Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Acid-Catalyzed Cleavage of C–C Bond Enabled Atropaldehyde Acetals as Masked C2 Electrophiles for Organic Synthesis

Shaomin Chen,[a] Minghao Li,[a]* and Yanlong Gu [a,b,c]*

[a] Key Laboratory for Large-Format Battery Materials and System, Ministry of Education, School of Chemistry and Chemical Engineering, Huazhong University of Science and Technology, 430074, Wuhan, China.

[b] School of Chemistry and Chemical Engineering, The Key Laboratory for Green Processing of Chemical Engineering of Xinjiang Bingtuan, Shihezi University, Shihezi City 832004, China.

[c] State Key Laboratory for Oxo Synthesis and Selective Oxidation, Lanzhou Institute of Chemical Physics, 730000, Lanzhou, China.

Corresponding authors: M. Li (liminghaochem@hust.edu.cn) and Y. Gu (klgyl@hust.edu.cn)

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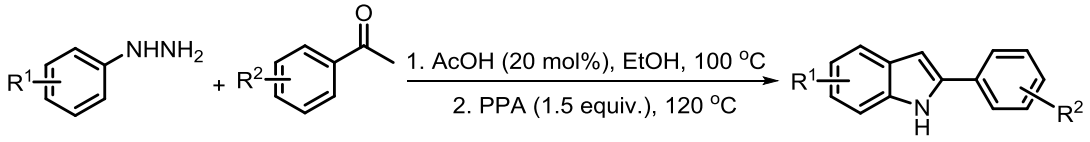
1. General information

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without further purification. The reactions were monitored by TLC with Haiyang GF-254 silica gel plates (Qingdao Haiyang chemical industry Co. Ltd, Qingdao, China) using UV light or $KMnO_4$ as visualizing agents as needed. Flash column chromatography was performed using 200-300 mesh silica gel at increased pressure. ^{1}H NMR spectra and ^{13}C NMR spectra were respectively recorded on Brüker AV-400 spectrometers. Chemical shifts (δ) were expressed in ppm relative to Me_4Si in $CDCl_3$, and coupling constants (*J*) were reported in Hz. High-resolution mass spectra (HRMS) were obtained on Brüker Compass Data Analysis 4.0. IR spectra were recorded on a Bruker FT-IR (EQUINOX 55) using KBr pellets or neat liquid technology.

2. Preparation of Substrates

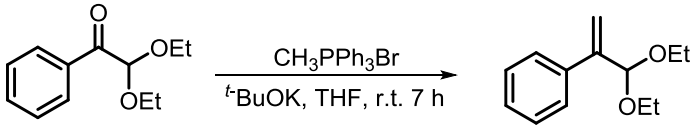
2.1 Preparation of 2-arylindole (1b–1s)



According to literature reports,[1] 2-arylindole (**1b–1s**) was synthesized by the methods below:

A mixture of acetophenone (10 mmol), phenylhydrazine (1.2 equiv), HOAc (2 mmol) and EtOH (6.0 mL) were taken in a 100 mL round bottom flask. Then, the reaction mixture was refluxed at 100 °C. When the reaction was completed (detected by TLC), it was cooled to room temperature. The EtOH was evaporated in vacuo to give the crude phenylhydrazone product. Next, the freshly prepared phenylhydrazone (10 mmol) were taken in a 100 mL round bottom flask and 1.5 equiv. of polyphosphoric acid was added at one time and the solution was refluxed. After completion, the reaction mixture was cooled to room temperature, quenched with cold H_2O (10 mL) and extracted with EtOAc (3 × 10mL). The combined organic layers were dried over anhydrous Na_2SO_4 and then evaporated in vacuo. The residue was purified by silica gel column chromatography using PE/ EtOAc as eluent to afford the corresponding 2-arylindole.

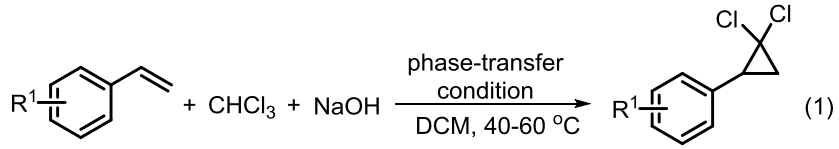
2.2 Preparation of 2-phenylpropenal diethyl acetal (2a)

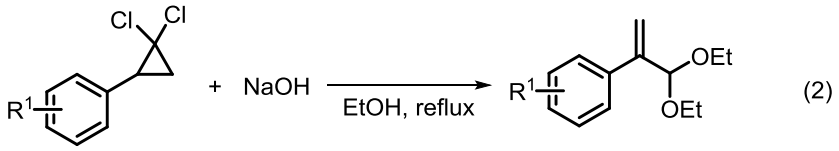


According to literature reports,[2] 2-phenylpropenal diethyl acetal (**2a**) was synthesized by the methods below:

A suspension of 8.57 g (24 mmol) of methyltriphenylphosphonium bromide and 2.69 g (24 mmol) of potassium *t*-butoxide in 35 mL of dried THF was stirred at room temperature for 30 min. Subsequently, 4.16 g (20 mmol) of 2,2- diethoxyacetophenone was added, and the reaction mixture was stirred at room temperature for 7 h. The reaction mixture was then filtered through a pad of Celite and the filtrate was concentrated on a rotary evaporator and then purified by silica gel column chromatography (PE/EtOAc = 20/1) to give the pure product.

2.3 Preparation of substituted atropaldehyde diethyl acetal (2b–2h)





According to literature reports,[3] the substituted atropaldehyde diethyl acetals (**2b–2h**) were synthesized by the two-step methods below:

Step 1: the synthesis of 1,1-dichloro-2-phenylcyclopropane.

In a 100 mL, three-necked, round-bottomed flask equipped with a thermometer and a reflux condenser were charged with 50 mmol of substituted styrene, 5 mL of chloroform, 0.2 g of triethylbenzylammonium chloride, 2.5 mL of methylene chloride, and a solution of 8 g of NaOH in 8 mL of water. The mixture was stirred vigorously. The temperature was allowed to rise to 40 °C and then kept between 40 and 45 °C by cooling with water. After about an hour, evolution of heat subsided, and the dark reaction mixture was heated to 55–60 °C for an additional hour. The products were transferred to a separatory funnel with 25 mL of water. The organic layer was separated and the aqueous phase extracted with petroleum ether. The organic fractions were combined, dried over anhydrous Na_2SO_4, filtered, concentrated in vacuo, and distilled through a Vigreux column.

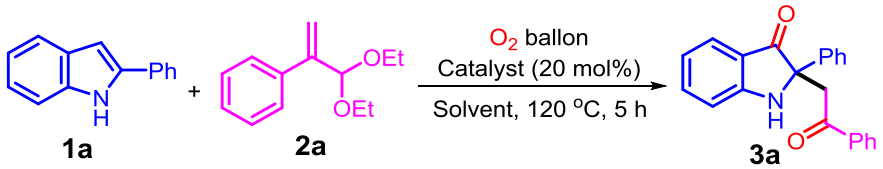
Step 2: the synthesis of atropaldehyde diethyl acetal.

A mixture of 10 mmol of 1,1-dichloro-2-arylcyclopropane, 1.6 g (40 mmol) of NaOH, and 16

mL of ethanol was placed in a flask fitted with a reflux condenser. The mixture was heated under reflux for 24 h. Some bumping might occur. Water (20 mL) was added, and the mixture was extracted with petroleum ether. The extracts were combined, dried over anhydrous Na_2SO_4, concentrated in vacuo, and distilled through a Vigreux column to give the corresponding substituted atropaldehyde diethyl acetal.

3. Optimization of the reaction conditions

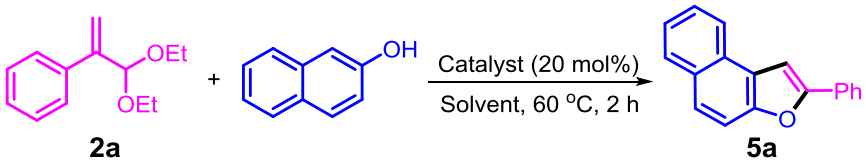
Table S1. Optimization of the reaction of **1a** and **2a** for the synthesis of **3a**.[a]



Entry	Catalyst	Oxidant	Solvent	Yield (%)[b]
1	—	O_2	DMSO	NR
2	$Sc(OTf)_3$	O_2	DMSO	Trace
3	$Fe(OTf)_3$	O_2	DMSO	ND
4	$Cu(OTf)_2$	O_2	DMSO	31
5	$CuCl_2$	O_2	DMSO	28
6	$Al(OTf)_3$	O_2	DMSO	58
7	$AlCl_3$	O_2	DMSO	37
8	$BF_3{\cdot}Et_2O$	O_2	DMSO	70
9	PTSA	O_2	DMSO	13
10[c]	$BF_3{\cdot}Et_2O$	TBHP	DMSO	41
11[c]	$BF_3{\cdot}Et_2O$	DTBP	DMSO	57
12[c]	$BF_3{\cdot}Et_2O$	$K_2S_2O_8$	DMSO	34
13	$BF_3{\cdot}Et_2O$	—	DMSO	43, (29)[d]
14	$BF_3{\cdot}Et_2O$	O_2	DMF	36
15	$BF_3{\cdot}Et_2O$	O_2	Toluene	39
16	$BF_3{\cdot}Et_2O$	O_2	PhCl	Messy
17	$BF_3{\cdot}Et_2O$	O_2	DMSO	(54, 30)[e]
18	$BF_3{\cdot}Et_2O$	O_2	DMSO	(39, 26)[f]

[a] Unless otherwise noted, all reactions were performed with **1a** (0.2 mmol), **2a** (0.2 mmol), catalyst (20 mol%), solvent (1 mL) at 120 °C under oxygen for 5 h. [b] Isolated yield; [c] Oxidant (1.2 equiv.). [d] Under nitrogen. [e] Performing the reaction at 100 °C and 140 °C. [f] Yields are with respect to the additives of ethanol and glycol (2.0 equiv.). TBHP = *tert*-Butyl hydroperoxide. DTBP = Di-*tert*-butyl peroxide.

Table S2. Optimization of the reaction of **2a** and β-naphthol for the synthesis of **5a**.[a]

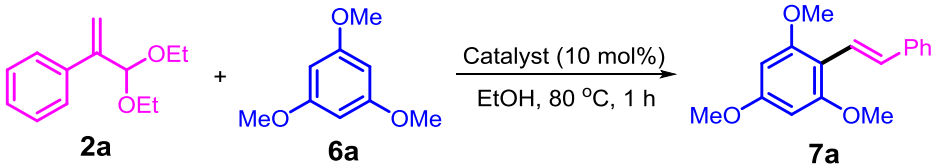


2a **5a**

Entry	Catalyst	Solvent	Yield (%)[b]
1	$Sc(OTf)_3$	EtOH	26
2	$Al(OTf)_3$	EtOH	76
3	$AlCl_3$	EtOH	22
4	$BiCl_3$	EtOH	ND
5	$BF_3{\cdot}Et_2O$	EtOH	8
6	PTSA	EtOH	ND
7	TFA	EtOH	18
8	$Al(OTf)_3$	CH_3CN	ND
9	$Al(OTf)_3$	1,4-Dioxane	39
10	$Al(OTf)_3$	DCE	24
11	$Al(OTf)_3$	IPA	68
12[c]	$Al(OTf)_3$	EtOH	43
13	$Al(OTf)_3$	EtOH	(36, 79)[d]

[a] Unless otherwise noted, all reactions were performed with **2a** (0.2 mmol), β-naphthol (0.3 mmol), catalyst (20 mol%), solvent (1 mL) at 60 °C under air condition for 2 h. [b] Isolated yield based on **2a**. [c] Performing the reaction at 80 °C. [d] Performing the reaction under nitrogen and oxygen atomosphere, respectively.IPA = Isopropyl alcohol. ND = No desired product.

Table S3. Optimization of the reaction of **2a** and **6a** for the synthesis of **7a**.[a]



2a **6a** **7a**

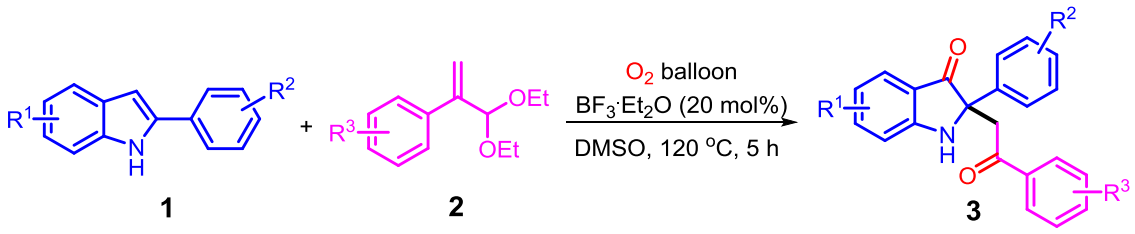
Entry	Catalyst	Solvent	Yield (%)[b]
1	$Sc(OTf)_3$	EtOH	22
2	$Fe(OTf)_3$	EtOH	Trace
3	$Al(OTf)_3$	EtOH	15
4	$Bi(OTf)_3$	EtOH	12
5	$Cu(OTf)_2$	EtOH	18
6	$AlCl_3$	EtOH	37
7	$BF_3{\cdot}Et_2O$	EtOH	31
8	PTSA	EtOH	11
9	$ZnBr_2$	EtOH	NR
10[c]	$AlCl_3$	EtOH	54
11[c]	$AlCl_3$	CH_3CN	Trace

12[c]	$AlCl_3$	1,4-Dioxane	Trace
13[c]	$AlCl_3$	DMSO	ND
14[c]	$AlCl_3$	Toluene	23
15[c,d]	$AlCl_3$	EtOH	72
16[c,d]	TFA	Toluene	(69, 65)[e]

[a] Unless otherwise noted, all reactions were performed with **2a** (0.2 mmol), **5a** (0.3 mmol), catalyst (10 mol%), solvent (1 mL) at 80 °C under air condition for 1 h. [b] Isolated yield based on **2a**. [c] $AlCl_3$ (0.04 mol, 20 mol%). [d] **5a**, 0.4 mmol. [e] Performing the reaction under nitrogen and oxygen atomosphere, respectively. ND = No desired product.

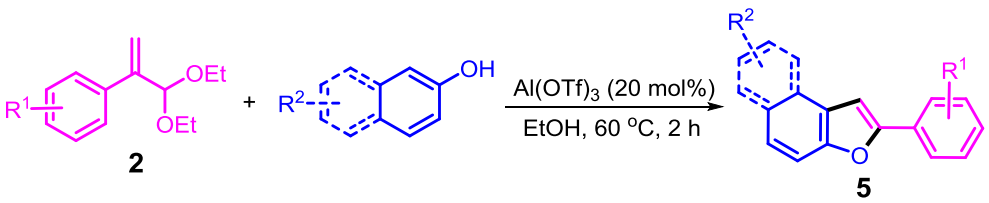
4. General procedure

4.1 General procedure for the synthesis of 2,2-disubstituted indolin-3-ones



The reactions were conducted in a 10 mL of V-type flask equipped with oil bath and triangle magnetic stirring. The mixture of **1** (0.2 mmol), **2** (0.2 mmol) and $BF_3{\cdot}Et_2O$ (0.04 mmol, 20 mol%) charged with an O_2 balloon in DMSO (1.0 mL) was stirred at 120 °C for 5 h. After the completion of the reaction, the mixture cooled to room temperature, and the resulting mixture was washed with saturated $NaHCO_3$ solution, extracted with ethyl acetate, dried over anhydrous sodium sulfate, and then concentrated by removing the solvent under vacuum. Finally, the residue was purified by silica gel column chromatography using PE/EtOAc as eluent to afford the desired product.

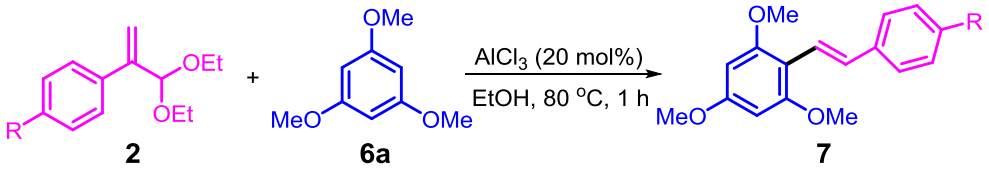
4.2 General procedure for the synthesis of naphthofurans



The reactions were conducted in a 10 mL of V-type flask equipped with oil bath and triangle magnetic stirring. The mixture of **2** (0.2 mmol), β-naphthol (0.3 mmol) and $Al(OTf)_3$ (0.04 mmol, 20 mol%) in EtOH (1.0 mL) was stirred at 60 °C for 2 h. After the completion of the reaction, the mixture cooled to room temperature, and the resulting mixture was washed with saturated

$NaHCO_3$ solution, extracted with ethyl acetate, dried over anhydrous sodium sulfate, and then concentrated by removing the solvent under vacuum. Finally, the residue was purified by silica gel column chromatography using PE as eluent to afford the desired product.

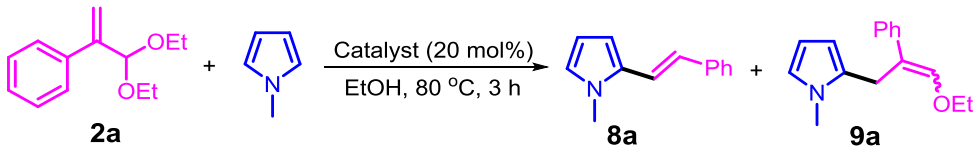
4.3 General procedure for the synthesis of stilbenes



The reactions were conducted in a 10 mL of V-type flask equipped with oil bath and triangle magnetic stirring. The mixture of **2** (0.2 mmol), **5a** (0.4 mmol) and $AlCl_3$ (0.04 mmol, 20 mol%) in EtOH (1.0 mL) was stirred at 80 °C for 1 h. After the completion of the reaction, the mixture cooled to room temperature, and the resulting mixture was washed with saturated $NaHCO_3$ solution, extracted with ethyl acetate, dried over anhydrous sodium sulfate, and then concentrated by removing the solvent under vacuum. Finally, the residue was purified by silica gel column chromatography using PE/EtOAc as eluent to afford the desired product.

5 Sluggish reactions of other nucleophiles with atropaldehyde acetal

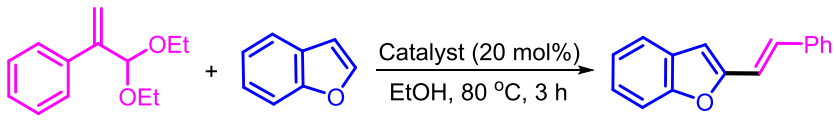
Table S4. Optimization of the reaction of **2a** and *N*-methyl pyrrole for the synthesis of **8a**.[a]



Entry	Catalyst	Yield (%)[b]
1	$Sc(OTf)_3$	Messy
2	$Al(OTf)_3$	Messy
3	$Fe(OTf)_3$	Messy
4	$AlCl_3$	23 (**9a**)
5	$BiCl_3$	ND
6	$BF_3{\cdot}Et_2O$	34 (**9a**)
7	PTSA	Trace
8	TFA	Trace

[a] Unless otherwise noted, all reactions were performed with **2a** (0.2 mmol), *N*-methyl pyrrole (0.4 mmol), catalyst (20 mol%), solvent (1 mL) at 80 °C under air condition for 3 h. [b] Isolated yield based on **2a**. ND = No desired product.

Table S5. Optimization of the reaction of **2a** and benzofuran for the synthesis of **10a**.[a]

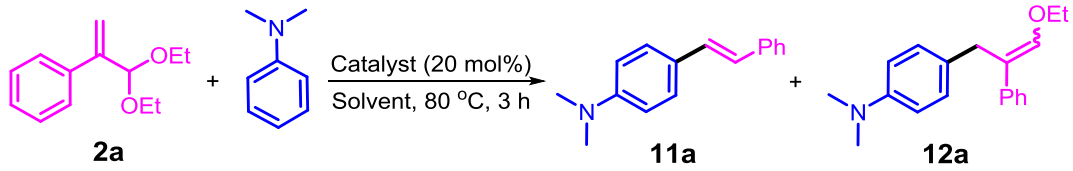


2a **10a**

Entry	Catalyst	Yield (%)[b]
1	$Sc(OTf)_3$	Trace
2	$Al(OTf)_3$	Trace
3	$Ni(OTf)_2$	Trace
4	$AlCl_3$	NR
5	$BiCl_3$	Messy
6	$CuCl_2$	ND
7	$BF_3{\cdot}Et_2O$	Trace
8	PTSA	ND
9	TFA	Trace

[a] Unless otherwise noted, all reactions were performed with **2a** (0.2 mmol), benzofuran (0.4 mmol), catalyst (20 mol%), solvent (1 mL) at 80 °C under air condition for 3 h. [b] Isolated yield based on **2a**. ND = No desired product.

Table S6. Optimization of the reaction of **2a** and *N*,*N*-dimethylaniline for the synthesis of **11a**.[a]



2a **11a** **12a**

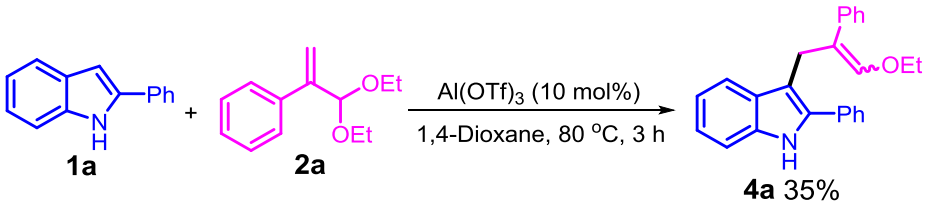
Entry	Catalyst	Solvent	Yield (%)[b]
1	$Al(OTf)_3$	EtOH	Messy
2	$Fe(OTf)_3$	EtOH	Messy
3	$Cu(OTf)_2$	EtOH	Messy
4	$Bi(OTf)_3$	EtOH	37 (**16a**)
5	$AlCl_3$	EtOH	Messy
6	$BF_3{\cdot}Et_2O$	EtOH	Trace
7	TFA	EtOH	Trace
8	$Bi(OTf)_3$	IPA	Trace
9	$Bi(OTf)_3$	1,4-Dioxane	ND
10	$Bi(OTf)_3$	Toluene	28 (**16a**)

[a] Unless otherwise noted, all reactions were performed with **2a** (0.2 mmol), *N*,*N*-dimethylaniline (0.4 mmol), catalyst (20 mol%), solvent (1 mL) at 80 °C under air condition for 3 h. [b] Isolated yield based on **2a**. ND = No desired product.

6 Mechanism study

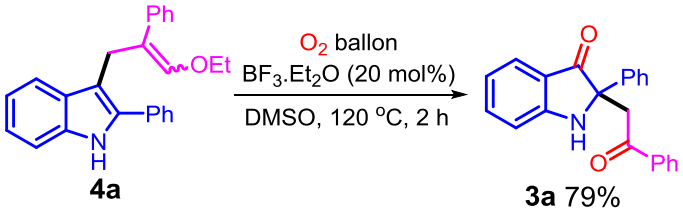
6.1 Control experiments

(1) The synthesis of **4a**



The reactions were conducted in a 10 mL of V-type flask equipped with oil bath and triangle magnetic stirring. The mixture of **1a** (0.2 mmol), **2a** (0.2 mmol) and $Al(OTf)_3$ (0.02 mmol, 10 mol%) in 1,4-Dioxane (1.0 mL) was stirred at 80 °C for 3 h. After the completion of the reaction, the mixture cooled to room temperature, and the resulting mixture was washed with saturated $NaHCO_3$ solution, extracted with ethyl acetate, dried over anhydrous sodium sulfate, and then concentrated by removing the solvent under vacuum. Finally, the residue was purified by silica gel column chromatography using PE/EtOAc as eluent to afford the desired product **4a** in 35% yield.

(2) The transformation of **4a** to **3a**



The reactions were conducted in a 10 mL of V-type flask equipped with oil bath and triangle magnetic stirring. The mixture of **4a** (0.2 mmol) and $BF_3{\cdot}Et_2O$ (0.04 mmol, 20 mol%) charged with an O_2 balloon in DMSO (1.0 mL) was stirred at 120 °C for 2 h. After the completion of the reaction, the mixture cooled to room temperature, and the resulting mixture was washed with saturated $NaHCO_3$ solution, extracted with ethyl acetate, dried over anhydrous sodium sulfate, and then concentrated by removing the solvent under vacuum. Finally, the residue was purified by silica gel column chromatography using PE/EtOAc as eluent to afford the desired product **3a** in 79% yield.

6.2 Kinetic analysis based on the conversion of 1a and yields of 3a over time

The reactions were conducted in seven 10 mL of V-type flasks equipped with oil bath and triangle magnetic stirring. The mixture of **1a** (0.2 mmol), **2a** (0.2 mmol) and $BF_3{\cdot}Et_2O$ (0.04 mmol, 20

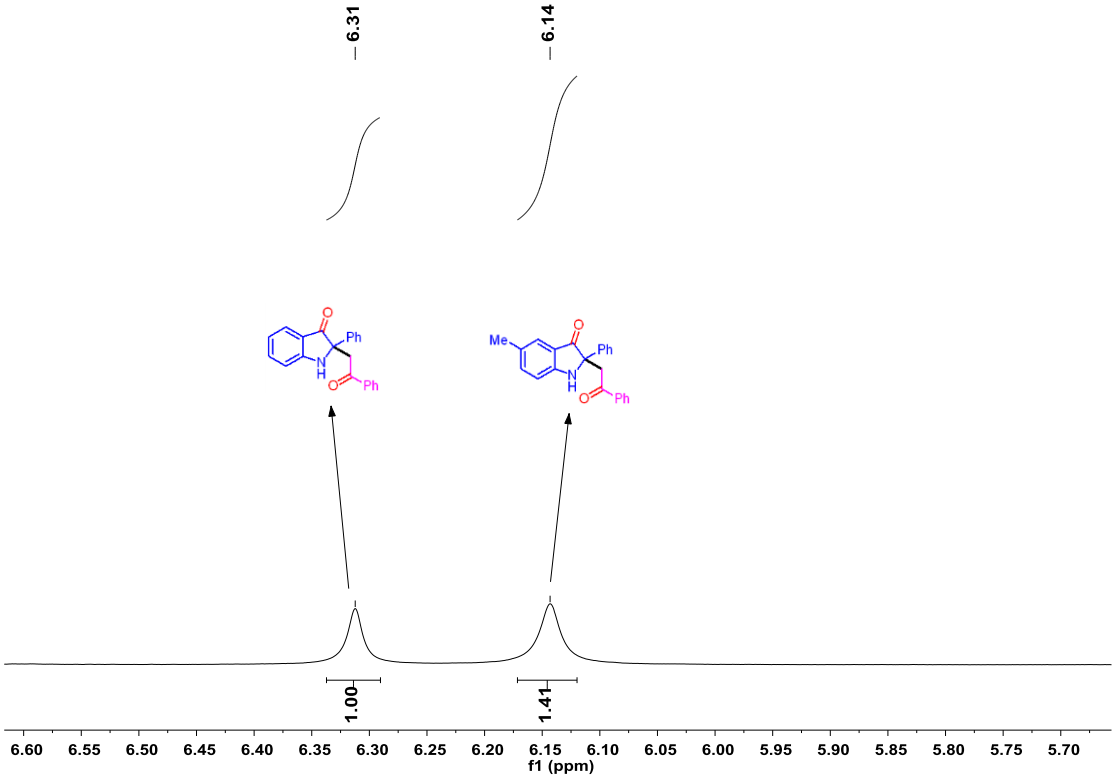
mol%) charged with an O_2 balloon in DMSO (1.0 mL) was stirred at 120 °C in each V-type flask. Each flask was taken out from the oil bath at the certain amount of time intervals. After the completion of the reaction, the mixture cooled to room temperature, and the resulting mixture was isolated by silica gel column chromatography to determine the conversion of 2-phenylindole **1a** and the yield of product **3a**.

Entry	Time (h)	Conversion (%)	Yield (%)
1	0.5	47	15
2	1	55	26
3	1.5	67	33
4	2	81	41
5	3	97	53
6	4	97	64
7	5	97	70

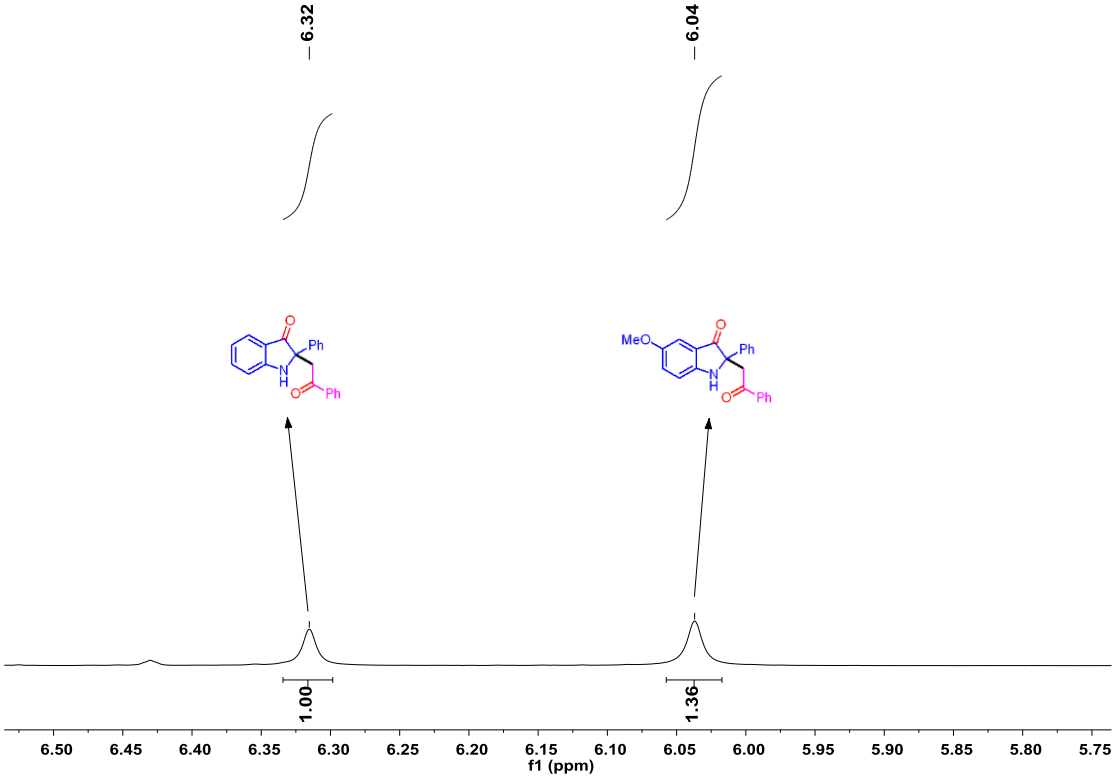
6.3 Competitive experiments

The mixture of **1a** (0.2 mmol), **1** (0.2 mmol), **2a** (0.2 mmol) and $BF_3{\cdot}Et_2O$ (0.04 mmol, 20 mol%) charged with an O_2 balloon in DMSO (1.0 mL) was stirred at 120 °C for 5 h. The product ratio of **3a** and **3** was determined based on the mixture ^{1}H NMR analyses in $CDCl_3$.

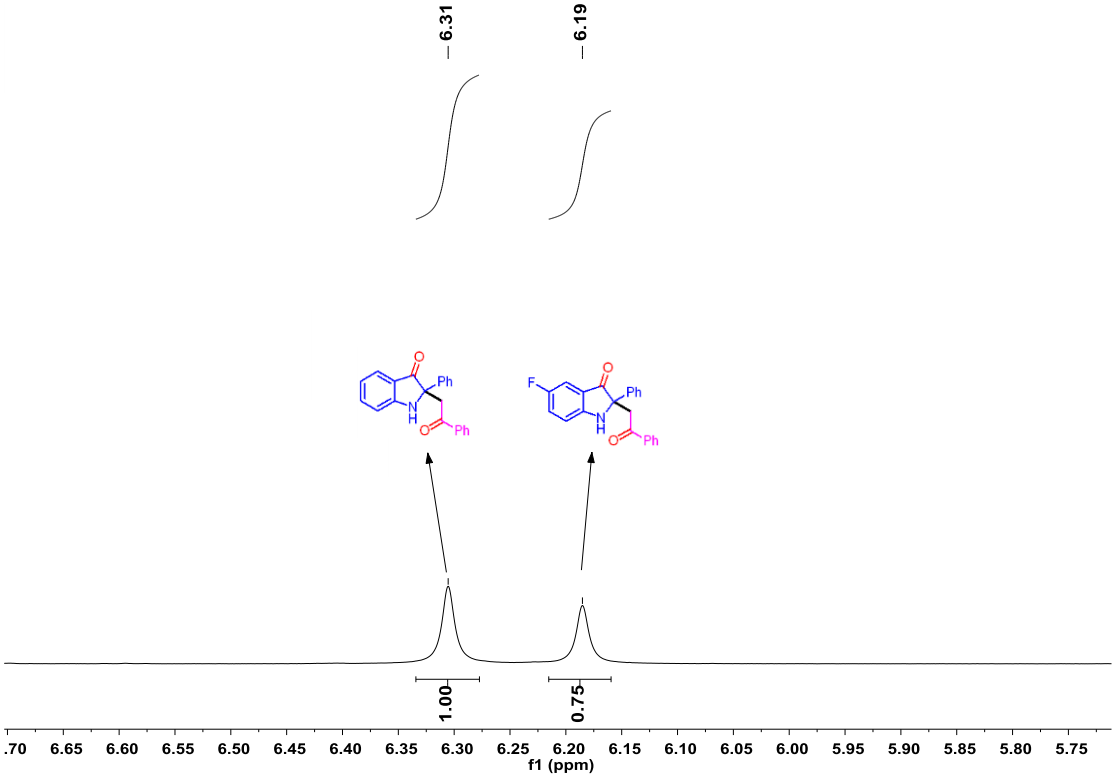
(1) ^{1}H NMR for the reaction of **1a**, **1l** and **2a** in $CDCl_3$



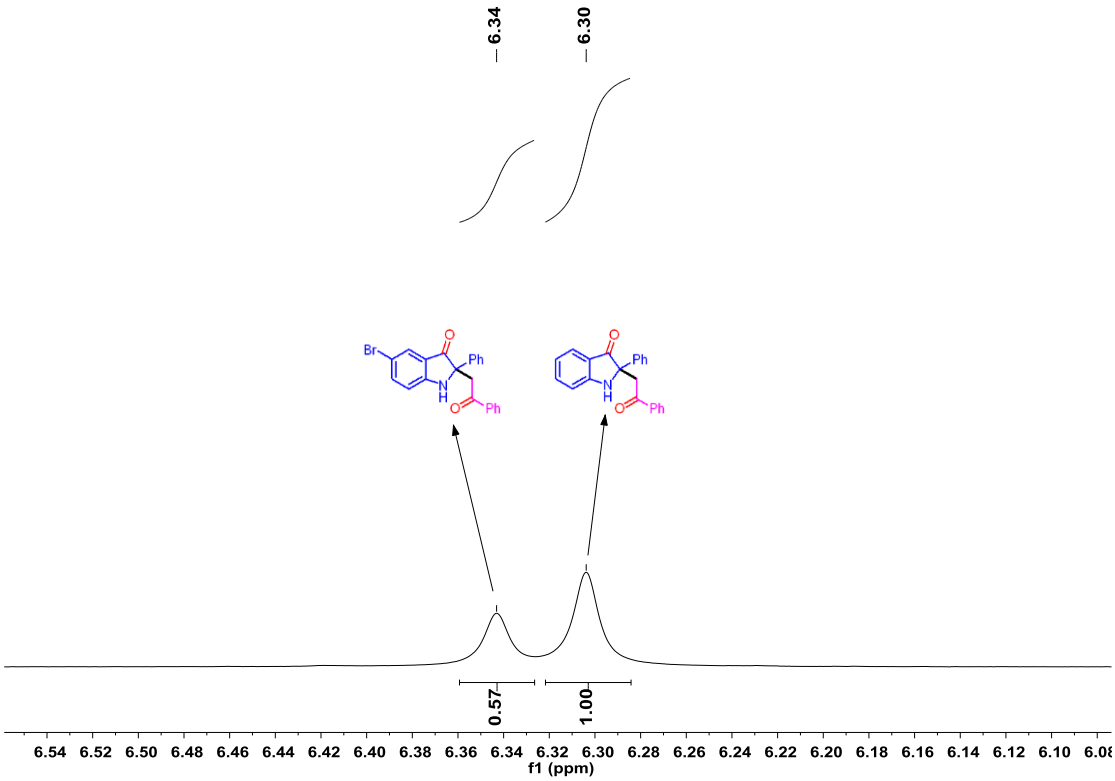
(2) ^{1}H NMR for the reaction of **1a**, **1m** and **2a** in $CDCl_3$



(3) ^{1}H NMR for the reaction of **1a**, **1n** and **2a** in $CDCl_3$



(4) ^{1}H NMR for the reaction of **1a**, **1p** and **2a** in $CDCl_3$



6.4 The key intermediates detected by HRMS for the synthesis of 2,2-disubstituted indolin-3-ones

The reactions were conducted in a 10 mL of V-type flask equipped with oil bath and triangle magnetic stirring. The mixture of **1a** (0.2 mmol), **2a** (0.2 mmol) and $BF_3{\cdot}Et_2O$ (0.04 mmol, 20 mol%) charged with an O_2 balloon in DMSO (1.0 mL) was stirred at 120 ℃ for 3 h. After the completion of the reaction, the mixture cooled to room temperature, and the resulting mixture was extracted with ethyl acetate, washed with water, and then the crude mixture was detected by HRMS.

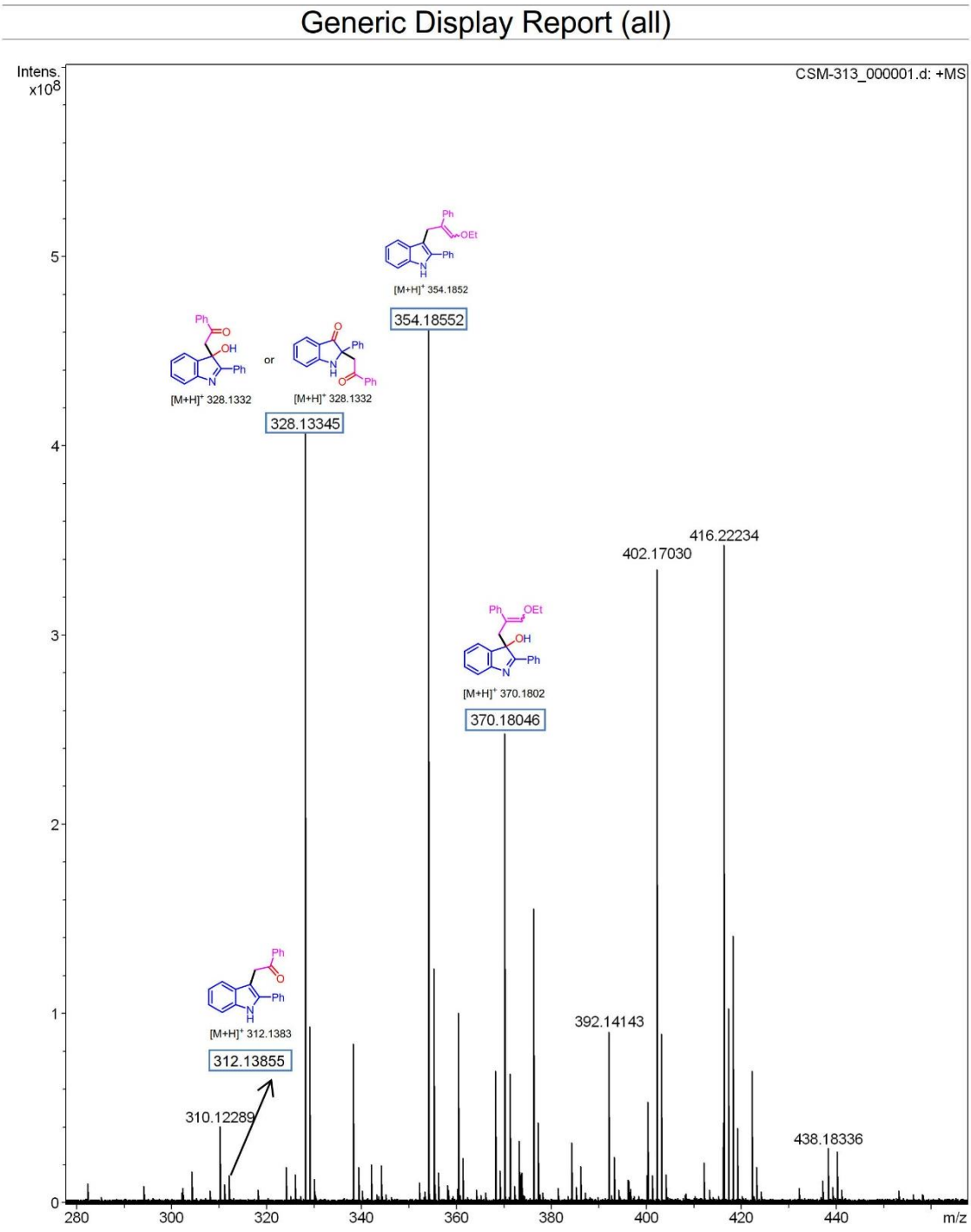


Figure S1. The key intermediates detected by HRMS after 3 h of the reaction.

6.5 The key intermediates detected by HRMS for the synthesis of stilbene

The reactions were conducted in a 10 mL of V-type flask equipped with oil bath and triangle magnetic stirring. The mixture of **2a** (0.2 mmol), **5a** (0.4 mmol) and $AlCl_3$ (0.04 mmol, 20 mol%) in EtOH (1.0 mL) was stirred at 80 °C for 20 min. After the completion of the reaction, the mixture cooled to room temperature, and the crude mixture was detected by HRMS.

