

Supplementary Information

Intramolecular Oxa-Michael Reaction on α,β -unsaturated α -amino- δ -hydroxycarboxylic Acid Esters. Synthesis of functionalized 1,3-dioxanes

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Computational Details

The DFT computations were carried out using the software Gaussian 09 series.¹ The M06-2X functional proposed by Truhlar and Zhao was used in all computations.² All the atoms were treated with 6-31+G(d) basis set. The geometries of the various critical points on the potential surface were fully optimized with the gradient method available in Gaussian 09 including the solvent effect (PCM calculations³) to simulate the experimental conditions (solvent emulated was the tetrahydrofuran, used experimentally, $\square = 7.4257$). Furthermore, with the purpose of evaluating the nature of all critical points, we computed harmonic vibrational frequencies for all of them. Geometry parameters refer to PCM optimized structures and energies values are Gibbs energies obtained with PCM frequency calculations.

In order to explore more carefully the potential energy surface and the conformational space of each structure, we also performed simulated annealing calculations using the PM7⁴ method available in MOPAC.⁵ We used the following protocol: 1. minimization, 2. heating from 0 to 450 K in 15 ps, 3. equilibration in 10 ps, 4. exploration between 25 and 30 ps depending on the size of the system, 5. cooling in 30 ps in all cases, 6. Minimization. In each process, the time step was 0.5 fs.

Table S-1. Model system 1. Gibbs energies of the critical points located on the potential energy surface, relative to reactants (M1) for different R and R'. Energy values are Gibbs energies obtained at the PCM level (kcal/mol)

	Model 1.1		Model 1.2		Model 1.3		Model 1.4		Model 1.5		Model 1.6	
	R	R'	R	R'	R	R'	R	R'	R	R'	R	R'
	NH ₂	H	NO ₂	H	OMe	H	F	H	H	CF ₃	H	H
M2	-2.7		-8.7		-3.1		-3.6		-17.6		-5.9	
TS2	30.7		16.0		22.0		20.3		8.3		20.1	
M3	20.3		5.8		11.5		9.6		2.2		9.9	

Table S-2: Model system 2. Energy values are Gibbs energies obtained at the PCM level (kcal/ mol)

			M2	TS2	M3
Model 2.1	R ₁	NCOCF ₃	-4.1	18.6	6.6
	R ₂	H			
	R ₃	H			
Model 2.2	R ₁	N-Succinimide	-2.0	2.2	-11.0
	R ₂	H			
	R ₃	H			
Model 2.3	R ₁	N-Phthalimide	-2.0	1.6	-11.5
	R ₂	H			
	R ₃	H			
Model 2.4	R ₁	N(CHO) ₂	-1.8	1.6	-11.0
	R ₂	H			
	R ₃	H			
Model 2.5	R ₁	NCOCH ₃	-3.5	18.4	10.0
	R ₂	F			
	R ₃	H			
Model 2.6	R ₁	NCOCH ₃	-1.8	27.0	19.6
	R ₂	H			
	R ₃	CF ₃			

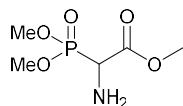
Table S-3: Model system 3. Energy values are Gibbs energies obtained at the PCM level (kcal mol⁻¹). In parenthesis values when K⁺ is used as counterion

	Model 3.1	Model 3.2	Model 3.3	Model 3.4	Model 3.5	Model 3.6
G group						
M2	-9.6 (-10.8)	-9.9	-10.7	-13.9	-12.2	-13.5
TS2	0.2 (6.3)	0.7	0.8	-1.6	1.9	-1.8
M3	-1.5 (4.9)	-1.7	-1.2	-1.7	-0.2	-2.3

Experimental procedures (Synthesis of Starting Material)

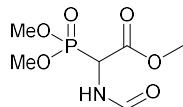
General information. NMR spectra were recorded on a 400 MHz spectrometer, and the data are expressed in parts per million (ppm) referenced to TMS and trifluoracetic acid (¹⁹F). Data are reported as follows: δ , chemical shift; multiplicity (recorded as br, broad; s, singlet; d, doublet; t, triplet; q, quadruplet and m, multiplet); coupling constants (J in Hertz, Hz); and integration. The chemical shifts for ¹³C spectra (101 MHz) are expressed in parts per million (ppm), referenced to TMS. Infrared spectra (IR) are reported in terms of absorption frequency (n , cm⁻¹) using KBr. High Resolution Mass Spectra (HRMS) were obtained on a Q-TOF LC/MS.

Methyl 2-amino-2-(dimethoxyphosphoryl)acetate⁶



A mixture of benzyloxycarbonyl- α -phosphonoglycine trimethyl ester (4.5 mmol, 1500 mg) and Pd/C (10% mol, 15 mg) in MeOH (0.1 M) was allowed to stir for 12 hours in hydrogen atmosphere. The mixture reaction was filtered through a short pad of celite and concentrated under reduced pressure. The crude extract was obtained as pale yellow oil (890 mg, 100%). ¹H NMR (400 MHz, CDCl₃) δ (ppm): 3.96 (d, J = 21.3 Hz, 1H), 3.86 (d, J = 2.6 Hz, 3H), 3.83 (d, J = 2.6 Hz, 6H), 1.78 (bs, 2H).

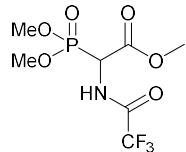
Methyl 2-(dimethoxyphosphoryl)-2-formamidoacetate⁷ (1c)



To a solution of methyl 2-amino-2-(dimethoxyphosphoryl)acetate (1.5 mmol, 341 mg) in dry dichloromethane (1 mL), a solution of formic acid (1.5 mmol, 0.060 mL) in dichloromethane (1.5 mL) were added at -10°C. Then, the cyclohexylcarbodiimide (1.7 mmol, 342 mg) was added and the mixture reaction was stirred to room temperature overnight. The precipitated urea was filtered and washed with cool DCM and the filtrate was washed with 1 mL of KHSO₄ 1 N, and with 1 mL of NaHCO₃ (sat), dried

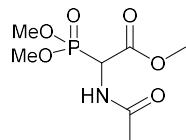
with Na₂SO₄ and concentrated *in vaccuo*. To remove traces of urea, the residue was dissolved in DCM (3 mL) the mixture was kept at -10°C overnight and washed with cool DCM. The product was purified with AcOEt to afford white solid (331 mg, 96 %). ¹H NMR (400 MHz, CDCl₃) δ (ppm), 8.26 (s, 1H), 6.75 (bs, 1H), 5.29 (dd, *J* = 21.8, 9.1 Hz), 3.79 – 3.88 (m, 9H).

Methyl 2-(dimethoxyphosphoryl)-2-(2,2,2-trifluoroacetamido)acetate (1d).



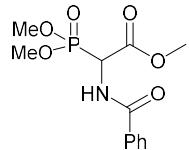
To a solution of methyl 2-amino-2-(dimethoxyphosphoryl)acetate (1.20 mmol, 225 mg) in dry CH₂Cl₂ (6 mL) at 0°C were added dry Et₃N (1.3 mmol, 0.19 mL) followed by trifluoroacetic anhydride added dropwise (1.2 mmol, 0.17 mL) within 5 min. The mixture was stirred for one hour at 0°C, then overnight at room temperature. The solvent was evaporated and the residue was dissolved in ethyl acetate and washed with water. The combined aqueous layers were extracted with ethyl acetate. The combined organic layers were washed with brine, then dried over MgSO₄ and concentrated *in vaccuo* to afford the product as colorless solid (212 mg, 63%). Mp: 89 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.38 (bs, 1H), 5.20 (dd, ²J_{H-P} = 22.2, *J* = 9.0 Hz, 1H), 3.85 (m, 9H); ¹³C NMR (δ, ppm) CDCl₃, 101 MHz: 165.5, 156.9 (qd, *J*_{C-F} = 38.1, ³J_{C-P} = 4.7 Hz), 115.5 (q, *J*_{C-F} = 287 Hz) 54.5 (d, ²J_{C-P} = 6.5 Hz), 54.1 (d, ²J_{C-P} = 6.9 Hz), 50.8 (d, ¹J_{C-P} = 150 Hz); IR: 3209, 3055, 1762, 1727, 1568, 1266, 1224, 1184, 1033; HRMS: Calculated for C₇H₁₂F₃NO₆P (M+H⁺): 294.0354; Found: 294.0397.

Methyl 2-acetamido-2-(dimethoxyphosphoryl)acetate (1e).



To a solution of benzyloxycarbonyl- α -phosphonoglycine trimethyl ester (3.0 mmol, 1.0 g) in methanol (8.6 mL) was added palladium on charcoal 10% (100 mg, 10 %) followed by acetic anhydride (8.2 mmol, 0.77 mL). The mixture was immediately hydrogenated at room temperature overnight. The catalyst was filtered off through a pad of celite and the solvent and excess acetic anhydride were removed *in vacuo*. Toluene was added to the mixture and the solvent was removed *in vacuo* (twice). The product was obtained as a colorless solid. (700 mg, 97%). Mp: 78 °C. ^1H NMR (400 MHz, CDCl_3) δ (ppm): 6.54 (d, $J = 8.2$ Hz, 1H), 5.25 (dd, $^2J_{H-P} = 22.2$, $J = 8.2$ Hz, 1H), 3.83 (m, 9H), 2.09 (s, 3H); ^{13}C NMR (δ , ppm) CDCl_3 , 100 MHz: 169.6 (d, $^3J_{C-P} = 6.0$ Hz), 167.2 (d, $^2J_{C-P} = 2.0$ Hz), 54.2 (d, $^2J_{C-P} = 6.5$ Hz), 53.9 (d, $^2J_{C-P} = 6.9$ Hz), 53.3, 49.2 (d, $^1J_{C-P} = 147$ Hz), 22.8; IR: 3297, 3245, 1738, 1669, 1541, 1492, 1447, 1291, 1233, 1040, 914; HRMS: Calculated for $\text{C}_7\text{H}_{15}\text{NO}_6\text{P}$ ($\text{M}+\text{H}^+$): 240.0637; Found: 240.0671.

Methyl 2-benzamido-2-(dimethoxyphosphoryl)acetate (1f)



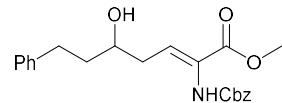
To a solution of benzyloxycarbonyl- α -phosphonoglycine trimethyl ester (4.5 mmol, 1.5 g) in dry AcOEt (26 mL) and palladium on charcoal 10 % (150 mg; 10%) under argon was added benzoic anhydride (9.1 mmol, 2.1 g). The mixture was immediately hydrogenated at room temperature for 24 h. The catalyst was filtered off through a pad of celite, the solvent was removed *in vacuo* and the crude product was purified by column chromatography on silica gel using $\text{CH}_2\text{Cl}_2/\text{AcOEt}$ (7:3) to afford the product as white solid (1.3 g, 95%). Mp: 113 °C. ^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.83 – 7.85 (m, 2H), 7.40 – 7.63 (m, 3H), 6.92 (d, $J = 8.1$ Hz, 1H), 5.46 (dd, $^2J_{H-P} = 21.9$, $J = 8.1$ Hz, 1H), 3.68 – 3.96 (m, 9H); ^{13}C NMR (δ , ppm) CDCl_3 , 101 MHz: 167.2 (d, $^2J_{C-P} = 1.8$ Hz), 166.7 (d, $^3J_{C-P} = 5.6$ Hz), 133.0, 132.2, 128.7, 127.2, 54.3 (d, $^2J_{C-P} = 6.4$ Hz), 54.0 (d, $^2J_{C-P} = 6.9$ Hz), 53.4, 50.4 (d, $^1J_{C-P} = 147$ Hz); IR: 3297, 3245, 1737, 1669,

1542, 1432, 1291, 1233, 1042, 708, 461; HRMS: Calculated for $C_{12}H_{16}NO_6PNa$ ($M+Na^+$): 324.0613; Found: 324.0559.

General procedure for HWE reaction.

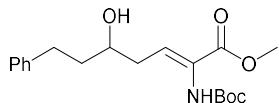
To a solution of phosphonate **1** (1.1 equiv) in dry CH_2Cl_2 (0.35 M) was added DBU (1.05 equiv) at 0°C. After 20 min of stirring a solution of 5-phenyl-3-((triethylsilyl)oxy)pentanal⁸ **2** (1 equiv) in dry CH_2Cl_2 was added drop wise at 0°C. The reaction was monitored by TLC. When the aldehyde was completely consumed, CH_2Cl_2 and a 1 M H_2SO_4 aqueous solution was added to the reaction mixture. This resulting mixture was stirred by 4 h. The aqueous layer was extracted with ethyl acetate and the organic phase was dried over $MgSO_4$, filtered and concentrated *in vacuo*. Purification was performed by flash chromatography.

Methyl (Z)-2-(((benzyloxy)carbonyl)amino)-5-hydroxy-7-phenylhept-2-enoate (3a).



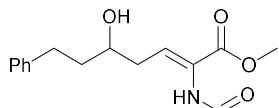
The general procedure for HWE reaction was applied to benzyloxycarbonyl- α -phosphonoglycine trimethyl ester **1a** (1.53 mmol, 507 mg). The crude residue was purified by silica gel column chromatography using $CH_2Cl_2/AcOEt$ (8:2) to provide the product as a white solid (458 mg, 85%). Mp: 97 °C. 1H NMR (400 MHz, $CDCl_3$) δ (ppm): 7.12 – 7.50 (m, 10H), 6.69 (t, $J = 7.8$ Hz, 1H), 6.56 (s, 1H), 5.14 (s, 2H), 3.79 – 3.83 (m, 1H), 3.75 (s, 3H), 2.56 – 2.90 (m, 2H), 2.32 – 2.50 (m, 2H), 1.75 – 1.90 (m, 2H); ^{13}C NMR (δ , ppm) $CDCl_3$, 101 MHz: 164.8, 154.4, 141.7, 135.8, 133.1, 128.5, 128.4, 128.3, 128.2, 125.8, 70.0, 67.5, 52.4, 39.3, 36.0, 31.9; IR: 3283, 3000, 3027, 2948, 1732, 1690, 1509, 1392, 1201, 1151, 1066, 1035, 770, 698; HRMS: Calculated for $C_{22}H_{25}NO_5Na$ ($M+Na^+$): 406.1630; found: 406.1663.

(Z)-Methyl 2-((tert-butoxycarbonyl)amino)-5-hydroxy-7-phenylhept-2-enoate (3b).



The general procedure for HWE reaction was applied to methyl 2-((tert-butoxycarbonyl)amino)-2-(dimethoxyphosphoryl)acetate **1b** (1.13 mmol, 335 mg). The crude residue was purified by silica gel column chromatography with CH₂Cl₂/Cyclohexane (1:1) to give the desired product as a white solid (305 mg, 85%). Mp: 90 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.15 – 7.36 (m, 5H), 6.64 (t, *J* = 6.8 Hz, 1H), 6.31 (s, 1H), 3.80 – 3.84 (m, 2H), 3.78 (s, 3H), 2.77 – 2.84 (m, 1H), 2.66 – 2.73 (m, 1H), 2.39 – 2.43 (m, 2H), 1.79 – 1.86 (m, 2H), 1.46 (s, 9H); ¹³C NMR (δ, ppm) CDCl₃, 101 MHz: 165.1, 153.7, 141.8, 132.4, 128.4, 128.4, 125.8, 81.0, 69.9, 52.3, 39.5, 36.0, 31.9, 28.1; IR: 3314, 3082, 3027, 1742, 1689, 1491, 1369, 1166, 1067, 1029, 896; HRMS: Calculated for C₁₉H₂₇NO₅Na (M+Na⁺): 372.1787; found: 372.1793.

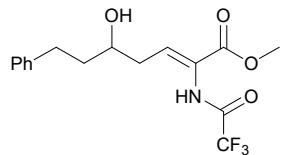
Methyl (Z)-2-formamido-5-hydroxy-7-phenylhept-2-enoate (3c).



The general procedure for HWE reaction was applied to Methyl 2-(dimethoxyphosphoryl)-2-formamidoacetate **1c** (2.07 mmol, 466 mg). The crude residue was purified by silica gel column chromatography using CH₂Cl₂/AcOEt (8:2) to provide the product as a yellow oil (510 mg, 88%). The presence of two rotamers was observed in NMR spectra in a 0.73 (M):0.27 (m) ratio. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.26 (m) (*d*, *J* = 10.5 Hz, 1H), 8.21 (M) (s, 1H), 7.76 (m) (*d*, *J* = 10.5 Hz, 1H), 7.48 (M) (s, 1H), 7.14 – 7.33 (m, 5H), 6.82 (M) (*t*, *J* = 7.6 Hz, 1H), 6.68 (m) (*t*, *J* = 7.6 Hz, 1H), 3.81 – 3.91 (m, 1H), 3.80 (m) (s, 3H) 3.78 (M) (s, 3H), 3.12 (s, 1H), 2.60 – 2.87 (m, 2H), 2.36- 2.45 (m, 2H), 1.79 – 1.86 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 164.4 (M), 164.4 (m), 159.5, 141.7, 134.8 (M), 130.8 (m), 128.5, 128.3, 128.3, 126.0, 125.8, 125.2, 70.5 (m), 69.7 (M), 52.6 (m), 52.5 (M), 39.4 (M), 38.8 (m), 36.6

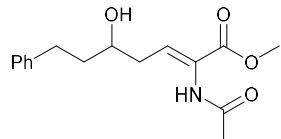
(M), 35.3 (m), 31.9; IR: 3380, 2929, 2859, 1721, 1779, 1652, 1495, 1436, 1394, 1282, 1278, 1207, 1057, 911, 748, 966; HRMS: Calculated for: C₁₅H₁₉NNaO₄ (M+Na⁺): 300.1212; found: 300.1206.

Methyl (Z)-5-hydroxy-7-phenyl-2-(2,2,2-trifluoroacetamido)hept-2-enoate (3d).



The general procedure for HWE reaction was applied to Methyl 2-(dimethoxyphosphoryl)-2-(2,2,2-trifluoroacetamido)acetate **1d** (3.08 mmol, 903 mg). The crude residue was purified by silica gel column chromatography using CH₂Cl₂/Cyclohexane (8:2) to provide the product as a pale yellow oil (923 mg, 96%). ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.41 (s, 1H), 7.12 – 7.39 (m, 5H), 6.87 (t, *J*=7.5 Hz, 1H), 3.86 – 3.89 (m, 1H), 3.81 (s, 3H), 2.63 – 2.90 (m, 2H), 2.26 – 2.47 (m, 2H), 1.74 – 1.96 (m, 2H); ¹³C NMR (δ, ppm) CDCl₃, 101 MHz: 163.5, 155.4 (*q*, *J*_{C-F} = 93.8), 141.2, 135.7, 128.5, 128.5, 128.3, 126.1, 115.6 (*q*, *J*_{C-F} = 288 Hz), 70.7, 52.8, 39.0, 35.8, 31.9; IR: 3300, 3028, 2954, 1719, 1655, 1541, 1439, 1291, 1213, 1171, 1053, 910. HRMS: Calculated for C₁₆H₁₈F₃NO₄ (M+H⁺): 368.1086; Found: 368.1080.

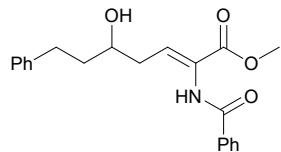
Methyl (Z)-2-acetamido-5-hydroxy-7-phenylhept-2-enoate (3e).



The typical procedure for HWE reaction was applied to methyl 2-acetamido-2-(dimethoxyphosphoryl)acetate **1e** (3.0 mmol, 720 mg). The crude residue was purified by silica gel column chromatography using pentane/AcOEt (8:2) to provide the product as a colorless solid (715 mg, 91%). Mp: 95 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.14 – 7.34 (m, 5H), 7.09 (s, 1H), 6.79 – 6.73 (t, *J* = 7.9 Hz, 1H), 3.81 – 3.86 (m, 1H), 3.77 (s, 3H), 3.10 (d, *J* = 5.1 Hz, 1H), 2.78 – 2.82 (m, 1H), 2.69 – 2.74 (m, 1H), 2.32 – 2.45 (m, 2H), 2.13 (s, 3H), 1.74 – 1.91 (m, 2H); ¹³C NMR (δ, ppm) CDCl₃, 101 MHz:

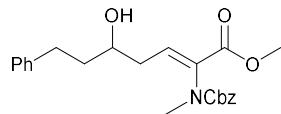
169.1, 164.8, 141.8, 134.4, 128.4, 128.3, 126.7, 125.8, 69.7, 52.5, 39.5, 36.4 32.0, 23.5; IR: 3495, 3277, 3025, 1710, 1646, 1520, 1439, 1307, 1094, 768, 695; HRMS Calculated for C₁₆H₂₂NO₄ (M+H⁺): 292.1549, found: 292.1545.

Methyl (Z)-2-benzamido-5-hydroxy-7-phenylhept-2-enoate (3f)



The typical procedure for HWE reaction was applied to methyl 2-benzamido-2-(dimethoxyphosphoryl)acetate **1f** (3.08 mmol, 929 mg). The crude residue was purified by silica gel column chromatography using CH₂Cl₂/AcOEt (8:2) to provide the product as a white solid (1.06 g, 100%). Mp: 100 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.05 (s, 1H), 7.87 (d, *J* = 7.5 Hz, 2H), 7.50 (m, 3H), 7.14 – 7.30 (m, 5H), 6.81 (t, *J* = 7.9 Hz, 1H), 3.85 – 3.94 (m, 1H), 3.79 (s, 3H), 2.64 – 2.86 (m, 3H), 2.40 – 2.50 (m, 2H), 1.77 – 1.93 (m, 2H); ¹³C NMR (δ, ppm) CDCl₃, 101 MHz: 166.0, 164.9, 141.8, 133.6, 133.4, 132.2, 128.7, 128.4, 128.4, 127.4, 127.3, 125.9, 70.2, 52.5, 39.5, 36.4, 32.0; IR: 3404, 3060, 3026, 1725, 1653, 1515, 1463, 1437, 1262, 1058, 700; HRMS: Calculated for C₂₁H₂₄NO₄ (M+H⁺): 354.1705; Found: 354.1737.

Methyl (Z)-2-(((benzyloxy)carbonyl)(methyl)amino)-5-hydroxy-7-phenylhept-2-enoate (6).

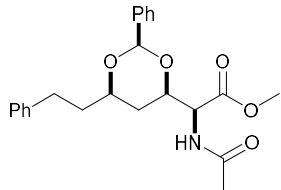


To a solution of methyl (Z)-2-(((benzyloxy)carbonyl)amino)-5-hydroxy-7-phenylhept-2-enoate **3a** (0.39 mmol, 150 mg), imidazole (1.2 mmol, 80 mg), DMAP (0.03 mmol, 10 mg) and dry DMF (1.3 mL) was added chlorotriethylsilane (0.59 mmol, 0.10 mL) to 0°C. The reaction mixture was stirred for 2 h and heated to room temperature overnight. The reaction mixture was quenched with MeOH. Water was added and the aqueous phase was extracted three times with CH₂Cl₂. The organic phase was washed with brine,

dried with anhydrous MgSO₄ and concentrated *in vacuo*. The crude product was dissolved in dry DMF (1 mL) with Ag₂O (1.2 mmol, 268 mg) and CH₃I (1.7 mmol, 0.10 mL) at 0°C. The mixture reaction was stirred overnight to room temperature. The solution was transferred to separatory funnel and water with AcOEt were added. The aqueous layer was extracted with AcOEt (3 x 10 mL) and organic layers were washed with brine, dried with MgSO₄ and concentrated under vacuum. The crude protected alcohol was dissolved in MeOH/THF (4:1) and a catalytic amount of pyridinium *p*-toluenesulfonate (0.04 mmol, 11 mg) was added and after stirring overnight the reaction mixture was quenched with saturated aqueous NaHCO₃. Water was added and the product was extracted with AcOEt, washed with brine and dried over MgSO₄, filtered and concentrated *in vacuo*. The crude product was purified by flash chromatography using petroleum ether/AcOEt (7:3) to afford the product **6** as a pale yellow oil (79 mg, 51%). The presence of two rotamers was observed in NMR spectra in a [0.63 (M): 0.37 (m)] ratio. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.12 – 7.44 (m, 10H), 6.98 (m) (t, *J* = 7.7 Hz, 0.37 H), 6.85 (M) (t, *J* = 7.7 Hz, 0.63 H), 5.19 (m) (d, *J* = 1.4 Hz, 0.74H), 5.06 (M) (s, 1.26H), 3.67 – 3.85 (m, 1H), 3.77 (m) (s, 1.1H), 3.64 (M) (s, 1.9H), 3.05 (m) (s, 1.1H), 3.03 (M) (s, 1.9H), 2.55 – 2.86 (m, 2H), 2.31 – 2.37 (m, 2H), 1.70 – 1.85 (m, 2H), 1.61 (bs, 1H); ¹³C NMR (δ, ppm) CDCl₃, 101 MHz. 164.5 (M), 164.0 (m), 156.2 (m), 155.6 (M), 141.7 (m), 141.4 (M), 139.8 (m), 138.1 (M), 136.4 (M), 136.2 (m), 134.2 (M), 134.0 (m), 128.4, 128.4, 128.4, 128.3, 128.3, 128.1, 128.0, 127.9, 127.8, 125.9, 125.8, 69.6 (M), 69.3 (m), 67.7 (m), 67.3 (M), 52.2 (m), 52.1 (M), 39.3 (m), 38.8 (M), 36.3 (M), 36.2 (m), 36.0 (m), 35.8 (M), 31.9 (m), 31.8 (M); IR: 3475, 3029, 2949, 1722, 1655, 1454, 1392, 1337, 1257, 1152, 1058, 915, 770, 747, 697; HRMS: Calculated for C₂₃H₂₇NO₅Na (M+Na⁺): 420.1787; found: 420.1781.

Experimental procedures (Intramolecular Oxa-Michael reaction)

Methyl (*R)-2-acetamido-2-((2*S**,4*S**,6*S**)-6-phenethyl-2-phenyl-1,3-dioxan-4-yl)acetate (4).**

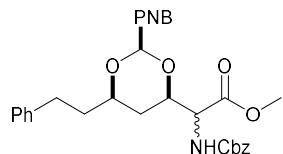


To a solution of methyl (*Z*)-2-formamido-5-hydroxy-7-phenylhept-2-enoate **3e** (0.68 mmol, 200 mg) in THF (7 mL) at 0°C was added benzaldehyde freshly distilled (2.1 mmol, 0.21 mL) followed by *t*BuOK (0.74 mmol, 84 mg). The resulting mixture was stirred for 15 min at 0°C and benzaldehyde (0.68 mmol, 0.07 mL) and *t*BuOK (0.068 mmol, 7.6 mg) were added. The same process – stirring for 15 min and adding benzaldehyde (0.68 mmol, 0.07 mL) and *t*BuOK (0.068 mmol, 7.6 mg) – was repeated twice. The resulting mixture was then stirred at room temperature for 24 h and quenched with a saturated aqueous NH₄Cl solution. The aqueous phase was extracted 3 times with AcOEt and the combined organic layers were dried over anhydrous MgSO₄, filtered and concentrated *in vacuo*. The crude residue was then purified by column chromatography using pentane/AcOEt to give the product as a colorless oil (23 mg, 9%). ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.00 – 7.60 (m, 10H), 6.25 (d, *J* = 9.3 Hz, 1H), 5.53 (s, 1H), 4.81 (dd, *J* = 9.3, 2.1 Hz, 1H), 4.34 – 4.52 (m, 1H), 3.81 – 3.86 (m, 1H), 3.78 (s, 3H), 2.69 – 2.90 (m, 2H), 2.07 (s, 3H), 1.96 - 2.06 (m, 2H), 1.79 – 1.96 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 170.9, 170.8, 141.8, 138.3, 129.1, 128.8, 128.7, 128.5, 126.2, 126.0, 100.4, 76.6, 75.6, 55.5, 53.0, 37.5, 33.1, 31.4, 23.5; IR: 2949, 2922, 2326, 1716, 1662, 1496, 1259, 1031; HRMS: Calculated for C₂₃H₂₇NO₅Na (M+Na⁺): 420.1787; found: 420.1779.

General procedure for conjugate intramolecular addition reaction. To a solution of homoallylic alcohol (1 equiv) in THF (0.1 M) at 0°C was added trifluoroacetophenone or *p*-nitrobenzaldehyde (3 equiv) followed by LiHMDS (1.1 equiv) and the resulting mixture was stirred for 15 min at 0°C. A second

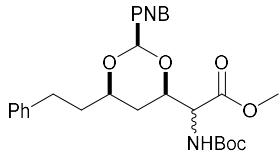
portion of trifluoroacetophenone (1 equiv) and LiHMDS (0.1 equiv) was added, after 15 min a third portion of trifluoroacetophenone (1.1 equiv) and LiHMDS (0.1 equiv) was made. The resulting mixture was then stirred at 0°C for 4 h and quenched with a saturated aqueous NH₄Cl solution. The aqueous phase was extracted 3 times with AcOEt and the combined organic layers were dried over anhydrous MgSO₄, filtered and concentrated *in vacuo*. The crude residue was then purified by column chromatography.

Methyl (R*)-2-(((benzyloxy)carbonyl)amino)-2-((2S*,4S*,6S*)-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4a).



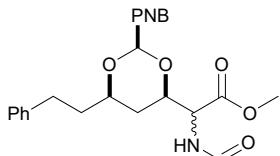
The typical procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3a** (0.21 mmol, 80 mg). The crude residue (*syn:anti* 54:46) was then purified by column chromatography using petroleum ether/Et₂O (8:2) to give the product **4a** as a yellow oil (22 mg, 20%). The presence of two isomers was observed in the NMR spectra, in a [0.60 (M):0.40 (m)] ratio. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.19 – 8.22 (m, 2H), 7.55 – 7.61 (m, 2H), 7.13 – 7.43 (m, 10H), 5.50 – 5.65 (m, 1.8H), 5.11 – 5.12 (m 2H), 4.51 (dd, *J* = 9.1, 2.1 Hz, 0.6H), 4.46 (dt, *J* = 11.2, 2.1 Hz, 0.6H), 3.83 – 3.91 (m, 1H), 3.79 (M) (s, 1.8H), 3.78 (m) (s, 1.2H), 2.60 – 2.96 (m, 2H), 1.80 - 2.11 (m, 2H), 1.61 – 1.71 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 170.3 (M), 169.5(m), 156.6, 148.1, 144.3, 141.2, 135.9, 130.4, 128.5, 128.5, 128.4, 128.3, 128.3, 128.2, 128.1, 127.1, 127.0, 126.0, 123.4, 99.1 (m), 98.8 (M), 77.6 (m), 77.2 (M), 75.9 (m), 76.6 (M), 67.3 (M), 67.3 (m), 57.4 (m), 57.3 (M), 52.8 (M), 52.6 (m), 37.0, 32.7 (m), 32.4 (M), 31.1; IR: 2954, 2858, 1722, 1604, 1596, 1454, 1437, 1340, 1212, 1123, 1054, 1028, 858, 748, 698; HRMS: Calculated for C₂₉H₃₀N₂O₈Na (M+Na⁺): 557.1900; found: 557.1886.

Methyl (R*)-2-((tert-butoxycarbonyl)amino)-2-((2S*,4S*,6S*)-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4b)



The general procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3b** (0.28 mmol, 100 mg). The crude residue (*syn:anti* 56:44) was then purified by column chromatography using pentane/AcOEt (9:1) to give the product **4b** as a colorless solid (50 mg, 36%). Mp: 110 °C The presence of two isomers was observed in the NMR spectra, in a [0.60 (M):0.40 (m)] ratio ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.22 (d, *J* = 8.6 Hz, 2H), 7.57– 7.60 (m, 2H), 7.15 – 7.35 (m, 5H), 5.56 (M) (s, 0.6H), 5.55 (m) (s, 0.4H), 5.37 – 7.42 (m) (m, 0.4H), 5.24 – 5.33 (M) (m, 0.6H), 4.44 – 4.46 (m, 1H), 3.74 – 3.94 (m, 1H), 3.79 (M) (s, 1.8H), 3.78 (m) (s, 1.2H), 2.61 – 2.98 (m, 2H), 2.10 – 1.76 – 2.10 (m, 4H), 1.45 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 170.7 (M), 169.9 (m), 155.9, 148.1, 144.5, 144.4, 141.3, 130.4, 128.5, 128.4, 127.1, 127.0, 126.0, 124.3, 123.3, 99.0 (m), 98.8 (M), 80.3, 75.9 (m), 75.7 (M), 56.8, 52.6 (M), 52.4 (m), 37.1 (M), 37.0 (m), 32.7 (m), 32.4 (M), 31.1 (M), 31.1 (m), 29.6, 28.2; IR: 1743, 1653, 1525, 1340, 1128, 1035, 858; HRMS: Calculated for C₂₆H₃₂N₂O₈Na (M+Na⁺): 523.2056 found: 523.2060

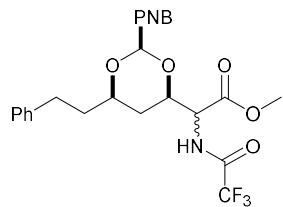
Methyl 2-formamido-2-((2R*,4R*,6R*)-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4c).



The typical procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3c** (0.34 mmol, 80 mg). The crude residue (*syn:anti* 78:22) was then purified by column chromatography using Et₂O/Petroleum ether (9:1) to give the products **4c** as a major diastereomer as a colorless solid (100

mg, 69%) Mp: 80 °C, and a minor diastereomer as a colorless solid. (15 mg, 10%). Mp: 85 °C Major diastereomer: ^1H NMR (400 MHz, CDCl_3) δ (ppm): 8.33 (s, 1H), 8.15 – 8.25 (m, 2H), 7.57 (d, J = 8.6 Hz, 2H), 7.19 – 7.32 (m, 5H), 6.40 (d, J = 9.2 Hz, 1H), 5.58 (s, 1H), 4.90 (dd, J = 9.2, 2.1 Hz, 1H), 4.50 (ddd, J = 9.2, 4.9, 2.1 Hz, 1H), 3.85 – 3.91 (m, 1H), 3.81 (s, 3H), 2.71 – 2.90 (m, 2H), 1.99 – 2.07 (m, 1H), 1.84 – 1.94 (m, 1H), 1.63 – 1.67 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ (ppm): 169.6, 161.1, 148.1, 144.2, 141.1, 128.4, 128.3, 126.9, 126.0, 123.3, 98.7, 76.3, 75.6, 53.5, 52.9, 36.9, 32.5, 31.0; IR: 3378, 2953, 2926, 2854, 1749, 1683, 1519, 1495, 1340, 1205, 1135, 1096; Minor diastereomer: ^1H NMR (400 MHz, CDCl_3) δ (ppm): 8.25 (s, 1H), 8.19 – 8.24 (m, 2H), 7.61 (d, J = 8.6 Hz, 2H), 7.15 – 7.33 (m, 5H), 6.56 (d, J = 8.1 Hz, 1H), 5.54 (s, 1H), 4.84 (dd, J = 8.1, 3.0 Hz, 1H), 4.16 (dt, J = 6.0, 3.0 Hz, 1H), 3.76 – 3.86 (m, 1H), 3.81 (s, 3H), 2.68 – 2.94 (m, 2H), 1.94 – 2.12 (m, 1H), 1.82 – 1.94 (m, 1H), 1.52 – 1.94 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ (ppm): 168.9, 160.4, 148.2, 144.3, 141.2, 128.4, 128.4, 127.1, 126.0, 123.4, 99.2, 77.4, 75.9, 54.2, 52.7, 37.0, 32.7, 31.1; HRMS: Calculated for $\text{C}_{22}\text{H}_{24}\text{N}_2\text{O}_7\text{Na} (\text{M}+\text{Na}^+)$: 451.1481; found: 451.1430.

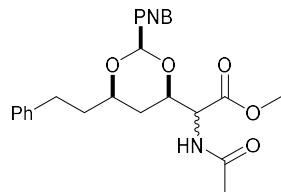
Methyl (R^*)-2-((2*S*^{*},4*S*^{*},6*S*^{*})-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)-2-(2,2,2-trifluoroacetamido)acetate (4d)



The general procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3d** (0.43 mmol, 150 mg). The crude residue (*syn:anti* 64:36) was then purified by column chromatography using pentane/AcOEt (8:2) to give the product **4d** as a colorless solid (68 mg, 32%). Mp: 88 °C The presence of two isomers was observed in the NMR spectra, in a [0.70 (M):0.30 (m)] ratio. ^1H NMR (400 MHz, CDCl_3) δ (ppm): 8.18 – 8.22 (m, 2H), 7.53 – 7.61 (m, 2H), 7.16 – 7.33 (m, 5H), 6.96 (d, J = 9.1 Hz,

1H), 5.59 (M) (s, 0.7H), 5.56 (m) (s, 0.3 H), 4.78 (M) (dd, $J = 9.1, 2.1$ Hz, 0.70H), 4.74 (m) (dd, $J = 8.0, 3.3$ Hz, 0.3H), 4.54 (M) (dt, $J = 11.8, 2.1$ Hz, 0.7H), 4.20 (m) (dt, $J = 12.0, 3.3$ Hz, 0.3H), 3.88 – 3.94 (m, 0.7H), 3.79 – 3.88, (m, 0.3H), 3.85 (m) (s, 0.9H), 3.84 (M) (s, 2.1H), 2.47 - 3.12 (m, 2H), 1.81 - 2.13 (m, 2H), 1.48 – 1.75 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ (ppm): 168.4 (M), 167.8 (m), 157.7 (d, $J_{\text{C}-\text{F}} = 38.3$ Hz), 148.2, 144.0, 143.8, 141.1, 141.0, 128.5, 128.4, 127.1, 127.0, 126.1, 123.5, 115.6 (d, $J_{\text{C}-\text{F}} = 38.3$ Hz), 99.3 (m), 99.0 (M), 75.9 (M), 75.8 (m), 75.5, 55.9 (m), 55.4 (M), 53.3 (M), 53.2 (m), 36.9, 32.5, 31.0; IR: HRMS: Calculated for $\text{C}_{23}\text{H}_{27}\text{F}_3\text{N}_3\text{O}_7$ ($\text{M}+\text{NH}_4^+$): 514.1801; found: 514.1805.

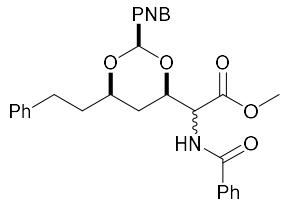
Methyl 2-acetamido-2-((2*R*^{*},4*R*^{*},6*R*^{*})-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4e).



The general procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3e** (0.27 mmol, 80 mg). The crude residue (*syn:anti* 77:23) was then purified by column chromatography using $\text{Et}_2\text{O}/\text{Petroleum ether}$ (7:3) to give the product **4e** as a major diastereomer as a colorless solid (90 mg, 71%) Mp: 90 °C, and minor diastereomer (5 mg, 4%) as a yellow oil. Major diastereomer: ^1H NMR (400 MHz, CDCl_3) δ (ppm): 8.22 (d, $J = 8.7$ Hz, 2H), 7.58 (d, $J = 8.7$ Hz, 2H), 7.16 – 7.34 (m, 5H), 6.18 (d, $J = 9.1$ Hz, 1H), 5.57 (s, 1H), 4.82 – 4.88 (m, 1H), 4.45 – 4.47 (m, 1H), 3.85 – 3.92 (m, 1H), 3.80 (s, 3H), 2.76 – 2.84 (m, 2H), 2.09 (s, 3H), 1.85 – 1.92 (m, 2H), 1.62 – 1.69 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ (ppm): 170.5, 170.2, 148.2, 144.3, 141.2, 128.5, 128.4, 126.9, 126.0, 123.4, 98.8, 76.6, 75.7, 55.0, 52.8, 37.0, 32.6, 31.1, 23.3; Minor diastereomer: ^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.99 (d, $J = 8.6$ Hz, 2H), 7.61 (d, $J = 8.6$ Hz, 2H), 7.10 – 7.38 (m, 5H), 4.75 (dd, $J = 8.1, 3.3$ Hz, 1H), 4.11 (dt, $J = 6.0, 3.3$ Hz, 1H), 3.79 – 3.83 (m, 1H), 3.80 (s, 3H), 2.78 (m, 2H), 2.05 (s, 3H), 1.93 – 1.61 (m, 4H); ^{13}C NMR (101 MHz, CDCl_3) δ (ppm): 169.7, 169.5, 148.2, 144.5, 141.2, 128.5, 128.4, 128.4, 127.1, 126.0,

123.8, 123.4, 99.2, 77.6, 76.0, 55.7, 52.6, 37.0, 32.9, 31.1, 23.1.IR: 3314, 2952, 2859, 1749, 1659, 1519, 1435, 1341, 1211, 1118, 1015, 859, 700; HRMS: Calculated for C₂₃H₂₆N₂O₇Na (M+Na⁺): 465.1638, found: 465.1617.

Methyl (R*)-2-benzamido-2-((2S*,4S*,6S*)-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4f).

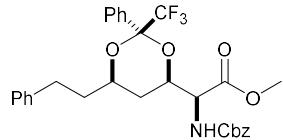


The typical procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3f** (0.22 mmol, 80 mg). The crude residue (*syn:anti* 69:31) was then purified by column chromatography using Et₂O/Petroleum ether (7:3) to give the product **4f** as a major diastereomer as a colorless solid (70 mg, 63%) Mp: 105 °C, and minor diastereomer as a colorless solid (13 mg, 12%) Mp: 112 °C.

Major diastereomer: ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.20 – 8.27 (m, 2H), 7.79 – 7.83 (m, 2H), 7.42 – 7.65 (m, 5H), 7.14 – 7.34 (m, 5H), 6.83 (d, *J* = 9.1 Hz, 1H), 5.62 (s, 1H), 5.07 (dd, *J* = 9.1, 2.2 Hz, 1H), 4.52 – 4.62 (m, 1H), 3.87 – 3.94 (m, 1H), 3.83 (s, 3H), 2.73 – 2.90 (m, 2H), 1.94 – 2.09 (m, 1H), 1.82 – 1.93 (m, 1H), 1.62 – 1.74 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 170.3, 167.7, 148.2, 144.4, 141.2, 133.5, 132.1, 128.7, 128.5, 128.4, 127.2, 127.0, 126.0, 123.4, 98.9, 76.9, 75.8, 55.5, 52.9 37.0, 32.8, 31.1; Minor diastereomer: ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.23 (d, *J* = 8.2 Hz, 2H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.41 – 7.66 (m, 5H), 7.17 – 7.33 (m, 5H), 7.07 (d, *J* = 7.9 Hz, 1H), 5.55 (s, 1H), 4.95 (dd, *J* = 7.9, 3.0 Hz, 1H), 4.26 (dt, *J* = 11.4, 3.0 Hz, 1H), 3.84 (s, 3H), 3.81 – 3.85 (m, 1H), 2.69 – 2.90 (m, 2H), 1.82 – 2.12 (m, 4H). ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 169.6, 166.8, 148.1 144.5, 141.2, 133.4, 132.0, 128.7, 128.4, 128.4, 127.2, 127.1, 126.0, 123.4, 99.2, 77.8, 76.1, 56.2, 52.7, 37.0, 33.0, 31.1.IR: 2954,

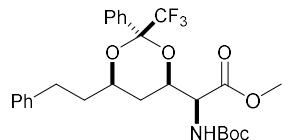
2927, 1746, 1661, 1581, 1486, 1295, 1125, 1104, 1015, 910, 859; HRMS: Calculated for C₂₈H₂₈N₂O₇Na (M+Na⁺): 527.1794; found: 527.1748

Methyl 2-(((benzyloxy)carbonyl)amino)-2-((2S*,4R*,6R*)-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5a).



The general procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3a** (0.21 mmol, 80 mg). The crude residue (*syn:anti* 96:4) was then purified by column chromatography using Et₂O/Petroleum ether (9:1) to give the product **5a** which was isolated as a single diastereoisomer and as a white solid (42 mg, 36%, 83% brsm). Mp: 102 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.16 – 7.47 (m, 15H), 5.60 (d, *J* = 9.9 Hz, 1H), 5.18 (m, 2H), 4.46 (dd, *J* = 9.9, 2.0 Hz, 1H), 4.41 (dt, *J* = 11.7, 2.1 Hz, 1H), 3.88 (s, 3H), 3.84 (m, 1H), 2.84 – 2.99 (m, 1H), 2.69 – 2.79 (m, 1H), 1.96 – 2.13 (m, 2H), 1.78 – 1.90 (m, 1H), 1.37 – 1.54 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 170.0, 156.7, 141.1, 136.0, 131.4, 130.0, 128.7, 128.6, 128.5, 128.3, 128.3, 128.1, 126.0, 121.2 (q, *J*_{C-F} = 284.5 Hz), 98.5 (q, *J*_{C-F} = 32.3 Hz), 71.0, 69.9, 67.4, 57.2, 52.6, 37.0, 31.9, 30.3; ¹⁹F NMR (376 MHz, CDCl₃) δ (ppm): -85.34; IR: 2929, 2851, 1727, 1509, 1452, 1325, 1193, 1123, 1058, 986, 725, 698; HRMS: Calculated for C₃₀H₃₀F₃NO₆Na (M+Na⁺): 580.1923; Found: 580.1930.

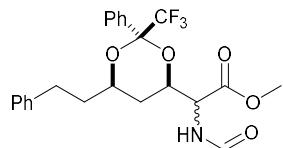
Methyl (R*)-2-((tert-butoxycarbonyl)amino)-2-((2S*,4S*,6S*)-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5b)



The typical procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3b** (0.28 mmol, 100 mg). The crude residue (*syn:anti* 96:4) was then purified by column chromatography

using pentane/AcOEt (9:1) to give the product **5b** which was isolated as a single diastereoisomer and as a pale yellow oil (44 mg, 28 %). ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.09 – 7.57 (m, 10H), 5.33 (d, *J* = 9.2 Hz, 1H), 4.39 (d, *J* = 10.0 Hz, 2H), 3.87 (s, 3H), 3.75 – 3.89 (m, 1H), 2.86 – 2.99 (m, 1H), 2.61 – 2.83 (m, 1H), 1.74 - 2.15 (m, 4H), 1.48 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 170.3, 156.1, 141.2, 131.4, 129.9, 128.7, 128.5, 128.4, 128.2, 126.0, 121.2 (q, *J*_{C-F} = 284 Hz), 98.4 (q, *J*_{C-F} = 32.2 Hz), 80.4, 71.0, 69.9, 56.6, 52.4, 37.0, 32.4, 30.9, 28.5. ¹⁹F NMR (376 MHz, CDCl₃) δ (ppm): -85.45; IR: 2930, 1750, 1718, 1497, 1452, 1367, 1193, 1123, 1059, 986, 724, 699; HRMS: Calculated: C₂₇H₃₂F₃NO₆ Na: 546,2079, Found: 546,2079.

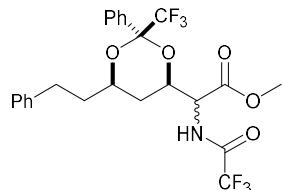
Methyl (*R*^{*})-2-formamido-2-((2*R*^{*},4*S*^{*},6*S*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5c).



The typical procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3c** (0.36 mmol, 100 mg). The crude residue (*syn:anti* 89:11) was then purified by column chromatography using Et₂O/Petroleum ether (8:2) to give the product **5c** as a pale yellow solid (128 mg, 79%). After purification, the presence of two isomers was observed in the NMR spectra, in a [0.88 (M):0.12 (m)] ratio. Mp: 139 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.41 (M) (s, 0.88H), 8.28 (m) (s, 0.12H) 7.11 – 7.51 (m, 10H), 6.71 (m) (d, *J* = 6.2 Hz, 0.12H), 6.47 (M) (d, *J* = 9.2 Hz, 0.88H), 4.85 (M) (dd, *J* = 9.2, 2.0 Hz, 0.88H), 4.74 (m) (dd, *J* = 8.1, 3.3 Hz, 0.12H), 4.44 (M) (dt, *J* = 11.8, 2.0 Hz, 0.88H), 4.07 (m) (dt, *J* = 12.0, 3.0 Hz, 0.12H), 3.89 (M) (s, 2.64H), 3.86 (m) (s, 0.36H), 3.75 – 3.93 (m, 1H), 2.88 – 2.96 (m, 2H), 1.85 – 2.06 (m, 2H), 1.55 – 1.71 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 169.7 (M), 169.2 (m), 161.6, (M), 160.7 (m), 141.4 (m), 141.3 (M), 131.7 (m), 131.6 (M), 130.1, 128.8, 128.7, 128.6, 128.4, 128.2, 126.0, 121.5 (q, *J*_{C-F} = 285 Hz), 98.8 (q, *J* = 32.3 Hz), 72.5 (m), 71.2 (M), 70.6, 70.2 (M), 54.8 (m), 53.5

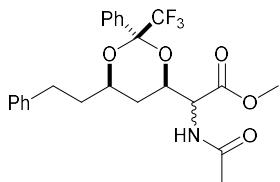
(M), 53.1 (M), 53.1 (m), 37.3 (m), 37.2 (M), 32.8 (m), 82.3 (M), 31.3 (m), 31.2 (M). ^{19}F NMR (376 MHz, CDCl_3) δ (ppm): -85.63 (m), -85.90 (M); IR: 3315, 2953, 3029, 1749, 1666, 1540, 1326, 1192, 1120, 985; HRMS: Calculated for $\text{C}_{23}\text{H}_{24}\text{F}_3\text{NO}_5\text{Na} (\text{M}+\text{Na}^+)$: 474.1504; Found: 474.1503.

Methyl (*R)-2-((2*S**,4*S**,6*S**)-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)-2-(2,2,2-trifluoroacetamido)acetate (5d).**



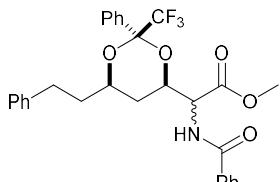
The general procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3d** (0.29 mmol, 100 mg). The crude residue (*syn:anti* 67:33) was then purified by column chromatography using $\text{CH}_2\text{Cl}_2/\text{cyclohexane}$ (7:3) to give the product **5d** as a pale yellow solid (34 mg, 23%). After purification, the presence of two isomers was observed in the NMR spectra, in a [0.60 (M):0.40 (m)] ratio. Mp: 99 °C. ^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.28 – 7.42 (m, 7H), 7.20 – 7.23 (m, 3.4H), 7.07 (M) (d, $J = 9.1$ Hz, 0.6H), 4.74 (M) (dd, $J = 9.1, 2.0$ Hz, 0.6H), 4.63 (m) (dd, $J = 8.1, 3.3$ Hz, 0.4H), 4.51 (M) (dt, $J = 11.8, 2.0$ Hz, 0.6H), 4.08 (m) (dt, $J = 12.0, 3.3$ Hz, 0.4H), 3.92 (m) (s, 1.2H), 3.90 (M) (s, 1.8H), 3.66 – 3.88 (m, 1H), 2.62 - 3.02 (m, 2H), 1.81 - 2.18 (m, 2H), 1.42 - 1.68 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ (ppm): 168.2 (m), 167.5 (M), 157.8 (q, $J_{\text{C}-\text{F}} = 38.3$ Hz), 156.6 (q, $J_{\text{C}-\text{F}} = 38.3$ Hz), 141.0 (m), 140.9 (M), 131.2 (M), 131.1 (m), 130.2, 130.2, 128.9, 128.8, 128.6, 128.6, 128.5, 128.4, 128.3, 128.3, 126.1, 126.1, 118.4 (q, $J_{\text{C}-\text{F}} = 286.1$ Hz), 98.5 (q, $J_{\text{C}-\text{F}} = 29.3$ Hz), 71.7 (M), 70.6 (m), 70.3 (m), 69.8 (M), 56.1 (M), 55.3 (m), 53.2 (m), 53.1 (M), 36.9 (m), 36.8 (M), 32.3 (M), 32.0 (m), 30.9 (m), 30.9 (M). ^{19}F NMR (376 MHz, CDCl_3) δ (ppm): -73.56 (M), -73.58 (m), -85.63 (m), 85.74 (M). IR: 1722, 1714, 1521, 1518, 1344, 1161, 1014, 854. HRMS: Calculated for $\text{C}_{24}\text{H}_{27}\text{F}_6\text{N}_2\text{O}_5 (\text{M}+\text{H}^+)$: 537.1824; found: 537.1824

Methyl 2-acetamido-2-((2*R*^{*},4*S*^{*},6*S*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5e).



