Table of Contents

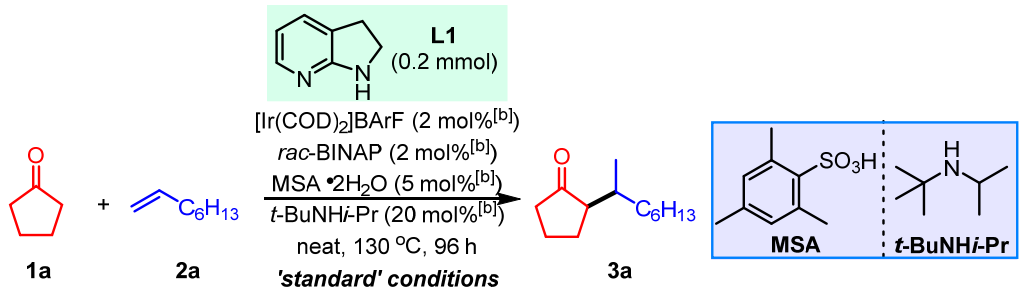
1. General Information

Unless otherwise noted, all solvents were dried by filtration through a Pure-Solv MD-5 Solvent Purification System (Innovative Technology). Toluene and 2-methyltetrahydrofuran (MeTHF) used for the key reactions were distilled freshly over sodium and carefully freeze-pump-thawed. Cyclopentanone used for the key reactions was fractionally distilled and carefully freeze-pump-thawed. 1-octene used for the key reactions was distilled freshly over calcium hydride and carefully freeze-pump-thawed. All the key reactions were carried out under nitrogen atmosphere with a stir bar in a sealed vial. Reaction temperatures were reported as the temperatures of the bather surrounding the vials. Sensitive ligands and metal catalysts and solvents were transferred under nitrogen into a nitrogen-filled glovebox with standard techniques. Analytical thin-layer chromatography (TLC) was carried out using 0.2 mm commercial silica gel plates (silica gel 60, F254, EMD chemical). Vials [15 x 45 mm 1 dram (4 mL) with PTFE lined cap attached] were purchased from Qorpak and flame-dried and cooled in a desiccator before use. High-resolution mass spectra were recorded on an Agilent 6530 LC Q-TOF mass spectrometer using electrospray ionization with fragmentation voltage set at 115 V and processed with an Agilent MassHunter Operating System. Infrared spectra were recorded on a Nicolet 380 FTIR using neat thin film technique. Nuclear magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded with Bruker Model DMX 500 (500 MHz, ^{1}H at 500 MHz, ^{13}C at 126 MHz) or Bruker Model DMX 400 (400 MHz, ^{1}H at 400 MHz, ^{13}C at 101 MHz). Unless otherwise noted, all spectrums were acquired in $CDCl_3$. Chemical shifts are reported in parts per million (ppm, δ), downfield from tetramethylsilane (TMS, δ = 0.00 ppm) and are referenced to residual solvent ($CDCl_3$, δ = 7.26 ppm (^{1}H) and 77.00 ppm (^{13}C)). Coupling constants were reported in Hertz (Hz). Data for ^{1}H NMR spectra were reported as follows: chemical shift (ppm, referenced to protium, s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, coupling constant (Hz), and integration). 2,2-Dimethyl-2,3-dihydro-1H-pyrrolo[2,3-b]pyridine (**L4**),[1] 3,4-dihydro-2H-pyrido[3,2-b][1,4]oxazine (**L7**),[2] Hex-5-en-1-ylbenzene (**2g**)[3] and 8-methylnona-1,7-diene (**2h**)[4] were synthesized by following literature procedures. 10-Methoxydec-1-ene (**2i**),[5] (dec-9-en-1-yloxy)triisopropylsilane (**2j**),[6] dec-9-en-1-yl acetate (**2k**)[7] and 2-(dec-9-en-1-yl)isoindoline-1,3-dione (**2m**)[8] were synthesized from dec-9-en-1-ol by following literature procedures. 3,3-Dimethylcyclopentan-1-one was synthesized from 3-methylcyclopent-2-en-1-one by following literature procedure.[9] 1-(1H-inden-2-yl)-2,3-dihydro-1H-pyrrolo[2,3-b]pyridine (**5**) was synthesized from 2-

indanone and 7-azaindoline by following literature procedure.[1] All other materials were obtained from commercial sources and were used as received.

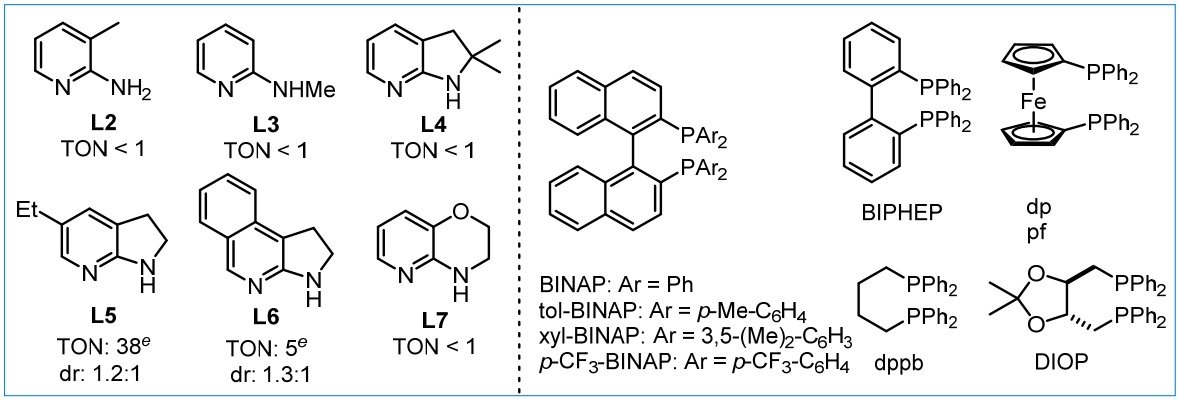
2. Experimental Procedure and Characterization Data

Table S1: Optimization study for the Ir(I)-catalyzed direct α-alkylation of cyclopentanone with 1-octene[a]



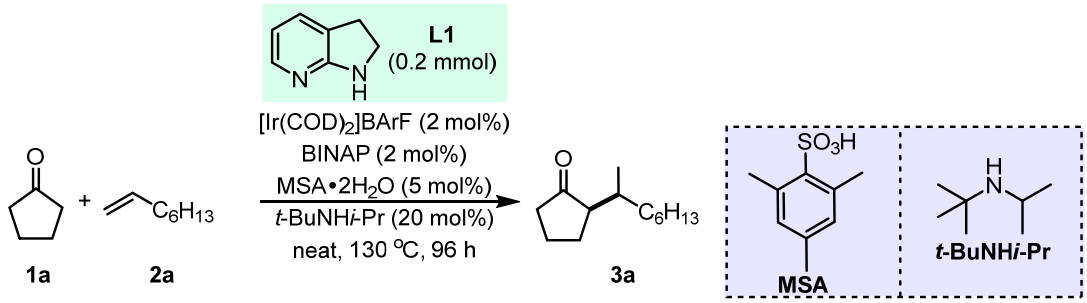
1a 2a 3a

entry	variations from the 'standard' conditions	TON of [Ir][c]	d.r. of **3a**[d]	branched/linear[e]
1	None	43 (40)	1.3:1	> 20:1
2	without **L1**	< 1	--	--
3	**L2-L7** instead of **L1**		listed below	
4	without MSA • $2H_2O$	26	1.4:1	> 20:1
5	TsOH•H_2O instead of MSA•$2H_2O$	33	1.3:1	> 20:1
6	MsOH instead of MSA•$2H_2O$	36	1.3:1	> 20:1
7	PPTS instead of MSA•$2H_2O$	35	1.3:1	> 20:1
8	without *t*-BuNH*i*-Pr	33	1.3:1	> 20:1
9	tol-BINAP instead of BINAP	33	1.3:1	>20:1
10	xyl-BINAP instead of BINAP	18	1.3:1	> 20:1
11	*p*-CF_3-BINAP instead of BINAP	13	1.3:1	> 20:1
12	BIPHEP instead of BINAP	22	1.3:1	> 20:1
13	dppf instead of BINAP	3	1.4:1	2:1
14	dppb instead of BINAP	6	1.3:1	11:1
15	DIOP instead of BINAP	8	1.3:1	17:1
16	$[Rh(COD)_2]$BArF instead of $[Ir(COD)_2]$BArF	< 1	--	--



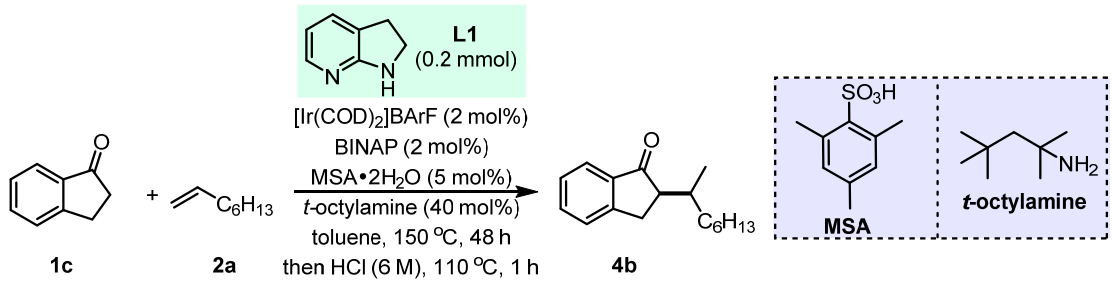
[a] Run with 0.2 mmol of **L1**, 0.5 mL of cyclopentanone and 0.5 mL of 1-octene. [b] Based on **L1**. [c] TON determined by GC using dodecane as the internal standard; value in parentheses is based on isolated products. [d] Determined by GC. d.r.= diastereomeric ratio. [e] Branched/linear > 20:1.

General procedure A: Ir(I)-catalyzed α-alkylation of cyclopentanone using 1-octene:



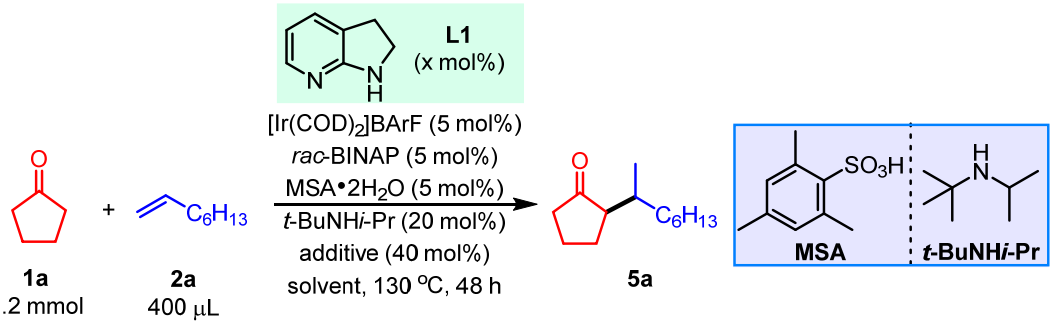
A 4-mL vial charged with a stir bar and *rac*-BINAP (2.5 mg, 0.004 mmol) was loosely capped and was transferred into a glove box. To this vial was added $[Ir(COD)_2]BArF$ (5.1 mg, 0.004 mmol) and 0.1 mL of cyclopentanone (**1a**). This mixture was stirred for 5 min before it was transferred to another vial containing 7-azaindoline (**L1**) (24 mg, 0.2 mmol) and 2-mesitylenesulfonic acid dihydrate ($MSA{\cdot}2H_2O$) (2.4 mg, 0.005 mmol) in 0.1 mL of cyclopentanone (**1a**). Another 0.3 mL of cyclopentanone (**1a**) was added to the first vial and was further transferred to the vial containing **L1**. *t*BuNH*i*Pr (4.6 mg, 0.04 mmol) was then added followed by the addition of 0.5 mL of 1-octene (**2a**). The vial was tightly capped, removed from glove box and heated at 130 °C for 96 h. After the completion of the reaction, the mixture was cooled to room temperature, diluted with ethyl acetate and passed through a short pad of silica gel. After concentration in vacuum, the crude mixture was subjected to flash chromatography (silica gel, Hexane/Et_2O=40:1 to 30:1) to give the desired product **3a (**31 mg, TON [based on iridium] = 40**)** as a colorless oil.

General procedure B: Ir(I)-catalyzed α-alkylation of 1-indanone using 1-octene:



A 4-mL vial charged with a stir bar, 1-indanone (**1c**) (264 mg, 2 mmol), 7-azaindoline (**L1**) (24 mg, 0.2 mmol) and 2-mesitylenesulfonic acid dihydrate (MSA·$2H_2O$) (2.4 mg, 0.005 mmol) was loosely capped and was transferred into a glove box. To this vial was added 0.2 mL of toluene and the resulted mixture was well stirred. Another 4-mL vial charged with a stir bar and *rac*-BINAP (2.5 mg, 0.004 mmol) was loosely capped and was transferred into the glove box. To this vial was added [$Ir(COD)_2$]BArF (5.1 mg, 0.004 mmol) and 0.1 mL of toluene. This mixture was stirred for 10 min before it was transferred to the first vial containing 1-indanone (**1c**). *t*-Octylamine (10.3 mg, 0.08 mmol) was then added to the same vial followed by the addition of 0.5 mL of 1-octene. The vial was tightly capped, removed from the glove box and heated at 150 ^{o}C for 48 h. After completion of the reaction, the mixture was cooled to room temperature. To this vial was further added 0.4 mL of HCl (6 M) and then was tightly capped and heated at 110 ^{o}C for 1 h. After cooling to room temperature, the reaction mixture was diluted with ethyl acetate and the organic layer was passed through a short pad of silica gel and K_2CO_3. After concentration in vacuum, the crude mixture was subjected to flash chromatography (silica gel, Hexane/Et_2O=25:1 to 10:1) to give the desired product **4b** (31 mg, TON [based on iridium] = 32) as a colorless oil and to recover the remaining 1-indanone **1c** (209 mg, recovering yield = 80%).

Table S2: Condition optimizations when cyclopentanone was used as the limiting reagent[a]

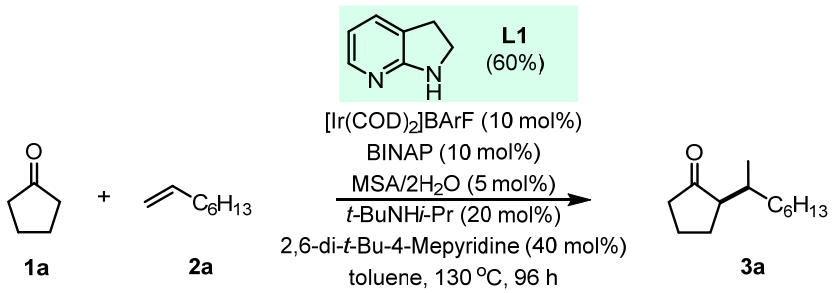


1a 0.2 mmol + **2a** 400 μL → **5a**

entry	x	additive	solvent	yield of **5a** (%)[b]	d.r. of **5a**[c]	branched/linear[c]
1	1	--	toluene	23	1.3:1	> 20:1
2	0.8	--	toluene	40	1.3:1	--
3	0.6	--	toluene	43	1.2:1	
4	0.4	--	toluene	38	1.2:1	> 20:1
5	0.2	--	toluene	29	1.1:1	> 20:1
6	0.6	--	1,4-dioxane	41	1.3:1	> 20:1
7	0.6	--	THF	21	1.3:1	> 20:1
8	0.6	--	MeTHF	33	1.3:1	> 20:1
9	0.6	H_2O	toluene	23	1.3:1	>20:1
10	0.6	$PhCO_2H$	toluene	21	1.3:1	> 20:1
11	0.6	4-Me-2-amino-$PhCO_2H$	toluene	26	1.2:1	> 20:1
12	0.6	2,6-lutidine	toluene	48	1.4:1	> 20:1
13	0.6	2,6-bi-*t*Bu-4-Me-pyridine	toluene	56	1.3:1	> 20:1
14	0.6	1,2,2,6,6-Me_5-piperidine	toluene	53	1.3:1	> 20:1
15[d]	0.6	**2,6-bi-*t*Bu-4-Me-pyridine**	toluene	**72**	1.3:1	> 20:1

[a] Unless otherwise noted, all reactions were conducted with 0.2 mmol of **1a**, 400 μL of octene (13 equiv) in 0.1 mL of toluene; [b] GC yield by using dodecane as an internal standard. [c] Selectivities were determined by GC of the crude products. [d] Reaction time = 96 h.

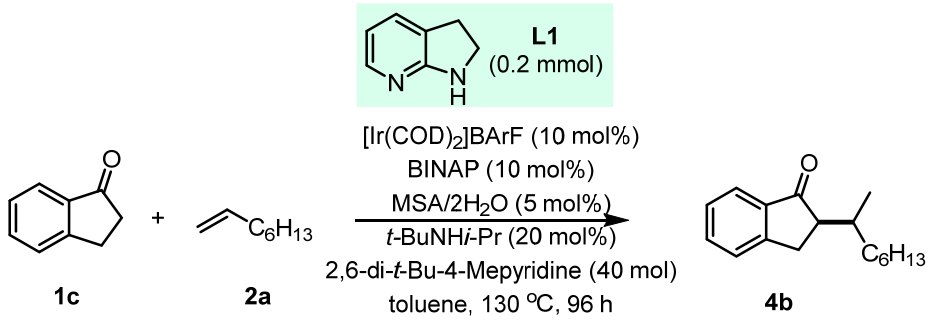
General procedure C: Ir(I)-catalyzed α-alkylation with cyclopentanone as the limiting reagent:



1a + **2a** → **3a**

A 4-mL vial charged with a stir bar and *rac*-BINAP (12.4 mg, 0.02 mmol) was loosely capped and was transferred into a glove box. To this vial was added [Ir(COD)$_2$]BArF (25.4 mg, 0.02 mmol) and 0.1 mL of toluene. This mixture was stirred for 5 min before it was transferred to another vial containing cyclopentanone (**1a**) (16.8 mg, 0.2 mmol), 7-azaindoline (**L1**) (14.4 mg, 0.12 mmol) and 2-mesitylenesulfonic acid dihydrate (MSA·2H$_2$O) (2.4 mg, 0.005 mmol). 2,6-di-*t*-Bu-4-methylpyridine (16.4 mg, 0.08 mmol) and *t*BuNH*i*Pr (4.6 mg, 0.04 mmol) was then added followed by the addition of 0.4 mL of 1-octene (**2a**) (2.6 mmol, 13 equiv). The vial was tightly capped, removed from glove box and heated at 130 ^{o}C for 96 h. After completion of the reaction, the mixture was cooled to room temperature, diluted with ethyl acetate and passed through a short pad of silica gel. After concentration in vacuum, the crude mixture was subjected to flash chromatography (silica gel, Hexane/Et$_2$O=40:1 to 30:1) to give the desired product **3a (**27 mg, 68% yield**)** as a colorless oil.

General procedure D: Ir(I)-catalyzed α-alkylation of 1-indanone with 1-indanone as the limiting reagent:

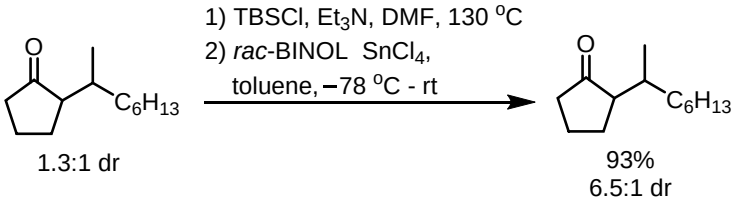


1c 2a 4b

A 4-mL vial charged with a stir bar and *rac*-BINAP (12.4 mg, 0.02 mmol) was loosely capped and was transferred into a glove box. To this vial was added [Ir(COD)$_2$]BArF (25.4 mg, 0.02 mmol) and 0.1 mL of toluene. This mixture was stirred for 5 min before it was transferred to another vial containing 1-indanone (**1c**) (26.4 mg, 0.2 mmol), 7-azaindoline (**L1**) (14.4 mg, 0.12 mmol) and 2-mesitylenesulfonic acid dihydrate (MSA·2H$_2$O) (2.4 mg, 0.005 mmol). 2,6-Di-*t*-Bu-4-methylpyridine (16.4 mg, 0.08 mmol) and *t*BuNH*i*Pr (4.6 mg, 0.04 mmol) was then added followed by the addition of 1-octene (**2a**) (400 μL mg, 2.6 mmol, 13 equiv). The vial was tightly capped, removed from glove box and heated at 130 ^{o}C for 96 h. After completion of the reaction, the mixture was cooled to room temperature. To this vial was further added 0.2 mL of HCl (6 M). The vial was tightly capped and was heated at 110 ^{o}C for 1 h. The

mixture was then cooled to room temperature, diluted with ethyl acetate and passed through a short pad of silica gel. After concentration in vacuum, the crude mixture was subjected to flash chromatography (silica gel, Hexane/Et_2O=25:1 to 10:1) to give the desired product **4b (**21 mg, 43% yield**)** as a colorless oil.

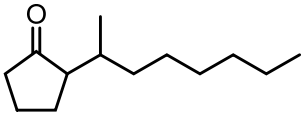
Example of increasing dr for product 3a:



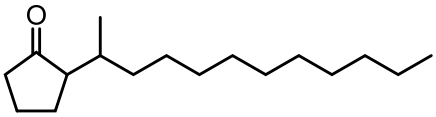
To a solution of **3a** (180 mg, 0.92 mmol) and triethylamine (2.2 mmol) in DMF (2 mL) was added TBSCl (1.1 mmol) dropwise with stirring. The mixture was heated at 130 ^oC for 90 h. After cooling, the mixture was diluted with Et_2O (10 mL) and washed with ice-cold aqueous $NaHCO_3$ solution (10 mL). The aqueous phase was re-extracted with Et_2O (3 × 10 mL). After drying over $MgSO_4$ and concentration in vacuo, the crude mixture wad directly used for the next step.

To a flame-dried 25 mL Schlenk tube containing *rac*-BINOL (1 mmol) and toluene (20 mL) was added a solution of $SnCl_4$ (1.0 mL, 1 mmol, 1.0 M solution in CH_2Cl_2) dropwise at room temperature. After being stirred for 5 min, the reaction mixture was cooled to – 78 ^oC. The crude silyl ether obtained above (considered as 0.9 mmol, dissolved in 1 mL of toluene) was added dropwise. After being stirred at – 78 ^oC for 6 h, the mixture was poured into saturated NH_4Cl, extracted with Et_2O twice, dried over $MgSO_4$, filtered, and concentrated in vacuo. Purification of the crude product by flash chromatography (eluent, 40:1 to 30:1 PE/Et_2O) gave **3a** (168 mg) with a 6.5:1 dr.

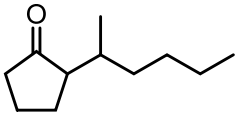
Characterization data of products



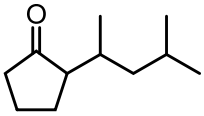
2-(octan-2-yl)cyclopentan-1-one 3a:[11] Synthesized from cyclopentanone and 1-octene by following general procedure A on a 0.2 mmol scale of **L1**. 31 mg obtained. TON (based on iridium) = 40. Or synthesized from cyclopentanone and 1-octene by following general procedure C on a 0.2 mmol scale of cyclopentanone. Yield = 68%. Isolated as a mixture with dr: 1.5:1. Colorless liquid. R_f = 0.4 (Hex:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.34 – 2.24 (m, 1H), 2.15 – 1.89 (m, 5H), 1.77 – 1.59 (m, 2H), 1.33 – 1.09 (m, 10H), 0.94 (d, *J* = 6.8 Hz, 1.2H), 0.90 – 0.83 (m, 3H), 0.74 (d, *J* = 6.7 Hz, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.70, 221.10, 54.94, 53.49, 39.37, 39.35, 35.40, 33.26, 32.49, 31.84, 31.72, 29.49, 29.37, 27.57, 27.29, 25.24, 23.63, 22.63, 20.72, 20.68, 18.05, 15.57, 14.07.



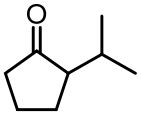
2-(dodecan-2-yl)cyclopentan-1-one 3b:[11] Synthesized from cyclopentanone and 1-dodecene by following general procedure A on a 0.2 mmol scale of **L1**. 38 mg obtained. TON (based on iridium) = 38. Isolated as a mixture with dr: 2.5:1. Colorless liquid. R_f = 0.45 (Hex:Et_2O=10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.38 – 2.24 (m, 1H), 2.18 – 1.91 (m, 5H), 1.82 – 1.62 (m, 2H), 1.37 – 1.11 (m, 18H), 0.95 (d, *J* = 6.9 Hz, 0.85H), 0.87 (t, *J* = 6.9 Hz, 3H), 0.74 (d, *J* = 6.8 Hz, 2.15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.78, 221.18, 54.95, 53.50, 39.37, 35.41, 33.28, 32.50, 31.90, 31.73, 29.85, 29.72, 29.64, 29.62, 29.33, 27.63, 27.34, 25.25, 23.62, 22.68, 20.73, 20.70, 18.07, 15.58, 14.11.



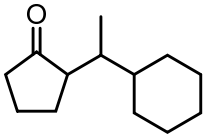
2-(hexan-2-yl)cyclopentan-1-one 3c:[11] Synthesized from cyclopentanone and 1-hexene by following general procedure A on a 0.2 mmol scale of **L1**. 24 mg obtained. TON (based on iridium) = 36. Or synthesized from cyclopentanone and 1-hexene by following general procedure C on a 0.2 mmol scale of cyclopentanone. Yield = 59%. Isolated as a mixture with dr: 1.5:1. Colorless liquid. R_f = 0.4 (pentane:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.34 – 2.25 (m, 1H), 2.19 – 1.89 (m, 5H), 1.78 – 1.63 (m, 2H), 1.35 – 1.08 (m, 6H), 0.95 (d, *J* = 6.9 Hz, 1.2H), 0.92 – 0.83 (m, 3H), 0.74 (d, *J* = 6.8 Hz, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.76, 221.18, 54.96, 53.51, 39.39, 39.37, 35.09, 32.94, 32.44, 31.71, 29.82, 29.56, 25.24, 23.63, 22.86, 22.76, 20.73, 20.69, 18.07, 15.59, 14.08.



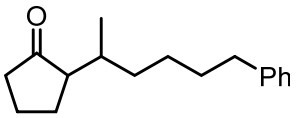
2-(4-methylpentan-2-yl)cyclopentan-1-one 3d:[11] Synthesized from cyclopentanone and 4-methylpent-1-ene by following general procedure A on a 0.2 mmol scale of **L1**. 22 mg obtained. TON (based on iridium) = 32. Isolated as a mixture with dr: 1:1. Colorless liquid. R_f = 0.4 (pentane:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.35 – 2.27 (m, 1H), 2.23 – 1.94 (m, 5H), 1.79 – 1.51 (m, 3.6H), 1.18 – 1.08 (m, 2H), 0.93 (d, *J* = 6.6 Hz, 1.5H), 0.90 – 0.83 (m, 5.4H), 0.73 (d, *J* = 6.7 Hz, 1.5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.68, 221.00, 55.00, 53.63, 44.71, 42.51, 39.49, 39.41, 30.02, 29.22, 25.33, 25.25, 25.16, 23.92, 23.55, 22.97, 22.42, 21.46, 20.76, 20.71, 18.00, 15.49.



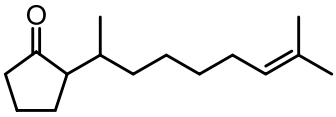
2-isopropylcyclopentan-1-one 3e:[11,12] Synthesized from cyclopentanone and pre-condensed propene by following general procedure A on a 0.8 mmol scale of **L1**. 85 mg obtained. C TON (based on iridium) = 42. olorless liquid. R_f = 0.45 (pentane:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.32 – 2.25 (m, 1H), 2.18 – 2.10 (m, 1H), 2.08 – 1.95 (m, 4H), 1.78 – 1.62 (m, 2H), 0.98 (d, *J* = 6.9 Hz, 3H), 0.81 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.12, 55.07, 39.20, 27.37, 24.62, 21.12, 20.61, 18.40.



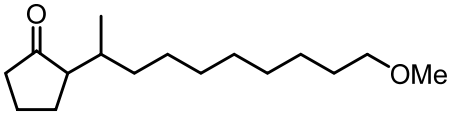
2-(1-cyclohexylethyl)cyclopentan-1-one 3f: Synthesized from cyclopentanone and vinylcyclohexane by following general procedure A on a 0.2 mmol scale of **L1**. 8.5 mg obtained. TON (based on iridium) = 11. Isolated as a mixture with dr: 1.7:1. Colorless liquid. R_f = 0.42 (Hex:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.39 – 2.16 (m, 2H), 2.13 – 1.86 (m, 3H), 1.81 – 1.46 (m, 7H), 1.29 – 1.08 (m, 6H), 0.98 – 0.82 (m, 2.2H), 0.72 (d, *J* = 6.9 Hz, 1.9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 222.50, 221.69, 51.81, 49.38, 41.44, 39.26, 38.22, 37.71, 37.02, 35.27, 33.42, 33.16, 31.01, 30.53, 29.60, 27.08, 26.67, 26.62, 26.52, 26.49, 26.37, 26.34, 24.04, 20.77, 20.74, 13.21. IR(KBr) 2958, 2924, 2853, 1738, 1465, 1406, 1378, 1268 cm^{-1}. HRMS: calcd. $C_{13}H_{22}O$ $[M]^+$: 194.1671. Found: 194.1704.



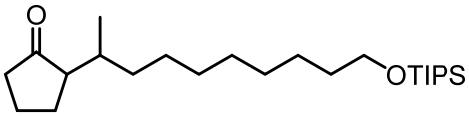
2-(6-phenylhexan-2-yl)cyclopentan-1-one 3g: Synthesized from cyclopentanone and hex-5-en-1-ylbenzene by following general procedure A on a 0.2 mmol scale of **L1**. 37 mg obtained. TON (based on iridium) = 38. Or synthesized from cyclopentanone and hex-5-en-1-ylbenzene by following general procedure C on a 0.2 mmol scale of cyclopentanone. Yield = 62%. Isolated as a mixture with dr: 1.3:1. Colorless liquid. R_f = 0.45 (Hex:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 2H), 7.19 – 7.14 (m, 3H), 2.68 – 2.52 (m, 2H), 2.39 – 2.24 (m, 1H), 2.16 – 1.92 (m, 5H), 1.78 – 1.51 (m, 4H), 1.41 – 1.11 (m, 4H), 0.95 (d, J = 6.8 Hz, 1.7H), 0.75 (d, J = 6.7 Hz, 1.3H). ^{13}C NMR (101 MHz, CDCl3) δ 221.61, 221.07, 142.72, 142.65, 128.37, 128.36, 128.22, 128.19, 125.59, 125.54, 54.90, 53.47, 39.36, 39.33, 35.89, 35.86, 35.20, 33.04, 32.38, 31.72, 31.56, 31.50, 27.23, 26.96, 25.22, 23.68, 20.71, 20.67, 18.05, 15.61. IR(KBr) 2957, 2930, 2856, 1735, 1496, 1453, 1153 cm^{-1}. HRMS: calcd. $C_{17}H_{25}O$ $[M+H]^+$: 245.1900. Found: 245.1894.



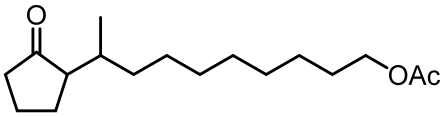
2-(8-methylnon-7-en-2-yl)cyclopentan-1-one 3h: Synthesized from cyclopentanone and hex-5-en-1-ylbenzene 8-methylnona-1,7-diene by following general procedure A on a 0.2 mmol scale of **L1**. 22 mg obtained. TON (based on iridium) = 25. Or synthesized from cyclopentanone and hex-5-en-1-ylbenzene 8-methylnona-1,7-diene by following general procedure C on a 0.2 mmol scale of cyclopentanone. Yield = 43%. Isolated as a mixture with dr: 1.3:1. Colorless liquid. R_f = 0.3 (Hex:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.13 – 5.06 (m, 1H), 2.38 – 2.22 (m, 1H), 2.16 – 1.90 (m, 7H), 1.78 – 1.62 (m, 5H), 1.59 (s, 3H), 1.35 – 1.10 (m, 6H), 0.95 (d, *J* = 6.9 Hz, 1.3H), 0.75 (d, *J* = 6.8 Hz, 1.7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.70, 221.11, 131.28, 131.21, 124.76, 124.70, 54.94, 53.50, 39.38, 39.37, 35.32, 33.17, 32.48, 31.77, 30.01, 29.92, 27.97, 27.26, 27.00, 25.71, 25.26, 23.65, 20.74, 20.70, 18.08, 17.67, 17.66, 15.61. IR(KBr) 2962, 2929, 2876, 1734, 1457, 1378, 1155 cm^{-1}. HRMS: calcd. $C_{15}H_{27}O$ $[M+H]^+$: 223.2056. Found: 223.2059.



2-(10-methoxydecan-2-yl)cyclopentan-1-one 3i:[11] Synthesized from cyclopentanone and 10-methoxydec-1-ene by following general procedure A on a 0.2 mmol scale of **L1**. 24 mg obtained. TON (based on iridium) = 24. Isolated as a mixture with dr: 1.1:1. Colorless liquid. R_f = 0.25 (Hex:Et_2O=5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.39 – 3.31 (m, 5H), 2.35 – 2.27 (m, 1H), 2.15 – 1.91 (m, 5H), 1.78 – 1.62 (m, 2H), 1.61 – 1.51 (m, 2H), 1.36 – 1.12 (m, 12H), 0.95 (d, J = 6.9 Hz, 1.4H), 0.74 (d, J = 6.7 Hz, 1.6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.75, 221.15, 72.95, 58.53, 54.95, 53.51, 39.39, 39.37, 35.39, 33.25, 32.49, 31.73, 29.75, 29.63, 29.55, 29.46, 27.59, 27.31, 26.13, 26.11, 25.26, 23.65, 20.73, 20.70, 18.07, 15.59.

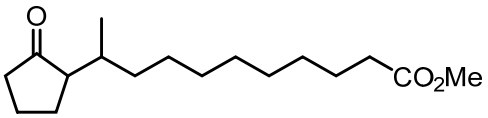


2-(10-((triisopropylsilyl)oxy)decan-2-yl)cyclopentan-1-one 3j:[11] Synthesized from cyclopentanone and (dec-9-en-1-yloxy)triisopropylsilane by following general procedure A on a 0.2 mmol scale of **L1**. 52 mg obtained. TON (based on iridium) = 33. Isolated as a mixture with dr: 1.5:1. Colorless liquid. R_f = 0.35 (Hex:Et_2O=20:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.66 (td, *J* = 6.7, 1.7 Hz, 2H), 2.36 – 2.25 (m, 1H), 2.18 – 1.91 (m, 5H), 1.80 – 1.62 (m, 2H), 1.56 – 1.48 (m, 2H), 1.39 – 1.13 (m, 12H), 1.13 – 1.01 (m, 21H), 0.95 (d, *J* = 6.9 Hz, 1.2H), 0.75 (d, *J* = 6.8 Hz, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.73, 221.13, 63.51, 54.94, 53.51, 39.39, 39.37, 35.41, 33.29, 33.04, 32.52, 31.75, 29.80, 29.68, 29.62, 29.45, 27.61, 27.34, 25.81, 25.29, 23.64, 20.74, 20.70, 18.06, 18.03, 15.59, 12.03.

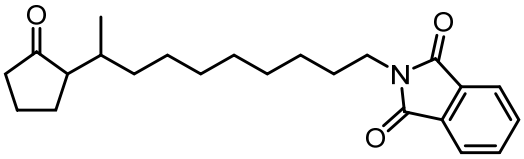


9-(2-oxocyclopentyl)decyl acetate 3k:[11] Synthesized from cyclopentanone and dec-9-en-1-yl acetate by following general procedure A on a 0.2 mmol scale of **L1**. 27 mg obtained. TON (based on iridium) = 24. Isolated as a mixture with dr: 1.1:1. Colorless liquid. R_f = 0.45 (CH_2Cl_2:Et_2O=10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.04 (td, *J* = 6.8, 2.0 Hz, 2H), 2.35 – 2.23 (m, 1H), 2.15 – 1.91 (m, 8H), 1.80 – 1.55 (m, 4H), 1.37 – 1.09 (m, 12H), 0.95 (d, *J* = 6.9 Hz, 1.6H), 0.74 (d, *J* = 6.8 Hz, 1.4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.69, 221.12, 171.22, 64.64, 64.63, 54.95, 53.51, 39.39, 39.36, 35.37, 33.22, 32.46, 31.73,

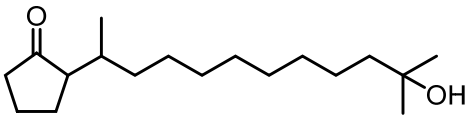
29.71, 29.61, 29.49, 29.47, 29.22, 28.59, 27.58, 27.30, 25.89, 25.25, 23.67, 21.02, 20.73, 20.69, 18.05, 15.60.



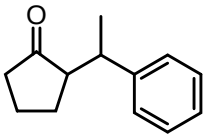
methyl 10-(2-oxocyclopentyl)undecanoate 3l: Synthesized from cyclopentanone and methyl undec-10-enoate by following general procedure A on a 0.2 mmol scale of **L1**. 34 mg obtained. TON (based on iridium) = 30. Isolated as a mixture with dr: 1.3:1. Colorless liquid. R_f = 0.4 (CH_2Cl_2:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.65 (s, 3H), 2.34 – 2.25 (m, 3H), 2.16 – 1.89 (m, 5H), 1.77 – 1.53 (m, 4H), 1.33 – 1.07 (m, 12H), 0.93 (d, *J* = 6.9 Hz, 1.3H), 0.73 (d, *J* = 6.8 Hz, 1.7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.64, 221.06, 174.27, 174.26, 54.91, 53.47, 51.38, 39.35, 39.33, 35.35, 34.07, 33.21, 32.45, 31.70, 29.70, 29.59, 29.38, 29.36, 29.19, 29.09, 27.54, 27.26, 25.24, 24.91, 23.63, 20.70, 20.67, 18.02, 15.56. IR(KBr) 2927, 2854, 1738, 1458, 1436, 1197, 1166 cm^{-1}. HRMS: calcd. $C_{17}H_{30}O_3$ $[M]^+$: 282.2195. Found: 282.2212.



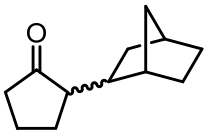
2-(9-(2-oxocyclopentyl)decyl)isoindoline-1,3-dione 3m: Synthesized from cyclopentanone and 2-(dec-9-en-1-yl)isoindoline-1,3-dione by following general procedure A on a 0.2 mmol scale of **L1**. 55 mg obtained. TON (based on iridium) = 37. Or synthesized from cyclopentanone and 2-(dec-9-en-1-yl)isoindoline-1,3-dione by following general procedure C on a 0.2 mmol scale of cyclopentanone. Yield = 39%. Isolated as a mixture with dr: 1.5:1. Colorless liquid. R_f = 0.42 (CH_2Cl_2:Et_2O=50:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.70 (dd, *J* = 5.5, 3.1 Hz, 2H), 3.66 (td, *J* = 7.4, 1.9 Hz, 2H), 2.35 – 2.24 (m, 1H), 2.16 – 1.89 (m, 5H), 1.75 – 1.61 (m, 4H), 1.35 – 1.09 (m, 12H), 0.94 (d, *J* = 6.9 Hz, 1.2H), 0.73 (d, *J* = 6.8 Hz, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.67, 221.08, 168.42, 133.79, 133.78, 132.17, 123.11, 54.90, 53.47, 39.36, 39.34, 38.04, 35.35, 33.22, 32.48, 31.73, 29.70, 29.60, 29.42, 29.14, 28.57, 27.53, 27.28, 26.83, 25.28, 23.63, 20.71, 20.67, 18.03, 15.57. IR(KBr) 2927, 2854, 1772, 1733, 1713, 1466, 1396, 1369 cm^{-1}. HRMS: calcd. $C_{23}H_{32}NO_3$ $[M+H]^+$: 370.2377. Found: 370.2375.



2-(11-hydroxy-11-methyldodecan-2-yl)cyclopentan-1-one 3n: Synthesized from cyclopentanone and 2-methyldodecan-2-ol by following general procedure A on a 0.2 mmol scale of **L1**. 24 mg obtained. TON (based on iridium) = 21. Isolated as a mixture with dr: 1.4:1. Colorless liquid. R_f = 0.4 (CH_2Cl_2:Et_2O=10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.34 – 2.25 (m, 1H), 2.15 – 1.90 (m, 5H), 1.77 – 1.61 (m, 2H), 1.49 – 1.41 (m, 2H), 1.37 – 1.12 (m, 21H), 0.95 (d, *J* = 6.8 Hz, 1.25H), 0.74 (d, *J* = 6.8 Hz, 1.75H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.75, 221.18, 71.03, 54.96, 53.50, 43.98, 39.39, 39.36, 35.38, 33.19, 32.44, 31.72, 30.16, 30.12, 29.75, 29.68, 29.59, 29.56, 29.49, 29.22, 29.19, 27.56, 27.30, 25.23, 24.32, 24.29, 23.66, 20.73, 20.69, 18.06, 15.60. IR(KBr) 3439, 2964, 2927, 2854, 1735, 1466, 1377, 1153 cm^{-1}. HRMS: calcd. $C_{18}H_{34}O_2$ $[M]^+$: 282.2559. Found: 282.2549.

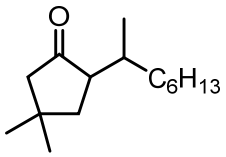


2-(1-phenylethyl)cyclopentan-1-one 3o:[11,13] Synthesized from cyclopentanone and styrene by following general procedure A on a 0.2 mmol scale of **L1**. 7.5 mg obtained. TON (based on iridium) = 10. Isolated as a mixture with dr: 1.3:1. Colorless liquid. R_f = 0.35 (Hex:Et_2O=10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.14 (m, 5H), 3.42 (qd, *J* = 7.2, 3.9 Hz, 0.43H), 3.22 (p, *J* = 7.0 Hz, 0.57H), 2.40 – 2.18 (m, 2H), 2.10 – 1.43 (m, 5H), 1.42 (d, *J* = 7.1 Hz, 1.7H), 1.20 (d, *J* = 7.2 Hz, 1.3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 220.26, 219.89, 145.38, 144.10, 128.36, 128.19, 127.96, 127.31, 126.29, 126.18, 55.88, 55.26, 39.12, 39.10, 38.88, 37.92, 26.60, 24.58, 20.44, 20.37, 20.01, 15.47.

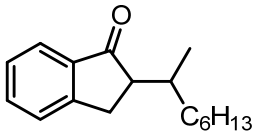


2-bicyclo[2.2.1]heptan-2-yl)cyclopentan-1-one 3p: Synthesized from cyclopentanone and norbornene by following general procedure A on a 0.2 mmol scale of **L1**. 25 mg obtained. TON (based on iridium) = 35. Or synthesized from cyclopentanone and norbornene by following general procedure C on a 0.2 mmol scale of cyclopentanone. Yield = 53%. Isolated as a mixture with dr: 1.1:1 (determined by ^{13}C

NMR). Colorless liquid. R_f = 0.45 (Hex:Et_2O=10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.51 – 2.47 (m, 0.4H), 2.29 – 1.82 (m, 6.6H), 1.80 – 1.67 (m, 1H), 1.66 – 1.54 (m, 2H), 1.54 – 1.36 (m, 3.5H), 1.32 – 1.24 (m, 1H), 1.21 – 1.05 (m, 3.5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 221.09, 220.73, 54.17, 53.38, 42.74, 42.31, 39.72, 39.23, 38.61, 38.37, 37.03, 36.86, 36.72, 35.97, 35.67, 35.50, 30.41, 30.27, 28.93, 28.64, 28.62, 27.46, 20.41. IR(KBr) 2922, 2360, 2341, 1734, 1653, 1559, 1457, 1260 cm^{-1}. HRMS: calcd. $C_{12}H_{19}O$ $[M+H]^+$: 179.1430. Found: 179.1424.

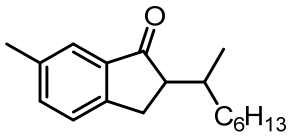


4,4-dimethyl-2-(octan-2-yl)cyclopentan-1-one 4a:[11] Synthesized from 3,3-dimethylcyclopentanone and 1-octene by following general procedure A and further treated with 0.5 mL of HCl (6 M) and 0.5 mL of toluene at 110 ^{o}C for 1 h on a 0.2 mmol scale of **L1**. 18 mg obtained. TON (based on iridium) = 20. Isolated as a mixture with dr: 1.3:1. Colorless liquid. R_f = 0.4 (Hex:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.48 – 2.40 (m, 0.56H), 2.35 – 2.29 (m, 0.44H), 2.17 – 1.87 (m, 3H), 1.85 – 1.68 (m, 1H), 1.62 – 1.56 (m, 1H), 1.35 – 1.13 (m, 13H), 1.05 – 1.00 (m, 3H), 0.93 (d, *J* = 6.9 Hz, 1.3H), 0.91 – 0.84 (m, 3H), 0.74 (d, *J* = 6.8 Hz, 1.7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.87, 221.23, 54.59, 54.55, 53.80, 52.39, 39.47, 37.67, 35.24, 33.64, 33.63, 33.21, 33.04, 32.09, 31.85, 29.85, 29.83, 29.51, 29.40, 27.73, 27.64, 27.54, 27.26, 22.66, 22.64, 17.84, 15.38, 14.09.

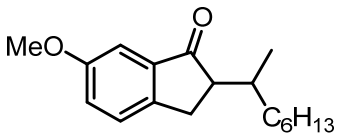


2-(octan-2-yl)-2,3-dihydro-1H-inden-1-one 4b: Synthesized from 1-indanone and 1-octene by following general procedure B on a 0.2 mmol scale of **L1**. 31 mg obtained. TON (based on iridium) = 32. Or synthesized from 1-indanone and 1-octene by following general procedure D on a 0.2 mmol scale of 1-indanone. Yield = 43%. Isolated as a mixture with dr: 2.1:1. Colorless liquid. R_f = 0.5 (Hex:Et_2O=10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 – 7.72 (m, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 – 7.44 (m, 1H), 7.35 (t, *J* = 7.4 Hz, 1H), 3.18 (dd, *J* = 17.4, 8.1 Hz, 0.38H), 3.09 (dd, *J* = 17.4, 8.1 Hz, 0.62H), 2.96 – 2.89 (m, 1H), 2.78 (dt, *J* = 8.1, 4.0 Hz, 0.62H), 2.70 (dt, *J* = 8.2, 4.1 Hz, 0.38H), 2.37 – 2.29 (m, 0.62H), 2.23 – 2.15 (m, 0.38H), 1.42 – 1.11 (m, 10H), 1.00 (d, *J* = 6.9 Hz, 1.14H), 0.93 – 0.81

(m, 3H), 0.70 (d, J = 6.8 Hz, 1.86H). ^{13}C NMR (101 MHz,$CDCl_3$) δ 209.42, 208.84, 154.37, 154.14, 137.77, 137.72, 134.49, 134.45, 127.17, 126.49, 126.45, 123.58, 123.55, 52.89, 51.51, 35.39, 34.37, 33.46, 32.22, 31.86, 31.81, 29.42, 29.15, 27.59, 27.52, 27.35, 22.65, 22.59, 17.74, 14.58, 14.10, 14.06. IR(KBr) 2956, 2925, 2854, 1712, 1609, 1464, 1281 cm^{-1}. HRMS: calcd. $C_{17}H_{25}O$ $[M+H]^+$: 245.1900. Found: 245.1905.

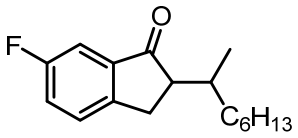


6-methyl-2-(octan-2-yl)-2,3-dihydro-1H-inden-1-one 4c: Synthesized from 6-methyl-1-indanone and 1-octene by following general procedure B on a 0.2 mmol scale of **L1**. 30 mg obtained. TON (based on iridium) = 29. Or synthesized from 6-methyl-1-indanone and 1-octene by following general procedure D on a 0.2 mmol scale of 6-methyl-1-indanone. Yield = 41%. Isolated as a mixture with dr: 1.5:1. Colorless liquid. R_f = 0.5 (Hex:EtOAc=10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.51 (m, 1H), 7.41 – 7.38 (m, 1H), 7.37 – 7.33 (m, 1H), 3.12 (dd, J = 17.2, 8.1 Hz, 0.4H), 3.04 (dd, J = 17.2, 8.0 Hz, 0.6H), 2.89 (t, J = 3.3 Hz, 0.6H), 2.85 (t, J = 3.4 Hz, 0.4H), 2.77 (dt, J = 8.0, 4.0 Hz, 0.6H), 2.69 (dt, J = 8.0, 4.0 Hz, 0.4H), 2.40 (s, 3H), 2.35 – 2.28 (m, 0.6H), 2.24 – 2.14 (m, 0.4H), 1.41 – 1.13 (m, 11H), 0.99 (d, J = 6.9 Hz, 1.2H), 0.88 (t, J = 7.0 Hz, 1.8H), 0.84 (t, J = 7.0 Hz, 1.2H), 0.69 (d, J = 6.8 Hz, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 209.52, 208.94, 151.74, 151.50, 137.94, 137.89, 137.06, 135.76, 135.71, 126.15, 126.11, 123.51, 123.49, 53.24, 51.84, 35.40, 34.40, 33.49, 32.18, 31.87, 31.81, 29.43, 28.76, 27.61, 27.36, 27.13, 22.65, 22.60, 21.06, 17.74, 14.55, 14.10, 14.06. IR(KBr) 2956, 2926, 2855, 1710, 1617, 1492, 1458, 1282, 1156 cm^{-1}. HRMS: calcd. $C_{18}H_{26}O$ $[M]^+$: 258.1984. Found: 258.1985.

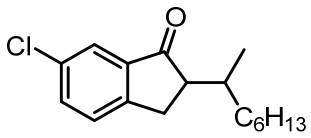


6-methoxy-2-(octan-2-yl)-2,3-dihydro-1H-inden-1-one 4d: Synthesized from 6-methoxyl-1-indanone and 1-octene by following general procedure B on a 0.2 mmol scale of **L1**. 30 mg obtained. TON (based on iridium) = 27. Isolated as a mixture with dr: 1.3:1. Colorless liquid. R_f = 0.25 (Hex:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.33 (m, 1H), 7.19 – 7.15 (m, 2H), 3.83 (s, 3H), 3.09 (dd, J = 17.0, 7.9 Hz, 0.4H), 3.01 (dd, J = 16.8, 7.7 Hz, 0.6H), 2.89 – 2.68 (m, 2H), 2.34 – 2.28 (m, 0.6H), 2.23 – 2.16

(m, 0.4H), 1.38 – 1.12 (m, 10H), 0.99 (d, J = 7.0 Hz, 1.2H), 0.88 (t, , J = 6.7 Hz, 1.8H), 0.84 (t, J = 6.9 Hz, 1.2H), 0.69 (d, J = 6.7 Hz, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 209.40, 208.82, 159.26, 147.21, 146.96, 138.88, 138.83, 127.17, 127.14, 123.95, 123.88, 104.70, 55.56, 53.73, 52.34, 35.38, 34.45, 33.56, 32.16, 31.86, 31.81, 29.42, 28.42, 27.60, 27.36, 26.81, 22.65, 22.59, 17.74, 14.54, 14.09, 14.05. IR(KBr) 2956, 2926, 2854, 1708, 1492, 1465, 1299, 1276, 1029 cm^{-1}. HRMS: calcd. $C_{18}H_{26}O_2$ $[M]^+$: 274.1933. Found: 274.1944.

