Supporting Information

Palladium/Norbornene Cooperative Catalysis Triple Functionalization: Carbamoylation/Double-annulation of (Hetero)aryl Iodides

Yi-Xin Chai,[a] Yu-Fan Yang,[a] Feng-Yu Zhang,[a] Ji-Yan Zhao,[a] Ya-Ting Wang,[a] Yanmei Chen,[c] Yuan-Yuan Sun,[a] Jin-Heng Li,[b,*] Yan-Ping Zhu [a,*]

[a] School of Pharmacy, Key Laboratory of Molecular Pharmacology and Drug Evaluation, Ministry of Education, Yantai University, Shandong, Yantai, 264005, P. R. China. E-mail: chemzyp@foxmail.com; chemzyp@ytu.edu.cn

[b] State Key Laboratory Base of Eco-Chemical Engineering, College of Chemical Engineering, Qingdao University of Science and Technology, Qingdao 266042, China.; orcid.org/0000-0001-7215-7152; E-mail: jhli@hnu.edu.cn.

[c] Hubei Key Laboratory of Processing and Application of Catalytic Materials, Huanggang Normal University, Huanggang 438000, P.R. China. E-mail: cingym@163.com

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1. General information

Materials and General Experimental: 2-iodobiphenyl, tri(2-furyl)phosphine and cesium carbonate were purchased from Shanghai Shaoyuan Co. Ltd. Palladium acetate was purchased from Energy Chemical. Unless stated otherwise, all solvents and commercially available reagents were obtained from commercial suppliers and used without further purification. In addition, petroleumether (b.p. 60-90 ºC), which was used for column chromatography, was distilled prior to use. Non-commercial starting materials were prepared as described below or according to literature procedures. Analytical thin layer chromatography (TLC) was performed using pre-coated silica gel HF254 glass plates. Column chromatography was performed using silica gel (200-300 mesh).

Instrumentation: Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Advance 400 MHz spectrometer at ambient temperature using the non or partly deuterated solvent as internal standard (^{1}H: δ 7.26 ppm and ^{13}C{1H}: δ 77.0 ppm for $CDCl_3$. Chemical shifts (δ) are reported in ppm, relative to the internal standard of tetramethylsilane (TMS). The coupling constants (*J*) are quoted in hertz (Hz). Resonances are described as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad) or combinations thereof. High resolution mass spectra were obtained on Thermo Scientific Q-Exactive (ESI mode, Q-Exactive Orbitrap MS system). Melting points were determined using SGW X-4 apparatus and not corrected. The X-ray diffraction data for the crystallized compound were collected on a Bruker Smart APEX CCD area detector diffractometer (graphite monochromator, Mo Kα radiation, λ = 0.71073 Å) at 296(2) K.

2. Experimental Procedures

2.1 General procedure for the catalytic process (3aa as an example)

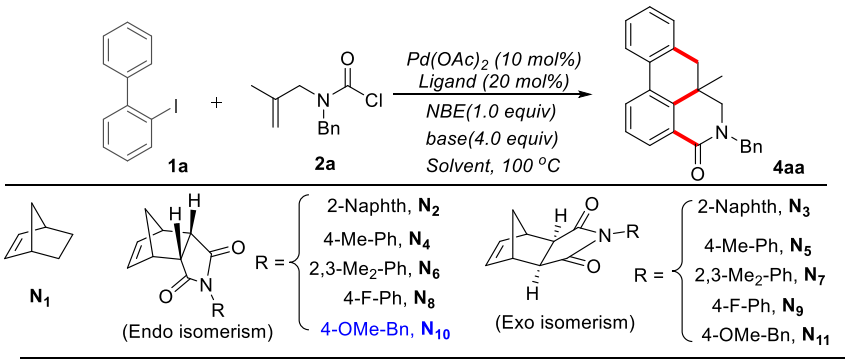
A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), carbamic chloride (89 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and **N_2** (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column chromatography (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1) to obtain the corresponding products.

2.2 Reaction Optimization

Our initial trial commenced with the reaction of 2-iodobiphenyl **1a** with carbamic chloride **2a** in the presence of palladium acetate, norbornene and tri(2-furyl)phosphine (TFP). The selected results are summarized in Table **S1**. To our delight, when the

reaction was performed with Cs_2CO_3 as the base, DMAc, MeCN or THF was used respectively at 100 °C for 24 h, The reaction afforded the target products in moderate yields. (Table S1, entry 1-3). Yield significantly decreased when the solvent was switched to NMP or DCM (entries 4 and 5). To our excitement, it was observed that toluene provided better result of the target product (entry 6). With Toluene as the most effective solvent, we went on to test other reaction conditions. Temperature screening proved that 80℃ was the better choice, thus providing **4aa** with 51% yield (entry 8). Replacing Cs_2CO_3 with several bases did not show superior results (entries 10-12). More gratifyingly, further optimization shows that using TFP as a phosphine ligand instead of PPh_3 did enhance the process to yield **4aa** in 78% (entry 17). Furthermore, we observed that NBE is a very essential and unique cocatalyst in the Pd/NBE catalysis. Thus, we explored the effects of different norbornene derivatives on the reaction (entries 18-27). Fortunately, we were pleasant to find that when $\mathbf{N_{10}}$ norbornene derivatives was added to the reaction system, the yield of the product reached 87%.

Table S1 Optimization of the reaction conditions[a, b]



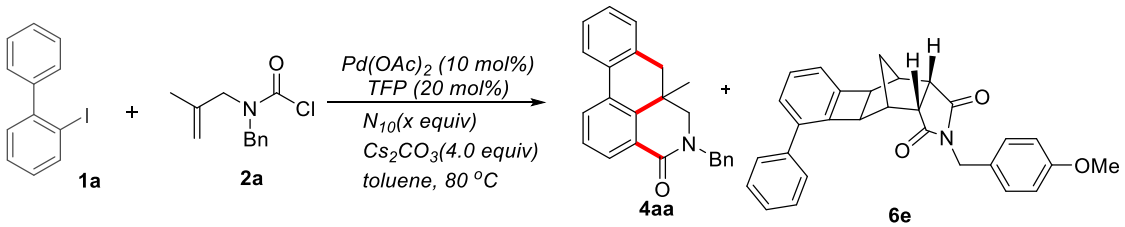
entry	Ligand	Base	NBEs	temp(℃)	solvent	yield (%)
1	PPh_3	Cs_2CO_3	N_1	100	DMAc	10
2	PPh_3	Cs_2CO_3	N_1	100	MeCN	14
3	PPh_3	Cs_2CO_3	N_1	100	THF	35
4	PPh_3	Cs_2CO_3	N_1	100	NMP	5
5	PPh_3	Cs_2CO_3	N_1	100	DCM	12
6	PPh_3	Cs_2CO_3	N_1	100	Toluene	50
7	PPh_3	Cs_2CO_3	N_1	90	Toluene	52
8	PPh_3	Cs_2CO_3	N_1	80	Toluene	51
9	PPh_3	Cs_2CO_3	N_1	110	Toluene	46
10	PPh_3	K_2CO_3	N_1	80	Toluene	33
11	PPh_3	K_3PO_4	N_1	80	Toluene	20
12	PPh_3	KOAc	N_1	80	Toluene	18
13	$P(4\text{-F-Ph})_3$	Cs_2CO_3	N_1	80	Toluene	35
14	$P(4\text{-Cl-Ph})_3$	Cs_2CO_3	N_1	80	Toluene	38
15	$P(4\text{-Me-Ph})_3$	Cs_2CO_3	N_1	80	Toluene	46
16	$P(4\text{-MeO-Ph})_3$	Cs_2CO_3	N_1	80	Toluene	43
17	TFP	Cs_2CO_3	N_1	80	Toluene	78
18	TFP	Cs_2CO_3	N_2	80	Toluene	77
19	TFP	Cs_2CO_3	N_3	80	Toluene	69

20	TFP	Cs_2CO_3	N_4	80	Toluene	73
21	TFP	Cs_2CO_3	N_5	80	Toluene	59
22	TFP	Cs_2CO_3	N_6	80	Toluene	64
23	TFP	Cs_2CO_3	N_7	80	Toluene	43
24	TFP	Cs_2CO_3	N_8	80	Toluene	76
25	TFP	Cs_2CO_3	N_9	80	Toluene	55
26	**TFP**	**Cs_2CO_3**	**N_{10}**	**80**	**Toluene**	**87**
27	TFP	Cs_2CO_3	N_{11}	80	Toluene	48

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2.0 equiv.), $Pd(OAc)_2$ (10 mol%), ligand (20 mol%), Base (4.0 equiv.) and NBEs (1.0 equiv.) were heated in solvent (2 mL) for 24 h under Ar atmosphere. [b] Isolated yields.

Next, we tried to reduce the amount of NBE equivalent to observe the effect on product yield. As shown in Table S2, the experimental results indicate that reducing the equivalent of NBE leads to residual raw material **1a** and a decrease in product yield. Some by-products **6e** in the reaction are formed through the coupling of NBE and **1a**. The formation of **6e** was confirmed by the analysis of HRMS and NMR.

Table S2 Optimization of the N_{10} equiv.[a, b]



entry	X equiv.	remaining **1a**	yield **4aa** (%)	**6e** (%)
1	0.1	70%	15	12
2	0.2	64%	20	16
3	0.3	48%	35	15
4	1.0	trace	87	10

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2.0 equiv.), $Pd(OAc)_2$ (10 mol%), TFP (20 mol%), Cs_2CO_3 (4.0 equiv.) and N_{10} (x equiv.) were heated in toluene (2 mL) for 24 h under Ar atmosphere. [b] Isolated yields.

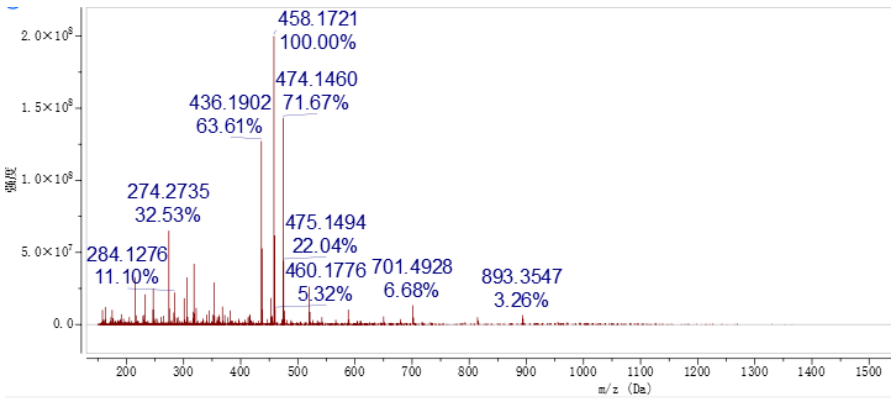
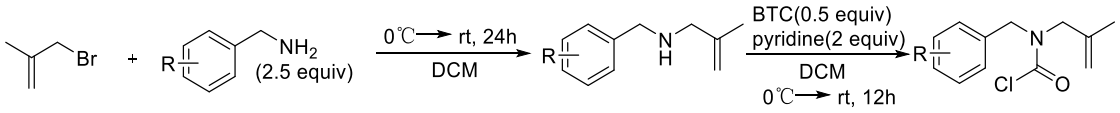


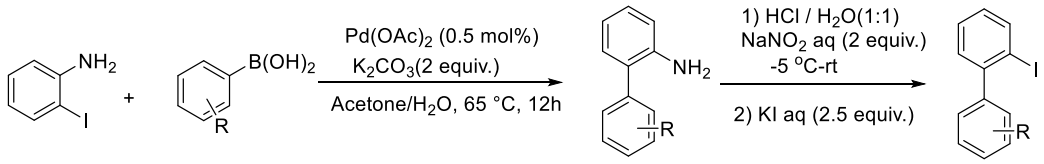
Figure S1. The HRMS results for the **6e.**

2.3 Synthesis of starting materials



Scheme S1 Synthesis of carbamic chloride

General procedure A: Alkyl halide (10 mmol, 1.0 equiv) was added slowly to a solution of the corresponding amine (25 mmol, 2.5 equiv) in CH_2Cl_2 (15 mL, 0.3 M) at 0 ℃. The mixture was allowed to stir at room temperature for 24 h, the reaction was quenched with water and the resulting mixture was extracted with dichloromethane. The combined organic layers were dried over Na_2SO_4, filtered and concentrated. Pure allylamines products were obtained by column chromatography (silica gel, with a mixture of petroleum ether/ethyl acetate as eluent). The pure allylamines products was dissolved in dichloromethane (15 mL, 0.3 M) and cooled to 0 ºC. Then pyridine (20 mmol, 2.0 equiv) was added followed by triphosgene (5 mmol, 0.5 equiv). The reaction was warmed to room temperature and stirred until TLC indicated completion. The reaction was quenched with water and extracted twice with dichloromethane. The organic layer was dried over magnesium sulfate, filtered, and concentrated under reduced pressure. The crude starting material was purified by flash column chromatography in an ethyl acetate / petroleum ether mixture to give the desired product.

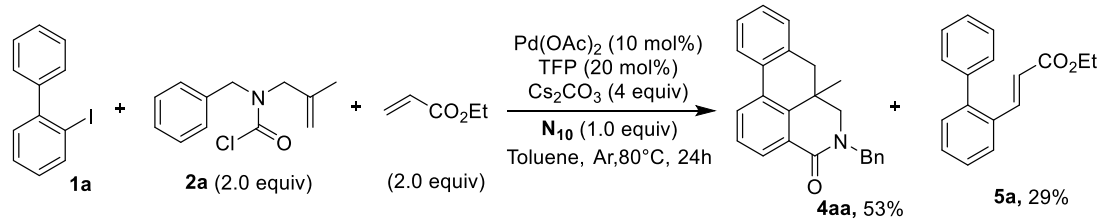


Scheme S2 Synthesis of iodobiphenyl derivative

General procedure B: To a 100 mL ground flask equipped with PTFE stopcock on side-arm were added a magnetic stir-bar, substituted 2-iodoaniline (10.0 mmol), substituted phenylboronic acid (12.0 mmol, 1.2 equiv), and K_2CO_3 (25 mmol, 2.5 equiv). The flask was equipped with a rubber septum and sealed up. The reaction flask was evacuated and back-filled with argon, followed by the addition of acetone (18.0 mL) and water (24.0 mL) via a syringe. The reaction mixture was stirred and heated to 65 °C. A solution of $Pd(OAc)_2$ (0.02 mmol, 20 mol %) in acetone (2.0 mL) was then introduced to the reaction mixture via a syringe. After the reaction mixture was stirred at 65 °C overnight, it was allowed to cool to room temperature. The reaction mixture was extracted with EtOAc (4×40 mL), and the combined organic phases were washed with 50 mL of water. The organic phases were dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude product was purified by silica gel column chromatography (petroleum ether/EtOAc) to give the corresponding substituted 2-aminobiphenyls. Subsequently, 2ml of concentrated hydrochloric acid/water (1:1) was added to the obtained product (2 mmol, 1.0 equiv) at room temperature and stirred for 15 min, then 1ml of sodium nitrite solution (4 mmol, 2 equiv) was added dropwise at -5 ℃, and stirring was continued for 20 min. After that, 1mL KI solution (5 mmol, 2.5 equiv) was added dropwise and stirred for 15 min, and then turned to room temperature

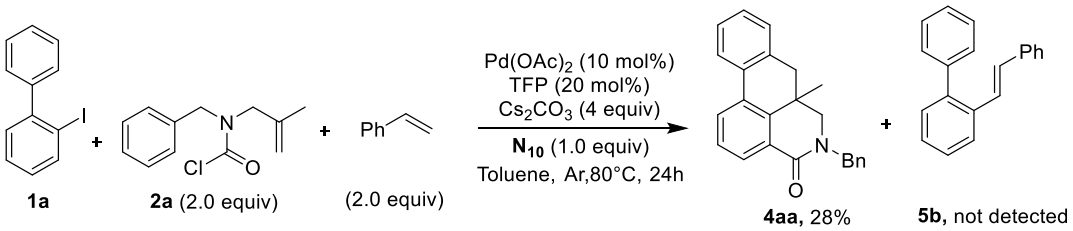
overnight. After the reaction is completed, add $NaHCO_3$ solution to the reaction solution and adjust it to pH = 9-10, and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phases were washed with saturated $Na_2S_2O_3$ solution and H_2O. After drying over Na_2SO_4 and concentration under reduced pressure, the crude product was purified by column chromatography using ethyl acetate/petroleum ether mixture.

2.4 Controlled Experiment



Scheme S3 With ethyl acrylate as trapping reagent

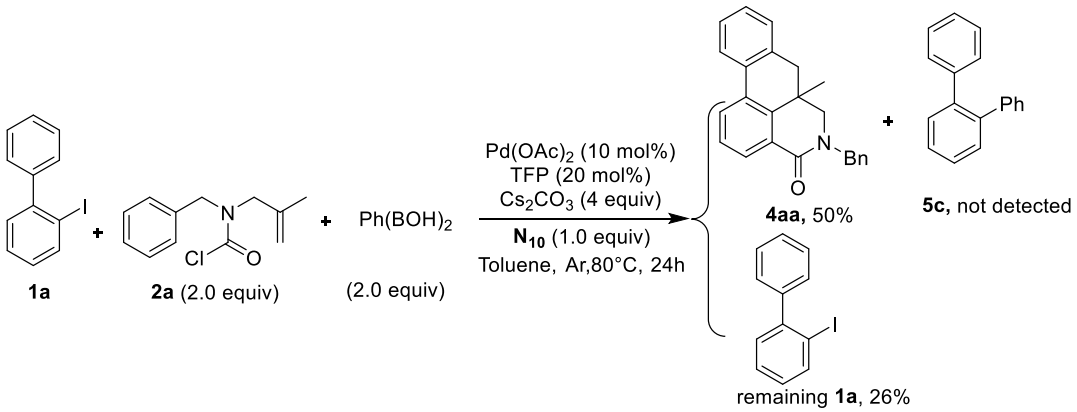
A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), benzoyl cyanide (89 mg, 0.4 mmol, 2.0 equiv), ethyl acrylate (40 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and **N_{10}** (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column chromatography using ethyl acetate/petroleum ether mixture to obtain the corresponding products **4aa** (53%) and **5a** (29%).



Scheme S4 With styrene as trapping reagent

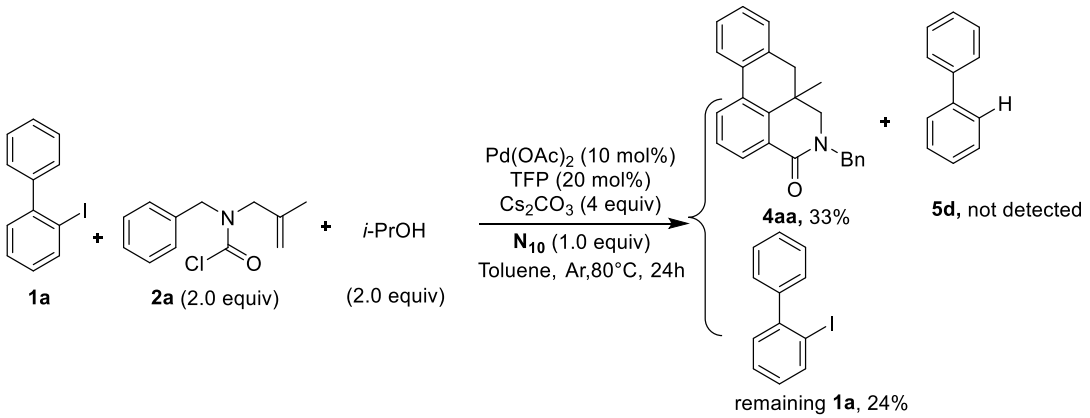
A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), benzoyl cyanide (89 mg, 0.4 mmol, 2.0 equiv), styrene (41 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and **N_{10}** (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column

chromatography using ethyl acetate/petroleum ether mixture to obtain the corresponding products **4aa**.



Scheme S5 With phenyl boronic acid as trapping reagent

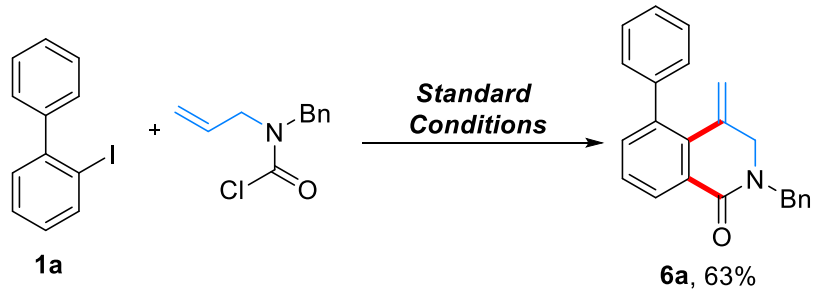
A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), benzoyl cyanide (89 mg, 0.4 mmol, 2.0 equiv), phenyl boronic acid (49 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and $\mathbf{N_{10}}$ (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column chromatography using ethyl acetate/petroleum ether mixture to obtain the corresponding products **4aa** and the reaction remaining **1a** 26%.



Scheme S6 With isopropyl alcohol as trapping reagent

A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), benzoyl cyanide (89 mg, 0.4 mmol, 2.0 equiv), isopropyl alcohol (24 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and $\mathbf{N_{10}}$ (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and

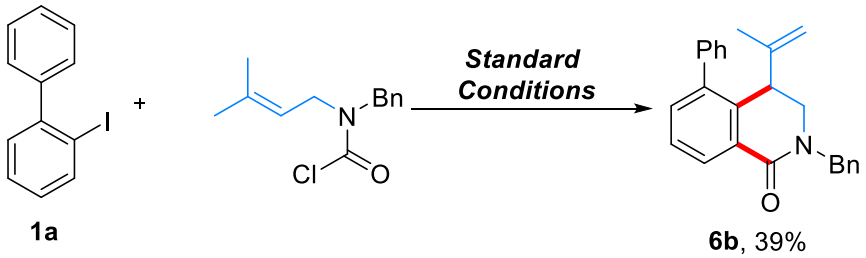
50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column chromatography using ethyl acetate/petroleum ether mixture to obtain the corresponding products **4aa** and the reaction remaining **1a** 24%.



1a **6a**, 63%

Scheme S7 Reaction of 2-iodobiphenyl with allyl(benzyl)carbamic chloride

A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), allyl(benzyl)carbamic chloride (54 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and **N₁₀** (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column chromatography using ethyl acetate/petroleum ether mixture to obtain the corresponding products **6a.**

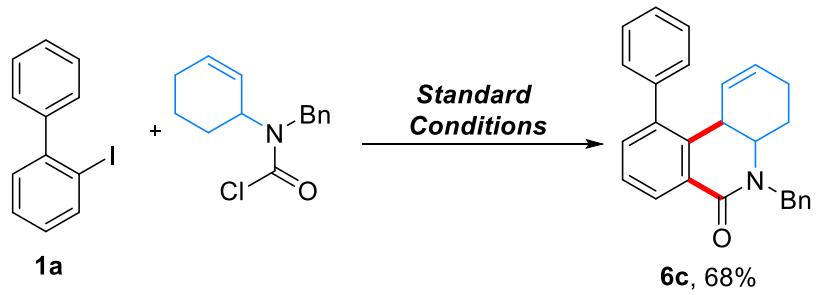


1a **6b**, 39%

Scheme S8 Reaction of 2-iodobiphenyl with benzyl(3-methylbut-2-en-1-yl)carbamic chloride.

A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), benzyl(3-methylbut-2-en-1-yl)carbamic chloride (94 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and **N₁₀** (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column

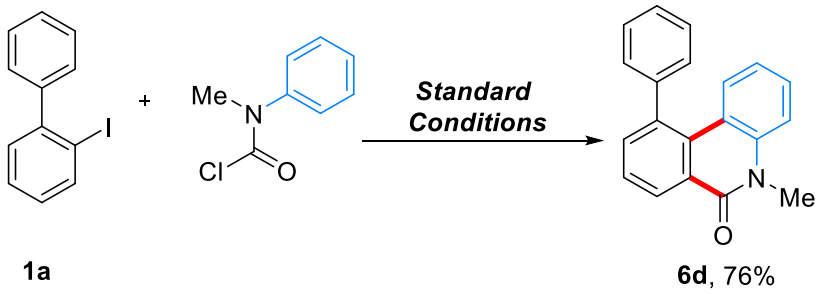
chromatography using ethyl acetate/petroleum ether mixture to obtain the corresponding products **6b**.



1a **6c**, 68%

Scheme S9 Reaction of 2-iodobiphenyl with benzyl(cyclohex-2-en-1-yl)carbamic chloride

A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), 5-(benzyl(chlorocarbonyl)amino)cyclohex-3-en-1-ylium (99 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and **N10** (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column chromatography using ethyl acetate/petroleum ether mixture to obtain the corresponding products **6c.**



1a **6d**, 76%

Scheme S10 Reaction of 2-iodobiphenyl with methyl(phenyl)carbamic chloride

A 25 mL pressure vial was charged with 2-iodobiphenyl (51 mg, 0.2 mmol, 1.0 equiv), methyl(phenyl)carbamic chloride (68 mg, 0.4 mmol, 2.0 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 10 mol%), TFP (9 mg, 0.04 mmol, 20 mol%), Cs_2CO_3 (261 mg, 0.8 mmol, 4.0 equiv) and **N10** (56 mg, 0.2 mmol, 1.0 equiv) in toluene (2.0 ml, 0.1 M) were added. The reaction was stirred at 80 °C in heating mantle under argon atmosphere for 24 h. After the reaction was completed (monitored by TLC), and 50 ml of water was added to the mixture, which was then extracted three times with EtOAc (3 × 50 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residues were purified by column chromatography using ethyl acetate/petroleum ether mixture to obtain the corresponding products **6d**.

3. Molecular structure and crystallographic data

The purified compound **4ad** is dissolved in dichloromethane and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a colorless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart APEX CCD area detector diffractometer at 293 K.

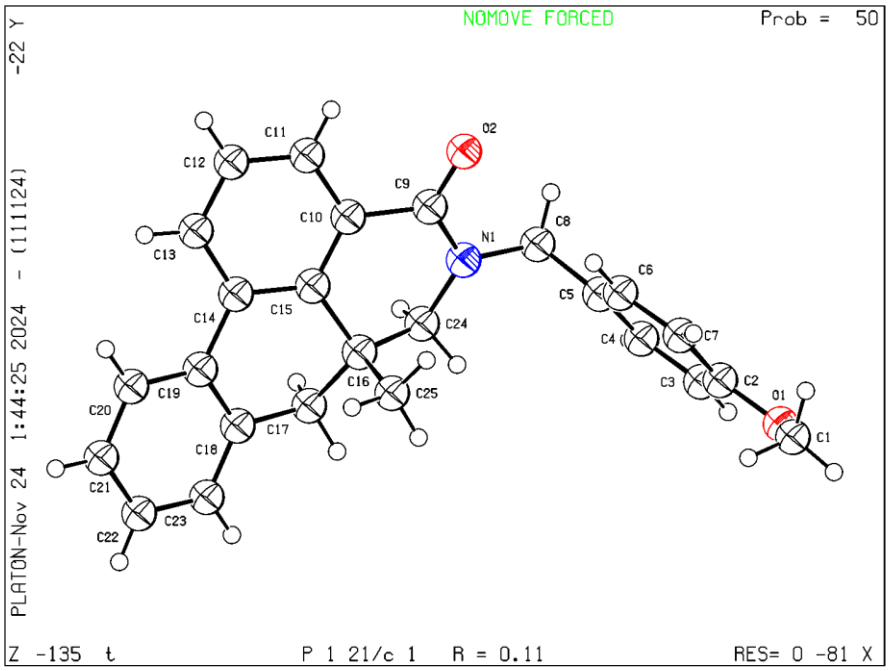


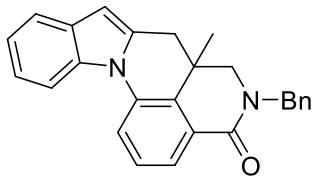
Figure S2 X-ray crystal structure of compound **4ad**

Table S3. Crystal data and structure refinement for compound 4ad

Identification code	CCDC: 2411797
Empirical formula	$C_{25}H_{22}NO_2$
Formula weight	368.459
Temperature/K	293 K
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.5319(14)
b/Å	6.0342(8)
c/Å	30.383(4)
α/°	90
β/°	93.080(5)
γ/°	90
Volume/Å^3	1928.1(4)
Z	4
ρ_{calc}g/cm^3	1.269
μ/mm^{-1}	0.080
F(000)	780.5

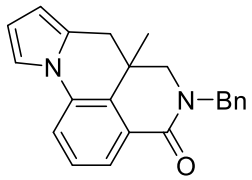
Crystal size/mm^3	0.28 x 0.26 x 0.25
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.88 to 50.28
Index ranges	-12 ≤ h ≤ 12, -7 ≤ k ≤ 7, -36 ≤ l ≤ 36
Reflections collected	34924
Independent reflections	3427 [R_{int} = 0.0946, R_{sigma} = 0.0447]
Data/restraints/parameters	3427/0/256
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.0478, wR_2 = 0.1116
Final R indexes [all data]	R_1 = 0.0613, wR_2 = 0.1199
Largest diff. peak/hole / e Å^{-3}	0.17/-0.20

4. Characterization Data for Products



3a

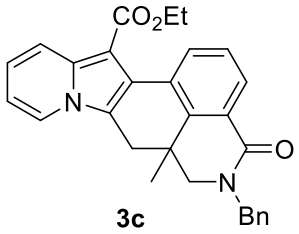
5-Benzyl-6a-methyl-5,6,6a,7-tetrahydro-4H-benzo[*ij*]indolo[1,2-*b*][2,6] naphthyridin-4-one (3a), (silica gel: 200−300 mesh, solvent system: petroleum ether/ ethyl acetate = 10:1-3:1), 36 mg, 48%, white solid, m.p. 136-137 °C. ^{1}H NMR (500 M Hz, $CDCl_3$) δ (ppm) 8.15 – 7.82 (m, 3H), 7.65 – 7.47 (m, 2H), 7.45 – 7.14 (m, 7H), 6. 43 (s, 1H), 4.84 (dd, J = 124.0, 14.5 Hz, 2H), 3.41 (dd, J = 174.4, 12.2 Hz, 2H), 2.88 (dd, J = 40.0, 15.0 Hz, 2H), 0.95 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 163.9, 136.6, 134.5, 134.1, 134.0, 132.8, 129.7, 128.7, 128.4, 128.0, 127.7, 126.0, 123.6, 12 2.4, 121.2, 120.6, 120.3, 111.1, 102.1, 56.9, 50.8, 34.4, 32.8, 22.0. HR-MS (ESI): calc d for $[M+Na]^+$ $C_{26}H_{22}N_2NaO$: 401.1624; found: 401.1619.



3b

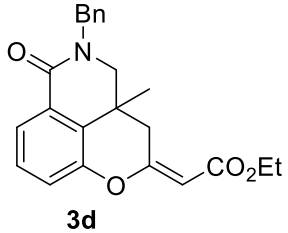
5-Benzyl-6a-methyl-5,6,6a,7-tetrahydro-4H-benzo[*ij*]pyrrolo[1,2-*b*][2,6] naphthyridin-4-one (3b), (silica gel: 200−300 mesh, solvent system: petroleum ether/

ethyl acetate = 10:1-3:1), 37 mg, 57%, white solid, m.p. 132-134 °C. ^{1}H NMR (500 M Hz, $CDCl_3$) δ (ppm) 7.96 (d, J = 7.6 Hz, 1H), 7.59 – 7.26 (m, 7H), 7.15 (s, 1H), 6.28 (t, J = 3.2 Hz, 1H), 6.04 (s, 1H), 4.83 (dd, J = 118.9, 14.5 Hz, 2H), 3.39 (dd, J = 185.0, 1 2.2 Hz, 2H), 2.72 (dd, J = 45.0, 15.0 Hz, 2H), 0.99 (s, 3H). ^{13}C NMR (126 MHz, CDC l_3) δ (ppm) 163.6, 136.7, 133.8, 131.5, 128.6, 128.4, 128.0, 127.7, 126.1, 124.1, 118.1, 114.8, 110.1, 107.5, 57.0, 50.8, 33.2, 32.4, 23.1. HR-MS (ESI): calcd for $[M+Na]^+$ C_2 $_2H_{20}N_2NaO$: 351.1468; found: 351.1467.



3c

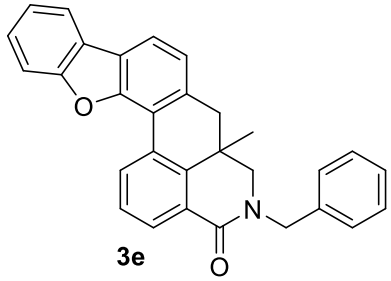
Ethyl 5-benzyl-6a-methyl-4-oxo-5,6,6a,7-tetrahydro-4H-benzo[*de*]indolizino[2,3-*g*]isoquinoline-13-carboxylate (3c), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 42 mg, 47%, white solid, m.p. 185-187 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.63 (d, J = 9.2 Hz, 1H), 8.22 (d, J = 9.2 Hz, 1H), 8.09 (d, J = 9.0 Hz, 1H), 7.73 (d, J = 6.9 Hz, 1H), 7.46 – 7.25 (m, 6H), 7.01 (dd, J = 9. 2, 6.6 Hz, 1H), 6.73 (t, J = 7.4 Hz, 1H), 4.98 (d, J = 14.6 Hz, 1H), 4.70 (d, J = 14.5 H z, 1H), 4.52 – 4.35 (m, 2H), 3.64 (d, J = 12.1 Hz, 1H), 3.25 (d, J = 12.1 Hz, 1H), 2.75 (d, J = 15.4 Hz, 2H), 1.45 (t, J = 7.1 Hz, 3H), 1.05 (s, 3H). ^{13}C NMR (126 MHz, CDC l_3) δ (ppm) 165.2, 164.4, 139.9, 137.3, 136.8, 131.6, 128.9, 128.6, 128.6, 127.6, 127.2, 127.2, 127.0, 122.1, 121.8, 121.7, 121.0, 120.7, 112.8, 99.9, 59.8, 57.1, 50.6, 35.0, 31. 1, 23.8, 14.5. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{29}H_{26}N_2NaO_3$: 473.1836; found: 473. 1840.



3d

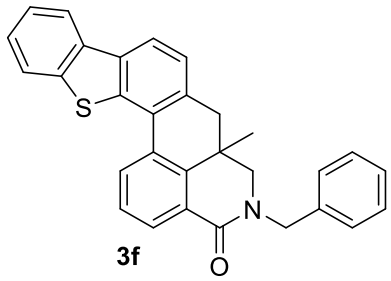
Ethyl (E)-2-(5-benzyl-3a-methyl-6-oxo-3a,4,5,6-tetrahydropyrano[4,3,2-*de*]isoqui

nolin-2(3H)-ylidene)acetate (3d), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 20 mg, 26%, white solid, m.p. 80-82 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.80 (dd, J = 7.7, 1.2 Hz, 1H), 7.45 – 7.13 (m, 7H), 5.04 (d, J = 1.6 Hz, 1H), 4.90 (d, J = 14.4 Hz, 1H), 4.63 (d, J = 14.4 Hz, 1H), 4.16 (q, J = 7.1 Hz, 2H), 3.40 (d, J = 12.2 Hz, 1H), 3.14 (d, J = 12.2 Hz, 1H), 2.49 – 2.41 (m, 1H), 2.26 (d, J = 14.2 Hz, 1H), 1.27 (t, J = 7.1 Hz, 3H), 1.10 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.2, 163.3, 159.4, 148.5, 136.4, 128.6, 128.6, 127.7, 127.4, 126.7, 123.1, 120.0, 98.7, 59.7, 56.5, 50.6, 38.3, 30.2, 23.2, 14.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{23}H_{23}NNaO_4$: 400.1519; found: 400.1522.



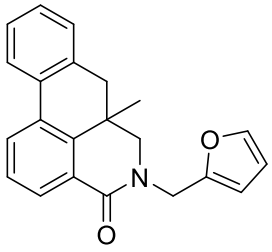
3e

2-Benzyl-3a-methyl-2,3,3a,4-tetrahydro-1H-benzo[*de*]benzo[2,3]benzofuro[7,6-*g*]isoquinolin-1-one (3e), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 59 mg, 69%, white solid, m.p. 187-188 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.86 (dd, J = 7.9, 1.3 Hz, 1H), 8.21 (dd, J = 7.8, 1.3 Hz, 1H), 7.97 – 7.91 (m, 1H), 7.81 (d, J = 7.7 Hz, 1H), 7.69 – 7.56 (m, 2H), 7.52 – 7.26 (m, 7H), 7.17 (dd, J = 7.8, 0.9 Hz, 1H), 4.87 (dd, J = 97.3, 14.5 Hz, 2H), 3.44 (dd, J = 148.4, 12.2 Hz, 2H), 2.86 (dd, J = 110.8, 14.9 Hz, 2H), 0.98 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.3, 156.0, 153.1, 141.2, 136.8, 133.4, 131.4, 128.9, 128.7, 128.6, 128.0, 127.6, 127.4, 127.3, 127.0, 124.2, 123.8, 123.8, 122.9, 120.3, 119.8, 117.9, 111.7, 57.4, 50.7, 40.2, 33.5, 22.0. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{30}H_{23}NNaO_2$: 452.1621; found: 452.1615.



3f

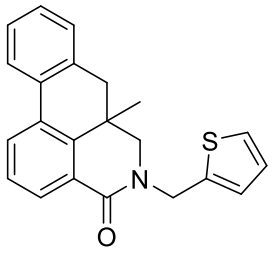
2-Benzyl-3a-methyl-2,3,3a,4-tetrahydro-1H-benzo[*de*]benzo[4',5']thieno[3',2':5,6] benzo[1,2-g]isoquinolin-1-one (3f), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 54 mg, 61%, white solid, m.p. 198-199 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.53 (dd, J = 7.9, 1.2 Hz, 1H), 8.22 – 8.13 (m, 2H), 8.08 (d, J = 7.8 Hz, 1H), 7.92 – 7.85 (m, 1H), 7.60 (t, J = 7.8 Hz, 1H), 7.51 – 7.44 (m, 2H), 7.42 – 7.27 (m, 8H), 4.86 (dd, J = 109.5, 14.5 Hz, 2H), 3.43 (dd, J = 172.2, 12.1 Hz, 2H), 2.85 (dd, J = 150.7, 14.6 Hz, 2H), 0.91 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 164.3, 142.3, 138.9, 136.8, 136.3, 136.1, 135.2, 133.6, 131.6, 129.0, 128.7, 128.6, 128.0, 127.9, 127.6, 127.6, 127.2, 126.8, 126.1, 124.6, 122.4, 121.2, 121.1, 57.3, 50.7, 40.6, 33.4, 21.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{30}H_{23}NNaOS$: 468.1393; found: 468.1396.



3g

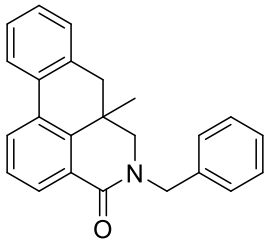
5-(Furan-2-ylmethyl)-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo [*de*,*g*]isoquinolin-4-one (3g), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 23 mg, 35%, white solid, m.p. 182-184 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.08 (d, J = 9.0 Hz, 1H), 7.90 (d, J = 9.2 Hz, 1H), 7.75 (d, J = 7.7 Hz, 1H), 7.49 – 7.13 (m, 5H), 6.39 – 6.28 (m, 2H), 4.82 (dd, J = 115.9, 15.2 Hz, 2H), 3.52 (dd, J = 137.3, 12.1 Hz, 2H), 2.77 (dd, J = 137.7, 14.8 Hz, 2H), 0.99 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 164.0, 150.6, 142.4, 141.0, 133.7, 132.5, 131.8, 129.0, 128.1, 127.9, 127.5, 127.4, 127.1, 123.8, 110.4, 110.4, 108.9, 57.6, 43.2, 39.8, 33.6, 21.8. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{22}H_{19}NNaO_2$: 352.1308; found:

352.1302.



3h

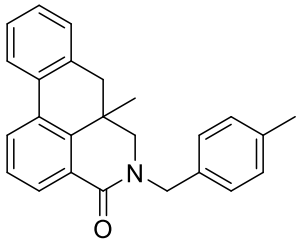
6a-Methyl-5-(thiophen-2-ylmethyl)-5,6,6a,7-tetrahydro-4H-dibenzo[*de*,*g*]isoquinolin-4-one (3h), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 54 mg, 79%, white solid, m.p. 181-182 °C. ^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm) 8.11 (dd, J = 7.7, 1.2 Hz, 1H), 7.91 (dd, J = 7.8, 1.3 Hz, 1H), 7.76 (dd, J = 7.7, 1.3 Hz, 1H), 7.44 (t, J = 7.8 Hz, 1H), 7.38 – 7.16 (m, 4H), 7.09 (dd, J = 3.4, 1.2 Hz, 1H), 6.97 (dd, J = 5.1, 3.4 Hz, 1H), 4.99 (dd, J = 63.2, 14.8 Hz, 2H), 3.49 (dd, J = 122.4, 12.1 Hz, 2H), 2.76 (dd, J = 113.3, 14.8 Hz, 2H), 1.00 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ (ppm) 164.1, 141.0, 139.3, 133.8, 132.6, 131.9, 129.1, 128.3, 128.1, 127.6, 127.6, 127.3, 127.3, 126.8, 125.8, 123.9, 57.6, 45.5, 39.9, 33.6, 22.2. HR-MS (ESI): calcd for [M+Na]$^+$ $C_{22}H_{19}NNaOS$: 368.1080; found: 368.1076.



4aa

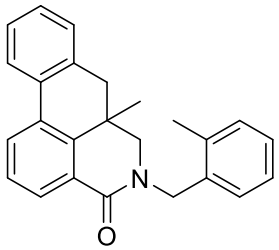
5-Benzyl-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de*,*g*]isoquinolin-4-one (4aa), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 58 mg, 87%, white solid, m.p. 182-183 °C. ^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm) 8.13 (dd, J = 7.7, 1.2 Hz, 1H), 7.92 (dd, J = 7.9, 1.3 Hz, 1H), 7.76 (dd, J = 7.8, 1.3 Hz, 1H), 7.48 – 7.27 (m, 7H), 7.26 – 7.16 (m, 2H), 4.84 (dd, J = 82.6, 14.5 Hz, 2H), 3.41 (dd, J = 148.6, 12.2 Hz, 2H), 2.72 (dd, J = 120.5, 14.8 Hz, 2H), 0.96 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ (ppm) 164.4, 141.0, 137.0, 133.8, 132.6, 131.9, 129.1, 128.8, 128.7, 128.3, 128.1, 127.7, 127.6, 127.5, 127.2, 123.9, 57.6, 50.9, 39.9, 33.5, 22.2. HR-MS (E

SI): calcd for $[M+Na]^+$ $C_{24}H_{21}NNaO$: 362.1515; found: 362.1515.



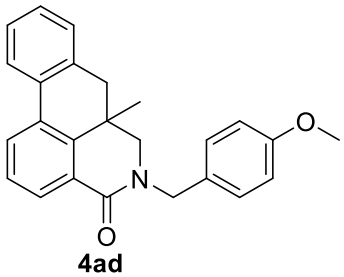
4ab

6a-Methyl-5-(4-methylbenzyl)-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4ab), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 52 mg, 74%, white solid, m.p. 185-186 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.12 (dd, J = 7.7, 1.2 Hz, 1H), 7.90 (dd, J = 7.8, 1.3 Hz, 1H), 7.75 (dd, J = 7.7, 1.3 Hz, 1H), 7.44 (t, J = 7.8 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.28 – 7.22 (m, 3H), 7.16 (d d, J = 9.8, 7.4 Hz, 3H), 5.09 – 4.48 (dd, J = 77.2, 14.4 Hz, 2H), 3.38 (dd, J = 140.1, 1 2.2 Hz, 2H), 2.71 (dd, J = 118.1, 14.8 Hz, 2H), 2.33 (s, 3H), 0.95 (s, 3H). ^{13}C NMR (1 01 MHz, $CDCl_3$) δ (ppm) 164.3, 141.0, 137.4, 133.9, 133.8, 132.6, 131.9, 129.4, 129. 1, 128.8, 128.2, 128.1, 127.8, 127.6, 127.5, 127.2, 123.9, 57.5, 50.6, 39.9, 33.5, 22.3, 21.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{25}H_{23}NNaO$: 376.1672; found: 376.1675.



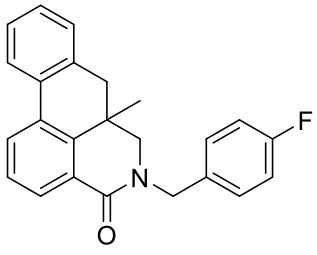
4ac

6a-Methyl-5-(2-methylbenzyl)-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4ac), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 55 mg, 79%, white solid, m.p. 181-183 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) δ 8.19 – 7.72 (m, 3H), 7.46 (t, J = 7.8 Hz, 1H), 7.37 – 7.26 (m, 2H), 7.26 – 7.15 (m, 5H), 4.89 (dd, J = 213.7, 14.7 Hz, 2H), 3.35 (dd, J = 135.2, 12.2 Hz, 2H), 2.70 (d d, J = 120.9, 14.8 Hz, 2H), 2.39 (s, 3H), 0.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.2, 141.0, 137.3, 134.5, 133.8, 132.6, 132.0, 130.8, 129.9, 129.2, 128.3, 128. 2, 127.9, 127.7, 127.7 127.6, 127.2, 126.1, 123.9, 56.9, 48.4, 39.9, 33.4, 22.1, 19.5. H R-MS (ESI): calcd for $[M+Na]^+$ $C_{25}H_{23}NNaO$: 376.1672; found: 376.1673.



4ad

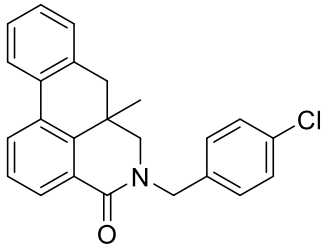
5-(4-Methoxybenzyl)-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de*,*g*]isoquinolin-4-one (4ad), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 53 mg, 73%, white solid, m.p. 181-182 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.23 – 7.57 (m, 3H), 7.49 – 7.26 (m, 4H), 7.26 – 7.16 (m, 2H), 6.88 (d, J = 8.7 Hz, 2H), 4.77 (dd, J = 110.7, 14.3 Hz, 2H), 3.79 (s, 3H), 3.39 (dd, J = 135.2, 12.2 Hz, 2H), 2.72 (dd, J = 117.0, 14.8 Hz, 2H), 0.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.3, 159.21, 141.0, 133.8, 132.6, 131.9, 130.1, 129.1, 129.9, 128.2, 128.1, 127.8, 127.6, 127.5, 127.2, 123.9, 114.1, 57.3, 55.4, 50.2, 39.9, 33.5, 22.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{25}H_{23}NNaO_2$: 392.1621; found: 392,1615.



4ae

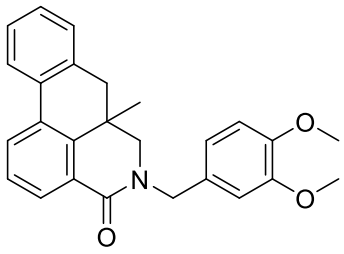
5-(4-Fluorobenzyl)-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4ae), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 44 mg, 62%, white solid, m.p. 182-184 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.10 (dd, J = 7.7, 1.2 Hz, 1H), 7.91 (dd, J = 7.8, 1.3 Hz, 1H), 7.75 (dd, J = 7.7, 1.3 Hz, 1H), 7.44 (t, J = 7.7 Hz, 1H), 7.39 – 7.30 (m, 3H), 7.28 – 7.22 (m, 1H), 7.18 (dt, J = 7.4, 1.3 Hz, 1H), 7.06 – 6.97 (m, 2H), 4.79 (dd, J = 109.0, 14.5 Hz, 2H), 3.39 (dd, J = 155.6, 12.1 Hz, 2H), 2.72 (dd, J = 118.9, 14.8 Hz, 2H), 0.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.4, 163.6, 161.2, 140.9, 133.7, 132.9, 132.8, 132.6, 132.0, 130.5, 130.42, 129.1, 128.3, 128.1, 127.7, 127.6, 127.6, 127.3, 124.0, 115.7, 115.5,

57.6, 50.2, 39.9, 33.5, 22.3. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{24}H_{20}FNNaO$: 380.142 1; found: 380.1424.