The typical procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3e** (0.18 mmol, 54 mg). The crude residue (*syn:anti* 90:10) was then purified by column chromatography using Et₂O/Petroleum ether (8:2) to give the product **5e** which was isolated as a single diastereoisomer and as a colorless solid (69 mg, 81%). Mp: 138 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.13 – 7.53 (m, 10H), 6.28 (d, *J* = 9.4 Hz, 1H), 4.79 (dd, *J* = 9.5, 1.9 Hz, 1H), 4.40 (dt, *J* = 11.8, 2.1 Hz, 1H), 3.88 (s, 1H), 3.82 (m, 1H), 2.67 - 2.96 (m, 2H), 2.15 (s, 3H), 1.98 – 2.08 (m, 2H), 1.83 – 1.88 (m, 2H), 1.60 – 1.69 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 170.6, 169.9, 141.0, 131.4, 130.0, 128.6, 128.6, 128.4, 128.4, 128.2, 126.0, 121.3 (q, *J*_{C-F} = 284 Hz), 98.6 (q, *J*_{C-F} = 32.2 Hz), 71.1, 69.9, 54.7, 52.6, 37.0, 32.0, 30.9, 23.1. ¹⁹F NMR (376 MHz, CDCl₃) δ (ppm): -85.28; IR: 1758, 1647, 1538, 1453, 1436, 1375, 1323, 1193, 1172, 1118, 1062, 910, 765, 728; HRMS: Calculated for C₂₄H₂₆F₃NO₅Na (M+Na⁺): 488.1643; Found: 488.1655.

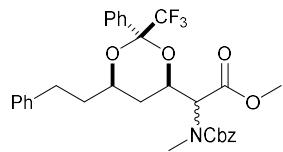
Methyl 2-benzamido-2-((2*R*^{*},4*R*^{*},6*R*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5f).



The general procedure for conjugate intramolecular addition reaction was applied to homoallylic alcohol **3f** (0.22 mmol, 80 mg). The crude residue (*syn:anti* 91:9) was then purified by column chromatography

using Et₂O/Petroleum ether (6:4) to give the product **5f** which as isolated as a single diastereoisomer and as a colorless solid (102 mg, 85%). Mp: 140 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.85 – 7.92 (m, 2H), 7.38 – 7.88 (m, 8H), 7.25 – 7.30 (m, 2H), 7.15 – 7.22 (m, 3H), 6.99 (d, *J* = 9.2 Hz, 1H), 5.01 (dd, *J* = 9.4, 1.9 Hz, 1H), 4.53 (d, *J* = 11.8, 2.3 Hz, 1H), 3.91 (s, 3H), 3.82 – 3.89 (m, 1H), 2.64 – 3.01 (m, 2H), 1.68 – 2.10 (m, 4H); ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 169.9, 167.6, 141.0, 133.4, 132.0, 131.4, 130.0, 128.7, 128.7, 128.6, 128.5, 128.3, 128.2, 128.2, 127.1, 126.9, 125.9, 121.4, (q, *J*_{C-F} = 284.4 Hz), 98.5 (q, *J*_{C-F} = 32.3 Hz), 71.4, 69.8, 55.1, 52.7, 36.8, 32.1, 30.8, 26.8; ¹⁹F NMR (376 MHz, CDCl₃) δ (ppm): -85.55; IR: 2927, 2851, 1743, 1654, 1522, 1488, 1193, 1124, 1063, 724, 699; HRMS: Calculated for C₂₉H₂₉F₃NO₅ (M+H⁺): 528.1998; Found: 528.1995.

Methyl (*R*^{*})-2-((2*R*^{*},4*S*^{*},6*S*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)-2-(2,2,2-trifluoroacetamido)acetate (7b).

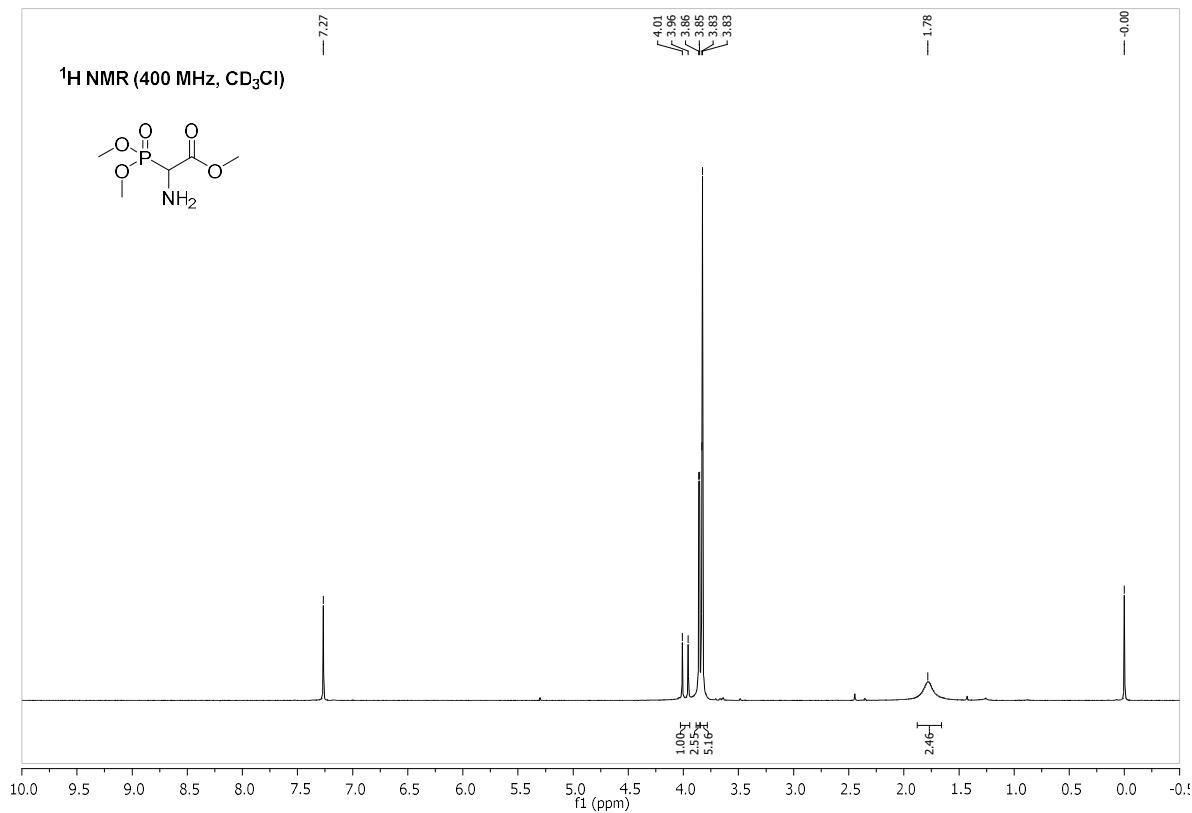


To a solution of homoallylic alcohol **6** (0.15 mmol, 60 mg) in THF (1.5 mL) at 0°C was added trifluoroacetophenone (0.45 mmol, 0.064 mL) followed by 2.16 M LiHMDS (0.045 mmol, 0.021 mL). The resulting mixture was stirred for 15 min at 0°C. A second portion of trifluoroacetophenone (0.15 mmol, 0.02 mL) and base (0.015 mmol, 0.007 mL) was added, after 15 min a third portion of trifluoroacetophenone (0.15 mmol, 0.02 mL) and base (0.015 mmol, 0.007 mL) was made; then a fourth addition of trifluoroacetophenone (0.15 mmol, 0.02 mL) and base (0.015 mmol, 0.007 mL) was added. The resulting mixture was then stirred at room temperature for 3 h and quenched with a saturated aqueous NH₄Cl solution. The aqueous phase was extracted 3 times with AcOEt and the combined organic layers were dried over anhydrous MgSO₄, filtered and concentrated in vacuo. The crude residue (*syn:anti* 56:44) was then purified by column chromatography using Et₂O/Petroleum ether (9:1) to give the product **7b** as

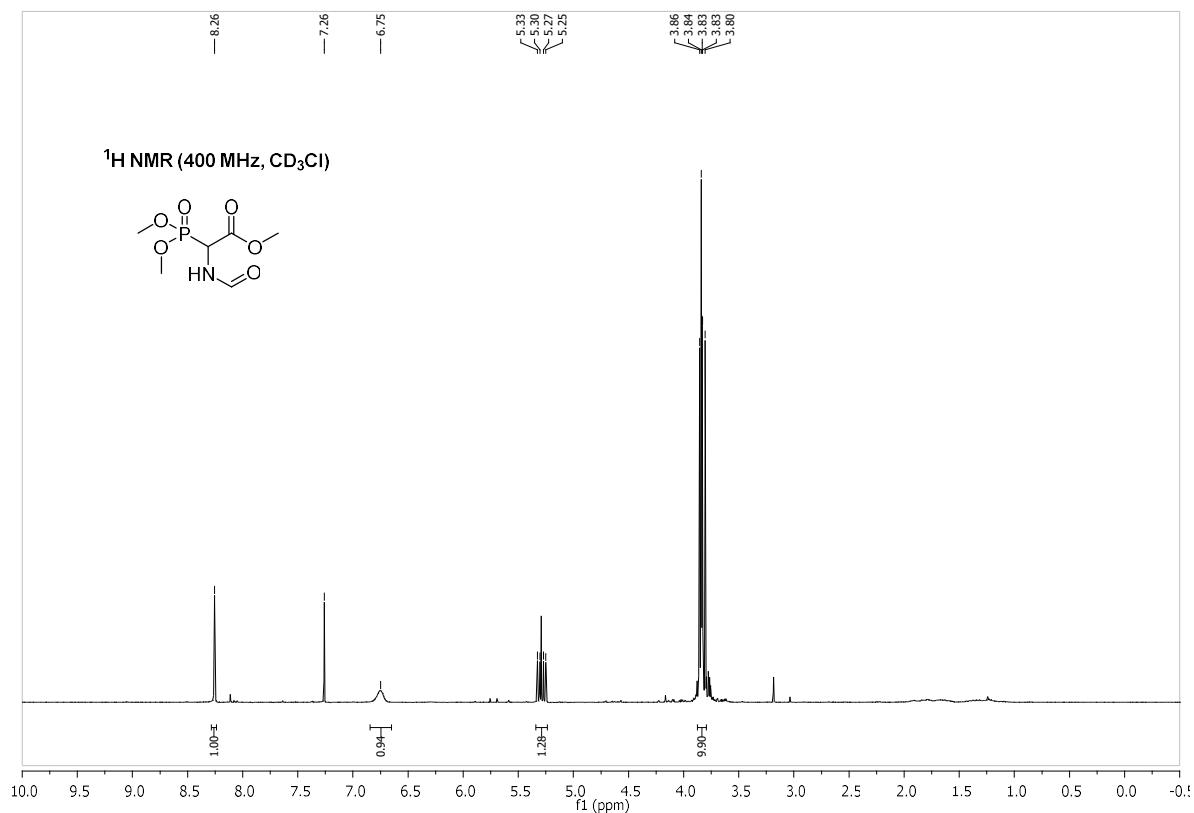
a pale yellow oil (19 mg, 22%). The crude residue (*syn:anti* 56:44) was then purified by column chromatography using Et₂O/Petroleum ether (9:1) to give the product **7b** as a pale yellow oil (19 mg, 22%). The presence of two isomers was observed in the NMR spectra, in a [0.77 (M):0.23 (m)]. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 6.81 - 7.89 (m, 15H), 5.14 – 5.32 (m, 2H), 5.03 (d, *J* = 3.3 Hz, 0.78H), 4.74 (d, *J* = 4.5 Hz, 0.22H), 4.58 (dt, *J* = 11.4, 3.3 Hz, 0.77H), 4.42 – 4.46 (m, 0.23 H), 3.87 (M) (s, 2.2H), 3.77 (m) (s, 0.8H), 3.80 – 3.84 (m, 1H), 3.18 (M) (s, 2.2H), 3.15 (m) (s, 0.8H), 2.89 – 2.97 (m, 2H), 2.60 – 2.76 (m, 2H), 1.97 – 2.04 (m, 1H), 1.79 – 1.88 (m, 1H), 1.48 – 1.58 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ (ppm): 169.5 (M), 169.2 (m), 158.0 (M), 156.4 (m), 141.5, 136.8 (M), 136.6 (m), 131.8 (m), 131.7 (M), 130.3, 129.3, 129.0, 128.9, 128.9, 128.8, 128.6, 128.5, 128.4, 127.9, 126.3, 121.8 (q, *J*_{C-F} = 284.5 Hz), 98.9 (q, *J*_{C-F} = 32.0 Hz), 71.4 (M), 70.8 (m), 70.2 (M), 70.1 (m), 68.1 (M), 68.0 (m), 62.3 (m), 61.9 (M), 52.7, 37.4 (M), 37.3 (m), 34.6 (m), 34.1 (M), 33.0 (m), 32.7 (M), 31.3 (m), 30.6 (M); IR: 2952, 2919, 1744, 1699, 1551, 1399, 1308, 1187, 1125, 1062, 998; HRMS: Calculated for C₃₁H₃₂F₃NO₆Na (M+Na⁺): 594.2079; Found: 594.2036.

COPY OF NMR SPECTRA

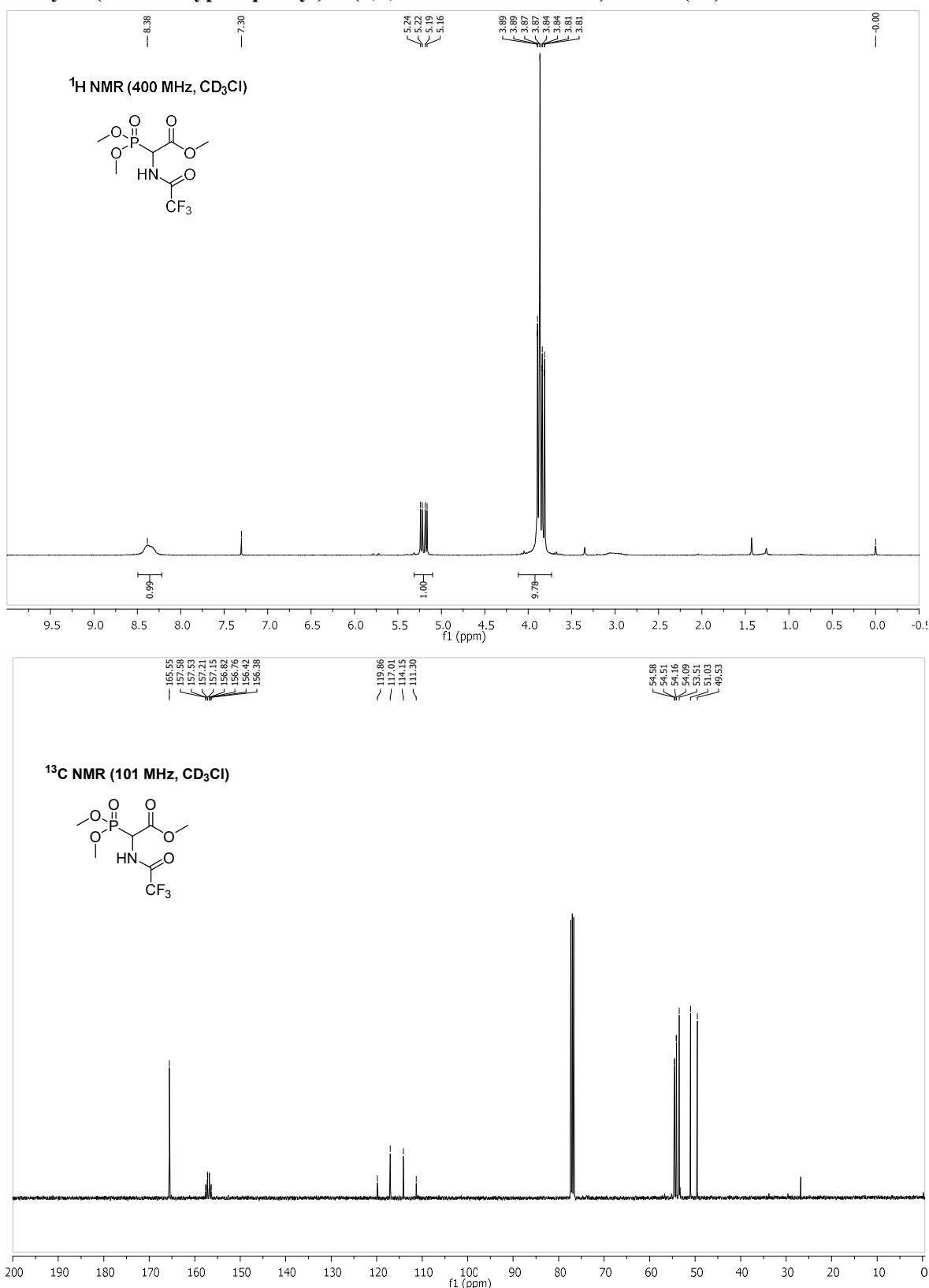
Methyl 2-amino-2-(dimethoxyphosphorylacetate)



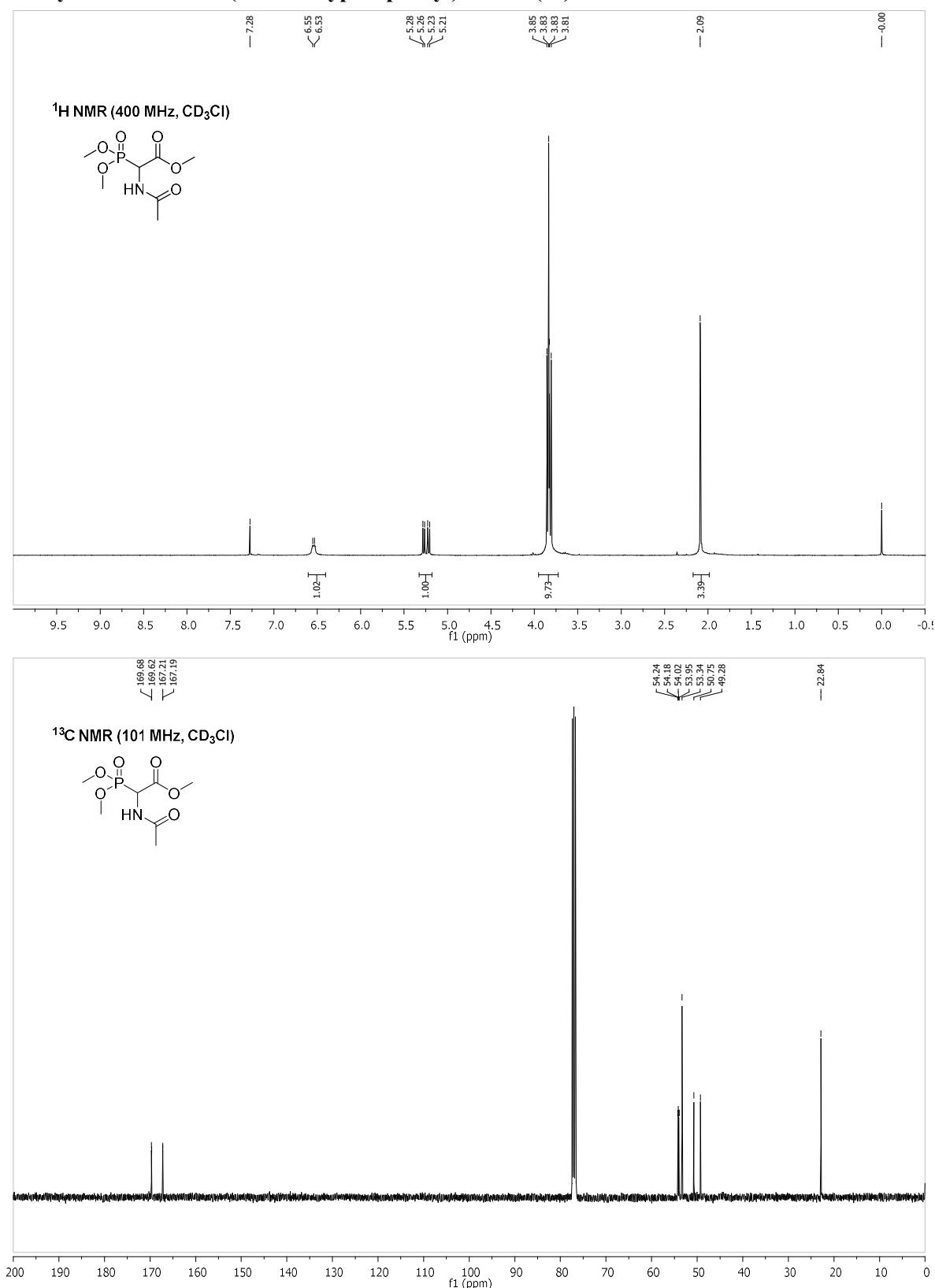
Methyl 2-(dimethoxyphosphoryl)-2-formamidoacetate (1c)



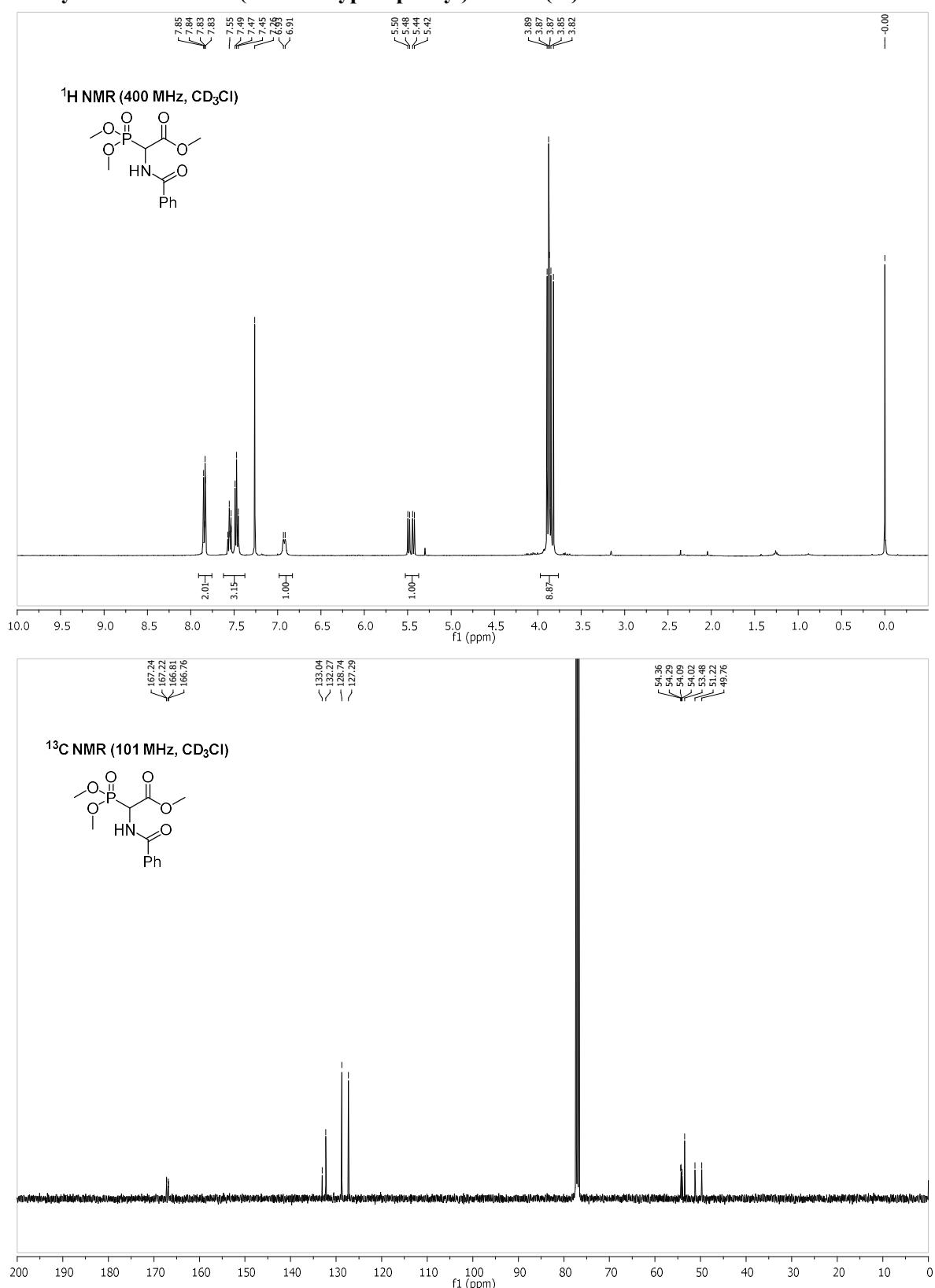
Methyl 2-(dimethoxyphosphoryl)-2-(2,2,2-trifluoroacetamido)acetate (1d)



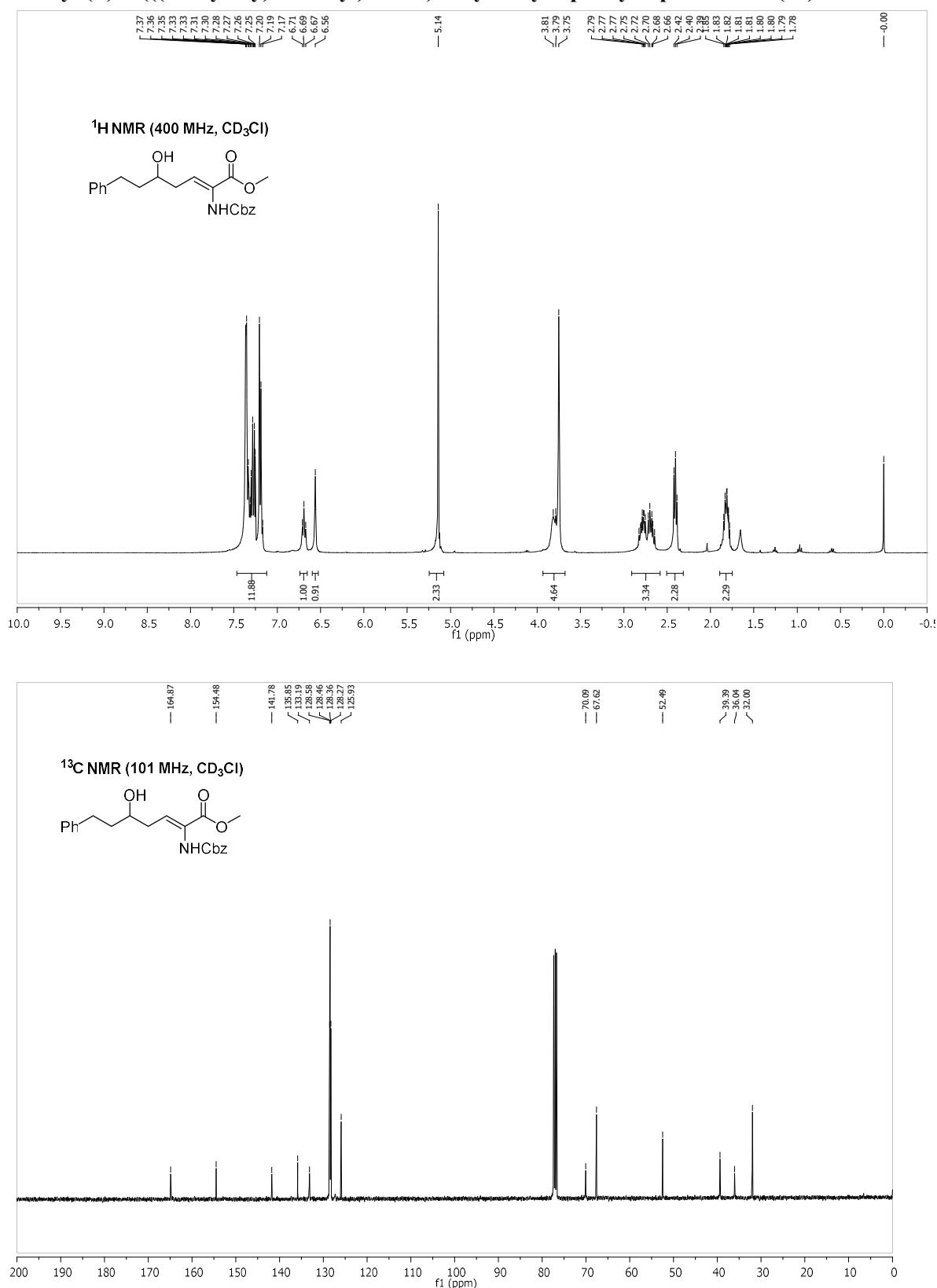
Methyl 2-acetamido-2-(dimethoxyphosphoryl)acetate (1e)



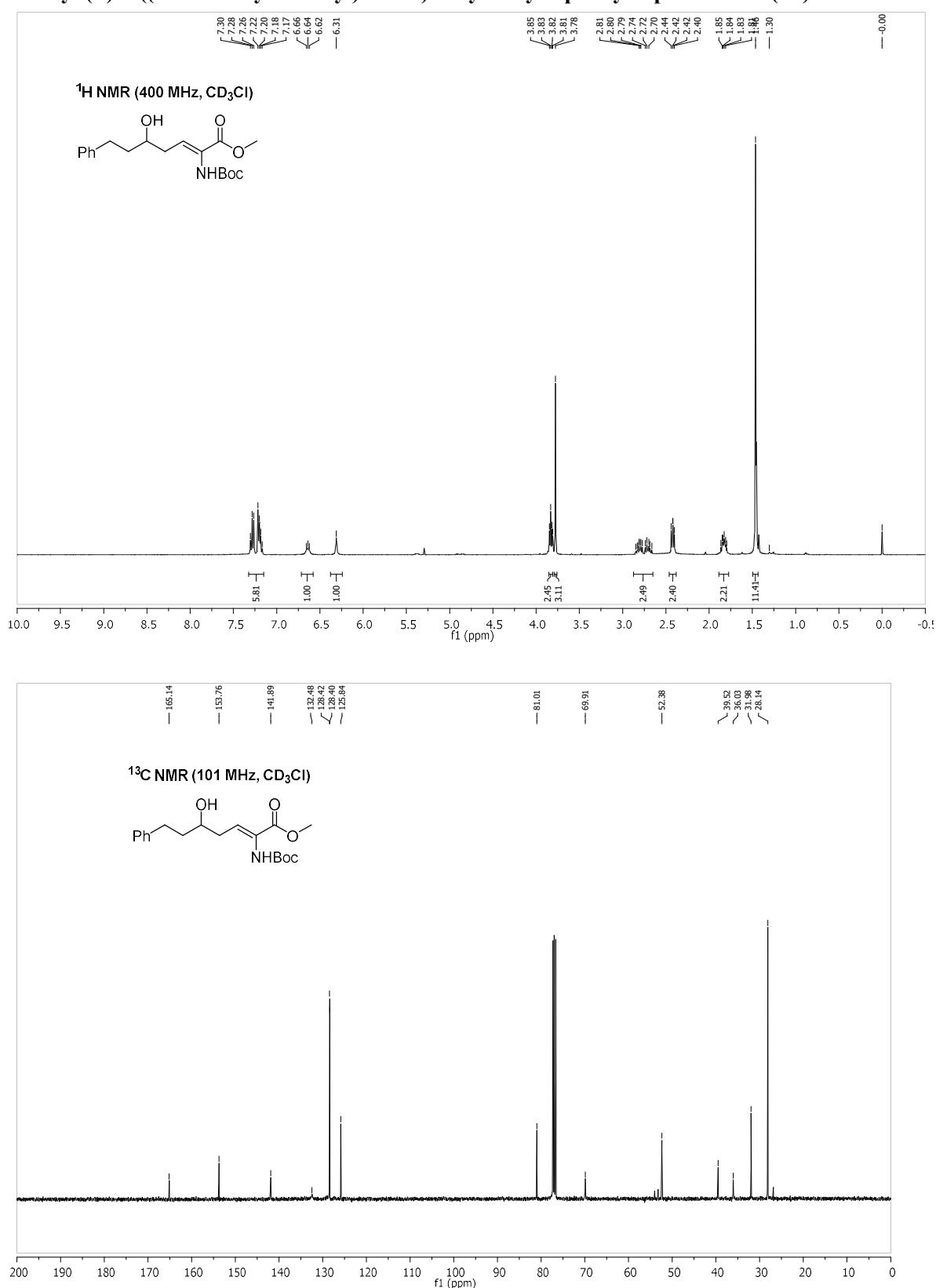
Methyl 2-benzamido-2-(dimethoxyphosphoryl)acetate (1f)



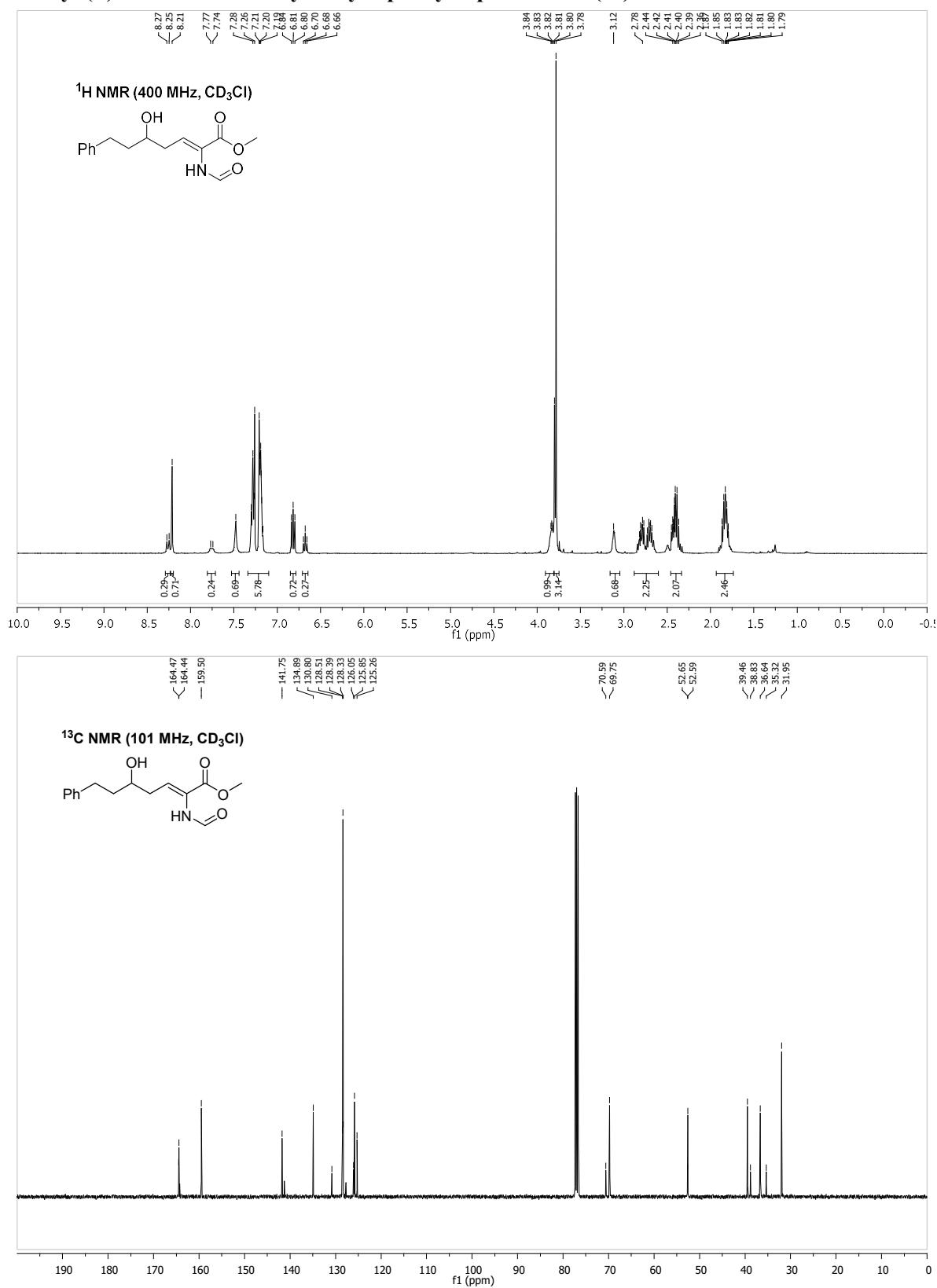
Methyl (Z)-2-((benzyloxy)carbonyl)amino)-5-hydroxy-7-phenylhept-2-enoate (3a)



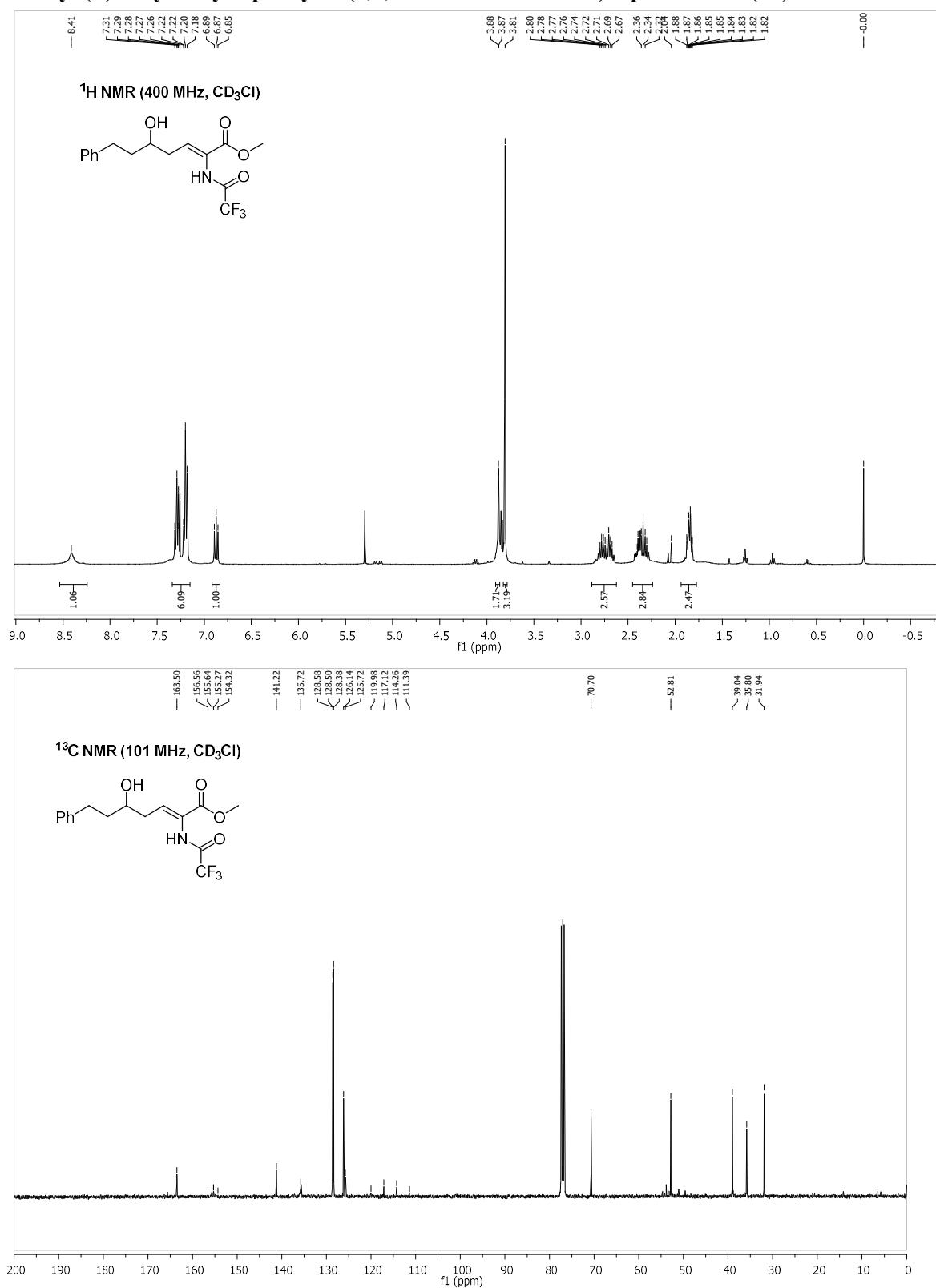
Methyl (*Z*) 2-((tert-butoxycarbonyl)amino)-5-hydroxy-7-phenylhept-2-enoate (3b)



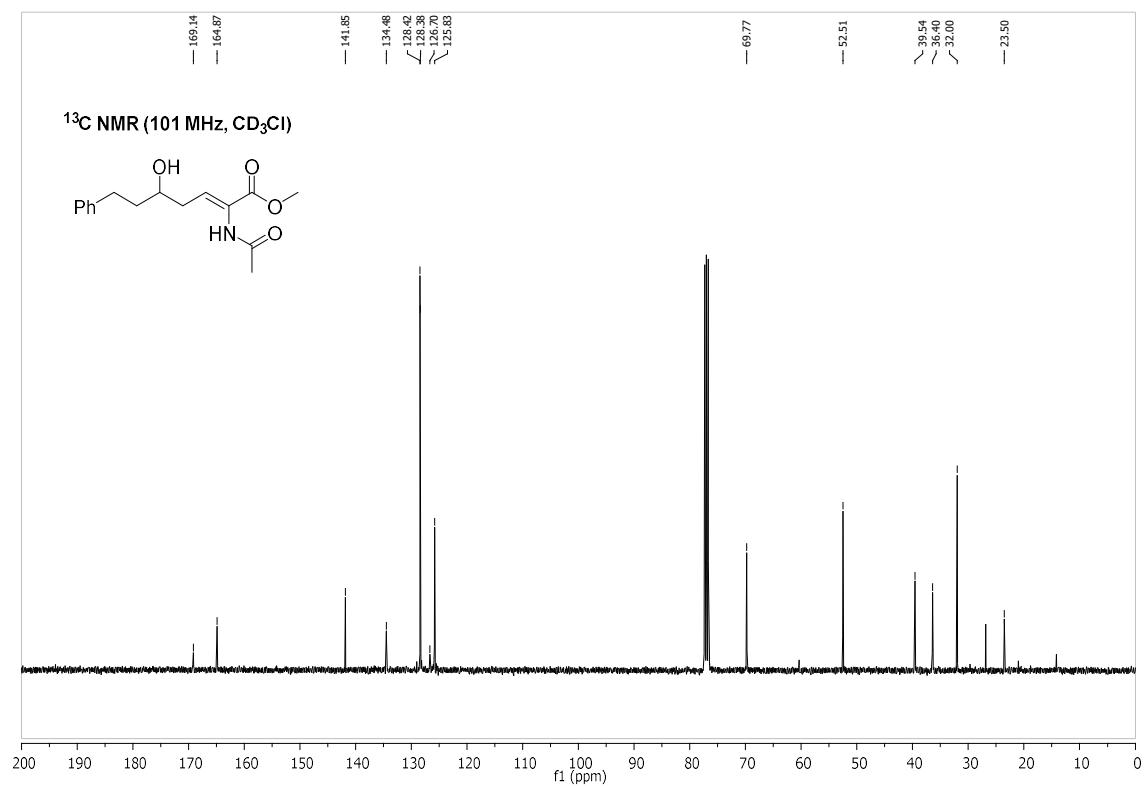
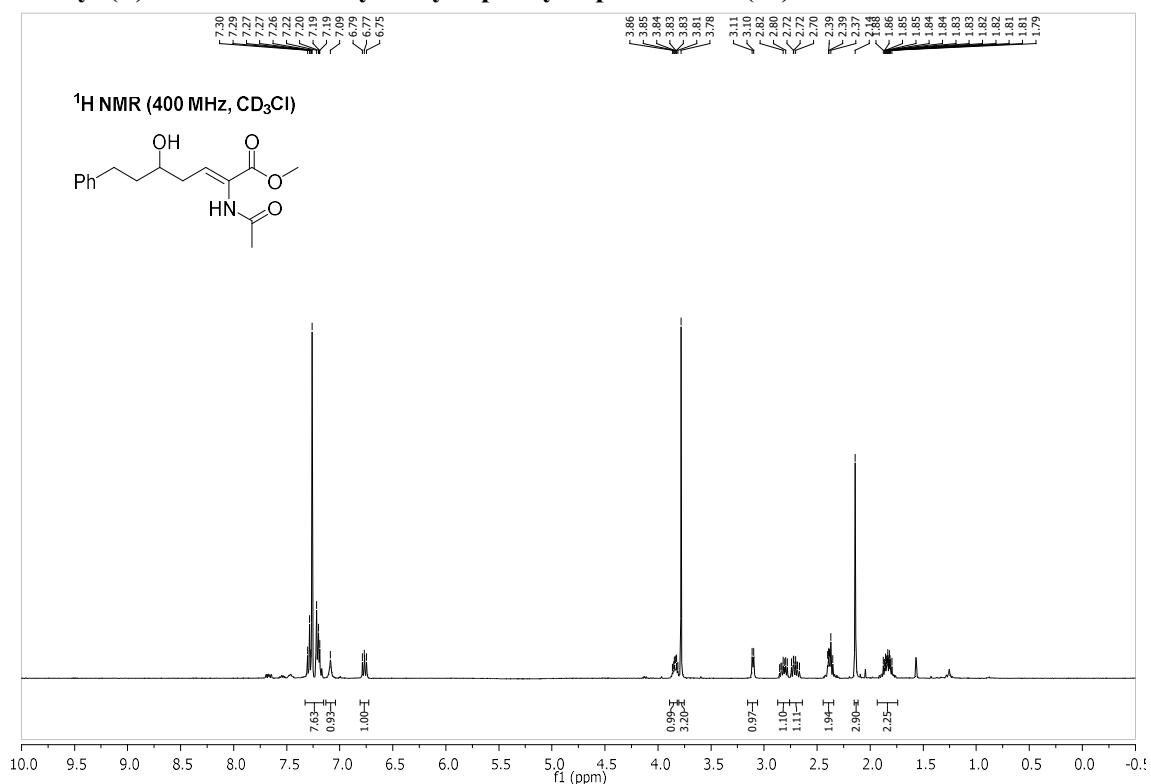
Methyl (*Z*)-2-formamido-5-hydroxy-7-phenylhept-2-enoate (3c)



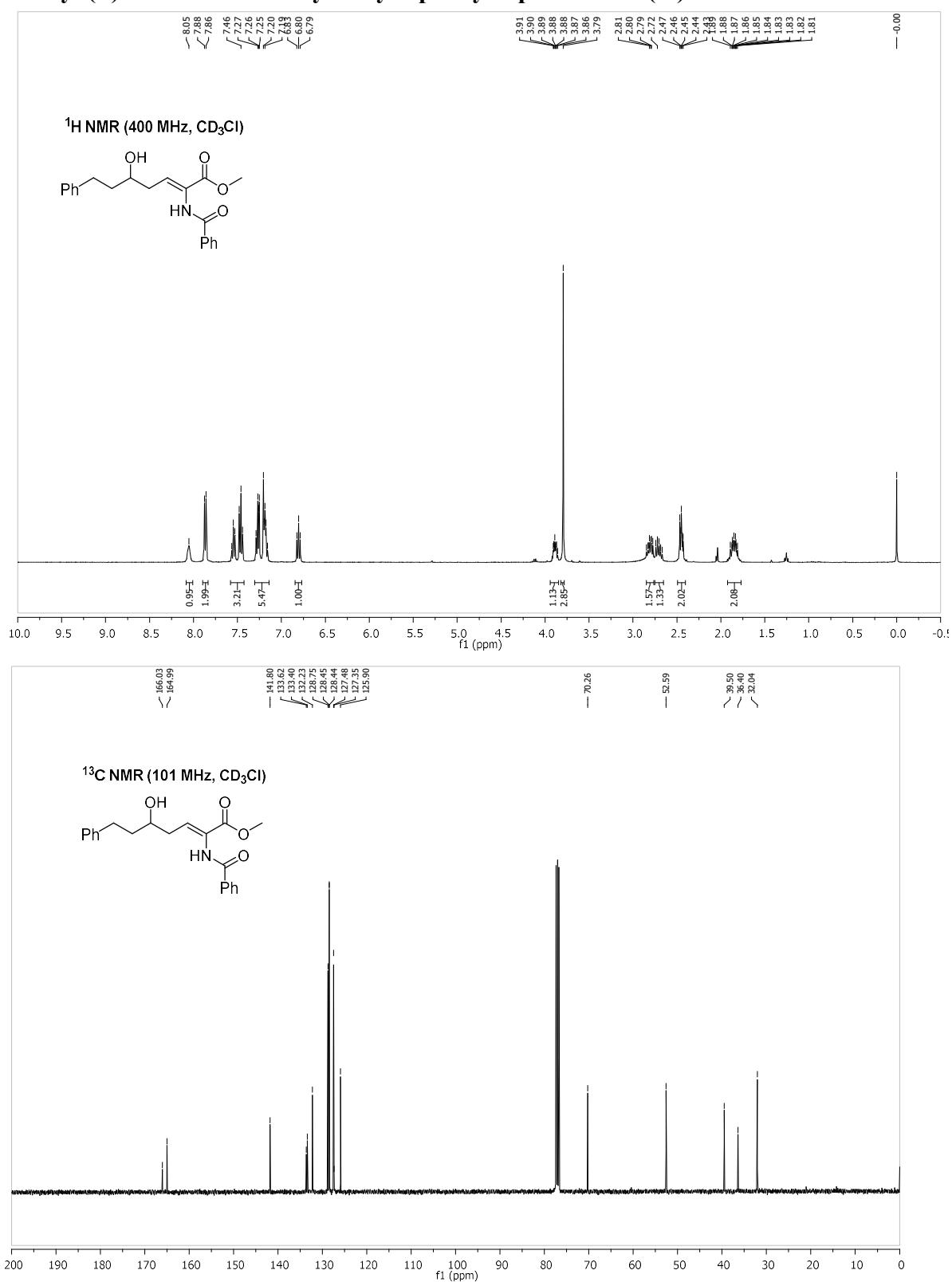
Methyl (Z)-5-hydroxy-7-phenyl-2-(2,2,2-trifluoroacetamido)hept-2-enoate (3d)



