Carbonyls as Potential Alkenyl Carbanions for Deoxygenative Cross-Coupling with Alkyl Electrophiles

Mei Bai,[1] Shasha Geng,[3] Cheng Ma,[2] Minghui Sun,[3] Chaoqun Shi,[3] Yun He,[3] Shao-Fei Ni,[2*] and Zhang Feng[1,4*]

[1]Key Laboratory of Biocatalysis & Chiral Drug Synthesis of Guizhou Province, Generic Drug Research Center of Guizhou Province, School of Pharmacy, Zunyi Medical University, Zunyi 563006, China

[2]Department of Chemistry and Key Laboratory for Preparation and Application of Ordered Structural Materials of Guangdong, Shantou University, Shantou 515063, Guangdong, P. R. China

[3]Chongqing Key Laboratory of Natural Product Synthesis and Drug Research, School of Pharmaceutical Sciences, Chongqing University, Chongqing 401331, P. R. China

[4]Affiliated Hospital of North Sichuan Medical College and Medical Imaging Key Laboratory of Sichuan Province, North Sichuan Medical College, Nanchong 637000, P. R. China

List of Contents

General Information and Materials

General Information: ^{1}H NMR and ^{13}C NMR spectra were recorded on Agilent 400MR DD2 (400 MHz) or 600MR DD2 (600 MHz) spectrometer at ambient temperature. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are reported in Hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, sept = septet. NMR yield was determined by ^{1}H NMR using mesitylene as an internal standard before working up the reaction. High resolution mass spectra (HRMS) were acquired on a 7 Tesla SolariX FT-ICR MS (Bruker Daltonics, Bremen, Germany) with an ESI source or GCT Premier (waters, United States) with an EI source. All air and moisture-sensitive manipulations were performed using oven-dried glassware, including standard Schlenk and glovebox techniques under an atmosphere of nitrogen.

Materials: All reagents from commercial sources were used as received, unless otherwise specified. All solvents were distilled with sodium/benzophenone or CaH_2 before use.

Optimization of the Deoxygenative Cross-Coupling with Alkyl Electrophiles (Table S1-S8, Figure S1-S3)

One-pot initial study

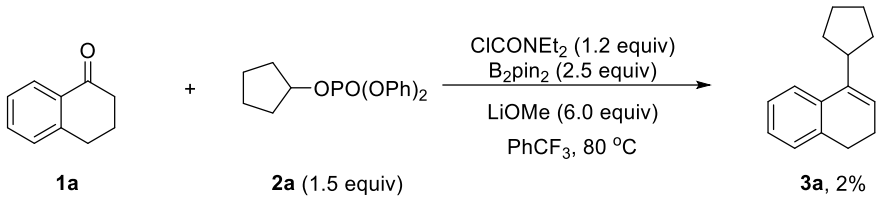
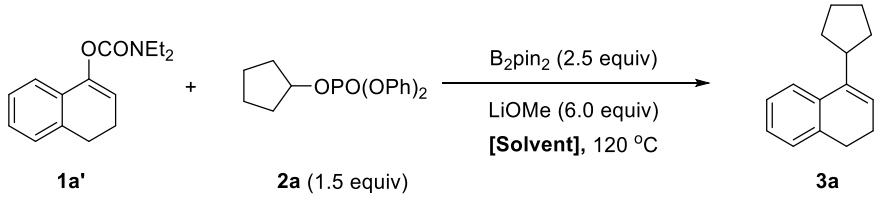


Figure S1. One-pot initial study[a]

Procedure: A 25 mL Schlenk tube equipped with a magnetic stir bar was added B_2pin_2 (66 mg, 0.26 mmol) and LiOMe (46 mg, 1.2 mmol). The tube was evacuated and backfilled nitrogen three times, followed by the addition of 1-tetralone **1a** (27 μL, 0.2 mmol), diethylcarbamoyl chloride (31 μL, 0.24 mmol), alkyl phosphate **2a** (83 μL, 0.3 mmol) and freshly distilled $PhCF_3$ (1.0 mL). The reaction mixture was heated at 80 ℃ for 16 h. The cooled solution was quenched with saturated NH_4Cl aqueous solution at 0 ℃, then diluted with ethyl acetate. The organic phase was added mesitylene (28 μL, 0.2 mmol) as an internal standard and analyzed by ^1H NMR to gain the 2% yield of product **3a**.

Table S1. Screening of Solvents [a]

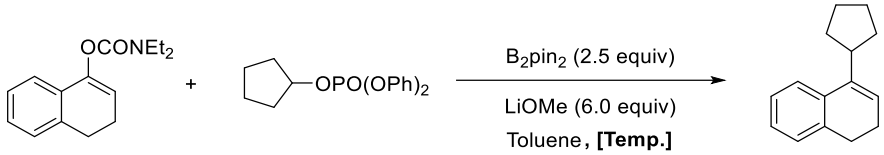


Entry	Solvent	Yield[b]
1	NMP	0%
2	**Toluene**	**6%**
3	DMF	0%
4	acetonitrile	0%
5	Hexane	trace
6	MTBE	trace

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (1.5 equiv), B_2pin_2 (2.5 equiv),

LiOMe (6.0 equiv), solvent (1.0 mL), 120 ℃, 16 h, under nitrogen atmosphere. [b]Determined by ^{1}H NMR using mesitylene as an internal standard.

Table S2. Screening of Temperature [a]

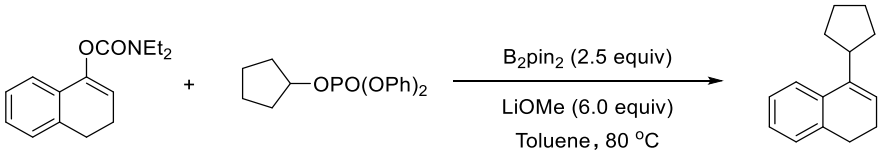


1a' **2a** (1.5 equiv) **3a**

Entry	Temp.	Yield[b]
1	60 ℃	0%
2	70 ℃	trace
3	**80** ℃	**11%**
4	90 ℃	trace
5	100 ℃	trace
6	110 ℃	trace

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (1.5 equiv), B_2pin_2 (2.5 equiv), LiOMe (6.0 equiv), toluene (1.0 mL), temp., 16 h, under nitrogen atmosphere. [b]Determined by ^{1}H NMR using mesitylene as an internal standard.

Table S3. Screening the Loading of Cyclopentyl Diphenyl Phosphate [a]

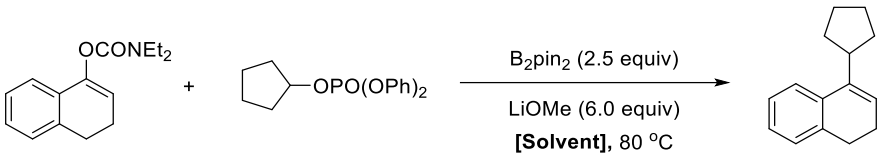


1a' **2a** (**X** equiv) **3a**

Entry	**2a** (equiv)	Yield[b]
1	1.0	8%
2	**1.2**	**13%**
3	1.5	11%
4	3.0	9%

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (X equiv), B_2pin_2 (2.5 equiv), LiOMe (6.0 equiv), toluene (1.0 mL), 80 ℃, 16 h, under nitrogen atmosphere. [b]Determined by ^{1}H NMR using mesitylene as an internal standard.

Table S4. Screening of Solvents [a]

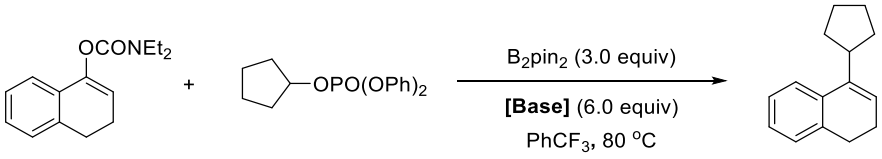


1a' **2a** (1.2 equiv) **3a**

Entry	Solvent	Yield[b]
1	**$PhCF_3$**	**18%**
2	*i*-Pr_2O	trace
3	MTBE	trace
4	Toluene	13%

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (1.2 equiv), B_2pin_2 (2.5 equiv), LiOMe (6.0 equiv), solvent (1.0 mL), 80 °C, 16 h, under nitrogen atmosphere. [b]Determined by ^1H NMR using mesitylene as an internal standard.

Table S5. Screening of Bases [a]

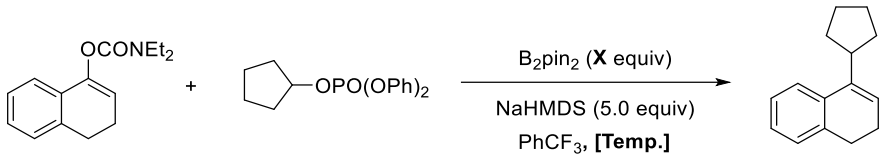


1a' **2a** (1.2 equiv) **3a**

Entry	Base	Yield[b]
1	KOMe	0%
2	*t*-BuOK	0%
3	*t*-BuOLi	0%
4	NaOMe	0%
5	**NaHMDS (5.0 equiv) (2.0 M in THF)**	**45%**
6	KHMDS (5.0 equiv) (1.0 M in THF)	32%

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (1.2 equiv), B_2pin_2 (3.0 equiv), base (6.0 equiv), $PhCF_3$ (1.0 mL), 80 °C, 16 h, under nitrogen atmosphere. [b]Determined by ^1H NMR using mesitylene as an internal standard.

Table S6. Screening of Temperature and Loading of B_2pin_2 [a]

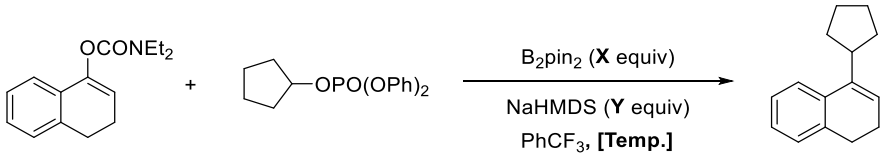


1a' **3a** (1.2 equiv) **3a**

Entry	Temp.	B_2pin_2 (equiv)	Yield[b]
1	RT	2.0	62%
2	**40 ℃**	**2.0**	**73%**
3	50 ℃	2.5	53%
4	**50 ℃**	**2.0**	**75%**
5	60 ℃	2.5	48%
6	60 ℃	2.0	53%
7	70 ℃	2.5	47%
8	70 ℃	2.0	57%
9	80 ℃	2.5	40%
10	80 ℃	2.0	56%

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (1.2 equiv), B_2pin_2 (X equiv), NaHMDS (5.0 equiv), $PhCF_3$ (1.0 mL), temp., 16 h, under nitrogen atmosphere. [b]Determined by ^1H NMR using mesitylene as an internal standard.

Table S7. Screening of Temperature, Concentration, Loading of NaHMDS and B_2pin_2 [a]



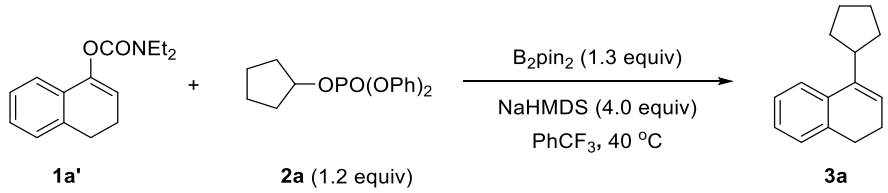
1a' **2a** (1.2 equiv) **3a**

Entry	Temp.	B_2pin_2 (equiv)	NaHMDS (equiv)	$PhCF_3$ (mL)	Yield[b]
1	30 ℃	1.3	4.0	0.5	55%
2	30 ℃	1.3	4.0	0.8	48%
3	30 ℃	1.3	4.0	1.0	68%
4	30 ℃	1.3	4.0	1.2	64%
5	40 ℃	1.3	4.0	0.8	76%
6	**40 ℃**	**1.3**	**4.0**	**1.0**	**81% (80%)**

7	40 ℃	1.3	4.0	1.2	73%
8	50 ℃	1.3	4.0	0.8	75%
9	50 ℃	1.3	4.0	1.0	75%
10	50 ℃	1.3	4.0	1.2	72%
11	50 ℃	1.3	4.0	1.5	70%
12	50 ℃	1.3	4.0	2.0	53%
13	50 ℃	1.3	3.0	1.0	59%
14	50 ℃	1.3	5.0	1.0	75%
15	50 ℃	1.4	5.0	1.0	51%
16	50 ℃	1.2	5.0	1.0	53%
17	50 ℃	1.1	5.0	1.0	66%
18	50 ℃	1.0	5.0	1.0	61%

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (1.2 equiv), B_2pin_2 (X equiv), NaHMDS (Y equiv), $PhCF_3$ (Z mL), temp., 16 h, under nitrogen atmosphere. [b]Determined by ^1H NMR using mesitylene as an internal standard. The isolated yield was shown in parentheses.

Table S8. Control Experiments [a]

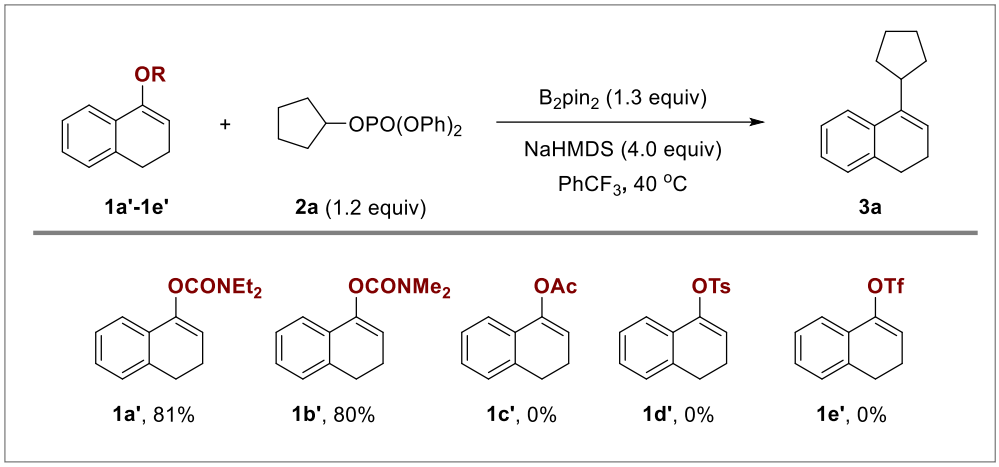


1a' **2a** (1.2 equiv) **3a**

Entry	B_2pin_2 (equiv)	NaHMDS (equiv)	$PhCF_3$ (mL)	Yield[b]
1	1.3	-	1.0	0%
2	-	4.0	1.0	0%

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (1.2 equiv), B_2pin_2 (1.3 equiv), NaHMDS (4.0 equiv), $PhCF_3$ (1.0 mL), 40 ℃, 16 h, under nitrogen atmosphere. [b]Determined by ^1H NMR using mesitylene as an internal standard.

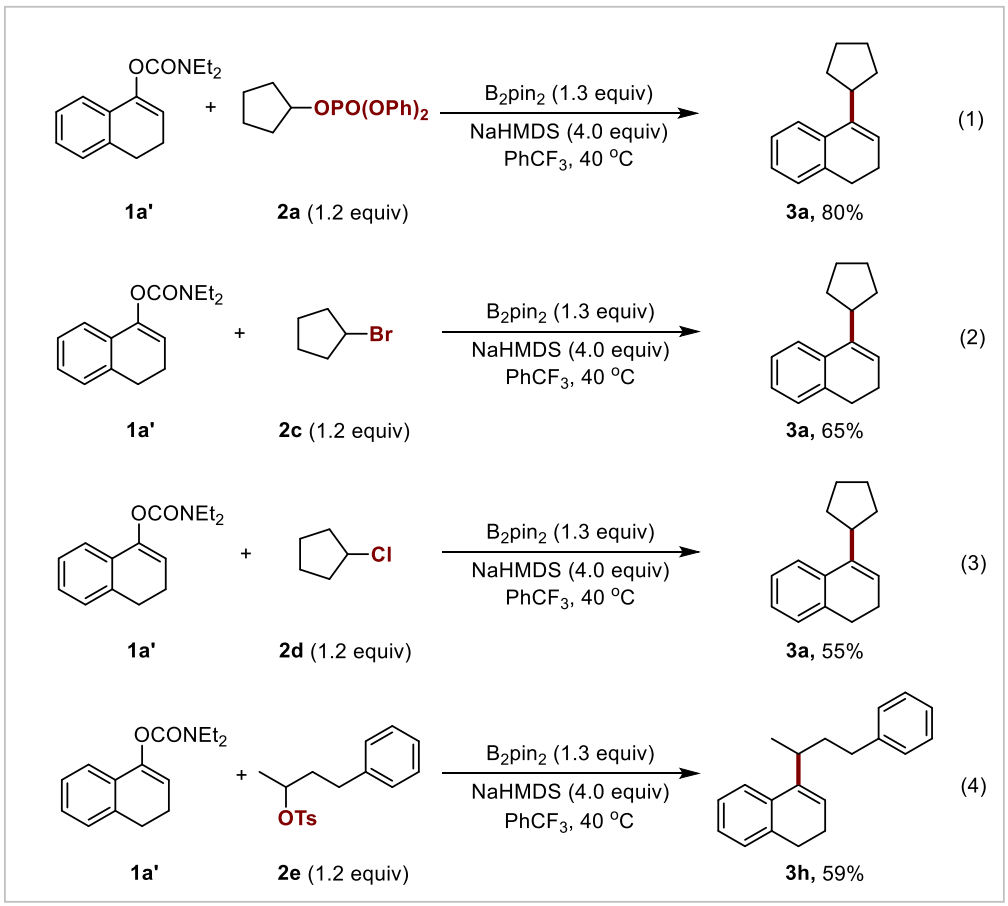
Evaluation of different alkenyl coupling partners



[a]Reaction conditions (unless otherwise specified): **1a'-1e'** (0.2 mmol, 1.0 equiv), **2** (0.24 mmol, 1.2 equiv), B_2pin_2 (1.3 equiv), NaHMDS (4.0 equiv), $PhCF_3$ (1.0 mL), 40 °C, 16 h, under nitrogen atmosphere. [b]Determined by ^1H NMR using mesitylene as an internal standard.

Figure S2. Reactivity of different coupling partners derived from 1-tetralone[a]

Evaluation of different alkyl coupling partners



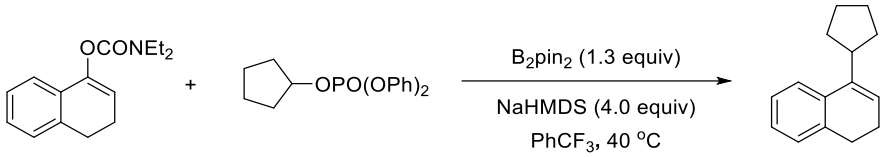
[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), alkyl electrophiles (0.24 mmol, 1.2 equiv), B_2pin_2 (1.3 equiv), NaHMDS (4.0 equiv), $PhCF_3$ (1.0 mL), 40 °C, 16 h, under nitrogen atmosphere. The isolated yield was shown.

Figure S3. Reactivity of other alkyl electrophiles [a]

Mechanistic Studies (Table S9-10, Figure S4-S6)

To gain insight into the mechanism of deoxygenative cross-coupling reactions, some experiments were conducted.

Table S9. Yield of Product 3a Formed over Time [a]



1a' **2a** (1.2 equiv) **3a**

Entry	Time (h)	Conc. of **3a** (mol/L)	Yield[b]
1	1.0	0.112	56%
2	2.0	0.114	57%
3	3.0	0.122	61%
4	4.0	0.136	68%
5	5.0	0.144	72%
6	6.0	0.158	79%
7	7.0	0.158	79%
8	8.0	0.158	79%
9	16.0	0.162	81%

[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), **2a** (1.2 equiv), B_2pin_2 (1.3 equiv), NaHMDS (4.0 equiv), $PhCF_3$ (1.0 mL), 40 °C, X h, under nitrogen atmosphere. [b]Determined by ^1H NMR using mesitylene as an internal standard.

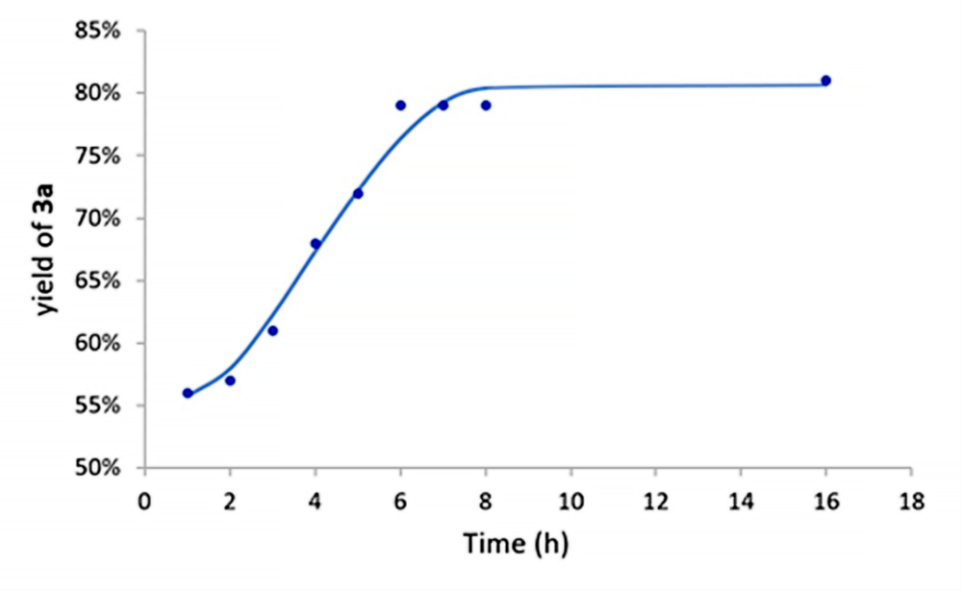


Figure S4. Yield of Product 3a Formed over Time

Representative Procedure for Reaction Rate Determination: A 25 mL of Schlenk tube equipped with a magnetic stir bar was added B_2pin_2 (66 mg, 0.26 mmol). The tube was evacuated and backfilled with nitrogen three times, followed by the addition of alkenyl carbamate **1a'** (48 μL, 0.2 mmol), alkyl phosphate **2a** (66 μL, 0.24 mmol) and freshly distilled $PhCF_3$ (1.0 mL). The solution of NaHMDS (2.0 M in THF, 0.4 mL, 0.8 mmol) was then added to the reaction mixture dropwise under nitrogen atmosphere. The reaction mixture was heated at 40 ℃. At regular intervals time (1, 2, 3, 4, 5, 6, 7, 8, 16 h *etc*.), the reaction tube was cooled to 0 ℃ and quenched with saturated NH_4Cl aqueous solution, then diluted with ethyl acetate. The organic phase was added mesitylene (28 μL, 0.2 mmol) as an internal standard and analyzed by ^1H NMR to gain the yield of product **3a**.

Potential intermediates of this reaction

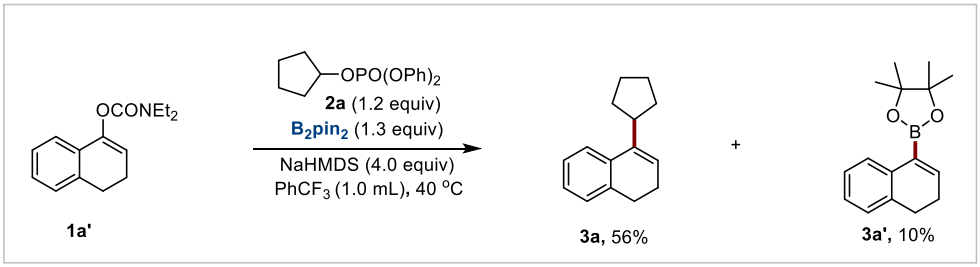


Figure S5. Research for the reaction intermediates[a]

Procedure: A 25 mL of Schlenk tube equipped with a magnetic stir bar was added B_2pin_2 (66 mg, 0.26 mmol). The tube was evacuated and backfilled with nitrogen three times, followed by the addition of alkenyl carbamate **1a'** (48 μL, 0.2 mmol), alkyl phosphate **2a** (66 μL, 0.24 mmol) and freshly distilled $PhCF_3$ (1.0 mL). The solution of NaHMDS (2.0 M in THF, 0.4 mL, 0.8 mmol) was then added to the reaction mixture dropwise under nitrogen atmosphere. The reaction mixture was heated at 40 ℃ for 1 h. The cooled solution was quenched with saturated NH_4Cl aqueous solution at 0 ℃, then diluted with ethyl acetate. The organic phase was added mesitylene (28 μL, 0.2 mmol) as an internal standard and analyzed by ^1H NMR to gain the yield of product **3a** (56% yield), **3a'** (10% yield).

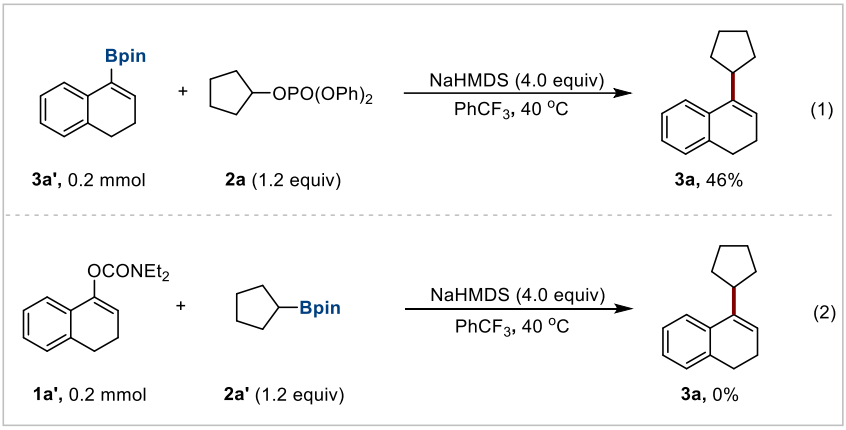


Figure S6. Research for the potential intermediates of this reaction[a]

Procedure 1: A 25 mL of Schlenk tube equipped with a magnetic stir bar was added alkenyl boronic ester **3a'** (51 mg, 0.2 mmol) and B_2pin_2 (66 mg, 0.26 mmol). The tube was evacuated and backfilled with nitrogen three times, followed by the addition of alkyl phosphate **2a** (66 μL, 0.24 mmol) and freshly distilled $PhCF_3$ (1.0 mL). The solution of NaHMDS (2.0 M in THF, 0.4 mL, 0.8 mmol) was then added to the reaction mixture dropwise under nitrogen atmosphere. The reaction mixture was heated at 40 ℃ for 16 h. The cooled solution was quenched with NH_4Cl saturated aqueous solution, then diluted with ethyl acetate. The organic phase was added mesitylene (28 μL, 0.2mmol) as an internal standard and analyzed by ^1H NMR to gain the 46% yield of product **3a**.

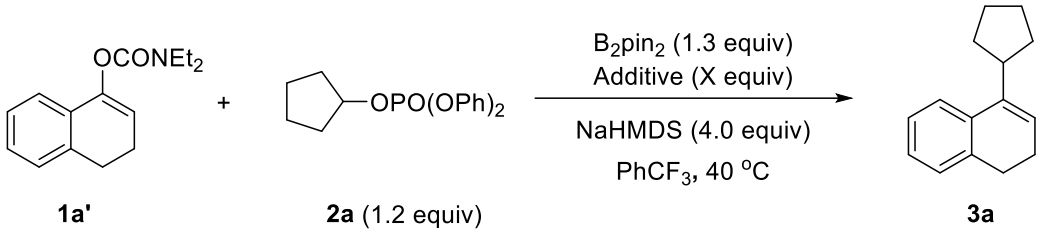
Procedure 2: A 25 mL of Schlenk tube equipped with a magnetic stir bar was added B_2pin_2 (66

mg, 0.26 mmol). The tube was evacuated and backfilled with nitrogen three times, followed by the addition of alkenyl carbamate **1a'** (48 μL, 0.2 mmol), alkyl boronic ester **2a'** (47 mg, 0.24 mmol) and freshly distilled $PhCF_3$ (1.0 mL). The solution of NaHMDS (2.0 M in THF, 0.4 mL, 0.8 mmol) was then added to the reaction mixture dropwise under nitrogen atmosphere. The reaction mixture was heated at 40 ℃ for 16 h. The cooled solution was quenched with NH_4Cl saturated aqueous solution, then diluted with ethyl acetate. The organic phase was added mesitylene (28 μL, 0.2 mmol) as an internal standard and analyzed by ^1H NMR to gain the 0% yield of product **3a**.

Conclusion: these results indicated that alkenyl boronic esters are the intermediate of this transformation.

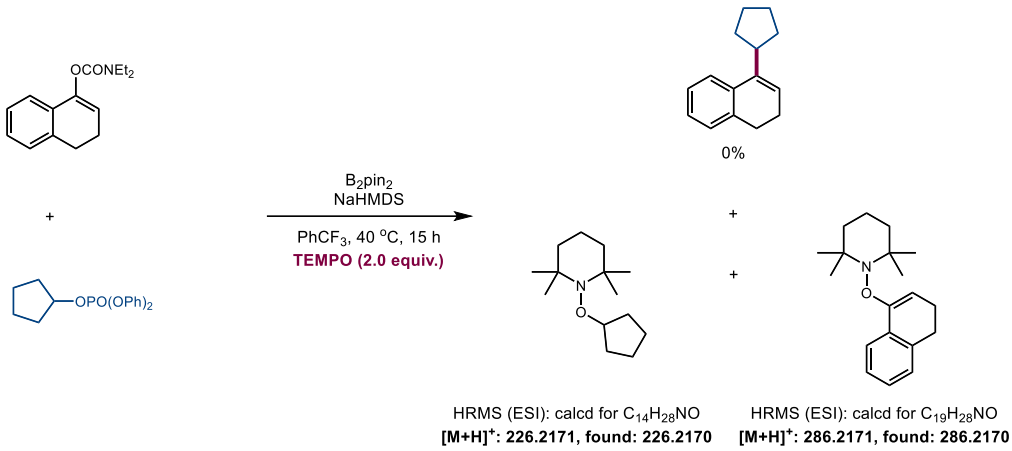
Radical experiments with TEMPO as a radical scavenger were also conducted to continue our research for the mechanism of deoxygenative cross-coupling reaction, which implied the possible involvement of organic radicals (Table S10).

Table S10. Radical Experiments[a]



1a' **2a** (1.2 equiv) **3a**

Entry	Additive (equiv)	Yield[b]
1	none	81% (80%)
2	TEMPO (0.5)	23%
3	TEMPO (1.0)	0%
4	TEMPO (2.0)	0%



Procedure: A 25 mL of Schlenk tube equipped with a magnetic stir bar was added B_2pin_2 (66 mg, 0.26 mmol) and TEMPO. The tube was evacuated and backfilled with nitrogen three times, followed by the addition of alkenyl carbamate **1a'** (48 μL, 0.2 mmol), alkyl phosphate **2a** (66 μL, 0.24 mmol) and freshly distilled $PhCF_3$ (1.0 mL). The solution of NaHMDS (2.0 M in THF, 0.4 mL, 0.8 mmol) was then added to the reaction mixture dropwise under nitrogen atmosphere. The reaction mixture was heated at 40 ℃ for 1 h. The cooled solution was quenched with saturated NH_4Cl aqueous solution at 0 ℃, then diluted with ethyl acetate. The organic phase was added mesitylene (28 μL, 0.2 mmol) as an internal standard and analyzed by ^1H NMR to gain the yield of product **3a**.

The addition of a radical scavenger (TEMPO) under the standard conditions almost completely suppressed the reaction. Moreover, TEMPO successfully trapped both the alkenyl and alkyl radicals generated from the alkenyl carbamate and alkyl electrophile, respectively, thereby supporting the involvement of organic radical intermediates in this transformation.

Applications of the Deoxygenative Cross-Coupling with Alkyl Electrophiles (Figure S7-S9)

Gram-scale experiments

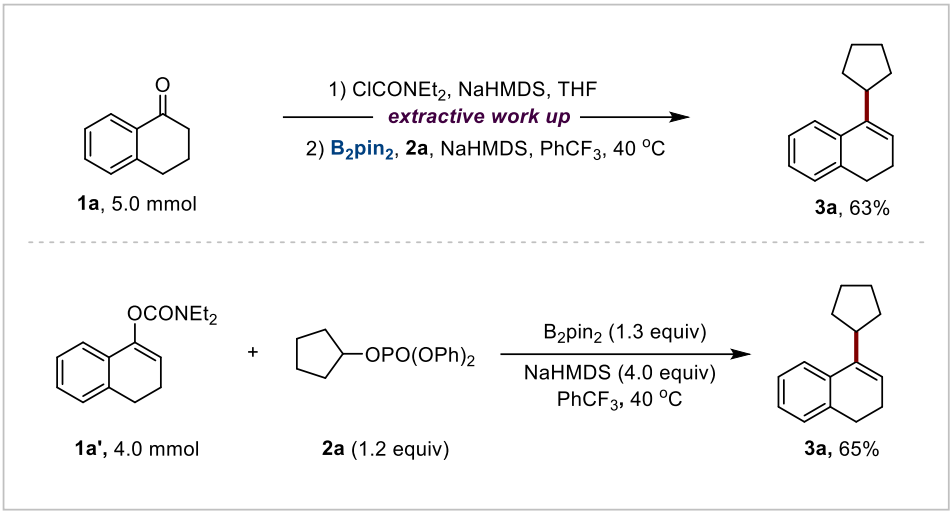


Figure S7. Gram-scale experiments

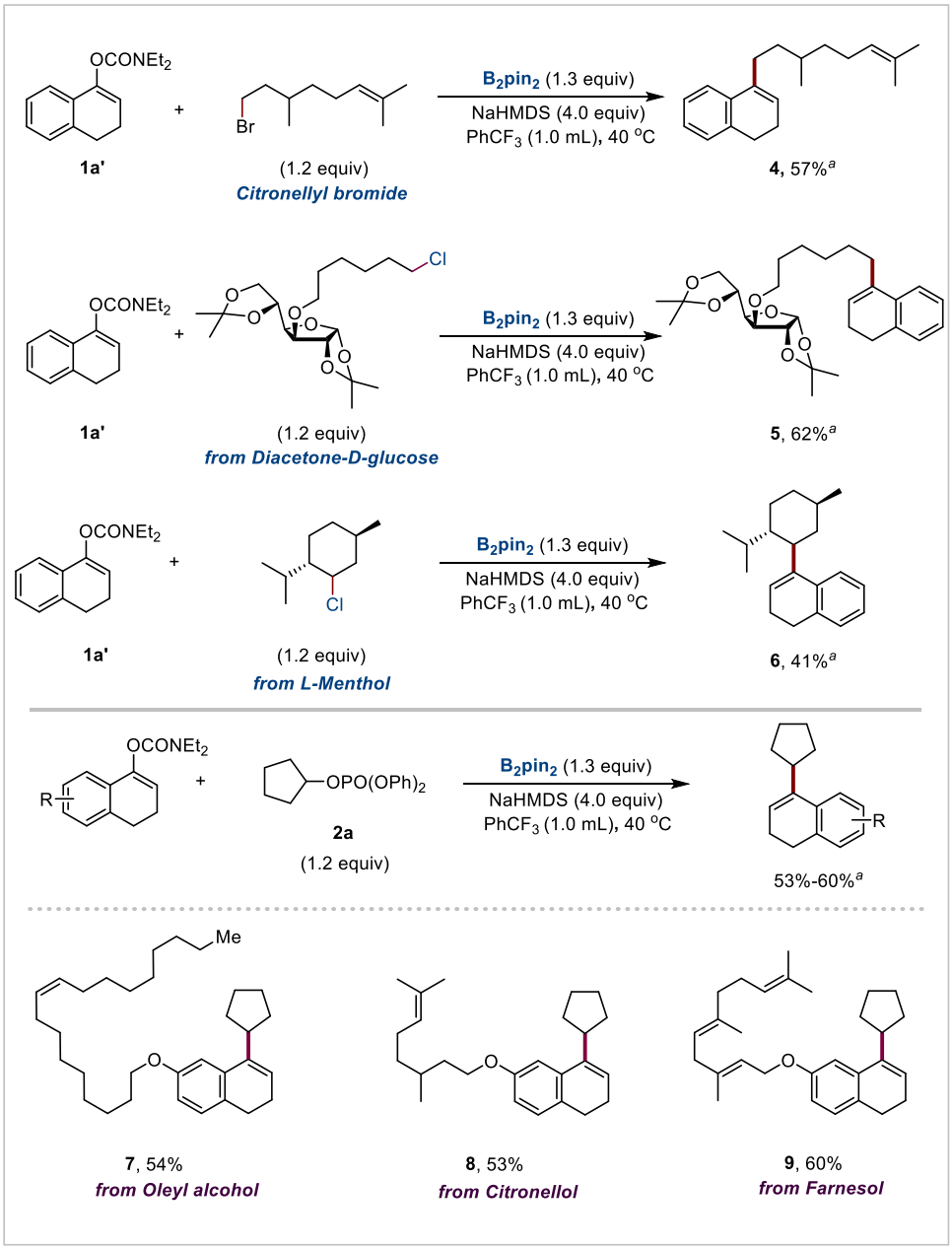
Procedure 1: Under nitrogen atmosphere, a solution of 1-tetralone **1a** (730 mg, 5.0 mmol) in dry THF (20 mL) was added KHMDS (1.0 M in THF, 6.0 mL, 6.0 mmol) dropwise over 15 min at -20 ℃. After stirring for 1 h, diethylcarbamoyl chloride (750 μL, 6.0 mmol) was added dropwise over another 15 min. The reaction system was raised to 0 ℃ and stirred for 30 min, then warmed to room temperature. After stirring overnight at room temperature, the reaction was quenched with saturated $NaHCO_3$ aqueous solution, separated and collected the organic phase with a separatory funnel. The aqueous phase was extracted with ethyl acetate three times. All these organic phases were combined and washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure to gain the crude product of alkenyl carbamate **1a'**, which was used for the next step without further purification. A 100 mL of Schlenk tube equipped with a magnetic stir bar was added B_2pin_2 (2.15 g, 6.5 mmol). The tube was evacuated and backfilled with nitrogen three times, followed by alkyl phosphate (1.98 mL, 6.0 mmol) and a solution of crude alkenyl carbamate in freshly distilled $PhCF_3$ (25 mL) in sequence. The solution of NaHMDS (2.0 M in THF, 10.0 mL, 20.0 mmol) was then added to the reaction mixture dropwise under nitrogen atmosphere. The reaction mixture was heated at 40 ℃ for 16 h. The cooled solution was quenched with NH_4Cl saturated aqueous solution at 0 ℃, then diluted with ethyl acetate, separated and collected the organic phase with a separatory funnel. The aqueous phase was extracted with ethyl acetate three times. All these organic phases were combined and washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash silica gel chromatography

to afford the coupling product **3a** (626 mg, 63% yield).

Procedure 2: A 100 mL of Schlenk tube equipped with a magnetic stir bar was added B_2pin_2 (1.32 g, 5.2 mmol). The tube was evacuated and backfilled with nitrogen three times, followed by alkyl phosphate (1.58 mL, 4.8 mmol) and a solution of crude alkenyl carbamate **1a'** in freshly distilled $PhCF_3$ (20.0 mL) in sequence. The solution of NaHMDS (2.0 M in THF, 8.0 mL, 16.0 mmol) was then added to the reaction mixture dropwise under nitrogen atmosphere. The reaction mixture was heated at 40 ℃ for 16 h. The cooled solution was quenched with NH_4Cl saturated aqueous solution at 0 ℃, then diluted with ethyl acetate, separated and collected the organic phase with a separatory funnel. The aqueous phase was extracted with ethyl acetate three times. All these organic phases were combined and washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash silica gel chromatography to afford the coupling product **3a** (515 mg, 65% yield).

Application for the synthesis of natural product derivatives

The deoxygenative cross-coupling product **4** was prepared from citronelly bromide. Natural product derivatives **5** and **6** were prepared by from alkyl chlorides. The method for product **7-9** was followed from alkyl phosphates (Figure S8).



[a]Reaction conditions (unless otherwise specified): **1a'** (0.2 mmol, 1.0 equiv), alkyl electrophilic substrate (1.2 equiv), B_2pin_2 (1.3 equiv), NaHMDS (4.0 equiv), $PhCF_3$ (1.0 mL), 40 °C, 16 h, under nitrogen atmosphere.

Figure S8. Application for the synthesis of natural product derivatives [a]

Carbonyl 1, 2-transposition alkylation

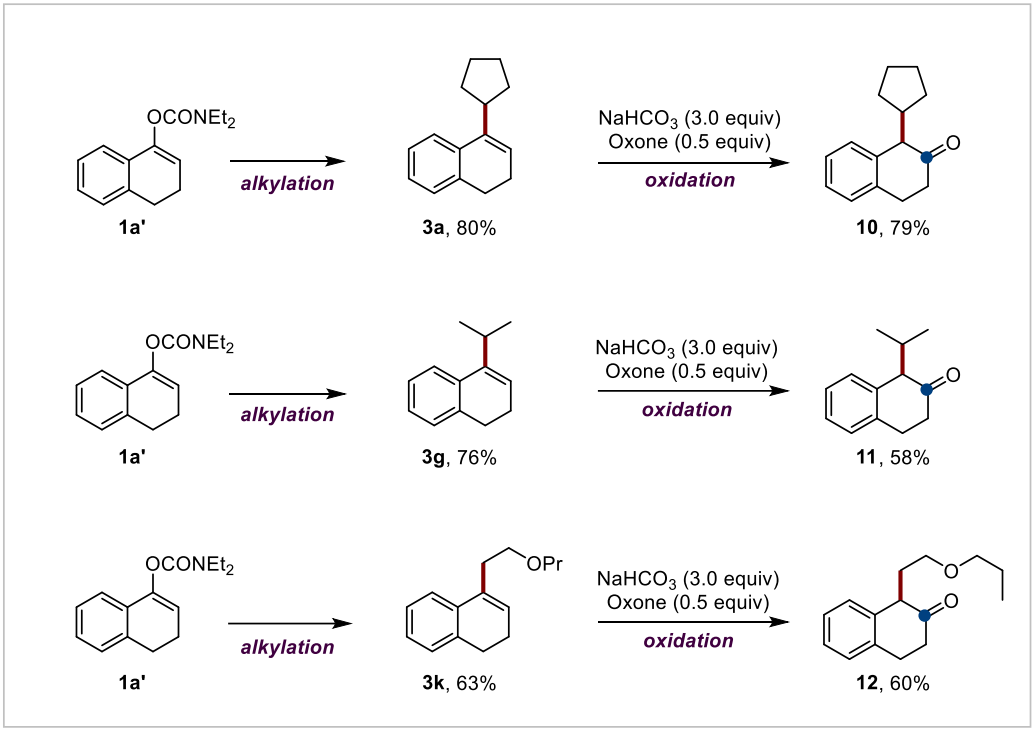


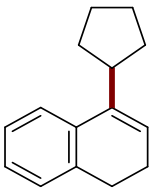
Figure S9. Carbonyl 1,2-transposition alkylation

General Procedure: The deoxygenative cross-coupling products **3a**, **3g**, **3k** were prepared by general procedure from alkyl phosphates, followed by the oxidation process: Add $NaHCO_3$ (3.0 equiv) to the coupling product dissolved in the mixed solvents of acetone/EA/water (2.5 mL/0.5 mL/0.5 mL). The mixture was stirred at room temperature for 1 h. Solid oxone (0.5 equiv) was then added in one portion at room temperature. The reaction system was stirred for 36 h at the same temperature. Evaporating the excess acetone under reduced pressure after completion of the reaction. The reaction was then diluted with water and ethyl acetate, then separated and collected the organic phase with a separatory funnel. The aqueous phase was extracted with ethyl acetate three times. The combined organic phase was washed with brine once and dried over Na_2SO_4. The result mixture was concentrated under reduced pressure and purified by flash silica gel chromatography to afford the desired ketone compound **10**, **11** and **12** respectively.

General Procedure for the Deoxygenative Cross-Coupling with Alkyl Electrophiles

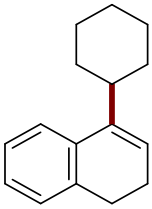
General procedure: A 25 mL of Schlenk tube equipped with a magnetic stir bar was added B_2pin_2 (66 mg, 0.26 mmol). The tube was evacuated and backfilled with nitrogen three times, followed by the addition of alkenyl carbamate (0.2 mmol), alkyl phosphates (or alkyl chlorides, alkyl bromides, alkyl tosylates) (0.24 mmol) and freshly distilled $PhCF_3$ (1.0 mL). The solution of NaHMDS (2.0 M in THF, 0.4 mL, 0.8 mmol) was then added to the reaction mixture dropwise under nitrogen atmosphere. The reaction mixture was heated at 40 ℃ for 16 h. The cooled solution was quenched with NH_4Cl saturated aqueous solution, separated and collected the organic phase with a separatory funnel. The aqueous phase was extracted with ethyl acetate three times. All these organic phases were combined and washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash silica gel chromatography to afford the coupling products.

Experimental Procedures and Characterization Data for Products



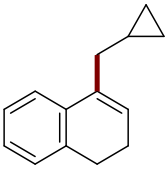
4-Cyclopentyl-1,2-dihydronaphthalene (3a).

This compound is known.[1] The product **3a** (31.7 mg, 80% yield) was from alkyl phosphate, **3a** (21.8 mg, 55% yield) was prepared from alkyl chloride, and **3a** (25.8 mg, 65% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.6 Hz, 1 H), 7.24-7.20 (m, 1 H), 7.16-7.13 (m, 2 H), 5.93 (t, *J* = 4.4 Hz, 1 H), 3.02 (m, 1 H), 2.73 (t, *J* = 7.9 Hz, 2 H), 2.26 (q, *J* = 7.6 Hz, 2 H), 2.04-1.99 (m, 2 H), 1.8-1.73 (m, 2 H), 1.71-1.64 (m, 2 H), 1.53-1.46 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 136.9, 135.8, 127.4, 126.3, 126.2, 123.1, 121.5, 41.1, 32.1, 28.5, 24.9, 23.2. HRMS (EI): Calculated for $C_{15}H_{18}$ $[M]^+$: 198.1403; Found: 198.1402.



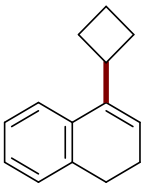
4-Cyclohexyl-1,2-dihydronaphthalene (3b).

This compound is known.[2] The product **3b** (25.4 mg, 60% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 7.7 Hz, 1 H), 7.22-7.19 (m, 1 H), 7.14-7.11 (m, 2 H), 5.86 (t, *J* = 4.8 Hz, 1 H), 2.70 (t, *J* = 7.9 Hz, 2 H), 2.56-2.50 (m, 1 H), 2.27-2.21 (m, 2H), 1.98-1.88 (m, 2 H), 1.88-1.70 (m, 3 H), 1.50-1.35 (m, 2 H), 1.33-1.17 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 137.1, 135.0, 127.6, 126.2, 126.1, 122.2, 121.9, 38.7, 33.1, 28.6, 27.1, 26.7, 23.1.



4-(Cyclopropylmethyl)-1,2-dihydronaphthalene (3c).

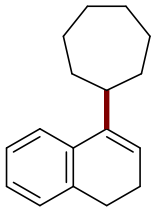
The product **3c** (23.6 mg, 64% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (t, *J* = 7.2 Hz, 1 H), 7.22-7.17 (m, 1 H), 7.17-7.12 (m, 2 H), 6.03 (t, *J* = 4.6 Hz, 1 H), 2.77 (t, *J* = 8.1 Hz, 2 H), 2.35 (d, *J* = 6.8 Hz, 2 H), 2.33-2.16 (m, 2 H), 1.08-0.87 (m, 1 H), 0.55-0.49 (m, 2 H), 0.19-0.12 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.6, 136.0, 135.4, 127.5, 126.5, 126.2, 124.6, 122.5, 37.1, 28.4, 23.2, 9.5, 4.9. HRMS (EI): Calculated for $C_{14}H_{16}[M]^{+}$: 184.1247; Found: 184.1245.



4-Cyclobutyl-1,2-dihydronaphthalene (3d).

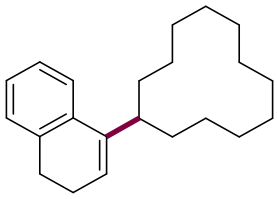
The product **3d** (25.0 mg, 68% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20-7.10

(m, 4 H), 5.84 (td, J = 4.8 Hz, 1.9 Hz, 1 H), 3.50-3.38 (m, 1 H), 2.74 (t, J = 8.0 Hz, 2 H), 2.32-2.23 (m, 4 H), 2.10-1.94 (m, 3H), 1.89-1.68 (m, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 136.7, 134.6, 127.5, 126.4, 126.2, 123.0, 122.2, 37.5, 28.3, 28.1, 23.1, 18.3. HRMS (EI): Calculated for $C_{14}H_{16}[M]^+$: 184.1247; Found: 184.1244.



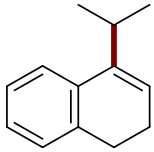
4-Cycloheptyl-1,2-dihydronaphthalene (3e).

The product **3e** (22.6 mg, 50% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, J = 7.7 Hz, 1 H), 7.26-7.20 (m, 1 H), 7.18-7.11 (m, 2 H), 5.89 (t, J = 4.7 Hz, 1 H), 2.78-2.67 (m, 3 H), 2.32-2.20 (m, 2 H), 2.00-1.87 (m, 2 H), 1.85-1.67 (m, 4 H), 1.66-1.46 (m, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 137.2, 135.2, 127.7, 126.3, 126.2, 122.3, 121.9, 40.5, 35.0, 28.6, 28.0, 27.3, 23.1. HRMS (EI): Calculated for $C_{17}H_{22}[M]^+$: 226.1716; Found: 226.1710.



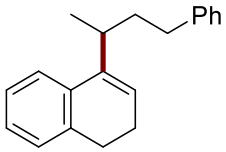
4-Cyclododecyl-1,2-dihydronaphthalene (3f).

The product **3f** (27.0 mg, 50% yield) was prepared from alkyl chloride, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, J = 7.8 Hz, 1 H), 7.23-7.17 (m, 1 H), 7.17-7.09 (m, 2H), 5.87 (t, J = 4.7 Hz, 1 H), 2.96-2.73 (m, 1 H), 2.69 (t, J = 7.9 Hz, 2 H), 2.27-2.21 (m, 2 H), 1.65-1.32 (m, 22 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.5, 140.4, 137.2, 127.6, 126.2, 126.1, 123.2, 122.3, 34.8, 29.7, 28.7, 28.4, 28.0, 24.5, 24.3, 23.3, 23.2, 23.1, 22.1. HRMS (ESI): Calculated for $C_{22}H_{33}[M+H]^+$: 297.2577; Found: 295.2587.



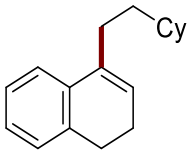
4-Isopropyl-1,2-dihydronaphthalene (3g).

This compound is known.[3] The product **3g** (26.1 mg, 76% yield) was from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 7.7 Hz, 1 H), 7.24-7.20 (m, 1 H), 7.16-7.12 (m, 2 H), 5.91 (t, *J* = 4.8 Hz, 1 H), 3.00-2.93 (m, 1 H), 2.72 (t, *J* = 7.9 Hz, 2 H), 2.28-2.23 (m, 2 H), 1.19 (s, 3 H), 1.18 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 137.1, 135.1, 127.6, 126.3, 126.2, 122.5, 121.4, 28.6, 28.2, 23.1, 22.3.



4-(4-Phenylbutan-2-yl)-1,2-dihydronaphthalene (3h).

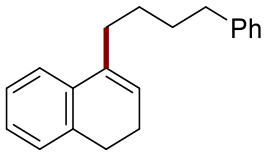
The product **3h** (35.6 mg, 68% yield) was prepared from alkyl phosphate, **3h** (30.9 mg, 59% yield) was prepared from alkyl tosylate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.27 (m, 2 H), 7.21-7.15 (m, 7 H), 5.95 (t, *J* = 4.8 Hz, 1 H), 2.85-2.81 (m, 1 H), 2.76-2.66 (m, 4 H), 2.31-2.26 (m, 2 H), 2.02-1.93 (m, 1 H), 1.78-1.69 (m, 1 H), 1.25 (d, *J* = 4.8 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 141.4, 137.1, 135.2, 128.5, 128.3, 127.7, 126.4, 126.3, 125.7, 122.5, 122.3, 38.2, 33.8, 33.1, 28.7, 23.1, 20.2. HRMS (EI): Calculated for $C_{20}H_{22}[M]^{+}$: 262.1716; Found: 262.1710.



4-(2-Cyclohexylethyl)-1,2-dihydronaphthalene (3i).

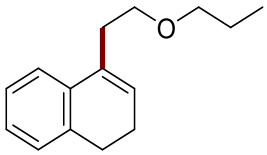
The product **3i** (25.9 mg, 54% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.6 Hz, 1 H), 7.24-7.20 (m, 1 H), 7.18-7.13 (m, 2 H), 5.87 (t, *J* = 4.6 Hz, 1 H), 2.76 (t, *J* = 8.0 Hz, 2 H), 2.47 (t, *J* = 8.1 Hz, 2 H), 2.29-2.24 (m, 2 H), 1.87-1.77 (m, 2 H), 1.72-1.68 (m, 3 H), 1.48-

1.42 (m, 2 H), 1.27-1.18 (m, 4 H), 1.00-0.92 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.0, 136.8, 135.1, 127.6, 126.5, 126.3, 124.4, 122.6, 37.8, 36.4, 33.4, 30.1, 28.5, 26.8, 26.5, 23.2. HRMS (ESI): Calculated for $C_{18}H_{25}[M+H]^+$: 241.1951; Found: 241.1959.



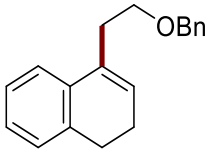
4-(4-Phenylbutyl)-1,2-dihydronaphthalene (3j).

This compound is known.[4] The product **3j** (37.7 mg, 72% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.27 (m, 3 H), 7.25-7.21 (m, 4 H), 7.19-7.16 (m, 2 H), 5.86 (t, *J* = 4.6 Hz, 1 H), 2.75 (t, *J* = 8.2 Hz, 2 H), 2.66 (t, *J* = 7.8 Hz, 2 H), 2.49 (t, *J* = 7.7 Hz, 2 H), 2.28-2.23 (m, 2 H), 1.75-1.68 (m, 2 H), 1.65-1.57 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 136.8, 136.3, 135.0, 128.4, 128.3, 127.6, 126.5, 126.3, 125.6, 124.9, 122.6, 35.8, 32.6, 31.3, 28.5, 28.1, 23.1.



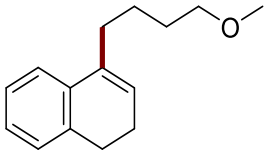
4-(2-Propoxyethyl)-1,2-dihydronaphthalene (3k).

The product **3k** (27.2 mg, 63% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA=20/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.27 (m, 1 H), 7.23-7.18 (m, 1 H), 7.16-7.12 (m, 2 H), 5.93 (t, *J* = 4.7 Hz, 1 H), 3.60 (t, *J* = 7.5 Hz, 2 H), 3.41 (t, *J* = 6.7 Hz, 2 H), 2.80-2.70 (m, 4 H), 2.28-2.23 (m, 2 H), 1.62 (t, *J* = 7.2 Hz, 2 H), 0.94 (t, *J* = 7.4 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.6, 134.8, 133.3, 127.6, 126.7, 126.4, 122.5, 72.7, 70.0, 33.1, 28.3, 23.1, 23.0, 10.6. HRMS (EI): Calculated for $C_{15}H_{20}O[M]^+$: 216.1509; Found: 216.1505.



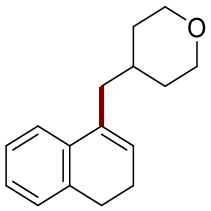
4-(2-(Benzyloxy)ethyl)-1,2-dihydronaphthalene (3l).

The product **3l** (31.7 mg, 60% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.32 (m, 4 H), 7.31-7.24 (m, 2 H), 7.22-7.16 (m, 1 H), 7.16-7.14 (m, 2 H), 5.94 (t, *J* = 4.6 Hz, 1 H), 4.55 (s, 2 H), 3.68 (td, *J* = 7.4, 2.3 Hz, 2 H), 2.81 (t, *J* = 7.0 Hz, 2 H), 2.75 (t, *J* = 8.0 Hz, 2 H), 2.29-2.24 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.6, 132.7, 130.8, 129.3, 124.4, 123.7, 123.6, 122.8, 122.6, 122.4, 118.6, 69.0, 65.6, 29.2, 24.4, 19.2. HRMS (EI): Calculated for $C_{19}H_{20}O[M]^+$: 264.1509; Found: 264.1503.



4-(4-Methoxybutyl)-1,2-dihydronaphthalene (3m).

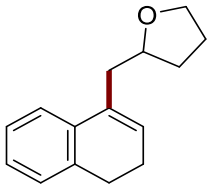
This compound is known.[5] The product **3m** (28.5 mg, 66% yield) was prepared from alkyl chloride, then purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 8.2 Hz, 1 H), 7.21-7.17 (m, 1 H), 7.15-7.10 (m, 2 H), 5.85 (t, *J* = 4.6 Hz, 1 H), 3.39 (t, *J* = 6.2 Hz, 2 H), 3.32 (s, 3 H), 2.73 (t, *J* = 8.0 Hz, 2 H), 2.46 (t, *J* = 6.8 Hz, 2 H), 2.26-2.21 (m, 2 H), 1.68-1.57 (m, 4 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.0, 131.5, 130.1, 122.8, 121.7, 121.5, 120.2, 117.9, 68.0, 53.8, 27.7, 24.7, 23.7, 20.1, 18.3.



4-((3,4-Dihydronaphthalen-1-yl)methyl)tetrahydro-*2H*-pyran (3n).

The product **3n** (28.3 mg, 62% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23-7.19 (m, 2 H), 7.15-7.14 (m, 2 H), 5.83 (t, *J* = 4.6 Hz, 1 H), 3.93 (dd, *J* = 11.5, 4.4 Hz, 2 H), 3.31 (t, *J* = 11.5 Hz, 2 H), 2.73 (t, *J* =7.8 Hz, 2 H), 2.38 (d, *J* = 7.0 Hz, 2 H), 2.28-2.23 (m, 2 H), 1.76-1.72

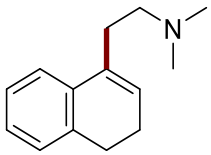
(m, 1 H), 1.64-1.61 (m, 2 H) 1.33-1.23 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.9, 134.8, 134.0, 127.7, 126.8, 126.6, 126.3, 122.8, 68.1, 40.6, 33.3, 28.5, 24.8, 23.1. HRMS (EI): Calculated for $C_{16}H_{20}O[M]^+$: 228.1509; Found: 228.1506.



2-((3,4-Dihydronaphthalen-1-yl)methyl)tetrahydrofuran (3o).

