Electronic Supplementary Information

Palladium-catalyzed mono and double carbonylation of indole with amine controllably leading to amide and α-ketoamide

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Electronic Supplementary Information Contents:

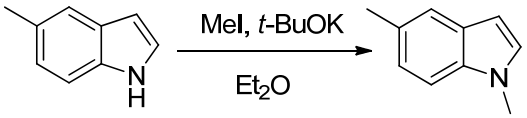
1) General Information

The reagents, free (NH)-indoles, 7-zazindole, and *N*-methyl indole were purchased and used as received without further purification. NMR spectra of the products were recorded using a Bruker Avance TM spectrometer operating at 400 MHz for ^{1}H and 100 MHz for ^{13}C in $CDCl_3$ unless otherwise noted. High resolution mass spectra (HRMS) of the products were obtained on a Bruker Daltonics micro TOF-spectrometer. High-performance liquid chromatography (HPLC) analysis (methanol/H_2O = 60/40, 0.8 mL/min, λ = 254 nm) was performed by Agilent 1260 Infinity with an Agilent ZORBAX C_{18} column using *N*-ethylbenzamide as inner standard for mono-carbonylated products. X-ray Single Crystal Diffraction measurement was conducted at 296 K on a Bruker APEX II diffractometer using Mo Kα radiation (γ = 0.71073Å). The data were corrected for Lorentz and polarization effects with the SMART suite of programs and for absorption effects with SADABS. The structure was solved by direct methods using the SHELXS program. Isolated yield was obtained by column chromatography (200-300 mesh), and Ethyl acetate/ Petroleum ether was used as the eluent.

2) General Procedures for the Synthesis of *N*-substituted Indoles

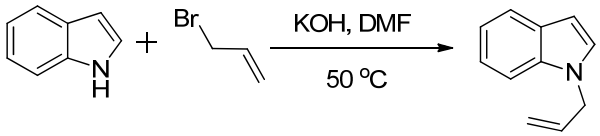
All of the *N*-substituted indoles were prepared according to literatures with slight modification.

General procedure for the preparation of *N*-methyl indoles[1]



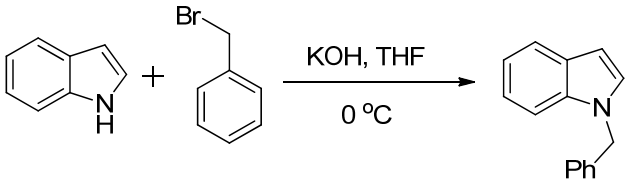
To a stirred solution of 5-methyl indole (1 mol) in ether (10 mL) was slowly added potassium *tert*-butanolate (2 mol) and iodomethane (2 mol) at 0 °C, after 24 hours the reaction mixture was poured into saturated aqueous $NaHCO_3$ solution (25 mL) and extracted with ether (10 mL) three times. The combined organic layers were dried over anhydrous Na_2SO_4 and concerntrated *in vacuo*. The crude product was purified by column chromatography (silica gel, pure hexane). The product was characterized and compared with the previously reported literature. Other *N*-methyl indoles were synthesized according to the above method.

General procedure for the preparation of *N*-allyl indole[2]



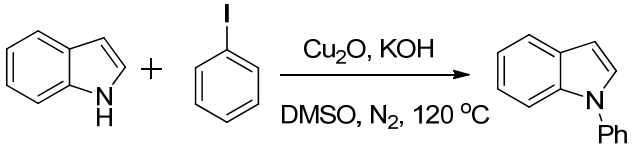
To a stirred solution of 1*H*-indole (1 mol) in DMF (10 mL) was slowly added potassium hydroxide (1.2 mol) and allyl bromide (1.2 mol). After 12 hours at 50 °C, the reaction mixture was cooled to room temperature, poured into saturated aqueous $NaHCO_3$ solution (10 mL) and extracted with ether (20 mL) three times. The combined organic layers were dried over anhydrous Na_2SO_4 and concerntrated *in vacuo*. The crude product was purified by column chromatography (silica gel, pure hexane). The product was characterized and compared with the previously reported literature. Other *N*-allyl indoles were synthesized according to the above method.

General procedure for the preparation of *N*-benzyl indoles[3]



To a stirred solution of 1*H*-indole (1 mol) in tetrahedrofuran (10 mL) was slowly added potassium hydroxide (4 mol) and benzyl bromide (1 mol) at 0 °C. After 24 hours, the mixture was poured into saturated aqueous $NaHCO_3$ solution (10 mL) and extracted with ether (20 mL) three times. The combined organic layers were dried over anhydrous Na_2SO_4 and concerntrated *in vacuo*. The crude product was purified by column chromatography (silica gel, pure hexane). The product was characterized and compared with the previously reported literature. Other *N*-benzyl indoles were synthesized according to the above method.

General procedure for the preparation of *N*-phenyl indole[4]



A mixture of iodobenzene (1 mol), 1*H*-Indole (1.5 mol), cuprous oxide (0.1 mol), potassium hydroxide (2 mol) and DMSO (2 mL) was stirred at 120 °C under N_2 atmosphere for 24 hours. Then the mixture was poured into 15 mL H_2O and extracted with ether (20 mL) three times. The combined organic layers were dried over anhydrous Na_2SO_4 and concerntrated *in vacuo*. The crude product was purified by column chromatography (silica gel, hexane:ethyl acetate = 50:1). The product was characterized and compared with the previously reported literature.

3) Experimental Procedure for Pd-catalyzed Carbonylation

Pd-catalyzed double carbonylation of indoles with amines (Scheme 1)

indole (0.5 mmol), I_2 (0.6 mmol), Cs_2CO_3 (0.25 mmol), and THF (5.0 mL) were introduced into an 100 mL stainless steel autoclave and stirred at room temperature for 3 h, then amine (2.0 mmol), $PdCl_2$(dppf) (0.025 mmol), and dppf (0.05 mmol), DBU (1.5 mmol), CuI (0.1mmol), LiCl (0.2 mmol) in THF (5.0 mL) were consecutively added. The autoclave was closed and purged three times with CO before it was finally pressurized with 40 atm CO gas. Then the reactor was immersed in an oil bath preheated at 60 ^oC for 36 h. After cooling to room temperature, excess CO was discharged and the resultant reaction mixture was purified by flash chromatography using silica gel (petroleum ether and ethyl acetate) to afford the corresponding product.

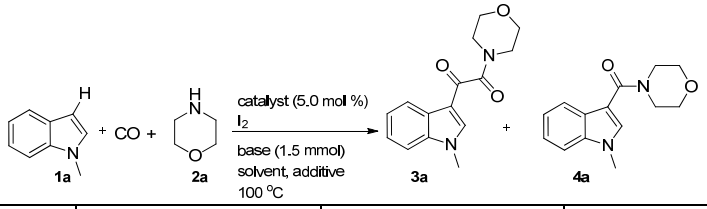
Pd-catalyzed monocarbonylation of indoles with amines (Scheme 2)

Indole (0.5 mmol), I_2 (1.0 mmol), K_2CO_3 (1.5 mmol), and THF (2.0 mL) were added to a 50 mL Schlenk tube with a magnetic bar. After stirring at room temperature for 0.5 h, amine (2.0 mmol), $PdCl_2$(dppf) (0.025 mmol), dppf (0.05 mmol), and THF (1.0 mL) were charged into the tube. The glass tube was vacuumed and purged with CO three times before it was finally pressurized with 1.0 atm CO gas. Then, the tube was tightly screw-capped, immersed in an oil bath preheated at 100 ^oC for 24 h. After cooling to room temperature, excess CO was discharged and the resultant reaction mixture was purified by the silica gel chromatography using petroleum ether and ethyl acetate as the eluent to afford the corresponding product.

Pd-catalyzed double carbonylation of indoles with *N*-benzoylpiperazine (Scheme 3)

A mixture of indole (0.5 mmol), I_2 (0.6 mmol), Cs_2CO_3 (0.25 mmol), in THF (5.0 mL) was stirred in an 100 mL stainless steel autoclave at room temperature for 3 h, then *N*-benzoylpiperazine (2.0 mmol), $PdCl_2(PhCN)_2$ (0.025 mmol), and Xantphos (0.05 mmol), DBU (1.5 mmol), CuI (0.1mmol), LiCl (0.2 mmol) and THF (5.0 mL) were added. The autoclave was closed and purged three times with CO before it was finally pressurized with 40 atm CO gas. After stirring at 60 ^oC for 48 h, the autoclave was cooled to room temperature and excess CO was discharged. Isolated yields of the desired product were obtained by silica gel chromatography using petroleum ether and ethyl acetate as the eluent.

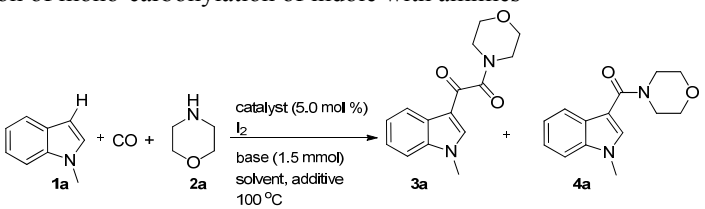
Table S1 Optimization of double-carbonylation of indole with amines[a]



Entry	Catalyst	Base	Additive	Solvent	Yield(%)	
					3a	4a
1	$PdCl_2(dppf)$	Cs_2CO_3/DBU	dppf	THF	74	16
2	$PdCl_2(dppf)$	Cs_2CO_3/DBU	dppf-CuI	THF	75	14
3	$PdCl_2(dppf)$	Cs_2CO_3/DBU	dppf- CuI/LiCl	THF	81	trace
4	$PdCl_2$	Cs_2CO_3/DBU	CuI/LiCl	THF	trace	trace
5	$PdCl_2$	Cs_2CO_3/DBU	bipyridine/CuI/LiCl	THF	37	6
6	$PdCl_2(PPh_3)_2$	Cs_2CO_3/DBU	PPh_3-CuI/LiCl	THF	64	trace
7	$PdCl_2(dppp)$	Cs_2CO_3/DBU	dppp-CuI/LiCl	THF	59	trace
8	$PdCl_2(dppf)$	Cs_2CO_3	dppf- CuI/LiCl	THF	60	10
9	$PdCl_2(dppf)$	Cs_2CO_3/ DABCO	dppf- CuI/LiCl	THF	73	12
10	$PdCl_2(dppf)$	Cs_2CO_3/ DMAP	dppf- CuI/LiCl	THF	42	15
11	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	1,4-Dioxane	48	5
12	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	DCE	trace	trace
13	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	Toluene	46	5
14	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	acetonitrile	trace	trace
15[b]	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	THF	76	8
16[c]	$PdCl_2(dppf)$	Cs_2CO_3/DBU	dppf- CuI/LiCl	THF	21	trace
17[d]	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	THF	80	trace
18[e]	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	THF	26	8
19[f]	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	THF	54	trace
20[g]	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	dppf- CuI/LiCl	THF	37	8
21	$PdCl_2(dppf)$	Cs_2CO_3/ DBU	CuI/LiCl	THF	45	trace

[a] Reaction conditions:**1a** (0.5 mmol), **2a** (2.0 mmol), Cs_2CO_3 (0.25 mmol), I_2 (0.6 mmol), DBU (1.5 mmol), $PdCl_2(dppf)$ (5 mol %), dppf (10 mol %), CuI (0.1 mmol), LiCl (0.2 mmol), THF (10 mL), CO (40 atm), 60 °C, 36 h, isolated yield. [b] THF (6mL). [c] I_2 (1 mmol). [d] Reaction was performed for 48 h. [e] CO (20 atm). [f] $PdCl_2(dppf)$ (2 mol %). [g] DBU (0.75 mmol).

Table S2 Optimization of mono-carbonylation of indole with amimes[a]

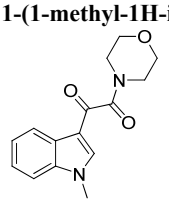


Entry	Catalyst	Base	Additive	Solvent	Yield(%)[b]	
					3a	4a
1[c]	$PdCl_2(dppf)$	K_2CO_3	dppf	THF	19	61
2	$PdCl_2(dppf)$	K_2CO_3	dppf	THF	trace	82 (90)
3	$PdCl_2(dppf)$	K_3PO_4	dppf	THF	trace	36
4	$PdCl_2(dppf)$	Cs_2CO_3	dppf	THF	trace	5
5	$PdCl_2(dppf)$	NEt_3	dppf	THF	trace	3
6	$PdCl_2(dppf)$	K_2CO_3	dppf	1,4-Dioxane	trace	trace
7	$PdCl_2(dppf)$	K_2CO_3	dppf	Toluene	trace	trace
8	$PdCl_2(dppf)$	K_2CO_3	dppf	Acetonitrile	trace	29
9[d]	$PdCl_2(dppf)$	K_2CO_3	dppf	THF	3	30

[a] Reaction conditions:**1a** (0.5 mmol), **2a** (2.0 mmol), I_2 (1.0 mmol), K_2CO_3 (1.5 mmol), $PdCl_2(dppf)$ (0.025 mmol), and dppf (0.05 mmol), THF (3 mL), CO (1 atm), 100 °C, 24 h. [b] HPLC yield, isolated yield in parenthesis. [c] CO (2 atm). [d] 80 °C.

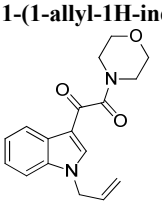
4) Characterization Data for Products

1-(1-methyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3a).



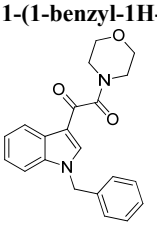
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.31 (m, 1H), 7.89 (s, 1H), 7.39 – 7.32 (m, 3H), 3.84 (s, 3H), 3.81 – 3.75 (m, 4H), 3.69 – 3.66 (m, 2H), 3.58 – 3.54 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.7 (C=O), 166.1 (C=O), 139.4, 137.7, 126.2, 124.1, 123.4, 122.3, 113.4, 110.0, 67.0, 66.7, 46.6, 41.9, 33.8. HRMS (ESI) Calcd for $C_{15}H_{16}N_2NaO_3$: $[M+Na]^+$, 295.1053; Found: 295.1058. IR: ν (cm^{-1}) = 1630.30 cm^{-1} (C=O stretch).

1-(1-allyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3b).



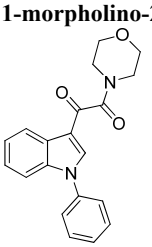
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 – 8.31 (m, 1H), 7.93 (s, 1H), 7.35 (m, 3H), 6.07 – 5.94 (m, 1H), 5.31 (d, *J* = 10.2 Hz, 1H), 5.21 (d, *J* = 17.1 Hz, 1H), 4.77 (d, *J* = 5.5 Hz, 2H), 3.78 (d, *J* = 3.4 Hz, 4H), 3.70 – 3.65 (m, 2H), 3.59 – 3.53 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.8 (C=O), 166.0 (C=O), 138.4, 137.1, 131.5, 126.4, 124.1, 123.5, 122.4, 119.3, 113.7, 110.5, 67.0, 66.8, 49.8, 46.6, 41.9. HRMS (ESI) Calcd for $C_{17}H_{18}N_2NaO_3$: $[M+Na]^+$, 321.1210; Found: 321.1201. IR: ν (cm^{-1}) = 1643.21 cm^{-1} (C=O stretch).

1-(1-benzyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3c).



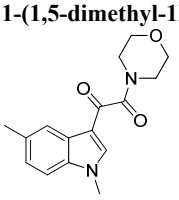
A white solid. Chromatography solvent (PE/EA = 1/1). 1H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.4 Hz, 1H), 7.97 (s, 1H), 7.37 – 7.28 (m, 6H), 7.20 – 7.13 (m, 2H), 5.34 (s, 2H), 3.78 – 3.73 (m, 4H), 3.67 – 3.64 (m, 2H), 3.58 – 3.54 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 184.9 (C=O), 165.9 (C=O), 138.7, 137.2, 135.2, 129.1, 128.4, 127.1, 126.4, 124.3, 123.5, 122.4, 113.9, 110.7, 67.0, 66.7, 51.2, 46.6, 41.9. HRMS (ESI) Calcd for $C_{21}H_{20}N_2NaO_3$: $[M+Na]^+$, 371.1366; Found: 371.1362. IR: ν (cm^{-1}) = 1636.77 cm^{-1} (C=O stretch).

1-morpholino-2-(1-phenyl-1H-indol-3-yl)ethane-1,2-dione (3d).



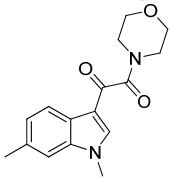
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 7.4 Hz, 1H), 8.04 (s, 1H), 7.52 – 7.40 (m, 6H), 7.29 (m, 2H), 3.74 – 3.68 (m, 4H), 3.65 – 3.61 (m, 2H), 3.55 – 3.51 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.2 (C=O), 165.8 (C=O), 138.2, 137.9, 137.3, 130.0, 128.5, 126.4, 125.0, 124.7, 123.9, 122.5, 115.1, 111.3, 67.1, 66.8, 46.6, 41.9. HRMS (ESI) Calcd for $C_{14}H_{17}NNaO_2$: $[M+Na]^+$, 357.1210; Found: 357.1201. IR: ν (cm^{-1}) = 1637.50 cm^{-1} (C=O stretch).

1-(1,5-dimethyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3e).



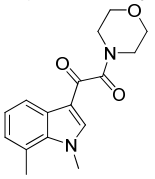
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.84 (s, 1H), 7.26 (d, *J* = 7.5 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 3.83 (s, 3H), 3.78 (m, 4H), 3.69 – 3.65 (m, 2H), 3.58 – 3.52 (m, 2H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.6 (C=O), 166.2 (C=O), 139.4, 136.1, 133.3, 126.5, 125.6, 122.1, 113.0, 109.7, 67.1, 66.8, 46.6, 41.9, 33.8, 21.5. HRMS (ESI) Calcd for $C_{16}H_{18}N_2NaO_3$: $[M+Na]^+$, 309.1210; Found: 309.1210. IR: ν (cm^{-1}) = 1625.44 cm^{-1} (C=O stretch).

1-(1,6-dimethyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3f).



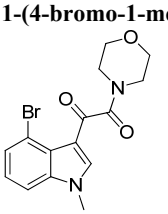
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.1 Hz, 1H), 7.83 (s, 1H), 7.20 – 7.13 (m, 2H), 3.81 (s, 3H), 3.80 – 3.75 (m, 4H), 3.70 – 3.64 (m, 2H), 3.58 – 3.53 (m, 2H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.4 (C=O), 166.2 (C=O), 139.1, 138.1, 134.3, 125.1, 123.9, 121.9, 113.3, 110.0, 67.0, 66.8, 46.6, 41.9, 33.7, 21.9. HRMS (ESI) Calcd for $C_{16}H_{18}N_2NaO_3$: $[M+Na]^+$, 309.1210; Found: 309.1198. IR: ν (cm^{-1}) = 1628.11 cm^{-1} (C=O stretch).

1-(1,7-dimethyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3g).



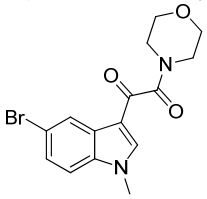
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 7.9 Hz, 1H), 7.78 (s, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 4.10 (s, 3H), 3.78 (m, 4H), 3.71 – 3.64 (m, 2H), 3.56 (d, *J* = 5.1 Hz, 2H), 2.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5 (C=O), 166.1 (C=O), 140.9, 136.4, 127.4, 127.0, 123.6, 121.9, 120.4, 112.9, 67.1, 66.8, 46.6, 41.9, 38.0, 19.5. HRMS (ESI) Calcd for $C_{16}H_{18}N_2NaO_3$: $[M+Na]^+$, 309.1210; Found: 309.1205. IR: ν (cm^{-1}) = 1628.42 cm^{-1} (C=O stretch).

1-(4-bromo-1-methyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3h).



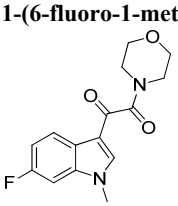
A light red solid. Chromatography solvent (PE/EA = 1/2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.18 (t, *J* = 7.9 Hz, 1H), 3.84 (s, 3H), 3.78 (d, *J* = 4.7 Hz, 2H), 3.76 – 3.69 (m, 4H), 3.63 – 3.57 (m, 2H). ^{13}C NMR (100 MHz $CDCl_3$) δ 183.9 (C=O), 166.8 (C=O), 141.0, 139.5, 128.4, 125.7, 124.8, 115.0, 113.7, 109.3, 66.9, 66.7, 46.6, 41.9, 34.0. HRMS (ESI) Calcd for $C_{15}H_{15}BrN_2NaO_3$: $[M+Na]^+$, 373.0158; Found: 373.0153. IR: ν (cm^{-1}) = 1657.11 cm^{-1}, 1629.17 cm^{-1} (C=O stretch).

1-(5-bromo-1-methyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3i).



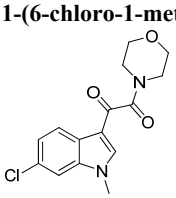
A yellow solid. Chromatography solvent (PE/EA = 1/2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 1.6 Hz, 1H), 7.82 (s, 1H), 7.36 (m, 1H), 7.15 (d, *J* = 8.7 Hz, 1H), 3.76 (s, 3H), 3.71 (m, 4H), 3.63 – 3.60 (m, 2H), 3.52 – 3.48 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.3 (C=O), 164.6 (C=O), 139.0, 135.3, 126.7, 126.1, 123.9, 116.2, 111.8, 110.5, 66.0, 65.7, 45.5, 40.9, 32.9. HRMS (ESI) Calcd for $C_{15}H_{15}BrN_2NaO_3$: $[M+Na]^+$, 373.0158; Found: 373.0163. IR: ν (cm^{-1}) = 1628.32 cm^{-1} (C=O stretch).

1-(6-fluoro-1-methyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3j).



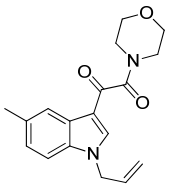
A pale yellow solid. Chromatography solvent (PE/EA = 1/2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (m, 1H), 7.82 (s, 1H), 7.05 – 6.94 (m, 2H), 3.73 (s, 3H), 3.70 (m, 4H), 3.63 – 3.58 (m, 2H), 3.51 – 3.46 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5 (C=O), 165.8 (C=O), 161.9, 159.5, 139.8, 139.8, 138.0, 137.9, 123.5, 123.4, 122.5, 113.5, 112.0, 111.8, 97.0, 96.7, 67.0, 66.7, 46.6, 41.9, 33.9. HRMS (ESI) Calcd for $C_{15}H_{15}FN_2NaO_3$: $[M+Na]^+$, 313.0959; Found: 313.0946. IR: ν (cm^{-1}) = 1628.01 cm^{-1} (C=O stretch).

1-(6-chloro-1-methyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3k).



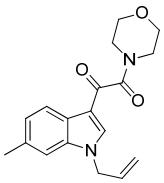
A pale yellow solid. Chromatography solvent (PE/EA = 1/2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.5 Hz, 1H), 7.91 (s, 1H), 7.36 (d, *J* = 1.6 Hz, 1H), 7.30 (m, 1H), 3.82 (s, 3H), 3.78 (m, 4H), 3.71 – 3.67 (m, 2H), 3.59 – 3.55 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.2 (C=O), 165.8 (C=O), 140.0, 138.1, 130.2, 124.7, 124.0, 123.3, 113.4, 110.3, 67.0,66.7, 46.7, 42.1, 33.9. HRMS (ESI) Calcd for $C_{15}H_{15}ClN_2NaO_3$: $[M+Na]^+$, 329.0663; Found: 329.0661. IR: ν (cm^{-1}) = 1627.94 cm^{-1} (C=O stretch).

1-(1-allyl-5-methyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3l)



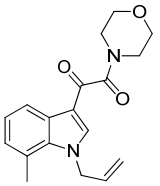
A white solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.88 (d, *J* = 2.1 Hz, 1H), 7.29 – 7.24 (m, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 6.11 – 5.89 (m, 1H), 5.31 (d, *J* = 10.2 Hz, 1H), 5.20 (d, *J* = 16.5 Hz, 1H), 4.80 – 4.70 (m, 2H), 3.83 – 3.75 (m, 4H), 3.71 – 3.64 (m, 2H), 3.56 (s, 2H), 2.48 (d, *J* = 1.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.8 (C=O), 166.1 (C=O), 138.4, 135.4, 133.3, 131.6, 126.6, 125.6, 122.2, 119.2, 113.3, 110.2, 67.0, 66.8, 49.8, 46.6, 41.9, 21.5. HRMS (ESI) Calcd for $C_{18}H_{20}N_2NaO_3$: $[M+Na]^+$, 335.1366; Found: 335.1357. IR: ν (cm^{-1}) = 1622.79 cm^{-1} (C=O stretch).

1-(1-allyl-6-methyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3m).



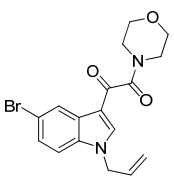
A white solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.0 Hz, 1H), 7.87 (s, 1H), 7.22 – 7.11 (m, 2H), 6.07 – 5.95 (m, 1H), 5.35 – 5.28 (m, 1H), 5.21 (m, 1H), 4.74 (d, *J* = 5.5 Hz, 2H), 3.78 (d, *J* = 2.9 Hz, 4H), 3.71 – 3.64 (m, 2H), 3.59 – 3.53 (m, 2H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.6 (C=O), 166.2 (C=O), 138.1, 137.5, 134.3, 131.6, 125.1, 124.1, 122.0, 119.2, 113.7, 110.5, 67.0, 66.8, 49.7, 46.6, 42.0, 21.9. HRMS (ESI) Calcd for $C_{18}H_{20}N_2NaO_3$: $[M+Na]^+$, 335.1366; Found: 335.1362. IR: ν (cm^{-1}) = 1629.57 cm^{-1} (C=O stretch).

1-(1-allyl-7-methyl-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3n).