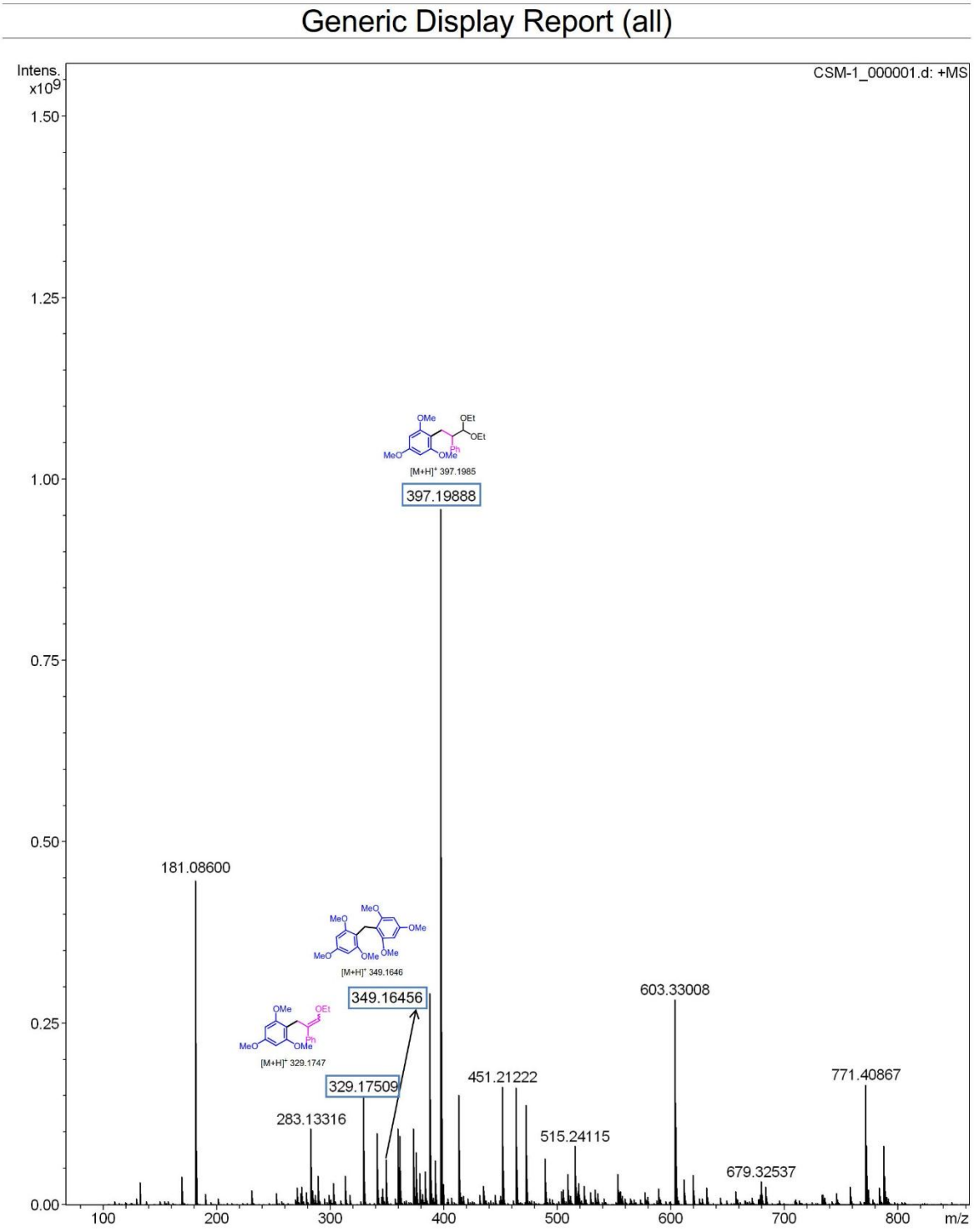


Figure S2. The key intermediates detected by HRMS after 20 min of the reaction.

7 X-ray crystallographic data

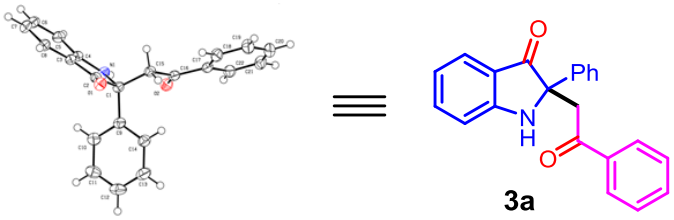
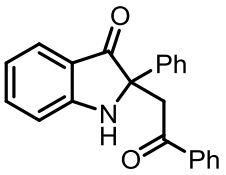


Figure S3. The X-ray diffraction structure of **3a**.

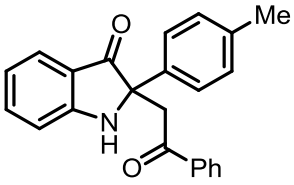
Table S7. Crystal data and structure refinement for 3a.

Identification code	2317
Empirical formula	$C_{22}H_{17}NO_2$
Formula weight	327.36
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.4881(8)
b/Å	12.4082(7)
c/Å	10.0756(6)
α/°	90
β/°	100.714(6)
γ/°	90
Volume/Å^3	1656.89(17)
Z	4
ρ_{calc}g/cm^3	1.312
μ/mm^{-1}	0.669
F(000)	688.0
Crystal size/mm^3	0.11 × 0.1 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.67 to 147.138
Index ranges	-16 ≤ h ≤ 12, -11 ≤ k ≤ 15, -11 ≤ l ≤ 12
Reflections collected	6716
Independent reflections	3252 [R_{int} = 0.0324, R_{sigma} = 0.0421]
Data/restraints/parameters	3252/0/226
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0511, wR_2 = 0.1287
Final R indexes [all data]	R_1 = 0.0618, wR_2 = 0.1379
Largest diff. peak and hole	0.25and -0.31 e.Å^{-3}

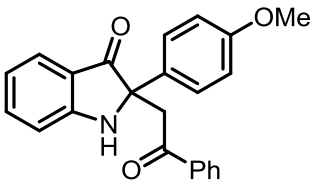
8 Characterization data of products



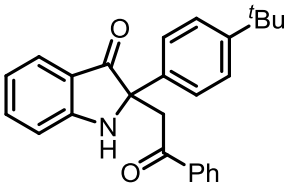
2-(2-Oxo-2-phenylethyl)-2-phenylindolin-3-one (**3a**)[4]: yellow solid (46 mg, 70% yield), mp: 148–150 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.91 (d, J = 7.4 Hz, 2H), 7.65–7.52 (m, 4H), 7.52–7.41 (m, 3H), 7.28 (t, J = 7.5 Hz, 2H), 7.21 (t, J = 7.2 Hz, 1H), 6.96 (d, J = 8.3 Hz, 1H), 6.80 (t, J = 7.4 Hz, 1H), 6.30 (s, 1H), 4.44 (d, J = 17.9 Hz, 1H), 3.18 ppm (d, J = 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.8, 197.9, 160.4, 138.2, 137.9, 136.7, 133.9, 128.9, 128.8, 128.2, 127.7, 125.8, 125.5, 119.0, 118.3, 111.9, 69.4, 44.9 ppm.



2-(2-Oxo-2-phenylethyl)-2-(p-tolyl)indolin-3-one (**3b**)[5]: yellow solid (40 mg, 58% yield), mp: 205–207 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.92 (d, J = 7.3 Hz, 2H), 7.57 (dd, J = 7.6, 5.4 Hz, 2H), 7.50–7.40 (m, 5H), 7.08 (d, J = 8.0 Hz, 2H), 6.95 (d, J = 8.2 Hz, 1H), 6.80 (t, J = 7.4 Hz, 1H), 6.27 (s, 1H), 4.42 (d, J = 18.0 Hz, 1H), 3.16 (d, J = 18.0 Hz, 1H), 2.26 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.9, 198.0, 160.4, 137.8, 137.4, 136.8, 135.1, 133.8, 129.6, 128.9, 128.3, 125.8, 125.3, 118.9, 118.3, 111.9, 69.3, 44.7, 21.1 ppm.

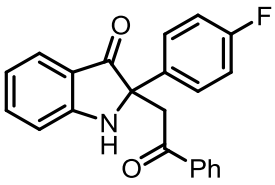


2-(4-Methoxyphenyl)-2-(2-oxo-2-phenylethyl)indolin-3-one (**3c**)[5]: yellow solid (34 mg, 47% yield), mp: 127–129 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.92 (d, J = 7.3 Hz, 2H), 7.57 (td, J = 7.3, 1.3 Hz, 2H), 7.51–7.42 (m, 5H), 6.95 (d, J = 8.2 Hz, 1H), 6.80 (dd, J = 8.2, 6.5 Hz, 3H), 6.28 (s, 1H), 4.39 (d, J = 17.9 Hz, 1H), 3.73 (s, 3H), 3.14 ppm (d, J = 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 201.1, 198.1, 160.3, 159.2, 137.9, 136.8, 133.9, 130.1, 128.9, 128.3, 126.7, 125.8, 118.9, 118.3, 114.3, 111.9, 69.0, 55.4, 44.7 ppm; IR (KBr) ν = 3384, 2932, 2836, 1687, 1618, 1510, 1251, 752, 690, 513 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{23}H_{20}NO_3$, $[M + H]^+$ 358.1438, found 358.1436.

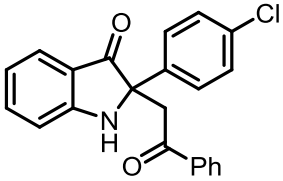


2-(4-(*tert*-Butyl)phenyl)-2-(2-oxo-2-phenylethyl)indolin-3-one (**3d**): yellow solid (34 mg, 44% yield), mp: 185–187 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.92 (d, J = 7.4 Hz, 2H), 7.56 (t, J = 7.5 Hz, 2H), 7.45 (p, J = 7.4 Hz, 5H), 7.29–7.25 (m, 2H), 6.95 (d, J = 8.2 Hz, 1H), 6.79 (t, J = 7.4 Hz, 1H), 6.27 (s, 1H), 4.42 (d, J = 17.9 Hz, 1H), 3.18 (d, J = 18.0 Hz, 1H), 1.23 ppm (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 201.1, 198.0, 160.4, 150.4, 137.8,

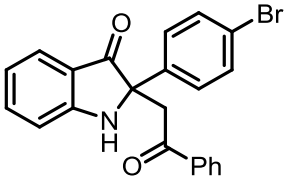
136.7, 135.0, 133.8, 128.8, 128.2, 125.8, 125.7, 125.0, 118.9, 118.4, 111.9, 69.3, 44.7, 34.5, 31.4 ppm; IR (KBr) ν = 3385, 2962, 2905, 2867, 1685, 1620, 1489, 1217, 754, 690, 508 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{26}H_{26}NO_2$, $[M + H]^+$ 384.1958, found 384.1956.



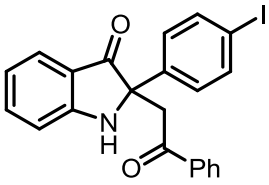
2-(4-Fluorophenyl)-2-(2-oxo-2-phenylethyl)indolin-3-one (**3e**)[6]: yellow solid (46 mg, 67% yield), mp: 151–153 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.90 (d, J = 7.3 Hz, 2H), 7.62–7.52 (m, 4H), 7.50 (ddd, J = 8.4, 7.0, 1.3 Hz, 1H), 7.45 (t, J = 7.8 Hz, 2H), 6.96 (dt, J = 8.7, 4.5 Hz, 3H), 6.82 (t, J = 7.4 Hz, 1H), 6.33 (s, 1H), 4.39 (d, J = 17.9 Hz, 1H), 3.14 ppm (d, J = 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.7, 198.0, 163.7 (d, $^1J_{C\text{-}F}$ = 245 Hz), 160.2, 138.1, 136.6, 134.0, 133.9 (d, $^4J_{C\text{-}F}$ = 3 Hz), 130.1 (d, $^3J_{C\text{-}F}$ = 8 Hz), 128.9, 128.2, 127.4 (d, $^3J_{C\text{-}F}$ = 8 Hz), 125.8, 119.9 (d, $^2J_{C\text{-}F}$ = 18 Hz), 119.2, 118.1, 115.7 (d, $^2J_{C\text{-}F}$ = 21 Hz), 112.0, 68.9, 45.0 ppm; ^{19}F NMR (377 MHz, $CDCl_3$, 25 °C) δ = -115.4 (m, 1F) ppm; IR (KBr) ν = 3385, 2921, 2849, 1687, 1619, 1507, 1219, 752, 513 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{22}H_{17}FNO_2$, $[M + H]^+$ 346.1238, found 346.1236.



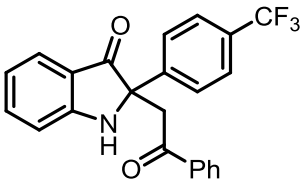
2-(4-Chlorophenyl)-2-(2-oxo-2-phenylethyl)indolin-3-one (**3f**)[5]: yellow solid (56 mg, 78% yield), mp: 153–155 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.90 (d, J = 7.4 Hz, 2H), 7.58 (dt, J = 7.5, 3.6 Hz, 2H), 7.48 (dt, J = 21.6, 8.1 Hz, 5H), 7.24 (d, J = 8.7 Hz, 2H), 6.96 (d, J = 8.3 Hz, 1H), 6.82 (t, J = 7.4 Hz, 1H), 6.31 (s, 1H), 4.38 (d, J = 18.0 Hz, 1H), 3.15 ppm (d, J = 18.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.4, 197.9, 160.2, 138.1, 136.9, 136.5, 134.1, 133.7, 128.9, 128.9, 128.2, 127.1, 125.8, 119.2, 118.1, 112.0, 69.0, 44.9 ppm.



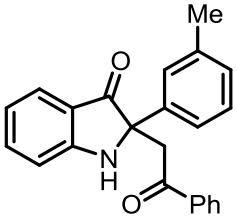
2-(4-Bromophenyl)-2-(2-oxo-2-phenylethyl)indolin-3-one (**3g**): yellow solid (53 mg, 66% yield), mp: 164–166 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.90 (d, J = 7.4 Hz, 2H), 7.62–7.55 (m, 2H), 7.53–7.43 (m, 5H), 7.40 (d, J = 8.6 Hz, 2H), 6.96 (d, J = 8.3 Hz, 1H), 6.82 (t, J = 7.4 Hz, 1H), 6.31 (s, 1H), 4.38 (d, J = 18.0 Hz, 1H), 3.15 ppm (d, J = 18.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.3, 197.8, 160.2, 138.1, 137.4, 136.5, 134.1, 131.9, 128.9, 128.2, 127.4, 125.8, 121.9, 119.3, 118.0, 112.0, 69.0, 44.9 ppm; IR (KBr) ν = 3385, 2923, 2852, 1685, 1618, 1487, 1217, 1006, 753, 516 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{22}H_{17}BrNO_2$, $[M + H]^+$ 406.0437, found 406.0436.



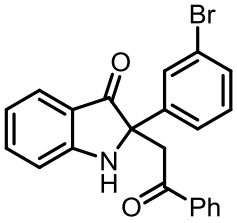
2-(4-Iodophenyl)-2-(2-oxo-2-phenylethyl)indolin-3-one (**3h**): yellow solid (34 mg, 38% yield), mp: 176–178 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.90 (d, J = 7.3 Hz, 2H), 7.62–7.56 (m, 4H), 7.50 (ddd, J = 8.4, 7.1, 1.3 Hz, 1H), 7.46 (t, J = 7.7 Hz, 2H), 7.32 (d, J = 8.6 Hz, 2H), 6.96 (d, J = 8.3 Hz, 1H), 6.82 (t, J = 7.5 Hz, 1H), 6.28 (s, 1H), 4.37 (d, J = 18.1 Hz, 1H), 3.14 ppm (d, J = 18.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.2, 197.8, 160.2, 138.2, 138.1, 137.8, 136.5, 134.1, 129.0, 128.2, 127.6, 125.8, 119.3, 118.0, 112.0, 93.6, 69.1, 44.8 ppm; IR (KBr) ν = 3384, 2920, 1684, 1618, 1486, 1218, 1003, 753, 515 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{22}H_{17}INO_2$, $[M + H]^+$ 454.0298, found 454.0297.



2-(2-Oxo-2-phenylethyl)-2-(4-(trifluoromethyl)phenyl)indolin-3-one (**3i**): yellow solid (46 mg, 59% yield), mp: 171–173 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.91 (d, J = 7.3 Hz, 2H), 7.71 (d, J = 8.2 Hz, 2H), 7.61–7.50 (m, 5H), 7.46 (t, J = 7.7 Hz, 2H), 6.99 (d, J = 8.3 Hz, 1H), 6.84 (t, J = 7.4 Hz, 1H), 6.35 (s, 1H), 4.44 (d, J = 18.1 Hz, 1H), 3.20 ppm (d, J = 18.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.0, 197.7, 160.3, 142.4, 138.3, 136.4, 134.2, 129.7, 128.8 (q, $^{2}J_{C\text{-}F}$ = 52.0 Hz), 127.4 (q, $^{1}J_{C\text{-}F}$ = 269.0 Hz), 126.4, 126.1, 125.9, 125.8 (q, $^{3}J_{C\text{-}F}$ = 4 Hz), 119.4, 117.9, 112.1, 69.2, 45.1 ppm; ^{19}F NMR (377 MHz, $CDCl_3$, 25 °C) δ = -62.6 (s, 3F) ppm; IR (KBr) ν = 3383, 2923, 2851, 1687, 1619, 1326, 1125, 1070, 753, 515 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{23}H_{17}F_3NO_2$, $[M + H]^+$ 396.1206, found 396.1204.

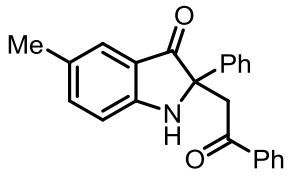


2-(2-Oxo-2-phenylethyl)-2-(m-tolyl)indolin-3-one (**3j**): yellow solid (30 mg, 45% yield), mp: 157–159 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.92 (d, J = 7.3 Hz, 2H), 7.57 (t, J = 7.4 Hz, 2H), 7.51–7.42 (m, 3H), 7.33 (d, J = 6.8 Hz, 2H), 7.17 (t, J = 8.0 Hz, 1H), 7.02 (d, J = 7.5 Hz, 1H), 6.96 (d, J = 8.3 Hz, 1H), 6.80 (t, J = 7.4 Hz, 1H), 6.27 (s, 1H), 4.43 (d, J = 17.9 Hz, 1H), 3.17 (d, J = 17.9 Hz, 1H), 2.28 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.9, 197.9, 160.4, 138.4, 138.0, 137.9, 136.7, 133.8, 128.9, 128.7, 128.6, 128.2, 126.1, 125.8, 122.5, 118.9, 118.3, 111.9, 69.4, 44.9, 21.8 ppm; IR (KBr) ν = 3384, 2920, 2859, 1687, 1618, 1488, 1217, 752, 689, 507 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{23}H_{20}NO_2$, $[M + H]^+$ 342.1489, found 342.1487.

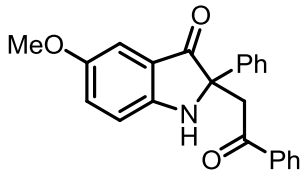


2-(3-Bromophenyl)-2-(2-oxo-2-phenylethyl)indolin-3-one (**3k**): yellow

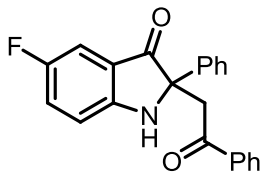
solid (62 mg, 77% yield), mp: 179–181 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.90 (d, *J* = 7.4 Hz, 2H), 7.73 (t, *J* = 1.9 Hz, 1H), 7.60–7.55 (m, 2H), 7.53–7.48 (m, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 1H), 7.15 (t, *J* = 7.9 Hz, 1H), 6.97 (d, *J* = 8.3 Hz, 1H), 6.82 (t, *J* = 7.4 Hz, 1H), 6.30 (s, 1H), 4.36 (d, *J* = 18.0 Hz, 1H), 3.16 ppm (d, *J* = 18.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.1, 197.7, 160.2, 140.7, 138.2, 136.5, 134.0, 130.8, 130.3, 128.9, 128.8, 128.2, 125.8, 124.3, 123.0, 119.3, 118.0, 112.1, 68.9, 45.1 ppm; IR (KBr) *v* = 3384, 2921, 2848, 1685, 1618, 1488, 1218, 753, 689, 507 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{22}H_{17}BrNO_2$, $[M + H]^+$ 406.0437, found 406.0436.



5-Methyl-2-(2-oxo-2-phenylethyl)-2-phenylindolin-3-one (**3l**)[5]: yellow solid (46 mg, 68% yield), mp: 181–183 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.91 (d, *J* = 7.3 Hz, 2H), 7.55 (dd, *J* = 15.3, 7.6 Hz, 3H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.37 (s, 1H), 7.33 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.27 (t, *J* = 6.8 Hz, 2H), 7.22–7.18 (m, 1H), 6.89 (d, *J* = 8.3 Hz, 1H), 6.14 (s, 1H), 4.42 (d, *J* = 17.9 Hz, 1H), 3.18 (d, *J* = 17.9 Hz, 1H), 2.28 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.9, 197.9, 158.9, 139.4, 138.4, 136.7, 133.8, 128.8, 128.8, 128.5, 128.2, 127.6, 125.4, 125.0, 118.4, 111.9, 69.8, 44.9, 20.6 ppm.

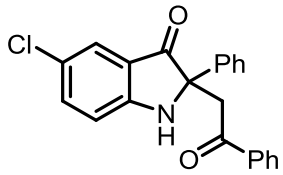


5-Methoxy-2-(2-oxo-2-phenylethyl)-2-phenylindolin-3-one (**3m**)[6]: yellow solid (39 mg, 56% yield), mp: 203–205 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.92 (d, *J* = 7.3 Hz, 2H), 7.56 (dd, *J* = 13.2, 7.4 Hz, 3H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.28 (s, 2H), 7.25–7.16 (m, 2H), 7.01 (d, *J* = 2.5 Hz, 1H), 6.94 (d, *J* = 8.8 Hz, 1H), 6.01 (s, 1H), 4.41 (d, *J* = 17.8 Hz, 1H), 3.76 (s, 3H), 3.21 ppm (d, *J* = 17.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 201.0, 197.9, 156.3, 153.5, 138.4, 136.8, 133.8, 128.9, 128.8, 128.6, 128.3, 127.7, 125.5, 118.5, 113.5, 105.4, 70.4, 56.0, 45.0 ppm; IR (KBr) *v* = 3392, 2920, 2849, 1685, 1497, 1448, 1216, 753, 527 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{23}H_{20}NO_3$, $[M + H]^+$ 358.1438, found 358.1436.

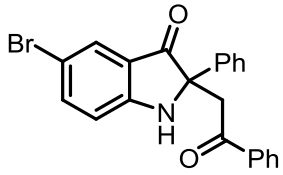


5-Fluoro-2-(2-oxo-2-phenylethyl)-2-phenylindolin-3-one (**3n**)[5]: yellow solid (43 mg, 62% yield), mp: 150–152 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.91 (d, *J* = 7.3 Hz, 2H), 7.60–7.52 (m, 3H), 7.44 (t, J = 7.7 Hz, 2H), 7.32–7.25 (m, 3H), 7.25–7.21 (m, 2H), 6.93 (dd, *J* = 8.7, 3.6 Hz, 1H), 6.18 (s, 1H), 4.40 (d, *J* = 17.9 Hz, 1H), 3.21 ppm (d, *J* = 17.9 Hz, 1H); ^{13}C NMR (100

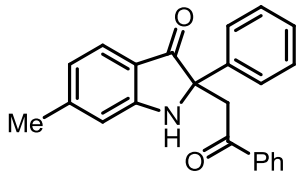
MHz, $CDCl_3$, 25 °C) δ = 200.6 (d, $^4J_{C\text{-}F}$ = 3.0 Hz, C=O), 197.7 (C=O), 157.7 (d, $^1J_{C\text{-}F}$ = 238.0 Hz), 157.0, 137.9, 136.6, 133.9, 128.9, 128.3, 127.9, 126.1 (d, $^2J_{C\text{-}F}$ = 26.0 Hz), 125.4, 118.8 (d, $^3J_{C\text{-}F}$ = 7.0 Hz), 113.1 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 110.5 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 70.5, 45.0 ppm; ^{19}F NMR (377 MHz, $CDCl_3$, 25 °C) δ = -125.0 (sextet, 1F) ppm.



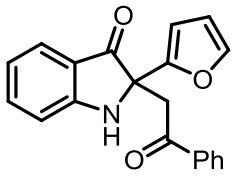
5-Chloro-2-(2-oxo-2-phenylethyl)-2-phenylindolin-3-one (**3o**)[5]: yellow solid (40 mg, 56% yield), mp: 146–148 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ = 7.91 (d, J = 7.4 Hz, 2H), 7.58 (t, J = 7.4 Hz, 1H), 7.52 (d, J = 8.6 Hz, 3H), 7.47–7.41 (m, 3H), 7.29 (t, J = 7.4 Hz, 2H), 7.23 (t, J = 7.2 Hz, 1H), 6.92 (d, J = 8.7 Hz, 1H), 6.32 (s, 1H), 4.42 (d, J = 17.9 Hz, 1H), 3.20 ppm (d, J = 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 199.6, 197.7, 158.6, 137.8, 137.7, 136.6, 134.0, 128.9, 128.9, 128.3, 127.9, 125.4, 125.0, 124.2, 119.4, 113.1, 70.2, 44.9 ppm.



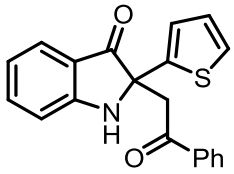
5-Bromo-2-(2-oxo-2-phenylethyl)-2-phenylindolin-3-one (**3p**): yellow solid (60 mg, 74% yield), mp: 154–156 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ = 7.91 (d, J = 7.3 Hz, 2H), 7.69 (d, J = 1.8 Hz, 1H), 7.60–7.50 (m, 4H), 7.45 (t, J = 7.7 Hz, 2H), 7.29 (t, J = 7.4 Hz, 2H), 7.23 (t, J = 7.2 Hz, 1H), 6.87 (d, J = 8.7 Hz, 1H), 6.34 (s, 1H), 4.42 (d, J = 17.9 Hz, 1H), 3.20 ppm (d, J = 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 199.4, 197.7, 158.8, 140.3, 137.6, 136.5, 134.0, 129.0, 128.9, 128.3, 128.1, 127.9, 125.34, 120.0, 113.5, 111.0, 70.1, 44.8 ppm; IR (KBr) ν = 3382, 2920, 2849, 1687, 1613, 1474, 1217, 1167, 753, 697, 509 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{22}H_{17}BrNO_2$, $[M + H]^+$ 406.0437, found 406.0436.



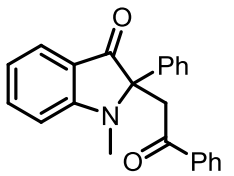
6-Methyl-2-(2-oxo-2-phenylethyl)-2-phenylindolin-3-one (**3q**)[6]: yellow solid (34 mg, 51% yield), mp: 160–162 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ = 7.92 (d, J = 7.3 Hz, 2H), 7.55 (dd, J = 12.2, 7.5 Hz, 3H), 7.48–7.42 (m, 3H), 7.28 (d, J = 7.2 Hz, 2H), 7.25 (s, 1H), 7.20 (t, J = 7.3 Hz, 1H), 6.77 (s, 1H), 6.64 (d, J = 7.9 Hz, 1H), 6.22 (s, 1H), 4.44 (d, J = 17.9 Hz, 1H), 3.16 (d, J = 17.9 Hz, 1H), 2.38 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 200.0, 198.1, 160.9, 149.7, 138.4, 136.8, 133.8, 128.9, 128.8, 128.3, 127.6, 125.5, 125.4, 120.9, 116.0, 111.9, 69.6, 44.9, 22.7 ppm; IR (KBr) ν = 3384, 2919, 2848, 1686, 1621, 1217, 753, 692, 539 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{23}H_{20}NO_2$, $[M + H]^+$ 342.1489, found 342.1487.



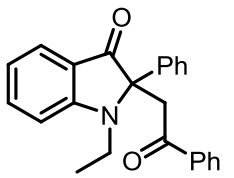
2-(Furan-2-yl)-2-(2-oxo-2-phenylethyl)indolin-3-one (**3r**): yellow solid (20 mg, 32% yield), mp: 104–106 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.96 (d, J = 7.3 Hz, 2H), 7.64 (d, J = 7.8 Hz, 1H), 7.59 (t, J = 7.4 Hz, 1H), 7.51–7.44 (m, 3H), 7.32–7.29 (m, 1H), 6.93 (d, J = 8.3 Hz, 1H), 6.86 (t, J = 7.4 Hz, 1H), 6.31–6.23 (m, 2H), 5.98 (s, 1H), 4.36 (d, J = 17.7 Hz, 1H), 3.22 ppm (d, J = 17.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 198.7, 197.4, 160.6, 150.9, 142.9, 137.9, 136.5, 133.8, 128.9, 128.3, 125.7, 119.5, 118.8, 112.4, 110.9, 106.4, 66.6, 43.1 ppm; IR (KBr) ν = 3379, 2921, 2850, 1690, 1618, 1487, 1219, 753, 690, 480 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{20}H_{15}NNaO_3$, $[M + Na]^+$ 340.0944, found 340.0944.



2-(2-Oxo-2-phenylethyl)-2-(thiophen-2-yl)indolin-3-one (**3s**)[7]: yellow solid (27 mg, 41% yield), mp: 122–124 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.93 (d, J = 7.3 Hz, 2H), 7.64–7.56 (m, 2H), 7.53–7.48 (m, 1H), 7.45 (t, J = 7.8 Hz, 2H), 7.12 (ddd, J = 8.7, 4.4, 1.2 Hz, 2H), 6.96 (d, J = 8.3 Hz, 1H), 6.91 (dd, J = 5.1, 3.7 Hz, 1H), 6.85 (t, J = 7.4 Hz, 1H), 6.41 (s, 1H), 4.31 (d, J = 17.6 Hz, 1H), 3.19 ppm (d, J = 17.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 199.4, 197.7, 160.1, 142.9, 138.0, 136.7, 133.9, 128.9, 128.3, 127.7, 125.9, 124.9, 123.9, 119.5, 118.0, 112.3, 68.1, 45.5 ppm.

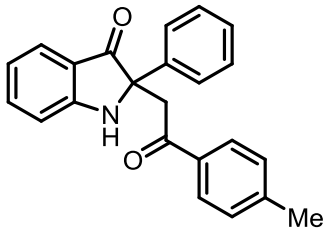


1-Methyl-2-(2-oxo-2-phenylethyl)-2-phenylindolin-3-one (**3t**): yellow solid (32 mg, 47% yield), mp: 150–152 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.90 (d, J = 7.3 Hz, 2H), 7.59–7.48 (m, 3H), 7.42 (t, J = 7.7 Hz, 2H), 7.37–7.28 (m, 5H), 6.82 (d, J = 8.3 Hz, 1H), 6.74 (t, J = 7.4 Hz, 1H), 4.21 (d, J = 17.0 Hz, 1H), 3.95 (d, J = 17.0 Hz, 1H), 2.93 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.3, 195.4, 161.2, 137.4, 137.2, 136.6, 133.5, 129.3, 128.8, 128.3, 128.2, 126.0, 125.5, 119.8, 117.4, 107.6, 73.1, 43.2, 29.1 ppm; IR (KBr) ν = 3061, 2918, 2830, 1702, 1617, 1492, 1320, 1220, 998, 750, 695, 574 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{23}H_{19}NNaO_2$, $[M + Na]^+$ 364.1308, found 364.1308.

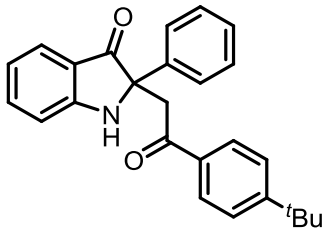


1-Ethyl-2-(2-oxo-2-phenylethyl)-2-phenylindolin-3-one (**3u**): yellow solid (24 mg, 34% yield), mp: 164–166 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.93 (d, J = 7.3 Hz, 2H), 7.63 (d, J = 7.6 Hz, 1H), 7.56 (t, J = 7.4 Hz,

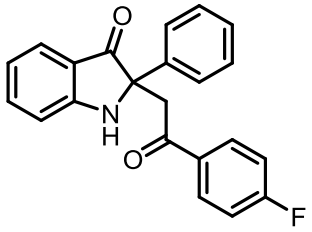
1H), 7.53–7.48 (m, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.35–7.25 (m, 5H), 6.84 (d, *J* = 8.3 Hz, 1H), 6.77 (t, *J* = 7.4 Hz, 1H), 4.21 (d, *J* = 17.6 Hz, 1H), 4.07 (d, *J* = 17.6 Hz, 1H), 3.54 (dq, *J* = 14.3, 7.1 Hz, 1H), 3.28 (dq, *J* = 14.7, 7.3 Hz, 1H), 0.99 ppm (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.4, 195.0, 160.5, 137.5, 137.2, 136.6, 133.5, 129.2, 128.8, 128.2, 128.2, 126.2, 125.6, 120.0, 117.3, 107.6, 73.3, 43.8, 38.5, 14.3 ppm; IR (KBr) *v* = 3060, 2927, 2871, 1692, 1616, 1489, 1322, 1219, 999, 750, 694, 581 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{24}H_{22}NO_2$, $[M + H]^+$ 356.1645, found 356.1644.



2-(2-Oxo-2-(*p*-tolyl)ethyl)-2-phenylindolin-3-one (**3v**)[4]: yellow solid (45 mg, 67% yield), mp: 182–184 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.82 (d, *J* = 8.2 Hz, 2H), 7.69–7.40 (m, 4H), 7.33–7.17 (m, 5H), 6.96 (d, *J* = 8.3 Hz, 1H), 6.80 (t, *J* = 7.4 Hz, 1H), 6.34 (s, 1H), 4.42 (d, *J* = 17.9 Hz, 1H), 3.13 (d, *J* = 17.9 Hz, 1H), 2.40 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.9, 197.6, 160.4, 144.9, 138.2, 137.9, 134.3, 129.6, 128.8, 128.4, 127.7, 125.8, 125.5, 118.9, 118.3, 111.9, 69.5, 44.7, 21.8 ppm.

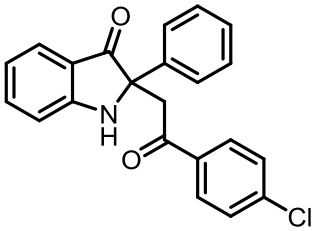


2-(2-(4-(*tert*-Butyl)phenyl)-2-oxoethyl)-2-phenylindolin-3-one (**3w**): yellow solid (37 mg, 49% yield), mp: 205–207 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.86 (d, *J* = 8.5 Hz, 2H), 7.56 (dd, *J* = 13.4, 7.7 Hz, 3H), 7.51–7.44 (m, 3H), 7.28 (d, *J* = 7.2 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 8.3 Hz, 1H), 6.80 (t, *J* = 7.4 Hz, 1H), 6.35 (s, 1H), 4.44 (d, *J* = 18.0 Hz, 1H), 3.13 (d, *J* = 17.9 Hz, 1H), 1.32 ppm (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.9, 197.6, 160.4, 157.8, 138.2, 137.9, 134.2, 128.8, 128.2, 127.6, 125.8, 125.7, 125.5, 118.9, 118.2, 111.9, 69.5, 44.7, 35.3, 31.2 ppm; IR (KBr) *v* = 3386, 2964, 2906, 2868, 1681, 1620, 1489, 1225, 833, 755, 511 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{26}H_{26}NO_2$, $[M + H]^+$ 384.1958, found 384.1956.

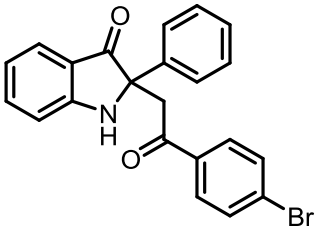


2-(2-(4-Fluorophenyl)-2-oxoethyl)-2-phenylindolin-3-one (**3x**)[7]: yellow solid (47 mg, 69% yield), mp: 167–169 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.98–7.90 (m, 2H), 7.56 (dd, *J* = 14.6, 7.6 Hz, 3H), 7.52–7.47 (m, 1H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.11 (t, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.81 (t, *J* = 7.4 Hz, 1H), 6.27 (s, 1H), 4.39 (d, *J* = 17.8 Hz, 1H), 3.16 ppm (d, *J* = 17.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25

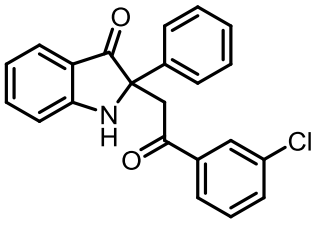
^{o}C) δ = 200.7, 196.3, 167.5 (d, $^{1}J_{C\text{-}F}$ = 255.0 Hz), 160.4, 138.1, 138.0, 133.2 (d, $^{4}J_{C\text{-}F}$ = 3.0 Hz), 131.0, (d, $^{3}J_{C\text{-}F}$ = 9.0 Hz), 128.9, 127.8, 125.8, 125.4, 119.1, 118.3, 116.1 (d, $^{2}J_{C\text{-}F}$ = 22.0 Hz), 111.93, 69.34, 44.83 ppm; ^{19}F NMR (377 MHz, $CDCl_3$, 25 °C) δ = -103.8 (m, 1F) ppm.



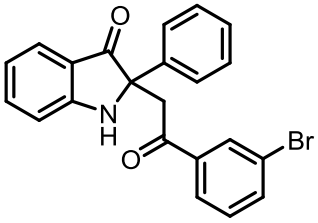
2-(2-(4-Chlorophenyl)-2-oxoethyl)-2-phenylindolin-3-one (**3y**)[7]: yellow solid (58 mg, 80% yield), mp: 172–174 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.85 (d, J = 8.5 Hz, 2H), 7.53 (td, J = 18.0, 7.5 Hz, 4H), 7.41 (d, J = 8.5 Hz, 2H), 7.28 (t, J = 7.5 Hz, 2H), 7.22 (t, J = 7.3 Hz, 1H), 6.97 (d, J = 8.2 Hz, 1H), 6.81 (t, J = 7.4 Hz, 1H), 6.24 (s, 1H), 4.38 (d, J = 17.9 Hz, 1H), 3.16 ppm (d, J = 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.6, 196.7, 160.3, 140.4, 138.0, 138.0, 135.0, 129.7, 129.2, 128.9, 127.8, 125.8, 125.4, 119.1, 118.3, 111.9, 69.3, 44.9 ppm.



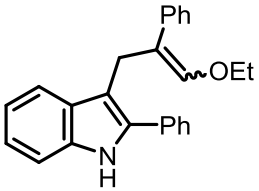
2-(2-(4-Bromophenyl)-2-oxoethyl)-2-phenylindolin-3-one (**3z**)[7]: yellow solid (76 mg, 61% yield), mp: 177–179 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.77 (d, J = 8.6 Hz, 2H), 7.57 (d, J = 2.4 Hz, 3H), 7.55–7.47 (m, 3H), 7.28 (t, J = 7.5 Hz, 2H), 7.22 (t, J = 7.2 Hz, 1H), 6.97 (d, J = 8.2 Hz, 1H), 6.81 (t, J = 7.4 Hz, 1H), 6.22 (s, 1H), 4.37 (d, J = 17.9 Hz, 1H), 3.15 ppm (d, J = 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.6, 196.9, 160.3, 138.0, 138.0, 135.4, 132.2, 129.7, 129.2, 128.9, 127.8, 125.8, 125.4, 119.2, 118.3, 111.9, 69.3, 44.9 ppm.



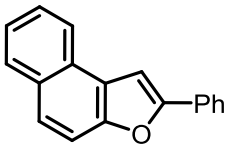
2-(2-(3-Chlorophenyl)-2-oxoethyl)-2-phenylindolin-3-one (**3aa**): yellow solid (34 mg, 47% yield), mp: 123–125 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.86 (s, 1H), 7.76 (d, J = 7.8 Hz, 1H), 7.55 (dd, J = 18.6, 7.8 Hz, 5H), 7.38 (q, J = 8.0 Hz, 2H), 7.28 (t, J = 7.5 Hz, 2H), 6.96 (d, J = 8.2 Hz, 1H), 6.81 (t, J = 7.4 Hz, 1H), 6.22 (s, 1H), 4.37 (d, J = 18.0 Hz, 1H), 3.16 ppm (d, J = 18.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.5, 196.7, 160.3, 138.0, 137.9, 135.3, 133.7, 130.2, 128.9, 128.8, 128.4, 128.3, 127.8, 126.3, 125.8, 125.4, 119.1, 111.9, 69.2, 45.1 ppm; IR (KBr) ν = 3382, 2922, 2848, 1687, 1619, 1489, 1212, 754, 699, 516 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{22}H_{16}ClNNaO_2$, $[M + Na]^+$ 384.0762, found 384.0761.



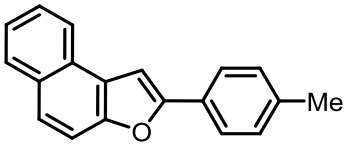
2-(2-(3-Bromophenyl)-2-oxoethyl)-2-phenylindolin-3-one (**3ab**)[7]: yellow solid (41 mg, 51% yield), mp: 133–135 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 8.03 (s, 1H), 7.83 (d, J = 7.8 Hz, 1H), 7.69 (d, J = 8.6 Hz, 1H), 7.59–7.48 (m, 4H), 7.31 (dd, J = 14.5, 7.3 Hz, 2H), 7.25 (dd, J = 13.4, 5.9 Hz, 2H), 6.97 (d, J = 8.3 Hz, 1H), 6.82 (t, J = 7.4 Hz, 1H), 6.21 (s, 1H), 4.38 (d, J = 17.9 Hz, 1H), 3.17 ppm (d, J = 18.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 200.4, 196.5, 160.2, 138.2, 137.9, 137.8, 136.6, 131.2, 130.3, 128.8, 127.7, 126.6, 125.7, 125.3, 123.1, 119.0, 118.2, 111.8, 69.1, 45.0 ppm.



