(2)	27(1)
C(18)	3401(2)	4830(2)	8938(1)	24(1)
C(19)	2748(2)	3945(2)	8353(2)	25(1)
C(20)	2933(2)	3834(2)	7342(1)	22(1)

Table S3C. Bond lengths [Å] and angles [°] for **3b**.

O(1)-C(1)	1.228(2)
O(2)-C(14)	1.214(2)
N(1)-C(1)	1.353(2)
N(1)-C(13)	1.458(2)
N(1)-C(8)	1.465(2)
C(1)-C(2)	1.504(2)
C(2)-C(7)	1.392(3)
C(2)-C(3)	1.394(3)
C(3)-C(4)	1.386(3)
C(4)-C(5)	1.391(3)
C(5)-C(6)	1.383(3)
C(6)-C(7)	1.391(3)
C(8)-C(9)	1.518(3)
C(9)-C(10)	1.515(3)
C(10)-C(11)	1.499(3)
C(10)-C(12)	1.509(3)
C(11)-C(12)	1.516(3)
C(12)-C(13)	1.536(3)
C(13)-C(14)	1.527(3)
C(14)-C(15)	1.499(2)
C(15)-C(16)	1.392(3)
C(15)-C(20)	1.393(3)
C(16)-C(17)	1.387(3)
C(17)-C(18)	1.386(3)

C(18)-C(19)	1.389(3)
C(19)-C(20)	1.388(3)
C(1)-N(1)-C(13)	117.24(15)
C(1)-N(1)-C(8)	124.59(14)
C(13)-N(1)-C(8)	117.44(15)
O(1)-C(1)-N(1)	122.31(16)
O(1)-C(1)-C(2)	119.87(17)
N(1)-C(1)-C(2)	117.77(15)
C(7)-C(2)-C(3)	119.61(17)
C(7)-C(2)-C(1)	119.12(17)
C(3)-C(2)-C(1)	121.03(16)
C(4)-C(3)-C(2)	119.94(17)
C(3)-C(4)-C(5)	120.27(18)
C(6)-C(5)-C(4)	119.99(17)
C(5)-C(6)-C(7)	119.97(18)
C(6)-C(7)-C(2)	120.19(18)
N(1)-C(8)-C(9)	111.04(16)
C(10)-C(9)-C(8)	111.08(16)
C(11)-C(10)-C(12)	60.53(14)
C(11)-C(10)-C(9)	120.38(18)
C(12)-C(10)-C(9)	119.11(17)
C(10)-C(11)-C(12)	60.05(14)
C(10)-C(12)-C(11)	59.42(14)
C(10)-C(12)-C(13)	120.65(16)
C(11)-C(12)-C(13)	120.22(16)
N(1)-C(13)-C(14)	112.45(14)
N(1)-C(13)-C(12)	112.70(15)
C(14)-C(13)-C(12)	107.46(15)
O(2)-C(14)-C(15)	121.59(17)
O(2)-C(14)-C(13)	121.92(17)
C(15)-C(14)-C(13)	116.24(15)
C(16)-C(15)-C(20)	119.64(17)
C(16)-C(15)-C(14)	121.68(16)
C(20)-C(15)-C(14)	118.68(17)
C(17)-C(16)-C(15)	120.23(17)
C(18)-C(17)-C(16)	119.94(18)
C(17)-C(18)-C(19)	120.10(17)
C(20)-C(19)-C(18)	120.11(18)
C(19)-C(20)-C(15)	119.91(18)

Symmetry transformations used to generate equivalent atoms:

Table S3D. Anisotropic displacement parameters ($Å^2$x 10^3)for **3b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	41(1)	25(1)	19(1)	-2(1)	5(1)	8(1)
O(2)	21(1)	44(1)	19(1)	-3(1)	-1(1)	1(1)
N(1)	24(1)	20(1)	14(1)	0(1)	3(1)	0(1)
C(1)	21(1)	22(1)	17(1)	-2(1)	1(1)	1(1)
C(2)	24(1)	15(1)	16(1)	-2(1)	1(1)	-3(1)
C(3)	23(1)	19(1)	20(1)	0(1)	1(1)	-1(1)
C(4)	26(1)	20(1)	23(1)	-2(1)	6(1)	-2(1)
C(5)	30(1)	22(1)	17(1)	1(1)	6(1)	-6(1)
C(6)	26(1)	23(1)	18(1)	3(1)	-2(1)	-4(1)
C(7)	21(1)	21(1)	21(1)	2(1)	3(1)	-1(1)
C(8)	32(1)	21(1)	17(1)	-2(1)	6(1)	-3(1)
C(9)	37(1)	26(1)	29(1)	2(1)	14(1)	6(1)
C(10)	28(1)	34(1)	29(1)	7(1)	8(1)	11(1)
C(11)	35(1)	28(1)	25(1)	10(1)	8(1)	7(1)
C(12)	22(1)	33(1)	19(1)	3(1)	2(1)	5(1)
C(13)	20(1)	25(1)	14(1)	-1(1)	2(1)	-1(1)
C(14)	22(1)	20(1)	17(1)	1(1)	1(1)	3(1)
C(15)	19(1)	20(1)	17(1)	1(1)	3(1)	4(1)
C(16)	25(1)	23(1)	21(1)	0(1)	6(1)	-4(1)
C(17)	29(1)	27(1)	24(1)	-7(1)	5(1)	-3(1)
C(18)	30(1)	28(1)	16(1)	-1(1)	7(1)	4(1)
C(19)	25(1)	25(1)	26(1)	2(1)	9(1)	-1(1)
C(20)	22(1)	22(1)	24(1)	-2(1)	3(1)	-1(1)

Table S3E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3b**.

	x	y	z	U(eq)
H(3)	7506	5026	3223	25

H(4)	8076	5394	1605	28
H(5)	6641	6351	413	27
H(6)	4651	6982	849	27
H(7)	4096	6670	2484	25
H(8A)	5418	3589	3191	28
H(8B)	4595	2981	4007	28
H(9A)	6413	1790	3917	36
H(9B)	7322	2958	4070	36
H(10)	7429	2013	5684	36
H(11A)	5555	1525	6476	35
H(11B)	4631	2034	5480	35
H(12)	6552	3484	6705	30
H(13)	5794	5209	5885	23
H(16)	5094	5952	7242	27
H(17)	4691	6207	8917	32
H(18)	3261	4913	9626	29
H(19)	2173	3414	8644	30
H(20)	2460	3250	6936	27

Table S3F. Torsion angles [°] for **3b**.

C(13)-N(1)-C(1)-O(1)	-9.6(3)
C(8)-N(1)-C(1)-O(1)	160.28(19)
C(13)-N(1)-C(1)-C(2)	167.81(15)
C(8)-N(1)-C(1)-C(2)	-22.3(3)
O(1)-C(1)-C(2)-C(7)	-53.6(3)
N(1)-C(1)-C(2)-C(7)	128.95(18)
O(1)-C(1)-C(2)-C(3)	120.9(2)
N(1)-C(1)-C(2)-C(3)	-56.6(2)
C(7)-C(2)-C(3)-C(4)	-0.5(3)
C(1)-C(2)-C(3)-C(4)	-174.93(18)
C(2)-C(3)-C(4)-C(5)	-0.7(3)
C(3)-C(4)-C(5)-C(6)	0.9(3)
C(4)-C(5)-C(6)-C(7)	0.2(3)
C(5)-C(6)-C(7)-C(2)	-1.4(3)
C(3)-C(2)-C(7)-C(6)	1.6(3)
C(1)-C(2)-C(7)-C(6)	176.07(16)
C(1)-N(1)-C(8)-C(9)	127.76(18)
C(13)-N(1)-C(8)-C(9)	-62.4(2)

N(1)-C(8)-C(9)-C(10)	52.9(2)
C(8)-C(9)-C(10)-C(11)	46.4(3)
C(8)-C(9)-C(10)-C(12)	-24.6(3)
C(9)-C(10)-C(11)-C(12)	-108.4(2)
C(9)-C(10)-C(12)-C(11)	110.5(2)
C(11)-C(10)-C(12)-C(13)	-109.2(2)
C(9)-C(10)-C(12)-C(13)	1.3(3)
C(10)-C(11)-C(12)-C(13)	109.9(2)
C(1)-N(1)-C(13)-C(14)	85.34(19)
C(8)-N(1)-C(13)-C(14)	-85.29(19)
C(1)-N(1)-C(13)-C(12)	-153.01(16)
C(8)-N(1)-C(13)-C(12)	36.4(2)
C(10)-C(12)-C(13)-N(1)	-5.6(3)
C(11)-C(12)-C(13)-N(1)	-75.8(2)
C(10)-C(12)-C(13)-C(14)	118.81(19)
C(11)-C(12)-C(13)-C(14)	48.6(2)
N(1)-C(13)-C(14)-O(2)	16.5(3)
C(12)-C(13)-C(14)-O(2)	-108.1(2)
N(1)-C(13)-C(14)-C(15)	-169.16(15)
C(12)-C(13)-C(14)-C(15)	66.3(2)
O(2)-C(14)-C(15)-C(16)	-142.35(19)
C(13)-C(14)-C(15)-C(16)	43.3(2)
O(2)-C(14)-C(15)-C(20)	36.8(3)
C(13)-C(14)-C(15)-C(20)	-137.53(18)
C(20)-C(15)-C(16)-C(17)	-1.2(3)
C(14)-C(15)-C(16)-C(17)	178.02(18)
C(15)-C(16)-C(17)-C(18)	2.5(3)
C(16)-C(17)-C(18)-C(19)	-1.3(3)
C(17)-C(18)-C(19)-C(20)	-1.2(3)
C(18)-C(19)-C(20)-C(15)	2.5(3)
C(16)-C(15)-C(20)-C(19)	-1.3(3)
C(14)-C(15)-C(20)-C(19)	179.46(16)

Symmetry transformations used to generate equivalent atoms:

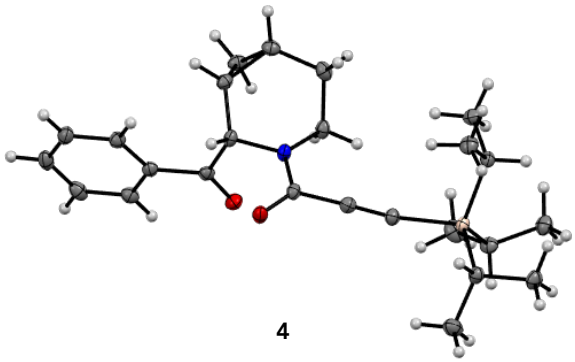


Figure S11. Single crystal XRD structure of **4**. Ortep drawn at 50% probability level.

Table S4A. Crystal data and structure refinement for **4**.

Identification code	CRoberts02_Sarpong	
Empirical formula	C25 H35 N O2 Si	
Formula weight	409.63	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.43610(10) Å	α= 87.3720(10)°.
	b = 9.47820(10) Å	β= 83.4540(10)°.
	c = 16.67800(10) Å	γ = 79.7650(10)°.
Volume	1148.84(2) $Å^3$	
Z	2	
Density (calculated)	1.184 Mg/m^3	
Absorption coefficient	1.048 mm^{-1}	
F(000)	444	
Crystal size	0.400 x 0.210 x 0.170 mm^3	
Theta range for data collection	4.743 to 74.503°.	
Index ranges	-9<=h<=9, -10<=k<=11, -20<=l<=20	
Reflections collected	45287	
Independent reflections	4698 [R(int) = 0.0314]	
Completeness to theta = 74.000°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.87599	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4698 / 0 / 268	

Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0336, wR2 = 0.0846
R indices (all data)	R1 = 0.0337, wR2 = 0.0847
Extinction coefficient	n/a
Largest diff. peak and hole	0.339 and -0.301 e.$Å^{-3}$

Table S4B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	3730(1)	2908(1)	8512(1)	15(1)
O(1)	48(1)	3814(1)	5955(1)	21(1)
O(2)	1915(1)	653(1)	4898(1)	22(1)
N(1)	2997(1)	2938(1)	5455(1)	17(1)
C(1)	2666(2)	3086(1)	7553(1)	18(1)
C(2)	2235(2)	3185(1)	6876(1)	18(1)
C(3)	1660(2)	3327(1)	6059(1)	16(1)
C(4)	4860(2)	2192(1)	5572(1)	19(1)
C(5)	6290(2)	2993(1)	5126(1)	22(1)
C(6)	5974(2)	3273(1)	4250(1)	20(1)
C(7)	5625(2)	2087(1)	3753(1)	21(1)
C(8)	4071(2)	3292(1)	4007(1)	18(1)
C(9)	2474(2)	3052(1)	4632(1)	16(1)
C(10)	1753(2)	1694(1)	4442(1)	17(1)
C(11)	936(2)	1664(1)	3661(1)	17(1)
C(12)	524(2)	365(1)	3435(1)	21(1)
C(13)	-160(2)	272(1)	2703(1)	24(1)
C(14)	-439(2)	1472(2)	2191(1)	25(1)
C(15)	-79(2)	2774(1)	2421(1)	23(1)
C(16)	598(2)	2878(1)	3156(1)	20(1)
C(17)	5577(2)	4053(1)	8359(1)	18(1)
C(18)	4766(2)	5652(1)	8264(1)	23(1)
C(19)	6988(2)	3578(1)	7634(1)	24(1)
C(20)	4680(2)	951(1)	8708(1)	21(1)
C(21)	6381(2)	771(1)	9176(1)	24(1)
C(22)	5095(2)	50(1)	7948(1)	28(1)
C(23)	1899(2)	3604(1)	9345(1)	19(1)
C(24)	2705(2)	3650(1)	10150(1)	23(1)

C(25)	306(2)	2758(2)	9438(1)	27(1)

Table S4C. Bond lengths [Å] and angles [°] for **4**.

Si(1)-C(1)	1.8512(12)
Si(1)-C(17)	1.8849(12)
Si(1)-C(23)	1.8853(12)
Si(1)-C(20)	1.8917(12)
O(1)-C(3)	1.2336(14)
O(2)-C(10)	1.2156(14)
N(1)-C(3)	1.3471(15)
N(1)-C(9)	1.4619(14)
N(1)-C(4)	1.4690(14)
C(1)-C(2)	1.2039(17)
C(2)-C(3)	1.4679(15)
C(4)-C(5)	1.5216(17)
C(5)-C(6)	1.5102(17)
C(6)-C(7)	1.5017(16)
C(6)-C(8)	1.5123(16)
C(7)-C(8)	1.5113(16)
C(8)-C(9)	1.5299(16)
C(9)-C(10)	1.5389(16)
C(10)-C(11)	1.5008(15)
C(11)-C(16)	1.3975(16)
C(11)-C(12)	1.3984(17)
C(12)-C(13)	1.3873(18)
C(13)-C(14)	1.3901(19)
C(14)-C(15)	1.3888(19)
C(15)-C(16)	1.3906(17)
C(17)-C(18)	1.5361(16)
C(17)-C(19)	1.5366(16)
C(20)-C(22)	1.5314(17)
C(20)-C(21)	1.5415(17)
C(23)-C(25)	1.5341(17)
C(23)-C(24)	1.5363(16)
C(1)-Si(1)-C(17)	105.25(5)
C(1)-Si(1)-C(23)	108.08(5)
C(17)-Si(1)-C(23)	111.30(5)
C(1)-Si(1)-C(20)	108.85(5)

C(17)-Si(1)-C(20)	112.66(5)
C(23)-Si(1)-C(20)	110.44(5)
C(3)-N(1)-C(9)	117.40(9)
C(3)-N(1)-C(4)	124.40(9)
C(9)-N(1)-C(4)	117.40(9)
C(2)-C(1)-Si(1)	170.35(11)
C(1)-C(2)-C(3)	178.45(12)
O(1)-C(3)-N(1)	124.00(10)
O(1)-C(3)-C(2)	120.16(10)
N(1)-C(3)-C(2)	115.81(10)
N(1)-C(4)-C(5)	110.44(9)
C(6)-C(5)-C(4)	111.49(10)
C(7)-C(6)-C(5)	120.09(10)
C(7)-C(6)-C(8)	60.19(8)
C(5)-C(6)-C(8)	118.80(10)
C(6)-C(7)-C(8)	60.26(8)
C(7)-C(8)-C(6)	59.56(8)
C(7)-C(8)-C(9)	121.69(10)
C(6)-C(8)-C(9)	121.24(10)
N(1)-C(9)-C(8)	112.08(9)
N(1)-C(9)-C(10)	109.82(9)
C(8)-C(9)-C(10)	110.20(9)
O(2)-C(10)-C(11)	121.16(10)
O(2)-C(10)-C(9)	120.42(10)
C(11)-C(10)-C(9)	118.35(9)
C(16)-C(11)-C(12)	119.44(11)
C(16)-C(11)-C(10)	122.35(10)
C(12)-C(11)-C(10)	118.21(10)
C(13)-C(12)-C(11)	120.21(11)
C(12)-C(13)-C(14)	120.11(12)
C(15)-C(14)-C(13)	119.98(11)
C(14)-C(15)-C(16)	120.24(12)
C(15)-C(16)-C(11)	119.98(11)
C(18)-C(17)-C(19)	110.03(10)
C(18)-C(17)-Si(1)	111.83(8)
C(19)-C(17)-Si(1)	111.85(8)
C(22)-C(20)-C(21)	110.60(10)
C(22)-C(20)-Si(1)	114.11(9)
C(21)-C(20)-Si(1)	111.49(8)

C(25)-C(23)-C(24)	111.22(10)
C(25)-C(23)-Si(1)	112.26(8)
C(24)-C(23)-Si(1)	111.63(8)

Symmetry transformations used to generate equivalent atoms:

Table S4D. Anisotropic displacement parameters ($Å^2$x 10^3)for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Si(1)	18(1)	15(1)	12(1)	-1(1)	-3(1)	-3(1)
O(1)	18(1)	26(1)	17(1)	-1(1)	-3(1)	0(1)
O(2)	25(1)	21(1)	22(1)	5(1)	-4(1)	-6(1)
N(1)	18(1)	19(1)	14(1)	-1(1)	-4(1)	1(1)
C(1)	20(1)	18(1)	17(1)	-2(1)	-3(1)	-3(1)
C(2)	18(1)	17(1)	18(1)	-2(1)	-1(1)	-2(1)
C(3)	20(1)	15(1)	15(1)	-1(1)	-3(1)	-4(1)
C(4)	19(1)	20(1)	18(1)	-1(1)	-4(1)	2(1)
C(5)	19(1)	22(1)	26(1)	-5(1)	-5(1)	-2(1)
C(6)	20(1)	18(1)	24(1)	-1(1)	0(1)	-5(1)
C(7)	23(1)	19(1)	20(1)	-3(1)	3(1)	-4(1)
C(8)	21(1)	16(1)	16(1)	-1(1)	-1(1)	-4(1)
C(9)	19(1)	17(1)	13(1)	-1(1)	-3(1)	0(1)
C(10)	14(1)	19(1)	16(1)	-1(1)	1(1)	-1(1)
C(11)	15(1)	21(1)	16(1)	-2(1)	0(1)	-2(1)
C(12)	18(1)	21(1)	23(1)	-2(1)	0(1)	-3(1)
C(13)	19(1)	26(1)	28(1)	-10(1)	-2(1)	-4(1)
C(14)	20(1)	37(1)	19(1)	-7(1)	-4(1)	-3(1)
C(15)	22(1)	29(1)	19(1)	1(1)	-3(1)	-2(1)
C(16)	19(1)	21(1)	18(1)	-1(1)	-2(1)	-3(1)
C(17)	20(1)	17(1)	16(1)	1(1)	-4(1)	-4(1)
C(18)	28(1)	17(1)	26(1)	1(1)	-5(1)	-4(1)
C(19)	22(1)	24(1)	24(1)	3(1)	1(1)	-5(1)
C(20)	22(1)	17(1)	23(1)	1(1)	-2(1)	-4(1)
C(21)	27(1)	21(1)	24(1)	4(1)	-6(1)	-1(1)
C(22)	29(1)	20(1)	36(1)	-9(1)	-6(1)	-1(1)
C(23)	20(1)	20(1)	16(1)	-2(1)	-1(1)	-2(1)
C(24)	27(1)	27(1)	16(1)	-4(1)	-1(1)	-4(1)
C(25)	22(1)	33(1)	27(1)	-5(1)	2(1)	-7(1)

Table S4E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) For **4**.

	x	y	z	U(eq)
H(4A)	5042	1206	5369	23
H(4B)	5013	2125	6155	23
H(5A)	6236	3918	5388	26
H(5B)	7531	2421	5159	26
H(6)	6677	3978	3952	24
H(7A)	5606	1135	4021	25
H(7B)	6134	2061	3178	25
H(8)	3720	4003	3566	21
H(9)	1457	3891	4599	19
H(12)	713	-457	3784	25
H(13)	-437	-612	2551	29
H(14)	-877	1401	1683	30
H(15)	-296	3598	2076	28
H(16)	831	3772	3314	23
H(17)	6243	3933	8853	21
H(18A)	4050	5796	7799	35
H(18B)	5765	6209	8177	35
H(18C)	3965	5970	8753	35
H(19A)	7520	2563	7706	35
H(19B)	7966	4156	7595	35
H(19C)	6380	3711	7138	35
H(20)	3708	550	9065	25
H(21A)	7388	1118	8838	36
H(21B)	6760	-245	9318	36
H(21C)	6077	1326	9670	36
H(22A)	3966	99	7689	42
H(22B)	5562	-949	8097	42
H(22C)	6021	425	7573	42
H(23)	1380	4614	9192	23
H(24A)	3218	2674	10323	35
H(24B)	1733	4073	10560	35
H(24C)	3679	4233	10079	35
H(25A)	-211	2776	8922	41

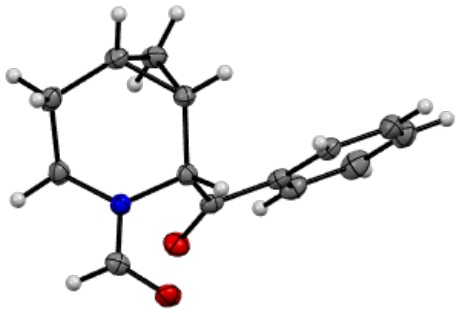
H(25B)	-649	3195	9851	41
H(25C)	760	1763	9600	41

Table S4F. Torsion angles [°] for **4**.

C(9)-N(1)-C(3)-O(1)	-2.55(17)
C(4)-N(1)-C(3)-O(1)	-171.97(11)
C(9)-N(1)-C(3)-C(2)	179.48(9)
C(4)-N(1)-C(3)-C(2)	10.06(16)
C(3)-N(1)-C(4)-C(5)	-127.25(12)
C(9)-N(1)-C(4)-C(5)	63.33(13)
N(1)-C(4)-C(5)-C(6)	-52.62(13)
C(4)-C(5)-C(6)-C(7)	-47.26(14)
C(4)-C(5)-C(6)-C(8)	23.04(14)
C(5)-C(6)-C(7)-C(8)	108.04(12)
C(6)-C(7)-C(8)-C(9)	-110.13(12)
C(5)-C(6)-C(8)-C(7)	-110.14(12)
C(7)-C(6)-C(8)-C(9)	110.86(12)
C(5)-C(6)-C(8)-C(9)	0.72(16)
C(3)-N(1)-C(9)-C(8)	152.62(10)
C(4)-N(1)-C(9)-C(8)	-37.20(13)
C(3)-N(1)-C(9)-C(10)	-84.55(12)
C(4)-N(1)-C(9)-C(10)	85.63(12)
C(7)-C(8)-C(9)-N(1)	76.08(13)
C(6)-C(8)-C(9)-N(1)	4.86(15)
C(7)-C(8)-C(9)-C(10)	-46.54(14)
C(6)-C(8)-C(9)-C(10)	-117.76(11)
N(1)-C(9)-C(10)-O(2)	-10.04(15)
C(8)-C(9)-C(10)-O(2)	113.90(12)
N(1)-C(9)-C(10)-C(11)	173.01(9)
C(8)-C(9)-C(10)-C(11)	-63.05(13)
O(2)-C(10)-C(11)-C(16)	174.78(11)
C(9)-C(10)-C(11)-C(16)	-8.30(16)
O(2)-C(10)-C(11)-C(12)	-5.91(16)
C(9)-C(10)-C(11)-C(12)	171.01(10)
C(16)-C(11)-C(12)-C(13)	2.04(17)
C(10)-C(11)-C(12)-C(13)	-177.29(10)
C(11)-C(12)-C(13)-C(14)	-0.04(18)
C(12)-C(13)-C(14)-C(15)	-1.67(19)

C(13)-C(14)-C(15)-C(16)	1.36(19)
C(14)-C(15)-C(16)-C(11)	0.66(18)
C(12)-C(11)-C(16)-C(15)	-2.35(17)
C(10)-C(11)-C(16)-C(15)	176.95(11)
C(1)-Si(1)-C(17)-C(18)	65.74(9)
C(23)-Si(1)-C(17)-C(18)	-51.11(10)
C(20)-Si(1)-C(17)-C(18)	-175.79(8)
C(1)-Si(1)-C(17)-C(19)	-58.19(9)
C(23)-Si(1)-C(17)-C(19)	-175.03(8)
C(20)-Si(1)-C(17)-C(19)	60.28(9)
C(1)-Si(1)-C(20)-C(22)	23.14(11)
C(17)-Si(1)-C(20)-C(22)	-93.21(10)
C(23)-Si(1)-C(20)-C(22)	141.64(9)
C(1)-Si(1)-C(20)-C(21)	149.33(9)
C(17)-Si(1)-C(20)-C(21)	32.98(10)
C(23)-Si(1)-C(20)-C(21)	-92.17(9)
C(1)-Si(1)-C(23)-C(25)	60.54(10)
C(17)-Si(1)-C(23)-C(25)	175.64(8)
C(20)-Si(1)-C(23)-C(25)	-58.43(10)
C(1)-Si(1)-C(23)-C(24)	-173.80(8)
C(17)-Si(1)-C(23)-C(24)	-58.69(10)
C(20)-Si(1)-C(23)-C(24)	67.23(10)

Symmetry transformations used to generate equivalent atoms:



5

Figure S12. Single crystal XRD structure of **4**. Ortep drawn at 50% probability level.

Table S5A. Crystal data and structure refinement for **5**.

Identification code	CRoberts03_Sarpong	
Empirical formula	C14 H15 N O2	
Formula weight	229.27	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 13.1623(2) Å	α= 90°.
	b = 7.55710(10) Å	β= 108.5650(10)°.
	c = 12.35190(10) Å	γ = 90°.
Volume	1164.69(3) $Å^3$	
Z	4	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	0.704 mm^{-1}	
F(000)	488	
Crystal size	0.180 x 0.120 x 0.070 mm^3	
Theta range for data collection	3.542 to 74.450°.	
Index ranges	-16<=h<=16, -9<=k<=9, -13<=l<=15	
Reflections collected	14327	
Independent reflections	2378 [R(int) = 0.0279]	
Completeness to theta = 74.000°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.69768	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2378 / 0 / 154	

Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0340, wR2 = 0.0887
R indices (all data)	R1 = 0.0357, wR2 = 0.0901
Extinction coefficient	n/a
Largest diff. peak and hole	0.243 and -0.182 e.$Å^{-3}$

Table S5B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4986(1)	4684(1)	3479(1)	26(1)
O(2)	2148(1)	4247(1)	2477(1)	26(1)
N(1)	3902(1)	2372(1)	3554(1)	19(1)
C(1)	4647(1)	3175(1)	3203(1)	21(1)
C(2)	3467(1)	639(1)	3114(1)	22(1)
C(3)	3602(1)	-664(1)	4092(1)	23(1)
C(4)	3206(1)	98(1)	5018(1)	22(1)
C(5)	2113(1)	923(1)	4713(1)	23(1)
C(6)	3096(1)	2086(1)	5100(1)	19(1)
C(7)	3392(1)	3323(1)	4270(1)	18(1)
C(8)	2409(1)	4339(1)	3513(1)	19(1)
C(9)	1773(1)	5398(1)	4090(1)	20(1)
C(10)	2198(1)	5937(1)	5227(1)	21(1)
C(11)	1582(1)	6925(1)	5731(1)	25(1)
C(12)	537(1)	7372(2)	5108(1)	29(1)
C(13)	110(1)	6853(2)	3976(1)	31(1)
C(14)	723(1)	5876(2)	3464(1)	26(1)

Table S5C. Bond lengths [Å] and angles [°] for **5**.

O(1)-C(1)	1.2320(13)
O(2)-C(8)	1.2166(13)
N(1)-C(1)	1.3377(13)
N(1)-C(7)	1.4578(12)
N(1)-C(2)	1.4629(13)
C(2)-C(3)	1.5243(15)
C(3)-C(4)	1.5128(15)
C(4)-C(5)	1.5017(15)

C(4)-C(6)	1.5156(14)
C(5)-C(6)	1.5100(15)
C(6)-C(7)	1.5272(13)
C(7)-C(8)	1.5388(13)
C(8)-C(9)	1.4933(14)
C(9)-C(10)	1.3967(15)
C(9)-C(14)	1.3992(15)
C(10)-C(11)	1.3869(15)
C(11)-C(12)	1.3881(16)
C(12)-C(13)	1.3872(18)
C(13)-C(14)	1.3855(17)
C(1)-N(1)-C(7)	119.94(8)
C(1)-N(1)-C(2)	121.78(8)
C(7)-N(1)-C(2)	117.74(8)
O(1)-C(1)-N(1)	124.66(10)
N(1)-C(2)-C(3)	110.52(8)
C(4)-C(3)-C(2)	111.83(9)
C(5)-C(4)-C(3)	120.10(9)
C(5)-C(4)-C(6)	60.06(7)
C(3)-C(4)-C(6)	119.40(9)
C(4)-C(5)-C(6)	60.43(7)
C(5)-C(6)-C(4)	59.52(7)
C(5)-C(6)-C(7)	121.35(8)
C(4)-C(6)-C(7)	120.77(8)
N(1)-C(7)-C(6)	111.74(8)
N(1)-C(7)-C(8)	109.75(8)
C(6)-C(7)-C(8)	111.59(8)
O(2)-C(8)-C(9)	121.28(9)
O(2)-C(8)-C(7)	120.75(9)
C(9)-C(8)-C(7)	117.95(8)
C(10)-C(9)-C(14)	119.29(10)
C(10)-C(9)-C(8)	121.99(9)
C(14)-C(9)-C(8)	118.72(9)
C(11)-C(10)-C(9)	120.28(10)
C(10)-C(11)-C(12)	119.98(10)
C(13)-C(12)-C(11)	120.16(11)
C(14)-C(13)-C(12)	120.15(10)
C(13)-C(14)-C(9)	120.13(11)

Symmetry transformations used to generate equivalent atoms:

Table S5D. Anisotropic displacement parameters ($Å^2$x 10^3)for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	27(1)	26(1)	25(1)	-2(1)	10(1)	-9(1)
O(2)	29(1)	28(1)	19(1)	2(1)	5(1)	0(1)
N(1)	20(1)	18(1)	20(1)	-2(1)	8(1)	-2(1)
C(1)	19(1)	25(1)	19(1)	1(1)	5(1)	-1(1)
C(2)	22(1)	20(1)	23(1)	-6(1)	9(1)	-4(1)
C(3)	24(1)	18(1)	28(1)	-2(1)	9(1)	-2(1)
C(4)	23(1)	19(1)	23(1)	3(1)	8(1)	0(1)
C(5)	22(1)	23(1)	26(1)	5(1)	10(1)	-1(1)
C(6)	22(1)	19(1)	18(1)	2(1)	7(1)	2(1)
C(7)	17(1)	17(1)	18(1)	-2(1)	6(1)	-1(1)
C(8)	20(1)	16(1)	20(1)	2(1)	5(1)	-4(1)
C(9)	20(1)	16(1)	24(1)	4(1)	7(1)	-1(1)
C(10)	21(1)	17(1)	24(1)	2(1)	6(1)	0(1)
C(11)	30(1)	19(1)	29(1)	1(1)	12(1)	1(1)
C(12)	29(1)	21(1)	42(1)	3(1)	18(1)	5(1)
C(13)	22(1)	26(1)	42(1)	7(1)	7(1)	6(1)
C(14)	23(1)	24(1)	28(1)	5(1)	4(1)	1(1)

Table S5E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) For **5**.

	x	y	z	U(eq)
H(1)	4936	2537	2706	25
H(2A)	3843	184	2593	26
H(2B)	2697	758	2673	26
H(3A)	3198	-1760	3791	28
H(3B)	4368	-979	4424	28
H(4)	3446	-544	5764	26
H(5A)	1698	749	5247	28
H(5B)	1677	962	3896	28

H(6)	3267	2552	5896	23
H(7)	3918	4210	4730	21
H(10)	2912	5625	5656	25
H(11)	1876	7295	6503	30
H(12)	112	8034	5457	35
H(13)	-605	7169	3550	37
H(14)	429	5531	2687	31

Table S5F. Torsion angles [°] for **5**.

C(7)-N(1)-C(1)-O(1)	3.15(15)
C(2)-N(1)-C(1)-O(1)	174.45(9)
C(1)-N(1)-C(2)-C(3)	124.66(10)
C(7)-N(1)-C(2)-C(3)	-63.85(11)
N(1)-C(2)-C(3)-C(4)	49.59(12)
C(2)-C(3)-C(4)-C(5)	50.23(13)
C(2)-C(3)-C(4)-C(6)	-20.17(13)
C(3)-C(4)-C(5)-C(6)	-108.72(10)
C(4)-C(5)-C(6)-C(7)	109.66(10)
C(3)-C(4)-C(6)-C(5)	109.86(11)
C(5)-C(4)-C(6)-C(7)	-110.62(10)
C(3)-C(4)-C(6)-C(7)	-0.76(14)
C(1)-N(1)-C(7)-C(6)	-147.78(9)
C(2)-N(1)-C(7)-C(6)	40.57(11)
C(1)-N(1)-C(7)-C(8)	87.89(10)
C(2)-N(1)-C(7)-C(8)	-83.76(10)
C(5)-C(6)-C(7)-N(1)	-78.49(11)
C(4)-C(6)-C(7)-N(1)	-7.68(13)
C(5)-C(6)-C(7)-C(8)	44.80(12)
C(4)-C(6)-C(7)-C(8)	115.62(10)
N(1)-C(7)-C(8)-O(2)	1.35(13)
C(6)-C(7)-C(8)-O(2)	-123.07(10)
N(1)-C(7)-C(8)-C(9)	179.80(8)
C(6)-C(7)-C(8)-C(9)	55.38(11)
O(2)-C(8)-C(9)-C(10)	-161.55(10)
C(7)-C(8)-C(9)-C(10)	20.01(14)
O(2)-C(8)-C(9)-C(14)	17.77(15)
C(7)-C(8)-C(9)-C(14)	-160.67(9)
C(14)-C(9)-C(10)-C(11) 0.45	

C(8)-C(9)-C(10)-C(11)	179.77(9)
C(9)-C(10)-C(11)-C(12)	0.42(16)
C(10)-C(11)-C(12)-C(13)	-0.87(17)
C(11)-C(12)-C(13)-C(14)	0.44(18)
C(12)-C(13)-C(14)-C(9)	0.45(17)
C(10)-C(9)-C(14)-C(13)	-0.89(16)
C(8)-C(9)-C(14)-C(13)	179.77(10)

Symmetry transformations used to generate equivalent atoms:

Computational Details

1.1 General

All calculations were conducted using DFT[1] implemented in the Jaguar 9.1 suite[2] of ab initio quantum chemistry programs with Becke's three-parameter exchange functional B3LYP including Grimme's D3 dispersion correction levels of theory.[3-8] Geometry optimizations were processed using Pople's 6-31G** basis set[9-14] for main group elements. Palladium was represented using the Los Alamos LACVP basis[15] that includes relativistic effective core potentials. The energies of the optimized structures were reevaluated by additional single point calculations on each optimized geometry using the same functional and Pople's 6-311G** basis set.[16-19] The LACV3P basis set, which is a triple-ζ contraction of the LACVP basis set developed and tested at Schrodinger, Inc., was used for palladium. Analytical vibrational frequencies within the harmonic approximation were calculated using the 6-31G** basis to confirm the proper convergence to well-defined minima or saddle points on the potential energy surface. Solvation energies were calculated using a self-consistent reaction field (SCRF)[20-22] approach based on accurate numerical solutions of the Poisson-Boltzmann equation and were performed with the 6-31G** basis at the optimized gas phase geometry with a dielectric constant of $\varepsilon = 2.379$ for toluene. As is the case for all continuum models, the solvation energies are subject to the empirical parametrization of the atomic radii that are used to generate the solute surface. The standard set of optimized radii in Jaguar was used for H (1.150 Å), C (1.900 Å), N (1.600 Å), O (1.600 Å), P (2.074 Å), and Pd (1.450 Å).[23] The Gibbs free energies in solution phase G(sol) were computed with the following protocol.

$$G(sol) = G(gas) + G^{solv} \quad (1)$$

$$G(gas) = H(gas) - TS(gas) \quad (2)$$

$$H(gas) = E(SCF) + ZPE \quad (3)$$

$$\Delta E(SCF) = \Sigma E(SCF) \text{ for products} - \Sigma E(SCF) \text{ for reactants} \quad (4)$$

$$\Delta G(sol) = \Sigma G(sol) \text{ for products} - \Sigma G(sol) \text{ for reactants} \quad (5)$$

G(gas) is the free energy in gas phase; G^{solv} is the free energy of solvation; H(gas) is the enthalpy in gas phase; T is the temperature (313.15K); S(gas) is the entropy in gas phase; E(SCF) is "raw" electronic energy computed from the SCF (self-consistent field) procedure; ZPE is the zero-point energy. The entropy we refer to is specifically the vibrational/rotational/translational entropy of the solute(s), and the entropy of the solvent is implicitly comprised in the continuum solvation model.

To better understand the role of the ligand in determining the product distribution, we conducted density functional theory (DFT) calculations. Figure S13 shows the calculated free energy profile using RuPhos. The calculations start from an alkoxide intermediate (**R1**), formed by sequential activation events involving base-assisted addition of phenyl bromide to RuPhos-Pd-G4. The reaction may then proceed via either proximal or distal C–C bond cleavage (refer to Figure 1D), ultimately leading to products **3a** or **3b**, respectively. Our calculations indicate that the proximal C–C bond cleavage *via* **R1'-TS$_{prox}$** is more favorable, with a free energy barrier of 10.60 kcal/mol, whereas the distal cleavage has an activation free energy of 14.05 kcal/mol. The calculated preference for proximal C–C bond cleavage over distal C–C bond cleavage of the β-lactam using the RuPhos ligated Pd(II)-complex is consistent with our previous computational findings and the experimental observations presented above.