A white solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.9 Hz, 1H), 7.84 (s, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 6.07 (m, 1H), 5.25 (d, *J* = 10.5 Hz, 1H), 5.00 – 4.95 (m, 2H), 4.89 (d, *J* = 17.1 Hz, 1H), 3.78 (m, 4H), 3.69 – 3.64 (m, 2H), 3.57 – 3.53 (m, 2H), 2.67 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.8 (C=O), 166.0 (C=O), 140.2, 135.9, 133.5, 127.2, 123.6, 121.7, 120.4, 117.6, 113.5, 67.0, 66.8, 51.8, 46.6, 41.9, 19.2. HRMS (ESI) Calcd for $C_{18}H_{20}N_2NaO_3$: $[M+Na]^+$, 335.1366; Found: 335.1365. IR: ν (cm^{-1}) = 1629.57 cm^{-1}, 1723.28 cm^{-1} (C=O stretch).

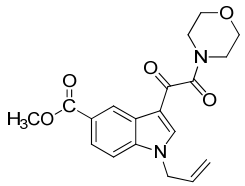
1-(1-allyl-5-bromo-1H-indol-3-yl)-2-morpholinoethane-1,2-dione (3o).



A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 1.7 Hz, 1H), 7.94 (s, 1H), 7.42 (m, 1H), 7.27 – 7.22 (m, 1H), 5.99 (m, 1H), 5.34 (d, *J* = 10.3 Hz, 1H), 5.21 (d, *J* = 17.1 Hz, 1H), 4.75 (d, *J* = 5.6 Hz, 2H), 3.81 – 3.75 (m, 4H), 3.72 – 3.67 (m, 2H), 3.60 – 3.56 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 184.4 (C=O), 165.5 (C=O), 139.0, 135.7, 131.1, 127.9, 127.1,

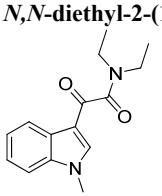
125.1, 119.6, 117.2, 113.2, 111.9, 67.0, 66.7, 49.9, 46.6, 41.9. HRMS (ESI) Calcd for $C_{17}H_{17}BrN_2NaO_3$: $[M+Na]^+$, 399.0315; Found: 399.0303. IR: ν (cm^{-1}) = 1638.80 cm^{-1} (C=O stretch).

methyl 1-allyl-3-(2-morpholino-2-oxoacetyl)-1H-indole-5-carboxylate (3p).



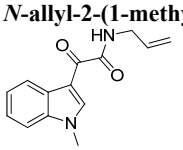
A white solid. Chromatography solvent (PE/EA = 1/2). ^1H NMR (400 MHz, $CDCl_3$) δ 9.05 (d, *J* = 1.1 Hz, 1H), 8.08 – 8.01 (m, 2H), 7.40 (d, *J* = 8.7 Hz, 1H), 6.11 – 5.91 (m, 1H), 5.35 (d, *J* = 10.3 Hz, 1H), 5.23 (d, *J* = 17.1 Hz, 1H), 4.80 (d, *J* = 5.6 Hz, 2H), 3.95 (s, 3H), 3.80 (m, 4H), 3.72 – 3.68 (m, 2H), 3.61 – 3.58 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5 (C=O), 167.5 (C=O), 165.5 (C=O), 139.6, 139.4, 131.1, 126.0, 125.6, 125.4,124.8, 119.7, 114.5, 110.3, 67.0, 66.7, 52.1, 49.9, 46.6, 42.0. HRMS (ESI) Calcd for $C_{19}H_{20}N_2NaO_5$: $[M+Na]^+$, 379.1264; Found: 379.1265. IR: ν (cm^{-1}) = 1637.10cm^{-1}, 1717.01 cm^{-1} (C=O stretch).

***N,N*-diethyl-2-(1-methylindol-3-yl)-2-oxoacetamide (3q).**



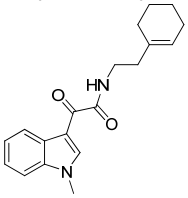
A yellow liquid. Chromatography solvent (PE/EA = 1/1). ^1H NMR (400 MHz, $CDCl_3$) δ 8.42 – 8.32 (m, 1H), 7.81 (s, 1H), 7.43 – 7.32 (m, 3H), 3.85 (s, 3H), 3.55 (m, 2H), 3.38 (m, 2H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.20 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100MHz, $CDCl_3$) δ 185.8 (C=O), 167.4 (C=O), 138.9, 137.7, 126.3, 123.9, 123.2, 122.4, 113.4, 109.9, 42.4, 39.1, 33.7, 14.5, 12.9. HRMS (ESI) Calcd for $C_{15}H_{18}N_2NaO_2$: $[M+Na]^+$, 281.1266; Found: 281.1260. IR: ν (cm^{-1}) = 1632.91cm^{-1} (C=O stretch).

***N*-allyl-2-(1-methylindol-3-yl)-2-oxoacetamide (3r).**



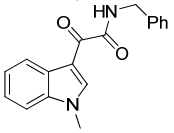
A pale yellow solid. Chromatography solvent (PE/EA = 5/1). ^1H NMR (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.42 (m, 1H), 7.64 (s, 1H), 7.40 – 7.33 (m, 3H), 5.90 (m, 1H), 5.28 (m, 1H), 5.20 (m, 1H), 4.02 (t, *J* = 5.8 Hz, 2H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.8 (C=O), 162.5 (C=O), 142.2, 137.1, 133.3, 127.7, 123.9, 123.5, 122.6, 116.8, 111.9, 109.9, 41.6, 33.8. HRMS (ESI) Calcd for $C_{14}H_{14}N_2NaO_2$: $[M+Na]^+$, 265.0947; Found: 265.0941. IR: ν (cm^{-1}) = 1677.75 cm^{-1}, 1622.99 cm^{-1} (C=O stretch) ; ν (cm^{-1}) = 3358.94 cm^{-1} (N-H stretch).

***N*-cyclohexenyl-2-(1-methylindol-3-yl)-2-oxoacetamide (3s).**



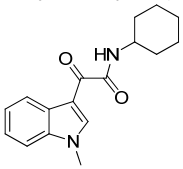
A white solid. Chromatography solvent (PE/EA = 5/1). ^1H NMR (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.47 – 8.37 (m, 1H), 7.54 (s, 1H), 7.39 – 7.32 (m, 3H), 5.54 (s, 1H), 3.86 (s, 3H), 3.45 (m, 2H), 2.23 (t, *J* = 6.8 Hz, 2H), 2.04 – 1.95 (m, 4H), 1.66 – 1.52 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 180.1 (C=O), 162.5 (C=O), 142.2, 137.0, 134.2, 127.7, 123.9, 123.8, 123.4, 122.6, 111.9, 109.9, 37.4, 37.2, 33.8, 28.0, 25.3, 22.9, 22.3. HRMS (ESI) Calcd for $C_{19}H_{22}N_2NaO_2$: $[M+Na]^+$, 333.1573; Found: 333.1562. IR: ν (cm^{-1}) = 1670.18 cm^{-1}, 1623.83 cm^{-1} (C=O stretch) ; ν (cm^{-1}) =3335.91 cm^{-1} (N-H stretch).

***N*-benzyl-2-(1-methylindol-3-yl)-2-oxoacetamide (3t).**



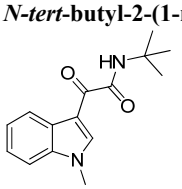
A white solid. Chromatography solvent (PE/EA = 5/1). ^1H NMR (400 MHz, $CDCl_3$) δ 9.00 (s, 1H), 8.43 – 8.39 (m, 1H), 7.89 (s, 1H), 7.37 – 7.34 (m, 8H), 4.57 (d, *J* = 6.1 Hz, 2H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.8 (C=O), 162.6 (C=O), 142.2, 137.5, 137.0, 128.8, 127.8, 127.7, 123.9, 123.5, 122.6, 111.9, 109.9, 43.3, 33.8. HRMS (ESI) Calcd for $C_{18}H_{16}N_2NaO_2$: $[M+Na]^+$, 315.1104; Found: 315.1101. IR: ν (cm^{-1}) = 1671.94 cm^{-1}, 1611.20 cm^{-1} (C=O stretch) ; ν (cm^{-1}) = 3332.99 cm^{-1} (N-H stretch).

_N_-cyclohexyl-2-(1-methylindol-3-yl)-2-oxoacetamide (3u).



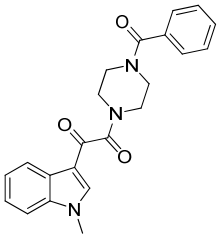
A yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (s, 1H), 8.36 – 8.31 (m, 1H), 7.38 (d, *J* = 7.9 Hz, 1H), 7.29 – 7.25 (m, 3H), 3.77 (s, 3H), 1.92 – 1.85 (m, 2H), 1.73 – 1.66 (m, 2H), 1.60 – 1.54 (m, 1H), 1.39 – 1.12 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.4 (C=O), 161.7 (C=O), 142.2, 137.0, 127.7, 123.8, 123.4, 122.6, 111.9, 109.9, 48.3, 33.8, 32.8, 25.5, 24.8. HRMS (ESI) Calcd for $C_{17}H_{20}N_2NaO_2$: $[M+Na]^+$, 307.1417; Found: 307.1417. IR: ν (cm^{-1}) = 1665.52 cm^{-1}, 1619.74 cm^{-1} (C=O stretch) ; ν (cm^{-1}) = 3330.31 cm^{-1} (N-H stretch).

***N-tert*-butyl-2-(1-methylindol-3-yl)-2-oxoacetamide (3v).**



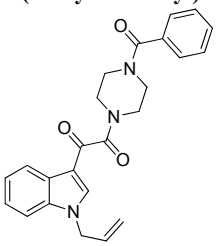
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, CD_3OD) δ 9.01 (s, 1H), 8.43 – 8.38 (m, 1H), 7.46 (s, 1H), 7.37 (m, 3H), 3.87 (s, 3H), 1.46 (s, 9H). ^{13}C NMR (101 MHz, CD_3OD) δ 185.8 (C=O), 167.5 (C=O), 145.5, 141.3, 131.2, 127.4, 126.7, 125.7, 115.2, 113.9, 54.8, 36.4, 31.2. HRMS (ESI) Calcd for $C_{15}H_{18}N_2NaO_2$: $[M+Na]^+$, 281.1260; Found: 281.1268. IR: ν (cm^{-1}) = 1679.02 cm^{-1}, 1616.66 cm^{-1} (C=O stretch) ; ν (cm^{-1}) = 3333.92 cm^{-1} (N-H stretch).

1-(1-methylindol-3-yl)-2-(4-benzoylpiperazin-1-yl)ethane-1,2-dione (3w).



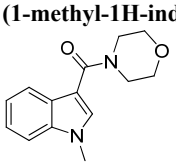
A pale yellow solid. Chromatography solvent (PE/EA = 1/2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.90 (s, 1H), 7.40 (d, *J* = 18.5 Hz, 8H), 3.72 (m, 11H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 184.3 (C=O), 170.7 (C=O), 166.2 (C=O), 139.5, 137.7, 135.1, 133.9, 130.2, 128.7, 128.5, 127.1, 126.2, 124.2, 123.5, 122.3, 113.3, 110.1, 50.1, 46.2, 41.7, 33.8, 28.4. HRMS (ESI) Calcd for $C_{22}H_{21}N_3NaO_3$: $[M+Na]^+$, 398.1475; Found: 398.1487. IR: ν (cm^{-1}) = 1617.24 cm^{-1}, 1601.36 cm^{-1}, 1674.25 cm^{-1} (C=O stretch).

1-(1-allylindol-3-yl)-2-(4-benzoylpiperazin-1-yl)ethane-1,2-dione (3x).



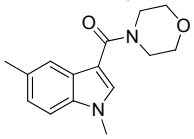
A white solid. Chromatography solvent (PE/EA = 1/2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.93 (s, 1H), 7.46 – 7.32 (m, 8H), 5.99 (m, 1H), 5.31 (m, 1H), 5.21 (m, 1H), 4.76 (d, *J* = 5.6 Hz, 2H), 3.69 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 184.5 (C=O), 170.7 (C=O), 166.2 (C=O), 138.5, 137.1, 135.1, 131.5, 130.2, 128.7, 127.1, 126.4, 124.2, 123.5, 122.4, 119.4, 113.6, 110.6, 65.8, 49.8, 46.2, 41.7, 15.3. HRMS (ESI) Calcd for $C_{24}H_{23}N_3NaO_3$: $[M+Na]^+$, 424.1632; Found: 424.1627. IR: ν (cm^{-1}) = 1620.26 cm^{-1}, 1607.46 cm^{-1}, 1676.23 cm^{-1} (C=O stretch).

(1-methyl-1H-indol-3-yl)(morpholino)methanone (4a).



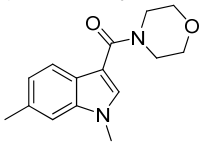
A red liquid. Chromatography solvent (PE/EA = 1/1).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.8 Hz, 1H), 7.44 (s, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.31 – 7.19 (m, 2H), 3.81 (s, 3H), 3.73 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8 (C=O), 136.5, 131.8, 125.8, 122.5, 121.0, 120.5, 110.0, 109.9, 67.2, 33.2. HRMS (ESI) Calcd for $C_{14}H_{16}N_2NaO_2$: $[M+Na]^+$, 267.1104; Found: 267.1097. IR: ν (cm^{-1}) = 1605.86 cm^{-1} (C=O stretch).

(1,5-dimethyl-1H-indol-3-yl)(morpholino)methanone (4b).



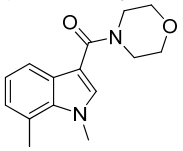
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (s, 1H), 7.37 (s, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.10 (d, *J* = 8.4 Hz, 1H), 3.78 (s, 3H), 3.74 (m, 8H), 2.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.9 (C=O), 134.9, 131.6, 130.5, 126.2, 124.2, 120.2, 109.5, 109.4, 67.2, 33.2, 21.6. HRMS (ESI) Calcd for $C_{15}H_{18}N_2NaO_2$: $[M+Na]^+$, 281.1260; Found: 281.1263. IR: ν (cm^{-1}) = 1642.65 cm^{-1} (C=O stretch).

(1,6-dimethyl-1H-indol-3-yl)(morpholino)methanone (4c).



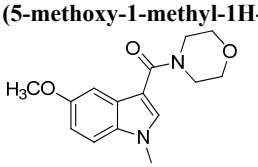
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.2 Hz, 1H), 7.30 (s, 1H), 7.06 (s, 1H), 6.98 (d, *J* = 8.2 Hz, 1H), 3.70 (s, 3H), 3.65 (m, 8H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.9 (C=O), 136.9, 132.5, 131.4, 123.7, 122.8, 120.1, 109.9, 109.8, 67.2, 33.1, 21.8. HRMS (ESI) Calcd for $C_{15}H_{18}N_2NaO_2$: $[M+Na]^+$, 281.1260; Found: 281.1256. IR: ν (cm^{-1}) = 1612.26 cm^{-1} (C=O stretch).

(1,7-dimethyl-1H-indol-3-yl)(morpholino)methanone (4d).



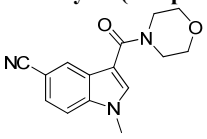
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.0 Hz, 1H), 7.30 (s, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 7.1 Hz, 1H), 4.05 (s, 3H), 3.71 (m, 8H), 2.75 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8 (C=O), 135.2, 133.1, 126.9, 125.2, 121.9, 121.2, 118.5, 109.8, 67.2, 37.3, 19.6. HRMS (ESI) Calcd for $C_{15}H_{18}N_2NaO_2$: $[M+Na]^+$, 281.1260; Found: 281.1258. IR: ν (cm^{-1}) = 1628.25 cm^{-1} (C=O stretch).

(5-methoxy-1-methyl-1H-indol-3-yl)(morpholino)methanone (4e).



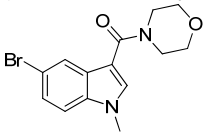
A yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.22 (d, *J* = 8.9 Hz, 1H), 7.18 (d, *J* = 2.4 Hz, 1H), 6.92 (m, 1H), 3.86 (s, 3H), 3.77 (s, 3H), 3.74 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8 (C=O), 155.2, 131.8, 126.7, 113.0, 110.6, 109.2, 102.1, 67.2, 55.8, 33.3. HRMS (ESI) Calcd for $C_{15}H_{18}N_2NaO_3$: $[M+Na]^+$, 297.1210; Found: 297.1217. IR: ν (cm^{-1}) =1620.26 cm^{-1} (C=O stretch).

1-methyl-3-(morpholine-4-carbonyl)-1H-indole-5-carbonitrile (4f).



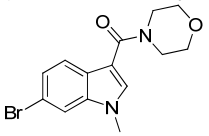
A white solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 0.7 Hz, 1H), 7.44 – 7.39 (m, 2H), 7.33 (d, *J* = 8.6 Hz, 1H), 3.79 (s, 3H), 3.67 (m, 8H) . ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1 (C=O), 137.9, 133.0, 126.2, 126.1, 125.5, 120.2, 110.8, 110.7, 104.3, 67.0, 33.5. HRMS (ESI) Calcd for $C_{15}H_{15}N_3NaO_2$: $[M+Na]^+$, 292.1056; Found: 292.1063. IR: ν (cm^{-1}) = 1628.25 cm^{-1} (C=O stretch).

(5-bromo-1-methyl-1H-indol-3-yl)(morpholino)methanone (4g).



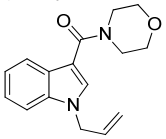
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 1.7 Hz, 1H), 7.38 (s, 1H), 7.33 (m, 1H), 7.19 (d, *J* = 8.7 Hz, 1H), 3.78 (s, 3H), 3.72 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9 (C=O), 135.2, 132.3, 127.7, 125.5, 123.1, 114.6, 111.3, 109.4, 67.1, 33.3. HRMS (ESI) Calcd for $C_{14}H_{15}BrN_2NaO_2$: $[M+Na]^+$, 345.0209; Found: 345.0199. IR: ν (cm^{-1}) = 1612.26 cm^{-1} (C=O stretch).

(6-bromo-1-methyl-1H-indol-3-yl)(morpholino)methanone (4h).



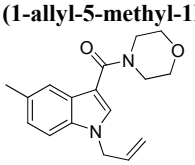
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.5 Hz, 1H), 7.49 (d, *J* = 1.4 Hz, 1H), 7.37 (s, 1H), 7.31 (m, 1H), 3.76 (s, 3H), 3.72 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1 (C=O), 137.3, 131.9, 124.9, 124.3, 121.8, 116.2, 112.9, 110.2, 67.1, 33.3. HRMS (ESI) Calcd for $C_{14}H_{15}BrN_2NaO_2$: $[M+Na]^+$, 345.0209; Found: 345.0211. IR: ν (cm^{-1}) = 1620.26 cm^{-1} (C=O stretch).

(1-allyl-1H-indol-3-yl)(morpholino)methanone (4i).



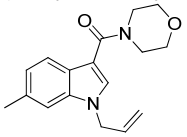
A red liquid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (m, 1H), 7.48 (s, 1H), 7.38 – 7.33 (m, 1H), 7.28 – 7.20 (m, 2H), 6.07 – 5.93 (m, 1H), 5.27 (m, 1H), 5.17 (m, 1H), 4.75 (m, 2H), 3.74 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7 (C=O), 135.9, 132.5, 130.7, 126.1, 122.6, 121.1, 120.6, 118.4, 110.4, 110.3, 67.2, 49.2. HRMS (ESI) Calcd for $C_{16}H_{18}N_2NaO_2$: $[M+Na]^+$, 293.1260; Found: 293.1260. IR: ν (cm^{-1}) = 1612.26 cm^{-1} (C=O stretch).

(1-allyl-5-methyl-1H-indol-3-yl)(morpholino)methanone (4j).



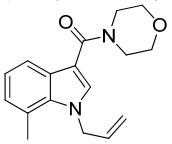
A red liquid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.41 (s, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 5.98 (m, 1H), 5.25 (m, 1H), 5.14 (m, 1.0 Hz, 1H), 4.71 (d, *J* = 5.5 Hz, 2H), 3.74 (m, 8H), 2.47 (s, 3H) . ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8 (C=O), 134.4, 132.6, 130.6, 130.6, 126.5, 124.2, 120.3, 118.2, 109.9, 109.8, 67.2, 49.2, 21.5. HRMS (ESI) Calcd for $C_{17}H_{20}N_2NaO_2$: $[M+Na]^+$, 307.1417; Found: 307.1414. IR: ν (cm^{-1}) = 1612.26 cm^{-1} (C=O stretch).

(1-allyl-6-methyl-1H-indol-3-yl)(morpholino)methanone (4k).



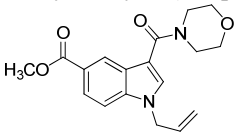
A red liquid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.2 Hz, 1H), 7.41 (s, 1H), 7.13 (s, 1H), 7.05 (d, *J* = 8.2 Hz, 1H), 6.00 (m, 1H), 5.26 (d, *J* = 10.2 Hz, 1H), 5.16 (d, *J* = 17.1 Hz, 1H), 4.71 (d, *J* = 5.0 Hz, 2H), 3.73 (m, 8H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.9 (C=O), 136.3, 132.6, 132.5, 130.3, 123.9, 122.9, 120.2, 118.2, 110.3, 110.1, 67.2, 49.0, 21.8. HRMS (ESI) Calcd for $C_{17}H_{20}N_2NaO_2$: $[M+Na]^+$, 307.1417; Found: 307.1422. IR: ν (cm^{-1}) = 1612.26 cm^{-1} (C=O stretch).

(1-allyl-7-methyl-1H-indol-3-yl)(morpholino)methanone (4l).



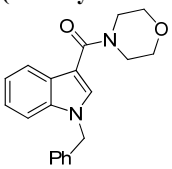
A red liquid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.36 (s, 1H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 7.1 Hz, 1H), 6.06 (m, 1H), 5.20 (d, *J* = 10.3 Hz, 1H), 4.97 (d, *J* = 2.7 Hz, 2H), 4.85 (d, *J* = 17.1 Hz, 1H), 3.72 (m, 8H), 2.68 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7 (C=O), 134.7, 134.5, 132.0, 126.9, 125.5, 121.5, 121.2, 118.6, 116.9, 110.6, 67.2, 51.2, 19.4. HRMS (ESI) Calcd for $C_{17}H_{20}N_2NaO_2$: $[M+Na]^+$, 307.1417; Found: 307.1417. IR: ν (cm^{-1}) = 1620.26 cm^{-1} (C=O stretch).

methyl 1-allyl-3-(morpholine-4-carbonyl)-1H-indole-5-carboxylate (4m).



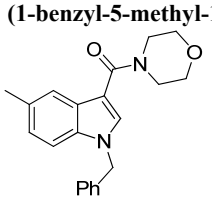
A red liquid. Chromatography solvent (PE/EA = 1/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 1.1 Hz, 1H), 7.96 (m, 1H), 7.52 (s, 1H), 7.37 (d, *J* = 8.7 Hz, 1H), 6.00 (m, 1H), 5.30 (m, 1H), 5.18 (m, 1H), 4.77 (m, 2H), 3.94 (s, 3H), 3.75 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.7 (C=O), 165.9 (C=O), 138.3, 131.9, 131.8, 125.7, 123.9, 123.3, 123.2, 118.8, 111.9, 110.0, 67.1, 52.0, 49.4. HRMS (ESI) Calcd for $C_{18}H_{20}N_2NaO_4$: $[M+Na]^+$, 351.1315; Found: 351.1307. IR: ν (cm^{-1}) = 1642.65 cm^{-1}, 1703.42 cm^{-1} (C=O stretch).

(1-benzyl-1H-indol-3-yl)(morpholino)methanone (4n).



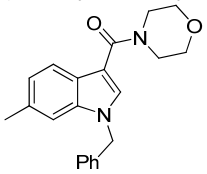
A white solid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.69 (m, 1H), 7.47 (s, 1H), 7.33 – 7.25 (m, 4H), 7.25 – 7.18 (m, 2H), 7.18 – 7.10 (m, 2H), 5.29 (s, 2H), 3.71 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6 (C=O), 136.2, 136.1, 131.1, 128.9, 128.1, 127.1, 126.2, 122.7, 121.2, 120.7, 110.6, 110.4, 67.1, 50.5. HRMS (ESI) Calcd for $C_{20}H_{20}N_2NaO_2$: $[M+Na]^+$, 343.1420; Found: 343.1417. IR: ν (cm^{-1}) = 1642.65 cm^{-1} (C=O stretch)

(1-benzyl-5-methyl-1H-indol-3-yl)(morpholino)methanone (4o).



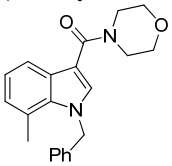
A white solid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.34 (s, 1H), 7.25 – 7.17 (m, 3H), 7.12 – 7.02 (m, 3H), 6.96 (m, 1H), 5.20 (s, 2H), 3.65 (m, 8H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8 (C=O), 136.4, 134.6, 130.9, 130.8,128.9, 128.0, 127.0, 126.6, 124.4, 120.4, 110.1,109.9,67.1, 50.5, 21.6. HRMS (ESI) Calcd for $C_{21}H_{22}N_2NaO_2$: $[M+Na]^+$, 357.1573; Found: 357.1570. IR: ν (cm^{-1}) = 1612.26 cm^{-1} (C=O stretch).

(1-benzyl-6-methyl-1H-indol-3-yl)(morpholino)methanone (4p).



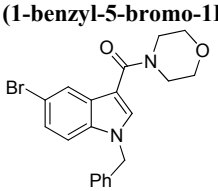
A white solid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.2 Hz, 1H), 7.41 (s, 1H), 7.36 – 7.26 (m, 3H), 7.17 – 7.02 (m, 4H), 5.28 (s, 2H), 3.72 (m, 8H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8 (C=O), 136.5, 136.4, 132.7, 130.6, 128.9, 127.9, 127.0, 124.0, 123.0, 120.3, 110.5, 110.2, 67.1, 50.3, 21.8. HRMS (ESI) Calcd for $C_{21}H_{22}N_2NaO_2$: $[M+Na]^+$, 357.1573; Found: 357.1567. IR: ν (cm^{-1}) = 1612.26 cm^{-1} (C=O stretch).

