Ruthenium(II)-catalyzed C–H olefination of indoles with alkynes: facile construction of tetrasubstituted alkenes under aqueous conditions

*Ming Li, Tian-Yu Yao, Sheng-Zheng Sun, Ting-Xun Yan, Li-Rong Wen, Lin-Bao Zhang**

State Key Laboratory Base of Eco-Chemical Engineering, College of Chemistry and Molecular Engineering, Qingdao University of Science & Technology, Qingdao 266042, China

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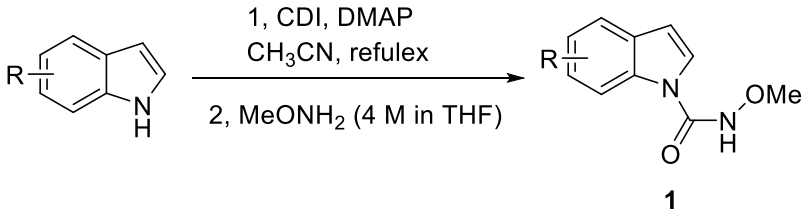
General methods

Unless noted, all commercial reagents and solvents were used without further purification. Melting points were recorded on a RY-1 microscopic melting apparatus and uncorrected. NMR spectra were recorded in DMSO on 400 MHz or 500 MHz spectrometers. ^{1}H NMR chemical shifts (δ) are reported in parts per million relative to tetramethylsilane (0 ppm) or residual DMSO (2.50 ppm). ^{13}C NMR chemical shifts are reported relative to the center line signal of the DMSO multiplet at 39.5 ppm. The following abbreviations are used for multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, and m = multiplet. Mass spectra were obtained on an Ultima Global spectrometer with an ESI source. The X-ray single-crystal diffraction was performed on Saturn 724+ instrument. Silica gel (200–300 mesh) for column chromatography and silica GF254 for TLC were produced by Qingdao Marine Chemical Company (China).

Preparation of the starting materials

Preparation of substrates 1

The *N*-methoxy-1*H*-indole-1-carboxamides **1** were prepared according to previously described methods.[1]



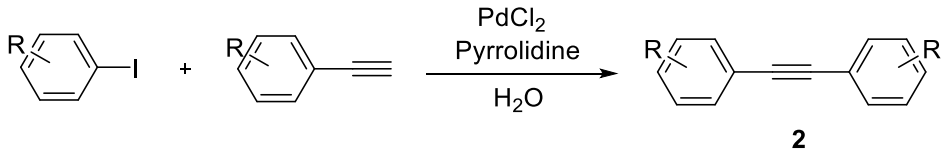
1

Preparation of $MeONH_2$ solution: To a 100 mL round bottle charged with a stirring bar was added $MeONH_2$·HCl (80.0 mmol) and THF (20 mL). To the system was then added sodium hydroxide (powder, 1.0 equiv). The system was then stirred at room temperature for about 3 h until the system became clear.

Preparation of *N*-methoxy-1*H*-indole-1-carboxamides: To a 100 mL round bottle charged with stirring bar, was added indole (5.0 mmol, 1.0 equiv), 1, 1'-carbonyldiimidazole (CDI, 7.5 mmol, 1.5 equiv) and 4-dimethylaminepyridine (DMAP, 5.0 mol %). Then anhydrous acetonitrile (20 mL) was added to the bottle under the protection of nitrogen. The system was refluxed at 85 ºC for 10 h. After cooled to room temperature, $MeONH_2$ solution (4 M in THF, 2 equiv) was added and then stirred at 80 ºC for another 6 h (when most of indole was consumed as detected by TLC). After cooled to room temperature, the solvents were removed under reduced pressure. The residue was purified by silica chromatography to afford the corresponding *N*-methoxy-1*H*-indole-1-carboxamides **1a-1w.**

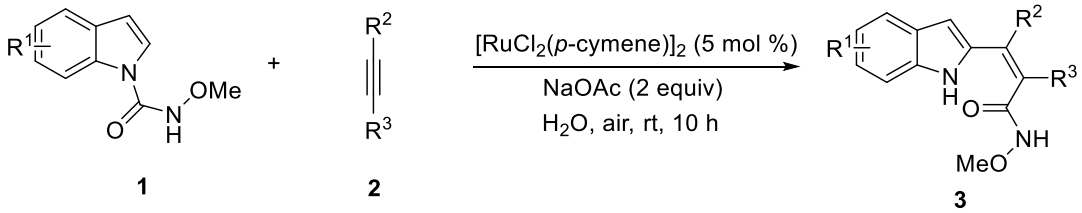
Preparation of substrates 2

The alkynes **2** were prepared according to previously described methods.[2]



To a 100 mL round bottle charged with a stirring bar was added iodobenzene (2.0 mmol, 1.0 equiv), $PdCl_2$ (2.0 mol %), H_2O (2.5 mL) and pyrrolidine (10 mmol, 5.0 equiv). The system was stirred at 50 °C for 5 min. To the system was then added terminal alkyne (2.2 mmol, 1.2 equiv). The system was then stirred at 50 °C for 12 h. After cooled to room temperature, the reaction mixture was then extracted with DCM, and the extract was dried over $MgSO_4$. The solvents were removed under reduced pressure. The residue was purified by silica chromatography to afford the corresponding alkynes **2b**-**2j**, **2l**-**2n**, **2p**.

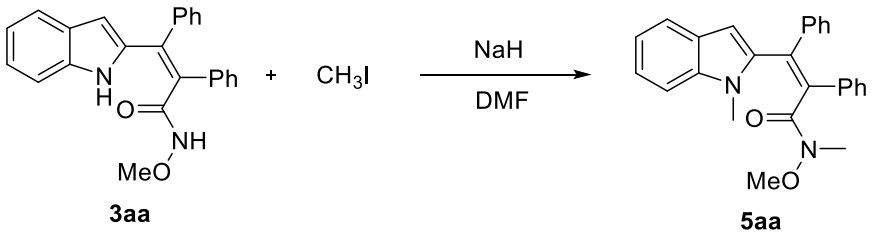
General procedure for the synthesis of compounds 3



To a solution of *N*-methoxy-1*H*-indole-1-carboxamides **1** (0.1 mmol, 1.0 equiv), alkynes **2** (0.1 mmol, 1.0 equiv), NaOAc (0.2 mmol, 2.0 equiv) in H_2O (1.0 mL) was added $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %). The reaction mixture was stirred at room temperature for 10 h. After filtration, the residual solids were purified by silica chromatography to afford the products **3**.

General procedure for the synthesis of compounds 5aa

The compounds **5aa** was prepared according to previously described methods.[3]



To a solution of NaH (60% dispersion oil in mineral oil, 3.0 mmol, 3.0 equiv) in DMF at 0 °C was added (*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide **3aa** (1.0 mmol, 1.0 equiv) and the mixture was stirred for 30 min at room temperature. The reaction mixture was cooled to 0 °C and was added methyl iodide (2.4 mmol, 2.4 equiv) dropwise. The mixture was stirred at room tempearture for 3 h. The crude reaction mixture was treated with saturated NH_4Cl solution (10 mL) and the aqueous phase was extracted with diethyl ether (3 x 20 mL). The combined organic phases were dried over $MgSO_4$ and the solvent was removed under reduced pressure. The residue was purified by silica chromatography to afford the product **5aa** (81%, 0.32 g) as a yellow solid.

References

[1] W. J. Kong, X. G. Chen, M. M. Wang, H. X. Dai, and J. Q. Yu, *Org. Lett.*, 2018**, 20**, 284.

[2] B. Liang, M. Dai, J. Chen and Z. Yang, *J. Org. Chem.*, 2005, **70**, 391.

[3] A. Acharya, D. Anumandla, and C. S. Jeffrey, *J. Am. Chem. Soc*., 2015, **137**, 14858.

Molecular structure and crystallographic data of 5aa

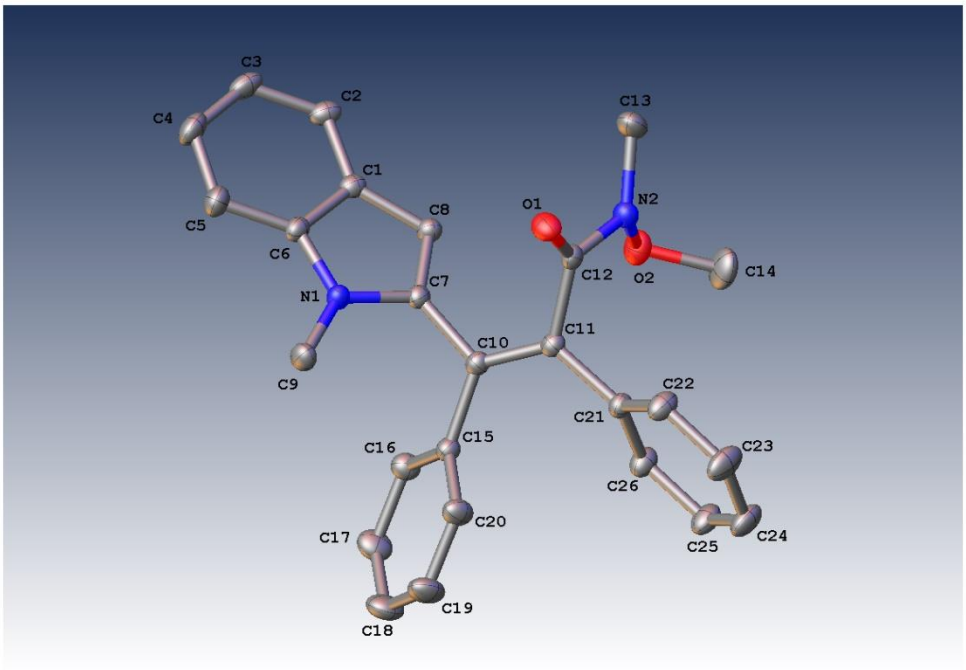


Figure S1. X-ray crystal structure

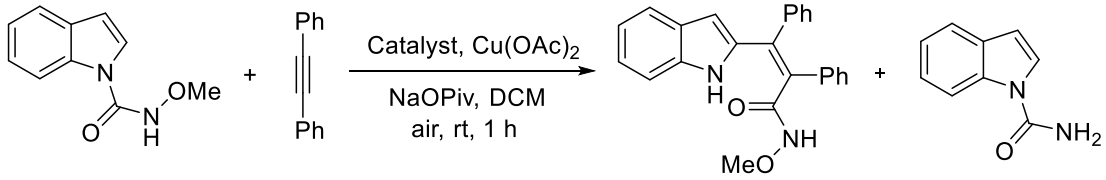
Table S1. Crystal data and structure refinement

Empirical formula	C26 H24 N2 O2	
CCDC number	1883916	
Formula weight	396.47	
Temperature	170.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.7780(2) Å	α= 103.0430(10)°.
	b = 10.6122(2) Å	β= 104.128(2)°.
	c = 11.1756(2) Å	γ = 92.353(2)°.
Volume	1089.87(4) $Å^3$	
Z	2	
Density (calculated)	1.208 Mg/m^3	
Absorption coefficient	0.607 mm^{-1}	
F(000)	420	

Crystal size	0.321 x 0.311 x 0.201 mm^3
Theta range for data collection	4.206 to 75.299°.
Index ranges	-12<=h<=12, -12<=k<=13, -13<=l<=13
Reflections collected	12136
Independent reflections	4259 [R(int) = 0.0164]
Completeness to theta = 67.684°	99.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.79521
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4259 / 0 / 274
Goodness-of-fit on F^2	1.066
Final R indices [I>2sigma(I)]	R1 = 0.0395, wR2 = 0.1026
R indices (all data)	R1 = 0.0430, wR2 = 0.1067
Extinction coefficient	n/a
Largest diff. peak and hole	0.248 and -0.174 e.$Å^{-3}$

Optimization of reaction conditions

Catalyst[a,b]

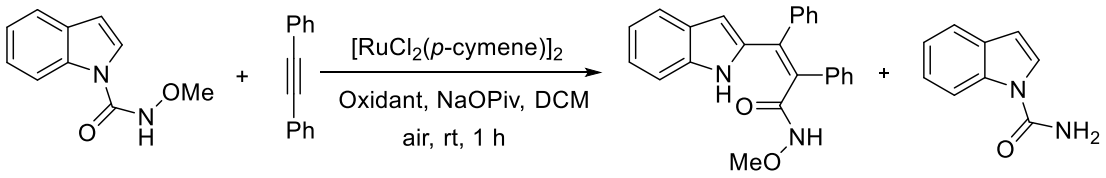


1a **2a** **3aa** **4**

Entry	Catalyst	**3aa**	**4**
1	**$[RuCl_2(p\text{-cymene})]_2$**	**43%**	**13%**
2	$[Cp^*RhCl_2]_2$	35%	9%
3	$[Cp^*IrCl_2]_2$	trace	-
4[c]	$Cp^*Co(CO)I_2$	n.r	-
5[c]	$RuCl_2(PPh_3)_3$	n.r	-
6[c]	$Ru(OAc)_2(PPh_3)_2$	n.r	-
7[d]	$[RuCl_2(p\text{-cymene})]_2$	27%	8%
8	none	n.r	-

[a]Conditions: **1a** (0.1 mmol, 1.0 equiv), **2a** (0.15 mmol, 1.5 equiv), catalyst (5.0 mol %), $Cu(OAc)_2$ (0.1 mmol, 1.0 equiv), NaOPiv (0.2 mmol, 2.0 equiv), DCM (1.0 mL), air, rt, 1 h. [b]Isolated yields. [c]Catalyst (10.0 mol %). [d]$[RuCl_2(p\text{-cymene})]_2$ (2.5 mol %).

Oxidant[a,b]

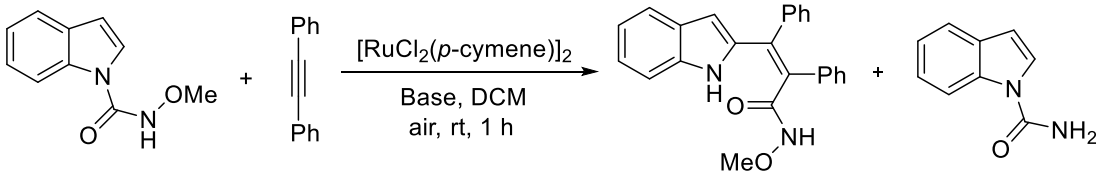


1a **2a** **3aa** **4**

Entry	Oxidant	**3aa**	**4**
1	$Cu(OAc)_2$	43%	13%
2	AgOAc	38%	16%
3	$Co(OAc)_2$	trace	-
4	*m*-CPBA	49%	14%
5	$K_2S_2O_8$	41%	11%
6	**none**	**54%**	**12%**

[a]Conditions: **1a** (0.1 mmol, 1.0 equiv), **2a** (0.15 mmol, 1.5 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %), Oxidant (0.1 mmol, 1.0 equiv), NaOPiv (0.2 mmol, 2.0 equiv), DCM (1.0 mL), air, rt, 1 h. [b]Isolated yields.

Base[a,b]

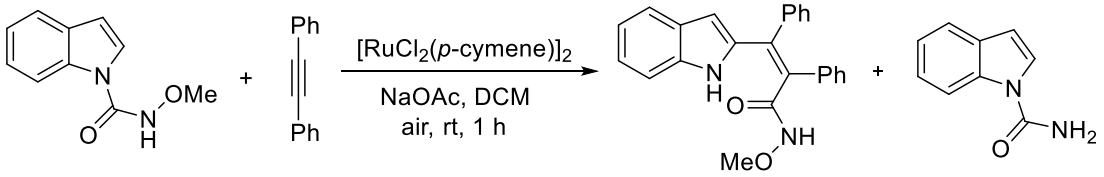


1a **2a** **3aa** **4**

Entry	Base	**3aa**	**4**
1	NaOPiv	54%	12%
2	Na_2CO_3	49%	11%
3	**NaOAc**	**76%**	**14%**
6	KOAc	71%	14%
7	CsOAc	65%	13%
6	*t*-BuOK	33%	8%
7	DABCO	43%	10%
8	Et_3N	41%	10%
9[c]	NaOAc	54%	9%
10	none	trace	-

[a]Conditions: **1a** (0.1 mmol, 1.0 equiv), **2a** (0.15 mmol, 1.5 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %), Base (0.2 mmol, 2.0 equiv), DCM (1.0 mL), air, rt, 1 h. [b]Isolated yields. [c]NaOAc (0.1 mmol, 1.0 equiv).

Proportion[a,b]

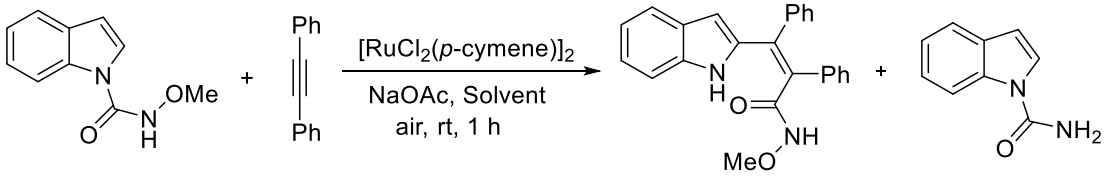


1a **2a** **3aa** **4**

Entry	**1a/2a**	**3aa**	**4**
1	0.1 mmol/0.15 mmol	76%	14%
2	0.1 mmol/0.12 mmol	76%	13%
3	**0.1 mmol/0.1 mmol**	**77%**	**13%**
4	0.15 mmol/0.1 mmol	73%	16%

[a]Conditions: $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %), NaOAc (0.2 mmol, 2.0 equiv), DCM (1.0 mL), air, rt, 1 h. [b]Isolated yields.

Solvent[a,b]

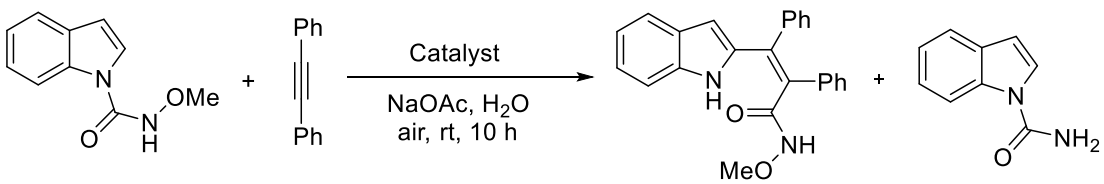


1a **2a** **3aa** **4**

Entry	Solvent	**3aa**	**4**
1	DCM	77%	13%
2	DCE	52%	12%
3	THF	49%	11%
4	DMF	35%	15%
5	Dioxane	63%	12%
6	Toluene	41%	13%
7	MeOH	73%	14%
8[c]	**H_2O**	**87%**	**-**

[a]Conditions: **1a** (0.1 mmol, 1.0 equiv), **2a** (0.1 mmol, 1.0 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %), NaOAc (0.2 mmol, 2.0 equiv), Solvent (1.0 mL), air, rt, 1 h. [b]Isolated yields. [c]Rection time: 10 h.

Complementary[a,b]



1a **2a** **3aa** **4**

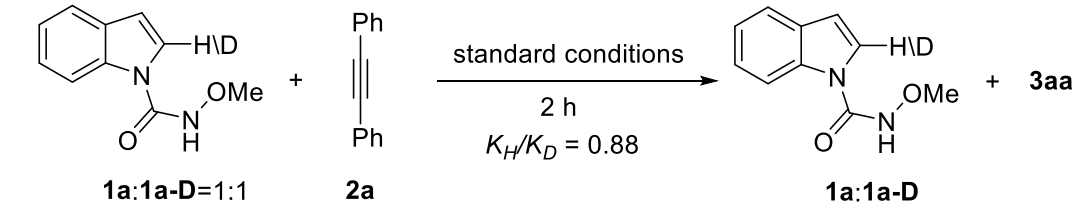
Entry	Catalyst	**3aa**	**4**
1	**[$RuCl_2$(*p*-cymene)]$_2$**	**87%**	**-**
2[c]	$Ru(O_2CMe)_2$(*p*-cymene)	82%	-
3[c]	$Ru(O_2CMes)_2$(*p*-cymene)	79%	-

[a]Conditions: **1a** (0.1 mmol, 1.0 equiv), **2a** (0.1 mmol, 1.0 equiv), Catalyst (5.0 mol %), NaOAc (0.2 mmol, 2.0 equiv), H_2O (1.0 mL), air, rt, 10 h. [b]Isolated yields. [c]Catalyst (10.0 mol %).

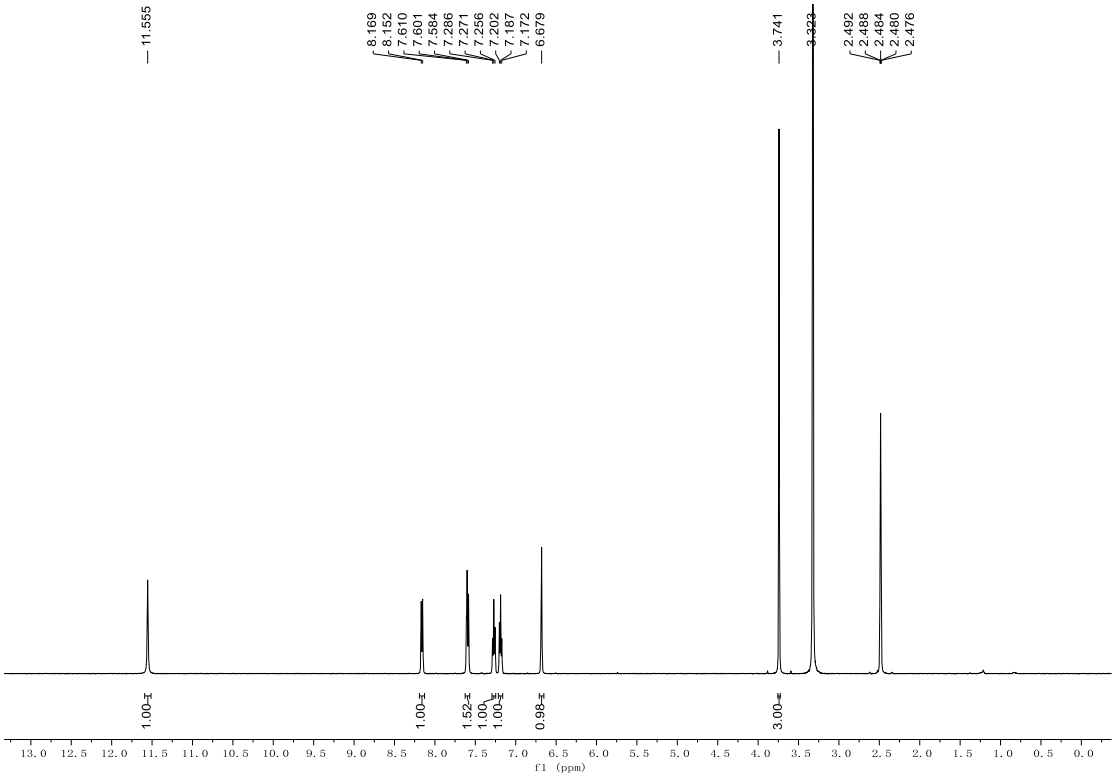
Control experiments

Kinetic Isotope Effect (KIE) study

The intermolecular competition

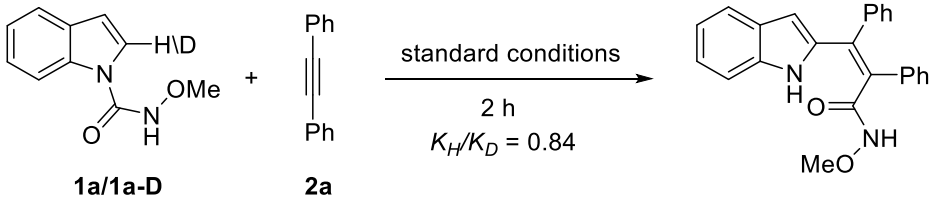


1a:**1a-D**=1:1 **2a** **1a**:**1a-D**



An equimolar mixture of **1a** (0.1 mmol, 1.0 equiv) and **1a-D** (95% D, 0.1 mmol, 1.0 equiv) were allowed to react with **2a** (0.1 mmol, 1.0 equiv) in H_2O (1.0 mL) in the presence of [$RuCl_2$(*p*-cymene)]$_2$ (5.0 mol %), NaOAc (0.2 mmol, 2.0 equiv). The reaction was stirred at room temperature and stopped after 2 h. After filtration, the starting materials was isolated by using column chromatography. A mixture of the starting materials was analyzed by ^{1}H NMR spectroscopy. *A Kinetic isotopic effect of this reaction was determined to be K_H/K_D = 0.88 (0.48/0.52*0.95)*

Two parallel reactions



1a/1a-D **2a**

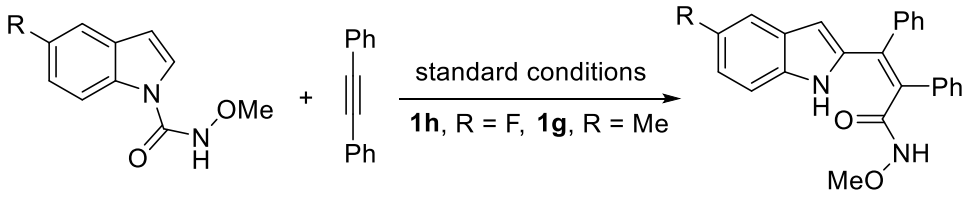
3aa, 24.2% yield starting from **1a**
3aa, 28.8% yield starting from **[D]-1a**

To a solution of *N*-methoxy-1*H*-indole-1-carboxamide **1a** (0.1 mmol, 1.0 equiv), alkyne **2a** (0.1 mmol, 1.0 equiv), NaOAc (0.2 mmol, 2.0 equiv) in H_2O (1.0 mL) was added $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %). The reaction mixture was stirred at room temperature for 2 h. After filtration, the residual solids were purified by silica chromatography to afford the product **3aa** (24.2%, 8.9 mg).

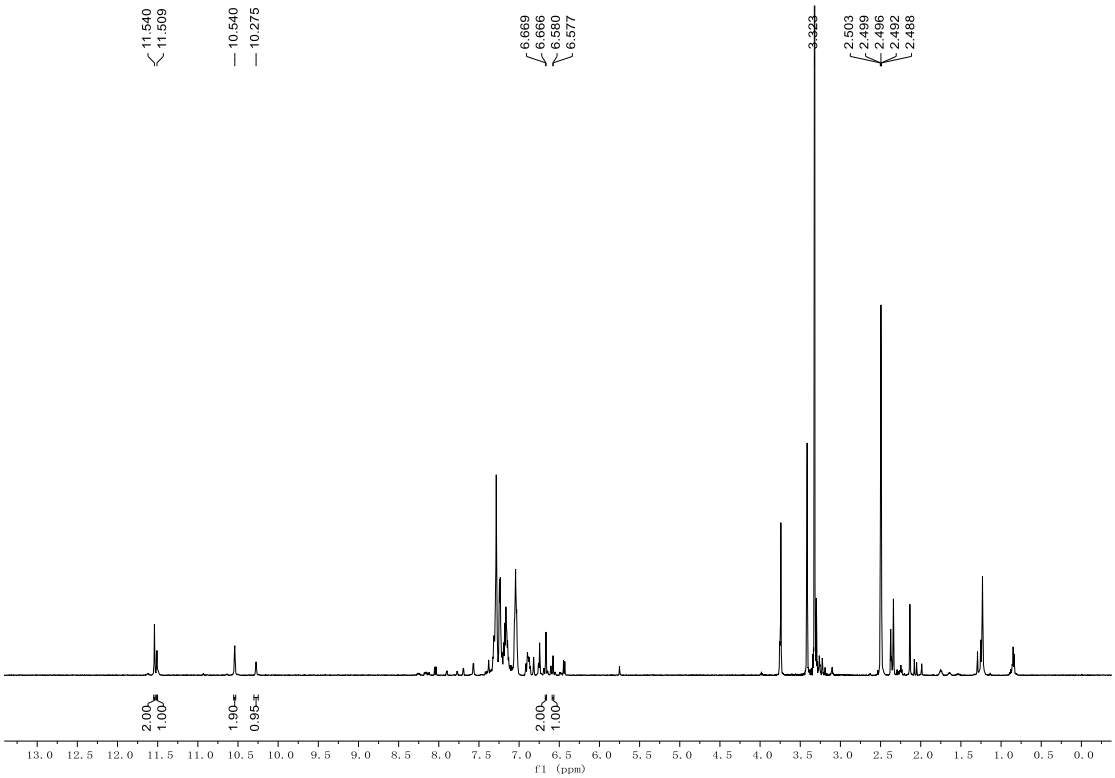
To a solution of *N*-methoxy-1*H*-indole-1-carboxamide **1a** (0.1 mmol, 1.0 equiv), alkyne **2a** (0.1 mmol, 1.0 equiv), NaOAc (0.2 mmol, 2.0 equiv) in H_2O (1.0 mL) was added $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %). The reaction mixture was stirred at room temperature for 2 h. After filtration, the residual solids were purified by silica chromatography to afford the product **3aa** (28.8%, 10.6 mg).

A kinetic isotopic effect of these two reactions was determined to be K_H/K_D = 0.84.

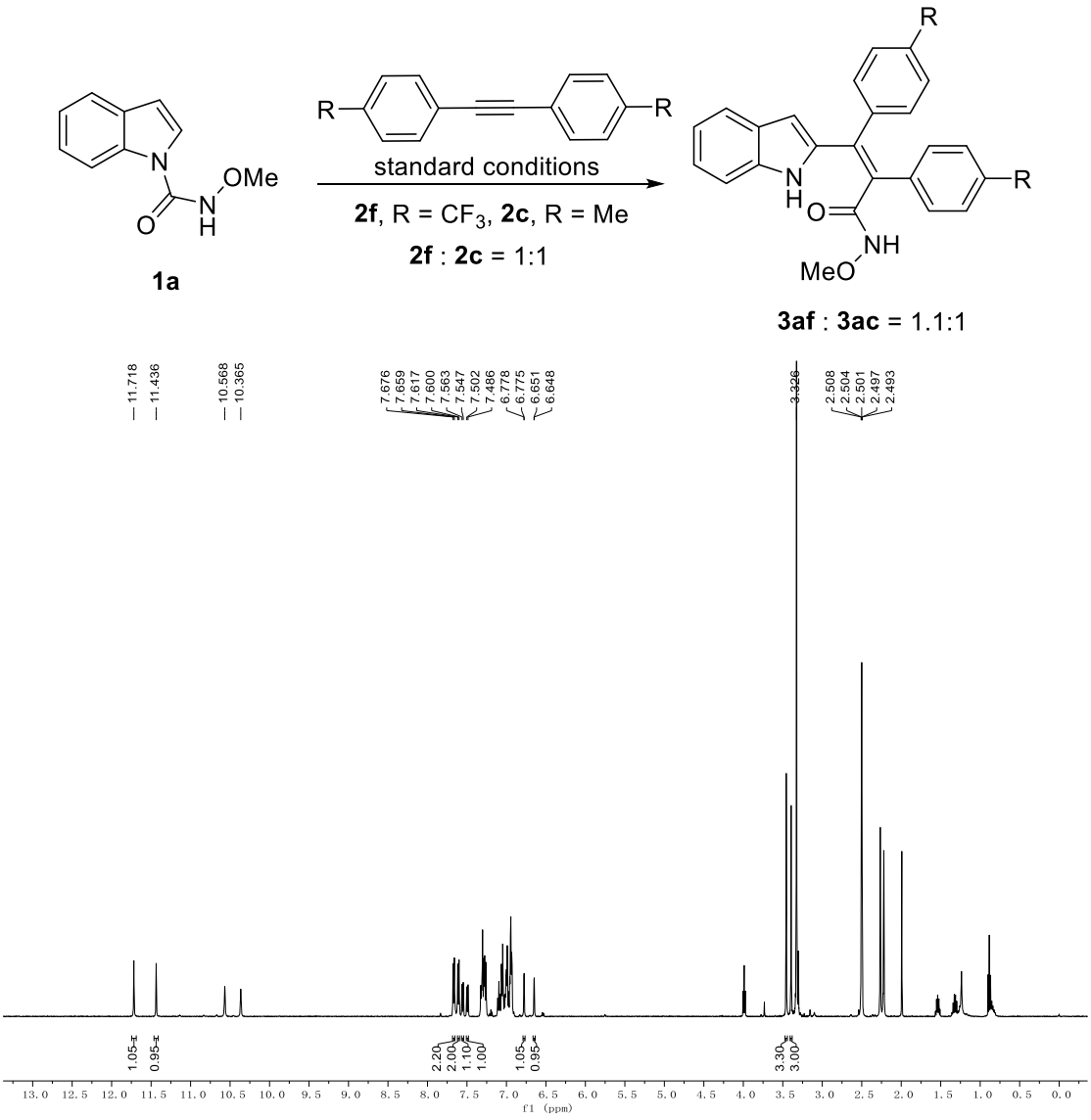
Competitive experiments



1h :**1g** = 1:1 **2a** **3ha** : **3ga** = 2:1

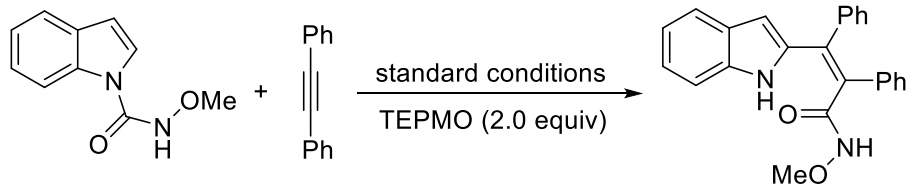


An equimolar mixture of **1h** (0.1 mmol, 1.0 equiv) and **1g** (0.1 mmol, 1.0 equiv) were allowed to react with **2a** (0.1 mmol, 1.0 equiv) in H_2O (1.0 mL) in the presence of $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %), NaOAc (0.2 mmol, 2.0 equiv). The reaction mixture was stirred at room temperature for 10 h. After filtration, the ratio of **3ha** and **3ga** of the same crude mixture was determined to be 2:1 by ^1H NMR.



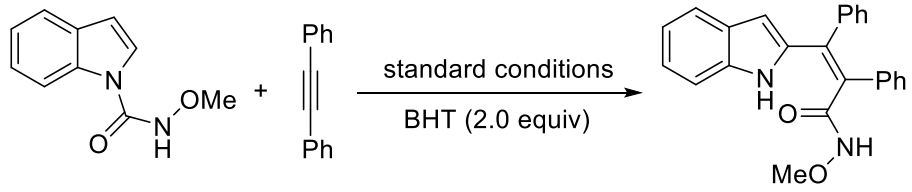
An equimolar mixture of **2f** (0.1 mmol, 1.0 equiv) and **2c** (0.1 mmol, 1.0 equiv) were allowed to react with **1a** (0.1 mmol, 1.0 equiv) in H_2O (1.0 mL) in the presence of $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %), NaOAc (0.2 mmol, 2.0 equiv). The reaction mixture was stirred at room temperature for 10 h. After filtration, the ratio of **3af** and **3ac** of the same crude mixture was determined to be 1.1:1 by ^1H NMR.

Radical inhibition experiments



1a **2a** **3aa**, 80%

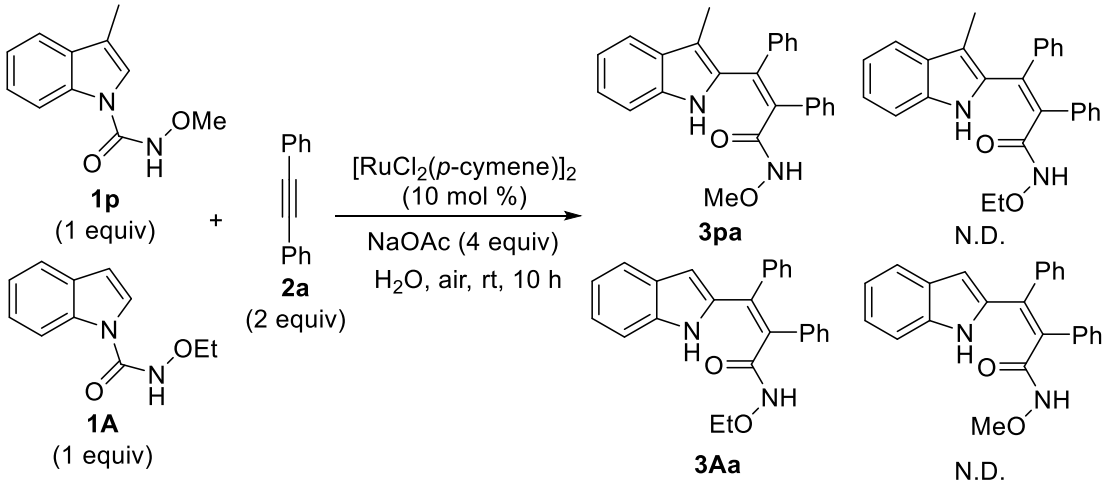
To a solution of *N*-methoxy-1*H*-indole-1-carboxamide **1a** (0.1 mmol, 1.0 equiv), alkyne **2a** (0.1 mmol, 1.0 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %), NaOAc (0.2 mmol, 2.0 equiv) in H_2O (1.0 mL) was added TEMPO (0.2 mmol, 2.0 equiv). The reaction mixture was stirred at room temperature for 10 h. After filtration, the residual solids were purified by silica chromatography to afford the product **3aa** (80%).



1a **2a** **3aa**, 83%

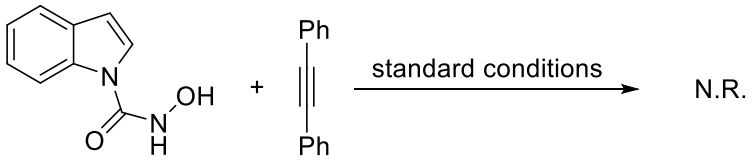
To a solution of *N*-methoxy-1*H*-indole-1-carboxamide **1a** (0.1 mmol, 1.0 equiv), alkyne **2a** (0.1 mmol, 1.0 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %), NaOAc (0.2 mmol, 2.0 equiv) in H_2O (1.0 mL) was added BHT (0.2 mmol, 2.0 equiv). The reaction mixture was stirred at room temperature for 10 h. After filtration, the residual solids were purified by silica chromatography to afford the product **3aa** (83%).

Directing group migration process study



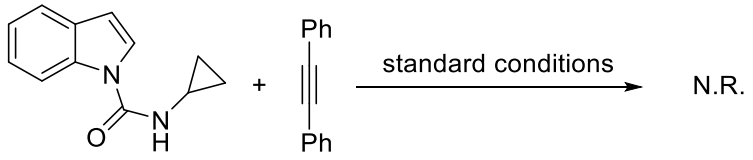
An equimolar mixture of **1p** (0.1 mmol, 1.0 equiv) and **1A** (0.1 mmol, 1.0 equiv) were allowed to react with **2a** (0.2 mmol, 2.0 equiv) in H_2O (2.0 mL) in the presence of $[RuCl_2(p\text{-cymene})]_2$ (10.0 mol %), NaOAc (0.4 mmol, 4.0 equiv). The reaction mixture was stirred at room temperature for 10 h. After the reaction was completed, only two products **3pa** and **3Aa** were observed in the system (detected by TLC).

Unsuccessful directing group study



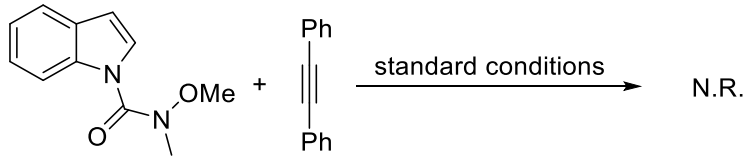
1B **2a**

To a solution of *N*-hydroxy-1*H*-indole-1-carboxamide **1B** (0.1 mmol, 1.0 equiv), alkyne **2a** (0.1 mmol, 1.0 equiv), NaOAc (0.2 mmol, 2.0 equiv) in H_2O (1.0 mL) was added $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %). The mixture was stirred at room temperature for 10 h, but no reaction occurred in the system.



1C **2a**

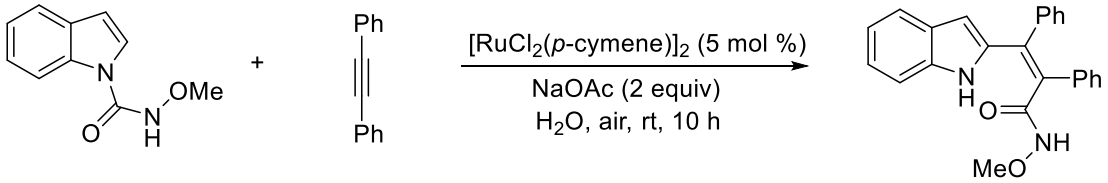
To a solution of *N*-cyclopropyl-1*H*-indole-1-carboxamide **1C** (0.1 mmol, 1.0 equiv), alkyne **2a** (0.1 mmol, 1.0 equiv), NaOAc (0.2 mmol, 2.0 equiv) in H_2O (1.0 mL) was added $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %). The reaction mixture was stirred at room temperature for 10 h, but no reaction occurred in the system.



1D **2a**

To a solution of *N*-methoxy-*N*-methyl-1*H*-indole-1-carboxamide **1D** (0.1 mmol, 1.0 equiv), alkyne **2a** (0.1 mmol, 1.0 equiv), NaOAc (0.2 mmol, 2.0 equiv) in H_2O (1.0 mL) was added $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %). The reaction mixture was stirred at room temperature for 10 h, but no reaction occurred in the system.

Gram scale synthesis of 3aa

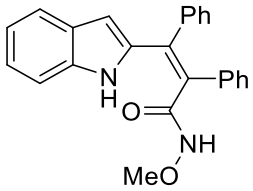


1a (5 mmol) **2a** (5 mmol) **3aa** (73%, 1.35 g)

To a solution of *N*-methoxy-1*H*-indole-1-carboxamides **1a** (5.0 mmol, 1.0 equiv), alkyne **2a** (5.0 mmol, 1.0 equiv), NaOAc (10.0 mmol, 2.0 equiv) in H_2O (25.0 mL) was added $[RuCl_2(p\text{-cymene})]_2$ (5.0 mol %). The reaction mixture was stirred at room temperature for 10 h. After filtration, the residual solids were purified by silica chromatography to afford the product **3aa** (73%, 1.35 g) as a white solid.

Characterization of products

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3aa)



3aa

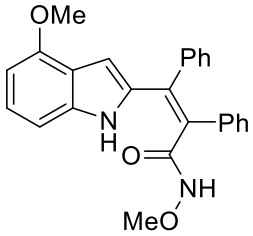
3aa: a white solid. Yeild: 87% (32 mg). Mp: 208-210 ºC.

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.53 (s, 1H), 10.44 (s, 1H), 7.51 (d, J = 7.8 Hz, 1H), 7.32 (d, J = 8.1 Hz, 1H), 7.24 (dd, J = 5.0, 1.7 Hz, 3H), 7.20 – 7.13 (m, 3H), 7.08 – 7.03 (m, 5H), 6.99 – 6.95 (m, 1H), 6.68 (d, J = 1.5 Hz, 1H), 3.42 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 166.5, 139.0, 137.6, 137.4, 137.3, 135.3, 134.6, 131.0, 129.6, 128.5, 128.3, 128.0, 127.7, 122.3, 120.6, 119.7, 112.1, 104.4, 62.8.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{20}N_2O_2Na$, 391.1422, Found: 391.1418.

(*Z*)-3-(4-methoxy-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ba)



3ba

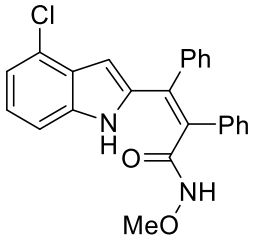
3ba: a light yellow solid. Yeild: 75% (30 mg). Mp: 218-220 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.52 (s, 1H), 10.40 (s, 1H), 7.22 (dd, J = 5.0, 1.7 Hz, 3H), 7.14 (dt, J = 11.5, 6.8 Hz, 3H), 7.02 (t, J = 7.6 Hz, 4H), 6.96 (t, J = 7.9 Hz, 1H), 6.90 (d, J = 8.0 Hz, 1H), 6.69 (d, J = 1.9 Hz, 1H), 6.44 (d, J = 7.6 Hz, 1H), 3.83 (s, 3H), 3.43 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.5, 153.1, 139.0, 138.6, 137.6, 135.7, 135.1, 134.0, 130.9, 129.5, 128.4, 128.4, 128.2, 127.5, 123.2, 118.7, 105.4, 101.8, 99.5, 62.7, 55.4.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{25}H_{22}N_2O_3Na$, 421.1528, Found: 421.1526.

(*Z*)-3-(4-chloro-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ca)



3ca

3ca: a white solid. Yeild: 77% (31 mg). Mp: 200-202 ºC.

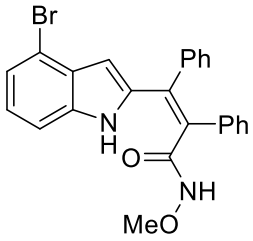
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.59 (s, 1H), 10.86 (s, 1H), 7.28 (dd, J = 5.4, 3.5 Hz, 1H), 7.24

(dd, *J* = 5.1, 1.8 Hz, 3H), 7.19 – 7.13 (m, 3H), 7.04 (dt, *J* = 4.1, 2.2 Hz, 5H), 7.03 – 7.02 (m, 1H), 6.76 (d, *J* = 1.9 Hz, 1H), 3.43 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.1, 138.6, 138.3, 138.0, 137.4, 135.7, 134.5, 130.9, 129.5, 128.6, 128.5, 128.4, 127.8, 126.5, 124.5, 123.0, 119.1, 111.2, 102.1, 62.6.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{19}N_2O_2NaCl$, 425.1033, Found: 425.1028.

(*Z*)-3-(4-bromo-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3da)



3da

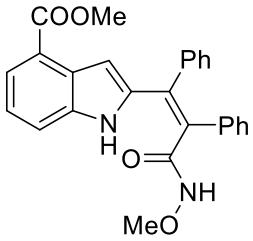
3da: a white solid. Yeild: 81% (36 mg). Mp: 192-194 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.60 (s, 1H), 10.89 (s, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.25 (dd, *J* = 5.0, 1.7 Hz, 3H), 7.22 – 7.16 (m, 4H), 7.06 (td, *J* = 6.5, 5.7, 2.7 Hz, 4H), 7.00 (t, *J* = 7.9 Hz, 1H), 6.73 (d, *J* = 1.9 Hz, 1H), 3.46 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.1, 138.6, 138.2, 137.5, 137.4, 135.7, 134.5, 130.9, 129.5, 128.6, 128.5, 128.4, 128.3, 127.8, 123.4, 122.2, 113.5, 111.7, 103.8, 62.6.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{19}N_2O_2NaBr$, 469.0528, Found: 469.0526.

Methyl (*Z*)-2-(3-(methoxyamino)-3-oxo-1,2-diphenylprop-1-en-1-yl)-1*H*-indole-4-carboxylate (3ea)



3ea

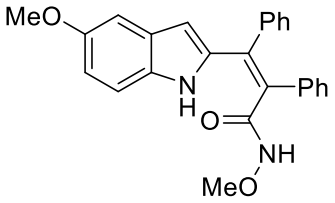
3ea: a light yellow solid. Yeild: 82% (35 mg). Mp: 198-200 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.57 (s, 1H), 10.90 (s, 1H), 7.72 (d, *J* = 7.5 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 1.7 Hz, 1H), 7.25 (dd, *J* = 5.0, 1.6 Hz, 3H), 7.19 (dt, *J* = 10.6, 7.1 Hz, 4H), 7.08 – 7.04 (m, 4H), 3.87 (s, 3H), 3.41 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 167.0, 165.5, 139.3, 138.4, 137.6, 137.0, 135.4, 134.4, 130.4, 129.1, 128.1, 128.1, 127.9, 127.3, 126.7, 122.5, 121.0, 120.1, 116.8, 104.7, 62.1, 51.6.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{22}N_2O_4Na$, 449.1477, Found: 449.1476.

(*Z*)-3-(5-methoxy-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3fa)



3fa

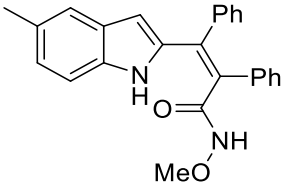
3fa: a light yellow solid. Yeild: 85% (34 mg). Mp: 218-220 ºC.

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.52 (s, 1H), 10.25 (s, 1H), 7.25 – 7.20 (m, 4H), 7.19 – 7.13 (m, 3H), 7.08 – 7.02 (m, 4H), 7.01 (d, J = 2.4 Hz, 1H), 6.71 (dd, J = 8.8, 2.4 Hz, 1H), 6.60 (d, J = 1.7 Hz, 1H), 3.74 (s, 3H), 3.45 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 166.5, 154.0, 139.1, 137.8, 137.7, 135.3, 134.2, 132.6, 131.0, 129.6, 128.5, 128.3, 128.3, 127.6, 112.9, 104.3, 101.8, 62.9, 55.7.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{25}H_{22}N_2O_3Na$, 421.1528, Found: 421.1528.

(*Z*)-3-(5-methyl-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ga)



3ga

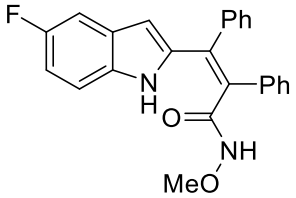
3ga: a white solid. Yeild: 86% (33 mg). Mp: 216-218 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.50 (s, 1H), 10.26 (s, 1H), 7.26 (s, 1H), 7.23 – 7.20 (m, 3H), 7.18 (d, J = 8.3 Hz, 1H), 7.17 – 7.11 (m, 3H), 7.05 – 6.99 (m, 4H), 6.86 (d, J = 8.3 Hz, 1H), 6.56 (s, 1H), 3.40 (s, 3H), 2.32 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.4, 139.0, 137.6, 137.3, 135.7, 135.3, 134.3, 130.9, 129.5, 128.4, 128.4, 128.2, 128.2, 128.0, 127.5, 123.9, 119.9, 111.8, 103.9, 62.8, 21.6.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{25}H_{22}N_2O_2Na$, 405.1579, Found: 405.1575.

(*Z*)-3-(5-fluoro-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ha)



3ha

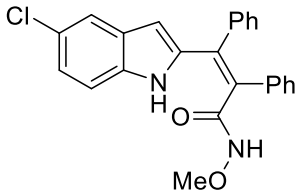
3ha: a light yellow solid. Yeild: 78% (30 mg). Mp: 204-206 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.53 (s, 1H), 10.53 (s, 1H), 7.28 (td, J = 9.8, 9.4, 3.5 Hz, 2H), 7.22 (d, J = 3.6 Hz, 3H), 7.15 (q, J = 10.2, 8.4 Hz, 3H), 7.03 (dt, J = 8.1, 4.2 Hz, 4H), 6.88 (td, J = 9.4, 2.3 Hz, 1H), 6.68 – 6.63 (m, 1H), 3.40 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.2, 157.4 (d, J = 231.4 Hz), 139.2, 138.8, 137.4, 135.0 (d, J = 24.8 Hz), 134.0, 130.9, 129.5, 128.5, 128.3, 128.1, 128.0, 127.7, 113.0, 110.4 (d, J = 25.6 Hz), 104.9, 104.8, 104.3, 62.8.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{19}N_2O_2NaF$, 409.1328, Found: 409.1328.

