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Supporting Information

A Striking Case of Enantioinversion in Gold Catalysis and Its Probable Origins

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NMR Studies

NMR spectra were recorded on an Avance III 500 spectrometer (499.89MHz) equipped with a $BBFO_{plus}$ $^{1}H/BB$(incl. ^{19}F) probehead and Z-gradient from Bruker Biospin GmbH. All NMR data were processed and analysed with Topspin 3.2 (Bruker) and presented with MNova 10 (Mestrelab Research).

Sample Preparation. The NMR sample was prepared by mixing methoxy-allene **2-OMe** (10 mg) with complex **1** (39 mg, 1.0 eq.) and $AgBF_4$ salt (6.7 mg, 1.0 eq.) in anhydrous CD_2Cl_2 (0.7 mL). The sample was stable in a flame-sealed 5mm NMR tube although traces of the *E*- and Z-1,3- diene isomers of **2-OMe** were detected after several days.

1D NMR signals at ambient temperatures were too broad for interpretation. By increasing or lowering the temperature, signals became sharper, indicating the presence of exchange (see Figure **S1**).

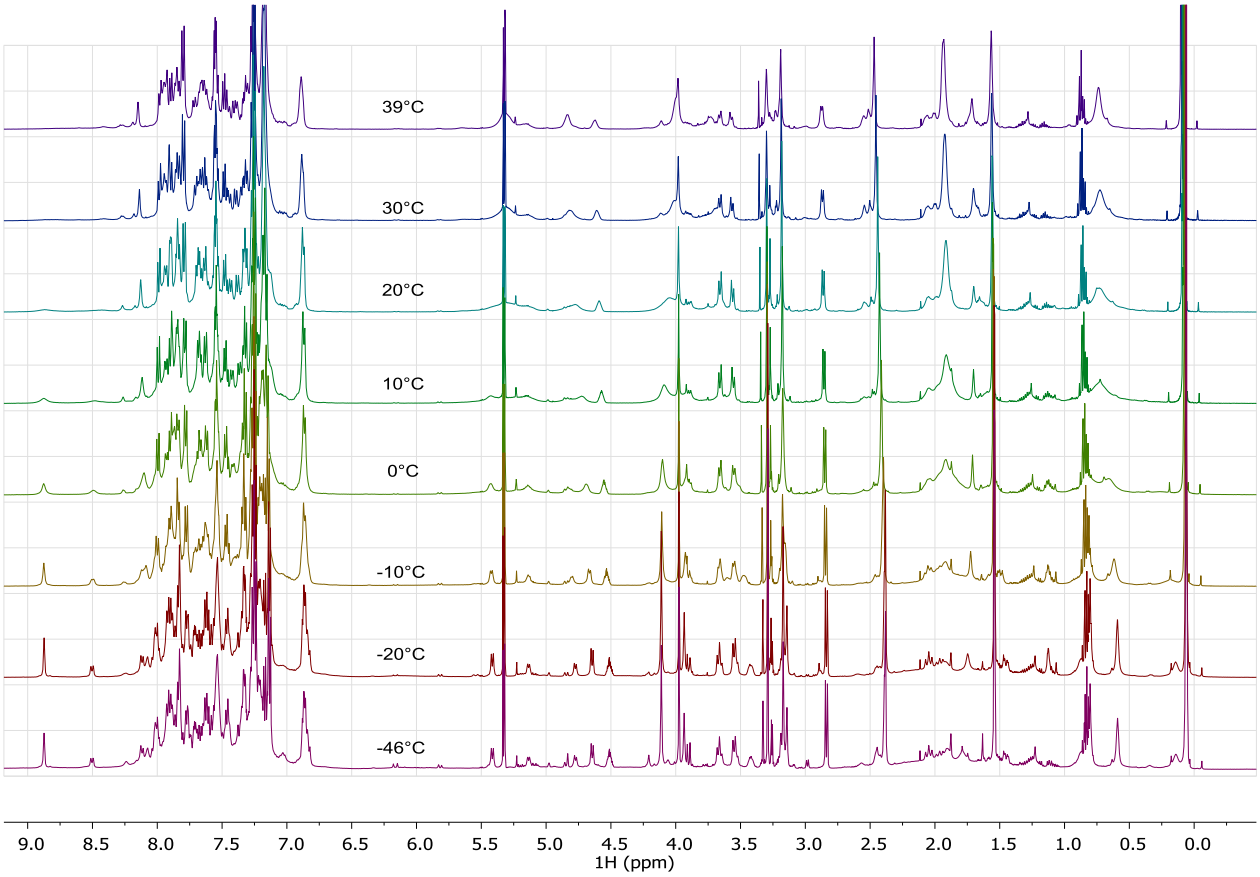
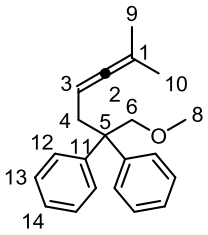


Figure S1. Variable temperature series of 1D ^{1}H NMR spectra of 2-OMe + **1** + $AgBF_4$ in CD_2Cl_2.

^{1}H and ^{13}C assignments were thus obtained at -46°C from standard 1D experiments as well as 2D correlation experiments. The correlation experiments included ^{1}H, ^{1}H DQF-COSY, ^{1}H, ^{1}H-TOCSY, ^{1}H,^{1}H-NOESY, ^{1}H,^{13}C-HSQC, ^{1}H,^{13}C-HMBC. The ^{1}H and ^{13}C spectra were referenced by setting the residual

solvent signal at their known chemical shift relative to TMS. Analysis of the spectra indicated that the substrate was slowly exchanging between its free and complexed forms, which were present in approximate ratio of ≈ 2:1. Furthermore, the complex exists in two exchanging conformations, in ratio of ≈ 3:2.



Assignment of the free substrate **2-OMe** could easily be completed by comparison with the spectra of a sample without the gold complex; it analyzed as follows: ^{1}H NMR (500 MHz, 25°C, CD_2Cl_2): δ = 7.29 (d, *J* = 7.6 Hz, 4H, 13), 7.15 (t, *J* = 7.8 Hz, 2H, 14), 7.20 (t, *J* = 7.4 Hz, 4H, 12), 4.43 (t, sept, *J* = 7.6, 2.8 Hz, 1H, 3), 3.98 (s, 2H, 6), 3.28 (s, 3H, 8), 2.81 (d, *J* = 7.6Hz, 2H, 4), 1.53 ppm (d, *J* = 2.8 Hz, 6H, 9+10). ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 203.2 (2), 146.4 (11), 128.0 (13), 127.7 (14), 126.0 (12), 94.2 (1), 84.0 (3), 77.0 (6), 59.2 (8), 49.8 (5), 36.7 (4), 20.3 ppm (9+10).

Table S1. Chemical shifts and assignments of ^{1}H and ^{13}C spectra recorded in CD_2Cl_2 (^{1}H: 5.32 ppm; ^{13}C: 54 ppm) at 227K (–46°C) for the major (red) and minor (blue) forms of the complex system formed in situ; unambiguously assigned correlations including COSY, NOESY and HMBC are also included.

Assign	^{13}C (J_{CP})				^{1}H (J_{HH})		Correlations		
	Major	minor	mult	$\|\Delta\delta\|^{a}$	Major	minor	HMBC (^{1}H↔^{13}C)	COSY	NOESY (τ_{mix} = 0.8s)^{b}
2	180.56 (14.5)	180.57 (14.5)	s	0.0					
11	145.4	145.3	s	0.1					
15	144.3	144.4	s	0.1					
75	142.5	--	s						
25	141.6	141.8	s	0.2					
55	139.8	140.7	s	**0.9**					
67	138.2	138.3	s	0.1					
35	136.1	136.1	s	0.0					
45	134.9	135.6	s	**0.7**					
47	133.0	128.5	d	**4.4**	7.56	8.14	45,53	46	**10**,23,49
48	132.8	133.1	s	**0.3**					
58	132.8	--	s						
53	131.8	--	s						
68+72	128.9	--	d		7.68	--	65		
52	128.7	--	d		8.01	--	48,54	51	54
56	128.5	--	d		7.98	--	22,58,64	57	
17	128.5	--	d		7.35	--	15		
64	128.3	--	d		7.15	--	22,56,58,62		
54	128.2	128.2	d	0.0	8.86	7.69	22,46,48,52	(46)	52,20,23,24
50	128.0	--	d		7.70	8.03		49,51	
51	128.0	--	d		8.01	--	53	50,52	
13	127.9	--	d		7.25	7.27	11		

49	127.5	--	d		7.88	8.00	47,53		47
12	127.1	127.1	d	0.0	6.84	6.81	5,12,14		
18	126.9	--	d		7.27	--	16		
16	126.7	--	d		6.85	--	5,16,18		
14	126.4	126.3	d	0.1	7.19	7.18	12		
27	126.2	--	d		7.25	7.60	25		
46	125.9	126.0	d	0.0	7.36	8.52	22,54,48	47,(54)	20,23,24,47
34	124.4	124.6	d	0.2	7.77	7.81	19,26		
1	106.1	106.0	s	0.1					
3	99.1	98.6	d	**0.5**	3.23	3.34	6	4	4ab,6ab,9,10,12,16, **(46),(47),(49),(34), (27)**
22	89.3	89.8	s	**0.5**					
19	86.4	86.2	s	0.2					
21	85.0	84.2	d	**0.8**	4.58 (d,7.7)	4.68 (d,7.0)	19,22,24,45,55	20	20,21,24,**10**
20	83.1	83.2	d	0.1	5.38 (d,7.7)	5.13 (d,7.0)	19,22,23,35,25	21	21,23,24,73
6	77.2	77.1	t	0.1	3.69, 3.53	3.68, 3.52	4,5,8,11,15	6	4ab,6,8,9,(10),27,46,49,50
23	62.1	62.0	q	0.1	4.12	3.97	20		20,21,24
24	61.1	60.9	q	0.2	2.34	2.33	21		21,20,23**,9,10,6**
8	59.4	59.4	q	0.0	3.14	3.10	6		6,9
65	55.9	55.8	d	0.0	6.13 (m)	6.13	66,67,68+72,73	66	66,74,(23),(20),73
73	50.6	50.5	d	0.2	4.32 (J_{HP}:33)	4.36	75	74	24,66,74,(20)
5	48.8	48.9	s	0.1					
4	36.6	36.5	t	0.0	2.02, 1.32	2.03, 1.32	2,3,5,11,15	3,4	(9),(10),4b,8,3,6ab,12,13,14, (**46),(49),(50),(34),(37)**
74	23.3	23.2	q	0.1	1.33	1.41	75	73	66,73,**(8)**
9	22.7	21.7	q	**1.0**	0.78	0.03	2,10		**(21),(24)**,8,(4a),10,12,16,**46,47,49**
10	22.3	23.2	q	**0.8**	0.51	0.86	2,9		**21,24**,(8),(4a),9,**47,49,52,54**
66	19.3	19.2	q	0.1	2.21	2.24	67	65	74,73,**(8)**
	^{31}P				^{19}F				
	109.1	109.5			-152.5 (-152.4)[d]				

Unassigned ^{13}C aromatic signals[c]

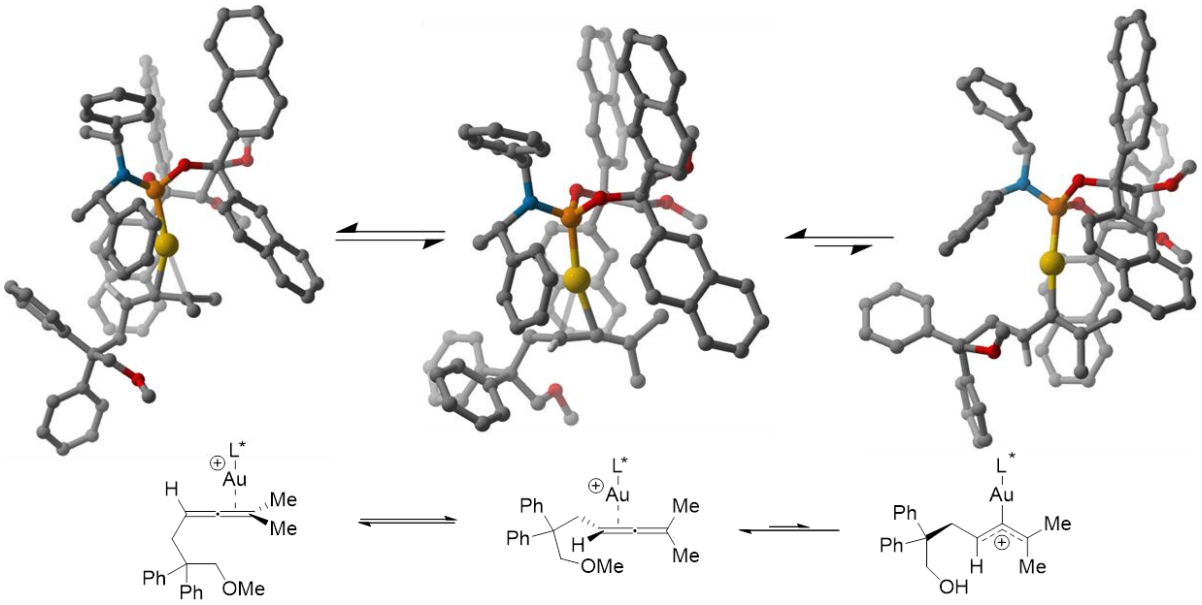
142.30, 140.71, 139.75, 136.54, 133.07, 132.74, 132.48, 132.19, 132.01, 131.94, 129.59, 128.96, 128.67, 127.42, 127.31,127.05, 126.50, 126.40, 123.68, 123.52

[a] Magnitude of the ^{13}C chemical shift difference between the major and minor forms. This value hints at the region of conformational exchange. Numbers in bold are larger than 0.5 ppm.

[b] NOESY includes NOE contacts cross peaks, exchange cross-peaks (EXSY) as well as some extent of correlations due to spin-diffusion due to low temperature. Values in bold indicate contacts between substrate and ligand. Values in parentheses are weak correlations

[c] Due to important overlap and broadening in the aromatic regions (minimum of 112 signals expected), it was not possible to assign all the aromatic carbons.

[d] Two signals due to the isotopic effect of ^{11}B and ^{10}B



Scheme S1. Pre-equilibrium of the loaded complex using 2–OMe as a dummy ligand.

Another distinctive feature of the loaded complex is the presence of two slowly exchanging conformers, which interconvert with an energy of activation of approximately 12 kcal·mol^{-1} (deduced from the temperature dependence of the ^{31}P NMR signals). Somewhat surprisingly, the ≈ 3:2 conformer ratio is fairly constant over a wide temperature range. A careful analysis of the spectra shows that the ligand's naphthyl group which is closest to the dimethyl-substituted allene terminus undergoes a 180° flip. Despite this rotatory movement, the position and orientation of the (dummy) substrate **2-OMe** within the catalyst binding site remains largely unaffected. This observation suggests that the naphthyl ring flip has little bearing on the stereochemical outcome of the reaction and therefore provides indirect support for the notion that the observed enantioinversions are not primarily caused by a conformational behavior of the ligand but by a more involved process with a strong entropic component.[1]

Independent of this naphthyl flip is an additional rotameric process involving the amine part of the phosphoramidite ligand scaffold which is fast (ms time scale at –20°C) and obviously quite unhindered by the naphthyl groups or the bound allenol. We had already previously implied such a process in the loading of the chiral complexes, where the rotational freedom of the P–N bond allows the amine to give way to the incoming substrate.[2]

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1 For cases of enantioinversion solely attributed to conformational changes, see: a) M. Messerer, H. Wennemers, *Synlett* **2011**, 499-502; b) M. Suginome, T. Yamamoto, Y. Nagata, T. Yamada, Y. Akai, *Pure Appl. Chem.* **2012**, *84*, 1759-1769.

2 H. Teller, M. Corbet, L. Mantilli, G. Gopakumar, R. Goddard, W. Thiel, A. Fürstner, *J. Am. Chem. Soc*. **2012**, *134*, 15331-15342.

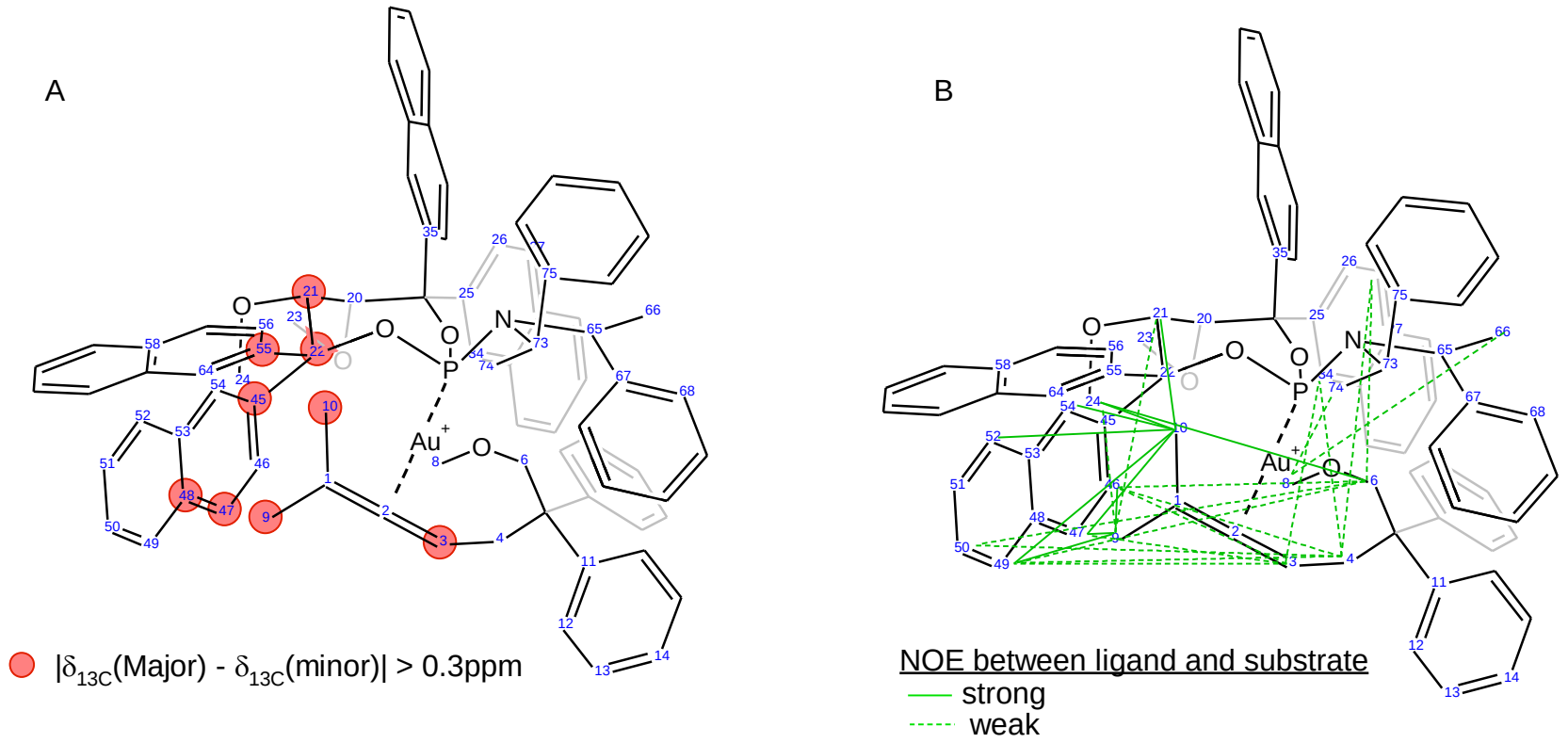
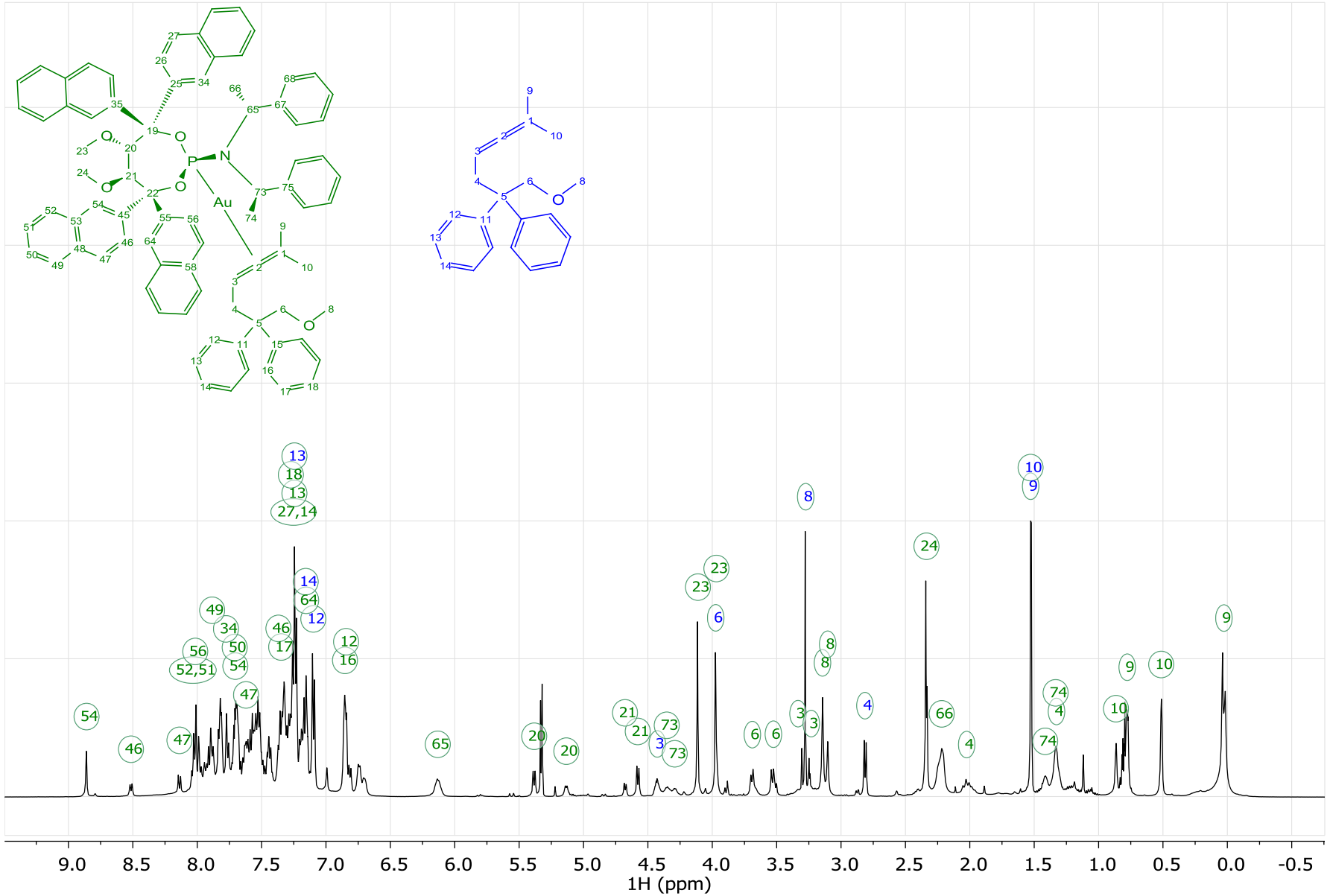


Figure S2. Summary of NMR data for 2-OMe + **1** + $AgBF_4$ in CD_2Cl_2 from Table S1. (A) conformational "hot spots" which exhibit the largest ^{13}C chemical shift changes between the 2 exchanging species (major and minor) of the complex. (B) Key NOE correlations between dummy substrate and ligand as observed in NOESY.

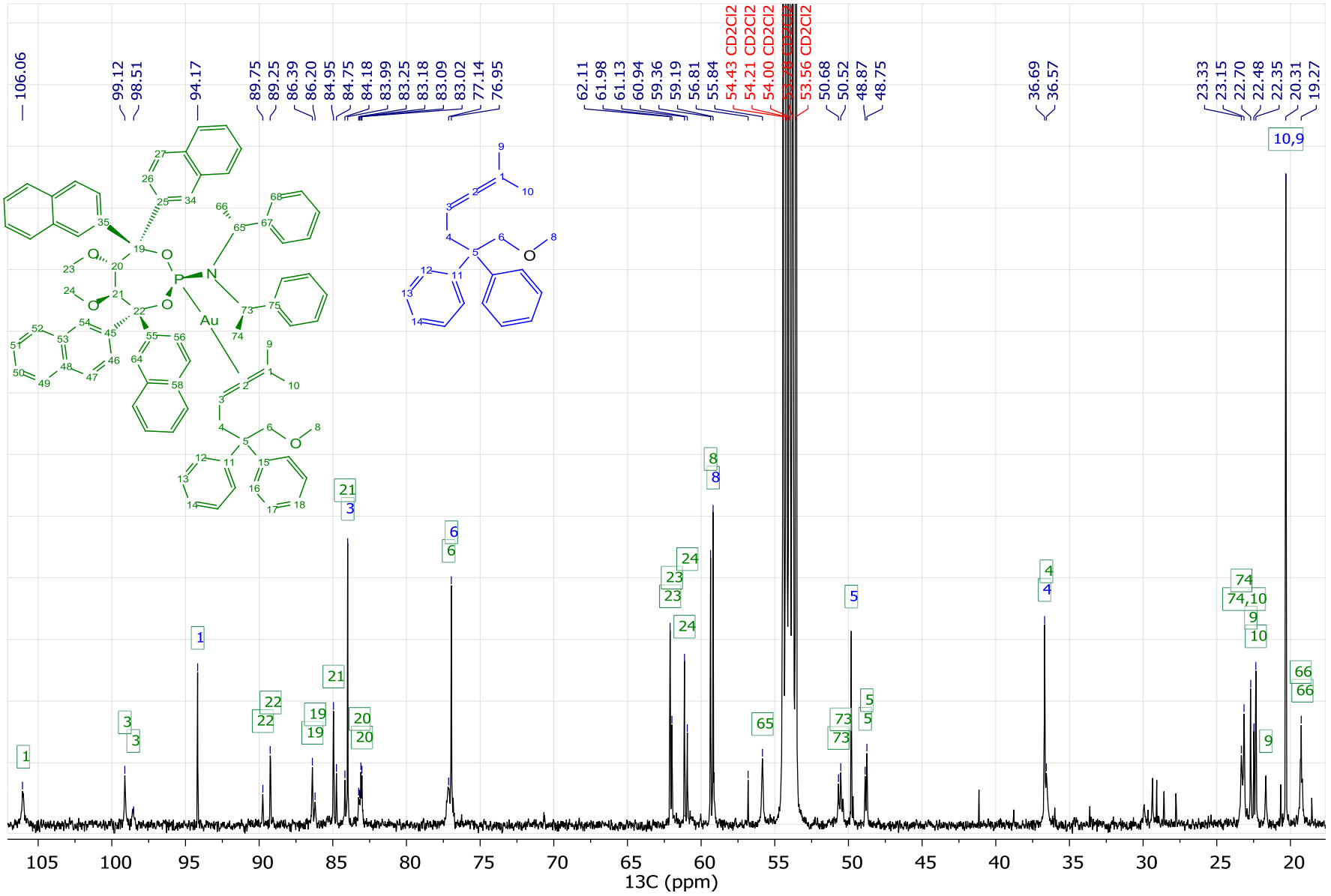
The following pages show assigned NMR Spectra:

1. ^{1}H,
2. $^{13}C\{^{1}H\}$ (upfield region),
3. $^{13}C\{^{1}H\}$ (downfield region),
4. HSQC-edited (upfield region),
5. HSQC-edited (downfield region)

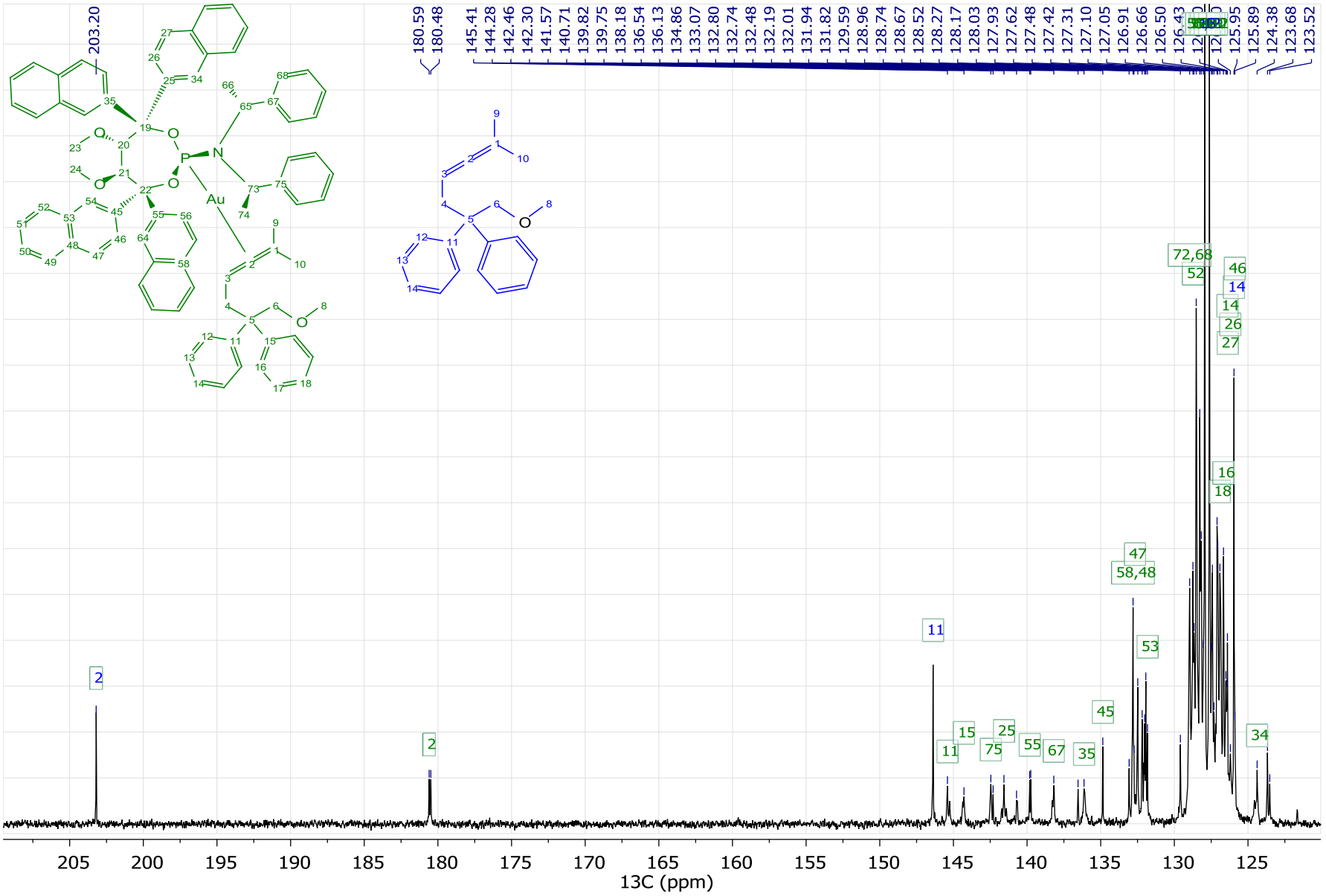
1 (AgBF4) + 2-OMe in CD2Cl2 — 1H (500MHz) — -46 °C

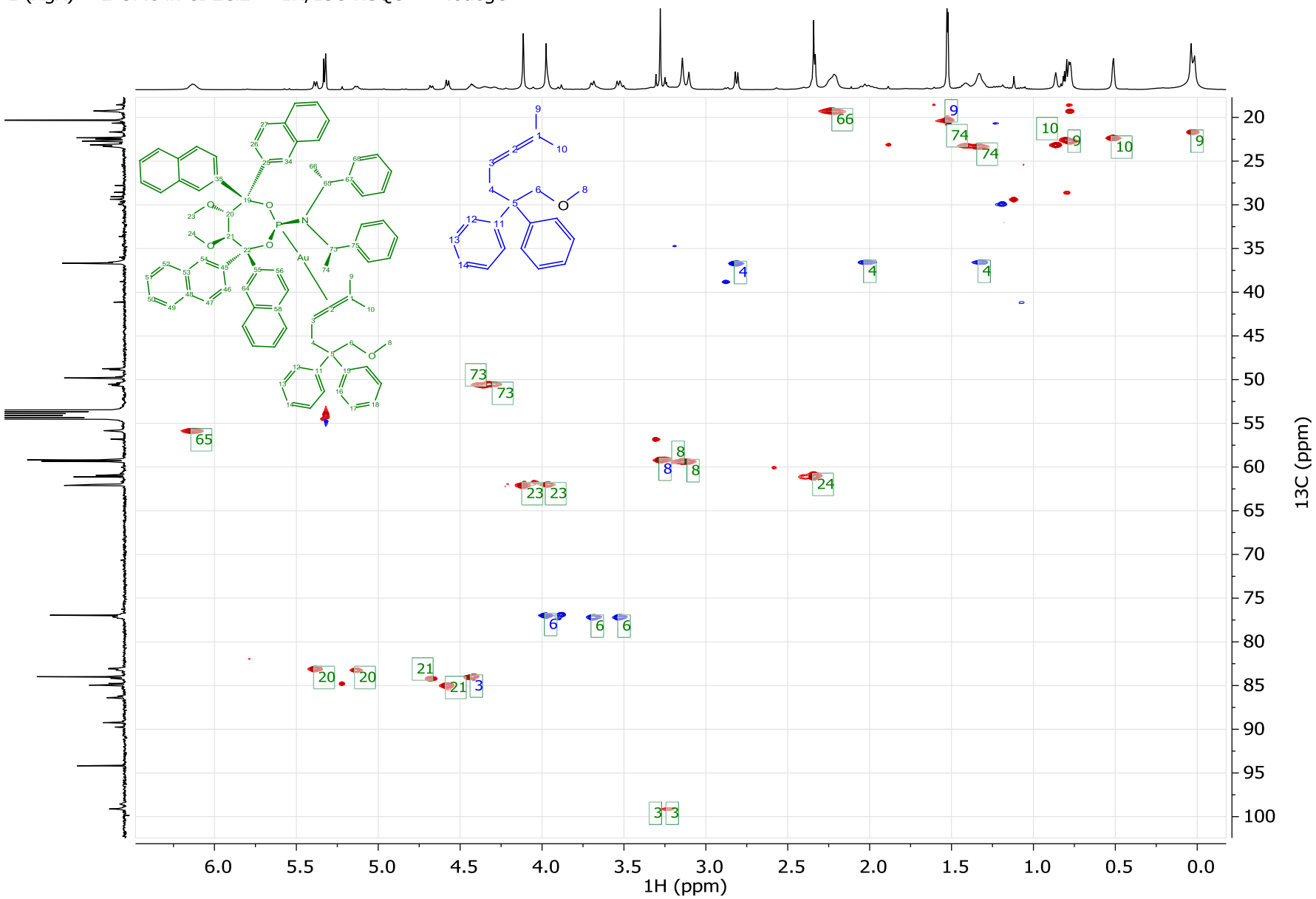


1 (AgBF4) + 2-OMe in CD2Cl2 — 13C{1H} — -46 °C

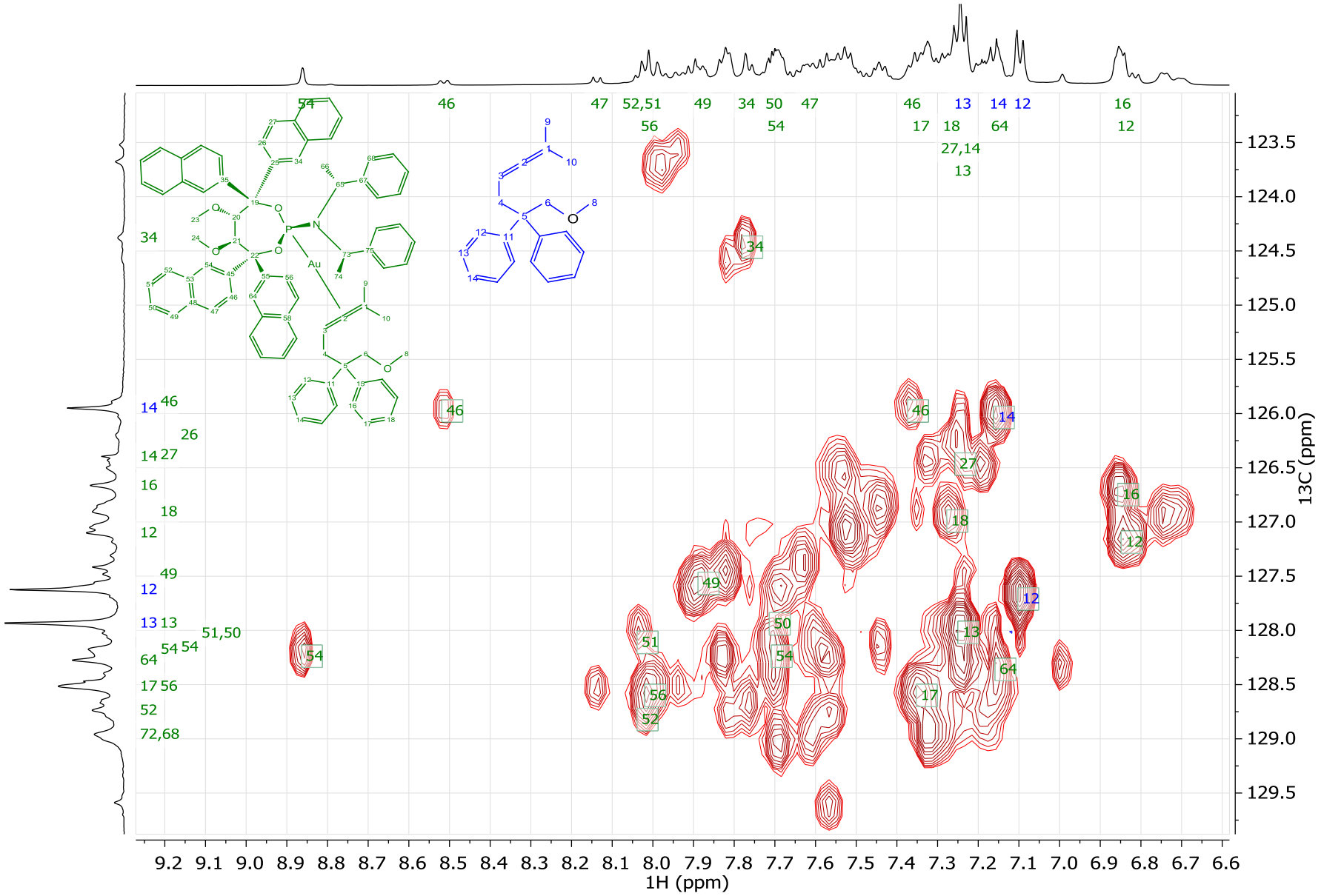


1 (AgBF4) + 2-OMe in CD2Cl2 — 13C{1H} — -46 °C




1 (AgX) + 2-OMe in CD2Cl2 — 1H/13C-HSQC — -46degC
1H (ppm)
13C (ppm)

1 (AgX) + 2-OMe in CD2Cl2 — 1H/13C-HSQC — -46degC



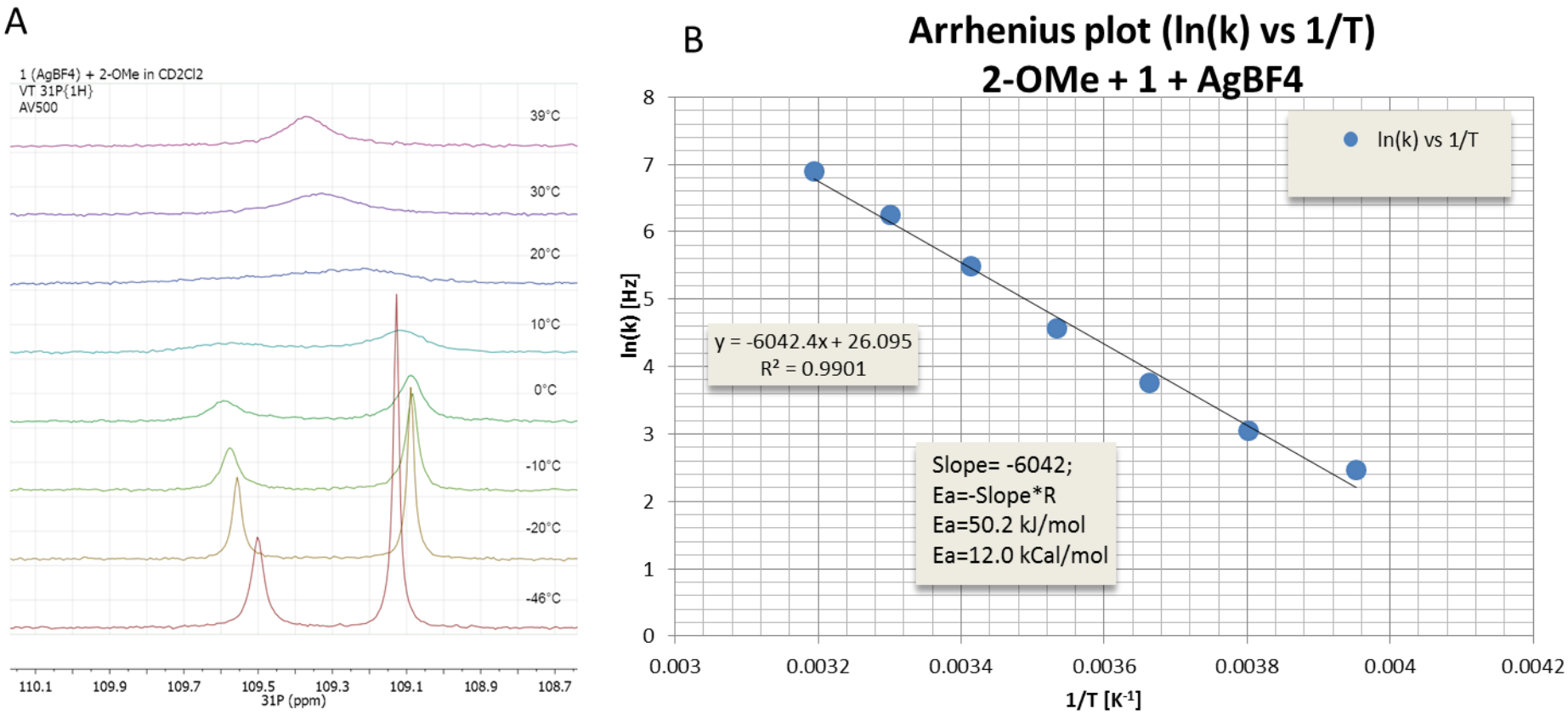


Figure S3. Thermodynamic study of activation energy based on coalescence of ^{31}P NMR signals. Exchange rates were extracted from peak fitting function with module DNMR of Topspin 3.2.

Screening Results

The results of screening different solvents, temperatures and counterions are summarized in Tables S2 – S4. The screening of different phosphoramidite ligands and various hydroxy-allenes is compiled in Table S5.

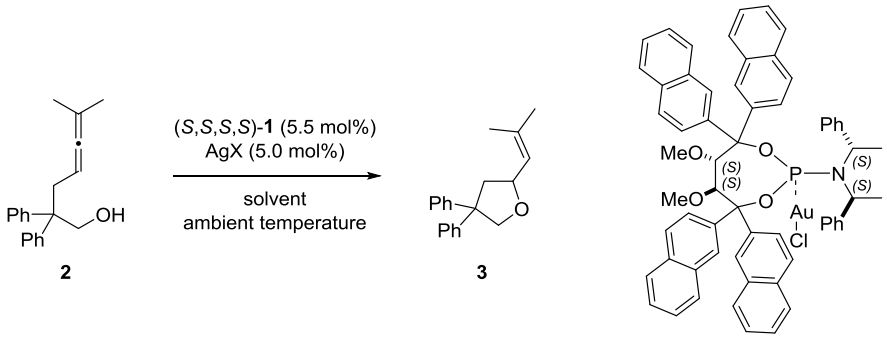
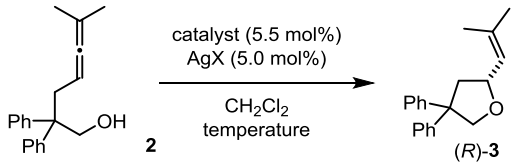


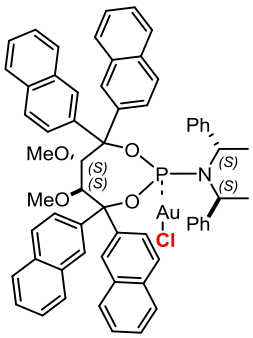
Table S2. Enantioinversion by solvent or counterion at ambient temperature (22 °C).

Entry	Solvent	X	(*R*) (*ee*, %)	(*S*) (*ee*, %)	Yield (%)
1	EtOAc	BF_4		(–)-68	77
2	EtOAc/H_2O (9:1)	BF_4	(+)-59		70
3	CH_2Cl_2	BF_4		(–)-59	95
4		ClO_4		(–)-43	68
5		NTf_2		(–)-36	79
6		CF_3COO	(+)-66		87
7		TsO	(+)-70		96
8	EtOH	BF_4	(+)-78		93
9		NTf_2	(+)-78		90
10		CF_3COO	(+)-77		95
11		TsO	(+)-77		91
12	DMA	BF_4	(+)-83		76
13	$CHCl_3$	BF_4		(–)-50	89
14	CCl_4	BF_4		(–)-28	73
15	$(CH_2Cl)_2$	BF_4		(–)-53	85
16	$PhCF_3$	BF_4		(–)-47	74
17	acetone	BF_4		(–)-21	86
18	MeCN	BF_4		(–)-7	72
19	$MeNO_2$	BF_4		(–)-7	81
20	hexane	BF_4	-	-	0[a]
21	pentane	BF_4	-	-	0[a]
22	HMDSO	BF_4	-	-	0[a]
23	H_2O	BF_4	-	-	0[a]

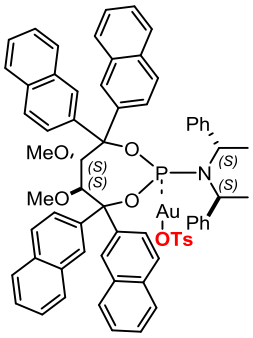
[a] insolubility of substrate and gold complex prevents the reaction from occurring

Table S3. Comparison of catalyst (*S*,*S*,*S*,*S*)-**1** ionized *in situ* with AgOTs with catalyst (*S*,*S*,*S*,*S*)-**16** prepared *ex situ*.





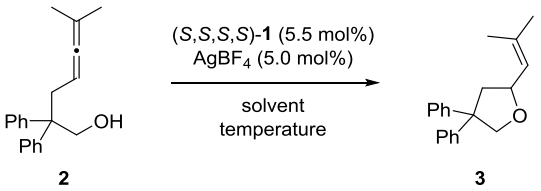
(*S*,*S*,*S*,*S*)-**1**



(*S*,*S*,*S*,*S*)-**16**

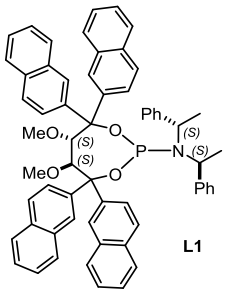
Entry	Catalyst	AgX	Temperature [°C]	(*R*) (*ee*, %)
1	(*S*,*S*,*S*,*S*)-**1**	OTs	22	(+)-70
2	(*S*,*S*,*S*,*S*)-**16**	-	22	(+)-73
3	(*S*,*S*,*S*,*S*)-**1**	OTs	–60	(+)-92
4	(*S*,*S*,*S*,*S*)-**16**	-	–60	(+)-94

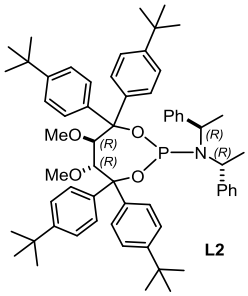
Table S4. Enantioinversion by changing the reaction temperature.

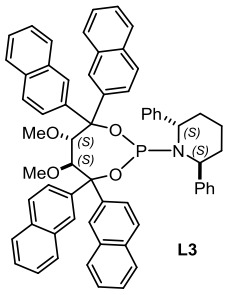


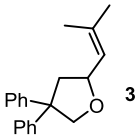
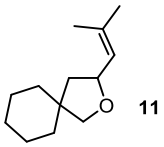
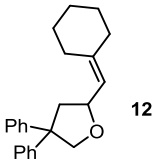
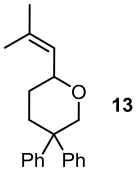
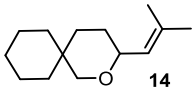
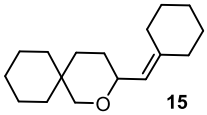
Entry	Solvent	T (°C)	(*R*) (*ee*, %)	(*S*) (*ee*, %)	Yield (%)
1	EtOAc	22		(–)-68	77
2		–60	(+)-77		80
3	CH_2Cl_2	22		(–)-59	95
4		–60	(+)-29		89
5	toluene	22		(–)-38	71
6		–60	(+)-33		71
7	EtOH	22	(+)-78		93
8		–30	(+)-92		90
9		–60	(+)-97		93
10	MeOH	22	(+)-72		86
11		–60	(+)-96		96
12	Et_2O	22	(+)-6		78
13		–60	(+)-74		80
14	THF	22	(+)-23		78
15		–60	(+)-86		88
16	DMA	22	(+)-83		76
17		–20	(+)-91		63

Table S5. Screening of gold complexes carrying different phosphoramidites in the cyclization of different hydroxy-allenols.[a]







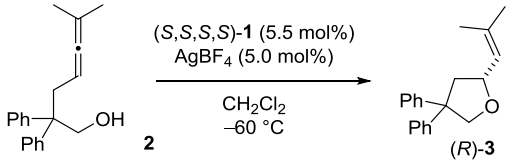
Entry	Product	Ligand	Solvent	T (°C)	(+) (ee, %)	(–) (ee, %)
1		**L1**	CH_2Cl_2	22		(–)-59
2		**L1**	CH_2Cl_2	–60	(+)-29	
3	 **3**	**L1**	EtOH	–60	(+)-97	
4		**L2**	CH_2Cl_2	22	(+)-26	
5		**L2**	CH_2Cl_2	–60	(+)-51	
6		**L3**	CH_2Cl_2	22		(–)-50
7		**L3**	CH_2Cl_2	–60		(–)-12
8		**L1**	CH_2Cl_2	22	(+)-1	
9		**L1**	CH_2Cl_2	–60	(+)-55	
10	 **11**	**L1**	EtOH	–60	(+)-92	
11		**L1**	EtOH	–78	(+)-95	
12		**L1**	CH_2Cl_2	22		(–)-25
13		**L1**	CH_2Cl_2	–60	(+)-26	
14	 **12**	**L1**	EtOAc	22		(–)-35
15		**L1**	EtOAc	–60	(+)-86	
16		**L1**	EtOH	–60	(+)-94	
17		**L1**	CH_2Cl_2	22	(+)-23	
18		**L1**	CH_2Cl_2	–60		(–)-35
19		**L1**	EtOH	–60		(–)-72
20	 **13**	**L2**	CH_2Cl_2	22	(+)-9	
21		**L2**	CH_2Cl_2	–60	(+)-77	
22		**L2**	EtOH	–60	(+)-96	
23		**L2**	EtOH	–78	(+)-98	
24	 **14**	**L2**	EtOH	–78		(–)-97
25	 **15**	**L2**	EtOH	–78		(–)-99

[a] Reactions carried out according to general procedure for gold catalysis; 5.5 mol% L-AuCl, 5.0 mol% $AgBF_4$, 0.1 M solution in indicated solvent.

Control Experiments

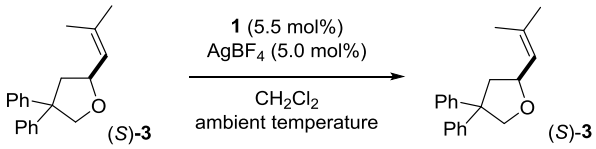
The *ee* of the product was determined at defined intervals while the reaction was in progress. Aliquots (100 µL) were taken and submitted to preparative TLC (hexane/*tert*-butyl methyl ether 9:1) and the *ee* of the resulting samples was determined by HPLC (*vide infra*). The *ee* was constant over the entire timeframe (Table S6). Likewise, even the prolonged exposure of product **3** (100 µmol, (–)-54% *ee*) to freshly prepared catalyst of either absolute configuration under the standard reaction conditions in CH_2Cl_2 did not lead to an erosion of the *ee* (Table S7).

Table S6. Continuous sampling and *ee* determination.



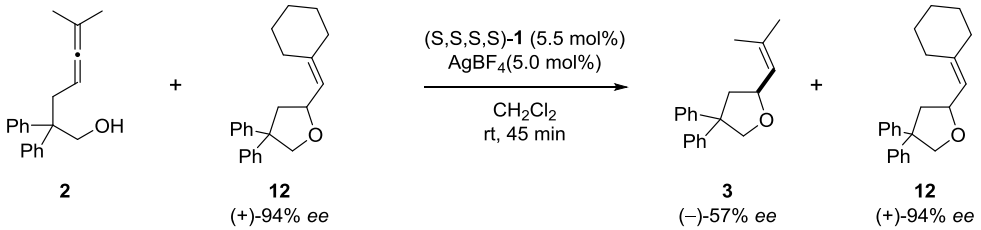
Entry	Time	(*R*) (*ee*, %)
1	30 min	(+)-27
2	60 min	(+)-26
3	90 min	(+)-27
4	120 min	(+)-27
5	180 min	(+)-27
6	17.5 h	(+)-25
7	24 h	(+)-26
8	48 h	(+)-26

Table S7. Investigation of possible product influence.



Entry	Time (h)	1	(*S*) (*ee*, %)	Entry	Time (h)	1	(*S*) (*ee*, %)
1	12	(*S*,*S*,*S*,*S*)	(–)-53	7	12	(*R*,*R*,*R*,*R*)	(–)-50
2	24		(–)-54	8	24		(–)-51
3	36		(–)-50	9	36		(–)-51
4	48		(–)-51	10	48		(–)-54
5	60		(–)-53	11	60		(–)-54
6	72		(–)-53	12	72		(–)-52

The gold-catalyzed hydroalkoxylation of allene **2** (50 µmol) to tetrahydrofuran **3** was also carried out in the presence of a different hydroalkoxylation product **12** (50 µmol, (+)-94% *ee*). No significant impairment of enantioselectivity was observed for tetrahydrofuran **3** and the *ee* of the added tetrahydrofuran **12** remained unchanged (Scheme S2).



Scheme S2. No product influence on enantioselectivity.

Search for Any Non-linear Effects

The correlation between the *ee* of the product and the *ee* of the precatalyst was investigated in CH_2Cl_2 at both 22 °C and –60 °C. To this end, a series of reactions was set up in parallel. Each flame-dried finger-Schlenck was loaded with allenol **2** (11.0 mg, 39.5 µmol) in anhydrous CH_2Cl_2 (0.2 mL) and stirred at the respective temperature. Accurately defined mixtures of (*S*,*S*,*S*,*S*)-**1** and (*R*,*R*,*R*,*R*)-**1** (total mass 2.25 mg, 2.19 µmol) were activated with $AgBF_4$ (0.40 mg, 2.05 µmol) in anhydrous CH_2Cl_2 (0.2 mL) at ambient temperature for 15 min. These activated catalyst solutions were transferred into the reaction vessels via cannula equipped with a PTFE filter (Perfect-Flow®, 0.45 µm pore size, Ø 13 mm) to retain the precipitates. The resulting solutions were stirred at ambient temperature for 45 min or at –60 °C for 16 h. The mixtures were submitted to flash chromatography (hexane/*tert*-butyl methyl ether 19:1) and the *ee* of the products determined by HPLC (*vide infra*) (Table S8). The *ee* of the product was then plotted against the *ee* of the precatalyst, resulting in a linear correlation at either temperature (Figures S4 and S5).

Table S8. Correlation between *ee* of precatalyst and *ee* of product.

Entry	T (°C)	1 (*ee*,%)	3 (*ee*, %)	Entry	T (°C)	1 (*ee*, %)	3 (*ee*, %)
1	22	> (+)-99	(–)-58	10	–60	> (+)-99	(+)-29
2		(+)-60	(–)-28	11		(+)-60	(+)-23
3		(+)-50	(–)-21	12		(+)-50	(+)-17
4		(+)-20	(–)-5	13		(+)-20	(+)-8
5		0	0	14		0	(+)-1
6		(–)-20	(+)-13	15		(–)-20	(–)-8
7		(–)-50	(+)-18	16		(–)-50	(–)-16
8		(–)-60	(+)-27	17		(–)-60	(–)-17
9		> (–)-99	(+)-59	18		> (–)-99	(–)-27

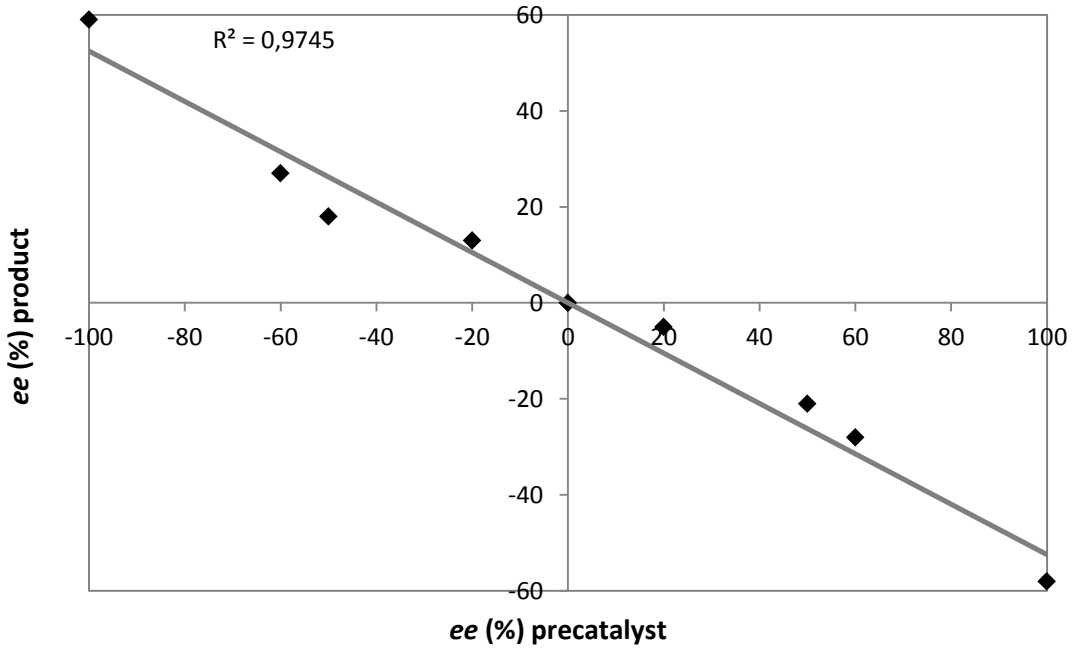


Figure S4. Correlation between *ee* precatalyst and *ee* product at 22 °C.

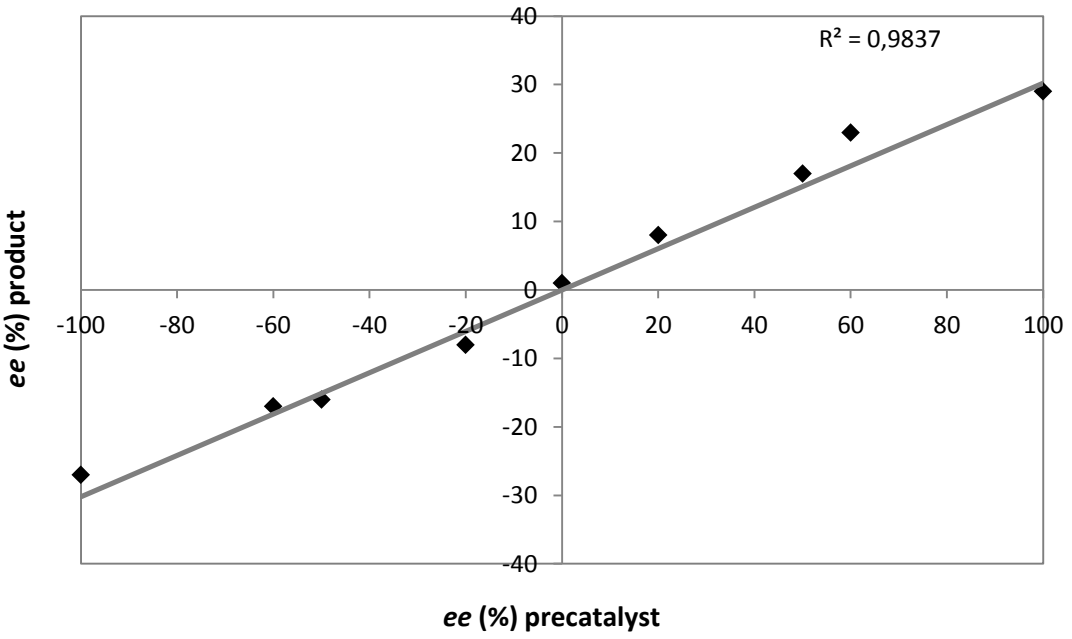


Figure S5. Correlation between *ee* precatalyst and *ee* product at –60 °C.

Eyring Plots

In transition state theory, the temperature-dependent variance of the rate of a chemical reaction is described by the Eyring equation (1):

$$k = \frac{k_B T}{h} e^{\frac{-\Delta G^{\ddagger}}{RT}} \quad (1)$$

The enantiomeric excess (*ee*) of an asymmetric reaction can be expressed as the natural logarithm of the relative rate constant for the formation of two enantiomers (*R*) and (*S*) as follows:

$$\ln \frac{k_R}{k_S} = \ln \frac{100 + \%\, ee}{100 - \%\, ee} \quad (2)$$

An alternative representation is provided by the differential Eyring equation (3):[3]

$$\ln \frac{k_R}{k_S} = - \frac{\Delta\Delta H^{\ddagger}}{R} \frac{1}{T} + \frac{\Delta\Delta S^{\ddagger}}{R} \quad (3)$$

Eyring studies were performed in both EtOH and CH_2Cl_2 using the gold precatalyst (*S*,*S*,*S*,*S*)-**1** and $AgBF_4$. Every data point was independently determined three times (Tables S9 and S10). For each reaction, complex (*S*,*S*,*S*,*S*)-**1** (1.58 mg, 1.40 µmol, 5.5 mol%) and $AgBF_4$ (0.24 mg, 1.30 µmol, 5.0 mol%) were dissolved in anhydrous EtOH or CH_2Cl_2 (0.1 mL) at ambient temperature and the resulting mixture was stirred for 15 min. In parallel, a solution of allenol **2** (7.00 mg, 25.1 µmol) in anhydrous EtOH or CH_2Cl_2 (0.15 mL) was placed in a flame-dried finger-Schlenck flask and equilibrated at the indicated temperature. The solution of the activated catalyst was then introduced via a cannula equipped with a PTFE filter (Perfect-Flow®, 0.45 µm pore size, Ø 13 mm) and the resulting mixture was stirred until complete conversion was achieved. In the case of EtOH, the reaction mixtures were then quickly filtered through a plug of silica, the filtrate was concentrated and the residue submitted to flash chromatography (hexane/*tert*-butyl methyl ether 19:1). For CH_2Cl_2, the reaction mixtures were directly submitted to flash chromatography (hexane/*tert*-butyl methyl ether 19:1). The enantiomeric excess of the resulting products was determined by HPLC (*vide infra*).

According to equation (2), the enantioselectivity was expressed as the natural logarithm of the relative rate constants for the formation of (*R*)-**3** and (*S*)-**3** (Table S9 and S10, data used for Eyring plot highlighted in blue for EtOH and red for CH_2Cl_2). These values were plotted against the reciprocal temperature and the differential Eyring equation (3) was applied, using at least four data points for each linear regression whilst minimizing the R^2 value (Figure S6).

[3] (a) J. Otera, K. Sakamoto, T. Tsukamoto, A. Orita, *Tetrahedron Lett.* **1998**, *39*, 3201–3204; (b) R. Saito, S. Naruse, K. Takano, K. Fukuda, A. Katoh, Y. Inoue, *Org. Lett.* **2006**, *8*, 2067–2070.

Table S9. Data for EtOH

Entry	T (°C)	T^{-1} ($10^3 \cdot K^{-1}$)	*ee* (%)	*ee* (%)	*ee* (%)	Ø *ee* (%)	$\ln(k_R/k_S)$
1	–85	5.3191	(+)-91	(+)-90	(+)-92	(+)-91	3.0550
2	–78	5.2182	(+)-95	(+)-92	(+)-92	(+)-93	3.3168
3	–70	4.9261	(+)-95	(+)-93	(+)-95	(+)-94	3.4761
4	–60	4.6948	(+)-96	(+)-95	(+)-97	(+)-96	3.8918
5	–50	4.4843	(+)-95	(+)-96	(+)-96	(+)-96	3.8918
6	–40	4.2918	(+)-95	(+)-95	(+)-94	(+)-95	3.6636
7	–21	3.9683	(+)-92	(+)-93	(+)-93	(+)-93	3.3168
8	0	3.6630	(+)-87	(+)-87	(+)-87	(+)-87	2.6662
9	10	3.5336	(+)-85	(+)-85	(+)-84	(+)-85	2.5123
10	22	3.3898	(+)-78	(+)-77	(+)-78	(+)-78	2.0907
11	38	3.2154	(+)-72	(+)-71	(+)-72	(+)-72	1.8153

Table S10. Data for CH_2Cl_2

Entry	T (°C)	$10^3\ T^{-1}$ (K^{-1})	*ee* (%)	*ee* (%)	*ee* (%)	Ø *ee* (%)	$\ln(k_R/k_S)$
1	–60	4.6948	(+)-29	(+)-28	(+)-29	(+)-29	0.5971
2	–50	4.4843	(+)-26	(+)-27	(+)-24	(+)-26	0.5322
3	–40	4.2918	(+)-24	(+)-26	(+)-22	(+)-24	0.4895
4	–21	3.9683	(+)-14	(+)-21	(+)-25	(+)-20	0.4055
5	–10	3.8023	(–)-14	(–)-26	(–)-17	(–)-19	–0.3847
6	0	3.6630	(–)-31	(–)-29	(–)-32	(–)-31	–0.6411
7	10	3.5336	(–)-41	(–)-41	(–)-43	(–)-42	–0.8954
8	22	3.3898	(–)-57	(–)-59	(–)-57	(–)-58	–1.3249

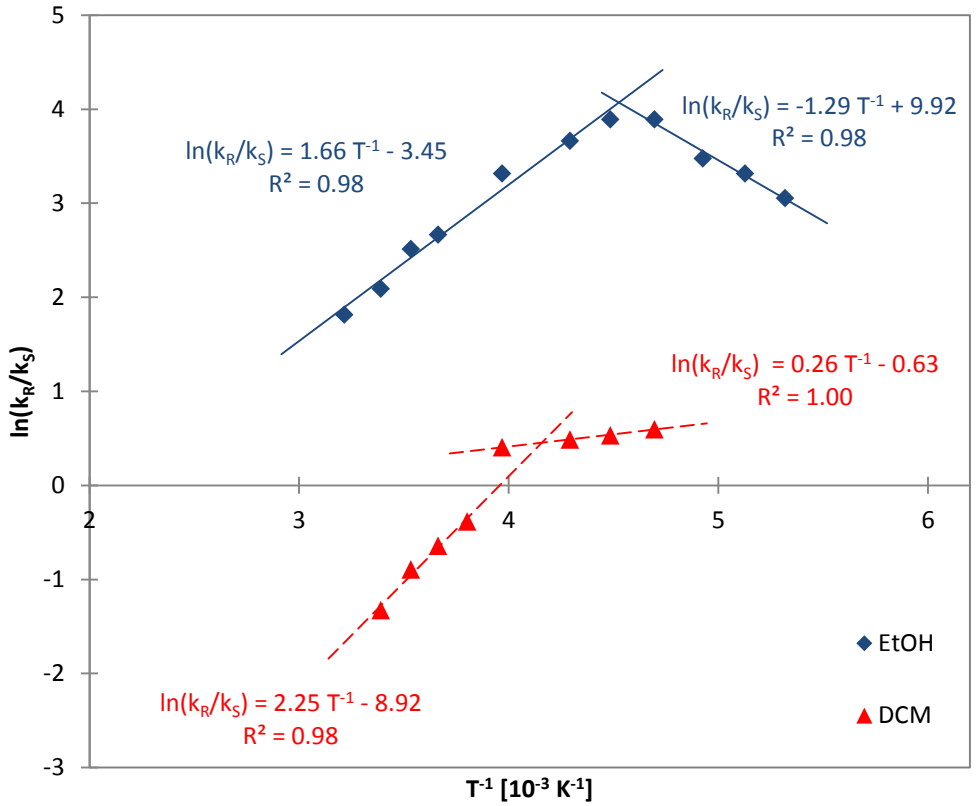


Figure S6. Eyring plot for the gold-catalyzed hydroalkoxylation in EtOH (blue squares) and CH_2Cl_2 (DCM, red triangles).

The temperature, at which the change in the selectivity-determining step occurs, is given by the interception of the two linear approximations (Table S11). Additionally, the thermodynamic parameters compiled in Table S11 were obtained from the linear equations.

Table S11. Linear regression equations, temperatures for the switch in mechanism, and thermodynamic parameters as deduced from the differential Eyring equation.

Solvent	Sector	$\ln(k_R/k_S)$	$\Delta\Delta H^{\ddagger}$ (kcal·mol^{-1})	$\Delta\Delta S^{\ddagger}$ (cal·mol^{-1}·K^{-1})
EtOH	left	$1.66\ T^{-1} - 3.45$	–3.3	–6.8
	right	$-1.29\ T^{-1} + 9.92$	2.6	19.7
CH_2Cl_2	left	$2.25\ T^{-1} - 8.92$	–4.5	–17.7
	right	$0.26\ T^{-1} - 0.63$	–0.5	–1.2

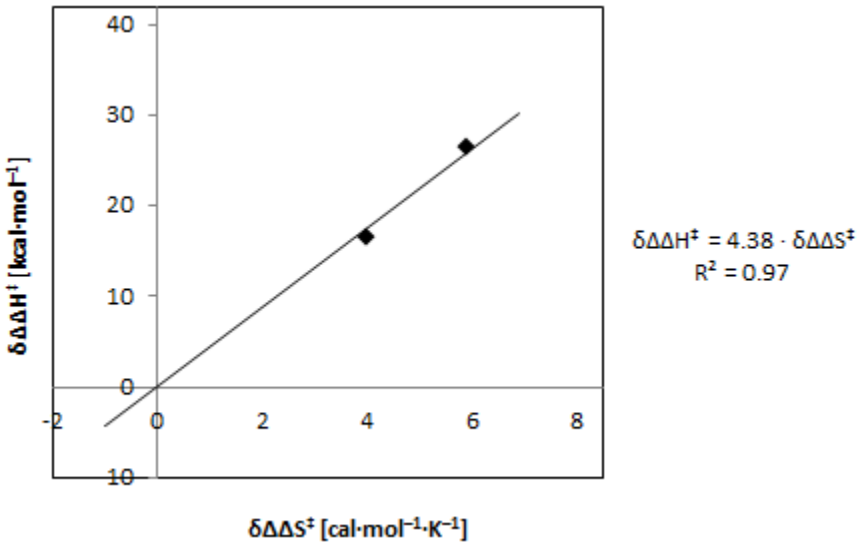


Figure S7. Isoinversion diagram gives a calculated T_i = 229 K; input data: $\delta\Delta\Delta H^{\ddagger}$ (kcal·mol^{-1}): 5.9 (EtOH), 26.5 (CH_2Cl_2); $\delta\Delta\Delta S^{\ddagger}$ (cal·mol^{-1}·K^{-1}): 4.0 (EtOH), 16.5 (CH_2Cl_2)

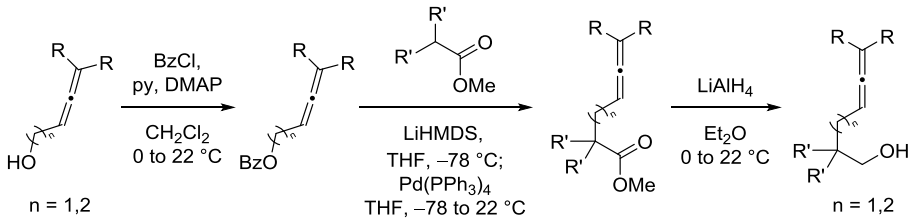
General Experimental Methods

All reactions were carried out under Argon in flame-dried glassware. The solvents were purified by distillation over the drying agents indicated and were transferred under Argon: THF, Et_2O (Mg/anthracene), CH_2Cl_2, $(CH_2Cl)_2$, EtOAc, MeCN (CaH_2), hexane, pentane, toluene (Na/K), MeOH, EtOH (Mg), DMF (MS 4Å), DMSO (distilled over CaH_2, stored over MS 4Å). Flash chromatography: Merck silica gel 60 (40-63 µm). NMR: Spectra were recorded on Bruker DPX 300, AV 400, AV 500 or AVIII 600 spectrometer in the solvents indicated; chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. The solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: $\delta_H \equiv 7.26$ ppm, $\delta_C \equiv 77.2$ ppm; CD_2Cl_2: $\delta_H \equiv 5.32$ ppm, $\delta_C \equiv 53.8$ ppm; C_6D_6: $\delta_H \equiv 7.16$ ppm, $\delta_C \equiv 128.0$ ppm; [D6]-DMSO: $\delta_H \equiv 2.50$ ppm, $\delta_C \equiv 39.5$ ppm). IR: Spectrum One (Perkin-Elmer) spectrometer, wavenumbers ($\tilde{\nu}$) in cm^{-1}. MS (EI): Finnigan MAT 8200 (70 eV), ESI MS: ESQ3000 (Bruker), accurate mass determinations: Bruker APEX III FT-MS (7 T magnet) or Mat 95 (Finnigan). Unless stated otherwise, all commercially available compounds (Acros, Alfa Aesar, Aldrich) were used as received.