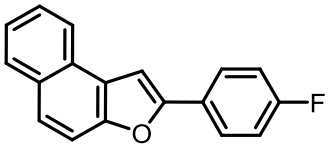
3-(3-Ethoxy-2-phenylallyl)-2-phenyl-1H-indole (**4a**): yellow oil (25 mg, 35% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 8.10 (s, 1H), 7.64 (d, J = 7.6 Hz, 3H), 7.57 (d, J = 7.4 Hz, 2H), 7.44 (t, J = 7.6 Hz, 2H), 7.40–7.34 (m, 2H), 7.32 (t, J = 7.6 Hz, 2H), 7.20 (q, J = 7.7 Hz, 2H), 7.12 (t, J = 7.4 Hz, 1H), 5.92 (s, 1H), 3.89 (s, 2H), 3.67 (q, J = 7.1 Hz, 2H), 1.14 ppm (t, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 144.9, 138.6, 136.0, 135.3, 132.9, 129.6, 128.9, 127.9, 127.8, 127.7, 127.5, 126.0, 122.3, 119.7, 119.7, 114.3, 110.7, 110.1, 68.3, 28.1, 15.3 ppm; IR (KBr) ν = 3362, 3055, 2976, 1601, 1493, 1454, 1304, 1136, 742, 697, 500 cm^{-1}; HRMS (ESI, TOF) m/z: calcd for $C_{25}H_{24}NO$, $[M + H]^+$ 354.1852, found 354.1855.



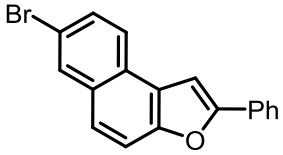
2-Phenylnaphtho[2,1-*b*]furan (**5a**)[8]: white solid (37 mg, 76% yield), mp: 145–147 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 8.17 (d, J = 8.2 Hz, 1H), 7.94 (t, J = 7.4 Hz, 3H), 7.75–7.66 (m, 2H), 7.59 (t, J = 7.1 Hz, 1H), 7.53–7.44 (m, 4H), 7.35 ppm (t, J = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 155.4, 152.4, 130.7, 130.4, 128.9, 128.8, 128.3, 127.6, 126.3, 125.2, 124.7, 124.6, 124.5, 123.5, 112.3, 100.5 ppm.



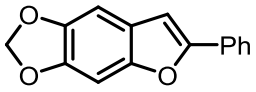
2-(*p*-Tolyl)naphtho[2,1-*b*]furan (**5b**)[9]: white solid (31 mg, 61% yield), mp: 149–151 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 8.17 (d, J = 8.2 Hz, 1H), 7.94 (d, J = 8.1 Hz, 1H), 7.82 (d, J = 7.9 Hz, 2H), 7.73–7.66 (m, 2H), 7.59 (t, J = 7.6 Hz, 1H), 7.48 (d, J = 6.4 Hz, 2H), 7.28 (d, J = 7.8 Hz, 2H), 2.41 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 155.7, 152.2, 138.3, 130.4, 129.6, 128.8, 127.9, 127.6, 126.2, 124.9, 124.6, 124.5, 123.5, 112.3, 99.7, 21.4 ppm.



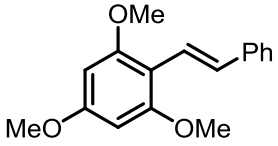
2-(4-Fluorophenyl)naphtho[2,1-*b*]furan (**5c**)[10]: off white solid (35 mg, 68% yield), mp: 120–122 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 8.15 (d, *J* = 8.1 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.89 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.70 (q, *J* = 8.9 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.44 (s, 1H), 7.16 ppm (t, *J* = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 164.0 (d, $^{1}J_{C\text{-}F}$ = 247 Hz), 154.5, 152.3, 130.5, 128.8, 127.6, 127.0 (d, $^{4}J_{C\text{-}F}$ = 3 Hz), 126.5 (d, $^{3}J_{C\text{-}F}$ = 8 Hz), 126.3, 125.2, 124.6, 124.5, 123.4, 116.1 (d, $^{2}J_{C\text{-}F}$ = 22 Hz), 112.2, 100.2 ppm; ^{19}F NMR (377 MHz, $CDCl_3$, 25 °C) δ = -112.8 (m, 1F) ppm.



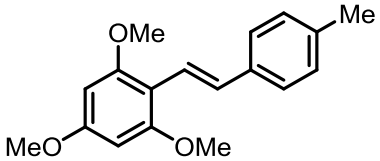
7-Bromo-2-phenylnaphtho[2,1-*b*]furan (**5d**)[8]: pale yellow solid (50 mg, 79% yield), mp: 115–117 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 8.09 (d, *J* = 2.0 Hz, 1H), 8.02 (d, *J* = 8.7 Hz, 1H), 7.91 (d, *J* = 7.1 Hz, 2H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.65 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.61 (d, *J* = 8.9 Hz, 1H), 7.50–7.44 (m, 3H), 7.37 ppm (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 155.9, 152.4, 131.7, 130.8, 130.4, 129.4, 128.9, 128.5, 126.1, 125.2, 124.8, 124.6, 124.1, 118.2, 113.4, 100.2 ppm.



4,5-Methylenedioxy-2-phenylbenzofuran (**5e**)[11]: white solid (15 mg, 32% yield), mp: 159–161 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.77 (d, *J* = 7.1 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.02 (s, 1H), 6.94 (s, 1H), 6.90 (s, 1H), 5.99 ppm (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 155.5, 150.2, 146.1, 144.6, 130.6, 128.8, 128.0, 124.3, 122.5, 101.8, 101.3, 99.3, 93.5 ppm.

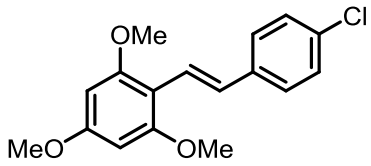


1,3,5-Trimethoxy-2-styrylbenzene (**7a**)[12]: colorless oil (38 mg, 72% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.51 (d, *J* = 7.5 Hz, 2H), 7.46 (d, *J* = 16.7 Hz, 1H), 7.39 (d, *J* = 16.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 6.17 (s, 2H), 3.88 (s, 6H), 3.83 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) δ = 160.3, 159.6, 139.8, 130.0, 128.5, 126.6, 126.3, 120.0, 108.3, 90.9, 55.9, 55.5 ppm.

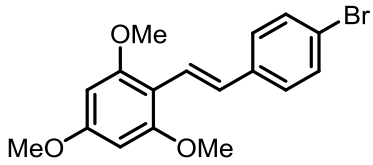


1,3,5-Trimethoxy-2-(4-methylstyryl)benzene (**7b**)[13]: white solid (42 mg, 74% yield), mp: 93–95 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C) δ = 7.46–7.31 (m, 4H), 7.12 (d, *J* = 7.7 Hz, 2H), 6.16 (s, 2H), 3.87 (s, 6H), 3.83 (s, 3H), 2.33 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$,

25 °C) δ = 160.0, 159.4, 136.9, 136.2, 129.9, 129.1, 126.1, 118.9, 108.3, 90.9, 55.8, 55.3, 21.2 ppm.



2-(4-Chlorostyryl)-1,3,5-trimethoxybenzene (**7c**)[13]: white solid (34 mg, 57% yield), mp: 97–99 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ = 7.40 (dd, J = 14.5, 6.6 Hz, 4H), 7.27 (d, J = 8.5 Hz, 2H), 6.16 (s, 2H), 3.88 (s, 6H), 3.84 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 160.4, 159.6, 138.2, 131.9, 128.51, 128.46, 127.3, 120.5, 107.8, 90.8, 55.8, 55.3 ppm.



(*E*)-2-(4-Bromostyryl)-1,3,5-trimethoxybenzene (**7d**)[13]: white solid (43 mg, 63% yield), mp: 94–96 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C) δ = 7.42 (d, J = 8.5 Hz, 2H), 7.39–7.34 (m, 4H), 6.16 (s, 2H), 3.88 (s, 6H), 3.84 ppm (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 160.5, 159.6, 138.7, 131.4, 128.5, 127.7, 120.6, 120.0, 107.8, 90.8, 55.8, 55.3 ppm.

9 References

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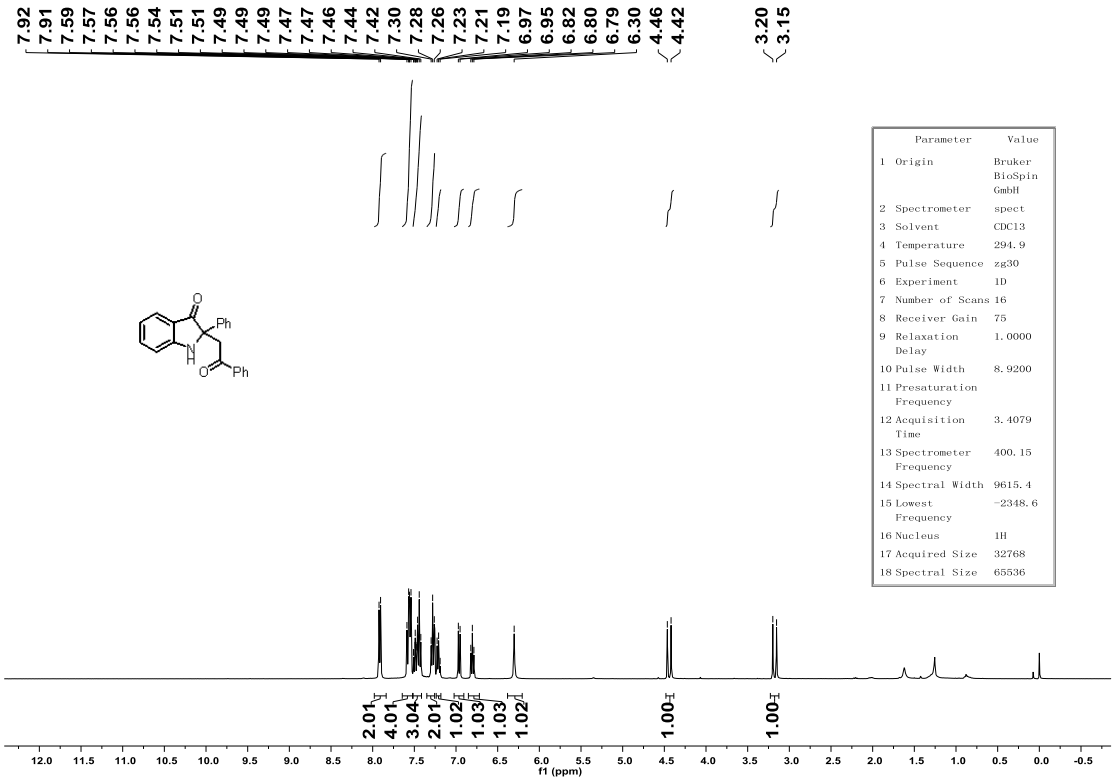
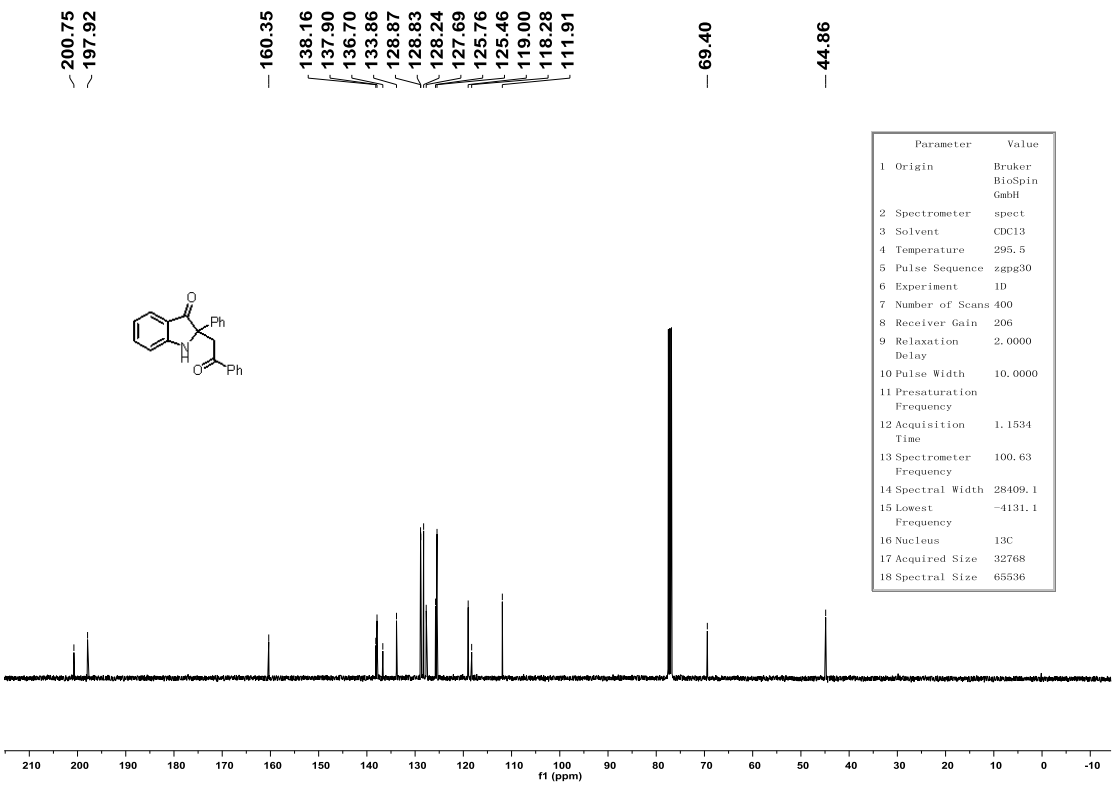
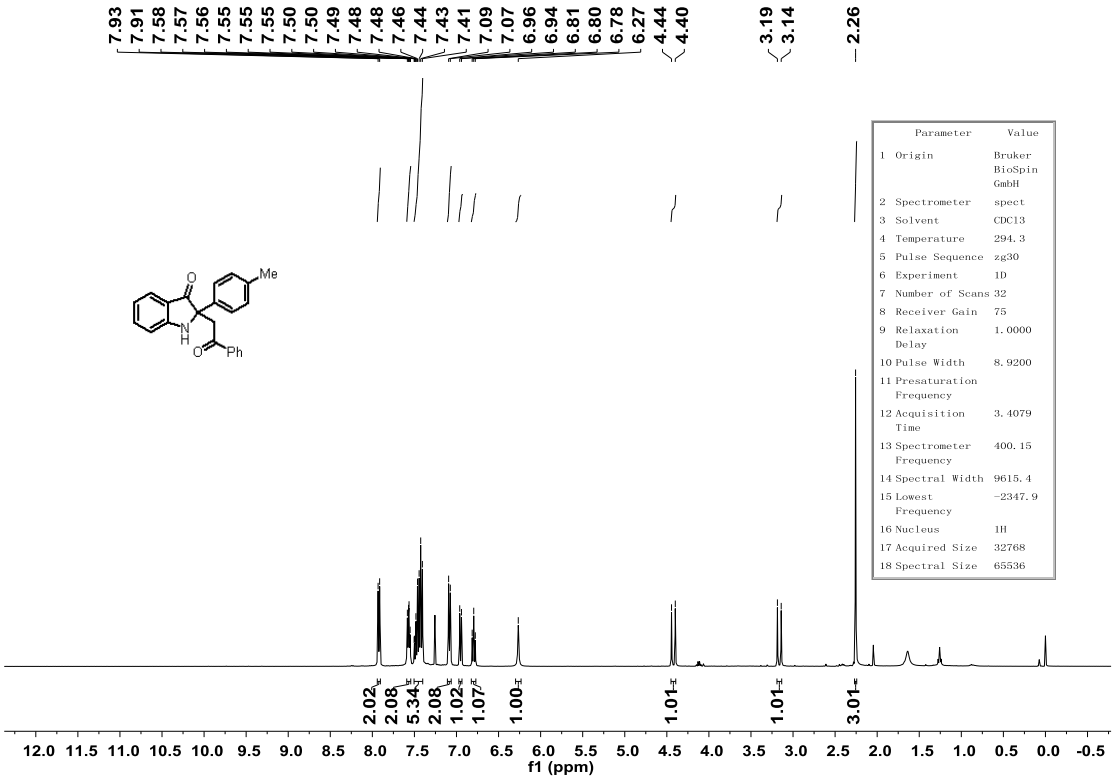
10 Copies of NMR spectra

3a





3b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7.55
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7.50
7.49
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6.80
6.78
6.27
4.44
4.40
3.19
3.14
2.26
Me
O
N
H
O
Ph
Parameter Value
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3 Solvent CDCl3
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5 Pulse Sequence zg30
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9 Relaxation Delay 1.0000
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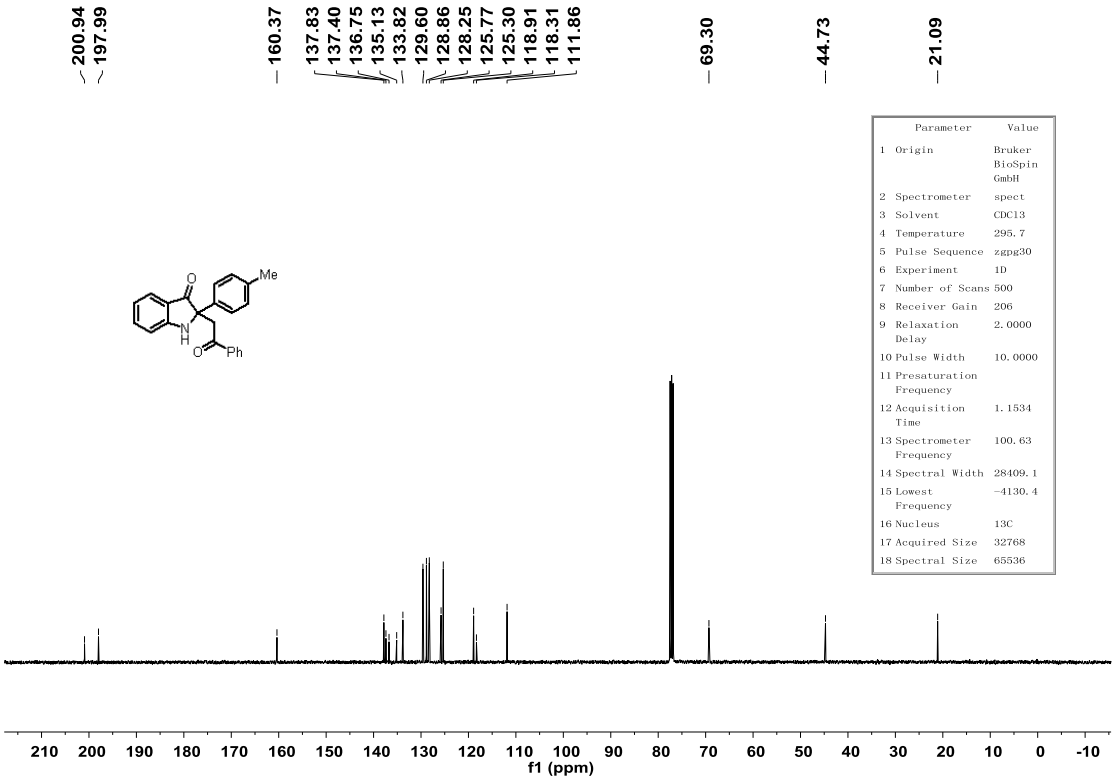
2.02
2.08
5.34
2.08
1.02
1.07
1.00
1.01
1.01
3.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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118.31
111.86
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44.73
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Ph
Parameter Value
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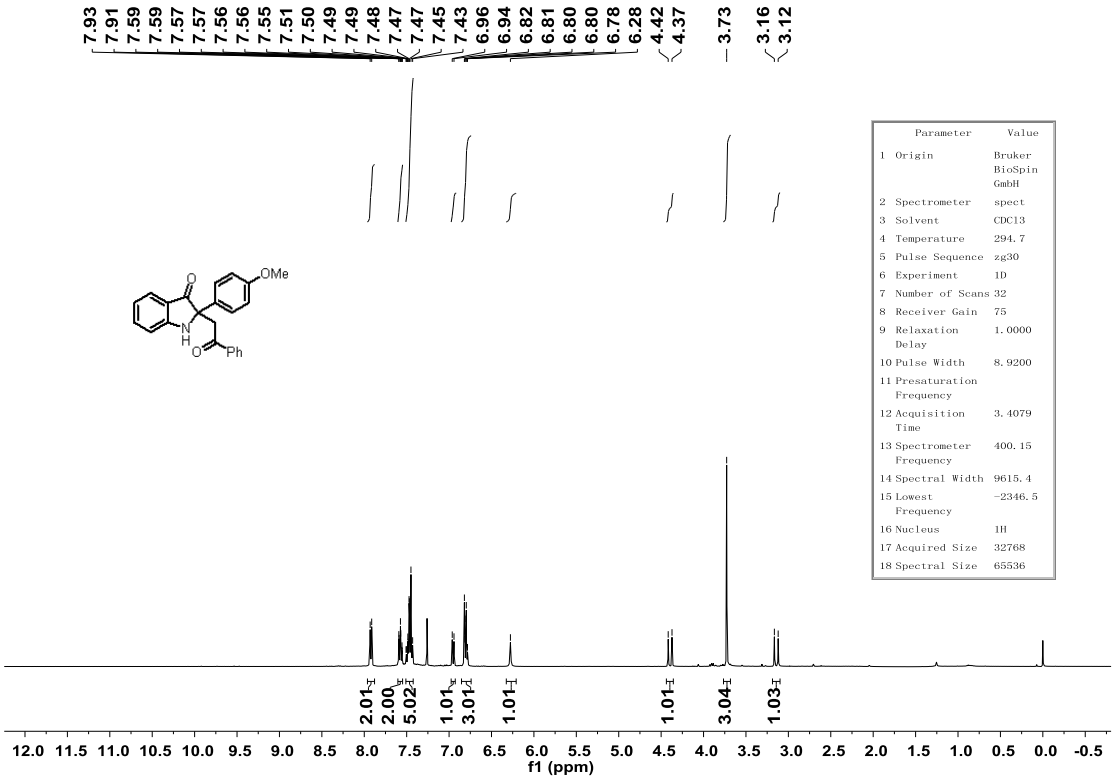
f1 (ppm)

3c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OMe
O
N
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O
Ph
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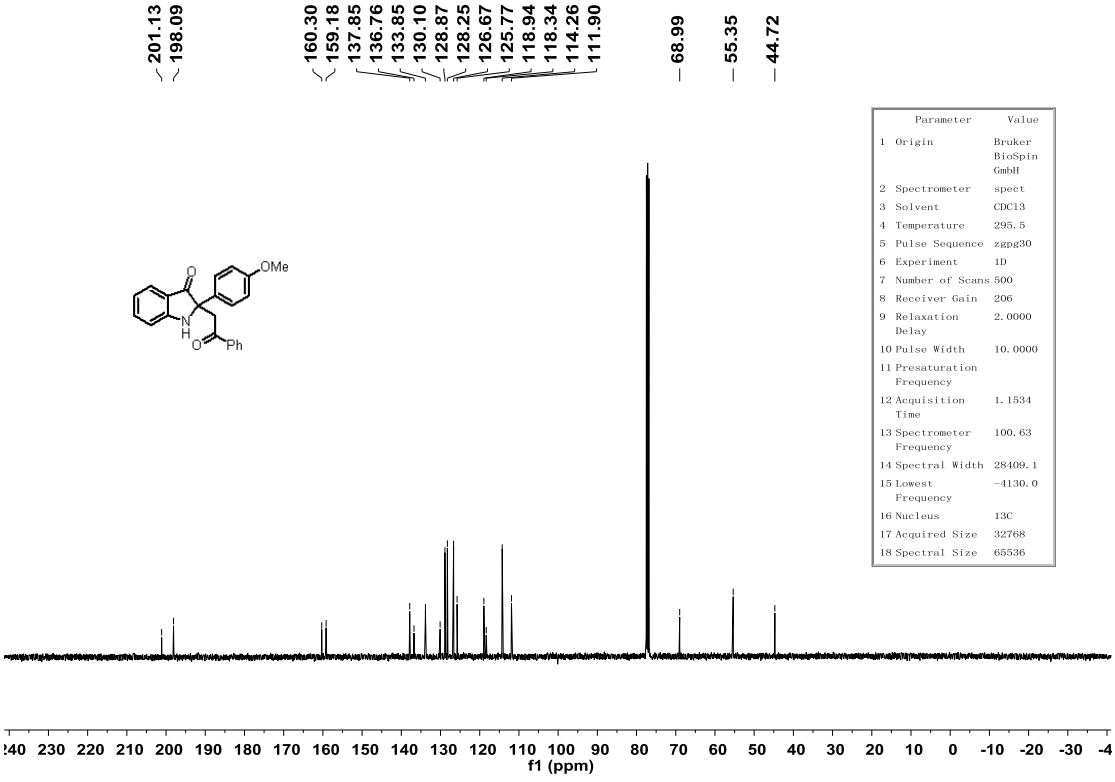
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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OMe
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Parameter Value
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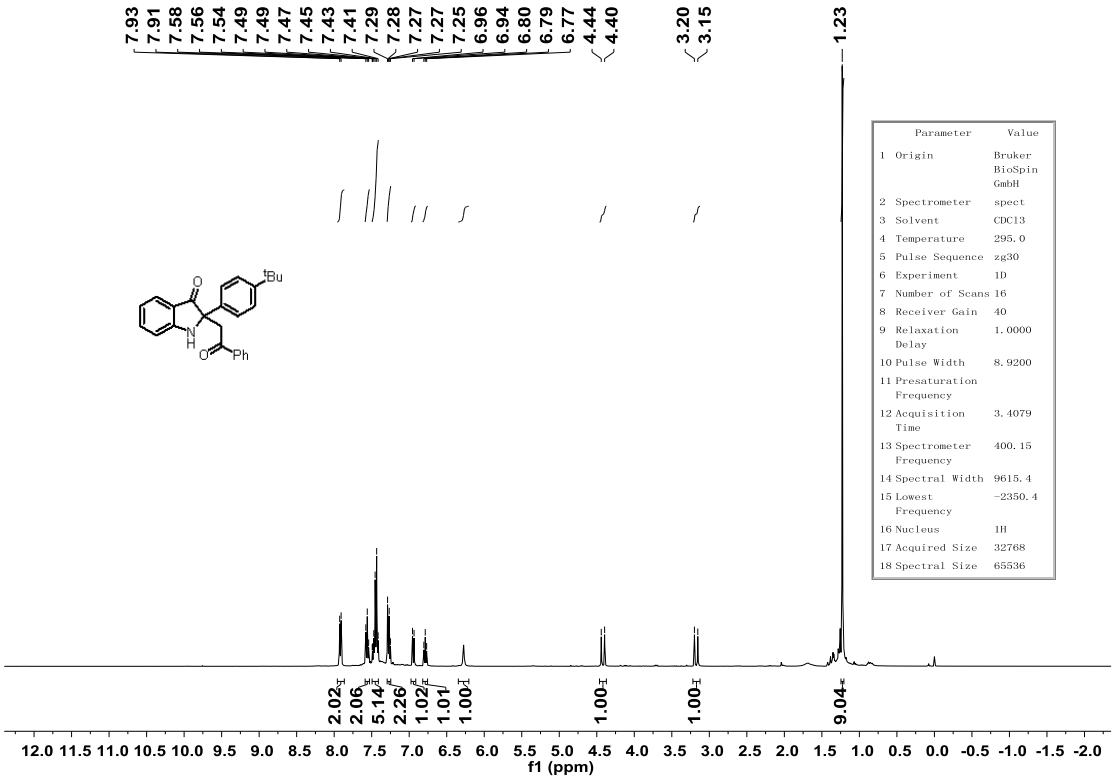
3d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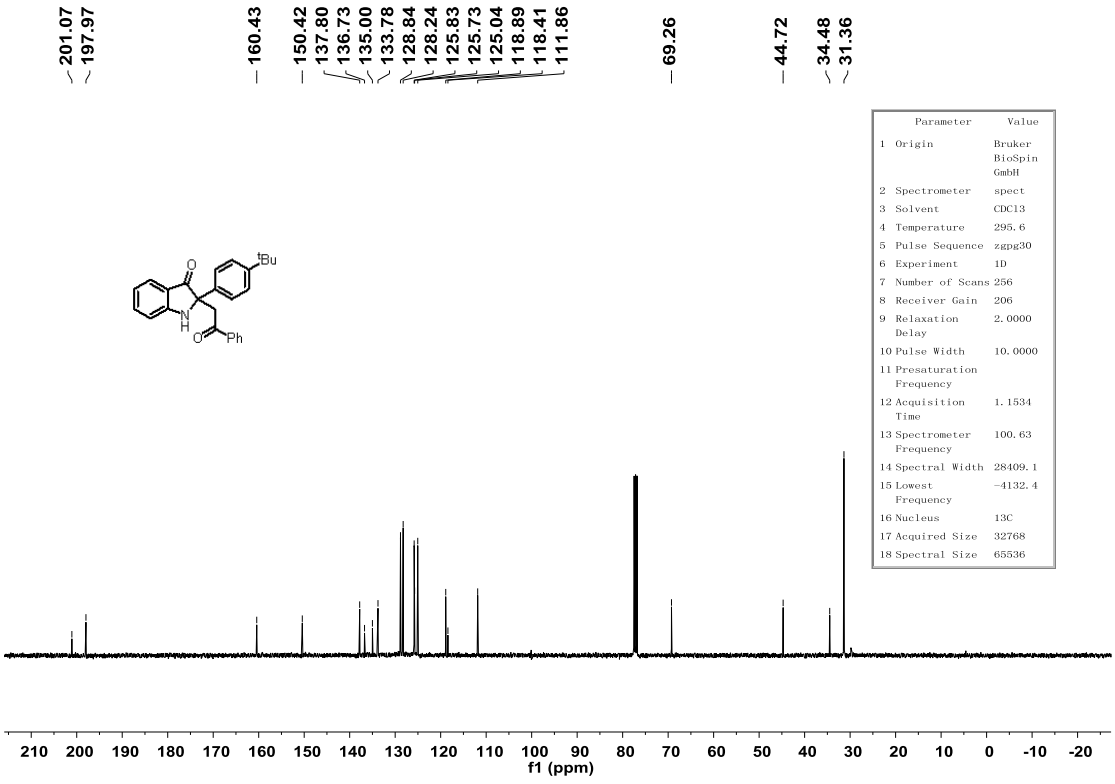
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.0
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 40
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2350.4
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
tBu
O
N
H
O
Ph
2.02
2.06
5.14
2.26
1.02
1.01
1.00
1.00
1.00
9.04
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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150.42
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136.73
135.00
133.78
128.84
128.24
125.83
125.73
125.04
118.89
118.41
111.86
69.26
44.72
34.48
31.36
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.6
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 256
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4132.4
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
tBu
O
N
H
O
Ph
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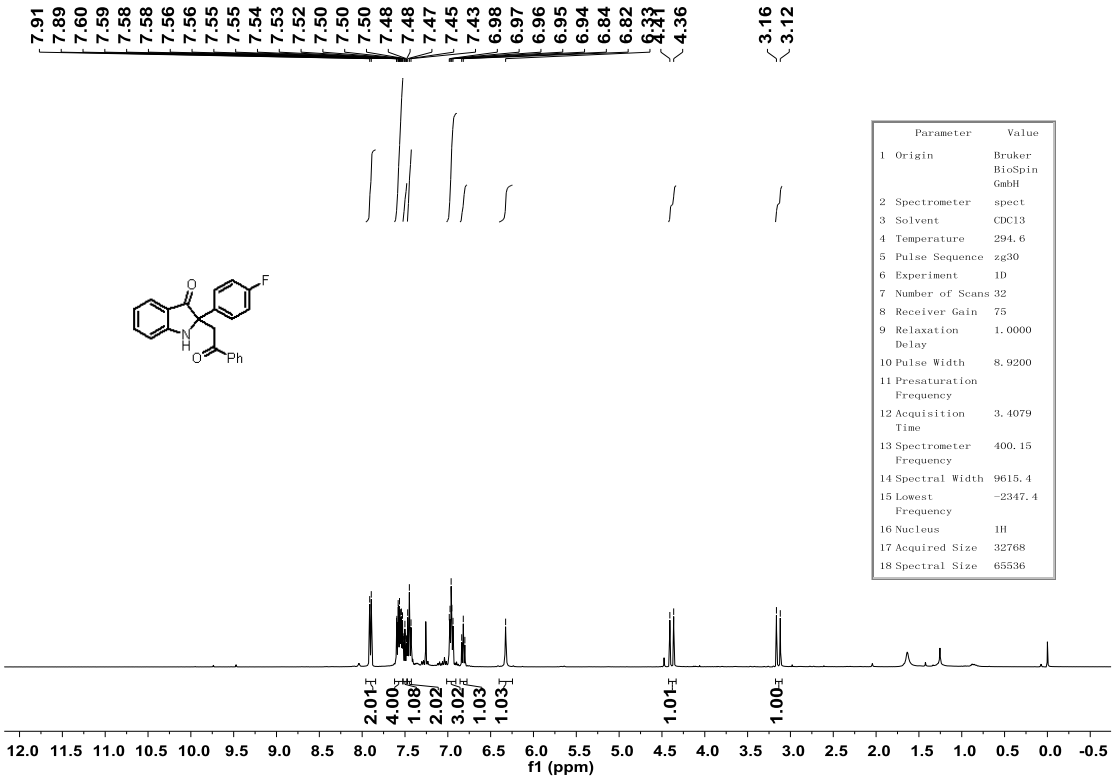
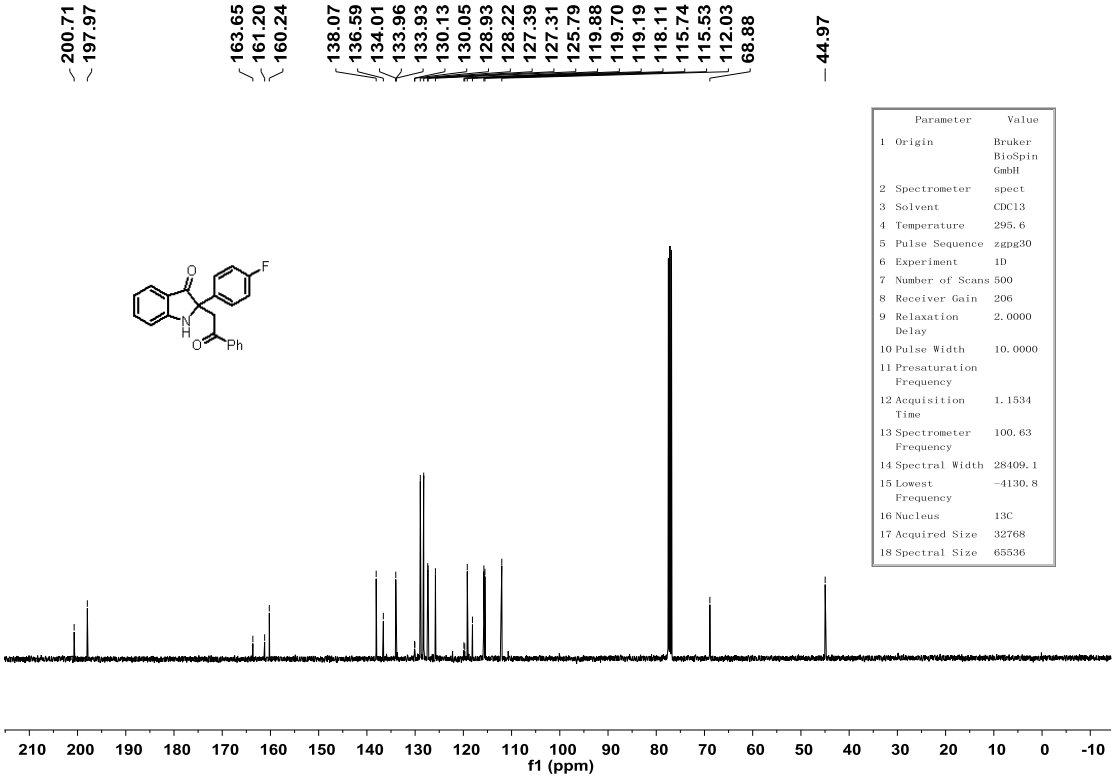
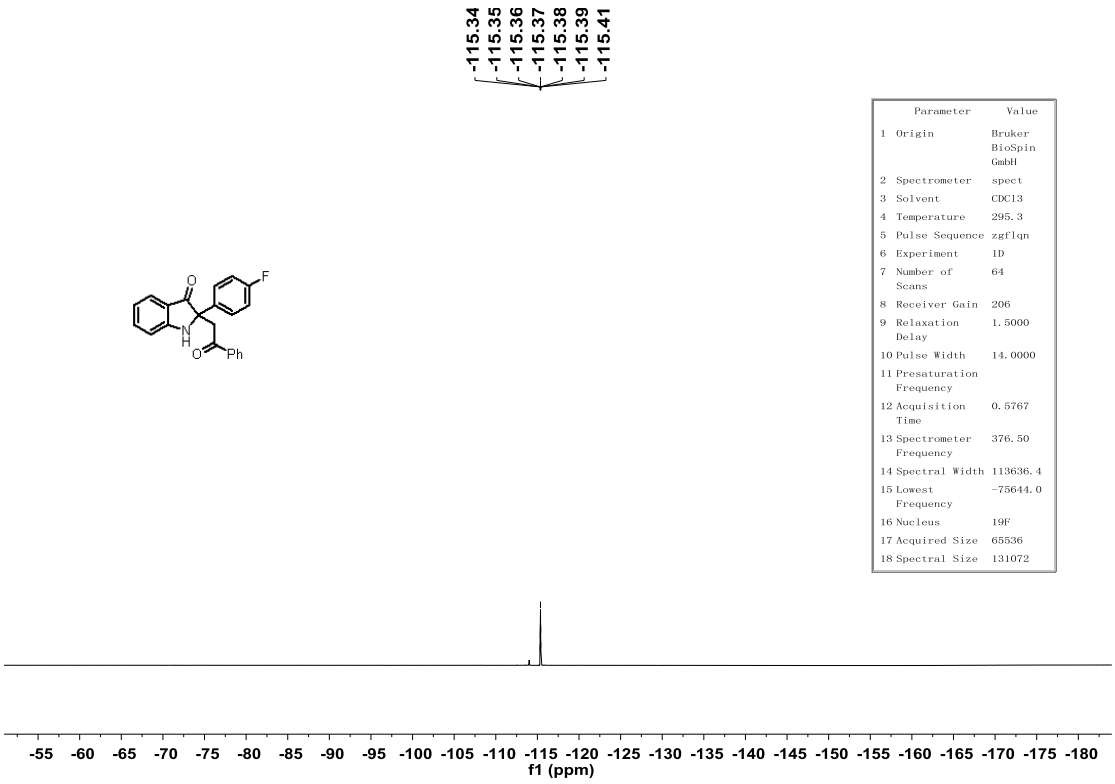
f1 (ppm)

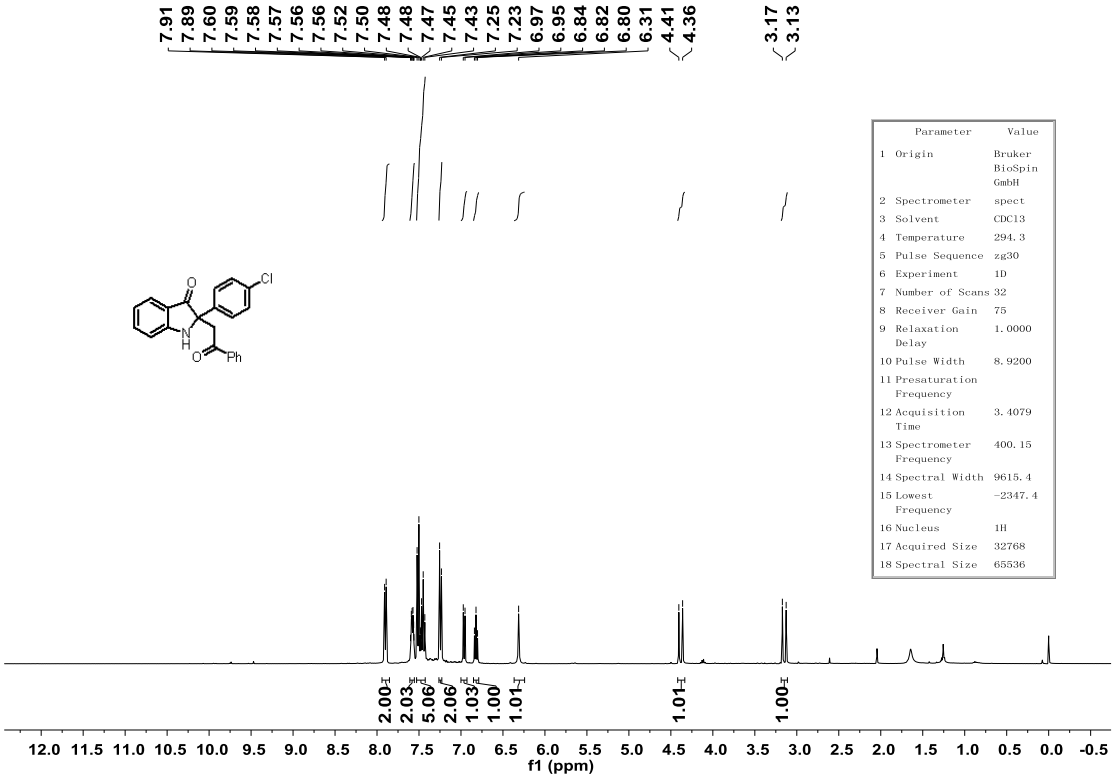
3e


7.91 7.89 7.60 7.59 7.58 7.58 7.56 7.56 7.55 7.55 7.54 7.53 7.52 7.50 7.50 7.50 7.48 7.48 7.47 7.45 7.43 6.98 6.97 6.96 6.95 6.94 6.84 6.82 6.33 4.41 4.36 3.16 3.12
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.6
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.4
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.01 4.00 1.08 2.02 3.02 1.03 1.03 1.01 1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


200.71 197.97 163.65 161.20 160.24 138.07 136.59 134.01 133.96 133.93 130.13 130.05 128.93 128.22 127.39 127.31 125.79 119.88 119.70 119.19 118.11 115.74 115.53 112.03 68.88 44.97
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.6
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4130.8
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-115.34
-115.35
-115.36
-115.37
-115.38
-115.39
-115.41
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.3
5 Pulse Sequence zgflqn
6 Experiment 1D
7 Number of Scans 64
8 Receiver Gain 206
9 Relaxation Delay 1.5000
10 Pulse Width 14.0000
11 Presaturation Frequency
12 Acquisition Time 0.5767
13 Spectrometer Frequency 376.50
14 Spectral Width 113636.4
15 Lowest Frequency -75644.0
16 Nucleus 19F
17 Acquired Size 65536
18 Spectral Size 131072
F
O
N
H
O
Ph
-55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170 -175 -180
f1 (ppm)