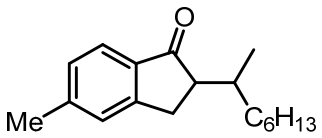


6-fluoro-2-(octan-2-yl)-2,3-dihydro-1H-inden-1-one 4e: Synthesized from 6-fluoro-1-indanone and 1-octene by following general procedure B on a 0.2 mmol scale of **L1**. 23 mg obtained. TON (based on iridium) = 22. Or synthesized from 6-fluoro-1-indanone and 1-octene by following general procedure D on a 0.2 mmol scale of 6-fluoro-1-indanone. Yield = 32%. Isolated as a mixture with dr: 2:1. Colorless liquid. R_f = 0.5 (Hex:Et_2O=10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 1H), 7.41 – 7.34 (m, 1H), 7.34 – 7.26 (m, 1H), 3.14 (dd, J = 17.2, 8.0 Hz, 0.35H), 3.06 (dd, J = 17.1, 8.0 Hz, 0.65H), 2.92 – 2.85 (m, 1H), 2.82 (dt, J = 8.0, 4.0 Hz, 0.63H), 2.75 (dt, J = 8.1, 4.0 Hz, 0.34H), 2.35 – 2.27 (m, 0.66H), 2.23 – 2.15 (m, 0.33H), 1.40 – 1.13 (m, 10H), 0.99 (d, J = 7.0 Hz, 1H), 0.92 – 0.82 (m, 3H), 0.70 (d, J = 6.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.39, 208.36, 207.80, 207.78, 163.45, 161.00, 160.99, 149.68, 149.66, 149.44, 149.42, 139.48, 139.42, 139.41, 139.35, 127.85, 127.81, 127.77, 127.73, 122.28, 122.24, 122.05, 122.00, 109.45, 109.43, 109.24, 109.22, 53.77, 52.46, 35.28, 34.47, 33.56, 32.29, 31.85, 31.79, 29.39, 28.67, 27.56, 27.33, 27.03, 22.64, 22.59, 17.64, 14.61, 14.09, 14.05. IR(KBr) 2957, 2927, 2855, 1714, 1486, 1466, 1290, 1264 cm^{-1}. HRMS: calcd. $C_{17}H_{24}FO$ $[M+H]^+$: 263.1806. Found: 263.1802.

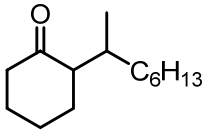


6-chloro-2-(octan-2-yl)-2,3-dihydro-1H-inden-1-one 4f: Synthesized from 6-chloro-1-indanone and 1-octene by following general procedure B on a 0.2 mmol scale of **L1**. 31 mg obtained. TON (based on iridium) = 28. Isolated as a mixture with dr: 1.5:1. Colorless liquid. R_f = 0.4 (Hex:Et_2O=10:1). ^{1}H NMR

(500 MHz, $CDCl_3$) δ 7.66 – 7.63 (m, 1H), 7.58 – 7.56 (m, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 3.18 (dd, *J* = 17.9, 8.2 Hz, 0.4H), 3.09 (dd, *J* = 17.9, 8.1 Hz, 0.6H), 2.92 – 2.85 (m, 1H), 2.81 (dt, *J* = 8.1, 4.0 Hz, 0.6H), 2.73 (dt, *J* = 8.2, 4.1 Hz, 0.4H), 2.39 – 2.29 (m, 0.6H), 2.25 – 2.18 (m, 0.4H), 1.42 – 1.16 (m, 10H), 1.02 (d, *J* = 6.9 Hz, 1.2H), 0.93 – 0.80 (m, 3H), 0.71 (d, *J* = 6.8 Hz, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.39, 207.80, 151.88, 151.66, 139.65, 139.60, 134.15, 134.12, 132.82, 132.77, 128.80, 121.85, 121.83, 52.88, 51.53, 35.28, 34.42, 33.54, 32.25, 31.86, 31.79, 29.39, 28.28, 27.56, 27.35, 26.69, 22.65, 22.59, 17.66, 14.61, 14.09, 14.05. IR(KBr) 2957, 2926, 2855, 1718, 1599, 1460, 1260, 1130 cm^{-1}. HRMS: calcd. $C_{17}H_{24}ClO$ $[M+H]^+$: 279.1510. Found: 279.1505.

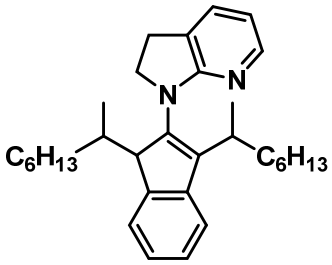


5-methyl-2-(octan-2-yl)-2,3-dihydro-1H-inden-1-one 4g: Synthesized from 5-methyl-1-indanone and 1-octene by following general procedure B on a 0.2 mmol scale of **L1**. 25 mg obtained. TON (based on iridium) = 24. Or synthesized from 5-methyl-1-indanone and 1-octene by following general procedure D on a 0.2 mmol scale of 5-methyl-1-indanone. Yield = 36%. Isolated as a mixture with dr: 1.5:1. Colorless liquid. R_f = 0.3 (Hex:Et_2O=10:1). ^1H NMR (500 MHz, $CDCl_3$) δ 7.66 – 7.60 (m, 1H), 7.27 – 7.25 (m, 1H), 7.16 (d, *J* = 7.8 Hz, 1H), 3.11 (dd, *J* = 17.4, 8.1 Hz, 0.4H), 3.03 (dd, *J* = 17.3, 8.1 Hz, 0.6H), 2.92 – 2.83 (m, 1H), 2.76 (dt, *J* = 8.0, 4.0 Hz, 0.6H), 2.68 (dt, *J* = 8.1, 4.0 Hz, 0.4H), 2.43 (s, 3H), 2.35 – 2.26 (m, 0.6H), 2.24 – 2.15 (m, 0.4H), 1.41 – 1.10 (m, 10H), 0.99 (d, *J* = 6.9 Hz, 1.2H), 0.92 – 0.81 (m, 3H), 0.69 (d, *J* = 6.8 Hz, 1.8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.90, 208.33, 154.90, 154.66, 145.61, 145.55, 135.57, 135.52, 128.46, 126.82, 126.78, 123.41, 123.39, 53.02, 51.62, 35.42, 34.38, 33.47, 32.14, 31.87, 31.82, 29.44, 28.94, 27.61, 27.37, 27.34, 22.66, 22.60, 22.05, 17.76, 14.51, 14.10, 14.06. IR(KBr) 2956, 2925, 2855, 1709, 1611, 1460, 1325, 1278 cm^{-1}. HRMS: calcd. $C_{18}H_{27}O$ $[M+H]^+$: 259.2056. Found: 259.2059.



2-(octan-2-yl)cyclohexan-1-one 4h:[11] Synthesized from cyclohexanone and 1-octene by following general procedure A on a 0.2 mmol scale of **L1**, and followed with hydrolysis with 0.5 mL of toluene

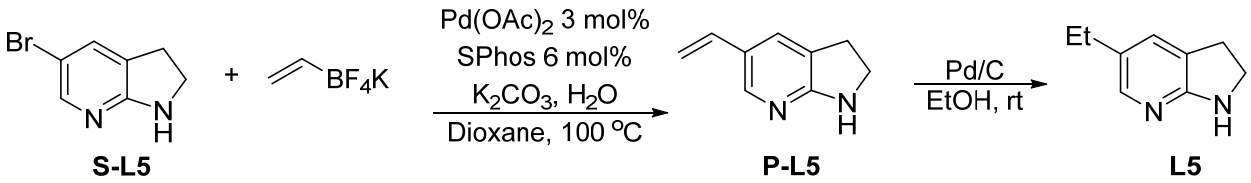
and 0.5 mL of HCl (6 M) at 110 °C for 1 h. 12 mg obtained. TON (based on iridium) = 14. Isolated as a mixture with dr: 1.3:1. Colorless liquid. R_f = 0.32 (Hex:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.41 – 2.33 (m, 1H), 2.30 – 2.10 (m, 2H), 2.08 – 1.82 (m, 4H), 1.78 – 1.60 (m, 2H), 1.58 – 1.48 (m, 1H), 1.42 – 1.00 (m, 10H), 0.90 – 0.80 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 213.40, 213.34, 56.41, 55.28, 42.07, 42.02, 34.83, 33.13, 31.90, 31.87, 31.36, 30.73, 29.63, 29.49, 29.18, 27.94, 27.75, 27.57, 27.34, 27.17, 24.50, 24.30, 22.68, 22.66, 17.47, 16.02, 14.10.



1-(1,3-di(octan-2-yl)-1H-inden-2-yl)-2,3-dihydro-1H-pyrrolo[2,3-b]pyridine 6: Synthesized from 1-(1H-inden-2-yl)-2,3-dihydro-1H-pyrrolo[2,3-b]pyridine **5** and 1-octene with the following procedure: A 4-mL vial charged with a stir bar and **5** (46.8 mg, 0.2 mmol) was loosely capped and was transferred into a glove box. Another 4-mL vial charged with a stir bar and *rac*-BINAP (6.2 mg, 0.01 mmol) was loosely capped and was transferred into the glove box. To this vial was added [Ir(COD)$_2$]BArF (12.7 mg, 0.01 mmol) and 0.2 mL of toluene. This mixture was stirred for 10 min at 50 °C before it was transferred to the first vial. The vial was tightly capped, removed from the glove box and heated at 130 °C for 48 h. After the completion of the reaction, the mixture was cooled to room temperature, diluted with ethyl acetate and passed through a short pad of silica gel. After concentration in vacuum, the crude mixture was subjected to ^{1}H NMR to determine the dr ratio and the NMR yield by using tetrachloroethane as internal standard. The crude mixture was then subjected to flash chromatography (silica gel, Hexane/Et_2O=25:1 to 10:1) to give the desired products. Three major diastereomers were observed with a 1.2:1.1:1 ratio. Two of them were isolated and characterized. **diastereomer 1**: Light yellow liquid. 21 mg, R_f = 0.40 (Hex:Et_2O=20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 5.2 Hz, 1H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 7.4 Hz, 1H), 7.24 (d, *J* = 7.0 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.51 – 6.45 (m, 1H), 4.43 (d, *J* = 2.6 Hz, 1H), 4.17 (td, *J* = 9.9, 6.8 Hz, 1H), 3.74 (q, *J* = 9.0 Hz, 1H), 3.22 – 3.06 (m, 2H), 2.98 – 2.88 (m, 1H), 1.94 – 1.71 (m, 3H), 1.69 – 1.60 (m, 1H), 1.50 – 1.15 (m, 20H), 0.90 – 0.83 (m, 6H), 0.43 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.92, 146.27, 144.08, 143.39, 143.35, 138.50, 131.06, 125.61, 123.94, 123.42, 122.42, 120.60, 112.92, 51.55, 50.29,

36.13, 34.92, 33.27, 32.56, 31.88, 31.87, 29.70, 29.30, 28.67, 27.71, 26.50, 22.67, 22.66, 19.05, 14.60, 14.11, 14.09. IR(KBr) 2956, 2927, 2855, 1605, 1486, 1461, 1433, 1378, 1325, 1248 cm^{-1}. HRMS: calcd. $C_{32}H_{47}N_2$ $[M+H]^+$: 459.3734. Found: 459.3732. **diastereomer 2**: Light yellow liquid. 14 mg obtained. ^1H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.3, 1.5 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 7.4 Hz, 1H), 7.24 (d, *J* = 7.1 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.48 (dd, *J* = 7.0, 5.3 Hz, 1H), 4.30 (d, *J* = 2.7 Hz, 1H), 4.16 (td, *J* = 9.8, 7.3 Hz, 1H), 3.73 (td, *J* = 9.8, 6.9 Hz, 1H), 3.15 (qt, *J* = 15.6, 8.3 Hz, 2H), 2.92 (q, *J* = 7.3 Hz, 1H), 1.94 – 1.84 (m, 2H), 1.78 – 1.69 (m, 1H), 1.48 – 1.38 (m, 1H), 1.33 – 1.17 (m, 14H), 1.14 – 0.99 (m, 9H), 0.87 – 0.79 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.06, 146.30, 144.52, 143.62, 142.81, 139.43, 131.01, 125.55, 123.64, 123.62, 122.33, 120.66, 112.73, 52.32, 51.44, 34.96, 34.57, 32.55, 31.91, 31.82, 31.31, 29.75, 29.52, 28.71, 28.04, 26.48, 22.68, 22.61, 19.17, 18.58, 14.09, 14.04. IR(KBr) 2957, 2927, 2855, 1605, 1461, 1433, 1377, 1325 cm^{-1}. HRMS: calcd. $C_{32}H_{47}N_2$ $[M+H]^+$: 459.3734. Found: 459.3732.

Synthesis of 5-ethyl-2,3-dihydro-1H-pyrrolo[2,3-b]pyridine L5:

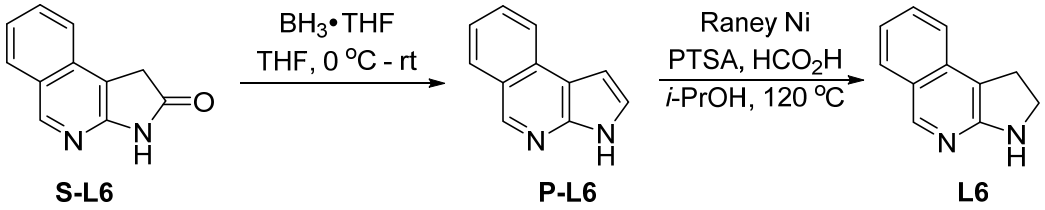


To a 20 mL vial with a stir bar was added $Pd(OAc)_2$ (33.6 mg, 0.15 mmol), SPhos (123 mg, 0.3 mmol), K_2CO_3 (1.38 g, 10 mmol), 5-bromo-2,3-dihydro-1H-pyrrolo[2,3-b]pyridine (**S-L5**) (1.0 g, 5 mmol), potassium vinyltrifluoroborate (1.0 g, 7.5 mmol), dioxane (6 mL) and H_2O (2 mL). The reaction mixture was heated at 100 °C for 3 h. The mixture was cooled to room temperature, passed through a short pad of Celite and further washed with EtOAc. The water layer of the filtrate was removed. The organic layer was dried and concentrated in vacuum. The obtained crude product **P-L5** was directly used for the next step.

The crude product **P-L5** obtained above was dissolved in 10 mL of EtOH and Pd/C (180 mg) was then added. The reaction mixture was stirred under 1 atm of H_2 (balloon) for 2 h. After completion, the reaction mixture as passed through a short pad of Celite and further washed with EtOH. After concentrated in vacuum, the crude mixture was subject to column chromatography (Hexane:EtOAc=1:1

to 0:1) to obtain the desired pure product (**L5**) as a light yellow solid. Yield for 2 steps: 68%. M.p. 114–116 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.12 (s, 1H), 4.42 (br, 1H), 3.57 (t, *J* = 8.3 Hz, 2H), 3.01 (tt, *J* = 8.4, 1.2 Hz, 2H), 2.46 (q, *J* = 7.6 Hz, 2H), 1.16 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.20, 144.39, 131.68, 128.90, 121.80, 44.63, 27.79, 25.56, 15.98. IR(KBr) 3201, 3166, 2958, 2926, 2360, 2341, 1592, 1512, 1436, 1408, 1263 cm^{-1}. HRMS: calcd. $C_9H_{13}N_2$ $[M+H]^+$: 149.1073. Found: 149.1074.

Synthesis of 2,3-dihydro-1H-pyrrolo[2,3-c]isoquinoline L6:



S-L6 **P-L6** **L6**

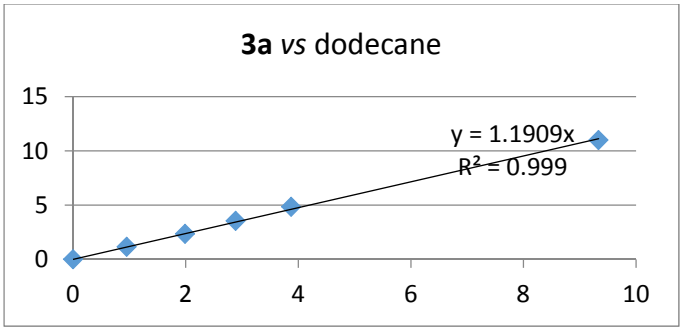
1,3-dihydro-2H-pyrrolo[2,3-c]isoquinolin-2-one (**S-L6**) was synthesized by following the literature procedure.[14] To a solution of 1,3-dihydro-2H-pyrrolo[2,3-c]isoquinolin-2-one (**S-L6**) (920 mg, 5.0 mmol) in 25 mL of THF at 0 °C was added a solution of BH_3/THF (1.0 M) (20 mL, 20 mmol). The reaction mixture was then warmed to room temperature and stirred for 2 h before 30 mL of 6 M HCl solution was added slowly. The resulted mixture was then stirred at 110 °C for another 2 h. After cooled to room temperature, aqueous NaOH solution (10%) was added till pH = 9. The resulting solution was extracted with EtOAc (50 mL × 3) and then dried over $MgSO_4$. The mixture was concentrated in vacuum and the crude product was purified by column chromatography (EtOAc:CH_2Cl_2=1:2 to 1:1) to give **P-L6** as the major product (470 mg, 56% yield) and **L6** as the minor product (85 mg, 10% yield).

To a solution of **P-L6** (340 mg, 2 mmol) in *i*PrOH (10 mL) was added Raney Nickel (3 mL of aqueous solution), PTSA (390 mg, 2.1 mmol) and HCO_2H (1.12 mL, 30 mmol). The reaction mixture was sealed and stirred at 120 °C for 12 h. The mixture was cooled to room temperature, passed through a short pad of Celite and washed with *i*PrOH. The filtrate was concentrated in vacuum and was further purified by column chromatography (EtOAc:CH_2Cl_2=1:2 to 1:1) to give **L6** as a yellow solid (163 mg, 48% yield). M.p. 118–120 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (s, 1H), 7.79 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.53 – 7.45 (m, 2H), 7.20 (ddd, *J* = 8.1, 6.5, 1.4 Hz, 1H), 4.38 (br, 1H), 3.77 (td, *J* = 8.7, 2.0 Hz, 2H), 3.33 (t, *J* = 8.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.97, 150.71, 134.59, 130.36, 128.67, 124.09, 122.26, 121.55,

110.75, 45.29, 26.75. IR(KBr) 3205, 2864, 1628, 1582, 1562, 1525, 1372, 1294, 1155 cm^{-1}. HRMS: calcd. $C_{11}H_{11}N_2$ $[M+H]^+$: 171.0917. Found: 171.0918.

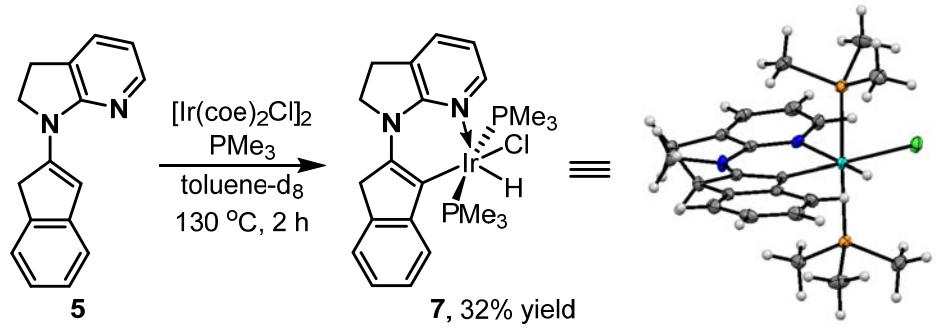
GC standard curve of **3a** with dodecane as the internal standard:

	m pro (mg)	m dode (mg)	Mole of pro	Mole of dode	Mole (dode) / Mole (pro)	GC area dode	GC area **5a** (dr 1)	GC area **5a** (dr 2)	y = area dode / area pro
0	0	0	0	0	0	0	0	0	0
1	10.3	8.5	0.052551	0.05	0.951456311	30240	10518.5	15773	1.150181618
2	10.2	17.6	0.0520408	0.1035294	1.989388697	56179	9573.6	14350.5	2.348217906
3	10.3	25.8	0.052551	0.1517647	2.887949743	73432	8299	12425	3.543331403
4	10.3	34.6	0.052551	0.2035294	3.872986865	83866	6935.5	10393	4.839772629
5	10.4	84.2	0.0530612	0.4952941	9.33438914	213650	7782	11653	10.99305377



3. Synthesis of the Ir–H Complex 7 and the X-Ray Data of 7

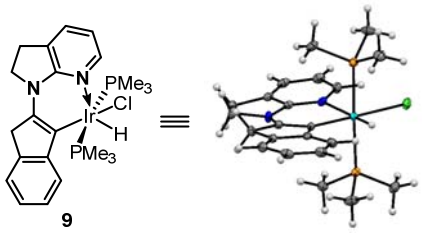
Synthesis of Ir–H complex 7:



Substrate **5** (12 mg, 0.05 mmol) and $[Ir(coe)_2Cl]_2$ (22.4 mg, 0.025 mmol, 0.5 equiv) were added to a J-Young tube in a glove box, followed by the addition of d_8-toluene (600 μL) and PMe_3 (7.6 mg, 10 μL, 0.1 mmol, 2 equiv). The J-Young tube was sealed and heated at 130 °C for 2 hours. After cooling, the reaction was subjected to ^1H NMR analysis, which showed about half conversion. The reaction mixture

was purified by flash chromatography (silica gel) in the glove box by using Hexane/Et_2O 3:1 to give 9 mg of desired product, yield 32%. Single crystal structure was obtained by dissolving the product in 500 μL of d_8-toluene in an NMR tube with slow evaporating in the glove box. ^{1}H NMR (500 MHz, Toluene-d_8) δ 9.60 (d, J = 5.9 Hz, 1H), 7.80 (d, J = 7.6 Hz, 1H), 7.38 (td, J = 7.5, 1.2 Hz, 1H), 7.25 (d, J = 7.1 Hz, 1H), 7.04 – 7.00 (m, 1H), 6.62 (dq, J = 6.8, 1.5 Hz, 1H), 6.06 (t, J = 6.5 Hz, 1H), 3.34 (t, J = 8.7 Hz, 2H), 3.11 (t, J = 2.7 Hz, 2H), 2.30 (t, J = 8.7 Hz, 2H), 1.11 (t, J = 3.5 Hz, 18H), –19.89 (t, J = 17.3 Hz, 1H).

X-Ray Data of 7:



9

Bond precision: C-C = 0.0040 A Wavelength=0.71073

Cell: a=12.8120(9) b=12.1811(8) c=15.4969(10)
alpha=90 beta=107.511(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2306.4(3)	2306.4(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H32 Cl Ir N2 P2	C22 H32 Cl Ir N2 P2
Sum formula	C22 H32 Cl Ir N2 P2	C22 H32 Cl Ir N2 P2
Mr	614.11	614.08
Dx,g cm-3	1.769	1.768
Z	4	4
Mu (mm-1)	6.054	6.054
F000	1208.0	1208.0
F000'	1204.13	
h,k,lmax	18,17,22	18,17,22
Nref	6972	6424
Tmin,Tmax	0.551,0.616	0.424,0.746
Tmin'	0.540	

Correction method= # Reported T Limits: Tmin=0.424 Tmax=0.746
AbsCorr = MULTI-SCAN

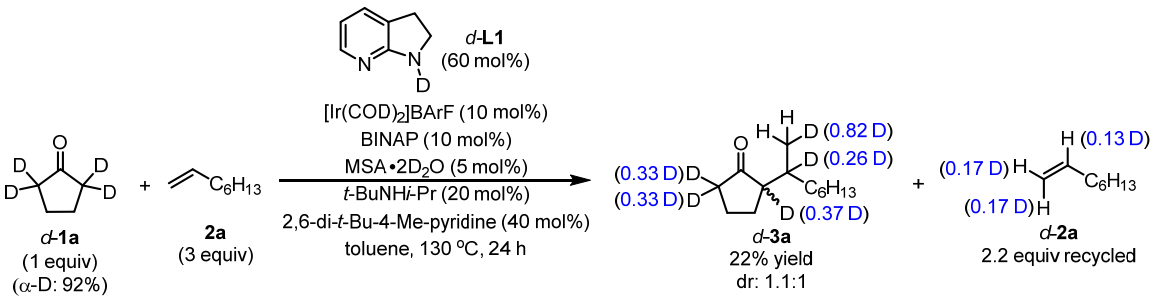
Data completeness= 0.921 Theta(max)= 30.396

R(reflections)= 0.0241(5793) wR2(reflections)= 0.0539(6424)

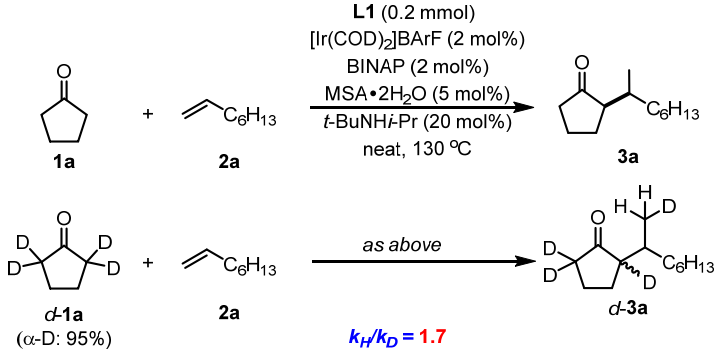
S = 1.064 Npar= 271

4. Deuterium experiments:

Deuterium experiment of *d*-1a and 2a:

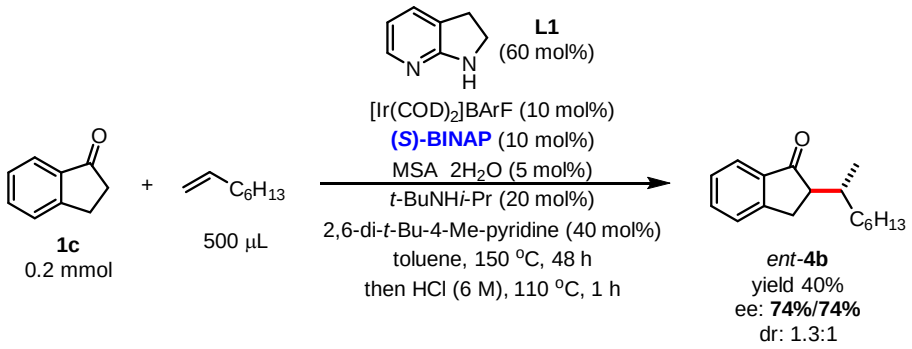


Side-by-side reactions using 1a and *d*-1a:



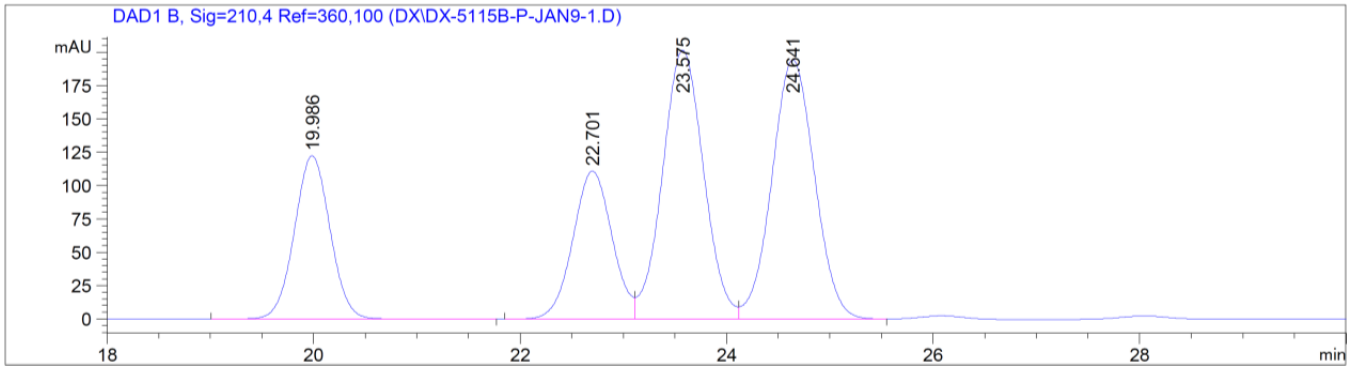
T (h)	internal standard (dodecane)	**3a** (peak 1)	**3a** (peak 2)	**3a**/IS	Internal standard (dodecane)	*d*-**3a** (peak 1)	*d*-**3a** (peak 2)	*d*-**3a**/IS	**3a**/*d*-**3a**
1	6644	10.6	20.7	0.004711017	0	0	0	0	0
2	6382	37	71	0.016922595	6619	22	43	0.00982	**1.723241**
4	7338	340	650	0.134914146	7434	203	385	0.079096	**1.7057**
6	7644	828	1392	0.290423862	7472	438	834	0.170236	**1.706012**
8	7747	1210	1924	0.404543694	7886	699	1319	0.255897	1.580888
10	9230	1838	2781	0.500433369	7490	875	1627	0.334045	1.4981
12	7925	1763	2589	0.549148265	7853	1137	2079	0.409525	1.340939
24	6764	2231	2912	0.760348906	6954	1737	2812	0.654156	1.162336

5. Enantioselective reaction [α-alkylation of 1-indanone by using (*S*)-BINAP]:



The enantio excess of compound ***ent*-4b** obtained by using (*S*)-BINAP as the ligand by following general procedure D was tested by chiral HPLC (Chiralpak IF, hexane:isopropanol = 99:1, 0.50 mL/min, 210 nm), first diastereomer: t_{minor} = 19.963 min, t_{major} = 22.637 min. at 74 % ee; second diastereomer: : t_{major} = 23.526 min, t_{minor} = 24.588 min.

Racemic 4b:

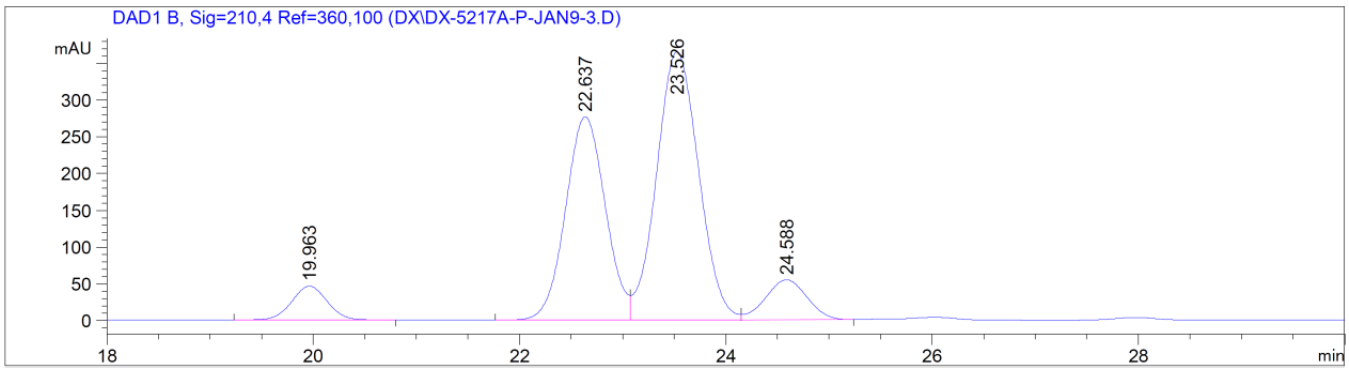



```
Signal 1: DAD1 B, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  19.986 BB    0.3744 2941.70923  122.37746  17.2767
   2  22.701 BV    0.4092 2923.59473  111.02409  17.1703
   3  23.575 VV    0.4327 5573.04932  201.51523  32.7305
   4  24.641 VB    0.4474 5588.71875  194.37410  32.8225

Totals :                 1.70271e4   629.29087
```

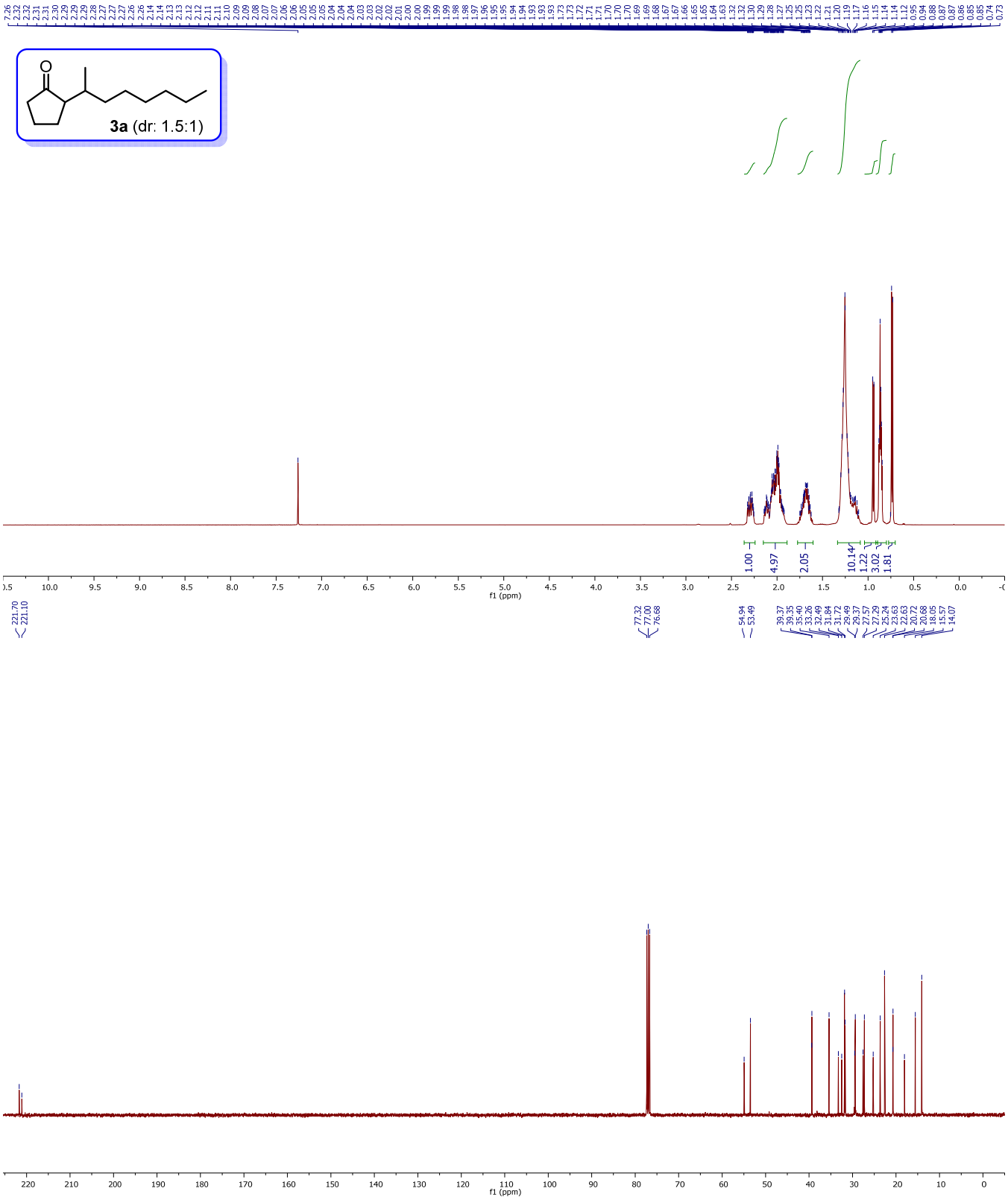
Enantiomeric 4b:

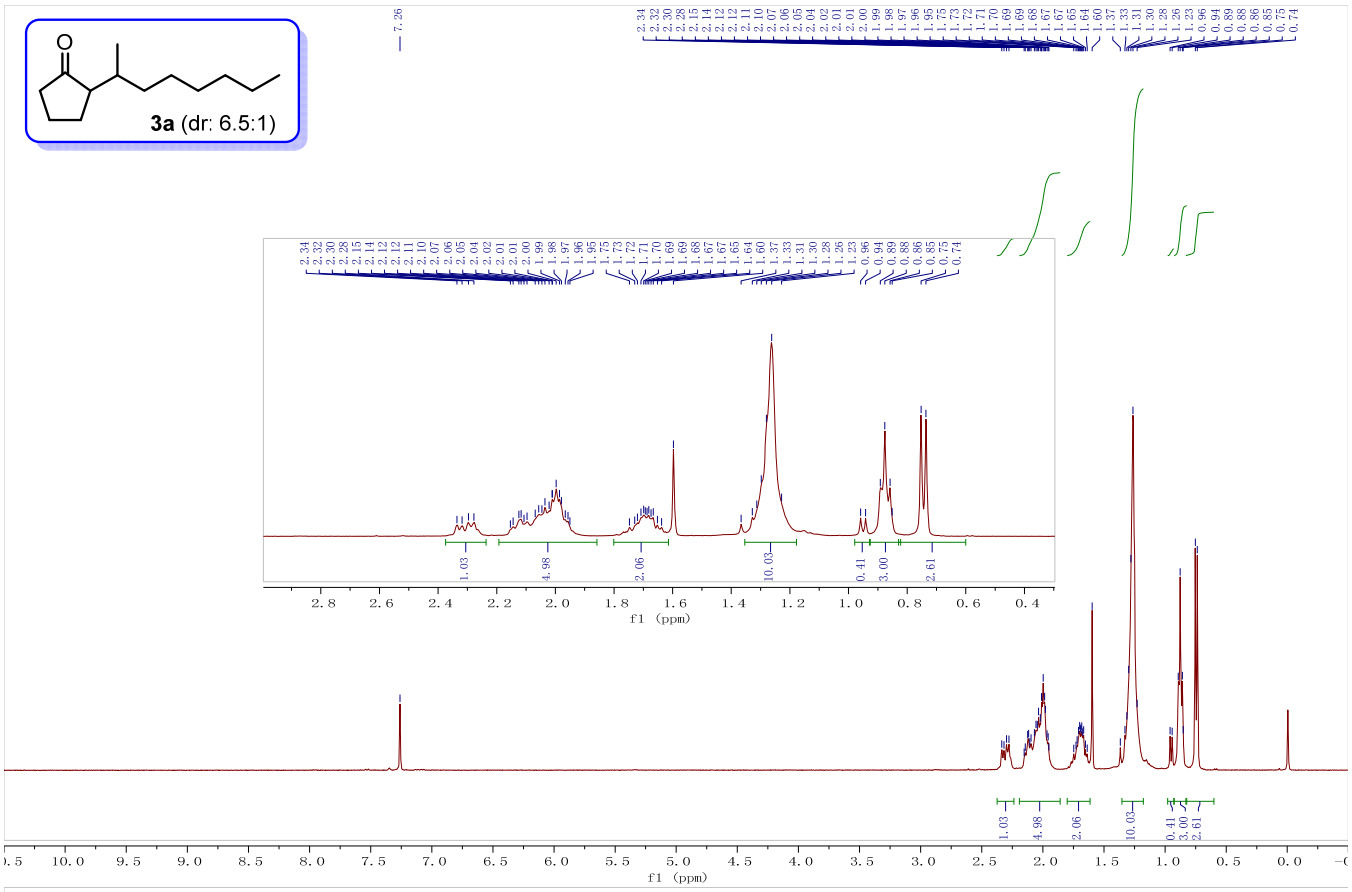


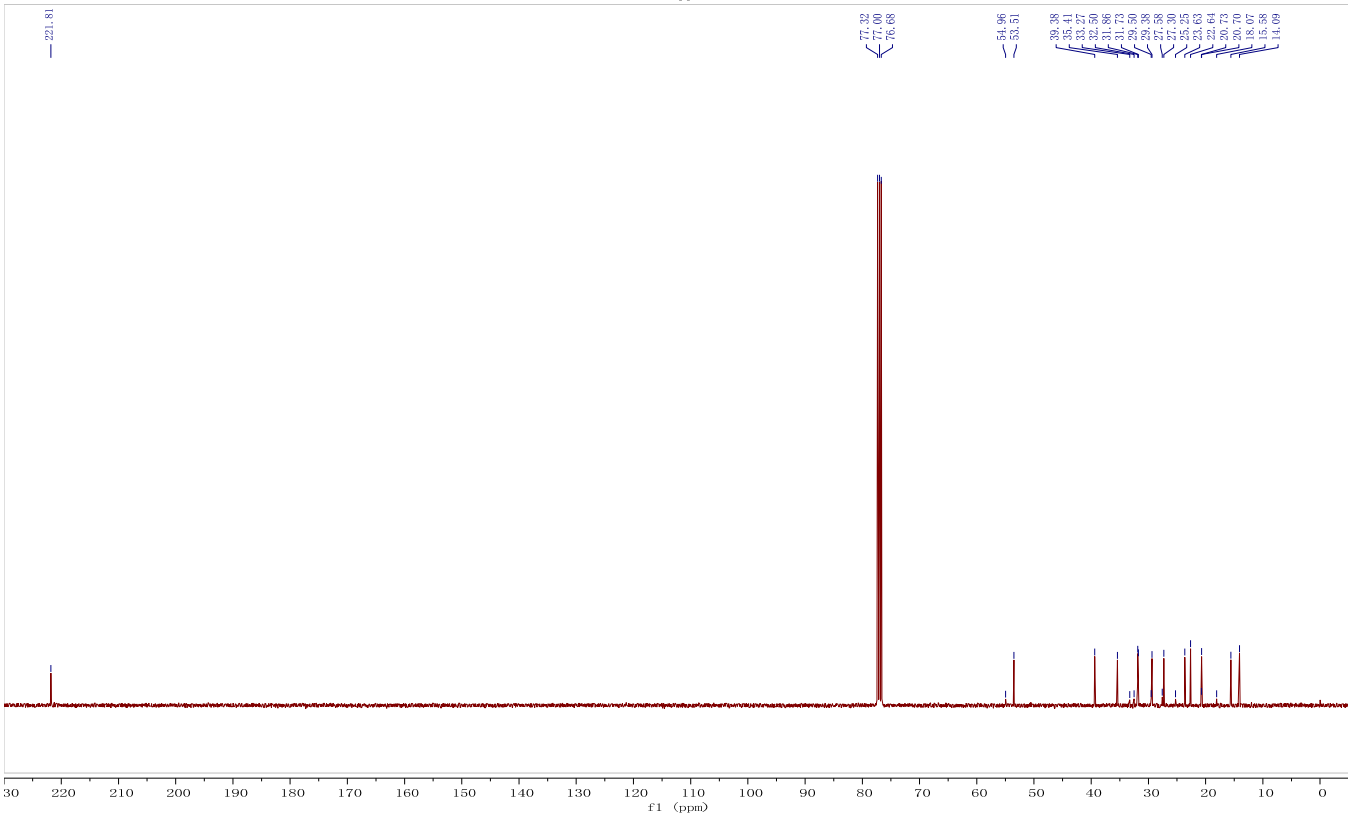
Signal 1: DAD1 B, Sig=210,4 Ref=360,100

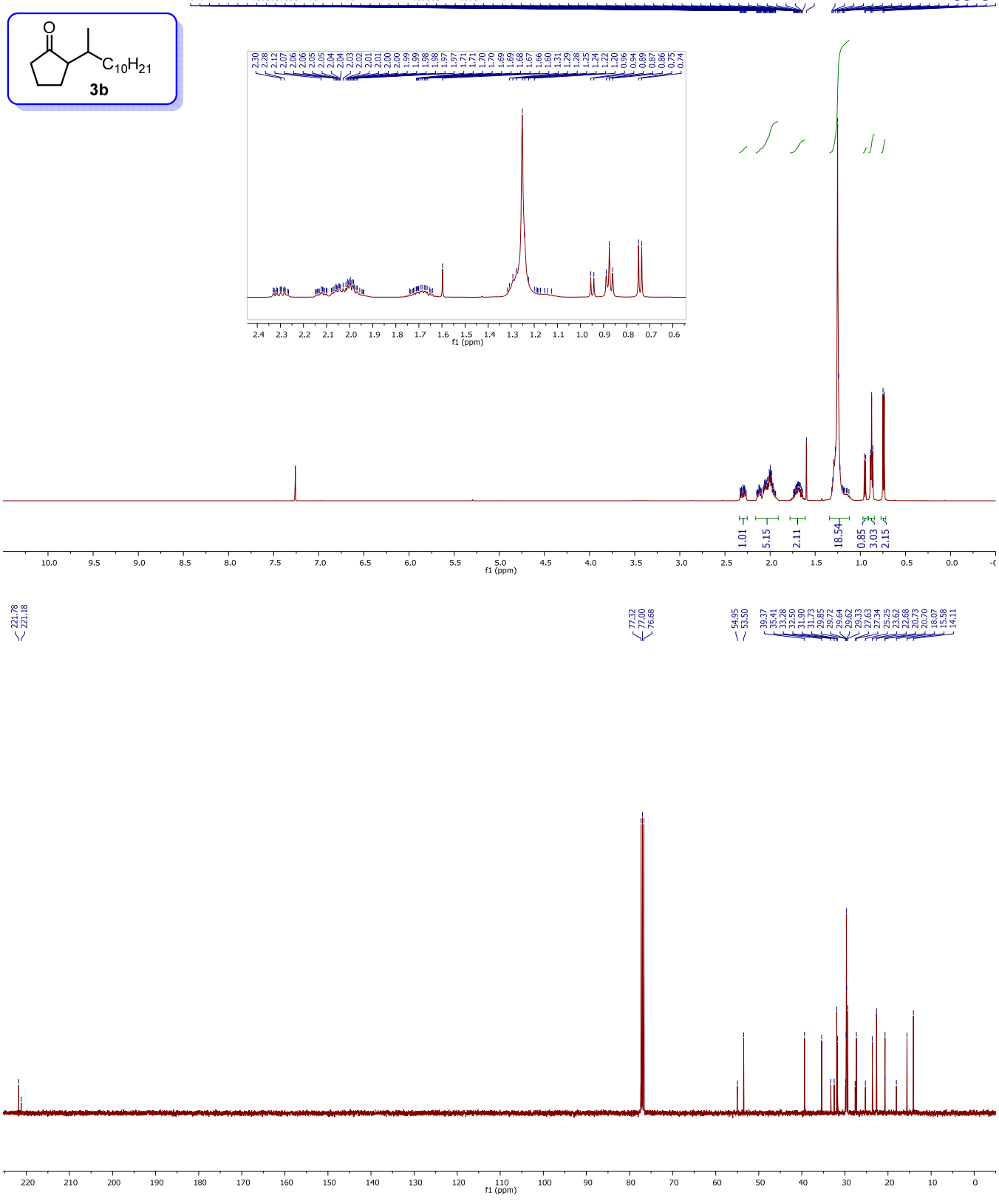
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.963	BB	0.3697	1093.43811	45.92932	5.3677
2	22.637	BV	0.4171	7422.47461	276.55185	36.4372
3	23.526	VV	0.4425	1.03397e4	364.94901	50.7581
4	24.588	VB	0.4358	1514.93445	54.25545	7.4369
Totals :				2.03706e4	741.68562	