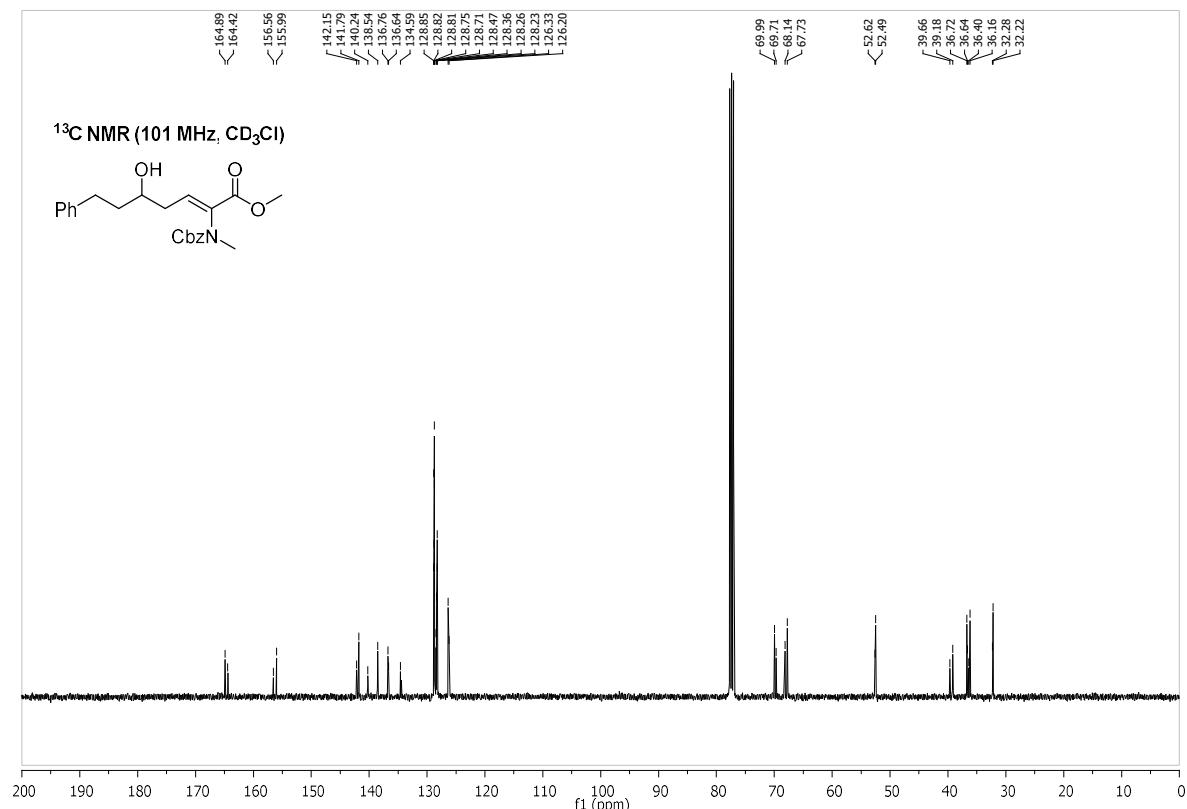
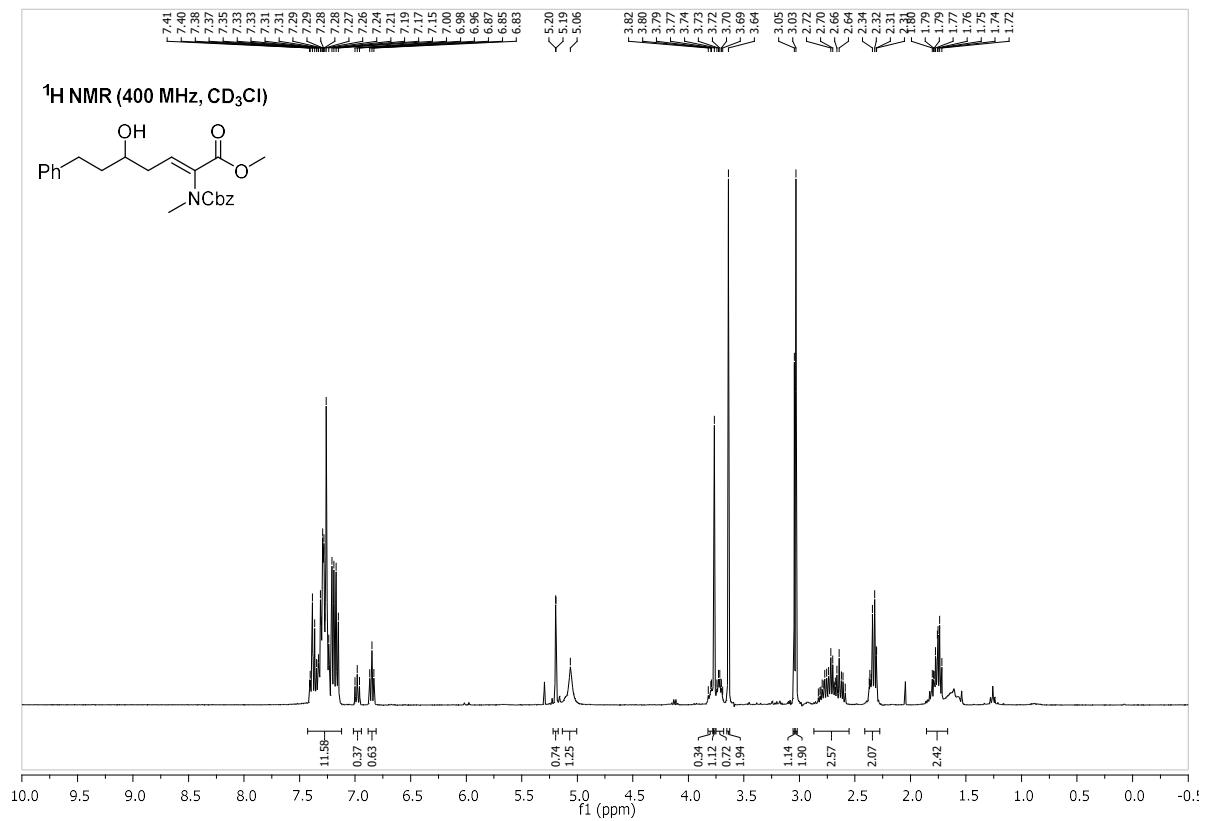
Methyl (Z)-2-acetamido-5-hydroxy-7-phenylhept-2-enoate (3e)



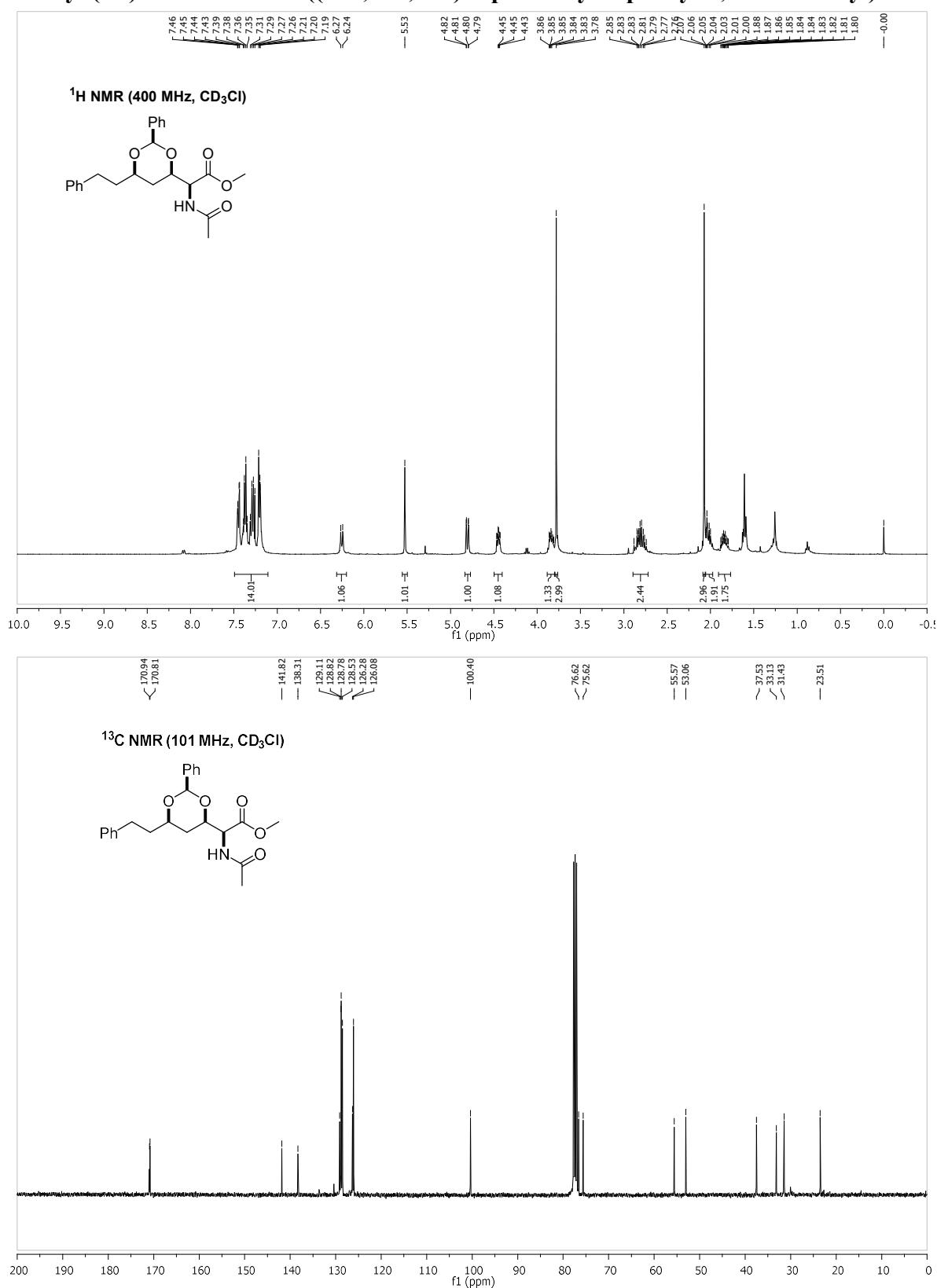
Methyl (Z)-2-benzamido-5-hydroxy-7-phenylhept-2-enoate (3f)



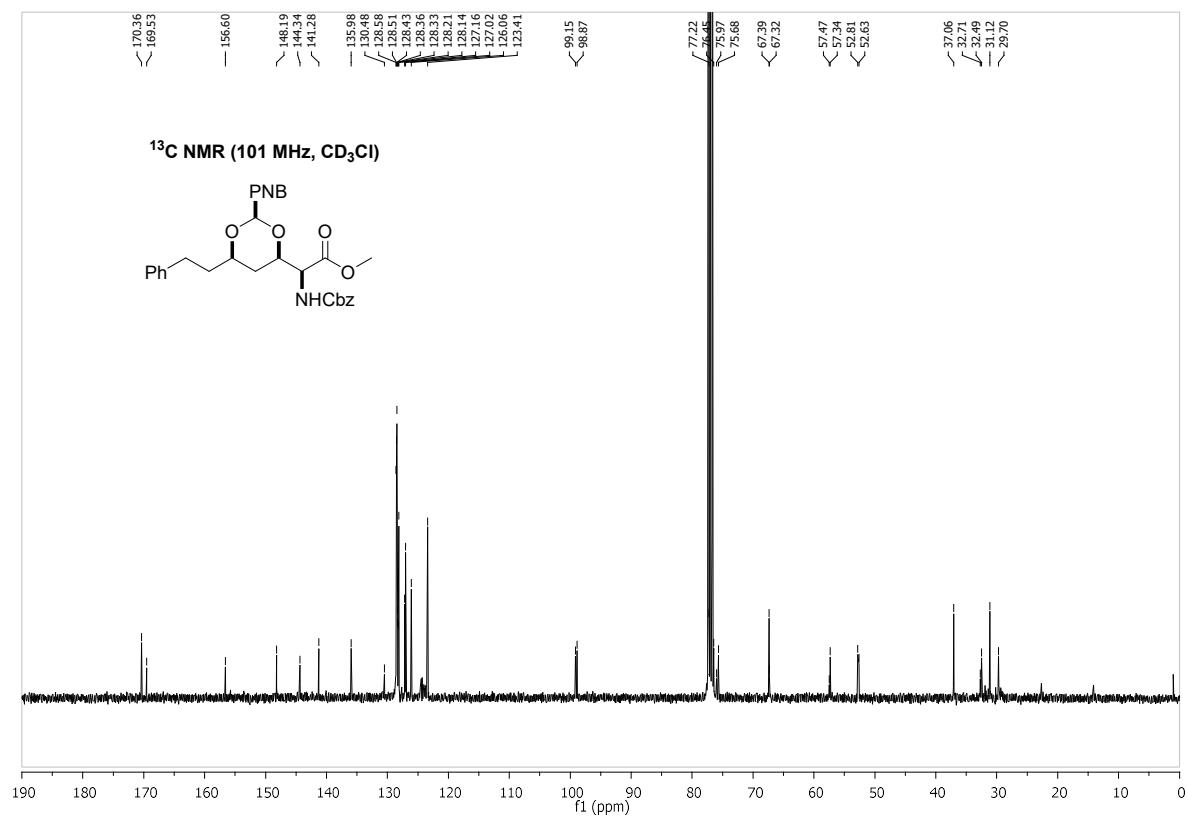
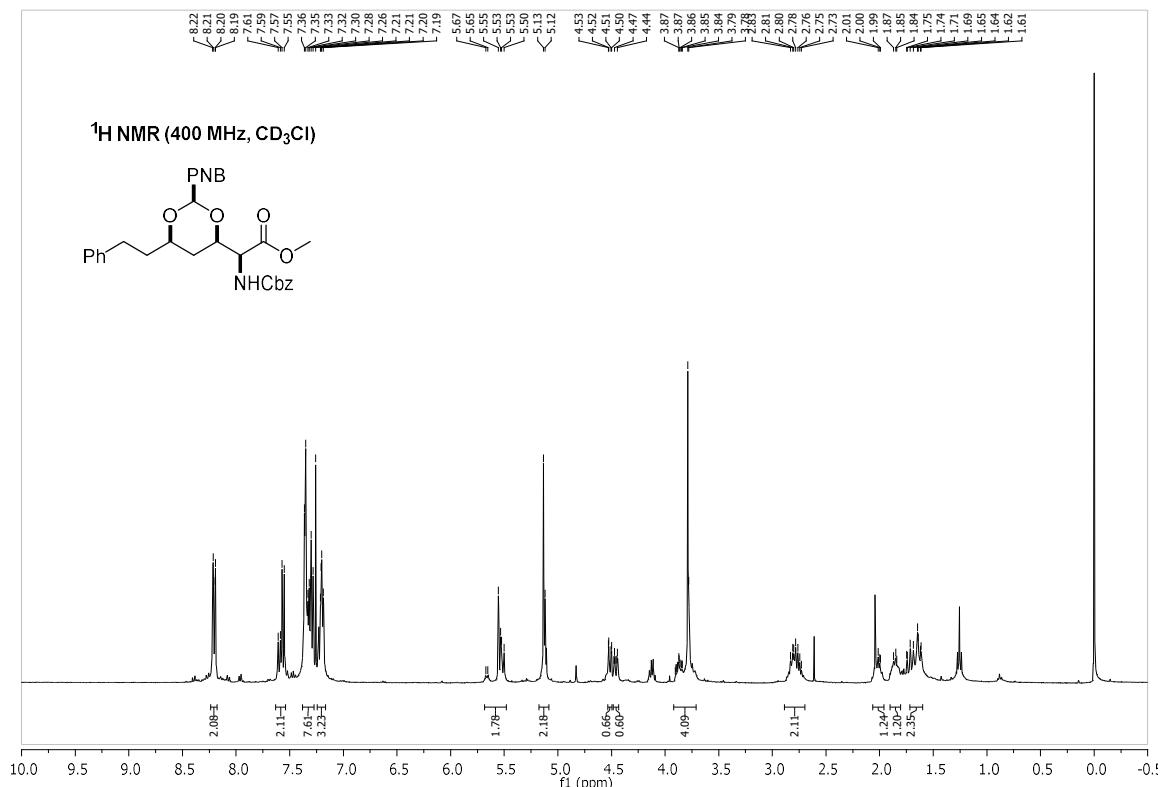
Methyl (Z)-2-(((benzyloxy)carbonyl)(methyl)amino)-5-hydroxy-7-phenylhept-2-enoate (6)



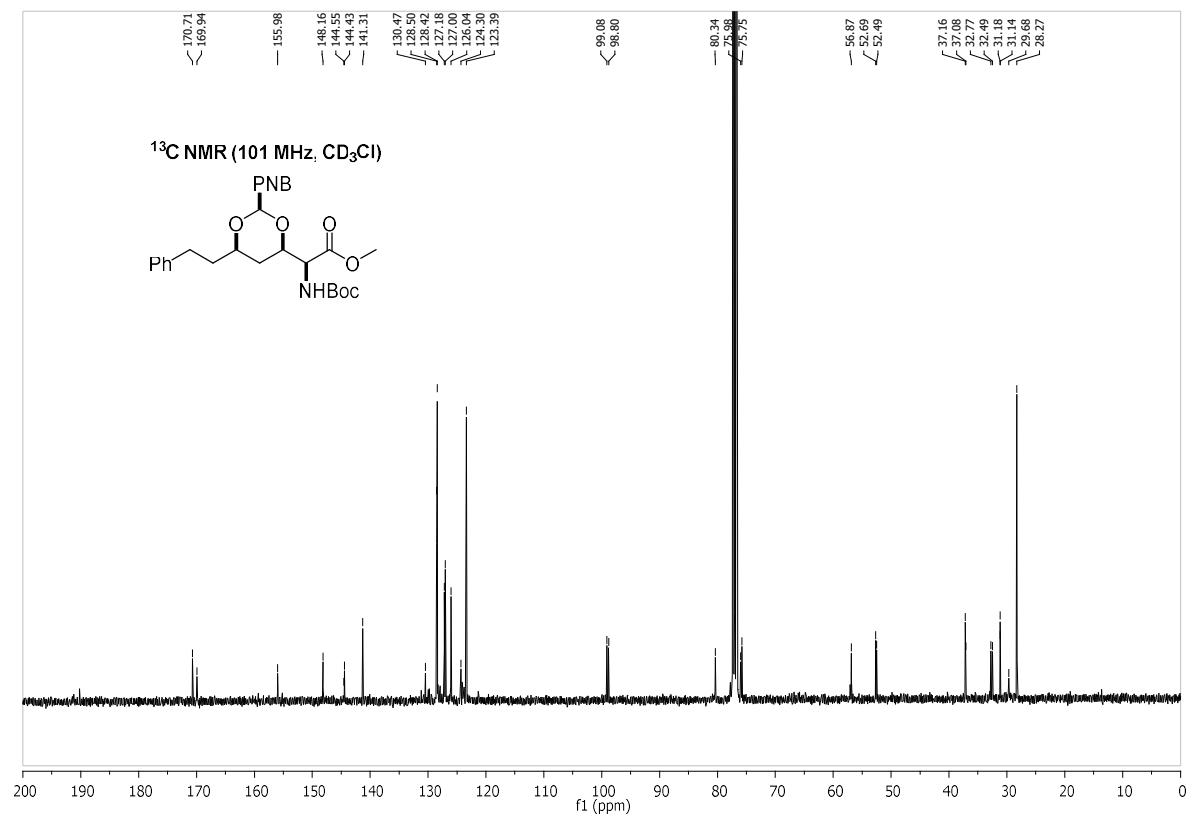
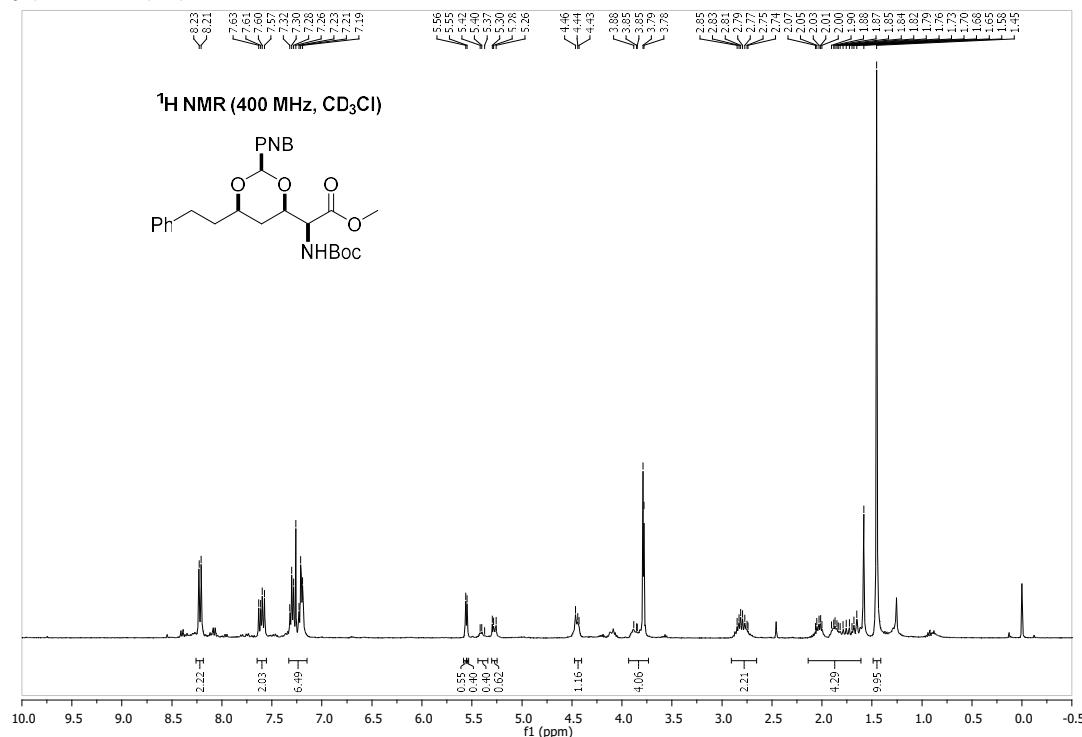
Methyl (*R)-2-acetamido-2-((2*S**,4*S**,6*S**)-6-phenethyl-2-phenyl-1,3-dioxan-4-yl)acetate (4)**



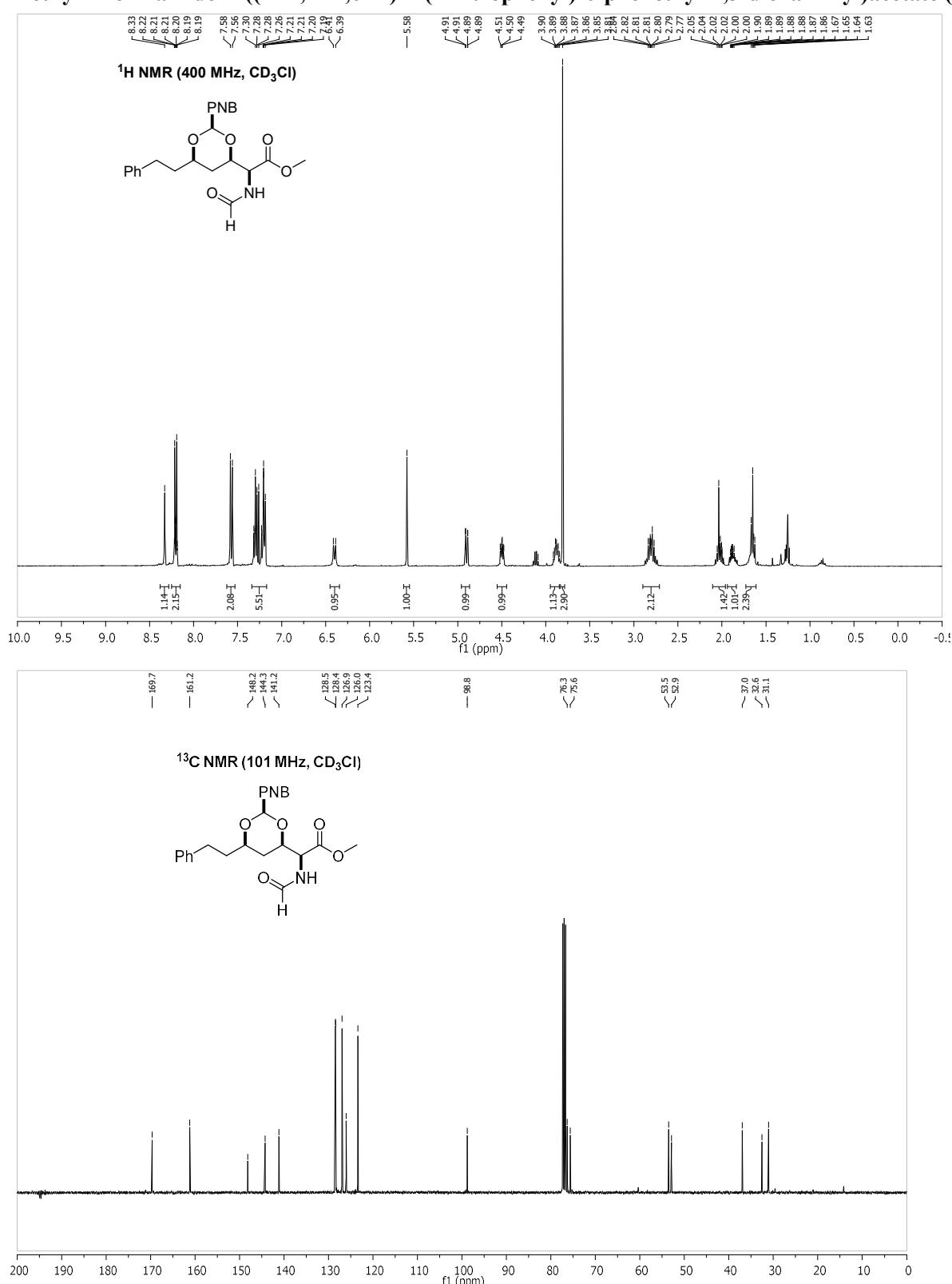
Methyl (*R*^{*})-2-(((benzyloxy)carbonyl)amino)-2-((2*S*^{*},4*S*^{*},6*S*^{*})-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4a)

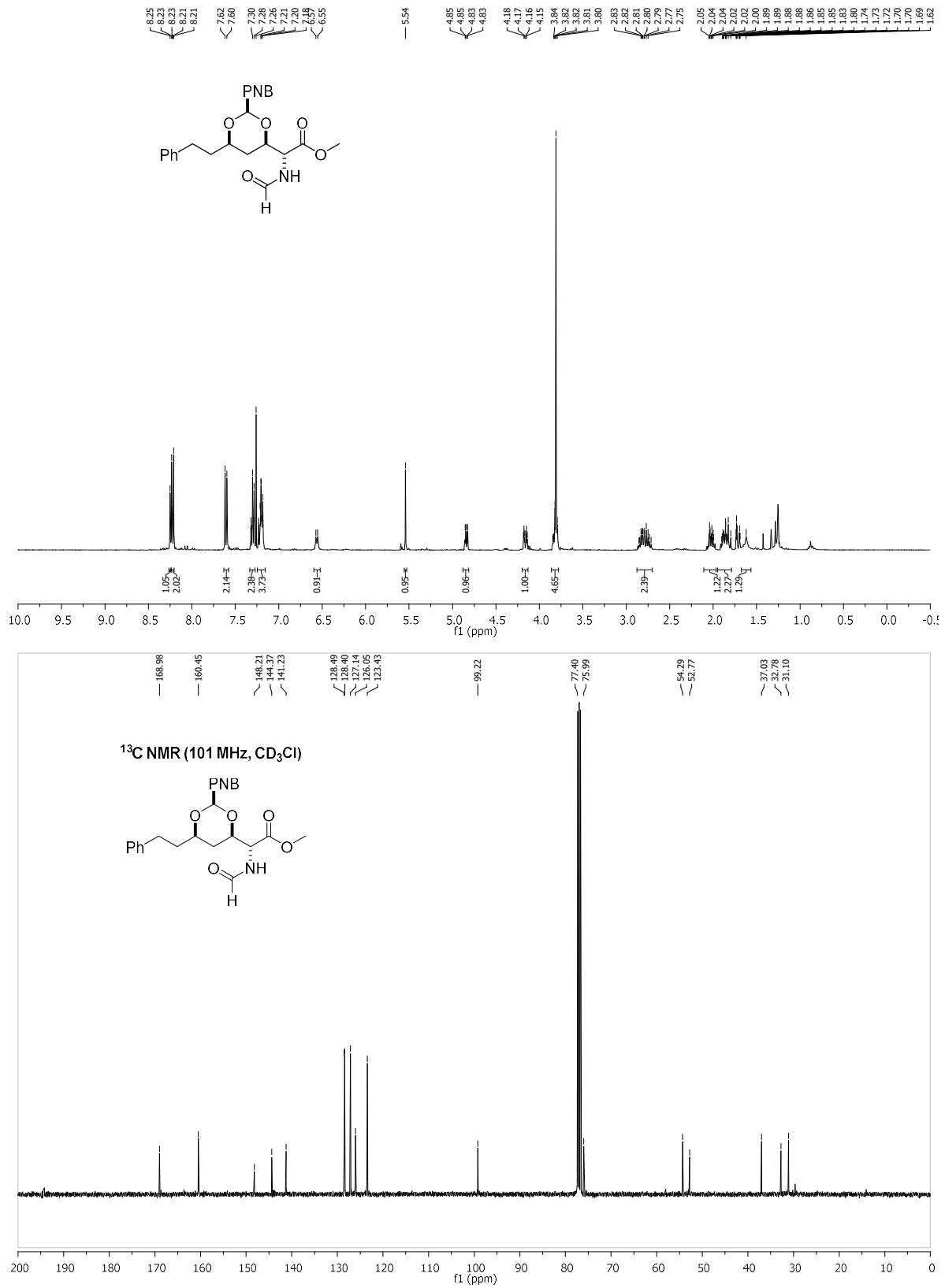


Methyl (*R*^{*})-2-((*tert*-butoxycarbonyl)amino)-2-((2*S*^{*},4*S*^{*},6*S*^{*})-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4b)

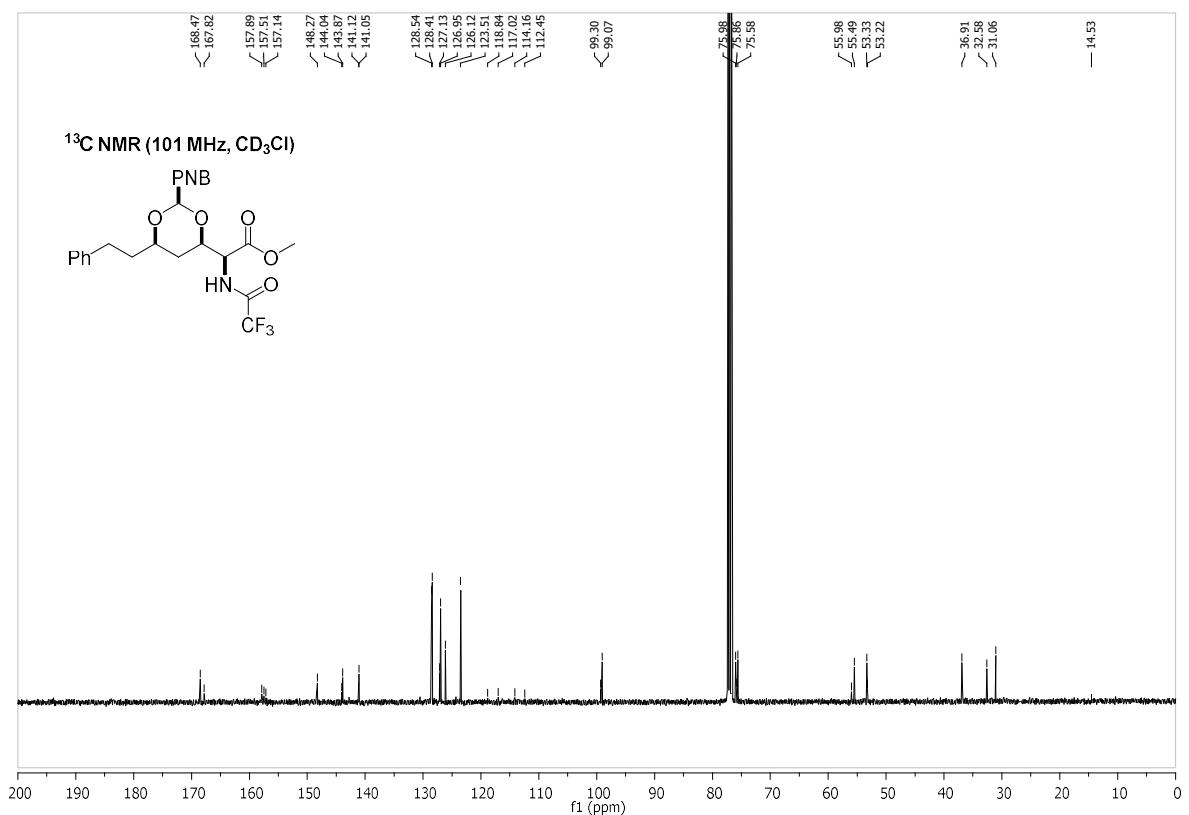
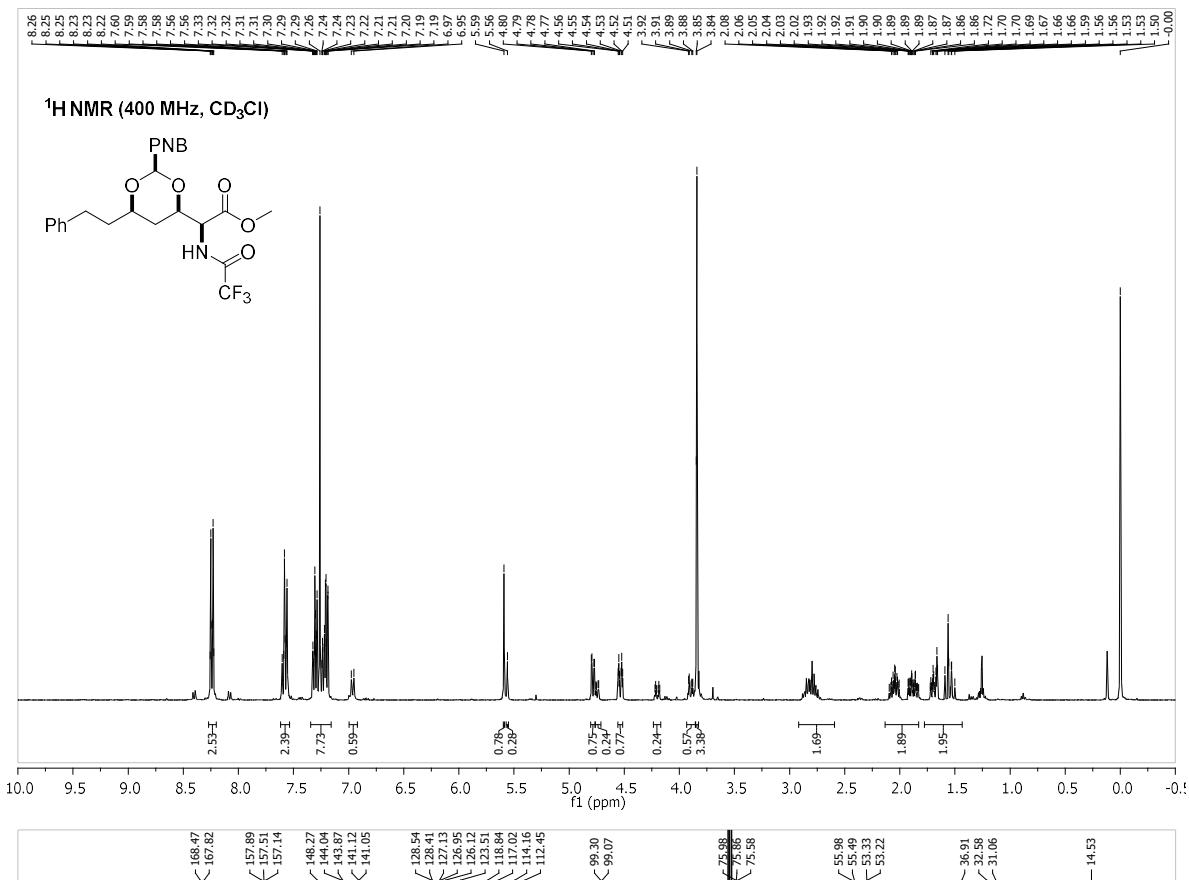


Methyl 2-formamido-2-((2R*,4R*,6R*)-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4c)

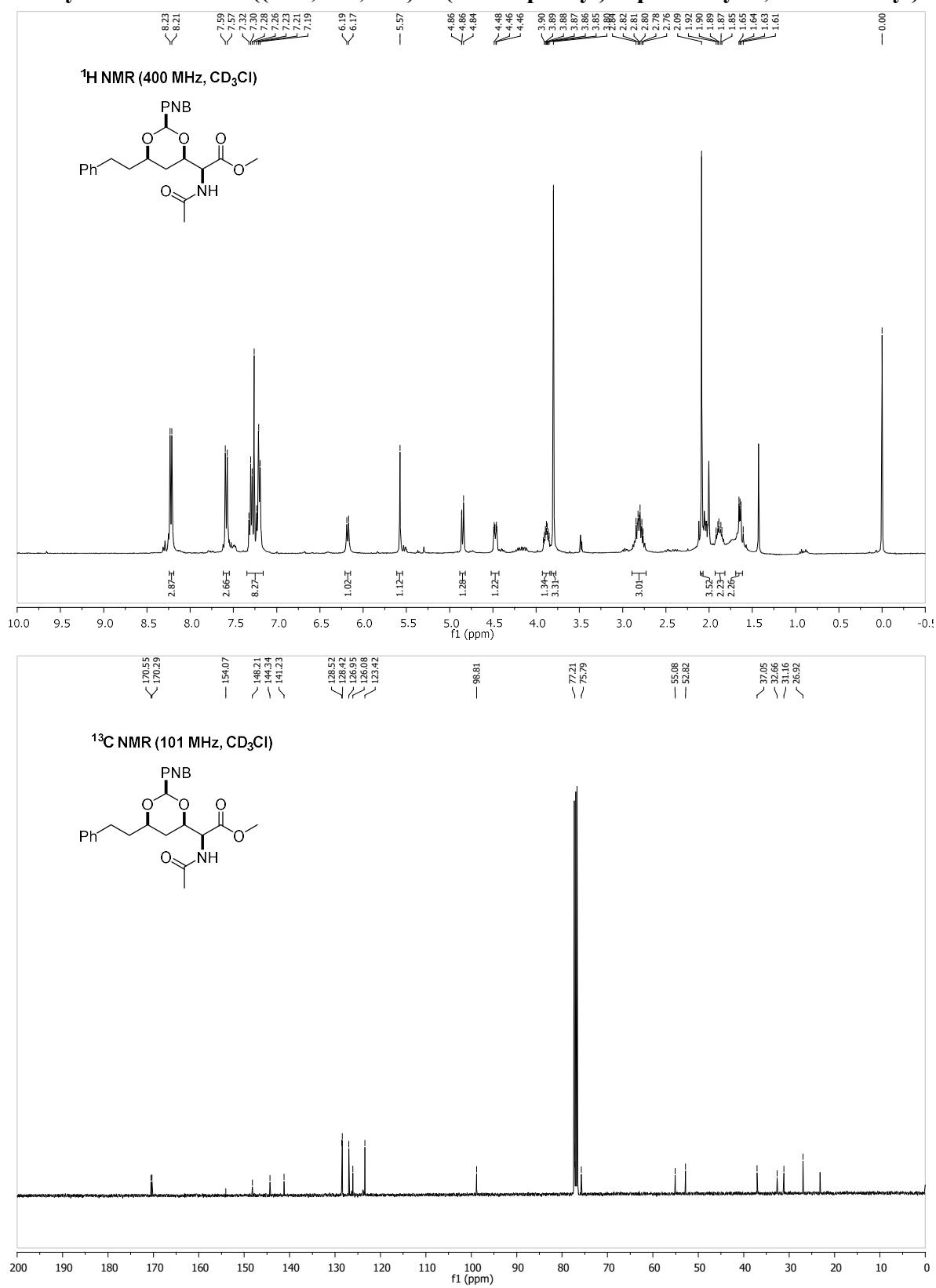


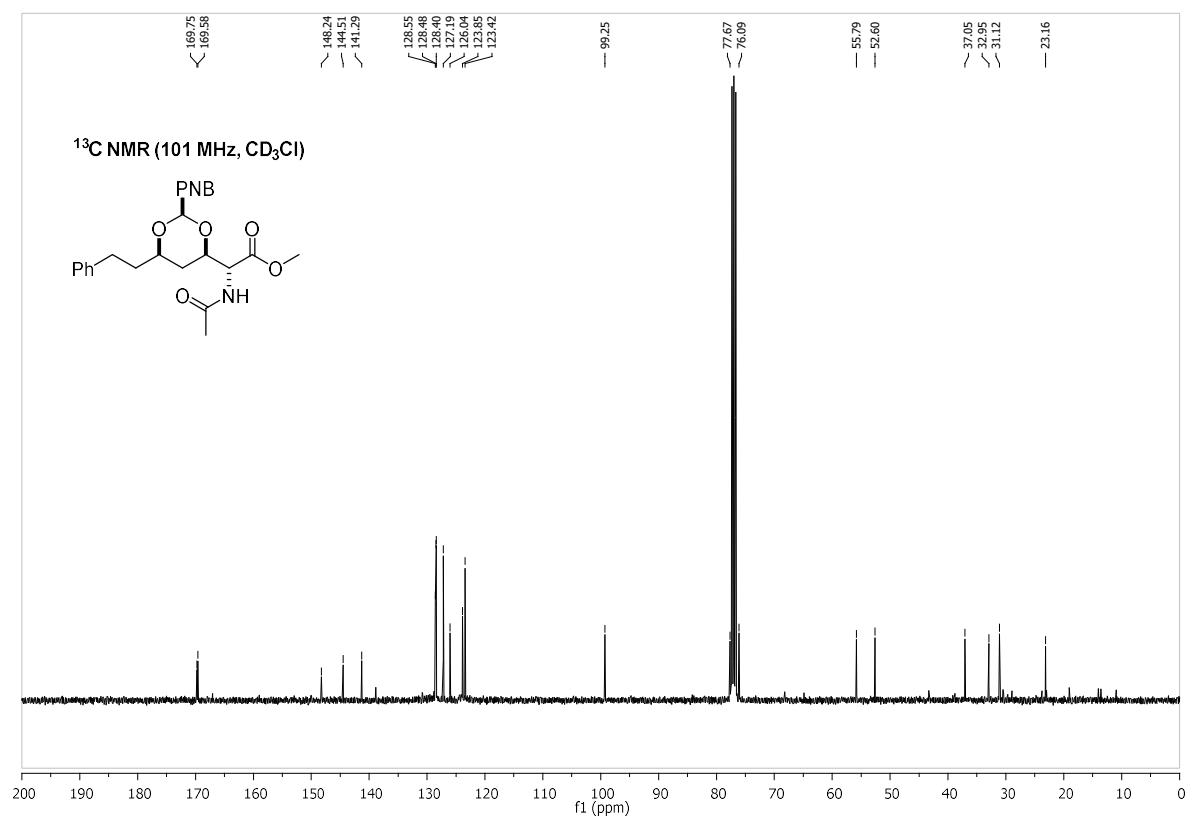
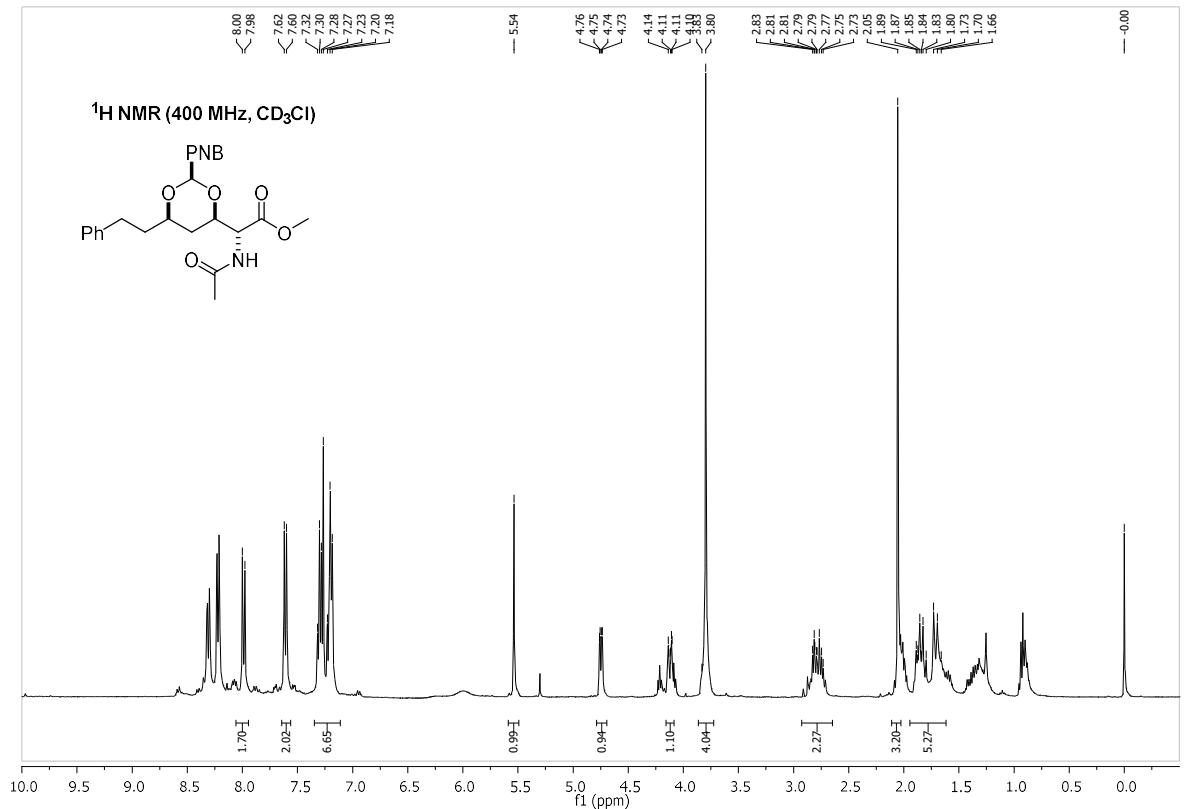


Methyl (*R*^{*})-2-((2*S*^{*},4*S*^{*},6*S*^{*})-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)-2-(2,2,2-trifluoroacetamido)acetate (4d)

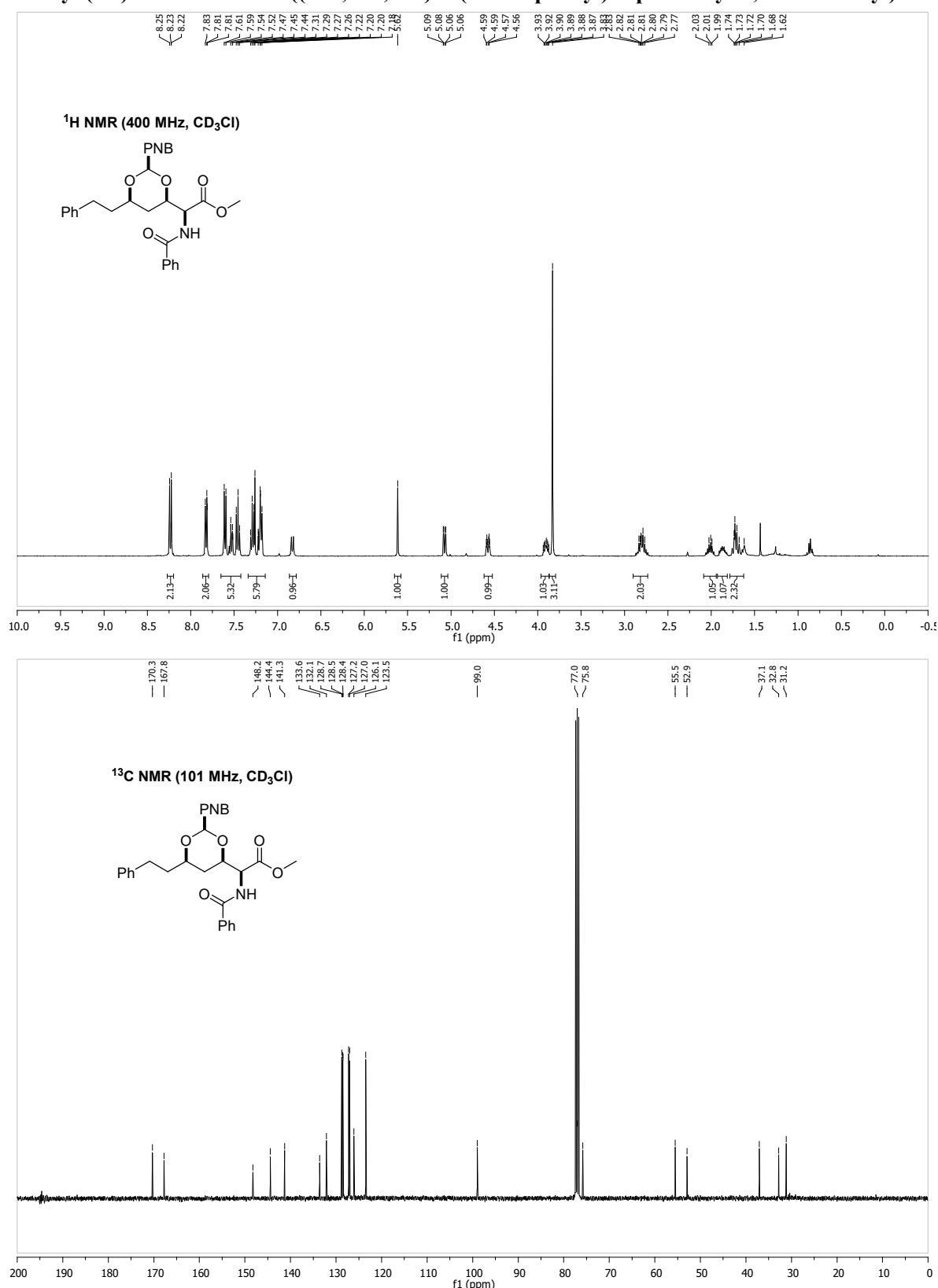


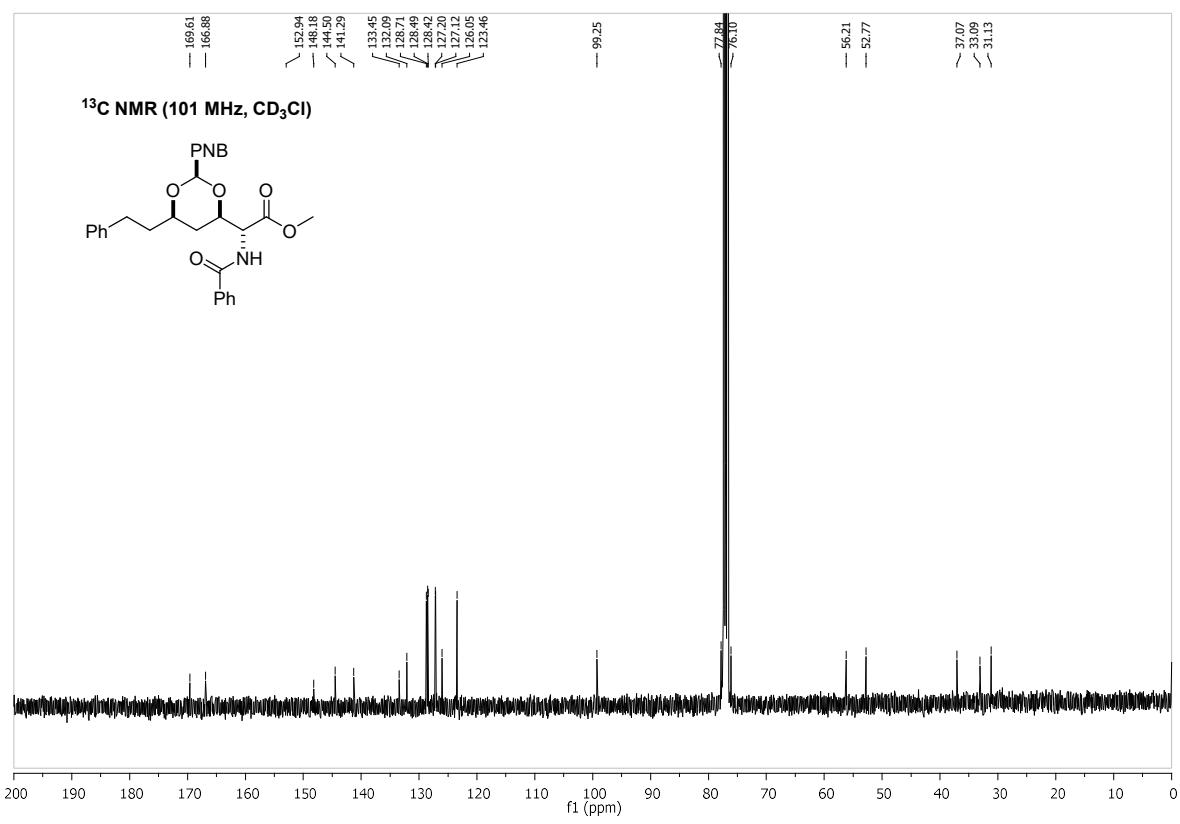
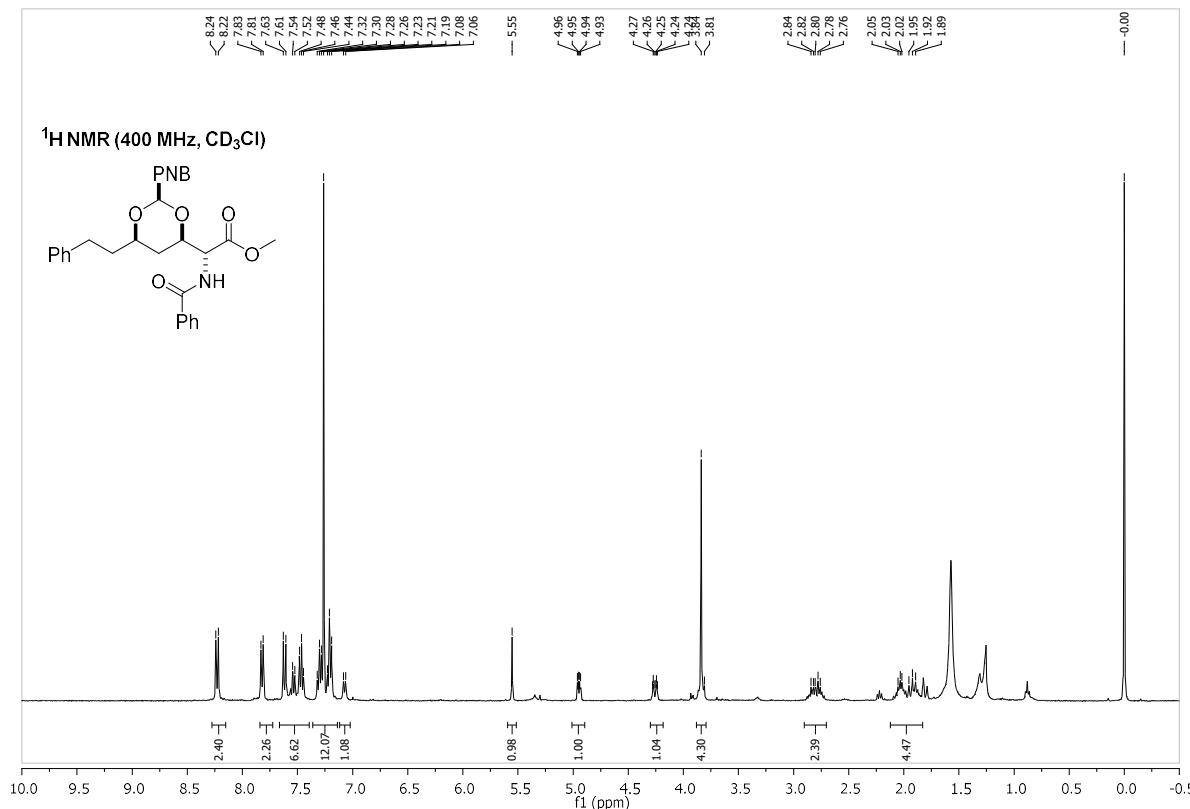
Methyl 2-acetamido-2-((2*R*^{*},4*R*^{*},6*R*^{*})-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4e)