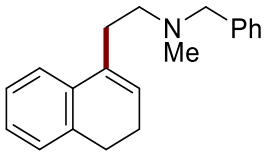
This compound is known.[6] The product **3o** (26.1 mg, 61% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, J = 7.6 Hz, 1 H), 7.22-7.16 (m, 1 H), 7.16-7.08 (m, 2 H), 5.95 (t, J = 4.6 Hz, 1 H), 4.08 (p, J = 6.5 Hz, 1 H), 3.92 (q, J = 7.2 Hz, 1 H), 3.73 (q, J = 7.6 Hz, 1 H), 2.86 (dd, J = 14.3, 6.0 Hz, 1 H), 2.74 (t, J = 8.1 Hz, 2 H), 2.50 (dd, J = 14.3, 7.1 Hz, 1 H), 2.29-2.24 (m, 2 H), 1.99-1.79 (m, 3 H), 1.62-1.49 (m, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 134.8, 133.7, 127.6, 126.7, 126.7, 126.3, 122.7, 77.7, 67.9, 39.0, 31.3, 28.3, 25.5, 23.1.

(1)



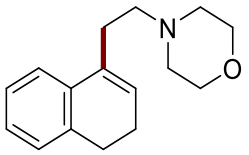
2-(3,4-Dihydronaphthalen-1-yl)-*N*,*N*-dimethylethan-1-amine (3p).

This compound is known.[7] The product **3p** (34.2 mg, 85% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.23 (m, 1 H), 7.22-7.16 (m, 1 H), 7.15-7.11 (m, 2 H), 5.89 (t, J = 4.6 Hz, 1 H), 2.72 (t, J = 8.0 Hz, 2 H), 2.69-2.64 (m, 2 H), 2.58-2.51 (m, 2 H), 2.36 (s, 6 H), 2.27-2.20 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 134.3, 129.2, 127.7, 126.7, 126.4, 126.2, 122.5, 58.9, 45.1, 30.7, 28.3, 23.1.



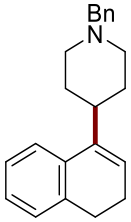
***N*-Benzyl-2-(3,4-dihydronaphthalen-1-yl)-*N*-methylethan-1-amine (3q).**

The product **3q** (28.8 mg, 52% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.28 (m, 4 H), 7.27-7.22 (m, 1 H), 7.21-7.10 (m, 4 H), 5.88 (t, *J* = 4.6 Hz, 1 H), 3.56 (s, 2 H), 2.75-2.65 (m, 4 H), 2.63-2.56 (m, 2 H), 2.30 (s, 3 H), 2.26-2.21 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.9, 136.6, 134.7, 134.7, 129.1, 128.2, 127.6, 127.0, 126.6, 126.4, 125.9, 122.6, 62.3, 56.8, 42.3, 30.8, 28.3, 23.1. HRMS (ESI): Calculated for $C_{20}H_{24}N[M+H]^+$: 278.1903; Found: 278.1913.



4-(2-(3,4-Dihydronaphthalen-1-yl)ethyl)morpholine (3r).

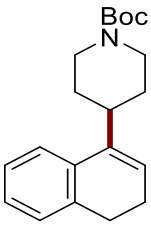
The product **3r** (24.8 mg, 51% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.21 (m, 1 H), 7.22 -7.15 (m, 1 H), 7.14-7.10 (m, 2 H), 5.89 (t, *J* = 4.7 Hz, 1 H), 3.74 (t, *J* = 4.7 Hz, 4 H), 2.72 (t, *J* = 8.0 Hz, 2 H), 2.68-2.62 (m, 2 H), 2.58-2.50 (m, 6 H), 2.24-2.21 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.9, 129.8, 129.7, 122.9, 122.0, 121.6, 121.3, 117.7, 62.2, 53.8, 49.0, 25.3, 23.6, 18.3. HRMS (ESI): Calculated for $C_{16}H_{22}ON[M+H]^+$: 244.1696 Found: 244.1704.



1-Benzyl-4-(3,4-dihydronaphthalen-1-yl)piperidine (3s).

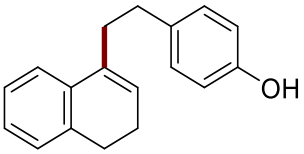
The product **3s** (30.3 mg, 50% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.32 (m, 4 H), 7.30-7.24 (m, 2 H), 7.21-7.18 (m, 1 H), 7.16-7.13 (m, 2 H), 5.90 (t, *J* = 4.7 Hz, 1 H), 3.58 (s,

2 H), 3.02 (d, *J* = 10.6 Hz, 2 H), 2.70 (t, *J* = 7.8 Hz, 2 H), 2.54 (t, *J* = 11.6 Hz, 1 H), 2.26-2.21 (m, 2 H), 2.13 (t, *J* = 11.7 Hz, 2 H), 1.85 (d, *J* = 12.3 Hz, 2 H), 1.61 (q, *J* = 10.5 Hz, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 138.4, 137.1, 134.7, 129.3, 128.2, 128.2, 127.8, 127.0, 126.4, 126.2, 122.5, 122.2, 63.5, 54.4, 37.0, 31.9, 28.5, 23.1. HRMS (ESI): Calculated for $C_{22}H_{26}N[M+H]^+$: 304.2060; Found: 304.2071.



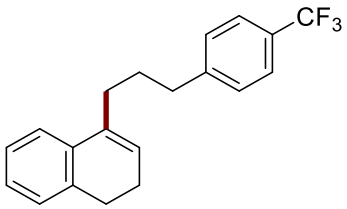
***tert*-Butyl 4-(3,4-dihydronaphthalen-1-yl)piperidine-1-carboxylate (3t).**

The product **3t** (39.4 mg, 63% yield) was prepared from alkyl chloride, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 7.3 Hz, 1 H), 7.23-7.17 (m, 1 H), 7.17-7.11 (m, 2 H), 5.84 (t, *J* = 4.7 Hz, 1 H), 4.21 (s, 2 H), 2.90-2.76 (m, 2 H), 2.74-2.64 (m, 3 H), 2.25-2.20 (m, 2 H), 1.84 (d, *J* = 13.0 Hz, 2 H), 1.47-1.43 (m, 11 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 140.0, 137.1, 134.3, 127.8, 126.5, 126.3, 122.8, 122.0, 79.3, 44.5, 37.0, 31.8, 28.5, 28.4, 23.0. HRMS (ESI): Calculated for $C_{20}H_{27}O_2NNa[M+Na]^+$: 336.1934; Found: 336.1947.



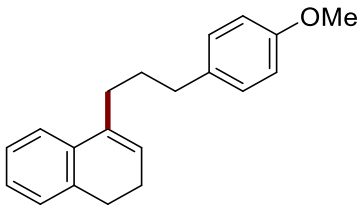
4-(2-(3,4-Dihydronaphthalen-1-yl)ethyl)phenol (3u).

The product **3u** (21.0 mg, 42% yield) was prepared from alkyl chloride, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.5 Hz, 1 H), 7.25-7.19 (m, 1 H), 7.18-7.14 (m, 2 H), 7.07 (d, *J* = 8.3 Hz, 2 H), 6.76 (d, *J* = 8.4 Hz, 2 H), 5.82 (t, *J* = 4.4 Hz, 1 H), 4.89 (s, 1 H), 2.79-2.68 (m, 6 H), 2.25-2.20 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 136.8, 135.8, 134.8, 134.5, 129.5, 127.7, 126.6, 126.4, 125.3, 122.5, 115.1, 35.0, 34.0, 28.4, 23.1. HRMS (EI): Calculated for $C_{18}H_{18}O[M]^+$: 250.1352; Found: 250.1353.



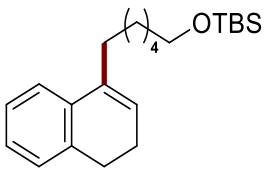
4-(3-(4-(Trifluoromethyl)phenyl)propyl)-1,2-dihydronaphthalene (3v).

The product **3v** (50.6 mg, 80% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.44 (m, 2 H), 7.40-7.38 (m, 2 H), 7.20-7.17 (m, 2 H), 7.16-7.14 (m, 2 H), 5.88 (t, J = 4.7 Hz, 1 H), 2.75 (t, J = 7.6 Hz, 4 H), 2.50 (t, J = 7.7 Hz, 2 H), 2.29-2.24 (m, 2 H), 1.95-1.87 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 136.8, 135.9, 134.7, 131.9, 130.6 (q, $^{2}J_{CF}$ = 32.0 Hz), 128.6, 127.6, 126.6, 126.5 (q, $^{1}J_{CF}$ = 174 Hz), 126.3, 125.3, 125.1 (q, $^{3}J_{CF}$ = 2.9 Hz), 122.6 (q, $^{4}J_{CF}$ = 3.9 Hz) 122.5, 35.4, 32.2, 29.8, 28.4, 23.1. HRMS (EI): Calculated for $C_{20}H_{19}F_3[M]^+$: 316.1433; Found: 316.1438.



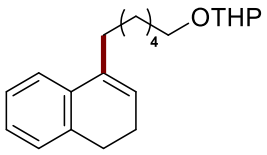
4-(3-(4-Methoxyphenyl)propyl)-1,2-dihydronaphthalene (3w).

This compound is known.[8] The product **3w** (34.5 mg, 62% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.19 (m, 2 H), 7.18-7.11 (m, 4 H), 6.90-6.81 (m, 2 H), 5.88 (t, J = 4.6 Hz, 1 H), 3.81 (s, 3 H), 2.76 (t, J = 8.0 Hz, 2 H), 2.65 (t, J = 7.7 Hz, 2 H), 2.49 (t, J = 7.7 Hz, 2 H), 2.29-2.24 (m, 2 H), 1.90-1.82 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 136.8, 136.3, 134.9, 134.5, 129.4, 127.6, 126.5, 126.3, 124.9, 122.6, 113.7, 55.3, 55.3, 34.8, 32.2, 30.3, 28.5, 23.1.



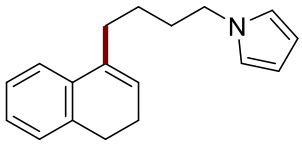
***tert*-Butyl((6-(3,4-dihydronaphthalen-1-yl)hexyl)oxy)dimethylsilane (3x).**

The product **3x** (48.2 mg, 70% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 7.6 Hz, 1 H), 7.23-7.19 (m, 1 H), 7.17-7.10 (m, 2 H), 5.87 (t, *J* = 4.6 Hz, 1 H), 3.63 (t, *J* = 6.6 Hz, 2 H), 2.75 (t, *J* = 8.0 Hz, 2 H), 2.45 (t, *J* = 7.7 Hz, 2 H), 2.29-2.24 (m, 2 H), 1.60-1.52 (m, 4 H), 1.42-1.36 (m, 4 H), 0.93 (s, 9 H), 0.08 (s, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 136.6, 135.0, 127.6, 126.5, 126.3, 124.6, 122.7, 63.3, 32.9, 32.7, 29.4, 28.5, 28.5, 26.0, 25.7, 23.1, 18.4, -5.2. HRMS (EI): Calculated for $C_{22}H_{36}OSi[M]^+$: 344.2530; Found: 344.2533.



2-((6-(3,4-Dihydronaphthalen-1-yl)hexyl)oxy)tetrahydro-*2H*-pyran (3y).

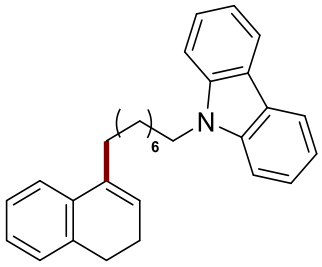
The product **3y** (32.7 mg, 52% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 7.5 Hz, 1 H), 7.22-7.18 (m, 1 H), 7.16-7.12 (m, 2 H), 5.85 (t, *J* = 4.7 Hz, 1 H), 4.59 (t, *J* = 3.6 Hz, 1 H), 3.98-3.83 (m, 1 H), 3.78-3.72 (m, 1 H), 3.52-3.48 (m, 1 H), 3.43-3.37 (m, 1 H), 2.74 (t, *J* = 8.0 Hz, 2 H), 2.45 (t, *J* = 7.7 Hz, 2 H), 2.27-2.22 (m, 2 H), 1.88-1.80 (m, 1 H), 1.76-1.70 (m, 1 H), 1.64-1.50 (m, 8 H), 1.45-1.38 (m, 4 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 136.6, 135.01 127.6, 126.5, 126.3, 124.6, 122.6, 98.8, 67.6, 62.3, 32.7, 30.8, 29.8, 29.7, 29.4, 28.5, 28.4, 26.2, 25.5, 23.1, 19.7. HRMS (EI): Calculated for $C_{21}H_{30}O_2[M]^+$: 314.2240; Found: 314.2245.



1-(4-(3,4-Dihydronaphthalen-1-yl)butyl)-*1H*-pyrrole (3z).

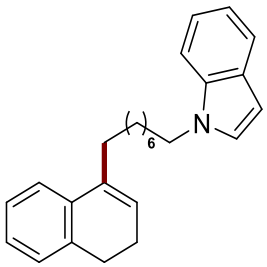
The product **3z** (21.1 mg, 42% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.20 (m, 2 H), 7.16-7.15 (m, 2 H), 6.66-6.65 (m, 2 H), 6.16-6.15 (m, 2 H), 5.84 (t, *J* = 4.8 Hz, 1 H), 3.89 (t, *J* = 7.2 Hz, 2 H), 2.74 (t, *J* = 8.0 Hz, 2 H), 2.47 (t, *J* = 7.6 Hz, 2 H), 2.27-2.22 (m, 2 H), 1.88-1.81 (m, 2 H), 1.60-1.52 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 135.8, 134.7, 127.6, 126.6,

126.3, 125.3, 122.5, 120.4, 107.8, 49.5, 32.2, 31.3, 28.4, 25.3, 23.0. HRMS (ESI): Calculated for $C_{18}H_{22}N[M+H]^+$: 252.1747; Found: 252.1755.



9-(8-(3,4-Dihydronaphthalen-1-yl)octyl)-*9H*-carbazole (3aa).

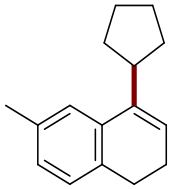
The product **3aa** (44.8 mg, 55% yield) was prepared from alkyl bromide, and was purified with silica gel chromatograph (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 7.7 Hz, 2 H), 7.52 (t, *J* = 7.0 Hz, 2 H), 7.45 (d, *J* = 8.1 Hz, 2 H), 7.35-7.24 (m, 4 H), 7.22-7.15 (m, 2 H), 5.89 (t, *J* = 4.6 Hz, 1 H), 4.32 (t, *J* = 7.2 Hz, 2 H), 2.79 (t, *J* = 7.5 Hz, 2 H), 2.47 (t, *J* = 6.9 Hz, 2 H), 2.32-2.27 (m, 2 H), 1.91 (p, *J* = 7.2 Hz, 2 H), 1.61-1.52 (m, 2 H), 1.47-1.28 (m, 8 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5, 136.9, 136.6, 135.1, 127.6, 126.5, 126.3, 125.6, 124.7, 122.9, 122.7, 120.4, 118.8, 108.7, 43.1, 32.8, 29.5, 29.4, 29.4, 29.0, 28.6, 28.4, 27.3, 23.2. HRMS (ESI): Calculated for $C_{30}H_{34}N[M+H]^+$: 408.2686; Found: 408.2698.



1-(8-(3,4-Dihydronaphthalen-1-yl)octyl)-*1H*-indole (3ab).

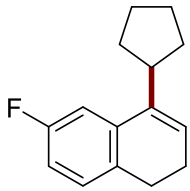
The product **3ab** (37.7 mg, 72% yield) was prepared from alkyl bromide, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.8 Hz, 1 H), 7.34 (d, *J* = 8.2 Hz, 1 H), 7.24-7.15 (m, 3 H), 7.15-7.02 (m, 4 H), 6.48 (d, *J* = 2.3 Hz, 1 H), 5.83 (t, *J* = 4.6 Hz, 1 H), 4.10 (t, *J* = 7.1 Hz, 2 H), 2.73 (t, *J* = 8.0 Hz, 2 H), 2.41 (t, *J* = 7.7 Hz, 2 H), 2.26-2.21 (m, 2 H), 1.83 (t, *J* = 7.0 Hz, 2 H), 1.52-1.44 (m, 2 H), 1.38-1.28 (m, 8 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 136.5, 135.9, 135.0, 128.5, 127.8, 127.5, 126.5, 126.2, 124.6,

122.6, 121.3, 120.9, 119.1, 109.4, 100.8, 46.4, 32.7, 30.2, 29.4, 29.3, 29.2, 28.5, 28.4, 27.0, 23.1. HRMS (ESI): Calculated for $C_{26}H_{32}N[M+H]^+$: 358.2529; Found: 358.2543.



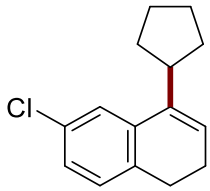
4-Cyclopentyl-6-methyl-1,2-dihydronaphthalene (3ac).

The product **3ac** (27.6 mg, 65% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (s, 1 H), 7.04 (d, *J* = 7.5 Hz, 1 H), 6.95 (d, *J* = 7.5 Hz, 1 H), 5.90 (t, *J* = 4.4 Hz, 1 H), 2.99 (p, *J* = 8.1 Hz, 1 H), 2.67 (t, *J* = 7.9 Hz, 2 H), 2.35 (s, 3 H), 2.25-2.20 (m, 2 H), 2.04-1.93 (m, 2 H), 1.78-1.62 (m, 4 H), 1.53- 1.40 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 135.6, 135.5, 133.9, 127.3, 126.8, 123.9, 121.6, 41.0, 32.1, 28.1, 24.9, 23.4, 21.5. HRMS (EI): Calculated for $C_{16}H_{20}[M]^+$: 212.1560; Found: 212.1554.



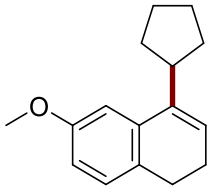
4-Cyclopentyl-6-fluoro-1,2-dihydronaphthalene (3ad).

The product **3ad** (22.5 mg, 52% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08-7.00 (m, 2 H), 6.83-6.78 (m, 1 H), 5.95 (t, *J* = 4.7 Hz, 1 H), 2.98-2.78 (m, 1 H), 2.65 (t, *J* = 7.9 Hz, 2 H), 2.25-2.20 (m, 2 H), 2.00-1.93 (m, 2 H), 1.78-1.62 (m, 4 H), 1.51-1.35 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0, 160.6, 139.6, 137.7, 137.6, 132.2, 128.3, 128.2, 122.8, 112.4, 112.2, 110.4, 110.1. 41.1, 31.9, 29.7, 27.6, 24.9, 23.3. HRMS (EI): Calculated for $C_{15}H_{17}F[M]^+$: 216.1309; Found: 216.1307.



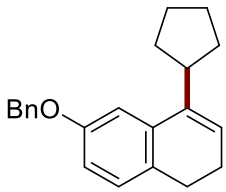
6-Chloro-4-cyclopentyl-1,2-dihydronaphthalene (3ae).

The product **3ae** (22.3 mg, 48% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (s, 1 H), 7.09-7.04 (m, 2 H), 5.94 (t, *J* = 4.4 Hz, 1 H), 2.91 (p, *J* = 8.1 Hz, 1 H), 2.65 (t, *J* = 7.9 Hz, 2 H), 2.25-2.20 (m, 2 H), 2.02-1.93 (m, 2 H), 1.76-1.60 (m, 4 H), 1.52-1.38 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 137.5, 135.1, 131.9, 128.5, 125.9, 123.3, 122.8, 40.9, 32.0, 27.8, 24.9, 23.1. HRMS (EI): Calculated for $C_{15}H_{17}Cl[M]^+$: 232.1013; Found: 232.1010.



4-Cyclopentyl-6-methoxy-1,2-dihydronaphthalene (3af).

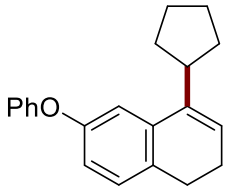
The product **3af** (33.3 mg, 73% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.1 Hz, 1 H), 6.91 (d, *J* = 2.3 Hz, 1 H), 6.67 (dd, *J* = 8.2, 2.6 Hz, 1 H), 5.92 (t, *J* = 4.1 Hz, 1 H), 3.80 (s, 3 H), 2.94 (p, *J* = 7.7 Hz, 1 H), 2.63 (t, *J* = 7.8 Hz, 2 H), 2.24-2.19 (m, 2 H), 2.03-1.92 (m, 2 H), 1.79-1.61 (m, 4 H), 1.52-1.39 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 140.0, 136.9, 129.2, 127.9, 122.3, 110.4, 110.2, 55.4, 41.1, 32.1, 27.6, 24.9, 23.5. HRMS (EI): Calculated for $C_{16}H_{20}O[M]^+$: 228.1509; Found: 228.1509.



6-(Benzyloxy)-4-cyclopentyl-1,2-dihydronaphthalene (3ag).

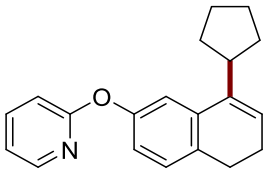
The product **3ag** (35.3 mg, 58% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* =

7.4 Hz, 2 H), 7.40 (t, *J* = 7.5 Hz, 2 H), 7.33 (t, *J* = 7.2 Hz, 1 H), 7.06 (d, *J* = 8.2 Hz, 1 H), 6.99 (d, *J* = 2.6 Hz, 1 H), 6.76 (dd, *J* = 8.2, 2.6 Hz, 1 H), 5.92 (t, *J* = 4.7 Hz, 1 H), 5.07 (s, 2 H), 2.96-2.88 (m, 1 H), 2.65 (t, *J* = 7.9 Hz, 2 H), 2.26-2.21 (m, 2 H), 2.02-1.86 (m, 2 H), 1.80-1.61 (m, 4 H), 1.51-1.38 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 139.9, 137.4, 136.9, 129.4, 128.6, 127.9, 127.5, 122.3, 111.5, 111.1, 70.2, 41.2, 32.0, 27.6, 24.9, 23.5. HRMS (EI): Calculated for $C_{22}H_{24}O[M]^+$: 304.1822; Found: 304.1829.



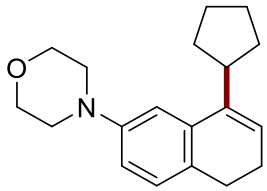
4-Cyclopentyl-6-phenoxy-1,2-dihydronaphthalene (3ah).

The product **3ah** (36.0 mg, 62% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (t, *J* = 7.9 Hz, 2 H), 7.12-7.05 (m, 2 H), 7.04 (d, *J* = 2.5 Hz, 1 H), 7.00 (d, *J* = 8.0 Hz, 2 H), 6.77 (dd, *J* = 8.1, 2.5 Hz, 1 H), 5.93 (t, *J* = 4.1 Hz, 1 H), 2.86 (p, *J* = 8.0 Hz, 1 H), 2.68 (t, *J* = 7.9 Hz, 2 H), 2.28-2.23 (m, 2 H), 1.97-1.87 (m, 2 H), 1.75-1.56 (m, 4 H), 1.50-1.40 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 155.1, 139.8, 137.3, 132.1, 129.6, 128.3, 122.6, 122.4, 118.0, 116.8, 114.9, 41.1, 31.9, 27.8, 24.8, 23.4. HRMS (EI): Calculated for $C_{21}H_{22}O[M]^+$: 290.1665; Found: 290.1671.



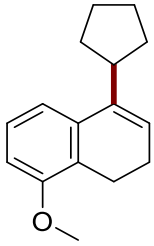
2-((8-Cyclopentyl-5,6-dihydronaphthalen-2-yl)oxy)pyridine (3ai).

The product **3ai** (37.7 mg, 72% yield) was prepared from alkyl phosphate as colorless oil, and was purified with silica gel chromatography (PE/EA, 20/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 4.3 Hz, 1 H), 7.65 (t, *J* = 7.0 Hz, 1 H), 7.14 (d, *J* = 8.0 Hz, 1 H), 7.09 (s, 1 H), 6.99-6.93 (m, 1 H), 6.88 (t, *J* = 8.6 Hz, 2 H), 5.92 (t, *J* = 4.4 Hz, 1 H), 2.87 (p, *J* = 8.0 Hz, 1 H), 2.69 (t, *J* = 7.9 Hz, 2 H), 2.27-2.22 (m, 2 H), 1.99-1.86 (m, 2 H), 1.75-1.55 (m, 4 H), 1.49-1.40 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 152.4, 147.8, 139.8, 139.3, 137.4, 133.3, 128.3, 122.2, 118.8, 118.1, 116.5, 111.0, 41.1, 31.9, 27.9, 24.8, 23.3.



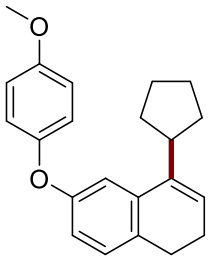
4-(8-Cyclopentyl-5,6-dihydronaphthalen-2-yl)morpholine (3aj).

The product **3aj** (27.2 mg, 48% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.1 Hz, 1 H), 6.93 (d, *J* = 2.5 Hz, 1 H), 6.71 (dd, *J* = 8.1, 2.5 Hz, 1 H), 5.91 (t, *J* = 4.1 Hz, 1 H), 3.93-3.76 (m, 4 H), 3.17-3.08 (m, 4 H), 2.96 (p, *J* = 8.1 Hz, 1 H), 2.62 (t, *J* = 7.8 Hz, 2 H), 2.23-2.18 (m, 2 H), 2.01-1.91 (m, 2 H), 1.80-1.63 (m, 4 H), 1.54-1.43 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.1, 140.1, 136.3, 129.2, 127.8, 122.1, 114.0, 112.1, 67.0, 50.3, 41.1, 32.1, 27.6, 25.0, 23.5.



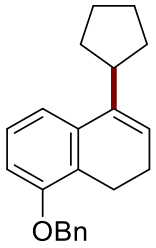
4-Cyclopentyl-8-methoxy-1,2-dihydronaphthalene (3ak).

The product **3ak** (23.2 mg, 51% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (t, *J* = 8.0 Hz, 1 H), 7.00 (d, *J* = 7.8 Hz, 1 H), 6.78 (d, *J* = 8.2 Hz, 1 H), 5.91 (t, *J* = 4.1 Hz, 1 H), 3.83 (s, 3 H), 2.97 (p, *J* = 7.9 Hz, 1 H), 2.71 (t, *J* = 8.1 Hz, 2 H), 2.24-2.16 (m, 2 H), 2.01-1.90 (m, 2 H), 1.79-1.61 (m, 4 H), 1.51-1.39 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.0, 139.9, 136.9, 126.1, 124.8, 121.7, 116.2, 109.2, 55.6, 41.4, 32.1, 24.9, 22.6, 19.9. HRMS (EI): Calculated for $C_{16}H_{20}O[M]^+$: 228.1509; Found: 228.1509.



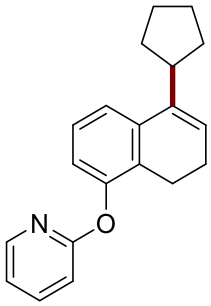
4-Cyclopentyl-6-(4-methoxyphenoxy)-1,2-dihydronaphthalene (3al).

The product **3al** (26.7 mg, 42% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.0 Hz, 1 H), 7.03-6.94 (m, 3 H), 6.91-6.84 (m, 2 H), 6.69 (dd, *J* = 8.1, 2.3 Hz, 1 H), 5.93 (t, *J* = 4.7 Hz, 1 H), 3.81 (s, 3 H), 2.87 (t, *J* = 8.2 Hz, 1 H), 2.66 (t, *J* = 7.9 Hz, 2 H), 2.29-2.19 (m, 2 H), 1.96-1.88 (m, 2 H), 1.78-1.57 (m, 4 H), 1.49-1.40 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.6, 155.4, 150.9, 139.8, 137.2, 131.3, 128.1, 122.3, 120.0, 115.4, 114.7, 113.8, 77.4, 77.0, 76.7, 55.7, 41.1, 31.9, 27.7, 24.9, 23.4. HRMS (ESI): Calculated for $C_{22}H_{25}O_2[M+H]^+$: 321.1849; Found: 321.1859.



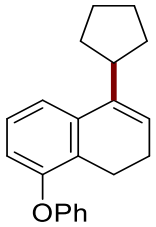
8-(Benzyloxy)-4-cyclopentyl-1,2-dihydronaphthalene (3am).

The product **3am** (44.3 mg, 73% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.5 Hz, 2 H), 7.39 (t, *J* = 7.5 Hz, 2 H), 7.35-7.30 (m, 1 H), 7.15 (t, *J* = 8.0 Hz, 1 H), 7.02 (d, *J* = 7.8 Hz, 1 H), 6.84 (d, *J* = 8.0 Hz, 1 H), 5.92 (t, *J* = 4.2 Hz, 1 H), 5.08 (s, 2 H), 2.98 (p, *J* = 7.8 Hz, 1 H), 2.79 (t, *J* = 8.1 Hz, 2 H), 2.24-2.19 (m, 2 H), 2.00-1.92 (m, 2 H), 1.77-1.61 (m, 4 H), 1.51-1.42 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 139.9, 137.6, 137.1, 128.5, 127.7, 127.2, 126.1, 121.8, 116.5, 110.7, 70.3, 41.4, 32.1, 24.9, 22.6, 20.2. HRMS (EI): Calculated for $C_{22}H_{24}O[M]^+$: 304.1822; Found: 304.1828.



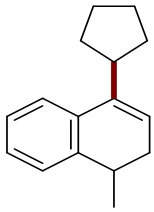
2-((5-Cyclopentyl-7,8-dihydronaphthalen-1-yl)oxy)pyridine (3an).

The product **3an** (26.2 mg, 45% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.16 (m, 1 H), 7.64 (t, *J* = 8.5 Hz, 1 H), 7.25-7.21 (m, 2 H), 6.98-6.92 (m, 2 H), 6.83 (d, *J* = 8.3 Hz, 1 H), 5.91 (t, *J* = 4.2 Hz, 1 H), 2.99 (p, *J* = 7.9 Hz, 1 H), 2.58 (t, *J* = 8.0 Hz, 2 H), 2.19-2.14 (m, 2 H), 2.02-1.93 (m, 2 H), 1.80-1.59 (m, 4 H), 1.54-1.44 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 150.4, 147.9, 139.9, 139.3, 137.8, 129.1, 126.56, 122.1, 120.3, 120.2, 117.9, 110.4, 41.3, 32.2, 24.9, 22.4, 21.1. HRMS (ESI): Calculated for $C_{20}H_{22}ON[M+H]^+$: 296.1696; Found: 296.1705.



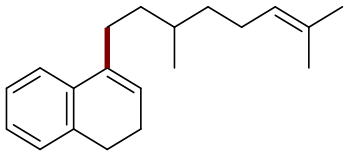
4-Cyclopentyl-8-phenoxy-1,2-dihydronaphthalene (3ao).

The product **3ao** (45.2 mg, 78% yield) was prepared from alkyl phosphate, and was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.8 Hz, 2 H), 7.19 (d, *J* = 6.6 Hz, 2 H), 7.10-7.01 (m, 1 H), 6.96-6.92 (m, 2 H), 6.85 (dd, *J* = 6.7, 2.1 Hz, 1 H), 5.96 (t, *J* = 4.7 Hz, 1 H), 3.08-2.96 (m, 1 H), 2.69 (t, *J* = 8.0 Hz, 2 H), 2.23-2.18 (m, 2 H), 2.04-1.96 (m, 2 H), 1.81-1.63 (m, 4 H), 1.54-1.46 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 152.4, 139.9, 137.8, 129.6, 128.7, 126.6, 122.3, 122.1, 119.5, 118.8, 116.9, 41.4, 32.2, 25.0, 22.5, 20.8. HRMS (EI): Calculated for $C_{22}H_{24}O[M]^+$: 290.1665; Found: 290.1664.



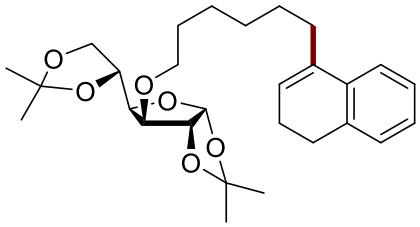
4-Cyclopentyl-1-methyl-1,2-dihydronaphthalene (3ap).

The product **3ap** (36.0 mg, 85% yield) was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.1 Hz, 1 H), 7.28-7.17 (m, 3 H), 5.84 (t, *J* = 4.3 Hz, 1 H), 3.04 (p, *J* = 7.8 Hz, 1 H), 2.90-2.82 (m, 1 H), 2.43 (dt, *J* = 16.5, 4.6 Hz, 1 H), 2.15-1.93 (m, 3 H), 1.84-1.64 (m, 4 H), 1.55-1.42 (m, 2 H), 1.24 (d, *J* = 6.9 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 139.3, 134.9, 126.6, 126.0, 126.0, 123.3, 119.9, 119.9, 41.0, 32.2, 32.1, 31.8, 31.1, 24.9, 24.9, 19.8. HRMS (EI): Calculated for $C_{16}H_{20}[M]^+$: 212.1560; Found: 212.1555.



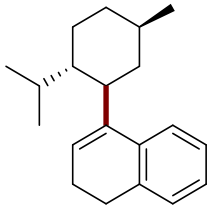
4-(3,7-Dimethyloct-6-en-1-yl)-1,2-dihydronaphthalene (4).

The product **4** (30.6 mg, 57% yield) was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.3 Hz, 1 H), 7.26-7.20 (m, 1 H), 7.19-7.13 (m, 2 H), 5.91-5.86 (m, 1 H), 5.14 (t, *J* = 6.7 Hz, 1 H), 2.76 (t, *J* = 7.9 Hz, 2 H), 2.59-2.36 (m, 2 H), 2.29-2.24 (m, 2 H), 2.11-1.92 (m, 2 H), 1.72 (s, 3 H), 1.64 (s, 3 H), 1.60-1.50 (m, 2 H), 1.49-1.33 (m, 2 H), 1.29-1.17 (m, 1 H), 1.02-0.95 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.0, 136.8, 135.1, 131.1, 127.6, 126.5, 126.3, 125.0, 124.5, 122.6, 37.0, 35.9, 32.5, 30.3, 28.5, 25.8, 25.6, 23.2, 19.6, 17.7. HRMS (EI): Calculated for $C_{20}H_{28}[M]^+$: 268.2186; Found: 268.2187.



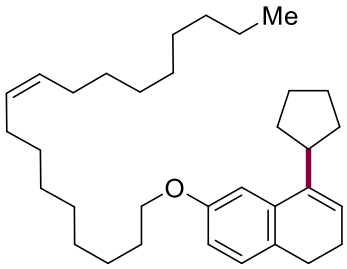
(*3aR,5R*)-6-((6-(3,4-Dihydronaphthalen-1-yl)hexyl)oxy)-5-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxole (5).

The product **5** (58.5 mg, 62% yield) was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.21 (m, 1 H), 7.21-7.16 (m, 1 H), 7.15-7.10 (m, 2 H), 5.87 (d, *J* = 3.4 Hz, 1 H), 5.83 (t, *J* = 4.0 Hz, 1 H), 4.52 (d, *J* = 3.5 Hz, 1 H), 4.30 (q, *J* = 6.3 Hz, 1 H), 4.16-4.04 (m, 2 H), 4.02-3.95 (m, 1 H), 3.85 (d, *J* = 2.7 Hz, 1 H), 3.64-3.44 (m, 2 H), 2.73 (t, *J* = 7.9 Hz, 2 H), 2.42 (t, *J* = 7.4 Hz, 2 H), 2.26-2.21 (m, 2 H), 1.63-1.46 (m, 6 H), 1.43-1.30 (m, 14 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 136.5, 135.0, 127.6, 126.5, 126.3, 124.7, 122.6, 111.7, 108.9, 105.3, 82.5, 82.1, 81.2, 72.5, 70.7, 67.2, 32.7, 29.7, 29.3, 28.5, 28.4, 26.8, 26.8, 26.3, 26.0, 25.4, 23.1. HRMS (ESI): Calculated for $C_{28}H_{40}O_6Na[M+Na]^+$: 495.2717; Found: 495.2737.



4-((*1R,2S,5R*)-2-Isopropyl-5-methylcyclohexyl)-1,2-dihydronaphthalene (6).

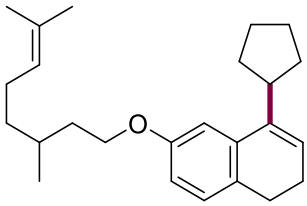
The product **4** (22.0 mg, 41% yield) was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.7 Hz, 1 H), 7.23-7.18 (m, 1 H), 7.18-7.08 (m, 2 H), 5.85 (t, *J* = 4.7 Hz, 1 H), 2.76-2.65 (m, 2 H), 2.60-2.50 (m, 1 H), 2.30-2.15 (m, 2 H), 2.03-1.96 (m, 1 H), 1.92-1.72 (m, 3 H), 1.47-1.38 (m, 2 H), 1.22-1.08 (m, 2 H), 0.88 (t, *J* = 6.6 Hz, 6 H), 0.73 (t, *J* = 7.6 Hz, 1 H), 0.63 (d, *J* = 6.9 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 136.9, 135.9, 127.6, 126.3, 126.2, 122.9, 121.6, 46.6, 45.1, 40.8, 35.4, 33.3, 28.7, 26.8, 24.8, 23.0, 22.5, 21.8, 16.3. HRMS (EI): Calculated for $C_{20}H_{28}[M]^+$: 268.2186; Found: 268.2187.



(*Z*)-4-Cyclopentyl-6-(octadec-9-en-1-yloxy)-1,2-dihydronaphthalene (7).

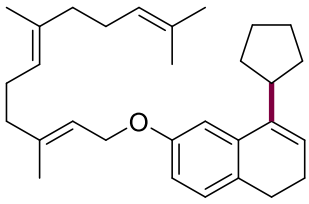
The product **7** (49.3 mg, 54% yield) was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (d, *J* = 8.1 Hz, 1 H), 6.91 (d, *J* = 2.5 Hz, 1 H),

6.67 (dd, *J* = 8.1, 2.5 Hz, 1 H), 5.92 (t, *J* = 4.6 Hz, 1 H), 5.36 (t, *J* = 5.0 Hz, 2 H), 3.95 (t, *J* = 6.6 Hz, 2 H), 2.96 (p, *J* = 8.1 Hz, 1 H), 2.63 (t, *J* = 7.9 Hz, 2 H), 2.32-2.15 (m, 2 H), 2.15-1.91 (m, 6 H), 1.87-1.59 (m, 4 H), 1.54-1.40 (m, 4 H), 1.41-1.21 (m, 23 H), 0.89 (t, *J* = 6.7 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 140.1, 136.8, 129.9, 129.8, 129.0, 127.8, 122.0, 111.2, 110.8, 68.1, 41.1, 32.1, 31.9, 29.8, 29.5, 29.5, 29.4, 29.3, 29.2, 27.6, 27.2, 26.1, 24.9, 23.6, 22.7, 14.1. HRMS (ESI): Calculated for $C_{33}H_{53}O[M+H]^+$: 465.4091; Found: 465.4094.

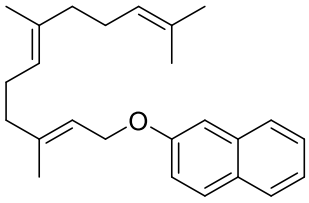


4-Cyclopentyl-6-((3,7-dimethyloct-6-en-1-yl)oxy)-1,2-dihydronaphthalene (8).

The product **8** (37.5 mg, 53% yield) was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 (d, *J* = 8.1 Hz, 1 H), 6.92 (d, *J* = 2.5 Hz, 1 H), 6.68 (dd, *J* = 8.1, 2.5 Hz, 1 H), 5.93 (t, *J* = 4.2 Hz, 1 H), 5.19-5.08 (m, 1 H), 4.06-3.94 (m, 2 H), 3.02-2.91 (m, 1 H), 2.64 (t, *J* = 7.9 Hz, 2 H), 2.27-2.18 (m, 2 H), 2.13-1.91 (m, 4 H), 1.89-1.81 (m, 1 H), 1.79-1.57 (m, 13 H), 1.51-1.43 (m, 2 H), 1.26-1.18 (m, 1 H), 0.97 (d, *J* = 6.6 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 140.1, 136.8, 131.2, 129.0, 127.8, 124.7, 122.1, 111.2, 110.8, 66.4, 41.1, 37.2, 36.3, 32.1, 30.0, 29.6, 27.6, 25.7, 25.5, 24.9, 23.6, 19.6, 17.6. HRMS (ESI): Calculated for $C_{25}H_{37}O[M+H]^+$: 353.2839; Found: 353.2840.



9



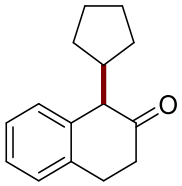
9'

4-Cyclopentyl-6-(((2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl)oxy)-1,2-dihydronaphthalene (9).

2-(((2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl)oxy)naphthalene (9').

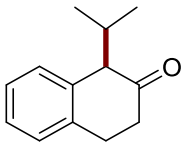
The mixture (71.4 mg in total) of **9** (51.3 mg, 60% yield) and **9′** (20.1 mg, 30% yield), was purified with silica gel chromatography (PE, 100%) as colorless oil. ^{1}H NMR (**9**, 400 MHz, $CDCl_3$) δ 7.05

(d, *J* = 8.1 Hz, 1 H), 6.95 (d, *J* = 2.6 Hz, 1 H), 6.70 (dd, *J* = 8.1, 2.6 Hz, 1 H), 5.93 (t, *J* = 4.7 Hz, 1 H), 5.53 (t, *J* = 6.6 Hz, 1 H), 5.19-5.07 (m, 2 H), 4.55 (d, *J* = 6.6 Hz, 2 H), 3.03-2.86 (m, 1 H), 2.65 (t, *J* = 7.8 Hz, 2 H), 2.28-1.78 (m, 14 H), 1.70 (s, 6 H), 1.63 (s, 3 H), 1.62 (s, 3 H), 1.53-1.42 (m, 2 H). ^{13}C NMR (**9** and **9'**, 150 MHz, $CDCl_3$) δ 160.2, 159.5, 144.0, 143.6, 143.6, 142.7, 139.5, 138.3, 138.2, 138.1, 138.0, 137.2, 134.2, 134.0, 132.0, 131.7, 131.6, 130.5, 130.3, 129.4, 128.9, 127.2, 127.2, 127.0, 127.0, 126.4, 126.4, 126.2, 124.8, 122.5, 122.1, 121.8, 114.0, 113.6, 109.5, 109.5, 67.6, 67.6, 67.2, 43.8, 42.5, 42.4, 42.3, 34.8, 34.7, 32.4, 30.3, 29.4, 29.3, 29.2, 28.9, 28.8, 28.4, 28.4, 27.6, 26.2, 26.0, 20.4, 20.3, 19.4, 19.3, 18.7, 18.7. HRMS (ESI) **9**: Calculated for $C_{29}H_{40}ONa[M+Na]^+$: 427.2971; Found: 427.2985. HRMS (ESI) **9′**: Calculated for $C_{24}H_{31}O[M+H]^+$: 335.2369; Found: 335.2374.



1-Cyclopentyl-3,4-dihydronaphthalen-2(*1H*)-one (10).

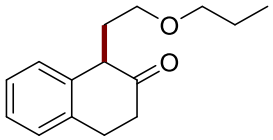
The product **10** (30.4 mg, 79% yield) was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.17 (m, 3 H), 7.11-7.04 (m, 1 H), 3.40-3.26 (m, 1 H), 3.18 (d, *J* = 9.5 Hz, 1 H), 2.99-2.87 (m, 1 H), 2.79-2.66 (m, 1 H), 2.52-2.36 (m, 1 H), 2.31-2.13 (m, 1 H), 1.75-1.56 (m, 3 H), 1.56-1.40 (m, 3 H), 1.32-1.15 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.6, 137.4, 136.2, 129.3, 127.9, 126.8, 126.5, 60.5, 42.4, 36.7, 31.2, 30.7, 27.4, 24.4, 24.1. HRMS (ESI): Calculated for $C_{15}H_{18}ONa[M+Na]^+$: 237.1250; Found: 237.1256.



1-Isopropyl-3,4-dihydronaphthalen-2(*1H*)-one (11).

This compound is known.[9] The product **11** (18.6 mg, 58% yield) was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.11 (m, 3 H), 7.11-6.98 (m, 1 H), 3.37-3.19 (m, 1 H), 3.07 (d, *J* = 8.3 Hz, 1 H), 2.97-2.83 (m, 1 H), 2.77-2.63 (m, 1 H), 2.52-2.36 (m, 1 H), 2.32-2.08 (m, 1 H), 1.01 (d, *J* = 6.8 Hz, 3 H), 0.83 (d, *J* = 6.8 Hz, 3

H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.9, 136.7, 136.5, 129.9, 128.0, 126.9, 126.4, 62.4, 37.2, 31.1, 27.5, 21.1, 20.7. HRMS (ESI): Calculated for $C_{13}H_{16}ONa[M+Na]^+$: 211.1093; Found: 211.1101.



1-(2-Propoxyethyl)-3,4-dihydronaphthalen-2(*1H*)-one (12).

The product **12** (17.7 mg, 60% yield) was purified with silica gel chromatography (PE/EA, 20/1) as colorless oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24-7.17 (m, 3 H), 7.17-7.13 (m, 1 H), 3.59 (t, *J* = 6.8 Hz, 1 H), 3.39 (t, *J* = 4.0 Hz, 2 H), 3.32 (t, *J* = 4.8 Hz, 2 H), 3.22-3.11 (m, 1 H), 3.04-2.93 (m, 1 H), 2.69-2.60 (m, 1 H), 2.58-2.45 (m, 1 H), 2.14 (q, *J* = 4.4 Hz, 2 H), 1.60-1.50 (m, 2 H), 0.90 (t, *J* = 4.8 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 214.9, 139.6, 139.4, 130.6, 130.5, 129.5, 129.4, 75.1, 70.1, 53.0, 40.4, 34.4, 30.5, 25.6, 13.3. HRMS (ESI): Calculated for $C_{15}H_{21}O_2[M+H]^+$: 233.1536; Found: 233.1546.

Reference

[1]. M. V. Mane, K. Vanka, *ChemCatChem*, **2017**, *9*, 3013-3022.

[2]. P. Peach, D. J. Cross, J. A. Kenny, I. Mann, I. Houson, L. Campbell, T. Walsgrove, M. Wills, *Tetrahedron*, **2006**, *62*, 1864-1876.

[3]. T. Si, B. Li, W. Xiong, B. Xu, W. Tang, *Org. Biomol. Chem.*, **2017**, *15*, 9903-9909.

[4]. G. M. Badger, R. W. L. Kimber, *J. Chem. Soc.*, **1958**, 2455-2458.

[5]. H.-C. Liu, X.-P. Gong, Y.-Z. Wang, Z.-J. Niu, H. Yue, X.-Y. Liu, Y.-M. Liang, *Org. Lett.*, **2022**, 24, 3043-3047.

[6]. Wang, L.; Chen, B.; Zhang, Y.; Wu, X. *Angew. Chem., Int. Ed.*, **2022**, *61*, e202207970.

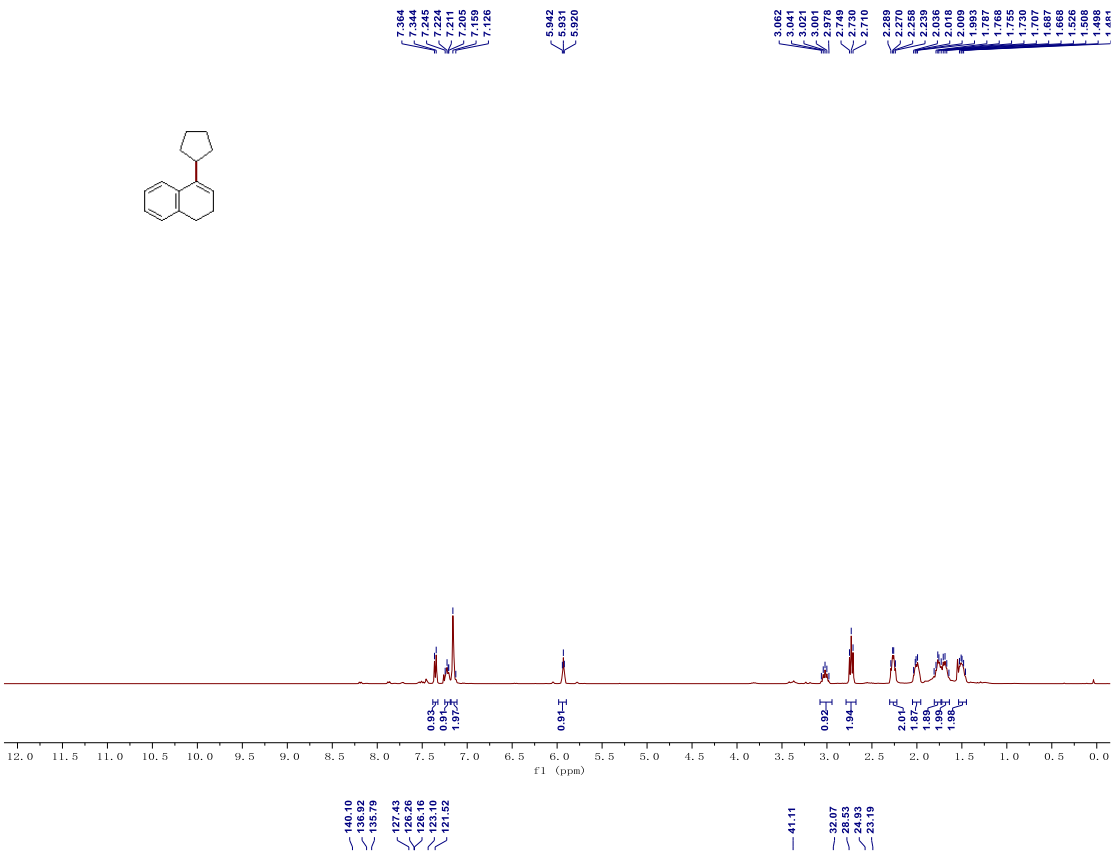
[7]. P. J. Hattersley, I. M. Lockhart, M. Wright, *Journal of the Chemical Society [Section] C: Organic,* **1969**, *2*, 217-222.

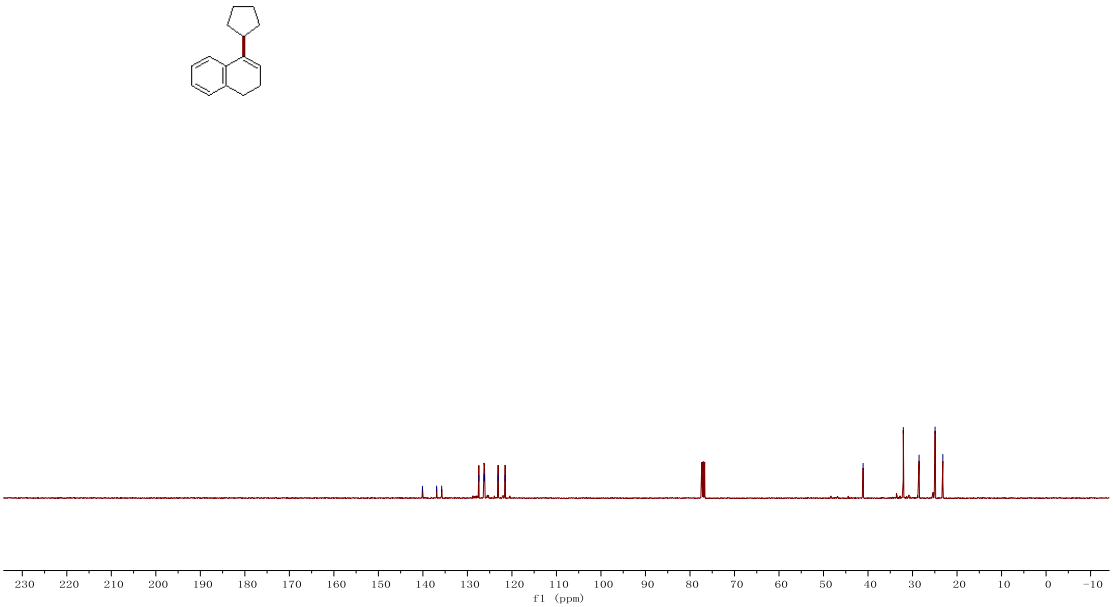
[8]. L. Guo, C.-C. Hsiao, H. Yue, X. Liu, M. Rueping, *ACS Catal.*, **2016**, *6*, 4438-4442.

[9]. T. P. Jonczyk, *Roczniki Chemii,* **1975**, *49*, 1425-1429.