3f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7.89
7.60
7.59
7.58
7.57
7.56
7.56
7.52
7.50
7.48
7.48
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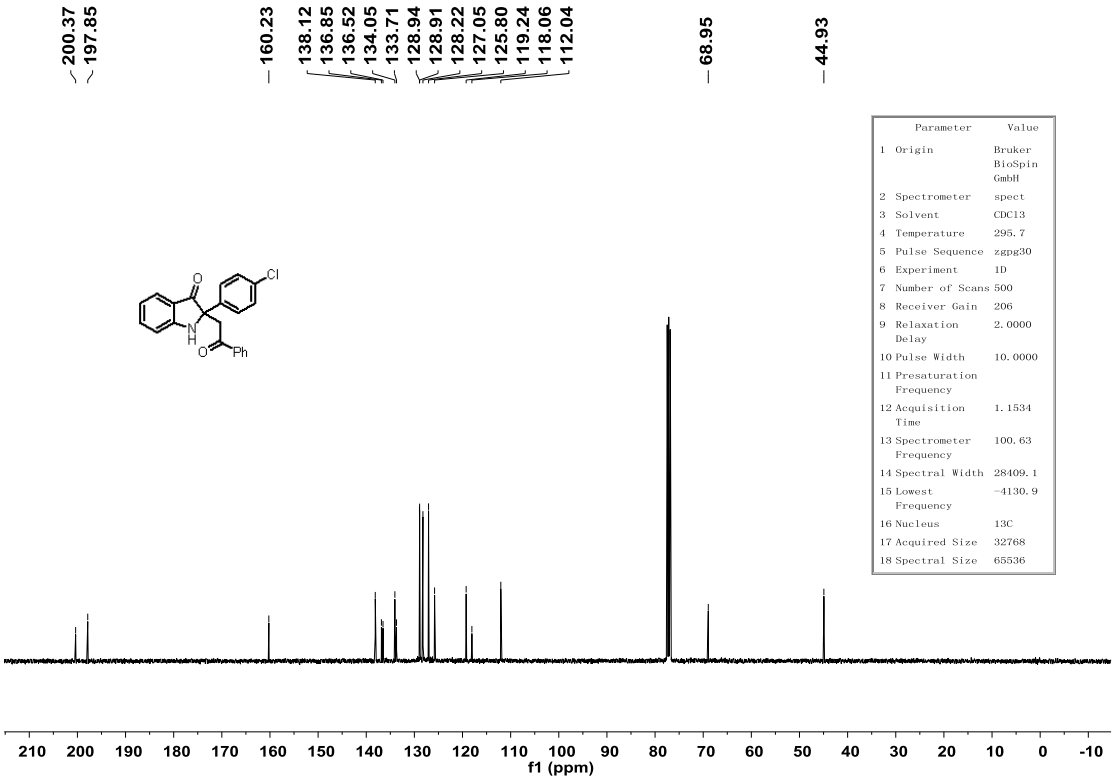
7.45
7.43
7.25
7.23
6.97
6.95
6.84
6.82
6.80
6.31
4.41
4.36
3.17
3.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.3
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.4
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
Cl
O
N
H
O
Ph
2.00
2.03
5.06
2.06
1.03
1.00
1.01
1.01
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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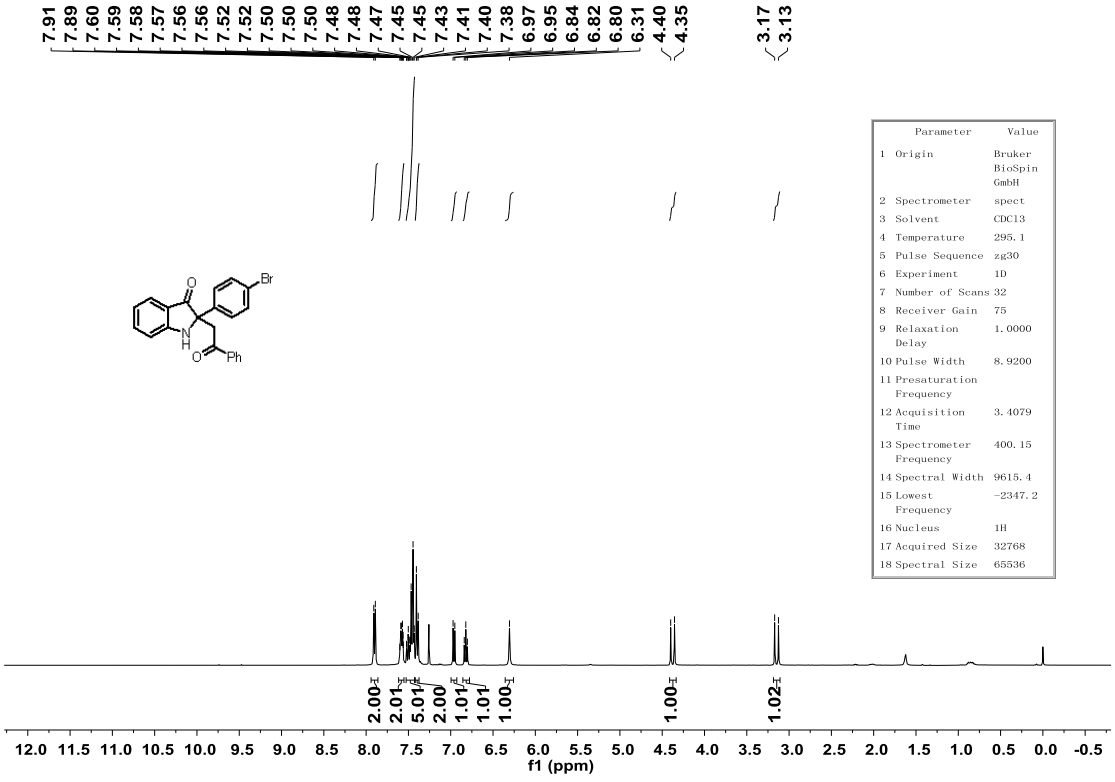
160.23
138.12
136.85
136.52
134.05
133.71
128.94
128.91
128.22
127.05
125.80
119.24
118.06
112.04
68.95
44.93
Cl
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.7
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4130.9
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3g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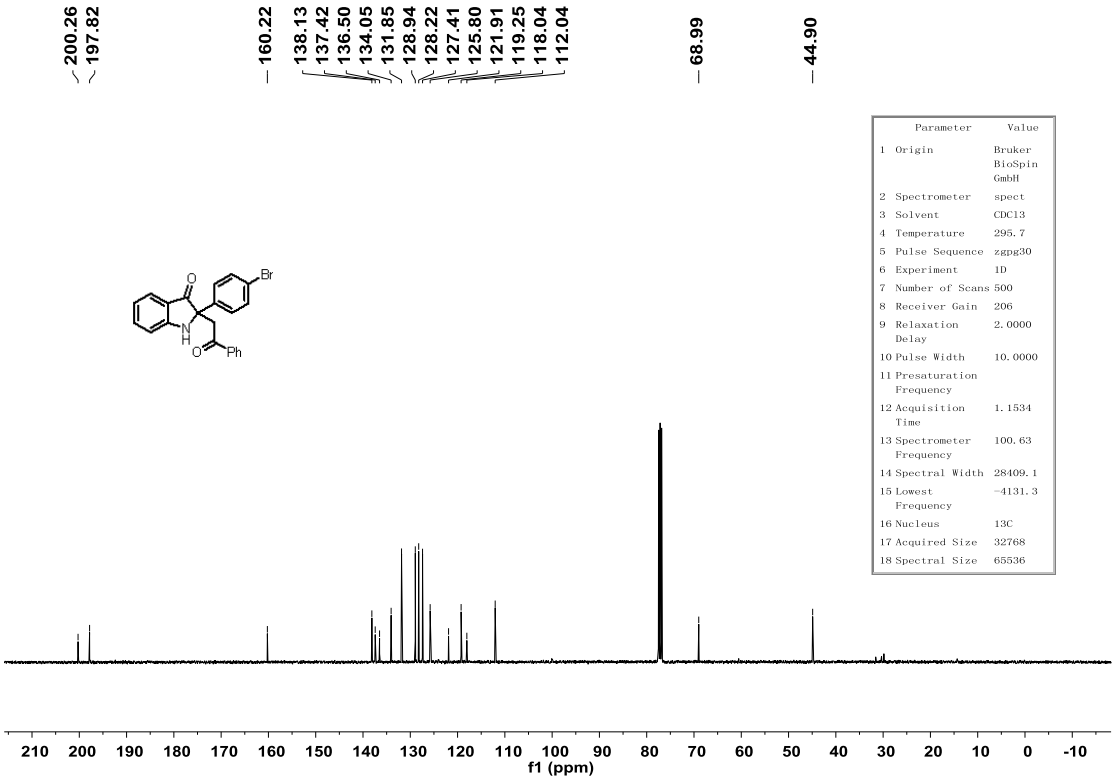
7.89
7.60
7.59
7.58
7.57
7.56
7.56
7.52
7.52
7.50
7.50
7.50
7.48
7.48
7.47
7.45
7.45
7.43
7.41
7.40
7.38
6.97
6.95
6.84
6.82
6.80
6.31
4.40
4.35
3.17
3.13
Br
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.1
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.2
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.00
2.01
5.01
2.00
1.01
1.01
1.00
1.00
1.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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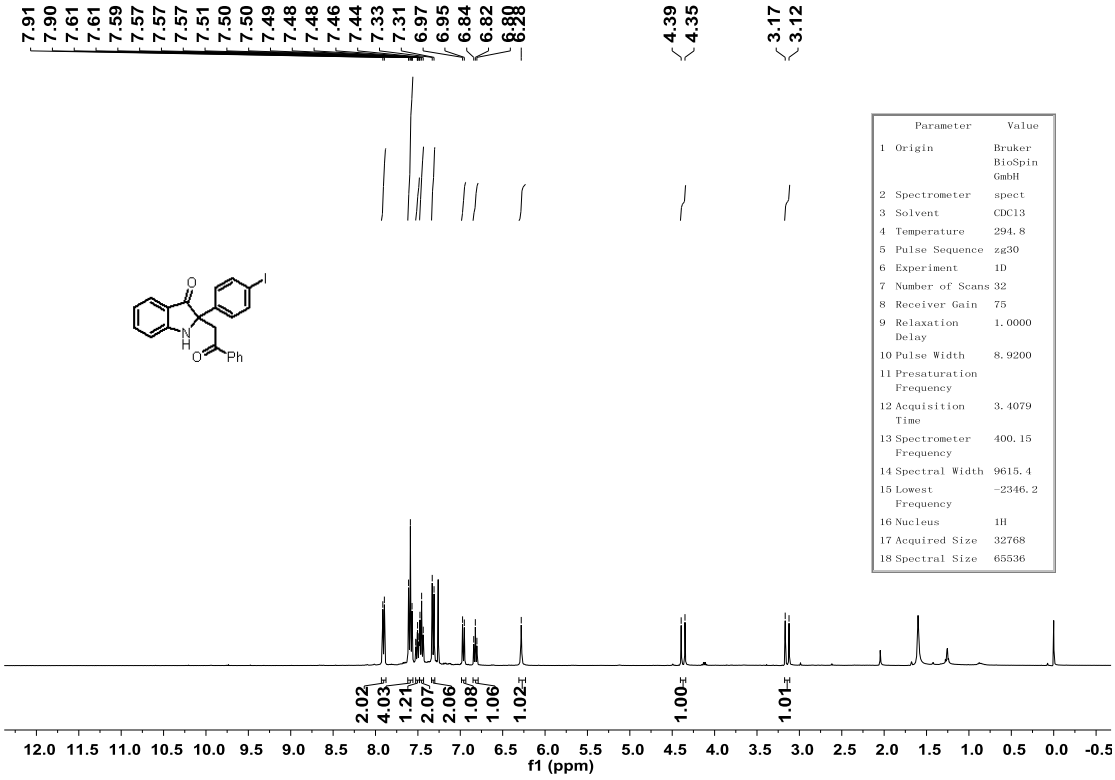
137.42
136.50
134.05
131.85
128.94
128.22
127.41
125.80
121.91
119.25
118.04
112.04
68.99
44.90
Br
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.7
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4131.3
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3h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7.59
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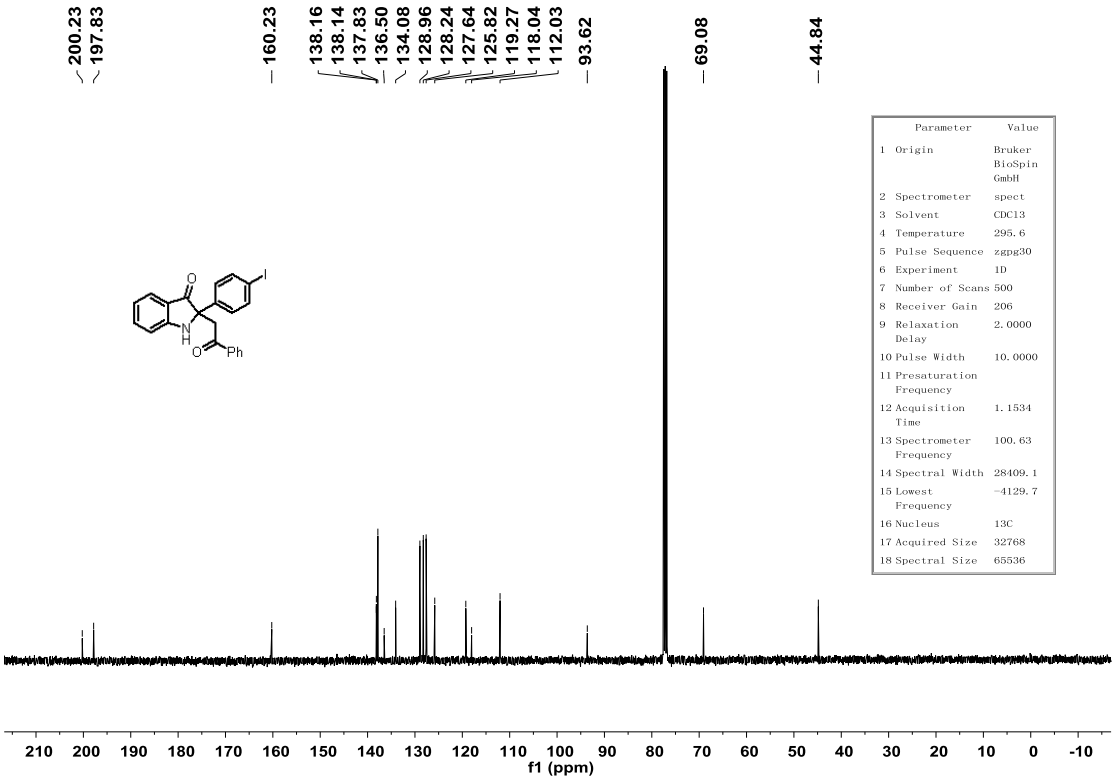
7.57
7.57
7.51
7.50
7.50
7.49
7.48
7.48
7.46
7.44
7.33
7.31
6.97
6.95
6.84
6.82
6.80
6.78
4.39
4.35
3.17
3.12
I
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.8
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2346.2
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.02
4.03
1.21
2.07
2.06
1.08
1.06
1.02
1.00
1.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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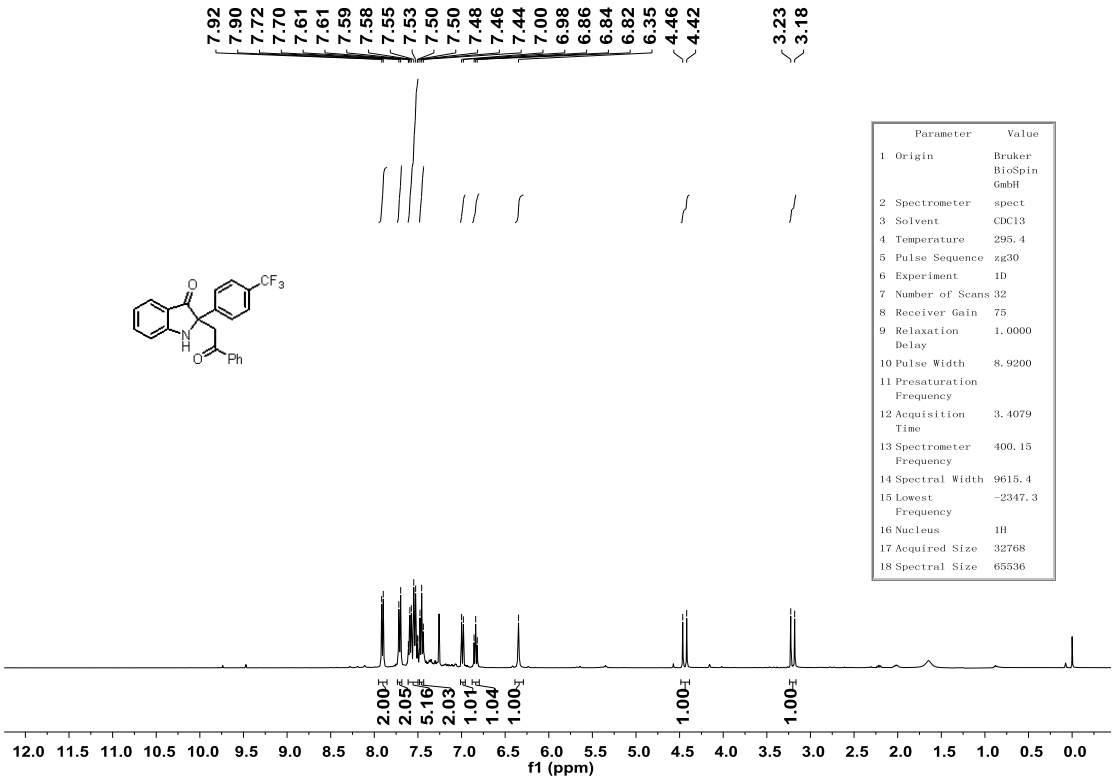
160.23
138.16
138.14
137.83
136.50
134.08
128.96
128.24
127.64
125.82
119.27
118.04
112.03
93.62
69.08
44.84
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.6
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4129.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
f1 (ppm)

3i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7.61
7.59
7.58
7.55
7.53
7.50
7.50
7.48
7.46
7.44
7.00
6.98
6.86
6.84
6.82
6.35
4.46
4.42
3.23
3.18
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.4
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.3
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
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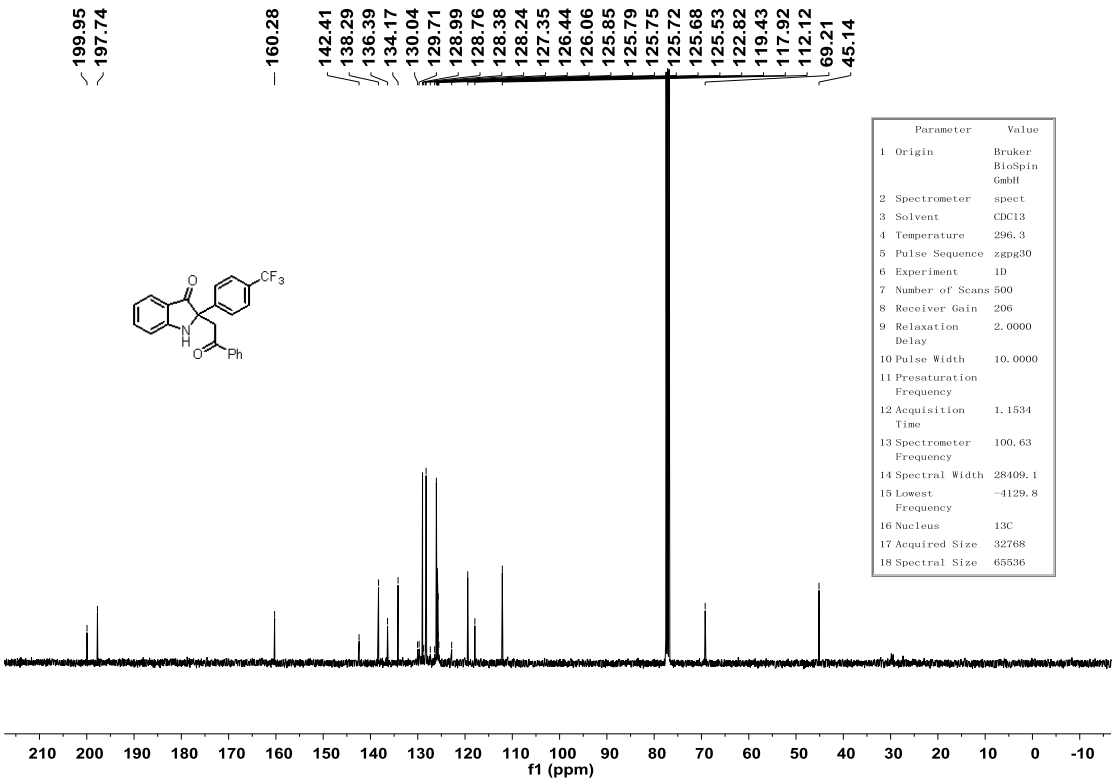
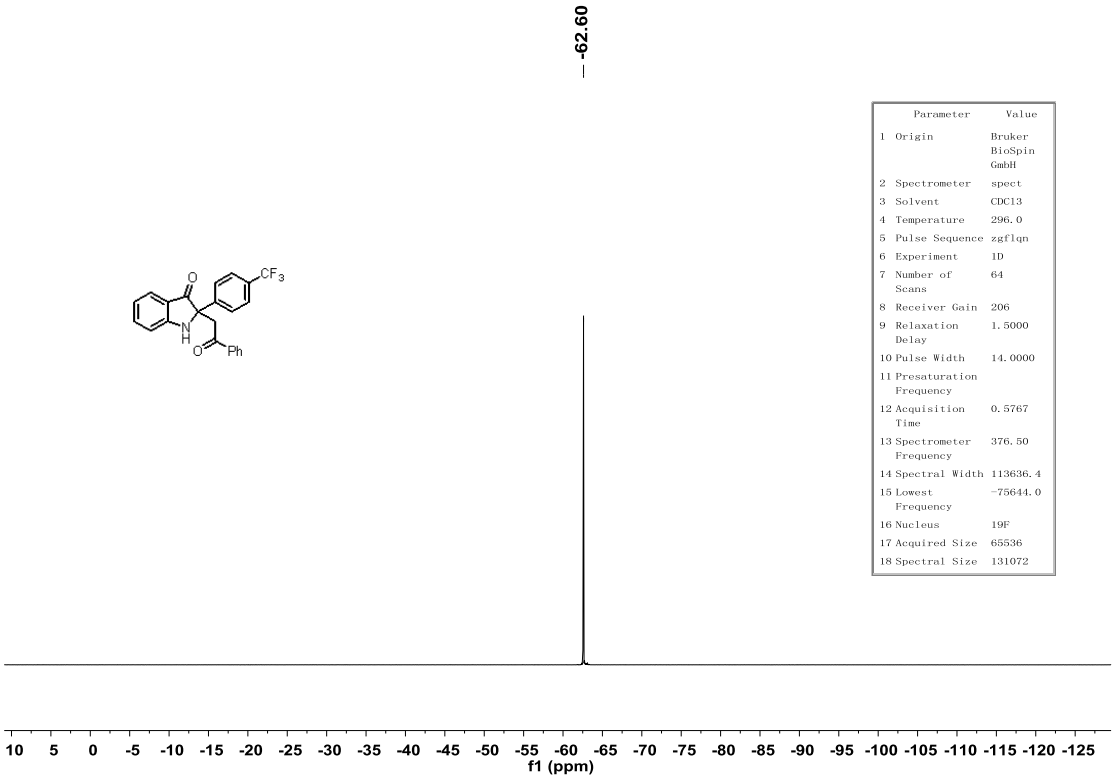
2.05
5.16
2.03
1.01
1.04
1.00
1.00
1.00
f1 (ppm)

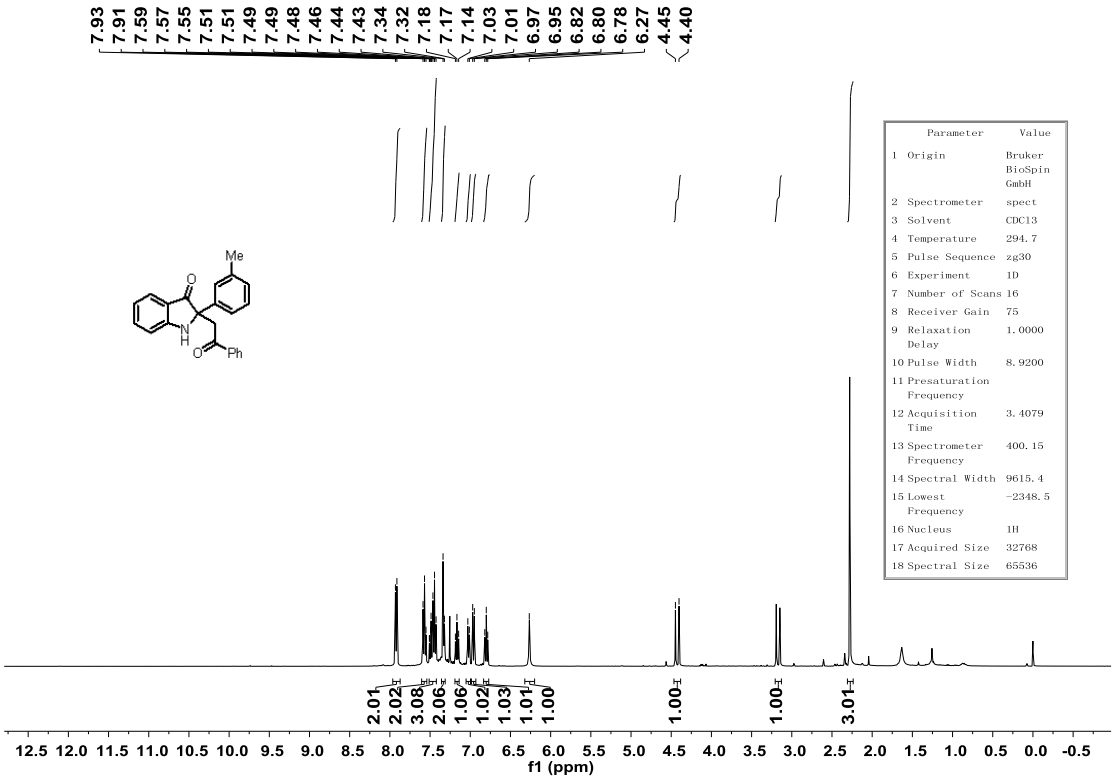


	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	296.3
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Number of Scans	500
8	Receiver Gain	206
9	Relaxation Delay	2.0000
10	Pulse Width	10.0000
11	Presaturation Frequency	
12	Acquisition Time	1.1534
13	Spectrometer Frequency	100.63
14	Spectral Width	28409.1
15	Lowest Frequency	-4129.8
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536



	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	296.0
5	Pulse Sequence	zgflqn
6	Experiment	1D
7	Number of Scans	64
8	Receiver Gain	206
9	Relaxation Delay	1.5000
10	Pulse Width	14.0000
11	Presaturation Frequency	
12	Acquisition Time	0.5767
13	Spectrometer Frequency	376.50
14	Spectral Width	113636.4
15	Lowest Frequency	-75644.0
16	Nucleus	19F
17	Acquired Size	65536
18	Spectral Size	131072

3j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7.51
7.49
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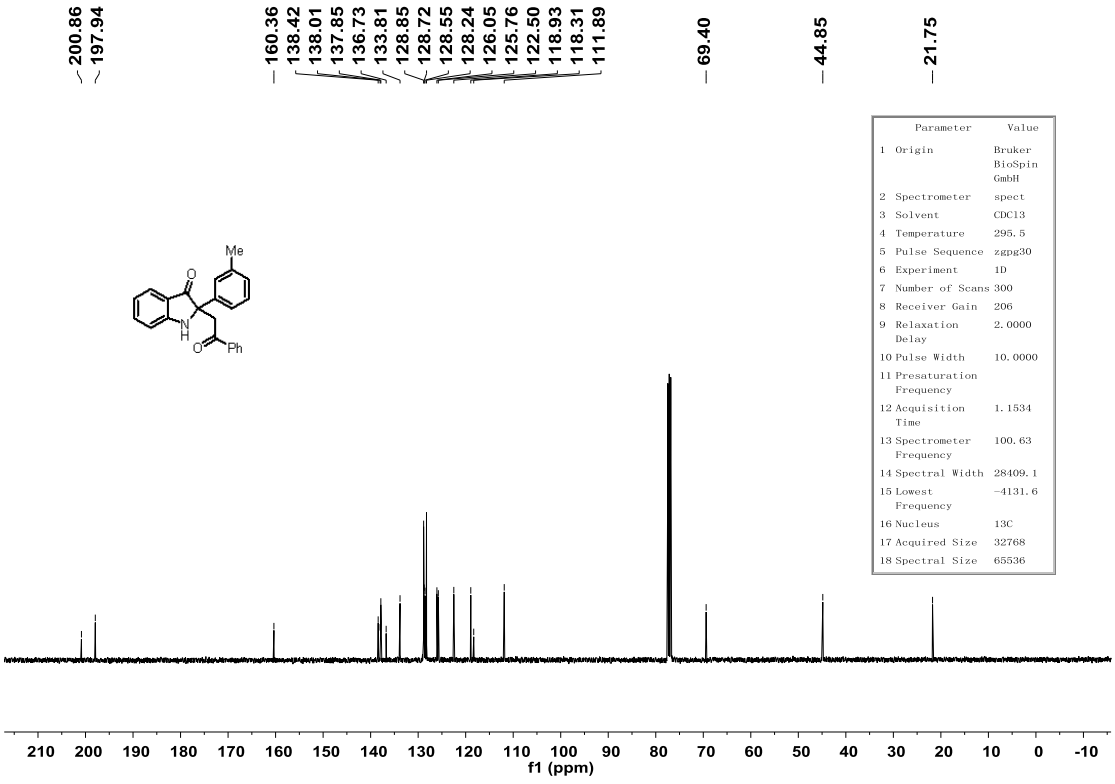
7.48
7.46
7.44
7.43
7.34
7.32
7.18
7.17
7.14
7.03
7.01
6.97
6.95
6.82
6.80
6.78
6.27
4.45
4.40
Me
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.7
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2348.5
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.01
2.02
3.08
2.06
1.06
1.02
1.03
1.01
1.00
1.00
1.00
3.01
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


200.86
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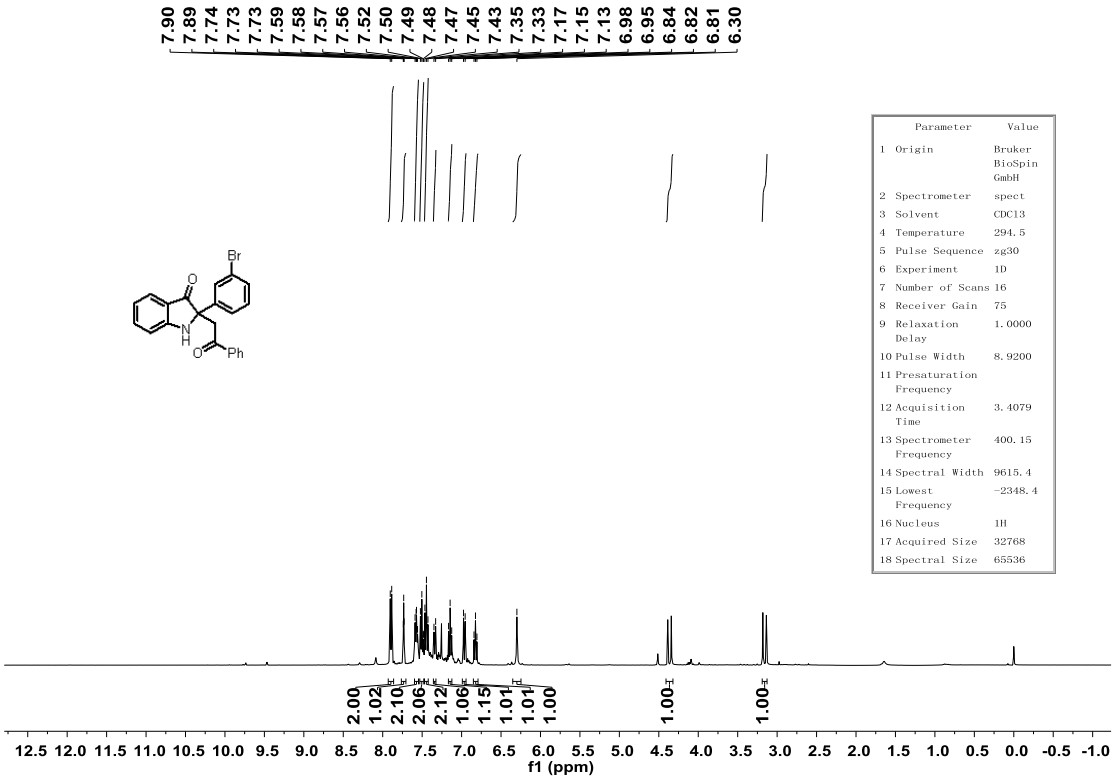
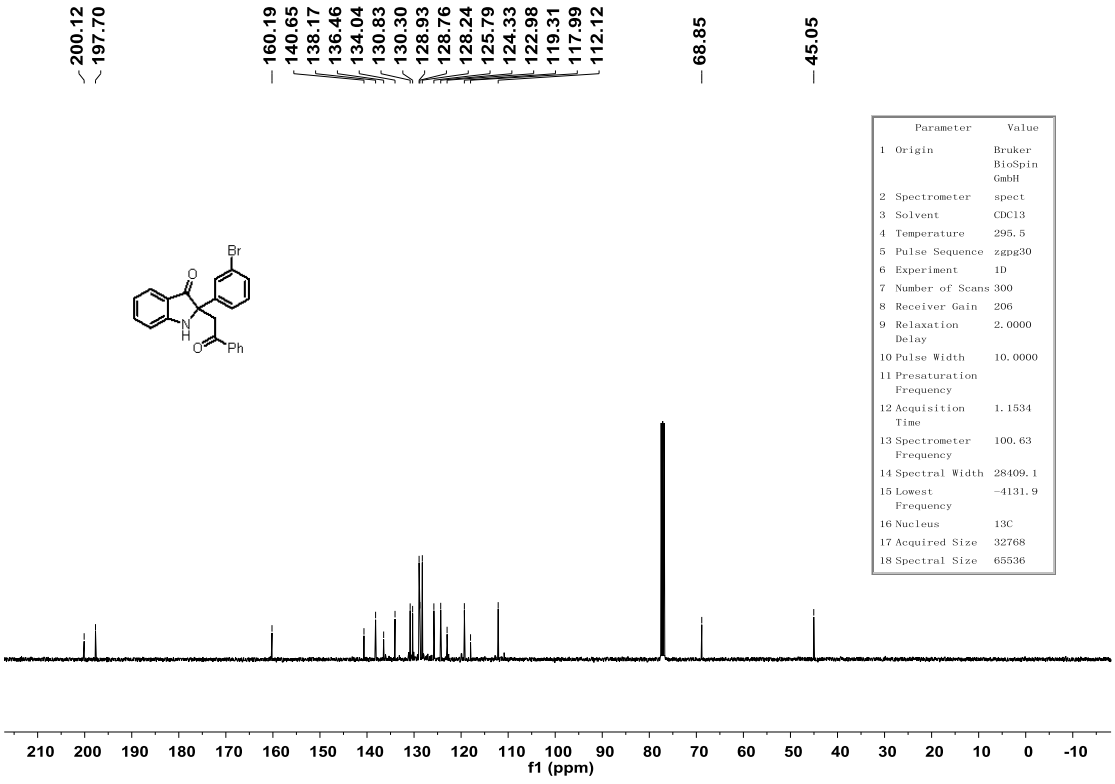
160.36
138.42
138.01
137.85
136.73
133.81
128.85
128.72
128.55
128.24
126.05
125.76
122.50
118.93
118.31
111.89
69.40
44.85
21.75
Me
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.5
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 300
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4131.6
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3k