(1-benzyl-6-methyl-1H-indol-3-yl)(morpholino)methanone (4q)



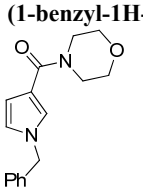
A white solid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.0 Hz, 1H), 7.31 (s, 1H), 7.24 – 7.15 (m, 3H), 7.03 (t, J = 7.6 Hz, 1H), 6.92 – 6.81 (m, 3H), 5.51 (s, 2H), 3.65 (m, 8H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7 (C=O), 138.4, 134.9, 132.5, 129.0, 127.7, 127.3, 125.7, 125.6, 121.7, 121.4, 118.7, 110.7, 67.1, 52.6, 19.5. HRMS (ESI) Calcd for $C_{21}H_{22}N_2NaO_2$: $[M+Na]^+$, 357.1573; Found: 357.1575. IR: ν (cm^{-1}) = 1620.26 cm^{-1} (C=O stretch).

(1-benzyl-5-bromo-1H-indol-3-yl)(morpholino)methanone (4r)



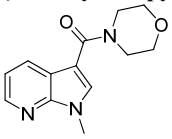
A pale yellow solid. Chromatography solvent (PE/EA = 1/1). 1H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 1.7 Hz, 1H), 7.44 (s, 1H), 7.33 – 7.26 (m, 4H), 7.17 – 7.09 (m, 3H), 5.29 (s, 2H), 3.72 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9 (C=O), 135.8, 134.8, 131.6, 129.1, 128.3, 128.0, 127.0, 125.8, 123.4, 114.8, 111.9, 110.1, 67.1, 50.7. HRMS (ESI) Calcd for $C_{22}H_{19}BrN_2NaO_2$: $[M+Na]^+$, 421.0546; Found: 421.0539. IR: ν (cm^{-1}) = 1612.26 cm^{-1} (C=O stretch).

(1-benzyl-1H-pyrrol-3-yl)(morpholino)methanone (4s)



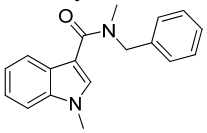
A red liquid. Chromatography solvent (PE/EA = 5/1).1H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 3H), 7.15 (d, *J* = 6.7 Hz, 2H), 7.07 (s, 1H), 6.62 (t, *J* = 2.5 Hz, 1H), 6.35 – 6.27 (m, 1H), 5.04 (s, 2H), 3.72 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4 (C=O), 136.8, 128.9, 128.1, 127.4, 124.4, 121.2, 118.4, 109.5, 67.0, 53.7. HRMS (ESI) Calcd for $C_{16}H_{18}N_2NaO_2$: $[M+Na]^+$, 293.1260; Found: 293.1261. IR: ν (cm^{-1}) = 1605.86 cm^{-1} (C=O stretch).

(1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)(morpholino)methanone (4t)



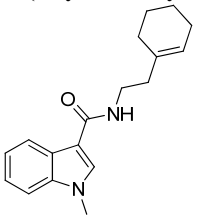
A yellow solid. Chromatography solvent (PE/EA = 1/1). ^1H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.35 (m, 1H), 8.05 (m, 1H), 7.57 (s, 1H), 7.18 (m, 1H), 3.92 (s, 3H), 3.75 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7 (C=O), 147.3, 143.9, 131.5, 128.9, 118.6, 117.1, 108.1, 67.0, 31.5. HRMS (ESI) Calcd for $C_{13}H_{15}N_3NaO_2$: $[M+Na]^+$, 268.1056; Found: 268.1066. IR: ν (cm^{-1}) = 1597.87 cm^{-1} (C=O stretch).

***N*-benzyl-N,1-dimethyl-1H-indole-3-carboxamide (4u)**



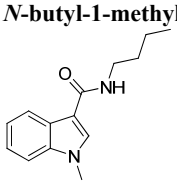
A white solid. Chromatography solvent (PE/EA = 1/1). ^1H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.8 Hz, 1H), 7.38 – 7.21 (m, 9H), 4.80 (s, 2H), 3.76 (s, 3H), 3.07 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.7 (C=O), 137.6, 136.5, 130.6, 128.8, 127.5, 127.4, 126.9, 122.5, 121.3, 120.9, 110.3, 109.6, 52.8, 35.5, 33.2. HRMS (ESI) Calcd for $C_{18}H_{18}N_2NaO$: $[M+Na]^+$, 301.1311; Found: 301.1311. IR: ν (cm^{-1}) = 1605.26 cm^{-1} (C=O stretch).

***N*-(2-cyclohexenylethyl)-1-methyl-1H-indole-3-carboxamide (4v)**



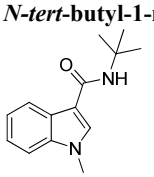
A colorless solid. Chromatography solvent (PE/EA = 5/1).^1H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.6 Hz, 1H), 7.68 (s, 1H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.28 (m, 2H), 6.01 (s, 1H), 5.63 (s, 1H), 3.82 (s, 3H), 3.59 (m, 2H), 2.30 (t, *J* = 6.4 Hz, 2H), 2.06 (m, 4H), 1.69 – 1.58 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9 (C=O), 137.3, 135.2, 132.8, 125.0, 124.2, 122.3, 121.3, 119.7, 111.2, 110.2, 37.7, 36.8, 33.3, 27.6, 25.4, 22.8, 22.4. HRMS (ESI) Calcd for $C_{18}H_{22}N_2NaO$: $[M+Na]^+$, 305.1624; Found: 305.1628. IR: ν (cm^{-1}) = 1628.25 cm^{-1} (C=O stretch); ν (cm^{-1})=3285.12 cm^{-1} (N-H stretch).

***N*-butyl-1-methyl-1H-indole-3-carboxamide (4w)**



A yellow solid. Chromatography solvent (PE/EA = 5/1). 1H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.88 (m, 1H), 7.65 (s, 1H), 7.37 – 7.23 (m, 3H), 5.98 (s, 1H), 3.79 (s, 3H), 3.50 (m, 2H), 1.67 – 1.58 (m, 2H), 1.44 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2 (C=O), 137.2, 132.3, 125.3, 122.4, 121.3, 119.9, 111.1, 110.1, 39.2, 33.2, 32.1, 20.3, 13.9. HRMS (ESI) Calcd for $C_{14}H_{18}N_2NaO$: $[M+Na]^+$, 253.1311; Found: 253.1310. IR: ν (cm^{-1}) = 1628.25 cm^{-1} (C=O stretch); ν (cm^{-1}) = 3384.27 cm^{-1} (N-H stretch).

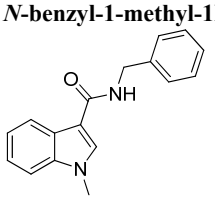
***N-tert*-butyl-1-methyl-1H-indole-3-carboxamide (4x)**



A white solid. Chromatography solvent (PE/EA = 10/1).1H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.2 Hz, 1H), 7.62 (s, 1H), 7.36 (d, *J* = 7.4 Hz, 1H), 7.29 (m, 2H), 5.81 (s, 1H), 3.82 (s, 3H), 1.52 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.6 (C=O), 137.3, 132.3, 125.1, 122.4,

121.2, 119.8, 112.2, 110.1, 51.3, 33.2, 29.3. HRMS (ESI) Calcd for $C_{14}H_{18}N_2O$: $[M+H]^+$, 231.1492; Found: 231.1497. IR: ν (cm^{-1}) = 1628.25 cm^{-1} (C=O stretch); ν (cm^{-1}) = 3384.27 cm^{-1} (N-H stretch).

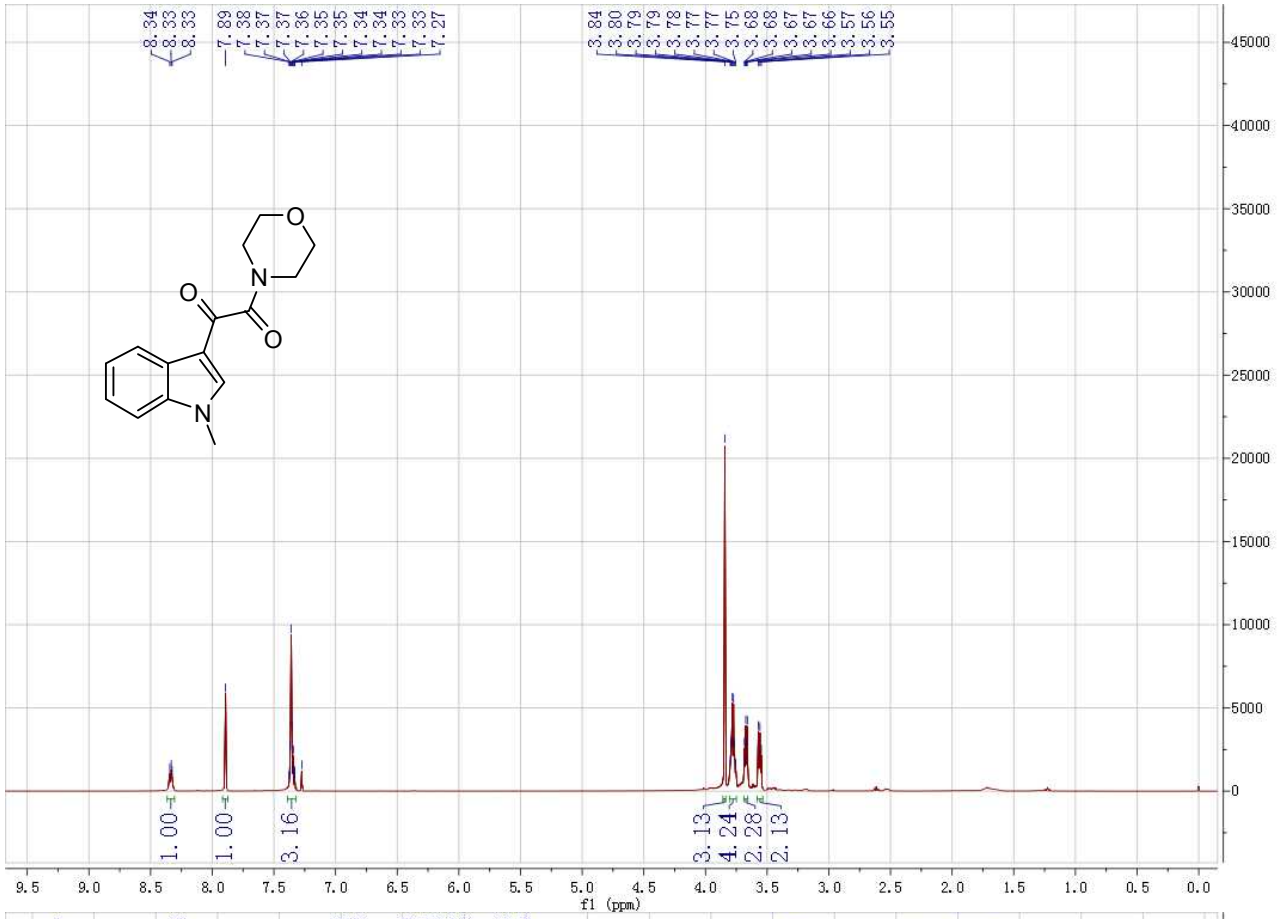
***N*-benzyl-1-methyl-1H-indole-3-carboxamide (4y)**

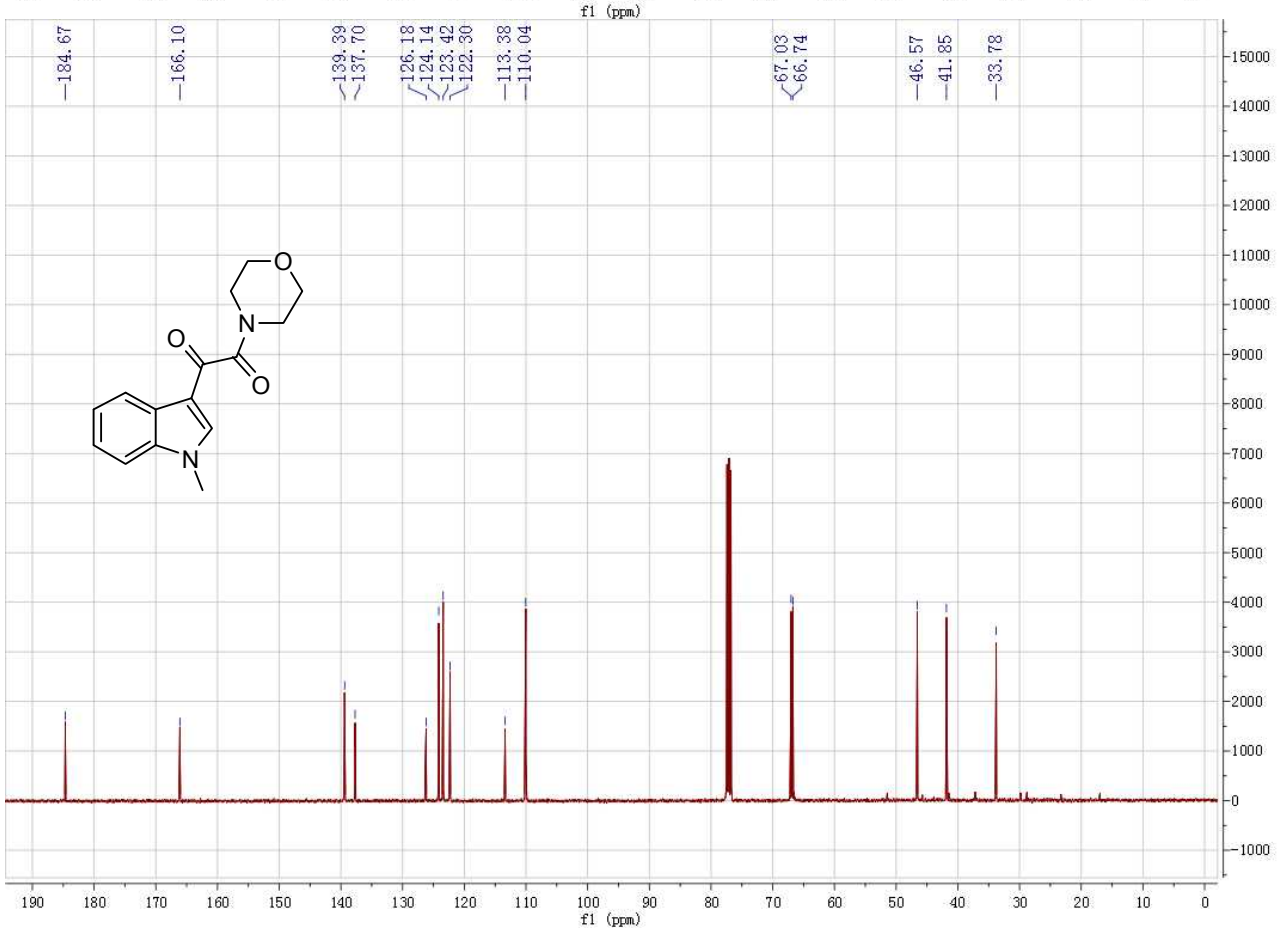


A pale yellow solid. Chromatography solvent (PE/EA = 5/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.90 (m, 1H), 7.67 (s, 1H), 7.44 – 7.32 (m, 5H), 7.31 – 7.22 (m, 3H), 6.24 (s, 1H), 4.70 (d, *J* = 5.7 Hz, 2H), 3.80 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0 (C=O), 138.9, 137.3, 132.4, 128.7, 127.8, 127.4, 125.3, 122.6, 121.5, 120.1, 110.7, 110.1, 43.5, 33.3. HRMS (ESI) Calcd for $C_{17}H_{16}N_2NaO$: $[M+Na]^+$, 287.1155; Found: 287.1153. IR: ν (cm^{-1}) = 1636.25 cm^{-1} (C=O stretch); ν (cm^{-1}) = 3445.05 cm^{-1} (N-H stretch).

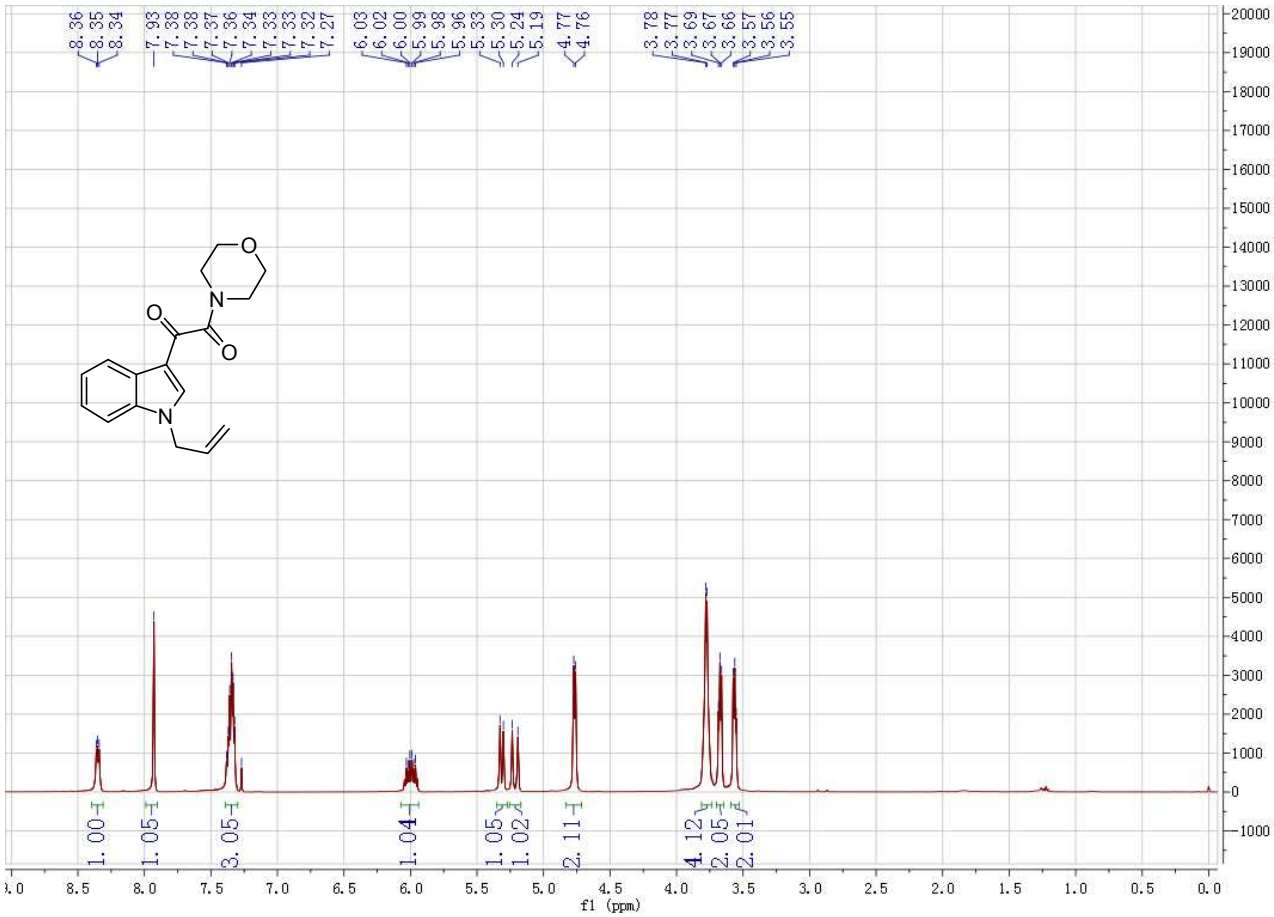
5) ^{1}H NMR and ^{13}C NMR Copies of Products

3a





3b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7.27
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6.02
6.00
5.99
5.98
5.96
5.33
5.30
5.24
5.19
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4.76
3.78
3.77
3.69
3.67
3.66
3.57
3.56
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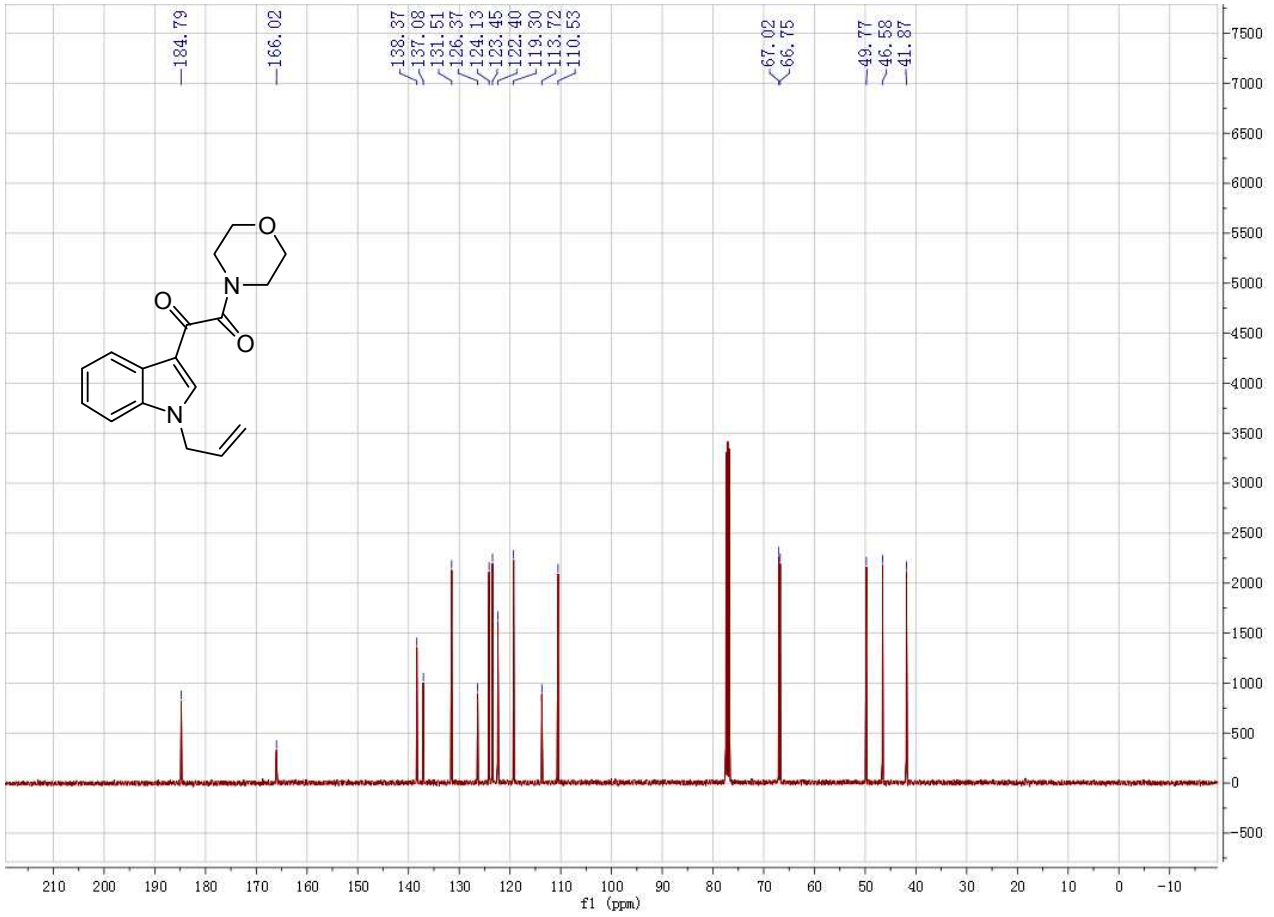
4.12
2.05
2.01
f1 (ppm)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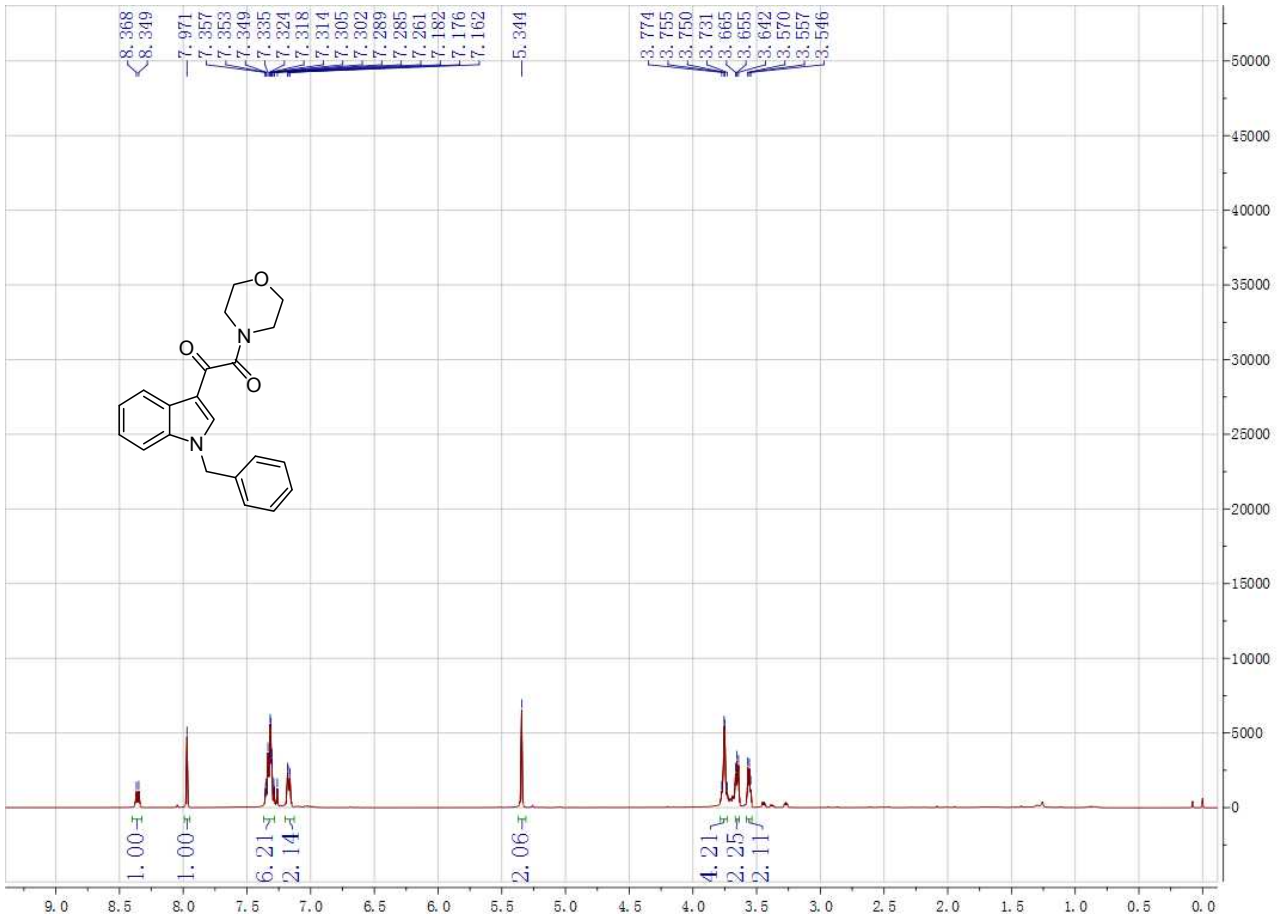
f1 (ppm)