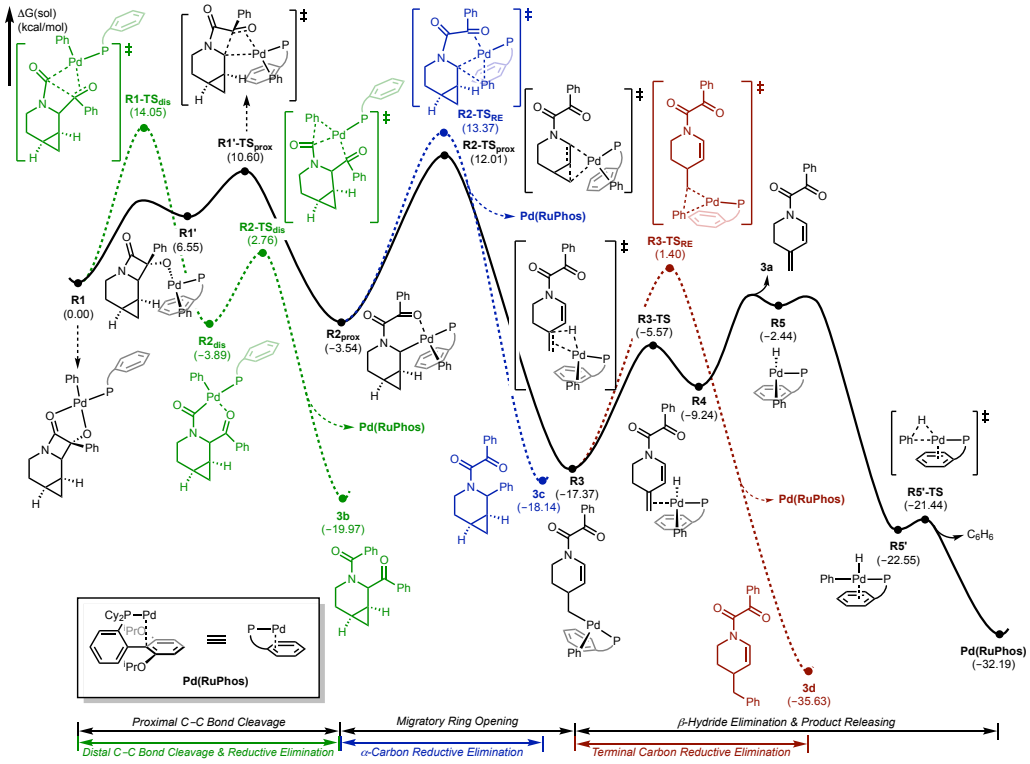


Figure S13. Calculated free energy profile for the formation of diene **3a** from lactam **2a** using **Pd(RuPhos)**. Dotted lines represent side pathways. Geometry optimization, vibration, solvation calculations: B3LYP-D3/6-31G** (LACVP for Pd). ε=2.379 for toluene. Single point calculations: B3LYP-D3/6-311G** (LACV3P for Pd).

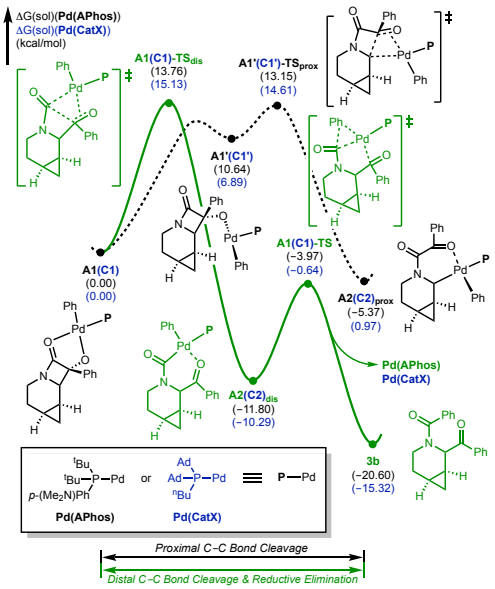


Figure S14. Calculated free energy profile for the distal/proximal C–C bond cleavage steps. Black and blue indicate profiles using APhos and CataCXium A, respectively.

In contrast, using monodentate phosphine ligands CataCXium A or APhos, we observed a reversal in the distal/proximal C–C cleavage selectivity leading to an α-benzoylated species (**3b**) as a major product. Specifically, the product ratio reversed by a factor of 26 (Table 2, entries 1, 2) upon switching from RuPhos to APhos. This experimental observation is in full agreement with our previous findings and corresponds to a 2 kcal/mol calculated difference between the free energy barriers for distal and proximal cleavage in comparing RuPhos to APhos or to CataCXiumA ($\Delta\Delta G^{\ddagger}$=$\Delta G$(**X1-TS$_{dis}$**)–$\Delta\Delta G$(**X1'-TS$_{prox}$**), where **X** = **A** (for APhos), **C** (for CataCxiumA), or **R** (for RuPhos) (see below for a derivation of this selectivity). Figure S14 shows the energy profiles of the C–C bond cleavage steps when APhos and CataCXium A are used as ligands. In agreement with our theoretical prediction, the $\Delta\Delta G^{\ddagger}$ values were calculated to be 0.61 and 0.52 kcal/mol, for APhos and CataCXium, respectively, showing a clear decrease of approximately 3 kcal/mol in selectivity to favor distal cleavage compared to the RuPhos case ($\Delta\Delta G^{\ddagger}$ = 3.45 kcal/mol).

Here, the $\Delta\Delta G^{\ddagger}$ values must be evaluated carefully when using the Curtin-Hammett principle because the calculations do not consider the effect of the frequency factor (pre-exponential factor).[24, 25, 26] In the case of distal C–C cleavage, **A1(C1)-TS$_{dis}$** is structurally very similar to complex **A1(C1)**, whereas in the case of proximal C–C cleavage, the related transition state **A1'(C1')-TS$_{prox}$** and **A1(C1)**, requires a significant structural change through **A1'(C1')**, including dissociation of a stabilizing Pd–carbonyl interaction, to approach the required geometry. Therefore, it is anticipated that **A1(C1)-TS$_{dis}$** would have a larger frequency factor compared to **A1'(C1')-TS$_{prox}$**. Overall, the proximal C–C bond cleavage should be less favorable than what is anticipated from the free energy calculations. On this basis, even though **A1(C1)-TS$_{dis}$** is very slightly higher in energy compared to **A1'(C1')-TS$_{prox}$**, we propose that the distal C–C bond cleavage should be favored in the APhos and CataCXium ligated

systems, and our interpretation matches our experimental observations (Table 2). Additionally, the above presented distal/proximal selectivity data for the RuPhos, APhos, and CataCXium A ligated systems are consistent with a distortion-interaction analysis,[22, 23] details of which can be found below.

Following lactam C–C bond cleavage, there are two possible mechanistic scenarios. In the case of APhos and CataCXium A, the distal C–C bond cleaved intermediate **A2(C2)$_{dis}$** (Figure S14) undergoes a RE with an energy demand of 7.83(9.65) kcal/mol to give α -benzoylated product **3b** with the regeneration of the Pd catalyst. With RuPhos, the proximal C–C bond cleaved intermediate **R2$_{prox}$** (Figure S13) could undergo RE (**R2-TS$_{RE}$**) to form an α-arylated product (**3c**), or proceed through β -carbon elimination (**R2-TS$_{prox}$**) to ring-opened terminal alkyl intermediate **R3**. Our calculations show that **R2-TS$_{prox}$** is favored over **R2-TS$_{RE}$** by 1.36 kcal/mol. The barrier associated with RE from **R3** was calculated to be 7.07 kcal/mol higher as compared to β-hydride elimination, via **R3-TS**, consistent with why **3d** was not observed experimentally. Ultimately, a β-hydride elimination (**R3-TS**) generates the observed diene product (**3a**) and benzene as a byproduct (via **R5'-TS**), with regeneration of **Pd(RuPhos)**.

1.2 Correlation Between Selectivity and ΔΔG‡

In this section, we derive the change of ΔΔG‡ of 2 kcal/mol from the experimentally observed selectivity change. The elementary reactions of interest have a common reactant (**R1**). The reaction is represented as shown below.

$$R2_{dis} \overset{k_{dis}}{\longleftarrow} R1 \overset{k_{prox}}{\longrightarrow} R2_{prox}$$

The product ratio can be written as

$$\frac{[R2_{dis}]}{[R2_{prox}]} = \frac{A_{R,dis}}{A_{R,prox}} \frac{exp\left(-\frac{\Delta G^{\ddagger}_{dis}}{RT}\right)}{exp\left(-\frac{\Delta G^{\ddagger}_{prox}}{RT}\right)} = \frac{A_{dis}}{A_{prox}} exp\left(-\frac{\Delta G^{\ddagger}_{dis} - \Delta G^{\ddagger}_{prox}}{RT}\right) \cdots (1)$$

Where

$\Delta G^{\ddagger}_{dis} = \Delta G$(**R1-TS$_{dis}$**) $- \Delta G$(**R1**) and $\Delta G^{\ddagger}_{prox} = \Delta G$(**R1'-TS$_{prox}$**) $- \Delta G$(**R1**), and A are the frequency factors.

Let $\Delta\Delta G^{\ddagger}_{R} = \Delta G$(**R1-TS$_{dis}$**)$-\Delta G$(**R1'-TS$_{prox}$**)

Thus,

$$\frac{[R2_{dis}]}{[R2_{prox}]} = \frac{A_{R,dis}}{A_{R,prox}} exp\,(-\Delta\Delta G_R/RT) \cdots (2)$$

With RuPhos-Pd-G4, [**R2$_{dis}$**]/[**R2$_{prox}$**] ≈ 0.2.

With APhos, $[\mathbf{A2_{dis}}]/[\mathbf{A2_{prox}}] \approx 5.2$.

Substitute $[\mathbf{R2_{dis}}]/[\mathbf{R2_{prox}}]$ with $[\mathbf{A2_{dis}}]/[\mathbf{A2_{prox}}]$ in equation (2) will give,

$$\frac{[A2_{dis}]}{[A2_{prox}]} = \frac{A_{A,dis}}{A_{A,prox}} exp\,(-\Delta\Delta G\ddagger_A/RT) \cdots (3)$$

Be dividing equation (2) by (3), we get,

$$\frac{[R2_{dis}]}{[R2_{prox}]}\frac{[A2_{prox}]}{[A2_{dis}]} = \frac{0.2}{5.2} = \frac{1}{26} = \frac{A_{R,dis}}{A_{R,prox}}\frac{A_{A,prox}}{A_{A,dis}} exp\,(-(\Delta\Delta G\ddagger_R - \Delta\Delta G\ddagger_A)/RT)$$

Assuming $\{(A_{R,dis})(A_{A,prox})\}/\{(A_{R,prox})(A_{A,dis})\} = 1$, then $exp\,(-(\Delta\Delta G\ddagger_R - \Delta\Delta G\ddagger_A)/RT) = 1/26$.
Therefore, the change of $\Delta\Delta G\ddagger$ ($\Delta\Delta G\ddagger_A - \Delta\Delta G\ddagger_R$) will be $-RT\ln(1/26) = 8479$ J/mol = 2.03 kcal/mol.

1.3 Distortion-Interaction Analysis

We analyzed two transition states to gain a deeper understanding of the dependency of distal/proximal selectivity on the ligand. A distortion-interaction analysis[27, 28] was conducted and the results are shown in Figure S15. For both RuPhos and CataCXium A, the distortions of ligands ([**L**]) are negligible, and the distortions of the remaining part ([**M**]) are greater in **1'-TS$_{prox}$** than **1-TS$_{dis}$**. This difference arises from a loss of Pd–carbonyl interaction. Notably, a significant difference in interaction energy changes between [**L**] and [**M**] (Δ**E(interact)**) of **R1'-TS$_{prox}$**. During the bond cleaving process, the Pd–carbamoyl bond and the Pd–alkyl bond are newly forming on the *trans*-site of the phosphine atom. On the basis of the *trans*-influence, the interaction between palladium and phosphine is assessed a penalty (Δ**E(interact)**>0). This is reflected in the distortion-interaction analysis as Δ**E(interact)**s; calculated to be 6.4 ~ 8.7 kcal/mol in all transition states except **R1'-TS$_{prox}$**, where it is approximately zero. This distinction is understandable considering its TS structure. At **1** and **1-TS$_{dis}$**, the palladium exists in a 16 e$^-$ square-planar structure, where RuPhos should be a monodentate ligand (Figure 2, S15 c). However, In **R1'**, which lacks the Pd–carbonyl interaction, there is a vacant site where RuPhos could serve as a bidentate ligand. The additional interaction between the palladium and an *ipso*-carbon of the biaryl ring (C(ipso) in Figure S15 c, d) enhances the interaction energy between [**M**] and [**L**]. With this functional feature of the biaryl phosphine ligand, there is no Δ**E(interact)** penalty on **R1'-TS$_{prox}$**. Other monodentate ligands cannot compensate for the lack of a coordinate site and thus make **1'-TS$_{prox}$** unfavorable over **1-TS$_{dis}$**. APhos also showed a similar trend as CataCXium. The optimized structures for **C1-TS$_{dis}$**, **C1'-TS$_{prox}$**, and the same analysis for the APhos case are shown below.

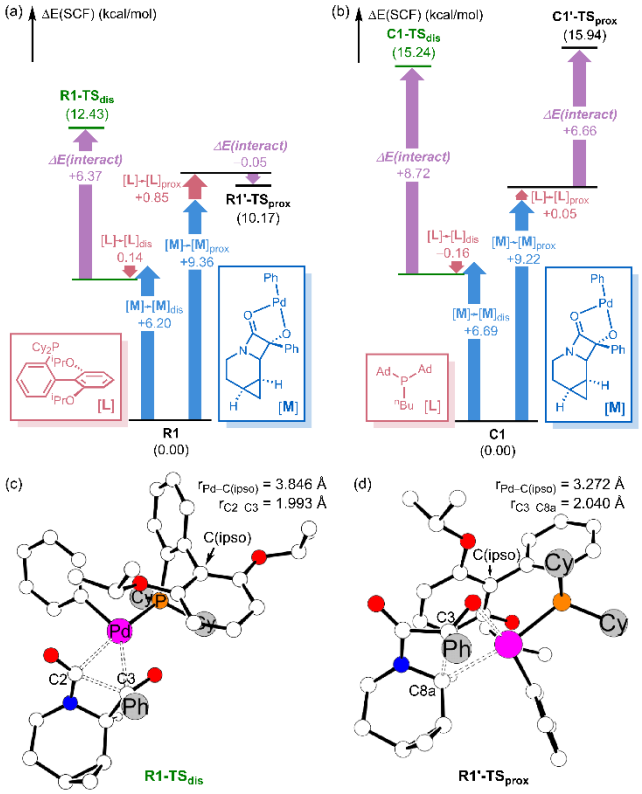


Figure S15. Distortion-interaction analysis of (a) **R1-TS$_{dis}$**, **R1'-TS$_{prox}$**, (b) **C1-TS$_{dis}$** and **C1'-TS$_{prox}$**. All species are fragmented into phosphine ligand and the remaining parts. (c) Optimized structure of **R1-TS$_{dis}$** and (d) **R1'-TS$_{prox}$**. Unimportant hydrogen atoms are omitted for clarity.

All molecules used for the distortion-interaction analysis were fragmented into a ligand part ([**L**]) and the remaining Pd(Ph)(substrate) part ([**M**]) as shown in Figure S16 a. Electronic energy (E(SCF)) of each geometry was reevaluated using the same method for single-point calculations (B3LYP-D3/6-311G**, LACV3P for Pd) without further geometry optimization. All energies used for the analysis were computed with the following protocol.

$$[\mathbf{L}]-[\mathbf{L}]_{dis} = E(SCF, [\mathbf{L}]_{dis}) - E(SCF, [\mathbf{L}]) \quad (9)$$
$$[\mathbf{M}]-[\mathbf{M}]_{dis} = E(SCF, [\mathbf{M}]_{dis}) - E(SCF, [\mathbf{M}]) \quad (10)$$
$$[\mathbf{L}]-[\mathbf{L}]_{prox} = E(SCF, [\mathbf{L}]_{prox}) - E(SCF, [\mathbf{L}]) \quad (11)$$
$$[\mathbf{M}]-[\mathbf{M}]_{prox} = E(SCF, [\mathbf{M}]_{prox}) - E(SCF, [\mathbf{M}]) \quad (12)$$
$$\mathbf{E(interact)} = E(SCF, \mathbf{1}) - (E(SCF, [\mathbf{L}])+E(SCF, [\mathbf{M}])) \quad (13)$$
$$\mathbf{E(interact)_{dis}} = E(SCF, \mathbf{1\text{-}TS_{dis}})-(E(SCF, [\mathbf{L}]_{dis})+E(SCF, [\mathbf{M}]_{dis})) \quad (14)$$
$$\mathbf{E(interact)_{prox}} = E(SCF, \mathbf{1'\text{-}TS_{prox}})-(E(SCF, [\mathbf{L}]_{prox})+E(SCF, [\mathbf{M}]_{prox})) \quad (15)$$
$$\Delta E(interact) = \mathbf{E(interact)_{dis}} - \mathbf{E(interact)} \text{ or } \mathbf{E(interact)_{prox}} - \mathbf{E(interact)} \quad (16)$$

A schematic diagram for the relationship is depicted in Figure S16 b, and all numeric data for the analysis is tabulated in Table S6. Lastly, the distortion-interaction analysis for the APhos system is depicted in Figure S17.

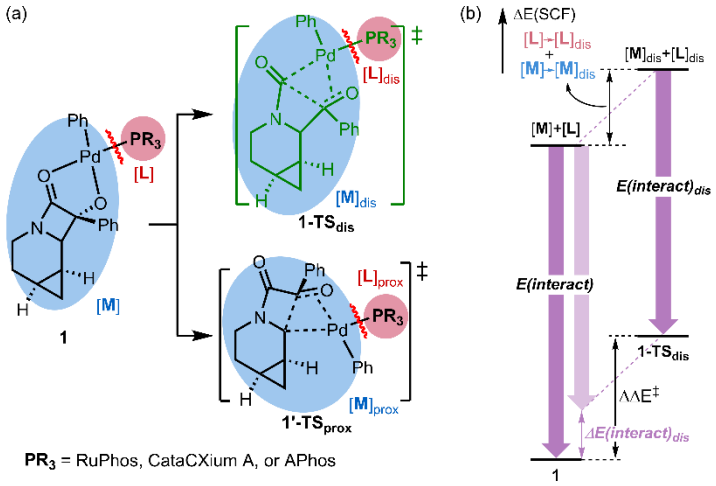


Figure S16. (a) Fragmentation for the resting state (**1**) and two transition states (**1-TS$_{dis}$** and **1'-TS$_{prox}$**). (b) Schematic diagram for energies used in distortion-interaction analysis. **1-TS$_{dis}$** was used for the example.

Table S6a. E(SCF) table for distortion-interaction analysis (sample, kcal/mol).

		1-TS$_{dis}$			**1'-TS$_{prox}$**		
		[L]$_{dis}$	**[M]$_{dis}$**	**E(interact)$_{dis}$**	**[L]$_{prox}$**	**[M]$_{prox}$**	**E(interact)$_{prox}$**
1	**[L]**	[L]–[L]$_{dis}$	-	-	[L]–[L]$_{prox}$	-	-
	[M]	-	[M]–[M]$_{dis}$	-	-	[M]–[M]$_{prox}$	-
	E(interact)	-	-	**ΔE(interact)**	-	-	**ΔE(interact)**

Table S6b. E(SCF) table for distortion-interaction analysis using RuPhos (kcal/mol).

		R1-TS$_{dis}$			**R1'-TS$_{prox}$**		
		–1042516.38	–693832.82	–78.68	–1042515.39	–693829.66	–85.09
R1	–1042516.25	–0.14	-	-	+0.85	-	-
	–693839.02	-	+6.20	-	-	+9.36	-
	–85.05	-	-	+6.37	-	-	–0.05

Table S6c. E(SCF) table for distortion-interaction analysis using CataCXium A (kcal/mol).

		C1-TS$_{dis}$			**C1'-TS$_{prox}$**		
		–803068.14	–693833.33	–70.20	–803067.94	–693830.79	–72.25
C1	–803067.98	–0.16	-	-	+0.04	-	-
	–693840.02	-	+6.69	-	-	+9.22	-
	–78.91	-	-	+8.72	-	-	+6.66

Table S6d. E(SCF) table for distortion-interaction analysis using APhos (kcal/mol).

		A1-TS$_{dis}$			**A1'-TS$_{prox}$**		
		–641885.70	–693831.78	–63.51	–641885.95	–693830.19	–65.56
A1	–641885.98	+0.28	-	-	+0.02	-	-
	–693842.83	-	+11.05	-	-	+12.64	-
	–69.07	-	-	+5.56	-	-	+3.51

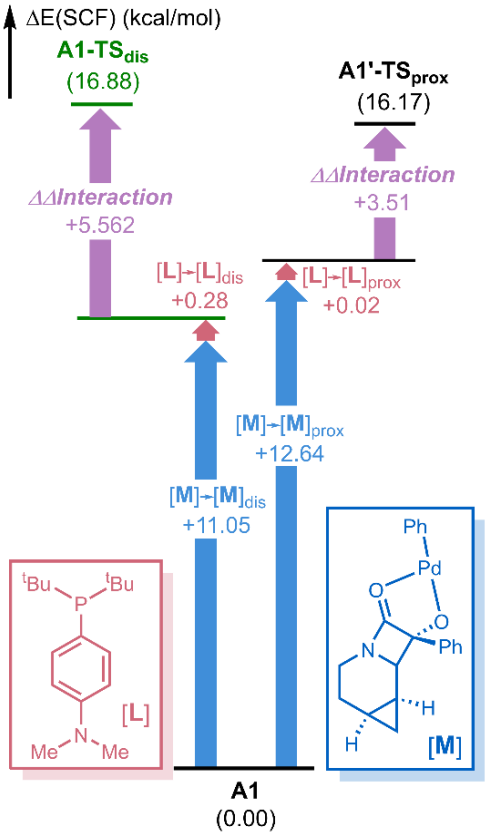


Figure S17. Distortion-interaction analysis of **A1-TS$_{dis}$**, **A1'-TS$_{prox}$**. Some hydrogen atoms are omitted for clarity.

1.4 Optimized Structure's Energy Components

Table S7. Computed Energy Components for Optimized Structures

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(cal/mol)	G^{solv}/(kcal/mol)
	B3LYP-D3 /LACV3P**	B3LYP-D3 /LACVP**	B3LYP-D3 /LACVP**	B3LYP-D3 /LACVP**
Pd(Ruphos)	-48658.210	423.411	218.34	-3.53
Pd(APhos)	-31284.875	258.959	156.73	-3.59
Pd(CatX)	-38274.483	373.530	162.55	-2.18
C6H6	-6321.578	63.159	64.09	-1.27
3a	-20319.129	151.39	122.64	-4.59
R1	-75299.197	641.928	306.57	-5.56
R1-TSdis	-75298.658	641.086	299.31	-5.37

R2dis	-75299.353	641.953	305.31	-6.27
R2-TSdis	-75299.121	641.572	300.58	-6.07
3b	-26640.900	217.73	144.22	-5.68
R1'	-75298.975	641.53	299.71	-5.87
R1'-TSprox	-75298.756	641.18	302.23	-5.74
R2prox	-75299.381	641.647	303.04	-5.68
R2-TSRE	-75298.569	640.399	301.99	-6.58
3c	-26640.834	217.578	143.66	-5.40
R2-TSprox	-75298.639	641.435	304.99	-6.42
R3	-75299.706	640.464	318.37	-6.03
R3-TSRE	-75298.950	639.454	307.77	-7.01
3d	-26641.485	217.383	150.70	-5.48
R3-TS	-75299.085	637.362	315.35	-6.40
R4	-75299.344	638.241	309.86	-6.69
R5	-54978.927	485.168	244.62	-5.35
R5'	-54979.754	484.402	247.92	-4.59
R5'-TS	-54979.707	483.585	248.30	-3.62
A1	-57925.692	476.483	250.05	-6.31
A1-TSdis	-57924.960	475.751	255.85	-6.88
A2dis	-57926.186	476.285	247.83	-7.21
A2-TSdis	-57925.743	475.833	254.78	-6.97
A1'	-57925.143	475.850	252.31	-6.99
A1'-TSprox	-57924.991	475.514	254.03	-7.11
A2prox	-57925.906	476.457	253.01	-5.79
C1	-64915.512	591.253	256.67	-5.25
C1-TSdis	-64914.851	590.454	255.02	-5.08

C2dis	-64915.994	590.969	252.98	-5.30
C2-TSdis	-64915.559	590.578	252.14	-5.55
C1'	-64915.116	590.554	259.25	-5.98
C1'-TSprox	-64914.821	590.268	255.67	-5.90
C2prox	-64915.496	590.888	256.43	-4.36
[**M**] of **R1**	-30087.715			
[**L**] of **R1**	-45207.794			
$[\mathbf{M}]_{dis}$ of **R1-TS$_{dis}$**	-30087.446			
$[\mathbf{L}]_{dis}$ of **R1-TS$_{dis}$**	-45207.800			
$[\mathbf{M}]_{prox}$ of **R1'-TS$_{prox}$**	-30087.309			
$[\mathbf{L}]_{prox}$ of **R1'-TS$_{prox}$**	-45207.757			
[**M**] of **C1**	-30087.880			
[**L**] of **C1**	-27834.817			
$[\mathbf{M}]_{dis}$ of **C1-TS$_{dis}$**	-30087.401			
$[\mathbf{L}]_{dis}$ of **C1-TS$_{dis}$**	-27834.805			
$[\mathbf{M}]_{prox}$ of **C1'-TS$_{prox}$**	-30087.332			
$[\mathbf{L}]_{prox}$ of **C1'-TS$_{prox}$**	-27834.816			
[**M**] of **A1**	-30087.758			
[**L**] of **A1**	-34824.332			
$[\mathbf{M}]_{dis}$ of **A1-TS$_{dis}$**	-30087.468			
$[\mathbf{L}]_{dis}$ of **A1-TS$_{dis}$**	-34824.339			
$[\mathbf{M}]_{prox}$ of **A1'-TS$_{prox}$**	-30087.358			
$[\mathbf{L}]_{prox}$ of **A1'-TS$_{prox}$**	-34824.330			

1.5 Cartesian coordinates of the optimized geometries

Table S8. Cartesian coordinates of the optimized geometries

The cartesian coordinates of optimized geometries are given below in the standard XYZ format, and units are in Å

==========

Pd(Ruphos)

==========

H	-2.457625235	-0.388491541	-6.346761356
O	-5.331909116	0.269983934	0.879182867
C	-6.079825261	-0.071822762	2.059525145
H	-5.813644342	-1.089594604	2.378573673
C	-5.617326392	0.915435188	3.123236242
H	-5.808413799	1.940275076	2.789736650
H	-6.152367018	0.744463743	4.062569353
H	-4.545526623	0.807867551	3.306836300
C	-7.580984260	0.022126138	1.785293183
H	-7.834649016	1.042475480	1.479705121
H	-7.882896621	-0.660817085	0.986903396
H	-8.151883426	-0.225385780	2.686357110
C	-1.866200591	0.745468267	0.945744242
C	-1.229969169	-0.478448158	1.633296993
C	-1.337358253	2.060520881	1.550181045
H	-2.947709330	0.697727870	1.131378625
C	-1.458584788	-0.433420533	3.153264729
H	-0.150801971	-0.505928560	1.432878736
H	-1.647553270	-1.395865750	1.202942050
C	-1.558124216	2.099989071	3.072870946
H	-0.261417153	2.154492707	1.349944439
H	-1.827404908	2.920434194	1.080036614
C	-0.935390567	0.876717180	3.762810830
H	-0.977814030	-1.295900455	3.631624468
H	-2.535736208	-0.524107466	3.356422278
H	-1.141031281	3.026398524	3.487840905
H	-2.637462563	2.124602984	3.276938938
H	-1.133106394	0.904779693	4.841639224
H	0.157355054	0.915159177	3.642449503
C	-0.220466548	1.545613560	-1.447303546
C	1.026103091	0.768591001	-0.975699530
C	-0.181600203	1.723251986	-2.979068725
H	-0.195804949	2.535947480	-0.973462687
C	2.323755254	1.454274742	-1.437143290
H	0.976046946	-0.252199063	-1.379406478
H	1.031489645	0.673487782	0.115003468
C	1.110808355	2.416438820	-3.437990148
H	-0.243400371	0.725824181	-3.435966275
H	-1.057389467	2.282410922	-3.325353343
C	2.352022716	1.648165525	-2.960372047
H	3.190142678	0.866498808	-1.109233884
H	2.407650319	2.435625578	-0.947143661
H	1.114941673	2.511219673	-4.531027546
H	1.138747324	3.439401957	-3.034320688
H	3.268249319	2.169644303	-3.263915581
H	2.372658663	0.662480242	-3.447369029
C	-3.871826194	4.194523079	-1.675188912
C	-5.195364394	3.773049041	-1.785515019
C	-5.486383132	2.415015469	-1.678852881
C	-4.892615787	0.029312869	-1.403856097
C	-4.839797049	-0.754765299	-2.574512614
C	-5.207262098	-2.109239767	-2.544018239
C	-5.636469285	-2.664936851	-1.338413846
C	-5.717944222	-1.907174632	-0.174068323
C	-5.343157032	-0.555727246	-0.213370226
P	-1.795263368	0.649416550	-0.943221083
H	-1.842702114	3.617741117	-1.360522919
H	-3.619833398	5.248435725	-1.759965756
H	-5.992146813	4.491090872	-1.958773332
H	-6.511467035	2.069012105	-1.773841511
O	-4.443085317	-0.087076800	-3.691614539
H	-5.179730823	-2.715526243	-3.440213060
H	-5.928502794	-3.711272537	-1.311750629
H	-6.061582260	-2.365135458	0.745083550
Pd	-1.996803158	-1.413889297	-1.798989164
C	-3.959209826	-0.804457129	-4.841743313
H	-3.496462948	-1.742075598	-4.502980929
C	-5.111820731	-1.089654186	-5.803410463
H	-4.753453092	-1.637529888	-6.681404837
H	-5.897822883	-1.679548877	-5.324436055
H	-5.554031059	-0.146344564	-6.139634125
C	-2.882696560	0.082312528	-5.454102383
H	-3.307816362	1.050453031	-5.737679680
H	-2.087499271	0.250345049	-4.724786781
C	-4.481467267	1.464420023	-1.461199549
C	-3.136635204	1.885234055	-1.332957413
C	-2.862433641	3.258930880	-1.448442821

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Pd(APhos)

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C	-2.303285000	-0.668579900	-1.808751700
C	-1.337923400	-0.440659300	-2.816848800
C	-0.028830621	-0.110864915	-2.390089500
C	0.274043900	0.014393071	-1.040067200
C	-0.686097900	-0.193312230	-0.033885438
C	-1.975734200	-0.545895000	-0.463696420
N	-1.659003000	-0.527723100	-4.159283000
C	-0.600290660	-0.451785620	-5.160090400
C	-2.967891700	-1.037600000	-4.553183600
P	-0.384324200	-0.022715164	1.776421200
C	1.230494400	-1.014291800	2.124459500
C	-0.098924720	1.865572300	1.988913900
C	0.858198460	2.515975700	0.972172100
C	-1.491118100	2.508988600	1.804744500
C	0.388400140	2.140075000	3.422614800
C	1.323101800	-1.259264100	3.647097600
C	1.043134800	-2.379269000	1.430270600
C	2.551893500	-0.379282060	1.655117300
H	-3.317133000	-0.946115260	-2.069974400
H	0.760797600	0.054482635	-3.112931000
H	1.290429600	0.283854900	-0.779026450
H	-2.739581600	-0.733548340	0.287431450
H	0.153430070	-1.260628200	-5.055885300
H	-1.049324800	-0.527543300	-6.154126600
H	-0.066553770	0.515743260	-5.107577300
H	-3.781607200	-0.398253020	-4.163443000
H	-3.035182700	-1.030548000	-5.644458000
H	-3.152102200	-2.073219800	-4.199357000
H	0.929939500	3.589718000	1.188934000
H	1.869720200	2.108795400	1.013853000
H	0.487211530	2.412998000	-0.050277174
H	-1.403795800	3.598992000	1.900298000
H	-2.198487300	2.148223000	2.557459800
H	-1.906112900	2.288564200	0.815868500
H	-0.245251500	1.633591800	4.158087000
H	1.422295000	1.817772200	3.576299200
H	0.348737120	3.218091700	3.622744000

H	2.191002400	-1.897676000	3.857642400
H	1.446818400	-0.332491600	4.212329400
H	0.424096300	-1.760095100	4.018957600
H	1.859706300	-3.050693500	1.723498600
H	1.049089300	-2.290776500	0.340908380
H	0.097169740	-2.843848700	1.728566200
H	2.572495000	-0.184988170	0.580632200
H	2.769892200	0.554143800	2.179803800
H	3.375950000	-1.071635000	1.871191300
Pd	-2.073656300	-0.773394000	3.071383000

Pd(CatX)

C	5.441222199	-1.352790825	1.172120726
C	4.311053186	-1.301566996	0.138810209
C	3.114961061	-0.466544946	0.615922056
C	1.984661502	-0.422277883	-0.422102324
P	0.657920212	0.866794148	-0.127322733
C	-0.471994317	0.633694588	-1.661182244
C	-1.503984124	1.795967793	-1.723294559
C	-2.357005322	1.704511367	-3.006519069
C	-3.097337698	0.351396297	-3.040063883
C	-2.068092141	-0.797310977	-3.029186425
C	-1.148662732	-0.674521718	-4.259755442
C	-0.414204799	0.680591322	-4.215589754
C	-1.442634204	1.825661155	-4.239273828
C	0.429709240	0.754255297	-2.925116457
C	-1.224694007	-0.718572014	-1.734973217
C	-0.231941997	0.253771055	1.460580654
C	-1.668552168	0.831708157	1.553988383
C	-2.336180419	0.433841511	2.888650961
C	-1.516689605	0.986952170	4.069357978
C	-0.090843352	0.407914998	4.008258744
C	-0.153543132	-1.129174649	4.110479338
C	-0.978680919	-1.684908330	2.932653916
C	-2.406008314	-1.103993715	2.982863028
C	-0.302255840	-1.291111168	1.598558987
C	0.568747425	0.816719110	2.673995748
H	6.288676360	-1.947352029	0.814537372
H	5.811020159	-0.346055271	1.399260275
H	5.095452018	-1.796468165	2.113334092
H	3.974376866	-2.321571291	-0.093584766
H	4.690497073	-0.882344489	-0.803222811
H	3.442450683	0.559258794	0.831343030
H	2.753040387	-0.881180654	1.564362936
H	1.539792998	-1.416461811	-0.551486427
H	2.425729488	-0.143765740	-1.382892646
H	-2.165042851	1.776757250	-0.853499626
H	-0.966404091	2.751676108	-1.689827171
H	-3.086913775	2.524196750	-3.004150748
H	-3.725072175	0.285260317	-3.938623242
H	-3.766430802	0.265943254	-2.173080121
H	-2.590294290	-1.762703576	-3.051864366
H	-0.421750343	-1.497967049	-4.270535900
H	-1.740087192	-0.755764142	-5.181327171
H	0.257622533	0.765563428	-5.079495363
H	-0.927534945	2.795127024	-4.231063624
H	-2.036643810	1.782189091	-5.162125989
H	0.990366366	1.697202501	-2.883752414
H	1.161973099	-0.059412876	-2.952749902
H	-0.513147613	-1.553689864	-1.708246359
H	-1.890680493	-0.836155179	-0.874356899
H	-1.630562860	1.924715890	1.462172907
H	-2.287803452	0.457258336	0.733217469
H	-3.350852669	0.852022889	2.912869336
H	-1.479776838	2.083202308	4.021642727
H	-1.996680674	0.720665036	5.020663312
H	0.508098071	0.810179408	4.835416879
H	-0.608384567	-1.427382732	5.064625375
H	0.860620002	-1.550303014	4.091575254
H	-1.022795383	-2.779997410	2.995462586
H	-3.005742817	-1.506347178	2.155048910
H	-2.903101232	-1.403193982	3.915102870
H	0.703681840	-1.723483640	1.574130124
H	-0.858356294	-1.731281921	0.765227666
H	1.602766960	0.460326362	2.651653119
H	0.616043949	1.909507744	2.594951847
Pd	1.480723474	2.942406939	0.013791381

C_6H_6

C	-2.207606262	0.000000000	-2.620451903
C	-3.363674954	-0.354690359	-1.922287903
C	-1.051537569	0.354690359	-1.922287903
H	-4.263100061	-0.630640582	-2.465460903
H	-0.152112462	0.630640582	-2.465460903
C	-3.363674954	-0.354690359	-0.525957903
C	-1.051537569	0.354690359	-0.525957903
H	-4.263100061	-0.630640582	0.017215097
H	-0.152112462	0.630640582	0.017215097
C	-2.207606262	0.000000000	0.172206097
H	-2.207606262	0.000000000	1.258553097
H	-2.207606262	0.000000000	-3.706798903

3a

C	2.333202035	0.471739219	0.920976225
C	2.577879454	1.880741583	0.372408914
H	1.473241572	0.012801012	0.417695931
H	3.196988045	-0.178550118	0.787451794
N	2.036588824	0.530666134	2.364250978
C	1.148205233	1.534798678	2.782627109
C	0.806803809	2.569136875	1.987533027
H	0.723173693	1.405653397	3.767395005
C	1.405168975	2.790543258	0.676520318
H	0.066546367	3.273705155	2.353336183
C	0.978407375	3.742577688	-0.170060621
H	3.479661211	2.287586410	0.849195654
H	2.772624865	1.828824628	-0.702812636
C	2.560752676	-0.444830074	3.176106827
C	2.192363587	-0.438308713	4.669448418
O	3.290938341	-1.342496203	2.764847035
O	1.016356719	-0.527908485	4.997597234
C	3.300901213	-0.394455779	5.657894230
C	2.952670169	-0.395608906	7.019419805
C	4.652044720	-0.297922611	5.287696103
C	3.937858081	-0.300067546	7.995241179
H	1.902772934	-0.467732984	7.283413193
C	5.635609826	-0.200053398	6.270164358
H	4.930110304	-0.322961326	4.240846229
C	5.281859983	-0.199834110	7.621013726
H	3.663645181	-0.300301389	9.046121615
H	6.680005112	-0.127824065	5.981834074
H	6.052315316	-0.121940685	8.383085625
H	0.155567012	4.402767529	0.089271905
H	1.438282091	3.885031979	-1.143155545

R1

H	-3.607822400	0.534107100	-7.085813500
O	-5.848005000	0.238084700	0.596510600
C	-6.661314000	-0.289434580	1.658653000
H	-6.363673700	-1.326349700	1.865886700
C	-6.330224000	0.570474450	2.872225300
H	-6.548762300	1.620901000	2.655571700
H	-6.924655400	0.257807970	3.736543400