The catalysts were prepared as previously reported by our group;[4] the preparation of (*S,S,S,S*)-**16** is described below:

Pre-activated catalyst (*S,S,S,S*)-16. To a solution of gold catalyst (*S,S,S,S*)-**1** (31 mg, 0.03 mmol, 1.0 equiv) in anhydrous CH_2Cl_2 (0.3 mL) at room temperature was added silver tosylate (7.6 mg, 0.03 mmol, 1.0 equiv). The resulting pale yellow solution was stirred at ambient temperature for 15 min, then filtered over a pad of Celite® eluting with CH_2Cl_2 (10 mL). The solvent was removed under reduced pressure affording the catalyst as an amorphous yellow solid (34 mg, 0.03 mmol, 98%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 8.47 (s, 1H), 8.28 (s, 1H), 8.01 (s, 1H), 7.97–7.73 (m, 14H), 7.73–7.64 (m, 4H), 7.58–7.45 (m, 12H), 7.44–7.34 (m, 2H), 7.21–7.15 (m, 3H), 7.03–6.93 (m, 4H), 5.65 (d, *J* = 7.3 Hz, 1H), 5.12 (dd, *J* = 19.1, 6.9 Hz, 2H), 4.87 (d, *J* = 7.3 Hz, 1H), 6.39 (s, 3H), 2.55 (s, 3H), 2.37 (s, 3H), 1.91 ppm (d, *J* = 7.1 Hz, 6H); ^{31}P NMR (162 MHz, CD_2Cl_2): δ = 95.8 ppm.[5]

All substrates were prepared by a three-step protocol starting from commercial 5-methyl-3,4-hexadien-1-ol or literature-known 4-cyclo-hexylidenebut-3-en-1-ol,[6] 3-cyclohexylidene-prop-2-en-1-ol[7] or 4-methylpenta-2,3-dien-1-ol[8] (Scheme S3).



Scheme S3. Preparation of the substrates.

4-Methylpenta-2,3-dien-1-yl benzoate (4). Pyridine (1.00 mL, 12.2 mmol, 1.2 equiv) and DMAP (125 mg, 1.02 mmol, 0.1 equiv) were added to a solution of 4-methylpenta-2,3-dien-1-ol (1.00 g, 10.2 mmol, 1.0 equiv) in CH_2Cl_2 (10 mL) at 0 °C. Finally, benzoyl chloride (1.78 mL, 15.3 mmol, 1.5 equiv) was added dropwise and the resulting yellow suspension stirred at ambient temperature for 15 h. The reaction was quenched by addition of sat. NH_4Cl solution (10 mL) and the aqueous layer extracted with CH_2Cl_2 (3 x 15 mL). The combined extracts were washed with HCl (1 M, 10 mL), NaOH (1 M, 10 mL) and brine (25 mL), dried over Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography (hexanes/*tert*-butyl methyl ether, 50:1) to yield the desired benzoate as a pale yellow oil (1.59 g, 77%). ^{1}H NMR

4 (a) H. Teller, A. Fürstner, *Chem. Eur. J.* **2011**, *17*, 7764–7767; (b) H. Teller, S. Flügge, R. Goddard, A. Fürstner, *Angew. Chem. Int. Ed.* **2010**, *49*, 1949–1953; (c) H. Teller, M. Corbet, L. Mantilli, G. Gopakumar, R. Goddard, W. Thiel, A. Fürstner, *J. Am. Chem. Soc.* **2012**, *134*, 15331–15342.

5 For comparison: ^{31}P NMR of (*S,S,S,S*)-**1** (162 MHz, CD_2Cl_2): δ = 113.8 ppm.

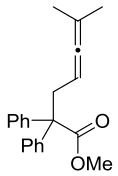
6 B. M. Trost, A. B. Pinkerton, M. Seidel, *J. Am. Chem. Soc.* **2001**, *123*, 12466–12476.

7 Z. Zhang, C. F. Bender, R. A. Widenhoefer, *Org. Lett.* **2007**, *9*, 2887–2889.

8 M. Murakami, S. Kadowaki, T. Matsuda, *Org. Lett.* **2005**, *7*, 3953–3956.

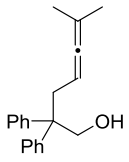
(400 MHz, $CDCl_3$): δ = 8.07–8.03 (m, 2H), 7.57–7.53 (m, 1H), 7.45–7.42 (m, 2H), 5.22 (tsept, *J* = 6.4, 2.8 Hz, 1H), 4.76 (d, *J* = 6.4 Hz, 2H), 1.70 ppm (d, *J* = 2.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 203.5, 166.5, 133.0, 130.6, 129.7, 129.7, 128.6, 128.4, 97.6, 85.0, 63.8, 20.4 ppm; IR (film): $\tilde{\nu}$ = 2938, 1715, 1602, 1584, 1451, 1362, 1315, 1268, 1176, 1108, 1068, 1025, 939, 804, 707, 686, 581, 543 cm^{-1}; MS (EI) *m/z* (%) = 202 [M^+], 105 (100), 77 (28); HRMS (EI): *m/z* calcd. for $C_{13}H_{14}O_2$ [M^+]: 202.0994, found: 202.0992. The analytical and spectroscopic data are in agreement with those reported in the literature.[9]

Allene ester 5. A solution of LiHMDS (1.24 g, 7.42 mmol) in THF (10 mL) was added dropwise over



15 min to a solution of methyl diphenylacetate (1.68 g, 7.42 mmol) in anhydrous THF (20 mL) at –78 °C and the resulting mixture was stirred at this temperature for 1.5 h. In a second flask, $Pd(PPh_3)_4$ (214 mg, 0.19 mmol, 0.05 equiv) was dissolved in THF (5 mL) and a solution of allene benzoate **4** (750 mg, 3.71 mmol, 1.0 equiv) in THF (5 mL) was added. The resulting mixture was stirred for 30 min at ambient temperature, before it was added to the enolate solution at –78 °C via syringe. The mixture was warmed to room temperature and stirred overnight. The reaction was quenched by addition of sat. NH_4Cl solution (20 mL) and the aqueous layer extracted with *tert*-butyl methyl ether (3 x 25 mL). The combined extracts were washed with brine (50 mL), dried over Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography (hexanes/*tert*-butyl methyl ether, 40:1) to furnish the title compound as a colorless oil (715 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.30–7.27 (m, 5H), 7.25–7.20 (m, 5H), 4.72–4.65 (m, 1H), 3.68 (s, 3H), 3.06 (d, *J* = 7.5 Hz, 2H), 1.46 ppm (d, *J* = 2.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 203.8, 174.7, 142.5, 129.2, 127.9, 126.9, 94.6, 84.6, 60.6, 52.6, 39.2, 20.3 ppm; IR (film): $\tilde{\nu}$ = 2958, 2853, 1730, 1599, 1495, 1446, 1362, 1275, 1218, 1036, 859, 813, 788, 750, 729, 697, 662, 612, 575, 501 cm^{-1}; MS (EI) *m/z* (%) = 306 [M^+] (33), 275 (12), 274 (27), 263 (15), 248 (21), 247 (100), 246 (20), 232 (19), 231 (36), 225 (39), 205 (37), 203 (10), 197 (44), 166 (15), 165 (52), 157 (11), 105 (26), 91 (25), 77 (12); HRMS (ESI): *m/z* calcd. for $C_{21}H_{22}O_2Na$ [M^+ + Na]: 329.1512, found: 329.1511.

Hydroxy-allene 2. A solution of ester **5** (840 mg, 2.74 mmol, 1.0 equiv) in Et_2O (4 mL) was added



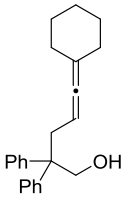
dropwise to a stirred suspension of $LiAlH_4$ (520 mg, 13.7 mmol, 5.0 equiv) in Et_2O (8 mL) at 0 °C. The mixture was allowed to warm to ambient temperature and stirred for 14 h. After cooling to 0 °C, the reaction was carefully quenched with H_2O (0.52 mL) followed by NaOH (10%, 0.52 mL) and H_2O (1.56 mL). The resulting suspension was stirred for 1 h before it was filtered through a pad of Celite®, eluting with *tert*-butyl methyl ether (20 mL). The combined filtrates were concentrated and the residue purified by flash chromatography (hexanes/*tert*-butyl methyl ether, 19:1) to give alcohol **2** as a colorless oil that solidified upon standing (735 mg, 96%). mp: 49–50 °C [*tert*-butyl methyl ether]. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.35–7.31 (m, 4H), 7.28–7.24 (m, 6H), 4.68–4.64 (m, 1H), 4.24 (s, 2H), 2.91 (d, *J* = 7.1, 2H), 1.61 (d, *J* = 2.5, 6H), 1.43 ppm (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 203.6, 145.3, 128.4, 128.3, 126.4, 94.5, 84.5, 68.4, 52.3, 37.4, 20.5 ppm; IR (film): $\tilde{\nu}$ = 3581, 3475, 3083, 3055, 2974, 2921, 2880, 1971, 1952, 1884,

[9] J. Löfstedt, J. Franzén, J.-E. Bäckvall, *J. Org. Chem.* **2001**, *66*, 8015–8025.

1807, 1598, 1577, 1493, 1443, 1377, 1363, 1308, 1227, 1189, 1154, 1121, 1105, 1072, 1035, 1017, 1004, 951, 907, 885, 818, 771, 755, 732, 691 cm^{-1}; MS (EI) *m/z* (%) = 278 [M^+] (23), 263 (34), 248 (34), 233 (63), 205 (100), 179 (28), 178 (32), 165 (31), 157 (24), 115 (41), 103 (25), 91 (61), 83 (34), 77 (22), 69 (80); HRMS (ESI): *m/z* calcd. for $C_{20}H_{22}ONa$ [M^+ + Na]: 301.1568, found: 301.1570. The analytical and spectroscopic data are in agreement with those reported in the literature.[10]

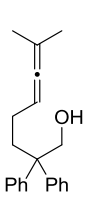
All other hydroxy-allenes were prepared analogously. Their spectral and analytical data are summarized below.

Hydroxy-allene 6. The crude material was purified by flash chromatography (pentane/*tert*-butyl methyl ether, 10:1) to give hydroxy-allene **6** (87%) as a colorless oil. ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 4.91 (thept, *J* = 10.9, 2.8, 1H), 3.41 (d, *J* = 3.7, 2H), 1.99 (d, *J* = 8.1, 2H), 1.67 (d, *J* = 3.2, 6H), 1.46–1.42 (m, 5H), 1.36–1.28 (m, 6H); ^{13}C NMR (100 MHz, CD_2Cl_2): d = 203.3, 94.2, 84.8, 68.9, 38.3, 35.5, 32.5, 26.8, 21.8, 20.7; IR (film): v = 3356, 2977, 2924, 2851, 1972, 1965, 1451, 1403, 1362, 1237, 1214, 1188, 1134, 1112, 1034, 1027, 1008, 975, 923, 894, 847, 829, 805, 704, 655 cm^{-1}; MS (EI) *m/z* (%) = 194 [M^+] (5), 180 (12), 179 (100), 95 (13), 85 (11), 83 (11), 81 (16), 69 (89), 67 (21), 55 (14), 41 (20); HRMS (ESI) calcd. for $C_{13}H_{22}O$ [M^+]: 194.1669, found: 194.1671.



Hydroxy-allene 7. The crude material was purified by flash chromatography (hexanes/EtOAc, 10:1) to give the title compound as a white solid (93%). mp 78–79 °C [EtOAc]; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.32–7.27 (m, 4H), 7.23–7.19 (m, 6H), 4.62 (tt, *J* = 7.6, 2.1 Hz, 1H), 4.20 (d, *J* = 6.7, 2H), 2.88 (d, *J* = 7.6 Hz, 2H), 1.98–1.95 (m, 4H), 1.54–1.46 (m, 6H), 1.30 ppm (t, *J* = 6.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.5, 145.9, 128.6, 128.4, 126.5, 102.1, 84.5, 68.4, 52.4, 37.8, 31.7, 27.8, 26.5 ppm; IR (film): ṽ = 3558, 3470, 3059, 3021, 2921, 2880, 2851, 2832, 1963, 1597, 1575, 1494, 1470, 1443, 1323, 1260, 1234, 1104, 1069, 1045, 1024, 977, 919, 897, 845, 834, 805, 769, 755, 695 cm^{-1}; MS (EI) *m/z* (%) = 318 [M^+] (5), 288 (20), 287 (81), 227 (37), 205 (33), 201 (27), 197 (59), 196 (35), 179 (18), 178 (19), 167 (23), 165 (35), 141 (23), 105 (91), 91 (100), 79 (20), 77 (34), 67 (15); HRMS (ESI) *m/z* calcd. for $C_{23}H_{26}O$ [M^+]: 318.1982, found: 318.1984. The analytical and spectroscopic data are in agreement with those reported in the literature.[11]

Hydroxy-allene 8. The crude material was purified by filtration through a short plug of SiO_2 (*tert*-butyl methyl ether) to give the title compound as a colorless oil (99%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.33–7.29 (m, 4H), 7.24–7.19 (m, 6H), 4.94–4.89 (m, 1H), 4.16 (bs, 2H), 2.28–2.23 (m, 2H), 1.75–1.69 (m, 2H), 1.68 (d, *J* = 2.9 Hz, 6H), 1.17 ppm (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.5, 145.6, 128.4, 128.3, 126.5, 95.6, 89.0, 68.5, 52.2, 36.0, 24.5, 20.9 ppm; IR (film): ṽ = 3553, 3411, 3087, 3057, 3024, 2976, 2930, 2907, 2861, 1970, 1958,

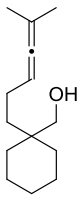


[10] K Aikawa, M. Kojima, K. Mikami, *Adv. Synth. Cat.* **2010**, *352*, 3131–3135; correction: Aikawa, M. Kojima, K. Mikami, *Adv. Synth. Cat.* **2011**, *353*, 2875–2883.

[11] J. L. Arbour, H. S. Rzepa, A. J. P. White, K. K. Hii, *Chem. Commun.* **2009**, 7125–7127.

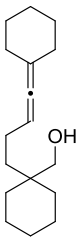
1950, 1878, 1807, 1598, 1579, 1495, 1444, 1386, 1361, 1232, 1188, 1157, 1039, 1023, 1003, 908, 847, 801, 755, 697 cm^{-1}; MS (EI) *m/z* (%) = 292 [M^+] (2), 205 (10), 183 (23), 180 (10), 179 (12), 178 (14), 167 (13), 165 (21), 158 (14), 157 (15), 143 (14), 105 (21), 98 (100), 91 (38), 81 (16), 79 (24), 77 (15), 41 (14); HRMS (ESI) *m/z* calcd. for $C_{21}H_{24}O$ [M^+]: 292.1830, found: 292.1827. The analytical and spectroscopic data are in agreement with those reported in the literature.[12]

Hydroxy-allene 9. The crude material was purified by flash chromatography (pentane/Et_2O, 5:1) to



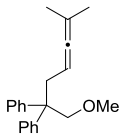
afford the title compound as a colorless oil (79%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 4.99–4.93 (m, 1H), 3.39 (d, *J* = 5.8 Hz, 2H), 1.92–1.86 (m, 2H), 1.67 (d, *J* = 2.9 Hz, 6H), 1.45–1.39 (m, 8H), 1.31–1.28 (m, 4H), 1.25–1.22 ppm (m, 1H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ = 201.7, 95.5, 89.9, 68.4, 37.3, 34.8, 32.8, 26.8, 23.5, 21.9, 20.9 ppm; IR (film): $\tilde{\nu}$ = 3395, 2924, 2851, 1969, 1728, 1451, 1375, 1361, 1262, 1230, 1189, 1135, 1044, 1034, 1022, 976, 848, 797, 713 cm^{-1}; MS (EI) *m/z* (%) = 208 [M^+] (>1), 121 (19), 98 (100), 96 (19), 95 (35), 93 (16), 82 (31), 81 (31), 79 (29), 67 (53), 55 (22), 41 (26); HRMS (ESI) *m/z* calcd. for $C_{14}H_{25}O$ [$M+H^+$]: 209.1903, found: 209.1905.

Hydroxy-allene 10. The crude material was purified by flash chromatography (pentane/Et_2O, 4:1) to



afford the title compound as a colorless oil (82%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 5.00–4.96 (m, 1H), 3.39 (s, 2H), 2.14-2.05 (m, 4H), 1.92–1.86 (m, 2H), 1.60-1.50 (m, 6H), 1.45-1.40 (m, 7H), 1.31-1.29 ppm (m, 5H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ = 198.3, 103.2, 89.8, 68.6, 37.3, 34.6, 32.9, 32.2, 28.0, 26.9, 26.6, 23.5, 21.9 ppm; IR (film): $\tilde{\nu}$ = 3382, 2924, 2851, 2358, 1996, 1967, 1714, 1446, 1344, 1264, 1238, 1130, 1034, 979, 931, 895, 850, 797, 737, 704 cm^{-1}; MS (EI) *m/z* (%) = 248 [M^+] (31), 205 (71), 187 (20), 167 (20), 166 (100), 109 (36), 108 (37), 107 (27), 97 (16), 96 (18), 95 (34), 93 (28), 911 (23), 81 (62), 80 (16), 79 (48), 67 (57), 55 (27), 41 (18); HRMS (ESI) *m/z* calcd. for $C_{17}H_{28}O$ [M^+]: 248.2141, found: 248.2140.

Allene ether 2-OMe. A solution of hydroxy-allene **2** (175 mg, 0.63 mmol) in THF (1 mL) was added



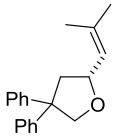
dropwise to a suspension of NaH (18.1 mg, 0.76 mmol) in THF (1 mL) at 0 °C. The mixture was stirred at ambient temperature for 2 h before methyl iodide (78.0 µL, 1.26 mmol) was introduced at 0 °C. The resulting solution was stirred at ambient temperature for another 2 h before it was diluted with *tert*-butyl methyl ether (5 mL) and the reaction was quenched with water (5 mL). The aqueous layer was extracted with *tert*-butyl methyl ether (3 x 10 mL), and the combined extracts were washed with brine (25 mL), dried over Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography (hexanes/*tert*-butyl methyl ether, 50:1) to afford the title compound as a colorless oil that solidified upon standing (128 mg, 70%). mp: 54–55 °C [$CHCl_3$]. ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 7.29–7.25 (m, 4H), 7.20–7.16 (m, 6H), 4.64–4.58 (m, 1H), 3.99 (s, 2H), 3.31 (s, 3H), 2.87 (d, *J* = 7.6 Hz, 2H), 1.57 ppm (d, *J* = 2.9 Hz, 6H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ = 203.9, 146.8, 128.4, 128.2, 126.3, 94.5, 85.0, 78.3, 59.4, 50.9, 37.7, 20.5 ppm; IR (film): $\tilde{\nu}$ = 2979, 2879, 2019, 1597, 1496, 1473, 1443, 1360, 1192, 1135, 1110, 1071, 1029, 985, 940, 795, 775, 754, 739, 698, 629, 615, 571, 504, 423 cm^{-1}; MS (EI) *m/z* (%) = 292

[12] Z. Zhang, C. F. Bender, R. A. Widenhoefer, *Org. Lett.* **2007**, *9*, 2887–2889.

[M$^+$], 248 (20), 247 (100), 245 (14), 212 (11), 211 (74), 210 (33), 205 (23), 201 (14), 180 (11), 179 (41), 178 (37), 175 (30), 169 (27), 167 (18), 165 (31), 152 (13), 115 (10), 105 (33), 91 (62), 77 (18), 41 (13); HRMS (EI): *m/z* calcd. for $C_{21}H_{24}O$ [M$^+$]: 292.1827, found: 292.1825.

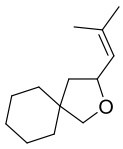
General Procedure for Gold Catalysis. A mixture containing the gold(I)-complex (2.0 µmol, 5.5 mol%) and AgX (1.8 µmol, 5.0 mol%) in EtOH (0.2 mL) was stirred for 15 min at ambient temperature before it was transferred to a solution of the hydroxy-allene substrate (36 µmol) in EtOH (0.2 mL) at the indicated temperature via a cannula equipped with a PTFE filter (Perfect-Flow®, 0.45 µm pore size, Ø 13 mm) to retain the precipitates. The resulting solution was stirred until TLC showed complete conversion. At this point, the solution was filtered through a plug of silica, the filtrate was concentrated and the residue purified by flash chromatography (hexane/*tert*-butyl methyl ether 19:1) to afford the title compound. Reactions performed in non-polar solvents were directly submitted to flash chromatography (hexane/*tert*-butyl methyl ether, 19:1) to yield the title compound.

Tetrahydrofuran 3. Colorless oil (93%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.41–7.30 (m, 6H), 7.27–7.22 (m, 4H), 5.32 (dt, *J* = 8.7, 1.4 Hz, 1H), 4.76 (td, *J* = 9.2, 5.9 Hz, 1H), 4.65 (dd, *J* = 8.7, 1.1 Hz, 1H), 4.20 (d, *J* = 8.7 Hz, 1H), 2.67 (ddd, *J* = 12.2, 5.9, 1.1 Hz, 1H), 2.41 (dd, *J* = 12.2, 9.6 Hz, 1H), 1.76 (d, *J* = 1.3 Hz, 3H), 1.68 ppm (d, *J* = 1.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.4, 146.3, 136.5, 128.5, 128.5, 127.3, 127.3, 126.5, 126.4, 125.9, 77.0, 75.3, 56.5, 45.6, 26.0, 18.4 ppm; IR (film): $\tilde{\nu}$ = 3459, 3058, 3026, 2976, 2924, 1784, 1730, 1598, 1579, 1494, 1446, 1378, 1316, 1275, 1157, 1028, 1001, 972, 912, 868, 841, 754, 731, 697, 660 cm^{-1}; MS (EI) *m/z* (%) = 278 [M$^+$] (69), 263 (38), 248 (46), 233 (70), 205 (100), 180 (21), 179 (35), 178 (29), 165 (41), 157 (31), 116 (23), 115 (32), 103 (29), 91 (71), 83 (32), 77 (20), 69 (81); HRMS (ESI): *m/z* calcd. for $C_{20}H_{22}O$ [M$^+$]: 278.1670, found: 278.1671; $[\alpha]_D^{20}$ = +146.9 (c = 1.0, $CHCl_3$) (97% *ee*). The *ee* was determined by HPLC (250 mm, Chiralcel IA (IA00CE-LH-028), 5 µm, Ø 4.6 mm, *n*-heptane/2-propanol 98:2, flow rate = 1.0 mL/min 4.0 MPa, 298 K, UV, 220 nm): major enantiomer t_R = 6.0 min; minor enantiomer t_R = 6.9 min.



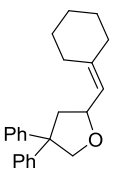
The absolute configuration was assigned to be (*R*) by comparison of the optical rotation of the sample ($[\alpha]_D^{20}$ = +146.9 (c = 1.0, $CHCl_3$) (97% *ee*)) with that of the (*S*)-enantiomer reported in the literature, which had the opposite sign ($[\alpha]_D^{20}$ = –74.9 (c = 0.36, $CHCl_3$) (70% *ee*)).[10]

Tetrahydrofuran 11. Colorless oil (89%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 5.21 (dt, *J* = 8.5, 1.4 Hz, 1H), 4.59 (td, *J* = 8.8, 6.6 Hz, 1H), 3.63 (d, *J* = 8.4 Hz, 1H), 3.50 (d, *J* = 8.4 Hz, 1H), 1.88 (dd, *J* = 12.4, 6.6 Hz, 1H), 1.72 (d, *J* = 1.4 Hz, 3H), 1.68 (d, *J* = 1.3 Hz, 3H), 1.47–1.39 (m, 10H), 1.34 ppm (dd, *J* = 12.4, 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 135.7, 126.6, 78.5, 75.4, 45.6, 44.3, 37.2, 35.8, 26.2, 25.9, 24.2, 23.8, 18.3 ppm; IR (film): $\tilde{\nu}$ = 2922, 2851, 1676, 1447, 1376, 1316, 1258, 1106, 1050, 1006, 979, 946, 891, 866, 849, 820, 668 cm^{-1}; MS (EI) *m/z* (%) = 194 [M$^+$] (2), 112 (48), 98 (15), 95 (25), 83 (26), 82 (100), 81 (23), 79 (28), 69 (20), 67 (62), 55 (22), 41 (36); HRMS (ESI): *m/z* calcd. for $C_{13}H_{22}O$ [M$^+$]: 194.1669, found: 194.1671; $[\alpha]_D^{20}$ = +6.2 (c = 1.0, $CHCl_3$) (95% *ee*). The *ee* was determined by HPLC (150 mm, Chiralcel OJ-3R (OJ3RCD-QD007),

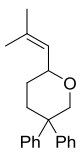


3 µm, Ø 4.6 mm, acetonitrile/H_2O 60:40, flow rate = 0.5 mL/min 10.6 MPa, 288 K, UV, 210 nm): major enantiomer t_R = 16.6 min; minor enantiomer t_R = 17.9 min.

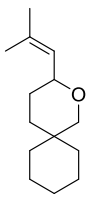
Tetrahydrofuran 12. Colorless oil (91%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.35–7.27 (m, 6H), 7.23–7.18 (m, 4H), 5.23 (dt, *J* = 8.7, 1.2 Hz, 1H), 4.77 (ddd, *J* = 9.7, 8.7, 5.9 Hz, 1H), 4.62 (dd, *J* = 8.7, 1.1 Hz, 1H), 4.16 (d, *J* = 8.7 Hz, 1H), 2.62 (ddd, *J* = 12.2, 5.9, 1.1 Hz, 1H), 2.38 (dd, *J* = 12.2, 9.7 Hz, 1H), 2.18–2.14 (m, 1H), 2.11–2.04 (m, 3H), 1.58–1.45 ppm (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.5, 146.3, 144.2, 128.5, 128.5, 127.3, 127.3, 126.5, 126.3, 122.7, 77.0, 74.4, 56.6, 46.0, 37.2, 29.4, 28.5, 28.0, 26.8 ppm; IR (film): $\tilde{\nu}$ = 3089, 3058, 3026, 2925, 2853, 1789, 1668, 1598, 1493, 1446, 1324, 1268, 1131, 1051, 1030, 1001, 970, 933, 909, 863, 756, 730, 697, 658 cm^{-1}; MS (EI) *m/z* (%) = 318 [M$^+$] (100), 288 (52), 241 (24), 206 (26), 205 (62), 197 (46), 194 (29), 193 (22), 180 (48), 179 (38), 178 (29), 167 (65), 165 (44), 125 (15), 124 (48), 123 (25), 116 (22), 115 (30), 103 (26), 91 (54), 81 (30), 77 (16); HRMS (ESI): *m/z* calcd. for $C_{23}H_{26}O$ [M$^+$]: 318.1980, found: 318.1984; $[\alpha]_D^{20}$ = +87.8 (c = 1.0, $CHCl_3$) (94% *ee*). The *ee* was determined by HPLC (250 mm, Chiralcel IA (IA00CE-LH-028), 5 µm, Ø 4.6 mm, *n*-heptane/2-propanol 98:2, flow rate = 1.0 mL/min 4.0 MPa, 298 K, UV, 220 nm): major enantiomer t_R = 5.9 min; minor enantiomer t_R = 6.6 min.



Tetrahydropyran 13. Colorless oil (93%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.45–7.42 (m, 2H), 7.30–7.23 (m, 4H), 7.19–7.16 (m, 4H), 5.15 (dt, *J* = 8.2, 1.4 Hz, 1H), 4.64 (dd, *J* = 12.1, 2.3 Hz, 1H), 4.14 (ddd, *J* = 10.9, 8.2, 2.5 Hz, 1 H), 3.61 (d, *J* = 12.1 Hz, 1H), 2.50–2.45 (m, 2H), 1.70 (s, 6H), 1.53–1.49 (m, 1H), 1.39–1.32 ppm (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.9, 145.9, 136.1, 129.1, 128.4, 128.1, 127.1, 126.4, 126.0, 125.8, 75.1, 75.0, 45.8, 34.8, 28.4, 25.9, 18.5 ppm; IR (film): $\tilde{\nu}$ = 3087, 3058, 3023, 2936, 2916, 2848, 1678, 1598, 1579, 1494, 1445, 1375, 1319, 1243, 1195, 1139, 1090, 1076, 1032, 1011, 972, 910, 870, 821, 764, 752, 731, 695, 661 cm^{-1}; MS (EI) *m/z* (%) = 292 [M+] (7), 214 (12), 201 (14), 194 (11), 181 (16), 180 (100), 179 (33), 178 (25), 165 (35), 115 (12), 91 (14), 82 (19), 67 (10); HRMS (ESI): *m/z* calcd. for $C_{21}H_{24}O$ [M$^+$]: 292.1828, found: 292.1827; $[\alpha]_D^{20}$ = +206.2 (c = 1.3, $CHCl_3$) (98% *ee*). The *ee* was determined by HPLC (250 mm, Chiralcel IA (IA00CE-LH-028), 5 µm, Ø 4.6 mm, *n*-heptane/2-propanol 98:2, flow rate = 1.0 mL/min 4.0 MPa, 298 K, UV, 220 nm): major enantiomer t_R = 4.2 min; minor enantiomer t_R = 4.6 min.

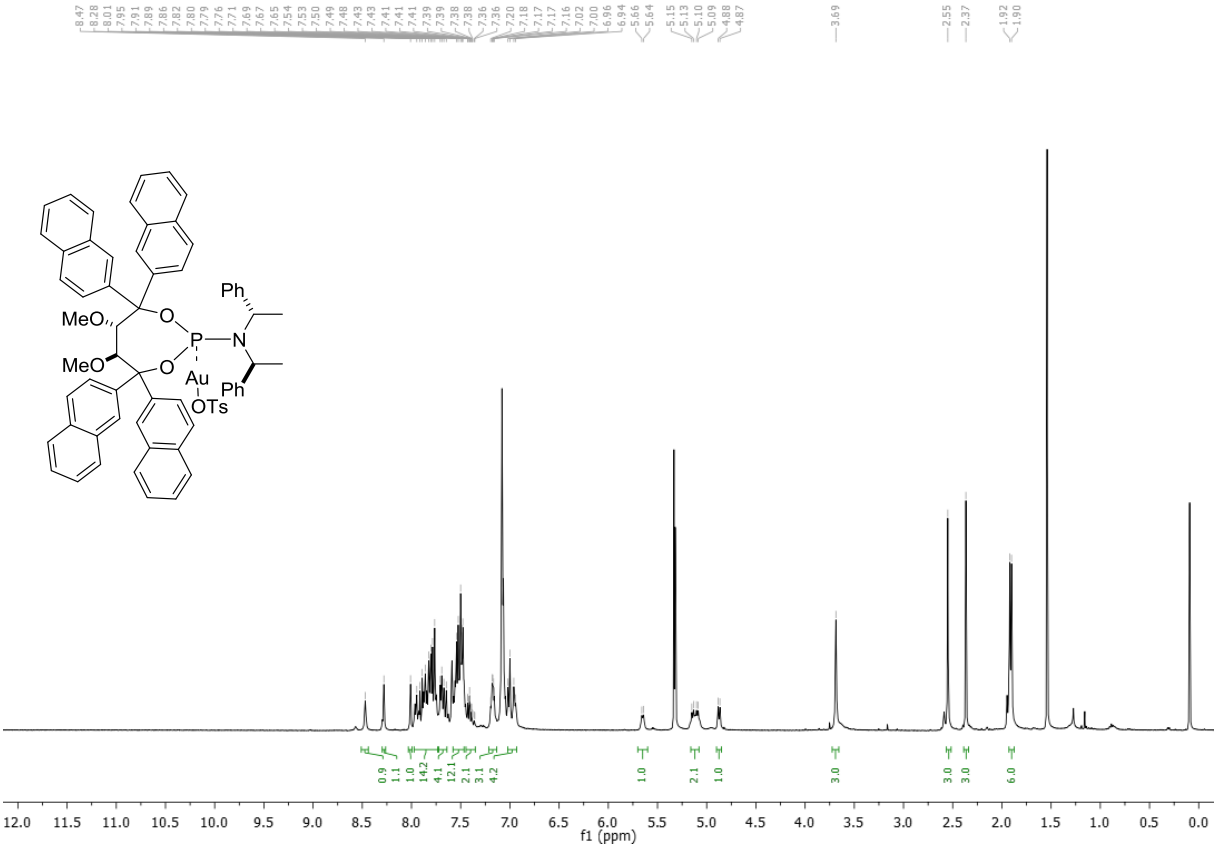


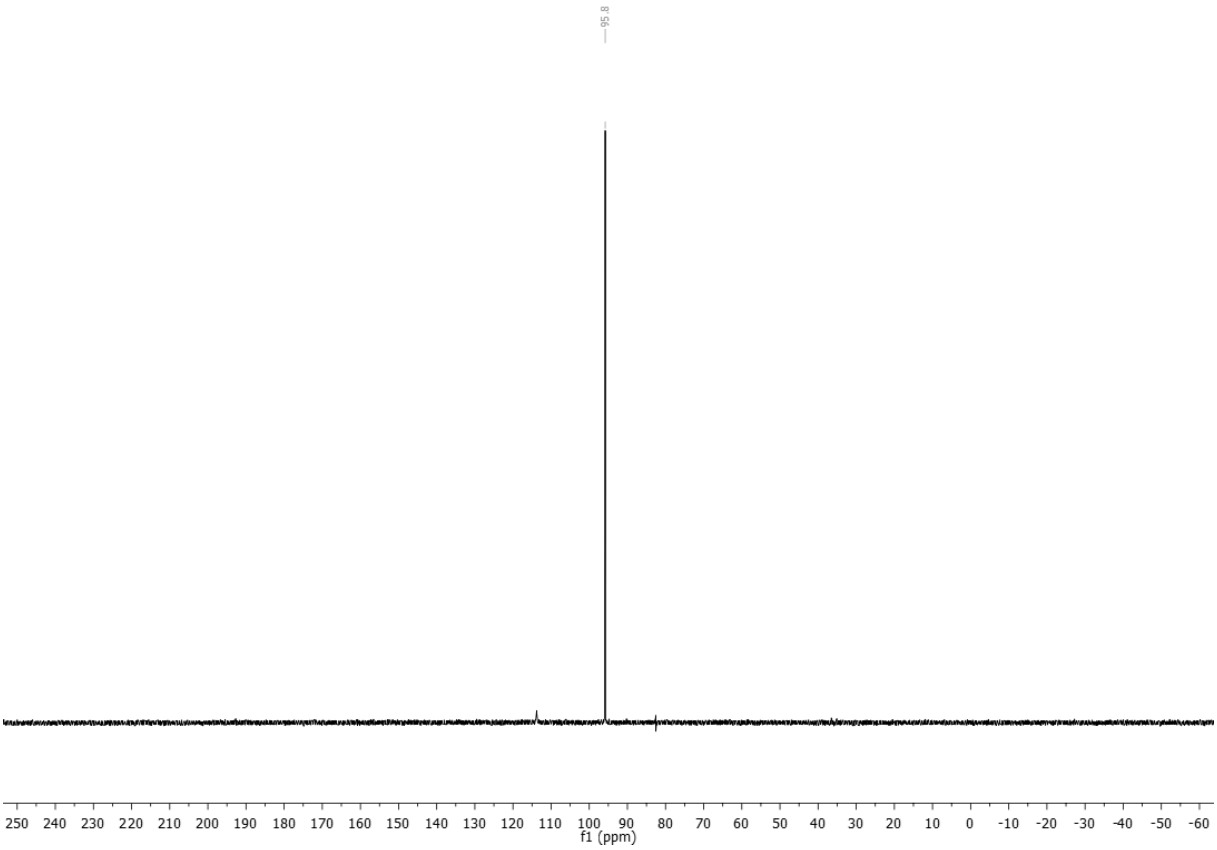
Tetrahydropyran 14. Colorless oil (89%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 5.15 (d, *J* = 7.9 Hz, 1H), 3.89 (ddd, *J* = 10.8, 7.8, 2.6 Hz, 1H), 3.69 (dd, J = 11.3, 2.6 Hz, 1H), 3.09 (d, *J* = 11.2 Hz, 1H), 1.76–1.72 (m, 1H), 1.70 (s, 3H), 1.65 (s, 3H), 1.56-1.53 (m, 1H), 1.49-1.32 (m, 9H), 1.23-1.19 (m, 1H), 1.14-1.11 ppm (m, 2H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ = 134.8, 127.0, 76.6, 75.8, 37.0, 34.5, 32.1, 31.6, 28.2, 27.3, 25.7, 21.9, 21.9, 18.4 ppm; IR (film): $\tilde{\nu}$ = 2923, 2848, 2162, 2024, 1736, 1678, 1450, 1375, 1345, 1326, 1270, 1259, 1222, 1184, 1157, 1129, 1080, 1071, 1054, 1007, 987, 952, 930, 906, 865, 846, 819, 713, 668 cm^{-1}; MS (EI) *m/z* (%) = 208 [M$^+$] (17), 193 (100), 175 (23), 109 (25), 95 (26), 85 (32), 82 (31), 81 (43), 69 (21), 67 (64), 55 (25), 41 (27); HRMS (ESI): *m/z* calcd. for $C_{14}H_{24}O$ [M$^+$]: 208.1827, found: 208.1827; $[\alpha]_D^{20}$ = –14.2 (c = 1.3, $CHCl_3$) (97% *ee*). The *ee* was determined by GC (30 m, BGB-176/SE-52 G/510, 220/80 1/min 150 12/min 220 5min iso/320, flow rate 0.50 bar H_2: minor enantiomer t_R = 62.5 min; major enantiomer t_R = 63.1 min).



Tetrahydropyran 15. Colorless oil (84%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 5.09 (dt, *J* = 7.9, 1.2 Hz, 1H), 3.93 (ddd, *J* = 10.8, 7.8, 2.8 Hz, 1H), 3.69 (dd, *J* = 11.2, 2.7 Hz, 1H), 3.08 (d, *J* = 11.3 Hz, 1H), 2.18–2.12 (m, 2H), 2.09–2.04 (m, 2H), 1.74 (dq, *J* = 13.1, 2.9 Hz, 1H), 1.61–1.53 (m, 4H), 1.52-1.29 (m, 12H), 1.26-1.18 (m, 1H), 1.15-1.10 (m, 2H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ = 142.6, 123.8, 76.6, 75.1, 37.2, 37.0, 34.5, 32.1, 31.6, 29.8, 28.9, 28.7, 28.3, 27.3, 27.1, 21.9, 21.9 ppm; IR (film): $\tilde{\nu}$ = 3391, 2924, 2851, 1729, 1449, 1258, 1187, 1157, 1071, 1050, 1011, 952, 905, 866, 846, 802, 736 cm^{-1}; MS (EI) *m/z* (%) = 248 [M^+] (18), 207 (19), 205 (56), 187 (18), 167 (19), 166 (98), 133 (15), 123 (17), 109 (49), 108 (53), 107 (38), 97 (27), 96 (33), 95 (54), 94 (17), 93 (43), 91 (40), 83 (17), 82 (17), 81 (100), 80 (25), 79 (79), 77 (28), 68 (20), 67 (97), 57 (22), 55 (47), 53 (18); HRMS (ESI): *m/z* calcd. for $C_{17}H_{28}ONa^+$ [M+Na^+]: 271.2030, found: 271.2032; $[\alpha]_D^{20}$ = –0.8 (c = 1.3, $CHCl_3$) (99% *ee*). The *ee* was determined by HPLC (150 mm, Chiralcel OJ-3R (OJ3RCD-QD007), 3 µm, Ø 4.6 mm, Acetonitrile, flow rate = 0.5 mL/min, 3.8 MPa, 298 K, UV, 210 nm): minor enantiomer t_R = 6.7 min; major enantiomer t_R = 18.1 min.

NMR Spectra





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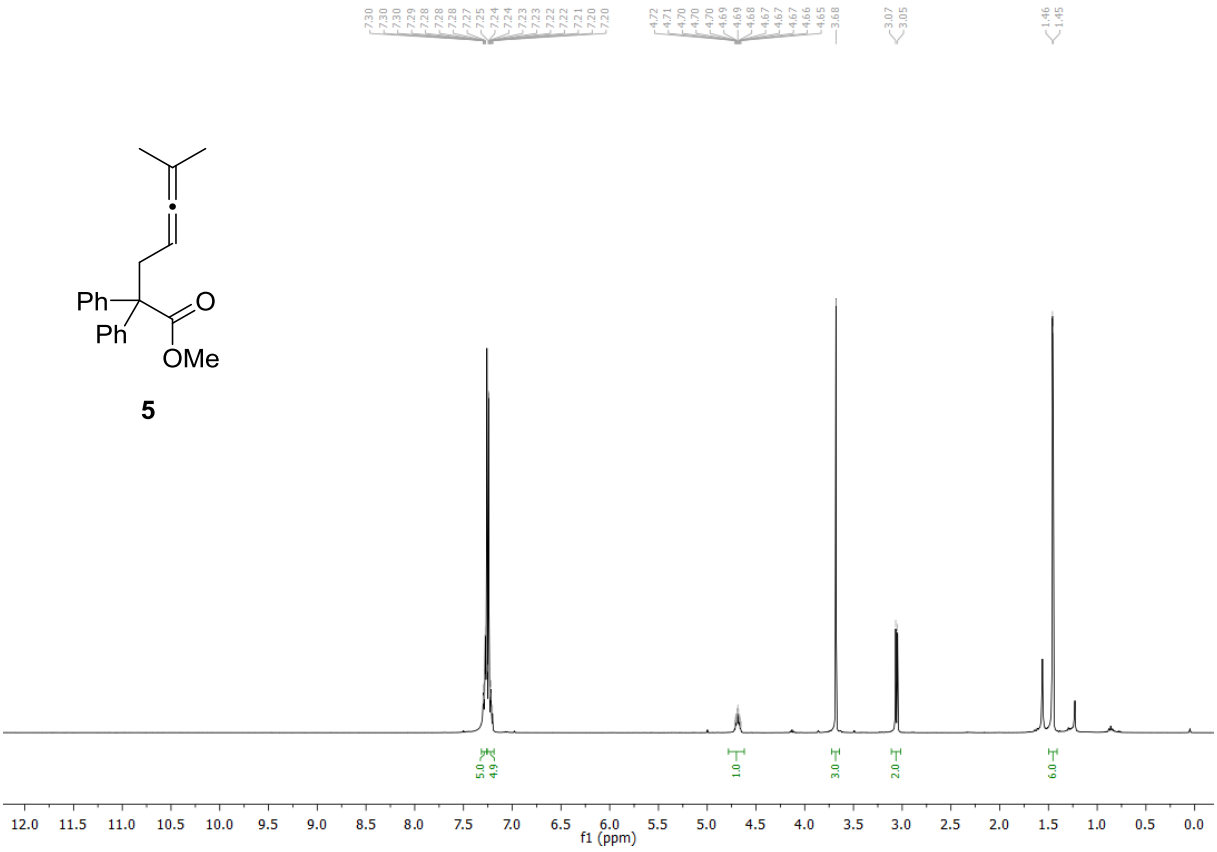

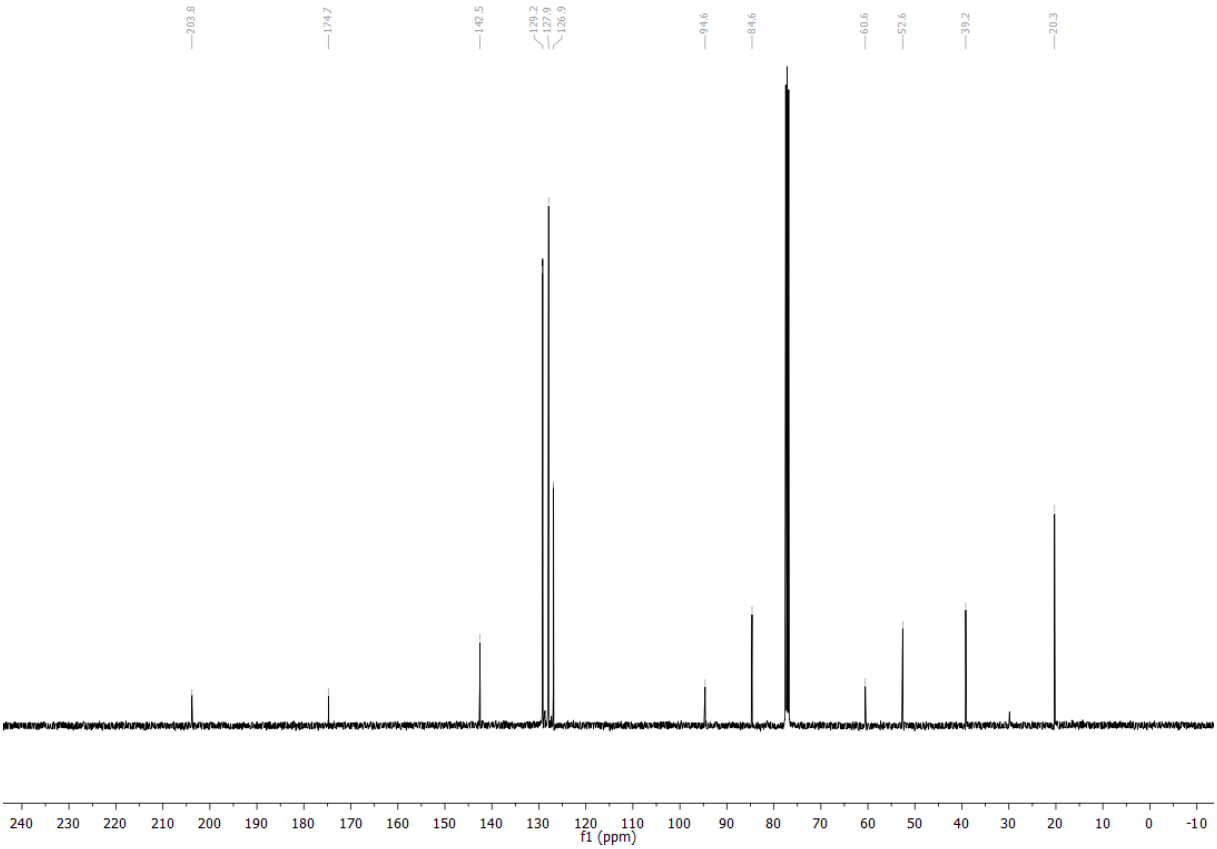

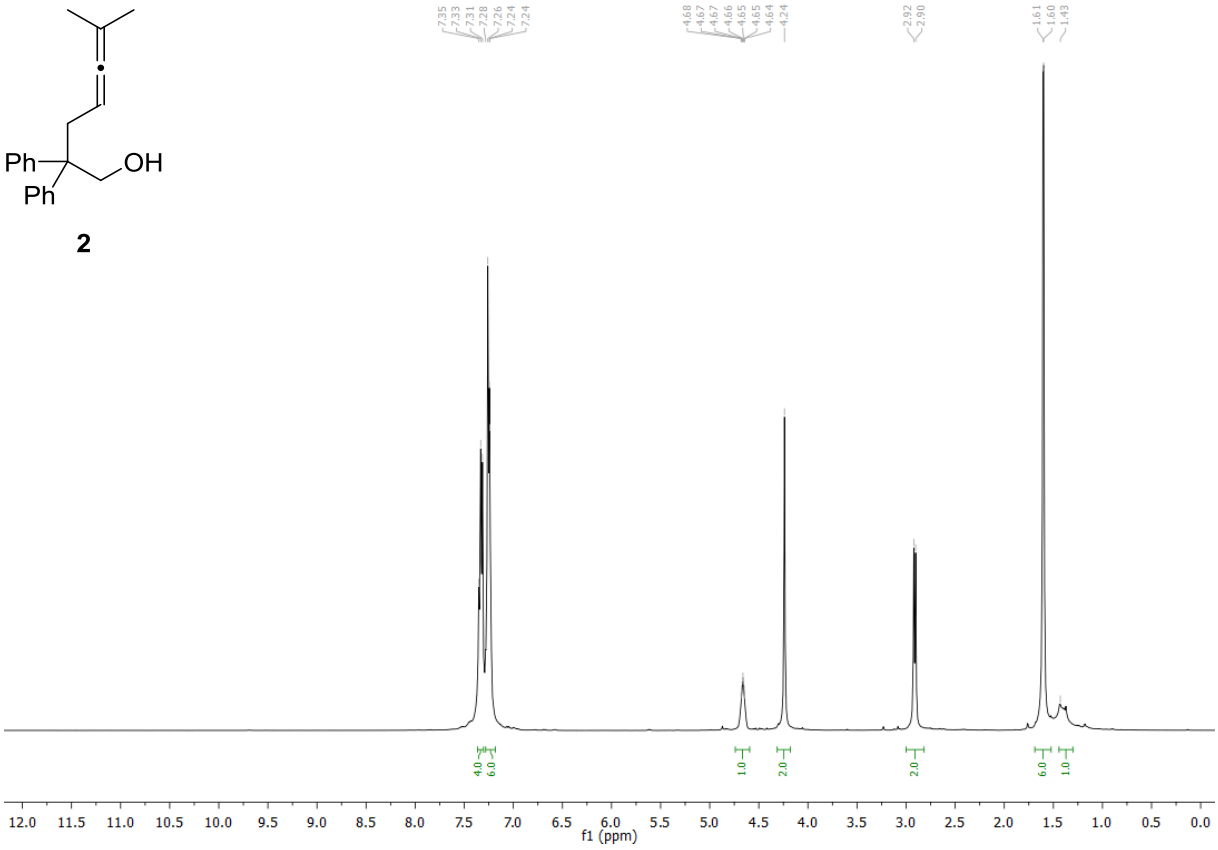
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Ph
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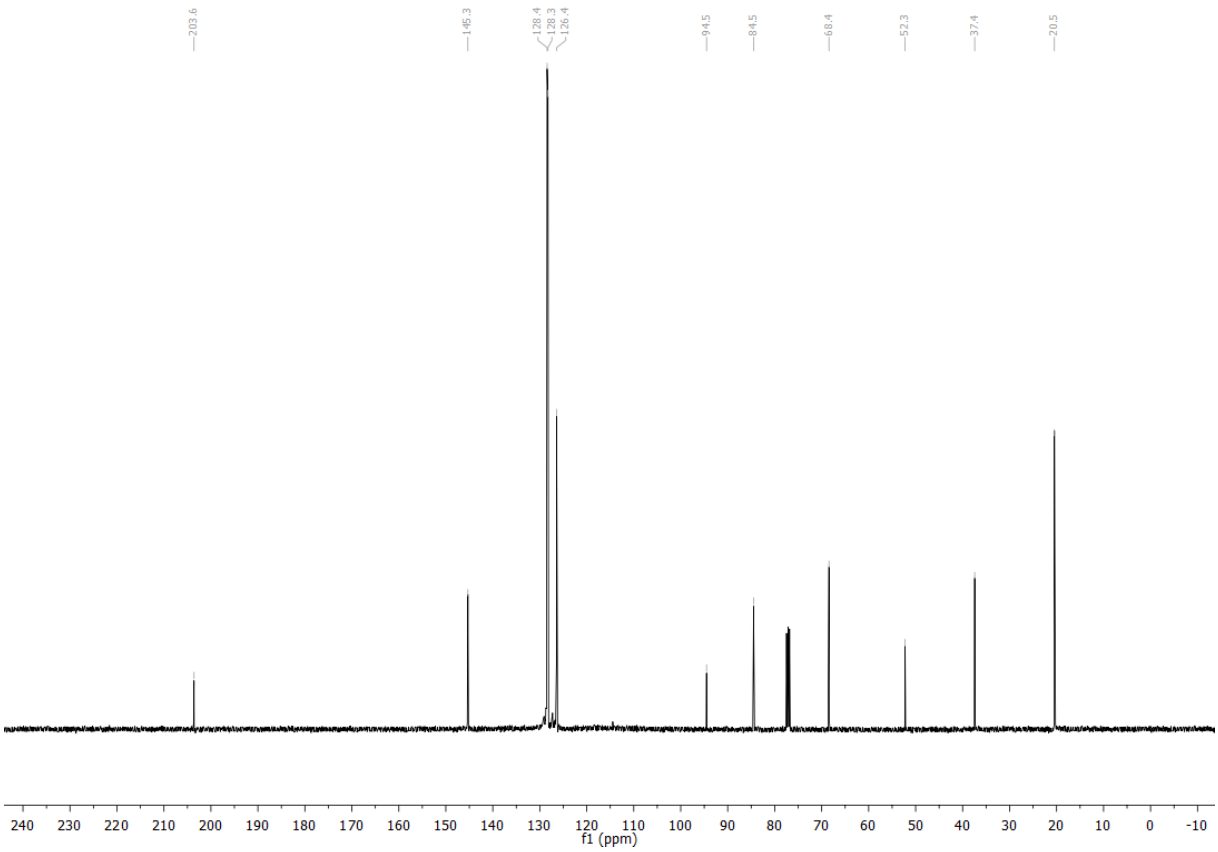
7.26
7.24
7.24
4.68
4.67
4.67
4.66
4.65
4.65
4.64
4.24
2.92
2.90
1.61
1.60
1.43
4.0
6.0
1.0
2.0
2.0
6.0
1.0
f1 (ppm)

2


203.6
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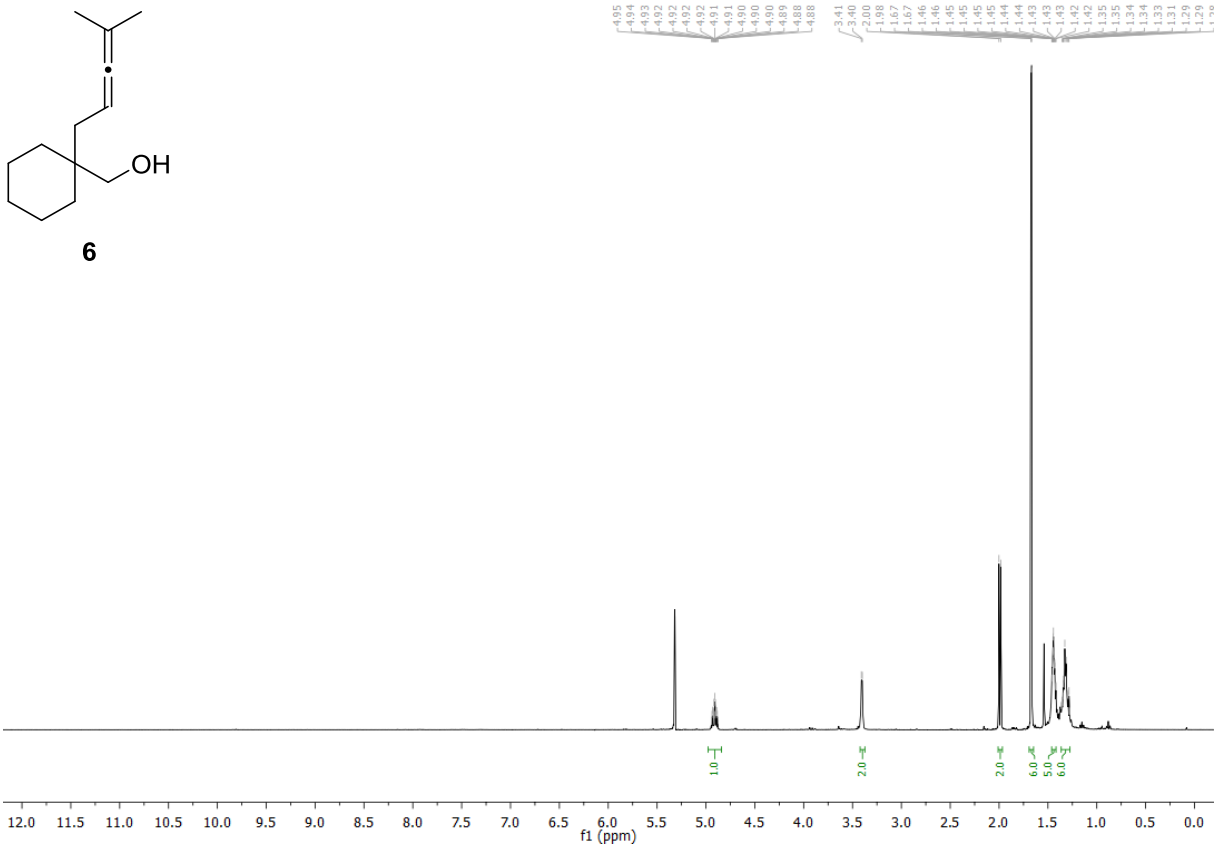
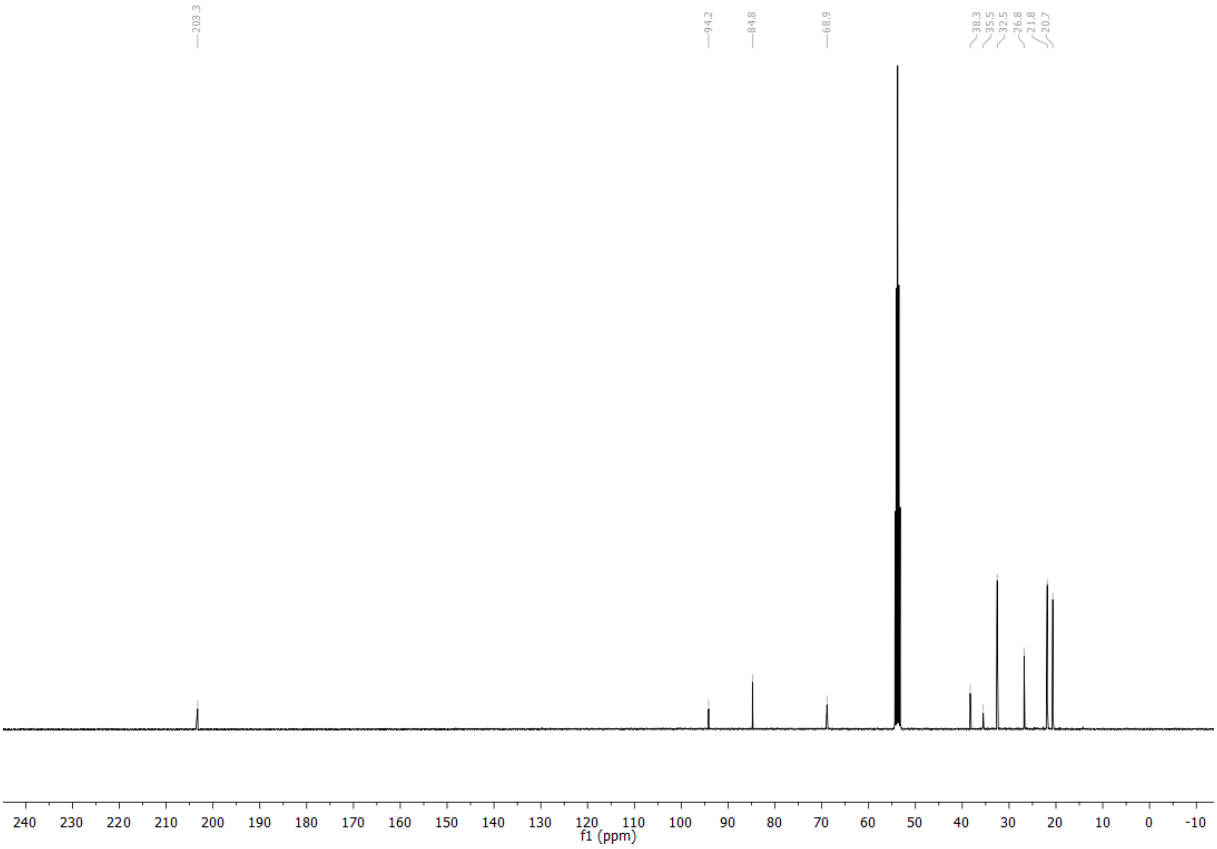
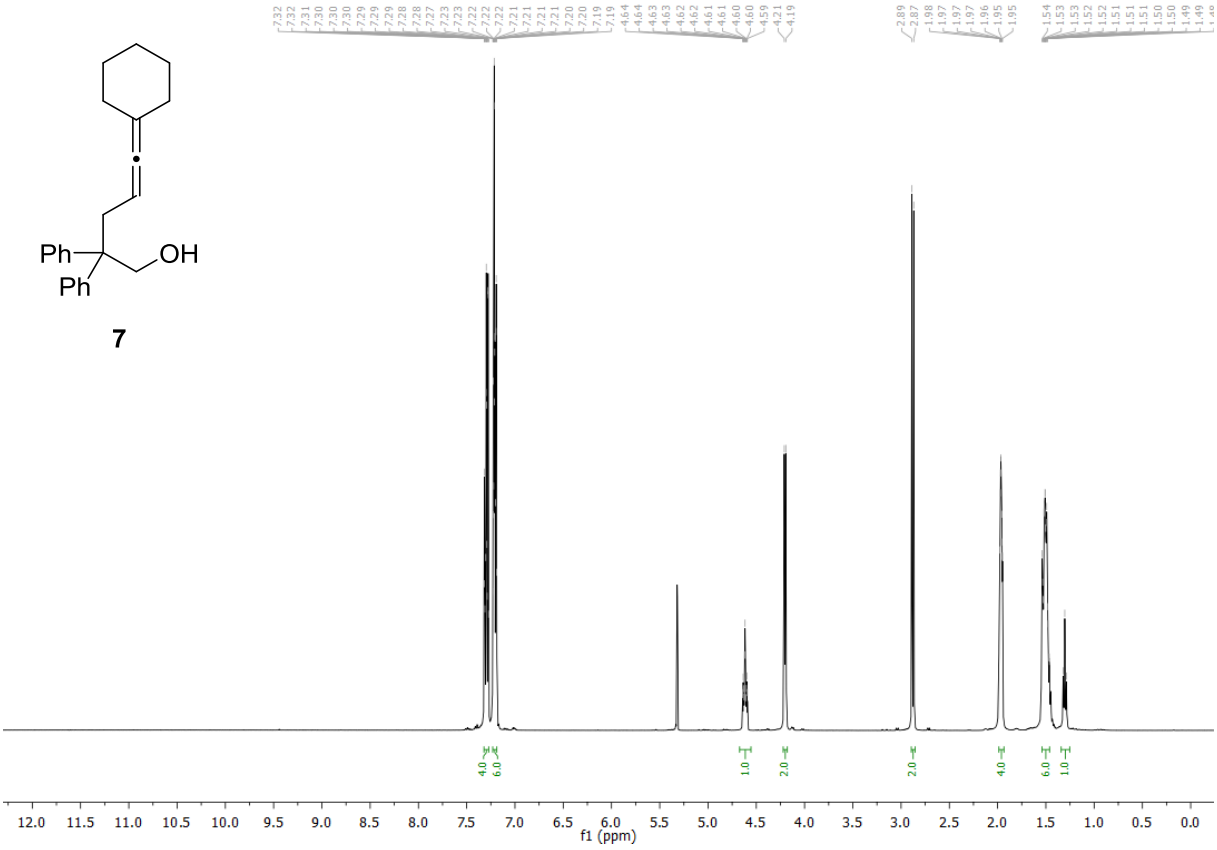
128.3
126.4
94.5
84.5
68.4
52.3
37.4
20.5
f1 (ppm)

6



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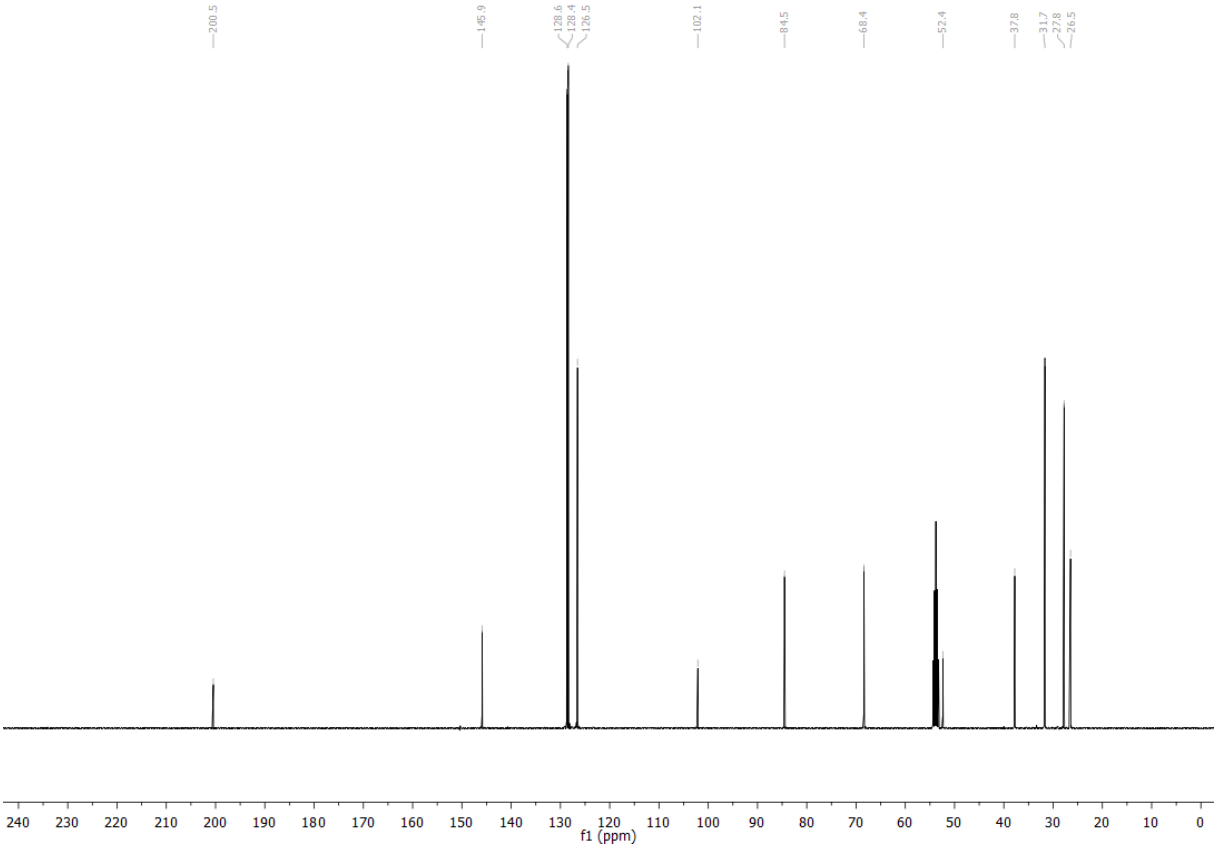
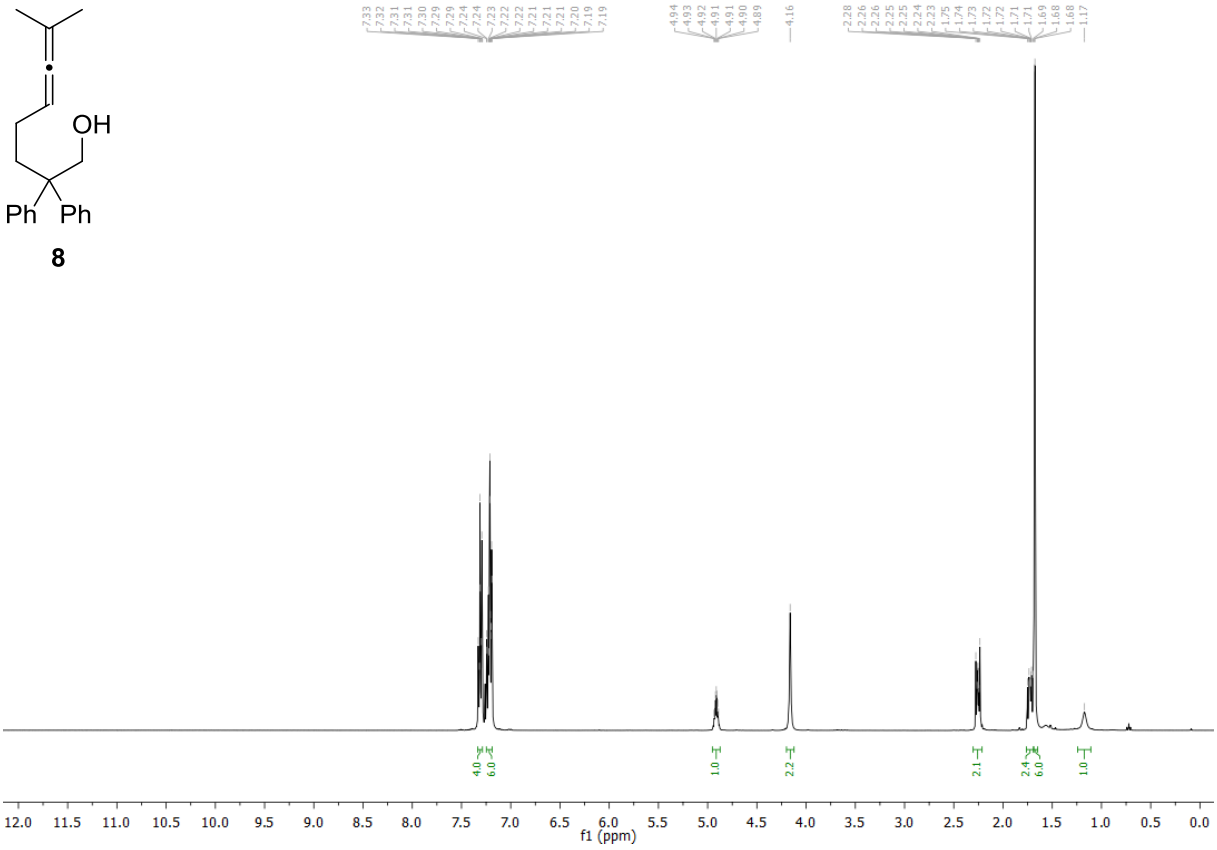
OH
Ph
7
f1 (ppm)


f1 (ppm)