4af

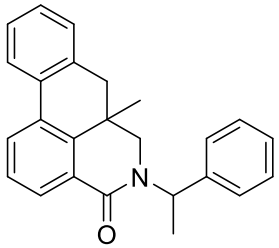
5-(4-Chlorobenzyl)-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de*,*g*]isoquinolin-4 -one (4af), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 56 mg, 76%, white solid, m.p. 176-177 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.17 – 7.70 (m, 3H), 7.45 (t, J = 7.8 Hz, 1H), 7.38 – 7.26 (m, 6H), 7.25 – 7.16 (m, 1H), 4.80 (dd, J = 96.8, 14.6 Hz, 2H), 3.40 (dd, J = 163.3, 12.2 Hz, 2H), 2.73 (dd, J = 119.3, 14.8 Hz, 2H), 0.96 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.4, 14 0.9, 135.7, 133.7, 132.5, 132.0, 130.1, 129.1, 128.9, 128.3, 128.1, 127.7, 127.6, 127.5, 127.3, 124.0, 57.8, 50.3, 39.9, 33.5, 22.3. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{24}H_{20}Cl NNaO_2$: 396.1126; found: 396.1124.



4ag

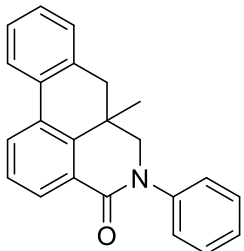
5-(3,4-Dimethoxybenzyl)-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de*,*g*] isoquinolin-4-one (4ag), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 48 mg, 61%, white solid, m.p. 189-192 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.12 (d, *J* = 9.0 Hz, 1H), 7.91 (d, *J* = 9.0 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.29 – 7.22 (m, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 6.98 – 6.74 (m, 3H), 4.77 (dd, *J* = 253.6, 14.3 Hz, 2H), 3.86 (d, *J* = 15.0 Hz, 6H), 3.39 (dd, *J* = 163.8, 12.1 Hz, 2H), 2.72 (dd, *J* = 149.7, 14.8 Hz, 2H), 0.94 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 164.2, 149.2, 148.6, 140.8,

133.6, 132.5, 131.8, 129.4, 129.0, 128.1, 127.9, 127.6, 127.5, 127.4, 127.0, 123.8, 121.1, 111.7, 110.8, 57.0, 55.9, 50.3, 39.7, 33.3, 22.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{26}H_{25}ClNNaO_3$: 422.1727; found: 422.1725.



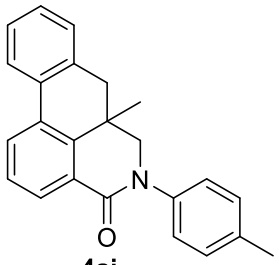
4ah

6a-Methyl-5-(1-phenylethyl)-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4ah), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 62 mg, 88%, white solid, m.p. 184-186 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.10 (d, J = 7.7 Hz, 1H), 7.87 (d, J = 7.8 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.45 – 7.14 (m, 8H), 7.10 (d, J = 7.4 Hz, 1H), 6.31 (q, J = 7.1 Hz, 1H), 3.22 (d, dd, J = 214.8, 12.0 Hz, 2H), 2.65 (dd, J = 182.4, 14.8 Hz, 2H), 1.60 (d, J = 7.1 Hz, 3H), 0.58 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 163.8, 140.7, 139.9, 133.8, 132.5, 131.7, 128.9, 128.3, 128.1, 128.1, 128.0, 127.6, 127.4, 127.4, 127.0, 123.8, 51.4, 50.2, 39.8, 32.9, 21.6, 14.8. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{25}H_{23}NNaO$: 376.1672; found: 376.1676.



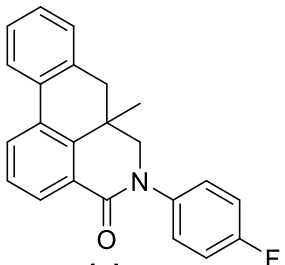
4ai

6a-Methyl-5-phenyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4ai), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 41 mg, 64%, white solid, m.p. 174-176 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.09 (d, J = 7.7 Hz, 1H), 7.91 (d, J = 7.8 Hz, 1H), 7.76 (d, J = 7.7 Hz, 1H), 7.47 – 7.18 (m, 8H), 3.90 (dd, J = 249.3, 12.0 Hz, 2H), 2.80 (dd, J = 155.6, 14.7 Hz, 2H), 1.23 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 163.9, 143.2, 141.1, 133.6, 132.5, 131.9, 129.1, 128.3, 128.2, 127.9, 127.6, 127.5, 127.4, 126.4, 125.4, 123.9, 61.4, 39.6, 34.1, 22.0. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{23}H_{19}NNaO$: 348.1359; found: 348.1353.



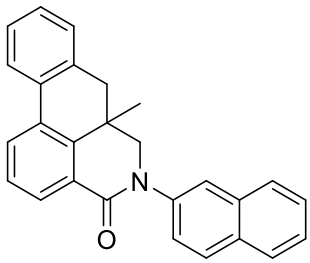
4aj

6a-Methyl-5-(p-tolyl)-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4aj), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 38 mg, 56%, white solid, m.p. 178-180 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.15 (dd, J = 7.8, 1.2 Hz, 1H), 7.97 (dd, J = 7.8, 1.3 Hz, 1H), 7.82 (dd, J = 7.7, 1.3 Hz, 1H), 7.49 (t, J = 7.8 Hz, 1H), 7.40 (t, J = 7.4 Hz, 1H), 7.33 (d, J = 8.5 Hz, 6H), 3.94 (dd, J = 206.2, 12.0 Hz, 2H), 2.86 (dd, J = 125.0, 14.8 Hz, 2H), 2.41 (s, 3H), 1.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.0, 141.2, 140.8, 136.4, 133.7, 132.7, 132.0, 129.8, 129.19, 128.3, 128.2, 127.7, 127.6, 127.4, 125.4, 124.0, 61.6, 39.8, 34.2, 22.1, 21.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{24}H_{21}NNaO$: 362.1515; found: 362.1515.



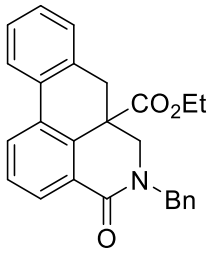
4ak

5-(4-Fluorophenyl)-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4ak), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 35 mg, 51%, white solid, m.p. 172-173 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.11 (dd, J = 7.7, 1.2 Hz, 1H), 7.97 (dd, J = 7.9, 1.2 Hz, 1H), 7.80 (d, J = 7.6 Hz, 1H), 7.51 – 7.26 (m, 6H), 7.13 (t, J = 8.6 Hz, 2H), 3.91 (dd, J = 214.1, 12.0 Hz, 2H), 2.85 (dd, J = 124.1, 14.8 Hz, 2H), 1.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.1, 159.6, 141.1, 139.2, 133.5, 132.5, 131.9, 129.1, 128.3, 128.2, 127.7, 127.6, 127.5, 127.2, 127.2, 123.9, 116.1, 115.8, 61.6, 39.6, 34.2, 22.1. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{23}H_{18}FNNaO$: 366.1265; found: 366.1259.



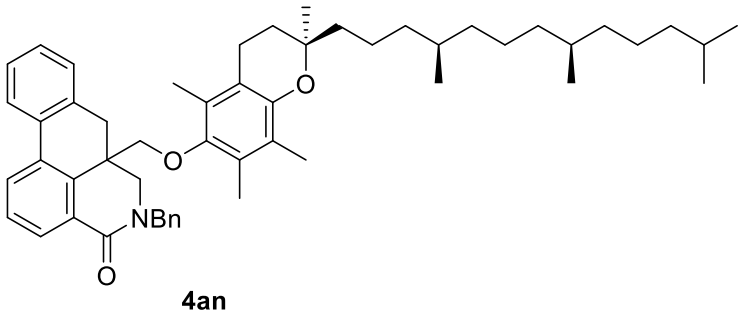
4al

6a-Methyl-5-(naphthalen-2-yl)-5,6,6a,7-tetrahydro-4*H*-dibenzo[*de,g*]isoquinolin-4-one (4al), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 40 mg, 53%, white solid, m.p. 200-202 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.17 (dd, J = 7.8, 1.2 Hz, 1H), 7.98 (dd, J = 7.9, 1.2 Hz, 1H), 7.95 – 7.79 (m, 5 H), 7.62 (dd, J = 8.7, 2.2 Hz, 1H), 7.54 – 7.27 (m, 6H), 4.05 (dd, J = 195.5, 12.0 Hz, 2 H), 2.88 (dd, J = 127.9, 14.7 Hz, 2H), 1.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (pp m) 164.2, 141.3, 141.1, 133.8, 133.7, 132.7, 132.1, 131.9, 129.2, 128.9, 128.4, 128.4, 128.1, 127.9, 127.8, 127.7, 127.6, 126.5, 126.1, 124.5, 124.0, 122.9, 61.7, 39.8, 34.4, 2 2.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{27}H_{21}NNaO$: 398.1515; found: 398.1516.



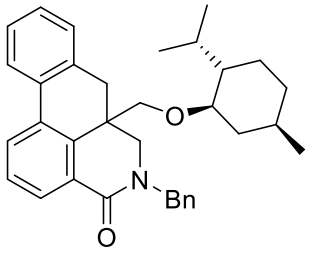
4am

Ethyl 5-benzyl-4-oxo-5,6-dihydro-4H-dibenzo[*de,g*]isoquinoline-6a-7*H*--carboxylate (4am), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 57 mg, 72%, white solid, m.p. 185-186 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.1 (dd, J = 7.8, 1.2 Hz, 1H), 7.9 (dd, J = 7.9, 1.2 Hz, 1H), 7.7 (d, J = 7.8 Hz, 1H), 7.5 (t, J = 7.8 Hz, 1H), 7.4 – 7.0 (m, 3H), 4.8 (d, J = 14.6 Hz, 5H), 4.6 (d, J = 14.6 Hz, 1H), 3.9 (d, J = 12.4 Hz, 1H), 3.7 – 3.5 (m, 3H), 3.1 (d, J = 14.9 Hz, 1H), 2.8 (d, J = 14.8 H z, 1H), 0.6 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 164.4, 136.8, 13 5.1, 133.4, 133.2, 132.0, 128.6, 128.6, 128.5, 128.4, 128.1, 127.9, 127.8, 127.6, 127.1, 124.0, 61.4, 54.3, 50.6, 45.3, 36.8, 13.5, 1.0. HR-MS (ESI): calcd for $[M+Na]^+$ C_2H_{23} $NNaO_3$: 420.1570; found: 420.1567.



4an

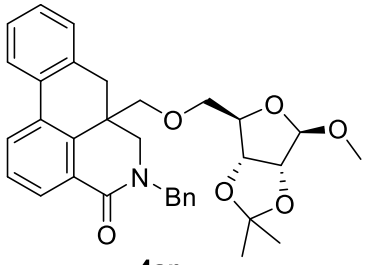
5-Benzyl-6a-((((R)-2,5,7,8-tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yl)oxymethyl)-5,6,6a,7-tetrahydro-4*H*-dibenzo[*de,g*]isoquinolin-4-one (**4an**), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 82 mg, 54%, colourless oil). ^{1}H NMR (400 MHz, Chloroform-d) δ 8.1 (d, J = 8.9 Hz, 1H), 7.9 (d, J = 9.2 Hz, 1H), 7.7 (d, J = 8.0 Hz, 1H), 7.5 – 7.2 (m, 9H), 5.9 (d, J = 14.4 Hz, 1H), 4.1 (d, J = 12.5 Hz, 2H), 4.0 (d, J = 14.4 Hz, 1H), 3.7 (d, J = 9.5 Hz, 2H), 3.5 – 3.4 (m, 1H), 3.3 (d, J = 9.5 Hz, 1H), 2.8 (d, J = 15.3 Hz, 2H), 2.5 (t, J = 6.9 Hz, 6H), 2.0 (d, J = 17.5 Hz, 3H), 1.3 – 1.1 (m, 23H), 0.9 – 0.7 (m, 15H). ^{13}C NMR (101 MHz, Chloroform-d) δ 164.3, 147.9, 146.9, 136.9, 133.4, 132.9, 132.6, 129.9, 128.7, 128.6, 128.5, 128.3, 128.2, 128.2, 127.6, 127.5, 127.1, 125.5, 123.7, 123.0, 74.7, 69.4, 52.4, 51.7, 39.4, 37.8, 37.4, 37.3, 34.4, 32.8, 32.7, 31.3, 28.0, 24.8, 24.4, 22.7, 22.6, 21.0, 20.6, 19.7, 12.7, 11.8, 11.7. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{53}H_{69}NNaO_3$: 790.5170; found: 790.5177.



4ao

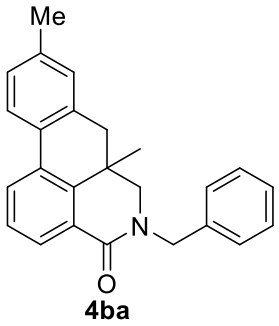
5-Benzyl-6a-((((1R,2R,5R)-2-isopropyl-5-methylcyclohexyl)oxy)methyl)-5,6,6a,7-tetrahydro-4*H*-dibenzo[de,g]isoquinolin-4-one (**4ao**), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 82 mg, 53%, white solid, m.p. 179-180 °C). ^{1}H NMR (400 MHz, Chloroform-d) δ 8.2 – 8.1 (m, 2H), 8.0 – 7.9 (m, 2H), 7.8 – 7.7 (m, 2H), 7.6 – 7.3 (m, 15H), 7.3 – 7.0 (m, 3H), 5.6 (d, J = 14.5 Hz, 1H), 5.1 (d, J = 14.5 Hz, 1H), 4.5 (d, J = 14.5 Hz, 1H), 4.1 (d, J = 14.5 Hz, 1H), 3.9 – 3.7

(m, 2H), 3.6 – 3.4 (m, 1H), 3.4 – 3.2 (m, 3H), 3.2 – 3.0 (m, 3H), 2.9 – 2.5 (m, 5H), 2.2 – 2.1 (m, 5H), 1.8 – 1.5 (m, 6H), 1.0 – 0.7 (m, 19H), 0.7 – 0.4 (m, 5H). ^{13}C NMR (101 MHz, Chloroform-d) δ 164.2, 137.4, 137.3, 137.0, 133.6, 132.9, 132.9, 132.5, 129.4, 128.8, 128.7, 128.6, 128.3, 128.2, 128.1, 127.9, 127.5, 127.5, 127.3, 127.3, 127.0, 126.9, 123.6, 78.7, 78.4, 64.9, 64.7, 52.3, 52.1, 51.2, 51.2, 48.3, 48.2, 40.1, 39.8, 37.8, 37.7, 34.5, 33.9, 33.9, 31.3, 31.3, 25.8, 25.5, 23.3, 23.1, 22.3, 22.2, 21.1, 21.0, 16.4, 16.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{34}H_{39}NNaO_2$: 516.2873; found: 516.2880.



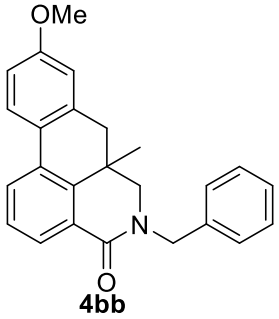
4ap

5-Benzyl-6a-((((3aR,4R,6R,6aR)-6-methoxy-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxol-4-yl)methoxy)methyl)-5,6,6a,7-tetrahydro-4H-dibenzo[de,g]isoquinolin-4-one (**4ap),** (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1),67 mg, 62%, white solid, m.p. 186-188 °C). ^{1}H NMR (500 MHz, Chloroform-d) δ 7.9 (d, J = 8.5 Hz, 2H), 7.7 – 7.6 (m, 4H), 7.6 – 7.5 (m, 2H), 7.4 – 7.2 (m, 12H), 5.0 (dd, J = 55.3, 14.5 Hz, 2H), 4.8 – 4.5 (m, 41H), 4.4 – 4.2 (m, 4H), 4.1 (d, J = 12.0 Hz, 1H), 4.0 – 3.6 (m, 11H), 3.6 – 3.2 (m, 6H), 3.1 – 2.9 (m, 2H), 1.6 – 1.4 (m, 9H), 1.4 (dd, J = 34.0, 5.7 Hz, 12H), 1.3 (s, 3H).^{13}C NMR (126 MHz, Chloroform-*d*) δ 164.1, 164.0, 137.4, 137.3, 136.7, 136.7, 133.5, 133.4, 132.9, 132.8, 132.5, 132.4, 129.2, 129.0, 128.7, 128.7, 128.6, 128.6, 128.3, 128.3, 127.9, 127.9, 127.6, 127.6, 127.5, 127.4, 127.1, 127.0, 123.7, 123.6, 112.2, 109.1, 109.0, 85.1, 84.9, 84.6, 82.2, 81.9, 71.5, 71.1, 67.9, 54.7, 54.4, 51.5, 51.4, 50.6, 50.5, 37.5, 37.4, 33.7, 33.7, 26.5, 26.4, 25.1, 25.0. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{33}H_{35}NNaO_6$: 564.2357; found: 564.2349.



4ba

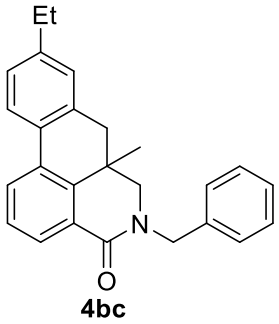
5-Benzyl-6a,9-dimethyl-5,6,6a,7-tetrahydro-4*H*-dibenzo[*de*,*g*]isoquinolin-4-one (4ba), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 54 mg, 77%, white solid, m.p. 182-183 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.37 (dd, J = 7.7, 1.2 Hz, 1H), 8.15 (dd, J = 7.9, 1.3 Hz, 1H), 7.91 (d, J = 7.9 Hz, 1H), 7.74 – 7.50 (m, 7H), 7.40 (d, J = 8.0 Hz, 1H), 5.11 (dd, J = 69.6, 14.4 Hz, 2H), 3.67 (dd, J = 147.5, 12.2 Hz, 2H), 2.94 (dd, J = 128.3, 14.8 Hz, 2H), 2.62 (s, 3H), 1.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.3, 140.5, 138.0, 136.9, 133.5, 131.9, 129.7, 129.7, 128.6, 128.6, 128.1, 127.5, 127.5, 127.4, 127.1, 126.7, 123.7, 57.5, 50.7, 39.7, 33.4, 22.1, 21.1. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{25}H_{23}NNaO_2$: 392.1621; found: 392,1612.



4bb

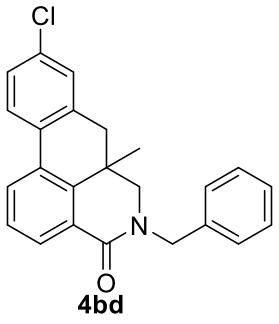
5-Benzyl-9-methoxy-6a-methyl-5,6,6a,7-tetrahydro-4*H*-dibenzo[*de*,*g*]isoquinolin-4-one (4bb), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 44 mg, 60%, white solid, m.p. 193-194 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.07 (dd, J = 7.7, 1.2 Hz, 1H), 7.89 – 7.61 (m, 2H), 7.49 – 7.27 (m, 6H), 6.93 – 6.68 (m, 2H), 4.84 (dd, J = 83.8, 14.5 Hz, 2H), 3.83 (s, 3H), 3.39 (dd, J = 151.4, 12.2 Hz, 2H), 2.68 (dd, J = 136.5, 14.8 Hz, 2H), 0.96 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.5, 159.7, 140.1, 137.0, 135.5, 131.9, 128.8, 128.7, 127.7, 127.6, 127.6, 127.2, 126.5, 125.5, 125.3, 114.7, 112.7, 57.6, 55.4, 50.9, 40.2, 33.5, 22.2. HR-MS

(ESI): calcd for $[M+Na]^+$ $C_{25}H_{23}NNaO$: 376.1672; found: 376.1670.



4bc

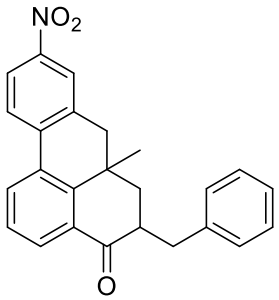
5-Benzyl-9-ethyl-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4bc), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 57 mg, 78%, white solid, m.p. 183-184 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.36 (dd, J = 7.8, 1.2 Hz, 1H), 8.13 (dd, J = 7.8, 1.3 Hz, 1H), 7.92 (d, J = 7.9 Hz, 1H), 7.72 – 7.48 (m, 7H), 7.41 (dd, J = 7.7, 1.8 Hz, 1H), 5.25 – 4.94 (m, 2H), 3.65 (dd, J = 146.4, 12.2 Hz, 2H), 3.09 (d, J = 14.8 Hz, 1H), 2.90 (q, J = 7.6 Hz, 2H), 2.78 (d, J = 14.8 Hz, 1H), 1.51 (t, J = 7.6 Hz, 3H), 1.21 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.4, 144.6, 140.8, 137.1, 133.7, 132.1, 130.1, 128.8, 128.7, 128.7, 127.7, 127.7, 127.7, 127.6, 127.0, 127.0, 123.9, 57.7, 50.9, 40.0, 33.5, 28.7, 22.3, 15.5. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{26}H_{25}NNaO$: 390.1828; found: 390.1832.



4bd

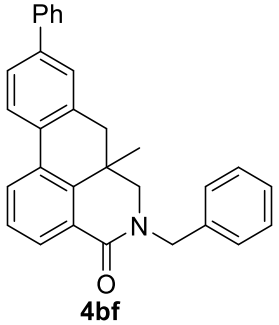
5-Benzyl-9-chloro-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4bd), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 34 mg, 46%, white solid, m.p. 186-187 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.14 (dd, J = 7.8, 1.3 Hz, 1H), 7.86 (dd, J = 8.0, 1.3 Hz, 1H), 7.68 (d, J = 8.4 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H), 7.40 – 7.27 (m, 6H), 7.18 (dd, J = 2.2, 1.2 Hz, 1H), 4.

83 (dd, J = 78.9, 14.5 Hz, 2H), 3.40 (dd, J = 144.2, 12.2 Hz, 2H), 2.69 (dd, J = 123.1, 14.9 Hz, 2H), 0.95 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.2, 140.7, 136.9, 135.6, 133.8, 131.2, 131.0, 129.0, 128.8, 128.4, 127.8, 127.7, 127.1, 125.3, 57.4, 50.9, 39.7, 33.5, 22.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{24}H_{20}ClNNaO$: 396.1126; found: 396.1120.



4be

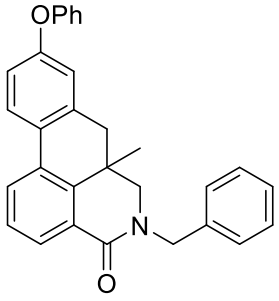
5-Benzyl-6a-methyl-9-nitro-5,6,6a,7-tetrahydro-4H-benzo[*de*]anthracen-4-one (4be), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 54 mg, 71%, white solid, m.p. 193-194 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.29 – 7.82 (m, 5H), 7.52 (t, J = 7.8 Hz, 1H), 7.43 – 7.27 (m, 5H), 4.85 (dd, J = 87.1, 14.4 Hz, 2H), 3.45 (dd, J = 140.7, 12.2 Hz, 2H), 3.08 – 2.60 (dd, J = 85.4, 15.1 Hz, 2H), 0.97 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 163.8, 147.3, 141.7, 139.0, 136.7, 135.2, 130.1, 129.9, 128.8, 128.2, 128.1, 127.9, 124.7, 124.1, 122.9, 57.2, 50.9, 39.7, 33.5, 22.4. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{24}H_{20}N_2NaO_3$: 407.1366; found: 407.1363.



4bf

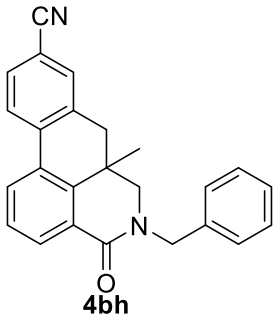
5-Benzyl-6a-methyl-9-phenyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de*,*g*]isoquinolin-4-one (4bf), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 62 mg, 75%, white solid, m.p. 192-193 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (p

pm) 8.15 (dd, J = 7.7, 1.2 Hz, 1H), 7.95 (dd, J = 7.8, 1.2 Hz, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.65 – 7.56 (m, 3H), 7.50 – 7.27 (m, 10H), 5.05 – 4.65 (dd, J = 72.4, 14.4 Hz, 2 H), 3.44 (dd, J = 149.4, 12.2 Hz, 2H), 2.79 (dd, J = 114.6, 14.8 Hz, 2H), 1.01 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.3, 141.0, 141.0, 140.5, 137.0, 134.2, 131.7, 131.6, 128.9, 128.8, 128.8, 128.1, 127.8, 127.7, 127.7, 127.6, 127.2, 127.0, 126.2, 124. 4, 57.6, 50.9, 40.1, 33.6, 22.4. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{30}H_{25}NNaO$: 438.18 28; found: 438.1821.



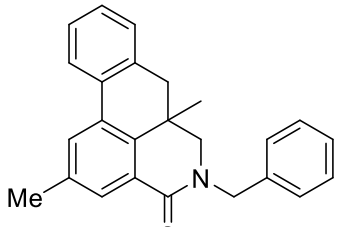
4bg

5-Benzyl-6a-methyl-9-phenoxy-5,6,6a,7-tetrahydro-4H-dibenzo[*de,g*]isoquinolin-4-one (4bg), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 47 mg, 55%, white solid, m.p. 180-181 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.10 (dd, J = 7.7, 1.2 Hz, 1H), 7.85 (dd, J = 7.8, 1.3 Hz, 1H), 7.71 (d, J = 8.5 H z, 1H), 7.47 – 7.26 (m, 8H), 7.19 – 6.80 (m, 5H), 4.84 (dd, J = 91.4, 14.4 Hz, 2H), 3.3 9 (dd, J = 151.5, 12.2 Hz, 2H), 2.67 (dd, J = 138.0, 14.9 Hz, 2H), 0.97 (s, 3H). ^{13}C NM R (101 MHz, $CDCl_3$) δ (ppm) 164.2, 157.4, 156.7, 140.3, 136.8, 135.6, 131.4, 129.8, 1 28.7, 128.6, 127.6, 127.6, 127.5, 126.7, 125.3, 123.6, 119.2, 118.8, 117.3, 57.4, 50.7, 3 9.9, 33.4, 22.1. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{30}H_{25}N_2NaO_2$: 454.1777; found: 45 4.1783.



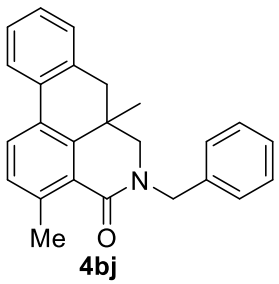
4bh

5-Benzyl-6a-methyl-4-oxo-5,6,6a,7-tetrahydro-4*H*-dibenzo[*de*,*g*]isoquinoline-9-carbonitrile (4bh), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 62 mg, 86%, white solid, m.p. 187-188 °C. ^{1}H NMR (500 MHz, CDCl$_3$) δ (ppm) 8.21 (d, J = 7.8 Hz, 1H), 7.92 (d, J = 9.1 Hz, 1H), 7.84 (d, J = 8.1 Hz, 1H), 7.62 (d, J = 8.1 Hz, 1H), 7.55 – 7.46 (m, 2H), 7.40 – 7.22 (m, 5H), 5.07 – 4.63 (dd, J = 115.7, 14.5 Hz, 2H), 3.42 (dd, J = 173.3, 12.3 Hz, 2H), 2.75 (dd, J = 122.3, 15.0 Hz, 2H), 0.94 (s, 3H). ^{13}C NMR (126 MHz, CDCl$_3$) δ (ppm) 163.7, 141.4, 137.0, 136.5, 134.7, 132.3, 131.3, 129.9, 129.7, 128.7, 127.9, 127.9, 127.7, 127.7, 124.4, 118.7, 111.3, 57.1, 50.7, 39.2, 33.3, 22.2. HR-MS (ESI): calcd for [M+Na]$^+$ $C_{25}H_{20}N_2NaO$: 387.1468; found: 387.1469.



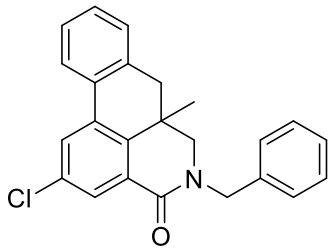
4bi

5-Benzyl-2,6a-dimethyl-5,6,6a,7-tetrahydro-4H-dibenzo[*de*,*g*]isoquinolin-4-one (4bi), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 43 mg, 62%, white solid, m.p. 190-191 °C. ^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm) 8.02 – 7.66 (m, 3H), 7.41 – 7.26 (m, 6H), 7.25 – 7.14 (m, 2H), 5.03 – 4.65 (dd, J = 62.8, 14.4 Hz, 2H), 3.39 (dd, J = 142.6, 12.2 Hz, 2H), 2.70 (dd, J = 114.4, 14.8 Hz, 2H), 2.46 (s, 3H), 0.94 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ (ppm) 164.6, 138.2, 137.3, 137.0, 133.9, 132.7, 131.9, 129.1, 128.8, 128.70, 128.6, 128.1, 127.9, 127.7, 127.5, 127.5, 123.8, 57.8, 50.9, 40.1, 33.2, 22.3, 21.5. HR-MS (ESI): calcd for [M+Na]$^+$ $C_{25}H_{23}NNaO$: 376.1672; found: 376.1664.



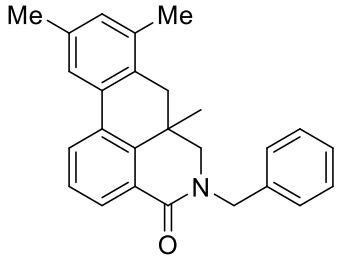
4bj

5-Benzyl-3,6a-dimethyl-5,6,6a,7-tetrahydro-4*H*-dibenzo[*de*,*g*]isoquinolin-4-one (4bj), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 52 mg, 75%, white solid, m.p. 180-181 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.74 (d, J = 8.0 Hz, 1H), 7.69 (dd, J = 7.7, 1.3 Hz, 1H), 7.42 – 7.27 (m, 6H), 7.26 – 7.13 (m, 3H), 5.00 – 4.66 (dd, J = 46.0, 14.8 Hz, 2H), 3.38 (dd, J = 167.6, 12.3 Hz, 2H), 2.88 – 2.45 (m, 5H), 0.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.9, 142.4, 140.7, 137.2, 133.4, 133.1, 131.5, 129.9, 128.8, 128.7, 128.7, 127.8, 127.6, 127.5, 126.6, 126.4, 123.7, 57.2, 50.7, 39.9, 34.5, 22.8, 21.5. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{25}H_{23}NNaO$: 376.1672; found: 376.1680.



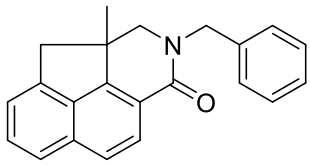
4bk

5-Benzyl-2-chloro-6a-methyl-5,6,6a,7-tetrahydro-4H-dibenzo[de,g]isoquinolin-4-one (4bk), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 34 mg, 46%, white solid, m.p. 183-184 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ(ppm) 8.08 (d, J = 2.2 Hz, 1H), 7.84 (d, J = 2.2 Hz, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.39 – 7.23 (m, 7H), 7.18 (d, J = 7.4 Hz, 1H), 4.82 (dd, J = 107.0, 14.5 Hz, 2H), 3.38 (dd, J = 166.3, 12.3 Hz, 2H), 2.69 (dd, J = 127.5, 14.9 Hz, 2H), 0.91 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 163.0, 139.1, 136.5, 133.9, 133.8, 133.7, 131.3, 129.2, 129.1, 128.8, 128.6, 127.7, 127.6, 127.5, 126.9, 123.9, 57.2, 50.8, 39.5, 33.1. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{24}H_{20}ClNNaO$: 396.1126; found: 396.1134.



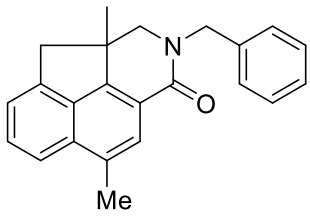
4bl

5-Benzyl-6a,8,10-trimethyl-5,6,6a,7-tetrahydro-4*H*-dibenzo[*de*,*g*]isoquinolin-4-one (4bl), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 49 mg, 67%, white solid, m.p. 187-189 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.10 (dd, J = 7.7, 1.2 Hz, 1H), 7.90 (dd, J = 8.0, 1.3 Hz, 1H), 7.48 – 7.26 (m, 7H), 6.98 (d, J = 1.7 Hz, 1H), 4.84 (dd, J = 89.9, 14.5 Hz, 2H), 3.42 (dd, J = 149.2, 12.2 Hz, 2H), 2.63 (dd, J = 92.3, 15.1 Hz, 2H), 2.37 (s, 3H), 2.26 (s, 3H), 0.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.5, 140.8, 137.0, 136.1, 136.0, 132.4, 131.0, 129.3, 128.8, 128.7, 127.7, 127.7, 127.5, 127.5, 122.6, 57.7, 50.9, 35.4, 33.3, 22.5, 21.33, 19.8. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{26}H_{25}NNaO$: 390.1820; found: 390.1828.



4bm

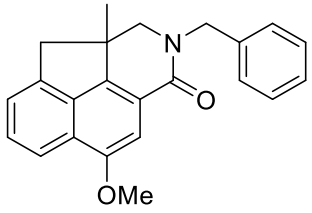
2-Benzyl-3a-methyl-2,3,3a,4-tetrahydro-1H-indeno[2,1,7-*def*]isoquinolin-1-one (4bm), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 48 mg, 78%, white solid, m.p. 191-192 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.94 (d, J = 8.5 Hz, 1H), 7.71 – 7.63 (m, 2H), 7.58 – 7.51 (m, 1H), 7.39 – 7.23 (m, 6H), 4.84 (dd, J = 141.7, 14.6 Hz, 2H), 3.62 (dd, J = 84.1, 11.9 Hz, 2H), 3.33 – 3.06 (dd, J = 85.0, 15.0 Hz, 2H), 1.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 164.1, 153.3, 144.3, 137.5, 134.7, 132.8, 130.5, 128.5, 128.5, 127.4, 124.3, 123.9, 122.9, 121.2, 120.2, 58.4, 51.0, 44.7, 40.5, 25.5. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{22}H_{219}NNaO$: 336.1359; found: 336.1358.



4bn

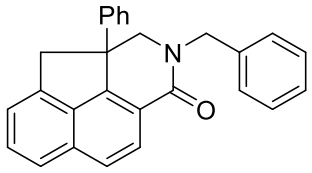
2-Benzyl-3a,8-dimethyl-2,3,3a,4-tetrahydro-1H-indeno[2,1,7-def]isoquinolin-1-one (4bn), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:

1-3:1), 49 mg, 75%, white solid, m.p. 194-195 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (pp m) 7.80 – 7.71 (m, 2H), 7.58 (dd, J = 8.3, 6.9 Hz, 1H), 7.40 – 7.26 (m, 6H), 4.85 (dd, J = 87.7, 14.6 Hz, 2H), 3.62 (dd, J = 62.3, 11.9 Hz, 2H), 3.2 (dd, J = 70.4, 16.0 Hz, 2 H), 2.68 (d, J = 1.0 Hz, 3H), 1.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.3, 151.3, 144.5, 137.6, 134.8, 132.5, 132.3, 130.2, 128.5, 128.5, 127.4, 123.6, 121.1, 12 0.5, 120.0, 58.6, 51.0, 45.0, 39.9, 25.6, 18.0. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{23}H_{21}$ NNaO: 350.1515; found: 350.1507.



4bo

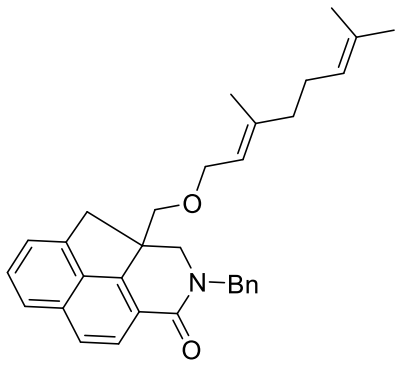
2-Benzyl-8-methoxy-3a-methyl-2,3,3a,4-tetrahydro-1H-indeno[2,1,7-def]isoquino lin-1-one (4bo), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acet ate = 10:1-3:1), 56 mg, 82%, white solid, m.p. 190-191 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.86 (d, J = 8.2 Hz, 1H), 7.52 (dd, J = 8.2, 6.9 Hz, 1H), 7.40 – 7.26 (m, 6H), 7.25 (d, J = 2.0 Hz, 1H), 4.83 (dd, J = 96.8, 14.6 Hz, 2H), 4.03 (s, 3H), 3.60 (dd, J = 6 8.4, 11.9 Hz, 2H), 3.17 (dd, J = 65.6, 16.0 Hz, 2H), 1.24 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.4, 154.9, 145.5, 143.6, 137.6, 135.9, 129.7, 128.5, 128.5, 127.4, 125.5, 121.9, 120.1, 119.0, 101.4, 58.9, 56.0, 51.1, 45.2, 39.6, 25.6. HR-MS (ESI): cal cd for $[M+Na]^+$ $C_{23}H_{21}NNaO_2$: 366.1464; found: 366.1463.



4bp

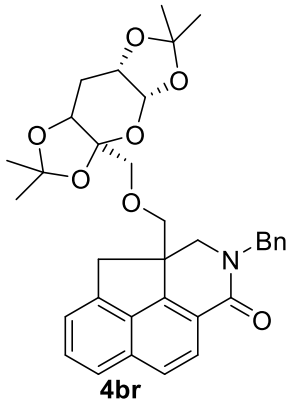
2-benzyl-3a-phenyl-2,3,3a,4-tetrahydro-1*H*-indeno[2,1,7-*def*]isoquinolin-1-one (4 bp), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3: 1), 46 mg, 62%, white solid, m.p. 60-62 °C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.1 (d, J = 8.5 Hz, 1H), 7.8 (d, J = 8.5 Hz, 1H), 7.7 (d, J = 8.2 Hz, 1H), 7.6 (dd, J = 8.2, 6.

9 Hz, 1H), 7.3 – 7.2 (m, 1H), 7.2 – 7.1 (m, 6H), 7.0 – 6.9 (m, 2H), 6.9 – 6.8 (m, 2H), 4.8 (d, J = 14.9 Hz, 1H), 4.4 (d, J = 14.9 Hz, 1H), 4.0 (q, J = 12.1 Hz, 2H), 3.7 (d, J = 16.3 Hz, 1H), 3.5 (dt, J = 16.3, 1.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-d) δ 164.5, 149.6, 144.8, 143.9, 137.0, 136.0, 132.8, 130.7, 128.4, 127.8, 126.9, 126.7, 126.6, 124.7, 124.3, 122.9, 122.4, 121.2, 59.3, 50.6, 48.8, 47.1. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{27}H_{21}NNaO$: 398.1515; found: 398.1517.



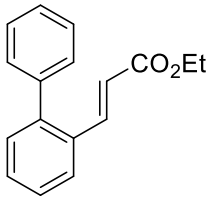
4bq

2-Benzyl-3a-(((3,7-dimethylocta-2,6-dien-1-yl)oxy)methyl)-2,3,3a,4-tetrahydro-1H-indeno[2,1,7-def]isoquinolin-1-one, (4bq), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 10:1-3:1), 72 mg, 78%, colourless oil). ^{1}H NMR (400 MHz, Chloroform-d) δ 7.9 (d, J = 8.5 Hz, 2H), 7.7 (dd, J = 18.7, 8.3 Hz,4H), 7.6 (dd, J = 8.2, 6.8 Hz, 2H), 7.5 – 7.4 (m, 4H), 7.4 – 7.2 (m, 9H), 5.2 – 4.9 (m, 6H), 4.6 (d, J = 14.4 Hz, 2H), 4.1 (d, J = 12.0 Hz, 2H), 3.8 – 3.6 (m, 8H), 3.5 (dd, J = 9.0, 1.6 Hz, 2H), 3.1 – 2.9 (m, 4H), 2.1 – 1.9 (m, 8H), 1.7 – 1.4 (m, 18H). ^{13}C NMR (101 MHz, Chloroform-d) δ 164.1, 148.9, 144.8, 140.0, 137.9, 135.9, 132.8, 131.6, 130.6, 128.7, 128.5, 128.2, 127.4, 124.4, 124.2, 123.9, 122.8, 121.3, 120.6, 71.8, 67.6, 53.7, 51.0, 45.4, 40.7, 39.5, 26.3, 25.6, 17.6, 16.4. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{32}H_{35}NNaO_2$: 488.2560; found: 488.2558.



4br

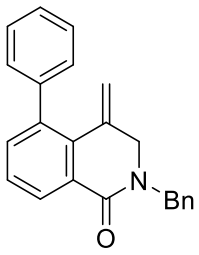
2-Benzyl-3a-((((3aS,4aR,7aS)-2,2,6,6-tetramethyltetrahydro-3aH-bis([1,3]dioxolo)[4,5-b:4',5'-e]pyran-3a-yl)methoxy)methyl)-2,3,3a,4-tetrahydro-1H-indeno[2,1,7-def]isoquinolin-1-one, **(4br).** (silica gel: 200−300 mesh, solvent system: petroleum et her/ethyl acetate = 10:1-5:1), 68 mg, 60%, colourless oil). ^{1}H NMR (500 MHz, Chloro form-*d*) δ 7.9 (d, *J* = 8.5 Hz, 2H), 7.7 – 7.6 (m, 4H), 7.6 – 7.5 (m, 2H), 7.4 – 7.2 (m, 12H), 5.0 (dd, *J* = 55.3, 14.5 Hz, 2H), 4.8 – 4.5 (m, 4H), 4.3 – 4.2 (m, 4H), 4.1 (d, *J* = 12.0 Hz, 1H), 4.0 – 3.6 (m, 11H), 3.5 – 3.2 (m, 3H), 3.0 (dd, *J* = 16.6, 12.3 Hz, 2H), 1.6 – 1.4 (m, 9H), 1.4 (dd, *J* = 34.0, 5.7 Hz, 12H), 1.3 (s, 3H). ^{13}C NMR (126 MHz, Chloroform-d) δ 164.1, 164.1, 148.5, 148.5, 144.6, 144.5, 137.6, 137.6, 135.9, 132.8, 130.7, 130.6, 128.7, 128.4, 128.3, 127.5, 124.6, 124.3, 124.2, 122.9, 122.8, 121.4, 121.4, 121.3, 109.0, 108.9, 108.5, 108.4, 102.3, 73.8, 73.8, 73.1, 73.0, 71.0, 70.9, 70.1, 70.1, 69.9, 61.0, 61.0, 54.1, 54.1, 51.3, 51.0, 45.7, 45.6, 40.7, 40.6, 26.6, 26.5, 26.0, 25.9, 25.5, 25.3, 24.1, 24.0. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{34}H_{37}NNaO_7$: 594.2462; found: 594.2446.



5a

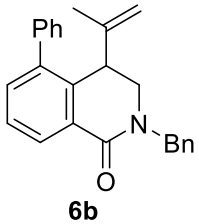
Ethyl (E)-3-([1,1'-biphenyl]-2-yl)acrylate (5a), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 20:1-10:1), 14 mg ,29%, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) *δ* (ppm) 7.80 – 7.62 (m, 2H), 7.49 – 7.35 (m, 6H), 7.35 – 7.25 (m, 2H), 6.40 (d, *J* = 15.9 Hz, 1H), 4.20 (q, *J* = 7.1 Hz, 2H), 1.28 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) *δ* (ppm) 166.9, 143.7, 142.9, 139.9, 132.6, 130.5, 129.8, 128.3,

127.6, 127.5, 126.8, 119.2, 60.4, 14.2. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{17}H_{16}NNaO_2$: 275.1043; found: 275.1048.



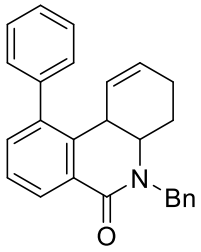
6a

2-Benzyl-4-methylene-5-phenyl-3,4-dihydroisoquinolin-1(2H)-one (6a), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 20:1-10:1), 40 mg, 63%, white solid, m.p. 116-118 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.21 (d, J = 7.4 Hz, 1H), 7.42 – 7.36 (m, 2H), 7.34 – 7.17 (m, 10H), 4.99 (s, 1H), 4.79 (s, 2H), 4.50 (s, 1H), 3.97 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 163.5, 141.1, 139.3, 136.7, 134.7, 134.5, 134.3, 129.7, 129.6, 129.1, 128.6, 128.4, 128.1, 128.0, 127.9, 127.5, 127.2, 120.1, 53.5, 50.3. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{23}H_{19}NNaO$: 348.1359; found: 348.1367.



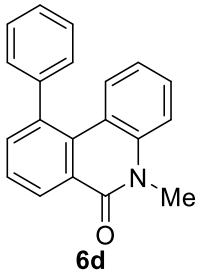
6b

2-Benzyl-5-phenyl-4-(prop-1-en-2-yl)-3,4-dihydroisoquinolin-1(2*H*)-one (6b), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 20:1-10:1), 28 mg, 39%, colorless oil. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.2 (dd, J = 7.3, 1.8 Hz, 1H), 7.5 – 7.2 (m, 12H), 4.9 (d, J = 14.6 Hz, 1H), 4.9 (s, 1H), 4.4 (d, J = 14.6 Hz, 1H), 4.2 (s, 1H), 3.6 (dd, J = 12.8, 4.4 Hz, 1H), 3.3 (dd, J = 12.8, 1.7 Hz, 1H), 3.2 (d, J = 4.2 Hz, 1H), 1.3 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 164.5, 144.5, 140.3, 140.1, 137.2, 136.8, 133.4, 130.3, 128.9, 128.6, 128.4, 128.1, 128.0, 127.5, 127.4, 127.3, 127.1, 116.1, 50.3, 47.6, 41.9, 21.2. HR-MS (ESI): calcd for $[M+H]^+$ $C_{25}H_{24}NO$: 354.1852; found: 354.1842.