(*Z*)-3-(5-chloro-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ia)



3ia

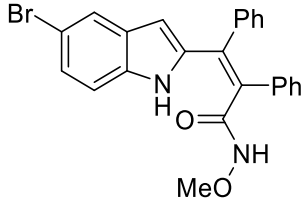
3ia: a white solid. Yeild: 84% (34 mg). Mp: 202-204 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.53 (s, 1H), 10.63 (s, 1H), 7.56 (d, J = 1.6 Hz, 1H), 7.29 (d, J = 8.6 Hz, 1H), 7.22 (dd, J = 4.9, 1.5 Hz, 3H), 7.18 – 7.12 (m, 3H), 7.04 – 6.99 (m, 5H), 6.64 (d, J = 1.6 Hz, 1H), 3.38 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 171.0, 143.8, 143.5, 142.2, 140.5, 140.2, 139.5, 135.7, 134.3, 133.8, 133.4, 133.3, 133.2, 132.6, 128.9, 127.0, 124.4, 114.8, 108.7, 67.6.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{19}N_2O_2NaCl$, 425.1033, Found: 425.1028.

(*Z*)-3-(5-bromo-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ja)



3ja

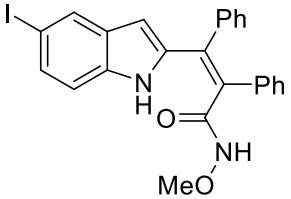
3ja: a white solid. Yeild: 83% (37 mg). Mp: 190-192 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.53 (s, 1H), 10.65 (s, 1H), 7.70 (d, J = 1.6 Hz, 1H), 7.25 (d, J = 8.7 Hz, 1H), 7.22 (dd, J = 5.0, 1.7 Hz, 3H), 7.14 (ddd, J = 6.7, 5.3, 3.2 Hz, 4H), 7.04 – 6.99 (m, 4H), 6.64 (d, J = 1.8 Hz, 1H), 3.39 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.2, 138.8, 138.7, 137.4, 135.9, 135.4, 134.7, 130.9, 129.7, 129.5, 128.6, 128.5, 128.4, 127.7, 124.7, 122.6, 114.0, 112.1, 103.7, 62.8.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{19}N_2O_2NaBr$, 469.0528, Found: 469.0528.

(*Z*)-3-(5-iodo-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ka)



3ka

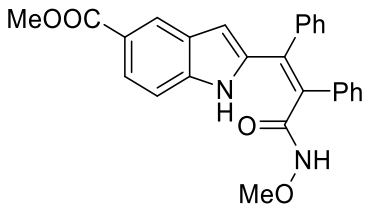
3ka: a light yellow solid. Yeild: 81% (40 mg). Mp: 168-170 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.53 (s, 1H), 10.63 (s, 1H), 7.88 (s, 1H), 7.30 – 7.28 (m, 1H), 7.22 (dt, J = 5.7, 3.0 Hz, 3H), 7.15 (td, J = 9.0, 4.4 Hz, 4H), 7.04 – 7.00 (m, 4H), 6.62 (d, J = 2.1 Hz, 1H), 3.39 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.2, 138.7, 138.3, 137.4, 136.2, 135.4, 134.7, 130.9, 130.7, 130.1, 129.5, 128.8, 128.5, 128.5, 128.3, 127.7, 114.5, 103.4, 83.4, 62.8.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{19}N_2O_2NaI$, 517.0389, Found: 517.0389.

Methyl (*Z*)-2-(3-(methoxyamino)-3-oxo-1,2-diphenylprop-1-en-1-yl)-1*H*-indole-5-carboxylate (3la)



3la

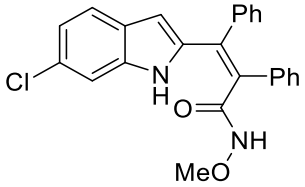
3la: a light yellow solid. Yeild: 77% (33 mg). Mp: 198-200 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.59 (s, 1H), 10.93 (s, 1H), 8.25 (s, 1H), 7.73 – 7.69 (m, 1H), 7.40 (d, J = 8.6 Hz, 1H), 7.27 – 7.24 (m, 3H), 7.19 (td, J = 9.5, 9.1, 4.5 Hz, 3H), 7.08 – 7.03 (m, 4H), 6.84 (s, 1H), 3.84 (s, 3H), 3.40 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 167.1, 165.7, 139.3, 138.7, 138.2, 136.9, 135.2, 134.2, 130.4, 129.1, 128.1, 128.1, 127.9, 127.3, 127.0, 122.7, 122.7, 120.7, 111.5, 104.9, 62.3, 51.6.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{22}N_2O_4Na$, 449.1477, Found: 449.1481.

(*Z*)-3-(6-chloro-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3na)



3na

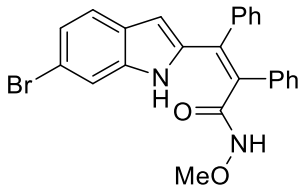
3na: a white solid. Yeild: 82% (33 mg). Mp: 204-206 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.55 (s, 1H), 10.57 (s, 1H), 7.53 (d, J = 8.5 Hz, 1H), 7.33 (s, 1H), 7.25 – 7.22 (m, 3H), 7.16 (p, J = 6.7 Hz, 3H), 7.03 (t, J = 7.2 Hz, 4H), 6.99 – 6.96 (m, 1H), 6.68 (s, 1H), 3.40 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 165.8, 138.3, 138.0, 137.1, 137.0, 134.7, 134.3, 130.4, 129.1, 128.1, 128.1, 127.9, 127.3, 126.3, 126.2, 121.5, 119.6, 111.1, 103.9, 62.3.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{19}N_2O_2NaCl$, 425.1033, Found: 425.1028.

(*Z*)-3-(6-bromo-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3oa)



3oa

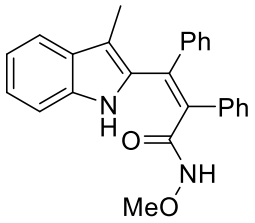
3oa: a white solid. Yeild: 81% (36 mg). Mp: 188-190 ºC.

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.58 (s, 1H), 10.60 (s, 1H), 7.53 – 7.48 (m, 2H), 7.26 (dd, J = 5.0, 1.7 Hz, 3H), 7.18 (t, J = 7.1 Hz, 3H), 7.11 (dd, J = 8.5, 1.7 Hz, 1H), 7.09 – 7.03 (m, 4H), 6.75 – 6.66 (m, 1H), 3.42 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 166.3, 138.7, 138.4, 138.1, 137.4, 135.3, 134.8, 131.0, 129.6,

128.6, 128.6, 128.4, 127.8, 127.0, 122.6, 122.4, 114.9, 114.6, 104.5, 62.8.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{19}N_2O_2NaBr$, 469.0528, Found: 469.0519.

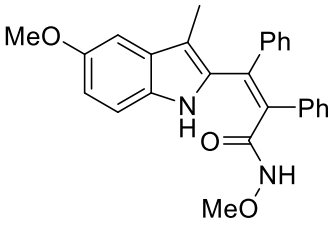
(*Z*)-3-(3-methyl-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3pa)



3pa

3pa: a light yellow solid. Yeild: 92% (35 mg). Mp: 212-214 ºC.
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.14 (s, 1H), 10.33 (s, 1H), 7.45 (d, J = 7.8 Hz, 1H), 7.30 (d, J = 8.0 Hz, 1H), 7.26 – 7.20 (m, 3H), 7.19 – 7.15 (m, 3H), 7.11 (d, J = 6.7 Hz, 2H), 7.06 (t, J = 7.5 Hz, 1H), 6.97 (dt, J = 6.9, 4.0 Hz, 3H), 3.11 (s, 3H), 2.12 (s, 3H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 165.3, 138.9, 136.8, 136.7, 136.1, 135.2, 134.1, 129.8, 129.3, 128.2, 128.1, 127.9, 127.5, 127.3, 121.5, 118.3, 118.3, 111.1, 109.9, 62.1, 9.3.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{25}H_{22}N_2O_2Na$, 405.1579, Found: 405.1576.

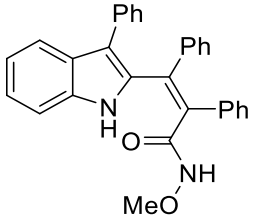
(*Z*)-3-(5-methoxy-3-methyl-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3qa)



3qa

3qa: a light yellow solid. Yeild: 70% (29 mg). Mp: 220-222 ºC.
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.10 (s, 1H), 10.14 (s, 1H), 7.20 (dd, J = 11.7, 7.7 Hz, 4H), 7.17 – 7.14 (m, 3H), 7.09 (d, J = 7.1 Hz, 2H), 6.95 (dd, J = 6.2, 2.6 Hz, 2H), 6.91 (d, J = 1.9 Hz, 1H), 6.70 (dd, J = 8.7, 2.2 Hz, 1H), 3.74 (s, 3H), 3.12 (s, 3H), 2.04 (s, 3H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 165.5, 153.0, 139.1, 137.0, 136.5, 135.4, 134.9, 131.3, 129.9, 129.3, 128.6, 128.2, 127.9, 127.6, 127.4, 111.9, 111.8, 109.9, 100.0, 62.3, 55.3, 9.4.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{24}N_2O_3Na$, 435.1685, Found: 435.1690.

(*Z*)-3-(3-phenyl-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ra)

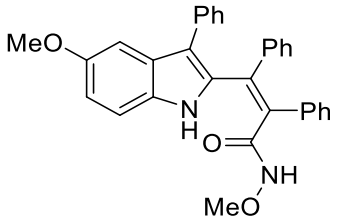


3ra

3ra: a light yellow solid. Yeild: 43% (19 mg). Mp: 210-212 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.01 (s, 1H), 10.96 (s, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 7.2 Hz, 2H), 7.45 (d, J = 8.1 Hz, 1H), 7.27 (t, J = 7.7 Hz, 2H), 7.21 (dd, J = 10.8, 7.1 Hz, 3H), 7.16 – 7.08 (m, 4H), 7.04 (t, J = 7.5 Hz, 1H), 6.98 (q, J = 5.9 Hz, 3H), 6.85 (dd, J = 7.8, 1.6 Hz, 2H), 3.14 (s, 3H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 165.3, 138.3, 137.6, 136.9, 136.0, 135.2, 134.6, 134.1, 129.9, 129.1, 128.6, 128.2, 127.9, 127.5, 126.5, 125.5, 122.0, 119.6, 118.7, 115.5, 111.7, 62.5.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{30}H_{24}N_2O_2Na$, 467.1735, Found: 467.1731.

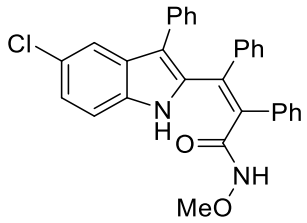
(*Z*)-3-(5-methoxy-3-phenyl-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3sa)



3sa

3sa: a light yellow solid. Yeild: 48% (23 mg). Mp: 226-228 ºC.
^{1}H NMR (500 MHz, DMSO-d_6) δ 10.99 (s, 1H), 10.79 (s, 1H), 7.54 (d, J = 7.7 Hz, 2H), 7.36 (d, J = 8.8 Hz, 1H), 7.28 – 7.18 (m, 5H), 7.10 (d, J = 6.4 Hz, 3H), 7.04 (s, 1H), 6.96 (q, J = 6.1, 5.6 Hz, 3H), 6.85 (d, J = 7.0 Hz, 2H), 6.82 – 6.78 (m, 1H), 3.72 (s, 3H), 3.17 (s, 3H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 165.8, 154.4, 138.7, 137.8, 137.3, 135.7, 135.2, 131.6, 130.4, 129.6, 129.0, 128.7, 128.4, 127.9, 127.2, 125.8, 115.9, 112.9, 112.7, 100.7, 63.0, 55.7.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{31}H_{26}N_2O_3Na$, 497.1841, Found: 497.1841.

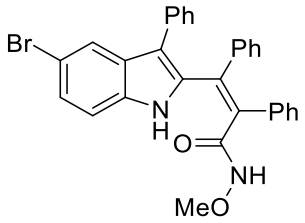
(*Z*)-3-(5-chloro-3-phenyl-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ta)



3ta

3ta: a light yellow solid. Yeild: 46% (22 mg). Mp: 218-220 ºC.
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.24 (s, 1H), 11.10 (s, 1H), 7.56 (d, J = 7.6 Hz, 3H), 7.52 (d, J = 8.6 Hz, 1H), 7.32 (t, J = 7.6 Hz, 2H), 7.29 – 7.23 (m, 3H), 7.20 – 7.15 (m, 2H), 7.13 (d, J = 6.6 Hz, 2H), 7.03 (t, J = 6.9 Hz, 3H), 6.90 – 6.86 (m, 2H), 3.19 (s, 3H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 165.6, 138.5, 137.2, 136.3, 135.2, 134.9, 134.3, 130.4, 129.6, 129.1, 128.8, 128.6, 128.2, 128.1, 126.3, 124.8, 122.4, 118.2, 115.7, 113.9, 63.0.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{30}H_{23}N_2O_2NaCl$, 501.1346, Found: 501.1345.

(*Z*)-3-(5-bromo-3-phenyl-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3ua)



3ua

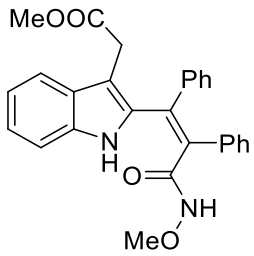
3ua: a light yellow solid. Yeild: 44% (23 mg). Mp: 216-218 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.20 (s, 1H), 11.04 (s, 1H), 7.66 (s, 1H), 7.51 (d, J = 7.6 Hz, 2H), 7.43 (d, J = 8.5 Hz, 1H), 7.30 – 7.25 (m, 3H), 7.21 (t, J = 8.0 Hz, 3H), 7.13 (t, J = 7.3 Hz, 1H), 7.09 (d, J = 6.9 Hz, 2H), 6.98 (q, J = 6.3, 5.9 Hz, 3H), 6.84 (d, J = 7.0 Hz, 2H), 3.15 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 165.6, 138.5, 137.1, 136.1, 135.2, 135.1, 134.2, 130.4, 129.6, 129.1, 128.7, 128.5, 128.1, 128.0, 126.2, 124.9, 121.2, 115.6, 114.3, 112.7, 62.9.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{30}H_{23}N_2O_2NaBr$, 545.0841, Found: 545.0848.

Methyl (*Z*)-2-(2-(3-(methoxyamino)-3-oxo-1,2-diphenylprop-1-en-1-yl)-1*H*-indol-3-yl)acetate (3va)



3va

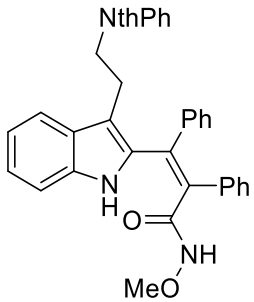
3va: a white solid. Yeild: 73% (32 mg). Mp: 218-220 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.07 (s, 1H), 10.72 (s, 1H), 7.48 (d, J = 7.8 Hz, 1H), 7.36 (d, J = 7.9 Hz, 1H), 7.25 (t, J = 8.1 Hz, 3H), 7.19 (s, 3H), 7.14 – 7.08 (m, 3H), 7.06 – 6.98 (m, 3H), 3.68 (s, 2H), 3.58 (s, 3H), 3.06 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 172.3, 165.4, 138.5, 137.1, 136.7, 136.1, 135.7, 134.8, 130.1, 129.4, 128.2, 127.9, 127.8, 127.6, 127.6, 121.8, 118.9, 118.6, 111.4, 107.3, 62.2, 51.6, 29.8.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{27}H_{24}N_2O_4Na$, 463.1634, Found: 463.1632.

(*Z*)-3-(3-(2-(1,3-dioxoisoindolin-2-yl)ethyl)-1*H*-indol-2-yl)-*N*-methoxy-2,3-diphenylacrylamide (3wa)



3wa

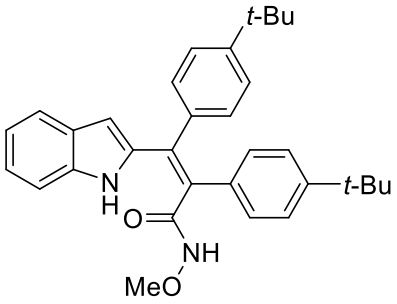
3wa: a light yellow solid. Yeild: 72% (39 mg). Mp: 220-222 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.07 (s, 1H), 10.46 (s, 1H), 7.87 – 7.81 (m, 4H), 7.61 (d, J = 7.7 Hz, 1H), 7.34 (d, J = 7.9 Hz, 1H), 7.27 (dt, J = 13.0, 6.9 Hz, 3H), 7.15 (dd, J = 16.5, 7.1 Hz, 3H), 7.09 (t, J = 7.2 Hz, 3H), 7.01 (dd, J = 12.4, 7.5 Hz, 3H), 3.82 – 3.76 (m, 2H), 3.05 (s, 3H), 3.02 (s, 2H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 167.7, 165.3, 138.6, 137.3, 136.9, 136.3, 134.9, 134.7, 134.3, 131.7, 129.9, 129.3, 128.2, 127.8, 127.6, 127.5, 127.4, 122.9, 121.7, 118.7, 118.3, 111.5, 111.2, 62.1, 38.0, 23.8.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{34}H_{27}N_3O_4Na$, 564.1899, Found: 564.1900.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-bis(4-(*tert*-butyl)phenyl)acrylamide (3ab)



3ab

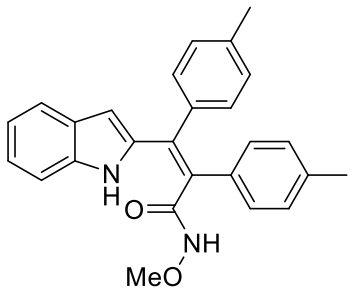
3ab: a white solid. Yeild: 73% (35 mg). Mp: 158-160 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.45 (s, 1H), 10.42 (s, 1H), 7.51 (d, J = 7.9 Hz, 1H), 7.34 (d, J = 8.1 Hz, 1H), 7.27 (d, J = 8.3 Hz, 2H), 7.20 (d, J = 8.4 Hz, 2H), 7.06 (t, J = 7.6 Hz, 1H), 6.98 (dd, J = 18.3, 8.4 Hz, 5H), 6.66 (d, J = 2.1 Hz, 1H), 3.41 (s, 3H), 1.25 (s, 9H), 1.23 (s, 9H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.2, 150.1, 149.4, 137.2, 136.8, 135.8, 134.3, 134.1, 133.9, 130.1, 128.8, 127.5, 124.7, 124.6, 121.6, 120.0, 119.1, 111.6, 103.7, 62.3, 34.3, 34.2, 31.0, 30.9.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{32}H_{36}N_2O_2Na$, 503.2674, Found: 503.2677.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-di-*p*-tolylacrylamide (3ac)



3ac

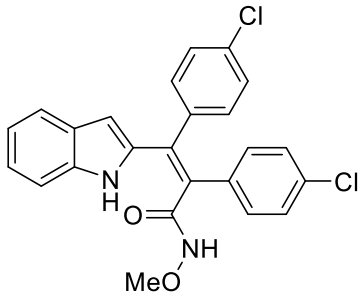
3ac: a white solid. Yeild: 76% (30 mg). Mp: 168-170 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.44 (s, 1H), 10.38 (s, 1H), 7.51 (d, J = 7.9 Hz, 1H), 7.33 (d, J = 8.1 Hz, 1H), 7.07 (d, J = 8.1 Hz, 3H), 7.01 (q, J = 9.6, 7.9 Hz, 3H), 6.97 – 6.94 (m, 4H), 6.66 (s, 1H), 3.41 (s, 3H), 2.28 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.2, 137.2, 137.0, 136.8, 136.4, 135.8, 134.4, 134.1, 133.7, 130.4, 129.0, 128.7, 127.5, 121.6, 120.0, 119.1, 111.6, 103.7, 62.2, 20.7.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{24}N_2O_2Na$, 419.1735, Found: 419.1736.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-bis(4-chlorophenyl)acrylamide (3ad)



3ad

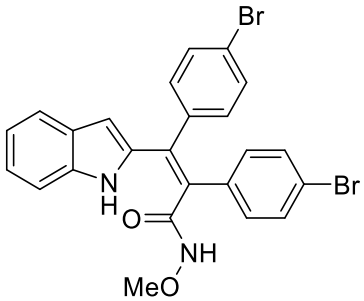
3ad: a light yellow solid. Yeild: 80% (35 mg). Mp: 188-190 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.58 (s, 1H), 10.49 (s, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.35 (d, J = 8.4 Hz, 2H), 7.32 – 7.27 (m, 3H), 7.08 – 7.03 (m, 5H), 6.97 (t, J = 7.5 Hz, 1H), 6.72 (d, J = 1.6 Hz, 1H), 3.43 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 165.5, 137.1, 136.9, 136.1, 135.6, 134.3, 133.0, 132.7, 132.4, 132.0, 130.9, 128.3, 127.4, 122.1, 120.2, 119.3, 111.6, 104.2, 62.4.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{18}N_2O_2NaCl_2$, 459.0643, Found: 459.0633.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-bis(4-bromophenyl)acrylamide (3ae)



3ae

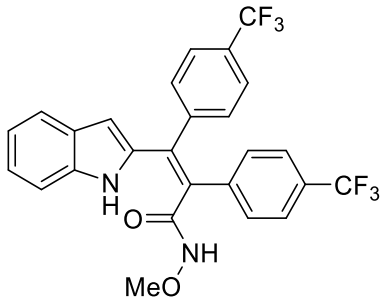
3ae: a light yellow solid. Yeild: 80% (42 mg). Mp: 198-200 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.63 (s, 1H), 10.54 (s, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.52 (d, J = 8.3 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 8.1 Hz, 1H), 7.10 (t, J = 7.5 Hz, 1H), 7.01 (q, J = 7.9 Hz, 5H), 6.78 – 6.72 (m, 1H), 3.45 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 165.9, 137.9, 137.4, 136.7, 136.6, 134.8, 133.5, 133.2, 131.8, 131.7, 127.9, 122.6, 122.0, 121.1, 120.7, 119.8, 112.1, 104.7, 62.9.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{24}H_{18}N_2O_2NaBr_2$, 546.9633, Found: 546.9634.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-bis(4-(trifluoromethyl)phenyl)acrylamide (3af)



3af

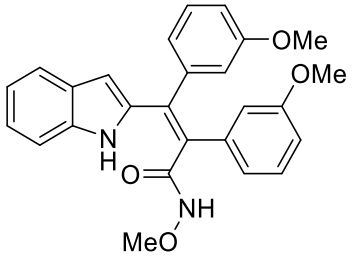
3af: a light yellow solid. Yeild: 81% (41 mg). Mp: 188-190 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.72 (s, 1H), 10.57 (s, 1H), 7.68 (d, J = 8.2 Hz, 2H), 7.62 (d, J = 8.2 Hz, 2H), 7.57 (d, J = 7.9 Hz, 1H), 7.34 – 7.27 (m, 5H), 7.11 (t, J = 7.5 Hz, 1H), 7.01 (t, J = 7.5 Hz, 1H), 6.82 – 6.76 (m, 1H), 3.47 (s, 3H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 165.6, 142.7, 141.5, 137.6, 136.2, 135.7, 134.1, 131.9, 130.5, 127.9, 127.1 (q, J = 252.0 Hz), 125.8, 125.7, 125.7, 122.8, 120.9, 119.9, 112.2, 105.1, 62.9.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{18}N_2O_2NaF_6$, 527.1170, Found: 527.1163.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-bis(3-methoxyphenyl)acrylamide (3ag)



3ag

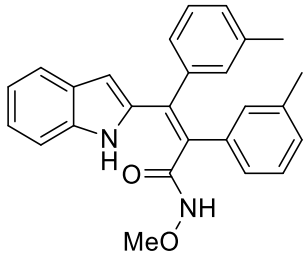
3ag: a white solid. Yeild: 89% (38 mg). Mp: 186-188 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.50 (s, 1H), 10.41 (s, 1H), 7.50 (d, J = 7.9 Hz, 1H), 7.32 (d, J = 8.1 Hz, 1H), 7.18 (t, J = 7.9 Hz, 1H), 7.12 (t, J = 7.9 Hz, 1H), 7.05 (t, J = 7.5 Hz, 1H), 6.96 (t, J = 7.4 Hz, 1H), 6.85 – 6.81 (m, 1H), 6.74 – 6.71 (m, 1H), 6.67 (d, J = 13.4 Hz, 3H), 6.62 (s, 1H), 6.58 (s, 1H), 3.57 (s, 3H), 3.53 (s, 3H), 3.43 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 165.8, 158.8, 158.7, 139.9, 138.4, 136.8, 136.5, 134.7, 133.9, 129.2, 129.1, 127.5, 122.7, 121.8, 121.2, 120.1, 119.2, 116.0, 114.5, 113.4, 113.0, 111.6, 103.8, 62.3, 54.9, 54.8.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{24}N_2O_4Na$, 451.1634, Found: 451.1634.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-di-*m*-tolylacrylamide (3ah)



3ah

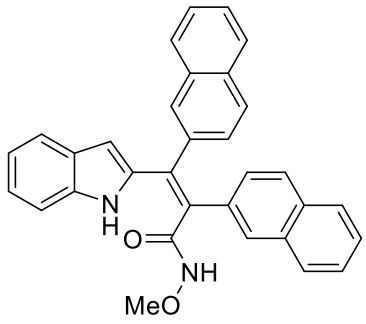
3ah: a white solid. Yeild: 88% (35 mg). Mp: 188-190 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.44 (s, 1H), 10.40 (s, 1H), 7.49 (d, J = 7.8 Hz, 1H), 7.31 (d, J = 8.1 Hz, 1H), 7.11 (t, J = 7.4 Hz, 1H), 7.04 (td, J = 9.2, 7.6, 5.1 Hz, 3H), 6.95 (d, J = 6.7 Hz, 2H), 6.88 (s, 2H), 6.84 (d, J = 7.4 Hz, 1H), 6.80 (d, J = 7.5 Hz, 1H), 6.65 (s, 1H), 3.38 (s, 3H), 2.16 (s, 3H), 2.14 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.5, 139.0, 137.5, 137.4, 137.4, 137.3, 137.2, 135.1, 134.6, 131.3, 129.9, 128.9, 128.3, 128.2, 128.1, 127.9, 126.8, 122.1, 120.5, 119.6, 112.0, 104.2, 62.7, 21.4.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{24}N_2O_2Na$, 419.1735, Found: 419.1734.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2,3-di(naphthalen-2-yl)acrylamide (3ai)



3ai

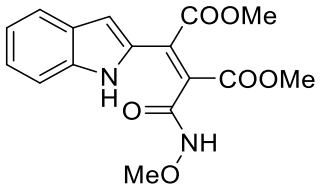
3ai: a yellow solid. Yeild: 85% (40 mg). Mp: 186-188 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.66 (s, 1H), 10.51 (s, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.75 – 7.68 (m, 6H), 7.59 (d, J = 8.6 Hz, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.47 (t, J = 7.5 Hz, 1H), 7.44 – 7.40 (m, 3H), 7.29 (d, J = 8.1 Hz, 1H), 7.21 (dd, J = 8.5, 1.4 Hz, 1H), 7.10 (dd, J = 8.6, 1.4 Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H), 6.99 (t, J = 7.4 Hz, 1H), 6.85 – 6.80 (m, 1H), 3.48 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.1, 137.0, 136.2, 135.1, 134.9, 134.2, 132.7, 132.6, 132.4, 131.8, 129.9, 128.5, 128.0, 127.8, 127.6, 127.4, 126.4, 126.3, 126.2, 121.9, 120.1, 119.2, 111.6, 104.2, 62.3.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{32}H_{24}N_2O_2Na$, 491.1735, Found: 491.1731.

Dimethyl 2-(1*H*-indol-2-yl)-3-(methoxycarbamoyl)maleate (3ak)



3ak

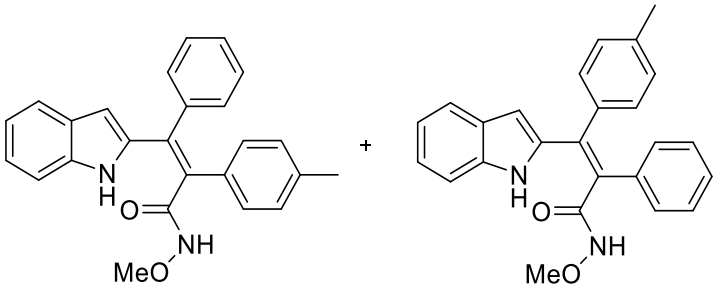
3ak: an orange solid. Yeild: 66% (22 mg). Mp: 170-172 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.79 (s, 1H), 11.04 (s, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 8.3 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 7.07 (t, J = 7.5 Hz, 1H), 6.95 (s, 1H), 3.89 (s, 3H), 3.76 (s, 3H), 3.62 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.8, 164.0, 161.5, 138.5, 129.0, 127.7, 124.9, 122.6, 121.7, 120.9, 112.9, 108.2, 63.1, 53.5, 53.2.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{16}H_{16}N_2O_6Na$, 355.0906, Found: 355.0910.

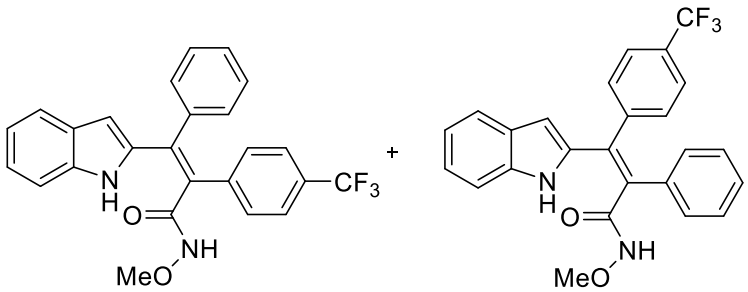
(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-3-phenyl-2-(*p*-tolyl)acrylamide (3al)
(*E*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2-phenyl-3-(*p*-tolyl)acrylamide (3al')



3al+3al' (52:48)

3al+3al': a white solid. Yeild: 92% (35 mg). Mp: 170-174ºC.
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.51 (s, 0.52H), 11.50 (s, 0.48H), 10.42 (s, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.27 – 7.16 (m, 3H), 7.10 – 7.04 (m, 4H), 6.99 (t, J = 6.5 Hz, 2H), 6.95 (t, J = 7.2 Hz, 2H), 6.69 (s, 0.52H), 6.67 (s, 0.48H), 3.42 (s, 3H), 2.27 (s, 1.56H), 2.23 (s, 1.44H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 166.1, 166.1, 138.7, 137.3, 137.0, 136.8, 136.5, 135.6, 134.6, 134.2, 134.1, 133.7, 130.5, 129.1, 129.0, 128.7, 128.6, 128.1, 127.7, 127.5, 127.1, 121.7, 120.0, 119.1, 111.6, 103.8, 103.8, 62.3, 20.8, 20.7.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{25}H_{22}N_2O_2Na$, 405.1579, Found: 405.1582.

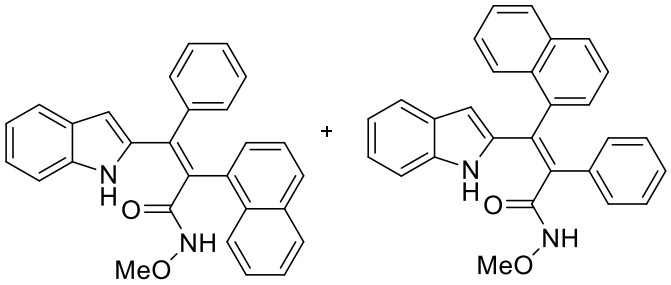
(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-3-phenyl-2-(4-(trifluoromethyl)phenyl)acrylamide (3am)
(*E*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2-phenyl-3-(4-(trifluoromethyl)phenyl)acrylamide (3am')



3am+3am' (3:2)

3am+3am': a light yellow solid. Yeild: 83% (36 mg). Mp: 184-188 ºC.
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.67 (s, 0.57H), 11.64 (s, 0.38H), 10.54 (s, 0.57H), 10.53 (s, 0.38H),7.64 (d, J = 8.0 Hz, 0.80H), 7.58 (d, J = 8.2 Hz, 1.20H), 7.55 (d, J = 8.0 Hz, 1H), 7.35 (d, J = 8.2 Hz, 0.60H), 7.33 (d, J = 8.6 Hz, 0.40H), 7.31 – 7.17 (m, 5H), 7.09 (t, J = 5.7 Hz, 3H), 7.00 (t, J = 7.4 Hz, 1H), 6.76 (s, 0.40H), 6.74 (s, 0.60H), 3.46 (s, 3H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 165.6, 165.5, 142.9, 141.6, 137.9, 137.0, 136.9, 136.6, 136.4, 136.1, 135.3, 133.5, 132.5, 131.4, 130.5, 129.9, 129.1, 128.2, 127.6, 127.4, 125.0, 124.1 (q, J = 272.8 Hz), 124.0 (q, J = 271.7 Hz), 122.1, 122.0, 120.2, 119.3, 111.7, 111.6, 104.3, 104.1, 62.4.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{25}H_{19}N_2O_2NaF_3$, 459.1296, Found: 459.1293.

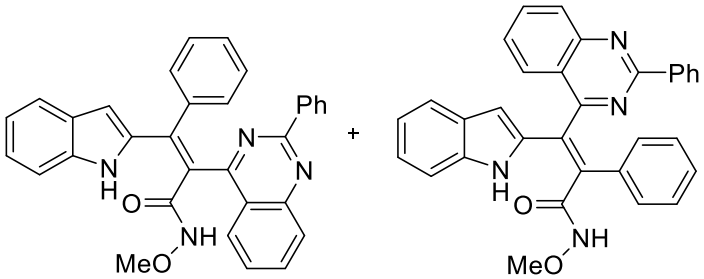
(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2-(naphthalen-1-yl)-3-phenylacrylamide (3an)
(*E*)-3-(1*H*-indol-2-yl)-*N*-methoxy-3-(naphthalen-1-yl)-2-phenylacrylamide (3an')



3an+3an' (11:1)

3an+3an': a yellow solid. Yeild: 81% (34 mg). Mp: 182-186 ºC.
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.73 (s, 0.88H), 11.53 (s, 0.08H), 10.64 (s, 0.08H), 10.25 (s, 0.88H), 8.16 (d, J = 8.2 Hz, 0.08H), 7.91 (d, J = 8.4 Hz, 0.88H), 7.88 (d, J = 8.2 Hz, 0.99H), 7.84 (d, J = 8.2 Hz, 0.88H), 7.81 (d, J = 8.0 Hz, 0.09H), 7.76 (d, J = 8.2 Hz, 0.08H), 7.55 (d, J = 7.7 Hz, 0.08H), 7.49 (d, J = 7.8 Hz, 0.88H), 7.45 – 7.31 (m, 4H), 7.21 (d, J = 8.0 Hz, 0.88H), 7.18 (d, J = 7.9 Hz, 0.08H), 7.00 – 6.91 (m, 7H), 6.77 (s, 0.08H), 6.75 (s, 0.88H), 3.52 (s, 2.75H), 3.34 (s, 0.25H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 166.35, 137.5, 137.5, 137.1, 136.1, 133.6, 132.3, 129.0, 128.7, 128.4, 128.2, 127.6, 126.7, 126.2, 125.9, 125.7, 122.2, 120.5, 119.7, 112.1, 103.2, 62.9.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{28}H_{22}N_2O_2Na$, 441.1579, Found: 441.1581.

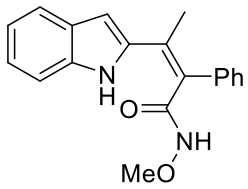
(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-3-phenyl-2-(2-phenylquinazolin-4-yl)acrylamide (3ao)
(*E*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2-phenyl-3-(2-phenylquinazolin-4-yl)acrylamide (3ao')



3ao+3ao' (2:1)

3ao+3ao': a yellow solid. Yeild: 70% (35 mg). Mp: 198-202 ºC.
^{1}H NMR (500 MHz, DMSO-d_6) δ 12.05 (s, 0.64H), 11.75 (s, 0.32H), 10.95 (s, 0.33H), 10.56 (s, 0.66H), 8.57 – 8.53 (m, 0.67H), 8.49 – 8.45 (m, 1.34H), 8.15 (d, J = 8.3 Hz, 0.66H), 8.06 (d, J = 8.2 Hz, 0.33H), 8.01 (d, J = 8.4 Hz, 0.66H), 7.94 (d, J = 8.4 Hz, 0.33H), 7.89 (t, J = 7.6 Hz, 0.68H), 7.85 (t, J = 7.6 Hz, 0.34H), 7.62 – 7.52 (m, 5H), 7.24 – 7.14 (m, 1H), 7.13– 6.97 (m, 7H), 6.95 (s, 0.66H), 6.88 (s, 0.33H), 3.68 (s, 2H), 3.47 (s, 1H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 166.9, 166.7, 165.0, 164.3, 159.1, 158.8, 150.7, 140.8, 138.1, 137.5, 137.3, 136.8, 136.7, 136.3, 135.6, 134.5, 134.4, 134.3, 130.8, 130.7, 130.0, 129.9, 129.6, 128.6, 128.3, 128.1, 128.0, 127.9, 127.8, 127.6, 127.5, 127.3, 126.5, 126.4, 122.4, 122.3, 121.5, 120.5, 120.4, 119.5, 119.5, 111.9, 111.5, 105.4, 103.4, 62.6, 62.3.
HRMS (ESI-TOF, [M + Na]$^+$): For $C_{32}H_{24}N_4O_2Na$, 519.1797, Found: 519.1796.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-3-methyl-2-phenylacrylamide (3ap)



3ap

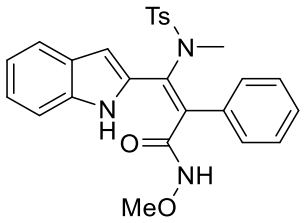
3ap: a white solid. Yeild: 82% (25 mg). Mp: 204-206 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.26 (s, 1H), 11.00 (s, 1H), 7.50 (d, J = 7.8 Hz, 1H), 7.44 (t, J = 7.5 Hz, 2H), 7.39 (d, J = 8.1 Hz, 1H), 7.36 (d, J = 7.5 Hz, 3H), 7.09 (t, J = 7.5 Hz, 1H), 6.98 (t, J = 7.4 Hz, 1H), 6.65 (s, 1H), 3.42 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 166.1, 137.2, 137.1, 136.3, 133.2, 129.1, 128.6, 128.3, 127.7, 127.5, 121.6, 120.0, 119.2, 111.2, 101.7, 62.2, 18.7.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{19}H_{18}N_2O_2Na$, 329.1266, Found: 329.1269.

(*E*)-3-(1*H*-indol-2-yl)-*N*-methoxy-3-((*N*,4-dimethylphenyl)sulfonamido)-2-phenylacrylamide (3aq)



3aq

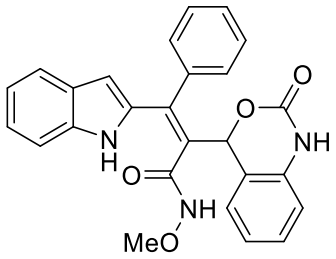
3aq: a white solid. Yeild: 67% (32 mg). Mp: 222-224 ºC.

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.36 (s, 1H), 10.53 (s, 1H), 7.46 (d, J = 7.9 Hz, 1H), 7.36 (dd, J = 12.8, 5.5 Hz, 5H), 7.18 (d, J = 8.1 Hz, 1H), 7.08 (t, J = 6.9 Hz, 3H), 6.99 (dd, J = 14.7, 7.6 Hz, 3H), 6.46 (s, 1H), 3.25 (s, 3H), 2.79 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 163.9, 143.0, 136.4, 135.6, 134.8, 133.9, 133.2, 132.7, 128.9, 128.4, 128.3, 127.8, 127.0, 126.9, 122.1, 120.2, 119.2, 111.6, 104.8, 62.3, 37.4, 20.9.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{25}N_3O_4NaS$, 498.1463, Found: 498.1465.

(*Z*)-3-(1*H*-indol-2-yl)-*N*-methoxy-2-(2-oxo-1,4-dihydro-2*H*-benzo[*d*][1,3]oxazin-4-yl)-3-phenylacrylamide (3ar)



3ar

3ar: a white solid. Yeild: 73% (32 mg). Mp: 228-230 ºC.

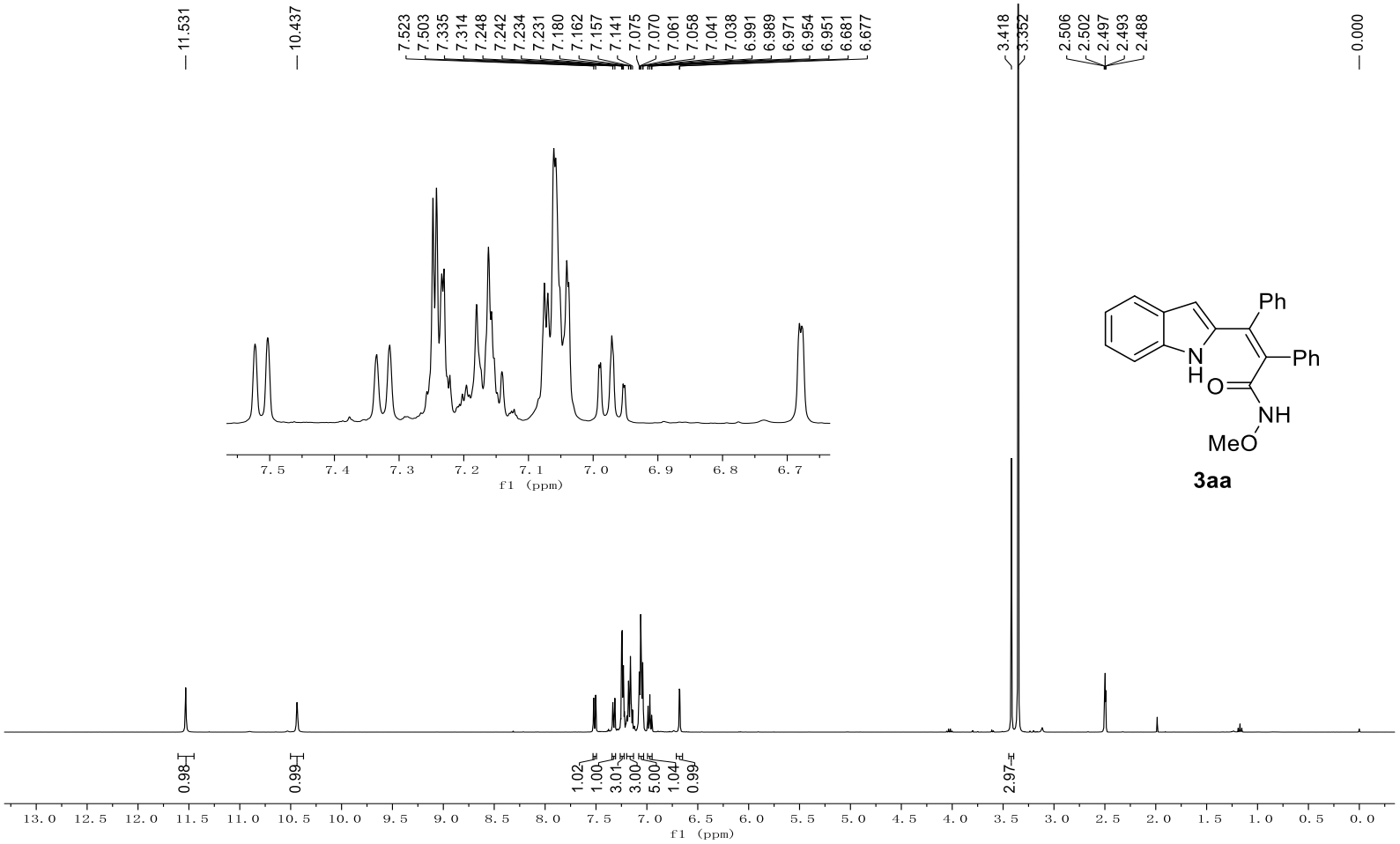
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.52 (s, 1H), 10.62 (s, 1H), 10.22 (s, 1H), 7.46 (dt, J = 18.8,

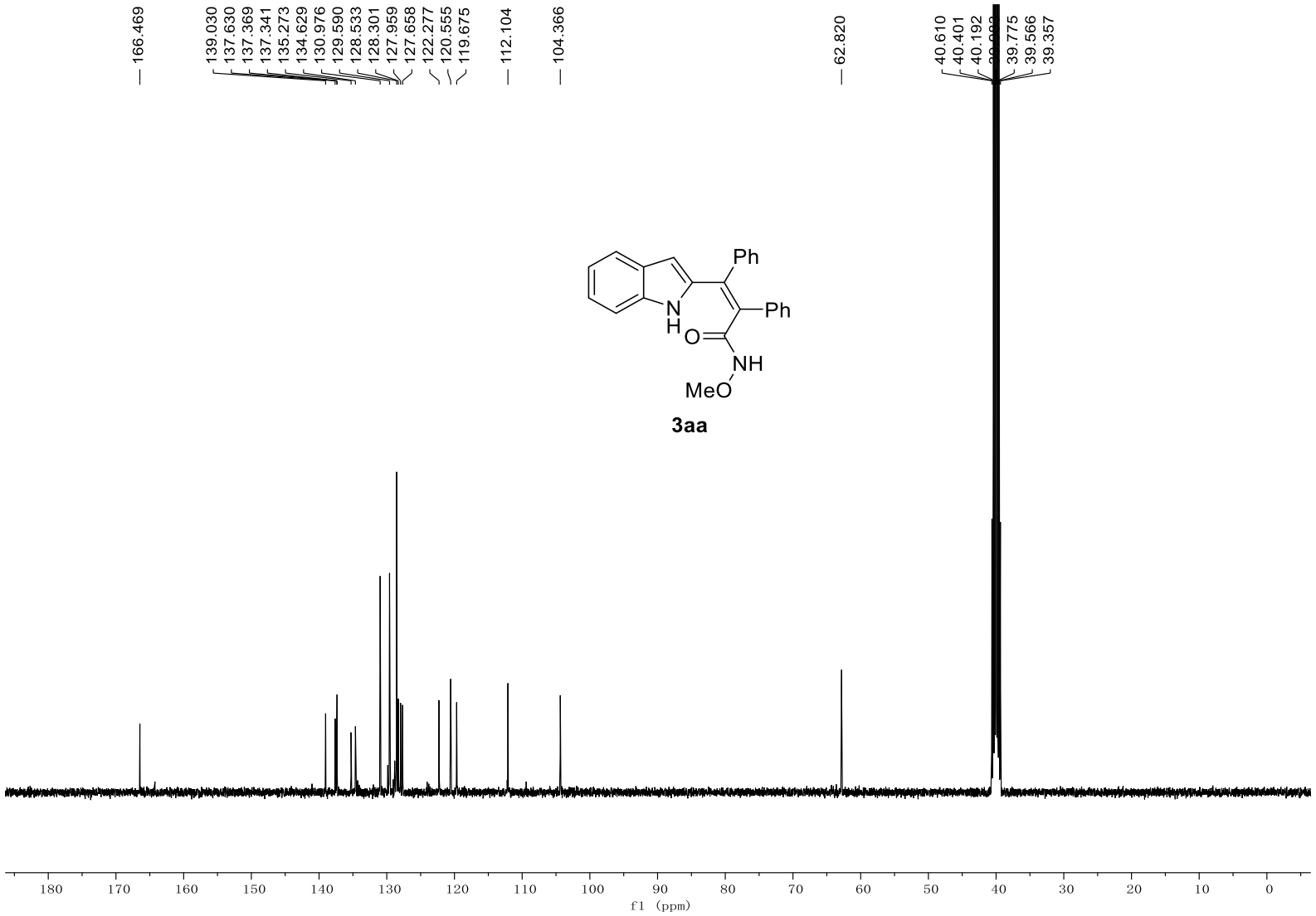
7.5 Hz, 6H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.35 (d, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.03 (dt, *J* = 10.2, 7.6 Hz, 2H), 6.94 (t, *J* = 7.4 Hz, 1H), 6.82 (d, *J* = 7.9 Hz, 1H), 6.43 (s, 1H), 6.14 (s, 1H), 3.23 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 164.1, 150.2, 141.2, 136.5, 136.3, 134.9, 131.8, 129.3, 128.8, 128.7, 127.8, 127.2, 125.0, 122.5, 121.6, 119.9, 119.1, 118.8, 113.8, 111.8, 103.9, 76.8, 62.5.

HRMS (ESI-TOF, [M + Na]$^+$): For $C_{26}H_{21}N_3O_4Na$, 462.1430, Found: 462.1436.