OH
Ph
Ph

8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7.21
7.20
7.19
7.19
4.94
4.93
4.92
4.91
4.91
4.90
4.89
4.16
2.28
2.26
2.26
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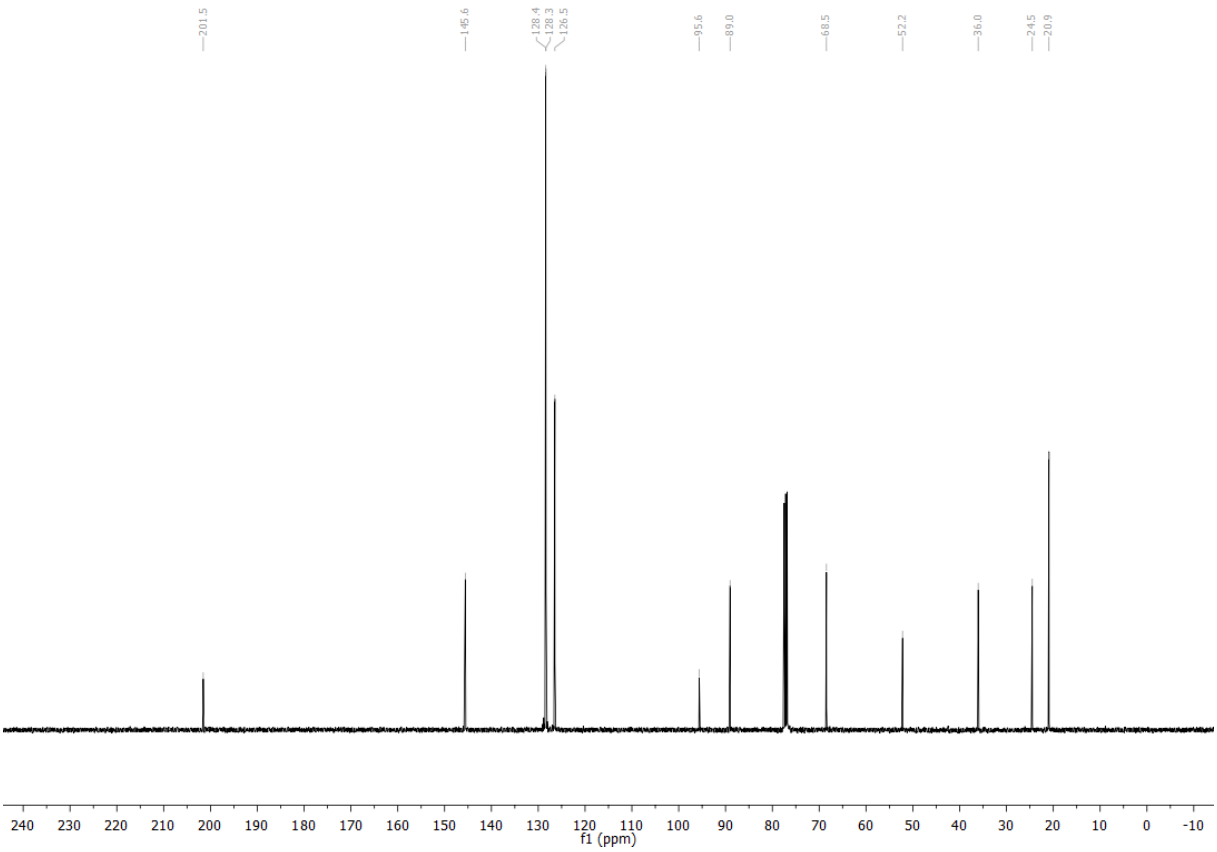
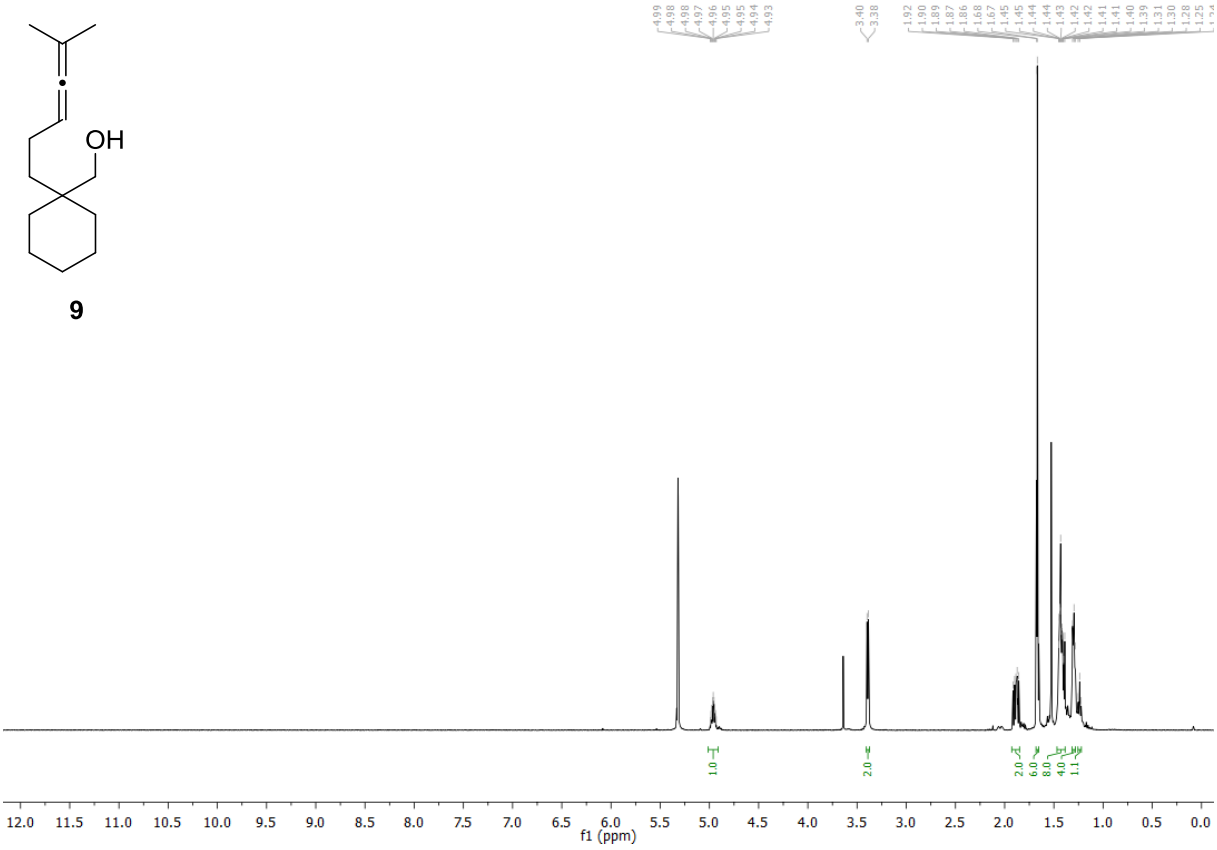
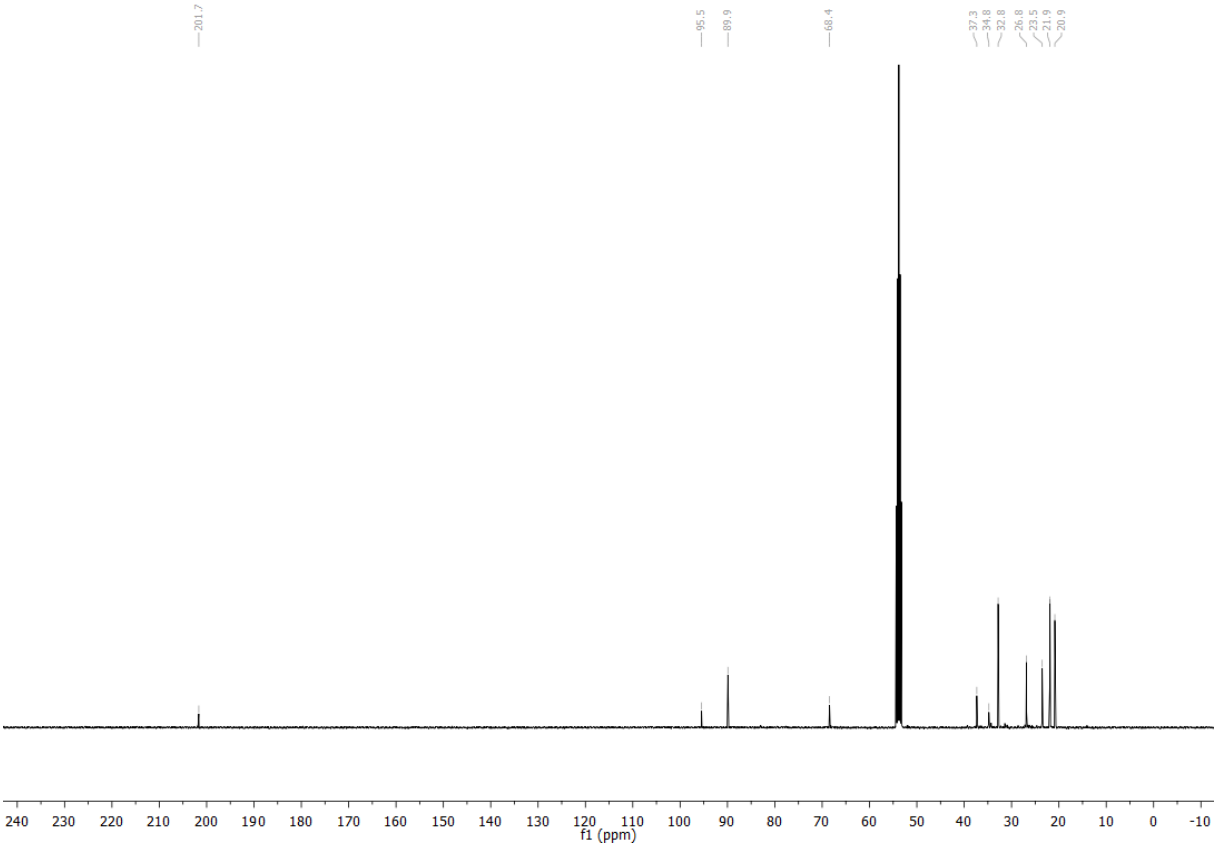
2.24
2.23
1.75
1.74
1.73
1.72
1.72
1.71
1.71
1.71
1.69
1.68
1.68
1.17
4.0
6.0
1.0
2.2
2.1
2.4
6.0
1.0
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


201.5
145.6
128.4
128.3
126.5
95.6
89.0
68.5
52.2
36.0
24.5
20.9
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

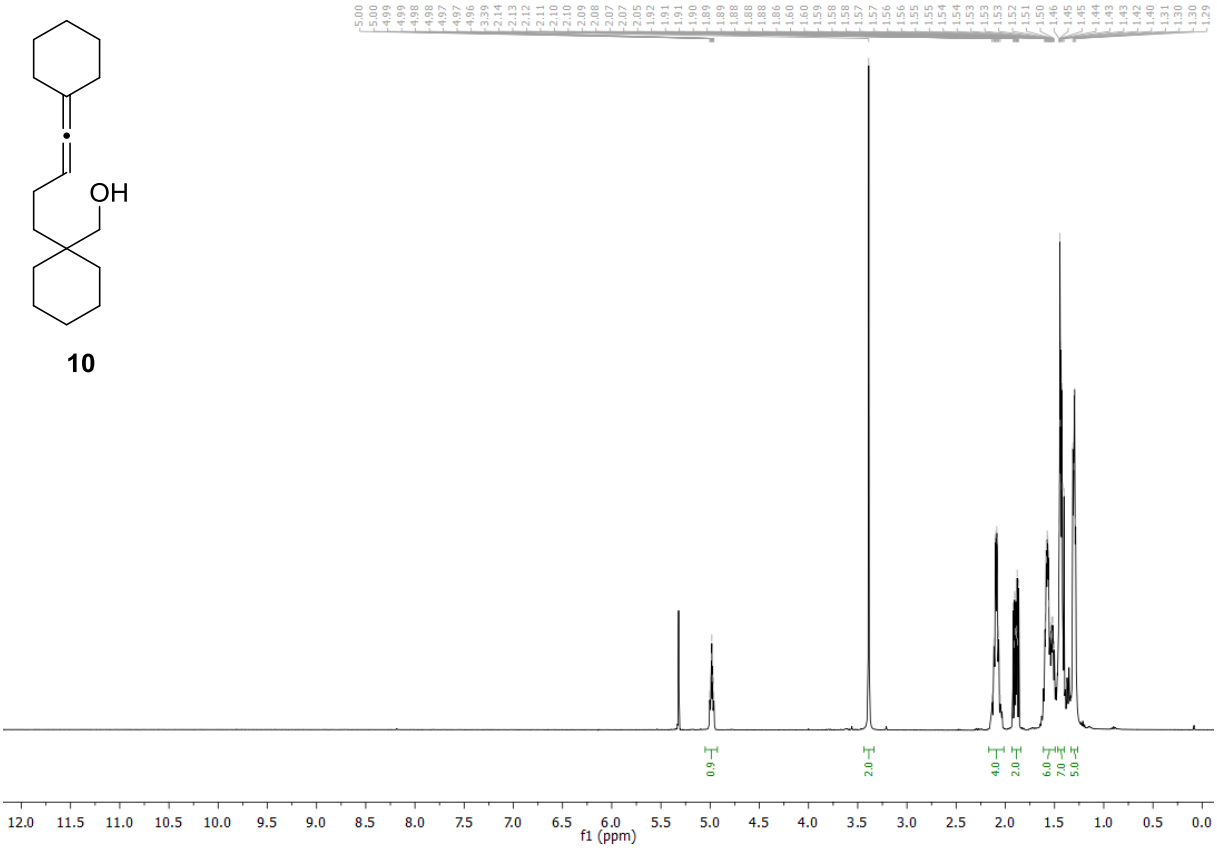
9





OH

10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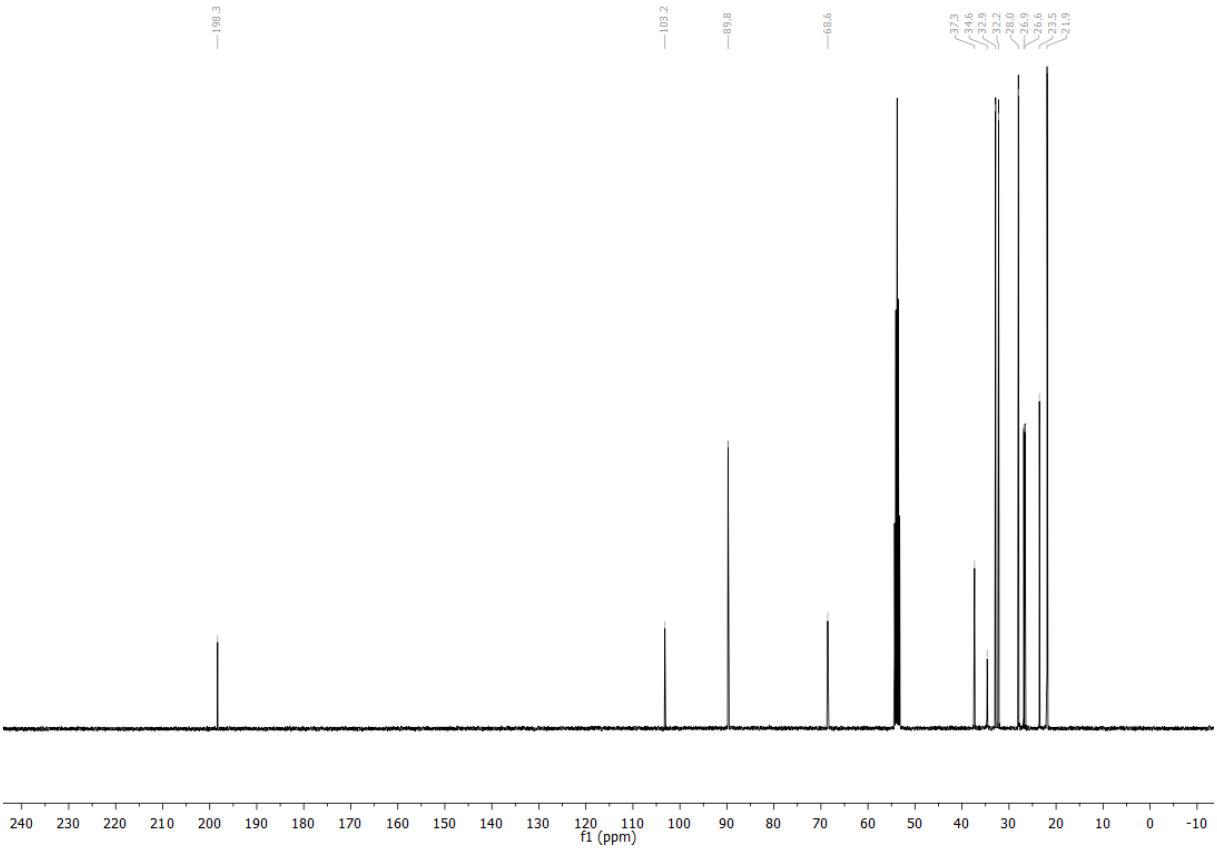
2.0
6.0
7.0
5.0
f1 (ppm)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37.3
34.6
32.9
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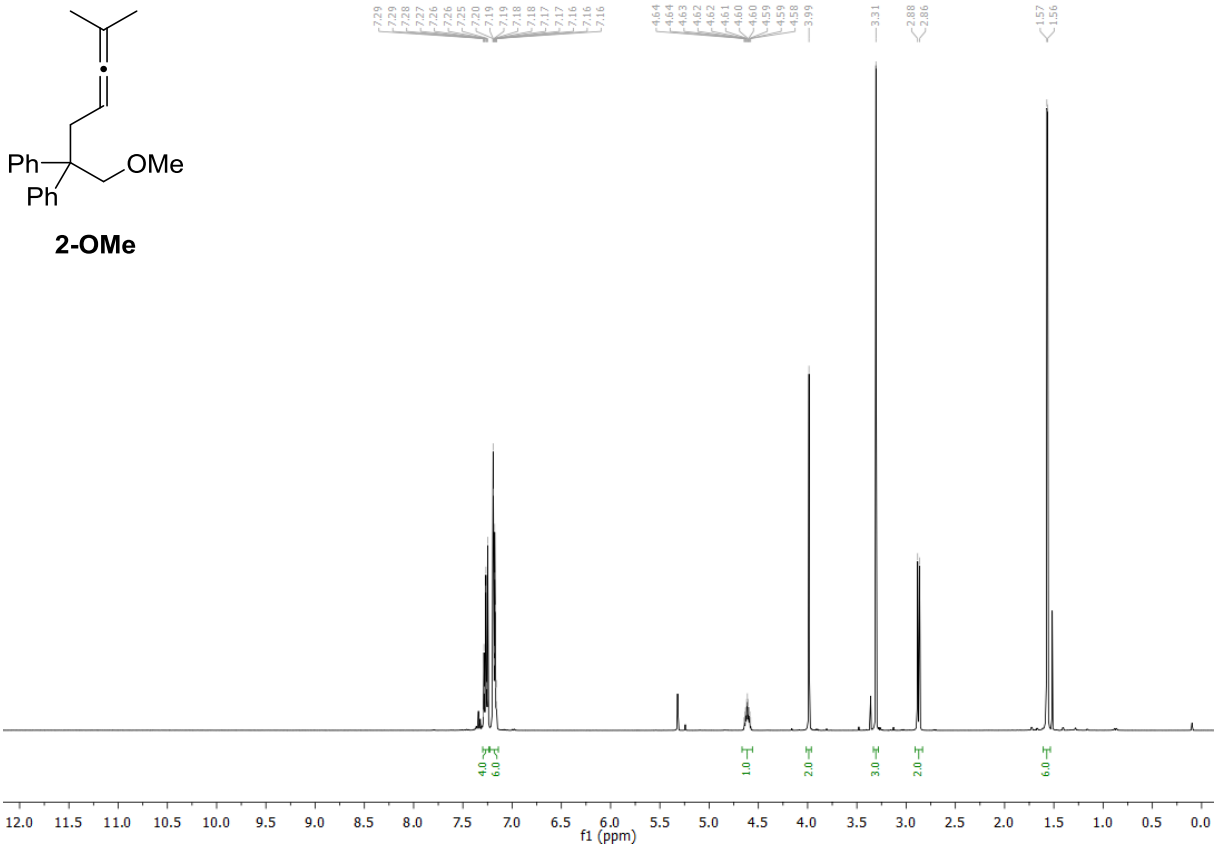
26.9
26.6
23.5
21.9
f1 (ppm)

Ph
OMe
Ph

2-OMe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7.25
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7.19
7.19
7.18
7.18
7.17
7.17
7.16
7.16
7.16
7.16
4.64
4.64
4.63
4.62
4.62
4.61
4.60
4.60
4.59
4.59
4.58
3.99
3.31
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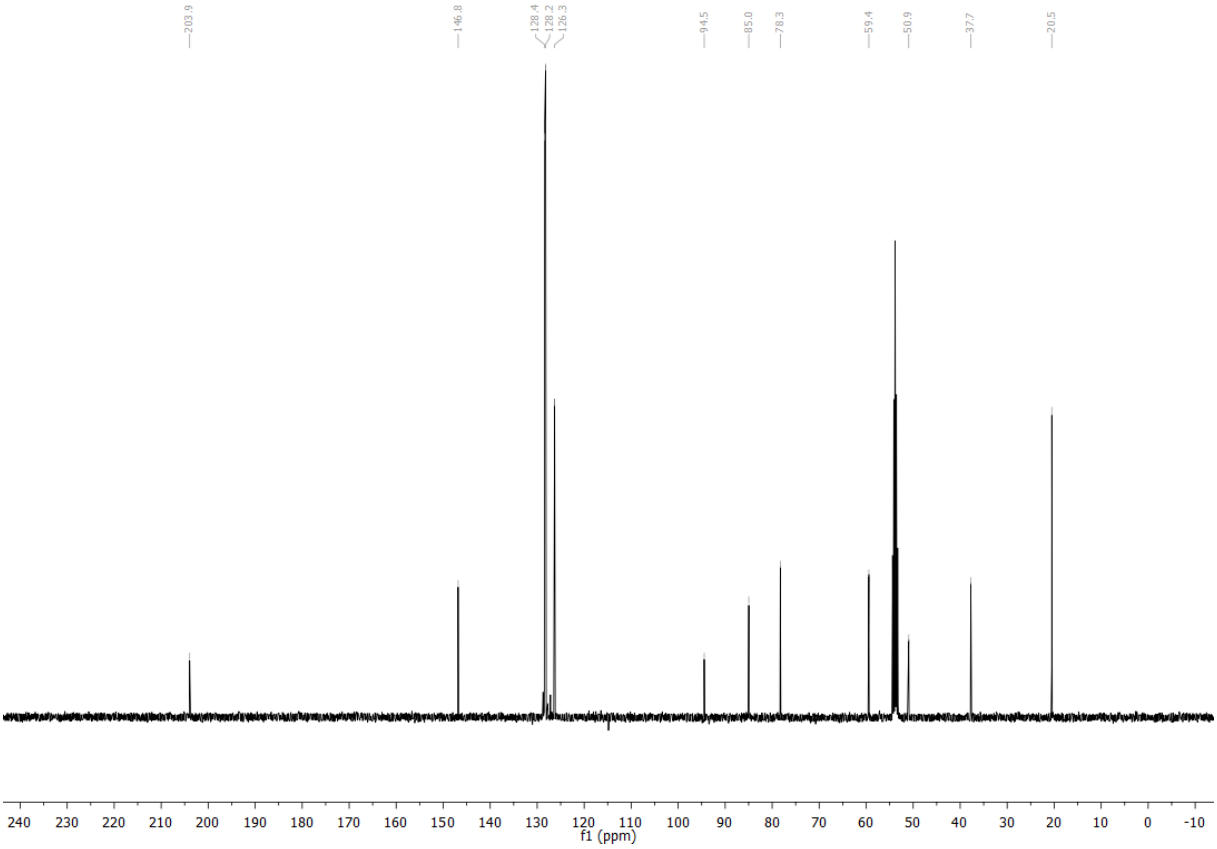
6.0
1.0
2.0
3.0
2.0
6.0
f1 (ppm)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78.3
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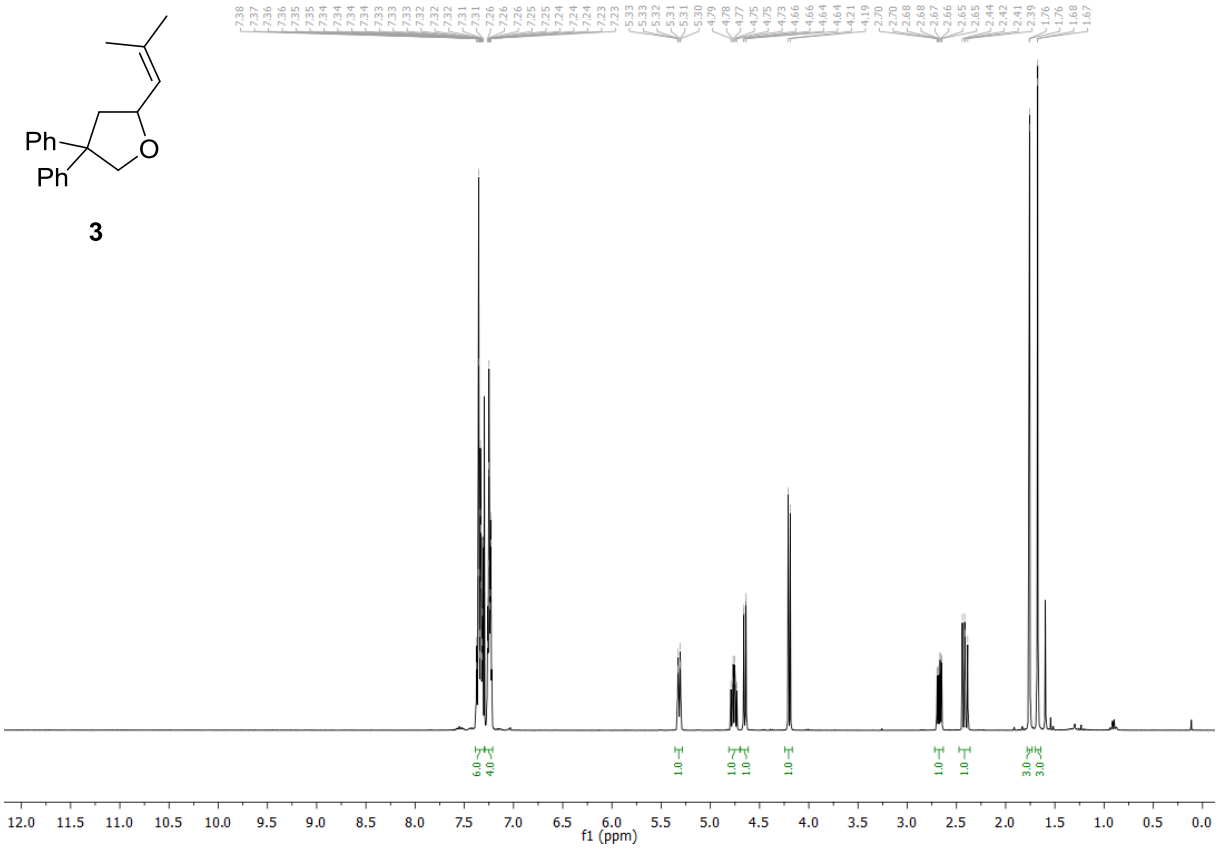
50.9
37.7
20.5
f1 (ppm)

Ph
Ph
O

3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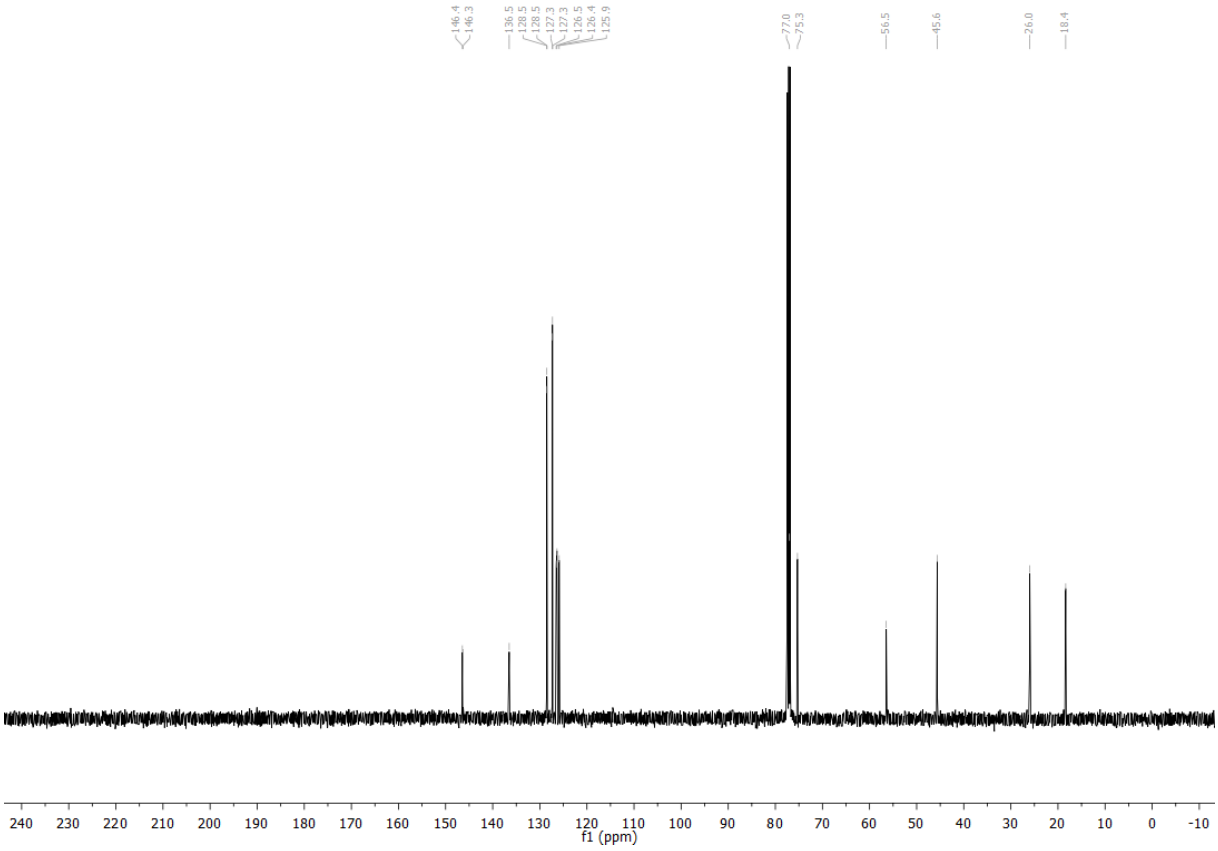
3.0
f1 (ppm)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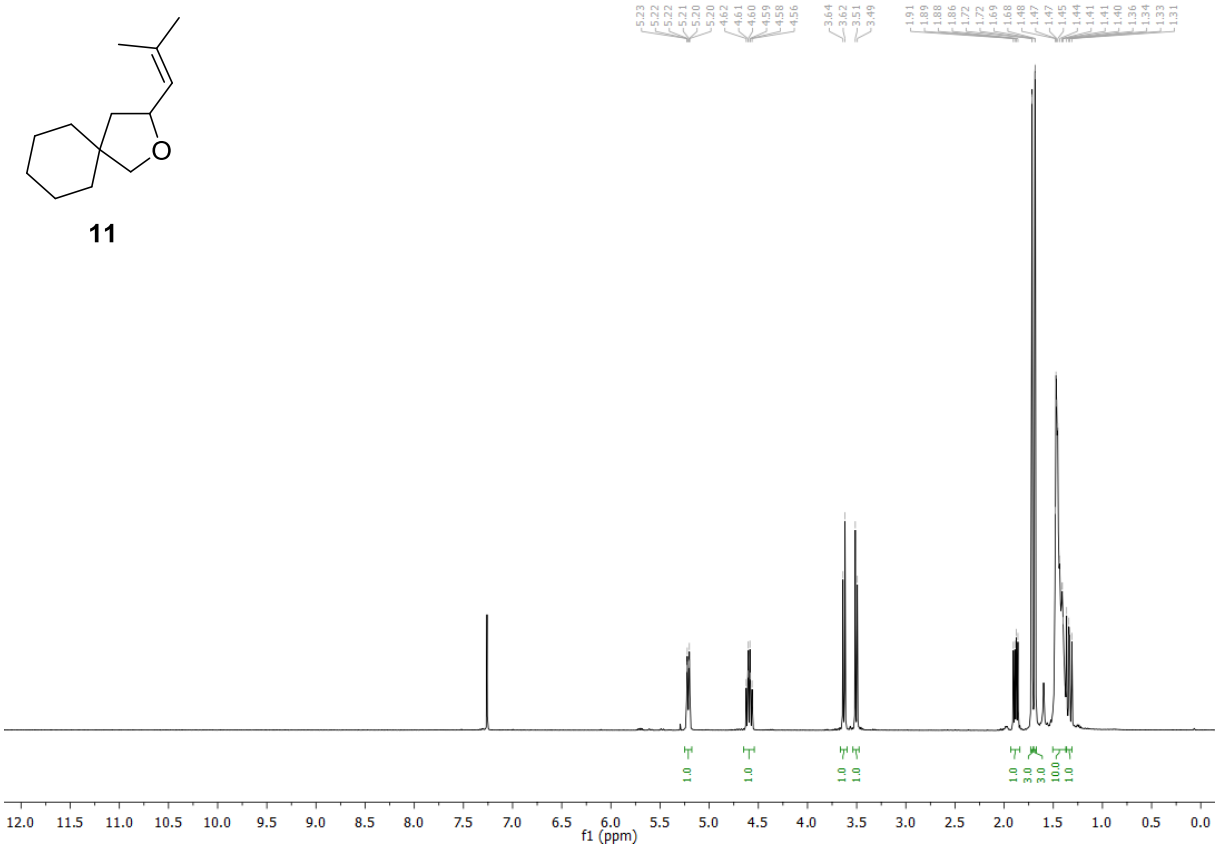
f1 (ppm)

11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1.47
1.45
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1.34
1.33
1.31
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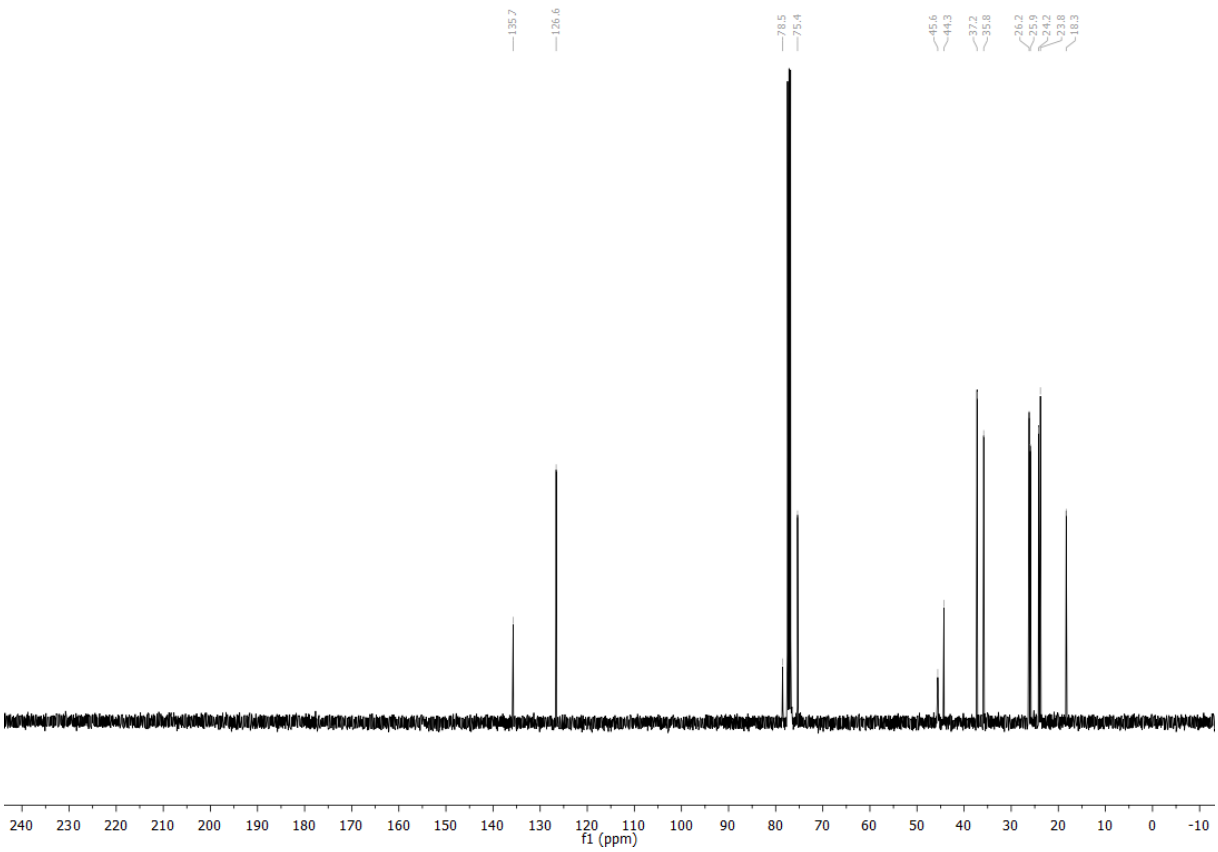
1.0
1.0
1.0
1.0
3.0
3.0
10.0
1.0
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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35.8
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25.9
24.2
23.8
18.3
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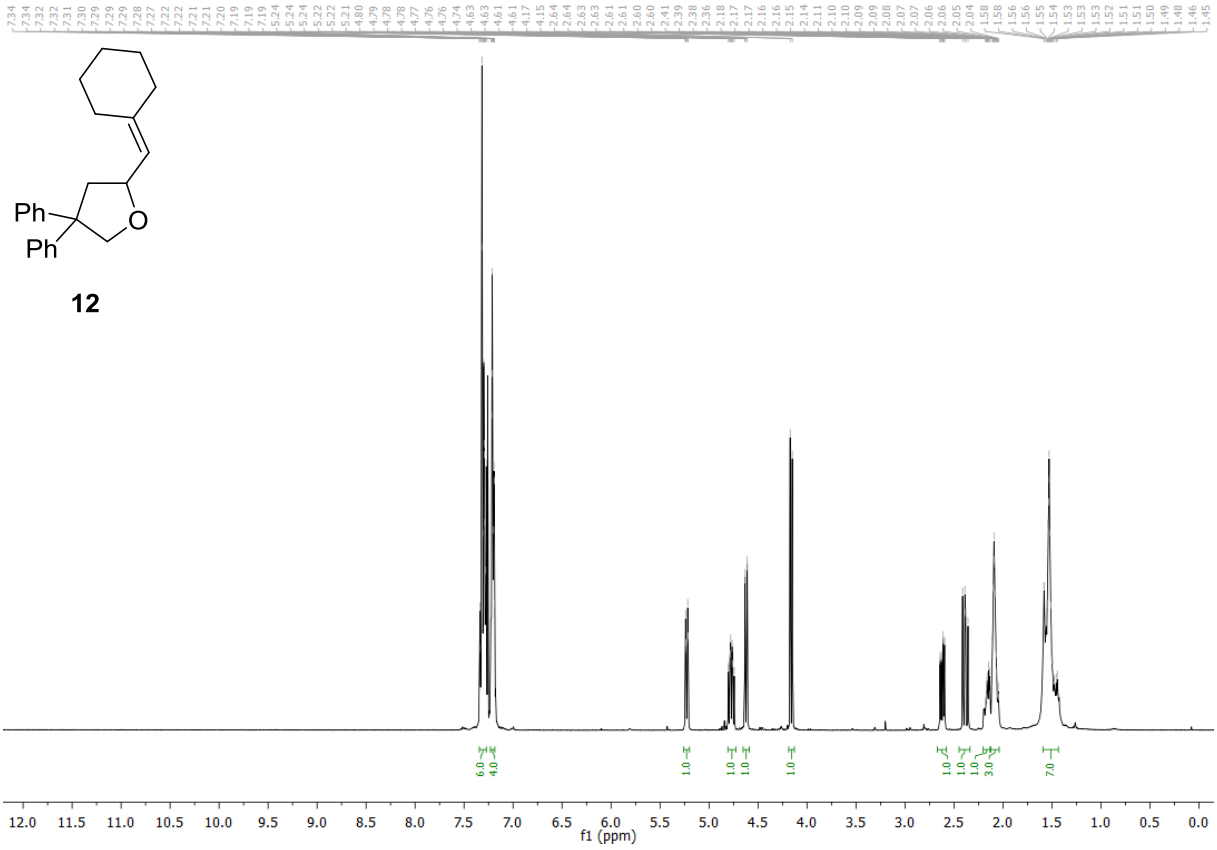
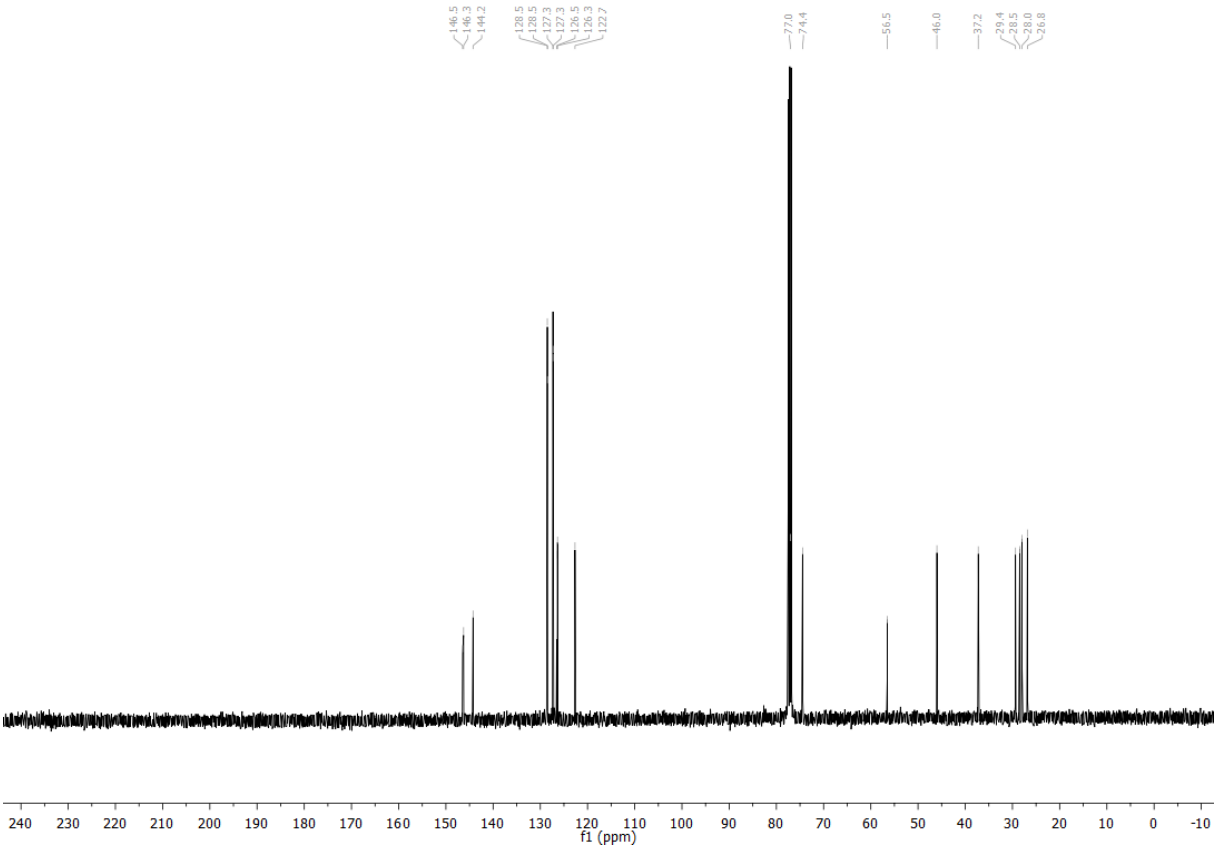
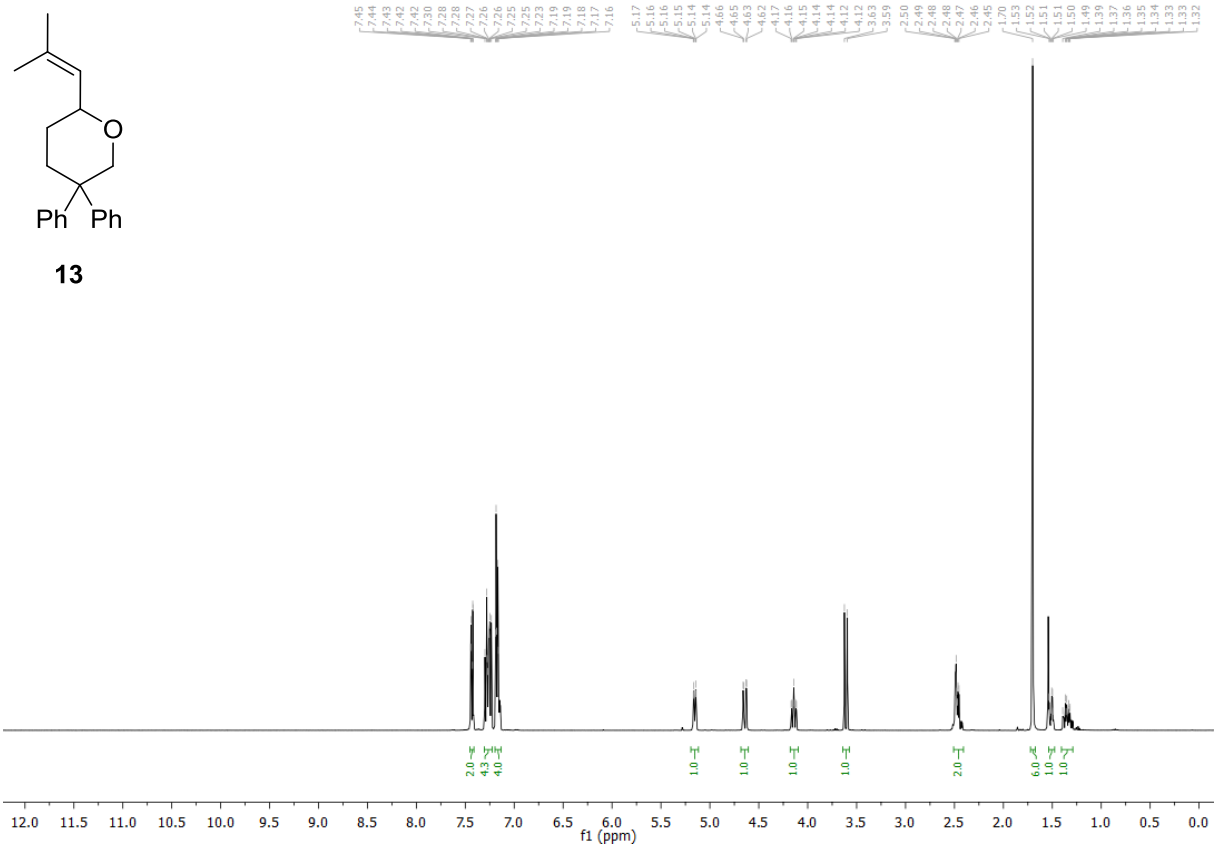
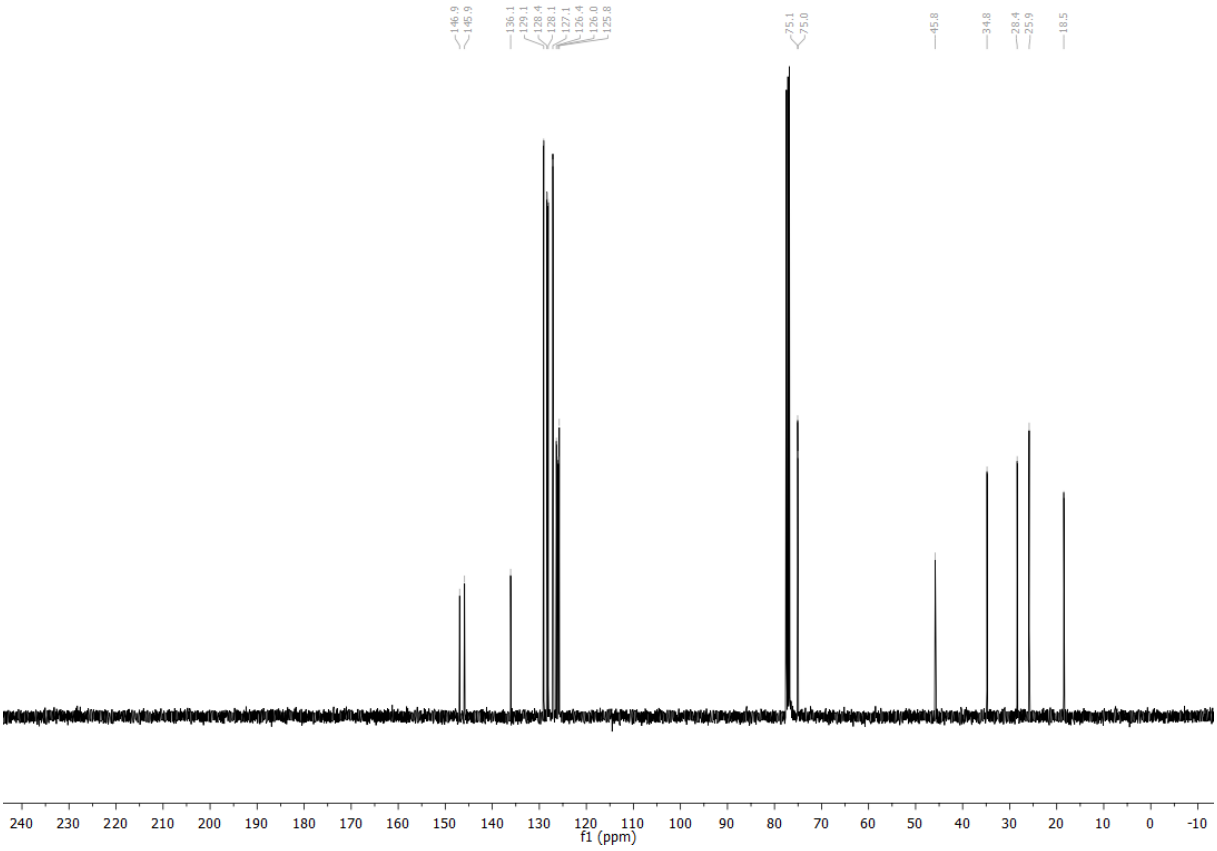
f1 (ppm)


Ph
Ph
O
12
f1 (ppm)

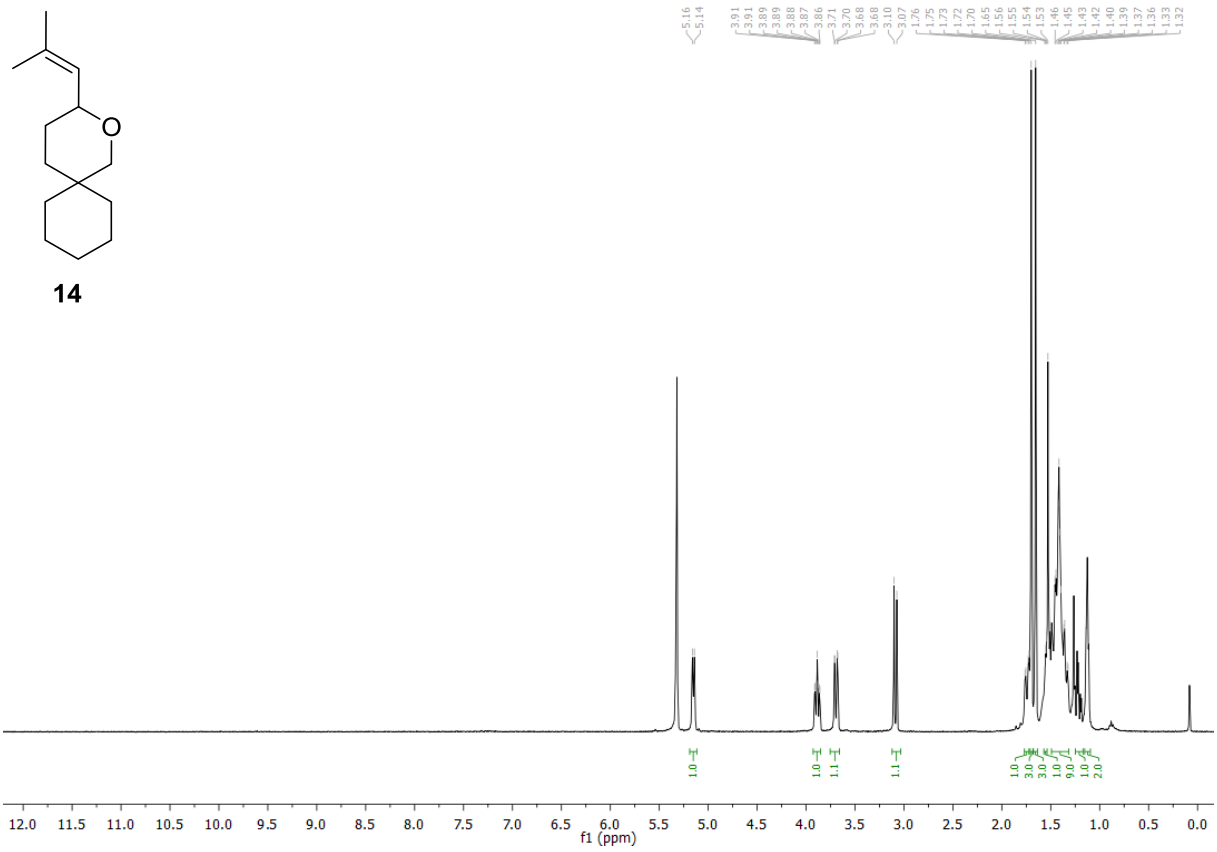

f1 (ppm)

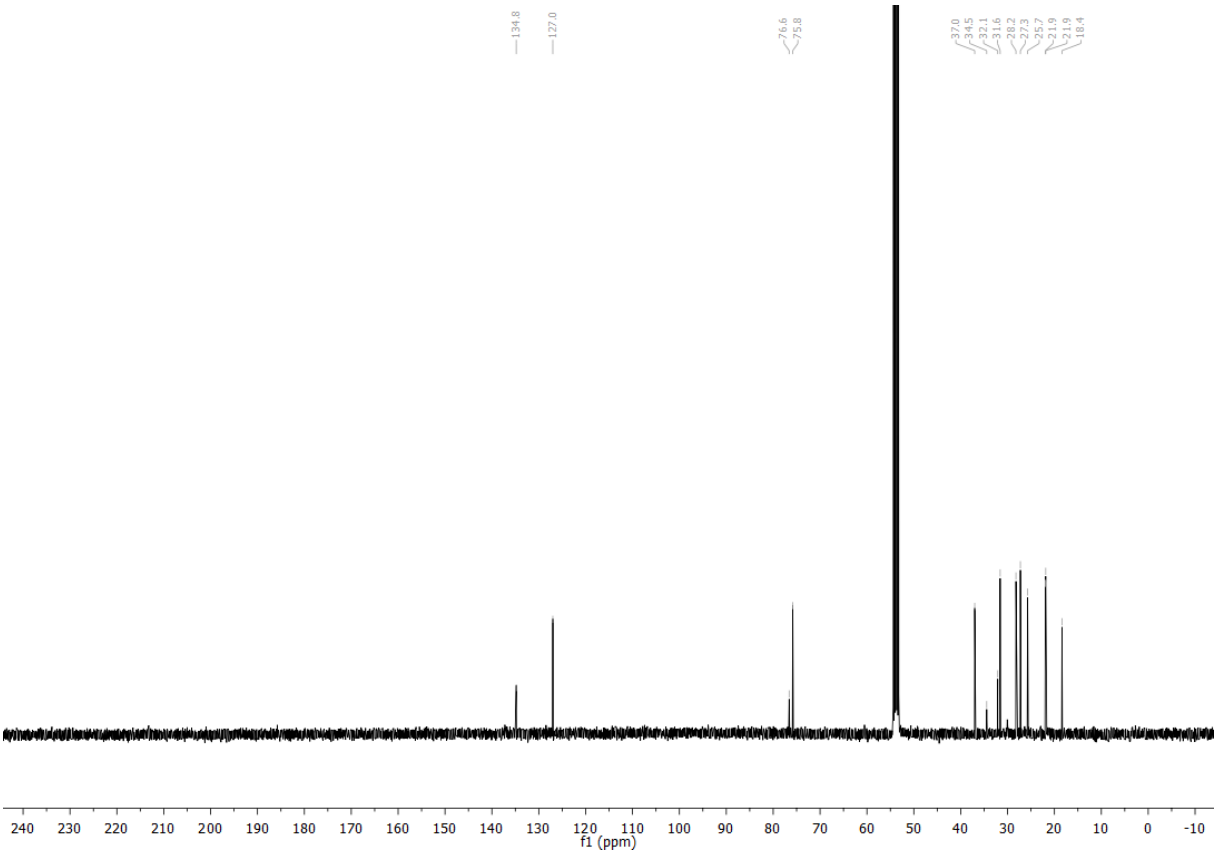
13





14





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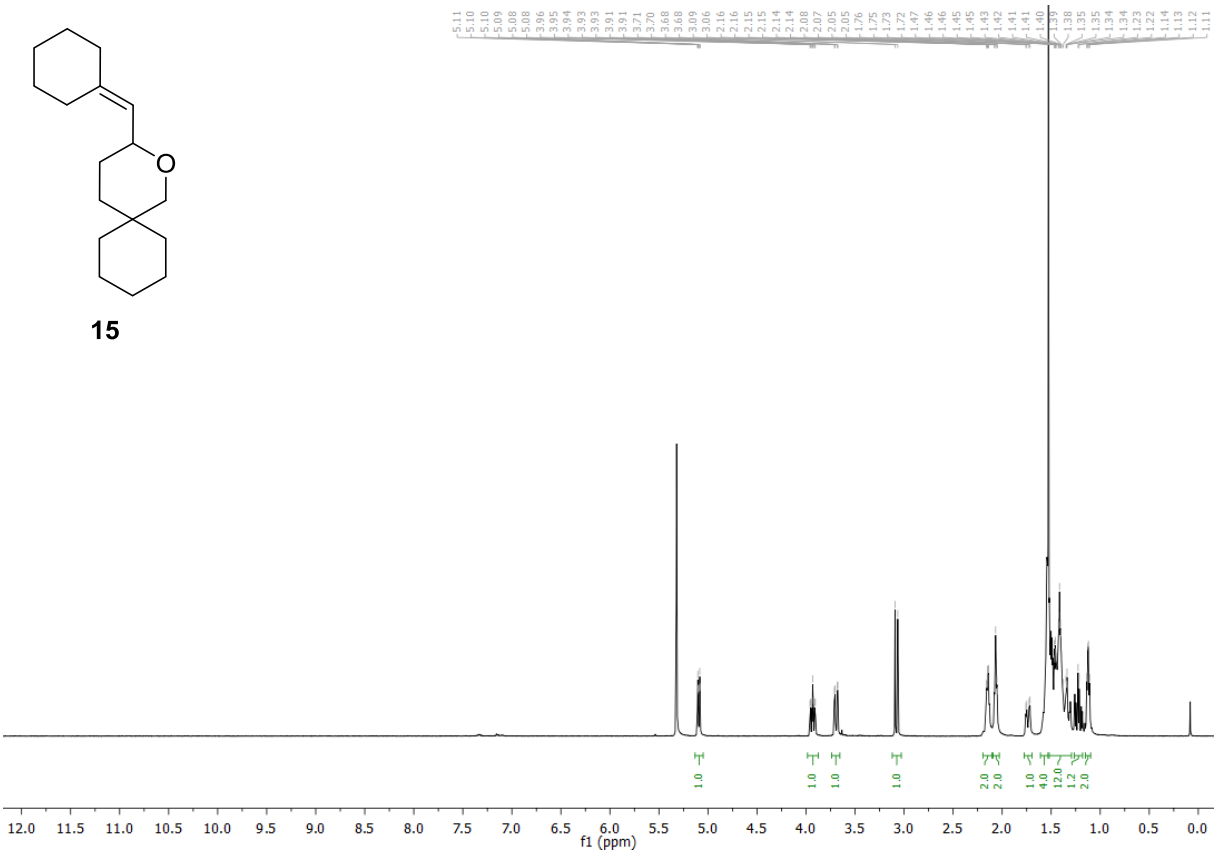
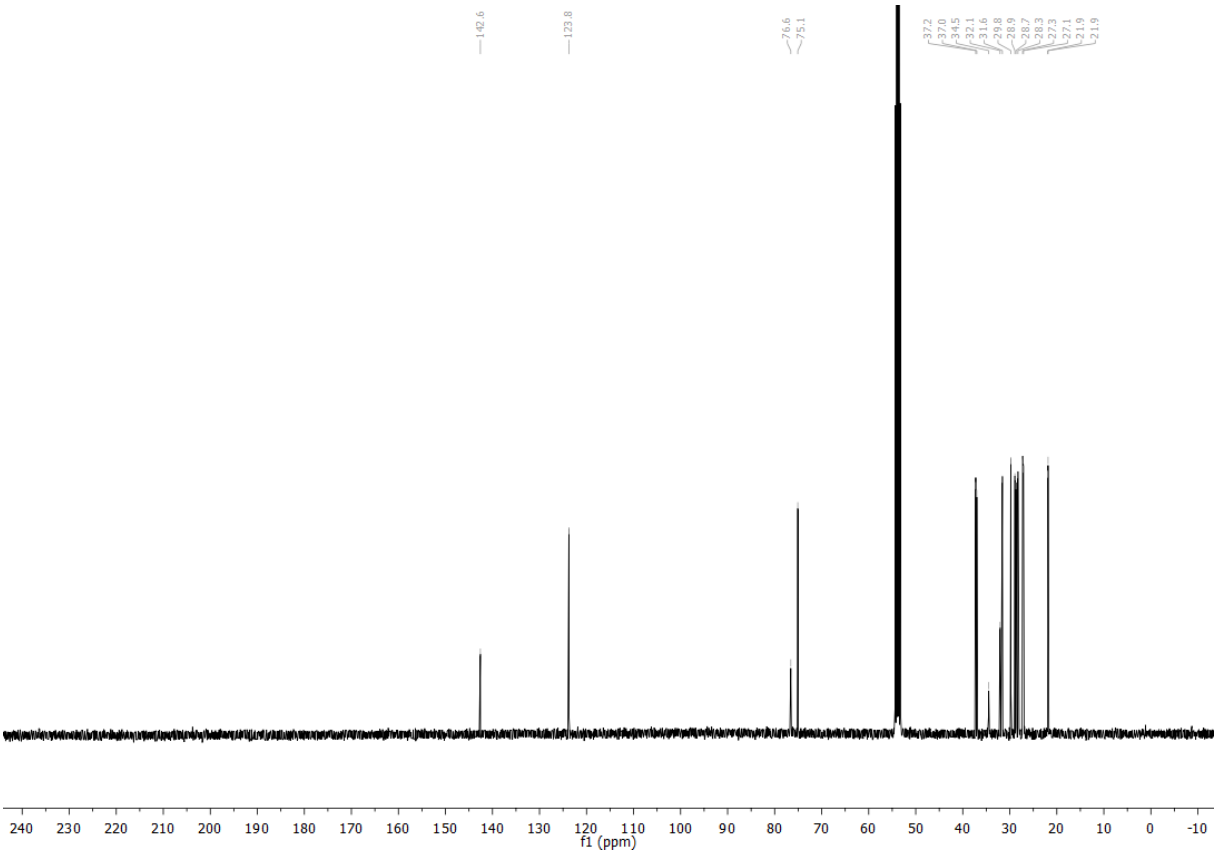
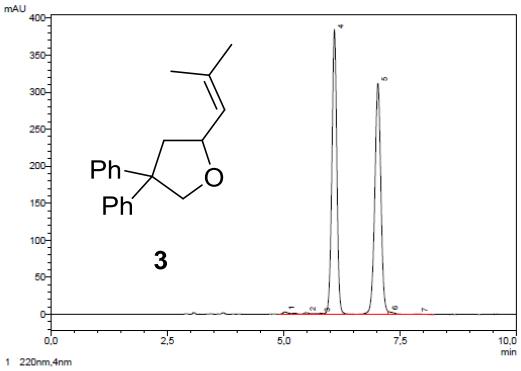




Representative HPLC Traces

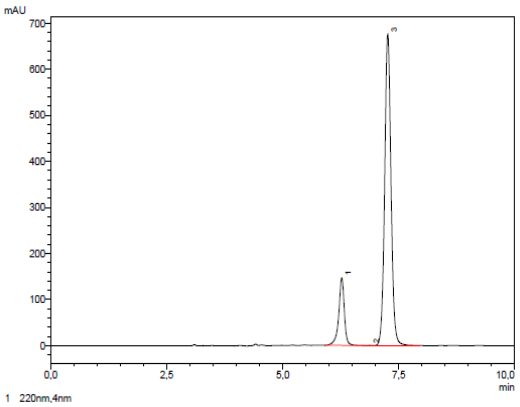
Racemate



PDA Ch1 220nm

Peak #	Ret. Time	Area %	Name
1	5,02	0,55	
2	5,48	0,27	
3	5,80	0,24	
4	6,09	49,09	enantiomer 1
5	7,02	49,29	enantiomer 2
6	7,25	0,46	
7	7,89	0,10	
Total		100,00	

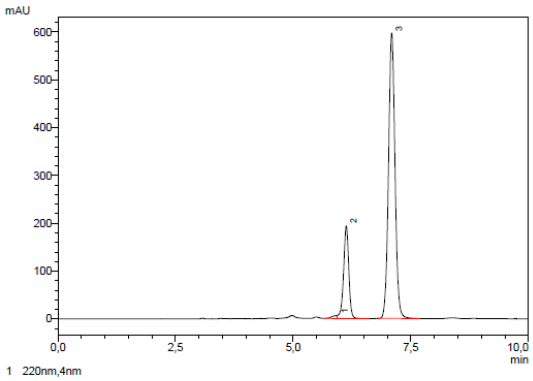
EtOAc, rt



PDA Ch1 220nm

Peak #	Ret. Time	Area %	Name
1	6,27	16,04	enantiomer 1
2	6,87	0,03	
3	7,26	83,92	enantiomer 2 68% ee
Total		100,00	

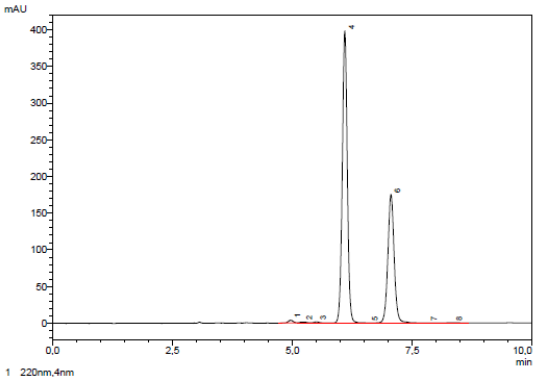
CH_2Cl_2, rt



PDA Ch1 220nm

Peak #	Ret. Time	Area %	Name
1	5,94	0,70	
2	6,13	20,55	enantiomer 1
3	7,09	78,75	enantiomer 2 59% ee
Total		100,00	

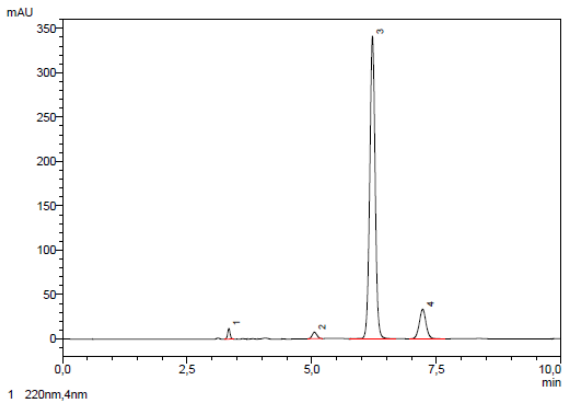
CH_2Cl_2, –60 °C



PDA Ch1 220nm

Peak #	Ret. Time	Area %	Name
1	4,96	0,63	
2	5,22	0,31	
3	5,50	0,28	
4	6,09	63,34	enantiomer 1 29% ee
5	6,58	0,06	
6	7,06	35,10	enantiomer 2
7	7,81	0,08	
8	8,34	0,20	
Total		100,00	

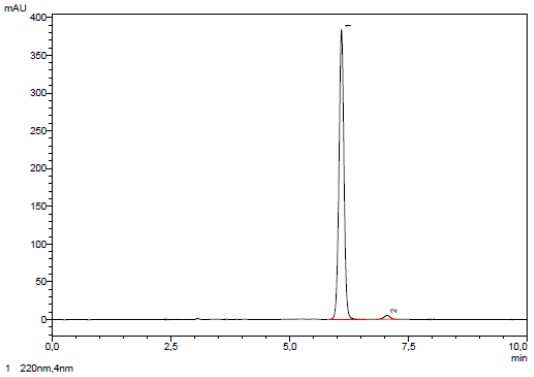
EtOH, rt



PDA Ch1 220nm

Peak #	Ret. Time	Area %	Name
1	3,34	1,35	
2	5,06	1,63	
3	6,22	86,36	enantiomer 1 78% ee
4	7,22	10,67	enantiomer 2
Total		100,00	

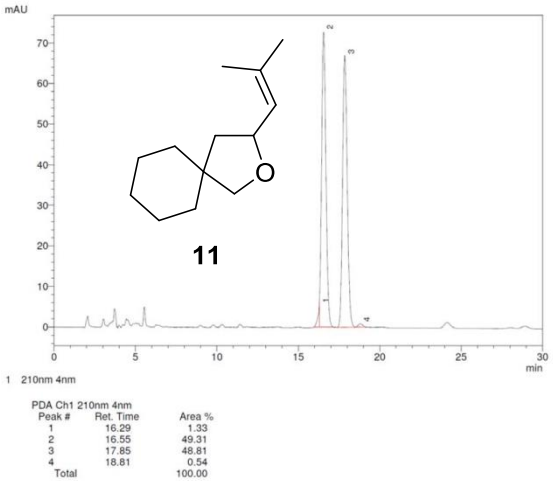
EtOH, –60 °C



PDA Ch1 220nm

Peak #	Ret. Time	Area %	Name
1	6,09	98,42	enantiomer 1 97% ee
2	7,05	1,58	enantiomer 2
Total		100,00	

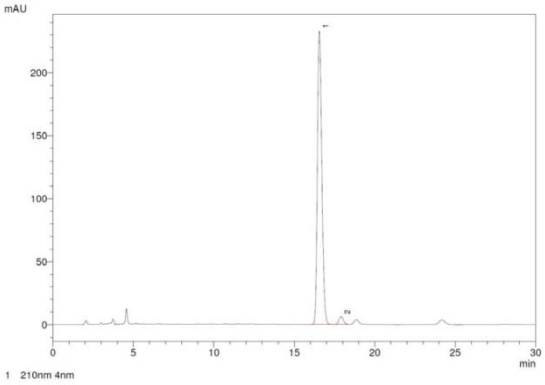
Racemate



PDA Ch1 210nm 4nm

Peak #	Ret. Time	Area %
1	16.29	1.33
2	16.55	49.31
3	17.85	48.81
4	18.81	0.54
Total		100.00

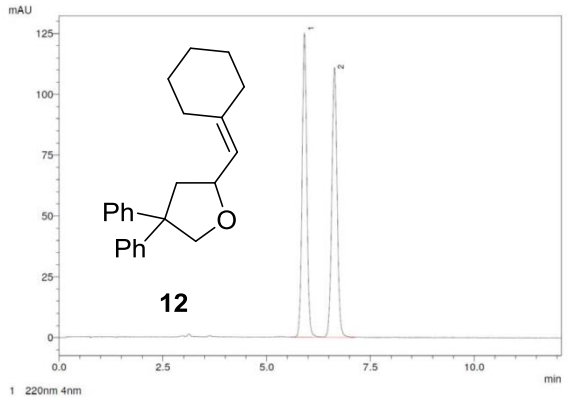
EtOH, –78 °C



PDA Ch1 210nm 4nm

Peak #	Ret. Time	Area %
1	16.55	97.35
2	17.90	2.65
Total		100.00

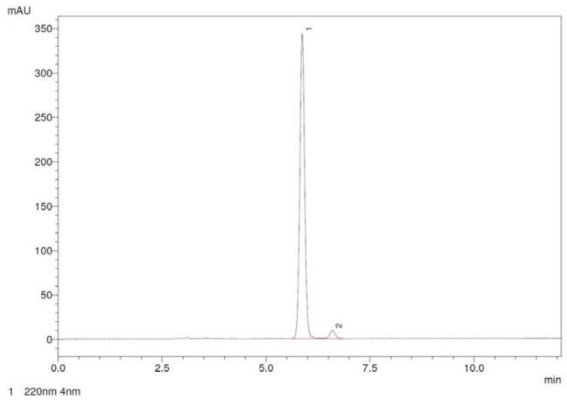
Racemate



PDA Ch1 220nm 4nm

Peak #	Ret. Time	Area %	Name
1	5.91	49.90	
2	6.63	50.10	
Total		100.00	

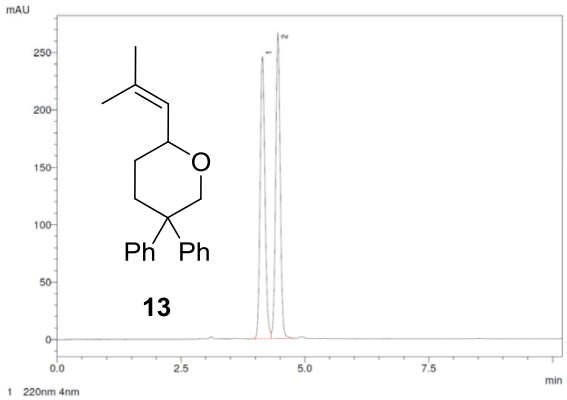
EtOH, –60 °C



PDA Ch1 220nm 4nm

Peak #	Ret. Time	Area %	Name
1	5.86	96.92	
2	6.59	3.08	
Total		100.00	

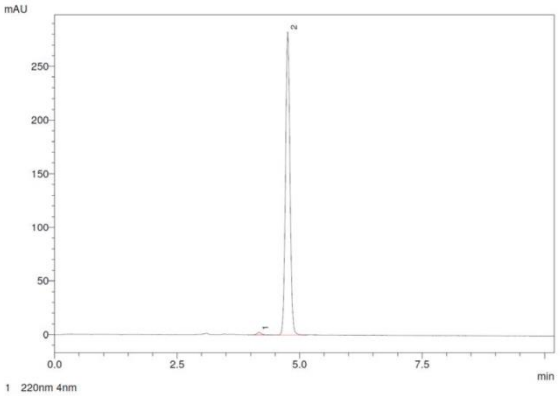
Racemate



PDA Ch1 220nm 4nm

Peak #	Ret. Time	Area %	Name
1	4.14	49.61	
2	4.45	50.39	
Total		100.00	

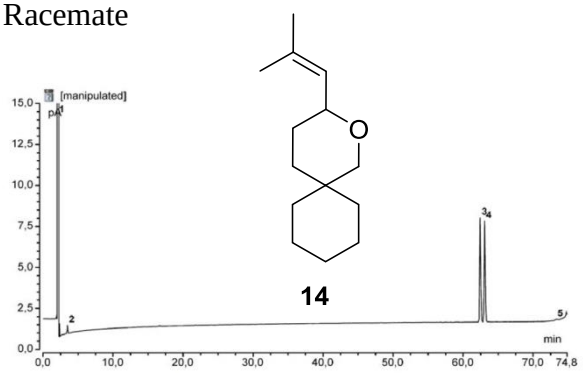
EtOH, –78 °C



PDA Ch1 220nm 4nm

Peak #	Ret. Time	Area %	Name
1	4.17	0.80	
2	4.75	99.20	
Total		100.00	

Racemate



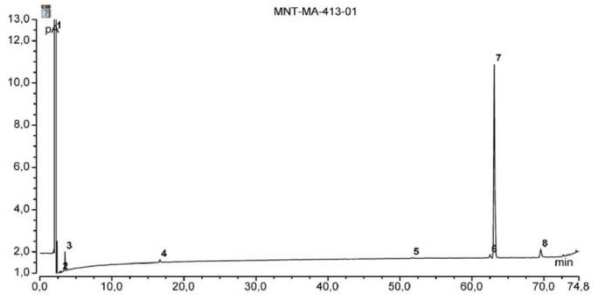
14

Sample: **MNT-MA-410-01**
Sequenz: **91761 MNT-MA SD**
Instrument: **GC_111**
Measured: **14.01.13 12:28**
Report-File: Verhältnis

chirale Messung
Racemt-Probe

No.	Ret.Time min	Rel.Area %	Peak Name
3	62,42	49,9	
4	63,07	50,1	

EtOH, –78 °C

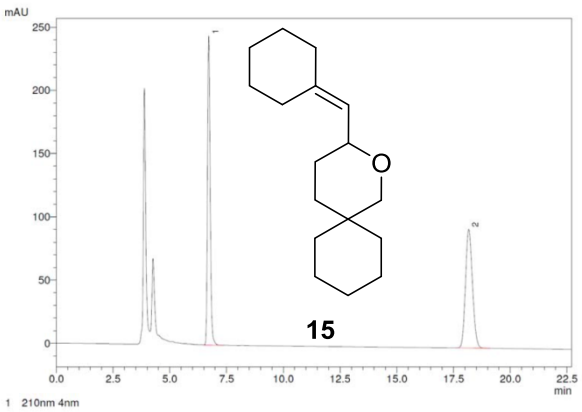


Sample: **MNT-MA-413-01**
Sequenz: **91761 MNT-MA SD**
Instrument: **GC_111**
Measured: **14.01.13 10:59**
Report-File: Verhältnis 413-01

chirale Messung
ee-Verhältnis

No.	Ret.Time min	Rel.Area %	Peak Name
6	62,49	1,5	
7	63,08	98,5	

Racemate



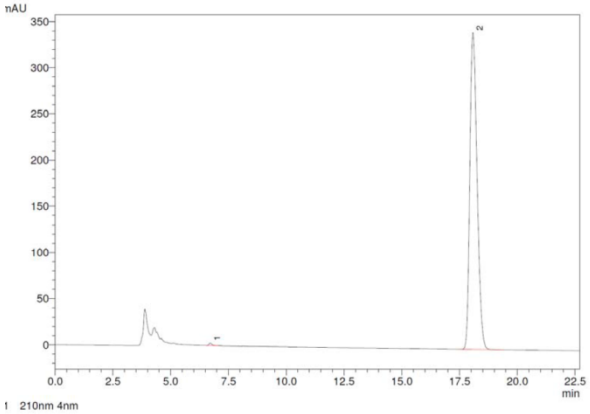
15

1 210nm 4nm

PDA Ch1 210nm 4nm

Peak #	Ret. Time	Area %
1	6.71	50.21
2	18.16	49.79
Total		100.00

EtOH, –78 °C



1 210nm 4nm

PDA Ch1 210nm 4nm

Peak #	Ret. Time	Area %
1	6.71	0.30
2	18.07	99.70
Total		100.00

Computational Part

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Computational Methods

Density functional theory (DFT) was used to investigate the mechanism for the solvent and temperature dependent enantioinversion phenomenon in the enantioselective gold catalyzed cycloetherification studied here. All geometry optimizations were performed using the TPSS[1] functional with the inclusion of Grimme's DFT-D3[2] empirical dispersion correction (TPSS-D3). For geometry optimizations, the triple-ζ quality def2-TZVP[3] basis set was used for Au and the double-ζ quality SVP basis set was used for all remaining atoms. The 60 inner-shell core electrons of the gold atom were described by the corresponding def2 effective core potential[4] accounting for scalar relativistic effects (def2-ecp). For the purpose of computational efficiency, the resolution-of-identity (RI) approximation[5] was applied using auxiliary basis sets to approximate Coulomb potentials in conjunction with the multipole-accelerated resolution of the identity approximation (MA-RI) method for geometry optimizations.[6]

Stationary points were characterized by evaluating the harmonic vibrational frequencies at the optimized geometries. Zero-point vibrational energies (ZPVE) were computed from the corresponding harmonic vibrational frequencies without scaling. Relative free energies (ΔG) were determined at standard pressure (1 bar) and at room (298 K) and cryogenic (213 K) temperatures. The thermal and entropic contributions were evaluated within the rigid-rotor harmonic-oscillator approximation. Single-point energies were computed at the TPSS-D3 and PBE0[7]-D3 level using the def2-TZVP basis set for all atoms. Solvation contributions were included for ethyl acetate and methanol on the optimized gas-phase geometries employing the SMD solvation model.[8] In addition, NMR chemical shifts were calculated using the Gauge-Independent Atomic Orbital (GIAO) method[9] at the SMD_{DCM}-PBE0/def2-TZVP//TPPS-D3/def2-SVP(TZVP for Au) level on selected intermediates for comparison with experimentally obtained chemical shift values.