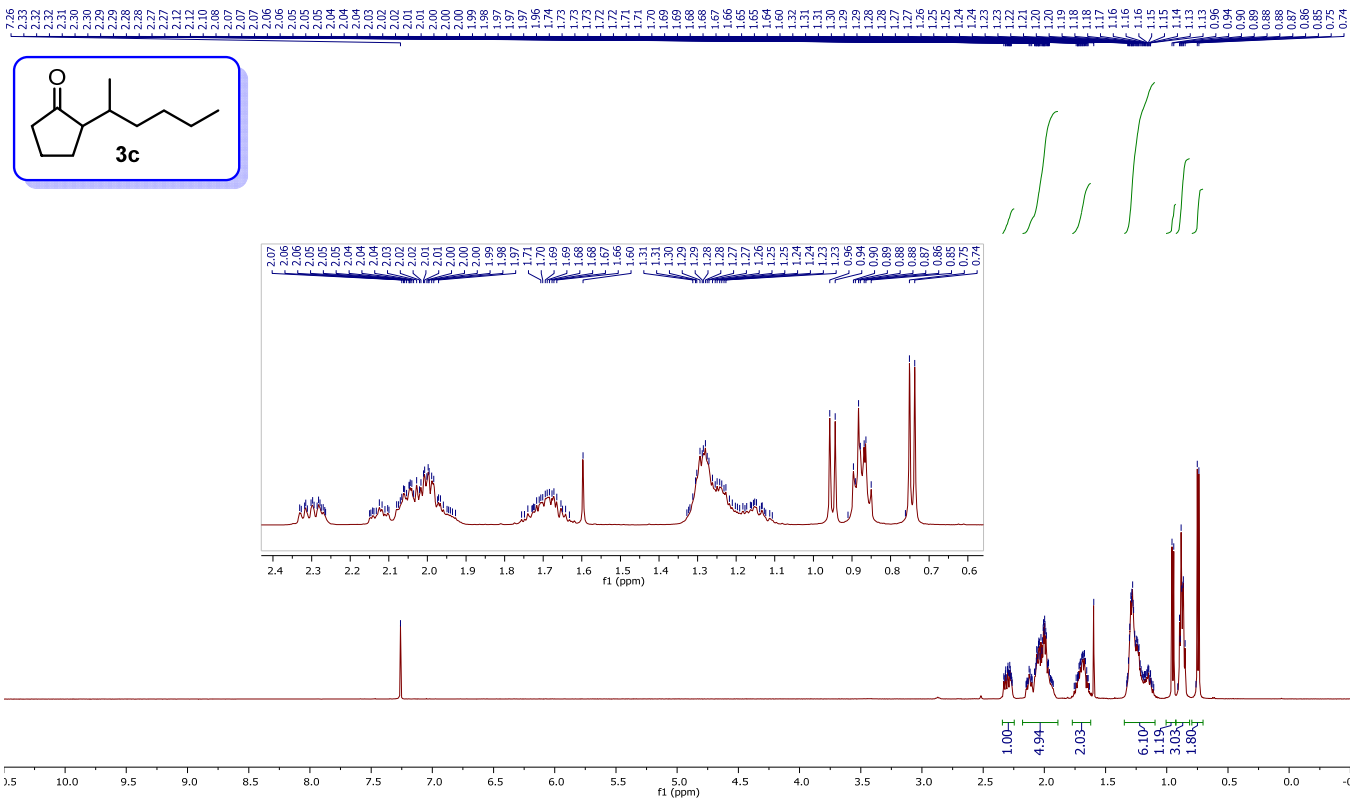
6. NMR Spectra

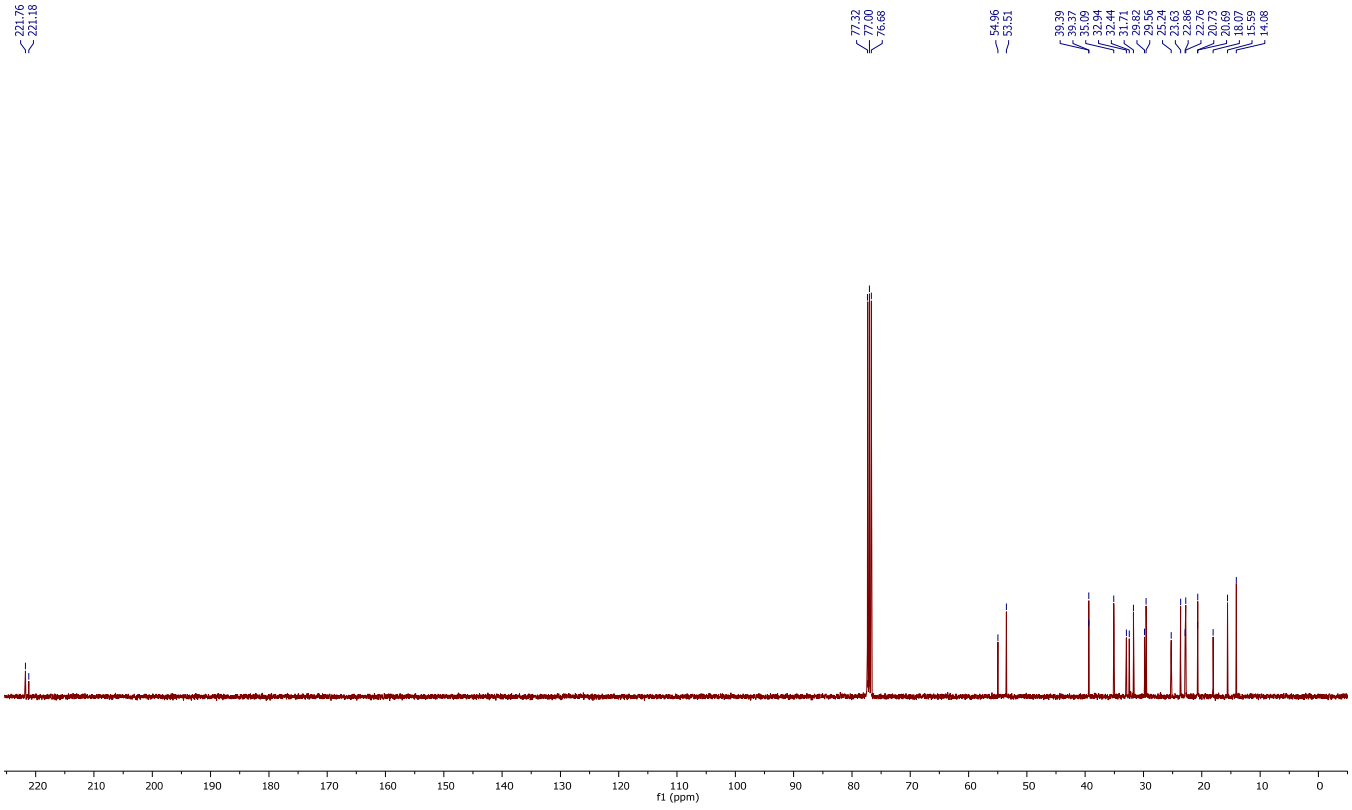


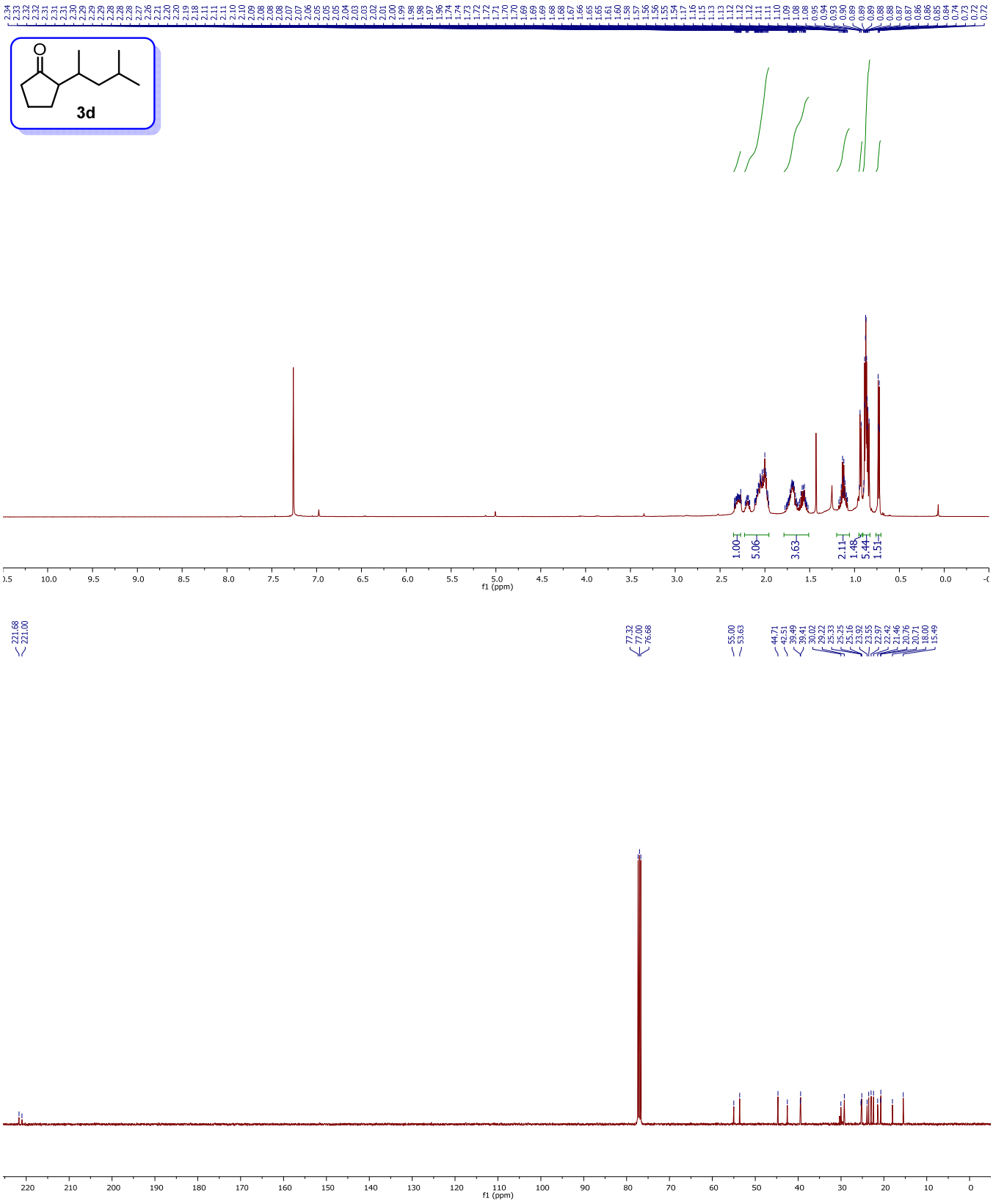

3a (dr: 6.5:1)
f1 (ppm)

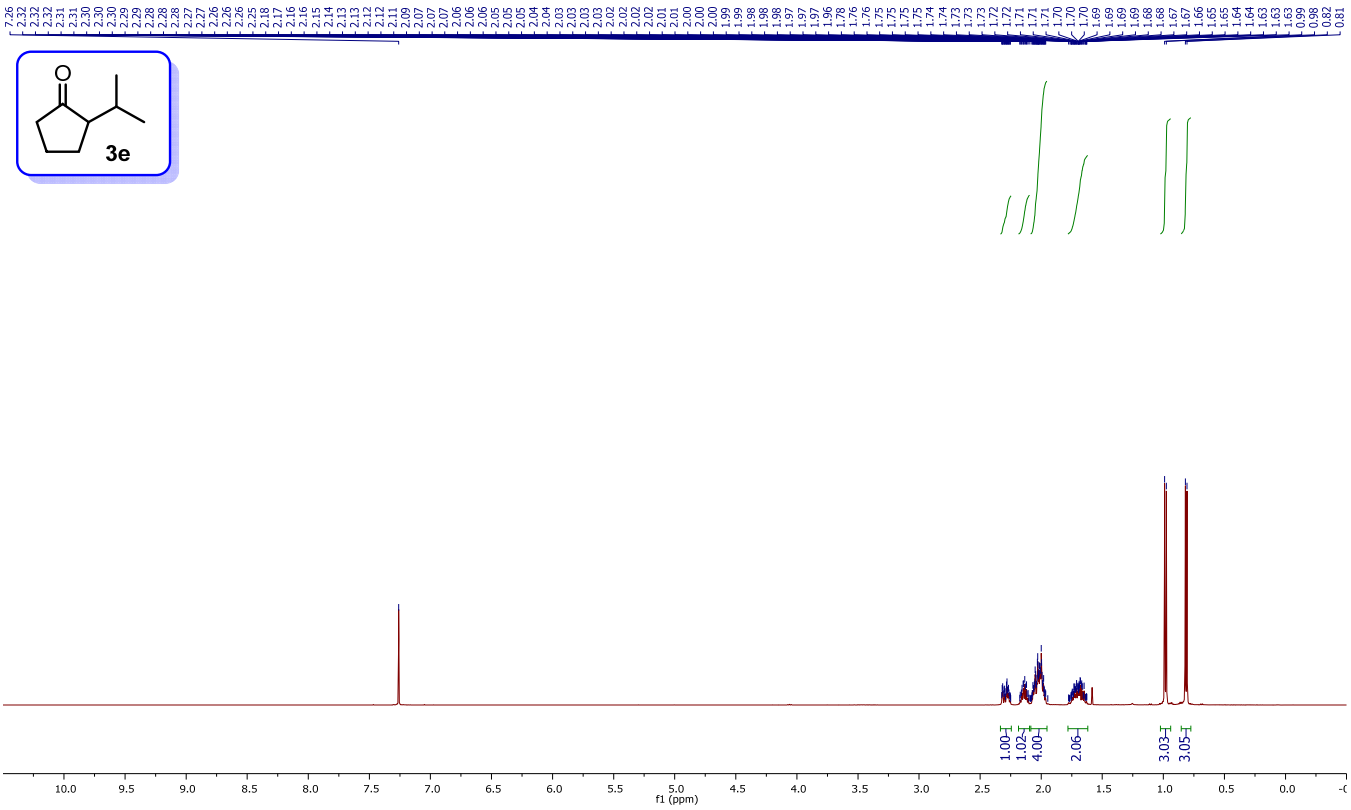

f1 (ppm)

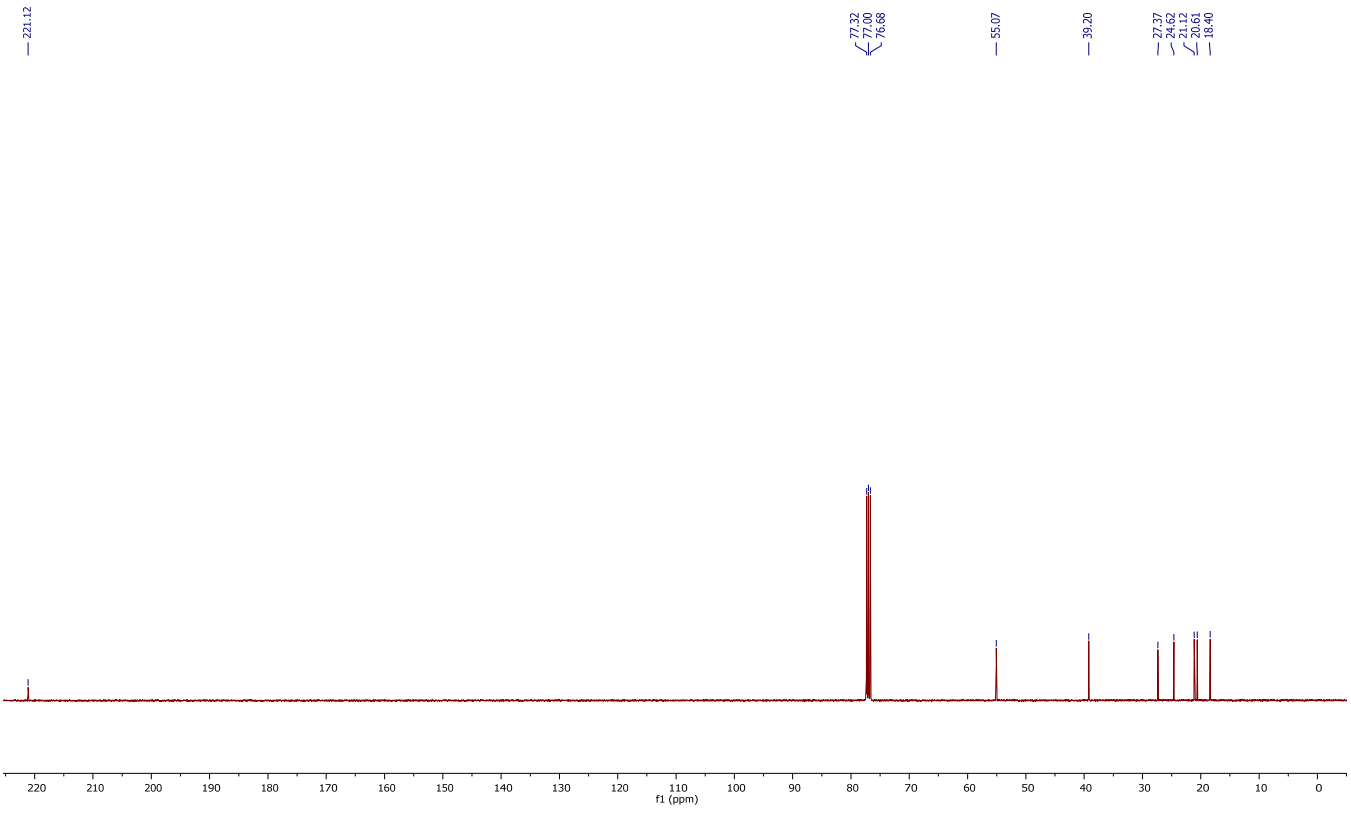

O
$C_{10}H_{21}$
3b
f1 (ppm)
1.01
5.15
2.11
18.54
0.85
3.03
2.15

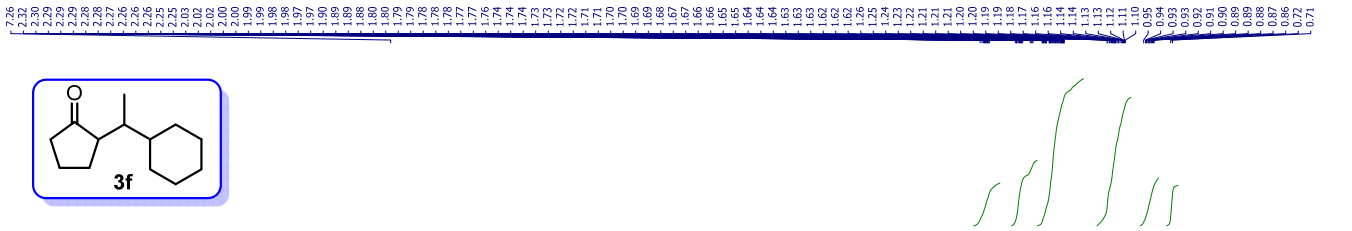

3c
f1 (ppm)
1.00
4.94
2.03
6.10
1.19
3.03
1.80


f1 (ppm)

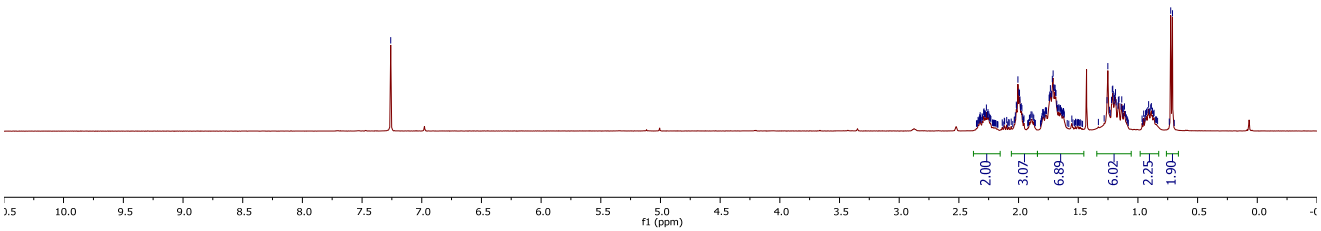

3d
1.00
5.06
3.63
2.11
1.48
5.44
1.51
f1 (ppm)
f1 (ppm)

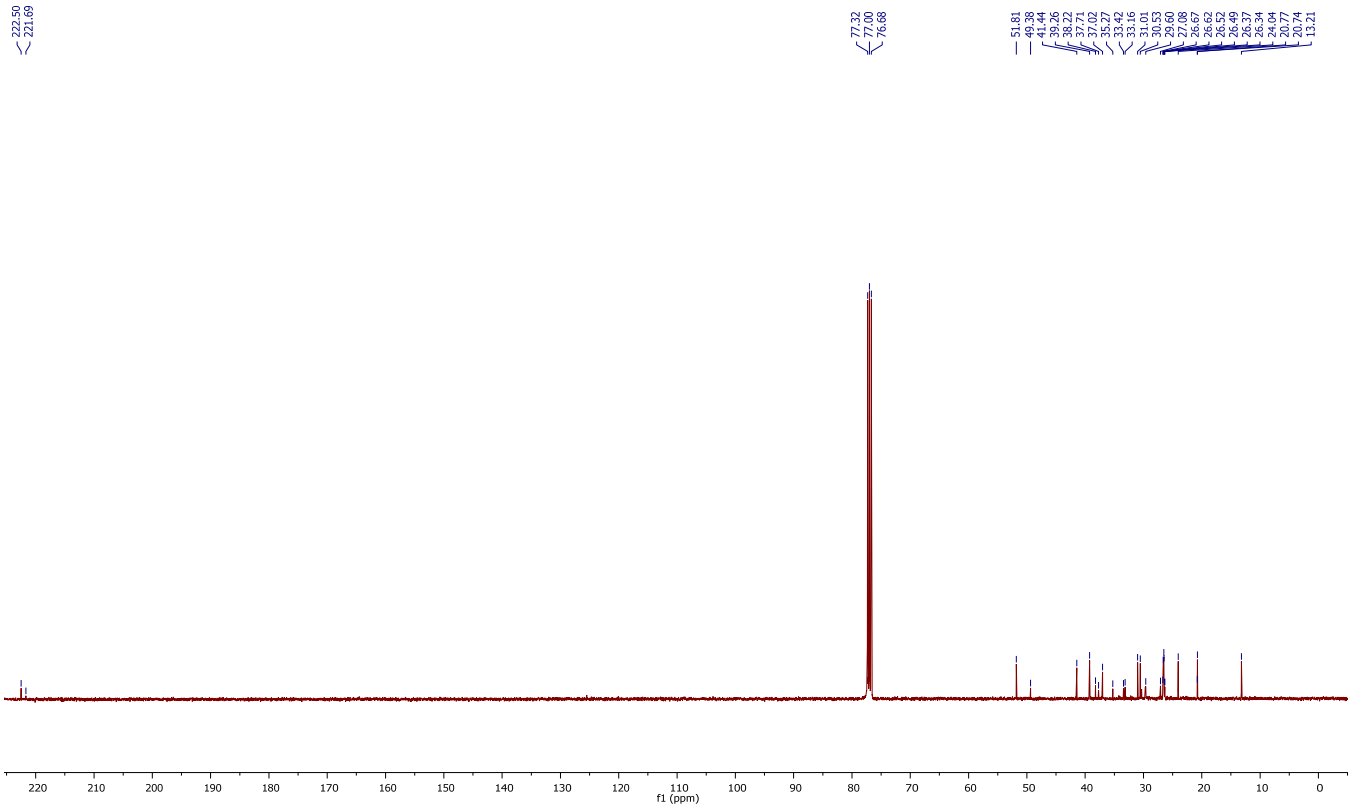

3e
1.00
1.02
4.00
2.06
3.03
3.05
f1 (ppm)

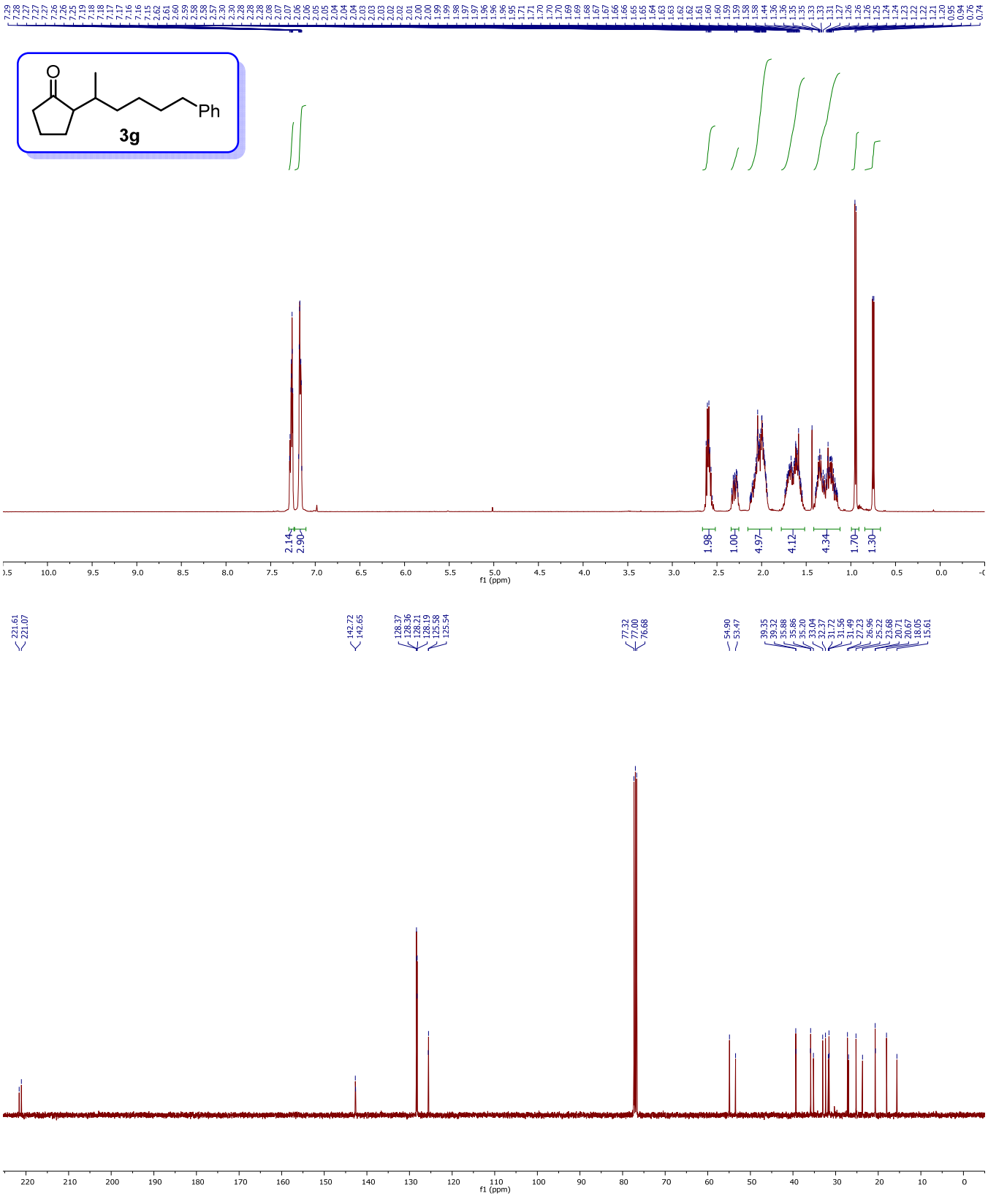

221.12
77.32
77.00
76.68
55.07
39.20
27.37
24.62
21.12
20.61
18.40
f1 (ppm)

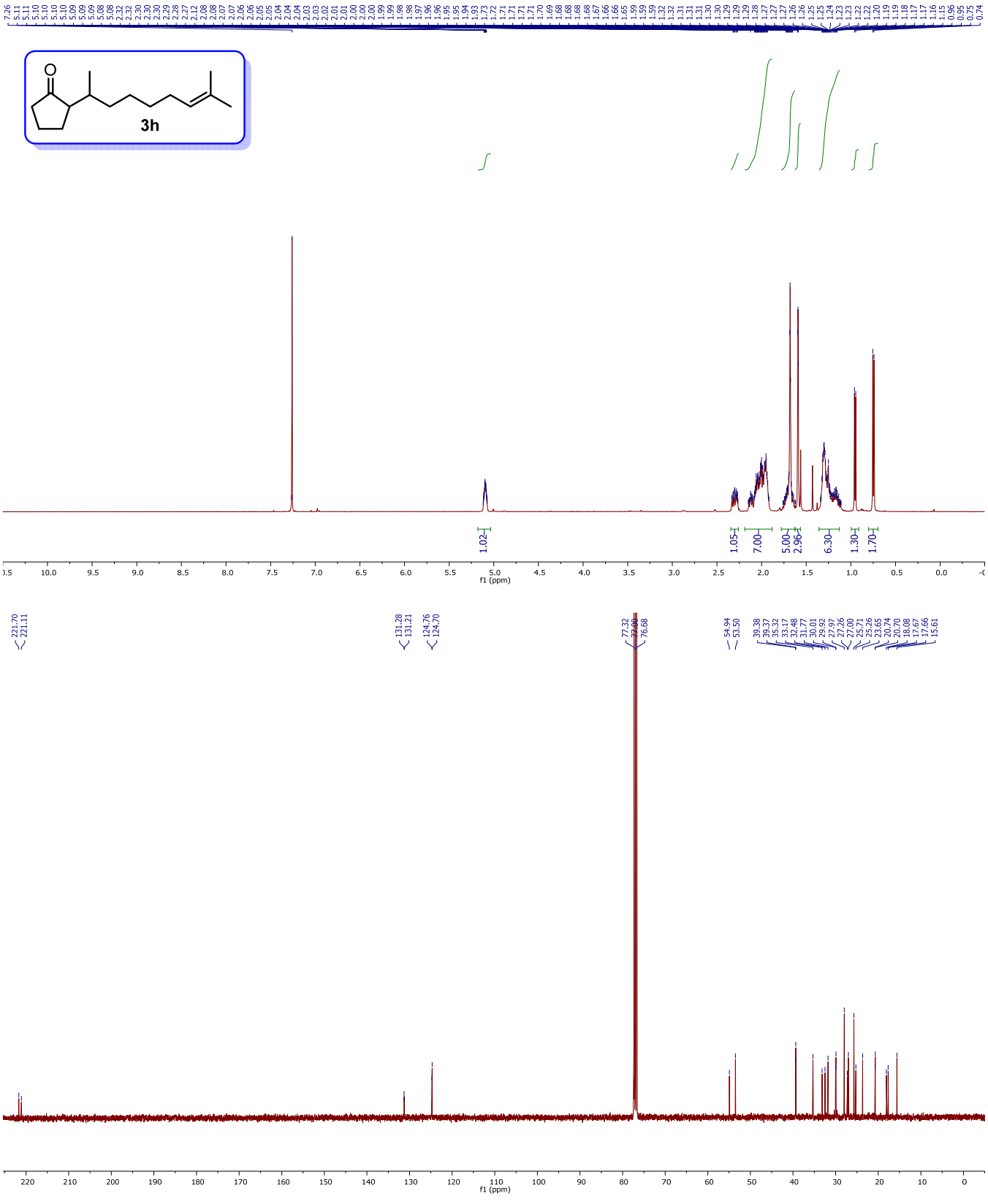


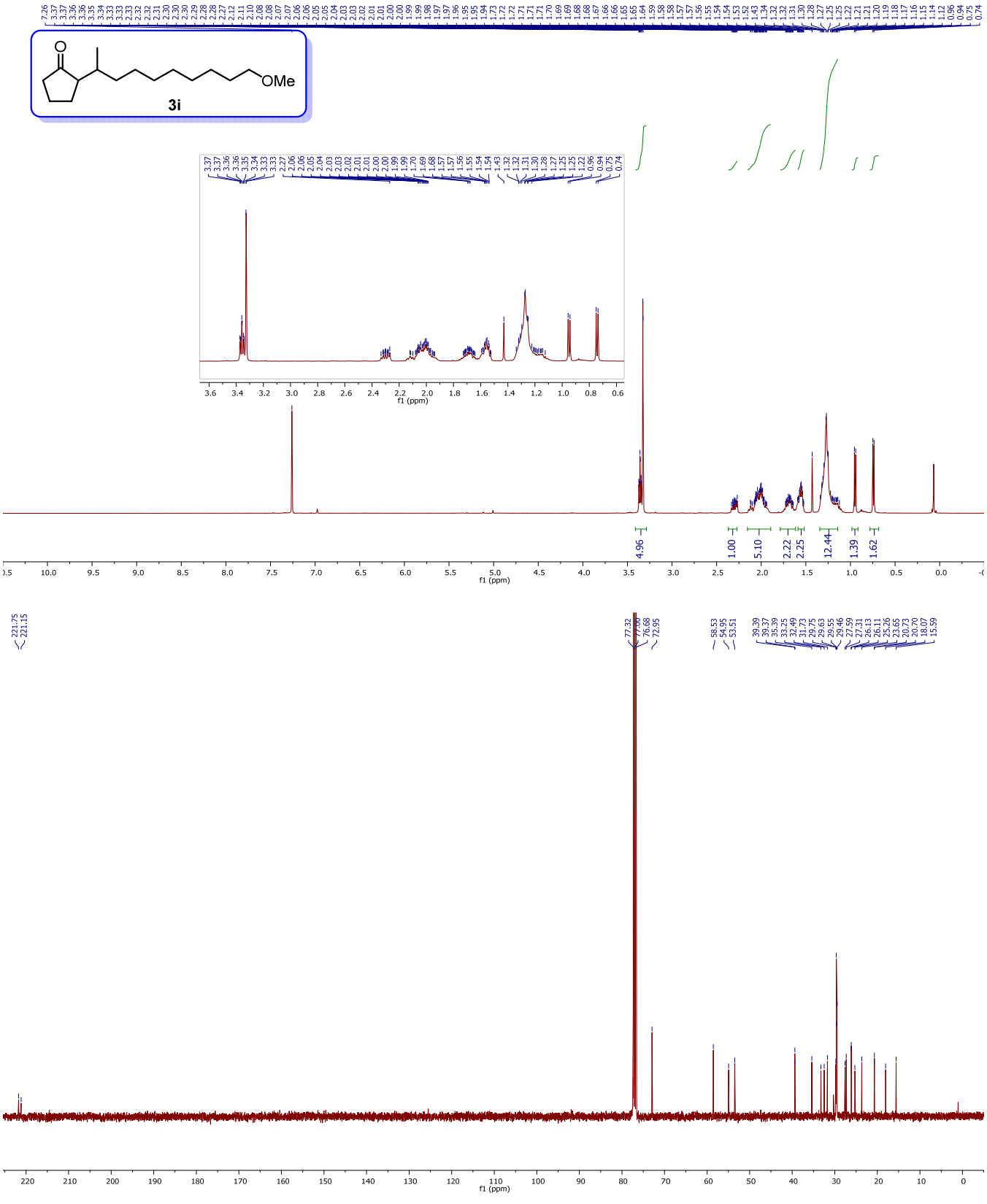
3f

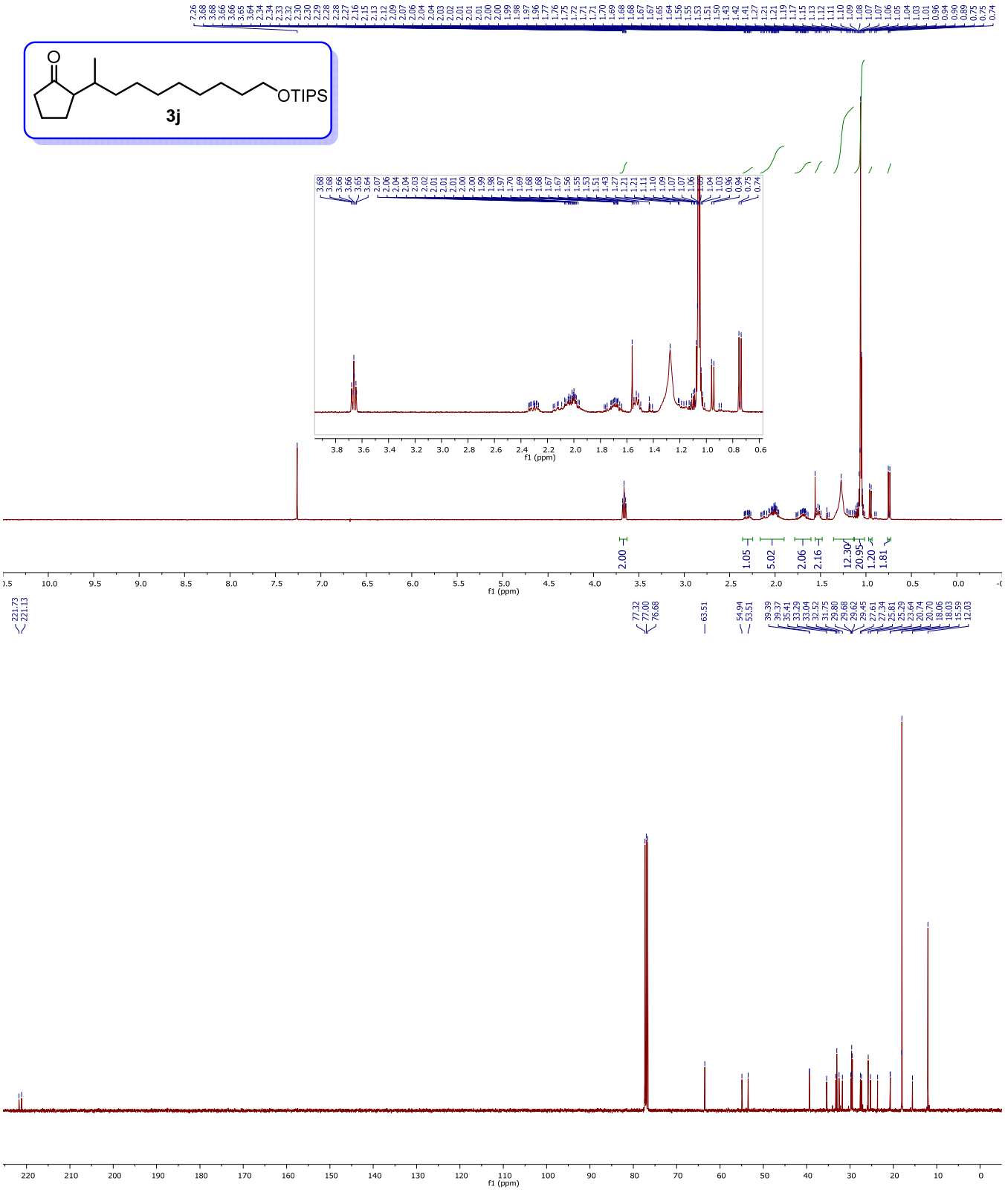

2.00
3.07
6.89
6.02
2.25
1.90
f1 (ppm)

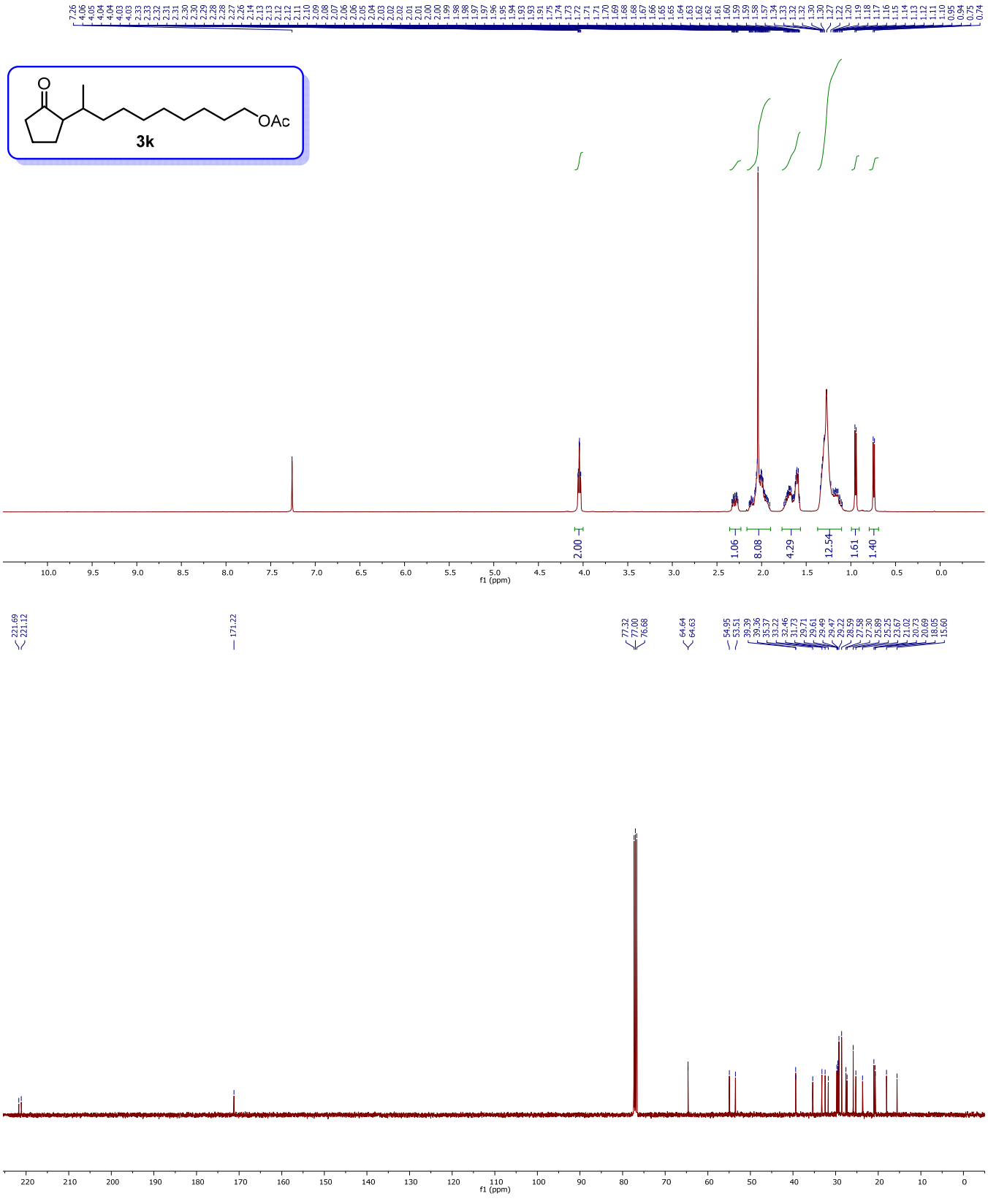

f1 (ppm)

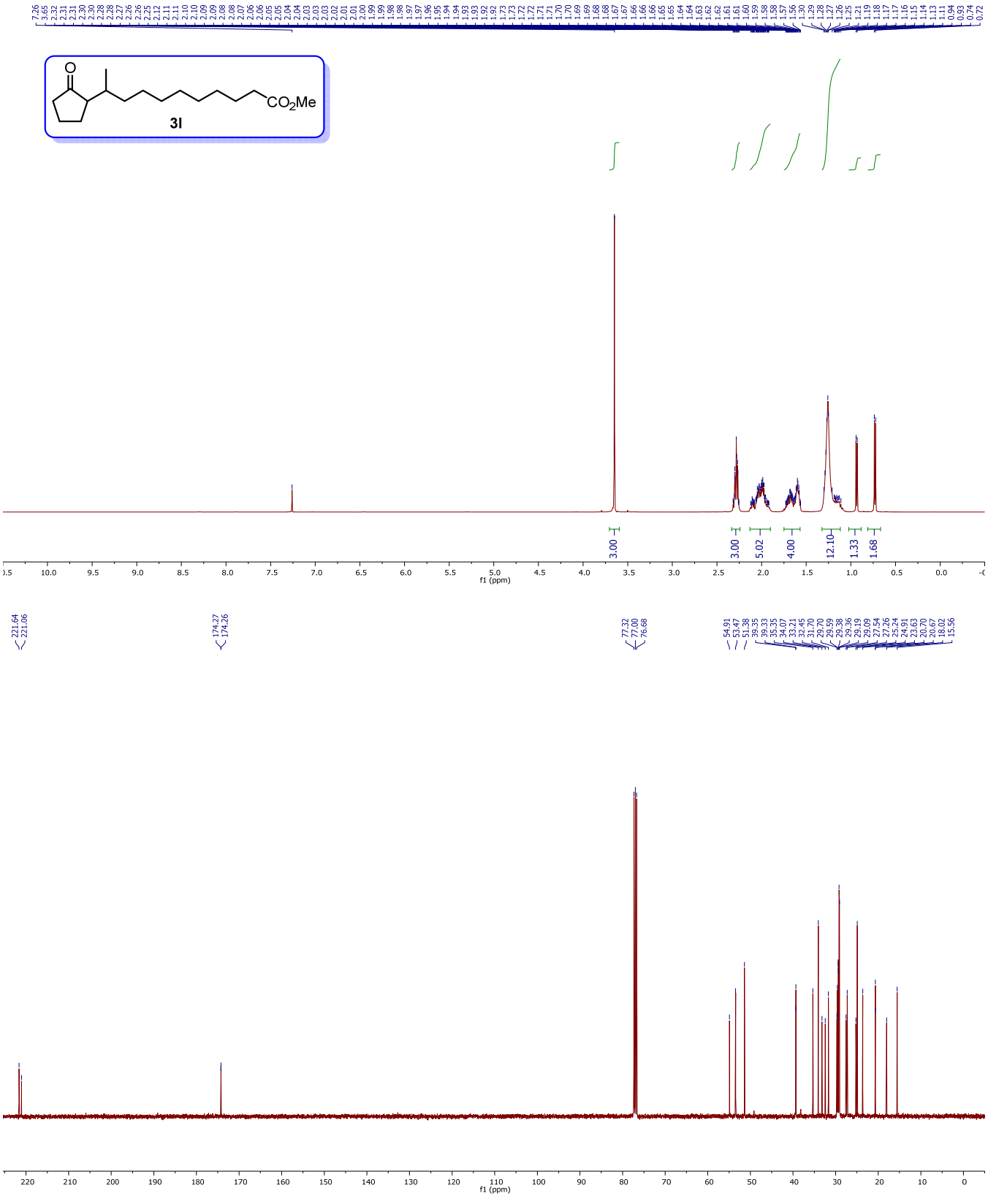

Ph
3g
f1 (ppm)

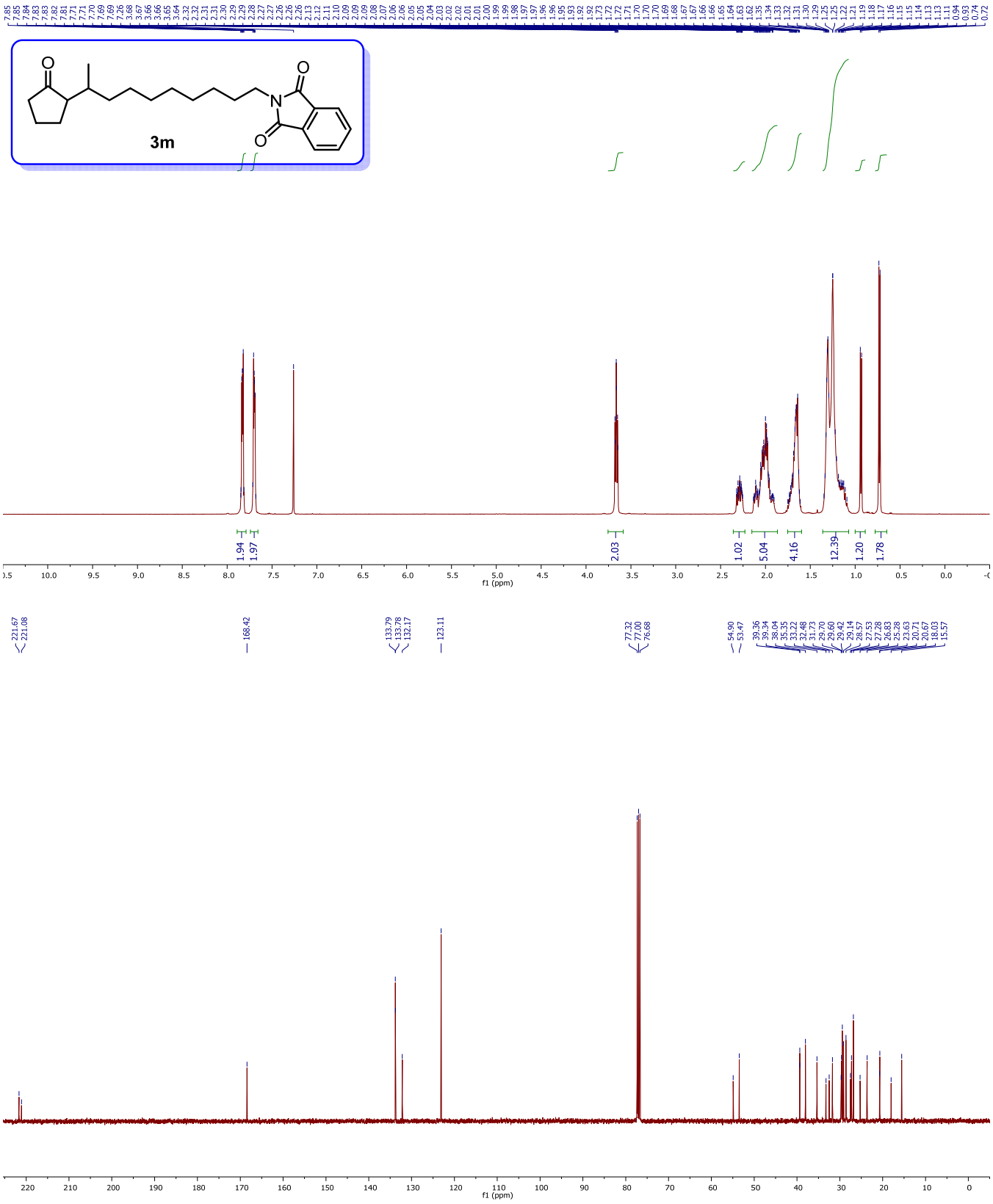

3h
1.02
1.05
7.00
5.00
2.96
6.30
1.30
1.70
f1 (ppm)
f1 (ppm)

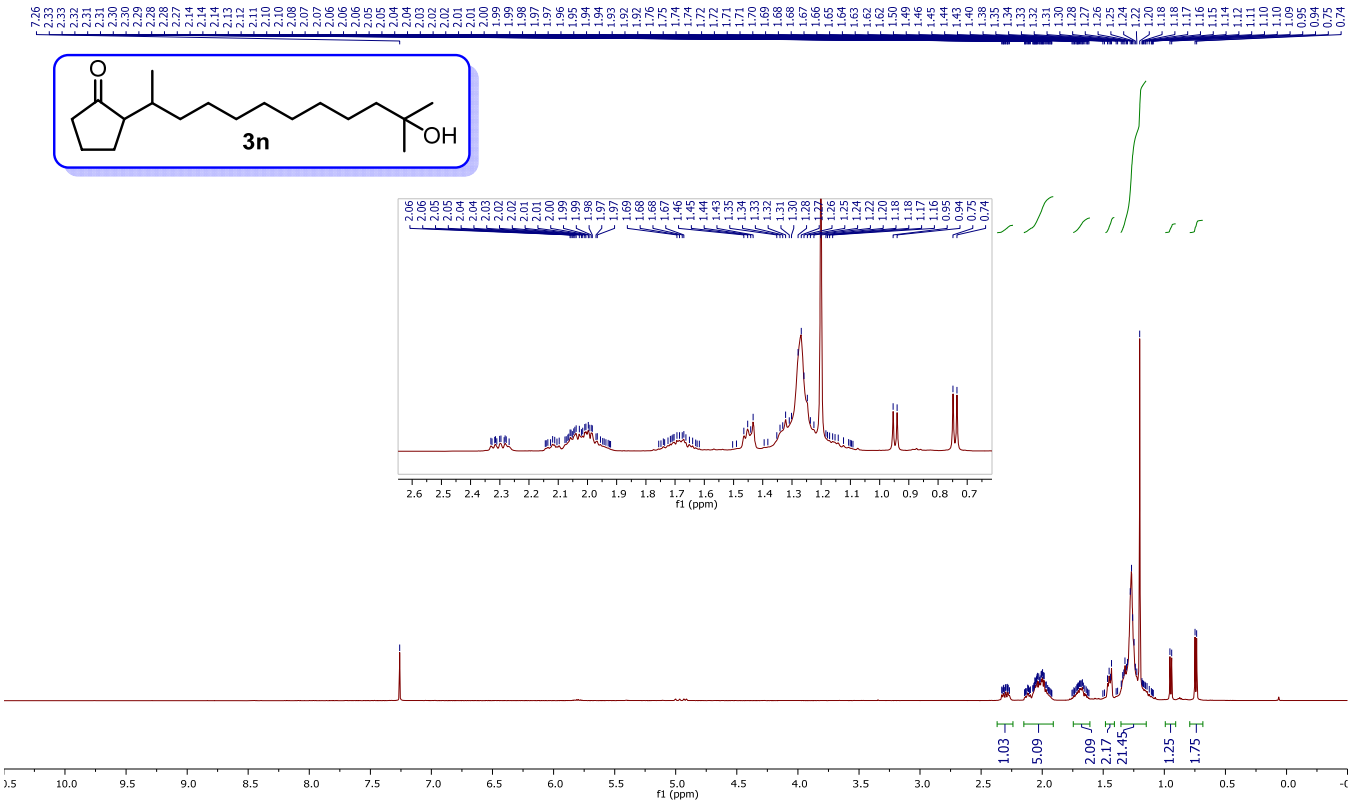

OMe
3i
f1 (ppm)