3c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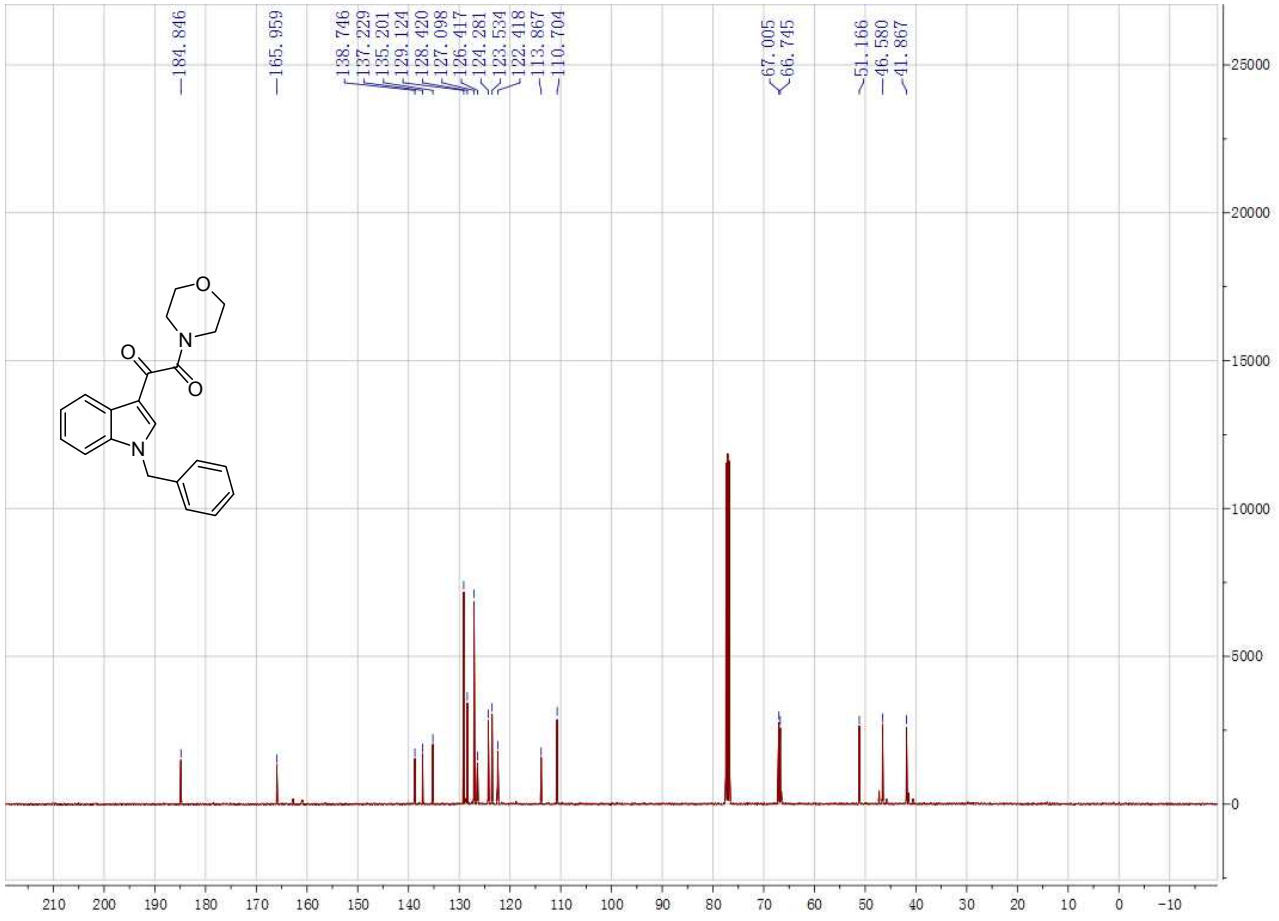
2.11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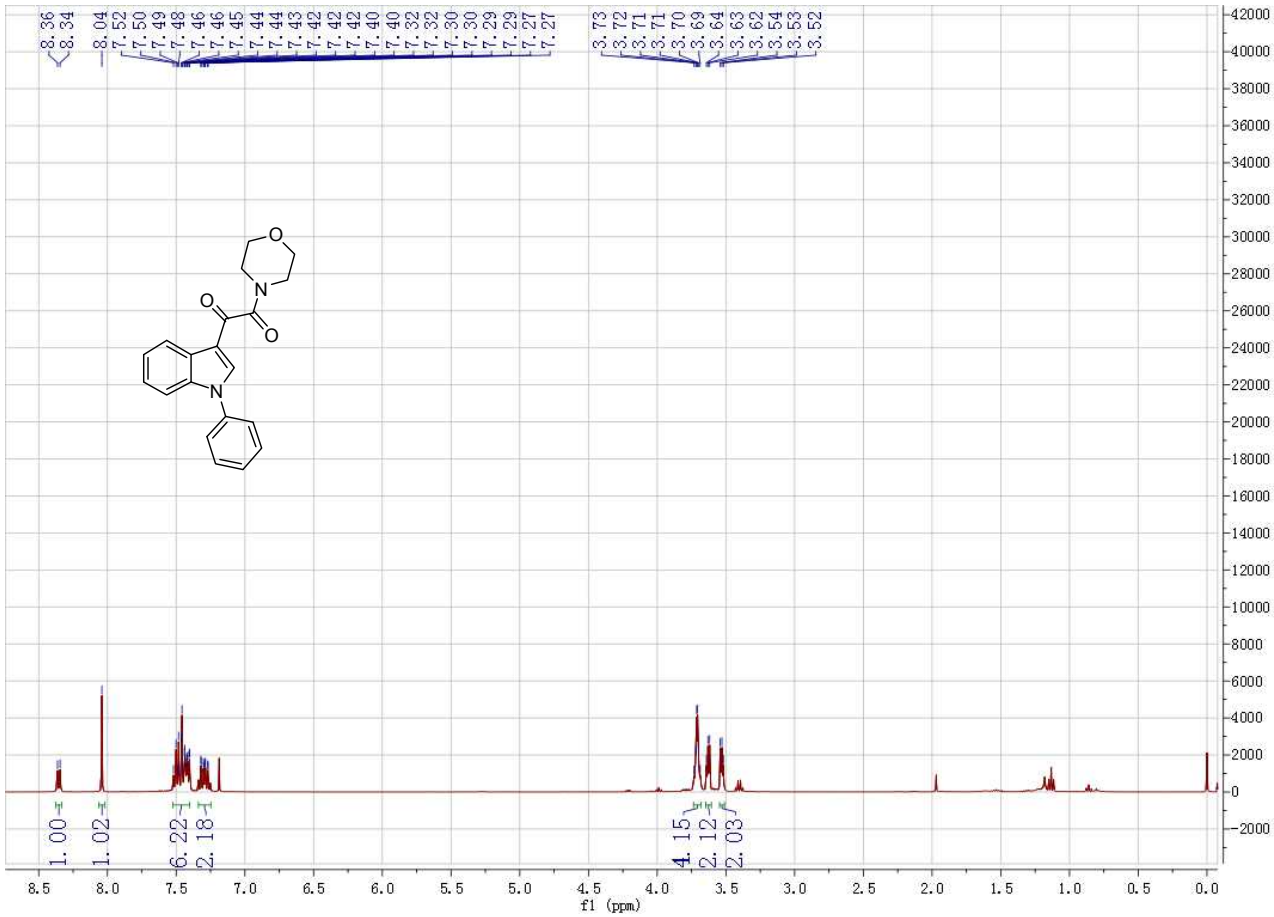
51.166
46.580
41.867

3d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3.63
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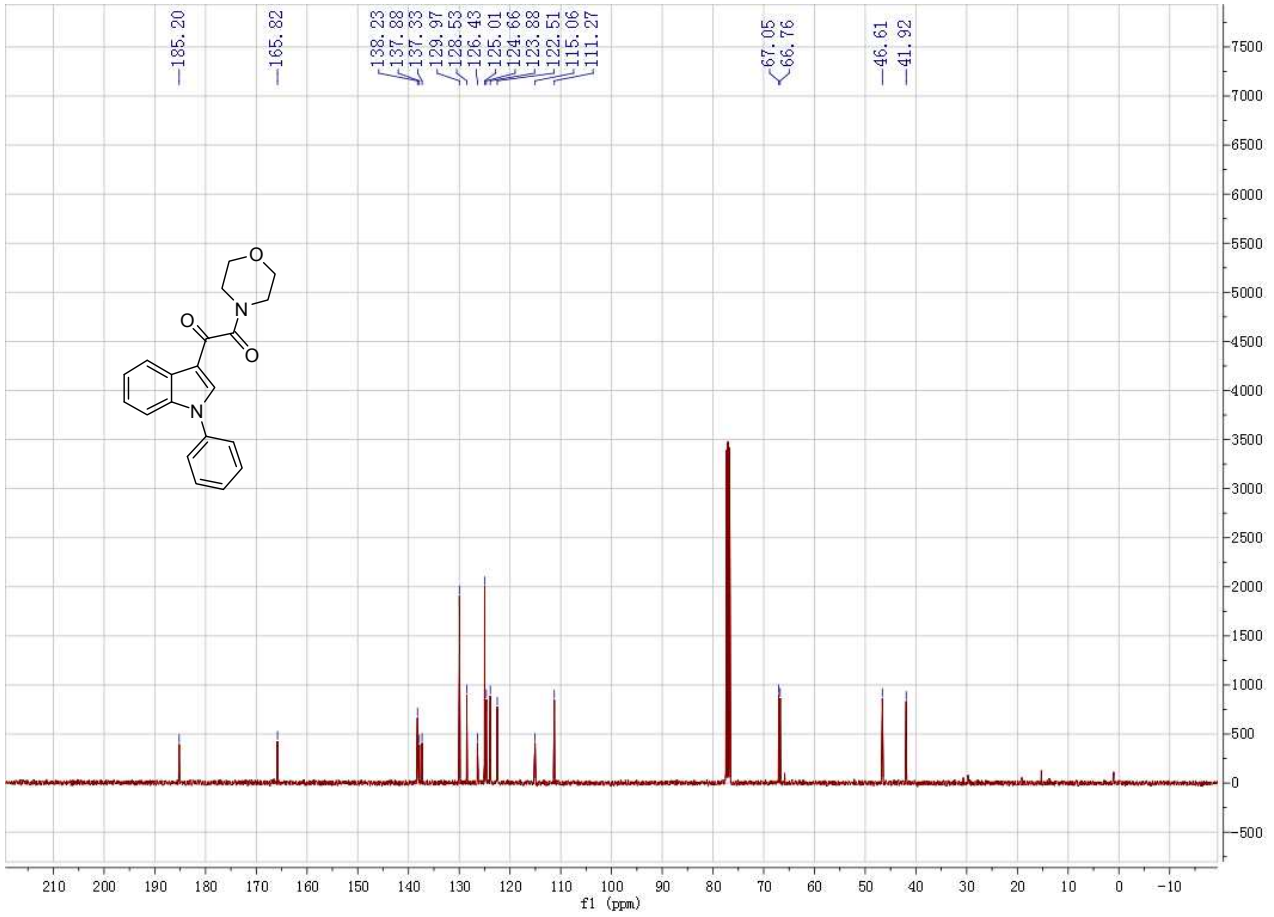
f1 (ppm)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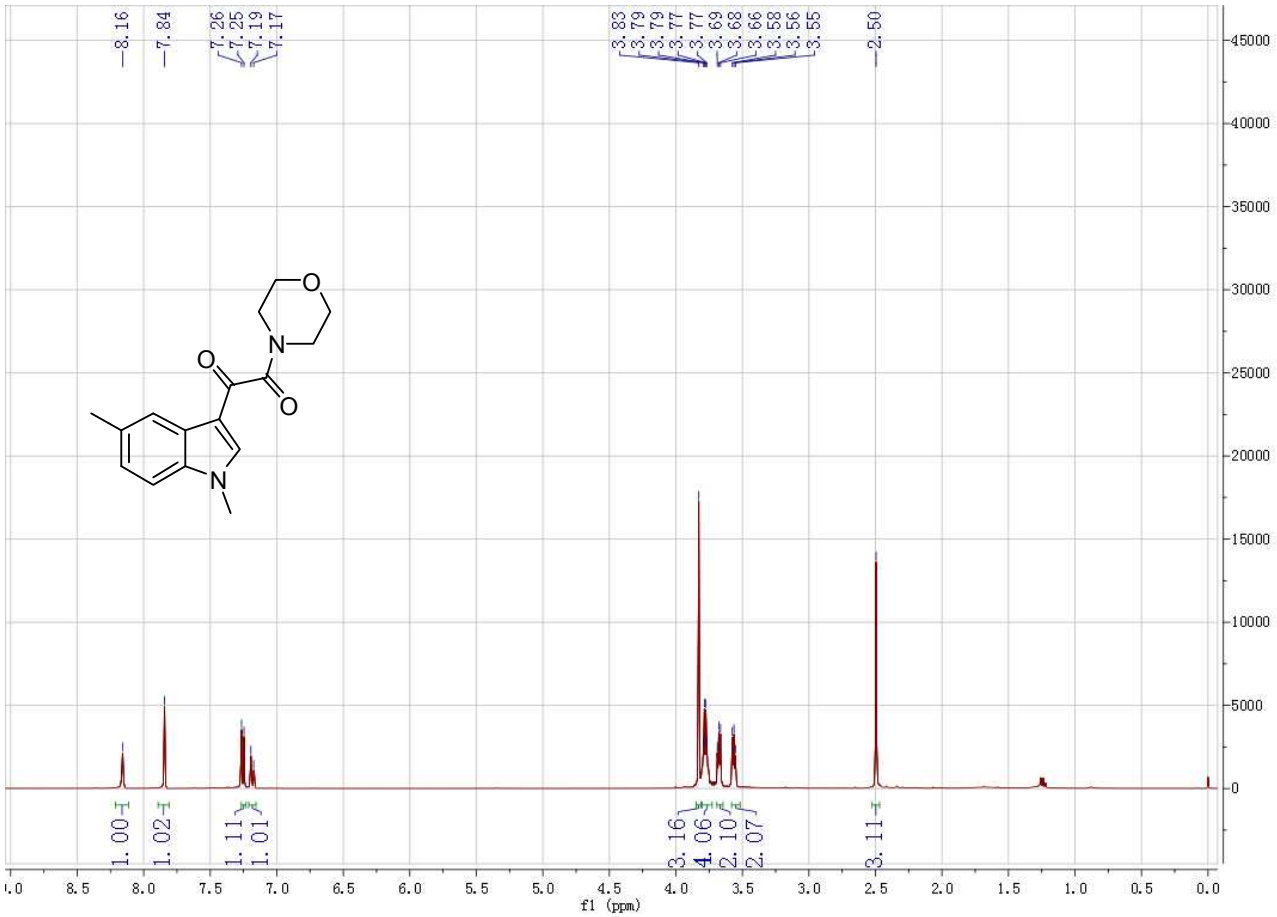
f1 (ppm)

3e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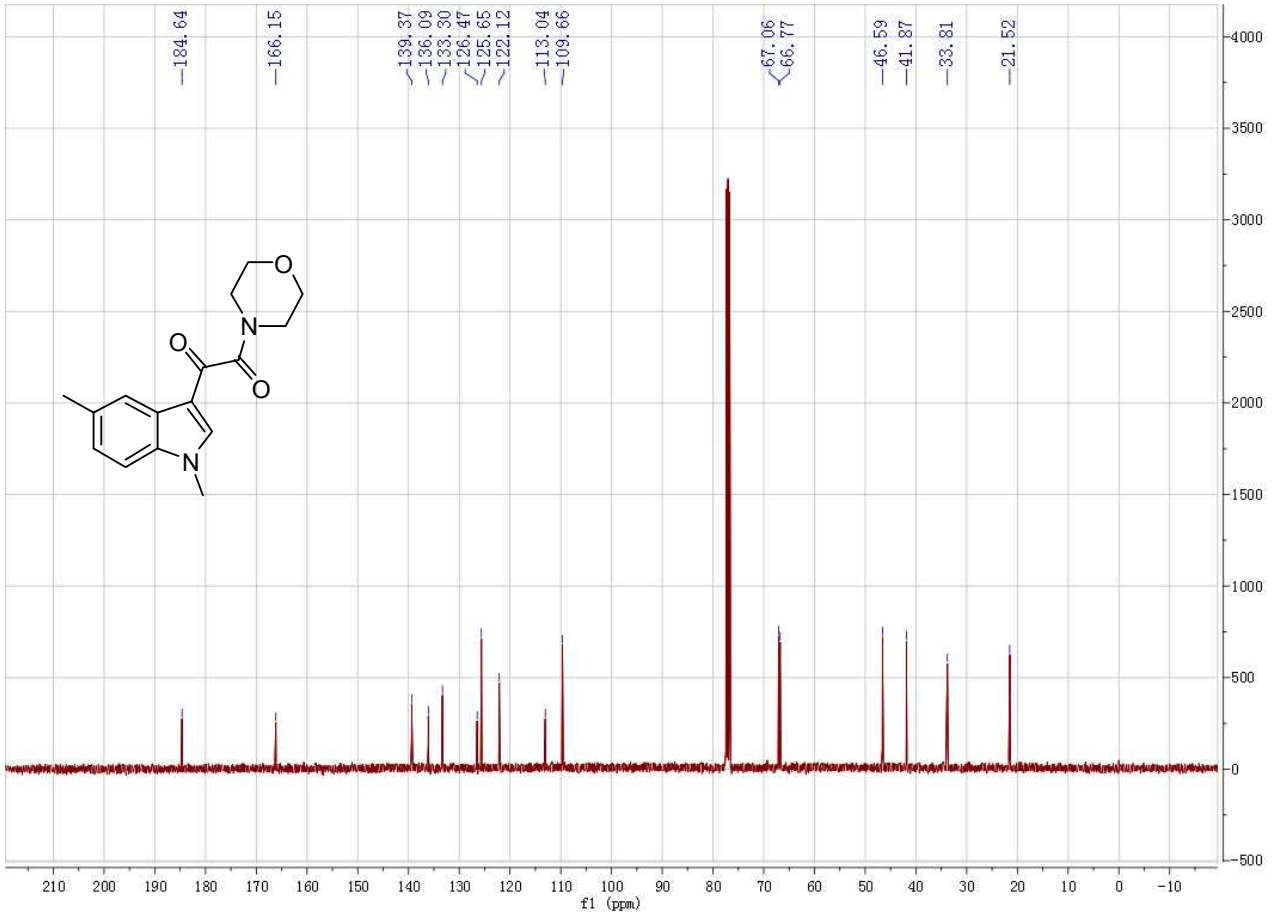
f1 (ppm)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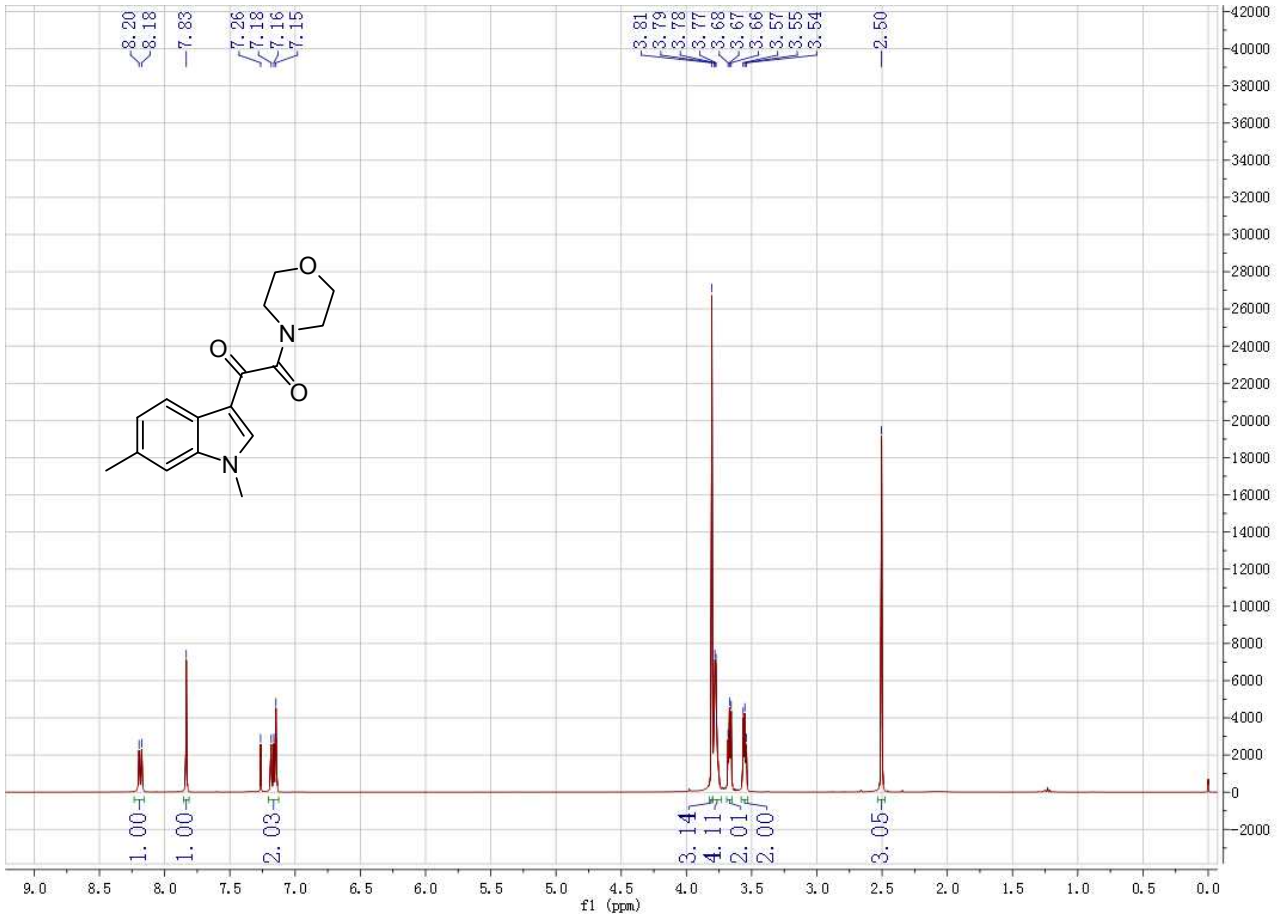
f1 (ppm)