All geometry optimizations were performed with TURBOMOLE (version-6.4)[10] and single-point SMD solvation and GIAO calculations were carried out with Gaussian09.[11]

Table S1. SCF energies and the corresponding enthalpies (*H*) and Gibbs free energies (*G*) for the aprotic process computed with the D3 dispersion correction. The thermally corrected *H* and *G* values were determined at the SMD-PBE0-D3/def2-TZVP level at the given temperature.

	SCF(TPSS)	SCF(TPSS-SMD)	SCF(PBE0-SMD)	*H(298K)*	*H(213K)*	*G(298K)*	*G(213K)*
cat-A	-3494.673574	-3498.056089	-3493.821844	-3492.674893	-3492.706315	-3492.850070	-3492.805256
cat-B	-3494.663892	-3498.049592	-3493.815484	-3492.668346	-3492.699731	-3492.844277	-3492.799239
INT1	-4076.595348	-4080.574103	-4075.507724	-4074.075227	-4074.113616	-4074.283081	-4074.230096
INT1`	-4076.590055	-4080.568034	-4075.501018	-4074.068521	-4074.106647	-4074.273628	-4074.221382
TS1-R	-4076.584430	-4080.564435	-4075.496548	-4074.065689	-4074.103796	-4074.271302	-4074.218909
TS1-S	-4076.578250	-4080.559697	-4075.492237	-4074.061633	-4074.099793	-4074.267100	-4074.214762
INT2-R	-4076.593511	-4080.572378	-4075.506053	-4074.073518	-4074.111923	-4074.279390	-4074.226975
INT2-S	-4076.594636	-4080.571421	-4075.503061	-4074.070705	-4074.109091	-4074.274923	-4074.222975
TS2-R	-4076.583701	-4080.558753	-4075.486953	-4074.056098	-4074.094156	-4074.257787	-4074.206513
TS2-S	-4076.574207	-4080.552460	-4075.481823	-4074.051017	-4074.089170	-4074.253518	-4074.202025
TS1-S`	-4076.578711	-4080.558700	-4075.489786	-4074.059495	-4074.097632	-4074.265145	-4074.212749
INT3-R	-4076.584931	-4080.562301	-4075.491221	-4074.059920	-4074.097844	-4074.263106	-4074.211381
INT3-S	-4076.583966	-4080.561635	-4075.490688	-4074.059014	-4074.097270	-4074.268211	-4074.214821
TS3-R	-4076.581567	-4080.558040	-4075.490013	-4074.056918	-4074.094572	-4074.259156	-4074.207660
TS3-S	-4076.584419	-4080.561099	-4075.489456	-4074.057927	-4074.095843	-4074.263337	-4074.210976
INT4-R	-4076.583424	-4080.558560	-4075.490184	-4074.058689	-4074.096419	-4074.259675	-4074.208549
INT4-S	-4076.586758	-4080.563339	-4075.494963	-4074.062058	-4074.100059	-4074.266709	-4074.214578
TS4-R	-4076.561155	-4080.536578	-4075.466505	-4074.039786	-4074.077634	-4074.242733	-4074.191063
TS4-S	-4076.566691	-4080.540934	-4075.470141	-4074.042862	-4074.080645	-4074.244009	-4074.192846
PRT-R	-4076.627432	-4080.606114	-4075.543128	-4074.109390	-4074.147283	-4074.314441	-4074.262178
PRT-S	-4076.624711	-4080.602682	-4075.539465	-4074.106812	-4074.144119	-4074.307326	-4074.256267
INT3-R-a	-4349.464373	-4353.729597	-4348.290963	-4346.687173	-4346.729252	-4346.910197	-4346.853489
INT3-S-a	-4349.473417	-4353.737710	-4348.299338	-4346.697243	-4346.738846	-4346.914669	-4346.859487
TS3-R-a	-4349.457268	-4353.721865	-4348.285148	-4346.683385	-4346.725232	-4346.904422	-4346.848245
TS3-S-a	-4349.461775	-4353.726327	-4348.289606	-4346.687225	-4346.728954	-4346.911063	-4346.854070
INT2-R-a	-4349.456164	-4353.728477	-4348.289088	-4346.682955	-4346.725191	-4346.907109	-4346.850106
INT2-S-a	-4349.457805	-4353.728486	-4348.290729	-4346.686303	-4346.728284	-4346.911560	-4346.854199
TS2-R-a	-4349.451468	-4353.722372	-4348.279441	-4346.673514	-4346.715537	-4346.898575	-4346.841278
TS2-S-a	-4349.449598	-4353.720254	-4348.276403	-4346.670907	-4346.712918	-4346.893607	-4346.83698
product	-850.167726	-851.0794658	-849.9038567	-849.5215942	-849.5307163	-849.5913572	-849.5729504
neopentanol	-272.8352073	-273.1423703	-272.7712142	-272.6002296	-272.6040841	-272.6402093	-272.6294275
MeOAc	-268.2364101	-268.5494612	-268.2028396	-268.1074254	-268.1101182	-268.1448705	-268.1346155

[a] The def2-TZVP basis set was used for Au (with def2-ecp), and the SVP basis set was used for all remaining atoms during geometry optimization. [b] The def2-TZVP basis set was used for all atoms and ethyl acetate was used for the SMD solvation correction.

Table S2. SCF energies and the corresponding enthalpies (*H*) and Gibbs free energies (*G*) for the protic process computed with the D3 dispersion correction. The thermally corrected *H* and *G* values were determined at the SMD-PBE0-D3/def2-TZVP level at the given temperature.

	SCF(TPSS)	SCF(TPSS-SMD)	SCF(PBE0-SMD)	*H(298K)*	*H(213K)*	*G(298K)*	*G(213K)*
cat-A-p	-3342.078333	-3345.302301	-3341.266554	-3340.160345	-3340.190355	-3340.329677	-3340.324653
cat-B-p	-3342.067076	-3345.293761	-3341.258549	-3340.152276	-3340.182285	-3340.321759	-3340.316742
INT-1-p	-4192.259177	-4196.382776	-4191.170949	-4189.681160	-4189.721290	-4189.901044	-4189.894320
TS-1-R-p	-4192.258499	-4196.374877	-4191.161023	-4189.673108	-4189.712860	-4189.887881	-4189.881224
TS-1-S-p	-4192.251204	-4196.370821	-4191.157107	-4189.669478	-4189.709272	-4189.885344	-4189.878684
INT-2-R-p	-4192.268969	-4196.384761	-4191.171667	-4189.680918	-4189.720861	-4189.897125	-4189.890438
INT-2-S-p	-4192.262263	-4196.379530	-4191.165793	-4189.674771	-4189.714740	-4189.892186	-4189.885489
TS-2-R-p	-4192.255421	-4196.374371	-4191.157031	-4189.669817	-4189.708876	-4189.879022	-4189.872490
TS-2-S-p	-4192.256083	-4196.369721	-4191.151478	-4189.662630	-4189.702208	-4189.876393	-4189.869768
INT-3-R-p	-4192.268419	-4196.381853	-4191.168850	-4189.681228	-4189.720847	-4189.893876	-4189.887247
INT-3-S-p	-4192.277517	-4196.387868	-4191.174897	-3340.160345	-3340.190355	-3340.329677	-3340.324653
TS-3-R-p	-4192.260967	-4196.371536	-4191.160014	-4189.675200	-4189.714598	-4189.885759	-4189.879172
TS-3-S-p	-4192.265194	-4196.375229	-4191.163734	-4189.680367	-4189.719521	-4189.889756	-4189.883211
PRT-R-p	-4192.298876	-4196.415448	-4191.206883	-4189.681228	-4189.720847	-4189.893876	-4189.887247
PRT-S-p	-4192.293300	-4196.409722	-4191.200388	-4189.710234	-4189.749251	-4189.921090	-4189.914567
MeOH	-115.646038	-115.793636	-115.645315	-115.590689	-115.592056	-115.617701	-115.617464
substrate-p	-965.802507	-966.853483	-965.526716	-965.088471	-965.099730	-965.170846	-965.168950

[a] The def2-TZVP basis set was used for Au (with def2-ecp), and the SVP basis set was used for all remaining atoms during geometry optimization. [b] The def2-TZVP basis set was used for all atoms and ethyl acetate was used for the SMD solvation correction.

Mechanism in the Protic Solvent Methanol

The pathway in a protic solvent medium (methanol) is computed to be similar to that of the substrate-assisted mechanism in aprotic media. In this case, entropy does not play an influential role since the concentration of the associating methanol is large and essentially constant. While a similar selectivity inversion is evident after cyclization, the selectivity is always dependent on the rate-determining cyclization step, and the pathways are never permitted to cross after **INT1-p** since a free allyl cation intermediate is never generated. This mechanism conforms reasonably well with the experimentally obtained activation parameters based on the difference in energy of the rate limiting transition states **TS2-p**. The predicted activation parameters are $\Delta\Delta H^{\ddagger}_{calc}$ = –4.5 kcal mol^{-1} and $\Delta\Delta S^{\ddagger}_{calc}$ = –9.6 cal mol^{-1} K^{-1} which are relatively close to the experimentally observed parameters obtained in ethanol ($\Delta\Delta H^{\ddagger}_{exp}$=–3.3 kcal mol^{-1}; $\Delta\Delta S^{\ddagger}_{exp.}$=–6.8 cal mol^{-1} K^{-1}).

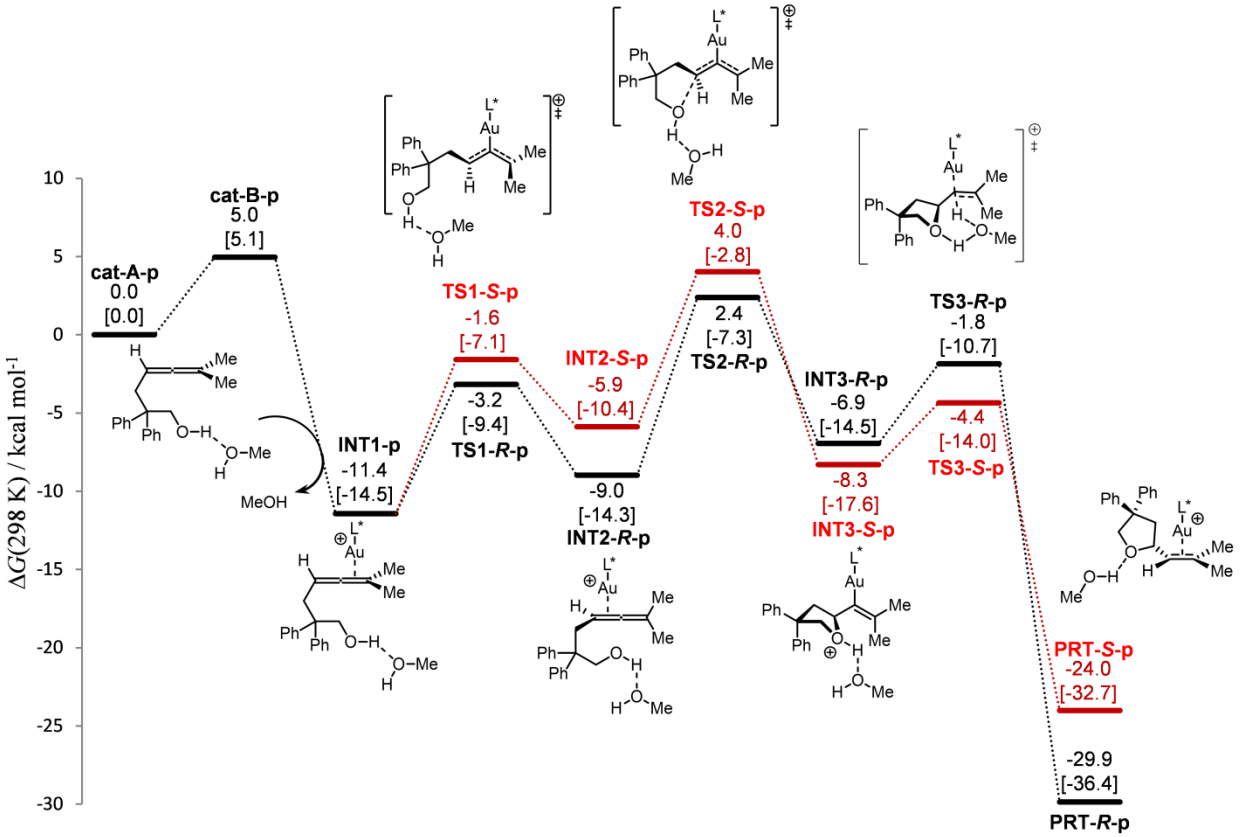


Figure S1. Gibbs free energy profile for the pathway in the protic solvent methanol computed at 298 K at the SMD$_{MeOH}$-PBE0-D3/def2-TZVP//TPSS-D3/def2-SVP(TZVP for Au) level of theory. An explicit methanol molecule is included in the gas-phase optimization for each stationary point.

Conversion of cat-A to cat-B

The conversion of **cat-A** to **cat-B** corresponds to a rotation of one of the benzyl groups of the bulky amino moiety which serves to expose the gold atom, thus facilitating displacement by the substrate. A mechanism involving the dissociation of the solvent molecule followed by association of the substrate is not energetically feasible.

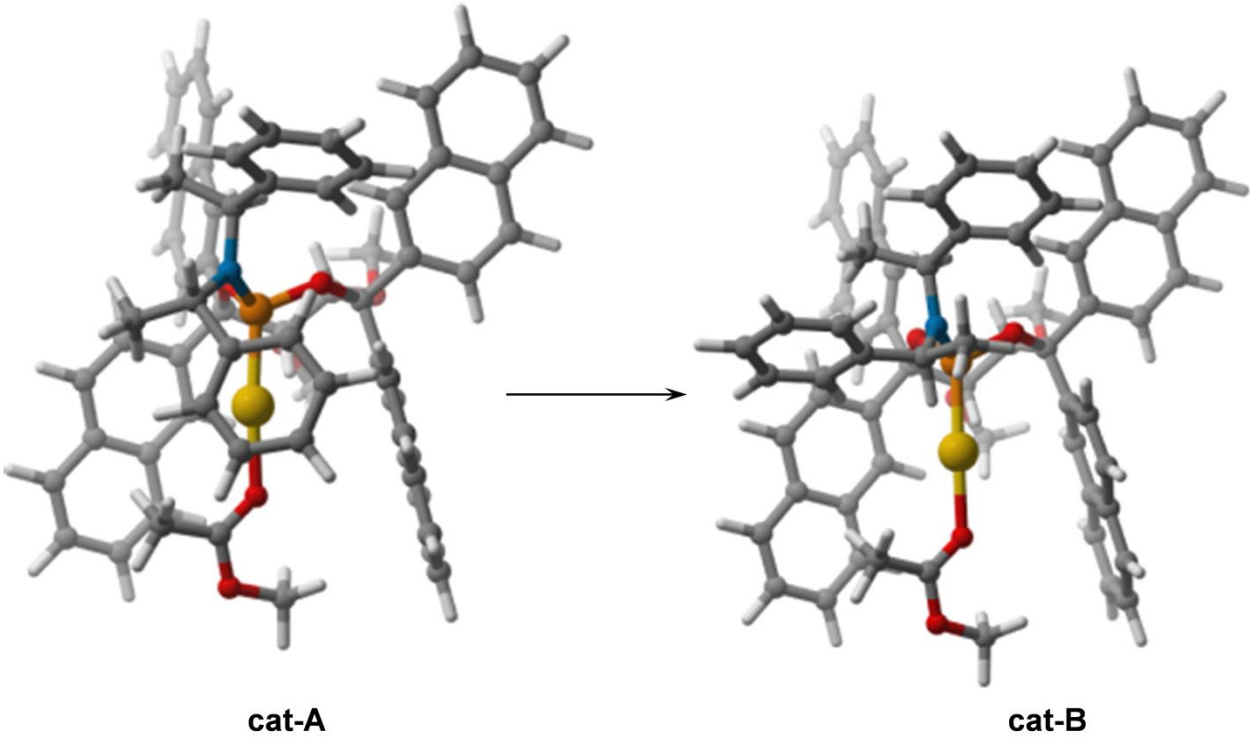


Figure S2. Geometries of **cat-A** and **cat-B** which differ by a rotation of one of the benzyl groups of the amino moiety.

Discussion of Selectivity-Dependent Transition States

In an aprotic solvent medium, at cryogenic temperatures, the selectivity-dependent step is cyclization (**TS3-a**, Figure S3). **TS3-S-a** is higher in energy than **TS3-R-a** by approximately 3 kcal/mol. This energy difference can be attributed to two factors. (1) The first one relates to the required rotation of the C=C bond which takes place concomitantly with C-O bond formation. Upon rotation, a destabilizing contact occurs between one of the phenyl rings of the substrate and one of the phenyl rings of the amino group bound to the ligand. This steric contact increases as the C=C rotation proceeds. The steric hindrance is reduced in **TS3-R-a**, because the direction of rotation is opposite, and there is less steric interaction between the phenyl group of the substrate and the methyl group of the amino group bound to the ligand. (2) The second factor is the difference in solvent exposure of the hydrogen atom of the associating alcohol. The partially positively charged hydrogen in **TS3-S-a** is less exposed as it is surrounded by both the phenyl ring of the substrate and the naphthyl ring of the ligand. The same hydrogen atom in **TS3-R-a** is much more exposed, which allows for a stronger stabilization by solvation as compared to **TS3-S-a**. The enhanced dielectric constant in the case of a protic solvent medium causes even a greater solvation preference favoring **TS3-R-a**.

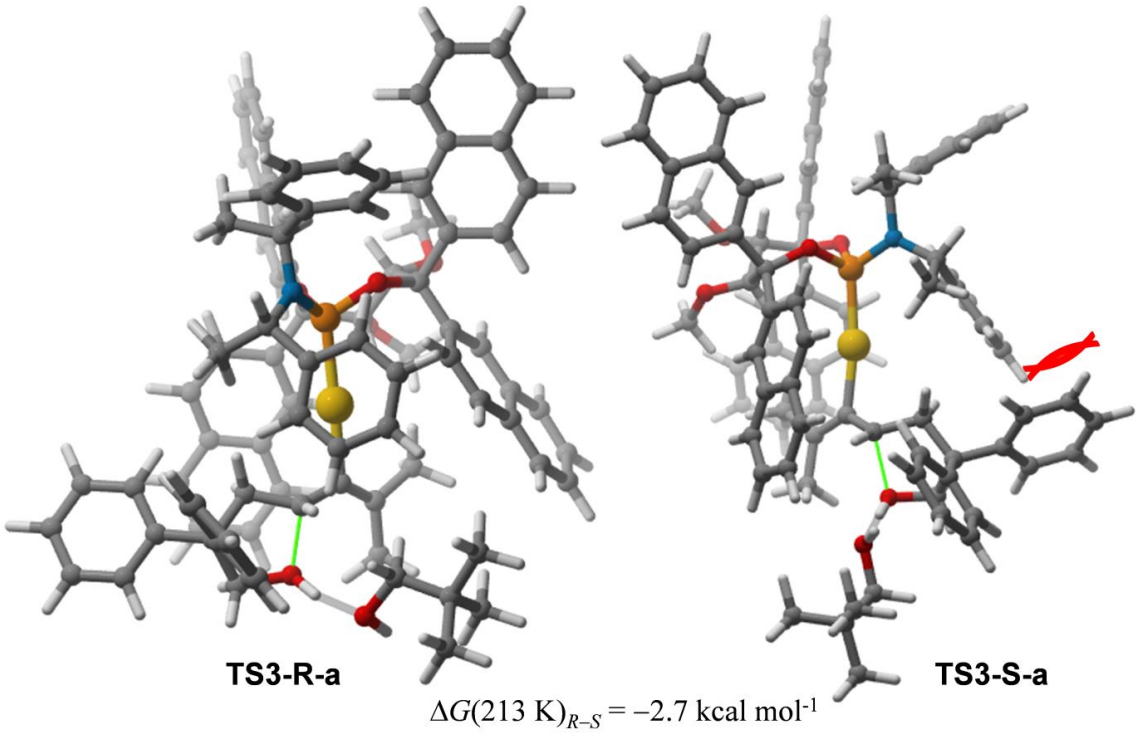


Figure S3. Comparison of the transition states **TS3-R-a** and **TS3-S-a**. Unfavorable steric interactions are depicted as red overlapping brackets.

In an aprotic solvent medium, at room temperature, the selectivity-dependent step after equilibration via **INT3** (see main paper) is protodeauration (**TS4-a**, Figure S4). In this case, **TS4-R-a** is higher in energy than **TS4-S-a** by approximately 3 kcal/mol. The origin of this energy difference can be primarily attributed to steric interactions. More free space is available in **TS4-S-a** for the phenyl groups of the substrate. In contrast, the phenyl groups in **TS4-R-a** are oriented in the direction of the phenyl groups of the amino ligand. In order to accommodate the association of the alcohol that facilitates the proton shuttle, there is necessarily an unfavorable steric interaction between one of the ligand naphthyl groups and the alcohol. To partly alleviate this steric interaction, the two phenyl groups of the amino ligand are forced together by the substrate.

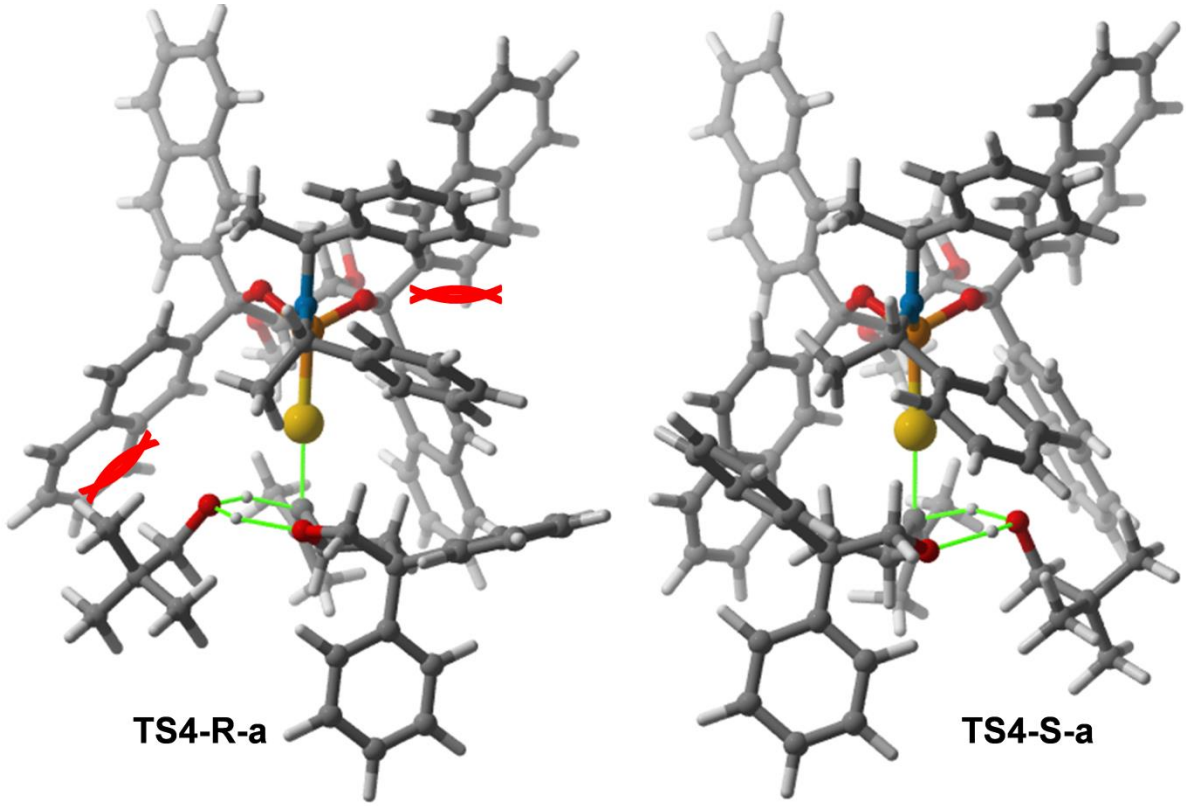
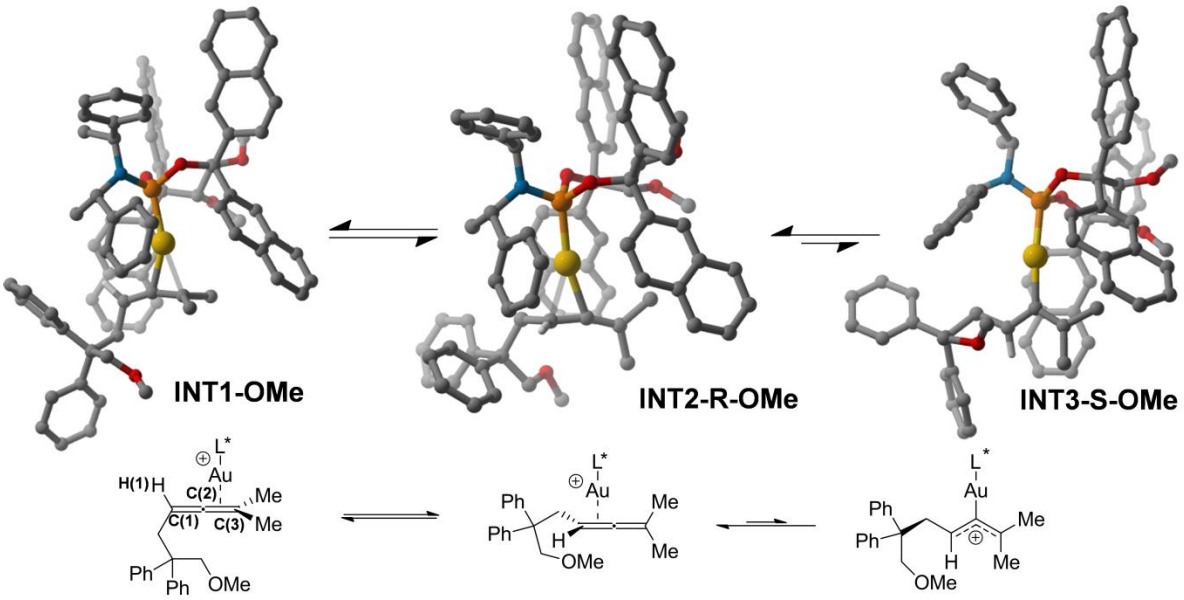


Figure S4. Comparison of transition states **TS4-R-a** and **TS4-S-a**. Unfavorable steric interactions are depicted as red overlapping brackets.

NMR chemical shifts

NMR chemical shifts were computed for the initially formed complexes of the model **OMe** substrate for comparison to the experimental values. The resulting chemical shift changes (Δδ) of selected atoms upon complexation are reported in Figure S5. According to the computed energy profile (Figure 2) possible intermediates prior to C-O bond formation include **INT1**, **INT2-R**, and **INT3-S**. **INT3-S** can be excluded since the observed shifts are inconsistent with the computations, which predict significant upfield shifts for the terminal carbon atoms C(1) and C(3) reflecting considerable partial positive charge accumulation. The computed Δδ values for **INT1** and **INT2-R** also do not closely match the experimental values by themselves. However, when they are Boltzmann averaged, the resulting Δδ values agree very well with experiment (see Figure S5). This much improved agreement suggests that the experimentally observed values correspond to an equilibrium between **INT1** and **INT2-R**, consistent with the predicted low barrier for their interconversion by slippage (~6 kcal mol^{-1}).



	C(1)	C(2)	C(3)	H(1)
INT1-OMe	19.0	-26.0	7.8	-1.5
INT2-R-OMe	4.3	-21.2	16.4	0.3
INT3-S-OMe	84.1	-5.0	42.0	
Boltz(INT1,INT2)	14.8	-24.6	10.2	-1.0
Exp	12.0	-20.0	8.0	-1.1

Figure S5. Experimental and computed (SMD_{DCM}-PBE0/def2-TZVP) changes in ^{13}C-NMR chemical shifts (Δδ (ppm)) upon complexation.

Coordinates

cat-A

Au	-0.8003440	-0.5577862	-0.5579949
C	-3.1091001	2.4174166	-3.0056201
C	-2.3221287	2.7280772	-1.8579695
C	-2.9725376	3.2606793	-0.6881712
C	-4.3831922	3.4672312	-0.7193416
C	-5.1224699	3.1482953	-1.8491120
C	-4.4816271	2.6158262	-3.0001748
C	-2.1734921	3.5538369	0.4583828
C	-0.8146790	3.3048877	0.4603027
C	-0.1685737	2.7455369	-0.6833696
C	-0.9164245	2.4923896	-1.8239369
C	1.3084799	2.3636754	-0.5356944
C	1.8473996	1.5337265	-1.7486688
O	2.0570680	2.4822279	-2.7771037
C	1.8774311	2.0605317	-4.1253799
O	1.3909752	1.5380363	0.6763212
P	0.9231584	-0.0345810	0.7577186
O	2.3225162	-0.8002164	0.3751163
C	2.9383892	-0.7808465	-0.9673874
C	2.0556179	-1.6336657	-1.8829490
C	1.8710022	-1.3499573	-3.2285021
C	0.9850372	-2.1221373	-4.0358781
C	0.2982289	-3.2456052	-3.4516089
C	0.5474632	-3.5528001	-2.0821882
C	1.4000330	-2.7743147	-1.3208614
C	-0.5904880	-4.0100380	-4.2623676
C	-0.8003845	-3.6761337	-5.5921227
C	-0.1299273	-2.5619192	-6.1671695
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C	2.4878337	-2.6637225	6.0020929
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C	3.1438497	-2.2523064	3.3123865
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C	-1.4823338	0.4368875	3.0622649
C	-1.0304390	-2.0026575	2.3444524
C	-2.3879384	-2.1491973	1.9977918
C	-2.8490856	-3.3240209	1.3807269
C	-1.9627976	-4.3744092	1.1093492
C	-0.6138935	-4.2492346	1.4774630
C	-0.1536966	-3.0771506	2.0880765
C	1.7481133	1.2426522	4.1113282
C	2.1959326	3.5758413	-0.2616260
C	2.0158611	4.7626920	-1.0318401
C	2.8405658	5.8549881	-0.8401778
C	3.8865138	5.8309702	0.1294847
C	4.0626140	4.6395975	0.9202683
C	3.1973048	3.5293052	0.6990848
C	5.0992374	4.6055197	1.8982502
C	5.9296491	5.6980826	2.0861838
C	5.7563745	6.8731265	1.3058232
C	4.7559233	6.9385691	0.3494394
C	3.1448493	0.7161206	-1.4100647
O	3.9996697	0.6878736	-2.5383171
C	5.0454174	1.6650577	-2.4990233
C	4.3278467	-1.3903331	-0.7484141
C	5.0613608	-1.0295812	0.3752374
C	6.3605512	-1.5569573	0.6162810
C	6.9320831	-2.4650997	-0.3463476
C	6.1686785	-2.7977863	-1.5027752
C	4.9004835	-2.2799241	-1.6997416
C	8.2331962	-2.9952815	-0.1048738
C	8.9371757	-2.6473219	1.0360115
C	8.3715667	-1.7540692	1.9868127
C	7.1105709	-1.2203992	1.7817356
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H	1.8203259	2.9801020	-4.7281573
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H	2.7229234	1.4419440	-4.4737051
H	5.7211767	1.4731378	-1.6428951
H	4.6294325	2.6868287	-2.4265786
H	5.6084550	1.5560601	-3.4382095
H	-0.2023669	-1.0057596	4.0369111
H	-1.8300567	0.7130605	2.0499719
H	-1.0048725	1.3232134	3.5057855
H	-2.3600452	0.1768532	3.6776418
H	0.9005018	-2.9819856	2.3651422
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H	3.3925019	-2.0956529	2.2576121
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H	-2.7057516	-0.6209305	-4.5974343

cat-B

Au	2.2910882	-1.1857620	5.3100187
C	4.0005418	-4.9532621	6.8211625
C	3.6744421	-4.7533374	5.4475776
C	2.6973490	-5.6117350	4.8289452
C	2.0857208	-6.6345103	5.6119161
C	2.4150360	-6.7964433	6.9497626
C	3.3787359	-5.9487274	7.5599249
C	2.3776893	-5.3944486	3.4545208
C	2.9565173	-4.3609680	2.7431223
C	3.8969773	-3.4819694	3.3599184
C	4.2612292	-3.7045926	4.6803987
C	4.3631419	-2.2702514	2.5449895
C	5.2969748	-1.3153955	3.3571234
O	6.5416379	-1.9854896	3.4040492
C	7.3602673	-1.8092685	4.5556240
O	3.1395629	-1.5436410	2.1782656
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O	3.0568629	0.8866393	2.8793591
C	4.4310548	1.2178032	3.3041887
C	4.3936594	1.3711209	4.8277032
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C	3.0985664	2.0771734	6.7825086
C	3.2386901	1.9845248	5.4097596
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C	4.9679575	1.0851560	9.8936252
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C	-3.1270598	-2.8382858	1.7275930
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C	4.7094021	-2.0081328	0.0412306
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C	7.5816475	0.4844101	1.8068394
C	4.7473444	2.5316580	2.5836472
C	4.2750030	2.7382149	1.2939458
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C	5.4089973	4.9267114	1.2000052
C	5.8980797	4.6778195	2.5157926
C	5.5741189	3.5162118	3.1943125
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C	5.2071176	6.3215101	-0.7946288
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H	1.2201328	-2.2004028	0.4458247
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H	-1.4442114	0.1235450	-0.6123042
H	-2.6870005	2.2033631	-1.1451799
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H	7.1660920	-3.3335360	-4.5218509
H	7.7049682	-4.5586669	-2.4241120
H	7.3305861	-4.9060417	0.0319117
H	6.1870349	-4.2624290	2.1381519
H	2.6889812	-4.1931279	1.6953959
H	1.6563991	-6.0591737	2.9672350
H	1.3474110	-7.2921459	5.1401833
H	1.9358026	-7.5838914	7.5403557
H	3.6313177	-6.0891365	8.6159746
H	4.7518833	-4.3033810	7.2844062
H	5.0032161	-3.0727233	5.1733226
H	5.9565539	3.3453903	4.2046085
H	6.5370495	5.4289390	2.9929588
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H	5.4458069	7.2414192	-1.3386289
H	3.9818376	5.5194689	-2.4109314
H	3.4203971	3.4174317	-1.1981464
H	3.6474604	1.9826922	0.8115294
H	2.4578131	2.3741372	4.7505134
H	2.2066553	2.5473119	7.2109048
H	3.0710536	2.0470618	9.5176235
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H	1.1037044	-4.1095464	6.4994009
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C	1.8211015	-2.7069587	7.9202162
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O	2.1512780	-2.9946386	9.1588215
C	3.2551762	-2.2437624	9.7504970
H	3.3352462	-2.6227264	10.7764959
H	3.0316958	-1.1666430	9.7304275
H	4.1757669	-2.4349782	9.1778004

INT1

Au	-1.4274140	-1.5983387	0.7036206
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C	-3.5580469	-1.3147553	0.6601296
C	-5.7269003	-0.5937127	1.5954020
H	-6.0531912	-0.7068566	0.5503152
H	-5.9557939	0.4342268	1.9217792
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C	-6.3880332	-3.0160505	1.8015360
O	-6.8337516	-3.0100235	0.4539953
H	-6.9335342	-3.7670915	2.4075595
H	-5.3251735	-3.3092910	1.7602807
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C	-3.6799685	-3.2963085	-0.8810860
C	-3.2160274	-0.9186266	-1.7985450
H	-4.1518381	-0.9796165	-2.3859205
H	-2.3946824	-1.2485307	-2.4559805
H	-3.0546399	0.1259742	-1.4936658
H	-4.7778458	-3.3762672	-0.9984974
H	-3.3805012	-3.9498646	-0.0488105
H	-3.1880121	-3.6306266	-1.8065766
H	-3.7277880	-0.5212833	2.6074978
C	-4.2760611	2.6881823	0.1800373
C	-3.2273358	2.3770682	1.0941665
C	-3.5043836	2.4135895	2.5066137
C	-4.8085402	2.7812427	2.9471055
C	-5.8039511	3.0921385	2.0328687
C	-5.5370575	3.0377546	0.6380491
C	-2.4515833	2.0860746	3.4125734
C	-1.1894888	1.7681867	2.9506718
C	-0.9004373	1.7438256	1.5507277
C	-1.9137448	2.0402829	0.6503283
C	0.5467568	1.4341435	1.1469644
C	0.7296554	1.0217665	-0.3552841
O	0.5598751	2.2025341	-1.1113512
C	0.0427682	2.0648835	-2.4327454
O	0.9904693	0.3138569	1.9786357
P	0.6493434	-1.2670115	1.6719118
O	1.9482792	-1.6954535	0.7645461
C	2.1813530	-1.2166610	-0.6075799
C	1.1677350	-1.9045498	-1.5228421
C	0.7814060	-1.3529004	-2.7368029
C	-0.1520471	-2.0112747	-3.5880586
C	-0.6851871	-3.2919457	-3.1947644
C	-0.2526109	-3.8524317	-1.9583723
C	0.6465271	-3.1824714	-1.1459442
C	-1.6283038	-3.9384943	-4.0466300
C	-2.0418168	-3.3402524	-5.2263419
C	-1.5214689	-2.0744351	-5.6113521
C	-0.5917945	-1.4273535	-4.8133155
N	0.9812729	-2.0209406	3.1034918
C	2.3457499	-1.8465782	3.7184754
C	3.0034403	-3.2125317	3.8924165
C	3.0177384	-3.8966130	5.1215603
C	3.5789382	-5.1801988	5.2185197
C	4.1419894	-5.7904578	4.0901994
C	4.1448474	-5.1106213	2.8615761

C	3.5767300	-3.8348066	2.7633164
C	-0.0986974	-2.7111532	3.8691565
C	-1.0814735	-1.7137901	4.5006374
C	-0.7548646	-3.8069805	3.0219651
C	-2.1503611	-3.9923901	2.9835429
C	-2.7108126	-5.0415475	2.2367990
C	-1.8897218	-5.9083616	1.5034485
C	-0.4978646	-5.7259784	1.5301103
C	0.0633421	-4.6905457	2.2868479
C	2.2992422	-0.9649183	4.9718643
C	1.4774798	2.5985370	1.4965223
C	1.1096951	3.9262538	1.1272463
C	1.9686796	4.9833538	1.3624780
C	3.2371966	4.7831450	1.9834483
C	3.6037799	3.4472340	2.3785775
C	2.6973955	2.3782339	2.1230828
C	4.8663193	3.2329410	3.0051970
C	5.7324677	4.2903358	3.2295012
C	5.3703692	5.6085856	2.8407509
C	4.1490565	5.8497296	2.2322612
C	2.1345796	0.3548216	-0.6065158
O	2.6681394	0.7862914	-1.8437824
C	3.5770881	1.8873505	-1.7304714
C	3.6309902	-1.6321881	-0.8984761
C	4.5969757	-1.4206458	0.0785797
C	5.9601886	-1.7664105	-0.1326188
C	6.3452525	-2.3317127	-1.4014918
C	5.3389678	-2.5231900	-2.3916208
C	4.0176333	-2.1876424	-2.1495264
C	7.7118951	-2.6779895	-1.6147863
C	8.6548489	-2.4779150	-0.6202562
C	8.2736232	-1.9234444	0.6326852
C	6.9550607	-1.5755157	0.8715391
H	-0.0751209	0.2962671	-0.6142709
H	2.8110453	0.6579376	0.2129495
H	-0.2992523	3.0669021	-2.7352474
H	-0.8147086	1.3608830	-2.4563202
H	0.8175373	1.7109833	-3.1342204
H	4.4618410	1.5961810	-1.1314437
H	3.0847142	2.7622552	-1.2681225
H	3.8947310	2.1338877	-2.7548298
H	0.4443416	-3.2309032	4.6798410
H	-1.6711771	-1.1921110	3.7262495
H	-0.5321613	-0.9517659	5.0739167
H	-1.7862445	-2.2176485	5.1823523
H	1.1500202	-4.5611554	2.3144084
H	0.1567017	-6.4015024	0.9688714
H	-2.3298681	-6.7243454	0.9207327
H	-3.7972396	-5.1795613	2.2305405
H	-2.8150290	-3.3212338	3.5338610
H	2.9242891	-1.3068685	2.9514333
H	1.6893333	-1.4095068	5.7761193
H	1.8756667	0.0207113	4.7174896
H	3.3200183	-0.8224648	5.3647391
H	2.5998734	-3.4305756	6.0203502
H	3.5804772	-5.6997925	6.1824140
H	4.5843447	-6.7889630	4.1682990
H	4.5952307	-5.5732483	1.9768557
H	3.5681184	-3.3130990	1.8005611
H	2.9769109	1.3679582	2.4355529
H	5.1429145	2.2152156	3.3045077
H	6.7012428	4.1149185	3.7088469
H	6.0638311	6.4357224	3.0251356
H	3.8693860	6.8661480	1.9336567
H	1.6768245	5.9987661	1.0728503
H	0.1419356	4.0975117	0.6499034
H	-0.3869411	1.5359242	3.6563315
H	-2.6552972	2.1003567	4.4888814
H	-5.0108593	2.8189924	4.0228897
H	-6.8014766	3.3775545	2.3826508
H	-6.3314385	3.2820315	-0.0748449
H	-4.0672743	2.6593252	-0.8956035
H	-1.7167181	2.0483301	-0.4230453
H	3.2640736	-2.3500049	-2.9246967
H	5.6242307	-2.9500597	-3.3593928
H	8.0050588	-3.1064525	-2.5794870
H	9.7016381	-2.7477693	-0.7949128
H	9.0302955	-1.7737143	1.4099460
H	6.6578069	-1.1511139	1.8373581
H	4.3147473	-0.9897143	1.0451969
H	0.9778543	-3.6423883	-0.2121658
H	-0.6419189	-4.8268832	-1.6446218
H	-2.0211416	-4.9187340	-3.7542489
H	-2.7676510	-3.8453746	-5.8719382
H	-1.8542839	-1.6163717	-6.5484196
H	-0.1831971	-0.4556141	-5.1120986
H	1.2120656	-0.4019247	-3.0574896
H	-7.7745067	-2.7443820	0.4579172
H	-5.3943437	0.6557285	6.4306828
C	-5.3607110	-0.2945714	5.8866553
C	-4.7387908	-1.4141796	6.4630890
H	-4.2814212	-1.3434930	7.4553724
C	-4.7269381	-2.6267775	5.7634033
H	-4.2633026	-3.5146076	6.2071812
C	-5.3128470	-2.7178269	4.4888838
H	-5.2887110	-3.6820183	3.9735728
C	-5.9253975	-1.6003155	3.8924217
C	-5.9516127	-0.3921275	4.6221514
H	-6.4494859	0.4821766	4.1894765
H	-8.0358635	0.0221311	0.7550388
C	-8.6321733	-0.4541419	1.5385206
C	-10.0183376	-0.2249040	1.5637871
H	-10.4737666	0.4146362	0.8000724
C	-10.8134625	-0.8050684	2.5592582
H	-11.8929782	-0.6235765	2.5797320
C	-10.2136068	-1.6185716	3.5335760
H	-10.8241323	-2.0756615	4.3194936
C	-8.8329123	-1.8457501	3.5084435
H	-8.3737234	-2.4744750	4.2794016
C	-8.0169359	-1.2662797	2.5127300

INT1′

Au	-1.0122541	-1.1641278	-0.0463075
C	-4.1390394	-0.9047720	-0.5252321
C	-3.0424115	-1.6053751	-0.7790959
C	-4.2918852	0.3570718	0.2741913
H	-4.5563119	1.1566368	-0.4376100
H	-3.3244546	0.6344892	0.7235985
C	-5.4186712	0.3207602	1.3662941
C	-4.8872101	-0.4111813	2.6295680
O	-4.1929829	-1.6284377	2.3616870
H	-5.7209758	-0.5624570	3.3448560
H	-4.1559075	0.2441696	3.1252336
C	-2.3061922	-2.6514309	-1.2766032
C	-1.7259128	-2.6143845	-2.6811910
C	-2.3366209	-4.0030334	-0.5833694
H	-1.3370200	-4.4618734	-0.5588809
H	-2.9993123	-4.6644496	-1.1736745
H	-2.7281149	-3.9225913	0.4400098
H	-0.6751536	-2.9437486	-2.6977470
H	-1.8070183	-1.6114388	-3.1247194
H	-2.3007695	-3.3252232	-3.3043591
H	-5.0494982	-1.2795091	-1.0196311
C	-3.8865627	1.2344486	-3.2793393
C	-2.9865768	1.9538409	-2.4406724
C	-3.4798346	3.0869189	-1.7006981
C	-4.8498848	3.4568639	-1.8311829
C	-5.6992931	2.7362226	-2.6569421
C	-5.2154190	1.6145563	-3.3837982
C	-2.5799765	3.7802950	-0.8380043
C	-1.2636545	3.3812077	-0.7183657
C	-0.7611998	2.2694857	-1.4622496
C	-1.6194298	1.5730024	-2.2986714
C	0.7163896	1.9291187	-1.2697366
C	1.2353473	0.7429969	-2.1524798
O	1.1166269	1.1780386	-3.4885373
C	0.9431867	0.1750708	-4.4863944
O	0.8807512	1.5690223	0.1460910
P	0.7831911	0.0564136	0.7810455
O	2.2837306	-0.5406225	0.4721256
C	2.8744769	-0.8811072	-0.8383186
C	2.2364181	-2.1780470	-1.3340482
C	2.2492036	-2.5286201	-2.6778695
C	1.7240826	-3.7760176	-3.1240794
C	1.2137696	-4.7143615	-2.1548307
C	1.2538121	-4.3484315	-0.7783955
C	1.7322830	-3.1131277	-0.3780422
C	0.6771097	-5.9546684	-2.6087335
C	0.6374209	-6.2537337	-3.9611556
C	1.1419807	-5.3298735	-4.9174688
C	1.6778326	-4.1198045	-4.5076623
N	0.8547003	0.3698342	2.4019087
C	1.8348606	1.4010427	2.8985614
C	2.8215599	0.7873598	3.8879065
C	2.6943167	0.9332789	5.2814621
C	3.6134520	0.3217511	6.1495315
C	4.6773519	-0.4317398	5.6355005
C	4.8192560	-0.5751358	4.2458543
C	3.8942339	0.0242007	3.3832823
C	-0.0123746	-0.3630733	3.3759403
C	-1.4453739	0.1770356	3.3785402
C	0.0992759	-1.8792348	3.1803843
C	-1.0180144	-2.6973939	2.9183570
C	-0.8563558	-4.0860031	2.7689645
C	0.4096361	-4.6738621	2.8803265
C	1.5255563	-3.8634293	3.1470751
C	1.3697846	-2.4808182	3.2949560
C	1.1061933	2.6585660	3.3853025
C	1.5940905	3.1635319	-1.4930892
C	1.4219921	3.9345100	-2.6822644
C	2.2690592	4.9922120	-2.9600476
C	3.3277122	5.3482902	-2.0721316
C	3.4845144	4.5937304	-0.8548035
C	2.5943760	3.5124506	-0.5954534
C	4.5338609	4.9400390	0.0463632
C	5.3969758	5.9843444	-0.2437148
C	5.2428457	6.7295022	-1.4446111
C	4.2294060	6.4199742	-2.3379098
C	2.7107760	0.3574713	-1.7742891
O	3.4942664	0.1363411	-2.9305233
C	4.2191911	1.2908658	-3.3696003
C	4.3677647	-1.0474707	-0.5097715
C	5.0586133	0.0317406	0.0317397
C	6.4202359	-0.0705982	0.4247249
C	7.1013314	-1.3284349	0.2478089
C	6.3801196	-2.4135698	-0.3271446
C	5.0512044	-2.2809591	-0.6950137
C	8.4631529	-1.4367571	0.6569436
C	9.1200268	-0.3537578	1.2170921
C	8.4470847	0.8873823	1.3907211
C	7.1259848	1.0268578	1.0020111
H	0.5703352	-0.1368125	-1.9848857
H	3.1341845	1.2035887	-1.2077818
H	0.5462925	0.6888704	-5.3756420
H	0.2194057	-0.5966498	-4.1551376
H	1.8993713	-0.3157640	-4.7343023
H	4.9450113	1.6087956	-2.5962937
H	3.5344188	2.1268233	-3.6017358
H	4.7622324	0.9888273	-4.2778401
H	0.4485942	-0.1387784	4.3542911
H	-1.9519732	-0.0493007	2.4242341
H	-1.4464365	1.2689455	3.5180824
H	-2.0334517	-0.2861363	4.1877974
H	2.2435764	-1.8549903	3.4986769
H	2.5207968	-4.3097299	3.2439548
H	0.5278140	-5.7577766	2.7751878
H	-1.7351440	-4.7123074	2.5833106
H	-2.0247190	-2.2733018	2.8448435
H	2.4175318	1.6768319	2.0046860
H	0.4566683	2.4526575	4.2525149
H	0.4815019	3.0578047	2.5699939
H	1.8379388	3.4275831	3.6843036
H	1.8820166	1.5336019	5.7038326
H	3.4994486	0.4431288	7.2317934

H	5.3970012	-0.9005934	6.3146935
H	5.6525408	-1.1507070	3.8288355
H	3.9929408	-0.1125131	2.3027374
H	2.7134559	2.9484690	0.3335314
H	4.6470287	4.3646159	0.9726590
H	6.2016414	6.2414537	0.4529422
H	5.9308837	7.5533712	-1.6604770
H	4.1097348	6.9962628	-3.2617855
H	2.1318887	5.5750507	-3.8772791
H	0.6208184	3.6697793	-3.3761126
H	-0.5790492	3.9255601	-0.0601383
H	-2.9505855	4.6405898	-0.2701933
H	-5.2249142	4.3101450	-1.2566480
H	-6.7503817	3.0286293	-2.7496508
H	-5.8984675	1.0515305	-4.0282250
H	-3.5126433	0.3696634	-3.8386788
H	-1.2609897	0.7294167	-2.8924351
H	4.5220170	-3.1330620	-1.1296541
H	6.8927824	-3.3708247	-0.4724641
H	8.9827685	-2.3917618	0.5215462
H	10.1656683	-0.4484262	1.5281254
H	8.9815155	1.7341617	1.8338823
H	6.6044671	1.9822007	1.1312317
H	4.5518607	0.9899602	0.1923186
H	1.7588292	-2.8655394	0.6854914
H	0.9013889	-5.0576331	-0.0216856
H	0.2945547	-6.6680817	-1.8702576
H	0.2222283	-7.2085521	-4.3001062
H	1.1095544	-5.5830527	-5.9822319
H	2.0716977	-3.4084575	-5.2418673
H	2.6944809	-1.8482609	-3.4064631
H	-4.7575184	-2.1866746	1.7964289
H	-4.3495314	4.8491559	2.2568827
C	-5.1127291	4.0631461	2.2849969
C	-6.3898204	4.3409085	2.7923664
H	-6.6334895	5.3434355	3.1590639
C	-7.3506660	3.3207083	2.8290604
H	-8.3507053	3.5213337	3.2277785
C	-7.0401572	2.0400101	2.3512154
H	-7.8043879	1.2559300	2.3748344
C	-5.7648186	1.7509581	1.8261271
C	-4.8015524	2.7801365	1.8129021
H	-3.7949708	2.5938654	1.4274620
H	-6.7975059	-2.0196219	2.1758503
C	-7.2094433	-1.5535892	1.2737317
C	-8.3158662	-2.1622918	0.6555203
H	-8.7267898	-3.0871999	1.0735360
C	-8.8954406	-1.5853843	-0.4806980
H	-9.7584520	-2.0577464	-0.9609067
C	-8.3665418	-0.3878766	-0.9906389
H	-8.8199107	0.0821698	-1.8700076
C	-7.2648229	0.2142190	-0.3730982
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C	-6.6597048	-0.3616571	0.7654674

TS1-R

Au	0.8428635	-0.5548740	0.3169456
C	3.6613908	-0.5574800	0.2100854
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C	4.9743271	0.1394072	0.3817810
H	5.2480793	0.1357663	1.4490148
H	4.8553796	1.1979279	0.0837893
C	6.1071253	-0.5095450	-0.4722070
C	6.3825114	-1.9268108	0.1197285
O	6.6976542	-1.8737385	1.5022787
H	7.1850376	-2.4245710	-0.4600847
H	5.4702424	-2.5456304	0.0469285
C	2.8053862	-0.8679224	2.5871850
C	3.6973146	-1.9189290	3.1888468
C	1.9576276	-0.0664396	3.5265402
H	2.6435061	0.5836598	4.1058620
H	1.4417166	-0.7074421	4.2606726
H	1.2224657	0.5594935	3.0013389
H	4.6518252	-2.0060615	2.6380152
H	3.1819463	-2.8964196	3.1290492
H	3.8821324	-1.7190669	4.2573887
H	3.3896712	-0.8298518	-0.8172269
C	3.2979199	3.2740904	2.0139992
C	2.4027221	3.1432627	0.9119959
C	2.9082029	3.3485215	-0.4208182
C	4.2780331	3.7033117	-0.5933733
C	5.1229401	3.8287117	0.4995245
C	4.6293497	3.6049277	1.8133286
C	2.0065597	3.2075926	-1.5172087
C	0.6773394	2.8954796	-1.3096388
C	0.1657468	2.6897920	0.0082814
C	1.0236186	2.8246286	1.0913506
C	-1.3199004	2.3244809	0.1309985
C	-1.7063121	1.6950012	1.5146056
O	-1.7360848	2.7665943	2.4360300
C	-1.4563318	2.4737615	3.8025026
O	-1.6001230	1.3323186	-0.9045363
P	-1.1397334	-0.2501713	-0.7878657
O	-2.4947306	-0.9058568	-0.1218801
C	-2.9824596	-0.6337156	1.2391897
C	-2.0650888	-1.3609437	2.2251763
C	-1.9430838	-0.9554044	3.5472247
C	-1.0678020	-1.6241225	4.4496422
C	-0.3104232	-2.7601352	3.9875299
C	-0.4910000	-3.1884418	2.6410599
C	-1.3450149	-2.5136452	1.7871971
C	0.5952605	-3.3975768	4.8854643
C	0.7587928	-2.9272474	6.1792524
C	0.0110066	-1.8070300	6.6358278
C	-0.8881709	-1.1747013	5.7914367
N	-1.2597539	-0.7897690	-2.3482815
C	-2.5504587	-0.5788628	-3.0929957
C	-3.1106678	-1.9234035	-3.5509826
C	-2.9726790	-2.3923919	-4.8700352
C	-3.4609540	-3.6579764	-5.2334021
C	-4.1027214	-4.4650735	-4.2848310

C	-4.2558760	-4.0012801	-2.9683120
C	-3.7594346	-2.7440690	-2.6042949
C	-0.0779431	-1.3550275	-3.0636559
C	0.9286008	-0.2653626	-3.4670791
C	0.5328729	-2.5147638	-2.2683335
C	1.9238152	-2.6629663	-2.1085307
C	2.4496109	-3.7172527	-1.3444523
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C	0.2085124	-4.5330894	-0.9297077
C	-0.3166176	-3.4772363	-1.6838066
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C	-2.2211760	3.5180607	-0.1905933
C	-1.9512383	4.7848632	0.4067090
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C	-3.3234846	3.3774200	-1.0234864
C	-5.3477177	4.3344899	-2.1182644
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C	-5.9339002	6.6632309	-1.7208151
C	-4.8310344	6.8247849	-0.8977019
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C	-4.7887497	2.2149938	2.4823091
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C	-6.2136396	-2.4878975	2.2375048
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C	-9.2252115	-2.3561971	-0.0096435
C	-8.7307547	-1.5353953	-1.0608235
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H	-8.7989118	-3.3074176	1.8799599
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TS1-S

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H	1.2978219	2.7072879	-4.6300613
H	0.5378890	1.2135334	-3.9612764
H	2.2789648	1.2108057	-4.4250705
H	5.5759412	1.4788820	-1.8271924
H	4.3799754	2.6462314	-2.5203848
H	5.3525434	1.5867271	-3.6120628
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H	-2.9592283	-1.1084541	2.9396278
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H	8.7969893	-3.5844474	-1.0229988
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H	4.6961197	-0.3256660	0.9222082
H	1.4939883	-3.1322567	-0.3232093
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H	-0.4772458	-5.4629563	-4.0460434
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H	0.4954657	-3.0171247	-7.4840684
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H	2.5673375	-0.7755783	-3.7751251
C	-6.1335119	0.2173239	0.3068675
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H	-7.2814707	0.9661774	-1.9142786
H	-5.7799266	-1.3266081	4.7371475
C	-5.5641603	-0.5138310	4.0358938
C	-4.8657206	0.6249692	4.4698095
H	-4.5357220	0.7064405	5.5107149
C	-4.6051273	1.6586303	3.5612047
C	-5.0322131	1.5564337	2.2270159
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C	-5.7269228	0.4165587	1.7767545
C	-5.9890695	-0.6128802	2.7056168
H	-6.5458021	-1.4988830	2.3798241
H	-7.2385302	-1.9155763	-1.1974039
C	-7.9794166	-1.3545856	-0.6207607
C	-9.3306917	-1.7285700	-0.7202663
H	-9.6125028	-2.5639682	-1.3699119
C	-10.3096327	-1.0422549	0.0070633
H	-11.3617220	-1.3351441	-0.0694918
C	-9.9299570	0.0233093	0.8390766
H	-10.6857155	0.5655483	1.4170057
C	-8.5845429	0.3932172	0.9387091
H	-8.2981483	1.2167307	1.6027120
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C	-2.8013612	-0.4464064	-1.2843538
C	-5.1248164	-0.7780238	-0.3488733
H	-5.3969874	-0.9702231	-1.4006818
H	-5.1635011	-1.7441624	0.1874797
C	-2.7783856	-0.6577926	-2.6450475
C	-3.5776337	0.2310329	-3.5577633
C	-1.8705877	-1.6652392	-3.2792369
H	-2.4391520	-2.2792048	-4.0014133
H	-1.0736748	-1.1664219	-3.8630673
H	-1.3863993	-2.3151859	-2.5355760
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H	-3.4370621	0.2921251	0.6077275

INT2-R

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C	-6.6820229	-1.5160568	0.9176231
O	-6.5057064	-0.1747742	0.5053910
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H	-2.4601858	-0.7511754	-3.5001288
H	-1.5283753	-0.4626585	-2.0026605
H	-5.3051827	0.1745173	-2.4638749
H	-5.7725584	-1.3967105	-1.7721039
H	-4.9500499	-1.3258733	-3.3698032
H	-3.7539540	-3.2330300	0.6957511
C	-4.2062916	2.4985242	-0.3767270
C	-3.2365758	2.2481466	0.6367066
C	-3.6384402	2.3223096	2.0171530
C	-4.9879696	2.6609832	2.3253399
C	-5.9044311	2.9082569	1.3147598
C	-5.5124282	2.8183625	-0.0475896
C	-2.6585320	2.0667138	3.0235223
C	-1.3498356	1.7765469	2.6878431
C	-0.9384494	1.7217704	1.3201725
C	-1.8772147	1.9492847	0.3239908
C	0.5414094	1.4360646	1.0454712
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O	0.7672922	2.2925990	-1.1579142
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O	0.9205772	0.2902964	1.8754186
P	0.5494444	-1.2729821	1.5316729
O	1.8166973	-1.7290470	0.5939703
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C	1.2454738	-1.7135226	-1.7747892
C	1.1319593	-1.1087214	-3.0206249
C	0.2281209	-1.6026226	-4.0042115
C	-0.5668259	-2.7691660	-3.7111008
C	-0.3975574	-3.3997284	-2.4466069
C	0.4850822	-2.8919892	-1.5078741
C	-1.5023592	-3.2311752	-4.6824228
C	-1.6558537	-2.5644511	-5.8876120
C	-0.8721910	-1.4132940	-6.1775236
C	0.0538999	-0.9467420	-5.2585670
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C	3.0177547	-3.0921464	3.7645943
C	3.1371186	-3.7300781	5.0131442

C	3.8234020	-4.9497433	5.1295820
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C	4.3020416	-4.9083387	2.7529794
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C	-1.1344607	-2.0675834	4.3947329
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C	-2.0021686	-4.3337328	2.7213278
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C	0.2244683	-4.6358445	1.8202294
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C	5.1974396	5.5535888	3.2633597
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C	2.2562423	0.3829889	-0.5961602
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C	3.8325647	1.9686529	-1.4219910
C	3.6481454	-1.6985385	-0.8927672
C	4.5846892	-1.4218683	0.0976982
C	5.9158862	-1.9149478	0.0292854
C	6.3044338	-2.7079543	-1.1103852
C	5.3333007	-2.9639845	-2.1202544
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C	7.6379627	-3.2091066	-1.1782789
C	8.5441466	-2.9447360	-0.1647945
C	8.1583020	-2.1673839	0.9624457
C	6.8726562	-1.6630518	1.0572802
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H	2.8433478	0.5918906	0.3159312
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H	-0.3745229	1.5315184	-2.7482975
H	1.3292422	1.9415915	-3.1491392
H	4.6272666	1.6407274	-0.7240444
H	3.2794716	2.8180996	-0.9815957
H	4.2871370	2.2719784	-2.3770572
H	0.5307888	-3.4422681	4.4093195
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H	-0.6469018	-1.3175083	5.0352352
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H	1.2876984	-4.3787320	1.8158604
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H	-2.0042602	-6.7171744	0.2614275
H	-3.5520383	-5.5805624	1.8783239
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H	2.8059369	-1.2035390	2.8138441
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H	2.7055812	-3.2761916	5.9114742
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H	4.9499060	-6.4875687	4.0960441
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H	3.5220132	-3.2112965	1.6596403
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INT2-S

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C	0.3888370	-3.5705621	-6.4159553
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N	0.7327219	-0.6497202	2.3747317
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C	2.1117840	-2.1441966	5.1702689
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H	2.2737300	-3.6600967	6.7094197
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H	8.5218015	-3.8831652	-0.2139087
H	9.6830409	-3.0995840	1.8426508
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H	6.4464415	-0.3474639	2.6743071
H	4.5130851	-0.2339769	1.1357038
H	1.0904952	-2.8616621	-0.6442631
H	-0.0564605	-4.1986850	-2.3687212
H	-0.5050707	-4.6866594	-4.7981514
H	-0.1269195	-4.1378442	-7.1978409
H	1.4364646	-2.2922625	-7.8396469
H	2.6351994	-0.9947821	-6.0836668
H	3.1189130	-0.5671089	-3.6837131
H	-6.3816996	-3.3048451	3.5612058
C	-6.4963162	-2.9347936	2.5371263
C	-7.0801016	-3.7490492	1.5542793
H	-7.4243950	-4.7573356	1.8059866
C	-7.2282899	-3.2560513	0.2509437
H	-7.6901277	-3.8781741	-0.5228483
C	-6.7925288	-1.9607879	-0.0712416
H	-6.9194527	-1.6008381	-1.0976296
C	-6.1982172	-1.1357576	0.9052768
C	-6.0609105	-1.6435379	2.2135505
H	-5.6215859	-1.0103252	2.9919578
H	-3.7951776	1.7795683	2.0883073
C	-4.8346558	1.9231738	2.3919129
C	-5.1102054	2.8251405	3.4323813
H	-4.2836195	3.3519876	3.9219783
C	-6.4296740	3.0493326	3.8449143
H	-6.6439508	3.7539696	4.6548999
C	-7.4744081	2.3537749	3.2161719
H	-8.5100149	2.5119587	3.5347640
C	-7.1967294	1.4475525	2.1859389
H	-8.0186269	0.8909765	1.7217822
C	-5.8727660	1.2240391	1.7506657
Au	-1.0788075	-0.4311450	-0.5427114
C	-3.8740280	-0.6977003	-1.0038639
C	-2.7524140	-0.5558256	-1.8345812
C	-4.1357463	0.1374008	0.2118782
H	-3.6603540	1.1262581	0.0795125
H	-3.6345434	-0.3525179	1.0648767
C	-5.6450429	0.2633033	0.5733562
C	-6.3284383	0.9020769	-0.6718259
H	-6.2229346	1.9958499	-0.6140751
H	-7.4003478	0.6477903	-0.7065253
O	-5.7191424	0.4242955	-1.8836613
C	-2.6180579	-0.6106402	-3.1950693
C	-3.8037115	-0.5510914	-4.1295677
C	-1.2785511	-0.6036326	-3.8755139
H	-1.1365851	0.3510423	-4.4199783
H	-1.2176810	-1.4028315	-4.6354969
H	-0.4454288	-0.7239454	-3.1644341
H	-3.8572961	0.4318032	-4.6380041

H	-4.7613208	-0.7308330	-3.6210808
H	-3.6707263	-1.3006366	-4.9314814
H	-4.4642937	-1.6241834	-1.0797635
H	-5.1912891	1.1611898	-2.2600484

TS2-S

C	1.2824853	2.9762239	4.2627038
C	0.2157993	2.3047598	3.5965240
C	-0.9474224	3.0583234	3.2111293
C	-0.9940650	4.4529854	3.4996385
C	0.0695157	5.0816511	4.1273322
C	1.2162730	4.3372110	4.5154827
C	-2.0031735	2.3776616	2.5341083
C	-1.9113734	1.0293963	2.2439554
C	-0.7461466	0.2804462	2.5971812
C	0.2828991	0.9187460	3.2770634
C	-0.6928983	-1.2006391	2.1995549
C	0.7730613	-1.7525445	2.0951958
O	1.2195045	-1.9428156	3.4231238
C	2.6223116	-1.8534636	3.6700201
O	-1.3144674	-1.3273207	0.8852812
P	-0.6217862	-0.8493709	-0.5374904
O	0.1824989	-2.2225833	-0.9697356
C	1.2892897	-2.8729127	-0.2458158
C	2.5556601	-2.0312772	-0.4232235
C	3.6534577	-2.1976484	0.4114004
C	4.8387563	-1.4271353	0.2400881
C	4.9155343	-0.4811195	-0.8448534
C	3.7935366	-0.3586598	-1.7119441
C	2.6472458	-1.1086816	-1.5083993
C	6.0970742	0.3021068	-0.9973224
C	7.1525952	0.1688887	-0.1095019
C	7.0756711	-0.7608581	0.9639314
C	5.9462269	-1.5454554	1.1308812
N	-1.9304135	-0.9083823	-1.5579827
C	-2.8628172	-2.0884834	-1.4746138
C	-2.9557820	-2.8082564	-2.8180103
C	-4.0332666	-2.6308612	-3.7060664
C	-4.0599203	-3.3012158	-4.9399657
C	-3.0168745	-4.1668672	-5.2963978
C	-1.9418127	-4.3588345	-4.4138640
C	-1.9108699	-3.6784471	-3.1910570
C	-2.1751075	0.1655523	-2.5599568
C	-2.8031049	1.4103194	-1.9138911
C	-0.9122708	0.4291465	-3.3891881
C	-0.4582968	1.7263290	-3.6886117
C	0.7034597	1.9196576	-4.4531502
C	1.4235778	0.8224070	-4.9423008
C	0.9627150	-0.4756438	-4.6730312
C	-0.1907090	-0.6685497	-3.9040684
C	-4.2056684	-1.6895801	-0.8505191
C	-1.5360881	-2.0758054	3.1308523
C	-1.4209674	-1.9201236	4.5441861
C	-2.1215682	-2.7475258	5.4018194
C	-2.9827795	-3.7705518	4.9056340
C	-3.1188729	-3.9186303	3.4794401
C	-2.3812181	-3.0531880	2.6214334
C	-3.9840251	-4.9297225	2.9678900
C	-4.6823333	-5.7629289	3.8263072
C	-4.5472848	-5.6177581	5.2337681
C	-3.7167917	-4.6421920	5.7616632
C	0.8439576	-3.0720861	1.2460138
O	1.7295729	-4.0052465	1.8348230
C	1.0914019	-4.9260902	2.7253516
C	1.3836215	-4.2441945	-0.9345649
C	0.2934705	-5.1059170	-0.8739254
C	0.2740909	-6.3414524	-1.5765499
C	1.4254315	-6.7136128	-2.3600101
C	2.5397504	-5.8272958	-2.3884135
C	2.5205745	-4.6247958	-1.7004830
C	1.3997265	-7.9444493	-3.0804446
C	0.2856515	-8.7662978	-3.0351974
C	-0.8521018	-8.3960497	-2.2654991
C	-0.8572442	-7.2105880	-1.5506031
H	1.3901079	-0.9706505	1.6001774
H	-0.1716292	-3.5045857	1.2029096
H	2.7326877	-1.7277865	4.7587053
H	3.0676097	-0.9810248	3.1519366
H	3.1476206	-2.7672195	3.3464943
H	0.3725374	-5.5627139	2.1731045
H	0.5677447	-4.3951584	3.5410519
H	1.8893836	-5.5584164	3.1429842
H	-2.9169141	-0.2753429	-3.2518501
H	-2.0986465	1.8736605	-1.1994229
H	-3.7074478	1.1277360	-1.3541259
H	-3.0829834	2.1610380	-2.6715539
H	-0.5355888	-1.6834394	-3.6903625
H	1.5054188	-1.3448877	-5.0590205
H	2.3280800	0.9759224	-5.5400119
H	1.0430576	2.9367309	-4.6776101
H	-1.0147084	2.5993663	-3.3396621
H	-2.3623182	-2.7821948	-0.7796770
H	-4.7471552	-0.9512206	-1.4657210
H	-4.0331935	-1.2550738	0.1473714
H	-4.8520286	-2.5772029	-0.7434957
H	-4.8696581	-1.9766001	-3.4385396
H	-4.9053376	-3.1512622	-5.6195926
H	-3.0449213	-4.6957208	-6.2548120
H	-1.1268338	-5.0433151	-4.6721479
H	-1.0634059	-3.8172932	-2.5137744
H	-2.4994908	-3.1647307	1.5405036
H	-4.0875349	-5.0377772	1.8817836
H	-5.3432580	-6.5375627	3.4234305
H	-5.1057451	-6.2824102	5.9012386
H	-3.6140363	-4.5290308	6.8466034
H	-2.0231575	-2.6197403	6.4853462
H	-0.7675435	-1.1410468	4.9436935
H	-2.7259018	0.5216718	1.7200498
H	-2.8942730	2.9448949	2.2448512
H	-1.8749369	5.0272225	3.1997000
H	0.0242748	6.1567814	4.3295121