6c

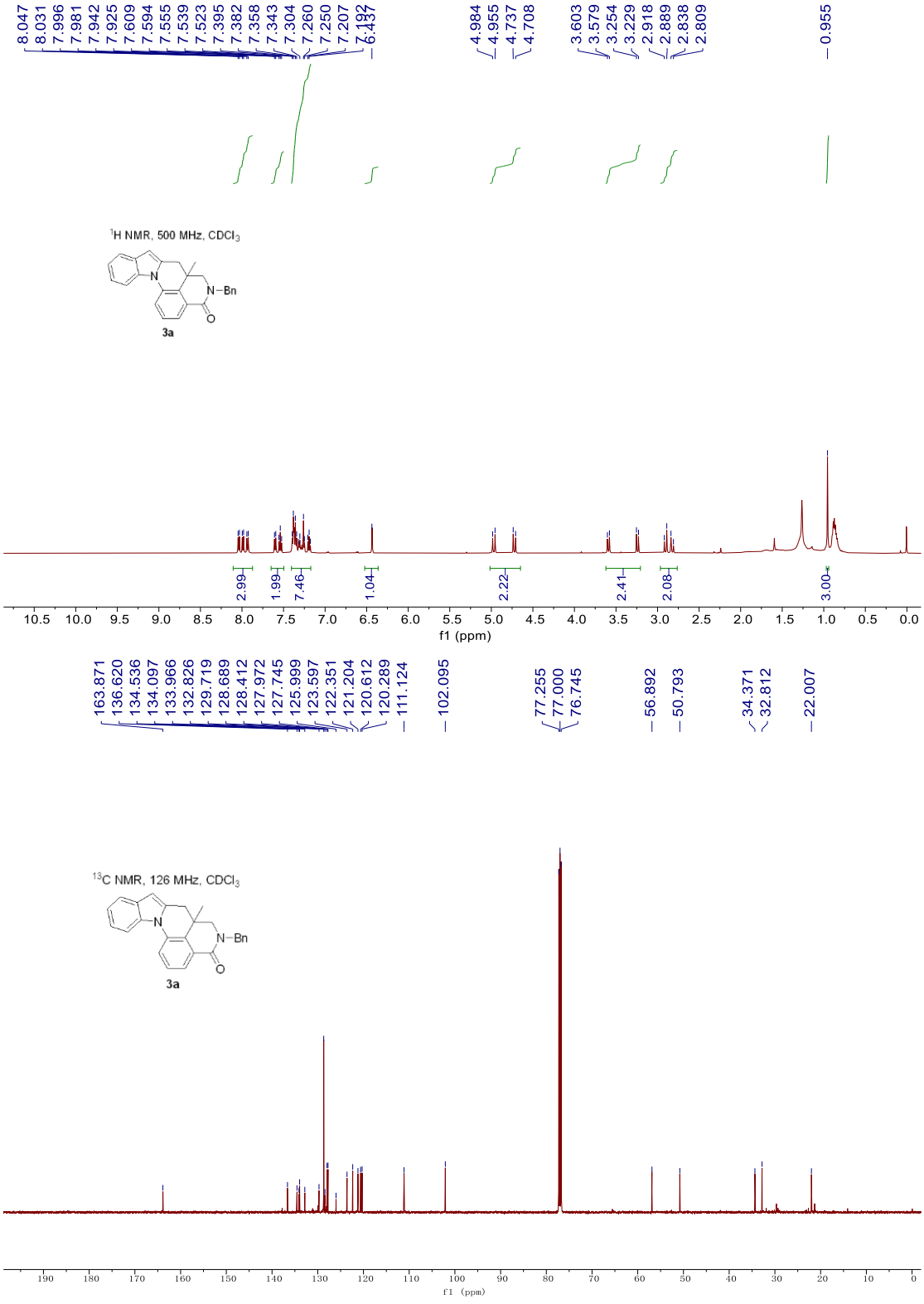
5-Benzyl-10-phenyl-3,4a,5,10b-tetrahydrophenanthridin-6(4*H*)-one (6c), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 20:1-10:1), 49 mg, 68%, white solid, m.p. 182-183 ℃. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.2 (dd, J = 7.6, 1.6 Hz, 1H), 7.5 – 7.3 (m, 10H), 7.3 – 7.2 (m, 3H), 5.9 – 5.5 (m, 3H), 4.1 (d, J = 16.2 Hz, 2H), 3.1 – 3.0 (m, 1H), 2.5 – 2.4 (m, 1H), 2.2 – 2.1 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-d) δ 166.3, 141.4, 140.1, 139.7, 138.4, 133.2, 129.2, 128.9, 128.8, 128.6, 128.3, 128.1, 127.4, 126.8, 126.7, 126.6, 122.1, 51.9, 45.4, 34.1, 29.5, 27.4. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{26}H_{23}NNaO$: 388.1672; found: 388.1664.

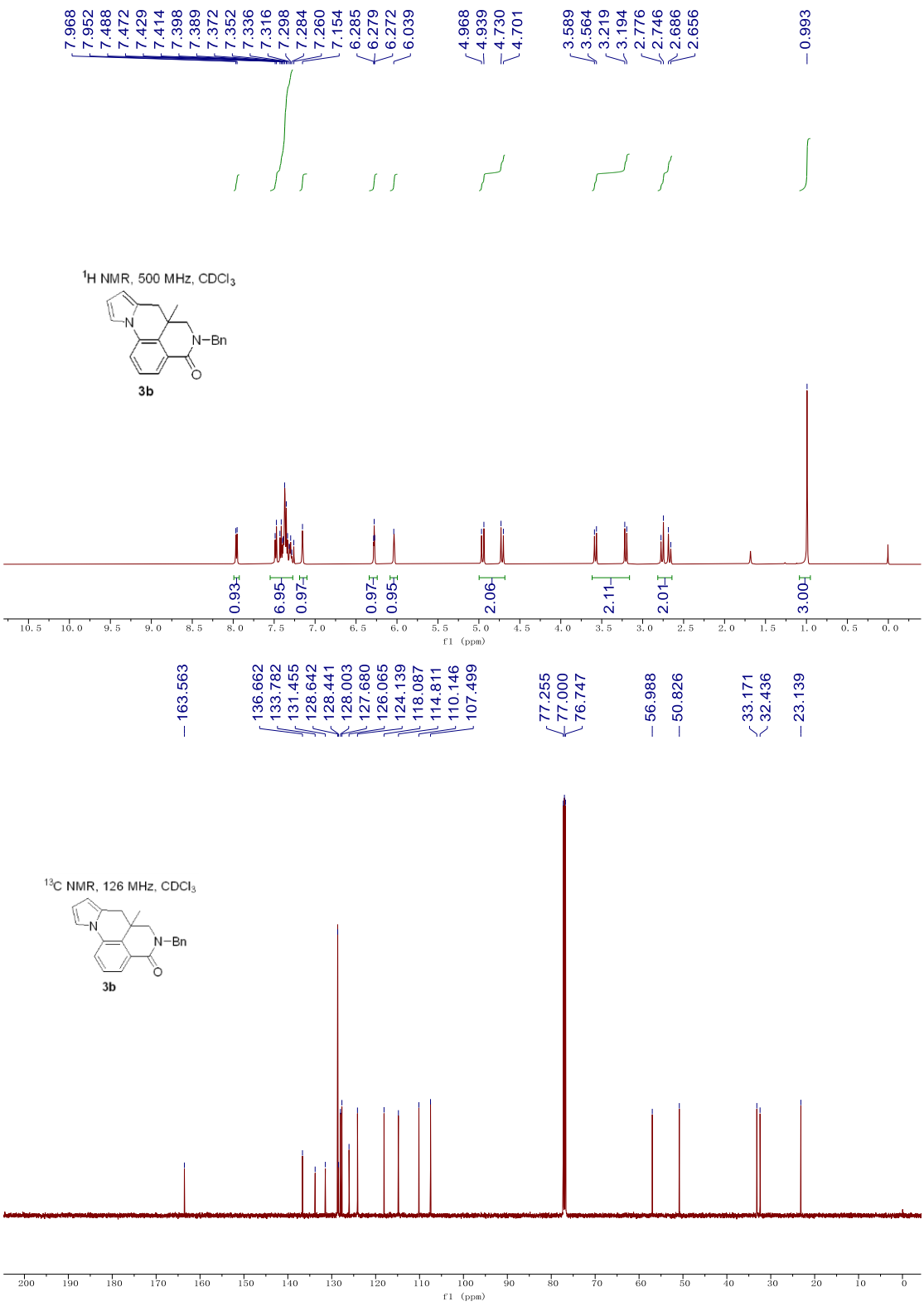


6d

5-Methyl-10-phenylphenanthridin-6(5H)-one (6d), (silica gel: 200−300 mesh, solvent system: petroleum ether/ethyl acetate = 20:1-10:1), 42 mg, 76%, white solid, m.p. 188-189 ℃. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 8.63 (p, J = 3.6 Hz, 1H), 7.59 (d, J = 4.9 Hz, 2H), 7.51 – 7.29 (m, 8H), 6.82 – 6.75 (m, 1H), 3.82 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 161.8, 143.4, 139.4, 138.4, 136.2, 131.7, 129.1, 128.9, 128.8, 128.3, 127.5, 127.3, 127.1, 121.0, 119.4, 114.6, 30.4. HR-MS (ESI): calcd for $[M+Na]^+$ $C_{20}H_{15}NNaO$: 308.1046; found: 308.1051.

5. ^{1}H-NMR and ^{13}C-NMR Spectra of Products

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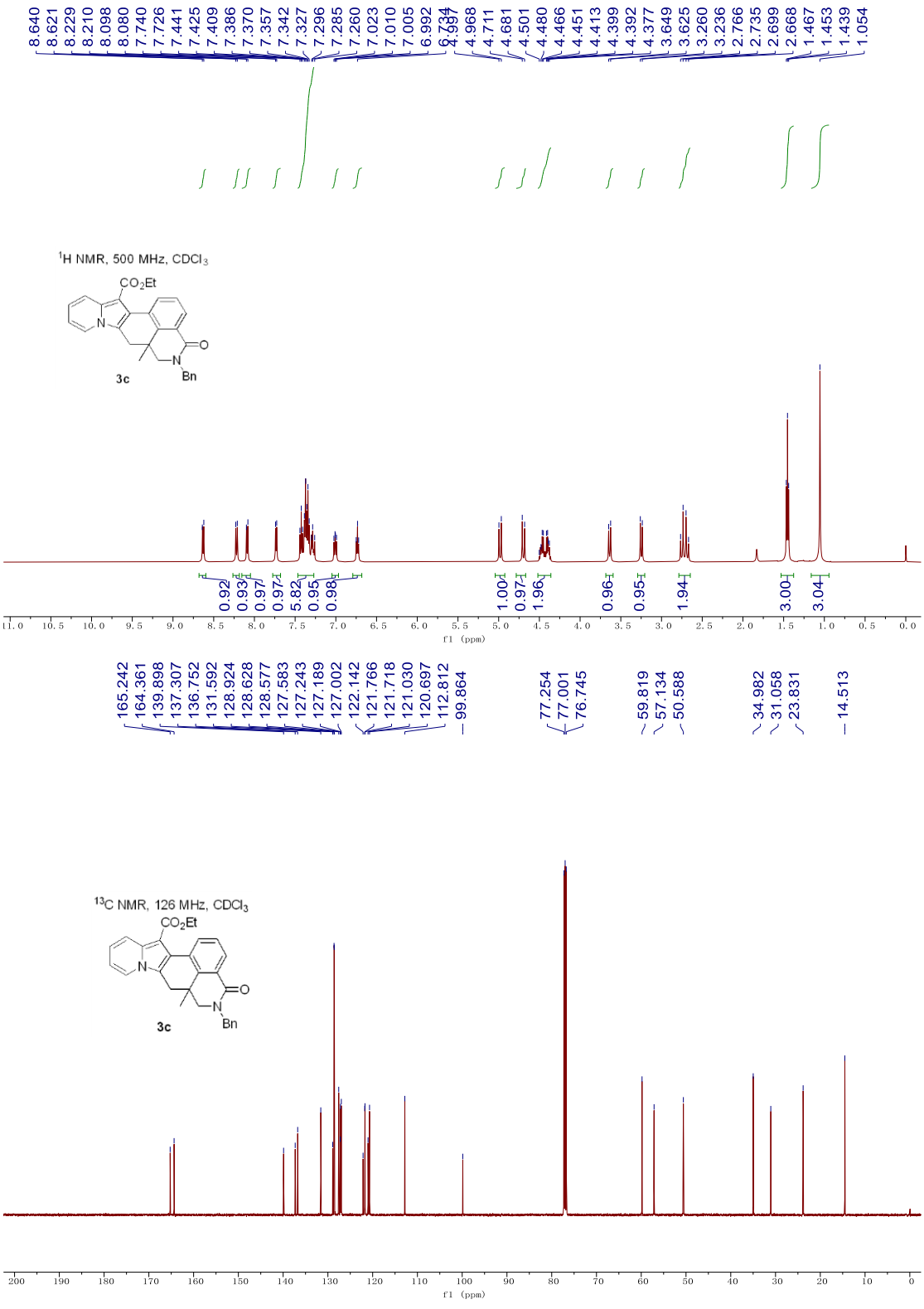
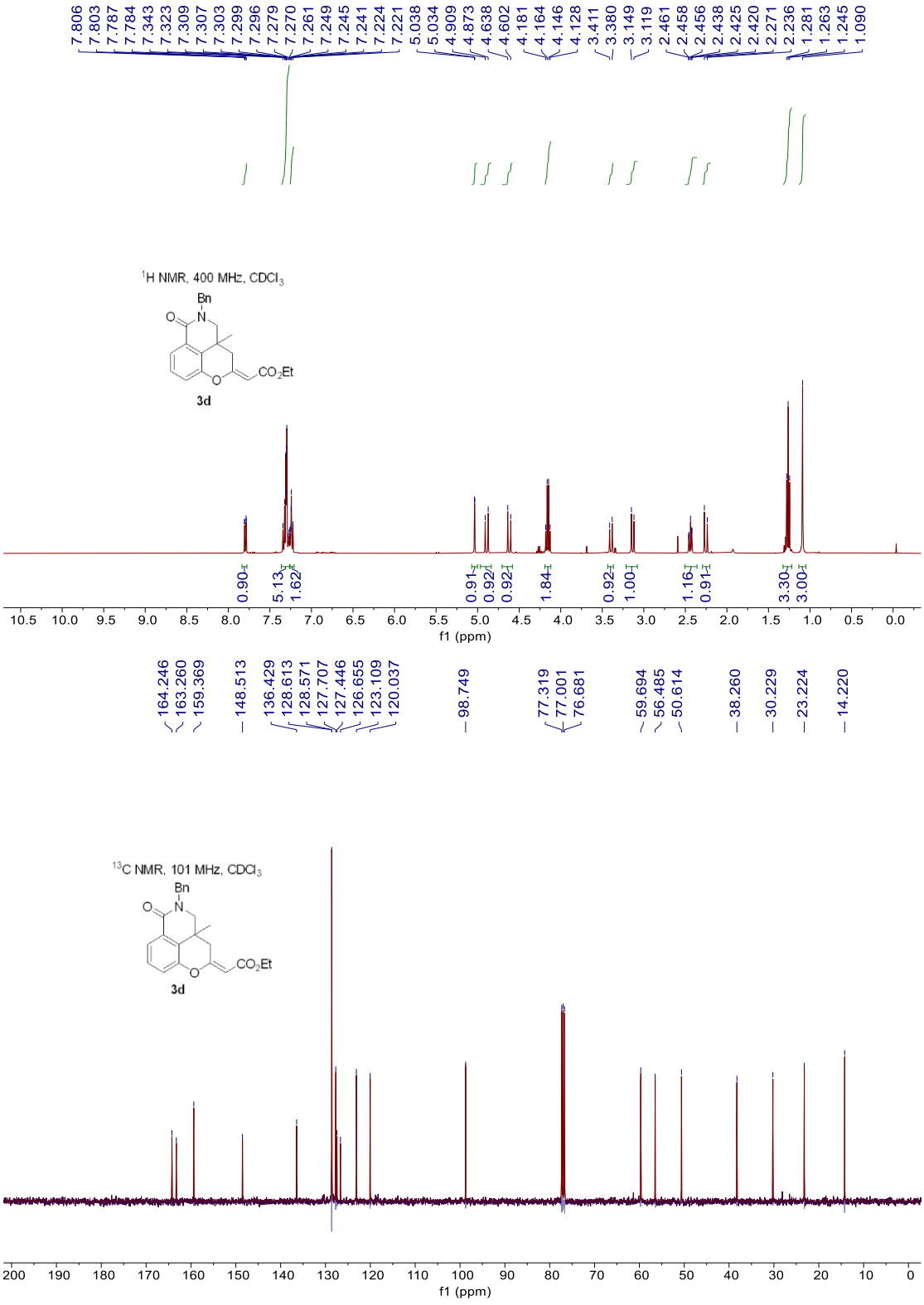
7.488
7.472
7.429
7.414
7.398
7.389
7.372
7.352
7.336
7.316
7.298
7.284
7.260
7.154
6.285
6.279
6.272
6.039
4.968
4.939
4.730
4.701
3.589
3.564
3.219
3.194
2.776
2.746
2.686
2.656
0.993
1H NMR, 500 MHz, CDCl3
N
N–Bn
O
3b
0.93
6.95
0.97
0.97
0.95
2.06
2.11
2.01
3.00
f1 (ppm)
163.563
136.662
133.782
131.455
128.642
128.441
128.003
127.680
126.065
124.139
118.087
114.811
110.146
107.499
77.255
77.000
76.747
56.988
50.826
33.171
32.436
23.139
13C NMR, 126 MHz, CDCl3
N
N–Bn
O
3b
f1 (ppm)


8.640
8.621
8.229
8.210
8.098
8.080
7.740
7.726
7.441
7.425
7.409
7.386
7.370
7.357
7.342
7.327
7.296
7.285
7.260
7.023
7.010
7.005
6.992
6.734
4.997
4.968
4.711
4.681
4.501
4.480
4.466
4.451
4.413
4.399
4.392
4.377
3.649
3.625
3.260
3.236
2.766
2.735
2.699
2.668
1.467
1.453
1.439
1.054
1H NMR, 500 MHz, CDCl3
CO2Et
N
O
N
Bn
3c
0.92
0.93
0.97
0.97
5.82
0.95
0.98
1.00
0.97
1.96
0.96
0.95
1.94
3.00
3.04
f1 (ppm)
165.242
164.361
139.898
137.307
136.752
131.592
128.924
128.628
128.577
127.583
127.243
127.189
127.002
122.142
121.766
121.718
121.030
120.697
112.812
99.864
77.254
77.001
76.745
59.819
57.134
50.588
34.982
31.058
23.831
14.513
13C NMR, 126 MHz, CDCl3
CO2Et
N
O
N
Bn
3c
f1 (ppm)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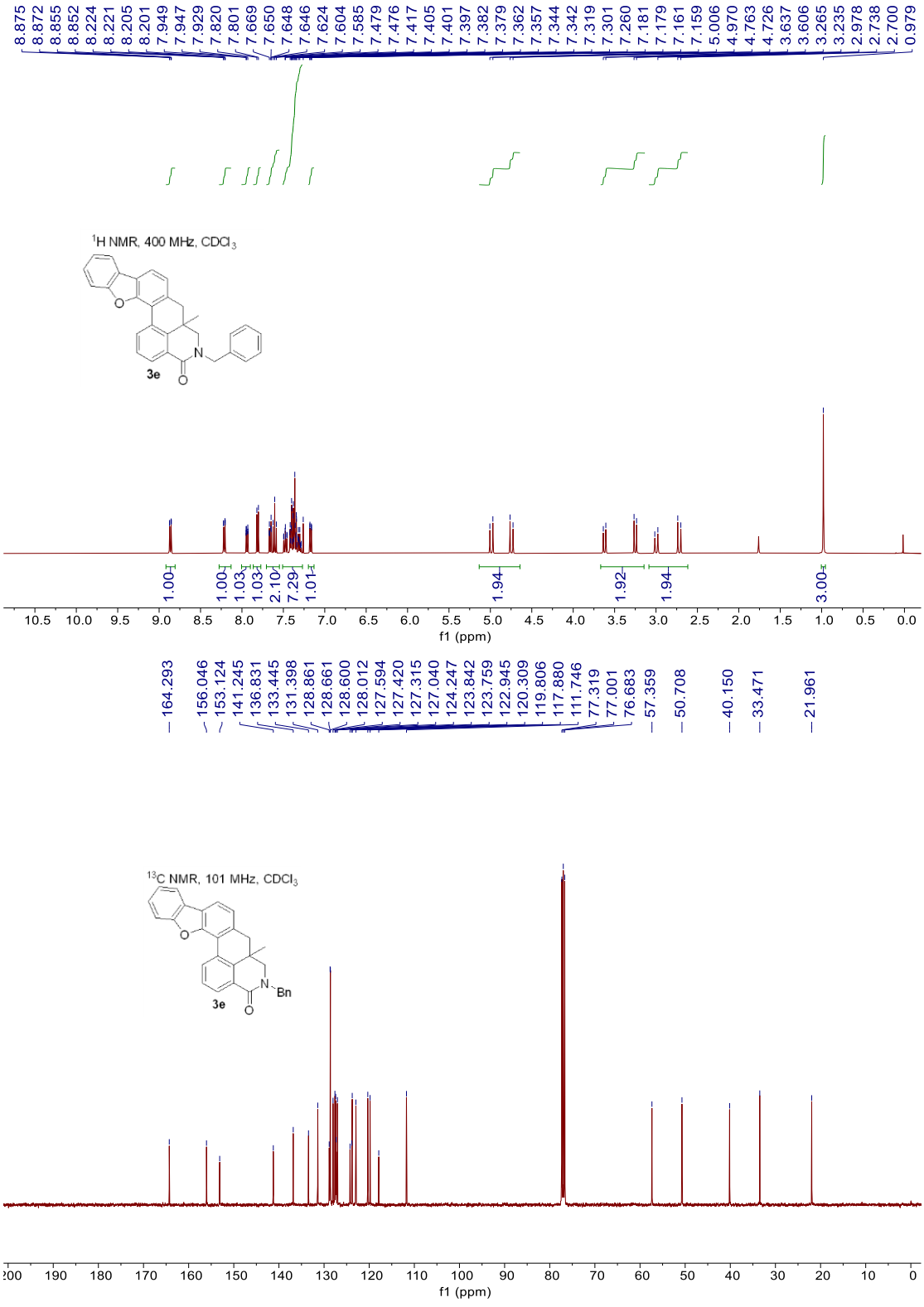
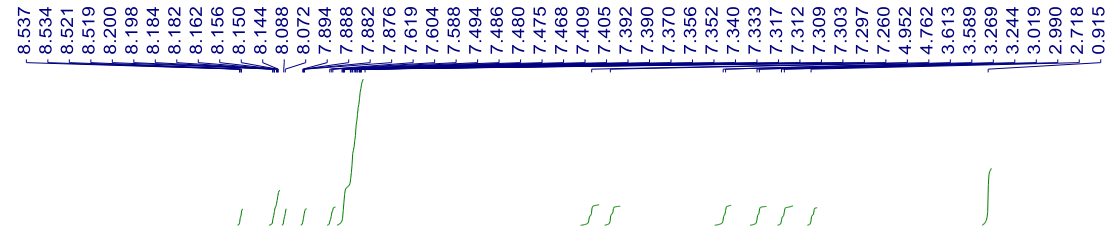
7.803
7.787
7.784
7.343
7.323
7.309
7.307
7.303
7.299
7.296
7.279
7.270
7.261
7.249
7.245
7.241
7.224
7.221
5.038
4.909
4.873
4.638
4.602
4.181
4.164
4.146
4.128
3.411
3.380
3.149
3.119
2.461
2.458
2.456
2.438
2.425
2.420
2.271
2.236
1.281
1.263
1.245
1.090
^{1}H NMR, 400 MHz, CDCl$_3$
Bn
N
O
CO$_2$Et
3d
0.90
5.13
1.62
0.91
0.92
0.92
1.84
0.92
1.00
1.16
0.91
3.30
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
164.246
163.260
159.369
148.513
136.429
128.613
128.571
127.707
127.446
126.655
123.109
120.037
98.749
77.319
77.001
76.681
59.694
56.485
50.614
38.260
30.229
23.224
14.220
^{13}C NMR, 101 MHz, CDCl$_3$
Bn
N
O
CO$_2$Et
3d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.875
8.872
8.855
8.852
8.224
8.221
8.205
8.201
7.949
7.947
7.929
7.820
7.801
7.669
7.650
7.648
7.646
7.624
7.604
7.585
7.479
7.476
7.417
7.405
7.401
7.397
7.382
7.379
7.362
7.357
7.344
7.342
7.319
7.301
7.260
7.181
7.179
7.161
7.159
5.006
4.970
4.763
4.726
3.637
3.606
3.265
3.235
2.978
2.738
2.700
0.979
1H NMR, 400 MHz, CDCl3
3e
1.00
1.00
1.03
1.03
2.10
7.29
1.01
1.94
1.92
1.94
3.00
f1 (ppm)
164.293
156.046
153.124
141.245
136.831
133.445
131.398
128.861
128.661
128.600
128.012
127.594
127.420
127.315
127.040
124.247
123.842
123.759
122.945
120.309
119.806
117.880
111.746
77.319
77.001
76.683
57.359
50.708
40.150
33.471
21.961
13C NMR, 101 MHz, CDCl3
3e
Bn
f1 (ppm)


8.537
8.534
8.521
8.519
8.200
8.198
8.184
8.182
8.162
8.156
8.150
8.144
8.088
8.072
7.894
7.888
7.882
7.876
7.619
7.604
7.588
7.494
7.486
7.480
7.475
7.468
7.409
7.405
7.392
7.390
7.370
7.356
7.352
7.340
7.333
7.317
7.312
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7.303
7.297
7.260
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3.269
3.244
3.019
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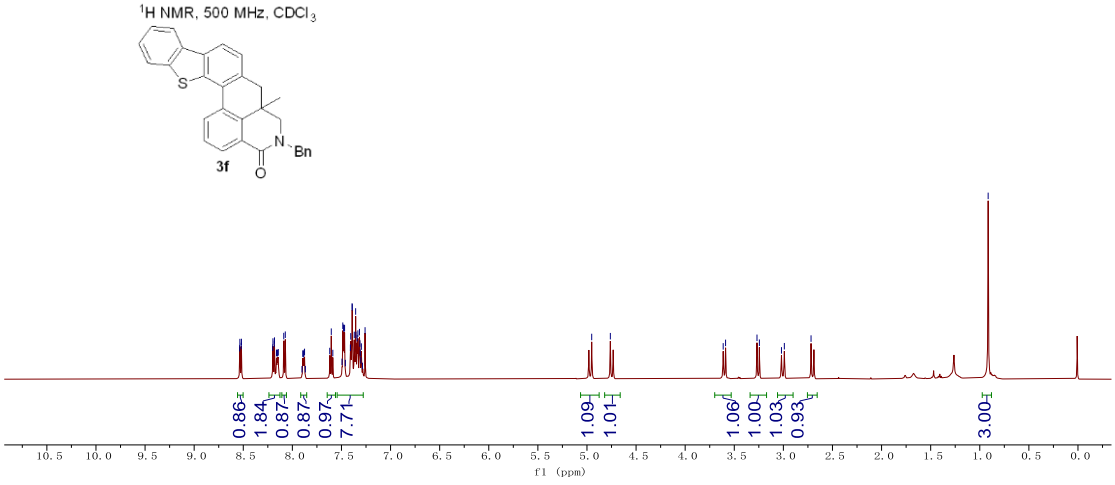
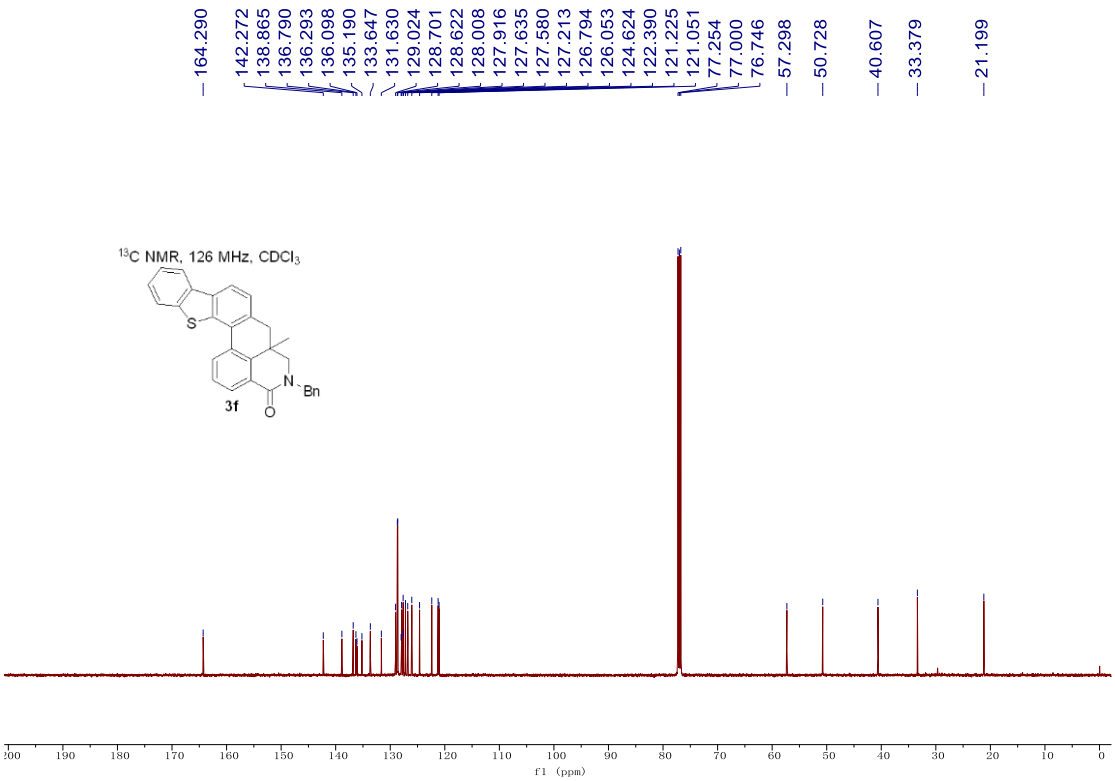
2.718
0.915


^{1}H NMR, 500 MHz, CDCl$_3$
S
N
Bn
O
3f
0.86
1.84
0.87
0.87
0.97
7.71
1.09
1.01
1.06
1.00
1.03
0.93
3.00
f1 (ppm)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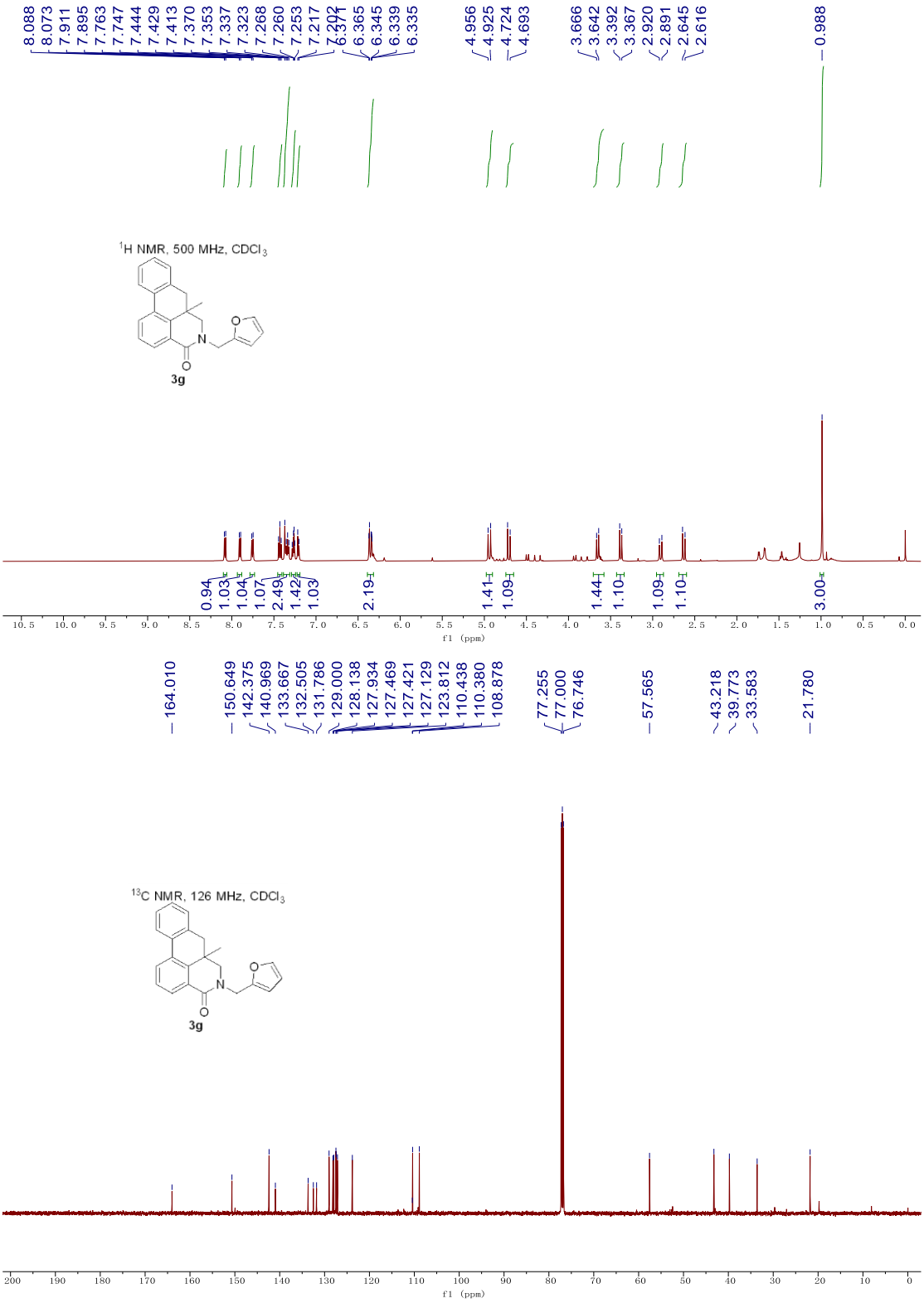
142.272
138.865
136.790
136.293
136.098
135.190
133.647
131.630
129.024
128.701
128.622
128.008
127.916
127.635
127.580
127.213
126.794
126.053
124.624
122.390
121.225
121.051
77.254
77.000
76.746
57.298
50.728
40.607
33.379
21.199
^{13}C NMR, 126 MHz, CDCl$_3$
S
N
Bn
O
3f
f1 (ppm)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7.895
7.763
7.747
7.444
7.429
7.413
7.370
7.353
7.337
7.323
7.268
7.260
7.253
7.217
7.202
6.371
6.365
6.345
6.339
6.335
4.956
4.925
4.724
4.693
3.666
3.642
3.392
3.367
2.920
2.891
2.645
2.616
0.988
1H NMR, 500 MHz, CDCl3
3g
0.94
1.03
1.04
1.07
2.49
1.42
1.03
2.19
1.41
1.09
1.44
1.10
1.09
1.10
3.00
f1 (ppm)
164.010
150.649
142.375
140.969
133.667
132.505
131.786
129.000
128.138
127.934
127.469
127.421
127.129
123.812
110.438
110.380
108.878
77.255
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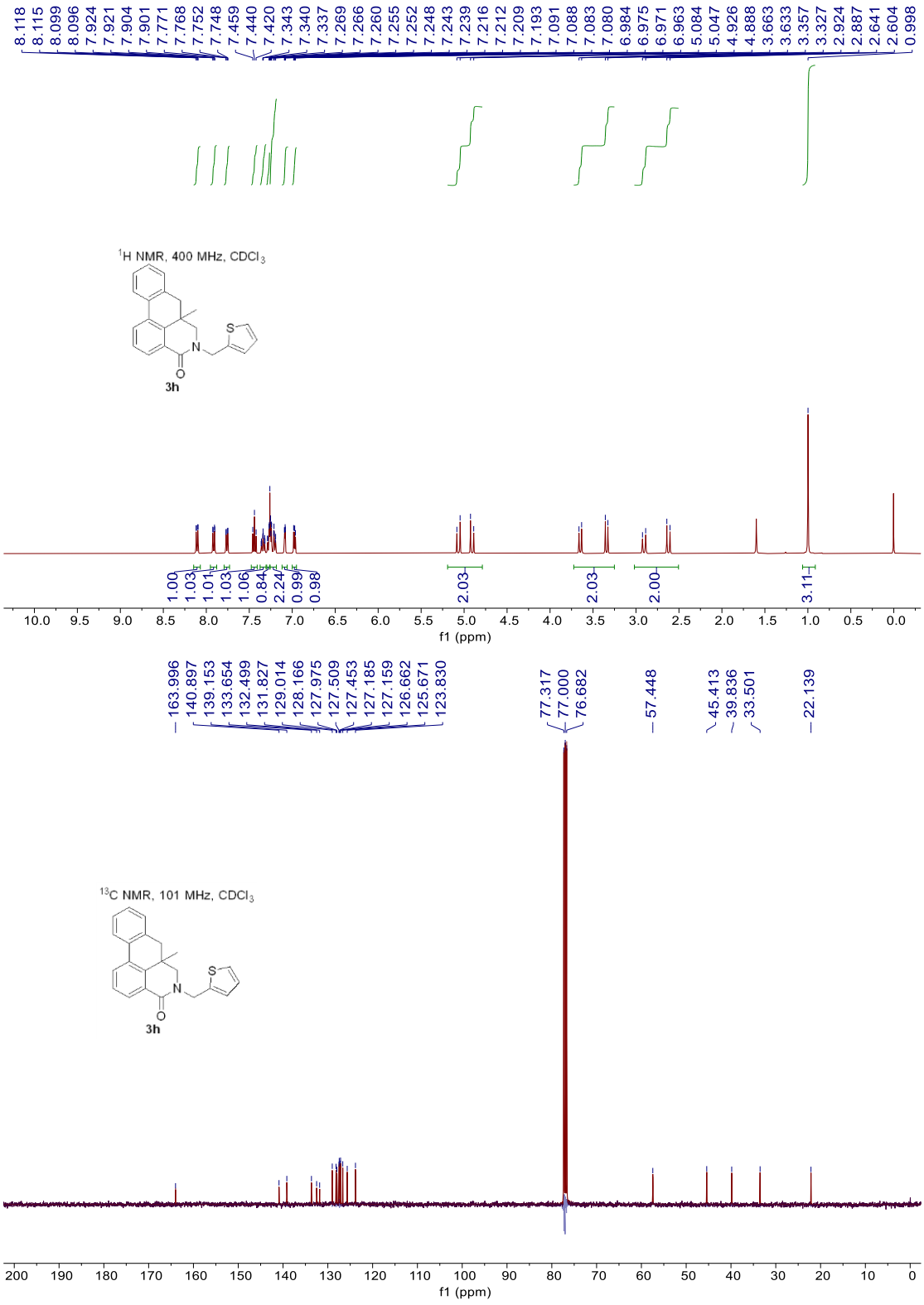
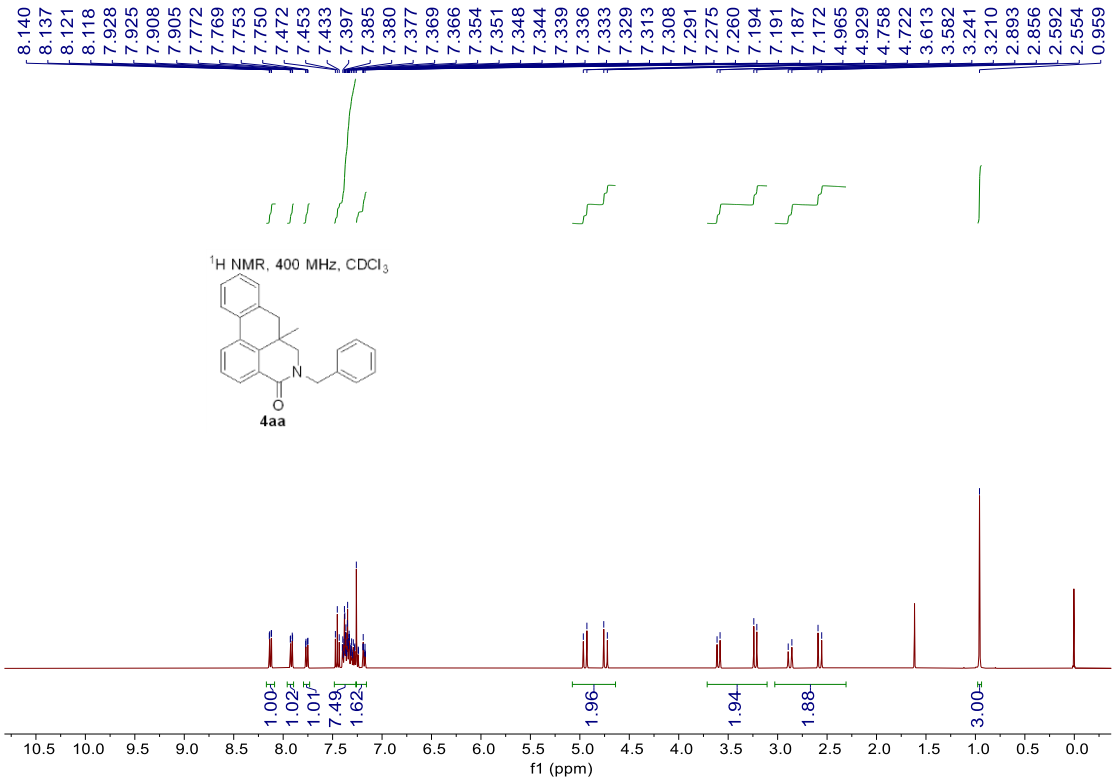
57.565
43.218
39.773
33.583
21.780
13C NMR, 126 MHz, CDCl3
3g
f1 (ppm)