7.90
7.89
7.74
7.73
7.73
7.59
7.58
7.57
7.56
7.52
7.50
7.49
7.48
7.47
7.45
7.43
7.35
7.33
7.17
7.15
7.13
6.98
6.95
6.84
6.82
6.81
6.30
Br
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.5
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2348.4
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.00
1.02
2.10
2.06
2.12
1.06
1.15
1.01
1.01
1.00
1.00
1.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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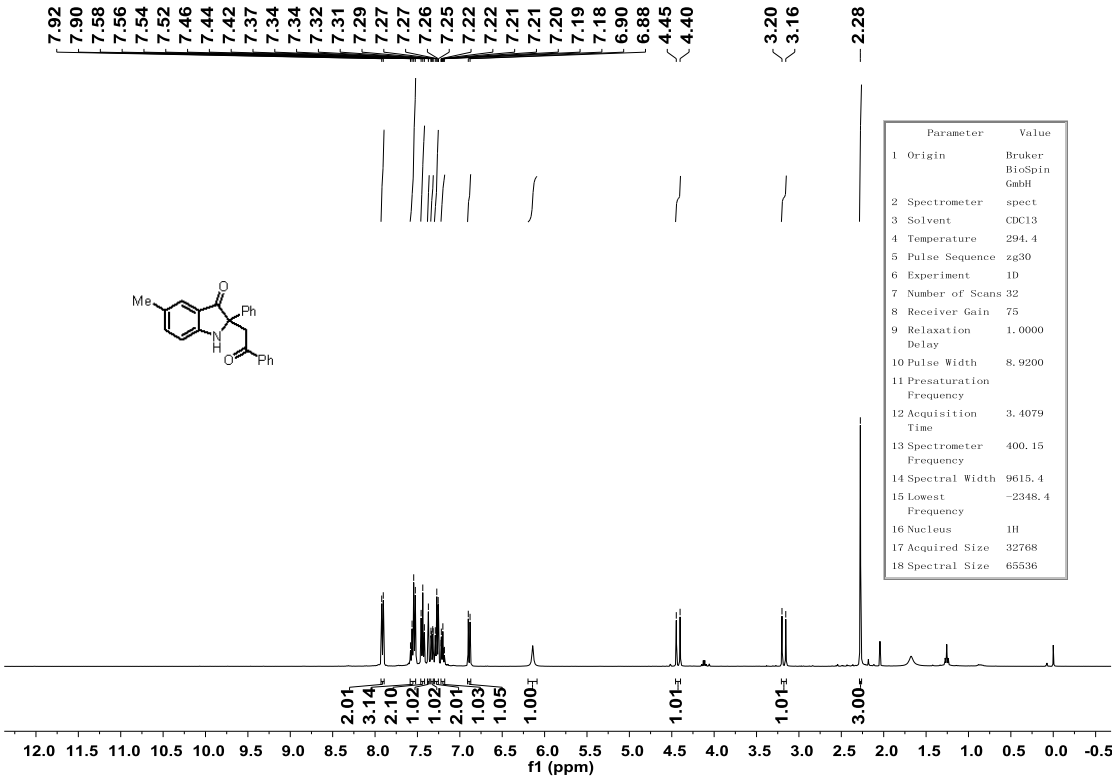
140.65
138.17
136.46
134.04
130.83
130.30
128.93
128.76
128.24
125.79
124.33
122.98
119.31
117.99
112.12
68.85
45.05
Br
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.5
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 300
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4131.9
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3l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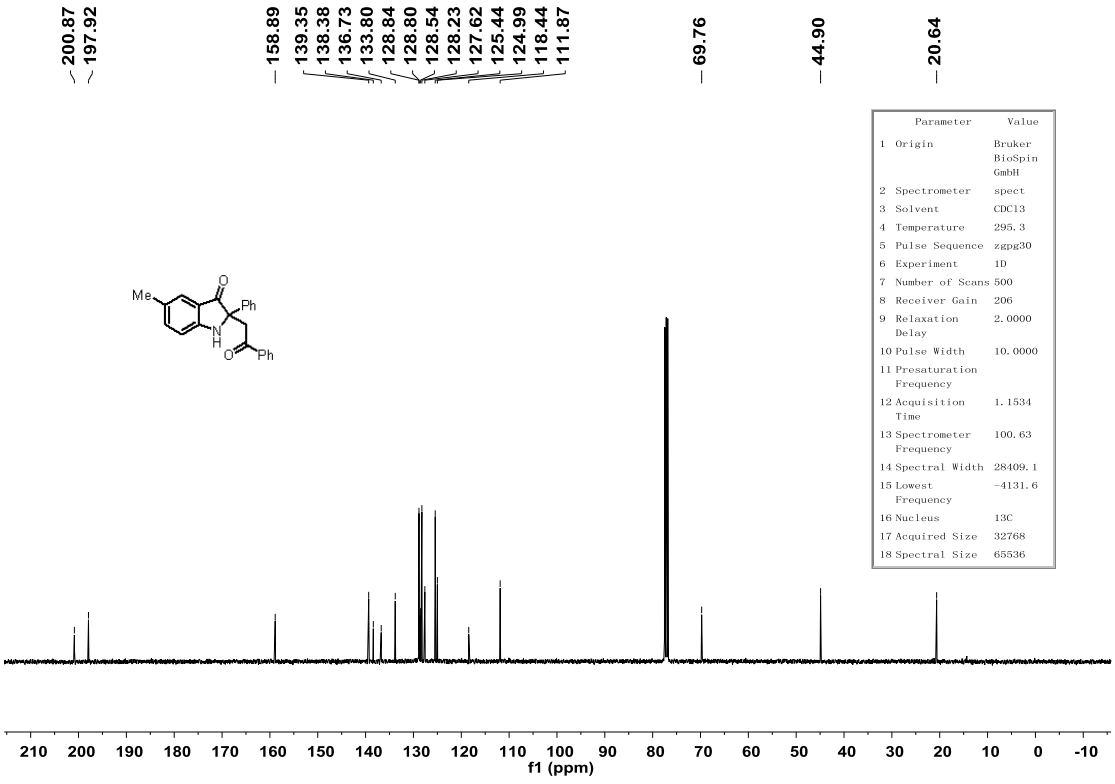
7.37
7.34
7.34
7.32
7.31
7.29
7.27
7.27
7.26
7.25
7.22
7.22
7.21
7.21
7.20
7.19
7.18
6.90
6.88
4.45
4.40
3.20
3.16
2.28
Me
O
Ph
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.4
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2348.4
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.01
3.14
2.10
1.02
1.02
2.01
1.03
1.05
1.00
1.01
1.01
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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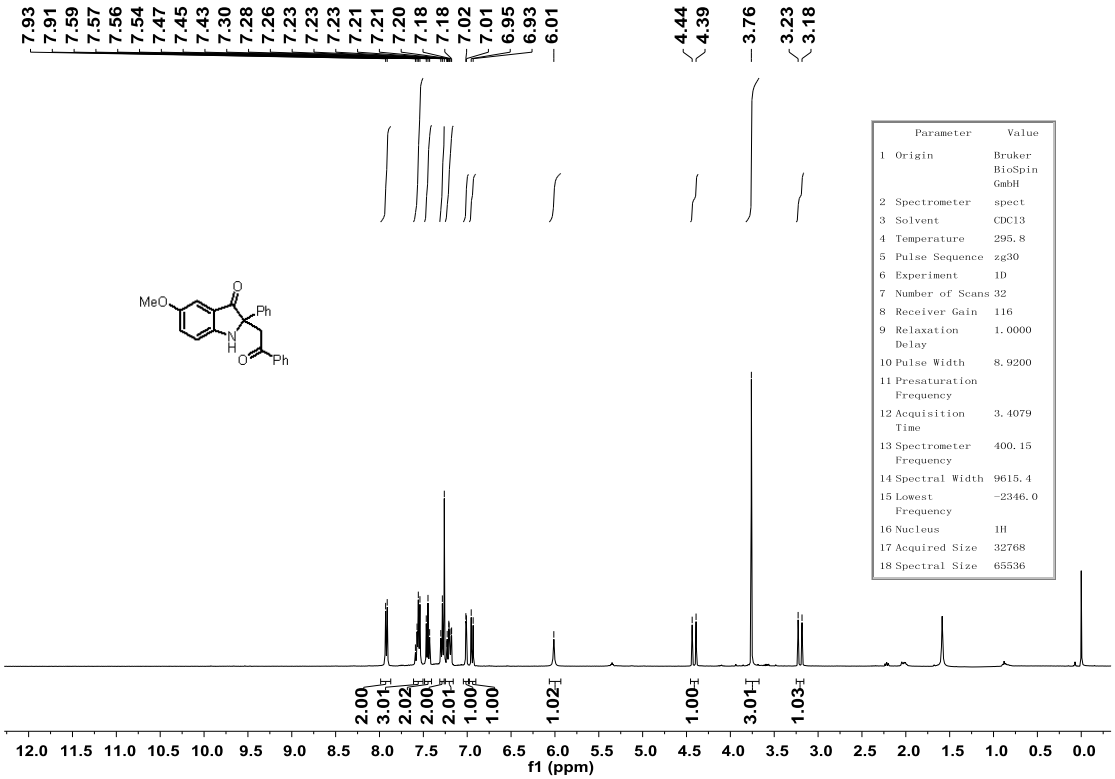
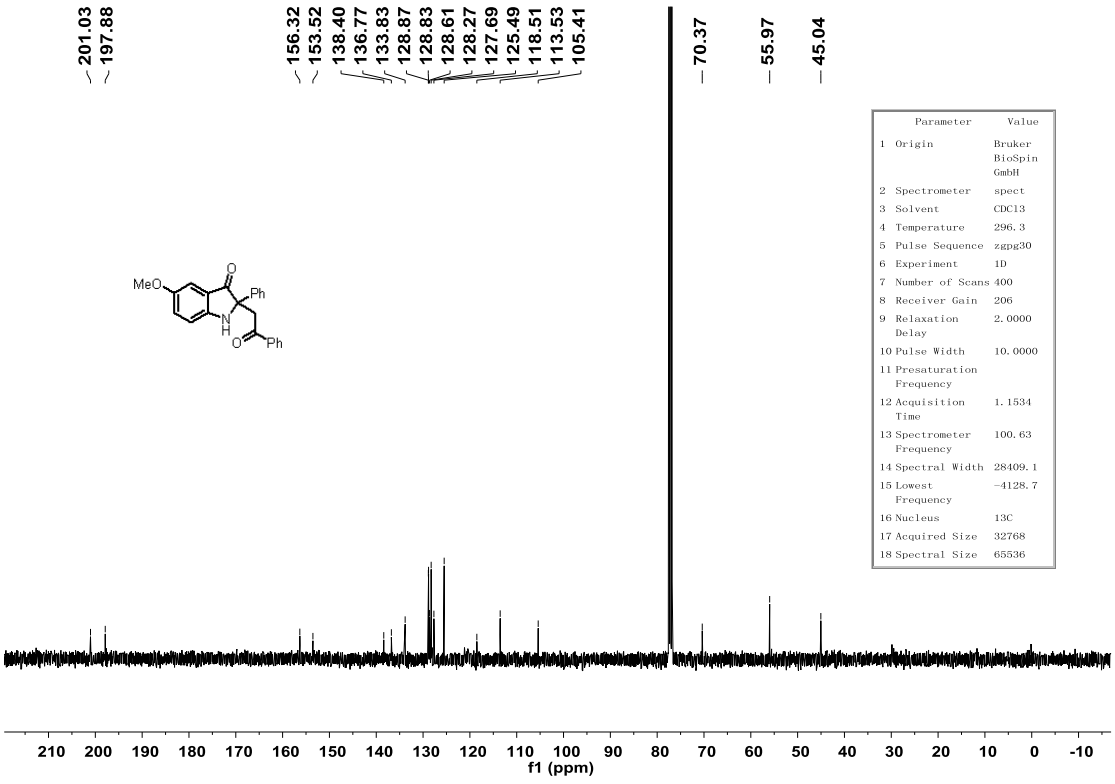
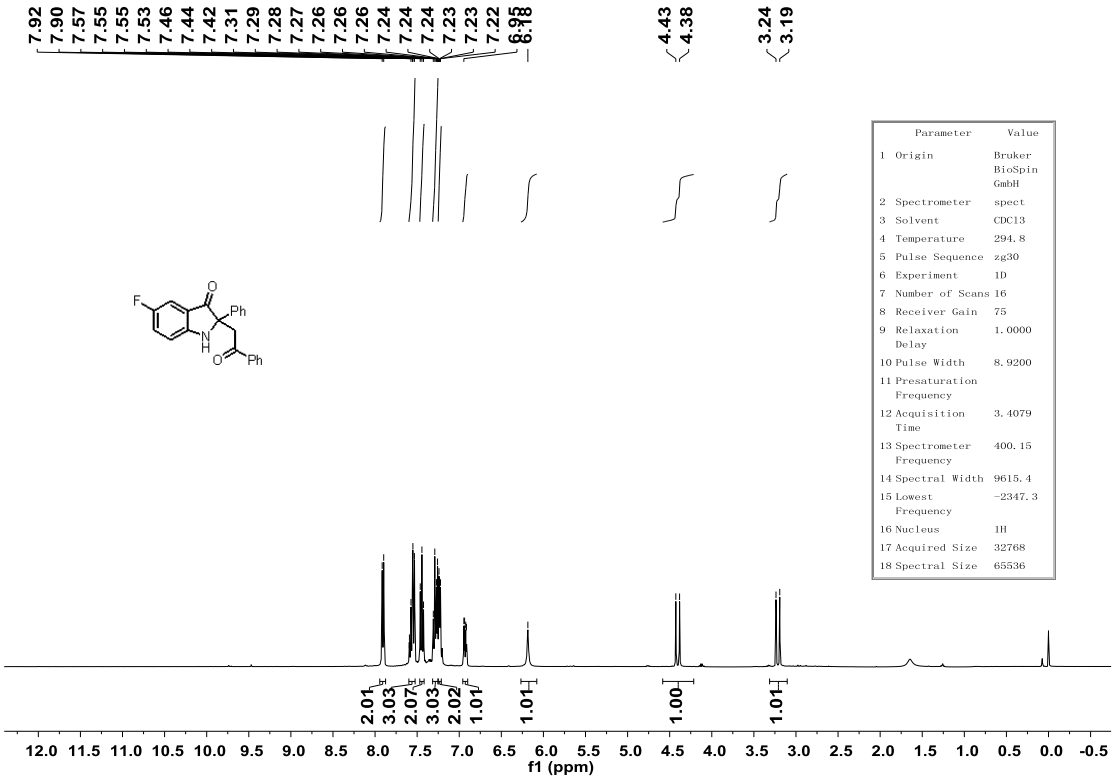
136.73
133.80
128.84
128.80
128.54
128.23
127.62
125.44
124.99
118.44
111.87
69.76
44.90
20.64
Me
O
Ph
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.3
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4131.6
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3m


7.93 7.91 7.59 7.57 7.56 7.54 7.47 7.45 7.43 7.30 7.28 7.26 7.23 7.23 7.23 7.21 7.21 7.20 7.18 7.18 7.02 7.01 6.95 6.93 6.01
4.44 4.39 3.76 3.23 3.18
MeO
Ph
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.8
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 116
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2346.0
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.00 3.01 2.02 2.00 2.01 1.00 1.00 1.02 1.00 3.01 1.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


201.03 197.88
156.32 153.52 138.40 136.77 133.83 128.87 128.83 128.61 128.27 127.69 125.49 118.51 113.53 105.41
70.37 55.97 45.04
MeO
Ph
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 296.3
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 400
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4128.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3n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7.90
7.57
7.55
7.55
7.53
7.46
7.44
7.42
7.31
7.29
7.28
7.27
7.26
7.26
7.26
7.24
7.24
7.24
7.23
7.23
7.22
6.95
6.18
4.43
4.38
3.24
3.19
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.8
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.3
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
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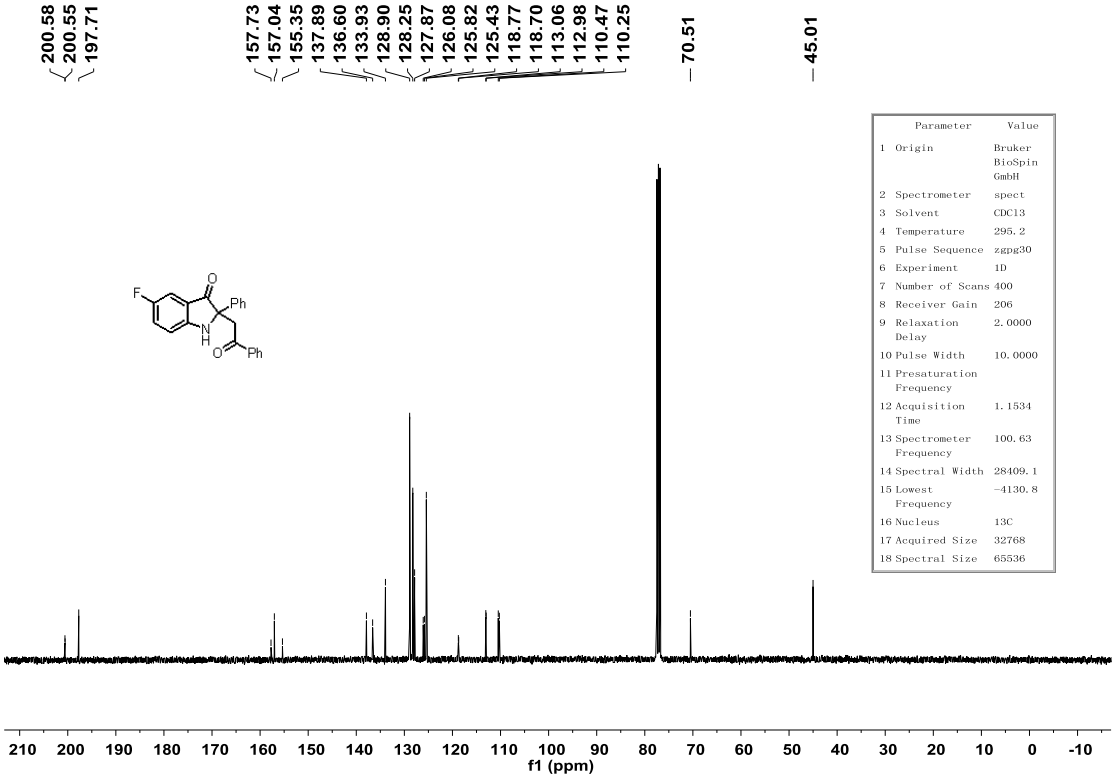
3.03
2.07
3.03
2.02
1.01
1.01
1.00
1.01
f1 (ppm)


200.58
200.55
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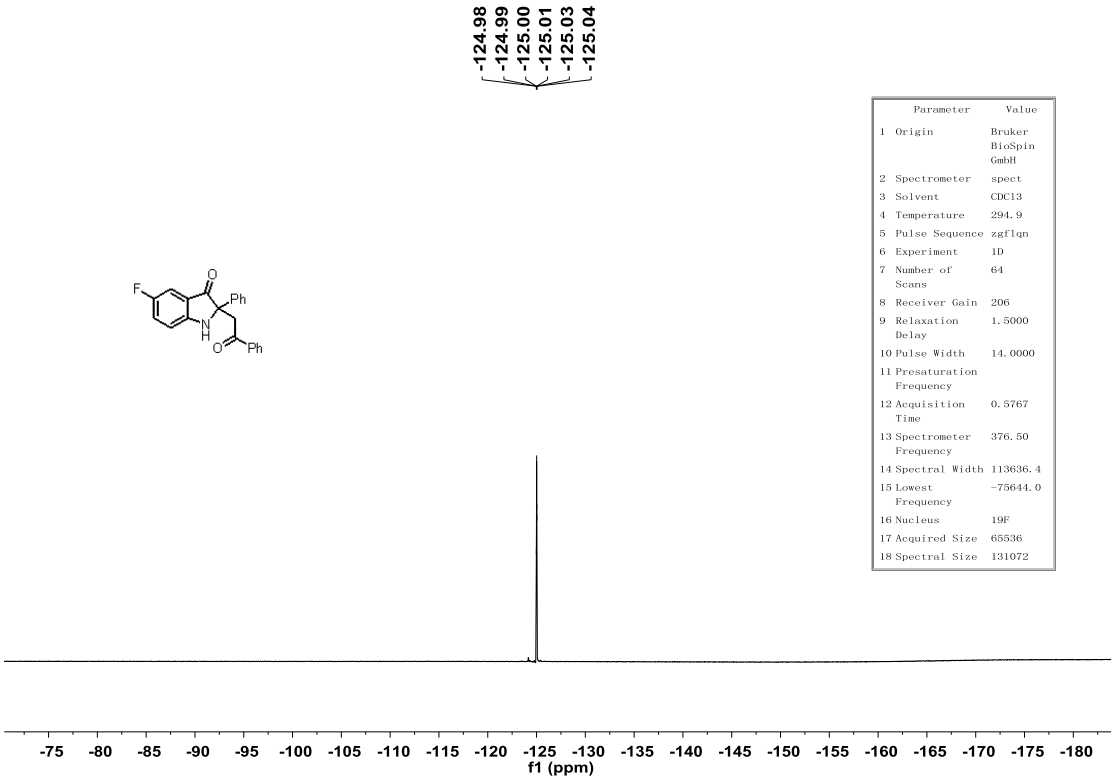
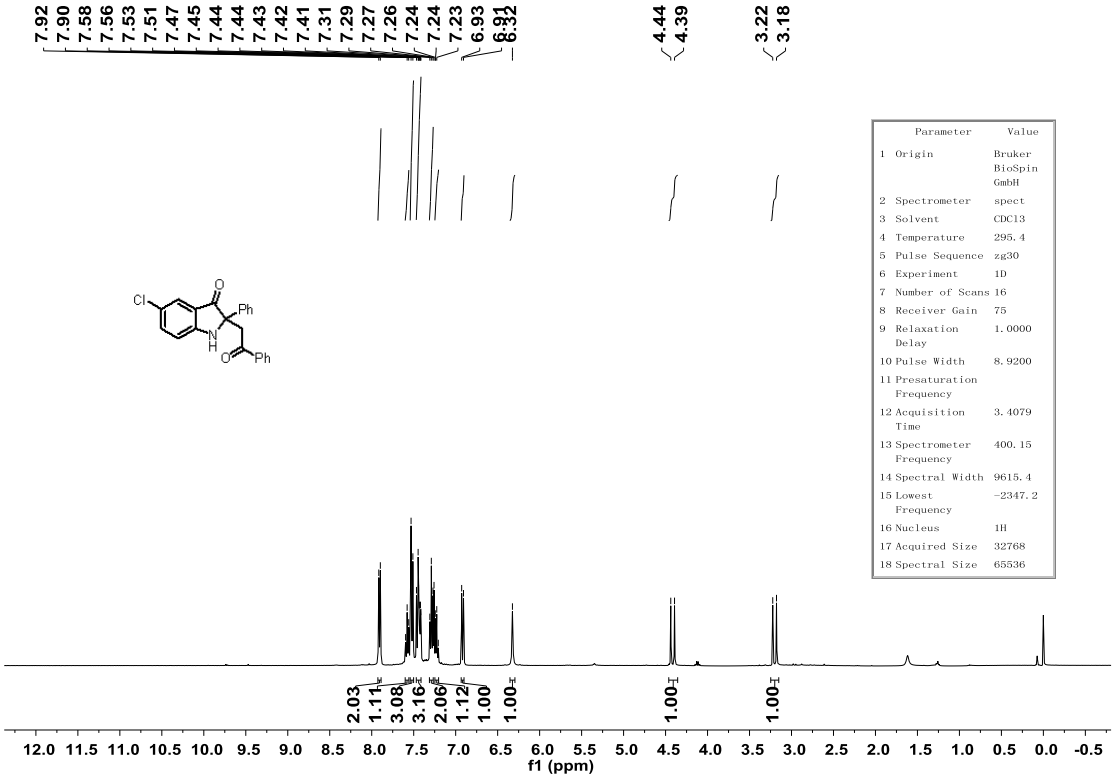
157.73
157.04
155.35
137.89
136.60
133.93
128.90
128.25
127.87
126.08
125.82
125.43
118.77
118.70
113.06
112.98
110.47
110.25
70.51
45.01
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.2
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 400
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4130.8
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
f1 (ppm)


-124.98
-124.99
-125.00
-125.01
-125.03
-125.04
F
O
Ph
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.9
5 Pulse Sequence zgflqn
6 Experiment 1D
7 Number of Scans 64
8 Receiver Gain 206
9 Relaxation Delay 1.5000
10 Pulse Width 14.0000
11 Presaturation Frequency
12 Acquisition Time 0.5767
13 Spectrometer Frequency 376.50
14 Spectral Width 113636.4
15 Lowest Frequency -75644.0
16 Nucleus 19F
17 Acquired Size 65536
18 Spectral Size 131072
-75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170 -175 -180
f1 (ppm)

3o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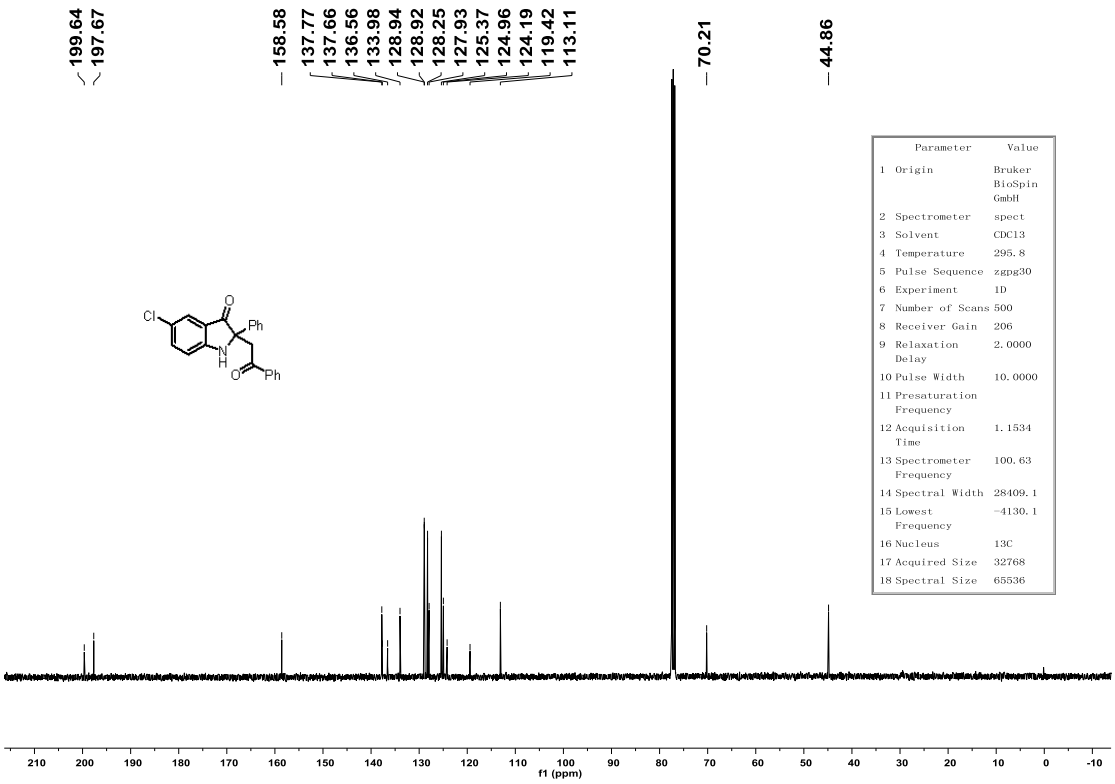
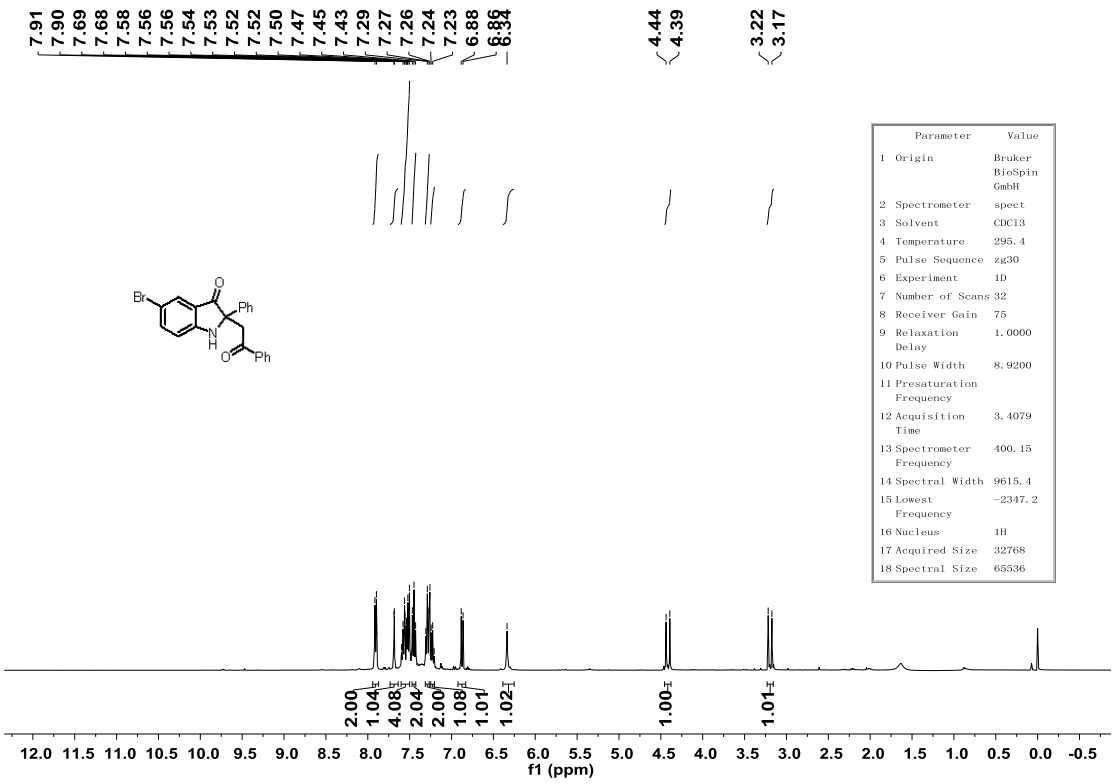
7.90
7.58
7.56
7.53
7.51
7.47
7.45
7.44
7.44
7.43
7.42
7.41
7.31
7.29
7.27
7.26
7.24
7.24
7.23
6.93
6.91
6.32
4.44
4.39
3.22
3.18
Cl
O
Ph
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.4
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.2
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.03
1.11
3.08
3.16
2.06
1.12
1.00
1.00
1.00
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

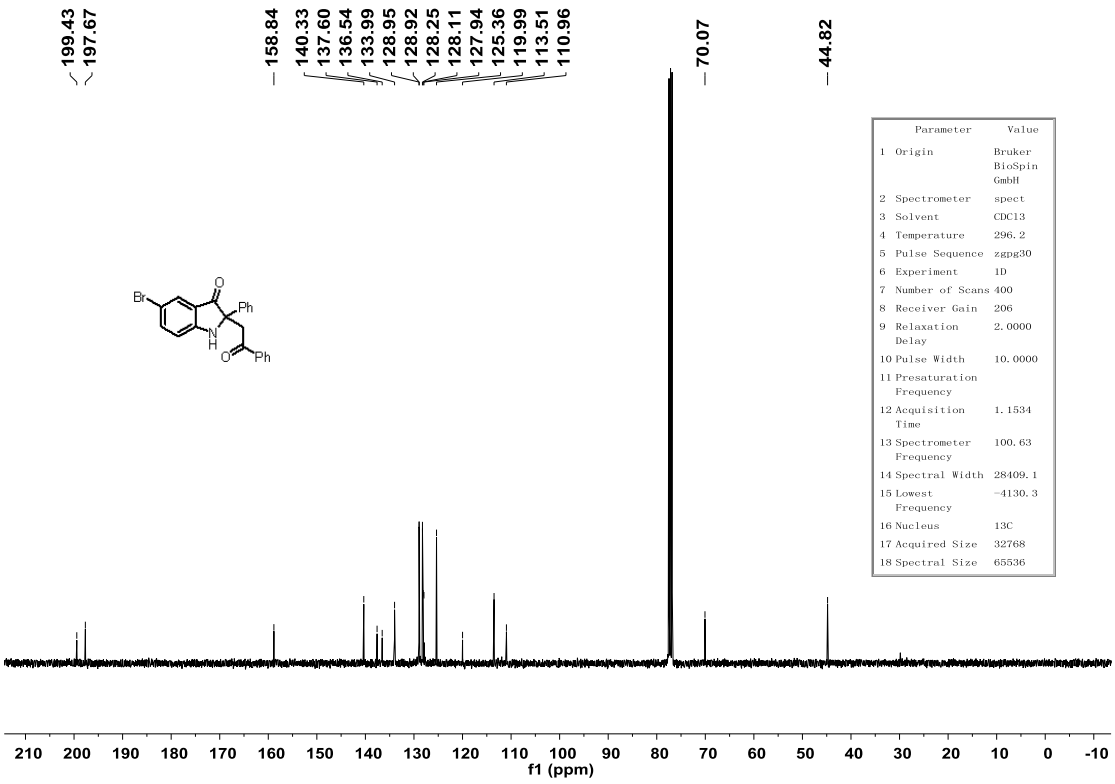


	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	295.8
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Number of Scans	500
8	Receiver Gain	206
9	Relaxation Delay	2.0000
10	Pulse Width	10.0000
11	Presaturation Frequency	
12	Acquisition Time	1.1534
13	Spectrometer Frequency	100.63
14	Spectral Width	28409.1
15	Lowest Frequency	-4130.1
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

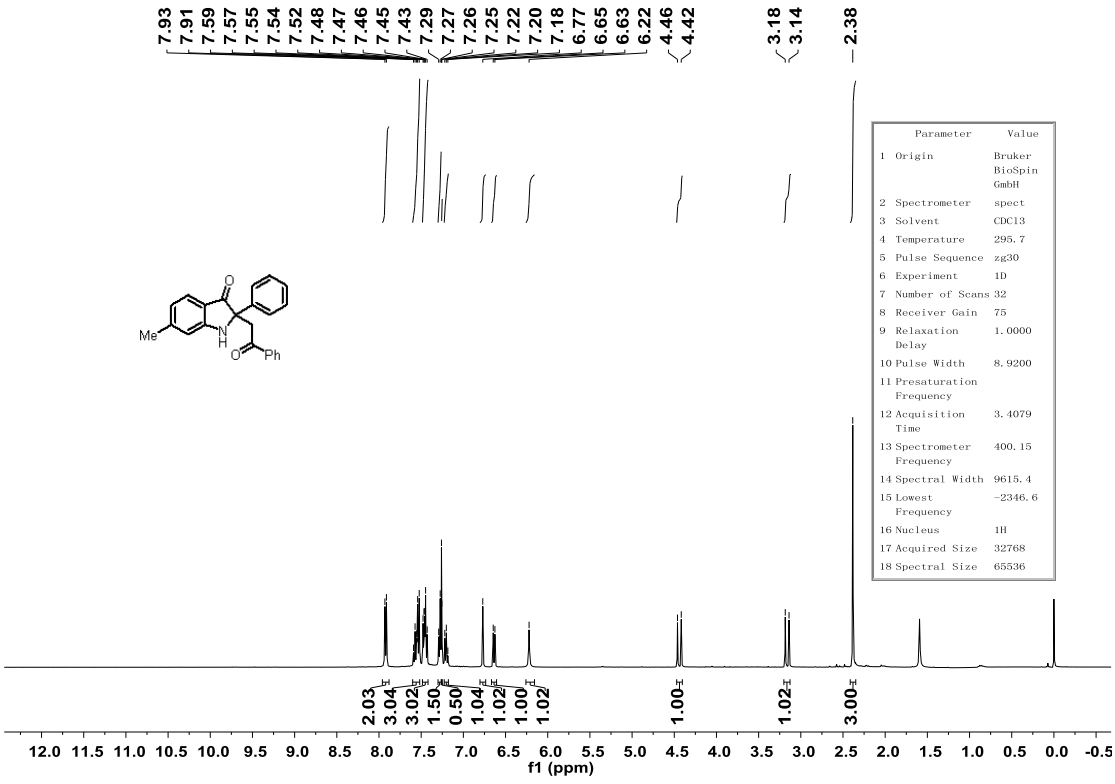
3p



	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	295.4
5	Pulse Sequence	zg30
6	Experiment	1D
7	Number of Scans	32
8	Receiver Gain	75
9	Relaxation Delay	1.0000
10	Pulse Width	8.9200
11	Presaturation Frequency	
12	Acquisition Time	3.4079
13	Spectrometer Frequency	400.15
14	Spectral Width	9615.4
15	Lowest Frequency	-2347.2
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536


199.43
197.67
158.84
140.33
137.60
136.54
133.99
128.95
128.92
128.25
128.11
127.94
125.36
119.99
113.51
110.96
70.07
44.82
Br
O
Ph
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 296.2
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 400
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4130.3
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3q


7.93
7.91
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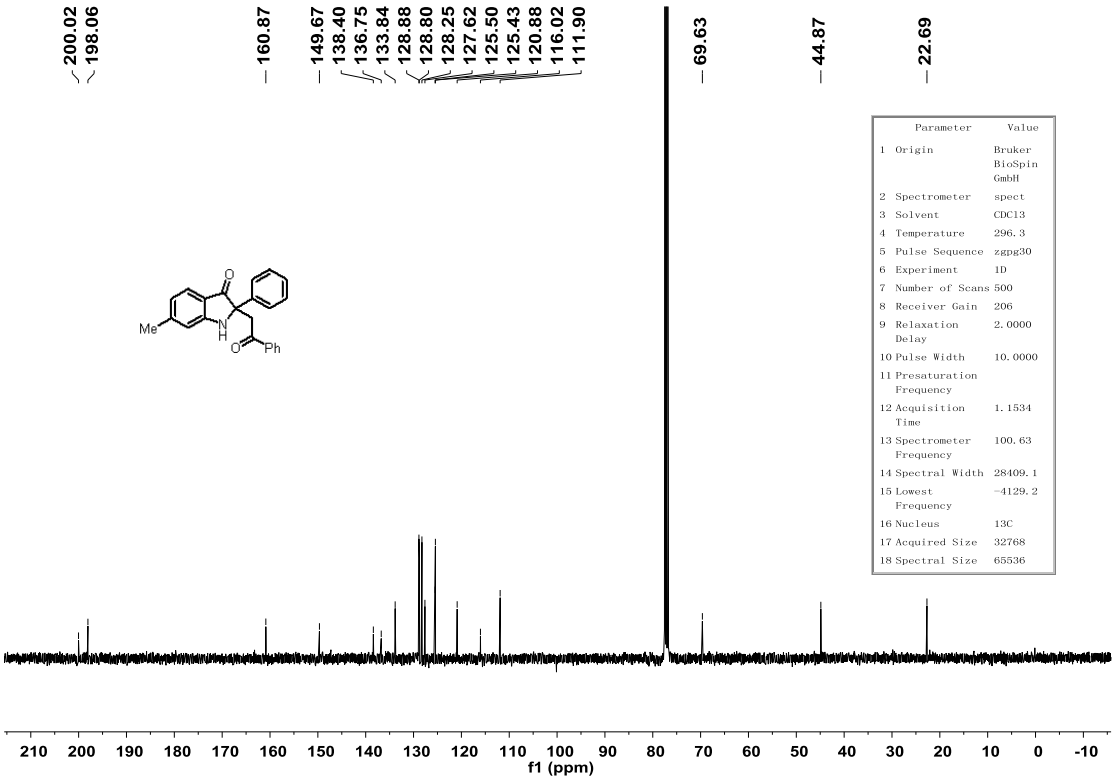
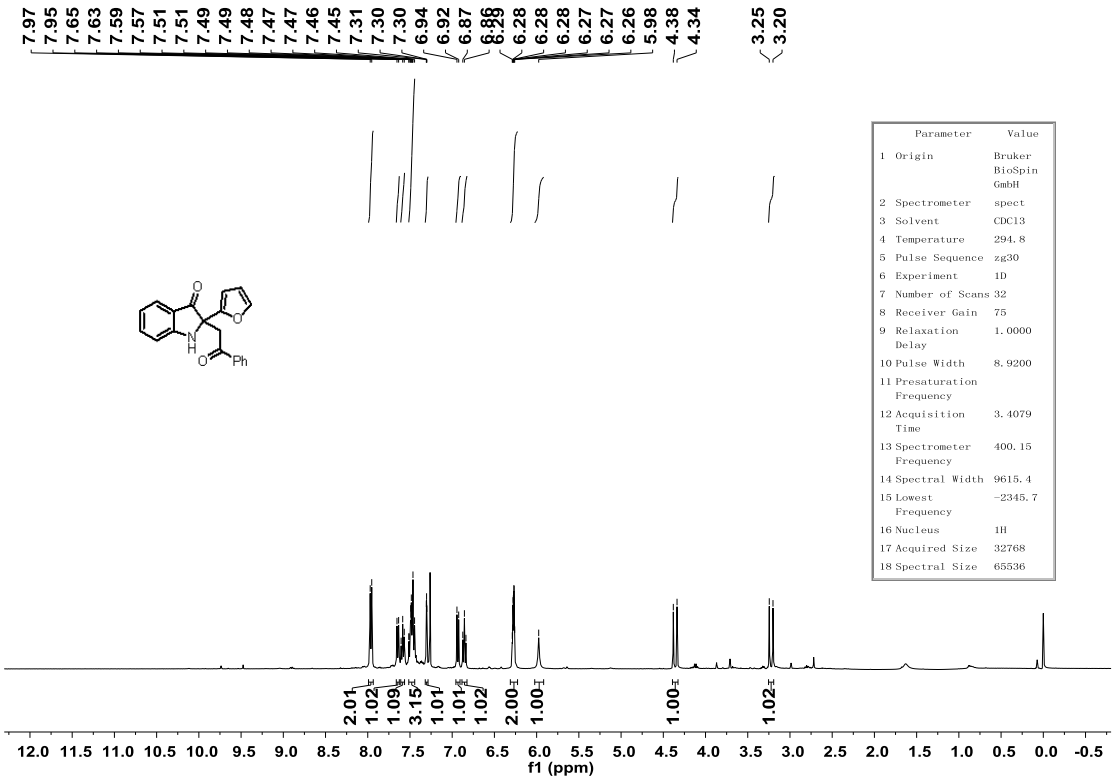
7.57
7.55
7.54
7.52
7.48
7.47
7.46
7.45
7.43
7.29
7.27
7.26
7.25
7.22
7.20
7.18
6.77
6.65
6.63
6.22
4.46
4.42
3.18
3.14
2.38
Me
O
N
H
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.7
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2346.6
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.03
3.04
3.02
1.50
0.50
1.04
1.02
1.00
1.02
1.00
1.02
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

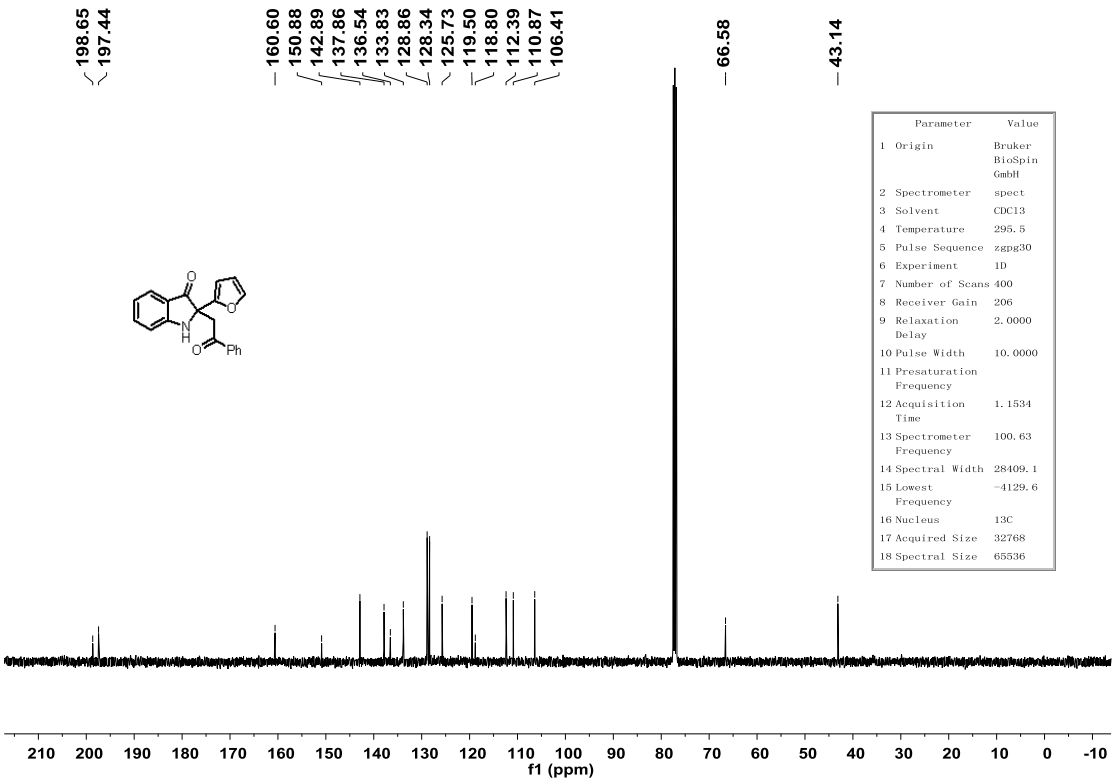


	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	296.3
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Number of Scans	500
8	Receiver Gain	206
9	Relaxation Delay	2.0000
10	Pulse Width	10.0000
11	Presaturation Frequency	
12	Acquisition Time	1.1534
13	Spectrometer Frequency	100.63
14	Spectral Width	28409.1
15	Lowest Frequency	-4129.2
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