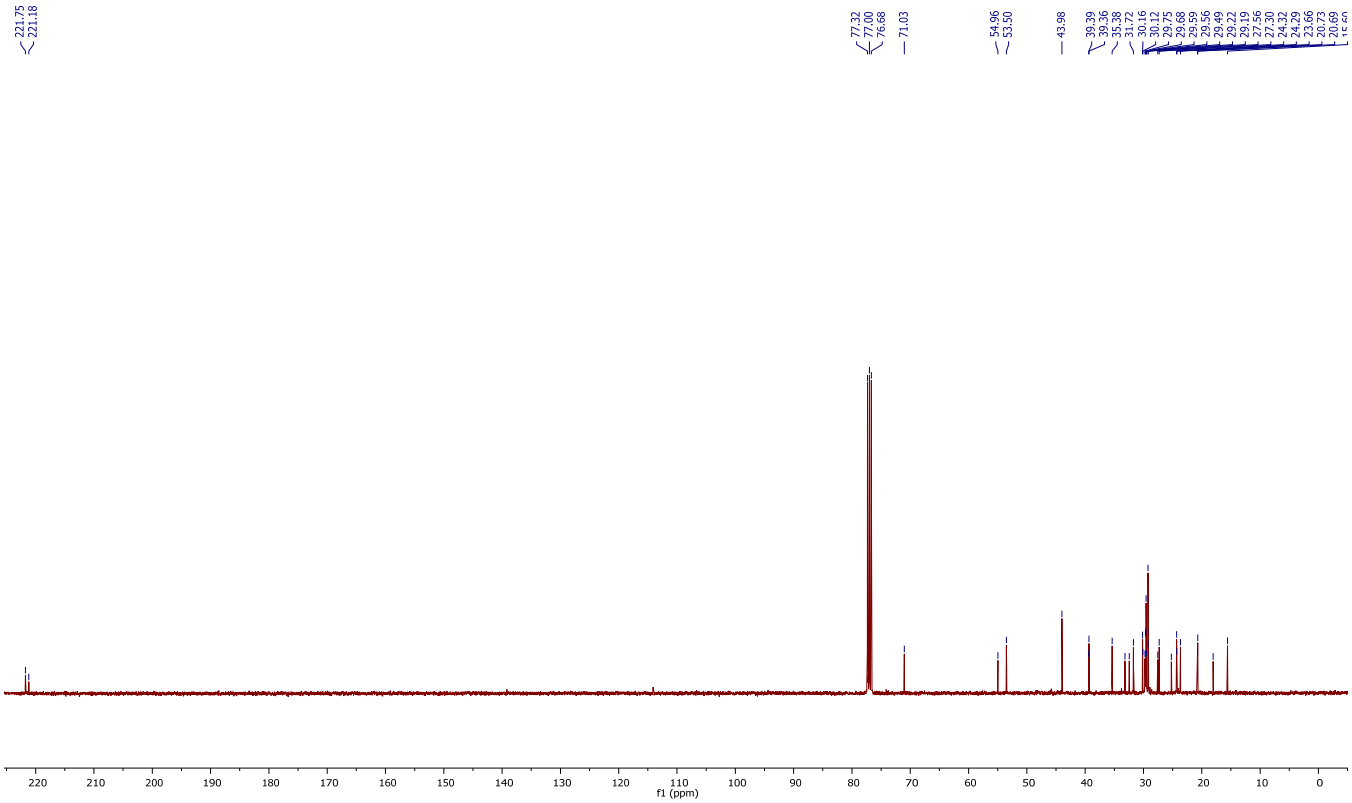

OTIPS
3j
f1 (ppm)

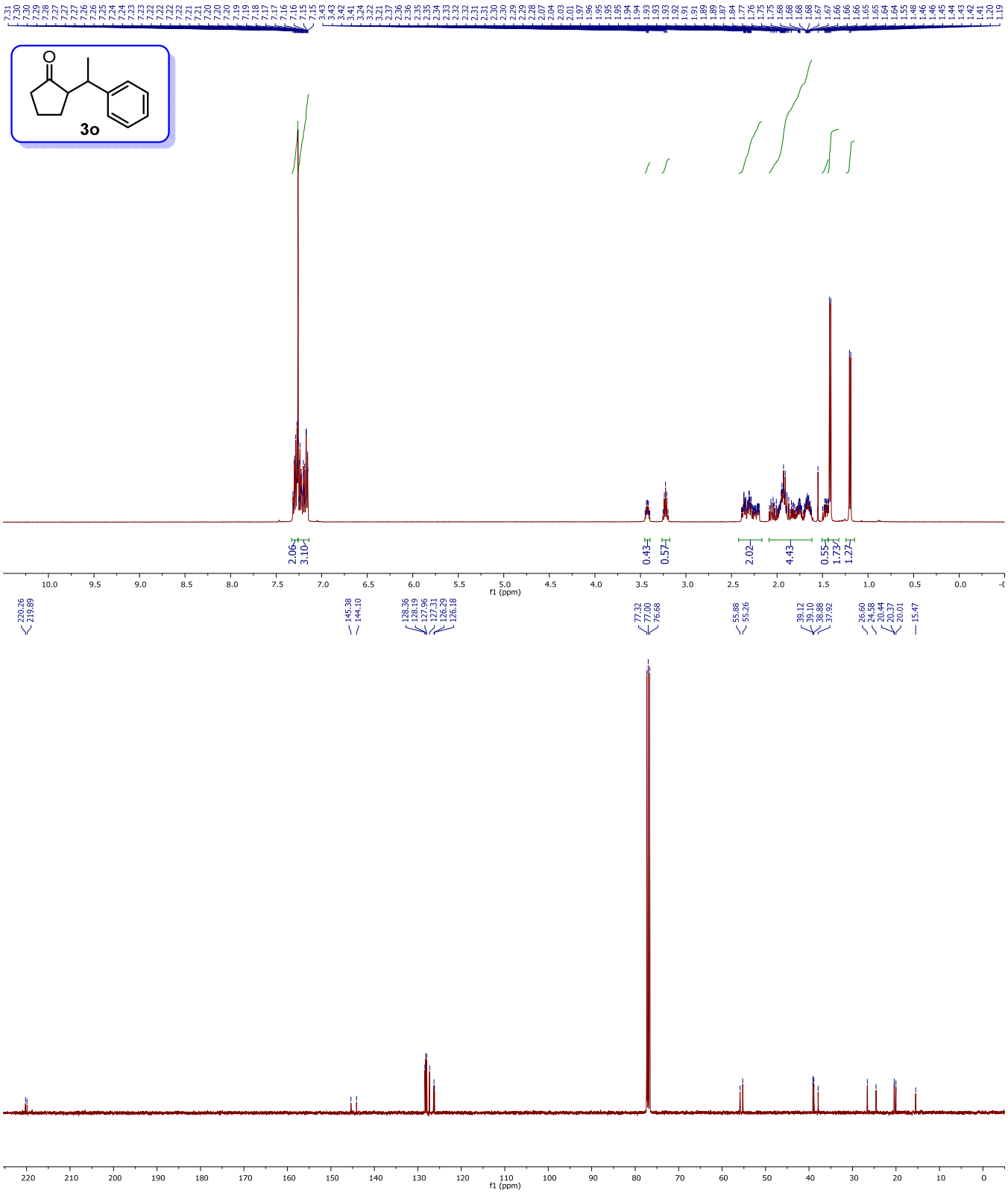

OAc
3k
f1 (ppm)

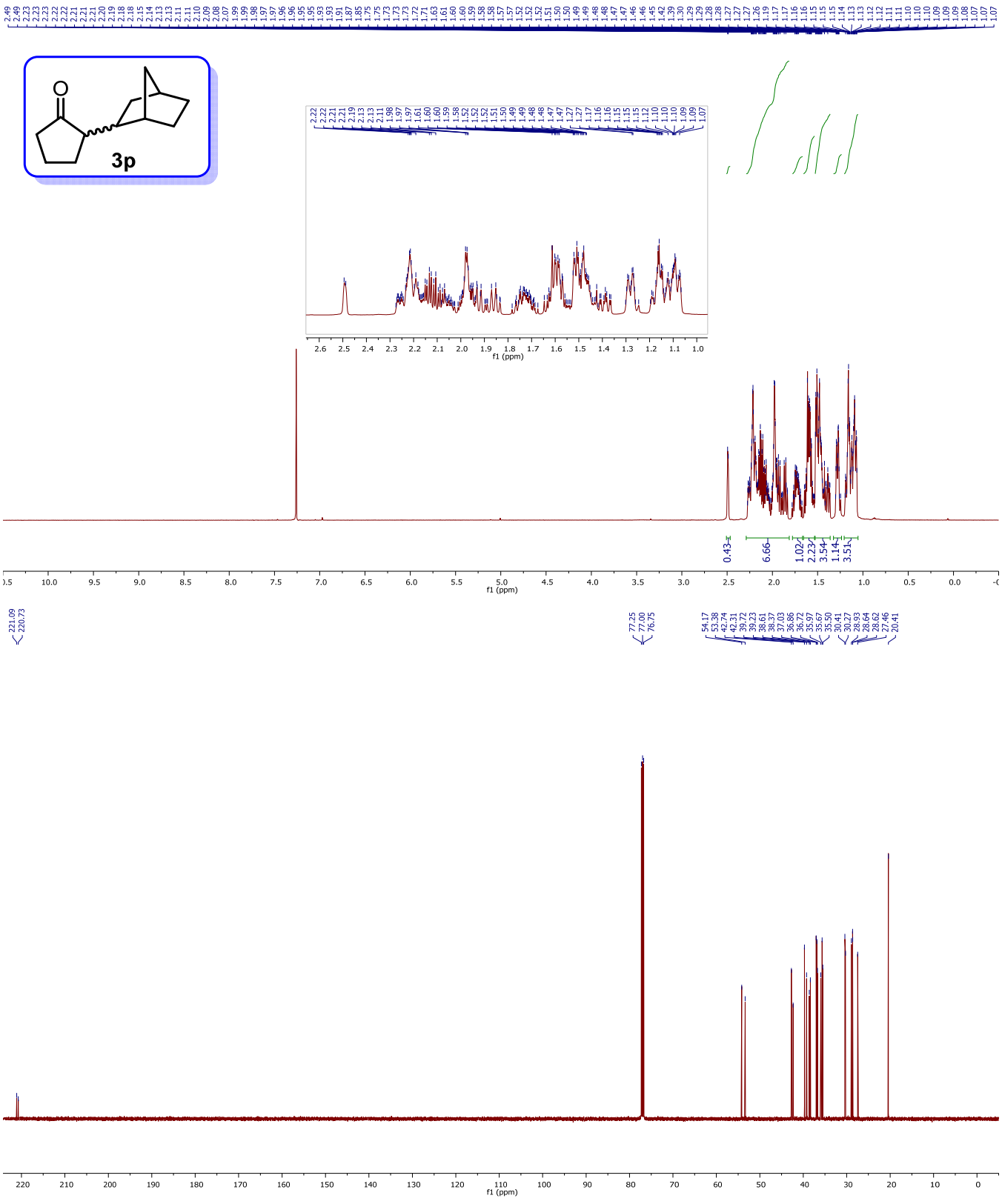

3l
CO2Me
f1 (ppm)

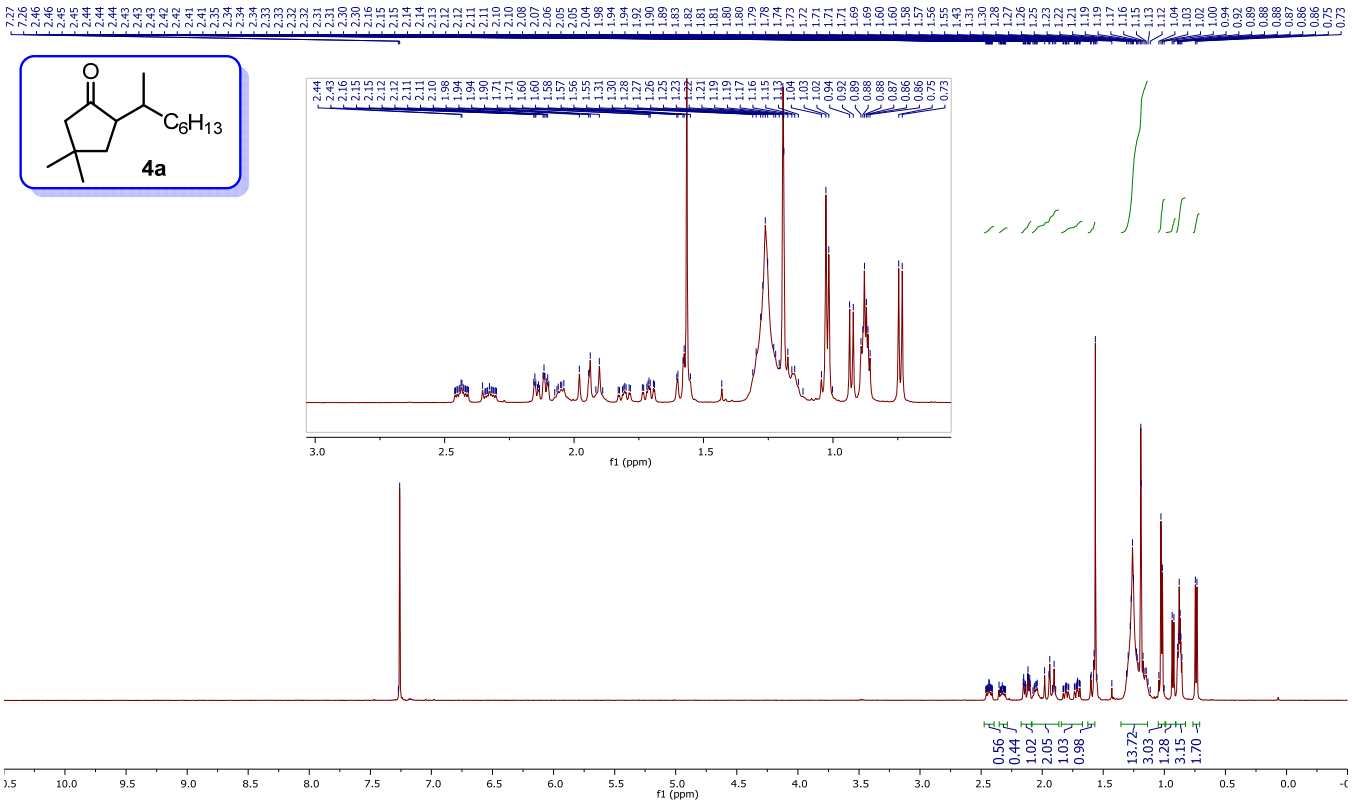

3m
1.94
1.97
2.03
1.02
5.04
4.16
12.39
1.20
1.78
f1 (ppm)
221.67
221.08
168.42
133.79
133.78
132.17
123.11
77.32
77.00
76.68
54.90
53.47
39.36
39.34
38.04
35.35
33.22
32.48
31.73
31.70
29.60
29.42
29.14
28.57
27.53
27.28
26.83
25.28
23.63
20.71
20.67
18.03
15.57
f1 (ppm)

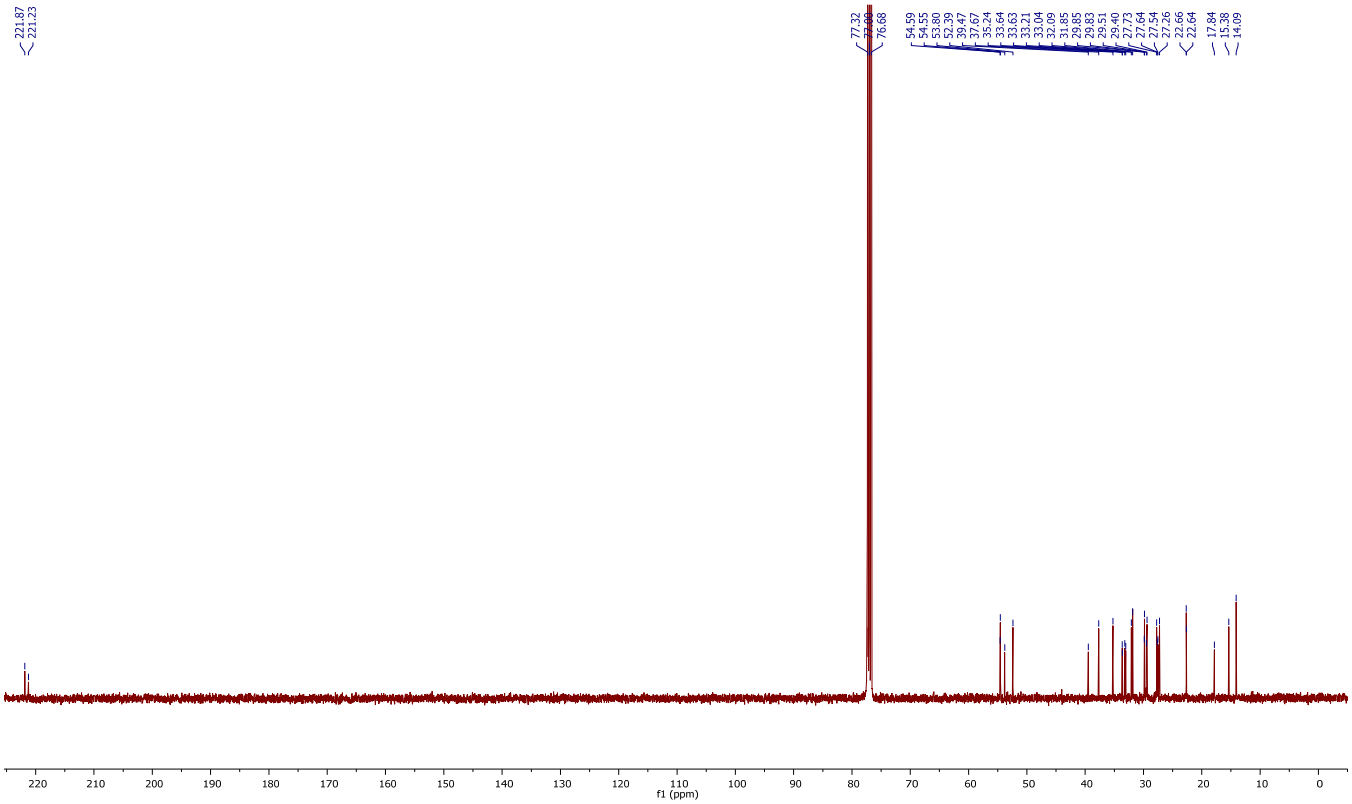

3n
OH
f1 (ppm)

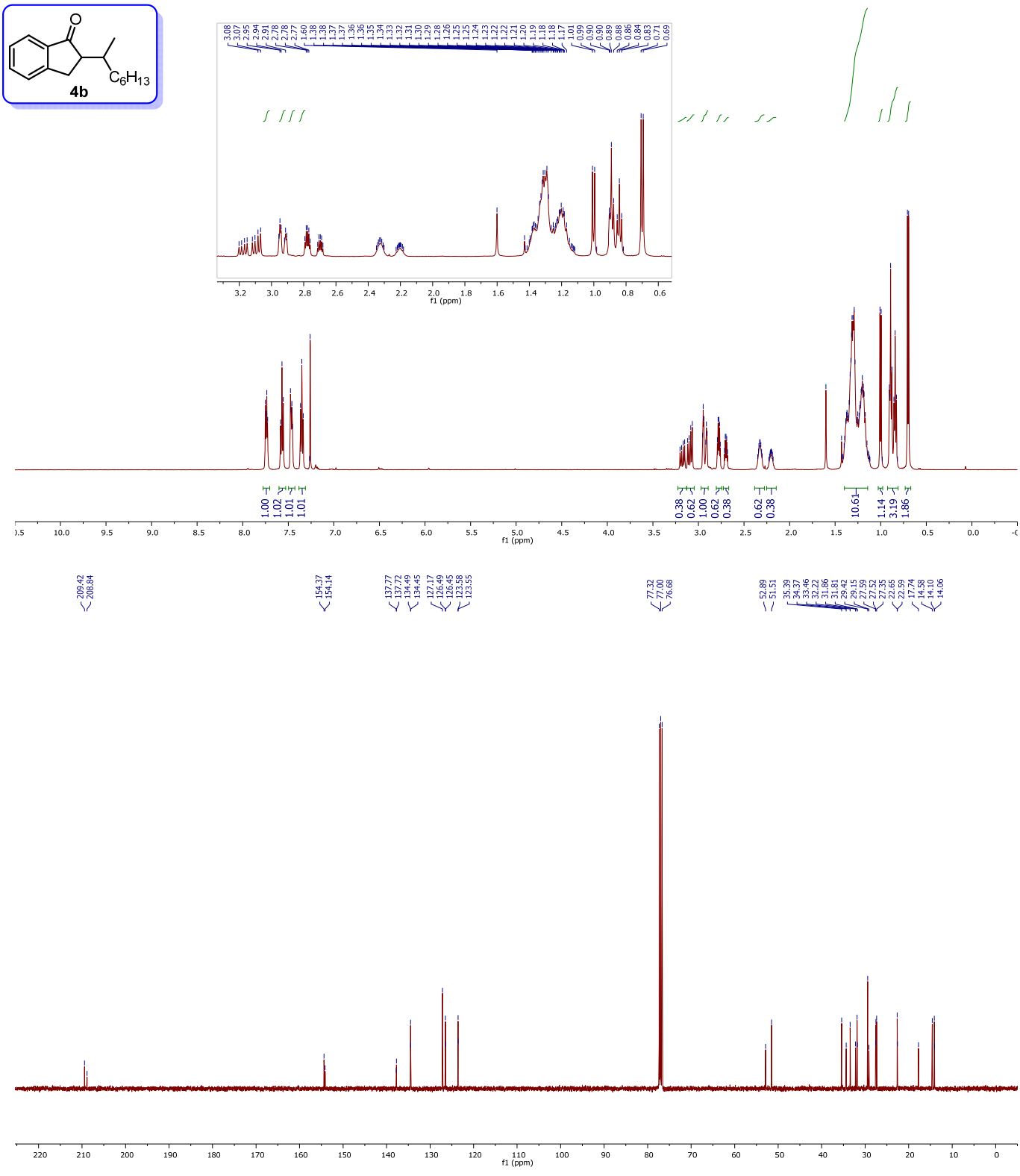

f1 (ppm)

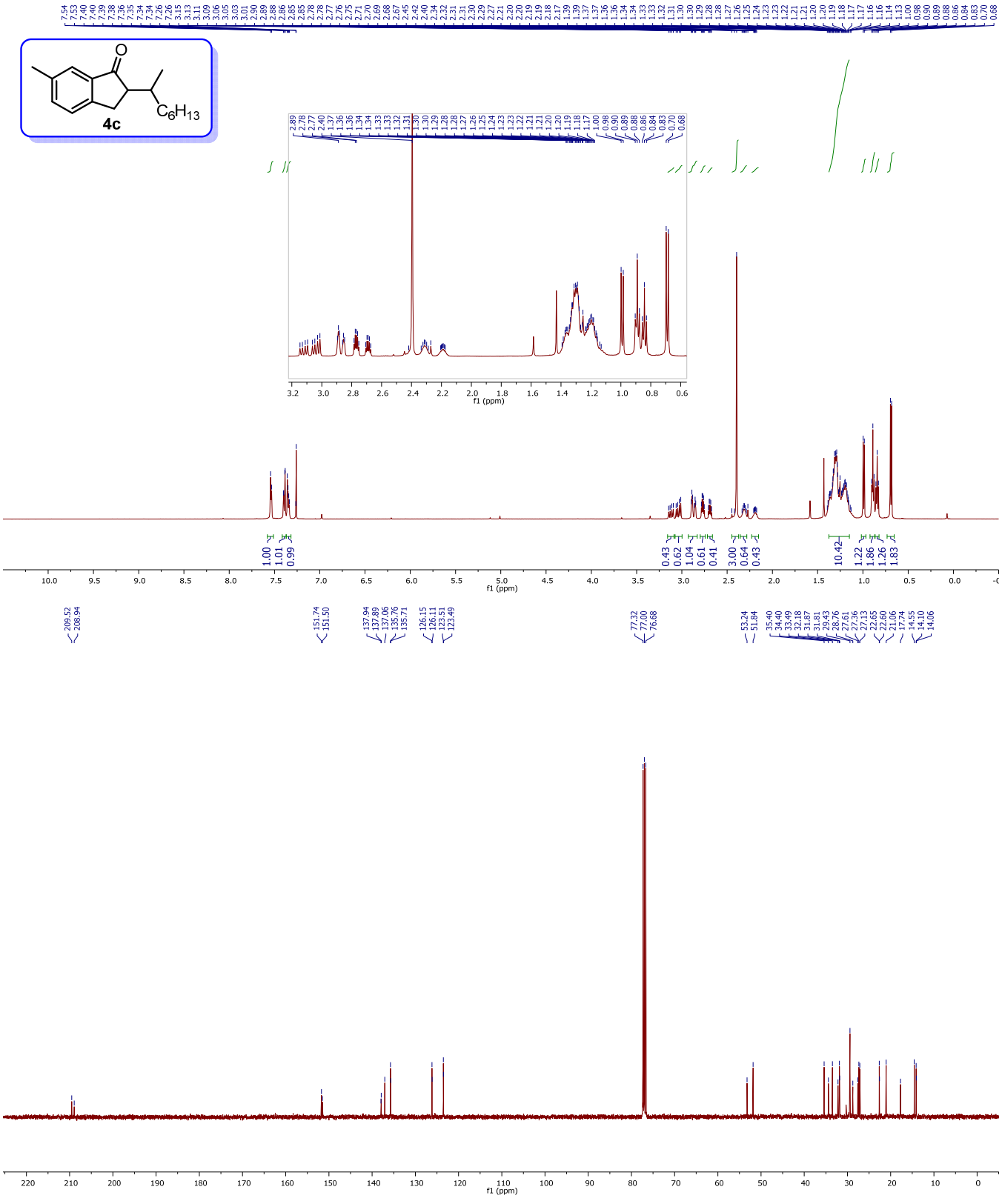

3o
f1 (ppm)
f1 (ppm)

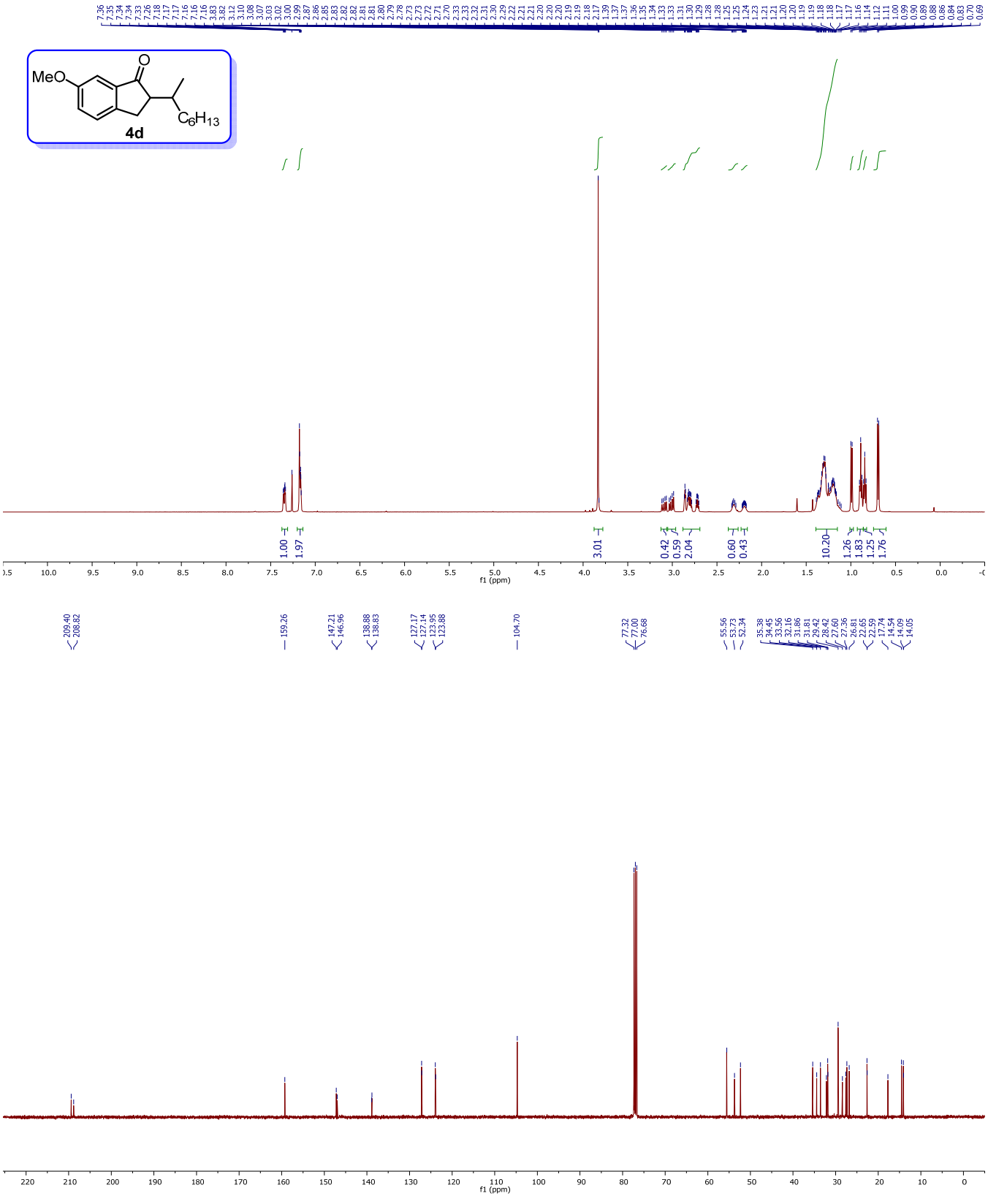

3p
f1 (ppm)
0.43
6.66
1.02
2.23
3.54
1.14
3.51

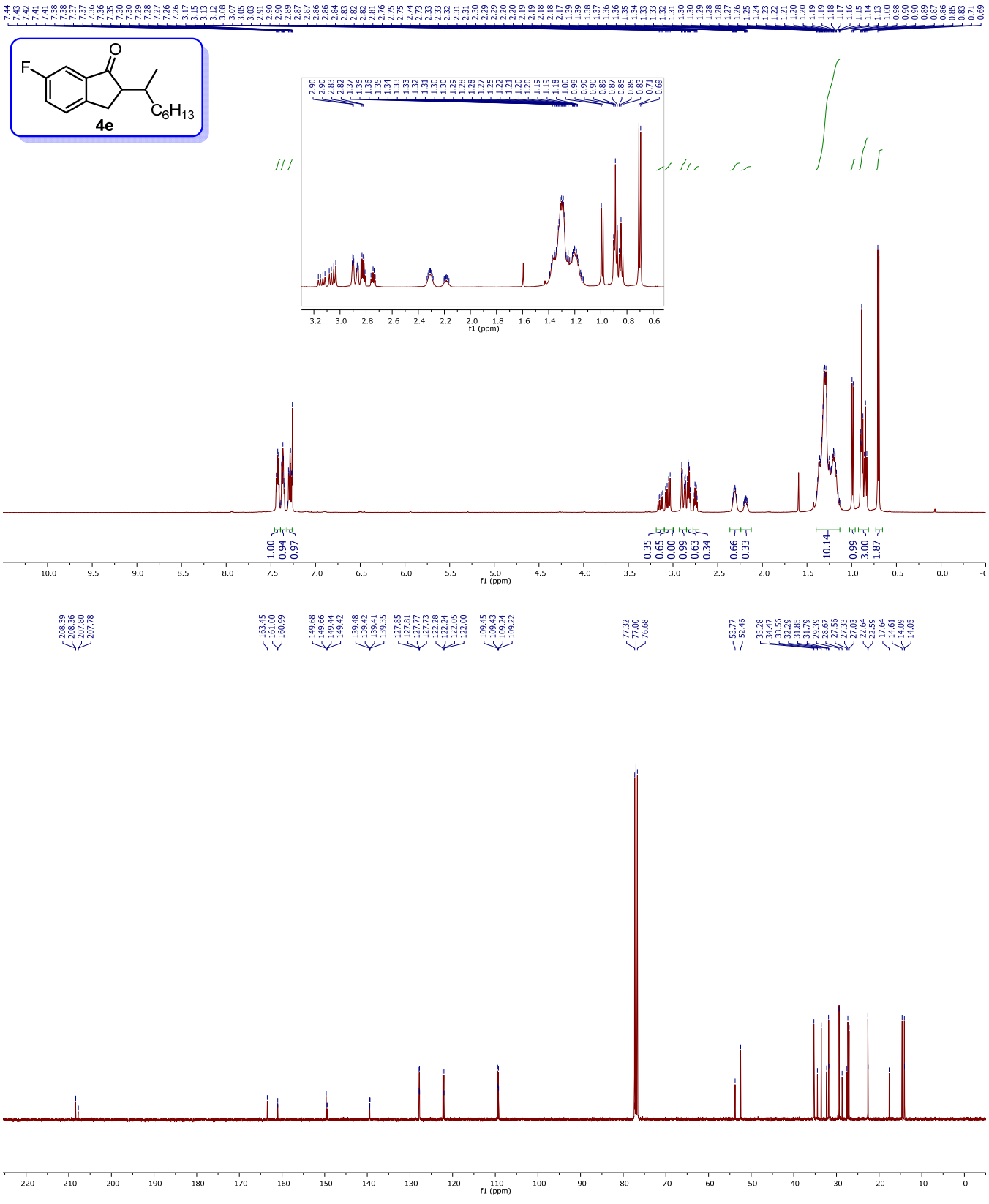

4a
f1 (ppm)


f1 (ppm)


4b
C6H13
f1 (ppm)

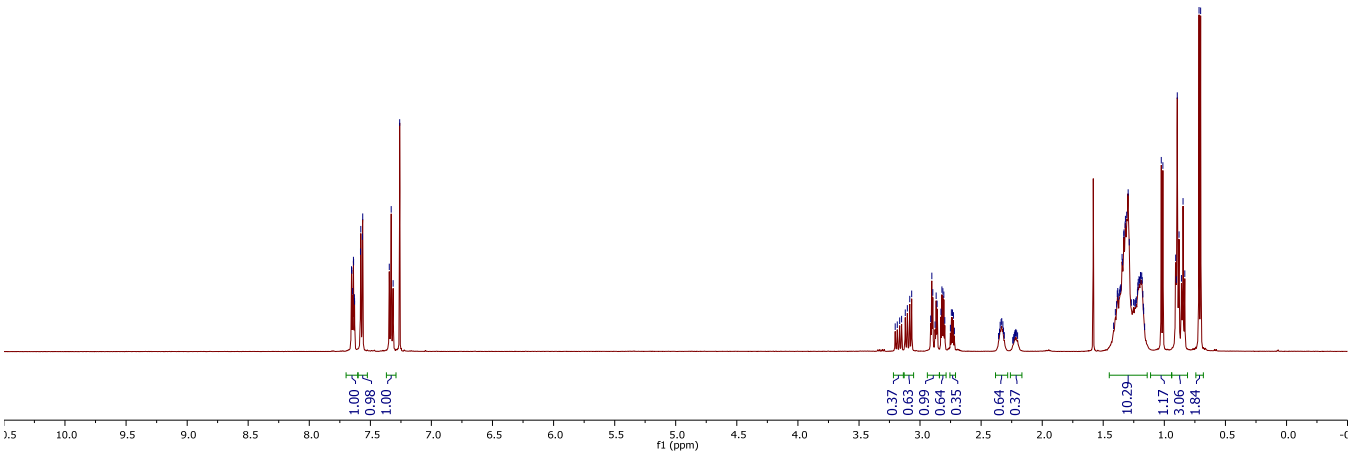

4c
f1 (ppm)

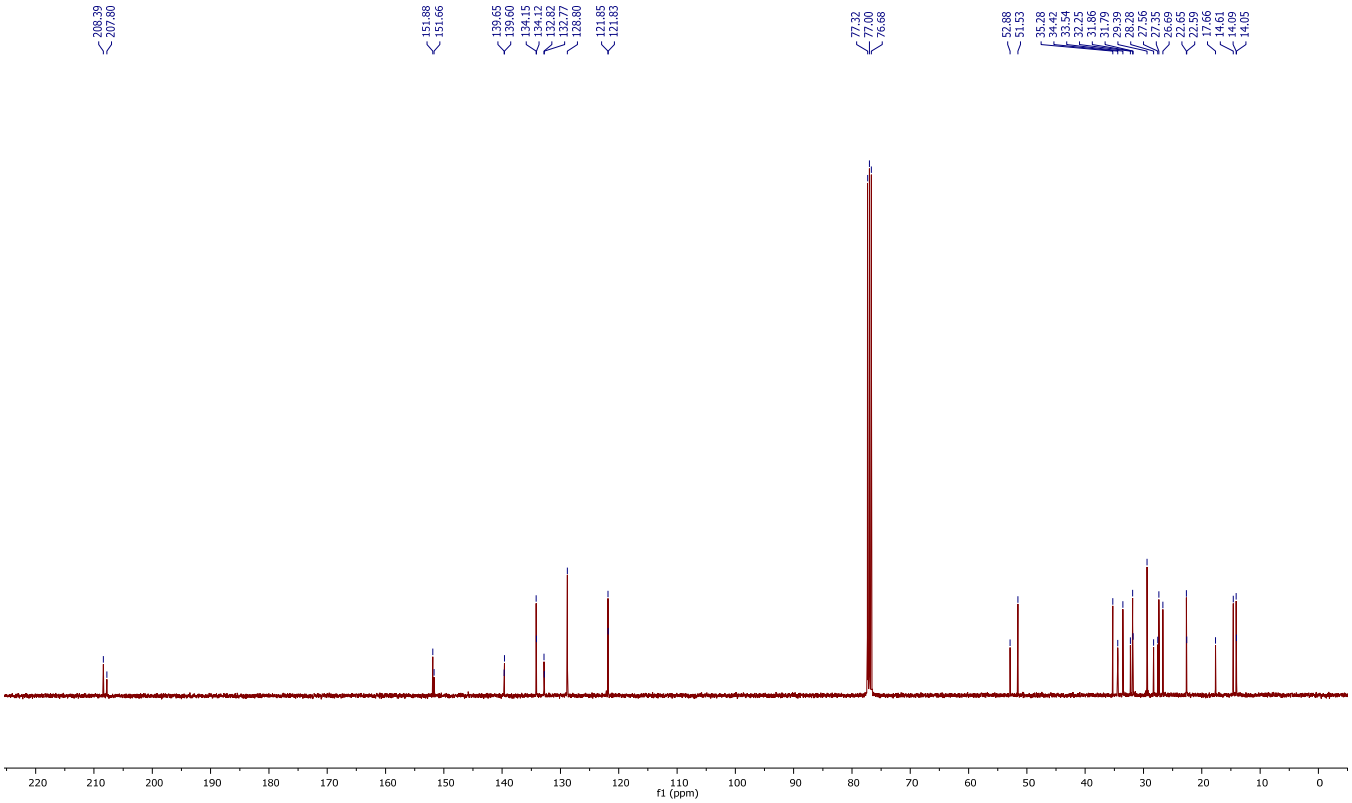

MeO
O
C6H13
4d
f1 (ppm)

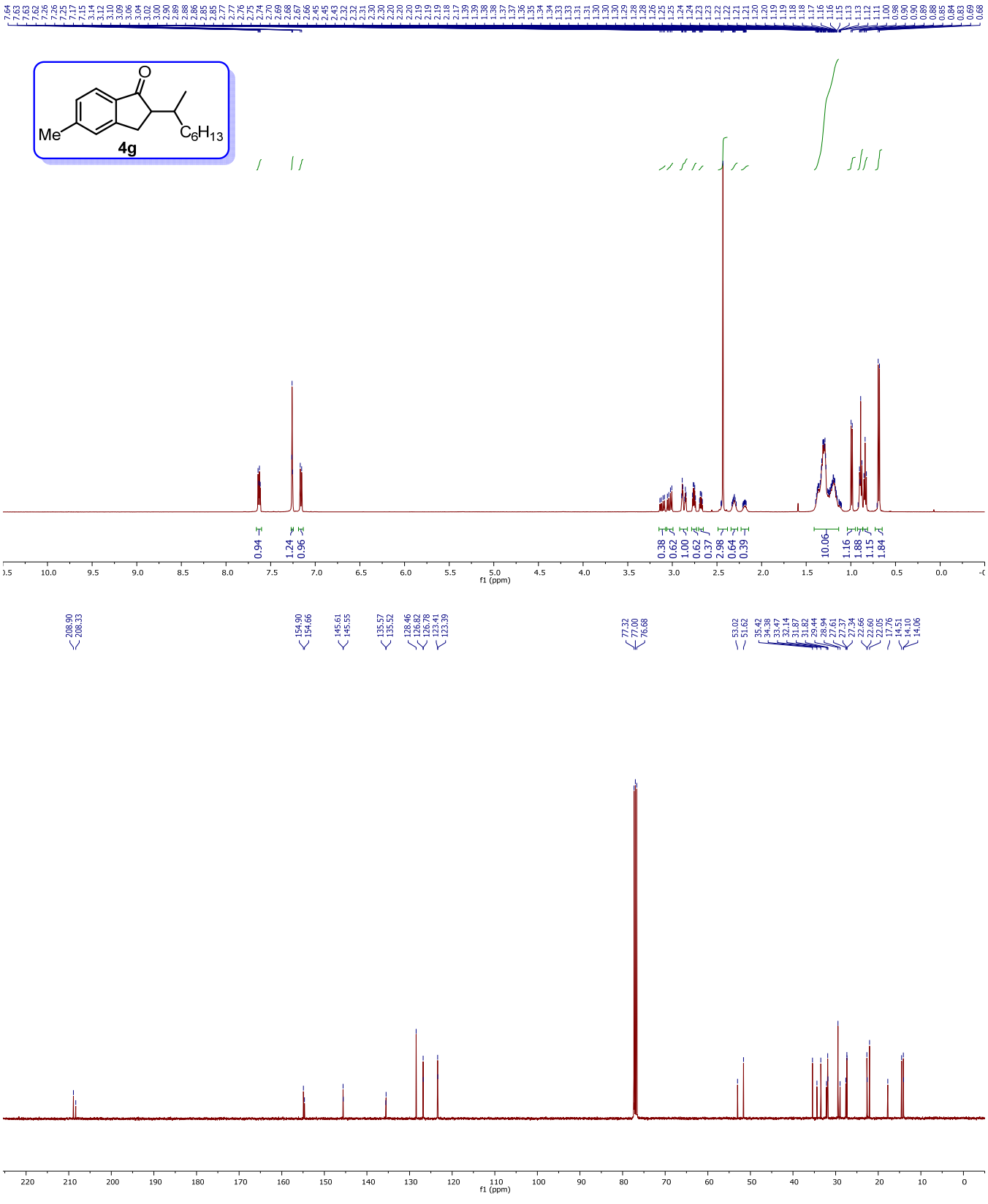

F
O
C_6H_{13}
4e
f1 (ppm)

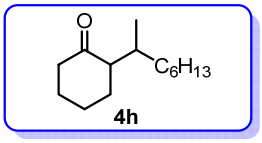
Cl
O
C_6H_{13}

4f


1.00
0.98
1.00
0.37
0.63
0.99
0.64
0.35
0.64
0.37
10.29
1.17
3.06
1.84
f1 (ppm)

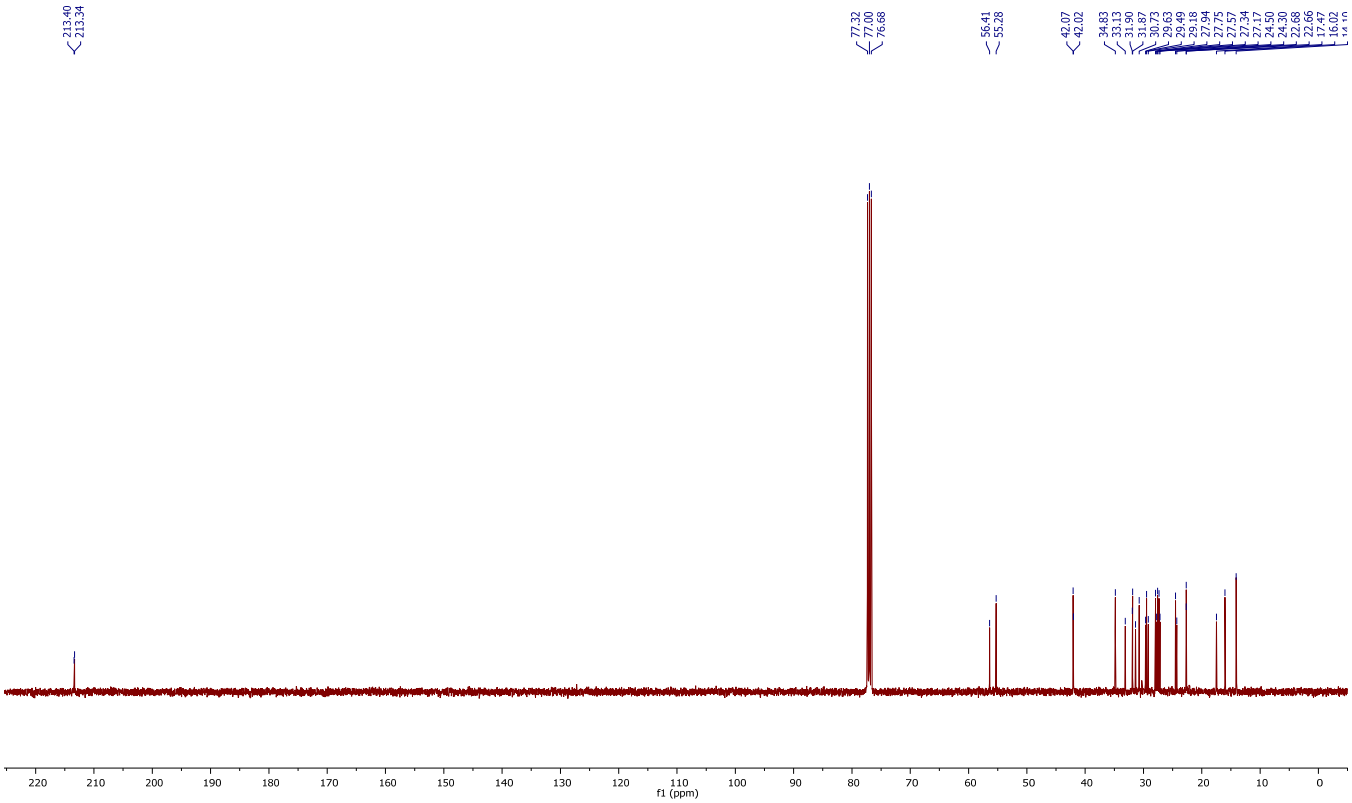

208.39
207.80
151.88
151.66
139.65
139.60
134.15
134.12
132.82
132.77
128.80
121.85
121.83
77.32
77.00
76.68
52.88
51.53
35.28
34.42
33.54
32.25
31.86
31.79
29.39
28.28
27.56
27.35
26.69
22.65
22.59
17.66
14.61
14.09
14.05
f1 (ppm)


Me
C6H13
4g
f1 (ppm)
f1 (ppm)