3f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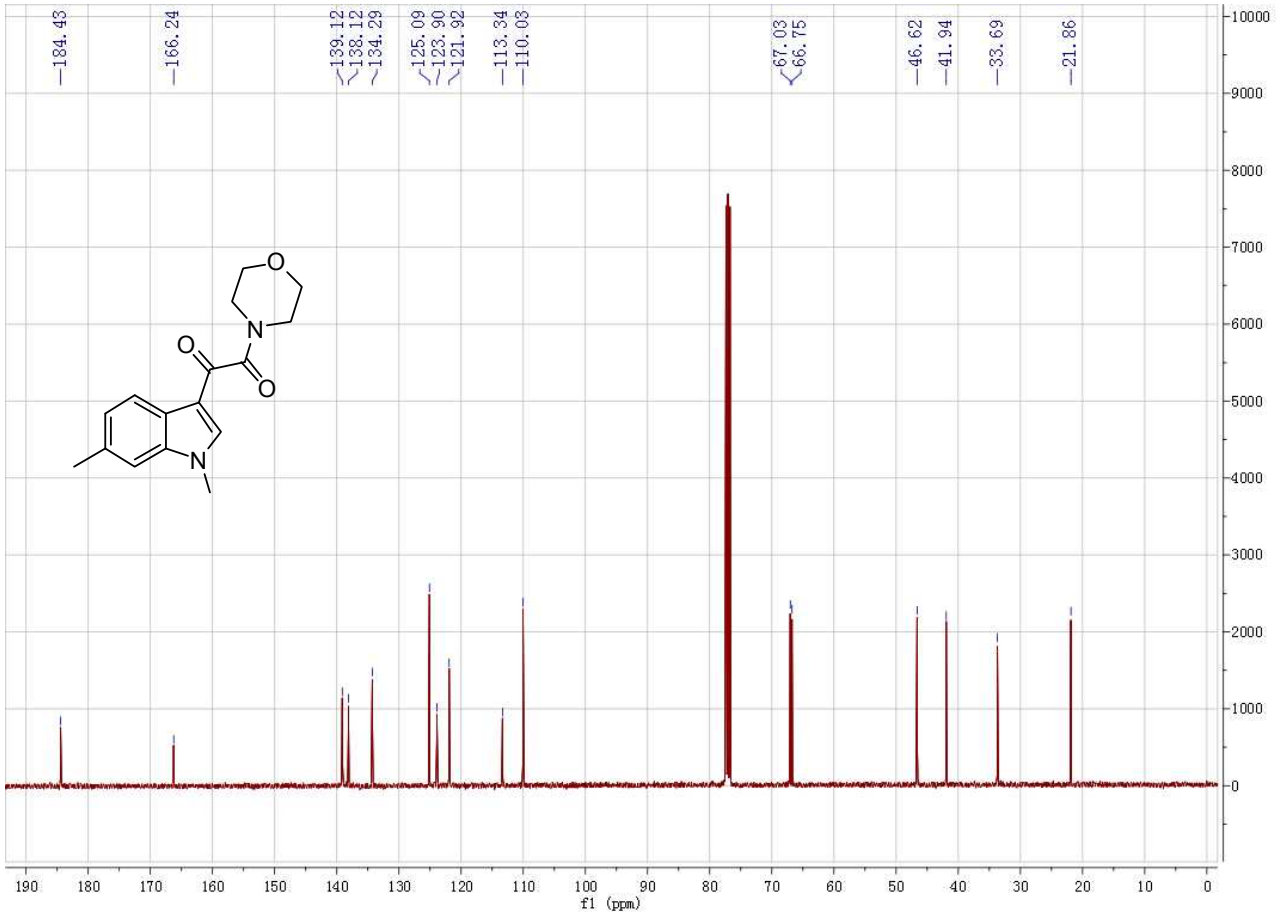
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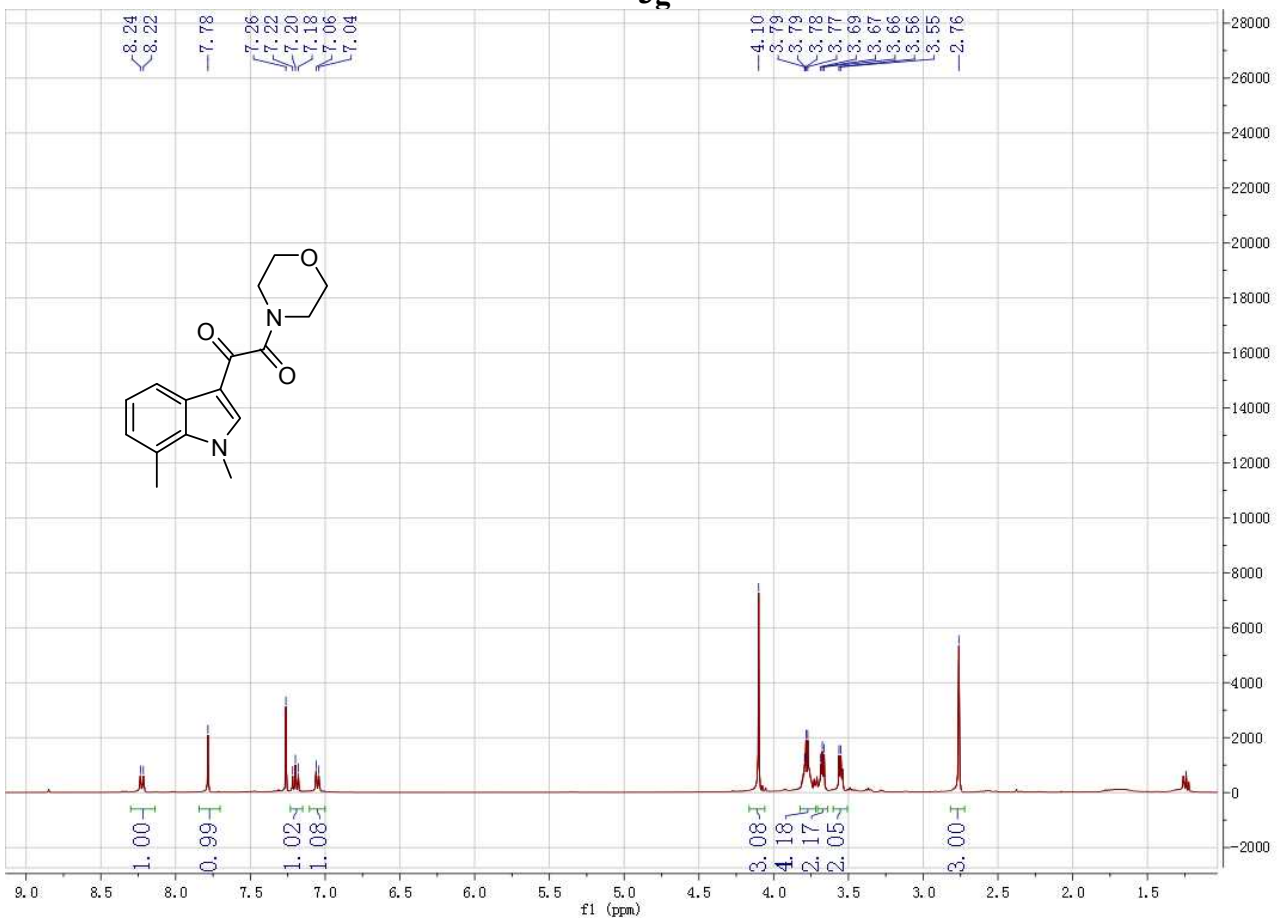
f1 (ppm)

3g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3.67
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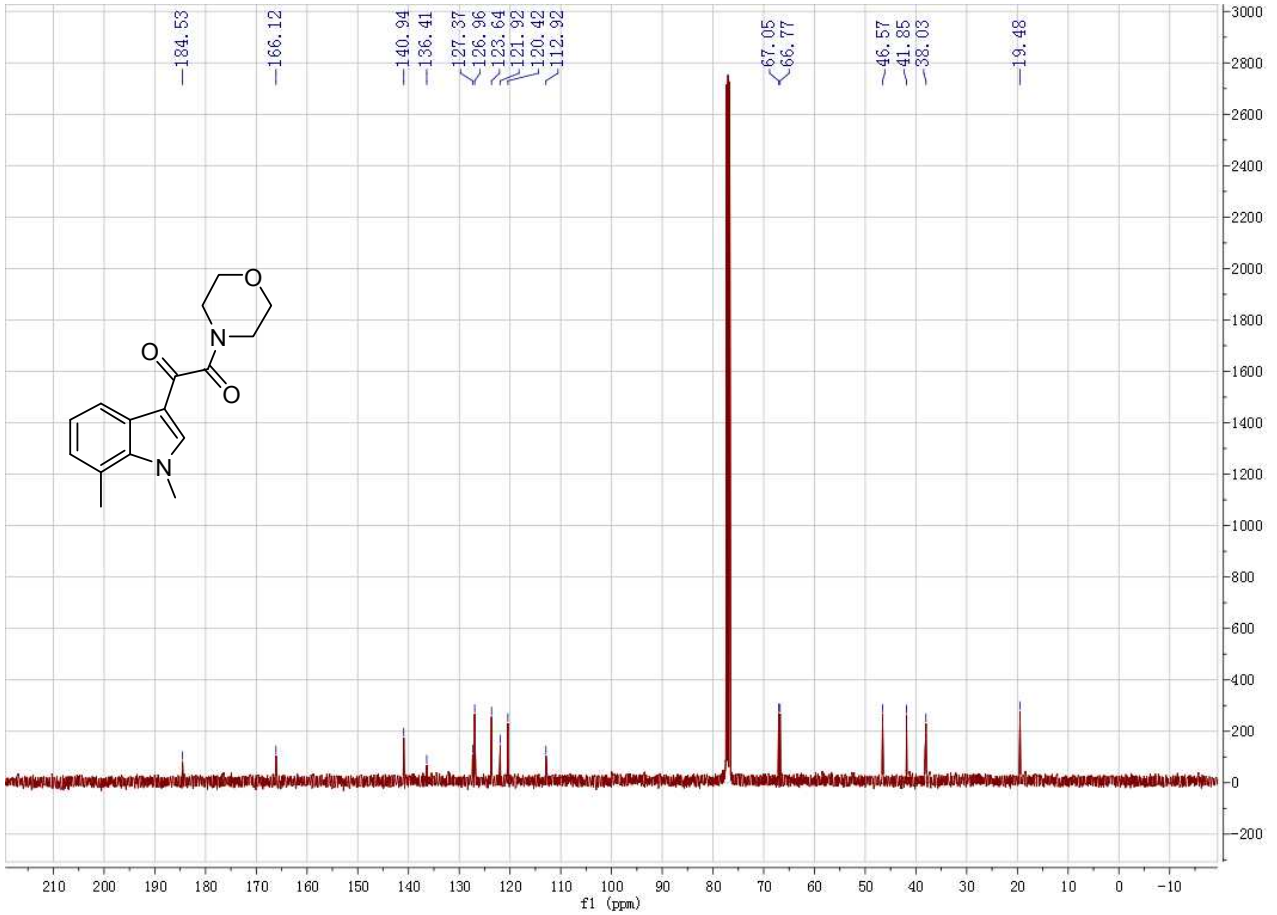
3.00
f1 (ppm)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38.03
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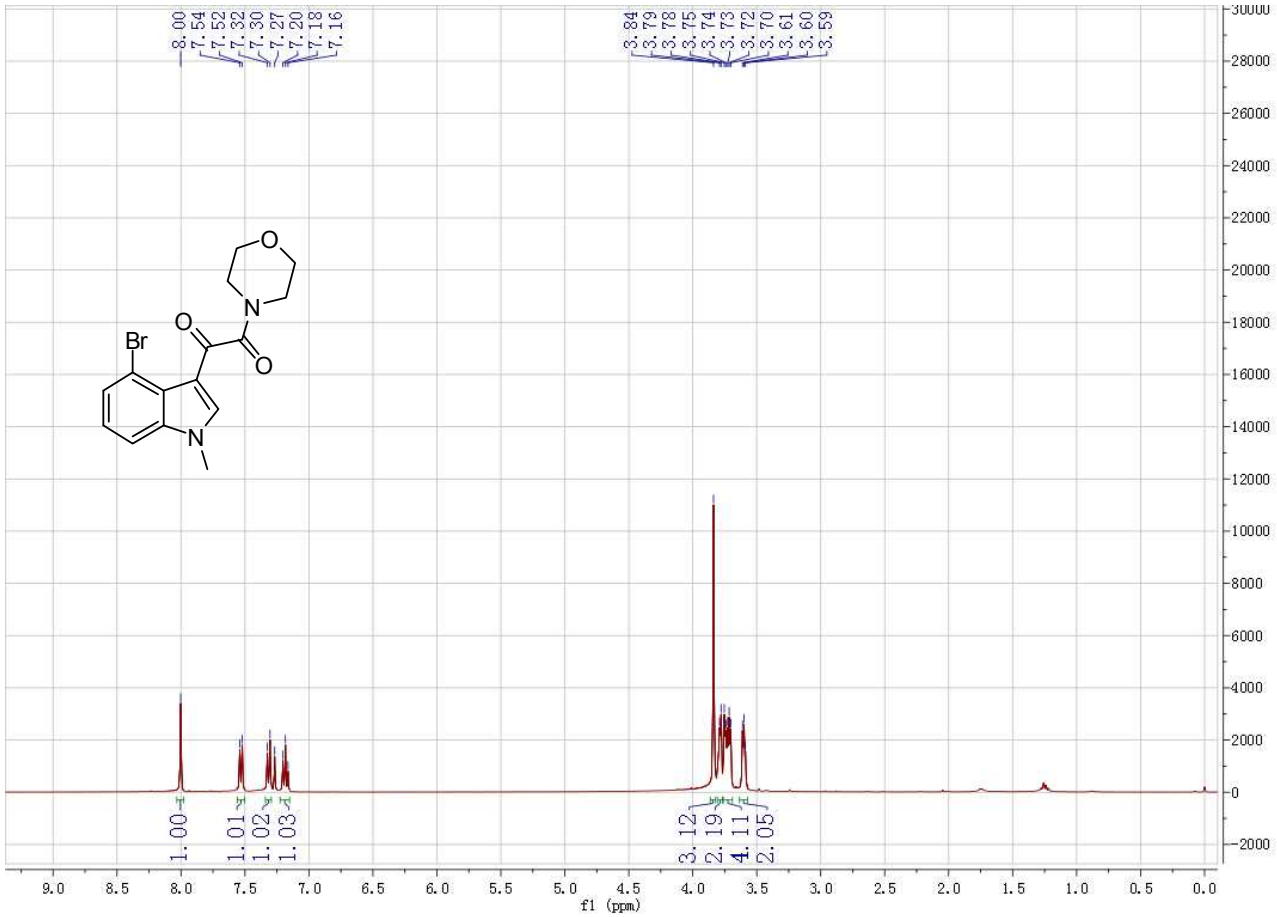
f1 (ppm)

3h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3.70
3.61
3.60
3.59
Br
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N
O
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N
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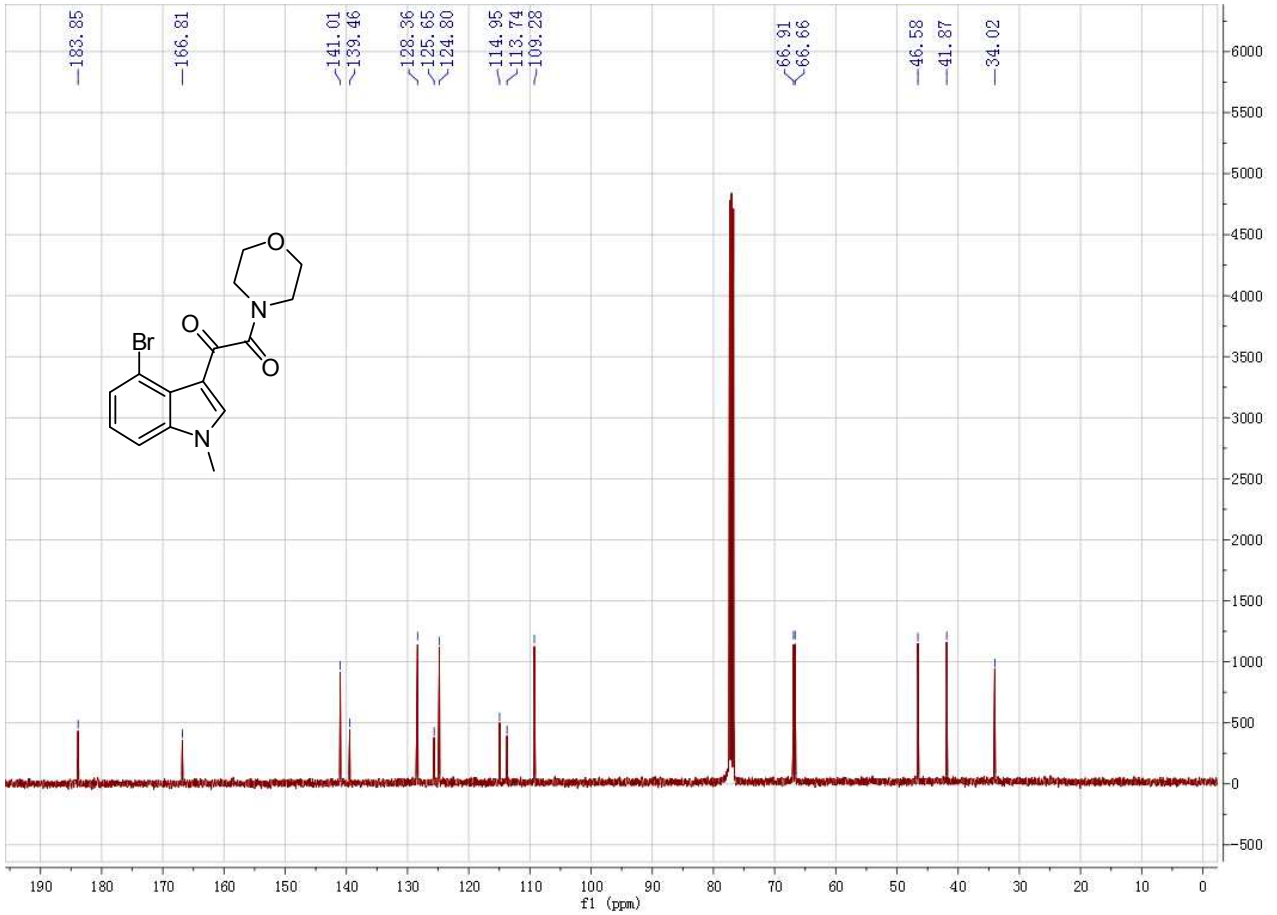
1.02
1.03
3.12
2.19
4.11
2.05
f1 (ppm)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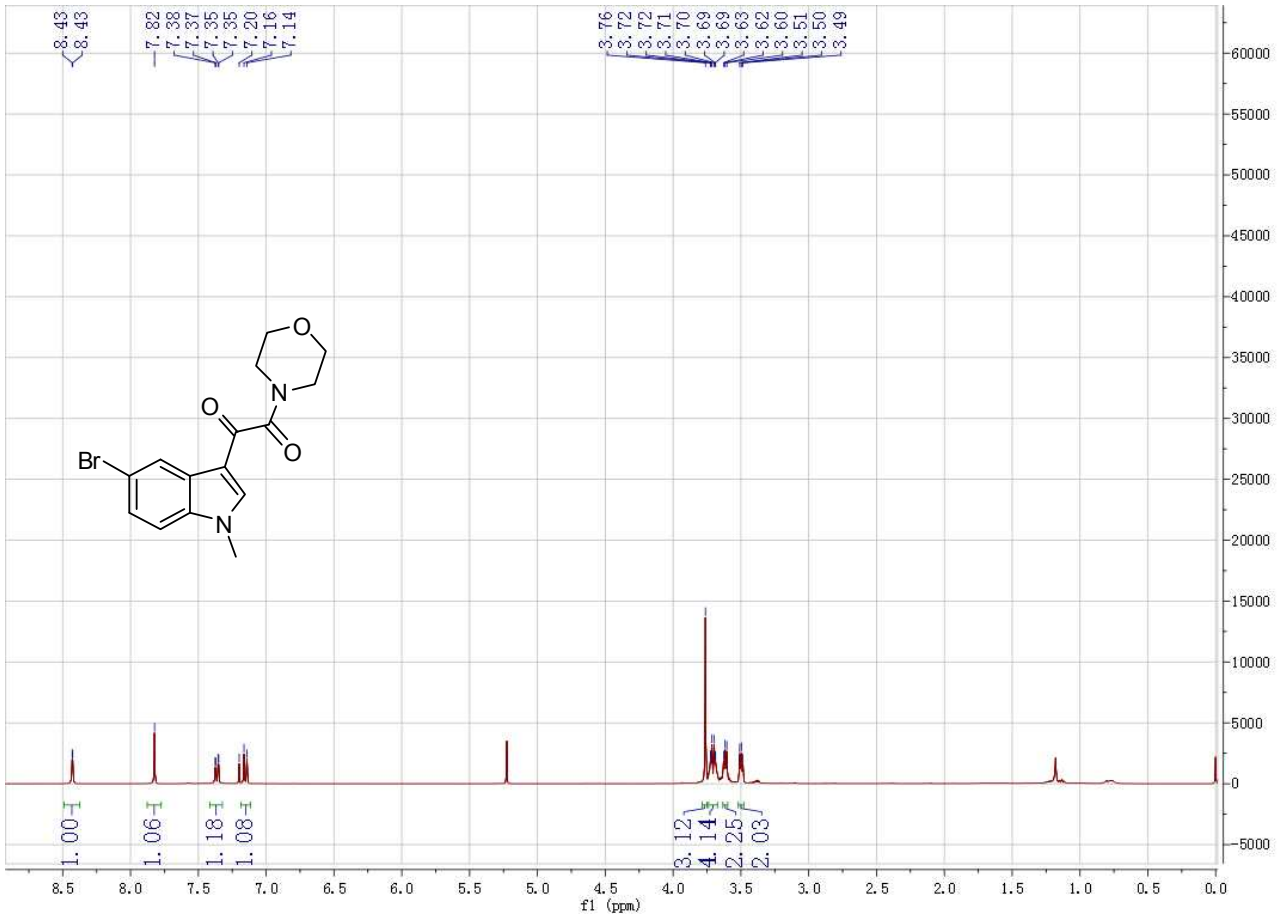
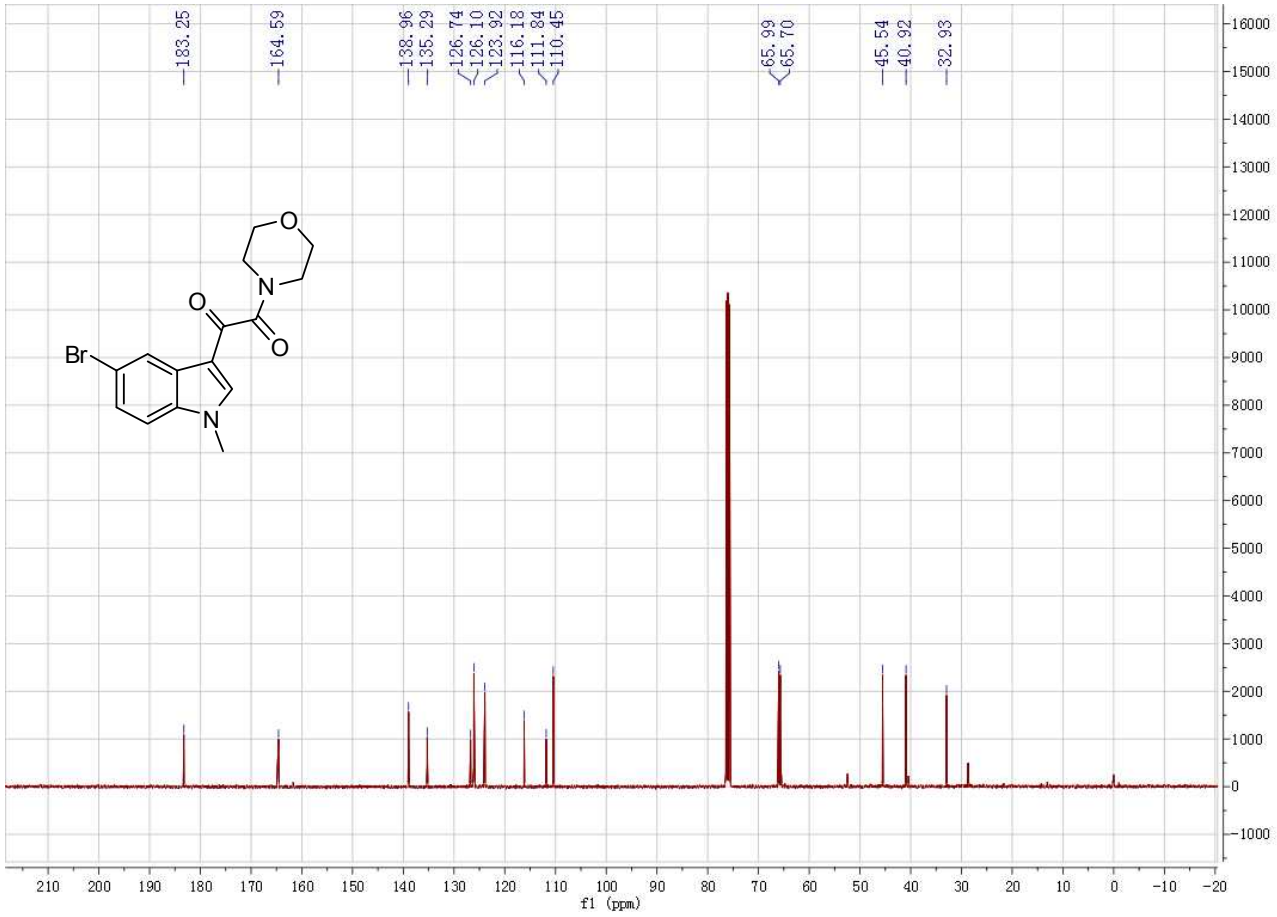
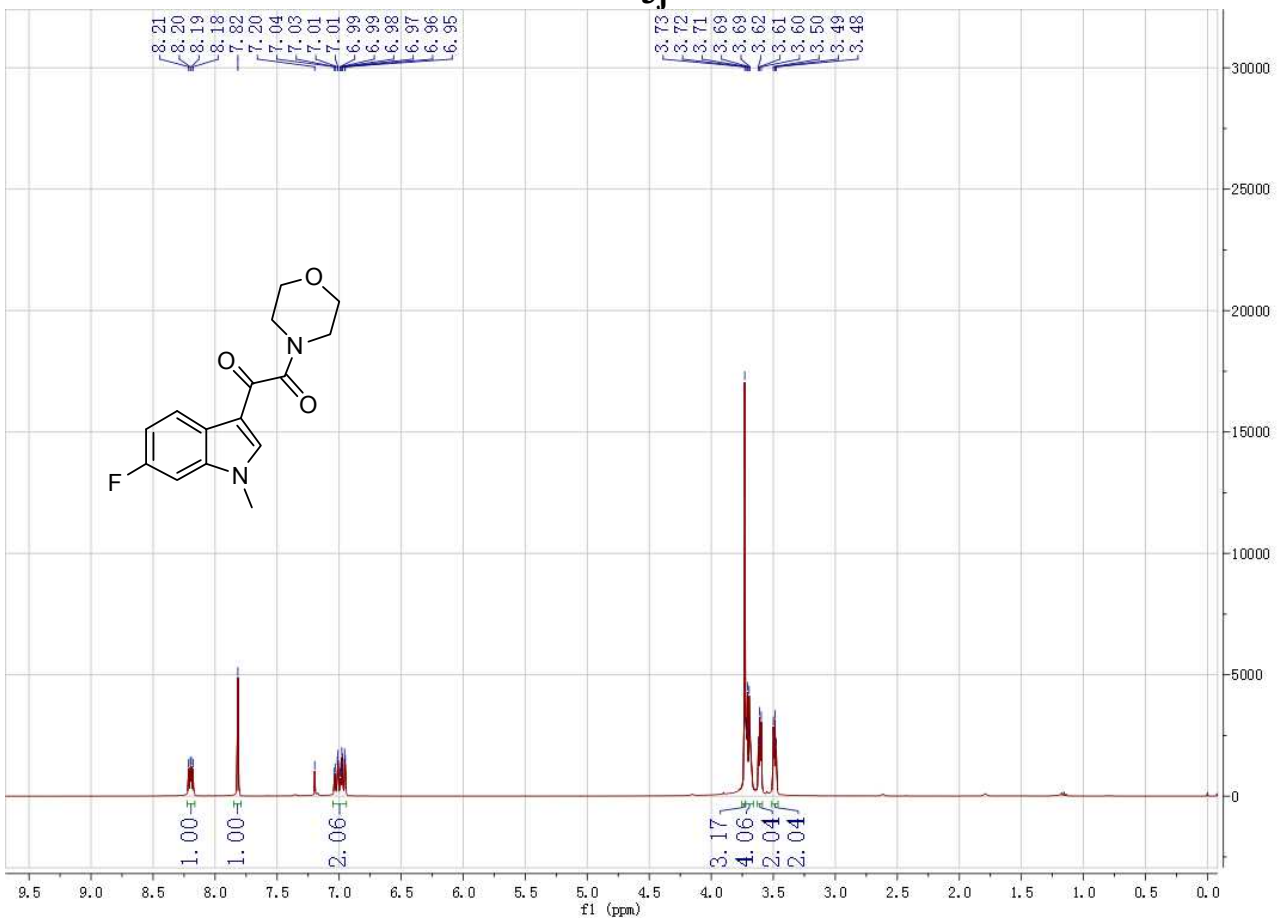
41.87
34.02
Br
O
N
O
O
N
f1 (ppm)