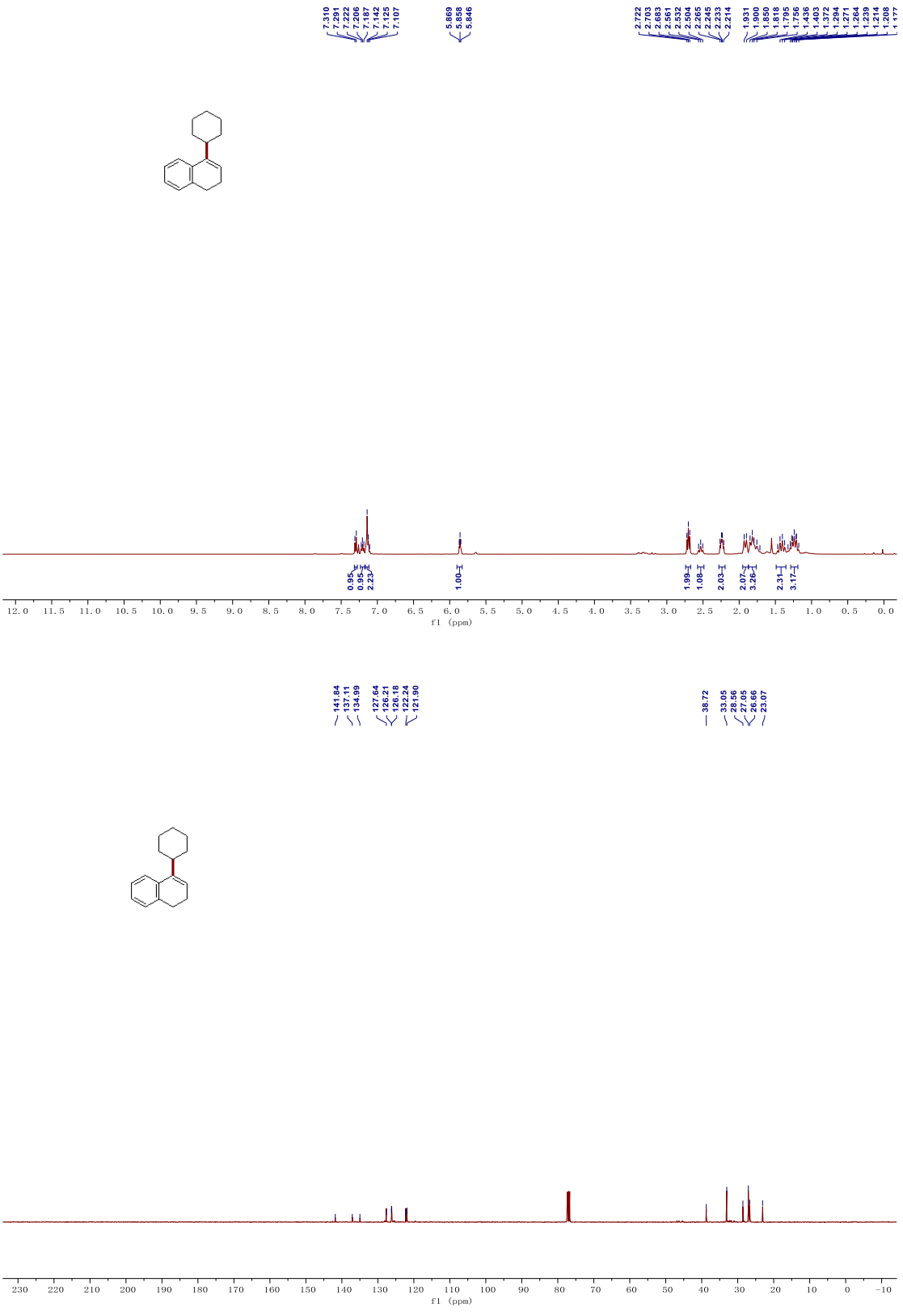
Spectra of Products

4-Cyclopentyl-1,2-dihydronaphthalene (3a)

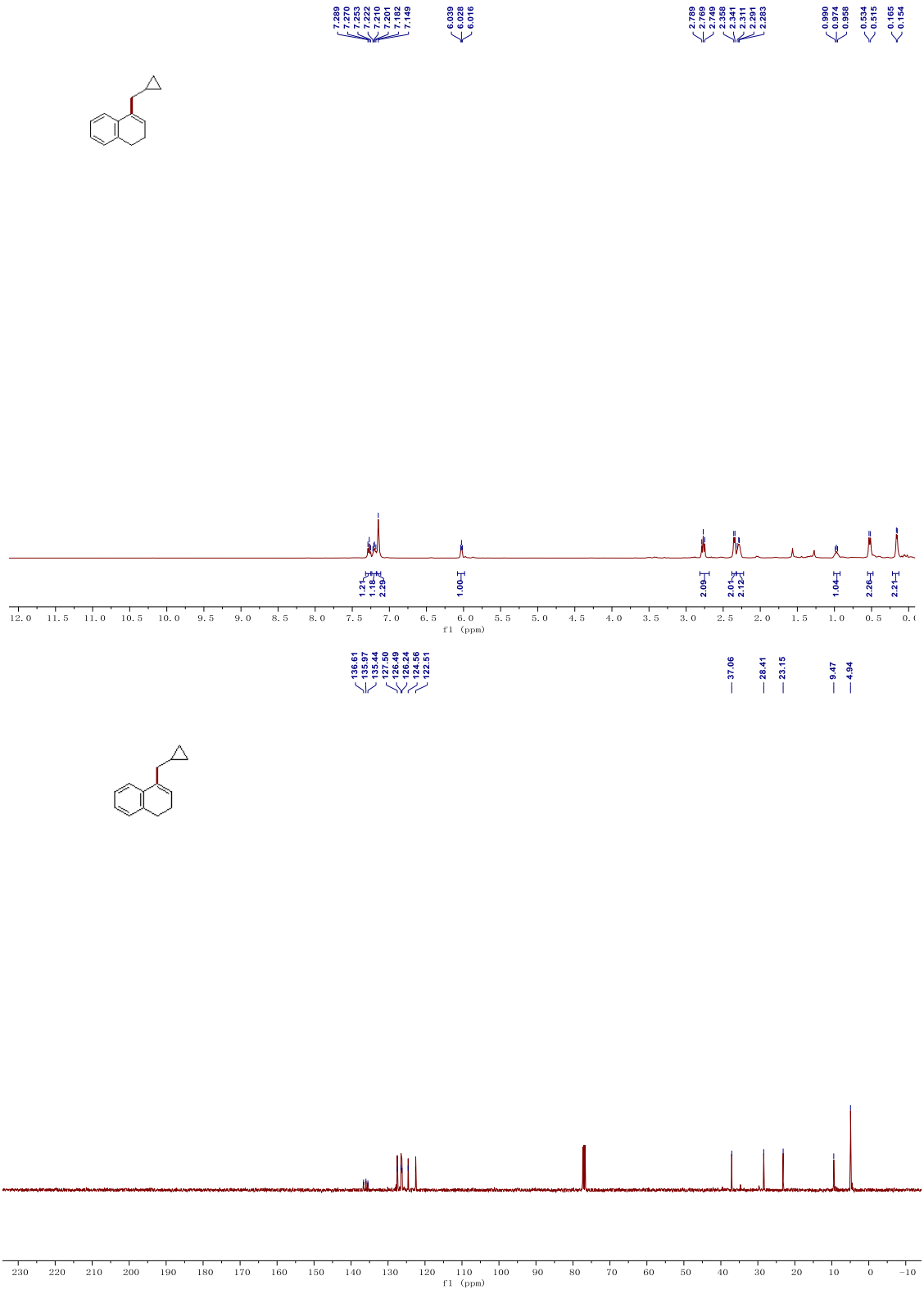




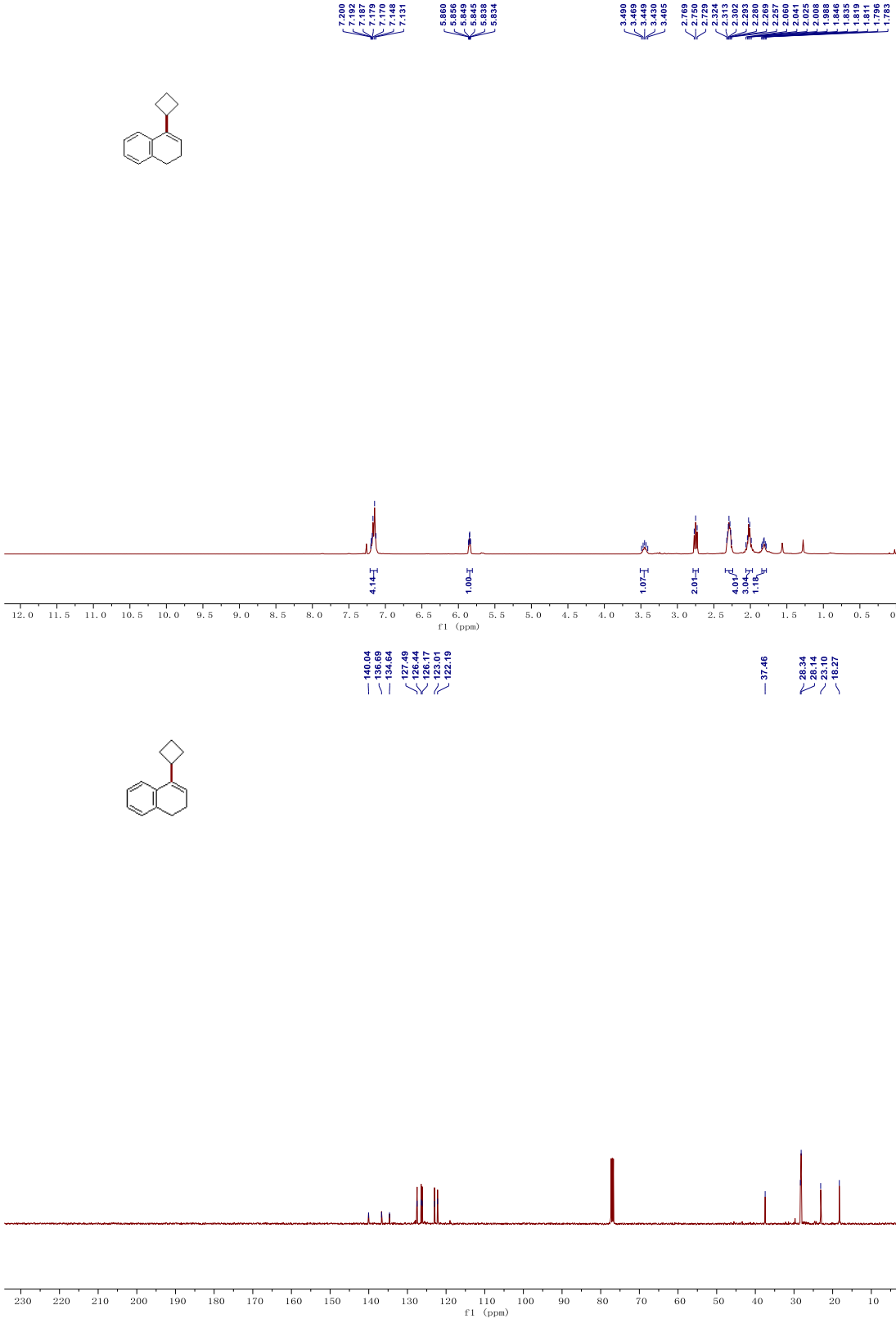
4-Cyclohexyl-1,2-dihydronaphthalene (3b)



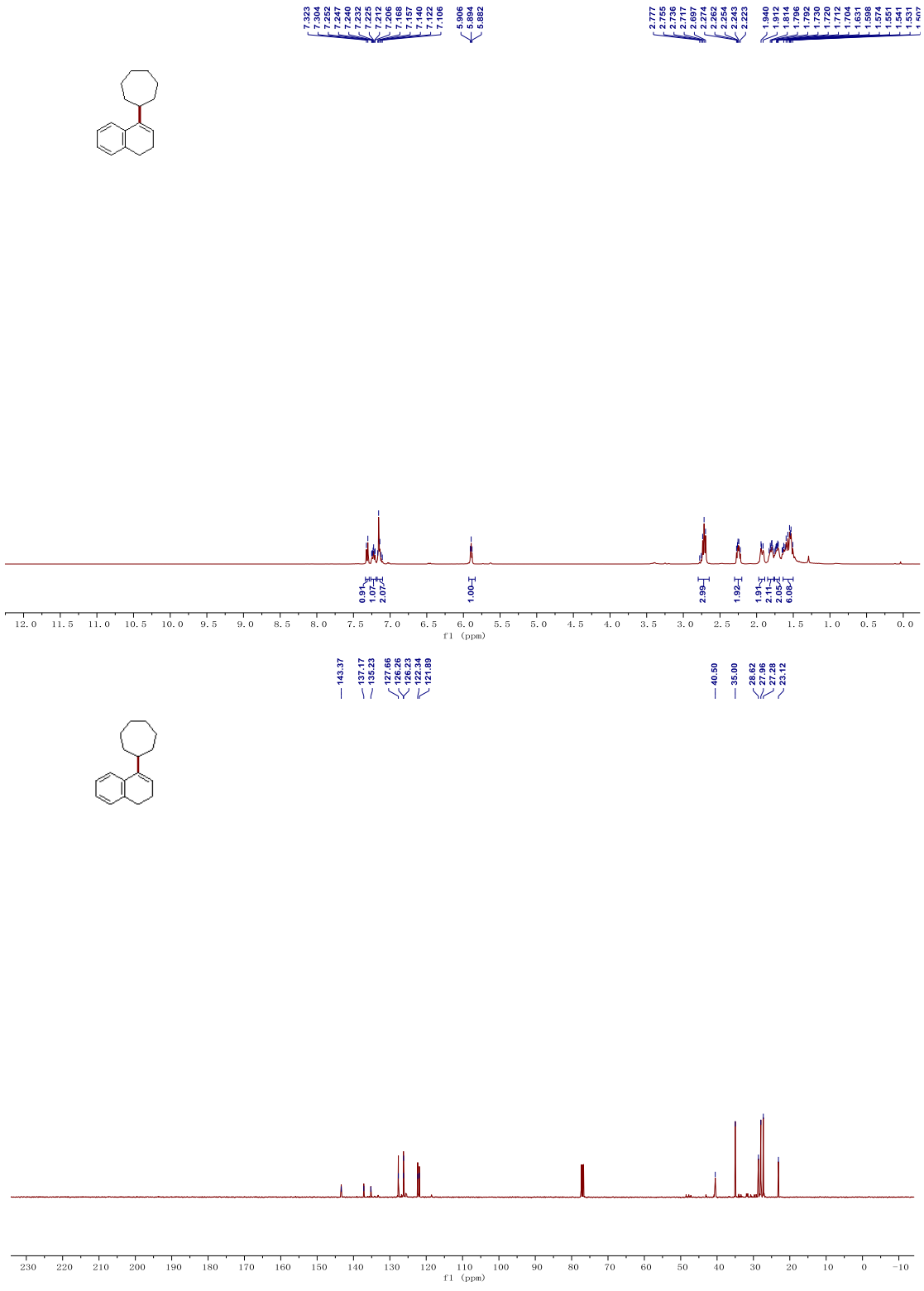
4-(Cyclopropylmethyl)-1,2-dihydronaphthalene (3c)



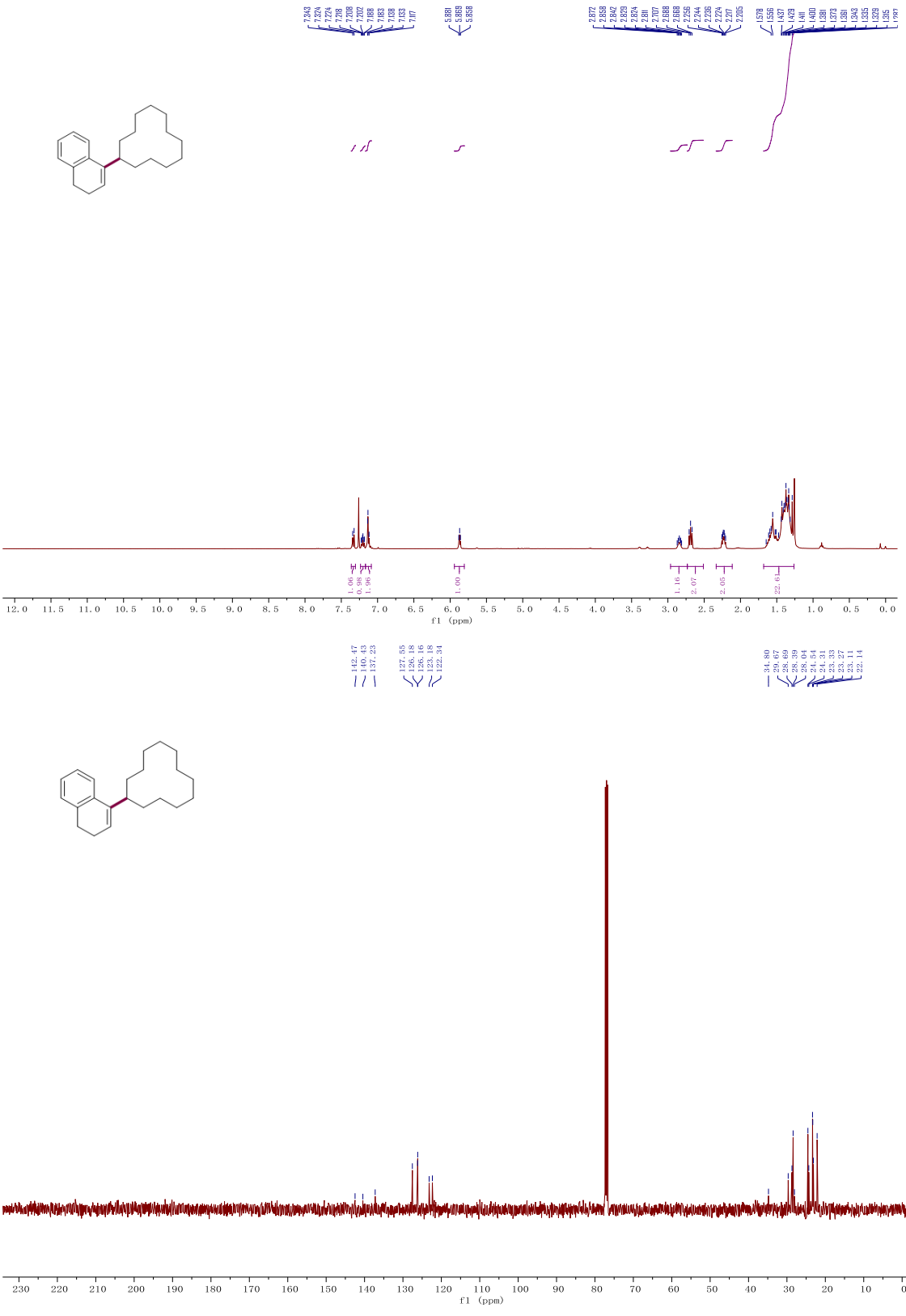
4-Cyclobutyl-1,2-dihydronaphthalene (3d)



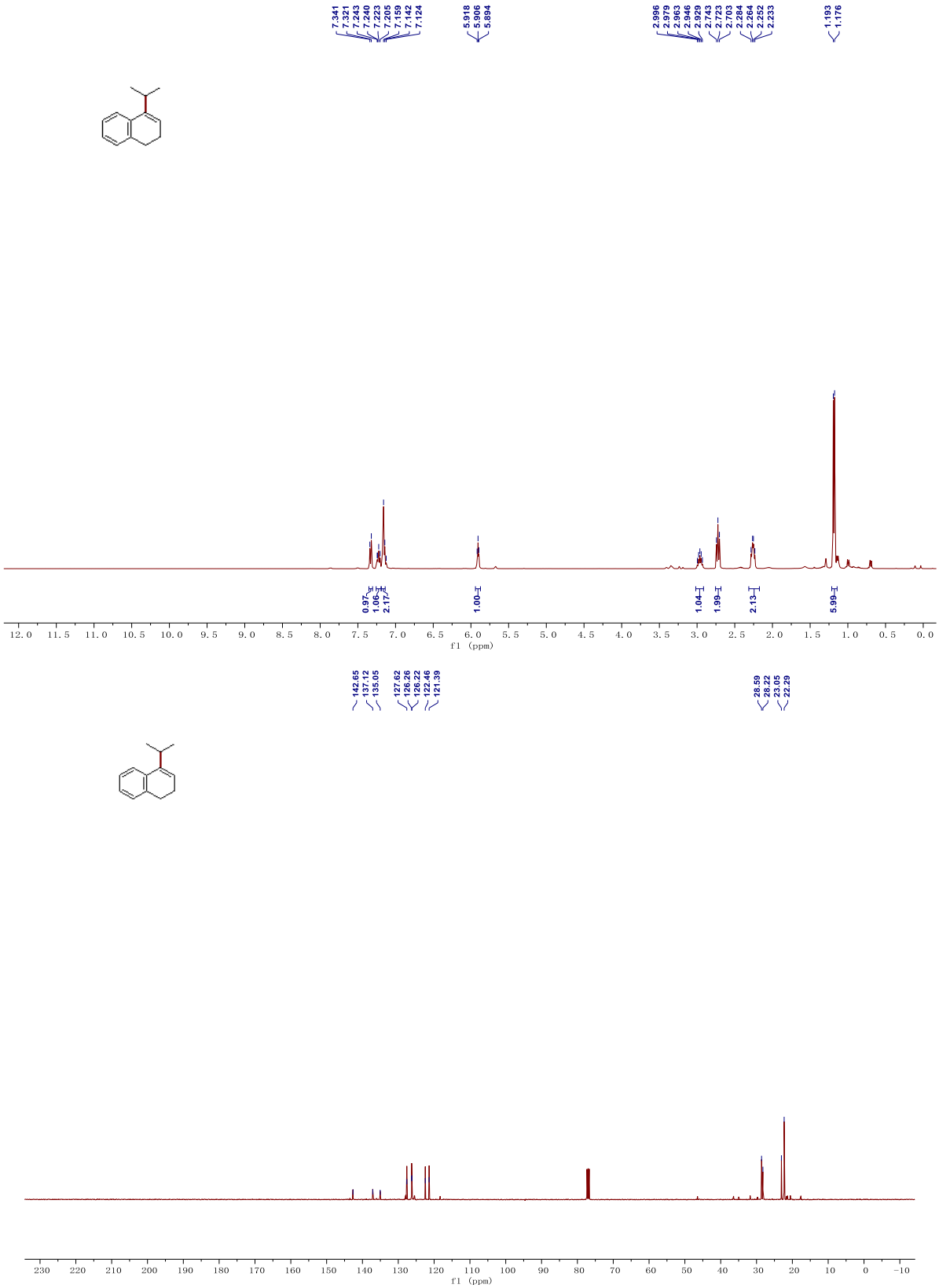
4-Cycloheptyl-1,2-dihydronaphthalene (3e)



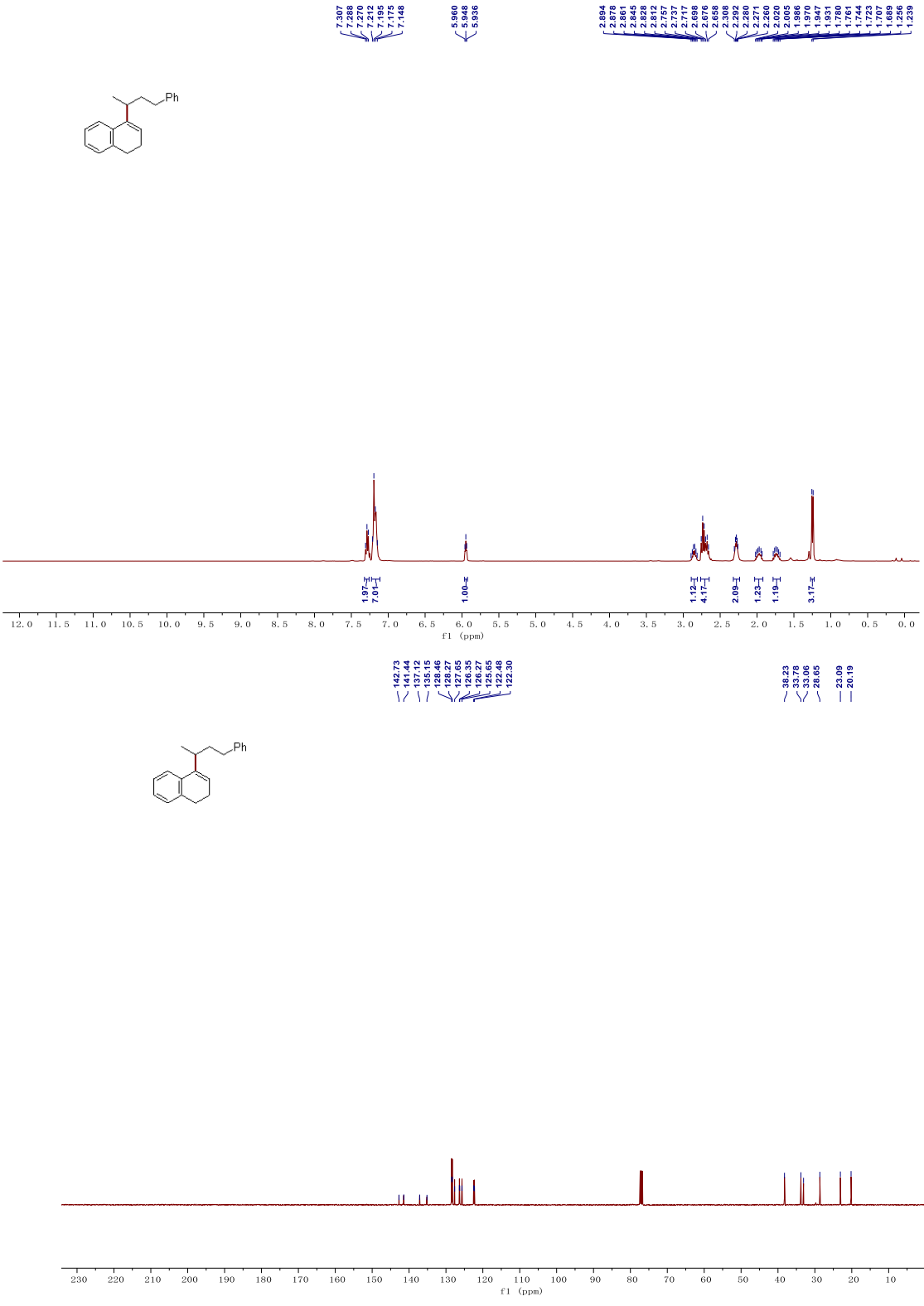
4-cyclododecyl-1,2-dihydronaphthalene (3f)



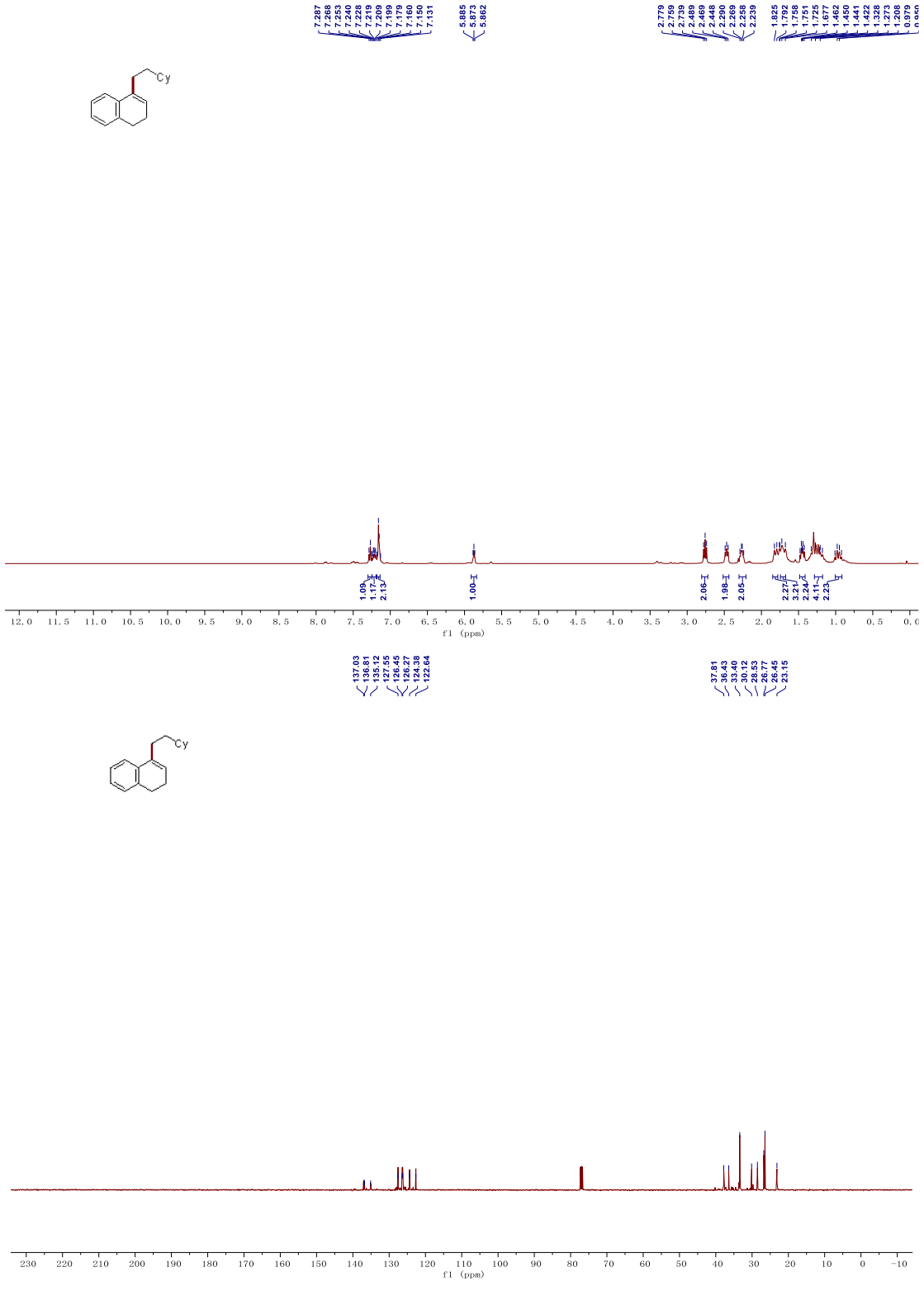
4-Isopropyl-1,2-dihydronaphthalene (3g)



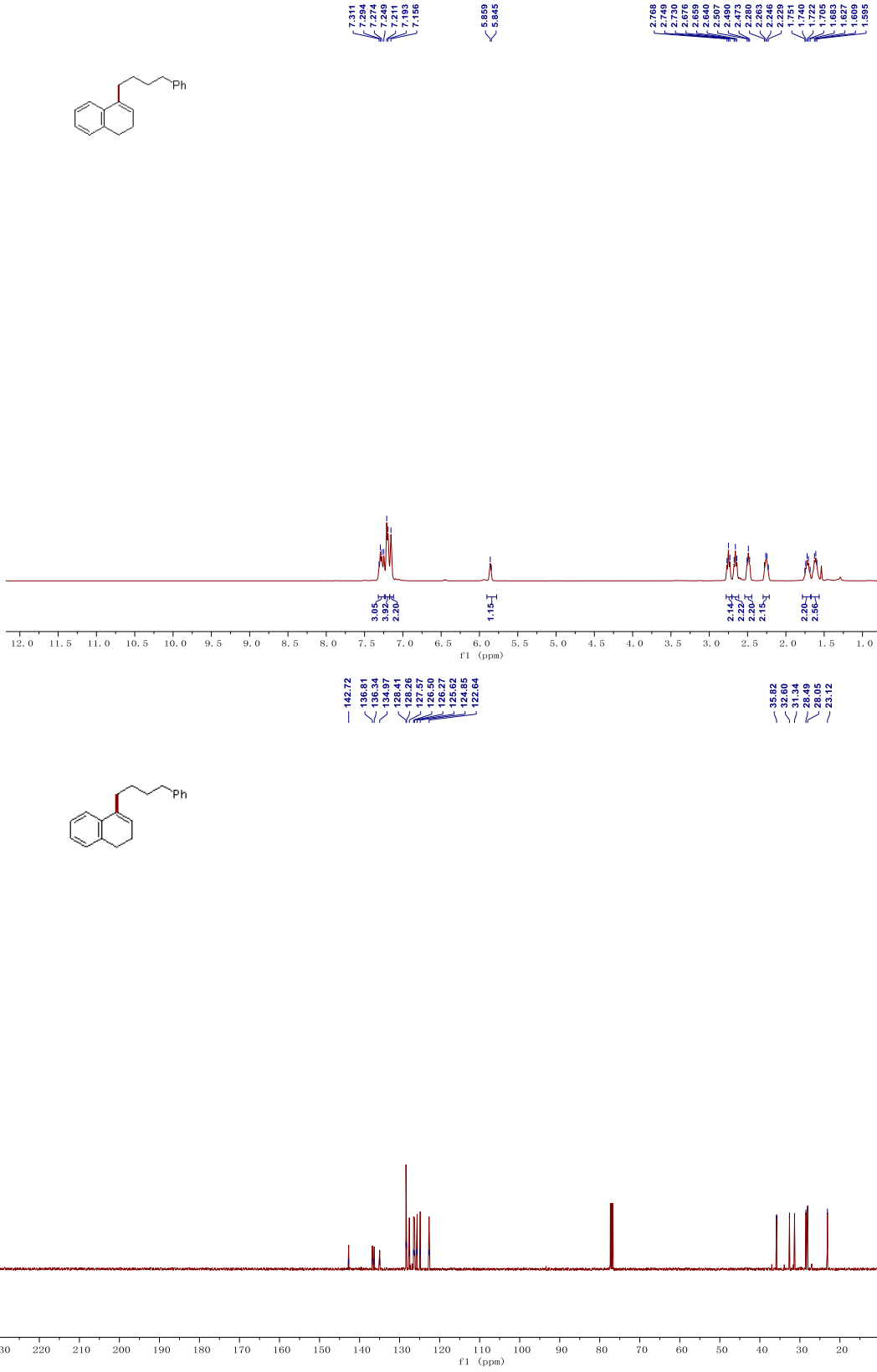
4-(4-Phenylbutan-2-yl)-1,2-dihydronaphthalene (3h)



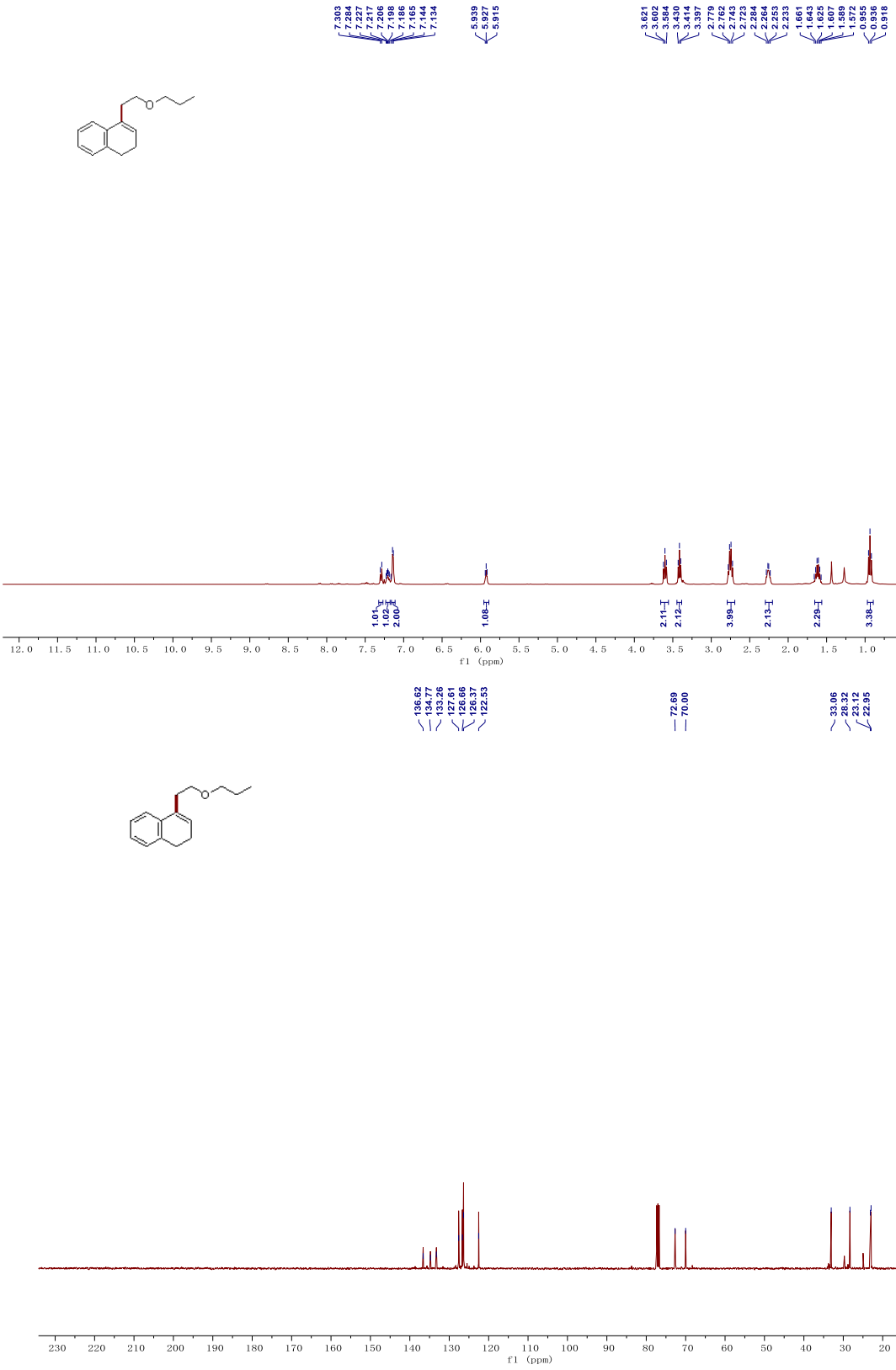
4-(2-Cyclohexylethyl)-1,2-dihydronaphthalene (3i)



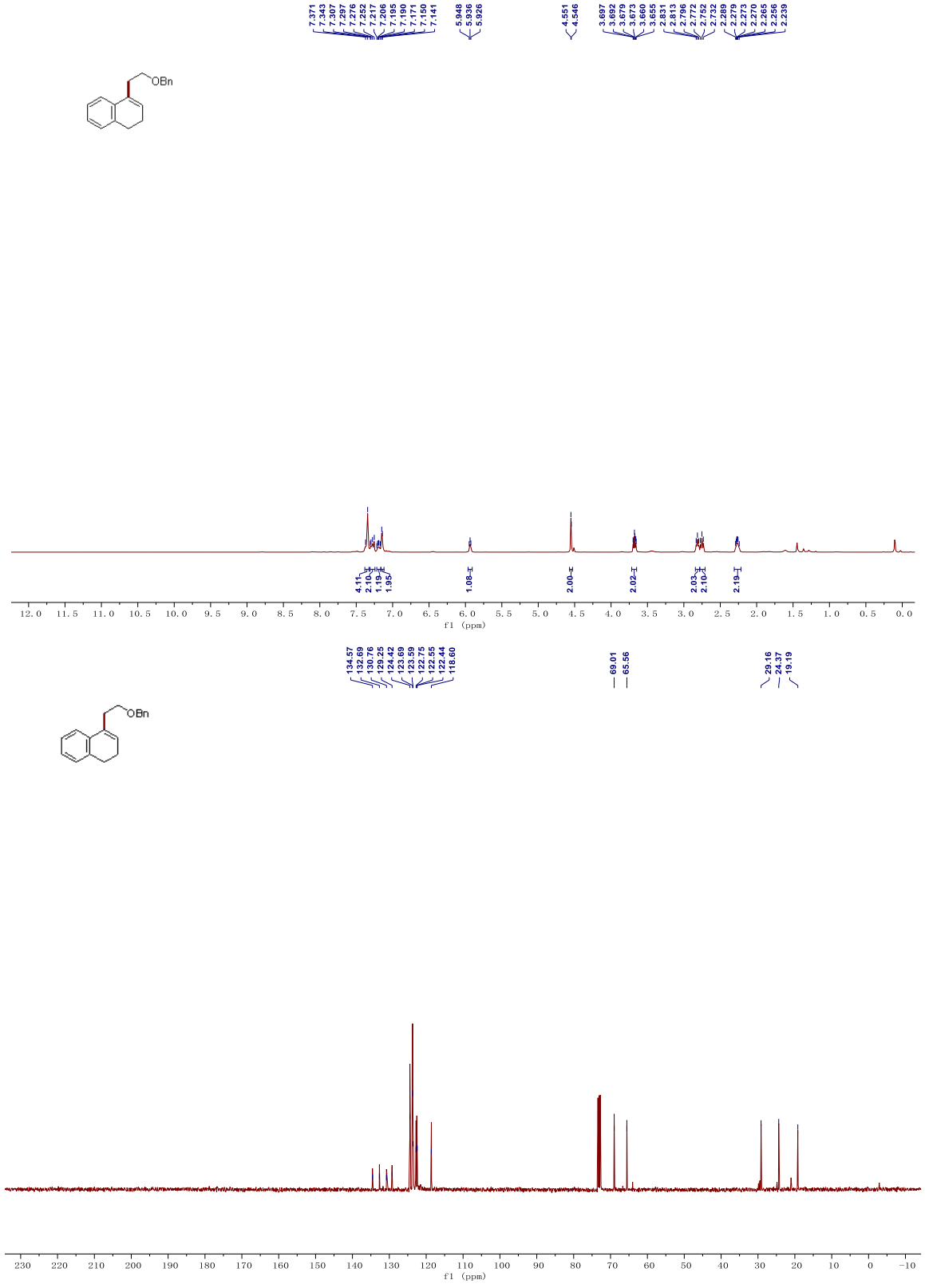
4-(4-Phenylbutyl)-1,2-dihydronaphthalene (3j)



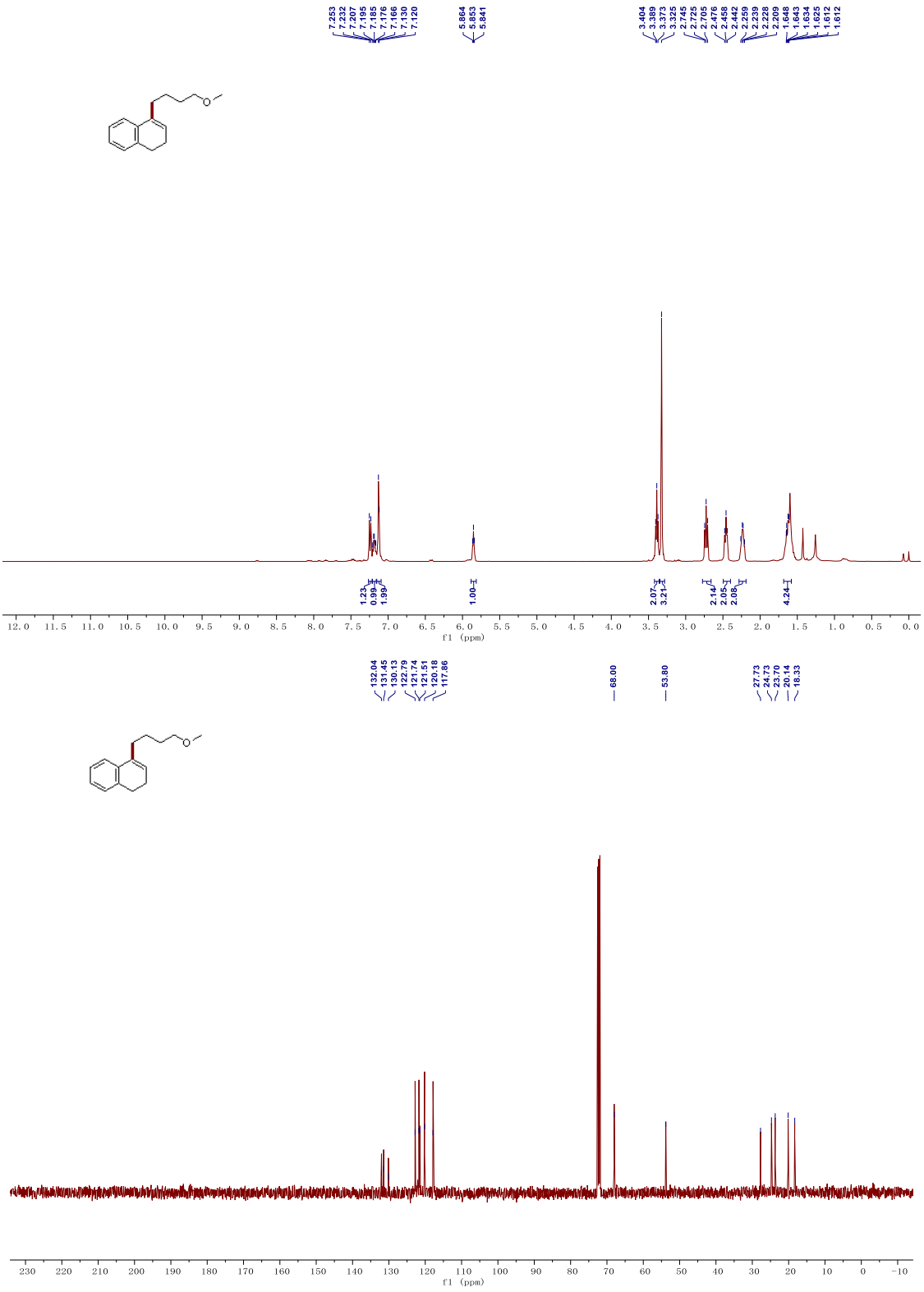
4-(2-Propoxyethyl)-1,2-dihydronaphthalene (3k)



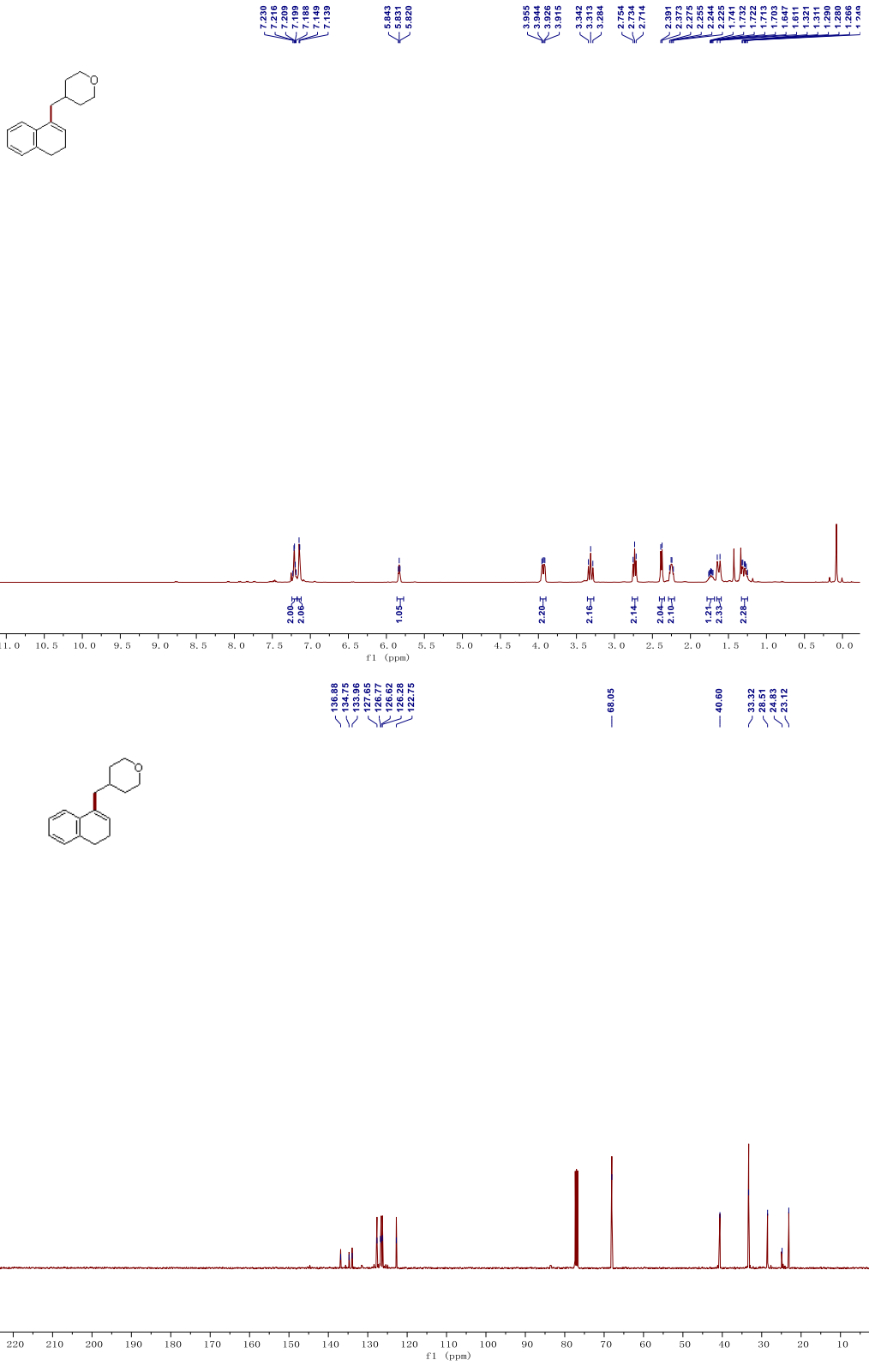
4-(2-(benzyloxy)ethyl)-1,2-dihydronaphthalene (3l)



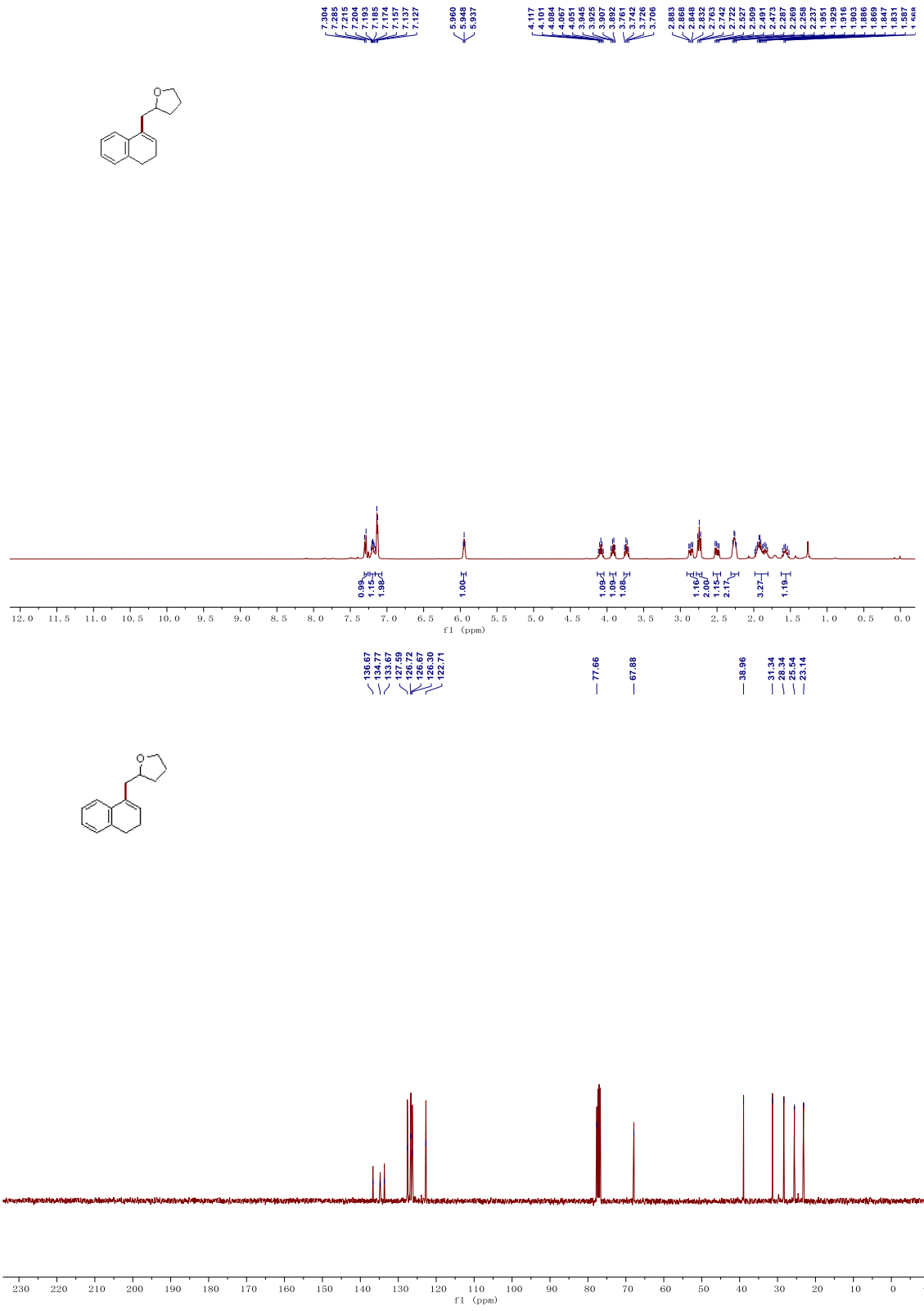
4-(4-Methoxybutyl)-1,2-dihydronaphthalene (3m)



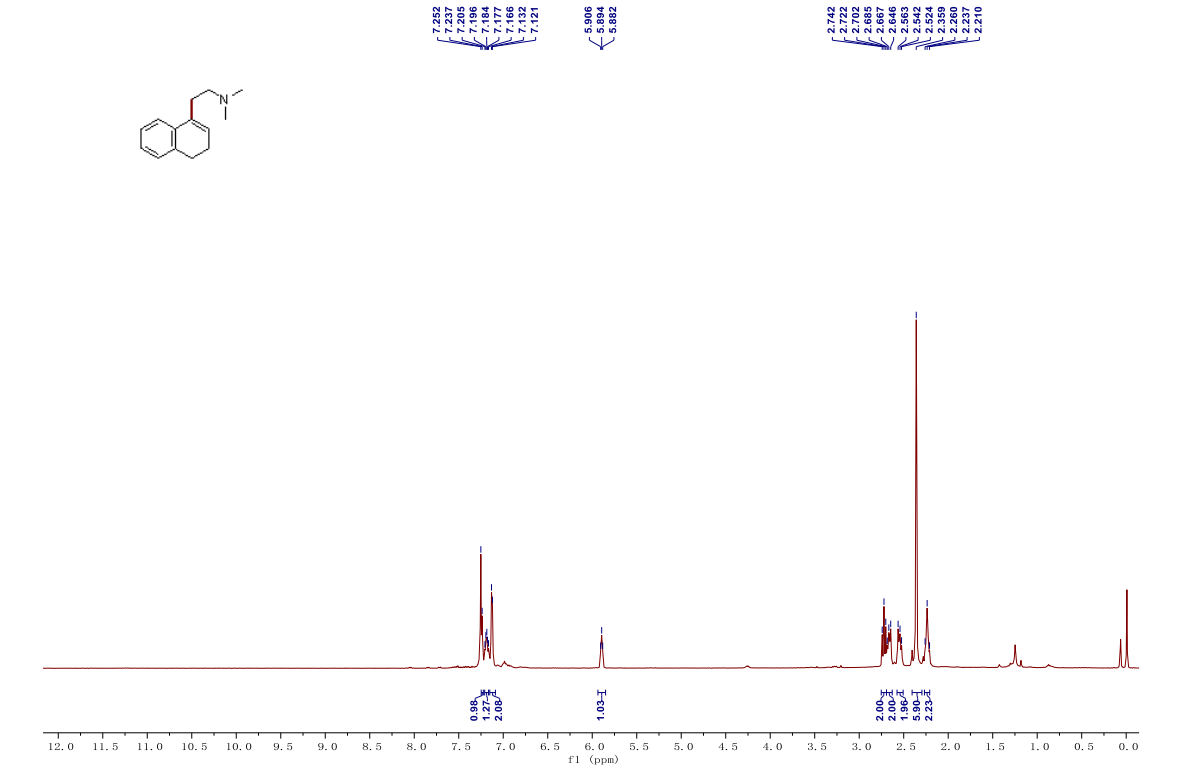
4-((3,4-Dihydronaphthalen-1-yl)methyl)tetrahydro-*2H*-pyran (3n)

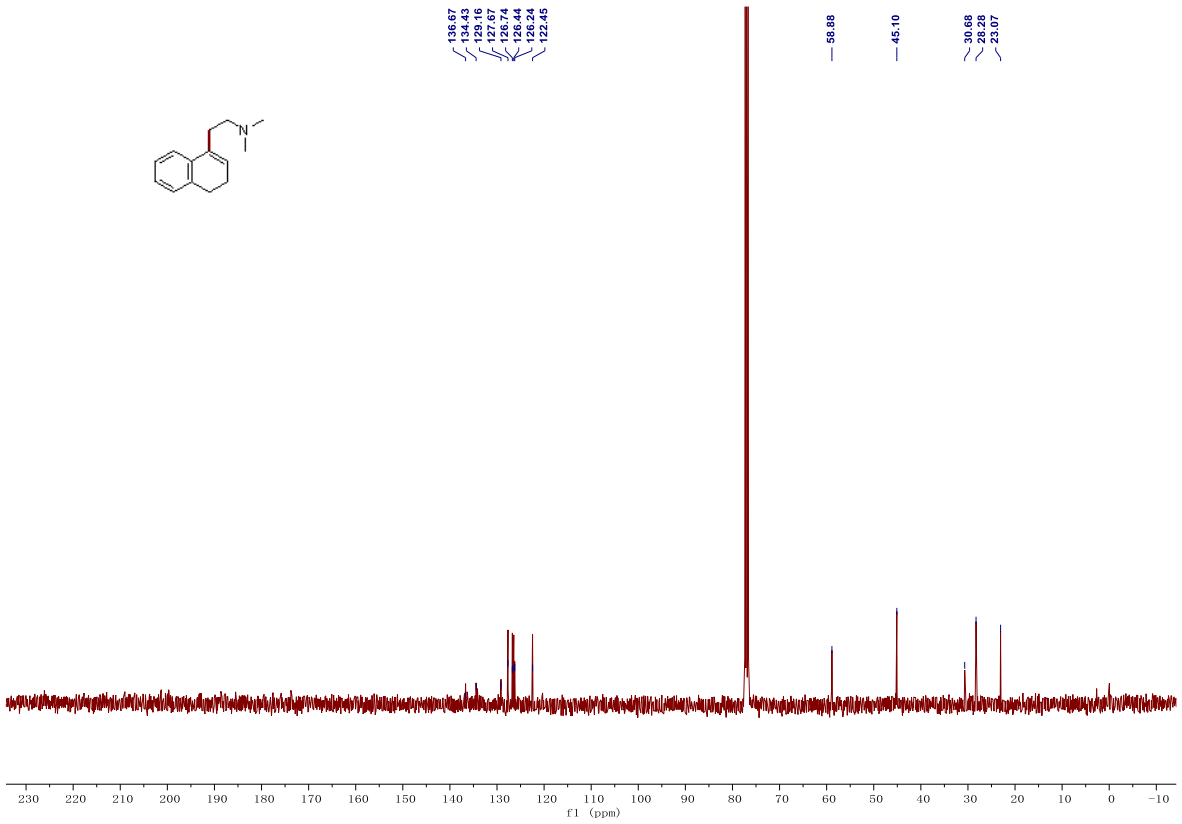


2-((3,4-Dihydronaphthalen-1-yl)methyl)tetrahydrofuran (3o)

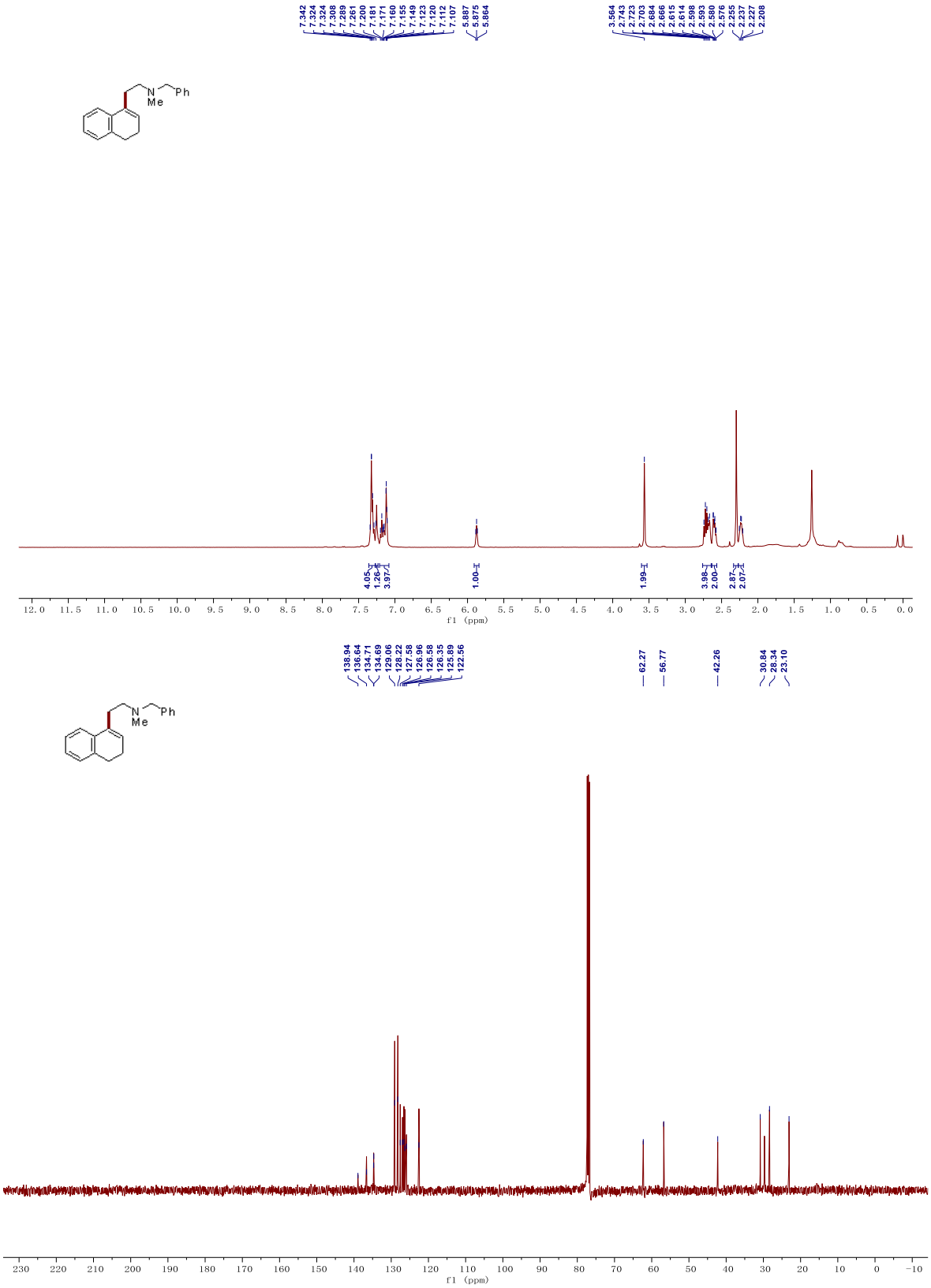


2-(3,4-Dihydronaphthalen-1-yl)-*N*,*N*-dimethylethan-1-amine (3p)