NMR spectra for products

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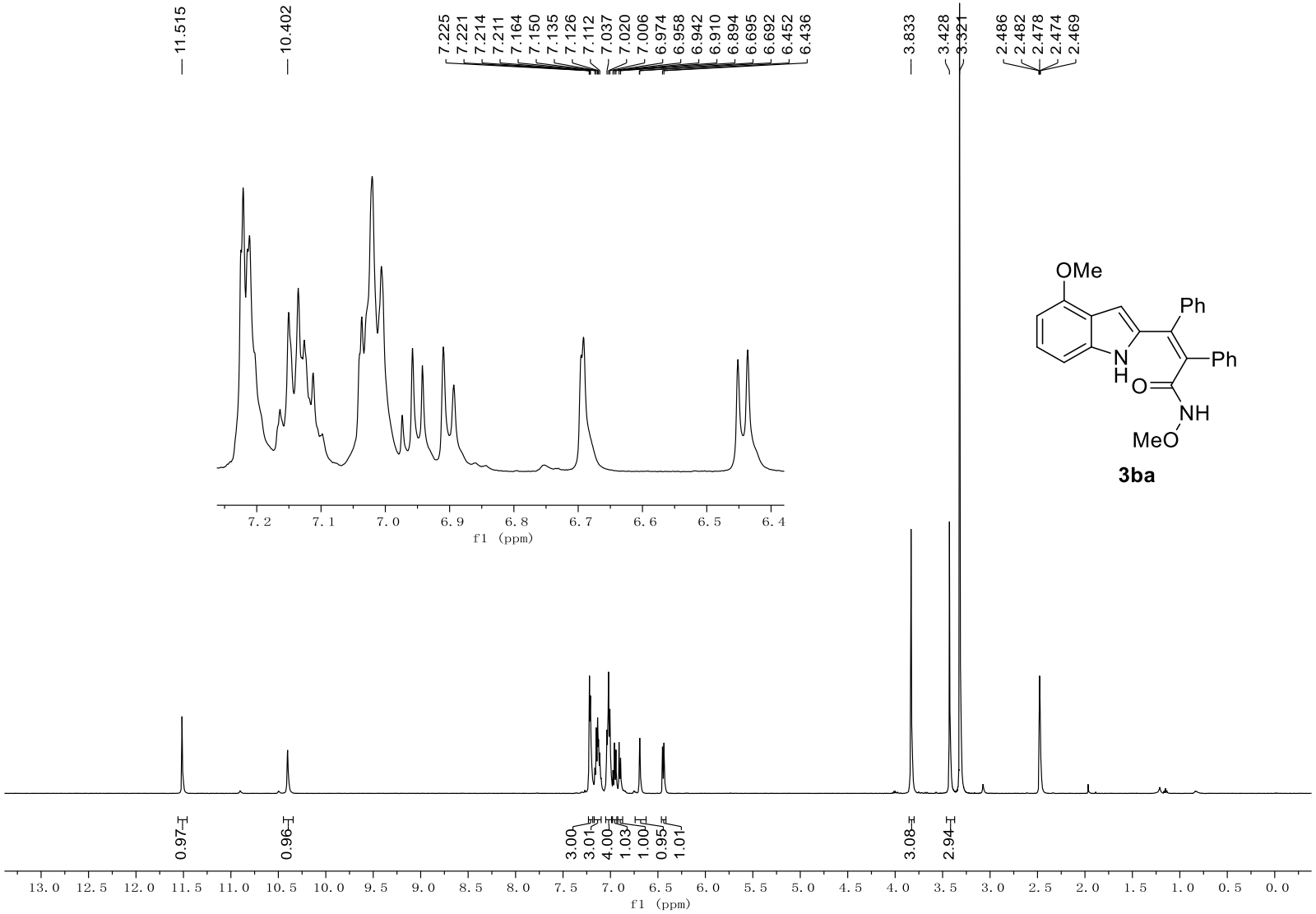
137.369
137.341
135.273
134.629
130.976
129.590
128.533
128.301
127.959
127.658
122.277
120.555
119.675
112.104
104.366
62.820
40.610
40.401
40.192
39.775
39.566
39.357
Ph
Ph
N
H
O
NH
MeO
3aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.221
7.214
7.211
7.164
7.150
7.135
7.126
7.112
7.037
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7.006
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6.894
6.695
6.692
6.452
6.436
3.833
3.428
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2.482
2.478
2.474
2.469
OMe
Ph
Ph
N
H
O
NH
MeO
3ba
f1 (ppm)
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0.96
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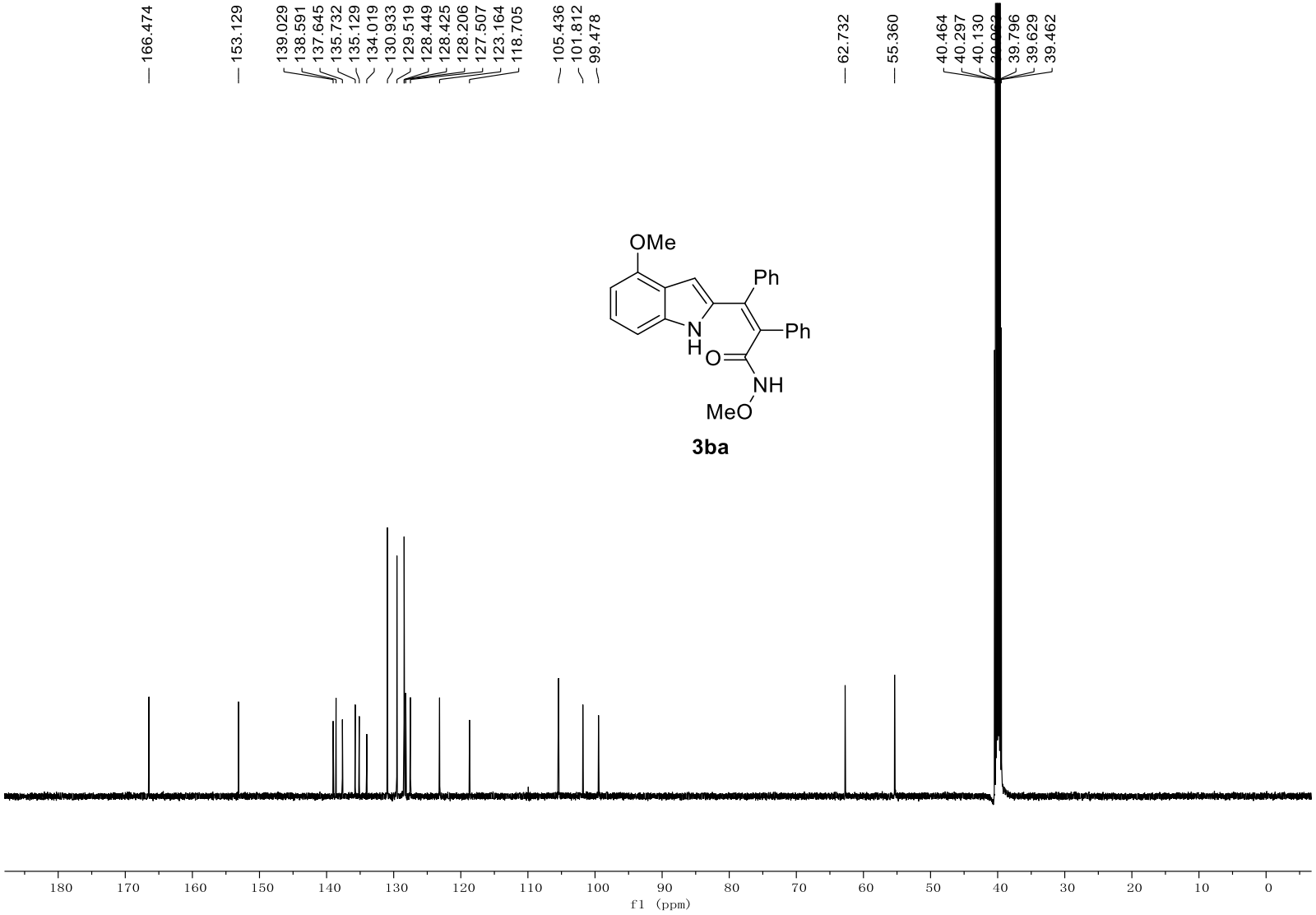
3.01
4.00
1.03
1.00
0.95
1.01
3.08
2.94
f1 (ppm)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127.507
123.164
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62.732
55.360
40.464
40.297
40.130
39.796
39.629
39.462
OMe
Ph
Ph
N
H
O
NH
MeO
3ba
180
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160
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130
120
110
100
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80
70
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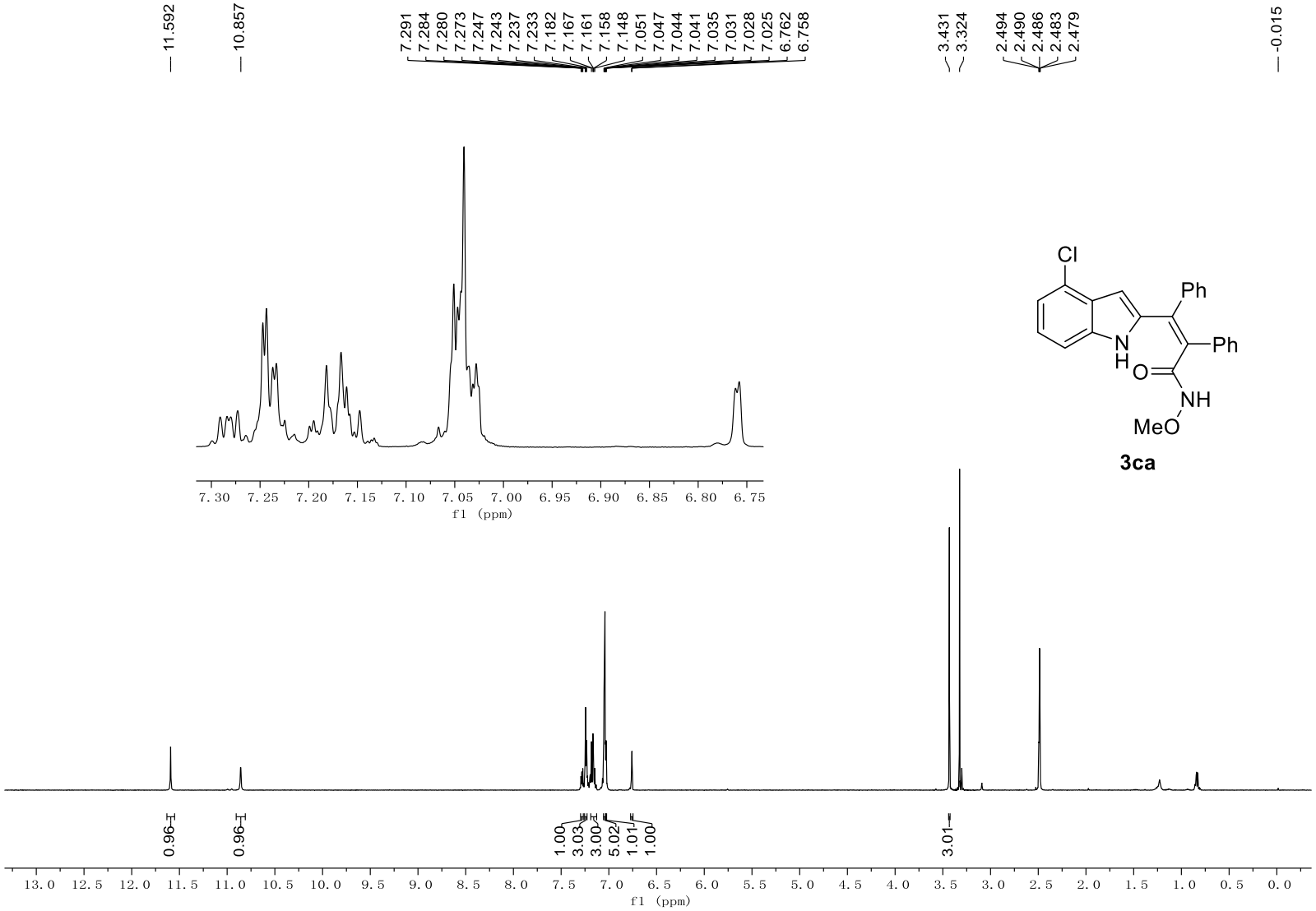
50
40
30
20
10
0
f1 (ppm)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7.044
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7.035
7.031
7.028
7.025
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6.758
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3.324
2.494
2.490
2.486
2.483
2.479
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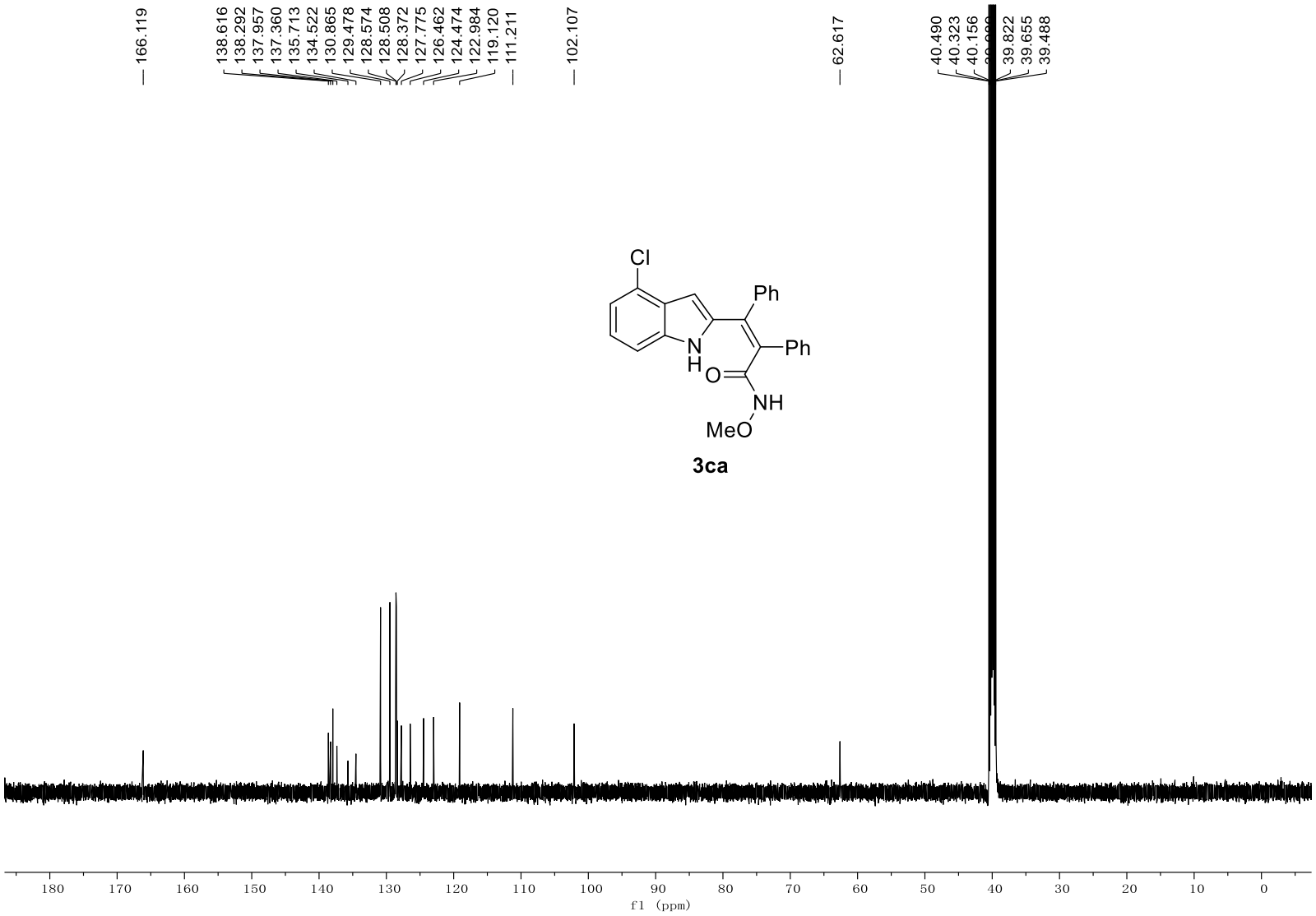
Cl
Ph
Ph
N
H
O
NH
MeO
3ca
7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75
f1 (ppm)
0.96
0.96
1.00
3.03
3.00
5.02
1.01
1.00
3.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.360
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127.775
126.462
124.474
122.984
119.120
111.211
102.107
62.617
40.490
40.323
40.156
39.822
39.655
39.488
Cl
Ph
Ph
N
H
O
NH
MeO
3ca
180
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160
150
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130
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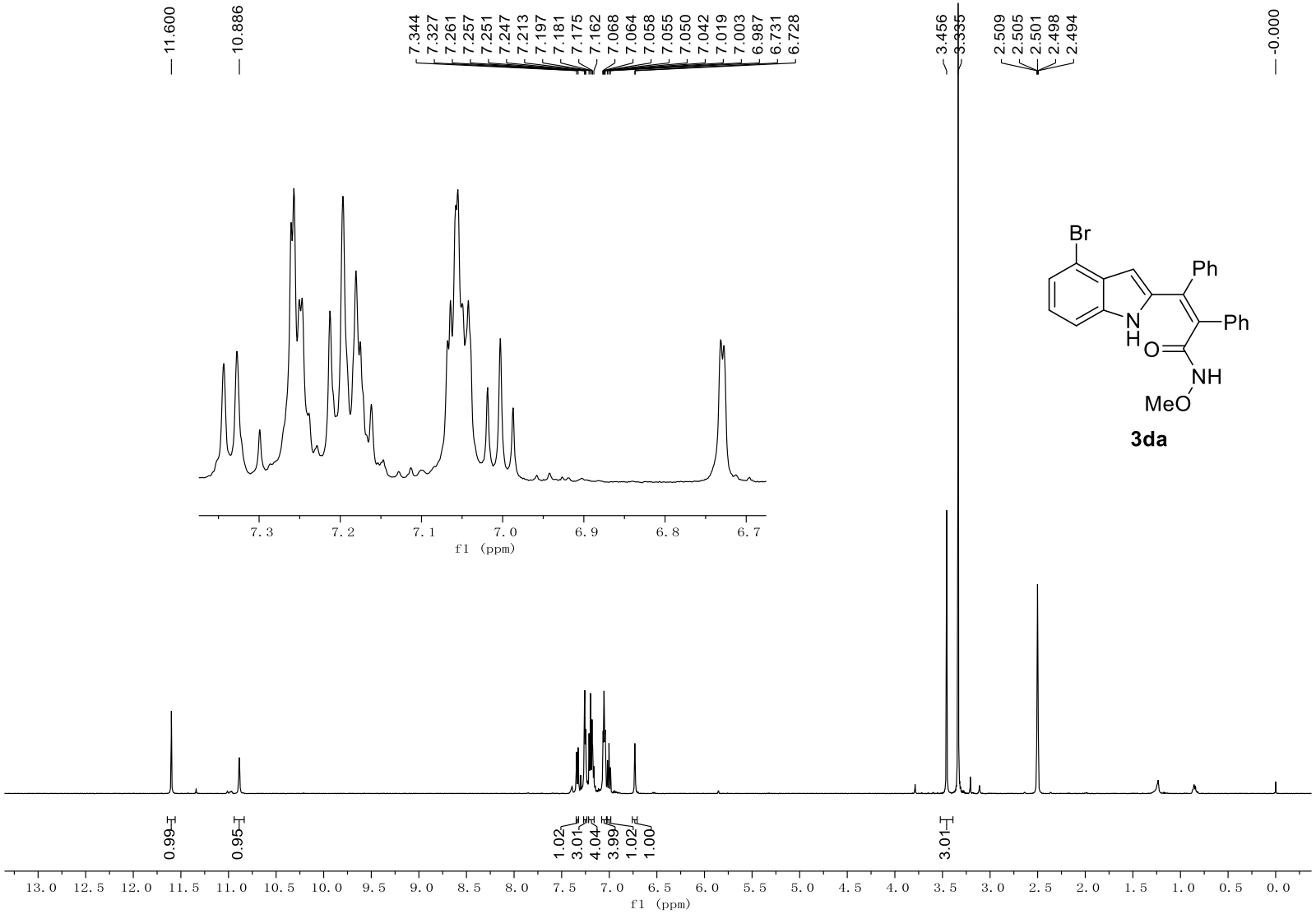
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.197
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7.068
7.064
7.058
7.055
7.050
7.042
7.019
7.003
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6.731
6.728
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3.335
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2.505
2.501
2.498
2.494
-0.000
Br
Ph
Ph
N
H
O
NH
MeO
3da
f1 (ppm)
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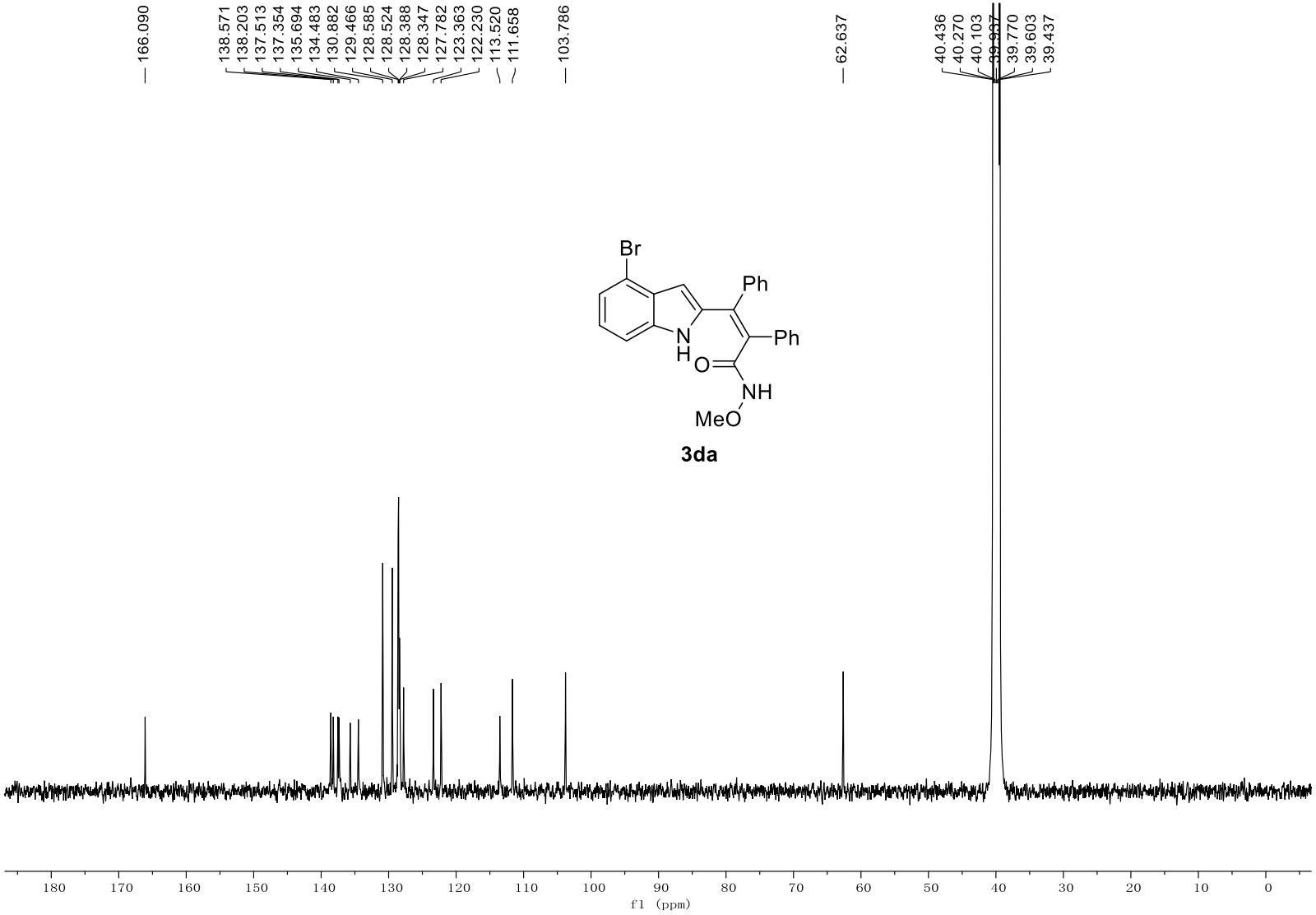
0.95
1.02
3.01
4.04
3.99
1.02
1.00
3.01
f1 (ppm)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128.388
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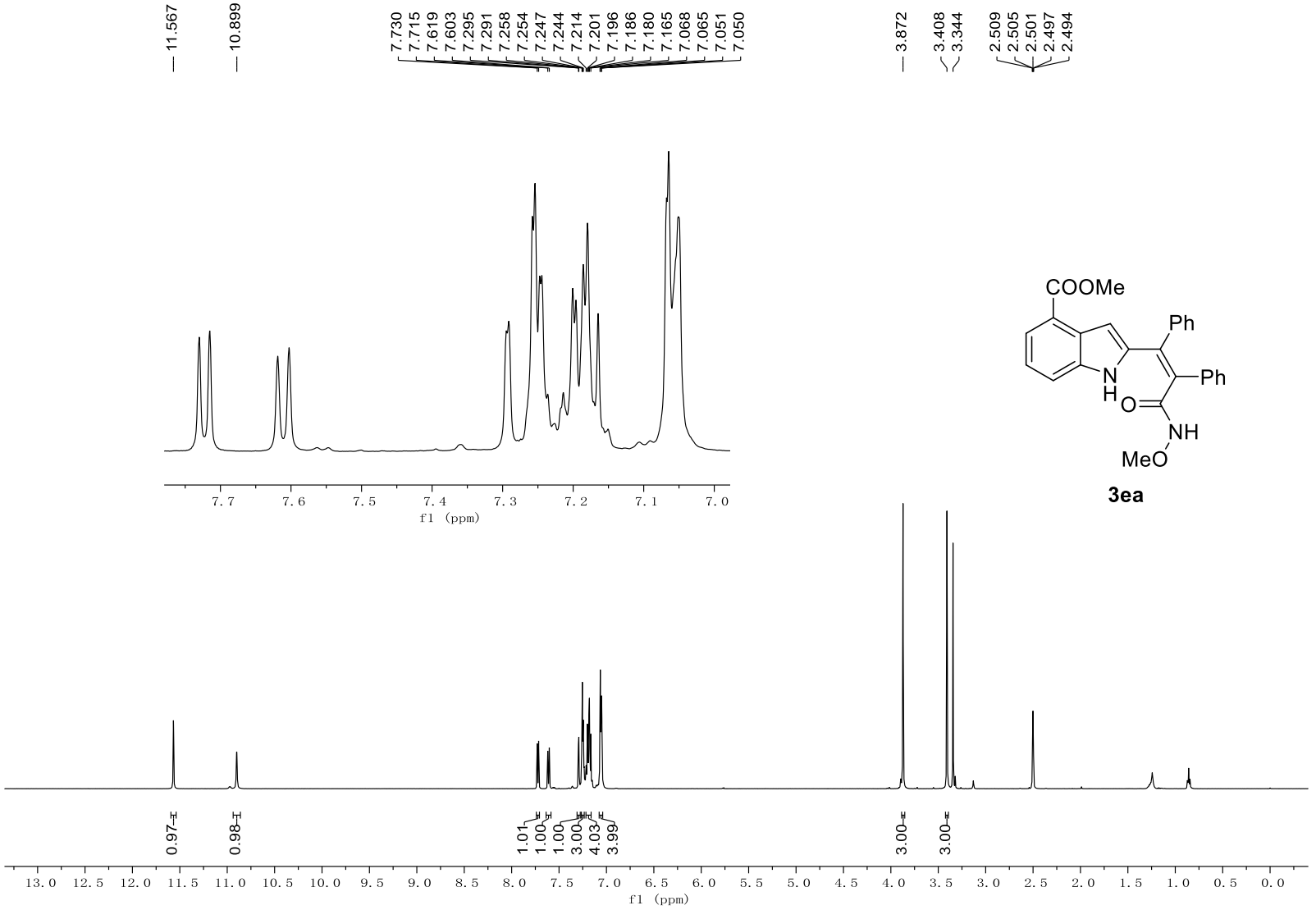
127.782
123.363
122.230
113.520
111.658
103.786
62.637
40.436
40.270
40.103
39.937
39.770
39.603
39.437
Br
Ph
Ph
N
H
O
NH
MeO
3da
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.603
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7.291
7.258
7.254
7.247
7.244
7.214
7.201
7.196
7.186
7.180
7.165
7.068
7.065
7.051
7.050
3.872
3.408
3.344
2.509
2.505
2.501
2.497
2.494
COOMe
Ph
Ph
N
H
O
NH
MeO
3ea
f1 (ppm)
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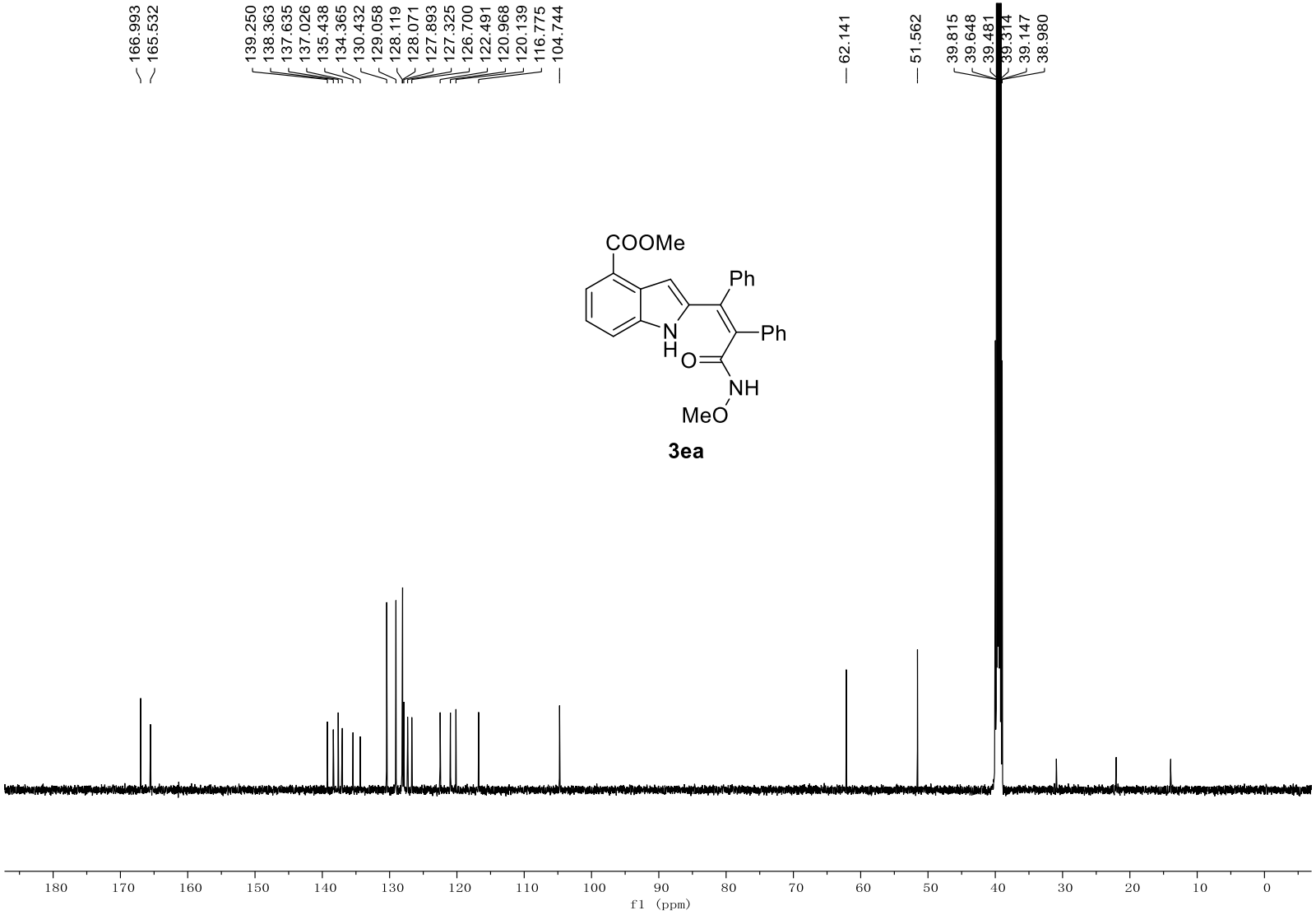
0.98
1.01
1.00
1.00
3.00
4.03
3.99
3.00
3.00
f1 (ppm)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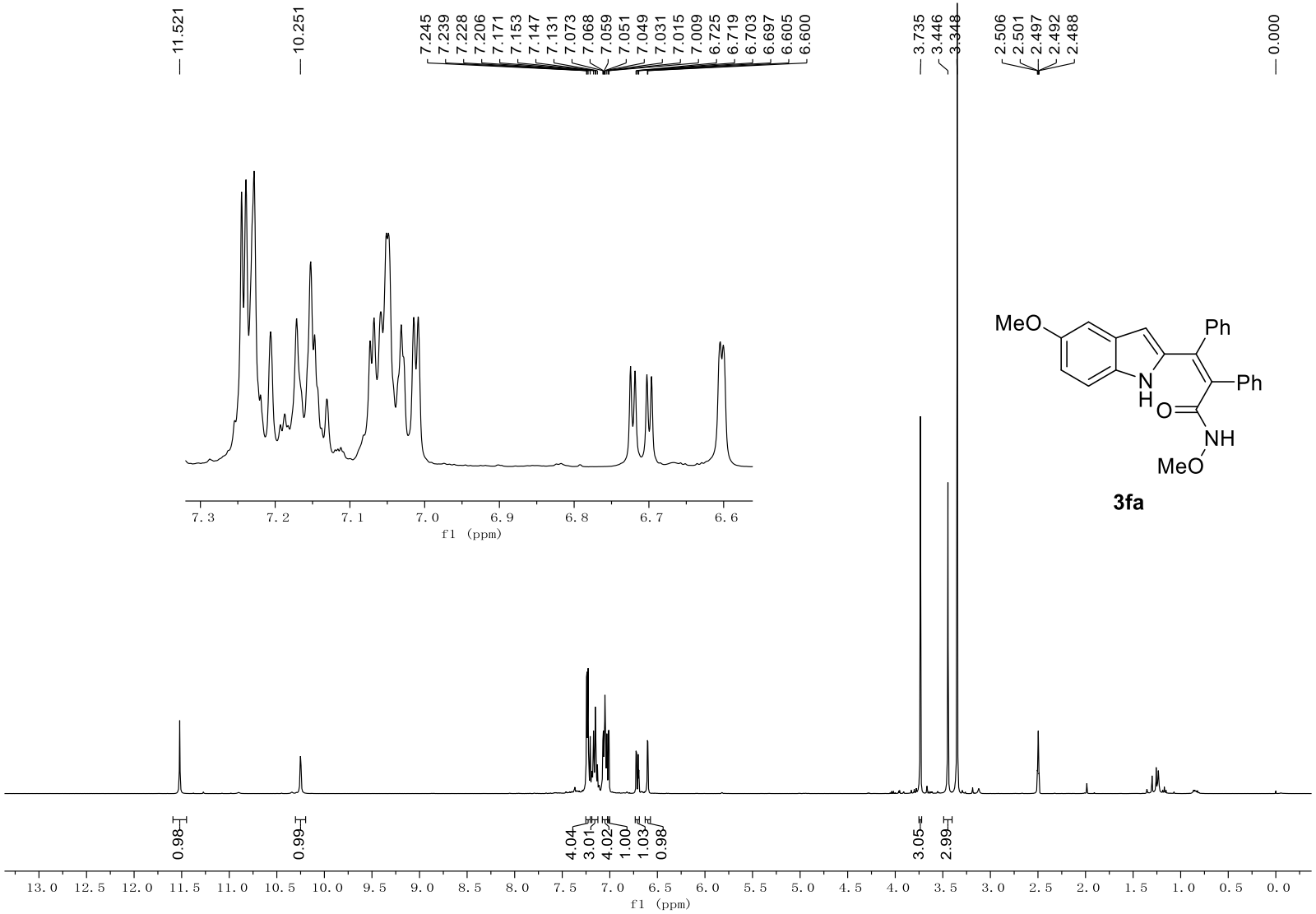
135.438
134.365
130.432
129.058
128.119
128.071
127.893
127.325
126.700
122.491
120.968
120.139
116.775
104.744
62.141
51.562
39.815
39.648
39.481
39.314
39.147
38.980
COOMe
Ph
Ph
N
H
O
NH
MeO
3ea
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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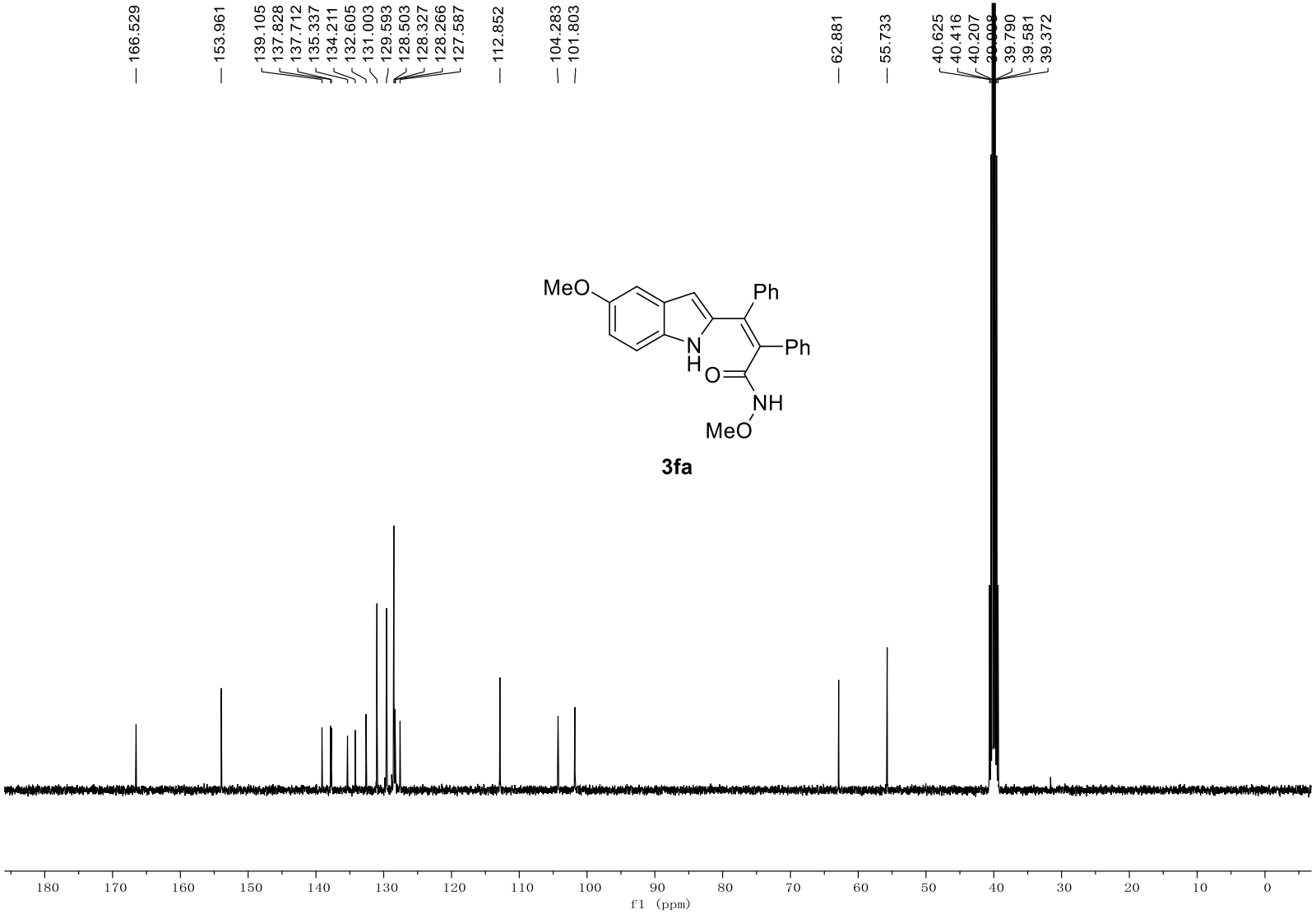
7.171
7.153
7.147
7.131
7.073
7.068
7.059
7.051
7.049
7.031
7.015
7.009
6.725
6.719
6.703
6.697
6.605
6.600
3.735
3.446
3.348
2.506
2.501
2.497
2.492
2.488
0.000
MeO
Ph
Ph
N
H
O
NH
MeO
3fa
f1 (ppm)
0.98
0.99
4.04
3.01
4.02
1.00
1.03
0.98
3.05
2.99
f1 (ppm)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139.105
137.828
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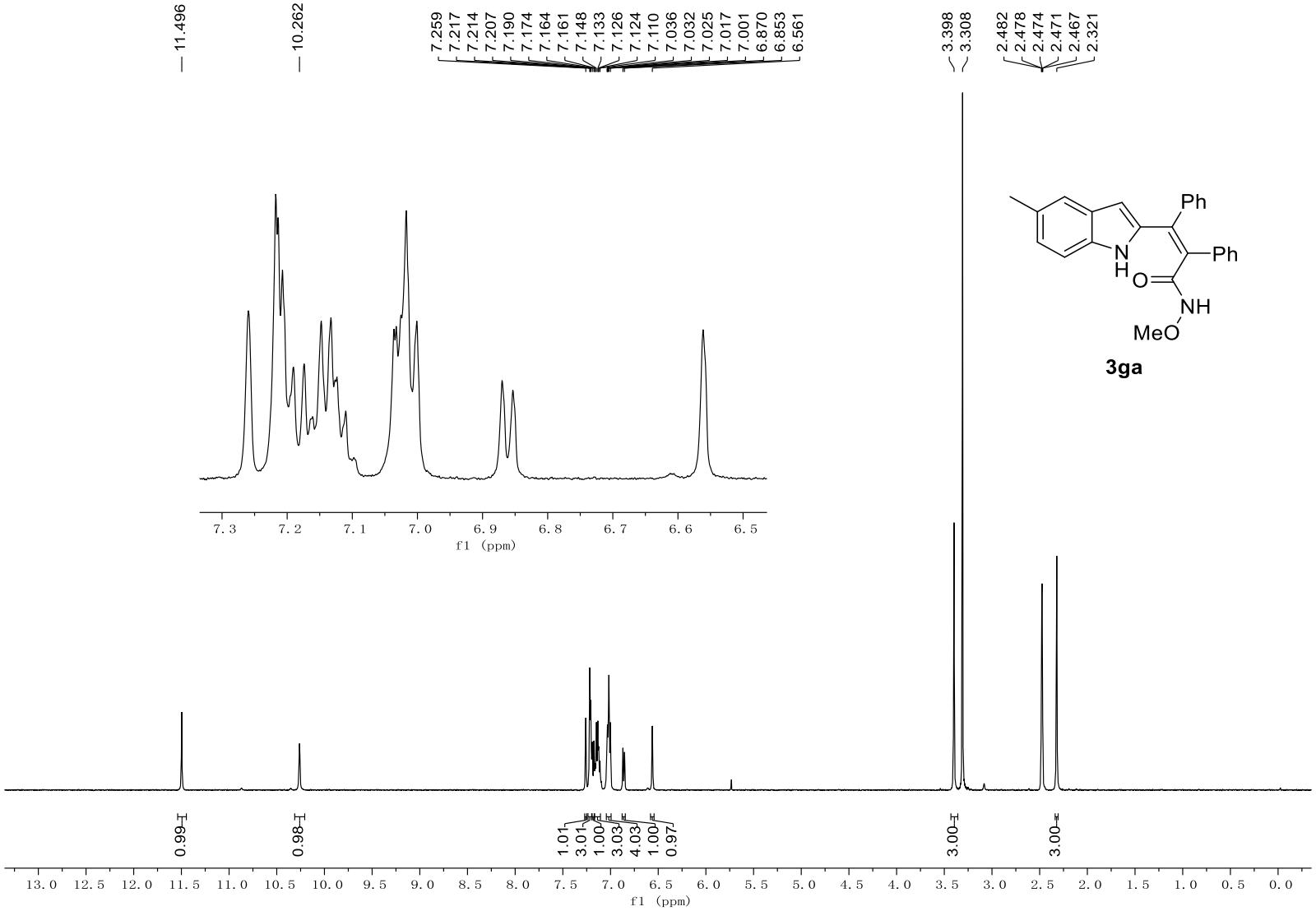
135.337
134.211
132.605
131.003
129.593
128.503
128.327
128.266
127.587
112.852
104.283
101.803
62.881
55.733
40.625
40.416
40.207
39.790
39.581
39.372
MeO
Ph
Ph
N
H
O
NH
MeO
3fa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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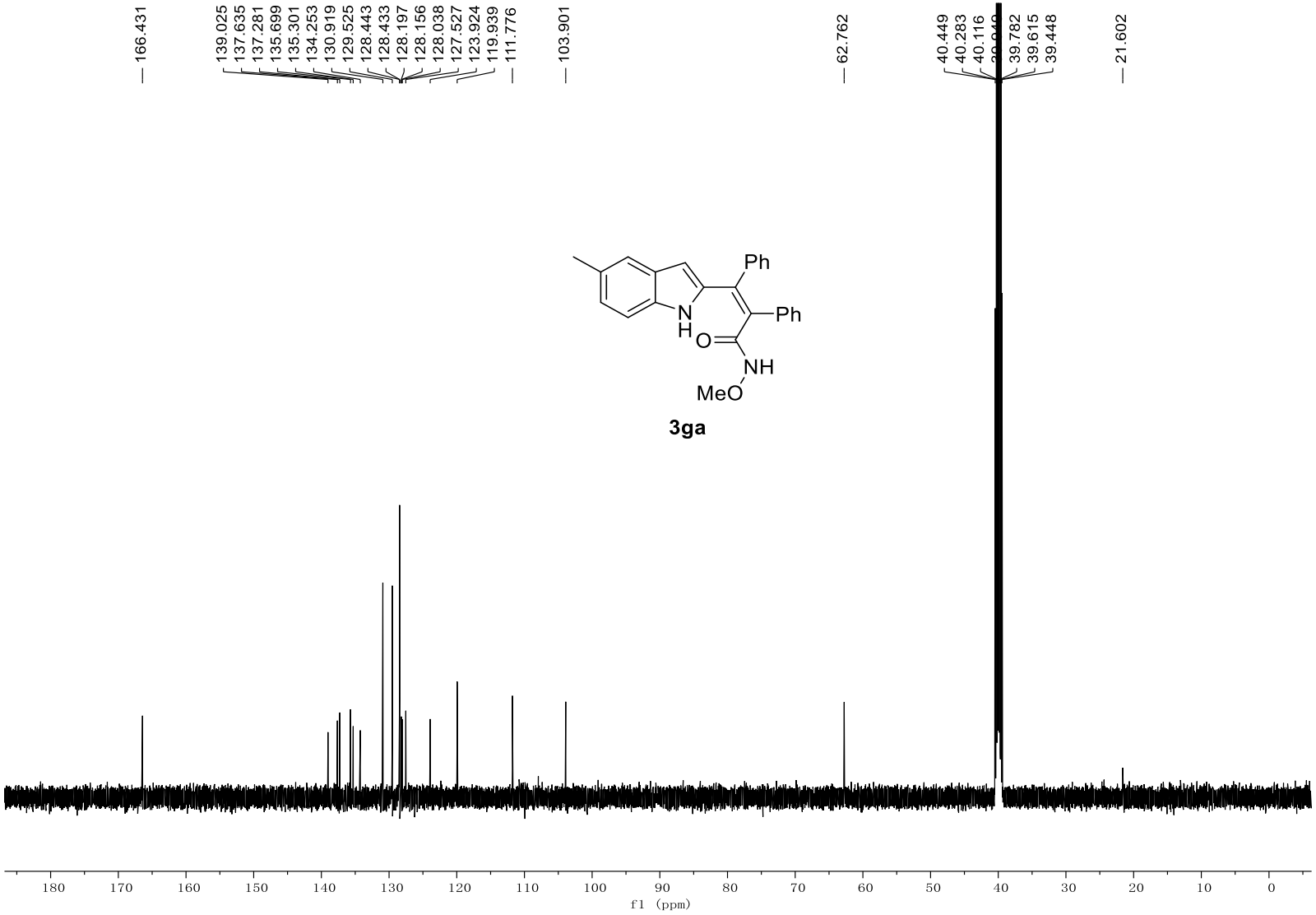
10.262
7.259
7.217
7.214
7.207
7.190
7.174
7.164
7.161
7.148
7.133
7.126
7.124
7.110
7.036
7.032
7.025
7.017
7.001
6.870
6.853
6.561
3.398
3.308
2.482
2.478
2.474
2.471
2.467
2.321
Ph
Ph
N
H
O
NH
MeO
3ga
f1 (ppm)
0.99
0.98
1.01
3.01
1.00
3.03
4.03
1.00
0.97
3.00
3.00
f1 (ppm)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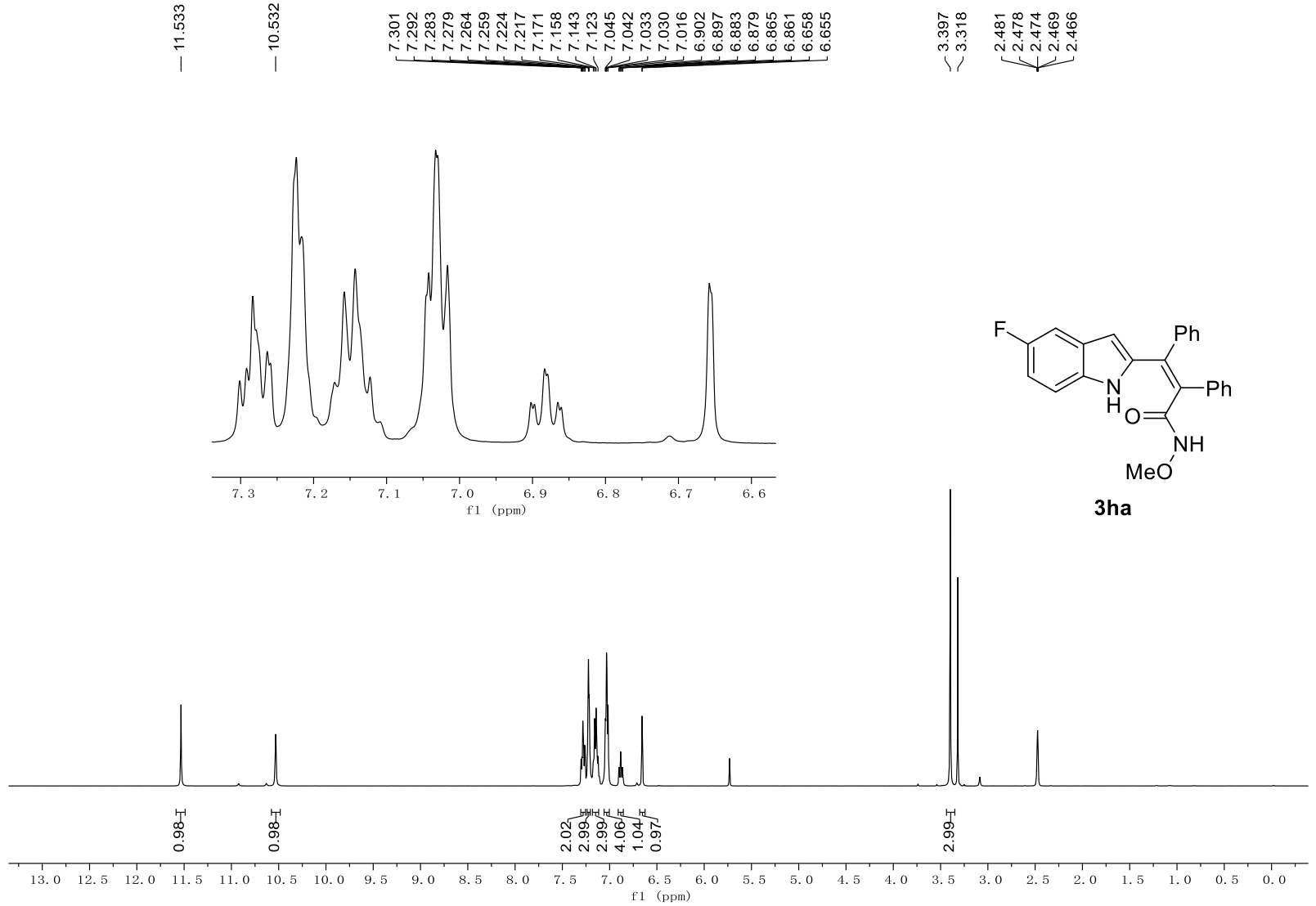
135.301
134.253
130.919
129.525
128.443
128.433
128.197
128.156
128.038
127.527
123.924
119.939
111.776
103.901
62.762
40.449
40.283
40.116
39.782
39.615
39.448
21.602
Ph
Ph
N
H
O
NH
MeO
3ga
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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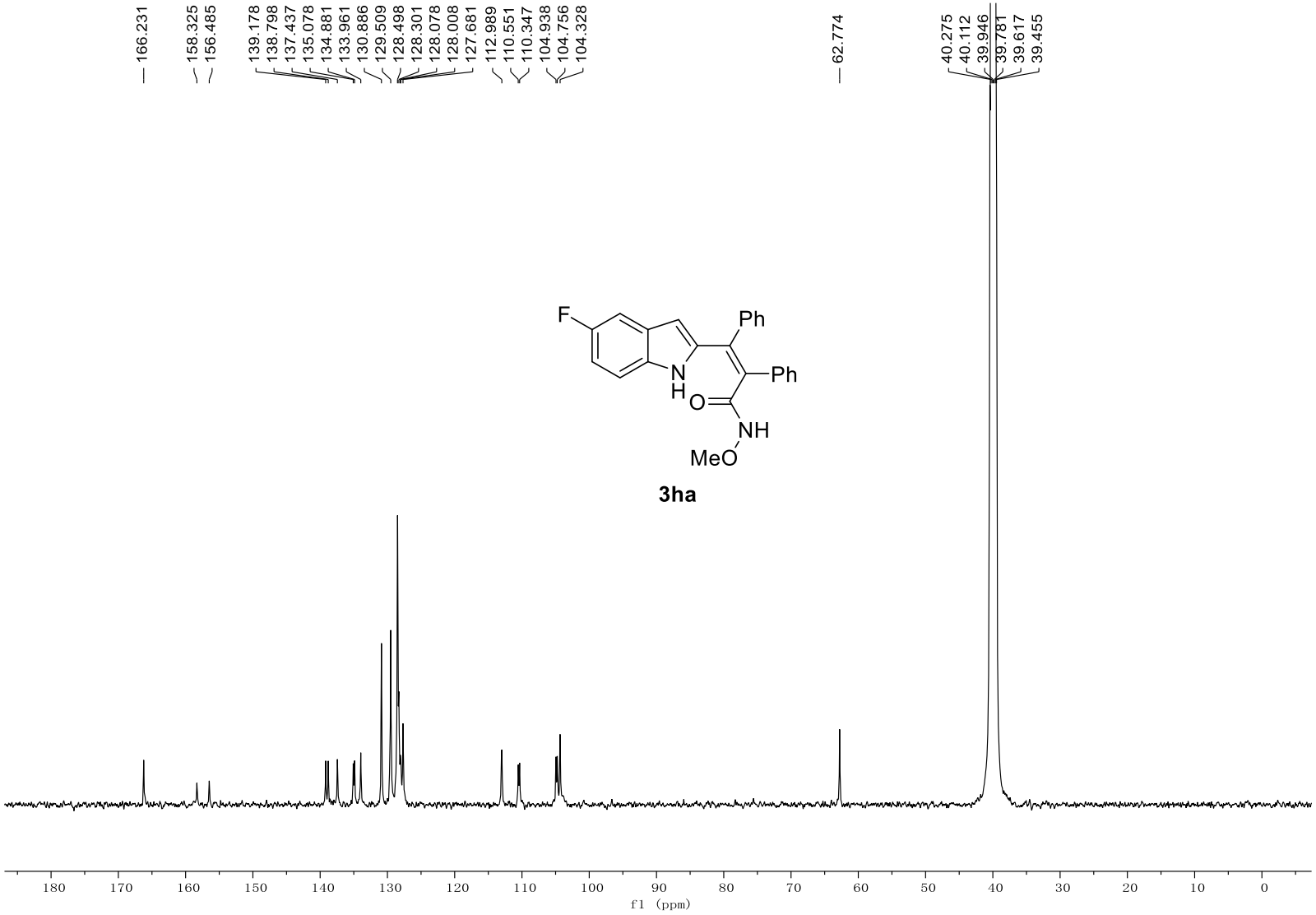
10.532
7.301
7.292
7.283
7.279
7.264
7.259
7.224
7.217
7.171
7.158
7.143
7.123
7.045
7.042
7.033
7.030
7.016
6.902
6.897
6.883
6.879
6.865
6.861
6.658
6.655
3.397
3.318
2.481
2.478
2.474
2.469
2.466
F
Ph
Ph
N
H
O
NH
MeO
3ha
f1 (ppm)
0.98
0.98
2.02
2.99
2.99
4.06
1.04
0.97
2.99
f1 (ppm)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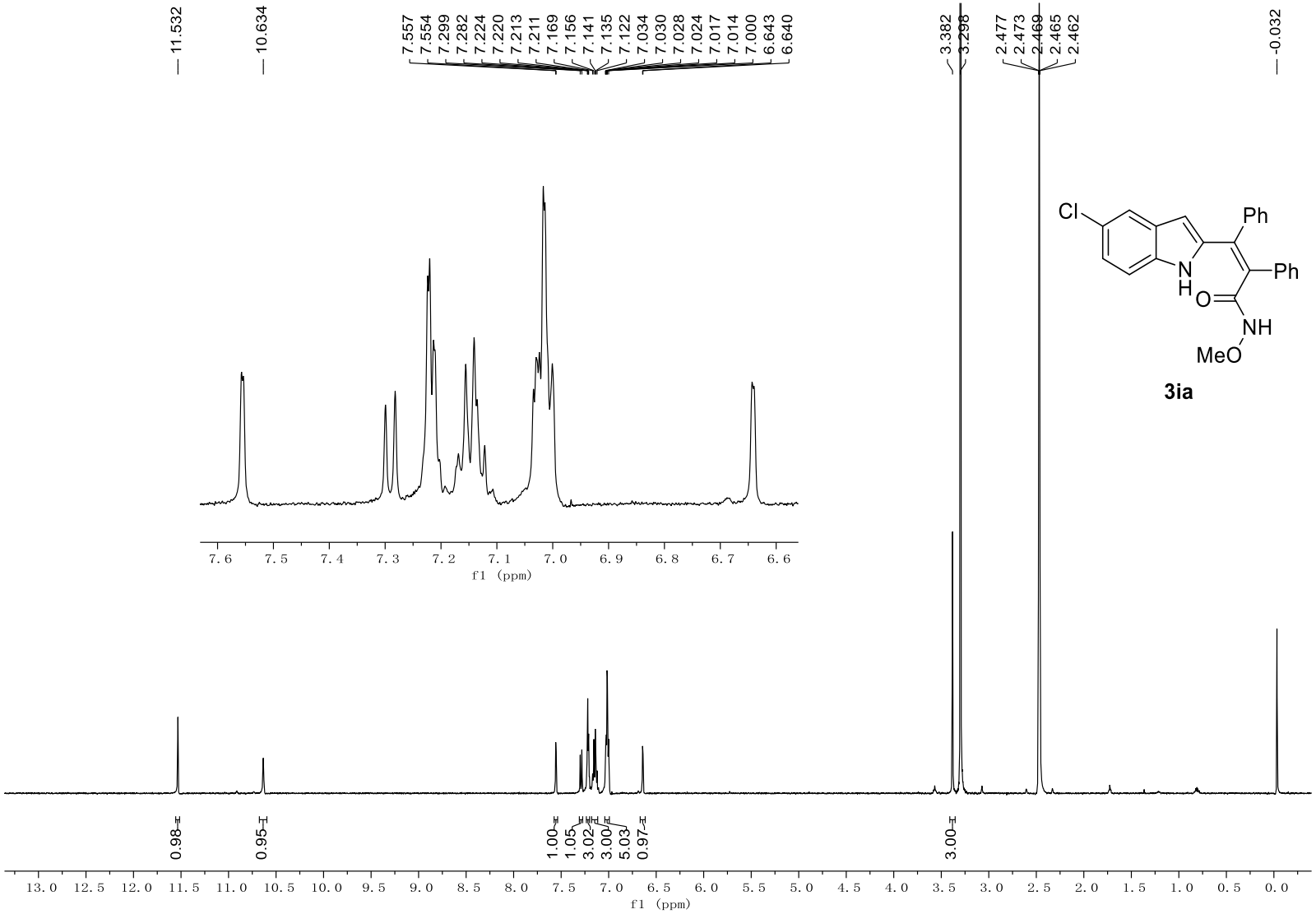
158.325
156.485
139.178
138.798
137.437
135.078
134.881
133.961
130.886
129.509
128.498
128.301
128.078
128.008
127.681
112.989
110.551
110.347
104.938
104.756
104.328
62.774
40.275
40.112
39.946
39.781
39.617
39.455
F
Ph
Ph
N
H
O
NH
MeO
3ha
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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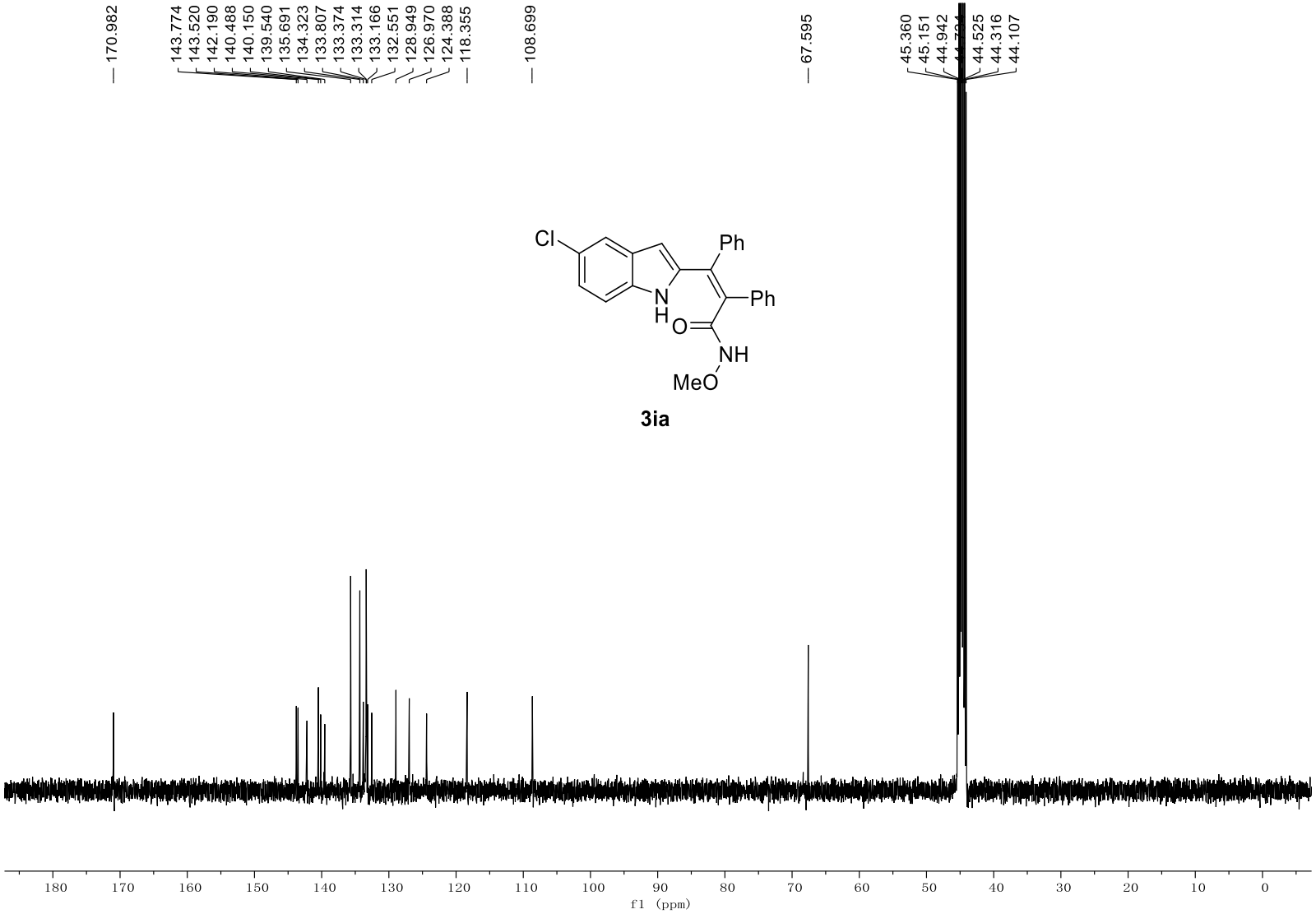
7.554
7.299
7.282
7.224
7.220
7.213
7.211
7.169
7.156
7.141
7.135
7.122
7.034
7.030
7.028
7.024
7.017
7.014
7.000
6.643
6.640
3.382
3.296
2.477
2.473
2.469
2.465
2.462
-0.032