H	-5.269888400	0.484514830	3.125271000
C	-8.139626500	-0.222199860	1.275257700
H	-8.424021000	0.819071350	1.091976300
H	-8.342467000	-0.796843000	0.367798630
H	-8.764958000	-0.617896300	2.082466000
C	-2.125270800	-0.565806600	-0.105851500
C	-0.902294930	-1.500164400	0.006190627
C	-2.780315200	-0.361056830	1.276633600
H	-2.846180000	-1.064177400	-0.763730800
C	-1.355381000	-2.859004000	0.570435700
H	-0.166047700	-1.060296200	0.692924400
H	-0.436777440	-1.632155500	-0.973914800
C	-3.234758000	-1.718206900	1.841448400
H	-2.051755000	0.081149110	1.965510200
H	-3.625605600	0.326075730	1.214727400
C	-2.062395600	-2.709173200	1.928317000
H	-0.492099550	-3.529862000	0.662998740
H	-2.041498700	-3.326010500	-0.150839910
H	-3.693095400	-1.576698500	2.829401700
H	-4.011709000	-2.131957800	1.185223100
H	-2.413577600	-3.684693300	2.288072300
H	-1.337655700	-2.342591800	2.670652200
C	-0.374522800	1.947369700	-0.230463920
C	-0.473939450	2.198338300	1.286245800
C	1.014599600	1.368211300	-0.586248800
H	-0.429656830	2.911115600	-0.752346460
C	0.621286200	3.185570700	1.728990600
H	-0.332872840	1.249397800	1.817992600
H	-1.464628100	2.573991500	1.563674000
C	2.115701400	2.347787600	-0.147657650
H	1.161283000	0.404148370	-0.086498484
H	1.076965700	1.174812400	-1.662178900
C	2.020336200	2.670966600	1.352510000
H	0.555043300	3.358629500	2.810173300
H	0.446513740	4.156610500	1.242827000
H	3.101692700	1.930089400	-0.385912240
H	2.017205700	3.276013100	-0.729228300
H	2.785081400	3.404581500	1.635410900
H	2.230802300	1.757977500	1.928645100
C	-4.136048000	4.360549000	-0.652444200
C	-5.402013300	3.936084300	-1.046769600
C	-5.602012600	2.594038500	-1.353277700
C	-4.940090000	0.232885570	-1.561469800
C	-4.737591700	-0.398689150	-2.802590000
C	-5.082499000	-1.750722600	-2.970295200
C	-5.693333000	-2.438470800	-1.930253100
C	-5.990989000	-1.813998100	-0.719840900
C	-5.618797300	-0.477063860	-0.545646100
P	-1.772510600	1.008286400	-1.045641900
H	-2.109831600	3.820742000	-0.324985000
H	-3.951269400	5.403643600	-0.411756370
H	-6.226632600	4.640540000	-1.114988300
H	-6.587535000	2.243714000	-1.644462100
O	-4.211379000	0.365561900	-3.800740700
H	-4.878249000	-2.258976200	-3.901803500
H	-5.959629500	-3.482992600	-2.069794000
H	-6.498062000	-2.361772800	0.064332955
Pd	-1.146265300	0.673218200	-3.188585800
C	-1.291533500	2.656449300	-3.440069700
C	-0.117479210	3.423466200	-3.459182000
C	-2.509536300	3.269072500	-3.762796900
C	-0.159401940	4.775983300	-3.815427300
H	0.839548470	2.968924800	-3.213688400
C	-2.547318200	4.617770000	-4.125586500
H	-3.429377000	2.696265000	-3.715654400
C	-1.374278500	5.375272000	-4.152417000
H	0.759556530	5.358433000	-3.833410300
H	-3.499893400	5.079571000	-4.377439000
H	-1.406853100	6.425921000	-4.430721800
C	-4.379449000	-0.067910040	-5.179941000
H	-4.000933000	-1.089484800	-5.276138300
C	2.630554000	-1.168909500	-6.061300300
C	1.045654800	-2.512126700	-4.534710000
C	1.410460500	-3.799440400	-5.230000000
C	2.370907800	-3.720095000	-6.428102500
C	2.795148400	-2.364664800	-7.025846500
H	3.455223800	-1.137307400	-5.335542000
H	2.611596800	-0.216014670	-6.597265000
H	1.579124600	-4.632459000	-4.551646000
H	3.134462400	-4.493030500	-6.466595600
H	2.197514300	-2.165003300	-7.923444300
H	3.840222600	-2.414629700	-7.350152500
H	1.534000800	-2.458583400	-3.553261500
N	1.387466000	-1.334719500	-5.345635000
C	0.234987530	-0.671446300	-5.138533600
C	-0.424154100	-1.828356000	-4.358143300
O	-0.118617670	0.504979250	-5.322847000
O	-0.776839500	-1.463587200	-3.094298600
C	-1.535811100	-2.549987800	-5.106107700
C	-1.877400300	-2.273007400	-6.435096000
C	-2.269561800	-3.515305800	-4.406433600
C	-2.919796000	-2.962521300	-7.061506000
H	-1.344489800	-1.498403500	-6.981567400
C	-3.299420400	-4.215825600	-5.032381000
H	-2.031876800	-3.681936000	-3.360040400
C	-3.630387300	-3.940702400	-6.363790500
H	-3.181921700	-2.727424000	-8.090496000
H	-3.856146300	-4.968933600	-4.478520000
H	-4.441581000	-4.478351600	-6.848445000
C	-5.855572000	0.000395000	-5.572843600
H	-5.979815000	-0.323449050	-6.611856500
H	-6.476799500	-0.639005660	-4.940472600
H	-6.216038000	1.031037200	-5.484063000
C	-3.518883200	0.844297230	-6.038908500
H	-3.845833800	1.884802600	-5.955723000
H	-2.467737200	0.788555260	-5.752620000
C	-4.563055500	1.655437000	-1.291999700
C	-3.268862500	2.087664100	-0.905825730
C	-3.089693800	3.445779300	-0.590626900
C	0.943746100	-4.171245600	-6.612304000
H	0.275531900	-3.488085500	-7.126291800
H	0.735373140	-5.219296500	-6.807723500

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R1-TS$_{dis}$

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H	-3.889391153	1.619723033	-7.090433581
O	-5.695224519	-0.081624227	0.458197835
C	-6.641873323	-0.692213139	1.352091304
H	-6.359052535	-1.740036243	1.525786192
C	-6.502669046	0.081224339	2.657000407
H	-6.730990582	1.138322966	2.488235593
H	-7.191538656	-0.312486971	3.410579409
H	-5.482121661	0.006783353	3.040515415
C	-8.054414543	-0.612332222	0.773752101
H	-8.326924774	0.436306082	0.614843779
H	-8.123666502	-1.135058199	-0.183475245
H	-8.776340481	-1.059327182	1.465032608
C	-2.052882993	-0.447564670	0.028996117
C	-0.808771824	-1.350900746	0.156684073
C	-2.693735157	-0.203286705	1.410058553
H	-2.768506697	-0.991466369	-0.597016969
C	-1.220720795	-2.700802876	0.769316271
H	-0.068678205	-0.872708989	0.812132518
H	-0.354918067	-1.507722474	-0.825032971
C	-3.107024262	-1.552012093	2.024982963
H	-1.971203583	0.288199656	2.072613298

H	-3.563084209	0.451345767	1.324782973
C	-1.913771272	-2.515815590	2.129426432
H	-0.340282982	-3.346998800	0.875341117
H	-1.903324919	-3.205806859	0.071716954
H	-3.553802413	-1.392652184	3.014741311
H	-3.884811078	-2.000598320	1.392047853
H	-2.240064956	-3.484710246	2.527839650
H	-1.187620724	-2.108942760	2.848970183
C	-0.343284547	2.081529074	-0.293860495
C	-0.407304694	2.434368025	1.205949649
C	1.044141738	1.485285396	-0.627641077
H	-0.418198919	3.004532934	-0.884170127
C	0.680270658	3.471272600	1.543326765
H	-0.231668961	1.525670515	1.795297385
H	-1.395456554	2.808485801	1.492105471
C	2.139889034	2.515199467	-0.309085915
H	1.213493601	0.577984163	-0.036667470
H	1.087631501	1.193054510	-1.679571867
C	2.080104435	2.961489740	1.161347562
H	0.642760137	3.719880944	2.611069166
H	0.468782942	4.401183399	0.995460268
H	3.126309098	2.092655313	-0.537382715
H	2.007679170	3.383850432	-0.969624766
H	2.832455501	3.735034302	1.357869465
H	2.333741592	2.105688452	1.804116779
C	-4.223382728	4.353800974	-0.595719703
C	-5.478665979	3.876209912	-0.963839990
C	-5.622701192	2.535386102	-1.308708247
C	-4.822601913	0.236019033	-1.692366596
C	-4.602614376	-0.222765733	-3.003563882
C	-4.831433158	-1.566550815	-3.333629727
C	-5.351858857	-2.423138011	-2.372926958
C	-5.673710882	-1.973133734	-1.091326875
C	-5.420575551	-0.637835300	-0.762755499
P	-1.744913218	1.072820970	-1.005389194
H	-2.166007607	3.899280220	-0.313941062
H	-4.083344404	5.399348291	-0.335863711
H	-6.337041907	4.542006847	-0.990851649
H	-6.594023747	2.148721484	-1.603471363
O	-4.160988765	0.709890044	-3.894979087
H	-4.591002641	-1.940598089	-4.320007445
H	-5.516083462	-3.465678094	-2.630797556
H	-6.112704542	-2.650466151	-0.369062366
Pd	-1.268481334	0.469785793	-3.142630963
C	-0.894382667	2.407275824	-3.564579688
C	0.427829002	2.801260118	-3.831955526
C	-1.911944147	3.365466278	-3.675154971
C	0.722278435	4.115231081	-4.207859085
H	1.238182820	2.078000809	-3.769670986
C	-1.617482580	4.679400466	-4.051821048
H	-2.940678418	3.081489771	-3.479899050
C	-0.300800621	5.060038252	-4.315436793
H	1.751198383	4.399103398	-4.419958564
H	-2.422350865	5.406470475	-4.138713988
H	-0.072655173	6.082489872	-4.606346238
C	-4.389466315	0.514312195	-5.318269969
H	-3.867955866	-0.397243768	-5.632260734
C	1.997078625	-0.661332978	-5.917779186
C	0.573747456	-2.021031648	-4.280211970
C	1.197708290	-3.294033831	-4.831879021
C	2.153627302	-3.216036489	-6.027463608
C	2.323991053	-1.891686633	-6.783718941
H	2.812765006	-0.466721054	-5.207656660
H	1.851019056	0.233198657	-6.528351526
H	1.487341920	-3.988465206	-4.046712323
H	3.048840602	-3.828988487	-5.955185083
H	1.668831477	-1.879336455	-7.662462843
H	3.350872626	-1.803076937	-7.155287866
H	0.993260912	-1.835197278	-3.281826045
N	0.780424842	-0.878046022	-5.158318760
C	-0.463116457	-0.357517395	-5.347174203
C	-0.990706790	-1.867142015	-4.157953529
O	-0.838002518	0.401094465	-6.223566627
O	-1.454560491	-1.645830694	-2.950450051
C	-1.892592600	-2.765848725	-4.982716444
C	-2.314876737	-2.504628931	-6.290884068
C	-2.368341989	-3.916607102	-4.335583055
C	-3.186618587	-3.383949133	-6.940693853
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C	-3.223969252	-4.799820016	-4.988811048
H	-2.070198823	-4.094352812	-3.307442879
C	-3.639715708	-4.534688879	-6.296937478
H	-3.514919781	-3.160525479	-7.952539143
H	-3.576019689	-5.690890323	-4.474829057
H	-4.316540102	-5.216294144	-6.805334109
C	-5.885731884	0.415394512	-5.616769435
H	-6.038359909	0.302664972	-6.694943141
H	-6.357135304	-0.432529916	-5.115050166
H	-6.387202395	1.333122214	-5.291112598
C	-3.757136269	1.712593481	-6.007245070
H	-4.239470957	2.637505079	-5.674386288
H	-2.690436417	1.764381169	-5.797781653
C	-4.538307930	1.649697409	-1.298959501
C	-3.260727995	2.128191197	-0.907943057
C	-3.132982265	3.488072853	-0.573509565
C	0.836442183	-3.937022486	-6.145883495
H	0.075014454	-3.467510099	-6.759459291
H	0.818969050	-5.022688222	-6.179164529

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H	-6.391354914	-1.888103530	1.590791878
C	-6.759186479	-0.072849540	2.680925371
H	-7.058198986	0.960693734	2.480320454
H	-7.468556247	-0.514868282	3.387225310
H	-5.767402943	-0.060628725	3.139295928
C	-8.106871092	-0.899072899	0.698904603
H	-8.444340590	0.124267256	0.504286099
H	-8.070328617	-1.435806158	-0.252319432
H	-8.841939667	-1.390858167	1.344546758
C	-2.041003336	-0.304739449	0.315739260
C	-0.735570969	-1.060713528	0.647236751
C	-2.832905021	-0.047529925	1.614813846
H	-2.636838738	-0.963565045	-0.327684617
C	-1.075911532	-2.413828909	1.296724076
H	-0.141444793	-0.468672559	1.355763682
H	-0.132487173	-1.212060093	-0.248665343
C	-3.184954988	-1.390909998	2.277988882
H	-2.222581518	0.546971217	2.305418574
H	-3.743740389	0.517998544	1.416322486
C	-1.929483205	-2.231010094	2.562343049
H	-0.153682308	-2.958276026	1.536079454
H	-1.624518539	-3.026081061	0.566502915
H	-3.741305133	-1.217739079	3.208200097
H	-3.854419880	-1.947296151	1.606923347
H	-2.208146189	-3.206269677	2.981468321
H	-1.325833883	-1.721616177	3.328030553
C	-0.459422481	2.276335173	-0.052092443
C	-0.570691003	2.624111083	1.445390261
C	0.967570131	1.769491652	-0.368920347
H	-0.577826296	3.195972629	-0.641109682
C	0.451946133	3.715936298	1.809791741
H	-0.362284261	1.726078252	2.040434559

H	-1.583219116	2.945992309	1.709053222
C	1.996059612	2.857004002	-0.019640251
H	1.183234241	0.863917447	0.209628061
H	1.043470943	1.497023137	-1.426036860
C	1.884210795	3.283127238	1.453720554
H	0.379963878	3.957173281	2.877671636
H	0.202796970	4.635934805	1.261015137
H	3.009676317	2.496272390	-0.235207419
H	1.823104249	3.725021181	-0.671518214
H	2.591888856	4.091909582	1.673452905
H	2.168033590	2.434079667	2.093126658
C	-4.446994550	4.320073141	-0.398344748
C	-5.667669677	3.776178764	-0.789830233
C	-5.727016105	2.433305955	-1.150860081
C	-4.778691844	0.189113833	-1.536761005
C	-4.473168873	-0.253178423	-2.835588893
C	-4.621372774	-1.601863872	-3.181317522
C	-5.132221087	-2.495796283	-2.249627999
C	-5.531323722	-2.071692568	-0.982739977
C	-5.376810270	-0.723604629	-0.642131553
P	-1.775279285	1.178160491	-0.804111038
H	-2.371723225	3.985216879	-0.092047824
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H	-6.563345144	4.390752095	-0.821524014
H	-6.669967417	1.993084347	-1.461060897
O	-4.048263876	0.692561537	-3.723658711
H	-4.350838230	-1.946094536	-4.168962581
H	-5.235940551	-3.542187431	-2.522932672
H	-5.966213643	-2.774762604	-0.282925171
Pd	-1.045429084	0.705646453	-3.078999224
C	-1.007930987	2.695603559	-3.389053576
C	0.219044085	3.371491112	-3.470298042
C	-2.195813785	3.430631255	-3.458559601
C	0.252603720	4.761527653	-3.607494796
H	1.153625325	2.819296227	-3.441276817
C	-2.156777759	4.821188245	-3.604738247
H	-3.150508792	2.925536499	-3.382387389
C	-0.936299779	5.491949614	-3.676146371
H	1.211423083	5.271660936	-3.672072536
H	-3.090524363	5.377712278	-3.650722330
H	-0.909205448	6.573050912	-3.787930605
C	-4.382994804	0.527086571	-5.130395399
H	-3.932455534	-0.405284941	-5.490222756
C	1.847703536	-0.295254477	-6.181150788
C	0.913721320	-1.399815912	-4.131610639
C	1.682077595	-2.661598944	-4.550884628
C	2.360001169	-2.751173093	-5.912188987
C	2.100550306	-1.618232244	-6.906207551
H	2.770162598	0.030701555	-5.672644020
H	1.542564732	0.488861163	-6.874995612
H	2.238535645	-3.077394271	-3.714781450
H	3.367291304	-3.161348451	-5.912716674
H	1.230574403	-1.848860066	-7.532514582
H	2.957557509	-1.507564826	-7.579943682
H	1.458654344	-0.968369664	-3.277101698
N	0.771596354	-0.426598214	-5.200640435
C	-0.201400584	0.580781901	-5.050701866
C	-0.482473843	-1.748980899	-3.582841963
O	-0.428139813	1.321772332	-5.999332794
O	-0.724302127	-1.574097498	-2.372904270
C	-1.480775109	-2.495023762	-4.413292739
C	-1.828530602	-2.160988565	-5.731444769
C	-2.078729065	-3.610191620	-3.807284677
C	-2.756566089	-2.939633385	-6.423794673
H	-1.400561039	-1.284784034	-6.201304689
C	-2.980770887	-4.402320437	-4.513608637
H	-1.824058688	-3.844091268	-2.778791010
C	-3.326469451	-4.065815148	-5.824184654
H	-3.036241107	-2.662195639	-7.436313945
H	-3.423969449	-5.273106121	-4.038023269
H	-4.042043231	-4.672105400	-6.372997120
C	-5.900958292	0.490092696	-5.308044087
H	-6.151166658	0.417341167	-6.371321549
H	-6.354975631	-0.358606320	-4.790194414
H	-6.338276959	1.412639748	-4.911543079
C	-3.748112790	1.692103376	-5.871223128
H	-4.193743268	2.639080962	-5.551542400
H	-2.670774728	1.736312899	-5.707333572
C	-4.591024152	1.615146598	-1.132309775
C	-3.347803840	2.158375497	-0.718738549
C	-3.308204307	3.519197475	-0.369378873
C	1.231686805	-3.684895790	-5.570255030
H	0.294457578	-3.532737681	-6.093147298
H	1.449138219	-4.725600164	-5.345573210

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C	-7.078051181	1.204284022	2.378534337
H	-7.261057784	2.206113465	1.977829825
H	-7.778545480	1.019635305	3.198869948
H	-6.058567267	1.172270574	2.771507444
C	-8.671707989	0.166401706	0.697169445
H	-8.912521814	1.166072805	0.321470914
H	-8.766158131	-0.541175263	-0.130533323
H	-9.403840621	-0.102031070	1.465739571
C	-2.494153290	-0.527194498	0.127664249
C	-1.395373607	-1.488219465	0.623877580
C	-3.262209260	0.052125163	1.334801356
H	-3.198215226	-1.135102069	-0.451873065
C	-2.025161396	-2.641482232	1.424689751
H	-0.698691580	-0.946792766	1.275936008
H	-0.814456158	-1.878769148	-0.215970908
C	-3.898885623	-1.089140301	2.148868061
H	-2.571805780	0.606454917	1.979959816
H	-4.032254287	0.755206628	1.012777719
C	-2.847237813	-2.110648189	2.611386348
H	-1.243192152	-3.325232528	1.779224821
H	-2.678234563	-3.223044032	0.757500498
H	-4.437091300	-0.679444302	3.013735682
H	-4.643990123	-1.597960768	1.522414941
H	-3.327033607	-2.939924012	3.146450585
H	-2.166822860	-1.626523304	3.327378199
C	-0.446478557	1.659598701	-0.413625241
C	-0.665843052	2.290758457	0.975082843
C	0.881228253	0.866211665	-0.431116087
H	-0.310479956	2.465762959	-1.147379987
C	0.501218453	3.229491170	1.328172975
H	-0.713128646	1.493128661	1.727121378
H	-1.618962033	2.827426778	1.023342704
C	2.056763944	1.788843558	-0.065434927
H	0.839175457	0.045950309	0.294608889
H	1.051488827	0.411222308	-1.409680473
C	1.842319157	2.478878734	1.291398851
H	0.338189297	3.677960981	2.316508094
H	0.526634816	4.057974313	0.604945123
H	2.990230817	1.212840021	-0.060426268
H	2.160400204	2.553392316	-0.846433738
H	2.670760036	3.164919398	1.508300943
H	1.846497109	1.719605915	2.087717344
C	-3.903013231	4.292390462	-1.480319806
C	-5.235074949	3.928911795	-1.667882898
C	-5.559650051	2.577248941	-1.714447821

C	-5.058712518	0.160813136	-1.691454483
C	-4.676692505	-0.681950388	-2.749182368
C	-5.043146683	-2.034728525	-2.757822419
C	-5.862407052	-2.533192247	-1.753782515
C	-6.330583933	-1.701940392	-0.735783566
C	-5.931507004	-0.362247636	-0.705050441
P	-1.862587412	0.686530545	-1.176379366
H	-1.905963712	3.634744374	-1.179276417
H	-3.613890078	5.339821706	-1.456177307
H	-6.008063798	4.683047859	-1.785613409
H	-6.590128264	2.272145266	-1.869230294
O	-3.874099183	-0.193438057	-3.751589967
H	-4.670538839	-2.670072013	-3.549843339
H	-6.151458145	-3.580598718	-1.760476217
H	-6.981782602	-2.104669866	0.029835843
Pd	-1.202885973	0.169508898	-3.494048534
C	-0.302201648	1.996748367	-4.136828446
C	1.010389836	2.243958109	-3.690474577
C	-1.199905802	3.078404244	-4.218935887
C	1.406391145	3.540948391	-3.349835672
H	1.713054269	1.432801237	-3.545421999
C	-0.806443620	4.362378396	-3.853702150
H	-2.197590478	2.896655329	-4.603688293
C	0.501986691	4.601468768	-3.421443609
H	2.424771136	3.715148018	-3.010808848
H	-1.523059498	5.178367013	-3.907737622
H	0.813776007	5.606007725	-3.147087844
C	-4.486224630	0.176303858	-5.031200964
H	-3.617665150	0.518794061	-5.592798781
C	0.544535577	0.381550289	-7.551705923
C	1.413527302	-0.472524442	-5.410347209
C	2.213248135	-1.505029223	-6.219859182
C	1.995086763	-1.675923725	-7.712050007
C	0.866074853	-0.873650582	-8.360762337
H	1.398030554	1.078942518	-7.592054356
H	-0.336476912	0.890939614	-7.939634151
H	3.238015625	-1.561544596	-5.863063477
H	2.892811914	-1.800714578	-8.312955855
H	-0.040655539	-1.484273946	-8.450863902
H	1.151545802	-0.578095520	-9.376547507
H	2.116809161	0.343045086	-5.193853959
N	0.272784659	0.054680233	-6.143384835
C	-0.765815880	0.743750294	-5.509313872
C	1.112037359	-1.112368723	-4.043312255
O	-1.726649566	1.132257672	-6.179858493
O	1.963149492	-0.946762731	-3.167952384
C	-0.018489189	-2.086897341	-3.821855003
C	-1.049690639	-2.377629855	-4.745330669
C	0.004548673	-2.799414350	-2.603190171
C	-2.012124141	-3.343961692	-4.445130461
H	-1.092381434	-1.859522499	-5.693806053
C	-0.960854907	-3.754574442	-2.311927970
H	0.804437966	-2.575091022	-1.906111145
C	-1.975715524	-4.031210613	-3.233350457
H	-2.793871536	-3.555017859	-5.169296054
H	-0.926961309	-4.283348941	-1.363312629
H	-2.734521357	-4.773902626	-3.003090993
C	-5.107140950	-1.021276636	-5.745598861
H	-5.403664627	-0.721252359	-6.756497665
H	-4.381798616	-1.835864478	-5.831346409
H	-5.997040425	-1.395200770	-5.229380073
C	-5.463804394	1.332844338	-4.861082963
H	-6.325695119	1.044189081	-4.249370042
H	-4.972926598	2.183263008	-4.384055981
C	-4.587660067	1.574250572	-1.584019443
C	-3.237087555	1.936553877	-1.338268160
C	-2.929312115	3.310005299	-1.314773013
C	1.647876777	-2.794679144	-6.761607807
H	0.594873567	-3.008354264	-6.614684945
H	2.286574820	-3.672582464	-6.720258474

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3b

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C	-2.008694004	0.717615266	-6.325371669
C	-2.368294350	-0.273469217	-7.248787480
C	-2.857790233	1.810661927	-6.117019400
C	-3.555032001	-0.158826023	-7.970937629
H	-1.728272255	-1.141436070	-7.372153924
C	-4.036318936	1.930796464	-6.849753787
H	-2.581642655	2.548673924	-5.370996582
C	-4.385648874	0.947409070	-7.779065921
H	-3.836101681	-0.935601991	-8.676278494
H	-4.687754857	2.785489096	-6.691827530
H	-5.308900968	1.037689998	-8.344607817
C	0.770564821	0.294071186	-7.388157866
C	1.409346743	-0.291742164	-5.077357029
C	2.495684525	-1.182664275	-5.686098399
C	2.498204300	-1.518322354	-7.169961895
C	1.409547854	-0.919152174	-8.057344122
H	1.504396360	1.114700104	-7.332304667
H	-0.079208415	0.658618078	-7.964406392
H	3.463009443	-1.051665376	-5.208006038
H	3.481409059	-1.599009458	-7.626741833
H	0.635096430	-1.664375472	-8.274591513
H	1.833385532	-0.608195969	-9.018415108
H	1.847082886	0.669680123	-4.780567241
N	0.322099423	-0.034047641	-6.026075432
C	-0.784703247	0.595506417	-5.472069424
C	0.853213155	-1.029440553	-3.840956625
O	-0.786298673	0.978284423	-4.304516903
O	0.016406142	-1.905785236	-3.987166261
C	1.421594443	-0.724467584	-2.492140787
C	2.532653686	0.105187615	-2.282462372
C	0.801609557	-1.325606383	-1.385489818
C	3.011712061	0.329022872	-0.991736875
H	3.037907422	0.575340793	-3.119179184
C	1.271877285	-1.092963207	-0.098023867
H	-0.053650494	-1.967483788	-1.567081475
C	2.379825465	-0.264298149	0.101982447
H	3.875097005	0.970233391	-0.839781240
H	0.776862348	-1.554605430	0.751606749
H	2.748733317	-0.081864228	1.107499575
C	2.145949455	-2.572410388	-6.151799457
H	1.100389357	-2.853324512	-6.062668636
H	2.851132890	-3.374580772	-5.956100657

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R1'

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C	-0.724649751	2.785790923	2.316867570
C	0.571479484	2.384683990	2.714381115
C	1.135182968	2.977202234	3.863167062
C	0.456954325	3.939630979	4.603598611
C	-0.820892098	4.335786973	4.208743674
C	-1.391278249	3.759413459	3.079972159
C	-1.456541705	2.288205485	1.112625768
C	-1.546339365	3.115321445	-0.023983266
C	-2.227717210	2.689859074	-1.169937130
C	-2.892207275	1.463222710	-1.135702769
C	-2.895899817	0.665503962	0.002750830
C	-2.171623470	1.075084937	1.134917798
P	1.563044394	1.060164940	1.889161201
H	2.122476213	2.674321694	4.195579581
H	0.924758921	4.371840042	5.483810523
H	-1.367094972	5.084944042	4.774983462
H	-2.382677451	4.063062436	2.757529096
O	-0.910101007	4.321724657	0.097843260

H	-2.255932152	3.299433031	-2.063794291
H	-3.438881547	1.132647816	-2.014245818
H	-3.427490352	-0.275575868	-0.001848326
Pd	0.799169043	0.413703914	-0.146249838
C	1.874877349	1.730525031	-1.208038517
C	2.730517139	1.129792444	-2.152816855
C	1.746950503	3.126615562	-1.224172423
C	3.403382860	1.897944255	-3.109195611
H	2.891466989	0.052676614	-2.143371160
C	2.424730766	3.894334643	-2.178071650
H	1.116906493	3.614661455	-0.490767420
C	3.253255553	3.286176421	-3.124132205
H	4.056143830	1.411140823	-3.830613954
H	2.310542181	4.976349699	-2.179317035
H	3.783287995	3.887260986	-3.858141657
C	-1.049983005	5.342333721	-0.906950570
H	-0.814983244	4.910679367	-1.890153871
C	-2.839769011	-1.820023399	-3.074909518
C	-0.602554098	-1.333173042	-1.927212301
C	0.152902333	-1.692059953	-3.186293272
C	-0.650633129	-2.230375991	-4.380463470
C	-2.159014898	-2.515891573	-4.274182424
H	-3.057731852	-0.770344855	-3.314998607
H	-3.778099313	-2.309989385	-2.800762362
H	0.962386423	-1.007799689	-3.429469677
H	-0.323079240	-1.872817408	-5.353600571
H	-2.314411875	-3.597312278	-4.182921940
H	-2.659813601	-2.203415025	-5.197325224
H	-0.626536707	-0.224209311	-1.827607813
N	-1.957252686	-1.856414847	-1.934505296
C	-1.920941004	-2.505741473	-0.731483444
C	-0.441237223	-2.052709586	-0.469852283
O	-2.779444522	-3.124030727	-0.126249469
O	-0.322517238	-1.199928506	0.597434357
C	0.578745408	-3.176340606	-0.426899609
C	1.909291805	-2.932573964	-0.796628575
C	0.234867807	-4.439009086	0.065512571
C	2.876617440	-3.927129291	-0.678406081
H	2.185354619	-1.953092172	-1.177391193
C	1.203844359	-5.439771478	0.184111745
H	-0.794233596	-4.630423068	0.355363065
C	2.524887201	-5.188148309	-0.186105933
H	3.903691003	-3.722916979	-0.971398823
H	0.924356174	-6.417269186	0.569123176
H	3.277293011	-5.967187947	-0.094290047
C	1.338281020	-0.427435581	3.014484901
C	2.203812332	-1.626536814	2.582091455
C	1.498305814	-0.168465828	4.526006544
H	0.294696514	-0.675883981	2.797359023
C	1.801998816	-2.888689667	3.357938031
H	3.259901309	-1.413003872	2.797090587
H	2.101388396	-1.801979394	1.511291217
C	1.156111373	-1.437683187	5.333144193
H	2.534227588	0.130272263	4.746987042
H	0.848912195	0.647213419	4.854428043
C	1.953682011	-2.665544051	4.869203212
H	2.415434624	-3.733868454	3.023986076
H	0.763687850	-3.142925300	3.109243118
H	1.331229224	-1.246523378	6.399509254
H	0.084422528	-1.642663054	5.224109644
H	1.634208380	-3.554257433	5.427572174
H	3.018379528	-2.514390904	5.103102218
C	3.366000848	1.583874008	2.025807890
C	4.278672297	0.706919617	1.135645620
C	3.643718156	3.072277381	1.718618482
H	3.628306286	1.389062201	3.077162045
C	5.760635928	1.034397578	1.387513775
H	4.034490188	0.909821049	0.088407764
H	4.097518886	-0.356576066	1.299627506
C	5.122758557	3.409983297	1.974184725
H	3.404937959	3.264822684	0.667552382
H	3.003787022	3.730206108	2.312093882
C	6.053824813	2.520819578	1.136916936
H	6.388246566	0.406014554	0.743873389
H	6.021043215	0.779121486	2.425561365
H	5.299973570	4.469189980	1.750878661
H	5.348665250	3.272359224	3.042435879
H	7.103952466	2.748624282	1.357570579
H	5.895578983	2.741789104	0.071756600
C	0.001319414	6.388701800	-0.554484559
H	1.002838556	5.952769995	-0.549809368
H	-0.020318724	7.208422467	-1.279211984
H	-0.197750088	6.795457189	0.441999080
C	-2.460272892	5.933690577	-0.892834362
H	-2.551064353	6.713611958	-1.656037102
H	-3.222485823	5.175303192	-1.082886218
H	-2.659480840	6.381438856	0.086273373
O	-2.103850025	0.381485642	2.297217497
C	-2.909416219	-0.813034358	2.461346282
H	-2.837703976	-1.421158896	1.557998053
C	-4.355683769	-0.416031250	2.755534330
H	-4.407104008	0.153128108	3.690084958
H	-4.772286565	0.202276102	1.955506582
H	-4.979718305	-1.310214230	2.855163287
C	-2.276062846	-1.593477617	3.601249148
H	-2.900926306	-2.454988233	3.857345174
H	-1.294495546	-1.960394383	3.298250481
H	-2.169529398	-0.961576108	4.489949820
C	0.316463239	-3.117414399	-3.638718182
H	-0.108987312	-3.892818399	-3.006816499
H	1.255566285	-3.397189531	-4.107668425

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R1'-TS$_{prox}$

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C	-0.951400039	3.544861620	1.824376234
C	0.384707167	3.209841650	2.128998053
C	0.941867238	3.698200400	3.329285922
C	0.213707822	4.482395768	4.217013637
C	-1.113299978	4.794073201	3.921355134
C	-1.674948403	4.329611812	2.738497082
C	-1.671353240	3.205848396	0.559316376
C	-1.794950000	4.204620102	-0.426793994
C	-2.526852729	3.976617318	-1.596600029
C	-3.178110327	2.752963893	-1.744923613
C	-3.118576895	1.765783731	-0.768974439
C	-2.365390314	1.991370457	0.395730650
P	1.436302058	2.082760043	1.104915488
H	1.967490920	3.456974158	3.584496110
H	0.678680105	4.840215906	5.131117806
H	-1.703861778	5.400392194	4.602938561
H	-2.701113227	4.582892596	2.488184927
O	-1.130121709	5.369202740	-0.146469042
H	-2.601536219	4.730693645	-2.369562238
H	-3.758080846	2.567464196	-2.644575955
H	-3.629768645	0.826633101	-0.928469975
Pd	0.684416994	1.569125536	-1.015697052
C	1.753580071	2.973518007	-1.986786231
C	2.838041080	2.560986337	-2.782659055
C	1.391305047	4.327493032	-2.019898057
C	3.531824860	3.470883492	-3.588306240
H	3.151429859	1.519242494	-2.788028703
C	2.079747446	5.236625067	-2.832159315
H	0.588564169	4.678573024	-1.385726412
C	3.155274108	4.815360323	-3.616728085
H	4.368248376	3.125588532	-4.192375745
H	1.778551508	6.282337956	-2.842848456

H	3.694189181	5.524167099	-4.239704064
C	-1.310229973	6.541022818	-0.963311543
H	-1.194192271	6.265384497	-2.021229566
C	-2.551061329	0.339528617	-4.460407978
C	-0.445111053	0.743181349	-3.142195553
C	0.402989903	0.650398083	-4.374918195
C	-0.295516772	0.310589019	-5.703894243
C	-1.789632778	-0.050336426	-5.744825484
H	-2.795974486	1.410254918	-4.471103368
H	-3.479358287	-0.227200036	-4.345639274
H	1.185094287	1.400396395	-4.429508579
H	0.064782368	0.863999270	-6.567957696
H	-1.897639202	-1.130280339	-5.902433202
H	-2.266714504	0.440316655	-6.600638258
H	-0.641555283	1.800760423	-2.893965992
N	-1.716699275	0.076103743	-3.307886850
C	-1.850794123	-0.786332776	-2.282790526
C	-0.462186864	-0.623554546	-1.627161880
O	-2.805245468	-1.476262224	-1.944938678
O	-0.418112525	-0.153120637	-0.405341974
C	0.537373346	-1.705600839	-1.964890919
C	1.905105689	-1.426357686	-2.068703787
C	0.100416653	-3.029301272	-2.095876473
C	2.824526062	-2.447378865	-2.291690627
H	2.238588144	-0.395476650	-1.985540195
C	1.022747685	-4.054451893	-2.321257283
H	-0.959711057	-3.250199429	-2.012185781
C	2.384210496	-3.767916483	-2.419147786
H	3.882838883	-2.213507717	-2.375174351
H	0.674220916	-5.079363021	-2.417491015
H	3.099530080	-4.566430005	-2.596857597
C	1.322896236	0.459710864	2.056957061
C	2.200469215	-0.657251490	1.456759557
C	1.525823991	0.525095866	3.583218305
H	0.276120812	0.206288190	1.856795101
C	1.846757222	-2.018792871	2.073535631
H	3.256252953	-0.447638416	1.672275944
H	2.080643606	-0.700990870	0.374536788
C	1.204039252	-0.841024900	4.223309510
H	2.566783610	0.799641967	3.810660193
H	0.883607096	1.286481641	4.032521756
C	2.013652056	-1.988443586	3.600044087
H	2.479171641	-2.797354376	1.629616604
H	0.811455129	-2.271070860	1.810101679
H	1.382021879	-0.788861085	5.304797410
H	0.132959812	-1.042701817	4.090522725
H	1.713421636	-2.946544199	4.042134514
H	3.078411053	-1.850744466	3.840920150
C	3.170648565	2.775008991	1.309613435
C	4.209656056	2.015898777	0.455079800
C	3.238614694	4.289229223	1.001405360
H	3.429564321	2.617441240	2.367171406
C	5.625851456	2.572359528	0.685211704
H	3.945608585	2.130160195	-0.599499832
H	4.194075998	0.946479399	0.674629780
C	4.656225600	4.837740329	1.232147877
H	2.957503841	4.448802899	-0.044170394
H	2.519667012	4.845158349	1.609434591
C	5.691095995	4.077798031	0.390194778
H	6.339191655	2.025485430	0.056385049
H	5.924792201	2.391900389	1.728717508
H	4.676708225	5.908231118	0.993785020
H	4.915245085	4.747600066	2.298013169
H	6.700474953	4.463251752	0.580003711
H	5.477890241	4.244777145	-0.675267263
C	-0.171214423	7.472851759	-0.566927425
H	0.796240880	6.993429923	-0.737275549
H	-0.214401619	8.397855802	-1.150300287
H	-0.246982350	7.723479411	0.495784259
C	-2.685796641	7.160301948	-0.720158466
H	-2.813804677	8.058033078	-1.334025830
H	-3.488509413	6.459488470	-0.962147065
H	-2.780933407	7.441759423	0.333559965
O	-2.258335144	1.112151307	1.422681887
C	-2.978983946	-0.145557913	1.361841953
H	-2.892492793	-0.560066897	0.354066545
C	-4.439877624	0.086460579	1.743888903
H	-4.505297057	0.461828927	2.770676635
H	-4.915124555	0.815223242	1.081724915
H	-5.001450952	-0.851197357	1.677640006
C	-2.265283252	-1.081502479	2.323660604
H	-2.811307068	-2.026976753	2.402415543
H	-1.260285959	-1.291786197	1.955437372
H	-2.199332628	-0.632404144	3.320699781
C	0.676673980	-0.655768425	-5.076415237
H	0.258966777	-1.559151593	-4.641164420
H	1.655513084	-0.794070388	-5.527380108

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R2$_{prox}$

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C	-3.026426992	2.057297440	2.764290453
C	-1.706852260	1.750380686	3.183597066
C	-1.079142181	2.631814522	4.085438073
C	-1.697856600	3.788494429	4.548909724
C	-2.982359259	4.101570591	4.109144614
C	-3.627061332	3.239421142	3.230292071
C	-3.897728330	1.215601568	1.883413391
C	-4.326684023	1.697804405	0.622686562
C	-5.257185499	0.985187622	-0.137300807
C	-5.769083777	-0.217898915	0.347691503
C	-5.394149678	-0.698978185	1.592422969
C	-4.486405030	0.035329532	2.362157437
P	-0.764707360	0.252856947	2.604429886
H	-0.074104343	2.419216321	4.431348361
H	-1.174385629	4.440853994	5.242540309
H	-3.480598004	5.004944895	4.450427762
H	-4.631463878	3.469810937	2.887676198
O	-3.779178978	2.886099027	0.227722163
H	-5.574020584	1.348524194	-1.106145986
H	-6.457572971	-0.791878758	-0.265045267
H	-5.776200491	-1.642351548	1.963780979
Pd	-1.577099375	-0.465235739	0.386817640
C	-0.390906572	0.828438825	-0.576932059
C	0.790469707	0.369335302	-1.183061089
C	-0.693270294	2.195370707	-0.641443856
C	1.665325844	1.264153130	-1.807929257
H	1.025281017	-0.691771608	-1.181804276
C	0.180232466	3.086038961	-1.277729090
H	-1.592935569	2.572531237	-0.170047314
C	1.366637779	2.629203115	-1.855731509
H	2.580768789	0.891364010	-2.262981098
H	-0.058908733	4.147580795	-1.299402742
H	2.048421990	3.324655061	-2.337949683
C	-4.358189835	3.626978886	-0.864898651
H	-4.488407061	2.958413681	-1.726646024
C	-4.544537021	-1.447127030	-2.701741919
C	-2.519393551	-0.637482699	-1.534343310
C	-1.721682302	-0.806167161	-2.809882815
C	-2.384713411	-1.413822146	-4.045210161
C	-3.811665307	-1.965467501	-3.950160966
H	-4.789876743	-0.383919817	-2.803361269
H	-5.460061172	-2.009187174	-2.505340062
H	-1.055545452	0.026649179	-3.004952254
H	-2.130531244	-0.951363222	-4.996391444
H	-3.797397268	-3.061764191	-3.909260415
H	-4.385107354	-1.691448318	-4.843787384