8.118
8.115
8.099
8.096
7.924
7.921
7.904
7.901
7.771
7.768
7.752
7.748
7.459
7.440
7.420
7.343
7.340
7.337
7.269
7.266
7.260
7.255
7.252
7.248
7.243
7.239
7.216
7.212
7.209
7.193
7.091
7.088
7.083
7.080
6.984
6.975
6.971
6.963
5.084
5.047
4.926
4.888
3.663
3.633
3.357
3.327
2.924
2.887
2.641
2.604
0.998
1H NMR, 400 MHz, CDCl3
3h
1.00
1.03
1.01
1.03
1.06
0.84
2.24
0.99
0.98
2.03
2.03
2.00
3.11
f1 (ppm)
163.996
140.897
139.153
133.654
132.499
131.827
129.014
128.166
127.975
127.509
127.453
127.185
127.159
126.662
125.671
123.830
77.317
77.000
76.682
57.448
45.413
39.836
33.501
22.139
13C NMR, 101 MHz, CDCl3
3h
f1 (ppm)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8.137
8.121
8.118
7.928
7.925
7.908
7.905
7.772
7.769
7.753
7.750
7.472
7.453
7.433
7.397
7.385
7.380
7.377
7.369
7.366
7.354
7.351
7.348
7.344
7.339
7.336
7.333
7.329
7.313
7.308
7.291
7.275
7.260
7.194
7.191
7.187
7.172
4.965
4.929
4.758
4.722
3.613
3.582
3.241
3.210
2.893
2.856
2.592
2.554
0.959
1H NMR, 400 MHz, CDCl3
4aa
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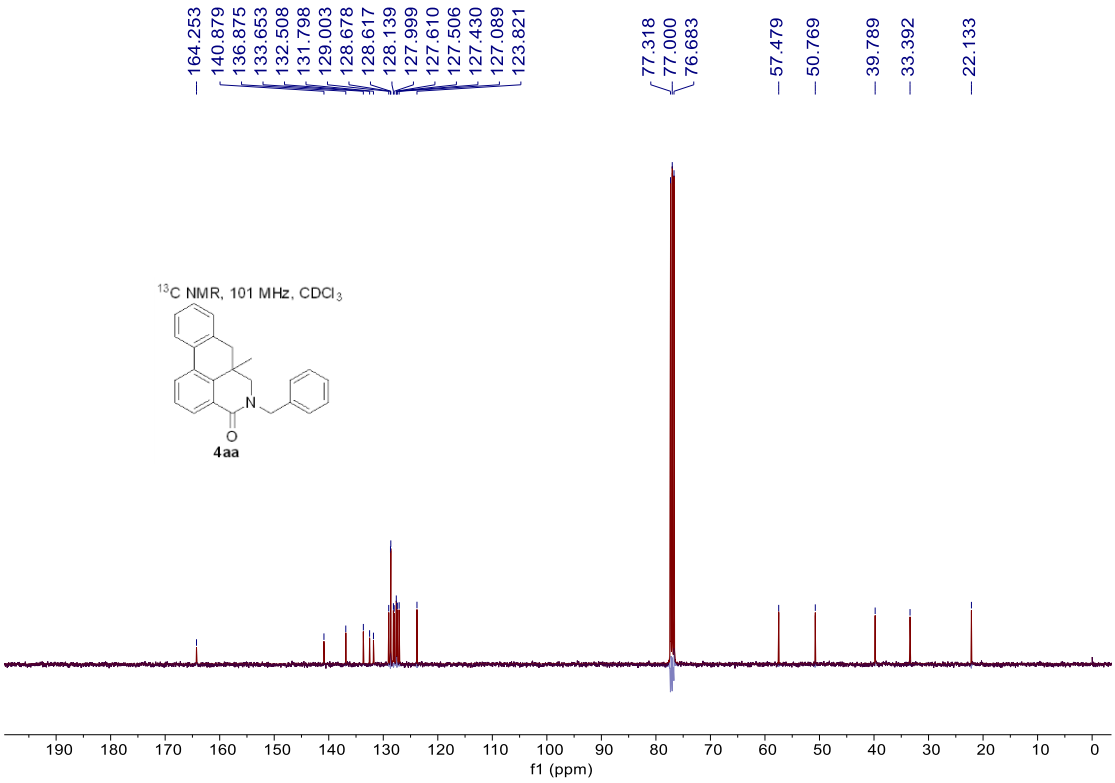
1.02
1.01
7.49
1.62
1.96
1.94
1.88
3.00
f1 (ppm)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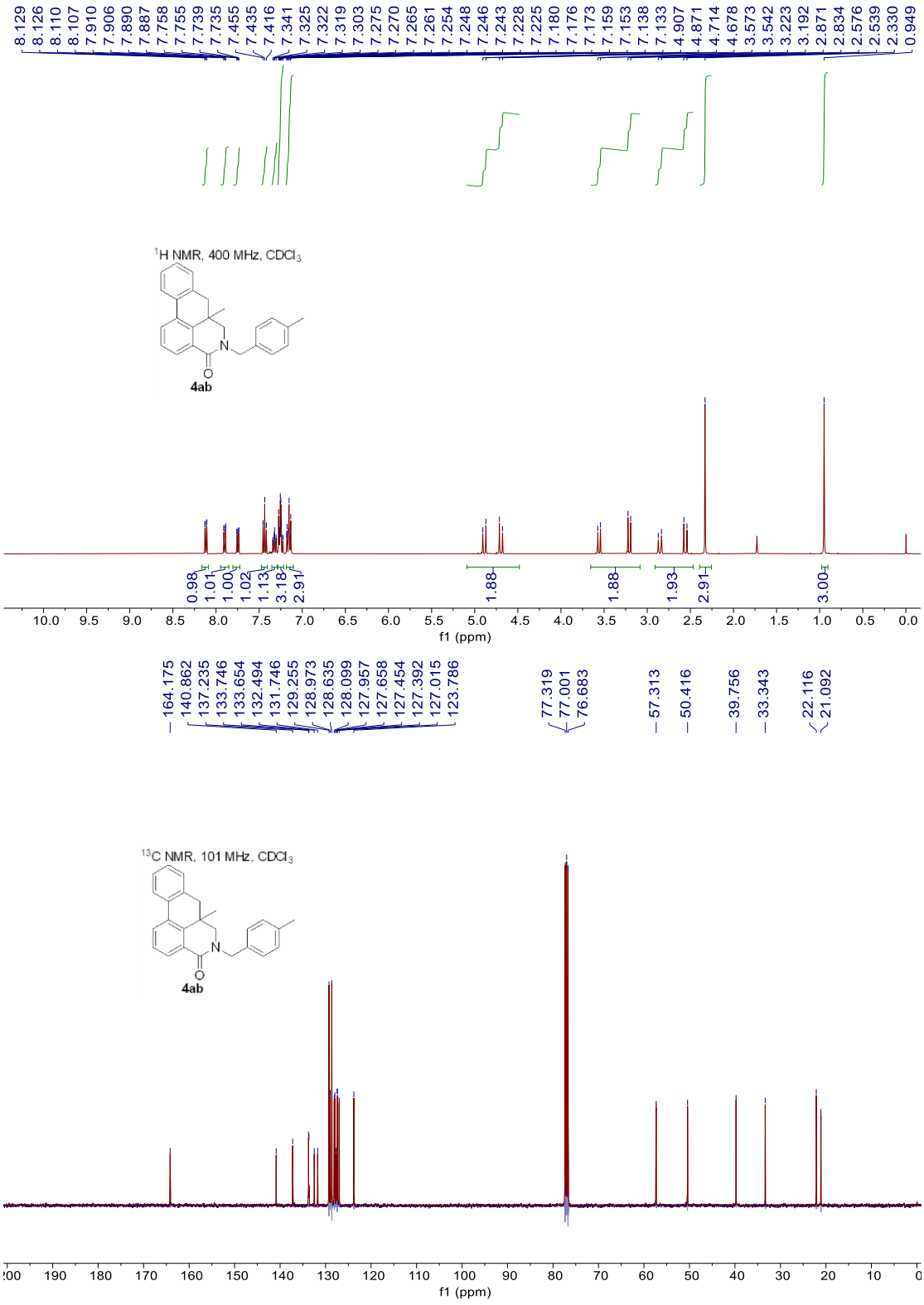
140.879
136.875
133.653
132.508
131.798
129.003
128.678
128.617
128.139
127.999
127.610
127.506
127.430
127.089
123.821
77.318
77.000
76.683
57.479
50.769
39.789
33.392
22.133
13C NMR, 101 MHz, CDCl3
4aa
f1 (ppm)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8.126
8.110
8.107
7.910
7.906
7.890
7.887
7.758
7.755
7.739
7.735
7.455
7.435
7.416
7.341
7.325
7.322
7.319
7.303
7.275
7.270
7.265
7.261
7.254
7.248
7.246
7.243
7.228
7.225
7.180
7.176
7.173
7.159
7.153
7.138
7.133
4.907
4.871
4.714
4.678
3.573
3.542
3.223
3.192
2.871
2.834
2.576
2.539
2.330
0.949
1H NMR, 400 MHz, CDCl3
4ab
0.98
1.01
1.00
1.02
1.13
3.18
2.91
1.88
1.88
1.93
2.91
3.00
f1 (ppm)
164.175
140.862
137.235
133.746
133.654
132.494
131.746
129.255
128.973
128.635
128.099
127.957
127.658
127.454
127.392
127.015
123.786
77.319
77.001
76.683
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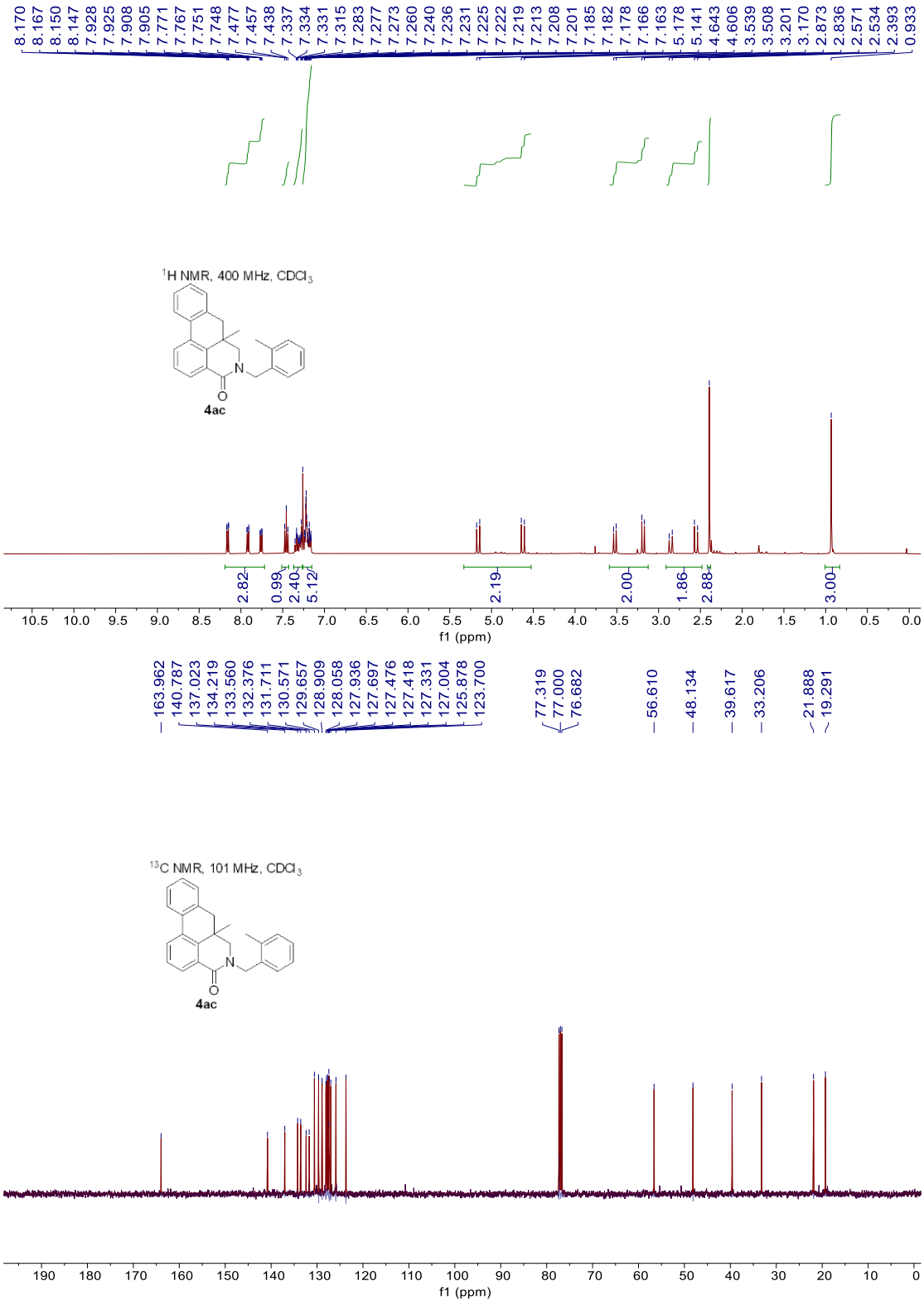
50.416
39.756
33.343
22.116
21.092
13C NMR, 101 MHz, CDCl3
4ab
f1 (ppm)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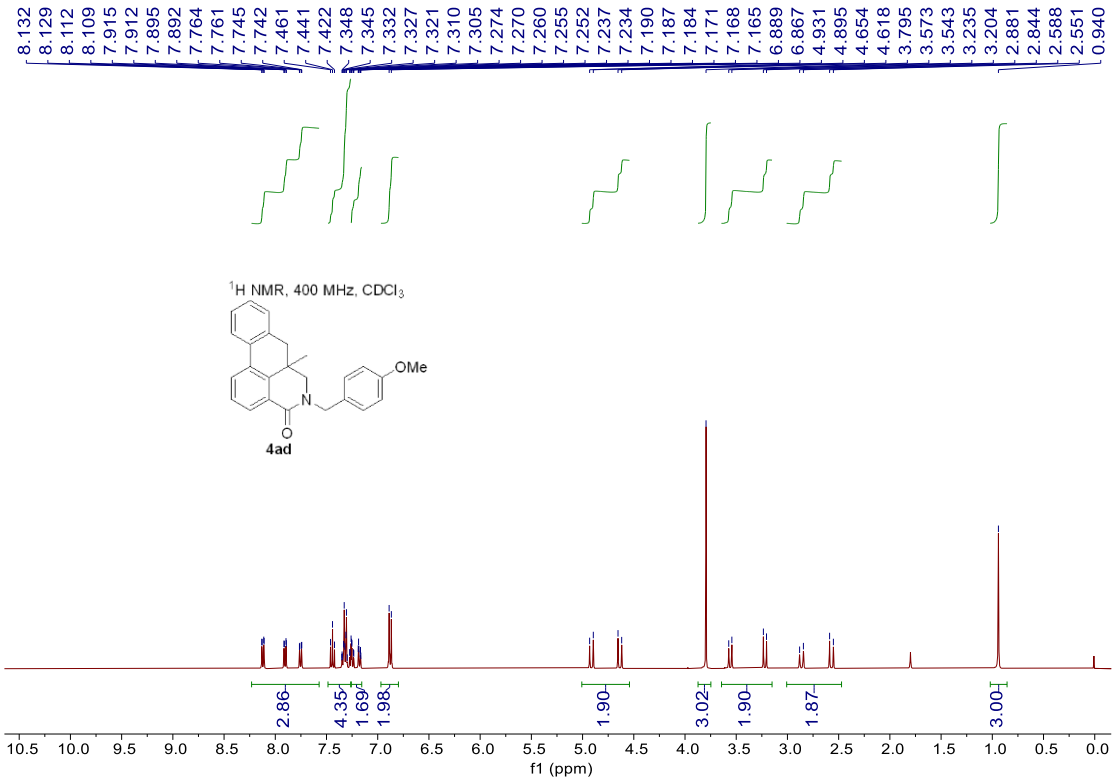
8.167
8.150
8.147
7.928
7.925
7.908
7.905
7.771
7.767
7.751
7.748
7.477
7.457
7.438
7.337
7.334
7.331
7.315
7.283
7.277
7.273
7.260
7.240
7.236
7.231
7.225
7.222
7.219
7.213
7.208
7.201
7.185
7.182
7.178
7.166
7.163
5.178
5.141
4.643
4.606
3.539
3.508
3.201
3.170
2.873
2.836
2.571
2.534
2.393
0.933
^{1}H NMR, 400 MHz, CDCl$_3$
4ac
2.82
0.99
2.40
5.12
2.19
2.00
1.86
2.88
3.00
f1 (ppm)
163.962
140.787
137.023
134.219
133.560
132.376
131.711
130.571
129.657
128.909
128.058
127.936
127.697
127.476
127.418
127.331
127.004
125.878
123.700
77.319
77.000
76.682
56.610
48.134
39.617
33.206
21.888
19.291
^{13}C NMR, 101 MHz, CDCl$_3$
4ac
f1 (ppm)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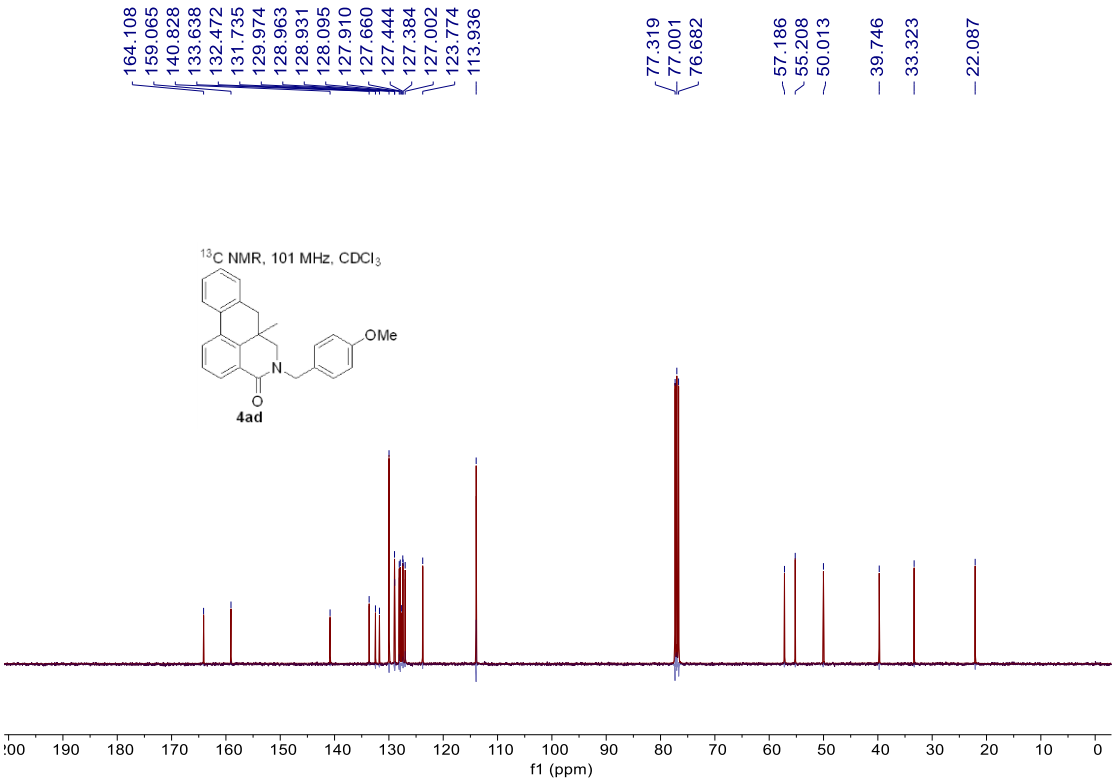
8.129
8.112
8.109
7.915
7.912
7.895
7.892
7.764
7.761
7.745
7.742
7.461
7.441
7.422
7.348
7.345
7.332
7.327
7.321
7.310
7.305
7.274
7.270
7.260
7.255
7.252
7.237
7.234
7.190
7.187
7.184
7.171
7.168
7.165
6.889
6.867
4.931
4.895
4.654
4.618
3.795
3.573
3.543
3.235
3.204
2.881
2.844
2.588
2.551
0.940
1H NMR, 400 MHz, CDCl3
OMe
N
O
4ad
2.86
4.35
1.69
1.98
1.90
3.02
1.90
1.87
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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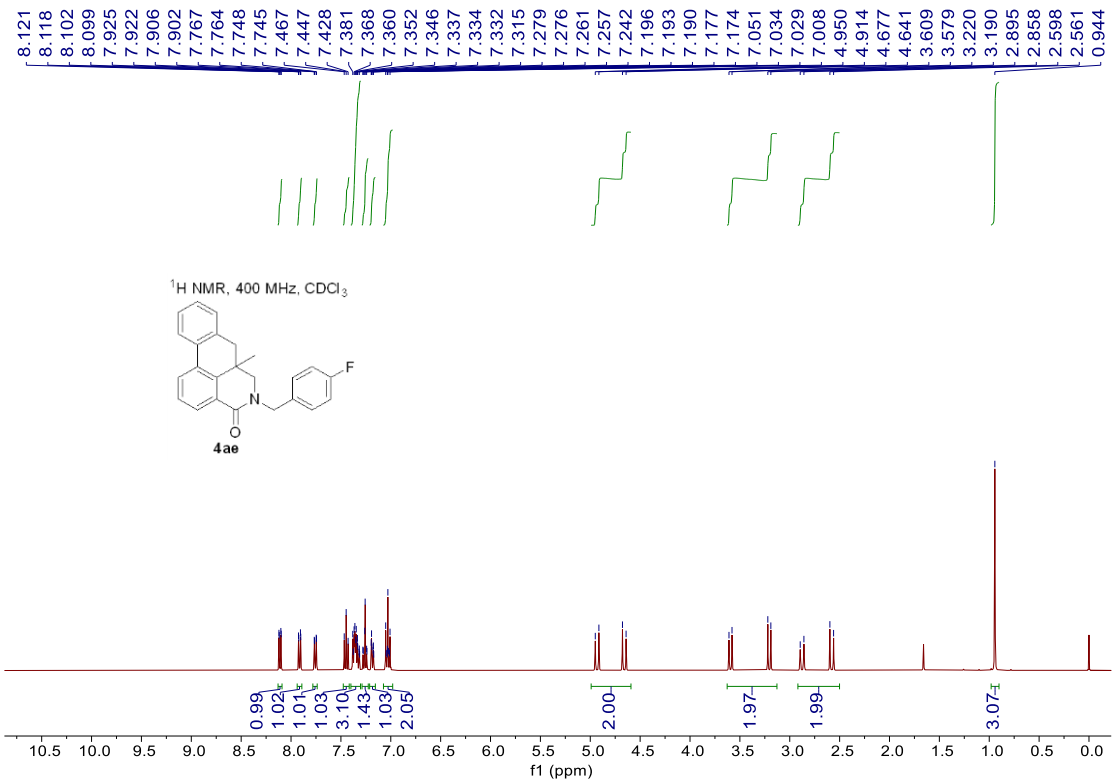
159.065
140.828
133.638
132.472
131.735
129.974
128.963
128.931
128.095
127.910
127.660
127.444
127.384
127.002
123.774
113.936
77.319
77.001
76.682
57.186
55.208
50.013
39.746
33.323
22.087
13C NMR, 101 MHz, CDCl3
OMe
N
O
4ad
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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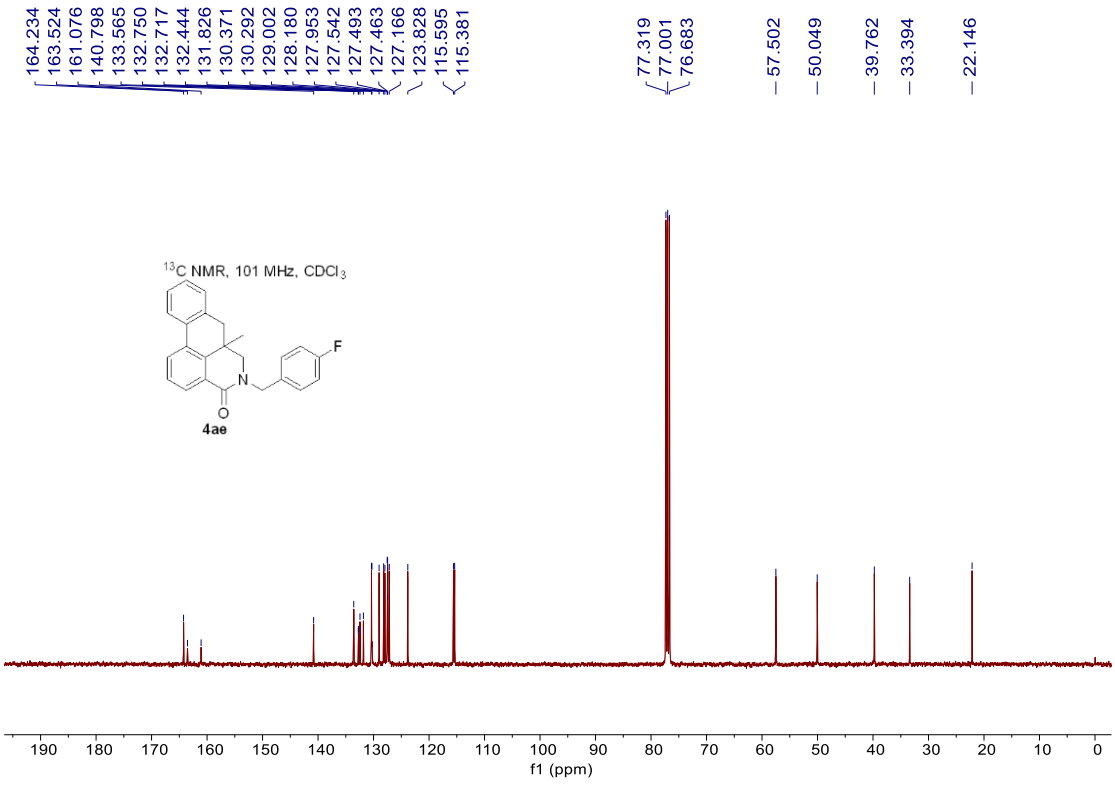
8.118
8.102
8.099
7.925
7.922
7.906
7.902
7.767
7.764
7.748
7.745
7.467
7.447
7.428
7.381
7.368
7.360
7.352
7.346
7.337
7.334
7.332
7.315
7.279
7.276
7.261
7.257
7.242
7.196
7.193
7.190
7.177
7.174
7.051
7.034
7.029
7.008
4.950
4.914
4.677
4.641
3.609
3.579
3.220
3.190
2.895
2.858
2.598
2.561
0.944
1H NMR, 400 MHz, CDCl3
F
N
O
4ae
0.99
1.02
1.01
1.03
3.10
1.43
1.03
2.05
2.00
1.97
1.99
3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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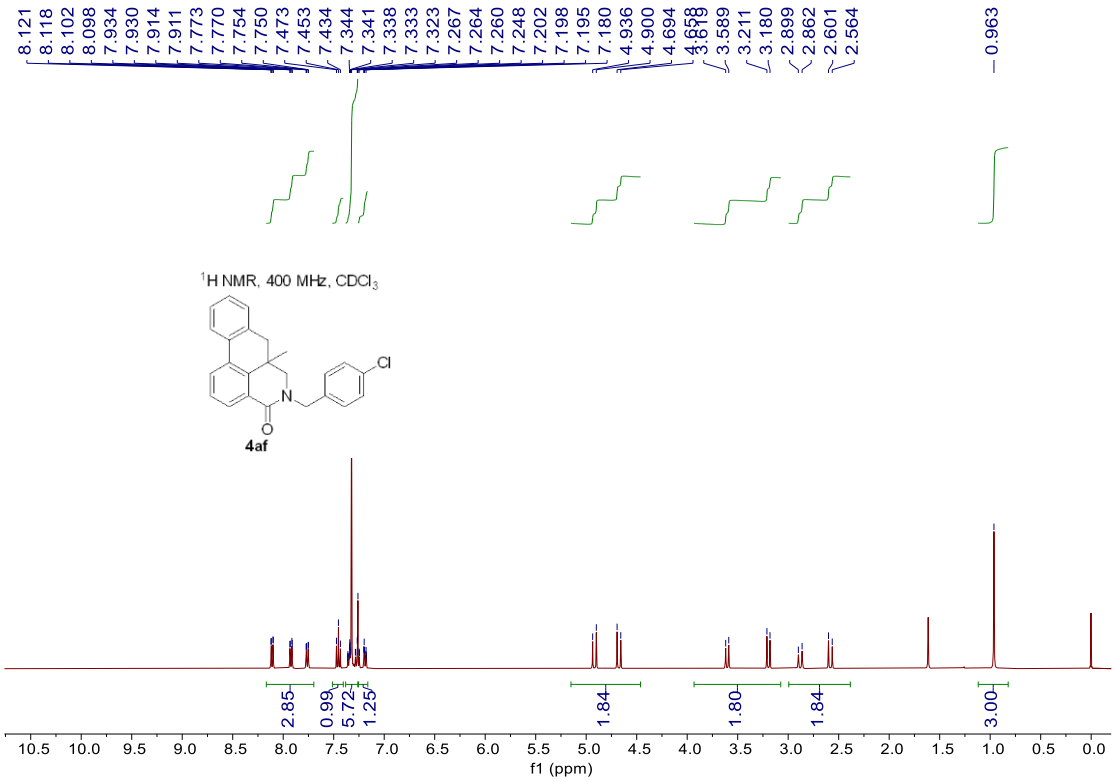
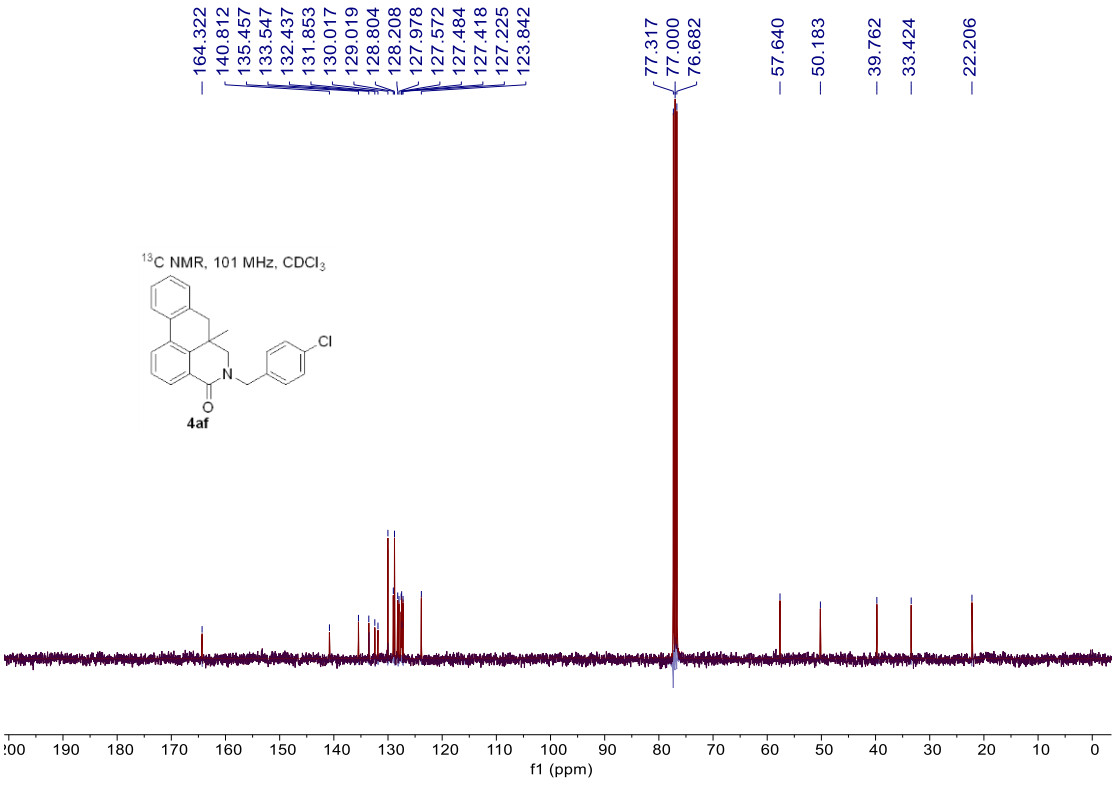
163.524
161.076
140.798
133.565
132.750
132.717
132.444
131.826
130.371
130.292
129.002
128.180
127.953
127.542
127.493
127.463
127.166
123.828
115.595
115.381
77.319
77.001
76.683
57.502
50.049
39.762
33.394
22.146
13C NMR, 101 MHz, CDCl3
F
N
O
4ae
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.121
8.118
8.102
8.098
7.934
7.930
7.914
7.911
7.773
7.770
7.754
7.750
7.473
7.453
7.434
7.344
7.341
7.338
7.333
7.323
7.267
7.264
7.260
7.248
7.202
7.198
7.195
7.180
4.936
4.900
4.694
3.589
3.211
3.180
2.899
2.862
2.601
2.564
0.963
^{1}H NMR, 400 MHz, CDCl$_3$
Cl
N
O
4af
2.85
0.99
5.72
1.25
1.84
1.80
1.84
3.00
f1 (ppm)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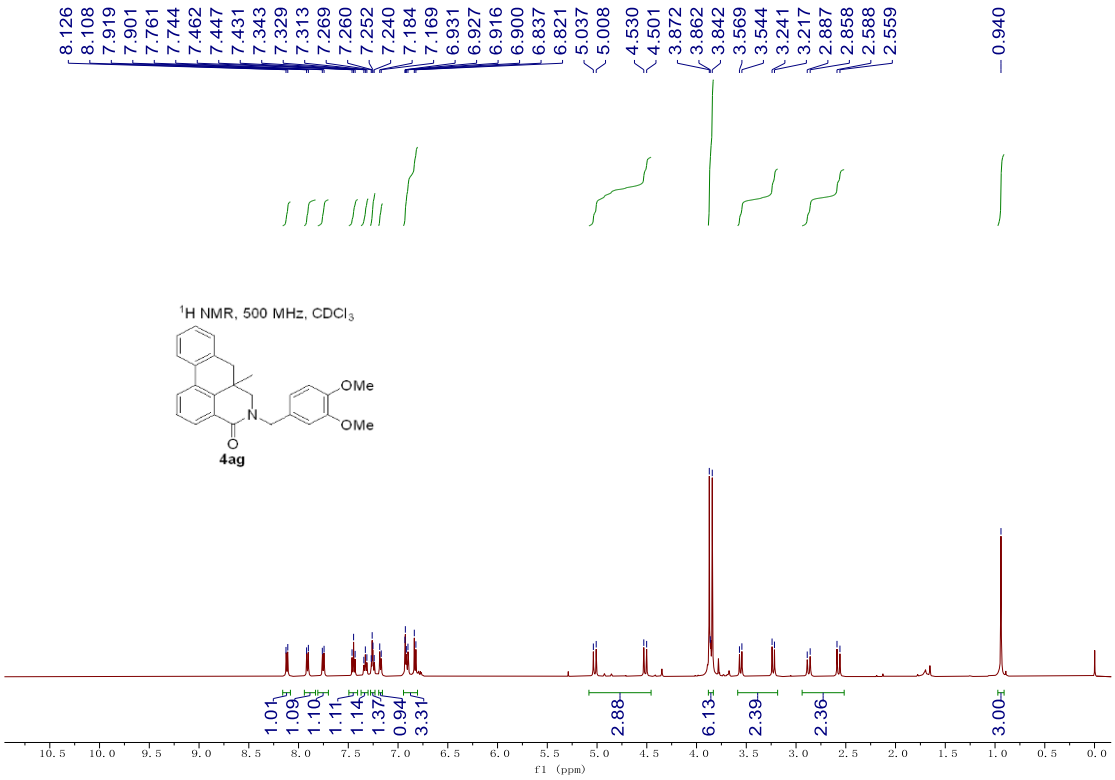
135.457
133.547
132.437
131.853
130.017
129.019
128.804
128.208
127.978
127.572
127.484
127.418
127.225
123.842
77.317
77.000
76.682
57.640
50.183
39.762
33.424
22.206
^{13}C NMR, 101 MHz, CDCl$_3$
Cl
N
O
4af
f1 (ppm)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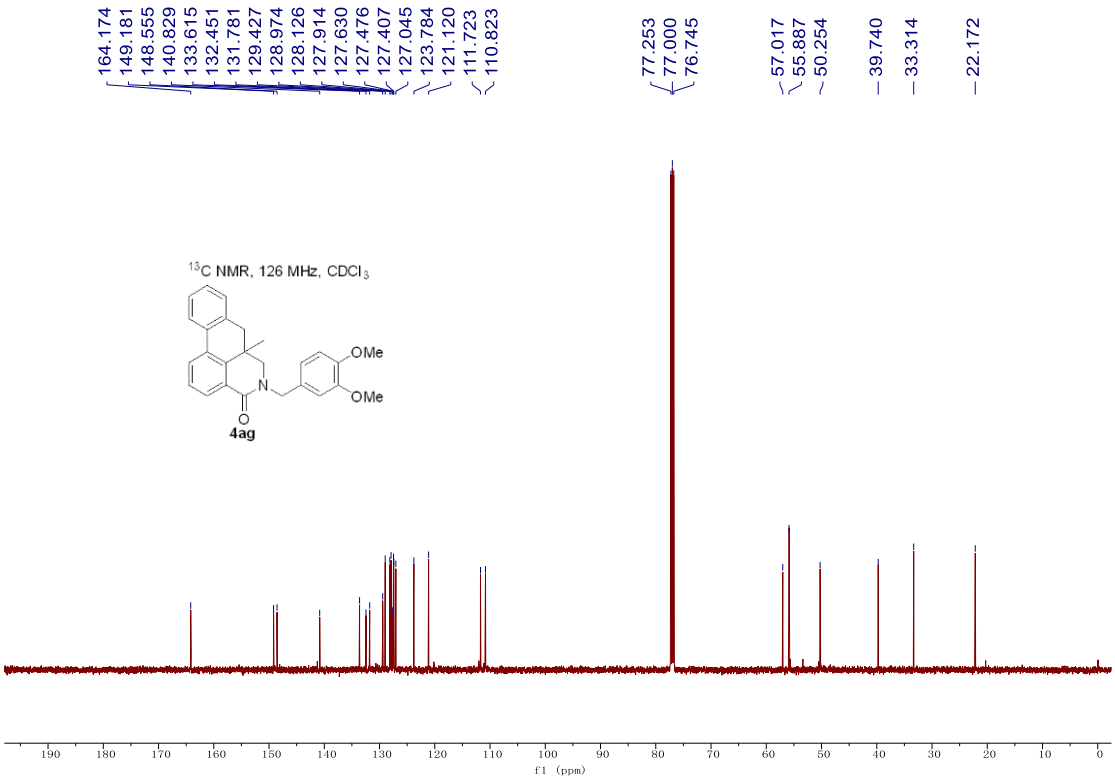
8.108
7.919
7.901
7.761
7.744
7.462
7.447
7.431
7.343
7.329
7.313
7.269
7.260
7.252
7.240
7.184
7.169
6.931
6.927
6.916
6.900
6.837
6.821
5.037
5.008
4.530
4.501
3.872
3.862
3.842
3.569
3.544
3.241
3.217
2.887
2.858
2.588
2.559
0.940
1H NMR, 500 MHz, CDCl3
OMe
OMe
N
O
4ag
1.01
1.09
1.10
1.11
1.14
1.37
0.94
3.31
2.88
6.13
2.39
2.36
3.00
f1 (ppm)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148.555
140.829
133.615
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131.781
129.427
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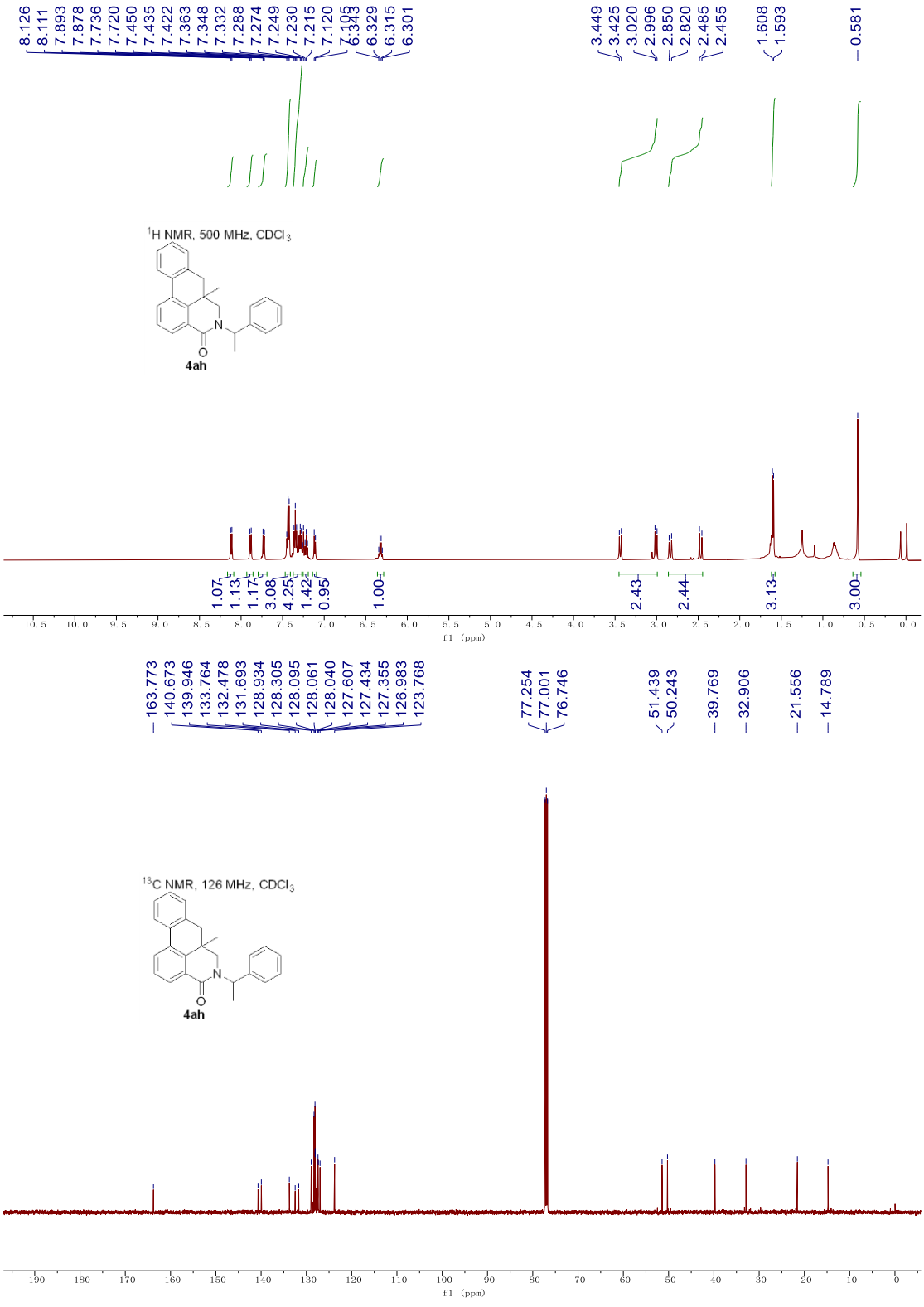
128.126
127.914
127.630
127.476
127.407
127.045
123.784
121.120
111.723
110.823
77.253
77.000
76.745
57.017
55.887
50.254
39.740
33.314
22.172
13C NMR, 126 MHz, CDCl3
OMe
OMe
N
O
4ag
f1 (ppm)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8.111
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7.878
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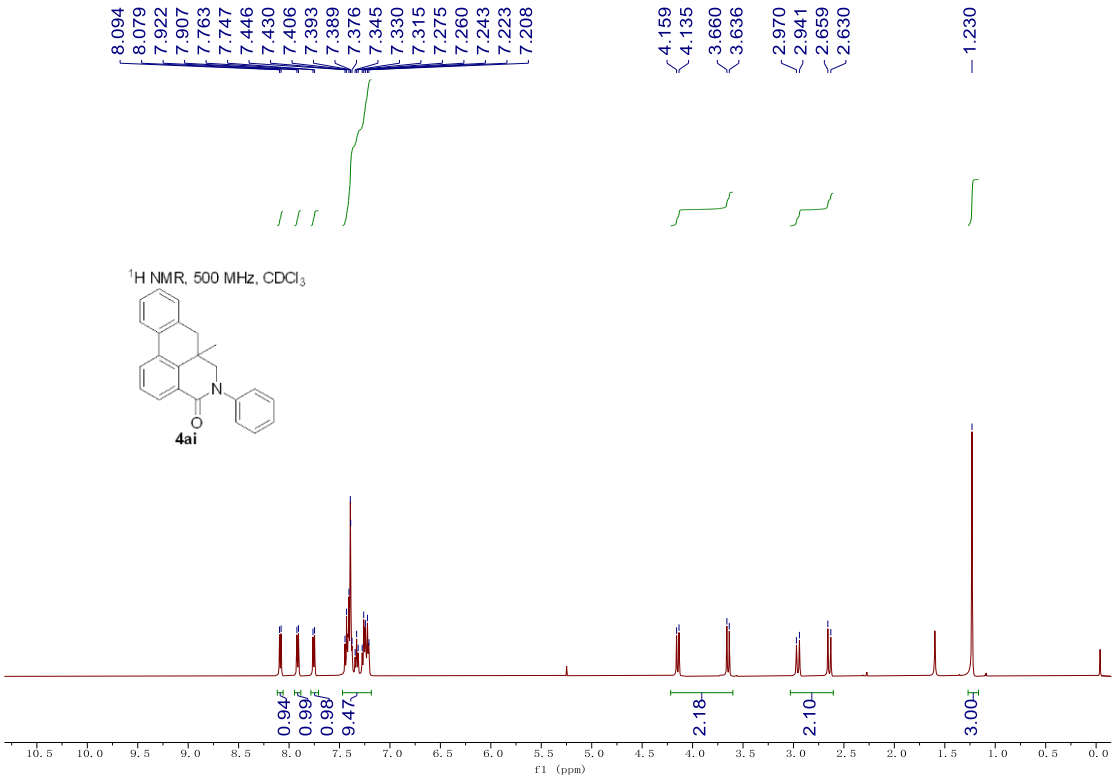
7.720
7.450
7.435
7.422
7.363
7.348
7.332
7.288
7.274
7.249
7.230
7.215
7.120
7.105
6.343
6.329
6.315
6.301
3.449
3.425
3.020
2.996
2.850
2.820
2.485
2.455
1.608
1.593
0.581
1H NMR, 500 MHz, CDCl3
4ah
1.07
1.13
1.17
3.08
4.25
1.42
0.95
1.00
2.43
2.44
3.13
3.00
f1 (ppm)
163.773
140.673
139.946
133.764
132.478
131.693
128.934
128.305
128.095
128.061
128.040
127.607
127.434
127.355
126.983
123.768
77.254
77.001
76.746
51.439
50.243
39.769
32.906
21.556
14.789
13C NMR, 126 MHz, CDCl3
4ah
f1 (ppm)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8.079
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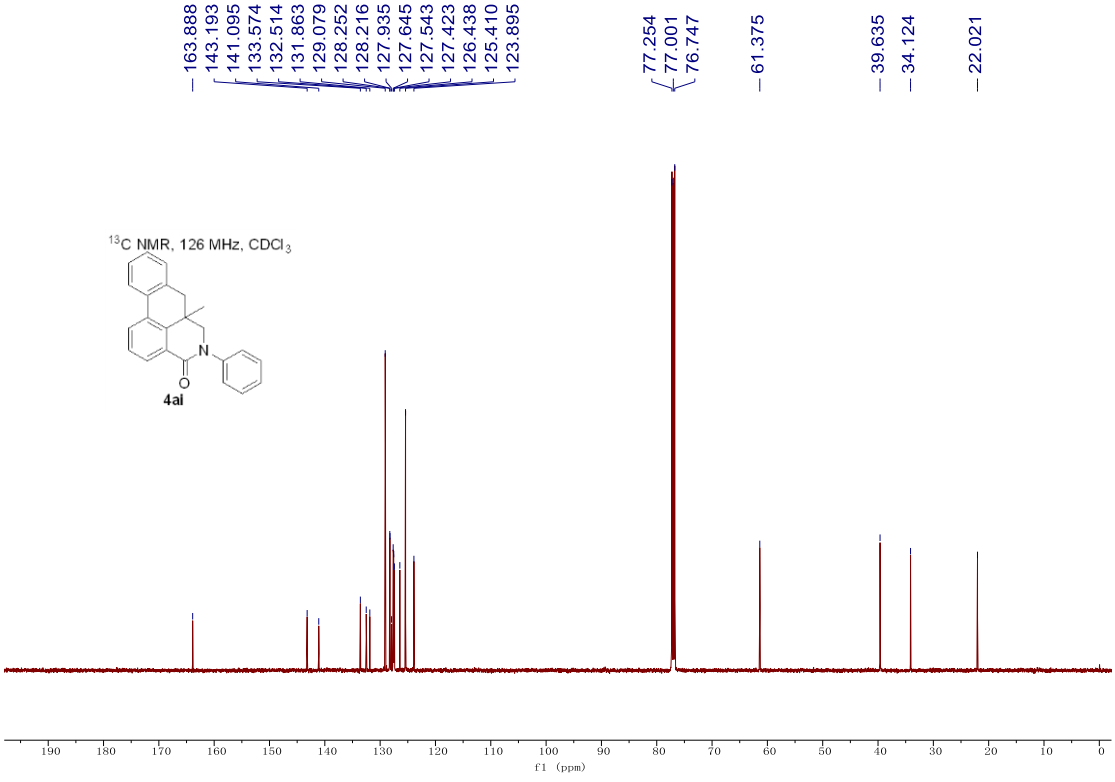
7.430
7.406
7.393
7.389
7.376
7.345
7.330
7.315
7.275
7.260
7.243
7.223
7.208
4.159
4.135
3.660
3.636
2.970
2.941
2.659
2.630
1.230
^{1}H NMR, 500 MHz, CDCl$_3$
4ai
0.94
0.99
0.98
9.47
2.18
2.10
3.00
f1 (ppm)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131.863
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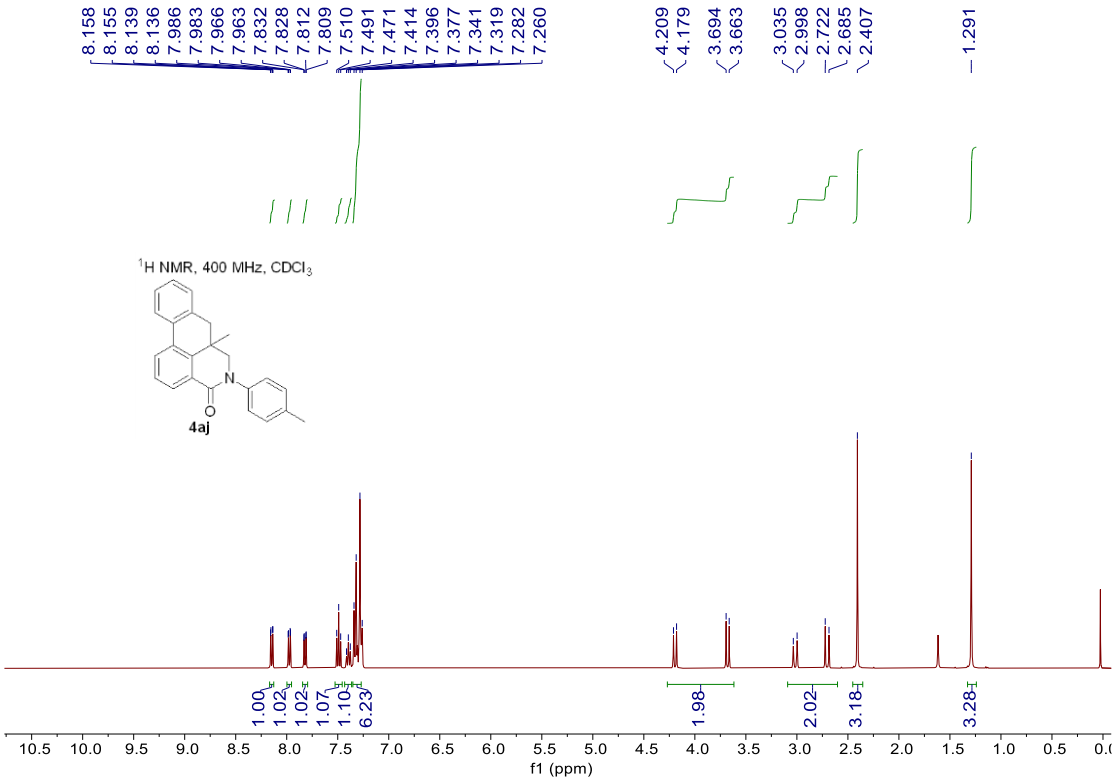
128.252
128.216
127.935
127.645
127.543
127.423
126.438
125.410
123.895
77.254
77.001
76.747
61.375
39.635
34.124
22.021
^{13}C NMR, 126 MHz, CDCl$_3$
4ai
f1 (ppm)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8.155
8.139
8.136
7.986
7.983
7.966
7.963
7.832
7.828
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7.809
7.510
7.491
7.471
7.414
7.396
7.377
7.341
7.319
7.282
7.260
4.209
4.179
3.694
3.663
3.035
2.998
2.722
2.685
2.407
1.291
1H NMR, 400 MHz, CDCl3
4aj
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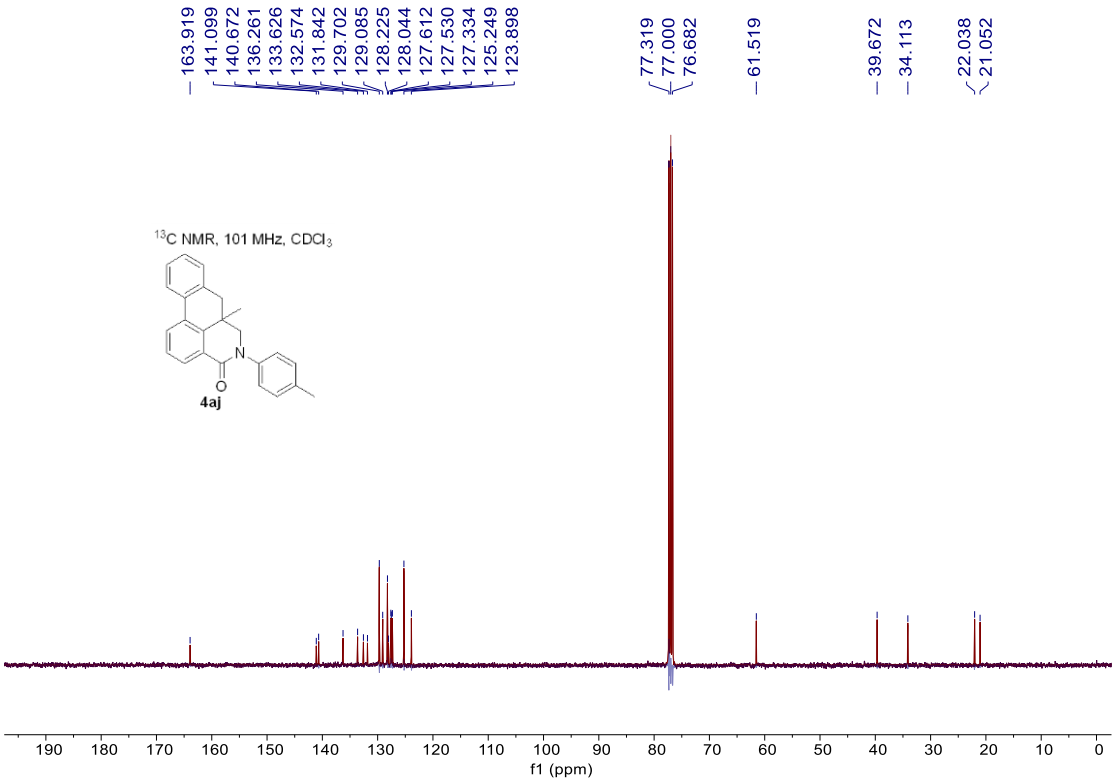
1.02
1.02
1.07
1.10
6.23
1.98
2.02
3.18
3.28
f1 (ppm)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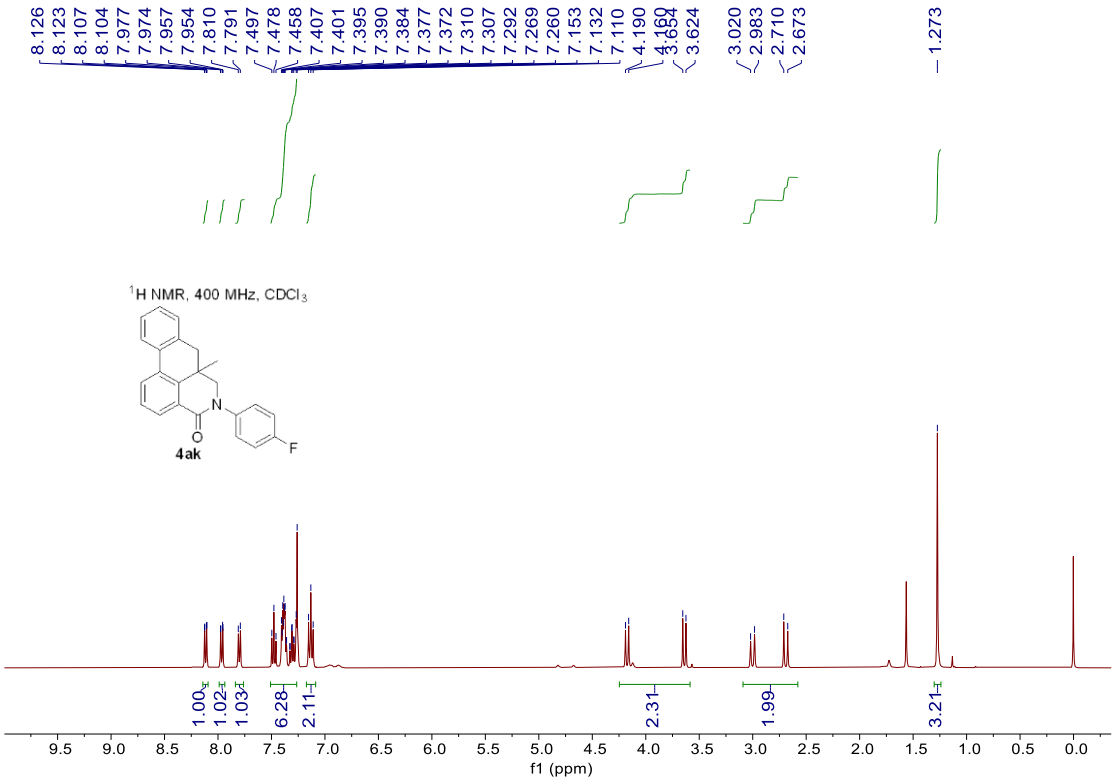
133.626
132.574
131.842
129.702
129.085
128.225
128.044
127.612
127.530
127.334
125.249
123.898
77.319
77.000
76.682
61.519
39.672
34.113
22.038
21.052
13C NMR, 101 MHz, CDCl3
4aj
f1 (ppm)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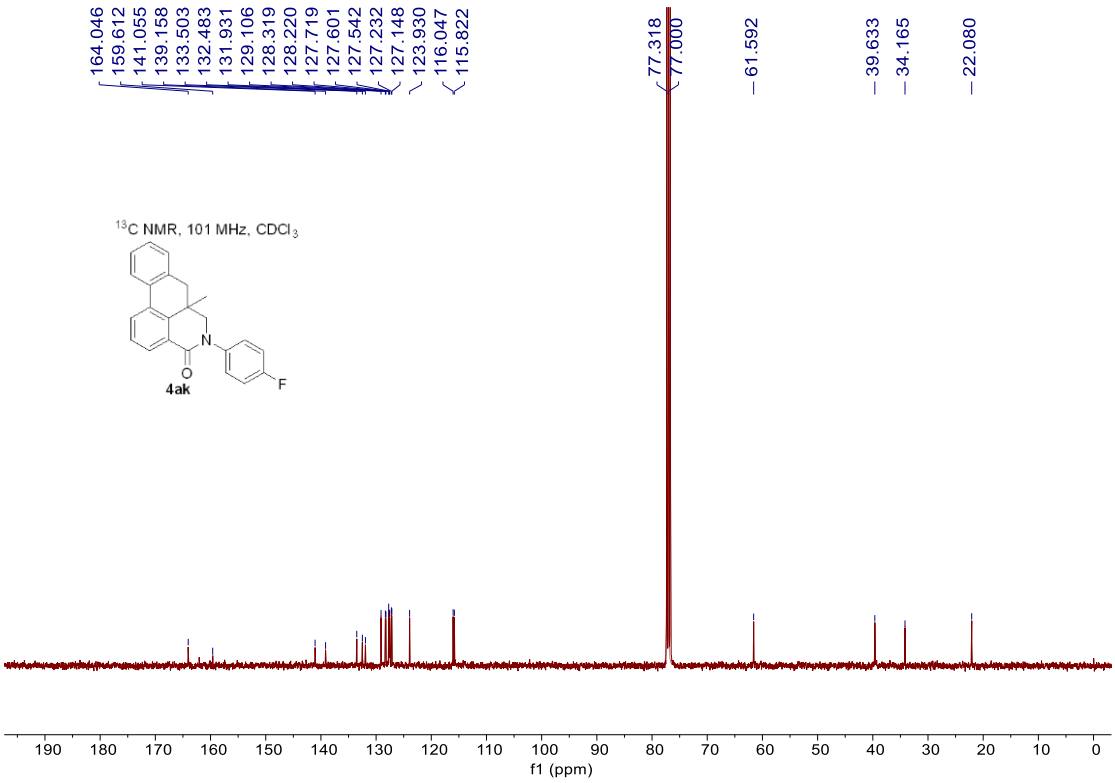
8.123
8.107
8.104
7.977