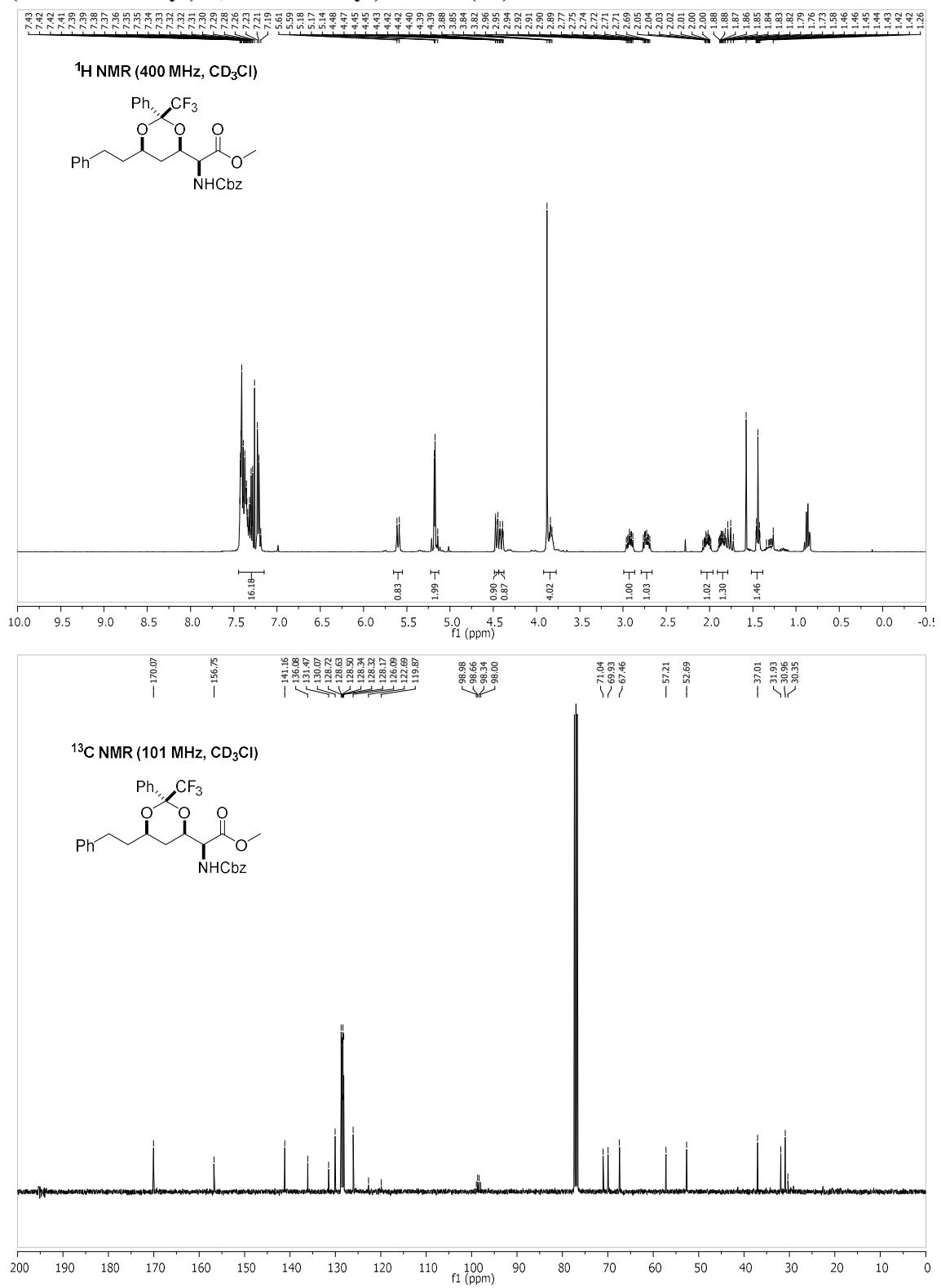


Methyl (R*)-2-benzamido-2-((2S*,4S*,6S*)-2-(4-nitrophenyl)-6-phenethyl-1,3-dioxan-4-yl)acetate (4f)

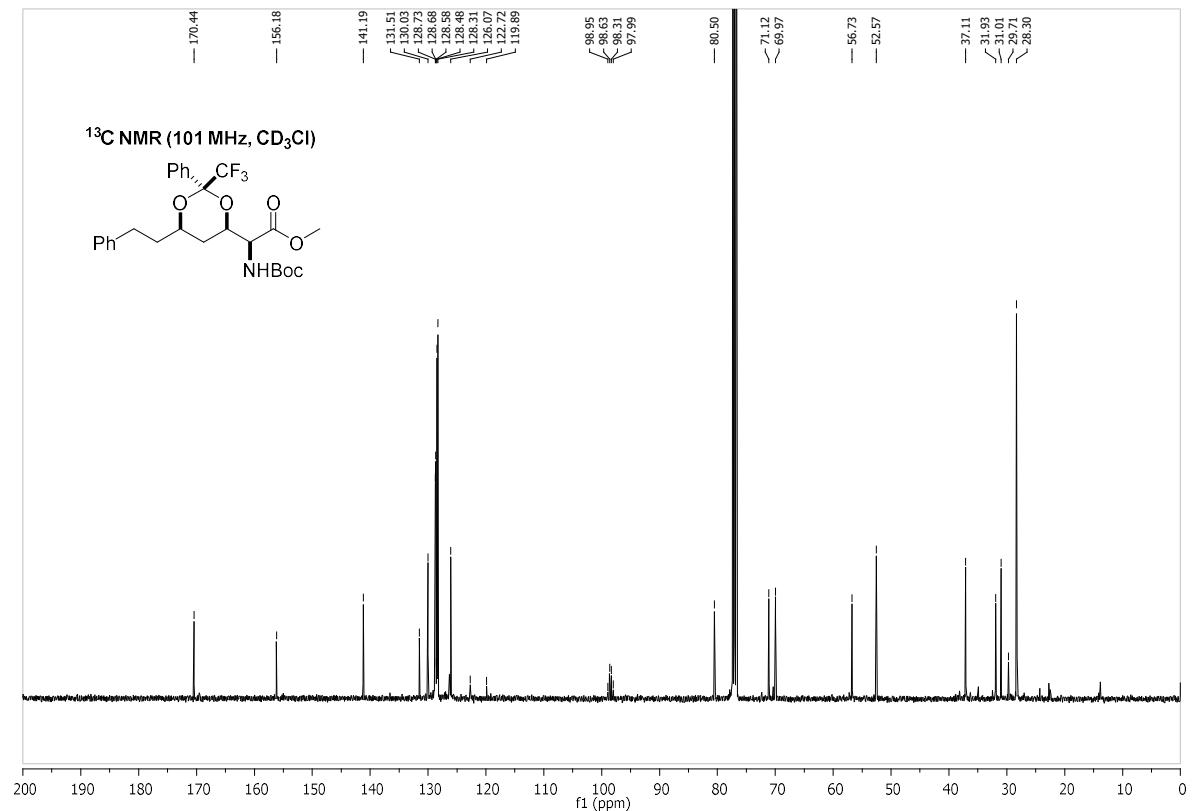
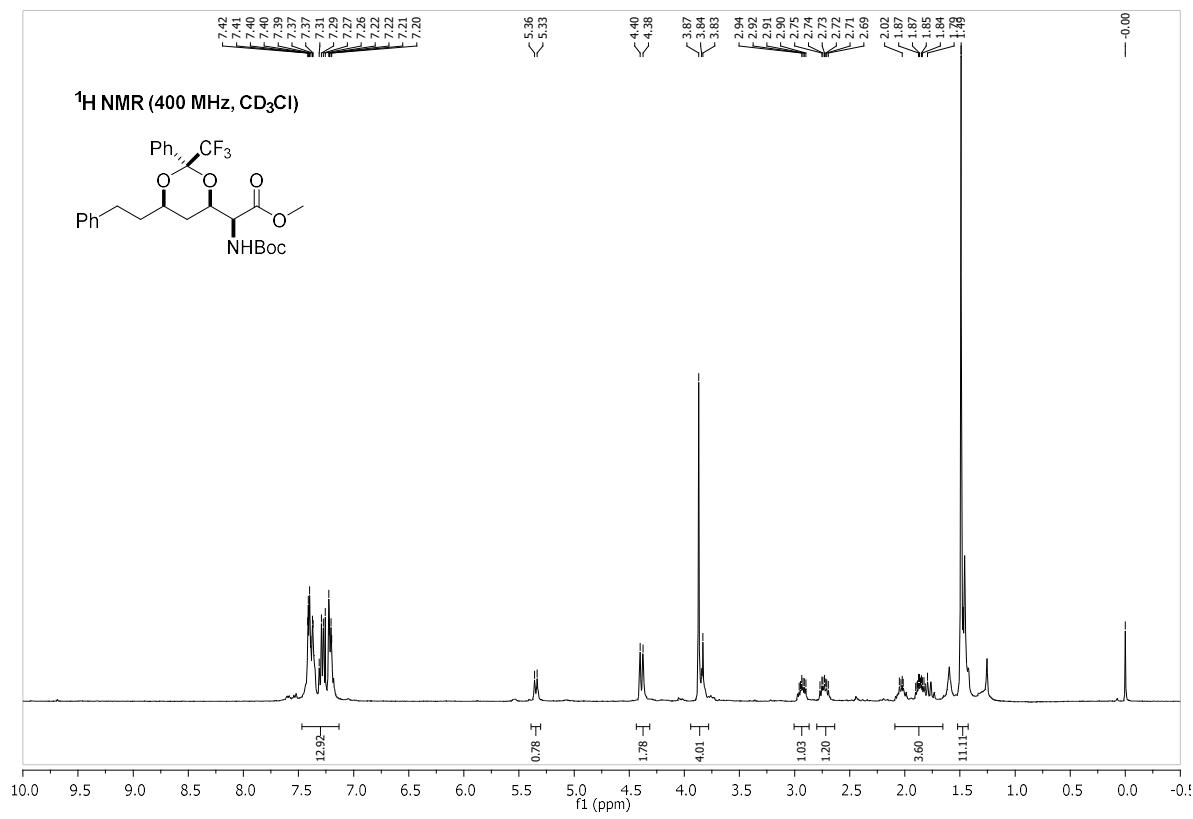




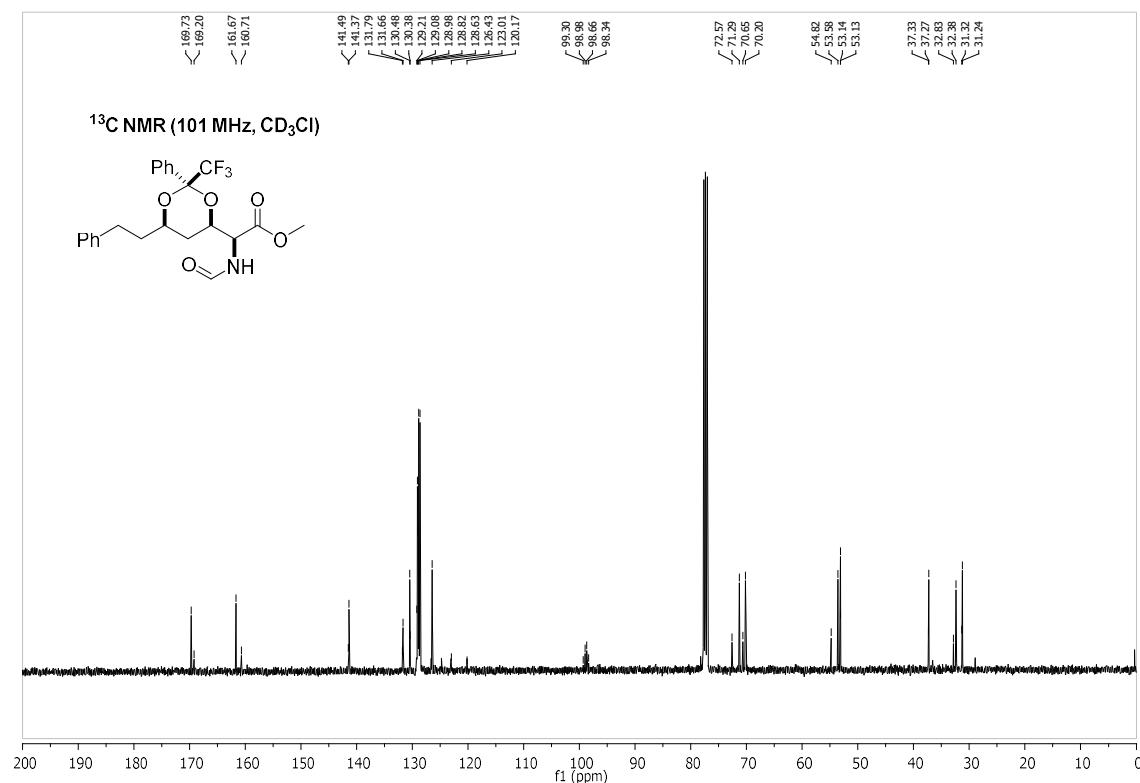
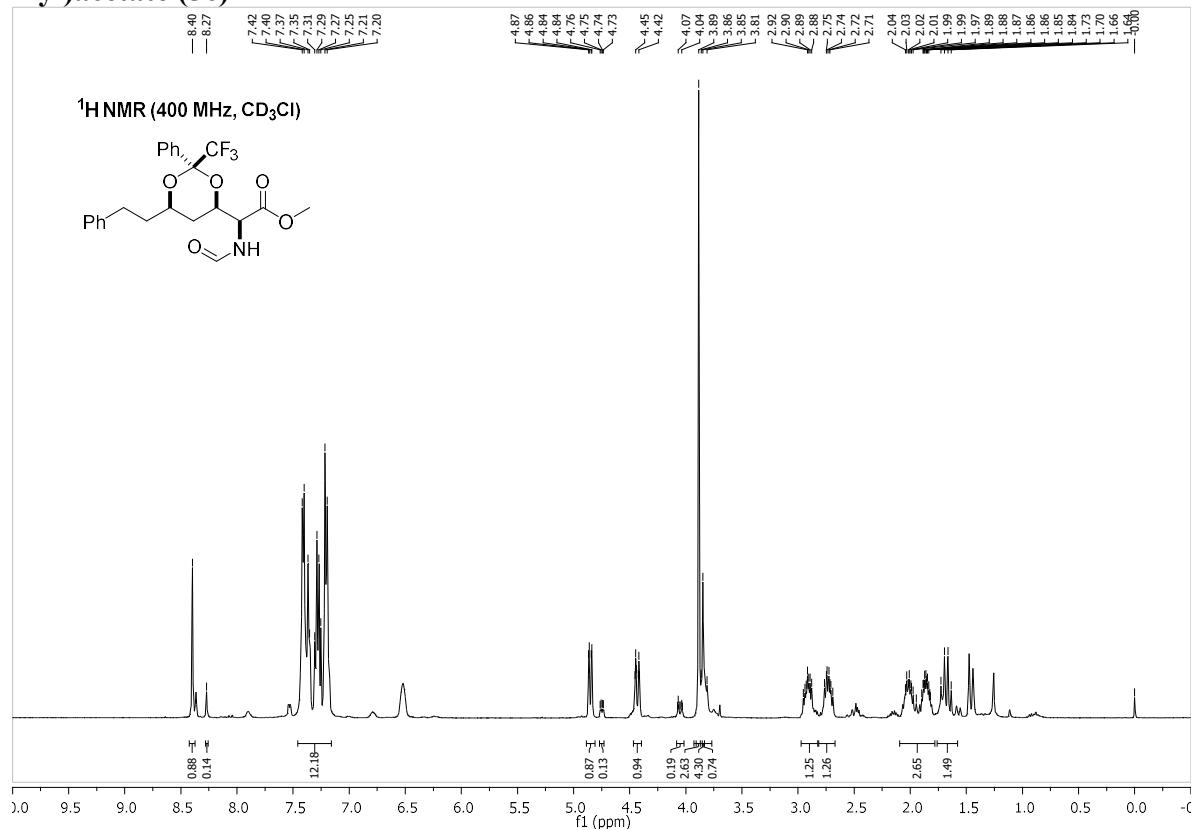
Methyl 2-(((benzyloxy)carbonyl)amino)-2-((2*S*^{*},4*R*^{*},6*R*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5a)



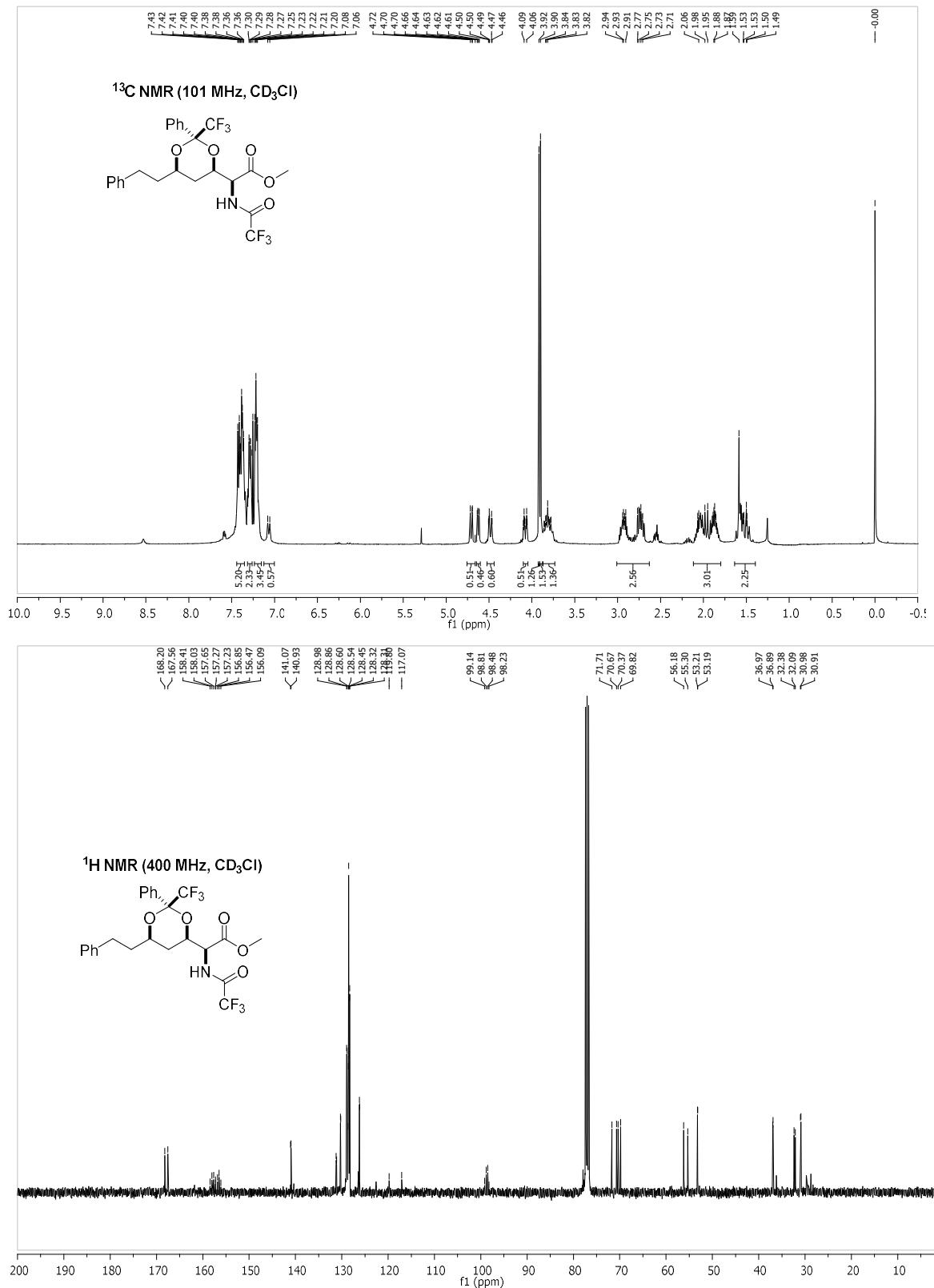
Methyl (R*)-2-((tert-butoxycarbonyl)amino)-2-((2S*,4S*,6S*)-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5b)



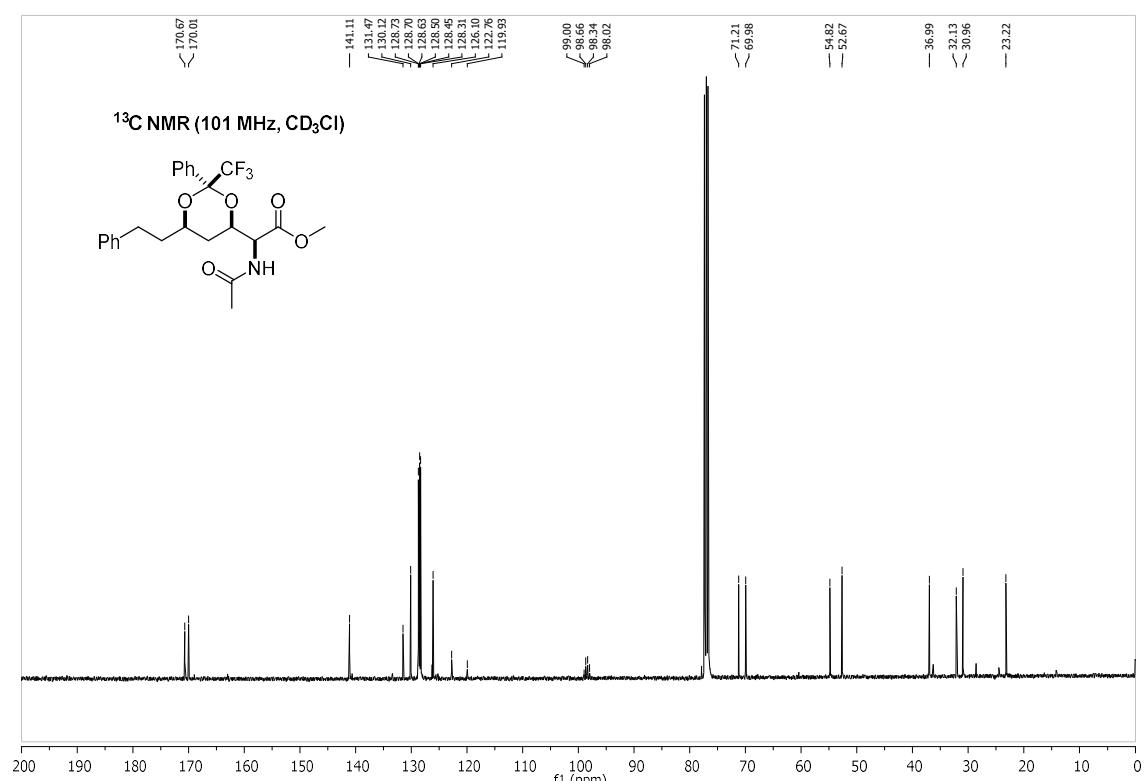
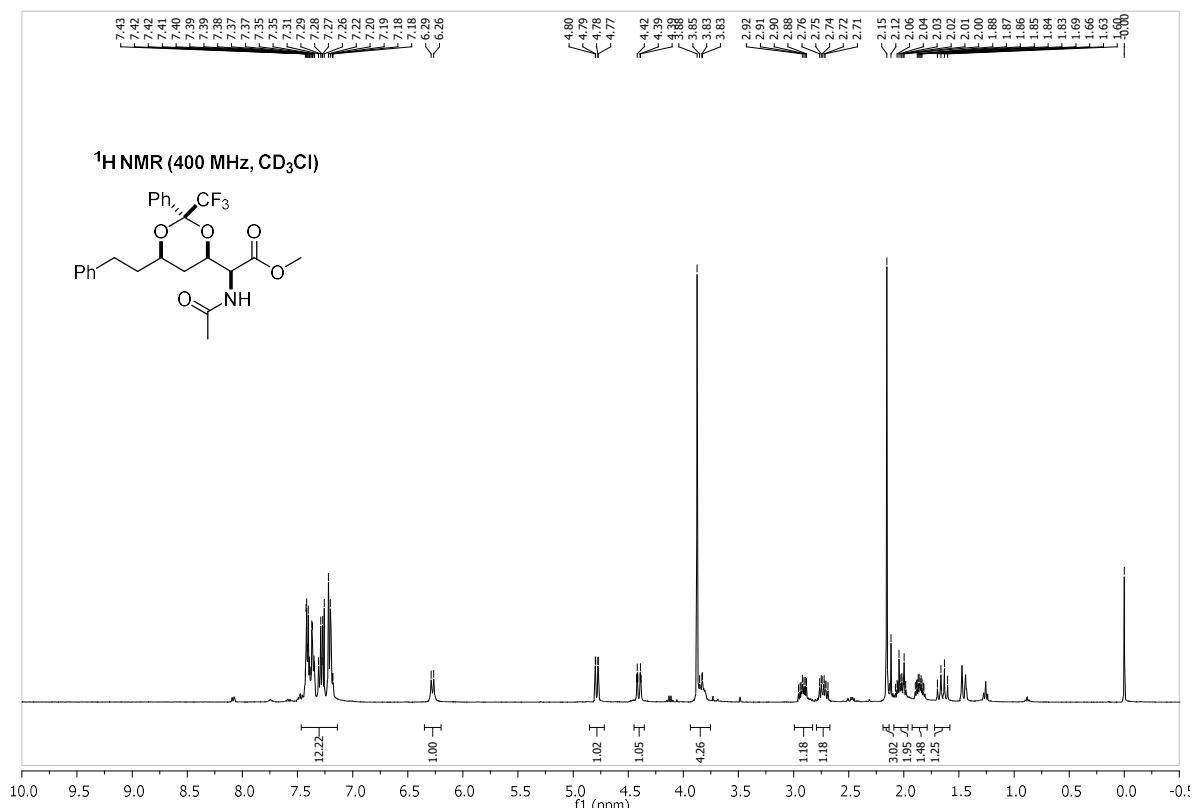
Methyl (*R*^{*})-2-formamido-2-((2*R*^{*},4*S*^{*},6*S*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5c)



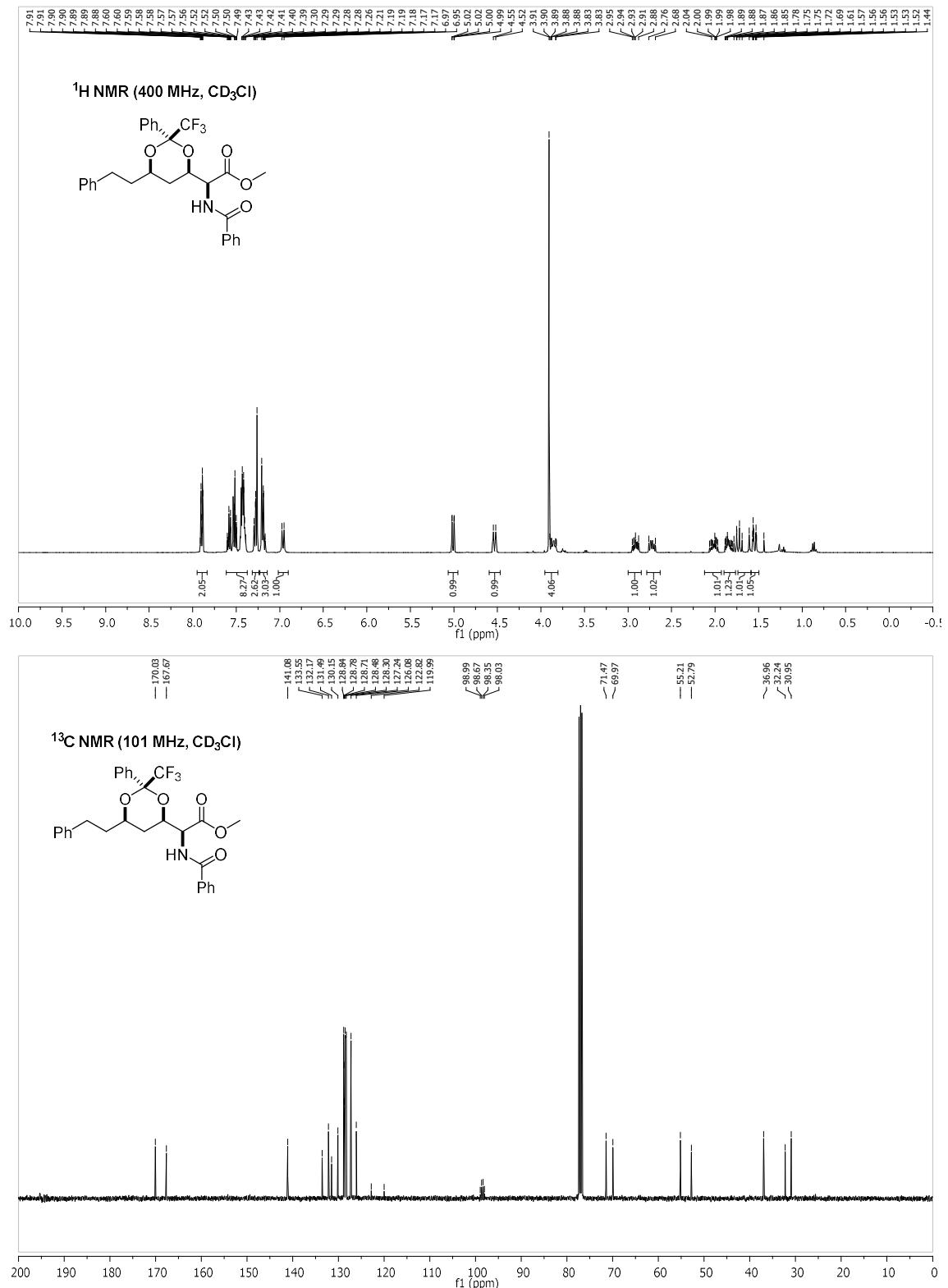
Methyl (*R)-2-((2*S**,4*S**,6*S**)-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)-2-(2,2,2-trifluoroacetamido)acetate (5d)**



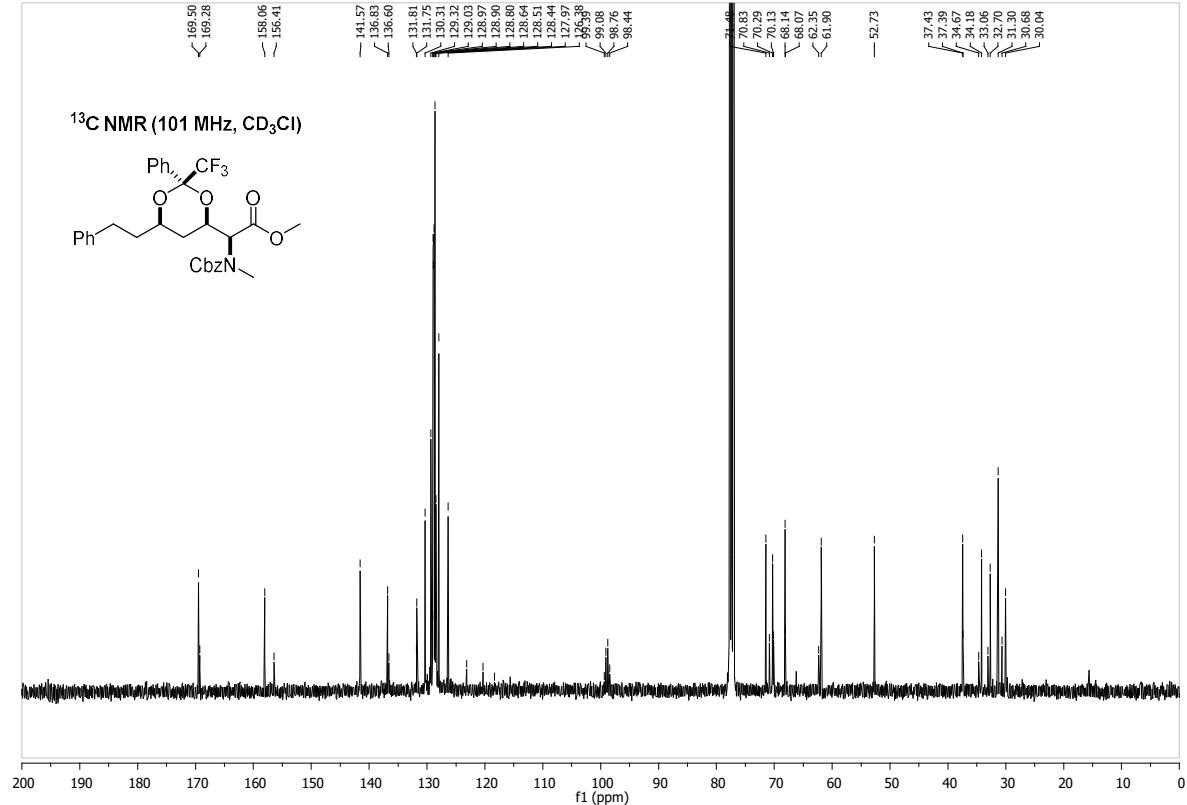
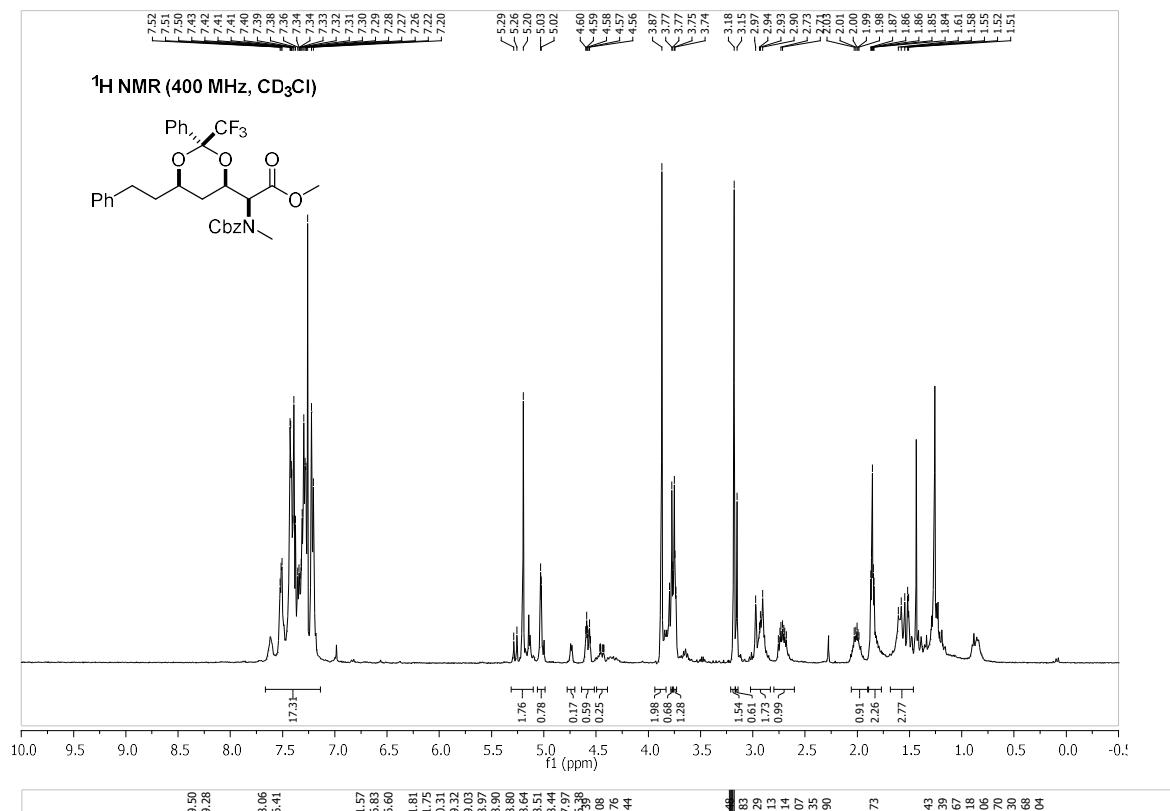
Methyl 2-acetamido-2-((2*R*^{*},4*S*^{*},6*S*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5e)



Methyl 2-benzamido-2-((2*R*^{*},4*R*^{*},6*R*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)acetate (5f)



Methyl (*R*^{*})-2-((2*R*^{*},4*S*^{*},6*S*^{*})-6-phenethyl-2-phenyl-2-(trifluoromethyl)-1,3-dioxan-4-yl)-2-(2,2,2-trifluoroacetamido)acetate (7b)



Computed Cartesian coordinates of all the molecules reported in this study-

Model 1.1

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M2, G= -3081.033176

O	3.253393	-1.086904	0.198505
C	0.919993	2.091942	0.956621
C	-0.141333	1.090997	0.610029
C	0.286586	-0.376076	0.745832
O	1.019558	-0.737996	-0.409788
H	1.721659	-2.372846	0.634720
H	1.280027	2.078133	1.983119
H	-0.507795	1.252914	-0.410523
H	0.935672	-0.479085	1.630914
H	-0.988216	1.263637	1.291056
C	-0.927393	-1.290861	0.892304
H	-1.484143	-1.071663	1.810335
H	-1.599138	-1.155765	0.035163
H	-0.615716	-2.340287	0.920161
C	2.207445	-2.512918	-1.452872
C	1.076367	-3.143203	-1.983967
C	1.156842	-3.949326	-3.114959
C	2.388393	-4.146756	-3.759382
C	3.522615	-3.514807	-3.238749
C	3.425710	-2.714652	-2.098801
H	0.112697	-2.995231	-1.499519
H	0.263149	-4.425571	-3.513768
H	4.484817	-3.655887	-3.727663
H	4.310712	-2.243534	-1.678349
C	1.384619	3.049762	0.130710
K	2.851491	0.923655	-1.512736
O	2.743385	3.878783	1.913005
C	2.284692	4.116829	0.676428
O	2.560341	5.144268	0.080539
C	3.562935	4.903336	2.473547
H	3.034047	5.859957	2.461363
H	3.773227	4.588793	3.495187
H	4.493891	4.993795	1.906695
N	1.124392	3.114821	-1.245203
K	0.687268	7.061702	-0.234254
O	-0.410765	4.807416	-0.889966
C	0.246521	4.018647	-1.638204
C	-0.030291	4.079616	-3.131833
H	0.693971	3.497854	-3.708117
H	-1.034570	3.683999	-3.325518
H	-0.020698	5.123903	-3.460912
C	2.135332	-1.694723	-0.152335
O	0.447059	6.369582	2.397819
O	1.351146	7.326928	-2.872201
O	4.476209	2.915697	-0.584708

O	1.589912	0.469798	-3.887732
C	1.907623	-0.564395	-4.798213
H	1.739828	-1.548497	-4.341705
H	1.299747	-0.477439	-5.710215
H	2.963604	-0.461420	-5.057817
C	0.235841	0.408844	-3.474377
H	0.093797	1.193618	-2.726469
H	-0.433757	0.582054	-4.329383
H	0.016938	-0.567718	-3.022030
C	1.040287	7.997263	-4.074092
H	1.881746	8.626473	-4.397670
H	0.806432	7.279146	-4.872497
H	0.168408	8.626187	-3.885339
C	2.479067	6.483829	-3.005328
H	2.311744	5.731437	-3.789353
H	3.373711	7.070525	-3.263594
H	2.632338	5.981037	-2.047205
C	-0.295180	5.166388	2.521275
H	0.280660	4.419550	3.085626
H	-1.247131	5.355547	3.036820
H	-0.480767	4.792255	1.510604
C	0.746208	6.938864	3.654541
H	-0.174557	7.201300	4.193039
H	1.329320	6.239360	4.270091
H	1.333818	7.842075	3.477148
O	3.080148	8.296125	-0.548032
C	4.381109	7.780395	-0.352678
H	4.858551	7.561344	-1.318994
H	5.005492	8.498206	0.197214
H	4.275809	6.854432	0.214746
C	3.077822	9.448778	-1.362950
H	3.674824	10.250649	-0.907273
H	3.483322	9.222713	-2.359404
H	2.042320	9.779007	-1.467624
C	5.654978	2.748053	0.173211
H	6.450084	2.292637	-0.433244
H	6.012626	3.714700	0.554748
H	5.412734	2.091149	1.010431
C	4.643230	3.815994	-1.661161
H	4.920685	4.814053	-1.293156
H	5.417037	3.455039	-2.353920
H	3.677470	3.882947	-2.169303
N	2.460927	-4.900781	-4.943593
H	3.375494	-5.306166	-5.112123
H	1.747397	-5.618388	-5.013384

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TS2, G= -3080.97996

O	2.933889	-1.017382	0.705985
C	0.891241	2.247348	1.059535
C	-0.262586	1.337069	0.767662

C	0.039322	-0.151839	0.973006
O	0.789951	-0.610263	-0.139601
H	1.351816	-2.310182	0.897509
H	1.262096	2.248712	2.082546
H	-0.622743	1.485470	-0.257901
H	0.645936	-0.270113	1.884151
H	-1.085580	1.616955	1.443194
C	-1.244374	-0.968594	1.091285
H	-1.820680	-0.680258	1.977203
H	-1.867340	-0.810861	0.202202
H	-1.014055	-2.036844	1.162774
C	2.064566	-2.306237	-1.138046
C	0.982692	-2.825062	-1.858650
C	1.169417	-3.395030	-3.110048
C	2.463990	-3.443820	-3.625441
C	3.566004	-2.972545	-2.921069
C	3.351539	-2.410282	-1.666321
H	-0.019494	-2.741252	-1.445741
H	0.337941	-3.778426	-3.690850
H	4.557869	-3.041794	-3.353244
H	4.178353	-2.022546	-1.078047
C	1.437190	3.114750	0.186358
K	2.783393	0.845414	-1.289546
O	2.988167	3.809769	1.865804
C	2.440116	4.109232	0.681096
O	2.734636	5.127140	0.077271
C	3.971088	4.732113	2.329565
H	3.536591	5.727411	2.450264
H	4.316146	4.344570	3.287257
H	4.799115	4.785961	1.617126
N	1.193368	3.135715	-1.195420
K	0.736169	6.922278	-0.221455
O	-0.469429	4.727257	-0.947611
C	0.252503	3.946610	-1.641459
C	-0.008965	3.900929	-3.138078
H	0.768718	3.347038	-3.670371
H	-0.975576	3.414964	-3.315918
H	-0.077743	4.921248	-3.528773
C	1.856333	-1.586866	0.210960
O	0.438659	5.804336	2.260622
O	1.278029	7.132692	-2.894211
O	4.565858	2.808329	-0.615245
O	1.708363	-0.119770	-3.614737
C	2.111525	-0.330066	-4.949667
H	1.623844	-1.223777	-5.366742
H	1.858469	0.535661	-5.577869
H	3.193920	-0.477888	-4.949628
C	0.303811	0.003471	-3.495120
H	0.074726	0.087544	-2.429250
H	-0.054857	0.893199	-4.030901
H	-0.193767	-0.888448	-3.901374

C	0.902496	7.778019	-4.090825
H	1.706729	8.437401	-4.447964
H	0.672222	7.043302	-4.875248
H	0.012312	8.373263	-3.879729
C	2.432299	6.331955	-3.056328
H	2.269665	5.569159	-3.831328
H	3.296457	6.949803	-3.344115
H	2.632268	5.841306	-2.100370
C	-0.661372	4.914019	2.360551
H	-0.376810	4.017307	2.927881
H	-1.503086	5.406721	2.867642
H	-0.931455	4.627427	1.342024
C	0.955032	6.143908	3.529284
H	0.167293	6.554088	4.176604
H	1.394092	5.261368	4.016162
H	1.727526	6.902004	3.383416
O	3.067061	8.239766	-0.683323
C	4.402601	7.806439	-0.522397
H	4.850333	7.567030	-1.498073
H	5.007120	8.584547	-0.036031
H	4.376346	6.905181	0.091501
C	2.968592	9.359773	-1.536932
H	3.521229	10.215248	-1.124674
H	3.365739	9.125347	-2.534988
H	1.911048	9.616426	-1.628395
C	5.787364	2.546506	0.043765
H	6.480528	2.006518	-0.616158
H	6.265726	3.482093	0.365567
H	5.560747	1.933212	0.917756
C	4.716618	3.688066	-1.711894
H	5.063762	4.673780	-1.371003
H	5.431928	3.281378	-2.440895
H	3.729041	3.796430	-2.166951
N	2.667544	-3.988838	-4.967831
O	3.805777	-4.023499	-5.412717
O	1.688340	-4.373441	-5.591017

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M3, G= -3080.996501

O	0.220191	0.330764	1.414538
C	-0.112784	1.698197	0.988120
C	-1.570858	1.645274	0.513274
C	-1.834776	0.354805	-0.291195
O	-0.602834	-0.243304	-0.693128
H	-0.284560	-1.526639	0.870421
H	-0.058293	2.220741	1.947292
H	-1.798494	2.535506	-0.078591
H	-2.363688	-0.375446	0.344179
H	-2.229053	1.650060	1.389837
C	-2.630944	0.607199	-1.556477
H	-3.594438	1.065263	-1.309147

H	-2.071644	1.294964	-2.200150
H	-2.813802	-0.325313	-2.100980
C	1.555542	-1.002484	-0.126195
C	1.683768	-1.771309	-1.285982
C	2.937674	-2.108834	-1.790812
C	4.104611	-1.696634	-1.128567
C	3.974311	-0.935664	0.043582
C	2.715147	-0.598363	0.537237
H	0.790282	-2.091921	-1.815014
H	3.017336	-2.690946	-2.706367
H	4.868631	-0.596884	0.562375
H	2.622078	0.024926	1.422363
C	0.855759	2.334214	0.022393
K	2.783112	1.175314	-2.107372
O	2.387847	2.313270	1.797927
C	2.135720	2.606638	0.449363
O	3.112164	3.083565	-0.238506
C	3.650308	2.714579	2.285019
H	3.797250	3.796834	2.183540
H	3.664900	2.439994	3.343129
H	4.466929	2.202188	1.763546
N	0.538877	2.461601	-1.378362
K	1.652131	5.323610	-0.484168
O	-0.770899	4.378004	-1.080272
C	-0.250614	3.436543	-1.775017
C	-0.581607	3.445896	-3.264354
H	-0.099170	2.619580	-3.791275
H	-1.668737	3.382701	-3.397882
H	-0.257377	4.394879	-3.708554
C	0.180186	-0.638565	0.402976
O	2.044645	5.735106	2.130384
O	1.443352	6.610465	-2.822742
O	3.925538	3.103272	-3.691746
O	1.464066	0.476692	-4.368054
C	1.773820	0.116645	-5.696022
H	1.798222	-0.976095	-5.810521
H	1.033350	0.530658	-6.394549
H	2.759183	0.527186	-5.927262
C	0.199124	-0.009149	-3.951741
H	0.034085	0.343831	-2.928652
H	-0.594711	0.375672	-4.609037
H	0.182443	-1.108507	-3.981257
C	0.138043	7.042965	-3.158512
H	0.026863	8.119937	-2.970916
H	-0.074423	6.841938	-4.218005
H	-0.554290	6.473410	-2.532729
C	2.441293	7.215274	-3.614729
H	2.301807	6.964898	-4.675769
H	2.422227	8.308556	-3.501663
H	3.405335	6.831136	-3.271262
C	1.191168	4.991412	2.978769