O
C6H13

4h

1.00
2.05
4.07
2.15
1.10
10.40
5.81
f1 (ppm)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213.34
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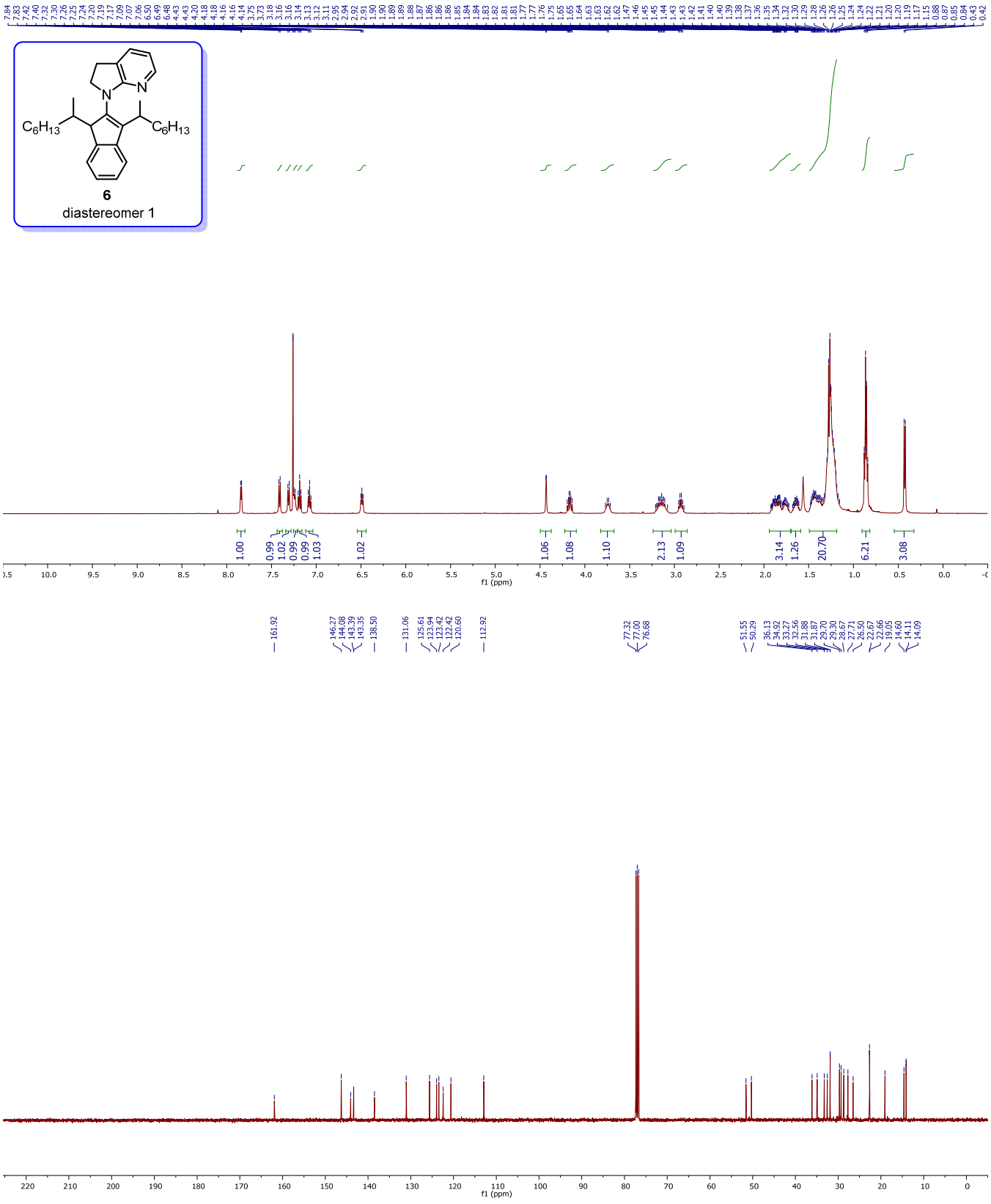
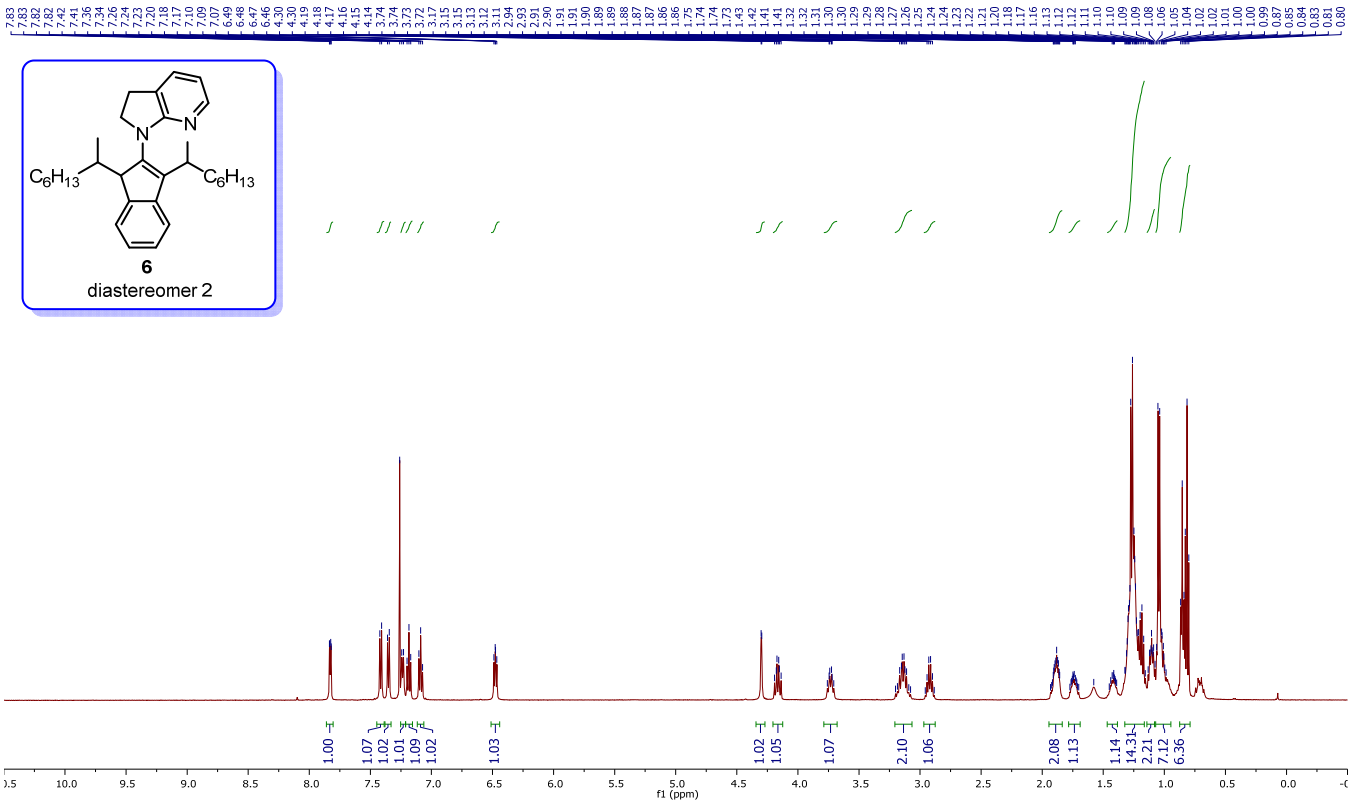
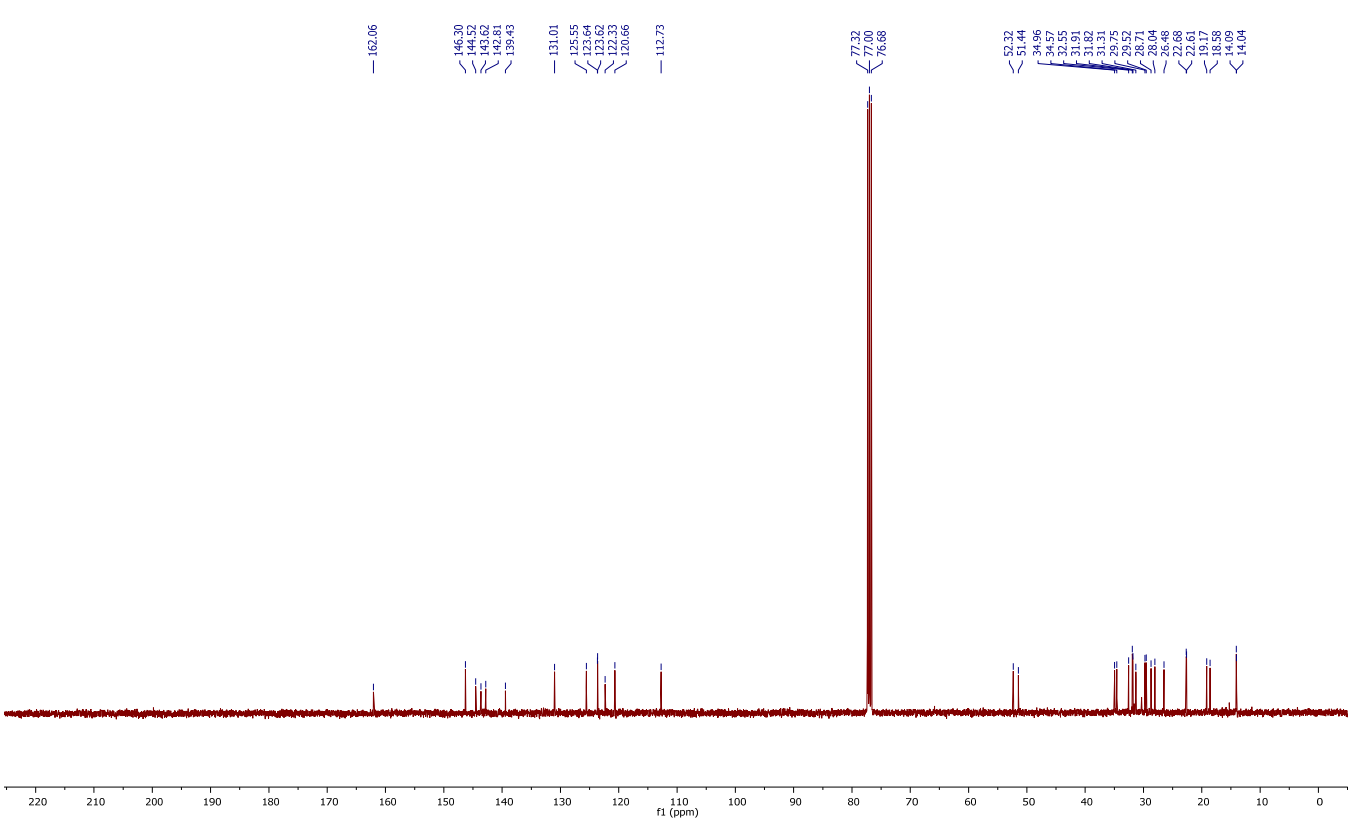
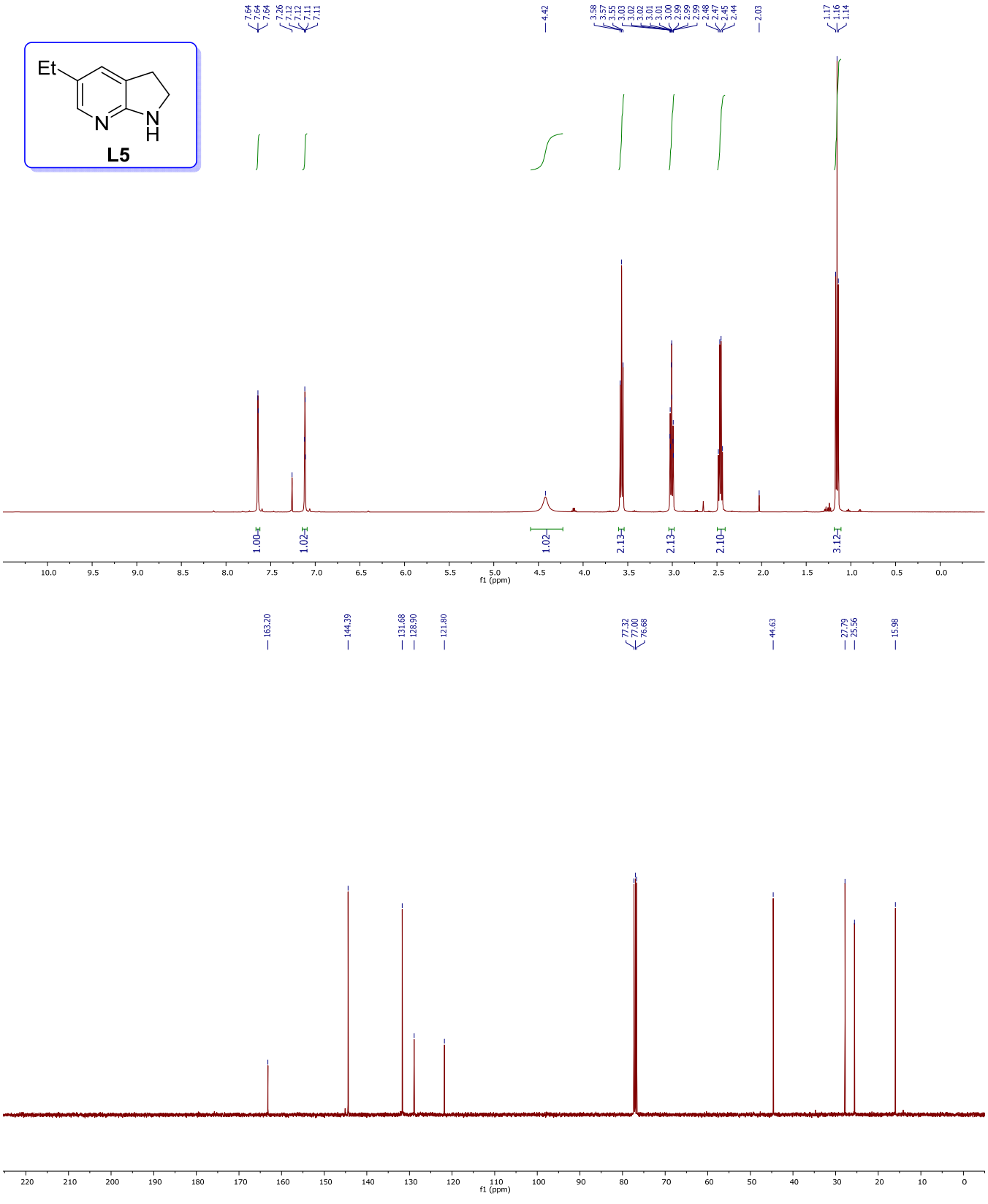
77.00
76.68
56.41
55.28
42.07
42.02
f1 (ppm)


6
diastereomer 1
f1 (ppm)
f1 (ppm)


C6H13
C6H13
6
diastereomer 2
f1 (ppm)


f1 (ppm)


Et
N
N
H
L5
7.64
7.64
7.64
7.26
7.12
7.12
7.11
7.11
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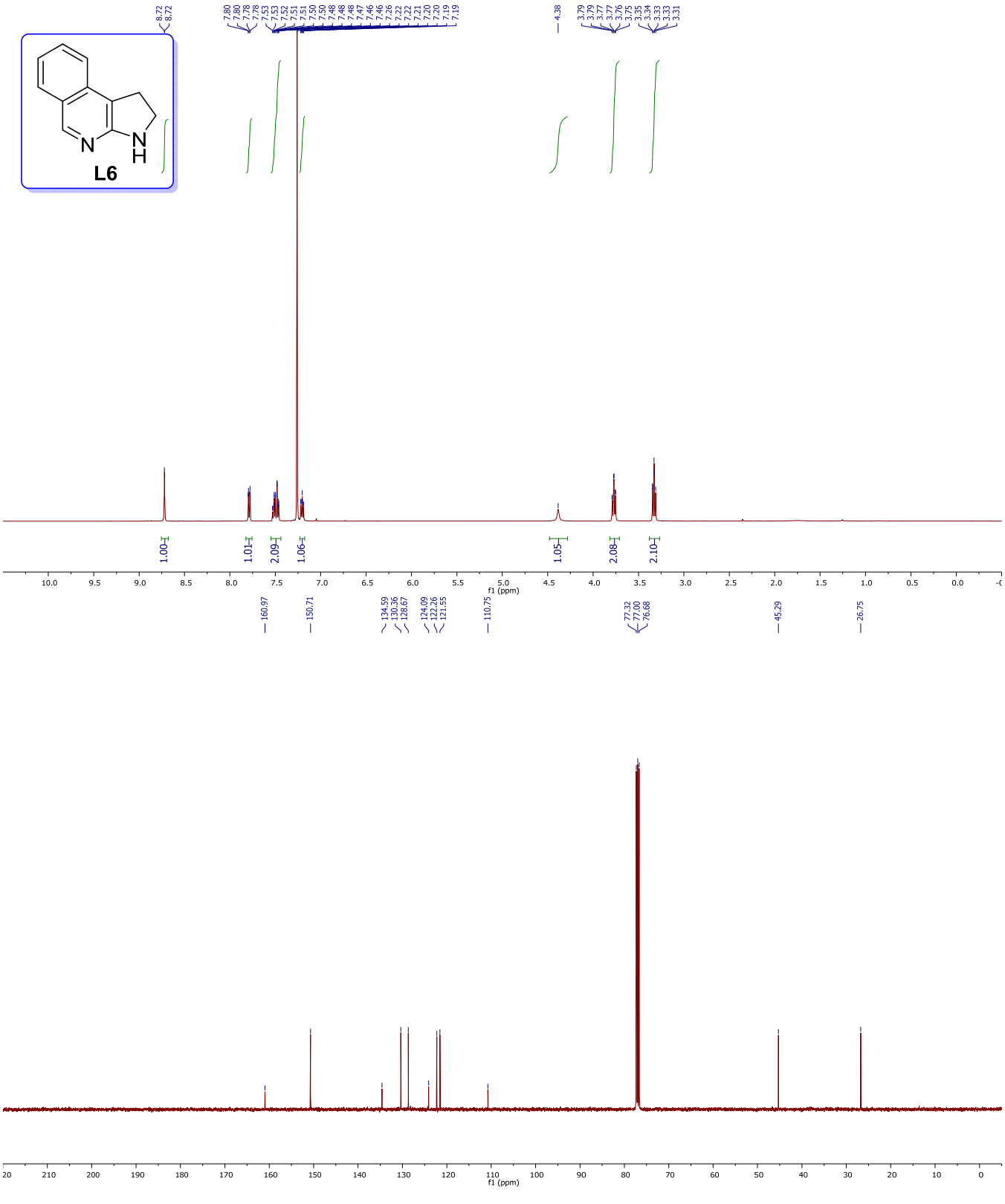
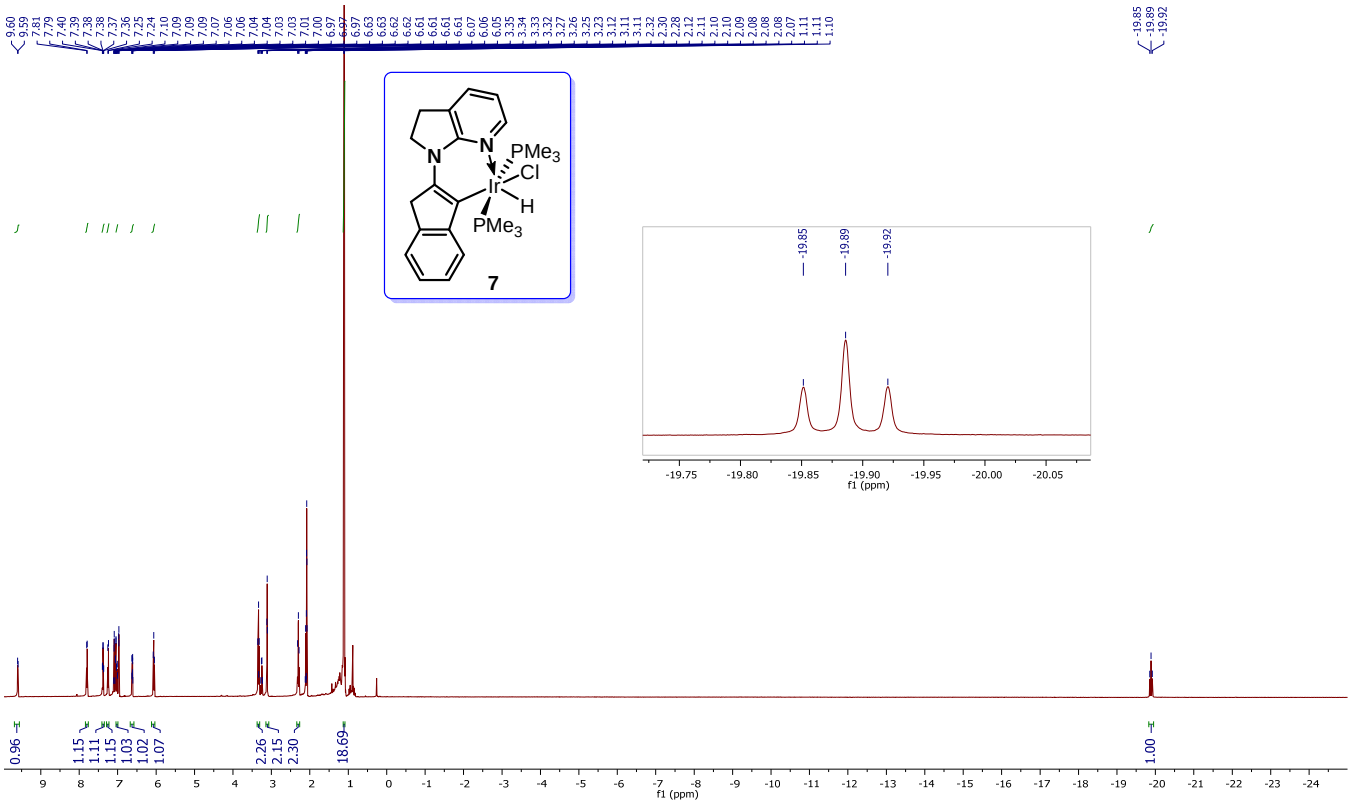
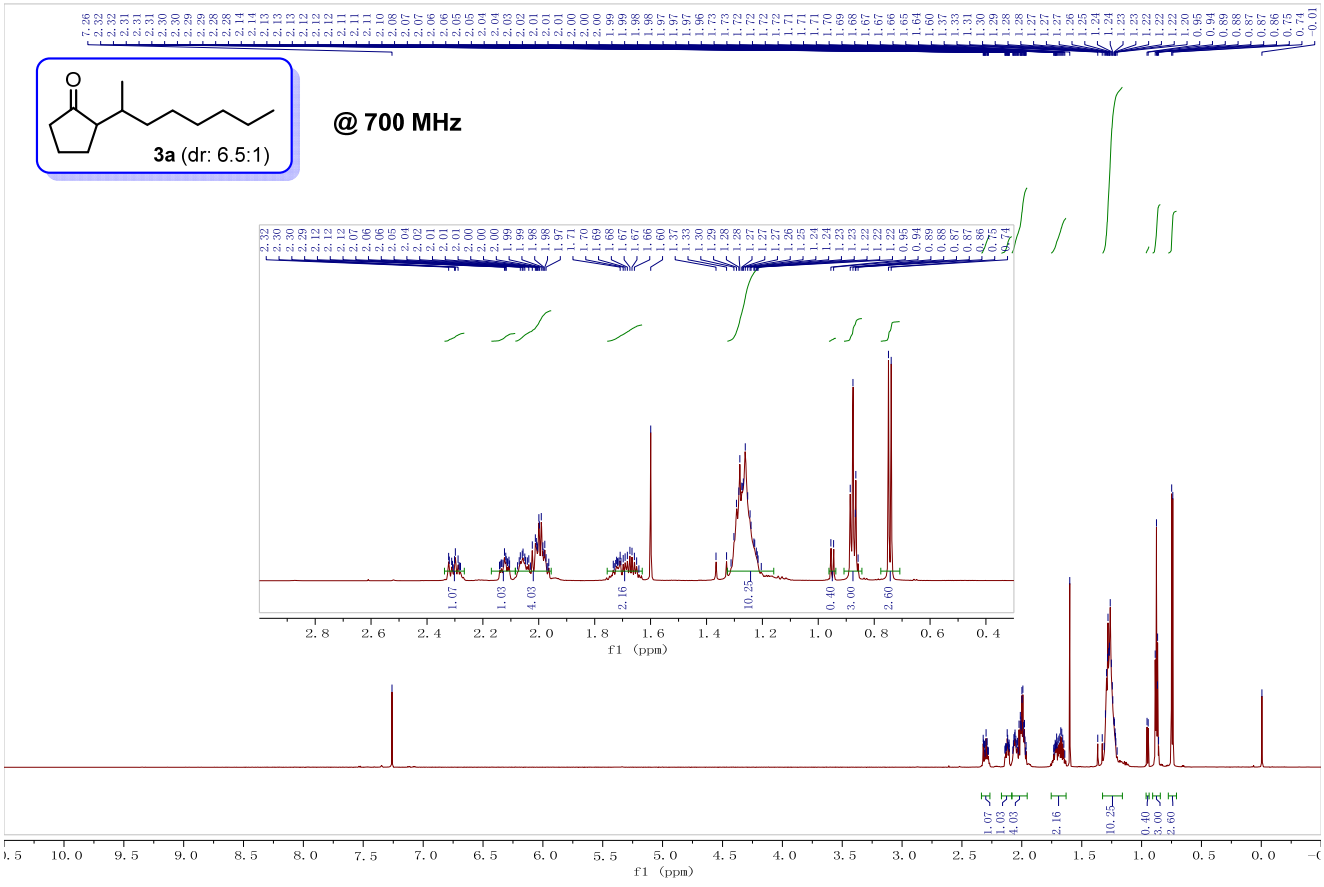
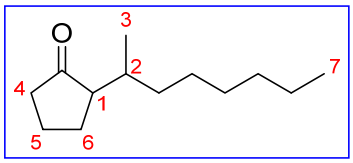
3.58
3.57
3.55
3.03
3.02
3.02
3.01
3.01
3.00
2.99
2.99
2.99
2.48
2.47
2.45
2.44
2.03
1.17
1.16
1.14
1.00
1.02
1.02
2.13
2.13
2.10
3.12
f1 (ppm)
163.20
144.39
131.68
128.90
121.80
77.32
77.00
76.68
44.63
27.79
25.56
15.98
f1 (ppm)

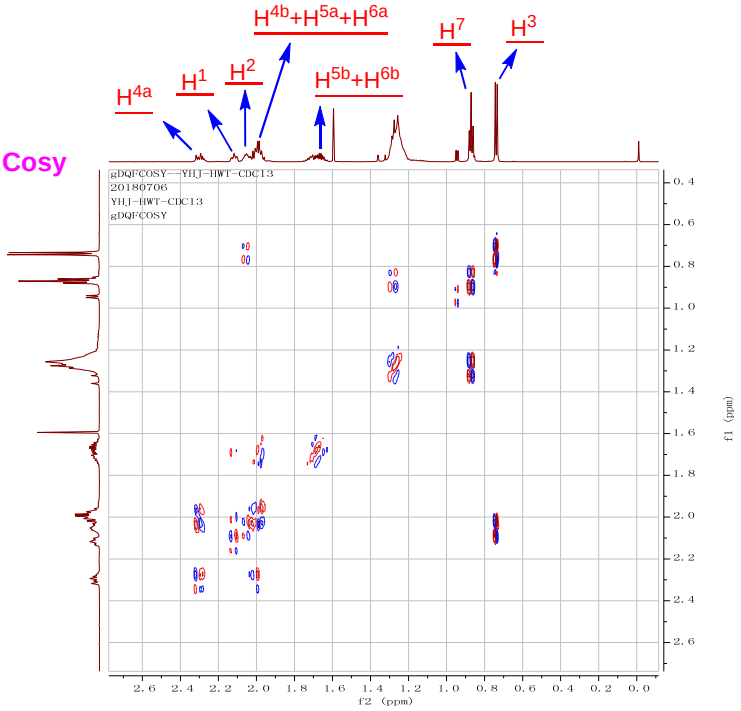

L6
f1 (ppm)
f1 (ppm)


PMe3
Cl
Ir
H
PMe3
7
f1 (ppm)

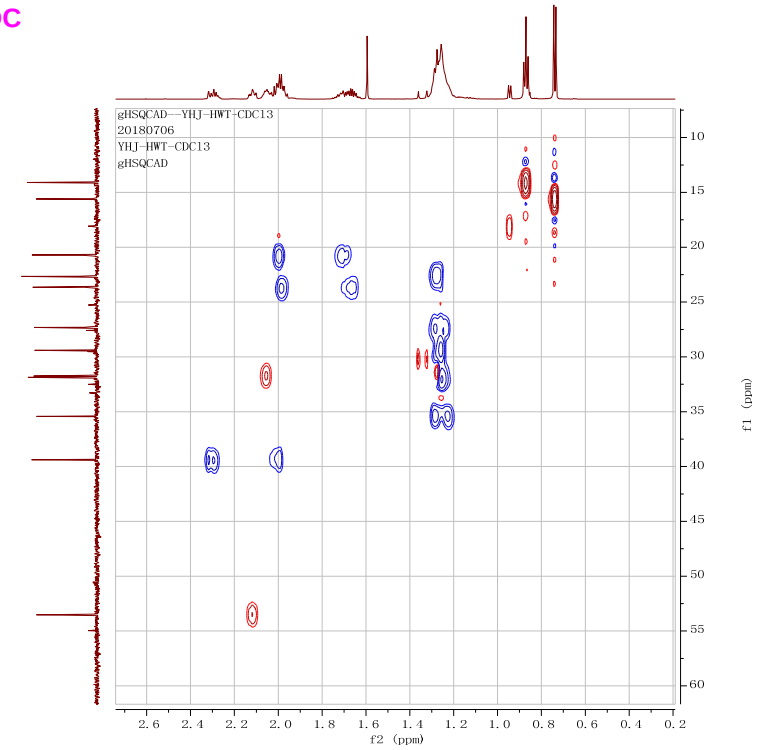

3a (dr: 6.5:1)
@ 700 MHz
f1 (ppm)

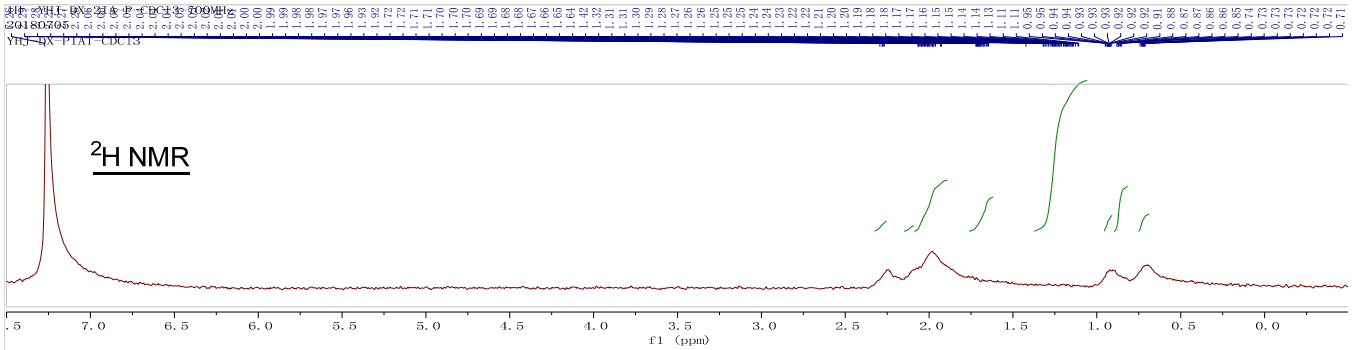

O
3
2
7
4
1
5
6

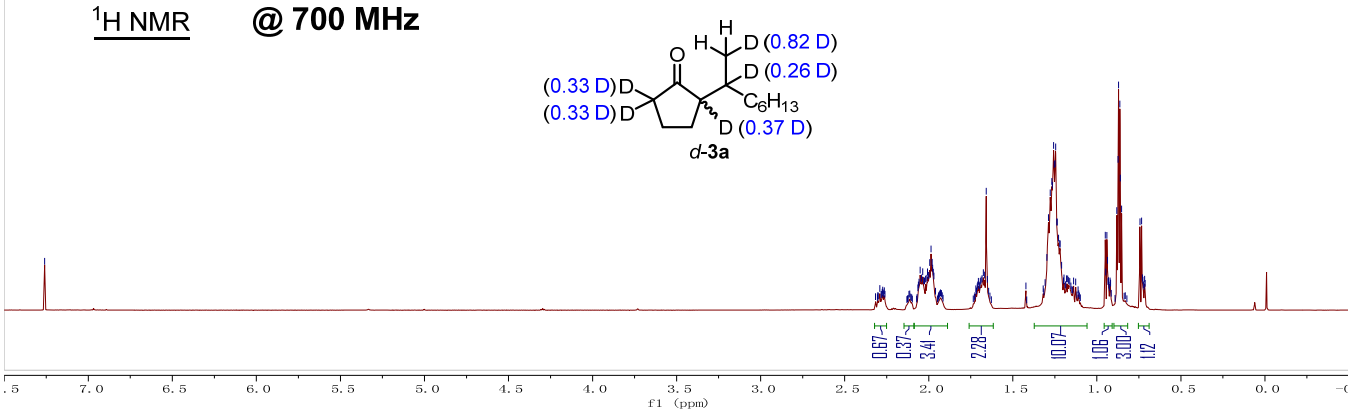
H-H Cosy

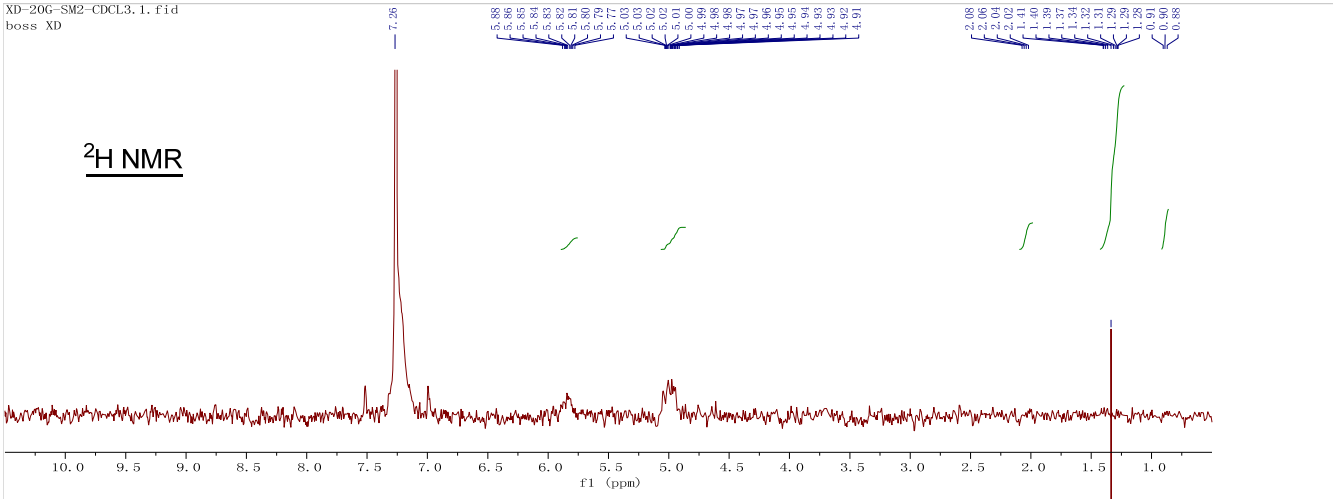

H4b+H5a+H6a
H7
H3
H4a
H1
H2
H5b+H6b
gDQFCOSY---YHJ-HWT-CDC13
20180706
YHJ-HWT-CDC13
gDQFCOSY
f2 (ppm)
f1 (ppm)

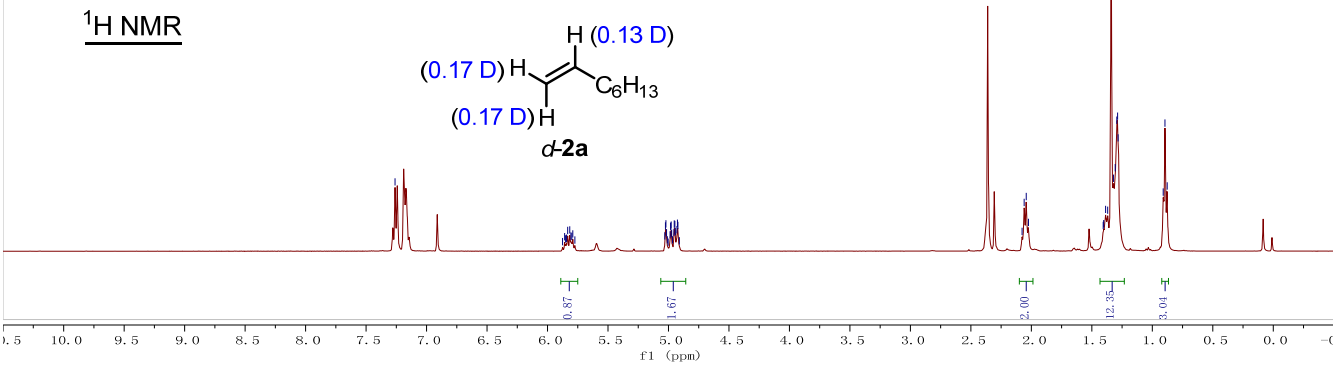
HSQC


gHSQCAD---YHJ-HWT-CDC13
20180706
YHJ-HWT-CDC13
gHSQCAD
f2 (ppm)
f1 (ppm)


^{2}H NMR
f1 (ppm)


^{1}H NMR
@ 700 MHz
H
D (0.82 D)
D (0.26 D)
(0.33 D)D
(0.33 D)D
C_6H_{13}
D (0.37 D)
d-3a
0.67
0.37
3.41
2.28
10.07
1.06
3.00
1.12
f1 (ppm)


XD-20G-SM2-CDCL3.1.fid
boss XD
^{2}H NMR
f1 (ppm)


^{1}H NMR
H (0.13 D)
(0.17 D) H
C_6H_{13}
(0.17 D) H
d-2a
0.87
1.67
2.00
12.35
3.04
f1 (ppm)

7 Density Functional Theory (DFT) Study

7.1 Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

7.2 Computational Methods

Geometry optimizations and single-point energy calculations were carried out using Gaussian 09. The geometries of intermediates and transition states were optimized using the B3LYP functional[15] with a mixed basis set of SDD for Ir and 6-31G(d) for other atoms in the gas phase. Vibrational frequency calculations were performed for all the stationary points to confirm if each optimized structure is a local minimum or a transition state structure. Solvation energy corrections were calculated in cyclopentanone solvent with the SMD continuum solvation model[16] based on the gas-phase optimized geometries. The DFT-D3(BJ) method

developed by Grimme and co-workers[17] with a mixed basis set of SDD for Ir and 6-311+G(d,p) for other atoms was used for solvation single-point energy calculations.

7.3 Complete free energy profiles of the reaction pathways shown in Figure 1

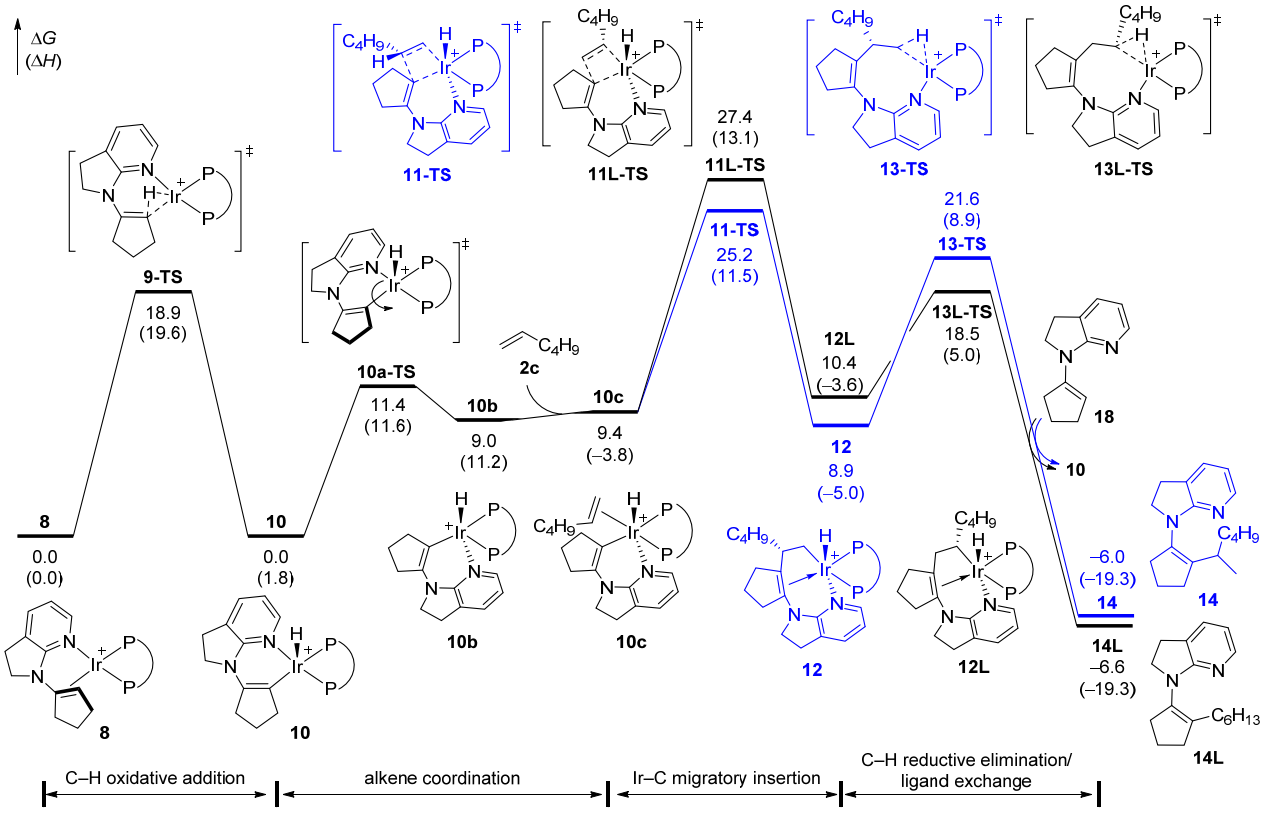


Figure S1. Free energy profile of Ir–C migratory insertion pathways to form the branched and linear alkylation products (shown in blue and black, respectively). The (*S*)-BINAP ligand was used in calculation. All energies are in kcal/mol and were performed at the B3LYP-D3(BJ)/6-311+G(d,p)−SDD/SMD(cyclopentanone)//B3LYP/6-31G(d)−SDD level of theory.

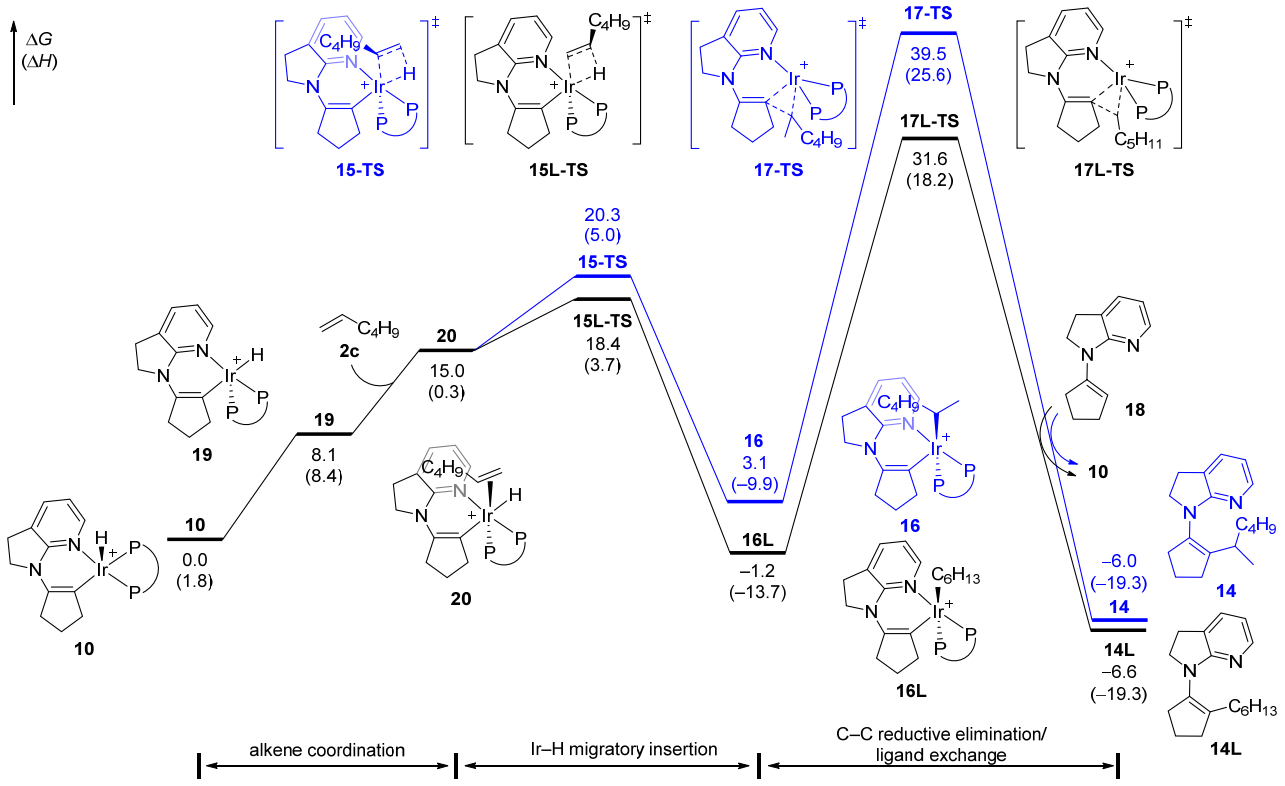


Figure S2. Free energy profile of Ir–H migratory insertion pathways to form the branched and linear alkylation products (shown in blue and black, respectively). The (*S*)-BINAP ligand was used in calculation. All energies are in kcal/mol and were performed at the B3LYP-D3(BJ)/6-311+G(d,p)−SDD/SMD(cyclopentanone)//B3LYP/6-31G(d)−SDD level of theory.

7.4 Other possible Ir–H or Ir–C insertion pathways from different configurations of Ir(III)-hydride complexes

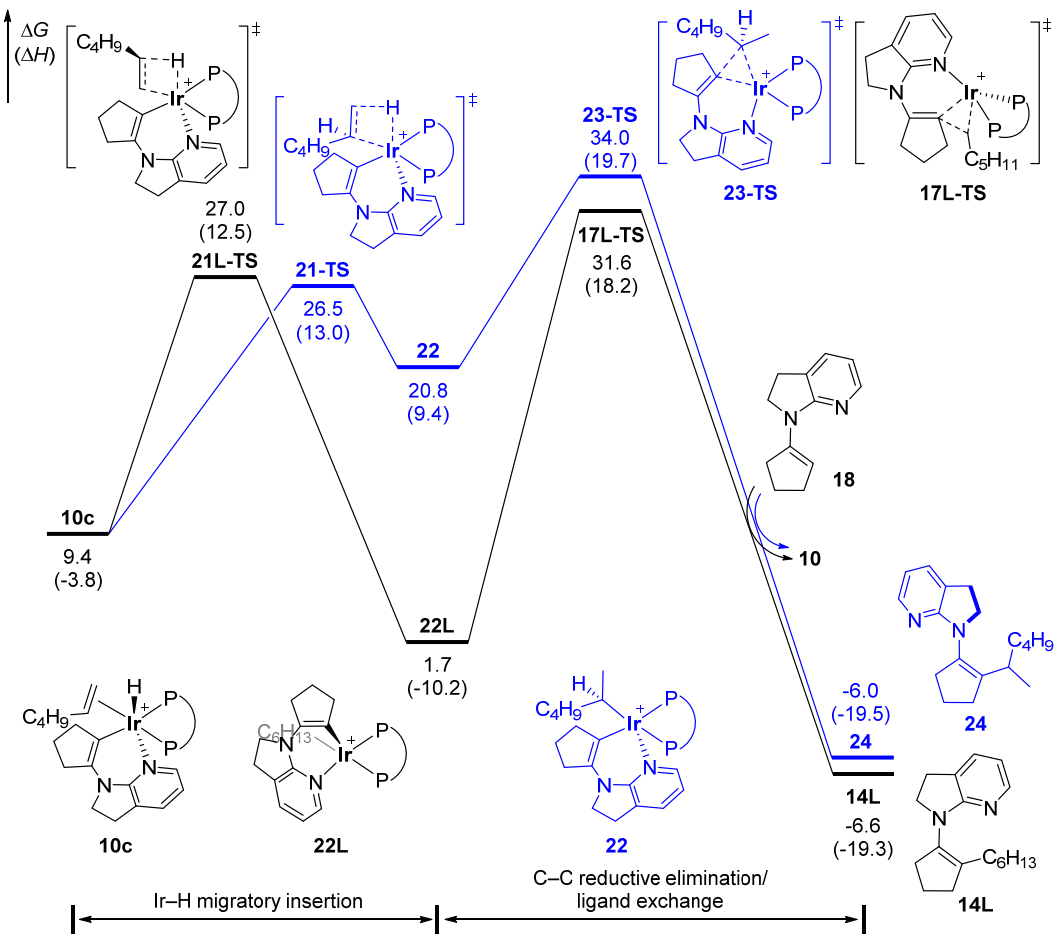


Figure S3. Free energy profile of Ir–H migratory insertion from complex **10c** to form the branched and linear alkylation products (shown in blue and black, respectively). The (*S*)-BINAP ligand was used in the calculations. All energies are in kcal/mol.

In addition to the free energy profiles shown in Figure 1 and 2, the Ir–H migratory insertion from complex **10c** is also calculated. As shown in Figure S3, the Ir–H migratory insertion occurs through transition state **21-TS** or **21L-TS**. The activation free energies are 26.5 and 27.0 kcal/mol, respectively. The rate-determining steps are the following C–C reductive elimination via transition state **17L-TS** or **23-TS**. The actiavtion free energies are much higher than the alkene insertion tration state **11-TS** (25.2 kcal/mol). The alkene insertion into Ir–C bond from intermediate **10** is also considered. As shown in Figure S4, the alkene lies at the *trans* position of hydride in transition state **25-TS**. The strong *trans*

effect of hydride suppressed the alkene insertion, thus result in the high activation free energy of **25-TS** (42.5 kcal/mol). Therefore, these possible reaction pathways could be ruled out in this reaction. These results are consistent with Huang's work.[18]

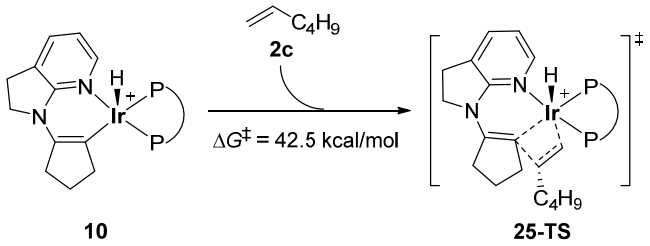


Figure S4. The Ir–C migratory insertion from intermediate **12**. The biphosphine ligand used in calculation is (*S*)-BINAP.