3r



	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	294.8
5	Pulse Sequence	zg30
6	Experiment	1D
7	Number of Scans	32
8	Receiver Gain	75
9	Relaxation Delay	1.0000
10	Pulse Width	8.9200
11	Presaturation Frequency	
12	Acquisition Time	3.4079
13	Spectrometer Frequency	400.15
14	Spectral Width	9615.4
15	Lowest Frequency	-2345.7
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536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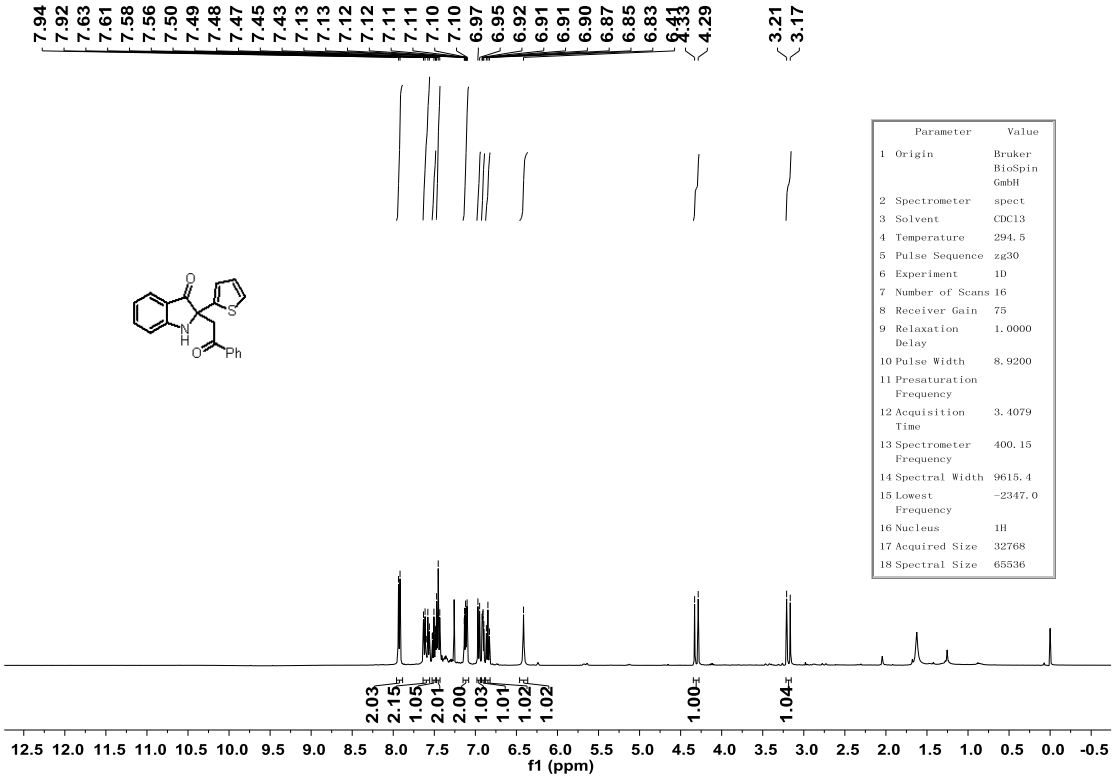
197.44
160.60
150.88
142.89
137.86
136.54
133.83
128.86
128.34
125.73
119.50
118.80
112.39
110.87
106.41
66.58
43.14
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.5
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 400
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4129.6
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
O
N
H
O
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3s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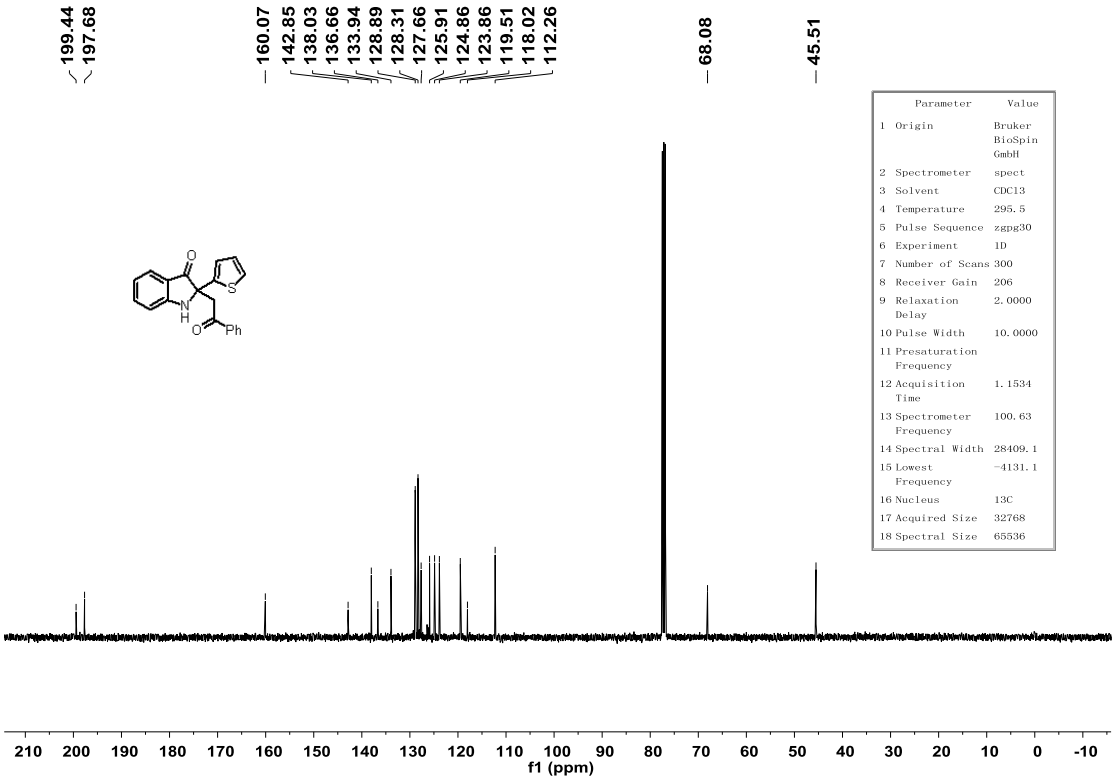
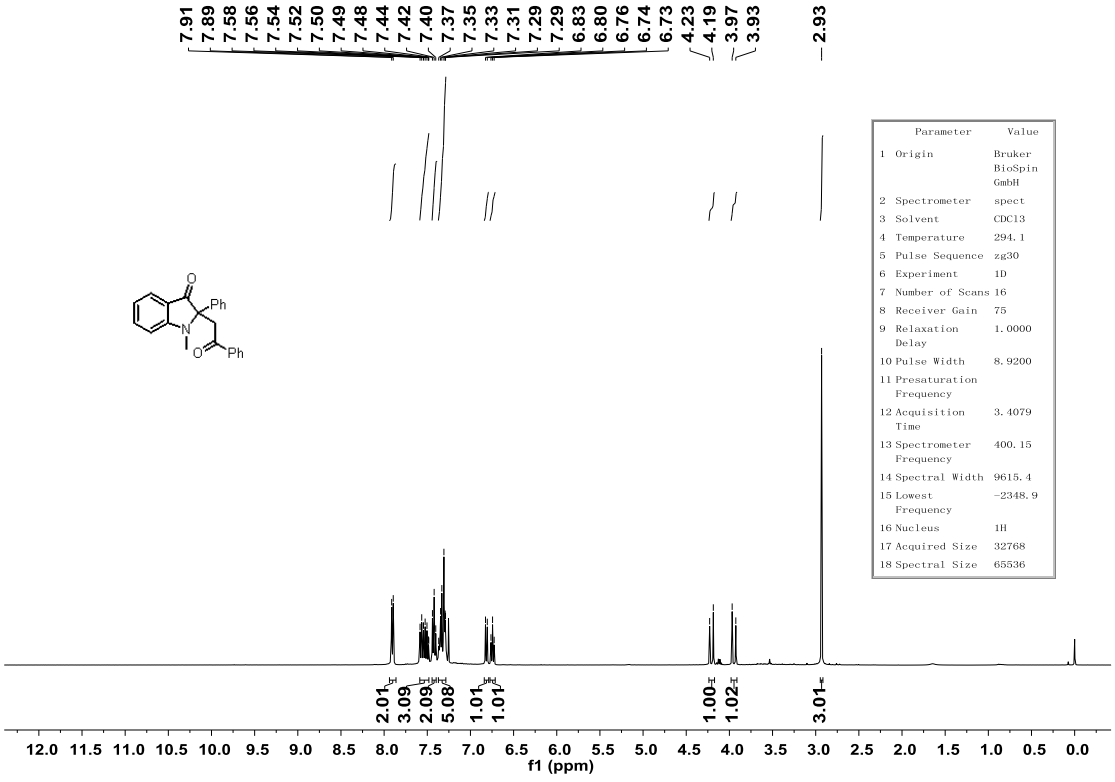
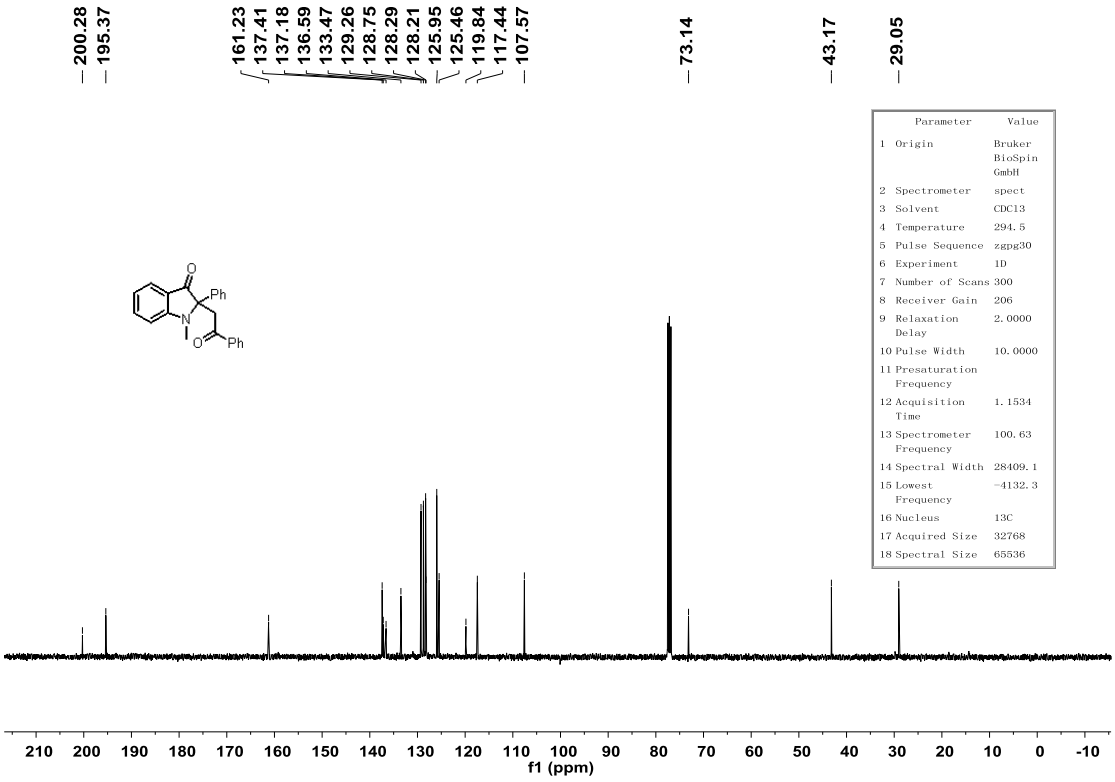
7.56
7.50
7.49
7.48
7.47
7.45
7.43
7.13
7.13
7.12
7.12
7.11
7.11
7.10
7.10
6.97
6.95
6.92
6.91
6.91
6.90
6.87
6.85
6.83
6.41
6.33
4.29
3.21
3.17
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.5
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.0
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
O
S
N
H
O
Ph
2.03
2.15
1.05
2.01
2.00
1.03
1.01
1.02
1.02
1.00
1.04
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

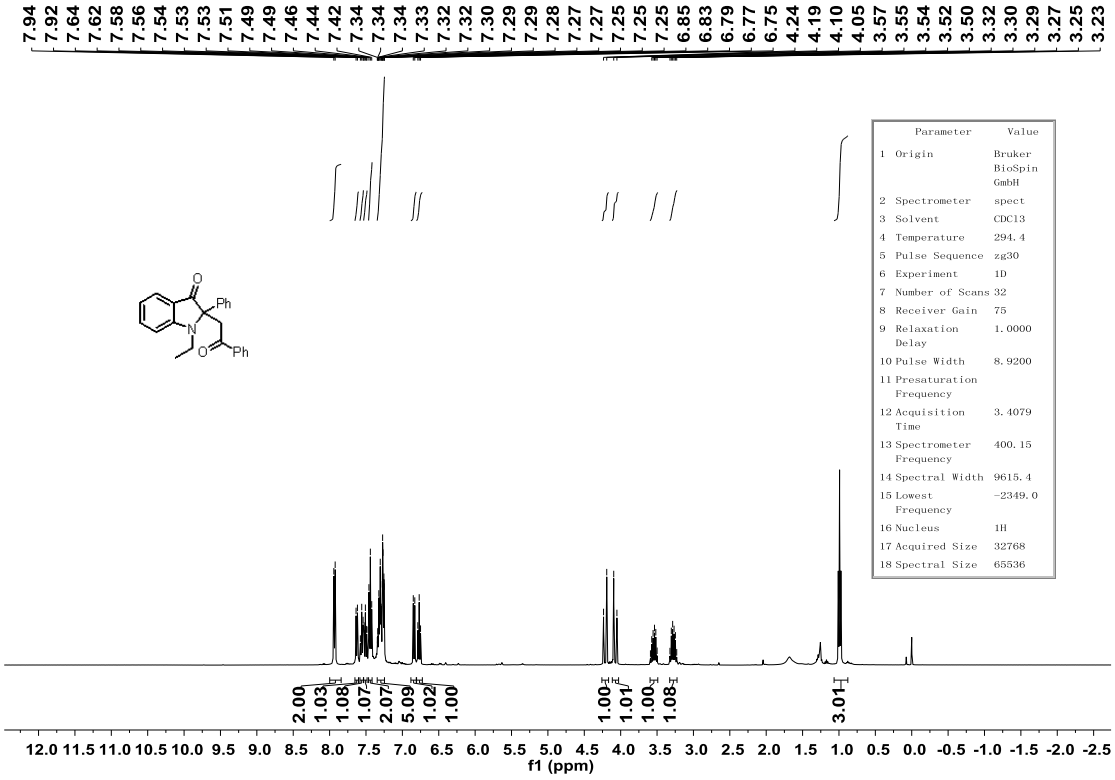

199.44
197.68
160.07
142.85
138.03
136.66
133.94
128.89
128.31
127.66
125.91
124.86
123.86
119.51
118.02
112.26
68.08
45.51
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.5
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 300
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4131.1
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
O
S
N
H
O
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

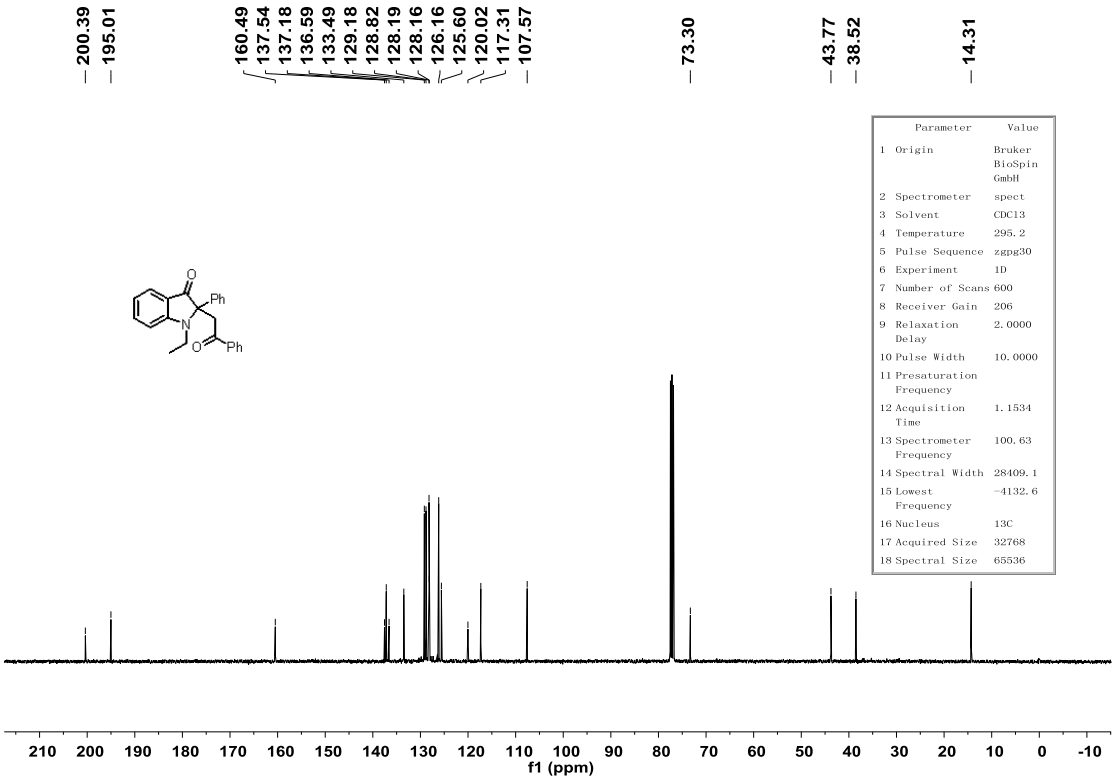
3t


7.91
7.89
7.58
7.56
7.54
7.52
7.50
7.49
7.48
7.44
7.42
7.40
7.37
7.35
7.33
7.31
7.29
7.29
6.83
6.80
6.76
6.74
6.73
4.23
4.19
3.97
3.93
2.93
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.1
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 16
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2348.9
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
O
Ph
N
O
Ph
2.01
3.09
2.09
5.08
1.01
1.01
1.00
1.02
3.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

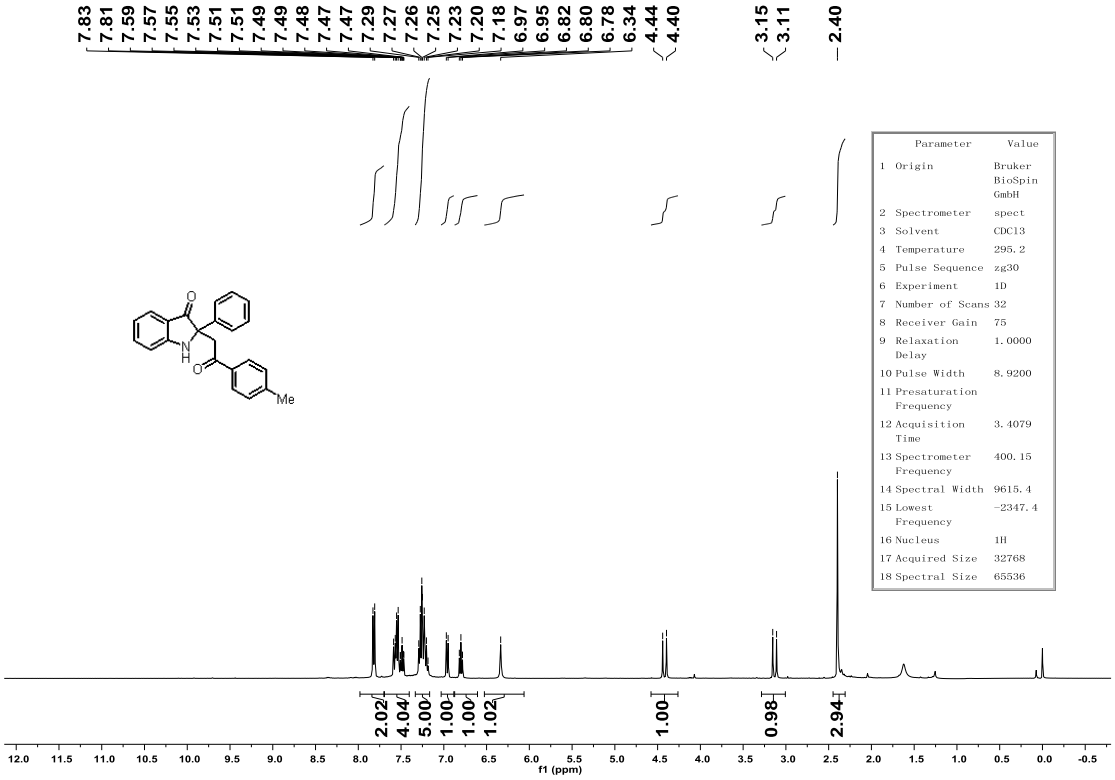

200.28
195.37
161.23
137.41
137.18
136.59
133.47
129.26
128.75
128.29
128.21
125.95
125.46
119.84
117.44
107.57
73.14
43.17
29.05
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.5
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 300
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4132.3
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
O
Ph
N
O
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

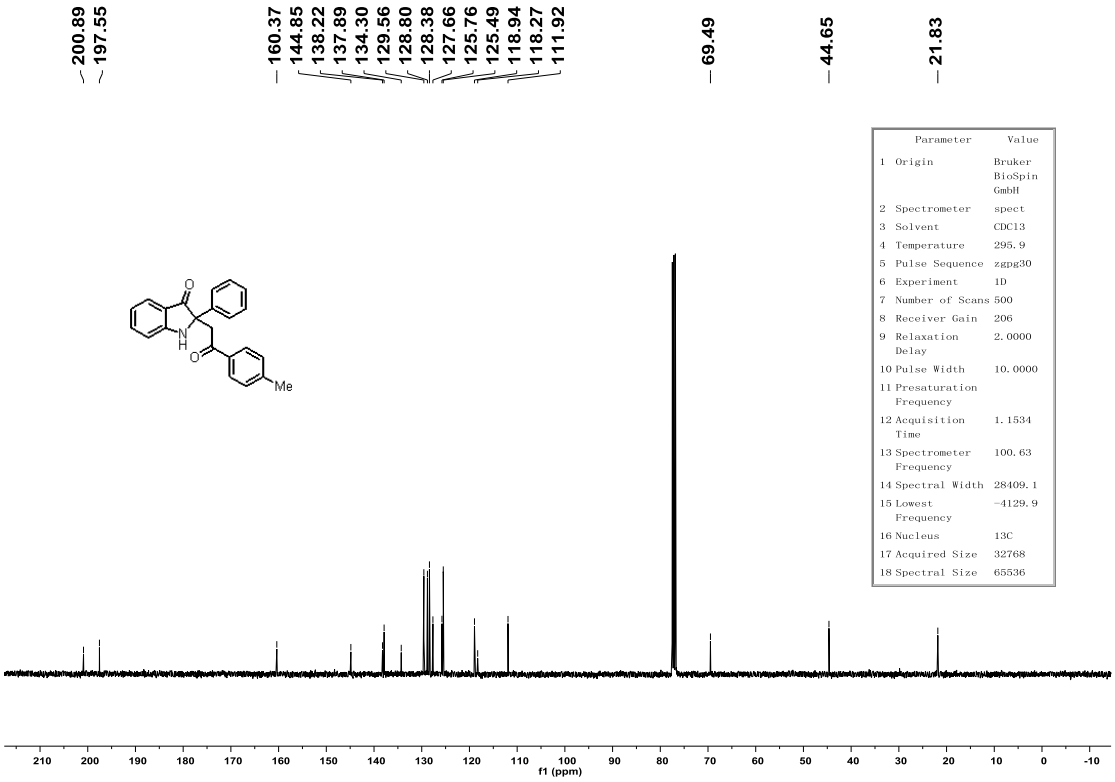
3u


7.94
7.92
7.64
7.62
7.58
7.56
7.54
7.53
7.53
7.51
7.49
7.49
7.46
7.44
7.42
7.34
7.34
7.34
7.33
7.32
7.32
7.30
7.29
7.29
7.28
7.27
7.27
7.25
7.25
7.25
6.85
6.83
6.79
6.77
6.75
4.24
4.19
4.10
4.05
3.57
3.55
3.54
3.52
3.50
3.32
3.30
3.29
3.27
3.25
3.23
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.4
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2349.0
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
O
Ph
N
O
Ph
2.00
1.03
1.08
1.07
2.07
5.09
1.02
1.00
1.00
1.01
1.00
1.08
3.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)


200.39
195.01
160.49
137.54
137.18
136.59
133.49
129.18
128.82
128.19
128.16
126.16
125.60
120.02
117.31
107.57
73.30
43.77
38.52
14.31
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.2
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 600
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4132.6
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
O
Ph
N
O
Ph
f1 (ppm)

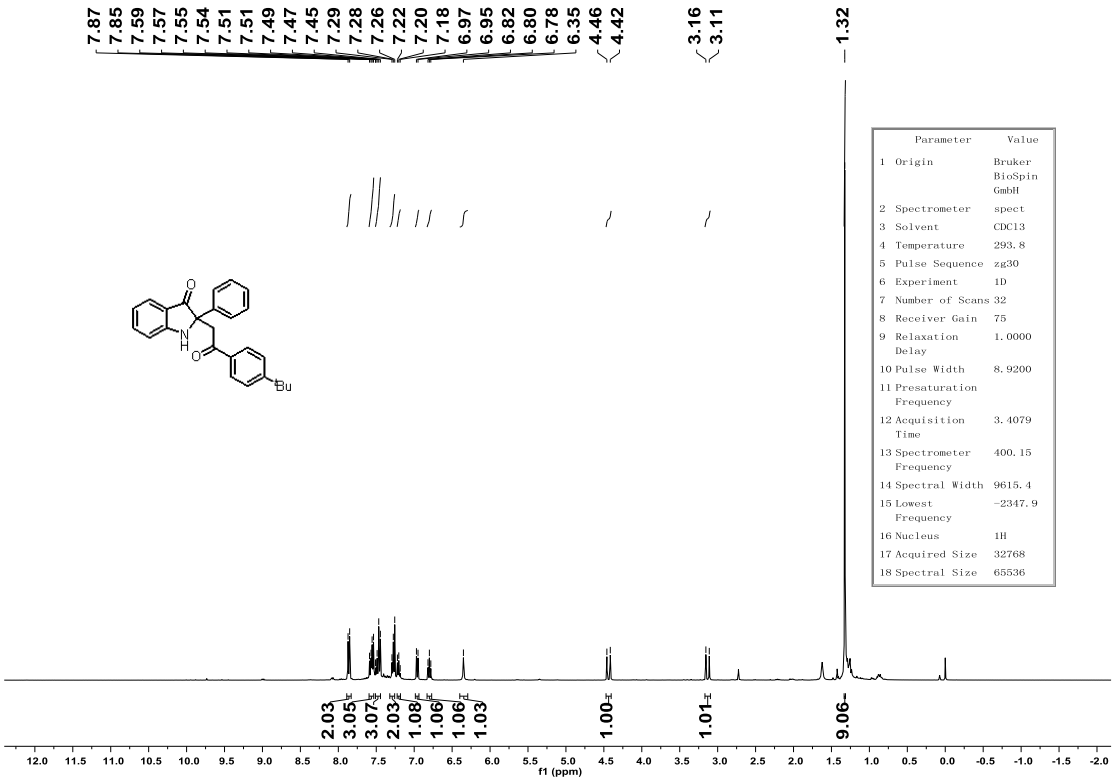
3v


7.83
7.81
7.59
7.57
7.55
7.53
7.51
7.51
7.49
7.49
7.48
7.47
7.47
7.29
7.27
7.26
7.25
7.23
7.20
7.18
6.97
6.95
6.82
6.80
6.78
6.34
4.44
4.40
3.15
3.11
2.40
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.2
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.4
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
O
N
H
O
Me
2.02
4.04
5.00
1.00
1.00
1.02
1.00
0.98
2.94
f1 (ppm)

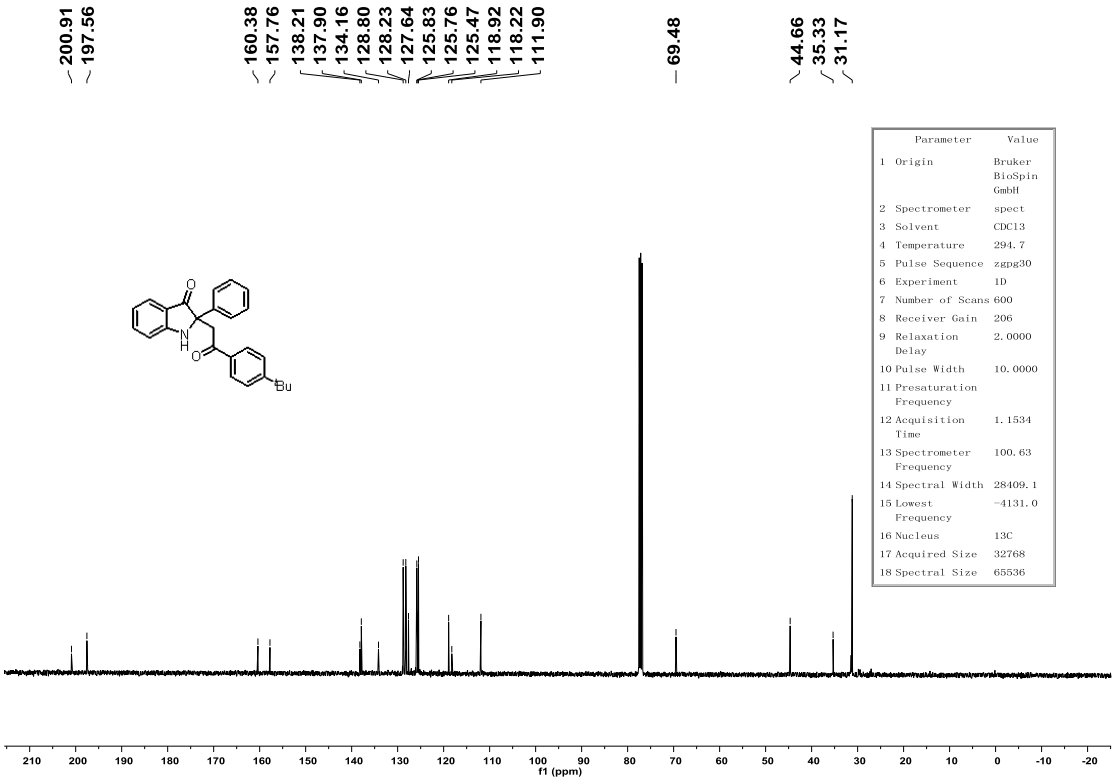


	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	295.9
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Number of Scans	500
8	Receiver Gain	206
9	Relaxation Delay	2.0000
10	Pulse Width	10.0000
11	Presaturation Frequency	
12	Acquisition Time	1.1534
13	Spectrometer Frequency	100.63
14	Spectral Width	28409.1
15	Lowest Frequency	-4129.9
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

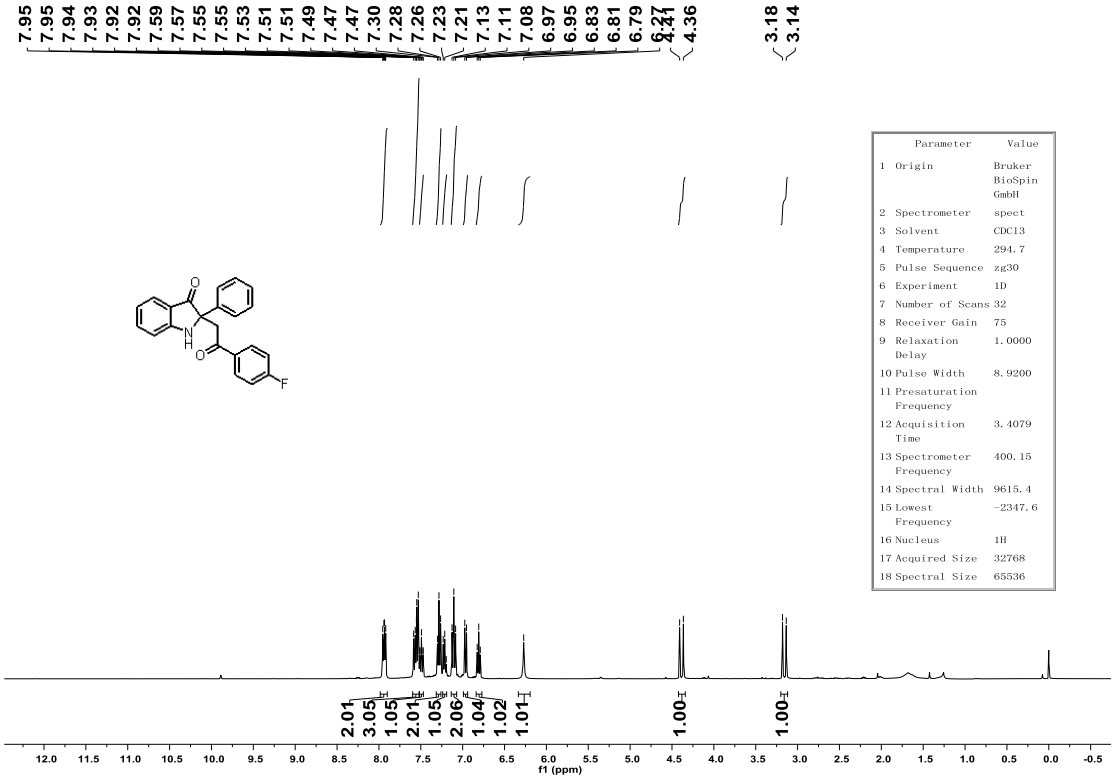
3w

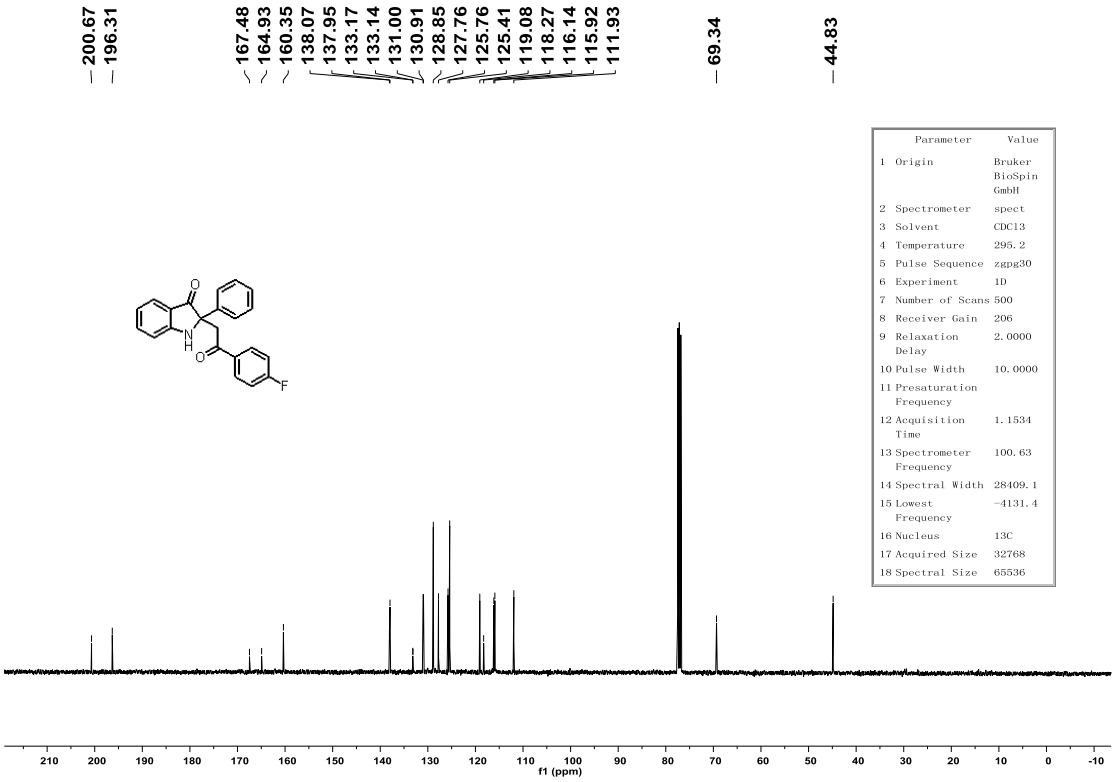


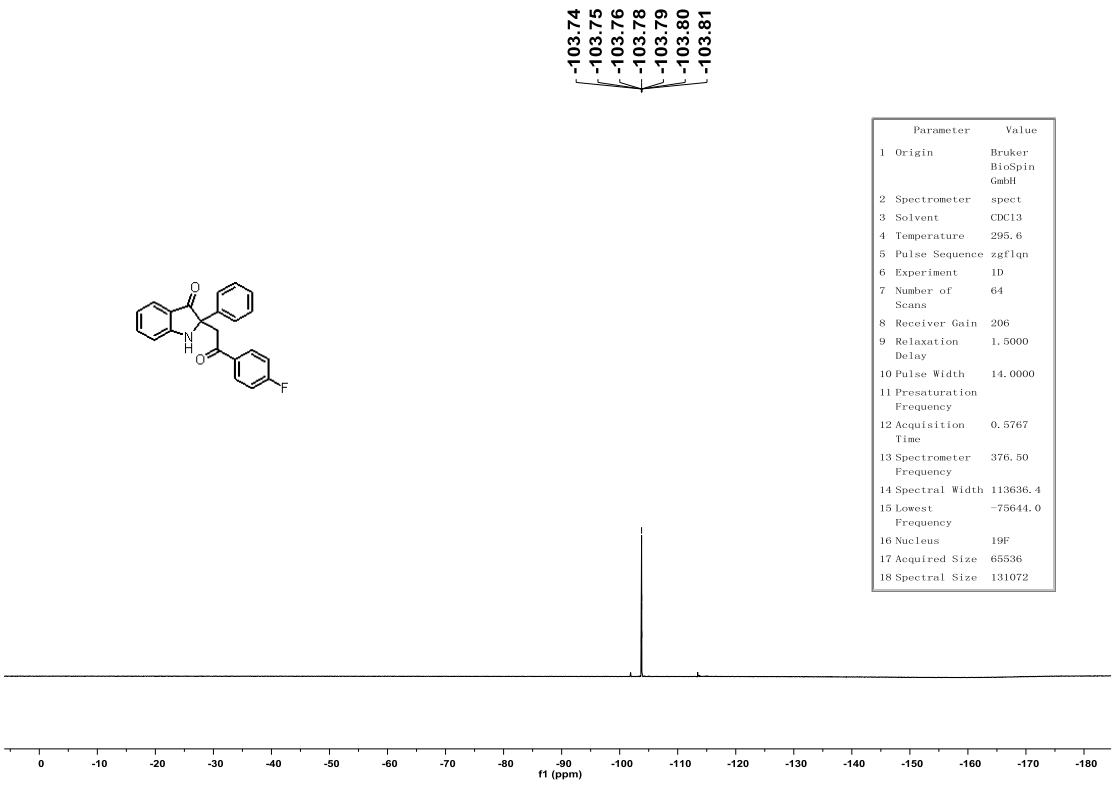
	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	293.8
5	Pulse Sequence	zg30
6	Experiment	1D
7	Number of Scans	32
8	Receiver Gain	75
9	Relaxation Delay	1.0000
10	Pulse Width	8.9200
11	Presaturation Frequency	
12	Acquisition Time	3.4079
13	Spectrometer Frequency	400.15
14	Spectral Width	9615.4
15	Lowest Frequency	-2347.9
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536


200.91
197.56
160.38
157.76
138.21
137.90
134.16
128.80
128.23
127.64
125.83
125.76
125.47
118.92
118.22
111.90
69.48
44.66
35.33
31.17
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.7
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 600
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4131.0
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
tBu
f1 (ppm)

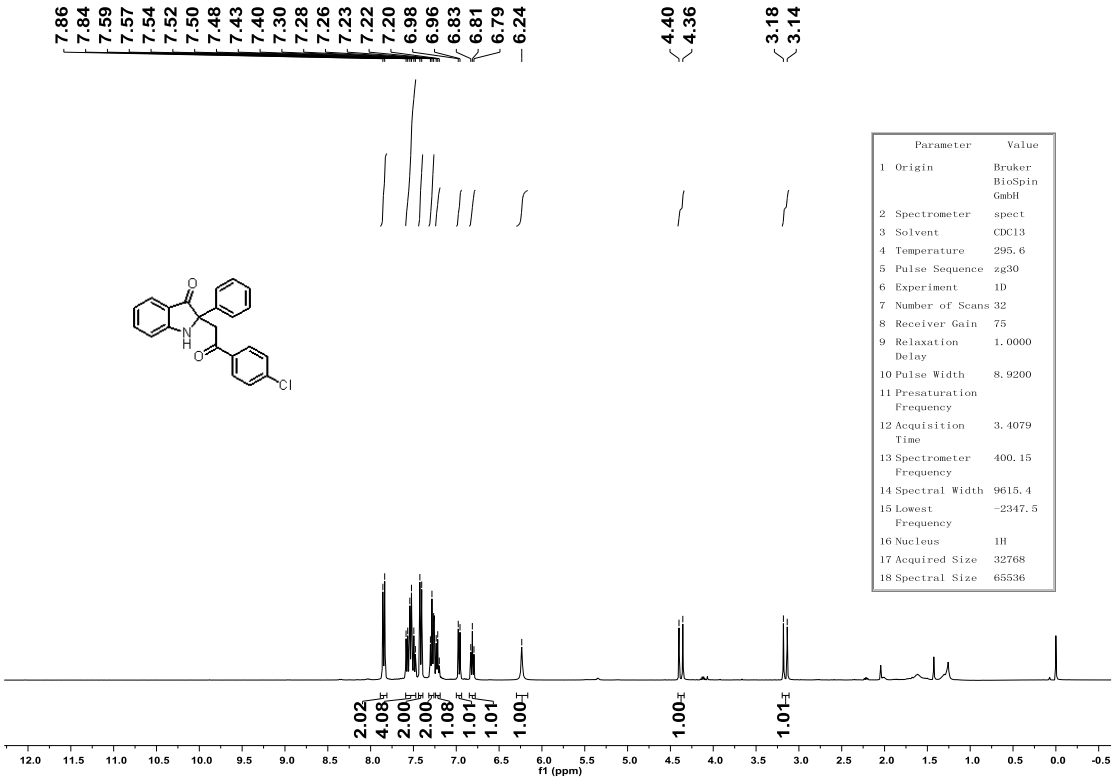
3x

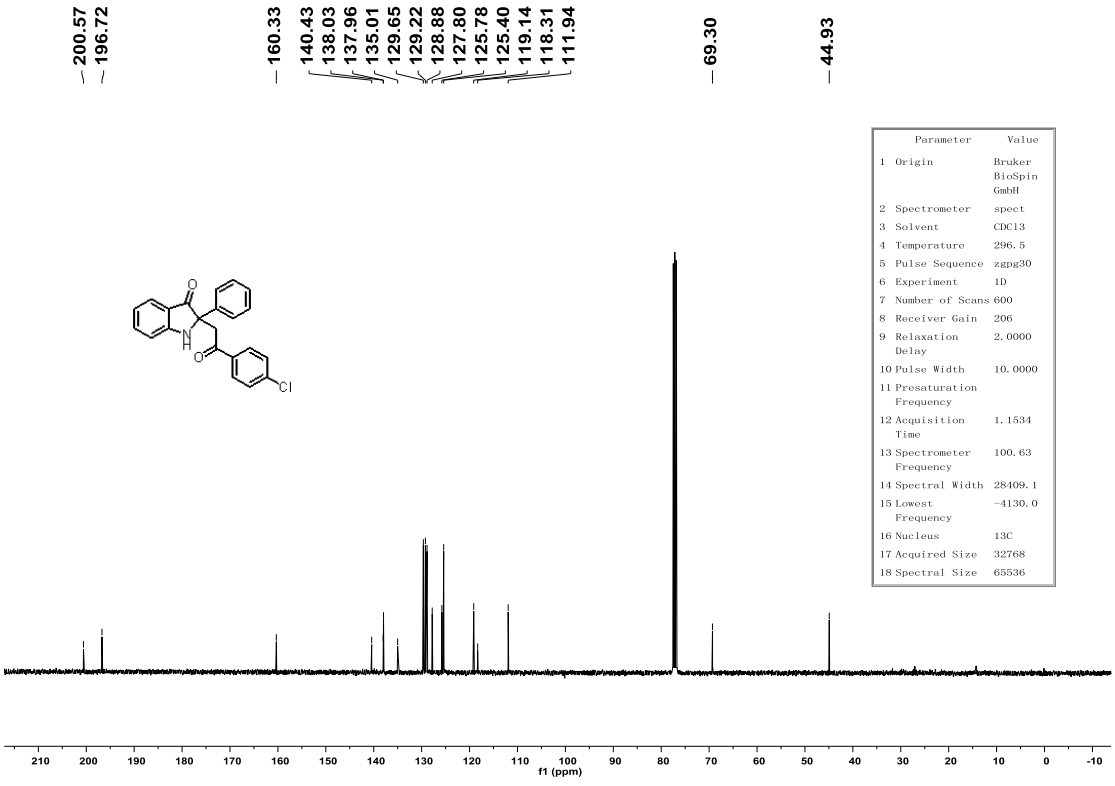

7.95
7.95
7.94
7.93
7.92
7.92
7.59
7.57
7.55
7.55
7.53
7.51
7.51
7.49
7.47
7.47
7.30
7.28
7.26
7.23
7.21
7.13
7.11
7.08
6.97
6.95
6.83
6.81
6.79
6.27
4.41
4.36
3.18
3.14
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.7
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.6
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
F
2.01
3.05
1.05
2.01
1.05
2.06
1.04
1.02
1.01
1.00
1.00
f1 (ppm)