H	2.0460577	4.8428002	5.0205971
H	2.1617615	2.3979332	4.5689724
H	1.1715194	0.3628503	3.5786669
H	3.3861274	-3.9586312	-1.7499209
H	3.4213281	-6.1053989	-2.9762269
H	2.2759116	-8.2291698	-3.6733172
H	0.2760168	-9.7077207	-3.5942728
H	-1.7262224	-9.0550531	-2.2416863
H	-1.7331829	-6.9208325	-0.9594869
H	-0.5975877	-4.8301943	-0.2994931
H	1.8135693	-1.0121449	-2.2068055
H	3.8362873	0.3420321	-2.5535618
H	6.1560181	1.0144477	-1.8282945
H	8.0555565	0.7756897	-0.2345507
H	7.9189245	-0.8585288	1.6556914
H	5.8879712	-2.2671375	1.9536775
H	3.6139609	-2.9432416	1.2092405
H	-4.5013590	5.4121680	1.3033372
C	-3.5358823	5.9179937	1.1970840
C	-3.2057843	6.9932992	2.0376759
H	-3.9097988	7.3312824	2.8047910
C	-1.9635265	7.6229051	1.8887190
H	-1.6879686	8.4546775	2.5455094
C	-1.0656298	7.2007789	0.8947035
H	-0.0998561	7.7050832	0.8107870
C	-1.3935861	6.1421261	0.0277456
C	-2.6357365	5.4956721	0.2118501
H	-2.9258604	4.6761357	-0.4560409
H	0.2231981	4.7356843	-3.6294613
C	-0.6691127	5.3678975	-3.6784623
C	-1.2608413	5.5937099	-4.9279481
H	-0.8378776	5.1202861	-5.8204226
C	-2.3859597	6.4238206	-5.0315227
H	-2.8528854	6.6032343	-6.0052860
C	-2.8981349	7.0305923	-3.8771885
H	-3.7654305	7.6956077	-3.9449713
C	-2.3075441	6.7954377	-2.6265296
H	-2.7233494	7.2827279	-1.7404279
C	-1.1928627	5.9430395	-2.5016145
Au	0.5694266	1.1082236	-0.2670371
C	0.6183804	3.8761496	0.2844352
C	1.5635803	2.8599549	0.4198402
C	-0.1347404	4.1894044	-0.9703235
H	0.4234641	3.7946180	-1.8352584
H	-1.0929597	3.6417697	-0.9398688
C	-0.4924177	5.7044339	-1.1419131
C	0.8408144	6.4771793	-1.1932609
H	1.3888770	6.1834441	-2.1062036
H	0.6503647	7.5659488	-1.2469306
O	1.5999215	6.1515812	-0.0216060
C	2.7283673	2.7907411	1.1345922
C	3.4576208	4.0471441	1.5480945
C	3.4164492	1.5029340	1.4776802
H	4.4311819	1.4695355	1.0402818
H	3.5484466	1.4415307	2.5742743
H	2.8638224	0.6190058	1.1228704
H	4.2265787	4.3167612	0.7975784
H	2.7659282	4.8943411	1.6730631
H	3.9940136	3.8776856	2.4977426
H	0.2546157	4.3733435	1.1970865
H	2.5470790	6.1644977	-0.2444235

TS1-S′

C	-3.7768385	1.3411014	-3.1683639
C	-2.8285679	2.0163832	-2.3468427
C	-3.2741266	3.1087239	-1.5210254
C	-4.6439191	3.4988893	-1.5709131
C	-5.5354352	2.8411403	-2.4055977
C	-5.1023917	1.7462468	-3.2011529
C	-2.3207968	3.7626448	-0.6847512
C	-0.9964820	3.3715040	-0.6803169
C	-0.5428638	2.3005094	-1.5083455
C	-1.4533674	1.6394869	-2.3191521
C	0.9396463	1.9367433	-1.4043950
C	1.3573675	0.6624652	-2.2146654
O	1.2628550	1.0134797	-3.5784710
C	1.0131813	-0.0433846	-4.5000851
O	1.2055970	1.6774480	0.0117661
P	0.8686007	0.2295084	0.7396197
O	2.2980682	-0.5581658	0.4949901
C	2.8555385	-1.0072029	-0.7878846
C	2.1287738	-2.2859316	-1.2095176
C	2.1564378	-2.7427394	-2.5212972
C	1.5821031	-3.9960238	-2.8833681
C	0.9902073	-4.8232290	-1.8601645
C	0.9800736	-4.3342439	-0.5207489
C	1.5245341	-3.1025201	-0.2051475
C	0.4178541	-6.0766753	-2.2292265
C	0.4192451	-6.4922681	-3.5512296
C	0.9995271	-5.6759254	-4.5607402
C	1.5722669	-4.4575021	-4.2327908
N	0.9929005	0.6230843	2.3449377
C	2.1527345	1.4698020	2.7941401
C	2.9656473	0.7500774	3.8676981
C	2.8827704	1.0787824	5.2331289
C	3.6327527	0.3701309	6.1858887
C	4.4837078	-0.6675534	5.7840883
C	4.5795703	-0.9986526	4.4227952
C	3.8215050	-0.3002775	3.4758516
C	-0.0283287	0.1690797	3.3368732
C	-1.3021155	1.0241319	3.2750134
C	-0.2593023	-1.3422273	3.2209461
C	-1.5153498	-1.8993303	2.9190300
C	-1.6817071	-3.2892136	2.8023645
C	-0.5902119	-4.1448271	2.9932876
C	0.6680395	-3.6011414	3.3042549
C	0.8310847	-2.2150870	3.4140920
C	1.6974654	2.8893919	3.1536765
C	1.8265051	3.1222476	-1.7871716
C	1.5697867	3.8204293	-3.0047756
C	2.4031623	4.8446483	-3.4138289

C	3.5325438	5.2363697	-2.6355591
C	3.7811922	4.5506551	-1.3937123
C	2.9033033	3.5015242	-0.9968881
C	4.9040950	4.9341100	-0.6037182
C	5.7478230	5.9500851	-1.0214611
C	5.5011486	6.6287924	-2.2454120
C	4.4167249	6.2804397	-3.0343663
C	2.7961345	0.1865910	-1.8011881
O	3.5643329	-0.1662697	-2.9349032
C	4.3544929	0.9109933	-3.4507086
C	4.3377929	-1.2612251	-0.4572541
C	5.0618595	-0.2408989	0.1503697
C	6.4228335	-0.4064021	0.5228064
C	7.0693997	-1.6648230	0.2482215
C	6.3129218	-2.6892412	-0.3894483
C	4.9839755	-2.4978661	-0.7307123
C	8.4329992	-1.8350945	0.6290398
C	9.1243529	-0.8115740	1.2554922
C	8.4843616	0.4288077	1.5291930
C	7.1624063	0.6273411	1.1704788
H	0.6262482	-0.1482902	-1.9871036
H	3.2881113	1.0247553	-1.2785187
H	0.7160939	0.4356099	-5.4457740
H	0.1883938	-0.6961699	-4.1464272
H	1.9119960	-0.6616014	-4.6605207
H	5.0957504	1.2410829	-2.6970346
H	3.7185936	1.7663504	-3.7443144
H	4.8804770	0.5157112	-4.3328748
H	0.4584743	0.3382036	4.3142308
H	-1.8036169	0.9129437	2.2977701
H	-1.0566159	2.0894743	3.4003408
H	-2.0136085	0.7355841	4.0665007
H	1.8162411	-1.7989536	3.6458174
H	1.5280110	-4.2603629	3.4628794
H	-0.7165006	-5.2303522	2.9154789
H	-2.6792380	-3.6778938	2.5765451
H	-2.3896771	-1.2638291	2.7754028
H	2.7986228	1.5416810	1.9038185
H	1.0103672	2.9007799	4.0167824
H	1.1803329	3.3370531	2.2900931
H	2.5700757	3.5139222	3.4106248
H	2.2381854	1.8984256	5.5668535
H	3.5550102	0.6380935	7.2448171
H	5.0748905	-1.2129251	6.5272304
H	5.2501843	-1.8002991	4.0950792
H	3.8826378	-0.5746373	2.4184700
H	3.0879277	2.9925833	-0.0467310
H	5.0909364	4.4086581	0.3402126
H	6.6094499	6.2352424	-0.4087105
H	6.1748184	7.4314759	-2.5630206
H	4.2261776	6.8044605	-3.9775267
H	2.1992928	5.3739241	-4.3511676
H	0.7109534	3.5285757	-3.6142000
H	-0.2693013	3.8848559	-0.0437946
H	-2.6533720	4.5935611	-0.0528011
H	-4.9818479	4.3289935	-0.9417764
H	-6.5812295	3.1625746	-2.4499489
H	-5.8207232	1.2259764	-3.8431377
H	-3.4381302	0.5001029	-3.7838893
H	-1.1329386	0.8272930	-2.9747774
H	4.4265691	-3.3052190	-1.2125693
H	6.7977016	-3.6478618	-0.6048064
H	8.9261951	-2.7907398	0.4189767
H	10.1711356	-0.9539249	1.5438271
H	9.0443433	1.2273169	2.0270150
H	6.6650107	1.5810284	1.3814681
H	4.5784911	0.7157061	0.3779752
H	1.5125745	-2.7599947	0.8314680
H	0.5296116	-4.9432655	0.2704056
H	-0.0241418	-6.7065982	-1.4489955
H	-0.0212940	-7.4570332	-3.8239317
H	0.9976834	-6.0191994	-5.6004976
H	2.0271633	-3.8307300	-5.0079003
H	2.6629436	-2.1495150	-3.2859477
H	-4.1554167	4.6519197	2.6327389
C	-4.9223595	3.8734873	2.7153373
C	-6.0917409	4.1128894	3.4486039
H	-6.2472535	5.0774067	3.9427359
C	-7.0640479	3.1058473	3.5395419
H	-7.9853416	3.2805548	4.1049777
C	-6.8667682	1.8761336	2.8990019
H	-7.6440122	1.1062707	2.9595084
C	-5.6932076	1.6210844	2.1594830
C	-4.7221284	2.6387636	2.0795445
H	-3.7998044	2.4904793	1.5123074
H	-7.3445637	-1.8330237	2.1520306
C	-7.5921004	-1.2776303	1.2391710
C	-8.7546181	-1.6448815	0.5399303
H	-9.3594018	-2.4833801	0.9011823
C	-9.1447951	-0.9363189	-0.6019705
H	-10.0509830	-1.2211784	-1.1462584
C	-8.3707909	0.1534731	-1.0309037
H	-8.6740352	0.7307151	-1.9112634
C	-7.2143333	0.5143317	-0.3324665
H	-6.6289751	1.3749796	-0.6683419
C	-6.7929225	-0.2009011	0.8063176
Au	-1.0857355	-0.7364850	-0.0258688
C	-4.1308221	-0.9772380	-0.3062211
C	-2.9235316	-1.5275728	-0.6716650
C	-4.3117397	0.2559374	0.5035983
H	-4.4825665	1.0870179	-0.2091661
H	-3.3651912	0.4898550	1.0219681
C	-5.4975856	0.2344238	1.5171822
C	-5.1033377	-0.7552078	2.6454538
H	-5.9179091	-0.8312750	3.3926086
O	-4.7279435	-2.0370020	2.1437706
H	-4.2201078	-0.3595355	3.1710828
C	-2.7867008	-2.7284837	-1.3778397
C	-1.7768936	-2.9033355	-2.4587057
C	-3.6095366	-3.9187499	-0.9933099
H	-3.1641089	-4.3531344	-0.0762646
H	-3.6276808	-4.7004130	-1.7696429

H	-4.6346125	-3.6108164	-0.7163425
H	-1.2616455	-1.9634641	-2.7084983
H	-2.2724130	-3.3256459	-3.3535769
H	-1.0163745	-3.6508495	-2.1639754
H	-5.5151799	-2.4309302	1.7230580
H	-5.0414096	-1.3484919	-0.8051148

INT3-R

Au	-1.04860	-0.32140	0.34180
C	-3.99530	-0.51710	0.88930
C	-2.76970	-1.14180	1.19870
C	-4.18400	0.44510	-0.22070
H	-3.41170	0.28690	-0.99330
H	-3.99990	1.46310	0.17710
C	-5.63000	0.38380	-0.81430
C	-5.76750	-1.06730	-1.33280
H	-5.09740	-1.21290	-2.19590
H	-6.80230	-1.26930	-1.66410
O	-5.40560	-1.96070	-0.27200
C	-2.73980	-2.20830	2.09640
C	-3.97080	-2.96220	2.51850
C	-1.45080	-2.75360	2.62450
H	-1.28430	-3.77680	2.23620
H	-1.49480	-2.84530	3.72510
H	-0.59180	-2.12520	2.34330
H	-3.93000	-3.19050	3.59830
H	-3.98940	-3.93580	1.99120
H	-4.91130	-2.44830	2.27150
H	-4.81120	-0.54170	1.62590
C	-2.35860	-4.72400	-0.47710
C	-1.60310	-3.79520	-1.25100
C	-2.21290	-3.20360	-2.41380
C	-3.55690	-3.54770	-2.74010
C	-4.27500	-4.44140	-1.95370
C	-3.66620	-5.03940	-0.81430
C	-1.43610	-2.30620	-3.20490
C	-0.14630	-1.97530	-2.83910
C	0.43780	-2.49440	-1.64370
C	-0.27540	-3.41820	-0.89270
C	1.80920	-1.93620	-1.23590
C	2.13410	-2.15320	0.28220
O	2.51320	-3.50880	0.40700
C	2.29380	-4.14960	1.66080
O	1.77040	-0.49730	-1.47970
P	0.89290	0.55060	-0.53600
O	2.03650	0.99110	0.57290
C	2.70230	0.11580	1.54430
C	1.72610	-0.17300	2.68890
C	1.87740	-1.27780	3.51770
C	0.97150	-1.53610	4.58670
C	-0.11390	-0.61860	4.82780
C	-0.22270	0.53070	3.99420
C	0.67030	0.74960	2.95950
C	-1.04530	-0.90750	5.86800
C	-0.91730	-2.05720	6.63240
C	0.15480	-2.96220	6.39620
C	1.08200	-2.70360	5.39890
N	0.86550	1.93310	-1.45920
C	2.16580	2.50550	-1.95280
C	2.27240	3.96680	-1.52210
C	2.17800	5.03720	-2.42930
C	2.24940	6.36490	-1.97710
C	2.42450	6.63690	-0.61430
C	2.52860	5.57470	0.29820
C	2.44810	4.25240	-0.15180
C	-0.38750	2.50400	-2.01350
C	-1.05570	1.53830	-3.01060
C	-1.34860	3.03820	-0.94500
C	-2.64230	3.45910	-1.31310
C	-3.52670	3.98860	-0.36250
C	-3.13950	4.09440	0.98290
C	-1.84870	3.69460	1.35800
C	-0.95950	3.18790	0.39900
C	2.37540	2.23220	-3.44760
C	2.93390	-2.47880	-2.11820
C	2.99440	-3.87570	-2.40040
C	4.03580	-4.39770	-3.14420
C	5.07280	-3.56110	-3.65370
C	5.00820	-2.14720	-3.38450
C	3.92250	-1.63860	-2.61390
C	6.03490	-1.29890	-3.89330
C	7.08220	-1.82260	-4.63360
C	7.14560	-3.21740	-4.89940
C	6.16180	-4.06780	-4.42090
C	3.23970	-1.15660	0.78910
O	4.14390	-1.81550	1.65470
C	5.32210	-2.29820	1.00100
C	3.92450	0.92860	2.00490
C	4.65220	1.64440	1.06200
C	5.79880	2.40580	1.42070
C	6.23000	2.40740	2.79570
C	5.48010	1.64920	3.74040
C	4.35640	0.93490	3.36110
C	7.38010	3.16920	3.15620
C	8.06920	3.90120	2.20330
C	7.63830	3.90570	0.84800
C	6.52720	3.17380	0.46460
H	1.19930	-1.97000	0.85940
H	3.78850	-0.75810	-0.08390
H	2.35890	-5.23180	1.46690
H	1.29080	-3.90830	2.06630
H	3.05800	-3.86050	2.40200
H	5.90020	-1.45450	0.57570
H	5.06710	-3.01570	0.19970
H	5.92340	-2.79950	1.77450
H	-0.04420	3.39080	-2.57810
H	-1.45350	0.65200	-2.48600
H	-0.31850	1.19730	-3.75420
H	-1.88500	2.02540	-3.54690
H	0.06010	2.92120	0.68860
H	-1.52140	3.79250	2.39860

H	-3.83170	4.50020	1.72830
H	-4.52310	4.31150	-0.68250
H	-2.97800	3.38240	-2.35080
H	2.93990	1.94830	-1.40180
H	1.61100	2.72070	-4.07610
H	2.33600	1.14690	-3.63350
H	3.36140	2.61160	-3.76490
H	2.05500	4.84730	-3.50040
H	2.17280	7.18730	-2.69650
H	2.48570	7.67250	-0.26380
H	2.67800	5.77730	1.36400
H	2.53000	3.42390	0.55960
H	3.87270	-0.56330	-2.42180
H	5.98350	-0.22350	-3.68710
H	7.86660	-1.16260	-5.01840
H	7.97840	-3.61810	-5.48690
H	6.20930	-5.14280	-4.62680
H	4.07290	-5.47230	-3.35420
H	2.20950	-4.53160	-2.01570
H	0.43980	-1.28160	-3.44740
H	-1.87700	-1.87930	-4.11260
H	-4.01240	-3.11090	-3.63610
H	-5.30130	-4.71080	-2.22510
H	-4.23240	-5.75970	-0.21480
H	-1.88540	-5.19730	0.39010
H	0.16340	-3.85850	0.00430
H	3.79390	0.37240	4.11040
H	5.80060	1.64360	4.78800
H	7.70970	3.16810	4.20110
H	8.95060	4.48370	2.49130
H	8.19010	4.49430	0.10760
H	6.18850	3.18070	-0.57770
H	4.33710	1.64860	0.01420
H	0.57400	1.64370	2.34190
H	-1.03410	1.24460	4.17280
H	-1.86780	-0.20720	6.05120
H	-1.63870	-2.27020	7.42810
H	0.24700	-3.86320	7.01150
H	1.91000	-3.39740	5.21570
H	2.71290	-1.96080	3.35320
H	-7.25490	3.17740	2.60740
C	-7.37820	2.23100	2.07010
C	-8.41300	1.35050	2.42010
H	-9.10150	1.60080	3.23380
C	-8.55560	0.14730	1.71810
H	-9.35690	-0.55100	1.98150
C	-7.67440	-0.17600	0.67410
H	-7.80280	-1.13180	0.15960
C	-6.63340	0.69760	0.30970
C	-6.49990	1.90490	1.03030
H	-5.70320	2.60780	0.76540
H	-3.99450	0.55840	-3.01950
C	-4.82580	1.26980	-3.06910
C	-4.92500	2.10750	-4.18670
H	-4.18110	2.03370	-4.98780
C	-5.97310	3.03500	-4.28040
H	-6.05280	3.69360	-5.15130
C	-6.92340	3.10030	-3.25330
H	-7.75550	3.80920	-3.31990
C	-6.82410	2.25640	-2.13640
H	-7.58100	2.31730	-1.34960
C	-5.76490	1.33710	-2.01780
H	-4.84670	-2.67780	-0.64360

INT3-S

Au	-1.1169270	-0.1532838	-0.6768774
C	-4.0777302	0.6027272	-0.8065537
C	-2.8516842	0.6280282	-1.5262558
C	-4.1841128	0.3974329	0.6551922
H	-4.1813004	1.4032417	1.1191873
H	-3.2936118	-0.1393619	1.0256227
C	-5.5023448	-0.3261668	1.0510541
C	-5.4379716	-1.6561150	0.2511612
O	-4.9288668	-1.3893114	-1.0728000
C	-2.8547588	1.3343020	-2.7337104
C	-4.0718543	1.8452616	-3.4623263
C	-1.5644480	1.7100759	-3.3949331
H	-1.4043260	2.8000324	-3.2654263
H	-1.5956403	1.5350771	-4.4850497
H	-0.7037038	1.1792402	-2.9590807
H	-4.0659069	1.4252124	-4.4855524
H	-4.0065840	2.9430132	-3.5850330
H	-5.0361923	1.5995215	-2.9972398
H	-4.1169799	-1.9258224	-1.2129794
H	-4.9749241	1.0410728	-1.2592527
H	-4.7690766	-2.3520610	0.7760425
H	-6.4346604	-2.1169922	0.1529962
C	-2.9808011	3.8686555	0.0597617
C	-2.0619266	3.2592382	0.9631849
C	-2.4817891	3.0030321	2.3170372
C	-3.7931499	3.3955618	2.7181687
C	-4.6606635	3.9948805	1.8161135
C	-4.2560771	4.2234740	0.4731743
C	-1.5699991	2.3489591	3.1993424
C	-0.3120679	1.9738874	2.7679145
C	0.1158236	2.2340451	1.4307994
C	-0.7515886	2.8713816	0.5561771
C	1.5062078	1.7249121	1.0390612
C	1.8516481	1.9170184	-0.4745399
O	2.0315385	3.3049651	-0.6583416
C	1.7821219	3.8343123	-1.9560946
O	1.5270666	0.2912233	1.3256615
P	0.8509807	-0.8435850	0.3207318
O	2.1404170	-1.1860843	-0.6574219
C	2.8028865	-0.2852088	-1.6077320
C	1.9373174	-0.1804423	-2.8655757
C	2.0551751	0.8851320	-3.7500096
C	1.2973850	0.9382072	-4.9557957
C	0.4132303	-0.1522114	-5.2817581
C	0.3242103	-1.2429013	-4.3698921
C	1.0597428	-1.2560947	-3.1982596

C	-0.3588419	-0.0821368	-6.4784525
C	-0.2723472	1.0225255	-7.3119743
C	0.5976977	2.1002881	-6.9891128
C	1.3698163	2.0556568	-5.8392334
N	0.8663637	-2.1992692	1.2837827
C	2.1421905	-2.6083210	1.9632257
C	2.4857033	-4.0491806	1.5904741
C	2.3156191	-5.1261870	2.4791431
C	2.6112156	-6.4388051	2.0767601
C	3.0892172	-6.6893816	0.7842100
C	3.2721705	-5.6202706	-0.1073177
C	2.9683404	-4.3137722	0.2915510
C	-0.3889843	-2.9066616	1.6349452
C	-1.2651453	-2.0712151	2.5875052
C	-1.1254668	-3.4125769	0.3879607
C	-2.5134383	-3.6475641	0.4024164
C	-3.1771825	-4.1308420	-0.7386472
C	-2.4627464	-4.3847139	-1.9196055
C	-1.0746323	-4.1867966	-1.9335946
C	-0.4152026	-3.7185110	-0.7901023
C	2.1135767	-2.3009254	3.4658441
C	2.5932341	2.3461075	1.9169339
C	2.6042802	3.7588589	2.1176628
C	3.6162651	4.3562971	2.8453690
C	4.6694666	3.5845304	3.4203018
C	4.6507997	2.1553472	3.2388744
C	3.5942470	1.5682201	2.4841074
C	5.6943045	1.3715676	3.8128714
C	6.7143933	1.9714832	4.5330131
C	6.7320299	3.3812028	4.7131742
C	5.7308572	4.1701939	4.1697226
C	3.1103330	1.0692410	-0.8779611
O	3.9849391	1.8177608	-1.6991096
C	5.0176952	2.4931048	-0.9725485
C	4.1561620	-0.9632600	-1.8847630
C	4.8779024	-1.4778715	-0.8139281
C	6.1445011	-2.0986260	-0.9925337
C	6.7025282	-2.1691931	-2.3195241
C	5.9532391	-1.6179654	-3.3984735
C	4.7137217	-1.0362697	-3.1917558
C	7.9745569	-2.7876634	-2.4996315
C	8.6613959	-3.3174247	-1.4198556
C	8.1067087	-3.2543517	-0.1117246
C	6.8748915	-2.6580696	0.0977161
H	0.9789772	1.5692488	-1.0760331
H	3.6413204	0.7743741	0.0457543
H	1.6573834	4.9210244	-1.8278695
H	0.8563632	3.4066148	-2.3917568
H	2.6228953	3.6351950	-2.6417196
H	5.6662650	1.7607467	-0.4531261
H	4.5909786	3.1969795	-0.2343366
H	5.6108963	3.0454761	-1.7170245
H	-0.0465012	-3.8083809	2.1777053
H	-1.6814009	-1.1952421	2.0592846
H	-0.6594508	-1.7013434	3.4283235
H	-2.1025115	-2.6550357	3.0031506
H	0.6698847	-3.5853832	-0.8017481
H	-0.4961445	-4.4088021	-2.8367038
H	-2.9798565	-4.7593071	-2.8090613
H	-4.2523596	-4.3414313	-0.6947528
H	-3.0841203	-3.4761754	1.3200031
H	2.9119032	-1.9657106	1.5062784
H	1.3354301	-2.8745701	3.9975369
H	1.9191898	-1.2269878	3.6181236
H	3.0860852	-2.5552340	3.9206687
H	1.9589351	-4.9517636	3.4995746
H	2.4720988	-7.2656578	2.7812527
H	3.3256091	-7.7125355	0.4738574
H	3.6590827	-5.8034981	-1.1154535
H	3.1115763	-3.4811713	-0.4054441
H	3.5784793	0.4821672	2.3579053
H	5.6782287	0.2844515	3.6723609
H	7.5124400	1.3607233	4.9679980
H	7.5433007	3.8425055	5.2859914
H	5.7431943	5.2567376	4.3095826
H	3.6169219	5.4420931	2.9912364
H	1.8062573	4.3633152	1.6796966
H	0.3803654	1.4704756	3.4495388
H	-1.8800795	2.1526050	4.2316120
H	-4.1092709	3.2078558	3.7500626
H	-5.6650735	4.2903186	2.1330401
H	-4.9560702	4.6865262	-0.2298169
H	-2.6610914	4.0523558	-0.9720899
H	-0.4504442	3.0905808	-0.4702421
H	4.1578569	-0.6293528	-4.0403134
H	6.3704148	-1.6650624	-4.4103862
H	8.4001276	-2.8388907	-3.5078758
H	9.6374006	-3.7905903	-1.5698016
H	8.6599062	-3.6825217	0.7307353
H	6.4420758	-2.6124586	1.1037078
H	4.4675935	-1.4235244	0.1997857
H	0.9785430	-2.1035502	-2.5170124
H	-0.3463934	-2.0777833	-4.6011270
H	-1.0263960	-0.9146711	-6.7274143
H	-0.8710003	1.0670659	-8.2277863
H	0.6590553	2.9647119	-7.6583952
H	2.0450393	2.8819290	-5.5903488
H	2.7612969	1.6885738	-3.5308676
H	-7.5818887	-2.3345411	4.7523427
C	-6.7157971	-1.7717467	4.3889022
C	-5.6840049	-1.4179280	5.2723444
H	-5.7388831	-1.7047007	6.3275504
C	-4.5901648	-0.6844380	4.7949391
H	-3.7850484	-0.3906401	5.4772379
C	-4.5180052	-0.3157811	3.4420159
H	-3.6564450	0.2650613	3.1024277
C	-5.5426210	-0.6728437	2.5454962
C	-6.6473296	-1.3967472	3.0416379
H	-7.4729462	-1.6519121	2.3676590
H	-6.5946587	1.7128685	2.4812725
C	-7.1148211	1.5809479	1.5271755
C	-8.1747788	2.4312511	1.1898907

H	-8.4738960	3.2258530	1.8819005
C	-8.8594538	2.2590380	-0.0226743
H	-9.6932892	2.9185649	-0.2844511
C	-8.4740535	1.2284193	-0.8899808
H	-9.0061324	1.0781505	-1.8353956
C	-7.4093503	0.3777181	-0.5521415
H	-7.1227167	-0.4115874	-1.2546571
C	-6.7128650	0.5434442	0.6625159

TS3-R

C	0.4182948	-4.0859184	3.2018342
C	-0.5684439	-3.5513063	2.3169973
C	-1.9116927	-3.3534476	2.8094090
C	-2.2108205	-3.7154883	4.1571820
C	-1.2275310	-4.2276554	4.9903661
C	0.0974268	-4.4112709	4.5103482
C	-2.8804911	-2.7853924	1.9257987
C	-2.5434318	-2.4429562	0.6312856
C	-1.2192065	-2.6430680	0.1343800
C	-0.2596812	-3.1918416	0.9696404
C	-0.9443906	-2.1810578	-1.3002367
C	0.5673304	-2.2180457	-1.7000262
O	0.9060731	-3.5847588	-1.8107949
C	2.2754450	-3.9434421	-1.6330598
O	-1.4081435	-0.8040033	-1.3969178
P	-0.5534820	0.5127322	-0.8424643
O	0.3651356	0.8570874	-2.1755496
C	1.4006211	0.0304751	-2.8110001
C	2.6739945	0.0959713	-1.9658446
C	3.6869111	-0.8437758	-2.1123865
C	4.8915627	-0.7595287	-1.3577619
C	5.0788087	0.3426684	-0.4481538
C	4.0409419	1.3107960	-0.3399136
C	2.8734417	1.1920139	-1.0738758
C	6.2756926	0.4054306	0.3240136
C	7.2412982	-0.5822683	0.2124203
C	7.0564089	-1.6705761	-0.6842032
C	5.9093167	-1.7535350	-1.4563407
N	-1.7039500	1.7046323	-0.9875245
C	-2.4640467	1.8327256	-2.2784573
C	-2.3169124	3.2428955	-2.8472595
C	-3.3266572	4.2163939	-2.7331045
C	-3.1373261	5.5081794	-3.2497112
C	-1.9402651	5.8400696	-3.8977835
C	-0.9299391	4.8739346	-4.0254181
C	-1.1154718	3.5905349	-3.4988526
C	-2.0562554	2.5903154	0.1495268
C	-2.8596544	1.8382888	1.2245615
C	-0.8320392	3.3394079	0.6873576
C	-0.7453559	3.7360412	2.0348875
C	0.3691742	4.4492158	2.5024817
C	1.4161547	4.7817305	1.6330423
C	1.3277913	4.4132759	0.2822435
C	0.2140793	3.7043714	-0.1849656
C	-3.9070710	1.3333369	-2.1294475
C	-1.7825421	-2.9755755	-2.3051455
C	-1.8047925	-4.4005697	-2.2332958
C	-2.4858830	-5.1400695	-3.1824867
C	-3.1884238	-4.5068478	-4.2507269
C	-3.1903867	-3.0676251	-4.3121553
C	-2.4804741	-2.3330212	-3.3193922
C	-3.8934043	-2.4202425	-5.3702024
C	-4.5624204	-3.1610531	-6.3307692
C	-4.5606121	-4.5811622	-6.2703942
C	-3.8899935	-5.2394362	-5.2519134
C	0.8161935	-1.4085928	-3.0204764
O	1.6757633	-2.1086830	-3.8987276
C	0.9858226	-2.9310108	-4.8453381
C	1.5716393	0.6823146	-4.1943032
C	0.4526850	0.8233575	-5.0081254
C	0.5216167	1.4635999	-6.2749798
C	1.7937008	1.9654562	-6.7308244
C	2.9291210	1.7954520	-5.8883240
C	2.8238124	1.1761182	-4.6535340
C	1.8630609	2.6167597	-7.9977684
C	0.7276938	2.7708382	-8.7757757
C	-0.5283263	2.2802884	-8.3225811
C	-0.6291115	1.6402019	-7.0994530
H	1.1532105	-1.7502423	-0.8751539
H	-0.1601523	-1.2560378	-3.5142760
H	2.2851624	-5.0276959	-1.4392163
H	2.7213177	-3.4095763	-0.7714417
H	2.8698893	-3.7213291	-2.5345011
H	0.3532894	-2.3092850	-5.5091057
H	0.3580916	-3.6857306	-4.3363505
H	1.7608013	-3.4329523	-5.4442654
H	-2.7166233	3.3552215	-0.3014307
H	-2.2055489	1.1162748	1.7463203
H	-3.6831690	1.2769383	0.7574609
H	-3.2853068	2.5238381	1.9746142
H	0.1482821	3.4295547	-1.2409205
H	2.1277274	4.6810542	-0.4162316
H	2.2863545	5.3357141	2.0003235
H	0.4117732	4.7467897	3.5554856
H	-1.5487630	3.4991113	2.7370498
H	-1.9407324	1.1542638	-2.9716059
H	-4.4835985	1.9340784	-1.4056732
H	-3.8985778	0.2867251	-1.7858915
H	-4.4286529	1.3869238	-3.0999633
H	-4.2781572	3.9726085	-2.2490610
H	-3.9339464	6.2532561	-3.1510362
H	-1.7976144	6.8450893	-4.3085256
H	0.0043654	5.1167483	-4.5425194
H	-0.3234872	2.8413693	-3.5979981
H	-2.4924846	-1.2409339	-3.3643638
H	-3.8943033	-1.3246672	-5.4121076
H	-5.0971891	-2.6547985	-7.1411990
H	-5.0944919	-5.1549188	-7.0351134
H	-3.8903240	-6.3340517	-5.2047370
H	-2.4918970	-6.2339540	-3.1221365
H	-1.2647619	-4.9007731	-1.4258889

H	-3.2905517	-2.0060324	-0.0378750
H	-3.9030793	-2.6332875	2.2882671
H	-3.2349187	-3.5826155	4.5242126
H	-1.4697191	-4.4947999	6.0240585
H	0.8644208	-4.8144190	5.1790754
H	1.4366444	-4.2307256	2.8269217
H	0.7597210	-3.3561714	0.6175821
H	3.7106407	1.0683186	-4.0237986
H	3.9003533	2.1720340	-6.2276179
H	2.8304294	2.9955811	-8.3459176
H	0.7921405	3.2740348	-9.7461870
H	-1.4173933	2.4129549	-8.9479056
H	-1.5957727	1.2637951	-6.7458882
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H	4.1663903	2.1575388	0.3439635
H	6.4179550	1.2461037	1.0125561
H	8.1559134	-0.5262680	0.8120965
H	7.8295429	-2.4419820	-0.7649323
H	5.7659613	-2.5887894	-2.1512389
H	3.5659594	-1.6555924	-2.8331021
H	1.4379249	1.3672551	9.2780284
C	0.6484123	0.8324226	8.7401681
C	-0.0795849	-0.1801693	9.3799329
H	0.1366166	-0.4446298	10.4199472
C	-1.0893511	-0.8476194	8.6742323
H	-1.6706545	-1.6373780	9.1613226
C	-1.3652756	-0.5081011	7.3423453
H	-2.1678733	-1.0442039	6.8273562
C	-0.6392480	0.5025217	6.6830869
C	0.3699645	1.1677462	7.4083803
H	0.9536848	1.9646050	6.9375288
H	-0.3723720	3.5579812	5.7393817
C	-1.4320346	3.4114779	5.5092031
C	-2.2853337	4.5212288	5.4968781
H	-1.8826582	5.5162999	5.7114822
C	-3.6482059	4.3602286	5.2046017
H	-4.3157852	5.2275036	5.1908702
C	-4.1489612	3.0788877	4.9400664
H	-5.2128113	2.9375635	4.7227839
C	-3.2914056	1.9680035	4.9546722
H	-3.7143912	0.9785049	4.7521190
C	-1.9182768	2.1204978	5.2243723
Au	0.5791030	0.1081728	1.1432832
C	1.0009037	-0.1403403	4.1682987
C	1.6140235	-0.4682276	2.8626075
C	0.3297307	1.1997765	4.3977843
H	0.0570975	1.6609049	3.4331734
H	1.0333836	1.8780939	4.9027193
C	-0.9625710	0.9227451	5.2285167
C	-1.5178018	-0.2551059	4.4146224
O	-0.3327372	-1.1115501	4.2732050
H	-1.8457179	0.0620300	3.4123734
H	-2.2881262	-0.8692164	4.8963449
C	2.7393260	-1.2546723	2.8350616
C	3.5110498	-1.7523900	4.0400122
C	3.3421674	-1.7213380	1.5358819
H	3.2449384	-2.8225381	1.4577579
H	4.4239024	-1.5026056	1.4929427
H	2.8581023	-1.2584923	0.6614089
H	3.6678388	-2.8441211	3.9581563
H	3.0384470	-1.5514331	5.0128845
H	4.5187589	-1.2963480	4.0499845
H	1.5277232	-0.4955007	5.0636631
H	-0.3631779	-1.6831696	3.4554048

TS3-S

C	-3.1135286	3.9278655	-0.3386827
C	-2.2267805	3.4281498	0.6587241
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C	-4.0837171	3.5498419	2.2805864
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C	-4.4364979	4.2122616	-0.0372345
C	-1.8344093	2.6973628	2.9771144
C	-0.5323465	2.3691793	2.6528732
C	-0.0320009	2.5602390	1.3293474
C	-0.8713236	3.0953479	0.3626259
C	1.3987338	2.0821057	1.0565750
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O	2.0023406	3.5534922	-0.7014141
C	1.7999496	4.0183749	-2.0314380
O	1.4492618	0.6720519	1.4468980
P	0.8276646	-0.5348593	0.4952218
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C	2.0349210	-0.0779064	-2.6862483
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C	1.3928151	0.9349790	-4.8278729
C	0.5800195	-0.2124931	-5.1397130
C	0.5426983	-1.2862683	-4.2039522
C	1.2488809	-1.2235065	-3.0165286
C	-0.1660574	-0.2212655	-6.3541470
C	-0.1200751	0.8610386	-7.2197466
C	0.6817511	1.9941235	-6.9117225
C	1.4260267	2.0273455	-5.7432547
N	0.8280775	-1.8373473	1.5335553
C	2.1051579	-2.1753815	2.2501934
C	2.4378943	-3.6471793	2.0149074
C	2.5720416	-4.5770847	3.0605351
C	2.8761810	-5.9206652	2.7853797
C	3.0537961	-6.3471454	1.4634838
C	2.9246694	-5.4241448	0.4127373
C	2.6145701	-4.0883923	0.6866133
C	-0.3967291	-2.5139191	2.0200633
C	-1.3645655	-1.5280905	2.7074344
C	-1.1076735	-3.3854339	0.9810990
C	-2.1067205	-4.2771758	1.4233587
C	-2.8380737	-5.0526788	0.5139550
C	-2.5889372	-4.9492500	-0.8638115
C	-1.5727559	-4.0944394	-1.3143358

C	-0.8307466	-3.3330736	-0.3958435
C	2.0709782	-1.7159712	3.7130888
C	2.4118297	2.8033070	1.9452456
C	2.3506929	4.2244580	2.0592762
C	3.2996190	4.9109756	2.7931809
C	4.3579136	4.2248458	3.4600771
C	4.4113301	2.7882198	3.3658392
C	3.4189639	2.1080530	2.6017398
C	5.4608997	2.0900381	4.0319879
C	6.4193867	2.7792558	4.7569691
C	6.3663194	4.1964984	4.8503043
C	5.3567775	4.9035252	4.2169018
C	3.1113032	1.3175830	-0.7342229
O	4.0048090	2.0277643	-1.5685020
C	5.0054327	2.7607770	-0.8529294
C	4.2136838	-0.7692518	-1.5842000
C	4.7955800	-1.4656027	-0.5335279
C	6.0735872	-2.0788499	-0.6582563
C	6.7920885	-1.9455281	-1.8994805
C	6.1818230	-1.2109821	-2.9576544
C	4.9281977	-0.6440058	-2.8106408
C	8.0751222	-2.5547398	-2.0213058
C	8.6210872	-3.2677060	-0.9662079
C	7.9069648	-3.4069008	0.2554934
C	6.6591344	-2.8254228	0.4065258
H	0.9899672	1.7822299	-1.0690547
H	3.6083413	1.0862611	0.2263433
H	1.6594033	5.1082704	-1.9584525
H	0.8973337	3.5612230	-2.4844158
H	2.6715481	3.8010340	-2.6723357
H	5.6488697	2.0714479	-0.2721963
H	4.5456486	3.5008334	-0.1722807
H	5.6129311	3.2774111	-1.6113827
H	-0.0269445	-3.2125970	2.7915547
H	-1.7459852	-0.7884362	1.9821873
H	-0.8447856	-0.9780035	3.5079186
H	-2.2302454	-2.0510249	3.1450054
H	-0.0045761	-2.7163942	-0.7555448
H	-1.3349288	-4.0313929	-2.3818348
H	-3.1636961	-5.5500162	-1.5761944
H	-3.6056532	-5.7412615	0.8827865
H	-2.3199857	-4.3664296	2.4950694
H	2.8781659	-1.5793520	1.7380626
H	1.3031823	-2.2460546	4.3020955
H	1.8594483	-0.6358816	3.7522600
H	3.0474949	-1.9003259	4.1920868
H	2.4469806	-4.2642364	4.1017816
H	2.9771053	-6.6329865	3.6111508
H	3.2953388	-7.3938664	1.2507632
H	3.0704591	-5.7468458	-0.6234370
H	2.5127250	-3.3664019	-0.1295521
H	3.4594343	1.0171340	2.5393320
H	5.4994530	0.9970184	3.9583811
H	7.2230240	2.2336460	5.2624683
H	7.1293411	4.7290905	5.4275266
H	5.3143494	5.9958985	4.2899160
H	3.2462811	6.0025102	2.8710151
H	1.5489284	4.7639218	1.5492339
H	0.1394906	1.9546285	3.4106989
H	-2.1990524	2.5521240	3.9999973
H	-4.4582991	3.4098467	3.3005464
H	-5.9688405	4.2618906	1.5151365
H	-5.1086888	4.5916571	-0.8138478
H	-2.7298144	4.0831100	-1.3523503
H	-0.5151445	3.2677958	-0.6553136
H	4.4814532	-0.0949653	-3.6431242
H	6.7202525	-1.1039397	-3.9057792
H	8.6232905	-2.4514787	-2.9642255
H	9.6075365	-3.7314993	-1.0705356
H	8.3485799	-3.9801273	1.0774835
H	6.1005912	-2.9383047	1.3427895
H	4.2651003	-1.5679114	0.4153111
H	1.2283587	-2.0685659	-2.3245818
H	-0.0558572	-2.1734012	-4.4387996
H	-0.7806589	-1.0964577	-6.5926447
H	-0.6982265	0.8448314	-8.1495513
H	0.7124323	2.8399611	-7.6064594
H	2.0470237	2.8978413	-5.5040427
H	2.7542898	1.8215936	-3.3825610
H	-6.4857872	-3.0011942	4.7598490
C	-5.9124369	-2.1660019	4.3441862
C	-5.2012875	-1.3066934	5.1966522
H	-5.2144737	-1.4692095	6.2792600
C	-4.4867091	-0.2322672	4.6516188
H	-3.9355456	0.4513823	5.3064816
C	-4.4699027	-0.0235140	3.2641002
H	-3.8992936	0.8164766	2.8622260
C	-5.1720366	-0.8822689	2.4009343
C	-5.9036563	-1.9503019	2.9606783
H	-6.4885488	-2.6077629	2.3074028
H	-6.9347399	1.0887600	1.8187767
C	-7.3492677	0.5468934	0.9610404
C	-8.6334043	0.8560702	0.4992507
H	-9.2141061	1.6416626	0.9940890
C	-9.1796168	0.1535730	-0.5867855
H	-10.1867205	0.3892975	-0.9456405
C	-8.4282397	-0.8540697	-1.2042816
H	-8.8451416	-1.4096320	-2.0508642
C	-7.1370518	-1.1605767	-0.7434644
H	-6.5665154	-1.9407061	-1.2571779
C	-6.5820414	-0.4653521	0.3474036
Au	-1.0688566	0.0529483	-0.6934391
C	-4.0363480	0.3363849	-1.0930354
C	-2.7817253	0.6439620	-1.7227542
C	-4.2213532	0.4193154	0.3862036
H	-3.2377545	0.3758216	0.8839129
H	-4.6667585	1.4077125	0.6074322
C	-5.1585801	-0.7194297	0.8758343
C	-4.4802481	-1.9681315	0.2719691
O	-4.1199371	-1.6369683	-1.0998163
H	-3.5681420	-2.2060795	0.8366925
H	-5.1372539	-2.8507451	0.2466283

C	-2.7842045	1.3957711	-2.8843157
C	-4.0163457	1.9132399	-3.5887759
C	-1.4976070	1.8733035	-3.4913109
H	-1.4590398	1.6399412	-4.5709686
H	-1.4283777	2.9765453	-3.4126974
H	-0.6198743	1.4312860	-2.9949922
H	-3.9118971	1.7631258	-4.6781548
H	-4.9596023	1.4536544	-3.2581663
H	-4.1057469	3.0057863	-3.4315851
H	-4.9673608	0.4154705	-1.6699223
H	-3.1810480	-1.8941676	-1.2574896

INT4-R

Au	0.5538478	0.1153727	1.1904140
C	0.8019718	-0.5445005	4.1577742
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C	0.4043018	0.7804023	4.7848621
H	0.3202208	1.5446241	3.9933640
H	1.1708073	1.0948843	5.5100669
C	-0.9782683	0.5403629	5.4689444
C	-1.6937257	-0.2875165	4.3801617
H	-2.1065021	0.3621910	3.5978125
H	-2.4496386	-0.9959036	4.7427206
O	-0.6282320	-1.1128006	3.7558678
C	2.8261571	-1.1089709	2.8488026
C	3.5732228	-1.6441986	4.0535145
C	3.6081540	-1.2270047	1.5675044
H	3.8147735	-2.2938098	1.3528381
H	4.5918501	-0.7313353	1.6470088
H	3.0721727	-0.7901768	0.7093493
H	3.9969636	-2.6402194	3.8278212
H	2.9643818	-1.7291949	4.9672325
H	4.4318375	-0.9855879	4.2854750
H	1.1111523	-1.2889478	4.9040395
C	0.8994247	-4.1387116	3.0608483
C	-0.1393919	-3.7371380	2.1715754
C	-1.5062190	-3.8010101	2.6209846
C	-1.7794147	-4.2941315	3.9297703
C	-0.7464993	-4.6857921	4.7675770
C	0.6045549	-4.5961963	4.3350843
C	-2.5317982	-3.3408654	1.7410215
C	-2.2233129	-2.8539315	0.4846939
C	-0.8713150	-2.7970624	0.0285720
C	0.1430615	-3.2368590	0.8667337
C	-0.6395208	-2.2064603	-1.3651256
C	0.8692603	-2.0094961	-1.7314655
O	1.4020806	-3.3063722	-1.8919519
C	2.8035813	-3.4692661	-1.6795387
O	-1.2930771	-0.8994426	-1.3878265
P	-0.6291206	0.4984951	-0.7922504
O	0.2252891	1.0168981	-2.1087925
C	1.3887334	0.3795605	-2.7425204
C	2.6153982	0.6070925	-1.8574161
C	3.7779242	-0.1364875	-2.0230474
C	4.9418057	0.1255564	-1.2445387
C	4.9246735	1.2032977	-0.2870988
C	3.7288370	1.9625722	-0.1491767
C	2.6080471	1.6744033	-0.9093316
C	6.0877112	1.4492377	0.4995611
C	7.2162353	0.6578769	0.3583596
C	7.2326146	-0.4087833	-0.5822043
C	6.1221265	-0.6654321	-1.3695911
N	-1.9372489	1.5224813	-0.8794592
C	-2.7544777	1.5499054	-2.1429266
C	-2.8022711	2.9615414	-2.7246592
C	-3.9191610	3.8063383	-2.5850357
C	-3.9039051	5.1058137	-3.1178338
C	-2.7769501	5.5727937	-3.8073634
C	-1.6606549	4.7349052	-3.9603342
C	-1.6726893	3.4449234	-3.4171534
C	-2.3248831	2.3807427	0.2707276
C	-3.0716912	1.5734166	1.3411184
C	-1.1224572	3.1797447	0.7855042
C	-0.8098831	3.2977214	2.1523810
C	0.3001804	4.0501296	2.5689491
C	1.1097250	4.7027789	1.6315307
C	0.7906599	4.6129496	0.2676738
C	-0.3121026	3.8588156	-0.1486278
C	-4.1176151	0.8753905	-1.9455240
C	-1.3440825	-3.0400723	-2.4381933
C	-1.1708472	-4.4564323	-2.4516335
C	-1.7345364	-5.2226102	-3.4552330
C	-2.5079136	-4.6275573	-4.4961360
C	-2.7053842	-3.2007603	-4.4731588
C	-2.1119760	-2.4384440	-3.4263778
C	-3.4817587	-2.5921624	-5.5026700
C	-4.0370803	-3.3578579	-6.5148167
C	-3.8430439	-4.7657513	-6.5372359
C	-3.0962836	-5.3869598	-5.5489469
C	1.0287504	-1.1191327	-3.0144454
O	2.0033764	-1.6508214	-3.8904101
C	1.4647681	-2.5316719	-4.8823073
C	1.4873299	1.1093737	-4.0941208
C	0.3967506	1.0676465	-4.9566702
C	0.3847970	1.7787914	-6.1869396
C	1.5435902	2.5542994	-6.5520945
C	2.6555594	2.5687467	-5.6624470
C	2.6299504	1.8708793	-4.4656493
C	1.5273544	3.2798615	-7.7800584
C	0.4160075	3.2456300	-8.6059795
C	-0.7287389	2.4829918	-8.2427918
C	-0.7437191	1.7645188	-7.0597178
H	1.3695408	-1.5022826	-0.8739343
H	0.0525847	-1.0949279	-3.5294580
H	2.9691053	-4.5489134	-1.5387146
H	3.1356449	-2.9243184	-0.7745186
H	3.3859288	-3.1114961	-2.5447471
H	0.7683909	-1.9841455	-5.5474463
H	0.9387915	-3.3847244	-4.4155910
H	2.3197213	-2.8968426	-5.4710619

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H	-3.9382298	1.0611994	0.8972232
H	-3.4285662	2.2136826	2.1652964
H	-0.5514254	3.7872078	-1.2134496
H	1.4042179	5.1299587	-0.4776226
H	1.9741271	5.2890338	1.9604793
H	0.5247449	4.1313284	3.6369759
H	-1.4332905	2.8185681	2.9127203
H	-2.1756877	0.9359071	-2.8516930
H	-4.7476673	1.4138030	-1.2177133
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H	-4.6647710	0.8426113	-2.9028273
H	-4.8181545	3.4548760	-2.0680025
H	-4.7811859	5.7503859	-2.9991996
H	-2.7704627	6.5828449	-4.2301919
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H	-0.7971733	2.7983938	-3.5271722
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H	-3.6317469	-1.5062598	-5.4805834
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H	-2.9484483	-6.4724305	-5.5655056
H	-1.5921248	-6.3088130	-3.4584900
H	-0.5775181	-4.9263472	-1.6636545
H	-3.0159578	-2.5056344	-0.1845220
H	-3.5753187	-3.3867233	2.0725415
H	-2.8207906	-4.3626235	4.2641628
H	-0.9695147	-5.0703181	5.7686207
H	1.4105471	-4.9027002	5.0097322
H	1.9377284	-4.0781522	2.7181465
H	1.1868949	-3.2002492	0.5497958
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H	3.5418168	3.1526378	-5.9338696
H	2.4089009	3.8672493	-8.0596462
H	0.4139089	3.8080218	-9.5454991
H	-1.6002154	2.4674635	-8.9056000
H	-1.6241419	1.1770219	-6.7757158
H	-0.5002795	0.5003098	-4.6849900
H	1.7150671	2.2925921	-0.8011084
H	3.6929112	2.7862963	0.5727393
H	6.0719822	2.2715919	1.2237858
H	8.1037476	0.8529969	0.9693828
H	8.1320871	-1.0247676	-0.6846905
H	6.1351042	-1.4839816	-2.0982894
H	3.8104039	-0.9238392	-2.7803936
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C	-0.2618331	-0.2526928	9.1672593
C	-0.3094074	-1.6546101	9.1924767
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H	-0.6371799	-3.4475583	8.0158598
C	-0.8321575	-1.6582752	6.8170109
H	-1.0400524	-2.2413804	5.9137373
C	-0.7879017	-0.2504734	6.7805920
C	-0.4998059	0.4412822	7.9741663
H	-0.4742153	1.5357768	7.9751212
H	-0.0343905	3.1468477	5.7678729
C	-1.1250738	3.0806442	5.8259633
C	-1.8671773	4.2532497	6.0312838
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C	-3.2642610	4.1973021	6.1192140
H	-3.8441071	5.1125475	6.2746352
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H	-5.0039962	2.9003212	6.0999742
C	-3.1703237	1.7872108	5.8197896
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H	-0.6086708	-1.0130540	2.7404284

INT4-S

Au	-1.0789371	0.3689957	-0.6300818
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C	-3.9815645	3.1901145	-2.6480622
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H	-4.9434362	0.9742783	-1.5245480
H	-3.4139678	-2.0602718	0.2869469
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C	-4.5127965	3.9025486	2.5204524
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C	-0.5794166	2.8161867	-6.6363360
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C	1.2342181	3.4000125	-5.1195987
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C	2.2820593	-4.2617021	-0.5694086
C	-0.4847172	-2.8259511	1.4054871
C	-1.3449428	-1.9338292	2.3251280
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C	-2.9356843	-4.5596215	-1.7598286
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C	3.7803526	3.8781792	3.7177148
C	4.8100223	2.9830226	4.1350569
C	4.7677603	1.6214369	3.6660904
C	3.7111807	1.2223051	2.7967870
C	5.7864824	0.7146068	4.0817877
C	6.8053702	1.1330014	4.9222210
C	6.8472192	2.4762759	5.3848503
C	5.8705012	3.3810239	5.0002211
C	3.1745462	1.2906419	-0.6331247
O	4.0818932	2.1137292	-1.3383178
C	5.1882626	2.5660449	-0.5499827
C	4.0192761	-0.5811796	-2.0781542
C	4.6324741	-1.5250214	-1.2646604
C	5.8310462	-2.1844466	-1.6544756
C	6.4376888	-1.8390738	-2.9142797
C	5.8013281	-0.8522969	-3.7221190
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H	1.1171306	4.0829991	-1.6013275
H	2.8950724	4.2225434	-1.8392324
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H	4.8428085	3.1533161	0.3205244
H	5.8003661	3.1992392	-1.2097730
H	-0.1350613	-3.6786002	2.0128986
H	-1.6980090	-1.0342450	1.7910465
H	-0.7502262	-1.5971618	3.1894787
H	-2.2304907	-2.4762400	2.6938147
H	-0.2690532	-2.4566780	-1.3657679
H	-1.7405576	-3.3830312	-3.1391746
H	-3.5681659	-4.9921981	-2.5418242
H	-3.8865260	-5.6599344	-0.1477723
H	-2.4636518	-4.6670174	1.6265135
H	2.8382411	-2.1385831	1.0163967
H	1.4010328	-3.2654875	3.5009914
H	2.1125183	-1.6382235	3.2950306
H	3.1616632	-3.0903975	3.2921103
H	2.1364297	-5.2906566	2.6927745
H	2.3097558	-7.5024454	1.5896394
H	2.4811155	-7.6615750	-0.8999826
H	2.4755423	-5.5712648	-2.2794376
H	2.2759175	-3.3457918	-1.1687183
H	3.6781439	0.1855333	2.4510996
H	5.7515887	-0.3204748	3.7230244
H	7.5839874	0.4289651	5.2337866
H	7.6576440	2.7940587	6.0490451
H	5.9020883	4.4164029	5.3571280
H	3.8006238	4.9118056	4.0799882
H	1.9850272	4.1590833	2.5635553
H	0.4385934	0.9758076	3.6906644
H	-1.8346446	1.5110621	4.5384146
H	-4.0300937	2.7040966	4.2488667
H	-5.5243617	4.1368330	2.8680030
H	-4.7126055	5.0757600	0.6918148
H	-2.4006836	4.5929340	-0.0928213
H	-0.2331539	3.4614204	0.2187910
H	4.1526570	0.5003476	-3.9683902
H	6.2548799	-0.5814506	-4.6819734
H	8.1021420	-2.2355099	-4.2613366
H	9.1372365	-3.9605710	-2.7970175
H	8.0728785	-4.5720500	-0.6165317
H	5.9700350	-3.4525034	0.1112949
H	4.1863608	-1.7933248	-0.3040185
H	0.8349903	-1.3996237	-2.8170766
H	-0.6451318	-0.8252094	-4.7181427
H	-1.4306468	0.8429973	-6.4271462
H	-1.2376304	3.0982024	-7.4648199
H	0.4661192	4.7303773	-6.6299223
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H	2.7205241	2.4696276	-3.0469488
H	-5.4694629	-4.2434189	3.8511661
C	-5.1891615	-3.1977559	3.6856084
C	-4.6944666	-2.4246838	4.7478785
H	-4.5828212	-2.8647337	5.7440893
C	-4.3572732	-1.0833009	4.5256418
H	-3.9809832	-0.4668866	5.3491354
C	-4.4939836	-0.5211800	3.2473707
H	-4.2152354	0.5240846	3.0918958

C	-4.9760900	-1.2901879	2.1745848
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H	-5.7453073	-3.2414980	1.5989119
H	-7.1058303	0.2844708	2.2821858
C	-7.4576332	0.0450629	1.2729392
C	-8.7903914	0.2967349	0.9254839
H	-9.4695305	0.7352899	1.6640220
C	-9.2577570	-0.0205914	-0.3593998
H	-10.3010958	0.1706224	-0.6299847
C	-8.3798704	-0.5879063	-1.2915653
H	-8.7320898	-0.8414305	-2.2968048
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TS4-R

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C	0.0896777	-4.3975933	-1.3519050
O	1.0138442	-4.0159406	-0.2962129
C	1.5201122	-2.7055464	2.7176680
C	1.8826718	-3.8273841	3.6640848
C	2.1694721	-1.3937388	3.0644322
H	2.1452920	-1.2066662	4.1497696
H	3.2358013	-1.4376844	2.7709436
H	1.7004364	-0.5385186	2.5522264
H	2.9827669	-3.8970033	3.7583681
H	1.4951660	-3.5939239	4.6734747
H	1.4912541	-4.8119069	3.3682035
H	1.0123664	-2.6500583	0.1334804
H	0.9144557	-5.0566486	1.5104425
H	-0.3956936	-3.4833492	-1.7315851
H	0.6904944	-4.8600608	-2.1462550
C	4.2493292	-3.0958509	0.1201522
C	3.5909777	-2.2591561	-0.8271775
C	3.1854127	-2.8232523	-2.0884924
C	3.4692052	-4.1932185	-2.3557701
C	4.0931944	-4.9856042	-1.4058111
C	4.4844897	-4.4327699	-0.1572789
C	2.4833855	-1.9902239	-3.0097075
C	2.1804027	-0.6789851	-2.6964584
C	2.5677984	-0.1158983	-1.4422969
C	3.2796125	-0.8967152	-0.5420702
C	2.1234508	1.3228043	-1.1633231
C	2.2702818	1.7580320	0.3336475
O	3.6528320	1.9352146	0.5540381
C	4.1348395	1.7948677	1.8896496
O	0.7038573	1.4003492	-1.5126152
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O	-0.8428301	2.1378310	0.3716367
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C	1.1037292	2.1350792	3.5587275
C	1.1442117	1.3574628	4.7514118
C	0.1259710	0.3625249	4.9821038
C	-0.8925792	0.2005612	4.0018111
C	-0.8992154	0.9649091	2.8464257
C	0.1921924	-0.4356250	6.1620007
C	1.2265171	-0.2698308	7.0694365
C	2.2325789	0.7099334	6.8415550
C	2.1883415	1.5100858	5.7110898
N	-1.8116655	0.9116079	-1.6252953
C	-2.0120857	2.1840705	-2.4073577
C	-3.4106643	2.7450123	-2.1612919
C	-4.4563968	2.6139049	-3.0936678
C	-5.7325405	3.1279723	-2.8129347
C	-5.9764663	3.7890832	-1.6019769
C	-4.9380123	3.9332617	-0.6687241
C	-3.6697256	3.4098765	-0.9449155
C	-2.7151011	-0.2434043	-1.8666280
C	-2.0470576	-1.3057278	-2.7524658
C	-3.3017007	-0.7786400	-0.5554707
C	-3.5878697	-2.1443128	-0.3703934
C	-4.1666615	-2.5987671	0.8253837
C	-4.4677186	-1.7000545	1.8565589
C	-4.2066634	-0.3334481	1.6737258
C	-3.6346399	0.1215792	0.4792969
C	-1.6247875	2.0032239	-3.8803561
C	2.8274002	2.3217320	-2.0831661
C	4.2443911	2.2522913	-2.2341388
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C	2.1201828	3.3246914	-2.7337761
C	2.0716301	5.3482697	-4.1887023
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C	4.1596548	6.2371043	-5.0694626
C	4.8793022	5.2329525	-4.4416411
C	1.4318128	3.0504230	0.6376122
O	2.1608808	3.9557593	1.4425478
C	2.8865922	4.9375623	0.6943305
C	-0.6346211	4.1529892	1.5716607
C	-0.8587248	4.9857324	0.4803442
C	-1.5493729	6.2209814	0.6083519
C	-2.0164928	6.6237738	1.9112984
C	-1.7621582	5.7629581	3.0167221
C	-1.0950645	4.5596840	2.8544033
C	-2.7189892	7.8581562	2.0399576
C	-2.9550702	8.6548471	0.9320816
C	-2.4985976	8.2541034	-0.3542079
C	-1.8102291	7.0638318	-0.5126751
H	1.8923312	0.9247411	0.9698727
H	1.1902103	3.5329881	-0.3264550
H	5.2269298	1.6798658	1.8087301
H	3.7060024	0.8988956	2.3782280
H	3.8967397	2.6814731	2.4995206

H	2.1895554	5.5785762	0.1194595
H	3.6061814	4.4608742	0.0035955
H	3.4260089	5.5528576	1.4302360
H	-3.5609445	0.1946924	-2.4289699
H	-1.2169948	-1.7899087	-2.2080707
H	-1.6288617	-0.8382967	-3.6565679
H	-2.7615237	-2.0854081	-3.0615652
H	-3.4455405	1.1894009	0.3398364
H	-4.4531228	0.3860900	2.4616013
H	-4.9169189	-2.0579388	2.7888830
H	-4.3800901	-3.6662188	0.9408411
H	-3.3709169	-2.8721711	-1.1565809
H	-1.3007827	2.8959597	-1.9572797
H	-2.2702433	1.2718993	-4.3953337
H	-0.5816249	1.6556377	-3.9464570
H	-1.7141488	2.9641751	-4.4143422
H	-4.2835813	2.1187153	-4.0548487
H	-6.5351854	3.0167352	-3.5496937
H	-6.9700201	4.1970900	-1.3889832
H	-5.1118199	4.4610210	0.2749405
H	-2.8629573	3.5207004	-0.2132646
H	1.0312208	3.3695941	-2.6476794
H	0.9802238	5.3891154	-4.0912836
H	2.1895551	7.0938132	-5.4456422
H	4.6798970	6.9910597	-5.6693370
H	5.9692707	5.1858844	-4.5419498
H	6.0040464	3.1312097	-3.1016726
H	4.7934365	1.4522859	-1.7319049
H	1.6306668	-0.0530759	-3.4055553
H	2.1791159	-2.4075623	-3.9761344
H	3.1756644	-4.6155200	-3.3237130
H	4.2909763	-6.0417950	-1.6159416
H	4.9824495	-5.0678958	0.5828356
H	4.5647920	-2.6658572	1.0774573
H	3.6038181	-0.4840562	0.4149896
H	-0.9233918	3.9146800	3.7198838
H	-2.1114742	6.0617714	4.0111703
H	-3.0711843	8.1660919	3.0306448
H	-3.4970393	9.5999564	1.0418127
H	-2.6958503	8.8939190	-1.2206614
H	-1.4595367	6.7514837	-1.5029207
H	-0.5266965	4.6864973	-0.5200461
H	-1.7139498	0.8434288	2.1300983
H	-1.6819657	-0.5416556	4.1636772
H	-0.5860747	-1.1869230	6.3369369
H	1.2709660	-0.8896970	7.9709483
H	3.0418905	0.8323646	7.5688061
H	2.9599623	2.2676246	5.5352195
H	1.8561934	2.9115071	3.4016391
H	-5.5480795	-6.2422611	-0.8359903
C	-4.6663794	-5.8905629	-1.3817466
C	-4.7823750	-5.4887768	-2.7213782
H	-5.7536742	-5.5216981	-3.2252099
C	-3.6419801	-5.0606000	-3.4130293
H	-3.7156722	-4.7624487	-4.4642690
C	-2.3979400	-5.0127672	-2.7644348
H	-1.5225179	-4.6774125	-3.3301347
C	-2.2752375	-5.3870733	-1.4130060
C	-3.4238582	-5.8464004	-0.7383818
H	-3.3441835	-6.1785560	0.3022507
H	0.2181549	-9.2871844	1.7062482
C	0.1846117	-8.7678678	0.7426679
C	-0.3137626	-7.4566334	0.6799411
H	-0.6652707	-6.9874984	1.6042530
C	-0.3683714	-6.7605618	-0.5408867
C	0.0716087	-7.4259984	-1.7036032
H	0.0070047	-6.9235879	-2.6755401
C	0.5700951	-8.7324192	-1.6456928
H	0.9034879	-9.2268206	-2.5641512
C	0.6331529	-9.4093235	-0.4179546
H	1.0215612	-10.4316408	-0.3700316

TS4-S

Au	-1.0967021	-0.3755195	0.5323499
C	-4.1197763	-0.7374988	1.0290459
C	-2.7840279	-1.2833446	1.4716642
C	-4.4601720	-0.6895476	-0.4587376
H	-5.0729536	-1.5500206	-0.7667435
H	-3.5279488	-0.6997153	-1.0507906
C	-5.1899301	0.6767982	-0.6096599
C	-4.2616168	1.5508522	0.2601936
O	-3.8888740	0.7011681	1.3943959
C	-2.5997150	-2.2470834	2.4161241
C	-3.7156907	-3.1562143	2.8777647
C	-1.2745062	-2.5103394	3.0767589
H	-0.9551958	-3.5550777	2.9138655
H	-1.3690883	-2.3684617	4.1688992
H	-0.4830176	-1.8362419	2.7122470
H	-3.8015867	-3.1243933	3.9797952
H	-3.4715927	-4.2017198	2.6105229
H	-4.6948200	-2.9193066	2.4358215
H	-2.5516202	0.2689851	1.4777358
H	-4.9693032	-1.0827645	1.6365111
H	-3.3456315	1.8177054	-0.2929651
H	-4.7204290	2.4613774	0.6681744
C	-2.5188064	-2.6437513	-3.2148395
C	-1.6993593	-3.0092705	-2.1054508
C	-2.2299727	-3.9152239	-1.1186397
C	-3.5640664	-4.3956459	-1.2642772
C	-4.3377027	-4.0150190	-2.3487696
C	-3.8066796	-3.1401767	-3.3361982
C	-1.3862211	-4.3060099	-0.0417228
C	-0.1056245	-3.7987956	0.0910844
C	0.4076199	-2.8530237	-0.8444146
C	-0.3794965	-2.5026853	-1.9400362
C	1.7913412	-2.2007633	-0.6763313
C	2.2094577	-2.0893873	0.8356407
O	2.7021149	-3.3652756	1.1925551
C	2.5752253	-3.7779277	2.5526876
O	1.7152357	-0.8492570	-1.2216557

P	0.8395022	0.3682128	-0.5280611
O	1.9575162	1.0552292	0.4701100
C	2.6725051	0.4190814	1.5883693
C	1.7126560	0.3054832	2.7758592
C	1.9085046	-0.6294220	3.7849840
C	0.9973911	-0.7525481	4.8728673
C	-0.1425275	0.1267655	4.9403306
C	-0.2903369	1.1167065	3.9278535
C	0.6116433	1.2081267	2.8816902
C	-1.0807340	-0.0371081	6.0009353
C	-0.9051215	-1.0307710	6.9513029
C	0.2218795	-1.8962446	6.8876665
C	1.1556355	-1.7563422	5.8733584
N	0.7897743	1.4973419	-1.7418643
C	2.0885786	1.8711574	-2.4080879
C	2.2640849	3.3879717	-2.3693841
C	2.2901422	4.1803517	-3.5309689
C	2.4373181	5.5742037	-3.4408205
C	2.5661746	6.1902114	-2.1896384
C	2.5466419	5.4066509	-1.0245756
C	2.3915897	4.0195281	-1.1147866
C	-0.4525073	2.0494673	-2.3359419
C	-1.3358824	0.9512547	-2.9532682
C	-1.2268916	2.9929213	-1.4119064
C	-2.3529719	3.6726578	-1.9207169
C	-3.0736903	4.5673359	-1.1195161
C	-2.6952148	4.7887302	0.2139020
C	-1.5770386	4.1203206	0.7296700
C	-0.8429941	3.2432079	-0.0836214
C	2.2037848	1.2162529	-3.7895998
C	2.8805122	-2.9055061	-1.4872915
C	2.9272903	-4.3302447	-1.5265527
C	3.9384669	-4.9830441	-2.2059756
C	4.9597494	-4.2578128	-2.8878583
C	4.9115542	-2.8183738	-2.8614625
C	3.8571907	-2.1745186	-2.1514186
C	5.9231852	-2.0803868	-3.5434248
C	6.9404423	-2.7340516	-4.2194502
C	6.9874929	-4.1543821	-4.2455825
C	6.0173887	-4.8998551	-3.5950710
C	3.2639560	-0.9488763	1.0845150
O	4.2232236	-1.3659770	2.0369495
C	5.4241863	-1.8884889	1.4590273
C	3.8499798	1.3675277	1.8621149
C	4.5270332	1.9319372	0.7880723
C	5.6221688	2.8196509	0.9762817
C	6.0600900	3.1083349	2.3184158
C	5.3678749	2.4950395	3.4025752
C	4.2887271	1.6554016	3.1851459
C	7.1574671	3.9988038	2.5079335
C	7.7879845	4.5835982	1.4218356
C	7.3483139	4.3060716	0.0980355
C	6.2882228	3.4424946	-0.1205723
H	1.2933100	-1.8622395	1.4255637
H	3.7689384	-0.7116718	0.1298720
H	2.7205153	-4.8697059	2.5542243
H	1.5701528	-3.5399853	2.9539159
H	3.3394110	-3.3028573	3.1908935
H	5.9377841	-1.1070308	0.8656144
H	5.2079525	-2.7625539	0.8180944
H	6.0680110	-2.1892256	2.2992720
H	-0.0841218	2.6826729	-3.1633084
H	-1.7433216	0.2839706	-2.1732694
H	-0.7436901	0.3453011	-3.6578215
H	-2.1896876	1.3862566	-3.4941675
H	0.0599477	2.7716433	0.3107630
H	-1.2571359	4.2946503	1.7627403
H	-3.2611779	5.4859455	0.8404425
H	-3.9389578	5.0887296	-1.5410705
H	-2.6769230	3.5068058	-2.9537011
H	2.8705474	1.4343214	-1.7640806
H	1.4233698	1.5711288	-4.4842825
H	2.1093464	0.1241593	-3.6865664
H	3.1850976	1.4442951	-4.2391944
H	2.2026139	3.7192566	-4.5197062
H	2.4550555	6.1769712	-4.3548738
H	2.6853015	7.2765093	-2.1208134
H	2.6556547	5.8779037	-0.0421443
H	2.3754972	3.4100097	-0.2060107
H	3.8227302	-1.0818782	-2.1459241
H	5.8843104	-0.9850204	-3.5231351
H	7.7134345	-2.1577778	-4.7385715
H	7.7961863	-4.6584763	-4.7849519
H	6.0514625	-5.9946972	-3.6166102
H	3.9628736	-6.0780499	-2.2283527
H	2.1566762	-4.9075585	-1.0101790
H	0.5200776	-4.1225963	0.9228561
H	-1.7658071	-5.0236335	0.6939578
H	-3.9652371	-5.0801891	-0.5087256
H	-5.3585962	-4.3958496	-2.4565408
H	-4.4230095	-2.8627644	-4.1977676
H	-2.1113246	-1.9678755	-3.9742929
H	0.0152346	-1.8079370	-2.6866767
H	3.7670098	1.2111040	4.0365969
H	5.6957016	2.7062064	4.4263381
H	7.4928537	4.2161812	3.5280362
H	8.6287376	5.2672635	1.5791138
H	7.8520104	4.7821598	-0.7497672
H	5.9401165	3.2342537	-1.1386272
H	4.2069250	1.7192867	-0.2359748
H	0.4855013	1.9839752	2.1252825
H	-1.1384754	1.8083919	3.9782097
H	-1.9458775	0.6332081	6.0510328
H	-1.6319100	-1.1496770	7.7616200
H	0.3505429	-2.6729088	7.6486942
H	2.0251873	-2.4209574	5.8219975
H	2.7797494	-1.2866815	3.7460039
H	-6.1617054	4.1248066	-3.6404727
C	-5.7785610	3.1072737	-3.5092362
C	-5.3451423	2.3690669	-4.6226737
H	-5.3882284	2.8069745	-5.6252797
C	-4.8761389	1.0615744	-4.4414033