Cl
Ph
Ph
N
H
O
NH
MeO
3ia
0.98
0.95
1.00
1.05
3.02
3.00
5.03
0.97
3.00
f1 (ppm)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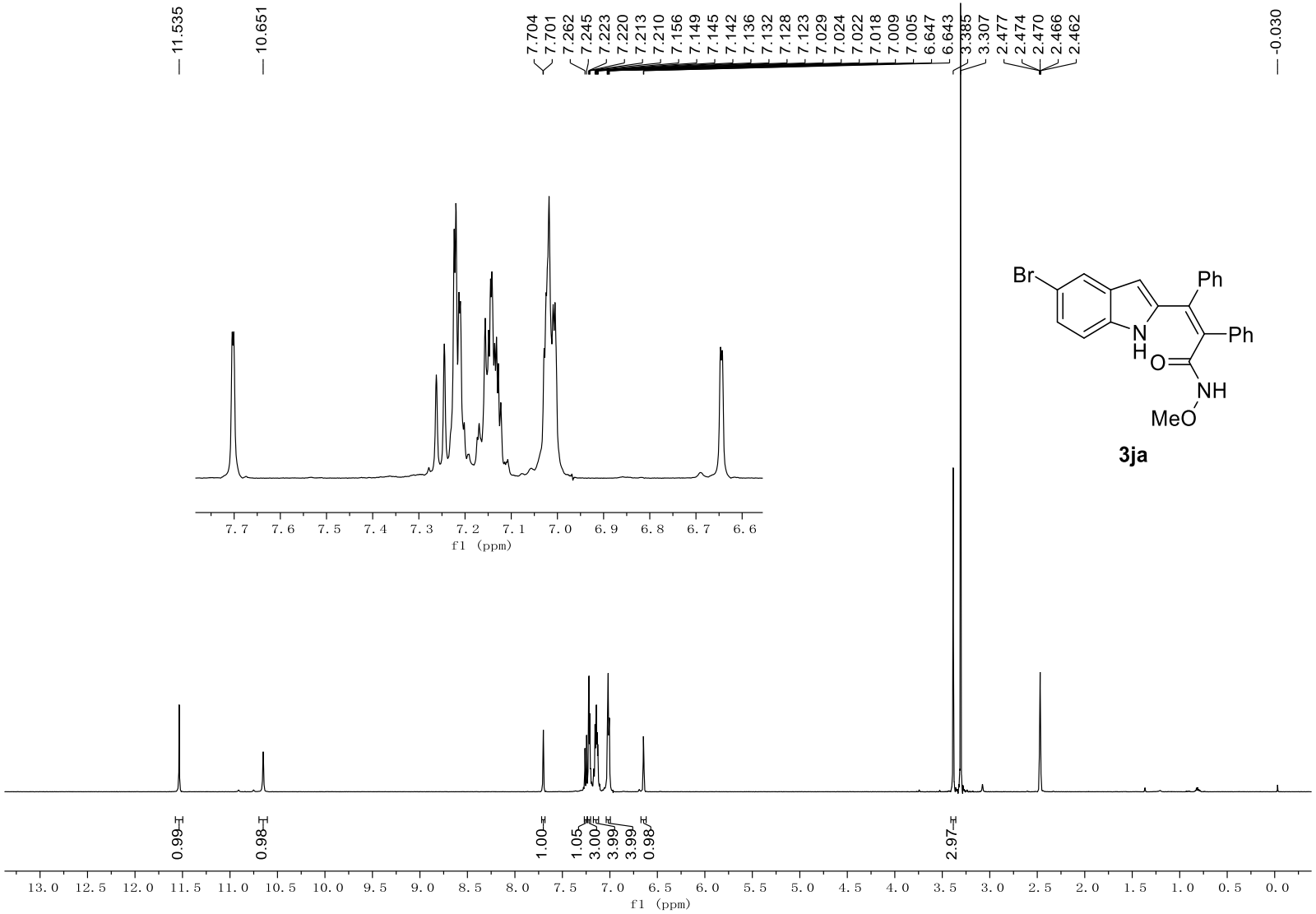
143.520
142.190
140.488
140.150
139.540
135.691
134.323
133.807
133.374
133.314
133.166
132.551
128.949
126.970
124.388
118.355
108.699
67.595
45.360
45.151
44.942
44.525
44.316
44.107
Cl
Ph
Ph
N
H
O
NH
MeO
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3ia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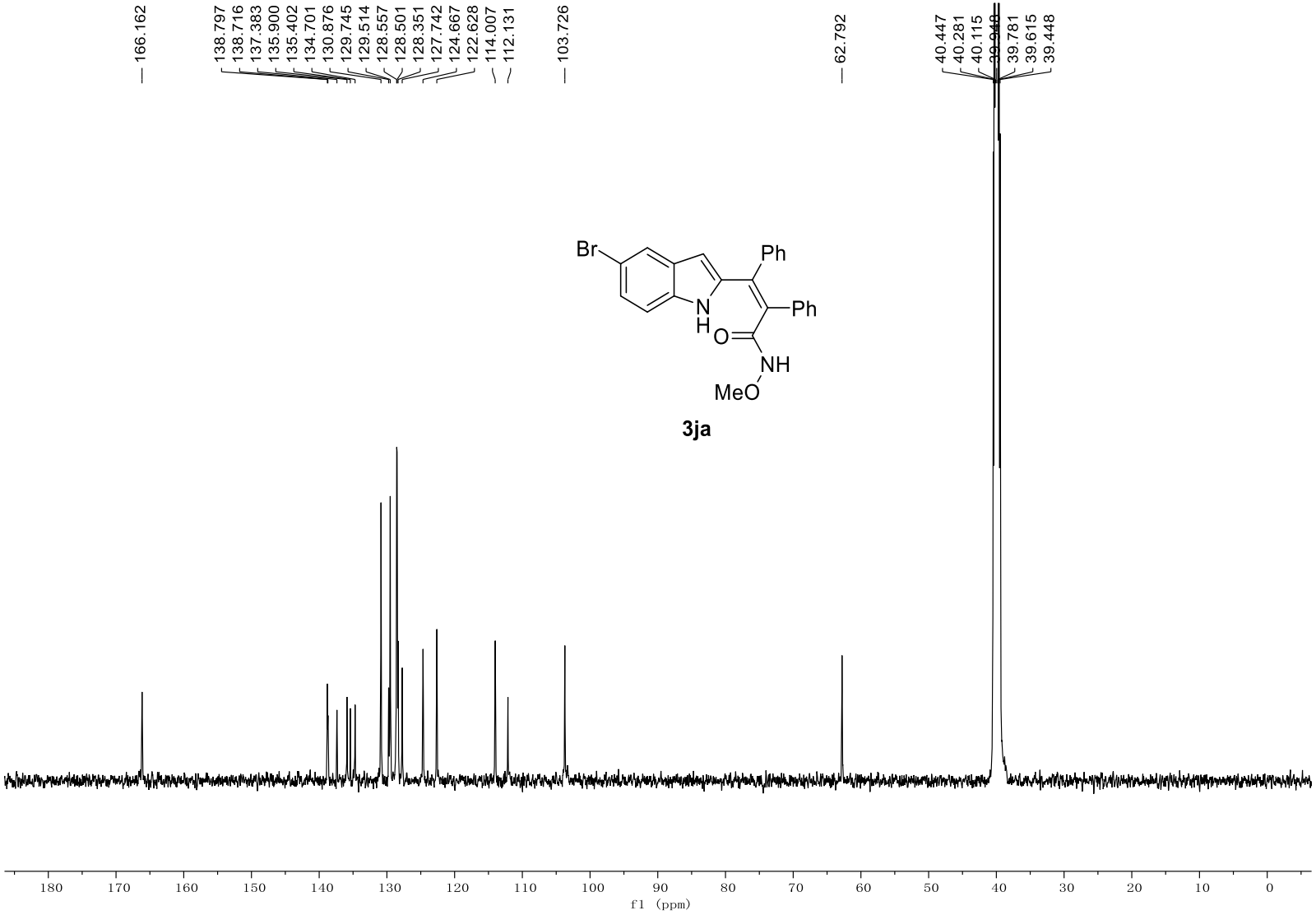
7.262
7.245
7.223
7.220
7.213
7.210
7.156
7.149
7.145
7.142
7.136
7.132
7.128
7.123
7.029
7.024
7.022
7.018
7.009
7.005
6.647
6.643
3.385
3.307
2.477
2.474
2.470
2.466
2.462
-0.030
f1 (ppm)
Br
Ph
Ph
N
H
O
NH
MeO
3ja
0.99
0.98
1.00
1.05
3.00
3.99
3.99
0.98
2.97
f1 (ppm)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138.716
137.383
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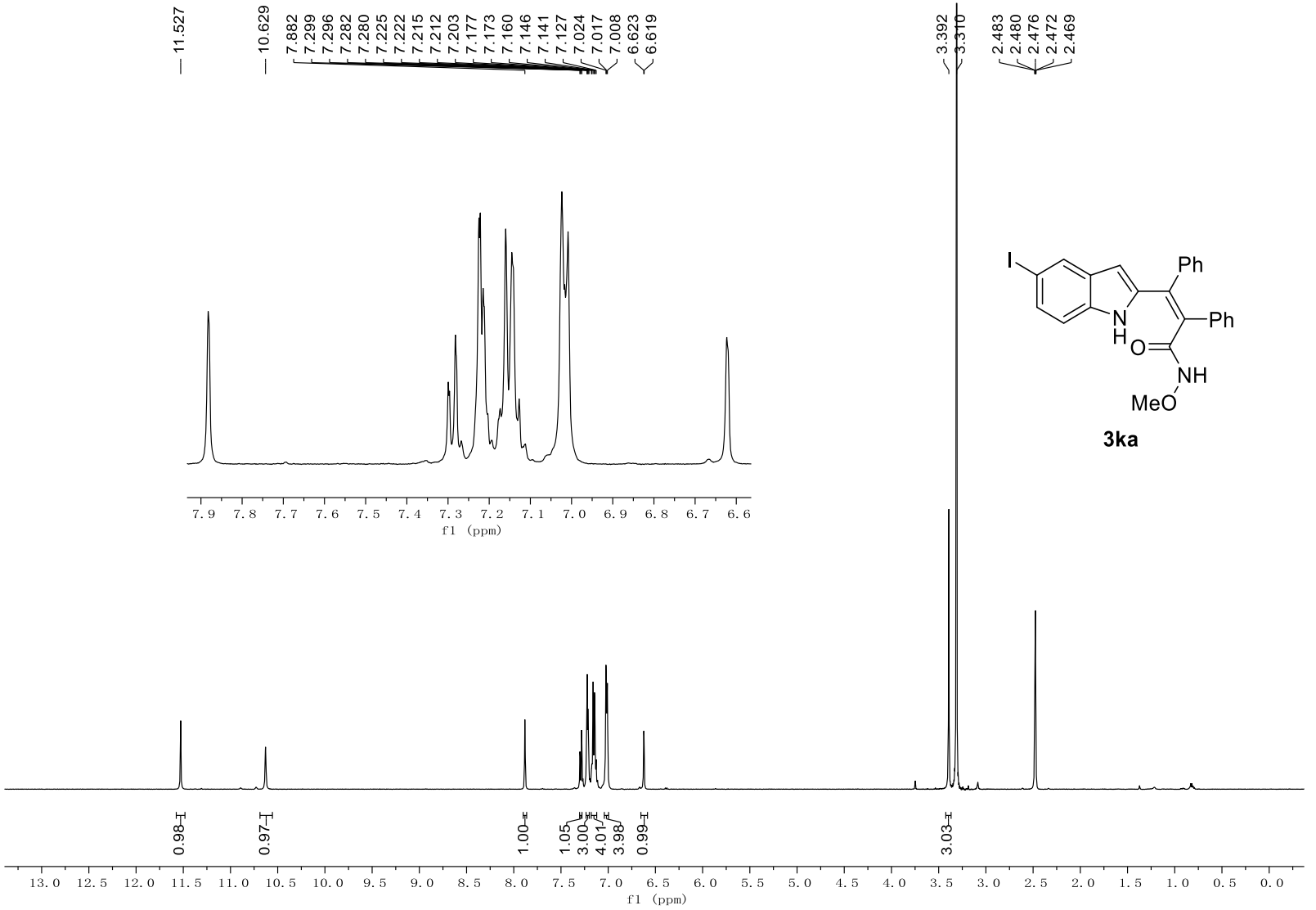
135.402
134.701
130.876
129.745
129.514
128.557
128.501
128.351
127.742
124.667
122.628
114.007
112.131
103.726
62.792
40.447
40.281
40.115
39.781
39.615
39.448
Br
Ph
Ph
N
H
O
NH
MeO
3ja
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.225
7.222
7.215
7.212
7.203
7.177
7.173
7.160
7.146
7.141
7.127
7.024
7.017
7.008
6.623
6.619
3.392
3.310
2.483
2.480
2.476
2.472
2.469
I
Ph
Ph
N
H
O
NH
MeO
3ka
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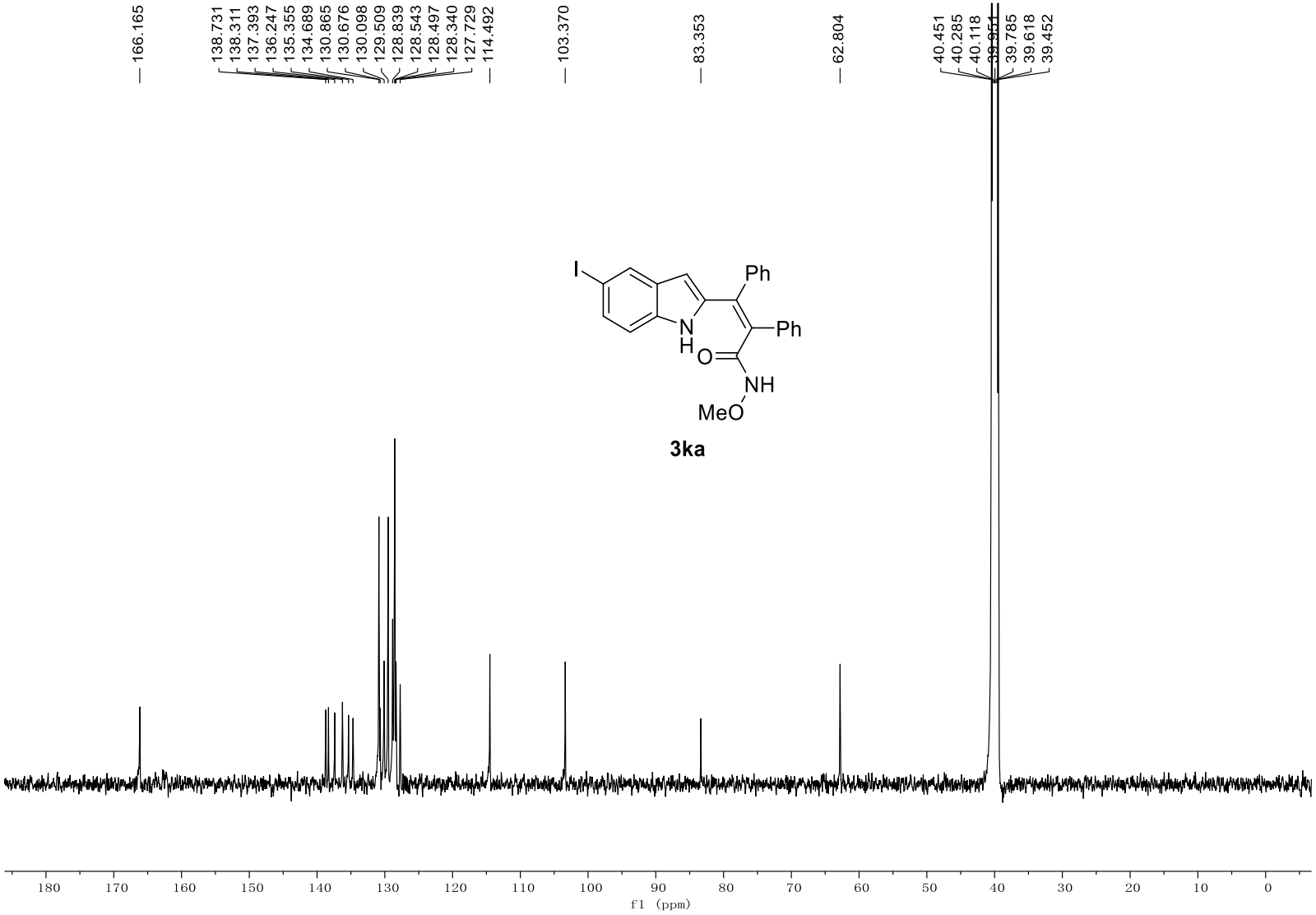
0.97
1.00
1.05
3.00
4.01
3.98
0.99
3.03
f1 (ppm)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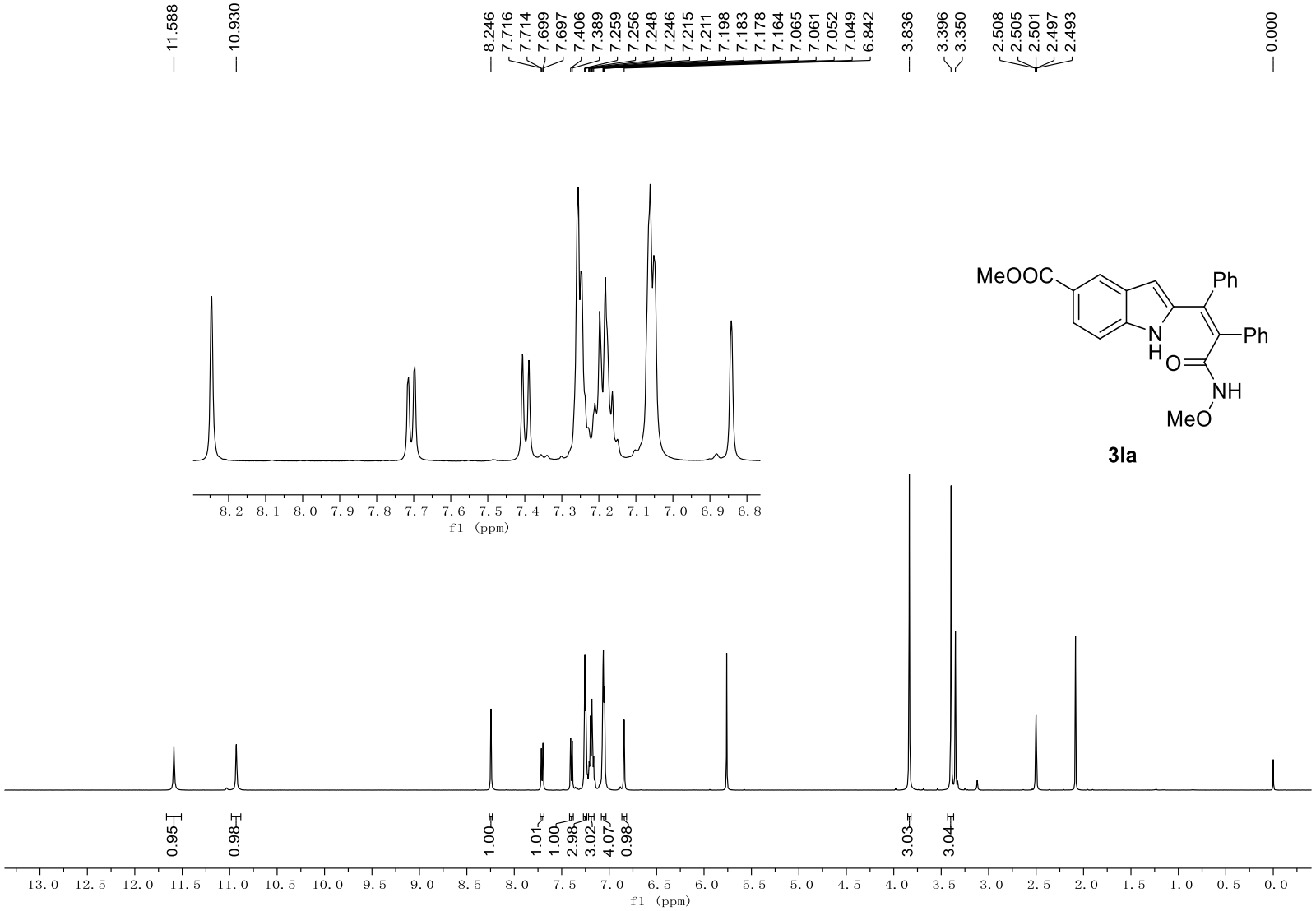
138.311
137.393
136.247
135.355
134.689
130.865
130.676
130.098
129.509
128.839
128.543
128.497
128.340
127.729
114.492
103.370
83.353
62.804
40.451
40.285
40.118
39.951
39.785
39.618
39.452
I
Ph
Ph
N
H
O
NH
MeO
3ka
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.714
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7.697
7.406
7.389
7.259
7.256
7.248
7.246
7.215
7.211
7.198
7.183
7.178
7.164
7.065
7.061
7.052
7.049
6.842
3.836
3.396
3.350
2.508
2.505
2.501
2.497
2.493
0.000
MeOOC
Ph
Ph
N
H
O
NH
MeO
3la
f1 (ppm)
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0.98
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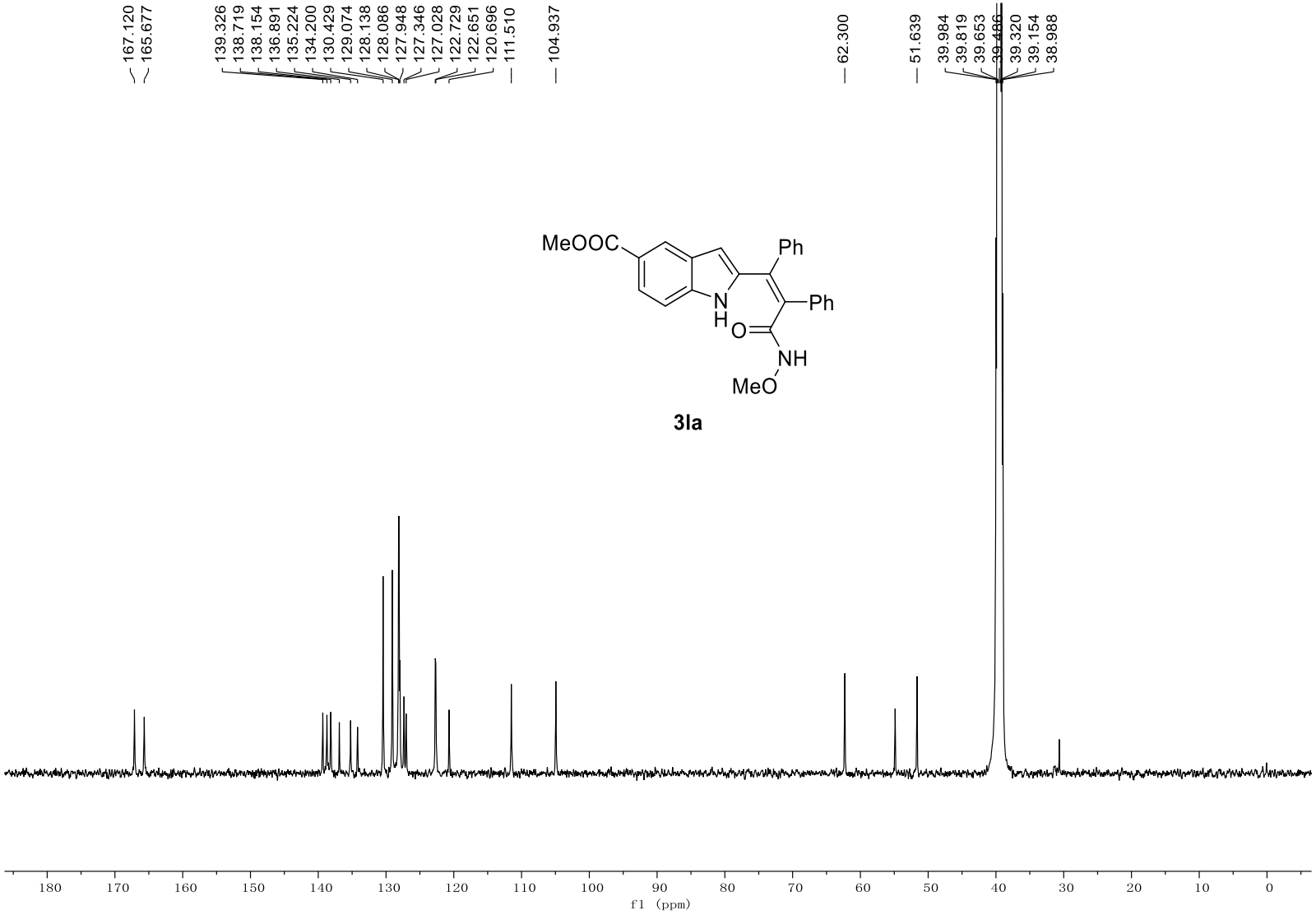
1.01
1.00
2.98
3.02
4.07
0.98
3.03
3.04
f1 (ppm)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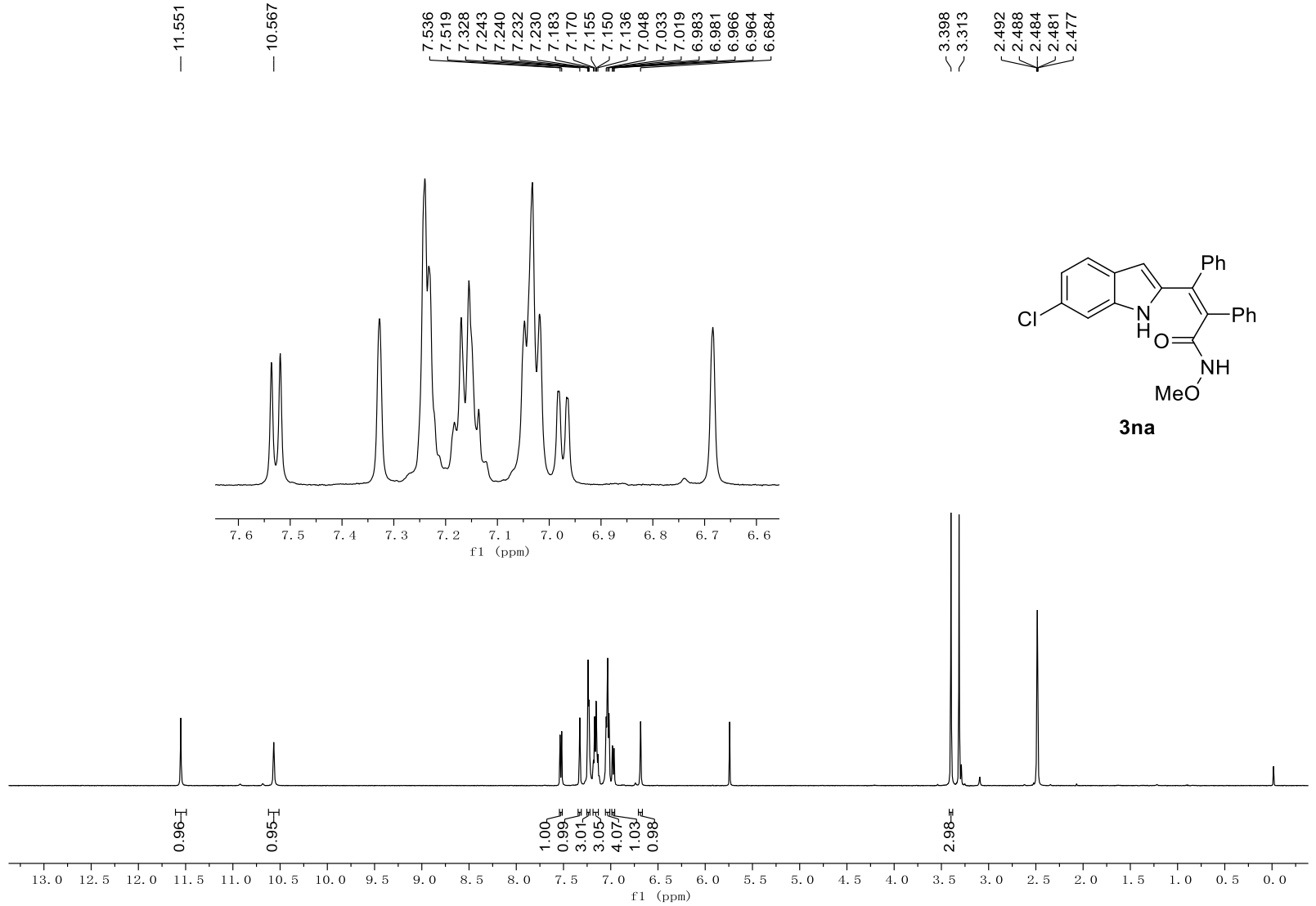
139.326
138.719
138.154
136.891
135.224
134.200
130.429
129.074
128.138
128.086
127.948
127.346
127.028
122.729
122.651
120.696
111.510
104.937
62.300
51.639
39.984
39.819
39.653
39.486
39.320
39.154
38.988
MeOOC
Ph
Ph
N
H
O
NH
MeO
3Ia
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.519
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7.243
7.240
7.232
7.230
7.183
7.170
7.155
7.150
7.136
7.048
7.033
7.019
6.983
6.981
6.966
6.964
6.684
3.398
3.313
2.492
2.488
2.484
2.481
2.477
Cl
N
H
O
Ph
Ph
NH
MeO
3na
f1 (ppm)
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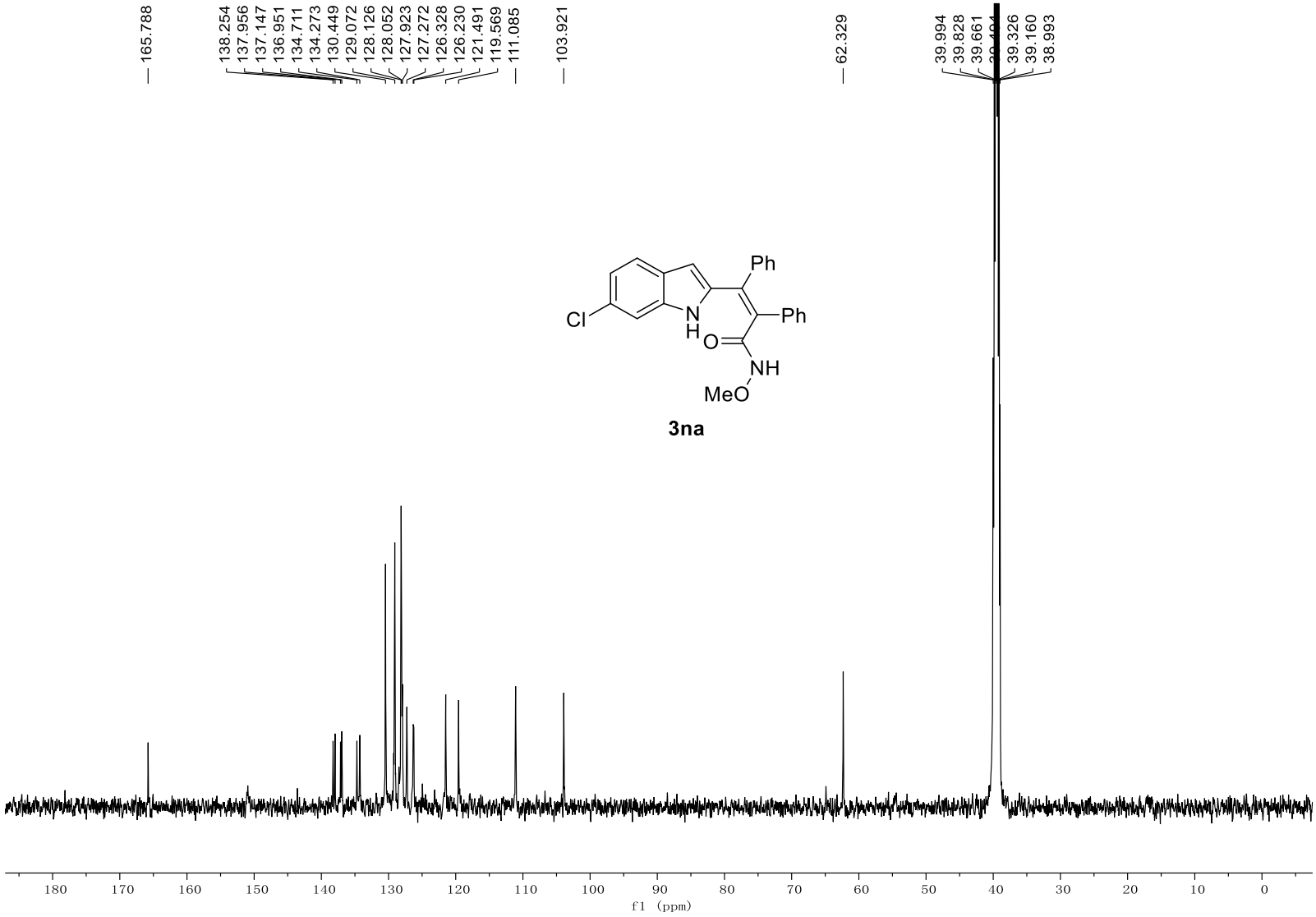
0.95
1.00
0.99
3.01
3.05
4.07
1.03
0.98
2.98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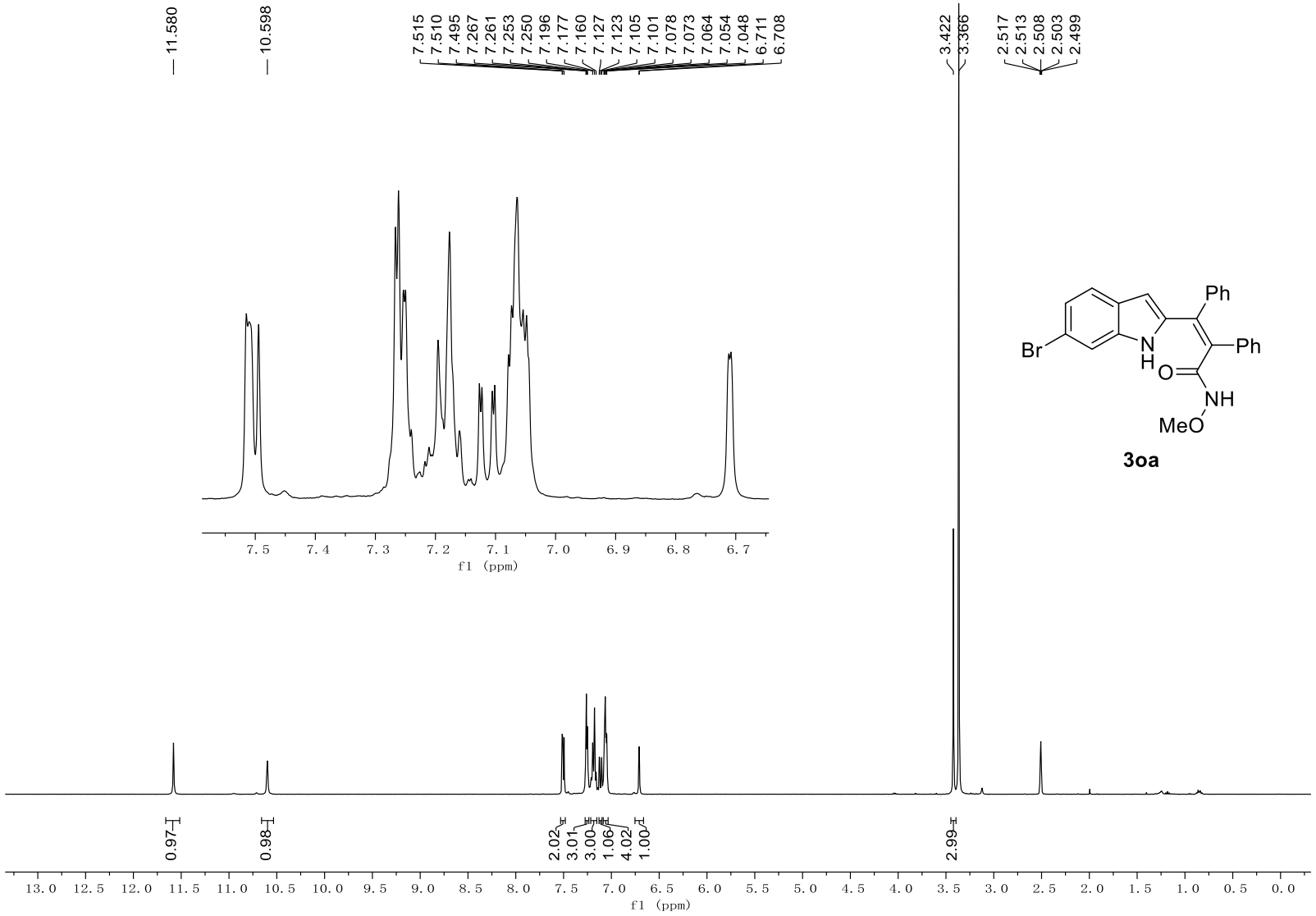
130.449
129.072
128.126
128.052
127.923
127.272
126.328
126.230
121.491
119.569
111.085
103.921
62.329
39.994
39.828
39.661
39.326
39.160
38.993
Ph
Cl
N
H
Ph
O
NH
MeO
3na
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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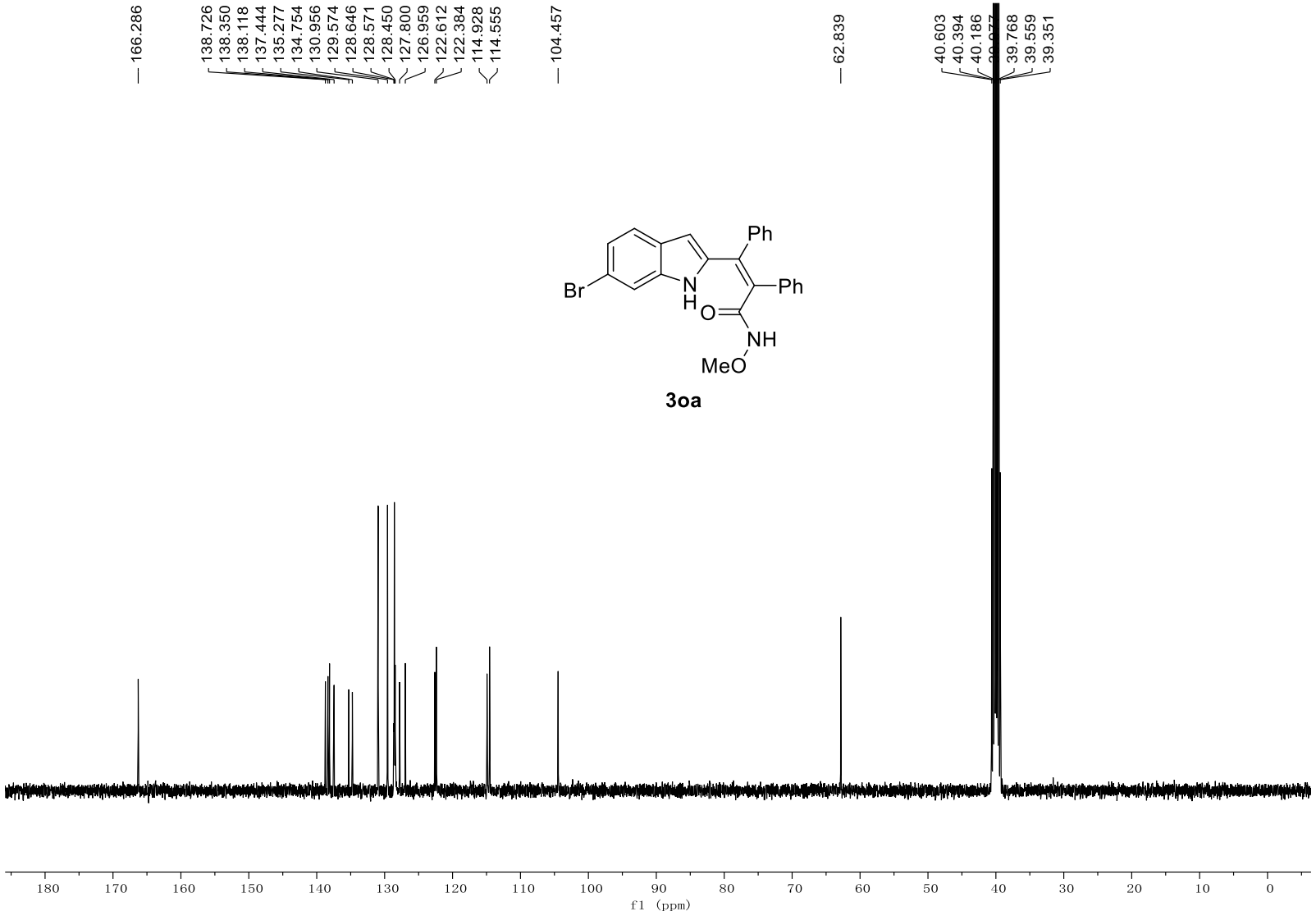
7.253
7.250
7.196
7.177
7.160
7.127
7.123
7.105
7.101
7.078
7.073
7.064
7.054
7.048
6.711
6.708
3.422
3.366
2.517
2.513
2.508
2.503
2.499
Ph
Br
N
H
O
NH
MeO
Ph
3oa
f1 (ppm)
0.97
0.98
2.02
3.01
3.00
1.06
4.02
1.00
2.99
f1 (ppm)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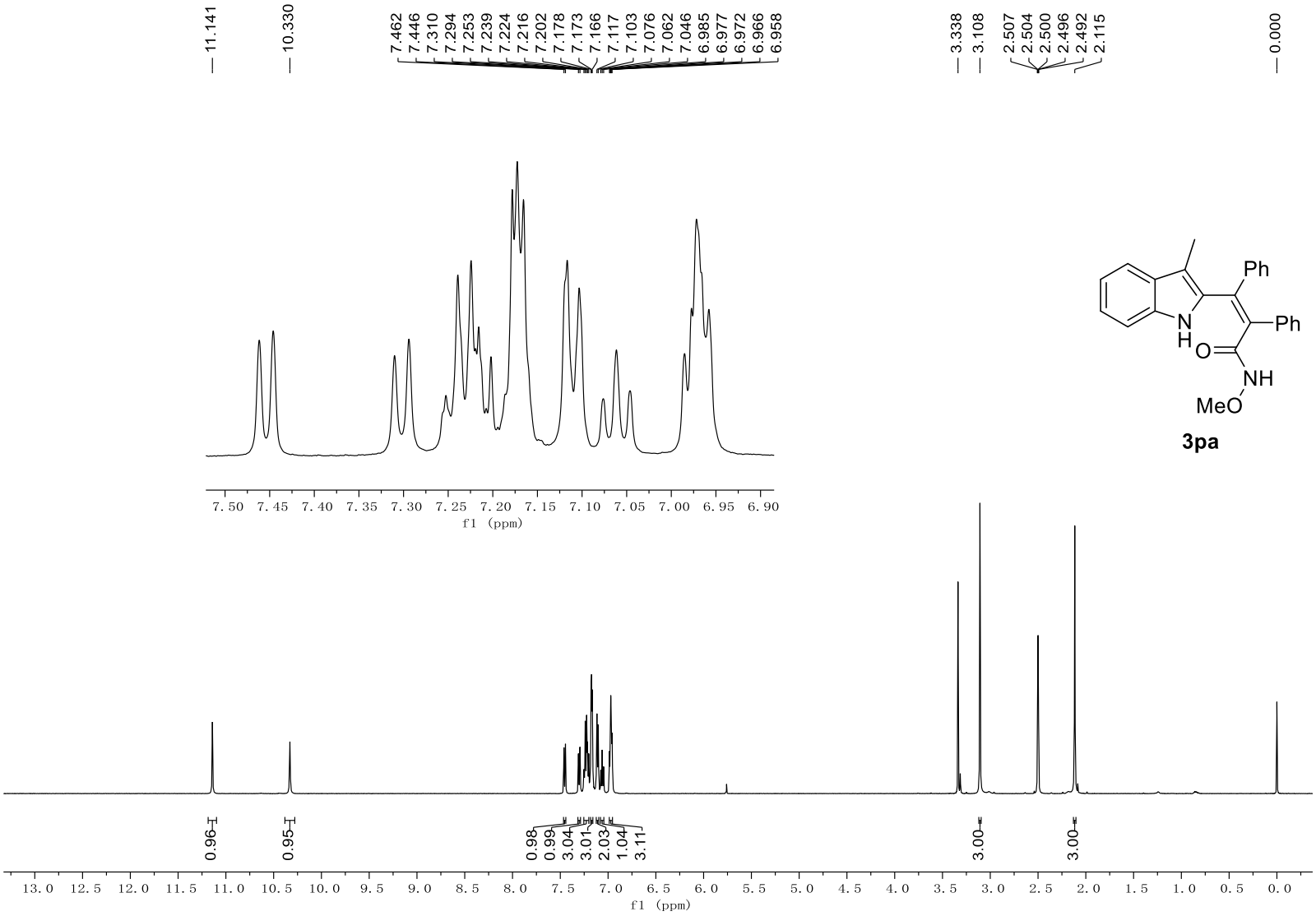
130.956
129.574
128.646
128.571
128.450
127.800
126.959
122.612
122.384
114.928
114.555
104.457
62.839
40.603
40.394
40.186
39.768
39.559
39.351
Ph
Ph
Br
N
H
O
NH
MeO
3oa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.141
10.330
7.462
7.446
7.310
7.294
7.253
7.239
7.224
7.216
7.202
7.178
7.173
7.166
7.117
7.103
7.076
7.062
7.046
6.985
6.977
6.972
6.966
6.958
3.338
3.108
2.507
2.504
2.500
2.496
2.492
2.115
0.000
Ph
Ph
N
H
O
NH
MeO
3pa
f1 (ppm)
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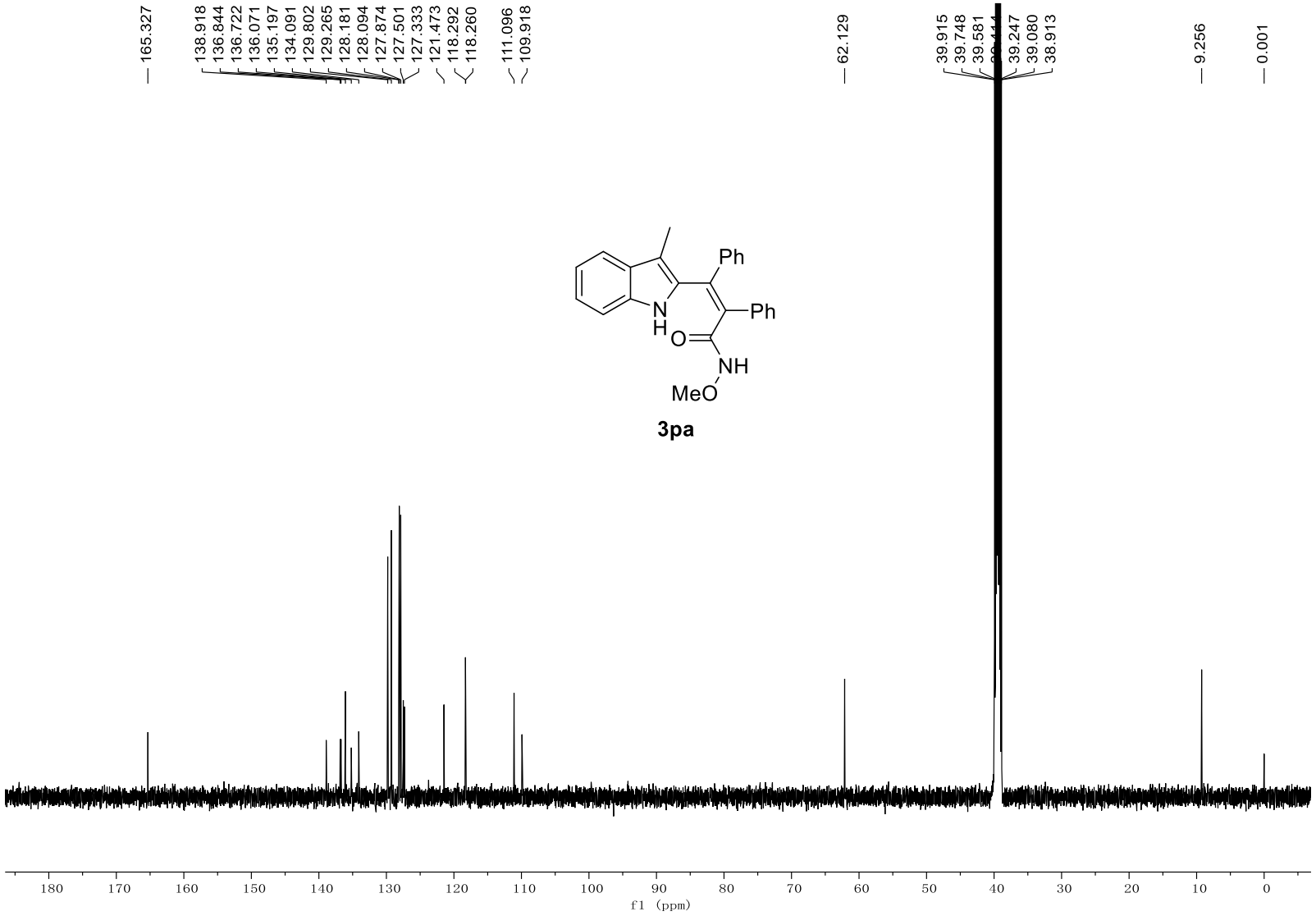
0.95
0.98
0.99
3.04
3.01
2.03
1.04
3.11
3.00
3.00
f1 (ppm)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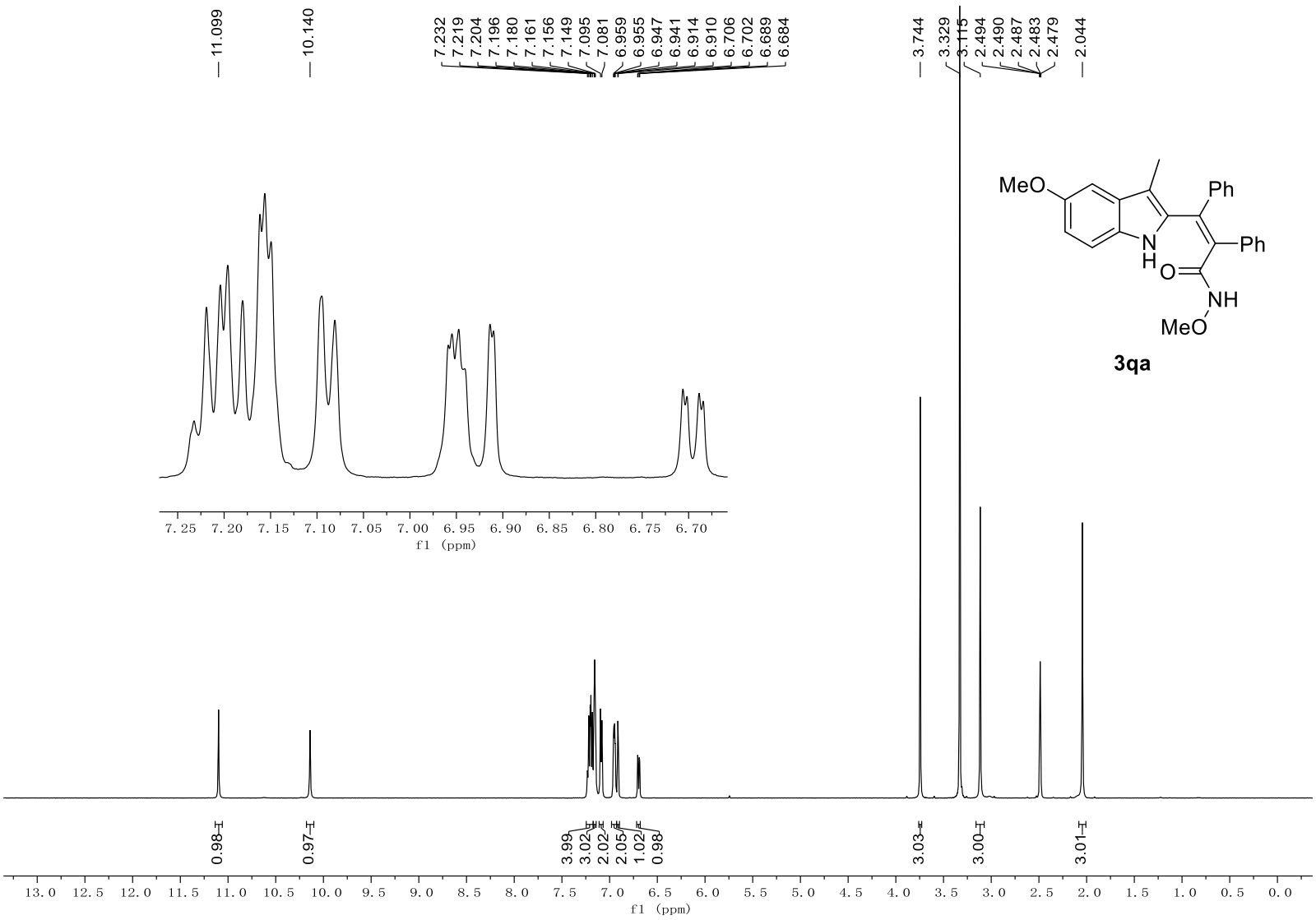
127.874
127.501
127.333
121.473
118.292
118.260
111.096
109.918
62.129
39.915
39.748
39.581
39.247
39.080
38.913
9.256
0.001
Ph
Ph
N
H
O
NH
MeO
3pa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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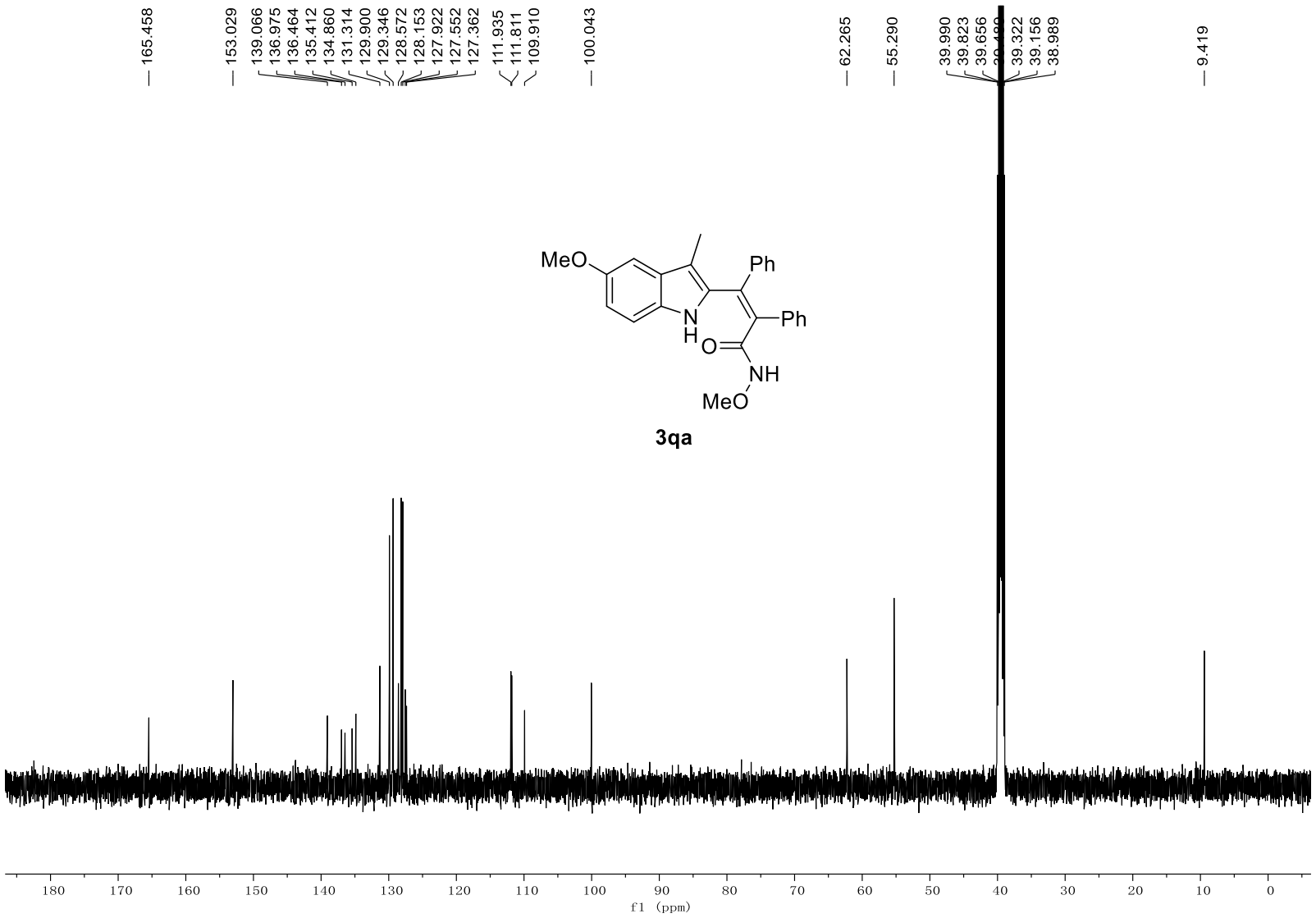
10.140
7.232
7.219
7.204
7.196
7.180
7.161
7.156
7.149
7.095
7.081
6.959
6.955
6.947
6.941
6.914
6.910
6.706
6.702
6.689
6.684
3.744
3.329
3.115
2.494
2.490
2.487
2.483
2.479
2.044
MeO
Ph
Ph
N
H
O
NH
MeO
3qa
f1 (ppm)
0.98
0.97
3.99
3.02
2.02
2.05
1.02
0.98
3.03
3.00
3.01
f1 (ppm)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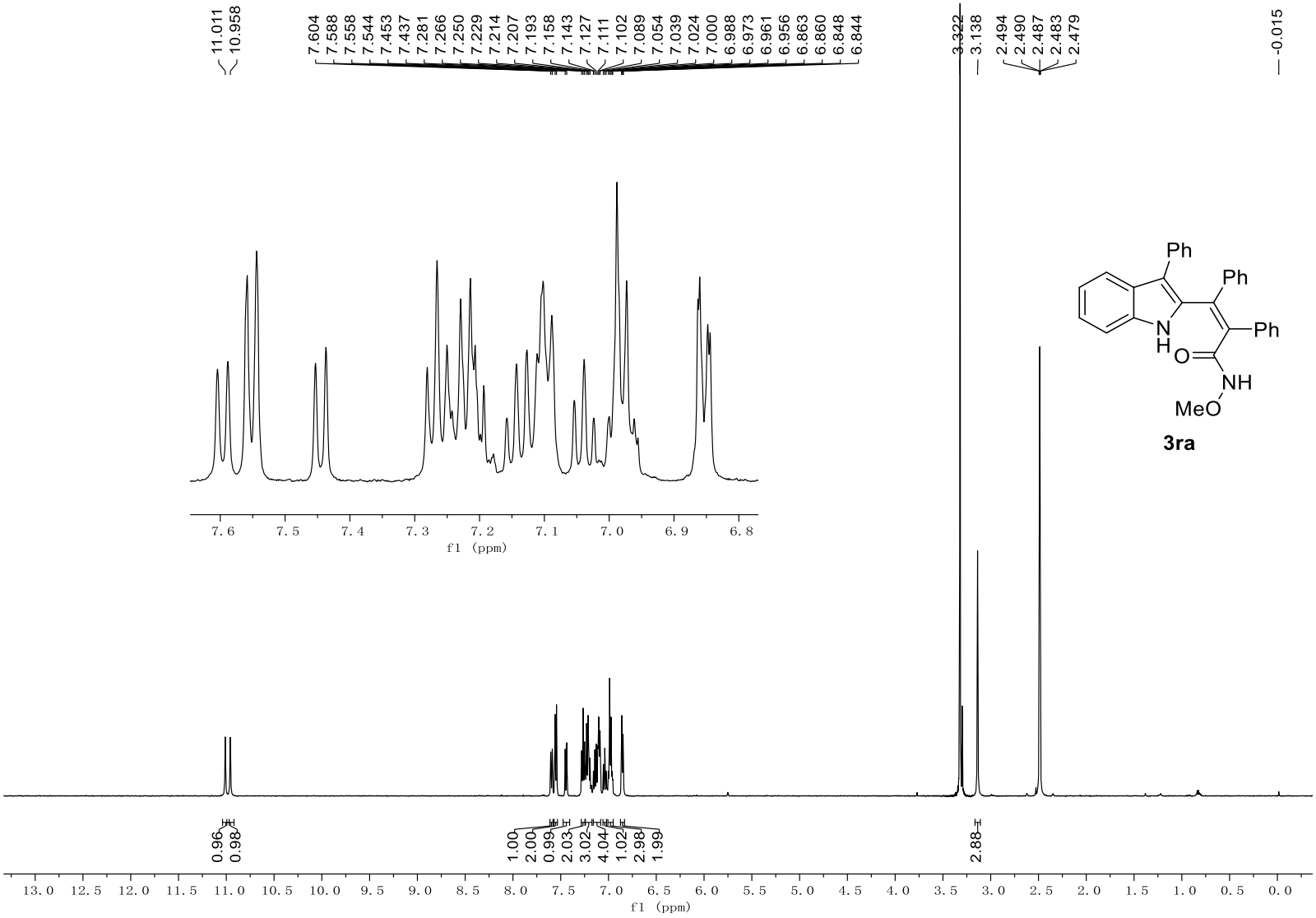
153.029
139.066
136.975
136.464
135.412
134.860
131.314
129.900
129.346
128.572
128.153
127.922
127.552
127.362
111.935
111.811
109.910
100.043
62.265
55.290
39.990
39.823
39.656
39.322
39.156
38.989
9.419
MeO
Ph
Ph
N
H
O
NH
MeO
3qa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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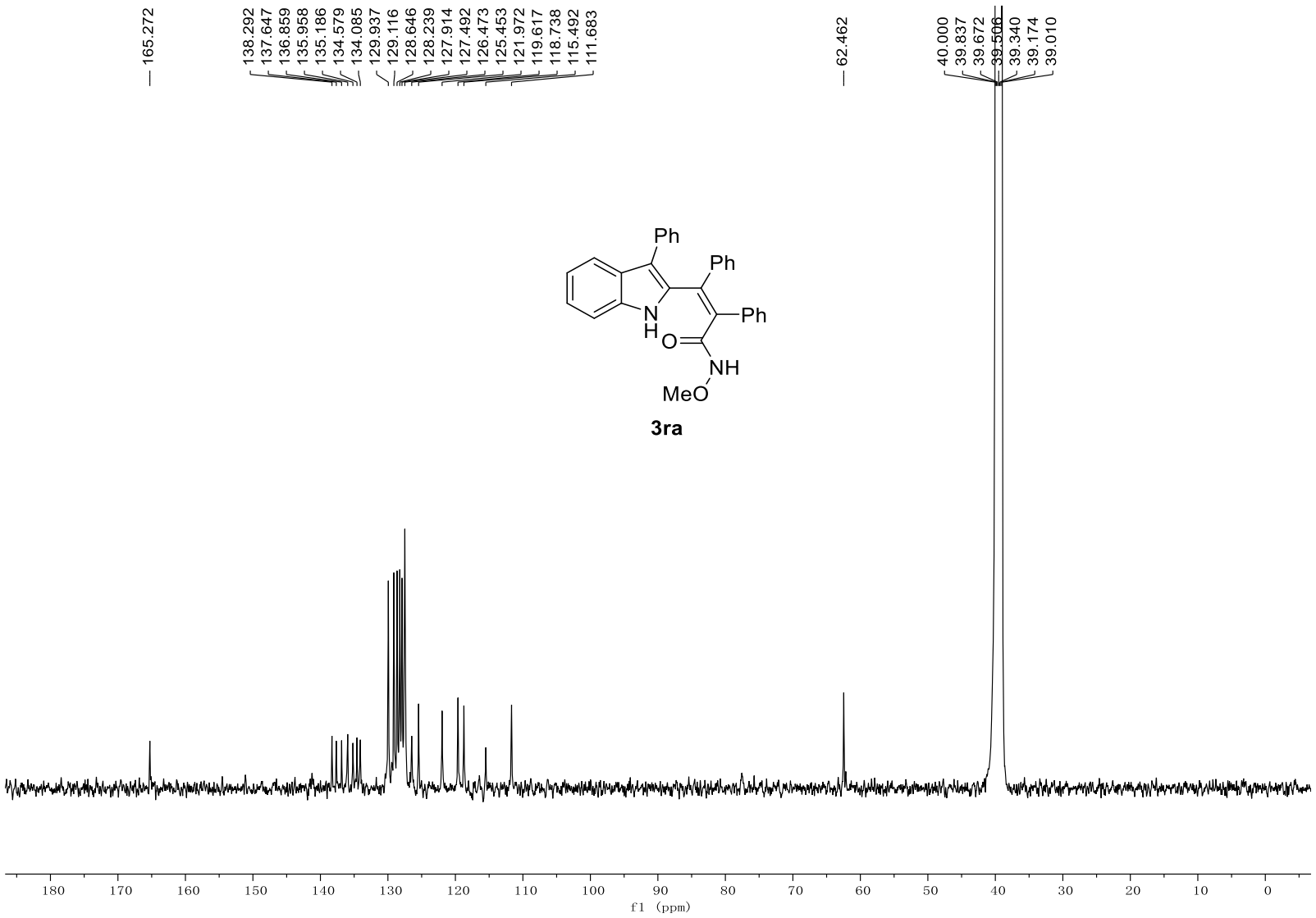
10.958
7.604
7.588
7.558
7.544
7.453
7.437
7.281
7.266
7.250
7.229
7.214
7.207
7.193
7.158
7.143
7.127
7.111
7.102
7.089
7.054
7.039
7.024
7.000
6.988
6.973
6.961
6.956
6.863
6.860
6.848
6.844
3.322
3.138
2.494
2.490
2.487
2.483
2.479
-0.015
Ph
Ph
Ph
N
H
O
NH
MeO
3ra
f1 (ppm)
0.96
0.98
1.00
2.00
0.99
2.03
3.02
4.04
1.02
2.98
1.99
2.88
f1 (ppm)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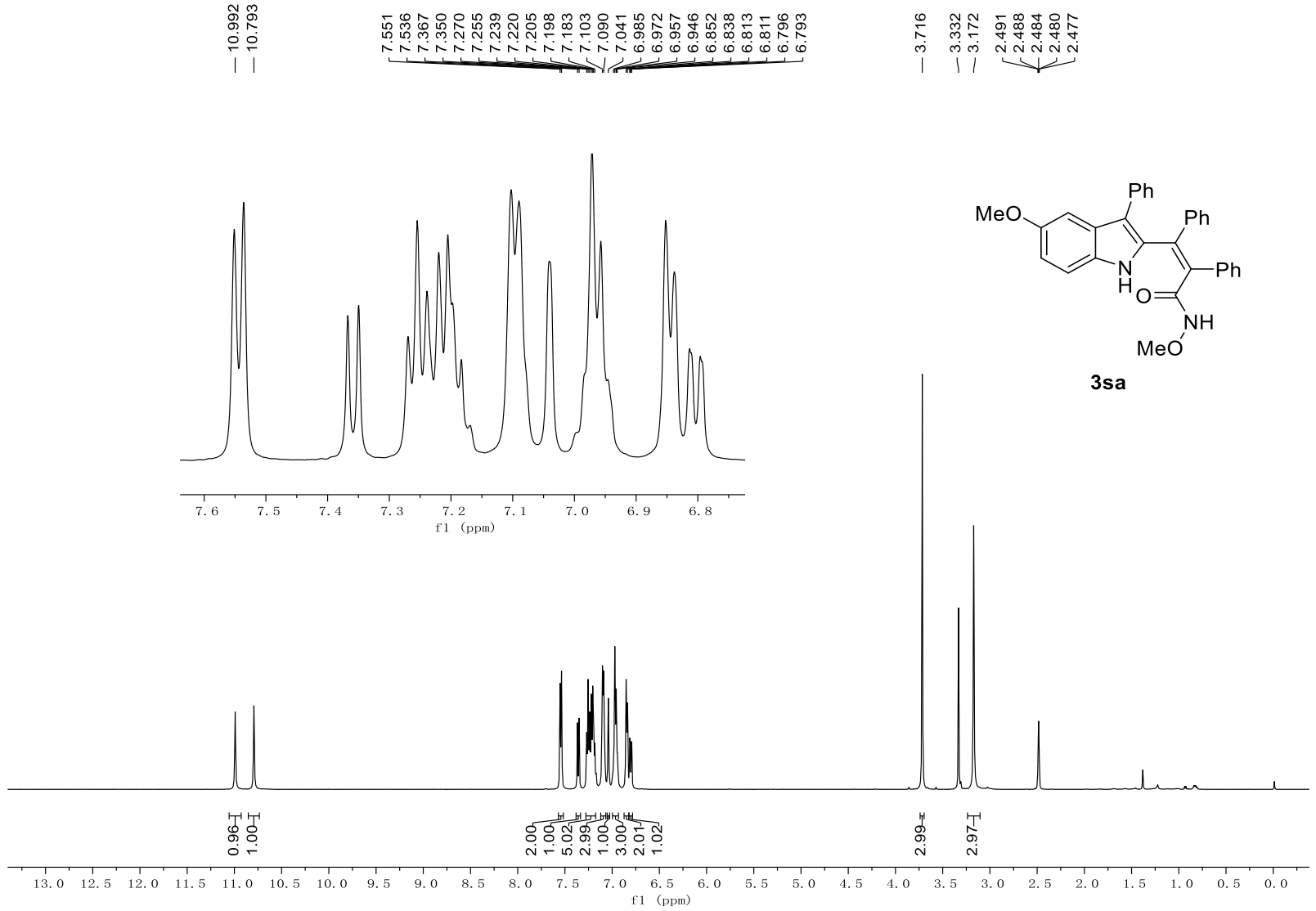
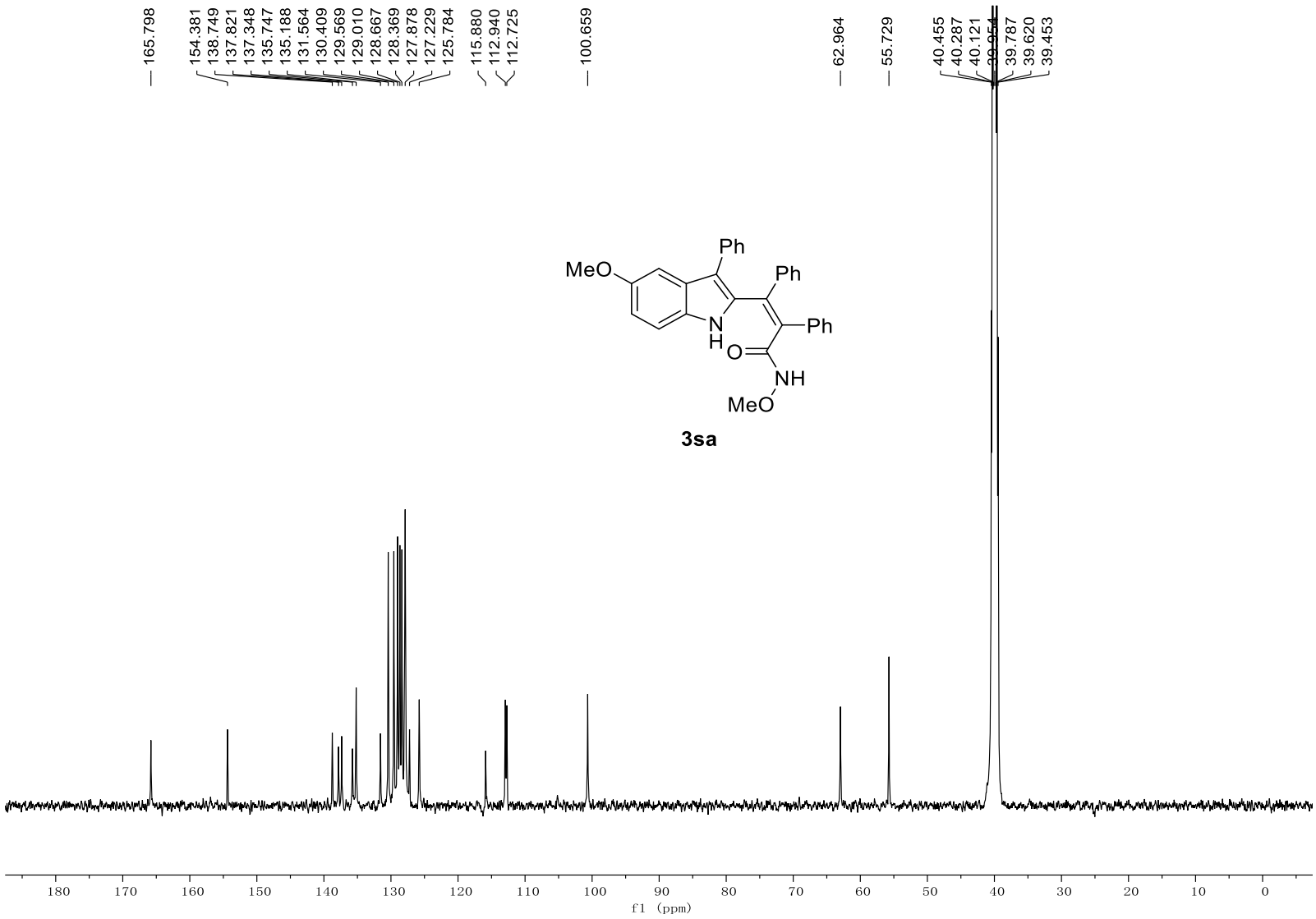
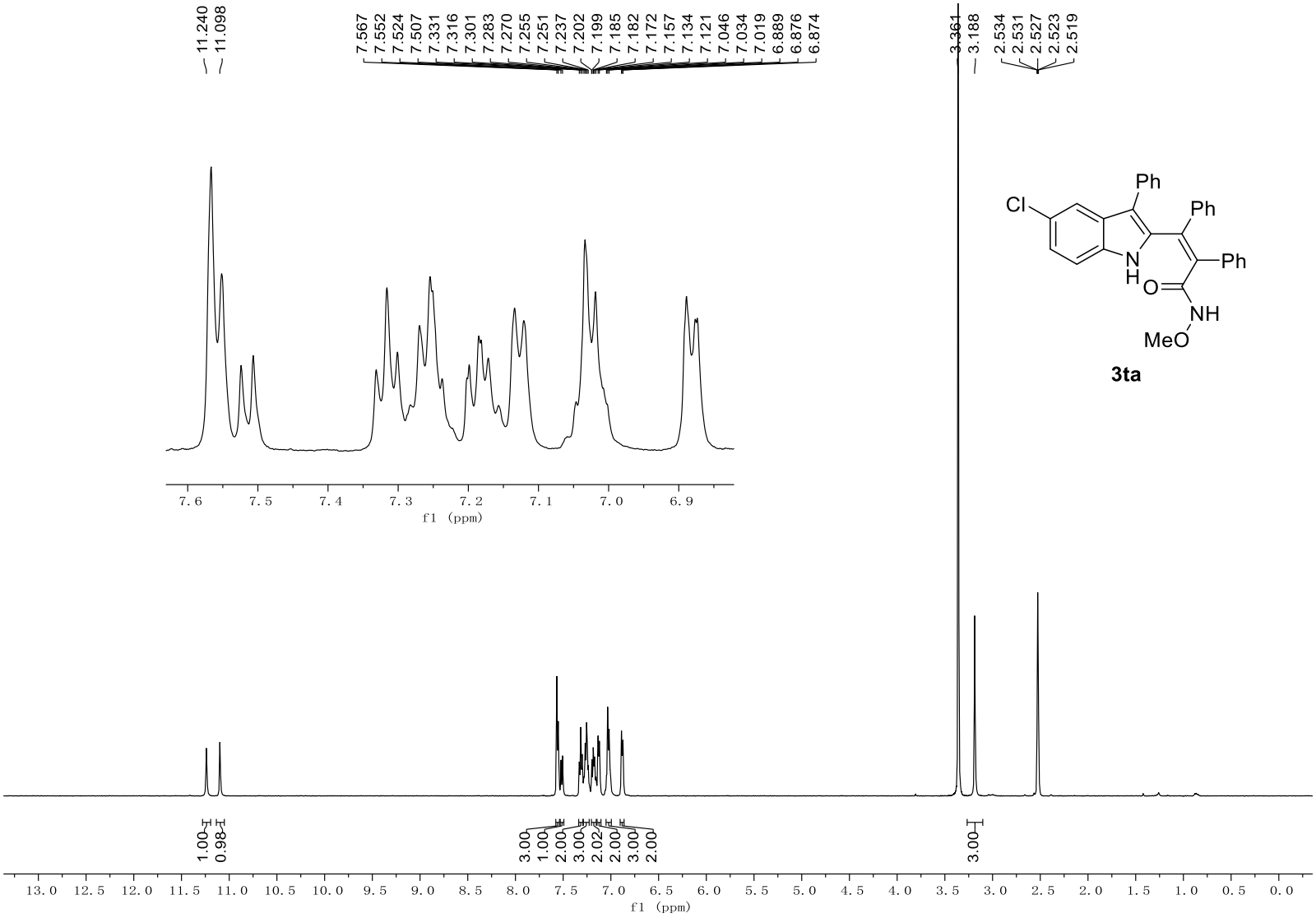
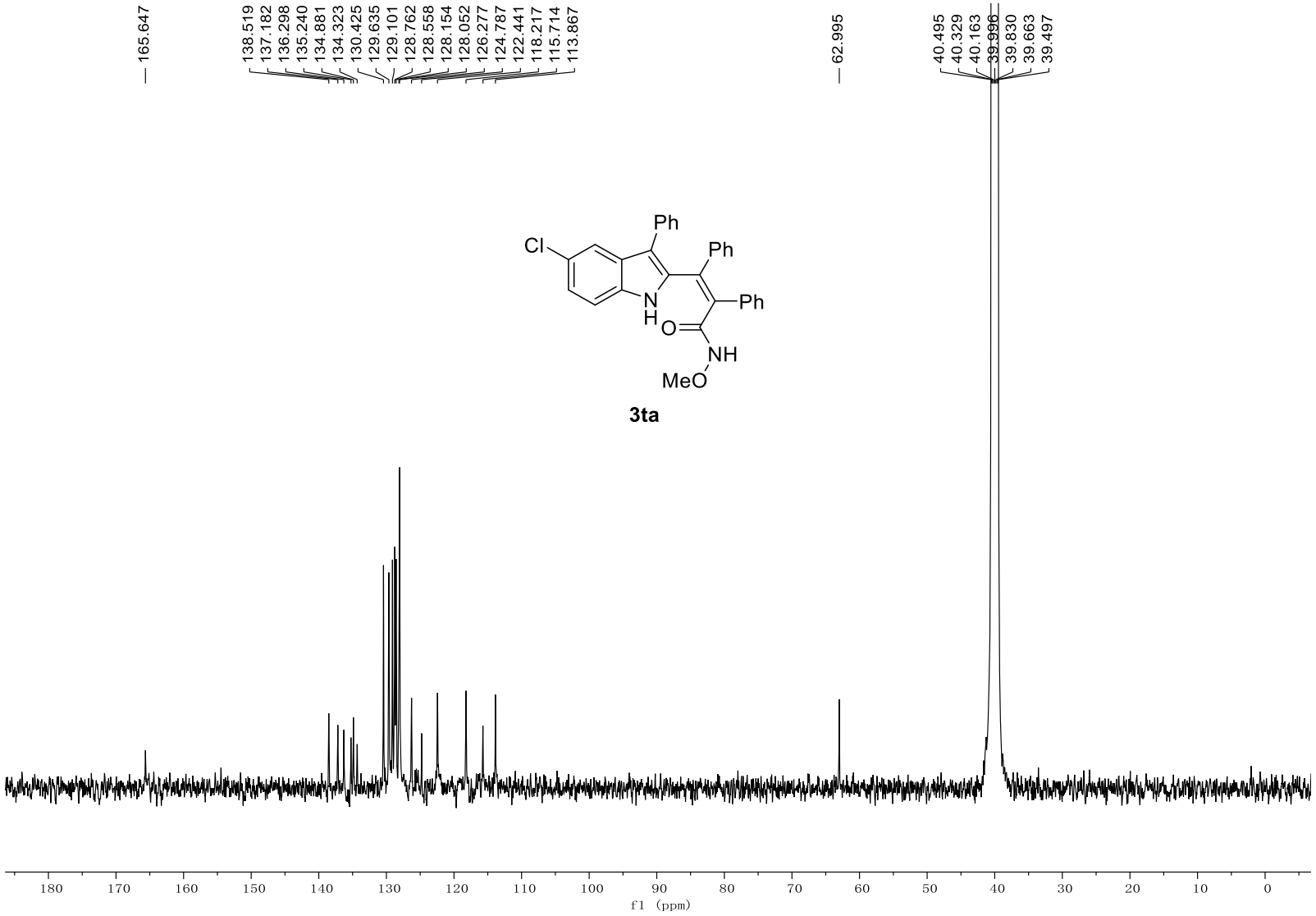
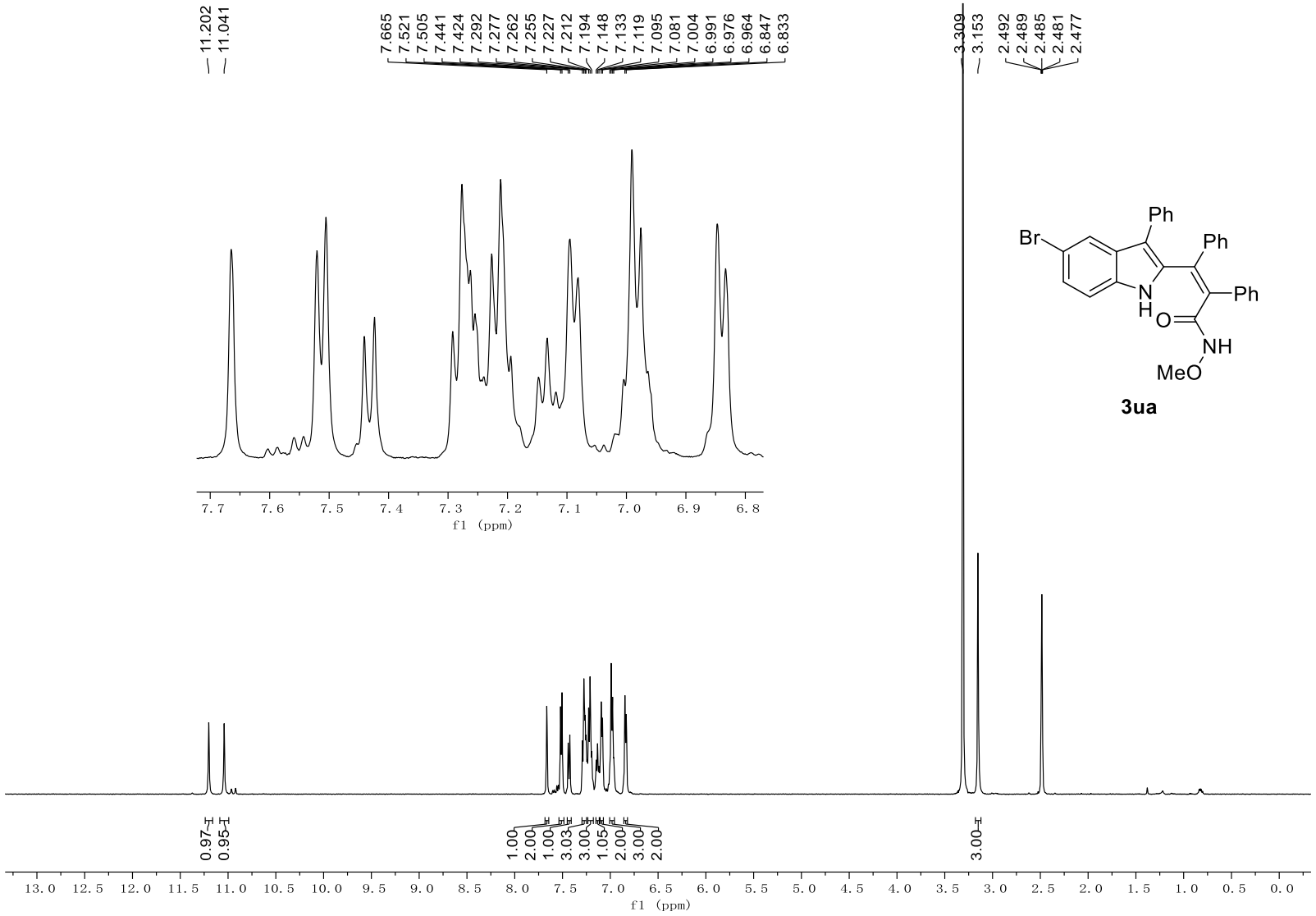
138.292
137.647
136.859
135.958
135.186
134.579
134.085
129.937
129.116
128.646
128.239
127.914
127.492
126.473
125.453
121.972
119.617
118.738
115.492
111.683
62.462
40.000
39.837
39.672
39.506
39.340
39.174
39.010
Ph
Ph
Ph
N
H
O
NH
MeO
3ra
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