200.67
196.31
167.48
164.93
160.35
138.07
137.95
133.17
133.14
131.00
130.91
128.85
127.76
125.76
125.41
119.08
118.27
116.14
115.92
111.93
69.34
44.83
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.2
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4131.4
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
O
N
H
O
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

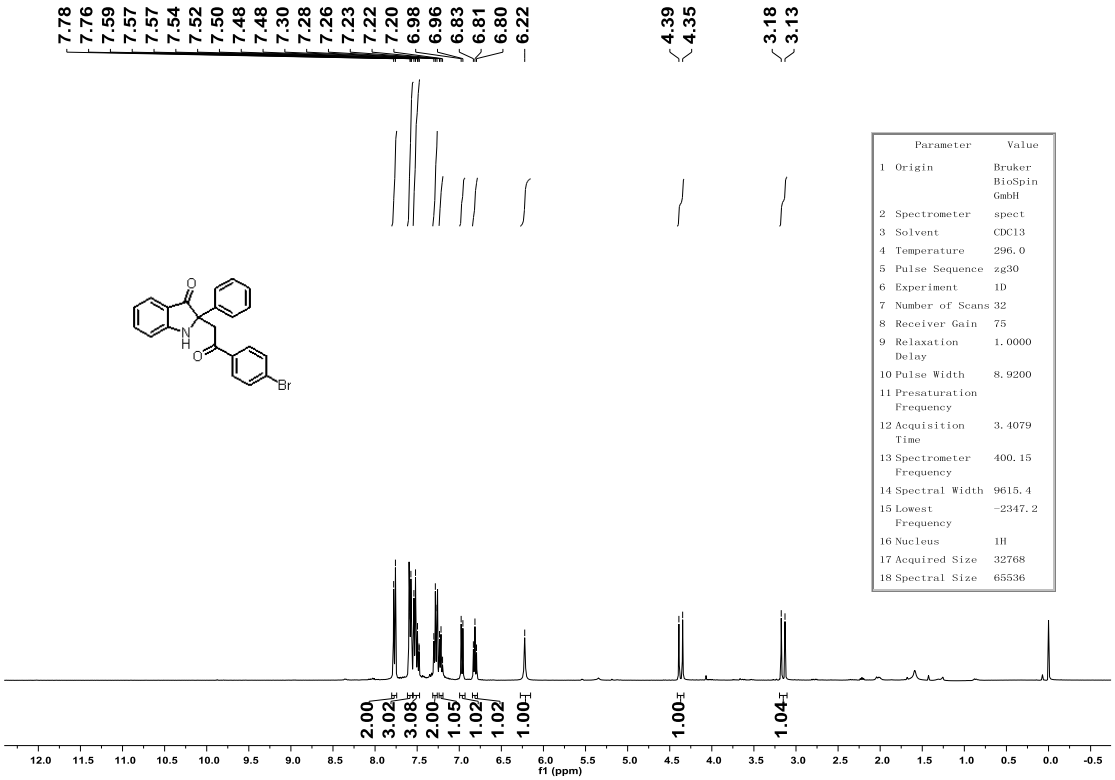

-103.74
-103.75
-103.76
-103.78
-103.79
-103.80
-103.81
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.6
5 Pulse Sequence zgflqn
6 Experiment 1D
7 Number of Scans 64
8 Receiver Gain 206
9 Relaxation Delay 1.5000
10 Pulse Width 14.0000
11 Presaturation Frequency
12 Acquisition Time 0.5767
13 Spectrometer Frequency 376.50
14 Spectral Width 113636.4
15 Lowest Frequency -75644.0
16 Nucleus 19F
17 Acquired Size 65536
18 Spectral Size 131072
O
N
H
O
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)

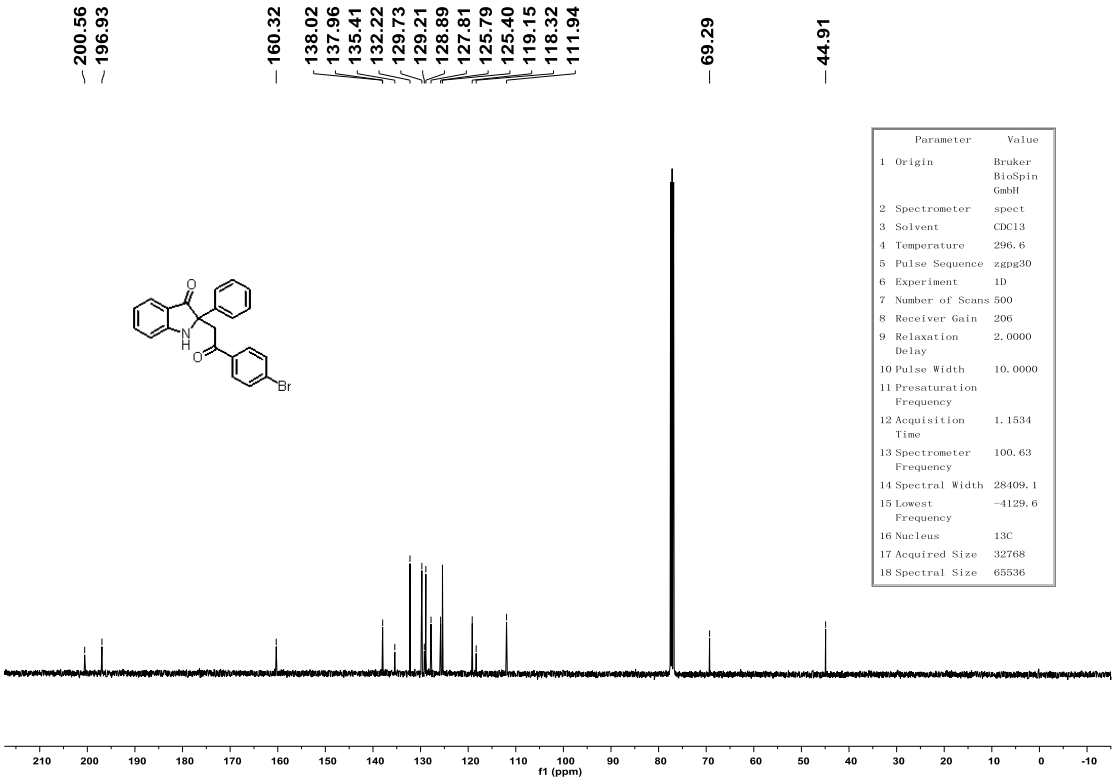
3y


7.86
7.84
7.59
7.57
7.54
7.52
7.50
7.48
7.43
7.40
7.30
7.28
7.26
7.23
7.22
7.20
6.98
6.96
6.83
6.81
6.79
6.24
4.40
4.36
3.18
3.14
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.6
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.5
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.02
4.08
2.00
2.00
1.08
1.01
1.01
1.00
1.00
1.01
f1 (ppm)

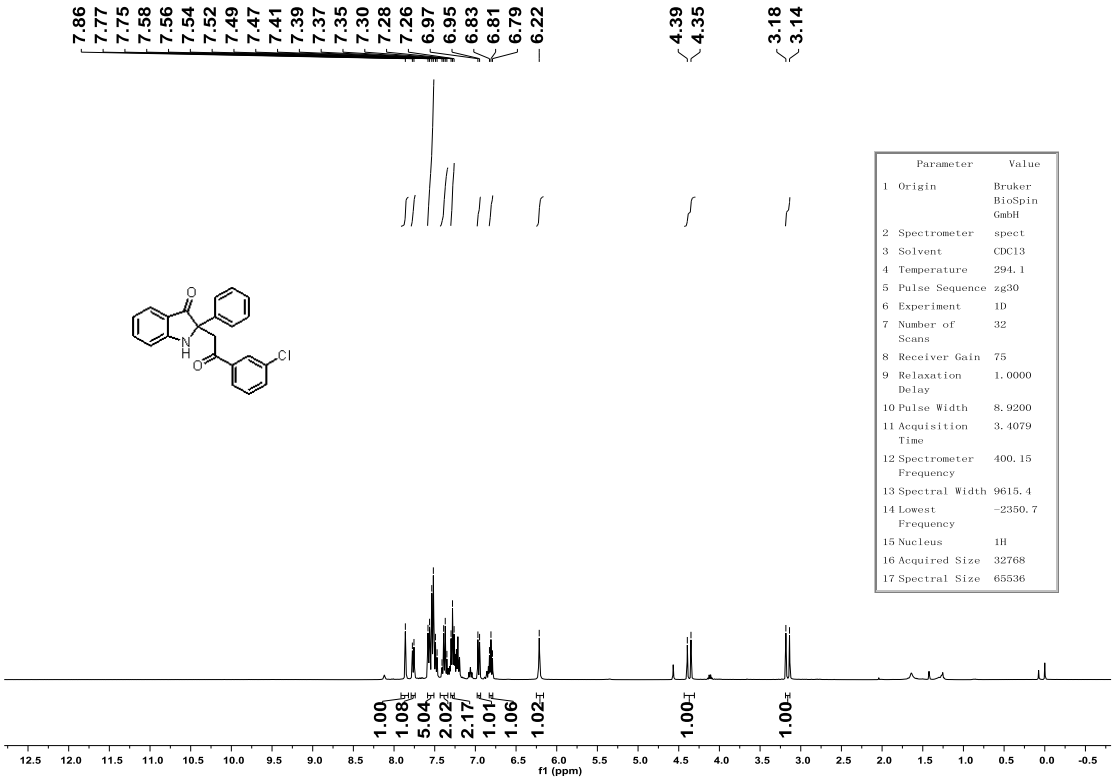

200.57
196.72
160.33
140.43
138.03
137.96
135.01
129.65
129.22
128.88
127.80
125.78
125.40
119.14
118.31
111.94
69.30
44.93
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 296.5
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 600
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4130.0
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
f1 (ppm)

3z

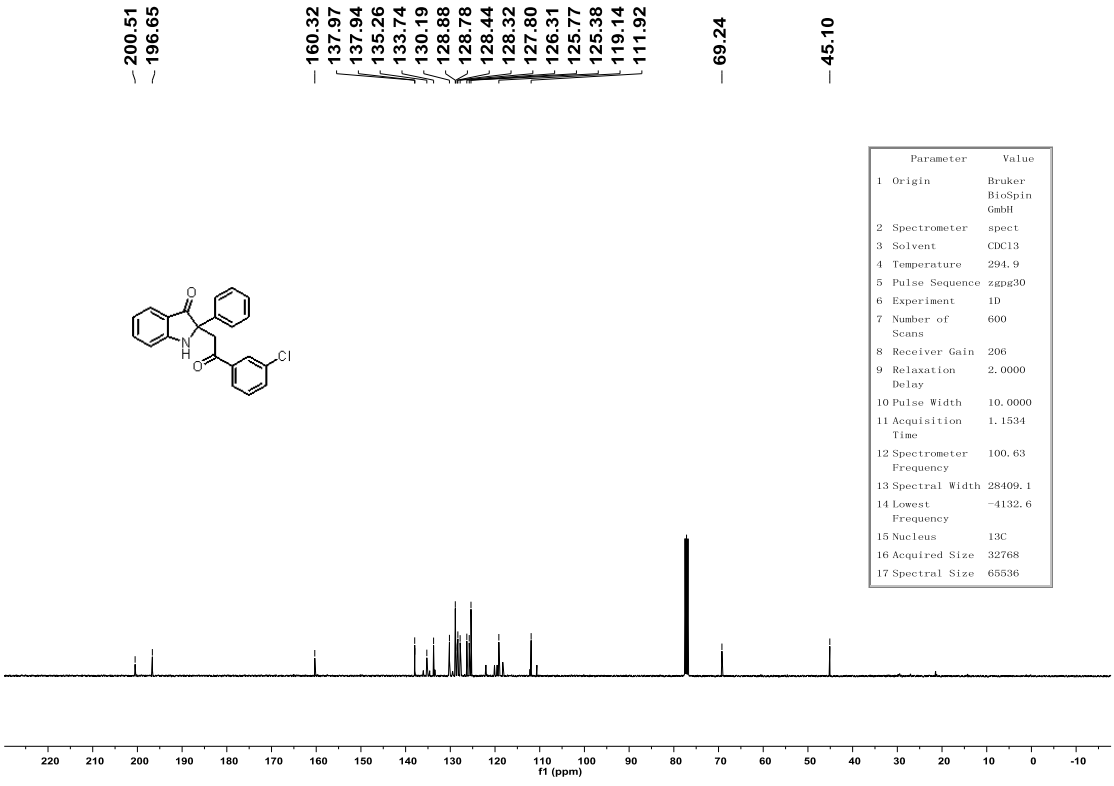

7.78
7.76
7.59
7.57
7.57
7.54
7.52
7.50
7.48
7.48
7.30
7.28
7.26
7.23
7.22
7.20
6.98
6.96
6.83
6.81
6.80
6.22
4.39
4.35
3.18
3.13
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 296.0
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.2
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.00
3.02
3.08
2.00
1.05
1.02
1.02
1.00
1.00
1.04
f1 (ppm)


200.56
196.93
160.32
138.02
137.96
135.41
132.22
129.73
129.21
128.89
127.81
125.79
125.40
119.15
118.32
111.94
69.29
44.91
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 296.6
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4129.6
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
f1 (ppm)

3aa

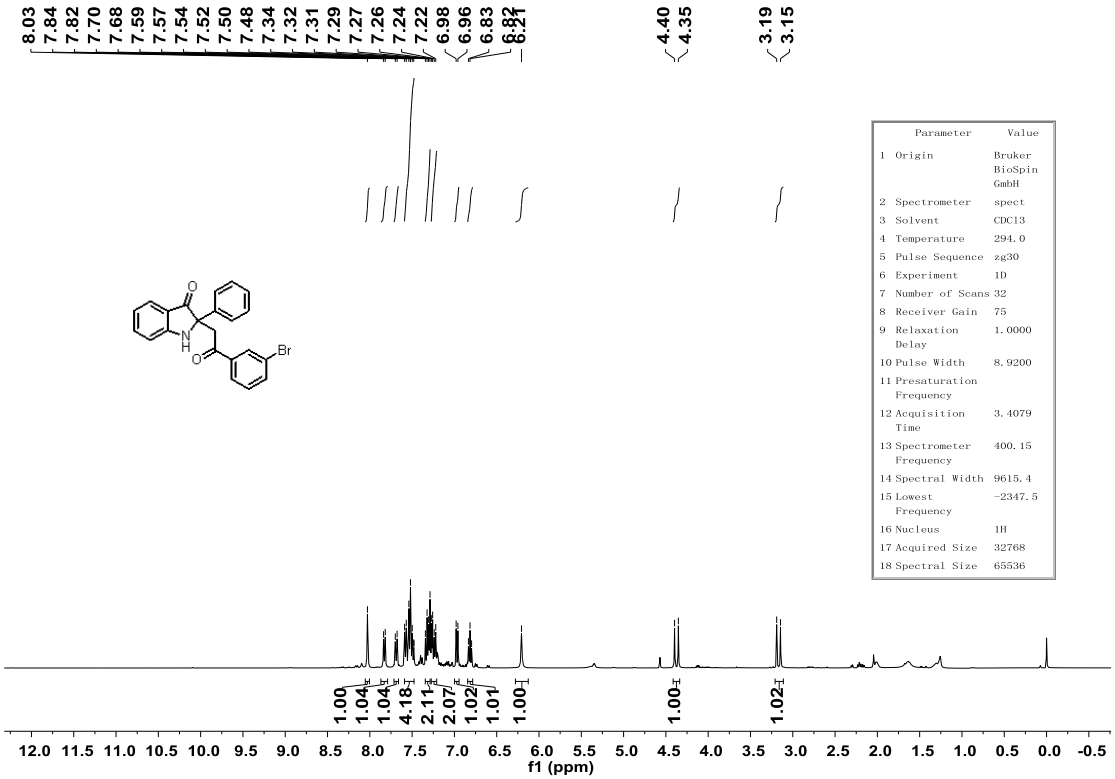


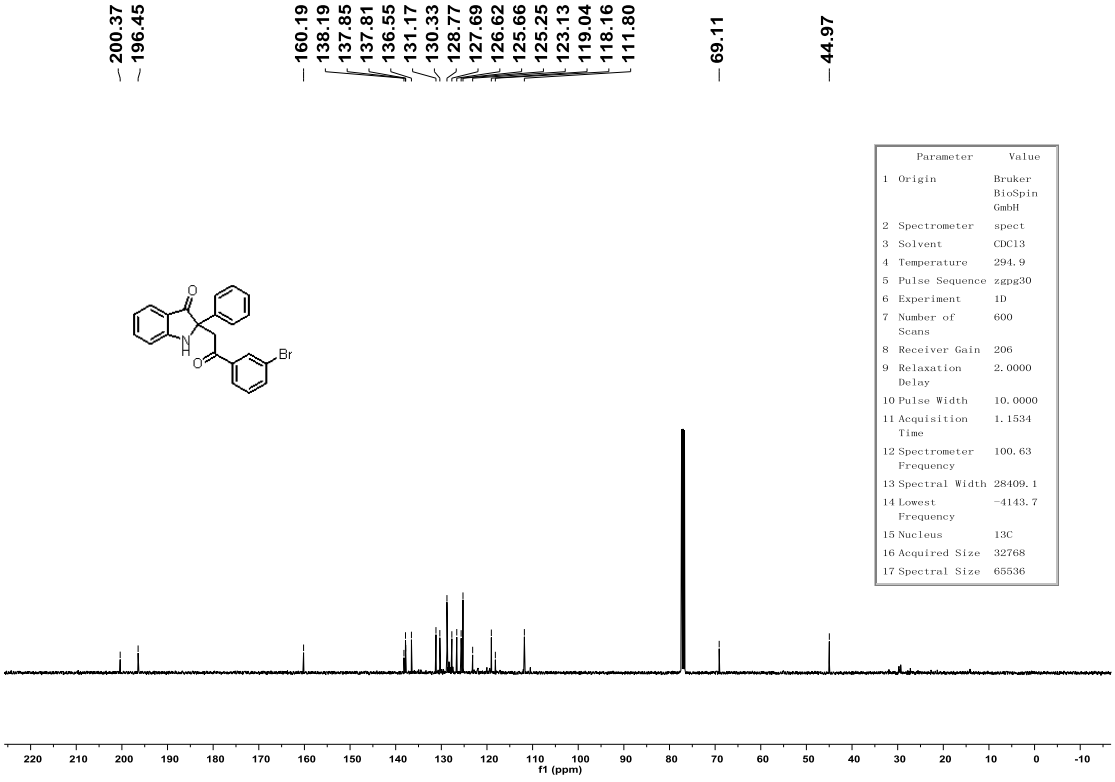
	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	294.1
5	Pulse Sequence	zg30
6	Experiment	1D
7	Number of Scans	32
8	Receiver Gain	75
9	Relaxation Delay	1.0000
10	Pulse Width	8.9200
11	Acquisition Time	3.4079
12	Spectrometer Frequency	400.15
13	Spectral Width	9615.4
14	Lowest Frequency	-2350.7
15	Nucleus	1H
16	Acquired Size	32768
17	Spectral Size	65536



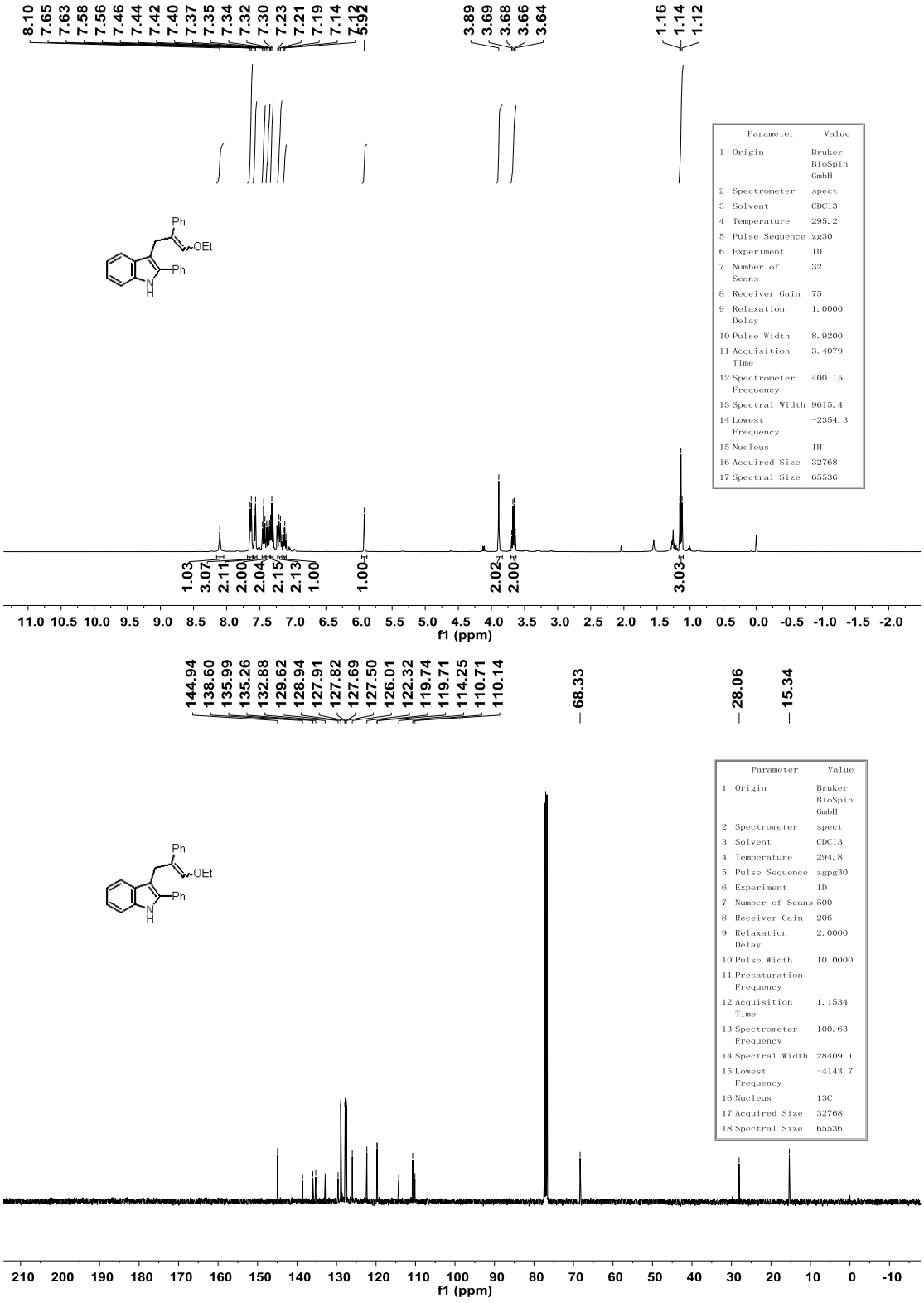
	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	294.9
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Number of Scans	600
8	Receiver Gain	206
9	Relaxation Delay	2.0000
10	Pulse Width	10.0000
11	Acquisition Time	1.1534
12	Spectrometer Frequency	100.63
13	Spectral Width	28409.1
14	Lowest Frequency	-4132.6
15	Nucleus	13C
16	Acquired Size	32768
17	Spectral Size	65536

3ab

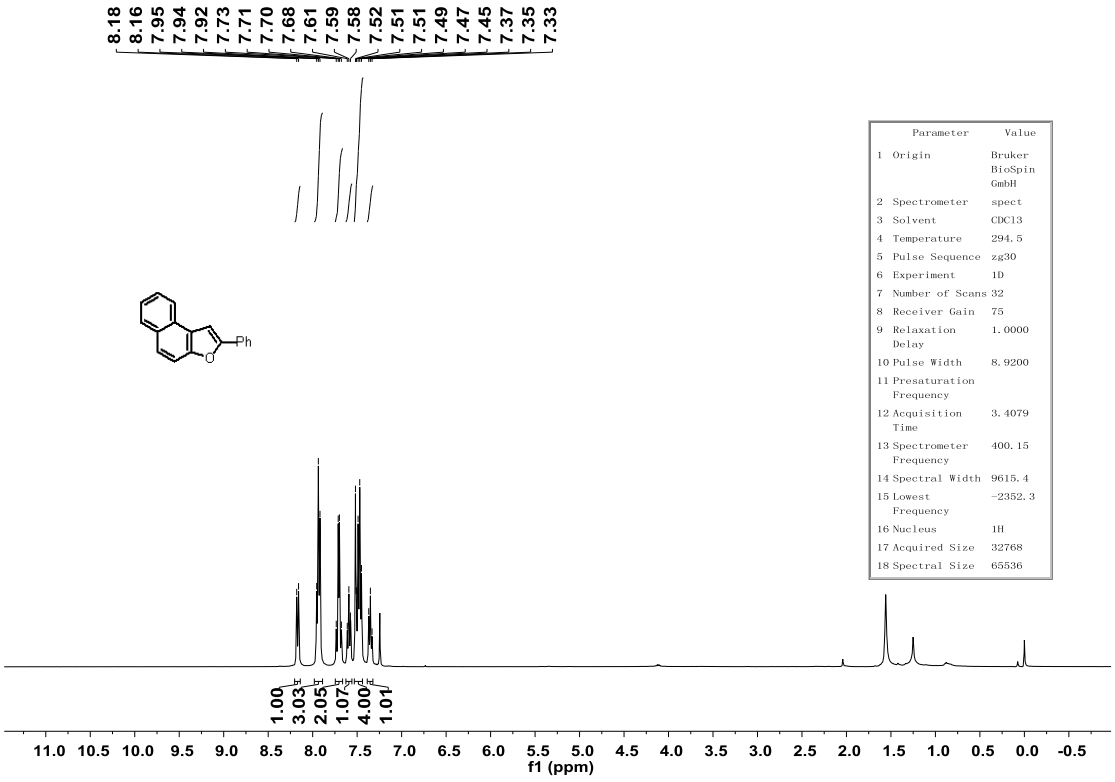

8.03
7.84
7.82
7.70
7.68
7.59
7.57
7.54
7.52
7.50
7.48
7.34
7.32
7.31
7.29
7.27
7.26
7.24
7.22
6.98
6.96
6.83
6.82
6.21
4.40
4.35
3.19
3.15
O
N
H
O
Br
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.0
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.5
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
1.00
1.04
1.04
4.18
2.11
2.07
1.02
1.01
1.00
1.00
1.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


200.37
196.45
160.19
138.19
137.85
137.81
136.55
131.17
130.33
128.77
127.69
126.62
125.66
125.25
123.13
119.04
118.16
111.80
69.11
44.97
O
N
H
O
Br
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.9
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 600
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.63
13 Spectral Width 28409.1
14 Lowest Frequency -4143.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

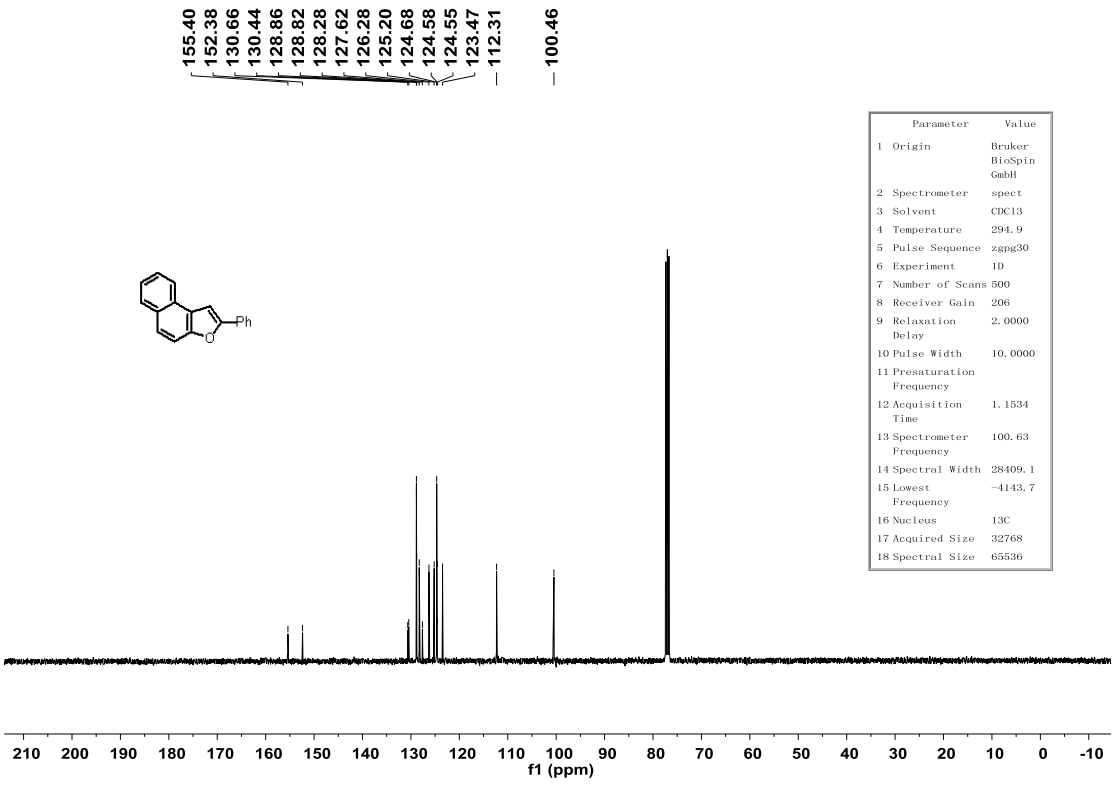
4a


8.10 7.65 7.63 7.58 7.56 7.46 7.44 7.42 7.40 7.37 7.35 7.34 7.32 7.30 7.23 7.21 7.19 7.14 7.12 5.92
3.89 3.69 3.68 3.66 3.64
1.16 1.14 1.12
Ph
OEt
Ph
N
H
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.2
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2354.3
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
1.03 3.07 2.11 2.00 2.04 2.15 2.13 1.00
1.00
2.02 2.00
3.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)
144.94 138.60 135.99 135.26 132.88 129.62 128.94 127.91 127.82 127.69 127.50 126.01 122.32 119.74 119.71 114.25 110.71 110.14
68.33
28.06
15.34
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.8
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4143.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5a

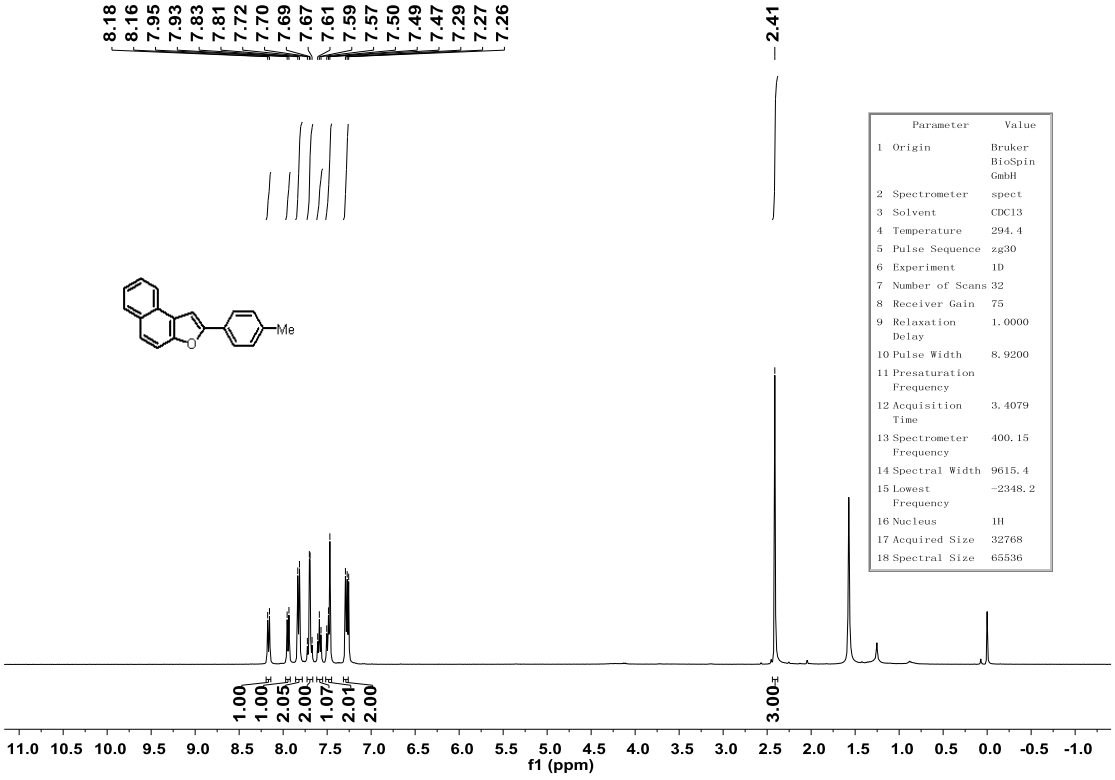


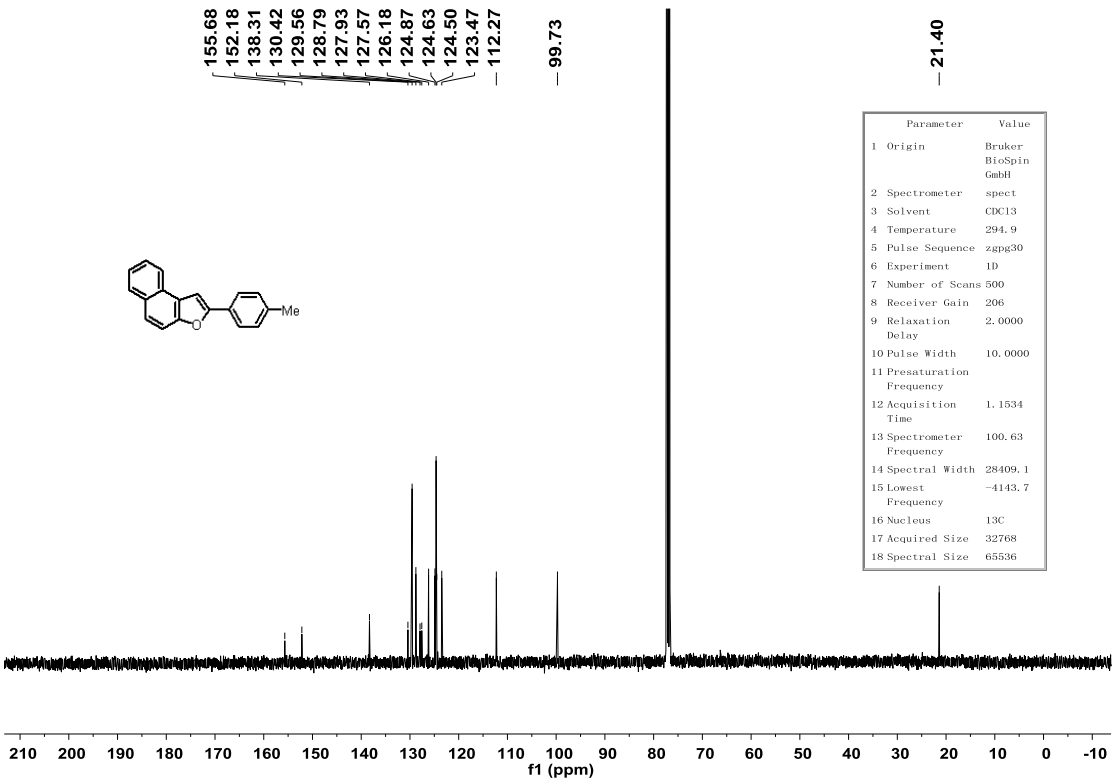
	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	294.5
5	Pulse Sequence	zg30
6	Experiment	1D
7	Number of Scans	32
8	Receiver Gain	75
9	Relaxation Delay	1.0000
10	Pulse Width	8.9200
11	Presaturation Frequency	
12	Acquisition Time	3.4079
13	Spectrometer Frequency	400.15
14	Spectral Width	9615.4
15	Lowest Frequency	-2352.3
16	Nucleus	1H
17	Acquired Size	32768
18	Spectral Size	65536



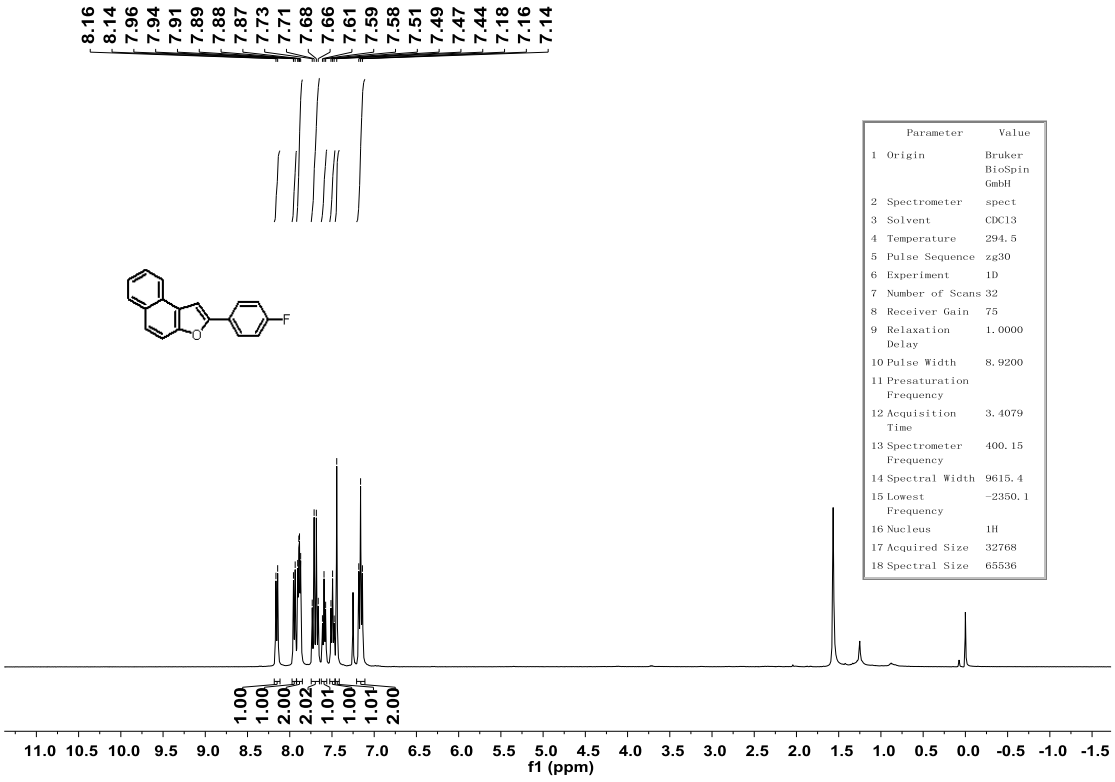
	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Spectrometer	spect
3	Solvent	CDCl3
4	Temperature	294.9
5	Pulse Sequence	zgpg30
6	Experiment	1D
7	Number of Scans	500
8	Receiver Gain	206
9	Relaxation Delay	2.0000
10	Pulse Width	10.0000
11	Presaturation Frequency	
12	Acquisition Time	1.1534
13	Spectrometer Frequency	100.63
14	Spectral Width	28409.1
15	Lowest Frequency	-4143.7
16	Nucleus	13C
17	Acquired Size	32768
18	Spectral Size	65536