H	-2.972793070	0.361115140	-1.560178656
N	-3.651969850	-1.579329509	-1.547403277
C	-3.748300443	-2.675304982	-0.776744942
C	-2.643589743	-2.906198412	0.250920352
O	-4.641101558	-3.530843499	-0.829249052
O	-2.663369427	-2.309934389	1.342826178
C	-1.653017988	-3.974351560	-0.050722017
C	-0.353805180	-3.847871802	0.469553657
C	-1.963271540	-5.062052457	-0.881544632
C	0.620599380	-4.790260387	0.158695800
H	-0.109808868	-2.985476547	1.076680208
C	-0.986739655	-6.012639908	-1.174021970
H	-2.969423726	-5.162950626	-1.272170181
C	0.305408566	-5.876292513	-0.662802989
H	1.627780970	-4.673517385	0.549320322
H	-1.234056077	-6.858331963	-1.809382921
H	1.066890408	-6.612278928	-0.906684875
C	-0.995400287	-0.918730390	4.086856612
C	-0.628143059	-2.386841748	3.792063167
C	-0.330086565	-0.448554878	5.396460054
H	-2.081798150	-0.877918304	4.212729821
C	-0.994241426	-3.300867507	4.973153758
H	0.449582297	-2.482489177	3.605364157
H	-1.158022539	-2.718157932	2.902245881
C	-0.689987338	-1.372993468	6.574843597
H	0.762645379	-0.452022063	5.279751347
H	-0.627445276	0.577088924	5.636597496
C	-0.330752411	-2.834978520	6.275801184
H	-0.706787052	-4.333928308	4.740310935
H	-2.086546416	-3.302015762	5.097757820
H	-0.177753757	-1.027805019	7.482005599
H	-1.766440387	-1.300099880	6.775359489
H	-0.625474590	-3.479998877	7.112982152
H	0.761272232	-2.925919737	6.176646361
C	1.051782286	0.768569484	2.737657540
C	1.960383158	-0.376198994	2.233134003
C	1.437067603	2.086449540	2.031688637
H	1.255062795	0.897734101	3.808806274
C	3.448359312	-0.039782151	2.441017918
H	1.763040516	-0.538152665	1.167561296
H	1.729451247	-1.313132649	2.747850474
C	2.914755507	2.426337330	2.287992214
H	1.290246585	1.980664463	0.959432009
H	0.796865737	2.911958425	2.354452660
C	3.827530331	1.297109013	1.787032450
H	4.068685856	-0.852926543	2.043167346
H	3.656424164	0.013369107	3.520226565
H	3.163789655	3.369331140	1.785943803
H	3.083396888	2.586044919	3.364171489
H	4.880988761	1.532628627	1.983889398
H	3.714727501	1.210975947	0.697387573
C	-3.336342537	4.698318791	-1.224884693
H	-2.417044325	4.246901861	-1.602490761
H	-3.741903240	5.360783415	-1.995834591
H	-3.095756649	5.296554567	-0.340095958
C	-5.702586442	4.219907375	-0.441815293
H	-6.152472154	4.776580738	-1.270405662
H	-6.403685906	3.441655778	-0.129119425
H	-5.552608528	4.906943729	0.397681653
O	-4.151296007	-0.375226101	3.630354853
C	-5.242886608	-0.558622753	4.562536382
H	-5.923637104	-1.326383334	4.169379807
C	-6.004987704	0.751409329	4.758988824
H	-5.322447962	1.530768230	5.112402346
H	-6.453165116	1.087688673	3.819376742
H	-6.806499441	0.619110319	5.493261656
C	-4.604331066	-1.064947344	5.846355055
H	-5.370315450	-1.261261963	6.602784380
H	-4.050291917	-1.989177852	5.661333179
H	-3.909090661	-0.315561228	6.238104493
C	-1.261995837	-2.137982359	-3.325679845
H	-1.539349121	-3.024301070	-2.761582904
H	-0.284718292	-2.201583755	-3.796894304

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R2-TS$_{RE}$

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C	-2.708568800	-1.719320900	4.512797000
C	-1.536634100	-0.938868500	4.400148400
C	-1.042710900	-0.299936200	5.547507300
C	-1.674734600	-0.434887260	6.783142000
C	-2.815549400	-1.227005100	6.893849000
C	-3.324367000	-1.859525600	5.761514700
C	-3.372472300	-2.354465700	3.334206600
C	-4.283372400	-1.588219400	2.575792800
C	-5.003348000	-2.169668200	1.522628300
C	-4.775601000	-3.506649700	1.205480800
C	-3.869367800	-4.280079400	1.926265400
C	-3.188479700	-3.708176600	3.009979200
P	-0.659567060	-0.885144700	2.772947000
H	-0.147967010	0.310859050	5.487307000
H	-1.271276200	0.073593340	7.654889000
H	-3.312848300	-1.344707100	7.852882400
H	-4.223927000	-2.464832500	5.831737500
O	-4.399408000	-0.287682980	2.964240300
H	-5.727284400	-1.596645100	0.958489060
H	-5.297637000	-3.953211500	0.366986450
H	-3.709144000	-5.312644500	1.651140200
C	-5.036379000	0.674293460	2.098896700
H	-4.902904500	0.355054530	1.061057600
C	0.410860420	-2.434546700	2.988241700
C	0.916549740	-3.012052500	1.652497900
C	1.541414500	-2.269335500	4.024204700
H	-0.307612800	-3.152754300	3.402353000
C	1.726859200	-4.302288500	1.861195300
H	1.532861400	-2.277549500	1.121871100
H	0.055868875	-3.215345100	1.007667800
C	2.317577400	-3.583416500	4.219298400
H	2.247602000	-1.497305600	3.693810700
H	1.126111700	-1.932983800	4.981234600
C	2.859156000	-4.112448700	2.881986100
H	2.129186000	-4.641334000	0.898713200
H	1.053507600	-5.099457300	2.205917400
H	3.138068000	-3.428245000	4.931384000
H	1.653027400	-4.333860000	4.668599600
H	3.399827500	-5.055093300	3.034344400
H	3.588533900	-3.392875400	2.481207100
C	0.486889450	0.590544900	2.920599700
C	1.563319400	0.568788770	1.812523500
C	-0.347851460	1.888043200	2.848859300
H	1.001158400	0.557996870	3.890427000
C	2.436103000	1.833388800	1.849339800
H	1.080901400	0.490199690	0.835370060
H	2.203159300	-0.312115850	1.918021400
C	0.539630500	3.142283200	2.891435900
H	-0.912584840	1.879543500	1.906639300
H	-1.085799500	1.911030800	3.659645800
C	1.585518800	3.108371700	1.767212000
H	3.156447200	1.800721300	1.022843700
H	3.021556400	1.849808800	2.781026400
H	-0.083324210	4.042164300	2.812926000
H	1.050495500	3.197439700	3.864258000
H	2.224139700	3.999562000	1.808543000
H	1.070704700	3.129002000	0.795894900
C	-4.283046000	1.982056700	2.305528600
H	-3.231506800	1.848309800	2.038608600
H	-4.710788700	2.772730400	1.680005200

H	-4.339529500	2.295011000	3.353297000
C	-6.520690400	0.773395360	2.441874000
H	-7.019159000	1.497153900	1.787692400
H	-7.018589500	-0.194055020	2.329077000
H	-6.643789000	1.100790000	3.479350600
O	-2.294237100	-4.377702700	3.800189300
C	-2.187073000	-5.813973400	3.725251700
H	-2.057781700	-6.112371000	2.675677800
C	-3.427252000	-6.474555500	4.328775400
H	-3.520748100	-6.186324000	5.380990000
H	-4.340105500	-6.174044600	3.808979700
H	-3.341940000	-7.564918000	4.273212000
C	-0.922317500	-6.162108400	4.498363500
H	-0.774022700	-7.246399400	4.514785300
H	-0.048072062	-5.698414000	4.037774600
H	-1.001223300	-5.803306600	5.529578000
C	-0.761100300	-0.445355420	-0.895052400
C	0.229597510	-1.358344800	-1.300339200
C	-0.523641400	0.923035260	-1.129597800
Pd	-1.915055500	-0.837503250	0.766992400
C	1.412185400	-0.922973040	-1.894617900
H	0.072430536	-2.419970000	-1.151471000
C	0.660988450	1.358260200	-1.733010200
H	-1.249635000	1.665713300	-0.816249300
C	1.636952200	0.439664400	-2.119129700
H	2.163057800	-1.653706700	-2.187022000
H	0.818890000	2.422909500	-1.890587900
H	2.556164500	0.776081440	-2.590391400
C	-2.121477400	-0.881373300	-3.707515200
C	-2.839215800	0.466565430	-3.494188500
H	-2.494641300	-1.389205200	-4.600236400
H	-1.047082000	-0.721760330	-3.852557000
N	-2.326472800	-1.818656200	-2.585399200
C	-2.729742500	-1.326780900	-1.281012800
C	-4.026076000	-0.546980300	-1.463560900
H	-2.936801700	-2.213718400	-0.673069830
C	-4.125116000	0.331817120	-2.691100000
H	-4.897811400	-1.149758000	-1.217561200
C	-4.205015000	0.948336800	-1.315915000
H	-5.047140000	0.269662740	-3.264482000
H	-2.159777200	1.151927200	-2.986317600
H	-3.040779000	0.903975800	-4.477654500
C	-2.129775500	-3.131104200	-2.859085000
C	-2.687037200	-4.193617000	-1.904484500
O	-1.633769900	-3.555026300	-3.906846300
O	-3.891632300	-4.222433000	-1.681764500
C	-1.758606700	-5.247550500	-1.415013600
C	-2.296265800	-6.304264000	-0.664202150
C	-0.373688900	-5.188183300	-1.632243500
C	-1.462366900	-7.275019600	-0.118483126
H	-3.372400800	-6.341541000	-0.528791800
C	0.460045840	-6.161795000	-1.083692300
H	0.041066326	-4.398741200	-2.248968000
C	-0.079755640	-7.200499500	-0.322029320
H	-1.884652000	-8.091660000	0.461275800
H	1.531622900	-6.113222000	-1.255030500
H	0.574223760	-7.955506000	0.106230680
H	-3.367895600	1.541954300	-0.965293100
H	-5.172870600	1.298578500	-0.967005000

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C	-1.473838453	-1.792341196	-1.219656942
C	-1.172630450	-3.046203602	-1.763130209
C	-0.542461340	-1.186349309	-0.370113761
C	0.033653634	-3.680535266	-1.465249188
H	-1.903067193	-3.544084504	-2.393237012
C	0.663754059	-1.816962377	-0.070218639
H	-0.778027453	-0.225930932	0.080930854
C	0.955855696	-3.068435594	-0.616721954
H	0.243757732	-4.661104029	-1.882445405
H	1.368785732	-1.339091019	0.604200074
H	1.888830631	-3.567666932	-0.371777671
C	-4.799474878	-2.018990430	-2.825875200
C	-2.775598639	-1.063958238	-1.535728348
C	-2.643411451	-0.144341804	-2.764620766
C	-3.256874705	-0.536875266	-4.094618996
C	-3.986749903	-1.872550612	-4.109642331
H	-5.527065304	-1.198631003	-2.749428263
H	-5.357230850	-2.955792435	-2.794290094
H	-2.697638064	0.908533764	-2.504085600
H	-3.742191132	0.261898952	-4.650841997
H	-3.281869307	-2.708279651	-4.189669440
H	-4.654188480	-1.939209839	-4.974685804
H	-2.993181921	-0.412118734	-0.685711274
N	-3.920221947	-2.012392374	-1.648763521
C	-4.260776098	-2.822788642	-0.606872248
C	-3.442364552	-2.725217523	0.690567762
O	-5.217114709	-3.599979261	-0.612799068
O	-3.449161417	-1.673100228	1.316349881
C	-2.720418461	-3.937748199	1.157293423
C	-1.789471940	-3.774634371	2.194651343
C	-2.875077481	-5.196086722	0.554835365
C	-1.015295919	-4.849977978	2.617252431
H	-1.678205391	-2.790875506	2.637837800
C	-2.103424573	-6.272087845	0.987548048
H	-3.607095059	-5.327740851	-0.233135054
C	-1.170418325	-6.100733820	2.012855939
H	-0.286643838	-4.715598582	3.411578386
H	-2.228725129	-7.246393161	0.524006422
H	-0.563365281	-6.940600460	2.339999606
C	-1.763214465	-0.474442078	-3.948123047
H	-1.215237126	-1.412142878	-3.924398372
H	-1.223365468	0.345116261	-4.413001718

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R2-TS$_{prox}$

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C	0.298460119	-2.726953823	-6.958940453
C	-0.320652627	-4.077732666	-6.601340747
H	-1.344082570	-4.131009658	-7.002346658
H	0.249616556	-4.887984101	-7.062474223
N	-0.379269454	-4.295341540	-5.148189112
C	-1.068363065	-1.964705725	-4.919689907
C	-0.996314297	-3.285661382	-4.321948639
H	-1.889033756	-3.635431197	-3.822266079
Pd	0.185080075	-2.086668294	-2.890134113
C	-0.355941371	-1.583014172	-6.176635440
H	-1.888822092	-1.330268944	-4.602962901
C	0.400349389	-1.028167878	-5.002723889
H	-0.865087874	-0.839522277	-6.786816022
H	1.375686664	-2.762463386	-6.756633755
H	0.184493808	-2.564367690	-8.035820456
C	-0.315177315	-5.563579049	-4.660415252
C	0.631795736	-6.540882265	-5.378139049
O	-0.877630968	-5.930278632	-3.629589740
O	0.208395740	-7.598553101	-5.814518024
C	2.089832568	-6.191522179	-5.398247027
C	2.979344771	-7.161272021	-5.887401914
C	2.599720962	-4.972692511	-4.914649743
C	4.349525500	-6.922682379	-5.889915748
H	2.567916568	-8.098386415	-6.249135552
C	3.974413548	-4.739779646	-4.912990733
H	1.931585074	-4.212673870	-4.527033283
C	4.849488844	-5.711174656	-5.401964477
H	5.031622377	-7.680332524	-6.265576768
H	4.357946666	-3.802384836	-4.520018245

H	5.920963597	-5.529291124	-5.395147568
H	1.386008173	-1.465241791	-4.854679784
H	0.321277852	0.029395279	-4.781658007
C	-0.600616528	-2.795917436	0.446873300
C	-1.907216847	-2.282552429	0.260688739
C	-2.672903812	-1.955535030	1.394206067
C	-2.607952644	-2.031932563	-1.041227692
C	-0.152914777	-2.992050838	1.768852486
P	0.532773249	-3.315682110	-0.932390795
C	-2.199347012	-2.131736606	2.687639459
H	-3.668214703	-1.550888273	1.235996873
C	-2.910212900	-0.707363503	-1.430908546
C	-3.197036611	-3.085641161	-1.767657675
C	-0.925498112	-2.663619923	2.876782620
H	0.823353134	-3.427540234	1.941542590
C	0.342409785	-5.214542474	-0.895147768
C	2.312641702	-3.121687927	-0.281641186
H	-0.534041750	-2.828057237	3.877001596
H	-2.821539509	-1.864443441	3.537635650
C	-3.677705813	-0.443446100	-2.573583307
O	-2.426716222	0.275622074	-0.620987678
C	-3.995160516	-2.822809552	-2.892925583
O	-2.951510708	-4.343728404	-1.304256306
C	-4.212247889	-1.508438610	-3.290980451
H	-3.881276675	0.574807968	-2.879534603
C	-3.005174758	1.596253624	-0.637328972
H	-4.823949961	-1.310846496	-4.167402264
H	-4.442926398	-3.630625832	-3.455415519
C	-3.777967623	-5.440794730	-1.764865963
C	1.475469326	-5.912575435	-1.671608712
C	0.211085317	-5.844605295	0.509237459
H	-0.590627811	-5.358843522	-1.440460803
C	3.318571103	-3.174543141	-1.460815574
C	2.675120609	-1.896104992	0.587975636
H	2.470930474	-4.020547383	0.331935737
H	-2.992459525	1.986665809	-1.664289408
C	-2.079804954	2.451567764	0.216790313
C	-4.433867909	1.560746685	-0.094670856
C	1.150088235	-0.415532757	-2.052408392
C	2.330020476	0.075432010	-2.645932780
C	0.687681892	0.278334204	-0.919020636
C	3.026024550	1.176597491	-2.134158441
H	2.748941685	-0.419197230	-3.522919762
C	1.373043550	1.385606902	-0.403189620
H	-0.200691886	-0.059650342	-0.401309078
C	2.549298066	1.840879898	-1.002371846
H	3.943783160	1.509577946	-2.616350019
H	1.000622373	1.877366008	0.493664769
H	3.088593581	2.690478637	-0.590712252
H	-1.080540099	2.481975250	-0.219914919
H	-2.467905407	3.472524643	0.289363288
H	-2.007497620	2.030410571	1.224857512
H	-4.865213991	2.567075369	-0.096634855
H	-5.077125468	0.909010547	-0.691460414
H	-4.424752102	1.189181531	0.935419072
C	1.263474393	-7.430551362	-1.767580024
H	2.433350449	-5.743384174	-1.163382701
H	1.561910318	-5.486961616	-2.669376902
C	0.081979066	-7.381822470	0.455236140
H	1.095608207	-5.596085196	1.113474879
H	-0.655569772	-5.431899966	1.032295240
C	1.197123567	-8.044723263	-0.364376035
H	2.082374205	-7.874515289	-2.348391316
H	0.337111394	-7.629658058	-2.317943858
H	0.071062003	-7.774145895	1.480377824
H	-0.883149132	-7.645924805	0.009715814
H	1.033069440	-9.128211007	-0.419127475
H	2.162779868	-7.897119653	0.142608958
C	4.758432968	-3.322688904	-0.940374423
H	3.226998701	-2.241754049	-2.024568535
H	3.095743196	-3.983590159	-2.157228156
C	4.099570801	-2.054818892	1.150287061
H	2.636662587	-0.994460335	-0.023163095
H	1.965776860	-1.743313443	1.403541857
C	5.129757029	-2.179805952	0.017018974
H	5.456046360	-3.355229057	-1.787634794
H	4.857857583	-4.286636897	-0.418767517
H	4.339423104	-1.194442913	1.787427861
H	4.149657900	-2.946905333	1.793513766
H	6.137720241	-2.330493402	0.424028616
H	5.148208633	-1.235550741	-0.545208658
H	-3.796700213	-5.435726622	-2.861398185
C	-5.188407054	-5.305060497	-1.189140124
C	-3.094036721	-6.715099908	-1.301718263
H	-5.147344877	-5.374930467	-0.097273982
H	-5.649358700	-4.351108937	-1.456418398
H	-5.827540269	-6.111688514	-1.562849275
H	-3.729943939	-7.578327099	-1.523060017
H	-2.141641521	-6.844400907	-1.814716561
H	-2.928948656	-6.675308863	-0.220590351

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C	-1.249527159	-0.651731500	-3.438766211
C	-2.309963301	-1.061966388	-2.609185822
C	-1.385686812	-0.735194208	-4.833031419
C	0.062441076	-0.113902953	-2.956747467
C	-3.487624185	-1.525697500	-3.221495402
P	-2.088040567	-1.024585437	-0.769473160
C	-3.615578590	-1.598553046	-4.607060795
H	-4.328507218	-1.838416351	-2.612665531
C	-2.555558049	-1.205289282	-5.422996933
H	-4.541566655	-1.962793551	-5.044122731
H	-2.640238313	-1.256628501	-6.504926637
H	-0.553547902	-0.414190055	-5.453914430
C	0.257504457	1.285210121	-2.897725122
C	1.180280759	-0.960315223	-2.837349153
C	1.551968692	1.816926764	-2.795552107
O	-0.881482210	2.019651928	-2.995223004
C	2.638013760	0.949764504	-2.706584914
H	1.712655863	2.887066822	-2.775682341
C	2.470794730	-0.434134035	-2.707487948
H	3.638450723	1.364164471	-2.617586515
H	3.328346235	-1.090080207	-2.615050732
O	0.905708276	-2.298449307	-2.845970604
Pd	-0.545204469	0.726540430	0.007676820
C	-1.492439837	-2.788516493	-0.481173624
C	-3.857944520	-0.917889051	-0.152380894
C	-0.894771095	3.421326887	-2.645745552
C	-1.361992734	1.004229233	1.809272018
C	-1.146304906	0.068034785	2.833017870
C	-2.224667680	2.082239312	2.053636788
C	-1.804687370	0.190328501	4.060530590
H	-0.471709868	-0.764690856	2.678379169
C	-2.898966791	2.189387016	3.276358849
H	-2.382352439	2.841163763	1.292180302
C	-2.696102513	1.242864249	4.283295424
H	-1.605256942	-0.533878283	4.845055192
H	-3.578236050	3.023427746	3.441472265
H	-3.212292176	1.333656926	5.235140054
H	-0.139710619	3.600168627	-1.871546946
C	-2.273822678	3.671610288	-2.048014118
C	-0.610744716	4.262634286	-3.887520783
C	2.595152366	0.744873744	3.739516226
C	1.771064782	1.784728697	2.972296327
H	3.669571003	0.906398924	3.581048040

H	2.384122073	0.787791210	4.805073548
N	2.276994766	-0.599993667	3.222558823
C	2.433764865	-0.741785813	1.821278110
C	2.386463997	0.317905684	1.008499083
H	2.574500469	-1.760430318	1.480853698
C	2.024436160	1.716907792	1.449463636
H	2.562223058	0.159750857	-0.051890067
H	2.893327072	2.363153695	1.229339583
C	0.821313894	2.216209024	0.612234165
H	0.717974958	1.602030333	3.185971157
H	2.009920872	2.786749370	3.347172450
C	1.721020961	-1.635976731	3.904603013
C	1.474548395	-1.514800686	5.413097766
O	1.348099971	-2.680040816	3.356815219
O	0.839508128	-0.565197740	5.856877733
C	1.927765845	-2.639724067	6.277993594
C	1.599033009	-2.576135343	7.642052885
C	2.691690575	-3.717602454	5.800876226
C	2.020169817	-3.573488944	8.514152444
H	1.012449513	-1.732500012	7.991320827
C	3.115936994	-4.712232838	6.679878375
H	2.927697978	-3.788028957	4.745900505
C	2.780103362	-4.644299181	8.033499684
H	1.759172803	-3.520032056	9.567329257
H	3.703427384	-5.546128743	6.306187274
H	3.109578161	-5.425049983	8.713974727
C	-0.787632551	-2.959917261	0.879063289
C	-2.553818063	-3.880323456	-0.719683722
H	-0.724686610	-2.891104454	-1.258929996
C	-0.191803200	-4.369729643	1.017479019
H	-1.493407462	-2.788309153	1.701229998
H	0.004170457	-2.213511767	0.989718570
C	-1.942199065	-5.285479223	-0.570420835
H	-3.371184928	-3.773130009	0.005527359
H	-2.995296876	-3.769941119	-1.716969777
C	-1.255229629	-5.455281113	0.794084798
H	0.275214066	-4.464060201	2.002015477
H	0.610570806	-4.492741351	0.273467134
H	-2.720864333	-6.046573038	-0.709250419
H	-1.204309810	-5.441407859	-1.370341836
H	-0.809593738	-6.454998679	0.874228577
H	-2.012694582	-5.385265890	1.588946936
C	-4.014106693	-1.230912937	1.350657108
C	-4.415946530	0.483239900	-0.487035141
H	-4.447164959	-1.668196735	-0.695743408
C	-5.478821568	-1.078122288	1.794322398
H	-3.395663647	-0.552295078	1.938312429
H	-3.664971546	-2.245347345	1.569341359
C	-5.871821349	0.638975198	-0.018324634
H	-3.792222025	1.231767792	0.015054600
H	-4.340800711	0.674523775	-1.564109425
C	-6.009376775	0.328690800	1.480281398
H	-5.555681563	-1.285016081	2.868676999
H	-6.102454494	-1.826140789	1.281263856
H	-6.222766887	1.655708941	-0.235908475
H	-6.515415005	-0.044967280	-0.592019065
H	-7.055407805	0.425014499	1.797277353
H	-5.428129672	1.062274246	2.056100249
H	-2.418019083	3.024792778	-1.178171205
H	-2.373101937	4.717291123	-1.739054743
H	-3.054212988	3.446059624	-2.782311040
H	-0.619285282	5.329133732	-3.638455462
H	0.362814984	4.017478979	-4.322131585
H	-1.378099015	4.076594888	-4.645981835
C	1.837140680	-3.234870328	-3.429258874
H	2.804639903	-3.156173813	-2.913652128
C	2.008477198	-2.950866619	-4.920051870
C	1.237594549	-4.606708832	-3.151344745
H	1.034262931	-3.002553480	-5.416962913
H	2.428458382	-1.954709743	-5.086544098
H	2.678092699	-3.687384167	-5.375799058
H	1.884363790	-5.394785718	-3.549450331
H	1.117486462	-4.761969145	-2.075733210
H	0.252597702	-4.686591162	-3.622471613
H	0.331778401	3.062105712	1.107615101
H	1.186702967	2.554984975	-0.364374503

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C	-1.144438700	-0.660737400	-3.593646800
C	-2.238567600	-1.036566600	-2.787961000
C	-1.273089300	-0.702059700	-4.990967000
C	0.176469420	-0.196808920	-3.074214000
C	-3.421550800	-1.453672500	-3.426629800
P	-2.143724400	-0.963002500	-0.939967500
C	-3.532432300	-1.501542800	-4.813184700
H	-4.284718000	-1.733164900	-2.832769900
C	-2.449257600	-1.119733900	-5.603999000
H	-4.462421000	-1.827614300	-5.271260700
H	-2.520876200	-1.142620600	-6.688168500
H	-0.424792560	-0.394002230	-5.595849500
C	0.527334150	1.165940900	-3.192083800
C	1.137253900	-1.097027500	-2.603185000
C	1.813616300	1.601354700	-2.850764300
O	-0.472213830	1.970005000	-3.640866300
C	2.751234000	0.674817700	-2.390561300
H	2.088032000	2.645230800	-2.943512400
C	2.426761400	-0.671610300	-2.261088400
H	3.748527800	1.015293000	-2.125743200
H	3.148981800	-1.387964200	-1.885000100
O	0.757171700	-2.410123600	-2.453379400
Pd	-0.650180160	0.469792780	0.205428850
C	-1.907450200	-2.787768800	-0.514425300
C	-3.903884400	-0.506561500	-0.463323920
C	-0.216242630	3.312715800	-4.090343500
C	-0.901895000	2.472497700	0.506805960
C	-2.036247700	2.873801700	1.242405000
C	-0.392829870	3.344519600	-0.475100300
C	-2.692156000	4.067414000	0.939773300
H	-2.413376300	2.240182900	2.041016600
C	-1.049143700	4.543018300	-0.760411100
H	0.509574530	3.073503000	-1.013016300
C	-2.207738600	4.907459700	-0.067654714
H	-3.586909300	4.342022400	1.495368100
H	-0.649984000	5.201976300	-1.529337900
H	-2.715320300	5.840484000	-0.297699960
H	0.360150430	3.848098300	-3.323420500
C	-1.593783400	3.951017000	-4.210861000
C	0.544390300	3.295845300	-5.416302000
C	3.388834200	0.013722697	3.498974800
C	2.596690400	1.238612700	3.025662400
H	4.278712700	-0.145425900	2.878418700
H	3.694603000	0.109805495	4.542122000
N	2.543154500	-1.182125300	3.386687300
C	2.062671200	-1.444124700	2.081090200
C	1.839611400	-0.431019200	1.234878400
H	1.957495000	-2.488393800	1.804392600
C	1.885065900	1.024084900	1.645676100
H	1.613171200	-0.653942350	0.196525420
H	2.421895300	1.576544000	0.863277700
C	0.460439150	1.638083700	1.761643500
H	1.839072700	1.455775500	3.788530600
H	3.254552800	2.114701300	2.984175400
C	2.082085400	-1.831306000	4.497231500
C	0.998406700	-2.900188000	4.255780000
O	2.440711300	-1.600678900	5.645848800

O	1.308774400	-4.065811000	4.056833300
C	-0.414194640	-2.439744500	4.344170600
C	-1.437916800	-3.394963700	4.429682300
C	-0.740962700	-1.078424200	4.269035300
C	-2.769781800	-2.992104800	4.430164300
H	-1.165029200	-4.443925400	4.486394000
C	-2.074950700	-0.677100500	4.251180600
H	0.046505682	-0.335331020	4.205908000
C	-3.089752000	-1.632964800	4.331861000
H	-3.561209700	-3.733552000	4.497195000
H	-2.322766300	0.377424030	4.168092300
H	-4.130345300	-1.320057700	4.312999000
C	-1.251651000	-2.971325400	0.869519200
C	-3.150046000	-3.683927000	-0.668608400
H	-1.168515200	-3.092062500	-1.265188500
C	-0.903706670	-4.446943000	1.121235800
H	-1.923334500	-2.618453000	1.661307600
H	-0.350686640	-2.353867500	0.937116270
C	-2.803901400	-5.158926500	-0.390390430
H	-3.930706500	-3.364027000	0.035123080
H	-3.568550300	-3.588144300	-1.676763800
C	-2.149099000	-5.335671000	0.989144600
H	-0.439384100	-4.563093000	2.106410700
H	-0.153709290	-4.768683400	0.383757230
H	-3.708166400	-5.775616600	-0.471903620
H	-2.109826000	-5.514576000	-1.165996800
H	-1.892564800	-6.388910300	1.157105300
H	-2.871218000	-5.056363000	1.771239400
C	-4.069907700	-0.531776600	1.069797500
C	-4.249388000	0.886256800	-1.037628900
H	-4.597381600	-1.245319500	-0.886929700
C	-5.469050400	-0.055131238	1.494336700
H	-3.307644100	0.115627274	1.520061700
H	-3.886279800	-1.538052800	1.460832500
C	-5.648547000	1.348397000	-0.600043800
H	-3.504615500	1.610256600	-0.687187850
H	-4.184685000	0.869642730	-2.130881000
C	-5.784009500	1.338621500	0.930082600
H	-5.542122400	-0.052180987	2.589988000
H	-6.223088300	-0.770295100	1.132968300
H	-5.843910700	2.352965600	-0.995254460
H	-6.410155300	0.684137500	-1.035908000
H	-6.790714300	1.655098300	1.230419300
H	-5.078414400	2.067757800	1.352783800
H	-2.106281300	3.924494500	-3.246472400
H	-1.504785500	4.992022000	-4.538188000
H	-2.194817000	3.402296000	-4.942963600
H	0.729269560	4.317898800	-5.762645700
H	1.506761800	2.785382000	-5.322601000
H	-0.049178872	2.773612000	-6.173919700
C	1.502249700	-3.413111200	-3.183491200
H	2.559006700	-3.361798300	-2.883663200
C	1.385658300	-3.177749400	-4.688125600
C	0.916155700	-4.746838000	-2.745624800
H	0.334194870	-3.198611300	-4.990561500
H	1.801511500	-2.203806000	-4.964056000
H	1.931234100	-3.951723600	-5.238059500
H	1.440971400	-5.574758000	-3.231878800
H	1.000478600	-4.865923000	-1.662005200
H	-0.143576440	-4.796243700	-3.016646400
H	-0.107009490	1.159772500	2.566657000
H	0.596749700	2.681665700	2.043749800

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C	0.731886677	3.780471164	-0.245713537
C	1.808983674	4.244212515	-1.013606301
C	-0.373022523	3.234439530	-0.911003655
C	1.784875673	4.161797055	-2.405255698
H	2.675210380	4.671138454	-0.513012011
C	-0.402486207	3.149930262	-2.304411871
H	-1.214973715	2.866638972	-0.329623672
C	0.677800108	3.612462148	-3.056093882
H	2.629809867	4.525911032	-2.983204854
H	-1.268637794	2.721507274	-2.801284753
H	0.658346633	3.546254118	-4.140174211
C	2.479821244	1.624916876	4.013792596
C	1.809939155	2.852862978	3.394842793
H	3.504794112	1.515096399	3.637190498
H	2.522471876	1.682093379	5.101458806
N	1.728798543	0.409155674	3.664251499
C	1.266022599	0.309893776	2.335964455
C	1.289273624	1.342065481	1.484521971
H	0.927116409	-0.671585521	2.034852299
C	1.729373349	2.733839279	1.863353239
H	0.963446898	1.167675658	0.464678559
H	2.732693819	2.908317845	1.443290132
C	0.795025946	3.817763458	1.265157512
H	0.797339079	2.945140182	3.807567422
H	2.360898599	3.754342951	3.684221492
C	1.458217918	-0.505908290	4.646292396
C	0.685968050	-1.776556817	4.257343729
O	1.827103270	-0.387539110	5.812601761
O	1.175165408	-2.551571640	3.446834337
C	-0.611437052	-2.031485698	4.935200771
C	-1.339901506	-3.165039079	4.537574480
C	-1.149204368	-1.162683007	5.897597525
C	-2.589498221	-3.423425281	5.088795570
H	-0.905661197	-3.821369847	3.790510361
C	-2.402449127	-1.426355164	6.447295952
H	-0.578380863	-0.302750931	6.228370180
C	-3.123657446	-2.551963200	6.043632148
H	-3.151151295	-4.298763348	4.775803539
H	-2.815887929	-0.754855818	7.193882423
H	-4.101694019	-2.751504307	6.472620219
H	-0.209114503	3.685375903	1.685433075
H	1.152200367	4.800550854	1.598393426

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C	-1.101058585	-0.409939099	-3.138562704
C	-2.230398753	-0.633715448	-2.329590286
C	-0.923367630	-1.171035155	-4.307196760
C	-0.069746730	0.651574500	-2.938829092
C	-3.166644362	-1.592094235	-2.766840657
P	-2.447701974	0.171446784	-0.666906445
C	-2.990050698	-2.325574257	-3.936500788
H	-4.060000753	-1.780108035	-2.184158024
C	-1.847865821	-2.127477220	-4.710464574
H	-3.741127313	-3.052388490	-4.233687190
H	-1.685940250	-2.697801433	-5.620963182
H	-0.039980670	-0.979532616	-4.910367049
C	-0.276022355	1.904977838	-3.542062803
C	1.188009295	0.352017171	-2.395207550
C	0.758255679	2.847565631	-3.604550838
O	-1.525515439	2.088494247	-4.053027488
C	2.014890490	2.498219212	-3.113561001
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C	2.248421048	1.260071164	-2.515846942
H	2.831882073	3.210762576	-3.191665667
H	3.232802581	1.015925784	-2.135762659
O	1.264478886	-0.844004335	-1.737981645
Pd	-1.413526033	2.226157297	-0.061406929
C	-1.730559415	-1.198681344	0.423988857
C	-4.313988382	0.126606900	-0.444378380
C	-1.780560655	3.049797283	-5.096689512

C	-2.953906068	3.573280306	-0.471091000
C	-3.831583000	4.059922503	0.515443750
C	-3.129608842	4.072354040	-1.774519497
C	-4.868578950	4.949669536	0.209234229
H	-3.719921292	3.733468375	1.548648868
C	-4.158157037	4.967636181	-2.089662020
H	-2.467142806	3.729100326	-2.561412295
C	-5.045015105	5.401254267	-1.100530533
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H	-4.272123126	5.323929715	-3.112420667
H	-5.851933062	6.088051780	-1.343632506
H	-1.491463879	4.051163764	-4.745297825
C	-3.290360305	3.001295263	-5.300938643
C	-1.012097183	2.688504834	-6.367125797
C	2.513493642	1.351309083	0.691422699
C	1.897701275	2.737397514	0.573180559
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H	3.560239425	1.347787460	0.381738848
N	2.455489688	0.835184006	2.077929996
C	1.466444204	1.322915624	2.947703486
C	0.529017603	2.205960975	2.565124595
H	1.479705227	0.909794638	3.946249217
C	0.520230828	2.792461950	1.210105751
H	-0.235877331	2.504505033	3.274139819
H	-0.043072653	1.415157347	0.373505705
C	-0.372578341	3.853353665	0.892647339
H	2.522462211	3.474224139	1.096218624
H	1.853994391	3.013876016	-0.480837978
C	3.276071996	-0.225751916	2.348988149
C	3.198914017	-0.887926343	3.730898390
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O	2.140788979	-1.381440651	4.099388852
C	4.438042206	-0.947792019	4.545121581
C	4.337147615	-1.508284872	5.829644214
C	5.664681210	-0.422244584	4.109741567
C	5.443282845	-1.536190376	6.670339996
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C	6.771048065	-0.454269431	4.956469190
H	5.754841898	-0.014068862	3.109645680
C	6.661753553	-1.004632310	6.235385910
H	5.359237576	-1.965497177	7.664703567
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H	-1.032729422	0.183227225	1.958132487
C	-1.646026793	-3.634042587	1.128517106
H	-3.445728578	-2.478291264	0.787220921
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H	-0.609889623	-1.534262810	3.711084529
H	0.276935763	-1.905476793	2.254378767
H	-2.173035728	-4.595458112	1.079014447
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H	-2.380219133	-3.179374789	3.109549086
C	-4.736393986	0.592502884	0.964392055
C	-5.014304909	0.961783572	-1.540404032
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C	-6.268255497	0.596606769	1.116083108
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H	0.068553845	2.701537164	-6.205196679
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C	3.077682503	-2.005340209	-2.878463043
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H	4.022396628	-2.538685313	-2.731667202
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R4

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C	-3.169492902	-1.804793485	-2.797568361
P	-2.142539179	-0.060829924	-0.842417285
C	-3.239114910	-2.477661053	-4.013517580
H	-3.894355244	-2.062882925	-2.035318898
C	-2.335632842	-2.163385230	-5.027178933
H	-3.997767160	-3.240987540	-4.163525325
H	-2.368646753	-2.681332372	-5.981653095
H	-0.714864693	-0.871703740	-5.598181634
C	-0.779344697	1.941585476	-4.003768662
C	1.005085708	0.456004788	-3.300960348
C	0.140157806	2.989699860	-4.151518354
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C	-2.236135226	3.312007182	-0.304211674
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H	-4.042217655	5.513558567	-2.229869069
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H	1.767390834	-0.120564896	0.479652712
H	3.485049542	0.061549809	0.876385014
N	2.170225972	0.651101584	2.384801478
C	1.287561025	1.661778019	2.790233410
C	0.802472944	2.601858862	1.954049742
H	0.973427220	1.616074435	3.822465575
C	1.224142827	2.685273140	0.560918834
H	0.072071654	3.310813586	2.328057451
H	0.274152294	0.587133836	-0.748415850
C	0.701960416	3.609137862	-0.315641152
H	3.330581709	2.495585974	0.606033856
H	2.588320210	1.753822065	-0.821133508
C	2.617593218	-0.359847951	3.197730442
C	2.221119290	-0.353618147	4.682970404
O	3.302594570	-1.293040439	2.783855594
O	1.036227937	-0.369357197	4.996941119
C	3.310855556	-0.401152354	5.689538031
C	2.936402711	-0.398822072	7.043937827
C	4.672049621	-0.396578522	5.345537318
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C	5.640491746	-0.384138567	6.347039285
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H	3.611908964	-0.384356211	9.084515866
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C	-2.282156603	-2.760947934	0.277296203
H	-0.525316009	-1.707905174	-0.398751124
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H	0.734352589	-2.340067266	1.766797225
H	-2.128711287	-4.776198396	1.071215995
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P	-2.070597968	-0.221851729	-0.851651593
C	-3.125904667	-2.613399902	-4.032783298
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C	-2.323282083	-2.180658951	-5.086495242
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C	0.909235766	0.617041977	-3.318415827
C	-0.130244917	3.094789340	-4.136614698
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Pd	-0.788679123	1.582893155	-0.603655239
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H	-0.639573139	-2.039866736	-0.375472007
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H	-1.683992659	-0.721702501	2.184300682
H	-0.160852173	-0.355040180	1.380426054
C	-1.807658598	-3.945120959	1.261327272
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H	-2.543062597	-4.739082034	1.440708483

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C	-5.591434669	0.866210280	1.228839851
H	-3.524208254	1.472421498	1.095483108
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H	-5.615337275	2.805135913	0.271798748
H	-4.617345811	3.049126909	-3.653632137
H	-4.972274970	3.730250276	-5.258444360
H	-4.773426415	1.973308685	-5.058516173
H	-3.034419416	3.826299434	-7.030882081
H	-1.483703488	3.066651119	-6.619950712
H	-2.918054009	2.056234131	-6.890569323
C	2.582749919	-0.832516736	-2.321031576
H	2.814199428	0.049816354	-1.710276416
C	3.662413935	-1.057527246	-3.379388204
C	2.399936170	-2.032524867	-1.398863843
H	3.426745548	-1.952419340	-3.964585792
H	3.727958643	-0.210883895	-4.068112922
H	4.641425028	-1.197398088	-2.908776988
H	3.342610919	-2.280629547	-0.900125117
H	1.647507829	-1.806248888	-0.638842618
H	2.068716884	-2.903669942	-1.973608963