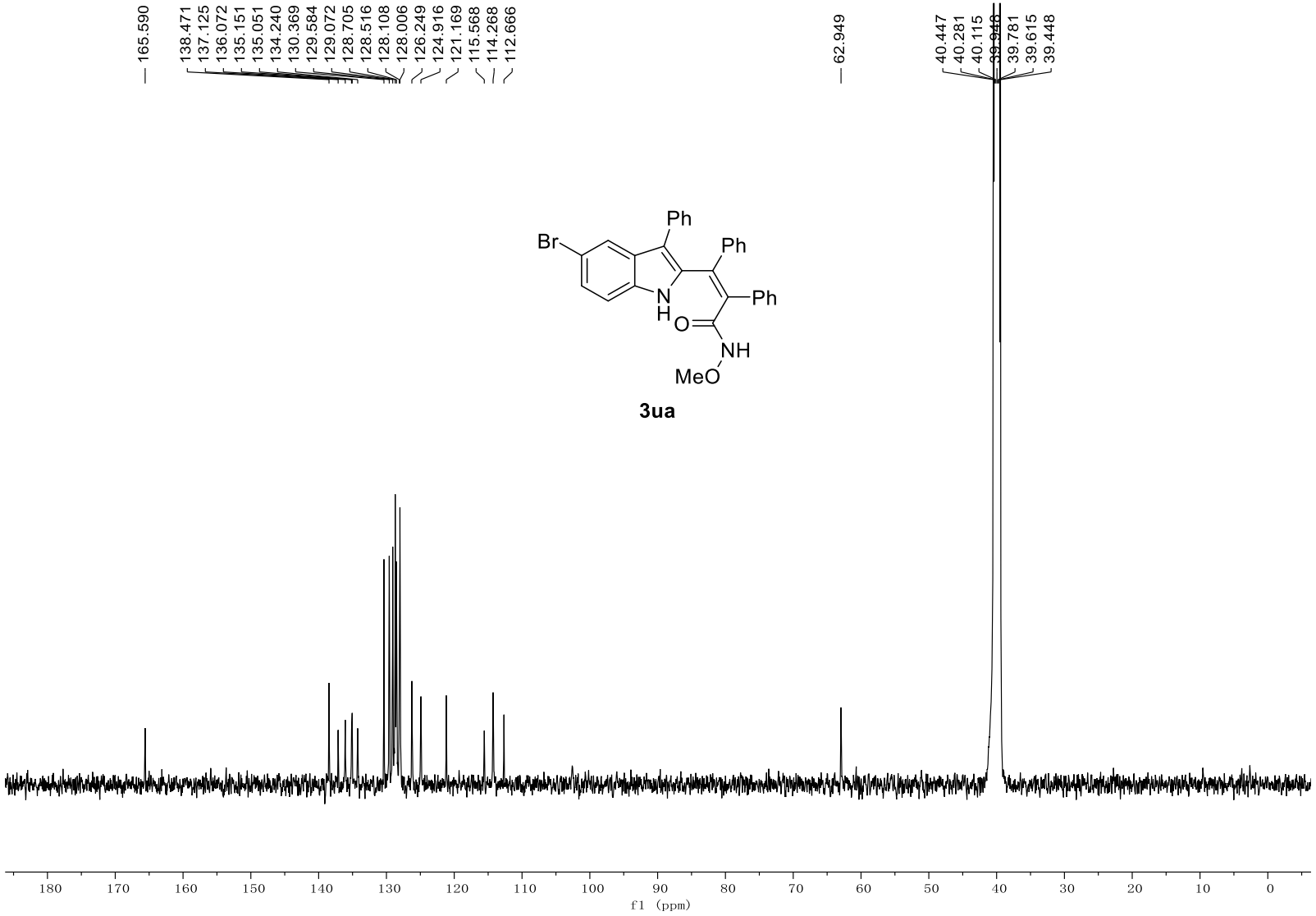

10.992
10.793
7.551
7.536
7.367
7.350
7.270
7.255
7.239
7.220
7.205
7.198
7.183
7.103
7.090
7.041
6.985
6.972
6.957
6.946
6.852
6.838
6.813
6.811
6.796
6.793
3.716
3.332
3.172
2.491
2.488
2.484
2.480
2.477
MeO
Ph
Ph
Ph
N
H
O
NH
MeO
3sa
f1 (ppm)
f1 (ppm)