7.974
7.957
7.954
7.810
7.791
7.497
7.478
7.458
7.407
7.401
7.395
7.390
7.384
7.377
7.372
7.310
7.307
7.292
7.269
7.260
7.153
7.132
7.110
4.190
4.160
3.654
3.624
3.020
2.983
2.710
2.673
1.273
1H NMR, 400 MHz, CDCl3
4ak
1.00
1.02
1.03
6.28
2.11
2.31
1.99
3.21
f1 (ppm)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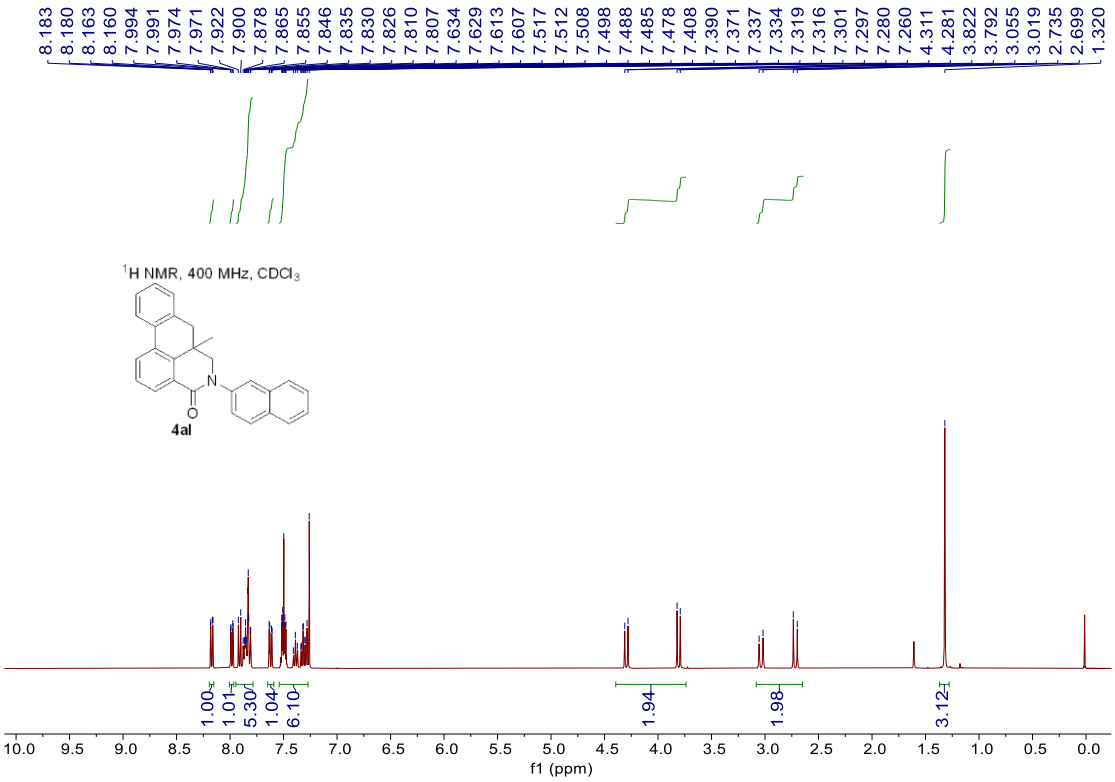
127.601
127.542
127.232
127.148
123.930
116.047
115.822
77.318
77.000
61.592
39.633
34.165
22.080
13C NMR, 101 MHz, CDCl3
4ak
f1 (ppm)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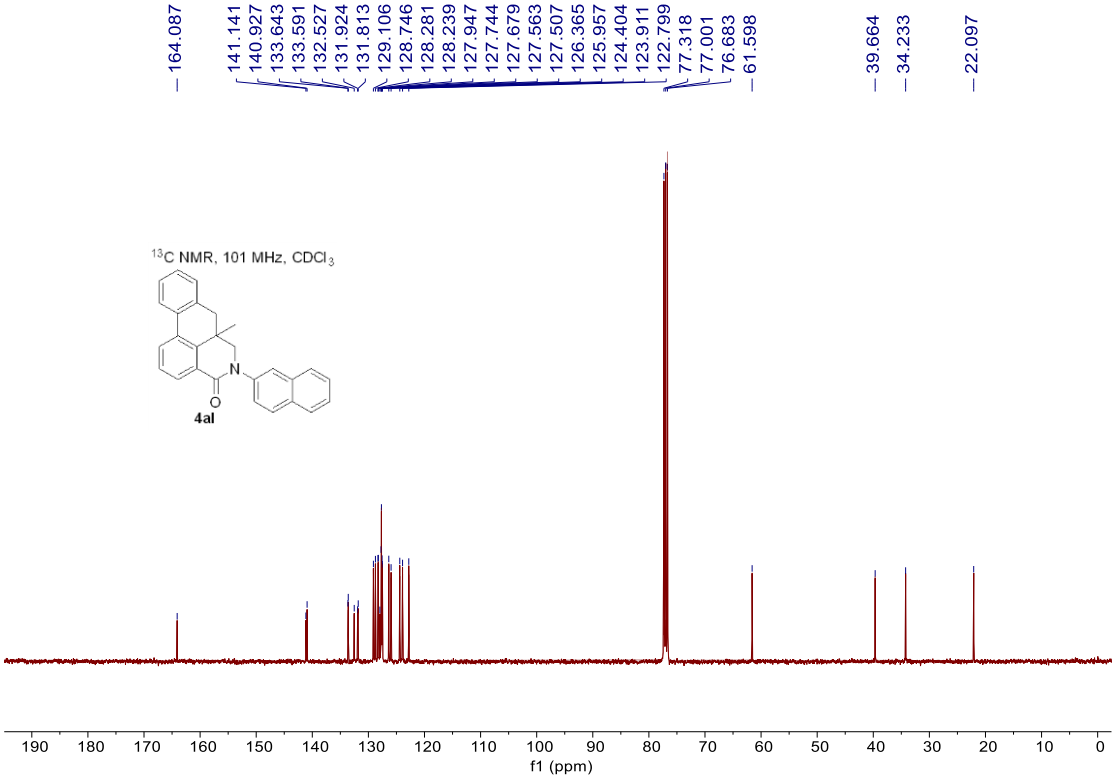
8.180
8.163
8.160
7.994
7.991
7.974
7.971
7.922
7.900
7.878
7.865
7.855
7.846
7.835
7.830
7.826
7.810
7.807
7.634
7.629
7.613
7.607
7.517
7.512
7.508
7.498
7.488
7.485
7.478
7.408
7.390
7.371
7.337
7.334
7.319
7.316
7.301
7.297
7.280
7.260
4.311
4.281
3.822
3.792
3.055
3.019
2.735
2.699
1.320
^{1}H NMR, 400 MHz, CDCl$_3$
4al
1.00
1.01
5.30
1.04
6.10
1.94
1.98
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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140.927
133.643
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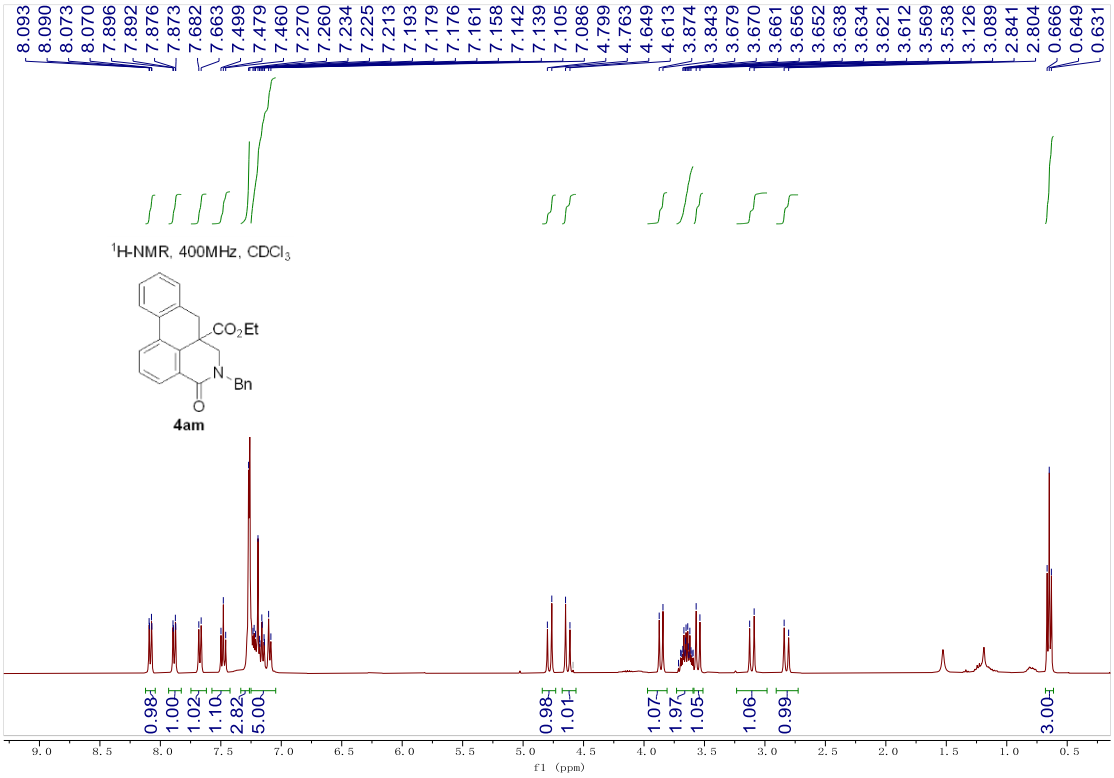
132.527
131.924
131.813
129.106
128.746
128.281
128.239
127.947
127.744
127.679
127.563
127.507
126.365
125.957
124.404
123.911
122.799
77.318
77.001
76.683
61.598
39.664
34.233
22.097
^{13}C NMR, 101 MHz, CDCl$_3$
4al
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.090
8.073
8.070
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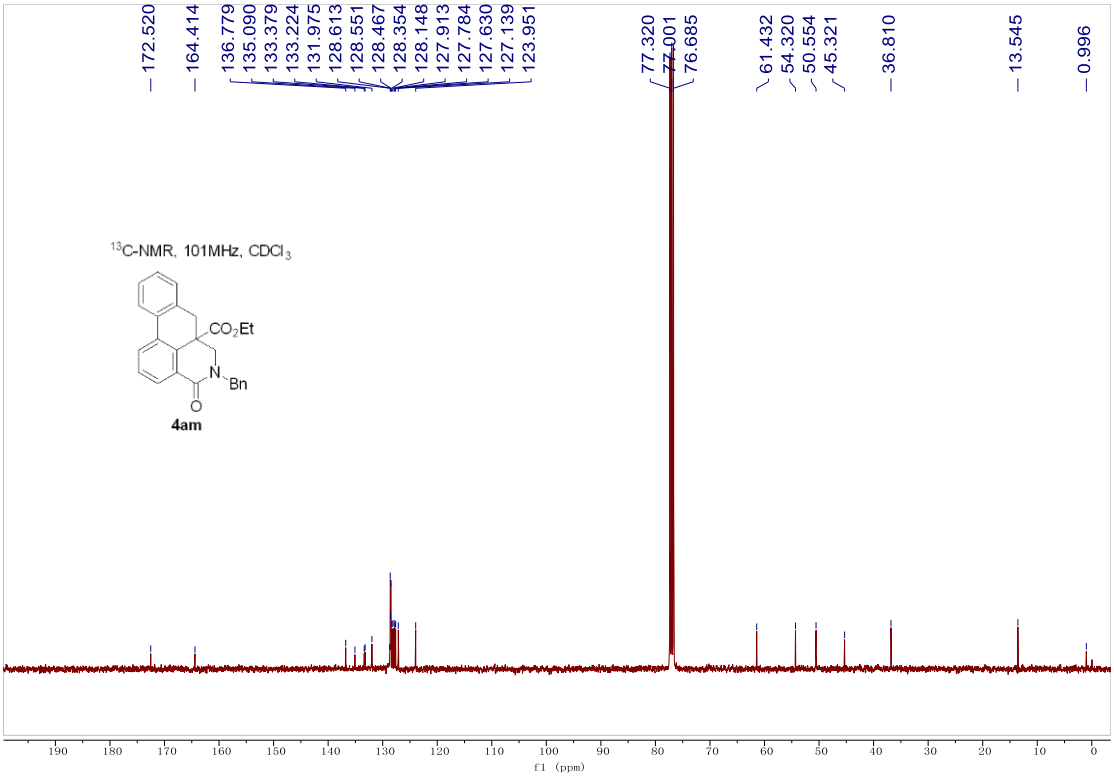
7.892
7.876
7.873
7.682
7.663
7.499
7.479
7.460
7.270
7.260
7.234
7.225
7.213
7.193
7.179
7.176
7.161
7.158
7.142
7.139
7.105
7.086
4.799
4.763
4.649
4.613
3.874
3.843
3.679
3.670
3.661
3.656
3.652
3.638
3.634
3.621
3.612
3.569
3.538
3.126
3.089
2.841
2.804
0.666
0.649
0.631
^{1}H-NMR, 400MHz, $CDCl_3$
CO_2Et
N
Bn
O
4am
0.98
1.00
1.02
1.10
2.82
5.00
0.98
1.01
1.07
1.97
1.05
1.06
0.99
3.00
f1 (ppm)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136.779
135.090
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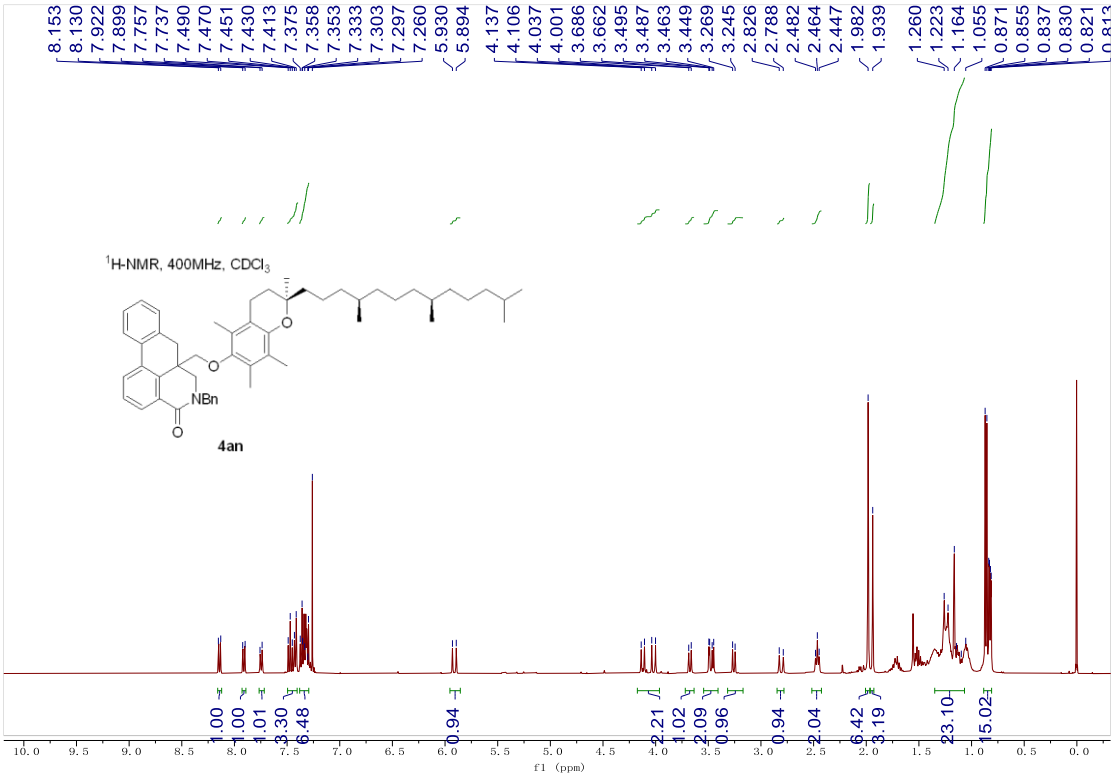
133.224
131.975
128.613
128.551
128.467
128.354
128.148
127.913
127.784
127.630
127.139
123.951
77.320
77.001
76.685
61.432
54.320
50.554
45.321
36.810
13.545
0.996
^{13}C-NMR, 101MHz, $CDCl_3$
CO_2Et
N
Bn
O
4am
f1 (ppm)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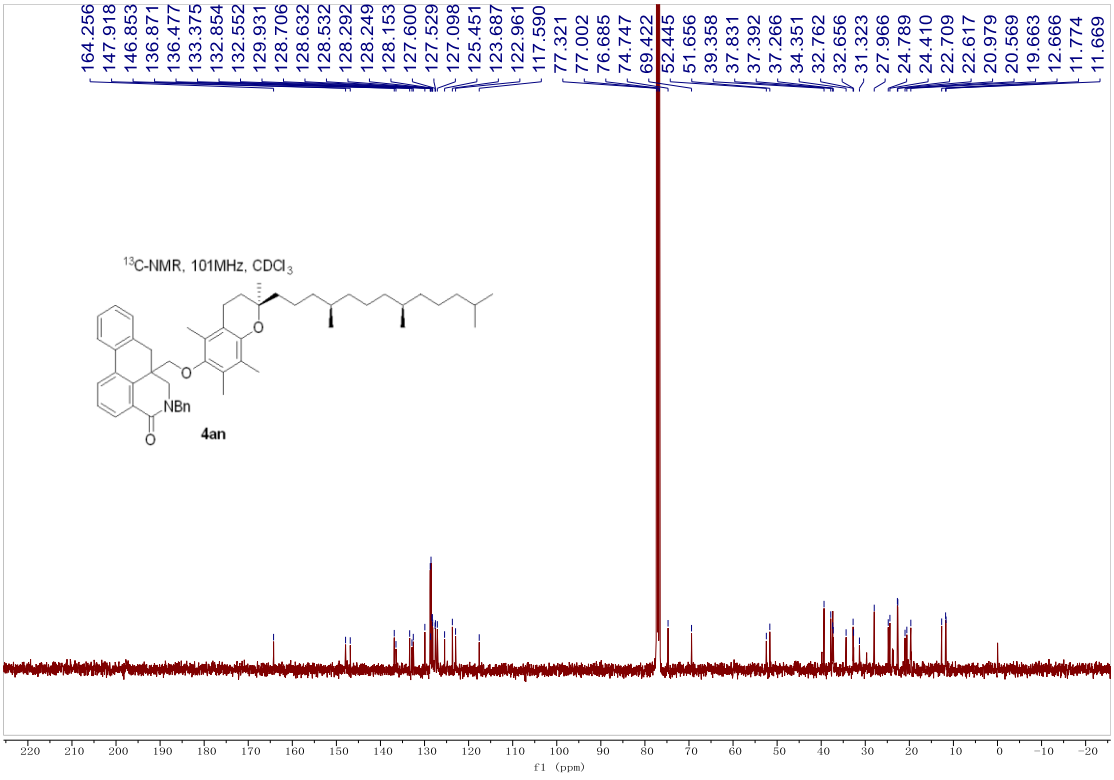
8.130
7.922
7.899
7.757
7.737
7.490
7.470
7.451
7.430
7.413
7.375
7.358
7.353
7.333
7.303
7.297
7.260
5.930
5.894
4.137
4.106
4.037
4.001
3.686
3.662
3.495
3.487
3.463
3.449
3.269
3.245
2.826
2.788
2.482
2.464
2.447
1.982
1.939
1.260
1.223
1.164
1.055
0.871
0.855
0.837
0.830
0.821
1H-NMR, 400MHz, CDCl3
NBn
4an
1.00
1.00
1.01
3.30
6.48
0.94
2.21
1.02
2.09
0.96
0.94
2.04
6.42
3.19
23.10
15.02
f1 (ppm)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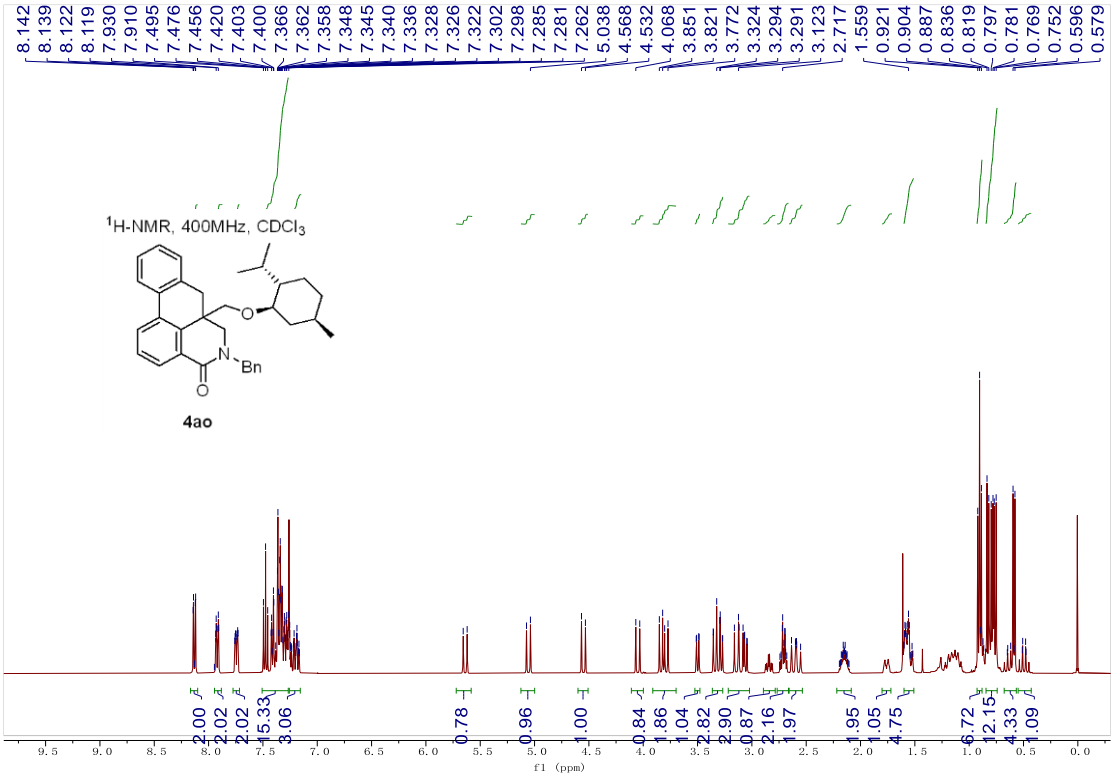
146.853
136.871
136.477
133.375
132.854
132.552
129.931
128.706
128.632
128.532
128.292
128.249
128.153
127.600
127.529
127.098
125.451
123.687
122.961
117.590
77.321
77.002
76.685
74.747
69.422
52.445
51.656
39.358
37.831
37.392
37.266
34.351
32.762
32.656
31.323
27.966
24.789
24.410
22.709
22.617
20.979
20.569
19.663
12.666
11.774
11.669
13C-NMR, 101MHz, CDCl3
NBn
4an
f1 (ppm)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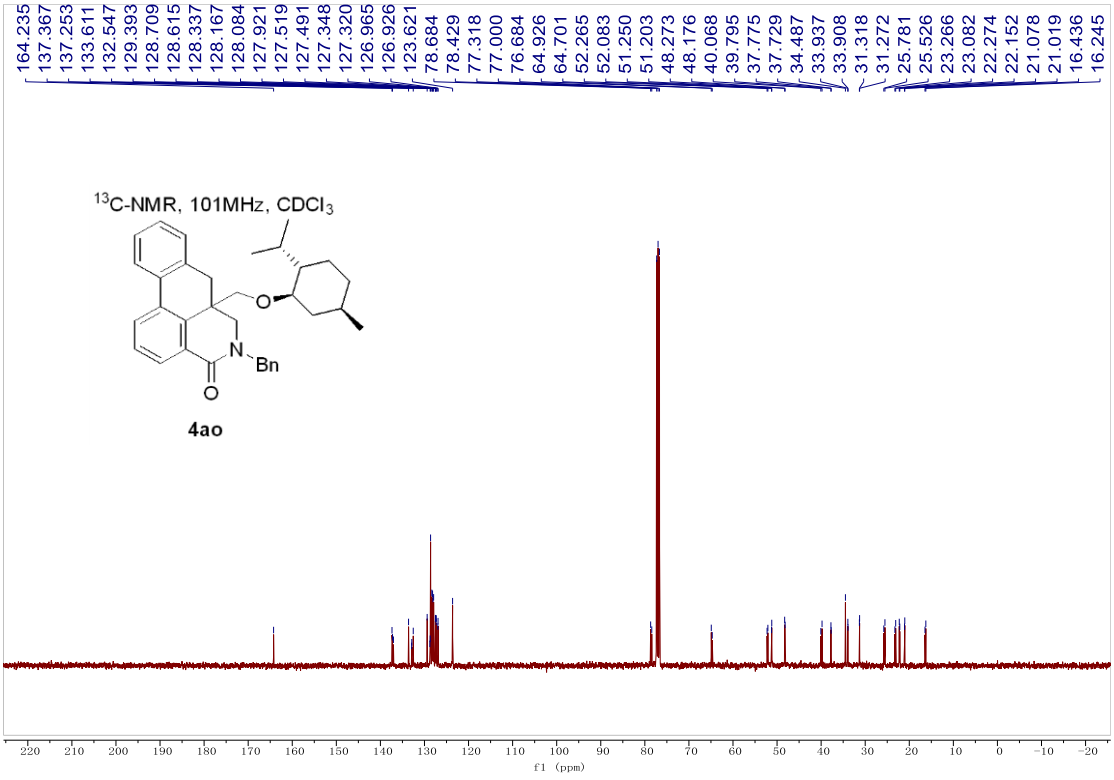
8.139
8.122
8.119
7.930
7.910
7.495
7.476
7.456
7.420
7.403
7.400
7.366
7.362
7.358
7.348
7.345
7.340
7.336
7.328
7.326
7.322
7.302
7.298
7.285
7.281
7.262
5.038
4.568
4.532
4.068
3.851
3.821
3.772
3.324
3.294
3.291
3.123
2.717
1.559
0.921
0.904
0.887
0.836
0.819
0.797
0.781
0.769
0.752
0.596
0.579
1H-NMR, 400MHz, CDCl3
Bn
4ao
2.00
2.02
2.02
15.33
3.06
0.78
0.96
1.00
0.84
1.86
1.04
2.82
2.90
0.87
2.16
1.97
1.95
1.05
4.75
6.72
12.15
4.33
1.09
f1 (ppm)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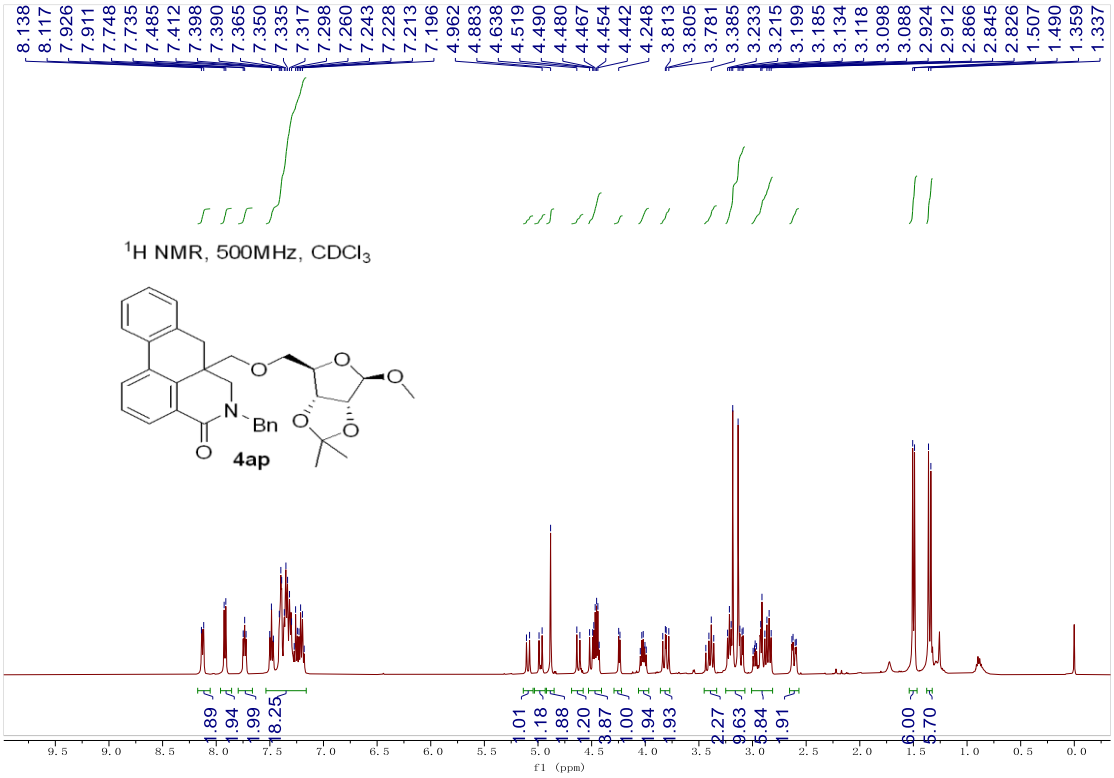
129.393
128.709
128.615
128.337
128.167
128.084
127.921
127.519
127.491
127.348
127.320
126.965
126.926
123.621
78.684
78.429
77.318
77.000
76.684
64.926
64.701
52.265
52.083
51.250
51.203
48.273
48.176
40.068
39.795
37.775
37.729
34.487
33.937
33.908
31.318
31.272
25.781
25.526
23.266
23.082
22.274
22.152
21.078
21.019
16.436
16.245
13C-NMR, 101MHz, CDCl3
Bn
4ao
f1 (ppm)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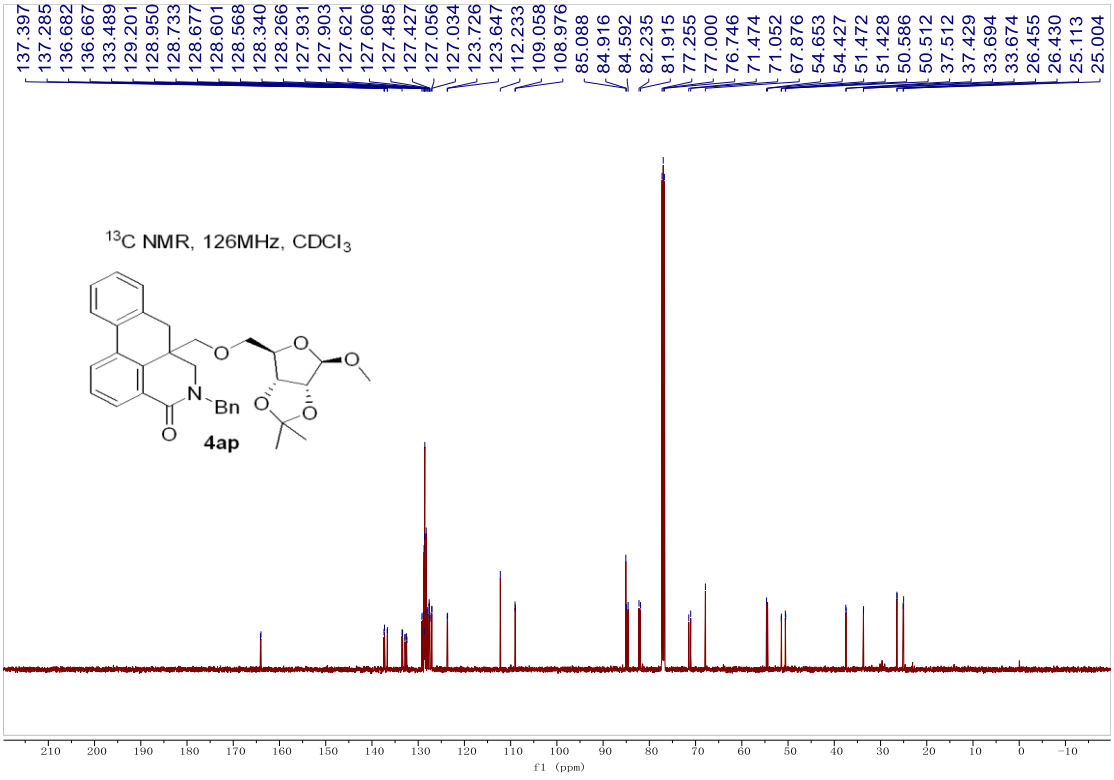
8.117
7.926
7.911
7.748
7.735
7.485
7.412
7.398
7.390
7.365
7.350
7.335
7.317
7.298
7.260
7.243
7.228
7.213
7.196
4.962
4.883
4.638
4.519
4.490
4.480
4.467
4.454
4.442
4.248
3.813
3.805
3.781
3.385
3.233
3.215
3.199
3.185
3.134
3.118
3.098
3.088
2.924
2.912
2.866
2.845
2.826
1.507
1.490
1.359
1.337
1H NMR, 500MHz, CDCl3
Bn
4ap
1.89
1.94
1.99
18.25
1.01
1.18
1.88
1.20
3.87
1.00
1.94
1.93
2.27
9.63
5.84
1.91
6.00
5.70
f1 (ppm)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136.682
136.667
133.489
129.201
128.950
128.733
128.677
128.601
128.568
128.340
128.266
127.931
127.903
127.621
127.606
127.485
127.427
127.056
127.034
123.726
123.647
112.233
109.058
108.976
85.088
84.916
84.592
82.235
81.915
77.255
77.000
76.746
71.474
71.052
67.876
54.653
54.427
51.472
51.428
50.586
50.512
37.512
37.429
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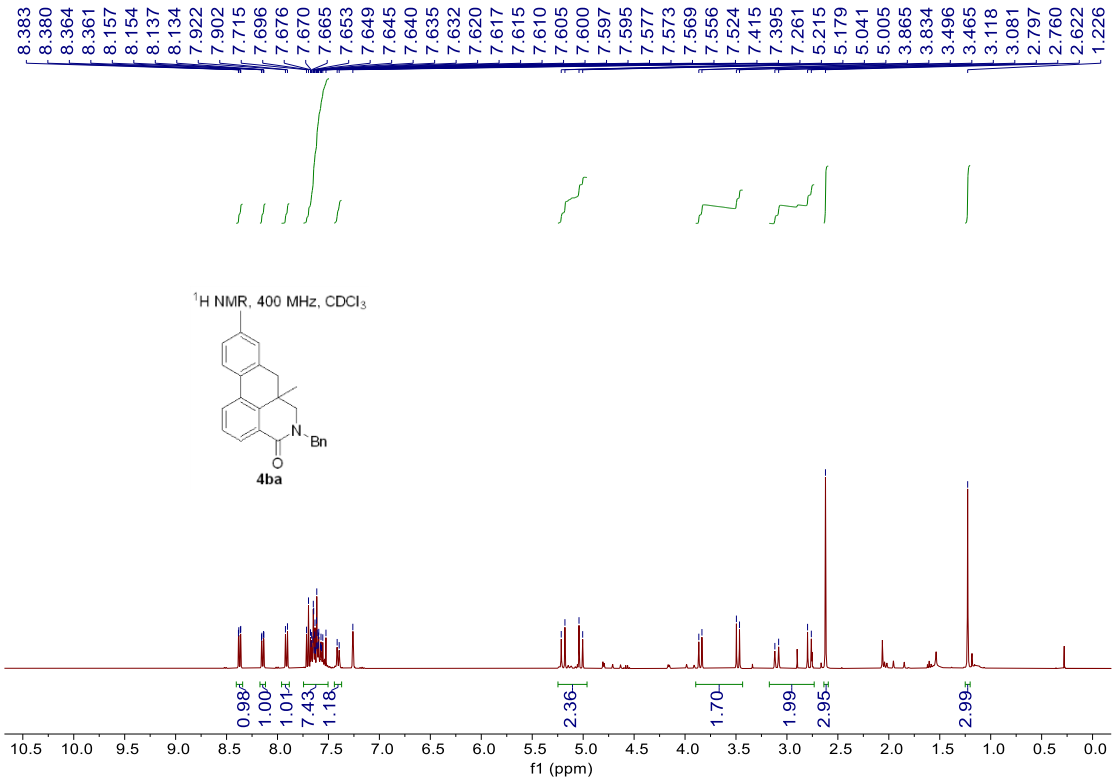
26.455
26.430
25.113
25.004
13C NMR, 126MHz, CDCl3
Bn
4ap
f1 (ppm)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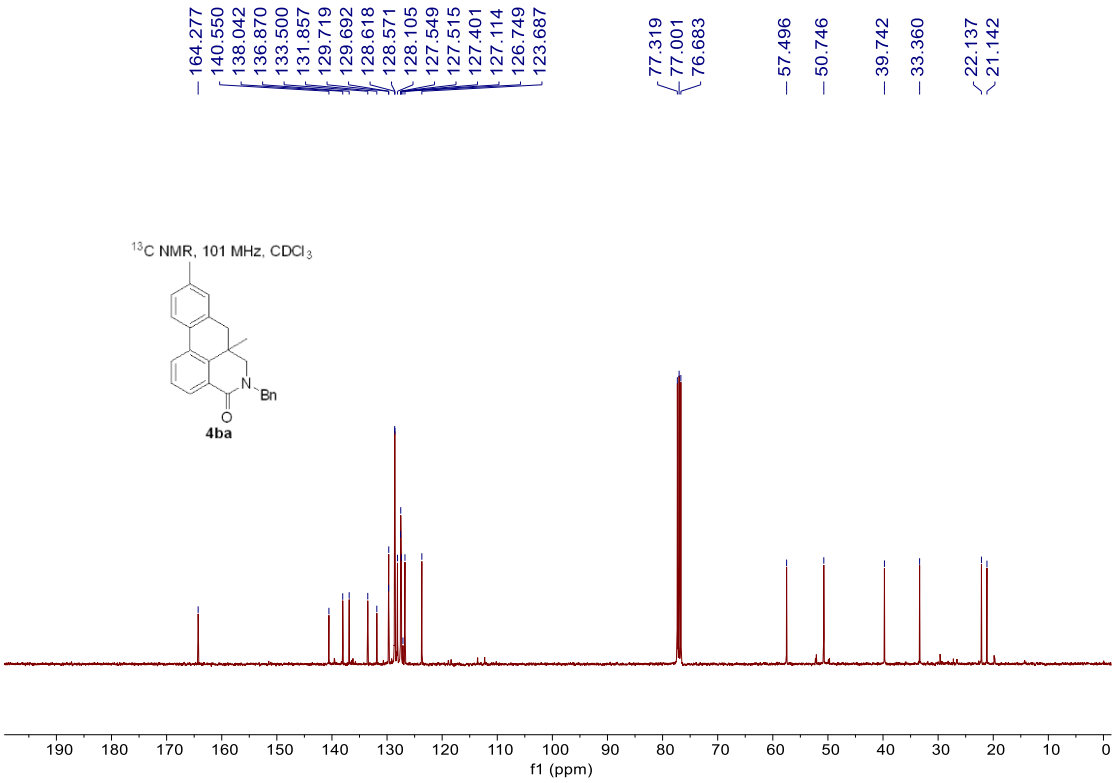
8.380
8.364
8.361
8.157
8.154
8.137
8.134
7.922
7.902
7.715
7.696
7.676
7.670
7.665
7.653
7.649
7.645
7.640
7.635
7.632
7.620
7.617
7.615
7.610
7.605
7.600
7.597
7.595
7.577
7.573
7.569
7.556
7.524
7.415
7.395
7.261
5.215
5.179
5.041
5.005
3.865
3.834
3.496
3.465
3.118
3.081
2.797
2.760
2.622
1.226
^{1}H NMR, 400 MHz, CDCl$_3$
N
Bn
O
4ba
0.98
1.00
1.01
7.43
1.18
2.36
1.70
1.99
2.95
2.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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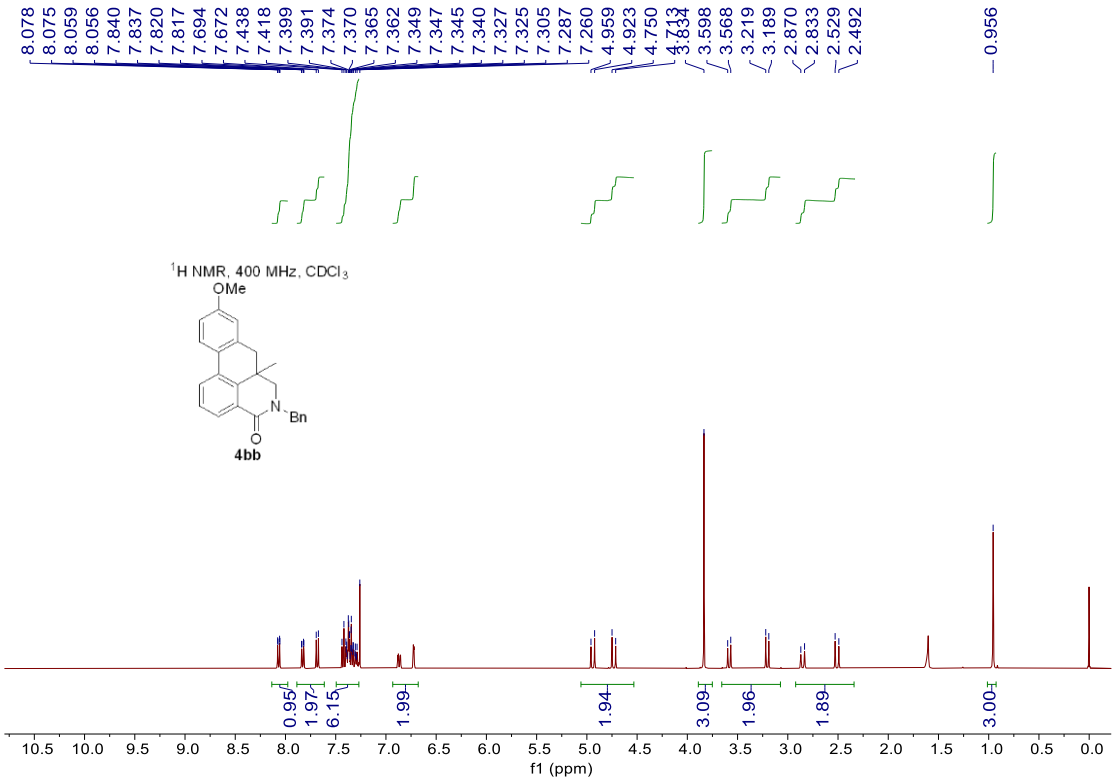
136.870
133.500
131.857
129.719
129.692
128.618
128.571
128.105
127.549
127.515
127.401
127.114
126.749
123.687
77.319
77.001
76.683
57.496
50.746
39.742
33.360
22.137
21.142
^{13}C NMR, 101 MHz, CDCl$_3$
N
Bn
O
4ba
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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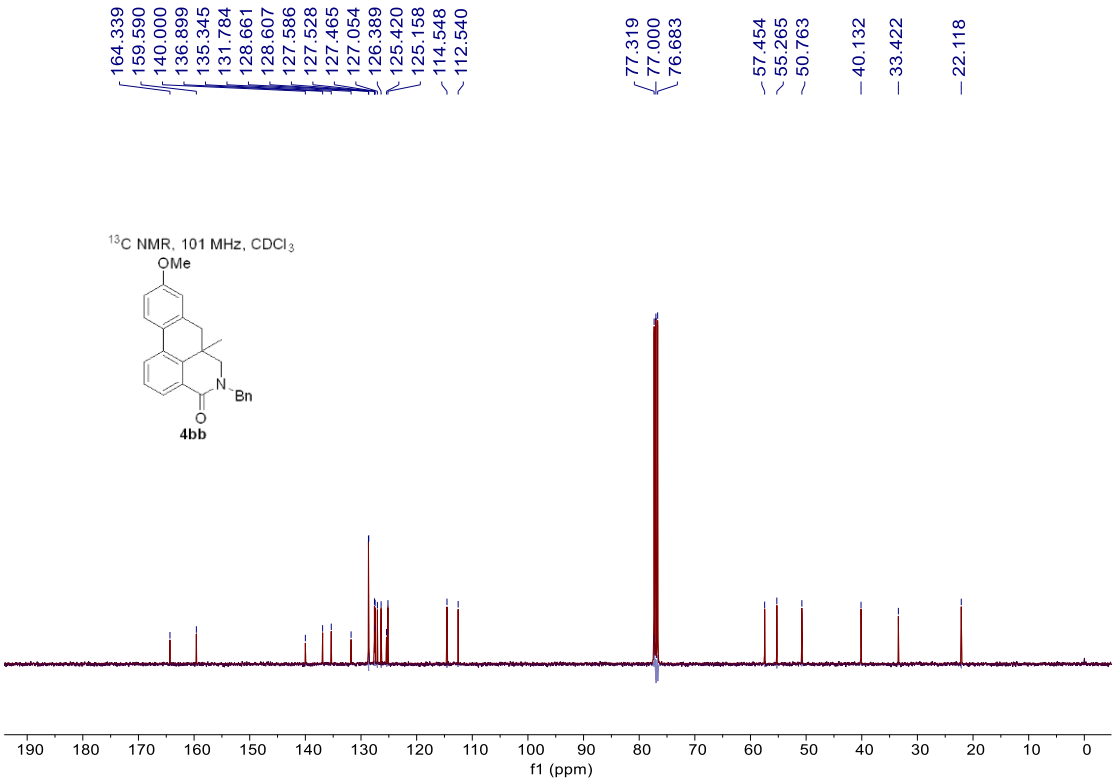
8.075
8.059
8.056
7.840
7.837
7.820
7.817
7.694
7.672
7.438
7.418
7.399
7.391
7.374
7.370
7.365
7.362
7.349
7.347
7.345
7.340
7.327
7.325
7.305
7.287
7.260
4.959
4.923
4.750
4.713
3.834
3.598
3.568
3.219
3.189
2.870
2.833
2.529
2.492
0.956
1H NMR, 400 MHz, CDCl3
OMe
N
Bn
O
4bb
0.95
1.97
6.15
1.99
1.94
3.09
1.96
1.89
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.345
131.784
128.661
128.607
127.586
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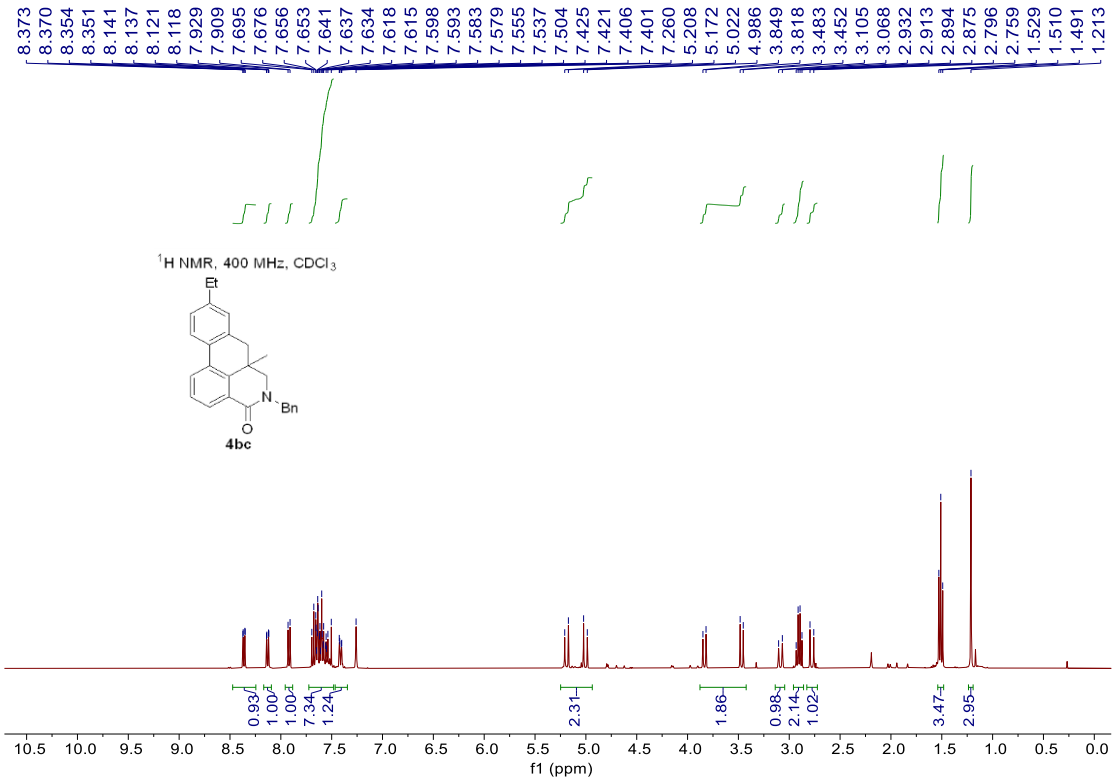
127.465
127.054
126.389
125.420
125.158
114.548
112.540
77.319
77.000
76.683
57.454
55.265
50.763
40.132
33.422
22.118
13C NMR, 101 MHz, CDCl3
OMe
N
Bn
O
4bb
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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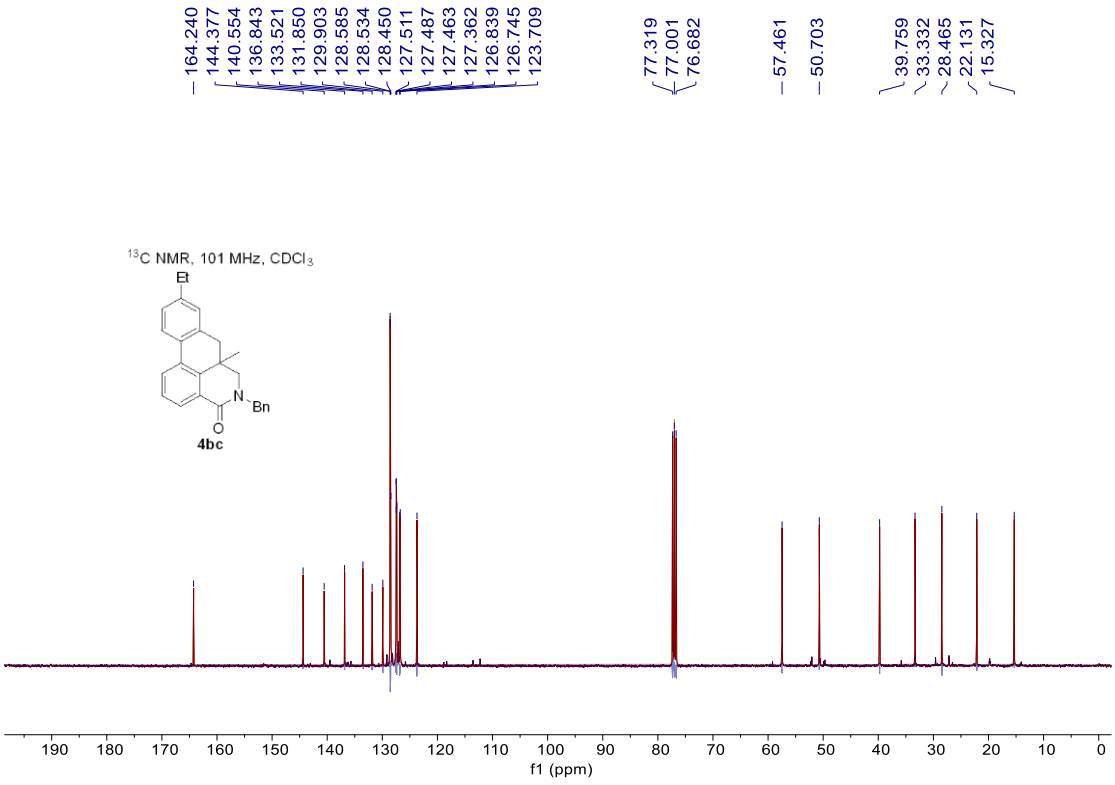
8.351
8.141
8.137
8.121
8.118
7.929
7.909
7.695
7.676
7.656
7.653
7.641
7.637
7.634
7.618
7.615
7.598
7.593
7.583
7.579
7.555
7.537
7.504
7.425
7.421
7.406
7.401
7.260
5.208
5.172
5.022
4.986
3.849
3.818
3.483
3.452
3.105
3.068
2.932
2.913
2.894
2.875
2.796
2.759
1.529
1.510
1.491
1.213
^{1}H NMR, 400 MHz, CDCl$_3$
Et
N
Bn
O
4bc
0.93
1.00
1.00
7.34
1.24
2.31
1.86
0.98
2.14
1.02
3.47
2.95
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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140.554
136.843
133.521
131.850
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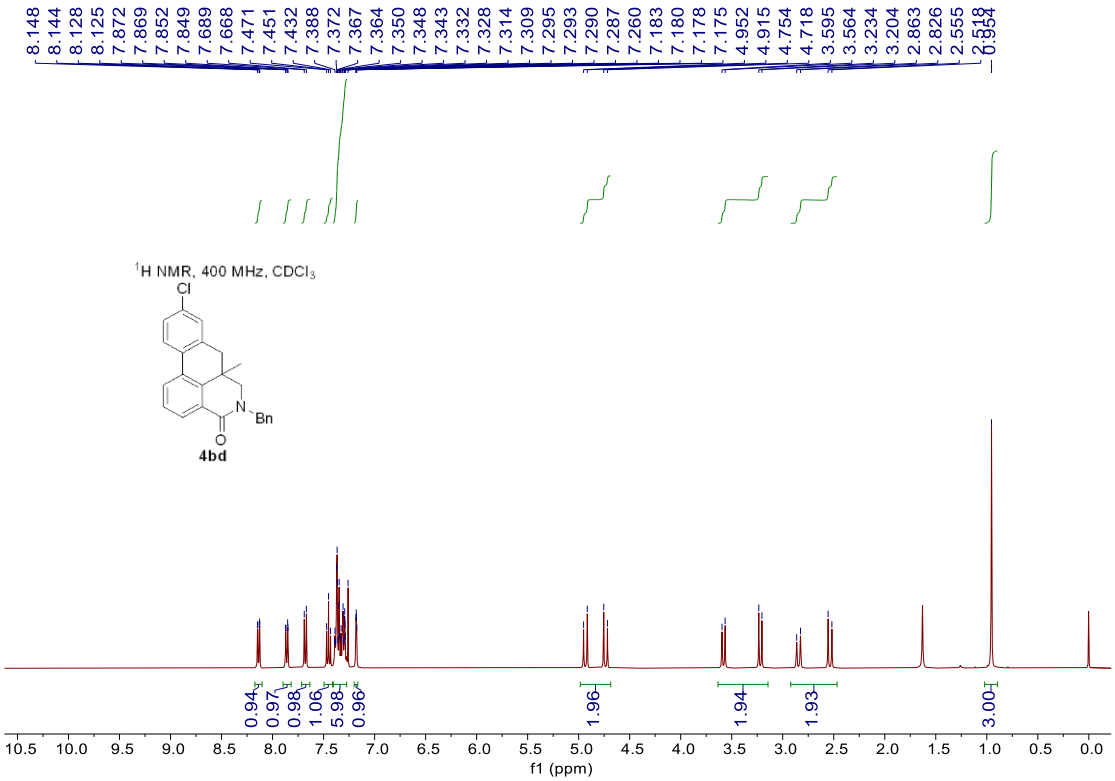
128.585
128.534
128.450
127.511
127.487
127.463
127.362
126.839
126.745
123.709
77.319
77.001
76.682
57.461
50.703
39.759
33.332
28.465
22.131
15.327
^{13}C NMR, 101 MHz, CDCl$_3$
Et
N
Bn
O
4bc
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.125
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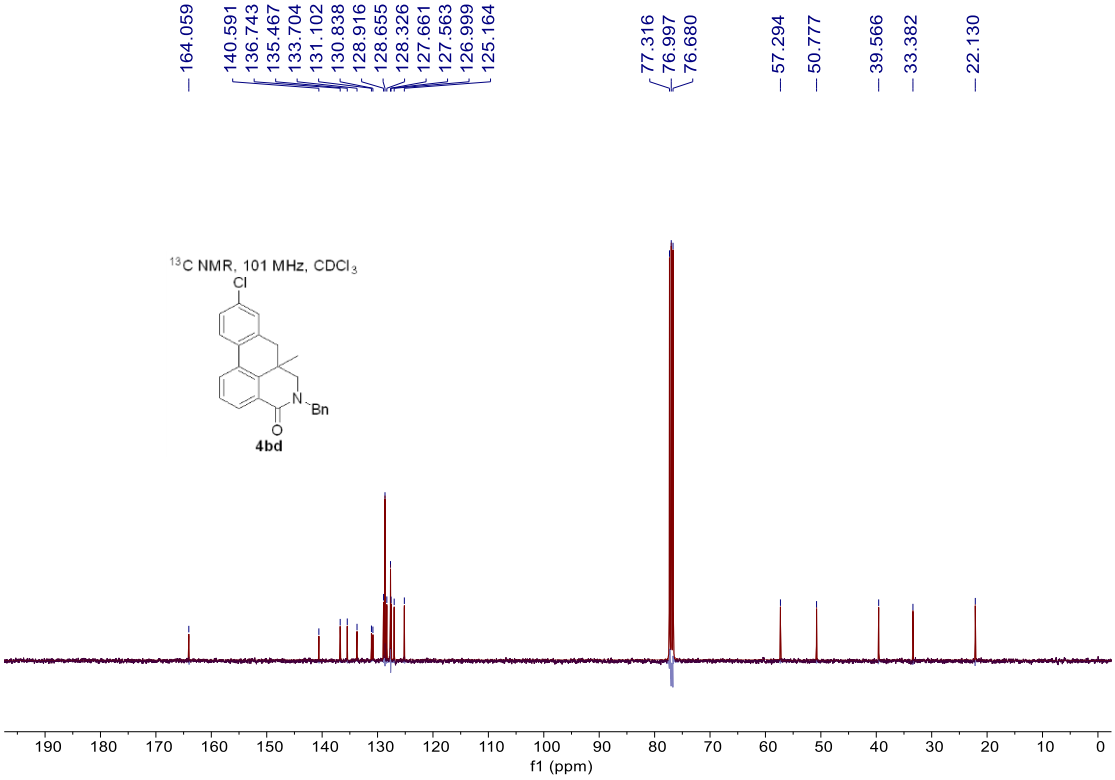
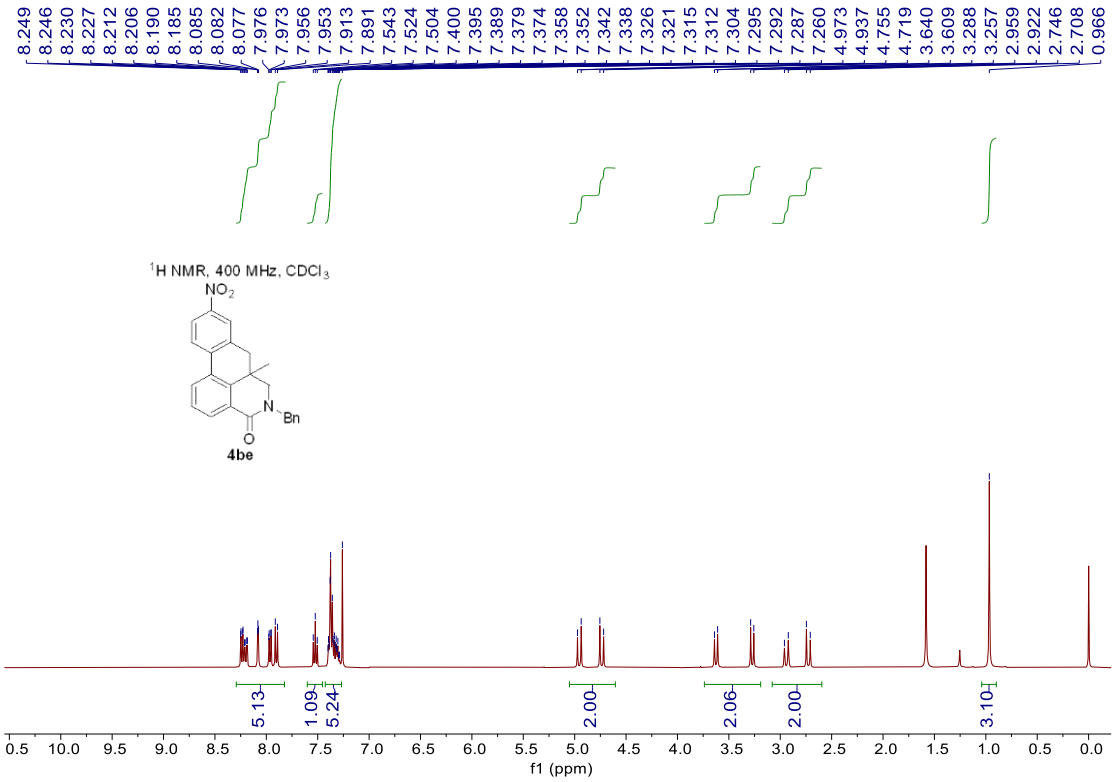
7.869
7.852
7.849
7.689
7.668
7.471
7.451
7.432
7.388
7.372
7.367
7.364
7.350
7.348
7.343
7.332
7.328
7.314
7.309
7.295
7.293
7.290
7.287
7.260
7.183
7.180
7.178
7.175
4.952
4.915
4.754
4.718
3.595
3.564
3.234
3.204
2.863
2.826
2.555
2.518
0.954
^{1}H NMR, 400 MHz, CDCl$_3$
Cl
N
Bn
O
4bd
0.94
0.97
0.98
1.06
5.98
0.96
1.96
1.94
1.93
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