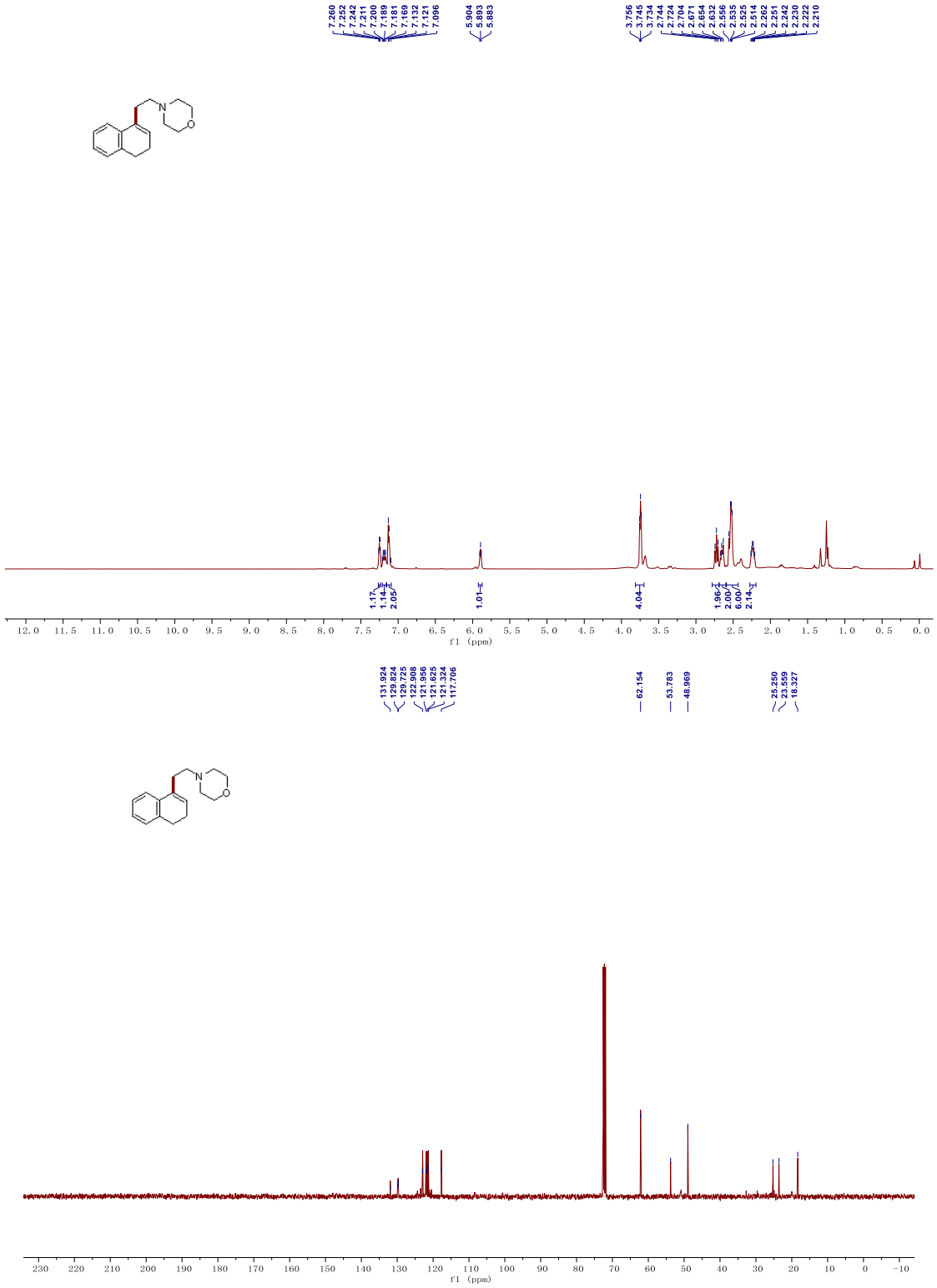




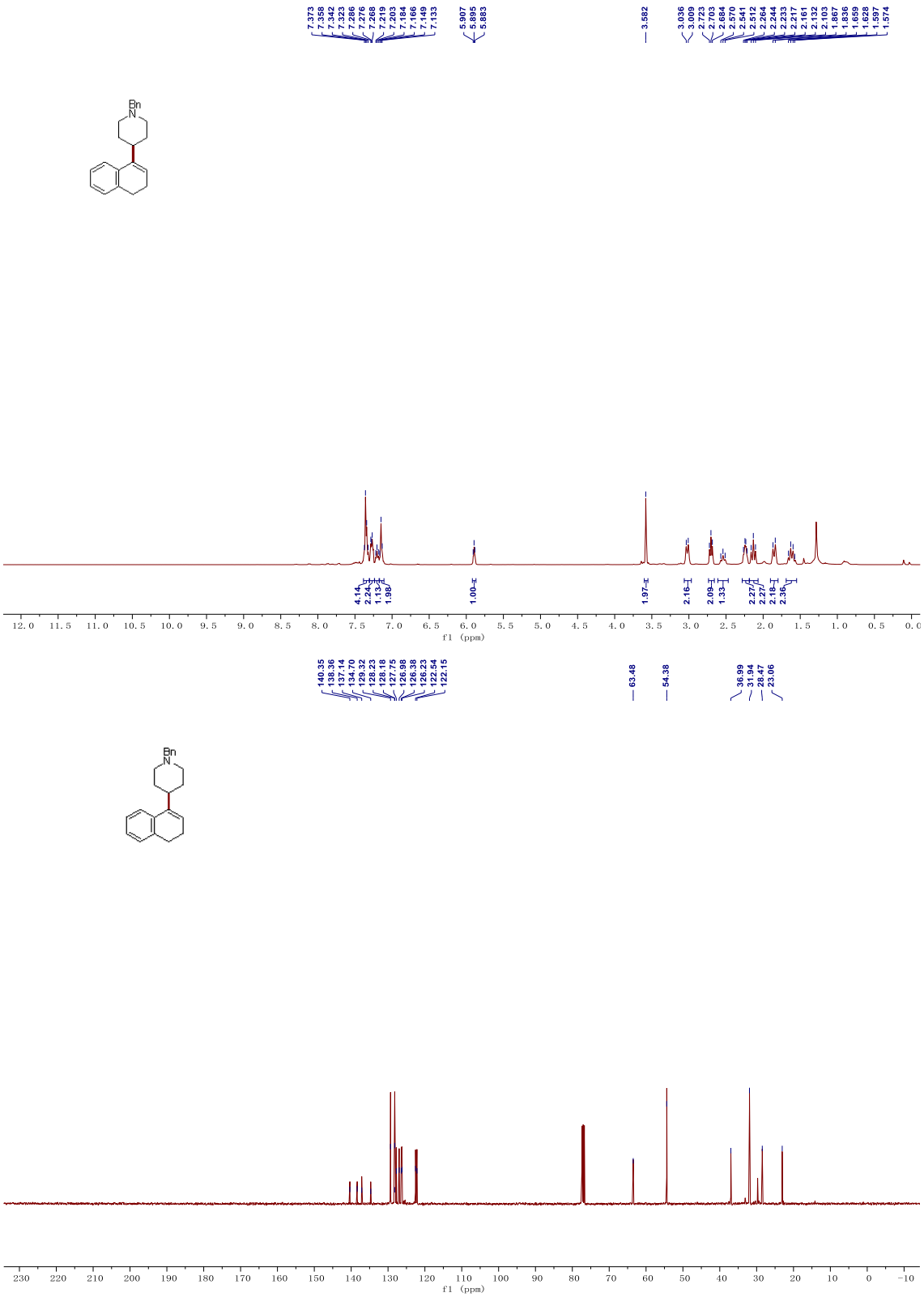
_N_-Benzyl-2-(3,4-dihydronaphthalen-1-yl)-N-methylethan-1-amine (3q)



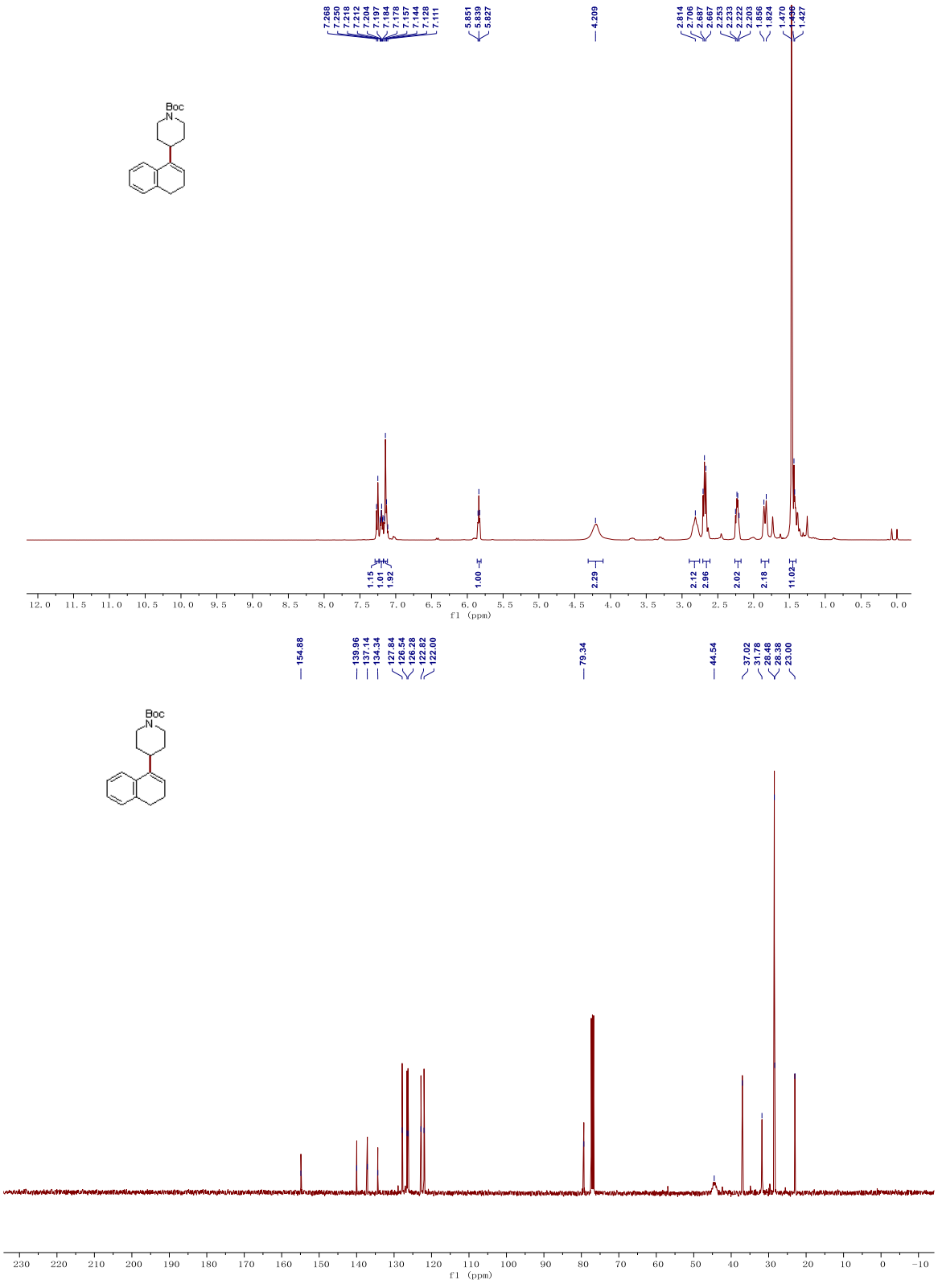
4-(2-(3,4-Dihydronaphthalen-1-yl)ethyl)morpholine (3r)



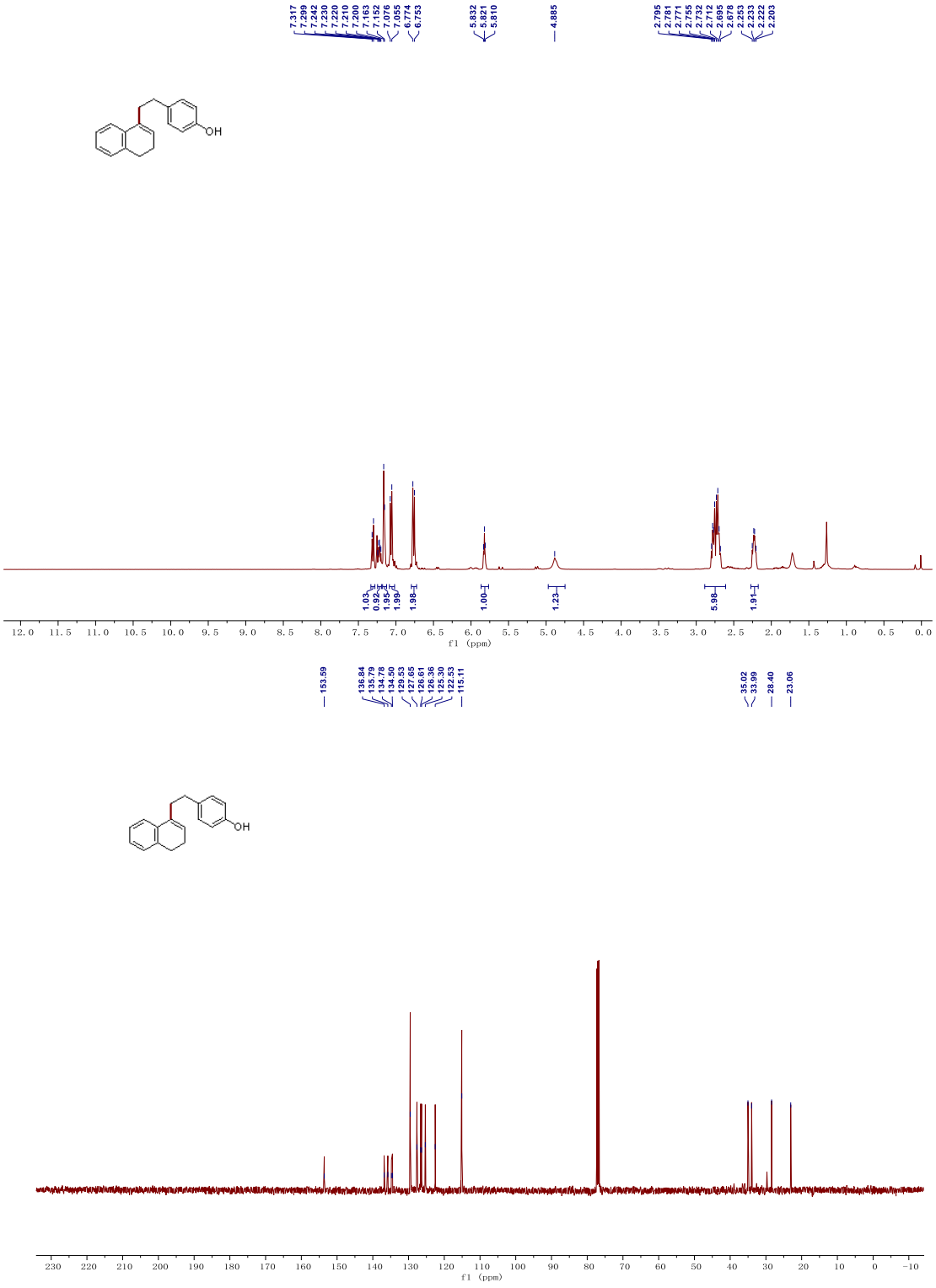
1-Benzyl-4-(3,4-dihydronaphthalen-1-yl)piperidine (3s)



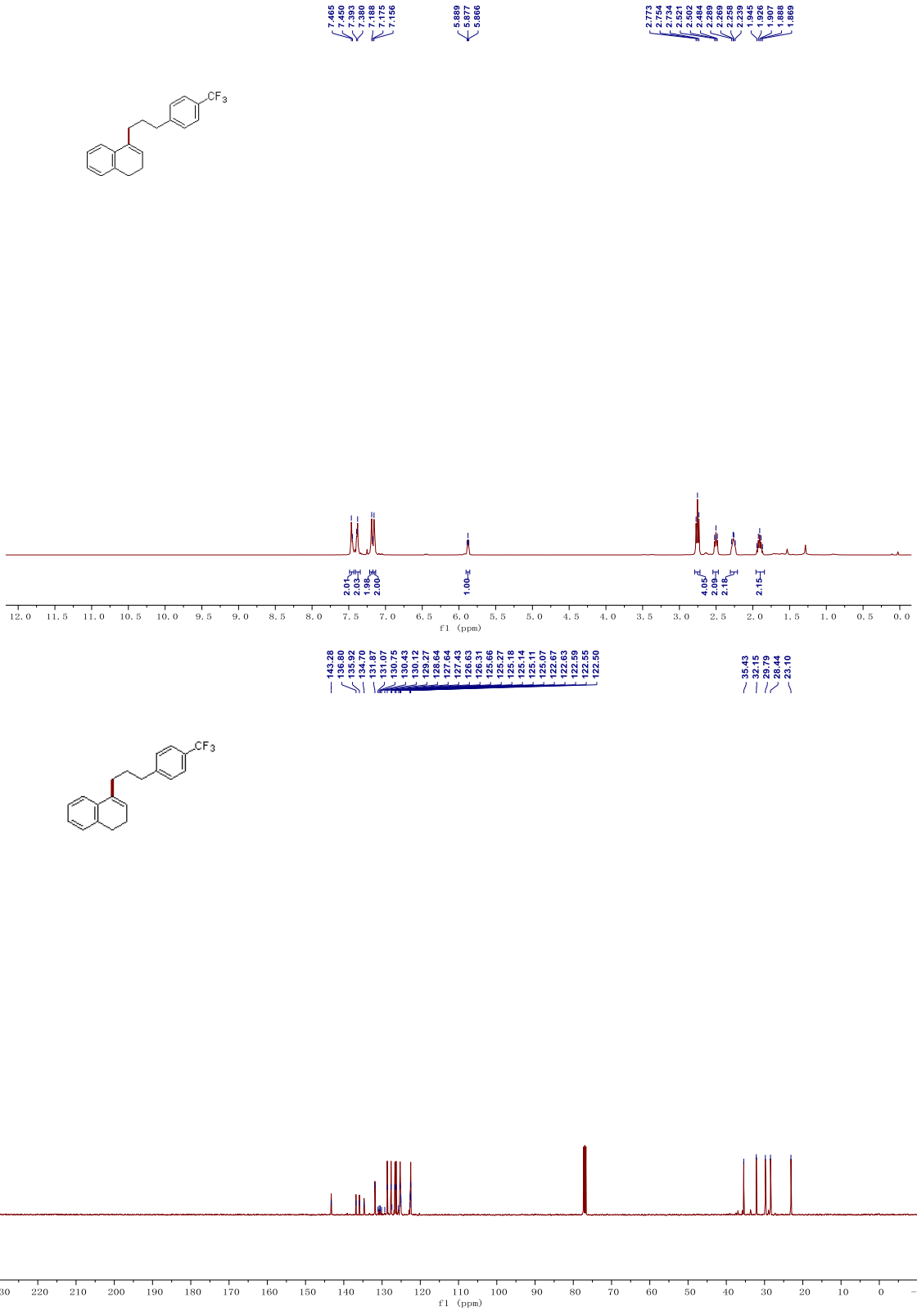
***tert*-Butyl 4-(3,4-dihydronaphthalen-1-yl)piperidine-1-carboxylate (3t)**



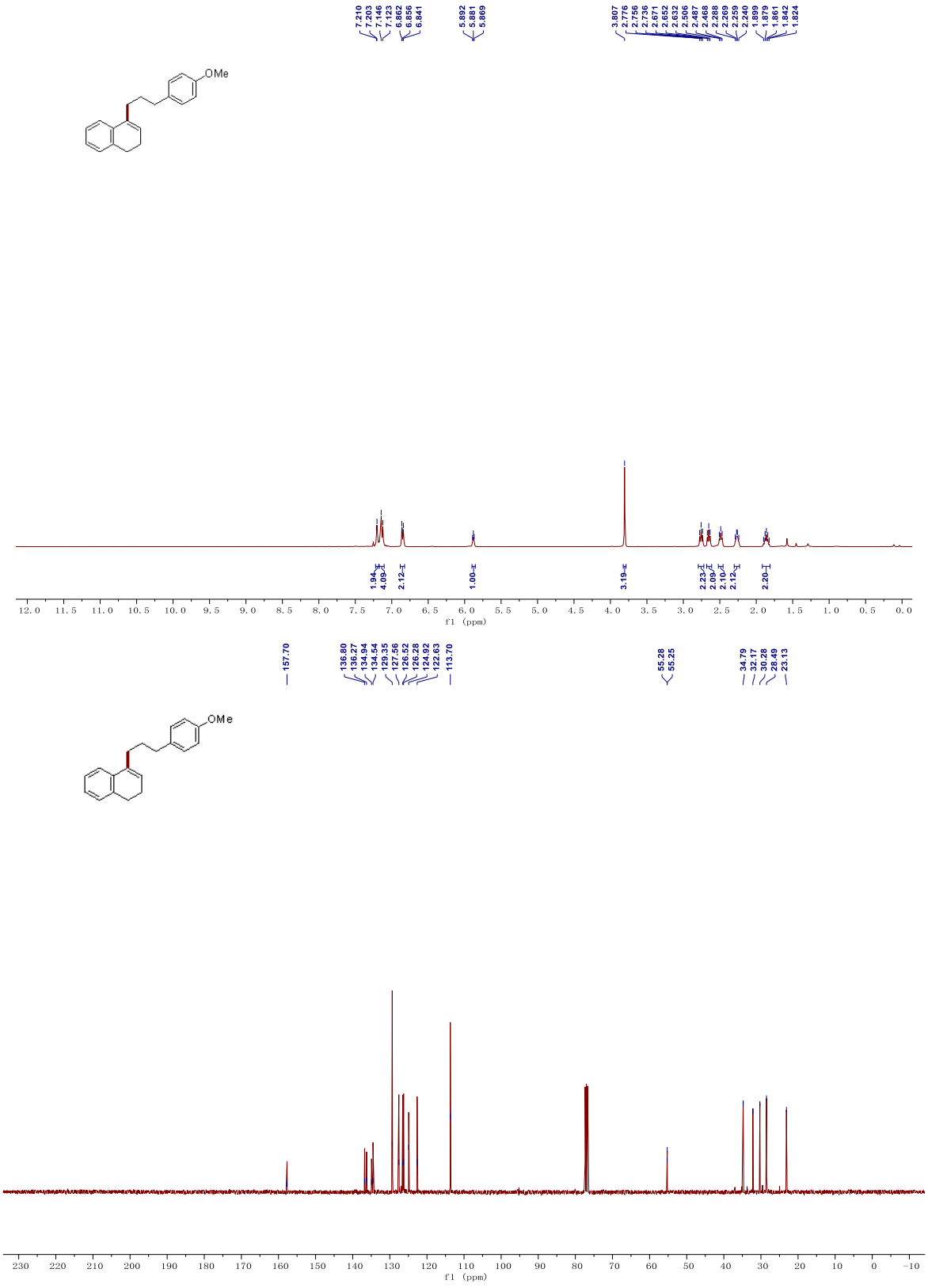
4-(2-(3,4-Dihydronaphthalen-1-yl)ethyl)phenol (3u)



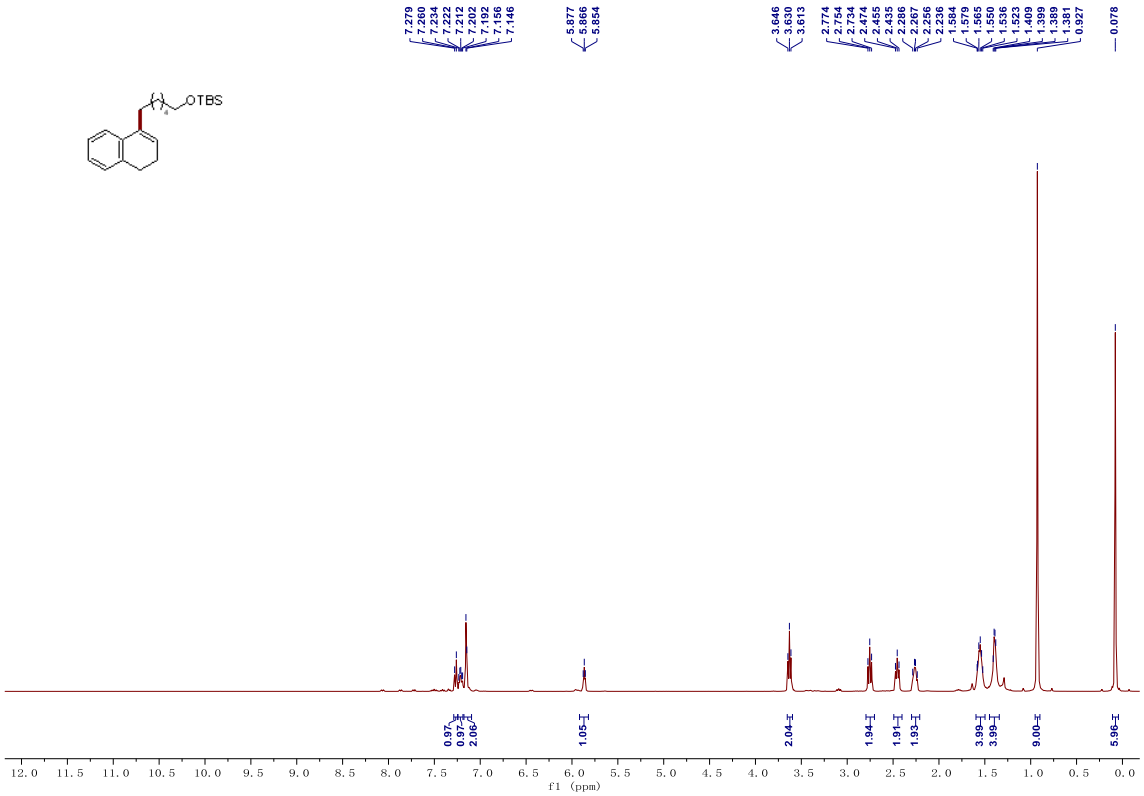
4-(3-(4-(Trifluoromethyl)phenyl)propyl)-1,2-dihydronaphthalene (3v)

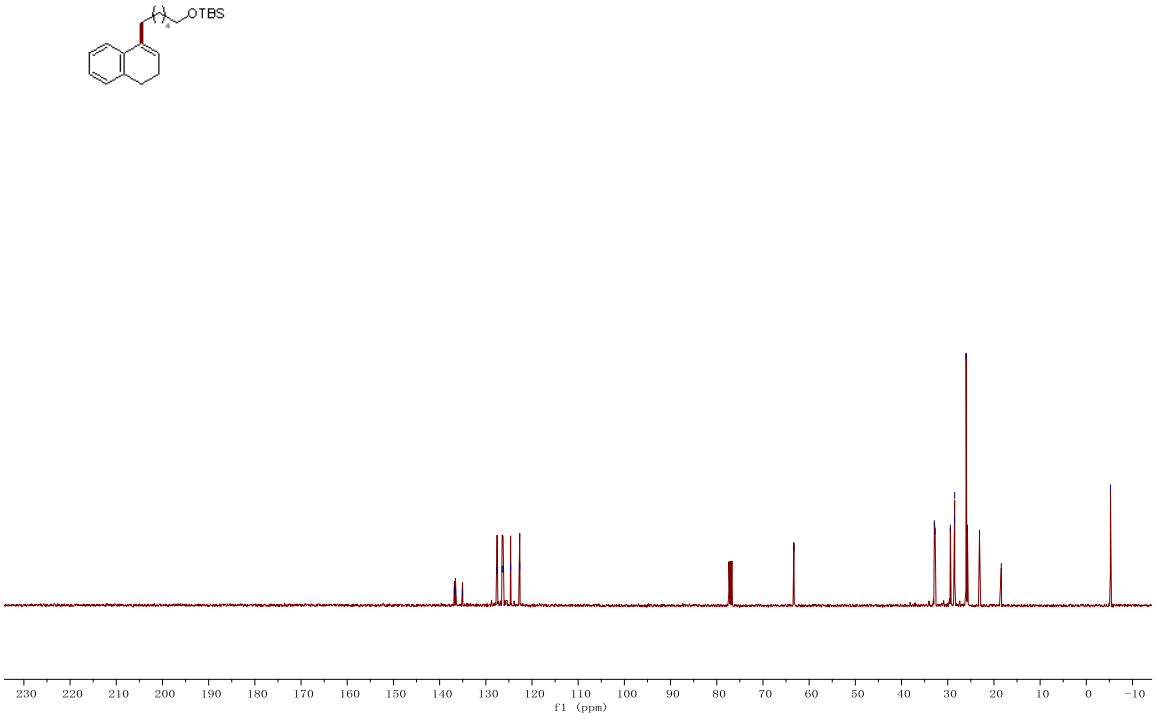


4-(3-(4-Methoxyphenyl)propyl)-1,2-dihydronaphthalene (3w)

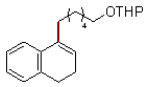


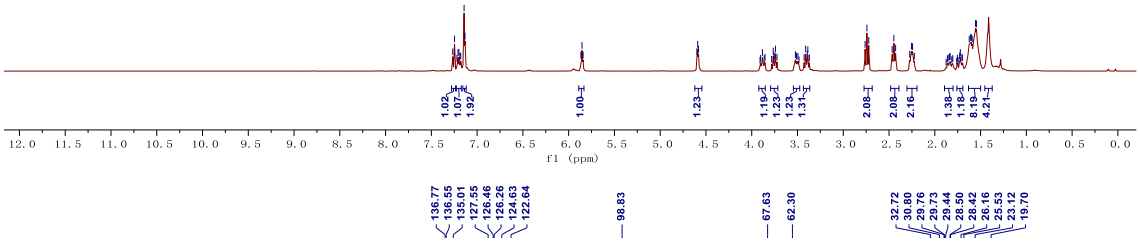
tert-Butyl((6-(3,4-dihydronaphthalen-1-yl)hexyl)oxy)dimethylsilane (3x)

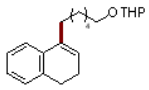


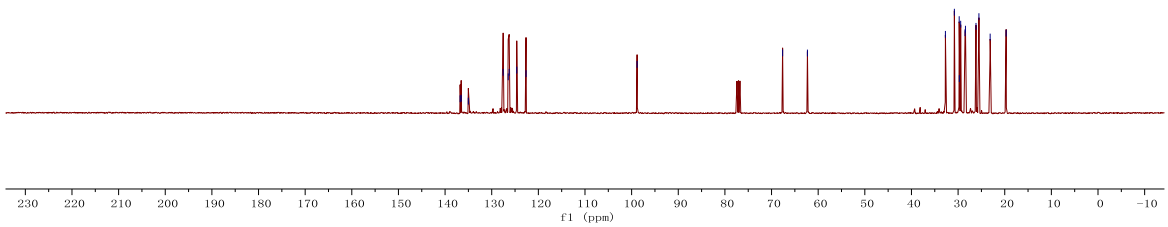


2-((6-(3,4-Dihydronaphthalen-1-yl)hexyl)oxy)tetrahydro-*2H*-pyran (3y)

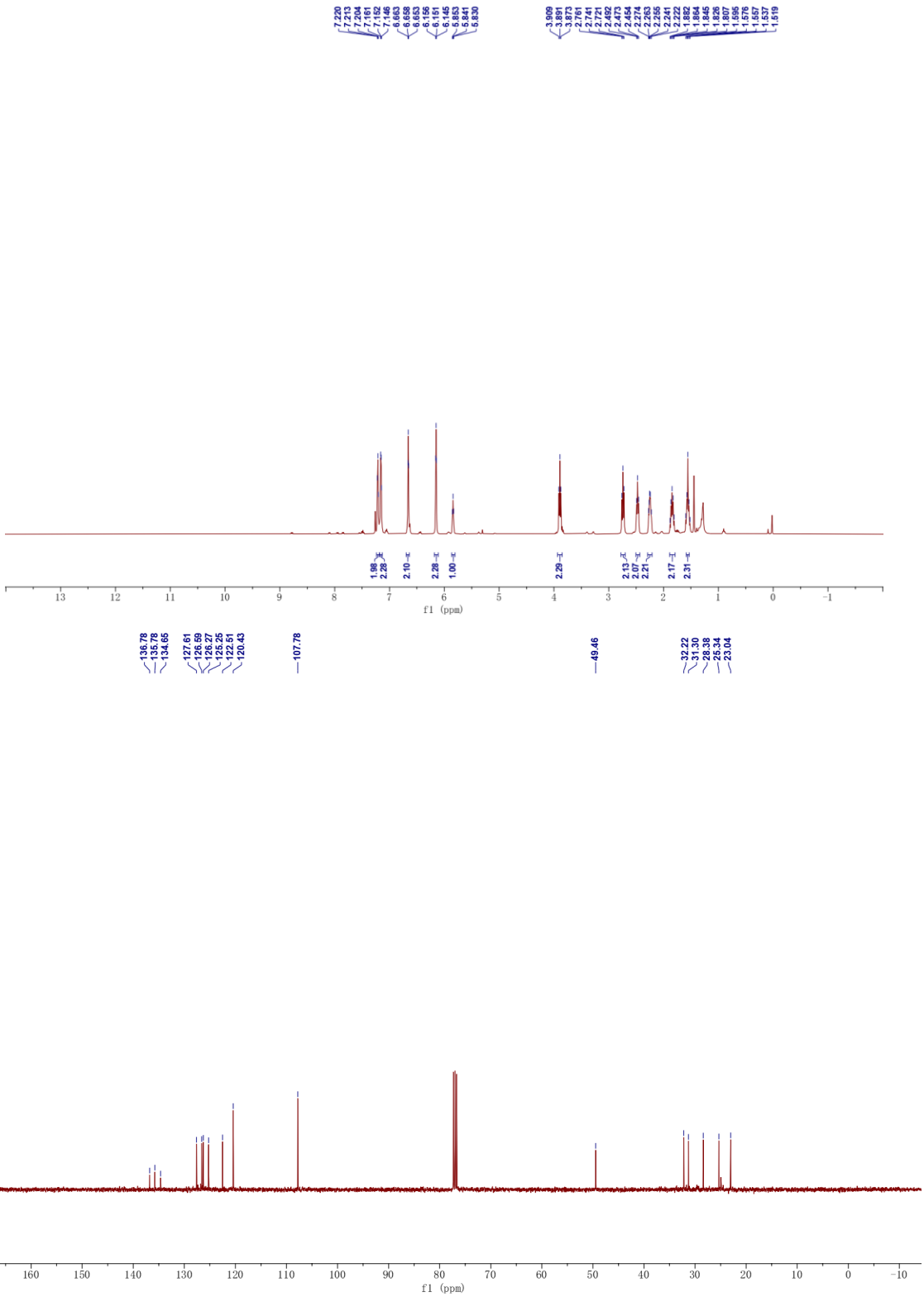




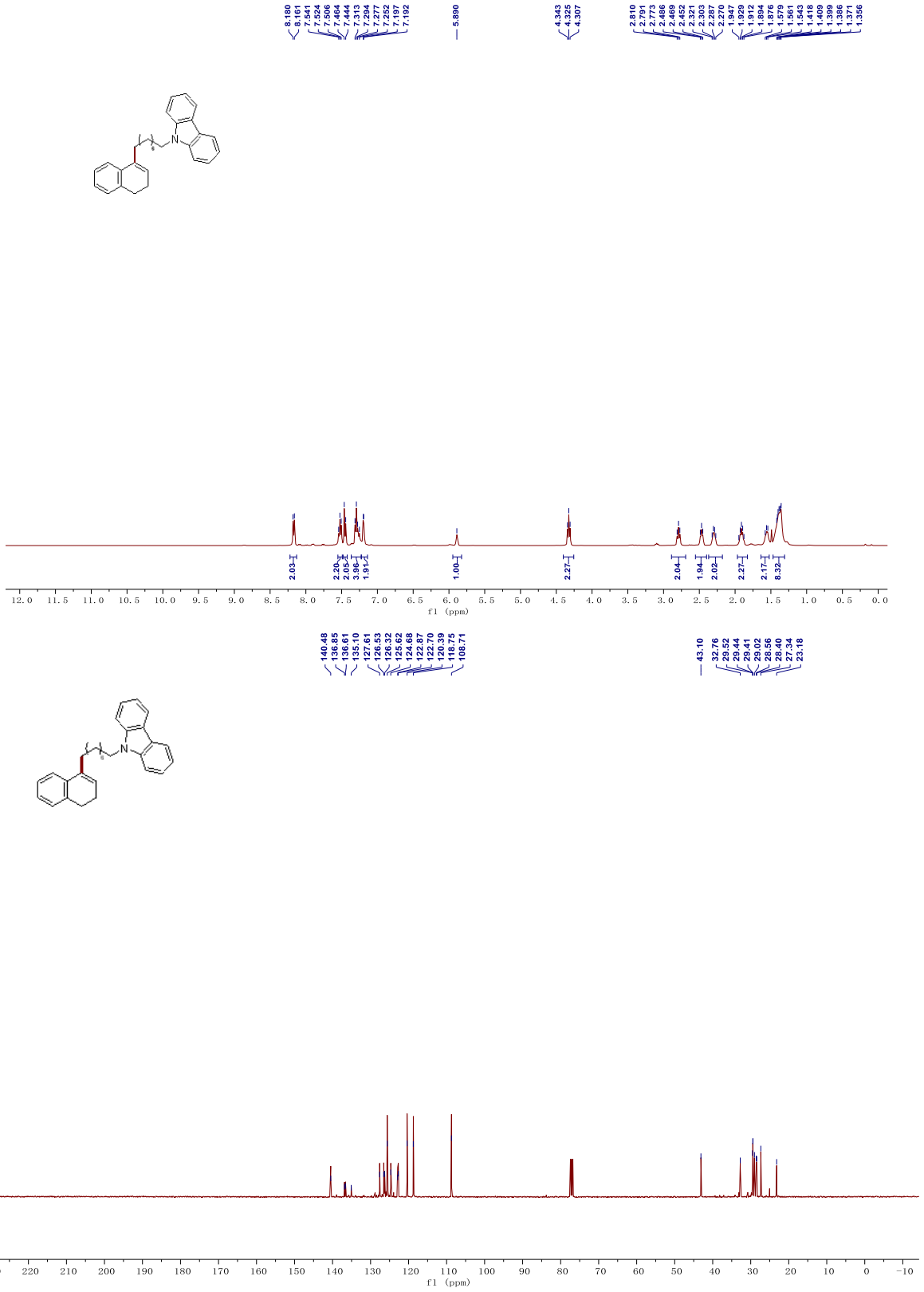




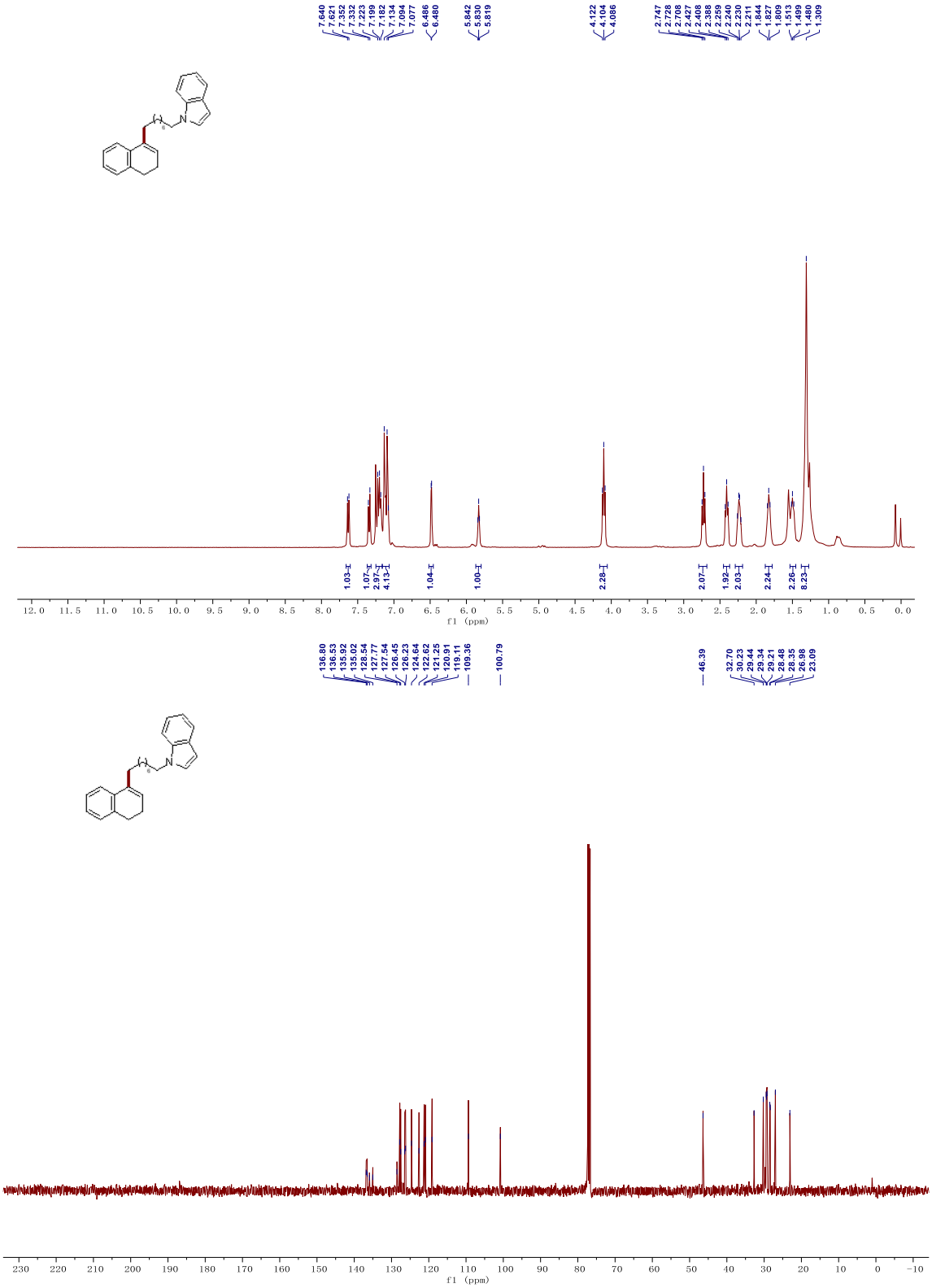
1-(4-(3,4-Dihydronaphthalen-1-yl)butyl)-*1H*-pyrrole (3z)



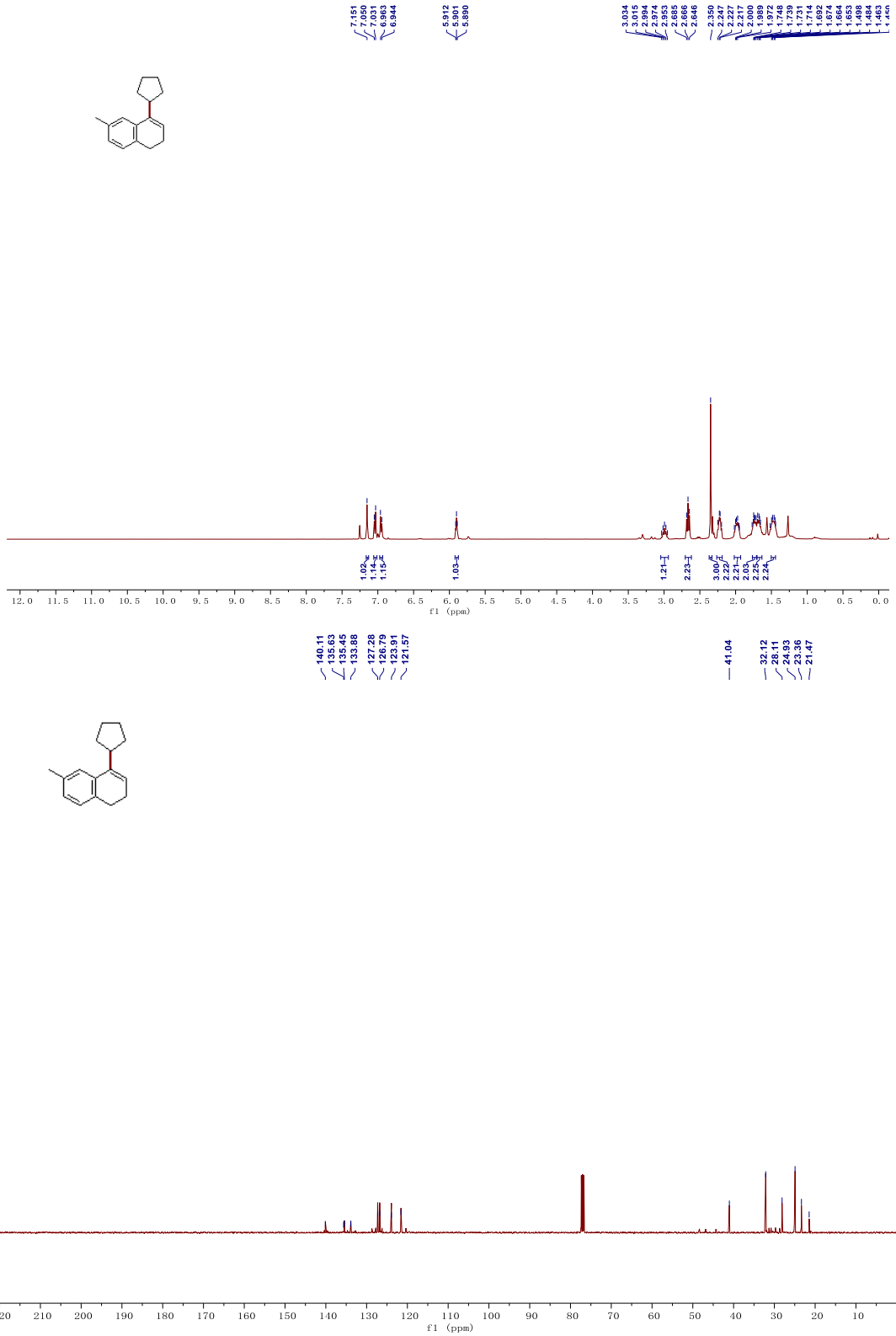
9-(8-(3,4-Dihydronaphthalen-1-yl)octyl)-*9H*-carbazole (3aa)



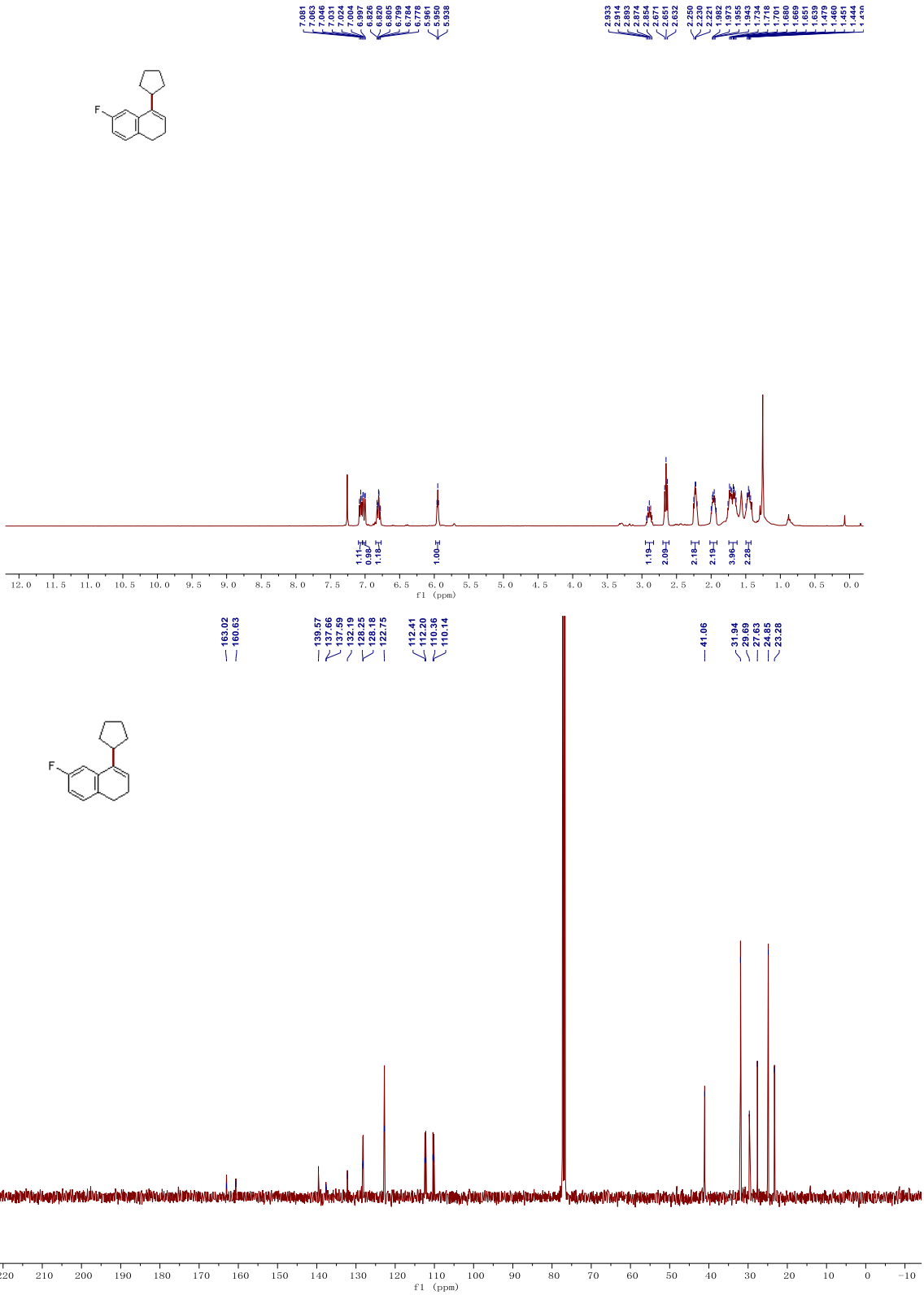
1-(8-(3,4-Dihydronaphthalen-1-yl)octyl)-*1H*-indole (3ab)



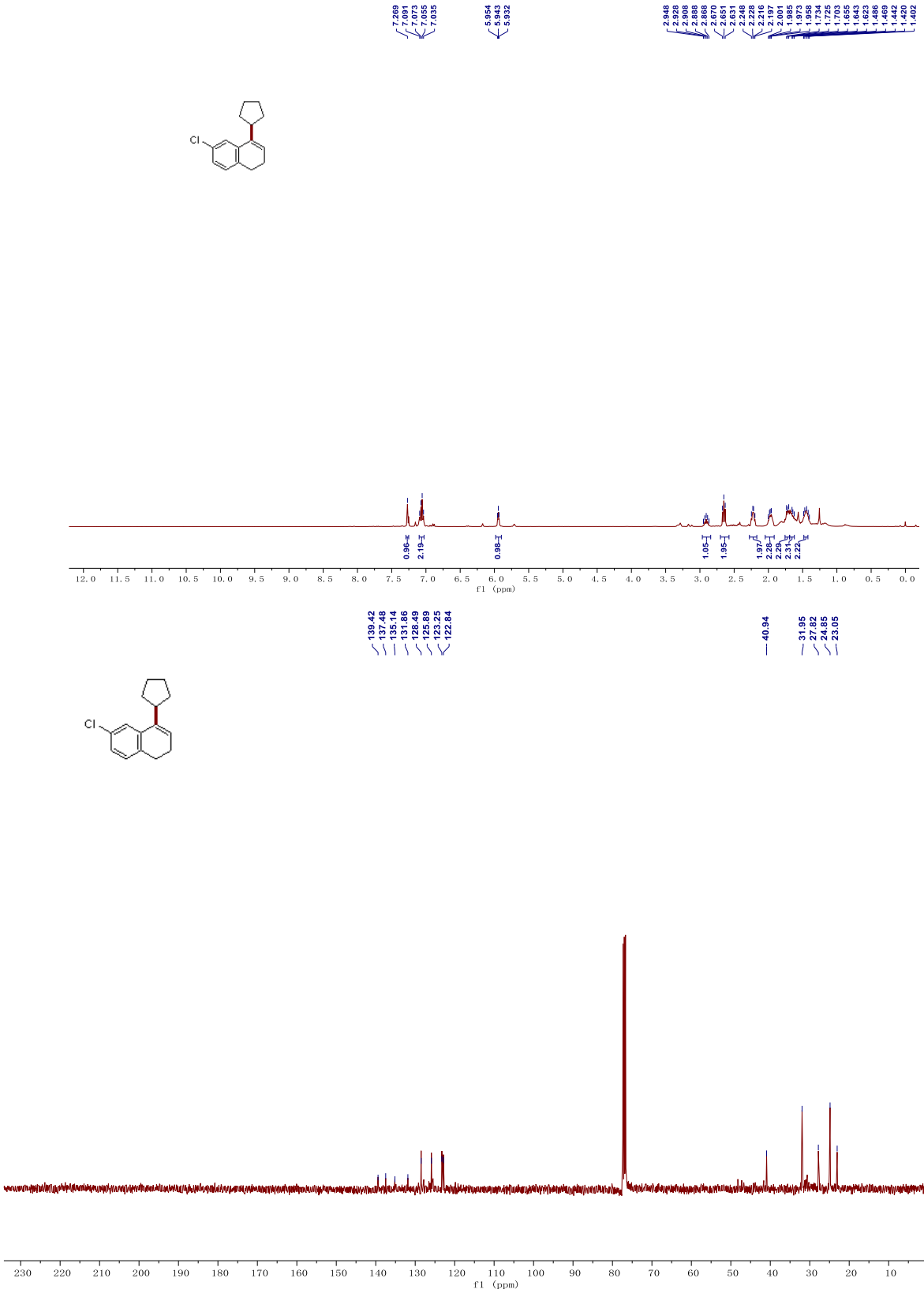
4-Cyclopentyl-6-methyl-1,2-dihydronaphthalene (3ac)



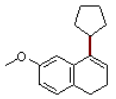
4-Cyclopentyl-6-fluoro-1,2-dihydronaphthalene (3ad)

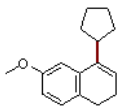


6-Chloro-4-cyclopentyl-1,2-dihydronaphthalene (3ae)

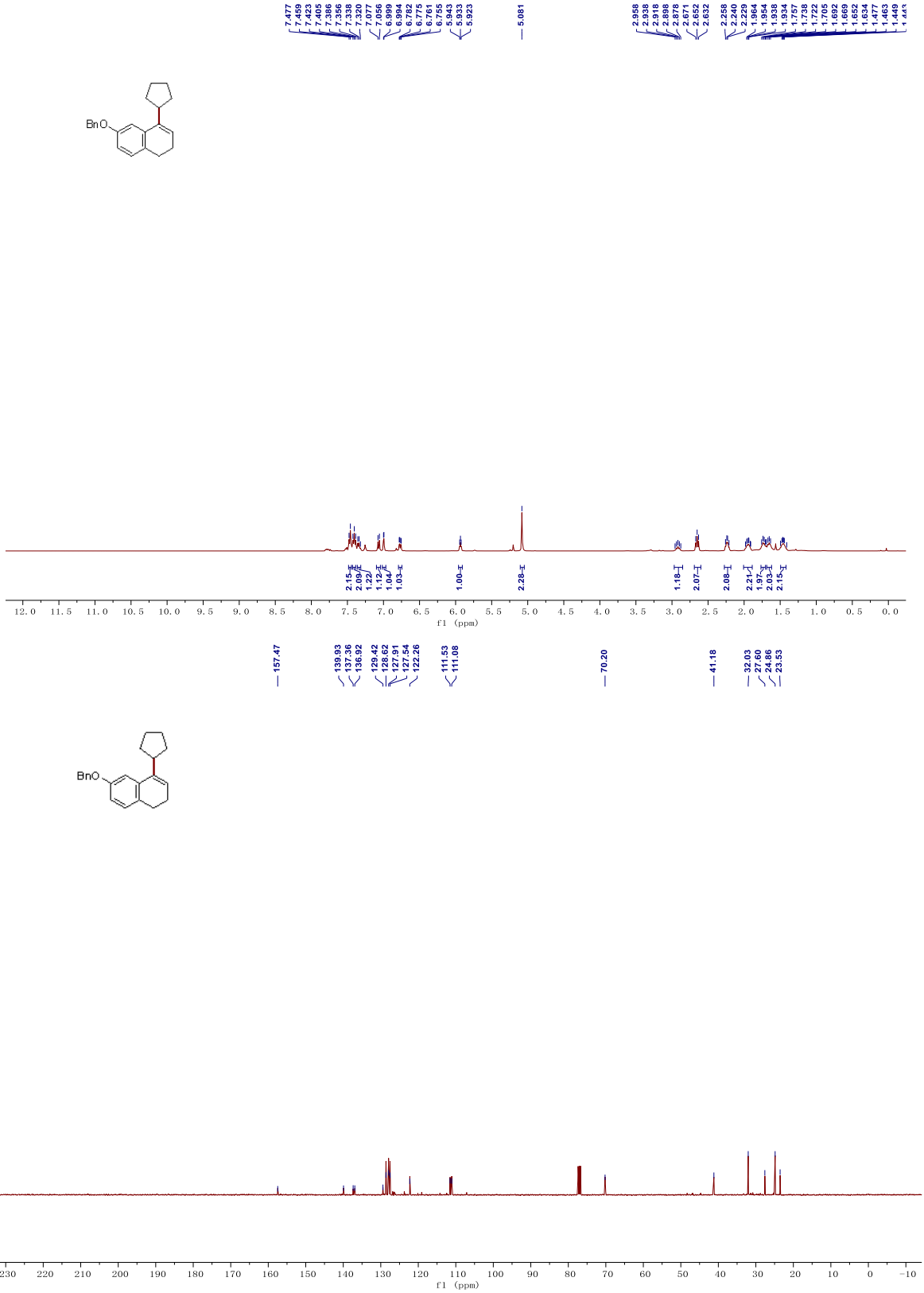


4-Cyclopentyl-6-methoxy-1,2-dihydronaphthalene (3af)