H	-4.5511024	0.4694102	-5.3037893
C	-4.8223203	0.4998019	-3.1552380
H	-4.4498256	-0.5207847	-3.0351847
C	-5.2378720	1.2360840	-2.0335353
C	-5.7326032	2.5417544	-2.2301653
H	-6.0941055	3.1168041	-1.3708371
H	-7.3750885	-0.3429294	-1.8599719
C	-7.6185316	-0.0317312	-0.8377669
C	-8.9201602	-0.2040079	-0.3524682
H	-9.6830639	-0.6568900	-0.9944141
C	-9.2491506	0.2116934	0.9471463
H	-10.2682104	0.0835106	1.3261931
C	-8.2636055	0.7947613	1.7534409
H	-8.5077758	1.1229097	2.7694297
C	-6.9569936	0.9631212	1.2670843
H	-6.2015281	1.4029698	1.9259531
C	-6.6173928	0.5554200	-0.0369189

PRT-R

Au	-0.6961092	0.9314131	-0.4710242
C	-1.0428362	4.0775527	-0.5127707
C	-0.6239544	2.9460616	-1.4369608
C	-0.0013655	4.4227577	0.5663394
H	-0.2627025	4.0116099	1.5509661
H	0.9823662	4.0110835	0.2902465
C	0.0862791	5.9719175	0.5346406
C	-0.1141482	6.1684479	-0.9916220
O	-1.1508582	5.2494103	-1.3512922
C	-1.5069375	2.2408475	-2.2621035
C	-3.0051175	2.4276174	-2.1789547
C	-0.9943112	1.5340165	-3.4974200
H	-1.4097548	0.5163964	-3.5827594
H	-1.3431727	2.0957836	-4.3850902
H	0.1053607	1.4889617	-3.5178580
H	-3.2530049	3.3593027	-2.7219949
H	-3.5319129	1.5921974	-2.6610824
H	-3.3670787	2.5328422	-1.1452611
H	0.4317231	2.9785563	-1.7473144
H	-2.0389360	3.8863500	-0.0815582
H	0.8263987	5.9372135	-1.5326303
H	-0.4599760	7.1744703	-1.2751087
C	2.9033759	3.1234942	-3.1839956
C	2.9352804	2.4102703	-1.9494073
C	3.2803045	3.1200087	-0.7441071
C	3.5906378	4.5080898	-0.8205411
C	3.5459081	5.1725519	-2.0363195
C	3.1974044	4.4778762	-3.2254962
C	3.2795249	2.4009744	0.4890602
C	2.9558100	1.0585805	0.5314293
C	2.6058235	0.3478367	-0.6591119
C	2.6117629	1.0229366	-1.8721012
C	2.2697172	-1.1416037	-0.5202015
C	1.4375809	-1.7236363	-1.7174360
O	2.3313596	-1.8366884	-2.8043690
C	1.7831767	-1.7497818	-4.1182789
O	1.4630331	-1.2906848	0.6925909
P	-0.1375822	-0.9183261	0.7932769
O	-0.8240835	-2.3530936	0.3906600
C	-0.7244299	-3.0495673	-0.9059935
C	-1.6698037	-2.3529585	-1.8845903
C	-1.5080098	-2.4541679	-3.2599227
C	-2.4235089	-1.8389601	-4.1623494
C	-3.5649253	-1.1316142	-3.6366452
C	-3.7305468	-1.0773821	-2.2222934
C	-2.8087767	-1.6601921	-1.3713969
C	-4.4679166	-0.5041296	-4.5442246
C	-4.2499642	-0.5638788	-5.9114025
C	-3.1254728	-1.2621480	-6.4305885
C	-2.2344767	-1.8898386	-5.5752074
N	-0.4089248	-0.8798212	2.4242909
C	0.0421337	-2.0497996	3.2602603
C	-1.1469278	-2.6447796	4.0101280
C	-1.3985294	-2.3748240	5.3679980
C	-2.5299120	-2.9097737	6.0049583
C	-3.4174264	-3.7293275	5.2952488
C	-3.1693866	-4.0139556	3.9429103
C	-2.0468462	-3.4718913	3.3059254
C	-0.9928957	0.3213975	3.0835251
C	0.0343462	1.4587584	3.2000761
C	-2.3185956	0.7167403	2.4225099
C	-2.6506021	2.0563581	2.1487825
C	-3.8833277	2.3932140	1.5668122
C	-4.8056426	1.3889709	1.2445713
C	-4.4918694	0.0495056	1.5257541
C	-3.2643408	-0.2826082	2.1111862
C	1.2581028	-1.6922857	4.1226421
C	3.5257712	-1.9829294	-0.2821163
C	4.6604312	-1.8035710	-1.1273811
C	5.7741954	-2.6100455	-0.9870259
C	5.8278767	-3.6333355	0.0053335
C	4.6947919	-3.8009507	0.8786146
C	3.5607444	-2.9558454	0.7086995
C	4.7374475	-4.8143705	1.8805277
C	5.8482078	-5.6312848	2.0123290
C	6.9657955	-5.4664152	1.1500603
C	6.9565176	-4.4877541	0.1692397
C	0.7822807	-3.1009878	-1.3377587
O	0.8776906	-4.0173415	-2.4107835
C	2.0146732	-4.8848241	-2.3324629
C	-1.1630119	-4.4845817	-0.5727101
C	-0.5493518	-5.1382016	0.4907227
C	-0.9160822	-6.4579891	0.8705910
C	-1.9389823	-7.1381835	0.1157366
C	-2.5402728	-6.4547640	-0.9801665
C	-2.1687759	-5.1629788	-1.3152145
C	-2.3096854	-8.4617089	0.4963382
C	-1.7015619	-9.0829696	1.5747323
C	-0.6959598	-8.4090450	2.3220331
C	-0.3116116	-7.1244509	1.9777077
H	0.6358640	-0.9911801	-1.9682333
H	1.3226008	-3.5044458	-0.4630170

H	2.6300475	-1.5440333	-4.7914081
H	1.0453716	-0.9247712	-4.1915684
H	1.2962627	-2.6941379	-4.4140764
H	1.9529543	-5.5197279	-1.4272092
H	2.9561450	-4.3059151	-2.3183123
H	1.9801873	-5.5224553	-3.2286659
H	-1.2449504	-0.0296742	4.1014343
H	0.3044137	1.8508702	2.2028535
H	0.9560279	1.0877935	3.6724827
H	-0.3537446	2.2900449	3.8128623
H	-3.0296591	-1.3282570	2.3331717
H	-5.2117565	-0.7432349	1.2954696
H	-5.7679494	1.6483963	0.7911206
H	-4.1202771	3.4457015	1.3748882
H	-1.9469687	2.8535109	2.3973050
H	0.3642991	-2.8016672	2.5215315
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H	2.0780869	-1.3364701	3.4781474
H	1.6011493	-2.5843161	4.6735078
H	-0.7076723	-1.7530613	5.9467964
H	-2.7116593	-2.6892169	7.0620587
H	-4.2952141	-4.1515750	5.7953251
H	-3.8483253	-4.6650102	3.3821672
H	-1.8612728	-3.6884829	2.2492185
H	2.7079453	-3.0827049	1.3816421
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H	5.8702596	-6.4086036	2.7834370
H	7.8379091	-6.1184106	1.2655787
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H	3.5388892	2.9360909	1.4092614
H	3.8519675	5.0483082	0.0951108
H	3.7787805	6.2411720	-2.0780420
H	3.1678070	5.0161205	-4.1785975
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H	-2.6507180	-4.6598719	-2.1574272
H	-3.3150185	-6.9669189	-1.5610720
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H	0.4601019	-6.6008904	2.5533760
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H	-2.9621581	-1.6084261	-0.2919165
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H	-4.9487669	-0.0777062	-6.5999551
H	-2.9700437	-1.3060801	-7.5134840
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H	-0.6755724	-3.0349557	-3.6626688
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C	3.9621867	7.3286558	2.0084386
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C	3.4122988	7.9027407	0.8536636
H	3.9585526	8.6843830	0.3152033
C	2.1623535	7.4761546	0.3788167
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C	1.4401874	6.4681683	1.0460805
C	1.9947488	5.9154073	2.2183635
H	1.4414702	5.1470194	2.7683932
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C	-1.1572691	8.0752017	1.2489251
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H	-2.2335184	9.8475799	1.8601994
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H	-3.9194753	8.5754875	3.2093100

PRT-S

Au	-0.7911058	0.8703993	-0.6450723
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C	3.7001555	4.7165182	0.0088644
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C	3.4661495	4.8017072	-2.4127290
C	3.2947299	2.5538396	1.1996955
C	2.9789659	1.2099804	1.1562556
C	2.7001555	0.5610621	-0.0854845
C	2.7429462	1.3002986	-1.2585930
C	2.4050034	-0.9387115	-0.0319293
C	1.8832982	-1.5355632	-1.3845122
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C	2.7875878	-1.4365905	-3.6402492
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C	-0.7045691	-2.2993845	-3.4062338
C	-1.5952533	-1.9392013	-4.4604867
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C	-2.8779638	2.3640377	2.0145149
C	-3.9578521	2.8866145	1.2860865
C	-4.7641653	2.0428981	0.5087900
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C	3.6208572	-1.7231657	0.4673998
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C	6.0086078	-2.1906822	0.3002055
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C	5.5792828	-5.2952402	3.1831679
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C	7.0106007	-4.0251770	1.6756692
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H	1.6929656	-3.3821535	-0.2485500
H	3.7696427	-1.2185693	-4.0875701
H	2.0942033	-0.5985818	-3.8652524
H	2.3837693	-2.3694525	-4.0707698
H	2.5031008	-5.3617179	-1.1874318
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H	-0.6661447	2.2389303	3.7252963
H	-3.2318193	-0.9360072	1.2111973
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H	-2.2712261	3.0506349	2.6111346
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H	-0.1745773	-1.0311674	4.9731425
H	1.1631244	-1.5642793	3.9136485
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H	-2.2309901	-1.7192929	5.5126798
H	-4.5495905	-2.4488887	5.9929189
H	-5.8476411	-3.7356557	4.2875957
H	-4.7914458	-4.2906806	2.0846191
H	-2.4717552	-3.5268207	1.5874140
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H	3.4919297	-4.7474558	3.2397928
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H	2.9465784	0.6183394	2.0763575
H	3.5106029	3.0377626	2.1587035
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H	2.9452669	2.9594901	-3.4093472
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H	-1.1188793	-5.0568733	-2.7616517
H	-1.4375528	-7.4730793	-2.3183165
H	-1.4191581	-9.4089952	-0.7185433
H	-1.0355159	-10.2842750	1.5784491
H	-0.3285030	-8.7422074	3.4177796
H	-0.0009747	-6.3151860	2.9641892
H	-0.0024692	-4.4216479	1.3662931
H	-2.9394763	-2.7328633	-0.8660519
H	-4.5432233	-2.1687336	-2.6732665
H	-4.9760935	-1.5341420	-5.0656611
H	-4.0973620	-0.9678785	-7.3239657
H	-1.6359521	-1.0163109	-7.7708751
H	-0.0445379	-1.6475378	-5.9608643
H	0.3561292	-2.4023070	-3.6344572
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C	-1.4317404	2.8470364	-1.4764371
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H	-0.6488458	3.5664490	0.8537936
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H	-0.6875603	2.5265593	-4.5034219
H	-0.2428397	0.8907894	-3.9675319
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H	-2.3716597	2.9586346	-0.9112071
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H	-2.6513522	5.3535105	-0.1337216
H	-1.9771518	6.8692833	-0.8247461
H	-0.5466019	4.6575574	5.1186596
C	-1.0197208	5.2316826	4.3142961

C	-2.1024715	6.0768892	4.5964917
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H	-2.6395595	7.3268207	1.4627217
C	-1.1163927	5.8523754	1.9467595
C	-0.5347874	5.1209442	3.0030191
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C	2.3563116	8.1822872	1.0374682
C	1.3585374	7.2257631	1.2748886
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C	1.7144690	8.2661453	-1.2908477
H	1.8427847	8.6671952	-2.3021057
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Au	-1.0033261	0.8567910	-0.0478356
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H	-3.9852695	2.7756823	-3.5675954
H	-4.9614543	2.7897053	-2.0812737
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H	-1.8590130	2.4241718	1.4657335
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C	-1.1244467	7.3099794	2.0694649
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C	1.0541880	4.1844184	0.1577352
C	2.5340563	2.0769580	0.3093364
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O	2.2619419	0.8637652	1.0559988
P	0.9403288	-0.1053541	0.8240343
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C	0.6332910	-0.8022694	-2.3938304
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C	-0.9177661	0.1624721	-4.0304416
C	-1.8922345	-0.8508971	-3.7203772
C	-1.5427361	-1.8579987	-2.7724704
C	-0.3206627	-1.8365957	-2.1295368
C	-3.1544070	-0.8203409	-4.3802125
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C	-1.3943264	-2.6526762	1.2980286
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C	9.0214668	2.2265304	1.5386254
C	8.1709211	3.2286180	1.0997626
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C	3.6258026	-2.7229740	-1.1898913
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H	1.2345739	-5.8619013	1.0111672
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H	10.0877460	2.4341118	1.6768598
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H	3.8411695	4.4720425	-0.0490348
H	1.9572220	2.3908733	2.9108963
H	0.6735101	4.1820010	4.0502183
H	-0.6073543	6.3360408	3.9258149
H	-1.6625160	8.1293938	2.5573060
H	-1.4845257	8.0765724	0.0593663
H	-0.2101420	6.2623254	-1.0674983
H	1.1828403	4.2167792	-0.9251213
H	2.2065673	-1.8757134	-4.1764751
H	3.6777374	-3.7088857	-4.9673206
H	5.3637381	-5.5036775	-4.4744048
H	6.7791371	-6.7186178	-2.8272371
H	6.7226892	-6.0909092	-0.4058656
H	5.2519777	-4.2380070	0.3763298
H	3.6226848	-2.4433749	-0.1332364
H	-0.0598964	-2.6209751	-1.4140092
H	-2.2565801	-2.6615423	-2.5629458
H	-3.8910368	-1.5985444	-4.1500308
H	-4.4185881	0.1778235	-5.8123431
H	-2.7094547	1.9168546	-6.3827051
H	-0.4846286	1.9009711	-5.2647208
H	1.0793477	0.9094743	-3.6202018
C	-1.5170154	3.3355767	-2.2404392
H	-6.1956624	-5.0836635	2.4313575
C	-5.8703310	-4.5965112	1.5063348
C	-5.7299269	-3.2040802	1.4684329
H	-5.9683687	-2.6173947	2.3620439
C	-5.3038928	-2.5525115	0.2945427
C	-5.0366243	-3.3329609	-0.8459177
H	-4.7092879	-2.8544038	-1.7742086
C	-5.1879373	-4.7275602	-0.8144848
H	-4.9804839	-5.3163263	-1.7143992
C	-5.6020796	-5.3643153	0.3630229
H	-5.7194596	-6.4525320	0.3895820
H	-7.0150157	-1.5476264	-1.7067245
C	-7.4026346	-0.8036616	-1.0015744
C	-8.6764163	-0.2626286	-1.2094315
H	-9.2640232	-0.5779373	-2.0781487
C	-9.2033958	0.6716407	-0.3043322
H	-10.2009329	1.0936185	-0.4638698
C	-8.4436863	1.0517359	0.8082941
H	-8.8424739	1.7756587	1.5270492
C	-7.1655595	0.5080786	1.0126785
H	-6.5946635	0.8313727	1.8862661
C	-6.6229263	-0.4239779	0.1104768
C	-5.4512464	3.4045513	2.7201951
C	-4.7562958	5.7832028	2.2319356
C	-3.6322860	4.4936350	4.0999311
H	-5.8811548	3.2641534	1.7131122
H	-6.2472995	3.7840362	3.3833766
H	-5.1435358	2.4165712	3.1053423
H	-3.2244469	3.5197635	4.4209501
H	-4.3868432	4.8119699	4.8392434
H	-2.8104824	5.2301243	4.1075151
H	-5.2258726	5.7315188	1.2331524
H	-3.9210814	6.5039775	2.1852836
H	-5.5075525	6.1733349	2.9396652

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Au	-0.9433185	-0.0356588	-0.4853264
C	-3.9358802	0.1944770	-0.9192400
C	-2.6745984	-0.1714688	-1.6424828
C	-3.9342138	1.5100941	-0.1447454
H	-4.3733640	2.3151205	-0.7524057
H	-2.8938344	1.7914836	0.0959797
C	-4.7292618	1.2291624	1.1624515
C	-4.1698147	-0.1598204	1.5053604
H	-4.7812590	-0.7731527	2.1798005
O	-4.1515429	-0.8407407	0.2076831
H	-3.1394526	-0.0930634	1.8871702
C	-2.7021924	-0.5118408	-2.9647351
C	-3.9293466	-0.5109472	-3.8548377
C	-1.4500079	-0.9164816	-3.6993582

H	-1.2351250	-0.2167436	-4.5303099
H	-1.5673808	-1.9158354	-4.1586507
H	-0.5758790	-0.9483478	-3.0292442
H	-4.0379156	-1.4929307	-4.3526014
H	-3.8071404	0.2336509	-4.6645410
H	-4.8718756	-0.2815693	-3.3358558
H	-3.4869031	-1.7346071	0.0939631
H	-4.8565130	0.0826246	-1.5094311
H	-1.9509297	-2.4009661	-0.6039339
O	-2.7789366	-2.8174021	-0.2565360
C	-3.4762428	-3.5101064	-1.3421800
C	-4.3342497	-4.6466853	-0.7693200
H	-4.0998356	-2.7733419	-1.8806696
H	-2.7148825	-3.8899548	-2.0409077
C	-2.5060526	2.9621359	-3.3603626
C	-1.5594412	3.2592770	-2.3381078
C	-1.8975151	4.2406376	-1.3404031
C	-3.1622916	4.8944633	-1.4168455
C	-4.0673045	4.5748937	-2.4185279
C	-3.7374134	3.5980001	-3.3969151
C	-0.9505289	4.5127704	-0.3071769
C	0.2577776	3.8458414	-0.2589636
C	0.5982029	2.8645753	-1.2394367
C	-0.2988972	2.5941845	-2.2631119
C	1.9271650	2.1270503	-1.0386318
C	2.1555059	0.9353041	-2.0231656
O	2.4555861	1.5267642	-3.2695796
C	2.1265523	0.8075881	-4.4529655
O	1.8984697	1.5811954	0.3158606
P	1.0252729	0.2327197	0.7268636
O	2.1624920	-0.9447555	0.4967393
C	2.7963075	-1.3273273	-0.7637610
C	1.8199556	-2.2173028	-1.5382982
C	1.8409319	-2.3153482	-2.9219586
C	0.9901746	-3.2209608	-3.6196173
C	0.1062149	-4.0762087	-2.8707549
C	0.1169965	-3.9751004	-1.4469585
C	0.9416429	-3.0703396	-0.8011524
C	-0.7357641	-4.9837687	-3.5776857
C	-0.7284160	-5.0245461	-4.9636935
C	0.1339291	-4.1700059	-5.7026406
C	0.9816368	-3.2938739	-5.0431779
N	1.0617083	0.3067532	2.3911104
C	2.3943344	0.4820418	3.0614189
C	2.5635536	-0.5893946	4.1383181
C	2.8566703	-0.2835587	5.4788609
C	3.0211676	-1.3079280	6.4259136
C	2.8989148	-2.6494475	6.0431806
C	2.6062505	-2.9650933	4.7065406
C	2.4354947	-1.9441683	3.7663493
C	-0.1334220	0.5644742	3.2286697
C	-0.8783483	1.8431752	2.7967749
C	-1.0713837	-0.6343434	3.3810122
C	-2.1144990	-0.5515359	4.3273719
C	-3.0161080	-1.6086435	4.5006841
C	-2.8940927	-2.7742515	3.7268771
C	-1.8507016	-2.8744532	2.7976490
C	-0.9445600	-1.8155774	2.6323697
C	2.6189465	1.9303191	3.5155813
C	3.1135778	3.0904505	-1.0783472
C	3.1978872	4.0512647	-2.1295706
C	4.2908031	4.8916302	-2.2262417
C	5.3578082	4.8295429	-1.2814595
C	5.2683381	3.8735887	-0.2077413
C	4.1298529	3.0199889	-0.1351183
C	6.3244692	3.8045531	0.7470715
C	7.4240602	4.6408606	0.6460954
C	7.5123187	5.5843661	-0.4128134
C	6.5006960	5.6776035	-1.3550495
C	3.2891961	-0.0289119	-1.5061541
O	4.1161948	-0.4274911	-2.5821937
C	5.2850189	0.3831526	-2.7461726
C	4.0404502	-2.1350427	-0.3484606
C	4.6045942	-1.9597392	0.9070267
C	5.7612656	-2.6822260	1.3149685
C	6.3777200	-3.5943644	0.3873322
C	5.7919978	-3.7418410	-0.9042487
C	4.6540916	-3.0418244	-1.2623156
C	7.5359110	-4.3159190	0.7984297
C	8.0577496	-4.1469676	2.0709267
C	7.4428538	-3.2527153	2.9892345
C	6.3173264	-2.5349297	2.6198440
H	1.2047443	0.3587141	-2.0972606
H	3.8957822	0.5057919	-0.7528135
H	2.1270817	1.5448439	-5.2713937
H	1.1220058	0.3466589	-4.3777071
H	2.8706808	0.0204785	-4.6669886
H	5.9328791	0.3131440	-1.8512320
H	5.0133363	1.4391245	-2.9272416
H	5.8217921	-0.0202112	-3.6181378
H	0.2832152	0.7436346	4.2359804
H	-1.2988483	1.7306424	1.7824146
H	-0.1882408	2.7016128	2.7812909
H	-1.7108759	2.0734056	3.4797476
H	-0.1154311	-1.9199624	1.9280511
H	-1.7320381	-3.7822621	2.1996250
H	-3.5958308	-3.6042821	3.8618875
H	-3.8142519	-1.5240333	5.2462413
H	-2.2245953	0.3515424	4.9372135
H	3.1346513	0.2711768	2.2714480
H	1.9194129	2.2336787	4.3128012
H	2.4882948	2.6066532	2.6569783
H	3.6447573	2.0514663	3.9025498
H	2.9657353	0.7567173	5.7998638
H	3.2482872	-1.0515457	7.4661645
H	3.0318412	-3.4471026	6.7816377
H	2.5137788	-4.0111184	4.3961548
H	2.2082714	-2.1886873	2.7243630
H	4.0629498	2.3024345	0.6873715
H	6.2541734	3.0753512	1.5627988
H	8.2313208	4.5780545	1.3835107
H	8.3866837	6.2401936	-0.4805027

H	6.5681994	6.4061841	-2.1708954
H	4.3462325	5.6249400	-3.0386755
H	2.3890796	4.1092551	-2.8625455
H	0.9762054	4.0578942	0.5386501
H	-1.1959101	5.2614993	0.4536748
H	-3.4098587	5.6579684	-0.6709399
H	-5.0369866	5.0814184	-2.4636826
H	-4.4570239	3.3572052	-4.1862515
H	-2.2420626	2.2202238	-4.1204217
H	-0.0637591	1.8584862	-3.0353191
H	4.2197072	-3.1851268	-2.2542230
H	6.2530895	-4.4333987	-1.6180841
H	8.0068983	-5.0097116	0.0931091
H	8.9478279	-4.7071432	2.3765165
H	7.8625922	-3.1365229	3.9940150
H	5.8317474	-1.8532092	3.3276663
H	4.1527366	-1.2686430	1.6197516
H	0.9558148	-3.0256824	0.2906670
H	-0.5237168	-4.6418357	-0.8596133
H	-1.3840528	-5.6607611	-3.0098201
H	-1.3798193	-5.7258525	-5.4954222
H	0.1329862	-4.2152028	-6.7966107
H	1.6553757	-2.6411570	-5.6093626
H	2.5421204	-1.7060356	-3.4950651
H	-3.1065361	5.3269258	2.8813618
C	-3.5594278	4.3530488	3.0965844
C	-3.8386144	3.4707203	2.0427090
H	-3.5907093	3.7657802	1.0199769
C	-4.4190840	2.2141488	2.2922437
C	-4.7285862	1.8668987	3.6223604
H	-5.2057810	0.9052462	3.8387703
C	-4.4386516	2.7415763	4.6775309
H	-4.6803848	2.4510649	5.7054514
C	-3.8500517	3.9893465	4.4184978
H	-3.6276047	4.6756289	5.2420089
H	-6.3041706	3.3702017	0.6147163
C	-6.8814582	2.4395106	0.5763093
C	-8.2451418	2.4864993	0.2650013
H	-8.7210044	3.4504069	0.0561777
C	-9.0020200	1.3047942	0.2304083
H	-10.0698726	1.3395118	-0.0082420
C	-8.3794195	0.0816272	0.5077967
H	-8.9585398	-0.8477472	0.4853753
C	-7.0101170	0.0361171	0.8168115
H	-6.5504024	-0.9368499	1.0135862
C	-6.2420754	1.2144013	0.8571380
C	-5.0981199	-5.2719936	-1.9563643
C	-5.3331615	-4.0799129	0.2637635
C	-3.4295555	-5.7044154	-0.1047851
H	-5.9667131	-3.2934139	-0.1844856
H	-4.8063061	-3.6474289	1.1326938
H	-5.9944775	-4.8808874	0.6358267
H	-2.7289163	-6.1462135	-0.8360055
H	-4.0354162	-6.5236943	0.3183251
H	-2.8381118	-5.2579706	0.7122494
H	-5.7643400	-4.5349933	-2.4399615
H	-5.7206337	-6.1145807	-1.6102283
H	-4.4007939	-5.6579240	-2.7217577

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Au	-0.8391958	0.6536831	-0.1415700
C	-3.9105537	0.4044870	-0.5064432
C	-2.7141167	1.2063245	-0.9949079
C	-3.9897997	-1.0614092	-0.9185849
H	-4.3919978	-1.1754762	-1.9369359
H	-2.9831803	-1.5130871	-0.8803983
C	-4.9014900	-1.6712278	0.1833762
C	-4.2716287	-0.9796056	1.4162338
H	-4.9581202	-0.8629486	2.2691724
O	-3.8860482	0.3450899	0.9641904
H	-3.3710589	-1.5279870	1.7442318
C	-2.7770187	1.8531663	-2.2088506
C	-3.9442722	1.7524948	-3.1598019
H	-1.2303355	2.2487396	-3.6406568
H	-1.9858696	3.7104917	-2.9680676
H	-0.8281873	2.7623271	-1.9701463
H	-4.1451136	2.7226648	-3.6474533
H	-3.6751106	1.0399595	-3.9637871
H	-4.8704072	1.3862788	-2.6913186
H	-4.8566370	0.9138873	-0.7752647
H	-3.4202732	1.8502817	1.4521282
H	-2.5064114	2.1525175	0.1302665
O	-2.8783834	2.6642991	1.1801499
C	-3.7214016	3.8413790	0.9555343
H	-4.3367252	3.6607014	0.0536258
H	-3.0104997	4.6555223	0.7528703
C	-0.7294973	5.9621052	-1.0054753
C	-0.0364675	5.1293213	-0.0781087
C	-0.2347201	5.3440608	1.3316101
C	-1.0846076	6.4072446	1.7544702
C	-1.7411853	7.2038147	0.8280979
C	-1.5710071	6.9717959	-0.5636703
C	0.4477050	4.4905210	2.2484239
C	1.2952269	3.4965478	1.8001842
C	1.5187020	3.2919675	0.4032231
C	0.8610431	4.1060496	-0.5064982
C	2.5264838	2.2066707	0.0004774
C	2.3437130	1.6758943	-1.4662523
O	2.8639921	2.6896711	-2.3075996
C	2.2952909	2.8338783	-3.6060437
O	2.3404560	1.0914024	0.9143402
P	1.1378011	-0.0347500	0.7987314
O	1.9360671	-1.1863964	-0.0745364
C	2.2953462	-1.0318540	-1.4877049
C	1.0104798	-1.2053198	-2.3002830
C	0.6839386	-0.4443445	-3.4118787
C	-0.5270040	-0.6676553	-4.1327479
C	-1.4235328	-1.7073444	-3.6993596
C	-1.0432430	-2.5052732	-2.5799074
C	0.1358720	-2.2655140	-1.9032723
C	-2.6352735	-1.9185925	-4.4186060

C	-2.9488518	-1.1437861	-5.5250518
C	-2.0574830	-0.1266441	-5.9624103
C	-0.8720326	0.1038063	-5.2809900
N	1.1752422	-0.6857336	2.3228737
C	2.5202195	-1.1144420	2.8564343
C	2.4731180	-2.5829982	3.2745421
C	2.6338704	-2.9967863	4.6079811
C	2.5374152	-4.3559055	4.9499559
C	2.2830360	-5.3149342	3.9618942
C	2.1279923	-4.9112897	2.6256873
C	2.2205334	-3.5580827	2.2872862
C	-0.0013343	-0.9692188	3.1923389
C	-1.0311301	0.1721933	3.2290891
C	-0.6417634	-2.3236845	2.8920334
C	-0.8709092	-3.2390802	3.9324433
C	-1.4193715	-4.5018964	3.6665069
C	-1.7458791	-4.8647059	2.3529871
C	-1.5371712	-3.9505863	1.3096684
C	-0.9959103	-2.6889657	1.5816319
C	3.0101522	-0.1268351	3.9213527
C	3.9673848	2.6809267	0.2245813
C	4.3671282	3.9758394	-0.2207030
C	5.6774108	4.3942422	-0.0812279
C	6.6644257	3.5526173	0.5123901
C	6.2628444	2.2503106	0.9792421
C	4.9049741	1.8479578	0.8219847
C	7.2371924	1.3988341	1.5782738
C	8.5526771	1.8130823	1.7090704
C	8.9488031	3.0986265	1.2496360
C	8.0246230	3.9501835	0.6653807
C	3.0922272	0.3082314	-1.6949371
O	3.6035786	0.2699944	-3.0164545
C	5.0033930	0.5556887	-3.1056879
C	3.2824848	-2.1768927	-1.7612110
C	4.1095126	-2.6394208	-0.7468174
C	5.0655409	-3.6689300	-0.9780254
C	5.1916784	-4.2185150	-2.3039099
C	4.3422655	-3.7122342	-3.3316149
C	3.4096187	-2.7240612	-3.0706092
C	6.1539321	-5.2448884	-2.5344745
C	6.9524141	-5.7101275	-1.5019416
C	6.8217452	-5.1724107	-0.1922605
C	5.8974386	-4.1733244	0.0645894
H	1.2547295	1.5459152	-1.6524708
H	3.9241695	0.2547567	-0.9699040
H	2.6685980	3.7931776	-3.9971190
H	1.1882398	2.8679236	-3.5571275
H	2.6059278	2.0154093	-4.2779408
H	5.5908784	-0.2197473	-2.5769725
H	5.2306098	1.5521447	-2.6839985
H	5.2568278	0.5372195	-4.1765480
H	0.4326357	-1.0390333	4.2040213
H	-1.5970131	0.2430042	2.2835419
H	-0.5397475	1.1428548	3.4152296
H	-1.7569914	-0.0270626	4.0347327
H	-0.8240591	-1.9885144	0.7551560
H	-1.8026063	-4.2238819	0.2843512
H	-2.1644296	-5.8521801	2.1375525
H	-1.5718162	-5.2108868	4.4870623
H	-0.5802028	-2.9771734	4.9560825
H	3.2045021	-1.0441799	1.9943843
H	2.3261810	-0.0748976	4.7861066
H	3.0891926	0.8772810	3.4767118
H	4.0049724	-0.4254495	4.2925684
H	2.8340208	-2.2641621	5.3960346
H	2.6636776	-4.6615562	5.9939576
H	2.2061866	-6.3739750	4.2295000
H	1.9263073	-5.6529289	1.8458986
H	2.0716584	-3.2407901	1.2509226
H	4.6051032	0.8626604	1.1883596
H	6.9287626	0.4077073	1.9306655
H	9.2940057	1.1504604	2.1678007
H	9.9915725	3.4138593	1.3600577
H	8.3295704	4.9414116	0.3119707
H	5.9722683	5.3908534	-0.4278105
H	3.6262665	4.6357222	-0.6782636
H	1.8170454	2.8548680	2.5152694
H	0.2986813	4.6410958	3.3232840
H	-1.2025213	6.5947006	2.8273153
H	-2.3857541	8.0219869	1.1660832
H	-2.0925464	7.6078838	-1.2864762
H	-0.5746775	5.8012178	-2.0782904
H	1.0461911	3.9978077	-1.5759814
H	2.7664522	-2.3513670	-3.8722475
H	4.4337109	-4.1235107	-4.3429166
H	6.2518274	-5.6619887	-3.5428831
H	7.6881941	-6.4988090	-1.6909933
H	7.4554832	-5.5543060	0.6149662
H	5.7875121	-3.7617392	1.0743231
H	4.0287755	-2.2210576	0.2597305
H	0.4232708	-2.8968469	-1.0580382
H	-1.6948202	-3.3280115	-2.2671072
H	-3.3125652	-2.7163617	-4.0930338
H	-3.8791872	-1.3210198	-6.0745721
H	-2.3076187	0.4695311	-6.8461166
H	-0.1773328	0.8789819	-5.6239559
H	1.3724178	0.3221671	-3.7700519
C	-1.6368232	2.6926569	-2.7137063
H	-5.5210159	-5.7035201	2.5220641
C	-5.2031234	-5.2278029	1.5884789
C	-5.2378587	-3.8328730	1.4747803
H	-5.5997529	-3.2347806	2.3177600
C	-4.8246082	-3.1935673	0.2896558
C	-4.3952254	-3.9929745	-0.7861704
H	-4.0838591	-3.5245988	-1.7250273
C	-4.3659557	-5.3918574	-0.6786637
H	-4.0313275	-5.9950033	-1.5294470
C	-4.7658473	-6.0139731	0.5115465
H	-4.7432408	-7.1052164	0.5981588
H	-6.6570221	-2.7087283	-1.6339930
C	-7.1038825	-1.8739628	-1.0833763
C	-8.4120945	-1.4748907	-1.3832411

H	-8.9701372	-1.9946265	-2.1692310
C	-9.0104245	-0.4224832	-0.6731072
H	-10.0357165	-0.1139527	-0.9019162
C	-8.2846899	0.2240116	0.3354145
H	-8.7388054	1.0452519	0.9005094
C	-6.9720831	-0.1764862	0.6312826
H	-6.4230553	0.3561871	1.4117243
C	-6.3610309	-1.2323544	-0.0709617
C	-5.6661138	3.0505720	2.3681169
C	-4.6051698	4.1556333	2.1747752
C	-5.3036870	5.5003534	1.8736172
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H	-4.3662720	4.5345110	4.3133927
H	-2.9779144	5.0720342	3.3224782
H	-3.2088470	3.3369398	3.6648626
H	-6.3291394	3.3011598	3.2131577
H	-5.2027124	2.0730928	2.5937895
H	-6.2907136	2.9313475	1.4648534
H	-5.9666354	5.7796875	2.7102316
H	-5.9210445	5.4371957	0.9593802
H	-4.5642437	6.3086481	1.7356620

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Au	-0.9009750	-0.1709608	-0.4096833
C	-3.9743795	-0.2104063	-0.6940741
C	-2.7180861	-0.5659409	-1.4778492
C	-4.0210386	1.2163822	-0.1327908
H	-4.4800865	1.9203023	-0.8439884
H	-2.9926612	1.5637436	0.0756588
C	-4.8165969	1.0633642	1.1977167
C	-4.2282891	-0.2788888	1.6821635
H	-4.8792280	-0.8429023	2.3669964
O	-4.0462371	-1.0760577	0.4942105
H	-3.2514427	-0.1174893	2.1667841
C	-2.7454393	-0.6979917	-2.8505392
C	-3.9826238	-0.5087067	-3.6976228
C	-1.5054937	-1.0618564	-3.6181591
H	-1.2846182	-0.2811035	-4.3703270
H	-1.6506126	-2.0031904	-4.1807655
H	-0.6278363	-1.1710756	-2.9613583
H	-3.9352994	-1.1291359	-4.6081592
H	-4.0514408	0.5468275	-4.0188486
H	-4.9145500	-0.7374956	-3.1565832
H	-3.1892745	-2.4259700	0.2573256
H	-4.8944554	-0.4190279	-1.2687278
H	-2.3286355	-1.8452984	-0.9992985
O	-2.6121776	-2.9460293	-0.4012739
C	-3.4884342	-3.7391774	-1.2561418
C	-4.1302436	-4.9146445	-0.4983039
H	-4.2672900	-3.0753347	-1.6790944
H	-2.8465780	-4.0933162	-2.0777422
C	-2.5335401	2.8568191	-3.6141824
C	-1.6632309	3.1463096	-2.5242596
C	-2.0986312	4.0778834	-1.5165531
C	-3.3873852	4.6742918	-1.6389070
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C	-3.7881690	3.4411225	-3.6989199
C	-1.2154519	4.3663937	-0.4329073
C	0.0235869	3.7636313	-0.3481543
C	0.4576484	2.8291190	-1.3374394
C	-0.3776393	2.5401404	-2.4057950
C	1.8309025	2.1858098	-1.1230158
C	2.1306681	0.9857165	-2.0793124
O	2.4080168	1.5660122	-3.3369892
C	2.1231258	0.8094442	-4.5079933
O	1.8461734	1.6769618	0.2465101
P	1.0509921	0.3033228	0.7065913
O	2.2288401	-0.8299888	0.4847413
C	2.8824405	-1.2094575	-0.7721695
C	1.9453597	-2.1505149	-1.5341729
C	1.9630840	-2.2537892	-2.9183704
C	1.1258198	-3.1782103	-3.6072317
C	0.2638669	-4.0471537	-2.8478074
C	0.2883046	-3.9475025	-1.4261498
C	1.0979761	-3.0255508	-0.7888004
C	-0.5776327	-4.9628049	-3.5454461
C	-0.5892886	-5.0014379	-4.9313435
C	0.2536876	-4.1357440	-5.6804846
C	1.0994511	-3.2502588	-5.0311122
N	1.0827163	0.4218513	2.3640648
C	2.4065213	0.6826503	3.0258758
C	2.6372854	-0.3571066	4.1217243
C	2.8830698	-0.0101302	5.4617791
C	3.0992626	-1.0056364	6.4288210
C	3.0764562	-2.3582614	6.0664550
C	2.8323168	-2.7145376	4.7302175
C	2.6102172	-1.7227944	3.7697950
C	-0.1249356	0.5814021	3.2123795
C	-0.9845782	1.7839045	2.7739712
C	-0.9470432	-0.6971601	3.3874034
C	-1.9712419	-0.7085671	4.3579803
C	-2.7770669	-1.8385925	4.5418789
C	-2.5758706	-2.9847552	3.7555080
C	-1.5459999	-2.9926375	2.8064879
C	-0.7343173	-1.8615501	2.6330616
C	2.5451594	2.1497794	3.4514331
C	2.9504168	3.2243364	-1.1989678
C	2.9555520	4.1640109	-2.2721739
C	3.9914995	5.0681453	-2.4088625
C	5.0774806	5.0935178	-1.4841738
C	5.0664663	4.1600897	-0.3869359
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C	6.1433212	4.1790014	0.5472810
C	7.1879282	5.0773419	0.4034985
C	7.1983679	5.9980426	-0.6788796
C	6.1647172	6.0069332	-1.6014585
C	3.3120691	0.0963450	-1.5373709
O	4.1637689	-0.2844484	-2.6005037
C	5.2946972	0.5761513	-2.7745946
C	4.1614008	-1.9468075	-0.3375989
C	4.7417342	-1.6759984	0.8933697

C	5.9301058	-2.3325225	1.3208079
C	6.5627605	-3.2756018	0.4355072
C	5.9611400	-3.5186450	-0.8339821
C	4.7917430	-2.8823635	-1.2096278
C	7.7527431	-3.9316460	0.8657627
C	8.2890131	-3.6717232	2.1166908
C	7.6578836	-2.7476758	2.9936490
C	6.5020570	-2.0912384	2.6045261
H	1.2133109	0.3573473	-2.1475656
H	3.8859062	0.6795404	-0.7947377
H	2.0896859	1.5309417	-5.3397561
H	1.1430021	0.2968025	-4.4294221
H	2.9075438	0.0577606	-4.7046480
H	5.9411407	0.5516389	-1.8761902
H	4.9756532	1.6151681	-2.9757315
H	5.8533928	0.1826249	-3.6372290
H	0.2858482	0.8115576	4.2116353
H	-1.4034367	1.6247275	1.7654848
H	-0.3735665	2.7001918	2.7461825
H	-1.8296392	1.9458127	3.4613745
H	0.0907317	-1.8992184	1.9177791
H	-1.3570044	-3.8848493	2.2019433
H	-3.2041118	-3.8702419	3.8985450
H	-3.5638637	-1.8259017	5.3038248
H	-2.1453033	0.1796093	4.9759669
H	3.1556532	0.4989926	2.2370489
H	1.8191069	2.4284801	4.2337488
H	2.3872395	2.8004336	2.5775902
H	3.5575663	2.3367130	3.8474678
H	2.9135262	1.0402873	5.7665222
H	3.2882371	-0.7181377	7.4684745
H	3.2489114	-3.1331869	6.8207875
H	2.8173972	-3.7691876	4.4362106
H	2.4188642	-1.9993215	2.7285804
H	3.9782134	2.5392038	0.5673264
H	6.1340633	3.4674515	1.3813968
H	8.0119608	5.0815337	1.1247754
H	8.0298856	6.7033661	-0.7805812
H	6.1713605	6.7175327	-2.4356317
H	3.9862692	5.7839046	-3.2385710
H	2.1318127	4.1542159	-2.9903167
H	0.6947085	3.9930730	0.4847581
H	-1.5322297	5.0791122	0.3357500
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H	-5.2094054	4.8175939	-2.7807977
H	-4.4463547	3.2124621	-4.5438112
H	-2.1879462	2.1687571	-4.3934556
H	-0.0664616	1.8417341	-3.1850638
H	4.3449659	-3.0992875	-2.1828195
H	6.4351997	-4.2338011	-1.5153092
H	8.2364028	-4.6485967	0.1928904
H	9.2030345	-4.1824276	2.4377248
H	8.0892626	-2.5596717	3.9825147
H	6.0043841	-1.3870229	3.2811581
H	4.2774245	-0.9591369	1.5724471
H	1.1111509	-2.9736304	0.3022619
H	-0.3492786	-4.6102034	-0.8341051
H	-1.2089286	-5.6480815	-2.9685996
H	-1.2394488	-5.7094729	-5.4557577
H	0.2397438	-4.1804440	-6.7744593
H	1.7586132	-2.5899013	-5.6058972
H	2.6470955	-1.6310854	-3.4971386
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C	-3.6846893	4.3678229	2.8352077
C	-3.9707323	3.3956088	1.8650080
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H	-4.7248236	2.6753858	5.6151797
C	-3.9431571	4.1123100	4.1883286
H	-3.7166174	4.8684165	4.9471067
H	-6.5648183	3.1373515	0.8491528
C	-7.0604085	2.1705547	0.7089008
C	-8.4201664	2.1348455	0.3748354
H	-8.9726888	3.0723838	0.2517145
C	-9.0752279	0.9050664	0.2096004
H	-10.1397212	0.8756192	-0.0447905
C	-8.3550121	-0.2846734	0.3780260
H	-8.8545228	-1.2516837	0.2535009
C	-6.9913904	-0.2474699	0.7091455
H	-6.4452631	-1.1895385	0.8183196
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C	-5.0082414	-5.6735622	-1.5174103
C	-5.0090670	-4.3878306	0.6575655
C	-3.0338120	-5.8495152	0.0519115
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H	-4.4098893	-3.8561098	1.4179131
H	-5.5151127	-5.2278414	1.1632224
H	-5.8059872	-5.0259615	-1.9241232
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H	-4.4059798	-6.0510146	-2.3634285
H	-2.4136068	-6.2601225	-0.7645242
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H	-2.3702558	-5.3111242	0.7488791

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C	-3.0270542	2.5824367	-3.9355090
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C	-0.0862512	4.2848635	-1.3848476
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C	-0.7387521	2.5464116	-2.9494371
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C	1.7990565	1.0801322	-2.5647630
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C	0.7882313	-3.3325348	-3.1733866
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C	-0.1837828	-3.3162655	-0.9149110
C	0.7309914	-2.3512730	-0.5286202
C	-1.1484401	-4.7894798	-2.6894985
C	-1.1472239	-5.2275992	-4.0043029
C	-0.1827064	-4.7332272	-4.9253426
C	0.7685330	-3.8126615	-4.5163707
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C	2.5493168	2.0547936	2.3806631
C	3.2072765	1.2719018	3.5145167
C	3.2134087	1.7203629	4.8481790
C	3.8247708	0.9558294	5.8554986
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C	4.4515870	-0.7131918	4.2118139
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C	-2.1920554	-1.8229233	2.6933278
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C	2.7135029	4.0921601	-3.4424239
C	3.7736948	4.8984936	-3.8136952
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C	4.9018040	4.4262132	-1.6752371
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C	7.0825092	6.0555709	-2.4458899
C	6.0128119	5.8998931	-3.3133490
C	3.0524106	0.3217311	-1.9987358
O	3.8274182	-0.2386708	-3.0392501
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C	4.0393992	-1.4633001	-0.5069248
C	5.0470415	-0.6487951	-0.0007715
C	6.2506028	-1.1870239	0.5296205
C	6.4320178	-2.6170201	0.5293756
C	5.3951008	-3.4303370	-0.0103300
C	4.2297482	-2.8729870	-0.5108801
C	7.6334771	-3.1587933	1.0745083
C	8.6076250	-2.3270515	1.6013934
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H	3.6651060	1.0520700	-1.4422008
H	1.4228522	0.8863066	-5.8405885
H	0.6842437	-0.1805753	-4.5918163
H	2.4264903	-0.3501318	-4.9943753
H	5.6070646	0.8075272	-2.6880080
H	4.4764314	1.5799015	-3.8688054
H	5.3786478	0.0819554	-4.3205526
H	0.7134560	1.3012295	3.9726301
H	-1.4588171	2.2774374	2.0141438
H	-0.4302071	3.3096020	3.0353578
H	-1.6111332	2.2038687	3.7951632
H	1.5958181	-1.0875384	3.2171542
H	0.7904757	-3.4372741	3.1115759
H	-1.6425222	-3.9212093	2.7613061
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H	-2.4666907	0.3111918	2.6878864
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H	1.7403489	3.7814202	3.4795461
H	1.9646477	4.0318580	1.7226391
H	3.3811931	4.0141176	2.8228257
H	2.7508327	2.6763909	5.1137366
H	3.8206098	1.3191480	6.8885693
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H	3.8209481	-0.3198582	2.1800154
H	3.7983814	3.1156877	-0.3421904
H	6.0115459	4.1106092	0.1725497
H	7.9357749	5.5397042	-0.5059919
H	7.9330477	6.6827728	-2.7322114
H	6.0105161	6.4026869	-4.2866399
H	3.7573375	5.4106635	-4.7818339
H	1.8599763	3.9564112	-4.1105639
H	0.6760020	4.7076780	-0.7229554
H	-1.5281854	5.8282846	-0.9754290
H	-3.8327594	5.8737928	-1.9789300
H	-5.5658981	4.8105312	-3.4059661
H	-5.0541282	2.6984884	-4.6532287
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H	3.4464073	-3.5229747	-0.9095820
H	5.5260074	-4.5179848	-0.0184454
H	7.7734769	-4.2454351	1.0710400
H	9.5257201	-2.7538665	2.0185073
H	9.2043033	-0.2722367	2.0273324
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H	4.9178890	0.4386434	0.0271050
H	0.7335669	-1.9999871	0.5048150
H	-0.9119837	-3.6878587	-0.1866087
H	-1.8861040	-5.1739453	-1.9769106
H	-1.8870957	-5.9624608	-4.3385795
H	-0.1918057	-5.0897939	-5.9604737
H	1.5155586	-3.4345692	-5.2230783
H	2.4948868	-2.0069779	-3.4382133
H	-4.1995670	1.0772109	5.0108598
C	-4.7672074	0.7973807	4.1171651
C	-5.5885608	-0.3408603	4.1321785

H	-5.6649130	-0.9558579	5.0346218
C	-6.3251630	-0.6673295	2.9868472
H	-6.9879947	-1.5394742	2.9867052
C	-6.2308394	0.1240689	1.8291714
H	-6.8321698	-0.1652730	0.9634035
C	-5.3912908	1.2533789	1.7901738
C	-4.6742163	1.5813122	2.9613546
H	-4.0512378	2.4823864	2.9683890
H	-3.5074910	4.3924389	0.2773816
C	-4.4617685	4.6231768	0.7565932
C	-4.7118642	5.9483413	1.1473915
H	-3.9497821	6.7153450	0.9694281
C	-5.9234440	6.2902317	1.7601417
H	-6.1184880	7.3242245	2.0629154
C	-6.8818526	5.2912819	1.9909943
H	-7.8297361	5.5413239	2.4789664
C	-6.6266063	3.9689244	1.6099350
H	-7.3711645	3.1942736	1.8238519
C	-5.4156995	3.6133376	0.9771290
Au	-1.1057070	0.3973637	-0.2908157
C	-3.4314660	0.4857366	-0.3189733
C	-2.9208073	-0.0533306	-1.4692304
C	-3.7906780	1.9392347	-0.0627500
H	-3.6831976	2.5161731	-0.9926539
H	-3.0718102	2.3478499	0.6692315
C	-5.2186540	2.1467555	0.5461531
C	-6.2611472	1.8632930	-0.5774391
H	-6.2203199	2.7071813	-1.2863136
H	-7.2800056	1.8425606	-0.1414712
O	-5.9874848	0.7047384	-1.3388809
C	-2.9252280	-0.6285282	-2.6723174
C	-4.2392021	-0.8763681	-3.3892509
C	-1.6889603	-1.0716049	-3.4069924
H	-1.5705486	-0.4810427	-4.3347937
H	-1.7883104	-2.1266306	-3.7153465
H	-0.7772601	-0.9755528	-2.7981964
H	-4.4502455	-1.9634847	-3.4052850
H	-4.1452366	-0.5583434	-4.4436704
H	-5.0688988	-0.3276627	-2.9233688
H	-3.6974453	-0.2134181	0.4909956
H	-6.1068397	-0.1333292	-0.8302853
C	-5.2750445	-4.2116037	-0.0473710
C	-5.0452417	-2.6851712	-0.0531209
H	-4.9848576	-2.3084025	0.9813131
H	-4.0873221	-2.4508070	-0.5627687
O	-6.1226337	-1.9434579	-0.6482538
H	-6.2377482	-2.2502027	-1.5665341
C	-4.0924385	-4.8557011	0.7050124
C	-5.3106979	-4.7340701	-1.5003631
C	-6.6017015	-4.5341586	0.6683156
H	-6.5726749	-4.1924787	1.7187207
H	-6.7953349	-5.6208890	0.6679423
H	-7.4469700	-4.0284616	0.1715645
H	-4.3757647	-4.4895407	-2.0378676
H	-6.1585295	-4.3063272	-2.0693402
H	-5.4383965	-5.8302374	-1.5198350
H	-3.1273829	-4.5959581	0.2337132
H	-4.1849252	-5.9554811	0.7076833
H	-4.0600416	-4.5176739	1.7562525

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C	0.3072048	3.4012241	3.5903362
C	-0.5999645	2.7291258	2.7221204
C	-1.5011954	3.5082635	1.9117478
C	-1.4365440	4.9298361	1.9844670
C	-0.5299079	5.5533652	2.8272620
C	0.3425282	4.7847070	3.6411533
C	-2.4076786	2.8129788	1.0544023
C	-2.4040464	1.4322567	0.9760995
C	-1.4767414	0.6566252	1.7399058
C	-0.6145515	1.3089446	2.6112824
C	-1.4618757	-0.8624035	1.5277072
C	-0.1076732	-1.5263962	1.9619087
O	-0.1284223	-1.5814636	3.3725830
C	1.1293225	-1.5714942	4.0492107
O	-1.6327382	-1.1033793	0.0934697
P	-0.4566984	-0.8263932	-1.0289229
O	0.3196035	-2.2741113	-1.0557904
C	1.0195371	-2.9569609	0.0476106
C	2.3809144	-2.2875947	0.2476455
C	3.1322722	-2.5134170	1.3953779
C	4.4263719	-1.9416570	1.5590725
C	4.9841750	-1.1390284	0.4989759
C	4.2054051	-0.9404875	-0.6757874
C	2.9424670	-1.4956237	-0.7988162
C	6.2740219	-0.5584924	0.6754584
C	6.9800605	-0.7520809	1.8517468
C	6.4294883	-1.5407173	2.8996948
C	5.1827153	-2.1264518	2.7544667
N	-1.3044861	-0.8984924	-2.4506568
C	-2.2522104	-2.0534446	-2.6525142
C	-1.9032000	-2.8163128	-3.9285419
C	-2.6457870	-2.6892003	-5.1170617
C	-2.2759389	-3.4006363	-6.2697280
C	-1.1662811	-4.2558147	-6.2457908
C	-0.4236817	-4.3961303	-5.0628974
C	-0.7865417	-3.6771789	-3.9184055
C	-1.2128755	0.1575798	-3.4938578
C	-1.9427034	1.4407304	-3.0585129
C	0.2316264	0.3713173	-3.9664503
C	0.6631728	1.6019259	-4.4980151
C	1.9837567	1.7773526	-4.9386002
C	2.8962399	0.7159623	-4.8727764
C	2.4692442	-0.5274917	-4.3847093
C	1.1517076	-0.6972061	-3.9394095
C	-3.7117908	-1.5991983	-2.5329257
C	-2.6477636	-1.5563464	2.1991890
C	-2.9838650	-1.2275042	3.5459442
C	-4.0070127	-1.8919961	4.1966330
C	-4.7583470	-2.9148762	3.5448386

C	-4.4355315	-3.2375697	2.1787386
C	-3.3740355	-2.5374773	1.5356669
C	-5.1835754	-4.2522014	1.5120078
C	-6.2043665	-4.9230223	2.1659006
C	-6.5225542	-4.6049630	3.5142548
C	-5.8160297	-3.6214113	4.1882252
C	0.0843347	-2.9402013	1.3064541
O	0.6045567	-3.8672531	2.2377668
C	-0.4009137	-4.6223353	2.9221079
C	1.1353906	-4.4025467	-0.4639980
C	-0.0277461	-5.0954145	-0.7839795
C	0.0065744	-6.4071796	-1.3303149
C	1.2854510	-7.0379053	-1.5429690
C	2.4621830	-6.3155174	-1.1948379
C	2.3929796	-5.0332148	-0.6749427
C	1.3224822	-8.3507321	-2.0993379
C	0.1509804	-9.0079026	-2.4363972
C	-1.1103737	-8.3824618	-2.2323070
C	-1.1813245	-7.1105374	-1.6907049
H	0.7192310	-0.8590692	1.6262543
H	-0.9013892	-3.2907627	0.9527608
H	0.9078101	-1.3280257	5.1000669
H	1.8050603	-0.8019347	3.6267659
H	1.6245046	-2.5547197	3.9906337
H	-0.9691946	-5.2475643	2.2055650
H	-1.0957010	-3.9583225	3.4681436
H	0.1301106	-5.2738572	3.6324084
H	-1.7610468	-0.2741505	-4.3522498
H	-1.4095872	1.9267155	-2.2216774
H	-2.9599232	1.1965560	-2.7153076
H	-2.0249365	2.1653473	-3.8848991
H	0.8278531	-1.6729407	-3.5693934
H	3.1624709	-1.3746770	-4.3479751
H	3.9276653	0.8538363	-5.2137420
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H	-2.0405798	-2.7313440	-1.8096935
H	-3.9866796	-0.8735159	-3.3164702
H	-3.8725272	-1.1289453	-1.5492505
H	-4.3866061	-2.4670818	-2.6256675
H	-3.5289560	-2.0429648	-5.1528254
H	-2.8646348	-3.2902165	-7.1864609
H	-0.8850636	-4.8167325	-7.1431571
H	0.4369515	-5.0723976	-5.0266618
H	-0.2041875	-3.7867857	-2.9983216
H	-3.1419896	-2.7801964	0.4952810
H	-4.9369890	-4.4942149	0.4714624
H	-6.7715748	-5.7015594	1.6452419
H	-7.3319480	-5.1418945	4.0196235
H	-6.0623189	-3.3747099	5.2269414
H	-4.2554856	-1.6323540	5.2315633
H	-2.4190614	-0.4467424	4.0607426
H	-3.1005191	0.9155706	0.3094075
H	-3.1169468	3.3934587	0.4541529
H	-2.1007145	5.5297355	1.3538233
H	-0.4825837	6.6445203	2.8528392
H	1.0503848	5.2925740	4.3041154
H	0.9840073	2.8034762	4.2108991
H	0.0839807	0.7398067	3.2265237
H	3.3137557	-4.4990410	-0.4275309
H	3.4383490	-6.7869684	-1.3525918
H	2.2942762	-8.8311774	-2.2572192
H	0.1906934	-10.0151582	-2.8638180
H	-2.0274970	-8.9138080	-2.5070547
H	-2.1515940	-6.6255987	-1.5350207
H	-1.0073399	-4.6242191	-0.6458716
H	2.3804238	-1.3463768	-1.7218367
H	4.6117529	-0.3363054	-1.4943787
H	6.6954772	0.0489297	-0.1330867
H	7.9693613	-0.3002364	1.9788629
H	7.0004657	-1.6865959	3.8225303
H	4.7587180	-2.7380040	3.5587707
H	2.7335834	-3.1594671	2.1810486
H	-3.3948626	5.2212644	-1.4733349
C	-2.5231378	5.7926467	-1.8093928
C	-2.6715718	7.1248459	-2.2147574
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C	-1.5410329	7.8365015	-2.6557729
H	-1.6415427	8.8749788	-2.9872055
C	-0.2843859	7.2196103	-2.6720373
H	0.5843462	7.7834144	-3.0290188
C	-0.1160596	5.8798706	-2.2535927
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H	3.9752086	5.5303959	-3.0540515
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C	3.8190405	5.5044215	-5.2003608
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C	2.9724540	5.4308138	-6.3152697
H	3.3884868	5.4478956	-7.3277715
C	1.5868651	5.3349825	-6.1197252
H	0.9127735	5.2704777	-6.9802607
C	1.0577369	5.3184925	-4.8222154
H	-0.0262060	5.2452283	-4.6864051
C	1.8958079	5.3987175	-3.6902952
Au	0.7566840	1.0826733	-0.5210723
C	1.0947362	3.3833636	-0.4780348
C	1.9648237	2.7052560	0.3371243
C	1.3521956	3.7600256	-1.9256341
H	2.3372620	3.3690924	-2.2245941
H	0.6164215	3.2593570	-2.5746646
C	1.3019480	5.2876438	-2.2701168
C	2.1488106	6.0583646	-1.2080955
H	3.1666957	5.6341699	-1.1707895
H	2.2423385	7.1219014	-1.5086345
O	1.6123481	5.9132621	0.0883319
C	2.8513139	2.5957576	1.3273515
C	3.5042265	3.8565117	1.8613593
C	3.2344596	1.2969908	1.9852151
H	4.3289296	1.1536132	1.9762408
H	2.9231811	1.3234236	3.0465905
H	2.7672397	0.4243625	1.5010505

H	4.5890376	3.8391273	1.6438557
H	3.0491856	4.7625135	1.4333368
H	3.3929204	3.8863912	2.9611610
H	0.1677272	3.7405750	-0.0074892
H	0.8035647	6.4882036	0.1902657
H	1.0271207	8.8493179	1.2810659
C	0.1761968	8.9913834	0.5928496
H	0.5811796	9.3316704	-0.3829773
C	-0.7958722	10.0492913	1.1593373
O	-0.4114761	7.6855484	0.4525954
H	-1.0531927	7.7092837	-0.2845809
C	-1.9612098	10.2745617	0.1722351
C	-0.0034520	11.3610552	1.3368438
C	-1.3486706	9.5736581	2.5180563
H	-1.9179574	8.6352912	2.4034419
H	-2.0227807	10.3328238	2.9518296
H	-0.5305976	9.3941320	3.2390902
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H	-0.6567169	12.1560679	1.7365397
H	-1.5904303	10.6098930	-0.8135174
H	-2.6518764	11.0462471	0.5545339
H	-2.5509872	9.3509761	0.0237693

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C	-2.5692129	2.6961159	-3.3309995
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C	-1.8999126	4.1388371	-1.4443390
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C	-4.1000671	4.3864792	-2.4800571
C	-3.8021408	3.3278355	-3.3804737
C	-0.9312815	4.4758139	-0.4503134
C	0.2679425	3.7945715	-0.3676745
C	0.5795697	2.7390020	-1.2786168
C	-0.3387895	2.4033878	-2.2618516
C	1.9110999	2.0113112	-1.0666981
C	2.1171393	0.7729992	-2.0020509
O	2.3395007	1.2991718	-3.2933639
C	2.0052295	0.4772169	-4.4093644
O	1.9235574	1.5411470	0.3195952
P	1.1365271	0.1780132	0.8342291
O	2.3166490	-0.9553507	0.6054259
C	2.8705407	-1.4014627	-0.6787261
C	1.8445729	-2.3107360	-1.3591197
C	1.8899005	-2.5760612	-2.7224721
C	0.9442758	-3.4447282	-3.3403653
C	-0.0636796	-4.0831840	-2.5310635
C	-0.0668876	-3.8236795	-1.1315539
C	0.8575442	-2.9659797	-0.5622292
C	-1.0265452	-4.9239318	-3.1623722
C	-1.0077057	-5.1147606	-4.5351010
C	-0.0160375	-4.4823212	-5.3345383
C	0.9423282	-3.6712446	-4.7484256
N	1.2140014	0.3469899	2.4853713
C	2.5336234	0.6753857	3.1247669
C	2.9031164	-0.3888052	4.1565496
C	2.7604176	-0.1874737	5.5416645
C	3.0818316	-1.2094861	6.4497663
C	3.5604108	-2.4414862	5.9852390
C	3.7156244	-2.6496622	4.6054331
C	3.3836883	-1.6343615	3.7008498
C	-0.0152879	0.2691784	3.3204285
C	-0.8588234	1.5499545	3.2190909
C	-0.7820937	-1.0287288	3.0389802
C	-2.1754976	-1.0574309	2.8505570
C	-2.8446877	-2.2666615	2.6030727
C	-2.1294030	-3.4683777	2.5384631
C	-0.7401146	-3.4545165	2.7433881
C	-0.0754195	-2.2485950	2.9936272
C	2.5752150	2.1235170	3.6279288
C	3.0929713	2.9737694	-1.1906997
C	3.1548588	3.8571456	-2.3093129
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C	5.3301377	4.6938975	-1.5624824
C	5.2616595	3.8201895	-0.4192919
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C	6.3372505	3.8211505	0.5164561
C	7.4349340	4.6456873	0.3314808
C	7.5018069	5.5080499	-0.7959728
C	6.4711701	5.5324419	-1.7216810
C	3.2962583	-0.1337376	-1.4992301
O	4.0981479	-0.5726544	-2.5789901
C	5.2305175	0.2650482	-2.8312540
C	4.1568720	-2.1440109	-0.2799259
C	5.0583269	-1.5032441	0.5630383
C	6.2617666	-2.1288195	0.9878797
C	6.5584849	-3.4574656	0.5136509
C	5.6275484	-4.0876513	-0.3609473
C	4.4574000	-3.4538277	-0.7453183
C	7.7650612	-4.0868351	0.9401344
C	8.6359486	-3.4363763	1.7983576
C	8.3397711	-2.1275725	2.2700719
C	7.1779983	-1.4877357	1.8737315
H	1.1771780	0.1757141	-1.9956036
H	3.9155664	0.4615856	-0.8049653
H	1.9305145	1.1520672	-5.2766887
H	1.0336750	-0.0315271	-4.2560254
H	2.7815764	-0.2841339	-4.5954454
H	5.9108671	0.2679854	-1.9570770
H	4.9174901	1.3002026	-3.0608366
H	5.7516353	-0.1688570	-3.6980530
H	0.3677437	0.1868661	4.3548296
H	-1.2618955	1.6681714	2.1975124
H	-0.2377204	2.4322466	3.4333180
H	-1.6999441	1.5350301	3.9326747
H	1.0073063	-2.2448820	3.1504979
H	-0.1695266	-4.3888464	2.7110660
H	-2.6483913	-4.4130662	2.3468361
H	-3.9323137	-2.2541854	2.4788661
H	-2.7637193	-0.1400202	2.9013590

H	3.2617464	0.5873592	2.3017786
H	1.8430982	2.3071878	4.4321933
H	2.3556148	2.8086367	2.7933473
H	3.5775188	2.3564969	4.0258033
H	2.4066486	0.7740357	5.9281312
H	2.9642117	-1.0359520	7.5247349
H	3.8184647	-3.2341061	6.6953185
H	4.1018456	-3.6034432	4.2306114
H	3.4929029	-1.8033861	2.6251584
H	4.0719347	2.3225260	0.6137576
H	6.2834524	3.1553555	1.3861746
H	8.2570889	4.6367886	1.0549275
H	8.3745236	6.1557482	-0.9300711
H	6.5215114	6.1980294	-2.5907512
H	4.2826307	5.3608739	-3.3520705
H	2.3316246	3.8606741	-3.0278204
H	1.0021088	4.0554602	0.4007836
H	-1.1538029	5.2876531	0.2507961
H	-3.3952109	5.6049828	-0.8468064
H	-5.0711450	4.8899046	-2.5336166
H	-4.5468427	3.0186839	-4.1215140
H	-2.3305219	1.8907081	-4.0318800
H	-0.1270497	1.6065295	-2.9770404
H	3.7575748	-3.9640535	-1.4123903
H	5.8469223	-5.0964627	-0.7278549
H	7.9930696	-5.0954827	0.5779237
H	9.5596522	-3.9291307	2.1193606
H	9.0370372	-1.6276675	2.9505553
H	6.9446834	-0.4804776	2.2374125
H	4.8411212	-0.4955590	0.9340094
H	0.8369755	-2.7933982	0.5151158
H	-0.8193749	-4.3031421	-0.4957167
H	-1.7847335	-5.4171688	-2.5442100
H	-1.7537396	-5.7604680	-5.0104645
H	-0.0101959	-4.6445069	-6.4174249
H	1.7090076	-3.1848265	-5.3618236
H	2.6707780	-2.1189631	-3.3346609
H	-4.8257747	0.5800977	5.3600404
C	-5.2393017	0.3199108	4.3802665
C	-6.0231081	-0.8342064	4.2315173
H	-6.2244091	-1.4812747	5.0910251
C	-6.5534909	-1.1426309	2.9729167
H	-7.1777819	-2.0328275	2.8398193
C	-6.2947510	-0.3118230	1.8702707
H	-6.7356387	-0.5928671	0.9097120
C	-5.5030371	0.8464200	2.0026182
C	-4.9872385	1.1487532	3.2805858
H	-4.3907609	2.0570021	3.4170370
H	-3.2424748	3.7225986	1.4561910
C	-4.2706843	4.0837430	1.5524111
C	-4.4856319	5.4040752	1.9756898
H	-3.6269184	6.0426345	2.2095493
C	-5.7879185	5.9064037	2.0941537
H	-5.9546369	6.9382577	2.4199351
C	-6.8776634	5.0733425	1.7994287
H	-7.9007040	5.4511387	1.8970071
C	-6.6618559	3.7515381	1.3905794
H	-7.5247812	3.1056927	1.1950651
C	-5.3556668	3.2403462	1.2497581
Au	-0.9023370	-0.1558384	-0.1860637
C	-3.6798164	0.1336004	-0.3405374
C	-2.6932540	-0.2680849	-1.3022854
C	-3.7210330	1.5011476	0.3061546
H	-3.4043536	2.2700492	-0.4151132
H	-3.0160838	1.5120211	1.1514243
C	-5.1649579	1.7813920	0.8197212
C	-6.0101561	1.4739354	-0.4359817
H	-5.9554615	2.3199411	-1.1387094
H	-7.0642016	1.2406339	-0.2186354
O	-5.3944189	0.3464777	-1.0980968
C	-2.7162896	-0.6668002	-2.5971982
C	-3.9422615	-0.6944632	-3.4923753
C	-1.4674340	-1.1164595	-3.3156108
H	-1.2044977	-0.3950381	-4.1137518
H	-1.6280893	-2.0886050	-3.8159937
H	-0.6064212	-1.2185470	-2.6362977
H	-3.6959776	-0.2488268	-4.4742928
H	-4.7975651	-0.1536093	-3.0735041
H	-4.2310028	-1.7438144	-3.7026319
H	-3.9785800	-0.6664075	0.3564911
H	-5.8459313	-0.5642631	-0.9928579
C	-5.4090086	-4.4670212	-0.9886536
C	-5.1855663	-3.0023812	-0.5674273
H	-5.2600334	-2.8930758	0.5266240
H	-4.1819471	-2.6634042	-0.8910130
O	-6.1970768	-2.1000841	-1.0983324
H	-6.3086054	-2.3018685	-2.0478665
C	-5.2504306	-4.5930605	-2.5210674
C	-6.8116730	-4.9370432	-0.5523646
C	-4.3222377	-5.3100379	-0.2888517
H	-7.6008919	-4.3224184	-1.0181520
H	-6.9276955	-4.8629482	0.5439127
H	-6.9780780	-5.9887309	-0.8426953
H	-6.0172524	-4.0107444	-3.0695418
H	-5.3738984	-5.6431315	-2.8374528
H	-4.2540521	-4.2486938	-2.8519736
H	-3.3088596	-4.9614652	-0.5563785
H	-4.4092585	-6.3704295	-0.5821054
H	-4.4246326	-5.2545804	0.8093312

TS3-S-a

C	0.6034330	2.9281288	3.6707938
C	-0.3872477	1.9869547	3.2664717
C	-1.7242182	2.4539223	3.0077684
C	-2.0181764	3.8366826	3.1871969
C	-1.0306345	4.7294215	3.5736192
C	0.2937837	4.2719961	3.8109605
C	-2.7060800	1.5082583	2.5844407
C	-2.3786345	0.1787030	2.4094071
C	-1.0474154	-0.2870677	2.6365171

C	-0.0829665	0.6069418	3.0768054
C	-0.7678686	-1.7573711	2.3081985
C	0.7535224	-2.1157549	2.2352728
O	1.2148523	-2.1419001	3.5693672
C	2.6014730	-1.8925466	3.7939598
O	-1.3432737	-2.0084486	0.9905321
P	-0.6597907	-1.4898203	-0.4283118
O	0.2794358	-2.7983404	-0.7953331
C	1.4128249	-3.3323280	-0.0249790
C	2.6296260	-2.4356448	-0.2640197
C	3.7329841	-2.4684336	0.5805862
C	4.8807093	-1.6625662	0.3327092
C	4.9114080	-0.8165442	-0.8339142
C	3.7814185	-0.8218523	-1.6995448
C	2.6748914	-1.6067799	-1.4250098
C	6.0521080	0.0074884	-1.0611095
C	7.1132168	0.0063593	-0.1701062
C	7.0832150	-0.8265029	0.9822467
C	5.9936070	-1.6467797	1.2248041
N	-1.9143836	-1.7210364	-1.4920631
C	-2.6577601	-3.0276164	-1.4670641
C	-2.6335131	-3.6812979	-2.8476188
C	-3.7451864	-3.6788844	-3.7099013
C	-3.6664823	-4.2737589	-4.9795171
C	-2.4788728	-4.8877062	-5.3985028
C	-1.3661658	-4.9031645	-4.5424591
C	-1.4428291	-4.3000684	-3.2820031
C	-2.3857251	-0.6351613	-2.3872018
C	-3.1289364	0.4623608	-1.6022628
C	-1.2626693	-0.1193700	-3.2944792
C	-1.2654358	1.1965699	-3.7907192
C	-0.2553314	1.6470698	-4.6534082
C	0.7810694	0.7856106	-5.0369939
C	0.7838532	-0.5363857	-4.5675674
C	-0.2299544	-0.9843559	-3.7112515
C	-4.0478991	-2.8688845	-0.8385682
C	-1.5010499	-2.6971774	3.2662419
C	-1.4119155	-2.4716928	4.6721914
C	-2.0077023	-3.3456645	5.5622571
C	-2.7318660	-4.4873427	5.1064206
C	-2.8433951	-4.7067323	3.6871379
C	-2.2172468	-3.7893348	2.7946394
C	-3.5708912	-5.8394266	3.2173448
C	-4.1601672	-6.7209106	4.1089728
C	-4.0497681	-6.5045733	5.5093103
C	-3.3519762	-5.4111488	5.9970238
C	0.9761756	-3.4723214	1.4767056
O	1.9419586	-4.2716138	2.1321620
C	1.3810759	-5.1966789	3.0686544
C	1.5929622	-4.7486947	-0.5984447
C	0.4935200	-5.5998126	-0.6252843
C	0.5704627	-6.9076390	-1.1763905
C	1.8312909	-7.3656582	-1.7039330
C	2.9476675	-6.4828911	-1.6508977
C	2.8340089	-5.2087345	-1.1189127
C	1.9088461	-8.6757546	-2.2624153
C	0.7917012	-9.4934692	-2.3036363
C	-0.4536701	-9.0382379	-1.7884840
C	-0.5618818	-7.7733100	-1.2365824
H	1.2705764	-1.3040284	1.6752902
H	0.0143477	-4.0138131	1.4511990
H	2.6975638	-1.6356300	4.8607957
H	2.9622178	-1.0463531	3.1775003
H	3.2123310	-2.7825075	3.5689655
H	0.7208766	-5.9192168	2.5494534
H	0.8093448	-4.6710305	3.8556171
H	2.2281427	-5.7356925	3.5193995
H	-3.1160480	-1.1358302	-3.0515891
H	-2.4258237	1.0290182	-0.9646839
H	-3.8873101	0.0065483	-0.9473448
H	-3.6401938	1.1679485	-2.2779901
H	-0.2269027	-2.0195854	-3.3613777
H	1.5762055	-1.2287010	-4.8721292
H	1.5722860	1.1371138	-5.7076103
H	-0.2870604	2.6765404	-5.0223216
H	-2.0603093	1.8924209	-3.5139420
H	-2.0588101	-3.6687984	-0.8002305
H	-4.6955677	-2.1964213	-1.4258346
H	-3.9467306	-2.4567345	0.1781586
H	-4.5499439	-3.8493686	-0.7770522
H	-4.6885811	-3.2210575	-3.3950613
H	-4.5410332	-4.2618348	-5.6385701
H	-2.4216896	-5.3584136	-6.3855571
H	-0.4367699	-5.3918602	-4.8535224
H	-0.5727911	-4.3110465	-2.6175294
H	-2.3140699	-3.9548226	1.7181792
H	-3.6545103	-6.0033057	2.1365345
H	-4.7145158	-7.5892098	3.7376530
H	-4.5207239	-7.2083302	6.2035448
H	-3.2674217	-5.2437056	7.0764936
H	-1.9306427	-3.1651312	6.6401372
H	-0.8585314	-1.6027758	5.0365869
H	-3.1343662	-0.5384458	2.0757807
H	-3.7300935	1.8518550	2.4005581
H	-3.0446160	4.1804296	3.0205171
H	-1.2691027	5.7891919	3.7101649
H	1.0666353	4.9853017	4.1131191
H	1.6211732	2.5730596	3.8636180
H	0.9378571	0.2727167	3.2713922
H	3.7051185	-4.5485744	-1.1013127
H	3.9101086	-6.8232770	-2.0485352
H	2.8678842	-9.0253138	-2.6606322
H	0.8625385	-10.4969869	-2.7360097
H	-1.3287374	-9.6951198	-1.8315245
H	-1.5207225	-7.4179962	-0.8423111
H	-0.4732471	-5.2602181	-0.2380075
H	1.8276629	-1.6001899	-2.1122512
H	3.7859058	-0.1871287	-2.5925960
H	6.0730303	0.6475767	-1.9503558
H	7.9836156	0.6454938	-0.3521478
H	7.9303566	-0.8191924	1.6761513
H	5.9701466	-2.2920611	2.1103959