164.059
140.591
136.743
135.467
133.704
131.102
130.838
128.916
128.655
128.326
127.661
127.563
126.999
125.164
77.316
76.997
76.680
57.294
50.777
39.566
33.382
22.130
^{13}C NMR, 101 MHz, CDCl$_3$
Cl
N
Bn
O
4bd
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.249
8.246
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8.190
8.185
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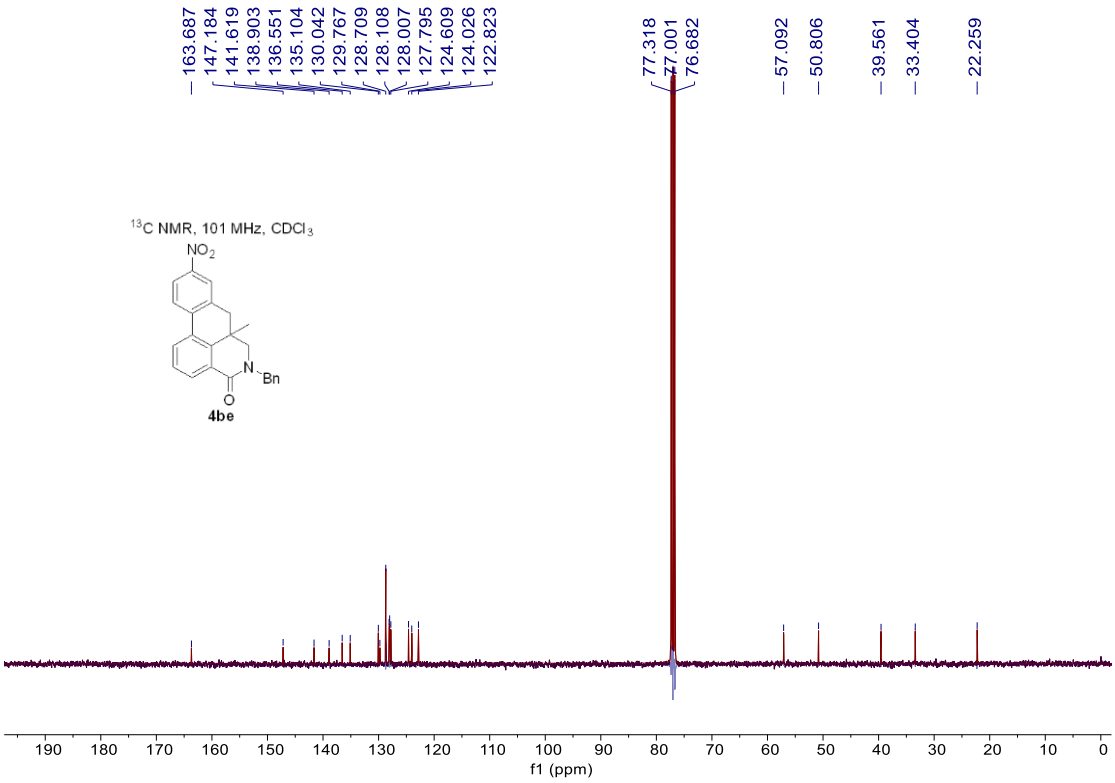
8.082
8.077
7.976
7.973
7.956
7.953
7.913
7.891
7.543
7.524
7.504
7.400
7.395
7.389
7.379
7.374
7.358
7.352
7.342
7.338
7.326
7.321
7.315
7.312
7.304
7.295
7.292
7.287
7.260
4.973
4.937
4.755
4.719
3.640
3.609
3.288
3.257
2.959
2.922
2.746
2.708
0.966
1H NMR, 400 MHz, CDCl3
NO2
N
Bn
O
4be
5.13
1.09
5.24
2.00
2.06
2.00
3.10
f1 (ppm)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135.104
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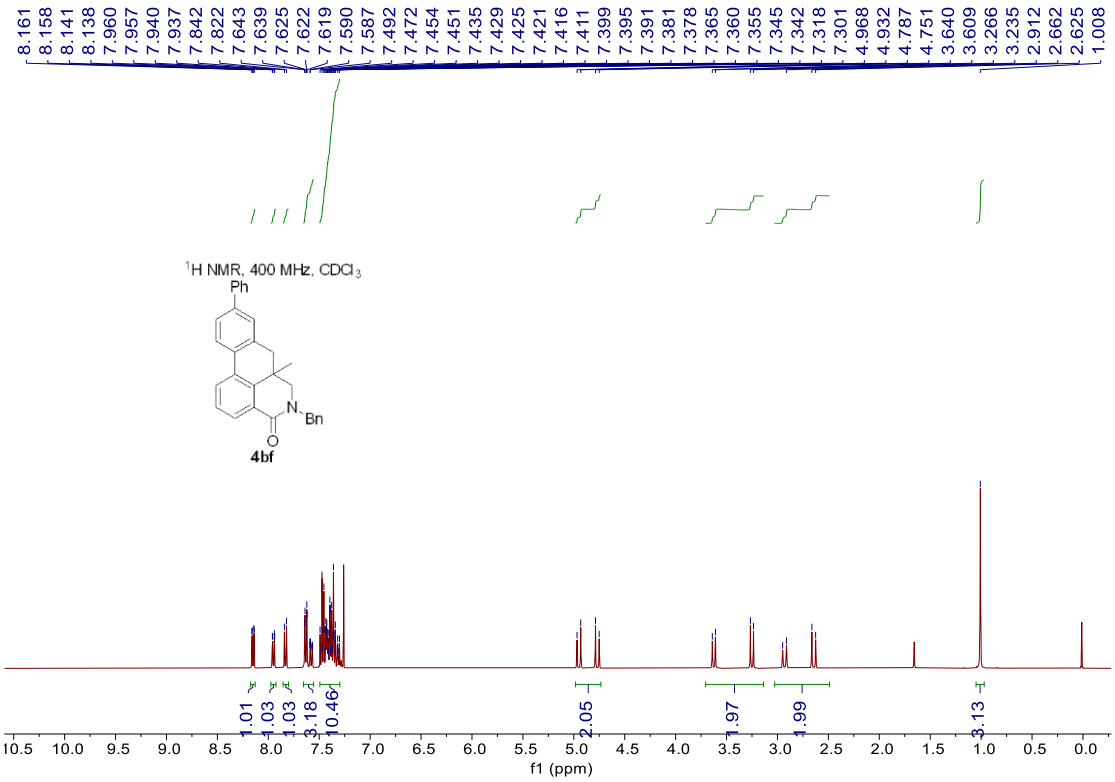
128.108
128.007
127.795
124.609
124.026
122.823
77.318
77.001
76.682
57.092
50.806
39.561
33.404
22.259
13C NMR, 101 MHz, CDCl3
NO2
N
Bn
O
4be
f1 (ppm)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8.158
8.141
8.138
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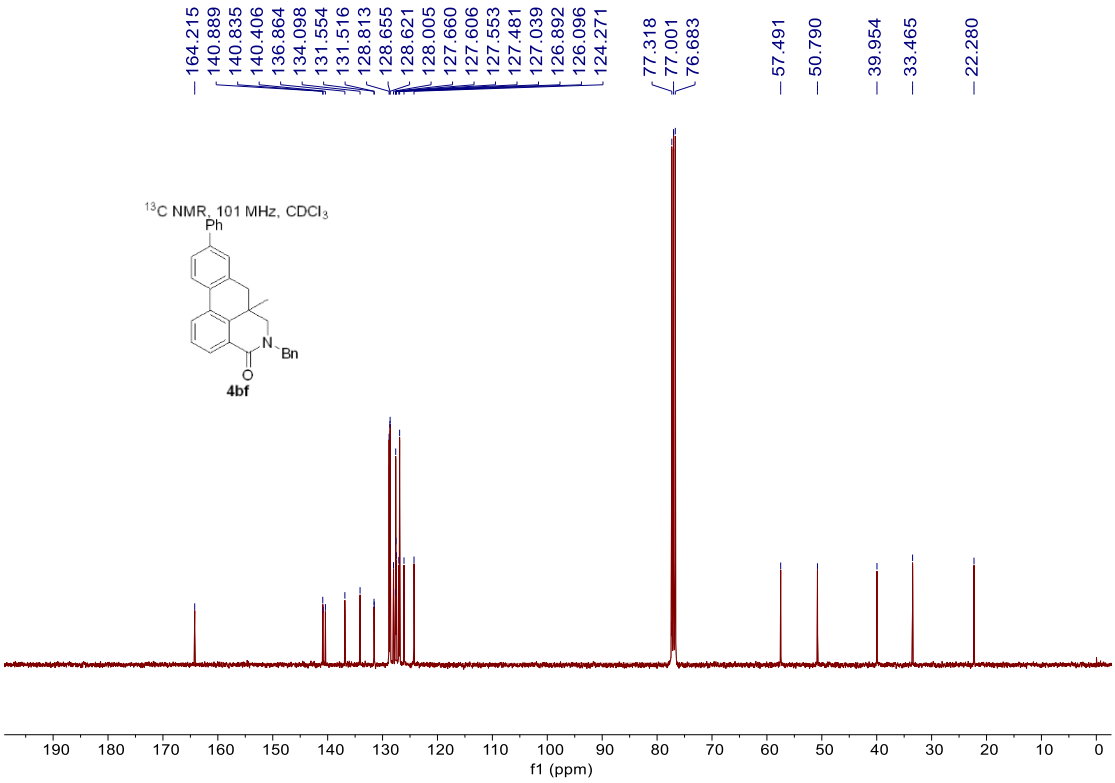
7.957
7.940
7.937
7.842
7.822
7.643
7.639
7.625
7.622
7.619
7.590
7.587
7.492
7.472
7.454
7.451
7.435
7.429
7.425
7.421
7.416
7.411
7.399
7.395
7.391
7.381
7.378
7.365
7.360
7.355
7.345
7.342
7.318
7.301
4.968
4.932
4.787
4.751
3.640
3.609
3.266
3.235
2.912
2.662
2.625
1.008
1H NMR, 400 MHz, CDCl3
Ph
N
Bn
O
4bf
1.01
1.03
1.03
3.18
10.46
2.05
1.97
1.99
3.13
f1 (ppm)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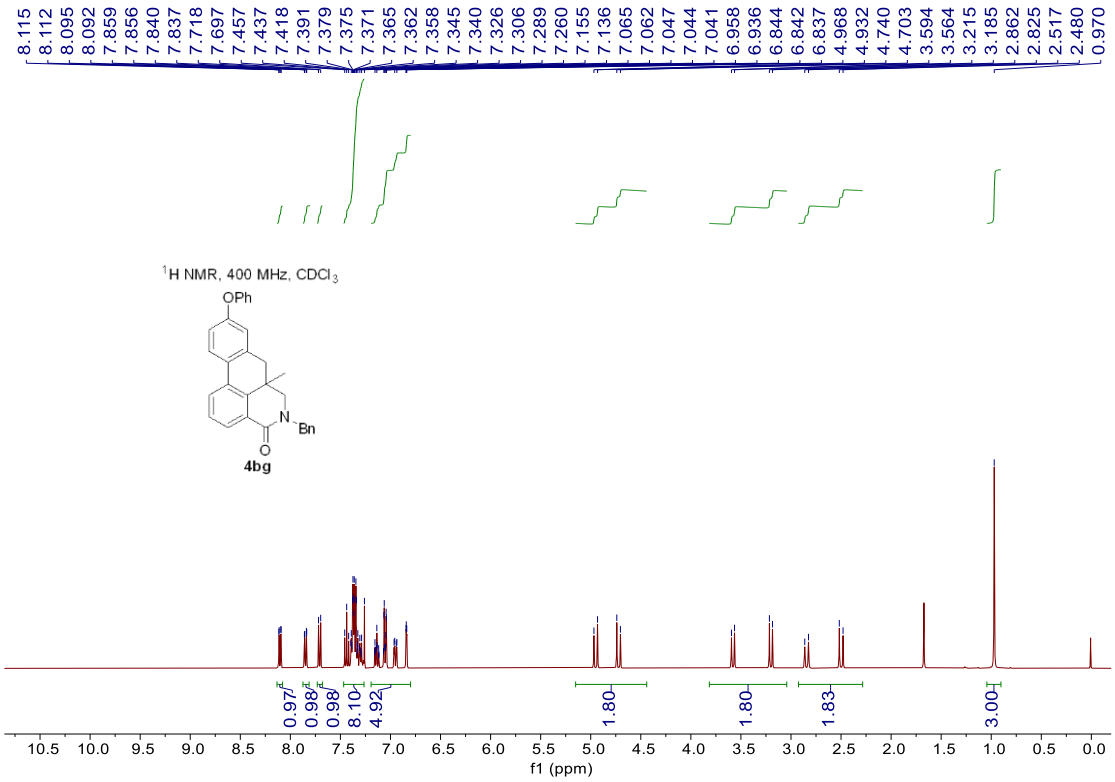
140.889
140.835
140.406
136.864
134.098
131.554
131.516
128.813
128.655
128.621
128.005
127.660
127.606
127.553
127.481
127.039
126.892
126.096
124.271
77.318
77.001
76.683
57.491
50.790
39.954
33.465
22.280
13C NMR, 101 MHz, CDCl3
Ph
N
Bn
O
4bf
f1 (ppm)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7.859
7.856
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7.837
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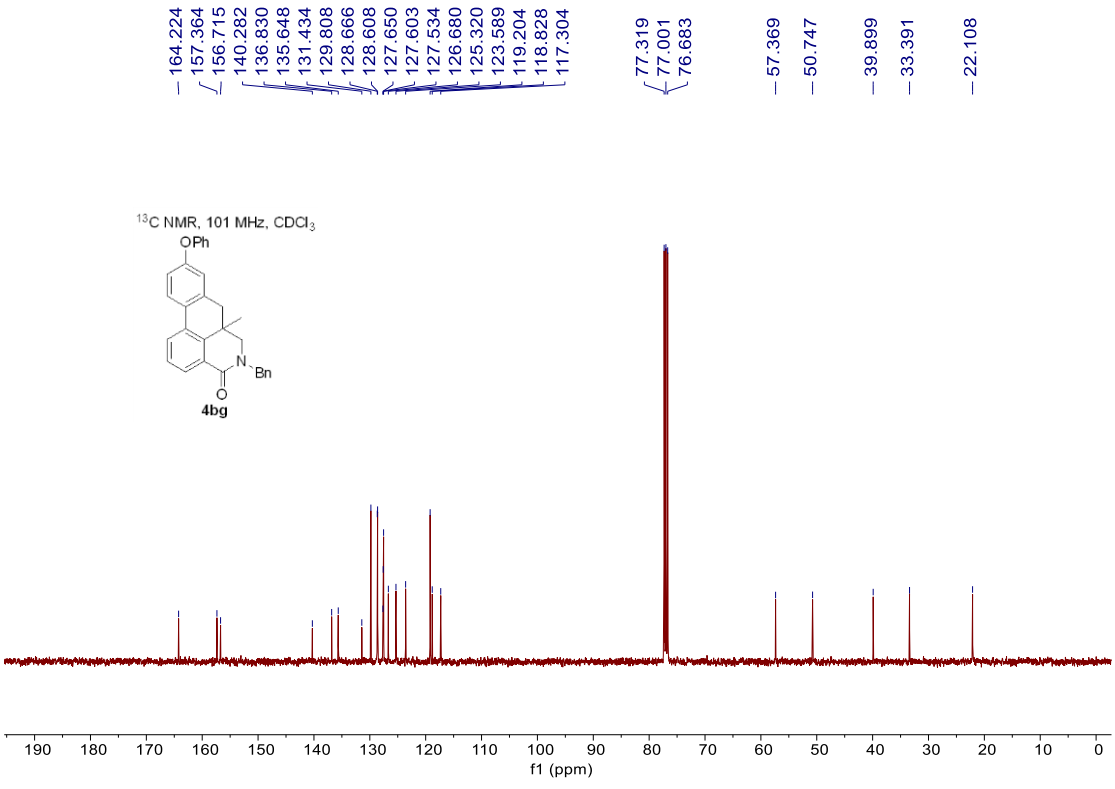
7.697
7.457
7.437
7.418
7.391
7.379
7.375
7.371
7.365
7.362
7.358
7.345
7.340
7.326
7.306
7.289
7.260
7.155
7.136
7.065
7.062
7.047
7.044
7.041
6.958
6.936
6.844
6.842
6.837
4.968
4.932
4.740
4.703
3.594
3.564
3.215
3.185
2.862
2.825
2.517
2.480
0.970
^{1}H NMR, 400 MHz, CDCl$_3$
OPh
N
Bn
O
4bg
0.97
0.98
0.98
8.10
4.92
1.80
1.80
1.83
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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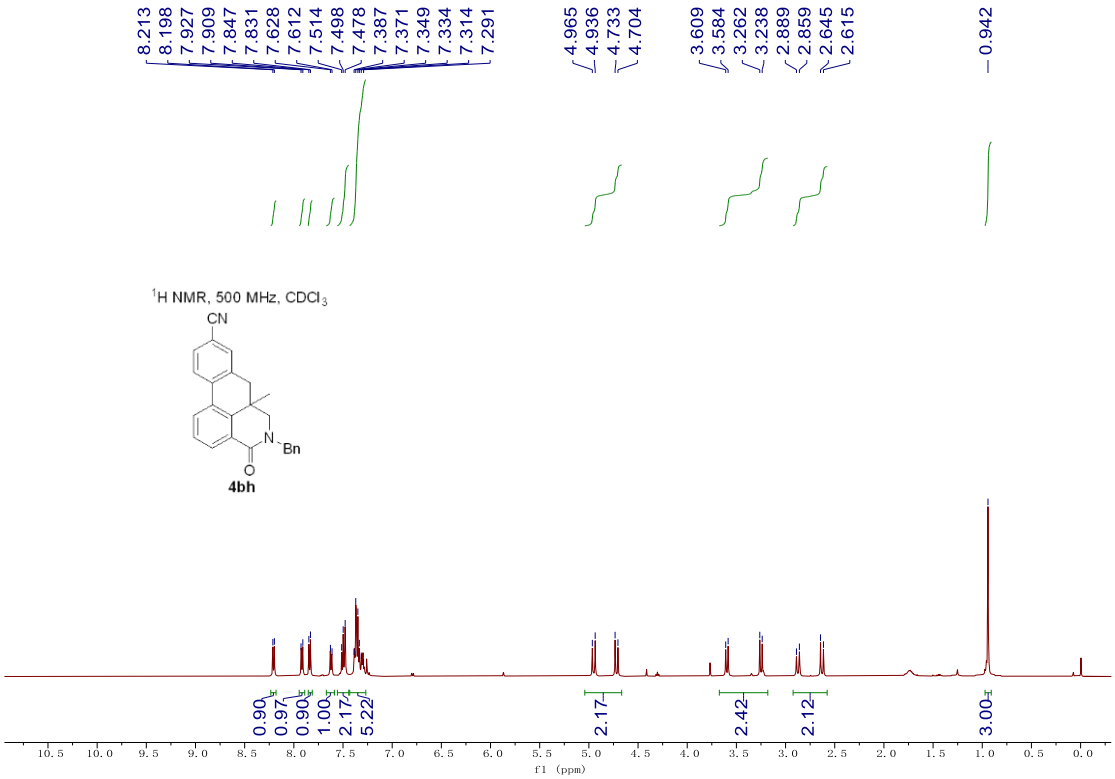
157.364
156.715
140.282
136.830
135.648
131.434
129.808
128.666
128.608
127.650
127.603
127.534
126.680
125.320
123.589
119.204
118.828
117.304
77.319
77.001
76.683
57.369
50.747
39.899
33.391
22.108
^{13}C NMR, 101 MHz, CDCl$_3$
OPh
N
Bn
O
4bg
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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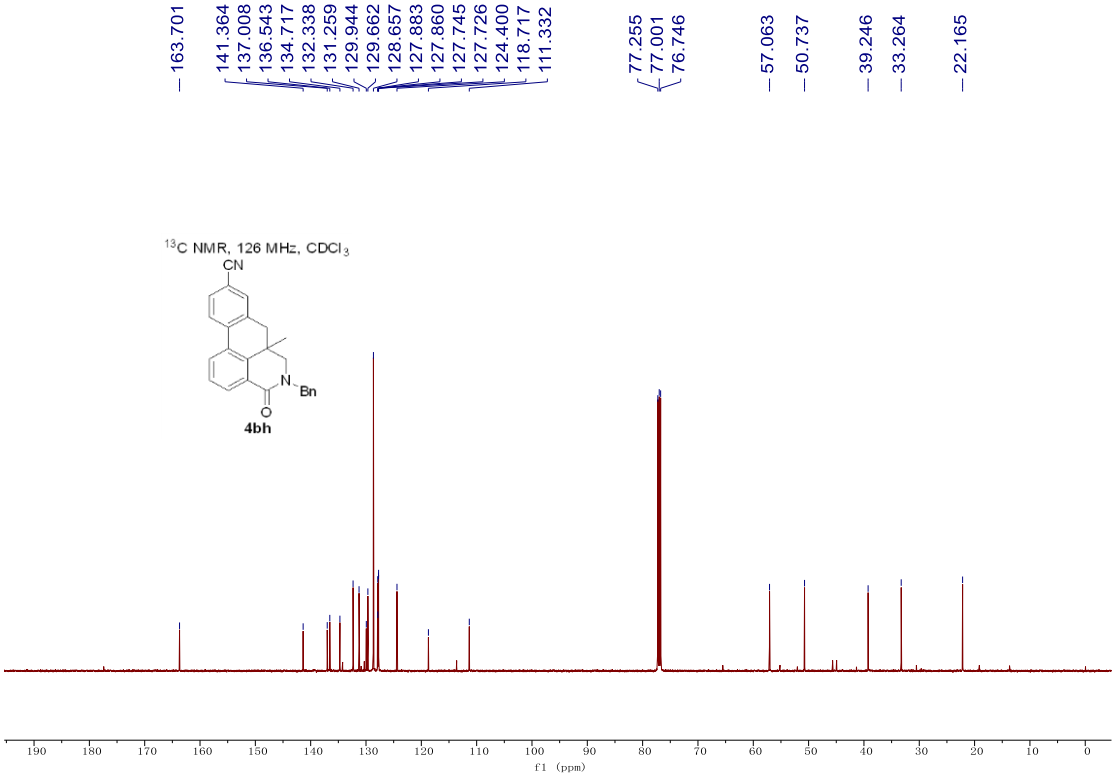
8.198
7.927
7.909
7.847
7.831
7.628
7.612
7.514
7.498
7.478
7.387
7.371
7.349
7.334
7.314
7.291
4.965
4.936
4.733
4.704
3.609
3.584
3.262
3.238
2.889
2.859
2.645
2.615
0.942
^{1}H NMR, 500 MHz, CDCl$_3$
CN
N
Bn
O
4bh
0.90
0.97
0.90
1.00
2.17
5.22
2.17
2.42
2.12
3.00
f1 (ppm)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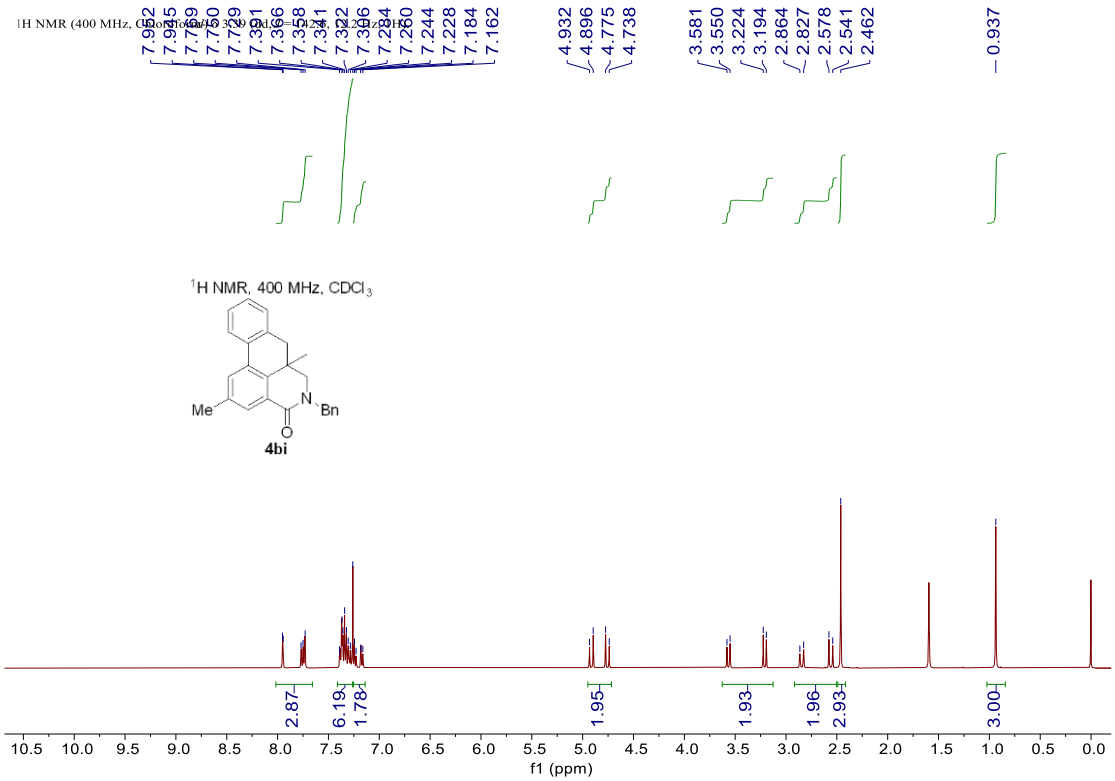
141.364
137.008
136.543
134.717
132.338
131.259
129.944
129.662
128.657
127.883
127.860
127.745
127.726
124.400
118.717
111.332
77.255
77.001
76.746
57.063
50.737
39.246
33.264
22.165
^{13}C NMR, 126 MHz, CDCl$_3$
CN
N
Bn
O
4bh
f1 (ppm)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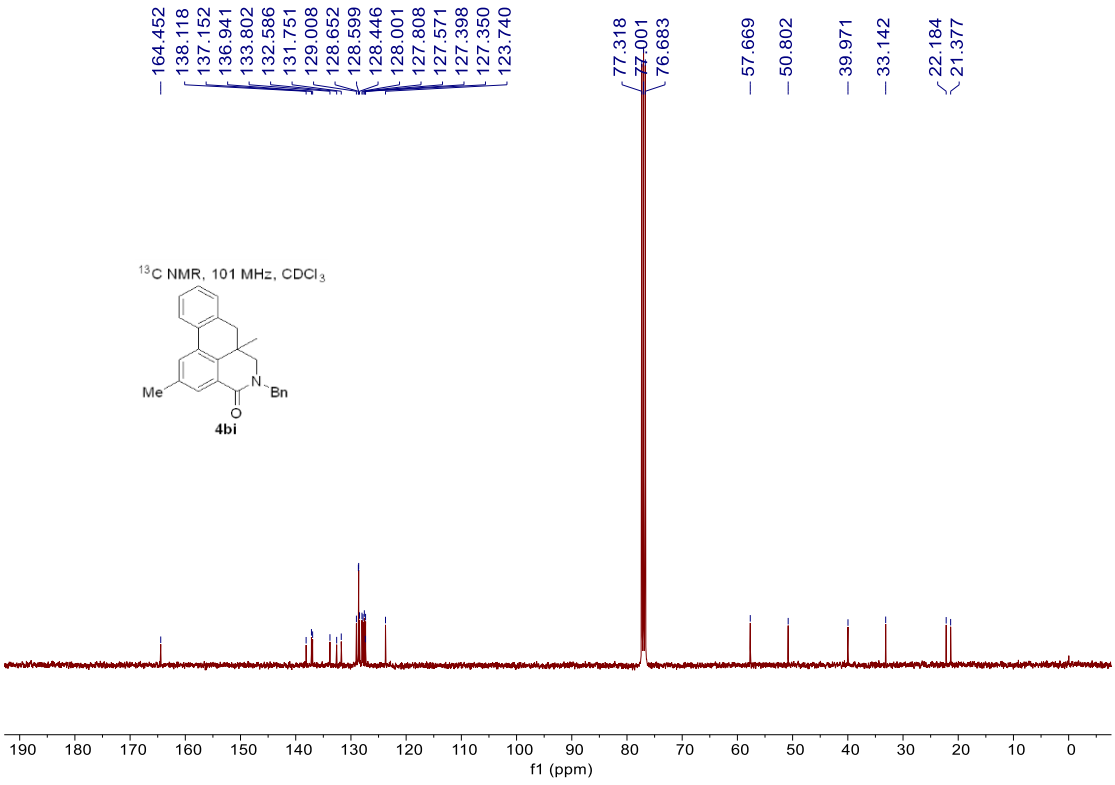
7.951
7.769
7.750
7.749
7.366
7.321
7.322
7.316
7.284
7.260
7.244
7.228
7.184
7.162
4.932
4.896
4.775
4.738
3.581
3.550
3.224
3.194
2.864
2.827
2.578
2.541
2.462
0.937
1H NMR, 400 MHz, CDCl3
Me
N
Bn
O
4bi
2.87
6.19
1.78
1.95
1.93
1.96
2.93
3.00
f1 (ppm)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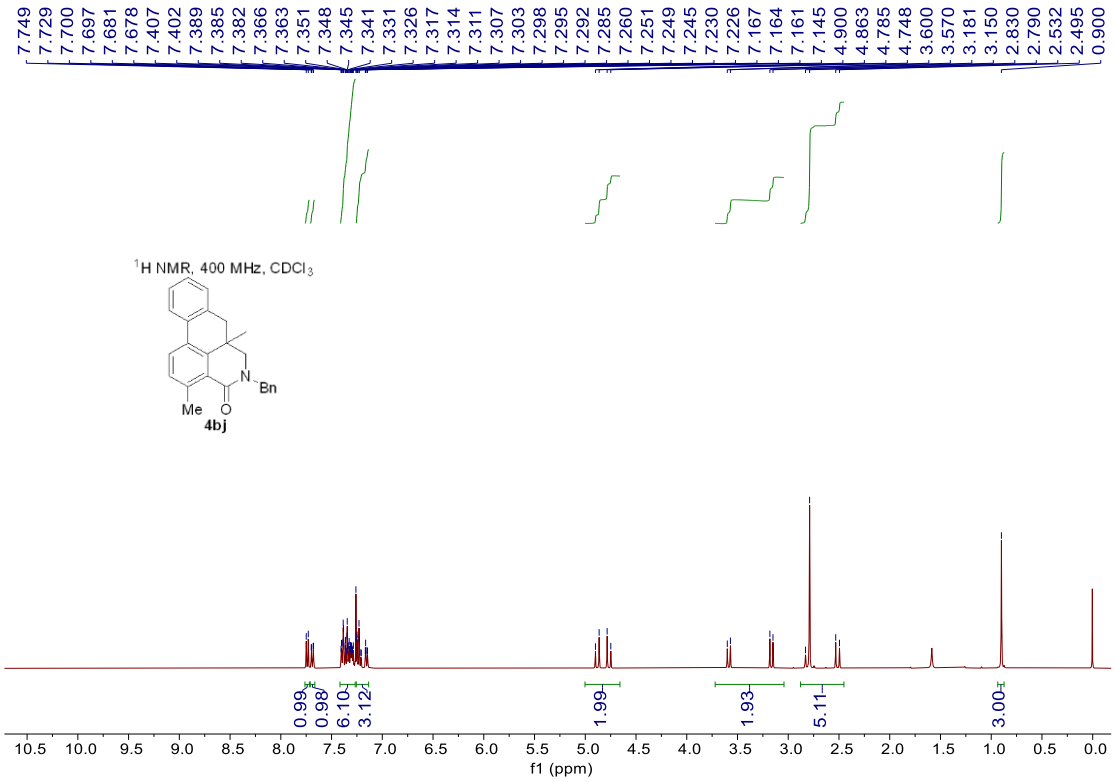
138.118
137.152
136.941
133.802
132.586
131.751
129.008
128.652
128.599
128.446
128.001
127.808
127.571
127.398
127.350
123.740
77.318
77.001
76.683
57.669
50.802
39.971
33.142
22.184
21.377
13C NMR, 101 MHz, CDCl3
Me
N
Bn
O
4bi
f1 (ppm)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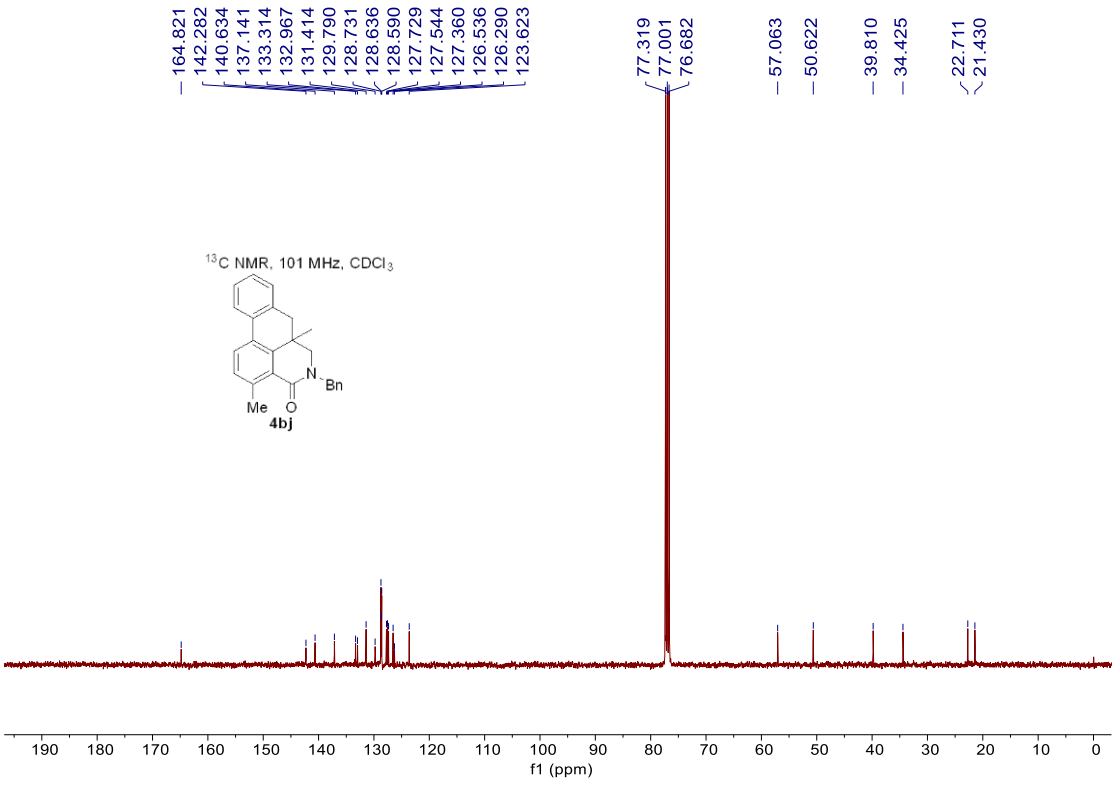
7.729
7.700
7.697
7.681
7.678
7.407
7.402
7.389
7.385
7.382
7.366
7.363
7.351
7.348
7.345
7.341
7.331
7.326
7.317
7.314
7.311
7.307
7.303
7.298
7.295
7.292
7.285
7.260
7.251
7.249
7.245
7.230
7.226
7.167
7.164
7.161
7.145
4.900
4.863
4.785
4.748
3.600
3.570
3.181
3.150
2.830
2.790
2.532
2.495
0.900
1H NMR, 400 MHz, CDCl3
N
Bn
Me
O
4bj
0.99
0.98
6.10
3.12
1.99
1.93
5.11
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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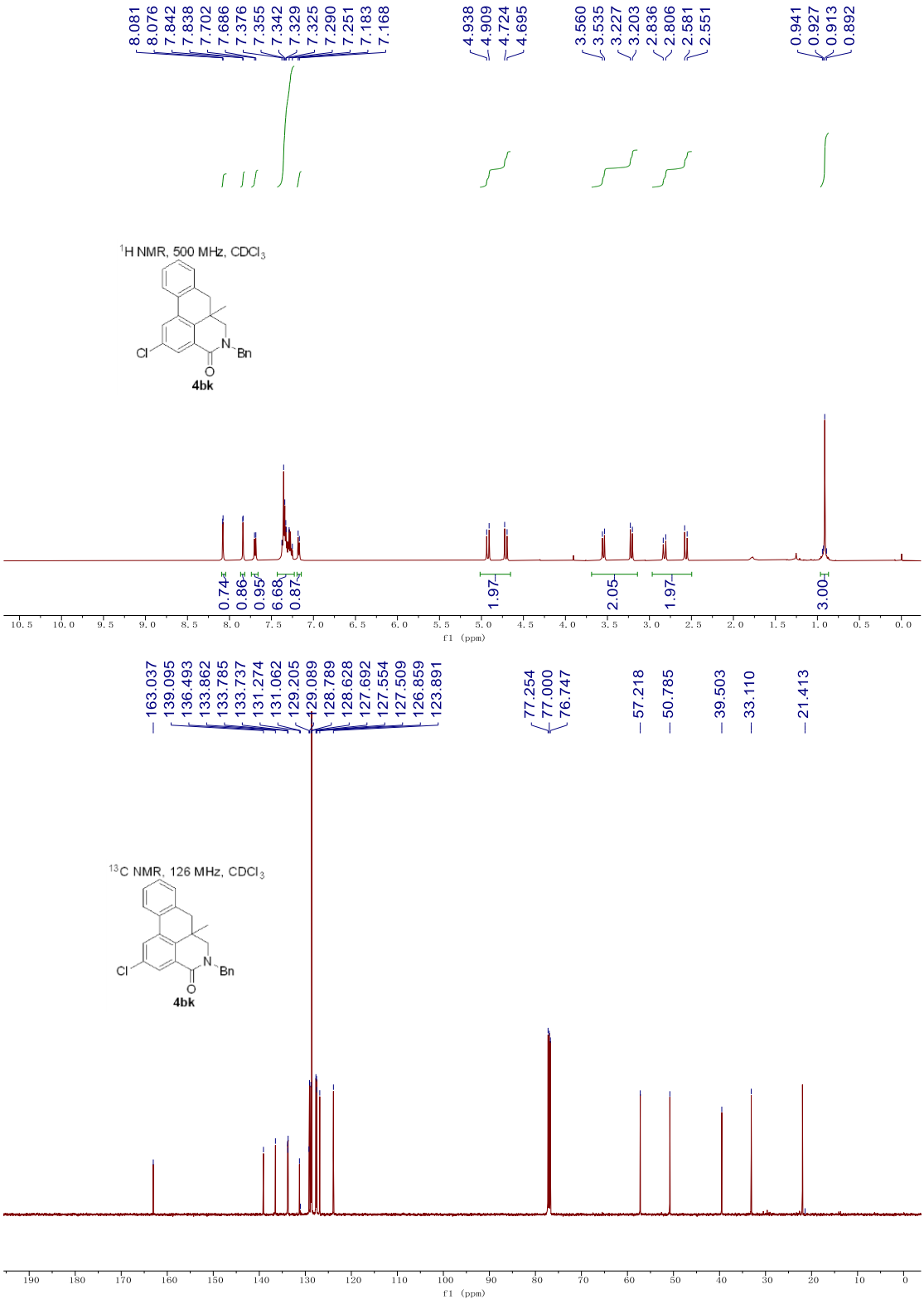
142.282
140.634
137.141
133.314
132.967
131.414
129.790
128.731
128.636
128.590
127.729
127.544
127.360
126.536
126.290
123.623
77.319
77.001
76.682
57.063
50.622
39.810
34.425
22.711
21.430
13C NMR, 101 MHz, CDCl3
N
Bn
Me
O
4bj
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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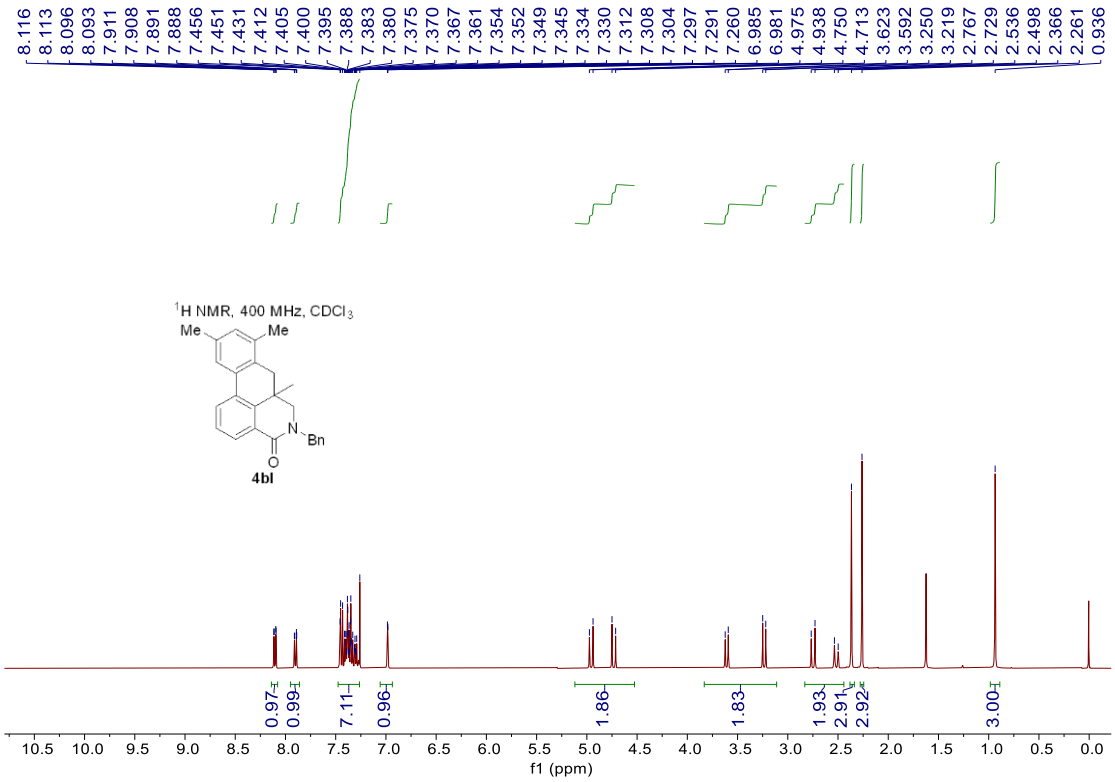
7.842
7.838
7.702
7.686
7.376
7.355
7.342
7.329
7.325
7.290
7.251
7.183
7.168
4.938
4.909
4.724
4.695
3.560
3.535
3.227
3.203
2.836
2.806
2.581
2.551
0.941
0.927
0.913
0.892
^{1}H NMR, 500 MHz, CDCl$_3$
Cl
N
Bn
O
4bk
0.74
0.86
0.95
6.68
0.87
1.97
2.05
1.97
3.00
f1 (ppm)
163.037
139.095
136.493
133.862
133.785
133.737
131.274
131.062
129.205
129.089
128.789
128.628
127.692
127.554
127.509
126.859
123.891
77.254
77.000
76.747
57.218
50.785
39.503
33.110
21.413
^{13}C NMR, 126 MHz, CDCl$_3$
Cl
N
Bn
O
4bk
f1 (ppm)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7.891