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R5'

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C	-1.284778272	-0.498060338	-3.579413603
C	-2.098853454	-1.026973822	-2.560928036
C	-1.405179266	-1.012077410	-4.880013297
C	-0.268635507	0.596651426	-3.391996590
C	-3.020951227	-2.039659840	-2.877115042
P	-1.944453465	-0.306287068	-0.875147890
C	-3.129959370	-2.541665354	-4.171774700
H	-3.679654489	-2.428816523	-2.107740620
C	-2.313222209	-2.023905345	-5.178386099
H	-3.851165508	-3.323144507	-4.394132945
H	-2.388569629	-2.400967103	-6.194807005
H	-0.776996781	-0.597409612	-5.663513517
C	-0.515353910	1.877403079	-3.957201910
C	1.064046485	0.271328519	-3.021316908
C	0.536090692	2.775894368	-4.184260577
O	-1.815451690	2.120341690	-4.266433964
C	1.826206408	2.410325797	-3.825068881
H	0.352844430	3.763282713	-4.584184495
C	2.108480652	1.176758519	-3.240323405
H	2.633458676	3.120151679	-3.975100235
H	3.125779314	0.939132268	-2.959431869
O	1.212452673	-0.967296558	-2.473714203
Pd	-0.691930323	1.698820851	-1.003939599
C	-1.300955635	-1.725148453	0.174448110
C	-3.730698548	0.004011132	-0.408367845
C	-2.237347646	3.451523225	-4.640289982
C	0.129048563	3.562039032	-1.066696331
C	1.506306064	3.788059286	-0.902998607
C	-0.660603681	4.648251611	-1.488851722
C	2.080332008	5.028090284	-1.206106348
H	2.148328312	2.980709033	-0.558806910
C	-0.090597860	5.886206664	-1.803396012
H	-1.736783304	4.523762224	-1.592512335
C	1.287037289	6.079895357	-1.669138566
H	3.151913586	5.173354309	-1.079519726
H	-0.723172266	6.703633899	-2.145529045
H	1.732871355	7.042907041	-1.905660828
H	-1.640582521	4.180168937	-4.079649843
C	-3.690841603	3.558402840	-4.197213066
C	-2.061594856	3.644308302	-6.145442685
H	-1.013819341	2.230073786	0.403002357
C	-0.606981881	-1.187110242	1.446600713
C	-2.310901259	-2.839864423	0.509764918
H	-0.523993729	-2.151544169	-0.474083447
C	0.023835411	-2.321418965	2.271371584
H	-1.337146742	-0.656040205	2.070709313
H	0.146964000	-0.443702667	1.164907959
C	-1.650498466	-3.962753016	1.329280832
H	-3.146842355	-2.422868361	1.086996074
H	-2.733927165	-3.259587253	-0.408048169
C	-1.001683320	-3.413958076	2.607924626
H	0.466051519	-1.911273819	3.187388770
H	0.847964528	-2.773076174	1.700852092
H	-2.393276383	-4.732711999	1.572150356
H	-0.880883329	-4.450505992	0.713288314
H	-0.526822163	-4.224454625	3.174068286
H	-1.783084814	-2.991272034	3.256394388
C	-3.873073204	0.498698731	1.045205625
C	-4.318198296	1.043573768	-1.389135899
H	-4.289927214	-0.936149331	-0.514015784
C	-5.337265476	0.834731400	1.378337723
H	-3.247786432	1.391689562	1.175913096
H	-3.500523841	-0.253821534	1.748895856
C	-5.779124205	1.377374840	-1.053136115
H	-3.710004409	1.955960227	-1.323150435
H	-4.233859090	0.687292821	-2.421131344
C	-5.918099499	1.863992023	0.397084173
H	-5.406590297	1.205247426	2.408352773
H	-5.938401991	-0.085664023	1.334034143
H	-6.154756045	2.135923891	-1.751342552
H	-6.400597878	0.481402580	-1.198528256
H	-6.969056614	2.068608377	0.635479885
H	-5.376168676	2.813890534	0.510475995
H	-3.767811142	3.436726362	-3.114045374
H	-4.100717904	4.535674830	-4.472147563
H	-4.292557726	2.779283127	-4.676613119
H	-2.373969343	4.651209036	-6.442067865
H	-1.019385870	3.505157913	-6.445348262
H	-2.673491115	2.916162463	-6.687845446
C	2.524125059	-1.457391106	-2.130776337
H	3.097708270	-0.648818270	-1.659392132
C	3.236011849	-1.958725358	-3.386339772
C	2.295951880	-2.555152216	-1.101009220
H	2.662712917	-2.777230753	-3.833314531
H	3.334061792	-1.163420757	-4.129982089
H	4.237349926	-2.326923436	-3.139740670
H	3.248446330	-3.009699414	-0.811085298
H	1.820053575	-2.143985815	-0.207853259
H	1.648356075	-3.334812494	-1.515053066

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C	-1.220738196	-0.628184242	-3.578163849
C	-2.149998950	-0.968711575	-2.575009541
C	-1.305005940	-1.255158582	-4.829158476
C	-0.119222323	0.372063470	-3.398064083
C	-3.140909706	-1.922010218	-2.864768993
P	-2.025556384	-0.132180834	-0.935252706

C	-3.216299035	-2.537117603	-4.112985968
H	-3.876245381	-2.182823481	-2.110379935
C	-2.290344472	-2.201015964	-5.100950347
H	-3.994481145	-3.268779714	-4.312255496
H	-2.337857093	-2.668538133	-6.080879809
H	-0.584722620	-0.983654693	-5.595996259
C	-0.273139517	1.693895150	-3.878805712
C	1.151267204	-0.042412606	-2.946202719
C	0.827628112	2.564318329	-3.935951242
O	-1.532585890	2.007898165	-4.288001262
C	2.063337567	2.121123887	-3.480831479
H	0.716946318	3.583194982	-4.282079856
C	2.242472526	0.832408984	-2.979153094
H	2.905650649	2.805936601	-3.499719745
H	3.217237874	0.522828593	-2.624311862
O	1.200252872	-1.327300998	-2.480546523
Pd	-0.933873129	1.965350013	-1.037523564
C	-1.182536454	-1.445387333	0.111168485
C	-3.811059510	-0.016436250	-0.386398280
C	-1.881175790	3.377376454	-4.587601635
C	-0.154588966	3.856440244	-0.952527500
C	1.221256323	4.022809145	-0.717265410
C	-0.875318470	4.950591540	-1.464277838
C	1.868128486	5.214269170	-1.057266586
H	1.798652986	3.205582188	-0.293031523
C	-0.228263723	6.141430587	-1.809636819
H	-1.949388725	4.865665472	-1.611399831
C	1.148847820	6.274613706	-1.615171425
H	2.937793860	5.316501721	-0.885197758
H	-0.801335091	6.968550810	-2.224141755
H	1.652309794	7.202054688	-1.876250062
H	-1.302399948	4.041807445	-3.936477331
C	-3.356124230	3.508067926	-4.231236164
C	-1.591373084	3.670697909	-6.057927355
H	-1.126981992	2.883888407	0.203845419
C	-0.558995412	-0.847219958	1.390861065
C	-2.029672153	-2.692100583	0.424162889
H	-0.357327247	-1.746760068	-0.548256736
C	0.249316459	-1.904752764	2.160360589
H	-1.348129543	-0.457105053	2.045999395
H	0.071874937	0.008589104	1.126974780
C	-1.205986482	-3.740190488	1.193441535
H	-2.898949338	-2.405875582	1.032532488
H	-2.416430060	-3.130931725	-0.502005453
C	-0.599820813	-3.146424569	2.474152315
H	0.647908115	-1.468933783	3.084717069
H	1.118904175	-2.204720343	1.557590318
H	-1.833251111	-4.608327615	1.431551361
H	-0.397325341	-4.105460802	0.544111129
H	0.001080497	-3.900197704	2.997575901
H	-1.413174684	-2.861907901	3.157842766
C	-3.926343035	0.507275269	1.059719866
C	-4.569332834	0.912323007	-1.360076841
H	-4.264630357	-1.016041824	-0.423578814
C	-5.396814805	0.695931793	1.470160036
H	-3.392219823	1.464100899	1.133409384
H	-3.438673561	-0.182132692	1.757126815
C	-6.036788935	1.093520020	-0.945034411
H	-4.067035052	1.889491542	-1.359923658
H	-4.506095733	0.527121785	-2.383379609
C	-6.143085850	1.617236425	0.494424763
H	-5.447400839	1.095814696	2.490314214
H	-5.894594574	-0.284917624	1.492266777
H	-6.537459636	1.777506356	-1.641512050
H	-6.559716149	0.128750622	-1.021657023
H	-7.194414556	1.717314335	0.791106693
H	-5.703370785	2.623931795	0.543103978
H	-3.502545930	3.296858369	-3.168779235
H	-3.711605007	4.521692662	-4.444040441
H	-3.953941663	2.797878430	-4.811908385
H	-1.850034100	4.706877396	-6.300840764
H	-0.534081208	3.516075702	-6.291097849
H	-2.182859208	3.005562725	-6.695623832
C	2.464749805	-1.990059117	-2.289523074
H	3.120526684	-1.352872640	-1.680128767
C	3.116943337	-2.289590696	-3.638796991
C	2.139730821	-3.256260552	-1.507718258
H	2.457480960	-2.933393830	-4.229739179
H	3.300038389	-1.373163855	-4.205212181
H	4.072695698	-2.803992902	-3.495799646
H	3.047835630	-3.842555829	-1.336930168
H	1.696669507	-3.010754741	-0.539344002
H	1.426063446	-3.868450929	-2.068281872

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Pd	0.634970100	0.889712300	-0.667164300
C	2.044223800	2.008650500	-1.563784000
C	3.383354700	1.613453500	-1.397926100
C	1.760203200	2.980715500	-2.536693600
C	4.401044400	2.162573600	-2.184857800
H	3.639943100	0.859454200	-0.657426000
C	2.777639600	3.529387700	-3.325294500
H	0.738393660	3.312599200	-2.694623700
C	4.103038000	3.125217000	-3.151111400
H	5.429050400	1.837323000	-2.038507500
H	2.531705900	4.277225500	-4.076658700
H	4.893669600	3.556640100	-3.759494000
C	-0.775082200	-4.977570500	0.854163700
C	-1.274068700	-2.914172200	-0.606556100
C	-1.386206300	-3.793586000	-1.833591500
C	-1.087450300	-5.292372700	-1.693170900
C	-0.536159750	-5.876064000	-0.380475850
H	-1.798420500	-5.107625000	1.232125200
H	-0.080273560	-5.220748400	1.663193500
H	-2.221452000	-3.542273000	-2.483251300
H	-1.752395600	-5.953793500	-2.243188900
H	0.542939070	-6.039307000	-0.485263560
H	-0.984818000	-6.858737000	-0.197020470
H	-2.262677700	-2.543561500	-0.309832480
N	-0.586905540	-3.592985000	0.495734630
C	0.414982000	-2.681143300	0.666095200
C	-0.208041500	-1.734057400	-0.437113460
O	1.391204800	-2.681744300	1.401886700
O	-0.758984450	-0.555709360	-0.009260545
C	0.730552500	-1.471360200	-1.619047400
C	0.207470950	-0.783103940	-2.735922600
C	2.087683200	-1.847636100	-1.633893400
C	1.014665800	-0.507883800	-3.846418000
H	-0.846247200	-0.518052600	-2.739707500
C	2.883916100	-1.563313700	-2.740106000
H	2.504775800	-2.349501800	-0.767106950
C	2.350870100	-0.897126560	-3.848513800
H	0.596255600	0.019462686	-4.698876000
H	3.931736500	-1.850905200	-2.735505300
H	2.983316200	-0.667931140	-4.701087000
C	-0.191187380	-4.405148500	-2.519448800
H	0.793912700	-4.193484000	-2.114167200
H	-0.212778780	-4.480834500	-3.602933000
C	0.223711150	-0.816992940	3.650112900
C	-0.731321330	-0.542178900	4.654545300
C	0.438750620	0.072014034	2.610430500
H	0.771995500	-1.749192700	3.625815400
C	-1.385596800	0.712711600	4.599807300
N	-1.025009200	-1.471948900	5.631551300
C	-1.149643000	1.595050700	3.551798300

H	-2.095781000	1.000473500	5.365861400
C	-0.253065100	1.290610100	2.513904000
H	-1.689490800	2.535121200	3.555533400
P	0.028969040	2.337584500	1.042584200
H	1.140973900	-0.222678590	1.841041200
C	-1.886942600	-1.102699000	6.747788400
C	-0.251066770	-2.706730800	5.704596500
H	-2.890023200	-0.792300700	6.396747000
H	-2.018172500	-1.973338700	7.396228000
H	-1.470277700	-0.274227680	7.358906700
H	0.822887900	-2.531717000	5.918208000
H	-0.663488860	-3.334802400	6.499391000
H	-0.315028520	-3.272576800	4.757807700
C	-1.651965400	3.095097500	0.509108070
C	1.258927500	3.665937200	1.647112500
C	-1.517117300	3.564200600	-0.956544500
C	-2.702913800	1.962229400	0.561374400
C	-2.137586000	4.290884500	1.351386400
C	0.838244900	4.278455300	3.000106000
C	2.601640500	2.932388300	1.851635300
C	1.440438400	4.782680500	0.604051200
H	1.618181600	4.981876000	3.317394700
H	-0.097859510	4.836199800	2.945295300
H	0.741613600	3.516744000	3.777308500
H	3.329302300	3.636428600	2.273710500
H	3.000900000	2.556733600	0.909140400
H	2.502573000	2.095732700	2.550401700
H	1.731086700	4.387168400	-0.370678450
H	0.536165360	5.386420700	0.483170600
H	2.237017900	5.457042700	0.942223700
H	-2.466477200	4.012116400	-1.275896500
H	-0.733228150	4.314186600	-1.089189600
H	-1.300224900	2.722339400	-1.620156400
H	-3.618382500	2.316615800	0.070221020
H	-2.955749800	1.687628400	1.587927200
H	-2.356904500	1.056337700	0.055840176
H	-2.244578100	4.053128000	2.411541500
H	-1.481502700	5.159903000	1.257848100
H	-3.128502600	4.590411000	0.987030270

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C	-0.739255755	2.322722778	-3.642190804
C	0.614930729	2.502621092	-3.983163087
C	-1.617197709	3.394130620	-3.844002320
C	1.073944679	3.713963985	-4.508240291
H	1.324402616	1.686730725	-3.856982381
C	-1.158232146	4.606534370	-4.371066731
H	-2.666569858	3.298270873	-3.591024970
C	0.187406488	4.775579315	-4.701454943
H	2.125293672	3.825566275	-4.765778407
H	-1.860655020	5.423554644	-4.522487244
H	0.541080682	5.719988693	-5.106675541
C	-5.195406279	2.918979413	-2.078188305
C	-5.477396722	3.871364331	-1.071322763
C	-4.085229365	2.091941412	-1.987733503
H	-5.825897077	2.836364514	-2.954667424
C	-4.604587536	3.906900700	0.041798759
N	-6.556681011	4.731442743	-1.174055331
C	-3.197784400	2.148110770	-0.899360351
H	-3.882413786	1.402346664	-2.803457910
C	-3.506653271	3.059078607	0.122541461
H	-4.774818241	4.605093065	0.852040225
C	-6.661734812	5.848276954	-0.249150792
C	-7.279758236	4.809715500	-2.434210426
H	-2.879479726	3.128160321	1.004191408
P	-1.766692696	1.011637958	-0.907152580
C	-0.300253575	1.817794567	0.029350009
C	-2.436975562	-0.530697025	0.021366515
H	-5.789890680	6.519217548	-0.295141991
H	-7.553873719	6.429627478	-0.486925346
H	-6.765160144	5.496280314	0.783777430
H	-7.734702410	3.845395824	-2.687146548
H	-8.087140121	5.537706885	-2.340981041
H	-6.635691663	5.113279098	-3.273983235
C	0.982376471	1.080120180	-0.420720424
C	-0.178946405	3.296710537	-0.397778981
C	-0.391279827	1.747391092	1.566695357
C	-3.113448302	-0.172466553	1.360291384
C	-3.509570089	-1.167164182	-0.893678208
C	-1.301854308	-1.549066787	0.241529945
H	1.839376598	1.492824255	0.126165204
H	0.943568162	0.006681324	-0.220615633
H	1.161969879	1.220931625	-1.488620829
H	0.744465586	3.704099309	0.032663002
H	-1.010566092	3.905836558	-0.038080075
H	-0.122037314	3.406065590	-1.480645437
H	-1.294414842	2.217665703	1.963139919
H	-0.347195897	0.721775041	1.939216711
H	0.466822462	2.284377691	1.989891407
H	-3.556632413	-1.085276206	1.777747290
H	-2.419420767	0.218263652	2.104771982
H	-3.920673529	0.552723590	1.224655923
H	-3.939206366	-2.030066883	-0.369154005
H	-3.081016241	-1.520967762	-1.832839758
H	-4.328525389	-0.472058248	-1.102071156
H	-0.806470653	-1.799463466	-0.699254767
H	-0.558476445	-1.193870709	0.961360613
H	-1.731666692	-2.472037267	0.650851159
C	0.578007051	-1.786999793	-4.688639095
C	1.211116513	-2.954870157	-5.431195114
C	1.873673637	-2.722550825	-6.794691237
C	1.731191101	-1.363657313	-7.492361511
C	1.469401578	-0.212782073	-6.505030482
H	2.391186088	0.047151426	-5.966215446
H	1.105595100	0.683967098	-7.012128148
H	1.740520712	-3.632417353	-4.765529571
H	2.826877803	-3.224035646	-6.944321700
H	0.902887271	-1.399011378	-8.209219910
H	2.637201661	-1.141905195	-8.067143557
H	1.174099133	-1.589096620	-3.786694699
N	0.472528514	-0.596606583	-5.524295426
C	-0.831212623	-0.217979991	-5.421763344
Pd	-1.184859667	0.432952085	-3.075021521
C	-0.936865219	-1.825380280	-4.250462396
O	-1.486994487	0.500129562	-6.147983529
O	-1.181570612	-1.707464548	-2.964776402
C	-1.869804195	-2.799165347	-4.943416677
C	-2.667365332	-2.504144430	-6.053092731
C	-1.930413774	-4.085904546	-4.384793692
C	-3.486162165	-3.490040158	-6.611680320
H	-2.657378496	-1.507415492	-6.478070621
C	-2.738532287	-5.068869542	-4.949028634
H	-1.332917790	-4.303185387	-3.504596374
C	-3.518430156	-4.774242456	-6.070755883
H	-4.102301235	-3.246742379	-7.473429796
H	-2.763607490	-6.064382397	-4.512968599
H	-4.151592906	-5.539126075	-6.512587375
C	0.650862353	-3.593583530	-6.675498541
H	-0.273915145	-3.200486518	-7.085002718
H	0.747985824	-4.671574944	-6.766369453

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Pd	-1.823817800	-0.121326160	-3.155177400
C	-1.431525000	1.755854200	-3.872622000

C	-0.165631010	2.317612200	-3.660966200
C	-2.433512700	2.520885000	-4.480751000
C	0.074105390	3.651317400	-4.013606000
H	0.635167900	1.730256900	-3.221323500
C	-2.187760800	3.853772200	-4.822679500
H	-3.394859300	2.076491800	-4.710786300
C	-0.936147000	4.425772000	-4.585392000
H	1.057758600	4.080819600	-3.835339500
H	-2.978323000	4.441761000	-5.284642700
H	-0.746592700	5.461744000	-4.854973000
C	-0.718187300	-0.714558900	-7.319345500
C	0.568744300	-0.673512940	-5.206330000
C	1.631665300	-1.530211600	-5.901621300
C	1.386895800	-2.116103400	-7.282033000
C	0.012429155	-1.913931500	-7.923548700
H	-0.215708400	0.220226440	-7.614492400
H	-1.755916700	-0.663789150	-7.650365400
H	2.632455300	-1.162072300	-5.692602000
H	2.234130600	-2.091269500	-7.963262000
H	-0.604677700	-2.811986400	-7.797257000
H	0.121957034	-1.754933800	-9.002194000
H	0.901628300	0.371737600	-5.262031600
N	-0.735139400	-0.790907600	-5.851991000
C	-1.871731900	-0.402706030	-5.172981000
C	0.619863300	-1.010555500	-3.702603000
O	-2.970047200	-0.329294400	-5.712331300
O	1.429561100	-0.370935800	-3.025900100
C	-0.001642417	-2.258863200	-3.109555000
C	-0.993159230	-3.057860000	-3.716647900
C	0.508165060	-2.664979000	-1.861163700
C	-1.458790200	-4.212602600	-3.083518500
H	-1.389205600	-2.791634800	-4.687323600
C	0.057992373	-3.828497600	-1.247221400
H	1.272172300	-2.047809000	-1.401877600
C	-0.934703700	-4.605322000	-1.852250800
H	-2.228267700	-4.809347600	-3.565590100
H	0.473441450	-4.127211600	-0.288486420
H	-1.295733900	-5.507973000	-1.366791600
C	1.508275000	-3.023263000	-6.082546700
H	0.600413400	-3.511700600	-5.743403400
H	2.406656500	-3.621016300	-5.956223000
C	-5.889050500	2.232739000	-2.724096000
C	-6.385353600	3.188833200	-1.809229400
C	-4.803611300	1.428264400	-2.401765300
H	-6.327458400	2.129053400	-3.709055700
C	-5.755436000	3.251378800	-0.544069200
N	-7.438298000	4.028115300	-2.137972400
C	-4.153857700	1.507652200	-1.157624800
H	-4.437343000	0.734102670	-3.154268000
C	-4.682242000	2.424772000	-0.233699550
H	-6.096365500	3.954782000	0.206103370
C	-7.753159000	5.145461600	-1.263147500
C	-7.887218000	4.087857000	-3.519960900
H	-4.248236700	2.516034600	0.755303140
P	-2.698644900	0.422155980	-0.874946950
C	-1.463686200	1.348280100	0.254679980
C	-3.475932800	-1.078890600	0.031355426
H	-6.906511300	5.838857700	-1.137358400
H	-8.592824000	5.704175000	-1.680544900
H	-8.054583000	4.795612000	-0.268827200
H	-8.266102000	3.114878200	-3.853932900
H	-8.706996000	4.803885000	-3.601777800
H	-7.088340800	4.396636500	-4.212235000
C	-0.101202470	0.633692500	0.090479510
C	-1.321341500	2.787897800	-0.287995000
C	-1.816403700	1.408106200	1.753399600
C	-4.493852600	-0.691896200	1.120066600
C	-4.212712300	-1.874224400	-1.070879600
C	-2.380570400	-1.980206300	0.626051700
H	0.657351100	1.172957800	0.672322500
H	-0.124164380	-0.396277870	0.457531000
H	0.229337130	0.608722900	-0.951230300
H	-0.493897770	3.281893000	0.237947420
H	-2.222814300	3.383834000	-0.128167540
H	-1.092684600	2.801694400	-1.355056900
H	-2.770595600	1.904807400	1.945867500
H	-1.850416300	0.419030900	2.216063000
H	-1.041951500	1.984481800	2.276149000
H	-4.921334000	-1.605683700	1.553703400
H	-4.040986500	-0.124418350	1.936354800
H	-5.316856000	-0.099816850	0.710780100
H	-4.724506400	-2.734193000	-0.619666040
H	-3.517693800	-2.261786500	-1.824561600
H	-4.968164400	-1.265552200	-1.577892100
H	-1.620927900	-2.234723000	-0.115555115
H	-1.885301600	-1.525091900	1.487928400
H	-2.832298500	-2.920092600	0.969861000

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A2-TS$_{dis}$

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Pd	-1.252964383	0.329952825	-3.452232779
C	-0.236730394	2.110296752	-4.111179956
C	1.000954125	2.230005295	-3.445172949
C	-0.932619597	3.283055220	-4.452785230
C	1.501752351	3.492474962	-3.113533781
H	1.557185643	1.354132801	-3.131830277
C	-0.421569702	4.537396484	-4.124904277
H	-1.868123619	3.191261815	-4.994436251
C	0.796491110	4.648059788	-3.449717699
H	2.445931105	3.564922766	-2.578894311
H	-0.976434616	5.431220724	-4.399989362
H	1.194349998	5.626548692	-3.193743235
C	0.500712195	0.587329408	-7.509987921
C	1.437880003	-0.272650628	-5.377301547
C	2.398323016	-1.117858961	-6.227809479
C	2.228744407	-1.233722497	-7.731842355
C	0.993015606	-0.584900948	-8.355177414
H	1.248936795	1.397415066	-7.524373960
H	-0.441693332	0.982799685	-7.887597363
H	3.415383955	-1.034494977	-5.855199611
H	3.142321191	-1.172831550	-8.318622780
H	0.183078150	-1.316613716	-8.460509826
H	1.226707800	-0.222770590	-9.362428440
H	2.020299620	0.593722283	-5.037712997
N	0.268670193	0.182494786	-6.114639039
C	-0.786803467	0.807344619	-5.445212090
C	1.130130582	-1.082905276	-4.104852662
O	-1.810168785	1.121234363	-6.051485933
O	1.883492625	-0.914736263	-3.146310410
C	0.134109884	-2.215876842	-4.086638050
C	-0.838621170	-2.464216226	-5.075700939
C	0.253351624	-3.128049940	-3.021820788
C	-1.650651482	-3.596268558	-4.999758500
H	-0.958609881	-1.775621768	-5.899852466
C	-0.561824368	-4.251360527	-2.947151598
H	1.009178101	-2.936969600	-2.269223803
C	-1.514345617	-4.493801235	-3.940461347
H	-2.394628413	-3.770074868	-5.772108755
H	-0.453721748	-4.942209356	-2.115793798
H	-2.149248527	-5.373826529	-3.883587928
C	2.054496480	-2.447629574	-6.855593430
H	1.047907136	-2.835516822	-6.742820807
H	2.826791640	-3.211650490	-6.848738939
C	-4.288302151	-3.260214712	-2.129236862
C	-5.174333336	-3.497351271	-1.055657699
C	-3.422510141	-2.173482840	-2.118114459

H	-4.272167715	-3.914909767	-2.991244035
C	-5.117647086	-2.594657676	0.032087662
N	-6.057887960	-4.567273564	-1.065331611
C	-3.375420042	-1.260121931	-1.053213765
H	-2.772387570	-2.029084307	-2.975664621
C	-4.239606084	-1.518468902	0.027260630
H	-5.767514416	-2.723843101	0.889279405
C	-7.125759047	-4.609534601	-0.079440606
C	-6.237555639	-5.317805386	-2.297148555
P	-2.286696450	0.212330690	-1.235756388
H	-4.244720052	-0.866485826	0.891696919
H	-7.788505225	-3.731292672	-0.131295028
H	-7.730091963	-5.503786121	-0.241661626
H	-6.720991156	-4.668690173	0.937259474
H	-5.297060569	-5.784352051	-2.612095995
H	-6.958891506	-6.119408723	-2.128532824
H	-6.601720606	-4.693807543	-3.128685693
C	-3.464755492	1.712951785	-1.002011528
C	-1.023325597	0.082547603	0.192015833
C	-2.736574166	2.999534621	-1.441402461
C	-4.634328256	1.468957425	-1.980663026
C	-4.019493419	1.934868216	0.416194014
C	-1.603223103	-0.281291397	1.571378961
C	-0.060455653	-1.045922698	-0.234853913
C	-0.229543639	1.399390015	0.288041137
H	-3.440765519	3.840108463	-1.390947286
H	-1.886390466	3.246664669	-0.802506696
H	-2.371735408	2.927738902	-2.465045003
H	-5.279960581	2.355820228	-1.999436156
H	-5.244330391	0.610161841	-1.687004165
H	-4.269392856	1.297859192	-2.999863181
H	-4.583346981	1.078783088	0.791613567
H	-3.228635683	2.175421523	1.131810822
H	-4.708575010	2.789510590	0.398155319
H	-0.786025061	-0.307415536	2.304113070
H	-2.339817817	0.439769971	1.932154639
H	-2.064348443	-1.272266114	1.562954750
H	0.666434718	-1.224946875	0.568140617
H	0.494911018	-0.790446098	-1.140470806
H	-0.597715423	-1.983454398	-0.413897639
H	0.127049957	1.732663045	-0.691875553
H	-0.822011504	2.203931580	0.734118766
H	0.646876239	1.245588226	0.930309913

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C	1.712639300	1.776241800	-1.132290100
C	3.095464500	2.001303000	-1.224890000
C	0.860853430	2.546968500	-1.944963200
C	3.610231400	2.958274000	-2.102511200
H	3.781338700	1.443259500	-0.597143770
C	1.374865400	3.505005800	-2.825297600
H	-0.219372960	2.415824400	-1.886804600
C	2.752217300	3.716895600	-2.901844700
H	4.685176400	3.117705600	-2.156751400
H	0.697462800	4.091253300	-3.442777400
H	3.153797400	4.467056800	-3.578647600
C	-3.046162100	-1.711735400	-2.793590800
C	-0.717449840	-1.279852500	-1.815590900
C	-0.077491350	-1.610015000	-3.146674000
C	-0.975759300	-2.111245900	-4.284933000
C	-2.471370700	-2.386711400	-4.058846000
H	-3.284613000	-0.658271500	-2.994277000
H	-3.960865000	-2.207349000	-2.457390500
H	0.721206670	-0.929512140	-3.433286000
H	-0.724888500	-1.731230900	-5.272318400
H	-2.628850000	-3.468628000	-3.978102000
H	-3.044497300	-2.051263300	-4.930423300
H	-0.680464300	-0.174023540	-1.677055600
N	-2.085194300	-1.764016400	-1.715070000
C	-1.901628600	-2.599033800	-0.634858250
C	-0.432951960	-2.084706500	-0.431477370
O	-2.644741800	-3.394516500	-0.099878660
O	-0.318803130	-1.265914900	0.673379600
C	0.662353500	-3.132887000	-0.475301770
C	1.945121500	-2.800303200	-0.933382100
C	0.443179160	-4.408794000	0.055262044
C	2.990180700	-3.718472500	-0.859634100
H	2.126736400	-1.811869700	-1.351463100
C	1.490356100	-5.330986500	0.129684150
H	-0.549955100	-4.668678300	0.409064920
C	2.764812200	-4.990257300	-0.324854250
H	3.978536000	-3.444315400	-1.220737900
H	1.308437800	-6.319085600	0.545174660
H	3.577660300	-5.709575700	-0.266381140
C	0.038865007	-3.024827000	-3.644839800
H	-0.342062740	-3.814756200	-3.002833000
H	0.937795640	-3.296399400	-4.190606600
C	1.970490700	4.988610700	1.095718300
C	3.198094400	5.403171500	1.665266200
C	3.920393700	4.434339500	2.397873400
C	3.446551600	3.134108500	2.540275000
C	2.237054600	2.716110000	1.966634000
C	1.519993000	3.688981000	1.242505100
N	3.668360000	6.690120000	1.499438400
C	5.001825000	7.034248400	1.976188700
C	3.021770700	7.567800500	0.528764550
P	1.537866700	1.020866600	1.988462300
C	2.837931400	-0.219524790	2.652622000
C	0.022127062	1.139853500	3.161395500
C	0.330582440	2.091053200	4.334586600
C	-1.165781900	1.699400300	2.348505300
C	-0.382932840	-0.251460300	3.684690700
C	2.299168000	-1.670596800	2.567878000
C	4.052901000	-0.134827390	1.700013900
C	3.259698600	0.048890382	4.112707000
H	1.378598500	5.669778000	0.497406930
H	4.872911000	4.682443600	2.849971300
H	4.064951400	2.444948000	3.099308300
H	0.610455330	3.411219400	0.725298640
H	5.799245400	6.449363700	1.480746000
H	5.186488600	8.093541000	1.786945600
H	5.087516000	6.872216700	3.062036500
H	1.980544100	7.784412400	0.814864460
H	3.557608800	8.518162000	0.494714620
H	3.013361000	7.137262300	-0.488685820
H	-0.540756400	2.115700000	5.000163600
H	1.188894400	1.763198600	4.926887500
H	0.525692400	3.110796500	3.993023900
H	-2.023805100	1.814374200	3.022380400
H	-1.447611600	1.008622000	1.549336300
H	-0.955725670	2.681999400	1.918466400
H	-0.511983700	-0.963683900	2.866316000
H	0.336669920	-0.645167770	4.406383000
H	-1.341107700	-0.152703400	4.209563300
H	3.155344700	-2.354985700	2.567530000
H	1.674327300	-1.927394200	3.423306200
H	1.711914800	-1.854385600	1.668898300
H	4.841288600	-0.797542040	2.075815700
H	4.473178400	0.868553340	1.609399400
H	3.774831800	-0.484790920	0.701470700
H	3.667552000	1.045518800	4.286076000
H	2.424679000	-0.094201826	4.802187400
H	4.033431500	-0.678643300	4.386476500
Pd	0.812950800	0.328249540	-0.065399150

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A1'-TS$_{prox}$

C	1.643063226	2.986758297	-1.924410855
C	2.829534667	2.678324839	-2.614027845
C	1.085712371	4.262246906	-2.111813492
C	3.434093181	3.608717803	-3.465387445
H	3.293433154	1.701354132	-2.494465854
C	1.688772196	5.193722808	-2.964092337
H	0.171775327	4.538601841	-1.592588104
C	2.865241879	4.871073476	-3.642451871
H	4.350046634	3.344828337	-3.989722182
H	1.237021178	6.174432582	-3.096499679
H	3.334623058	5.596102681	-4.302019961
C	-2.637282122	0.425821767	-4.409939301
C	-0.504861386	0.787928084	-3.116119054
C	0.325916339	0.638165747	-4.358418527
C	-0.394680474	0.304953181	-5.676360318
C	-1.899149449	-0.007620912	-5.694929895
H	-2.863339693	1.499887520	-4.439858786
H	-3.574925886	-0.121468310	-4.280587896
H	1.140929016	1.353641110	-4.424917117
H	-0.022336142	0.828080533	-6.554042317
H	-2.041929289	-1.086262949	-5.831726554
H	-2.370055439	0.481829495	-6.554696699
H	-0.635240557	1.859272274	-2.893778167
N	-1.809227564	0.172198696	-3.247446595
C	-1.858006320	-0.845166152	-2.356584289
C	-0.505227658	-0.628474621	-1.641541773
O	-2.713454763	-1.692985015	-2.166271047
O	-0.542224275	-0.149403017	-0.421946608
C	0.546953919	-1.687153805	-1.901600430
C	1.879395234	-1.375107120	-2.190751387
C	0.182264668	-3.029309751	-1.730707964
C	2.841678867	-2.379695081	-2.279668564
H	2.154674008	-0.337876646	-2.357991026
C	1.145855621	-4.036091781	-1.820413040
H	-0.856056014	-3.271156716	-1.526564352
C	2.477880737	-3.715335043	-2.087846392
H	3.873288187	-2.121311891	-2.504842611
H	0.853546735	-5.073708979	-1.680954303
H	3.226505400	-4.500121418	-2.158827195
C	0.542115884	-0.689221380	-5.039485932
H	0.090106004	-1.569430235	-4.589983525
H	1.512657075	-0.876102555	-5.490941369
C	2.359370826	-1.935747052	1.642278755
C	2.082624644	-2.279675554	2.985192236
C	2.121005446	-0.654041596	1.175566535
H	2.720617356	-2.672371874	0.935358419
C	1.603553226	-1.248103598	3.828499566
N	2.267872535	-3.569921367	3.447671502
C	1.380873769	0.034934009	3.341769984
H	1.385090687	-1.446667586	4.870764730
C	1.609162827	0.364074720	1.995982193
H	1.007193750	0.779223065	4.036159529
P	1.266983052	1.988177337	1.227019338
H	2.312710416	-0.454857362	0.129424664
C	1.767898796	-3.933243991	4.762798237
C	2.536904143	-4.629615993	2.486887589
H	0.679703427	-3.793501415	4.855915582
H	1.995806100	-4.982374377	4.957923524
H	2.254127419	-3.340888291	5.546988138
H	3.490842088	-4.462634874	1.972618763
H	2.608850099	-5.582609008	3.013563174
H	1.751497505	-4.713457592	1.720817162
C	-0.289245444	2.754298249	2.045005405
C	2.845309781	2.997761358	1.602490090
Pd	0.643456871	1.523297012	-0.972000261
C	-0.827608249	3.844320137	1.089474891
C	-1.358484085	1.643847792	2.156027863
C	-0.060567996	3.390301703	3.429633087
C	3.253614056	2.914883484	3.088567870
C	3.972387591	2.355215537	0.765954468
C	2.677942375	4.469359589	1.184028220
H	4.212504199	3.433408963	3.212945086
H	2.537443583	3.394972799	3.756347310
H	3.391420767	1.880785584	3.414464837
H	4.913478210	2.875223734	0.983268335
H	3.779212428	2.441844447	-0.303234429
H	4.110758175	1.299152811	1.017021474
H	2.384064627	4.564620673	0.136910807
H	1.945233318	4.994259449	1.803642309
H	3.637713653	4.985453001	1.310416609
H	-1.705843721	4.316230555	1.547178156
H	-0.094730059	4.628763058	0.884752182
H	-1.138125972	3.410489444	0.134457986
H	-2.307010238	2.106698743	2.456490440
H	-1.098487589	0.894707041	2.906682127
H	-1.512066536	1.123286511	1.207761325
H	0.357188077	2.691047647	4.157232631
H	0.590477932	4.266744418	3.382389824
H	-1.029064818	3.725200288	3.821599180

A2$_{prox}$

C	1.054011600	2.992792100	-2.490706700
C	2.411744000	2.886465000	-2.840840800
C	0.352376300	4.134638300	-2.907170000
C	3.056393100	3.910924000	-3.539583000
H	2.977398600	1.999823700	-2.567250700
C	0.998930800	5.162157000	-3.604534100
H	-0.706405900	4.234296300	-2.681105100
C	2.355631600	5.060085000	-3.916652400
H	4.110841300	3.811256200	-3.788688700
H	0.437165230	6.044410700	-3.903859000
H	2.858589400	5.859075000	-4.454646600
C	-2.019397300	-0.544501070	-4.600418600
C	-0.423138900	0.843001840	-3.332099200
C	0.660464900	0.537545740	-4.353055000
C	0.368220750	-0.435895030	-5.492768000
C	-0.983087300	-1.156007300	-5.561116700
H	-2.382775800	0.417249650	-4.976484000
H	-2.868628300	-1.212799700	-4.449100500
H	1.257523200	1.404332300	-4.611356300
H	0.797217400	-0.176346030	-6.458335400
H	-0.864472150	-2.216883000	-5.309525000
H	-1.378734100	-1.117306600	-6.582665400
H	-1.004341600	1.692269700	-3.708797200
N	-1.373483800	-0.289311770	-3.303461600
C	-1.344497200	-1.317613400	-2.430831200
C	-0.510152800	-1.164023600	-1.167438100
O	-1.981088300	-2.373383300	-2.541283000
O	-0.765007260	-0.237588930	-0.376371650
C	0.516056840	-2.178112300	-0.845731000
C	1.427821600	-1.861853200	0.177254300
C	0.671039300	-3.375416000	-1.567818300
C	2.482768800	-2.718515000	0.467862520
H	1.320685500	-0.925561600	0.709644560
C	1.722999200	-4.234845600	-1.262199200
H	-0.043466255	-3.628827000	-2.341696700
C	2.631374600	-3.907655500	-0.251475660
H	3.194379300	-2.445977000	1.241816800
H	1.837524300	-5.161749400	-1.816695900
H	3.456927500	-4.578599000	-0.028180731
C	1.365421900	-0.789385400	-4.405488500
H	1.072572100	-1.558000100	-3.694186200
H	2.424438200	-0.802937150	-4.651232700