H	3.7305946	-3.1372410	1.4441397
H	-3.6989170	5.9109464	1.4968742
C	-3.0784404	6.2997386	0.6834815
C	-3.1348098	7.6586883	0.3493616
H	-3.7918925	8.3367852	0.9028078
C	-2.3479942	8.1390073	-0.7110485
H	-2.3940129	9.1953225	-0.9950712
C	-1.5083492	7.2665229	-1.4105867
H	-0.9171498	7.6494043	-2.2500173
C	-1.4212085	5.8983915	-1.0691167
C	-2.2319507	5.4247414	-0.0220146
H	-2.2140248	4.3710711	0.2697291
H	0.9639867	5.7215227	-4.2161983
C	-0.0665631	5.4051848	-4.4034276
C	-0.5318150	5.3922130	-5.7288565
H	0.1385913	5.6981473	-6.5385732
C	-1.8417235	4.9880977	-6.0148077
H	-2.2011855	4.9724914	-7.0485336
C	-2.6929236	4.6111553	-4.9636536
H	-3.7219697	4.3018419	-5.1745671
C	-2.2316686	4.6377513	-3.6429659
H	-2.9111659	4.3666658	-2.8267798
C	-0.9078326	5.0204721	-3.3427953
Au	0.3749698	0.5659179	-0.2512727
C	0.4042180	3.4296787	-0.0460812
C	1.3427652	2.3886218	0.2128794
C	-0.3458628	3.5437455	-1.3587741
H	0.1635670	2.9358403	-2.1237501
H	-1.3538559	3.1125695	-1.2382202
C	-0.4530798	5.0113868	-1.8765759
C	0.9905660	5.5247071	-1.6711850
H	1.6917710	4.9919239	-2.3332900
H	1.0905823	6.6109486	-1.8411914
O	1.3735508	5.2020817	-0.3357520
C	2.5154119	2.4237464	0.9069400
C	3.2016800	3.7181563	1.3075296
C	3.2567367	1.1791582	1.3122020
H	4.2939728	1.1932243	0.9319765
H	3.3348880	1.1398835	2.4166192
H	2.7723193	0.2576522	0.9515075
H	3.6423414	4.2267301	0.4337828
H	2.4910637	4.4250807	1.7672365
H	4.0120709	3.5147318	2.0274954
H	-0.1015532	3.8410825	0.8438153
H	0.9437170	5.8556717	0.3211289
H	1.9717515	8.1362994	1.0771921
C	0.8890999	8.2556617	1.2532697
H	0.4434431	8.7546032	0.3704004
C	0.6452794	9.0907521	2.5270991
O	0.3784593	6.9060457	1.3525470
H	-0.5996106	6.9245479	1.3386568
C	-0.8710745	9.2494685	2.7694768
C	1.2819690	10.4775731	2.2976080
C	1.3037697	8.3958429	3.7359595
H	0.8686038	7.3951594	3.8963088
H	1.1557662	8.9895740	4.6543671
H	2.3907187	8.2738517	3.5797917
H	0.8290153	10.9901259	1.4293904
H	2.3692629	10.3945687	2.1195413
H	1.1334403	11.1194214	3.1828284
H	-1.3642941	9.7402992	1.9118212
H	-1.0566953	9.8630854	3.6677475
H	-1.3630718	8.2726115	2.9320275

Product

C	-1.0613499	4.5781153	-1.1183929
C	-0.8308241	3.4707111	-2.1065563
C	-0.0144337	4.6297263	0.0171781
H	-0.3120025	4.0203748	0.8849440
H	0.9552885	4.2406522	-0.3387813
C	0.1439227	6.1452353	0.3038691
C	0.0692275	6.6355242	-1.1675639
O	-0.9541213	5.8648120	-1.7834350
C	-1.5759307	2.3578260	-2.2873144
C	-2.8221874	2.0283934	-1.4974697
C	-1.1893842	1.3240520	-3.3212404
H	-1.0239610	0.3356487	-2.8493552
H	-2.0029864	1.1861749	-4.0599706
H	-0.2720558	1.6049575	-3.8649456
H	-3.6643960	1.8032720	-2.1791487
H	-2.6630007	1.1201685	-0.8840006
H	-3.1340296	2.8403912	-0.8220386
H	0.0641829	3.6136660	-2.7291885
H	-2.0795111	4.5214788	-0.6934454
H	1.0512956	6.4703339	-1.6624252
H	-0.1989854	7.6999547	-1.2730890
H	3.2839045	5.4761650	3.7434500
C	3.0142966	6.0530140	2.8518262
C	3.8488485	7.0887069	2.4049729
H	4.7733816	7.3245463	2.9429063
C	3.4863785	7.8208087	1.2673556
H	4.1270475	8.6346412	0.9100324
C	2.3024449	7.5174663	0.5778707
H	2.0392391	8.1090539	-0.3052444
C	1.4591813	6.4765364	1.0120551
C	1.8324596	5.7545290	2.1635668
H	1.1805304	4.9550338	2.5322474
H	-3.7314171	5.9128568	3.0590737
C	-2.9958924	6.5495535	2.5549822
C	-1.9751545	5.9573761	1.7939599
H	-1.9381549	4.8658907	1.7280538
C	-1.0159101	6.7423349	1.1294945
C	-1.1036433	8.1434432	1.2660149
H	-0.3531125	8.7796373	0.7834461
C	-2.1190300	8.7391942	2.0220344
H	-2.1610343	9.8303865	2.1096509
C	-3.0754072	7.9423919	2.6703706
H	-3.8718395	8.4049189	3.2631177

neopentanol

C	0.1649778	-0.5926712	1.0959314
O	1.5833455	-0.6691213	1.2164035
H	-0.2381257	-1.4566785	0.5208152
C	-0.2061297	0.7135970	0.3665700
H	-0.3258555	-0.6010561	2.0947798
C	0.4362748	0.7141346	-1.0368398
C	0.3105832	1.9179084	1.1817870
C	-1.7415017	0.7800865	0.2432141
H	1.5309745	0.6092350	-0.9589317
H	0.2084803	1.6538062	-1.5716622
H	0.0539736	-0.1262888	-1.6454624
H	-2.1355999	-0.0766171	-0.3339841
H	-2.0474302	1.7058033	-0.2761255
H	-2.2258489	0.7752149	1.2370420
H	1.4020421	1.8488580	1.3213592
H	-0.1615723	1.9480612	2.1810320
H	0.0789450	2.8672964	0.6663606
H	1.7995073	-1.4894914	1.6909589

MeOAc

H	1.5791957	-0.1301082	0.7079103
C	1.0700952	-0.2308626	-0.2658568
H	1.3593357	0.6400795	-0.8783674
H	1.3804311	-1.1618577	-0.7596467
C	-0.4297437	-0.2427988	-0.0632179
O	-1.1895578	-1.1371141	-0.3774367
O	-0.8405468	0.9086644	0.5353877
C	-2.2574663	1.0032527	0.7757236
H	-2.4129141	1.9775669	1.2604521
H	-2.5952795	0.1833225	1.4321047
H	-2.8164475	0.9471844	-0.1737936

cat-A-p

Au	-0.8113495	-0.4055956	-0.4772301
C	-3.0053323	2.1911339	-2.9938493
C	-2.2384769	2.5928083	-1.8550459
C	-2.9276176	3.0097526	-0.6611196
C	-4.3527675	3.0144626	-0.6549942
C	-5.0725846	2.6034023	-1.7671115
C	-4.3952935	2.1869098	-2.9448310
C	-2.1486152	3.3805966	0.4761985
C	-0.7719092	3.2650208	0.4621890
C	-0.0879568	2.7758944	-0.6913773
C	-0.8151078	2.5076510	-1.8425712
C	1.3956578	2.4166299	-0.5310421
C	1.9326900	1.5642017	-1.7308211
O	2.1756803	2.5012938	-2.7627819
C	2.0020653	2.0763827	-4.1120586
O	1.4723108	1.6087672	0.6937445
P	0.9597901	0.0488252	0.8026469
O	2.3344254	-0.7590714	0.4229476
C	2.9414897	-0.7770520	-0.9246126
C	2.0090687	-1.5925262	-1.8251843
C	1.8264317	-1.3077230	-3.1707833
C	0.8517729	-1.9964713	-3.9509850
C	0.0714593	-3.0422056	-3.3397309
C	0.3397698	-3.3778646	-1.9801960
C	1.2788595	-2.6769278	-1.2442527
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C	-1.1581317	-3.3354508	-5.4305409
C	-0.3845300	-2.3081083	-6.0361857
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C	2.4577262	-1.1297498	4.0753883
C	2.1515296	-1.3138256	5.4358223
C	2.5287421	-2.4923300	6.0996987
C	3.2253039	-3.4959931	5.4143199
C	3.5445297	-3.3180714	4.0585260
C	3.1590529	-2.1474850	3.3947597
C	-0.4509462	-0.6276447	3.0542776
C	-1.4536232	0.5333736	3.1255459
C	-0.9929427	-1.9004859	2.3919132
C	-2.3270715	-2.0207031	1.9538284
C	-2.7796684	-3.2080877	1.3538444
C	-1.9076391	-4.2905767	1.1802843
C	-0.5799365	-4.1840834	1.6250696
C	-0.1295738	-3.0029886	2.2252695
C	1.7893676	1.3723207	4.1336753
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C	2.0845775	4.8147606	-1.0474173
C	2.9061157	5.9119338	-0.8704881
C	3.9631810	5.8969976	0.0871718
C	4.1542549	4.7101080	0.8815272
C	3.2914371	3.5949545	0.6761264
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C	6.0313563	5.7822174	2.0184116
C	5.8433676	6.9526197	1.2344624
C	4.8305772	7.0092910	0.2906856
C	3.2022766	0.7103190	-1.3769079
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C	5.1378949	1.5844186	-2.4666760
C	4.3056330	-1.4405651	-0.7115407
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C	6.3431863	-1.6769935	0.6351678
C	6.8649806	-2.6213878	-0.3208687
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C	4.8288812	-2.3667670	-1.6560964
C	8.1444960	-3.2041591	-0.0854015
C	8.8748719	-2.8721933	1.0436233
C	8.3581673	-1.9434375	1.9882284
C	7.1192245	-1.3584072	1.7887305
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H	1.0449395	1.5298597	-4.2451516
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H	5.6965994	1.4525503	-3.4054602
H	-0.1631775	-0.9089503	4.0840607
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H	-2.3363954	0.2538645	3.7249645
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H	-2.2626864	-5.2175437	0.7175411
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H	1.5519199	2.2175740	3.4679296
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H	1.6235074	-0.5346795	5.9949855
H	2.2816448	-2.6204493	7.1587718
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H	4.6845603	7.9120467	-0.3126940
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H	-4.1409838	-1.5159479	-1.0860663
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Au	2.2665059	-1.2180559	5.3372015
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C	2.2721187	-6.3070332	7.2157770
C	3.3308311	-5.5374231	7.7688631
C	2.3095662	-5.0804206	3.6554702
C	2.9467038	-4.1179369	2.8959207
C	3.9630871	-3.2912781	3.4621761
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C	4.4347273	-2.0896703	2.6325072
C	5.3370058	-1.1111466	3.4531075
O	6.6085244	-1.7296740	3.4817961
C	7.4335433	-1.5273148	4.6257482
O	3.2121307	-1.3787962	2.2375004
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C	4.3208516	1.4586445	5.0013008
C	5.3914418	1.0848772	5.8003402
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C	5.0040402	0.9651654	10.0376726
C	6.2197582	0.5579041	9.4243518
C	6.3600311	0.6096739	8.0464588
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C	5.4811282	-2.2165335	-1.0786634
C	4.8234465	-1.8556006	0.1330238
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C	6.8240722	-2.9745416	-3.4512031

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C	4.1606450	2.9627109	1.5171753
C	4.4074863	4.1952778	0.8504395
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C	5.3885727	3.7326609	3.4665835
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C	4.1675242	5.6695356	-1.0805275
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H	7.8786157	-0.5172522	4.6322630
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H	7.6481931	-0.2360516	1.5826610
H	8.4869811	1.2377038	2.2028746
H	-0.0817733	-0.9235236	4.1645040
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H	2.6549226	-3.9525094	1.8544457
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Au	-1.5292199	-1.4716125	0.6103348
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C	-6.2932585	-2.9451656	1.9970416
O	-6.7391777	-3.0456529	0.6575696
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C	-3.4515046	-1.6166548	-0.7067515
C	-3.7822755	-3.0614031	-1.0426970
C	-3.2751062	-0.6633756	-1.8779352
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H	-4.8815750	-3.1166565	-1.1431413
H	-3.4902542	-3.7497264	-0.2371132
H	-3.3048169	-3.3675904	-1.9852956
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C	-3.1923149	2.4906948	1.0822023
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C	-4.7984154	2.8536145	2.9213843
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C	-5.4847332	3.1970112	0.6106569
C	-2.4628787	2.1006330	3.4012905
C	-1.1994863	1.7725660	2.9495846
C	-0.8873436	1.7923784	1.5545211
C	-1.8779955	2.1451952	0.6489862
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C	-0.7922438	-3.0740566	-3.3478975
C	-0.3939151	-3.6918237	-2.1277150
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C	-1.5588824	-1.7426289	-5.7271430
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C	2.1873087	-1.9181098	3.6675783
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C	-1.2611772	-1.8356305	4.3649549
C	-0.8845156	-3.8556876	2.7965597
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C	-1.9553581	-5.8761078	1.1316667
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H	4.4448803	-6.8610583	4.0171028
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H	-0.4150511	1.4958636	3.6597135
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H	-5.0178292	2.8554189	3.9938086
H	-6.7739421	3.4932447	2.3446302
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H	-3.9933898	2.8536175	-0.9104399
H	-1.6620368	2.1883078	-0.4198755
H	3.1835940	-2.3600767	-2.9714259
H	5.5261148	-3.0425862	-3.3815701
H	7.8919292	-3.2811580	-2.5771475
H	9.5821351	-2.9778526	-0.7763787
H	8.9232528	-1.9764528	1.4200380
H	6.5696206	-1.2713246	1.8228058
H	4.2409118	-1.0324121	1.0077077
H	0.8187722	-3.5858210	-0.3610285
H	-0.8225003	-4.6607108	-1.8492710
H	-2.1808940	-4.6294074	-3.9759052
H	-2.8676932	-3.4546817	-6.0609554
H	-1.8653301	-1.2393831	-6.6499558
H	-0.1657341	-0.1944161	-5.1603184
H	1.2120867	-0.2653745	-3.0947523
H	-6.5793633	-3.9820288	0.3964320
H	-5.7365231	1.1825213	6.2785161
C	-5.5996140	0.1972871	5.8188531

C	-4.8996207	-0.8075714	6.5060223
H	-4.4830697	-0.6114501	7.4995900
C	-4.7607175	-2.0690671	5.9154203
H	-4.2388944	-2.8714682	6.4484461
C	-5.2964627	-2.3201591	4.6406496
H	-5.1769306	-3.3194309	4.2131859
C	-5.9874509	-1.3179865	3.9336355
C	-6.1407885	-0.0603914	4.5545797
H	-6.7075594	0.7219979	4.0393110
H	-8.2004571	-0.1279513	0.6883385
C	-8.7547447	-0.5608096	1.5250716
C	-10.1488498	-0.4020084	1.5636993
H	-10.6509225	0.1549419	0.7650514
C	-10.8966404	-0.9532094	2.6117984
H	-11.9840198	-0.8271877	2.6414702
C	-10.2380452	-1.6659512	3.6251439
H	-10.8088118	-2.0999210	4.4532301
C	-8.8468742	-1.8179831	3.5865716
H	-8.3418339	-2.3643592	4.3913049
C	-8.0817356	-1.2680276	2.5370818
H	-4.9814639	-5.7903169	-1.4244456
C	-5.6905823	-6.4032187	-0.8472104
H	-6.6100739	-6.5442807	-1.4466511
H	-5.2272393	-7.3886861	-0.6516433
O	-5.9481113	-5.6936631	0.3717783
H	-6.5278962	-6.2409599	0.9326413

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Au	0.8460947	-0.5615136	0.3565316
C	3.6548739	-0.6037704	0.3206495
C	2.7331299	-0.7494781	1.3136782
C	4.9543030	0.1165668	0.4989007
H	5.2114151	0.1422882	1.5699055
H	4.8214663	1.1642447	0.1688546
C	6.1117401	-0.5428520	-0.3082680
C	6.3693522	-1.9451186	0.3457656
O	6.6010466	-1.8545166	1.7297218
H	7.2056385	-2.4474841	-0.1814069
H	5.4628672	-2.5659220	0.2070050
C	2.7640329	-0.8583361	2.6875096
C	3.6636351	-1.8836676	3.3209665
C	1.8850767	-0.0528950	3.5929688
H	2.5463980	0.5444583	4.2509549
H	1.2880124	-0.6995707	4.2583340
H	1.2154361	0.6190565	3.0369124
H	4.6542954	-1.9137249	2.8258284
H	3.2056960	-2.8831872	3.1959345
H	3.7720318	-1.7083130	4.4035489
H	3.4058919	-0.9064866	-0.7042173
C	3.2474844	3.2713116	2.0499916
C	2.3697075	3.1339774	0.9349727
C	2.8956955	3.3311693	-0.3911658
C	4.2681843	3.6843367	-0.5448356
C	5.0944273	3.8213293	0.5607582
C	4.5808028	3.6052569	1.8681179
C	2.0108183	3.1855488	-1.5005141
C	0.6785263	2.8750290	-1.3116543
C	0.1471641	2.6751455	-0.0007121
C	0.9878984	2.8161826	1.0947330
C	-1.3377028	2.3009945	0.0999573
C	-1.7441293	1.6769216	1.4802126
O	-1.7959957	2.7522373	2.3962409
C	-1.5416899	2.4644234	3.7689815
O	-1.5929573	1.2990201	-0.9322015
P	-1.1149230	-0.2772389	-0.7937392
O	-2.4776408	-0.9412414	-0.1503829
C	-3.0005220	-0.6611344	1.1958392
C	-2.1045868	-1.3762198	2.2100566
C	-2.0248710	-0.9660202	3.5339034
C	-1.1699157	-1.6242980	4.4632175
C	-0.3893386	-2.7548024	4.0265598
C	-0.5276687	-3.1887191	2.6770209
C	-1.3624827	-2.5239457	1.7968910
C	0.4998156	-3.3782783	4.9503417
C	0.6249545	-2.9001464	6.2454593
C	-0.1460389	-1.7859605	6.6772539
C	-1.0296942	-1.1669324	5.8070910
N	-1.2004153	-0.8299597	-2.3523831
C	-2.4774556	-0.6346077	-3.1237848
C	-3.0191675	-1.9869569	-3.5813465
C	-2.8520067	-2.4663685	-4.8932447
C	-3.3243382	-3.7384263	-5.2550727
C	-3.9792488	-4.5417848	-4.3123472
C	-4.1616921	-4.0676133	-3.0032975
C	-3.6811520	-2.8038752	-2.6406365
C	-0.0012132	-1.3919984	-3.0402520
C	1.0063899	-0.2981701	-3.4303356
C	0.6015922	-2.5440863	-2.2279878
C	1.9912697	-2.6934309	-2.0587887
C	2.5104560	-3.7419572	-1.2826056
C	1.6508317	-4.6673113	-0.6771269
C	0.2655353	-4.5497701	-0.8731774
C	-0.2530585	-3.5000293	-1.6402050
C	-2.3224750	0.4233733	-4.2232398
C	-2.2419430	3.4852866	-0.2461282
C	-1.9943822	4.7575319	0.3493349
C	-2.8380814	5.8240821	0.1020970
C	-3.9697370	5.6896782	-0.7558922
C	-4.2115840	4.4124252	-1.3764186
C	-3.3254741	3.3313004	-1.1009918
C	-5.3338257	4.2660028	-2.2433014
C	-6.1842300	5.3323239	-2.4850699
C	-5.9459477	6.5924615	-1.8725679
C	-4.8617889	6.7674464	-1.0275614
C	-3.1081144	0.8975238	1.3816949
O	-3.8977940	1.1284270	2.5329430
C	-4.8467519	2.1892498	2.3793539
C	-4.4290746	-1.2237762	1.1537442
C	-5.2428942	-0.8999948	0.0737910
C	-6.5709758	-1.3955986	-0.0359507

C	-7.0869600	-2.2391059	1.0133671
C	-6.2397916	-2.5412151	2.1181712
C	-4.9459533	-2.0522997	2.1876388
C	-8.4175549	-2.7397322	0.9029946
C	-9.2020895	-2.4247466	-0.1941060
C	-8.6912550	-1.5958375	-1.2309761
C	-7.4040046	-1.0923334	-1.1537900
H	-0.9427046	0.9658921	1.7842525
H	-3.6483433	1.2577852	0.4872963
H	-1.3182565	3.4301534	4.2487543
H	-0.6711127	1.7874321	3.8839879
H	-2.4186729	2.0028268	4.2536778
H	-5.5775494	1.9411005	1.5852185
H	-4.3420170	3.1419872	2.1357209
H	-5.3710037	2.2788093	3.3427996
H	-0.4124834	-1.8372631	-3.9650494
H	1.4853432	0.1389612	-2.5358233
H	0.4953817	0.5130310	-3.9706408
H	1.8003106	-0.6993295	-4.0821601
H	-1.3343886	-3.4088837	-1.7828627
H	-0.4171599	-5.2796971	-0.4248056
H	2.0562755	-5.4837100	-0.0701799
H	3.5944960	-3.8295306	-1.1564815
H	2.6874187	-1.9947088	-2.5308383
H	-3.1883664	-0.2401835	-2.3798034
H	-1.5862685	0.1280327	-4.9892225
H	-1.9957818	1.3762283	-3.7759237
H	-3.2898555	0.5814700	-4.7298043
H	-2.3598805	-1.8466723	-5.6498301
H	-3.1843357	-4.0969285	-6.2802545
H	-4.3528025	-5.5307662	-4.5978067
H	-4.6847970	-4.6815463	-2.2624785
H	-3.8135042	-2.4417476	-1.6164883
H	-3.5069263	2.3671716	-1.5837986
H	-5.5145421	3.2933079	-2.7154047
H	-7.0447252	5.2086905	-3.1510245
H	-6.6254100	7.4275003	-2.0728737
H	-4.6768972	7.7393699	-0.5568336
H	-2.6399402	6.7964284	0.5662099
H	-1.1312822	4.8778529	1.0084764
H	0.0095373	2.7697101	-2.1703437
H	2.4021276	3.3335214	-2.5130259
H	4.6599946	3.8592111	-1.5529702
H	6.1468258	4.0912916	0.4283982
H	5.2417078	3.7156734	2.7343789
H	2.8472181	3.1198650	3.0587140
H	0.5975516	2.7044159	2.1081752
H	-4.3138624	-2.3050724	3.0429605
H	-6.6251102	-3.1791868	2.9210411
H	-8.8098061	-3.3796063	1.7010567
H	-10.2224101	-2.8151715	-0.2684606
H	-9.3228594	-1.3588819	-2.0934840
H	-7.0064492	-0.4567395	-1.9532314
H	-4.8603833	-0.2634999	-0.7315179
H	-1.4528009	-2.8771028	0.7682076
H	0.0470118	-4.0543447	2.3296846
H	1.0877241	-4.2416205	4.6186011
H	1.3147048	-3.3840843	6.9448354
H	-0.0418488	-1.4222470	7.7047082
H	-1.6269315	-0.3099112	6.1379427
H	-2.6329168	-0.1249892	3.8741195
H	7.5564151	-1.6045943	1.8740342
H	4.6560520	1.4137572	-4.3261691
C	4.9227012	0.4837383	-3.8124683
C	4.8422559	-0.7440983	-4.4900588
H	4.5130587	-0.7798110	-5.5336872
C	5.2002069	-1.9207543	-3.8208394
H	5.1496992	-2.8847987	-4.3378490
C	5.6226653	-1.8761295	-2.4806419
H	5.8931104	-2.8149895	-1.9898357
C	5.6988231	-0.6540016	-1.7857775
C	5.3508304	0.5246734	-2.4812933
H	5.4208333	1.4887190	-1.9664455
H	6.8045916	1.4852792	1.5181023
C	7.6069467	1.2390205	0.8195327
C	8.8452364	1.8892458	0.9587460
H	8.9803530	2.6312683	1.7530651
C	9.9075147	1.5854926	0.0937230
H	10.8727054	2.0901541	0.2043939
C	9.7145230	0.6359419	-0.9244976
H	10.5312414	0.3962690	-1.6134862
C	8.4774089	-0.0055359	-1.0621788
H	8.3368089	-0.7413566	-1.8615046
C	7.4055401	0.2778029	-0.1890946
H	9.7519733	-3.2836694	1.7482014
C	10.0812951	-2.3039561	1.3676839
H	11.1388425	-2.1497170	1.6543264
H	10.0042217	-2.3029301	0.2626660
O	9.2303414	-1.3217174	1.9636169
H	9.4686721	-0.4399096	1.6151908

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C	-4.4132717	-1.3988809	-2.0048758
C	-3.2846214	-0.7731856	-1.4001852
C	-3.4678076	0.4926731	-0.7380437
C	-4.7667923	1.0792371	-0.7150841
C	-5.8432776	0.4419078	-1.3128708
C	-5.6665725	-0.8101774	-1.9592878
C	-2.3295206	1.1223175	-0.1525138
C	-1.0780611	0.5454952	-0.2345630
C	-0.8863655	-0.7124262	-0.8853440
C	-1.9799976	-1.3519249	-1.4513143
C	0.5490848	-1.2482107	-0.9237570
C	0.6867372	-2.7622453	-1.3110353
O	0.3846426	-2.8575926	-2.6867953
C	-0.1590902	-4.0932564	-3.1388036
O	1.0966082	-1.0925682	0.4253179
P	0.7744437	-2.1485422	1.6541017
O	2.0493624	-3.1720270	1.5081012
C	2.3046455	-4.0770077	0.3773492

C	1.4288566	-5.3170568	0.5644398
C	1.0775640	-6.1379112	-0.4992540
C	0.3686814	-7.3572483	-0.2948404
C	0.0317787	-7.7601806	1.0468928
C	0.4106021	-6.9051940	2.1231499
C	1.0821161	-5.7183308	1.8920762
C	-0.6860232	-8.9753766	1.2436108
C	-1.0604313	-9.7582487	0.1627195
C	-0.7271078	-9.3624519	-1.1613623
C	-0.0245794	-8.1891005	-1.3848006
N	1.1997846	-1.3128279	3.0180174
C	2.6072408	-0.7988625	3.1623697
C	3.2522568	-1.4195286	4.3988004
C	3.3428789	-0.7423264	5.6282624
C	3.8895570	-1.3766353	6.7553311
C	4.3621340	-2.6921480	6.6634889
C	4.2895469	-3.3720302	5.4371271
C	3.7364425	-2.7423457	4.3160032
C	0.1713428	-0.9152946	4.0233439
C	-0.7432195	0.2017425	3.4963159
C	-0.5769510	-2.1363956	4.5707549
C	-1.9539900	-2.0995678	4.8631738
C	-2.5995908	-3.2278323	5.3928820
C	-1.8890834	-4.4121884	5.6242279
C	-0.5137291	-4.4541935	5.3451706
C	0.1363203	-3.3249060	4.8348646
C	2.6720126	0.7306587	3.0751693
C	1.4299063	-0.3853492	-1.8306721
C	0.9859072	-0.0779046	-3.1514069
C	1.7967210	0.6339116	-4.0158274
C	3.0891412	1.0869005	-3.6155266
C	3.5316447	0.8000326	-2.2748376
C	2.6737764	0.0647565	-1.4069511
C	4.8188389	1.2511068	-1.8591775
C	5.6363484	1.9537910	-2.7292904
C	5.1990031	2.2386491	-4.0514777
C	3.9523992	1.8155387	-4.4844979
C	2.1303939	-3.2879113	-0.9707271
O	2.6228196	-4.1148037	-2.0079774
C	3.4258622	-3.4180801	-2.9683810
C	3.8036403	-4.4028922	0.5046423
C	4.6946809	-3.3616636	0.7392225
C	6.0953822	-3.5830472	0.8383372
C	6.5995429	-4.9238250	0.6774520
C	5.6678311	-5.9719689	0.4274515
C	4.3080794	-5.7229499	0.3444231
C	8.0045150	-5.1472608	0.7736306
C	8.8721641	-4.0956741	1.0176845
C	8.3738947	-2.7731345	1.1775606
C	7.0152369	-2.5224165	1.0905415
H	-0.0653703	-3.3419857	-0.7266388
H	2.7898421	-2.4085871	-0.8660198
H	-0.5864963	-3.8985350	-4.1349019
H	-0.9614924	-4.4492786	-2.4577533
H	0.6179877	-4.8733650	-3.2158844
H	4.3261737	-2.9942245	-2.4826215
H	2.8506616	-2.6096800	-3.4558283
H	3.7304201	-4.1647985	-3.7170418
H	0.7670390	-0.5141622	4.8646269
H	-1.4099910	-0.1731198	2.6990010
H	-0.1402305	1.0202527	3.0748812
H	-1.3727364	0.6148887	4.3004995
H	1.2114180	-3.3576792	4.6318884
H	0.0601135	-5.3674832	5.5366959
H	-2.3974396	-5.2923410	6.0320784
H	-3.6669626	-3.1663983	5.6282443
H	-2.5430280	-1.1959221	4.6850859
H	3.1392074	-1.2039224	2.2876199
H	2.1171251	1.2251712	3.8902613
H	2.2501640	1.0678616	2.1140538
H	3.7226381	1.0611117	3.1381279
H	2.9976658	0.2931480	5.7166260
H	3.9515233	-0.8353121	7.7052706
H	4.7940116	-3.1838013	7.5415199
H	4.6709193	-4.3951233	5.3516908
H	3.6753892	-3.2759389	3.3618092
H	3.0093939	-0.1410866	-0.3865660
H	5.1528883	1.0296720	-0.8387897
H	6.6242278	2.2936549	-2.4013569
H	5.8541721	2.7964479	-4.7287540
H	3.6149796	2.0361827	-5.5031206
H	1.4474320	0.8630678	-5.0285540
H	-0.0011903	-0.4180570	-3.4733212
H	-0.2097244	1.0457509	0.2033940
H	-2.4581157	2.0861748	0.3523146
H	-4.8996003	2.0498173	-0.2242043
H	-6.8365856	0.9017423	-1.2878746
H	-6.5265022	-1.3114779	-2.4129252
H	-4.2724240	-2.3541993	-2.5210403
H	-1.8594656	-2.3067265	-1.9675297
H	3.6154325	-6.5463398	0.1521342
H	6.0426973	-6.9934436	0.3011539
H	8.3879539	-6.1661083	0.6502596
H	9.9494085	-4.2788885	1.0889205
H	9.0725974	-1.9524423	1.3708311
H	6.6282874	-1.5045598	1.2152611
H	4.3223914	-2.3385131	0.8600647
H	1.3684255	-5.0822850	2.7319716
H	0.1573301	-7.1968802	3.1485236
H	-0.9392428	-9.2812391	2.2648206
H	-1.6111225	-10.6906200	0.3253825
H	-1.0238945	-9.9940034	-2.0051948
H	0.2387654	-7.8841723	-2.4039881
H	1.3867679	-5.8690365	-1.5113909
C	-6.3207443	-2.0028022	2.7943066
C	-6.6037686	-1.6104962	1.3030784
O	-7.1182052	-2.6899412	0.5602677
H	-7.2672280	-0.7234318	1.2718134
H	-5.6522012	-1.3209447	0.8225311
H	-8.1027342	-2.7412321	0.7137675
H	-4.8945728	-0.0651152	6.8395653
C	-4.9350979	0.0286570	5.7493540

C	-4.3331558	1.1268132	5.1135254
H	-3.8228505	1.8948134	5.7040933
C	-4.4004897	1.2336433	3.7184968
C	-5.0587303	0.2511470	2.9608796
H	-5.0899007	0.3632042	1.8738478
C	-5.6606430	-0.8597931	3.5848134
C	-5.5895798	-0.9497647	4.9916574
H	-6.0675248	-1.7956330	5.4985567
H	-7.3482506	-4.5395141	3.5105277
C	-8.0408837	-3.7161479	3.7015517
C	-9.3165531	-4.0156606	4.2085223
H	-9.5878277	-5.0576893	4.4085658
C	-10.2415936	-2.9918079	4.4504690
H	-11.2372508	-3.2251278	4.8413632
C	-9.8728464	-1.6578708	4.1979885
H	-10.5808533	-0.8455839	4.3933497
C	-8.5958418	-1.3633828	3.7023653
H	-8.3158074	-0.3204945	3.5177798
C	-7.6601690	-2.3882835	3.4368038
H	-3.9386999	2.0859169	3.2083609
Au	-1.3227846	-3.0537670	1.5342257
C	-4.0681825	-2.8304022	2.0319941
C	-3.3425366	-3.6761841	1.2500245
C	-5.3323768	-3.2094179	2.7420609
H	-5.7936550	-4.0554322	2.2054972
H	-5.0964561	-3.5454825	3.7691562
C	-3.5703835	-4.7619771	0.4359367
C	-4.6925749	-4.7356937	-0.5647444
C	-2.6467649	-5.9406485	0.4118929
H	-3.2301008	-6.8767316	0.4866245
H	-2.1014593	-5.9970195	-0.5492874
H	-1.9011939	-5.9006511	1.2201081
H	-5.4643372	-3.9862980	-0.3210729
H	-4.2804805	-4.5041516	-1.5662499
H	-5.1401320	-5.7432123	-0.6450295
H	-3.6842256	-1.8207782	2.2349082
H	-10.1544347	-4.3532997	-0.2993249
C	-10.3834619	-4.0763547	0.7418684
H	-11.4824810	-4.0365358	0.8626897
H	-9.9745530	-4.8519704	1.4185631
O	-9.7882790	-2.7963882	0.9718696
H	-9.9866374	-2.5197646	1.8887142

INT2-R-p

Au	-0.9689432	-0.5804191	-0.3386785
C	-3.1673421	-1.0309867	-0.5411122
C	-2.7016162	-0.6798222	-1.7761466
C	-3.9655884	-0.1164568	0.3771080
H	-4.0807145	0.8622480	-0.1121259
H	-3.4401308	0.0251517	1.3367639
C	-5.3714754	-0.7344048	0.6711818
C	-6.1025073	-0.9168246	-0.6997735
O	-6.0945723	0.2544896	-1.4757762
H	-7.1267691	-1.3055364	-0.5199305
H	-5.5688960	-1.6810050	-1.2935622
C	-2.6618545	-0.3746183	-3.0681562
C	-3.9393042	-0.4663947	-3.8858732
C	-1.4235631	0.0635540	-3.8042466
H	-1.5397503	1.1080953	-4.1487513
H	-1.2800014	-0.5559770	-4.7058971
H	-0.5172141	-0.0159003	-3.1848297
H	-4.0047950	0.4166387	-4.5476131
H	-4.8389391	-0.4838927	-3.2535962
H	-3.9060173	-1.3604070	-4.5360635
H	-3.1777794	-2.1036486	-0.2839065
C	-3.3997904	2.9178230	-2.0802477
C	-2.4755408	3.1038749	-1.0119269
C	-2.9432246	3.6907313	0.2175835
C	-4.3070640	4.0925306	0.3121498
C	-5.1856834	3.8792128	-0.7384717
C	-4.7298081	3.2779741	-1.9409548
C	-2.0195893	3.8387764	1.2958604
C	-0.7038875	3.4383839	1.1654850
C	-0.2267954	2.8728734	-0.0560748
C	-1.1067230	2.7141691	-1.1173804
C	1.2373295	2.4325520	-0.0890935
C	1.6855651	1.8097214	-1.4519811
O	1.6945958	2.8824493	-2.3669215
C	1.5353507	2.5870609	-3.7535588
O	1.3933622	1.4111655	0.9576270
P	1.0248541	-0.1790543	0.7751364
O	2.4016830	-0.7809090	0.1079217
C	2.9886869	-0.4711091	-1.2121144
C	2.1481123	-1.1495938	-2.2952585
C	2.2558408	-0.7737523	-3.6288529
C	1.4961898	-1.4226184	-4.6441384
C	0.6220841	-2.5122858	-4.2861352
C	0.5617242	-2.9068446	-2.9202488
C	1.3024554	-2.2479184	-1.9529397
C	-0.1619605	-3.1336358	-5.3017432
C	-0.0974429	-2.6906345	-6.6132178
C	0.7626149	-1.6144087	-6.9671096
C	1.5469411	-0.9987546	-6.0050011
N	1.1337502	-0.7292023	2.3337330
C	2.3027539	-0.2723282	3.1694404
C	3.1203874	-1.4642170	3.6604367
C	3.0095423	-1.9800100	4.9649794
C	3.7698686	-3.0928860	5.3590664
C	4.6588265	-3.6958652	4.4592570
C	4.7836358	-3.1838005	3.1580267
C	4.0147627	-2.0830792	2.7632250
C	0.1287849	-1.6702216	2.9114696
C	-1.1491370	-0.9460384	3.3559027
C	-0.0991488	-2.8614639	1.9745660
C	-1.3823418	-3.2784817	1.5717970
C	-1.5401719	-4.3692484	0.7003768
C	-0.4210539	-5.0698842	0.2339700
C	0.8616720	-4.6792151	0.6526632
C	1.0201067	-3.5848211	1.5099749
C	1.8543136	0.7131881	4.2549818

C	2.1819888	3.5685731	0.3045409
C	2.0298978	4.8463310	-0.3127767
C	2.9271924	5.8641887	-0.0477613
C	4.0194163	5.6743389	0.8503069
C	4.1596055	4.3959482	1.4987494
C	3.2189599	3.3670254	1.2058435
C	5.2411422	4.1938151	2.4054774
C	6.1505471	5.2080745	2.6574491
C	6.0126817	6.4697000	2.0175795
C	4.9691328	6.6983102	1.1348902
C	3.0760785	1.0868705	-1.3308846
O	3.9158522	1.3991343	-2.4232567
C	4.7522531	2.5408060	-2.2004556
C	4.4018618	-1.0626249	-1.0990114
C	5.2807597	-0.5446277	-0.1534618
C	6.5613387	-1.1179783	0.0725390
C	6.9598952	-2.2608273	-0.7098209
C	6.0525007	-2.7615009	-1.6862459
C	4.8079792	-2.1837104	-1.8750158
C	8.2371251	-2.8481103	-0.4707847
C	9.0795319	-2.3345665	0.5009934
C	8.6845235	-1.2088055	1.2752692
C	7.4533959	-0.6122989	1.0646289
H	0.9198358	1.0591219	-1.7575743
H	3.5528066	1.4288207	-0.3951001
H	1.2526335	3.5355308	-4.2360980
H	0.7348431	1.8415924	-3.9160328
H	2.4720755	2.2071540	-4.1941397
H	5.4534651	2.3494320	-1.3649441
H	4.1495866	3.4399636	-1.9783327
H	5.3239935	2.6914922	-3.1284602
H	0.6308334	-2.0705106	3.8104502
H	-1.6930758	-0.5368207	2.4864151
H	-0.9007813	-0.1071321	4.0231470
H	-1.8256736	-1.6328731	3.8902194
H	2.0230410	-3.2762122	1.8190002
H	1.7447725	-5.2247745	0.3045055
H	-0.5449881	-5.9232999	-0.4410422
H	-2.5492573	-4.6719106	0.4031524
H	-2.2766506	-2.7672915	1.9381658
H	2.9444053	0.2781836	2.4623369
H	1.1717745	0.2461918	4.9851682
H	1.3339432	1.5635020	3.7855478
H	2.7314133	1.0913112	4.8067768
H	2.3369753	-1.5113381	5.6910342
H	3.6713645	-3.4826227	6.3776956
H	5.2574427	-4.5576376	4.7726675
H	5.4845186	-3.6360008	2.4481583
H	4.1006579	-1.6989756	1.7424628
H	3.3238260	2.4027697	1.7101398
H	5.3424885	3.2205625	2.9000327
H	6.9795813	5.0422406	3.3533679
H	6.7372846	7.2634849	2.2268554
H	4.8616224	7.6716914	0.6436499
H	2.8042302	6.8399704	-0.5302021
H	1.2006174	5.0053234	-1.0061719
H	-0.0030630	3.5593101	1.9976257
H	-2.3692162	4.2823452	2.2347729
H	-4.6559522	4.5604634	1.2394855
H	-6.2406772	4.1519487	-0.6453757
H	-5.4375586	3.0955423	-2.7547100
H	-3.0443675	2.4716199	-3.0132771
H	-0.7660942	2.3020431	-2.0693091
H	4.1279592	-2.5960155	-2.6251140
H	6.3486640	-3.6266392	-2.2898085
H	8.5411942	-3.7147053	-1.0682482
H	10.0573339	-2.7947541	0.6775443
H	9.3613169	-0.8152131	2.0407734
H	7.1464387	0.2553031	1.6601300
H	4.9880714	0.3087667	0.4685201
H	1.2650040	-2.5986436	-0.9195636
H	-0.0819850	-3.7438171	-2.6287297
H	-0.8232728	-3.9625599	-5.0264050
H	-0.7069160	-3.1711101	-7.3856965
H	0.8053192	-1.2771017	-8.0079084
H	2.2125694	-0.1715934	-6.2758163
H	2.9438924	0.0277017	-3.9074135
H	-6.7149559	0.9276352	-1.0834128
H	-4.2719358	-3.1349343	4.5646632
C	-4.5831467	-3.1969112	3.5164675
C	-4.7800740	-4.4493214	2.9130291
H	-4.6208621	-5.3695795	3.4838505
C	-5.1907155	-4.5081940	1.5758467
H	-5.3584801	-5.4779766	1.0954705
C	-5.3942736	-3.3278458	0.8401295
H	-5.7180116	-3.4112226	-0.2010309
C	-5.1950251	-2.0643866	1.4300787
C	-4.7914672	-2.0232846	2.7833029
H	-4.6527478	-1.0516044	3.2711716
H	-4.7971003	1.8547293	1.6627715
C	-5.7840945	1.4868324	1.9479715
C	-6.6239394	2.3275480	2.7006684
H	-6.2689916	3.3208340	2.9948140
C	-7.9085511	1.9033718	3.0685921
H	-8.5627170	2.5594409	3.6520176
C	-8.3412437	0.6189816	2.6933310
H	-9.3357754	0.2672820	2.9867113
C	-7.5017360	-0.2136964	1.9452961
H	-7.8454464	-1.2166678	1.6701302
C	-6.2152340	0.2112117	1.5449002
H	-9.3416655	1.4912738	-1.8237502
C	-9.2457965	1.6764949	-0.7424031
H	-9.9473481	2.4824872	-0.4557512
H	-9.5134355	0.7526675	-0.1938898
O	-7.8869095	2.0594950	-0.5075296
H	-7.7565632	2.1952030	0.4518845

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C	2.1260542	4.3426585	1.8100834
C	1.3524824	3.9350582	0.6854400

C	1.9483225	3.9920818	-0.6244904
C	3.3026215	4.4160549	-0.7524851
C	4.0373381	4.7763588	0.3662892
C	3.4412779	4.7510267	1.6556183
C	1.1615176	3.5942914	-1.7464416
C	-0.1223847	3.1127072	-1.5789240
C	-0.6876434	2.9673413	-0.2741060
C	0.0320485	3.4133092	0.8269360
C	-2.0375389	2.2460414	-0.1724769
C	-2.3303768	1.6742417	1.2583388
O	-2.7190956	2.7769831	2.0470499
C	-2.5221854	2.6866224	3.4581610
O	-1.9755960	1.1001930	-1.0911303
P	-1.0596441	-0.2385730	-0.7963217
O	-2.1029366	-1.1951832	0.0302551
C	-2.8378477	-0.9203595	1.2794914
C	-1.8936987	-1.1910731	2.4527441
C	-2.1911320	-0.7416603	3.7341641
C	-1.3482530	-1.0452699	4.8411990
C	-0.1788853	-1.8626960	4.6355990
C	0.0929420	-2.3304728	3.3191642
C	-0.7367841	-2.0054651	2.2594053
C	0.6716359	-2.1457812	5.7440522
C	0.3871420	-1.6344268	7.0000164
C	-0.7649367	-0.8254738	7.2033061
C	-1.6166480	-0.5418970	6.1484461
N	-1.0396107	-1.0326075	-2.2511603
C	-2.3601632	-1.3926092	-2.8853166
C	-2.4134280	-2.8971782	-3.1354587
C	-2.2720820	-3.4603655	-4.4164877
C	-2.2977291	-4.8534460	-4.5904993
C	-2.4738069	-5.6983448	-3.4871293
C	-2.6251906	-5.1449648	-2.2056362
C	-2.5907427	-3.7573388	-2.0317351
C	0.1946376	-1.2490887	-3.0479497
C	0.7753037	0.0855248	-3.5529703
C	1.2206060	-2.1486461	-2.3468569
C	2.5274047	-2.2734840	-2.8636835
C	3.4702314	-3.1114968	-2.2513095
C	3.1240940	-3.8445370	-1.1067104
C	1.8200393	-3.7555980	-0.6021222
C	0.8757463	-2.9252386	-1.2238995
C	-2.6629847	-0.5008570	-4.0949565
C	-3.1984924	3.1068943	-0.6650896
C	-3.3022685	4.4572546	-0.2177253
C	-4.3801715	5.2384874	-0.5894683
C	-5.4106073	4.7250704	-1.4320658
C	-5.3000244	3.3679803	-1.9024360
C	-4.1788883	2.5862363	-1.4997877
C	-6.3193306	2.8454556	-2.7516744
C	-7.4031898	3.6263456	-3.1184170
C	-7.5121369	4.9650677	-2.6538623
C	-6.5365854	5.5027393	-1.8297141
C	-3.4140056	0.5375787	1.2112721
O	-4.3505990	0.6742492	2.2603516
C	-5.5074174	1.4396270	1.9051559
C	-4.0071753	-1.9172249	1.2102918
C	-4.8588224	-1.8713070	0.1113547
C	-5.9207593	-2.8002643	-0.0555778
C	-6.1243018	-3.8095596	0.9533811
C	-5.2484046	-3.8306881	2.0759088
C	-4.2154995	-2.9155378	2.2020822
C	-7.1859009	-4.7470985	0.7851525
C	-8.0053556	-4.6933356	-0.3300149
C	-7.8010263	-3.6998271	-1.3276167
C	-6.7814862	-2.7733166	-1.1931737
H	-1.3813519	1.2457601	1.6541400
H	-3.9410087	0.6043947	0.2432066
H	-2.5813099	3.7174530	3.8409147
H	-1.5290603	2.2608928	3.6972351
H	-3.3000727	2.0669102	3.9336369
H	-6.0631977	0.9414706	1.0868362
H	-5.2282453	2.4632406	1.5955105
H	-6.1409093	1.4794227	2.8040112
H	-0.1591693	-1.8225420	-3.9249055
H	1.1759617	0.6841883	-2.7157531
H	-0.0125285	0.6742221	-4.0481103
H	1.5865703	-0.0784963	-4.2799603
H	-0.1517233	-2.8952364	-0.8502191
H	1.5255521	-4.3423517	0.2748858
H	3.8675831	-4.4842024	-0.6210971
H	4.4848434	-3.1759083	-2.6575079
H	2.8217362	-1.7184027	-3.7596639
H	-3.1089828	-1.1720510	-2.1096283
H	-1.9284473	-0.6284815	-4.9080753
H	-2.6576436	0.5572663	-3.7869118
H	-3.6577164	-0.7488438	-4.5024188
H	-2.1511264	-2.8176522	-5.2946207
H	-2.1857983	-5.2763802	-5.5943696
H	-2.5003607	-6.7843585	-3.6252159
H	-2.7771328	-5.7966249	-1.3387551
H	-2.7124587	-3.3255769	-1.0333107
H	-4.0963097	1.5598844	-1.8682912
H	-6.2322354	1.8128857	-3.1096421
H	-8.1814746	3.2149333	-3.7696069
H	-8.3733394	5.5721827	-2.9517984
H	-6.6192123	6.5351995	-1.4726805
H	-4.4513074	6.2739655	-0.2389587
H	-2.5212832	4.8652267	0.4286297
H	-0.7122316	2.7985356	-2.4445112
H	1.5989930	3.6638551	-2.7478054
H	3.7607320	4.4339086	-1.7462786
H	5.0815062	5.0868605	0.2566310
H	4.0285754	5.0517355	2.5294070
H	1.6677981	4.3119869	2.8047347
H	-0.3917570	3.3443938	1.8313655
H	-3.5529059	-2.9631466	3.0700760
H	-5.3966184	-4.5940462	2.8475498
H	-7.3425868	-5.5127487	1.5529068
H	-8.8169758	-5.4185382	-0.4494019
H	-8.4559127	-3.6720918	-2.2047429
H	-6.6205477	-2.0075596	-1.9606477

H	-4.7097499	-1.1176976	-0.6696928
H	-0.5169603	-2.3962689	1.2650345
H	0.9765669	-2.9545308	3.1461702
H	1.5586684	-2.7691545	5.5853284
H	1.0483394	-1.8544045	7.8446664
H	-0.9778867	-0.4304906	8.2020202
H	-2.5067729	0.0778710	6.3031076
H	-3.0998627	-0.1590797	3.9011585
Au	0.9589331	0.2519785	0.2272475
C	3.1228711	0.7872464	0.4586671
C	2.5606529	0.8827350	1.6982902
C	3.9889189	-0.3656112	-0.0137331
H	4.1010951	-1.0782703	0.8134410
H	3.5212396	-0.9045190	-0.8519193
C	5.3991453	0.1425733	-0.4601970
C	6.0816598	0.8118200	0.7861388
O	6.0046137	0.0092574	1.9449224
H	7.1354303	1.0443847	0.5495503
H	5.5602065	1.7707093	0.9822121
C	2.4087002	1.1317145	2.9925818
C	3.6252397	1.5820248	3.7832456
C	1.0990552	1.0688833	3.7309287
H	1.1980961	0.4750310	4.6546822
H	0.8060704	2.0919602	4.0344420
H	0.2923091	0.6352786	3.1196850
H	4.5641371	1.3961385	3.2413444
H	3.5368314	2.6576441	4.0243224
H	3.6595580	1.0274495	4.7381367
H	3.1530393	1.7093416	-0.1488230
H	6.8929256	-0.4244849	2.0358092
H	3.3691928	1.8399792	-4.3787096
C	4.1702626	1.9581022	-3.6409025
C	5.0991841	3.0007952	-3.7713751
H	5.0328211	3.7021881	-4.6095053
C	6.1149328	3.1312130	-2.8146741
H	6.8504794	3.9380155	-2.9011718
C	6.2002565	2.2308563	-1.7416285
H	7.0141638	2.3556114	-1.0227893
C	5.2790656	1.1716351	-1.5989107
C	4.2647508	1.0572942	-2.5719312
H	3.5401439	0.2427372	-2.5005803
H	5.7394426	-2.2586152	0.8564834
C	6.2788487	-2.2388034	-0.0933694
C	7.0330204	-3.3590950	-0.4761208
H	7.0600290	-4.2396422	0.1756252
C	7.7401328	-3.3580540	-1.6886137
H	8.3227175	-4.2340745	-1.9915880
C	7.6869449	-2.2220109	-2.5082639
H	8.2325459	-2.2042134	-3.4576213
C	6.9355477	-1.1008104	-2.1227311
H	6.9060447	-0.2271285	-2.7797087
C	6.2174608	-1.0848978	-0.9100837
H	9.1625180	-1.4790422	3.5884983
C	9.0846296	-1.9836655	2.6128517
H	10.1001363	-2.2730776	2.2828638
H	8.4700164	-2.8979312	2.7322186
O	8.4888299	-1.0497735	1.7066995
H	8.3649029	-1.4924280	0.8434395

TS2-R-p

C	-3.0471597	2.2833030	-3.2667800
C	-2.1699737	2.7318270	-2.2378586
C	-2.6664916	3.6569818	-1.2527673
C	-4.0147316	4.1096070	-1.3486156
C	-4.8467491	3.6459658	-2.3564544
C	-4.3608999	2.7214241	-3.3205400
C	-1.7904224	4.0591350	-0.1989975
C	-0.4999868	3.5711245	-0.1226916
C	0.0012130	2.6588682	-1.1009879
C	-0.8278005	2.2610248	-2.1385136
C	1.4320152	2.1468413	-0.9081363
C	1.8649784	1.0658018	-1.9549880
O	2.0108175	1.7516768	-3.1795996
C	1.8360422	1.0045870	-4.3807676
O	1.5003256	1.5432323	0.4239353
P	0.9480470	0.0198166	0.7693176
O	2.2976911	-0.8787503	0.4528353
C	2.9560290	-1.0774604	-0.8451061
C	2.1237288	-2.0633286	-1.6672818
C	2.2593164	-2.1574503	-3.0469553
C	1.5091957	-3.1036723	-3.8029406
C	0.6139551	-4.0033683	-3.1193219
C	0.5151776	-3.9076904	-1.7023619
C	1.2462297	-2.9680181	-0.9970999
C	-0.1514195	-4.9304539	-3.8852010
C	-0.0487106	-4.9617172	-5.2668987
C	0.8316058	-4.0718956	-5.9422598
C	1.5976302	-3.1673633	-5.2249688
N	0.9904367	0.0094039	2.4310241
C	2.2517813	0.4256615	3.1338072
C	2.7376155	-0.6980267	4.0471115
C	2.5633529	-0.6732969	5.4430220
C	2.9961217	-1.7476889	6.2372461
C	3.6185976	-2.8550978	5.6468514
C	3.8062359	-2.8857629	4.2556868
C	3.3639484	-1.8197277	3.4637526
C	-0.2272221	-0.2867813	3.2297149
C	-1.2003708	0.9042735	3.2442124
C	-0.8592147	-1.6165668	2.8012423
C	-2.2516234	-1.7788934	2.6917151
C	-2.8096016	-3.0056918	2.3001620
C	-1.9789439	-4.0940728	2.0052039
C	-0.5874979	-3.9518950	2.1349166
C	-0.0343955	-2.7296882	2.5353326
C	2.1094558	1.8010613	3.7979038
C	2.4329551	3.3029412	-0.8928450
C	2.3651147	4.2939191	-1.9172119
C	3.2969731	5.3131763	-1.9708739
C	4.3433117	5.4106477	-1.0060171
C	4.4031488	4.4250682	0.0428291

C	3.4288128	3.3856997	0.0713112
C	5.4398149	4.5155735	1.0176077
C	6.3791912	5.5320553	0.9587997
C	6.3192768	6.5045907	-0.0756773
C	5.3224106	6.4454418	-1.0362243
C	3.1751862	0.3282840	-1.5031621
O	4.0690938	0.1642560	-2.5871822
C	5.0283208	1.2204460	-2.7038097
C	4.3368515	-1.6370838	-0.4630677
C	5.0978575	-0.9464106	0.4739139
C	6.3704481	-1.4151524	0.8992454
C	6.8889450	-2.6324627	0.3266526
C	6.0990403	-3.3142668	-0.6428401
C	4.8565790	-2.8356035	-1.0258067
C	8.1639875	-3.1063816	0.7555769
C	8.8911729	-2.4133683	1.7091335
C	8.3765292	-1.2149696	2.2774107
C	7.1433963	-0.7264436	1.8808784
H	1.0447918	0.3164677	-2.0393288
H	3.6610566	0.9388304	-0.7210367
H	1.6558295	1.7423991	-5.1782971
H	0.9659566	0.3235186	-4.3064769
H	2.7339384	0.4099198	-4.6192270
H	5.6758761	1.2547356	-1.8056368
H	4.5304201	2.1981965	-2.8384287
H	5.6413660	0.9877077	-3.5875224
H	0.1548435	-0.4373977	4.2569820
H	-1.6197770	1.0722335	2.2359838
H	-0.6734140	1.8228018	3.5412130
H	-2.0304368	0.7399208	3.9516792
H	1.0502556	-2.6261448	2.6362764
H	0.0733400	-4.8003283	1.9276394
H	-2.4084379	-5.0532812	1.6963404
H	-3.8999166	-3.0977633	2.2454302
H	-2.9270838	-0.9532098	2.9194740
H	2.9938360	0.5219257	2.3250854
H	1.3574239	1.8024047	4.6055573
H	1.8114784	2.5450552	3.0418707
H	3.0735258	2.1073560	4.2381841
H	2.0962898	0.1906776	5.9273463
H	2.8515544	-1.7122872	7.3222079
H	3.9633832	-3.6881668	6.2683315
H	4.3050578	-3.7396745	3.7849117
H	3.5036886	-1.8487657	2.3786617
H	3.4711606	2.6469892	0.8768348
H	5.4833782	3.7649541	1.8159323
H	7.1728925	5.5910379	1.7110421
H	7.0669795	7.3040075	-0.1102548
H	5.2747444	7.1956797	-1.8335169
H	3.2370313	6.0669029	-2.7639944
H	1.5701820	4.2298772	-2.6640839
H	0.1628384	3.8817869	0.6911372
H	-2.1577976	4.7664361	0.5529084
H	-4.3916686	4.8168531	-0.6035701
H	-5.8821634	3.9982283	-2.4137010
H	-5.0261194	2.3626809	-4.1132653
H	-2.6661458	1.5804805	-4.0138016
H	-0.4742311	1.5676534	-2.9033235
H	4.2680743	-3.3837471	-1.7660318
H	6.4862636	-4.2389070	-1.0847907
H	8.5595099	-4.0299123	0.3186412
H	9.8688679	-2.7865396	2.0313221
H	8.9620345	-0.6799214	3.0323801
H	6.7430158	0.1953123	2.3183149
H	4.7114723	-0.0249695	0.9229849
H	1.1586888	-2.9205345	0.0894820
H	-0.1589216	-4.5830487	-1.1639789
H	-0.8259531	-5.6177039	-3.3618770
H	-0.6419165	-5.6771802	-5.8462095
H	0.9050118	-4.1092705	-7.0341973
H	2.2794626	-2.4834824	-5.7426556
H	2.9662286	-1.5046751	-3.5636599
H	-5.2096357	-0.8423770	5.1663818
C	-5.5712233	-1.0441649	4.1528204
C	-6.2682930	-2.2306202	3.8777199
H	-6.4529970	-2.9610803	4.6717680
C	-6.7362540	-2.4626316	2.5787176
H	-7.2954916	-3.3758245	2.3487451
C	-6.5002074	-1.5238922	1.5605045
H	-6.8930242	-1.7477944	0.5647801
C	-5.7921810	-0.3338274	1.8188680
C	-5.3414796	-0.1092518	3.1368202
H	-4.8156346	0.8222511	3.3728424
H	-3.7727239	2.7408121	1.6606362
C	-4.8309033	3.0117460	1.7163530
C	-5.1796575	4.2692202	2.2314399
H	-4.3926653	4.9482825	2.5766060
C	-6.5238921	4.6584574	2.2984129
H	-6.7956354	5.6416911	2.6958352
C	-7.5207481	3.7738626	1.8595170
H	-8.5754429	4.0627912	1.9151065
C	-7.1718629	2.5130562	1.3593754
H	-7.9650748	1.8234213	1.0506794
C	-5.8218526	2.1180981	1.2689778
Au	-0.9998822	-0.5321725	-0.3230028
C	-3.8090838	-0.6704472	-0.5118714
C	-2.7440953	-0.8423517	-1.4684519
C	-3.9971682	0.6109427	0.2764720
H	-3.7126855	1.4763199	-0.3427489
H	-3.3337722	0.5821367	1.1533870
C	-5.4813600	0.7223329	0.7341349
C	-6.2267737	0.4515475	-0.5887925
H	-6.1988250	1.3489454	-1.2250588
H	-7.2669824	0.1143513	-0.4626437
O	-5.4790860	-0.5741026	-1.2901344
C	-2.6901995	-1.1402029	-2.7904069
C	-3.8838028	-1.3041280	-3.7146922
C	-1.3754383	-1.3199461	-3.5136807
H	-1.2273844	-0.5034657	-4.2475613
H	-1.3657086	-2.2620456	-4.0906101
H	-0.5147891	-1.3301038	-2.8255292
H	-3.7109369	-0.7460925	-4.6539139

H	-4.8244984	-0.9522332	-3.2787162
H	-3.9846734	-2.3683890	-4.0099345
H	-4.0147447	-1.5666524	0.0969757
H	-5.8692066	-1.5173331	-1.2640008
H	-5.4829876	-5.0058272	-1.1495173
C	-5.1755896	-3.9614341	-0.9711094
H	-5.0863886	-3.7943307	0.1121986
H	-4.2022590	-3.7600364	-1.4547557
O	-6.1973709	-3.0507921	-1.4392920
H	-6.3824811	-3.2373751	-2.3788011

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C	1.0297029	2.8880491	4.0300123
C	-0.0217131	2.0119307	3.6317308
C	-1.3645320	2.5256319	3.5613660
C	-1.6031536	3.8835658	3.9211554
C	-0.5581672	4.7130920	4.2955595
C	0.7714819	4.2137941	4.3408389
C	-2.4079417	1.6507031	3.1338089
C	-2.1355596	0.3444562	2.7810257
C	-0.8029530	-0.1671005	2.8293819
C	0.2242526	0.6558961	3.2662810
C	-0.6003805	-1.5983436	2.3233373
C	0.8975565	-1.9870095	2.0911434
O	1.4590649	-2.1597074	3.3747746
C	2.8674649	-1.9761825	3.5108305
O	-1.2874310	-1.6855710	1.0374324
P	-0.6930442	-1.0498403	-0.3716603
O	0.1704918	-2.3382435	-0.9375253
C	1.3421777	-2.9825824	-0.3212466
C	2.5672619	-2.0985754	-0.5634096
C	3.7338602	-2.2574779	0.1751414
C	4.8880677	-1.4638470	-0.0828805
C	4.8572559	-0.4989532	-1.1532475
C	3.6608019	-0.3751489	-1.9140573
C	2.5494193	-1.1494123	-1.6290757
C	6.0071430	0.3096110	-1.3895335
C	7.1357386	0.1818130	-0.5959326
C	7.1660969	-0.7675161	0.4625570
C	6.0687067	-1.5761724	0.7094264
N	-2.0310420	-1.1325839	-1.3507358
C	-2.8230508	-2.4113854	-1.3880564
C	-2.9209451	-2.9376068	-2.8184896
C	-4.0821337	-2.8012832	-3.6017578
C	-4.1148539	-3.2802644	-4.9213870
C	-2.9911178	-3.9115295	-5.4708309
C	-1.8307634	-4.0614044	-4.6948631
C	-1.7959218	-3.5726557	-3.3839397
C	-2.5104877	0.0436450	-2.1199675
C	-3.1671557	1.0907588	-1.2020585
C	-1.4199735	0.5978671	-3.0439783
C	-1.3668780	1.9605120	-3.3876880
C	-0.3861932	2.4489072	-4.2637769
C	0.5625530	1.5780994	-4.8155635
C	0.5062349	0.2121183	-4.5004297
C	-0.4766219	-0.2725855	-3.6283127
C	-4.1588188	-2.2636054	-0.6486883
C	-1.2901223	-2.6178367	3.2306629
C	-1.0846705	-2.5502864	4.6408497
C	-1.6434552	-3.4982045	5.4775817
C	-2.4447404	-4.5602944	4.9622694
C	-2.6725698	-4.6201390	3.5410554
C	-2.0811179	-3.6303105	2.7041286
C	-3.4787024	-5.6711087	3.0132558
C	-4.0338851	-6.6248720	3.8506369
C	-3.8090699	-6.5658016	5.2527757
C	-3.0323473	-5.5551843	5.7965084
C	1.0148248	-3.2657279	1.1863181
O	1.9970190	-4.1555542	1.6811702
C	1.4755017	-5.1492845	2.5695092
C	1.4230090	-4.3290333	-1.0611435
C	0.3123745	-5.1660893	-1.0459596
C	0.2868188	-6.3919873	-1.7644873
C	1.4541957	-6.7811775	-2.5152095
C	2.5870642	-5.9183454	-2.5002878
C	2.5735194	-4.7238037	-1.7985097
C	1.4254208	-8.0048340	-3.2475206
C	0.2942515	-8.8040262	-3.2435543
C	-0.8591632	-8.4166217	-2.5063996
C	-0.8625659	-7.2369532	-1.7821944
H	1.3965202	-1.1363100	1.5746342
H	0.0340505	-3.7730497	1.1832810
H	3.0544407	-1.8262563	4.5858597
H	3.2116834	-1.0858349	2.9498513
H	3.4246494	-2.8586206	3.1548142
H	0.7505854	-5.7982525	2.0398922
H	0.9866976	-4.6847958	3.4454528
H	2.3340764	-5.7544433	2.8975249
H	-3.2950204	-0.3722515	-2.7806828
H	-2.4111823	1.5723349	-0.5552461
H	-3.9093580	0.6051944	-0.5501373
H	-3.6816126	1.8729781	-1.7843168
H	-0.5181208	-1.3398586	-3.3963213
H	1.2292084	-0.4849259	-4.9378489
H	1.3309567	1.9576693	-5.4973636
H	-0.3730799	3.5150579	-4.5106193
H	-2.0948635	2.6652006	-2.9797018
H	-2.2056877	-3.1307914	-0.8260775
H	-4.8180610	-1.5175443	-1.1240332
H	-3.9715161	-1.9507229	0.3911494
H	-4.6945901	-3.2278794	-0.6395888
H	-4.9784788	-2.3290362	-3.1861349
H	-5.0262671	-3.1648929	-5.5175045
H	-3.0207719	-4.2915832	-6.4973480
H	-0.9508345	-4.5659868	-5.1079586
H	-0.8880116	-3.6851868	-2.7831983
H	-2.2671706	-3.6741042	1.6275986
H	-3.6515185	-5.7130415	1.9313970
H	-4.6499776	-7.4291362	3.4350177
H	-4.2548214	-7.3251233	5.9037858
H	-2.8598231	-5.5087791	6.8774521

H	-1.4771394	-3.4390666	6.5587977
H	-0.4725717	-1.7428133	5.0499559
H	-2.9388550	-0.3178193	2.4456311
H	-3.4351031	2.0302434	3.0917398
H	-2.6316793	4.2594820	3.9013041
H	-0.7512164	5.7565164	4.5642655
H	1.5883952	4.8822841	4.6292980
H	2.0515557	2.4977477	4.0783793
H	1.2490255	0.2840157	3.3227793
H	3.4537918	-4.0756934	-1.8146912
H	3.4794888	-6.2081366	-3.0656716
H	2.3133313	-8.3021761	-3.8163509
H	0.2826911	-9.7403344	-3.8111787
H	-1.7469571	-9.0575176	-2.5157808
H	-1.7504907	-6.9333171	-1.2163997
H	-0.5884932	-4.8752244	-0.4945010
H	1.6507499	-1.0425422	-2.2381537
H	3.6171192	0.3516091	-2.7329794
H	5.9807129	1.0405973	-2.2055910
H	8.0126207	0.8105027	-0.7830956
H	8.0655696	-0.8592690	1.0802714
H	6.0916224	-2.3107664	1.5225108
H	3.7753786	-3.0169336	0.9597048
H	-3.4547358	5.9943181	2.4566314
C	-2.8680457	6.4874131	1.6756847
C	-2.9301740	7.8792669	1.5260403
H	-3.5611754	8.4791025	2.1896389
C	-2.1923053	8.4932460	0.4993021
H	-2.2488218	9.5770630	0.3541406
C	-1.3889550	7.7193011	-0.3447446
H	-0.8352412	8.2082135	-1.1538283
C	-1.2897259	6.3190941	-0.1856022
C	-2.0574780	5.7123202	0.8253432
H	-2.0322326	4.6296845	0.9764559
H	0.9917604	6.4584039	-3.4476873
C	-0.0545912	6.1920127	-3.6233300
C	-0.5694424	6.3236925	-4.9235899
H	0.0794759	6.6903347	-5.7255885
C	-1.9011250	5.9861436	-5.1951668
H	-2.2992828	6.0839911	-6.2100448
C	-2.7237378	5.5297701	-4.1529739
H	-3.7690921	5.2712274	-4.3515706
C	-2.2125513	5.4123179	-2.8556492
H	-2.8692189	5.0790881	-2.0436720
C	-0.8673741	5.7279027	-2.5721103
Au	0.4253491	0.9459259	-0.0657928
C	0.5523071	3.7172415	0.4389464
C	1.5066245	2.6756463	0.5165836
C	-0.2352324	4.0231755	-0.8179904
H	0.2410246	3.5220649	-1.6758369
H	-1.2459254	3.5900984	-0.7262474
C	-0.3539487	5.5472931	-1.1357383
C	1.0953315	6.0484641	-0.9261797
H	1.7719096	5.5930160	-1.6677783
H	1.1784301	7.1478555	-1.0002029
O	1.5377340	5.5983499	0.3482769
C	2.7336859	2.5981538	1.0991690
C	3.5033143	3.8250964	1.5538967
C	3.4580930	1.2966900	1.3065187
H	4.4569635	1.3208076	0.8355978
H	3.6316672	1.1402215	2.3893427
H	2.9083956	0.4324715	0.8999104
H	3.9254488	4.3742619	0.6947721
H	2.8561525	4.5293080	2.0995850
H	4.3399184	3.5275768	2.2086288
H	0.0986456	4.0245446	1.3959668
H	1.1230107	6.1608927	1.0847156
H	2.0905990	8.3982657	2.3818751
C	0.9901955	8.4187637	2.3989403
H	0.6213472	9.0312479	1.5552951
H	0.6547203	8.8671234	3.3512923
O	0.5506102	7.0558885	2.2940209
H	-0.4275527	7.0278473	2.2811785

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Au	-0.9759398	0.8633483	-0.0306236
C	-4.0027938	1.0332999	-0.4412676
C	-2.7061364	1.6704137	-0.8501525
C	-4.2599900	-0.4125834	-0.8497415
H	-4.7265564	-0.4439185	-1.8452663
H	-3.3069775	-0.9680595	-0.8842732
C	-5.1759917	-0.9784162	0.2731830
C	-4.4074001	-0.4447107	1.4955083
H	-4.9893693	-0.3641681	2.4244124
O	-4.0609606	0.9199020	1.0852154
H	-3.4861036	-1.0260691	1.6659978
C	-2.7135227	2.6784567	-1.7730051
C	-3.9371929	3.1941907	-2.5044852
H	-1.3250386	3.3278332	-3.3010495
H	-1.4796322	4.4392951	-1.9207343
H	-0.5619337	2.9144858	-1.7308850
H	-3.9278595	4.2987583	-2.5459716
H	-3.9082471	2.8353545	-3.5508896
H	-4.8980741	2.8716327	-2.0742475
H	-4.8843740	1.6535494	-0.6650484
H	-3.3667363	1.6394956	1.6448498
H	-1.8064385	2.5624183	1.6886072
O	-2.6867122	2.6279181	2.1388091
C	-3.3268124	3.8885082	1.7812192
H	-4.3404550	3.8472763	2.2041948
H	-3.3687726	3.9948333	0.6841919
H	-2.7579284	4.7169358	2.2256830
C	-0.2106746	6.3015687	-0.0387741
C	0.3058219	5.2089408	0.7187427
C	0.0149367	5.1434317	2.1278398
C	-0.7568650	6.1836058	2.7253778
C	-1.2428591	7.2331955	1.9605252
C	-0.9733922	7.2880812	0.5659465
C	0.5271566	4.0396631	2.8722579
C	1.3067775	3.0719777	2.2662526
C	1.6170882	3.1383349	0.8720303