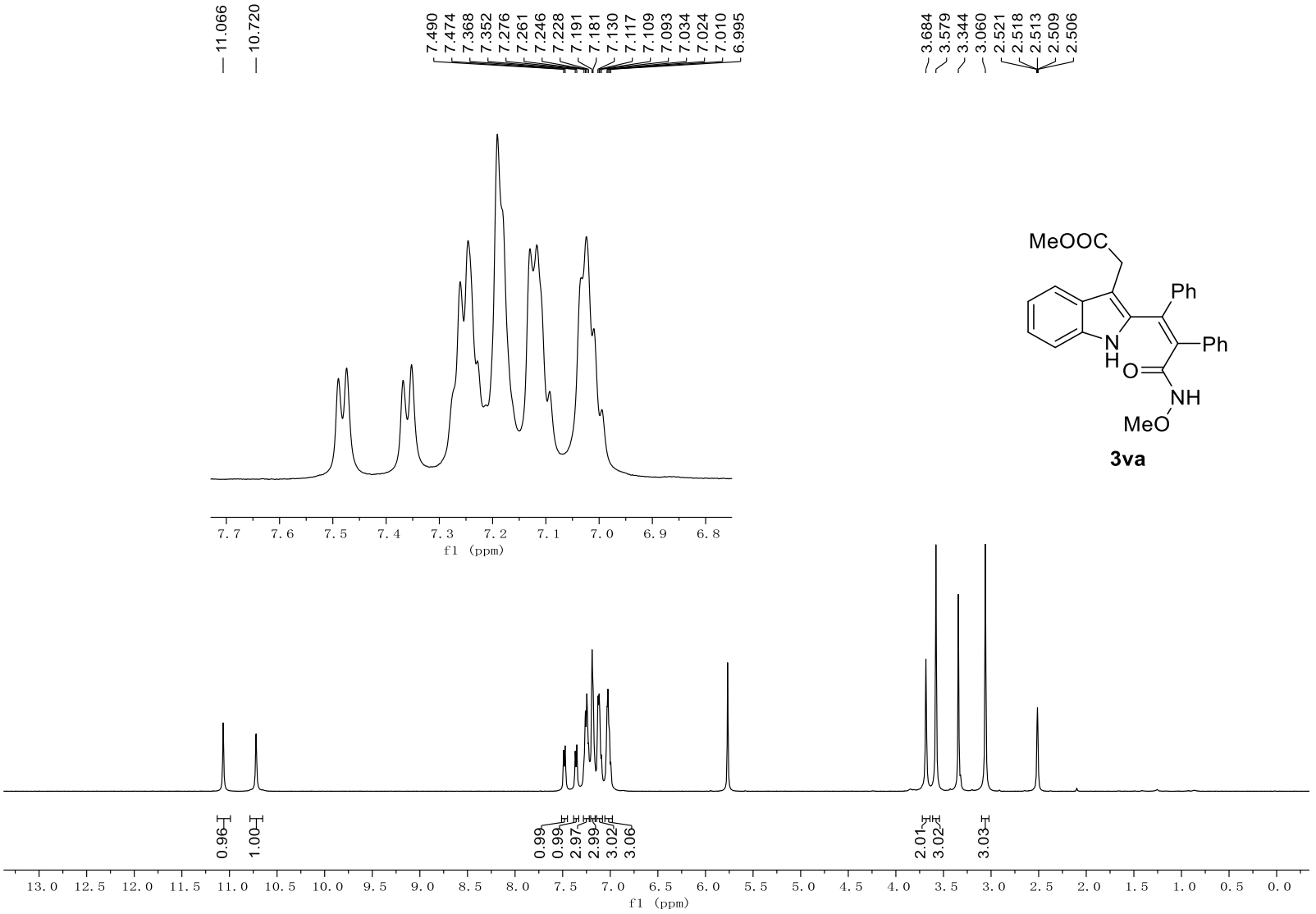

165.798
154.381
138.749
137.821
137.348
135.747
135.188
131.564
130.409
129.569
129.010
128.667
128.369
127.878
127.229
125.784
115.880
112.940
112.725
100.659
62.964
55.729
40.455
40.287
40.121
39.787
39.620
39.453
MeO
Ph
Ph
Ph
N
H
O
NH
MeO
3sa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

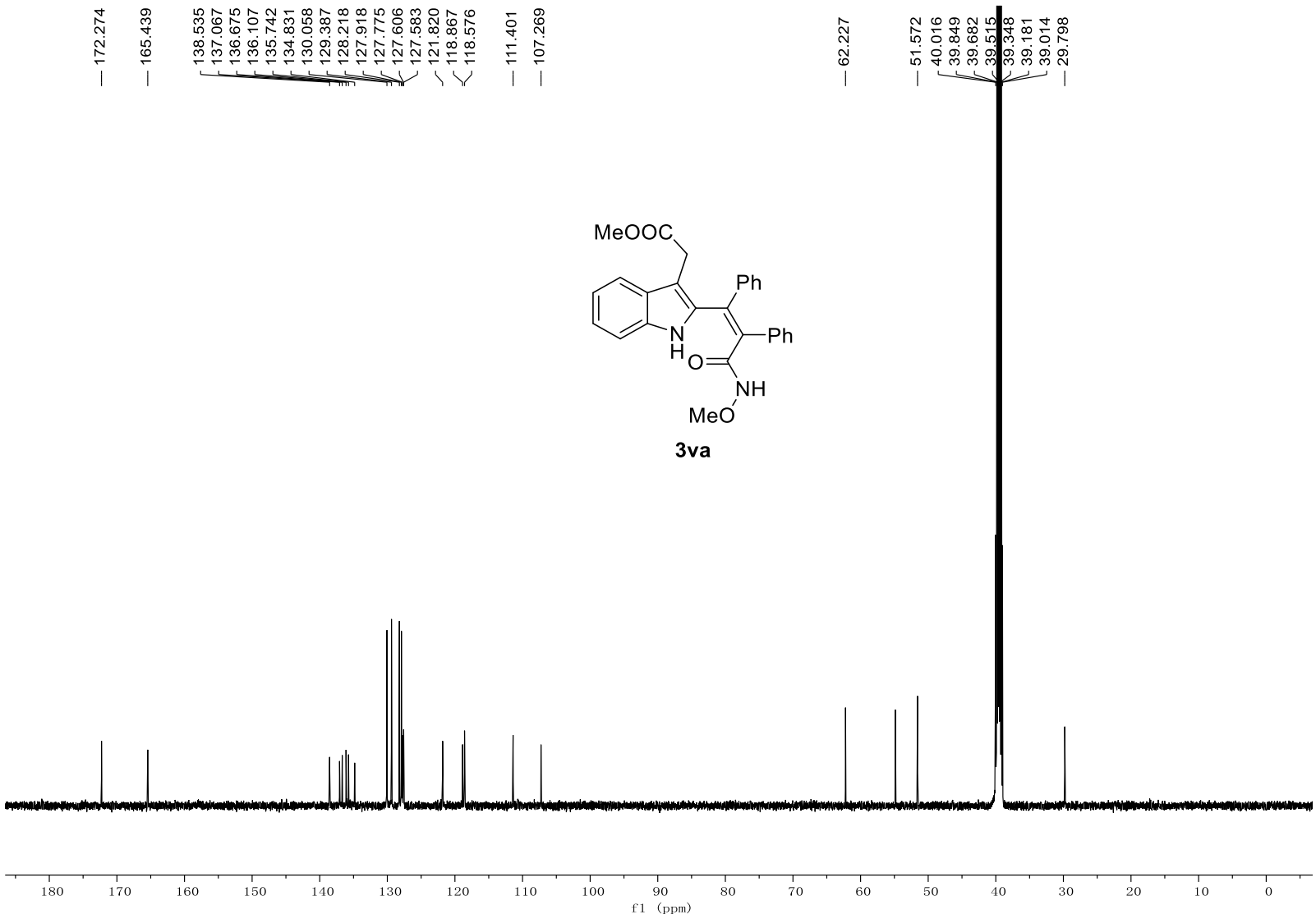

11.240
11.098
7.567
7.552
7.524
7.507
7.331
7.316
7.301
7.283
7.270
7.255
7.251
7.237
7.202
7.199
7.185
7.182
7.172
7.157
7.134
7.121
7.046
7.034
7.019
6.889
6.876
6.874
3.361
3.188
2.534
2.531
2.527
2.523
2.519
Cl
Ph
Ph
Ph
N
H
O
NH
MeO
3ta
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
1.00
0.98
3.00
1.00
2.00
3.00
2.02
2.00
3.00
2.00
3.00
13.0
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
f1 (ppm)

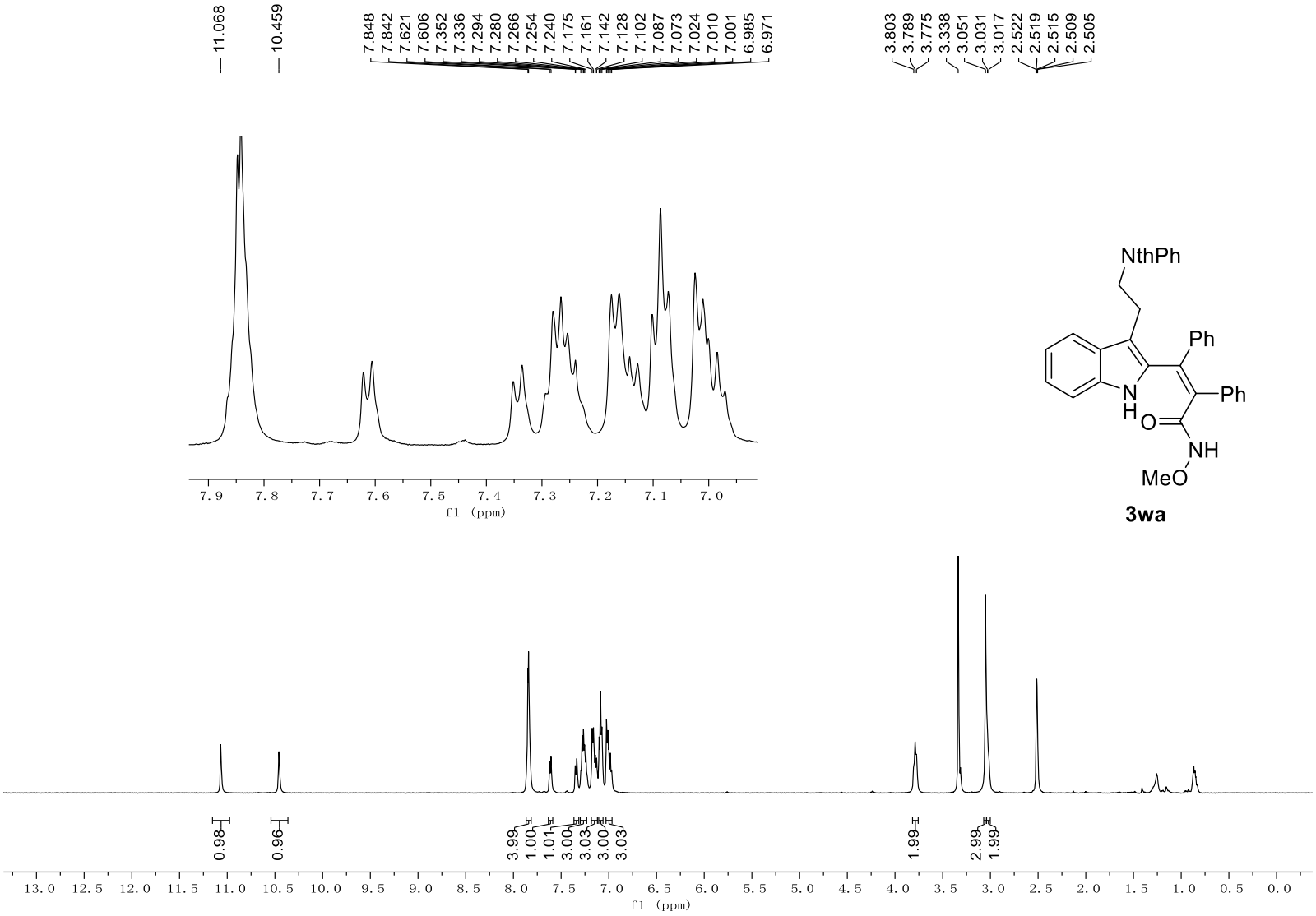

165.647
138.519
137.182
136.298
135.240
134.881
134.323
130.425
129.635
129.101
128.762
128.558
128.154
128.052
126.277
124.787
122.441
118.217
115.714
113.867
62.995
40.495
40.329
40.163
39.996
39.830
39.663
39.497
Cl
Ph
Ph
Ph
N
H
O
NH
MeO
3ta
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

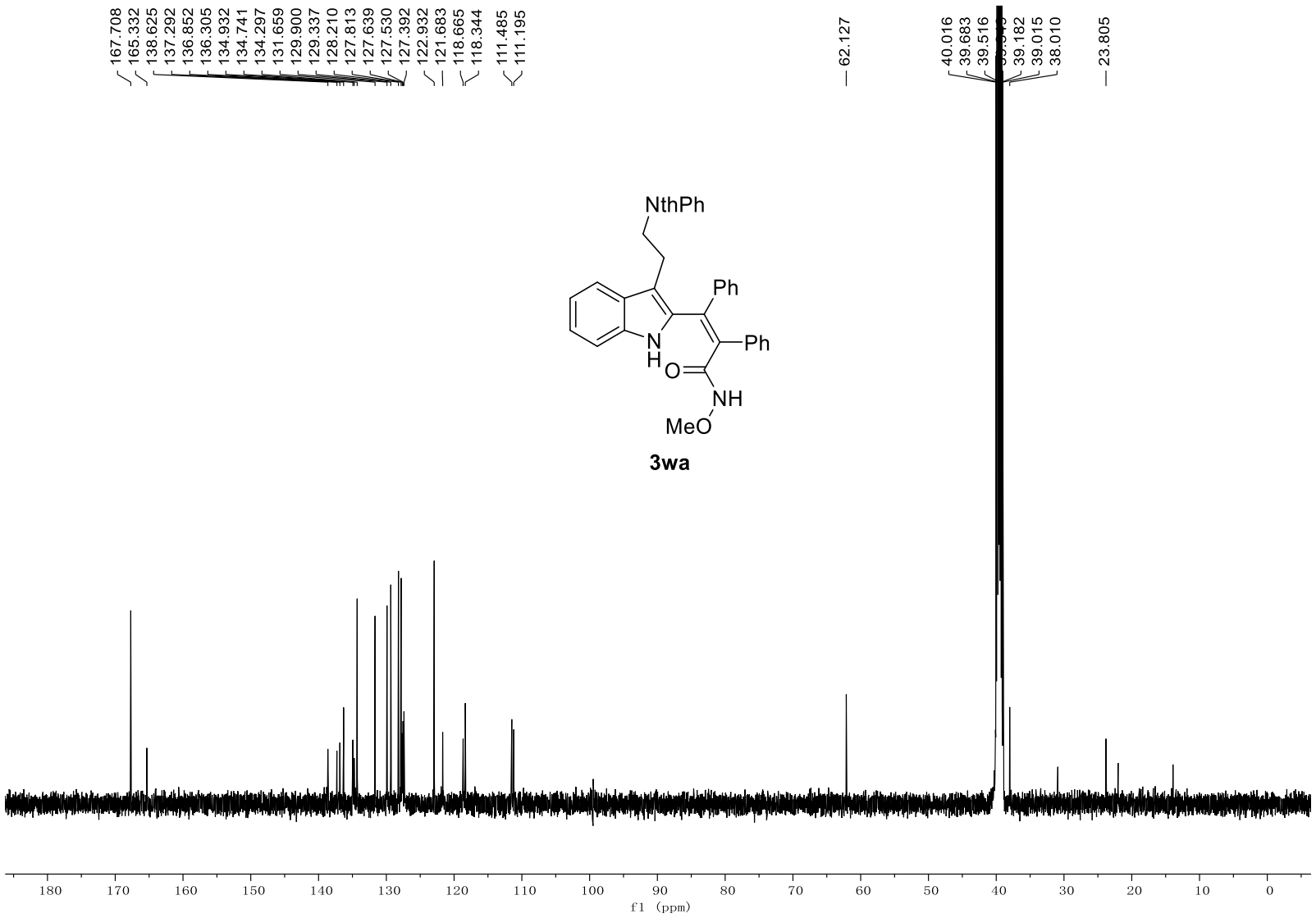

11.202
11.041
7.665
7.521
7.505
7.441
7.424
7.292
7.277
7.262
7.255
7.227
7.212
7.194
7.148
7.133
7.119
7.095
7.081
7.004
6.991
6.976
6.964
6.847
6.833
3.309
3.153
2.492
2.489
2.485
2.481
2.477
Br
Ph
Ph
Ph
N
H
O
NH
MeO
3ua
f1 (ppm)
0.97
0.95
1.00
2.00
1.00
3.03
3.00
1.05
2.00
3.00
2.00
3.00
f1 (ppm)

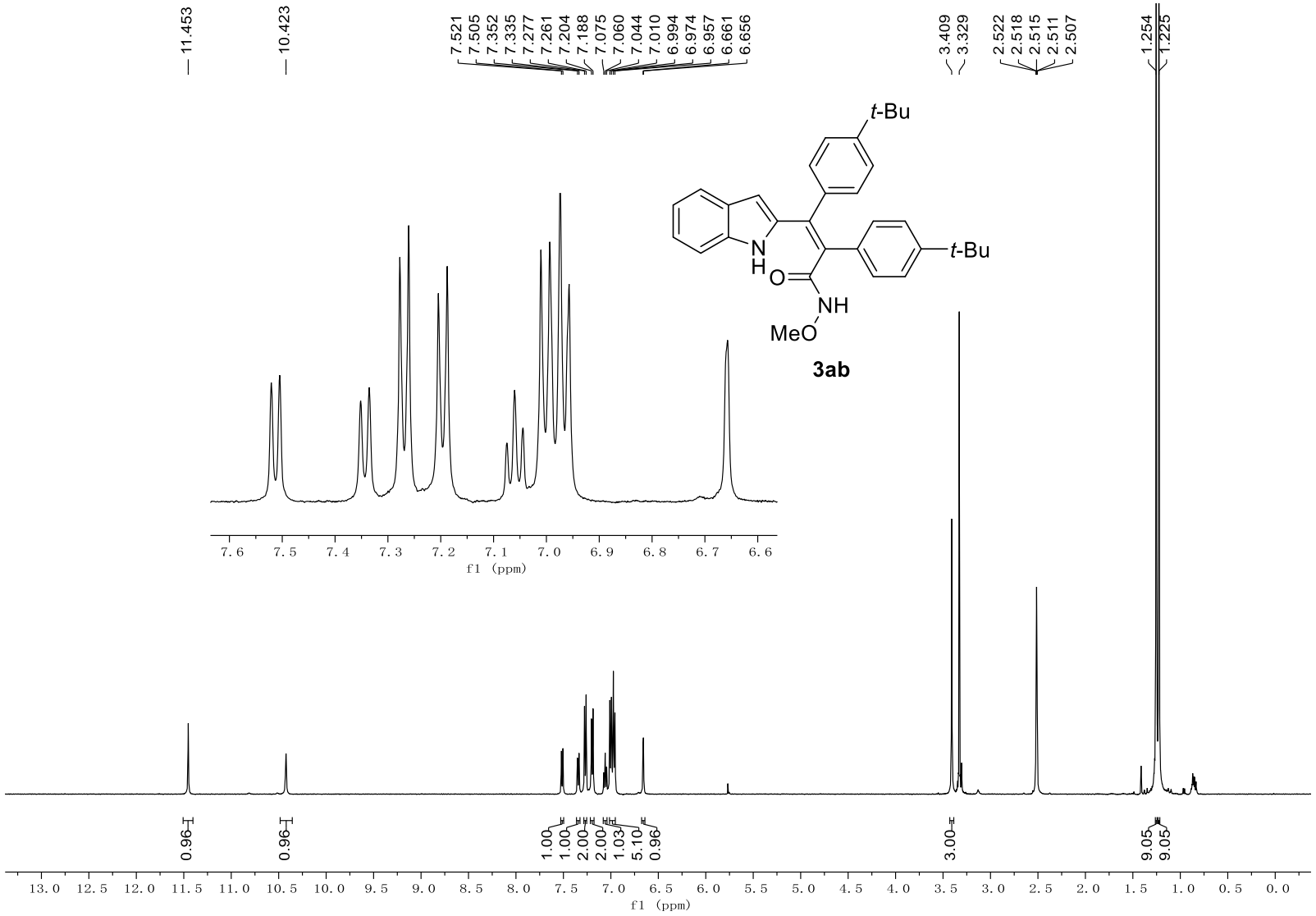

165.590
138.471
137.125
136.072
135.151
135.051
134.240
130.369
129.584
129.072
128.705
128.516
128.108
128.006
126.249
124.916
121.169
115.568
114.268
112.666
62.949
40.447
40.281
40.115
39.948
39.781
39.615
39.448
Br
Ph
Ph
Ph
N
H
O
NH
MeO
3ua
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.066
10.720
7.490
7.474
7.368
7.352
7.276
7.261
7.246
7.228
7.191
7.181
7.130
7.117
7.109
7.093
7.034
7.024
7.010
6.995
3.684
3.579
3.344
3.060
2.521
2.518
2.513
2.509
2.506
MeOOC
Ph
Ph
N
H
O
NH
MeO
3va
f1 (ppm)
0.96
1.00
0.99
0.99
2.97
2.99
3.02
3.06
2.01
3.02
3.03
f1 (ppm)


172.274
165.439
138.535
137.067
136.675
136.107
135.742
134.831
130.058
129.387
128.218
127.918
127.775
127.606
127.583
121.820
118.867
118.576
111.401
107.269
62.227
51.572
40.016
39.849
39.682
39.515
39.348
39.181
39.014
29.798
MeOOC
Ph
Ph
N
H
O
NH
MeO
3va
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.068
10.459
7.848
7.842
7.621
7.606
7.352
7.336
7.294
7.280
7.266
7.254
7.240
7.175
7.161
7.142
7.128
7.102
7.087
7.073
7.024
7.010
7.001
6.985
6.971
3.803
3.789
3.775
3.338
3.051
3.031
3.017
2.522
2.519
2.515
2.509
2.505
f1 (ppm)
NthPh
Ph
Ph
N
H
O
NH
MeO
3wa
0.98
0.96
3.99
1.00
1.01
3.00
3.03
3.00
3.03
1.99
2.99
1.99
f1 (ppm)


167.708
165.332
138.625
137.292
136.852
136.305
134.932
134.741
134.297
131.659
129.900
129.337
128.210
127.813
127.639
127.530
127.392
122.932
121.683
118.665
118.344
111.485
111.195
62.127
40.016
39.683
39.516
39.182
39.015
38.010
23.805
NthPh
Ph
Ph
N
H
O
NH
MeO
3wa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.453
10.423
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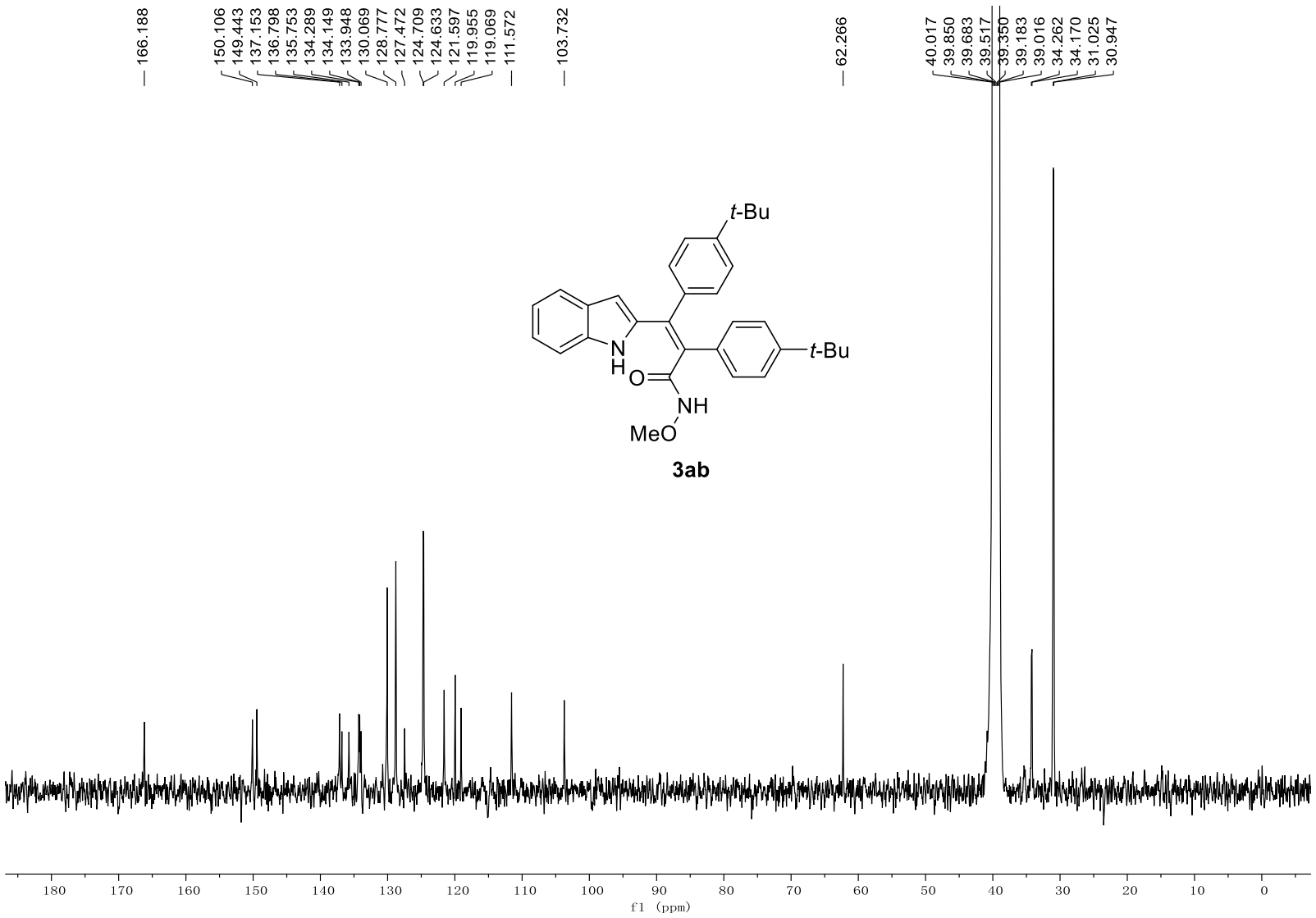
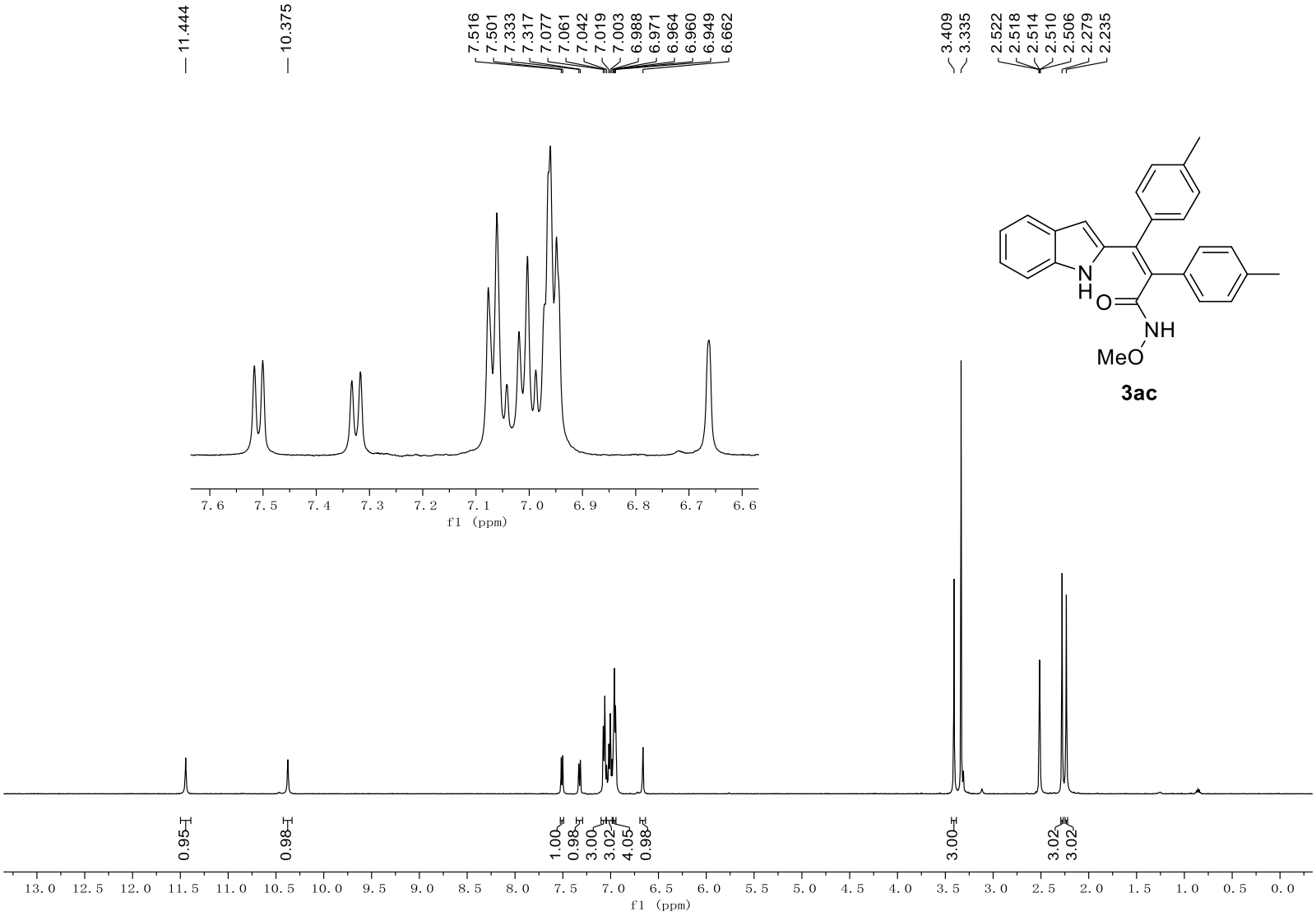
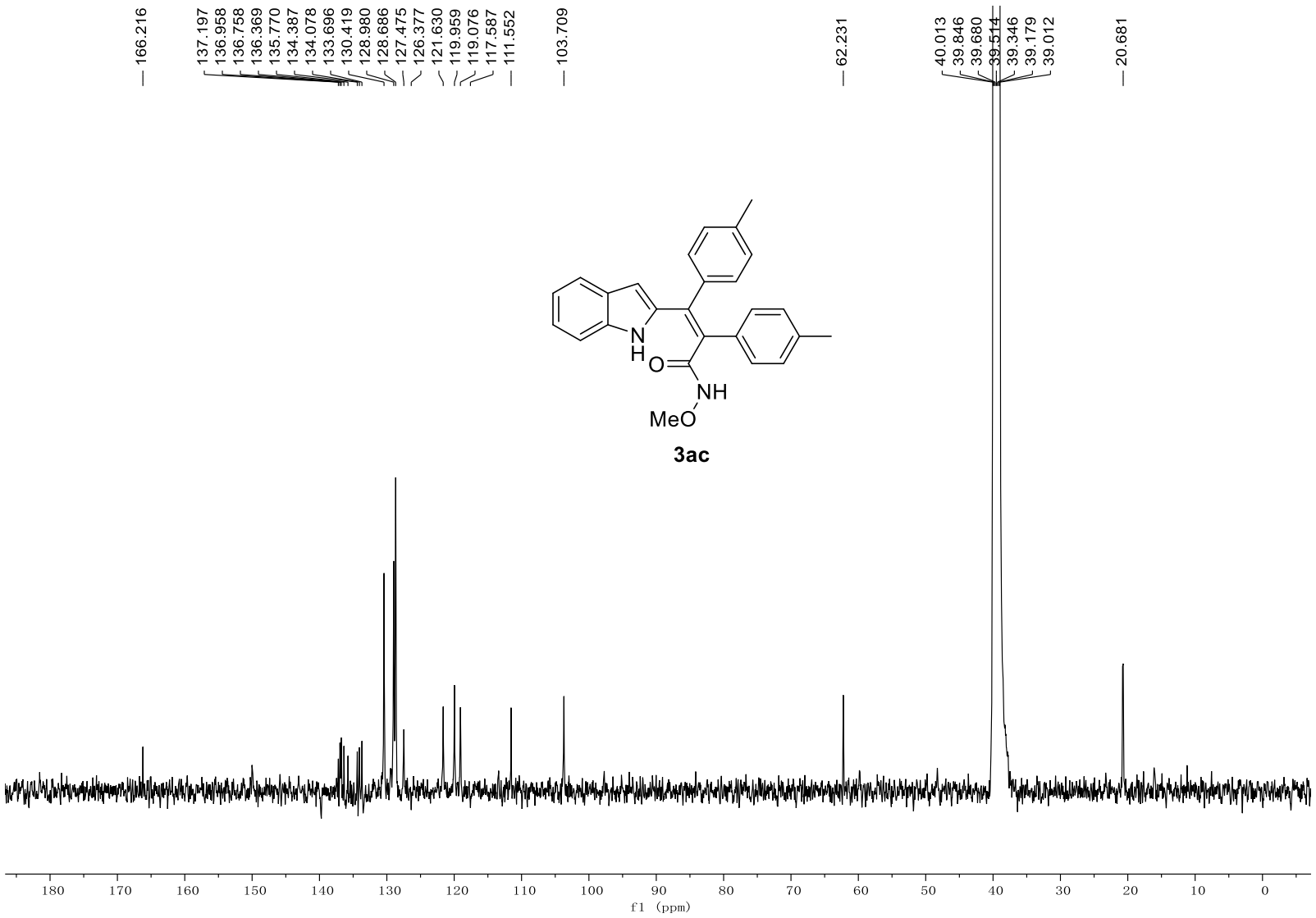
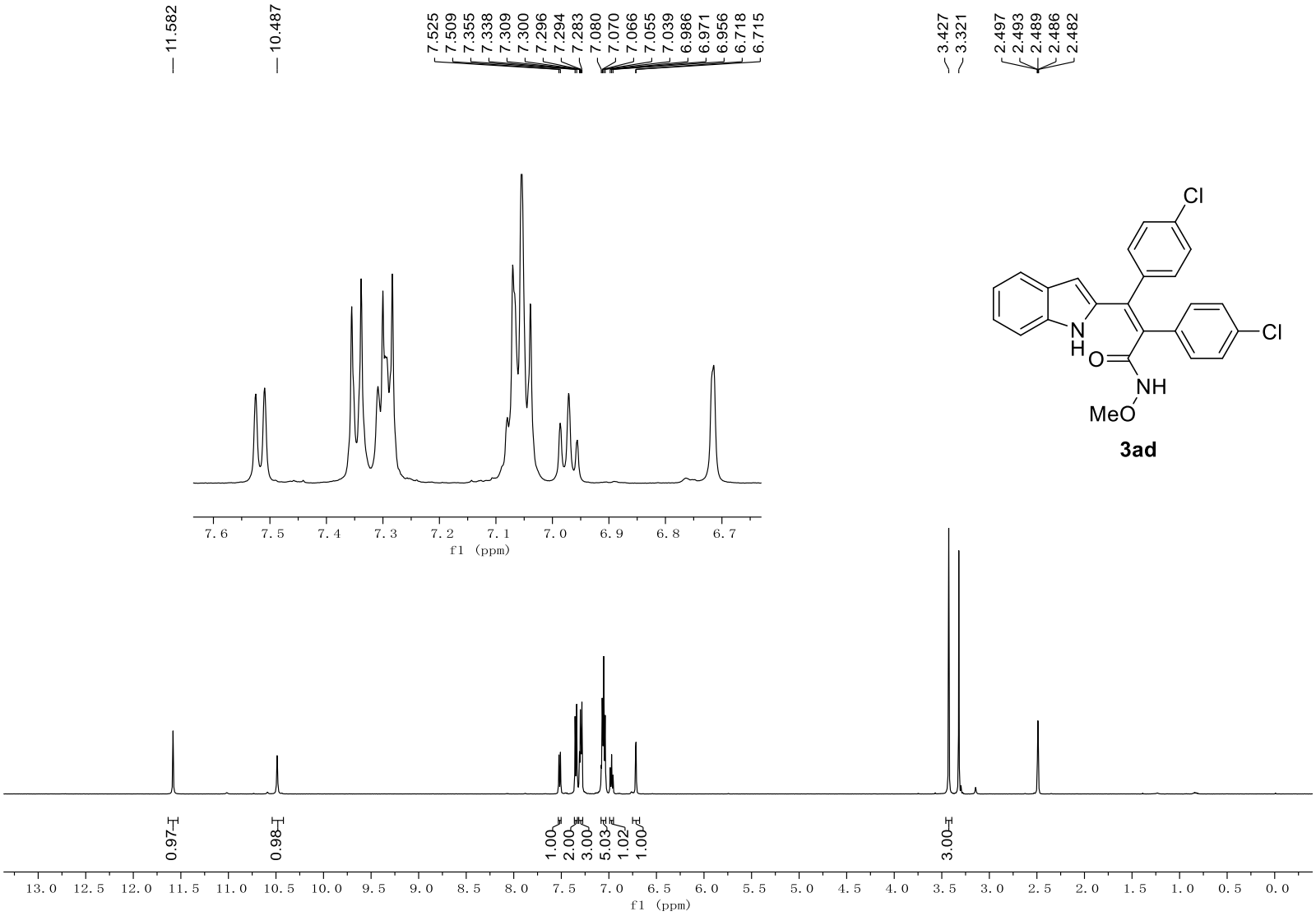
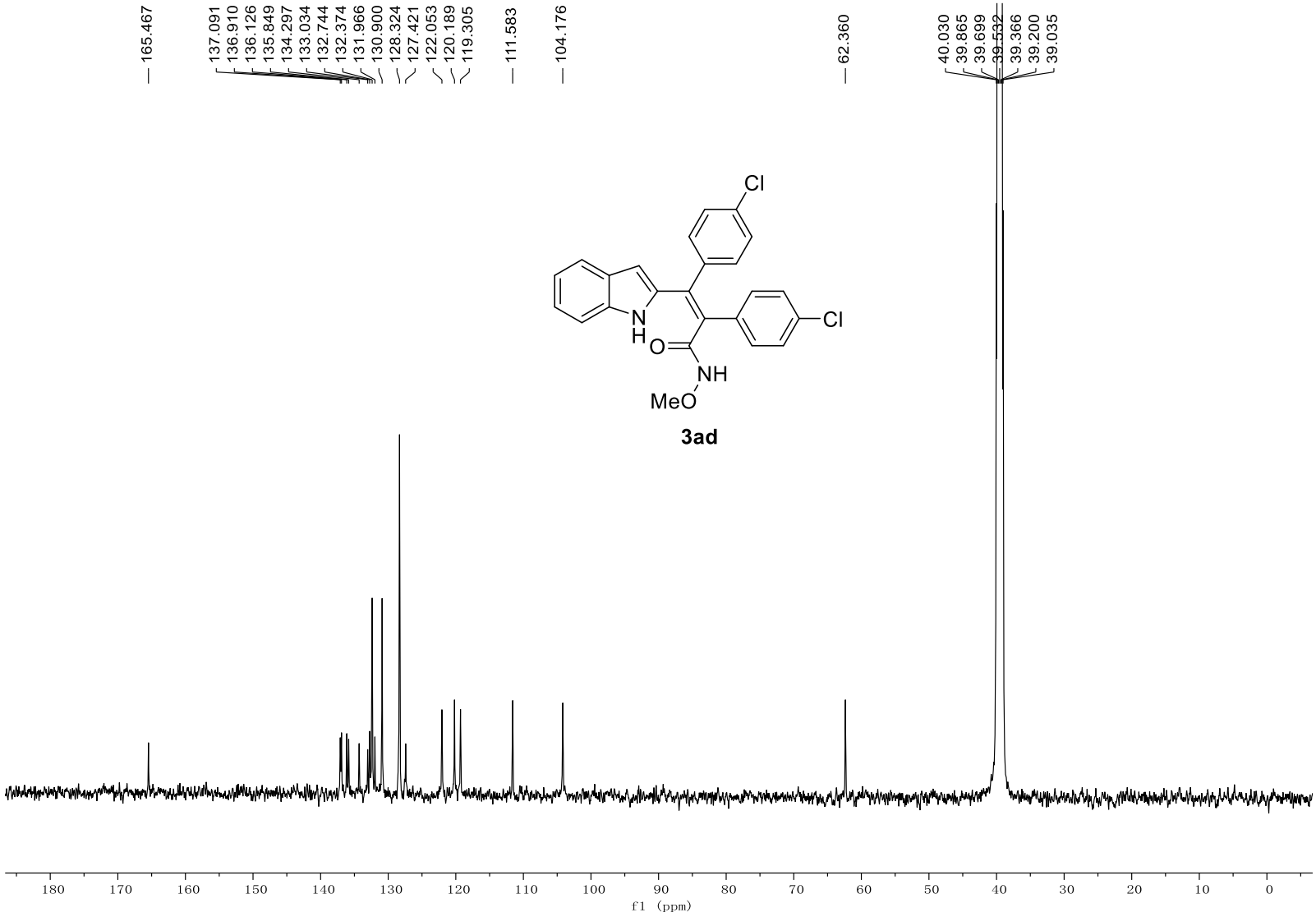
7.505
7.352
7.335
7.277
7.261
7.204
7.188
7.075
7.060
7.044
7.010
6.994
6.974
6.957
6.661
6.656
3.409
3.329
2.522
2.518
2.515
2.511
2.507
1.254
1.225
t-Bu
t-Bu
N
H
O
NH
MeO
3ab
f1 (ppm)
0.96
0.96
1.00
1.00
2.00
2.00
1.03
5.10
0.96
3.00
9.05
9.05
f1 (ppm)

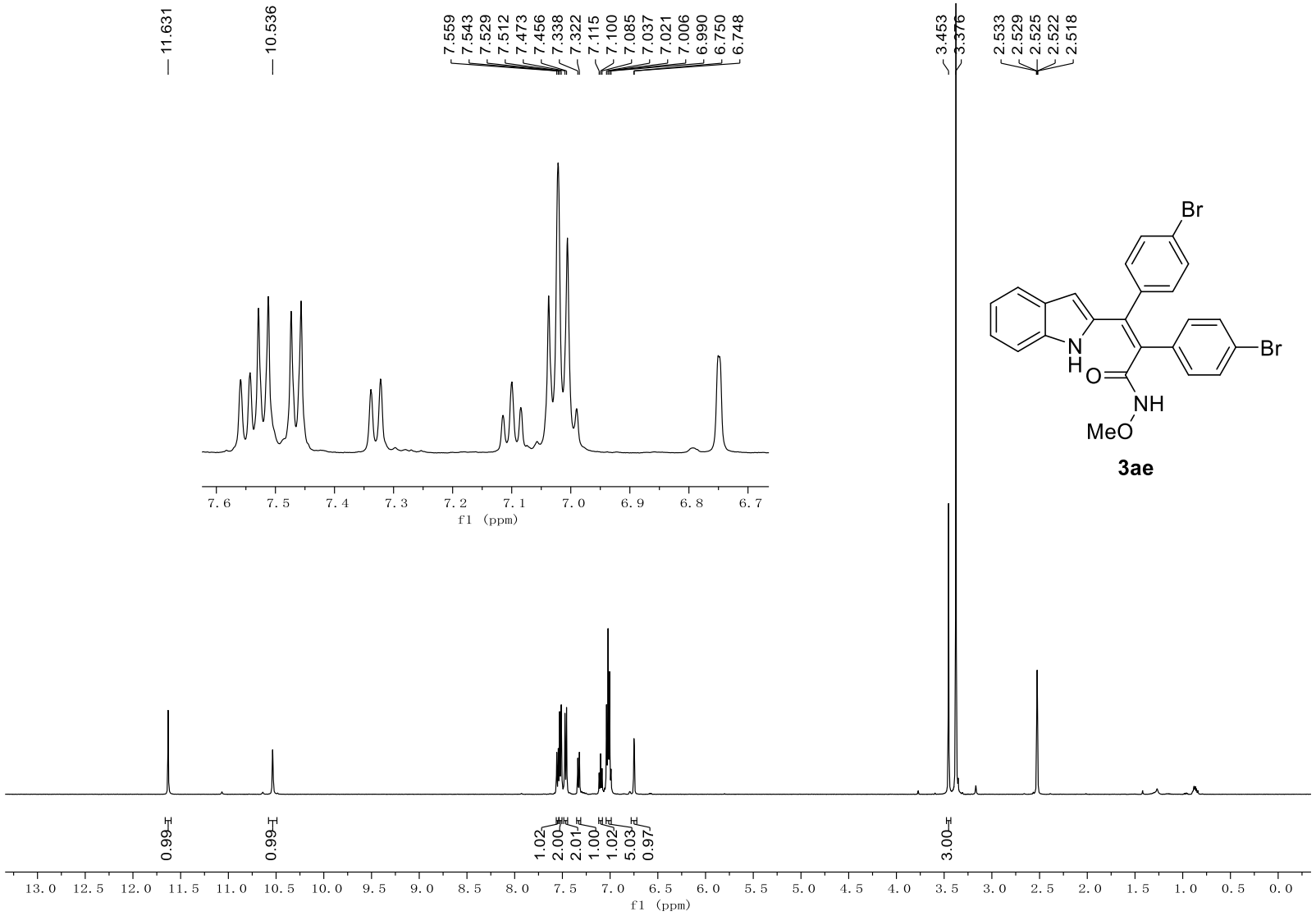

166.188
150.106
149.443
137.153
136.798
135.753
134.289
134.149
133.948
130.069
128.777
127.472
124.709
124.633
121.597
119.955
119.069
111.572
103.732
62.266
40.017
39.850
39.683
39.517
39.350
39.183
39.016
34.262
34.170
31.025
30.947
t-Bu
t-Bu
N
H
O
NH
MeO
3ab
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

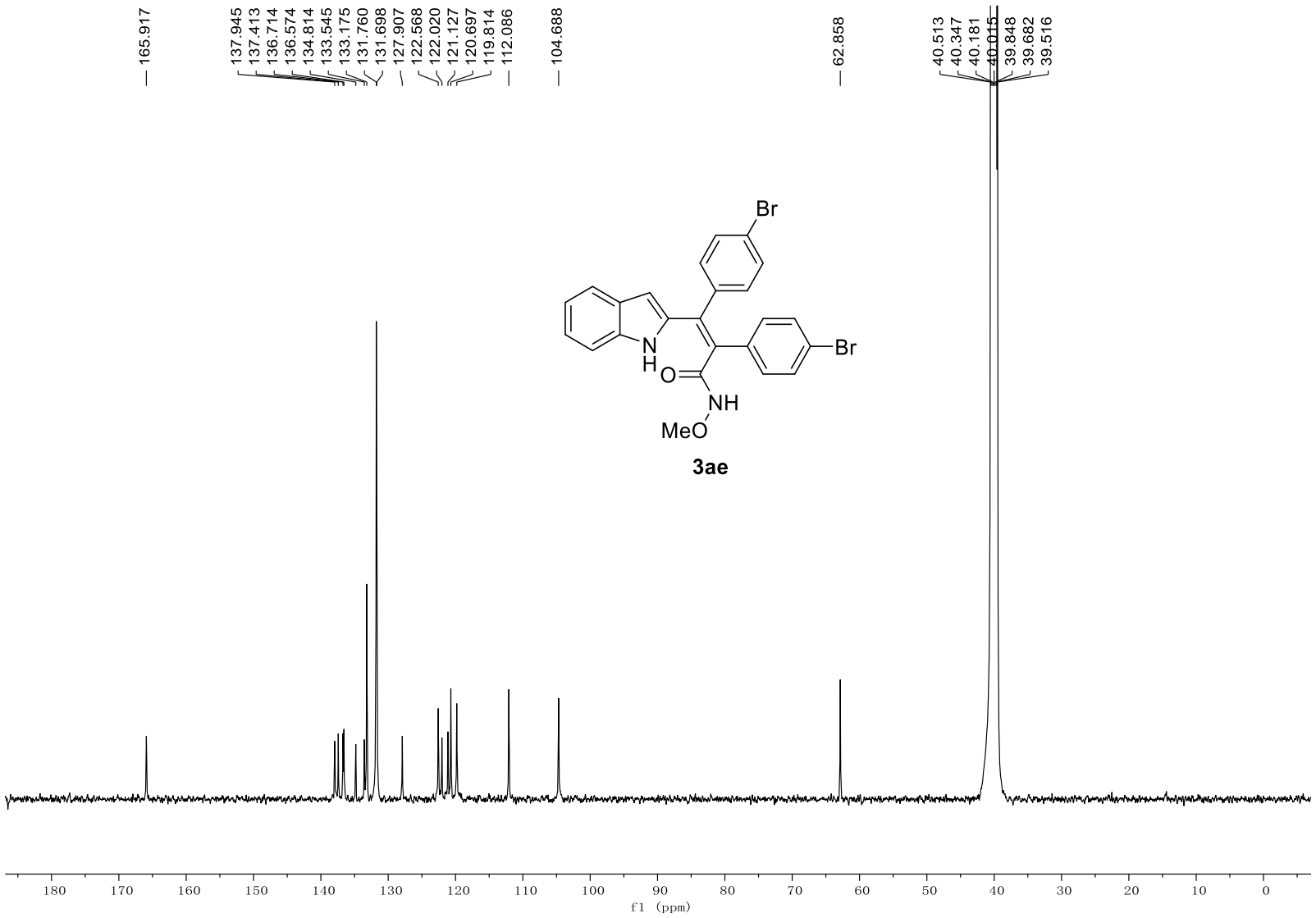

11.444
10.375
7.516
7.501
7.333
7.317
7.077
7.061
7.042
7.019
7.003
6.988
6.971
6.964
6.960
6.949
6.662
3.409
3.335
2.522
2.518
2.514
2.510
2.506
2.279
2.235
N
H
O
NH
MeO
3ac
0.95
0.98
1.00
0.98
3.00
3.02
4.05
0.98
3.00
3.02
3.02
f1 (ppm)