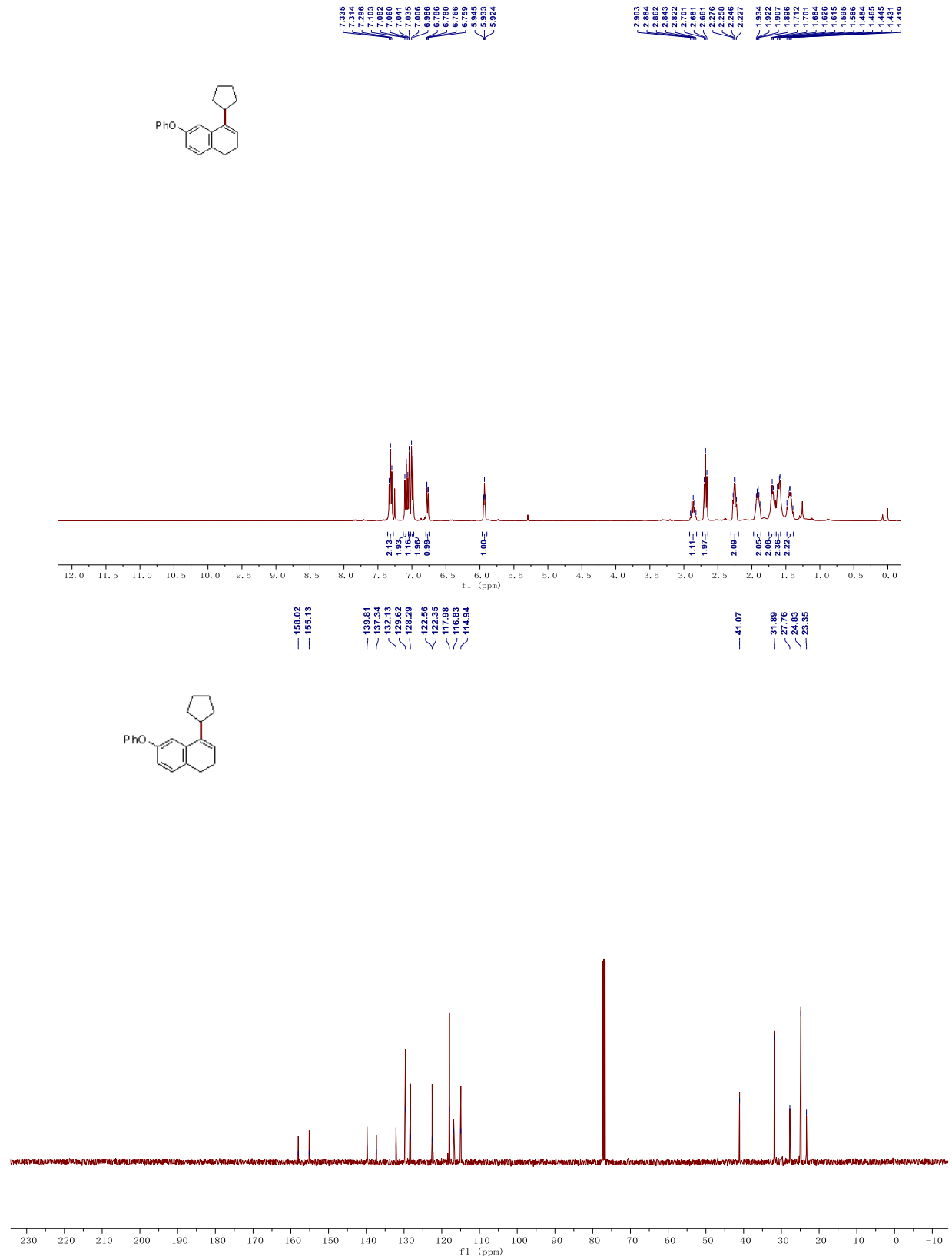




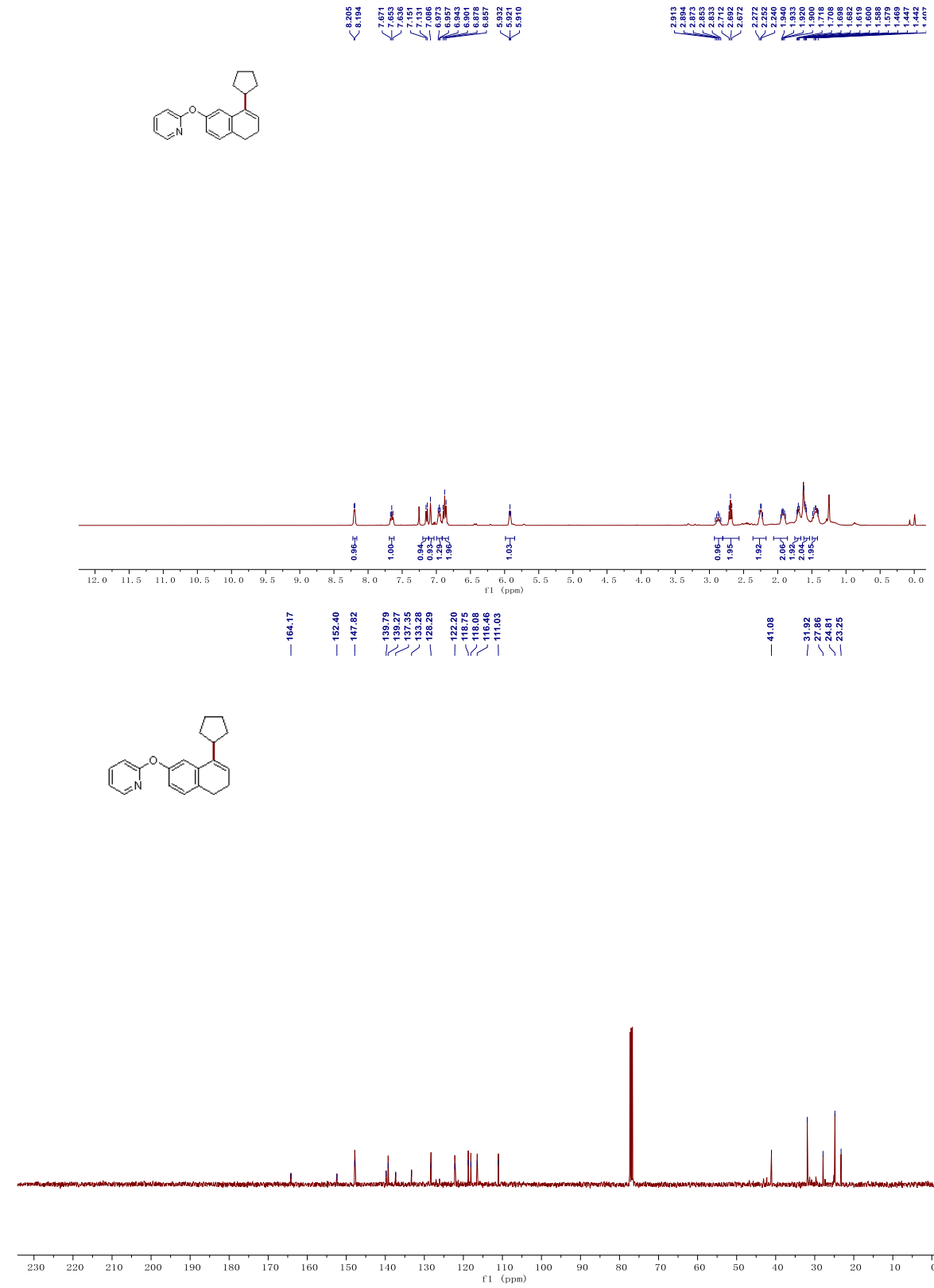
6-(Benzyloxy)-4-cyclopentyl-1,2-dihydronaphthalene (3ag)



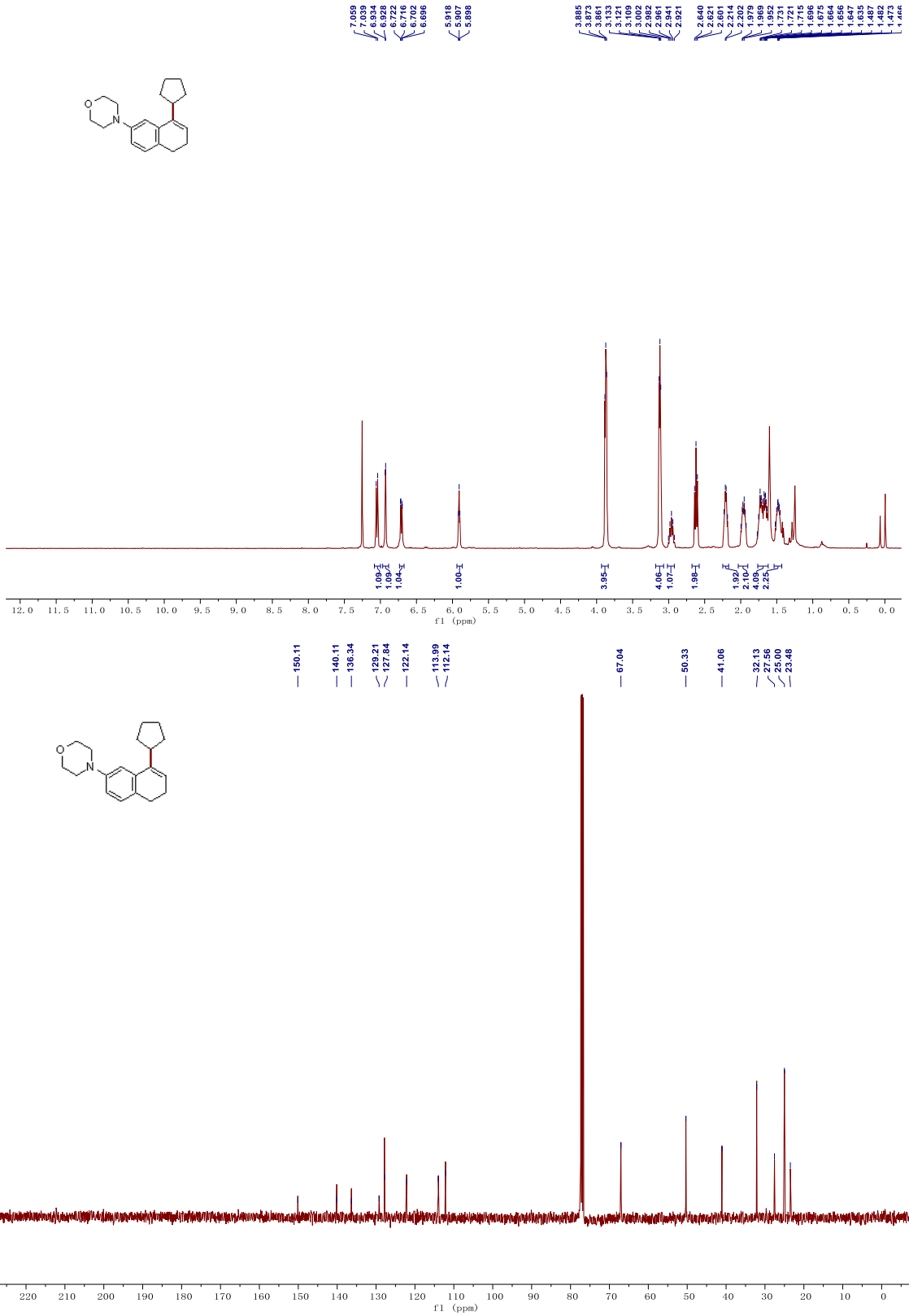
4-Cyclopentyl-6-phenoxy-1,2-dihydronaphthalene (3ah)



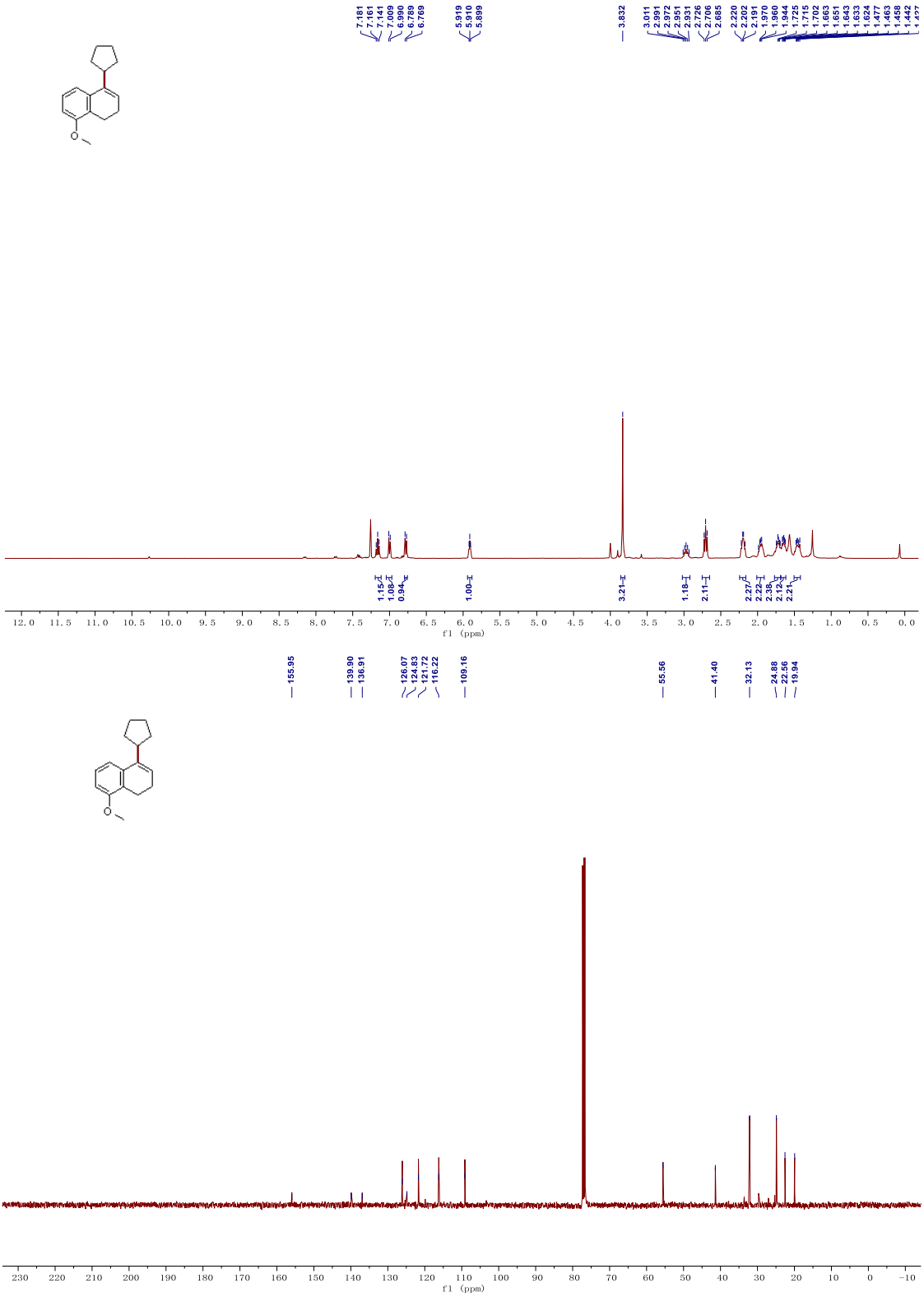
2-((8-Cyclopentyl-5,6-dihydronaphthalen-2-yl)oxy)pyridine (3ai)



4-(8-Cyclopentyl-5,6-dihydronaphthalen-2-yl)morpholine (3aj)

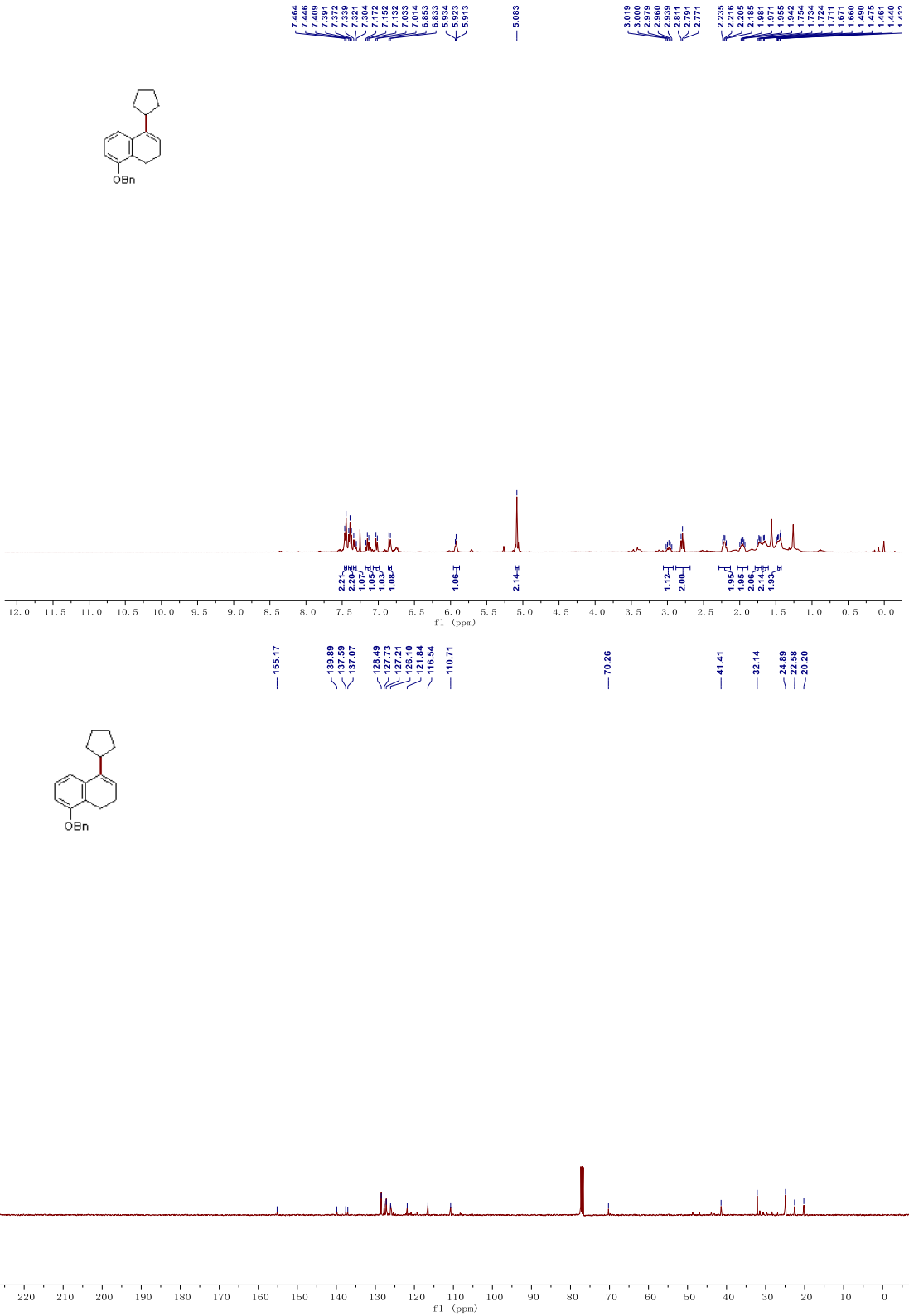


4-Cyclopentyl-8-methoxy-1,2-dihydronaphthalene (3ak)

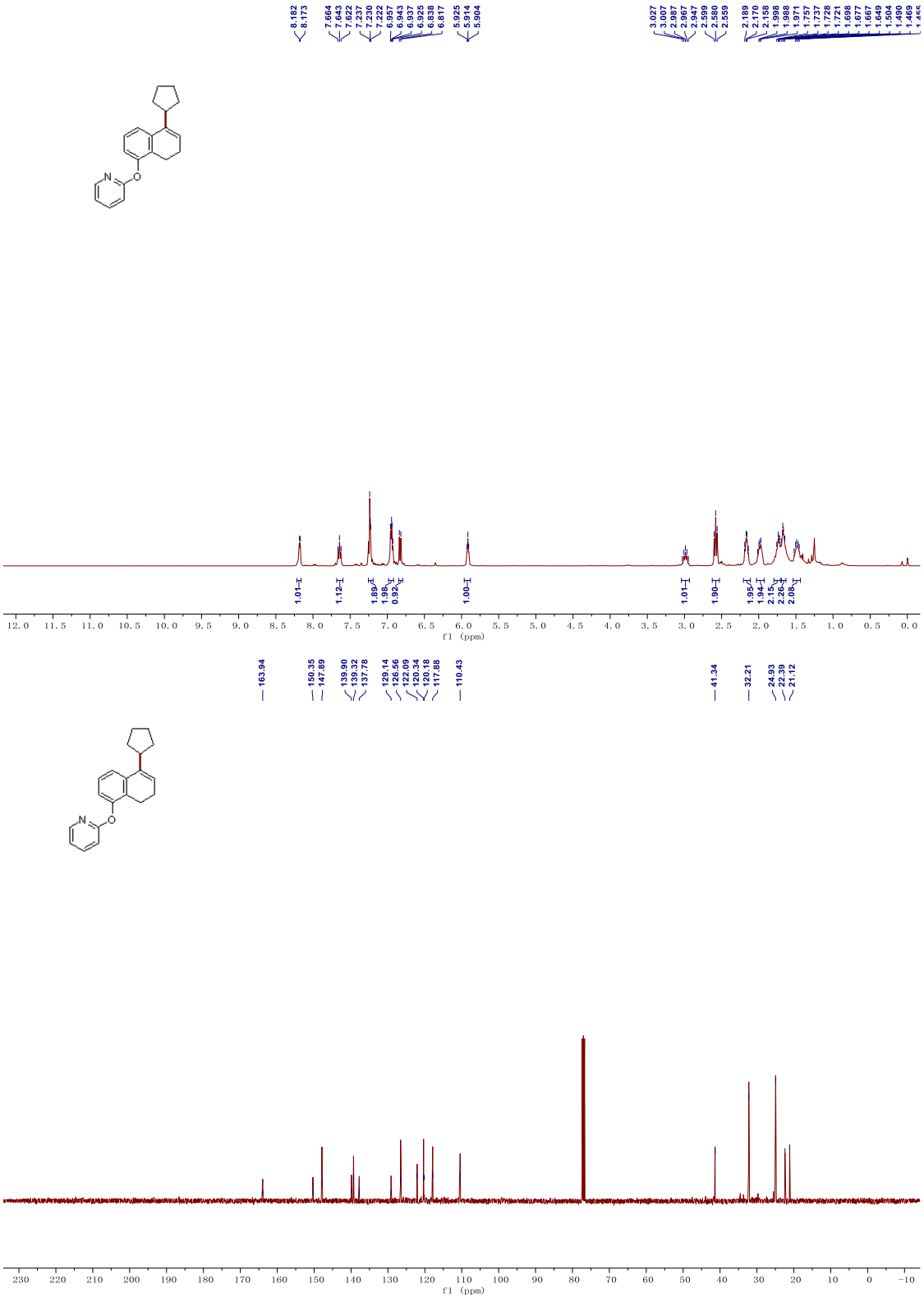


4-Cyclopentyl-6-(4-methoxyphenoxy)-1,2-dihydronaphthalene (3al)

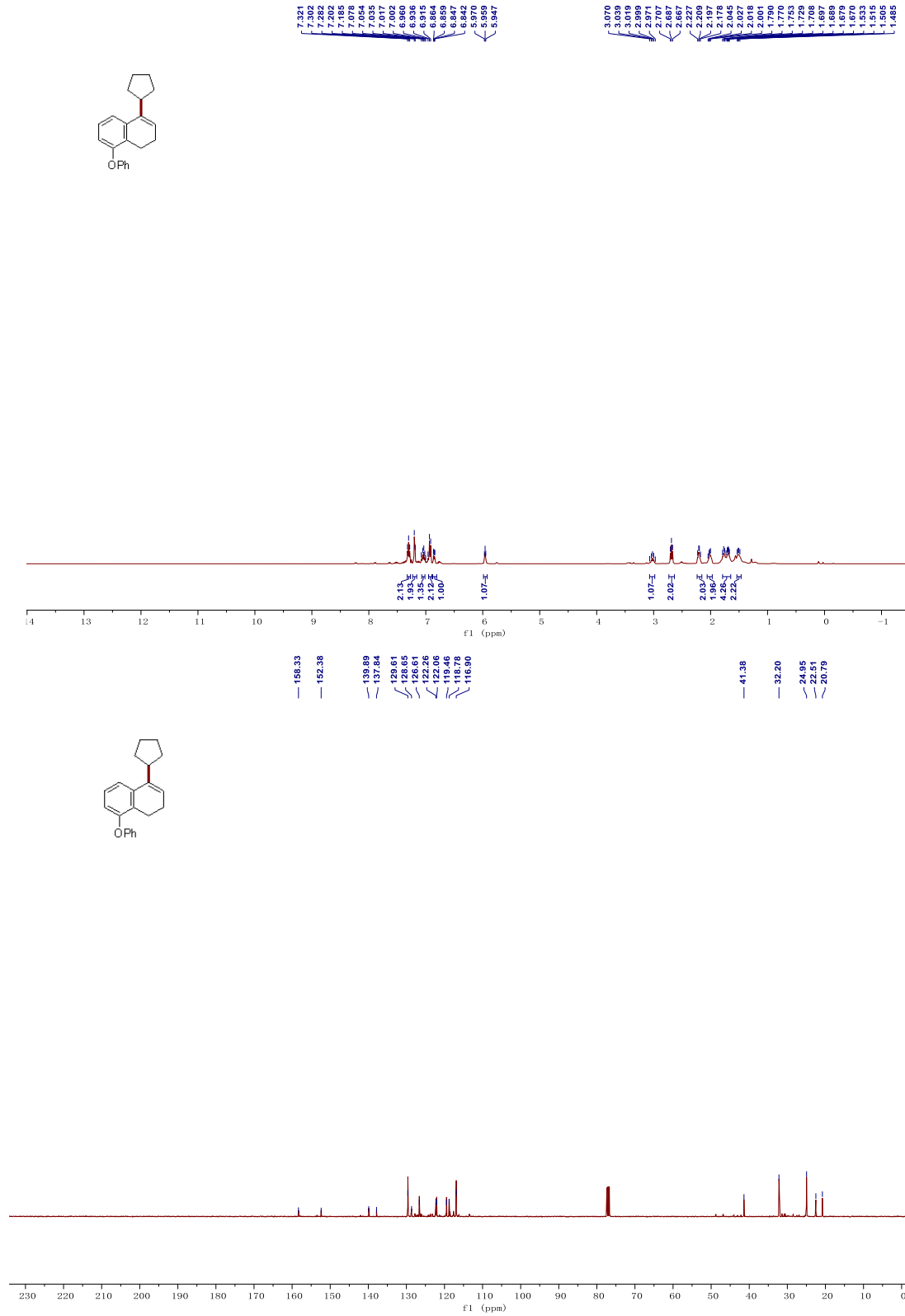
8-(Benzyloxy)-4-cyclopentyl-1,2-dihydronaphthalene (3am)



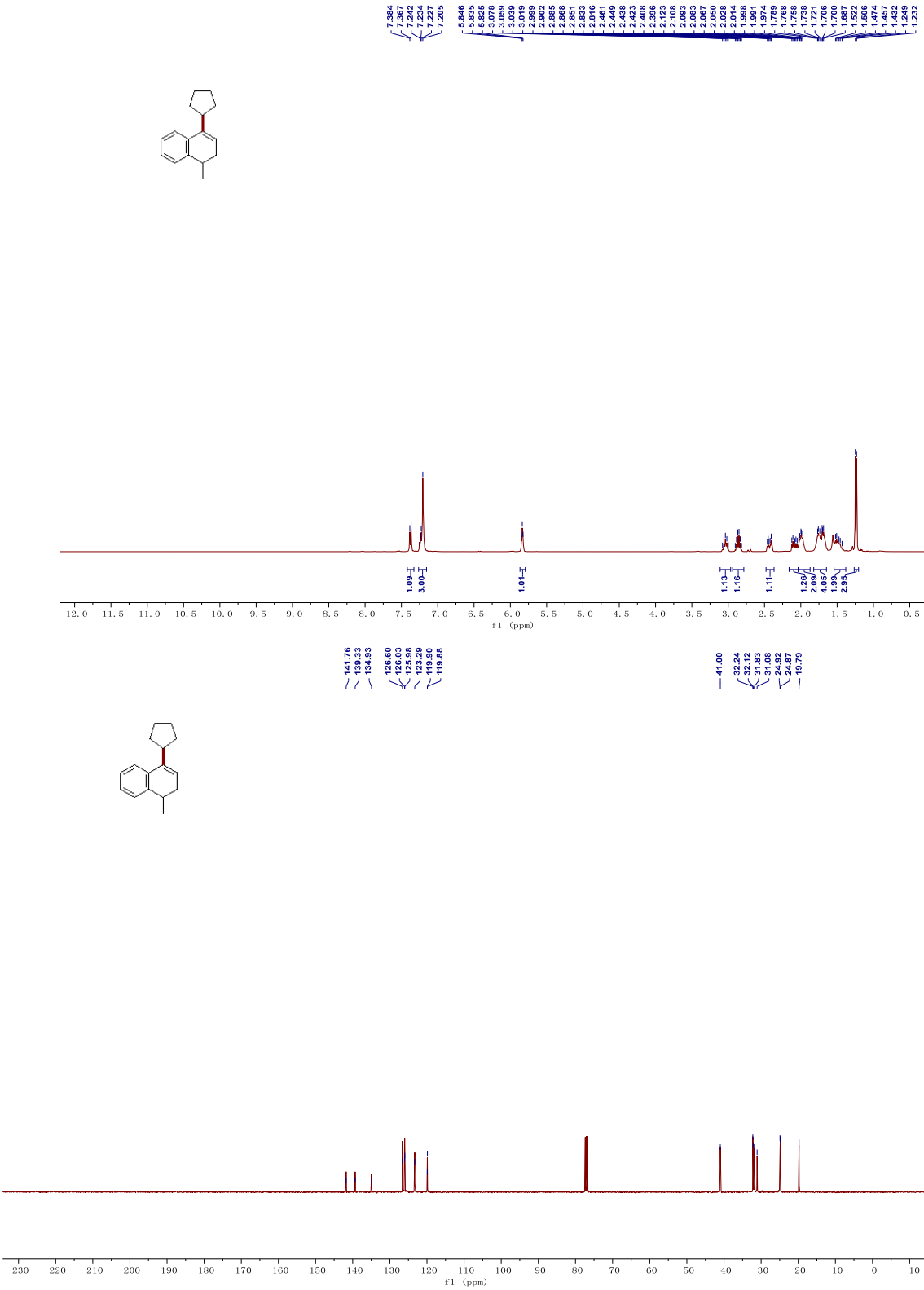
2-((5-Cyclopentyl-7,8-dihydronaphthalen-1-yl)oxy)pyridine (3an)



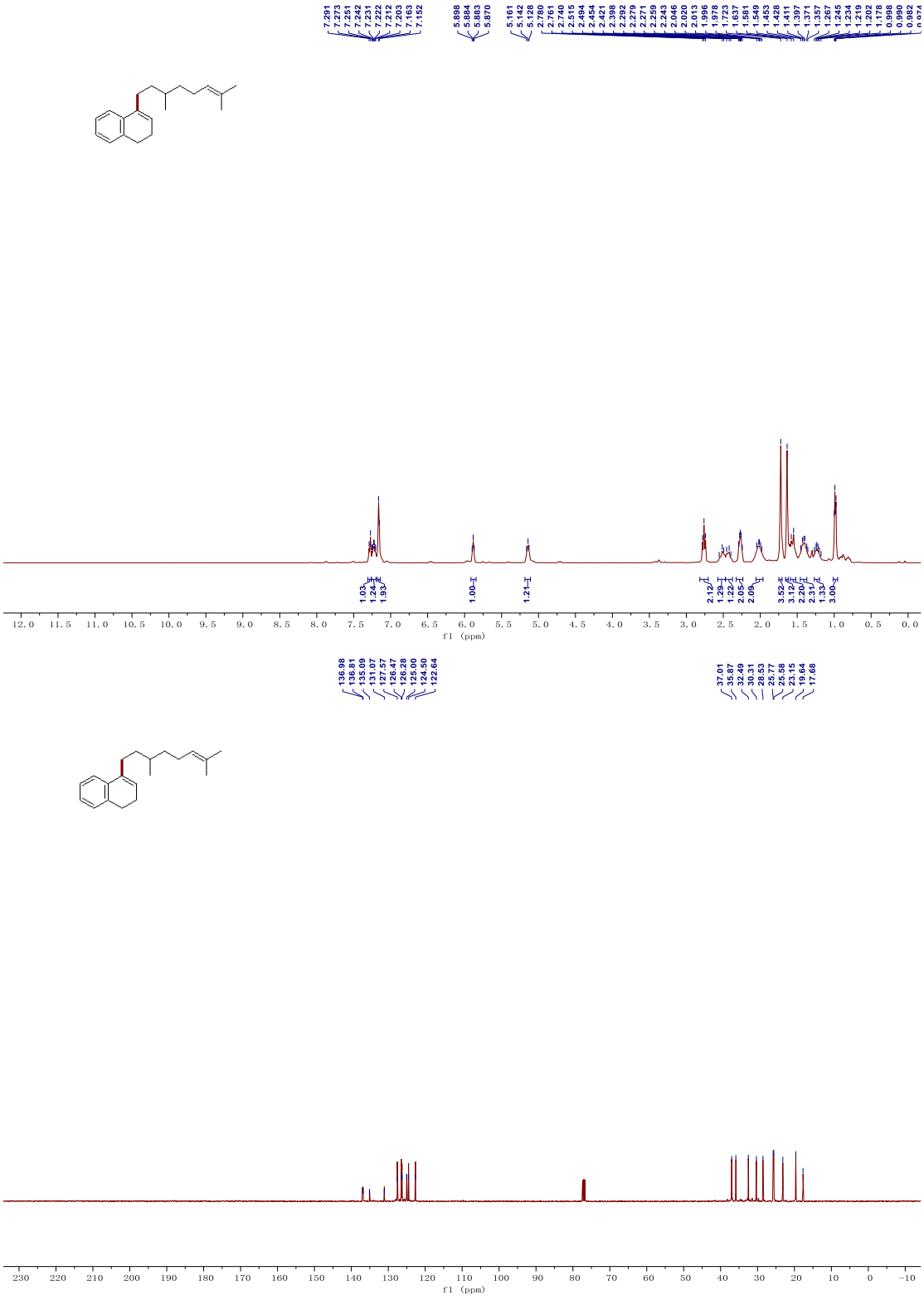
4- Cyclopentyl-8-phenoxy-1,2-dihydronaphthalene (3ao)



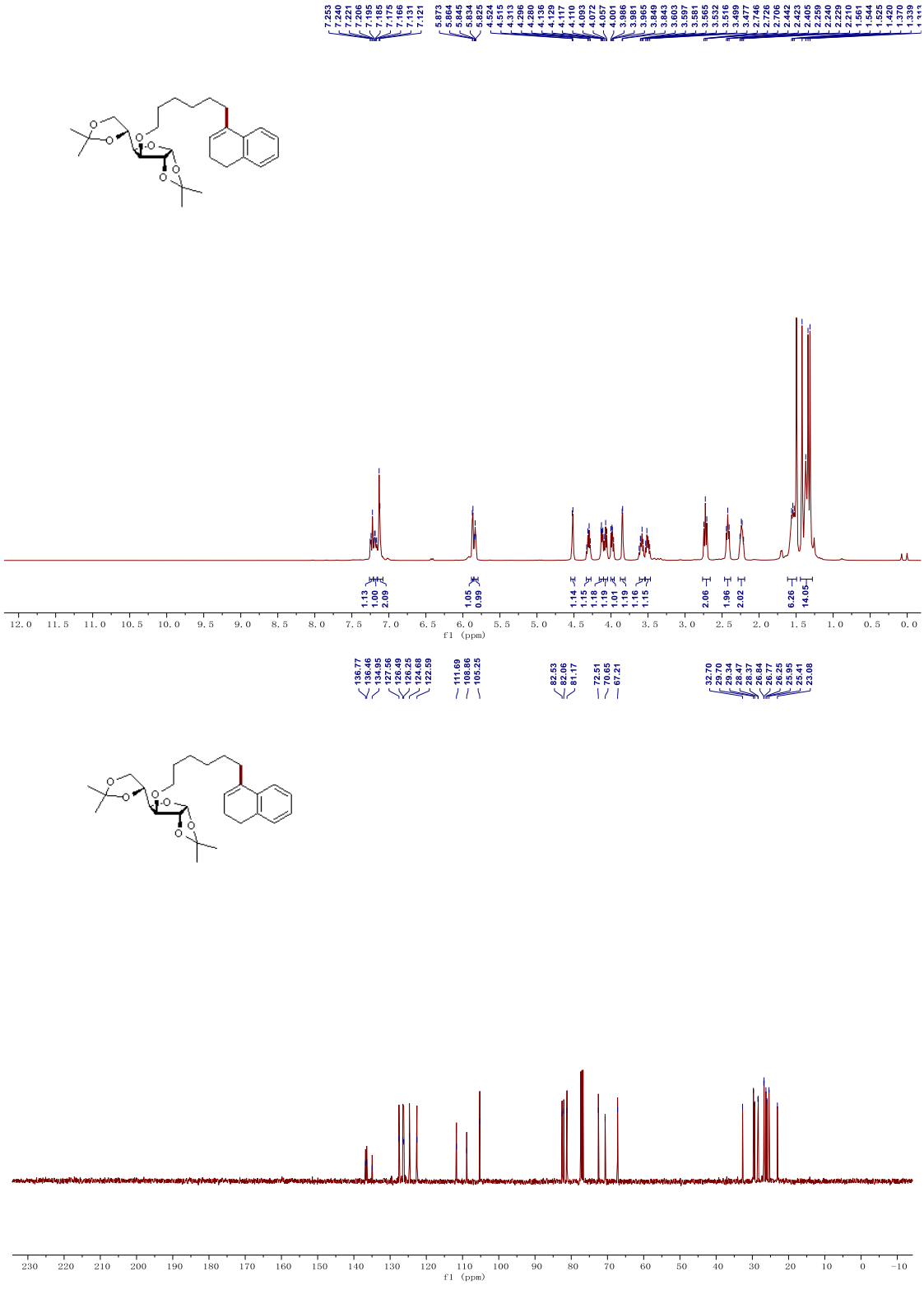
4-Cyclopentyl-1-methyl-1,2-dihydronaphthalene (3ap)



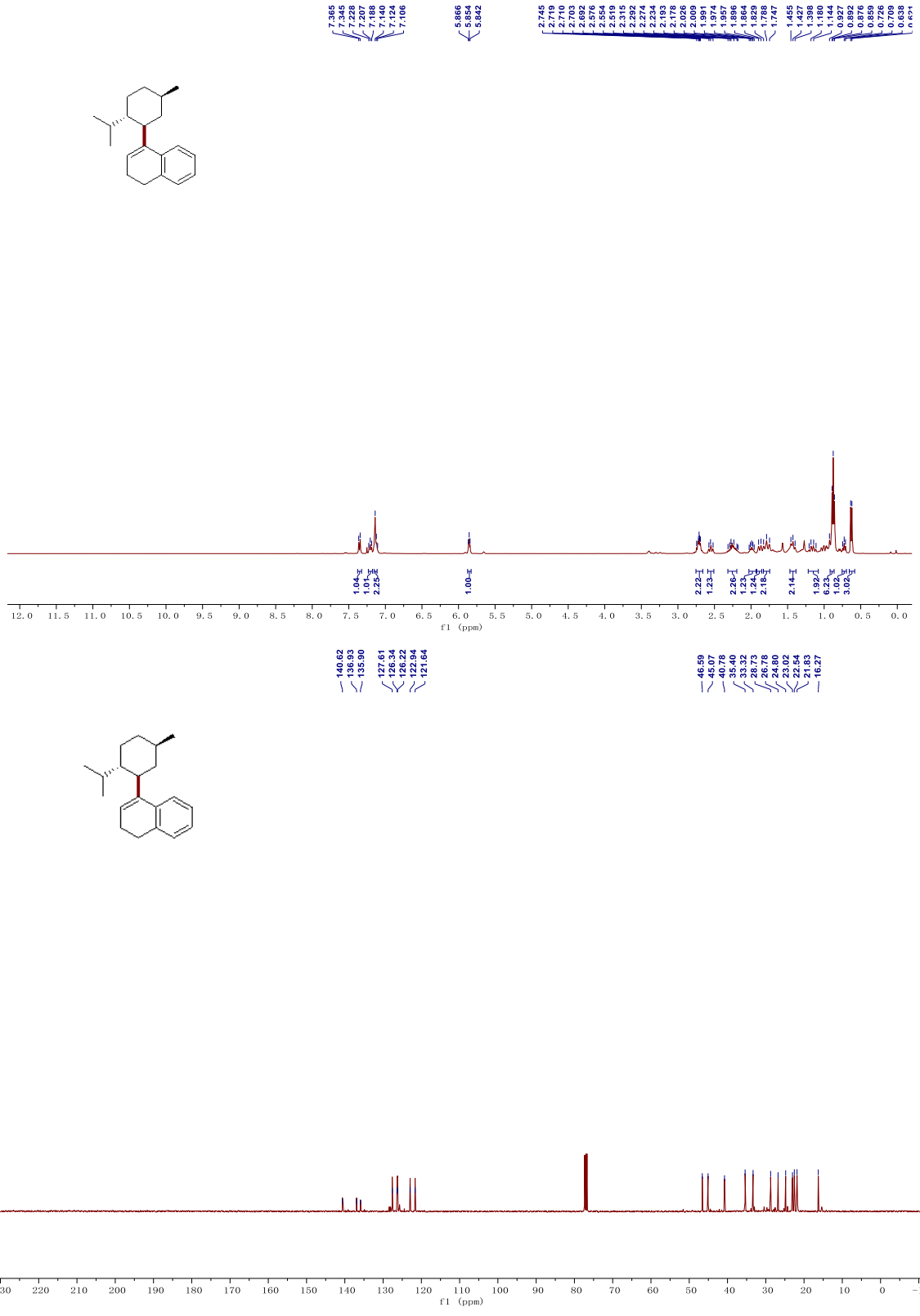
4-(3,7-Dimethyloct-6-en-1-yl)-1,2-dihydronaphthalene (4)



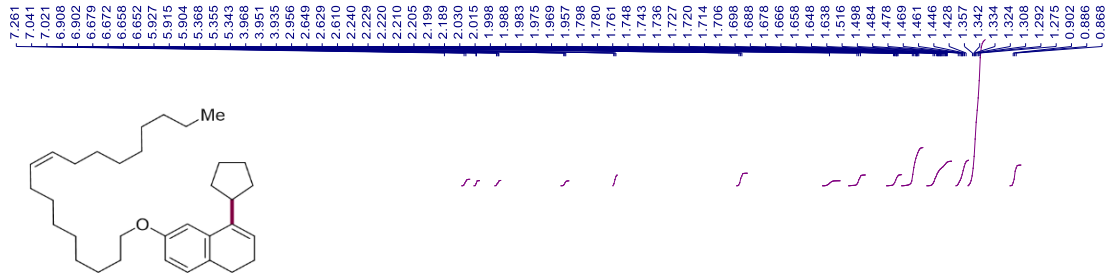
(*3aR,5R*)-6-((6-(3,4-Dihydronaphthalen-1-yl)hexyl)oxy)-5-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxole (5)

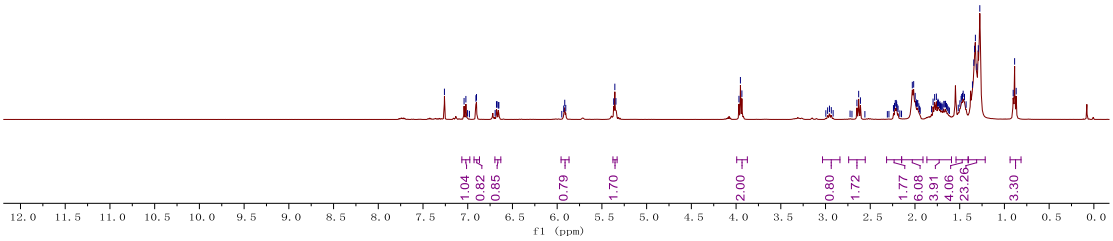


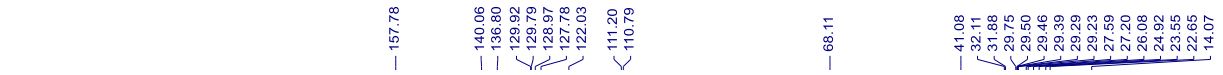
4-((*1R,2S,5R*)-2-Isopropyl-5-methylcyclohexyl)-1,2-dihydronaphthalene (6)

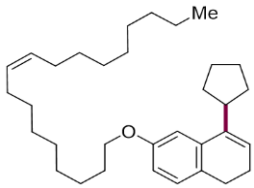


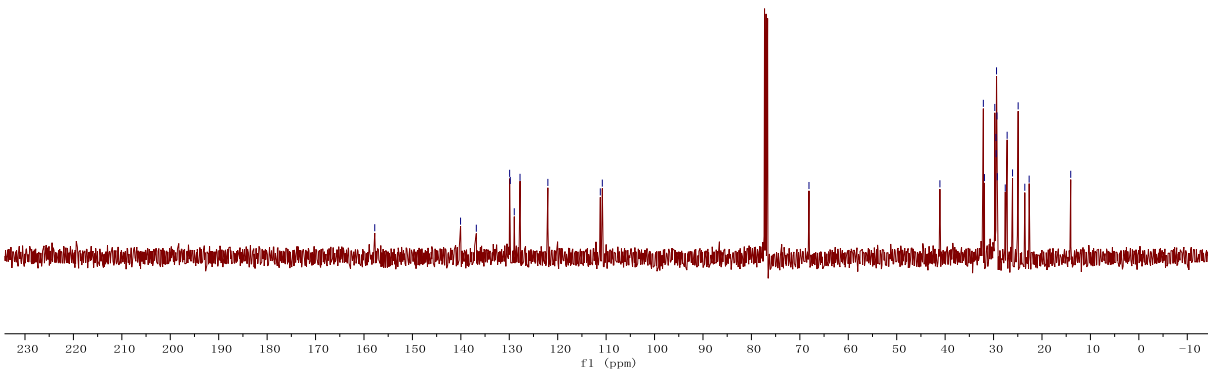
(*Z*)-4-Cyclopentyl-6-(octadec-9-en-1-yloxy)-1,2-dihydronaphthalene (7).



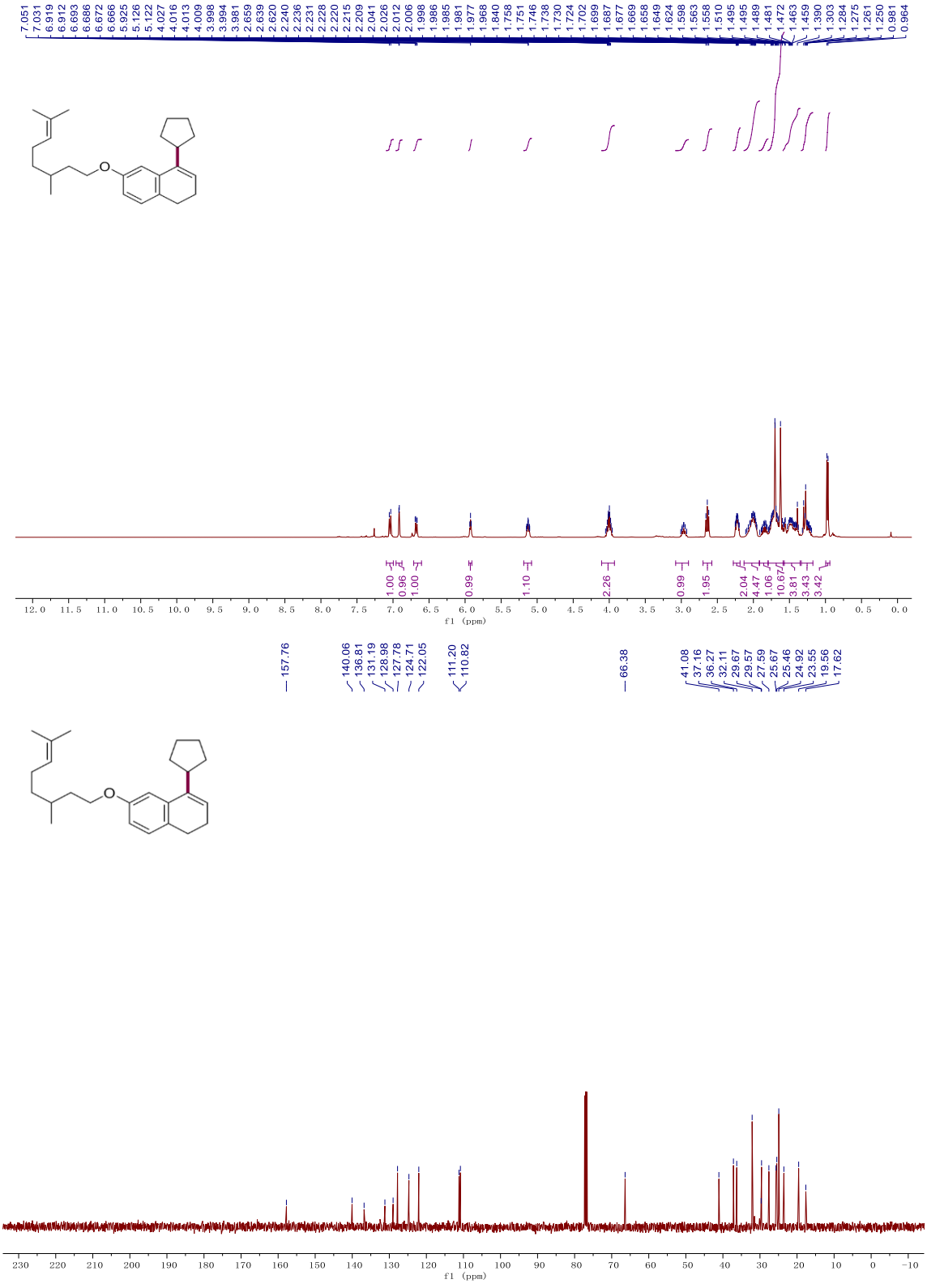






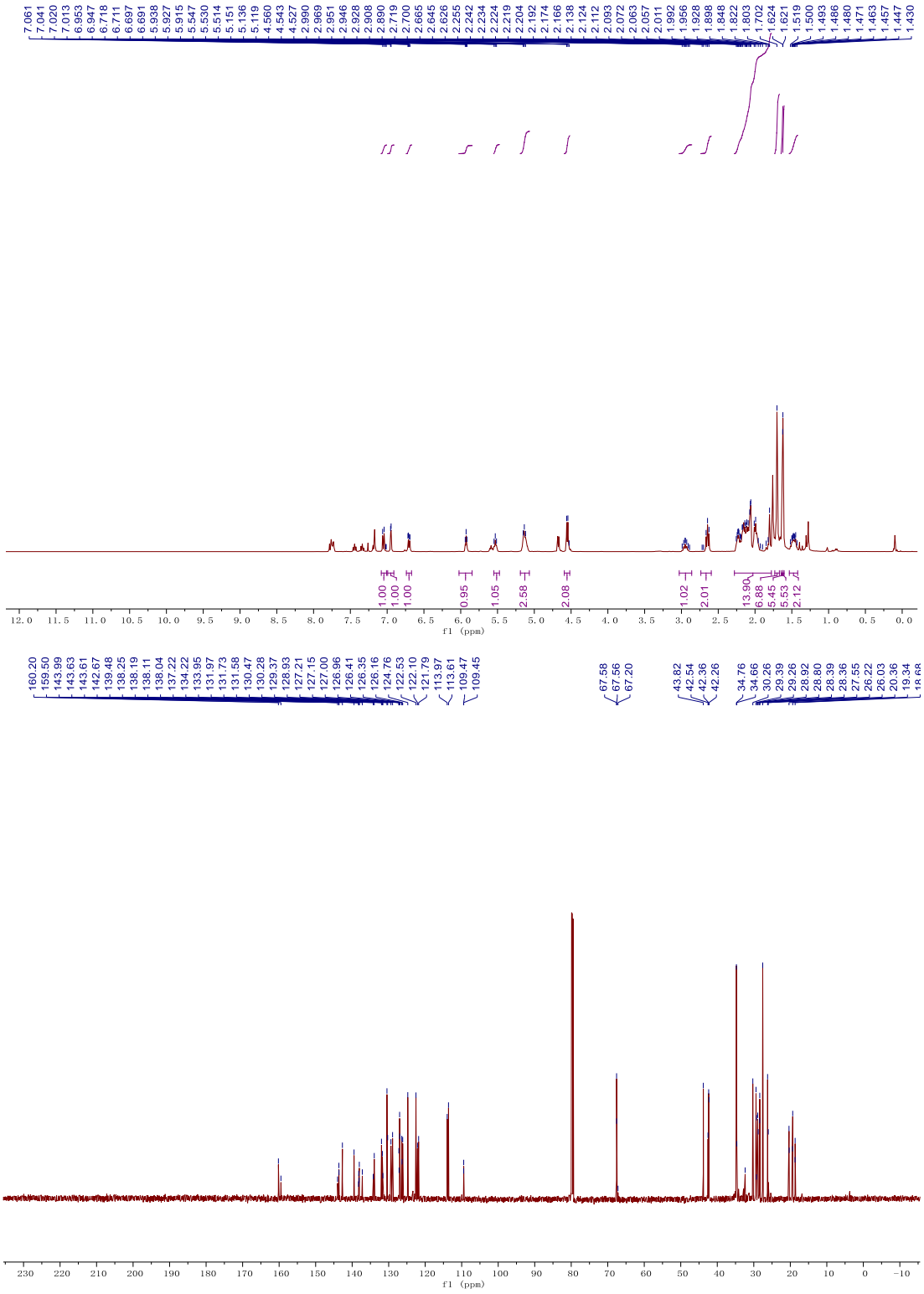


4-Cyclopentyl-6-((3,7-dimethyloct-6-en-1-yl)oxy)-1,2-dihydronaphthalene (8).

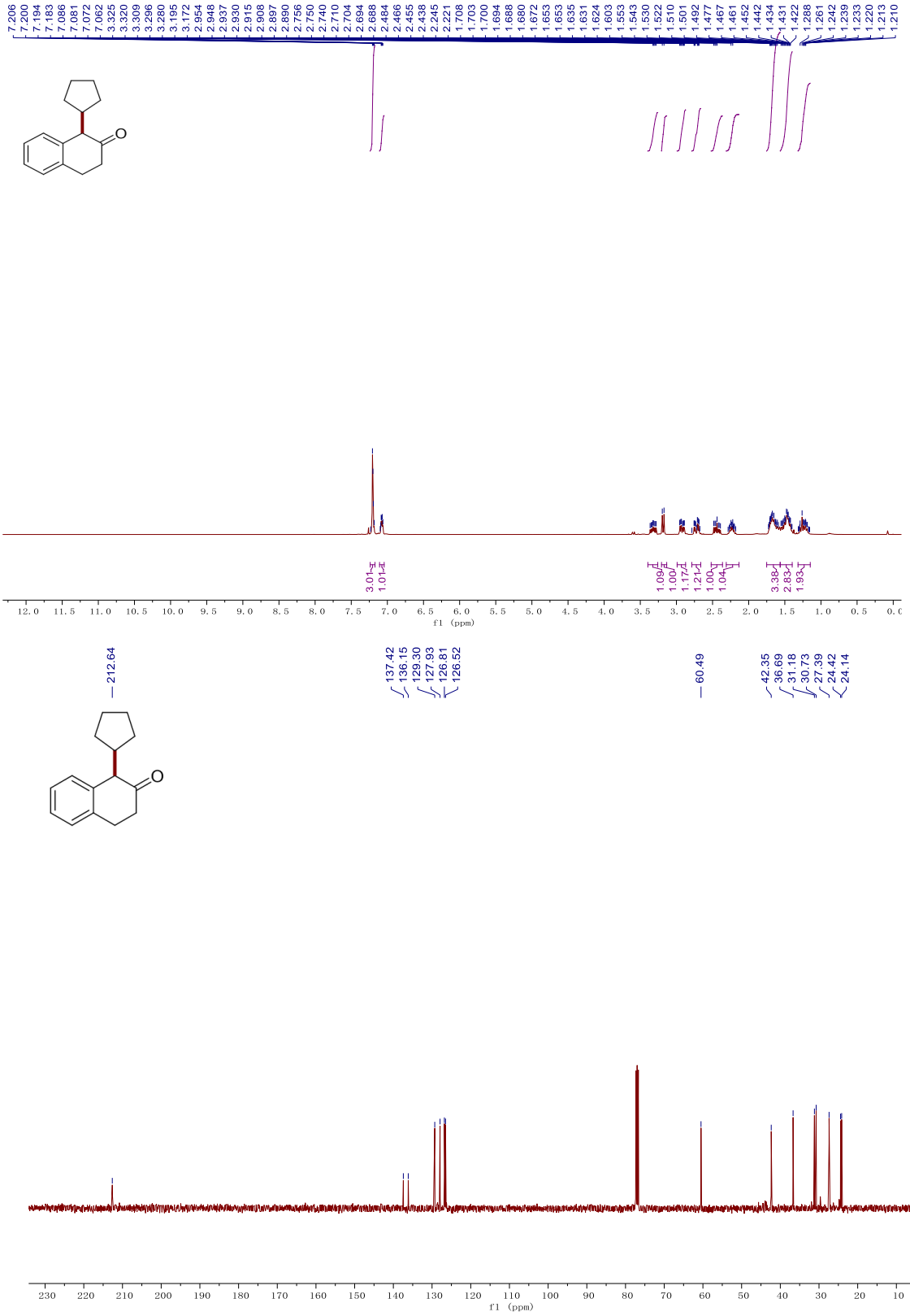


4-Cyclopentyl-6-(((2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl)oxy)-1,2-dihydronaphthalene (9).

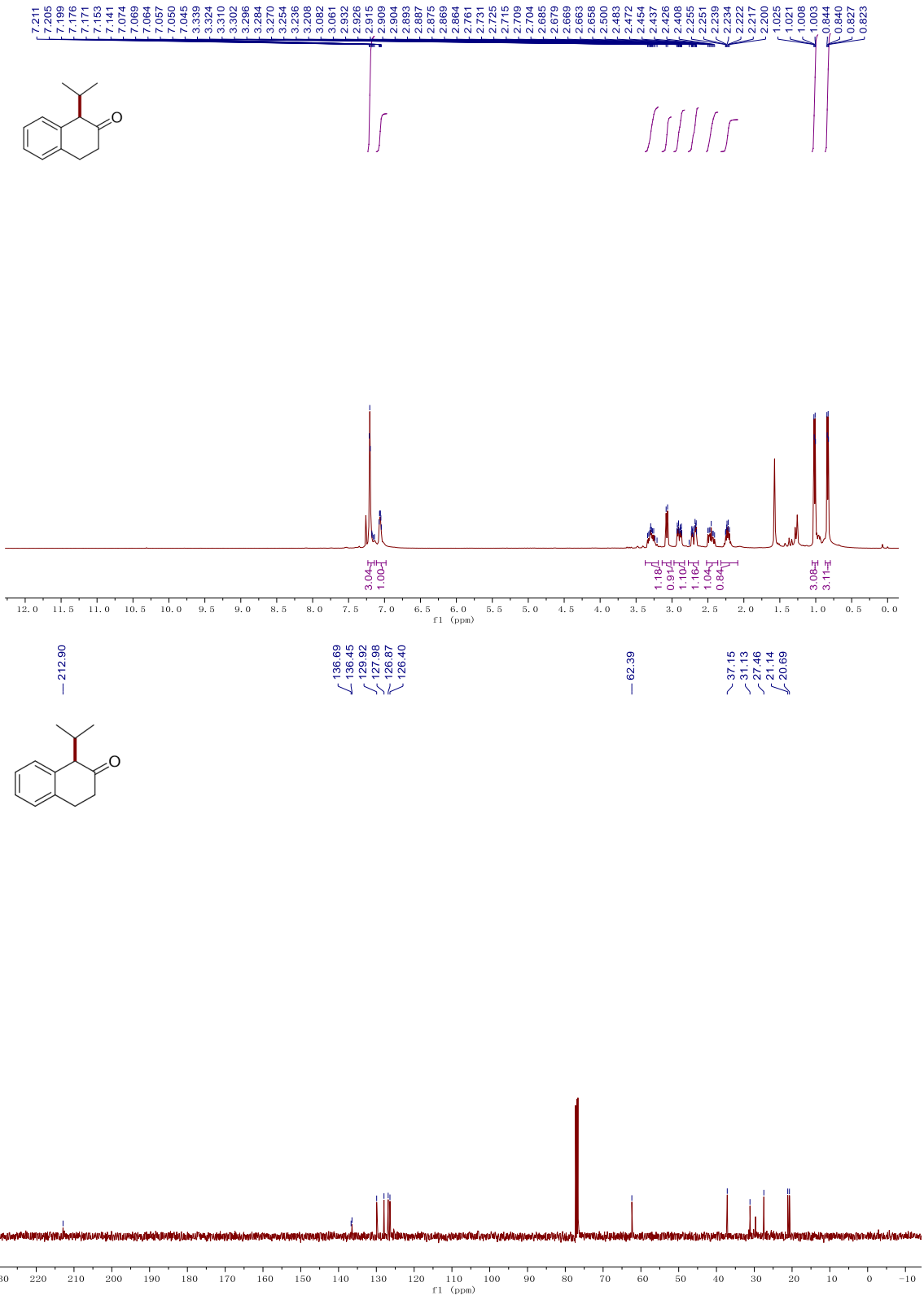
2-(((2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl)oxy)naphthalene (9').