H	1.775103	4.341706	3.644357
H	0.566106	5.664010	3.582299
H	0.562196	4.368316	2.338977
C	2.940724	6.551953	2.849970
H	2.395903	7.249534	3.501329
H	3.614504	5.940969	3.468057
H	3.524381	7.115390	2.119001
O	4.054583	6.564706	-0.460560
C	5.074323	5.716957	0.038035
H	5.911064	5.662785	-0.674327
H	5.454142	6.094347	0.998612
H	4.631146	4.724999	0.167400
C	4.516901	7.872220	-0.717538
H	4.932748	8.326329	0.193181
H	5.292728	7.866385	-1.496606
H	3.663609	8.462193	-1.058353
C	4.704647	4.039595	-2.974162
H	5.079741	4.826896	-3.645097
H	4.114055	4.493180	-2.166885
H	5.549527	3.501893	-2.537917
C	2.750772	3.699033	-4.210162
H	2.159963	4.156948	-3.403691
H	3.002730	4.469769	-4.953285
H	2.161441	2.907913	-4.679790
N	5.366466	-1.969399	-1.668889
H	6.116526	-1.980723	-0.986679
H	5.400432	-2.801456	-2.247466

Model 1.2

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M2, G= -3230.150467

O	2.933889	-1.017382	0.705985
C	0.891241	2.247348	1.059535
C	-0.262586	1.337069	0.767662
C	0.039322	-0.151839	0.973006
O	0.789951	-0.610263	-0.139601
H	1.351816	-2.310182	0.897509
H	1.262096	2.248712	2.082546
H	-0.622743	1.485470	-0.257901
H	0.645936	-0.270113	1.884151
H	-1.085580	1.616955	1.443194
C	-1.244374	-0.968594	1.091285
H	-1.820680	-0.680258	1.977203
H	-1.867340	-0.810861	0.202202
H	-1.014055	-2.036844	1.162774
C	2.064566	-2.306237	-1.138046
C	0.982692	-2.825062	-1.858650
C	1.169417	-3.395030	-3.110048
C	2.463990	-3.443820	-3.625441
C	3.566004	-2.972545	-2.921069

C	3.351539	-2.410282	-1.666321
H	-0.019494	-2.741252	-1.445741
H	0.337941	-3.778426	-3.690850
H	4.557869	-3.041794	-3.353244
H	4.178353	-2.022546	-1.078047
C	1.437190	3.114750	0.186358
K	2.783393	0.845414	-1.289546
O	2.988167	3.809769	1.865804
C	2.440116	4.109232	0.681096
O	2.734636	5.127140	0.077271
C	3.971088	4.732113	2.329565
H	3.536591	5.727411	2.450264
H	4.316146	4.344570	3.287257
H	4.799115	4.785961	1.617126
N	1.193368	3.135715	-1.195420
K	0.736169	6.922278	-0.221455
O	-0.469429	4.727257	-0.947611
C	0.252503	3.946610	-1.641459
C	-0.008965	3.900929	-3.138078
H	0.768718	3.347038	-3.670371
H	-0.975576	3.414964	-3.315918
H	-0.077743	4.921248	-3.528773
C	1.856333	-1.586866	0.210960
O	0.438659	5.804336	2.260622
O	1.278029	7.132692	-2.894211
O	4.565858	2.808329	-0.615245
O	1.708363	-0.119770	-3.614737
C	2.111525	-0.330066	-4.949667
H	1.623844	-1.223777	-5.366742
H	1.858469	0.535661	-5.577869
H	3.193920	-0.477888	-4.949628
C	0.303811	0.003471	-3.495120
H	0.074726	0.087544	-2.429250
H	-0.054857	0.893199	-4.030901
H	-0.193767	-0.888448	-3.901374
C	0.902496	7.778019	-4.090825
H	1.706729	8.437401	-4.447964
H	0.672222	7.043302	-4.875248
H	0.012312	8.373263	-3.879729
C	2.432299	6.331955	-3.056328
H	2.269665	5.569159	-3.831328
H	3.296457	6.949803	-3.344115
H	2.632268	5.841306	-2.100370
C	-0.661372	4.914019	2.360551
H	-0.376810	4.017307	2.927881
H	-1.503086	5.406721	2.867642
H	-0.931455	4.627427	1.342024
C	0.955032	6.143908	3.529284
H	0.167293	6.554088	4.176604
H	1.394092	5.261368	4.016162
H	1.727526	6.902004	3.383416

O	3.067061	8.239766	-0.683323
C	4.402601	7.806439	-0.522397
H	4.850333	7.567030	-1.498073
H	5.007120	8.584547	-0.036031
H	4.376346	6.905181	0.091501
C	2.968592	9.359773	-1.536932
H	3.521229	10.215248	-1.124674
H	3.365739	9.125347	-2.534988
H	1.911048	9.616426	-1.628395
C	5.787364	2.546506	0.043765
H	6.480528	2.006518	-0.616158
H	6.265726	3.482093	0.365567
H	5.560747	1.933212	0.917756
C	4.716618	3.688066	-1.711894
H	5.063762	4.673780	-1.371003
H	5.431928	3.281378	-2.440895
H	3.729041	3.796430	-2.166951
N	2.667544	-3.988838	-4.967831
O	3.805777	-4.023499	-5.412717
O	1.688340	-4.373441	-5.591017

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TS2, G= -3230.111173

O	0.164627	-0.113922	1.549055
C	-0.109203	1.801522	1.054657
C	-1.556446	1.622878	0.672239
C	-1.839529	0.322604	-0.133792
O	-0.657649	-0.285130	-0.621303
H	-0.339093	-1.862113	0.655500
H	0.107776	1.970171	2.102383
H	-1.856255	2.495529	0.079397
H	-2.343182	-0.397904	0.531346
H	-2.170042	1.606167	1.578870
C	-2.724304	0.603570	-1.336220
H	-3.663364	1.068492	-1.016236
H	-2.210398	1.294082	-2.014153
H	-2.955854	-0.319273	-1.878526
C	1.489082	-1.133617	-0.199435
C	1.587916	-1.843963	-1.402486
C	2.827235	-2.116483	-1.970756
C	3.968873	-1.668616	-1.306561
C	3.905799	-0.958498	-0.109290
C	2.652132	-0.692557	0.437169
H	0.681959	-2.183329	-1.896665
H	2.917370	-2.659924	-2.904406
H	4.818237	-0.624952	0.372485
H	2.546105	-0.129017	1.359923
C	0.805463	2.317649	0.133251
K	2.706860	1.172474	-2.258378
O	2.416675	2.282626	1.862370
C	2.151785	2.554633	0.554804

O	3.073021	2.977896	-0.180045
C	3.715125	2.636207	2.318031
H	3.891942	3.707542	2.179946
H	3.735538	2.382046	3.378572
H	4.486021	2.072678	1.783688
N	0.562673	2.407418	-1.275714
K	1.557253	5.304580	-0.429858
O	-0.831593	4.272575	-1.085945
C	-0.244034	3.343519	-1.734351
C	-0.482278	3.310842	-3.239681
H	0.158193	2.577967	-3.736972
H	-1.532194	3.061795	-3.438096
H	-0.302128	4.303802	-3.665769
C	0.122679	-0.867195	0.444080
O	2.066657	5.511257	2.201392
O	1.455295	6.596544	-2.777913
O	3.696866	3.193401	-3.756910
O	1.260855	0.221545	-4.286672
C	1.497713	-0.057198	-5.649654
H	1.325328	-1.120387	-5.866215
H	0.840702	0.547954	-6.289684
H	2.539606	0.191086	-5.862135
C	-0.066021	-0.087408	-3.892192
H	-0.172012	0.187736	-2.838314
H	-0.787752	0.479854	-4.497430
H	-0.261684	-1.161849	-4.022155
C	0.131626	6.962269	-3.129122
H	-0.033536	8.032969	-2.947913
H	-0.057839	6.746600	-4.189977
H	-0.542422	6.364534	-2.509704
C	2.422771	7.272628	-3.552980
H	2.295660	7.043235	-4.620278
H	2.346199	8.359510	-3.410943
H	3.405865	6.930458	-3.220987
C	1.205952	4.851927	3.112139
H	1.780387	4.205897	3.789751
H	0.637567	5.583853	3.701776
H	0.522956	4.235796	2.524037
C	2.997897	6.345247	2.858117
H	2.482349	7.093684	3.475240
H	3.665140	5.753268	3.500873
H	3.582264	6.849698	2.086222
O	3.979659	6.495102	-0.424092
C	5.062910	5.666431	-0.041535
H	5.844742	5.672632	-0.815049
H	5.500976	6.014734	0.904754
H	4.666934	4.654916	0.079817
C	4.369724	7.839438	-0.610425
H	4.793900	8.253973	0.314874
H	5.117508	7.921615	-1.411497
H	3.477436	8.405254	-0.885434

C	4.415992	4.079205	-2.922329
H	5.045360	4.752908	-3.522006
H	3.731069	4.676679	-2.305304
H	5.046834	3.476891	-2.265153
C	2.807967	3.886509	-4.612531
H	2.106599	4.496743	-4.026413
H	3.366317	4.536247	-5.301568
H	2.253120	3.139331	-5.184182
N	5.282937	-1.954909	-1.891201
O	6.274376	-1.549009	-1.304938
O	5.322393	-2.581715	-2.938631

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M3, G= -3230.127376

O	0.215493	0.333029	1.422713
C	-0.111803	1.699732	0.978692
C	-1.568451	1.640662	0.501701
C	-1.834941	0.337065	-0.279731
O	-0.601798	-0.267024	-0.679394
H	-0.229998	-1.539773	0.888637
H	-0.056336	2.231581	1.932135
H	-1.793581	2.520444	-0.106208
H	-2.357481	-0.384683	0.369187
H	-2.228465	1.662131	1.376282
C	-2.635580	0.566386	-1.545844
H	-3.601374	1.020342	-1.300665
H	-2.084391	1.250187	-2.200644
H	-2.813408	-0.374717	-2.076731
C	1.571965	-0.973025	-0.123953
C	1.688802	-1.729140	-1.296126
C	2.941278	-2.078229	-1.790653
C	4.067620	-1.661016	-1.085822
C	3.981637	-0.914254	0.087416
C	2.719855	-0.574059	0.566346
H	0.793174	-2.034797	-1.827195
H	3.050741	-2.655975	-2.701350
H	4.884417	-0.602403	0.600182
H	2.610426	0.038816	1.455947
C	0.863072	2.311480	0.005577
K	2.806081	1.229486	-2.173751
O	2.395023	2.299432	1.781497
C	2.142331	2.590207	0.434049
O	3.118086	3.062847	-0.255989
C	3.649547	2.724327	2.274723
H	3.778147	3.807822	2.167107
H	3.661331	2.455538	3.334075
H	4.476901	2.222420	1.760622
N	0.544559	2.436113	-1.394492
K	1.670983	5.325960	-0.489197
O	-0.745917	4.361786	-1.086458
C	-0.238269	3.419811	-1.786917

C	-0.579030	3.431050	-3.273489
H	-0.086963	2.614756	-3.806988
H	-1.665747	3.348664	-3.399654
H	-0.275484	4.387330	-3.716100
C	0.190698	-0.632988	0.415749
O	2.047363	5.716306	2.128168
O	1.449506	6.624923	-2.818801
O	3.927473	3.157226	-3.746553
O	1.458298	0.423022	-4.361386
C	1.757729	0.099238	-5.702113
H	1.739951	-0.988554	-5.855621
H	1.034957	0.567074	-6.384781
H	2.758358	0.480074	-5.917206
C	0.171204	-0.022028	-3.967316
H	0.010584	0.315686	-2.938489
H	-0.600898	0.408544	-4.621528
H	0.110439	-1.118792	-4.024615
C	0.139608	7.042044	-3.157167
H	0.014189	8.116686	-2.965719
H	-0.066516	6.842592	-4.218176
H	-0.547611	6.461894	-2.535767
C	2.441640	7.252871	-3.600492
H	2.308225	7.014354	-4.664961
H	2.407673	8.344160	-3.473454
H	3.409740	6.877314	-3.259221
C	1.181656	4.980180	2.970762
H	1.755186	4.324099	3.639229
H	0.559410	5.657924	3.571193
H	0.549730	4.364705	2.326668
C	2.944771	6.526878	2.854133
H	2.400363	7.225912	3.504023
H	3.612036	5.910865	3.474129
H	3.535024	7.088586	2.127153
O	4.075470	6.551343	-0.455062
C	5.094723	5.698925	0.036801
H	5.932375	5.651089	-0.674730
H	5.473105	6.067076	1.001409
H	4.651762	4.705775	0.156747
C	4.538301	7.861619	-0.698873
H	4.952688	8.306643	0.216807
H	5.315166	7.862972	-1.476802
H	3.685390	8.454651	-1.035232
C	4.707393	4.088994	-3.022489
H	5.049607	4.901762	-3.679881
H	4.129090	4.509094	-2.188320
H	5.573607	3.555863	-2.624338
C	2.738358	3.747763	-4.237569
H	2.152074	4.184610	-3.416090
H	2.969576	4.534161	-4.970348
H	2.152862	2.958479	-4.715751
N	5.393965	-2.021621	-1.599936

O	6.371761	-1.671344	-0.959314
O	5.452345	-2.652546	-2.643514

Model 1.3

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M2, G=-3140.160087

O	3.004941	-0.972164	0.887419
C	0.889042	2.253959	1.111313
C	-0.238378	1.307361	0.832938
C	0.103209	-0.168532	1.076629
O	0.869022	-0.633161	-0.018785
H	1.455297	-2.304408	1.047715
H	1.245454	2.294646	2.138691
H	-0.590558	1.418921	-0.200139
H	0.706888	-0.248289	1.994448
H	-1.075563	1.582361	1.492966
C	-1.161596	-1.013167	1.212553
H	-1.746727	-0.719358	2.091209
H	-1.787210	-0.891780	0.319429
H	-0.904607	-2.073425	1.307661
C	2.229532	-2.304659	-0.971720
C	1.198520	-2.871589	-1.717795
C	1.435175	-3.482602	-2.950869
C	2.738149	-3.519937	-3.455541
C	3.787934	-2.978215	-2.709269
C	3.528501	-2.384884	-1.478181
H	0.179192	-2.812861	-1.340665
H	0.604547	-3.904173	-3.507364
H	4.795870	-3.031220	-3.112657
H	4.335997	-1.962599	-0.884900
C	1.436840	3.100383	0.218924
K	2.854032	0.810190	-1.171946
O	2.962178	3.859453	1.894568
C	2.422754	4.119054	0.696518
O	2.714769	5.122474	0.066909
C	3.944611	4.794315	2.332464
H	3.508701	5.790993	2.436586
H	4.297405	4.427409	3.295480
H	4.767408	4.836259	1.613022
N	1.218046	3.074098	-1.167108
K	0.677206	6.853613	-0.313121
O	-0.492290	4.625537	-1.001120
C	0.262189	3.840680	-1.655440
C	0.027404	3.734343	-3.153381
H	0.831017	3.186697	-3.652159
H	-0.919817	3.210617	-3.328920
H	-0.067242	4.737658	-3.581449
C	1.960895	-1.582115	0.360895
O	0.350657	5.807021	2.194355

O	1.249063	7.003476	-2.981895
O	4.605705	2.806489	-0.498487
O	1.891425	-0.038048	-3.564955
C	2.326487	-0.430438	-4.846997
H	1.906948	-1.409749	-5.116403
H	2.028011	0.308694	-5.604730
H	3.415159	-0.508505	-4.816493
C	0.481483	-0.016916	-3.461345
H	0.232369	0.251529	-2.430966
H	0.052203	0.720650	-4.153974
H	0.066998	-1.010368	-3.682349
C	0.882649	7.619960	-4.196187
H	1.682738	8.283895	-4.554429
H	0.674357	6.867164	-4.969444
H	-0.018867	8.206527	-4.009934
C	2.416644	6.215891	-3.111156
H	2.275190	5.434763	-3.871698
H	3.275740	6.840204	-3.400233
H	2.610129	5.749109	-2.141987
C	-0.750284	4.919458	2.305583
H	-0.468028	4.031147	2.886786
H	-1.592628	5.420703	2.803215
H	-1.018693	4.616542	1.291355
C	0.869784	6.160274	3.458028
H	0.083547	6.578123	4.102350
H	1.309767	5.283201	3.953744
H	1.641997	6.916636	3.301897
O	2.999288	8.197389	-0.777659
C	4.340087	7.790035	-0.593395
H	4.798230	7.524489	-1.557475
H	4.929236	8.593495	-0.129872
H	4.323023	6.909837	0.050347
C	2.892101	9.290547	-1.664087
H	3.431959	10.164587	-1.274304
H	3.297698	9.031803	-2.652771
H	1.832114	9.531532	-1.768635
C	5.822859	2.557017	0.173012
H	6.513936	1.991296	-0.467209
H	6.307231	3.498789	0.467018
H	5.589368	1.972667	1.064788
C	4.765782	3.651041	-1.620671
H	5.103480	4.649226	-1.307370
H	5.491840	3.225475	-2.328092
H	3.783560	3.739131	-2.091563
O	3.076195	-4.054789	-4.667952
C	2.038773	-4.625075	-5.443666
H	1.276243	-3.877910	-5.696256
H	2.508339	-4.987499	-6.357974
H	1.565985	-5.462411	-4.917460

TS2, G= -3140.120185

O	0.060158	-0.145411	1.541038
C	-0.183170	1.793304	1.048080
C	-1.625764	1.623887	0.648649
C	-1.898116	0.337485	-0.186518
O	-0.712348	-0.277776	-0.648495
H	-0.508130	-1.866941	0.629543
H	0.027909	1.939280	2.100193
H	-1.920903	2.507922	0.069971
H	-2.428345	-0.385538	0.456047
H	-2.247992	1.589646	1.548916
C	-2.750408	0.646647	-1.406296
H	-3.691713	1.119045	-1.103682
H	-2.210923	1.339032	-2.061929
H	-2.979899	-0.265842	-1.967096
C	1.388970	-1.225559	-0.166369
C	1.508115	-1.972343	-1.347021
C	2.753880	-2.270712	-1.885178
C	3.919576	-1.834785	-1.236505
C	3.818962	-1.090135	-0.058383
C	2.551448	-0.795378	0.463833
H	0.608848	-2.314815	-1.854425
H	2.850925	-2.843284	-2.803592
H	4.705263	-0.739887	0.459827
H	2.449623	-0.202911	1.369811
C	0.743114	2.309314	0.140412
K	2.566532	1.000693	-2.168117
O	2.345314	2.222618	1.877013
C	2.095563	2.502325	0.568435
O	3.032296	2.895930	-0.161995
C	3.655570	2.521998	2.334417
H	3.875129	3.586552	2.203295
H	3.666338	2.260395	3.393362
H	4.403741	1.931683	1.796246
N	0.503849	2.427397	-1.267228
K	1.583749	5.255829	-0.426404
O	-0.856765	4.314214	-1.045362
C	-0.291300	3.381410	-1.708682
C	-0.543717	3.369446	-3.212102
H	0.062246	2.614746	-3.719298
H	-1.605191	3.166794	-3.401328
H	-0.326492	4.357511	-3.633120
C	0.020190	-0.901221	0.434764
O	2.097319	5.441754	2.204216
O	1.558454	6.537576	-2.784153
O	3.678719	2.968975	-3.686693
O	1.172776	0.326418	-4.354499
C	1.363220	0.097832	-5.733114
H	1.197402	-0.959714	-5.980689
H	0.675183	0.714801	-6.328306
H	2.393730	0.367562	-5.973809

C	-0.128032	-0.034348	-3.918088
H	-0.204713	0.213594	-2.854763
H	-0.890624	0.523585	-4.480805
H	-0.294736	-1.111337	-4.064296
C	0.265560	6.989901	-3.145584
H	0.178427	8.074028	-2.991942
H	0.057817	6.760635	-4.200018
H	-0.449684	6.459978	-2.511071
C	2.572611	7.115162	-3.578721
H	2.432195	6.855716	-4.637381
H	2.572444	8.209344	-3.477090
H	3.528383	6.717722	-3.229135
C	1.218498	4.812111	3.118709
H	1.775701	4.158715	3.803645
H	0.666897	5.563436	3.699899
H	0.522679	4.206908	2.534242
C	3.050911	6.255058	2.854162
H	2.556881	7.026487	3.460531
H	3.698300	5.651233	3.506193
H	3.653289	6.732063	2.078315
O	4.052131	6.348156	-0.426349
C	5.112064	5.497714	-0.027942
H	5.893007	5.466502	-0.801931
H	5.560871	5.852418	0.911057
H	4.686822	4.500805	0.113037
C	4.476449	7.679040	-0.632194
H	4.904216	8.098560	0.289261
H	5.231530	7.729519	-1.429161
H	3.600157	8.261677	-0.923081
C	4.440909	3.845908	-2.882450
H	5.068838	4.498633	-3.506743
H	3.787441	4.463856	-2.252083
H	5.075503	3.236204	-2.235956
C	2.777758	3.675920	-4.517528
H	2.107928	4.304491	-3.913849
H	3.327378	4.310980	-5.227394
H	2.188047	2.937599	-5.065212
O	5.096629	-2.179625	-1.832886
C	6.298001	-1.785616	-1.193161
H	6.370649	-2.221307	-0.190292
H	7.108077	-2.164648	-1.815574
H	6.369728	-0.693768	-1.124413

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M3, G= -3140.136858

O	0.175978	0.372612	1.463510
C	-0.145635	1.731706	1.002872
C	-1.596972	1.671696	0.508698
C	-1.850825	0.362861	-0.269496
O	-0.613457	-0.242440	-0.645081
H	-0.304286	-1.496524	0.944518
H	-0.105651	2.273001	1.951752

H	-1.815439	2.548589	-0.106008
H	-2.384801	-0.353742	0.376858
H	-2.268176	1.697140	1.374982
C	-2.635025	0.584574	-1.547880
H	-3.603496	1.042532	-1.321103
H	-2.071863	1.261367	-2.199506
H	-2.806879	-0.360486	-2.074220
C	1.543642	-0.975564	-0.032382
C	1.694273	-1.764952	-1.172107
C	2.959618	-2.113077	-1.644670
C	4.096266	-1.680246	-0.958207
C	3.955291	-0.901424	0.193112
C	2.687642	-0.552803	0.649792
H	0.813444	-2.090399	-1.718615
H	3.051777	-2.701482	-2.550548
H	4.845683	-0.564772	0.717275
H	2.574870	0.084317	1.522372
C	0.843257	2.341371	0.040602
K	2.827314	1.184054	-2.069390
O	2.342236	2.359815	1.843838
C	2.114758	2.625401	0.484610
O	3.103239	3.087591	-0.194139
C	3.600392	2.764518	2.341400
H	3.752499	3.844164	2.223255
H	3.600473	2.507133	3.404033
H	4.421228	2.240563	1.838283
N	0.548948	2.441181	-1.367559
K	1.658357	5.340121	-0.488066
O	-0.745391	4.374096	-1.123376
C	-0.223146	3.416179	-1.793518
C	-0.538844	3.396452	-3.285723
H	-0.043427	2.564495	-3.792694
H	-1.623852	3.320030	-3.429083
H	-0.220634	4.340759	-3.743571
C	0.156557	-0.611769	0.468098
O	2.011119	5.773722	2.132841
O	1.482006	6.591904	-2.848247
O	3.977288	3.092638	-3.658325
O	1.517212	0.373970	-4.290332
C	1.844290	0.021497	-5.616456
H	1.842097	-1.070053	-5.744108
H	1.128547	0.463041	-6.323819
H	2.844141	0.408865	-5.824096
C	0.233104	-0.086254	-3.905944
H	0.048905	0.270071	-2.887945
H	-0.536615	0.314072	-4.582683
H	0.195159	-1.185414	-3.937638
C	0.176494	6.994371	-3.219439
H	0.039392	8.070482	-3.044692
H	-0.005686	6.779612	-4.281943
H	-0.519418	6.416543	-2.605703

C	2.485217	7.209776	-3.623380
H	2.373022	6.949788	-4.685369
H	2.443787	8.303315	-3.518806
H	3.448759	6.846014	-3.256901
C	1.162635	5.037542	2.993006
H	1.748944	4.406090	3.672970
H	0.529977	5.715995	3.581875
H	0.541154	4.397117	2.363870
C	2.897880	6.610801	2.840595
H	2.345065	7.308506	3.484958
H	3.581100	6.015917	3.464191
H	3.472060	7.173516	2.101481
O	4.064162	6.566901	-0.448635
C	5.080696	5.707523	0.036718
H	5.916145	5.659807	-0.677420
H	5.463677	6.068241	1.002504
H	4.632564	4.715985	0.151931
C	4.533266	7.874498	-0.693216
H	4.951087	8.317789	0.221943
H	5.309184	7.872092	-1.472145
H	3.683100	8.472047	-1.028787
C	4.743513	4.034753	-2.933408
H	5.114565	4.827457	-3.599858
H	4.145332	4.480518	-2.126946
H	5.591456	3.503529	-2.495431
C	2.799566	3.676240	-4.183562
H	2.197938	4.126652	-3.380905
H	3.046974	4.450631	-4.923984
H	2.222902	2.879903	-4.660153
O	5.370784	-1.936410	-1.395766
C	5.630780	-3.249139	-1.876505
H	5.109616	-3.455906	-2.816818
H	6.705705	-3.295253	-2.048964
H	5.348729	-3.997815	-1.125244

Model 1.4

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M2, G= -3124.928848

O	2.921184	-1.010077	0.700751
C	0.887742	2.241761	1.074372
C	-0.267831	1.336054	0.776298
C	0.033320	-0.157272	0.949950
O	0.785473	-0.595715	-0.167102
H	1.340851	-2.306391	0.848683
H	1.257849	2.240231	2.097676
H	-0.634002	1.503766	-0.244056
H	0.635044	-0.294900	1.861811
H	-1.085831	1.603672	1.462895
C	-1.254113	-0.972175	1.047575
H	-1.832976	-0.701546	1.937606

H	-1.873104	-0.793038	0.159639
H	-1.026592	-2.042312	1.095488
C	2.088194	-2.285481	-1.173614
C	1.022888	-2.797651	-1.921611
C	1.240136	-3.436325	-3.139843
C	2.546734	-3.547235	-3.595560
C	3.630336	-3.061665	-2.886079
C	3.384766	-2.432273	-1.662474
H	0.008683	-2.677796	-1.547536
H	0.424417	-3.833143	-3.737184
H	4.633775	-3.179308	-3.283975
H	4.204131	-2.043406	-1.063537
C	1.436242	3.108526	0.202071
K	2.795619	0.848188	-1.275825
O	2.991190	3.799379	1.879156
C	2.441377	4.100477	0.695544
O	2.736440	5.118632	0.092018
C	3.977119	4.719194	2.341180
H	3.545376	5.715570	2.463044
H	4.323113	4.330625	3.298134
H	4.803909	4.771289	1.627169
N	1.192657	3.127230	-1.179538
K	0.732429	6.901743	-0.221162
O	-0.482159	4.708737	-0.942539
C	0.246263	3.927780	-1.630401
C	-0.013149	3.868009	-3.126810
H	0.763426	3.304699	-3.650853
H	-0.980921	3.382777	-3.301181
H	-0.078666	4.884729	-3.527734
C	1.853349	-1.576440	0.174753
O	0.435011	5.796500	2.266652
O	1.276365	7.099665	-2.894183
O	4.576685	2.815359	-0.601471
O	1.683335	0.206246	-3.660803
C	2.020602	-0.310466	-4.929865
H	1.537316	-1.282481	-5.097280
H	1.713981	0.383636	-5.725446
H	3.104310	-0.441553	-4.955846
C	0.283283	0.308529	-3.485521
H	0.107435	0.751383	-2.501972
H	-0.156874	0.951575	-4.260917
H	-0.181863	-0.685951	-3.528551
C	0.901557	7.737447	-4.094904
H	1.705916	8.394767	-4.455683
H	0.671833	6.997945	-4.875003
H	0.011160	8.333929	-3.888079
C	2.430726	6.297800	-3.050329
H	2.268534	5.529809	-3.820258
H	3.295013	6.913932	-3.341618
H	2.630075	5.813411	-2.091084
C	-0.666501	4.908324	2.369217

H	-0.382639	4.011544	2.936726
H	-1.506458	5.403122	2.877231
H	-0.938615	4.621105	1.351361
C	0.955199	6.135432	3.533840
H	0.170108	6.548233	4.182751
H	1.392986	5.252054	4.020338
H	1.729426	6.891328	3.385642
O	3.063430	8.220672	-0.688344
C	4.399731	7.789834	-0.526928
H	4.846705	7.546779	-1.502070
H	5.003706	8.571038	-0.044816
H	4.375402	6.891240	0.090903
C	2.962730	9.335623	-1.548142
H	3.516063	10.193704	-1.142188
H	3.357672	9.095434	-2.545729
H	1.904927	9.591520	-1.638717
C	5.809505	2.568234	0.041360
H	6.493266	2.018689	-0.620527
H	6.290444	3.510638	0.338946
H	5.599261	1.969262	0.929322
C	4.705849	3.679448	-1.713007
H	5.047304	4.673715	-1.391413
H	5.416356	3.268474	-2.444378
H	3.711892	3.771300	-2.157973
F	2.766597	-4.152038	-4.792976

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TS2, G= -3124.890724

O	0.162031	-0.119198	1.544283
C	-0.126281	1.806189	1.054396
C	-1.567203	1.609083	0.660637
C	-1.818133	0.317610	-0.172383
O	-0.620983	-0.272694	-0.640168
H	-0.363747	-1.855749	0.637351
H	0.084219	1.963601	2.105053
H	-1.880450	2.487291	0.082590
H	-2.329574	-0.416528	0.472448
H	-2.184974	1.563447	1.563454
C	-2.681572	0.607569	-1.388652
H	-3.631040	1.060372	-1.081805
H	-2.159855	1.310457	-2.047484
H	-2.894679	-0.310209	-1.947236
C	1.507186	-1.163421	-0.173415
C	1.631353	-1.900695	-1.356006
C	2.884802	-2.180879	-1.901595
C	4.008987	-1.716660	-1.230629
C	3.928043	-0.980566	-0.057981
C	2.660642	-0.708099	0.466255
H	0.735609	-2.255044	-1.860313
H	2.998715	-2.747669	-2.820644
H	4.836949	-0.635921	0.426282

H	2.541962	-0.123546	1.374768
C	0.786579	2.339078	0.142109
K	2.656630	1.108479	-2.188264
O	2.392833	2.296812	1.876379
C	2.133395	2.569093	0.567823
O	3.058345	2.987643	-0.164259
C	3.695340	2.633429	2.331474
H	3.887666	3.701837	2.190583
H	3.712221	2.381554	3.392674
H	4.458397	2.057584	1.798746
N	0.543775	2.442996	-1.265911
K	1.544756	5.312862	-0.423895
O	-0.860861	4.298766	-1.056354
C	-0.270979	3.377184	-1.713912
C	-0.514891	3.354741	-3.218426
H	0.109499	2.610494	-3.718735
H	-1.570963	3.130891	-3.413854
H	-0.313180	4.345188	-3.641157
C	0.132110	-0.874553	0.438009
O	2.071339	5.523041	2.202088
O	1.425930	6.563186	-2.791431
O	3.687544	3.095935	-3.716956
O	1.250328	0.360776	-4.346281
C	1.432117	0.172195	-5.732377
H	1.281772	-0.881085	-6.006746
H	0.727793	0.792741	-6.304389
H	2.455557	0.466128	-5.974895
C	-0.040498	-0.034274	-3.909353
H	-0.118394	0.197156	-2.842400
H	-0.817667	0.514907	-4.460351
H	-0.184499	-1.112332	-4.071525
C	0.110873	6.979348	-3.116863
H	-0.010914	8.054868	-2.929650
H	-0.107010	6.774148	-4.174225
H	-0.572548	6.404359	-2.486152
C	2.404707	7.197273	-3.587282
H	2.258338	6.955918	-4.649447
H	2.363771	8.288079	-3.461021
H	3.380475	6.829737	-3.260153
C	1.210293	4.873358	3.119440
H	1.783678	4.228457	3.798966
H	0.647507	5.611700	3.706496
H	0.522663	4.256918	2.536897
C	3.012311	6.352907	2.849716
H	2.506167	7.109530	3.464697
H	3.677572	5.759215	3.492962
H	3.597835	6.847938	2.072365
O	3.980500	6.473980	-0.452909
C	5.063621	5.650149	-0.059958
H	5.840318	5.637488	-0.838645
H	5.509066	6.016982	0.875860

H	4.664687	4.642955	0.084722
C	4.373251	7.812774	-0.669804
H	4.804117	8.245472	0.244070
H	5.116321	7.875816	-1.477062
H	3.480964	8.375468	-0.951262
C	4.421326	3.988960	-2.903525
H	5.043138	4.654701	-3.520037
H	3.747052	4.593661	-2.282152
H	5.060020	3.392414	-2.248741
C	2.783147	3.782995	-4.560711
H	2.096888	4.403327	-3.967273
H	3.328932	4.422868	-5.269176
H	2.211777	3.031439	-5.109906
F	5.232502	-1.990875	-1.747365

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M3, G= -3124.907801

O	0.224098	0.331243	1.415231
C	-0.108876	1.699534	0.986409
C	-1.566393	1.644262	0.511158
C	-1.829323	0.352669	-0.291606
O	-0.595446	-0.245668	-0.692428
H	-0.265147	-1.529663	0.870725
H	-0.053997	2.222666	1.945005
H	-1.794333	2.533507	-0.081915
H	-2.356614	-0.377842	0.344232
H	-2.224860	1.649514	1.387326
C	-2.624855	0.601881	-1.557605
H	-3.590011	1.056279	-1.310364
H	-2.068250	1.291876	-2.201151
H	-2.804226	-0.331413	-2.101855
C	1.565233	-0.995709	-0.126801
C	1.684845	-1.763686	-1.288793
C	2.940009	-2.120070	-1.784258
C	4.062846	-1.702018	-1.084322
C	3.981306	-0.942841	0.074351
C	2.716932	-0.593404	0.552473
H	0.789939	-2.071754	-1.821369
H	3.052427	-2.706990	-2.690531
H	4.889380	-0.630602	0.580698
H	2.614870	0.031324	1.435211
C	0.860774	2.330064	0.019060
K	2.785889	1.197337	-2.127900
O	2.394749	2.307105	1.793149
C	2.141121	2.602702	0.445760
O	3.116783	3.078985	-0.243147
C	3.653840	2.718441	2.282967
H	3.792222	3.801585	2.180859
H	3.668109	2.444319	3.341060
H	4.475196	2.212146	1.763213
N	0.543820	2.457338	-1.381397

K	1.654218	5.323430	-0.484284
O	-0.767176	4.371895	-1.082199
C	-0.246148	3.432463	-1.777970
C	-0.574980	3.442002	-3.267555
H	-0.086696	2.618635	-3.793797
H	-1.661416	3.372216	-3.403169
H	-0.255745	4.393297	-3.710288
C	0.186789	-0.635027	0.404034
O	2.045381	5.731918	2.130483
O	1.442122	6.611178	-2.822584
O	3.932117	3.118586	-3.705448
O	1.457209	0.435277	-4.351897
C	1.765658	0.124125	-5.693041
H	1.754655	-0.962574	-5.855637
H	1.044170	0.593247	-6.376437
H	2.765458	0.511893	-5.899889
C	0.172077	-0.023387	-3.968043
H	0.005023	0.297793	-2.935148
H	-0.600747	0.410591	-4.619382
H	0.119116	-1.119719	-4.039530
C	0.135385	7.041855	-3.155721
H	0.022114	8.117952	-2.964641
H	-0.077609	6.843685	-4.215628
H	-0.555195	6.469088	-2.531016
C	2.437636	7.223138	-3.612347
H	2.298822	6.976659	-4.674365
H	2.414260	8.315811	-3.494737
H	3.403279	6.841524	-3.270640
C	1.191787	4.988408	2.978919
H	1.775477	4.337988	3.644052
H	0.567283	5.660933	3.582996
H	0.561859	4.366328	2.339119
C	2.940659	6.549870	2.850198
H	2.394892	7.247674	3.500419
H	3.614171	5.939691	3.469307
H	3.524580	7.112930	2.119180
O	4.055059	6.564769	-0.461108
C	5.077080	5.718918	0.036061
H	5.913791	5.667683	-0.676495
H	5.456195	6.095756	0.997075
H	4.636470	4.725717	0.164333
C	4.514091	7.874006	-0.716026
H	4.929173	8.327428	0.195323
H	5.289571	7.871343	-1.495415
H	3.659166	8.462405	-1.055406
C	4.707915	4.056004	-2.984885
H	5.077470	4.848030	-3.653035
H	4.116433	4.503113	-2.174601
H	5.556442	3.520731	-2.552904
C	2.754896	3.711315	-4.221975
H	2.160761	4.162270	-3.413923

H	3.003342	4.486581	-4.961251
H	2.169875	2.920324	-4.697572
F	5.285913	-2.042501	-1.555156

Model 1.5

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M2, G=-3362.676680

O	3.183027	-0.941057	0.396615
C	0.916600	1.950884	1.152963
C	-0.091994	0.871493	0.895946
C	0.394501	-0.568733	1.136032
O	0.902434	-1.098913	-0.092557
H	1.374224	1.962984	2.139415
H	-0.489344	0.949433	-0.122457
H	1.202090	-0.558647	1.876812
H	-0.935959	1.057525	1.577061
C	-0.763573	-1.443423	1.609558
H	-1.138337	-1.093941	2.577775
H	-1.585116	-1.392260	0.884375
H	-0.459710	-2.487065	1.710991
C	2.415113	-2.158708	-1.552428
C	1.350555	-2.610753	-2.337449
C	1.556903	-2.972724	-3.667658
C	2.831989	-2.889214	-4.228311
C	3.900471	-2.447107	-3.448055
C	3.690240	-2.088320	-2.115635
H	0.355068	-2.659655	-1.906417
H	0.718626	-3.312287	-4.271359
H	4.897576	-2.383031	-3.875895
H	4.508638	-1.738052	-1.491664
C	1.222416	2.941138	0.289710
K	2.542724	0.886888	-1.512441
O	2.547497	3.932049	2.007409
C	2.142100	4.040626	0.733615
O	2.489598	4.975971	0.033193
C	3.383256	4.983237	2.490851
H	2.900291	5.949644	2.329308
H	3.517149	4.787241	3.554395
H	4.351486	4.965514	1.982172
N	0.823921	2.950000	-1.052182
K	0.812306	7.032653	-0.468007
O	-0.506294	4.810908	-0.710416
C	0.002091	3.906527	-1.441440
C	-0.400025	3.875485	-2.906737
H	0.190798	3.147554	-3.469098
H	-1.460945	3.608622	-2.980285
H	-0.282063	4.873918	-3.340780
C	2.235622	-1.713874	-0.076005
O	0.528005	6.661869	2.226367
O	1.380462	6.835361	-3.127809

O	4.316008	2.520357	-0.265176
O	1.135113	0.445646	-3.770504
C	1.255925	0.422909	-5.175150
H	1.012088	-0.574087	-5.568299
H	0.587922	1.164729	-5.635986
H	2.291900	0.663439	-5.421248
C	-0.179986	0.147207	-3.346126
H	-0.166167	0.070371	-2.255941
H	-0.876480	0.939280	-3.654503
H	-0.510973	-0.813177	-3.765352
C	1.087565	7.393675	-4.389778
H	1.982335	7.859603	-4.827102
H	0.715411	6.624131	-5.080647
H	0.317499	8.153487	-4.245065
C	2.391960	5.848645	-3.201251
H	2.097746	5.042254	-3.888126
H	3.335693	6.288611	-3.557239
H	2.528517	5.437088	-2.198077
C	-0.268160	5.527273	2.534404
H	0.256731	4.874253	3.245555
H	-1.225453	5.841628	2.973136
H	-0.442853	4.992312	1.597173
C	0.800983	7.444134	3.369706
H	-0.128299	7.833501	3.806963
H	1.329097	6.851475	4.130189
H	1.433053	8.278480	3.058343
O	3.274831	8.004341	-1.020615
C	4.509668	7.376345	-0.740166
H	4.906812	6.885623	-1.640778
H	5.244929	8.108808	-0.379523
H	4.319490	6.620643	0.023186
C	3.381640	8.957080	-2.056848
H	4.085353	9.754756	-1.781849
H	3.724035	8.483660	-2.987899
H	2.390138	9.384656	-2.219318
C	4.831673	1.848527	0.871058
H	5.814730	1.410894	0.646855
H	4.932902	2.546254	1.714133
H	4.128671	1.049307	1.119610
C	5.163581	3.548854	-0.724272
H	5.364600	4.276647	0.074133
H	6.118866	3.138324	-1.080427
H	4.649048	4.059323	-1.541068
H	2.991623	-3.165686	-5.267219
C	2.139416	-3.026470	0.765439
F	1.113065	-3.836663	0.415539
F	2.003280	-2.794471	2.086852
F	3.261090	-3.764175	0.627457

O	0.135916	-0.073614	1.543497
C	-0.125428	1.767542	1.036539
C	-1.576508	1.620304	0.652735
C	-1.918389	0.317701	-0.123757
O	-0.772526	-0.411049	-0.567319
H	0.079627	1.982760	2.078852
H	-1.852103	2.492042	0.048233
H	-2.508185	-0.331431	0.534098
H	-2.186617	1.637769	1.561396
C	-2.723422	0.619825	-1.375800
H	-3.644310	1.149997	-1.110150
H	-2.134329	1.258063	-2.042330
H	-2.988156	-0.301726	-1.904670
C	1.464303	-1.106592	-0.207080
C	1.570313	-1.771699	-1.433311
C	2.823841	-2.034658	-1.988633
C	3.983790	-1.630557	-1.322845
C	3.880087	-0.950230	-0.107108
C	2.624539	-0.693635	0.449285
H	0.670339	-2.083846	-1.953612
H	2.894007	-2.551381	-2.942129
H	4.778051	-0.623735	0.411035
H	2.519961	-0.159968	1.389604
C	0.793440	2.273230	0.105570
K	2.716136	1.150057	-2.274336
O	2.392831	2.262771	1.839632
C	2.131488	2.524290	0.526293
O	3.055543	2.954597	-0.204883
C	3.689364	2.616838	2.296624
H	3.868361	3.688034	2.158876
H	3.708339	2.363801	3.357669
H	4.461254	2.052055	1.764734
N	0.536050	2.342613	-1.304243
K	1.570812	5.284502	-0.438312
O	-0.797421	4.253280	-1.116661
C	-0.240491	3.304297	-1.763771
C	-0.489702	3.273407	-3.267385
H	0.152275	2.546333	-3.770638
H	-1.539530	3.018567	-3.459705
H	-0.319657	4.268864	-3.691266
C	0.100438	-0.865249	0.469142
O	2.058648	5.504093	2.193765
O	1.518162	6.606073	-2.773383
O	3.671100	3.197759	-3.772576
O	1.217987	0.274324	-4.332055
C	1.424597	0.039764	-5.707635
H	1.261027	-1.018783	-5.952731
H	0.744368	0.654552	-6.313793
H	2.457787	0.308719	-5.937480
C	-0.091796	-0.073282	-3.914291
H	-0.179595	0.183455	-2.854322

H	-0.840688	0.487895	-4.491830
H	-0.266101	-1.149392	-4.058582
C	0.195394	6.939806	-3.157990
H	0.005284	8.009624	-2.997100
H	0.032981	6.704320	-4.219276
H	-0.480412	6.338586	-2.543807
C	2.487859	7.291148	-3.537358
H	2.379306	7.055425	-4.605409
H	2.395166	8.377564	-3.401492
H	3.470220	6.962948	-3.190163
C	1.186575	4.839686	3.089750
H	1.751391	4.182834	3.764972
H	0.617010	5.568224	3.682500
H	0.505112	4.233957	2.489200
C	2.990873	6.322676	2.867802
H	2.476281	7.067378	3.490264
H	3.648730	5.717816	3.508200
H	3.585061	6.832135	2.106835
O	3.993270	6.479699	-0.410760
C	5.062318	5.630957	-0.033086
H	5.849044	5.636918	-0.801775
H	5.499371	5.960117	0.920631
H	4.651530	4.623354	0.072017
C	4.401249	7.821669	-0.572865
H	4.820349	8.217708	0.362805
H	5.158765	7.906838	-1.364484
H	3.518766	8.401998	-0.849183
C	4.390788	4.085442	-2.940832
H	5.024668	4.753417	-3.542349
H	3.706165	4.689570	-2.330011
H	5.016871	3.484457	-2.277976
C	2.785399	3.889208	-4.632558
H	2.087848	4.507178	-4.050101
H	3.346632	4.531611	-5.326285
H	2.226178	3.140837	-5.198339
H	4.960191	-1.838506	-1.751824
C	-0.427809	-2.258909	0.934342
F	-1.586073	-2.170229	1.613754
F	-0.656359	-3.113904	-0.086938
F	0.453738	-2.869301	1.751913

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M3, G=-3362.645199

O	0.205346	0.337513	1.446199
C	-0.122165	1.711308	0.991290
C	-1.583524	1.664538	0.537926
C	-1.906833	0.382773	-0.258941
O	-0.711576	-0.355166	-0.587186
H	-0.050395	2.237417	1.945925
H	-1.805470	2.558242	-0.050912
H	-2.549781	-0.271435	0.339922

H	-2.221984	1.683038	1.427807
C	-2.584935	0.663608	-1.585013
H	-3.525930	1.195711	-1.410639
H	-1.933394	1.289059	-2.200943
H	-2.802160	-0.267906	-2.118286
C	1.524177	-0.972318	-0.134523
C	1.613399	-1.707558	-1.319072
C	2.863281	-2.040724	-1.844484
C	4.027338	-1.648655	-1.181242
C	3.936272	-0.917607	0.006305
C	2.687620	-0.582451	0.531770
H	0.705976	-2.010564	-1.831407
H	2.925121	-2.603928	-2.771554
H	4.839230	-0.604249	0.522889
H	2.601202	0.014094	1.435475
C	0.844527	2.309203	0.011234
K	2.797492	1.208171	-2.163079
O	2.375038	2.319926	1.784650
C	2.123589	2.597063	0.435314
O	3.094313	3.070954	-0.258570
C	3.638851	2.723893	2.269568
H	3.783574	3.805706	2.163941
H	3.654058	2.452351	3.328112
H	4.454105	2.209675	1.748285
N	0.520498	2.400532	-1.390060
K	1.645615	5.332786	-0.477749
O	-0.738575	4.354022	-1.124534
C	-0.243599	3.390646	-1.804355
C	-0.578106	3.382802	-3.292409
H	-0.100842	2.547537	-3.810312
H	-1.665655	3.323936	-3.422991
H	-0.251180	4.325113	-3.748424
C	0.157899	-0.639022	0.466587
O	2.031404	5.719025	2.142022
O	1.484225	6.616356	-2.823151
O	3.931194	3.141113	-3.739249
O	1.455371	0.427993	-4.372440
C	1.792580	0.153074	-5.714971
H	1.830741	-0.930228	-5.894962
H	1.059913	0.602294	-6.399664
H	2.777184	0.586757	-5.902586
C	0.187808	-0.093037	-4.014016
H	0.001843	0.188583	-2.973178
H	-0.598285	0.331062	-4.655758
H	0.179472	-1.187773	-4.118790
C	0.175883	7.012005	-3.192225
H	0.032465	8.086983	-3.015604
H	-0.006016	6.798307	-4.254947
H	-0.516316	6.429487	-2.578572
C	2.482636	7.245998	-3.595043
H	2.365931	6.999241	-4.659656

H	2.439053	8.337950	-3.476452
H	3.448233	6.879468	-3.238008
C	1.176512	4.987256	2.999125
H	1.758072	4.331800	3.661098
H	0.564200	5.668096	3.606291
H	0.534028	4.371600	2.366015
C	2.934964	6.535302	2.853866
H	2.396080	7.238846	3.503558
H	3.607957	5.924053	3.472409
H	3.518264	7.092189	2.117696
O	4.061519	6.545811	-0.440790
C	5.082269	5.694126	0.048615
H	5.923477	5.655981	-0.659370
H	5.454664	6.056043	1.018040
H	4.642522	4.698545	0.159024
C	4.518116	7.861449	-0.666252
H	4.924915	8.297734	0.257108
H	5.299548	7.876905	-1.439492
H	3.663736	8.453687	-1.000304
C	4.707883	4.079017	-3.019753
H	5.037757	4.895810	-3.678513
H	4.131596	4.492496	-2.180855
H	5.582089	3.553298	-2.629157
C	2.732061	3.721984	-4.217517
H	2.152382	4.155364	-3.389800
H	2.948333	4.509556	-4.953628
H	2.146123	2.928036	-4.687178
H	5.000459	-1.909012	-1.588379
C	-0.346831	-1.901183	1.222560
F	-1.514146	-1.688485	1.851483
F	-0.536383	-2.933698	0.382722
F	0.533305	-2.302362	2.155642

Model 1.6

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M2, G=-2113,068212

O	3.275345	-0.852301	0.320862
C	0.846605	2.026711	1.151665
C	-0.188697	0.974115	0.896307
C	0.350509	-0.461191	0.958187
O	1.012318	-0.741103	-0.261648
H	1.937203	-2.383728	0.586260
H	1.295709	2.031688	2.142185
H	-0.661730	1.127661	-0.080556
H	1.077091	-0.534587	1.782236
H	-0.971340	1.079642	1.661834
C	-0.776695	-1.469017	1.169026
H	-1.267073	-1.323151	2.137973
H	-1.527127	-1.357373	0.376679
H	-0.387006	-2.491642	1.129126

C	2.407194	-2.174219	-1.510448
C	1.348158	-2.836267	-2.139649
C	1.493865	-3.351247	-3.425674
C	2.707037	-3.206616	-4.104303
C	3.772038	-2.560565	-3.479436
C	3.621131	-2.056834	-2.184748
H	0.395772	-2.921403	-1.618985
H	0.660082	-3.856298	-3.907964
H	4.722423	-2.453921	-3.997170
H	4.441170	-1.558247	-1.673164
C	1.219412	2.984243	0.278942
K	2.634517	0.993874	-1.600278
O	2.637903	3.882643	1.975550
C	2.171234	4.052202	0.729820
O	2.487704	5.020488	0.059299
C	3.480465	4.920985	2.473040
H	2.971162	5.885259	2.398898
H	3.681564	4.665065	3.513009
H	4.416086	4.956702	1.908075
N	0.832776	3.016819	-1.068024
K	0.778719	7.061269	-0.365679
O	-0.532822	4.840918	-0.669271
C	-0.013319	3.963836	-1.426483
C	-0.436242	3.958573	-2.886503
H	0.174734	3.276047	-3.482621
H	-1.484862	3.645607	-2.952037
H	-0.369438	4.973334	-3.292173
C	2.246855	-1.561542	-0.104631
O	0.596536	6.649454	2.333753
O	1.306033	6.938931	-3.040120
O	4.381151	2.632171	-0.320144
O	1.319868	0.086787	-3.795948
C	1.534958	-0.018595	-5.184399
H	1.215440	-1.003855	-5.551357
H	0.985630	0.764698	-5.727209
H	2.606108	0.097589	-5.362199
C	-0.038450	-0.099830	-3.449459
H	-0.097060	-0.106968	-2.358138
H	-0.658145	0.711017	-3.859179
H	-0.402526	-1.063114	-3.833089
C	0.988477	7.518969	-4.286029
H	1.872454	8.000140	-4.728890
H	0.610717	6.760019	-4.985540
H	0.215280	8.270076	-4.114395
C	2.322126	5.960004	-3.149539
H	2.021085	5.166131	-3.847710
H	3.257334	6.412849	-3.512034
H	2.477560	5.529123	-2.157311
C	-0.137751	5.470573	2.629245
H	0.455283	4.802498	3.269523
H	-1.075825	5.724025	3.142408