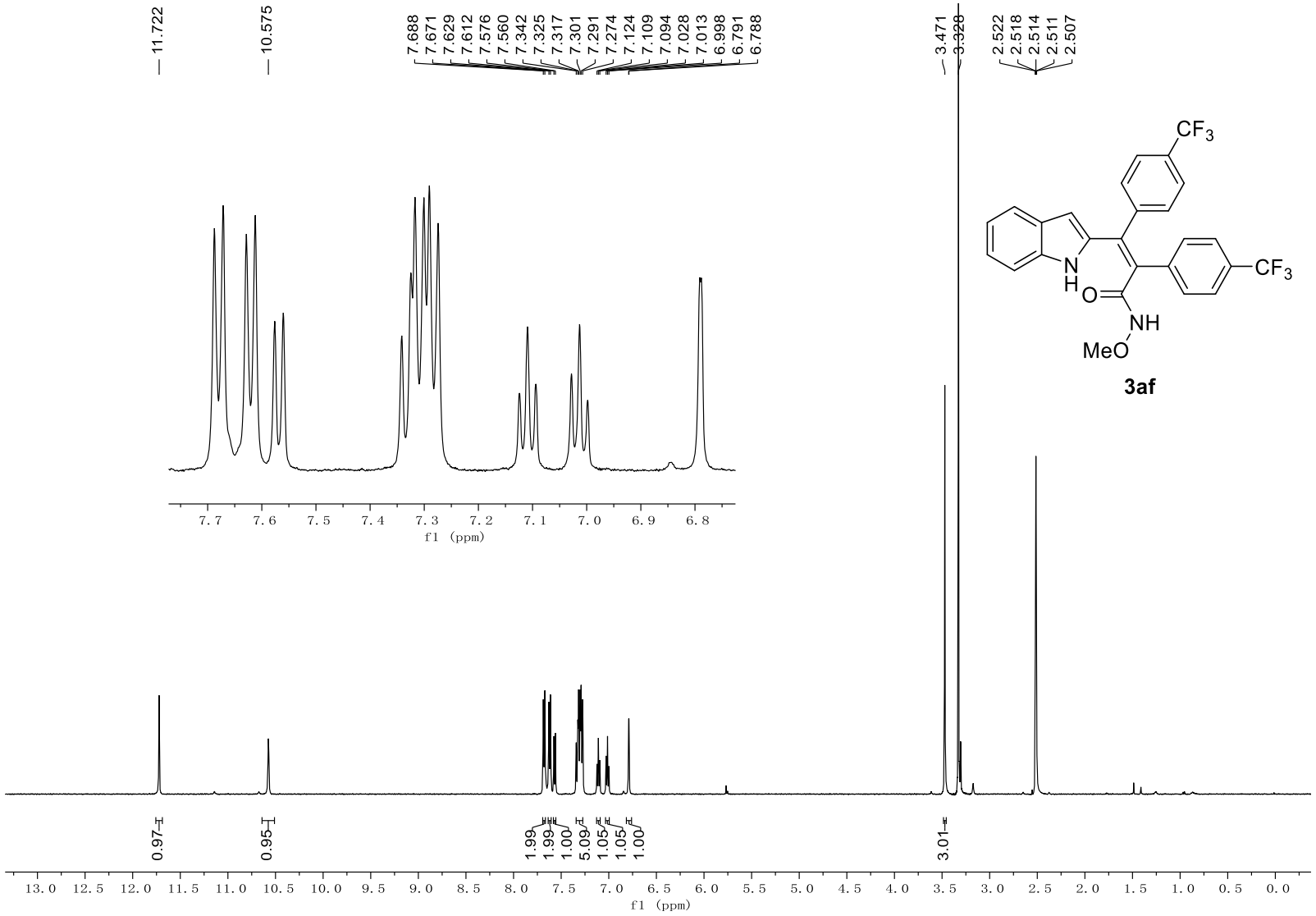

166.216
137.197
136.958
136.758
136.369
135.770
134.387
134.078
133.696
130.419
128.980
128.686
127.475
126.377
121.630
119.959
119.076
117.587
111.552
103.709
62.231
40.013
39.846
39.680
39.514
39.346
39.179
39.012
20.681
N
H
O
NH
MeO
3ac
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

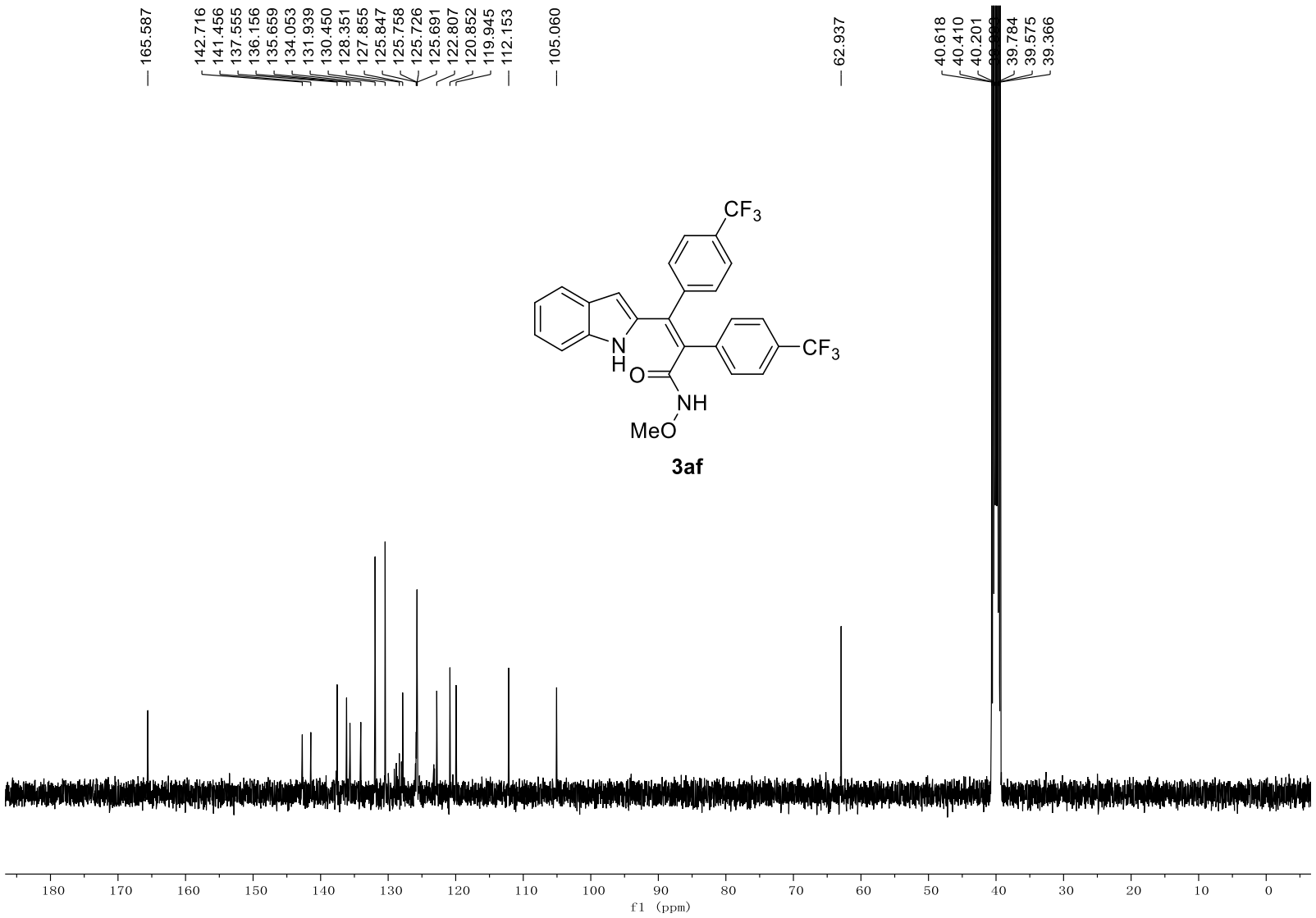

11.582
10.487
7.525
7.509
7.355
7.338
7.309
7.300
7.296
7.294
7.283
7.080
7.070
7.066
7.055
7.039
6.986
6.971
6.956
6.718
6.715
3.427
3.321
2.497
2.493
2.489
2.486
2.482
Cl
Cl
N
H
O
NH
MeO
3ad
f1 (ppm)
0.97
0.98
1.00
2.00
3.00
5.03
1.02
1.00
3.00
f1 (ppm)

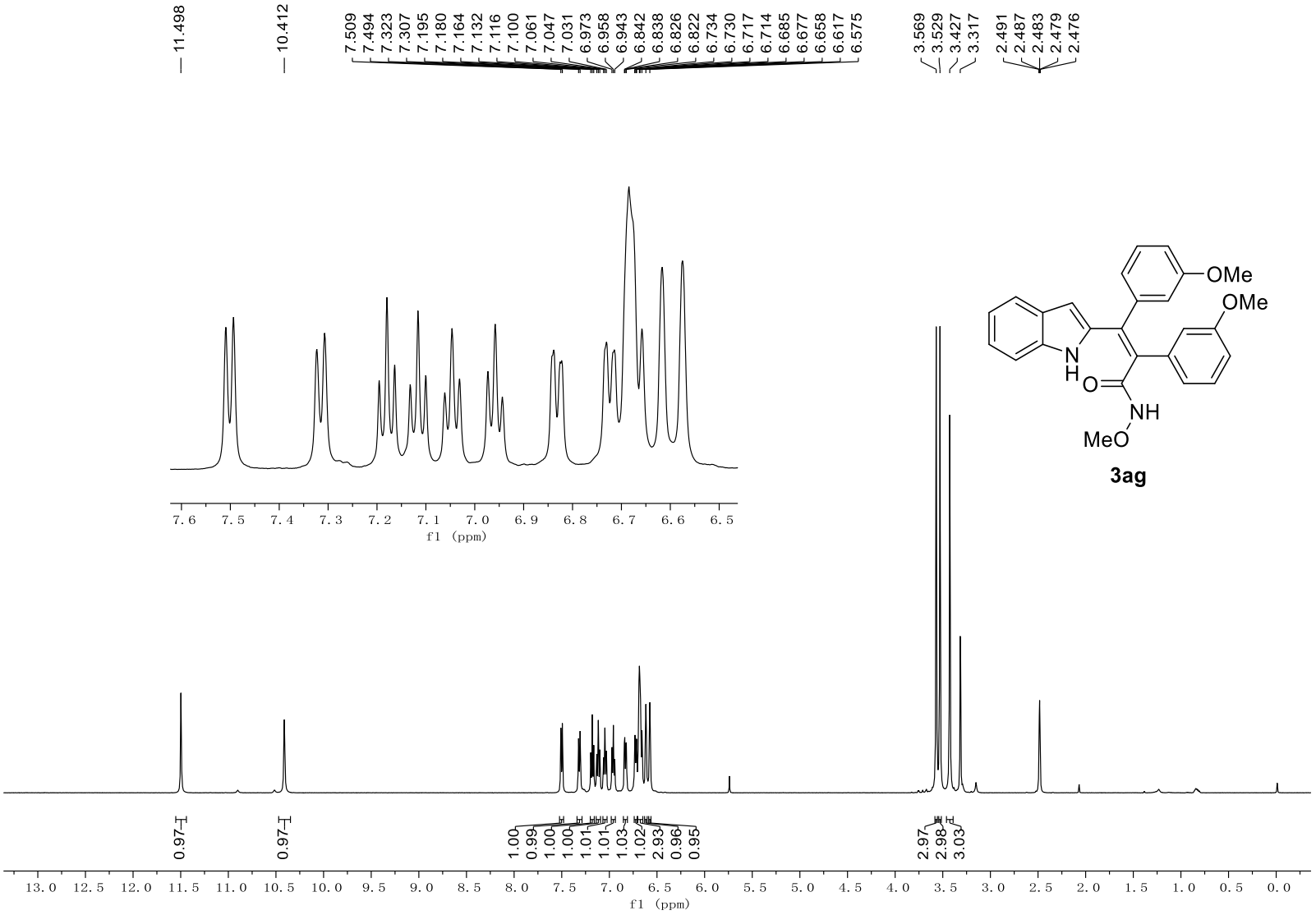

165.467
137.091
136.910
136.126
135.849
134.297
133.034
132.744
132.374
131.966
130.900
128.324
127.421
122.053
120.189
119.305
111.583
104.176
62.360
40.030
39.865
39.699
39.532
39.366
39.200
39.035
Cl
Cl
N
H
O
NH
MeO
3ad
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

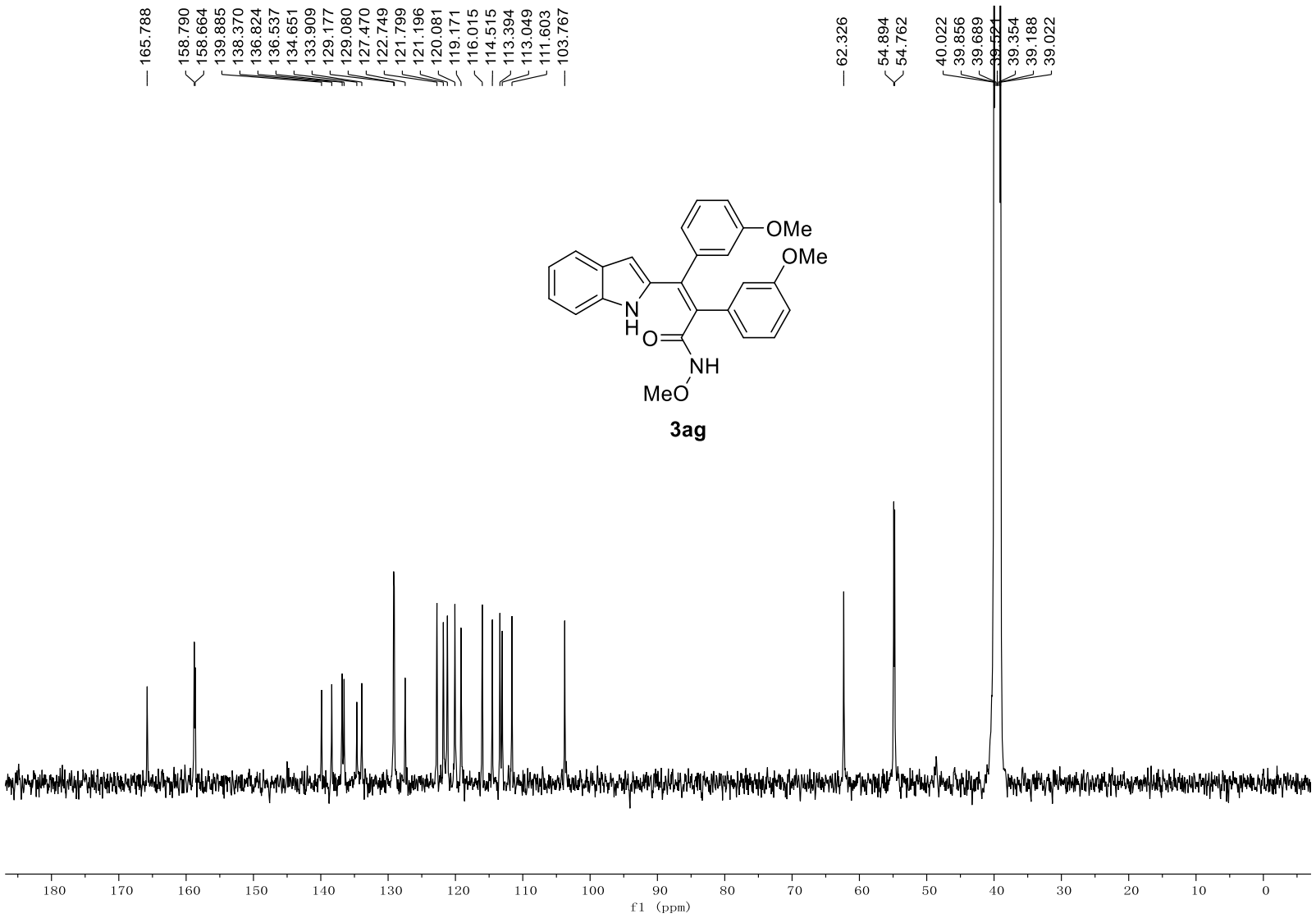

11.631
10.536
7.559
7.543
7.529
7.512
7.473
7.456
7.338
7.322
7.115
7.100
7.085
7.037
7.021
7.006
6.990
6.750
6.748
3.453
3.376
2.533
2.529
2.525
2.522
2.518
Br
Br
N
H
O
NH
MeO
3ae
f1 (ppm)
0.99
0.99
1.02
2.00
2.01
1.00
1.02
5.03
0.97
3.00
f1 (ppm)

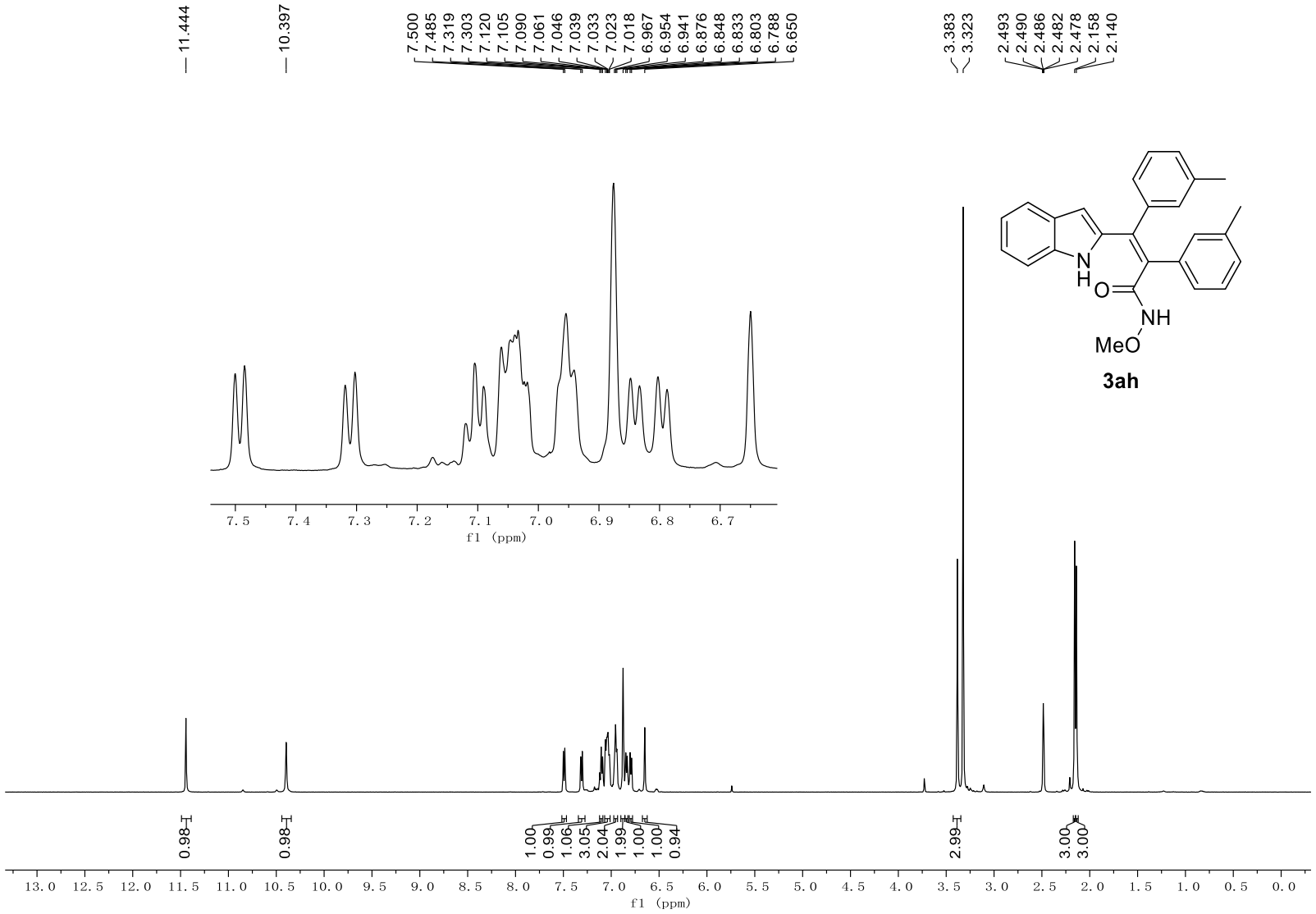

165.917
137.945
137.413
136.714
136.574
134.814
133.545
133.175
131.760
131.698
127.907
122.568
122.020
121.127
120.697
119.814
112.086
104.688
62.858
40.513
40.347
40.181
40.015
39.848
39.682
39.516
Br
Br
N
H
O
NH
MeO
3ae
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

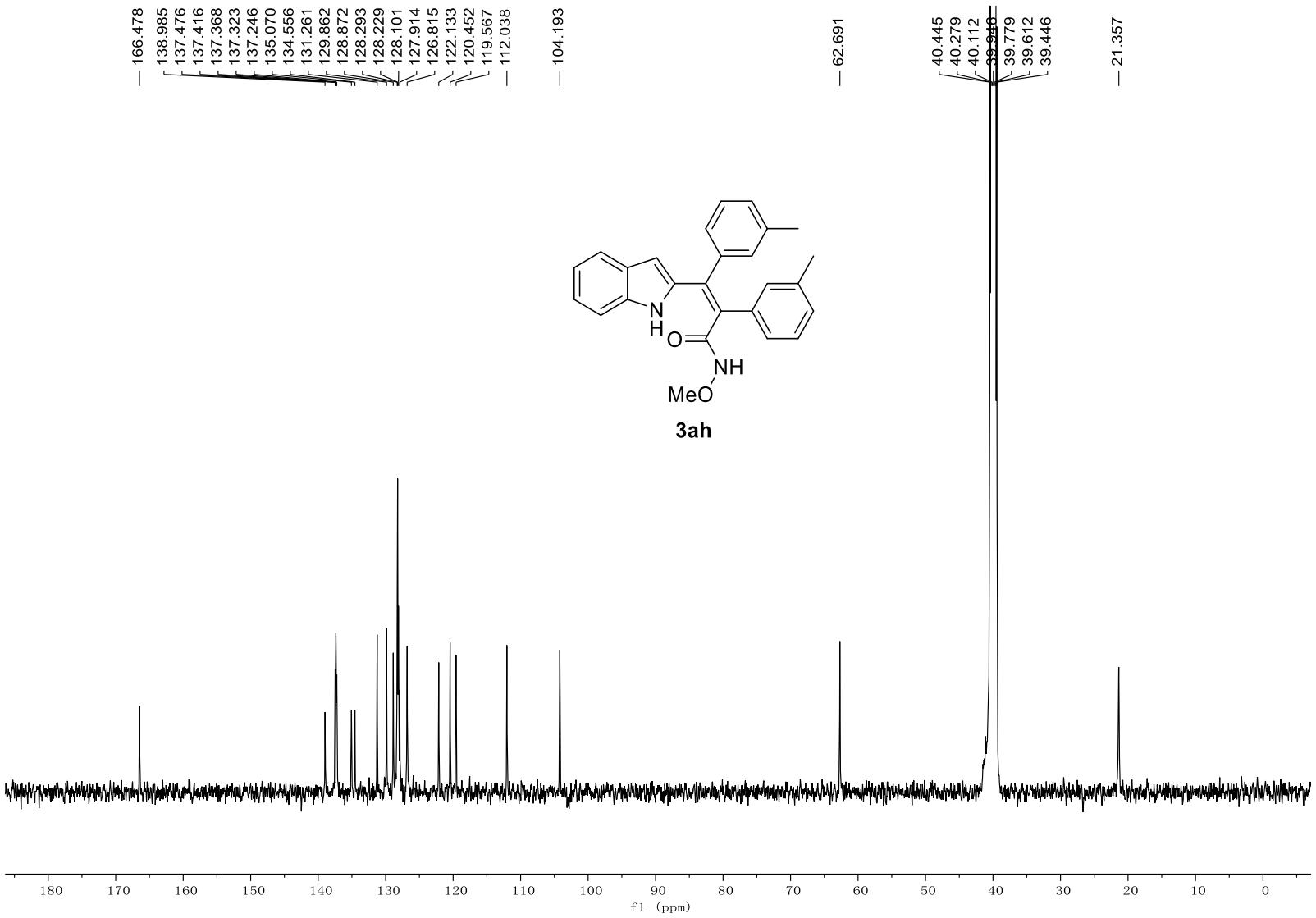

11.722
10.575
7.688
7.671
7.629
7.612
7.576
7.560
7.342
7.325
7.317
7.301
7.291
7.274
7.124
7.109
7.094
7.028
7.013
6.998
6.791
6.788
3.471
3.328
2.522
2.518
2.514
2.511
2.507
CF3
CF3
N
H
O
NH
MeO
3af
f1 (ppm)
0.97
0.95
1.99
1.99
1.00
5.09
1.05
1.05
1.00
3.01
f1 (ppm)

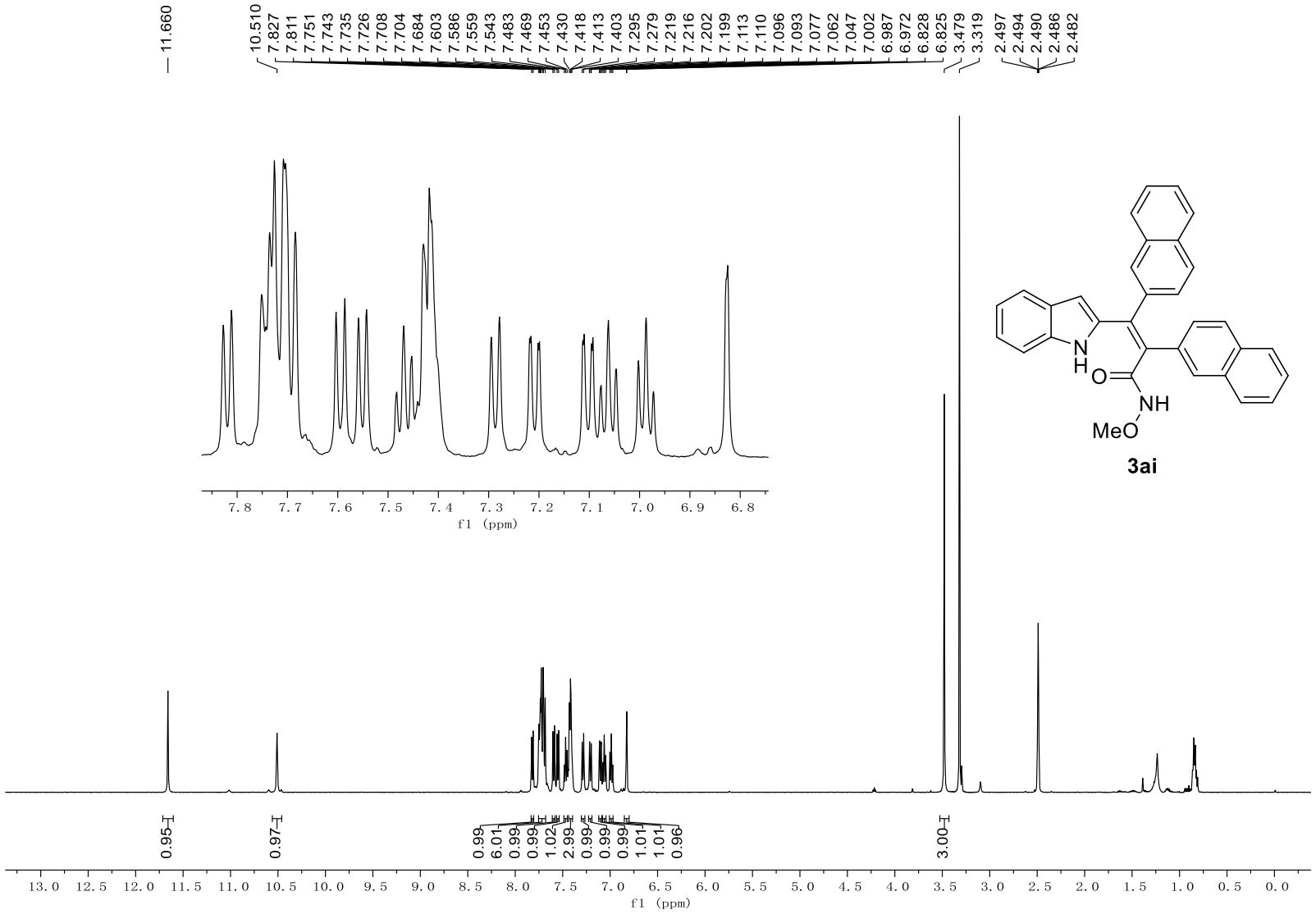

165.587
142.716
141.456
137.555
136.156
135.659
134.053
131.939
130.450
128.351
127.855
125.847
125.758
125.726
125.691
122.807
120.852
119.945
112.153
105.060
62.937
40.618
40.410
40.201
39.784
39.575
39.366
CF3
CF3
N
H
O
NH
MeO
3af
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

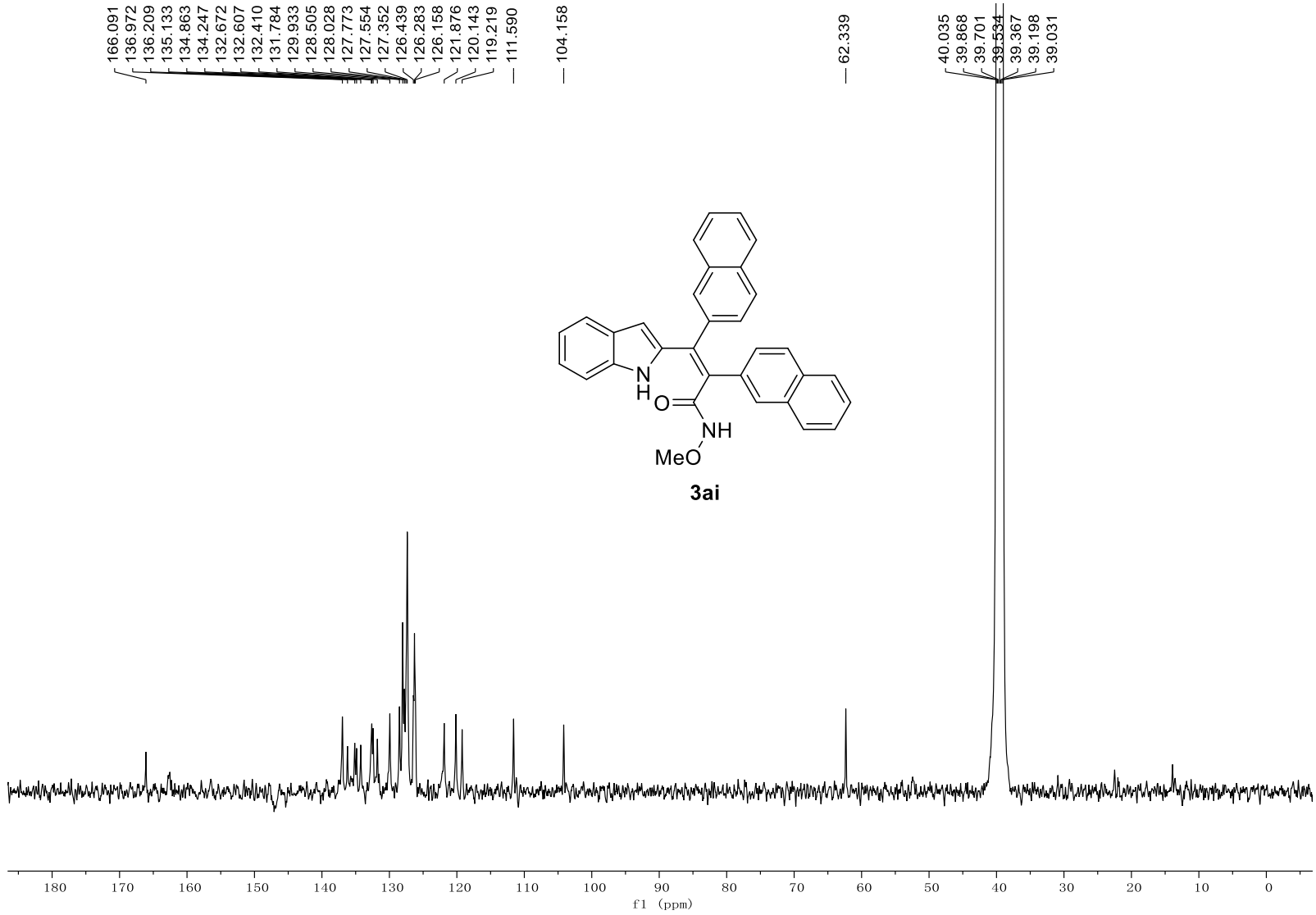

11.498
10.412
7.509
7.494
7.323
7.307
7.195
7.180
7.164
7.132
7.116
7.100
7.061
7.047
7.031
6.973
6.958
6.943
6.842
6.838
6.826
6.822
6.734
6.730
6.717
6.714
6.685
6.677
6.658
6.617
6.575
3.569
3.529
3.427
3.317
2.491
2.487
2.483
2.479
2.476
OMe
OMe
N
H
O
NH
MeO
3ag
f1 (ppm)
0.97
0.97
1.00
0.99
1.00
1.00
1.01
1.01
1.03
1.02
2.93
0.96
0.95
2.97
2.98
3.03
f1 (ppm)

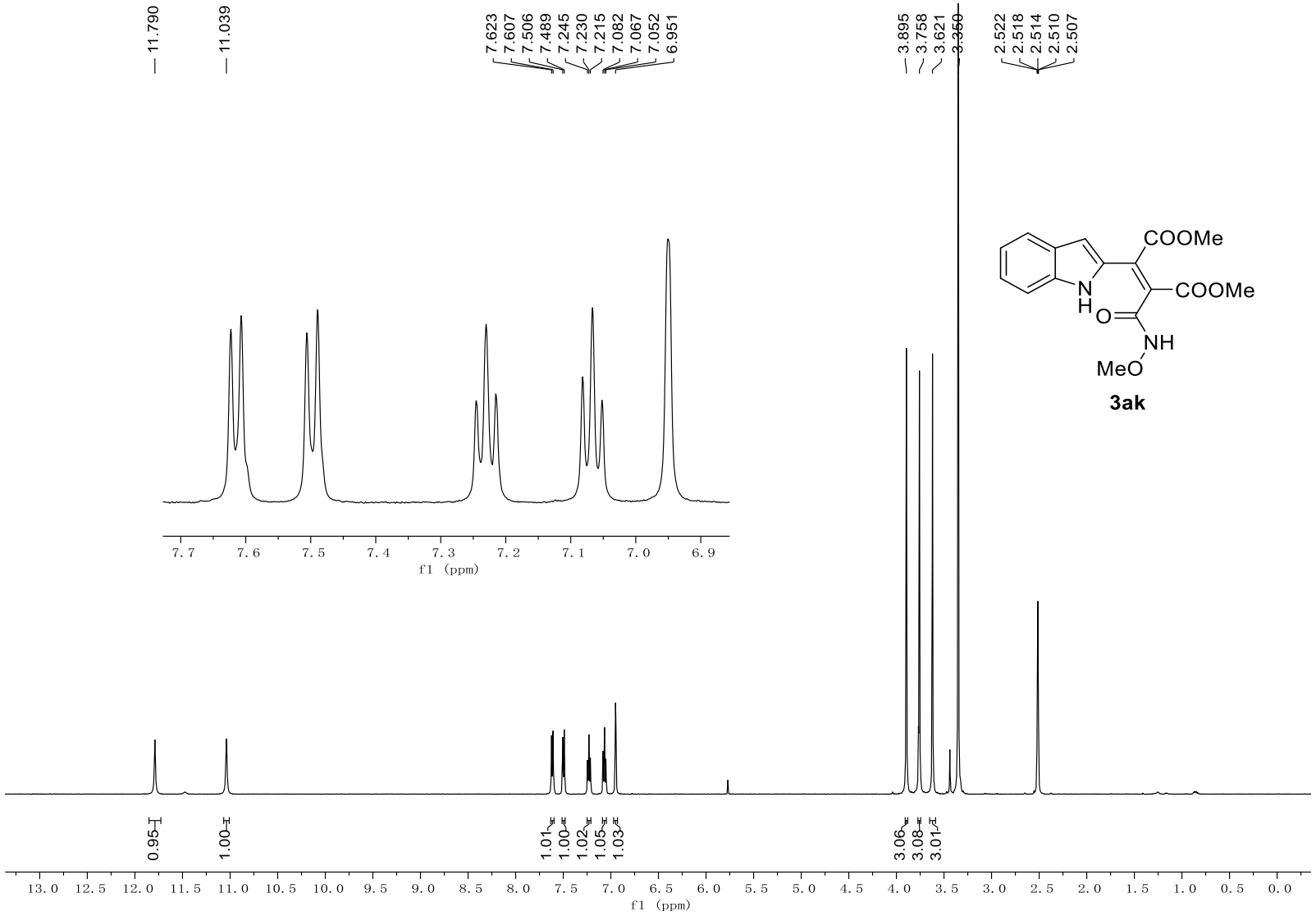

165.788
158.790
158.664
139.885
138.370
136.824
136.537
134.651
133.909
129.177
129.080
127.470
122.749
121.799
121.196
120.081
119.171
116.015
114.515
113.394
113.049
111.603
103.767
62.326
54.894
54.762
40.022
39.856
39.689
39.521
39.354
39.188
39.022
OMe
OMe
N
H
O
NH
MeO
3ag
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

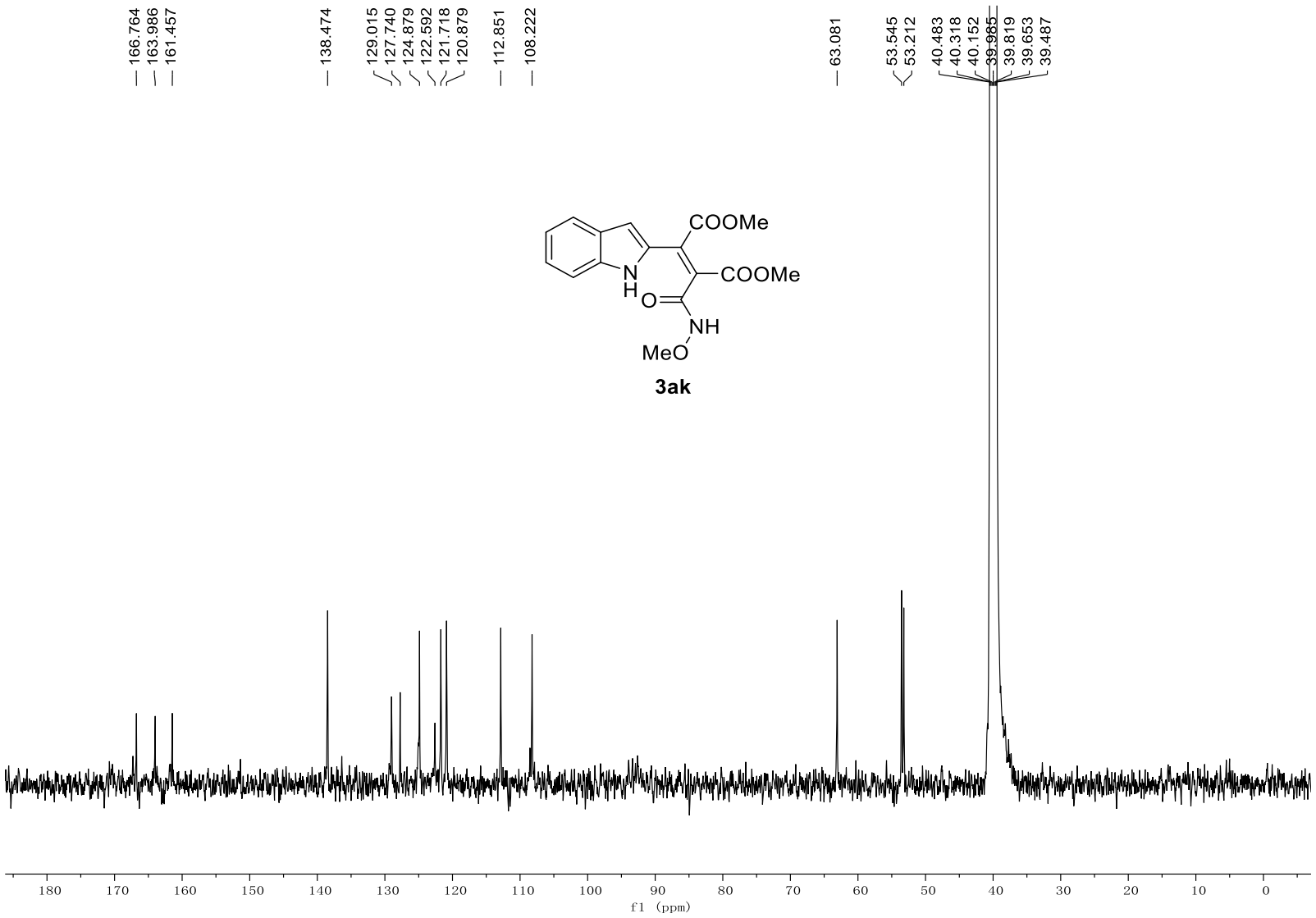

11.444
10.397
7.500
7.485
7.319
7.303
7.120
7.105
7.090
7.061
7.046
7.039
7.033
7.023
7.018
6.967
6.954
6.941
6.876
6.848
6.833
6.803
6.788
6.650
3.383
3.323
2.493
2.490
2.486
2.482
2.478
2.158
2.140
f1 (ppm)
0.98
0.98
1.00
0.99
1.06
3.05
2.04
1.99
1.00
1.00
0.94
2.99
3.00
3.00
f1 (ppm)
3ah

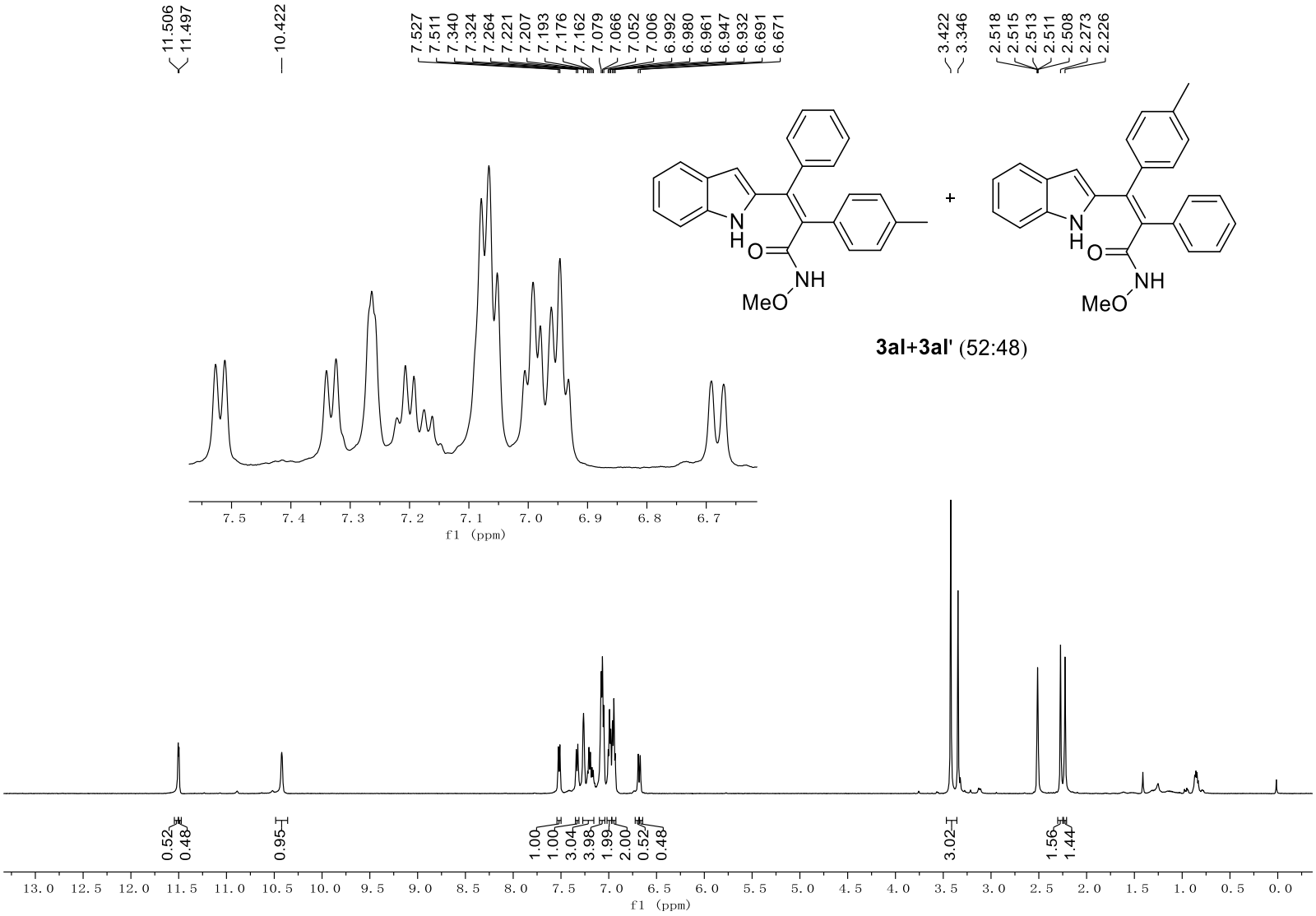

166.478
138.985
137.476
137.416
137.368
137.323
137.246
135.070
134.556
131.261
129.862
128.872
128.293
128.229
128.101
127.914
126.815
122.133
120.452
119.567
112.038
104.193
62.691
40.445
40.279
40.112
39.946
39.779
39.612
39.446
21.357
N
H
O
NH
MeO
3ah
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

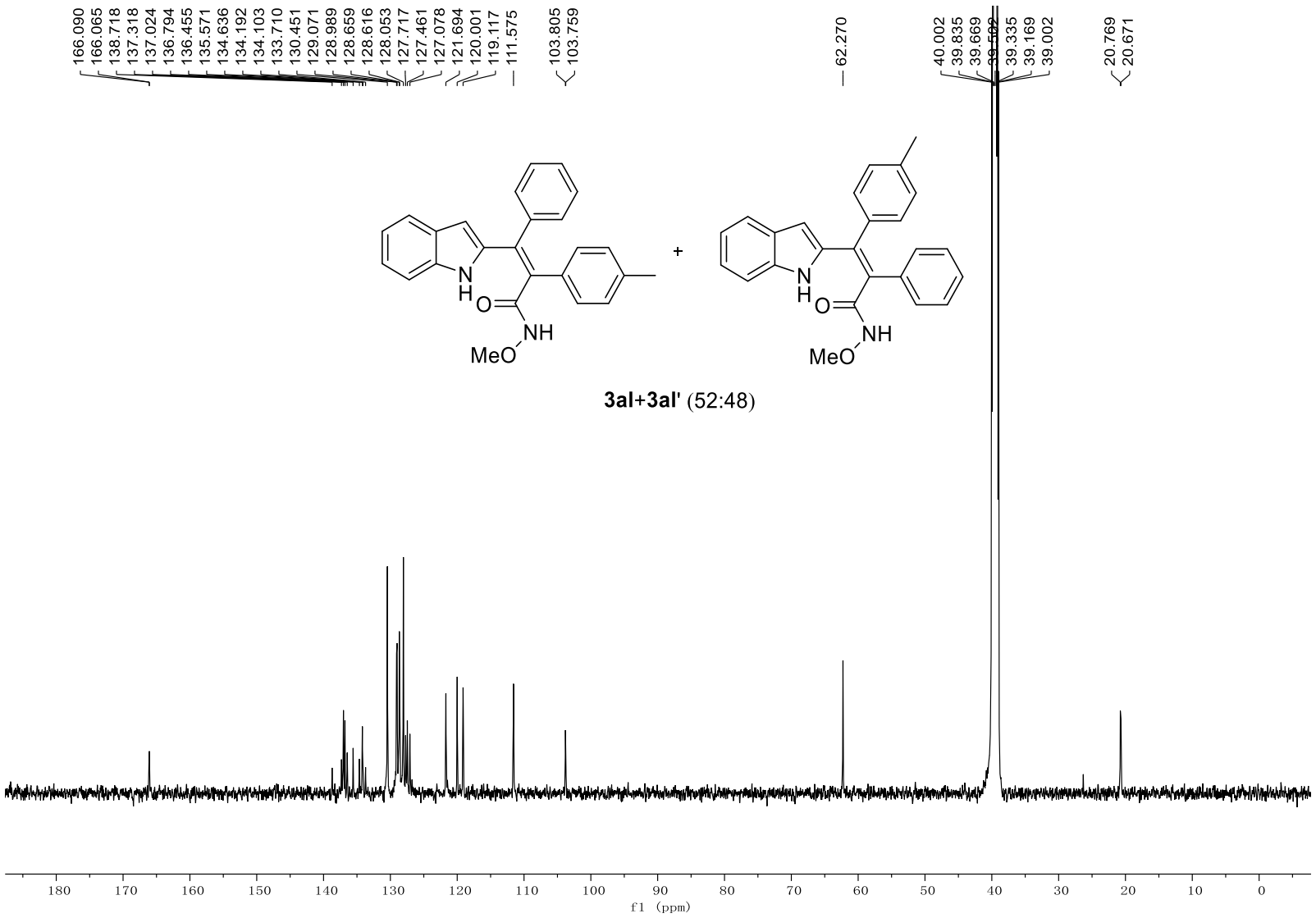

11.660
10.510
7.827
7.811
7.751
7.743
7.735
7.726
7.708
7.704
7.684
7.603
7.586
7.559
7.543
7.483
7.469
7.453
7.430
7.418
7.413
7.403
7.295
7.279
7.219
7.216
7.202
7.199
7.113
7.110
7.096
7.093
7.077
7.062
7.047
7.002
6.987
6.972
6.828
6.825
3.479
3.319
2.497
2.494
2.490
2.486
2.482
f1 (ppm)
NH
O
NH
MeO
3ai
0.95
0.97
0.99
6.01
0.99
0.99
1.02
2.99
0.99
0.99
0.99
1.01
1.01
0.96
3.00
f1 (ppm)


166.091
136.972
136.209
135.133
134.863
134.247
132.672
132.607
132.410
131.784
129.933
128.505
128.028
127.773
127.554
127.352
126.439
126.283
126.158
121.876
120.143
119.219
111.590
104.158
62.339
40.035
39.868
39.701
39.534
39.367
39.198
39.031
N
H
O
NH
MeO
3ai
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