C	4.290322000	0.534957300	1.001018000
C	4.675732000	0.479954500	2.361082300
C	3.085095200	1.114089700	0.622873960
H	4.928752000	0.124240816	0.228363020
C	3.766619700	1.010559900	3.309250600
N	5.887518400	-0.057970807	2.746087800
C	2.572055800	1.595057500	2.907926800
H	3.995237600	0.978129800	4.367755000
C	2.191693500	1.666803700	1.555982700
H	1.924676800	2.002710800	3.677230000
P	0.687678040	2.499087300	0.913457800
H	2.822702000	1.128763100	-0.430908700
C	6.180510500	-0.240383580	4.163896600
C	6.731071500	-0.716298340	1.753923800
H	5.458493000	-0.914412740	4.669142200
H	7.179876000	-0.671363950	4.265574000
H	6.176477400	0.725064930	4.703398700
H	7.021805000	-0.018505543	0.946883140
H	7.647623500	-1.059557900	2.240692600
H	6.238782000	-1.591963300	1.282045800
C	-0.768209400	2.084013200	2.119083400
C	1.154391500	4.363648400	1.081899400
Pd	0.153934700	1.563523300	-1.416823100
C	-2.069444400	2.241443400	1.297239400
C	-0.643311600	0.616473900	2.585523400
C	-0.893729750	2.960297800	3.380264000
C	1.619652200	4.801228000	2.486099200
C	2.342178000	4.624169300	0.130966810
C	-0.048597075	5.210263700	0.625223930
H	1.944713100	5.847904700	2.428685200
H	0.843291760	4.748902300	3.246242000
H	2.479335800	4.215979000	2.823779800
H	2.665888300	5.665130000	0.254418220
H	2.078355600	4.480183600	-0.911409000
H	3.197301000	3.982606000	0.365159660
H	-0.381410450	4.919550400	-0.374815640
H	-0.897505200	5.134144000	1.310934100
H	0.244571500	6.267006400	0.583139100
H	-2.931371000	2.042673800	1.946789400
H	-2.183137400	3.254356000	0.898947360
H	-2.108036000	1.539597600	0.463027420
H	-1.554449000	0.348902850	3.136143400
H	0.204092380	0.470485000	3.259703000
H	-0.548255300	-0.072052660	1.748677400
H	-0.007568038	2.914068200	4.018363500
H	-1.100056300	4.007224000	3.148305200
H	-1.738580500	2.589199500	3.974736700

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C1

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Pd	-1.409562608	0.695961314	-3.486759124
C	-2.919996547	1.800964814	-4.183185392
C	-2.988319396	3.195522623	-4.057791729
C	-3.881634466	1.149062845	-4.972360716
C	-4.001065387	3.920992872	-4.697402820
H	-2.252445848	3.726322110	-3.458188870
C	-4.895373366	1.873543253	-5.605709514
H	-3.845425051	0.068703548	-5.090262233
C	-4.964208773	3.262600784	-5.464662640
H	-4.037613964	5.003209123	-4.591864741
H	-5.635094573	1.350689274	-6.208325262
H	-5.754445693	3.824978727	-5.954669983
C	2.187845106	0.052986116	-7.143679135
C	2.130962169	-1.031183880	-4.803014934
C	3.021587503	-2.156347026	-5.271394470
C	3.409202335	-2.196917944	-6.758779219
C	2.806164390	-1.212766362	-7.778789915
H	2.969415619	0.780372873	-6.885929093
H	1.477878403	0.539917919	-7.817334657
H	3.810506959	-2.422405165	-4.571918618
H	4.438871555	-2.481680932	-6.960416619
H	2.027111097	-1.725735661	-8.354919633
H	3.576107073	-0.906743738	-8.495262492
H	2.688136239	-0.326098876	-4.174507098
N	1.500959880	-0.333968950	-5.933229720
C	0.254923153	-0.327284795	-5.426177434
C	0.627995220	-1.162518487	-4.189385409
O	-0.780524367	0.300959211	-5.706285468
O	0.361566489	-0.482286063	-3.033919660
C	0.110166938	-2.588495411	-4.169284287
C	-0.975581259	-3.003360214	-4.946449968
C	0.724003271	-3.510733732	-3.310193363
C	-1.413394838	-4.331386824	-4.899425715
H	-1.474198178	-2.287090747	-5.594185117
C	0.294155765	-4.834390003	-3.267205882
H	1.552941099	-3.181818672	-2.690281959
C	-0.772538865	-5.251893384	-4.070918181
H	-2.254852572	-4.644608077	-5.512156728
H	0.786322147	-5.543616141	-2.606470778
H	-1.109759827	-6.284389054	-4.036394381
C	2.527211302	-3.264275499	-6.161829686
H	1.477794871	-3.253554849	-6.441846694
H	2.928210293	-4.260677384	-6.000505799
C	-7.199141965	2.575185974	-2.247930269
C	-5.862130641	2.863143682	-1.558506908
C	-4.937139135	1.636778795	-1.557983179
C	-3.560301578	1.973713791	-0.963006123
P	-2.112042927	0.852557261	-1.313288420
C	-0.746455130	1.637764276	-0.227667297
C	0.629249703	0.945549659	-0.440396495
C	1.727118004	1.665456056	0.371427638
C	1.374468854	1.642818056	1.871847284
C	0.025233425	2.357353764	2.085067704
C	0.133627141	3.816815187	1.601169225
C	0.503594595	3.835615521	0.104859922
C	1.851147895	3.122756019	-0.108094388
C	-0.600853680	3.116467460	-0.697295717
C	-1.077212602	1.621997437	1.287471966
C	-2.631676511	-0.874219539	-0.709918949
C	-1.393059388	-1.775105733	-0.461246048
C	-1.838770023	-3.205493659	-0.085948973
C	-2.679697991	-3.816440288	-1.221504168
C	-3.924423840	-2.940990939	-1.453256929
C	-4.772385653	-2.874857729	-0.168490032
C	-3.925165517	-2.272613557	0.969292094
C	-2.679479790	-3.150762489	1.205985077
C	-3.489379289	-0.839878849	0.584382829
C	-3.472015909	-1.521569102	-1.853684450
H	-7.854638045	3.452739007	-2.236191213
H	-7.033085861	2.294003752	-3.293749129
H	-7.733412822	1.752487016	-1.757423915
H	-6.030959821	3.204863220	-0.527431160
H	-5.356379705	3.681246574	-2.086505331
H	-4.825824711	1.289958619	-2.586457703
H	-5.413748622	0.824990410	-0.996167385
H	-3.638600470	2.101325357	0.122639408
H	-3.250681416	2.937265842	-1.372608406
H	0.585846689	-0.098927005	-0.128011066
H	0.887005132	0.927281666	-1.500599906
H	2.676585312	1.140349282	0.206690486
H	2.159836466	2.139243548	2.457563101
H	1.311845791	0.606109718	2.228946707
H	-0.242902858	2.339514238	3.149265533
H	-0.819144826	4.340082168	1.760767428
H	0.894870819	4.350695445	2.185034101
H	0.570437372	4.873132334	-0.246993659

H	2.124501804	3.145475791	-1.171190313
H	2.645969145	3.642894304	0.443427737
H	-0.365136042	3.134287678	-1.769318216
H	-1.538022136	3.665788685	-0.557959646
H	-2.045799119	2.096588340	1.486503156
H	-1.142310858	0.588511860	1.643907021
H	-0.746694904	-1.775795989	-1.345724371
H	-0.807532662	-1.371799608	0.372348635
H	-0.941663138	-3.816298345	0.076774819
H	-2.086804937	-3.873694821	-2.138572084
H	-2.977908669	-4.841287303	-0.960530392
H	-4.524023644	-3.358827342	-2.272240049
H	-5.117063407	-3.879526400	0.110667528
H	-5.669043484	-2.262469780	-0.336752172
H	-4.522631638	-2.219218332	1.888833238
H	-2.081803110	-2.739658553	2.031346634
H	-2.986119672	-4.162234598	1.504571234
H	-4.381420418	-0.220243512	0.446558439
H	-2.921762192	-0.401433744	1.410720366
H	-4.346245160	-0.909039438	-2.089456457
H	-2.863076105	-1.574584903	-2.762894812

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C1-TS$_{dis}$

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C	-1.068094389	2.311515940	-3.294780232
C	-0.251606285	3.079278519	-2.450416605
C	-1.648015994	2.938068677	-4.409872628
C	-0.005983911	4.431246858	-2.720472265
H	0.207604984	2.629506246	-1.574171004
C	-1.414680775	4.289929415	-4.672330987
H	-2.260496244	2.361358090	-5.095978081
C	-0.592377418	5.042208700	-3.828826503
H	0.640079138	5.005181177	-2.059384794
H	-1.870883274	4.755779384	-5.543230507
H	-0.411678712	6.094011931	-4.035377274
C	0.602008644	-2.127654502	-4.617283479
C	0.962515358	-3.222397625	-5.614707029
C	1.803515002	-2.897039902	-6.853522952
C	2.156931206	-1.440643601	-7.175576041
C	2.119262889	-0.539568842	-5.930071608
H	2.994299686	-0.724328949	-5.294712539
H	2.109234061	0.518244750	-6.203427808
H	1.186800485	-4.171367113	-5.133119167
H	2.566979669	-3.629299690	-7.104822089
H	1.453080097	-1.039986490	-7.913584366
H	3.154124851	-1.386210171	-7.626029416
H	1.099946144	-2.328698063	-3.660957302
N	0.932398848	-0.797297927	-5.126954718
C	-0.289806564	-0.202410490	-5.263708758
Pd	-1.297901876	0.328972174	-3.039540583
C	-0.915485028	-1.839480462	-4.330322730
O	-0.622037336	0.663013269	-6.049204618
O	-1.242870326	-1.796271117	-3.055675131
C	-2.000019354	-2.454505177	-5.190792086
C	-2.804668083	-1.708911636	-6.056436991
C	-2.269916494	-3.819206697	-5.012242551
C	-3.849932289	-2.325833582	-6.750276224
H	-2.609675430	-0.650887563	-6.191726863
C	-3.304843467	-4.434965887	-5.711700847
H	-1.658533478	-4.394115868	-4.322267886
C	-4.099507744	-3.687718904	-6.586303841
H	-4.470486655	-1.735453787	-7.419258248
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H	-4.911328791	-4.164836224	-7.128662758
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H	-0.341758826	-2.567510998	-7.307281863
H	0.135031050	-4.322515705	-7.366321612
C	-4.584637828	5.391728651	-2.694371015
C	-3.806815673	4.592775733	-1.644987441
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C	-1.816849860	-0.070384607	0.364371076
C	-1.102083317	-1.426297404	0.100677657
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C	-1.979540933	-0.668871089	2.827348144
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C	0.749532698	-0.835444192	1.706147110
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C	-2.771817132	-0.223413342	1.576232993
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C	-7.127661238	-0.407106493	-2.518331923
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C2$_{dis}$

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C	0.303534109	-0.670572241	-5.316798724
C	1.481232504	-1.247363240	-6.115404119
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C	-0.169920055	-2.190632839	-7.899920944
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H	-0.506599942	-3.197817223	-7.625830856
H	-0.228979059	-2.123498569	-8.992114441
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C	-0.464399132	-3.344564220	-3.746661077
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H	-1.222701708	-5.342066033	-3.522997443
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H	0.101438738	-5.819180971	-1.474161865
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C	-6.335307787	3.716706520	-0.523828039
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H	2.675321446	0.405442586	1.069772562
H	1.273702094	-1.645777694	0.677953343
H	1.320464791	-0.673035586	2.993865222
H	-0.242750493	-1.418169651	2.646293325
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H	-0.211221720	-0.636565298	-1.037935923
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C	-0.589201061	4.390923751	-3.364991490
H	-1.966737317	3.142318270	-4.461028311
C	0.663187408	4.469619215	-2.746609178
H	2.458493440	3.386203093	-2.240914838
H	-1.232558436	5.266590006	-3.408171001
H	0.996689805	5.401901689	-2.298909449
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C	1.512796620	-0.207802862	-5.491717538
C	2.368943953	-1.076681118	-6.425155022
C	2.188115495	-1.033403493	-7.932058144
C	1.049077391	-0.178666637	-8.488879103
H	1.503204879	1.664459577	-7.447865465
H	-0.218882566	1.471720402	-7.850920624
H	3.387121691	-1.156351873	-6.054135241
H	3.103606856	-1.043576701	-8.518899663
H	0.163809873	-0.795570081	-8.684448062
H	1.345870920	0.263976899	-9.446147674
H	2.181709295	0.568628282	-5.096716836
N	0.390282141	0.414830174	-6.177316320
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C	-1.928431130	-3.238614333	-5.187147316
H	-1.094515541	-1.445024802	-6.013236439
C	-0.715700339	-4.243487023	-3.358523245
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H	-0.595947016	-5.042434990	-2.631764443
H	-2.519651681	-5.068868188	-4.213329141
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C	-2.753179161	1.697699878	-0.963053876
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C	2.052062429	-0.598002397	0.664499000
C	0.096357451	0.889741395	0.066970698
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C	-4.640611818	-0.734229856	-0.117739787
C	-4.374063409	-1.092302116	-2.607359612
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C1'

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C	1.774853168	3.974610448	-2.122836218
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C	2.682101090	3.521034985	-3.083094245
H	3.809586992	1.827825335	-3.802711029
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C	-0.832231795	-1.263327874	-1.734875238
C	-0.335382934	-1.531942780	-3.139338827
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C	-2.812389977	-2.275013641	-3.831559475
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H	-4.128177028	-2.161658662	-2.079061921
H	0.431010576	-0.837491109	-3.477062099
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H	-2.962552004	-3.359703163	-3.779526756
H	-3.471582162	-1.905157092	-4.624730610
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C	2.874585686	-3.841196795	-1.383408904
H	2.018001425	-1.891826493	-1.676942221
C	1.482001185	-5.438183601	-0.228005184
H	-0.463492778	-4.718475780	0.382559162
C	2.682366931	-5.125838789	-0.868064714
H	3.805792559	-3.587364270	-1.883963712
H	1.325535750	-6.435159565	0.175849651
H	3.463542802	-5.875207869	-0.964034914
C	-0.274622404	-2.923624554	-3.708778583
H	-0.588527521	-3.741732341	-3.065816066
H	0.561744293	-3.169879067	-4.356679586
P	1.809242042	0.909011434	1.910805709
Pd	0.817026015	0.301606535	-0.039774077
C	5.952556792	3.668659527	-0.261193442
C	4.707175856	3.725408052	0.627888991
C	4.190427716	2.325717987	0.990300133
C	2.911132498	2.403493542	1.838103375
C	2.865585721	-0.518815036	2.580963022
C	1.970875419	-1.657919601	3.139301049
C	2.847016980	-2.847629434	3.589660640
C	3.813444538	-2.379573371	4.696663572
C	4.721280860	-1.262105345	4.142840871
C	5.529465360	-1.800795823	2.944367638

C	4.557422661	-2.274553369	1.845050231
C	3.649330172	-3.392063202	2.393082440
C	3.682452621	-1.090539219	1.383465629
C	3.855575480	-0.061746656	3.687607215
C	0.412184219	1.453443290	3.091109997
C	-0.737489894	0.406726594	3.129572451
C	-1.891260471	0.912765997	4.020926186
C	-2.458066957	2.220807442	3.438794723
C	-1.340682971	3.279210449	3.401240313
C	-0.815476386	3.537603646	4.828220122
C	-0.258871079	2.224243329	5.414306606
C	-1.377249931	1.162709984	5.452552519
C	0.908454300	1.709457615	4.537964417
C	-0.177344270	2.778023107	2.519810037
H	6.318002716	4.671870953	-0.504927758
H	6.769326065	3.126315046	0.230138047
H	5.726951699	3.156211153	-1.203188353
H	3.909998186	4.265345487	0.100741155
H	4.922090407	4.291450212	1.545312371
H	4.973344200	1.774366976	1.524118298
H	3.990877709	1.781893990	0.063973645
H	2.273935302	3.181415083	1.412999823
H	3.147400737	2.707423360	2.864676170
H	1.411431000	-1.297089272	4.009128518
H	1.244745799	-1.965468113	2.378453235
H	2.187325068	-3.632897215	3.979474116
H	4.426729877	-3.220010906	5.047891895
H	3.247188419	-2.010450494	5.562993000
H	5.407202182	-0.916511935	4.927256177
H	6.192663976	-1.016672661	2.553465205
H	6.170127289	-2.631720403	3.268246782
H	5.120443406	-2.646786072	0.979650097
H	2.969597552	-3.741086533	1.609292591
H	4.256732114	-4.252482590	2.705359128
H	2.994076242	-1.431798494	0.605926882
H	4.318094558	-0.317163717	0.942254650
H	4.513017823	0.733112386	3.319471435
H	3.314025028	0.341789997	4.548998189
H	-1.099151144	0.200349084	2.119568128
H	-0.379312853	-0.548796207	3.514309017
H	-2.674314458	0.145003687	4.036368126
H	-2.843679359	2.043816273	2.426095347
H	-3.298523137	2.580122980	4.047469338
H	-1.724079217	4.213944730	2.971946349
H	-1.624582408	3.918622877	5.464650418
H	-0.031327385	4.306992440	4.809240271
H	0.120965990	2.403359058	6.428274221
H	-0.995535911	0.227833851	5.883990397
H	-2.197241201	1.504737156	6.097865089
H	1.724999051	2.442275347	4.549489589
H	1.295675140	0.781691251	4.971904922
H	0.586357203	3.562006485	2.480671213
H	-0.529526264	2.605844445	1.494935634

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C1'-TS$_{prox}$

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Pd	0.266521666	1.604661700	-0.822076970
C	1.453241798	3.049959064	-1.577696211
C	2.853679719	2.993541203	-1.475160244
C	0.892399632	4.078872904	-2.355405627
C	3.665134430	3.925076270	-2.132949154
H	3.325689848	2.216509468	-0.877987158
C	1.701712748	5.014500248	-3.008572080
H	-0.188697060	4.164766428	-2.448321940
C	3.092632952	4.944051140	-2.897157431
H	4.747144254	3.855793668	-2.043117631
H	1.243041839	5.802808718	-3.601613553
H	3.721364680	5.673057780	-3.400820024
C	-2.118604818	0.099627417	-4.857937311
C	-0.400517302	0.755699877	-3.128500124
C	0.700789564	0.714399627	-4.147108545
C	0.350624937	0.271566843	-5.578664641
C	-1.055602294	-0.244598948	-5.923413721
H	-2.470835551	1.132077321	-4.984914905
H	-2.981648597	-0.568945313	-4.918695680
H	1.408443883	1.533760710	-4.053493264
H	0.841514402	0.832832781	-6.370351613
H	-1.021630897	-1.334172902	-6.042777815
H	-1.376518670	0.165952298	-6.887388667
H	-0.712686452	1.798386256	-2.956855253
N	-1.552488205	-0.025375967	-3.529467664
C	-1.694759371	-1.011434836	-2.614904837
C	-0.574430540	-0.611567755	-1.628572511
O	-2.473786695	-1.948392987	-2.572271706
O	-0.953020079	-0.110944924	-0.472807834
C	0.636247361	-1.526279333	-1.616039157
C	1.946298182	-1.034176550	-1.572721395
C	0.428702561	-2.911689040	-1.573923122
C	3.030927965	-1.903405210	-1.477548605
H	2.113682845	0.037556896	-1.640335933
C	1.516055552	-3.782571113	-1.472671389
H	-0.585386948	-3.295731013	-1.624605402
C	2.818280678	-3.283377011	-1.423391729
H	4.041583401	-1.503792868	-1.452513700
H	1.343175466	-4.854894460	-1.434366422
H	3.662773072	-3.963362848	-1.348732322
C	1.240604064	-0.576889421	-4.707469983
H	0.819713129	-1.506542212	-4.333916457
H	2.304528751	-0.629869663	-4.920800730
C	2.008422693	7.376448448	0.274924589
C	2.397405029	6.047475575	0.929311589
C	1.202267729	5.091436107	1.056125176
C	1.624452508	3.741245959	1.658297471
P	0.524814186	2.269726485	1.367763448
C	1.388599425	0.890010319	2.374455992
C	0.734616830	-0.501532200	2.137204553
C	1.508849362	-1.598988185	2.900193145
C	1.511662574	-1.285067743	4.409521788
C	2.194501282	0.077838734	4.643587053
C	3.643398862	0.026509802	4.119135917
C	3.632080481	-0.303431599	2.613221983
C	2.957186221	-1.667929477	2.382374695
C	2.857077346	0.799962747	1.860254797
C	1.407088951	1.181031163	3.897964600
C	-1.186534738	2.724821599	2.062029657
C	-2.025993946	1.451351793	2.350741351
C	-3.448903365	1.840038146	2.810046450
C	-4.154213757	2.653211266	1.707946104
C	-3.341785668	3.932575301	1.428062398
C	-3.243619051	4.782491889	2.710997739
C	-2.544275572	3.963257554	3.814610862
C	-3.356503962	2.682996584	4.098282983
C	-1.116611002	3.583693483	3.354033787
C	-1.925046214	3.542070137	0.957606305
H	2.867198904	8.051896794	0.197359860
H	1.625106989	7.205430724	-0.737361396
H	1.228485271	7.891972865	0.848375082
H	2.836435649	6.227245551	1.920961127
H	3.170662387	5.559278039	0.322780773
H	0.776884218	4.939854006	0.061931458
H	0.423786518	5.560718434	1.669293724
H	1.805660915	3.840241753	2.734601633
H	2.573458539	3.453654784	1.199887564
H	-0.303996877	-0.505272860	2.470218769
H	0.709762830	-0.730503582	1.071497966
H	1.007489513	-2.557807984	2.719967370

H	2.043838282	-2.071115489	4.961731071
H	0.482866424	-1.261353206	4.793640646
H	2.196882041	0.315179724	5.715297028
H	4.142289137	0.990091238	4.292914161
H	4.214152317	-0.733915602	4.667982989
H	4.661171225	-0.325551115	2.231331781
H	2.962562669	-1.919407933	1.315578841
H	3.513269372	-2.456059360	2.908007462
H	2.851420469	0.582690682	0.785338149
H	3.382960606	1.749731207	2.006082868
H	1.862331432	2.157155982	4.106494276
H	0.383949154	1.209663212	4.287287452
H	-2.067769115	0.817489431	1.458417042
H	-1.556418605	0.868967240	3.149666260
H	-4.012216800	0.919719177	3.008430099
H	-4.237775492	2.052237946	0.793388142
H	-5.174181051	2.911389900	2.022358406
H	-3.825698616	4.514713677	0.633409611
H	-4.246061548	5.082324142	3.043744540
H	-2.681298678	5.704767045	2.511080283
H	-2.466834873	4.564594659	4.729619045
H	-2.876318171	2.101019541	4.896808349
H	-4.361861228	2.946262776	4.452572603
H	-0.541240478	4.498762280	3.181192225
H	-0.611475306	3.034768847	4.154728313
H	-1.361441388	4.444469021	0.703053932
H	-1.992114559	2.937975324	0.045065595

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C2$_{prox}$

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Pd	-1.700811026	-0.353752985	0.153587982
C	-0.771582534	1.017961162	-0.964797924
C	0.508461009	0.743805182	-1.478001969
C	-1.363302939	2.250438123	-1.278078486
C	1.193031978	1.695765617	-2.239097124
H	0.978423335	-0.215395546	-1.282804462
C	-0.676944752	3.202201972	-2.042330418
H	-2.364320123	2.480858271	-0.922601465
C	0.608859616	2.935297829	-2.516842163
H	2.187013783	1.466802931	-2.617834394
H	-1.151244113	4.155812249	-2.264601775
H	1.142752507	3.675887385	-3.105989015
C	-4.736582389	-1.796214144	-2.699279495
C	-2.770093910	-0.711782848	-1.663844634
C	-2.003458793	-0.876174433	-2.966439003
C	-2.638213933	-1.634318876	-4.131189047
C	-4.014247363	-2.287546734	-3.965885550
H	-5.099827423	-0.771291645	-2.829505876
H	-5.576829824	-2.442549938	-2.439229256
H	-1.424738088	-0.000942174	-3.235290756
H	-2.439942164	-1.229155180	-5.121221737
H	-3.917873838	-3.378568334	-3.907782530
H	-4.640853615	-2.073008526	-4.839349048
H	-3.340393626	0.223535491	-1.727066586
N	-3.784755618	-1.781642351	-1.578894227
C	-3.658355417	-2.916631406	-0.865737993
C	-2.579642283	-2.975254879	0.206279959
O	-4.378664887	-3.918041458	-0.959885732
O	-2.651306511	-2.202266890	1.180065356
C	-1.568666438	-4.054056924	0.152627480
C	-0.513068917	-4.008176561	1.079771111
C	-1.589118594	-5.065820096	-0.822473687
C	0.515056023	-4.941877509	1.022021614
H	-0.506581976	-3.222125463	1.824597972
C	-0.558272463	-6.000835356	-0.873487256
H	-2.420997604	-5.126966492	-1.514385996
C	0.495801987	-5.938239719	0.041003191
H	1.333347081	-4.891364778	1.734278979
H	-0.577790250	-6.781676157	-1.628127076
H	1.301659090	-6.665451119	-0.009383231
C	-1.434732982	-2.197691553	-3.400416948
H	-1.603598968	-3.060782346	-2.761803863
H	-0.471158840	-2.206431089	-3.903508919
C	3.503539494	-2.564019421	0.567407265
C	2.820355323	-2.021840020	1.826898988
C	1.632918972	-1.107377250	1.500482137
C	0.879545299	-0.658557318	2.763845845
P	-0.667917900	0.334234652	2.402635346
C	-1.943958528	-0.110088940	3.785308555
C	-3.357038344	0.185397935	3.197323452
C	-4.462766095	-0.274568657	4.169895869
C	-4.323039813	0.481086661	5.504468136
C	-2.941132806	0.178871569	6.116023674
C	-2.825979068	-1.333242984	6.383999145
C	-2.958724409	-2.087274433	5.047559572
C	-4.329793590	-1.791779458	4.408377390
C	-1.828096665	-1.629771050	4.101592974
C	-1.831987478	0.639390535	5.137535226
C	-0.063524764	2.140560632	2.620115729
C	-1.268424182	3.086808790	2.376500568
C	-0.814524951	4.562407525	2.403155618
C	0.232441972	4.801667635	1.297045656
C	1.455721278	3.898367663	1.550207327
C	2.078600059	4.238370545	2.915509890
C	1.031385014	3.976623410	4.013019556
C	-0.197335974	4.880680952	3.780069544
C	0.591072527	2.491490614	3.986943570
C	1.019530021	2.416950996	1.537114684
H	4.360232406	-3.200842241	0.814343802
H	2.802252921	-3.160097709	-0.028448240
H	3.866812703	-1.746572086	-0.066643349
H	3.547358705	-1.474575881	2.443222875
H	2.471061035	-2.861697539	2.445536364
H	0.939626840	-1.637139469	0.835407752
H	1.983562143	-0.239306958	0.931179366
H	1.544818354	-0.090479661	3.423455218
H	0.582849395	-1.549354497	3.322603329
H	-3.460616683	1.260247010	3.004833440
H	-3.486582864	-0.323892427	2.240425305
H	-5.439360796	-0.056162431	3.718788250
H	-5.116506335	0.177436858	6.200597982
H	-4.435935250	1.561464058	5.339088693
H	-2.822888370	0.732811510	7.056743775
H	-1.859718297	-1.564036546	6.853345329
H	-3.609099321	-1.650952493	7.085450088
H	-2.855141176	-3.167135327	5.216582801
H	-4.423180254	-2.329364651	3.456581788
H	-5.135086369	-2.144646824	5.066658030
H	-1.865926709	-2.212431026	3.181720513
H	-0.870888599	-1.831257806	4.597894573
H	-0.847259647	0.466930115	5.589853240
H	-1.943855154	1.717159030	4.987840379
H	-1.730395809	2.851865503	1.411218594
H	-2.032072206	2.933482089	3.148468246
H	-1.688848080	5.203961331	2.231719625
H	-0.196979423	4.578219890	0.313840962
H	0.538994763	5.856657401	1.290540575
H	2.192737708	4.045962484	0.750609182
H	2.400809530	5.288245641	2.941157161
H	2.971337746	3.621936896	3.089755194
H	1.464150462	4.191140174	4.999259422
H	-0.940454011	4.720247157	4.573589401
H	0.100254617	5.936825912	3.826803293
H	1.467288944	1.854848744	4.163917758
H	-0.093550798	2.328656026	4.816126150
H	1.898259692	1.786939564	1.725664533

H 0.647868845 2.163334218 0.548468105

1.6 Vibrational Frequencies of the Optimized Geometries

Table S7. Vibrational Frequencies (in cm^{-1}) of the Optimized Geometries

Pd(Ruphos)

24.84 35.12 39.23 42.09 50.44 55.79
60.95 63.64 66.91 69.80 74.15 79.04
84.39 90.45 93.99 105.77 130.32 145.37
158.40 171.99 191.60 197.68 209.34 221.05
224.85 228.82 238.46 245.31 248.46 255.78
265.05 272.90 274.27 291.71 299.58 334.00
337.44 344.94 380.80 391.59 401.15 405.02
424.74 430.82 440.50 446.66 451.77 458.37
475.37 479.93 485.56 494.13 511.44 531.95
533.25 567.58 582.52 603.79 637.37 638.34
687.29 719.53 737.27 745.28 753.84 764.25
772.64 779.76 782.43 807.65 811.79 823.81
826.41 826.69 844.15 862.26 866.66 870.85
890.27 899.65 903.95 907.19 909.84 920.64
937.97 943.61 944.90 948.53 952.35 958.82
959.31 964.92 980.67 989.31 1021.34 1022.40
1026.12 1044.25 1048.28 1061.34 1065.32 1069.74
1095.84 1096.82 1099.00 1099.20 1106.31 1109.29
1129.38 1135.72 1149.25 1153.30 1156.95 1159.45
1164.14 1167.43 1201.31 1204.35 1207.26 1209.51
1210.11 1222.70 1224.91 1256.55 1274.41 1282.09
1295.01 1296.93 1301.37 1304.91 1309.75 1315.74
1317.28 1318.95 1325.20 1336.93 1342.50 1350.90
1366.92 1368.97 1369.74 1376.41 1379.14 1386.14
1388.27 1389.84 1391.89 1392.00 1394.17 1395.25
1396.50 1399.83 1419.23 1422.42 1431.46 1433.91
1471.12 1492.25 1493.06 1494.39 1496.39 1498.64
1499.01 1499.33 1499.99 1500.84 1501.24 1503.72
1505.63 1506.43 1507.89 1509.10 1510.39 1520.90
1523.46 1526.49 1528.27 1530.62 1614.64 1633.99
1639.73 1645.05 3011.20 3012.47 3012.92 3016.29
3018.30 3019.20 3019.42 3024.21 3025.19 3025.56
3028.18 3032.81 3037.20 3046.74 3047.84 3048.91
3051.70 3054.74 3063.72 3064.20 3064.33 3065.22
3071.03 3071.37 3080.47 3085.87 3088.43 3093.74
3118.54 3121.35 3125.82 3130.90 3132.35 3135.32
3143.44 3152.44 3173.09 3182.16 3185.63 3199.42
3207.63 3223.85 3231.58

Pd(APhos)

37.66 60.82 65.48 72.14 81.27 102.06
113.31 129.86 130.42 149.27 175.99 198.73
232.60 239.84 245.96 255.45 257.42 268.26
283.69 295.97 298.16 312.79 318.57 323.35
330.57 339.50 366.70 380.74 390.82 410.12
415.75 431.69 438.07 450.98 480.72 496.19
524.86 546.71 579.60 599.96 626.81 655.30
733.77 779.46 817.04 817.29 818.89 829.29
944.09 945.30 951.65 956.97 960.76 966.90
972.61 978.59 980.84 1018.84 1041.43 1048.17
1050.47 1054.15 1094.81 1121.13 1158.38 1164.22
1167.01 1211.00 1212.30 1214.48 1221.71 1227.78
1236.41 1239.30 1245.88 1274.50 1329.34 1363.87
1397.27 1409.65 1412.23 1415.54 1417.44 1441.90
1448.43 1455.16 1475.29 1488.32 1489.62 1497.00
1498.36 1501.41 1502.52 1505.84 1506.05 1507.42
1512.85 1517.30 1522.99 1526.84 1535.03 1535.12
1539.46 1548.44 1559.37 1588.61 1660.11 2912.54
2922.60 2974.17 2979.07 3024.26 3026.33 3029.51
3030.56 3036.78 3038.84 3095.67 3097.88 3099.30
3101.94 3106.91 3110.05 3114.96 3120.40 3122.07
3122.16 3131.96 3137.38 3145.12 3157.70 3164.01
3211.83 3222.74 3229.09

Pd(CatX)

40.33 49.83 54.08 64.92 72.40 77.03
87.95 92.69 145.47 158.28 173.83 177.76
190.19 201.39 220.01 228.95 262.90 321.68
329.18 336.20 341.21 345.15 357.51 375.13
408.81 411.76 413.92 418.23 429.11 438.47
453.14 461.36 464.40 469.85 476.05 496.66
507.14 656.45 656.88 658.77 661.63 678.36
683.90 726.35 745.11 756.19 771.62 786.13
815.43 816.07 818.59 823.63 826.88 829.72
900.14 903.01 903.91 904.34 907.48 909.10
910.34 918.97 938.99 944.68 949.45 951.94
980.20 982.48 983.91 986.03 987.60 989.14
1025.91 1050.27 1053.49 1054.21 1055.74 1058.02
1058.65 1059.56 1061.46 1065.11 1081.16 1117.34
1129.63 1130.63 1132.38 1133.16 1135.18 1135.30
1147.31 1147.64 1158.49 1159.02 1211.66 1215.70
1216.44 1218.69 1238.85 1253.81 1282.60 1291.05
1292.05 1298.75 1317.89 1321.89 1322.46 1324.71
1325.46 1330.57 1332.49 1340.30 1343.77 1344.82
1345.86 1351.66 1355.84 1356.50 1357.50 1357.81
1362.31 1384.06 1384.96 1385.79 1388.48 1395.95
1400.39 1404.75 1405.23 1407.15 1410.56 1411.99
1429.91 1475.35 1494.52 1495.63 1496.61 1498.66
1503.28 1508.62 1509.09 1510.09 1510.59 1511.03
1512.61 1514.28 1514.37 1523.20 1534.68 1536.05
3016.17 3016.37 3017.31 3017.59 3017.86 3018.66
3018.74 3028.14 3029.03 3030.73 3031.21 3034.13
3035.58 3037.35 3039.00 3041.31 3043.51 3044.18
3046.84 3048.16 3050.61 3050.96 3058.57 3058.90
3060.41 3060.82 3063.22 3065.58 3065.82 3075.87
3085.30 3088.77 3095.75 3102.75 3106.02 3108.01
3108.74 3115.35 3119.26

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413.73 413.74 620.41 620.43 693.39 717.25
864.03 864.04 975.58 975.60 1013.71 1015.64
1020.08 1067.73 1067.85 1189.19 1208.43 1208.56
1357.61 1378.09 1523.60 1523.78 1653.97 1653.99
3171.42 3181.46 3181.51 3198.04 3198.17 3209.17

3a

25.47 41.26 52.16 70.96 147.04 155.91
167.36 183.23 260.90 283.67 318.84 344.28
358.39 397.40 411.75 417.80 451.97 473.20
518.62 617.23 629.58 634.06 688.78 699.29
711.08 733.54 751.75 770.74 798.41 814.99
819.04 864.23 867.78 902.45 958.11 960.69
963.27 990.51 994.91 1014.52 1016.23 1017.63
1054.69 1069.85 1084.80 1121.60 1170.19 1198.53
1215.88 1227.34 1243.26 1295.91 1321.53 1331.42
1351.88 1364.28 1373.08 1397.45 1416.91 1437.38
1478.82 1490.23 1491.77 1517.42 1534.44 1634.21
1655.97 1674.83 1710.47 1738.66 1749.26 3034.99
3052.87 3105.83 3154.50 3158.82 3181.58 3194.43
3199.43 3204.75 3218.02 3231.54 3242.49 3269.38

R1

10.50 14.60 28.53 33.77 36.08 39.54
44.48 45.83 47.94 55.13 59.09 61.64

66.53 68.25 71.62 76.35 78.18 82.59
86.91 91.60 93.43 97.65 100.93 105.05
109.96 120.57 127.71 138.09 149.51 155.81
160.58 172.28 174.19 194.87 195.47 202.85
204.47 213.32 228.79 229.20 230.02 238.86
241.09 248.76 253.45 261.16 264.40 264.49
267.80 273.06 281.41 289.52 293.39 295.39
302.38 305.41 308.50 318.24 344.29 347.14
352.67 380.04 389.74 399.58 405.68 409.32
412.83 416.67 418.98 427.54 433.14 440.10
446.30 450.52 453.86 461.06 472.03 488.10
489.11 497.81 501.98 513.70 519.40 519.91
534.93 535.58 547.47 574.76 580.18 616.69
616.89 626.78 629.60 632.55 654.19 675.01
677.83 686.94 711.13 716.81 718.18 727.57
738.07 741.66 752.04 754.66 756.45 758.18
760.90 767.10 773.48 784.75 786.93 794.55
816.05 822.24 824.31 825.06 827.95 830.97
858.01 859.36 859.78 866.32 867.98 868.10
870.10 874.95 885.83 898.88 904.23 905.44
910.06 912.04 916.16 916.95 923.45 938.65
943.57 947.78 949.44 951.59 957.78 962.45
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1047.05 1050.55 1064.05 1065.41 1070.29 1072.98
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1101.00 1101.64 1103.95 1111.23 1111.61 1112.26
1128.63 1135.57 1144.68 1145.65 1149.83 1154.00
1157.19 1159.96 1164.28 1167.55 1169.24 1185.76
1191.16 1193.02 1204.59 1206.15 1208.42 1211.05
1213.00 1215.45 1216.00 1227.80 1235.79 1243.59
1247.44 1256.37 1270.08 1271.02 1275.34 1282.13
1294.42 1300.39 1302.05 1306.58 1315.19 1315.69
1316.60 1319.15 1321.26 1323.12 1330.96 1339.24
1342.65 1347.52 1350.98 1353.33 1355.00 1362.29
1365.88 1368.38 1369.47 1372.92 1375.69 1377.73
1381.89 1387.99 1391.99 1393.19 1393.46 1393.90
1394.50 1394.72 1396.84 1410.28 1411.01 1417.35
1422.71 1424.49 1435.23 1442.92 1467.18 1469.41
1472.24 1486.81 1491.93 1494.35 1495.83 1497.19
1498.42 1500.33 1500.85 1501.16 1503.01 1503.77
1504.29 1505.17 1506.54 1508.02 1509.62 1510.37
1510.44 1512.72 1513.70 1515.33 1523.06 1527.49
1527.85 1529.97 1531.73 1534.82 1615.86 1620.21
1625.01 1634.56 1638.15 1640.74 1648.59 1656.45
1751.55 3009.43 3013.92 3016.02 3017.75 3019.48
3021.08 3023.60 3024.90 3031.37 3038.31 3040.38
3042.91 3044.30 3045.68 3047.70 3052.54 3053.87
3054.05 3057.62 3061.55 3067.66 3068.79 3068.88
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3100.25 3115.21 3116.01 3117.89 3121.10 3127.91
3130.38 3133.41 3135.15 3136.37 3142.15 3144.41
3151.74 3153.39 3161.26 3161.82 3161.86 3165.50
3168.17 3173.94 3176.66 3179.60 3181.12 3187.01
3191.31 3191.92 3202.52 3203.89 3215.59 3226.73
3232.38 3232.57 3253.49