7.5 Cartesian coordinates and energies of optimized structures

2c
B3LYP SCF energy: -235.84430838 a.u.
B3LYP enthalpy: -235.669191 a.u.
B3LYP free energy: -235.710183 a.u.
B3LYP-D3(BJ) SCF energy in solution: -235.94575929 a.u.
B3LYP-D3(BJ) enthalpy in solution: -235.770642 a.u.
B3LYP-D3(BJ) free energy in solution: -235.811634 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	3.088717	-0.176480	-0.440044
H	3.096365	0.455824	-1.326095
C	2.045666	-0.203765	0.390784
H	2.083984	-0.856003	1.265709
C	0.777206	0.588104	0.222563
H	0.862902	1.240581	-0.656730
H	0.643176	1.250766	1.092101
C	-0.474134	-0.300900	0.088728
H	-0.539141	-0.970111	0.959439
H	-0.358396	-0.952511	-0.788548
C	-1.776351	0.501021	-0.033032
H	-1.883026	1.153325	0.845572

H	-1.709304	1.170616	-0.902311
C	-3.019446	-0.385080	-0.165847
H	-3.134210	-1.040508	0.706375
H	-3.931739	0.216212	-0.252812
H	-2.956652	-1.025654	-1.054193
H	3.976095	-0.779936	-0.267420

8

B3LYP SCF energy: -3058.13057527 a.u.
B3LYP enthalpy: -3057.210058 a.u.
B3LYP free energy: -3057.345829 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3059.23437508 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3058.313858 a.u.
B3LYP-D3(BJ) free energy in solution: -3058.449629 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	5.303907	-2.884406	-1.175392
C	4.332793	-2.167297	-0.512883
C	3.646935	-1.089951	-1.147180
C	3.994454	-0.791568	-2.504291
C	5.002401	-1.547651	-3.161397
C	5.649326	-2.572489	-2.512125
H	5.812049	-3.698220	-0.665605
H	4.086937	-2.428323	0.509110
C	2.629608	-0.314808	-0.480976
C	3.322710	0.266705	-3.158581
H	5.252437	-1.297048	-4.189149
H	6.421594	-3.143640	-3.019263
C	2.343728	0.984782	-2.517500
C	1.967833	0.705847	-1.172619
H	3.594258	0.514059	-4.181885
H	1.866484	1.793111	-3.053133
C	2.352859	-0.636402	0.959496
C	3.366339	-0.330493	1.935849
C	1.181173	-1.283584	1.358862
C	4.574440	0.347968	1.602918
C	3.173367	-0.716178	3.302522
C	1.015177	-1.660834	2.721236
C	5.530760	0.610742	2.558076
H	4.742879	0.662072	0.579820
C	4.178895	-0.431234	4.265305
C	1.981118	-1.390749	3.659100
H	0.121176	-2.187003	3.028899

C	5.337130	0.215838	3.903421
H	6.444425	1.126608	2.276433
H	4.014264	-0.738492	5.294964
H	1.839110	-1.703322	4.690702
H	6.103073	0.425399	4.644526
P	0.551211	1.680133	-0.413298
P	-0.227396	-1.546028	0.173388
C	0.382623	3.102488	-1.589959
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C	0.824189	4.405181	-1.323415
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H	-0.647120	1.855628	-3.024764
C	0.644518	5.423513	-2.265230
H	1.296459	4.643752	-0.377766
C	0.030488	5.154867	-3.487818
H	-0.914521	3.642924	-4.706530
H	0.988245	6.428372	-2.036636
H	-0.102391	5.947049	-4.218982
C	1.295048	2.376615	1.120090
C	0.642107	2.198363	2.347138
C	2.515690	3.072740	1.093785
C	1.177176	2.732350	3.520355
H	-0.275286	1.620395	2.376824
C	3.042754	3.616556	2.264925
H	3.061337	3.184662	0.161258
C	2.371943	3.452332	3.479274
H	0.662824	2.582181	4.465504
H	3.983576	4.158287	2.230645
H	2.787197	3.872687	4.390693
C	-1.354481	-2.714377	1.071674
C	-2.172378	-2.192491	2.090736
C	-1.436417	-4.084074	0.783264
C	-3.021924	-3.023191	2.820288
H	-2.146465	-1.127930	2.306476
C	-2.299782	-4.912480	1.506477
H	-0.834569	-4.516624	-0.007265
C	-3.088059	-4.388752	2.530069
H	-3.634902	-2.602596	3.613038
H	-2.349458	-5.970862	1.266356
H	-3.751998	-5.036546	3.095449
C	0.463209	-2.547462	-1.209975
C	1.288486	-3.660147	-0.977679
C	0.132770	-2.212514	-2.532113
C	1.748003	-4.433518	-2.043748
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C	0.595764	-2.985464	-3.598573

H	-0.472092	-1.329731	-2.725551
C	1.398610	-4.100863	-3.354813
H	2.386609	-5.290616	-1.850916
H	0.335794	-2.711590	-4.617262
H	1.760115	-4.703509	-4.183028
C	-6.275593	-0.323103	1.155753
C	-5.421271	0.942087	1.464929
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H	-6.354621	-0.964275	2.042996
H	-5.797820	1.810567	0.906559
H	-5.404960	1.190218	2.527494
C	-5.471781	-1.013668	0.075830
C	-4.198905	-0.432305	0.076649
C	-5.706363	-2.035008	-0.823293
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C	-4.650605	-2.417145	-1.678787
H	-4.786870	-3.210583	-2.404972
C	-3.419821	-1.784919	-1.590762
H	-2.589273	-2.074244	-2.222409
N	-3.176954	-0.783489	-0.705346
N	-4.055142	0.589976	0.978251
C	-3.107660	1.611980	0.612091
C	-2.940058	2.108469	-0.704256
H	-3.521517	1.721748	-1.539219
C	-2.859584	2.701384	1.638037
H	-3.838306	3.028648	2.020665
H	-2.282230	2.369732	2.505614
C	-2.201311	3.835898	0.829304
H	-2.464003	4.826817	1.210886
H	-1.114083	3.748061	0.881655
C	-2.685668	3.608779	-0.618044
H	-3.657585	4.104599	-0.771138
H	-2.007147	4.016658	-1.365597
Ir	-1.417301	0.424263	-0.367948

9-TS

B3LYP SCF energy: -3058.09317076 a.u.
B3LYP enthalpy: -3057.177462 a.u.
B3LYP free energy: -3057.314338 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3059.19826898 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3058.282560 a.u.
B3LYP-D3(BJ) free energy in solution: -3058.419436 a.u.
Imaginary frequency: -846.4266 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.196539	0.925592	1.231702
C	5.018928	0.685790	0.558946
C	4.024472	-0.181929	1.098336
C	4.282556	-0.779682	2.374255
C	5.513386	-0.524919	3.037073
C	6.454263	0.309146	2.480031
H	6.936653	1.592942	0.799337
H	4.843739	1.167291	-0.395995
C	2.777865	-0.443703	0.427002
C	3.287264	-1.600699	2.955121
H	5.692625	-0.996602	3.999894
H	7.391099	0.501269	2.994919
C	2.086539	-1.808239	2.322818
C	1.808605	-1.236519	1.049031
H	3.478589	-2.060299	3.921509
H	1.343920	-2.428408	2.806822
C	2.562115	0.153631	-0.931185
C	3.347536	-0.335496	-2.040033
C	1.625078	1.162098	-1.147286
C	4.307870	-1.377420	-1.901115
C	3.163376	0.230019	-3.343574
C	1.423633	1.671864	-2.466289
C	5.055663	-1.806881	-2.975901
H	4.455697	-1.838759	-0.932335
C	3.950832	-0.231019	-4.431281
C	2.178644	1.234789	-3.522989
H	0.660889	2.423970	-2.637569
C	4.884430	-1.226125	-4.253814
H	5.785039	-2.600402	-2.839806
H	3.799230	0.217817	-5.409657
H	2.021836	1.649943	-4.515413
H	5.485027	-1.570626	-5.090643
P	0.132086	-1.558173	0.281551
P	0.347506	1.700334	0.074193
C	-0.606563	-2.788386	1.463819
C	-1.392631	-2.286897	2.514946
C	-0.427089	-4.176697	1.366104
C	-1.967986	-3.144825	3.452487
H	-1.563263	-1.217819	2.597303
C	-1.011960	-5.036436	2.298772
H	0.159496	-4.598107	0.557665
C	-1.779578	-4.524363	3.346056
H	-2.568227	-2.736038	4.260666
H	-0.863872	-6.108662	2.204755

H	-2.230487	-5.195078	4.071872
C	0.574787	-2.535361	-1.225932
C	-0.101169	-2.306596	-2.433864
C	1.584008	-3.514010	-1.188264
C	0.202116	-3.059093	-3.570623
H	-0.850636	-1.521842	-2.482055
C	1.879808	-4.268781	-2.323095
H	2.152418	-3.677878	-0.277406
C	1.186393	-4.046226	-3.515353
H	-0.327591	-2.867122	-4.499563
H	2.660336	-5.023041	-2.278830
H	1.422391	-4.631898	-4.399249
C	0.243164	3.548489	-0.078379
C	-0.735703	4.193092	0.698913
C	1.188720	4.331147	-0.753813
C	-0.783987	5.582958	0.774702
H	-1.464583	3.601011	1.246344
C	1.135043	5.727006	-0.680546
H	1.978929	3.866657	-1.332889
C	0.149917	6.356005	0.078273
H	-1.548714	6.063333	1.378668
H	1.873399	6.318013	-1.215148
H	0.113260	7.440015	0.136150
C	0.960862	1.730748	1.819714
C	2.181219	2.331147	2.163509
C	0.086269	1.336391	2.840748
C	2.530573	2.498023	3.502279
H	2.859813	2.675067	1.389142
C	0.431287	1.515632	4.182472
H	-0.878462	0.906507	2.582702
C	1.656972	2.091663	4.515056
H	3.484309	2.952483	3.754552
H	-0.259540	1.209666	4.963409
H	1.928568	2.233209	5.557281
C	-6.676874	-0.716805	0.622212
C	-6.305515	0.660785	0.032685
H	-7.616320	-1.096718	0.211469
H	-6.793777	-0.660176	1.711914
H	-6.793193	0.810219	-0.937101
H	-6.571262	1.495440	0.684676
C	-5.480139	-1.559032	0.262238
C	-4.406781	-0.700590	-0.070974
C	-5.297816	-2.919866	0.197320
H	-6.103844	-3.610942	0.426814
C	-4.033508	-3.385706	-0.212324
H	-3.832536	-4.444718	-0.326300

C	-3.020144	-2.479613	-0.444914
H	-2.047806	-2.827824	-0.753075
N	-3.151539	-1.123583	-0.316085
N	-4.833500	0.606918	-0.156484
C	-4.138260	1.620233	-0.798515
C	-2.787952	1.694940	-1.027442
C	-4.887188	2.849181	-1.286127
H	-5.873596	2.625697	-1.705324
H	-5.046335	3.557443	-0.458497
C	-3.913681	3.416480	-2.332668
H	-4.111139	2.942051	-3.301473
H	-4.011807	4.498385	-2.463127
C	-2.528753	2.994877	-1.806707
H	-1.799556	2.866890	-2.614516
H	-2.130366	3.770625	-1.149236
Ir	-1.435740	0.259586	-0.233504
H	-1.931726	0.724245	-1.712766

10

B3LYP SCF energy: -3058.11821345 a.u.
B3LYP enthalpy: -3057.200333 a.u.
B3LYP free energy: -3057.338949 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3059.22881556 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3058.310935 a.u.
B3LYP-D3(BJ) free energy in solution: -3058.449551 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	6.021895	1.194905	1.621337
C	4.913564	0.896480	0.860161
C	3.932826	-0.031926	1.317134
C	4.131122	-0.632406	2.602389
C	5.291032	-0.313837	3.359000
C	6.220312	0.580363	2.881393
H	6.753182	1.907443	1.250427
H	4.784106	1.377978	-0.102147
C	2.755789	-0.354067	0.552937
C	3.149864	-1.525010	3.095072
H	5.425397	-0.787098	4.328309
H	7.103067	0.820015	3.467013
C	2.016266	-1.797780	2.370084
C	1.795422	-1.217968	1.088428
H	3.298768	-1.991121	4.065807
H	1.282938	-2.476491	2.785393

C	2.616815	0.248665	-0.814146
C	3.496977	-0.209553	-1.863626
C	1.678707	1.240062	-1.094296
C	4.474286	-1.223692	-1.656593
C	3.395560	0.360135	-3.174509
C	1.566305	1.760623	-2.420002
C	5.310641	-1.626942	-2.674619
H	4.564384	-1.683371	-0.680040
C	4.272241	-0.074899	-4.203175
C	2.405416	1.345055	-3.420804
H	0.804035	2.499843	-2.642288
C	5.216480	-1.045775	-3.960438
H	6.051246	-2.399268	-2.487237
H	4.181464	0.375253	-5.188374
H	2.314211	1.765166	-4.419240
H	5.885865	-1.369982	-4.751901
P	0.196872	-1.611480	0.196308
P	0.293332	1.724007	0.025094
C	-0.596455	-2.851562	1.328011
C	-1.390126	-2.366968	2.381961
C	-0.454065	-4.239467	1.181594
C	-2.013724	-3.241921	3.270918
H	-1.519337	-1.296851	2.513662
C	-1.086610	-5.116248	2.066584
H	0.144934	-4.645931	0.374333
C	-1.865283	-4.621926	3.113562
H	-2.617598	-2.846529	4.083060
H	-0.965882	-6.188014	1.935618
H	-2.353394	-5.305762	3.802110
C	0.776814	-2.615025	-1.244885
C	0.133585	-2.519710	-2.488914
C	1.850462	-3.512868	-1.108546
C	0.541777	-3.312498	-3.564232
H	-0.681263	-1.815929	-2.627116
C	2.253465	-4.306770	-2.181890
H	2.378143	-3.587525	-0.162257
C	1.598205	-4.210472	-3.411831
H	0.034595	-3.222076	-4.520657
H	3.084191	-4.995840	-2.058815
H	1.915737	-4.826714	-4.248045
C	0.086451	3.555273	-0.168575
C	-1.043280	4.144715	0.424347
C	1.082119	4.386462	-0.700873
C	-1.185052	5.530264	0.458810
H	-1.820158	3.515071	0.849036
C	0.934460	5.776166	-0.668824

H	1.979069	3.963171	-1.139686
C	-0.197451	6.351101	-0.092934
H	-2.067197	5.969662	0.915874
H	1.711998	6.405783	-1.092108
H	-0.308748	7.431244	-0.067914
C	0.768361	1.783032	1.809238
C	1.938565	2.425176	2.240330
C	-0.165769	1.360893	2.763973
C	2.181250	2.605155	3.600823
H	2.662563	2.787975	1.517644
C	0.070393	1.554115	4.126901
H	-1.092579	0.891994	2.439937
C	1.248437	2.171466	4.546991
H	3.098237	3.090589	3.921843
H	-0.665802	1.226168	4.855590
H	1.436674	2.322973	5.605997
C	-6.509362	-0.739129	0.937668
C	-6.153290	0.681326	0.428964
H	-7.491620	-1.065509	0.584077
H	-6.532750	-0.768448	2.034014
H	-6.781733	0.964824	-0.421421
H	-6.260790	1.448312	1.200586
C	-5.377426	-1.584537	0.407774
C	-4.340710	-0.720951	-0.024764
C	-5.223762	-2.939621	0.257702
H	-6.008890	-3.633791	0.543847
C	-4.017390	-3.405184	-0.314424
H	-3.850633	-4.462065	-0.487510
C	-3.023203	-2.506261	-0.624566
H	-2.086955	-2.845890	-1.041188
N	-3.128061	-1.151026	-0.439392
N	-4.741050	0.586428	-0.005432
C	-4.104758	1.568552	-0.782405
C	-2.783540	1.574470	-1.100520
C	-4.904981	2.690446	-1.420902
H	-5.882551	2.367790	-1.797511
H	-5.098323	3.502313	-0.703911
C	-3.970317	3.137145	-2.566529
H	-4.275781	2.635601	-3.491432
H	-4.016601	4.214883	-2.749679
C	-2.554209	2.658923	-2.153612
H	-2.001603	2.263151	-3.014062
H	-1.958692	3.488432	-1.762095
Ir	-1.415188	0.217746	-0.401883
H	-0.846322	0.180475	-1.835691

10a-TS

B3LYP SCF energy: -3058.11181512 a.u.
B3LYP enthalpy: -3057.194103 a.u.
B3LYP free energy: -3057.330129 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3059.21312918 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3058.295417 a.u.
B3LYP-D3(BJ) free energy in solution: -3058.431443 a.u.
Imaginary frequency: -26.6016 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	5.708348	1.782012	2.091591
C	4.649432	1.486145	1.261721
C	3.955135	0.244215	1.361598
C	4.400525	-0.683049	2.356471
C	5.504636	-0.356848	3.189095
C	6.148317	0.851709	3.063377
H	6.214857	2.738206	1.995618
H	4.337584	2.214837	0.523029
C	2.826736	-0.084775	0.521684
C	3.723042	-1.918186	2.476453
H	5.827080	-1.082334	3.931557
H	6.990270	1.095483	3.704682
C	2.625175	-2.196921	1.702687
C	2.128753	-1.278087	0.730007
H	4.077661	-2.650639	3.197273
H	2.140170	-3.153170	1.833538
C	2.540719	0.879450	-0.591871
C	3.489896	0.925120	-1.679736
C	1.476771	1.780320	-0.573802
C	4.576178	0.009847	-1.788287
C	3.352194	1.916664	-2.704736
C	1.364422	2.760013	-1.606121
C	5.465055	0.078587	-2.838242
H	4.705923	-0.755371	-1.032877
C	4.288300	1.967258	-3.771410
C	2.278076	2.836716	-2.624728
H	0.544585	3.466554	-1.586267
C	5.326836	1.068091	-3.839726
H	6.283060	-0.633757	-2.896832
H	4.166088	2.731444	-4.534592
H	2.178300	3.602798	-3.389404
H	6.038783	1.113045	-4.658656
P	0.547479	-1.731029	-0.188070

P	-0.044222	1.532844	0.447988
C	0.109490	-3.344374	0.622021
C	-0.285957	-3.346657	1.974275
C	0.091402	-4.554940	-0.085359
C	-0.672212	-4.529488	2.600611
H	-0.279208	-2.420581	2.542361
C	-0.311591	-5.738824	0.542435
H	0.389706	-4.583091	-1.127324
C	-0.690081	-5.731093	1.884218
H	-0.961807	-4.514394	3.647719
H	-0.319945	-6.666869	-0.022172
H	-0.994802	-6.652751	2.371791
C	1.143827	-2.262114	-1.852385
C	0.293159	-2.149440	-2.963497
C	2.408844	-2.847622	-2.022980
C	0.700305	-2.606410	-4.218668
H	-0.688483	-1.697986	-2.847992
C	2.814546	-3.301125	-3.278139
H	3.077920	-2.954294	-1.174738
C	1.962167	-3.180772	-4.378253
H	0.031792	-2.509824	-5.069487
H	3.797342	-3.748560	-3.396567
H	2.280954	-3.533253	-5.355060
C	-0.761229	3.222190	0.699151
C	-2.126939	3.370409	0.981272
C	0.078639	4.343404	0.814997
C	-2.645762	4.616456	1.338340
H	-2.786092	2.513353	0.918270
C	-0.444321	5.587951	1.167410
H	1.143673	4.256242	0.626164
C	-1.808606	5.729412	1.426248
H	-3.706723	4.714767	1.550767
H	0.218253	6.445561	1.241201
H	-2.214203	6.698729	1.701307
C	0.345494	1.155503	2.212132
C	1.400767	1.790820	2.881204
C	-0.547690	0.357139	2.941158
C	1.576050	1.604374	4.252158
H	2.093358	2.425350	2.338095
C	-0.376318	0.182083	4.316258
H	-1.381548	-0.119694	2.431884
C	0.688939	0.800908	4.972387
H	2.406866	2.089029	4.756606
H	-1.078083	-0.432796	4.873297
H	0.824124	0.664148	6.041469
C	-6.699491	-0.454667	0.664638

C	-6.235575	0.696494	-0.257982
H	-7.615128	-0.927385	0.297679
H	-6.907311	-0.087744	1.677107
H	-6.728934	0.659666	-1.235172
H	-6.415921	1.682719	0.176505
C	-5.516860	-1.389642	0.664633
C	-4.405501	-0.727779	0.074985
C	-5.380671	-2.684205	1.089037
H	-6.214763	-3.229011	1.522280
C	-4.119120	-3.299696	0.913582
H	-3.951516	-4.332011	1.198059
C	-3.078709	-2.573216	0.386850
H	-2.113661	-3.028122	0.253447
N	-3.161290	-1.256799	-0.000673
N	-4.779699	0.480044	-0.437742
C	-4.010761	1.276865	-1.277064
C	-2.656721	1.215527	-1.429836
C	-4.693129	2.284618	-2.186712
H	-5.203619	1.770157	-3.015925
H	-5.454253	2.888249	-1.678367
C	-3.507320	3.133460	-2.686307
H	-3.648464	3.493883	-3.709474
H	-3.392571	4.009693	-2.038160
C	-2.278652	2.211689	-2.527306
H	-2.067417	1.667726	-3.459736
H	-1.369696	2.773313	-2.294893
Ir	-1.337319	-0.045875	-0.544089
H	-0.396320	0.387979	-1.712257

10b

B3LYP SCF energy: -3058.11686277 a.u.
B3LYP enthalpy: -3057.197920 a.u.
B3LYP free energy: -3057.337080 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3059.21500579 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3058.296063 a.u.
B3LYP-D3(BJ) free energy in solution: -3058.435223 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-5.917215	-1.472093	1.887736
C	-4.761789	-1.308947	1.155318
C	-4.082608	-0.055195	1.108913
C	-4.653733	1.028449	1.849522
C	-5.854993	0.835743	2.583258

C	-6.477571	-0.389968	2.606744
H	-6.406633	-2.441667	1.908319
H	-4.360682	-2.155080	0.610275
C	-2.852922	0.137307	0.368550
C	-4.004525	2.284588	1.817417
H	-6.269298	1.678717	3.130340
H	-7.394052	-0.530808	3.172189
C	-2.814062	2.439161	1.155605
C	-2.188348	1.365709	0.451053
H	-4.455103	3.129713	2.331741
H	-2.347223	3.414574	1.162349
C	-2.471702	-1.007815	-0.533435
C	-3.318980	-1.220297	-1.682426
C	-1.443406	-1.918132	-0.274308
C	-4.327210	-0.290662	-2.072844
C	-3.151796	-2.395150	-2.487822
C	-1.300951	-3.081808	-1.085155
C	-5.115656	-0.515622	-3.178713
H	-4.467790	0.615208	-1.496204
C	-3.991821	-2.606447	-3.613848
C	-2.143897	-3.326345	-2.138710
H	-0.505595	-3.785657	-0.871944
C	-4.956224	-1.687893	-3.955420
H	-5.869568	0.214727	-3.458114
H	-3.851444	-3.508417	-4.203910
H	-2.029132	-4.229984	-2.731947
H	-5.591915	-1.855104	-4.819984
P	-0.515154	1.707490	-0.324009
P	0.037648	-1.471531	0.730324
C	0.009487	3.293595	0.487795
C	-0.002759	3.431774	1.889610
C	0.541634	4.339037	-0.281712
C	0.481617	4.590840	2.496391
H	-0.404450	2.637337	2.513081
C	1.039825	5.493124	0.329987
H	0.559927	4.264344	-1.363979
C	1.007300	5.625880	1.717794
H	0.443822	4.685934	3.578302
H	1.442149	6.292810	-0.285539
H	1.382834	6.528983	2.190353
C	-0.956513	2.271546	-2.032790
C	-0.084111	2.025106	-3.103534
C	-2.135242	2.996596	-2.273556
C	-0.380821	2.493061	-4.385667
H	0.827130	1.456227	-2.938615
C	-2.431861	3.460260	-3.555054

H	-2.826910	3.199582	-1.461957
C	-1.555794	3.209794	-4.614003
H	0.304800	2.291783	-5.204053
H	-3.348781	4.017303	-3.726197
H	-1.789667	3.570659	-5.611577
C	0.883847	-3.062993	1.148256
C	2.274771	-3.199662	1.066751
C	0.125753	-4.121181	1.681336
C	2.896199	-4.375768	1.495894
H	2.868590	-2.389362	0.660435
C	0.747482	-5.296388	2.098374
H	-0.953046	-4.034228	1.767640
C	2.135992	-5.426541	2.007443
H	3.976601	-4.468047	1.427168
H	0.147363	-6.108822	2.497933
H	2.619625	-6.341624	2.336871
C	-0.465631	-0.959706	2.427937
C	-1.663693	-1.400309	3.007356
C	0.449726	-0.242950	3.212565
C	-1.950821	-1.104984	4.340670
H	-2.379939	-1.968162	2.424327
C	0.162562	0.046276	4.547374
H	1.393967	0.075139	2.784269
C	-1.041474	-0.379629	5.112513
H	-2.888431	-1.442346	4.772873
H	0.882736	0.596921	5.146350
H	-1.266472	-0.153848	6.150922
C	6.685895	0.489322	0.287360
C	6.166712	-0.266223	-0.954591
H	7.449873	1.226596	0.024782
H	7.135463	-0.202079	1.011011
H	6.385588	0.279976	-1.879944
H	6.581212	-1.271590	-1.044919
C	5.434284	1.112681	0.849717
C	4.301790	0.547756	0.207765
C	5.253761	2.049173	1.835642
H	6.097823	2.501375	2.348537
C	3.927042	2.403964	2.159586
H	3.711689	3.146133	2.920002
C	2.883236	1.801088	1.494028
H	1.866028	2.066129	1.728209
N	3.024513	0.862395	0.507622
N	4.695470	-0.336200	-0.769826
C	3.886993	-1.073477	-1.609338
C	2.514173	-1.182024	-1.563814
C	4.528553	-1.953067	-2.669220

H	5.305996	-1.446518	-3.252388
H	5.007942	-2.822400	-2.191050
C	3.323004	-2.381912	-3.525391
H	3.196890	-1.674544	-4.353361
H	3.446316	-3.379380	-3.957278
C	2.120707	-2.270380	-2.564799
H	1.185130	-2.056823	-3.086781
H	1.969101	-3.217393	-2.022220
Ir	1.226493	-0.024722	-0.540976
H	0.194992	-0.515004	-1.621131

10c

B3LYP SCF energy: -3293.96722501 a.u.
B3LYP enthalpy: -3292.869596 a.u.
B3LYP free energy: -3293.024702 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.18734312 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.089714 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.244820 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-5.906158	-2.580323	-0.110230
C	-4.826195	-1.774537	-0.393440
C	-4.139370	-1.072656	0.638666
C	-4.610532	-1.232686	1.981421
C	-5.729804	-2.068260	2.242872
C	-6.367502	-2.730031	1.219860
H	-6.411120	-3.106229	-0.915603
H	-4.487425	-1.675177	-1.418115
C	-3.002211	-0.231430	0.371250
C	-3.957229	-0.522283	3.015143
H	-6.073398	-2.171568	3.268983
H	-7.223844	-3.365219	1.427051
C	-2.855122	0.254025	2.750145
C	-2.328835	0.385365	1.434621
H	-4.342437	-0.589249	4.029676
H	-2.407838	0.804124	3.565826
C	-2.665353	0.048658	-1.067560
C	-3.570770	0.906533	-1.801961
C	-1.538538	-0.459474	-1.708746
C	-4.742881	1.467407	-1.220201
C	-3.296360	1.220888	-3.172348
C	-1.242175	-0.059116	-3.046984
C	-5.603700	2.249468	-1.959775

H	-4.967064	1.274774	-0.178612
C	-4.202099	2.027337	-3.909660
C	-2.100106	0.736088	-3.759814
H	-0.319521	-0.386624	-3.511326
C	-5.340636	2.527432	-3.320431
H	-6.494685	2.656998	-1.490583
H	-3.976474	2.243262	-4.950919
H	-1.866701	1.008341	-4.786196
H	-6.031773	3.139418	-3.892734
P	-0.743795	1.348201	1.148164
P	-0.235298	-1.444278	-0.841221
C	-0.299045	2.145233	2.775518
C	-0.150229	1.411539	3.968692
C	0.061460	3.505360	2.801398
C	0.315905	2.013943	5.138300
H	-0.426005	0.363628	4.007431
C	0.541553	4.104615	3.968108
H	-0.045791	4.115231	1.911870
C	0.668345	3.364099	5.142677
H	0.399073	1.424280	6.047021
H	0.807100	5.157924	3.954980
H	1.032929	3.832994	6.051833
C	-1.422005	2.817943	0.229431
C	-0.911512	3.271122	-0.993476
C	-2.503317	3.511840	0.804283
C	-1.457091	4.395316	-1.620989
H	-0.098476	2.740093	-1.473145
C	-3.043009	4.634175	0.180668
H	-2.924514	3.176946	1.747713
C	-2.518382	5.082092	-1.034950
H	-1.049439	4.727598	-2.571666
H	-3.875273	5.157748	0.642589
H	-2.939734	5.956719	-1.522176
C	0.394471	-2.688650	-2.063408
C	1.510459	-3.448498	-1.674365
C	-0.263083	-3.024168	-3.257038
C	1.975304	-4.491035	-2.475525
H	2.011362	-3.239454	-0.735870
C	0.207691	-4.067118	-4.059434
H	-1.151653	-2.487440	-3.568611
C	1.331213	-4.798121	-3.676339
H	2.837321	-5.070178	-2.155985
H	-0.313944	-4.308616	-4.981234
H	1.695202	-5.609120	-4.300527
C	-1.079476	-2.641709	0.295397
C	-1.905558	-3.637474	-0.254886

C	-0.853526	-2.644448	1.675288
C	-2.493443	-4.600869	0.562008
H	-2.085331	-3.672384	-1.324115
C	-1.434678	-3.615705	2.492663
H	-0.223374	-1.886874	2.115719
C	-2.256673	-4.596165	1.938604
H	-3.133918	-5.358902	0.120665
H	-1.240450	-3.603887	3.561609
H	-2.708247	-5.354085	2.572297
C	5.322570	-3.269233	1.682161
C	5.438318	-2.550684	0.321321
H	6.244831	-3.196286	2.265347
H	5.105591	-4.336809	1.546195
H	6.234046	-1.793520	0.334185
H	5.638385	-3.237307	-0.502893
C	4.153312	-2.569467	2.325758
C	3.465380	-1.817787	1.331433
C	3.695365	-2.570913	3.617925
H	4.206007	-3.130405	4.396844
C	2.544184	-1.806192	3.905360
H	2.147915	-1.737807	4.912318
C	1.924274	-1.129822	2.877360
H	1.058994	-0.518836	3.073943
N	2.333218	-1.129485	1.577481
N	4.127776	-1.885899	0.133230
C	3.816586	-1.211330	-1.062081
C	2.749795	-0.416462	-1.300625
C	4.652141	-1.503276	-2.298613
H	5.733175	-1.429616	-2.130997
H	4.454666	-2.523963	-2.663346
C	4.143307	-0.443617	-3.294599
H	4.780496	0.446961	-3.235448
H	4.163112	-0.793423	-4.331306
C	2.723897	-0.100318	-2.793787
H	2.440602	0.932383	-3.017949
H	1.977386	-0.739493	-3.290649
Ir	1.266190	0.195552	-0.005384
H	0.700588	1.007369	-1.230483
C	2.320745	2.410673	0.067180
H	1.471600	3.049941	0.292430
C	2.792917	1.591344	1.068421
H	2.388283	1.647649	2.073500
H	3.764804	1.118306	0.964035
C	3.121134	2.837870	-1.134329
H	3.877671	2.083496	-1.370207
H	2.470029	2.939050	-2.010767

C	3.806082	4.196507	-0.866499
H	3.047022	4.946927	-0.602280
H	4.465757	4.102981	0.007249
C	4.615500	4.695105	-2.072052
H	3.950610	4.782040	-2.942915
H	5.370153	3.941236	-2.336626
C	5.302383	6.040195	-1.814648
H	4.569871	6.821859	-1.579721
H	6.000755	5.974872	-0.971656
H	5.869765	6.368772	-2.692059

11-TS

B3LYP SCF energy: -3293.94512989 a.u.
B3LYP enthalpy: -3292.849681 a.u.
B3LYP free energy: -3293.004666 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.16160909 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.066160 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.221145 a.u.
Imaginary frequency: -314.7382 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.272485	2.000654	0.854428
C	5.132102	1.464908	0.297976
C	4.366376	0.480269	0.987113
C	4.829110	0.060676	2.274694
C	6.012932	0.625061	2.820811
C	6.722684	1.577877	2.128040
H	6.835013	2.752986	0.308683
H	4.808172	1.802109	-0.679660
C	3.157606	-0.081529	0.436429
C	4.097313	-0.936543	2.960595
H	6.346737	0.287895	3.798880
H	7.627097	2.004834	2.551766
C	2.930799	-1.437258	2.438912
C	2.408033	-0.990740	1.190258
H	4.470305	-1.308727	3.911626
H	2.418083	-2.212337	2.990166
C	2.855184	0.259473	-0.995652
C	3.696842	-0.353523	-1.998745
C	1.858490	1.150644	-1.385854
C	4.706626	-1.305017	-1.677180
C	3.518162	-0.016691	-3.379473
C	1.678931	1.439470	-2.771989

C	5.496014	-1.866633	-2.656778
H	4.852567	-1.599455	-0.645255
C	4.353961	-0.604012	-4.365755
C	2.491044	0.893937	-3.731744
H	0.880610	2.103354	-3.079384
C	5.327993	-1.509843	-4.014910
H	6.256820	-2.591765	-2.382195
H	4.205062	-0.325304	-5.405990
H	2.344623	1.147019	-4.779013
H	5.963377	-1.955041	-4.775109
P	0.767053	-1.671718	0.574656
P	0.494138	1.679946	-0.250306
C	0.158258	-2.764585	1.954692
C	0.093961	-2.321808	3.290257
C	-0.382335	-4.026863	1.654653
C	-0.458737	-3.124576	4.290201
H	0.490404	-1.348031	3.562721
C	-0.949877	-4.822273	2.653103
H	-0.347535	-4.405485	0.638984
C	-0.984639	-4.378793	3.975210
H	-0.472310	-2.768103	5.316760
H	-1.353665	-5.796914	2.393557
H	-1.412599	-5.004649	4.752932
C	1.383937	-2.943987	-0.636975
C	0.992202	-2.976642	-1.981418
C	2.308705	-3.903732	-0.184656
C	1.500451	-3.947741	-2.849628
H	0.301240	-2.233656	-2.361421
C	2.811225	-4.873770	-1.048933
H	2.638445	-3.896686	0.849887
C	2.406201	-4.899829	-2.386370
H	1.186470	-3.952474	-3.889706
H	3.521413	-5.607842	-0.678566
H	2.799430	-5.654990	-3.061054
C	-0.033944	3.357244	-0.846957
C	-1.268359	3.842987	-0.389155
C	0.786890	4.218913	-1.593893
C	-1.683526	5.141487	-0.690223
H	-1.900467	3.209697	0.222874
C	0.367523	5.514647	-1.901370
H	1.761224	3.888861	-1.937707
C	-0.870982	5.978829	-1.456414
H	-2.638893	5.502636	-0.318129
H	1.016522	6.163333	-2.483076
H	-1.194197	6.988260	-1.694075
C	1.223667	2.221706	1.362628

C	2.280730	3.144038	1.408247
C	0.628495	1.815017	2.563254
C	2.743478	3.629631	2.629714
H	2.747977	3.485235	0.489919
C	1.086979	2.308306	3.787511
H	-0.201220	1.118217	2.538361
C	2.146888	3.214107	3.823156
H	3.569987	4.334131	2.649534
H	0.611343	1.987572	4.710645
H	2.504898	3.599341	4.773738
C	-5.424242	2.538134	1.796983
C	-5.246302	2.477620	0.263823
H	-6.452096	2.312020	2.095651
H	-5.186853	3.536445	2.185226
H	-6.071052	1.934626	-0.212631
H	-5.183859	3.467376	-0.192775
C	-4.428296	1.523056	2.293918
C	-3.571665	1.140288	1.237652
C	-4.244073	0.976233	3.545612
H	-4.889503	1.244869	4.377370
C	-3.201881	0.048824	3.703018
H	-3.020926	-0.444925	4.651342
C	-2.388809	-0.235654	2.618333
H	-1.585747	-0.949239	2.713207
N	-2.525441	0.311972	1.385061
N	-3.978606	1.734659	0.046286
C	-3.469845	1.530452	-1.221143
C	-2.433740	0.700656	-1.582728
C	-4.037287	2.329941	-2.381840
H	-5.133056	2.363229	-2.396551
H	-3.686673	3.371733	-2.322659
C	-3.442699	1.610768	-3.607605
H	-4.133182	0.828303	-3.945834
H	-3.273704	2.285883	-4.451584
C	-2.148733	0.976959	-3.060810
H	-1.836260	0.085344	-3.617350
H	-1.316606	1.689570	-3.137640
Ir	-0.985193	-0.202878	-0.329689
H	-0.200457	-0.507640	-1.651896
C	-3.168669	-1.315395	-1.469566
H	-2.976962	-1.372668	-2.538661
C	-2.225099	-1.989639	-0.628588
H	-1.598963	-2.725876	-1.130048
H	-2.604783	-2.335851	0.333793
C	-4.630786	-1.264152	-1.102709
H	-4.752168	-0.992477	-0.047835

H	-5.156690	-0.516428	-1.705938
C	-5.280910	-2.649497	-1.337913
H	-5.131680	-2.951136	-2.384217
H	-4.772768	-3.401843	-0.721663
C	-6.783138	-2.651349	-1.017961
H	-7.287528	-1.895445	-1.636004
H	-6.930088	-2.343377	0.027085
C	-7.435677	-4.018719	-1.246655
H	-7.335753	-4.336476	-2.291229
H	-6.973169	-4.789274	-0.618375
H	-8.504285	-3.991050	-1.007923

12

B3LYP SCF energy: -3293.97636281 a.u.
B3LYP enthalpy: -3292.878352 a.u.
B3LYP free energy: -3293.033017 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.19045696 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.092446 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.247111 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	6.554393	1.015157	0.848174
C	5.318023	0.735080	0.309149
C	4.385771	-0.102216	0.989768
C	4.782961	-0.637799	2.255699
C	6.068728	-0.342181	2.782228
C	6.941152	0.468721	2.094882
H	7.241883	1.659939	0.308068
H	5.049280	1.165838	-0.647796
C	3.076878	-0.401454	0.454161
C	3.873757	-1.467978	2.951329
H	6.346937	-0.768101	3.742811
H	7.922357	0.692008	2.503542
C	2.620555	-1.710735	2.451206
C	2.179633	-1.160849	1.209454
H	4.176339	-1.913073	3.895883
H	1.963812	-2.355072	3.017812
C	2.826497	0.085229	-0.945439
C	3.542251	-0.580751	-2.006220
C	2.031315	1.192770	-1.239922
C	4.302895	-1.766056	-1.790236
C	3.489952	-0.056038	-3.339008
C	1.997347	1.694414	-2.574153

C	4.970427	-2.382244	-2.825303
H	4.343845	-2.198763	-0.797787
C	4.201868	-0.705710	-4.382692
C	2.720231	1.107748	-3.582554
H	1.391587	2.563574	-2.800431
C	4.930019	-1.845775	-4.134278
H	5.535376	-3.290173	-2.634586
H	4.155523	-0.284884	-5.383971
H	2.694161	1.524555	-4.586451
H	5.469725	-2.338083	-4.938068
P	0.459863	-1.616865	0.611957
P	0.687043	1.770279	-0.106505
C	-0.322832	-2.433078	2.080824
C	-0.323706	-1.804877	3.340745
C	-1.010005	-3.649374	1.941814
C	-0.969319	-2.390248	4.430822
H	0.203532	-0.865321	3.480331
C	-1.671302	-4.223906	3.030591
H	-1.020372	-4.164486	0.988053
C	-1.649156	-3.601067	4.278124
H	-0.937424	-1.899761	5.399941
H	-2.193843	-5.167338	2.900563
H	-2.151481	-4.056638	5.126578
C	0.889524	-3.058964	-0.481223
C	0.563466	-3.112788	-1.841860
C	1.625910	-4.121536	0.075240
C	0.952895	-4.201310	-2.626912
H	0.008490	-2.299585	-2.293296
C	2.009616	-5.209054	-0.707120
H	1.903996	-4.104517	1.124219
C	1.673294	-5.252610	-2.062694
H	0.691416	-4.221591	-3.681123
H	2.573796	-6.021083	-0.257121
H	1.973980	-6.099682	-2.672634
C	0.411235	3.558540	-0.531349
C	-0.828291	4.132045	-0.210640
C	1.442216	4.399486	-0.983382
C	-1.039635	5.504870	-0.355578
H	-1.633647	3.502791	0.151736
C	1.226279	5.769196	-1.138966
H	2.421061	3.991899	-1.214306
C	-0.015226	6.326627	-0.826389
H	-2.005609	5.931516	-0.099052
H	2.033722	6.401703	-1.497099
H	-0.179465	7.393958	-0.943058
C	1.390328	2.080198	1.579617

C	2.665861	2.636797	1.755660
C	0.562933	1.917523	2.698893
C	3.112187	2.995555	3.026720
H	3.319990	2.787629	0.903102
C	1.006743	2.288350	3.971308
H	-0.437764	1.519489	2.575899
C	2.284044	2.823207	4.138700
H	4.108115	3.412262	3.147040
H	0.349541	2.164752	4.828080
H	2.631162	3.111211	5.126928
C	-5.302508	2.970260	0.348661
C	-4.648622	2.662870	-1.029655
H	-6.379908	2.780071	0.333459
H	-5.165550	4.023577	0.622523
H	-5.306256	2.051647	-1.661344
H	-4.393903	3.571259	-1.581118
C	-4.553927	2.065433	1.301076
C	-3.460979	1.500083	0.610520
C	-4.723822	1.742799	2.628146
H	-5.549644	2.145430	3.208420
C	-3.794222	0.857370	3.214121
H	-3.890946	0.551680	4.249935
C	-2.746353	0.367253	2.454466
H	-2.033323	-0.324066	2.880634
N	-2.542727	0.689079	1.149450
N	-3.425484	1.894134	-0.696451
C	-2.604930	1.297432	-1.697917
C	-2.662893	-0.022929	-2.155796
C	-2.101656	2.212082	-2.815085
H	-2.978236	2.676594	-3.293168
H	-1.468430	3.027536	-2.463203
C	-1.403082	1.257946	-3.799524
H	-1.479761	1.594084	-4.837594
H	-0.342514	1.173268	-3.552986
C	-2.094199	-0.092779	-3.560117
H	-2.966630	-0.219501	-4.223136
H	-1.448469	-0.959900	-3.729202
Ir	-0.987682	-0.046789	-0.389629
H	-0.098344	-0.449955	-1.621636
C	-3.375237	-1.251134	-1.615656
H	-3.399175	-1.974368	-2.442165
C	-2.370774	-1.712545	-0.549231
H	-1.885786	-2.644606	-0.839569
H	-2.830876	-1.844380	0.433611
C	-4.834159	-1.067066	-1.157525
H	-4.873870	-0.479638	-0.232763

H	-5.385664	-0.496793	-1.920343
C	-5.547271	-2.407336	-0.924115
H	-5.541141	-2.987885	-1.858391
H	-4.980720	-2.999630	-0.191659
C	-6.992854	-2.247600	-0.434795
H	-7.558884	-1.651684	-1.164924
H	-6.996065	-1.669021	0.500315
C	-7.702953	-3.586351	-0.208512
H	-7.749867	-4.172398	-1.134273
H	-7.178469	-4.191705	0.540904
H	-8.729798	-3.437754	0.142983

13-TS

B3LYP SCF energy: -3293.94769526 a.u.
B3LYP enthalpy: -3292.852589 a.u.
B3LYP free energy: -3293.008997 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.16549903 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.070393 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.226801 a.u.
Imaginary frequency: -943.3217 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.605190	0.889713	0.969123
C	5.410527	0.555483	0.372343
C	4.418415	-0.184253	1.078146
C	4.695797	-0.558107	2.433597
C	5.940851	-0.202912	3.019478
C	6.878749	0.504077	2.304076
H	7.347038	1.454012	0.411142
H	5.217639	0.858167	-0.650566
C	3.163401	-0.549677	0.482911
C	3.715244	-1.280331	3.155050
H	6.136717	-0.501062	4.046282
H	7.828583	0.770049	2.758870
C	2.505477	-1.595049	2.583567
C	2.202334	-1.225054	1.243377
H	3.929244	-1.586097	4.176222
H	1.777857	-2.145124	3.167049
C	2.919815	-0.248713	-0.966124
C	3.638161	-1.008235	-1.960041
C	1.981312	0.699881	-1.365881
C	4.624381	-1.979456	-1.625306
C	3.355373	-0.797644	-3.348807

C	1.674599	0.846339	-2.751114
C	5.306244	-2.669914	-2.603492
H	4.848333	-2.174732	-0.583789
C	4.073578	-1.525668	-4.333886
C	2.343656	0.127543	-3.708436
H	0.904131	1.544353	-3.056487
C	5.035758	-2.440391	-3.972652
H	6.060398	-3.398662	-2.319862
H	3.847269	-1.344874	-5.381696
H	2.103879	0.264815	-4.760015
H	5.584375	-2.989059	-4.732751
P	0.498251	-1.587291	0.572794
P	0.924083	1.650064	-0.169917
C	-0.268526	-2.661770	1.878385
C	-0.814966	-2.034223	3.013569
C	-0.367419	-4.056274	1.772532
C	-1.420139	-2.780592	4.023094
H	-0.776933	-0.951601	3.098711
C	-0.983275	-4.803203	2.781689
H	0.025101	-4.570252	0.902868
C	-1.505590	-4.171184	3.909236
H	-1.831590	-2.276753	4.893310
H	-1.053224	-5.882459	2.679571
H	-1.981696	-4.754650	4.692024
C	0.817907	-2.735696	-0.832042
C	0.097245	-2.622344	-2.028059
C	1.769543	-3.762847	-0.707345
C	0.303555	-3.528807	-3.070238
H	-0.609458	-1.809281	-2.151159
C	1.972876	-4.668367	-1.747641
H	2.358058	-3.852125	0.201322
C	1.236825	-4.555906	-2.929963
H	-0.260547	-3.426454	-3.993181
H	2.711396	-5.457229	-1.637927
H	1.398384	-5.260849	-3.740412
C	0.591467	3.225804	-1.099568
C	-0.628935	3.898719	-0.947119
C	1.581275	3.819817	-1.906393
C	-0.852425	5.129932	-1.570108
H	-1.410065	3.461122	-0.341732
C	1.356018	5.046163	-2.530742
H	2.528881	3.317405	-2.070546
C	0.137954	5.708232	-2.362466
H	-1.804856	5.634736	-1.432689
H	2.134094	5.482294	-3.150899
H	-0.036273	6.664050	-2.848198

C	1.983165	2.281403	1.222164
C	3.002667	3.228825	1.035309
C	1.700545	1.857057	2.529876
C	3.715773	3.731101	2.123415
H	3.241025	3.591890	0.042563
C	2.409581	2.363015	3.620396
H	0.937575	1.102310	2.696320
C	3.419132	3.304226	3.419397
H	4.501523	4.462518	1.957034
H	2.174663	2.016900	4.623137
H	3.971767	3.702835	4.265310
C	-5.899685	2.823363	0.757148
C	-5.604701	2.351693	-0.679742
H	-6.575190	2.125248	1.268318
H	-6.370060	3.810488	0.782217
H	-6.351280	1.654860	-1.068682
H	-5.532877	3.199812	-1.373329
C	-4.534858	2.796167	1.396504
C	-3.645066	2.057310	0.560969
C	-4.092752	3.311481	2.586928
H	-4.755446	3.880854	3.232809
C	-2.744643	3.090836	2.943041
H	-2.326427	3.494343	3.858137
C	-1.950253	2.351731	2.098321
H	-0.909232	2.182421	2.340853
N	-2.366286	1.800853	0.910350
N	-4.288950	1.670009	-0.588052
C	-3.765784	1.111996	-1.787939
C	-3.533578	-0.192787	-2.010846
C	-3.607666	1.968770	-3.034062
H	-4.586676	2.274506	-3.432591
H	-3.043303	2.889584	-2.841433
C	-2.876233	1.012861	-4.004397
H	-3.186593	1.145135	-5.044719
H	-1.798677	1.205001	-3.954925
C	-3.164002	-0.408934	-3.465722
H	-4.006638	-0.886232	-3.990265
H	-2.308968	-1.084744	-3.590997
Ir	-0.904298	0.224669	0.322016
H	-1.629596	-0.663774	-0.759198
C	-3.638302	-1.344765	-1.030729
H	-3.227289	-2.226344	-1.542938
C	-2.777973	-1.123534	0.247347
H	-2.508533	-2.082399	0.685892
H	-3.340291	-0.549159	0.987574
C	-5.115755	-1.671576	-0.694467

H	-5.544450	-0.828339	-0.135144
H	-5.679822	-1.738629	-1.635803
C	-5.314773	-2.971175	0.096846
H	-4.850914	-3.804258	-0.452483
H	-4.789034	-2.908214	1.059385
C	-6.793264	-3.295944	0.353277
H	-7.321662	-3.360801	-0.608288
H	-7.256998	-2.462112	0.899777
C	-6.996607	-4.596396	1.137475
H	-6.577337	-5.454280	0.597843
H	-6.506550	-4.549723	2.117850
H	-8.060150	-4.797443	1.306326

14

B3LYP SCF energy: -811.06434751 a.u.
B3LYP enthalpy: -810.633035 a.u.
B3LYP free energy: -810.704588 a.u.
B3LYP-D3(BJ) SCF energy in solution: -811.39757683 a.u.
B3LYP-D3(BJ) enthalpy in solution: -810.966264 a.u.
B3LYP-D3(BJ) free energy in solution: -811.037817 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.485542	-1.029100	2.159496
C	1.499131	0.153103	1.970236
H	1.947188	-1.939962	2.455365
H	3.226080	-0.822247	2.939053
H	0.564842	0.017128	2.520750
H	1.951226	1.100455	2.302012
C	3.077116	-1.184821	0.778580
C	2.288470	-0.452167	-0.137702
C	4.143375	-1.907816	0.285904
H	4.783275	-2.490150	0.945294
C	4.384323	-1.869834	-1.101751
H	5.213474	-2.415554	-1.540492
C	3.534114	-1.119314	-1.906595
H	3.695543	-1.078992	-2.982700
N	2.482787	-0.407046	-1.453783
N	1.248236	0.199053	0.512974
C	0.531023	1.284592	-0.053339
C	-0.800118	1.459746	0.045786
C	1.215291	2.394872	-0.832274
H	2.141158	2.735359	-0.350415
H	1.497276	2.036876	-1.829525

C	0.126375	3.491157	-0.878182
H	0.290364	4.203154	-0.060489
H	0.134805	4.062215	-1.812230
C	-1.212722	2.746842	-0.645987
H	-1.922135	3.344682	-0.058995
H	-1.718147	2.521834	-1.597692
C	-1.788468	0.505464	0.671897
H	-1.227145	-0.387997	0.977746
C	-2.843450	0.046906	-0.366733
H	-3.477848	0.900861	-0.645969
H	-2.315813	-0.256710	-1.281290
C	-3.733021	-1.115281	0.096493
H	-3.096371	-1.950336	0.425640
H	-4.323184	-0.816267	0.973722
C	-4.689466	-1.613018	-0.996689
H	-4.104816	-1.924219	-1.873881
H	-5.320990	-0.778262	-1.333002
C	-5.578739	-2.773324	-0.537564
H	-4.975547	-3.633998	-0.222832
H	-6.205570	-2.480507	0.314029
H	-6.244704	-3.109439	-1.340678
C	-2.440459	1.114924	1.931378
H	-3.052376	1.989564	1.678576
H	-3.089013	0.391192	2.436600
H	-1.678633	1.439682	2.649347

11L-TS

B3LYP SCF energy: -3293.93794310 a.u.
B3LYP enthalpy: -3292.842089 a.u.
B3LYP free energy: -3292.996139 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.15940375 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.063550 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.217600 a.u.
Imaginary frequency: -371.2607 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-6.019073	-1.494649	1.963054
C	-4.978683	-1.108456	1.147749
C	-4.041037	-0.119749	1.565092
C	-4.220540	0.459605	2.861587
C	-5.306067	0.045160	3.679565
C	-6.189779	-0.913362	3.242469
H	-6.718094	-2.252439	1.620439

H	-4.868156	-1.567842	0.172706
C	-2.935413	0.292137	0.736849
C	-3.313807	1.458830	3.283503
H	-5.423692	0.502623	4.658640
H	-7.018061	-1.224724	3.872383
C	-2.248109	1.820658	2.496649
C	-2.009339	1.222510	1.226093
H	-3.470516	1.947260	4.242160
H	-1.599316	2.608470	2.850379
C	-2.908709	-0.233446	-0.671124
C	-3.898884	0.284043	-1.588822
C	-2.006002	-1.200236	-1.109005
C	-4.852180	1.274002	-1.215847
C	-3.943041	-0.203646	-2.935012
C	-2.036005	-1.625074	-2.470762
C	-5.799470	1.726143	-2.108469
H	-4.835185	1.678948	-0.211702
C	-4.931807	0.279588	-3.832162
C	-2.979785	-1.157563	-3.347729
H	-1.295610	-2.329438	-2.827895
C	-5.848681	1.222480	-3.428759
H	-6.517294	2.478294	-1.793537
H	-4.948846	-0.111500	-4.846358
H	-2.993698	-1.512491	-4.375342
H	-6.604863	1.584130	-4.119531
P	-0.471641	1.704897	0.252737
P	-0.551388	-1.722948	-0.091633
C	0.313614	3.073277	1.247148
C	0.697708	2.895586	2.589922
C	0.650768	4.289325	0.628207
C	1.372692	3.896016	3.290272
H	0.436572	1.983591	3.116955
C	1.335646	5.287678	1.325711
H	0.374868	4.470728	-0.403874
C	1.697571	5.098155	2.659057
H	1.637351	3.736689	4.331985
H	1.577123	6.219288	0.821746
H	2.220664	5.879097	3.203203
C	-1.244592	2.697112	-1.119755
C	-0.865868	2.586440	-2.463873
C	-2.229394	3.642433	-0.777645
C	-1.452937	3.396398	-3.440716
H	-0.120665	1.858168	-2.759497
C	-2.810812	4.452279	-1.750724
H	-2.543135	3.750573	0.256348
C	-2.423794	4.331701	-3.087874