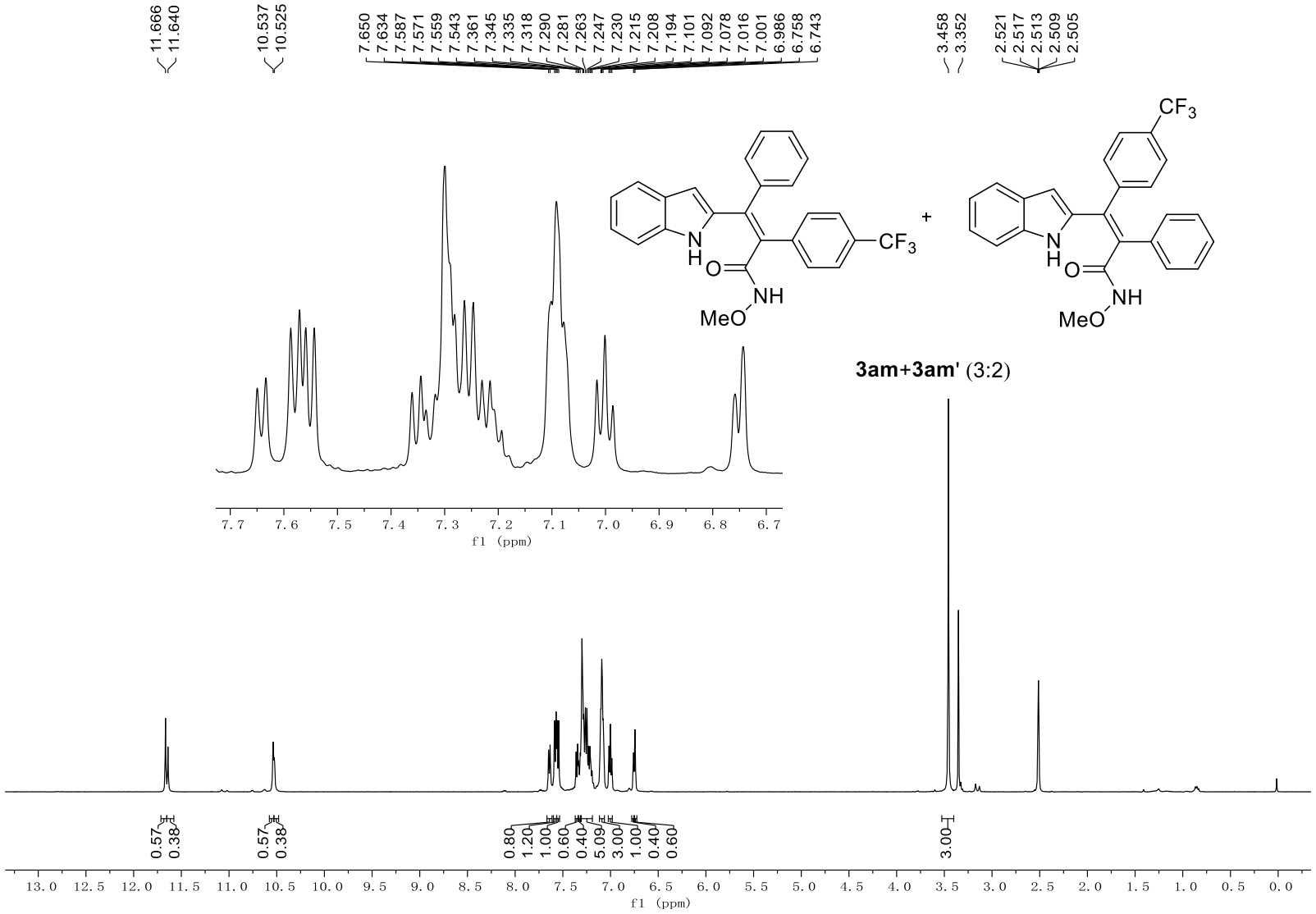

11.790
11.039
7.623
7.607
7.506
7.489
7.245
7.230
7.215
7.082
7.067
7.052
6.951
3.895
3.758
3.621
3.350
2.522
2.518
2.514
2.510
2.507
COOMe
COOMe
N
H
O
NH
MeO
3ak
f1 (ppm)
0.95
1.00
1.01
1.00
1.02
1.05
1.03
3.06
3.08
3.01
f1 (ppm)

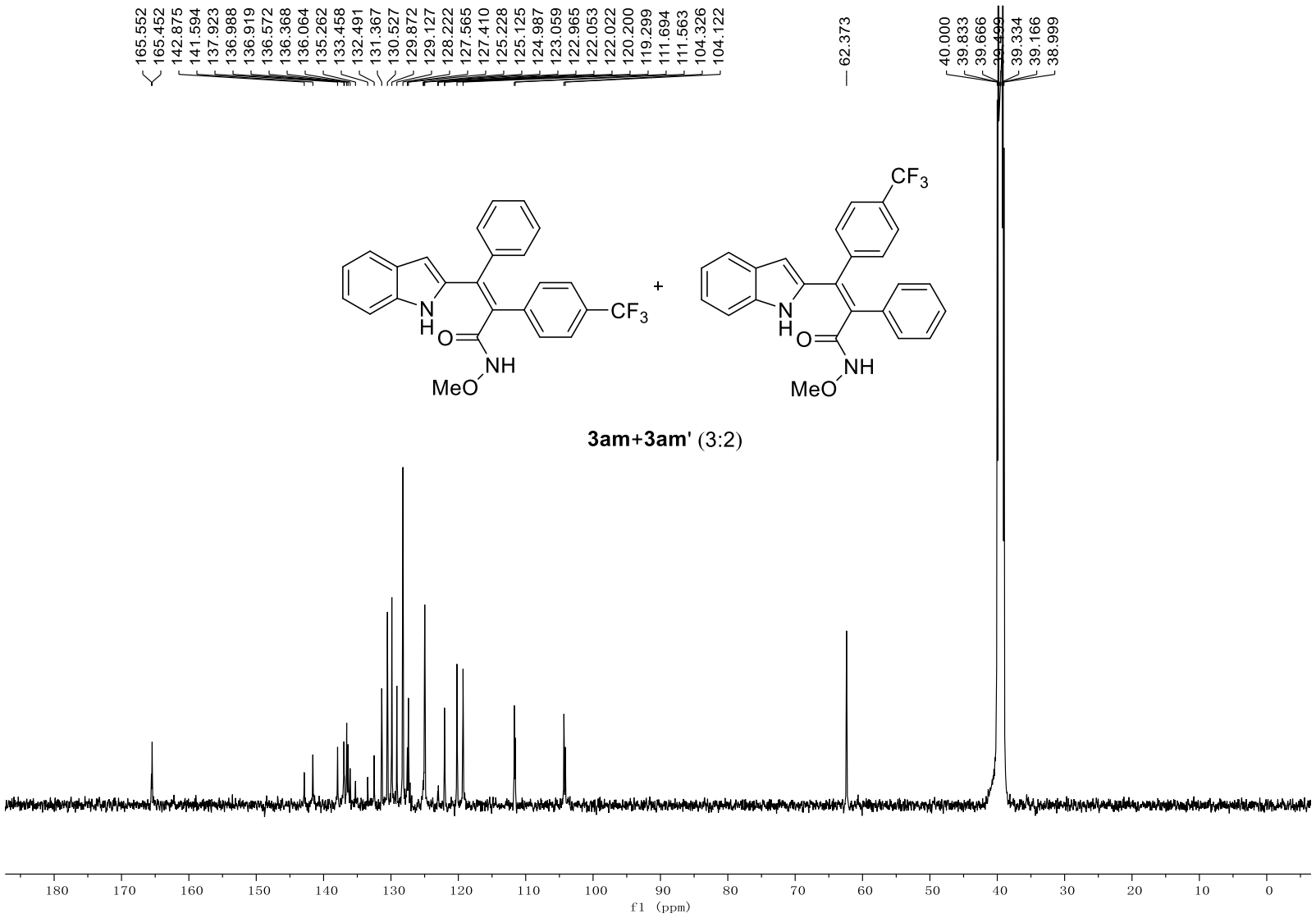

166.764
163.986
161.457
138.474
129.015
127.740
124.879
122.592
121.718
120.879
112.851
108.222
63.081
53.545
53.212
40.483
40.318
40.152
39.985
39.819
39.653
39.487
COOMe
COOMe
N
H
O
NH
MeO
3ak
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

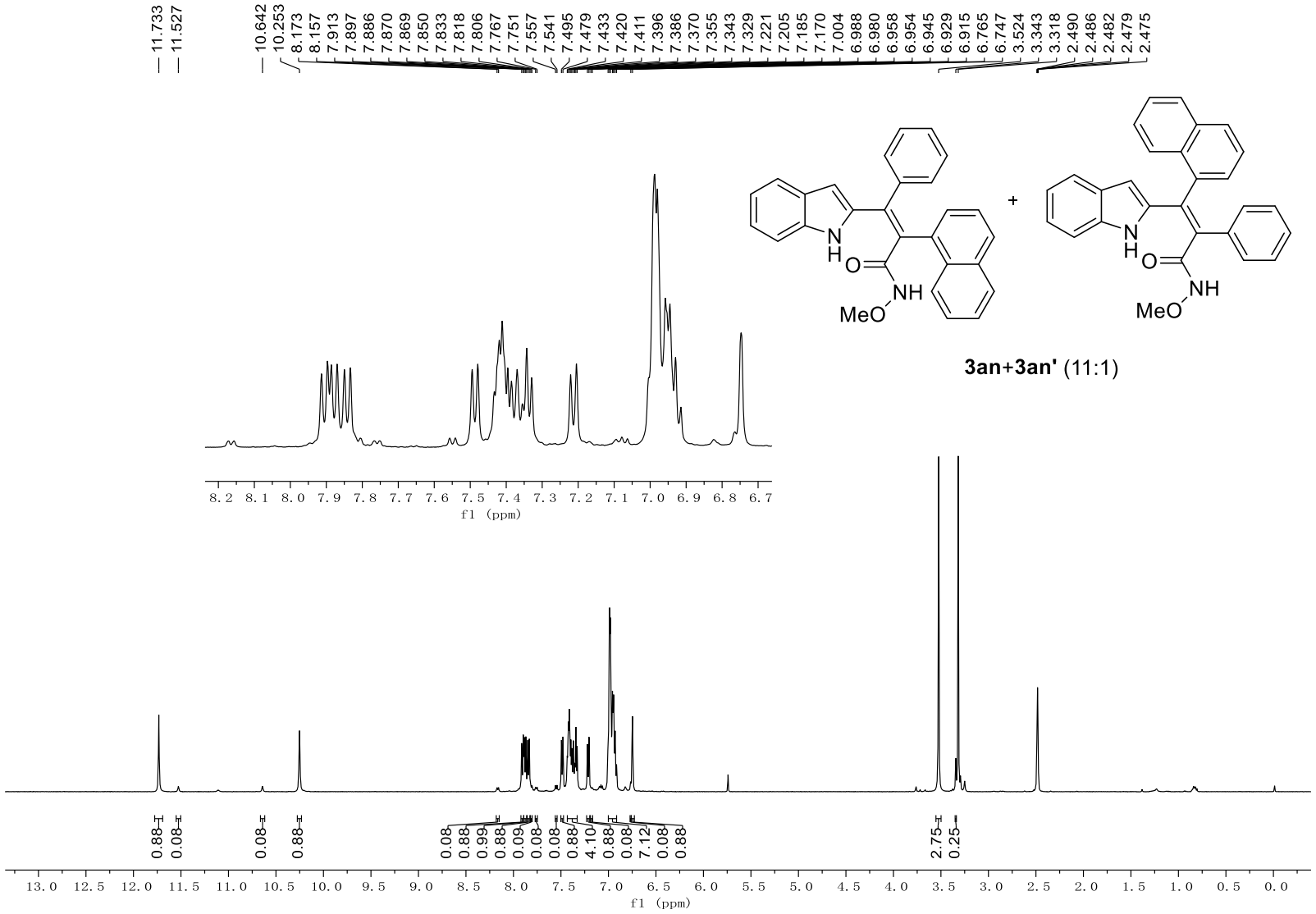

11.506
11.497
10.422
7.527
7.511
7.340
7.324
7.264
7.221
7.207
7.193
7.176
7.162
7.079
7.066
7.052
7.006
6.992
6.980
6.961
6.947
6.932
6.691
6.671
3.422
3.346
2.518
2.515
2.513
2.511
2.508
2.273
2.226
N
H
O
NH
MeO
+
3al+3al' (52:48)
f1 (ppm)
0.52
0.48
0.95
1.00
1.00
3.04
3.98
1.99
2.00
0.52
0.48
3.02
1.56
1.44

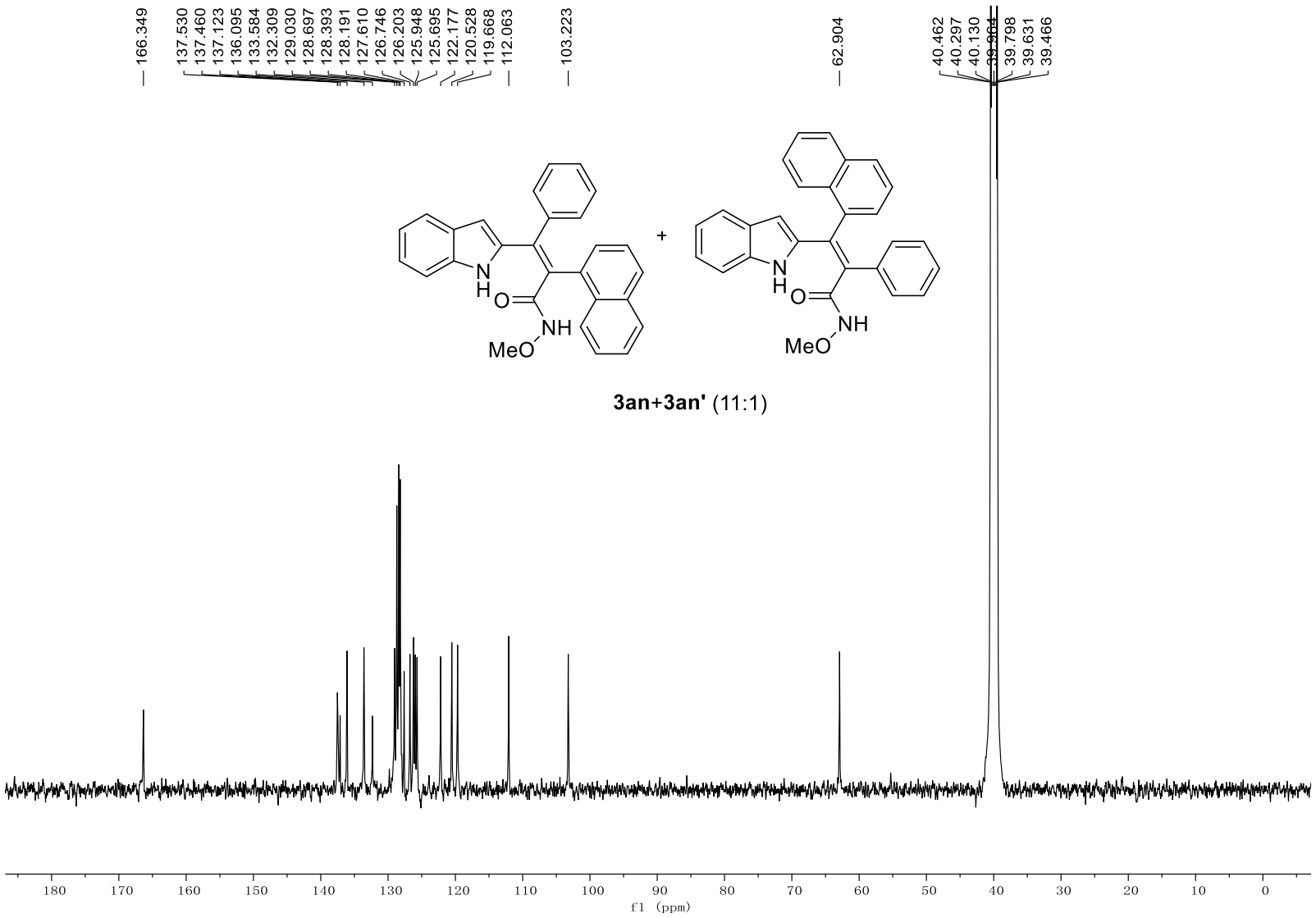

166.090
166.065
138.718
137.318
137.024
136.794
136.455
135.571
134.636
134.192
134.103
133.710
130.451
129.071
128.989
128.659
128.616
128.053
127.717
127.461
127.078
121.694
120.001
119.117
111.575
103.805
103.759
62.270
40.002
39.835
39.669
39.502
39.335
39.169
39.002
20.769
20.671
N
H
O
NH
MeO
+
N
H
O
NH
MeO
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

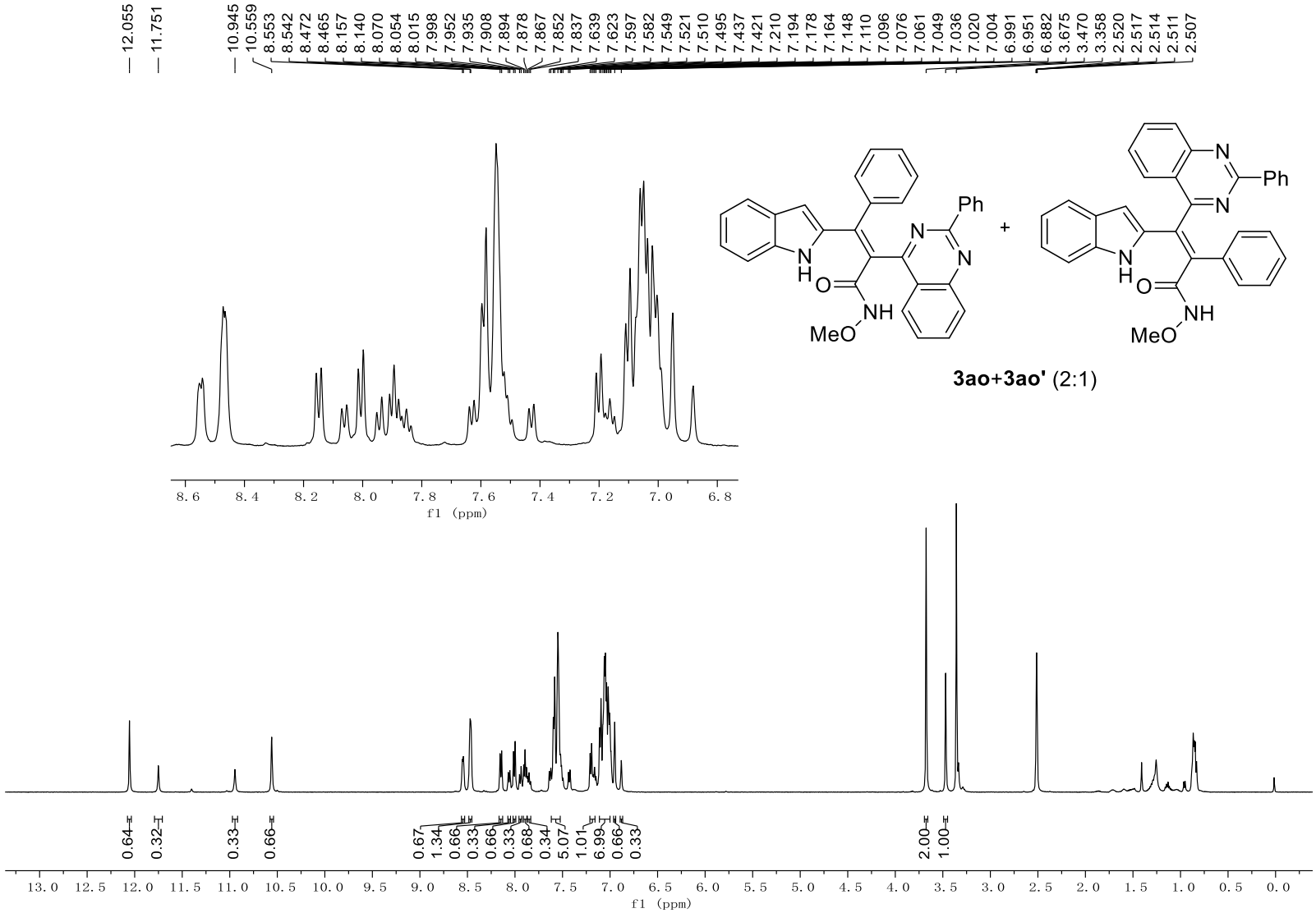
3al+**3al'** (52:48)

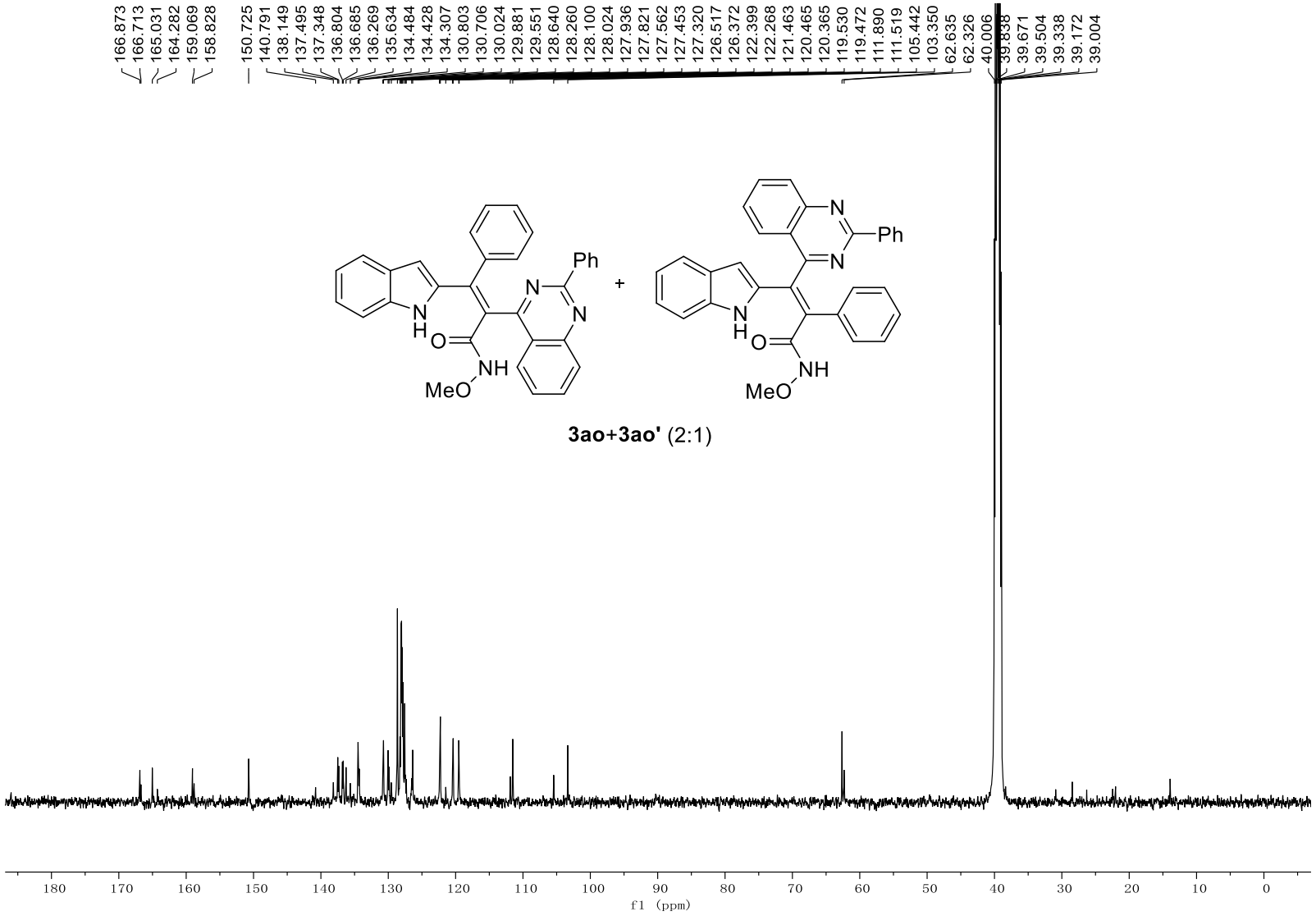

11.666
11.640
10.537
10.525
7.650
7.634
7.587
7.571
7.559
7.543
7.361
7.345
7.335
7.318
7.290
7.281
7.263
7.247
7.230
7.215
7.208
7.194
7.101
7.092
7.078
7.016
7.001
6.986
6.758
6.743
3.458
3.352
2.521
2.517
2.513
2.509
2.505
CF3
N
H
O
NH
MeO
+
CF3
N
H
O
NH
MeO
3am+3am' (3:2)
f1 (ppm)
f1 (ppm)

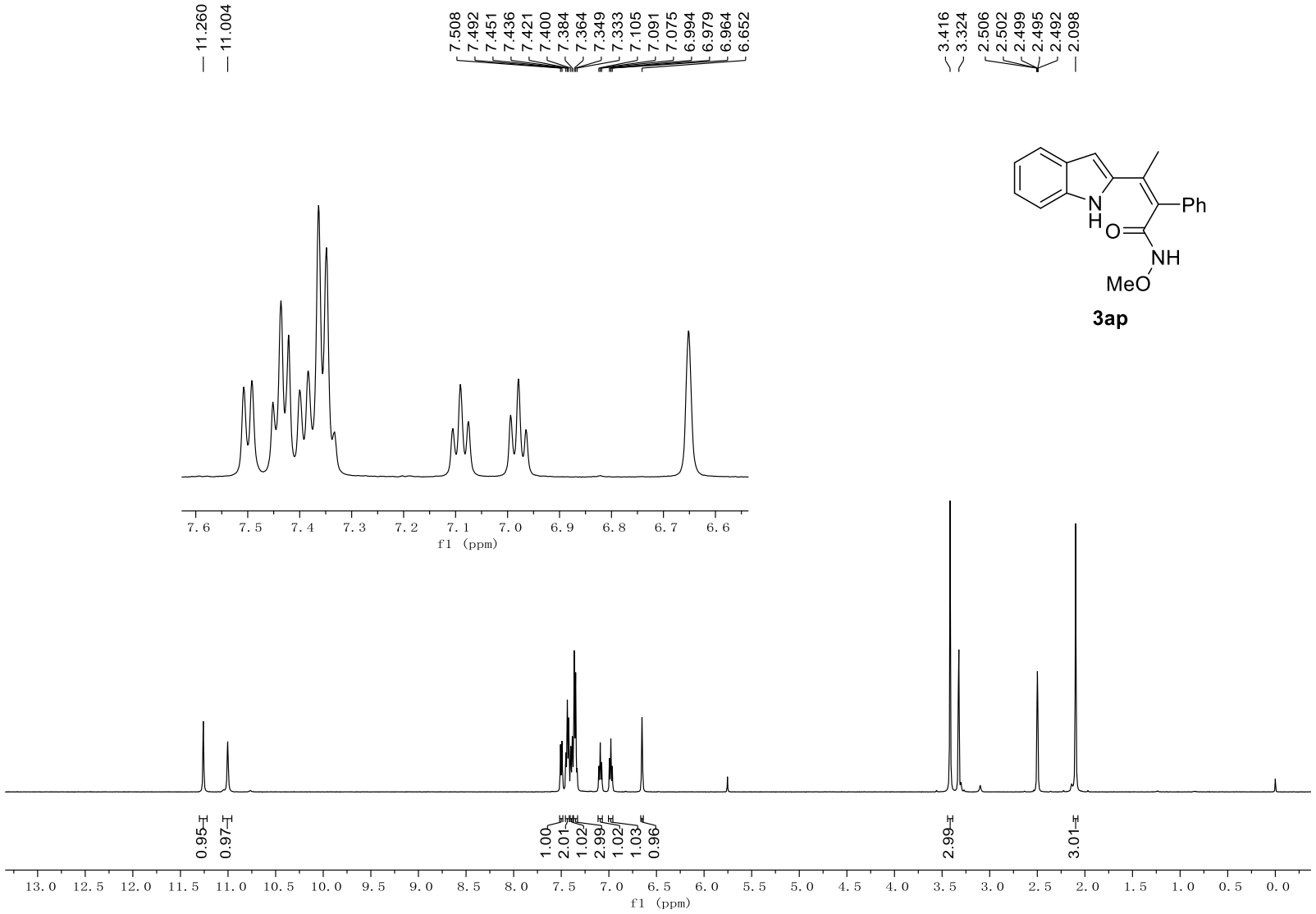

165.552
165.452
142.875
141.594
137.923
136.988
136.919
136.572
136.368
136.064
135.262
133.458
132.491
131.367
130.527
129.872
129.127
128.222
127.565
127.410
125.228
125.125
124.987
123.059
122.965
122.053
122.022
120.200
119.299
111.694
111.563
104.326
104.122
62.373
40.000
39.833
39.666
39.499
39.334
39.166
38.999
CF3
N
H
O
NH
MeO
CF3
N
H
O
NH
MeO
3am+3am' (3:2)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

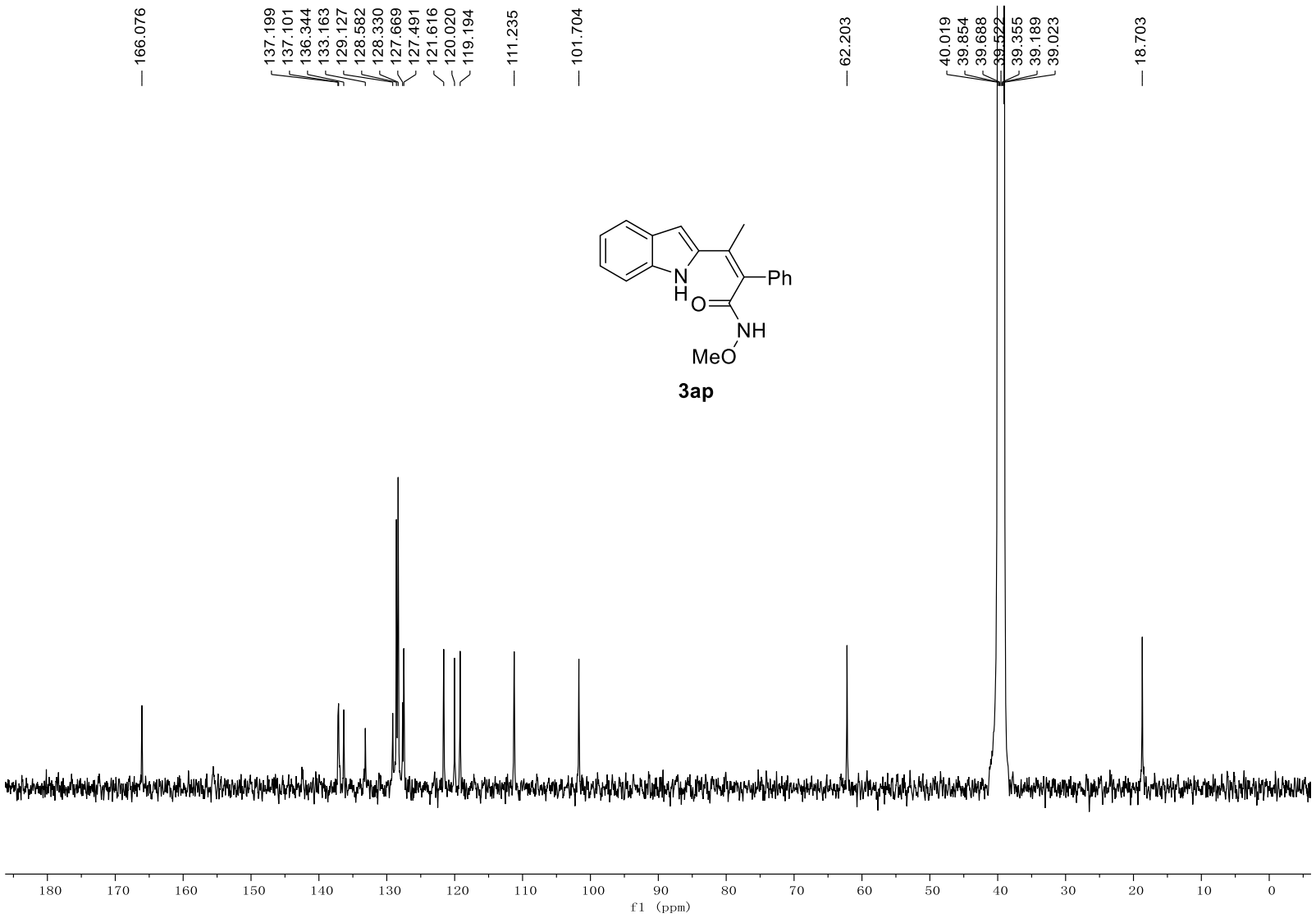

11.733
11.527
10.642
10.253
8.173
8.157
7.913
7.897
7.886
7.870
7.869
7.850
7.833
7.818
7.806
7.767
7.751
7.557
7.541
7.495
7.479
7.433
7.420
7.411
7.396
7.386
7.370
7.355
7.343
7.329
7.221
7.205
7.185
7.170
7.004
6.988
6.980
6.958
6.954
6.945
6.929
6.915
6.765
6.747
3.524
3.343
3.318
2.490
2.486
2.482
2.479
2.475
N
H
O
NH
MeO
+
3an+3an' (11:1)
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
0.88
0.08
0.08
0.88
0.08
0.88
0.99
0.88
0.09
0.08
0.08
0.88
4.10
0.88
0.08
7.12
0.08
0.88
2.75
0.25
13.0 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
f1 (ppm)

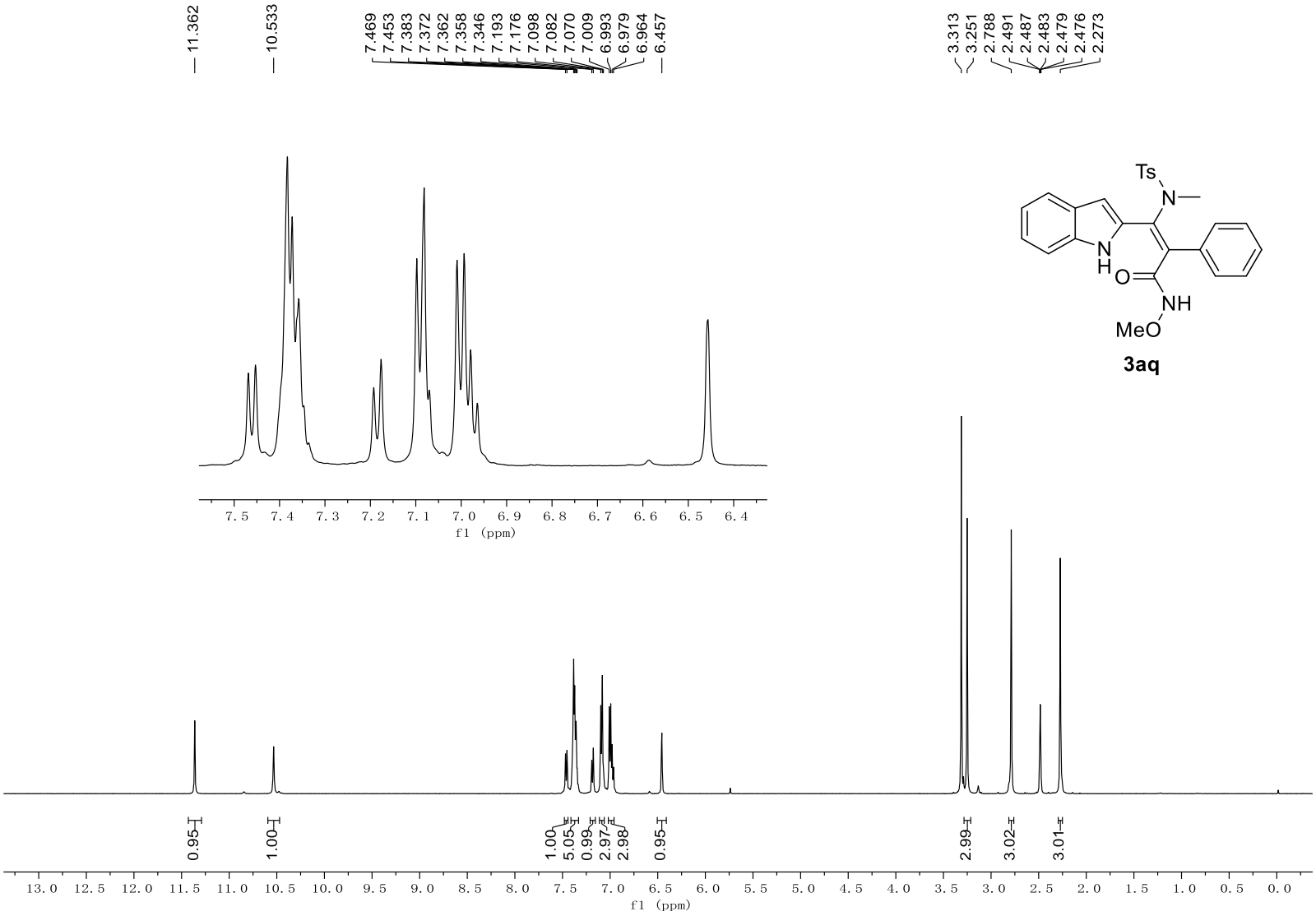

166.349
137.530
137.460
137.123
136.095
133.584
132.309
129.030
128.697
128.393
128.191
127.610
126.746
126.203
125.948
125.695
122.177
120.528
119.668
112.063
103.223
62.904
40.462
40.297
40.130
39.964
39.798
39.631
39.466
MeO
NH
O
N
H
+
3an+3an' (11:1)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

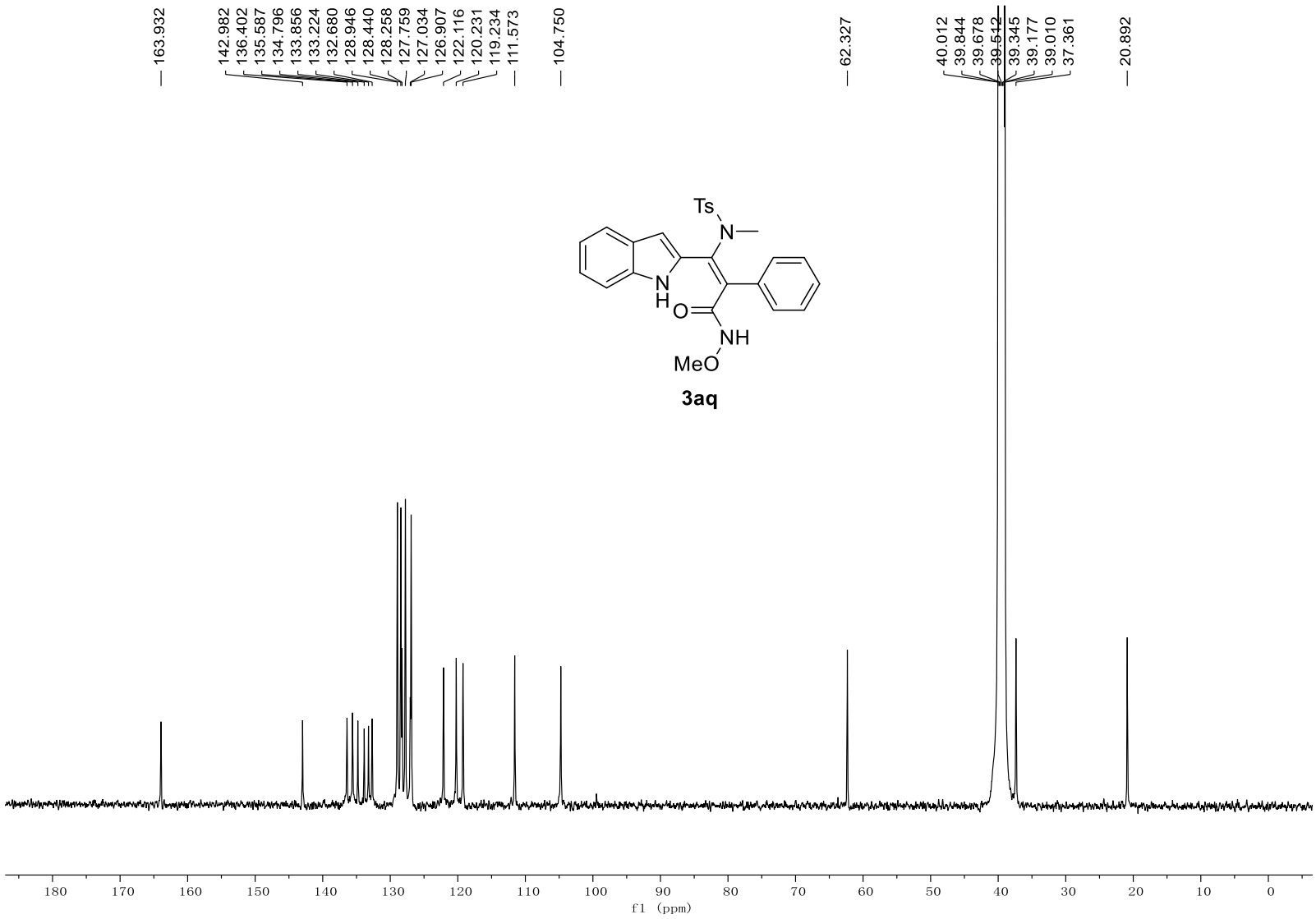

12.055
11.751
10.945
10.559
8.553
8.542
8.472
8.465
8.157
8.140
8.070
8.054
8.015
7.998
7.952
7.935
7.908
7.894
7.878
7.867
7.852
7.837
7.639
7.623
7.597
7.582
7.549
7.521
7.510
7.495
7.437
7.421
7.210
7.194
7.178
7.164
7.148
7.110
7.096
7.076
7.061
7.049
7.036
7.020
7.004
6.991
6.951
6.882
3.675
3.470
3.358
2.520
2.517
2.514
2.511
2.507
Ph
N
H
O
NH
MeO
+
3ao+3ao' (2:1)
f1 (ppm)
0.64
0.32
0.33
0.66
0.67
1.34
0.66
0.33
0.66
0.33
0.68
0.34
5.07
1.01
6.99
0.66
0.33
2.00
1.00
f1 (ppm)

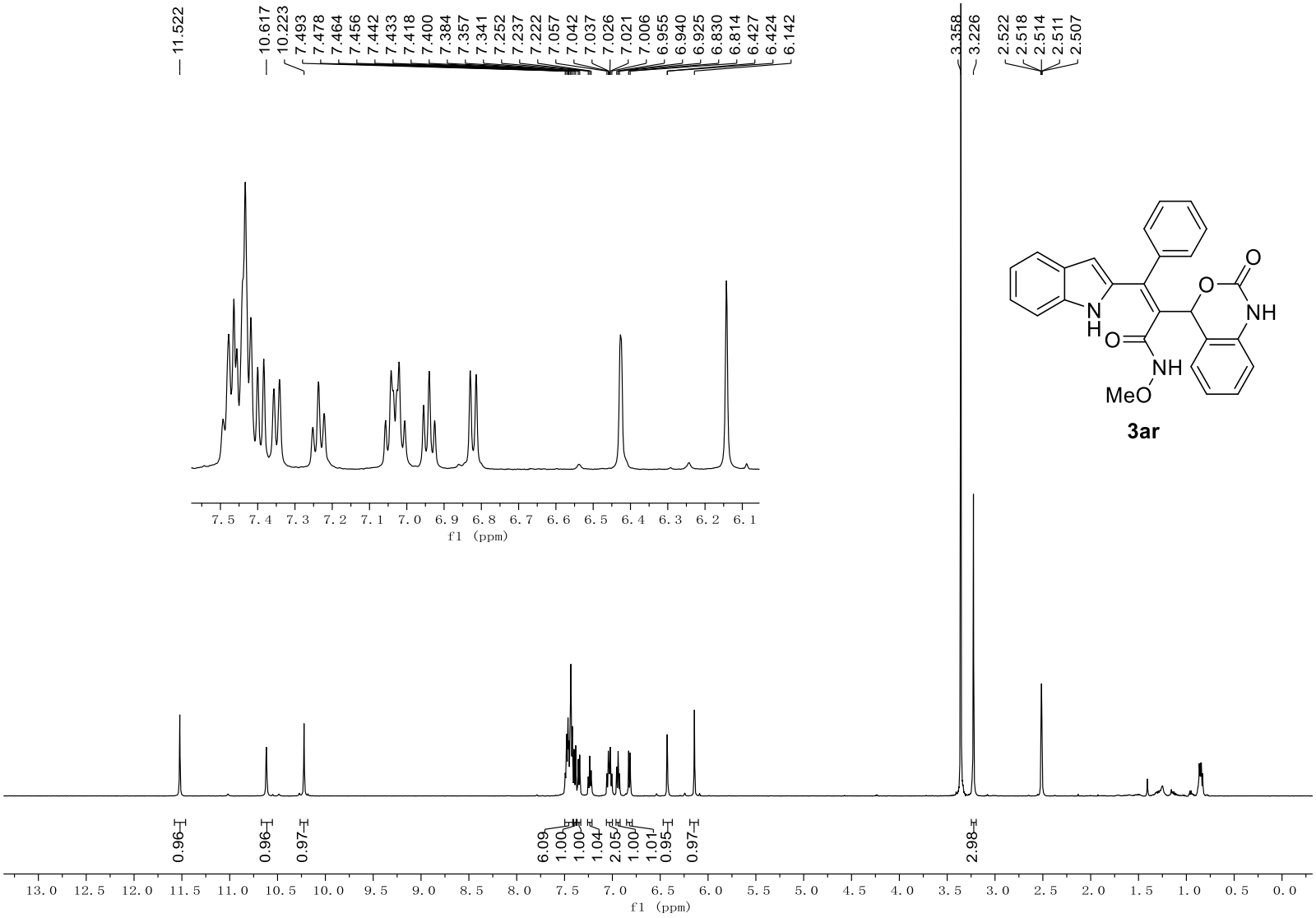

166.873
166.713
165.031
164.282
159.069
158.828
150.725
140.791
138.149
137.495
137.348
136.804
136.685
136.269
135.634
134.484
134.428
134.307
130.803
130.706
130.024
129.881
129.551
128.640
128.260
128.100
128.024
127.936
127.821
127.562
127.453
127.320
126.517
126.372
122.399
122.268
121.463
120.465
120.365
119.530
119.472
111.890
111.519
105.442
103.350
62.635
62.326
40.006
39.838
39.671
39.504
39.338
39.172
39.004
Ph
N
N
H
O
NH
MeO
+
Ph
N
N
H
O
NH
MeO
3ao+3ao' (2:1)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.260
11.004
7.508
7.492
7.451
7.436
7.421
7.400
7.384
7.364
7.349
7.333
7.105
7.091
7.075
6.994
6.979
6.964
6.652
3.416
3.324
2.506
2.502
2.499
2.495
2.492
2.098
Ph
N
H
O
NH
MeO
3ap
f1 (ppm)
0.95
0.97
1.00
2.01
1.02
2.99
1.02
1.03
0.96
2.99
3.01
f1 (ppm)

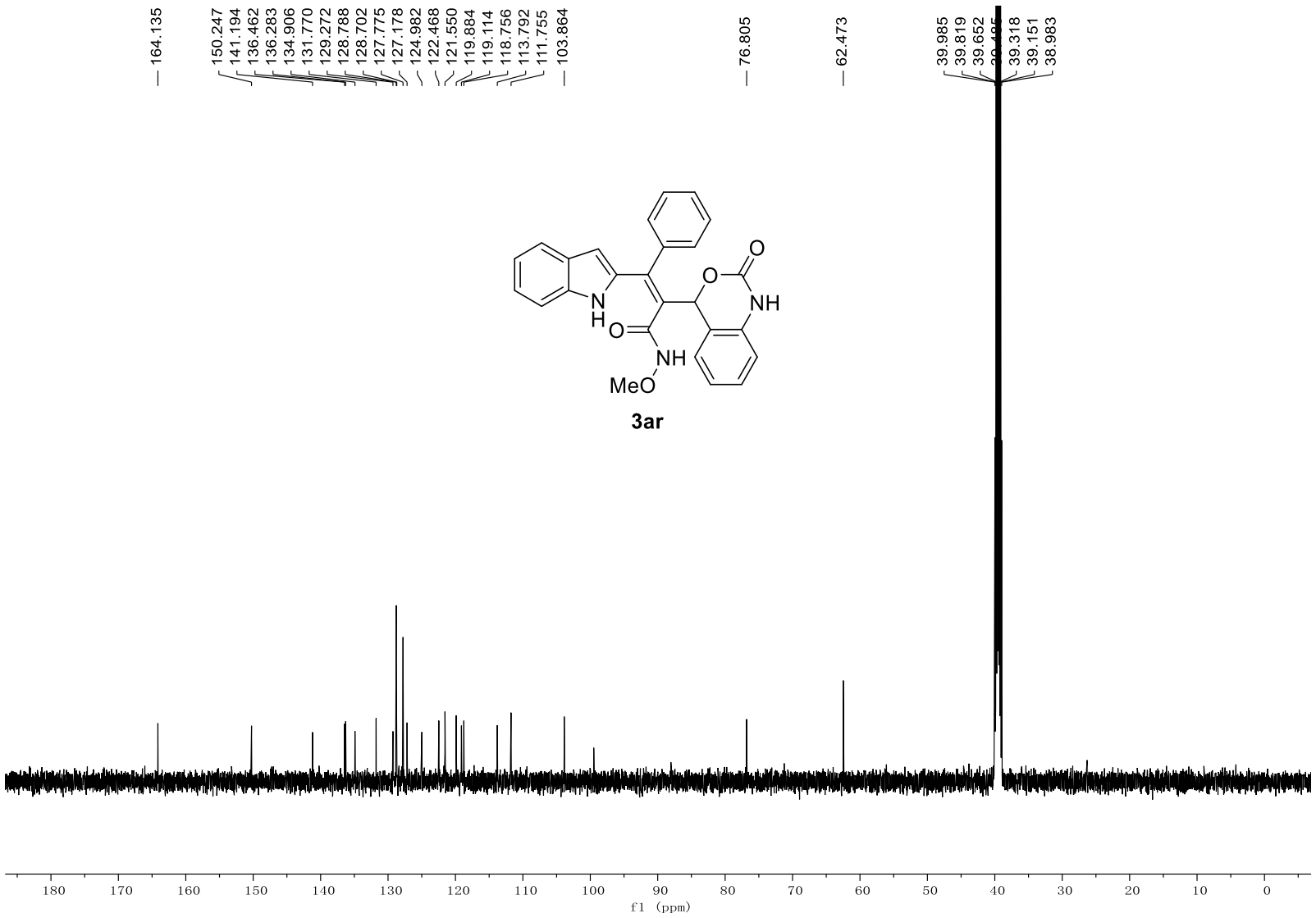

166.076
137.199
137.101
136.344
133.163
129.127
128.582
128.330
127.669
127.491
121.616
120.020
119.194
111.235
101.704
62.203
40.019
39.854
39.688
39.522
39.355
39.189
39.023
18.703
N
H
O
NH
MeO
Ph
3ap
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.362
10.533
7.469
7.453
7.383
7.372
7.362
7.358
7.346
7.193
7.176
7.098
7.082
7.070
7.009
6.993
6.979
6.964
6.457
3.313
3.251
2.788
2.491
2.487
2.483
2.479
2.476
2.273
Ts
N
N
H
O
NH
MeO
3aq
f1 (ppm)
0.95
1.00
1.00
5.05
0.99
2.97
2.98
0.95
2.99
3.02
3.01
f1 (ppm)


163.932
142.982
136.402
135.587
134.796
133.856
133.224
132.680
128.946
128.440
128.258
127.759
127.034
126.907
122.116
120.231
119.234
111.573
104.750
62.327
40.012
39.844
39.678
39.512
39.345
39.177
39.010
37.361
20.892
Ts
N
N
H
O
NH
MeO
3aq
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.522
10.617
10.223
7.493
7.478
7.464
7.456
7.442
7.433
7.418
7.400
7.384
7.357
7.341
7.252
7.237
7.222
7.057
7.042
7.037
7.026
7.021
7.006
6.955
6.940
6.925
6.830
6.814
6.427
6.424
6.142
3.358
3.226
2.522
2.518
2.514
2.511
2.507
f1 (ppm)
0.96
0.96
0.97
6.09
1.00
1.00
1.04
2.05
1.00
1.01
0.95
0.97
2.98
f1 (ppm)
O
O
NH
N
H
O
NH
MeO

3ar


164.135
150.247
141.194
136.462
136.283
134.906
131.770
129.272
128.788
128.702
127.775
127.178
124.982
122.468
121.550
119.884
119.114
118.756
113.792
111.755
103.864
76.805
62.473
39.985
39.819
39.652
39.318
39.151
38.983
O
O
NH
N
H
O
NH
MeO
3ar
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)