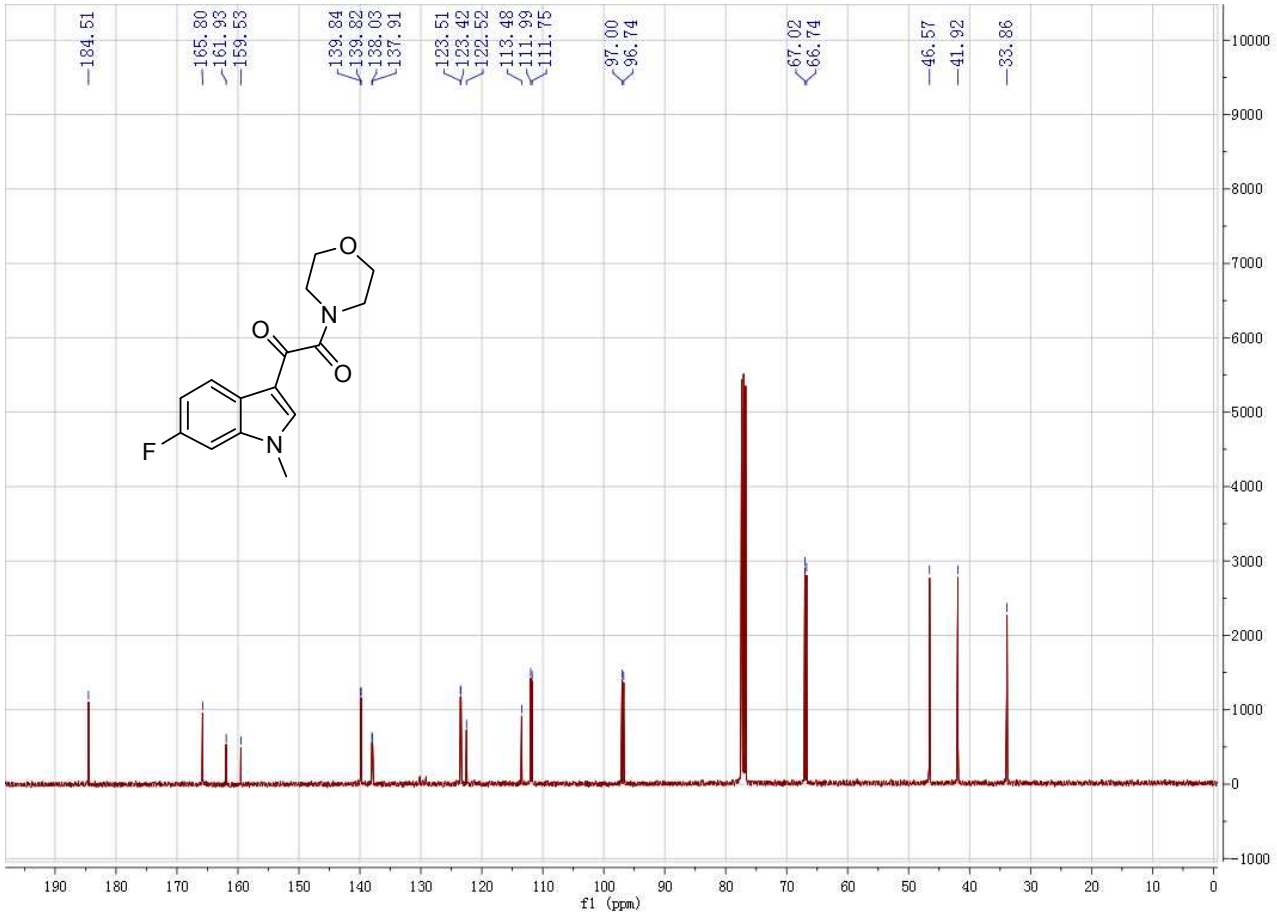
3i


8.43
8.43
7.82
7.38
7.37
7.35
7.35
7.20
7.16
7.14
3.76
3.72
3.72
3.71
3.70
3.69
3.69
3.63
3.62
3.60
3.51
3.50
3.49
O
N
O
O
Br
N
1.00
1.06
1.18
1.08
3.12
4.14
2.25
2.03
f1 (ppm)

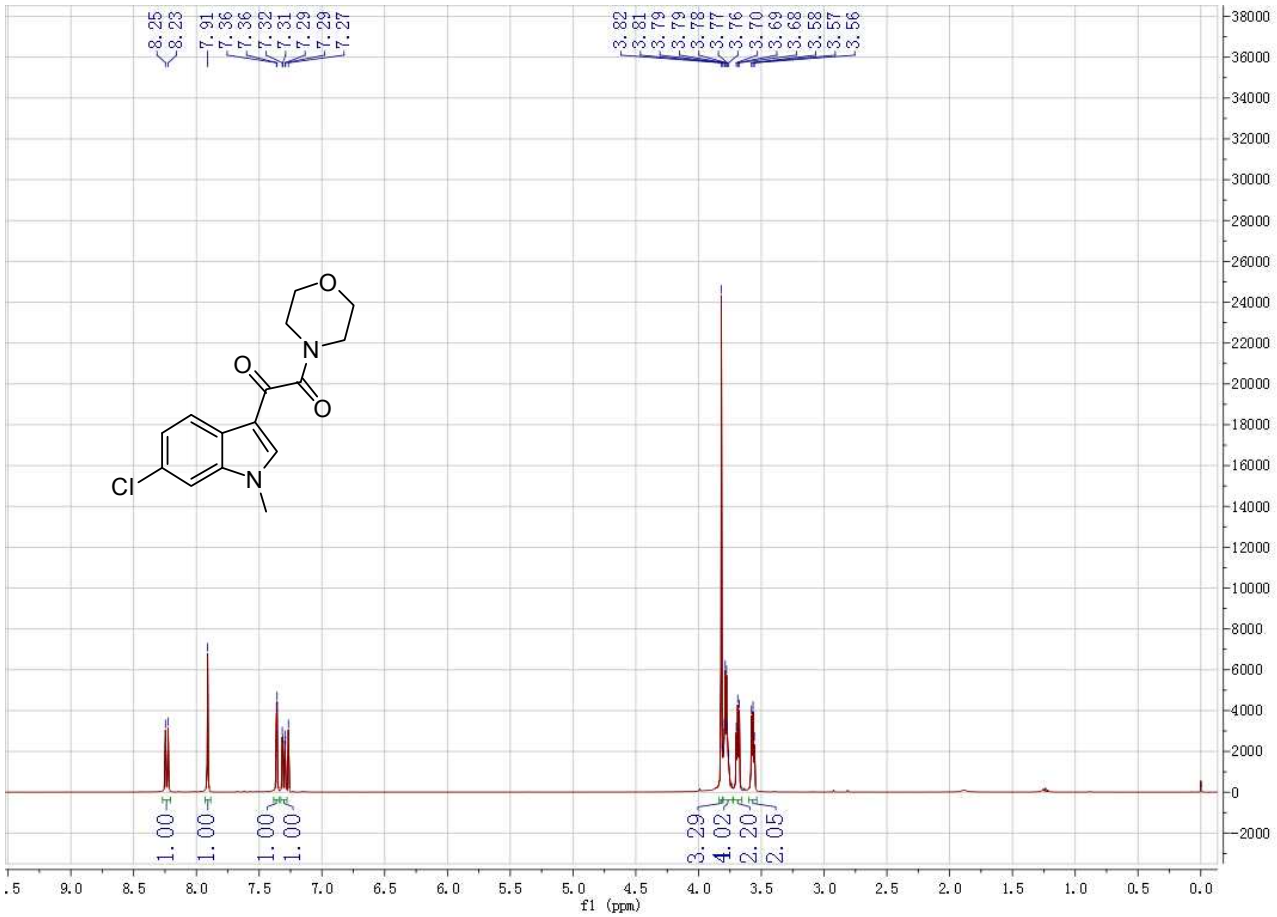

183.25
164.59
138.96
135.29
126.74
126.10
123.92
116.18
111.84
110.45
65.99
65.70
45.54
40.92
32.93
O
N
O
O
Br
N
f1 (ppm)

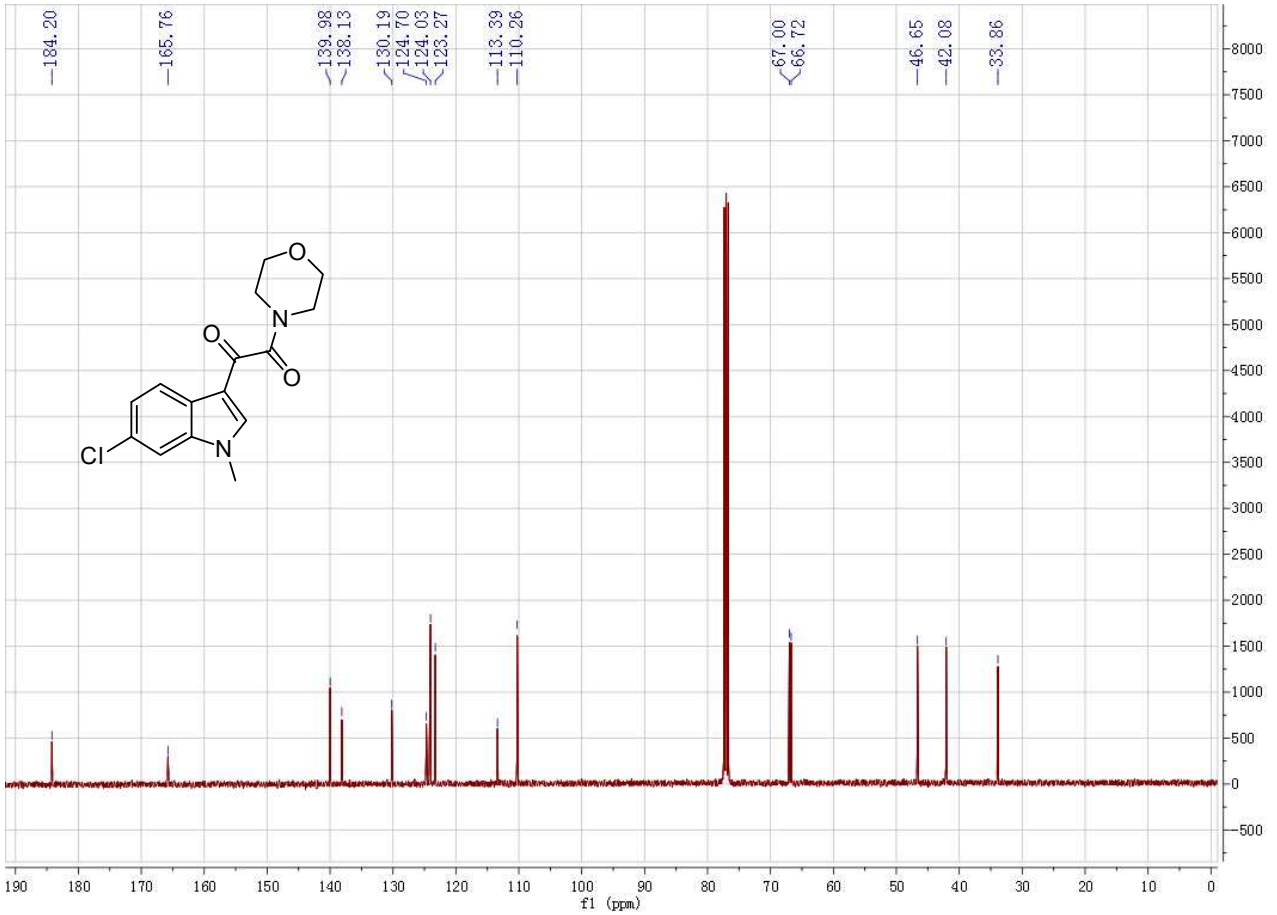
3j


8.21
8.20
8.19
8.18
7.82
7.20
7.04
7.03
7.01
7.01
6.99
6.99
6.98
6.97
6.96
6.95
3.73
3.72
3.71
3.69
3.69
3.62
3.61
3.60
3.50
3.49
3.48
1.00
1.00
2.06
3.17
4.06
2.04
2.04
f1 (ppm)

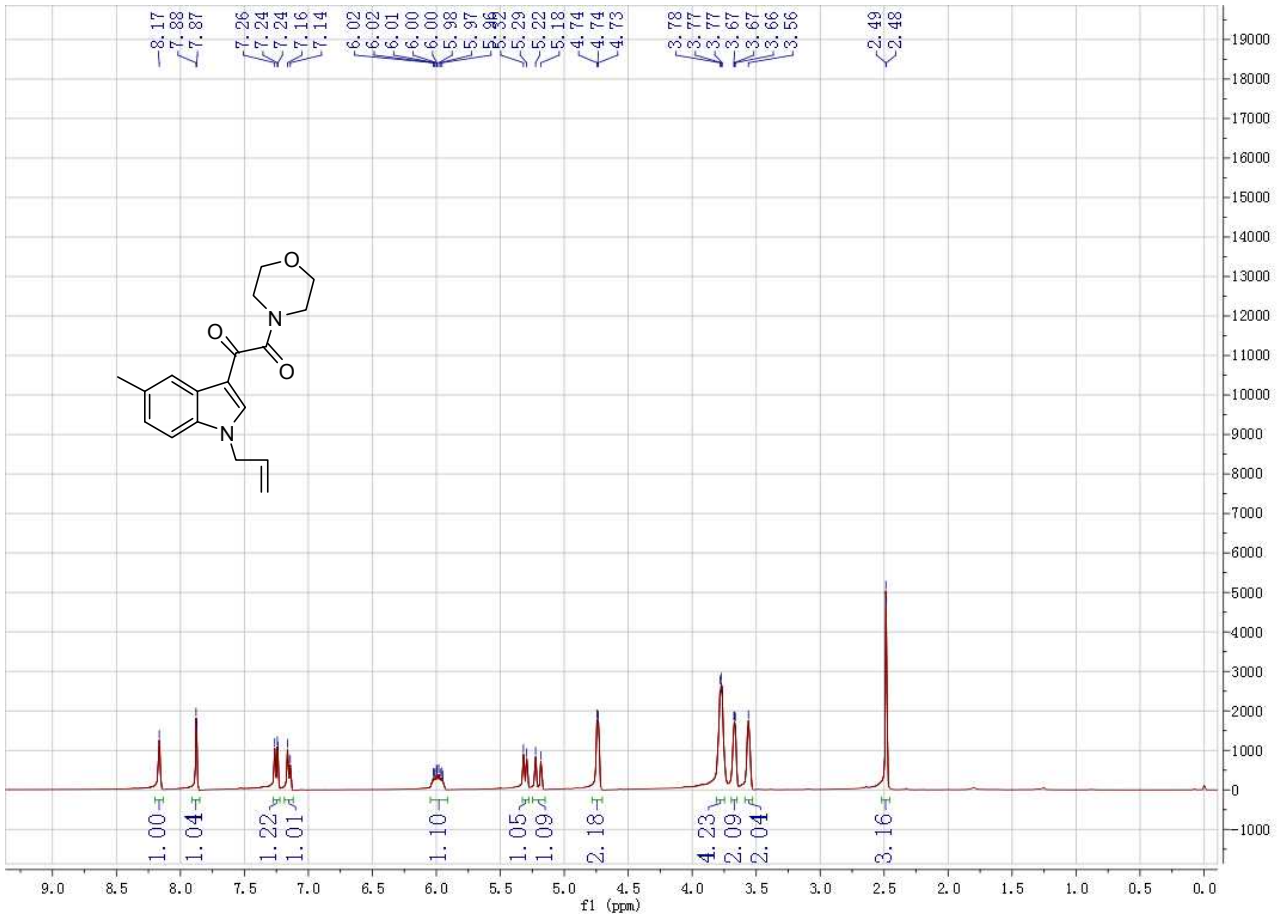

184.51
165.80
161.93
159.53
139.84
139.82
138.03
137.91
123.51
123.42
122.52
113.48
111.99
111.75
97.00
96.74
67.02
66.74
46.57
41.92
33.86
f1 (ppm)

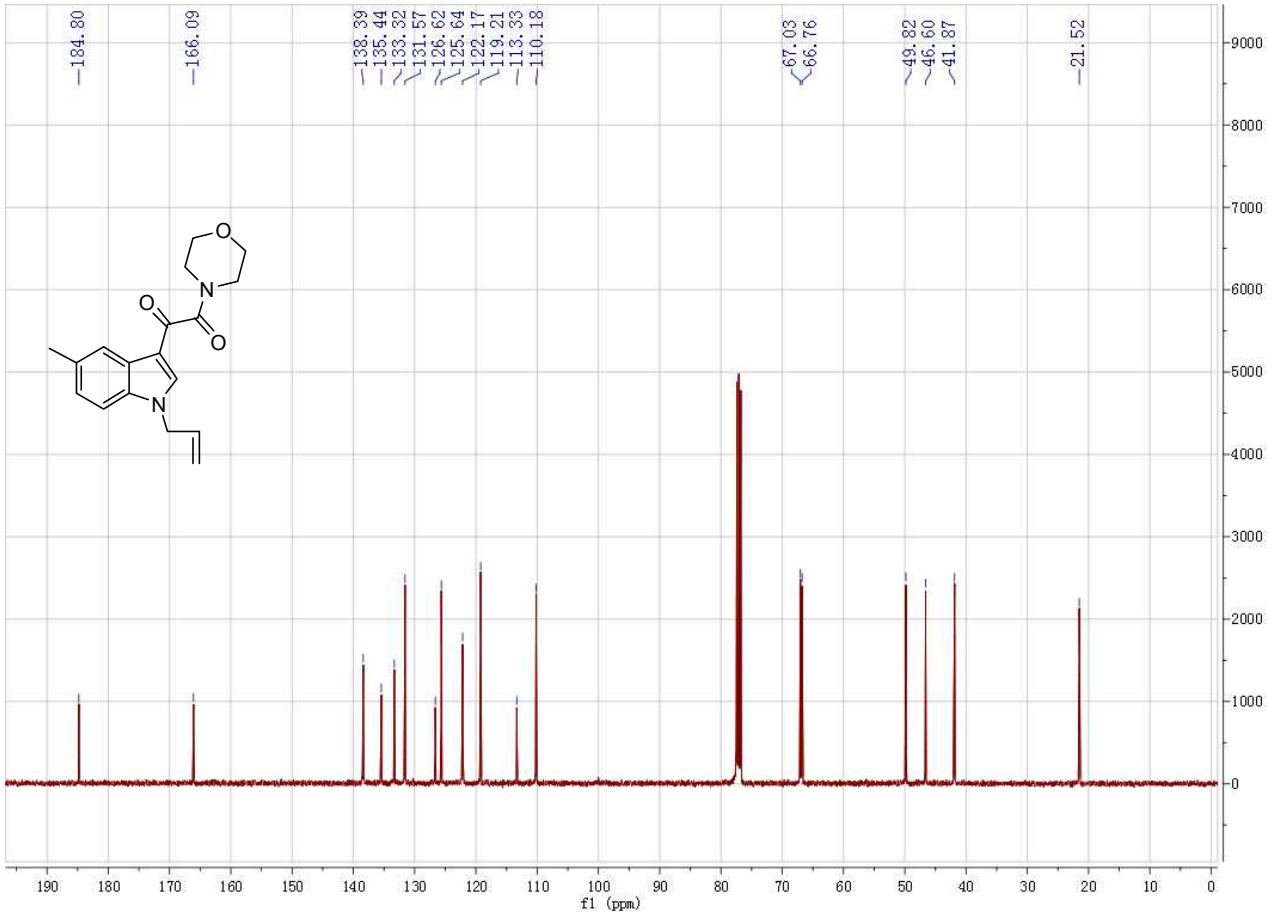
3k


8.25
8.23
7.91
7.36
7.36
7.32
7.31
7.29
7.29
7.27
3.82
3.81
3.79
3.79
3.78
3.77
3.76
3.70
3.69
3.68
3.58
3.57
3.56
O
N
O
O
Cl
N
1.00
1.00
1.00
1.00
3.29
4.02
2.20
2.05
f1 (ppm)

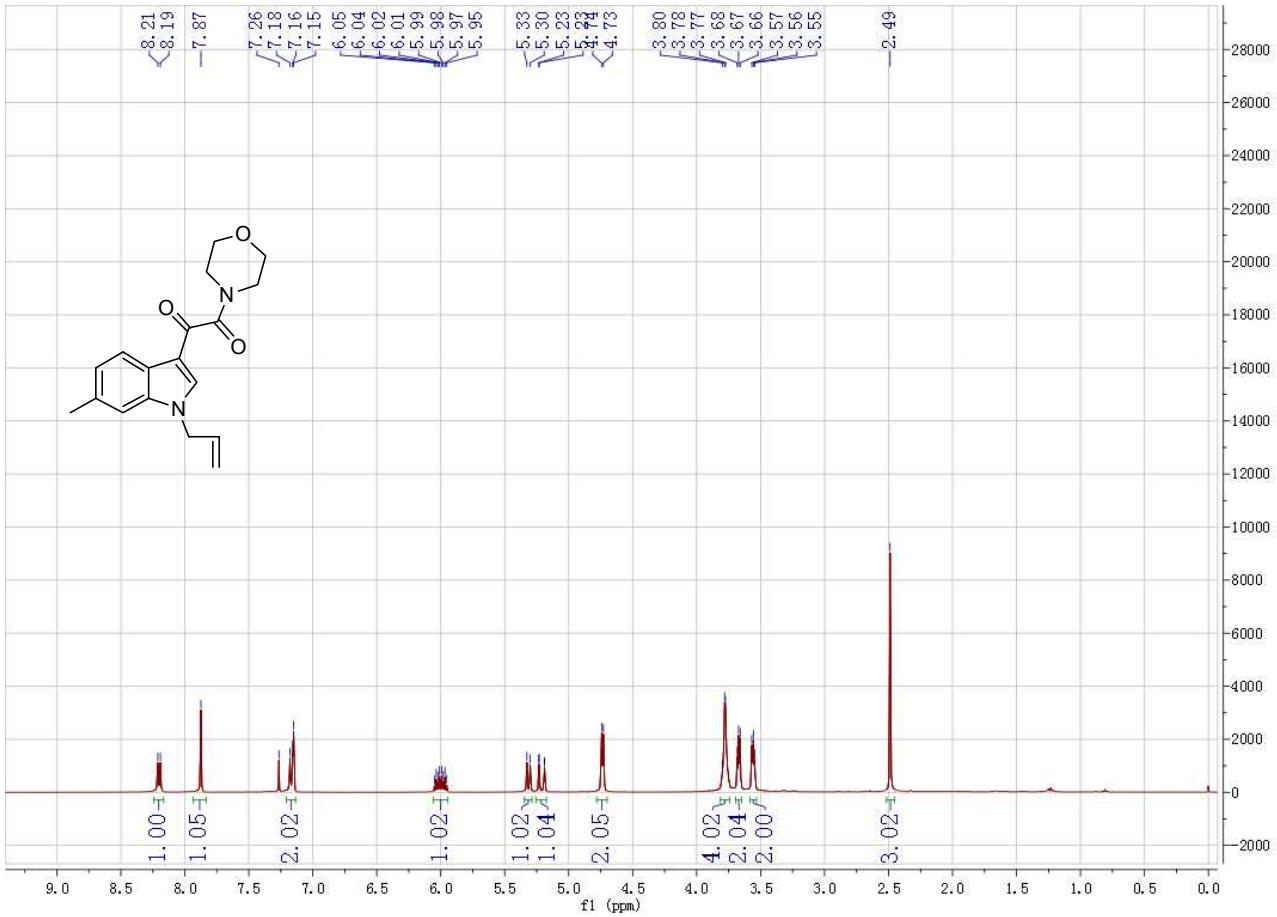

184.20
165.76
139.98
138.13
130.19
124.70
124.03
123.27
113.39
110.26
67.00
66.72
46.65
42.08
33.86
O
N
O
O
Cl
N
f1 (ppm)

3l


8.17
7.88
7.87
7.26
7.24
7.24
7.16
7.14
6.02
6.02
6.01
6.00
6.00
5.98
5.97
5.96
5.29
5.22
5.18
4.74
4.74
4.73
3.78
3.77
3.77
3.67
3.67
3.66
3.56
2.49
2.48
1.00
1.04
1.22
1.01
1.10
1.05
1.09
2.18
4.23
2.09
2.04
3.16
f1 (ppm)