C	1.1164104	4.1956877	0.1260353
C	2.5426666	2.0578561	0.2930698
C	2.2990752	1.7683943	-1.2329149
O	2.9246008	2.8310106	-1.9301265
C	2.3762766	3.2230971	-3.1872203
O	2.2915777	0.8358549	1.0291531
P	0.9606636	-0.1259583	0.8136974
O	1.6188176	-1.2200525	-0.2400678
C	1.9604982	-0.8941120	-1.6279922
C	0.6436747	-0.8179197	-2.4044765
C	0.3491164	0.1464782	-3.3564976
C	-0.9112079	0.1671349	-4.0251427
C	-1.8895801	-0.8430007	-3.7170298
C	-1.5396226	-1.8596043	-2.7793296
C	-0.3141696	-1.8489796	-2.1428986
C	-3.1557980	-0.7995211	-4.3684449
C	-3.4477480	0.1966912	-5.2876050
C	-2.4752025	1.1824866	-5.6072408
C	-1.2324315	1.1625520	-4.9930850
N	0.9918423	-0.9874469	2.2349395
C	2.3044936	-1.6119960	2.6411162
C	2.1271687	-3.1154210	2.8477218
C	2.2833374	-3.7320097	4.1007702
C	2.0635158	-5.1113390	4.2494571
C	1.6884968	-5.8884551	3.1465521
C	1.5370756	-5.2819676	1.8891949
C	1.7529402	-3.9087263	1.7432792
C	-0.1770417	-1.2953318	3.1005642
C	-1.0868736	-0.0820059	3.3435262
C	-0.9582956	-2.5218387	2.6300957
C	-1.2564551	-3.5542748	3.5353410
C	-1.9278452	-4.7084849	3.1078742
C	-2.3098416	-4.8439184	1.7662051
C	-2.0332781	-3.8101619	0.8595524
C	-1.3697561	-2.6561223	1.2923432
C	2.9188717	-0.8404634	3.8147111
C	4.0182562	2.3921634	0.5501769
C	4.5089247	3.7078175	0.3004531
C	5.8470623	4.0061423	0.4766630
C	6.7750440	3.0158491	0.9152611
C	6.2835978	1.6883737	1.1817286
C	4.8988022	1.4121409	0.9911851
C	7.1983660	0.6881792	1.6244365
C	8.5409129	0.9841301	1.7949999
C	9.0253850	2.2946644	1.5333772
C	8.1609634	3.2888790	1.1038878
C	2.8897194	0.3751327	-1.6735466
O	3.3622516	0.4706766	-3.0069782
C	4.7832367	0.6048503	-3.1126353
C	2.8146429	-2.0791720	-2.1034627
C	3.6268836	-2.7567226	-1.2048227
C	4.4599360	-3.8331538	-1.6220474
C	4.4773820	-4.2021548	-3.0148557
C	3.6483937	-3.4758674	-3.9198473
C	2.8347806	-2.4473075	-3.4797206
C	5.3166422	-5.2762951	-3.4315190
C	6.1006571	-5.9573237	-2.5143987
C	6.0776311	-5.5971318	-1.1393178
C	5.2736377	-4.5577231	-0.7020055
H	1.2015517	1.7859371	-1.4098872
H	3.7274465	0.1339936	-0.9940261
H	2.8852111	4.1608314	-3.4594208
H	1.2871536	3.4112401	-3.1093592
H	2.5621295	2.4634416	-3.9651919
H	5.2876736	-0.2981696	-2.7172065
H	5.1364217	1.5014208	-2.5698856
H	5.0075443	0.7057722	-4.1854692
H	0.2727196	-1.5576532	4.0733251
H	-1.6157327	0.2019872	2.4168682
H	-0.5054267	0.7890489	3.6903208
H	-1.8458655	-0.3362044	4.1008901
H	-1.1416653	-1.8654162	0.5670060
H	-2.3336913	-3.9068719	-0.1874898
H	-2.8214215	-5.7481957	1.4241927
H	-2.1314486	-5.5132057	3.8218973
H	-0.9219711	-3.4735836	4.5756839
H	2.9656499	-1.4780367	1.7689496
H	2.2686937	-0.8540402	4.7067391
H	3.0829260	0.2067216	3.5158524
H	3.8906452	-1.2792962	4.0974716
H	2.5765749	-3.1444593	4.9762295
H	2.1887830	-5.5768638	5.2329737
H	1.5156891	-6.9634469	3.2643243
H	1.2422040	-5.8797314	1.0208035
H	1.6083965	-3.4307956	0.7695976
H	4.5323285	0.4052224	1.2077460
H	6.8223228	-0.3216396	1.8251237
H	9.2358803	0.2082717	2.1328449
H	10.0887766	2.5155552	1.6731507
H	8.5334616	4.2994000	0.9026712
H	6.2100939	5.0209096	0.2805934
H	3.8163100	4.4828961	-0.0348904
H	1.7069412	2.2433154	2.8556933
H	0.3109049	3.9765636	3.9445556
H	-0.9551094	6.1429570	3.8024474
H	-1.8295913	8.0294923	2.4302498
H	-1.3585671	8.1242364	-0.0268178
H	0.0179633	6.3575656	-1.1089844
H	1.3596302	4.2826443	-0.9342776
H	2.2043485	-1.9029664	-4.1878594
H	3.6589855	-3.7484360	-4.9809486
H	5.3313814	-5.5565422	-4.4906284
H	6.7419868	-6.7806917	-2.8461807
H	6.6989178	-6.1485647	-0.4256573
H	5.2462567	-4.2822863	0.3584030
H	3.6293439	-2.4756178	-0.1485419
H	-0.0537208	-2.6394902	-1.4340332
H	-2.2560407	-2.6615675	-2.5723145
H	-3.8950489	-1.5762915	-4.1413206
H	-4.4238162	0.2182871	-5.7834202
H	-2.7089118	1.9532632	-6.3489838
H	-0.4763293	1.9136897	-5.2474352

H	1.0925848	0.8990343	-3.6225224
C	-1.4450758	3.3702818	-2.2038158
H	-6.1782000	-5.0455502	2.4118369
C	-5.8485999	-4.5538095	1.4908414
C	-5.7029806	-3.1617923	1.4623414
H	-5.9436697	-2.5804641	2.3588617
C	-5.2713947	-2.5047561	0.2935020
C	-5.0038043	-3.2782192	-0.8513228
H	-4.6732551	-2.7952491	-1.7759661
C	-5.1615240	-4.6722947	-0.8293631
H	-4.9547128	-5.2558752	-1.7327255
C	-5.5811557	-5.3148900	0.3429048
H	-5.7036471	-6.4026550	0.3618498
H	-7.0612896	-1.5921233	-1.5892659
C	-7.4167122	-0.8056998	-0.9142346
C	-8.6944299	-0.2671249	-1.1030102
H	-9.3173750	-0.6271425	-1.9285524
C	-9.1801602	0.7201151	-0.2322754
H	-10.1815041	1.1389875	-0.3747452
C	-8.3734985	1.1600940	0.8237942
H	-8.7405479	1.9278158	1.5133070
C	-7.0900613	0.6216929	1.0081799
H	-6.4796031	0.9999992	1.8336307
C	-6.5914738	-0.3697493	0.1428175

INT3-S-p

Au	-1.0475908	-0.4268443	-0.5393176
C	-4.0365372	-0.6688284	-1.0033751
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C	-4.2392827	0.6030620	-0.1839447
H	-4.7903459	1.3527845	-0.7707657
H	-3.2542493	1.0287603	0.0785586
C	-4.9934047	0.1653864	1.1038508
C	-4.2371839	-1.1352594	1.4139333
H	-4.7560150	-1.8535585	2.0617870
O	-4.1091389	-1.7676285	0.0938094
H	-3.2295619	-0.9300793	1.8077932
C	-2.6922032	-1.0805847	-3.0564953
C	-3.8979603	-1.2370661	-3.9631605
C	-1.3848274	-1.2096697	-3.7965146
H	-1.2845288	-0.4105160	-4.5570884
H	-1.3293892	-2.1674925	-4.3460858
H	-0.5230350	-1.1518164	-3.1124967
H	-3.8329092	-2.1896641	-4.5220780
H	-3.9039354	-0.4342285	-4.7252651
H	-4.8682935	-1.2070478	-3.4456171
H	-3.3210134	-2.5153542	-0.0350186
H	-4.9243236	-0.9010104	-1.6081609
H	-1.6178927	-3.0006752	-0.6703123
O	-2.4148269	-3.5067307	-0.3758195
C	-2.9017925	-4.3381723	-1.4548712
H	-2.2681137	-5.2337477	-1.5469219
H	-3.9241330	-4.6394425	-1.1821438
H	-2.9137349	-3.7801780	-2.4057691
C	-3.0780293	2.3828923	-3.3370689
C	-2.2073482	2.8005797	-2.2902906
C	-2.7176063	3.6784039	-1.2700549
C	-4.0733599	4.1128242	-1.3483140
C	-4.8999711	3.6780539	-2.3739629
C	-4.3983886	2.8032740	-3.3753020
C	-1.8429224	4.0696466	-0.2119077
C	-0.5417210	3.6105662	-0.1612840
C	-0.0292520	2.7341677	-1.1659187
C	-0.8544890	2.3534814	-2.2136993
C	1.4059333	2.2329759	-0.9718777
C	1.8515303	1.1417581	-1.9988416
O	2.0540098	1.8289229	-3.2147738
C	1.8709283	1.1170169	-4.4334167
O	1.4637101	1.6352574	0.3595586
P	0.8396409	0.1367502	0.7016286
O	2.1641250	-0.8157781	0.4367426
C	2.8704948	-1.0253980	-0.8251675
C	2.0691182	-2.0311048	-1.6567426
C	2.1156794	-2.0534205	-3.0429279
C	1.4149128	-3.0376161	-3.7978947
C	0.6592263	-4.0497967	-3.1066578
C	0.6604544	-4.0326015	-1.6794147
C	1.3366635	-3.0516224	-0.9754858
C	-0.0494578	-5.0212714	-3.8708508
C	-0.0309248	-4.9838741	-5.2569768
C	0.7095063	-3.9806013	-5.9386986
C	1.4234150	-3.0324479	-5.2231333
N	0.8566202	0.1403361	2.3682951
C	2.1374987	0.5082289	3.0606799
C	2.4760531	-0.5594555	4.1015392
C	2.7681840	-0.2513971	5.4419364
C	3.1010536	-1.2677754	6.3526915
C	3.1493531	-2.6033829	5.9340679
C	2.8588631	-2.9214188	4.5975773
C	2.5216263	-1.9090079	3.6937332
C	-0.3701507	0.1774957	3.2007590
C	-1.3089882	1.3323572	2.8000447
C	-1.1041362	-1.1599046	3.3104039
C	-2.1347466	-1.2779301	4.2670481
C	-2.8539386	-2.4711228	4.4079859
C	-2.5577963	-3.5741618	3.5909073
C	-1.5261664	-3.4738007	2.6485875
C	-0.8030847	-2.2777124	2.5151323
C	2.1158847	1.9558898	3.5701949
C	2.4002365	3.3945223	-0.9605635
C	2.3106128	4.3942222	-1.9745605
C	3.2304024	5.4241188	-2.0288254
C	4.2869601	5.5227922	-1.0752384
C	4.3716874	4.5255368	-0.0391621
C	3.4091018	3.4747789	-0.0098580
C	5.4200423	4.6162913	0.9230692
C	6.3464255	5.6447199	0.8643753
C	6.2616223	6.6289992	-0.1571532
C	5.2531933	6.5695863	-1.1055639
C	3.1339662	0.3726225	-1.5005214
O	4.0305366	0.1806870	-2.5773325

C	5.0382386	1.1933016	-2.6802344
C	4.2288768	-1.6275415	-0.4207391
C	4.7099004	-1.4773847	0.8717245
C	5.9689540	-2.0107151	1.2686897
C	6.7748808	-2.6976937	0.2932915
C	6.2653414	-2.8268953	-1.0324645
C	5.0275316	-2.3171005	-1.3809520
C	8.0368274	-3.2261284	0.6930420
C	8.4783565	-3.0871119	1.9993639
C	7.6766783	-2.4174701	2.9639761
C	6.4465635	-1.8898180	2.6068972
H	1.0208624	0.4080926	-2.1133659
H	3.6258620	0.9711278	-0.7127361
H	1.7398467	1.8787943	-5.2180091
H	0.9690301	0.4751580	-4.3935744
H	2.7491677	0.4914685	-4.6718573
H	5.6819013	1.1912364	-1.7794374
H	4.5842389	2.1923109	-2.8115027
H	5.6443357	0.9383403	-3.5625665
H	0.0068093	0.3898167	4.2172017
H	-1.7058841	1.1821442	1.7811146
H	-0.7649814	2.2897586	2.8121250
H	-2.1684905	1.4052001	3.4845358
H	0.0201644	-2.2201437	1.7985239
H	-1.2775467	-4.3281091	2.0124601
H	-3.1157913	-4.5097410	3.7022459
H	-3.6441166	-2.5426653	5.1634104
H	-2.3771529	-0.4268418	4.9126804
H	2.9083521	0.4534987	2.2728252
H	1.3788967	2.1055883	4.3776897
H	1.8699478	2.6325016	2.7375055
H	3.1078448	2.2346331	3.9632049
H	2.7451334	0.7850677	5.7917447
H	3.3246288	-1.0093605	7.3931868
H	3.4125933	-3.3940418	6.6444252
H	2.8980736	-3.9619451	4.2589444
H	2.2960235	-2.1558975	2.6521300
H	3.4728392	2.7265845	0.7852332
H	5.4839028	3.8560653	1.7105134
H	7.1494435	5.7036022	1.6066313
H	6.9994477	7.4375432	-0.1916661
H	5.1864559	7.3285097	-1.8931693
H	3.1531246	6.1852009	-2.8133360
H	1.5075094	4.3299666	-2.7128664
H	0.1207021	3.9130842	0.6555545
H	-2.2184406	4.7430464	0.5663534
H	-4.4551026	4.7984833	-0.5835877
H	-5.9408459	4.0145841	-2.4201137
H	-5.0578692	2.4709348	-4.1840244
H	-2.6840568	1.7218657	-4.1152934
H	-0.4881451	1.6953982	-3.0043206
H	4.6574904	-2.4428040	-2.4007826
H	6.8686361	-3.3513941	-1.7815913
H	8.6529305	-3.7471544	-0.0483323
H	9.4495393	-3.4973644	2.2957170
H	8.0360260	-2.3229756	3.9941084
H	5.8190533	-1.3818500	3.3481901
H	4.1139080	-0.9560255	1.6208528
H	1.3463005	-3.0677557	0.1172757
H	0.1379386	-4.8285170	-1.1364680
H	-0.6052755	-5.8079973	-3.3484155
H	-0.5793807	-5.7362956	-5.8332178
H	0.7202317	-3.9661622	-7.0334076
H	2.0013185	-2.2616122	-5.7449376
H	2.7155883	-1.3120587	-3.5733413
H	-4.0526933	4.4149924	2.9548689
C	-4.3416165	3.3745188	3.1387114
C	-4.4729524	2.4906619	2.0577611
H	-4.2753210	2.8528551	1.0456836
C	-4.8425796	1.1497277	2.2663202
C	-5.0921870	0.7165739	3.5837299
H	-5.4069345	-0.3157381	3.7697893
C	-4.9482896	1.5946369	4.6660971
H	-5.1398591	1.2375444	5.6834726
C	-4.5701770	2.9285281	4.4476097
H	-4.4625959	3.6164683	5.2924534
H	-6.8532586	2.0729286	0.5956007
C	-7.2911700	1.0709687	0.5245376
C	-8.6447841	0.9321693	0.1984681
H	-9.2516408	1.8239454	0.0101579
C	-9.2247461	-0.3437333	0.1226502
H	-10.2848706	-0.4548570	-0.1272678
C	-8.4359413	-1.4730579	0.3726664
H	-8.8761731	-2.4743453	0.3163924
C	-7.0766448	-1.3318474	0.6958710
H	-6.4832699	-2.2349035	0.8675587
C	-6.4857482	-0.0582472	0.7791478

TS3-R-p

Au	-0.9020553	0.8905757	0.1011120
C	-3.9859799	1.0385633	-0.1508113
C	-2.7175638	1.7453044	-0.6050309
C	-4.2711999	-0.3479865	-0.7151435
H	-4.7313777	-0.2917240	-1.7136260
H	-3.3308364	-0.9221506	-0.7858254
C	-5.2047982	-0.9672283	0.3644851
C	-4.4379975	-0.5104555	1.6275784
H	-5.0658029	-0.4157686	2.5269535
O	-3.9149122	0.8071607	1.3048812
H	-3.5969148	-1.1945436	1.8352886
C	-2.7469491	2.5556382	-1.7176322
C	-3.9524229	2.7369669	-2.6063548
H	-1.2017979	2.9563082	-3.1493788
H	-1.7762090	4.3977324	-2.2821064
H	-0.7055277	3.2180356	-1.4476175
H	-4.1383815	3.8094462	-2.7988114
H	-3.7352772	2.2738173	-3.5881213
H	-4.8729722	2.2780066	-2.2167813
H	-4.8687754	1.6864154	-0.3105132
H	-3.2441103	2.1429508	1.9340490
H	-2.3812562	2.5392614	0.6122686

O	-2.6891558	2.9687684	1.7121748
C	-3.5349537	4.1449957	1.5896987
H	-3.8478264	4.4494355	2.5990810
H	-4.4128024	3.9264163	0.9578410
H	-2.9178281	4.9333694	1.1387755
C	-0.3547226	6.1786232	0.0429554
C	0.2440810	5.1259721	0.7963264
C	-0.0000372	5.0614181	2.2140149
C	-0.8157460	6.0593028	2.8220722
C	-1.3751253	7.0772460	2.0641845
C	-1.1482525	7.1333089	0.6618477
C	0.6065333	4.0058009	2.9565494
C	1.4103065	3.0691091	2.3375037
C	1.6559063	3.1218112	0.9302885
C	1.0861266	4.1468461	0.1892975
C	2.5807257	2.0539588	0.3283386
C	2.3201371	1.7740366	-1.1962167
O	2.9221725	2.8494263	-1.8937372
C	2.3460882	3.2417850	-3.1368841
O	2.3405818	0.8202543	1.0563975
P	1.0137390	-0.1416574	0.8413857
O	1.6494740	-1.2200953	-0.2345167
C	1.9865972	-0.8799841	-1.6200795
C	0.6684981	-0.7863563	-2.3932010
C	0.4153287	0.1505767	-3.3836931
C	-0.8316705	0.1781125	-4.0767007
C	-1.8464118	-0.7871425	-3.7414859
C	-1.5441249	-1.7700977	-2.7525869
C	-0.3254126	-1.7742882	-2.1029271
C	-3.0943319	-0.7444560	-4.4281299
C	-3.3313514	0.2033070	-5.4124549
C	-2.3247204	1.1470998	-5.7550289
C	-1.1013919	1.1320254	-5.1018919
N	1.0298794	-1.0191758	2.2470995
C	2.3360291	-1.6640334	2.6431063
C	2.1395315	-3.1673254	2.8312067
C	2.2975999	-3.8023901	4.0746126
C	2.0590674	-5.1802507	4.2069225
C	1.6632935	-5.9369824	3.0971882
C	1.5102121	-5.3118924	1.8491568
C	1.7450911	-3.9402197	1.7193952
C	-0.1413062	-1.3077131	3.1221300
C	-1.0298989	-0.0809001	3.3854600
C	-0.9433959	-2.5209014	2.6535845
C	-1.2296511	-3.5629000	3.5514294
C	-1.9289652	-4.7017306	3.1266495
C	-2.3503284	-4.8125787	1.7946306
C	-2.0840590	-3.7696921	0.8948703
C	-1.3933199	-2.6311848	1.3261485
C	2.9637167	-0.9138653	3.8234421
C	4.0561762	2.3915076	0.5736103
C	4.5345896	3.7123484	0.3266598
C	5.8712609	4.0203164	0.4970096
C	6.8090035	3.0354882	0.9274842
C	6.3296862	1.7028638	1.1907709
C	4.9461895	1.4161676	1.0055338
C	7.2544076	0.7088026	1.6264807
C	8.5950304	1.0154270	1.7935471
C	9.0675071	2.3309580	1.5351887
C	8.1932733	3.3193833	1.1122118
C	2.9189225	0.3884037	-1.6507605
O	3.3991192	0.4997866	-2.9797539
C	4.8182269	0.6628759	-3.0727706
C	2.8350598	-2.0632550	-2.1106659
C	3.6424499	-2.7551760	-1.2183796
C	4.4721514	-3.8297471	-1.6464351
C	4.4913213	-4.1824512	-3.0433565
C	3.6665419	-3.4427290	-3.9411212
C	2.8558887	-2.4161777	-3.4907694
C	5.3275026	-5.2547429	-3.4708017
C	6.1066513	-5.9495178	-2.5598919
C	6.0816541	-5.6055807	-1.1806565
C	5.2807192	-4.5682923	-0.7329732
H	1.2201519	1.7798009	-1.3630137
H	3.7531641	0.1385384	-0.9701922
H	2.8067063	4.2082641	-3.3945040
H	1.2492912	3.3746982	-3.0461913
H	2.5601941	2.5079248	-3.9326574
H	5.3368484	-0.2329489	-2.6794126
H	5.1492079	1.5621471	-2.5207120
H	5.0490521	0.7760363	-4.1429696
H	0.3161746	-1.5822575	4.0876508
H	-1.5998108	0.2104042	2.4853222
H	-0.4242402	0.7827396	3.7086764
H	-1.7589914	-0.3292422	4.1740276
H	-1.1827978	-1.8272396	0.6100732
H	-2.4206943	-3.8455162	-0.1428438
H	-2.8874703	-5.7026795	1.4544721
H	-2.1254125	-5.5129249	3.8353325
H	-0.8672838	-3.5008296	4.5836045
H	2.9970713	-1.5277531	1.7709294
H	2.3177060	-0.9317402	4.7182216
H	3.1372694	0.1353594	3.5374508
H	3.9319038	-1.3670051	4.0957030
H	2.6059403	-3.2306357	4.9553410
H	2.1852614	-5.6605411	5.1831957
H	1.4750464	-7.0106522	3.2024048
H	1.1985997	-5.8936731	0.9758179
H	1.5996506	-3.4475253	0.7532009
H	4.5884232	0.4057541	1.2209256
H	6.8875521	-0.3047295	1.8253438
H	9.2975877	0.2442473	2.1263741
H	10.1293677	2.5604106	1.6726617
H	8.5564588	4.3338087	0.9137631
H	6.2254090	5.0387938	0.3039733
H	3.8326680	4.4825147	-0.0010132
H	1.8742204	2.2711033	2.9225256
H	0.4342070	3.9514277	4.0371390
H	-0.9871775	6.0146695	3.9033904
H	-1.9912491	7.8449087	2.5440484
H	-1.5924268	7.9429688	0.0732984
H	-0.1648497	6.2315145	-1.0350987

H	1.2971069	4.2351902	-0.8780454
H	2.2281422	-1.8634215	-4.1946336
H	3.6774457	-3.7033401	-5.0052154
H	5.3436873	-5.5225775	-4.5330791
H	6.7455348	-6.7714506	-2.8998132
H	6.6988630	-6.1680199	-0.4720754
H	5.2517432	-4.3054279	0.3305759
H	3.6437027	-2.4875299	-0.1586841
H	-0.0992446	-2.5458360	-1.3624880
H	-2.2889282	-2.5388462	-2.5217689
H	-3.8623506	-1.4851025	-4.1773415
H	-4.2914547	0.2209007	-5.9385295
H	-2.5166663	1.8810033	-6.5445415
H	-0.3193486	1.8502232	-5.3736412
H	1.1877087	0.8668253	-3.6671955
C	-1.5344089	3.3253025	-2.1629907
H	-6.2263969	-5.1475296	2.2593322
C	-5.8955888	-4.6040542	1.3682275
C	-5.7506589	-3.2125368	1.4190143
H	-5.9878000	-2.6823262	2.3474291
C	-5.3176169	-2.4889333	0.2907106
C	-5.0498133	-3.1972157	-0.8957433
H	-4.7231511	-2.6613722	-1.7926252
C	-5.2028999	-4.5910242	-0.9529756
H	-4.9940736	-5.1224034	-1.8877199
C	-5.6227739	-5.2997107	0.1806442
H	-5.7423815	-6.3872153	0.1382439
H	-7.2362804	-1.6497096	-1.3401375
C	-7.5117366	-0.7943389	-0.7141031
C	-8.7694553	-0.2009492	-0.8786937
H	-9.4573009	-0.5922307	-1.6357698
C	-9.1525205	0.8803343	-0.0714902
H	-10.1381510	1.3408927	-0.1943467
C	-8.2632104	1.3605067	0.8979552
H	-8.5497635	2.2018415	1.5383322
C	-7.0016997	0.7667292	1.0586412
H	-6.3199030	1.1722140	1.8130643
C	-6.6051316	-0.3218240	0.2569178

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Au	-0.9995696	-0.5553252	-0.4312346
C	-4.0332443	-1.1078225	-0.6250048
C	-2.7565593	-1.2420707	-1.4450795
C	-4.2849055	0.2815721	-0.0249374
H	-4.8677648	0.9203266	-0.7059334
H	-3.3164602	0.7809868	0.1647845
C	-5.0079307	-0.0176372	1.3214498
C	-4.2090374	-1.2630217	1.7590154
H	-4.7468742	-1.9321593	2.4470566
O	-3.9443566	-2.0033492	0.5463476
H	-3.2528528	-0.9637152	2.2187550
C	-2.8101579	-1.3638885	-2.8168384
C	-4.1027910	-1.3779500	-3.6056843
C	-1.5574260	-1.4971911	-3.6365757
H	-1.4915422	-0.6654875	-4.3642022
H	-1.5710518	-2.4293010	-4.2319862
H	-0.6497982	-1.4831273	-3.0131422
H	-3.9504189	-1.7829308	-4.6192104
H	-4.4939345	-0.3494845	-3.7061707
H	-4.8913921	-1.9665654	-3.1061834
H	-2.8721111	-3.1440796	0.2925708
H	-4.9248091	-1.4440087	-1.1842357
H	-2.1349204	-2.4630820	-0.9759307
O	-2.2081348	-3.5630194	-0.3695961
C	-2.9055703	-4.5357948	-1.1855191
H	-3.0839949	-5.4377746	-0.5796908
H	-3.8642708	-4.1260358	-1.5483480
H	-2.2523143	-4.7747829	-2.0364110
C	-3.2626319	2.1652015	-3.4645133
C	-2.4046138	2.6101050	-2.4183656
C	-2.9457868	3.4626658	-1.3924323
C	-4.3219254	3.8291528	-1.4538433
C	-5.1366922	3.3627466	-2.4743848
C	-4.6011634	2.5266225	-3.4904940
C	-2.0767952	3.9062915	-0.3507519
C	-0.7511504	3.5222181	-0.3214113
C	-0.2096110	2.6671658	-1.3293516
C	-1.0300638	2.2331376	-2.3591697
C	1.2578863	2.2600923	-1.1699517
C	1.7248707	1.1474108	-2.1643141
O	1.8507168	1.7893891	-3.4154921
C	1.6651851	1.0135205	-4.5937363
O	1.4001384	1.7340664	0.1861857
P	0.8778597	0.2325777	0.6364310
O	2.2300459	-0.6692365	0.3520033
C	2.8947463	-0.9062775	-0.9333457
C	2.1117208	-1.9861602	-1.6846766
C	2.0996844	-2.0627118	-3.0707141
C	1.4176598	-3.1113164	-3.7524075
C	0.7516391	-4.1323651	-2.9854501
C	0.8049244	-4.0502509	-1.5633961
C	1.4578112	-3.0082453	-0.9315687
C	0.0666849	-5.1748597	-3.6760703
C	0.0158090	-5.1943038	-5.0616818
C	0.6626587	-4.1790668	-5.8176355
C	1.3563496	-3.1653627	-5.1759086
N	0.9438597	0.3217987	2.2945244
C	2.2271991	0.7844929	2.9267466
C	2.6556630	-0.2273003	3.9885334
C	2.8347703	0.1149960	5.3402626
C	3.2261721	-0.8561859	6.2767234
C	3.4470739	-2.1784707	5.8713906
C	3.2729015	-2.5293024	4.5226050
C	2.8758723	-1.5632363	3.5926627
C	-0.2461132	0.2755043	3.1808567
C	-1.3021800	1.3273602	2.7874163
C	-0.8461449	-1.1195269	3.3652597
C	-1.8103568	-1.3022604	4.3792994
C	-2.4207973	-2.5465843	4.5766418
C	-2.0820909	-3.6368360	3.7585878
C	-1.1085879	-3.4733658	2.7646905

C	-0.4893533	-2.2270663	2.5795300
C	2.1351252	2.2448940	3.3877089
C	2.1859466	3.4736144	-1.2467061
C	2.0091028	4.4236330	-2.2965680
C	2.8712259	5.4966145	-2.4256714
C	3.9534584	5.6900866	-1.5158914
C	4.1259940	4.7430423	-0.4439011
C	3.2215039	3.6465675	-0.3375214
C	5.1999049	4.9272285	0.4760047
C	6.0685996	5.9983901	0.3429750
C	5.8976486	6.9334602	-0.7139705
C	4.8622436	6.7829024	-1.6228851
C	3.0605886	0.4674972	-1.6808782
O	3.9286599	0.2621055	-2.7787448
C	4.8902383	1.3081251	-2.9595410
C	4.3000641	-1.4087012	-0.5571722
C	4.8763938	-1.0331579	0.6480751
C	6.1818499	-1.4619266	1.0196466
C	6.9345926	-2.2785045	0.1030802
C	6.3300351	-2.6326079	-1.1385806
C	5.0492655	-2.2191984	-1.4595768
C	8.2430711	-2.7041622	0.4758314
C	8.7802476	-2.3437383	1.7013186
C	8.0318139	-1.5458159	2.6094722
C	6.7586770	-1.1138331	2.2763380
H	0.9287244	0.3697533	-2.2183529
H	3.5494137	1.1284560	-0.9422795
H	1.4667055	1.7300865	-5.4061610
H	0.8007558	0.3268109	-4.4923287
H	2.5663083	0.4231055	-4.8359883
H	5.5629045	1.3710129	-2.0822375
H	4.3920656	2.2821528	-3.1172832
H	5.4770353	1.0388583	-3.8506723
H	0.1530420	0.5602302	4.1704284
H	-1.7282595	1.1091394	1.7931010
H	-0.8463528	2.3293266	2.7489508
H	-2.1370559	1.3468839	3.5058707
H	0.2996831	-2.1258773	1.8307818
H	-0.8156341	-4.3170240	2.1316613
H	-2.5594454	-4.6103458	3.9122244
H	-3.1628514	-2.6671606	5.3732785
H	-2.0907687	-0.4593767	5.0208338
H	2.9712496	0.7446929	2.1135883
H	1.3944103	2.3846723	4.1934407
H	1.8495402	2.8809006	2.5353755
H	3.1134381	2.5847647	3.7668183
H	2.6750520	1.1433271	5.6786820
H	3.3597062	-0.5734416	7.3261960
H	3.7552480	-2.9337997	6.6018688
H	3.4486339	-3.5593582	4.1954169
H	2.7358102	-1.8358724	2.5419938
H	3.3527020	2.9382526	0.4848535
H	5.3292854	4.2046039	1.2899317
H	6.8917786	6.1291615	1.0530506
H	6.5904288	7.7762951	-0.8072510
H	4.7294074	7.5033804	-2.4373947
H	2.7271749	6.2191044	-3.2364016
H	1.1857566	4.2874973	-3.0018418
H	-0.0920841	3.8686522	0.4803111
H	-2.4754610	4.5622846	0.4305073
H	-4.7290947	4.4907373	-0.6813690
H	-6.1927920	3.6490940	-2.5085420
H	-5.2490674	2.1810682	-4.3032741
H	-2.8432002	1.5361506	-4.2573039
H	-0.6386943	1.5926024	-3.1524242
H	4.6067761	-2.5175800	-2.4129989
H	6.8945779	-3.2530041	-1.8433338
H	8.8180260	-3.3238028	-0.2214797
H	9.7861802	-2.6766323	1.9778029
H	8.4666751	-1.2760833	3.5776178
H	6.1732526	-0.5078654	2.9773024
H	4.3212898	-0.4076499	1.3492175
H	1.4959456	-2.9697601	0.1593867
H	0.3162029	-4.8261523	-0.9653196
H	-0.4091360	-5.9733342	-3.0948059
H	-0.5124679	-6.0011412	-5.5804364
H	0.6201036	-4.2090356	-6.9112758
H	1.8665053	-2.3882679	-5.7562238
H	2.6424674	-1.3187955	-3.6557374
H	-4.1016573	4.4154907	2.7091457
C	-4.3618504	3.3929010	3.0037820
C	-4.5194433	2.4054843	2.0198086
H	-4.3721475	2.6677202	0.9696081
C	-4.8547140	1.0856836	2.3686173
C	-5.0464389	0.7811628	3.7319929
H	-5.3342887	-0.2328513	4.0289328
C	-4.8791039	1.7625318	4.7179926
H	-5.0274882	1.5040310	5.7719163
C	-4.5325996	3.0742825	4.3575099
H	-4.4061117	3.8429410	5.1269766
H	-7.0516670	1.7780589	1.0634081
C	-7.4033099	0.7514508	0.9154516
C	-8.7519156	0.5210323	0.6170776
H	-9.4400259	1.3686132	0.5294795
C	-9.2231409	-0.7888801	0.4422461
H	-10.2788943	-0.9711561	0.2160162
C	-8.3304328	-1.8614731	0.5637494
H	-8.6851745	-2.8891118	0.4298972
C	-6.9781129	-1.6290516	0.8592344
H	-6.2955341	-2.4817933	0.9304224
C	-6.4948938	-0.3189016	1.0444737

PRT-R-p

Au	-0.6234629	0.9619268	-0.5386944
C	-0.9596665	4.0598447	-0.5377773
C	-0.5227781	2.9694082	-1.4979072
C	0.1009755	4.4678070	0.4975638
H	-0.1138651	4.0618069	1.4958044
H	1.0903228	4.0916602	0.1956280
C	0.1292724	6.0214106	0.4545927
C	-0.1807634	6.2117869	-1.0521530

O	-1.2169606	5.2567062	-1.3322560
C	-1.4099323	2.2946224	-2.3454679
C	-2.9038576	2.5028708	-2.2759494
C	-0.8911481	1.5857228	-3.5755874
H	-1.3319022	0.5798665	-3.6742376
H	-1.2124371	2.1614847	-4.4646354
H	0.2070343	1.5126891	-3.5786624
H	-3.1314244	3.4663758	-2.7692724
H	-3.4361913	1.7025841	-2.8081119
H	-3.2864722	2.5746052	-1.2476597
H	0.5354237	2.9982317	-1.7991337
H	-1.9161271	3.7902241	-0.0630431
H	0.7159283	5.9942717	-1.6663114
H	-0.5762906	7.2050627	-1.3121968
C	3.0021419	3.0567597	-3.2502222
C	3.0155678	2.3680962	-2.0012967
C	3.3356198	3.1025282	-0.8041193
C	3.6356634	4.4919758	-0.9020901
C	3.6035979	5.1334490	-2.1306513
C	3.2838202	4.4129486	-3.3126105
C	3.3148262	2.4066111	0.4420879
C	2.9883918	1.0655225	0.5051443
C	2.6580720	0.3314409	-0.6767486
C	2.6901823	0.9827232	-1.9025874
C	2.3030365	-1.1518695	-0.5140626
C	1.4896034	-1.7451548	-1.7198241
O	2.4051938	-1.8893256	-2.7851350
C	1.8870273	-1.8119964	-4.1120110
O	1.4727285	-1.2629246	0.6858031
P	-0.1296698	-0.8834158	0.7515600
O	-0.8169368	-2.3194770	0.3564276
C	-0.7089971	-3.0246694	-0.9342058
C	-1.6223061	-2.3171522	-1.9358185
C	-1.4355083	-2.4320462	-3.3069489
C	-2.3152200	-1.7980838	-4.2316020
C	-3.4480012	-1.0573972	-3.7338367
C	-3.6415871	-0.9898784	-2.3237422
C	-2.7536039	-1.5921469	-1.4506912
C	-4.3137742	-0.4102900	-4.6638029
C	-4.0675532	-0.4820036	-6.0256461
C	-2.9511993	-1.2126717	-6.5171451
C	-2.0968886	-1.8607728	-5.6398207
N	-0.4306304	-0.8175305	2.3757821
C	0.0106009	-1.9724118	3.2379343
C	-1.1874437	-2.5553253	3.9830086
C	-1.4508684	-2.2697754	5.3354088
C	-2.5886502	-2.7961808	5.9680956
C	-3.4708633	-3.6224240	5.2595609
C	-3.2115568	-3.9216887	3.9125021
C	-2.0827537	-3.3879588	3.2796460
C	-1.0382424	0.3907624	3.0041940
C	-0.0199761	1.5349159	3.1271372
C	-2.3485692	0.7685488	2.3036738
C	-2.6586447	2.0954421	1.9517979
C	-3.8715512	2.4213696	1.3212696
C	-4.7977612	1.4083979	1.0370113
C	-4.5117062	0.0825483	1.4010604
C	-3.3002232	-0.2351637	2.0273774
C	1.2145863	-1.5988540	4.1103810
C	3.5417044	-2.0058464	-0.2328599
C	4.6992358	-1.8571248	-1.0527891
C	5.7954016	-2.6803485	-0.8747250
C	5.8072118	-3.6915992	0.1312242
C	4.6511548	-3.8273792	0.9795417
C	3.5367602	-2.9648394	0.7718616
C	4.6509996	-4.8289241	1.9941180
C	5.7424652	-5.6650143	2.1616119
C	6.8828668	-5.5316807	1.3240740
C	6.9153426	-4.5649379	0.3319456
C	0.8045193	-3.1064222	-1.3355422
O	0.9073349	-4.0394885	-2.3938622
C	2.0295062	-4.9222044	-2.2805993
C	-1.1796922	-4.4489961	-0.5990420
C	-0.5954629	-5.1058313	0.4786617
C	-0.9942116	-6.4150980	0.8627350
C	-2.0182453	-7.0810469	0.0968009
C	-2.5884983	-6.3946916	-1.0137927
C	-2.1866158	-5.1130030	-1.3525628
C	-2.4212798	-8.3938152	0.4818826
C	-1.8429895	-9.0180387	1.5748878
C	-0.8363647	-8.3579564	2.3330250
C	-0.4210924	-7.0840868	1.9848115
H	0.7037675	-1.0064574	-2.0004644
H	1.3203486	-3.5067053	-0.4445902
H	2.7522488	-1.6346215	-4.7697671
H	1.1686107	-0.9728023	-4.2137811
H	1.3862416	-2.7502558	-4.4037613
H	1.9403153	-5.5437573	-1.3684520
H	2.9790589	-4.3570618	-2.2551681
H	2.0036087	-5.5717194	-3.1685759
H	-1.3108073	0.0521576	4.0208160
H	0.2772987	1.9071566	2.1298700
H	0.8897817	1.1802216	3.6340474
H	-0.4323465	2.3767329	3.7088030
H	-3.0824095	-1.2712441	2.3051461
H	-5.2381060	-0.7121097	1.1989958
H	-5.7418644	1.6548436	0.5401240
H	-4.0833713	3.4596718	1.0349520
H	-1.9454826	2.8933452	2.1714596
H	0.3431591	-2.7371850	2.5170506
H	0.9750511	-0.8030249	4.8346030
H	2.0425586	-1.2528240	3.4708897
H	1.5510824	-2.4812389	4.6804911
H	-0.7647808	-1.6418349	5.9131711
H	-2.7796833	-2.5634699	7.0209301
H	-4.3537908	-4.0378150	5.7562971
H	-3.8867704	-4.5772656	3.3525393
H	-1.8898215	-3.6139165	2.2263405
H	2.6658123	-3.0678404	1.4251734
H	3.7702085	-4.9292498	2.6394471
H	5.7313499	-6.4334144	2.9418456
H	7.7392553	-6.1987822	1.4676737

H	7.7953942	-4.4610804	-0.3124779
H	6.6776628	-2.5597407	-1.5130784
H	4.7077049	-1.0898353	-1.8306015
H	2.9721214	0.5463395	1.4674353
H	3.5567804	2.9589894	1.3568119
H	3.8765461	5.0532257	0.0065557
H	3.8284955	6.2030463	-2.1883740
H	3.2676763	4.9324507	-4.2764560
H	2.7629827	2.4974321	-4.1618236
H	2.4698048	0.4398419	-2.8226058
H	-2.6454718	-4.6070718	-2.2059294
H	-3.3640390	-6.8960935	-1.6029853
H	-3.1975382	-8.9018781	-0.1007677
H	-2.1603668	-10.0259405	1.8618147
H	-0.3912530	-8.8635754	3.1961977
H	0.3512246	-6.5709349	2.5689552
H	0.1812856	-4.6085910	1.0705140
H	-2.9292636	-1.5283543	-0.3752225
H	-4.5048878	-0.4459325	-1.9247808
H	-5.1785756	0.1455624	-4.2844006
H	-4.7381698	0.0192474	-6.7312534
H	-2.7730678	-1.2655826	-7.5961786
H	-1.2391451	-2.4290950	-6.0166003
H	-0.6102317	-3.0367514	-3.6886374
H	3.8258896	6.0926747	3.3641329
C	3.3719150	6.4973521	2.4533681
C	4.0552388	7.4615454	1.6949198
H	5.0453387	7.8092107	2.0067128
C	3.4535264	7.9838871	0.5418622
H	3.9723533	8.7439930	-0.0517571
C	2.1854791	7.5345514	0.1402827
H	1.7404185	7.9539903	-0.7678729
C	1.4996225	6.5529400	0.8801367
C	2.1061508	6.0527534	2.0503793
H	1.5788400	5.3083741	2.6561343
H	-3.6388186	6.0280569	3.3563972
C	-2.9159578	6.6210255	2.7867182
C	-1.9194039	5.9669396	2.0452407
H	-1.8943414	4.8753675	2.0615110
C	-0.9797871	6.6901273	1.2922943
C	-1.0676822	8.0984814	1.3029516
H	-0.3379117	8.6905184	0.7392514
C	-2.0566526	8.7570652	2.0423045
H	-2.0978742	9.8513200	2.0382211
C	-2.9880836	8.0187182	2.7901807
H	-3.7626302	8.5317475	3.3692224
H	-5.4824077	6.5884759	-0.2977107
C	-4.4157088	6.5931402	-0.5761073
H	-4.3242873	7.0493125	-1.5836585
H	-3.8684201	7.2270051	0.1488991
O	-3.9677685	5.2433351	-0.5590332
H	-3.0225283	5.2490523	-0.8161629

PRT-S-p

Au	-0.7183826	0.8673391	-0.7068080
C	3.1263624	3.5161210	-2.2386238
C	3.1168957	2.6945319	-1.0730671
C	3.4321663	3.2907617	0.2006811
C	3.7335652	4.6821560	0.2560763
C	3.7176309	5.4564578	-0.8924054
C	3.4121079	4.8696529	-2.1488596
C	3.4119214	2.4627872	1.3629188
C	3.1075339	1.1191186	1.2721060
C	2.7934146	0.5204419	0.0138592
C	2.7984436	1.3051233	-1.1296381
C	2.4666167	-0.9728103	0.0289797
C	1.9717699	-1.5384675	-1.3453739
O	3.1138447	-1.5506598	-2.1772825
C	2.9186715	-1.3979508	-3.5788060
O	1.3908533	-1.1573252	1.0114661
P	-0.1985629	-0.8975618	0.6822804
O	-0.6716001	-2.3804508	0.1764790
C	-0.2116648	-3.0866195	-1.0336833
C	-1.0695144	-2.5857761	-2.1920684
C	-0.5675013	-2.3003655	-3.4516348
C	-1.4299428	-1.9598817	-4.5354535
C	-2.8548207	-1.9532563	-4.3236523
C	-3.3476852	-2.2493264	-3.0162822
C	-2.4840099	-2.5394306	-1.9790950
C	-3.7120360	-1.6207122	-5.4117637
C	-3.1860893	-1.2971362	-6.6530417
C	-1.7805920	-1.2992210	-6.8614295
C	-0.9208607	-1.6294614	-5.8255669
N	-0.9305842	-0.8394510	2.1678249
C	-0.8977943	-2.0477609	3.0652915
C	-2.3295146	-2.4704978	3.3793804
C	-2.9760546	-2.1333215	4.5817655
C	-4.3174159	-2.4892741	4.7950520
C	-5.0240921	-3.1957017	3.8132808
C	-4.3825456	-3.5514474	2.6160961
C	-3.0481670	-3.1887584	2.4007733
C	-1.3998775	0.4523133	2.7412461
C	-0.2186438	1.3916986	3.0428056
C	-2.5169345	1.0942347	1.9090026
C	-2.7548077	2.4825261	1.9650620
C	-3.8061802	3.0600232	1.2376417
C	-4.6370882	2.2657725	0.4354838
C	-4.4243359	0.8793063	0.3916107
C	-3.3822890	0.2978083	1.1268933
C	0.0229526	-1.8476567	4.2750430
C	3.6468688	-1.7935287	0.5527111
C	4.9527434	-1.5513883	0.0311283
C	6.0243397	-2.3246754	0.4373561
C	5.8609996	-3.3764928	1.3873013
C	4.5484231	-3.6112684	1.9322299
C	3.4636942	-2.7970923	1.4955084
C	4.3710903	-4.6568334	2.8851594
C	5.4429047	-5.4392974	3.2828077
C	6.7386252	-5.2063513	2.7470436
C	6.9432753	-4.1964544	1.8204338
C	1.3457692	-2.9705288	-1.1759175

O	1.7132131	-3.7981358	-2.2643833
C	2.8231737	-4.6611424	-1.9871346
C	-0.4955612	-4.5697538	-0.7456932
C	-0.3205498	-5.0731385	0.5363808
C	-0.5066396	-6.4530715	0.8290226
C	-0.8629835	-7.3480862	-0.2427492
C	-1.0166175	-6.8099335	-1.5538712
C	-0.8411906	-5.4598864	-1.8024780
C	-1.0446099	-8.7317924	0.0487762
C	-0.8821616	-9.2095465	1.3390496
C	-0.5325168	-8.3251470	2.3960750
C	-0.3493091	-6.9755263	2.1463701
H	1.2070652	-0.8417207	-1.7593060
H	1.7430406	-3.3973664	-0.2383871
H	3.9073271	-1.1649146	-4.0034868
H	2.2238805	-0.5597607	-3.7992775
H	2.5287012	-2.3242929	-4.0359929
H	2.5688746	-5.3681703	-1.1742540
H	3.7192205	-4.0769908	-1.7081679
H	3.0163432	-5.2233641	-2.9131714
H	-1.8666931	0.1603826	3.7000796
H	0.2343401	1.7680327	2.1079785
H	0.5594745	0.8504210	3.6015602
H	-0.5351321	2.2587281	3.6438106
H	-3.2320311	-0.7857822	1.0976796
H	-5.0739103	0.2410720	-0.2165347
H	-5.4361363	2.7242386	-0.1539406
H	-3.9701581	4.1404361	1.3048194
H	-2.1252603	3.1337573	2.5772232
H	-0.4589506	-2.8415913	2.4435026
H	-0.3092267	-1.0269527	4.9328415
H	1.0464827	-1.6230052	3.9320895
H	0.0446781	-2.7708170	4.8783362
H	-2.4361819	-1.5977629	5.3699246
H	-4.8073704	-2.2175208	5.7359391
H	-6.0685432	-3.4770331	3.9836070
H	-4.9222836	-4.1192933	1.8507313
H	-2.5464500	-3.4657303	1.4673153
H	2.4715173	-2.9721237	1.9209154
H	3.3702614	-4.8352030	3.2951689
H	5.2958501	-6.2419599	4.0129813
H	7.5775512	-5.8309909	3.0709390
H	7.9421697	-4.0161374	1.4081095
H	7.0227511	-2.1317401	0.0298603
H	5.0932513	-0.7504532	-0.6987021
H	3.1058214	0.4890231	2.1669818
H	3.6522044	2.9090974	2.3342572
H	3.9630727	5.1380636	1.2251531
H	3.9253528	6.5280386	-0.8323997
H	3.4050366	5.4953842	-3.0470636
H	2.9101346	3.0587649	-3.2111391
H	2.5790966	0.8709148	-2.1073724
H	-0.9598586	-5.0693010	-2.8165655
H	-1.2801467	-7.4860087	-2.3744207
H	-1.3150968	-9.4136819	-0.7650308
H	-1.0236940	-10.2744929	1.5509071
H	-0.4100127	-8.7173531	3.4109838
H	-0.0841973	-6.2897571	2.9592845
H	-0.0333722	-4.4034048	1.3526893
H	-2.8754962	-2.7661354	-0.9833364
H	-4.4295023	-2.2359575	-2.8437290
H	-4.7957238	-1.6184227	-5.2509451
H	-3.8548048	-1.0416472	-7.4814470
H	-1.3797442	-1.0463592	-7.8484060
H	0.1633043	-1.6443182	-5.9860289
H	0.5015270	-2.3841204	-3.6458661
C	-0.4901332	4.0138270	-1.4319826
C	-1.3974721	2.8015619	-1.5720539
C	-0.0223752	4.3057733	0.0056436
H	1.0673988	4.2189026	0.0996300
H	-0.4889937	3.5839189	0.6952642
C	-0.5368332	5.7467866	0.3458181
C	-1.7444310	5.8262013	-0.6200679
O	-1.3379129	5.1375049	-1.8171378
C	-1.4623273	1.9512023	-2.6814901
C	-0.3867416	1.8880274	-3.7408765
C	-2.7674699	1.2822371	-3.0289070
H	-2.6154369	0.2858387	-3.4637368
H	-3.2595557	1.9259105	-3.7825736
H	-3.4438112	1.2224607	-2.1642437
H	-0.7252251	2.4721930	-4.6178468
H	-0.2484277	0.8479793	-4.0812199
H	0.5781548	2.2911349	-3.3997317
H	-2.3305387	2.9063220	-0.9948443
H	0.3483169	3.9935531	-2.1437093
H	-2.6281441	5.3241134	-0.1832541
H	-2.0154699	6.8508671	-0.9176512
H	-0.1295314	4.6820007	4.9292105
C	-0.6868934	5.2283671	4.1604612
C	-1.7943820	6.0113794	4.5170933
H	-2.1133063	6.0746522	5.5624513
C	-2.4818276	6.7227515	3.5238650
H	-3.3403831	7.3478886	3.7907344
C	-2.0704084	6.6447565	2.1852451
H	-2.6089489	7.2289504	1.4314443
C	-0.9777474	5.8403483	1.8076009
C	-0.2858384	5.1427156	2.8195323
H	0.5828647	4.5286136	2.5602676
H	2.8199627	8.8799256	1.5165046
C	2.2374229	8.4241792	0.7087010
C	1.2960664	7.4297390	1.0138243
H	1.1561814	7.1363947	2.0579459
C	0.5167596	6.8291046	0.0054598
C	0.7230841	7.2511900	-1.3260934
H	0.1452812	6.7972801	-2.1363024
C	1.6580241	8.2504414	-1.6310596
H	1.7873889	8.5660493	-2.6720747
C	2.4194172	8.8462824	-0.6153531
H	3.1439932	9.6322232	-0.8527037
H	-5.8917465	4.6800192	-2.5443217
C	-4.9103532	5.1811309	-2.5987382
H	-4.8620290	5.7324742	-3.5608767

H	-4.8625545	5.9244035	-1.7735824
H	-3.0283152	4.6111325	-2.5074532

MeOH

H	-5.0855899	-5.7189514	-1.4776853
C	-5.7838986	-6.3464445	-0.8983149
H	-6.7402681	-6.3966889	-1.4640200
H	-5.3576263	-7.3728943	-0.8540411
O	-5.9220166	-5.7437953	0.3782718
H	-6.5364804	-6.2932649	0.8953904

Substrate-p

C	-4.9998704	-1.4975147	1.0131004
C	-4.3705155	-2.3063010	0.1839877
C	-6.5010195	-1.3982036	1.1959985
H	-7.0203285	-1.8972023	0.3623675
H	-6.7887057	-0.3313837	1.1797276
C	-7.0094423	-2.0410343	2.5345175
C	-6.9992665	-3.5988384	2.3544443
O	-7.9373794	-4.0318813	1.3987273
H	-7.2581605	-4.0580063	3.3271902
H	-5.9692650	-3.9206901	2.0912471
C	-3.7199371	-3.1229673	-0.6346181
C	-3.2983268	-4.5172221	-0.1974348
C	-3.3567704	-2.7192138	-2.0539828
H	-3.7866634	-3.4344278	-2.7815418
H	-2.2587904	-2.7451867	-2.1879020
H	-3.7163970	-1.7071214	-2.2965423
H	-3.7906612	-5.2814554	-0.8281077
H	-3.5612202	-4.7096666	0.8542850
H	-2.2058045	-4.6416210	-0.3191493
H	-4.3898839	-0.8455369	1.6572311
H	-7.4831099	-4.1138085	0.5248580
H	-5.2595855	1.3367561	5.2969014
C	-5.2255031	0.2763626	5.0232060
C	-4.3146581	-0.5856699	5.6548930
H	-3.6323674	-0.2042954	6.4223422
C	-4.2903987	-1.9383141	5.2952344
H	-3.5867907	-2.6232168	5.7816424
C	-5.1627179	-2.4283680	4.3092657
H	-5.1108505	-3.4877856	4.0446043
C	-6.0813295	-1.5773668	3.6672771
C	-6.0968589	-0.2170765	4.0461622
H	-6.8160423	0.4589068	3.5699242
H	-9.0312220	-1.2500721	0.7667771
C	-9.3643820	-1.2829092	1.8071909
C	-10.7034917	-0.9821705	2.0965173
H	-11.3837600	-0.7080189	1.2823697
C	-11.1734195	-1.0378163	3.4151601
H	-12.2191851	-0.8019168	3.6410278
C	-10.2908034	-1.4030367	4.4422886
H	-10.6431530	-1.4567648	5.4783159
C	-8.9535393	-1.6987402	4.1494572
O	-3.9111075	4.1786743	-2.4898083

H	-8.2737381	-1.9801361	4.9610346
C	-8.4627615	-1.6347755	2.8290167
H	-8.2286814	-4.0324807	-2.2904513
C	-7.2988150	-3.4730707	-2.1001959
H	-6.6885575	-3.4779669	-3.0248733
H	-7.5651040	-2.4236726	-1.8577835
O	-6.6249191	-4.1228404	-1.0241575
H	-5.7945185	-3.6277601	-0.8317942

INT1-OMe

Au	-1.4288532	-1.6043493	0.6806925
C	-4.2525751	-0.8541242	1.6444704
C	-3.5696181	-1.3383668	0.6177842
C	-5.7459084	-0.6501248	1.5764053
H	-6.0936922	-0.7754574	0.5404322
H	-5.9654096	0.3836526	1.8912124
C	-6.5262166	-1.6481422	2.4940218
C	-6.4324701	-3.0560018	1.8580524
O	-6.9318114	-2.9886928	0.5323794
H	-7.0238137	-3.7715480	2.4649148
H	-5.3759440	-3.4031348	1.8433535
C	-3.3435097	-1.8376990	-0.6409408
C	-3.6421953	-3.2948179	-0.9515380
C	-3.1736631	-0.9054880	-1.8301167
H	-4.0972993	-0.9622425	-2.4367953
H	-2.3375028	-1.2237981	-2.4745716
H	-3.0232683	0.1357787	-1.5095565
H	-4.7283074	-3.3608235	-1.1493757
H	-3.4052692	-3.9542996	-0.1041296
H	-3.0952554	-3.6300830	-1.8451669
H	-3.7451943	-0.5926371	2.5794598
C	-4.2869950	2.6486776	0.1376616
C	-3.2421894	2.3459554	1.0590591
C	-3.5294905	2.3790420	2.4695230
C	-4.8387060	2.7394078	2.9009033
C	-5.8305901	3.0410753	1.9798896
C	-5.5540818	2.9871548	0.5869478
C	-2.4813031	2.0568414	3.3826631
C	-1.2137020	1.7477831	2.9298004
C	-0.9141752	1.7286011	1.5320343
C	-1.9226189	2.0208492	0.6247127
C	0.5371608	1.4282441	1.1371767
C	0.7317308	1.0178336	-0.3643581
O	0.5644215	2.1989587	-1.1202463
C	0.0589945	2.0623135	-2.4462063
O	0.9821651	0.3088577	1.9697338
P	0.6417949	-1.2715495	1.6618224
O	1.9452554	-1.6998368	0.7609216
C	2.1916108	-1.2164405	-0.6075027
C	1.1905750	-1.9071753	-1.5343664
C	0.8108471	-1.3538498	-2.7496264
C	-0.1090510	-2.0167054	-3.6121243

C	-0.6339485	-3.3038838	-3.2293140
C	-0.2083499	-3.8652747	-1.9908444
C	0.6758390	-3.1902451	-1.1667578
C	-1.5629167	-3.9553480	-4.0929449
C	-1.9711945	-3.3556459	-5.2737272
C	-1.4591561	-2.0833377	-5.6482927
C	-0.5431715	-1.4312465	-4.8386412
N	0.9655411	-2.0258333	3.0949393
C	2.3240856	-1.8453648	3.7211312
C	2.9890258	-3.2077985	3.8958586
C	2.9998445	-3.8943484	5.1237062
C	3.5694593	-5.1741272	5.2219612
C	4.1450636	-5.7778421	4.0964512
C	4.1514543	-5.0954362	2.8692662
C	3.5745154	-3.8236984	2.7695590
C	-0.1167631	-2.7235012	3.8505378
C	-1.1089628	-1.7332655	4.4775976
C	-0.7604942	-3.8197120	2.9942796
C	-2.1547129	-4.0111491	2.9418603
C	-2.7028052	-5.0584516	2.1833632
C	-1.8710410	-5.9179601	1.4536797
C	-0.4801594	-5.7307424	1.4961826
C	0.0687785	-4.6966499	2.2634777
C	2.2627120	-0.9676223	4.9765175
C	1.4604539	2.5965895	1.4923628
C	1.0877110	3.9227325	1.1225361
C	1.9417373	4.9834391	1.3595495
C	3.2103228	4.7883528	1.9820381
C	3.5812457	3.4541629	2.3789976
C	2.6794955	2.3815009	2.1224479
C	4.8439568	3.2450281	3.0070309
C	5.7062356	4.3057040	3.2307926
C	5.3401142	5.6221429	2.8396734
C	4.1183668	5.8583544	2.2301262
C	2.1400625	0.3548173	-0.6053819
O	2.6824442	0.7884712	-1.8380973
C	3.5874828	1.8920129	-1.7166975
C	3.6455037	-1.6269066	-0.8842271
C	4.6011309	-1.4127777	0.1024242
C	5.9672319	-1.7554227	-0.0948458
C	6.3665165	-2.3194748	-1.3599070
C	5.3708706	-2.5127126	-2.3604180
C	4.0462518	-2.1807973	-2.1315404
C	7.7360520	-2.6626743	-1.5592771
C	8.6683266	-2.4607713	-0.5550684
C	8.2730440	-1.9075839	0.6940926
C	6.9513415	-1.5625815	0.9195109
H	-0.0692121	0.2904117	-0.6299748
H	2.8092188	0.6593614	0.2195007
H	-0.2841001	3.0637353	-2.7494139
H	-0.7957645	1.3554400	-2.4785268
H	0.8409412	1.7128424	-3.1419840
H	4.4681674	1.6027921	-1.1108295
H	3.0890436	2.7651318	-1.2575481
H	3.9124967	2.1402039	-2.7383317
H	0.4229027	-3.2432775	4.6634997
H	-1.6933539	-1.2097915	3.7004810
H	-0.5682615	-0.9717737	5.0597165
H	-1.8184914	-2.2426201	5.1498983
H	1.1545765	-4.5626221	2.3024711
H	0.1829342	-6.4014259	0.9391474
H	-2.3013903	-6.7331872	0.8624823
H	-3.7887815	-5.1999034	2.1666086
H	-2.8283612	-3.3468344	3.4897787
H	2.9052266	-1.2997412	2.9601442
H	1.6498311	-1.4183414	5.7750841
H	1.8348171	0.0159805	4.7216472
H	3.2796805	-0.8197189	5.3771414
H	2.5727518	-3.4330840	6.0206205
H	3.5679371	-5.6957085	6.1847785
H	4.5944075	-6.7731331	4.1756906
H	4.6117446	-5.5526740	1.9868412
H	3.5689695	-3.3001811	1.8078394
H	2.9622987	1.3725489	2.4362707
H	5.1239780	2.2286077	3.3076047
H	6.6751520	4.1342669	3.7112973
H	6.0307452	6.4518355	3.0232018
H	3.8354863	6.8733946	1.9298857
H	1.6461155	5.9976377	1.0695037
H	0.1202900	4.0898409	0.6430380
H	-0.4150801	1.5189893	3.6410369
H	-2.6931854	2.0675210	4.4574180
H	-5.0478794	2.7788628	3.9752318
H	-6.8330660	3.3172859	2.3226093
H	-6.3462714	3.2227396	-0.1312046
H	-4.0706956	2.6213878	-0.9365509
H	-1.7163357	2.0353987	-0.4469055
H	3.3010042	-2.3446595	-2.9143707
H	5.6671517	-2.9380426	-3.3255419
H	8.0400854	-3.0901501	-2.5210501
H	9.7174620	-2.7281676	-0.7190891
H	9.0213825	-1.7564821	1.4790998
H	6.6432207	-1.1391746	1.8823397
H	4.3081162	-0.9822820	1.0660093
H	1.0000653	-3.6494163	-0.2301872
H	-0.5917912	-4.8444997	-1.6846540
H	-1.9486893	-4.9408987	-3.8087943
H	-2.6858996	-3.8646888	-5.9286379
H	-1.7874804	-1.6241825	-6.5863919
H	-0.1412033	-0.4542542	-5.1291293
H	1.2366590	-0.3982358	-3.0627515
C	-7.3305912	-4.2473193	0.0140791
H	-5.2559235	0.6715015	6.3760014
C	-5.2561755	-0.2903540	5.8514203
C	-4.6560683	-1.4144794	6.4420053
H	-4.1810477	-1.3362264	7.4253843
C	-4.6898783	-2.6411154	5.7680433
H	-4.2446831	-3.5325553	6.2233762
C	-5.2992758	-2.7419758	4.5051505
H	-5.3104263	-3.7172522	4.0105037
C	-5.8906989	-1.6207032	3.8947113
C	-5.8710073	-0.3978223	4.5993562

H	-6.3566160	0.4788447	4.1584330
H	-8.0858131	-0.0601674	0.7718481
C	-8.6519293	-0.4640312	1.6150389
C	-10.0226273	-0.1775288	1.7066373
H	-10.4956751	0.4484032	0.9421664
C	-10.7851300	-0.6902713	2.7640189
H	-11.8543378	-0.4647198	2.8347899
C	-10.1655640	-1.4945613	3.7320766
H	-10.7485631	-1.9013677	4.5652506
C	-8.7964518	-1.7747054	3.6414548
H	-8.3209821	-2.3937875	4.4105353
C	-8.0172938	-1.2628430	2.5837249
H	-7.7005015	-4.0732470	-1.0085965
H	-8.1431502	-4.6961388	0.6214282
H	-6.4830483	-4.9658756	-0.0264796

INT2-R-OMe

Au	1.088915	-0.471403	0.348580
C	3.307910	-0.822445	0.641192
C	2.818185	-0.217785	1.764597
C	4.033133	-0.091466	-0.477343
H	3.965513	0.992928	-0.305961
H	3.551635	-0.326803	-1.441210
C	5.537798	-0.507019	-0.586992
C	6.246009	-0.163472	0.741771
O	6.062180	1.213238	1.007437
H	7.322318	-0.418707	0.665291
H	5.826635	-0.769004	1.575148
C	2.759787	0.369972	2.954068
C	4.033273	0.510096	3.766103
C	1.511987	0.940392	3.573164
H	1.610857	2.036355	3.669142
H	1.373232	0.534432	4.589495
H	0.612827	0.710216	2.981826
H	4.267927	1.583652	3.887243
H	4.890555	0.020777	3.284341
H	3.886359	0.079383	4.772783
H	3.364417	-1.923810	0.623454
C	3.078134	3.961116	1.730333
C	2.304410	3.534031	0.612555
C	2.910233	3.534717	-0.693697
C	4.262034	3.962762	-0.827890
C	4.988555	4.367651	0.279238
C	4.391991	4.368964	1.567608
C	2.119790	3.115304	-1.806075
C	0.802429	2.730802	-1.642525
C	0.192793	2.734602	-0.349541
C	0.943711	3.131100	0.747879
C	-1.280368	2.324544	-0.259289
C	-1.737156	1.935001	1.189129
O	-1.874640	3.153214	1.890124
C	-1.722395	3.133635	3.309259
O	-1.457173	1.151665	-1.116822
P	-0.962007	-0.366894	-0.733147
O	-2.272671	-0.958645	0.060080
C	-2.866520	-0.457910	1.314556
C	-1.968387	-0.885150	2.476783
C	-2.056265	-0.272573	3.720921
C	-1.210349	-0.660603	4.798879
C	-0.261416	-1.728419	4.603448
C	-0.226739	-2.375582	3.336541
C	-1.057557	-1.970904	2.305037
C	0.614054	-2.080500	5.672110
C	0.563613	-1.401256	6.879087
C	-0.372214	-0.347580	7.072702
C	-1.244185	0.010253	6.057014
N	-1.083804	-1.149373	-2.187915
C	-2.350324	-0.972728	-2.986152
C	-2.990216	-2.327917	-3.277321
C	-2.903259	-2.955560	-4.533819
C	-3.492775	-4.212221	-4.747136
C	-4.185733	-4.851992	-3.711014
C	-4.285254	-4.231099	-2.455783
C	-3.686842	-2.984054	-2.241183
C	0.033343	-1.968963	-2.734844
C	1.138773	-1.094456	-3.346664
C	0.517320	-2.981628	-1.691704
C	1.883022	-3.225431	-1.455722
C	2.292453	-4.164416	-0.495030
C	1.339978	-4.878944	0.241962
C	-0.026226	-4.663736	-0.003583
C	-0.432587	-3.726723	-0.959991
C	-2.123783	-0.074240	-4.207549
C	-2.206545	3.393713	-0.843371
C	-2.016695	4.760194	-0.481849
C	-2.887575	5.733601	-0.934413
C	-3.991981	5.406137	-1.775912
C	-4.175880	4.030475	-2.161262
C	-3.261984	3.049912	-1.678308
C	-5.271057	3.689352	-3.008015
C	-6.150493	4.662878	-3.452699
C	-5.969360	6.020332	-3.072349
C	-4.912339	6.384079	-2.253400
C	-3.063265	1.092924	1.176425
O	-3.935248	1.503556	2.211169
C	-4.891377	2.488779	1.803030
C	-4.249832	-1.124637	1.338601
C	-5.100664	-0.937870	0.254317
C	-6.373891	-1.565535	0.183812
C	-6.797105	-2.401585	1.279396
C	-5.916364	-2.564026	2.386824
C	-4.675140	-1.949476	2.416251
C	-8.072349	-3.036297	1.208598
C	-8.888949	-2.859293	0.104019
C	-8.467582	-2.039910	-0.979885
C	-7.237437	-1.406299	-0.940690
H	-0.926852	1.323961	1.647106
H	-3.558692	1.243234	0.200630
H	-1.565752	4.180858	3.611700
H	-0.845596	2.529797	3.612781
H	-2.621817	2.733301	3.805945

H	-5.561328	2.075815	1.023885
H	-4.389586	3.395547	1.419077
H	-5.481794	2.737314	2.697731
H	-0.438988	-2.552700	-3.546595
H	1.652707	-0.504605	-2.565893
H	0.706164	-0.386447	-4.069504
H	1.890022	-1.708023	-3.871074
H	-1.498093	-3.561913	-1.143332
H	-0.781162	-5.229832	0.552552
H	1.657080	-5.611485	0.991777
H	3.362088	-4.333370	-0.336730
H	2.652046	-2.688155	-2.015458
H	-3.031046	-0.441857	-2.300401
H	-1.418827	-0.520324	-4.929018
H	-1.721266	0.898240	-3.881273
H	-3.079430	0.095364	-4.731911
H	-2.383929	-2.465324	-5.363985
H	-3.415325	-4.686443	-5.731090
H	-4.652617	-5.827474	-3.882119
H	-4.835977	-4.714356	-1.641714
H	-3.758224	-2.507804	-1.258349
H	-3.401138	2.009744	-1.985557
H	-5.407257	2.641739	-3.301154
H	-6.989639	4.390424	-4.101254
H	-6.671161	6.780189	-3.431524
H	-4.771271	7.430866	-1.962162
H	-2.733192	6.779941	-0.649134
H	-1.176545	5.028233	0.163210
H	0.205093	2.423667	-2.505714
H	2.568209	3.119845	-2.805957
H	4.723120	3.969803	-1.819889
H	6.027434	4.691765	0.160395
H	4.971342	4.705915	2.433775
H	2.611901	3.981444	2.721634
H	0.492987	3.169718	1.740135
H	-4.015039	-2.100191	3.274333
H	-6.231435	-3.196089	3.224165
H	-8.395901	-3.668637	2.042572
H	-9.865771	-3.352081	0.059928
H	-9.122911	-1.913197	-1.847884
H	-6.908709	-0.777004	-1.775426
H	-4.789061	-0.311674	-0.589140
H	-1.027753	-2.504504	1.352995
H	0.470847	-3.204765	3.174646
H	1.331874	-2.894274	5.521593
H	1.241503	-1.677306	7.693474
H	-0.403507	0.177829	8.032833
H	-1.967130	0.820396	6.204064
H	-2.790061	0.521354	3.878597
C	7.027811	1.743870	1.901307
H	5.161787	-4.117889	-3.581380
C	5.411696	-3.804731	-2.562243
C	5.828910	-4.755135	-1.616577
H	5.905359	-5.811985	-1.891488
C	6.152000	-4.335573	-0.320348
H	6.484926	-5.063890	0.426513
C	6.056628	-2.978487	0.032050
H	6.319382	-2.687336	1.052892
C	5.646760	-2.012400	-0.908020
C	5.328771	-2.452494	-2.211305
H	5.035975	-1.715337	-2.967989
H	4.490078	1.425554	-2.371019
C	5.550359	1.219063	-2.529812
C	6.223001	1.905205	-3.554539
H	5.674656	2.625036	-4.172470
C	7.583710	1.674008	-3.787344
H	8.108777	2.210721	-4.584067
C	8.265802	0.737674	-2.994245
H	9.327298	0.535515	-3.171996
C	7.589962	0.050312	-1.979853
H	8.129712	-0.698559	-1.389507
C	6.223757	0.287839	-1.721338
H	6.756564	2.794657	2.080823
H	8.046721	1.699213	1.464757
H	7.035870	1.205448	2.872284

INT3-S-OMe

C	-2.657969	-4.408645	0.952040
C	-1.890809	-3.788267	-0.075411
C	-2.533794	-3.464758	-1.322736
C	-3.923240	-3.737401	-1.478195
C	-4.646394	-4.318344	-0.449325
C	-4.007059	-4.667687	0.769827
C	-1.752375	-2.861167	-2.352941
C	-0.423000	-2.546545	-2.145546
C	0.198369	-2.784595	-0.879952
C	-0.523291	-3.429715	0.115783
C	1.617756	-2.240768	-0.681170
C	2.003285	-2.048845	0.827610
O	2.297904	-3.337121	1.321147
C	2.157969	-3.559722	2.724230
O	1.655840	-0.914460	-1.310071
P	0.890101	0.405098	-0.685933
O	2.042668	1.034481	0.297290
C	2.779310	0.409419	1.412491
C	1.902281	0.494130	2.662845
C	2.188604	-0.259245	3.795964
C	1.416371	-0.132451	4.986031
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C	0.830547	1.436477	2.714671
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C	-3.295602	3.959811	-1.155523
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C	2.457412	1.221579	-3.911031
C	2.672875	-3.070036	-1.410678
C	2.640115	-4.491784	-1.302699
C	3.624531	-5.263190	-1.891494
C	4.693403	-4.666061	-2.623671
C	4.721240	-3.231135	-2.750237
C	3.692344	-2.463089	-2.132501
C	5.782039	-2.621801	-3.482762
C	6.775045	-3.394059	-4.063009
C	6.746746	-4.809735	-3.939333
C	5.727322	-5.431999	-3.236660
C	3.197024	-1.041074	0.987840
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C	5.204418	-2.271785	1.352028
C	4.046144	1.275568	1.512157
C	4.862776	1.393893	0.392176
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C	6.352658	2.950539	1.585266
C	5.509108	2.806410	2.723504
C	4.384751	1.997293	2.690211
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C	8.290859	3.903282	0.445070
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H	-7.314975	-1.822862	2.649962

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