H	-0.352434	4.974584	1.678623
C	0.907526	7.385337	3.498055
H	-0.007970	7.719563	4.004603
H	1.496639	6.775953	4.198133
H	1.493352	8.255312	3.194462
O	3.218995	8.080947	-0.940157
C	4.462208	7.459619	-0.683117
H	4.858171	6.995139	-1.598059
H	5.192355	8.190945	-0.309940
H	4.284617	6.683509	0.062622
C	3.305840	9.051891	-1.960928
H	4.002193	9.853446	-1.678446
H	3.646193	8.598053	-2.902441
H	2.307843	9.469359	-2.108383
C	4.966019	1.912078	0.752058
H	5.950385	1.520327	0.458464
H	5.086474	2.564116	1.628735
H	4.298901	1.076638	0.982597
C	5.201216	3.677628	-0.789773
H	5.454708	4.374703	0.021389
H	6.132440	3.280792	-1.218370
H	4.639672	4.217984	-1.554895
H	2.819369	-3.600072	-5.111555

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M2, G=-2113,061501

O	0.164158	-0.124991	1.555807
C	-0.131534	1.801588	1.055100
C	-1.571596	1.597436	0.661755
C	-1.816025	0.301631	-0.166544
O	-0.616821	-0.286882	-0.629572
H	-0.349787	-1.866685	0.651482
H	0.077822	1.963966	2.105074
H	-1.889361	2.472105	0.080814
H	-2.328243	-0.430945	0.479580
H	-2.189434	1.551995	1.564577
C	-2.675753	0.584922	-1.386932
H	-3.626437	1.039145	-1.085950
H	-2.150783	1.284051	-2.046986
H	-2.886402	-0.335777	-1.941783
C	1.516510	-1.165284	-0.160162
C	1.642091	-1.905155	-1.341476
C	2.899665	-2.167253	-1.886768
C	4.051231	-1.697831	-1.246478
C	3.931729	-0.964327	-0.064049
C	2.668736	-0.699987	0.474783
H	0.745315	-2.269224	-1.838126
H	2.983877	-2.737121	-2.808553
H	4.823508	-0.595906	0.437228
H	2.547057	-0.117229	1.384179
C	0.780751	2.333059	0.142792

K	2.658990	1.092882	-2.183094
O	2.380389	2.308535	1.880491
C	2.125926	2.569182	0.570057
O	3.053083	2.983410	-0.161416
C	3.683550	2.648193	2.326041
H	3.873262	3.716331	2.177775
H	3.705821	2.402179	3.388360
H	4.443795	2.069792	1.791715
N	0.539849	2.431891	-1.266199
K	1.544069	5.306577	-0.445427
O	-0.863316	4.289816	-1.063294
C	-0.275180	3.364401	-1.717510
C	-0.520356	3.337798	-3.222078
H	0.099828	2.588148	-3.719432
H	-1.577892	3.119456	-3.415569
H	-0.313911	4.325883	-3.648845
C	0.140352	-0.882483	0.450908
O	2.053792	5.539193	2.183886
O	1.438696	6.563219	-2.804248
O	3.704255	3.083940	-3.708643
O	1.239979	0.370450	-4.355553
C	1.362102	0.272451	-5.757225
H	1.188466	-0.758691	-6.094651
H	0.641017	0.935734	-6.256166
H	2.377730	0.573342	-6.023125
C	-0.030464	-0.060186	-3.892419
H	-0.079350	0.128458	-2.815249
H	-0.832699	0.498662	-4.395790
H	-0.164445	-1.132999	-4.093183
C	0.125694	6.976125	-3.140932
H	0.001256	8.052857	-2.962690
H	-0.085822	6.762066	-4.197771
H	-0.560636	6.405102	-2.509719
C	2.423648	7.187082	-3.600310
H	2.278008	6.942440	-4.661768
H	2.390494	8.278635	-3.478453
H	3.395691	6.812829	-3.269232
C	1.188320	4.889288	3.096920
H	1.758735	4.245774	3.780197
H	0.621161	5.627489	3.680017
H	0.505084	4.271232	2.510927
C	2.989847	6.370543	2.836389
H	2.479233	7.125028	3.450389
H	3.654005	5.777742	3.481632
H	3.577369	6.868182	2.062275
O	3.991615	6.450120	-0.451812
C	5.070277	5.631594	-0.036324
H	5.858800	5.615034	-0.803023
H	5.500690	6.005838	0.903565
H	4.670894	4.624727	0.108981
C	4.386099	7.786950	-0.677329

H	4.809327	8.227846	0.236243
H	5.135972	7.842955	-1.478859
H	3.496148	8.347135	-0.971033
C	4.473902	3.958323	-2.908244
H	5.060720	4.645040	-3.536053
H	3.833048	4.538880	-2.230866
H	5.149683	3.346648	-2.306391
C	2.772690	3.790183	-4.505725
H	2.104086	4.395477	-3.877560
H	3.295488	4.447303	-5.215854
H	2.184385	3.051795	-5.054857
H	5.031883	-1.904445	-1.666411

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M2, G=-2113,082596

O	0.221932	0.331887	1.416755
C	-0.111040	1.699482	0.987207
C	-1.568948	1.644165	0.512862
C	-1.832673	0.351011	-0.287105
O	-0.600256	-0.248133	-0.688823
H	-0.265305	-1.530466	0.875339
H	-0.055971	2.223369	1.945451
H	-1.797071	2.532226	-0.081952
H	-2.359856	-0.378012	0.350740
H	-2.227059	1.651456	1.389356
C	-2.629560	0.598610	-1.552696
H	-3.593762	1.055246	-1.305719
H	-2.072190	1.286266	-2.198179
H	-2.810797	-0.335543	-2.094810
C	1.561972	-0.998305	-0.127879
C	1.674484	-1.764541	-1.292331
C	2.930891	-2.108657	-1.793358
C	4.086625	-1.699210	-1.124147
C	3.975339	-0.947004	0.047602
C	2.717846	-0.598774	0.546055
H	0.774124	-2.073005	-1.816069
H	3.006758	-2.693133	-2.706449
H	4.870608	-0.621426	0.570719
H	2.619171	0.022331	1.431877
C	0.857744	2.331128	0.019449
K	2.783553	1.179689	-2.111063
O	2.389333	2.313022	1.794831
C	2.137510	2.605530	0.446600
O	3.113435	3.082166	-0.241836
C	3.650995	2.716354	2.283157
H	3.796233	3.798727	2.181267
H	3.664722	2.442164	3.341304
H	4.468754	2.204739	1.762820
N	0.539739	2.459117	-1.381019
K	1.652945	5.324532	-0.484630
O	-0.768742	4.375140	-1.078417

C	-0.249526	3.435456	-1.775690
C	-0.581061	3.447966	-3.264743
H	-0.096287	2.624769	-3.794286
H	-1.668002	3.381703	-3.398174
H	-0.259832	4.399182	-3.706186
C	0.185449	-0.636070	0.406478
O	2.044588	5.734437	2.129904
O	1.441547	6.611089	-2.822804
O	3.929247	3.106614	-3.690719
O	1.466454	0.476329	-4.371077
C	1.776709	0.115991	-5.699147
H	1.796265	-0.976686	-5.814556
H	1.039183	0.534102	-6.398206
H	2.764146	0.522495	-5.928646
C	0.196876	-0.001532	-3.958917
H	0.030743	0.353480	-2.936712
H	-0.592127	0.388160	-4.618966
H	0.173177	-1.100704	-3.988271
C	0.135932	7.044265	-3.156727
H	0.025329	8.121100	-2.968185
H	-0.077870	6.844051	-4.216088
H	-0.555921	6.474588	-2.530540
C	2.438676	7.216787	-3.615255
H	2.298887	6.966326	-4.676225
H	2.418718	8.310018	-3.502110
H	3.403229	6.833556	-3.272204
C	1.190238	4.991940	2.978462
H	1.773335	4.341426	3.643991
H	0.566134	5.665344	3.582038
H	0.560096	4.369889	2.338835
C	2.940390	6.551783	2.849452
H	2.395189	7.249947	3.499818
H	3.613636	5.941189	3.468466
H	3.524556	7.114562	2.118399
O	4.054190	6.566229	-0.460920
C	5.075274	5.720279	0.037892
H	5.912316	5.667565	-0.674206
H	5.454188	6.098101	0.998618
H	4.633830	4.727550	0.167133
C	4.514277	7.874649	-0.717734
H	4.929045	8.329416	0.193115
H	5.290287	7.870168	-1.496605
H	3.659993	8.463060	-1.058734
C	4.706465	4.045693	-2.974423
H	5.081397	4.831687	-3.646860
H	4.114403	4.500593	-2.168999
H	5.551520	3.510248	-2.535789
C	2.754705	3.700219	-4.212694
H	2.161596	4.158454	-3.408058
H	3.007476	4.470226	-4.956190
H	2.167470	2.907808	-4.682805

H 5.065708 -1.964691 -1.513152

Model 2.1

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M2, G= -3323.396213

C	3.622650	-2.100349	-2.078431
C	2.402081	-2.191092	-1.411783
C	1.348352	-2.875726	-2.025550
C	1.505573	-3.437466	-3.290489
C	2.725481	-3.320358	-3.962058
C	3.785613	-2.653610	-3.351250
C	2.230654	-1.529451	-0.030308
O	0.991331	-0.720874	-0.219641
C	0.318502	-0.417657	0.987999
C	-0.813556	-1.418014	1.205949
C	-0.217376	1.017653	0.895052
C	0.820560	2.068602	1.143564
C	1.208344	3.007817	0.261430
N	0.814730	3.013359	-1.088713
C	0.019905	3.972790	-1.471116
C	-0.430970	3.829673	-2.940405
C	2.166283	4.079810	0.677083
O	2.475239	5.026808	-0.025779
O	2.642859	3.933596	1.918652
C	3.550861	4.943638	2.356827
O	-0.499936	4.927862	-0.842541
O	3.251841	-0.797829	0.373967
K	0.815771	7.139129	-0.332389
O	3.297293	8.111235	-0.841700
C	3.386575	9.166304	-1.776115
C	4.522441	7.421080	-0.699321
K	2.620548	0.968263	-1.619508
O	1.367723	-0.042163	-3.789437
C	-0.001790	-0.176172	-3.465388
C	1.603309	-0.170217	-5.172130
O	4.328084	2.669612	-0.343848
C	5.157477	3.658605	-0.911380
C	4.973733	1.926922	0.677527
O	1.316895	7.233628	-2.990482
C	2.250325	6.193809	-3.206047
C	0.947729	7.873010	-4.192104
O	0.572915	6.525062	2.319956
C	0.963807	7.131614	3.534126
C	-0.267036	5.401601	2.533867
H	1.922400	-2.327314	0.688702
H	1.261021	2.093275	2.137601
H	-0.680933	1.154264	-0.088797
H	1.036190	-0.476893	1.820866
H	-1.005729	1.141555	1.651416
H	-1.316116	-1.250815	2.165105

H	-1.552842	-1.322738	0.401260
H	-0.424314	-2.441441	1.193110
H	0.390860	-2.940962	-1.511712
H	0.675117	-3.958103	-3.761835
H	4.741325	-2.567511	-3.863048
H	4.438983	-1.583476	-1.579432
H	3.093480	5.931127	2.258960
H	3.765384	4.715738	3.400272
H	4.470493	4.905099	1.766146
F	0.440013	3.171377	-3.724036
F	-1.599503	3.150806	-3.001919
F	-0.652448	5.021663	-3.521386
H	1.253516	-1.146434	-5.536208
H	1.093255	0.627367	-5.731814
H	2.681250	-0.096808	-5.331371
H	-0.082558	-0.137409	-2.375555
H	-0.588122	0.634855	-3.918652
H	-0.384828	-1.144457	-3.817014
H	1.824950	8.324036	-4.678462
H	0.482414	7.159350	-4.885047
H	0.230242	8.656921	-3.942310
H	1.855871	5.462703	-3.924385
H	3.197259	6.597608	-3.595616
H	2.431078	5.701812	-2.245911
H	0.265556	4.630024	3.106813
H	-1.172907	5.699101	3.079715
H	-0.534647	5.004576	1.551462
H	0.088736	7.507937	4.080886
H	1.499782	6.414991	4.172305
H	1.625636	7.965372	3.290295
H	4.856466	7.022528	-1.668335
H	5.299768	8.087736	-0.301020
H	4.344343	6.591367	-0.014486
H	4.120296	9.915024	-1.447311
H	3.679379	8.786590	-2.765108
H	2.400137	9.627552	-1.852070
H	5.913595	1.497194	0.303036
H	5.194856	2.573835	1.538141
H	4.298225	1.116504	0.965375
H	5.545306	4.339136	-0.139854
H	6.007993	3.200414	-1.435478
H	4.549712	4.231905	-1.614905
H	2.846623	-3.750530	-4.953031

O	0.310102	-0.181694	1.582763
C	-0.092124	1.758990	1.124856
C	-1.541288	1.504431	0.800544
C	-1.778244	0.193006	-0.005162
O	-0.584752	-0.324257	-0.557945

H	0.176940	1.900392	2.163744
H	-1.918697	2.361258	0.227827
H	-2.191629	-0.563323	0.681735
H	-2.117209	1.450167	1.729739
C	-2.749397	0.416889	-1.151452
H	-3.695048	0.824530	-0.777218
H	-2.323581	1.132731	-1.862511
H	-2.954680	-0.521566	-1.677229
C	1.596022	-1.147960	-0.229174
C	1.678437	-1.899776	-1.406180
C	2.905497	-2.096510	-2.040817
C	4.070377	-1.546467	-1.496835
C	3.995563	-0.802323	-0.316991
C	2.762947	-0.607569	0.313474
H	0.771416	-2.324280	-1.831466
H	2.953670	-2.674005	-2.960273
H	4.898781	-0.375048	0.111179
H	2.674112	-0.029167	1.229038
C	0.751931	2.322805	0.177870
K	2.424185	1.124395	-2.423328
O	2.452671	2.375199	1.804121
C	2.116705	2.610200	0.512377
O	2.968779	3.048056	-0.286265
C	3.766067	2.761167	2.184135
H	3.918411	3.828316	1.999871
H	3.840235	2.546270	3.250817
H	4.517280	2.186960	1.632929
N	0.431851	2.433973	-1.214946
K	1.470642	5.376532	-0.571292
O	-1.022963	4.263208	-0.950941
C	-0.407066	3.357351	-1.581535
C	-0.645040	3.396847	-3.104715
C	0.251003	-0.921142	0.468239
O	1.869083	5.426510	2.094859
O	1.792686	7.006703	-2.705820
O	3.607405	3.216147	-3.735738
O	1.076615	-0.186111	-4.351597
C	1.225123	-0.511877	-5.715347
H	1.001894	-1.573695	-5.889500
H	0.556424	0.099192	-6.337411
H	2.261755	-0.310350	-5.992598
C	-0.240157	-0.419694	-3.882680
H	-0.277286	-0.140950	-2.825484
H	-0.962967	0.182872	-4.450040
H	-0.498481	-1.483852	-3.987339
C	0.608551	7.542815	-3.268544
H	0.648877	8.640182	-3.276574
H	0.468920	7.177079	-4.294269
H	-0.230857	7.211942	-2.654294
C	2.942021	7.408302	-3.423409
H	2.869930	7.101372	-4.475968

H	3.066271	8.499184	-3.377516
H	3.803223	6.922847	-2.959829
C	0.902805	4.834194	2.944058
H	1.383699	4.150075	3.656160
H	0.350412	5.607278	3.495357
H	0.217256	4.268346	2.310164
C	2.793654	6.213983	2.814960
H	2.285557	7.043277	3.325770
H	3.322428	5.607097	3.563672
H	3.509821	6.611847	2.094056
O	3.927074	6.480801	-0.365623
C	5.097690	5.735579	-0.087111
H	5.847758	5.886914	-0.877027
H	5.532267	6.039966	0.876009
H	4.806249	4.683509	-0.046270
C	4.164279	7.873877	-0.384877
H	4.497195	8.227108	0.601125
H	4.930989	8.130457	-1.129075
H	3.223296	8.360524	-0.651007
C	4.428411	4.000638	-2.895015
H	5.124232	4.608148	-3.492172
H	3.819777	4.662023	-2.263813
H	4.990594	3.323096	-2.249381
C	2.826408	4.020533	-4.598668
H	2.171832	4.687218	-4.019192
H	3.472839	4.625347	-5.250116
H	2.214189	3.354246	-5.208333
H	5.027871	-1.700375	-1.986906
H	-0.202713	-1.922207	0.670197
F	0.103599	2.535327	-3.816906
F	-1.932318	3.144351	-3.419890
F	-0.370851	4.628871	-3.593477

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M3, G= -3323.379082

O	0.278677	0.302206	1.453595
C	-0.123912	1.647990	1.025078
C	-1.594999	1.533323	0.598901
C	-1.828401	0.222149	-0.182180
O	-0.580735	-0.315707	-0.624347
H	-0.055308	2.184950	1.975297
H	-1.886370	2.404669	0.006588
H	-2.287559	-0.524339	0.486509
H	-2.223455	1.522852	1.496195
C	-2.688916	0.404219	-1.415480
H	-3.653529	0.843999	-1.141401
H	-2.183851	1.079111	-2.113675
H	-2.867292	-0.554008	-1.914001
C	1.608487	-1.016437	-0.108252

C	1.707674	-1.801602	-1.261118
C	2.957668	-2.110439	-1.798624
C	4.119462	-1.647404	-1.176366
C	4.021532	-0.880000	-0.013463
C	2.770031	-0.566616	0.521502
H	0.801349	-2.150842	-1.747933
H	3.023698	-2.705160	-2.705781
H	4.922147	-0.513165	0.471751
H	2.678468	0.064587	1.400339
C	0.783483	2.305982	0.018353
K	2.628261	1.177269	-2.165843
O	2.404029	2.369765	1.695609
C	2.068172	2.647643	0.368932
O	2.973932	3.162603	-0.381460
C	3.668445	2.834686	2.122129
H	3.741986	3.925744	2.044779
H	3.760055	2.533592	3.168795
H	4.481332	2.387268	1.538890
N	0.369696	2.447063	-1.358695
K	1.584310	5.447036	-0.540866
O	-0.870368	4.407538	-0.956442
C	-0.410193	3.446841	-1.644107
C	-0.876622	3.493153	-3.113398
C	0.238596	-0.679790	0.454248
O	1.947094	5.754435	2.090424
O	1.702259	6.953865	-2.785254
O	3.760608	3.100263	-3.748957
O	1.492864	0.232572	-4.377629
C	1.874933	0.035862	-5.721039
H	1.957101	-1.035427	-5.952494
H	1.144462	0.492727	-6.402814
H	2.847609	0.512237	-5.860248
C	0.241017	-0.357127	-4.076677
H	-0.014244	-0.086114	-3.048085
H	-0.535751	0.020998	-4.754669
H	0.302496	-1.451066	-4.173889
C	0.528064	7.508876	-3.345985
H	0.578565	8.606195	-3.338171
H	0.390829	7.159663	-4.378167
H	-0.316596	7.173625	-2.741879
C	2.859717	7.319410	-3.506094
H	2.790614	6.983640	-4.550149
H	2.999798	8.409824	-3.492500
H	3.710269	6.837358	-3.020307
C	1.097443	4.977277	2.913298
H	1.686680	4.317162	3.563835
H	0.460905	5.625330	3.531069
H	0.479874	4.364323	2.253113
C	2.842678	6.546260	2.838584
H	2.297320	7.234623	3.498916
H	3.503545	5.915388	3.450299

H	3.441026	7.119128	2.127248
O	4.038696	6.565164	-0.441241
C	5.062922	5.704653	0.023530
H	5.921128	5.721590	-0.664477
H	5.404635	6.015144	1.022098
H	4.635586	4.699054	0.068152
C	4.462422	7.906819	-0.546168
H	4.806064	8.287218	0.426161
H	5.282331	8.002878	-1.272197
H	3.606689	8.495092	-0.884505
C	4.625220	4.007840	-3.094582
H	4.947433	4.800590	-3.785378
H	4.125212	4.453981	-2.224110
H	5.498883	3.445361	-2.757684
C	2.547833	3.719798	-4.132153
H	2.054097	4.174703	-3.261604
H	2.726514	4.499023	-4.886425
H	1.898959	2.945015	-4.547698
H	5.093501	-1.881738	-1.596199
H	-0.184686	-1.576963	0.941619
F	-0.457099	2.482086	-3.888849
F	-2.227403	3.498176	-3.190920
F	-0.463189	4.633891	-3.718111

Model 2.2

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M2, G=-2113.068212

C	1.882540	3.529957	-0.545713
C	1.058386	3.550643	-1.789580
C	-0.385233	3.063535	-1.594924
O	-0.394145	1.671213	-1.358888
H	1.463300	4.003362	0.337451
H	1.522811	2.952927	-2.581819
H	-0.822160	3.584375	-0.730727
H	1.038002	4.592873	-2.141188
C	-1.211928	3.349050	-2.843248
H	-1.251426	4.422773	-3.055950
H	-0.775687	2.838676	-3.709688
H	-2.232913	2.980167	-2.707530
C	3.124902	3.035987	-0.444308
K	2.160168	0.663185	1.684379
O	3.268458	3.443676	1.868643
C	3.972435	3.154667	0.770506
O	5.175705	2.989048	0.765829
C	4.037708	3.634868	3.065916
H	4.822032	4.373163	2.889722
H	3.327668	3.992202	3.808917
H	4.470568	2.681326	3.379646
C	4.255153	3.000773	-2.678894
C	4.194615	1.058768	-1.404079

C	5.004555	1.962188	-3.491979
C	4.995077	0.692186	-2.633962
H	4.494285	1.836889	-4.450539
H	6.008758	2.340652	-3.696716
H	4.519710	-0.161669	-3.122866
H	5.993430	0.380806	-2.315306
N	3.788132	2.380446	-1.516971
O	4.061449	4.162309	-2.951783
O	3.923380	0.354659	-0.450382
C	-0.731057	1.314399	0.021501
C	-0.610616	-0.210437	0.058078
C	0.470946	-0.861942	-0.546345
C	-1.513211	-0.966374	0.808904
C	0.652990	-2.236220	-0.391324
H	1.167956	-0.278983	-1.144667
C	-1.338822	-2.342783	0.965206
H	-2.358370	-0.468239	1.281113
C	-0.252121	-2.982058	0.367426
H	1.497265	-2.728034	-0.868186
H	-2.051447	-2.916852	1.551792
H	-0.114321	-4.053252	0.486395
O	0.041413	1.909447	0.927128
H	-1.812619	1.578154	0.126153
O	4.473232	0.131024	3.017909
O	1.950605	1.716648	4.141189
C	4.231311	-0.978270	3.859944
H	4.371728	-1.921453	3.314461
H	4.905120	-0.964732	4.727783
H	3.197182	-0.910373	4.208069
C	5.786253	0.118113	2.486563
H	6.527751	0.162721	3.296093
H	5.954261	-0.792077	1.895348
H	5.884551	0.994807	1.844605
C	2.585520	1.726407	5.400401
H	2.725298	2.755969	5.760468
H	1.993000	1.172401	6.141621
H	3.562316	1.253218	5.278784
C	0.733848	2.446031	4.141784
H	0.301550	2.366637	3.139493
H	0.037249	2.033514	4.884648
H	0.923870	3.502020	4.382813

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TS2, G= -2113.061501

C	1.944361	3.050501	-0.494457
C	1.219599	3.040024	-1.804149
C	-0.295412	2.820749	-1.713413
O	-0.647651	1.490514	-1.392477
H	1.417691	3.449007	0.368670
H	1.654597	2.285523	-2.471168
H	-0.695466	3.490216	-0.929330

H	1.395772	4.020124	-2.271946
C	-0.964250	3.146860	-3.039485
H	-0.792534	4.192449	-3.313838
H	-0.558392	2.508157	-3.832024
H	-2.041699	2.972635	-2.973140
C	3.303979	2.986323	-0.402102
K	3.073343	0.226714	1.407531
O	3.285137	3.378120	1.906569
C	4.065514	3.226130	0.817390
O	5.285975	3.257432	0.878540
C	3.979509	3.605475	3.135621
H	4.668278	4.446459	3.033612
H	3.208160	3.830799	3.870823
H	4.527055	2.705186	3.429874
C	4.386236	3.464141	-2.600815
C	4.838338	1.445965	-1.559818
C	5.332368	2.737930	-3.537476
C	5.693245	1.440274	-2.809183
H	4.813537	2.564434	-4.484430
H	6.190650	3.381811	-3.741632
H	5.477850	0.536715	-3.384156
H	6.742818	1.399967	-2.504710
N	4.111283	2.625673	-1.519763
O	3.919311	4.572423	-2.741906
O	4.778714	0.580817	-0.706756
C	-0.225932	1.105802	-0.065389
C	-0.815916	-0.275200	0.179210
C	-0.536334	-1.321011	-0.707017
C	-1.578762	-0.537764	1.316497
C	-1.015899	-2.604632	-0.460734
H	0.057942	-1.113253	-1.593051
C	-2.055666	-1.826219	1.573354
H	-1.802226	0.272411	2.008672
C	-1.776334	-2.862129	0.684217
H	-0.800853	-3.408252	-1.160350
H	-2.647237	-2.018473	2.464645
H	-2.150257	-3.863896	0.877205
O	1.109603	1.118554	0.078048
H	-0.735072	1.827115	0.621727
O	5.254876	-0.000606	3.010245
O	2.127608	1.265939	3.706698
C	5.400269	-1.001257	3.997038
H	6.091266	-1.784786	3.658126
H	5.780343	-0.571770	4.934192
H	4.415257	-1.439615	4.172043
C	6.491274	0.607382	2.680990
H	6.933233	1.083101	3.567589
H	7.194626	-0.138905	2.287750
H	6.292203	1.365902	1.921446
C	2.400945	1.213309	5.088948
H	2.430376	2.223935	5.521032

H	1.638368	0.625541	5.618160
H	3.378582	0.742675	5.210772
C	0.923182	1.949375	3.413848
H	0.802267	1.933571	2.327195
H	0.069070	1.451950	3.894286
H	0.973813	2.990130	3.765100

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M3, G= -2113.082596

C	2.277758	3.555379	-0.741285
C	1.847438	4.028430	-2.127728
C	0.329842	4.163375	-2.218578
O	-0.287285	2.938100	-1.805247
H	1.994479	4.306849	0.010336
H	2.178558	3.301150	-2.881274
H	-0.005749	4.956749	-1.528984
H	2.327415	4.987622	-2.349011
C	-0.156977	4.463095	-3.621334
H	0.270381	5.406187	-3.975650
H	0.148949	3.663428	-4.303976
H	-1.247666	4.543057	-3.642284
C	3.719565	3.249532	-0.611053
K	2.950795	0.698877	1.166515
O	3.622201	3.566588	1.685536
C	4.412762	3.217009	0.596747
O	5.593847	2.864071	0.792784
C	4.288124	3.592305	2.940629
H	5.179721	4.223228	2.900997
H	3.569453	4.005986	3.650073
H	4.570736	2.582175	3.257524
C	5.042379	3.505192	-2.713429
C	4.675408	1.373186	-1.920778
C	5.735412	2.593645	-3.708504
C	5.541888	1.183810	-3.148252
N	4.426670	2.723165	-1.735767
O	5.002520	4.716289	-2.754646
O	4.259326	0.484597	-1.196965
C	0.097736	2.587002	-0.498650
C	-0.615405	1.322693	-0.096547
C	-0.250583	0.107456	-0.683939
C	-1.634156	1.352013	0.854328
C	-0.902682	-1.068212	-0.320096
H	0.545640	0.092547	-1.424231
C	-2.288262	0.174284	1.220403
H	-1.917802	2.297465	1.312156
C	-1.922938	-1.036030	0.633852
H	-0.617775	-2.010133	-0.780372
H	-3.081244	0.204116	1.962211
H	-2.431190	-1.953100	0.917731
O	1.479935	2.359357	-0.421329
H	-0.172541	3.420708	0.177613

O	4.785959	-0.132123	2.982019
O	1.951954	1.689082	3.447646
C	4.631040	-1.241088	3.842188
H	5.214406	-2.099172	3.481944
H	4.957746	-0.992376	4.861646
H	3.571082	-1.504908	3.855849
C	6.138336	0.285675	2.887318
H	6.510166	0.599312	3.872890
H	6.766536	-0.534372	2.513664
H	6.170766	1.128779	2.193041
C	2.234127	1.516269	4.819540
H	2.556571	2.464884	5.271419
H	1.350696	1.147228	5.358291
H	3.044851	0.789260	4.894457
C	0.970771	2.678496	3.215162
H	0.896134	2.812270	2.133495
H	-0.001715	2.368098	3.621753
H	1.264169	3.634092	3.671251
H	6.479004	0.712869	-2.838528
H	5.038484	0.500425	-3.836659
H	6.782766	2.893627	-3.789756
H	5.272414	2.733777	-4.689188

Model 2.3

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M2, G=-2265.417140

C	2.064518	3.678787	-0.691361
C	1.250214	3.471722	-1.923364
C	-0.098258	2.838867	-1.563269
O	0.149337	1.607841	-0.908450
H	1.577466	4.178817	0.144519
H	1.777678	2.834351	-2.642166
H	-0.616655	3.511808	-0.863563
H	1.073686	4.442276	-2.406110
C	-0.951394	2.620162	-2.807419
H	-1.171143	3.568384	-3.310149
H	-0.425779	1.963222	-3.509987
H	-1.899826	2.144616	-2.538185
C	3.327203	3.271431	-0.515549
K	1.985608	1.070290	1.370994
O	3.286605	3.639739	1.803666
C	4.090467	3.442003	0.756119
O	5.297780	3.365011	0.827533
C	3.937607	3.796940	3.074872
H	4.672904	4.601330	3.018560
H	3.141865	4.040306	3.775808
H	4.417268	2.855194	3.353197
C	4.584449	3.188397	-2.693646
C	4.461855	1.275046	-1.376473

C	5.375196	2.107328	-3.353898
C	5.306431	0.962689	-2.561737
N	4.060807	2.605923	-1.527164
O	4.394577	4.327152	-3.046752
O	4.133500	0.571611	-0.444107
C	-0.805572	1.362402	0.209986
C	-0.770936	-0.168239	0.373088
C	-0.853507	-1.021666	-0.733456
C	-0.692946	-0.728049	1.649281
C	-0.845795	-2.404994	-0.567294
H	-0.913572	-0.589450	-1.729725
C	-0.679614	-2.115188	1.822030
H	-0.650021	-0.055216	2.503631
C	-0.754922	-2.957141	0.713721
H	-0.905572	-3.056345	-1.435452
H	-0.616253	-2.537110	2.821970
H	-0.746576	-4.035806	0.844201
O	-0.500591	2.051006	1.294438
H	-1.799995	1.619561	-0.227921
O	4.304401	0.346410	2.652209
O	1.850548	1.625559	4.034667
C	3.864460	-0.898430	3.158379
H	3.907887	-1.672995	2.379945
H	4.481524	-1.214933	4.010751
H	2.831778	-0.773054	3.497071
C	5.655553	0.291224	2.231537
H	6.308245	0.044184	3.080261
H	5.784316	-0.460469	1.442185
H	5.914959	1.274889	1.837353
C	2.636469	1.489777	5.199127
H	2.755487	2.460106	5.702674
H	2.172264	0.783591	5.901909
H	3.616005	1.118113	4.893061
C	0.580119	2.193990	4.315820
H	0.032818	2.254082	3.370846
H	0.030060	1.565219	5.030601
H	0.700846	3.196908	4.749904
C	6.087049	2.127823	-4.540357
H	6.134544	3.022243	-5.153517
C	5.946649	-0.210861	-2.920631
H	5.888706	-1.099184	-2.299519
C	6.673090	-0.200436	-4.117146
H	7.193191	-1.098870	-4.434334
C	6.741820	0.947650	-4.912236
H	7.314109	0.922071	-5.834165

C	1.858972	3.004575	-0.535200
C	1.230264	2.795996	-1.878629
C	-0.295483	2.625918	-1.867410

O	-0.722589	1.376928	-1.362334
H	1.260056	3.489389	0.231054
H	1.690243	1.937164	-2.382112
H	-0.724582	3.424829	-1.234682
H	1.464725	3.686466	-2.481957
C	-0.859320	2.747151	-3.274734
H	-0.632403	3.729528	-3.700714
H	-0.423079	1.978253	-3.922263
H	-1.944492	2.612590	-3.261727
C	3.202514	2.972702	-0.329221
K	2.706345	-0.344333	1.296934
O	3.010692	3.869369	1.830956
C	3.866268	3.421798	0.893434
O	5.076542	3.417093	1.059967
C	3.606769	4.302258	3.052589
H	4.361591	5.068420	2.862902
H	2.792930	4.713278	3.649122
H	4.064862	3.454563	3.569840
C	4.528770	3.299872	-2.416858
C	4.789657	1.304135	-1.279314
C	5.560155	2.492415	-3.131632
C	5.725809	1.296198	-2.441184
N	4.091526	2.509014	-1.341431
O	4.121604	4.407858	-2.679353
O	4.637008	0.443934	-0.434935
C	-0.357341	1.179038	0.023940
C	-1.047801	-0.101563	0.470471
C	-0.863417	-1.291492	-0.243263
C	-1.795894	-0.128709	1.647478
C	-1.422232	-2.483311	0.212703
H	-0.282081	-1.271095	-1.161965
C	-2.352115	-1.322762	2.113575
H	-1.943403	0.794104	2.206330
C	-2.166848	-2.503155	1.396530
H	-1.279596	-3.400882	-0.352543
H	-2.932337	-1.328349	3.032394
H	-2.600237	-3.433417	1.753459
O	0.969368	1.126466	0.204631
H	-0.828230	2.032872	0.573660
O	5.071525	-0.633989	2.643162
O	2.454927	1.298086	3.447128
C	6.033671	-1.648584	2.440078
H	6.506635	-1.541952	1.454405
H	6.810639	-1.607347	3.215616
H	5.518455	-2.609188	2.496026
C	5.650194	0.658404	2.596377
H	6.373756	0.786690	3.413890
H	6.146008	0.830435	1.633287
H	4.840599	1.383100	2.704923
C	2.877511	1.032508	4.768686
H	3.005528	1.968714	5.330861

H	2.146041	0.402536	5.293821
H	3.832257	0.505451	4.708787
C	1.194703	1.946192	3.406409
H	0.946457	2.091183	2.352630
H	0.429004	1.321099	3.888680
H	1.242584	2.913777	3.925182
C	6.627323	0.333214	-2.862009
H	6.752570	-0.599550	-2.320600
C	6.287236	2.783233	-4.272580
H	6.152099	3.720506	-4.803404
C	7.370033	0.615282	-4.014893
H	8.088998	-0.111721	-4.379576
C	7.203230	1.818556	-4.707642
H	7.795605	2.006869	-5.597724

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M3, G= -2265.432220

C	2.297464	3.495798	-0.740984
C	1.888252	3.937743	-2.143812
C	0.374080	4.094670	-2.253493
O	-0.266517	2.891153	-1.812781
H	2.017515	4.270573	-0.012142
H	2.214750	3.185384	-2.874150
H	0.044698	4.912164	-1.589527
H	2.385322	4.883348	-2.386169
C	-0.094277	4.362659	-3.668910
H	0.350997	5.289046	-4.044562
H	0.206055	3.539775	-4.325836
H	-1.183358	4.458578	-3.703060
C	3.733910	3.172963	-0.590696
K	2.923702	0.676183	1.228398
O	3.628319	3.564145	1.695120
C	4.419150	3.168261	0.623604
O	5.592766	2.802595	0.837539
C	4.284027	3.605737	2.955294
H	5.186624	4.220366	2.909875
H	3.566576	4.046992	3.649248
H	4.545983	2.598030	3.296509
C	5.108179	3.360881	-2.678323
C	4.675520	1.251407	-1.862071
C	5.787833	2.374535	-3.572630
C	5.532575	1.101439	-3.074872
N	4.440826	2.614289	-1.695935
O	5.108953	4.568458	-2.768778
O	4.250490	0.365788	-1.142625
C	0.100775	2.568339	-0.494322
C	-0.636853	1.327671	-0.064605
C	-0.325959	0.099171	-0.655596
C	-1.622781	1.391579	0.918572
C	-0.999286	-1.054949	-0.262754
H	0.443094	0.056557	-1.422831

C	-2.297504	0.235241	1.314497
H	-1.864873	2.347745	1.377824
C	-1.985991	-0.988199	0.724407
H	-0.758097	-2.007244	-0.726581
H	-3.064545	0.292684	2.081448
H	-2.510748	-1.888864	1.030009
O	1.479012	2.319977	-0.398430
H	-0.160192	3.423782	0.157816
O	4.735865	-0.129117	3.079156
O	1.928110	1.738419	3.477864
C	4.561732	-1.213763	3.966379
H	5.149477	-2.082519	3.640835
H	4.869917	-0.937859	4.984619
H	3.501066	-1.474929	3.967555
C	6.091398	0.282020	2.998756
H	6.444826	0.623470	3.981809
H	6.723748	-0.550599	2.661975
H	6.140220	1.104145	2.280763
C	2.198883	1.583205	4.854206
H	2.531607	2.534269	5.293247
H	1.306819	1.235041	5.392562
H	2.998740	0.846261	4.945833
C	0.960601	2.735957	3.224232
H	0.894470	2.854366	2.140272
H	-0.018040	2.443298	3.629334
H	1.262494	3.694567	3.668249
C	6.559640	2.571926	-4.704370
H	6.755410	3.569225	-5.086517
C	6.036962	-0.033724	-3.686248
H	5.835651	-1.024645	-3.290659
C	6.819437	0.151959	-4.831855
H	7.236444	-0.711312	-5.341506
C	7.076651	1.432429	-5.331983
H	7.688828	1.541865	-6.222100

Model 2.4

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M2, G= -2035.682350

C	2.127394	3.637828	-0.670045
C	1.352457	3.440768	-1.928943
C	-0.006964	2.807146	-1.617494
O	0.218059	1.577180	-0.952240
H	1.596236	4.081685	0.171368
H	1.902863	2.809530	-2.636276
H	-0.548670	3.480176	-0.936199
H	1.196536	4.416603	-2.408725
C	-0.818069	2.586783	-2.888727
H	-1.021308	3.534542	-3.399265
H	-0.269982	1.929217	-3.573264
H	-1.774666	2.111423	-2.649813

C	3.403810	3.290831	-0.477178
K	2.010494	1.063758	1.379835
O	3.302412	3.607579	1.844455
C	4.134422	3.456049	0.811821
O	5.341901	3.419167	0.907587
C	3.919678	3.774894	3.131379
H	4.639198	4.594366	3.093645
H	3.102589	4.000148	3.813343
H	4.412247	2.842763	3.419280
C	4.654808	3.426993	-2.596490
C	4.567650	1.368794	-1.340085
N	4.199171	2.693620	-1.503674
O	4.369504	4.583025	-2.790209
O	4.183117	0.697470	-0.406333
C	-0.756114	1.350921	0.153582
C	-0.729272	-0.177078	0.341136
C	-0.790192	-1.048216	-0.752912
C	-0.681237	-0.716575	1.627536
C	-0.790425	-2.428788	-0.564170
H	-0.827436	-0.632259	-1.757161
C	-0.676068	-2.100754	1.823070
H	-0.655042	-0.030270	2.471680
C	-0.729435	-2.960443	0.727154
H	-0.833799	-3.093811	-1.422847
H	-0.636529	-2.506364	2.830957
H	-0.727409	-4.036867	0.875145
O	-0.467171	2.055845	1.231884
H	-1.742396	1.604078	-0.305156
O	4.288778	0.326847	2.701680
O	1.809462	1.610551	4.039089
C	3.869418	-0.912581	3.238179
H	3.957996	-1.711249	2.488974
H	4.469356	-1.181432	4.118600
H	2.823666	-0.806096	3.541305
C	5.650354	0.296747	2.314378
H	6.289864	0.095704	3.185068
H	5.819697	-0.476823	1.554475
H	5.892182	1.274543	1.894786
C	2.570253	1.472261	5.219828
H	2.671905	2.439930	5.732242
H	2.095674	0.758332	5.907725
H	3.558935	1.109337	4.933116
C	0.532901	2.177769	4.293189
H	0.009013	2.245117	3.335425
H	-0.035004	1.544782	4.989991
H	0.643370	3.177877	4.736374
H	5.293962	2.837392	-3.269643
H	5.229754	0.985066	-2.127904

C	2.164452	2.872538	-0.502999
C	1.508699	2.877554	-1.851902
C	-0.013585	2.702835	-1.836244
O	-0.419099	1.409988	-1.438913
H	1.580915	3.230225	0.341371
H	1.957742	2.106050	-2.489562
H	-0.435146	3.436390	-1.124969
H	1.729100	3.850367	-2.314949
C	-0.600014	2.949008	-3.216947
H	-0.380799	3.966529	-3.555461
H	-0.175274	2.241904	-3.937978
H	-1.684997	2.812641	-3.197286
C	3.524030	2.910741	-0.357188
K	3.347036	0.146145	1.288679
O	3.393338	3.118160	1.962912
C	4.212875	3.210423	0.891258
O	5.396380	3.490639	0.988999
C	3.949212	3.512569	3.219139
H	4.026106	4.602199	3.266820
H	3.252693	3.145393	3.973502
H	4.933076	3.062204	3.352719
C	4.620031	3.713301	-2.413657
C	5.180397	1.570403	-1.539313
N	4.402821	2.709484	-1.473810
O	4.069994	4.788607	-2.394331
O	5.127669	0.668538	-0.727484
C	0.000858	1.083600	-0.098645
C	-0.780807	-0.170038	0.299441
C	-2.024412	-0.466241	-0.267158
C	-0.275228	-1.020352	1.286892
C	-2.741201	-1.593441	0.136138
H	-2.423054	0.188309	-1.035578
C	-0.992286	-2.144555	1.698712
H	0.687091	-0.789999	1.737493
C	-2.228338	-2.437189	1.121652
H	-3.702147	-1.813201	-0.321786
H	-0.584463	-2.795494	2.468287
H	-2.786283	-3.314779	1.436282
O	1.332246	0.960225	0.014344
H	-0.387660	1.924678	0.532537
O	5.465433	0.736531	2.813814
O	1.815381	0.566332	3.498202
C	5.417328	0.543185	4.212606
H	5.950845	-0.373182	4.498795
H	5.868307	1.395338	4.740536
H	4.364224	0.463444	4.493493
C	6.781577	0.961736	2.344250
H	7.196197	1.875696	2.790564
H	7.429387	0.109384	2.590231
H	6.719513	1.087744	1.262966
C	1.415653	-0.326843	4.518102

H	1.291890	0.201988	5.472884
H	0.466396	-0.814969	4.255246
H	2.196536	-1.083049	4.621972
C	0.857009	1.590094	3.289335
H	1.199267	2.182016	2.438950
H	-0.126541	1.156387	3.060122
H	0.772097	2.221476	4.184896
H	5.342340	3.426410	-3.192712
H	5.862952	1.545682	-2.400308

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M3, G= -2035.696971

C	2.270941	3.602625	-0.767460
C	1.828188	4.077671	-2.149407
C	0.308320	4.194142	-2.231375
O	-0.291868	2.959307	-1.822054
H	1.978326	4.345231	-0.010270
H	2.163655	3.358301	-2.908536
H	-0.033151	4.979526	-1.535663
H	2.293507	5.044501	-2.367969
C	-0.189151	4.495601	-3.630015
H	0.224331	5.446024	-3.981153
H	0.123342	3.703697	-4.318689
H	-1.280843	4.561815	-3.644900
C	3.717079	3.317876	-0.640059
K	2.957141	0.732112	1.121550
O	3.608716	3.570139	1.662575
C	4.409427	3.268221	0.567001
O	5.597351	2.936149	0.755679
C	4.275438	3.593512	2.917982
H	5.154761	4.241544	2.884410
H	3.549813	3.985073	3.632748
H	4.577264	2.585084	3.222372
C	5.030836	3.716292	-2.690331
C	4.691592	1.495276	-1.963954
N	4.446959	2.841090	-1.781698
O	4.940563	4.921969	-2.640536
O	4.272727	0.609497	-1.243196
C	0.104672	2.604722	-0.520007
C	-0.589179	1.328013	-0.122918
C	-0.207400	0.121413	-0.717334
C	-1.607196	1.337259	0.829179
C	-0.841357	-1.065753	-0.358831
H	0.587545	0.122649	-1.459240
C	-2.243115	0.148035	1.189874
H	-1.904817	2.275955	1.291975
C	-1.860457	-1.053722	0.596734
H	-0.543263	-2.000870	-0.824585
H	-3.035593	0.161943	1.932716
H	-2.354529	-1.979721	0.876668
O	1.490082	2.394349	-0.452239

H	-0.172456	3.430169	0.163567
O	4.819487	-0.105945	2.902850
O	1.958104	1.674128	3.420525
C	4.677240	-1.236921	3.736413
H	5.242262	-2.089903	3.336804
H	5.033905	-1.019017	4.752784
H	3.615515	-1.491620	3.771771
C	6.172863	0.302014	2.781743
H	6.577315	0.577476	3.765845
H	6.780884	-0.510316	2.360874
H	6.193699	1.168281	2.116245
C	2.243411	1.486638	4.789935
H	2.555258	2.433008	5.253809
H	1.364852	1.100288	5.324451
H	3.062733	0.768304	4.855087
C	0.967721	2.657459	3.201169
H	0.893970	2.807047	2.121422
H	-0.002521	2.331620	3.600742
H	1.251063	3.608812	3.672287
H	5.318329	1.272101	-2.840111
H	5.585993	3.205278	-3.492614

Model 2.5

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M2, G=-3224.166121

O	3.375236	-0.851029	0.258684
C	0.919854	2.003722	1.223626
C	-0.092836	0.909894	1.082135
C	0.449627	-0.519912	0.998727
O	1.091419	-0.670005	-0.240511
H	2.014078	-2.356976	0.525605
H	1.357860	2.047185	2.215233
F	-0.956232	1.127535	0.045712
H	1.180529	-0.615455	1.817010
F	-0.885745	0.972240	2.224713
C	-0.664985	-1.551492	1.156320
H	-1.144760	-1.487055	2.136321
H	-1.420646	-1.410041	0.377043
H	-0.237776	-2.552356	1.042971
C	2.429873	-2.116280	-1.572923
C	1.322210	-2.679767	-2.215615
C	1.442758	-3.226796	-3.491404
C	2.678243	-3.216420	-4.144717
C	3.788203	-2.662604	-3.509315
C	3.661443	-2.121053	-2.226806
H	0.357900	-2.670144	-1.711858
H	0.572452	-3.655385	-3.982873
H	4.754032	-2.657593	-4.008610
H	4.516539	-1.693775	-1.708324
C	1.264134	2.927637	0.306311

K	2.758853	0.981349	-1.673369
O	2.623844	3.915323	2.011281
C	2.190883	4.039699	0.752571
O	2.502748	4.986012	0.054662
C	3.449340	4.975053	2.497024
H	2.943052	5.933161	2.360378
H	3.609178	4.763404	3.553615
H	4.405174	4.983439	1.965962
N	0.923901	2.914922	-1.037660
K	0.754437	6.996024	-0.436878
O	-0.471384	4.732298	-0.756970
C	0.093239	3.847889	-1.467783
C	-0.251480	3.797467	-2.945302
H	0.400599	3.109290	-3.489606
H	-1.289152	3.459546	-3.051708
H	-0.186430	4.803504	-3.372157
C	2.326026	-1.526961	-0.152968
O	0.521786	6.557257	2.254430
O	1.342788	6.837787	-3.095171
O	4.406416	2.624214	-0.268802
O	1.180853	0.506910	-3.820612
C	1.270772	0.125002	-5.175219
H	0.984247	-0.928015	-5.300530
H	0.619777	0.753509	-5.799824
H	2.309112	0.254312	-5.487726
C	-0.127457	0.330464	-3.306176
H	-0.115926	0.644975	-2.259834
H	-0.845285	0.943796	-3.869595
H	-0.422880	-0.725474	-3.372150
C	1.052765	7.417418	-4.348317
H	1.932709	7.940745	-4.749350
H	0.736947	6.650455	-5.069434
H	0.241644	8.133022	-4.201956
C	2.406276	5.907559	-3.168793
H	2.178549	5.115304	-3.896047
H	3.337733	6.409232	-3.471310
H	2.530098	5.464807	-2.177303
C	-0.271538	5.412446	2.531845
H	0.261090	4.734373	3.213122
H	-1.223993	5.710540	2.991513
H	-0.457250	4.908525	1.579769
C	0.795394	7.307784	3.418861
H	-0.133831	7.682498	3.868750
H	1.326557	6.695471	4.161396
H	1.424677	8.152096	3.129354
O	3.194918	8.033031	-0.980255
C	4.453166	7.465942	-0.677046
H	4.901385	7.018696	-1.576462
H	5.138036	8.227087	-0.278610
H	4.281922	6.683682	0.063824
C	3.279465	9.022957	-1.982969

H	3.900318	9.865435	-1.648930
H	3.709490	8.608274	-2.905786
H	2.265967	9.373246	-2.189648
C	4.991751	1.923508	0.816242
H	5.991111	1.557391	0.541333
H	5.079832	2.581725	1.692105
H	4.343504	1.071497	1.036440
C	5.216182	3.678657	-0.737998
H	5.447809	4.387399	0.069501
H	6.158829	3.292020	-1.150119
H	4.657099	4.202937	-1.515988
H	2.772373	-3.639015	-5.141633

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TS2, G= -3224.131217

O	0.285599	-0.165334	1.608510
C	-0.130279	1.678345	1.082882
C	-1.564163	1.273773	0.845955
C	-1.776404	0.003654	-0.031674
O	-0.563015	-0.513205	-0.519518
H	0.102070	1.925953	2.111241
H	-2.245593	-0.733295	0.639405
C	-2.671329	0.266191	-1.230754
C	1.678648	-1.115194	-0.130782
C	1.829774	-1.862094	-1.304450
C	3.081122	-1.991169	-1.908463
C	4.200887	-1.379718	-1.335101
C	4.056370	-0.638651	-0.160394
C	2.798943	-0.507071	0.437495
H	0.957682	-2.335511	-1.749829
H	3.185068	-2.567498	-2.824145
H	4.923202	-0.161540	0.289928
H	2.659761	0.075000	1.344712
C	0.591267	2.287425	0.065984
K	2.435104	1.202791	-2.275432
O	2.281151	2.651762	1.672353
C	1.903167	2.781310	0.372037
O	2.705198	3.264968	-0.453946
C	3.584756	3.111159	1.996344
H	3.698958	4.169389	1.744910
H	3.689820	2.966028	3.072709
H	4.345277	2.528289	1.465447
N	0.143378	2.257022	-1.289157
K	1.746770	5.811728	-0.461363
O	-0.326819	4.544072	-1.259503
C	-0.313638	3.386203	-1.790568
C	-0.949297	3.270496	-3.171465
C	0.310072	-0.975848	0.537872
O	1.670443	5.626212	2.208047
O	2.075197	6.830111	-2.909065
O	3.446620	3.212113	-3.828902