H	-1.147699	3.289845	-4.477958
H	-3.569145	5.175670	-1.464624
H	-2.879023	4.961138	-3.847169
C	-0.170871	-3.480355	-0.549778
C	1.038918	-3.998040	-0.057767
C	-1.057228	-4.355152	-1.198547
C	1.365411	-5.343593	-0.231922
H	1.715457	-3.350262	0.489986
C	-0.724663	-5.699719	-1.380445
H	-2.018972	-4.002718	-1.554284
C	0.488728	-6.197302	-0.904769
H	2.299633	-5.728653	0.168581
H	-1.424366	-6.359585	-1.885750
H	0.742090	-7.244494	-1.042715
C	-1.158928	-2.081057	1.622822
C	-2.201388	-3.000788	1.823866
C	-0.507207	-1.547119	2.739543
C	-2.587465	-3.362659	3.112649
H	-2.712904	-3.441125	0.973707
C	-0.888910	-1.914957	4.032123
H	0.303037	-0.844446	2.597721
C	-1.930578	-2.822402	4.221376
H	-3.401138	-4.068624	3.251408
H	-0.369268	-1.493194	4.888345
H	-2.228303	-3.111410	5.225305
C	5.818504	-2.452730	1.270907
C	5.236122	-2.871725	-0.097536
H	6.759259	-1.902490	1.149689
H	6.032572	-3.319469	1.903753
H	5.946005	-2.713265	-0.911726
H	4.938218	-3.926055	-0.109006
C	4.746746	-1.565380	1.846141
C	3.745708	-1.325772	0.875929
C	4.645712	-0.977467	3.087207
H	5.399872	-1.144567	3.851272
C	3.539655	-0.146008	3.326707
H	3.406717	0.359138	4.276906
C	2.616427	0.041047	2.314035
H	1.780170	0.704331	2.458075
N	2.677460	-0.536777	1.087605
N	4.036499	-2.017652	-0.296673
C	3.292512	-2.086742	-1.460560
C	2.258479	-1.262657	-1.828645
C	3.621138	-3.141989	-2.502759
H	4.696367	-3.259482	-2.679820
H	3.241797	-4.124073	-2.183437

C	2.870838	-2.626468	-3.746706
H	3.538711	-1.987459	-4.337231
H	2.528431	-3.435675	-4.398284
C	1.719452	-1.786046	-3.159211
H	1.385076	-0.986741	-3.831194
H	0.844207	-2.422522	-2.978206
Ir	1.082136	-0.014275	-0.551660
H	0.192963	0.204487	-1.825559
C	3.001384	0.603867	-2.093474
H	2.675359	0.606923	-3.129819
C	2.487574	1.605132	-1.210402
H	1.831346	2.332629	-1.688270
C	3.454461	2.235206	-0.216289
H	4.168000	1.479499	0.136138
H	2.926716	2.601391	0.669915
C	4.240814	3.405822	-0.839718
H	4.792195	3.048014	-1.722141
H	3.531857	4.161044	-1.209213
C	5.217804	4.067036	0.141202
H	4.656410	4.430417	1.013336
H	5.917780	3.309224	0.522185
C	6.006987	5.223961	-0.481053
H	5.336304	6.013609	-0.841457
H	6.692291	5.675555	0.244826
H	6.604625	4.883449	-1.335363
H	4.039170	0.313572	-1.949837

12L

B3LYP SCF energy: -3293.96780157 a.u.
B3LYP enthalpy: -3292.869268 a.u.
B3LYP free energy: -3293.023687 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.18872683 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.090193 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.244612 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	6.317571	0.713759	1.579318
C	5.158315	0.523814	0.859994
C	4.115797	-0.320468	1.344304
C	4.318333	-0.956354	2.610045
C	5.528691	-0.751904	3.324952
C	6.512408	0.067240	2.823085
H	7.092635	1.365216	1.185592

H	5.038259	1.031386	-0.089193
C	2.881523	-0.525681	0.621055
C	3.292780	-1.785361	3.118420
H	5.658510	-1.253663	4.280420
H	7.434927	0.221029	3.375316
C	2.113084	-1.944362	2.437361
C	1.867109	-1.304180	1.186027
H	3.445128	-2.299420	4.064130
H	1.365567	-2.594792	2.866094
C	2.813092	0.112603	-0.736201
C	3.641520	-0.442207	-1.777867
C	2.077214	1.271752	-0.981970
C	4.371041	-1.654099	-1.611085
C	3.748222	0.232308	-3.037644
C	2.200532	1.922095	-2.244782
C	5.156188	-2.157686	-2.624235
H	4.296482	-2.193463	-0.674719
C	4.575061	-0.305927	-4.059761
C	3.022748	1.433391	-3.229225
H	1.639885	2.828868	-2.434981
C	5.267821	-1.477254	-3.860044
H	5.697138	-3.087443	-2.473053
H	4.647224	0.226435	-5.004844
H	3.114560	1.961961	-4.174938
H	5.897279	-1.883253	-4.646577
P	0.224966	-1.648116	0.327196
P	0.659503	1.780816	0.093218
C	-0.644152	-2.740850	1.549248
C	-0.965617	-2.241729	2.825326
C	-1.050075	-4.042836	1.222116
C	-1.664314	-3.022327	3.745441
H	-0.629133	-1.251567	3.119257
C	-1.756300	-4.822479	2.143087
H	-0.822603	-4.458220	0.247625
C	-2.066337	-4.317069	3.404899
H	-1.886659	-2.623544	4.731451
H	-2.059513	-5.828749	1.868561
H	-2.609571	-4.926495	4.121207
C	0.798153	-2.866472	-0.956221
C	0.423420	-2.801928	-2.303785
C	1.648381	-3.911538	-0.547360
C	0.878116	-3.755608	-3.218942
H	-0.217681	-1.999780	-2.646202
C	2.095961	-4.865981	-1.458812
H	1.964239	-3.984784	0.488693
C	1.711197	-4.791175	-2.799927

H	0.577481	-3.683690	-4.260422
H	2.748722	-5.665889	-1.120692
H	2.062254	-5.533219	-3.511279
C	0.488961	3.620686	-0.124377
C	-0.732496	4.207236	0.242407
C	1.561773	4.464060	-0.458085
C	-0.887005	5.594275	0.251049
H	-1.566632	3.576408	0.527495
C	1.402812	5.851119	-0.459495
H	2.530023	4.048166	-0.715804
C	0.178259	6.421148	-0.108251
H	-1.839552	6.028484	0.542623
H	2.242938	6.485504	-0.727969
H	0.058674	7.500710	-0.105894
C	1.221860	1.865004	1.858457
C	2.468397	2.406780	2.206094
C	0.315490	1.547674	2.877934
C	2.807290	2.600295	3.544202
H	3.182044	2.676686	1.434583
C	0.651014	1.752020	4.219007
H	-0.663220	1.159172	2.623298
C	1.899536	2.274184	4.555246
H	3.781667	3.008768	3.796532
H	-0.067092	1.508654	4.997676
H	2.163274	2.433685	5.596887
C	-5.240170	3.399930	0.007212
C	-4.435719	3.186366	-1.309421
H	-6.313518	3.256876	-0.151394
H	-5.105854	4.418955	0.389467
H	-5.047082	2.708869	-2.086463
H	-4.045396	4.123777	-1.714170
C	-4.645324	2.383190	0.956082
C	-3.525761	1.790534	0.332635
C	-4.959891	1.994086	2.237407
H	-5.809358	2.417823	2.766210
C	-4.145824	1.015480	2.848864
H	-4.359899	0.658718	3.850112
C	-3.068245	0.496788	2.154877
H	-2.453778	-0.278706	2.589840
N	-2.723923	0.877086	0.895183
N	-3.324079	2.285854	-0.923805
C	-2.394937	1.761808	-1.868196
C	-2.507512	0.513260	-2.481846
C	-1.674511	2.733246	-2.801615
H	-2.436955	3.348663	-3.303794
H	-1.002183	3.423947	-2.291339

C	-0.970979	1.817596	-3.824084
H	-0.905684	2.271409	-4.817133
H	0.044114	1.596341	-3.491679
C	-1.801177	0.522365	-3.818046
H	-2.603620	0.555560	-4.573873
H	-1.217601	-0.379739	-4.025363
Ir	-1.107038	0.121026	-0.550297
H	-0.124126	-0.211763	-1.734449
C	-3.456826	-0.587108	-2.114435
H	-3.767545	-1.153664	-3.001509
C	-2.650665	-1.394852	-1.089546
H	-2.132066	-2.210280	-1.599343
C	-3.568499	-1.975226	-0.006235
H	-4.245880	-1.193012	0.358114
H	-3.005766	-2.319925	0.862399
C	-4.420171	-3.149171	-0.529784
H	-3.754675	-3.959577	-0.862303
H	-4.987423	-2.836746	-1.418853
C	-5.398501	-3.696513	0.519294
H	-6.062890	-2.885558	0.850765
H	-4.832698	-4.009806	1.407850
H	-4.365685	-0.172244	-1.658740
C	-6.240906	-4.869535	0.006729
H	-6.925487	-5.237161	0.779347
H	-6.845340	-4.576034	-0.860233
H	-5.606483	-5.709288	-0.302717

13L-TS

B3LYP SCF energy: -3293.94878743 a.u.
B3LYP enthalpy: -3292.853062 a.u.
B3LYP free energy: -3293.008255 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.17232436 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.076599 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.231792 a.u.
Imaginary frequency: -842.6316 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-6.371487	1.383120	-1.016815
C	-5.164014	1.086815	-0.424779
C	-4.346594	0.025907	-0.911103
C	-4.818954	-0.720562	-2.038580
C	-6.072414	-0.395551	-2.623557
C	-6.835508	0.634525	-2.125671

H	-6.976527	2.197440	-0.628217
H	-4.826839	1.669592	0.424736
C	-3.074565	-0.298558	-0.324643
C	-4.019536	-1.775580	-2.538025
H	-6.415213	-0.977076	-3.475548
H	-7.792557	0.876601	-2.578659
C	-2.793618	-2.055239	-1.985032
C	-2.286169	-1.308458	-0.884523
H	-4.385920	-2.366499	-3.373801
H	-2.214438	-2.871384	-2.395575
C	-2.651843	0.424253	0.919819
C	-3.347875	0.133972	2.150852
C	-1.594872	1.331468	0.922448
C	-4.419405	-0.800583	2.226768
C	-2.952598	0.793866	3.359792
C	-1.174443	1.920002	2.153477
C	-5.076798	-1.036204	3.414561
H	-4.722746	-1.336321	1.335775
C	-3.654006	0.535971	4.566697
C	-1.843041	1.676654	3.325370
H	-0.314140	2.579103	2.161863
C	-4.700840	-0.356656	4.596396
H	-5.893421	-1.751978	3.443112
H	-3.344163	1.056021	5.469739
H	-1.522131	2.156460	4.246921
H	-5.233774	-0.546750	5.523546
P	-0.591599	-1.716422	-0.201118
P	-0.487423	1.610707	-0.535683
C	-0.014064	-3.124477	-1.258084
C	0.221333	-2.893585	-2.627190
C	0.303298	-4.383637	-0.729048
C	0.725924	-3.901557	-3.446836
H	-0.004321	-1.922812	-3.058263
C	0.824662	-5.389328	-1.549532
H	0.145235	-4.590938	0.323305
C	1.030865	-5.155592	-2.908514
H	0.885042	-3.707685	-4.503962
H	1.062256	-6.358693	-1.120526
H	1.425592	-5.941844	-3.545527
C	-1.037003	-2.514608	1.403384
C	-0.466749	-2.090157	2.609381
C	-1.988217	-3.550516	1.429846
C	-0.817696	-2.702262	3.815587
H	0.231376	-1.261017	2.607450
C	-2.332752	-4.164402	2.632625
H	-2.461077	-3.880625	0.509205

C	-1.744506	-3.743835	3.828879
H	-0.371126	-2.357216	4.744015
H	-3.063758	-4.968009	2.636923
H	-2.016143	-4.221065	4.766126
C	-0.011225	3.405304	-0.413830
C	1.069007	3.868673	-1.181162
C	-0.794614	4.351908	0.269767
C	1.377523	5.228960	-1.237807
H	1.660511	3.173062	-1.763761
C	-0.482149	5.711340	0.216075
H	-1.658109	4.038465	0.845639
C	0.608372	6.155303	-0.532768
H	2.216448	5.561840	-1.842846
H	-1.101165	6.423286	0.755008
H	0.847211	7.214101	-0.577111
C	-1.471676	1.734205	-2.097706
C	-2.569891	2.599802	-2.217678
C	-1.011554	1.061422	-3.237903
C	-3.205029	2.767874	-3.446558
H	-2.930971	3.146980	-1.352442
C	-1.641240	1.238236	-4.472272
H	-0.152181	0.400104	-3.159034
C	-2.741037	2.089648	-4.577130
H	-4.060972	3.432179	-3.522807
H	-1.271312	0.712576	-5.348370
H	-3.233011	2.229377	-5.535481
C	5.099955	3.724586	0.655467
C	4.304598	3.292796	1.910115
H	6.170927	3.518555	0.769717
H	4.996391	4.796182	0.459403
H	4.960607	3.024436	2.741518
H	3.622614	4.079092	2.251818
C	4.498006	2.884650	-0.441201
C	3.568529	1.963913	0.121171
C	4.743341	2.876929	-1.791174
H	5.465705	3.557314	-2.233846
C	4.038125	1.950069	-2.589330
H	4.198792	1.885742	-3.659470
C	3.114531	1.127723	-1.983775
H	2.531900	0.423530	-2.567286
N	2.831414	1.133616	-0.643789
N	3.523112	2.098677	1.489803
C	3.139388	1.177501	2.488590
C	3.305278	-0.160896	2.488224
C	2.594856	1.699939	3.804727
H	3.379422	2.207887	4.384825

H	1.789253	2.431163	3.663275
C	2.112252	0.411854	4.511721
H	2.271351	0.439676	5.593498
H	1.036425	0.293126	4.340967
C	2.878559	-0.742332	3.821971
H	3.772157	-1.039594	4.392866
H	2.270229	-1.650087	3.723435
Ir	1.094715	-0.121329	-0.241401
H	1.623055	-0.786632	1.098219
C	3.851605	-1.008411	1.376770
H	4.471689	-1.805693	1.807495
C	2.758623	-1.661730	0.485065
H	2.323745	-2.514220	1.019456
H	4.518573	-0.414588	0.741454
C	3.349120	-2.184410	-0.837093
H	3.831899	-1.361555	-1.378753
H	2.554703	-2.567388	-1.481283
C	4.386895	-3.309616	-0.628341
H	5.228098	-2.942956	-0.025044
H	3.925487	-4.127353	-0.055616
C	4.931606	-3.863342	-1.952702
H	5.369749	-3.040445	-2.535942
H	4.096343	-4.252939	-2.550586
C	5.980872	-4.962907	-1.755785
H	6.349066	-5.339134	-2.716721
H	6.844604	-4.590972	-1.191396
H	5.565279	-5.813579	-1.202002

14L

B3LYP SCF energy: -811.06657399 a.u.
B3LYP enthalpy: -810.635047 a.u.
B3LYP free energy: -810.707469 a.u.
B3LYP-D3(BJ) SCF energy in solution: -811.39782318 a.u.
B3LYP-D3(BJ) enthalpy in solution: -810.966296 a.u.
B3LYP-D3(BJ) free energy in solution: -811.038718 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.720056	-1.412372	2.046932
C	1.869150	-0.115850	2.008010
H	2.087478	-2.285674	2.257386
H	3.488435	-1.373226	2.826011
H	0.932290	-0.206094	2.563712
H	2.428356	0.734970	2.426686

C	3.274014	-1.481692	0.643418
C	2.560982	-0.572422	-0.170823
C	4.246831	-2.259643	0.051173
H	4.825707	-2.976538	0.629378
C	4.473451	-2.098434	-1.330028
H	5.230903	-2.681350	-1.844092
C	3.703089	-1.176104	-2.029888
H	3.855264	-1.037280	-3.099110
N	2.743518	-0.405883	-1.478792
N	1.607410	0.113853	0.570097
C	1.006099	1.324640	0.141722
C	-0.292653	1.634525	0.309441
C	1.791493	2.433607	-0.537515
H	2.761538	2.615251	-0.056472
H	2.007347	2.160858	-1.577281
C	0.833080	3.642438	-0.423920
H	1.103889	4.241587	0.453516
H	0.877608	4.304605	-1.294607
C	-0.575009	3.030758	-0.210406
H	-1.187895	3.624249	0.482389
H	-1.141766	2.982076	-1.152737
C	-1.369196	0.747013	0.866567
H	-0.941644	-0.233536	1.108565
C	-2.564137	0.547163	-0.088608
H	-3.016139	1.520474	-0.324308
H	-2.196300	0.138752	-1.040004
C	-3.638733	-0.382160	0.489383
H	-3.187677	-1.358410	0.721747
H	-3.993049	0.024408	1.448777
C	-4.837201	-0.588438	-0.446411
H	-4.483383	-0.993455	-1.406238
H	-5.290027	0.387330	-0.678126
C	-5.912032	-1.519734	0.129350
H	-5.459989	-2.495174	0.359224
H	-6.265258	-1.115368	1.088836
H	-1.749400	1.169805	1.811179
C	-7.105766	-1.719243	-0.810729
H	-7.854869	-2.388265	-0.371614
H	-7.600014	-0.764924	-1.031543
H	-6.789015	-2.155185	-1.766412

15-TS

B3LYP SCF energy: -3293.95115384 a.u.

B3LYP enthalpy: -3292.856333 a.u.

B3LYP free energy: -3293.008684 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.17135402 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.076533 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.228884 a.u.
Imaginary frequency: -732.0190 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.473020	-1.243105	-0.234474
C	5.172248	-1.009821	0.154661
C	4.430469	0.096754	-0.355376
C	5.097276	0.957349	-1.283979
C	6.442750	0.700339	-1.659503
C	7.122014	-0.379921	-1.147961
H	7.007926	-2.097740	0.170006
H	4.708544	-1.687501	0.860101
C	3.053672	0.356782	0.023250
C	4.393324	2.071753	-1.794923
H	6.923174	1.376374	-2.362054
H	8.150660	-0.571596	-1.439113
C	3.077415	2.273245	-1.473409
C	2.360322	1.400037	-0.595059
H	4.903486	2.766779	-2.456908
H	2.577723	3.133850	-1.893589
C	2.560832	-0.506461	1.153415
C	3.168372	-0.272755	2.439621
C	1.740615	-1.623620	0.976176
C	3.912285	0.907710	2.729628
C	3.034831	-1.249539	3.480202
C	1.665771	-2.603110	2.006881
C	4.475191	1.108113	3.969807
H	4.024305	1.665847	1.963522
C	3.642161	-1.021629	4.744777
C	2.314823	-2.436927	3.206299
H	1.094473	-3.507306	1.844402
C	4.346862	0.133324	4.988795
H	5.026492	2.022581	4.169160
H	3.533782	-1.778553	5.517347
H	2.260655	-3.211886	3.966810
H	4.804469	0.302246	5.959170
P	0.539985	1.787199	-0.365470
P	0.574979	-1.729864	-0.463667
C	0.244270	2.905249	-1.829306
C	0.491277	2.427330	-3.131061
C	-0.249276	4.207621	-1.678106
C	0.252404	3.231231	-4.243262

H	0.890868	1.427914	-3.275183
C	-0.500025	5.009932	-2.797711
H	-0.435255	4.612001	-0.689469
C	-0.250673	4.526747	-4.080131
H	0.460848	2.848267	-5.238460
H	-0.884374	6.016208	-2.657622
H	-0.439052	5.152602	-4.947622
C	0.513188	3.006867	1.029563
C	-0.668423	3.243417	1.750707
C	1.645771	3.787203	1.313903
C	-0.716292	4.240608	2.725974
H	-1.541373	2.626175	1.573232
C	1.596294	4.778959	2.294919
H	2.569704	3.630824	0.767670
C	0.415142	5.011074	3.000901
H	-1.637624	4.408060	3.276886
H	2.482957	5.370824	2.503798
H	0.377460	5.784486	3.762695
C	-0.174074	-3.419553	-0.324337
C	-1.061471	-3.693658	0.733062
C	0.093423	-4.435231	-1.254345
C	-1.643383	-4.953230	0.865944
H	-1.291470	-2.916045	1.454584
C	-0.502566	-5.693178	-1.125803
H	0.768464	-4.257183	-2.083070
C	-1.367678	-5.958025	-0.065654
H	-2.314549	-5.150122	1.697626
H	-0.280707	-6.465884	-1.856499
H	-1.823700	-6.938652	0.036879
C	1.648957	-1.905331	-1.956593
C	2.865747	-2.601393	-1.870174
C	1.225213	-1.445442	-3.210923
C	3.643325	-2.816862	-3.008098
H	3.208645	-2.977982	-0.911891
C	1.999436	-1.667562	-4.351845
H	0.284700	-0.909705	-3.295353
C	3.212696	-2.350345	-4.251860
H	4.586943	-3.347323	-2.920026
H	1.654491	-1.305704	-5.316582
H	3.818594	-2.519216	-5.137435
C	-5.619215	-2.491031	1.261744
C	-4.879877	-1.527940	2.224790
H	-6.652193	-2.175297	1.087322
H	-5.658259	-3.508809	1.668646
H	-5.433340	-0.591001	2.367543
H	-4.712201	-1.971795	3.207756

C	-4.777480	-2.442835	0.010317
C	-3.608900	-1.678340	0.277831
C	-4.939049	-3.024060	-1.219714
H	-5.814227	-3.625556	-1.449394
C	-3.918263	-2.834678	-2.181854
H	-3.980162	-3.287398	-3.164843
C	-2.831307	-2.056512	-1.859277
H	-2.037811	-1.887791	-2.575348
N	-2.665211	-1.431948	-0.651061
N	-3.586827	-1.243337	1.565450
C	-2.513600	-0.613120	2.228795
C	-1.381181	-0.118571	1.668837
C	-2.527045	-0.592195	3.750735
H	-3.470594	-0.231963	4.178346
H	-2.360038	-1.601542	4.162870
C	-1.345663	0.343133	4.059148
H	-1.706580	1.376838	4.128983
H	-0.843715	0.102791	5.001804
C	-0.432228	0.194057	2.827781
H	0.201334	1.067436	2.675545
H	0.246438	-0.652855	2.979889
Ir	-1.089542	0.048711	-0.434051
H	-1.060571	0.125186	-2.132749
C	-2.650752	1.622414	-0.736981
H	-2.218888	2.597326	-0.519782
C	-2.337866	1.130556	-2.050407
H	-1.827844	1.776518	-2.754487
H	-3.043623	0.444790	-2.514810
C	-4.047171	1.491436	-0.153204
H	-3.986556	1.405198	0.938619
H	-4.531921	0.580340	-0.521289
C	-4.934020	2.700397	-0.512635
H	-5.000829	2.792327	-1.606412
H	-4.453701	3.623760	-0.156903
C	-6.347197	2.606308	0.078504
H	-6.275188	2.509391	1.171636
H	-6.828392	1.684999	-0.280484
C	-7.227501	3.810965	-0.270808
H	-7.345057	3.914038	-1.356297
H	-8.228001	3.713373	0.164611
H	-6.790089	4.743734	0.105311

16

B3LYP SCF energy: -3293.97111076 a.u.

B3LYP enthalpy: -3292.871931 a.u.
B3LYP free energy: -3293.027978 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.19938392 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.100204 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.256251 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-6.545588	1.051666	0.089345
C	-5.225520	0.828957	0.414943
C	-4.454348	-0.171809	-0.247609
C	-5.111215	-0.936830	-1.263245
C	-6.476151	-0.693336	-1.571679
C	-7.184657	0.282225	-0.910580
H	-7.103067	1.823909	0.611784
H	-4.769724	1.433312	1.189077
C	-3.059307	-0.418828	0.064927
C	-4.376239	-1.940997	-1.936062
H	-6.948376	-1.295199	-2.343834
H	-8.228298	0.462947	-1.150871
C	-3.048248	-2.134369	-1.663449
C	-2.350127	-1.362865	-0.680770
H	-4.873717	-2.555516	-2.682019
H	-2.519858	-2.905460	-2.207456
C	-2.552254	0.343761	1.260295
C	-3.080054	-0.054682	2.540799
C	-1.786073	1.510998	1.167149
C	-3.770174	-1.287395	2.730952
C	-2.915012	0.799937	3.680151
C	-1.680427	2.365949	2.301316
C	-4.249155	-1.652089	3.968903
H	-3.906555	-1.954397	1.887953
C	-3.436492	0.403312	4.941459
C	-2.247294	2.036405	3.508612
H	-1.147720	3.303765	2.211374
C	-4.088298	-0.798512	5.087183
H	-4.759573	-2.603318	4.089519
H	-3.305525	1.069160	5.790653
H	-2.169760	2.718985	4.351247
H	-4.480068	-1.096333	6.055355
P	-0.525830	-1.742750	-0.509760
P	-0.667641	1.822827	-0.279151
C	-0.183737	-2.513536	-2.166410
C	-0.397781	-1.751419	-3.329156
C	0.328805	-3.811327	-2.296062
C	-0.105023	-2.275807	-4.587606

H	-0.830309	-0.758024	-3.257482
C	0.627763	-4.331932	-3.558804
H	0.490484	-4.426605	-1.417604
C	0.414595	-3.567506	-4.705917
H	-0.289453	-1.678011	-5.476027
H	1.021530	-5.341045	-3.640842
H	0.642277	-3.977111	-5.685767
C	-0.467846	-3.189547	0.642636
C	0.725091	-3.519880	1.307588
C	-1.587726	-4.020214	0.811372
C	0.795588	-4.655961	2.114913
H	1.595487	-2.882916	1.206115
C	-1.514255	-5.153319	1.623355
H	-2.520669	-3.791751	0.307546
C	-0.323374	-5.475276	2.275583
H	1.725901	-4.896477	2.621767
H	-2.390783	-5.783595	1.743825
H	-0.267863	-6.357549	2.906765
C	0.015513	3.524062	0.002404
C	0.987204	3.713676	1.002041
C	-0.376434	4.630014	-0.767782
C	1.534026	4.975068	1.235519
H	1.305988	2.871953	1.607819
C	0.183895	5.889879	-0.541001
H	-1.121925	4.519115	-1.546577
C	1.137003	6.067935	0.461036
H	2.272171	5.103879	2.022709
H	-0.134243	6.732886	-1.147948
H	1.566190	7.049729	0.639710
C	-1.738880	2.089148	-1.755197
C	-3.040484	2.600925	-1.646973
C	-1.206681	1.866171	-3.034863
C	-3.796373	2.863566	-2.790542
H	-3.466866	2.794718	-0.668462
C	-1.957956	2.138103	-4.179624
H	-0.193639	1.486882	-3.143073
C	-3.257855	2.632985	-4.058146
H	-4.806844	3.248500	-2.688429
H	-1.529029	1.964213	-5.162594
H	-3.846748	2.841085	-4.946786
C	5.507854	2.730059	1.196681
C	4.851056	1.710722	2.164367
H	6.567457	2.510657	1.036541
H	5.444960	3.750355	1.594839
H	5.465524	0.809100	2.280801
H	4.674069	2.131010	3.156417

C	4.682470	2.596664	-0.061078
C	3.565259	1.772354	0.223841
C	4.804554	3.150409	-1.310173
H	5.639657	3.797726	-1.562599
C	3.797952	2.867424	-2.264045
H	3.837252	3.285873	-3.263120
C	2.754877	2.040718	-1.912068
H	1.975491	1.795483	-2.624138
N	2.627134	1.457658	-0.683443
N	3.567253	1.355231	1.520349
C	2.565494	0.604835	2.151183
C	1.472015	0.034613	1.584649
C	2.583216	0.476055	3.664390
H	3.560623	0.179004	4.063169
H	2.323257	1.433711	4.144176
C	1.500828	-0.592398	3.911976
H	1.965895	-1.585326	3.924059
H	0.979436	-0.457563	4.864480
C	0.561011	-0.476810	2.694042
H	0.063610	-1.419200	2.468626
H	-0.227844	0.254726	2.892895
Ir	1.093939	-0.006509	-0.399835
C	2.628819	-1.481659	-0.851811
H	2.158050	-2.468049	-0.817730
C	2.972180	-1.197480	-2.327993
H	2.107193	-0.859629	-2.917246
H	3.329188	-2.103565	-2.834951
C	3.896556	-1.582316	0.009707
H	3.624217	-1.664291	1.069152
H	4.491089	-0.663871	-0.084144
C	4.799479	-2.778819	-0.350083
H	5.132606	-2.700130	-1.393782
H	4.213772	-3.708627	-0.285928
C	6.031946	-2.897092	0.557498
H	5.704803	-2.983730	1.604064
H	6.615278	-1.966551	0.496454
C	6.933287	-4.085142	0.204486
H	7.305558	-4.007925	-0.824276
H	7.802365	-4.139803	0.869575
H	6.389546	-5.034039	0.288926
H	3.751798	-0.433912	-2.420552

17-TS

B3LYP SCF energy: -3293.92221196 a.u.

B3LYP enthalpy: -3292.824111 a.u.
B3LYP free energy: -3292.978792 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.14177377 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.043673 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.198354 a.u.
Imaginary frequency: -307.1495 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-6.598933	0.452746	-0.136299
C	-5.297457	0.269372	0.275267
C	-4.376553	-0.501981	-0.493912
C	-4.856988	-1.065119	-1.718723
C	-6.207200	-0.867665	-2.114807
C	-7.066685	-0.125400	-1.340038
H	-7.274854	1.046763	0.472462
H	-4.970824	0.726071	1.201046
C	-3.001987	-0.706638	-0.091072
C	-3.958943	-1.809367	-2.516380
H	-6.544496	-1.314221	-3.046645
H	-8.098058	0.020905	-1.647552
C	-2.647593	-1.958460	-2.145506
C	-2.129972	-1.406555	-0.935828
H	-4.314613	-2.255657	-3.441681
H	-1.996159	-2.515253	-2.802419
C	-2.627351	-0.161331	1.258985
C	-3.228513	-0.768847	2.423583
C	-1.823087	0.970998	1.412996
C	-4.068861	-1.920266	2.349689
C	-2.991653	-0.209087	3.721290
C	-1.634677	1.526414	2.710356
C	-4.615824	-2.482412	3.481967
H	-4.283130	-2.363555	1.384380
C	-3.573737	-0.808799	4.871086
C	-2.196824	0.956648	3.824890
H	-1.055257	2.431246	2.828603
C	-4.368932	-1.924489	4.759268
H	-5.250717	-3.359304	3.391959
H	-3.378560	-0.362946	5.843001
H	-2.043675	1.407548	4.802195
H	-4.811024	-2.375672	5.642682
P	-0.278387	-1.617466	-0.654421
P	-0.868449	1.691487	-0.012717
C	0.290245	-2.292039	-2.300713
C	0.827742	-1.410719	-3.253819
C	0.156173	-3.647546	-2.652023

C	1.223305	-1.864578	-4.513901
H	0.952130	-0.361492	-2.996711
C	0.555116	-4.102547	-3.909831
H	-0.268102	-4.354338	-1.947143
C	1.090119	-3.213657	-4.844776
H	1.639402	-1.163806	-5.232477
H	0.444094	-5.154270	-4.158376
H	1.400585	-3.570639	-5.822577
C	-0.132273	-3.123916	0.425580
C	0.999286	-3.956150	0.341404
C	-1.109498	-3.431290	1.378856
C	1.144088	-5.053558	1.190184
H	1.763366	-3.767551	-0.403352
C	-0.961678	-4.524879	2.234795
H	-1.997794	-2.824266	1.462292
C	0.166323	-5.339084	2.146437
H	2.020418	-5.689291	1.097944
H	-1.738433	-4.736426	2.964193
H	0.280663	-6.193538	2.807258
C	-0.374529	3.388753	0.566823
C	0.614260	3.511158	1.561635
C	-0.929170	4.562892	0.036064
C	1.004596	4.763336	2.033853
H	1.084328	2.619884	1.965050
C	-0.525705	5.818184	0.500601
H	-1.677159	4.513092	-0.745384
C	0.434548	5.924079	1.504739
H	1.757314	4.832249	2.814717
H	-0.970747	6.712367	0.073320
H	0.739701	6.900174	1.871046
C	-2.106486	2.058427	-1.332589
C	-3.328573	2.683396	-1.033425
C	-1.800101	1.776941	-2.671093
C	-4.213453	3.030815	-2.053895
H	-3.590597	2.900167	-0.001939
C	-2.686017	2.124849	-3.692838
H	-0.872275	1.266646	-2.914037
C	-3.892101	2.755875	-3.385495
H	-5.156700	3.509647	-1.807899
H	-2.435517	1.897192	-4.725141
H	-4.582874	3.027144	-4.178672
C	5.258931	3.677676	0.549229
C	4.963592	2.567682	1.593849
H	6.231889	3.524996	0.069482
H	5.283966	4.669489	1.012903
H	5.779624	1.841129	1.668088

H	4.790423	2.978499	2.593370
C	4.124249	3.548717	-0.438309
C	3.288969	2.474470	-0.040373
C	3.810859	4.261712	-1.566647
H	4.429446	5.089225	-1.902590
C	2.647777	3.891373	-2.282287
H	2.344416	4.423741	-3.176451
C	1.892638	2.831437	-1.832800
H	1.001835	2.520674	-2.363836
N	2.195101	2.089945	-0.723187
N	3.738866	1.892574	1.108656
C	3.167068	0.802957	1.773356
C	2.296811	-0.111499	1.241277
C	3.368788	0.645106	3.269443
H	4.415088	0.752142	3.582457
H	2.798844	1.405119	3.830538
C	2.822192	-0.773223	3.525504
H	3.639744	-1.498580	3.447554
H	2.375781	-0.882100	4.518562
C	1.807397	-1.003942	2.385523
H	1.702510	-2.056753	2.122433
H	0.806637	-0.666500	2.685096
Ir	1.003212	0.338328	-0.329874
C	3.141719	-1.072881	-0.471079
H	2.466678	-1.643358	-1.106471
C	4.062552	-0.231237	-1.346111
H	3.527630	0.428824	-2.029149
H	4.667127	-0.908027	-1.963964
C	3.947274	-2.063962	0.384645
H	3.299033	-2.591175	1.086549
H	4.680484	-1.512640	0.985697
C	4.685633	-3.135199	-0.449553
H	5.451240	-2.669858	-1.082293
H	3.982294	-3.628429	-1.137523
C	5.356786	-4.196179	0.435585
H	4.594015	-4.685210	1.058465
H	6.045116	-3.700104	1.134073
C	6.119003	-5.254375	-0.369150
H	6.918594	-4.799381	-0.965892
H	6.578990	-5.998939	0.289706
H	5.452496	-5.786168	-1.059223
H	4.762994	0.362501	-0.751537

15L-TS

B3LYP SCF energy: -3293.95426891 a.u.
B3LYP enthalpy: -3292.859829 a.u.
B3LYP free energy: -3293.013070 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.17308766 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.078648 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.231889 a.u.
Imaginary frequency: -747.9765 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.092447	-0.775845	-2.288482
C	4.966693	-0.792027	-1.494679
C	4.203721	0.390640	-1.262421
C	4.659058	1.594857	-1.886876
C	5.830163	1.585980	-2.690606
C	6.536915	0.424001	-2.891446
H	6.647907	-1.695586	-2.448729
H	4.657725	-1.727321	-1.045476
C	3.005932	0.400508	-0.443843
C	3.928893	2.785065	-1.666097
H	6.154149	2.518588	-3.145300
H	7.431301	0.423217	-3.507656
C	2.767109	2.767743	-0.940395
C	2.250402	1.571485	-0.349831
H	4.292602	3.719261	-2.086347
H	2.241609	3.701084	-0.801627
C	2.769396	-0.882776	0.304964
C	3.717653	-1.198854	1.343638
C	1.843513	-1.848749	-0.095360
C	4.606990	-0.227247	1.887506
C	3.789137	-2.533205	1.862058
C	1.974935	-3.180676	0.390512
C	5.493487	-0.554639	2.888551
H	4.573311	0.790039	1.515882
C	4.726543	-2.844256	2.883847
C	2.933220	-3.518770	1.314867
H	1.311736	-3.951329	0.021444
C	5.560884	-1.876509	3.391436
H	6.150993	0.208104	3.295808
H	4.767204	-3.863662	3.258918
H	3.025207	-4.548212	1.651996
H	6.271462	-2.120946	4.175589
P	0.599898	1.722136	0.527944
P	0.329705	-1.376373	-1.061380
C	0.018333	3.375236	-0.108687
C	-0.139972	3.571885	-1.494966

C	-0.315451	4.424678	0.757217
C	-0.614332	4.782661	-1.994141
H	0.122591	2.777881	-2.187495
C	-0.804545	5.636360	0.254349
H	-0.192611	4.311446	1.828384
C	-0.954286	5.819999	-1.118351
H	-0.717231	4.918824	-3.067201
H	-1.059636	6.435880	0.944038
H	-1.326364	6.763343	-1.507534
C	1.069248	2.160586	2.266393
C	0.157210	1.988891	3.319737
C	2.300943	2.780814	2.532992
C	0.468256	2.433050	4.606240
H	-0.782978	1.480114	3.141455
C	2.612034	3.216285	3.821884
H	3.018871	2.935176	1.734600
C	1.695822	3.047042	4.861089
H	-0.248318	2.291037	5.410481
H	3.570622	3.691242	4.010761
H	1.937872	3.389107	5.863275
C	-0.476011	-3.005995	-1.431859
C	-1.080004	-3.726278	-0.383511
C	-0.523341	-3.541169	-2.727348
C	-1.695273	-4.952977	-0.625891
H	-1.068184	-3.320304	0.623537
C	-1.151735	-4.766610	-2.968882
H	-0.070191	-3.011023	-3.556868
C	-1.735955	-5.476530	-1.921514
H	-2.146194	-5.500516	0.197356
H	-1.176741	-5.163944	-3.979703
H	-2.218682	-6.431341	-2.109786
C	0.943967	-0.848363	-2.721375
C	2.065841	-1.471677	-3.291897
C	0.250673	0.111247	-3.471698
C	2.485564	-1.136129	-4.579183
H	2.614344	-2.221102	-2.730114
C	0.667594	0.442853	-4.762832
H	-0.615247	0.602946	-3.038045
C	1.787107	-0.178639	-5.318168
H	3.360870	-1.620846	-5.001698
H	0.118629	1.187856	-5.332418
H	2.114782	0.081654	-6.320585
C	-5.520038	-2.496629	1.887881
C	-4.365140	-2.259452	2.896273
H	-6.352193	-1.806772	2.072203
H	-5.923072	-3.511459	1.961137

H	-4.656100	-1.593442	3.713699
H	-4.017464	-3.199382	3.337350
C	-4.877555	-2.217026	0.551696
C	-3.595726	-1.651724	0.779279
C	-5.305674	-2.416035	-0.736435
H	-6.270489	-2.869679	-0.946251
C	-4.447071	-2.023519	-1.789871
H	-4.726322	-2.170194	-2.826891
C	-3.250184	-1.414988	-1.487682
H	-2.590150	-1.063959	-2.269352
N	-2.812455	-1.184482	-0.212476
N	-3.273715	-1.648843	2.103163
C	-1.963824	-1.498760	2.619213
C	-0.914301	-0.912677	1.995393
C	-1.621414	-2.163739	3.944044
H	-2.344363	-1.956781	4.742720
H	-1.577019	-3.260642	3.838716
C	-0.230336	-1.573277	4.236471
H	-0.340276	-0.661903	4.836495
H	0.416329	-2.259098	4.793045
C	0.321821	-1.212243	2.842392
H	1.046287	-0.397590	2.884471
H	0.855475	-2.072298	2.420644
Ir	-1.123106	0.122470	0.149265
H	-1.633507	0.972885	-1.257004
C	-2.610140	1.492657	1.026247
H	-2.155106	2.220275	1.691232
C	-2.736921	1.853874	-0.353081
H	-2.215518	2.753764	-0.653059
H	-3.421211	0.932837	1.486002
C	-4.014636	1.635122	-1.137808
H	-3.801606	1.504932	-2.205973
H	-4.539478	0.739481	-0.796685
C	-4.936422	2.861030	-0.956981
H	-5.158158	2.994714	0.110770
H	-4.407019	3.768925	-1.278884
C	-6.249686	2.731530	-1.741504
H	-6.021884	2.594072	-2.807840
H	-6.775220	1.821127	-1.420641
C	-7.170046	3.943905	-1.565681
H	-8.096647	3.823420	-2.137172
H	-7.443553	4.086083	-0.513231
H	-6.683756	4.864643	-1.909806

16L

B3LYP SCF energy: -3293.98321495 a.u.
B3LYP enthalpy: -3292.883842 a.u.
B3LYP free energy: -3293.040601 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.20571419 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.106341 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.263100 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-6.423509	0.113556	1.791386
C	-5.257616	-0.035644	1.072717
C	-4.237145	0.960839	1.096164
C	-4.475806	2.123848	1.896385
C	-5.691541	2.256029	2.619122
C	-6.650456	1.271786	2.571041
H	-7.179737	-0.665401	1.753440
H	-5.118433	-0.931261	0.480447
C	-2.995674	0.826226	0.358926
C	-3.485490	3.133251	1.939694
H	-5.846577	3.152955	3.213204
H	-7.577991	1.379694	3.125700
C	-2.299442	2.975641	1.272930
C	-2.015751	1.812784	0.489862
H	-3.670784	4.035739	2.516524
H	-1.561833	3.764292	1.339156
C	-2.944978	-0.370732	-0.555720
C	-3.805544	-0.332304	-1.710456
C	-2.288396	-1.563312	-0.230914
C	-4.418527	0.871620	-2.165015
C	-4.072118	-1.535437	-2.444119
C	-2.605144	-2.752883	-0.946374
C	-5.229121	0.881861	-3.277579
H	-4.229515	1.796682	-1.633082
C	-4.926843	-1.494893	-3.578888
C	-3.488496	-2.745863	-1.998725
H	-2.143403	-3.687578	-0.654130
C	-5.493583	-0.312138	-3.991473
H	-5.673703	1.815282	-3.610720
H	-5.120535	-2.419487	-4.116678
H	-3.730728	-3.672379	-2.513339
H	-6.142739	-0.289028	-4.861864
P	-0.322738	1.756813	-0.294812
P	-0.815747	-1.576211	0.895060
C	0.613239	2.952024	0.771173
C	0.737725	2.677595	2.145707

C	1.262198	4.076113	0.243978
C	1.491934	3.511430	2.971231
H	0.207379	1.836683	2.583051
C	2.021744	4.906506	1.073281
H	1.173199	4.313707	-0.810608
C	2.140409	4.627182	2.435334
H	1.566481	3.294320	4.033229
H	2.514164	5.777782	0.650816
H	2.726029	5.278852	3.077254
C	-0.529993	2.662495	-1.894008
C	0.369980	2.465004	-2.954604
C	-1.553801	3.613220	-2.043859
C	0.250988	3.206244	-4.131464
H	1.158293	1.726722	-2.869178
C	-1.671677	4.348390	-3.224066
H	-2.261377	3.787525	-1.240354
C	-0.769098	4.148838	-4.269895
H	0.956203	3.041837	-4.941315
H	-2.470205	5.078199	-3.323176
H	-0.861484	4.722856	-5.187443
C	-0.363659	-3.364722	1.069273
C	0.301023	-4.004631	0.006572
C	-0.631582	-4.100379	2.233766
C	0.668755	-5.346312	0.102427
H	0.524163	-3.451033	-0.900231
C	-0.248644	-5.440676	2.331942
H	-1.141254	-3.634920	3.069580
C	0.398989	-6.067975	1.268242
H	1.170100	-5.827948	-0.732792
H	-0.464523	-5.993055	3.242174
H	0.691177	-7.111432	1.344819
C	-1.420109	-1.158903	2.585605
C	-2.724466	-1.460338	3.004817
C	-0.526964	-0.598640	3.512093
C	-3.126499	-1.195438	4.314860
H	-3.429270	-1.900749	2.307380
C	-0.924937	-0.341492	4.825198
H	0.491208	-0.365587	3.210780
C	-2.228878	-0.637160	5.227297
H	-4.142968	-1.425574	4.620640
H	-0.219492	0.088795	5.530586
H	-2.543614	-0.434355	6.246887
C	5.010696	-3.479866	-1.601060
C	4.119771	-2.806990	-2.680848
H	6.064103	-3.211270	-1.724063
H	4.947841	-4.573118	-1.659573

H	4.657870	-2.015424	-3.217242
H	3.749066	-3.522310	-3.418231
C	4.429694	-2.975347	-0.301116
C	3.254572	-2.239510	-0.590585
C	4.803128	-3.149291	1.008132
H	5.690580	-3.717714	1.271786
C	3.988412	-2.578309	2.014455
H	4.230235	-2.693663	3.064699
C	2.873456	-1.858442	1.646655
H	2.235926	-1.400623	2.394051
N	2.498266	-1.651506	0.350210
N	2.991223	-2.218018	-1.927812
C	1.838365	-1.698047	-2.533773
C	0.884522	-0.924113	-1.958461
C	1.477222	-2.123469	-3.946350
H	2.309816	-2.032064	-4.654021
H	1.155725	-3.177503	-3.969857
C	0.314490	-1.168700	-4.284402
H	0.712227	-0.267428	-4.765420
H	-0.416642	-1.614163	-4.965756
C	-0.293352	-0.797299	-2.914369
H	-0.762600	0.187220	-2.921223
H	-1.074688	-1.514197	-2.640196
Ir	1.022107	-0.167694	-0.093095
C	2.720364	0.969973	-0.756149
H	2.423032	1.920189	-1.209284
C	3.719046	1.275774	0.372698
H	3.213824	1.772000	1.212276
H	3.224208	0.400496	-1.546933
C	4.880940	2.176884	-0.092186
H	5.388277	1.700090	-0.944235
H	4.474336	3.126031	-0.468906
C	5.904471	2.464497	1.014161
H	5.394375	2.943773	1.863180
H	6.303359	1.512702	1.396638
C	7.070818	3.352514	0.558443
H	7.575489	2.876784	-0.294467
H	6.674130	4.306294	0.182348
C	8.091463	3.625256	1.668273
H	8.911379	4.257789	1.310363
H	7.625447	4.135315	2.520430
H	8.529988	2.691640	2.041814
H	4.145605	0.348375	0.774587

17L-TS

B3LYP SCF energy: -3293.94145785 a.u.
B3LYP enthalpy: -3292.843686 a.u.
B3LYP free energy: -3292.999143 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.15329405 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.055522 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.210979 a.u.
Imaginary frequency: -421.4516 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-6.681398	0.630477	-0.600033
C	-5.414923	0.454032	-0.087983
C	-4.493086	-0.456997	-0.683800
C	-4.933306	-1.169974	-1.843908
C	-6.247943	-0.974557	-2.345930
C	-7.110437	-0.093858	-1.737231
H	-7.359318	1.332686	-0.122973
H	-5.117067	1.024604	0.782609
C	-3.153251	-0.656947	-0.174319
C	-4.031583	-2.058124	-2.472695
H	-6.556263	-1.535513	-3.224422
H	-8.114788	0.049776	-2.124986
C	-2.752505	-2.208577	-2.004120
C	-2.275407	-1.510173	-0.854615
H	-4.357842	-2.615471	-3.347165
H	-2.094555	-2.879432	-2.536388
C	-2.827464	0.072306	1.099546
C	-3.507519	-0.343132	2.303599
C	-2.005398	1.202292	1.129365
C	-4.372160	-1.477680	2.351157
C	-3.332713	0.403084	3.514522
C	-1.887193	1.950531	2.334498
C	-4.994906	-1.855891	3.520130
H	-4.546755	-2.053669	1.449918
C	-3.991895	-0.009476	4.704410
C	-2.525311	1.564642	3.486587
H	-1.297270	2.856378	2.348145
C	-4.804991	-1.117918	4.713040
H	-5.646575	-2.725050	3.523681
H	-3.842473	0.574771	5.608807
H	-2.423369	2.160101	4.390482
H	-5.306166	-1.425133	5.626207
P	-0.459917	-1.755463	-0.428849
P	-0.904951	1.648223	-0.305691
C	0.192992	-2.616613	-1.951494

C	0.854514	-1.871711	-2.941332
C	0.012917	-3.994691	-2.170802
C	1.328311	-2.477970	-4.106974
H	1.016730	-0.808780	-2.787338
C	0.489103	-4.602527	-3.333350
H	-0.505180	-4.600247	-1.435076
C	1.149520	-3.847251	-4.304748
H	1.841099	-1.879592	-4.854999
H	0.341720	-5.669030	-3.478223
H	1.521384	-4.323274	-5.207506
C	-0.432081	-3.143603	0.804769
C	0.671349	-4.015915	0.877354
C	-1.469642	-3.306640	1.730204
C	0.730519	-5.010009	1.854127
H	1.478986	-3.941219	0.158159
C	-1.407738	-4.299248	2.710604
H	-2.335559	-2.661376	1.696196
C	-0.306619	-5.151875	2.779384
H	1.586843	-5.677943	1.886781
H	-2.227749	-4.401948	3.415649
H	-0.258992	-5.926471	3.539385
C	-0.383371	3.406379	0.008093
C	0.503875	3.686630	1.064520
C	-0.814453	4.473730	-0.794780
C	0.913758	4.992579	1.329628
H	0.878828	2.877885	1.682931
C	-0.390007	5.780321	-0.536844
H	-1.483202	4.298991	-1.628438
C	0.467804	6.046648	0.528538
H	1.585556	5.185914	2.161753
H	-0.738651	6.588851	-1.173197
H	0.789180	7.064010	0.732863
C	-2.001407	1.825968	-1.778923
C	-3.232979	2.496927	-1.697512
C	-1.565047	1.362949	-3.027740
C	-4.004557	2.700706	-2.841082
H	-3.590727	2.862767	-0.739603
C	-2.336381	1.568810	-4.173488
H	-0.623760	0.826287	-3.105086
C	-3.556733	2.239216	-4.081528
H	-4.957827	3.214995	-2.761743
H	-1.985765	1.200636	-5.133582
H	-4.159195	2.398984	-4.971157
C	5.145565	3.396214	1.001316
C	4.648108	2.397437	2.078642
H	6.205716	3.247893	0.773737

H	5.031114	4.433421	1.337385
H	5.382937	1.606962	2.272582
H	4.423163	2.887526	3.029070
C	4.251848	3.112264	-0.181086
C	3.265112	2.171830	0.208295
C	4.224893	3.626376	-1.452601
H	4.965358	4.348437	-1.785142
C	3.191127	3.201207	-2.319954
H	3.113997	3.582610	-3.331615
C	2.268178	2.286696	-1.864604
H	1.463352	1.938562	-2.500451
N	2.291934	1.738001	-0.612207
N	3.418391	1.795008	1.512419
C	2.688767	0.816194	2.195589
C	1.870589	-0.132092	1.642542
C	2.675742	0.801500	3.712014
H	3.668486	0.936449	4.158619
H	2.041664	1.609584	4.112726
C	2.084523	-0.589079	4.017670
H	2.900978	-1.313780	4.119079
H	1.506669	-0.610097	4.946382
C	1.235142	-0.935568	2.774916
H	1.212188	-2.009013	2.579291
H	0.193222	-0.618324	2.908070
Ir	0.902524	0.166034	-0.179206
C	2.735831	-1.234438	0.213351
C	4.225155	-0.904448	0.136475
H	4.404795	-0.078784	-0.561979
C	5.036157	-2.128730	-0.332358
H	4.860084	-2.965173	0.359795
H	4.669948	-2.460197	-1.314798
C	6.544395	-1.855356	-0.419958
H	6.724244	-1.026450	-1.120910
H	6.909529	-1.512372	0.559767
C	7.359586	-3.078066	-0.862315
H	7.179367	-3.904616	-0.160562
H	6.992598	-3.422762	-1.839464
C	8.864084	-2.801234	-0.949742
H	9.414544	-3.693157	-1.268421
H	9.080233	-2.002244	-1.669584
H	9.268148	-2.490871	0.021651
H	4.600835	-0.590644	1.117143
H	2.409730	-1.501247	-0.806183
H	2.561849	-2.117752	0.825430

18

B3LYP SCF energy: -575.18734061 a.u.
B3LYP enthalpy: -574.935109 a.u.
B3LYP free energy: -574.986894 a.u.
B3LYP-D3(BJ) SCF energy in solution: -575.41708279 a.u.
B3LYP-D3(BJ) enthalpy in solution: -575.164851 a.u.
B3LYP-D3(BJ) free energy in solution: -575.216636 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.575346	2.178057	0.076806
C	-0.047886	2.011787	-0.142172
H	-2.021596	2.833171	-0.678640
H	-1.784713	2.627056	1.056635
H	0.240411	2.316903	-1.157767
H	0.535066	2.609657	0.562889
C	-2.082647	0.759120	0.014933
C	-0.983679	-0.129891	0.030615
C	-3.354587	0.227597	-0.008777
H	-4.232665	0.869342	-0.021469
C	-3.486433	-1.174998	-0.014305
H	-4.464100	-1.645472	-0.036257
C	-2.334400	-1.951024	0.013654
H	-2.406677	-3.037325	0.017065
N	-1.079622	-1.457706	0.034797
N	0.216027	0.572241	0.048678
C	1.507572	0.037960	-0.001048
C	1.886141	-1.255332	-0.025769
H	1.203013	-2.091987	-0.026219
C	2.703834	0.975298	-0.069128
H	2.774495	1.444333	-1.062692
H	2.654137	1.794793	0.658313
C	3.899175	0.033461	0.207330
H	4.792389	0.311990	-0.361069
H	4.159111	0.088296	1.270551
C	3.386335	-1.390849	-0.122048
H	3.692749	-1.707129	-1.132709
H	3.795085	-2.142492	0.566493

19

B3LYP SCF energy: -3058.11779916 a.u.
B3LYP enthalpy: -3057.199434 a.u.
B3LYP free energy: -3057.335655 a.u.