184.80
166.09
138.39
135.44
133.32
131.57
126.62
125.64
122.17
119.21
113.33
110.18
67.03
66.76
49.82
46.60
41.87
21.52
f1 (ppm)

3m


8.21
8.19
7.87
7.26
7.18
7.16
7.15
6.05
6.04
6.02
6.01
5.99
5.98
5.97
5.95
5.33
5.30
5.23
4.73
3.80
3.78
3.77
3.68
3.67
3.66
3.57
3.56
3.55
2.49
1.00
1.05
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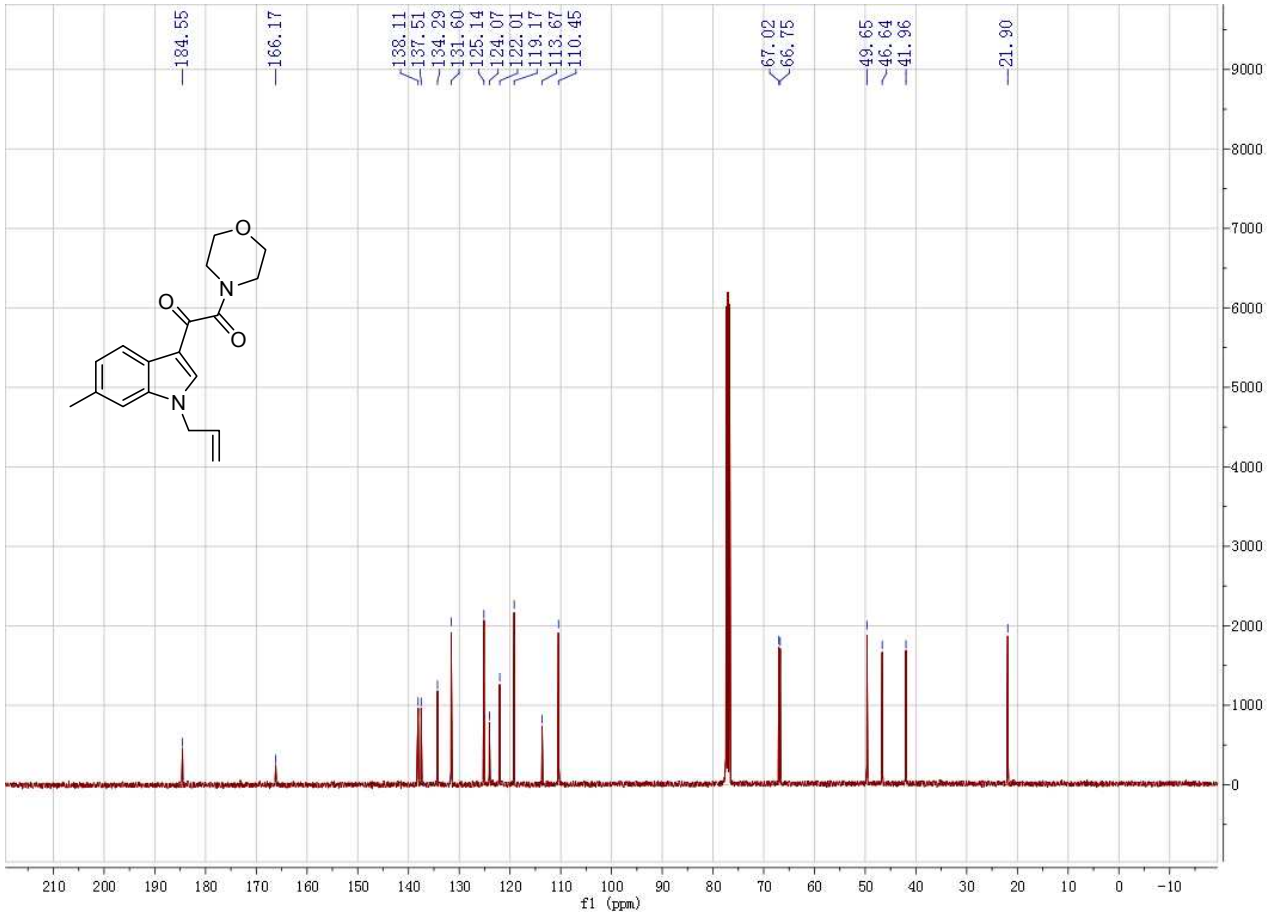
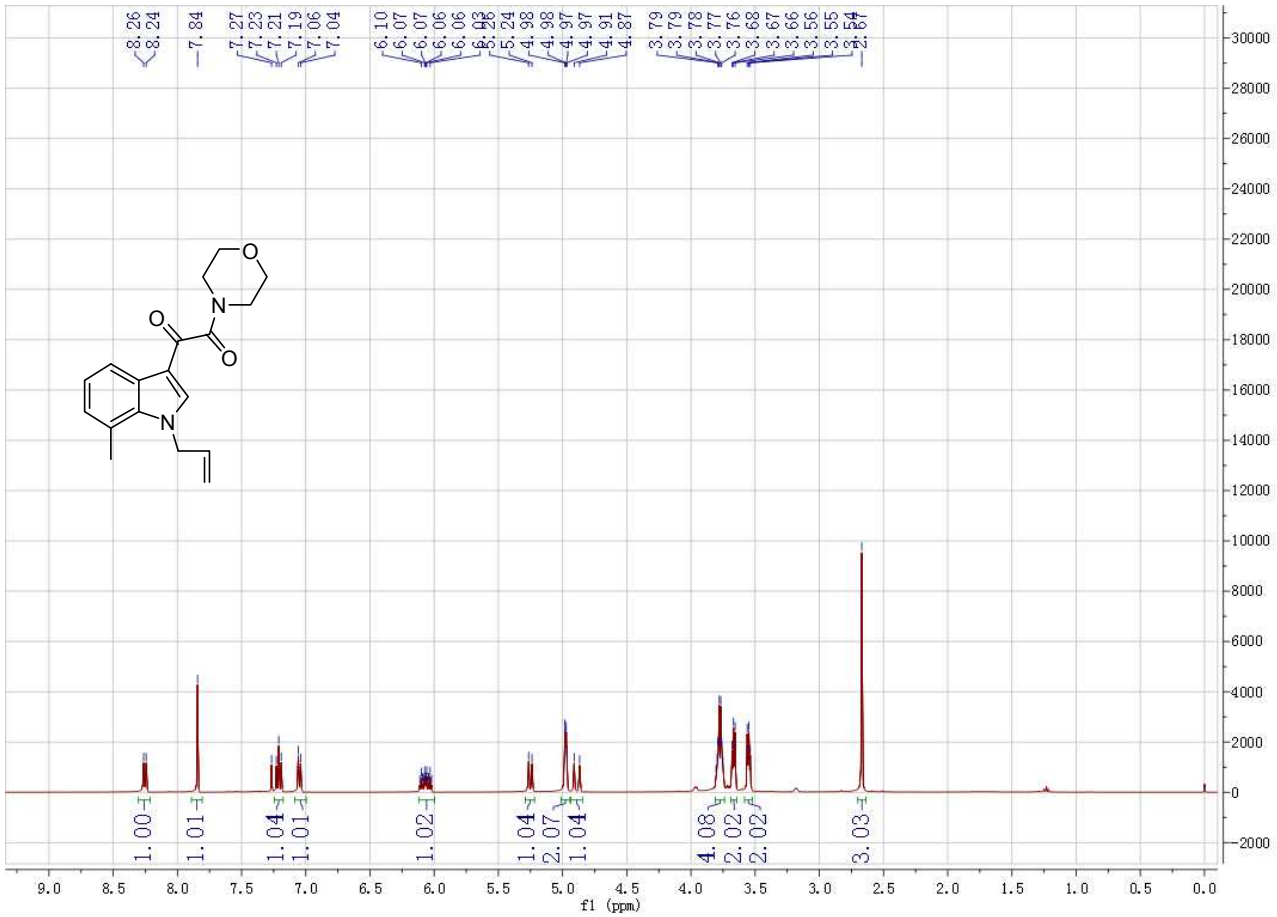
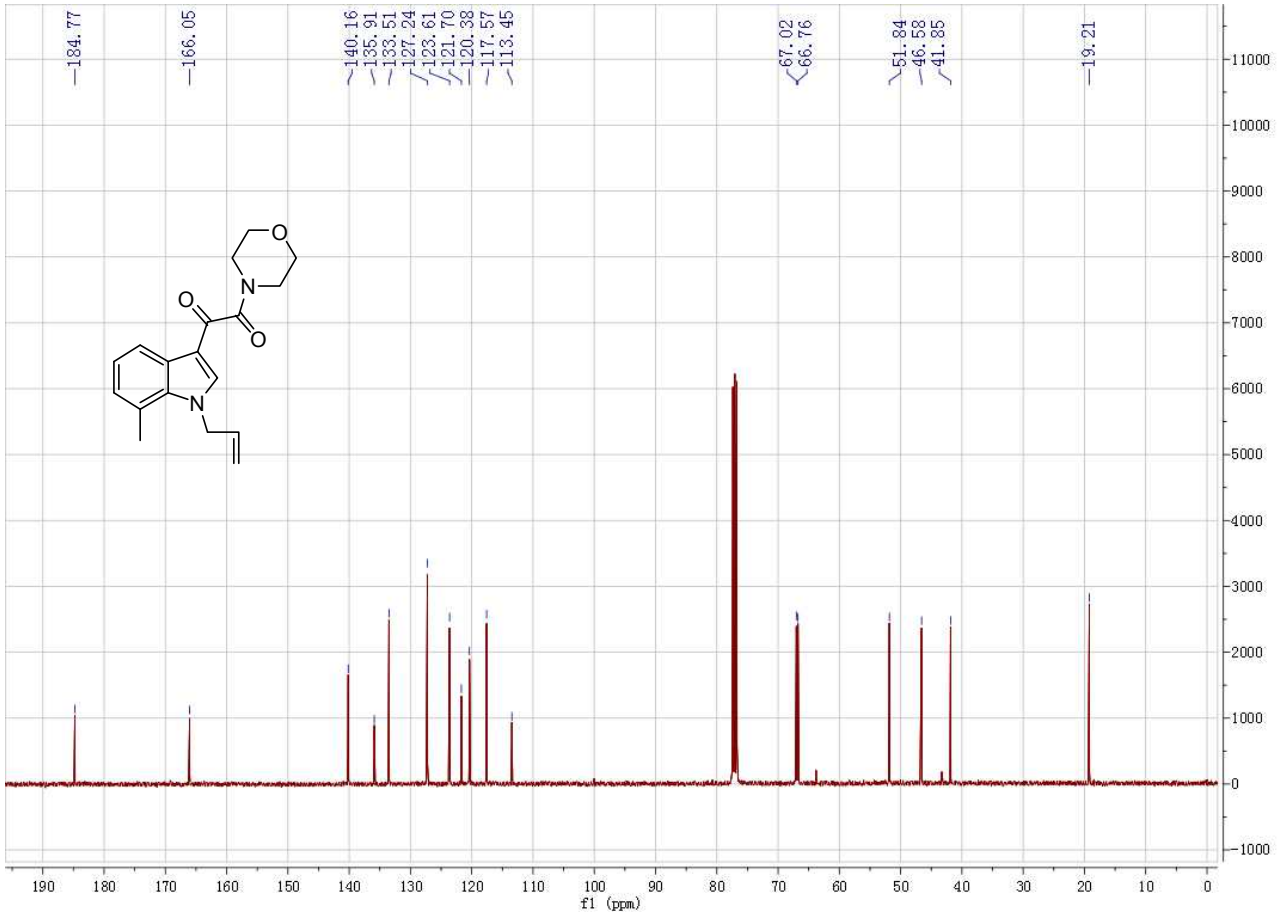
1.02
1.02
1.04
2.05
4.02
2.04
2.00
3.02
f1 (ppm)

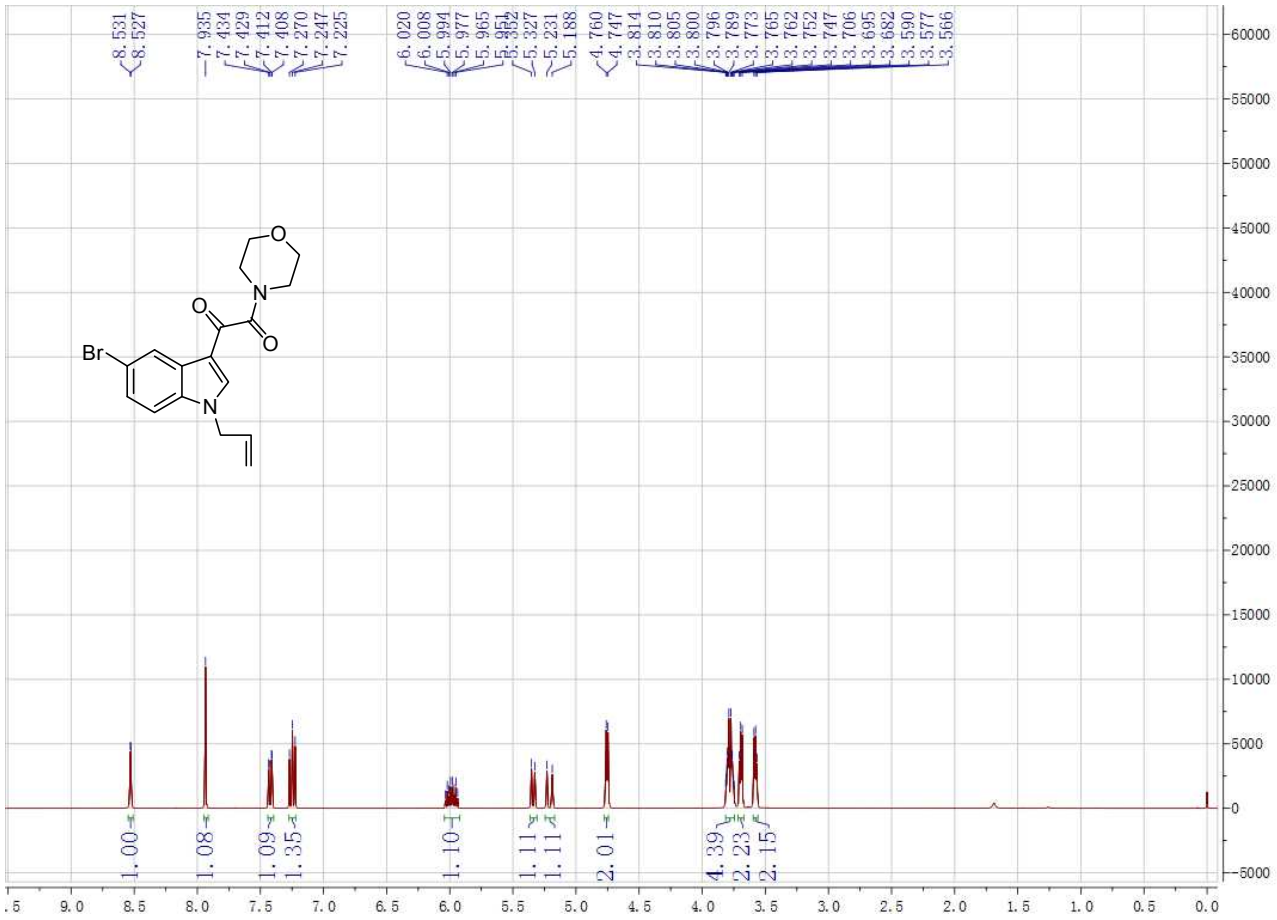

184.55
166.17
138.11
137.51
134.29
131.60
125.14
124.07
122.01
119.17
113.67
110.45
67.02
66.75
49.65
46.64
41.96
21.90
f1 (ppm)

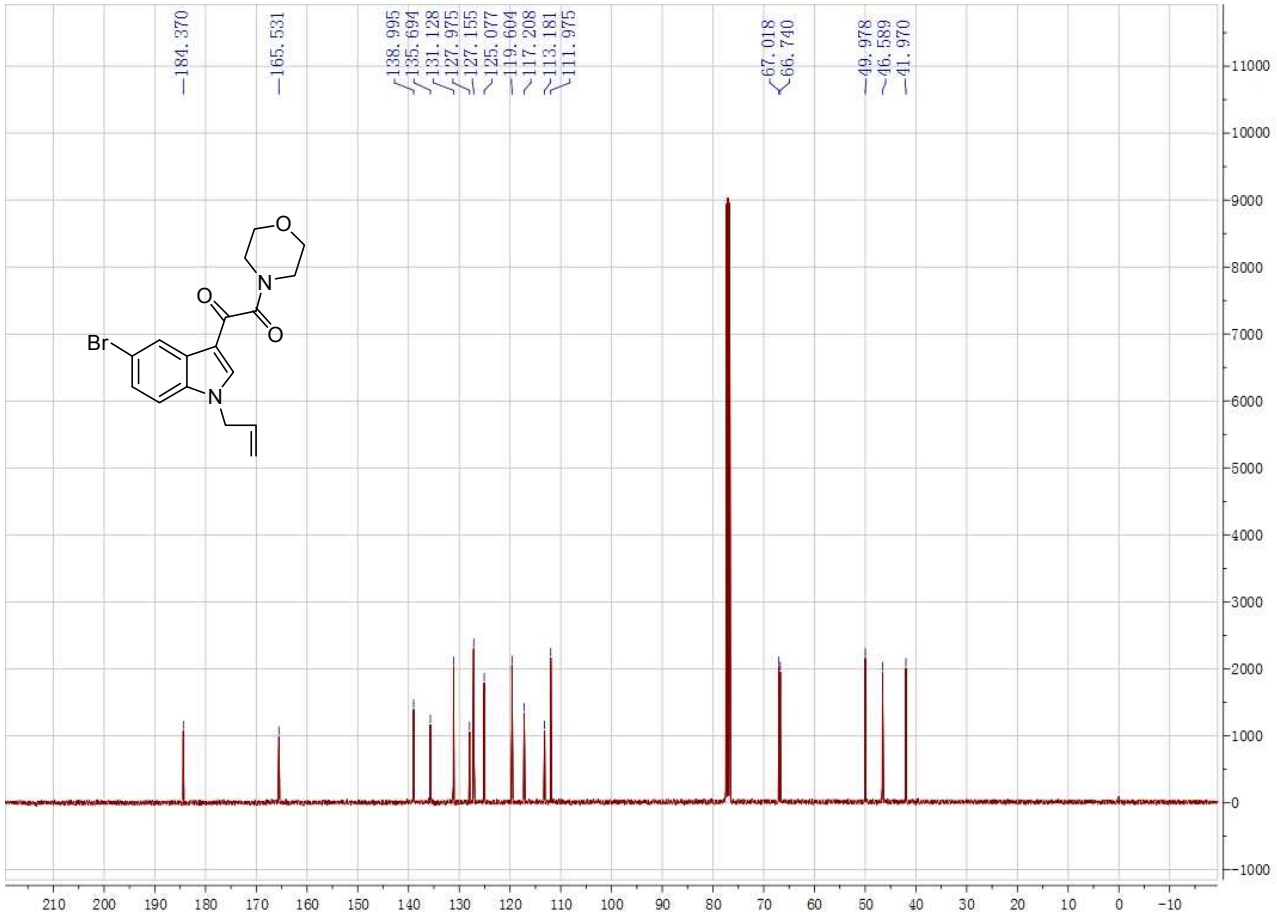
3n


8.26
8.24
7.84
7.27
7.23
7.21
7.19
7.06
7.04
6.10
6.07
6.07
6.06
6.06
5.26
5.24
4.98
4.98
4.97
4.97
4.91
4.87
3.79
3.79
3.78
3.77
3.76
3.68
3.67
3.66
3.56
3.55
3.54
2.67
1.00
1.01
1.04
1.01
1.02
1.04
2.07
1.04
4.08
2.02
2.02
3.03
f1 (ppm)

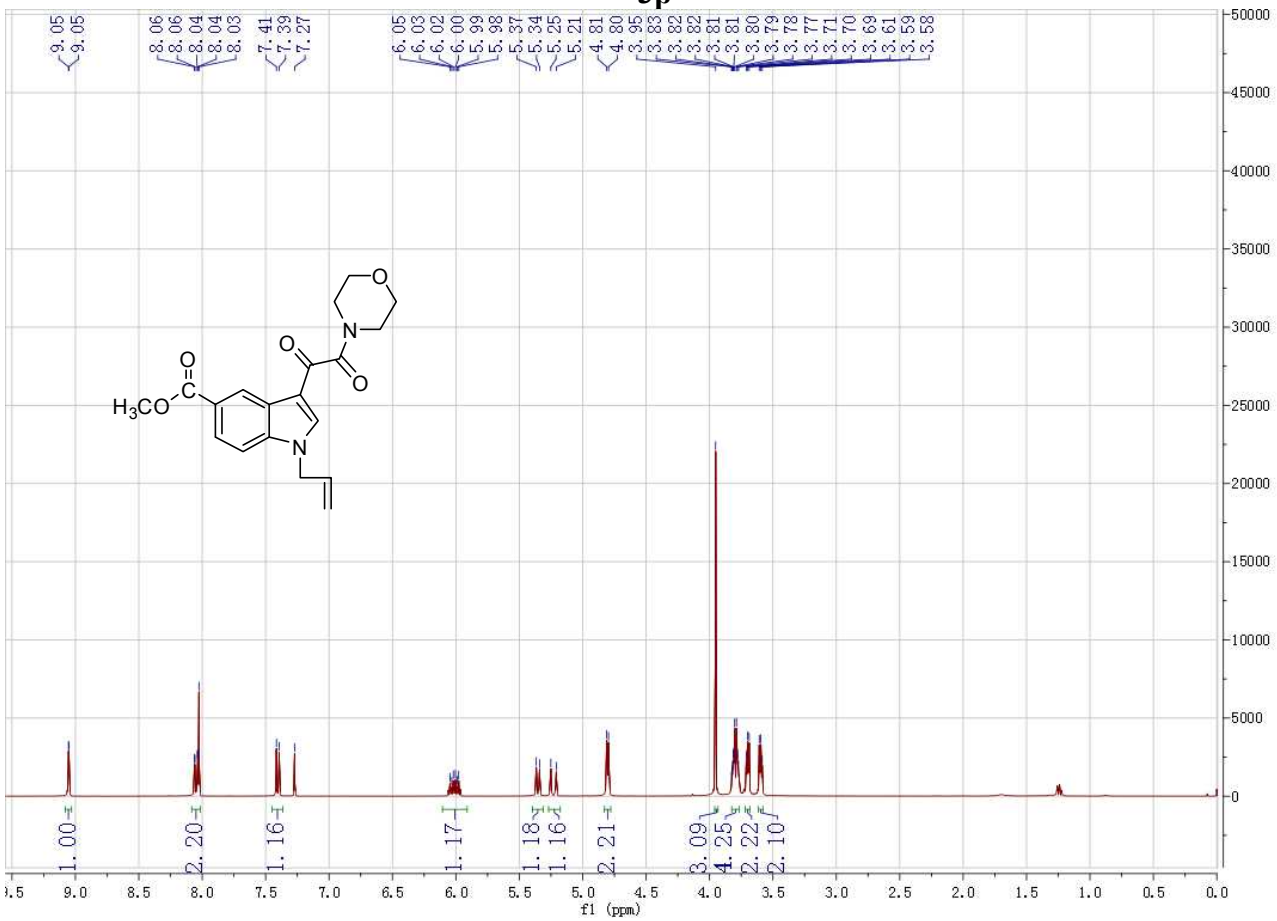

184.77
166.05
140.16
135.91
133.51
127.24
123.61
121.70
120.38
117.57
113.45
67.02
66.76
51.84
46.58
41.85
19.21
f1 (ppm)

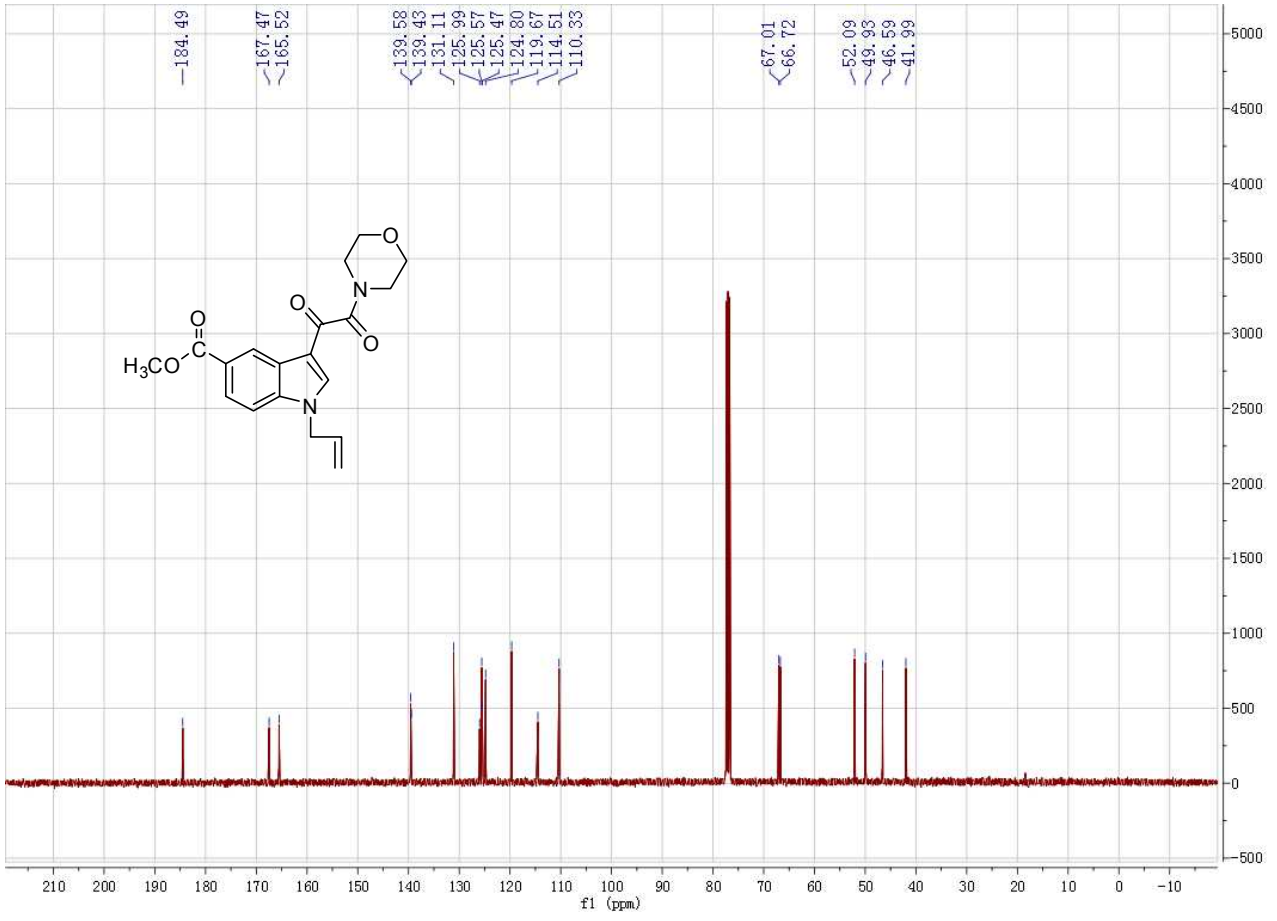
3o


8.531
8.527
7.935
7.434
7.429
7.412
7.408
7.270
7.247
7.225
6.020
6.008
5.994
5.977
5.965
5.951
5.352
5.327
5.231
5.188
4.760
4.747
3.814
3.810
3.805
3.800
3.796
3.789
3.773
3.765
3.762
3.752
3.747
3.706
3.695
3.682
3.590
3.577
3.566
Br
O
N
O
O
N
1.00
1.08
1.09
1.35
1.10
1.11
1.11
2.01
4.39
2.23
2.15