O	1.000677	0.386779	-4.371335
C	1.105417	0.240264	-5.770718
H	1.163143	-0.820685	-6.050065
H	0.239871	0.694627	-6.272836
H	2.017885	0.749284	-6.088579
C	-0.148145	-0.255041	-3.840990
H	-0.195652	-0.021119	-2.772771
H	-1.057626	0.116852	-4.335315
H	-0.082291	-1.342253	-3.991848
C	0.829211	6.911280	-3.576979
H	0.475734	7.950635	-3.614014
H	0.914449	6.527796	-4.603728
H	0.123167	6.293225	-3.013824
C	3.093562	7.560526	-3.556042
H	3.234453	7.202952	-4.586085
H	2.853281	8.632348	-3.580447
H	4.014514	7.403864	-2.988996
C	0.648992	4.953395	2.921144
H	1.081201	4.202437	3.595540
H	0.051471	5.667914	3.503486
H	0.016390	4.451382	2.185728
C	2.576511	6.290093	3.062971
H	2.071995	7.087397	3.625284
H	3.029728	5.584948	3.773542
H	3.359902	6.723663	2.435525
O	4.412863	6.251734	-0.262604
C	5.433549	5.275473	-0.178142
H	6.166364	5.413560	-0.986082
H	5.952296	5.342699	0.788783
H	4.950797	4.301067	-0.273407
C	4.920546	7.565488	-0.148209
H	5.405293	7.713561	0.826466
H	5.650789	7.772370	-0.942709
H	4.079155	8.256011	-0.243100
C	4.304428	4.165240	-3.231315
H	4.543044	4.967844	-3.943992
H	3.835755	4.602201	-2.339580
H	5.222488	3.646192	-2.946679
C	2.198284	3.787250	-4.166423
H	1.712841	4.208077	-3.274320
H	2.329892	4.585591	-4.911276
H	1.571649	2.994552	-4.584477
H	5.177150	-1.484356	-1.800140
H	-0.050282	-1.994638	0.809154
H	-2.040125	3.282361	-3.051993
H	-0.660466	2.344804	-3.675309
H	-0.681399	4.131110	-3.794160
H	-3.654741	0.625819	-0.916470
H	-2.799301	-0.667543	-1.786660
H	-2.203134	1.013404	-1.877775
F	-2.177526	1.055496	2.065400

F -2.270252 2.344032 0.335521

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M3, G= -3224.144592

O	0.269824	0.276947	1.454390
C	-0.153301	1.610313	1.020736
C	-1.622325	1.384321	0.661789
C	-1.831725	0.118406	-0.203822
O	-0.573787	-0.390848	-0.614125
H	-0.133461	2.157857	1.967702
H	-2.325118	-0.622873	0.442955
C	-2.648419	0.373280	-1.453593
C	1.653585	-0.973218	-0.119538
C	1.785255	-1.741067	-1.280647
C	3.047709	-1.987310	-1.822445
C	4.188132	-1.476070	-1.198438
C	4.057682	-0.723242	-0.029451
C	2.794520	-0.474258	0.511515
H	0.895169	-2.127804	-1.768906
H	3.139811	-2.573064	-2.733097
H	4.940992	-0.319327	0.457734
H	2.678331	0.140784	1.399270
C	0.682983	2.308262	-0.013951
K	2.581562	1.267840	-2.177366
O	2.258185	2.454788	1.708389
C	1.950584	2.694347	0.362198
O	2.876554	3.199342	-0.369441
C	3.538414	2.870768	2.135431
H	3.664888	3.953791	2.027165
H	3.604888	2.596508	3.191548
H	4.335301	2.367034	1.575774
N	0.240046	2.337168	-1.380813
K	1.721145	5.566143	-0.475034
O	-0.492302	4.563689	-1.292522
C	-0.326558	3.430461	-1.851642
C	-0.890012	3.302508	-3.264924
C	0.274403	-0.711976	0.458634
O	1.998016	5.815293	2.175748
O	1.946882	6.831320	-2.826748
O	3.575295	3.228895	-3.794725
O	1.300903	0.408992	-4.384538
C	1.642459	0.087506	-5.715091
H	1.769347	-0.997394	-5.835569
H	0.866096	0.434617	-6.410859
H	2.584353	0.590805	-5.943495
C	0.085590	-0.192148	-3.973029
H	-0.107558	0.134626	-2.946283
H	-0.741281	0.127356	-4.624193
H	0.165801	-1.288240	-4.015850
C	0.729103	6.896698	-3.544306
H	0.406534	7.939575	-3.668784

H	0.842231	6.438650	-4.538118
H	-0.011655	6.335461	-2.967333
C	3.008182	7.478241	-3.493013
H	3.160754	7.046548	-4.492686
H	2.807292	8.553839	-3.597478
H	3.907342	7.328859	-2.891027
C	1.090400	5.086723	2.981320
H	1.629655	4.393679	3.641075
H	0.481527	5.769611	3.589465
H	0.448565	4.510520	2.310909
C	2.921336	6.555601	2.942887
H	2.402357	7.269906	3.596979
H	3.536930	5.888107	3.563152
H	3.561894	7.098165	2.244308
O	4.211445	6.640674	-0.313283
C	5.135464	5.638062	0.069179
H	5.987973	5.615333	-0.625447
H	5.511828	5.827069	1.085597
H	4.604373	4.681899	0.040165
C	4.789455	7.927483	-0.333418
H	5.180769	8.197236	0.658001
H	5.612057	7.976139	-1.061129
H	4.008650	8.635422	-0.619700
C	4.397593	4.183790	-3.152277
H	4.719610	4.956408	-3.865038
H	3.863386	4.657223	-2.317469
H	5.273151	3.657086	-2.766099
C	2.355091	3.800182	-4.227443
H	1.818545	4.254323	-3.382059
H	2.536993	4.572271	-4.989742
H	1.748142	2.996027	-4.651610
H	5.171214	-1.661384	-1.622125
H	-0.096807	-1.624046	0.957751
H	-1.986235	3.306220	-3.206281
H	-0.598917	4.167201	-3.872636
H	-0.561253	2.382929	-3.755508
H	-3.641788	0.749636	-1.194228
H	-2.758753	-0.563615	-2.007619
H	-2.134921	1.110197	-2.077729
F	-2.325158	1.193668	1.841037
F	-2.197926	2.489724	0.114200

Model 2.6

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M2, G=-3323.407771

O	3.366591	-0.676580	0.126399
C	0.858496	1.974296	1.025537
C	-0.151423	0.916231	0.695741
C	0.418934	-0.507708	0.735231
O	1.092290	-0.822635	-0.446281

H	2.181823	-2.293137	0.534866
H	1.315886	1.928949	2.010561
H	-0.578566	1.092345	-0.295828
H	1.075599	-0.628706	1.610709
H	-0.968147	0.989067	1.427424
C	-0.718998	-1.509933	0.903629
C	2.638045	-2.240937	-1.568899
C	1.694369	-3.151118	-2.060995
C	1.934764	-3.855266	-3.239272
C	3.120870	-3.648113	-3.950164
C	4.060099	-2.736280	-3.472053
C	3.819465	-2.043962	-2.281785
H	0.769510	-3.305970	-1.509169
H	1.198065	-4.563994	-3.608729
H	4.986694	-2.573438	-4.016815
H	4.555514	-1.357140	-1.870626
C	1.171829	2.997947	0.206244
K	2.618624	1.125390	-1.718535
O	2.577503	3.862115	1.929032
C	2.096015	4.075114	0.697373
O	2.378412	5.077803	0.065336
C	3.406009	4.896922	2.458759
H	2.875672	5.852582	2.432400
H	3.628665	4.601428	3.483540
H	4.330815	4.976141	1.880370
N	0.759791	3.079190	-1.128072
K	0.661425	7.110489	-0.382786
O	-0.627064	4.862979	-0.637381
C	-0.105287	4.028413	-1.437743
C	-0.543337	4.076907	-2.892192
C	2.428715	-1.519559	-0.226853
O	0.548003	6.725208	2.317228
O	1.230487	7.002123	-3.051920
O	4.329224	2.781871	-0.399054
O	1.078439	0.619168	-3.912554
C	1.453937	-0.396683	-4.821927
H	1.543171	-1.364157	-4.310263
H	0.716396	-0.482702	-5.632412
H	2.422442	-0.119215	-5.244043
C	-0.176407	0.348049	-3.310856
H	-0.365652	1.152293	-2.595054
H	-0.970067	0.329404	-4.071233
H	-0.149616	-0.612266	-2.777959
C	0.929066	7.578059	-4.304111
H	1.820119	8.053549	-4.738703
H	0.556250	6.817425	-5.004337
H	0.157289	8.333128	-4.144236
C	2.245439	6.020492	-3.145963
H	1.950833	5.223893	-3.843851
H	3.186137	6.469882	-3.498638
H	2.387785	5.592712	-2.150399

C	-0.134659	5.529002	2.659764
H	0.495066	4.899826	3.304528
H	-1.070568	5.760506	3.186742
H	-0.354368	5.001701	1.727158
C	0.846769	7.510033	3.452736
H	-0.073429	7.822875	3.964190
H	1.471493	6.947667	4.161344
H	1.391630	8.392522	3.111446
O	3.093674	8.162416	-0.924223
C	4.337513	7.554820	-0.640266
H	4.754800	7.088812	-1.544991
H	5.054000	8.294927	-0.258123
H	4.153708	6.781538	0.107167
C	3.189693	9.126736	-1.950631
H	3.872029	9.937658	-1.660985
H	3.552283	8.669489	-2.882106
H	2.190055	9.531747	-2.120143
C	4.993130	2.057910	0.623472
H	5.969003	1.698794	0.266968
H	5.147251	2.696418	1.504780
H	4.364173	1.200617	0.874505
C	5.098262	3.855891	-0.891678
H	5.381435	4.541960	-0.080583
H	6.012517	3.489510	-1.379745
H	4.482222	4.397865	-1.612434
H	3.309151	-4.196342	-4.869316
H	-0.467876	5.104780	-3.261938
H	0.052508	3.408848	-3.519047
H	-1.596874	3.780234	-2.956606
F	-0.285306	-2.783977	0.876764
F	-1.643578	-1.396237	-0.070298
F	-1.367728	-1.346069	2.077017

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TS2, G= -3323.361829

O	0.170320	-0.065293	1.514753
C	-0.119123	1.807693	1.020753
C	-1.569669	1.653866	0.617306
C	-1.844462	0.277678	-0.032205
O	-0.713387	-0.302563	-0.617791
H	0.073890	1.994049	2.070046
H	-1.819491	2.465666	-0.074185
H	-2.275535	-0.407320	0.713781
H	-2.214911	1.750738	1.495405
C	-2.883518	0.391063	-1.128124
C	1.488849	-1.111845	-0.232865
C	1.573091	-1.820600	-1.436156
C	2.814015	-2.103396	-2.007909
C	3.988220	-1.689832	-1.370819
C	3.908863	-0.983430	-0.168418
C	2.662952	-0.693758	0.395990

H	0.658571	-2.146371	-1.925699
H	2.866819	-2.647126	-2.947585
H	4.818218	-0.655996	0.329367
H	2.574893	-0.131593	1.321966
C	0.802017	2.333303	0.107248
K	2.722523	1.145427	-2.236648
O	2.387131	2.290500	1.856964
C	2.142322	2.565321	0.545419
O	3.074964	2.988844	-0.175130
C	3.683552	2.628028	2.327414
H	3.875757	3.697188	2.192364
H	3.689502	2.372669	3.387966
H	4.453131	2.054811	1.801067
N	0.574020	2.427825	-1.304740
K	1.554616	5.309745	-0.439975
O	-0.836068	4.278079	-1.104109
C	-0.232237	3.366141	-1.762745
C	-0.445139	3.366675	-3.270636
C	0.137707	-0.854970	0.432733
O	2.055283	5.514861	2.195568
O	1.463344	6.598368	-2.787496
O	3.762863	3.151947	-3.730312
O	1.276749	0.385639	-4.371125
C	1.494583	-0.018449	-5.704636
H	1.372024	-1.105531	-5.809221
H	0.792019	0.485021	-6.383428
H	2.516884	0.257838	-5.971555
C	-0.026670	0.059347	-3.912918
H	-0.118601	0.423623	-2.884940
H	-0.785466	0.545761	-4.542255
H	-0.181345	-1.028668	-3.944656
C	0.148751	7.008325	-3.122830
H	0.018906	8.082006	-2.930707
H	-0.058400	6.807526	-4.183119
H	-0.537549	6.426089	-2.502016
C	2.445047	7.240103	-3.573445
H	2.308173	7.001725	-4.637542
H	2.397886	8.330276	-3.443695
H	3.419952	6.875949	-3.240246
C	1.179066	4.860660	3.095036
H	1.740598	4.209836	3.778853
H	0.608706	5.596083	3.678464
H	0.498643	4.250243	2.498107
C	2.980539	6.345589	2.864141
H	2.459839	7.097718	3.472431
H	3.635972	5.751811	3.517362
H	3.578519	6.846021	2.100054
O	3.987724	6.480851	-0.425199
C	5.069667	5.659458	-0.024449
H	5.858819	5.660913	-0.790659
H	5.498122	6.018163	0.922380

H	4.674928	4.648162	0.102229
C	4.374874	7.824705	-0.619574
H	4.788584	8.248941	0.306106
H	5.130038	7.902575	-1.414233
H	3.483326	8.384963	-0.908189
C	4.472766	4.045964	-2.897351
H	5.097995	4.723502	-3.497398
H	3.781327	4.638675	-2.283284
H	5.106433	3.450592	-2.236610
C	2.865395	3.834683	-4.585155
H	2.166078	4.447999	-3.999450
H	3.416301	4.480914	-5.283713
H	2.307933	3.079836	-5.143988
H	4.955961	-1.916681	-1.809660
H	-0.313526	-1.843896	0.677918
H	-1.488307	3.111165	-3.488980
H	0.211397	2.654784	-3.775668
H	-0.264534	4.372265	-3.665931
F	-2.480544	1.141167	-2.165653
F	-3.224944	-0.812683	-1.628256
F	-4.017137	0.950815	-0.653168

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M3, G= -3323.373583

O	0.205707	0.344307	1.392216
C	-0.104301	1.718280	0.949852
C	-1.565423	1.690162	0.460640
C	-1.854672	0.313747	-0.156079
O	-0.679662	-0.275893	-0.668381
H	-0.052401	2.239539	1.908590
H	-1.729800	2.495800	-0.257345
H	-2.312483	-0.362065	0.582566
H	-2.246807	1.842393	1.303076
C	-2.831725	0.391187	-1.310086
C	1.545326	-0.957294	-0.190832
C	1.634919	-1.704099	-1.368718
C	2.882566	-2.052586	-1.888749
C	4.049023	-1.669196	-1.223633
C	3.959295	-0.934345	-0.038343
C	2.711667	-0.579741	0.478418
H	0.725938	-2.000704	-1.883600
H	2.942350	-2.618857	-2.814255
H	4.863646	-0.625369	0.478894
H	2.628330	0.024367	1.377620
C	0.879325	2.329849	-0.009573
K	2.856764	1.218216	-2.175196
O	2.386095	2.318014	1.787465
C	2.153690	2.605080	0.436500
O	3.135888	3.078339	-0.241614
C	3.641829	2.722858	2.291911
H	3.785639	3.805478	2.192385

H	3.643103	2.447434	3.349616
H	4.465594	2.212896	1.779865
N	0.597038	2.445862	-1.418010
K	1.657857	5.324161	-0.494424
O	-0.747989	4.336739	-1.142872
C	-0.186215	3.418915	-1.836036
C	-0.438726	3.464628	-3.338023
C	0.184283	-0.630193	0.395502
O	2.023944	5.727729	2.129863
O	1.423951	6.602834	-2.837097
O	4.072310	3.155931	-3.685880
O	1.466856	0.454547	-4.373147
C	1.766442	0.021880	-5.681777
H	1.730992	-1.074513	-5.750187
H	1.054831	0.445091	-6.404210
H	2.774335	0.367500	-5.922129
C	0.165657	0.068612	-3.959113
H	0.013715	0.464770	-2.950293
H	-0.591000	0.488586	-4.637169
H	0.073289	-1.027152	-3.961150
C	0.121560	7.051641	-3.164077
H	0.018618	8.125151	-2.953862
H	-0.092328	6.874097	-4.227367
H	-0.574767	6.474009	-2.550744
C	2.425277	7.215659	-3.619043
H	2.290060	6.975607	-4.682964
H	2.405818	8.307680	-3.495118
H	3.388238	6.828445	-3.275737
C	1.170712	4.988400	2.981928
H	1.754229	4.338551	3.647792
H	0.548524	5.663690	3.585272
H	0.537880	4.366605	2.345076
C	2.915095	6.552989	2.846845
H	2.365383	7.249620	3.494921
H	3.591843	5.948333	3.467889
H	3.495615	7.117085	2.114093
O	4.059349	6.564856	-0.430430
C	5.085872	5.733743	0.081551
H	5.930978	5.689631	-0.621443
H	5.450110	6.118830	1.045019
H	4.655712	4.735961	0.209017
C	4.506885	7.876940	-0.692043
H	4.911822	8.341018	0.218525
H	5.286931	7.876309	-1.466784
H	3.648133	8.454291	-1.040658
C	4.791549	4.097896	-2.914055
H	5.162806	4.916660	-3.548280
H	4.156042	4.506722	-2.117361
H	5.638544	3.577014	-2.462088
C	2.904142	3.730157	-4.242660
H	2.267833	4.158519	-3.453947

H	3.164982	4.519254	-4.962540
H	2.355029	2.933884	-4.751376
H	5.020928	-1.936873	-1.628465
H	-0.219511	-1.535488	0.881560
H	-1.513908	3.384813	-3.533747
H	-0.105652	4.432653	-3.731184
H	0.087776	2.665991	-3.863719
F	-2.385249	1.138975	-2.327761
F	-3.115900	-0.825984	-1.812045
F	-3.996873	0.929472	-0.898045

Model 3.1

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M2, G=-1983,467905

C	-2.669625	3.409743	2.021060
C	-2.611559	3.147972	3.497672
C	-1.205285	2.735674	3.982863
C	-0.481001	0.641615	3.046036
H	-2.915334	4.075887	4.008321
H	-1.746437	3.723795	1.539853
H	-0.485421	3.039438	3.208511
H	-3.336543	2.383775	3.792414
O	-1.019546	0.876911	1.857049
O	-1.114191	1.325047	4.147398
C	-0.729562	-0.840498	3.442482
F	-0.329633	-1.167842	4.689112
F	-2.038786	-1.149020	3.368035
F	-0.087262	-1.679613	2.604095
C	1.035381	0.919804	3.100246
C	1.750398	1.042571	1.909154
C	1.710825	1.053054	4.317044
C	3.122681	1.295836	1.928319
H	1.207754	0.943107	0.973648
C	3.082213	1.305606	4.340667
H	1.154331	0.970793	5.246841
C	3.792140	1.427444	3.145039
H	3.668984	1.392635	0.993768
H	3.596098	1.412491	5.292331
H	4.860116	1.626994	3.162478
C	-3.767664	3.342562	1.246869
C	-0.739360	3.404096	5.282843
H	0.352745	3.301245	5.306596
H	-0.946547	4.481395	5.214005
C	-3.691477	3.750215	-0.180997
O	-4.698089	3.858880	-0.880795
O	-2.480825	4.010491	-0.654024
C	-2.414840	4.463888	-2.011101
H	-1.353650	4.547537	-2.238222
H	-2.897487	3.744782	-2.676347
H	-2.906461	5.435015	-2.105001

C	-1.266640	2.858789	6.615338
H	-1.113376	1.774107	6.638375
H	-0.620081	3.270620	7.399599
C	-2.712827	3.215670	6.996226
H	-2.796514	3.152648	8.090200
H	-2.902176	4.268010	6.744396
C	-3.824321	2.366177	6.415635
C	-3.716819	0.974836	6.316514
C	-5.018189	2.967261	6.001832
C	-4.771567	0.209043	5.824485
H	-2.796701	0.478096	6.611372
C	-6.075115	2.206728	5.503520
H	-5.114467	4.050270	6.056494
C	-5.955750	0.820446	5.415293
H	-4.659756	-0.868620	5.742844
H	-6.987732	2.699259	5.176750
H	-6.771489	0.222707	5.017504
N	-5.087485	3.022134	1.635352
C	-5.322789	1.795359	2.073063
O	-4.520068	0.832566	2.183811
Li	-2.788535	0.749028	1.484156
H	-6.371457	1.619013	2.359127
O	-2.945991	0.967191	-0.450401
C	-1.743963	0.948918	-1.203161
H	-1.822456	1.630765	-2.059650
H	-0.948716	1.269476	-0.528828
H	-1.538208	-0.065836	-1.567819
C	-4.079499	0.571902	-1.200031
H	-4.229978	1.252605	-2.048130
H	-3.958706	-0.453557	-1.572526
H	-4.940167	0.620815	-0.530305
Li	-6.332009	3.769107	0.228362
O	-7.297120	5.326869	-0.380864
C	-8.600965	5.667385	0.086286
H	-9.335469	4.969504	-0.324326
H	-8.605606	5.610622	1.176356
H	-8.861660	6.683627	-0.218540
C	-6.805073	6.189649	-1.400078
H	-5.828130	5.811934	-1.699025
H	-7.482023	6.186776	-2.260726
H	-6.707043	7.208908	-1.013124

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TS2, G= -1983,452280

C	-2.535256	2.557000	1.573032
C	-2.668480	2.322031	3.053477
C	-1.308944	2.263525	3.749778
C	-0.321605	1.065160	1.931767
H	-3.245115	3.155096	3.483853
H	-1.759061	3.268891	1.296764
H	-0.743950	3.173194	3.487606

H	-3.237779	1.405755	3.236839
O	-1.463271	1.097316	1.190862
O	-0.550426	1.126276	3.328572
C	0.291922	-0.342245	1.750831
F	1.341786	-0.565052	2.555520
F	-0.618303	-1.302812	2.006943
F	0.709892	-0.531377	0.487207
C	0.707601	2.115354	1.494109
C	0.611519	2.683787	0.223512
C	1.752821	2.489356	2.342122
C	1.551309	3.624481	-0.196098
H	-0.220543	2.402017	-0.415835
C	2.692560	3.429987	1.922505
H	1.820418	2.048869	3.333702
C	2.594122	3.998402	0.651631
H	1.466802	4.068955	-1.183990
H	3.500184	3.721376	2.588071
H	3.325407	4.732568	0.325205
C	-3.670536	2.604846	0.742758
C	-1.425999	2.182954	5.265927
H	-0.432069	2.333210	5.702461
H	-2.035970	3.040396	5.577340
C	-3.634539	3.379422	-0.446020
O	-4.646273	3.667160	-1.132161
O	-2.414855	3.825905	-0.839203
C	-2.386723	4.648541	-2.000953
H	-1.337068	4.899343	-2.154896
H	-2.776914	4.108692	-2.867844
H	-2.972666	5.559110	-1.849586
C	-2.034782	0.867905	5.789623
H	-2.444343	0.283153	4.957040
H	-1.247883	0.247878	6.231782
C	-3.155588	1.079476	6.823225
H	-3.416812	0.110901	7.265983
H	-2.797561	1.721962	7.637289
C	-4.383992	1.683802	6.184381
C	-5.220138	0.883712	5.394930
C	-4.687783	3.043016	6.304812
C	-6.321242	1.425998	4.737526
H	-4.997281	-0.176534	5.287000
C	-5.787364	3.594443	5.643179
H	-4.058875	3.678409	6.925402
C	-6.606811	2.787505	4.856156
H	-6.955715	0.786425	4.130068
H	-6.002685	4.654658	5.745659
H	-7.462536	3.214293	4.340216
N	-4.993296	2.172900	1.086494
C	-5.205295	0.962076	1.534985
O	-4.376446	0.015024	1.732487
Li	-2.767039	-0.203209	0.898276
H	-6.263003	0.751912	1.763523

O	-2.921861	-0.340866	-1.047195
C	-1.936927	0.395748	-1.759637
H	-2.080506	1.473072	-1.606947
H	-0.963269	0.105897	-1.362489
H	-1.994095	0.155635	-2.829015
C	-4.231034	-0.069207	-1.527065
H	-4.474700	0.991808	-1.386476
H	-4.301033	-0.329122	-2.590839
H	-4.922961	-0.683655	-0.949172
Li	-6.189423	3.216551	-0.105789
O	-7.325997	4.776354	-0.279963
C	-8.355214	5.135034	0.627098
H	-9.272307	5.387571	0.081629
H	-8.538396	4.276232	1.274635
H	-8.044281	5.993382	1.234577
C	-6.970340	5.842139	-1.148774
H	-6.135898	5.494294	-1.757598
H	-7.823452	6.110436	-1.783655
H	-6.661749	6.717897	-0.564946

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M3, G= -1983,454840

C	-2.338207	2.438881	1.526180
C	-2.594439	2.378080	3.021042
C	-1.290919	2.257807	3.798810
C	-0.311201	1.156530	1.926571
H	-3.116012	3.293025	3.324037
H	-1.670397	3.271397	1.279477
H	-0.693424	3.170397	3.651415
H	-3.245883	1.528845	3.241409
O	-1.503081	1.220117	1.189948
O	-0.528310	1.141461	3.299683
C	0.253831	-0.254145	1.636513
F	1.316622	-0.536282	2.394486
F	-0.681653	-1.197226	1.877779
F	0.617359	-0.389442	0.353338
C	0.707620	2.209239	1.491396
C	0.647170	2.745743	0.204398
C	1.731731	2.590200	2.359505
C	1.607143	3.666274	-0.209795
H	-0.173768	2.468202	-0.451254
C	2.692457	3.511092	1.942607
H	1.770832	2.164715	3.359224
C	2.631789	4.049179	0.657198
H	1.551160	4.089824	-1.208531
H	3.486267	3.808693	2.621406
H	3.378555	4.768044	0.332370
C	-3.549564	2.527522	0.681162
C	-1.480697	2.014390	5.288104
H	-0.502918	2.081214	5.779275
H	-2.082611	2.849524	5.669713

C	-3.537625	3.310585	-0.459615
O	-4.563233	3.632719	-1.148420
O	-2.301870	3.754976	-0.886794
C	-2.310045	4.665338	-1.973875
H	-1.263053	4.911567	-2.160237
H	-2.751464	4.213858	-2.866946
H	-2.865429	5.575502	-1.726792
C	-2.151835	0.668960	5.618648
H	-2.599032	0.236134	4.715679
H	-1.396148	-0.050485	5.950912
C	-3.238471	0.783462	6.700128
H	-3.610789	-0.222012	6.931281
H	-2.798911	1.181569	7.623251
C	-4.390420	1.663668	6.272756
C	-5.251033	1.259142	5.243762
C	-4.603720	2.913170	6.863590
C	-6.296113	2.079232	4.824025
H	-5.095458	0.296235	4.758463
C	-5.647152	3.740578	6.444266
H	-3.945023	3.241865	7.665232
C	-6.497936	3.324553	5.422306
H	-6.955481	1.748093	4.026883
H	-5.793918	4.707475	6.917812
H	-7.312273	3.963817	5.093022
N	-4.868913	2.158164	1.121133
C	-5.091897	0.970195	1.615598
O	-4.275337	0.001127	1.790926
Li	-2.741325	-0.221801	0.846497
H	-6.135881	0.795168	1.923268
O	-2.974467	-0.353188	-1.079255
C	-2.019839	0.355335	-1.859732
H	-2.158365	1.437112	-1.741809
H	-1.029148	0.071709	-1.502051
H	-2.122744	0.074971	-2.915707
C	-4.304821	-0.076833	-1.501165
H	-4.516977	0.994272	-1.400803
H	-4.434803	-0.390737	-2.544505
H	-4.973801	-0.648232	-0.855950
Li	-6.055052	3.202138	-0.091078
O	-7.324561	4.633335	-0.380313
C	-8.543888	4.857153	0.305456
H	-9.381667	4.879811	-0.402245
H	-8.681483	4.036237	1.010806
H	-8.504304	5.807068	0.852181
C	-7.021775	5.661688	-1.311399
H	-6.056159	5.413647	-1.753219
H	-7.797162	5.709962	-2.086086
H	-6.961817	6.628949	-0.797284

C	-2.825265	1.922246	1.115851
C	-3.282114	2.307135	2.522368
C	-2.082146	2.417268	3.455503
C	-0.961056	0.753451	2.195012
H	-3.798682	3.273636	2.481966
H	-2.113909	2.678572	0.753440
H	-1.393045	3.187469	3.076168
H	-3.980651	1.558753	2.897992
O	-2.021019	0.671971	1.281056
O	-1.381500	1.159276	3.461399
C	-0.524502	-0.711434	2.399501
F	0.481476	-0.803643	3.278242
F	-1.529298	-1.469110	2.853590
F	-0.106481	-1.251036	1.242298
C	0.216594	1.582268	1.681049
C	0.420129	1.753578	0.310971
C	1.120194	2.129621	2.595604
C	1.524168	2.478388	-0.138993
H	-0.290704	1.339468	-0.401443
C	2.221868	2.851876	2.141903
H	0.952973	1.992484	3.660486
C	2.425860	3.026786	0.772393
H	1.676152	2.615481	-1.205733
H	2.919507	3.278184	2.856683
H	3.283707	3.590978	0.418094
C	-2.424860	2.740451	4.902512
H	-1.484043	2.789259	5.468480
H	-2.859735	3.747815	4.927754
C	-3.368402	1.740878	5.571846
H	-4.361817	1.791608	5.108612
H	-2.993335	0.723176	5.413983
C	-3.511794	1.993598	7.081226
H	-4.151159	1.213639	7.511411
H	-2.528208	1.901294	7.557901
C	-4.097904	3.351817	7.389126
C	-5.461830	3.593644	7.182489
C	-3.298339	4.404396	7.845280
C	-6.012071	4.851287	7.424024
H	-6.099263	2.783233	6.833143
C	-3.843083	5.666528	8.088794
H	-2.236709	4.233143	8.011568
C	-5.202358	5.894168	7.878180
H	-7.073704	5.017036	7.262924
H	-3.204843	6.470584	8.444600
H	-5.629283	6.874381	8.069479
C	-3.851703	1.746761	0.048612
C	-5.158872	1.317307	0.247845
N	-3.623544	2.382800	-1.240073
O	-6.099669	1.438585	-0.599760
O	-5.441150	0.695150	1.441472
C	-2.686676	1.864564	-1.991656

Li	-5.495898	2.920310	-1.634783
C	-6.796560	0.325982	1.647617
O	-1.949253	0.847032	-1.755936
H	-2.528726	2.382235	-2.952086
O	-5.811110	4.480388	-0.469168
H	-7.124798	-0.402907	0.901609
H	-6.831692	-0.119375	2.642914
H	-7.457720	1.196987	1.606019
Li	-2.502915	-0.257178	-0.366597
C	-4.634646	5.210774	-0.157444
C	-6.596792	4.227272	0.685117
H	-4.899008	6.157939	0.328849
H	-3.984783	4.618611	0.498833
H	-4.110913	5.406112	-1.093001
H	-6.028423	3.629470	1.410481
H	-6.902116	5.174364	1.146762
H	-7.475274	3.665913	0.366819
O	-3.751366	-1.625525	-0.873625
C	-3.708658	-3.029185	-0.691333
H	-4.701956	-3.405528	-0.418596
H	-3.371462	-3.525235	-1.609856
H	-3.006359	-3.236395	0.117122
C	-4.654105	-1.233937	-1.898229
H	-4.635618	-0.144095	-1.950871
H	-4.347950	-1.668728	-2.858049
H	-5.669465	-1.565386	-1.648528

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M2-K, G= -3168,148905

C	-2.829944	2.836127	1.957245
C	-2.728794	2.694744	3.453118
C	-1.281976	2.457650	3.917060
C	0.004188	0.605929	2.950303
H	-3.122811	3.617345	3.904160
H	-1.901050	2.826793	1.390820
H	-0.630348	2.931991	3.169648
H	-3.383768	1.896127	3.834425
O	-0.395198	0.654151	1.702063
O	-0.999908	1.060030	3.920285
C	0.146841	-0.878851	3.411933
F	0.461353	-1.056668	4.711601
F	-1.008249	-1.565359	3.215972
F	1.089821	-1.522766	2.699203
C	1.347054	1.322264	3.229281
C	2.083283	1.796021	2.143576
C	1.851801	1.504601	4.520677
C	3.301890	2.447379	2.338801
H	1.671497	1.646900	1.149984
C	3.071329	2.150691	4.721080
H	1.282209	1.150961	5.375308
C	3.800518	2.624653	3.629475

H	3.863510	2.814287	1.483567
H	3.451035	2.287342	5.730285
H	4.750825	3.128117	3.785025
C	-3.986180	2.999102	1.288331
C	-0.911552	3.095621	5.282758
H	0.116340	3.460751	5.184087
H	-1.534654	3.987708	5.435019
C	-3.958709	3.220132	-0.189790
O	-4.966099	3.273367	-0.881737
O	-2.740206	3.400311	-0.706230
C	-2.686210	3.557006	-2.123093
H	-1.627767	3.603587	-2.375134
H	-3.164312	2.706048	-2.614680
H	-3.191549	4.478404	-2.423228
C	-0.965856	2.202574	6.535124
H	-0.841893	1.155335	6.237365
H	-0.107186	2.447597	7.172851
C	-2.229178	2.350732	7.393980
H	-2.089498	1.774748	8.318418
H	-2.345069	3.400422	7.692261
C	-3.489709	1.883687	6.709928
C	-3.642454	0.534657	6.363057
C	-4.523448	2.770358	6.402421
C	-4.796644	0.086422	5.727769
H	-2.844049	-0.169402	6.591138
C	-5.681720	2.327879	5.759726
H	-4.416770	3.822420	6.660599
C	-5.821910	0.984398	5.422918
H	-4.896779	-0.962634	5.461546
H	-6.469464	3.036497	5.516834
H	-6.714641	0.636914	4.911169
N	-5.264708	3.064444	1.868939
C	-5.790998	1.919357	2.263971
O	-5.333390	0.751794	2.157573
K	-2.919749	-0.168226	1.824904
H	-6.784883	2.039280	2.737515
O	-3.125939	0.482768	-0.865537
C	-1.761307	0.427466	-1.240874
H	-1.600443	0.941103	-2.199222
H	-1.184691	0.910801	-0.448333
H	-1.431617	-0.616944	-1.342995
C	-3.975263	-0.115240	-1.819854
H	-3.879370	0.383270	-2.795151
H	-3.739103	-1.181510	-1.945430
H	-4.999538	-0.006296	-1.458668
K	-7.185915	4.277219	0.270688
O	-8.068400	6.637609	-0.728479
C	-9.399379	7.099489	-0.592527
H	-9.834437	7.321008	-1.575636
H	-9.975747	6.306832	-0.112133
H	-9.433786	8.003685	0.028617

C	-7.235144	7.600093	-1.347746
H	-6.234606	7.170607	-1.423262
H	-7.604848	7.841756	-2.352608
H	-7.194237	8.518671	-0.748440

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TS2-K, G= -3168,121568

C	-2.753152	2.754847	2.066524
C	-2.757130	2.940180	3.562637
C	-1.345437	2.879188	4.149219
C	-0.691019	1.120398	2.685945
H	-3.178366	3.932974	3.781194
H	-1.948861	3.265447	1.540047
H	-0.726206	3.580028	3.562310
H	-3.418274	2.200006	4.016234
O	-1.879180	1.114103	2.042961
O	-0.768680	1.579304	4.028920
C	-0.261567	-0.356298	2.855622
F	0.910674	-0.501011	3.502441
F	-1.169983	-1.071768	3.534454
F	-0.118244	-0.949078	1.651532
C	0.424708	1.870376	1.931858
C	0.282996	2.136268	0.569817
C	1.588741	2.274527	2.591446
C	1.294630	2.796054	-0.129304
H	-0.640602	1.853339	0.072016
C	2.600617	2.933698	1.894860
H	1.692208	2.078362	3.655371
C	2.457083	3.193419	0.530854
H	1.171699	3.004572	-1.189031
H	3.500698	3.246285	2.417033
H	3.245325	3.708186	-0.011294
C	-3.972280	2.667728	1.369760
C	-1.197996	3.300477	5.614394
H	-0.144418	3.576736	5.748719
H	-1.778600	4.220983	5.765371
C	-3.995327	2.906345	-0.032249
O	-4.996675	3.126183	-0.740729
O	-2.751581	2.870833	-0.628423
C	-2.679800	3.394841	-1.946609
H	-1.632780	3.306909	-2.243525
H	-3.314201	2.826059	-2.630184
H	-2.982125	4.447020	-1.963113
C	-1.529268	2.286037	6.719987
H	-1.063450	1.324925	6.478933
H	-1.017927	2.643258	7.621911
C	-3.004004	2.100288	7.104944
H	-3.029443	1.708977	8.131904
H	-3.487565	3.085339	7.153867
C	-3.859276	1.182425	6.254902
C	-3.336696	0.062813	5.601141

C	-5.232850	1.431461	6.144733
C	-4.158403	-0.769473	4.840404
H	-2.271721	-0.143756	5.639445
C	-6.061145	0.593894	5.400228
H	-5.655895	2.303717	6.640004
C	-5.524059	-0.510336	4.738762
H	-3.723159	-1.616476	4.316996
H	-7.122147	0.815522	5.318597
H	-6.159721	-1.149586	4.132371
N	-5.210134	2.452605	2.064602
C	-5.826557	1.315462	1.821916
O	-5.498942	0.349438	1.069654
K	-3.116109	-0.095357	0.141457
H	-6.784471	1.218777	2.371644
O	-2.915409	0.268872	-2.537560
C	-1.692619	0.391018	-3.233783
H	-1.708798	1.267251	-3.896521
H	-0.902369	0.517131	-2.490217
H	-1.492252	-0.506820	-3.833752
C	-4.022165	0.177097	-3.412581
H	-4.075897	1.062342	-4.061378
H	-3.949854	-0.721276	-4.040190
H	-4.923498	0.126408	-2.799458
K	-6.593203	4.513770	0.915718
O	-7.637186	6.728886	-0.265702
C	-8.619011	7.588481	0.280418
H	-9.517654	7.600506	-0.349808
H	-8.875680	7.207405	1.270424
H	-8.230516	8.611102	0.372782
C	-7.234887	7.137064	-1.559842
H	-6.488495	6.423418	-1.913331
H	-8.090222	7.140187	-2.247861
H	-6.794150	8.142074	-1.528625

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M3-K, G= -3168,141025

C	-2.338207	2.438881	1.526180
C	-2.594439	2.378080	3.021042
C	-1.290919	2.257807	3.798810
C	-0.311201	1.156530	1.926571
H	-3.116012	3.293025	3.324037
H	-1.670397	3.271397	1.279477
H	-0.693424	3.170397	3.651415
H	-3.245883	1.528845	3.241409
O	-1.503081	1.220117	1.189948
O	-0.528310	1.141461	3.299683
C	0.253831	-0.254145	1.636513
F	1.316622	-0.536282	2.394486
F	-0.681653	-1.197226	1.877779
F	0.617359	-0.389442	0.353338
C	0.707620	2.209239	1.491396

C	0.647170	2.745743	0.204398
C	1.731731	2.590200	2.359505
C	1.607143	3.666274	-0.209795
H	-0.173768	2.468202	-0.451254
C	2.692457	3.511092	1.942607
H	1.770832	2.164715	3.359224
C	2.631789	4.049179	0.657198
H	1.551160	4.089824	-1.208531
H	3.486267	3.808693	2.621406
H	3.378555	4.768044	0.332370
C	-3.549564	2.527522	0.681162
C	-1.480697	2.014390	5.288104
H	-0.502918	2.081214	5.779275
H	-2.082611	2.849524	5.669713
C	-3.537625	3.310585	-0.459615
O	-4.563233	3.632719	-1.148420
O	-2.301870	3.754976	-0.886794
C	-2.310045	4.665338	-1.973875
H	-1.263053	4.911567	-2.160237
H	-2.751464	4.213858	-2.866946
H	-2.865429	5.575502	-1.726792
C	-2.151835	0.668960	5.618648
H	-2.599032	0.236134	4.715679
H	-1.396148	-0.050485	5.950912
C	-3.238471	0.783462	6.700128
H	-3.610789	-0.222012	6.931281
H	-2.798911	1.181569	7.623251
C	-4.390420	1.663668	6.272756
C	-5.251033	1.259142	5.243762
C	-4.603720	2.913170	6.863590
C	-6.296113	2.079232	4.824025
H	-5.095458	0.296235	4.758463
C	-5.647152	3.740578	6.444266
H	-3.945023	3.241865	7.665232
C	-6.497936	3.324553	5.422306
H	-6.955481	1.748093	4.026883
H	-5.793918	4.707475	6.917812
H	-7.312273	3.963817	5.093022
N	-4.868913	2.158164	1.121133
C	-5.091897	0.970195	1.615598
O	-4.275337	0.001127	1.790926
Li	-2.741325	-0.221801	0.846497
H	-6.135881	0.795168	1.923268
O	-2.974467	-0.353188	-1.079255
C	-2.019839	0.355335	-1.859732
H	-2.158365	1.437112	-1.741809
H	-1.029148	0.071709	-1.502051
H	-2.122744	0.074971	-2.915707
C	-4.304821	-0.076833	-1.501165
H	-4.516977	0.994272	-1.400803
H	-4.434803	-0.390737	-2.544505

H	-4.973801	-0.648232	-0.855950
Li	-6.055052	3.202138	-0.091078
O	-7.324561	4.633335	-0.380313
C	-8.543888	4.857153	0.305456
H	-9.381667	4.879811	-0.402245
H	-8.681483	4.036237	1.010806
H	-8.504304	5.807068	0.852181
C	-7.021775	5.661688	-1.311399
H	-6.056159	5.413647	-1.753219
H	-7.797162	5.709962	-2.086086
H	-6.961817	6.628949	-0.797284

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M4_{syn}, G= -1983.912087

C	-2.403806	2.633721	1.810237
C	-2.593976	2.397865	3.303297
C	-1.241603	2.122213	3.947850
C	-0.428352	1.307160	1.868348
H	-3.043294	3.288290	3.761270
H	-1.768448	3.515944	1.658477
H	-0.610532	3.018548	3.869340
H	-3.271506	1.556424	3.455103
O	-1.677277	1.522538	1.220460
O	-0.589378	1.055127	3.222264
C	0.070616	-0.033210	1.288947
F	1.197296	-0.430933	1.869979
F	-0.852002	-1.003646	1.478078
F	0.275223	0.049467	-0.030226
C	0.602163	2.391458	1.568414
C	0.573069	3.081168	0.355846
C	1.633499	2.625948	2.480146
C	1.562488	4.018105	0.064749
H	-0.230535	2.890866	-0.348555
C	2.621807	3.563352	2.186875
H	1.661095	2.073230	3.415245
C	2.586550	4.261391	0.979995
H	1.536975	4.556799	-0.877589
H	3.419778	3.745215	2.900015
H	3.356995	4.991509	0.751404
C	-3.725909	2.957669	1.089411
C	-1.298336	1.690419	5.404062
H	-0.266479	1.558544	5.747778
H	-1.703291	2.542136	5.964001
C	-3.569849	3.278525	-0.397250
O	-4.493862	3.198279	-1.192678
O	-2.393376	3.786062	-0.716415
C	-2.269244	4.354244	-2.033606
H	-1.260485	4.758328	-2.082448
H	-2.414109	3.583921	-2.791426
H	-3.009564	5.145659	-2.161016
C	-2.123039	0.417440	5.680875

H	-2.544437	0.023319	4.747674
H	-1.467338	-0.368150	6.069496
C	-3.265722	0.641565	6.689913
H	-3.737400	-0.323512	6.907632
H	-2.845619	1.014632	7.632024
C	-4.305336	1.609196	6.176861
C	-5.262490	1.187937	5.244720
C	-4.305412	2.952102	6.568109
C	-6.181302	2.086136	4.707318
H	-5.276614	0.146228	4.928762
C	-5.219455	3.858758	6.027717
H	-3.584444	3.292969	7.308540
C	-6.158180	3.428580	5.091356
H	-6.916963	1.740927	3.986173
H	-5.200622	4.897936	6.344320
H	-6.873985	4.129815	4.671747
N	-4.980459	2.241448	1.271619
C	-5.084585	0.999253	1.668205
O	-4.196791	0.145771	1.962509
Li	-2.769314	-0.135850	0.877120
H	-6.134767	0.670657	1.756128
O	-3.326600	0.327282	-0.907791
C	-2.438330	0.687516	-1.956450
H	-2.948518	1.360459	-2.655850
H	-1.586648	1.196819	-1.501425
H	-2.096507	-0.203885	-2.495113
C	-4.544790	-0.210994	-1.405970
H	-5.088504	0.555754	-1.971453
H	-4.344019	-1.069142	-2.057535
H	-5.136243	-0.533720	-0.548353
Li	-6.172388	2.826562	-0.237507
O	-7.190232	4.429857	-0.541384
C	-8.181458	4.928880	0.345364
H	-9.137882	5.038352	-0.178185
H	-8.286335	4.210036	1.159144
H	-7.872052	5.899000	0.750536
C	-6.933297	5.315739	-1.622742
H	-6.149730	4.867332	-2.233795
H	-7.841615	5.455520	-2.219977
H	-6.594024	6.285940	-1.241245
H	-3.926219	3.967600	1.498670

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M4_anti, G= -1983.914002

C	-2.773580	2.407173	1.185536
C	-3.229668	2.780949	2.594197
C	-2.095715	2.556951	3.584643
C	-1.278175	0.815470	2.207360
H	-3.527186	3.835390	2.608378
H	-1.960882	3.075826	0.870361
H	-1.238741	3.187743	3.305605

H	-4.094187	2.166114	2.867490
O	-2.254397	1.058260	1.210413
O	-1.692073	1.179185	3.479007
C	-1.239668	-0.725649	2.269729
F	-0.275315	-1.174595	3.065013
F	-2.400989	-1.230755	2.688528
F	-1.020742	-1.228487	1.028247
C	0.085378	1.389373	1.836501
C	0.400713	1.702856	0.513192
C	1.042311	1.557210	2.841247
C	1.672830	2.180444	0.198073
H	-0.344043	1.596456	-0.271876
C	2.311547	2.032546	2.522108
H	0.788265	1.315897	3.869686
C	2.629274	2.342462	1.198977
H	1.912643	2.427826	-0.831537
H	3.051689	2.160414	3.305922
H	3.619111	2.713081	0.950373
C	-2.439890	2.809192	5.043314
H	-1.548190	2.566518	5.637482
H	-2.616194	3.884783	5.167461
C	-3.636154	2.012639	5.565306
H	-4.564269	2.390820	5.117955
H	-3.539230	0.962292	5.266452
C	-3.757120	2.084139	7.096338
H	-4.612461	1.475727	7.412463
H	-2.862147	1.638167	7.546793
C	-3.924499	3.497866	7.602535
C	-5.148773	4.161568	7.455669
C	-2.860060	4.188171	8.190448
C	-5.305235	5.479302	7.882556
H	-5.990272	3.635218	7.008486
C	-3.010111	5.507802	8.619621
H	-1.903212	3.685325	8.315479
C	-4.233710	6.158134	8.465779
H	-6.264898	5.975205	7.766452
H	-2.171383	6.025522	9.076543
H	-4.354260	7.183594	8.802517
C	-3.908813	2.582788	0.150388
C	-4.867555	1.401323	-0.037631
N	-3.537181	3.136783	-1.146047
O	-5.561231	1.300686	-1.039149
O	-4.958988	0.579415	0.987810
C	-2.749045	2.374367	-1.872275
Li	-5.416430	3.034705	-2.115457
C	-5.937475	-0.471284	0.883328
O	-2.313142	1.217882	-1.599670
H	-2.456915	2.811195	-2.839163
O	-6.433559	4.144282	-0.822023
H	-5.757505	-1.048406	-0.024206
H	-5.798011	-1.083118	1.771922

H	-6.939801	-0.042043	0.858895
Li	-2.287875	-0.136916	-0.410430
C	-5.946992	5.444492	-0.516933
C	-7.467135	3.727675	0.056480
H	-6.760005	6.176515	-0.581108
H	-5.515712	5.468397	0.492740
H	-5.172283	5.681175	-1.245262
H	-7.083121	3.641852	1.082175
H	-8.294001	4.446497	0.037599
H	-7.821377	2.756525	-0.287944
O	-3.452860	-1.548782	-0.929293
C	-3.590836	-2.840300	-0.350202
H	-4.651376	-3.085239	-0.218087
H	-3.122026	-3.592929	-0.993925
H	-3.095203	-2.823432	0.620329
C	-4.069373	-1.455783	-2.209993
H	-3.891144	-0.445059	-2.576831
H	-3.628213	-2.191212	-2.892410
H	-5.146372	-1.639070	-2.122429
H	-4.573028	3.328227	0.616641

Model 3.2

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M2, G=-2022.744776

C	-2.726216	3.349585	1.976768
C	-2.686067	3.004476	3.436917
C	-1.252605	2.712058	3.939486
C	-0.521017	0.556078	3.188797
H	-3.119292	3.852329	3.990231
H	-1.794805	3.687934	1.527598
H	-0.562511	2.948771	3.117577
H	-3.326175	2.143735	3.660332
O	-1.075474	0.737579	1.998524
O	-1.094922	1.336429	4.260232
C	-0.816521	-0.884998	3.686145
F	-0.377710	-1.144315	4.936672
F	-2.136263	-1.145263	3.680508
F	-0.239422	-1.802634	2.883413
C	1.005913	0.777176	3.195764
C	1.708600	0.750854	1.991038
C	1.704306	0.995619	4.387262
C	3.090936	0.940813	1.971637
H	1.150875	0.587680	1.073935
C	3.085874	1.186405	4.372275
H	1.155821	1.025739	5.324917
C	3.783113	1.158157	3.163329
H	3.628142	0.919946	1.027210
H	3.618488	1.359372	5.303541
H	4.859333	1.306796	3.150797
C	-3.812130	3.342093	1.180087