B3LYP-D3(BJ) SCF energy in solution: -3059.21885586 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3058.300491 a.u.
B3LYP-D3(BJ) free energy in solution: -3058.436712 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	5.685499	2.591603	0.106949
C	4.573897	1.878135	-0.282698
C	3.917985	0.979423	0.609583
C	4.447801	0.865942	1.936061
C	5.597825	1.613152	2.308852
C	6.211109	2.457148	1.413847
H	6.164568	3.265207	-0.598056
H	4.193263	2.005879	-1.288282
C	2.752780	0.212149	0.231143
C	3.802922	0.008849	2.857466
H	5.982223	1.502336	3.319502
H	7.092096	3.021703	1.705029
C	2.686769	-0.700508	2.493916
C	2.142038	-0.619042	1.180269
H	4.199662	-0.080335	3.865585
H	2.212105	-1.337041	3.228519
C	2.277369	0.356772	-1.191263
C	3.111830	-0.152646	-2.251023
C	1.108893	1.055573	-1.522912
C	4.324665	-0.863688	-2.006325
C	2.739041	0.064223	-3.619399
C	0.775216	1.280752	-2.887451
C	5.097547	-1.340414	-3.040789
H	4.652468	-1.021883	-0.985767
C	3.558519	-0.440140	-4.665929
C	1.566161	0.802849	-3.902302
H	-0.109732	1.852746	-3.135012
C	4.713326	-1.131250	-4.387481
H	6.016590	-1.876559	-2.821668
H	3.253070	-0.263413	-5.693942
H	1.298584	0.994247	-4.938346
H	5.334153	-1.511632	-5.193255
P	0.555097	-1.549307	0.879646
P	-0.106864	1.586382	-0.232148
C	0.224390	-2.470400	2.470008
C	-0.803807	-2.094525	3.347578
C	1.000338	-3.600128	2.793505
C	-1.053800	-2.827310	4.511310
H	-1.409548	-1.224010	3.122910
C	0.759390	-4.320027	3.962364

H	1.797165	-3.922501	2.131314
C	-0.272776	-3.938776	4.823773
H	-1.860653	-2.522828	5.172197
H	1.374522	-5.184547	4.195539
H	-0.465060	-4.506331	5.729862
C	0.974334	-3.013319	-0.168642
C	-0.028486	-3.979634	-0.370118
C	2.255410	-3.253696	-0.673284
C	0.246711	-5.147533	-1.076490
H	-1.026750	-3.815315	0.026044
C	2.528505	-4.423026	-1.390375
H	3.050274	-2.540332	-0.501365
C	1.527071	-5.370124	-1.594656
H	-0.536260	-5.886704	-1.221321
H	3.528312	-4.588850	-1.781266
H	1.740515	-6.280781	-2.147041
C	-1.280013	2.773995	-1.043422
C	-2.247901	2.293547	-1.946028
C	-1.258578	4.147963	-0.753923
C	-3.142210	3.166926	-2.562331
H	-2.307170	1.230098	-2.152746
C	-2.166655	5.017660	-1.363861
H	-0.538916	4.552141	-0.053280
C	-3.105746	4.533627	-2.272688
H	-3.872987	2.778123	-3.266323
H	-2.133050	6.076492	-1.123680
H	-3.807261	5.212645	-2.748918
C	0.840474	2.662569	0.926816
C	1.745100	3.594836	0.387358
C	0.617546	2.657331	2.309446
C	2.400621	4.505530	1.214792
H	1.936948	3.613715	-0.681385
C	1.280275	3.566461	3.136690
H	-0.061406	1.929177	2.739780
C	2.168844	4.494012	2.592155
H	3.098166	5.217164	0.783161
H	1.101739	3.545140	4.208066
H	2.682496	5.201664	3.236575
C	-6.705468	-0.074480	-0.315495
C	-5.862794	-1.099688	-1.108702
H	-7.499785	-0.560824	0.258526
H	-7.186831	0.647784	-0.985785
H	-6.040822	-2.126425	-0.768082
H	-6.056134	-1.059654	-2.181918
C	-5.686500	0.603551	0.564848
C	-4.386694	0.172453	0.189253

C	-5.828774	1.533734	1.560937
H	-6.808252	1.889985	1.866743
C	-4.652806	2.026763	2.172001
H	-4.700767	2.766245	2.963477
C	-3.428329	1.555490	1.764202
H	-2.513580	1.906039	2.219731
N	-3.255240	0.605329	0.784230
N	-4.450086	-0.736781	-0.833940
C	-3.390465	-1.315433	-1.515519
C	-2.049141	-1.170907	-1.237668
C	-3.688028	-2.107153	-2.780504
H	-4.474276	-2.860399	-2.652951
H	-4.030023	-1.429731	-3.580135
C	-2.317435	-2.723220	-3.113874
H	-2.244123	-3.721023	-2.665021
H	-2.154280	-2.833585	-4.190354
C	-1.311391	-1.776064	-2.430933
H	-0.375644	-2.271439	-2.173988
H	-1.036104	-0.954834	-3.112445
Ir	-1.289335	-0.207122	0.444467
H	-0.921333	0.365566	1.947114

20

B3LYP SCF energy: -3293.96292966 a.u.
B3LYP enthalpy: -3292.865817 a.u.
B3LYP free energy: -3293.019238 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.18110259 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.083990 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.237411 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	6.079579	-1.066490	-2.176409
C	4.973141	-0.957465	-1.363277
C	4.170229	0.221726	-1.353909
C	4.559634	1.283626	-2.231250
C	5.711413	1.148292	-3.051894
C	6.461549	-0.003315	-3.027828
H	6.667650	-1.979806	-2.160478
H	4.710906	-1.791607	-0.725252
C	2.993867	0.363759	-0.518914
C	3.783013	2.464266	-2.248875
H	5.984927	1.975697	-3.701540
H	7.341260	-0.100863	-3.657292

C	2.647595	2.567509	-1.488256
C	2.206380	1.512434	-0.633201
H	4.092076	3.295071	-2.878148
H	2.088545	3.490167	-1.531762
C	2.782224	-0.764064	0.454735
C	3.751446	-0.905838	1.512072
C	1.843626	-1.778600	0.249017
C	4.671467	0.128579	1.848035
C	3.821797	-2.129480	2.255930
C	1.970195	-3.004691	0.959751
C	5.584817	-0.032913	2.865195
H	4.642325	1.061837	1.299043
C	4.784648	-2.270924	3.291742
C	2.943810	-3.184649	1.911945
H	1.291586	-3.819379	0.744030
C	5.647682	-1.244593	3.594994
H	6.267153	0.776189	3.109473
H	4.823307	-3.208040	3.841120
H	3.032586	-4.137978	2.426732
H	6.378514	-1.359438	4.390160
P	0.610532	1.782920	0.307055
P	0.351066	-1.495080	-0.815385
C	0.012994	3.403549	-0.397247
C	-0.317710	3.492039	-1.764221
C	-0.164772	4.538601	0.405350
C	-0.797596	4.680795	-2.308499
H	-0.195880	2.624224	-2.404310
C	-0.664365	5.727442	-0.139635
H	0.085559	4.511096	1.459420
C	-0.978427	5.804419	-1.494226
H	-1.034685	4.729995	-3.367677
H	-0.798967	6.592797	0.503008
H	-1.358828	6.729837	-1.916979
C	1.203197	2.336010	1.975316
C	0.390040	2.234067	3.114754
C	2.437277	2.998922	2.089627
C	0.799682	2.778487	4.333871
H	-0.555577	1.708475	3.063064
C	2.847364	3.536983	3.309752
H	3.078664	3.112492	1.222090
C	2.029493	3.429672	4.435736
H	0.156803	2.685518	5.204667
H	3.805752	4.044094	3.376840
H	2.348407	3.850495	5.384993
C	-0.463675	-3.158627	-0.940638
C	-1.092771	-3.712522	0.189733

C	-0.488291	-3.883074	-2.142263
C	-1.704777	-4.963016	0.122305
H	-1.109165	-3.155460	1.120286
C	-1.113563	-5.131412	-2.208778
H	-0.022027	-3.484325	-3.034841
C	-1.718445	-5.677807	-1.078548
H	-2.173966	-5.379444	1.009660
H	-1.120194	-5.674724	-3.149470
H	-2.197827	-6.651264	-1.130257
C	1.030028	-1.268529	-2.521566
C	2.134773	-2.042791	-2.916568
C	0.421659	-0.433585	-3.467981
C	2.619663	-1.975923	-4.222141
H	2.618436	-2.702997	-2.203582
C	0.907513	-0.367992	-4.775953
H	-0.429285	0.173849	-3.178171
C	2.007177	-1.137702	-5.156222
H	3.480007	-2.574916	-4.505783
H	0.424659	0.287198	-5.495789
H	2.386025	-1.084975	-6.172896
C	-5.658399	-2.353628	1.675686
C	-4.580441	-2.056894	2.748401
H	-6.507105	-1.665309	1.767170
H	-6.058039	-3.368220	1.768863
H	-4.932475	-1.354959	3.509820
H	-4.258961	-2.970450	3.259359
C	-4.925171	-2.131705	0.376649
C	-3.660034	-1.551833	0.660134
C	-5.279264	-2.383048	-0.924497
H	-6.232005	-2.844301	-1.169859
C	-4.363116	-2.029338	-1.940601
H	-4.582833	-2.213654	-2.985992
C	-3.185608	-1.407515	-1.592989
H	-2.485120	-1.079222	-2.348175
N	-2.817353	-1.129200	-0.305045
N	-3.437811	-1.474257	2.006612
C	-2.177721	-1.280043	2.624109
C	-1.083774	-0.727856	2.049979
C	-1.953044	-1.835490	4.023660
H	-2.746495	-1.579637	4.736280
H	-1.885729	-2.936578	4.011812
C	-0.598584	-1.200584	4.387630
H	-0.771012	-0.235432	4.881046
H	-0.004384	-1.818896	5.068385
C	0.073590	-0.974994	3.018815
H	0.823714	-0.183417	3.039760

H	0.609246	-1.886059	2.725008
Ir	-1.119479	0.169072	0.063323
H	-1.214793	0.699237	-1.496317
C	-2.594314	1.593878	1.140015
H	-1.979072	2.250512	1.741210
C	-2.825392	1.901706	-0.192472
H	-2.260582	2.716504	-0.622966
H	-3.300803	0.985765	1.694617
C	-4.091511	1.589210	-0.947834
H	-3.865116	1.301706	-1.980830
H	-4.638840	0.761555	-0.487617
C	-4.993837	2.844359	-0.967634
H	-5.228164	3.139193	0.064675
H	-4.441251	3.684948	-1.410488
C	-6.298213	2.625534	-1.747437
H	-6.057972	2.331148	-2.778801
H	-6.846120	1.780467	-1.307245
C	-7.196186	3.866894	-1.763313
H	-8.117374	3.682846	-2.326667
H	-7.480548	4.164015	-0.746680
H	-6.686211	4.719501	-2.227768

21-TS

B3LYP SCF energy: -3293.93885607 a.u.
B3LYP enthalpy: -3292.843868 a.u.
B3LYP free energy: -3292.999030 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.15881311 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.063825 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.218987 a.u.
Imaginary frequency: -268.5506 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	5.952213	2.326253	1.170878
C	4.898802	1.695165	0.547569
C	4.186652	0.642294	1.190411
C	4.610899	0.251231	2.500403
C	5.703737	0.917484	3.116869
C	6.362208	1.936423	2.468584
H	6.476186	3.130242	0.661659
H	4.599400	2.008424	-0.446084
C	3.068667	-0.017920	0.568992
C	3.943825	-0.825167	3.131712
H	6.010920	0.603901	4.111288

H	7.197717	2.440475	2.945675
C	2.859217	-1.424723	2.540420
C	2.362533	-0.998539	1.275863
H	4.303115	-1.180796	4.094229
H	2.397787	-2.262421	3.043988
C	2.824611	0.261258	-0.888117
C	3.783277	-0.302232	-1.818273
C	1.752223	1.001464	-1.376628
C	4.889441	-1.093782	-1.398317
C	3.624509	-0.081613	-3.224539
C	1.575598	1.136956	-2.789411
C	5.791819	-1.601498	-2.308249
H	5.026507	-1.306389	-0.345674
C	4.574642	-0.608688	-4.137768
C	2.487698	0.634783	-3.679603
H	0.705112	1.659992	-3.168240
C	5.643856	-1.351506	-3.691501
H	6.626776	-2.200852	-1.956778
H	4.437615	-0.416709	-5.199095
H	2.343944	0.776532	-4.748061
H	6.367933	-1.750533	-4.395919
P	0.807781	-1.778423	0.569563
P	0.355005	1.646842	-0.345723
C	0.152537	-2.926452	1.877825
C	0.047244	-2.563827	3.234936
C	-0.437410	-4.141251	1.478913
C	-0.582612	-3.400794	4.158940
H	0.457716	-1.622456	3.585236
C	-1.077826	-4.970552	2.401829
H	-0.379816	-4.460660	0.443758
C	-1.147046	-4.608689	3.747498
H	-0.626282	-3.104780	5.203616
H	-1.514617	-5.906190	2.064379
H	-1.634570	-5.259897	4.466947
C	1.571221	-2.975040	-0.635773
C	1.582340	-2.715431	-2.013496
C	2.247463	-4.115493	-0.163999
C	2.209844	-3.593781	-2.901352
H	1.133578	-1.809063	-2.403507
C	2.873901	-4.989809	-1.050229
H	2.281991	-4.328338	0.899546
C	2.848055	-4.736957	-2.424072
H	2.208228	-3.371518	-3.964367
H	3.385294	-5.867722	-0.665515
H	3.333242	-5.421010	-3.114348
C	-0.031495	3.321487	-1.049022

C	-1.177027	3.963972	-0.549879
C	0.807329	4.032824	-1.921457
C	-1.487938	5.268579	-0.933625
H	-1.821859	3.451746	0.156025
C	0.490405	5.337471	-2.309460
H	1.718959	3.583217	-2.298603
C	-0.660065	5.957215	-1.823006
H	-2.374831	5.750651	-0.531170
H	1.152658	5.869017	-2.987155
H	-0.903997	6.971956	-2.124145
C	1.037845	2.224620	1.279680
C	1.949805	3.292631	1.328228
C	0.574457	1.682521	2.484733
C	2.395052	3.790126	2.551412
H	2.307771	3.748302	0.410738
C	1.014459	2.186125	3.710876
H	-0.135368	0.866069	2.468324
C	1.927018	3.240103	3.747118
H	3.105313	4.611660	2.569827
H	0.638060	1.756405	4.635340
H	2.268143	3.635802	4.699570
C	-5.270712	2.583353	2.206636
C	-5.237404	2.634716	0.664776
H	-6.275406	2.385192	2.589956
H	-4.936017	3.535215	2.639274
H	-6.075175	2.073755	0.229921
H	-5.266651	3.652233	0.270579
C	-4.284348	1.486622	2.519536
C	-3.506920	1.235184	1.355983
C	-4.047464	0.775064	3.667216
H	-4.634723	0.940818	4.565983
C	-3.023484	-0.196013	3.632984
H	-2.804456	-0.821624	4.490771
C	-2.289443	-0.354691	2.479136
H	-1.513100	-1.099427	2.424937
N	-2.476321	0.364830	1.333343
N	-3.962014	1.975226	0.298307
C	-3.585374	1.808069	-1.044353
C	-2.579685	1.033173	-1.499887
C	-4.243032	2.654790	-2.117171
H	-5.338229	2.662593	-2.066531
H	-3.911091	3.701846	-2.040787
C	-3.724860	1.993737	-3.410514
H	-4.442879	1.235861	-3.744665
H	-3.593639	2.708533	-4.228401
C	-2.405544	1.306399	-2.992623

H	-2.201011	0.417190	-3.598998
H	-1.553005	1.985318	-3.146720
Ir	-1.316087	-0.145197	-0.415241
H	-0.804526	-0.818030	-1.943600
C	-1.672222	-1.830200	-1.972390
H	-0.922058	-2.602782	-2.131365
C	-2.494499	-1.923658	-0.767798
H	-2.169727	-2.692195	-0.062872
H	-2.192025	-1.551267	-2.888994
C	-4.008197	-1.841355	-0.861162
H	-4.412463	-1.541101	0.115392
H	-4.297876	-1.058117	-1.570919
C	-4.653655	-3.179820	-1.270329
H	-4.267130	-3.486997	-2.253638
H	-4.346781	-3.964122	-0.562643
C	-6.186151	-3.117874	-1.323766
H	-6.567851	-2.803536	-0.341713
H	-6.491705	-2.336948	-2.034693
C	-6.830761	-4.450467	-1.719233
H	-7.923111	-4.371624	-1.745596
H	-6.496744	-4.774670	-2.712372
H	-6.571370	-5.243325	-1.007082

22

B3LYP SCF energy: -3293.93718115 a.u.
B3LYP enthalpy: -3292.838701 a.u.
B3LYP free energy: -3292.997376 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.16798394 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.069504 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.228179 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-6.130478	-1.640157	1.565621
C	-5.041683	-1.188888	0.853445
C	-4.183364	-0.180763	1.379456
C	-4.496862	0.355693	2.669466
C	-5.627605	-0.128581	3.380260
C	-6.430188	-1.107472	2.842518
H	-6.768170	-2.411499	1.143012
H	-4.829364	-1.610335	-0.122317
C	-3.030532	0.299220	0.662913
C	-3.681177	1.388816	3.187925
H	-5.848202	0.294123	4.357123

H	-7.294839	-1.470402	3.390563
C	-2.574209	1.824675	2.502272
C	-2.199737	1.261630	1.248624
H	-3.945137	1.845585	4.138591
H	-1.997441	2.636416	2.923298
C	-2.869814	-0.154126	-0.762446
C	-3.779711	0.420884	-1.727437
C	-1.931409	-1.099727	-1.179340
C	-4.759206	1.393573	-1.375129
C	-3.712657	0.016004	-3.100377
C	-1.852380	-1.442046	-2.564950
C	-5.625265	1.907331	-2.315354
H	-4.826758	1.737182	-0.350503
C	-4.622550	0.558492	-4.045684
C	-2.718912	-0.916336	-3.488180
H	-1.102790	-2.149494	-2.895320
C	-5.565896	1.483890	-3.663527
H	-6.363911	2.645690	-2.016673
H	-4.557344	0.227580	-5.079160
H	-2.651351	-1.215493	-4.531325
H	-6.261102	1.892399	-4.391211
P	-0.622844	1.816841	0.406694
P	-0.579200	-1.764822	-0.097063
C	0.156391	3.062037	1.542257
C	0.375977	2.790335	2.907135
C	0.690471	4.251320	1.015591
C	1.074889	3.686373	3.717260
H	-0.016026	1.882670	3.356405
C	1.398512	5.142046	1.826037
H	0.546600	4.497386	-0.030067
C	1.590165	4.867181	3.179416
H	1.209791	3.461535	4.771750
H	1.794360	6.056116	1.392750
H	2.133132	5.565095	3.809901
C	-1.280699	2.863689	-0.967453
C	-1.117464	2.474278	-2.301748
C	-2.014504	4.030404	-0.687387
C	-1.642411	3.246294	-3.340652
H	-0.597413	1.551960	-2.538850
C	-2.535648	4.802634	-1.723559
H	-2.171819	4.341972	0.340956
C	-2.344732	4.415660	-3.053288
H	-1.505794	2.927877	-4.369882
H	-3.093277	5.705992	-1.492957
H	-2.750621	5.019910	-3.859488
C	-0.280749	-3.495714	-0.687688

C	0.940156	-4.088103	-0.325703
C	-1.235223	-4.281386	-1.355334
C	1.204965	-5.423454	-0.634511
H	1.685553	-3.509010	0.209002
C	-0.964648	-5.614150	-1.671280
H	-2.195402	-3.860218	-1.635094
C	0.256333	-6.188610	-1.314752
H	2.152780	-5.866339	-0.340639
H	-1.714312	-6.204315	-2.190971
H	0.463729	-7.226354	-1.559554
C	-1.284058	-2.156019	1.569941
C	-2.319343	-3.093508	1.718246
C	-0.702782	-1.606931	2.720062
C	-2.770188	-3.455981	2.986004
H	-2.771626	-3.551673	0.844858
C	-1.150461	-1.974634	3.990939
H	0.107899	-0.895064	2.624764
C	-2.186614	-2.898235	4.126284
H	-3.576259	-4.177430	3.083360
H	-0.684531	-1.542950	4.872656
H	-2.534518	-3.188338	5.113616
C	5.453432	-2.657718	1.634341
C	5.254875	-2.707901	0.102072
H	6.480588	-2.399913	1.906433
H	5.226915	-3.628776	2.092451
H	6.030316	-2.136992	-0.424266
H	5.250941	-3.724916	-0.295389
C	4.446723	-1.621366	2.073469
C	3.563831	-1.368789	0.986210
C	4.271486	-0.972202	3.265676
H	4.935386	-1.146090	4.107379
C	3.201646	-0.051390	3.360492
H	3.022342	0.516944	4.265768
C	2.376049	0.133323	2.278246
H	1.571747	0.850123	2.306206
N	2.508029	-0.528071	1.087018
N	3.939665	-2.067679	-0.119283
C	3.358524	-1.940973	-1.386691
C	2.259243	-1.204908	-1.643593
C	3.849418	-2.751359	-2.566546
H	4.936081	-2.716713	-2.711011
H	3.573194	-3.812068	-2.457574
C	3.083656	-2.086257	-3.732145
H	3.692826	-1.277193	-4.150518
H	2.852225	-2.784295	-4.542348
C	1.814382	-1.486856	-3.076877

H	1.446703	-0.609308	-3.619217
H	1.004393	-2.230141	-3.077204
Ir	1.218225	0.002301	-0.418193
C	2.452854	1.828077	-2.457454
H	2.737656	2.847101	-2.754118
C	2.514271	1.656104	-0.931534
H	2.050711	2.537089	-0.469938
H	3.130897	1.129541	-2.959868
C	3.969543	1.617551	-0.438066
H	3.989841	1.524492	0.654551
H	4.476137	0.729666	-0.843056
C	4.796467	2.866702	-0.803304
H	4.898351	2.948998	-1.893345
H	4.256067	3.767516	-0.474977
C	6.196886	2.864284	-0.174361
H	6.102880	2.798805	0.919390
H	6.733061	1.957032	-0.489490
C	7.026505	4.098788	-0.543266
H	8.019222	4.067143	-0.080433
H	7.167213	4.171705	-1.628528
H	6.533893	5.020982	-0.211313
H	1.451131	1.665021	-2.871254

23-TS

B3LYP SCF energy: -3293.92802464 a.u.
B3LYP enthalpy: -3292.830097 a.u.
B3LYP free energy: -3292.984014 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.15110655 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.053179 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.207096 a.u.
Imaginary frequency: -322.9651 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-6.099715	1.875584	-1.617478
C	-5.031265	1.429389	-0.871828
C	-4.152536	0.422863	-1.368275
C	-4.411373	-0.095104	-2.678578
C	-5.522820	0.383200	-3.423393
C	-6.355405	1.346984	-2.905091
H	-6.754399	2.642041	-1.212231
H	-4.856819	1.853545	0.109351
C	-3.029727	-0.074365	-0.611643
C	-3.549401	-1.088873	-3.198055

H	-5.702005	-0.030734	-4.412473
H	-7.205654	1.704777	-3.478558
C	-2.470792	-1.535938	-2.475478
C	-2.180135	-1.028704	-1.177355
H	-3.753105	-1.504268	-4.182062
H	-1.845125	-2.305140	-2.906732
C	-2.858689	0.450735	0.785550
C	-3.834271	0.076478	1.776838
C	-1.844289	1.351240	1.120778
C	-4.857845	-0.880637	1.520805
C	-3.789302	0.675758	3.078115
C	-1.826453	1.940352	2.416113
C	-5.781444	-1.209722	2.487189
H	-4.899954	-1.365699	0.553224
C	-4.762594	0.322376	4.051072
C	-2.774300	1.622621	3.357756
H	-1.071702	2.675248	2.662439
C	-5.742420	-0.598861	3.763667
H	-6.549212	-1.946223	2.268000
H	-4.716526	0.795860	5.028552
H	-2.753776	2.102969	4.332987
H	-6.484035	-0.862270	4.512306
P	-0.708871	-1.705963	-0.231643
P	-0.446541	1.682854	-0.059375
C	-0.036960	-3.006395	-1.388024
C	0.538258	-2.583993	-2.603119
C	0.000328	-4.373952	-1.082000
C	1.103789	-3.497919	-3.490713
H	0.541054	-1.527805	-2.857756
C	0.578065	-5.290318	-1.966742
H	-0.412604	-4.738938	-0.149194
C	1.126163	-4.859101	-3.173328
H	1.528869	-3.146903	-4.426969
H	0.595894	-6.344511	-1.704855
H	1.569154	-5.573878	-3.860815
C	-1.634788	-2.696359	1.039722
C	-1.525456	-2.426763	2.407607
C	-2.546703	-3.684279	0.619393
C	-2.262653	-3.159554	3.342113
H	-0.884080	-1.626563	2.745856
C	-3.276245	-4.419546	1.551424
H	-2.689340	-3.882131	-0.438546
C	-3.128158	-4.165682	2.918114
H	-2.163870	-2.932887	4.399846
H	-3.965239	-5.186945	1.209545
H	-3.697471	-4.739608	3.643704

C	0.415214	3.186874	0.611714
C	1.140900	3.073137	1.812483
C	0.418475	4.423190	-0.051820
C	1.806546	4.172621	2.353662
H	1.193359	2.115737	2.320023
C	1.101059	5.519330	0.483649
H	-0.107279	4.543342	-0.990980
C	1.787524	5.402520	1.691117
H	2.342758	4.066708	3.293049
H	1.087901	6.466733	-0.047885
H	2.306243	6.259398	2.111775
C	-1.280886	2.318992	-1.584068
C	-2.228449	3.353698	-1.503692
C	-0.964686	1.792200	-2.843288
C	-2.820081	3.863903	-2.658971
H	-2.506110	3.762221	-0.536081
C	-1.557964	2.300648	-4.000043
H	-0.274232	0.956995	-2.916775
C	-2.481500	3.342838	-3.910110
H	-3.550915	4.663618	-2.580946
H	-1.304892	1.876761	-4.967830
H	-2.944216	3.740614	-4.808670
C	5.767402	2.614108	0.713694
C	5.321613	1.608364	1.804648
H	6.783343	2.407365	0.363757
H	5.759517	3.641747	1.095564
H	6.007088	0.755463	1.879580
H	5.250339	2.071641	2.791323
C	4.732150	2.437186	-0.368963
C	3.713170	1.574335	0.109590
C	4.628174	2.971471	-1.627226
H	5.392129	3.633282	-2.025348
C	3.487086	2.638202	-2.392492
H	3.347693	3.027607	-3.394494
C	2.538645	1.798561	-1.853848
H	1.661294	1.523161	-2.420744
N	2.623563	1.240899	-0.606217
N	3.989561	1.129253	1.368553
C	3.235813	0.230501	2.123129
C	2.194544	-0.551869	1.695362
C	3.466065	0.165776	3.622638
H	4.525810	0.111875	3.898887
H	3.056999	1.057551	4.127308
C	2.692407	-1.103993	4.013076
H	3.356025	-1.974188	3.944097
H	2.295661	-1.067937	5.032448

C	1.591320	-1.199123	2.941292
H	1.236850	-2.218227	2.793747
H	0.723614	-0.600542	3.252690
Ir	1.062370	-0.116230	-0.014471
C	2.542912	-3.193725	0.855151
H	1.501972	-3.396542	1.109315
C	2.736229	-1.880846	0.106751
H	2.223911	-1.945138	-0.862143
H	2.878107	-4.023826	0.222517
C	4.208833	-1.582230	-0.179900
H	4.303098	-0.641038	-0.725988
H	4.765136	-1.473841	0.759641
C	4.894221	-2.670075	-1.037600
H	4.940543	-3.617254	-0.485928
H	4.293712	-2.865034	-1.938231
C	6.317005	-2.270276	-1.455026
H	6.277733	-1.331082	-2.025649
H	6.911114	-2.057222	-0.554639
C	7.022658	-3.345519	-2.287917
H	8.033788	-3.031345	-2.569189
H	7.109446	-4.285757	-1.730243
H	6.470767	-3.557512	-3.211823
H	3.134842	-3.223883	1.776544

24

B3LYP SCF energy: -811.06436615 a.u.
B3LYP enthalpy: -810.633064 a.u.
B3LYP free energy: -810.704423 a.u.
B3LYP-D3(BJ) SCF energy in solution: -811.39782286 a.u.
B3LYP-D3(BJ) enthalpy in solution: -810.966521 a.u.
B3LYP-D3(BJ) free energy in solution: -811.037880 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.662950	-2.408994	-0.915047
C	-0.673039	-1.244161	-1.177355
H	-1.225218	-3.141791	-0.223310
H	-1.917603	-2.943712	-1.835961
H	0.367174	-1.522186	-0.990396
H	-0.746181	-0.892190	-2.217891
C	-2.833602	-1.703591	-0.272481
C	-2.426920	-0.404188	0.107394
C	-4.119740	-2.097676	0.032397
H	-4.485651	-3.086325	-0.236025

C	-4.952159	-1.179514	0.702342
H	-5.974463	-1.436535	0.960386
C	-4.437885	0.069380	1.033445
H	-5.059213	0.794279	1.557018
N	-3.184982	0.479964	0.751997
N	-1.105088	-0.172726	-0.253037
C	-0.537465	1.124031	-0.349870
C	0.704541	1.450686	0.054477
C	-1.289230	2.299739	-0.950296
H	-1.826240	2.029237	-1.868851
H	-2.044992	2.663733	-0.244290
C	-0.160882	3.326737	-1.197834
H	0.187992	3.242445	-2.233939
H	-0.484946	4.361586	-1.047233
C	0.984334	2.914017	-0.239356
H	1.975174	3.084113	-0.680644
H	0.960993	3.499655	0.692512
C	1.684306	0.553253	0.772118
H	1.163716	-0.390128	0.987091
C	2.101601	1.170558	2.123206
H	2.688251	2.086262	1.979157
H	1.220141	1.425111	2.721743
C	2.908082	0.225381	-0.121434
H	2.542629	-0.108296	-1.103121
H	3.478411	1.146825	-0.308474
C	3.850573	-0.846240	0.445078
H	4.290114	-0.501055	1.390574
H	3.269436	-1.748383	0.690717
C	4.984235	-1.223847	-0.519048
H	4.552149	-1.582162	-1.464380
H	5.560082	-0.322019	-0.771566
C	5.928205	-2.289552	0.048046
H	5.387096	-3.215332	0.280109
H	6.724649	-2.538463	-0.662689
H	6.404051	-1.944739	0.974427
H	2.710927	0.473293	2.707616

21L-TS

B3LYP SCF energy: -3293.93897868 a.u.
B3LYP enthalpy: -3292.844150 a.u.
B3LYP free energy: -3292.997754 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.15939743 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.064569 a.u.
B3LYP-D3(BJ) free energy in solution: -3294.218173 a.u.

Imaginary frequency: -289.3300 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-5.882006	-2.622434	-0.412329
C	-4.783071	-1.814629	-0.601772
C	-4.150966	-1.158708	0.493692
C	-4.703121	-1.363005	1.798662
C	-5.838962	-2.200495	1.964065
C	-6.419656	-2.819729	0.882186
H	-6.342456	-3.113153	-1.265211
H	-4.386759	-1.679499	-1.601205
C	-2.992653	-0.318578	0.322031
C	-4.116436	-0.684879	2.892182
H	-6.242188	-2.338472	2.964052
H	-7.289396	-3.456468	1.015723
C	-2.997038	0.091350	2.720008
C	-2.378482	0.249478	1.447448
H	-4.568335	-0.774929	3.876915
H	-2.608765	0.623199	3.576339
C	-2.604414	0.026857	-1.091271
C	-3.492536	0.921024	-1.805885
C	-1.468618	-0.462012	-1.733090
C	-4.659411	1.483437	-1.214752
C	-3.201040	1.279021	-3.162159
C	-1.156472	-0.017647	-3.054799
C	-5.496322	2.311236	-1.931562
H	-4.896681	1.260364	-0.182208
C	-4.086363	2.126289	-3.878734
C	-2.002843	0.802935	-3.753229
H	-0.232681	-0.340270	-3.520677
C	-5.218400	2.630275	-3.280353
H	-6.381109	2.721959	-1.453616
H	-3.848899	2.371829	-4.910901
H	-1.758834	1.102593	-4.769623
H	-5.892749	3.275642	-3.835760
P	-0.793922	1.247230	1.305218
P	-0.165733	-1.461460	-0.884077
C	-0.334162	1.831753	3.013093
C	-0.344197	1.011548	4.157668
C	0.236754	3.113409	3.139095
C	0.156749	1.466468	5.379612
H	-0.751165	0.007079	4.114715
C	0.748240	3.562521	4.357659
H	0.266544	3.783105	2.286256
C	0.704934	2.744164	5.486667

H	0.112401	0.815963	6.248832
H	1.172827	4.560403	4.421679
H	1.092671	3.097887	6.437359
C	-1.494599	2.809813	0.566173
C	-1.321697	3.133175	-0.786528
C	-2.308241	3.643965	1.355357
C	-1.907637	4.280955	-1.327356
H	-0.752775	2.478004	-1.436834
C	-2.892137	4.788149	0.815003
H	-2.483217	3.405943	2.399613
C	-2.685863	5.115591	-0.527513
H	-1.764055	4.509471	-2.379351
H	-3.510993	5.422168	1.443723
H	-3.139240	6.008876	-0.947484
C	0.469081	-2.673547	-2.140687
C	1.602022	-3.418992	-1.771350
C	-0.177099	-2.991279	-3.345294
C	2.090310	-4.431093	-2.597680
H	2.100210	-3.219055	-0.828660
C	0.317554	-4.001792	-4.174237
H	-1.074310	-2.462169	-3.646512
C	1.455117	-4.720036	-3.807558
H	2.964289	-4.999745	-2.291701
H	-0.196156	-4.229183	-5.104178
H	1.837417	-5.506115	-4.452368
C	-1.038703	-2.711388	0.179601
C	-1.912342	-3.639058	-0.413502
C	-0.764045	-2.832439	1.546109
C	-2.501874	-4.647261	0.345979
H	-2.128870	-3.584412	-1.475335
C	-1.349374	-3.846876	2.307384
H	-0.087936	-2.138324	2.023365
C	-2.220623	-4.756550	1.709936
H	-3.179461	-5.350331	-0.129734
H	-1.118158	-3.925191	3.366293
H	-2.674416	-5.548320	2.299152
C	5.524149	-2.902962	1.853114
C	5.620123	-2.264237	0.450949
H	6.412617	-2.700887	2.457859
H	5.417601	-3.993135	1.783270
H	6.346387	-1.440541	0.432656
H	5.899680	-2.980985	-0.323401
C	4.269368	-2.284429	2.416605
C	3.558700	-1.650499	1.359239
C	3.759033	-2.275720	3.688271
H	4.286331	-2.749015	4.511708

C	2.526176	-1.619596	3.892103
H	2.076737	-1.549136	4.875978
C	1.888540	-1.048435	2.814767
H	0.959018	-0.523771	2.948095
N	2.356344	-1.057618	1.531945
N	4.264148	-1.730718	0.190794
C	3.931316	-1.124793	-1.029209
C	2.831429	-0.382985	-1.272452
C	4.758388	-1.421821	-2.266205
H	5.837541	-1.295966	-2.118481
H	4.599435	-2.460117	-2.597683
C	4.184858	-0.413964	-3.283430
H	4.776535	0.509012	-3.253890
H	4.209454	-0.789280	-4.310945
C	2.752736	-0.130617	-2.776858
H	2.404715	0.869914	-3.048955
H	2.043785	-0.837523	-3.231071
Ir	1.383050	0.192128	0.050806
H	1.122655	1.545908	-1.041602
C	1.919063	2.469234	-0.438789
H	1.108315	3.134304	-0.143145
C	2.609468	1.829561	0.673766
H	2.364719	2.163468	1.680797
H	3.669310	1.618670	0.529099
C	2.716886	3.036744	-1.608278
H	3.530290	2.353164	-1.869011
H	2.078509	3.148141	-2.494095
C	3.300928	4.411213	-1.229651
H	2.486949	5.087417	-0.930163
H	3.949767	4.298527	-0.350187
C	4.095588	5.052177	-2.376014
H	3.441523	5.163451	-3.252125
H	4.903264	4.372118	-2.680872
C	4.686596	6.415288	-2.001284
H	3.899471	7.127607	-1.725825
H	5.371629	6.330626	-1.149093
H	5.247317	6.846232	-2.837602

22L

B3LYP SCF energy: -3293.97661190 a.u.
B3LYP enthalpy: -3292.877209 a.u.
B3LYP free energy: -3293.035040 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.20009414 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.100691 a.u.

B3LYP-D3(BJ) free energy in solution: -3294.258522 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-6.643696	0.405754	0.248258
C	-5.310473	0.234238	0.548557
C	-4.450886	-0.522810	-0.300921
C	-5.026206	-1.097706	-1.479414
C	-6.406267	-0.909923	-1.760168
C	-7.203241	-0.173422	-0.915690
H	-7.273684	0.988167	0.914563
H	-4.909367	0.685548	1.448065
C	-3.046645	-0.709540	-0.017685
C	-4.197047	-1.853132	-2.341817
H	-6.818926	-1.360392	-2.659144
H	-8.257616	-0.035138	-1.136500
C	-2.861659	-2.007418	-2.072771
C	-2.253935	-1.428731	-0.917482
H	-4.630235	-2.312486	-3.226630
H	-2.260304	-2.595364	-2.753654
C	-2.542246	-0.150069	1.283715
C	-2.976486	-0.795550	2.500435
C	-1.750651	0.999178	1.357207
C	-3.769437	-1.979818	2.503486
C	-2.613306	-0.239345	3.770962
C	-1.374144	1.508341	2.636017
C	-4.174915	-2.566762	3.681446
H	-4.066826	-2.422973	1.561380
C	-3.052101	-0.863808	4.969462
C	-1.809026	0.925813	3.799313
H	-0.729021	2.375514	2.694413
C	-3.817935	-2.005194	4.930168
H	-4.779125	-3.468993	3.651830
H	-2.767586	-0.420252	5.920247
H	-1.524855	1.348367	4.759944
H	-4.149034	-2.476639	5.850784
P	-0.422679	-1.747689	-0.711668
P	-0.856218	1.712510	-0.096978
C	0.076882	-2.282173	-2.416512
C	0.126955	-1.302291	-3.424260
C	0.478041	-3.588428	-2.725198
C	0.576216	-1.618972	-4.706437
H	-0.229337	-0.296678	-3.219851
C	0.928421	-3.903350	-4.010722
H	0.440881	-4.365111	-1.969279
C	0.983912	-2.922271	-5.001350

H	0.597720	-0.852427	-5.476336
H	1.233337	-4.921501	-4.235254
H	1.333620	-3.172387	-5.998691
C	-0.361116	-3.317608	0.264842
C	0.871099	-3.842835	0.693196
C	-1.529180	-4.050790	0.522815
C	0.928634	-5.063957	1.364416
H	1.790019	-3.303645	0.499830
C	-1.469056	-5.270291	1.200904
H	-2.490596	-3.679509	0.189509
C	-0.242190	-5.779666	1.624502
H	1.890431	-5.453928	1.685304
H	-2.385383	-5.820962	1.393250
H	-0.196291	-6.728874	2.150531
C	-0.597590	3.509639	0.319469
C	0.415014	4.208291	-0.355690
C	-1.485570	4.240819	1.128106
C	0.562627	5.588388	-0.197219
H	1.079680	3.684094	-1.031581
C	-1.332303	5.617687	1.292169
H	-2.307062	3.742481	1.631682
C	-0.303472	6.296275	0.635734
H	1.351220	6.107458	-0.735235
H	-2.026999	6.161445	1.926321
H	-0.189559	7.369274	0.760838
C	-2.026447	2.007332	-1.499810
C	-3.361304	2.390576	-1.309010
C	-1.498219	2.029323	-2.798853
C	-4.157824	2.746317	-2.396848
H	-3.785335	2.412431	-0.311033
C	-2.292149	2.394582	-3.888180
H	-0.450491	1.788612	-2.960797
C	-3.627377	2.745890	-3.689258
H	-5.194213	3.026865	-2.232365
H	-1.865562	2.409224	-4.887365
H	-4.248931	3.028274	-4.534089
C	4.230966	4.104127	1.341564
C	3.718538	3.062682	2.366470
H	5.292735	4.326176	1.480344
H	3.680800	5.048652	1.437217
H	4.546214	2.479861	2.788636
H	3.164806	3.517400	3.190248
C	3.921976	3.455618	0.014515
C	3.052624	2.360805	0.252792
C	4.276475	3.762716	-1.274658
H	4.944209	4.590676	-1.495263

C	3.746753	2.965887	-2.319560
H	4.004383	3.155117	-3.355289
C	2.888279	1.934608	-2.007963
H	2.460647	1.308483	-2.784015
N	2.510209	1.624504	-0.731100
N	2.833582	2.167996	1.582923
C	2.186842	1.058646	2.154536
C	1.459934	0.111586	1.518482
C	2.238321	0.865376	3.656354
H	3.254837	0.937632	4.062054
H	1.642832	1.634624	4.171028
C	1.643921	-0.550581	3.851006
H	2.444872	-1.255431	4.095147
H	0.925435	-0.581981	4.674597
C	0.989518	-0.942963	2.498200
H	1.305283	-1.942911	2.194355
H	-0.102933	-0.975211	2.561537
Ir	1.084421	0.076316	-0.458369
C	3.942384	-1.237631	0.035389
H	3.645409	-1.633402	1.016882
C	2.731541	-1.209139	-0.903528
H	2.415439	-2.237878	-1.100075
H	3.054798	-0.824730	-1.887760
C	5.105332	-2.084971	-0.511248
H	4.756881	-3.114520	-0.683243
H	5.403491	-1.698103	-1.497083
C	6.329151	-2.111914	0.414661
H	6.683149	-1.082420	0.577194
H	6.029543	-2.489465	1.404198
C	7.487936	-2.964413	-0.119913
H	7.784231	-2.590838	-1.110341
H	7.136566	-3.994189	-0.276511
C	8.707099	-2.976323	0.808258
H	9.103569	-1.964106	0.955849
H	8.450051	-3.378111	1.796193
H	9.514840	-3.592957	0.398725
H	4.306060	-0.219200	0.224575

25-TS

B3LYP SCF energy: -3293.91407551 a.u.
B3LYP enthalpy: -3292.819370 a.u.
B3LYP free energy: -3292.974474 a.u.
B3LYP-D3(BJ) SCF energy in solution: -3295.13307224 a.u.
B3LYP-D3(BJ) enthalpy in solution: -3294.038367 a.u.

B3LYP-D3(BJ) free energy in solution: -3294.193471 a.u.
Imaginary frequency: -399.3275 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	6.615326	1.274316	0.167842
C	5.354427	0.876594	-0.218326
C	4.483361	0.200093	0.685013
C	4.958664	-0.030137	2.015577
C	6.269545	0.377539	2.381239
C	7.085835	1.016386	1.477595
H	7.256553	1.790088	-0.541334
H	5.018368	1.085689	-1.226674
C	3.154222	-0.219173	0.312930
C	4.092684	-0.650397	2.945708
H	6.610864	0.181855	3.394578
H	8.085618	1.328541	1.765200
C	2.813395	-0.999518	2.593026
C	2.313965	-0.790224	1.274701
H	4.447121	-0.838341	3.956120
H	2.182193	-1.457924	3.341381
C	2.743867	-0.013787	-1.114979
C	3.390260	-0.801530	-2.139475
C	1.781630	0.924208	-1.479247
C	4.354002	-1.806034	-1.842501
C	3.057313	-0.585246	-3.515739
C	1.427139	1.081126	-2.852775
C	4.965446	-2.527804	-2.844571
H	4.612696	-2.005087	-0.809878
C	3.708341	-1.339896	-4.526733
C	2.061187	0.371974	-3.838069
H	0.626365	1.759400	-3.124291
C	4.648722	-2.290613	-4.201963
H	5.699434	-3.286707	-2.588719
H	3.445966	-1.153034	-5.565050
H	1.790820	0.521530	-4.880466
H	5.143371	-2.862193	-4.981960
P	0.557392	-1.353067	0.906172
P	0.636915	1.708981	-0.259387
C	0.059465	-2.111701	2.537452
C	-0.371474	-1.260841	3.572160
C	0.055180	-3.495444	2.770516
C	-0.775251	-1.774827	4.804265
H	-0.397429	-0.189812	3.411881
C	-0.359610	-4.010504	4.002397
H	0.367188	-4.182486	1.993294

C	-0.772982	-3.155070	5.023383
H	-1.096538	-1.097198	5.590427
H	-0.355202	-5.085604	4.159652
H	-1.092425	-3.557539	5.980400
C	0.903011	-2.846632	-0.143371
C	0.076298	-3.212958	-1.214023
C	2.006110	-3.664747	0.162676
C	0.338944	-4.368918	-1.953560
H	-0.755270	-2.577085	-1.489050
C	2.263730	-4.820797	-0.573423
H	2.669476	-3.401079	0.980456
C	1.429104	-5.177589	-1.634651
H	-0.308161	-4.631009	-2.786330
H	3.120996	-5.438472	-0.320624
H	1.633209	-6.074745	-2.212233
C	0.332358	3.455311	-0.828260
C	-0.533392	4.231745	-0.035076
C	1.033404	4.085687	-1.865100
C	-0.723168	5.585694	-0.297479
H	-1.057575	3.777270	0.800799
C	0.841075	5.446412	-2.127078
H	1.744684	3.534139	-2.468416
C	-0.040452	6.197788	-1.352764
H	-1.398255	6.165179	0.325963
H	1.393051	5.915626	-2.936718
H	-0.186085	7.254232	-1.558537
C	1.588252	2.265460	1.237674
C	2.773961	2.999549	1.069860
C	1.040410	2.154554	2.519236
C	3.403864	3.585433	2.165364
H	3.207393	3.120059	0.081855
C	1.664768	2.753773	3.616618
H	0.117084	1.606928	2.654722
C	2.848540	3.468592	3.442844
H	4.327141	4.138750	2.019685
H	1.221787	2.660855	4.604599
H	3.334987	3.936939	4.293765
C	-4.916669	-3.017826	-2.352666
C	-4.330866	-1.809041	-3.127859
H	-4.721401	-3.960860	-2.872720
H	-6.003854	-2.931947	-2.239902
H	-3.676282	-2.129784	-3.945429
H	-5.112383	-1.174311	-3.547208
C	-4.221999	-2.944547	-1.016874
C	-3.409195	-1.795466	-0.974731
C	-4.315833	-3.739872	0.105989

H	-4.941297	-4.628115	0.119091
C	-3.601739	-3.338658	1.246060
H	-3.655045	-3.897893	2.173081
C	-2.796472	-2.213431	1.182335
H	-2.237827	-1.893970	2.045931
N	-2.632877	-1.457604	0.064883
N	-3.538425	-1.047763	-2.127471
C	-3.249885	0.295654	-2.258673
C	-2.612443	1.137825	-1.368200
C	-3.640361	0.957917	-3.567979
H	-3.454207	0.322187	-4.440479
H	-4.716817	1.196027	-3.571325
C	-2.787716	2.229826	-3.556581
H	-1.815509	2.018545	-4.018363
H	-3.244065	3.060519	-4.103735
C	-2.608400	2.516051	-2.059654
H	-1.720434	3.107453	-1.865634
H	-3.461884	3.116337	-1.701253
Ir	-1.078817	0.143014	-0.052039
H	-0.520757	-0.478041	-1.444433
C	-3.233316	1.559134	0.495271
H	-3.094954	2.613191	0.267959
C	-2.350982	1.079125	1.546271
H	-1.845731	1.871340	2.096470
H	-2.782976	0.334284	2.216616
C	-4.700161	1.160513	0.485263
H	-5.161828	1.435655	-0.470819
H	-4.801325	0.075204	0.599068
C	-5.465818	1.856994	1.630950
H	-5.023367	1.572919	2.594264
H	-5.342726	2.946101	1.542494
C	-6.962827	1.515047	1.630832
H	-7.084475	0.425434	1.712930
H	-7.400786	1.800808	0.664071
C	-7.731346	2.203134	2.763986
H	-7.339253	1.909380	3.745163
H	-7.654742	3.294517	2.689116
H	-8.794790	1.941614	2.738005

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