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R1-TS$_{dis}$

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-221.01 7.85 21.51 22.55 26.96 30.97
36.79 39.65 40.68 43.19 45.90 54.85
60.11 62.79 66.12 70.70 73.37 76.61
79.96 83.93 87.77 92.17 100.68 103.04
109.08 113.83 118.76 129.75 147.16 154.31
159.15 163.56 168.85 181.32 191.15 193.46
204.93 211.41 217.27 226.96 227.55 229.59
231.60 246.83 250.73 255.19 257.05 266.31
271.73 273.53 275.35 284.28 287.87 293.81
302.34 306.81 310.38 317.77 341.86 347.79
351.82 354.81 380.72 395.45 397.11 408.88
411.56 416.24 421.96 431.25 439.93 446.31
449.64 453.88 456.20 459.89 472.76 481.72
492.06 494.98 500.54 513.25 518.45 531.57
534.57 540.35 544.54 573.11 581.44 586.77
608.60 614.70 625.78 627.89 632.09 661.32
664.15 670.92 676.96 686.70 717.81 719.85
728.76 738.61 742.22 751.41 753.07 754.75
758.82 762.87 772.90 775.34 783.37 795.82
796.97 816.03 817.34 820.92 821.62 823.71
830.28 848.45 859.94 862.23 868.54 869.32
871.97 873.46 885.71 888.57 903.25 905.14
909.28 913.05 915.83 917.94 923.17 942.33
943.04 946.25 949.61 953.63 960.04 961.68
963.31 965.12 966.06 972.71 978.23 982.89
985.93 992.24 999.94 1000.76 1011.58 1016.15
1018.42 1022.80 1025.70 1030.25 1035.51 1039.78
1043.48 1045.53 1063.10 1066.32 1067.38 1068.76
1080.82 1087.76 1088.63 1091.35 1092.02 1093.56
1099.79 1100.34 1109.07 1109.93 1111.12 1117.79
1129.98 1130.84 1145.30 1148.66 1149.35 1156.14
1158.87 1164.25 1167.19 1168.11 1188.93 1190.89
1195.61 1204.64 1205.23 1207.49 1210.16 1214.26
1216.17 1221.07 1223.53 1228.06 1234.64 1243.66
1246.28 1257.37 1270.08 1276.39 1278.32 1294.62
1300.10 1302.63 1307.02 1312.67 1314.65 1315.07
1317.04 1319.74 1325.59 1330.14 1330.85 1336.82
1342.89 1345.75 1347.54 1354.31 1355.92 1366.26
1367.58 1367.89 1371.09 1374.23 1375.71 1376.46
1379.62 1384.81 1390.74 1391.06 1391.33 1393.21
1393.99 1394.62 1398.40 1399.27 1403.11 1406.88
1421.59 1421.96 1427.13 1434.57 1441.78 1466.16
1472.30 1483.35 1490.38 1492.42 1493.75 1495.21
1497.01 1499.06 1500.75 1500.89 1501.17 1502.22
1502.60 1503.19 1504.78 1506.48 1507.69 1510.61
1511.02 1512.12 1513.03 1514.12 1521.77 1525.88
1527.50 1529.00 1530.27 1535.66 1614.76 1619.11
1625.03 1633.72 1636.26 1642.98 1648.21 1656.24
1764.80 3010.88 3013.87 3016.83 3017.76 3020.95
3021.29 3023.51 3024.27 3026.48 3029.34 3034.85
3042.36 3046.48 3047.50 3048.28 3052.86 3053.38
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3070.98 3073.86 3077.67 3083.65 3089.96 3095.84
3114.50 3117.91 3120.95 3120.96 3123.03 3124.58
3131.50 3135.42 3137.83 3140.01 3143.47 3144.44
3149.15 3150.41 3159.64 3160.40 3169.51 3170.14
3176.56 3179.71 3186.34 3187.18 3189.49 3195.09
3195.31 3201.39 3208.88 3209.23 3218.77 3221.60
3232.97 3233.49 3240.74

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R2$_{dis}$

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15.77 22.62 27.98 31.60 34.41 36.08
40.48 44.90 47.09 50.34 55.73 62.89
68.39 71.34 73.92 77.70 82.23 84.91
87.76 92.19 98.25 103.14 107.65 112.92
120.06 123.35 129.60 132.11 146.03 156.61
160.66 167.14 174.36 184.19 191.68 200.65
207.16 215.73 225.09 226.04 229.33 234.93
238.99 249.10 251.88 266.45 270.15 272.16
278.58 279.39 280.33 290.44 293.19 297.95
303.15 307.70 316.38 323.39 340.26 346.22
353.68 378.84 392.16 396.36 402.27 409.43
414.62 415.06 422.99 424.71 430.86 440.31
447.99 450.59 452.98 456.13 461.28 472.19
488.38 494.87 495.80 506.63 513.69 518.79
525.63 534.87 537.27 569.13 574.87 582.94
605.14 608.15 625.87 627.43 630.36 649.82
664.34 667.79 685.43 695.80 710.67 717.58
728.34 735.66 738.07 749.01 750.97 760.73

762.14 769.27 775.31 779.86 784.43 794.38
799.35 816.47 816.74 820.31 822.65 824.66
828.23 839.78 858.23 860.00 866.33 869.20
873.53 876.26 885.80 886.41 903.02 904.64
908.29 913.98 917.10 922.79 925.58 942.95
945.20 948.54 949.67 953.69 957.71 959.12
962.46 964.09 965.38 970.91 977.28 984.74
989.28 1003.92 1004.51 1009.82 1013.76 1016.45
1023.89 1024.68 1026.88 1029.09 1039.85 1042.41
1044.88 1048.33 1062.96 1063.65 1068.31 1078.64
1083.65 1086.14 1088.79 1089.55 1090.34 1091.58
1100.48 1102.55 1106.29 1107.10 1110.63 1120.89
1131.55 1133.37 1140.64 1145.62 1148.84 1155.79
1158.57 1162.60 1166.55 1167.16 1182.53 1190.99
1197.77 1204.42 1205.00 1208.23 1210.95 1211.90
1217.73 1220.36 1223.28 1230.03 1243.15 1249.90
1266.31 1268.83 1276.66 1278.24 1290.27 1296.75
1299.73 1302.35 1307.05 1311.24 1315.02 1316.48
1318.44 1318.90 1326.07 1329.70 1336.21 1342.07
1342.68 1344.32 1347.36 1355.76 1361.59 1365.12
1366.25 1366.75 1368.66 1371.57 1375.26 1376.80
1379.39 1386.03 1390.84 1391.45 1392.81 1393.35
1394.39 1394.74 1401.50 1401.75 1405.08 1420.98
1421.33 1421.97 1434.91 1446.50 1468.27 1472.58
1482.80 1492.74 1493.35 1494.03 1498.06 1499.38
1499.88 1500.83 1501.36 1502.37 1504.09 1505.94
1506.43 1507.60 1508.48 1510.30 1511.07 1512.14
1513.09 1513.42 1513.76 1524.94 1527.35 1528.46
1530.52 1533.49 1534.05 1615.58 1620.93 1622.55
1624.41 1636.90 1643.86 1644.28 1649.20 1655.85
1700.21 2978.13 2980.25 3011.88 3012.22 3016.64
3017.94 3019.37 3022.31 3022.54 3031.22 3034.41
3041.63 3044.75 3046.29 3048.66 3050.82 3051.38
3054.36 3055.77 3058.88 3060.47 3062.84 3065.94
3066.96 3067.87 3073.84 3076.66 3088.52 3094.50
3101.97 3115.08 3121.05 3124.78 3131.99 3133.57
3138.03 3143.18 3143.65 3144.22 3145.42 3148.72
3149.70 3156.62 3161.22 3165.59 3171.98 3175.50
3176.51 3183.20 3185.57 3187.76 3189.32 3191.68
3200.23 3201.25 3212.32 3221.92 3234.52 3235.67
3238.30 3242.55 3258.91

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R2-TS$_{dis}$

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-361.11 18.29 24.21 25.75 31.29 34.72
43.48 48.04 48.80 54.35 60.46 62.02
66.18 73.53 74.67 77.15 79.08 83.50
83.92 96.03 101.06 106.68 109.33 113.22
116.26 124.24 128.89 133.29 143.68 152.79
160.71 165.83 172.82 174.56 180.42 189.73
192.23 198.75 206.90 214.97 225.68 228.19
230.69 236.85 248.82 254.54 267.10 268.52
272.59 280.20 285.22 287.34 292.85 301.89
303.68 306.83 320.61 325.43 328.40 342.83
366.44 378.94 384.37 388.53 398.56 401.90
403.09 419.11 430.35 432.22 433.64 436.48
442.33 448.83 451.42 460.76 464.17 466.73
472.73 494.21 497.04 502.81 511.80 514.80
517.93 532.57 532.94 558.66 572.86 579.03
586.99 607.37 625.18 628.93 631.88 640.67
656.00 677.33 678.48 683.53 708.34 709.50
724.17 725.47 732.20 743.64 752.51 755.76
761.09 765.48 772.62 774.13 778.51 780.99
801.61 815.75 819.41 820.48 822.37 823.71
828.37 842.20 853.43 868.24 869.87 871.48
875.10 879.37 886.08 886.76 902.46 904.24
908.40 916.06 921.27 932.84 934.50 935.79
943.07 944.47 949.80 954.89 957.05 957.38
959.30 960.78 963.87 969.18 984.83 987.09
998.77 1002.71 1005.42 1006.87 1009.84 1013.01
1016.22 1018.60 1026.53 1028.83 1036.07 1040.20
1045.76 1051.91 1061.36 1066.36 1067.39 1068.66
1071.48 1074.69 1078.37 1089.20 1089.44 1093.04
1099.92 1106.78 1108.20 1111.18 1115.10 1117.48
1128.64 1134.91 1140.80 1141.36 1150.81 1155.46
1157.28 1161.33 1161.76 1166.47 1189.56 1193.99
1196.66 1202.25 1204.35 1205.64 1209.35 1210.78
1212.49 1215.77 1217.04 1226.67 1241.98 1249.67
1260.31 1261.21 1268.65 1274.01 1282.69 1295.05
1298.46 1302.19 1305.06 1309.01 1314.13 1315.35
1317.30 1326.76 1329.93 1332.74 1339.84 1339.88
1340.34 1343.45 1344.45 1357.30 1367.05 1368.14
1368.23 1369.26 1374.72 1375.63 1379.10 1381.27
1387.19 1390.90 1391.89 1392.62 1393.39 1393.72
1395.70 1397.91 1399.79 1406.44 1422.56 1423.14
1423.92 1426.80 1435.52 1445.14 1468.24 1469.12
1480.34 1489.78 1493.65 1493.89 1498.40 1499.38
1500.10 1500.36 1501.11 1501.51 1503.59 1505.90
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1511.96 1512.22 1515.37 1520.80 1523.52 1524.94
1526.84 1528.25 1531.66 1611.10 1613.84 1618.21
1623.94 1628.89 1640.26 1642.02 1645.54 1646.89
1698.74 2978.16 3010.23 3012.50 3013.82 3014.42
3017.29 3024.15 3030.80 3030.95 3036.97 3039.85
3040.87 3042.11 3042.38 3046.84 3049.37 3054.67
3057.64 3060.04 3061.04 3063.30 3065.53 3067.40
3067.98 3081.73 3084.83 3086.58 3093.94 3108.46
3113.29 3120.61 3122.55 3126.06 3132.04 3132.34
3136.09 3140.09 3141.23 3144.83 3146.42 3152.90
3155.28 3157.58 3165.49 3169.89 3174.70 3175.55
3176.38 3184.49 3187.30 3187.66 3192.11 3200.70
3202.46 3213.91 3220.07 3226.21 3228.75 3233.85
3234.92 3243.66 3249.21

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3b

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21.71 35.47 38.32 46.82 58.65 91.63
122.45 151.15 152.60 168.78 199.82 242.29
263.32 283.95 314.01 339.93 376.31 390.89
407.76 415.79 421.95 433.80 451.03 493.55
517.22 561.39 628.04 629.99 634.79 675.06
683.34 694.13 705.80 708.68 725.08 759.53
782.85 786.10 812.49 831.12 839.10 860.98
869.09 870.41 919.52 934.95 945.92 949.43
974.54 988.61 989.24 1006.35 1006.98 1008.20
1010.87 1014.37 1018.45 1050.52 1057.59 1062.74
1083.36 1091.34 1111.64 1119.03 1120.92 1131.84
1144.57 1178.71 1196.46 1196.98 1211.07 1214.89
1223.47 1242.01 1246.84 1260.68 1290.27 1318.49
1344.58 1345.84 1362.40 1365.92 1368.77 1384.34
1390.74 1406.05 1421.68 1435.00 1488.71 1488.88
1496.30 1511.37 1517.29 1535.21 1536.00 1636.48
1637.85 1658.78 1661.29 1734.39 1771.75 2984.11
3035.72 3045.71 3090.56 3140.92 3148.18 3153.53
3164.25 3178.21 3178.28 3189.23 3189.48 3199.70
3200.32 3209.20 3211.00 3215.21 3221.65 3231.11

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R1'

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9.38 24.68 27.87 28.81 32.73 41.66
42.89 46.35 50.37 53.91 60.19 64.36
67.34 68.61 71.03 75.47 77.11 80.39
84.77 90.50 92.98 98.01 100.06 105.07
109.23 114.69 118.39 126.84 130.42 154.62
161.75 168.33 171.79 178.67 190.72 195.87
204.00 208.22 214.02 218.31 225.95 234.72
235.87 242.89 244.40 256.50 257.14 261.52
267.27 270.40 273.24 276.66 283.44 294.43
301.35 302.66 311.64 332.13 335.17 340.74
350.84 377.97 388.16 392.94 400.00 409.06

411.56 414.49 416.30 432.32 440.71 447.46
450.31 461.00 464.66 468.05 475.44 483.78
488.14 494.21 496.45 505.26 512.40 533.00
533.66 537.09 543.69 573.07 581.73 621.28
624.52 626.70 628.80 633.52 648.42 670.35
675.02 688.47 712.29 714.24 717.86 721.15
734.12 740.92 749.75 751.13 755.23 763.07
764.09 765.89 782.86 784.13 791.01 795.05
811.26 814.38 823.14 825.44 827.66 828.30
852.94 858.91 861.98 862.30 864.91 868.18
870.48 873.02 896.40 901.72 905.27 908.11
910.08 915.92 917.87 918.53 923.79 933.08
937.67 943.56 949.59 950.40 961.09 962.28
967.09 970.64 973.40 974.07 978.30 978.53
981.27 997.94 999.73 1005.12 1007.34 1014.05
1017.34 1019.84 1025.45 1028.91 1040.87 1046.09
1047.64 1049.29 1055.48 1062.13 1063.02 1067.16
1081.15 1086.60 1091.69 1092.53 1093.89 1097.59
1098.67 1103.05 1104.06 1109.82 1110.47 1116.12
1132.35 1133.07 1144.05 1147.25 1149.30 1153.75
1157.01 1158.42 1163.13 1166.20 1172.45 1185.17
1193.26 1194.28 1204.51 1204.88 1209.51 1210.24
1212.39 1219.06 1220.13 1225.30 1237.82 1239.23
1256.33 1260.30 1263.43 1267.93 1272.28 1284.13
1295.92 1296.42 1302.50 1307.69 1311.09 1315.64
1320.13 1321.72 1323.79 1325.30 1329.65 1338.02
1338.98 1339.96 1346.54 1349.10 1359.53 1359.99
1365.93 1366.83 1366.97 1367.75 1373.31 1377.73
1378.63 1380.93 1389.03 1391.37 1394.13 1395.44
1395.61 1396.92 1400.98 1402.47 1404.65 1414.27
1422.60 1426.85 1434.86 1435.90 1443.24 1464.00
1466.67 1487.28 1491.66 1492.76 1493.21 1495.35
1496.51 1499.61 1500.75 1501.57 1502.04 1504.17
1504.45 1506.45 1507.15 1507.84 1509.07 1510.24
1511.95 1512.07 1513.23 1513.95 1522.08 1529.85
1530.53 1530.97 1532.47 1537.01 1611.22 1613.65
1621.47 1635.45 1635.71 1640.88 1646.00 1658.71
1828.38 2831.78 3000.74 3008.02 3009.11 3009.74
3013.59 3022.22 3022.97 3023.72 3025.24 3038.95
3040.95 3043.76 3043.87 3049.23 3050.25 3056.55
3062.73 3064.90 3065.83 3071.83 3078.74 3082.42
3086.59 3088.99 3090.85 3099.87 3109.87 3114.40
3115.17 3115.97 3120.40 3121.19 3128.81 3130.52
3134.06 3142.14 3144.04 3144.24 3145.33 3146.54
3151.66 3152.93 3160.66 3160.84 3162.80 3164.72
3171.62 3174.55 3178.25 3184.35 3186.44 3189.85
3192.79 3194.18 3201.19 3203.01 3208.30 3218.93
3230.21 3231.45 3249.20

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R1'-TS$_{prox}$

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-228.59 18.09 25.99 31.50 35.80 37.23
46.26 49.20 50.31 52.98 58.19 59.48
67.25 70.69 72.38 73.83 78.62 80.82
81.80 85.40 88.36 97.79 102.77 107.15
110.07 114.25 116.94 122.49 131.91 137.64
152.32 159.00 168.84 171.88 188.70 190.94
203.45 207.80 212.83 214.30 225.59 228.18
233.38 239.68 241.47 244.77 257.10 261.33
262.70 267.37 269.00 274.32 280.88 287.34
300.50 303.62 308.46 334.18 336.55 337.92
350.19 357.12 387.89 389.09 393.08 402.38
408.86 413.72 416.88 431.27 437.09 442.17
446.46 452.72 453.46 463.34 474.33 479.14
485.07 488.32 493.59 500.93 502.98 510.03
527.72 530.26 535.91 572.03 574.31 581.86
625.21 626.42 629.40 631.93 636.06 645.88
660.47 670.69 688.49 715.94 718.45 718.90
725.78 738.40 743.82 752.29 753.58 757.23
759.88 765.93 780.76 781.41 785.58 792.86
794.91 807.91 811.85 823.67 825.82 827.57
828.42 856.00 862.24 864.48 867.34 868.54
869.63 870.06 878.28 894.32 899.35 907.26
909.34 911.01 915.25 918.61 922.12 936.84
938.16 943.26 944.46 949.98 951.74 963.98
969.08 971.07 974.61 977.39 977.83 980.52
982.51 996.18 997.15 1000.65 1006.72 1012.72
1017.28 1020.90 1024.80 1029.59 1042.78 1045.25
1046.68 1048.90 1060.43 1063.14 1064.85 1065.21
1082.72 1091.13 1091.44 1092.80 1093.47 1098.24
1098.56 1104.68 1108.52 1109.47 1112.20 1115.24
1129.03 1134.79 1137.62 1141.61 1148.78 1154.27
1155.72 1158.27 1159.21 1168.37 1173.27 1192.65
1194.23 1204.24 1206.04 1209.82 1210.29 1211.16
1211.51 1217.00 1222.61 1229.24 1235.69 1236.92
1251.53 1262.89 1266.19 1271.76 1286.09 1297.02
1298.03 1300.76 1307.64 1309.96 1314.83 1320.12
1321.25 1323.33 1327.85 1329.04 1334.19 1338.53
1341.10 1342.13 1351.41 1358.93 1360.38 1364.65
1366.24 1368.29 1369.05 1375.53 1378.10 1379.53
1380.01 1384.26 1388.52 1393.30 1393.93 1395.56
1396.02 1397.81 1400.81 1403.29 1407.11 1414.74
1423.10 1427.93 1436.02 1438.53 1464.31 1466.46
1480.95 1488.50 1492.15 1493.71 1494.24 1494.71
1497.38 1498.81 1500.68 1501.28 1502.33 1505.02
1505.32 1506.68 1507.16 1507.31 1508.07 1510.03
1510.67 1512.12 1512.89 1515.20 1521.89 1527.72
1529.93 1530.45 1534.04 1534.41 1613.99 1615.97
1622.08 1634.91 1638.23 1642.98 1647.06 1657.81
1806.10 2955.31 3006.55 3008.45 3010.60 3011.28
3014.68 3020.99 3022.42 3024.84 3033.17 3034.27
3037.69 3040.81 3045.06 3048.78 3050.06 3054.22
3062.85 3064.91 3065.48 3071.96 3075.96 3079.96
3081.57 3084.14 3089.52 3096.27 3104.69 3112.23
3114.56 3115.99 3121.24 3122.62 3129.91 3130.41
3131.46 3135.64 3138.77 3140.74 3141.27 3151.26
3154.02 3156.57 3160.62 3161.79 3167.34 3173.10
3176.67 3177.03 3184.99 3186.07 3190.00 3191.17
3192.85 3196.26 3200.40 3204.11 3212.80 3222.67
3228.58 3248.13 3255.58

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R2$_{prox}$

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9.59 12.14 22.09 31.55 33.06 34.26
39.69 48.09 48.65 50.33 54.97 62.12
64.62 67.71 73.01 74.32 77.77 80.89
84.77 88.83 91.21 92.69 96.30 100.61
108.51 119.67 121.74 133.18 138.66 157.49
162.95 167.66 169.35 173.17 180.98 186.27
194.61 205.69 219.42 221.59 231.49 233.31
235.79 239.64 245.62 256.02 265.13 267.63
268.79 274.23 277.58 278.81 284.89 295.12
307.59 309.27 334.54 337.47 339.53 345.52
349.74 373.78 382.78 391.78 396.05 400.98
412.48 413.75 416.58 416.97 427.96 435.56
444.27 449.16 452.55 466.62 468.97 473.62
485.14 488.78 492.60 495.05 497.61 508.91
521.38 524.94 531.09 568.68 584.39 597.74
609.04 626.32 629.24 630.51 647.43 665.33
671.43 677.38 681.10 702.72 713.27 716.75
717.97 733.77 743.25 746.80 752.96 754.22
762.23 766.03 776.69 782.24 785.34 800.82
802.43 807.35 813.13 818.96 822.82 828.90
830.13 854.20 855.19 865.61 866.30 868.40
870.63 873.57 874.61 894.73 902.38 904.41
910.08 911.06 914.22 918.06 919.18 937.94
939.99 942.47 947.04 950.97 956.19 960.68
963.08 966.94 971.21 971.75 974.98 979.63
990.71 996.51 997.50 1009.68 1010.25 1016.56
1019.71 1021.74 1025.17 1030.98 1042.42 1046.03

1047.90 1052.62 1062.37 1062.71 1064.91 1067.71
1070.88 1080.36 1084.06 1090.01 1092.42 1097.09
1098.18 1102.01 1109.73 1111.81 1112.03 1121.31
1129.18 1130.67 1144.02 1151.60 1155.17 1156.59
1157.89 1158.50 1162.47 1166.68 1168.51 1182.52
1190.66 1198.06 1203.49 1205.68 1208.58 1209.75
1213.27 1217.36 1220.30 1220.59 1239.63 1244.31
1244.87 1258.55 1264.93 1267.95 1272.05 1299.68
1301.40 1302.20 1308.11 1309.38 1311.80 1313.63
1314.03 1317.06 1320.07 1322.46 1340.96 1343.21
1344.53 1346.61 1348.77 1358.74 1360.83 1368.90
1369.39 1370.20 1372.67 1375.21 1376.95 1381.35
1385.05 1389.35 1391.31 1393.31 1393.85 1395.26
1396.32 1398.92 1399.94 1401.95 1412.11 1420.53
1422.63 1431.92 1435.03 1465.42 1467.52 1485.82
1491.14 1492.31 1494.87 1495.24 1495.90 1497.67
1498.47 1499.32 1500.32 1501.24 1502.40 1504.26
1506.30 1506.99 1507.50 1508.00 1509.22 1509.96
1512.33 1513.56 1513.67 1522.53 1524.39 1526.36
1529.31 1532.23 1533.69 1612.83 1615.87 1619.56
1624.25 1636.21 1645.55 1647.75 1648.45 1662.26
1714.06 3004.31 3009.86 3011.27 3019.00 3021.33
3024.08 3026.51 3028.18 3033.30 3033.48 3034.15
3035.61 3035.86 3046.01 3047.61 3051.85 3052.50
3056.55 3056.69 3063.43 3064.19 3067.46 3070.18
3075.01 3078.97 3079.44 3091.63 3092.75 3101.11
3114.47 3120.07 3122.17 3127.63 3129.35 3130.76
3131.85 3131.93 3134.90 3136.98 3146.53 3155.93
3158.42 3162.73 3175.34 3177.85 3180.48 3181.64
3188.15 3190.11 3191.70 3193.56 3196.19 3196.62
3200.53 3201.77 3213.69 3218.64 3223.01 3225.76
3227.87 3231.10 3238.44

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R2-TS$_{RE}$

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-227.94 2.89 12.05 23.62 35.20 38.50
41.93 46.10 48.74 51.13 55.19 57.54
63.82 64.69 67.21 70.69 73.63 78.20
79.16 80.85 86.48 91.88 96.43 100.79
102.26 109.36 119.33 130.88 133.42 142.28
148.41 160.26 163.25 168.95 178.42 182.78
186.08 192.50 199.10 202.58 210.06 220.47
221.89 228.06 236.32 237.50 245.21 251.04
256.90 263.18 266.15 273.41 275.16 283.23
290.94 295.23 298.45 317.35 331.80 339.04
346.59 352.93 379.06 392.34 397.54 402.89
408.13 416.15 421.77 425.05 428.24 434.54
436.17 446.29 447.39 449.51 457.48 458.75
470.48 478.19 483.90 486.05 495.18 509.99
515.18 527.57 530.46 541.98 569.76 581.85
611.71 624.70 629.26 632.99 638.09 639.19
649.11 680.50 681.63 700.17 710.83 714.95
720.89 738.07 739.63 748.56 752.37 755.72
764.43 765.01 775.67 779.08 781.92 792.93
806.14 809.04 809.32 817.55 820.56 824.29
825.88 839.40 854.38 858.66 862.77 865.83
868.82 871.57 873.46 890.13 899.15 901.12
903.71 908.07 910.24 914.00 920.25 938.93
943.97 946.54 949.54 959.93 960.41 961.50
961.58 964.88 968.90 971.89 973.55 978.26
986.59 991.54 999.20 1000.57 1007.09 1010.19
1014.76 1017.26 1017.54 1021.16 1024.37 1034.23
1045.15 1048.48 1055.69 1055.80 1062.09 1063.86
1064.83 1066.70 1072.97 1096.45 1096.93 1099.39
1099.95 1100.64 1101.26 1109.72 1112.26 1117.65
1127.48 1132.38 1134.87 1137.64 1147.56 1155.65
1156.09 1157.90 1160.54 1165.56 1168.72 1190.63
1196.55 1201.90 1204.79 1208.14 1209.64 1212.62
1212.90 1216.80 1217.24 1229.94 1230.04 1239.08
1254.52 1256.56 1274.09 1279.18 1286.59 1298.17
1299.37 1300.43 1302.43 1306.10 1310.63 1311.28
1318.15 1320.67 1323.66 1326.01 1341.30 1341.63
1344.51 1348.99 1350.35 1350.52 1369.66 1370.41
1370.62 1374.62 1379.54 1381.06 1383.15 1383.91
1389.54 1391.07 1394.97 1395.64 1396.17 1396.87
1398.14 1401.95 1405.67 1409.26 1417.34 1422.87
1423.61 1434.01 1434.56 1465.01 1470.33 1472.96
1489.82 1490.72 1491.54 1493.65 1495.86 1496.55
1497.62 1498.78 1499.42 1500.05 1501.18 1501.42
1501.95 1503.94 1505.07 1507.50 1508.07 1508.31
1509.53 1511.00 1520.24 1522.09 1522.54 1525.78
1528.25 1530.60 1534.25 1608.46 1617.54 1621.13
1633.81 1634.09 1641.31 1646.13 1654.36 1710.32
1743.27 3008.14 3011.92 3012.38 3020.91 3024.82
3025.74 3027.59 3029.96 3031.31 3038.60 3043.33
3048.22 3048.73 3051.80 3056.27 3057.03 3057.51
3061.46 3063.40 3063.79 3065.32 3068.43 3070.39
3071.54 3073.49 3078.67 3080.76 3088.96 3091.92
3104.49 3107.25 3116.14 3119.96 3124.69 3128.92
3129.40 3133.60 3137.75 3139.53 3140.69 3143.55
3144.15 3153.72 3157.48 3162.14 3168.97 3173.09
3175.79 3184.17 3187.59 3191.92 3196.70 3198.85
3200.17 3205.17 3212.89 3218.58 3218.66 3224.36
3231.42 3236.68 3253.16

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3c

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26.10 32.93 38.87 53.23 66.82 78.46
110.16 160.35 166.29 181.91 199.79 233.92
255.36 271.63 300.20 326.78 354.69 368.66
405.25 413.08 416.26 439.19 450.14 484.82
494.09 535.36 598.33 625.91 632.11 634.13
681.72 698.53 713.54 725.33 747.38 753.16
780.75 789.67 807.93 814.68 840.75 850.69
858.25 866.87 897.20 928.60 950.51 955.80
959.66 973.92 992.73 995.74 1002.82 1009.15
1010.97 1013.33 1017.77 1047.17 1059.74 1064.60
1083.33 1088.42 1112.38 1119.69 1125.22 1132.06
1156.83 1191.78 1196.50 1197.33 1212.73 1218.67
1220.68 1237.28 1256.73 1272.43 1305.48 1319.02
1348.88 1351.59 1366.41 1369.67 1371.96 1391.46
1399.70 1405.03 1426.92 1441.52 1489.34 1496.87
1498.09 1514.96 1522.80 1533.58 1539.43 1634.61
1644.10 1657.14 1663.28 1724.70 1750.03 3020.72
3053.36 3080.64 3099.33 3138.42 3139.01 3151.17
3168.05 3173.71 3177.32 3181.25 3190.18 3190.27
3198.79 3201.18 3207.72 3218.99 3225.51 3230.07

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R2-TS$_{prox}$

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-106.78 3.35 21.56 27.53 31.38 32.07
35.08 46.27 50.38 55.85 59.09 63.86
66.38 71.04 75.20 78.36 83.11 86.76
92.26 93.24 96.68 99.77 107.90 111.81
118.12 122.95 125.05 136.08 145.43 149.55
162.38 165.05 170.33 177.54 181.26 193.65
207.03 209.65 214.26 221.03 225.37 229.09
231.86 235.76 238.61 244.14 257.05 267.20
270.81 272.16 278.60 285.73 293.52 293.84
305.07 309.83 315.10 335.13 343.17 348.47
355.00 370.94 381.38 390.67 401.35 407.42
412.31 419.23 420.20 421.74 430.72 443.79
446.43 448.20 453.70 460.92 467.39 470.99
475.62 484.77 489.10 492.55 495.76 499.06
506.83 513.94 531.15 537.99 557.33 573.73
584.30 618.45 626.71 629.50 631.91 644.60
654.36 656.91 661.48 682.75 706.00 715.13
717.29 723.13 733.59 737.46 743.74 748.38
754.65 756.31 761.18 778.66 782.30 785.83
795.96 811.16 813.25 821.66 822.99 827.70

828.69 832.42 855.62 857.38 860.96 861.65
869.74 870.04 872.98 877.51 896.54 900.80
905.49 908.16 915.32 916.08 919.56 921.92
939.51 944.74 951.21 956.78 959.28 961.17
964.82 969.89 969.96 974.10 976.63 979.36
984.94 1000.04 1000.60 1003.38 1004.36 1012.29
1014.08 1017.74 1018.63 1021.67 1025.48 1028.63
1032.40 1044.11 1048.33 1049.63 1053.66 1060.89
1063.72 1064.03 1067.40 1084.68 1088.74 1092.84
1098.10 1098.23 1102.37 1109.44 1116.62 1119.81
1124.76 1129.74 1135.22 1143.97 1152.44 1153.10
1156.48 1159.32 1164.22 1169.24 1171.63 1190.66
1197.83 1205.07 1206.03 1207.13 1209.03 1210.57
1214.16 1215.62 1226.80 1228.74 1232.86 1249.55
1250.64 1252.22 1265.29 1272.56 1279.36 1293.08
1297.68 1301.54 1305.11 1306.40 1306.86 1309.19
1313.04 1320.39 1321.29 1322.44 1337.56 1339.11
1341.98 1344.52 1346.74 1363.37 1364.88 1365.83
1369.00 1369.19 1373.03 1376.41 1378.99 1384.04
1389.91 1391.04 1393.63 1394.80 1395.01 1396.39
1399.68 1402.08 1402.46 1410.27 1421.41 1422.30
1424.33 1435.23 1436.18 1456.38 1459.81 1465.29
1466.44 1488.97 1492.69 1494.33 1495.16 1495.91
1499.09 1500.50 1501.39 1502.28 1502.80 1505.97
1508.10 1508.37 1508.59 1509.22 1511.73 1511.92
1512.75 1515.73 1518.01 1525.77 1527.90 1531.23
1533.29 1535.11 1535.95 1613.47 1613.98 1620.07
1631.77 1635.82 1638.31 1647.91 1652.34 1723.18
1770.82 3002.74 3003.42 3006.09 3007.33 3010.37
3015.84 3020.70 3024.60 3036.07 3038.86 3041.26
3047.63 3047.74 3049.21 3049.47 3052.11 3054.92
3057.20 3061.87 3062.05 3069.38 3093.53 3094.54
3096.09 3099.10 3106.20 3107.61 3111.67 3118.51
3119.47 3119.52 3124.07 3127.55 3127.68 3135.32
3137.75 3140.28 3146.55 3151.28 3151.81 3158.57
3165.06 3167.49 3168.77 3174.68 3178.33 3180.27
3182.32 3184.80 3188.04 3190.43 3200.17 3200.92
3212.62 3213.47 3220.91 3224.66 3227.67 3239.07
3239.98 3240.97 3253.15

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R3

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10.00 16.06 17.72 20.21 29.02 31.77
36.25 38.63 45.39 46.53 51.56 55.22
60.92 62.99 63.67 67.05 70.29 73.88
75.96 80.99 84.72 89.40 91.99 98.33
104.26 121.54 126.13 127.70 136.18 146.57
153.29 157.25 163.62 180.56 184.90 189.22
192.68 200.18 204.16 207.65 222.08 227.07
231.91 234.00 239.03 249.43 252.35 258.40
263.69 268.75 272.17 273.37 277.59 290.06
296.10 304.55 307.89 331.23 339.05 344.43
357.87 377.38 380.06 381.31 393.40 399.61
408.37 414.07 420.51 423.49 423.90 428.65
437.57 446.52 448.06 451.43 457.14 467.33
472.73 478.03 483.92 486.64 491.10 496.64
511.63 525.00 526.46 533.31 566.84 576.73
587.89 608.48 625.08 629.93 633.56 645.99
656.90 669.61 685.33 690.99 699.90 716.24
717.66 720.83 724.66 736.90 742.92 747.11
753.92 755.31 758.26 766.16 773.34 777.10
781.30 786.53 808.73 812.91 820.27 824.41
827.26 828.23 835.70 857.21 863.24 866.35
866.96 868.96 869.70 883.41 888.69 899.95
906.87 909.44 911.93 917.97 919.66 940.02
943.54 947.45 949.07 956.55 960.37 960.44
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1742.18 2933.07 3003.78 3005.55 3008.59 3013.88
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R3-TS$_{RE}$

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3204.04 3204.48 3207.52 3216.85 3227.48 3259.30

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R4

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401.01 406.04 408.47 410.21 415.74 425.73
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994.41 1010.01 1014.87 1017.12 1020.67 1022.51
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R5

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19.33 29.22 36.38 41.42 43.16 44.54
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3227.27 3230.13 3233.91

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R5'

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3171.51 3175.25 3185.69 3186.60 3197.20 3198.95
3206.90 3235.30 3248.17

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R5'-$_{TS}$

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172.71 188.63 194.22 200.76 204.77 222.11
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756.67 770.32 777.45 779.06 780.96 806.46
810.00 824.96 825.30 829.71 858.02 859.67
861.19 866.80 871.33 891.51 899.22 904.45
907.92 909.87 911.12 919.07 937.75 943.12
946.75 948.97 955.60 961.62 963.19 964.73
970.69 976.07 991.70 993.12 1010.02 1020.65
1023.86 1027.72 1037.30 1045.11 1049.37 1063.21
1066.52 1068.50 1077.81 1094.08 1096.80 1097.43
1097.81 1101.78 1107.33 1109.70 1131.88 1137.85
1150.12 1153.62 1157.22 1160.02 1166.86 1168.90
1190.27 1200.84 1204.43 1208.48 1209.64 1209.67
1211.25 1226.66 1227.85 1253.13 1271.04 1284.41
1295.79 1298.13 1298.68 1305.62 1309.43 1313.49
1315.83 1317.45 1325.10 1327.10 1338.26 1342.39
1342.61 1349.12 1369.08 1369.66 1375.34 1381.92
1382.59 1386.92 1390.28 1391.67 1392.26 1392.90
1396.16 1397.70 1401.34 1404.81 1422.81 1424.96
1433.20 1434.10 1465.19 1470.67 1492.20 1493.03
1495.21 1495.66 1496.60 1498.45 1499.14 1499.78
1501.07 1501.52 1504.09 1505.00 1506.32 1506.66
1508.03 1508.31 1509.53 1520.46 1522.52 1524.96
1527.29 1529.07 1616.36 1616.45 1623.03 1630.72
1638.77 1645.10 1999.13 3011.47 3013.08 3014.15
3017.33 3019.60 3020.52 3023.60 3025.51 3027.40
3031.89 3036.75 3041.25 3044.70 3049.18 3049.29
3050.20 3055.06 3065.82 3066.15 3067.34 3067.75
3070.57 3072.44 3072.64 3086.63 3087.60 3090.49
3095.05 3117.73 3123.10 3126.12 3129.24 3131.42
3138.49 3138.68 3142.03 3153.34 3159.71 3173.85
3174.46 3180.83 3184.92 3190.50 3193.78 3195.26
3204.30 3227.79 3240.68

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A1

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13.42 25.01 30.05 39.19 46.44 46.51
53.34 57.93 69.30 74.27 82.59 83.96
94.46 98.43 102.14 113.13 117.68 123.98
131.56 134.32 137.40 143.70 154.54 171.03
183.15 198.85 203.38 218.68 234.80 235.18
240.28 242.00 250.23 255.74 256.23 260.30
265.88 273.75 276.67 285.50 290.69 296.33
300.59 308.51 315.26 321.40 332.94 337.39
338.71 365.09 384.15 385.87 396.35 410.83
412.23 413.45 417.48 418.08 435.34 440.79
455.74 459.14 484.61 496.22 501.05 503.35
521.11 525.28 553.01 566.11 584.00 612.12
619.32 626.45 629.15 633.31 654.83 668.61
675.29 706.51 714.70 718.95 729.66 729.83
750.61 760.91 762.55 779.80 785.58 808.72
816.16 818.61 824.34 852.47 854.50 854.82
858.31 869.37 904.09 912.15 924.14 940.39
942.82 946.35 948.44 954.73 958.69 967.65
971.88 973.08 983.86 984.78 989.59 990.02
991.89 1001.39 1004.85 1006.07 1006.90 1013.55
1018.77 1039.97 1045.71 1049.33 1051.28 1053.26
1061.71 1065.89 1079.65 1085.22 1092.14 1095.64
1097.17 1104.79 1110.35 1123.33 1130.83 1146.13
1157.84 1162.02 1164.59 1176.70 1184.10 1191.24
1197.05 1212.67 1214.04 1214.36 1216.00 1216.97
1222.50 1227.13 1235.06 1237.73 1238.16 1241.90
1248.84 1253.61 1264.21 1278.64 1309.48 1331.19
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1368.63 1389.16 1396.78 1403.36 1412.26 1415.60
1418.86 1419.96 1429.34 1442.88 1450.91 1456.60
1460.61 1462.88 1476.83 1480.58 1492.96 1493.43
1493.91 1498.22 1500.07 1504.21 1505.41 1505.79
1506.35 1507.17 1510.52 1511.83 1512.38 1518.60
1521.23 1524.76 1527.37 1527.96 1534.99 1538.68
1543.49 1547.96 1561.34 1590.98 1615.66 1621.12
1623.20 1648.76 1659.78 1815.77 2911.10 2930.19
2965.36 2990.17 3022.75 3029.66 3033.92 3037.42
3038.44 3040.81 3042.68 3045.86 3048.78 3085.66
3104.15 3105.97 3107.24 3107.40 3110.12 3111.23
3115.35 3119.34 3120.78 3138.69 3138.84 3145.58
3146.64 3148.91 3155.31 3155.63 3159.17 3160.55
3161.47 3168.69 3175.01 3177.94 3184.51 3188.74
3194.96 3196.36 3204.62 3205.95 3213.91 3223.06
3223.80 3227.92 3248.13