7.888
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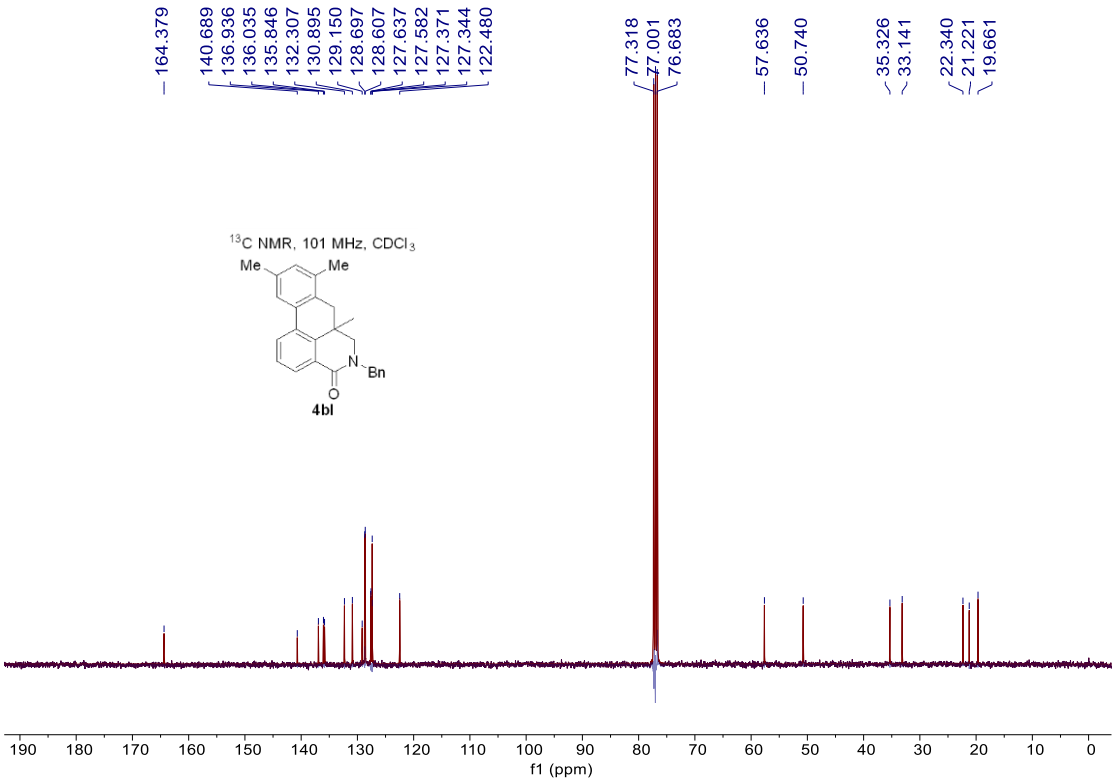
7.451
7.431
7.412
7.405
7.400
7.395
7.388
7.383
7.380
7.375
7.370
7.367
7.361
7.354
7.352
7.349
7.345
7.334
7.330
7.312
7.308
7.304
7.297
7.291
7.260
6.985
6.981
4.975
4.938
4.750
4.713
3.623
3.592
3.250
3.219
2.767
2.729
2.536
2.498
2.366
2.261
0.936
^{1}H NMR, 400 MHz, CDCl$_3$
Me
Me
N
Bn
O
4bl
0.97
0.99
7.11
0.96
1.86
1.83
1.93
2.91
2.92
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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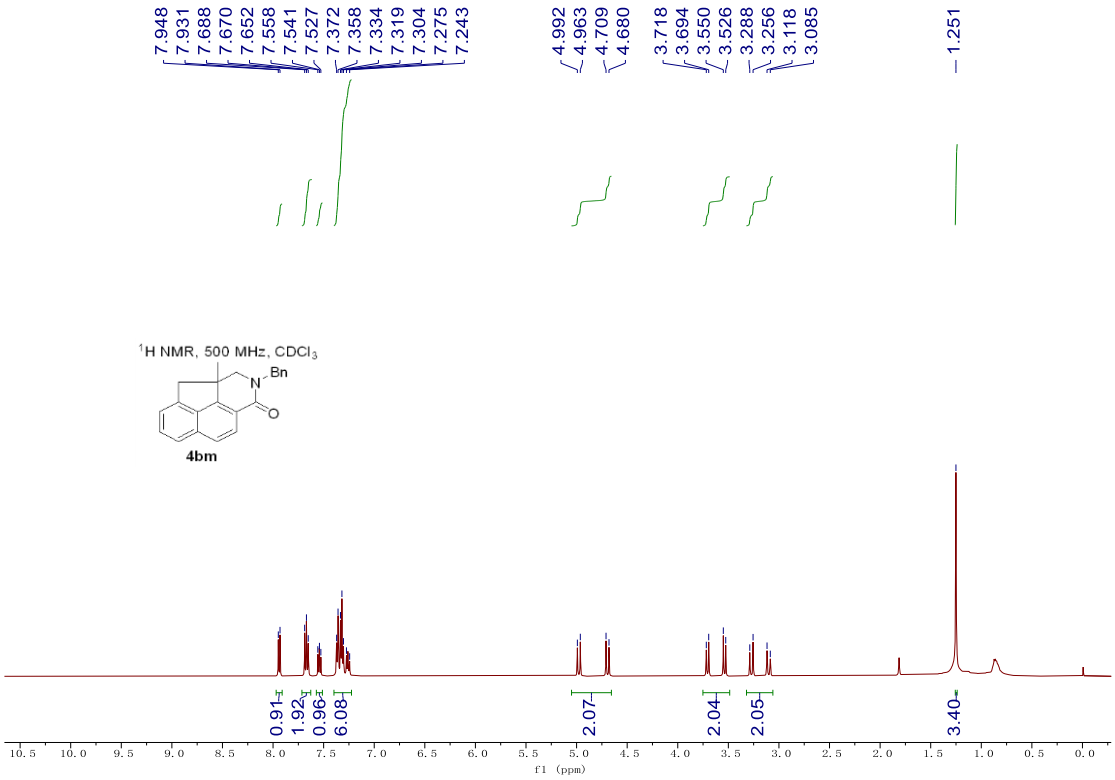
136.936
136.035
135.846
132.307
130.895
129.150
128.697
128.607
127.637
127.582
127.371
127.344
122.480
77.318
77.001
76.683
57.636
50.740
35.326
33.141
22.340
21.221
19.661
^{13}C NMR, 101 MHz, CDCl$_3$
Me
Me
N
Bn
O
4bl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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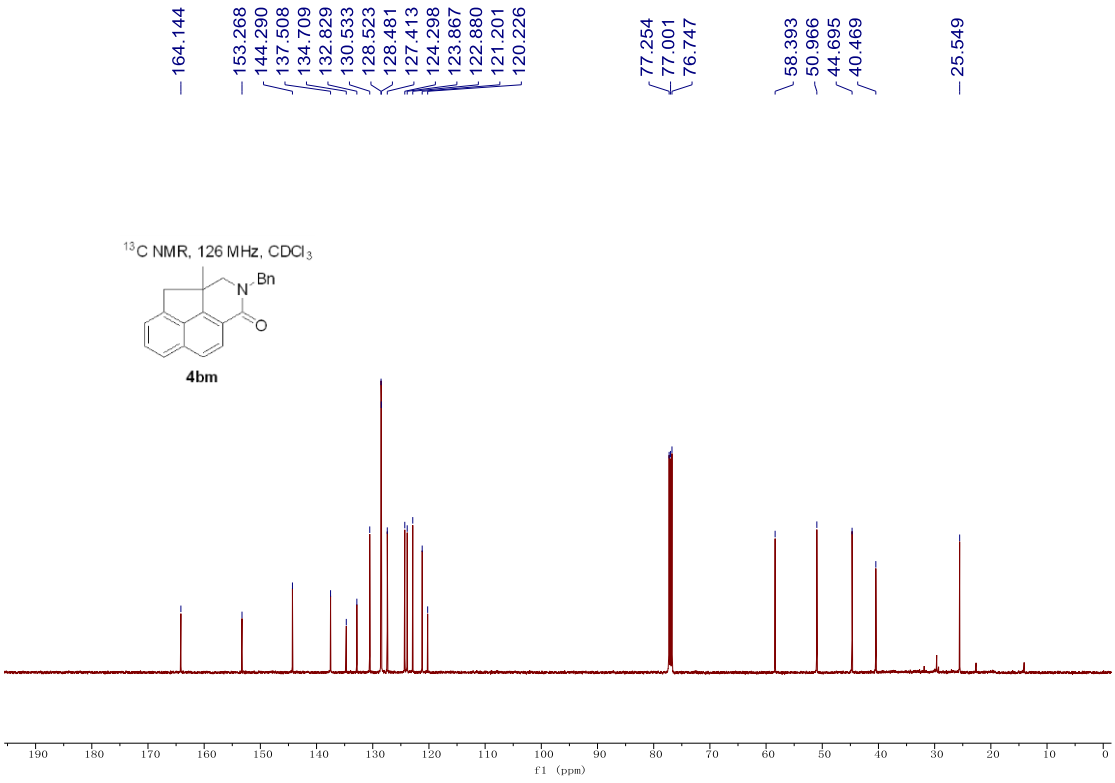
7.527
7.372
7.358
7.334
7.319
7.304
7.275
7.243
4.992
4.963
4.709
4.680
3.718
3.694
3.550
3.526
3.288
3.256
3.118
3.085
1.251
^{1}H NMR, 500 MHz, CDCl$_3$
Bn
N
O
4bm
0.91
1.92
0.96
6.08
2.07
2.04
2.05
3.40
f1 (ppm)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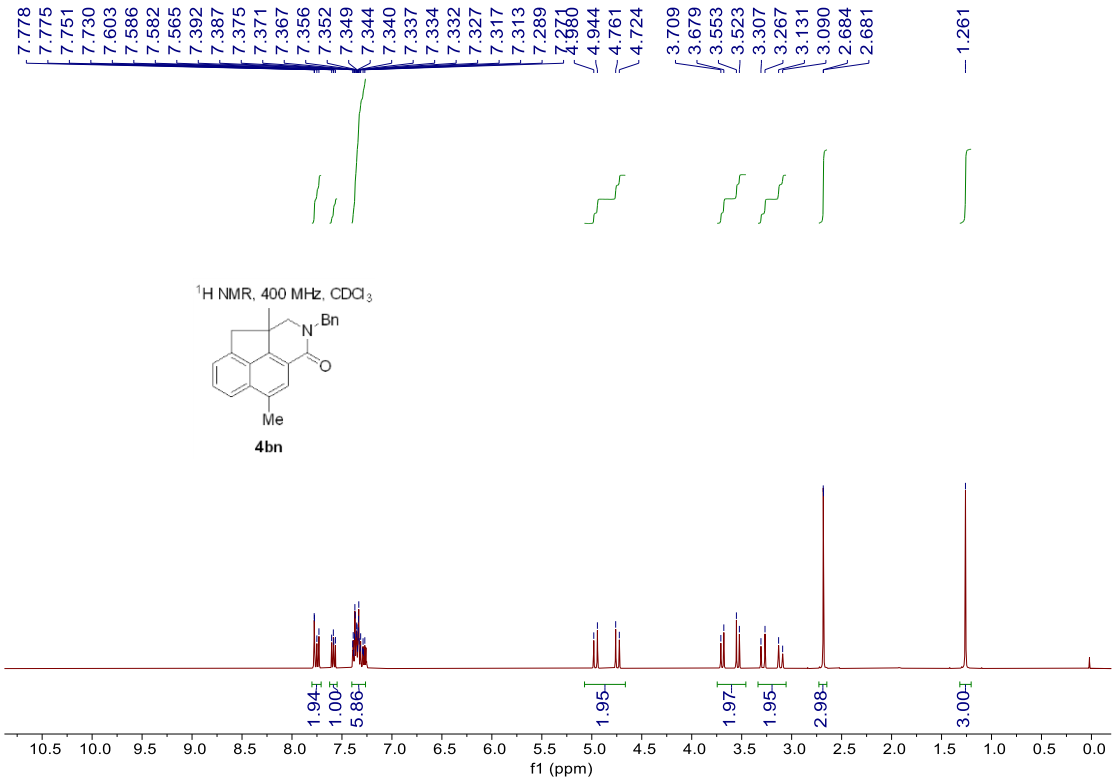
128.523
128.481
127.413
124.298
123.867
122.880
121.201
120.226
77.254
77.001
76.747
58.393
50.966
44.695
40.469
25.549
^{13}C NMR, 126 MHz, CDCl$_3$
Bn
N
O
4bm
f1 (ppm)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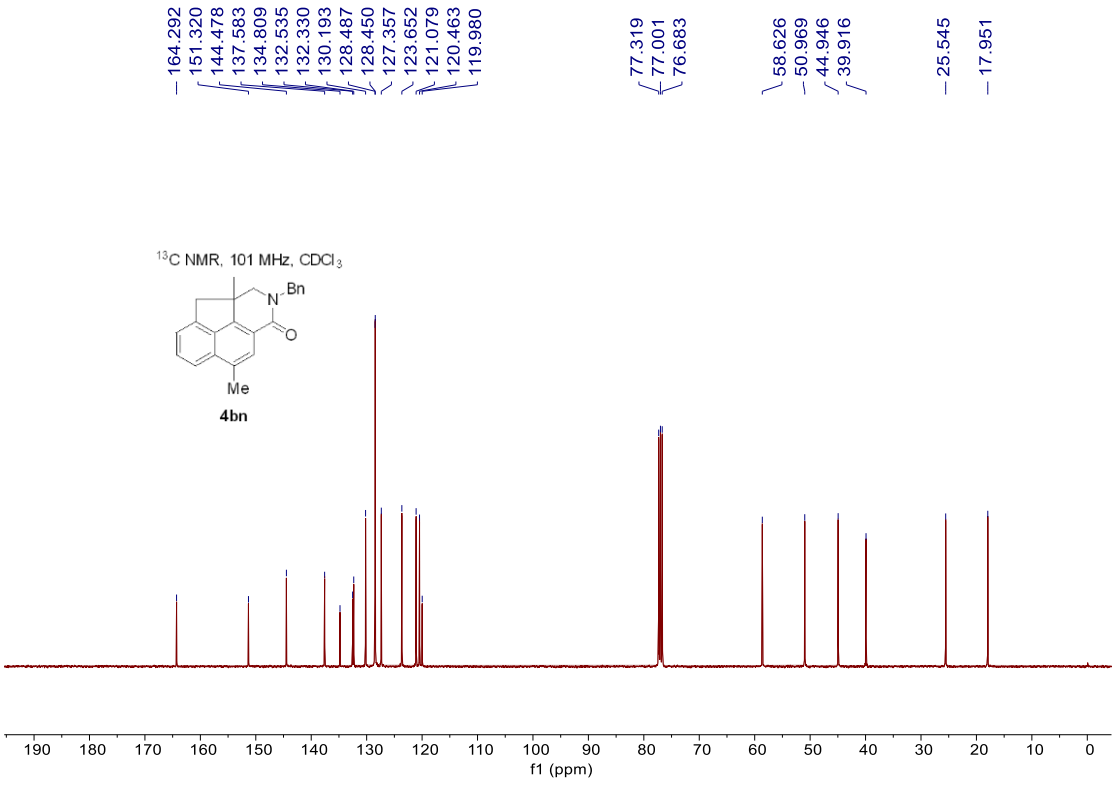
7.730
7.603
7.586
7.582
7.565
7.392
7.387
7.375
7.371
7.367
7.356
7.352
7.349
7.344
7.340
7.337
7.334
7.332
7.327
7.317
7.313
7.289
7.271
4.980
4.944
4.761
4.724
3.709
3.679
3.553
3.523
3.307
3.267
3.131
3.090
2.684
2.681
1.261
1H NMR, 400 MHz, CDCl3
N
Bn
O
Me
4bn
1.94
1.00
5.86
1.95
1.97
1.95
2.98
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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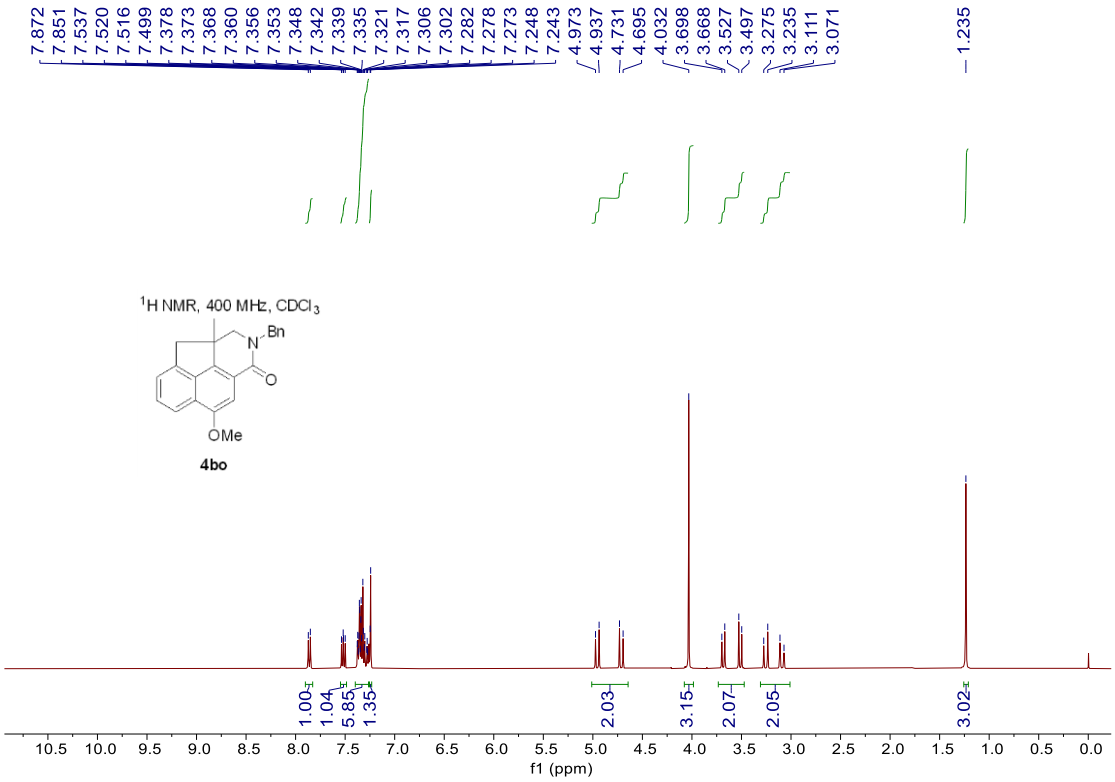
132.535
132.330
130.193
128.487
128.450
127.357
123.652
121.079
120.463
119.980
77.319
77.001
76.683
58.626
50.969
44.946
39.916
25.545
17.951
13C NMR, 101 MHz, CDCl3
N
Bn
O
Me
4bn
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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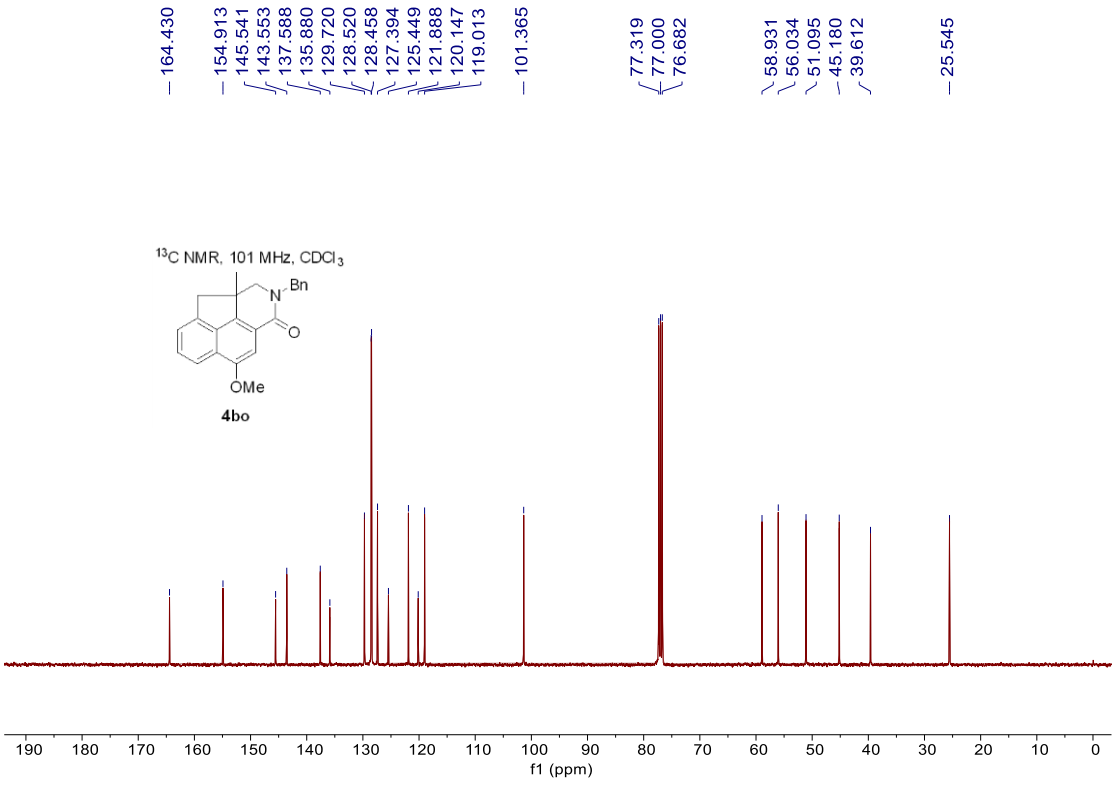
7.499
7.378
7.373
7.368
7.360
7.356
7.353
7.348
7.342
7.339
7.335
7.321
7.317
7.306
7.302
7.282
7.278
7.273
7.248
7.243
4.973
4.937
4.731
4.695
4.032
3.698
3.668
3.527
3.497
3.275
3.235
3.111
3.071
1.235
1H NMR, 400 MHz, CDCl3
Bn
N
O
OMe
4bo
1.00
1.04
5.85
1.35
2.03
3.15
2.07
2.05
3.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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143.553
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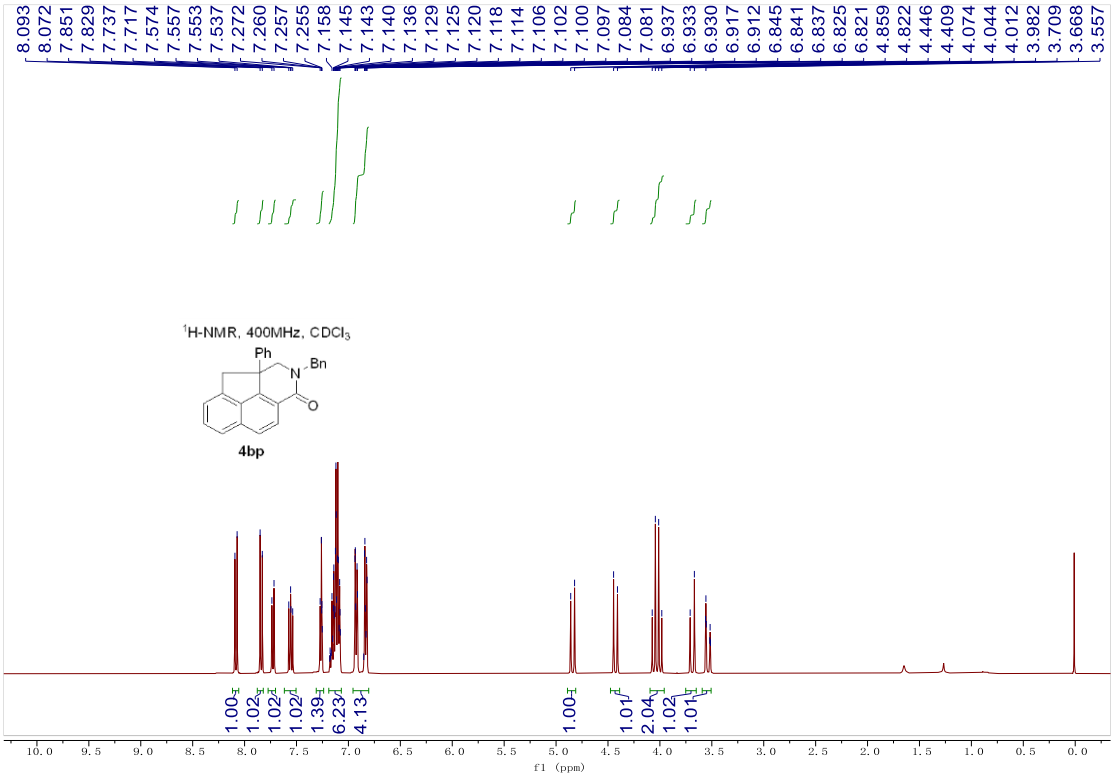
135.880
129.720
128.520
128.458
127.394
125.449
121.888
120.147
119.013
101.365
77.319
77.000
76.682
58.931
56.034
51.095
45.180
39.612
25.545
13C NMR, 101 MHz, CDCl3
Bn
N
O
OMe
4bo
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.717
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7.537
7.272
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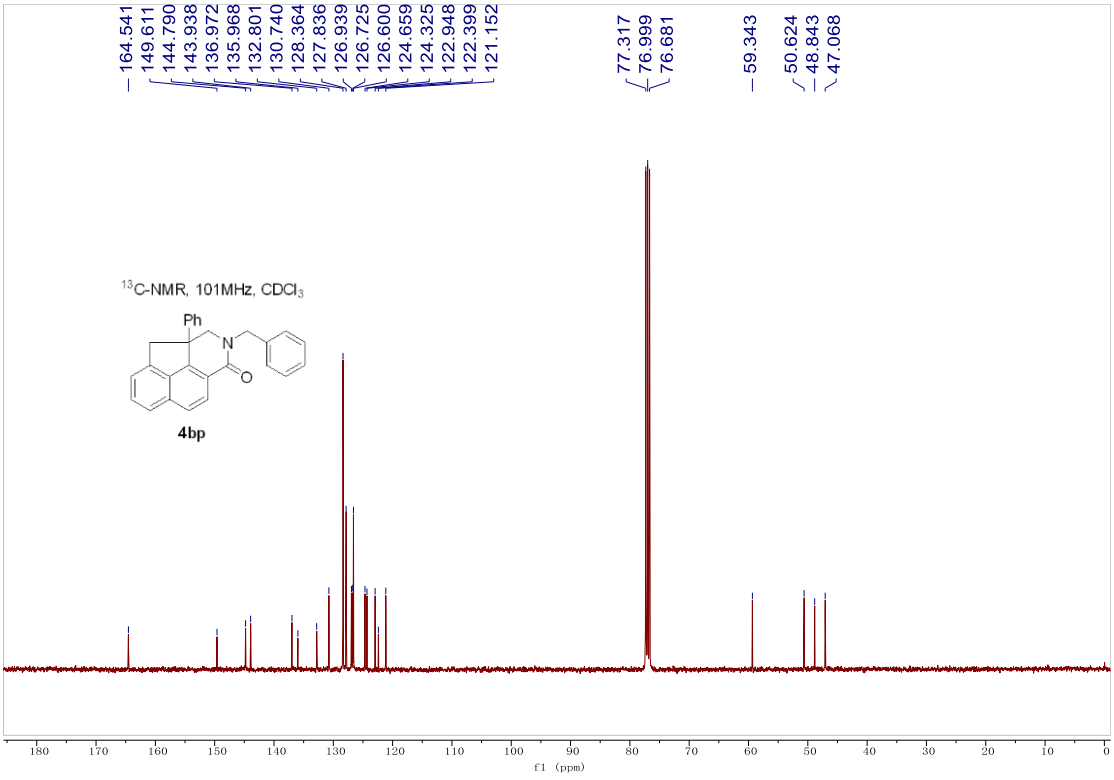
7.257
7.255
7.158
7.145
7.143
7.140
7.136
7.129
7.125
7.120
7.118
7.114
7.106
7.102
7.100
7.097
7.084
7.081
6.937
6.933
6.930
6.917
6.912
6.845
6.841
6.837
6.825
6.821
4.859
4.822
4.446
4.409
4.074
4.044
4.012
3.982
3.709
3.668
3.557
^{1}H-NMR, 400MHz, CDCl$_3$
Ph
N
Bn
O
4bp
1.00
1.02
1.02
1.02
1.39
6.23
4.13
1.00
1.01
2.04
1.02
1.01
f1 (ppm)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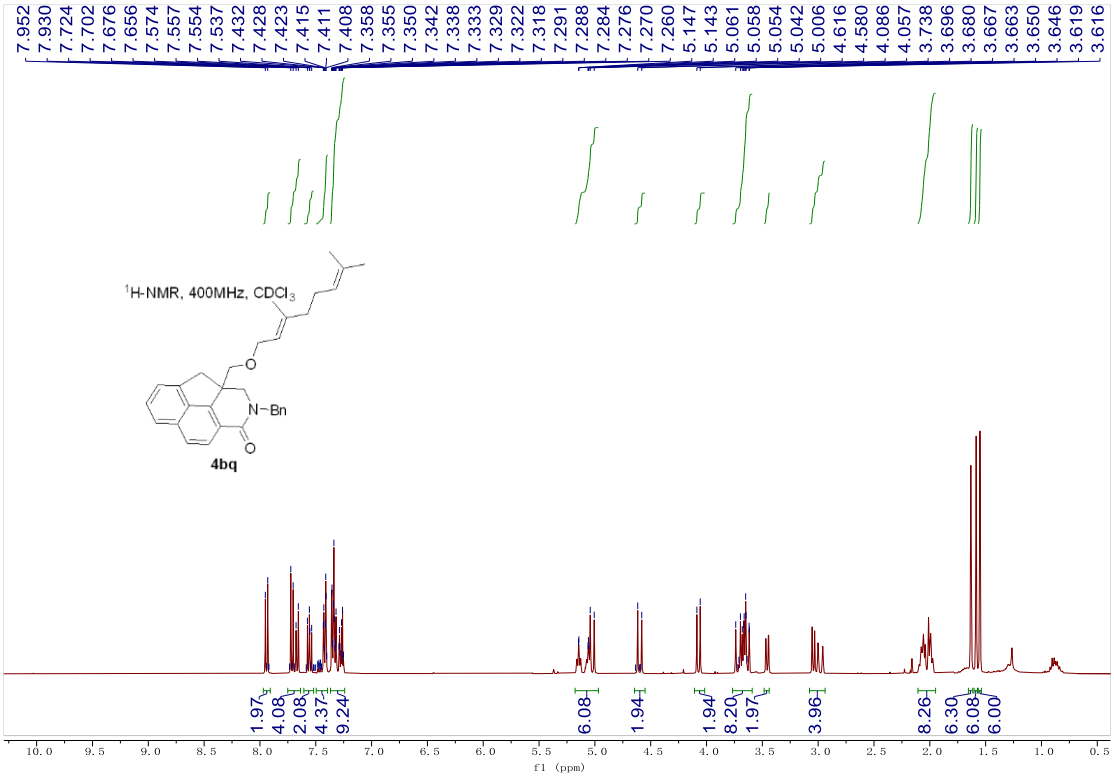
149.611
144.790
143.938
136.972
135.968
132.801
130.740
128.364
127.836
126.939
126.725
126.600
124.659
124.325
122.948
122.399
121.152
77.317
76.999
76.681
59.343
50.624
48.843
47.068
^{13}C-NMR, 101MHz, CDCl$_3$
Ph
N
O
4bp
f1 (ppm)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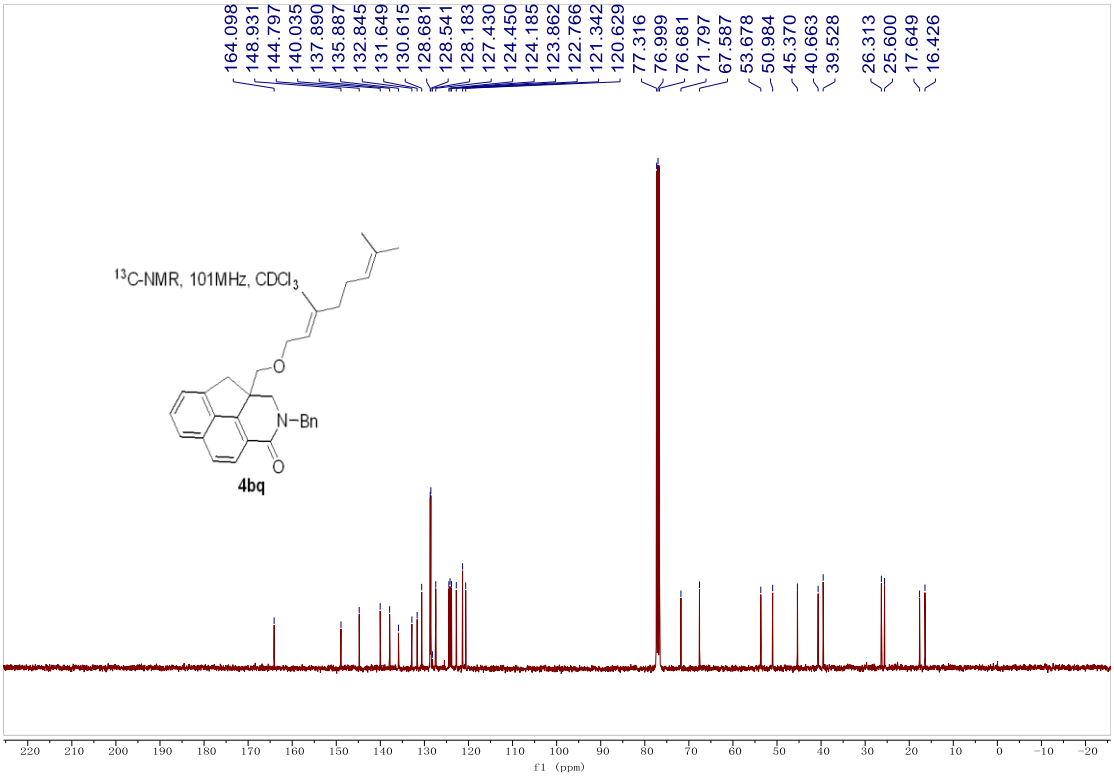
7.930
7.724
7.702
7.676
7.656
7.574
7.557
7.554
7.537
7.432
7.428
7.423
7.415
7.411
7.408
7.358
7.355
7.350
7.342
7.338
7.333
7.329
7.322
7.318
7.291
7.288
7.284
7.276
7.270
7.260
5.147
5.143
5.061
5.058
5.054
5.042
5.006
4.616
4.580
4.086
4.057
3.738
3.696
3.680
3.667
3.663
3.650
3.646
3.619
3.616
1H-NMR, 400MHz, CDCl3
N−Bn
O
4bq
1.97
4.08
2.08
4.37
9.24
6.08
1.94
1.94
8.20
1.97
3.96
8.26
6.30
6.08
6.00
f1 (ppm)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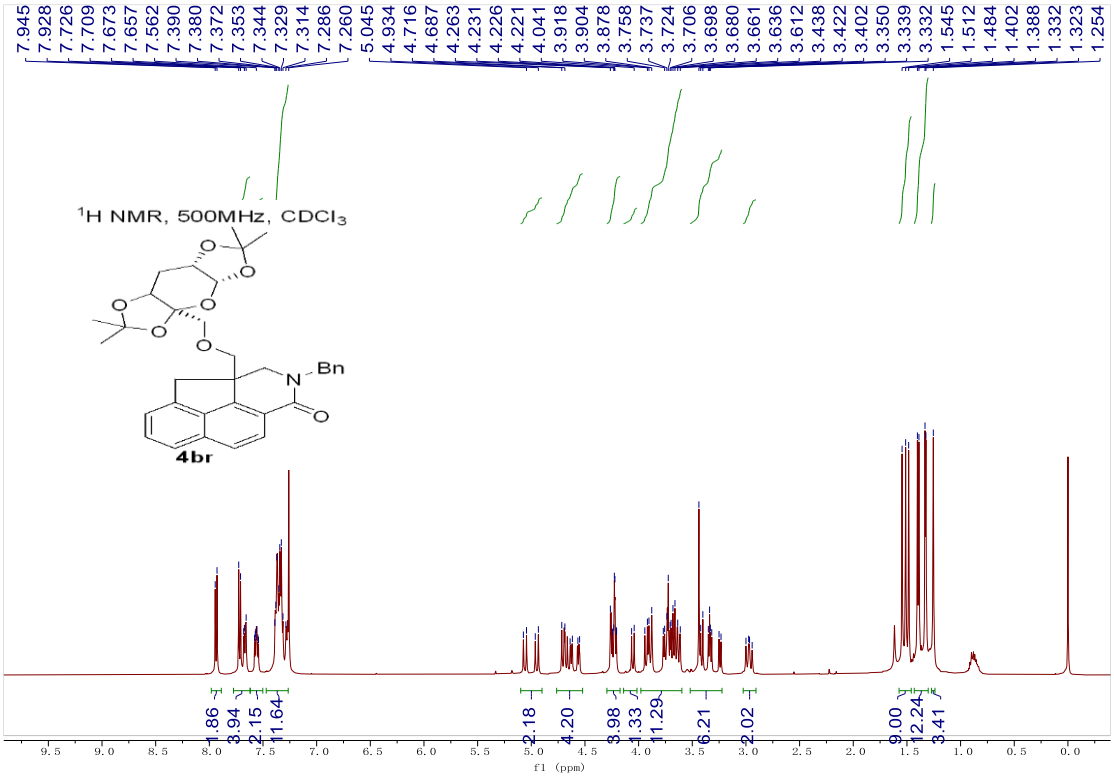
148.931
144.797
140.035
137.890
135.887
132.845
131.649
130.615
128.681
128.541
128.183
127.430
124.450
124.185
123.862
122.766
121.342
120.629
77.316
76.999
76.681
71.797
67.587
53.678
50.984
45.370
40.663
39.528
26.313
25.600
17.649
16.426
13C-NMR, 101MHz, CDCl3
N−Bn
O
4bq
f1 (ppm)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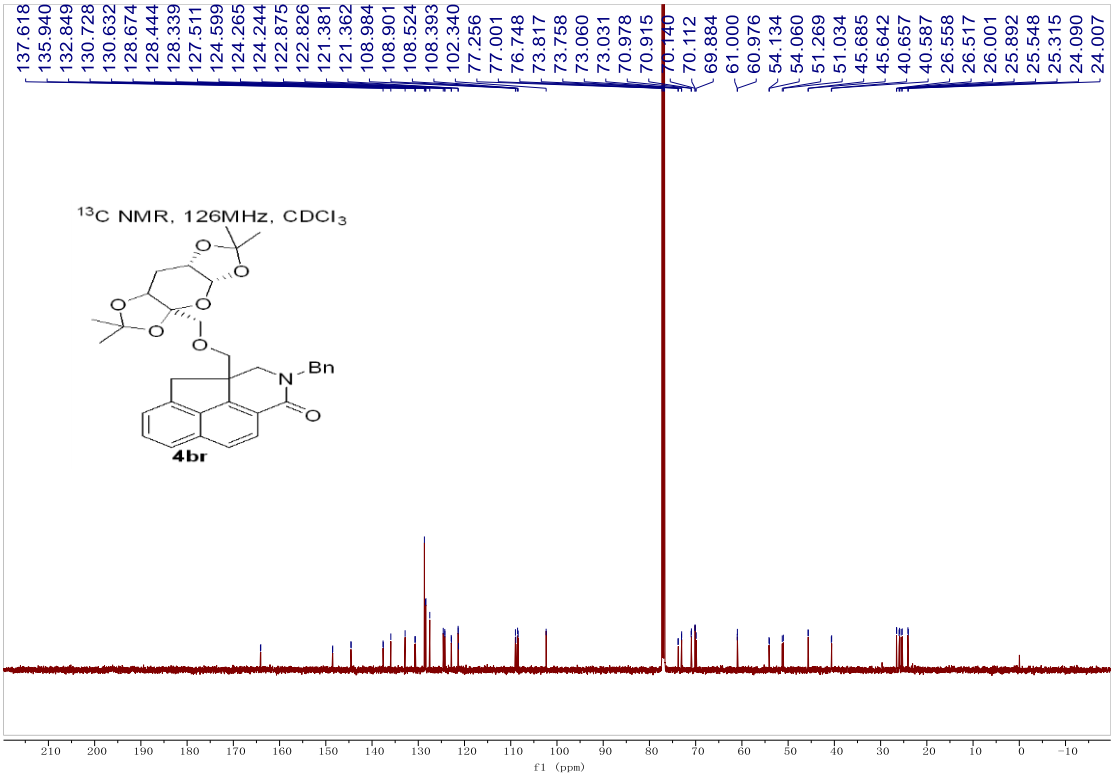
7.928
7.726
7.709
7.673
7.657
7.562
7.390
7.380
7.372
7.353
7.344
7.329
7.314
7.286
7.260
5.045
4.934
4.716
4.687
4.263
4.231
4.226
4.221
4.041
3.918
3.904
3.878
3.758
3.737
3.724
3.706
3.698
3.680
3.661
3.636
3.612
3.438
3.422
3.402
3.350
3.339
3.332
1.545
1.512
1.484
1.402
1.388
1.332
1.323
1.254
1H NMR, 500MHz, CDCl3
Bn
N
O
4br
1.86
3.94
2.15
11.64
2.18
4.20
3.98
1.33
11.29
6.21
2.02
9.00
12.24
3.41
f1 (ppm)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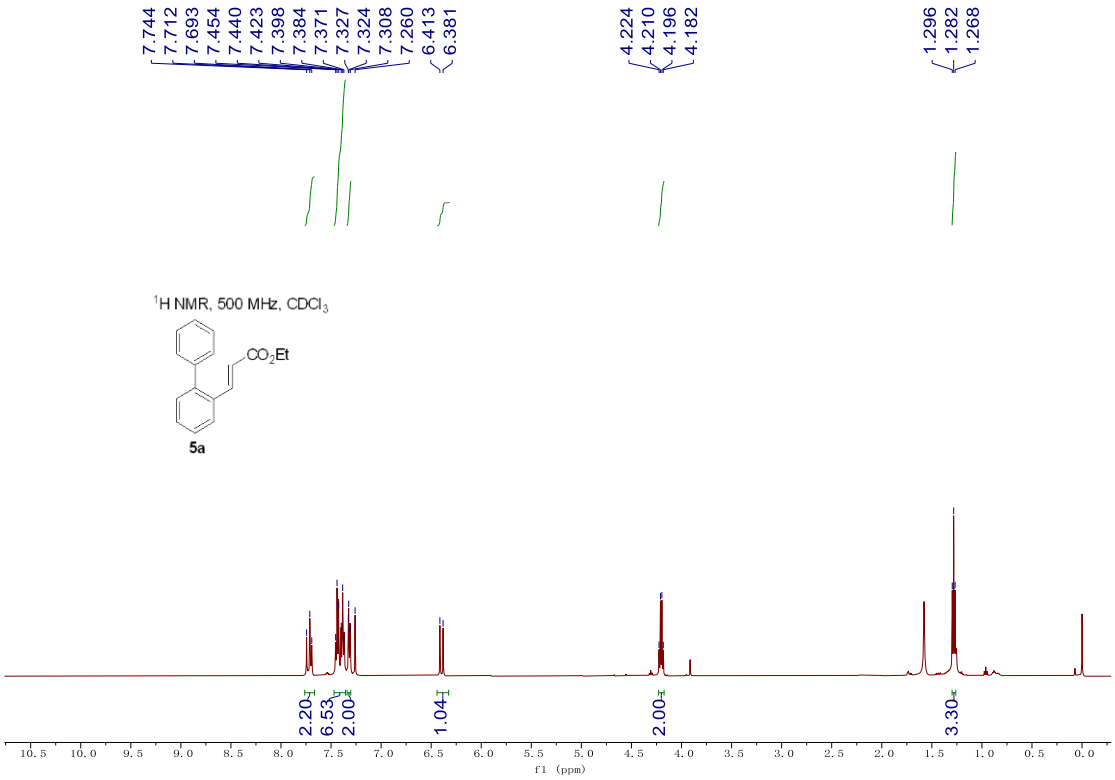
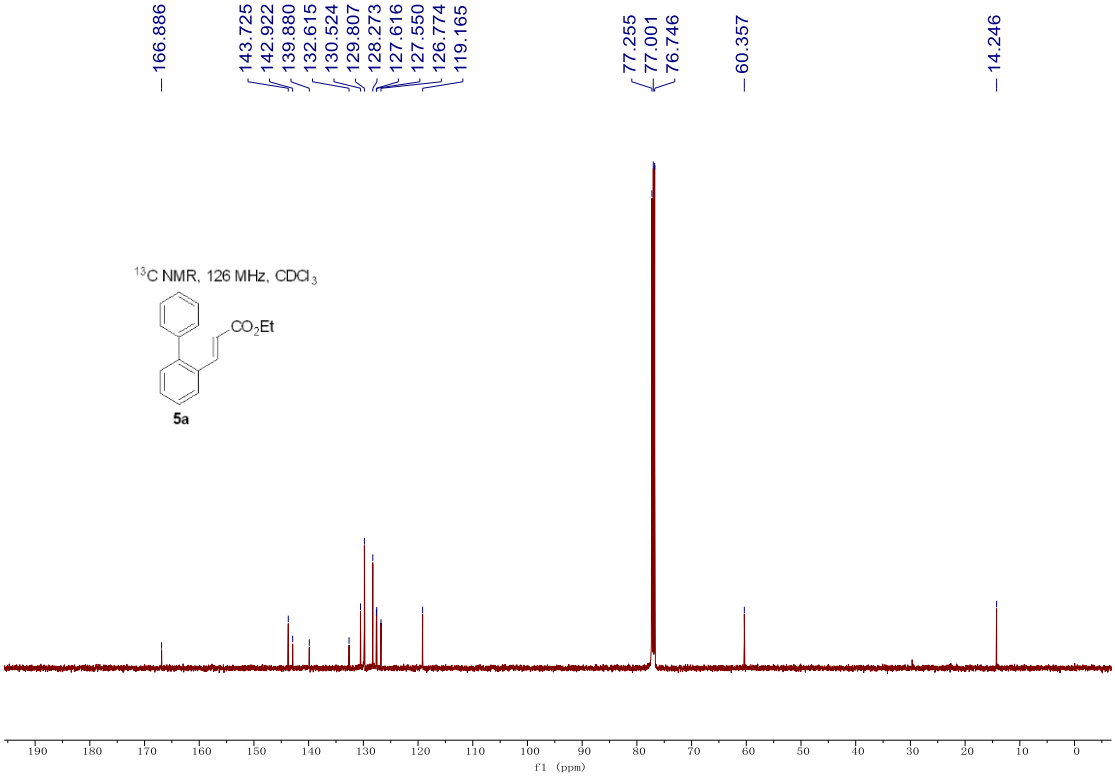
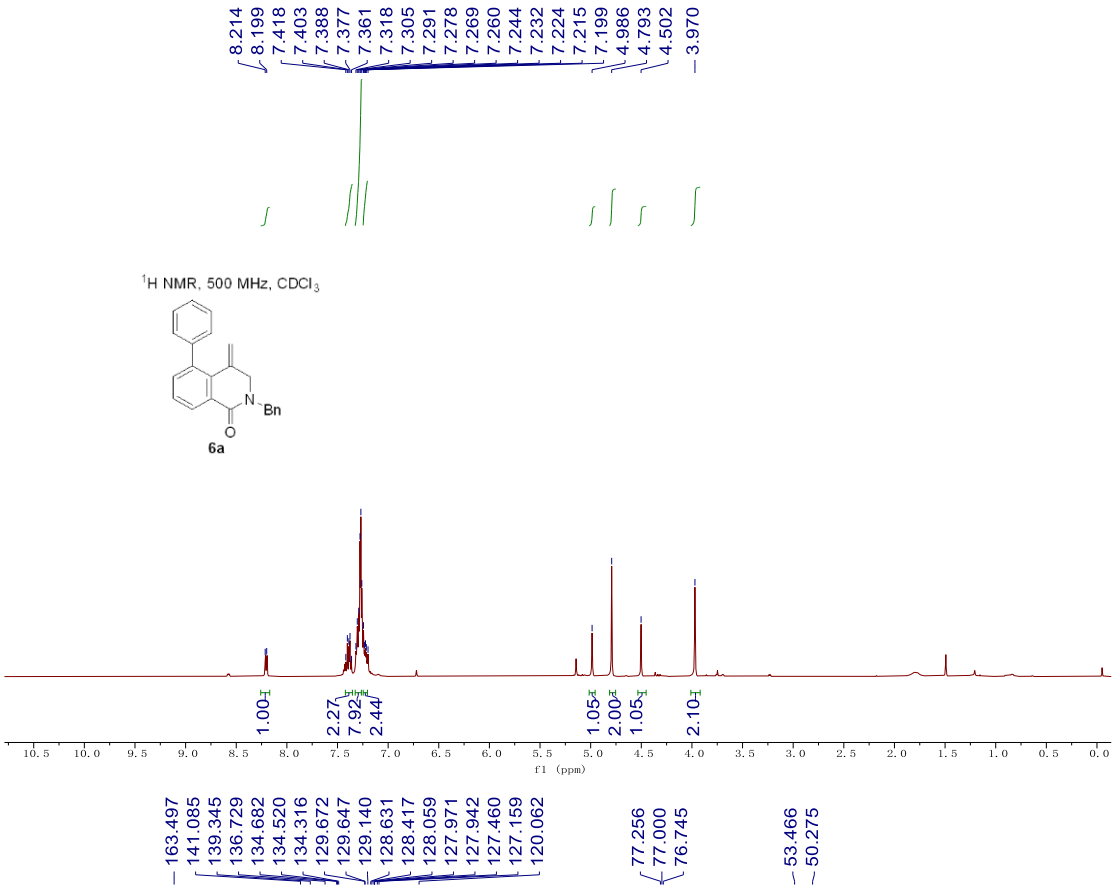
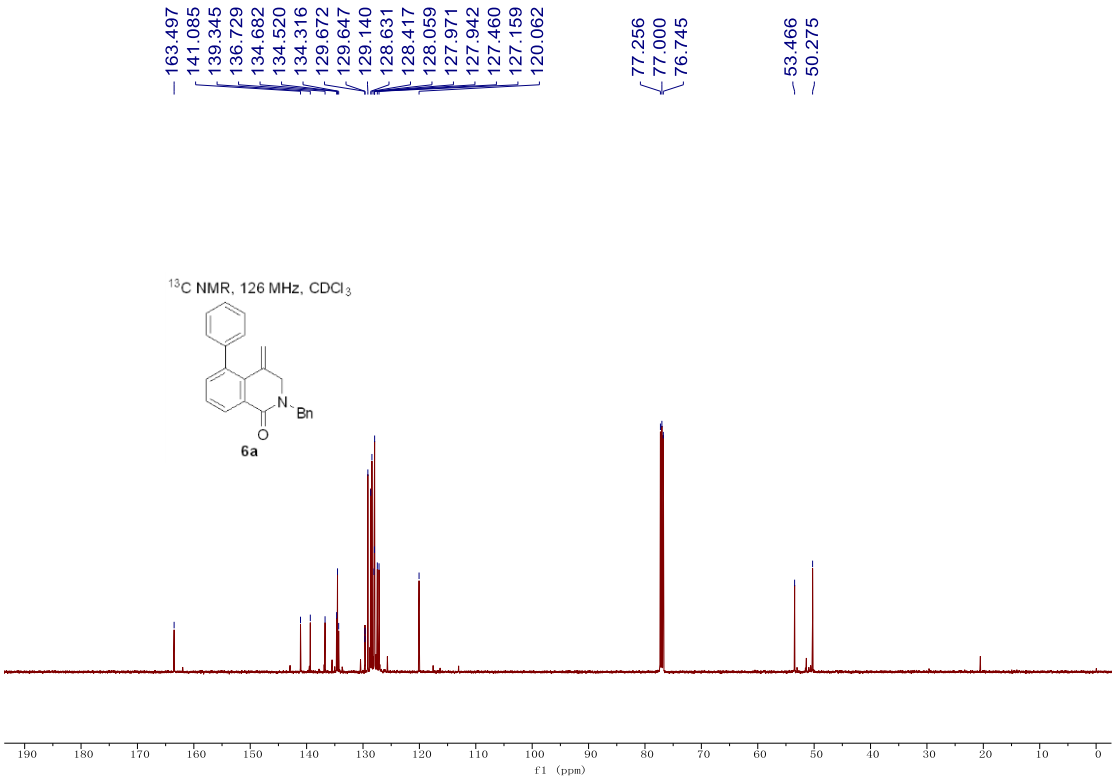
135.940
132.849
130.728
130.632
128.674
128.444
128.339
127.511
124.599
124.265
124.244
122.875
122.826
121.381
121.362
108.984
108.901
108.524
108.393
102.340
77.256
77.001
76.748
73.817
73.758
73.060
73.031
70.978
70.915
70.140
70.112
69.884
61.000
60.976
54.134
54.060
51.269
51.034
45.685
45.642
40.657
40.587
26.558
26.517
26.001
25.892
25.548
25.315
24.090
24.007
13C NMR, 126MHz, CDCl3
Bn
N
O
4br
f1 (ppm)