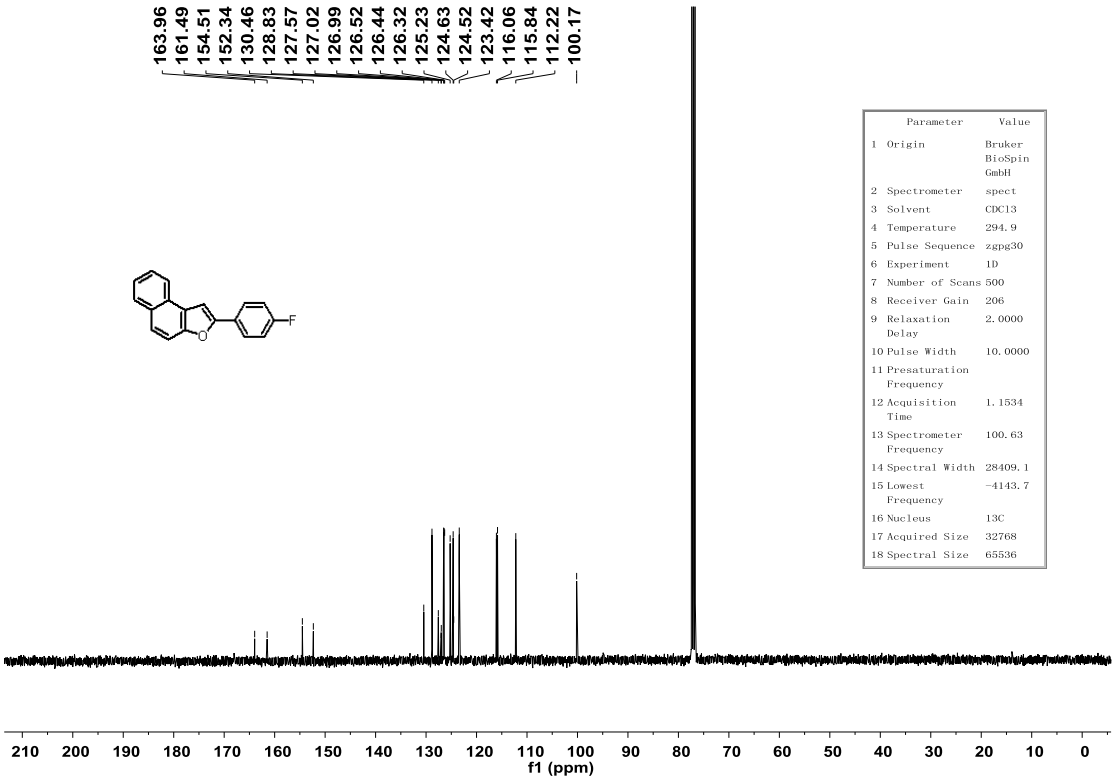
5b

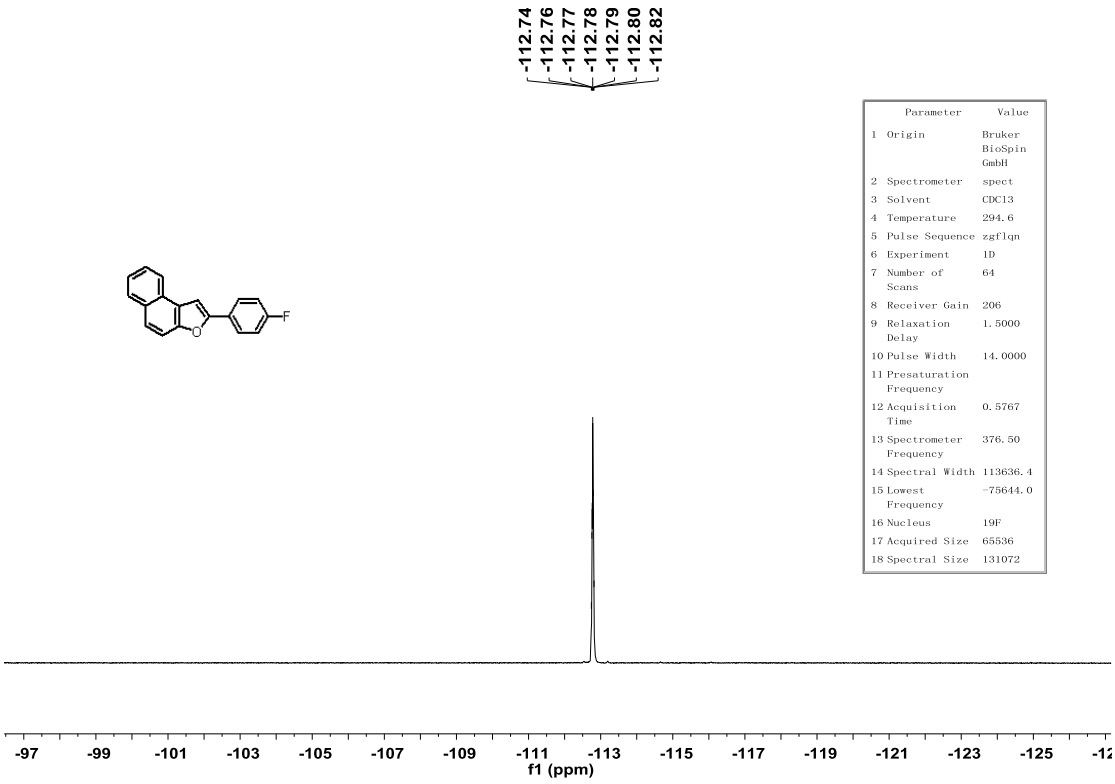

8.18
8.16
7.95
7.93
7.83
7.81
7.72
7.70
7.69
7.67
7.61
7.59
7.57
7.50
7.49
7.47
7.29
7.27
7.26
2.41
Me
1.00
1.00
2.05
2.00
1.07
2.01
2.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.4
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2348.2
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536


155.68
152.18
138.31
130.42
129.56
128.79
127.93
127.57
126.18
124.87
124.63
124.50
123.47
112.27
99.73
21.40
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.9
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4143.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536

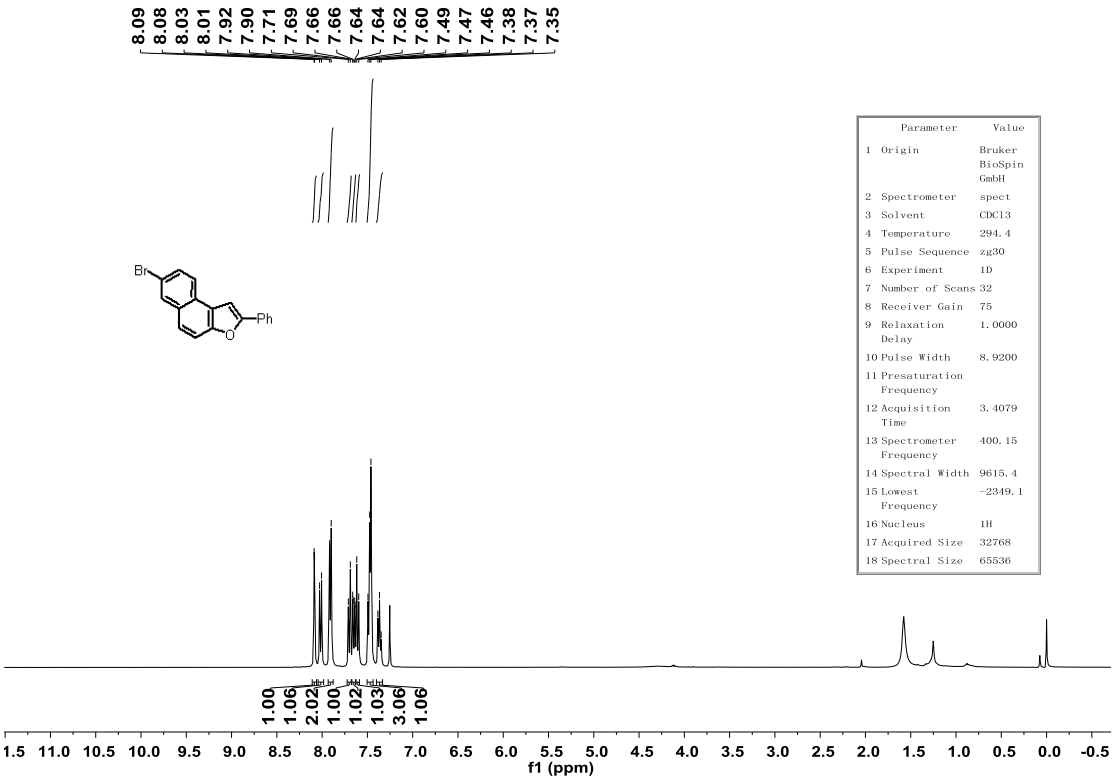
5c

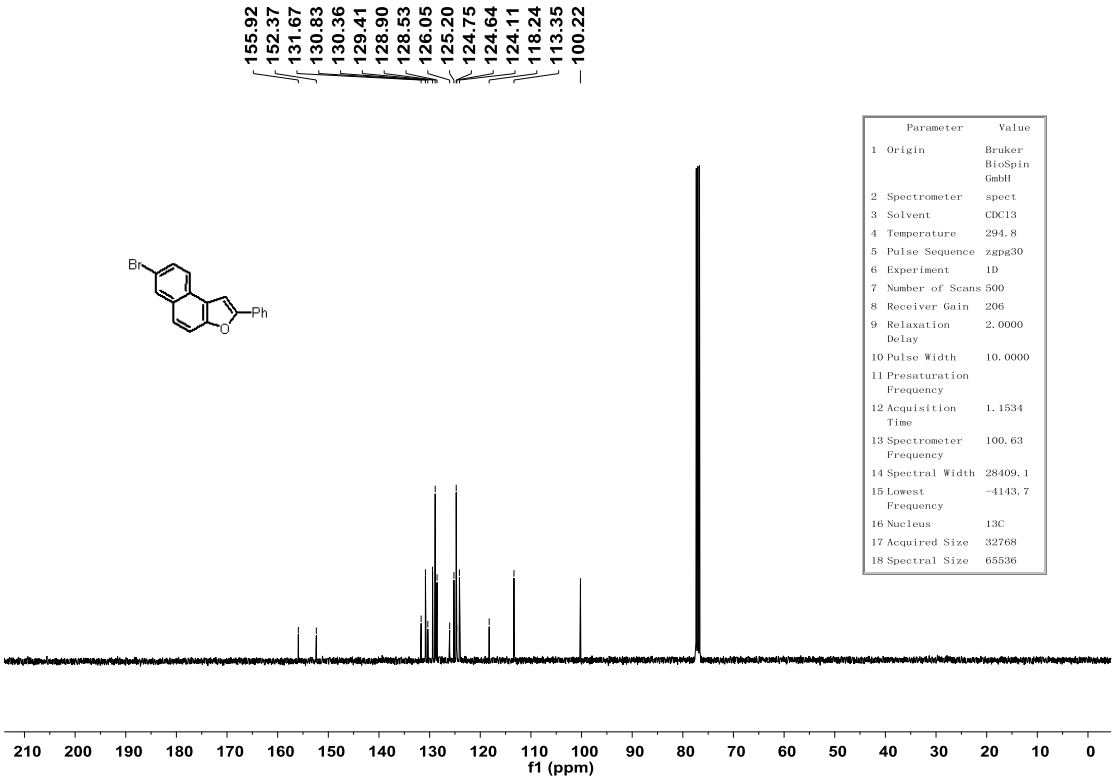

8.16
8.14
7.96
7.94
7.91
7.89
7.88
7.87
7.73
7.71
7.68
7.66
7.61
7.59
7.58
7.51
7.49
7.47
7.44
7.18
7.16
7.14
F
O
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.5
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2350.1
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
1.00
1.00
2.00
2.02
1.01
1.00
1.01
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


163.96
161.49
154.51
152.34
130.46
128.83
127.57
127.02
126.99
126.52
126.44
126.32
125.23
124.63
124.52
123.42
116.06
115.84
112.22
100.17
F
O
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.9
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4143.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

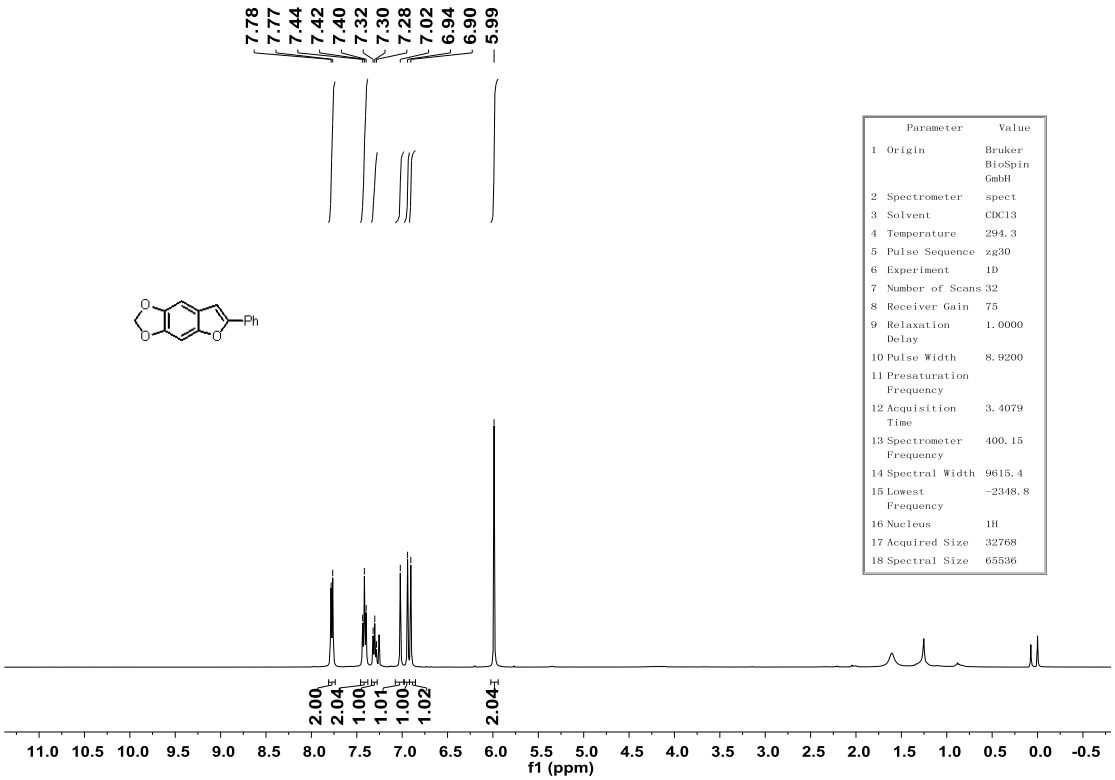

-112.74
-112.76
-112.77
-112.78
-112.79
-112.80
-112.82
F
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.6
5 Pulse Sequence zgflqn
6 Experiment 1D
7 Number of Scans 64
8 Receiver Gain 206
9 Relaxation Delay 1.5000
10 Pulse Width 14.0000
11 Presaturation Frequency
12 Acquisition Time 0.5767
13 Spectrometer Frequency 376.50
14 Spectral Width 113636.4
15 Lowest Frequency -75644.0
16 Nucleus 19F
17 Acquired Size 65536
18 Spectral Size 131072
-97 -99 -101 -103 -105 -107 -109 -111 -113 -115 -117 -119 -121 -123 -125
f1 (ppm)

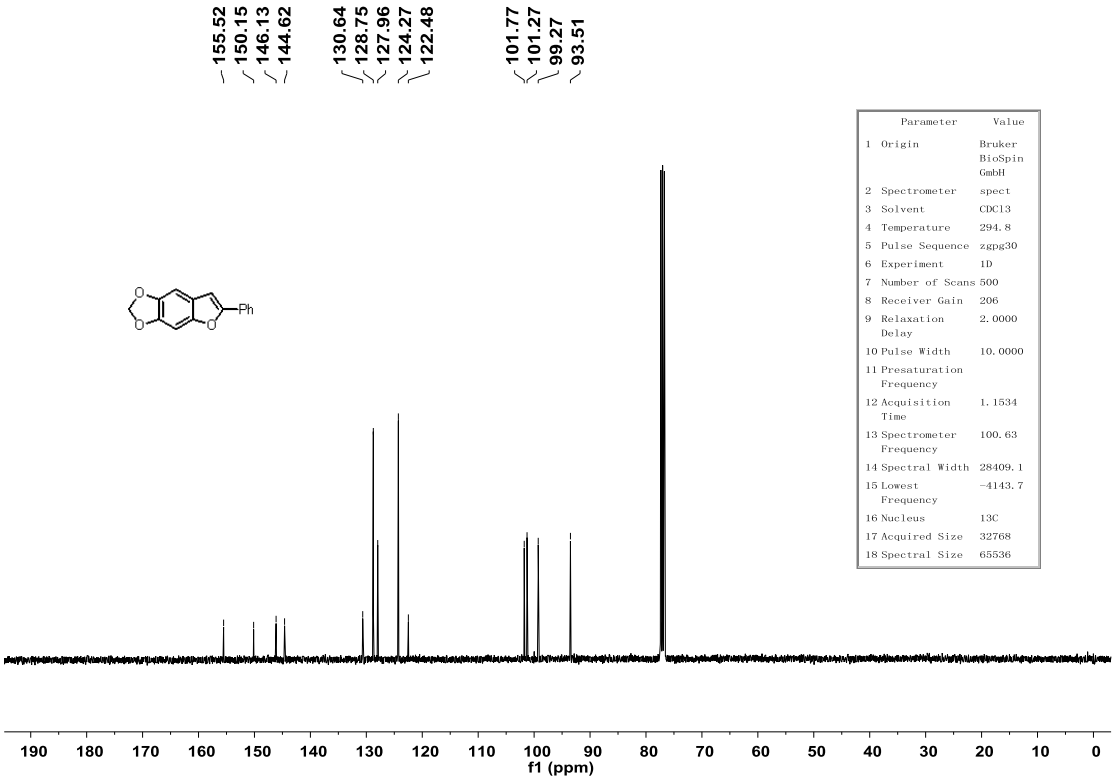
5d


8.09
8.08
8.03
8.01
7.92
7.90
7.71
7.69
7.66
7.66
7.64
7.64
7.62
7.60
7.49
7.47
7.46
7.38
7.37
7.35
Br
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.4
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2349.1
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
1.00
1.06
2.02
1.00
1.02
1.03
3.06
1.06
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

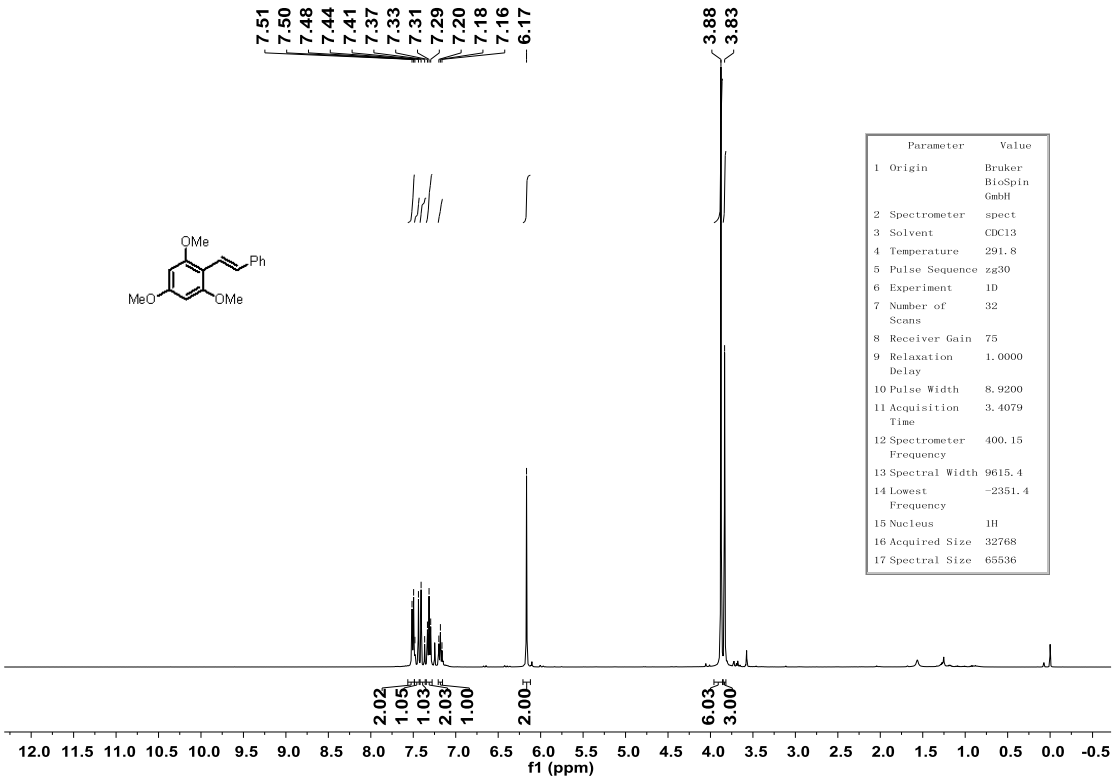

155.92
152.37
131.67
130.83
130.36
129.41
128.90
128.53
126.05
125.20
124.75
124.64
124.11
118.24
113.35
100.22
Br
Ph
O
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.8
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4143.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

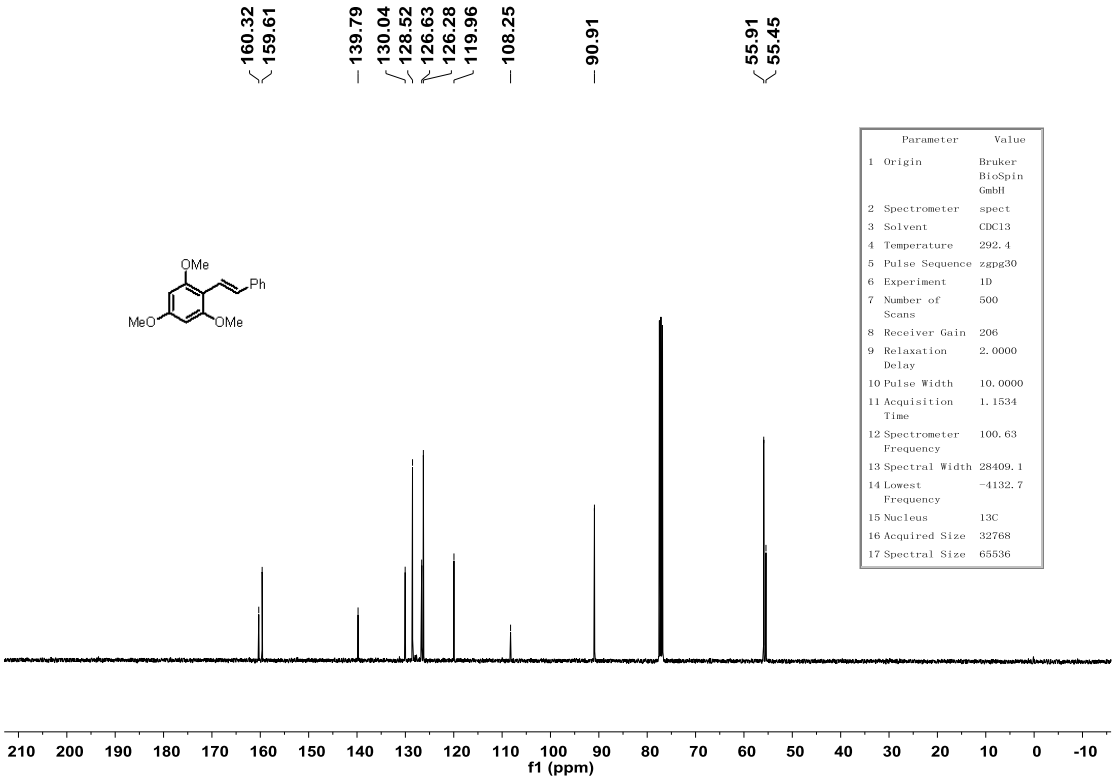
5e


7.78
7.77
7.44
7.42
7.40
7.32
7.30
7.28
7.02
6.94
6.90
5.99
O
O
Ph
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.3
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2348.8
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.00
2.04
1.00
1.01
1.00
1.02
2.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

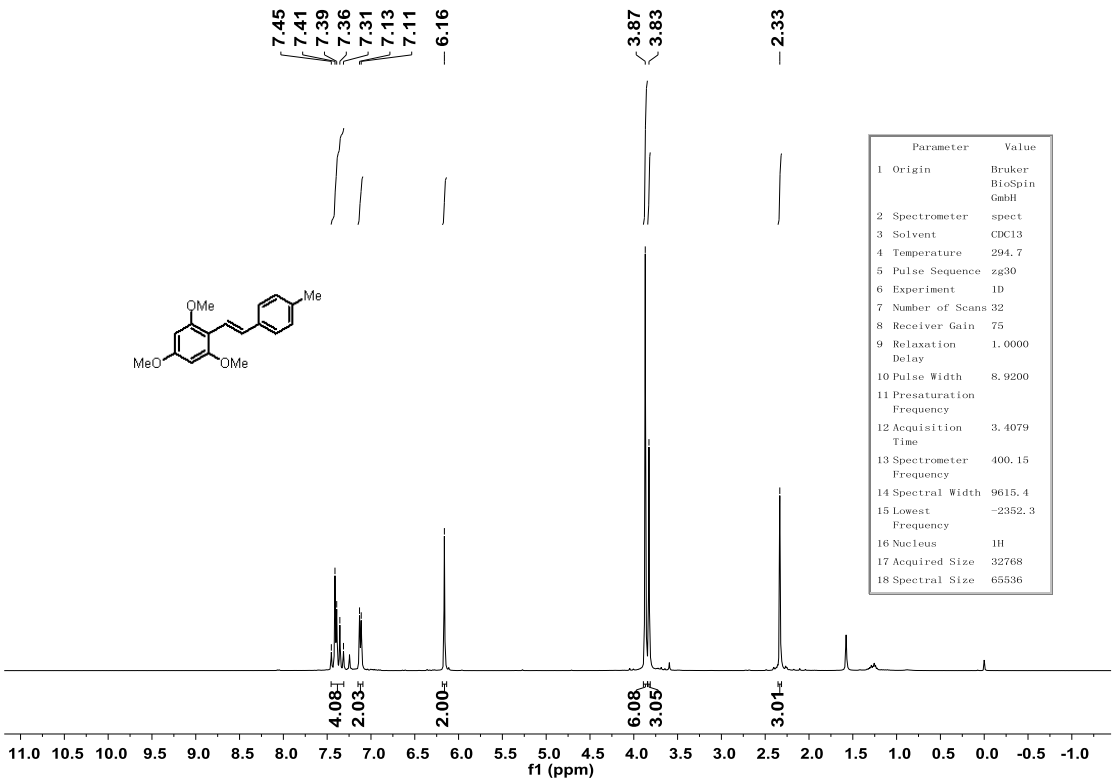

155.52
150.15
146.13
144.62
130.64
128.75
127.96
124.27
122.48
101.77
101.27
99.27
93.51
Ph
O
O
O
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.8
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4143.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

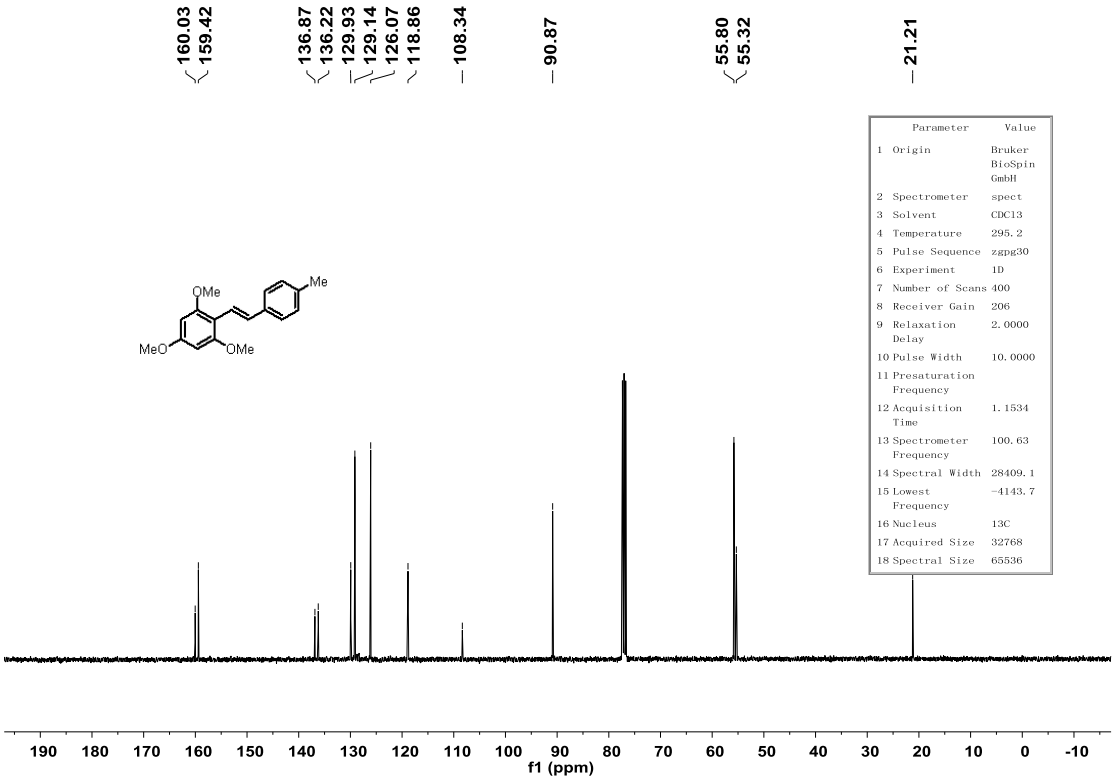
7a


7.51
7.50
7.48
7.44
7.41
7.37
7.33
7.31
7.29
7.20
7.18
7.16
6.17
3.88
3.83
OMe
Ph
MeO
OMe
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 291.8
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Acquisition Time 3.4079
12 Spectrometer Frequency 400.15
13 Spectral Width 9615.4
14 Lowest Frequency -2351.4
15 Nucleus 1H
16 Acquired Size 32768
17 Spectral Size 65536
2.02
1.05
1.03
2.03
1.00
2.00
6.03
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

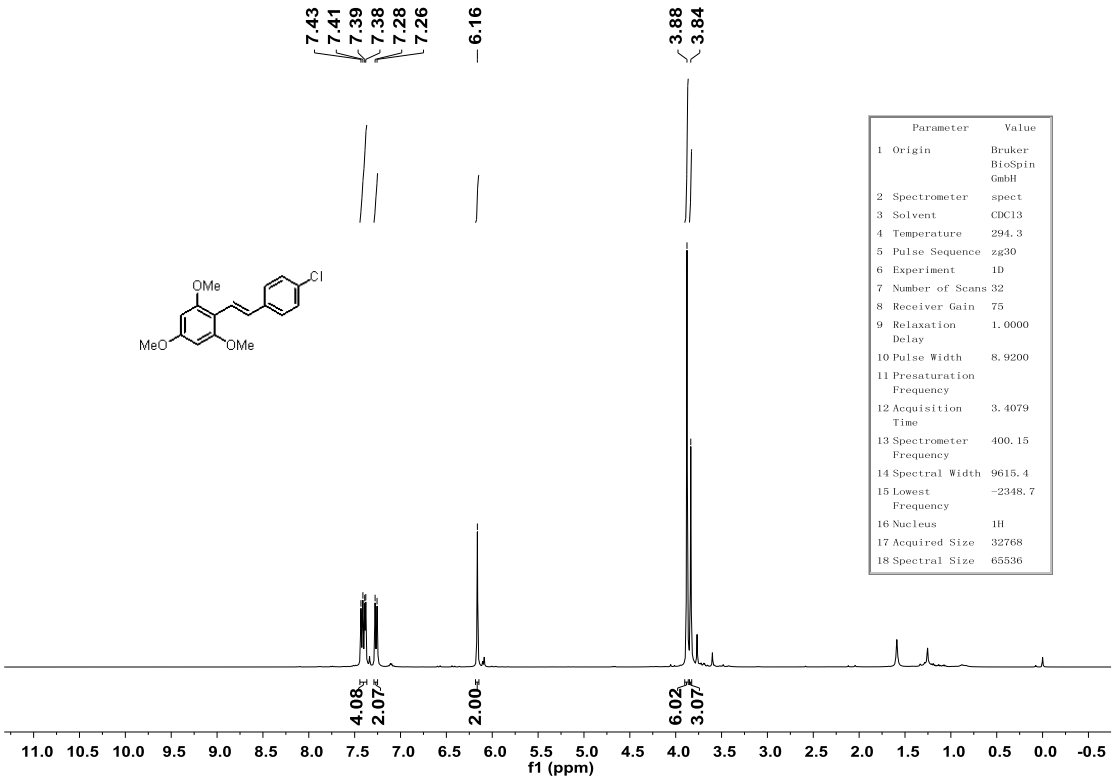

160.32
159.61
139.79
130.04
128.52
126.63
126.28
119.96
108.25
90.91
55.91
55.45
OMe
Ph
MeO
OMe
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 292.4
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Acquisition Time 1.1534
12 Spectrometer Frequency 100.63
13 Spectral Width 28409.1
14 Lowest Frequency -4132.7
15 Nucleus 13C
16 Acquired Size 32768
17 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

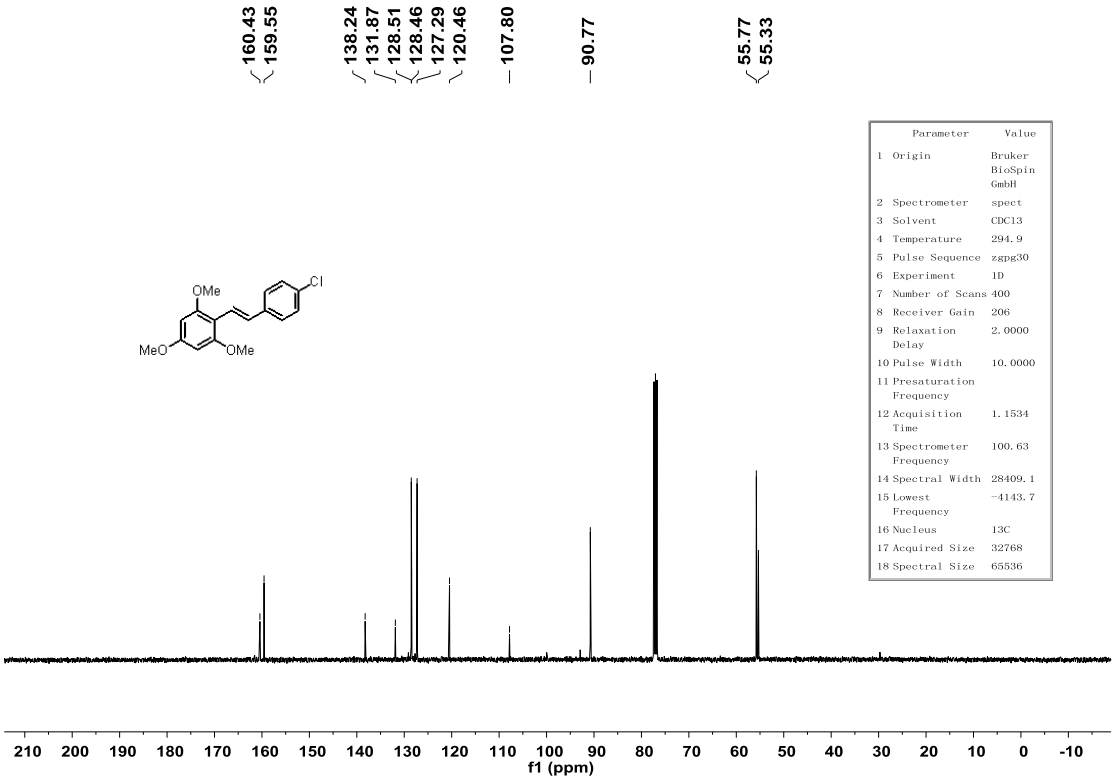
7b


7.45
7.41
7.39
7.36
7.31
7.13
7.11
6.16
3.87
3.83
2.33
OMe
Me
MeO
OMe
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.7
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2352.3
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
4.08
2.03
2.00
6.08
3.05
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

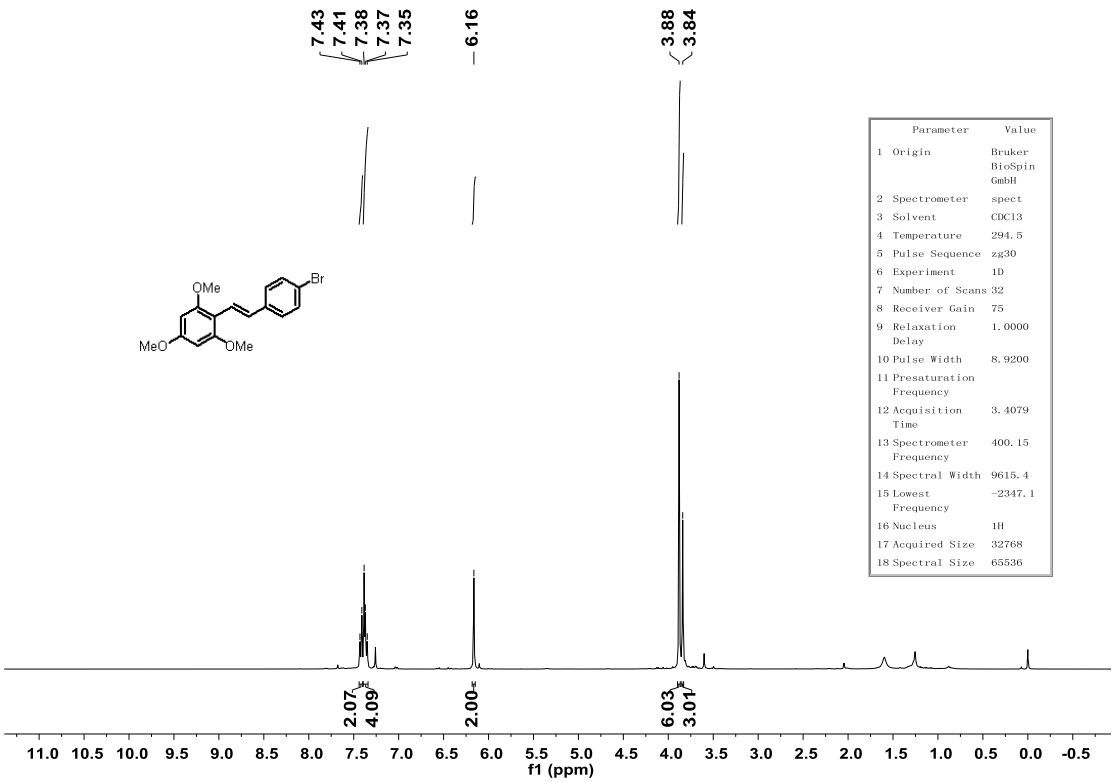

160.03
159.42
136.87
136.22
129.93
129.14
126.07
118.86
108.34
90.87
55.80
55.32
21.21
OMe
Me
MeO
OMe
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 295.2
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 400
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4143.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

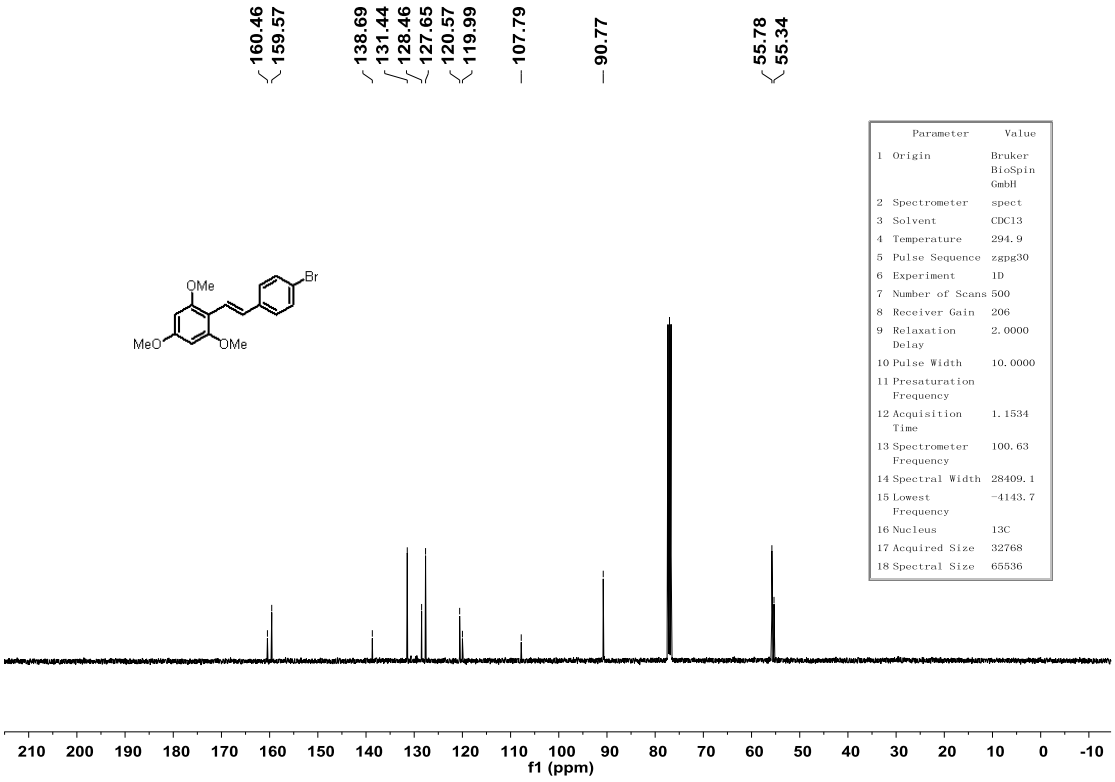
7c


7.43
7.41
7.39
7.38
7.28
7.26
6.16
3.88
3.84
OMe
Cl
MeO
OMe
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.3
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2348.7
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
4.08
2.07
2.00
6.02
3.07
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


160.43
159.55
138.24
131.87
128.51
128.46
127.29
120.46
107.80
90.77
55.77
55.33
OMe
Cl
MeO
OMe
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.9
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 400
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4143.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
f1 (ppm)

7d


7.43
7.41
7.38
7.37
7.35
6.16
3.88
3.84
OMe
Br
MeO
OMe
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.5
5 Pulse Sequence zg30
6 Experiment 1D
7 Number of Scans 32
8 Receiver Gain 75
9 Relaxation Delay 1.0000
10 Pulse Width 8.9200
11 Presaturation Frequency
12 Acquisition Time 3.4079
13 Spectrometer Frequency 400.15
14 Spectral Width 9615.4
15 Lowest Frequency -2347.1
16 Nucleus 1H
17 Acquired Size 32768
18 Spectral Size 65536
2.07
4.09
2.00
6.03
3.01
f1 (ppm)


160.46
159.57
138.69
131.44
128.46
127.65
120.57
119.99
107.79
90.77
55.78
55.34
OMe
Br
MeO
OMe
Parameter Value
1 Origin Bruker BioSpin GmbH
2 Spectrometer spect
3 Solvent CDCl3
4 Temperature 294.9
5 Pulse Sequence zgpg30
6 Experiment 1D
7 Number of Scans 500
8 Receiver Gain 206
9 Relaxation Delay 2.0000
10 Pulse Width 10.0000
11 Presaturation Frequency
12 Acquisition Time 1.1534
13 Spectrometer Frequency 100.63
14 Spectral Width 28409.1
15 Lowest Frequency -4143.7
16 Nucleus 13C
17 Acquired Size 32768
18 Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)