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A1-TS$_{dis}$

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-213.39 14.16 17.72 20.28 28.23 31.57
39.76 42.68 44.05 58.59 61.72 70.92
75.95 83.02 99.41 101.27 107.44 112.72
123.07 127.94 132.71 145.51 149.84 152.37
164.81 171.38 202.39 207.74 218.37 218.84
224.91 227.21 240.46 247.69 252.35 254.39
258.31 263.11 265.31 274.81 280.11 282.07
295.52 305.40 312.62 318.67 333.45 336.75
341.44 354.25 359.20 388.51 394.32 398.52
407.49 411.94 415.27 425.71 435.91 439.79
454.46 456.45 480.75 484.55 495.18 499.63
523.31 530.81 539.58 550.60 582.89 583.85
607.33 620.07 627.67 632.74 634.66 653.52
664.09 668.74 681.14 709.83 714.51 731.24
744.66 750.27 752.07 773.73 784.19 796.73
813.46 817.54 818.31 820.74 836.45 849.00
852.15 863.07 884.56 909.54 913.33 938.32
944.95 946.72 951.68 956.01 960.09 960.61
968.73 971.44 974.57 982.90 985.87 989.08
991.67 993.27 997.73 1009.61 1015.85 1016.62
1019.44 1035.30 1040.97 1046.47 1050.76 1053.90
1063.46 1067.45 1080.82 1082.72 1086.73 1095.54
1101.69 1109.97 1117.94 1127.31 1130.73 1146.61
1149.14 1150.24 1173.92 1186.73 1190.62 1195.70
1205.64 1209.64 1213.36 1217.53 1220.92 1222.50
1224.32 1226.82 1234.66 1238.41 1242.78 1246.34
1249.70 1256.86 1281.89 1310.76 1324.24 1330.53
1335.97 1341.67 1352.66 1353.26 1367.96 1370.51
1371.19 1391.52 1394.30 1398.64 1404.98 1417.51
1419.69 1421.72 1426.63 1427.00 1450.86 1454.05
1458.33 1463.31 1472.45 1483.76 1489.31 1492.24
1495.00 1497.53 1497.96 1499.42 1501.83 1505.42
1505.93 1507.72 1511.34 1514.13 1514.53 1519.74
1521.34 1526.52 1529.13 1530.70 1536.01 1538.35
1541.84 1547.67 1560.46 1591.94 1617.22 1623.29
1634.97 1657.96 1662.52 1791.91 2992.32 3000.11
3013.98 3021.35 3032.68 3035.47 3037.94 3039.47
3043.67 3046.36 3047.60 3066.27 3070.74 3090.85
3101.28 3104.24 3110.01 3114.35 3121.61 3126.80
3128.77 3135.62 3144.54 3144.73 3146.61 3146.74
3149.09 3149.64 3154.05 3156.96 3159.48 3160.93
3164.46 3169.28 3169.64 3173.16 3177.82 3180.09
3190.62 3193.78 3202.39 3206.68 3219.09 3227.11
3227.86 3228.05 3232.30

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A2$_{dis}$

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2.87 24.00 30.23 37.23 42.69 48.95
52.22 55.15 60.60 67.63 73.91 78.79
89.28 98.17 103.67 106.64 108.20 117.39
123.01 124.55 133.34 140.56 149.85 162.10
163.46 180.11 189.03 204.40 208.59 214.11
217.85 228.32 233.17 236.42 242.89 252.44
253.33 266.43 270.38 272.27 281.27 288.02
301.79 304.46 306.77 318.58 324.97 327.63
332.15 360.86 383.45 387.97 389.00 402.21
406.77 414.95 421.03 422.36 432.62 437.25
444.58 449.85 456.19 474.68 480.48 496.02
504.08 513.69 527.33 551.14 578.03 600.01

608.80 612.73 626.10 629.91 632.35 654.67
655.76 660.08 675.53 710.13 710.43 733.13
733.84 748.15 772.94 782.33 784.00 787.87
816.49 818.68 820.20 823.26 835.40 848.59
860.82 877.25 878.59 925.25 933.12 942.98
946.46 949.76 952.86 958.20 961.25 963.66
972.57 978.09 978.93 982.59 996.73 997.86
1000.55 1003.78 1008.15 1011.18 1014.70 1018.94
1035.81 1042.88 1043.36 1051.25 1052.89 1053.33
1056.61 1074.02 1079.02 1081.27 1087.13 1090.44
1107.11 1115.28 1117.27 1123.49 1135.05 1146.22
1147.56 1150.01 1173.37 1192.56 1196.76 1203.14
1205.63 1211.60 1215.16 1217.45 1220.31 1221.25
1225.33 1226.47 1236.63 1239.90 1246.67 1249.20
1257.85 1281.99 1284.30 1317.79 1330.27 1333.09
1341.32 1344.68 1359.32 1363.46 1365.42 1369.31
1381.54 1391.98 1397.88 1409.02 1416.04 1420.37
1423.02 1426.08 1427.24 1449.84 1452.57 1458.65
1466.61 1471.36 1482.02 1491.85 1495.67 1496.18
1497.32 1499.89 1500.36 1503.28 1504.97 1506.25
1507.85 1510.30 1512.34 1513.79 1517.61 1522.81
1524.45 1526.01 1527.12 1528.60 1537.62 1539.58
1542.37 1558.93 1591.37 1618.24 1620.81 1622.44
1647.32 1660.79 1686.49 1708.65 2987.94 2995.40
2996.38 3023.82 3028.36 3030.89 3033.08 3033.51
3035.94 3040.53 3041.31 3063.03 3065.70 3085.68
3090.04 3105.89 3106.60 3110.41 3113.94 3118.06
3121.31 3130.72 3140.78 3141.90 3142.24 3143.97
3144.99 3146.61 3153.30 3155.22 3157.87 3162.07
3166.27 3168.25 3170.48 3176.39 3186.82 3187.18
3194.55 3200.70 3207.37 3219.45 3223.59 3223.71
3225.41 3230.34 3245.37

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A2-TS$_{dis}$

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-347.99 11.50 25.08 28.68 34.57 40.11
45.00 46.54 53.50 57.88 61.59 70.62
81.00 83.76 89.47 96.00 106.38 112.26
113.13 119.10 129.55 136.32 150.03 156.00
161.08 169.85 185.72 192.55 201.41 216.21
220.83 225.55 235.81 240.36 244.30 250.80
254.45 268.32 268.46 270.07 278.08 293.44
306.52 308.38 317.19 318.01 325.80 337.07
341.38 361.16 377.90 379.73 388.22 403.19
411.14 415.83 423.17 426.16 430.08 433.27
435.95 446.53 450.82 458.06 476.45 494.11
499.04 511.83 513.13 551.81 569.81 578.23
605.91 606.46 619.86 621.78 625.45 630.34
646.68 651.66 679.69 710.59 711.55 724.10
733.78 753.21 765.63 777.49 778.73 785.17
818.77 820.91 821.79 824.65 833.06 841.50
874.45 876.47 883.77 935.22 946.34 946.39
949.09 950.57 958.87 961.38 963.57 965.99
967.48 975.71 978.98 988.02 992.69 997.22
1004.45 1006.91 1008.41 1013.49 1013.93 1015.19
1017.34 1034.21 1043.11 1049.32 1051.73 1053.73
1056.64 1066.52 1072.32 1080.82 1085.85 1090.87
1108.97 1115.08 1117.05 1117.75 1134.46 1141.91
1145.83 1150.98 1170.31 1190.63 1194.67 1196.83
1202.87 1212.63 1215.72 1217.12 1218.39 1221.45
1227.00 1231.21 1237.75 1239.81 1248.53 1251.84
1259.14 1280.25 1281.61 1321.93 1330.33 1332.12
1342.30 1345.69 1359.36 1366.90 1368.61 1369.24
1374.72 1387.89 1393.93 1407.91 1414.34 1416.91
1420.23 1423.75 1423.86 1447.57 1449.90 1454.77
1467.72 1469.45 1483.00 1492.85 1494.59 1496.53
1496.90 1498.30 1501.67 1503.02 1504.39 1508.15
1509.59 1510.19 1511.47 1513.93 1518.90 1519.08
1525.68 1526.34 1527.38 1530.40 1537.03 1540.74
1543.52 1556.41 1591.52 1614.49 1623.78 1624.77
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2995.22 3026.65 3026.72 3028.21 3029.62 3032.50
3036.34 3040.74 3044.97 3065.20 3067.84 3089.29
3095.02 3095.64 3098.04 3103.37 3110.10 3124.44
3125.79 3131.32 3131.56 3142.29 3143.86 3144.42
3146.06 3150.35 3152.76 3153.02 3166.34 3170.85
3175.32 3176.62 3181.61 3189.82 3190.93 3193.29
3200.94 3211.04 3213.35 3215.35 3229.63 3231.02
3233.00 3234.65 3255.16

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A1'

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5.53 10.69 20.09 21.46 29.39 43.56
46.04 55.22 58.35 60.36 71.00 74.32
81.53 82.34 87.38 94.89 107.95 113.38
117.86 122.25 127.75 145.82 159.59 167.72
180.71 182.41 185.74 198.84 211.33 221.78
235.17 239.55 243.43 252.29 255.57 257.59
265.64 272.39 273.03 283.45 289.42 294.44
295.02 311.36 312.70 316.95 324.08 335.14
362.97 367.52 374.86 392.01 396.55 402.49
408.04 415.14 416.60 423.30 433.75 437.74
458.41 476.29 479.85 490.68 496.61 502.32
526.25 538.78 548.25 550.42 581.26 607.05
618.15 625.30 632.47 633.01 656.98 671.69
672.85 706.78 708.40 715.37 729.29 732.07
749.16 764.25 767.82 782.92 796.74 811.53
814.00 815.63 825.41 828.13 847.19 848.80
862.84 866.13 906.61 908.40 921.74 935.75
943.99 949.11 950.74 954.79 959.04 965.38
965.84 968.48 976.12 977.67 979.88 990.14
991.97 994.61 1002.28 1007.40 1013.20 1015.81
1018.37 1041.23 1044.44 1046.00 1051.11 1053.49
1065.19 1066.53 1079.06 1084.65 1088.68 1089.19
1098.36 1099.89 1116.40 1118.71 1130.25 1138.34
1153.22 1154.73 1155.45 1178.21 1181.18 1192.26
1194.68 1208.00 1209.97 1212.37 1214.00 1216.09
1221.75 1225.87 1236.58 1237.95 1241.24 1251.84
1257.18 1263.78 1269.32 1277.82 1310.64 1321.24
1336.37 1337.30 1343.92 1351.50 1358.36 1369.21
1371.53 1376.96 1396.45 1402.29 1410.77 1414.76
1421.09 1423.89 1428.03 1430.21 1451.18 1456.54
1462.07 1463.93 1475.35 1487.16 1490.40 1491.78
1494.82 1497.98 1499.78 1502.80 1503.11 1503.88
1504.94 1505.68 1506.97 1511.41 1512.24 1517.07
1519.53 1523.01 1531.13 1532.04 1536.42 1537.94
1545.78 1552.60 1564.25 1591.82 1616.25 1622.98
1635.36 1659.01 1664.48 1851.66 2814.24 2951.69
2966.28 3020.97 3022.33 3023.63 3034.76 3037.58
3042.09 3043.92 3044.12 3047.22 3055.26 3086.58
3107.42 3110.04 3112.04 3114.64 3116.89 3122.64
3127.63 3135.72 3137.64 3139.72 3141.08 3143.37
3144.29 3147.29 3148.34 3151.37 3152.23 3157.65
3158.48 3159.62 3169.08 3169.30 3179.15 3187.26
3187.96 3193.57 3207.18 3214.82 3217.95 3219.95
3220.58 3235.21 3244.04

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A1'-TS$_{prox}$

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79.94 91.76 93.50 96.24 98.51 105.32
114.99 122.24 124.31 124.88 142.70 146.87
160.31 174.88 182.26 207.96 216.61 225.40
227.22 236.57 240.83 244.52 247.84 252.64
259.72 261.67 265.70 277.73 281.17 283.55
305.58 309.36 312.74 314.30 324.00 328.12
335.98 359.13 360.67 383.65 393.44 395.60
410.55 414.88 416.37 418.78 430.28 437.97
455.24 467.92 477.67 482.05 485.81 497.92

503.15 520.80 539.85 548.00 562.76 585.53
612.41 626.48 627.64 633.60 637.04 655.84
663.64 670.54 717.03 718.07 724.52 729.56
738.62 750.87 758.03 785.62 786.59 798.61
813.54 817.51 818.44 823.65 836.69 854.20
859.63 864.10 866.83 909.21 913.82 934.19
942.97 945.89 946.16 949.48 954.89 958.92
972.34 973.05 974.80 978.27 981.08 984.80
989.13 994.81 998.81 1005.31 1009.12 1016.51
1018.11 1043.26 1044.92 1045.80 1050.89 1052.93
1060.02 1063.97 1081.27 1087.26 1087.76 1089.50
1098.79 1107.58 1114.68 1125.06 1126.35 1135.19
1148.35 1148.88 1154.18 1175.53 1193.12 1194.02
1206.68 1207.87 1211.91 1215.15 1216.53 1218.38
1222.05 1226.86 1235.07 1236.06 1241.85 1249.43
1250.09 1266.29 1283.84 1309.17 1318.12 1333.45
1335.79 1336.94 1351.93 1354.02 1363.55 1365.90
1370.97 1376.02 1395.96 1396.83 1412.76 1416.02
1419.02 1420.44 1429.07 1451.23 1454.55 1460.28
1464.03 1470.21 1473.39 1484.26 1491.99 1492.42
1494.06 1496.88 1499.66 1500.24 1503.67 1504.76
1507.05 1507.58 1510.02 1511.33 1511.91 1518.47
1521.89 1525.57 1527.17 1528.32 1533.40 1539.48
1542.14 1543.84 1560.76 1592.54 1617.26 1623.29
1632.60 1656.09 1661.96 1828.76 2974.23 2993.42
3004.65 3029.87 3034.66 3036.81 3038.57 3039.42
3041.89 3042.78 3046.53 3062.58 3064.94 3085.41
3105.65 3106.52 3109.33 3111.27 3118.29 3119.03
3122.46 3132.21 3133.80 3138.35 3143.53 3145.15
3151.40 3152.98 3153.44 3155.42 3162.85 3163.83
3168.55 3171.90 3173.04 3173.78 3178.54 3184.09
3189.26 3194.92 3197.61 3204.08 3211.05 3217.45
3223.28 3224.64 3237.21

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$A2_{prox}$

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11.71 20.25 25.00 37.12 41.92 49.35
54.15 58.69 67.05 71.13 78.29 84.46
91.03 96.88 104.76 111.30 114.19 117.94
123.87 130.48 134.96 143.63 166.87 172.22
180.24 189.53 196.01 207.59 219.53 222.84
226.90 233.07 234.62 247.48 256.11 261.53
264.34 273.33 280.97 287.58 293.49 301.09
304.16 311.49 313.84 319.25 331.46 351.42
363.80 366.50 381.82 389.40 391.21 394.73
409.96 414.14 417.15 425.65 435.15 437.08
442.45 449.18 479.14 485.90 494.09 499.35
500.95 514.46 517.08 547.56 576.97 596.14
612.72 626.37 629.12 630.06 652.13 653.84
669.88 686.48 698.07 716.42 720.35 732.95
749.11 751.20 760.96 773.08 780.21 811.61
815.45 816.53 818.84 820.08 828.13 851.62
856.13 865.70 871.49 905.50 908.26 934.16
942.21 947.65 950.46 955.31 959.86 964.94
966.77 968.27 971.05 974.06 977.93 985.70
990.63 999.57 1009.03 1013.36 1017.74 1019.75
1020.53 1041.64 1044.52 1048.32 1051.01 1055.75
1058.66 1060.99 1065.31 1077.60 1088.11 1093.91
1096.09 1109.22 1125.27 1126.12 1128.28 1157.09
1158.19 1160.22 1164.16 1168.35 1177.47 1190.89
1198.21 1207.89 1211.87 1212.59 1213.05 1220.43
1221.19 1228.17 1235.49 1238.29 1239.74 1247.01
1247.57 1266.47 1274.77 1306.98 1316.06 1331.27
1345.89 1348.08 1353.14 1360.09 1365.55 1371.19
1372.70 1395.24 1400.59 1408.27 1414.67 1417.04
1421.75 1423.48 1448.12 1454.23 1457.40 1464.80
1475.91 1485.25 1487.79 1491.54 1495.10 1497.86
1498.31 1500.76 1503.44 1505.82 1506.05 1506.44
1506.47 1507.90 1509.96 1511.79 1516.43 1521.91
1528.61 1529.25 1533.25 1534.83 1540.34 1545.67
1548.40 1561.07 1587.42 1615.13 1618.59 1622.69
1645.36 1660.67 1665.33 1707.39 2917.00 2925.52
2977.82 2979.91 3032.51 3034.67 3035.69 3036.99
3041.07 3041.55 3042.91 3045.31 3064.07 3085.28
3102.23 3103.22 3106.64 3109.90 3113.79 3114.13
3119.67 3125.76 3126.95 3138.16 3141.26 3144.24
3144.48 3156.84 3160.71 3162.04 3176.11 3178.37
3180.54 3188.11 3188.19 3192.76 3194.52 3194.81
3199.04 3200.41 3203.30 3212.27 3222.75 3223.89
3232.89 3234.59 3248.12

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C1

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13.08 16.08 30.25 36.83 38.45 50.79
54.09 57.33 60.27 66.71 67.93 70.58
72.12 77.84 86.92 91.36 101.77 106.15
117.00 131.49 151.25 153.61 156.36 163.78
176.63 186.85 193.37 201.80 210.44 222.93
229.44 241.13 244.86 256.08 270.32 273.69
275.48 298.92 317.38 322.33 331.09 335.81
338.49 342.07 344.27 358.01 381.62 382.29
403.18 411.26 412.25 412.28 415.21 417.28
421.54 422.89 435.59 440.50 453.63 459.62
463.75 466.20 479.69 489.96 496.42 500.16
513.33 526.87 541.99 617.25 625.28 632.11
658.28 658.63 660.29 662.47 672.80 675.71
683.43 688.03 712.25 714.50 718.84 726.09
736.02 746.75 752.78 761.68 769.29 773.17
774.50 786.12 796.51 818.69 820.03 820.59
828.04 829.88 830.04 833.97 852.94 859.89
863.83 868.60 895.14 901.60 902.68 904.62
905.23 907.35 908.23 911.65 916.83 918.11
923.23 936.00 940.10 947.71 952.49 954.87
969.83 970.43 975.26 977.04 980.62 984.02
985.68 986.53 988.84 989.20 992.80 995.24
1006.80 1014.97 1016.94 1030.92 1040.72 1051.50
1052.49 1053.71 1056.66 1059.28 1059.66 1061.37
1061.78 1063.27 1064.24 1072.79 1084.36 1087.18
1093.90 1094.96 1096.39 1105.93 1111.61 1120.93
1128.78 1129.22 1131.85 1132.76 1133.80 1136.15
1137.41 1144.37 1149.12 1150.29 1153.00 1162.98
1166.91 1183.45 1190.58 1194.60 1209.97 1213.63
1214.02 1217.62 1219.58 1221.67 1234.10 1241.82
1249.32 1261.71 1263.71 1279.06 1287.85 1297.05
1299.69 1303.09 1312.33 1320.58 1321.50 1324.60
1326.48 1331.40 1331.92 1334.35 1337.75 1341.26
1341.91 1346.10 1346.37 1348.30 1352.79 1354.01
1357.78 1358.01 1358.97 1361.37 1363.61 1364.59
1366.69 1369.92 1385.19 1386.75 1388.10 1389.82
1390.42 1394.59 1402.71 1406.47 1407.24 1410.68
1412.42 1414.55 1415.39 1417.16 1429.19 1464.38
1471.05 1471.39 1487.53 1490.54 1495.37 1496.01
1496.12 1500.95 1503.94 1505.41 1506.38 1506.75
1509.15 1509.63 1511.28 1512.34 1512.44 1513.73
1517.49 1522.67 1523.24 1533.87 1536.31 1544.26
1616.99 1620.79 1635.84 1658.10 1750.65 3013.77
3015.01 3016.91 3017.51 3018.58 3020.11 3023.89
3028.19 3030.06 3032.85 3033.11 3035.21 3036.74
3040.71 3041.79 3043.60 3045.59 3049.39 3050.01
3051.08 3051.49 3055.91 3058.08 3058.92 3059.83
3060.26 3060.82 3065.59 3067.86 3069.57 3085.18
3089.28 3090.44 3099.98 3102.73 3107.41 3110.48
3112.50 3116.07 3119.29 3121.01 3127.08 3140.50
3141.98 3151.72 3151.77 3155.86 3160.86 3161.46
3168.56 3174.27 3176.28 3178.61 3187.15 3193.86
3193.92 3200.86 3225.25

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$C1\text{-}TS_{dis}$

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-209.01 13.44 18.23 31.98 35.80 44.80

48.07 50.93 54.88 58.45 64.50 66.16
70.30 73.55 77.29 83.18 91.30 99.21
102.83 116.41 137.34 152.55 155.80 162.94
174.15 182.13 188.71 203.18 207.29 216.46
219.83 228.68 249.95 254.47 261.43 269.32
272.14 279.05 319.46 321.70 329.97 335.69
339.23 341.34 345.07 347.97 359.10 380.34
397.72 410.79 411.98 412.91 414.45 416.34
420.54 434.84 436.67 441.71 454.88 460.28
463.73 467.98 479.67 482.87 496.00 496.93
513.03 537.30 545.29 555.54 626.32 628.27
631.05 657.74 658.90 660.58 663.02 668.60
670.66 674.63 683.15 687.99 711.63 715.88
729.26 735.34 749.90 754.35 755.73 771.99
774.47 776.94 790.83 796.73 816.88 819.07
819.18 820.68 826.48 829.40 832.45 851.55
852.92 864.27 886.40 898.07 902.19 904.24
904.85 907.14 909.81 910.47 912.81 917.48
922.46 938.36 940.22 946.89 951.85 952.78
961.41 966.32 978.88 980.42 983.59 984.04
985.19 986.93 987.42 988.84 990.82 999.51
1011.40 1016.52 1020.21 1025.38 1035.46 1042.88
1051.52 1054.27 1055.82 1058.51 1058.97 1060.14
1060.56 1063.04 1064.12 1066.67 1077.58 1087.64
1092.69 1094.40 1099.32 1104.55 1116.95 1121.43
1130.27 1130.69 1132.14 1132.77 1134.10 1136.43
1137.20 1149.01 1149.65 1149.88 1162.92 1164.19
1184.88 1191.95 1195.77 1213.76 1215.27 1216.36
1217.82 1220.00 1220.52 1223.17 1242.37 1245.11
1247.54 1257.63 1263.33 1287.08 1295.19 1299.19
1301.49 1308.82 1315.17 1319.08 1323.11 1324.82
1325.30 1329.22 1330.53 1333.60 1334.57 1339.49
1341.09 1345.20 1345.73 1352.01 1353.21 1354.18
1357.60 1358.06 1358.24 1361.58 1362.06 1365.72
1367.19 1368.30 1382.45 1384.96 1386.62 1387.68
1389.71 1398.51 1401.45 1405.44 1405.88 1407.88
1408.56 1411.40 1412.34 1413.63 1422.41 1428.45
1464.41 1471.02 1483.81 1488.94 1492.89 1495.60
1496.24 1500.58 1502.12 1505.46 1507.64 1507.78
1509.84 1510.60 1511.01 1511.91 1512.92 1514.46
1515.66 1521.77 1522.05 1534.37 1536.80 1543.81
1617.73 1623.60 1635.02 1658.07 1776.64 3013.62
3016.31 3018.02 3018.77 3018.91 3019.33 3024.39
3031.75 3032.22 3035.87 3036.89 3037.95 3042.48
3042.85 3043.70 3044.01 3045.79 3046.17 3050.34
3051.42 3053.57 3055.08 3056.62 3060.01 3061.13
3061.18 3065.02 3066.23 3069.22 3073.31 3085.49
3092.72 3093.49 3094.36 3095.32 3102.42 3109.21
3111.29 3112.04 3113.79 3121.34 3126.80 3131.89
3141.37 3143.02 3148.95 3156.60 3159.37 3164.82
3170.43 3179.81 3180.52 3189.63 3190.41 3198.62
3199.75 3220.60 3226.45

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$C2_{dis}$

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19.82 28.94 35.43 35.53 44.46 48.97
55.18 58.81 65.01 65.88 74.78 79.00
85.14 90.61 103.28 104.99 110.81 117.97
120.92 132.14 143.56 152.05 164.98 168.53
175.58 178.37 186.27 199.12 199.62 210.69
214.97 224.19 245.44 257.54 273.11 280.26
288.59 300.48 305.11 309.45 319.63 322.36
325.79 342.16 344.34 357.37 383.03 388.91
406.70 410.37 412.67 413.14 416.75 417.40
423.35 427.35 438.76 440.59 449.53 451.83
458.21 460.25 465.58 482.68 483.36 499.75
504.00 521.26 525.37 606.13 610.81 623.83
633.04 652.80 656.22 657.01 658.55 661.74
663.46 664.73 681.44 687.08 689.69 714.54
716.35 735.83 750.01 750.68 768.52 769.84
775.14 784.56 786.11 792.03 816.20 819.02
819.40 825.65 826.08 831.69 837.89 846.54
866.39 878.33 883.00 888.97 898.18 902.50
905.73 908.58 909.01 911.30 918.74 925.41
933.40 936.66 947.08 948.71 953.62 964.20
966.52 980.65 983.49 984.23 986.03 987.35
989.38 992.40 996.88 1007.47 1008.60 1010.17
1014.87 1015.49 1018.58 1036.24 1041.38 1050.59
1052.91 1053.52 1057.47 1058.36 1059.58 1061.92
1062.21 1065.19 1065.68 1076.28 1081.20 1082.34
1085.90 1091.57 1100.80 1101.22 1115.81 1119.60
1129.51 1132.09 1132.24 1134.28 1135.36 1136.30
1139.26 1145.41 1149.49 1154.35 1159.69 1164.61
1192.25 1196.27 1198.65 1213.47 1215.25 1215.86
1218.18 1219.02 1220.31 1220.94 1227.27 1243.37
1249.15 1260.32 1281.67 1284.38 1285.61 1296.14
1299.54 1299.87 1315.36 1322.61 1325.66 1327.59
1329.34 1329.84 1330.72 1332.88 1334.54 1337.34
1341.55 1342.73 1345.31 1346.03 1354.03 1356.61
1357.18 1357.91 1358.91 1360.48 1360.93 1362.74
1366.02 1380.63 1384.38 1385.88 1386.79 1389.38
1395.16 1399.78 1402.87 1405.00 1407.75 1408.49
1409.13 1412.11 1413.42 1425.63 1434.80 1466.17
1473.18 1484.91 1486.82 1491.61 1493.37 1495.08
1496.59 1497.70 1505.74 1506.66 1508.40 1509.31
1509.93 1510.22 1511.97 1512.47 1513.45 1513.57
1515.34 1524.43 1530.36 1533.73 1537.28 1617.56
1618.27 1629.00 1652.81 1682.74 1705.93 2857.69
2990.92 3014.90 3015.57 3016.45 3016.73 3022.02
3022.76 3024.55 3028.79 3033.10 3034.45 3035.13
3036.53 3041.20 3041.62 3042.11 3042.36 3044.60
3047.82 3049.62 3051.51 3056.25 3056.96 3057.47
3057.61 3061.47 3061.75 3062.76 3074.21 3076.00
3078.56 3081.59 3086.01 3086.02 3089.10 3101.41
3106.53 3110.14 3114.30 3118.95 3135.69 3141.64
3149.75 3151.56 3160.51 3167.66 3168.53 3175.27
3182.65 3186.78 3188.40 3195.95 3199.83 3204.56
3225.57 3230.62 3252.02

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$C2\text{-}TS_{dis}$

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-353.22 17.33 28.26 37.40 38.97 44.32
49.38 51.09 58.90 62.16 64.31 72.68
74.54 84.41 89.29 101.06 106.43 111.13
112.95 128.32 138.36 152.09 156.72 169.97
173.16 178.04 186.31 188.83 195.18 203.84
207.43 221.18 224.58 229.96 231.26 268.06
272.70 279.52 306.80 318.88 325.92 327.06
336.54 340.69 343.16 358.40 374.44 381.02
400.63 408.06 409.63 413.81 419.21 419.93
427.12 432.23 434.28 435.38 446.20 452.09
460.28 461.69 463.82 473.48 474.30 495.64
503.25 508.43 513.39 569.74 606.60 622.96
630.11 634.82 654.68 656.71 658.45 660.02
661.89 673.11 678.91 685.60 710.02 711.06
718.54 734.04 747.92 755.00 762.70 765.32
769.63 777.67 780.83 788.74 816.71 817.40
819.10 822.24 823.19 831.43 835.59 842.52
873.52 875.75 881.81 901.03 903.68 904.31
908.63 909.67 910.50 914.52 922.43 932.10
938.50 944.06 945.82 949.87 951.21 960.51
961.01 981.23 983.91 984.21 987.68 989.20
990.14 994.70 1000.18 1000.51 1005.86 1007.47
1009.65 1012.97 1015.25 1026.28 1036.03 1048.23
1051.98 1054.37 1057.07 1057.87 1058.79 1060.70
1061.73 1063.20 1065.29 1066.23 1070.69 1080.49
1087.55 1090.07 1107.86 1116.23 1117.21 1118.96
1130.87 1131.22 1133.32 1134.55 1135.00 1135.28
1136.44 1142.09 1148.73 1149.72 1160.62 1163.48
1191.90 1193.57 1197.65 1212.91 1214.86 1217.64

1218.34 1218.87 1219.76 1226.33 1242.22 1249.69
1255.39 1259.74 1278.92 1285.66 1295.10 1296.81
1301.26 1321.41 1323.88 1325.44 1326.09 1328.50
1329.44 1330.32 1332.57 1335.58 1340.10 1341.29
1343.04 1344.97 1345.99 1353.64 1355.28 1357.79
1357.87 1357.96 1358.24 1359.16 1364.75 1366.59
1368.10 1375.80 1384.41 1386.19 1387.12 1388.62
1394.03 1400.30 1404.47 1407.36 1408.00 1408.24
1408.89 1410.72 1412.27 1422.84 1429.61 1467.68
1475.68 1480.58 1494.23 1494.65 1497.05 1498.17
1499.81 1506.38 1506.45 1508.69 1509.89 1510.99
1511.38 1511.73 1512.87 1513.21 1514.25 1514.51
1518.08 1523.13 1523.41 1536.16 1539.23 1613.35
1619.52 1623.24 1645.14 1664.88 1690.87 2981.40
3012.18 3014.48 3014.66 3016.79 3018.70 3019.60
3021.22 3023.17 3026.77 3029.82 3032.85 3033.86
3035.54 3036.57 3037.54 3040.41 3042.38 3044.23
3044.85 3048.45 3054.36 3056.30 3057.18 3057.89
3059.57 3060.70 3062.03 3063.36 3069.45 3071.50
3080.25 3081.19 3087.92 3089.24 3100.72 3100.90
3105.31 3105.86 3106.71 3108.99 3114.77 3131.44
3143.62 3152.06 3153.22 3166.37 3169.59 3174.44
3177.93 3189.40 3194.80 3202.34 3212.41 3218.90
3227.85 3233.03 3250.16

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C1'

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15.28 20.11 27.75 34.32 40.62 46.97
50.89 52.31 54.89 60.33 63.04 64.17
70.26 78.68 83.41 85.82 94.92 98.18
99.68 106.04 118.48 155.01 157.46 168.82
176.43 183.47 186.16 194.36 208.74 222.04
225.82 233.70 245.69 248.00 258.40 271.63
272.26 294.50 314.42 318.43 331.23 335.31
336.07 341.99 344.56 357.74 376.95 379.53
408.03 409.00 412.73 414.12 416.55 419.75
420.96 433.93 440.56 452.78 458.58 462.93
466.17 476.80 479.28 485.24 496.87 497.61
512.17 538.40 544.74 618.19 624.91 633.55
656.98 658.67 659.28 663.37 669.19 673.03
681.66 686.83 707.76 713.14 718.11 729.78
732.69 749.10 753.10 764.08 767.40 770.02
774.12 788.88 796.35 817.62 818.49 819.72
825.77 826.40 826.86 831.26 848.02 855.39
865.32 868.62 893.82 902.73 904.37 905.26
908.18 909.21 910.00 911.40 917.81 921.79
923.04 938.50 940.10 946.38 951.19 953.58
965.86 970.24 976.16 979.44 981.19 982.57
985.05 985.59 988.24 990.36 993.82 1002.09
1004.11 1013.11 1017.07 1028.90 1039.45 1045.02
1051.07 1052.46 1055.68 1057.00 1057.70 1060.06
1060.63 1061.39 1064.06 1066.97 1079.15 1083.15
1090.26 1092.96 1097.82 1098.06 1115.95 1121.07
1128.85 1131.65 1132.23 1132.52 1134.34 1136.00
1136.80 1139.63 1149.20 1150.03 1154.92 1163.96
1165.55 1177.74 1193.04 1194.81 1211.31 1213.67
1217.64 1219.69 1221.56 1222.29 1237.76 1246.53
1250.48 1262.46 1263.71 1268.86 1287.82 1295.92
1299.85 1302.19 1308.46 1319.37 1320.75 1323.72
1325.08 1330.24 1330.64 1333.93 1335.38 1337.64
1340.47 1344.45 1345.44 1345.95 1349.21 1353.75
1357.23 1357.67 1358.11 1358.26 1360.50 1363.74
1368.34 1369.54 1376.87 1384.50 1386.15 1387.43
1389.70 1396.57 1401.71 1405.02 1407.35 1410.83
1411.06 1411.42 1413.16 1415.01 1428.12 1429.77
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1509.40 1510.00 1511.52 1511.93 1512.31 1513.18
1516.11 1522.21 1523.00 1533.57 1538.30 1545.66
1614.44 1620.20 1635.29 1658.66 1851.53 2796.33
3015.02 3015.99 3017.86 3020.18 3020.41 3021.25
3025.79 3026.43 3030.72 3032.88 3033.54 3036.40
3039.36 3042.71 3043.74 3044.76 3047.58 3049.45
3051.80 3053.72 3056.28 3057.58 3061.70 3061.83
3062.74 3063.31 3065.22 3067.77 3077.94 3086.50
3087.61 3089.58 3098.12 3102.85 3103.69 3104.90
3106.32 3110.87 3118.45 3121.88 3125.67 3134.25
3134.97 3146.01 3148.13 3150.98 3157.42 3160.60
3165.46 3171.16 3175.79 3179.14 3184.50 3194.48
3196.41 3209.41 3219.67

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C1'-TS$_{prox}$

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-233.80 11.06 22.04 31.22 33.27 42.93
48.38 53.47 56.40 60.21 63.24 63.89
68.23 76.74 78.50 91.04 94.75 99.81
105.81 107.58 124.62 133.19 154.31 160.92
174.88 181.78 183.62 188.19 204.55 220.06
225.64 230.31 241.13 245.93 253.07 267.01
272.20 284.23 310.75 317.79 330.82 332.22
334.47 341.89 343.24 359.14 363.65 380.21
394.32 409.72 412.05 414.22 415.36 416.07
421.00 434.81 437.95 453.48 459.13 462.93
465.77 476.24 477.79 481.53 495.46 498.53
508.14 513.30 538.25 567.73 627.14 627.22
636.91 657.97 658.29 659.93 661.06 664.81
669.00 683.10 687.87 715.68 716.65 724.55
729.91 738.50 748.57 752.73 757.02 771.58
773.34 787.91 789.37 799.03 818.31 818.74
819.37 822.42 826.77 828.13 832.73 855.35
859.34 864.19 867.87 897.50 901.36 904.09
904.47 909.12 910.89 911.37 913.06 914.06
922.75 936.59 939.52 946.73 947.54 951.48
953.33 972.91 976.87 980.47 983.06 983.63
984.36 986.51 988.11 990.71 993.35 1000.58
1005.13 1007.71 1016.83 1028.32 1040.81 1044.16
1051.50 1053.16 1055.30 1058.09 1058.31 1059.60
1060.54 1061.93 1063.84 1064.76 1081.65 1085.91
1089.91 1092.93 1097.37 1104.79 1116.74 1120.82
1124.32 1129.98 1131.68 1132.90 1132.96 1133.91
1136.15 1137.22 1149.28 1151.30 1153.11 1163.01
1164.84 1191.46 1195.63 1207.50 1213.93 1215.75
1217.76 1219.82 1221.16 1221.97 1235.06 1246.74
1247.27 1262.50 1265.47 1287.03 1296.08 1298.62
1302.07 1306.78 1319.70 1322.00 1323.78 1326.02
1329.09 1329.47 1331.18 1333.66 1335.34 1336.71
1340.78 1345.37 1345.81 1350.21 1352.38 1353.85
1357.67 1358.08 1358.66 1360.94 1361.28 1363.66
1366.96 1367.44 1377.17 1384.79 1386.45 1387.15
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1411.04 1411.72 1412.55 1413.44 1429.17 1462.21
1471.08 1471.23 1484.95 1491.79 1492.34 1494.82
1496.74 1499.69 1503.67 1505.30 1507.11 1507.23
1509.10 1510.95 1511.14 1511.38 1512.34 1512.75
1516.35 1518.43 1522.72 1533.39 1535.14 1539.49
1614.52 1621.43 1632.32 1656.04 1831.48 2978.71
3015.85 3017.65 3018.09 3018.42 3020.37 3023.23
3024.44 3027.10 3031.59 3032.74 3034.67 3037.78
3039.97 3041.77 3044.16 3045.72 3047.57 3048.77
3051.08 3052.16 3058.69 3059.11 3059.29 3060.48
3063.28 3063.54 3067.73 3068.82 3070.53 3084.91
3086.36 3088.29 3091.42 3103.10 3106.86 3109.33
3110.61 3110.96 3117.82 3119.66 3121.18 3133.75
3134.17 3150.82 3151.15 3157.93 3165.69 3165.93
3171.32 3171.67 3175.65 3176.64 3184.26 3196.14
3196.95 3210.48 3219.64

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C2$_{prox}$

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16.08 23.35 26.49 38.12 44.22 45.36

52.30 60.08 64.58 65.91 68.55 75.11
81.49 83.84 89.77 93.66 111.37 114.48
121.53 126.57 132.29 153.64 166.03 168.55
178.03 179.20 184.11 186.48 193.53 211.92
220.43 223.88 236.95 241.14 254.10 271.08
276.37 291.94 310.55 315.46 318.76 336.69
340.49 344.14 355.85 361.68 374.90 378.78
390.65 404.34 411.40 412.11 415.12 415.88
420.62 425.22 429.69 431.27 449.03 457.55
462.95 469.25 480.53 486.61 490.68 496.34
498.57 502.09 514.26 605.82 622.00 626.96
646.67 654.94 656.25 657.33 664.02 664.83
670.27 680.67 684.40 696.25 714.45 718.08
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904.89 907.42 908.57 911.50 913.03 916.88
919.33 932.98 938.25 947.16 950.13 952.52
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