C	-0.784912	3.545822	5.139361
H	0.312156	3.509267	5.130333
H	-1.062085	4.594533	4.960699
C	-3.702027	3.891305	-0.199826
O	-4.692771	4.187738	-0.869266
O	-2.472869	4.062357	-0.665164
C	-2.358313	4.649407	-1.967870
H	-1.290248	4.695522	-2.170937
H	-2.864434	4.027025	-2.709016
H	-2.795319	5.649824	-1.968587
C	-1.232025	3.123281	6.543207
H	-0.996314	2.062530	6.682977
H	-0.598168	3.668875	7.252792
C	-2.690502	3.407903	6.934285
H	-2.747187	3.411806	8.031891
H	-2.955911	4.426058	6.619252
C	-3.749095	2.448780	6.429951
C	-3.539794	1.066375	6.407726
C	-4.996016	2.934321	6.019893
C	-4.544549	0.195440	5.987695
H	-2.578398	0.658011	6.705713
C	-6.005014	2.069645	5.598080
H	-5.173770	4.008255	6.020281
C	-5.783291	0.692446	5.586547
H	-4.355598	-0.874176	5.969842
H	-6.962657	2.472523	5.277731
H	-6.564137	0.011263	5.260265
N	-5.139789	3.004273	1.506599
C	-5.395596	1.758811	1.897325
O	-4.562700	0.816728	2.007386
Li	-2.789087	0.698222	1.448348
O	-2.764294	0.898029	-0.485400
C	-1.523516	0.934439	-1.168645
H	-1.482184	1.806950	-1.833501
H	-0.751532	1.008633	-0.401109
H	-1.385447	0.019541	-1.759029
C	-3.881926	0.842537	-1.347551
H	-3.882402	1.701134	-2.033238
H	-3.874681	-0.084881	-1.934440
H	-4.774863	0.875292	-0.718901
Li	-6.327913	3.872140	0.166821
O	-7.490958	5.285936	-0.403134
C	-8.623554	5.745190	0.319241
H	-9.512962	5.729817	-0.321193
H	-8.769324	5.073710	1.166460
H	-8.452417	6.764558	0.683777
C	-7.198367	6.099510	-1.530917
H	-6.316334	5.678928	-2.013784
H	-8.045515	6.096169	-2.226655
H	-6.992646	7.127443	-1.210431
C	-6.851227	1.436878	2.164922

H	-6.932086	0.825993	3.065642
H	-7.460219	2.336802	2.278035
H	-7.242440	0.841896	1.330913

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TS2, G= -2022.728003

C	-2.615642	2.531270	1.421535
C	-2.788387	2.299504	2.897427
C	-1.463878	2.227623	3.660515
C	-0.352843	1.104848	1.867299
H	-3.372914	3.139506	3.303375
H	-1.872660	3.281192	1.159094
H	-0.894479	3.150992	3.465803
H	-3.375834	1.392426	3.055649
O	-1.449458	1.117129	1.066019
O	-0.667098	1.113545	3.249677
C	0.324439	-0.273270	1.681180
F	1.341155	-0.485088	2.529665
F	-0.560119	-1.275047	1.864672
F	0.809778	-0.411221	0.435340
C	0.658660	2.207076	1.524690
C	0.605439	2.828496	0.276459
C	1.646364	2.577448	2.440671
C	1.532225	3.817701	-0.053174
H	-0.180087	2.544036	-0.418801
C	2.573994	3.564308	2.110349
H	1.676222	2.098823	3.416067
C	2.519145	4.185470	0.861605
H	1.481672	4.303596	-1.023671
H	3.337234	3.850739	2.828224
H	3.240461	4.956137	0.605201
C	-3.723555	2.495843	0.557515
C	-1.655545	2.086909	5.165901
H	-0.671823	2.158587	5.644000
H	-2.230087	2.961570	5.496553
C	-3.689887	3.256236	-0.643426
O	-4.689958	3.474960	-1.369818
O	-2.485125	3.770924	-0.998484
C	-2.467185	4.587474	-2.164559
H	-1.432549	4.911514	-2.277773
H	-2.782133	4.017160	-3.042169
H	-3.122719	5.453891	-2.044639
C	-2.362374	0.789199	5.600472
H	-2.802775	0.285061	4.732437
H	-1.631757	0.085291	6.012441
C	-3.463599	1.029440	6.647877
H	-3.886479	0.062624	6.947178
H	-3.021170	1.477027	7.546471
C	-4.564905	1.929009	6.134303
C	-5.412714	1.501765	5.103979
C	-4.734372	3.222741	6.637850

C	-6.394894	2.346201	4.590759
H	-5.292630	0.500908	4.690317
C	-5.716619	4.073683	6.127352
H	-4.084821	3.570294	7.438734
C	-6.549625	3.637281	5.099296
H	-7.038140	1.999357	3.787417
H	-5.828135	5.075328	6.533229
H	-7.315019	4.295684	4.697776
N	-5.031031	1.994734	0.862243
C	-5.205056	0.773363	1.312258
O	-4.310817	-0.109266	1.545000
Li	-2.666004	-0.245248	0.770967
O	-2.794646	-0.419692	-1.163034
C	-1.839388	0.332478	-1.897810
H	-2.062150	1.404766	-1.825553
H	-0.862059	0.141471	-1.454541
H	-1.845734	0.016694	-2.948700
C	-4.106848	-0.253452	-1.677661
H	-4.400133	0.803531	-1.637328
H	-4.151607	-0.610509	-2.714293
H	-4.778447	-0.843733	-1.052189
Li	-6.226347	2.867602	-0.422573
O	-7.271829	4.430406	-0.003703
C	-7.489137	4.680850	1.377057
H	-8.324509	5.378989	1.507626
H	-7.729432	3.726558	1.848137
H	-6.584355	5.095891	1.837803
C	-6.933231	5.612154	-0.715781
H	-6.759854	5.330681	-1.754262
H	-7.756069	6.334133	-0.654982
H	-6.019382	6.056308	-0.303136
C	-6.642036	0.348853	1.552352
H	-6.748852	-0.060288	2.562330
H	-7.337337	1.182066	1.423132
H	-6.903629	-0.453268	0.852507

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M3, G=2022.731784

C	-2.351771	2.440431	1.427432
C	-2.633115	2.416804	2.922068
C	-1.352184	2.273487	3.737830
C	-0.329909	1.164633	1.897959
H	-3.133427	3.351411	3.202540
H	-1.702086	3.284777	1.176743
H	-0.734514	3.175200	3.610787
H	-3.313906	1.592454	3.139007
O	-1.498630	1.231171	1.130493
O	-0.589135	1.144731	3.268750
C	0.234135	-0.241330	1.611816
F	1.278961	-0.529209	2.390565
F	-0.706378	-1.183048	1.826161

F	0.624968	-0.364704	0.335941
C	0.701755	2.217963	1.499594
C	0.681177	2.773129	0.218734
C	1.703291	2.580234	2.402045
C	1.657725	3.695424	-0.153252
H	-0.115355	2.502696	-0.469895
C	2.679882	3.501580	2.026798
H	1.710509	2.143283	3.397043
C	2.658515	4.059495	0.748415
H	1.634703	4.132629	-1.147227
H	3.455238	3.783762	2.732769
H	3.418121	4.778879	0.456740
C	-3.555107	2.481630	0.565129
C	-1.607060	2.040234	5.220568
H	-0.656437	2.111284	5.761833
H	-2.229659	2.876278	5.564888
C	-3.544460	3.249220	-0.587956
O	-4.566630	3.535933	-1.298317
O	-2.315597	3.722850	-1.001229
C	-2.328024	4.605415	-2.111544
H	-1.286136	4.884906	-2.277548
H	-2.729156	4.115339	-3.003064
H	-2.922435	5.500102	-1.902144
C	-2.293451	0.698681	5.533084
H	-2.776455	0.300198	4.633647
H	-1.541678	-0.044875	5.817474
C	-3.340537	0.809016	6.652856
H	-3.759858	-0.186395	6.845731
H	-2.856402	1.134136	7.582064
C	-4.454697	1.775637	6.312257
C	-5.240881	1.586992	5.167694
C	-4.697356	2.902771	7.103240
C	-6.229518	2.505239	4.819228
H	-5.065666	0.720212	4.531397
C	-5.692888	3.821529	6.764950
H	-4.093194	3.066976	7.993121
C	-6.459986	3.627219	5.617926
H	-6.814982	2.352503	3.916721
H	-5.862042	4.690820	7.394432
H	-7.228848	4.344185	5.344436
N	-4.872805	2.077398	0.974439
C	-5.095406	0.888412	1.476274
O	-4.231992	-0.035937	1.704164
Li	-2.687100	-0.266201	0.789257
O	-2.860103	-0.397066	-1.140147
C	-1.914156	0.327595	-1.915416
H	-2.090113	1.405855	-1.817905
H	-0.922444	0.085159	-1.532134
H	-1.987209	0.026391	-2.967933
C	-4.191100	-0.161867	-1.583161
H	-4.420956	0.909692	-1.537692

H	-4.310977	-0.529780	-2.609912
H	-4.856574	-0.709613	-0.913407
Li	-6.051428	3.069154	-0.254876
O	-7.369756	4.466824	-0.311138
C	-8.414083	4.703705	0.617503
H	-9.320908	5.028880	0.093895
H	-8.610198	3.766848	1.140544
H	-8.114417	5.472311	1.339986
C	-7.029932	5.628811	-1.055896
H	-6.192635	5.361557	-1.701054
H	-7.888343	5.955070	-1.655154
H	-6.729639	6.436838	-0.377568
C	-6.535970	0.535584	1.801085
H	-6.613194	0.155911	2.825483
H	-7.208960	1.388845	1.682242
H	-6.863239	-0.274714	1.137874

Model 3.3

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M2, G=2328,834338

C	-2.636485	3.521358	1.998852
C	-2.583172	3.218070	3.465527
C	-1.183031	2.743231	3.921013
C	-0.536724	0.599434	3.031297
H	-2.841927	4.146154	4.000821
H	-1.719542	3.896944	1.548839
H	-0.473998	2.998039	3.121024
H	-3.331379	2.472840	3.747133
O	-0.978851	0.896754	1.815512
O	-1.168652	1.333942	4.101495
C	-0.952367	-0.849229	3.405114
F	-0.643147	-1.209840	4.667692
F	-2.282616	-1.021433	3.271916
F	-0.362667	-1.751470	2.595711
C	0.992881	0.725138	3.173070
C	1.780438	0.798913	2.024225
C	1.610766	0.758776	4.426694
C	3.168094	0.908147	2.121613
H	1.282284	0.777318	1.059318
C	2.997139	0.867886	4.528353
H	0.997364	0.711273	5.322834
C	3.779742	0.942455	3.374763
H	3.772079	0.967003	1.219954
H	3.467251	0.897944	5.507773
H	4.860089	1.028925	3.453545
C	-3.715625	3.446791	1.198215
C	-0.656879	3.404957	5.198763
H	0.423403	3.215199	5.228405
H	-0.777267	4.493244	5.100960
C	-3.624146	3.955213	-0.200519

O	-4.627116	4.139395	-0.889530
O	-2.407936	4.222625	-0.652086
C	-2.326949	4.765834	-1.975970
H	-1.263199	4.868367	-2.182000
H	-2.795148	4.086740	-2.692054
H	-2.822582	5.738225	-2.013567
C	-1.236848	2.934917	6.537215
H	-1.165460	1.843631	6.595449
H	-0.570073	3.318271	7.318889
C	-2.655609	3.413888	6.879873
H	-2.748985	3.447073	7.974255
H	-2.770789	4.454311	6.545859
C	-3.833461	2.606454	6.366237
C	-3.774968	1.223773	6.162251
C	-5.057404	3.252981	6.153682
C	-4.911040	0.507873	5.782343
H	-2.835239	0.693149	6.279500
C	-6.195174	2.542858	5.773924
H	-5.117789	4.331576	6.289775
C	-6.128362	1.161147	5.596254
H	-4.839294	-0.565772	5.627710
H	-7.135236	3.066344	5.618143
H	-7.018376	0.604047	5.314380
N	-5.026835	3.054183	1.515630
C	-5.228402	1.814856	1.928646
O	-4.407049	0.884124	2.089887
Li	-2.712094	0.860218	1.335731
O	-2.849317	1.143263	-0.583024
C	-1.616506	1.166632	-1.286115
H	-1.635764	1.945419	-2.059195
H	-0.841230	1.379325	-0.547578
H	-1.430403	0.193555	-1.758319
C	-3.960441	0.860608	-1.412161
H	-4.058420	1.626984	-2.192448
H	-3.853808	-0.126022	-1.880100
H	-4.849574	0.873772	-0.777452
Li	-6.245570	3.840007	0.151237
O	-7.397468	5.255797	-0.455859
C	-8.730614	5.371773	0.019129
H	-9.435939	4.942758	-0.703236
H	-8.790784	4.829239	0.963218
H	-8.977167	6.425920	0.191389
C	-7.176030	6.029406	-1.626090
H	-6.170384	5.801492	-1.980070
H	-7.912398	5.771183	-2.396793
H	-7.258495	7.096209	-1.387347
O	-6.550979	1.573861	2.158330
C	-6.905172	0.229958	2.447080
H	-6.228471	-0.166934	3.210444
H	-6.783021	-0.386539	1.547521
C	-8.336610	0.189955	2.919116

C	-9.015832	-1.033224	2.912699
C	-8.989755	1.325700	3.402509
C	-10.322169	-1.122151	3.387993
H	-8.515884	-1.923859	2.536123
C	-10.301196	1.238720	3.873691
H	-8.465877	2.277120	3.406033
C	-10.970883	0.016470	3.870217
H	-10.835967	-2.079555	3.378925
H	-10.797653	2.130792	4.246743
H	-11.990906	-0.050483	4.238028

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TS2, G= -2328,816034

C	-2.482643	2.530579	1.595207
C	-2.604704	2.326530	3.082680
C	-1.239750	2.294599	3.770833
C	-0.248407	1.115606	1.942258
H	-3.185748	3.164668	3.496142
H	-1.734355	3.264468	1.300803
H	-0.695117	3.215808	3.507388
H	-3.166004	1.410625	3.290165
O	-1.405302	1.105067	1.217999
O	-0.460683	1.174297	3.339477
C	0.409317	-0.271113	1.758602
F	1.508577	-0.432591	2.509177
F	-0.443265	-1.261240	2.086371
F	0.766354	-0.473458	0.478874
C	0.737540	2.197254	1.481762
C	0.615233	2.743948	0.203865
C	1.774521	2.617695	2.318106
C	1.520871	3.709669	-0.234081
H	-0.210488	2.427403	-0.427392
C	2.680158	3.582751	1.879986
H	1.862164	2.192855	3.314822
C	2.555497	4.129517	0.601920
H	1.415957	4.137649	-1.227248
H	3.481635	3.909388	2.536478
H	3.260128	4.882707	0.260760
C	-3.630295	2.537418	0.774612
C	-1.331286	2.203178	5.287962
H	-0.329090	2.354819	5.704970
H	-1.939702	3.054275	5.619393
C	-3.621491	3.276970	-0.432245
O	-4.645584	3.520454	-1.121302
O	-2.416544	3.753492	-0.844989
C	-2.431693	4.586098	-1.999310
H	-1.393896	4.877888	-2.162952
H	-2.811577	4.041127	-2.867597
H	-3.049565	5.472967	-1.833442
C	-1.922761	0.881964	5.813754
H	-2.352582	0.301120	4.988701

H	-1.124550	0.260478	6.233160
C	-3.008758	1.095629	6.882418
H	-3.282824	0.125441	7.314002
H	-2.605678	1.708823	7.698166
C	-4.238315	1.755854	6.304358
C	-5.111911	1.019611	5.493657
C	-4.511060	3.111180	6.511786
C	-6.220993	1.620069	4.903647
H	-4.914744	-0.037861	5.321087
C	-5.617425	3.721698	5.916339
H	-3.850573	3.697785	7.147475
C	-6.475001	2.977743	5.108782
H	-6.891978	1.032533	4.283895
H	-5.808158	4.777623	6.088149
H	-7.337632	3.447680	4.644060
N	-4.938700	2.084698	1.139880
C	-5.112486	0.860707	1.558397
O	-4.278497	-0.063596	1.773152
Li	-2.656386	-0.245951	0.937262
O	-6.447166	0.572263	1.769266
O	-2.907028	-0.390205	-0.978884
C	-1.962818	0.325697	-1.763593
H	-2.162766	1.403730	-1.711020
H	-0.974570	0.125800	-1.348276
H	-2.010257	-0.014844	-2.805547
C	-4.237449	-0.181024	-1.430783
H	-4.499313	0.882435	-1.359253
H	-4.338569	-0.520902	-2.469143
H	-4.895394	-0.765513	-0.785069
Li	-6.169097	3.033632	-0.081286
O	-7.407256	4.509267	-0.324779
C	-8.593292	4.703483	0.427557
H	-9.410955	5.024316	-0.229049
H	-8.849873	3.749908	0.891381
H	-8.432839	5.459546	1.205641
C	-6.977574	5.696819	-0.975089
H	-6.055942	5.455643	-1.504940
H	-7.745456	6.037395	-1.680313
H	-6.787806	6.484444	-0.235504
C	-6.743933	-0.728357	2.243541
C	-8.227885	-0.830080	2.501888
H	-6.430837	-1.483069	1.512137
H	-6.182379	-0.925891	3.166499
C	-8.806420	-2.097029	2.633288
C	-10.164634	-2.232755	2.910505
C	-10.965760	-1.098805	3.056155
C	-10.396500	0.166267	2.922904
C	-9.034191	0.300920	2.648251
H	-8.187131	-2.984219	2.514665
H	-10.599557	-3.223394	3.008458
H	-12.025946	-1.202606	3.268209

H	-11.013023	1.054530	3.031402
H	-8.591969	1.286730	2.538278

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M3, G=-2328,819242

C	-2.334623	2.451322	1.605161
C	-2.540473	2.403543	3.111421
C	-1.194621	2.335076	3.825207
C	-0.278578	1.184861	1.954190
H	-3.074641	3.307325	3.429164
H	-1.685787	3.292629	1.340275
H	-0.621403	3.246652	3.595728
H	-3.158163	1.539017	3.371552
O	-1.495295	1.236421	1.263522
O	-0.442456	1.205498	3.340883
C	0.261703	-0.231473	1.672140
F	1.353176	-0.502790	2.389739
F	-0.666958	-1.162770	1.971577
F	0.568214	-0.392464	0.377253
C	0.724152	2.224834	1.458099
C	0.615205	2.740497	0.165525
C	1.780738	2.619256	2.280991
C	1.558553	3.655345	-0.298338
H	-0.226398	2.450783	-0.457925
C	2.724187	3.533108	1.813550
H	1.856566	2.214730	3.286850
C	2.614383	4.051531	0.523168
H	1.465566	4.063412	-1.300689
H	3.542841	3.840824	2.457360
H	3.347589	4.765712	0.159644
C	-3.559801	2.510213	0.782360
C	-1.295578	2.181994	5.334352
H	-0.296820	2.309276	5.767618
H	-1.899430	3.026968	5.689123
C	-3.577102	3.263965	-0.377592
O	-4.617693	3.545590	-1.062351
O	-2.358109	3.734775	-0.826336
C	-2.406002	4.659546	-1.900577
H	-1.368682	4.935635	-2.099119
H	-2.848766	4.208865	-2.793311
H	-2.980937	5.551529	-1.632214
C	-1.906414	0.849498	5.804770
H	-2.365666	0.318489	4.961962
H	-1.114421	0.192390	6.178995
C	-2.968343	1.038090	6.902331
H	-3.245805	0.056673	7.304988
H	-2.540749	1.616967	7.730648
C	-4.201258	1.731396	6.371643
C	-5.113170	1.022883	5.578778
C	-4.441567	3.088582	6.605958
C	-6.229245	1.651147	5.032083

H	-4.940276	-0.035865	5.388818
C	-5.553368	3.727472	6.052191
H	-3.752257	3.653566	7.230595
C	-6.449540	3.010622	5.262213
H	-6.930773	1.084959	4.426336
H	-5.718682	4.784467	6.242659
H	-7.316106	3.502987	4.829294
N	-4.863475	2.098170	1.222502
C	-5.044267	0.884732	1.658721
O	-4.213949	-0.053298	1.853345
Li	-2.668168	-0.276396	0.913429
O	-6.374236	0.613510	1.923518
O	-2.955724	-0.375896	-0.997453
C	-2.052545	0.360985	-1.812809
H	-2.221779	1.437691	-1.688841
H	-1.040981	0.110708	-1.490592
H	-2.185341	0.076632	-2.864124
C	-4.307703	-0.141450	-1.374603
H	-4.546954	0.924443	-1.275635
H	-4.465698	-0.468860	-2.409788
H	-4.938583	-0.726409	-0.702587
Li	-6.088619	3.095608	0.023955
O	-7.362346	4.536411	-0.233597
C	-8.556373	4.780119	0.488426
H	-9.413319	4.827050	-0.194746
H	-8.691548	3.956518	1.190861
H	-8.480714	5.724429	1.041363
C	-7.066993	5.565745	-1.165952
H	-6.119111	5.303067	-1.636682
H	-7.863489	5.634523	-1.917407
H	-6.974097	6.528057	-0.647190
C	-6.670140	-0.682582	2.405913
C	-8.156541	-0.791056	2.648864
H	-6.346987	-1.442932	1.684807
H	-6.117991	-0.871611	3.336775
C	-8.716991	-2.057370	2.849683
C	-10.078545	-2.199720	3.105173
C	-10.901910	-1.073137	3.160528
C	-10.350673	0.190614	2.959135
C	-8.984801	0.332008	2.705097
H	-8.080358	-2.938888	2.802693
H	-10.499405	-3.189833	3.255993
H	-11.964761	-1.182589	3.355758
H	-10.983865	1.072801	2.997139
H	-8.555835	1.316220	2.542912

Model 3.4

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M2, G=-1860.816665

C	-2.281261	3.704796	1.939450
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C	-2.146938	3.705139	3.426660
C	-0.908851	2.967705	3.964251
C	-0.560229	0.791224	2.973896
H	-2.066788	4.762591	3.724568
H	-1.390592	3.916313	1.352653
H	-0.072836	3.157630	3.274352
H	-3.049385	3.301904	3.892225
O	-0.945739	1.149237	1.757201
O	-1.140576	1.569654	4.041820
C	-1.143128	-0.612596	3.300609
F	-0.997380	-1.008032	4.578638
F	-2.470976	-0.641197	3.035930
F	-0.583256	-1.566814	2.532970
C	0.967488	0.745439	3.158927
C	1.789916	0.783641	2.033324
C	1.547497	0.645168	4.427039
C	3.177298	0.727009	2.168121
H	1.319253	0.864723	1.057965
C	2.933823	0.586185	4.565396
H	0.907950	0.621439	5.305534
C	3.752221	0.626778	3.435218
H	3.809830	0.759300	1.285114
H	3.376151	0.508741	5.554910
H	4.832416	0.580918	3.543003
C	-3.433032	3.543344	1.274261
C	-0.480814	3.448490	5.355998
H	0.553320	3.113524	5.503117
H	-0.455799	4.546809	5.358513
C	-3.557084	3.670133	-0.205476
O	-4.594100	3.474146	-0.805397
O	-2.423712	4.063723	-0.792948
C	-2.484008	4.190168	-2.215855
H	-1.466637	4.409168	-2.535766
H	-2.839359	3.258499	-2.661277
H	-3.157979	5.004105	-2.492787
C	-1.295237	2.947949	6.555632
H	-1.285985	1.852788	6.561481
H	-0.740607	3.253225	7.450312
C	-2.728754	3.485504	6.704755
H	-2.947923	3.567416	7.778020
H	-2.771228	4.516389	6.325066
C	-3.880966	2.702576	6.096083
C	-3.793127	1.360559	5.713150
C	-5.119058	3.346796	5.959948
C	-4.912154	0.680947	5.227137
H	-2.842654	0.839405	5.759665
C	-6.239603	2.672456	5.480188
H	-5.203864	4.395219	6.242537
C	-6.141096	1.328105	5.116060
H	-4.815620	-0.358735	4.926335
H	-7.188987	3.194998	5.392028

H	-7.011188	0.794752	4.742106
N	-4.669636	3.266279	1.937182
C	-5.137470	2.009891	1.938780
O	-4.509554	1.031621	1.521568
C	-5.475377	4.395320	2.387316
H	-6.416438	4.022875	2.796842
H	-4.941390	4.941927	3.170291
H	-5.684097	5.063890	1.546607
Li	-2.637877	0.859758	1.169984
H	-6.146019	1.904614	2.356763
O	-2.539619	1.099953	-0.767939
C	-1.233513	1.054476	-1.322666
H	-1.206643	1.600556	-2.274135
H	-0.565676	1.514662	-0.593756
H	-0.929261	0.013846	-1.495284
C	-3.519032	0.505603	-1.603732
H	-3.560323	1.022265	-2.571017
H	-3.288783	-0.554578	-1.770053
H	-4.478836	0.606940	-1.095752

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TS2, G= -1860.796986

C	-1.586999	3.201085	2.338726
C	-1.898982	3.188084	3.811100
C	-0.706800	2.825683	4.700533
C	0.156260	1.237057	3.133396
H	-2.237412	4.196653	4.091803
H	-0.644566	3.659472	2.049721
H	0.121635	3.517550	4.482237
H	-2.731116	2.500246	4.003710
O	-0.830712	1.462157	2.230445
O	-0.252436	1.490154	4.467731
C	0.430907	-0.285548	3.135728
F	1.241648	-0.682468	4.126400
F	-0.723532	-0.978219	3.266102
F	0.988089	-0.680116	1.979791
C	1.460727	1.975219	2.805562
C	1.669099	2.463422	1.515263
C	2.450722	2.141295	3.777294
C	2.858004	3.120622	1.198816
H	0.882324	2.342217	0.775217
C	3.640148	2.795764	3.460244
H	2.280228	1.767295	4.783765
C	3.845903	3.286108	2.169844
H	3.011177	3.507625	0.195101
H	4.404600	2.926538	4.220733
H	4.771097	3.799549	1.924078
C	-2.609233	3.291314	1.403467
C	-1.028301	2.897902	6.191585
H	-0.142567	2.530732	6.721849
H	-1.155405	3.949861	6.478021

C	-2.374877	3.520105	0.002382
O	-3.237791	3.589673	-0.867894
O	-1.053719	3.660146	-0.298672
C	-0.751141	3.897300	-1.670645
H	0.335029	3.976095	-1.722031
H	-1.100223	3.068005	-2.291768
H	-1.214121	4.824816	-2.016536
C	-2.266417	2.079730	6.597577
H	-2.318000	1.198201	5.947905
H	-2.117523	1.695231	7.611214
C	-3.589635	2.879235	6.546495
H	-3.930978	3.063864	7.573873
H	-3.409199	3.874588	6.123919
C	-4.744821	2.254344	5.791221
C	-4.955285	0.871052	5.759593
C	-5.683497	3.078946	5.157360
C	-6.068369	0.329212	5.115675
H	-4.249564	0.204420	6.248858
C	-6.806083	2.544103	4.527264
H	-5.535027	4.157497	5.167532
C	-7.002621	1.163033	4.501873
H	-6.208346	-0.748135	5.100341
H	-7.524499	3.206663	4.050874
H	-7.872442	0.740862	4.006752
N	-3.981874	3.095359	1.772727
C	-4.520816	1.880240	1.882860
O	-3.916144	0.808712	1.725017
C	-4.805281	4.290371	1.923014
H	-5.844676	4.006725	2.103648
H	-4.443840	4.887079	2.766655
H	-4.746815	4.882387	1.005657
Li	-2.155421	0.249524	1.747615
O	-1.440814	-0.678600	0.235190
C	-0.660087	0.119754	-0.640886
H	-0.922615	-0.098696	-1.683340
H	-0.875507	1.164676	-0.407531
H	0.407710	-0.073633	-0.478041
C	-1.226182	-2.066396	0.051659
H	-1.502543	-2.361140	-0.967946
H	-0.173654	-2.315990	0.233079
H	-1.856828	-2.594369	0.768377
H	-5.586363	1.878108	2.146336

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M3, G= -1860.797049

C	-4.639339	-1.244906	4.475453
C	-3.953412	-1.264494	5.691473
C	-3.614703	-0.071003	6.323739
C	-3.952597	1.167756	5.761894
C	-4.641536	1.171084	4.547048
C	-4.981047	-0.021771	3.903964

C	-3.638067	2.451700	6.501365
C	-2.163709	2.619551	6.936519
C	-1.327100	3.648463	6.166979
C	-1.024763	3.359245	4.695074
C	-2.064164	3.835627	3.682904
C	-1.601789	3.479708	2.276168
O	-1.350477	1.995989	2.291064
C	-0.443952	1.563246	3.267600
O	-0.830779	1.943451	4.554921
C	-2.548722	3.787344	1.184483
N	-3.897087	4.196099	1.465982
C	-4.198806	5.626049	1.466549
C	-0.568293	0.024741	3.265503
F	-0.087799	-0.496473	2.125656
C	0.999073	1.955888	2.953503
C	1.390699	2.207800	1.638255
C	2.719159	2.523787	1.357883
C	3.658896	2.580187	2.387342
C	3.267245	2.322026	3.701122
C	1.938963	2.008359	3.984528
F	0.123250	-0.514075	4.278280
F	-1.840604	-0.371500	3.383213
C	-2.140482	3.942259	-0.151999
O	-0.804311	3.635744	-0.339271
C	-0.321231	3.770873	-1.668589
O	-2.834067	4.294193	-1.118538
C	-4.885381	3.304185	1.542224
O	-4.740670	2.070526	1.490553
Li	-3.009193	1.316573	1.498220
O	-2.422878	-0.096942	0.396149
C	-2.760720	-1.470167	0.483505
C	-1.419053	0.171805	-0.571370
H	-2.176482	4.922487	3.769298
H	-0.615502	3.915709	2.077849
H	-0.074648	3.856779	4.445735
H	-3.036108	3.370535	3.879315
H	0.647300	2.183828	0.845743
H	1.625012	1.809190	5.005860
H	3.019020	2.730270	0.334428
H	3.994886	2.366600	4.506177
H	4.693410	2.827281	2.167001
H	-0.367149	3.738366	6.689534
H	-1.803078	4.636414	6.222161
H	0.724808	3.460358	-1.636869
H	-0.881623	3.131977	-2.357421
H	-0.391712	4.807076	-2.010680
H	-1.653375	1.651979	6.891273
H	-2.138746	2.930055	7.986662
H	-4.266960	2.471127	7.400432
H	-3.960291	3.311101	5.901236
H	-3.089190	-0.102574	7.276297

H	-4.932432	2.116517	4.095336
H	-3.683242	-2.212414	6.149356
H	-5.509815	0.020078	2.955230
H	-4.901776	-2.175425	3.979333
H	-5.272861	5.786297	1.591692
H	-3.665997	6.117593	2.285104
H	-3.878014	6.055950	0.513849
H	-5.886273	3.735127	1.678907
H	-1.784492	-0.081006	-1.574073
H	-1.191896	1.239340	-0.514391
H	-0.515506	-0.407825	-0.348683
H	-3.151198	-1.827263	-0.476856
H	-1.879147	-2.058560	0.764556
H	-3.527763	-1.571117	1.253516

Model 3.5

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M2, G= -1900.091891

C	-2.019887	3.861972	1.877002
C	-1.972867	3.853568	3.369665
C	-0.846806	2.999703	3.977444
C	-0.533498	0.885779	2.812418
H	-1.803361	4.895232	3.684859
H	-1.079987	3.945827	1.338527
H	0.076635	3.201635	3.413604
H	-2.942987	3.544712	3.770542
O	-0.864909	1.321346	1.606321
O	-1.145634	1.612962	3.902495
C	-1.163609	-0.519432	3.032378
F	-1.075631	-0.999631	4.285130
F	-2.485259	-0.487576	2.724954
F	-0.607790	-1.438210	2.222551
C	0.982210	0.794175	3.059475
C	1.854258	0.894829	1.976217
C	1.502721	0.598318	4.342477
C	3.233376	0.806805	2.168070
H	1.430172	1.049112	0.988512
C	2.880508	0.509132	4.537389
H	0.823620	0.523820	5.187766
C	3.749088	0.613368	3.449636
H	3.905850	0.888827	1.318406
H	3.277553	0.360318	5.537839
H	4.822735	0.544796	3.601696
C	-3.152533	3.828255	1.162031
C	-0.585241	3.330554	5.453993
H	0.387268	2.892537	5.708846
H	-0.477076	4.418459	5.561425
C	-3.190197	3.897019	-0.326131
O	-4.219508	3.834875	-0.967992
O	-1.982528	4.055450	-0.873567

C	-1.957796	4.101857	-2.302273
H	-0.905121	4.132082	-2.578059
H	-2.441591	3.213885	-2.715101
H	-2.474965	4.995724	-2.658791
C	-1.616074	2.802013	6.461671
H	-1.749474	1.728195	6.291436
H	-1.166091	2.893991	7.456109
C	-2.988584	3.518647	6.485432
H	-3.159461	3.939644	7.482309
H	-2.962644	4.387652	5.814149
C	-4.198394	2.668249	6.137100
C	-4.140742	1.626185	5.200873
C	-5.426264	2.926188	6.760105
C	-5.271614	0.861282	4.912047
H	-3.203962	1.397362	4.698204
C	-6.559956	2.166069	6.470460
H	-5.492207	3.726607	7.494764
C	-6.484965	1.123550	5.547042
H	-5.197906	0.059506	4.181440
H	-7.497553	2.382046	6.975731
H	-7.363531	0.525407	5.321016
N	-4.440700	3.746961	1.777449
C	-5.053347	2.540470	1.808384
O	-4.441351	1.508555	1.491009
C	-5.125735	5.010485	2.043466
H	-5.889862	4.875497	2.808507
H	-4.390713	5.726589	2.415610
H	-5.584819	5.406468	1.130493
Li	-2.610866	1.181680	1.082138
O	-2.587126	1.097219	-0.840911
C	-1.340565	0.736835	-1.419095
H	-1.244063	1.179099	-2.418652
H	-0.565784	1.114768	-0.751251
H	-1.260561	-0.354914	-1.499230
C	-3.699637	0.658751	-1.602843
H	-3.677189	1.112257	-2.602031
H	-3.688553	-0.434318	-1.700371
H	-4.597910	0.979295	-1.074300
C	-6.497420	2.489161	2.230749
H	-6.617498	2.840777	3.260228
H	-7.110770	3.117011	1.576566
H	-6.834545	1.454588	2.172997

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TS2, G= -1900.069378

C	-1.643875	3.571075	2.280620
C	-2.019240	3.737304	3.730489
C	-0.926537	3.242643	4.680112
C	-0.360812	1.413825	3.267669
H	-2.180914	4.806756	3.926933
H	-0.622169	3.845502	2.026980

H	0.009999	3.745712	4.388824
H	-2.960966	3.215368	3.916933
O	-1.272228	1.769788	2.318946
O	-0.729745	1.833458	4.569500
C	-0.391000	-0.129373	3.368705
F	0.305376	-0.599074	4.414639
F	-1.651076	-0.586954	3.493258
F	0.123365	-0.695600	2.263431
C	1.070388	1.855324	2.933200
C	1.407134	2.181062	1.619031
C	2.047025	1.905319	3.930867
C	2.712437	2.558741	1.304145
H	0.633725	2.159136	0.855585
C	3.351705	2.281516	3.615564
H	1.778357	1.660515	4.955268
C	3.687069	2.607565	2.300697
H	2.967053	2.818094	0.280169
H	4.105665	2.324017	4.396570
H	4.703584	2.902075	2.055640
C	-2.584872	3.820255	1.279418
C	-1.166967	3.552125	6.158164
H	-0.195771	3.488714	6.664537
H	-1.491552	4.598259	6.236683
C	-2.240789	3.929986	-0.107824
O	-3.026349	4.125858	-1.033740
O	-0.901915	3.788319	-0.341508
C	-0.493029	3.912815	-1.699713
H	0.585260	3.749785	-1.697765
H	-0.987512	3.163778	-2.324145
H	-0.722681	4.908996	-2.086677
C	-2.137103	2.641774	6.920083
H	-1.777984	1.611141	6.838906
H	-2.050850	2.912892	7.977995
C	-3.627639	2.713891	6.512879
H	-4.232494	2.771631	7.426937
H	-3.830307	3.644702	5.968624
C	-4.146897	1.536704	5.711755
C	-3.920685	0.224686	6.148494
C	-4.925631	1.720919	4.564809
C	-4.442167	-0.865247	5.456344
H	-3.333937	0.051320	7.047874
C	-5.452291	0.632877	3.865855
H	-5.126251	2.733514	4.214406
C	-5.209703	-0.665984	4.307925
H	-4.250214	-1.872876	5.815038
H	-6.045809	0.799994	2.971520
H	-5.618722	-1.514329	3.766394
N	-3.990448	3.903612	1.564817
C	-4.787303	2.850481	1.289810
O	-4.325711	1.720393	1.047444
C	-4.538739	5.244795	1.770257

H	-5.482278	5.207695	2.317030
H	-3.820689	5.816233	2.359465
H	-4.691806	5.752261	0.810293
Li	-2.787803	0.872663	1.682562
O	-2.132903	-0.358575	0.376179
C	-1.181503	0.211646	-0.508054
H	-1.422013	-0.055757	-1.544472
H	-1.227933	1.295875	-0.381025
H	-0.172286	-0.139644	-0.258306
C	-2.151843	-1.773224	0.326697
H	-2.434057	-2.113819	-0.677089
H	-1.165772	-2.176439	0.587390
H	-2.891126	-2.118066	1.051304
C	-6.284160	3.055671	1.288459
H	-6.570781	3.886760	0.637913
H	-6.752875	2.137657	0.934483
H	-6.652422	3.276859	2.296545

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M3, G=-1900.072823

C	-1.618642	3.439537	2.253307
C	-2.089738	3.803519	3.654232
C	-1.053328	3.356293	4.681902
C	-0.420069	1.558628	3.280084
H	-2.219733	4.889462	3.728491
H	-0.646775	3.901377	2.042512
H	-0.109031	3.870097	4.442850
H	-3.056250	3.328205	3.846979
O	-1.322028	1.963250	2.289945
O	-0.829081	1.943341	4.559192
C	-0.519551	0.018317	3.288184
F	0.158431	-0.503667	4.318877
F	-1.788546	-0.395410	3.381858
F	-0.007800	-0.503924	2.162249
C	1.018080	1.976367	2.978210
C	1.413707	2.241856	1.666737
C	1.949734	2.040426	4.016050
C	2.738588	2.581348	1.396933
H	0.675565	2.208635	0.869334
C	3.274516	2.377097	3.742993
H	1.632048	1.832331	5.034454
C	3.670488	2.647706	2.432976
H	3.041627	2.798151	0.376536
H	3.996077	2.429901	4.553013
H	4.702386	2.912227	2.220677
C	-2.585222	3.692326	1.164752
C	-1.386410	3.651444	6.145262
H	-0.438216	3.744067	6.688542
H	-1.863910	4.639469	6.185245
C	-2.190201	3.834560	-0.175990
O	-2.899050	4.141950	-1.147682

O	-0.843597	3.567184	-0.366441
C	-0.370524	3.703028	-1.698580
H	0.685174	3.426215	-1.668121
H	-0.912513	3.039404	-2.378860
H	-0.475096	4.732657	-2.052210
C	-2.239851	2.626049	6.901211
H	-1.725849	1.659611	6.878707
H	-2.243523	2.946171	7.948789
C	-3.702361	2.446963	6.431414
H	-4.350914	2.457212	7.316608
H	-4.019568	3.305691	5.827837
C	-3.988969	1.161147	5.683344
C	-3.658728	-0.073905	6.257861
C	-4.646253	1.155693	4.450937
C	-3.976191	-1.271782	5.623112
H	-3.157795	-0.098936	7.223793
C	-4.965661	-0.041591	3.805542
H	-4.928040	2.098576	3.986032
C	-4.633526	-1.260539	4.391439
H	-3.712974	-2.216301	6.091876
H	-5.469735	-0.005945	2.843514
H	-4.880816	-2.194337	3.893704
N	-3.944763	4.061937	1.454212
C	-4.920581	3.133124	1.419874
O	-4.668224	1.913926	1.330856
C	-4.245058	5.495191	1.447224
H	-5.214220	5.706849	1.898856
H	-3.474801	6.010045	2.023837
H	-4.226963	5.872740	0.418818
Li	-2.922315	1.256109	1.440752
O	-2.305895	-0.168526	0.370208
C	-1.280879	0.080115	-0.579822
H	-1.621584	-0.199171	-1.584244
H	-1.059915	1.149922	-0.544609
H	-0.380714	-0.490009	-0.321664
C	-2.644105	-1.539708	0.480406
H	-3.022717	-1.916137	-0.477342
H	-1.765921	-2.122246	0.783920
H	-3.420217	-1.625539	1.243148
C	-6.362627	3.573347	1.520721
H	-6.616213	4.285882	0.730631
H	-6.992956	2.689273	1.428979
H	-6.560848	4.052658	2.484918

Model 3.6

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M3, G=-2206.182911

C	-2.103199	4.193869	1.944923
C	-2.262751	3.811529	3.381728
C	-1.078353	2.989671	3.927353

C	-0.566392	1.046932	2.591642
H	-2.338813	4.748085	3.956361
H	-1.105032	4.452223	1.598367
H	-0.184168	3.300655	3.367389
H	-3.201820	3.271241	3.524437
O	-0.776360	1.658585	1.434191
O	-1.290017	1.602528	3.709574
C	-1.180855	-0.379832	2.533461
F	-1.180394	-1.045250	3.704271
F	-2.467615	-0.328682	2.118742
F	-0.527513	-1.155568	1.646739
C	0.922177	0.928788	2.969859
C	1.893303	1.148861	1.993124
C	1.321615	0.592424	4.266623
C	3.248638	1.037408	2.304660
H	1.563875	1.413485	0.992682
C	2.675336	0.478093	4.581287
H	0.566686	0.430271	5.031540
C	3.642696	0.700264	3.599788
H	3.997904	1.212864	1.537344
H	2.975532	0.218526	5.592878
H	4.697824	0.612860	3.844108
C	-3.100252	4.281754	1.054855
C	-0.751234	3.208644	5.418030
H	0.315267	2.975759	5.526654
H	-0.856100	4.276816	5.653664
C	-2.905677	4.699681	-0.364605
O	-3.809793	4.713844	-1.175643
O	-1.654332	5.073876	-0.643376
C	-1.419197	5.452714	-2.001910
H	-0.345062	5.610993	-2.082850
H	-1.746408	4.657342	-2.675362
H	-1.962435	6.371234	-2.235634
C	-1.489962	2.364445	6.466050
H	-1.526270	1.323749	6.124905
H	-0.867977	2.363715	7.369464
C	-2.886013	2.835353	6.895626
H	-3.157277	2.284569	7.806956
H	-2.836214	3.893177	7.185003
C	-4.000147	2.654583	5.888997
C	-4.140183	1.465277	5.164994
C	-4.932051	3.675903	5.674091
C	-5.172964	1.306196	4.242239
H	-3.416938	0.664752	5.294788
C	-5.974904	3.518852	4.761540
H	-4.834488	4.609905	6.224296
C	-6.098514	2.331294	4.040996
H	-5.251678	0.380580	3.677616
H	-6.690411	4.323701	4.614033
H	-6.908739	2.207357	3.328231
N	-4.462795	3.999380	1.382207

C	-4.949653	2.816523	0.940354
O	-6.283977	2.776194	0.873918
C	-5.332638	5.142023	1.654676
H	-6.273885	4.789906	2.073206
H	-4.832561	5.779224	2.387226
H	-5.527146	5.711219	0.738392
O	-4.244091	1.853065	0.640002
C	-6.842451	1.547323	0.377157
H	-6.435989	0.705771	0.944818
H	-7.909283	1.645155	0.590115
C	-6.585971	1.378255	-1.101112
C	-6.710058	2.468625	-1.966306
C	-6.224455	0.132560	-1.615207
C	-6.468823	2.314203	-3.330235
H	-6.975522	3.444615	-1.567305
C	-5.994559	-0.026516	-2.981768
H	-6.105808	-0.713231	-0.941700
C	-6.112289	1.065428	-3.841398
H	-6.555251	3.169906	-3.993765
H	-5.707353	-0.999110	-3.371190
H	-5.922774	0.945362	-4.904224
Li	-2.350398	1.672288	0.556759
O	-2.007929	2.177762	-1.270068
C	-0.647357	2.083809	-1.664207
H	-0.389828	1.043997	-1.903279
H	-0.462683	2.712049	-2.544777
H	-0.049586	2.424473	-0.817824
C	-2.916743	1.821284	-2.301950
H	-2.792296	2.490101	-3.163522
H	-2.748404	0.783545	-2.618646
H	-3.924595	1.930247	-1.897671

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TS2, G = -2206,164266

C	-1.177456	3.100180	1.983396
C	-1.831499	3.529385	3.267515
C	-1.112787	3.043542	4.526627
C	-0.494746	0.959627	3.553127
H	-1.833972	4.629088	3.285375
H	-0.104697	3.264314	1.919341
H	-0.060765	3.365834	4.463943
H	-2.871737	3.198002	3.257553
O	-1.027425	1.285567	2.344385
O	-1.136436	1.618720	4.631614
C	-0.829229	-0.527549	3.811660
F	-0.413668	-0.960522	5.011900
F	-2.152948	-0.750912	3.748520
F	-0.255775	-1.311855	2.881046
C	1.024532	1.169549	3.620189
C	1.754553	1.392143	2.452489
C	1.684490	1.148785	4.852470

C	3.135503	1.585624	2.513728
H	1.232009	1.435841	1.500718
C	3.063169	1.339503	4.913330
H	1.113019	0.995929	5.763973
C	3.792425	1.555764	3.742724
H	3.695330	1.765578	1.600047
H	3.568658	1.323246	5.874697
H	4.867068	1.706694	3.790854
C	-1.877694	3.237641	0.782677
C	-1.686948	3.594279	5.830031
H	-0.991191	3.308523	6.628448
H	-1.663885	4.690837	5.771844
C	-1.239435	3.269041	-0.504977
O	-1.791619	3.480977	-1.580998
O	0.105743	3.040452	-0.437776
C	0.835962	3.277453	-1.637346
H	1.875177	3.046562	-1.401100
H	0.483479	2.636229	-2.448967
H	0.743503	4.322744	-1.944986
C	-3.092072	3.121564	6.229725
H	-3.115141	2.027046	6.218335
H	-3.233842	3.408058	7.277272
C	-4.271530	3.697362	5.409791
H	-4.959923	4.218050	6.084597
H	-3.900717	4.476610	4.728850
C	-5.091287	2.700404	4.607480
C	-4.551356	1.508250	4.108875
C	-6.440145	2.975517	4.342063
C	-5.343414	0.607776	3.394230
H	-3.506650	1.265933	4.285963
C	-7.233016	2.082633	3.623670
H	-6.876316	3.899808	4.716853
C	-6.688436	0.884791	3.160198
H	-4.903244	-0.315374	3.024957
H	-8.275978	2.317794	3.423595
H	-7.310591	0.180150	2.614312
N	-3.301020	3.397368	0.790310
C	-4.085174	2.347674	0.484015
O	-5.376948	2.683235	0.393779
C	-3.901736	4.720650	0.977999
H	-4.603015	4.709403	1.820014
H	-3.093197	5.419823	1.188541
H	-4.432172	5.044259	0.077311
O	-3.688357	1.189462	0.296642
C	-6.285413	1.665688	-0.032755
H	-6.109497	1.470084	-1.097209
H	-6.086900	0.745172	0.521960
C	-7.691262	2.150544	0.211748
C	-7.982787	3.499577	0.419630
C	-8.730210	1.216175	0.232085
C	-9.297173	3.906590	0.652182

H	-7.177787	4.228274	0.418502
C	-10.042843	1.621697	0.463102
H	-8.509168	0.161370	0.078758
C	-10.329982	2.970886	0.677152
H	-9.511787	4.958262	0.820291
H	-10.839976	0.883949	0.485016
H	-11.351634	3.288467	0.864696
Li	-2.017455	0.588395	0.944896
O	-1.074325	-0.027991	-0.586473
C	-1.543886	0.169404	-1.911928
H	-0.993870	0.985999	-2.393095
H	-1.421440	-0.753405	-2.492189
H	-2.597709	0.439213	-1.843405
C	0.312392	-0.319603	-0.535188
H	0.894134	0.545413	-0.879377
H	0.561270	-0.539190	0.504053
H	0.539521	-1.191532	-1.160742

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M3, G = -2206, 165041

C	-1.586320	3.114159	2.146697
C	-1.996139	3.534382	3.551068
C	-0.974252	3.068084	4.582678
C	-0.419052	1.230093	3.184110
H	-2.069797	4.627844	3.589694
H	-0.625688	3.559108	1.870081
H	-0.011748	3.553403	4.358328
H	-2.983069	3.114775	3.759613
O	-1.344940	1.631802	2.215256
O	-0.785791	1.644356	4.466754
C	-0.541766	-0.305669	3.232539
F	0.269304	-0.829283	4.159452
F	-1.791209	-0.694522	3.520649
F	-0.218713	-0.847282	2.048702
C	1.011174	1.622232	2.817493
C	1.357561	1.818068	1.480025
C	1.981746	1.744838	3.813155
C	2.667872	2.145990	1.138388
H	0.592991	1.725192	0.713795
C	3.292559	2.072670	3.470478
H	1.706287	1.589340	4.853016
C	3.637144	2.273917	2.133690
H	2.929630	2.305672	0.096227
H	4.044203	2.173569	4.247669
H	4.658302	2.532253	1.868909
C	-2.583885	3.368755	1.091798
C	-1.312775	3.358521	6.040565
H	-0.427897	3.092085	6.631615
H	-1.438238	4.445132	6.139400
C	-2.280556	3.990081	-0.136483
O	-3.084236	4.406377	-0.983340

O	-0.919182	4.098731	-0.374116
C	-0.559785	4.747527	-1.586147
H	0.530201	4.717681	-1.626262
H	-0.982041	4.228552	-2.451614
H	-0.905024	5.785081	-1.595156
C	-2.526517	2.634404	6.638620
H	-2.424329	1.559626	6.456772
H	-2.459809	2.755711	7.724942
C	-3.918563	3.133991	6.181649
H	-4.481282	3.482471	7.054522
H	-3.800581	4.023881	5.547169
C	-4.789436	2.124296	5.453600
C	-4.253330	1.092257	4.674460
C	-6.184390	2.219416	5.551236
C	-5.083772	0.168387	4.037790
H	-3.176774	0.991696	4.568623
C	-7.018077	1.303458	4.912743
H	-6.621585	3.017271	6.149055
C	-6.467572	0.262910	4.164209
H	-4.640734	-0.628628	3.445368
H	-8.097823	1.396996	5.000286
H	-7.117540	-0.461202	3.679810
N	-3.975311	3.306298	1.439242
C	-4.677037	2.197873	1.148678
O	-5.985302	2.330088	1.404892
C	-4.679426	4.482179	1.960677
H	-5.135055	4.261110	2.933601
H	-3.943246	5.276746	2.077045
H	-5.459774	4.814589	1.269682
O	-4.204024	1.147962	0.686818
C	-6.830461	1.244126	1.025363
H	-6.406715	0.305050	1.391098
H	-6.865553	1.196239	-0.069581
C	-8.203141	1.477357	1.602421
C	-8.605347	2.722542	2.086857
C	-9.100500	0.406422	1.643064
C	-9.889610	2.892211	2.606619
H	-7.908467	3.554899	2.072284
C	-10.382527	0.574706	2.161413
H	-8.788701	-0.569884	1.276200
C	-10.780888	1.821521	2.647039
H	-10.191446	3.864616	2.985738
H	-11.067051	-0.268161	2.192294
H	-11.777728	1.954824	3.057145
Li	-2.317911	1.022615	0.613927
O	-1.141403	0.172623	-0.661181
C	-1.036012	-1.225660	-0.876989
H	-1.440035	-1.488186	-1.862045
H	0.013307	-1.537689	-0.813785
H	-1.612144	-1.725690	-0.097930
C	-0.454689	0.931019	-1.646420

H	0.608301	0.657742	-1.658232
H	-0.889493	0.751976	-2.636981
H	-0.561499	1.984401	-1.377603

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