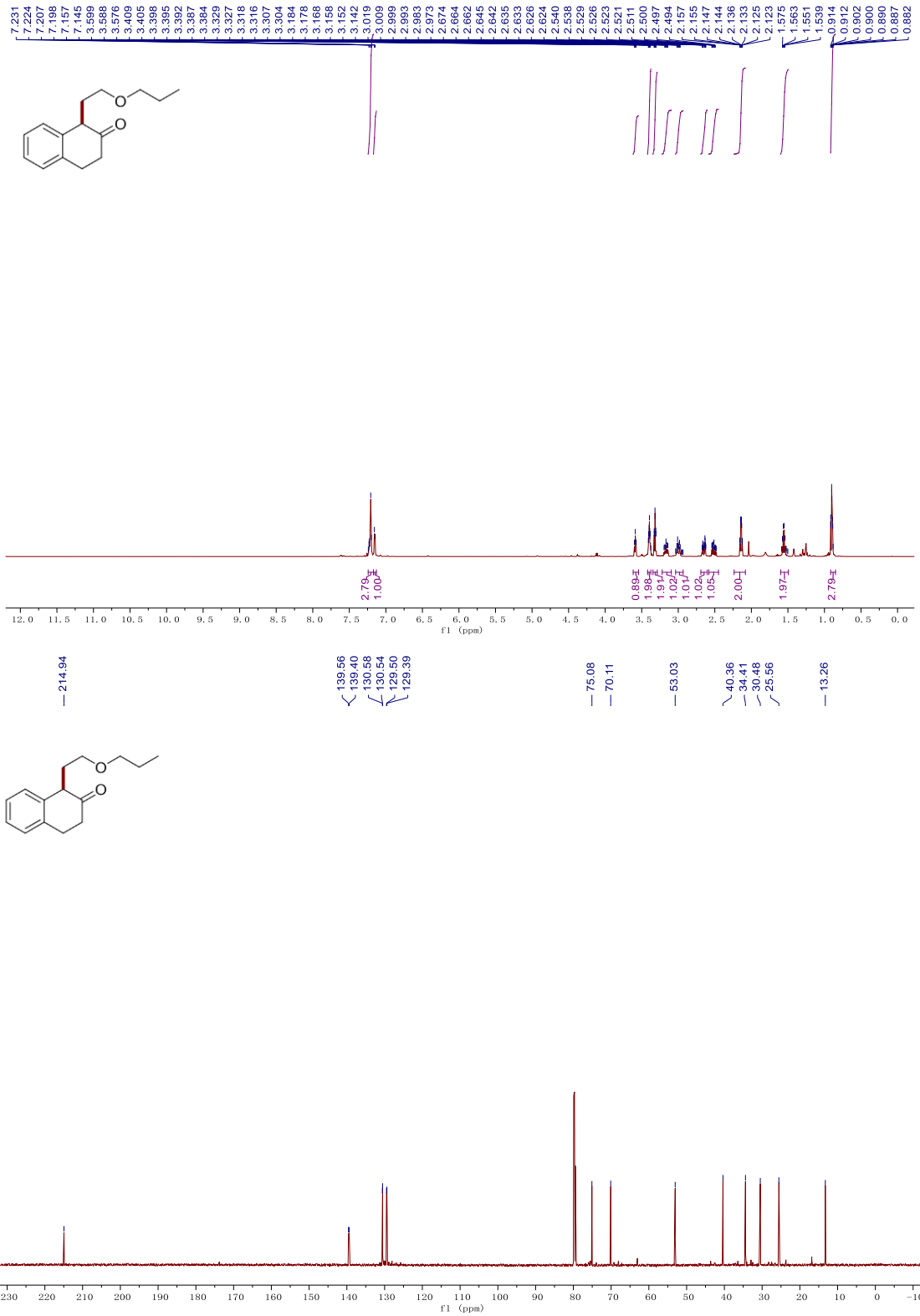
1-Cyclopentyl-3,4-dihydronaphthalen-2(*1H*)-one (10).



1-Isopropyl-3,4-dihydronaphthalen-2(*1H*)-one (11).



1-(2-Propoxyethyl)-3,4-dihydronaphthalen-2(*1H*)-one (12).



Computational studies Computational details:

All calculations were performed using Gaussian 16, Revision A.03 package [1] All of the intermediates were optimized by the DFT with the B3LYP-D3(BJ) functional.[2] For geometry optimizations and frequency calculations, BS-I basis set system was employed. In BS-I, we employed 6-311G(d) basis sets for H, C, O, N, P, Si, B and Na. All the stationary structures were characterized with no imaginary frequency and the transition state structures (TSs) were characterized with a single imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were performed on the TSs. The solvent effect of toluene was evaluated through the SMD method,[3] in which a better basis system BS-II was used. In BSII, we employed 6-311++G(d,p) basis sets for all atoms. All reported energies are free energies at a concentration of 1 M and a temperature of 298.15 K.

$$\%\text{Ionic Character} = 16|\Delta\chi| + 3.5(\Delta\chi)^2$$

$\Delta\chi$ is the difference in electronegativity of sodium (0.93) and carbon (2.55). Here %Ionic character can be calculated as 35.1 for Na-C bond.[4]

1 Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

2 Grimme, S. Semiempirical GGA-type density functional constructed with a long- range dispersion correction. J. Comp. Chem. 2006, 27, 1787.

3 A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B.,* **2009**, *113*, 6378.

4 J. D. Lee, *Concise Inorganic Chemistry*, 4th ed., Chapman & Hall, London New York **1991**.

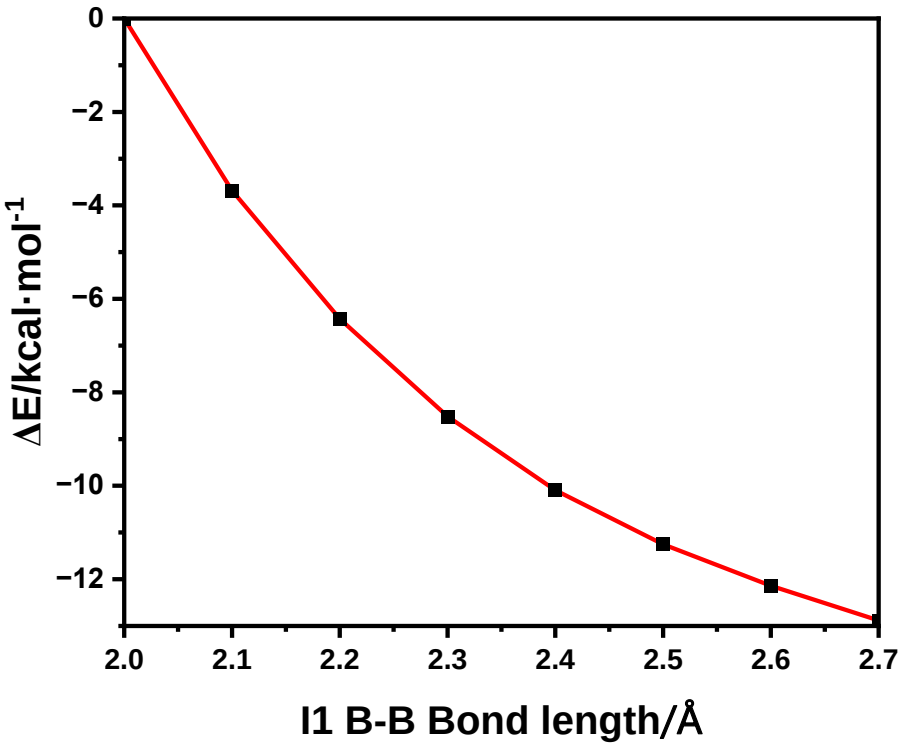


Figure DFT-S1. The energy plot of the potential energy surface relaxed scan of the **I1** B–B bond cleavage.

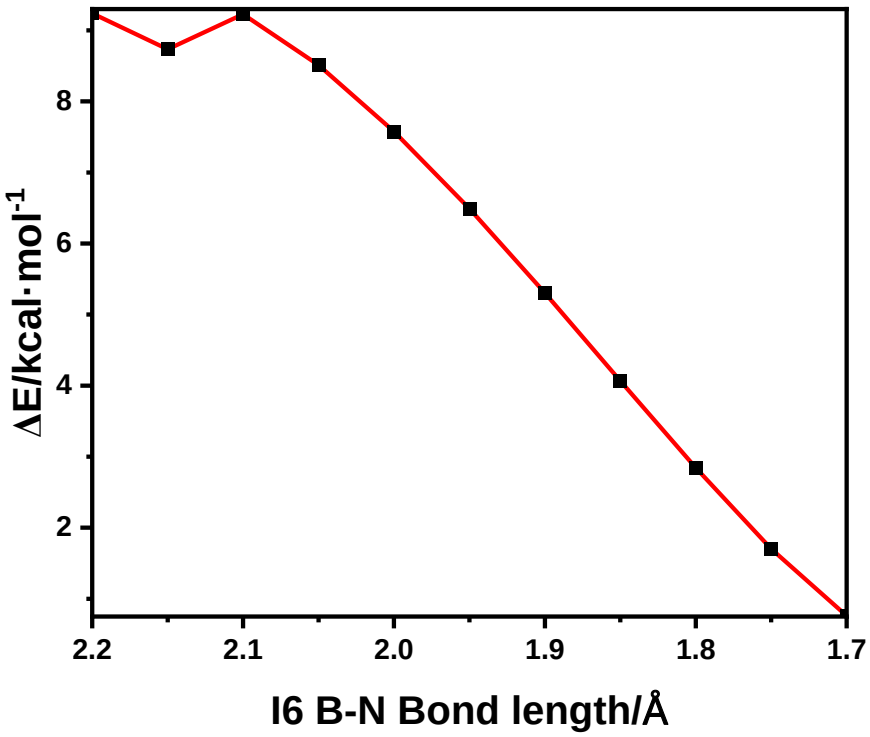


Figure DFT-S2. The energy plot of the potential energy surface relaxed scan of the **I6** B–N bond.

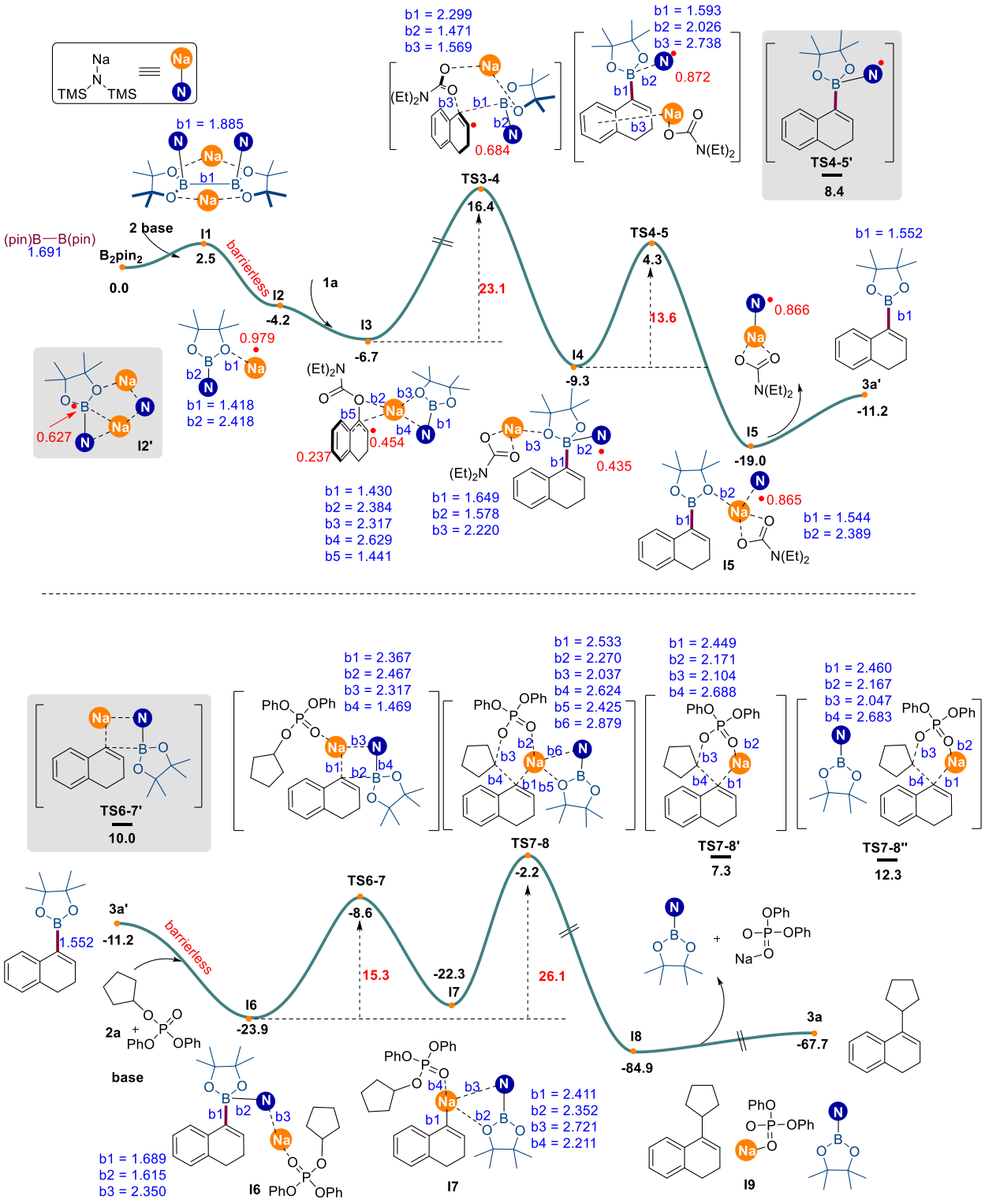


Figure DFT-S3. DFT calculated Gibbs free energy profile for the deoxygenative reductive coupling reaction pathway

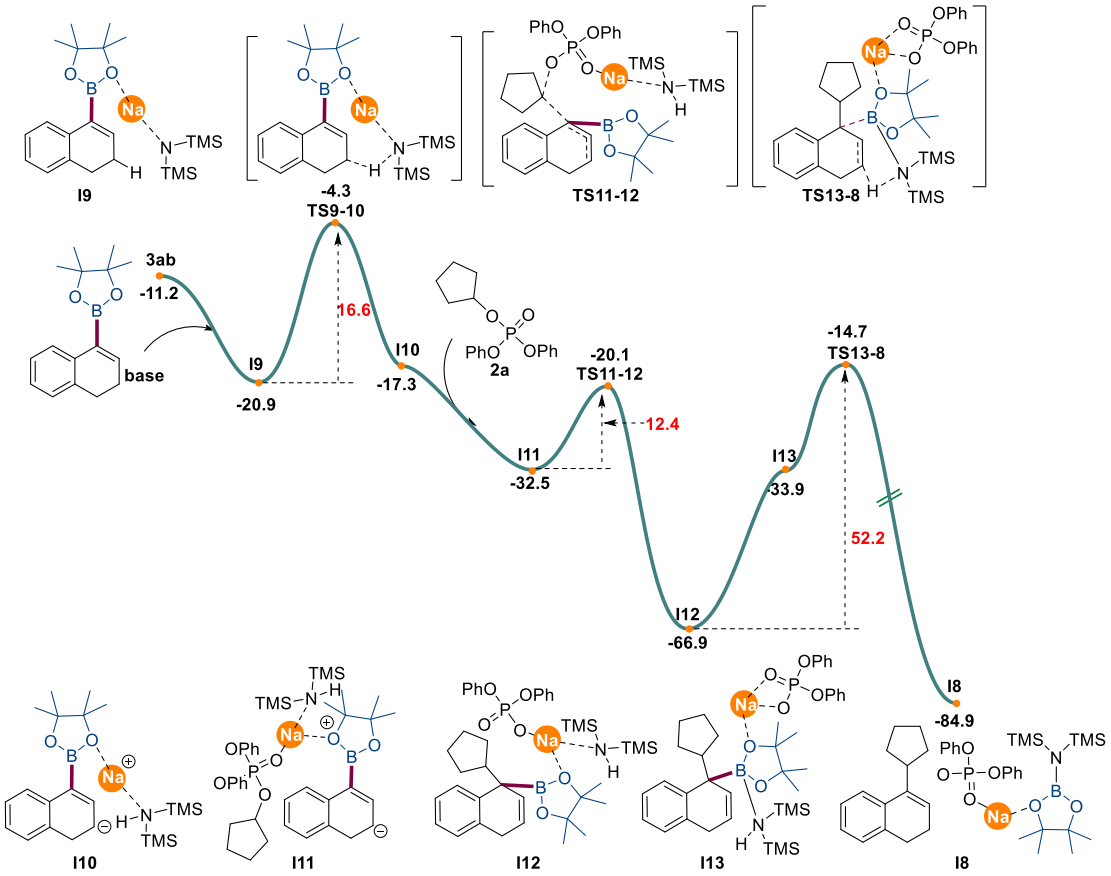


Figure DFT-S4. The potential energy surfaces for deprotonation process.

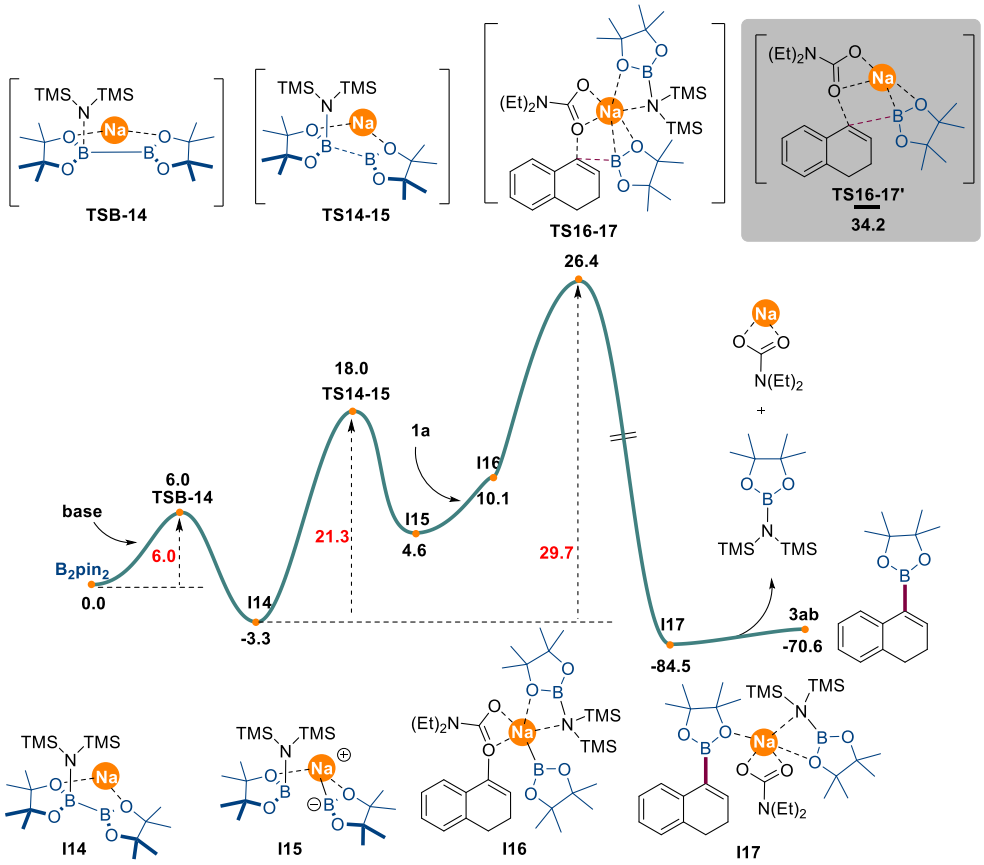


Figure DFT-S5. The potential energy surfaces for without radical process.

Cartesian coordinates of the optimized structures:

B_2pin_2

E = -822.809043507 a.u.

0 1

B	-2.50459900	1.98886200	-2.21829600
B	-2.55694700	3.67809500	-2.17843300
C	-2.12541900	5.82800300	-1.52403500
C	-3.12386500	5.82442700	-2.73391400
C	-3.05032700	-0.18946000	-1.77804300
C	-1.83000200	-0.12911100	-2.76192800
C	-4.58021800	6.03632100	-2.31846900
H	-4.86065400	5.36788800	-1.50254100
H	-4.76700400	7.06575800	-2.00433300
H	-5.22583000	5.81305500	-3.16957600
C	-2.75777600	6.76032600	-3.87619900
H	-3.49390100	6.66681800	-4.67701200
H	-2.75209200	7.80139000	-3.54146400
H	-1.77932500	6.52346800	-4.29191600
C	-2.54790300	6.68556400	-0.34051100
H	-1.80616400	6.60193500	0.45620200

H	-2.61962700	7.73846700	-0.62709800
H	-3.50888000	6.36873400	0.06252400
C	-0.68584800	6.14968400	-1.92729200
H	-0.56439800	7.20209500	-2.19379100
H	-0.02626100	5.92864200	-1.08637900
H	-0.36530500	5.53813100	-2.77252900
C	-2.21582800	-0.37235100	-4.22151100
H	-1.36968000	-0.10917800	-4.85855300
H	-2.47341800	-1.41805100	-4.40441000
H	-3.06209100	0.25056800	-4.51647100
C	-0.64497800	-1.00125300	-2.37503400
H	-0.25387600	-0.73547600	-1.39386400
H	-0.92527800	-2.05822200	-2.36442700
H	0.15863700	-0.87192800	-3.10263100
C	-4.18173500	-1.11114100	-2.20827200
H	-4.99074900	-1.06483700	-1.47664300
H	-4.58917200	-0.82238900	-3.17621200
H	-3.83915800	-2.14789400	-2.26899500
C	-2.64856600	-0.47946100	-0.33133900
H	-1.84033800	0.17763100	-0.00549800
H	-3.50791800	-0.29795500	0.31644600
H	-2.32917000	-1.51565000	-0.19854700
O	-3.53705400	1.18592600	-1.80391200
O	-2.13562000	4.42871500	-1.11014100
O	-1.42639900	1.27011500	-2.66898500
O	-3.02635400	4.44910500	-3.21165100

I1

E = -2894.57123619 a.u.

0 1

B	0.91891500	0.21059100	-0.25162000
B	1.14098100	2.08258000	-0.21802500
C	0.47810700	3.78438300	1.38979400
C	-0.67158200	3.67927700	0.31677200
C	-0.97082200	-1.08656600	0.61663400
C	-1.25572400	-0.80620100	-0.90018800
C	-1.94747500	3.07234700	0.91369700
H	-2.37964100	3.71241500	1.68623100
H	-2.70102500	2.95519200	0.13345200
H	-1.74742300	2.09063300	1.34009300
C	-1.04787500	5.00965800	-0.33339000
H	-1.82789700	4.84286300	-1.08114900
H	-1.44126500	5.71800400	0.40186300
H	-0.20034800	5.47051800	-0.83125600

C	-0.01152800	3.83288800	2.84210300
H	0.85230600	3.85289300	3.51367400
H	-0.59793500	4.73228900	3.04464000
H	-0.63989600	2.97644300	3.10333600
C	1.41390400	4.97867800	1.18106400
H	0.90659700	5.93102800	1.35578600
H	2.24585700	4.90754100	1.88499800
H	1.82846600	4.97986700	0.18205300
C	-2.32132200	0.27507400	-1.12694600
H	-2.44777300	0.43122100	-2.20655300
H	-3.30391900	-0.00460800	-0.74174200
H	-2.01742200	1.21120800	-0.67465000
C	-1.69349900	-2.04623800	-1.67955100
H	-0.98752700	-2.86549800	-1.60320400
H	-2.66693200	-2.39550100	-1.32141900
H	-1.80364000	-1.79753700	-2.73845500
C	-2.16817000	-0.85188600	1.53671300
H	-1.88843300	-1.07792500	2.57065800
H	-2.51664400	0.17887100	1.49766300
H	-3.00445500	-1.50684300	1.27745200
C	-0.45357700	-2.50953300	0.84735200
H	0.37426300	-2.73329100	0.18302900
H	-0.09902500	-2.60381500	1.87568000
H	-1.23606500	-3.25754600	0.69907800
O	0.04262600	-0.13721600	0.94183700
O	1.19024900	2.56342500	1.21345600
O	-0.00807300	-0.30765800	-1.39074500
O	-0.14274600	2.79814200	-0.67524600
N	2.35231700	2.76272900	-1.05978400
Si	2.27032300	3.81912400	-2.44723600
Si	3.96000700	2.66065300	-0.34873300
C	0.76767000	3.62719500	-3.61840400
H	0.86439900	4.43065700	-4.35350300
H	1.36443800	-0.04836000	-3.78142100
H	-0.20354700	3.77655500	-3.13992400
C	2.29315100	5.69838000	-2.15816700
H	1.34561200	6.10625300	-1.80362600
H	3.06999700	6.01848700	-1.46397300
H	2.50406600	6.18193400	-3.11847000
C	3.70751100	3.53391600	-3.65295000
H	3.55266100	4.16267700	-4.53641000
H	4.68612100	3.79478600	-3.24811700
H	3.75852900	2.49858000	-3.99484400
C	4.86574000	4.33184900	-0.30680400

H	5.06946000	4.77325700	-1.28370000
H	4.32916800	5.07513800	0.28813000
H	5.83667800	4.17432100	0.17599300
C	5.09575700	1.47206400	-1.26121500
H	5.23215100	1.73031000	-2.31170000
H	6.08615600	1.43880100	-0.79559800
H	4.67793100	0.47144300	-1.21693700
C	3.99244400	2.14697200	1.46917800
H	5.03437800	2.01567200	1.77902600
H	3.53723900	2.90345900	2.10663800
H	3.48274400	1.20211800	1.63517700
Na	0.95417700	0.92648700	2.55851000
N	2.20477600	-0.75725100	-0.34444700
Si	3.06111700	-1.58140600	0.92462500
Si	2.52189100	-1.34461400	-1.97309500
C	4.29591800	-1.99755800	-2.20520500
H	4.50830500	-2.89625500	-1.62170700
H	4.38316900	-2.28608700	-3.25882400
H	5.08846900	-1.27759000	-2.00780600
C	2.32516500	0.03046500	-3.26157200
H	0.77426400	2.70866100	-4.22063700
H	2.42290100	1.00359300	-2.77978500
H	3.10414800	-0.03070100	-4.02575600
C	1.51333500	-2.83203000	-2.57974800
H	2.08642300	-3.37623400	-3.33779400
H	1.28356200	-3.54479600	-1.78402400
H	0.57329200	-2.52484700	-3.03406000
C	4.92585600	-1.26125700	1.02271900
H	5.18753300	-0.20522500	1.03533100
H	5.30802200	-1.70582000	1.94884200
H	5.47188100	-1.72337900	0.20009300
C	2.49635000	-1.20537600	2.71557300
H	1.42384500	-1.33380300	2.87577100
H	2.99025600	-1.94320200	3.35437000
H	2.84535200	-0.23660000	3.09422900
C	2.93396900	-3.47817800	0.84882800
H	1.97548100	-3.85544300	1.20996000
H	3.07850000	-3.87729400	-0.15692300
H	3.71451900	-3.91743500	1.47946100
Na	-0.06792200	1.55275200	-2.46649300

I2

E = -1447.27239711 a.u.

0 2

B	1.22417200	3.74270600	0.05683300
C	-0.54657700	4.59749900	1.25698400
C	-0.78146500	4.81666600	-0.27774800
C	-1.73920800	3.79363700	-0.88737800
H	-1.46215900	2.77172300	-0.61825200
H	-2.76929700	3.96588200	-0.56864800
H	-1.70206000	3.87324000	-1.97486200
C	-1.19320300	6.22905100	-0.66344600
H	-1.32183700	6.29121700	-1.74562900
H	-2.14282000	6.50048000	-0.19481900
H	-0.43927500	6.95968300	-0.37319600
C	-1.74892700	4.07037000	2.02224000
H	-1.49079300	3.92049800	3.07292300
H	-2.57193000	4.78913000	1.98020400
H	-2.10741500	3.12004200	1.62582700
C	0.03157400	5.82593600	1.95757800
H	-0.71488400	6.61620300	2.05885700
H	0.36884400	5.54292700	2.95562100
H	0.88742000	6.22948800	1.41335100
O	0.50766800	3.58016200	1.24809400
O	0.53970100	4.55687100	-0.82279100
N	2.46985300	3.12998300	-0.23267100
Si	2.77959700	2.80148800	-1.96121500
Si	3.74766700	2.99617100	0.99492200
C	1.21217200	2.14932600	-2.76678500
H	1.43567400	1.76189000	-3.76580200
H	0.77981000	1.32730400	-2.18804700
H	0.45352700	2.92469200	-2.86999100
C	3.34983800	4.37048400	-2.82119600
H	2.60017600	5.15681600	-2.70269700
H	4.29102200	4.74159500	-2.40723200
H	3.49997600	4.20855500	-3.89328300
C	4.08079500	1.45280300	-2.13716000
H	4.24326100	1.26449300	-3.20345600
H	5.05281800	1.69672500	-1.70587900
H	3.74159900	0.51377400	-1.69261000
C	5.28459400	3.89001400	0.37046800
H	5.69902000	3.46921300	-0.54743900
H	5.06773800	4.94509100	0.17961800
H	6.07406300	3.85023900	1.12766100
C	4.15721200	1.20346300	1.37849200
H	4.59376100	0.67719000	0.52787000
H	4.87402800	1.14690100	2.20423400
H	3.26740200	0.64379000	1.68609800

C	3.23713900	3.85123800	2.58979600
H	4.08430600	3.83264600	3.28327800
H	2.96946600	4.89864800	2.42926200
H	2.39365800	3.36897300	3.08596800
Na	0.25819800	1.29544200	1.99999200

I2’

E = -2483.13592772 a.u.

0 2

B	0.23708700	3.29993800	0.09485600
C	-1.33342600	3.90985700	1.69953700
C	-1.52542700	4.84385500	0.45183400
C	-2.71344500	4.42399900	-0.41369300
H	-2.67344900	3.35770900	-0.63694200
H	-3.66911700	4.64269600	0.06950800
H	-2.67935000	4.97127500	-1.35789000
C	-1.61446900	6.33037600	0.77254800
H	-1.72434400	6.90625700	-0.15017300
H	-2.48143300	6.54616000	1.40273100
H	-0.72632700	6.68896900	1.29547100
C	-2.63450900	3.37844600	2.29087600
H	-2.41037500	2.72697600	3.13817600
H	-3.26822500	4.19401600	2.65154200
H	-3.19724300	2.79601200	1.56263500
C	-0.49321400	4.55200600	2.80960900
H	-1.01447100	5.37357300	3.30677800
H	-0.26279600	3.79116600	3.55796500
H	0.45696600	4.91842800	2.42078300
O	-0.59931100	2.81356500	1.15222500
O	-0.31731900	4.60382900	-0.31312300
N	3.90276200	4.98336900	0.23823700
Si	5.06852800	4.74429700	-0.97991400
Si	4.01474600	5.77139900	1.74486200
C	4.78133600	3.02649700	-1.76310600
H	5.41769200	2.87191800	-2.63965900
H	5.03036700	2.21426500	-1.06575200
H	3.75312300	2.87627700	-2.10615700
C	4.94936800	6.01280400	-2.38518800
H	5.12731600	7.02311600	-2.00112200
H	5.68888900	5.82900700	-3.17163400
H	3.96541500	6.01788300	-2.86536400
C	6.87931100	4.72818400	-0.42709200
H	7.52877300	4.39198500	-1.24249700
H	7.22892100	5.71665700	-0.11995900

H	7.03741800	4.04945000	0.41726600
C	2.64745500	7.10364300	1.89383200
H	2.71766300	7.84674500	1.08919300
H	1.62777200	6.69829800	1.90339900
H	2.74285400	7.65795100	2.83261400
C	5.62707700	6.68731500	2.11468400
H	5.86454100	7.42120700	1.33823200
H	5.55609700	7.22757300	3.06457500
H	6.47742200	6.00529400	2.18967700
C	3.71083000	4.56676000	3.17926800
H	3.71660700	5.06617800	4.15372500
H	2.74178800	4.06276400	3.08563700
H	4.48574100	3.79221500	3.21015100
Na	2.85173800	2.88864300	0.38645500
N	0.64390500	2.27662200	-0.96338800
Na	1.71421500	5.61423300	-0.32702700
Si	0.48505100	0.60573800	-0.40365000
Si	0.55871800	2.73316600	-2.66167300
C	1.44539700	0.42723600	1.22162200
H	1.22098600	-0.54151600	1.67927200
H	2.53446300	0.42970400	1.07101800
H	1.17428200	1.19628400	1.94639100
C	-1.30029700	0.07023800	-0.15666500
H	-1.77273000	0.66179500	0.62690000
H	-1.87827800	0.20693000	-1.07589800
H	-1.36415100	-0.98865100	0.11602900
C	1.27803200	-0.64986300	-1.56661200
H	1.32176800	-1.60846000	-1.03756700
H	0.70514300	-0.81988000	-2.47999600
H	2.29939500	-0.39332400	-1.85617300
C	-1.18798200	2.65033100	-3.36168600
H	-1.60929200	1.64555400	-3.26044400
H	-1.86250300	3.34093000	-2.85450700
H	-1.19351100	2.89941500	-4.42839100
C	1.63748100	1.65665800	-3.77696800
H	1.18930200	0.68927600	-4.00531600
H	1.76878500	2.17977900	-4.73019300
H	2.63507200	1.47139900	-3.37479200
C	1.20306800	4.49337700	-2.93994100
H	1.27882500	4.68047900	-4.01523200
H	0.52409700	5.24210500	-2.52925200
H	2.21217300	4.63631700	-2.54226600

I3

E = -2235.80708687 a.u.

0 2

C	-3.52320800	7.10376100	4.22398900
C	-2.72112000	6.04145100	4.70681400
C	-2.81673500	4.76431600	4.20651700
C	-3.72866200	4.48202200	3.11912700
C	-4.59694400	5.54982700	2.69526100
C	-4.48035700	6.82128400	3.24670200
H	-1.26752600	3.92939000	5.44462200
H	-3.43525100	8.09749800	4.64753800
H	-2.02358700	6.23060200	5.51999000
C	-2.07697800	3.58839600	4.79135800
C	-3.62040100	3.21974700	2.48465200
H	-5.41335000	5.34001200	2.01103100
H	-5.16437400	7.60013500	2.91878100
C	-2.58460100	2.31480900	2.66582200
C	-1.53950400	2.63333200	3.70692300
H	-2.65689300	1.31717900	2.26024900
H	-0.64536000	3.09204000	3.25561000
H	-1.18409800	1.71078700	4.17909100
H	-2.77690800	3.02135200	5.42036300
O	-4.51120800	3.11778800	1.35641400
C	-5.10506600	1.94731900	0.98934200
O	-4.89018900	0.86861000	1.49301100
N	-5.97156300	2.14690300	-0.05421800
C	-6.30877200	3.46450800	-0.58273900
C	-5.47836400	3.87981000	-1.79921500
H	-6.20021500	4.19338200	0.21842200
H	-7.36986800	3.45282100	-0.84800400
H	-5.75662900	4.88419700	-2.13244300
H	-4.41093600	3.87725200	-1.57098600
H	-5.63570200	3.19777400	-2.63824500
C	-6.61622400	0.95639000	-0.61201200
C	-5.71308400	0.14931900	-1.54312900
H	-7.51024600	1.29227400	-1.14251700
H	-6.94199100	0.32464000	0.21599100
H	-6.24340500	-0.72845700	-1.92335400
H	-5.38602800	0.74398100	-2.40000400
H	-4.83234600	-0.19725500	-1.00128300
B	-0.89011600	5.00565500	-0.86873200
C	-1.29987400	2.85834000	-1.62282400
C	0.17059400	2.98480500	-1.07573000
C	0.33387500	2.39703900	0.32313700
H	-0.45301100	2.72445400	1.00437000

H	0.31063700	1.30580900	0.29695300
H	1.29806800	2.70548600	0.73056400
C	1.24548100	2.45222500	-2.00954800
H	2.22699400	2.59045000	-1.55267900
H	1.10583200	1.38350600	-2.19059000
H	1.24383400	2.97133900	-2.96734900
C	-2.08517500	1.67453300	-1.08441200
H	-3.09107100	1.67386000	-1.50589500
H	-1.60595600	0.73418600	-1.36802100
H	-2.17421000	1.70671900	0.00055900
C	-1.38966900	2.92075000	-3.14530900
H	-0.98965900	2.01379300	-3.60205300
H	-2.43588800	3.01497300	-3.44057900
H	-0.84744900	3.77744200	-3.54848700
O	-1.91083400	4.08952400	-1.11471600
O	0.34646000	4.43428500	-0.96142500
N	-1.20767800	6.33856400	-0.45904100
Si	-0.17657900	7.07547100	0.81546100
Si	-2.27123100	7.32281900	-1.49516200
C	0.21762600	5.75832900	2.08702500
H	0.83455800	6.19292000	2.88006800
H	-0.68365200	5.38122700	2.57879600
H	0.76859500	4.91724200	1.66689600
C	1.40173000	7.74068400	0.04788900
H	1.91784500	6.94829900	-0.50096400
H	1.21213800	8.56107700	-0.64834400
H	2.08640000	8.11273400	0.81636800
C	-1.15832300	8.41482000	1.68861700
H	-0.50761200	8.90339600	2.42152300
H	-1.55079200	9.20030500	1.04122500
H	-1.99187100	7.98741900	2.25453900
C	-1.45972300	8.96759700	-1.90399400
H	-1.25033900	9.59766100	-1.03933500
H	-0.51764400	8.80924900	-2.43585500
H	-2.11518200	9.53848700	-2.56935900
C	-3.92427000	7.59212100	-0.63296000
H	-3.81561600	7.90020800	0.40920800
H	-4.50063100	8.36850900	-1.14573800
H	-4.55246300	6.69388600	-0.64680800
C	-2.57600500	6.44520600	-3.12828000
H	-3.18489200	7.08690800	-3.77306600
H	-1.64293200	6.24591200	-3.66302300
H	-3.10195600	5.49831300	-3.01088600
Na	-3.09239400	4.91754000	0.69895200

TS3-4

E = -2235.78251113 a.u.

0 2

C	-3.46445000	0.64862500	2.84576100
C	-2.85109500	1.63359200	3.61427800
C	-2.72658700	2.94352100	3.15596100
C	-3.25645000	3.29624800	1.89323900
C	-3.84476400	2.28747300	1.11854600
C	-3.95367600	0.98392400	1.58564800
H	-1.95365200	3.66988200	5.02414800
H	-3.54911600	-0.36602300	3.22041000
H	-2.45583300	1.38346800	4.59529500
C	-2.02433300	3.99094800	3.98078900
C	-3.15525600	4.69597600	1.43846200
H	-4.22793700	2.54007100	0.14172200
H	-4.42040700	0.22790600	0.96151300
C	-2.99444900	5.69407000	2.43855900
C	-2.73702300	5.34118300	3.87155400
H	-3.21761600	6.73165500	2.21629900
H	-3.68592300	5.28876100	4.43541800
H	-2.15008400	6.11993200	4.36981600
H	-1.00153000	4.10697700	3.60867800
O	-4.30714100	5.05983100	0.43702900
C	-5.24652300	5.93792600	0.86100300
O	-5.16060000	7.13442200	0.52477000
N	-6.26823800	5.49205500	1.61226800
C	-6.54329900	4.07773400	1.86988800
C	-6.35199900	3.66576900	3.32467300
H	-5.89388600	3.49180100	1.23092400
H	-7.57518200	3.88453000	1.55423800
H	-6.52824600	2.59264300	3.42739800
H	-5.33150600	3.86314400	3.64859500
H	-7.04241000	4.18796500	3.99245200
C	-7.21509300	6.48423400	2.13731000
C	-6.66166800	7.25479500	3.33359100
H	-8.12125100	5.94244900	2.41564900
H	-7.47388800	7.17494400	1.33349100
H	-7.40577000	7.96547000	3.70428600
H	-6.39316800	6.58108100	4.14932900
H	-5.77163600	7.81424900	3.04456200
B	-1.39231700	4.56609200	-0.03159300
C	-1.62687000	5.20660200	-2.27758800
C	-2.01810600	3.69209700	-2.12819800

C	-3.52312500	3.44454500	-2.25550700
H	-4.08974500	4.06933100	-1.56826800
H	-3.87308100	3.61954900	-3.27634600
H	-3.72534500	2.40031400	-2.01181700
C	-1.28290500	2.76034800	-3.08805800
H	-1.56696400	1.72808100	-2.87508200
H	-1.54827400	2.97597900	-4.12727500
H	-0.20249400	2.83569800	-2.98517600
C	-2.58258800	6.03275100	-3.13270900
H	-2.25443700	7.07792500	-3.16035900
H	-2.59657800	5.67882300	-4.16583500
H	-3.60836400	5.98830500	-2.76042700
C	-0.18942500	5.42117000	-2.75775800
H	-0.05542200	5.12614600	-3.80081600
H	0.06184900	6.48087600	-2.66907700
H	0.51464500	4.86120200	-2.14469300
O	-1.69955300	5.68260300	-0.91608000
O	-1.59572900	3.38788900	-0.79005400
N	-0.22146600	4.62547200	0.85730000
Si	0.75293100	3.14366400	0.97447100
Si	0.48812700	6.16029500	1.33334200
C	-0.22672500	1.56992100	1.24022100
H	0.44430700	0.71542400	1.09474500
H	-0.63166100	1.50083600	2.24933900
H	-1.05687000	1.47581300	0.54410100
C	1.82541100	2.90900300	-0.56472300
H	1.21861300	2.62464000	-1.42589300
H	2.38878200	3.80723500	-0.82809700
H	2.55039100	2.10463000	-0.40108700
C	1.94362000	3.24380300	2.44161100
H	2.51887100	2.31203400	2.46415400
H	2.66556700	4.06151700	2.40168100
H	1.41086300	3.30998100	3.39356400
C	2.15752800	6.40881600	0.47843900
H	2.89562300	5.64715600	0.73801200
H	2.04422200	6.39418100	-0.60945100
H	2.58560300	7.37909700	0.75141600
C	0.75273200	6.35513600	3.18941500
H	1.33371200	5.55174100	3.64018200
H	1.29160500	7.29047500	3.37664800
H	-0.19787300	6.41701400	3.72066700
C	-0.51135700	7.70187500	0.85544900
H	0.01724100	8.58068100	1.23757600
H	-0.60475000	7.81296000	-0.22566000

H	-1.49337600	7.69725300	1.33530400
Na	-3.15024900	7.20555700	-0.38232500

I4

E = -2235.81754904 a.u.

0 2

C	-1.67097500	-3.99773000	1.96049500
C	-1.41112700	-2.93524500	2.82354100
C	-0.86847300	-1.74621500	2.34974300
C	-0.55417300	-1.61608600	0.97107000
C	-0.83035000	-2.69778200	0.11786200
C	-1.38773400	-3.87087300	0.60180700
H	-1.24022900	-0.67114000	4.17017700
H	-2.10235500	-4.91538200	2.34687400
H	-1.65071400	-3.02576100	3.87872000
C	-0.63003000	-0.57850200	3.26861500
C	-0.00490100	-0.35879500	0.45816300
H	-0.57401200	-2.60185000	-0.92301600
H	-1.59700700	-4.68997200	-0.07791600
C	-0.19505800	0.75548800	1.24383500
C	-0.93724600	0.72906000	2.53304800
H	0.17783000	1.71386200	0.91098700
H	-2.01517400	0.78825700	2.33041100
H	-0.69281300	1.60440900	3.13940900
H	0.41989200	-0.57105300	3.59244100
O	-3.00381700	0.54998100	-0.61995500
C	-3.31109000	1.43203400	0.23585000
O	-2.80076600	2.59662700	0.28235800
N	-4.23682300	1.10707700	1.22846100
C	-4.91722800	-0.17999100	1.20138900
C	-4.77078900	-0.95866600	2.50805400
H	-4.48525700	-0.74170400	0.37696800
H	-5.98324700	-0.02831000	0.97655700
H	-5.31174100	-1.90817000	2.45131300
H	-3.71989900	-1.18293800	2.70200000
H	-5.16746500	-0.40206600	3.36219900
C	-4.81716700	2.18034700	2.03283100
C	-3.98741600	2.57256800	3.25425000
H	-5.81096800	1.84865800	2.34973000
H	-4.95166700	3.05946900	1.39870200
H	-4.49627500	3.35249900	3.82983000
H	-3.82074000	1.71728600	3.91490200
H	-3.02146700	2.96080100	2.93191200
B	0.91711200	-0.19044100	-0.89916400

C	0.72758800	0.57151700	-3.12941600
C	0.48372900	-0.97237900	-3.09158500
C	-1.00979400	-1.32430400	-3.15302400
H	-1.58839000	-0.81747900	-2.37810400
H	-1.44374100	-1.08660100	-4.12751000
H	-1.13023900	-2.39927300	-3.00379100
C	1.23637800	-1.75791500	-4.15996200
H	1.03712900	-2.82455600	-4.03645700
H	0.91368800	-1.47071100	-5.16500500
H	2.31281400	-1.60974100	-4.08668700
C	-0.22967300	1.35374500	-4.02481100
H	-0.02511200	2.42647900	-3.94820000
H	-0.10204100	1.07622900	-5.07354400
H	-1.27761700	1.17215600	-3.77486700
C	2.17062200	0.93048900	-3.49810600
H	2.38514600	0.71696400	-4.54737600
H	2.33554400	1.99721500	-3.33484900
H	2.87897100	0.37983400	-2.88209500
O	0.48265800	0.93783600	-1.75871300
O	1.00307600	-1.32971500	-1.80728000
N	2.29897500	0.06664200	-0.18147000
Si	3.35086600	-1.36424200	0.05698200
Si	2.91470500	1.68532100	0.23870700
C	2.43888600	-2.95592300	0.43242400
H	3.19065000	-3.73974700	0.57760800
H	1.84322400	-2.90389600	1.34501700
H	1.78555700	-3.25779800	-0.38253200
C	4.38082600	-1.61313400	-1.50038000
H	3.73504900	-1.90241500	-2.33019400
H	4.93786200	-0.72100300	-1.79241200
H	5.10528000	-2.41869400	-1.34145300
C	4.51564800	-1.12002500	1.52433200
H	5.14631900	-2.01177100	1.60378900
H	5.18549900	-0.26234500	1.45606900
H	3.96052400	-1.03939600	2.46257100
C	4.62813200	1.88863500	-0.53215200
H	5.35509900	1.13921500	-0.21874100
H	4.56978800	1.85872000	-1.62307600
H	5.03043600	2.86827200	-0.25417200
C	3.02847000	1.91694700	2.10684800
H	3.77274300	1.27323300	2.57534400
H	3.29752700	2.95298600	2.33683100
H	2.06853600	1.71272900	2.58769200
C	1.93200600	3.15538700	-0.42128600

H	2.50553600	4.05577200	-0.17354700
H	1.81202100	3.11997800	-1.50173800
H	0.94305000	3.28715900	0.02132900
Na	-1.44457000	1.96939700	-1.37282900

TS4-5

E = -2235.79575759 a.u.

0 2

C	-1.68593800	-3.71341200	2.11585600
C	-1.73170200	-2.46972400	2.75321200
C	-1.22368700	-1.32405200	2.13864900
C	-0.65170100	-1.41372600	0.84204400
C	-0.64301400	-2.66506500	0.20241000
C	-1.14259600	-3.80518100	0.83369700
H	-1.95281200	0.01769500	3.64668700
H	-2.08408000	-4.59363200	2.60973900
H	-2.15484100	-2.38818400	3.74973500
C	-1.21102400	0.00695000	2.84391700
C	-0.13704900	-0.19340900	0.17669100
H	-0.24325400	-2.72672500	-0.79929800
H	-1.11830700	-4.75943500	0.31753700
C	-0.57660600	0.99678000	0.64455300
C	-1.45340500	1.14554600	1.85316100
H	-0.32417000	1.89408400	0.09392700
H	-2.50744800	1.16017100	1.53487100
H	-1.27360900	2.11239900	2.33336600
H	-0.23107000	0.12485100	3.32145400
O	3.11756200	-2.73891900	3.89693800
C	2.63908500	-1.73548400	4.52364800
O	1.51587500	-1.20649000	4.24050200
N	3.39415400	-1.20258100	5.54964500
C	4.65673500	-1.83285300	5.91690100
C	5.83348400	-1.42353600	5.03009200
H	4.53196500	-2.91619200	5.87082300
H	4.86305500	-1.56868900	6.95913900
H	6.75863800	-1.90020300	5.37047800
H	5.64960700	-1.73659600	4.00212000
H	5.98371100	-0.34121300	5.04094100
C	2.87481900	-0.12845500	6.38086400
C	3.68945300	1.16278800	6.29738500
H	2.83409300	-0.46921000	7.42533000
H	1.85305700	0.04944200	6.05398900
H	3.23667100	1.94217200	6.91826300
H	4.71611700	1.01976800	6.64562200

H	3.72951600	1.52253300	5.26734100
B	0.76705900	-0.17066500	-1.13523000
C	1.03048700	0.78437700	-3.23645700
C	0.56879700	-0.70959100	-3.37966200
C	-0.93746300	-0.84084600	-3.62862500
H	-1.50618300	-0.26219600	-2.89890700
H	-1.22049100	-0.51251100	-4.63140000
H	-1.22288300	-1.88913800	-3.51955200
C	1.33723800	-1.52415600	-4.41012900
H	0.97477200	-2.55459300	-4.41304600
H	1.19594000	-1.11573100	-5.41453400
H	2.40456400	-1.54408700	-4.19645500
C	0.23271500	1.77825500	-4.07288500
H	0.61065000	2.78863200	-3.90191900
H	0.32640900	1.55997800	-5.14050200
H	-0.82285200	1.76725700	-3.80517500
C	2.52679900	0.98792200	-3.48380100
H	2.79445300	0.85002400	-4.53402300
H	2.79544800	2.00694200	-3.19716400
H	3.12083800	0.30486200	-2.88148200
O	0.76529500	1.04738000	-1.84809400
O	0.82732700	-1.24489300	-2.06271400
N	2.58484700	-0.25911100	-0.24446700
Si	3.58059000	-1.74706300	-0.33897900
Si	3.23849000	1.21303600	0.54458500
C	2.56501600	-3.32212300	-0.46468400
H	3.26121800	-4.16355900	-0.54154600
H	1.92175900	-3.52413900	0.39334000
H	1.92996900	-3.30814100	-1.34807600
C	4.60140000	-1.63724600	-1.92401200
H	3.98173300	-1.76459400	-2.81132100
H	5.15735200	-0.70437800	-2.01866100
H	5.32876100	-2.45556400	-1.90639200
C	4.75353000	-1.95627500	1.11258900
H	5.34674200	-2.86007500	0.93221600
H	5.45801600	-1.13113400	1.22885300
H	4.23783800	-2.10714100	2.06485500
C	4.94071800	1.52960900	-0.21961200
H	5.64644600	0.70948600	-0.08286500
H	4.86212100	1.73579000	-1.29009900
H	5.37447800	2.41704800	0.25229100
C	3.37741000	0.91494600	2.39354500
H	4.20254400	0.25979300	2.66946300
H	3.54525200	1.88413700	2.87545300

H	2.46855500	0.48670700	2.82184000
C	2.24070600	2.77886400	0.27531300
H	2.91221500	3.63528600	0.39940100
H	1.79529700	2.82601100	-0.71643200
H	1.44436200	2.88353900	1.01336000
Na	1.24639700	-2.81420700	2.71100000

I5

E = -2235.82738475 a.u.

0 2

C	-1.88951300	-2.97248600	3.00871100
C	-1.72771400	-1.68635800	3.52059700
C	-1.49449300	-0.60227700	2.68200400
C	-1.42091500	-0.80481000	1.28790900
C	-1.60093900	-2.10024600	0.78204700
C	-1.82914300	-3.17887300	1.63405700
H	-1.65547500	0.88811800	4.22429200
H	-2.06259300	-3.80695400	3.68019900
H	-1.76797100	-1.52477400	4.59383000
C	-1.22624800	0.77734800	3.22479400
C	-1.14325600	0.35158800	0.40275500
H	-1.56128300	-2.26607000	-0.28813200
H	-1.96385300	-4.17387500	1.22264400
C	-1.31750200	1.60338200	0.87524700
C	-1.75344300	1.86821300	2.28742300
H	-1.13241800	2.45063700	0.22159800
H	-2.85333900	1.90029300	2.32046600
H	-1.40964400	2.85338400	2.61413500
H	-0.13895900	0.87035300	3.32328700
O	3.06562600	-2.24444600	2.12636500
C	2.50302500	-1.47141900	2.97197100
O	1.58703300	-0.65247200	2.67370200
N	2.92115200	-1.52024400	4.29211600
C	3.88764300	-2.51015100	4.74160000
C	5.18778500	-1.89908600	5.26507100
H	4.08970800	-3.15841000	3.89204300
H	3.43000400	-3.12997000	5.52521400
H	5.87921900	-2.68426300	5.58613100
H	5.67880600	-1.30922700	4.48791200
H	5.01071000	-1.24352400	6.12235300
C	2.20978200	-0.72339000	5.28557500
C	2.63450900	0.74470900	5.31589300
H	2.38613700	-1.18377800	6.26263300
H	1.13815700	-0.78752500	5.08257500

H	2.06899300	1.29560000	6.07460400
H	3.69850200	0.84595300	5.54328500
H	2.44644700	1.20610300	4.34624600
B	-0.53990000	0.18481300	-1.00864000
C	0.30952200	0.70451800	-3.07053400
C	0.47347800	-0.83230300	-2.80875800
C	-0.60898200	-1.68135200	-3.47196500
H	-1.60758400	-1.29350200	-3.26247400
H	-0.47577900	-1.72404700	-4.55473600
H	-0.55277800	-2.69951200	-3.08237700
C	1.85488000	-1.38453500	-3.11176300
H	1.87331700	-2.46278000	-2.94349700
H	2.11851500	-1.20936900	-4.15775800
H	2.61246800	-0.92994000	-2.47688800
C	-0.30890800	1.06306700	-4.41241200
H	-0.38975700	2.14804600	-4.49962100
H	0.31351400	0.70349600	-5.23604100
H	-1.30784500	0.64259700	-4.52050400
C	1.60555100	1.48242500	-2.84971100
H	2.31282900	1.32190200	-3.66608600
H	1.37719500	2.54820600	-2.79796700
H	2.09042900	1.19335900	-1.91830500
O	-0.61774100	1.10314800	-2.01639700
O	0.23353900	-0.91473400	-1.36365800
N	3.75854000	-0.60111200	-0.02138500
Si	4.82615200	-1.95665100	-0.33035500
Si	4.08433200	0.99146900	0.64196900
C	3.84362600	-3.54786200	-0.54562400
H	4.48437300	-4.34484400	-0.93634300
H	3.44215200	-3.87319200	0.41476500
H	3.01575900	-3.43316300	-1.25182000
C	5.65112100	-1.55086900	-1.98999800
H	4.92151900	-1.41224300	-2.79160000
H	6.26102700	-0.64633700	-1.93568900
H	6.30862000	-2.37630800	-2.28275000
C	6.16291000	-2.21344900	0.96448700
H	6.71261900	-3.14053600	0.77209600
H	6.88991100	-1.39740400	0.97993500
H	5.70340300	-2.28978700	1.95045400
C	5.08615200	1.90562100	-0.67971500
H	6.08820100	1.48484200	-0.79323700
H	4.59883300	1.87647200	-1.65755600
H	5.19748700	2.95752300	-0.39722700
C	5.06950600	0.91343800	2.24178500

H	6.08103000	0.53404800	2.08349600
H	5.15091400	1.91101600	2.68528600
H	4.58052700	0.26825700	2.97268000
C	2.48667400	1.92578700	0.96288400
H	2.70512100	2.91345800	1.38290500
H	1.89150400	2.08296700	0.06069300
H	1.87686800	1.37782900	1.68281300
Na	1.57458400	-1.46458800	0.53542100

TS4-5’

E = -1671.48140139 a.u.

0 2

C	-1.77047300	-3.88968300	1.72848500
C	-1.34948200	-2.87320800	2.58435100
C	-0.79779400	-1.69957000	2.08068500
C	-0.63668300	-1.54159000	0.68633700
C	-1.08337600	-2.56306200	-0.16250800
C	-1.64656200	-3.72505700	0.35170700
H	-0.81528600	-0.66877300	3.96932100
H	-2.20158200	-4.79840800	2.13579200
H	-1.46044300	-2.99034100	3.65866700
C	-0.35436300	-0.57575500	2.98275600
C	-0.05928200	-0.28855300	0.15973900
H	-0.95734500	-2.44626300	-1.22928000
H	-1.98161800	-4.50591400	-0.32316800
C	-0.14617400	0.81769000	0.94311000
C	-0.68614500	0.77461800	2.34181900
H	0.16310200	1.77522100	0.54382500
H	-1.77719300	0.91831100	2.32291500
H	-0.28142200	1.59966200	2.93529100
H	0.73298300	-0.63434000	3.13095400
B	0.61487900	-0.15136100	-1.26466300
C	0.93038800	0.81982800	-3.32359100
C	0.59111300	-0.70048200	-3.50459100
C	-0.87082900	-0.93866400	-3.89424500
H	-1.54778400	-0.40714600	-3.22320400
H	-1.07875500	-0.62277800	-4.91904900
H	-1.08947400	-2.00590700	-3.81827500
C	1.51027900	-1.45821500	-4.45158200
H	1.22556400	-2.51231400	-4.47563200
H	1.43302000	-1.06454100	-5.46888700
H	2.55117800	-1.39910500	-4.13872100
C	0.15463700	1.76395400	-4.23192400
H	0.45050000	2.79546600	-4.02862600

H	0.36223800	1.55547700	-5.28525500
H	-0.91879300	1.68531700	-4.06458000
C	2.43080300	1.10976000	-3.42631200
H	2.79257300	0.99910600	-4.45106700
H	2.61951000	2.13745500	-3.11105500
H	3.00487700	0.44843700	-2.77925500
O	0.50925300	1.05467700	-1.96123800
O	0.76169600	-1.21788100	-2.16427100
N	2.48986100	-0.08678400	-0.26320200
Si	3.30502000	-1.64886900	-0.05177900
Si	3.15726400	1.42321000	0.38207500
C	2.16844900	-3.13499100	-0.01106900
H	2.79711600	-4.03244000	0.00109400
H	1.53522500	-3.16769600	0.87612700
H	1.52595200	-3.17840200	-0.88780400
C	4.43559000	-1.81652600	-1.55638100
H	3.84130500	-1.92197300	-2.46537300
H	5.11085900	-0.96929300	-1.68455500
H	5.04713400	-2.71876600	-1.45183100
C	4.35654000	-1.75386400	1.51567900
H	4.85618600	-2.72790600	1.54485400
H	5.13365300	-0.99018900	1.58557800
H	3.73869600	-1.68572000	2.41537800
C	4.93738100	1.53178300	-0.25498800
H	5.57231800	0.70908100	0.07740300
H	4.96576000	1.55919100	-1.34720900
H	5.38670100	2.46235100	0.10734700
C	3.17936400	1.45190100	2.26855100
H	3.78699200	0.65899500	2.70504400
H	3.58263900	2.40961100	2.61465300
H	2.16872600	1.35876200	2.67258500
C	2.27235600	2.98406400	-0.20127200
H	3.00388200	3.70375800	-0.58188000
H	1.55573400	2.77802500	-0.99361300
H	1.74153400	3.47348100	0.62022200

3a'

E = -798.026005367 a.u.