7.744
7.712
7.693
7.454
7.440
7.423
7.398
7.384
7.371
7.327
7.324
7.308
7.260
6.413
6.381
4.224
4.210
4.196
4.182
1.296
1.282
1.268
^{1}H NMR, 500 MHz, $CDCl_3$
CO_2Et
5a
2.20
6.53
2.00
1.04
2.00
3.30
f1 (ppm)


166.886
143.725
142.922
139.880
132.615
130.524
129.807
128.273
127.616
127.550
126.774
119.165
77.255
77.001
76.746
60.357
14.246
^{13}C NMR, 126 MHz, $CDCl_3$
CO_2Et
5a
f1 (ppm)


8.214
8.199
7.418
7.403
7.388
7.377
7.361
7.318
7.305
7.291
7.278
7.269
7.260
7.244
7.232
7.224
7.215
7.199
4.986
4.793
4.502
3.970
1H NMR, 500 MHz, CDCl3
N
Bn
O
6a
1.00
2.27
7.92
2.44
1.05
2.00
1.05
2.10
f1 (ppm)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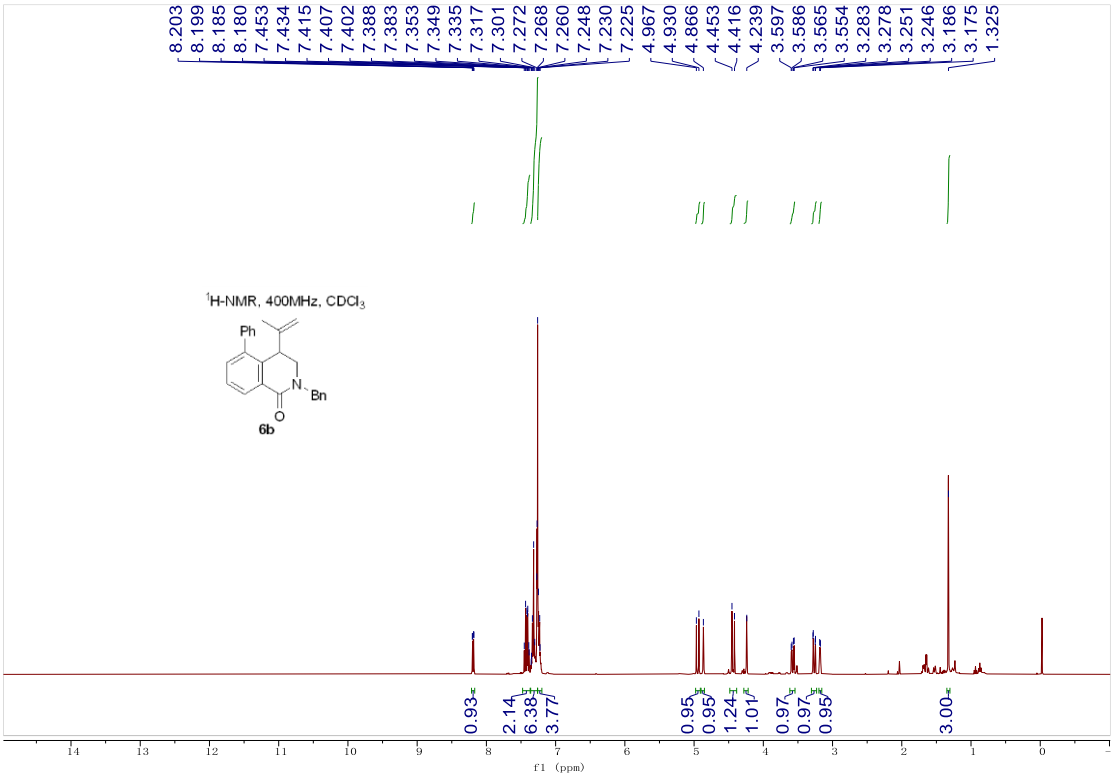
141.085
139.345
136.729
134.682
134.520
134.316
129.672
129.647
129.140
128.631
128.417
128.059
127.971
127.942
127.460
127.159
120.062
77.256
77.000
76.745
53.466
50.275
13C NMR, 126 MHz, CDCl3
N
Bn
O
6a
f1 (ppm)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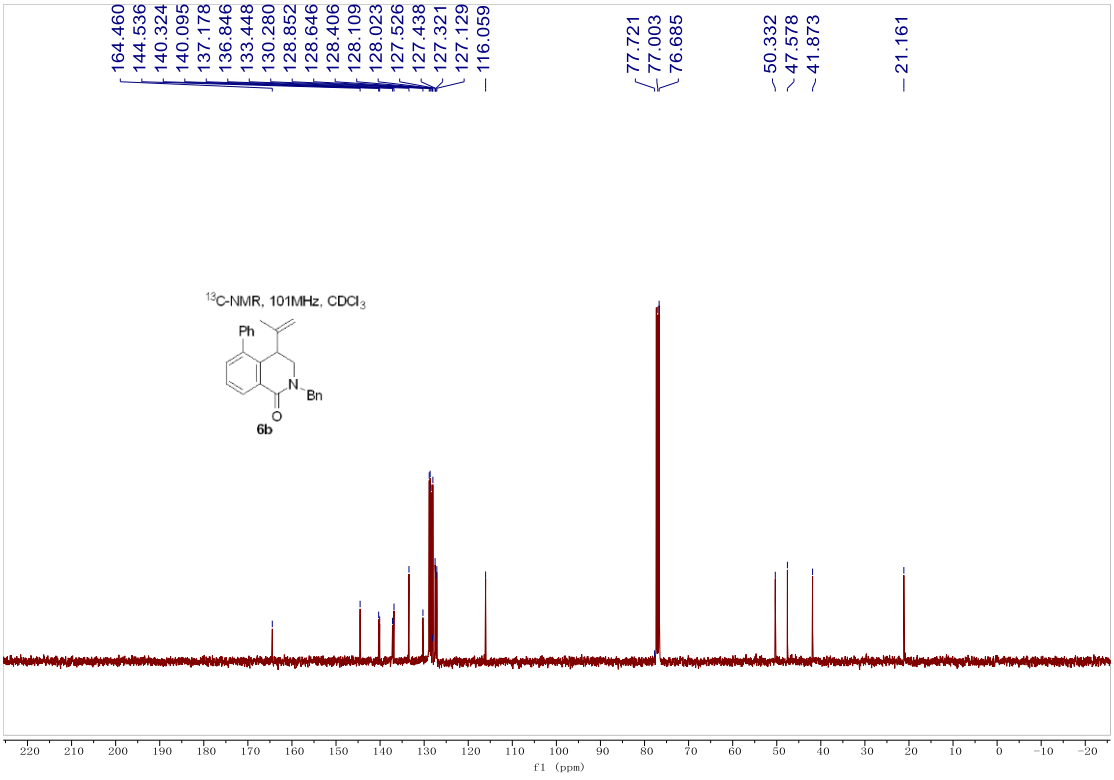
8.199
8.185
8.180
7.453
7.434
7.415
7.407
7.402
7.388
7.383
7.353
7.349
7.335
7.317
7.301
7.272
7.268
7.260
7.248
7.230
7.225
4.967
4.930
4.866
4.453
4.416
4.239
3.597
3.586
3.565
3.554
3.283
3.278
3.251
3.246
3.186
3.175
1.325
^{1}H-NMR, 400MHz, CDCl$_3$
Ph
N
Bn
O
6b
0.93
2.14
6.38
3.77
0.95
0.95
1.24
1.01
0.97
0.97
0.95
3.00
f1 (ppm)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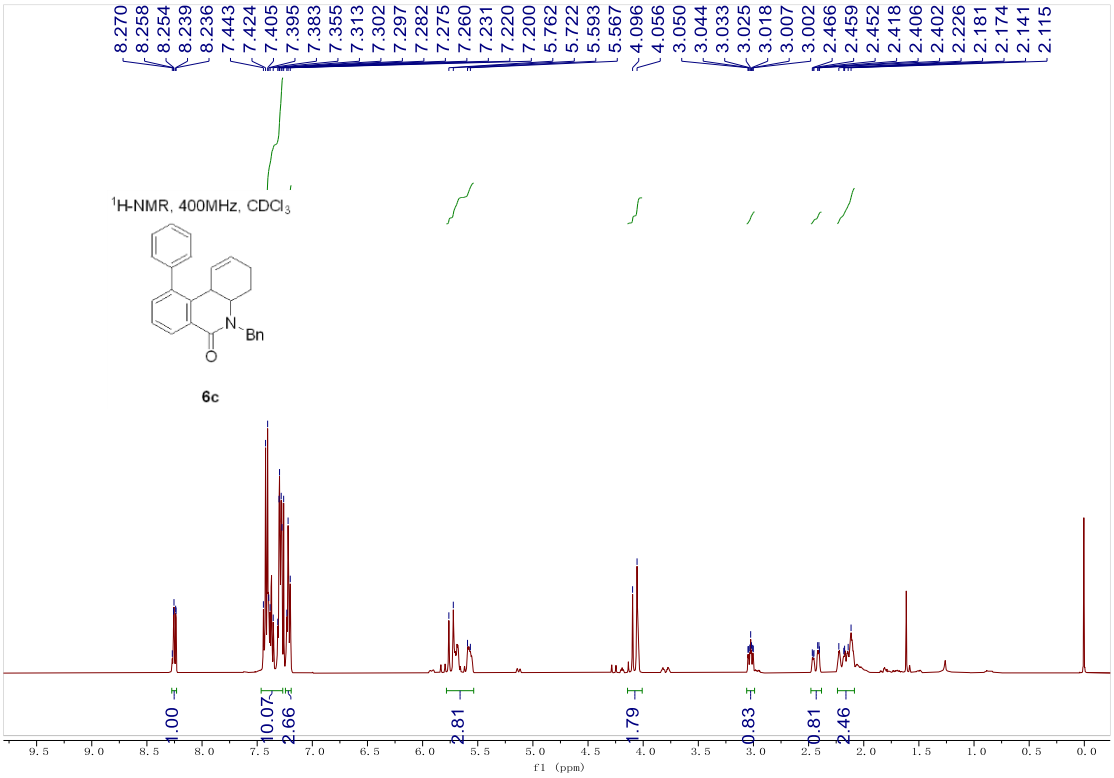
144.536
140.324
140.095
137.178
136.846
133.448
130.280
128.852
128.646
128.406
128.109
128.023
127.526
127.438
127.321
127.129
116.059
77.721
77.003
76.685
50.332
47.578
41.873
21.161
^{13}C-NMR, 101MHz, CDCl$_3$
Ph
N
Bn
O
6b
f1 (ppm)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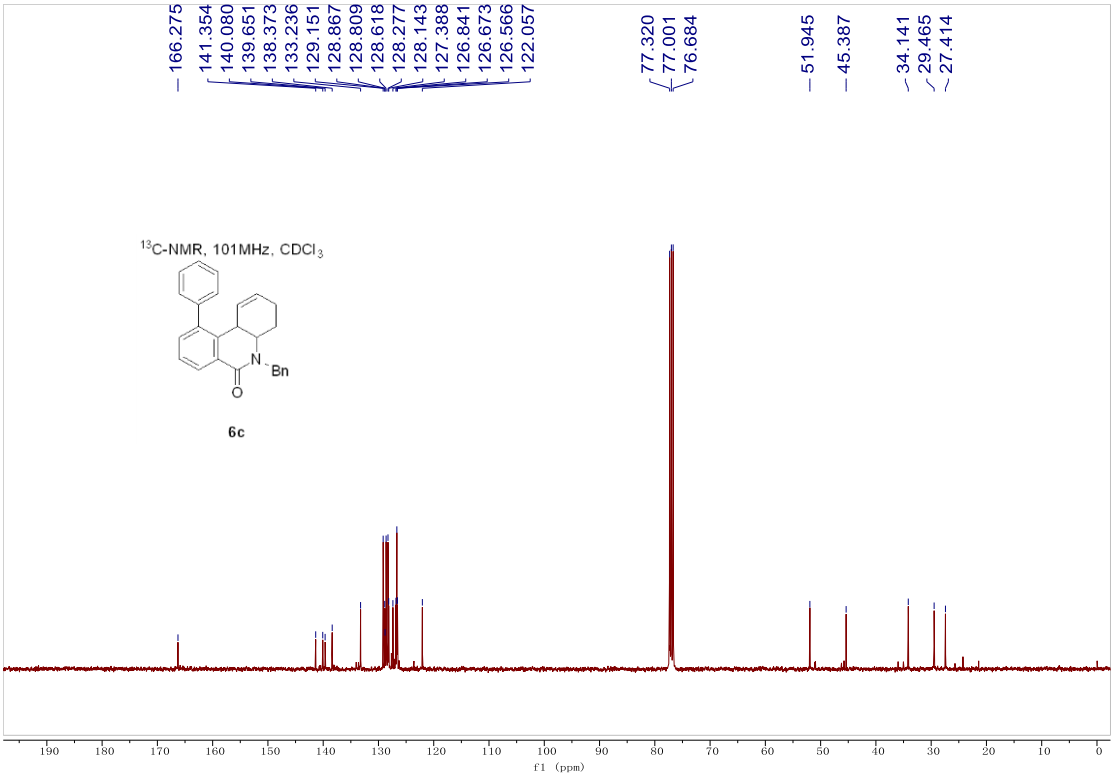
8.258
8.254
8.239
8.236
7.443
7.424
7.405
7.395
7.383
7.355
7.313
7.302
7.297
7.282
7.275
7.260
7.231
7.220
7.200
5.762
5.722
5.593
5.567
4.096
4.056
3.050
3.044
3.033
3.025
3.018
3.007
3.002
2.466
2.459
2.452
2.418
2.406
2.402
2.226
2.181
2.174
2.141
2.115
^{1}H-NMR, 400MHz, CDCl$_3$
N
Bn
O
6c
1.00
10.07
2.66
2.81
1.79
0.83
0.81
2.46
f1 (ppm)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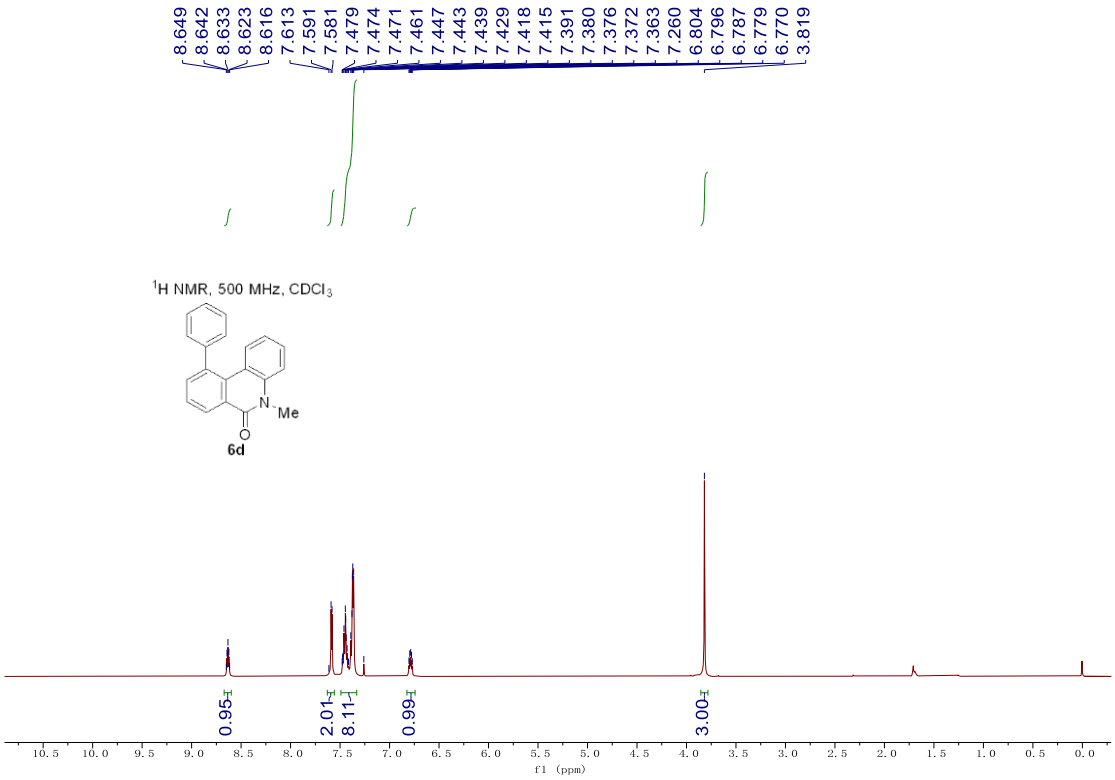
141.354
140.080
139.651
138.373
133.236
129.151
128.867
128.809
128.618
128.277
128.143
127.388
126.841
126.673
126.566
122.057
77.320
77.001
76.684
51.945
45.387
34.141
29.465
27.414
^{13}C-NMR, 101MHz, CDCl$_3$
N
Bn
O
6c
f1 (ppm)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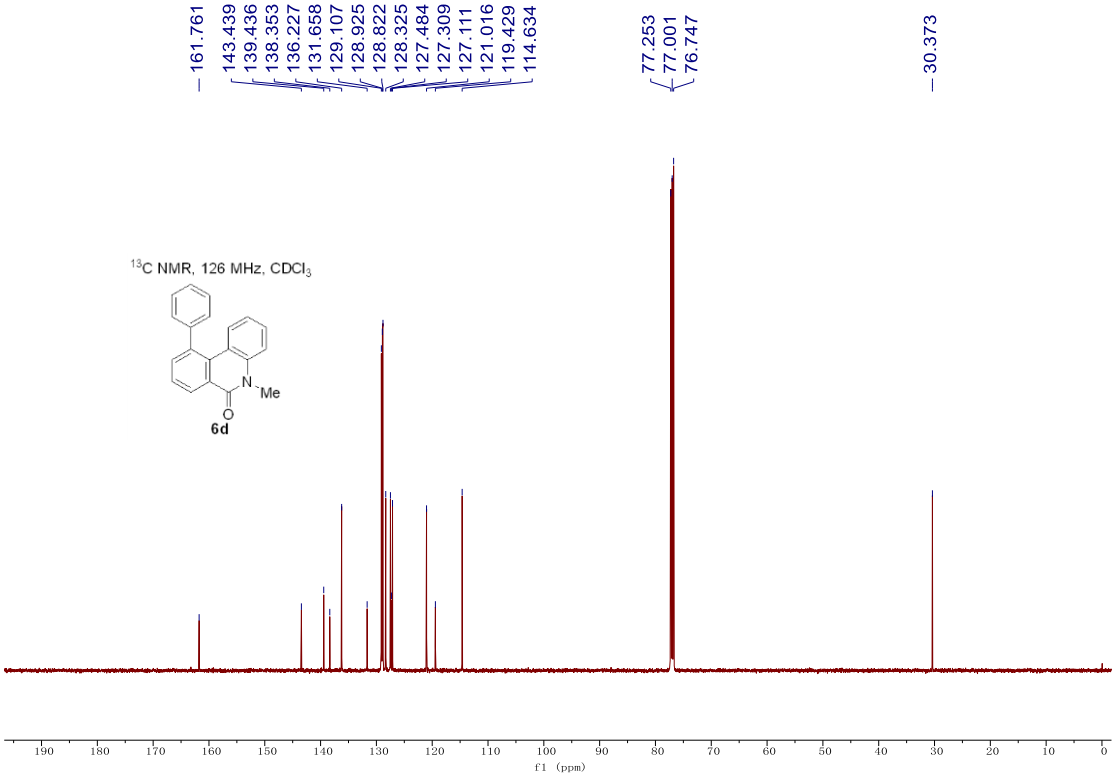
8.633
8.623
8.616
7.613
7.591
7.581
7.479
7.474
7.471
7.461
7.447
7.443
7.439
7.429
7.418
7.415
7.391
7.380
7.376
7.372
7.363
7.260
6.804
6.796
6.787
6.779
6.770
3.819
1H NMR, 500 MHz, CDCl3
N
Me
O
6d
0.95
2.01
8.11
0.99
3.00
f1 (ppm)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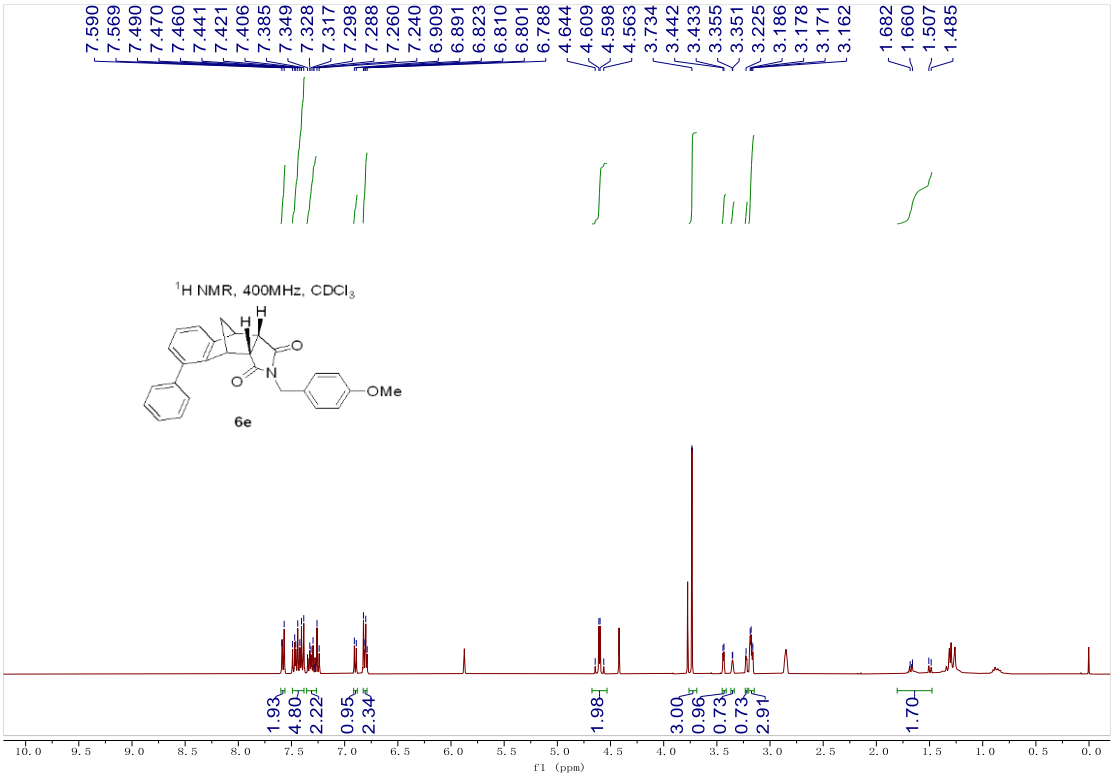
139.436
138.353
136.227
131.658
129.107
128.925
128.822
128.325
127.484
127.309
127.111
121.016
119.429
114.634
77.253
77.001
76.747
30.373
13C NMR, 126 MHz, CDCl3
N
Me
O
6d
f1 (ppm)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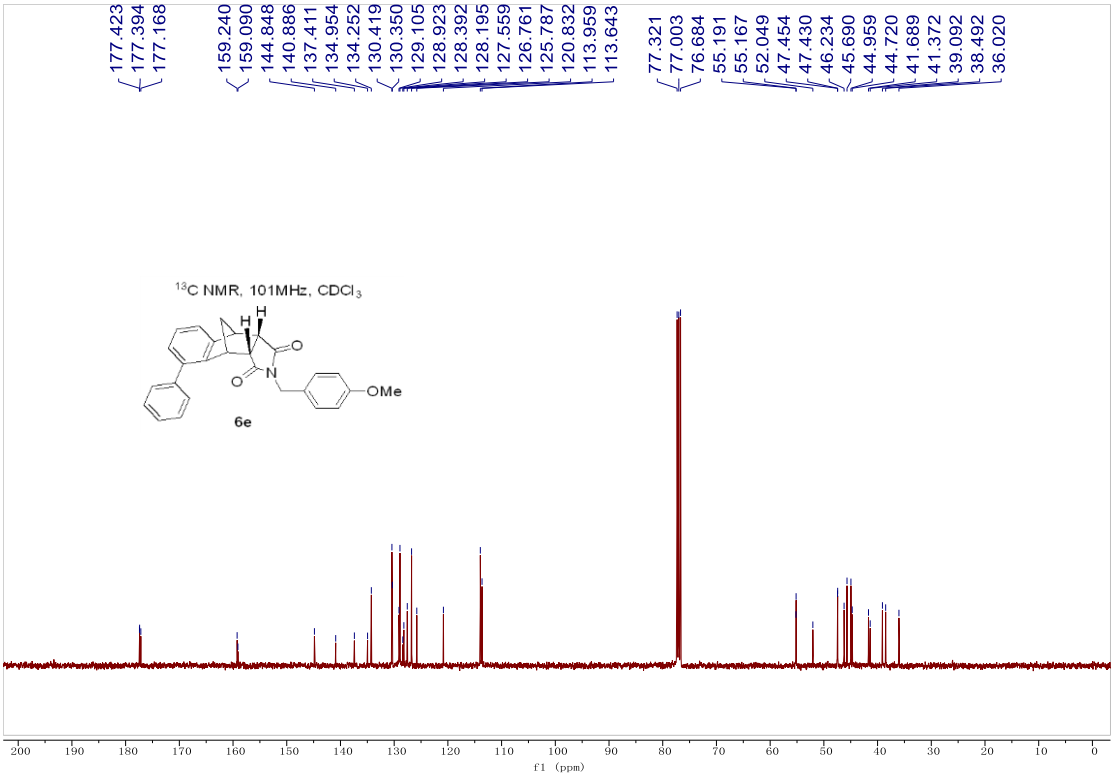
7.569
7.490
7.470
7.460
7.441
7.421
7.406
7.385
7.349
7.328
7.317
7.298
7.288
7.260
7.240
6.909
6.891
6.823
6.810
6.801
6.788
4.644
4.609
4.598
4.563
3.734
3.442
3.433
3.355
3.351
3.225
3.186
3.178
3.171
3.162
1.682
1.660
1.507
1.485
^{1}H NMR, 400MHz, CDCl$_3$
OMe
6e
1.93
4.80
2.22
0.95
2.34
1.98
3.00
0.96
0.73
0.73
2.91
1.70
f1 (ppm)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177.394
177.168
159.240
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144.848
140.886
137.411
134.954
134.252
130.419
130.350
129.105
128.923
128.392
128.195
127.559
126.761
125.787
120.832
113.959
113.643
77.321
77.003
76.684
55.191
55.167
52.049
47.454
47.430
46.234
45.690
44.959
44.720
41.689
41.372
39.092
38.492
36.020
^{13}C NMR, 101MHz, CDCl$_3$
OMe
6e
f1 (ppm)