0 1

C	-1.25300700	0.92702500	-0.47918100
C	-0.33576900	0.01205800	0.03451900
C	0.72846600	0.43209400	0.82606700
C	0.88720200	1.80448600	1.11818100
C	-0.04371300	2.71338800	0.59854800

C	-1.10354300	2.28001400	-0.19299600
H	1.37690900	-0.79288200	2.44954700
H	-2.07587700	0.58339900	-1.09767900
H	-0.44903400	-1.04642600	-0.18331000
C	1.70090500	-0.55504700	1.42658800
C	2.04397000	2.24031500	1.93640700
H	0.06180700	3.76513200	0.82767100
H	-1.81178900	3.00251900	-0.58584800
C	3.08895800	1.39956900	2.09269900
C	3.11467900	0.02574900	1.48667200
H	3.95656500	1.73141700	2.65457500
H	3.77997800	-0.63411200	2.05075800
H	3.53584200	0.09091200	0.47174400
H	1.68832800	-1.49444300	0.86743800
B	2.15766200	3.63263600	2.61167100
C	1.77243100	5.81542300	3.17697200
C	2.97324900	5.24452000	4.01171300
C	2.57795200	4.83598700	5.43167600
H	3.39399500	4.26167700	5.87371100
H	2.38537300	5.70429800	6.06564500
H	1.68744200	4.20468500	5.42930800
C	4.21404800	6.12452700	4.03982900
H	4.60510500	6.29846100	3.03825400
H	3.99716000	7.09089200	4.50309400
H	4.99628000	5.63750400	4.62539500
C	0.70881800	6.54070400	3.98727300
H	-0.08983300	6.88094400	3.32518000
H	0.26500900	5.89050200	4.73991200
H	1.13001400	7.41725700	4.48702400
C	2.21699500	6.67252100	1.99120700
H	2.97805400	6.16334500	1.39713500
H	1.35687800	6.85924500	1.34575000
H	2.61766300	7.63538400	2.31551700
O	1.18623800	4.60471200	2.62018100
O	3.28772600	4.02038800	3.29512400

I6

E = -3135.86722510 a.u.

0 1

C	3.30678800	-2.12369200	-4.43300100
C	3.44020100	-0.99576100	-3.62318000
C	3.66195700	-1.11525500	-2.25377300
C	3.75008700	-2.39567700	-1.65450600
C	3.65262400	-3.51537000	-2.49205500

C	3.42486400	-3.38608200	-3.85993700
H	4.95699600	0.26598400	-1.28563900
H	3.13132900	-2.01332500	-5.49839100
H	3.37624000	-0.00442700	-4.06418400
C	3.87545200	0.10885500	-1.39832400
C	3.92723600	-2.52564800	-0.17998200
H	3.80094800	-4.48926900	-2.05880200
H	3.35369600	-4.27597500	-4.47776900
C	3.68052100	-1.41796700	0.55320000
C	3.27121300	-0.07991600	-0.01128000
H	3.81095700	-1.45928100	1.62746200
H	3.59771800	0.72516200	0.65530900
H	2.17429600	-0.00165600	-0.06207100
H	3.47786800	1.00027500	-1.89284700
C	-0.29264800	3.44094100	3.75110800
C	0.71987300	2.99529700	2.66616800
C	0.84781300	1.49112900	2.84317700
C	0.74212000	1.28698200	4.34882000
C	-0.35685100	2.27582200	4.78030200
H	0.02032000	4.37786600	4.21553100
H	-1.27477400	3.61832500	3.31060800
H	1.70457200	3.43842800	2.84167800
H	0.41958000	3.25586700	1.65070800
H	1.72990400	1.04674500	2.38539200
H	0.54527000	0.25247600	4.63333900
H	1.71040400	1.55655300	4.78305700
H	-1.33013600	1.78403100	4.73708400
H	-0.21460600	2.61678500	5.80704500
B	4.53467000	-3.88628000	0.61641000
O	5.06962100	-4.86702100	-0.33658700
O	5.70234800	-3.47788400	1.42089600
C	6.47787900	-5.01388400	-0.16436000
C	6.87402000	-3.72737900	0.65014200
C	7.13045300	-5.11611300	-1.54210000
C	6.73878400	-6.30698800	0.61611700
C	7.15809900	-2.51915400	-0.25852400
C	8.05979800	-3.91288200	1.59327400
H	6.80404700	-6.03550300	-2.03552300
H	6.84574700	-4.27912500	-2.17863000
H	8.22188600	-5.14544400	-1.46714300
H	6.30908300	-6.25268400	1.61475800
H	6.26408500	-7.13662800	0.08670900
H	7.80530500	-6.53059000	0.70737200
H	7.18738500	-1.61922000	0.35988700

H	8.11788500	-2.61558800	-0.77321300
H	6.38173400	-2.38052100	-1.00946100
H	7.88018800	-4.70183400	2.32154000
H	8.96977000	-4.15875600	1.03798200
H	8.24028300	-2.98441400	2.14091100
O	-0.33347100	0.91087300	2.15668200
P	-0.55842000	-0.64187000	2.10567200
O	0.65471000	-1.49079500	2.21926300
O	-1.38441000	-0.87669300	0.74510600
O	-1.64947700	-0.89201000	3.26045400
C	-0.92989400	-1.80807600	-0.20549300
C	-2.13707900	-2.20165300	3.43711600
C	-0.12855000	-1.36823000	-1.25131800
C	-1.27528200	-3.14727100	-0.05852400
C	-1.32464900	-3.16603700	4.01955700
C	-3.42296400	-2.48975100	3.00234300
C	0.35015300	-2.29761300	-2.17303300
H	0.12643200	-0.31831900	-1.32734700
C	-0.79265300	-4.06766700	-0.99027200
H	-1.89666600	-3.45657400	0.77370200
C	-1.81668300	-4.46108100	4.16010700
H	-0.32333200	-2.90715400	4.33748100
C	-3.90653200	-3.78797200	3.15560800
H	-4.01848700	-1.70903400	2.54519400
C	0.02008800	-3.64537800	-2.04146800
H	1.00239300	-1.97436600	-2.97369400
H	-1.03753900	-5.11720300	-0.87758200
C	-3.10392300	-4.77409100	3.72715300
H	-1.18504100	-5.22314100	4.60124000
H	-4.90942600	-4.02751300	2.82009800
H	0.41336300	-4.36316600	-2.75035200
H	-3.48126500	-5.78456000	3.83633800
N	3.44916200	-4.53340300	1.62226200
Na	1.70964200	-3.04540700	1.08919400
Si	3.82844300	-4.31274800	3.33523500
Si	2.62318700	-6.01475500	1.15817400
C	4.05280300	-2.51084600	3.84963500
H	4.25514800	-2.48609000	4.92622900
H	4.89794200	-2.05189100	3.33845200
H	3.15578300	-1.90666100	3.67997000
C	2.34550600	-4.86736500	4.39447600
H	1.40850300	-4.39566200	4.08793700
H	2.18582300	-5.94765700	4.40727900
H	2.53737700	-4.56288700	5.42886900

C	5.28741300	-5.29374100	4.01343000
H	6.23044300	-4.85513400	3.69199400
H	5.26423400	-5.28525900	5.10873100
H	5.27356400	-6.33864600	3.69662400
C	0.80161000	-5.98726000	1.74618200
H	0.68877300	-6.23967000	2.79982200
H	0.27250400	-5.03892200	1.59837800
H	0.23980500	-6.73431800	1.17540700
C	3.36014700	-7.59199100	1.88175500
H	3.36231100	-7.59553700	2.97446700
H	2.78125000	-8.46241300	1.55505100
H	4.38940300	-7.73474300	1.54811800
C	2.45619000	-6.27076700	-0.69856400
H	2.00606700	-5.41523700	-1.20527500
H	3.42117900	-6.46292900	-1.16216900
H	1.80174300	-7.13208400	-0.87153600

TS6-7

E = -3135.83668248 a.u.

0 1

C	3.80287800	-2.64650200	-4.80165500
C	4.14032000	-1.41577300	-4.23385600
C	4.15417400	-1.24161900	-2.85261800
C	3.80495900	-2.31281200	-1.99433300
C	3.50667000	-3.54907600	-2.58644100
C	3.49682200	-3.72018300	-3.96856400
H	5.62710700	-0.01361300	-1.92988700
H	3.79615100	-2.76546300	-5.88074600
H	4.39785300	-0.57864900	-4.87901700
C	4.56974100	0.06519000	-2.22060400
C	3.71653100	-2.15551400	-0.52232200
H	3.29469600	-4.38186800	-1.93149200
H	3.25632100	-4.69030800	-4.39412200
C	3.66650100	-0.87514200	-0.08438100
C	3.74895000	0.36173400	-0.96505500
H	3.58081400	-0.66082500	0.98661300
H	4.19693000	1.19908700	-0.41721900
H	2.73846800	0.69413600	-1.24949600
H	4.50566700	0.88348200	-2.94533300
C	-0.26825400	2.72715700	4.09774200
C	0.56040700	2.41577500	2.82513500
C	0.73875600	0.90577500	2.83022400
C	0.87508500	0.55872200	4.30718100
C	-0.16842800	1.45884200	4.99292500

H	0.11683100	3.61347900	4.60548500
H	-1.30777400	2.93578200	3.84101000
H	1.55324000	2.87140400	2.88001200
H	0.09321400	2.76098200	1.90214000
H	1.54838400	0.53978700	2.19986500
H	0.75880500	-0.50595200	4.51252400
H	1.89155800	0.82704600	4.61241000
H	-1.13086300	0.94492900	5.02882000
H	0.10970000	1.69367800	6.02174300
B	4.48393800	-4.22621700	1.02276000
O	4.78547000	-5.10186600	-0.01550600
O	5.62761400	-3.59818300	1.50296100
C	6.22368700	-5.18294200	-0.14404400
C	6.73246100	-3.89705700	0.62111700
C	6.58090800	-5.22432900	-1.62379300
C	6.64004400	-6.49102400	0.53459600
C	6.97494800	-2.69477900	-0.29083900
C	7.96874200	-4.12513200	1.48659500
H	6.17122900	-6.13188700	-2.07348600
H	6.16659900	-4.37284200	-2.15933400
H	7.66544600	-5.23909100	-1.76391900
H	6.36860200	-6.49083200	1.59187900
H	6.11471900	-7.31908000	0.05409200
H	7.71389600	-6.67452600	0.45256000
H	7.12108600	-1.80826100	0.32934100
H	7.86858100	-2.83952500	-0.90362900
H	6.12646100	-2.50313000	-0.93942800
H	7.80418700	-4.89298800	2.24150200
H	8.82709900	-4.41699400	0.87543300
H	8.22429700	-3.19665500	2.00180000
O	-0.52291400	0.35770800	2.27662100
P	-0.77323300	-1.19555900	2.18310500
O	0.44109100	-2.04593500	2.27393400
O	-1.61240400	-1.40267600	0.82717700
O	-1.87156600	-1.47651500	3.31096800
C	-0.89292000	-1.57737500	-0.37449200
C	-2.17632400	-2.81009100	3.65458800
C	-0.36842400	-0.47036800	-1.02699400
C	-0.70900200	-2.86915800	-0.85582000
C	-1.60310900	-3.34123300	4.79975000
C	-3.03514200	-3.54715600	2.85122300
C	0.36917500	-0.66818400	-2.19341300
H	-0.52758200	0.51924400	-0.61611000
C	0.03317200	-3.04811600	-2.02363300

H	-1.13080200	-3.70833300	-0.31378500
C	-1.89714100	-4.65647700	5.14860200
H	-0.93182400	-2.73451900	5.39438300
C	-3.31955700	-4.86298100	3.21052700
H	-3.46119300	-3.09453000	1.96447200
C	0.57949500	-1.95138600	-2.68862500
H	0.80358200	0.18317600	-2.70328400
H	0.20506400	-4.04839100	-2.40309300
C	-2.75092200	-5.41870700	4.35450600
H	-1.44665600	-5.08593000	6.03621000
H	-3.98685000	-5.45263700	2.59179900
H	1.19023100	-2.10156400	-3.56940700
H	-2.97156500	-6.44493700	4.62581900
N	3.32440800	-4.43251000	1.91750000
Na	1.93450600	-2.79182300	0.84914700
Si	3.60863100	-3.81335700	3.56736200
Si	2.29699000	-5.85003600	1.60998400
C	3.86151300	-1.95151000	3.51122800
H	4.16076000	-1.58155400	4.49759200
H	4.63405800	-1.67792100	2.79376700
H	2.93223200	-1.44160000	3.24244900
C	2.11476600	-4.10090700	4.68081600
H	1.19945000	-3.68581500	4.25964600
H	1.93860700	-5.15142700	4.92199000
H	2.30961500	-3.58488500	5.62788800
C	5.07094100	-4.66805700	4.38843200
H	6.00882700	-4.37909200	3.91540000
H	5.12703400	-4.40909300	5.45098800
H	4.98190600	-5.75646700	4.32125500
C	0.56052400	-5.61187100	2.32524100
H	0.47719300	-5.85673100	3.38320300
H	0.17630400	-4.59511300	2.21130500
H	-0.12477200	-6.27688700	1.78956700
C	3.05983000	-7.40211000	2.34787400
H	3.17531500	-7.31838700	3.43249000
H	2.44195800	-8.28401500	2.15099700
H	4.04954200	-7.58545200	1.92277400
C	1.99367000	-6.10438900	-0.23026700
H	1.55057000	-5.22421100	-0.70531800
H	2.90889100	-6.33978400	-0.76801600
H	1.28407200	-6.92874900	-0.35880800

TS6-7’

E = -1833.86016198 a.u.

0 1

C	4.17788200	-2.74277400	-4.74668000
C	4.52954400	-1.53961400	-4.13477000
C	4.29768100	-1.32898300	-2.77815500
C	3.71545900	-2.35142100	-1.98876100
C	3.37475500	-3.55377700	-2.62526600
C	3.59035300	-3.75033700	-3.98613100
H	5.68179300	-0.13667000	-1.66575900
H	4.36079600	-2.88856500	-5.80677700
H	4.98149400	-0.74680400	-4.72629400
C	4.67909000	-0.03216300	-2.10348200
C	3.50619700	-2.18491300	-0.53226500
H	2.96599800	-4.35169300	-2.02095600
H	3.31529400	-4.69376600	-4.44838300
C	3.48820300	-0.90188800	-0.09453000
C	3.69257500	0.31269900	-0.98630400
H	3.38502100	-0.67315200	0.97351700
H	4.06025100	1.16632500	-0.40686000
H	2.73605500	0.62937400	-1.42874400
H	4.74258000	0.77590300	-2.83883300
B	4.39770400	-4.16002300	0.96764100
O	4.70016000	-5.03739800	-0.06417700
O	5.53452400	-3.50471000	1.42806000
C	6.13943800	-5.10533600	-0.20335200
C	6.64102400	-3.80708100	0.54502000
C	6.48620200	-5.15741500	-1.68491000
C	6.57171700	-6.40277400	0.48567200
C	6.86584000	-2.61292100	-0.37921300
C	7.88401900	-4.01418000	1.40544700
H	6.08356600	-6.07373100	-2.12248300
H	6.05828200	-4.31744900	-2.22728100
H	7.56991500	-5.16175800	-1.83164500
H	6.30787700	-6.39499400	1.54502200
H	6.05099900	-7.24008800	0.01652600
H	7.64642100	-6.57763500	0.39822800
H	6.99873800	-1.71747700	0.23081100
H	7.76089600	-2.75001600	-0.99108900
H	6.01828100	-2.44682600	-1.03469700
H	7.73836200	-4.78314000	2.16271400
H	8.74194400	-4.29489700	0.78881800
H	8.13015800	-3.08038600	1.91561500
N	3.27900500	-4.40639000	1.91993400
Na	1.87715700	-2.73596000	1.00340200
Si	3.67557800	-3.86133900	3.57383400

Si	2.26581500	-5.83906300	1.63357100
C	3.86495100	-1.98860300	3.57152700
H	4.23972500	-1.64398300	4.54052100
H	4.56476100	-1.66366300	2.80248400
H	2.91008700	-1.47139700	3.41256700
C	2.26338100	-4.23673300	4.77024200
H	1.31207600	-3.78061100	4.48538400
H	2.09034000	-5.30332600	4.92921600
H	2.53890200	-3.81367100	5.74215000
C	5.20132400	-4.70460200	4.27507500
H	6.10944200	-4.31916800	3.81458700
H	5.26920600	-4.54659600	5.35615100
H	5.16994500	-5.78437400	4.10390800
C	0.51925900	-5.53512300	2.31308900
H	0.43443400	-5.58804600	3.39704600
H	0.09712600	-4.56767600	2.00688900
H	-0.15048000	-6.29448000	1.89734900
C	2.99663200	-7.36136600	2.45659800
H	3.10198500	-7.23915800	3.53794000
H	2.37306000	-8.24413300	2.28526300
H	3.98898900	-7.57280500	2.04975000
C	1.97112200	-6.16881000	-0.19076000
H	1.48840000	-5.32470100	-0.69279200
H	2.89324600	-6.38058800	-0.72588000
H	1.29635000	-7.02598800	-0.28772200

I7

E = -3135.85495917 a.u.

0 1

C	4.53086500	-0.18170700	-3.65417300
C	5.41202400	0.25794700	-2.66475100
C	5.11088400	0.10677500	-1.31402200
C	3.91325000	-0.53966700	-0.91507100
C	3.03632100	-0.95718400	-1.93007700
C	3.32848300	-0.77608700	-3.27931000
H	6.69079100	-0.20401800	0.09821500
H	4.77668600	-0.04802500	-4.70318100
H	6.34205400	0.74425300	-2.95120200
C	6.02992700	0.61239900	-0.22813800
C	3.60592600	-0.81254700	0.51123000
H	2.10619800	-1.44061500	-1.64339700
H	2.62505800	-1.10956200	-4.03572800
C	4.23836200	-0.00025800	1.38810400
C	5.21810200	1.08878700	0.97968900

H	4.07554200	-0.10522900	2.46338000
H	5.88861600	1.34228100	1.80805300
H	4.68713900	2.01725700	0.71724300
H	6.67708900	1.40603900	-0.61541700
C	-0.64486900	2.26340700	2.17281700
C	0.27994900	1.58450100	1.12556500
C	0.49733300	0.16505300	1.62078300
C	0.41763700	0.27986200	3.13536300
C	-0.73037700	1.27491100	3.36744800
H	-0.23154900	3.22530200	2.48451500
H	-1.63503200	2.46532100	1.76039400
H	1.25933500	2.06782900	1.08316300
H	-0.12360900	1.58977100	0.11249400
H	1.40616800	-0.30455000	1.23978000
H	0.29233100	-0.68047700	3.63901600
H	1.37356200	0.69135000	3.47524200
H	-1.68348000	0.74102100	3.34841800
H	-0.65911300	1.77641600	4.33479400
B	4.44702500	-4.76188600	1.40465900
O	3.81089200	-4.73566000	0.16375600
O	5.80315900	-4.89674300	1.27528300
C	4.80390700	-5.06379800	-0.85458900
C	6.14117400	-4.67754100	-0.12860700
C	4.50427500	-4.26262500	-2.10972300
C	4.67006600	-6.56253400	-1.12056900
C	6.49063300	-3.19878800	-0.27994800
C	7.33245600	-5.55491400	-0.47700800
H	3.54475800	-4.57402700	-2.52825200
H	4.44797000	-3.19405000	-1.91473100
H	5.27262800	-4.43495200	-2.86783800
H	4.87256000	-7.14829800	-0.22147300
H	3.64905700	-6.77858000	-1.44156600
H	5.35040500	-6.89363300	-1.90750400
H	7.31339400	-2.95802100	0.39497000
H	6.80011800	-2.96003200	-1.29903600
H	5.64884400	-2.55484800	-0.02358100
H	7.15167800	-6.60043000	-0.22885300
H	7.56697200	-5.48304500	-1.54231800
H	8.20814800	-5.22210300	0.08318000
O	-0.66649400	-0.62578900	1.10847300
P	-0.80415500	-2.16395700	1.37721700
O	0.43804700	-2.91350500	1.69238600
O	-1.58683200	-2.71933800	0.08092300
O	-1.93441900	-2.27552800	2.50864900

C	-0.88465700	-2.83849400	-1.13113900
C	-2.09487600	-3.42889200	3.28788000
C	-0.88864000	-1.77425700	-2.02239800
C	-0.21412700	-4.02310000	-1.40931000
C	-2.03161300	-3.27892200	4.66585300
C	-2.33321300	-4.66415100	2.69886100
C	-0.20703700	-1.90783400	-3.22982200
H	-1.40749800	-0.86116200	-1.75924400
C	0.46764800	-4.14178200	-2.61832200
H	-0.22792900	-4.83188800	-0.69037600
C	-2.21190600	-4.39723700	5.47533100
H	-1.84125000	-2.29780300	5.08411600
C	-2.50365500	-5.77631600	3.51949300
H	-2.39108300	-4.74747700	1.62059800
C	0.47129300	-3.08747300	-3.52873300
H	-0.19247900	-1.07920400	-3.92833400
H	0.99621500	-5.06116800	-2.84373300
C	-2.44482400	-5.64684800	4.90528700
H	-2.16218000	-4.29010800	6.55317200
H	-2.68762600	-6.74574500	3.06953700
H	1.01066800	-3.18128200	-4.46409500
H	-2.57973500	-6.51646800	5.53869600
N	3.69619700	-4.60363900	2.61260300
Na	2.48365100	-2.91968800	0.85261200
Si	4.35258100	-3.56041500	3.90831600
Si	2.42781500	-5.80992600	2.95600300
C	5.89068800	-2.66168100	3.33397500
H	6.22231500	-1.99091800	4.13396900
H	6.70765400	-3.34222300	3.09565500
H	5.68583600	-2.04272100	2.45794900
C	3.05646200	-2.26525700	4.33418500
H	2.78034700	-1.69860300	3.44150800
H	2.14381800	-2.68382200	4.75827800
H	3.46399900	-1.55127400	5.05720800
C	4.78617500	-4.59343200	5.42302800
H	5.55049200	-5.33569400	5.17527100
H	5.19686900	-3.95276100	6.20997400
H	3.93442700	-5.12561800	5.85207800
C	1.26561900	-5.21529100	4.30118400
H	1.74314200	-5.00622900	5.25941700
H	0.73326100	-4.32079100	3.97515800
H	0.50980300	-5.98610500	4.47748600
C	3.27717800	-7.40904200	3.47283100
H	3.89353900	-7.26939100	4.36436800

H	2.54965700	-8.19739200	3.69103400
H	3.93474500	-7.78042300	2.68027300
C	1.36343900	-6.15126300	1.44538000
H	0.77865000	-5.26367000	1.20070500
H	1.93704600	-6.44697800	0.56737600
H	0.65747800	-6.95411000	1.68258300

TS7-8

E = -3135.82725937 a.u.

0 1

C	-0.32350200	0.67256000	0.18909900
C	0.41935500	1.71667900	0.74113500
C	0.15028200	2.19649300	2.02080700
C	-0.87637500	1.60663800	2.79952200
C	-1.61964800	0.56625700	2.21439300
C	-1.35582000	0.10247100	0.92938500
H	1.81235300	2.88652700	3.17728800
H	-0.09847300	0.31204300	-0.80946600
H	1.21936200	2.17119500	0.16130400
C	0.95932400	3.31627800	2.63372000
C	-1.12407800	2.01896800	4.20277900
H	-2.41438300	0.09592800	2.78551100
H	-1.93899300	-0.71725600	0.52374200
C	-0.64219300	3.22710800	4.55769600
C	0.12181300	4.13836600	3.61566400
H	-0.82132100	3.62280100	5.56016700
H	0.76189000	4.83416800	4.16774700
H	-0.59210600	4.76319400	3.05382000
H	1.38204200	3.95152100	1.84938300
C	-4.66238800	4.32708500	4.04775400
C	-4.08399600	3.05564600	3.39843200
C	-3.71947000	2.18275500	4.55458200
C	-3.71836100	2.97749900	5.83050900
C	-3.88129300	4.44252300	5.36929700
H	-4.56007200	5.20904200	3.41268700
H	-5.72672000	4.18023800	4.25102300
H	-3.16266700	3.27277700	2.84907000
H	-4.75984100	2.54872700	2.70953200
H	-3.25119300	1.23815200	4.43969700
H	-4.58403600	2.66983000	6.42233500
H	-2.82418400	2.79146700	6.42399500
H	-4.38983300	5.05880900	6.11321400
H	-2.89760700	4.88090100	5.18391600
B	0.19181100	-2.38854900	5.48925000

O	0.65345600	-1.11406700	5.81349300
O	0.98932600	-3.00047800	4.55663000
C	1.99222200	-0.97045400	5.23743800
C	1.95671100	-2.02322600	4.06916600
C	2.98771300	-1.32546700	6.33941300
C	2.17867300	0.46777400	4.79074300
C	3.27385400	-2.74361000	3.82321200
C	1.41203400	-1.45339200	2.76254000
H	2.82101500	-0.66976800	7.19602200
H	2.87111900	-2.35715200	6.67438800
H	4.01700300	-1.18762000	6.00283800
H	1.38418800	0.78773700	4.12313800
H	2.17030600	1.13257800	5.65631400
H	3.13787300	0.58739000	4.27985400
H	3.15040300	-3.46037500	3.00929500
H	4.05468600	-2.03578600	3.53308100
H	3.60787500	-3.29019400	4.70426200
H	0.47057800	-0.92358600	2.89834500
H	2.11552000	-0.75917800	2.30054700
H	1.23520800	-2.27195900	2.06281300
O	-5.45661700	1.13725000	4.74971200
P	-5.17455000	-0.23493400	5.34217900
O	-3.73999200	-0.66577400	5.49256900
O	-6.01511100	-1.37423300	4.51562200
O	-5.97131100	-0.28042400	6.75181500
C	-5.66023400	-1.79535000	3.24440500
C	-5.89725100	-1.30934000	7.68165300
C	-5.13907600	-0.92783600	2.28681800
C	-5.87814100	-3.13593400	2.94215800
C	-5.34390300	-1.02211700	8.92483700
C	-6.42838800	-2.56534400	7.40679600
C	-4.81129300	-1.42278300	1.02686600
H	-5.01176100	0.12032400	2.52008700
C	-5.55382100	-3.61696700	1.67777900
H	-6.29555700	-3.78338400	3.70312100
C	-5.32284800	-2.00695200	9.90799000
H	-4.94579400	-0.03118300	9.10668000
C	-6.39563800	-3.54552400	8.39601200
H	-6.85900400	-2.75766200	6.43327000
C	-5.01136900	-2.76522900	0.71688400
H	-4.40352300	-0.74457300	0.28572200
H	-5.72275100	-4.66324500	1.44581300
C	-5.84756400	-3.27109300	9.64691500
H	-4.89290400	-1.78487000	10.87881600

H	-6.80398500	-4.52786100	8.18459400
H	-4.75450400	-3.14348100	-0.26633700
H	-5.82469100	-4.03914100	10.41196900
N	-1.01725200	-2.90006900	6.04284900
Na	-1.53621600	-0.12246500	5.49054800
Si	-1.96124400	-3.95584400	4.94877000
Si	-1.21576200	-2.68535200	7.79652900
C	-1.07166100	-5.60172800	4.76694300
H	-1.60432300	-6.27144200	4.08410300
H	-0.06166300	-5.45391600	4.37885900
H	-0.98676900	-6.11462900	5.73034600
C	-3.70369900	-4.24741300	5.57171100
H	-3.77156400	-4.95492300	6.39723700
H	-4.18326100	-3.31521100	5.86946000
H	-4.28205900	-4.65768900	4.73911700
C	-2.10470700	-3.07441100	3.29914200
H	-1.13888900	-2.81877700	2.86301400
H	-2.64064500	-3.69537400	2.57606900
H	-2.69044400	-2.16007400	3.41264100
C	-2.43128000	-3.91213100	8.52076500
H	-3.46487800	-3.70355600	8.25267000
H	-2.20068500	-4.94285700	8.23934100
H	-2.36580300	-3.85212900	9.61187000
C	-1.79066700	-0.94038500	8.21692800
H	-2.72071700	-0.69105000	7.70149300
H	-1.99038900	-0.86461600	9.28979000
H	-1.02595000	-0.18883000	7.99163700
C	0.44741200	-2.97468100	8.63074400
H	0.87120600	-3.94446500	8.35308700
H	1.17607500	-2.20420200	8.37546700
H	0.33281600	-2.96762700	9.71934100

I8

E = -3135.95897252 a.u.

0 1

C	-1.12028600	-0.38812700	0.58369800
C	-0.16937300	0.62981300	0.65276700
C	-0.28843400	1.66752400	1.57232200
C	-1.39137400	1.69283700	2.45859600
C	-2.36807800	0.68846500	2.34501800
C	-2.22682600	-0.35032300	1.42539500
H	1.49801200	2.49755600	2.41249200
H	-1.00779200	-1.19264100	-0.13531600
H	0.68250600	0.61798000	-0.02170500

C	0.74546800	2.76533100	1.65882500
C	-1.49865700	2.79045900	3.45061600
H	-3.28253400	0.74801500	2.92437300
H	-2.99809800	-1.10625800	1.35308000
C	-0.78849800	3.91285900	3.25339600
C	0.10959400	4.09725900	2.06018600
H	-0.88867800	4.74322700	3.94651100
H	0.88648400	4.83711700	2.27261700
H	-0.47464700	4.49931000	1.21948000
H	1.27706300	2.85749000	0.70785700
C	-4.06744900	3.44009800	6.22572700
C	-3.53300600	3.67673900	4.80084200
C	-2.41322100	2.63126700	4.64791600
C	-1.72325100	2.68952600	6.02688400
C	-2.89202700	2.80467700	7.02602900
H	-4.42392500	4.36474900	6.68549000
H	-4.91049000	2.75026700	6.18128700
H	-3.11413400	4.68323500	4.69570600
H	-4.30399200	3.54324000	4.04256000
H	-2.94968500	1.68395500	4.57622200
H	-1.06094400	1.83838300	6.23052200
H	-1.08429700	3.57692200	6.06873400
H	-3.17798300	1.81713700	7.39576500
H	-2.61201700	3.39487100	7.90191900
B	0.15202200	-2.24088500	5.65059600
O	0.35304600	-0.86233900	5.81553200
O	1.14959900	-2.80439600	4.89853400
C	1.70015500	-0.55029800	5.34219400
C	1.96194300	-1.73045400	4.33801400
C	2.62047800	-0.57571800	6.55922100
C	1.67611900	0.83266600	4.71620600
C	3.40502600	-2.20430800	4.27450000
C	1.43039400	-1.44347500	2.93648900
H	2.24682300	0.12788600	7.30534700
H	2.65866200	-1.56565000	7.01549800
H	3.63741600	-0.28119700	6.29326600
H	0.90893500	0.91479600	3.94919200
H	1.47160500	1.58706100	5.47796300
H	2.64212600	1.06777100	4.26293000
H	3.48724400	-3.03192800	3.56777700
H	4.06275000	-1.40128500	3.93168200
H	3.75795700	-2.55437600	5.24356700
H	0.39227600	-1.11130600	2.94356400
H	2.01942800	-0.67632300	2.43212300

H	1.47834400	-2.35490600	2.33886100
O	-5.20159300	0.98995800	4.15934000
P	-5.18765200	-0.33885100	4.82728200
O	-3.86950600	-0.98409700	5.20365000
O	-6.04667800	-1.46024100	3.95855200
O	-6.13735800	-0.27459800	6.15880500
C	-5.70455900	-1.71715700	2.64402900
C	-6.11516500	-1.22192200	7.16294600
C	-5.91875300	-0.76039300	1.65223000
C	-5.17564200	-2.96467600	2.32434400
C	-5.80738300	-0.79395900	8.45161200
C	-6.43384400	-2.55523800	6.91573600
C	-5.60858700	-1.06946200	0.33077400
H	-6.30233600	0.21101000	1.93509500
C	-4.87063500	-3.26417600	0.99835900
H	-5.01033100	-3.67966800	3.11962200
C	-5.81884800	-1.70724700	9.50210600
H	-5.56743800	0.25098600	8.61044800
C	-6.43733700	-3.46175600	7.97265000
H	-6.67388700	-2.86278600	5.90629800
C	-5.08710700	-2.31917800	-0.00285100
H	-5.76958100	-0.32469600	-0.44135600
H	-4.46004500	-4.23752000	0.75015500
C	-6.13235600	-3.04465300	9.26706400
H	-5.58154400	-1.37127900	10.50626300
H	-6.68203300	-4.50107300	7.77984700
H	-4.84815500	-2.55260900	-1.03484200
H	-6.13744300	-3.75649100	10.08533500
N	-1.01979700	-2.86367400	6.15583000
Na	-1.83595200	-0.38934700	5.19151500
Si	-1.73078500	-4.17132400	5.16189000
Si	-1.39838700	-2.52290500	7.86887600
C	-0.76924100	-5.75765700	5.46291700
H	-1.14888300	-6.58263900	4.85195000
H	0.28757600	-5.61821400	5.22007000
H	-0.82973400	-6.07074200	6.50969300
C	-3.55155500	-4.39239000	5.53461200
H	-3.76117300	-4.92220400	6.46240700
H	-4.05084200	-3.42209700	5.56439100
H	-3.99970600	-4.97632100	4.72389600
C	-1.59657400	-3.65932600	3.35843800
H	-0.56532800	-3.53645700	3.02903700
H	-2.05623300	-4.42246000	2.72269600
H	-2.13888100	-2.73029200	3.16328400

C	-2.55969200	-3.79875400	8.59508900
H	-3.58771100	-3.66750000	8.26048300
H	-2.25212300	-4.82723900	8.39113500
H	-2.56068000	-3.67162000	9.68252100
C	-2.16246600	-0.81927100	8.06590400
H	-3.06781700	-0.72190100	7.46292900
H	-2.45695300	-0.65874700	9.10691400
H	-1.45927000	-0.01997400	7.81307600
C	0.21766300	-2.58336600	8.83429700
H	0.73748900	-3.53464500	8.68668000
H	0.89945800	-1.78016700	8.54819200
H	0.02645800	-2.47678700	9.90665700

TS7-8’

E = -1850.79956410 a.u.

0 1

C	-1.56560500	1.08732100	-0.76152000
C	-0.42610700	1.58256400	-0.12723000
C	-0.32076300	1.58614800	1.26037100
C	-1.37517300	1.07355700	2.05524800
C	-2.50553300	0.56703500	1.39475300
C	-2.60829000	0.57779300	0.00624400
H	1.57480000	1.21577700	2.16426000
H	-1.63458100	1.09841600	-1.84463800
H	0.39383300	1.97553300	-0.72346400
C	0.92303000	2.07788600	1.96074800
C	-1.29629700	1.06892500	3.53586900
H	-3.32512100	0.15961900	1.97979400
H	-3.49899900	0.18456400	-0.47108100
C	-0.37741400	1.88778500	4.08971600
C	0.58112100	2.74878600	3.29107500
H	-0.31630000	2.00151600	5.17475200
H	1.49346500	2.95287100	3.86078400
H	0.11599900	3.73006800	3.10156200
H	1.48920800	2.75214900	1.31125100
C	-3.98037500	4.21683200	4.47756700
C	-4.04647100	2.94012300	3.61700900
C	-3.66622500	1.84000500	4.54330900
C	-3.13950300	2.39472300	5.83121300
C	-2.90038600	3.88795300	5.52492600
H	-3.75045900	5.10835800	3.89166800
H	-4.94376300	4.37790700	4.96939400
H	-3.30207800	2.95678100	2.81270600
H	-5.01232900	2.74172300	3.15001500

H	-3.56490500	0.83987500	4.20957000
H	-3.93351100	2.29269100	6.57563400
H	-2.26901200	1.85667400	6.20152600
H	-2.96753000	4.51117900	6.41863500
H	-1.90525000	4.01971200	5.09294300
O	-5.54932000	1.16878300	5.20069500
P	-5.44626900	-0.29047500	5.60427300
O	-4.07386900	-0.91225700	5.67920000
O	-6.38310100	-1.21009200	4.61093500
O	-6.26760800	-0.46867600	6.98376000
C	-5.89938000	-1.50165900	3.34538500
C	-6.31419300	-1.69166900	7.65089800
C	-6.24641200	-0.68231200	2.27608800
C	-5.08390100	-2.61616000	3.15912200
C	-5.36738200	-1.96595000	8.63020500
C	-7.32811700	-2.59429500	7.35323900
C	-5.78164800	-0.99393600	1.00001600
H	-6.87315600	0.18180500	2.45990000
C	-4.61838000	-2.91380000	1.88018500
H	-4.84024700	-3.23457900	4.01475400
C	-5.44428600	-3.16680400	9.33095500
H	-4.58776400	-1.24058500	8.82852700
C	-7.39483700	-3.79344900	8.05852900
H	-8.03983300	-2.35075700	6.57448800
C	-4.96562100	-2.10480600	0.79906600
H	-6.05231100	-0.35888700	0.16352000
H	-3.98882100	-3.78401200	1.72649100
C	-6.45610600	-4.08241400	9.04722500
H	-4.71121700	-3.38620300	10.10004600
H	-8.18442500	-4.50248800	7.83355000
H	-4.59726500	-2.33786500	-0.19338800
H	-6.51403000	-5.01620300	9.59599300
Na	-2.16059000	-0.93188200	4.65377900

TS7-8”

E = -3135.79502182 a.u.

0 1

C	-0.84040800	-0.28532300	-0.34933400
C	0.15432500	0.53576000	0.18386600
C	0.00980300	1.11744000	1.43958100
C	-1.14856800	0.85872000	2.21459100
C	-2.14260800	0.03841400	1.65339800
C	-1.99691200	-0.52436100	0.38744900
H	1.75152600	1.40832800	2.64380900

H	-0.71382700	-0.72736900	-1.33249200
H	1.05229100	0.73789700	-0.39506500
C	1.07272700	2.01527800	2.02669200
C	-1.28565300	1.40153600	3.58878300
H	-3.05762900	-0.15224200	2.20924900
H	-2.78730900	-1.14634600	-0.01599800
C	-0.52409100	2.47259300	3.88736900
C	0.45368200	3.09934600	2.91243300
H	-0.59614900	2.95666700	4.86425800
H	1.23798200	3.64931500	3.44185900
H	-0.06939200	3.83868800	2.28738800
H	1.68159200	2.45446000	1.23058600
C	-4.66565300	4.06676600	4.55094200
C	-4.29629500	2.89824200	3.62552500
C	-3.73861500	1.88449500	4.56172600
C	-3.25884400	2.54664500	5.82708200
C	-3.53546500	4.05106200	5.59388700
H	-4.75049100	5.00839200	4.01511600
H	-5.62453200	3.85745700	5.03080100
H	-3.48876000	3.19243300	2.94683700
H	-5.10390100	2.50047600	3.01672300
H	-3.52006700	0.89531000	4.25197500
H	-3.84672700	2.16800800	6.66391000
H	-2.21180800	2.32697300	6.03004100
H	-3.79532000	4.57287700	6.51641800
H	-2.64318400	4.53077500	5.18111200
B	-4.78072100	4.90348100	0.31954400
O	-3.59276500	5.23955200	-0.30270000
O	-5.27182600	3.68858000	-0.13506600
C	-3.13222000	4.06955300	-1.03087300
C	-4.47639100	3.30689500	-1.29399900
C	-2.18660300	3.30497700	-0.10999900
C	-2.40106000	4.53399100	-2.28071800
C	-4.34603000	1.79378200	-1.32874200
C	-5.21796400	3.81058800	-2.53238800
H	-1.37239600	3.96426600	0.19475900
H	-2.69238900	2.96294500	0.79266500
H	-1.75154900	2.43217200	-0.59559400
H	-3.01232600	5.20954000	-2.87824200
H	-1.49079900	5.06579400	-1.99646300
H	-2.11209000	3.68113400	-2.90072700
H	-5.31805800	1.34360100	-1.54180300
H	-3.65340000	1.48398500	-2.11564400
H	-3.98358400	1.39737600	-0.38329800

H	-5.31311300	4.89798400	-2.52563200
H	-4.71197200	3.51330100	-3.45340400
H	-6.22306600	3.38475600	-2.54448100
O	-5.49826900	1.13071400	5.28625100
P	-5.34286600	-0.34990900	5.60009700
O	-3.95222800	-0.93265500	5.56937300
O	-6.32246400	-1.21672100	4.61239600
O	-6.07141900	-0.61448400	7.01659200
C	-6.07588300	-1.17086800	3.24409300
C	-6.02814200	-1.85165000	7.65747000
C	-6.47905300	-0.06162800	2.50577600
C	-5.43984300	-2.24824900	2.63754200
C	-5.16613000	-2.01198000	8.73512200
C	-6.87157700	-2.87828900	7.24844700
C	-6.23919000	-0.03669600	1.13494400
H	-6.96266600	0.76385000	3.01142600
C	-5.21759800	-2.21870800	1.26236200
H	-5.13349200	-3.08956400	3.24772300
C	-5.14957700	-3.22536800	9.41812600
H	-4.52563400	-1.18757600	9.02530400
C	-6.84396300	-4.08908700	7.93614400
H	-7.52546600	-2.72027300	6.40036400
C	-5.61281600	-1.11388600	0.51072600
H	-6.53762700	0.83091500	0.55836500
H	-4.72690000	-3.05808400	0.78123900
C	-5.98612800	-4.26641200	9.02000600
H	-4.48154500	-3.35579800	10.26294000
H	-7.49929700	-4.89504900	7.62342900
H	-5.42955900	-1.08922200	-0.55752200
H	-5.97185400	-5.21034500	9.55399700
N	-5.42724300	5.72616800	1.28814700
Na	-1.91114500	-0.55046900	4.94879900
Si	-7.17412000	5.43849800	1.45085900
Si	-4.44468800	7.08524400	1.88450300
C	-7.52101100	3.73283700	2.15856000
H	-8.59396400	3.51814500	2.12388300
H	-7.00624900	2.96906000	1.57503800
H	-7.20289900	3.64435500	3.19951900
C	-8.01848700	6.70673100	2.55233600
H	-7.67975100	6.68295100	3.58884000
H	-7.91453200	7.72995900	2.18388100
H	-9.08919200	6.47639700	2.55664500
C	-7.96893100	5.58116400	-0.25089500
H	-7.60397400	4.80810500	-0.92864100

H	-9.05714300	5.48165000	-0.18639300
H	-7.75426400	6.55319500	-0.70566600
C	-5.15147900	7.87343200	3.44390000
H	-6.04256200	8.47520700	3.26541200
H	-5.38659800	7.15183200	4.22919500
H	-4.38595800	8.54479300	3.84721600
C	-4.34207300	8.40690100	0.55119900
H	-5.33434300	8.79446400	0.29951800
H	-3.72673700	9.25552400	0.86649700
H	-3.90410600	7.99343700	-0.36019600
C	-2.71355700	6.48870800	2.33088200
H	-2.73528800	5.60140900	2.96840700
H	-2.13636500	6.24040200	1.44157500
H	-2.17868300	7.27013500	2.88016800

3a

E = -582.621787571 a.u.

0 1

C	-2.41254100	-5.92971300	-0.99992800
C	-1.11706100	-5.85797900	-0.49262800
C	-0.84046300	-5.16653800	0.68272300
C	-1.88426000	-4.52098100	1.38425600
C	-3.18195100	-4.60685200	0.86119700
C	-3.44627400	-5.29999100	-0.31644900
H	0.64565800	-5.91643200	2.01559900
H	-2.60949400	-6.47086800	-1.91947000
H	-0.30380600	-6.34947900	-1.01907600
C	0.55519200	-5.12801300	1.25519700
C	-1.55915500	-3.77257700	2.62475300
H	-4.00408900	-4.12342900	1.36814600
H	-4.46155300	-5.34401800	-0.69693400
C	-0.28135700	-3.42320200	2.85265400
C	0.83917400	-3.78015800	1.91617600
H	-0.04094200	-2.83741600	3.73599200
H	1.79234900	-3.81184000	2.45162300
H	0.94402100	-3.00035300	1.14701100
H	1.29269500	-5.35075400	0.47948500
C	-4.78578900	-3.80660300	4.63787100
C	-3.51090100	-4.51529100	4.16440700
C	-2.62936000	-3.36741700	3.61426000
C	-3.63725700	-2.27110500	3.12447600
C	-5.04282400	-2.76084400	3.54050600
H	-5.62782100	-4.48778800	4.78512100
H	-4.60166800	-3.30650700	5.59598600

H	-3.75042900	-5.23586400	3.37885600
H	-3.00015500	-5.06653200	4.95763800
H	-2.09867700	-2.94575100	4.47273700
H	-3.39739800	-1.32107600	3.60797300
H	-3.56220500	-2.09195900	2.05122200
H	-5.69148600	-1.94615400	3.87118400
H	-5.54800300	-3.23908100	2.69428900

I9

E = -1833.89995352 a.u.

0 1

C	1.86954500	0.50501400	-0.82837500
C	1.59662700	-0.60524300	-0.03192300
C	1.73417800	-0.54750000	1.35083200
C	2.15354600	0.65477400	1.95801500
C	2.41383800	1.76671400	1.14834500
C	2.27661600	1.69457200	-0.23386500
H	0.37870300	-1.65119200	2.57613700
H	1.76985600	0.43701200	-1.90649400
H	1.28359100	-1.53669300	-0.49420200
C	1.41611800	-1.73803100	2.22415400
C	2.37608300	0.69030800	3.42174900
H	2.72390200	2.69812800	1.60456100
H	2.49425200	2.56493200	-0.84380400
C	2.45830200	-0.47471900	4.10414800
C	2.34838400	-1.81005600	3.43442000
H	2.65401800	-0.46226500	5.17460600
H	2.01478300	-2.57691600	4.13829500
H	3.36273600	-2.09377800	3.12199300
H	1.47311600	-2.66134300	1.64277800
B	2.64508100	2.00440500	4.19223500
C	2.88769600	4.21789000	4.73433200
C	3.44573300	3.33518100	5.90569100
C	2.47057500	3.17657400	7.06923400
H	2.83631900	2.39850500	7.74200600
H	2.37336200	4.10199100	7.63984100
H	1.47989900	2.88078900	6.72029000
C	4.82570900	3.72933500	6.40766500
H	5.57113900	3.70256500	5.61245300
H	4.81263400	4.73922900	6.82377800
H	5.14272800	3.05206900	7.20483400
C	1.93177500	5.31837200	5.16539200
H	1.57832500	5.85942600	4.28629500
H	1.06199800	4.91740600	5.68376300

H	2.43310900	6.03310300	5.82330600
C	3.98113800	4.77907500	3.82535100
H	4.67000100	4.00175900	3.48932100
H	3.51461300	5.21313500	2.93972500
H	4.55646600	5.56207900	4.32355500
O	2.14481000	3.24477100	3.93853000
O	3.54420800	2.02095300	5.26264700
N	6.15648100	-1.02958600	3.66379300
Na	5.22459100	0.50754600	4.90371100
Si	6.38544700	-2.54077700	4.37252900
Si	6.53059800	-0.34936300	2.16644300
C	5.37179500	-2.60915700	5.99109300
H	5.48027500	-3.56564400	6.51247100
H	5.69268700	-1.83393800	6.70115000
H	4.30123100	-2.46817200	5.80202000
C	5.81707300	-4.01559700	3.31798700
H	4.76535100	-3.92790700	3.02826200
H	6.39881400	-4.07784500	2.39220600
H	5.93741200	-4.97003500	3.84208200
C	8.18029800	-2.91024200	4.86755900
H	8.56629600	-2.14351600	5.54797400
H	8.29015900	-3.88087700	5.36398100
H	8.83347100	-2.91321800	3.98888600
C	5.52565500	-1.02463100	0.70893100
H	5.81602300	-0.56559400	-0.24243200
H	5.66374400	-2.10611500	0.60755200
H	4.45631300	-0.84397600	0.84413300
C	8.35914000	-0.46379100	1.67235700
H	8.66112300	-1.50776900	1.53563900
H	8.57510000	0.06254100	0.73603300
H	9.00543100	-0.04425600	2.45006000
C	6.11899000	1.52171800	2.24924400
H	6.35603100	2.03385700	1.31171100
H	5.04910600	1.68729900	2.42211000
H	6.68880800	2.03387500	3.03714300

TS9-10

E = -1833.87177874 a.u.

0 1

C	2.00516300	0.94863900	-0.82772400
C	2.07121200	-0.25799000	-0.13446900
C	2.16117200	-0.30103400	1.25512100
C	2.19316300	0.90885500	1.98699200
C	2.11646000	2.11799500	1.27491400

C	2.02128200	2.14172400	-0.11194300
H	1.12939600	-1.99875600	2.04401900
H	1.93968400	0.95384300	-1.91081000
H	2.04974200	-1.19413200	-0.68619400
C	2.16950600	-1.64262900	1.96632900
C	2.39045700	0.88550100	3.45108700
H	2.12213500	3.05100000	1.82517800
H	1.96332600	3.09323400	-0.63143500
C	2.60836900	-0.34726400	4.05029500
C	2.80146700	-1.56498100	3.34598700
H	2.78519700	-0.36664600	5.12696100
H	2.68644800	-2.47338900	3.93871800
H	4.22209300	-1.48562400	3.24023200
H	2.68499600	-2.38407600	1.34653200
B	2.59637000	2.13064500	4.29710300
C	2.81871800	4.30716800	5.00878900
C	3.43078600	3.34867900	6.08948100
C	2.47924400	3.06083100	7.24946700
H	2.87899400	2.23719700	7.84411100
H	2.36296800	3.92870600	7.90171400
H	1.49290700	2.76590600	6.88761300
C	4.80132200	3.75298200	6.60982900
H	5.53543500	3.82709600	5.80663200
H	4.75591500	4.72020100	7.11613700
H	5.15747500	3.01638200	7.33389600
C	1.86995300	5.36217900	5.55614800
H	1.48164100	5.96728000	4.73503300
H	1.02148800	4.90981900	6.06743900
H	2.38548100	6.02814000	6.25352000
C	3.87571000	4.95288700	4.11090900
H	4.56152500	4.20862500	3.69967100
H	3.37712800	5.43850500	3.27083900
H	4.45985500	5.70603600	4.64406900
O	2.06211300	3.39066100	4.17410200
O	3.56431900	2.10965600	5.33356800
N	5.58143900	-1.33432100	3.28181300
Na	5.05599300	0.68552900	4.26771900
Si	6.16462200	-2.52621200	4.38813000
Si	6.24697800	-0.88152800	1.74951200
C	5.12730100	-2.42015700	5.97201800
H	5.44925900	-3.17093100	6.70048800
H	5.22791100	-1.44532400	6.46598400
H	4.06312700	-2.58337900	5.78670400
C	6.02703000	-4.27962200	3.70342600

H	4.99486000	-4.50609700	3.41906400
H	6.64199300	-4.40061400	2.80571700
H	6.34765100	-5.03787900	4.42495200
C	7.95498000	-2.23619700	4.92784500
H	8.10967700	-1.21037900	5.28041900
H	8.21955700	-2.90463400	5.75424700
H	8.67214900	-2.41256500	4.12381300
C	5.50881200	-1.83797000	0.30463600
H	6.04356600	-1.62593900	-0.62691900
H	5.56345800	-2.91660200	0.48047100
H	4.46200400	-1.57577700	0.14551300
C	8.12519900	-1.08027700	1.65533100
H	8.42904000	-2.12946500	1.71552300
H	8.50011100	-0.69148100	0.70265000
H	8.64232800	-0.54366300	2.45553000
C	5.87831500	0.96361700	1.48079700
H	6.21545400	1.29420600	0.49395400
H	4.80717300	1.18410500	1.52504900
H	6.40585300	1.60586500	2.20249300

I10

E = -1833.89447668 a.u.

0 1

C	1.81187600	0.66264900	-0.75659700
C	1.78122400	-0.49188900	0.01830500
C	1.95186400	-0.46155000	1.40346100
C	2.16331200	0.77679400	2.06217600
C	2.17966100	1.93833200	1.25735300
C	2.00964300	1.88648900	-0.11820500
H	0.86365500	-2.20103400	2.05467600
H	1.67782900	0.60922400	-1.83210800
H	1.61897300	-1.45410800	-0.46310900
C	1.87838800	-1.78168000	2.15821700
C	2.41757800	0.83553500	3.50477500
H	2.32039900	2.89718500	1.74016200
H	2.02821900	2.80697800	-0.69485400
C	2.41157100	-0.43302300	4.19468800
C	2.22927500	-1.64505800	3.61450000
H	2.55093100	-0.41538600	5.27787400
H	2.18162500	-2.53891400	4.23075000
H	4.56556100	-1.48855000	3.21730800
H	2.52577900	-2.52319800	1.66192400
B	2.66663400	2.08052000	4.28086500
C	3.14746000	4.26171700	4.87388000

C	3.32769100	3.33971800	6.12947600
C	2.10562600	3.33834800	7.04851900
H	2.20800200	2.52965200	7.77493100
H	2.00412400	4.27920300	7.59388900
H	1.18991600	3.16521800	6.48106600
C	4.59593100	3.58572200	6.93385700
H	5.49306500	3.46056700	6.32528500
H	4.60768000	4.59720800	7.34768500
H	4.64945100	2.88320300	7.76900600
C	2.34015500	5.52760200	5.12404900
H	2.25712900	6.09947600	4.19775800
H	1.33153700	5.29313500	5.46134500
H	2.82271800	6.16249900	5.87263800
C	4.47482500	4.60883600	4.19245500
H	5.07360100	3.71398600	4.00465600
H	4.26447500	5.06648400	3.22470400
H	5.07314200	5.30772600	4.78157100
O	2.41132500	3.41372400	3.97051000
O	3.40678600	2.03046600	5.51786100
N	5.57844800	-1.31191200	3.27580600
Na	4.81653700	0.57541200	4.49159500
Si	6.31427900	-2.54443000	4.30115600
Si	6.19046000	-0.64839200	1.74714000
C	5.15608000	-2.79705400	5.76262700
H	5.51590700	-3.60212200	6.41046000
H	5.07282900	-1.90082200	6.38759400
H	4.14694000	-3.05772300	5.43707500
C	6.54756400	-4.17120300	3.38805300
H	5.58915100	-4.55558300	3.02665400
H	7.20124600	-4.05805300	2.51838600
H	6.98878200	-4.93892200	4.03119900
C	7.96935900	-1.92947600	4.95451800
H	7.89682900	-0.91577700	5.36290800
H	8.31114500	-2.57726000	5.76790800
H	8.75375300	-1.92220800	4.19638400
C	5.35893500	-1.47922000	0.29180900
H	5.78339200	-1.13195800	-0.65528400
H	5.47898300	-2.56589600	0.33165600
H	4.29082100	-1.25255500	0.26766800
C	8.05447200	-0.88764300	1.65678300
H	8.35141700	-1.93916200	1.68571600
H	8.42112000	-0.47828800	0.71031600
H	8.58406200	-0.36674200	2.45809600
C	5.83466500	1.20165700	1.73238400

H	6.16999200	1.65029600	0.79256100
H	4.76535200	1.41738000	1.81081200
H	6.36949900	1.73481100	2.53005600

I11

E = -3135.87046549 a.u.

0 1

C	3.05671100	-1.20175000	-3.38288800
C	3.30941900	-0.44520800	-2.24012000
C	3.83182500	-1.01955500	-1.08315900
C	4.15980300	-2.40056500	-1.05557700
C	3.91911600	-3.14372500	-2.23171800
C	3.36679500	-2.56201400	-3.36558000
H	4.13538700	0.86399000	-0.08489000
H	2.63578200	-0.73832700	-4.26928300
H	3.07313700	0.61656700	-2.23675500
C	3.98203600	-0.18824700	0.17795800
C	4.77497200	-2.98569000	0.13684500
H	4.19578600	-4.19053400	-2.24906800
H	3.19893100	-3.16984500	-4.25041500
C	5.38338700	-2.02924600	1.03885200
C	5.09864500	-0.70427000	1.05125400
H	6.16470300	-2.40407300	1.70104200
H	5.69323900	-0.00232900	1.62894200
H	3.02195500	-0.21189800	0.72796100
C	0.24581500	-4.36156300	-2.17793500
C	1.15980000	-4.79891400	-1.00441400
C	1.13114200	-3.64409300	0.00515400
C	0.54596300	-2.45631500	-0.73678100
C	-0.47837100	-3.09449600	-1.68341200
H	0.86119200	-4.11377800	-3.04532800
H	-0.44731900	-5.15032800	-2.47739900
H	2.18621000	-4.96464200	-1.32583500
H	0.81409300	-5.72194400	-0.54125300
H	2.09038100	-3.44346400	0.47890600
H	0.14210800	-1.70727100	-0.05282500
H	1.34895000	-1.99000200	-1.31005000
H	-1.38631100	-3.36396000	-1.13335000
H	-0.76898500	-2.42870500	-2.49862700
B	4.97250300	-4.43849600	0.38087600
O	4.77633900	-5.53506100	-0.46167000
O	5.34277000	-4.92181300	1.68239400
C	4.86036100	-6.75398000	0.30641500
C	5.70560300	-6.31710100	1.55431800

C	5.50905100	-7.82673100	-0.55783900
C	3.43407000	-7.16629900	0.67364600
C	7.21354500	-6.36877300	1.30524400
C	5.35525600	-7.03846500	2.84898700
H	4.85726100	-8.05996100	-1.40240800
H	6.46468900	-7.49083200	-0.95805300
H	5.67026700	-8.74765400	0.01000100
H	2.94831200	-6.41954700	1.30163000
H	2.84994900	-7.26382400	-0.24208300
H	3.40979800	-8.12289900	1.20172400
H	7.72753000	-5.87259700	2.13107000
H	7.58281600	-7.39470300	1.23971900
H	7.47603900	-5.84496300	0.38456000
H	4.31015100	-6.88985300	3.12394700
H	5.53300800	-8.11316900	2.75743600
H	5.97844000	-6.66620100	3.66491100
O	0.14839700	-3.95770100	1.09131700
P	0.49056500	-4.73170500	2.41354800
O	1.81303600	-4.45498800	3.02513400
O	0.32536900	-6.30509800	2.17236400
O	-0.78595100	-4.42859900	3.33903000
C	-0.60005600	-6.93266700	1.33105300
C	-1.20550800	-3.15005400	3.73551600
C	-1.88692400	-6.44638200	1.13509300
C	-0.15757300	-8.08883100	0.70111100
C	-1.73234600	-2.26093600	2.80670800
C	-1.13845700	-2.84096000	5.08576700
C	-2.73655800	-7.13252300	0.26966700
H	-2.22360900	-5.55701400	1.64961700
C	-1.01919700	-8.76657200	-0.15587100
H	0.85234200	-8.43317100	0.88252300
C	-2.18535100	-1.02112800	3.25075900
H	-1.76657000	-2.53229000	1.76051300
C	-1.59638700	-1.59860300	5.51695300
H	-0.72995000	-3.56775600	5.77579400
C	-2.30874500	-8.28789500	-0.37886000
H	-3.74091700	-6.75698400	0.10759000
H	-0.67712000	-9.66735900	-0.65335400
C	-2.11661400	-0.68578200	4.60161600
H	-2.59026300	-0.31543600	2.53403000
H	-1.54489300	-1.34620400	6.57035600
H	-2.97663500	-8.81363800	-1.05184000
H	-2.46947900	0.28205000	4.93972100
N	4.33993500	-1.60776800	4.17862500

Na	3.87402700	-3.69059400	2.94543200
Si	2.77581200	-1.13581600	4.83913500
Si	5.85318400	-1.92079500	5.02948500
C	1.62999000	-0.89004600	3.37404500
H	1.98221400	-0.07330200	2.73776000
H	1.55724200	-1.78103600	2.74794100
H	0.61899000	-0.63962700	3.70168300
C	2.19982100	-2.53368500	5.96024200
H	1.93256900	-3.41933800	5.37852700
H	2.97503200	-2.82277000	6.67498600
H	1.32159300	-2.23860100	6.53921500
C	2.83292800	0.46977700	5.82199200
H	3.30026500	1.27093500	5.24156200
H	1.82106500	0.80057400	6.07859300
H	3.38999600	0.36886800	6.75622600
C	6.23058000	-3.76757800	4.93637600
H	5.43308700	-4.36559500	5.39283700
H	6.36135100	-4.10764900	3.90482500
H	7.15279100	-4.01212300	5.47235200
C	5.74813300	-1.43016300	6.84323900
H	4.93170000	-1.92041400	7.37866000
H	6.67661100	-1.70800900	7.35209900
H	5.62353500	-0.35113200	6.96158700
C	7.23629700	-0.95105900	4.21064200
H	7.35898700	-1.21124900	3.15680700
H	7.04781900	0.12509300	4.26337800
H	8.19229100	-1.14184500	4.70813200
H	4.51164900	-1.18810100	3.25828000

TS11-12

E = -3135.84715792 a.u.

0 1

C	3.99433000	-1.44224900	-4.20733200
C	4.03887200	-0.59104900	-3.10727300
C	4.29439600	-1.05974700	-1.81924000
C	4.50493600	-2.44768800	-1.60158600
C	4.49246500	-3.28896200	-2.73741500
C	4.23698700	-2.80101300	-4.01079600
H	5.13373400	0.71460000	-0.94317600
H	3.78801600	-1.05125900	-5.19823800
H	3.87438400	0.47485500	-3.24985600
C	4.37037100	-0.03844300	-0.69121100
C	4.70801500	-2.97302700	-0.25404200
H	4.69547500	-4.34310600	-2.60139500

H	4.23104700	-3.48453600	-4.85482500
C	4.86985400	-1.99018800	0.78354600
C	4.69457700	-0.65664200	0.64056600
H	5.19524900	-2.35099000	1.75776400
H	4.89592800	0.01822900	1.46969900
H	3.43201800	0.53597300	-0.64321500
C	1.01393000	-2.84584000	-2.04639600
C	1.55515700	-4.08386200	-1.29288200
C	1.79285200	-3.61470500	0.10779800
C	1.45041300	-2.17376800	0.23916100
C	0.50180600	-1.90393600	-0.94073400
H	1.82634100	-2.37172400	-2.59670600
H	0.23687100	-3.10920500	-2.76636200
H	2.47520100	-4.47812300	-1.72823200
H	0.83160400	-4.90187200	-1.26953800
H	2.47906500	-4.11121100	0.76463100
H	1.04304600	-1.92222000	1.21565100
H	2.38518300	-1.60645300	0.13638400
H	-0.51981000	-2.16803900	-0.65270500
H	0.50610700	-0.85590200	-1.24578000
B	4.81313500	-4.41358700	0.12030500
O	4.82571800	-5.53593400	-0.70007300
O	4.82146000	-4.83722500	1.48765800
C	4.66498800	-6.72625500	0.10315300
C	5.15558700	-6.25316400	1.51458000
C	5.49435900	-7.84172200	-0.51857900
C	3.18309600	-7.10338900	0.08275400
C	6.67195200	-6.35474500	1.68142100
C	4.44176900	-6.90515300	2.69122000
H	5.08370300	-8.09913400	-1.49688000
H	6.53011500	-7.53698500	-0.66187400
H	5.47443800	-8.74115800	0.10306100
H	2.56575700	-6.33925800	0.55080000
H	2.86218200	-7.20589700	-0.95538200
H	2.99086300	-8.04723900	0.59660700
H	6.96922600	-5.85437300	2.60469800
H	7.00302000	-7.39363700	1.73971400
H	7.19189700	-5.87044800	0.85319400
H	3.36921100	-6.71375700	2.68164400
H	4.59477200	-7.98715100	2.68428000
H	4.85069200	-6.52793300	3.63292100
O	0.23065700	-4.42028000	1.02183600
P	0.45201800	-4.94835800	2.43937600
O	1.65988000	-4.46284600	3.17972200

O	0.49636200	-6.56672700	2.44608600
O	-0.91118800	-4.72309400	3.30266700
C	-0.47652200	-7.35557800	1.83068500
C	-1.40417000	-3.45549800	3.59002700
C	-1.45183400	-7.94581100	2.62431600
C	-0.43024800	-7.57448000	0.45919200
C	-1.84327300	-2.61062000	2.57477600
C	-1.48565400	-3.07968800	4.92602300
C	-2.39569400	-8.77974400	2.03061700
H	-1.46255600	-7.73883100	3.68734500
C	-1.37962000	-8.40952900	-0.12454900
H	0.33535900	-7.09196000	-0.13283400
C	-2.36988600	-1.36665900	2.91368100
H	-1.76222500	-2.93278900	1.54494500
C	-2.02343700	-1.83765400	5.25232000
H	-1.12912400	-3.76352500	5.68669600
C	-2.36187600	-9.01389600	0.65723800
H	-3.16053400	-9.24408700	2.64380100
H	-1.35015900	-8.58516200	-1.19458200
C	-2.46485900	-0.97741400	4.24838000
H	-2.71177700	-0.70214400	2.12752900
H	-2.09454800	-1.54207700	6.29376400
H	-3.09880500	-9.66375600	0.19805000
H	-2.88147100	-0.00951100	4.50482600
N	4.06524200	-1.54509200	4.23335200
Na	3.65611400	-3.68416700	3.07131000
Si	2.56355200	-1.20102400	5.11870400
Si	5.68680200	-1.82495500	4.88244900
C	1.26510100	-0.87073500	3.81365500
H	1.60354900	-0.13743900	3.07533500
H	1.01359800	-1.79142200	3.28734400
H	0.33858100	-0.49630400	4.25286000
C	2.13321700	-2.72309800	6.13144400
H	1.86044700	-3.55691900	5.47903800
H	2.95615300	-3.04391500	6.77727200
H	1.27515800	-2.52356500	6.78003900
C	2.71520700	0.30297600	6.24193800
H	3.09654900	1.17096900	5.69538100
H	1.73332300	0.57762300	6.64112800
H	3.37579100	0.13106300	7.09415300
C	6.09286000	-3.66085700	4.70052000
H	5.36173500	-4.29422200	5.21697100
H	6.14812000	-3.97746900	3.65466500
H	7.06648200	-3.88971700	5.14376400

C	5.79673900	-1.39328200	6.70783700
H	5.05332900	-1.91744100	7.31395000
H	6.78125800	-1.67406100	7.09483300
H	5.67156200	-0.32194300	6.87984800
C	6.90881100	-0.80494500	3.89176500
H	6.85159700	-1.01650500	2.82069800
H	6.72980300	0.26606400	4.02559600
H	7.93614500	-1.00648000	4.20982700
H	4.09615300	-1.01155700	3.36649700

I12

E = -3135.92750850 a.u.

0 1

C	4.97435700	-1.88733300	-4.47983600
C	5.34762900	-1.01746600	-3.46497900
C	5.07976300	-1.30444400	-2.12311000
C	4.42595000	-2.50050900	-1.78183100
C	4.06739300	-3.37520200	-2.81790100
C	4.33171200	-3.07672900	-4.14894200
H	6.49810700	0.09897600	-1.33980900
H	5.18974100	-1.64461100	-5.51531500
H	5.85877600	-0.09038800	-3.71055400
C	5.51077200	-0.29878400	-1.07842600
C	4.06913300	-2.81674400	-0.32884700
H	3.59441700	-4.31480600	-2.57554400
H	4.04034700	-3.77753900	-4.92456300
C	4.89790500	-1.98375900	0.62831900
C	5.53495000	-0.86378300	0.30617800
H	4.95665200	-2.34748500	1.64591800
H	6.09755900	-0.32302700	1.06325200
H	4.83729900	0.57103600	-1.10408900
C	0.19150300	-2.60542100	-0.40953300
C	1.49265300	-3.34427400	-0.74312900
C	2.55234700	-2.48766300	-0.03646500
C	2.11492700	-1.04860600	-0.36863600
C	0.56609800	-1.10087300	-0.43555700
H	-0.62112200	-2.84843000	-1.09933300
H	-0.12369800	-2.89864300	0.59251700
H	1.66957000	-3.34301000	-1.82221700
H	1.48336000	-4.37688000	-0.39446800
H	2.39231300	-2.63737200	1.03630300
H	2.48810000	-0.32688800	0.36081800
H	2.52320100	-0.76221900	-1.34056700
H	0.10615700	-0.57142500	0.40156700

H	0.20794300	-0.61828000	-1.34833300
B	4.28341000	-4.33437500	0.08241100
O	4.35586300	-5.40771100	-0.74770500
O	4.41360500	-4.70737500	1.41926000
C	4.32700200	-6.62342600	0.06589200
C	4.88030000	-6.10753200	1.43120500
C	5.18394000	-7.67584800	-0.61632800
C	2.86785600	-7.06290200	0.14745800
C	6.40511100	-6.03823100	1.48738800
C	4.33261900	-6.83211700	2.64803400
H	4.72560200	-7.96244400	-1.56440100
H	6.18745100	-7.30656700	-0.82521100
H	5.26121300	-8.57220800	0.00452900
H	2.25768000	-6.32217100	0.66211800
H	2.47255000	-7.18379300	-0.86217100
H	2.75780200	-8.01419400	0.67028000
H	6.70620500	-5.47874800	2.37543800
H	6.84707800	-7.03440200	1.54857800
H	6.81620500	-5.53023900	0.61316300
H	3.24828200	-6.80601700	2.71166700
H	4.63746100	-7.88126700	2.61852600
H	4.73737500	-6.40652600	3.56822400
O	1.04128400	-4.50562300	2.18323500
P	0.77549800	-5.36176100	3.40093400
O	1.76965800	-5.19995900	4.51615000
O	0.72671400	-6.95153500	3.02256300
O	-0.77809900	-5.19156300	3.89528800
C	-0.04995600	-7.53473600	2.03776300
C	-1.37970500	-3.94606000	3.96963100
C	-0.27485400	-8.90239800	2.17291800
C	-0.55210600	-6.83854200	0.93865900
C	-1.95541600	-3.38531000	2.83369900
C	-1.43660500	-3.29343200	5.19616300
C	-1.00574500	-9.58030200	1.20284500
H	0.12575000	-9.41157100	3.04165500
C	-1.28653900	-7.52986100	-0.02256200
H	-0.34888600	-5.78185300	0.83169500
C	-2.59257500	-2.15189600	2.93044200
H	-1.89733200	-3.91892600	1.89407500
C	-2.07972400	-2.06091300	5.28449700
H	-0.98048800	-3.76077700	6.05998500
C	-1.51655600	-8.89751100	0.10014700
H	-1.17995900	-10.64556800	1.31327300
H	-1.67600600	-6.98736500	-0.87793300

C	-2.65639100	-1.48569200	4.15368700
H	-3.03876800	-1.71072300	2.04560600
H	-2.13097200	-1.55127100	6.24111300
H	-2.08874700	-9.42654800	-0.65415400
H	-3.15673300	-0.52596400	4.22540200
N	3.80854500	-1.70764400	4.04665100
Na	3.08643500	-3.86647000	3.12006600
Si	2.26967700	-1.08991700	4.70493300
Si	5.23945600	-2.13078500	5.00131800
C	1.01697800	-1.15506300	3.31617800
H	1.33358900	-0.52503300	2.47974200
H	0.84716000	-2.16089100	2.92716800
H	0.04628900	-0.78397400	3.65343700
C	1.79945100	-2.18318100	6.15156700
H	1.67915900	-3.22712000	5.85195600
H	2.53568600	-2.14358000	6.95894100
H	0.84624200	-1.84804200	6.56901400
C	2.45142700	0.69870200	5.26674600
H	2.80559600	1.33815100	4.45179400
H	1.48875900	1.10204300	5.59716100
H	3.15359600	0.80292600	6.09730000
C	5.07308800	-3.92060400	5.55555800
H	4.08317300	-4.15577100	5.95381700
H	5.26378400	-4.61456700	4.73055700
H	5.80423500	-4.15801200	6.33400300
C	5.46332500	-1.02217400	6.50476500
H	4.62872200	-1.08937300	7.20665000
H	6.36852900	-1.30179600	7.05304000
H	5.56689300	0.02691000	6.21430700
C	6.74239300	-1.95705300	3.88446600
H	6.69910000	-2.62196000	3.01812300
H	6.85876400	-0.93536900	3.51063300
H	7.65526000	-2.20252200	4.43575000
H	4.06167400	-1.19988000	3.20193700

I13

E = -3135.87621241 a.u.

0 1

C	5.72192500	-2.28068700	-5.25098200
C	5.69419900	-1.22584200	-4.35218100
C	5.16303300	-1.37190500	-3.06517900
C	4.64518700	-2.61161200	-2.65644700
C	4.68845300	-3.66707500	-3.57960700
C	5.21003200	-3.51432100	-4.85564200

H	6.23144700	0.18826500	-2.04716600
H	6.13841400	-2.14539400	-6.24364100
H	6.09392500	-0.25838100	-4.64492800
C	5.19471200	-0.16163500	-2.16124300
C	4.03154000	-2.84467400	-1.27575500
H	4.33504300	-4.63761800	-3.27738600
H	5.22692400	-4.35982200	-5.53590000
C	4.08311000	-1.57603400	-0.44986200
C	4.58713200	-0.40196400	-0.82029200
H	3.62407500	-1.64555400	0.53320300
H	4.54235700	0.44173500	-0.13615000
H	4.67433600	0.67478500	-2.64740400
C	0.35722400	-4.02511200	-2.03671300
C	1.85851600	-4.34813900	-1.96523500
C	2.47337800	-3.06500400	-1.39051600
C	1.73294300	-1.98145500	-2.20516600
C	0.28889900	-2.50902400	-2.36510200
H	-0.16502900	-4.64408700	-2.76917300
H	-0.12010000	-4.22112900	-1.06963400
H	2.24494300	-4.52611200	-2.97070900
H	2.07081900	-5.23839400	-1.37540700
H	2.08960900	-2.95610800	-0.36445600
H	1.77557700	-1.00341100	-1.72580800
H	2.21719200	-1.88281100	-3.17997700
H	-0.39663900	-1.99828000	-1.68551200
H	-0.08459800	-2.33523500	-3.37654300
B	4.84819200	-4.09853600	-0.46196200
O	5.60784300	-5.06497600	-1.20364300
O	3.99227700	-4.86490700	0.41382100
C	5.20406800	-6.40897600	-0.90134800
C	4.41735600	-6.25535600	0.45063200
C	6.43925200	-7.30152400	-0.80029800
C	4.35632400	-6.94595600	-2.06147900
C	5.28660800	-6.45990100	1.68928600
C	3.18810900	-7.15332700	0.57806000
H	6.98063100	-7.27598300	-1.74837900
H	7.11929700	-6.98743300	-0.01643300
H	6.15133900	-8.33855900	-0.60778000
H	3.44627500	-6.37496500	-2.21635500
H	4.94633300	-6.89074800	-2.97838600
H	4.07891900	-7.99060400	-1.90603800
H	4.70763100	-6.21929600	2.58076700
H	5.62110700	-7.49510600	1.77801400
H	6.16530500	-5.82174400	1.66103800

H	2.46631900	-6.98793100	-0.22406200
H	3.48062300	-8.20485700	0.53259100
H	2.69840000	-6.99765400	1.54245200
O	0.62080600	-3.44156900	2.63191100
P	0.96151800	-4.44696700	3.70314400
O	1.80973900	-5.60873700	3.25110900
O	-0.35892100	-5.07287600	4.44251800
O	1.65406500	-3.59800600	4.92609300
C	-1.20210200	-4.32655500	5.25165700
C	1.96749900	-4.14430600	6.15942800
C	-1.59946600	-4.90863700	6.45131400
C	-1.64493500	-3.05663500	4.88983600
C	2.68561900	-5.33176000	6.27959700
C	1.55940600	-3.43713700	7.28649800
C	-2.45137500	-4.21140900	7.30155400
H	-1.21831700	-5.89024600	6.70605200
C	-2.49143800	-2.36583700	5.75437300
H	-1.31522400	-2.62422100	3.95334800
C	2.99631100	-5.80717900	7.55199000
H	2.96491000	-5.87433500	5.38560800
C	1.88194400	-3.91934000	8.55075600
H	0.97876600	-2.53246500	7.15208500
C	-2.89823500	-2.93621700	6.95867900
H	-2.75764400	-4.66305800	8.23936400
H	-2.83538500	-1.37404200	5.47919500
C	2.60160600	-5.10545400	8.68895200
H	3.55018300	-6.73518700	7.65135700
H	1.55933200	-3.37140800	9.42990600
H	-3.55843800	-2.39155500	7.62525200
H	2.84767300	-5.48255700	9.67591200
N	6.13343000	-3.17656000	0.46131700
Na	1.92464300	-4.58354500	1.16864200
Si	5.95270800	-2.83218100	2.26984100
Si	7.84037900	-3.39085000	-0.19353800
C	4.25572400	-3.19540200	2.95107300
H	3.45842000	-2.64531000	2.44749700
H	3.98616800	-4.24675100	2.96200400
H	4.23339400	-2.85384200	3.99062200
C	7.23604300	-3.75090000	3.28955800
H	7.07434100	-4.82827300	3.32826100
H	8.26467500	-3.57333400	2.97295900
H	7.14870900	-3.38344900	4.31737400
C	6.22603500	-0.98335300	2.50010300
H	7.20825800	-0.63305600	2.18381600

H	5.47534700	-0.39444700	1.96921100
H	6.12079900	-0.74673400	3.56366500
C	8.69805700	-4.93983500	0.43765200
H	8.19535600	-5.43250400	1.26738000
H	8.81362700	-5.66800700	-0.36534300
H	9.70040700	-4.67372700	0.78608000
C	8.83000400	-1.90019100	0.41368700
H	9.00169000	-1.87917600	1.49131000
H	9.81379500	-1.92465800	-0.06674000
H	8.36365100	-0.95229800	0.13038000
C	7.90862900	-3.30336700	-2.05749400
H	7.34028300	-4.09900500	-2.53131100
H	7.54332800	-2.35412100	-2.45159600
H	8.95977900	-3.39459300	-2.35485300
H	5.90780900	-2.24238900	0.09871500

TS13-8

E = -3135.83881985 a.u.

0 1

C	5.39702700	-2.47138900	-5.12710300
C	5.71037400	-1.53808300	-4.14615400
C	5.14636400	-1.57779200	-2.87173000
C	4.20002900	-2.58399900	-2.54235000
C	3.89796500	-3.51457100	-3.55775300
C	4.47845000	-3.47038500	-4.81769000
H	6.67563300	-0.50317300	-1.80182800
H	5.85583400	-2.41800900	-6.10868000
H	6.42269600	-0.74730800	-4.37121200
C	5.57610600	-0.50602100	-1.88404900
C	3.54816700	-2.62774900	-1.21618100
H	3.18409400	-4.29762300	-3.35705800
H	4.20435500	-4.21427300	-5.55992300
C	3.89532600	-1.54600500	-0.35267700
C	4.91809500	-0.65958800	-0.53930100
H	3.32399400	-1.45294500	0.57160400
H	5.07775900	0.12601500	0.19113400
H	5.34186900	0.48543400	-2.30226600
C	-0.07315900	-4.09420200	-1.23662500
C	1.43233300	-4.36565300	-1.35298400
C	2.05085700	-2.96689800	-1.10940600
C	1.14021000	-2.08451400	-2.00495200
C	-0.26901100	-2.72243200	-1.93461400
H	-0.68057200	-4.88760300	-1.67794500
H	-0.34958200	-4.02453600	-0.18021400

H	1.66036900	-4.72430900	-2.35775100
H	1.76091100	-5.16022500	-0.67366000
H	1.75260300	-2.69207300	-0.08625400
H	1.16078600	-1.04616600	-1.66873100
H	1.52620100	-2.09633400	-3.02692600
H	-0.96992400	-2.09875600	-1.37585600
H	-0.69040400	-2.85049800	-2.93499300
B	5.49822400	-4.31847100	-0.02482900
O	6.03573700	-5.12144000	-1.00161100
O	4.67933000	-5.04351000	0.83783300
C	5.44020800	-6.44938700	-0.91006000
C	4.88648400	-6.47470700	0.56264900
C	6.52386600	-7.48047300	-1.19201000
C	4.35578900	-6.53570500	-1.97473800
C	5.89857900	-6.95887300	1.59762100
C	3.57022500	-7.21220700	0.75268900
H	6.89762600	-7.34616200	-2.20855800
H	7.36517200	-7.39820400	-0.50656100
H	6.11686400	-8.49172000	-1.11406400
H	3.58101600	-5.79547800	-1.80238600
H	4.79830200	-6.32756300	-2.94880800
H	3.89884000	-7.52696600	-2.00113500
H	5.50123900	-6.76379000	2.59482500
H	6.08127000	-8.03121700	1.50788700
H	6.85300000	-6.44174400	1.49785700
H	2.80398800	-6.88267200	0.05145700
H	3.71377300	-8.28393900	0.59619500
H	3.19380300	-7.05873400	1.76546200
O	1.07310500	-3.24051200	2.55091100
P	1.23332600	-4.31870400	3.59141800
O	2.11616800	-5.47572900	3.19605800
O	-0.18953300	-4.94684300	4.09711700
O	1.77004100	-3.56490900	4.95155600
C	-1.14263700	-4.20324000	4.77979000
C	1.84169000	-4.17473100	6.19187600
C	-1.64599400	-4.74801900	5.95657900
C	-1.59294500	-2.97359100	4.30684600
C	2.35661500	-5.45818000	6.36114300
C	1.38967000	-3.43716900	7.28245200
C	-2.61875300	-4.05440200	6.66937300
H	-1.25340700	-5.69641600	6.30302200
C	-2.56226600	-2.28602700	5.03402000
H	-1.17090200	-2.56736600	3.39624000
C	2.41079100	-6.00096600	7.64344500

H	2.68567600	-6.01586100	5.49350900
C	1.45713400	-3.98745100	8.55790900
H	0.97271300	-2.45258700	7.10794900
C	-3.07936700	-2.82072200	6.21220600
H	-3.00932100	-4.47596400	7.58967400
H	-2.91439000	-1.32527700	4.67269400
C	1.96608000	-5.27210400	8.74417800
H	2.80412900	-7.00341400	7.77880900
H	1.09883100	-3.41436400	9.40671500
H	-3.83491100	-2.27916600	6.77145800
H	2.01169200	-5.70242700	9.73893500
N	6.30680900	-3.11276600	0.42549500
Na	2.59708100	-4.31199800	1.23678000
Si	6.22097800	-2.69162500	2.26338200
Si	8.03171300	-3.18766100	-0.32784200
C	4.55880400	-3.01035600	3.03789500
H	3.73437000	-2.48635500	2.55171400
H	4.30563900	-4.06230000	3.14970800
H	4.60000700	-2.59118200	4.04944700
C	7.50320700	-3.70477300	3.17890400
H	7.33470500	-4.77822100	3.08046000
H	8.53512200	-3.48769400	2.90081800
H	7.39870900	-3.46617500	4.24240300
C	6.56621000	-0.85386200	2.43506500
H	7.13984800	-0.40811700	1.62719000
H	5.62541600	-0.30538500	2.51024800
H	7.11700700	-0.68228900	3.36568400
C	8.89645700	-4.75806300	0.22099400
H	8.70699000	-5.05298200	1.25098500
H	8.62244400	-5.58632400	-0.43036300
H	9.97657200	-4.60550300	0.12537700
C	8.99378500	-1.69902900	0.28907000
H	9.15577600	-1.66616500	1.36715400
H	9.98090100	-1.74076600	-0.18422600
H	8.53797800	-0.75533800	-0.01770900
C	7.97405400	-3.11912200	-2.19046200
H	7.10485900	-3.61675000	-2.61212500
H	7.99952700	-2.09934500	-2.57218900
H	8.86615500	-3.63365800	-2.56498700
H	5.84071800	-2.22535400	0.03140600

TSB-14

E = -1858.67555182 a.u.

0 1

B	0.38739700	2.18167200	0.88398300
B	1.99813500	2.67766200	0.64312800
C	4.16096500	2.09063600	0.12044900
C	3.99566200	2.10960700	1.68362900
C	-1.49703700	1.85054100	2.20608400
C	-1.46812300	0.81124600	1.02372000
C	3.79188500	0.71492800	2.28167100
H	3.00032200	0.17731800	1.75653800
H	4.70335400	0.11437700	2.24437100
H	3.49462800	0.81873000	3.32776400
C	5.10062700	2.84277000	2.42937500
H	4.88463500	2.85437600	3.50055200
H	6.05948600	2.33685000	2.28811400
H	5.20632100	3.87179300	2.09157700
C	4.81723800	0.83034800	-0.42832300
H	4.87362300	0.89642100	-1.51639100
H	5.83504300	0.71814800	-0.04358900
H	4.24654500	-0.06299000	-0.17762500
C	4.85989300	3.33096100	-0.42796100
H	5.91144000	3.37134400	-0.13394700
H	4.80944700	3.31583500	-1.51691600
H	4.35439300	4.23202000	-0.09379900
C	-2.46544300	1.11808700	-0.09221800
H	-2.25162600	0.46662000	-0.94107500
H	-3.49302400	0.93397700	0.22971600
H	-2.38512300	2.14639300	-0.43998000
C	-1.60618500	-0.64343100	1.45444000
H	-0.81519600	-0.93967300	2.14225400
H	-2.57260400	-0.82140400	1.93386800
H	-1.54218900	-1.28691500	0.57552500
C	-2.80827100	2.60368800	2.36880400
H	-2.72795300	3.31739300	3.19223000
H	-3.06790600	3.15613400	1.46730100
H	-3.62536800	1.91658900	2.60266600
C	-1.04601300	1.26566700	3.54482200
H	-0.07872100	0.76842200	3.45532000
H	-0.94326700	2.07312400	4.27430300
H	-1.76891000	0.54951800	3.93985200
O	-0.46212200	2.80147500	1.80812300
O	2.78705300	2.11343600	-0.33668100
O	-0.13084100	0.98861500	0.47270400
O	2.73799100	2.81516200	1.85832800
N	1.67188800	4.93548000	0.22077200
Si	2.47347000	6.32690500	0.82694900

Si	1.02091700	4.96774800	-1.37694800
C	3.03195800	6.04465100	2.64562100
H	3.77521500	6.80411800	2.90477300
H	2.22483400	6.19538000	3.38107200
H	3.49226200	5.07288900	2.82956300
C	4.01441200	6.92809900	-0.10144500
H	4.88525800	6.28428800	0.04183500
H	3.82893900	6.98137500	-1.17824300
H	4.29352100	7.93389400	0.23033400
C	1.36698300	7.86416900	1.01963600
H	1.83454600	8.58584000	1.69951100
H	1.17812800	8.38051700	0.07751700
H	0.38918700	7.60363600	1.44111300
C	2.22685400	4.35140800	-2.69880400
H	3.14399200	4.94867000	-2.71297000
H	2.51050300	3.31469300	-2.51197600
H	1.78083400	4.41045900	-3.69766900
C	0.47011000	6.68523600	-1.98016700
H	1.29479100	7.40082500	-2.04691100
H	0.04748000	6.59398900	-2.98680900
H	-0.29913800	7.12742000	-1.34114800
C	-0.53371500	3.89707200	-1.53221000
H	-1.03051700	4.09217100	-2.48829900
H	-0.31748000	2.82715300	-1.50256500
H	-1.24847600	4.12726500	-0.73650900
Na	1.05422700	4.34297300	2.39452000

I14

E = -1858.69227448 a.u.

0 1

B	0.43443300	2.45602300	0.80549500
B	1.94624400	3.27585100	0.51236600
C	4.03064700	2.18373200	0.24144900
C	3.65356200	2.17609700	1.76873200
C	-1.39156600	1.89436200	2.16948100
C	-1.22530400	0.84148900	1.01304200
C	3.00396100	0.85359200	2.20110900
H	2.20447600	0.56135600	1.52203200
H	3.73056600	0.03908400	2.24917500
H	2.58036800	0.98226700	3.20157100
C	4.81076500	2.48687700	2.71264900
H	4.45495800	2.50105700	3.74671200
H	5.58743300	1.72064400	2.63789000
H	5.26616900	3.45212400	2.50259900

C	4.49047200	0.82873000	-0.29234500
H	4.74649500	0.92251800	-1.35023300
H	5.37593900	0.46459100	0.23829000
H	3.69748600	0.08643800	-0.20892900
C	5.08669900	3.24424200	-0.10048700
H	6.08258800	2.97902000	0.26586900
H	5.13663800	3.34445000	-1.18637600
H	4.81645900	4.21660800	0.30683800
C	-2.26534200	0.98162200	-0.09871900
H	-1.96812800	0.34816600	-0.93603000
H	-3.25728800	0.66681300	0.23411000
H	-2.32853000	2.00406800	-0.46851600
C	-1.16200600	-0.60832000	1.47855100
H	-0.33257800	-0.77691000	2.16429000
H	-2.09134300	-0.90668300	1.97182700
H	-1.01533000	-1.25785000	0.61391600
C	-2.79588600	2.45763100	2.33126000
H	-2.81077600	3.19554100	3.13738000
H	-3.13922700	2.94691700	1.42107300
H	-3.50687800	1.66864100	2.59000300
C	-0.85848100	1.40748400	3.51790600
H	0.16586500	1.04369800	3.43172300
H	-0.86522700	2.23818800	4.22980800
H	-1.47522000	0.61005300	3.93700000
O	-0.50603700	2.96816400	1.73543300
O	2.80649800	2.52633400	-0.39453400
O	0.06429600	1.18652800	0.44343700
O	2.67884400	3.22272200	1.84887500
N	1.71751000	4.82467300	0.14601700
Si	2.59303500	6.22688200	0.71972500
Si	1.00887700	4.96543600	-1.46787800
C	3.61914800	5.98137900	2.29582400
H	3.98854600	6.96961000	2.59206900
H	3.08541800	5.57801600	3.16294000
H	4.47951800	5.33399700	2.14745900
C	3.77086200	7.01126400	-0.52847400
H	4.52738100	6.29369800	-0.85534500
H	3.26402400	7.37762600	-1.42321600
H	4.29287600	7.86172000	-0.07803500
C	1.35164700	7.55491800	1.28852500
H	1.88052600	8.43040400	1.67978600
H	0.68194500	7.89901200	0.50157300
H	0.70887300	7.19600400	2.10623700
C	2.27319800	4.59219000	-2.81147800

H	3.10832200	5.29714000	-2.79951400
H	2.68169900	3.59386700	-2.64826700
H	1.82010700	4.62927600	-3.80792100
C	0.28603500	6.68285800	-1.81246700
H	1.00386100	7.50364900	-1.76319000
H	-0.11776000	6.67800800	-2.83059700
H	-0.54329500	6.92089600	-1.14037200
C	-0.44878600	3.79649500	-1.71322900
H	-0.92192600	4.02462800	-2.67452800
H	-0.16082400	2.74517800	-1.73370000
H	-1.20697200	3.93361200	-0.93767300
Na	0.95059000	4.47939700	2.50325400

TS14-15

E = -1858.65723220 a.u.

0 1

B	0.68685600	2.13335700	1.03159700
B	2.82284900	3.89659100	0.43514000
C	4.39714400	2.24631900	0.11417100
C	4.43477800	2.72454500	1.64230900
C	-1.40309400	1.43400200	1.94251300
C	-1.12685900	0.70772500	0.58729700
C	4.00364800	1.65350300	2.64267000
H	3.00170200	1.29254500	2.41414900
H	4.69437600	0.80740700	2.64805200
H	3.99770000	2.08300400	3.64913100
C	5.76889900	3.32199000	2.08549400
H	5.66337200	3.72015900	3.09736600
H	6.56044300	2.56923700	2.10039600
H	6.08459100	4.13902400	1.43800500
C	3.85354600	0.83198800	-0.09065900
H	3.81412000	0.62791600	-1.16258400
H	4.49739700	0.07987600	0.37311100
H	2.84157200	0.73726200	0.29649900
C	5.73280100	2.38725800	-0.61457700
H	6.49527900	1.72818200	-0.19147700
H	5.59151000	2.11239000	-1.66126300
H	6.10189800	3.41249600	-0.59012600
C	-1.90946100	1.29552800	-0.58922500
H	-1.51526400	0.87669800	-1.51664100
H	-2.97518200	1.05833700	-0.53085500
H	-1.79581000	2.37827600	-0.64397700
C	-1.30294000	-0.80429300	0.62171200
H	-0.64171500	-1.27006400	1.35148400

H	-2.33530600	-1.07816100	0.86079300
H	-1.06207100	-1.22050200	-0.35847000
C	-2.77482200	2.08212700	2.06106000
H	-2.86552600	2.58569000	3.02681200
H	-2.93976300	2.82301400	1.27986000
H	-3.57089800	1.33370000	2.00005800
C	-1.12414200	0.56277900	3.16841700
H	-0.13693100	0.10253100	3.10696800
H	-1.14929700	1.18765600	4.06451100
H	-1.86974700	-0.22772100	3.28785000
O	-0.38182000	2.48519000	1.92872700
O	3.48241900	3.16257700	-0.52014400
O	0.28262700	1.00010700	0.34533600
O	3.45903200	3.79644100	1.69436400
N	2.02294000	5.09287800	0.17495000
Si	2.55374500	6.56772000	0.97533100
Si	0.83367200	5.02641800	-1.14652800
C	2.22988500	6.48721000	2.85105000
H	2.54365100	7.42755400	3.31373000
H	1.16255800	6.38865900	3.09476600
H	2.80411400	5.69899700	3.34604300
C	4.38728700	6.87998600	0.71779200
H	4.69070400	7.84614900	1.13356000
H	4.99099700	6.10541500	1.19247100
H	4.63124800	6.88512800	-0.34831000
C	1.60432300	8.08870800	0.40273100
H	1.81770200	8.90693700	1.09849100
H	1.90802200	8.42273900	-0.58973000
H	0.52100200	7.94972100	0.39288100
C	0.94779800	3.44471300	-2.14524300
H	1.91047600	3.38341300	-2.65653100
H	0.83862500	2.54364000	-1.54563200
H	0.15839100	3.45653500	-2.90594200
C	1.10457100	6.42474300	-2.39122900
H	2.16839400	6.58183700	-2.59313700
H	0.63827800	6.14519200	-3.34157600
H	0.67359500	7.38045200	-2.09139200
C	-0.88534500	5.21934300	-0.39236700
H	-1.66633200	5.15828900	-1.15706500
H	-1.07404200	4.43526900	0.34426600
H	-1.00225000	6.18479600	0.11000400
Na	1.25103700	3.96599400	2.51458600

I15

E = -1858.67099656 a.u.

0 1

B	0.43402700	1.18483200	1.32814800
B	3.45597100	4.18856000	0.21081300
C	5.00251900	2.58073200	-0.30143500
C	5.11747900	2.94216400	1.22603200
C	-1.79104500	1.64135000	2.02446300
C	-1.77627500	0.51348500	0.94924300
C	5.11956100	1.74520200	2.16365600
H	4.21755800	1.14314100	2.05138300
H	5.98584400	1.10706400	1.97216300
H	5.18112400	2.08587000	3.20034300
C	6.27741300	3.88276600	1.54324200
H	6.18804100	4.23073600	2.57411200
H	7.24010000	3.37895700	1.43822800
H	6.27282100	4.75760400	0.89094300
C	4.23110600	1.28698600	-0.55578200
H	4.02456200	1.20347400	-1.62399000
H	4.81516700	0.41399500	-0.25540600
H	3.27410500	1.25719400	-0.02721100
C	6.32589300	2.57311500	-1.05119800
H	7.00025800	1.81674700	-0.64126000
H	6.14742300	2.33027200	-2.10014300
H	6.82174400	3.54251300	-1.01014000
C	-2.16687600	1.00623000	-0.44720800
H	-1.91990000	0.22935600	-1.17293700
H	-3.23641200	1.22206600	-0.52395000
H	-1.60772400	1.90259400	-0.71949100
C	-2.58319200	-0.72665600	1.30840200
H	-2.21977000	-1.18853000	2.22558900
H	-3.64391900	-0.48648200	1.43400400
H	-2.49653400	-1.46409900	0.50770000
C	-2.81289100	2.74487300	1.79277900
H	-2.71236500	3.51191700	2.56504300
H	-2.68596200	3.22594400	0.82478700
H	-3.83218300	2.34945000	1.84768200
C	-1.91271400	1.11315100	3.45603800
H	-1.19028600	0.31762700	3.64236200
H	-1.70383500	1.92720100	4.15410500
H	-2.91574200	0.73280300	3.66879500
O	-0.43837400	2.18830600	1.88807900
O	4.19339800	3.67888300	-0.82107600
O	-0.36626400	0.14590500	0.88767700
O	3.88694200	3.70183600	1.44985500

N	2.33056800	5.05571400	0.11833100
Si	2.16387900	6.34384300	1.32299900
Si	1.17835000	4.83038300	-1.23313900
C	1.13380500	5.74661400	2.79367600
H	0.79296700	6.59584500	3.39337400
H	0.23880000	5.19590400	2.48935200
H	1.71745700	5.12062500	3.48019800
C	3.85610300	6.86942600	1.94731200
H	3.75915500	7.72577000	2.62205500
H	4.36213700	6.07098500	2.49028300
H	4.50566700	7.17739800	1.12264400
C	1.35064900	7.86428400	0.57561900
H	1.27386000	8.63949800	1.34476300
H	1.95944400	8.27298500	-0.23469600
H	0.34630900	7.69644800	0.18578700
C	1.36790300	3.12476900	-1.97909300
H	2.32175900	2.99832200	-2.49081400
H	1.28016900	2.34358300	-1.21754900
H	0.56645500	2.96356800	-2.70794000
C	1.45878700	6.13565800	-2.55641400
H	2.49619100	6.11093400	-2.90268200
H	0.81954400	5.94588500	-3.42459200
H	1.24737600	7.14902100	-2.20919700
C	-0.55515100	4.93287500	-0.51109400
H	-1.29691400	4.76047300	-1.29747300
H	-0.68183800	4.14476200	0.23511900
H	-0.80272400	5.88620100	-0.04067500
Na	1.78145400	2.98421500	2.15323100

I16

E = -2647.20160626 a.u.

0 1

B	0.86400000	-0.13311500	0.44238200
B	1.89931300	4.48282000	0.75701700
C	1.08992600	5.63071600	2.57881500
C	0.47901500	6.21634800	1.25790200
C	2.16340800	-2.08751800	0.15272600
C	1.01077000	-2.06795100	-0.90337500
C	-0.94472000	5.72740800	0.99154300
H	-1.01250600	4.64174500	1.04052700
H	-1.65539500	6.15095500	1.70429300
H	-1.24598800	6.03313000	-0.01210000
C	0.54867400	7.73115400	1.13778100
H	0.11847700	8.04365000	0.18427400

H	-0.01873600	8.21244600	1.93898700
H	1.57625000	8.08988700	1.17440000
C	0.09762500	5.39943900	3.70546200
H	0.61921400	5.00974000	4.58244700
H	-0.37834200	6.34156900	3.99188900
H	-0.67000900	4.67897300	3.43497800
C	2.28462500	6.43795800	3.08558300
H	1.96706600	7.39005200	3.51571600
H	2.79512300	5.86738100	3.86323500
H	3.00200100	6.64228300	2.28966900
C	-0.13811500	-3.01817000	-0.56087600
H	-0.95764100	-2.85309500	-1.26082000
H	0.16129700	-4.06796100	-0.63178700
H	-0.52312800	-2.82749700	0.44084800
C	1.45183400	-2.29981600	-2.34437800
H	2.17213000	-1.55157200	-2.67284200
H	1.89969100	-3.29107000	-2.46889500
H	0.58490600	-2.23923900	-3.00709600
C	2.27493500	-3.37232100	0.96595200
H	3.08156200	-3.27175100	1.69592600
H	1.35594600	-3.57847900	1.51338700
H	2.50244400	-4.23266800	0.32788800
C	3.53486500	-1.73346700	-0.42870700
H	3.48845400	-0.81808700	-1.01761800
H	4.23414500	-1.56631600	0.39338900
H	3.93460500	-2.53100800	-1.06176700
O	1.78674300	-1.00814800	1.04929900
O	1.60499000	4.34359000	2.11706300
O	0.49317900	-0.71066800	-0.79076000
O	1.33792500	5.63420700	0.24140800
N	2.64321900	3.51677500	0.03381500
Si	2.24794300	3.36218900	-1.70017400
Si	4.06078100	2.84600400	0.88340500
C	0.38275400	3.47504700	-1.89363600
H	0.11019900	3.36899800	-2.94890800
H	-0.08116900	2.64422900	-1.35510400
H	-0.03245400	4.41433400	-1.52985600
C	3.11386700	4.74655400	-2.63572200
H	2.80832500	5.72110100	-2.24601600
H	4.20155800	4.67595100	-2.53470000
H	2.88107700	4.72166900	-3.70506800
C	2.70651900	1.69445900	-2.42096600
H	2.27767700	1.64417200	-3.42816800
H	3.77449700	1.50479800	-2.51475600

H	2.24153700	0.89493100	-1.84086100
C	5.04216700	4.29793400	1.58252700
H	5.26907200	5.03753000	0.80864000
H	4.50564800	4.80668200	2.38514700
H	5.99447000	3.95322300	1.99809700
C	5.20828500	1.93866200	-0.29376400
H	5.47421100	2.52892000	-1.17423100
H	6.13808800	1.72667400	0.24448100
H	4.80441300	0.98369400	-0.62697700
C	3.60535200	1.69827000	2.29482800
H	4.52140600	1.35917300	2.79199400
H	3.00887300	2.21536900	3.05224400
H	3.06477200	0.80978000	1.95931000
Na	0.48706900	2.02255100	1.73484800
O	-1.99169500	2.34833600	0.95920600
O	-1.54595100	2.61565000	3.10407000
C	-3.56323300	-2.58166000	1.04282400
C	-3.47724500	-2.16195000	-0.28304600
C	-3.07715300	-0.87082900	-0.60396200
C	-2.79788500	0.04595900	0.43431200
C	-2.83598400	-0.39859000	1.75930100
C	-3.21559900	-1.70297700	2.06204700
H	-1.69303600	-0.54937700	-2.14292500
H	-3.86848600	-3.59674000	1.27354700
H	-3.69065200	-2.86170100	-1.08523300
C	-2.78070800	-0.46240700	-2.02358600
C	-2.51685800	1.43060000	0.03009500
H	-2.54005900	0.24828400	2.57189400
H	-3.23033600	-2.02892000	3.09641100
C	-2.70373700	1.88764600	-1.20982600
C	-3.17989900	0.98465600	-2.30998100
H	-2.51162300	2.93200500	-1.42082200
H	-2.75708600	1.30704700	-3.26556600
H	-4.27239000	1.07577400	-2.41265500
H	-3.25226400	-1.14757700	-2.73258500
C	-2.41844300	2.53510400	2.24837300
N	-3.73869500	2.67345400	2.48249900
C	-4.74265100	2.90257100	1.43136400
H	-5.71218300	2.86315800	1.92931400
H	-4.72462900	2.07684900	0.72170100
C	-4.57536200	4.23572700	0.70743900
H	-5.34625300	4.34285500	-0.06007000
H	-4.66051200	5.07754200	1.39742600
H	-3.60420900	4.29715600	0.21709200

C	-4.15593700	2.81401100	3.88466900
H	-5.11948700	2.30883500	3.98703800
H	-3.43359800	2.27498100	4.49467800
C	-4.24979700	4.26651000	4.34438200
H	-4.99634000	4.82462500	3.77434900
H	-4.53477400	4.31130500	5.39873900
H	-3.28475200	4.76437300	4.23247900

TS16-17

E = -2647.18516071 a.u.

0 1

B	0.17140000	0.31970500	-0.31671300
B	1.86399000	4.38610600	0.51191600
C	0.82099000	5.57122000	2.18990000
C	0.39221700	6.12173700	0.78235100
C	1.44366700	-1.52721900	0.46235100
C	0.79133200	-1.85458500	-0.93339400
C	-0.98133900	5.62259600	0.33761900
H	-1.07367900	4.54179200	0.43677900
H	-1.78095300	6.09207600	0.91526300
H	-1.12964900	5.87806300	-0.71285500
C	0.48428200	7.63274900	0.63467800
H	0.18347200	7.91951100	-0.37461300
H	-0.18350700	8.13356500	1.34061900
H	1.49883100	7.99430200	0.79771000
C	-0.32344100	5.33048100	3.15821500
H	0.05413600	4.87990400	4.07746600
H	-0.80491000	6.27761200	3.41568500
H	-1.07388100	4.66172000	2.74851000
C	1.91017200	6.40978400	2.85646000
H	1.51636500	7.36231000	3.21597100
H	2.30898700	5.86172800	3.71223100
H	2.73335000	6.61724600	2.17154300
C	-0.38535700	-2.82432800	-0.85148800
H	-0.87323700	-2.87006600	-1.82655600
H	-0.05920200	-3.83377100	-0.58541400
H	-1.12949600	-2.49919900	-0.12973600
C	1.76775800	-2.33048300	-2.00354300
H	2.56573100	-1.61147000	-2.18332700
H	2.21800600	-3.29000200	-1.73253900
H	1.22734000	-2.46627200	-2.94229300
C	1.07490800	-2.48604000	1.58696600
H	1.52615500	-2.14234600	2.52096400
H	-0.00284500	-2.53420300	1.73286000

H	1.44529000	-3.49595700	1.38714700
C	2.95898200	-1.34884900	0.40959100
H	3.24489800	-0.58972500	-0.31734500
H	3.32564600	-1.03409300	1.38840200
H	3.46652200	-2.28138900	0.15090300
O	0.85945800	-0.21467200	0.79207700
O	1.43444800	4.29038500	1.83573200
O	0.24755100	-0.56714000	-1.36713700
O	1.38072300	5.51591100	-0.09885900
N	2.69272800	3.38962000	-0.08281700
Si	2.51728500	3.21459900	-1.86166400
Si	4.09318000	2.91089600	0.89388700
C	0.71011900	3.37804200	-2.31697700
H	0.57950400	3.16055100	-3.38210500
H	0.11687000	2.64128800	-1.76430600
H	0.30897000	4.37238500	-2.12576100
C	3.56802700	4.54816300	-2.67476800
H	3.24839100	5.53924800	-2.34207800
H	4.62827500	4.44015700	-2.42422700
H	3.48513600	4.51782000	-3.76566400
C	3.04926200	1.52107500	-2.47110700
H	2.83035500	1.47891500	-3.54367800
H	4.10519800	1.28621700	-2.34890200
H	2.44578200	0.74092100	-2.00557100
C	4.98094700	4.45758900	1.49631100
H	5.23900600	5.11438500	0.66043400
H	4.37244900	5.03381500	2.19588300
H	5.91109300	4.19917200	2.01210600
C	5.33549400	1.89135100	-0.07444000
H	5.67962700	2.39084000	-0.98278800
H	6.21387200	1.73938600	0.56138700
H	4.95993800	0.90581900	-0.34898000
C	3.56802100	1.91131300	2.40590800
H	4.45394800	1.60578000	2.97098400
H	2.94857900	2.49976100	3.08812600
H	3.04343700	0.98993500	2.13936200
Na	0.81237100	1.94588000	1.68237700
O	-1.40681800	2.23032100	1.05406200
O	-1.00046100	2.04993100	3.21723900
C	-3.76953700	-2.36830700	0.66048600
C	-3.80074800	-1.77198600	-0.59865400
C	-3.14415000	-0.57039400	-0.84820500
C	-2.45271300	0.07713200	0.20119700
C	-2.37868500	-0.55927600	1.44622300

C	-3.03728400	-1.76459500	1.67792500
H	-2.07503700	-0.19710700	-2.62487700
H	-4.28845000	-3.30489800	0.83583700
H	-4.33328600	-2.25624000	-1.41222200
C	-3.07198000	0.02751500	-2.22638600
C	-1.85890600	1.40299400	-0.10296800
H	-1.77806100	-0.14091000	2.24141600
H	-2.96803200	-2.23082400	2.65560300
C	-2.40909600	2.16240700	-1.10696100
C	-3.24683200	1.54940900	-2.19266600
H	-2.09715800	3.19382100	-1.21049700
H	-2.97565600	1.96239300	-3.17206600
H	-4.31708300	1.78686800	-2.05838100
H	-3.80584800	-0.44301000	-2.88759400
C	-1.85987100	2.16828400	2.33583300
N	-3.17170700	2.28977800	2.61447600
C	-4.22644500	2.55896600	1.63407900
H	-4.94145400	1.73071000	1.67045500
H	-3.78026100	2.55050100	0.64141000
C	-4.92918500	3.89255200	1.87345600
H	-5.67491500	4.05762000	1.09143400
H	-5.44625500	3.93245000	2.83530700
H	-4.21323400	4.71791900	1.83625500
C	-3.57003500	2.09542900	4.01511500
H	-4.63442400	1.85116800	4.00650300
H	-3.03769500	1.22340700	4.39919800
C	-3.29761100	3.30130300	4.91185100
H	-3.81716900	4.19286400	4.55534700
H	-3.63681700	3.09546400	5.93119700
H	-2.22885900	3.51021300	4.94373000

I17

E = -2647.36159514 a.u.

0 1

B	-0.30775200	-0.85938000	-0.40343000
B	1.76076400	4.49030100	0.76051000
C	0.78890600	5.02352600	2.77485700
C	0.36557400	6.06437900	1.66418500
C	1.87151400	-1.31476000	0.18375500
C	0.89845000	-2.34989100	0.84829500
C	-1.04974600	5.84502100	1.13604800
H	-1.22489600	4.80522600	0.85771300
H	-1.79268300	6.13516700	1.88301300
H	-1.19760300	6.47323400	0.25501100

C	0.57075700	7.52206100	2.04982000
H	0.27518000	8.16257200	1.21681200
H	-0.04715500	7.78539600	2.91210800
H	1.61161200	7.73932200	2.28795700
C	-0.36772300	4.42197500	3.55621800
H	0.00933000	3.67389400	4.25584200
H	-0.88466400	5.19461300	4.13167100
H	-1.08252300	3.93462300	2.89943000
C	1.86542800	5.54799200	3.72424100
H	1.47853700	6.33056700	4.37957700
H	2.21898400	4.72618700	4.34968000
H	2.72189700	5.95001400	3.17859800
C	0.58706100	-2.04177100	2.31352100
H	-0.20724800	-2.71332400	2.64617100
H	1.45658400	-2.20975300	2.95394500
H	0.22797500	-1.01927000	2.44101800
C	1.30843500	-3.80467600	0.67635500
H	1.38571400	-4.08278000	-0.37410900
H	2.26878400	-3.99872200	1.16206800
H	0.56048200	-4.45002100	1.14005700
C	2.88053400	-0.69732200	1.13717600
H	3.49274100	0.03712500	0.61101800
H	2.39203500	-0.21324700	1.98339100
H	3.55463200	-1.45871100	1.53640900
C	2.57259700	-1.84404900	-1.06606800
H	1.85699300	-2.27901700	-1.76560300
H	3.07507900	-1.01794000	-1.57306600
H	3.32053700	-2.60065800	-0.82043200
O	0.95225800	-0.27065400	-0.26602200
O	1.42155900	3.96684600	1.99067200
O	-0.33176000	-2.12697700	0.10573800
O	1.28776700	5.75678900	0.57061900
N	2.53484300	3.70935600	-0.17445400
Si	2.07274700	3.82392300	-1.89662000
Si	4.21098900	3.43794200	0.35212300
C	0.25673200	4.27161600	-1.99894800
H	-0.10837200	4.09837600	-3.01600000
H	-0.36297100	3.68334800	-1.31798800
H	0.09690700	5.32326600	-1.75929800
C	3.10794700	5.11944600	-2.78408200
H	3.00511100	6.09350700	-2.29819900
H	4.17197700	4.86765800	-2.80501400
H	2.78191200	5.23155400	-3.82299300
C	2.34122300	2.14379900	-2.71025000

H	1.73812000	2.07788700	-3.62121300
H	3.37902800	1.97563400	-3.00181000
H	2.04037600	1.31593700	-2.06388200
C	5.11396100	5.08830300	0.39958000
H	5.15197800	5.55735200	-0.58660200
H	4.61394100	5.79325500	1.07083700
H	6.14308500	4.97271900	0.75396000
C	5.10532100	2.28421600	-0.83205400
H	5.25271000	2.72421600	-1.82055800
H	6.09853400	2.06507800	-0.42766700
H	4.58965100	1.33152100	-0.96741600
C	4.26474000	2.70467400	2.08304500
H	5.30107700	2.46657100	2.34459300
H	3.88495400	3.40477100	2.82741300
H	3.68684600	1.78475900	2.18478900
Na	0.88995000	1.84946800	0.84997500
O	-1.23683600	2.62824500	0.62961100
O	-0.77822100	0.98373700	2.08716700
C	-5.61499600	-0.98039500	-0.29710800
C	-5.24737800	-0.19995100	-1.39175900
C	-3.90880200	0.05414700	-1.67375900
C	-2.90300500	-0.48188600	-0.84183600
C	-3.28539500	-1.27102000	0.24885900
C	-4.62682800	-1.51790400	0.52163800
H	-3.27534200	0.16385700	-3.70705100
H	-6.66377000	-1.16432200	-0.08707200
H	-6.01369700	0.22130000	-2.03677100
C	-3.49882100	0.85776100	-2.88425100
C	-1.48455000	-0.14962100	-1.10785200
H	-2.52157600	-1.68900800	0.88973700
H	-4.89787700	-2.12436500	1.37981500
C	-1.19683400	0.87906200	-1.93036200
C	-2.25471700	1.69958300	-2.60181100
H	-0.16496200	1.17186900	-2.08028100
H	-1.87502500	2.14798000	-3.52441700
H	-2.49832500	2.53360800	-1.92970100
H	-4.32570400	1.48789700	-3.22304000
C	-1.58758400	1.78133900	1.51362800
N	-2.91623700	1.72448700	1.88854900
C	-3.93342600	2.46558500	1.16238700
H	-4.72195100	1.76937800	0.85515100
H	-3.46261000	2.84208100	0.25773300
C	-4.53352000	3.62595800	1.95762200
H	-5.27672100	4.16218700	1.35869800

H	-5.03062800	3.27843700	2.86761800
H	-3.75372100	4.33408300	2.24908600
C	-3.32411300	0.81939800	2.95358900
H	-4.39923200	0.65135100	2.84709900
H	-2.83287700	-0.14286200	2.80568500
C	-2.99845100	1.34388000	4.35244300
H	-3.48705300	2.30284200	4.54364500
H	-3.32567600	0.63465400	5.12020800
H	-1.92058100	1.48006100	4.45025200

TS16-17'

E = -1362.16852800 a.u.

0 1

B	0.19481700	0.22537700	-0.13751200
C	1.54567200	-1.64514400	0.39238400
C	0.79855100	-1.86784700	-0.96573800
C	-0.40680700	-2.79893900	-0.84501600
H	-0.98438300	-2.75144800	-1.76922800
H	-0.10114000	-3.83676400	-0.68662900
H	-1.06668700	-2.50217900	-0.03198300
C	1.68760300	-2.30911300	-2.12012200
H	2.47060100	-1.58101300	-2.32871600
H	2.15507300	-3.27635700	-1.91195800
H	1.08263200	-2.41527800	-3.02263400
C	1.39262100	-2.77002700	1.40506100
H	1.92475200	-2.51574800	2.32525300
H	0.34670000	-2.94012900	1.65600600
H	1.81537200	-3.70450700	1.02376700
C	3.01897600	-1.27188600	0.22889600
H	3.14134500	-0.44500200	-0.47191600
H	3.41989300	-0.95768100	1.19592500
H	3.61693800	-2.11672500	-0.12255300
O	0.86434600	-0.45228800	0.91885300
O	0.27727000	-0.53694300	-1.27673700
Na	0.66303900	1.44957100	2.09387300
O	-1.34058600	2.18582400	1.20188800
O	-1.11452600	2.13436700	3.39178200
C	-3.83074700	-2.34669500	0.75996200
C	-3.81682200	-1.75724100	-0.50195200
C	-3.13172100	-0.56847100	-0.74060000
C	-2.45378600	0.06947100	0.32236500
C	-2.44332500	-0.55173600	1.57712800
C	-3.12739400	-1.74383700	1.79834900
H	-2.03572500	-0.25945600	-2.51739200

H	-4.36960200	-3.27381800	0.92516100
H	-4.33619600	-2.23645500	-1.32689000
C	-3.02059600	0.01737500	-2.12226500
C	-1.77630300	1.35702100	0.02165500
H	-1.88131600	-0.12539500	2.39717900
H	-3.10501500	-2.19858500	2.78348400
C	-2.23092900	2.11862000	-1.02420300
C	-3.11437300	1.54549500	-2.09586800
H	-1.82052900	3.11338200	-1.15475400
H	-2.83585700	1.94018700	-3.07976700
H	-4.16990400	1.83825600	-1.94855500
H	-3.77704800	-0.41714600	-2.78291800
C	-1.90429100	2.22865400	2.43556600
N	-3.22926200	2.37343900	2.61653700
C	-4.21451200	2.61686900	1.55912800
H	-4.90201600	1.76492300	1.53238900
H	-3.68941100	2.63188500	0.60639300
C	-4.97979500	3.92342700	1.74943500
H	-5.66510000	4.06644600	0.90993300
H	-5.57579000	3.93722700	2.66517900
H	-4.29479500	4.77448300	1.77471500
C	-3.72640800	2.22517400	3.99206500
H	-4.78664700	1.97456400	3.91558000
H	-3.22066300	1.36898300	4.44167500
C	-3.52031100	3.46085800	4.86476300
H	-4.02356900	4.33574900	4.44933100
H	-3.92030600	3.28307900	5.86730900
H	-2.45688900	3.68080000	4.95524800