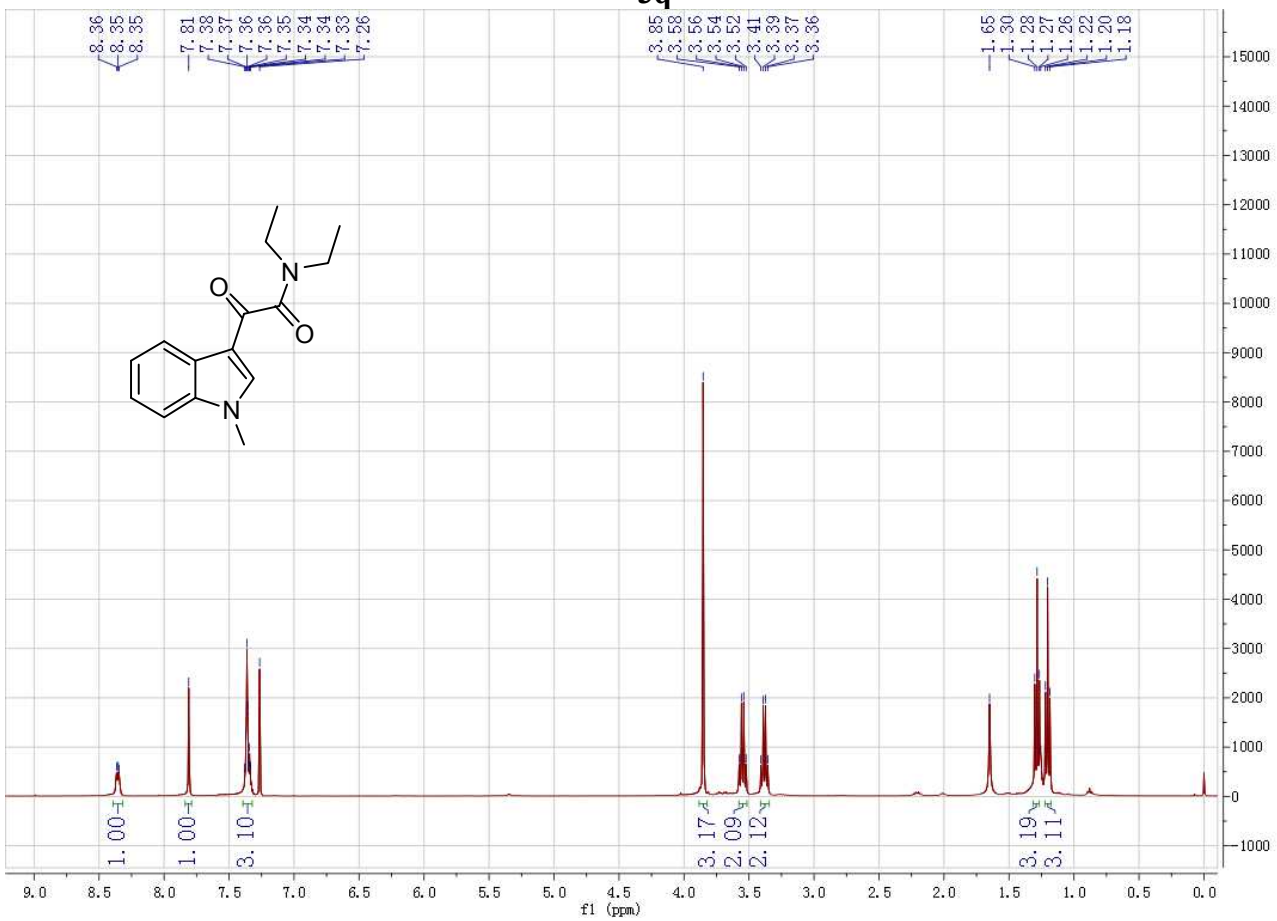

184.370
165.531
138.995
135.694
131.128
127.975
127.155
125.077
119.604
117.208
113.181
111.975
67.018
66.740
49.978
46.589
41.970
Br
O
N
O
O
N

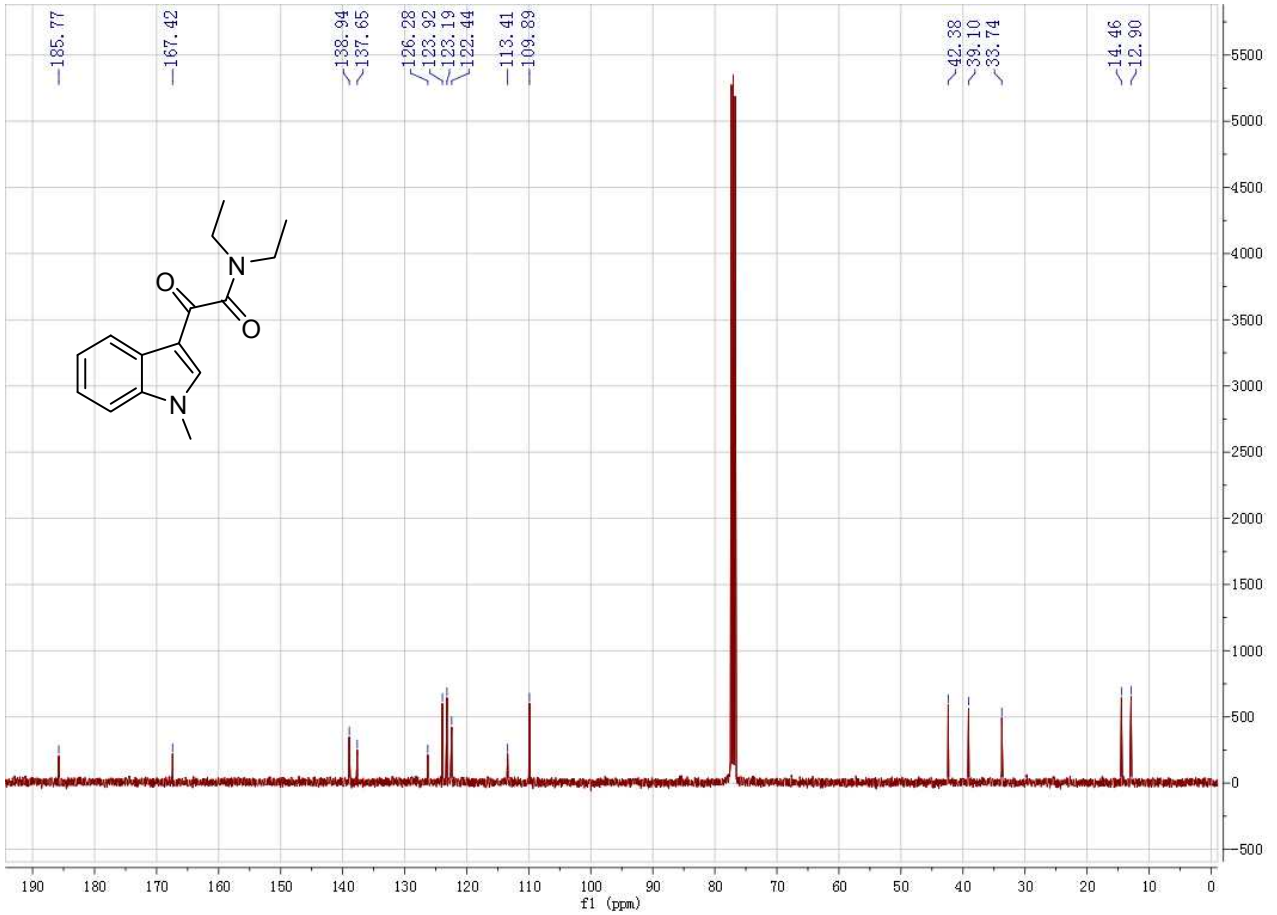
3p


9.05
9.05
8.06
8.06
8.04
8.04
8.03
7.41
7.39
7.27
6.05
6.03
6.02
6.00
5.99
5.98
5.37
5.34
5.25
5.21
4.81
4.80
3.95
3.83
3.82
3.82
3.81
3.81
3.80
3.79
3.78
3.77
3.71
3.70
3.69
3.61
3.59
3.58
1.00
2.20
1.16
1.17
1.18
1.16
2.21
3.09
4.25
2.22
2.10
f1 (ppm)

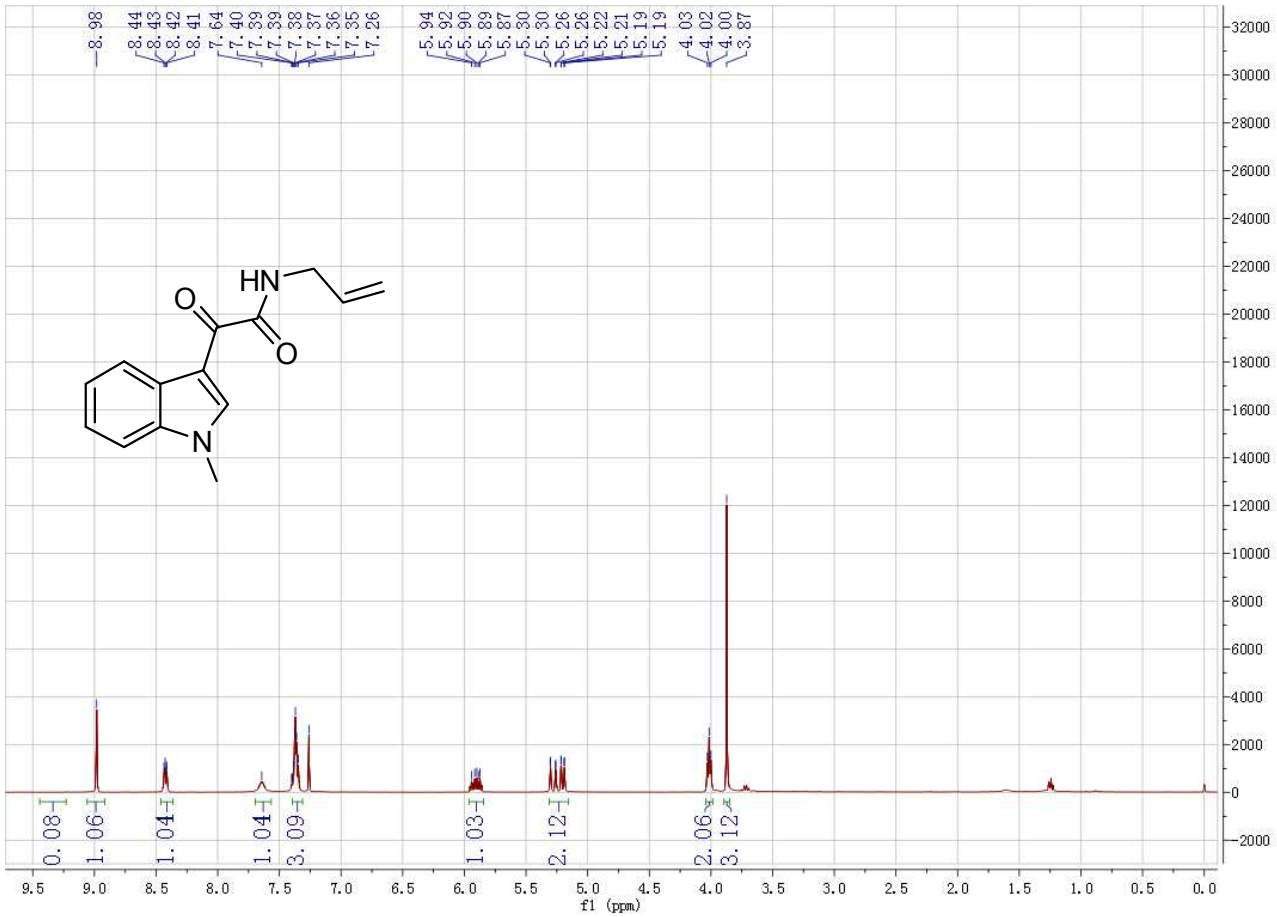

184.49
167.47
165.52
139.58
139.43
131.11
125.99
125.57
125.47
124.80
119.67
114.51
110.33
67.01
66.72
52.09
49.93
46.59
41.99
f1 (ppm)

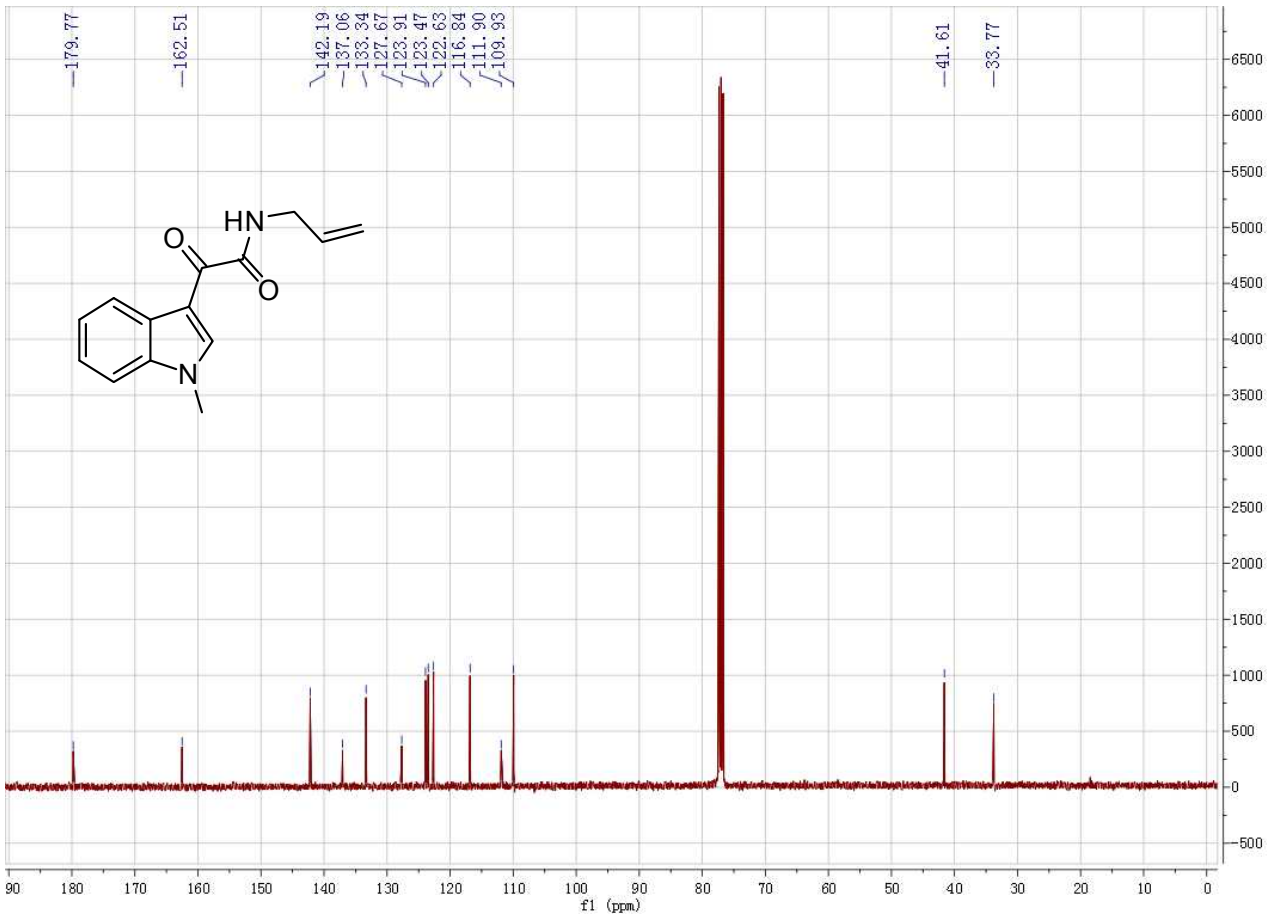
3q


8.36
8.35
8.35
7.81
7.38
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.26
3.85
3.58
3.56
3.54
3.52
3.41
3.39
3.37
3.36
1.65
1.30
1.28
1.27
1.26
1.22
1.20
1.18
1.00
1.00
3.10
3.17
2.09
2.12
3.19
3.11
f1 (ppm)

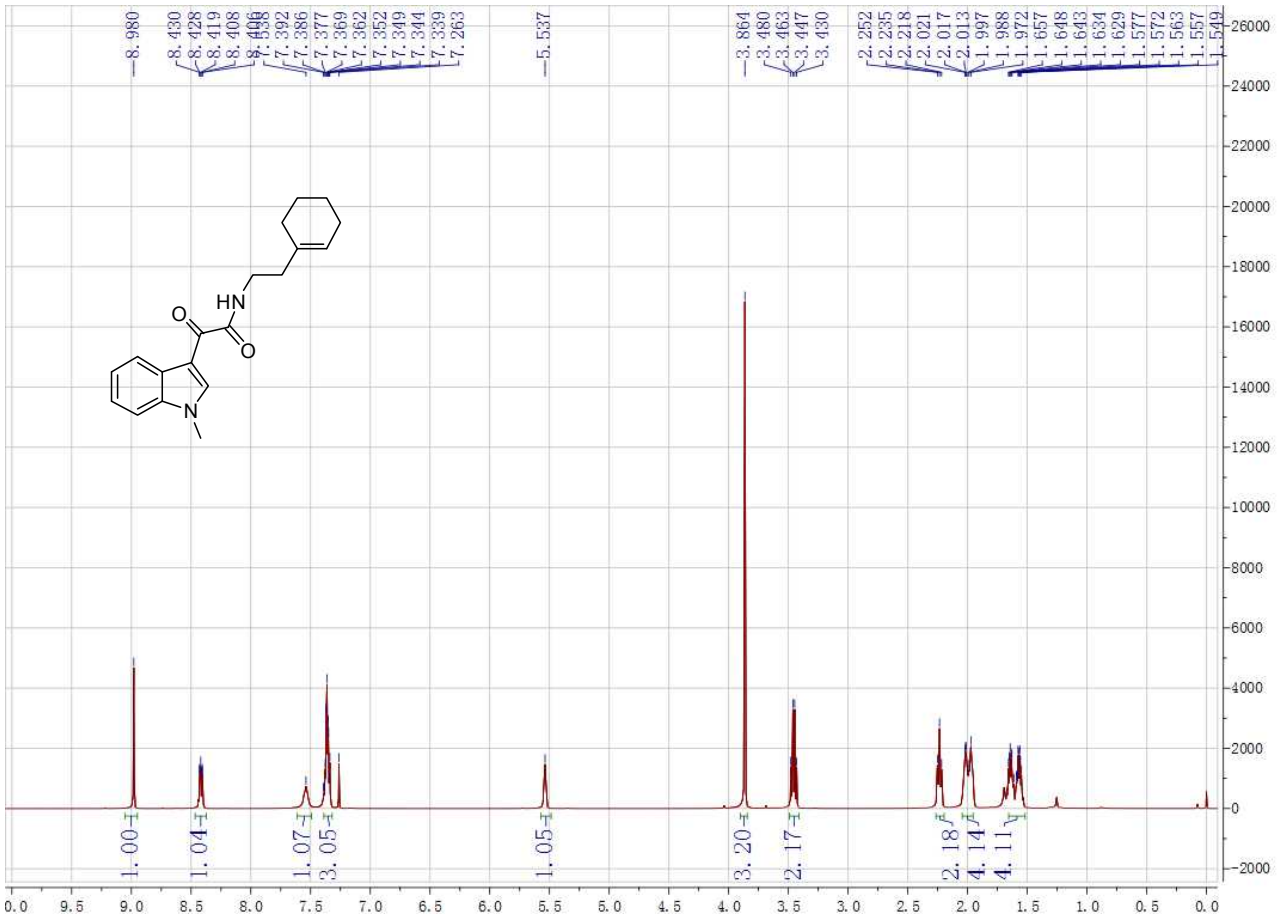

185.77
167.42
138.94
137.65
126.28
123.92
123.19
122.44
113.41
109.89
42.38
39.10
33.74
14.46
12.90
f1 (ppm)

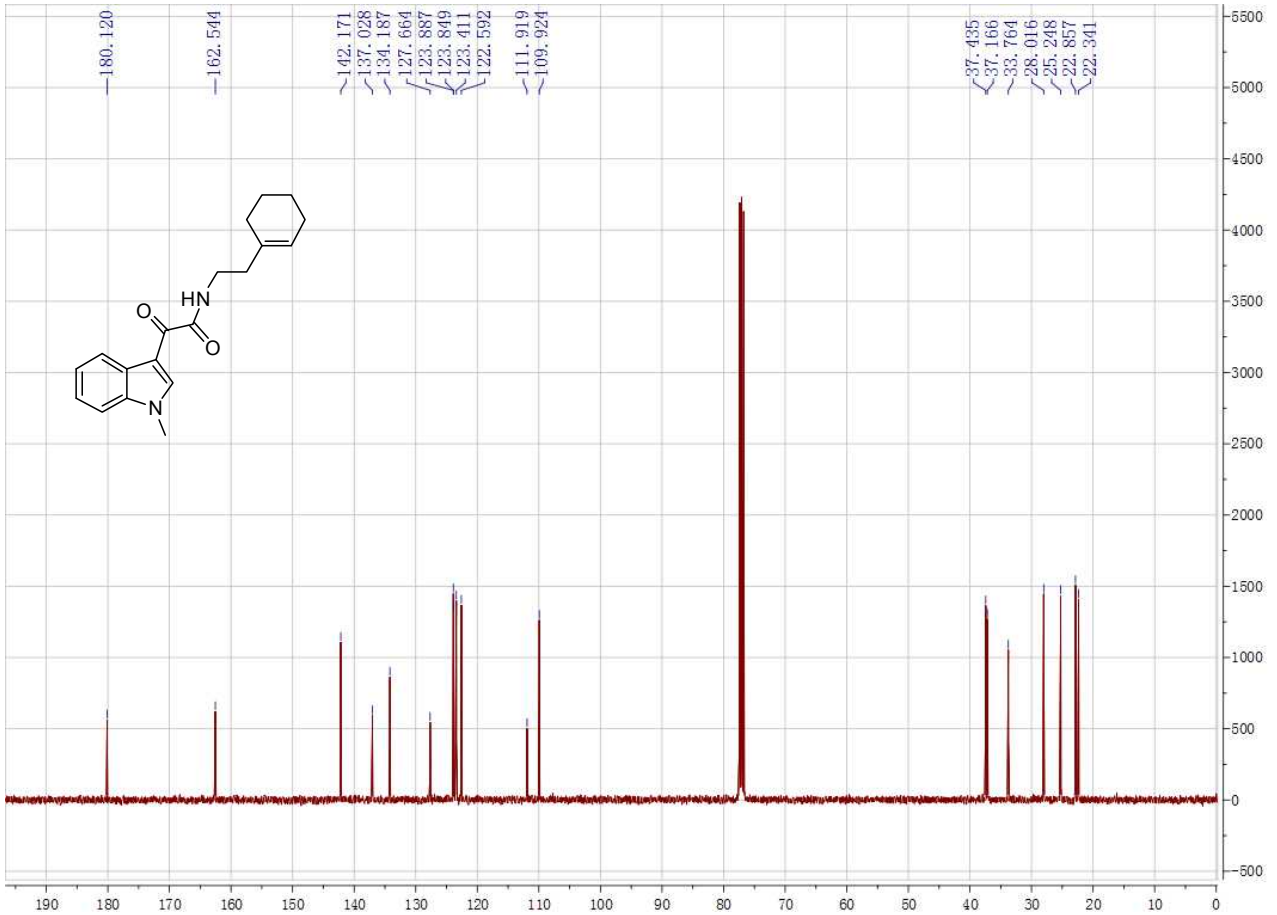
3r


8.98
8.44
8.43
8.42
8.41
7.64
7.40
7.39
7.39
7.38
7.37
7.36
7.35
7.26
5.94
5.92
5.90
5.89
5.87
5.30
5.30
5.26
5.26
5.22
5.21
5.19
5.19
4.03
4.02
4.00
3.87
HN
O
O
N
0.08
1.06
1.04
1.04
3.09
1.03
2.12
2.06
3.12
f1 (ppm)

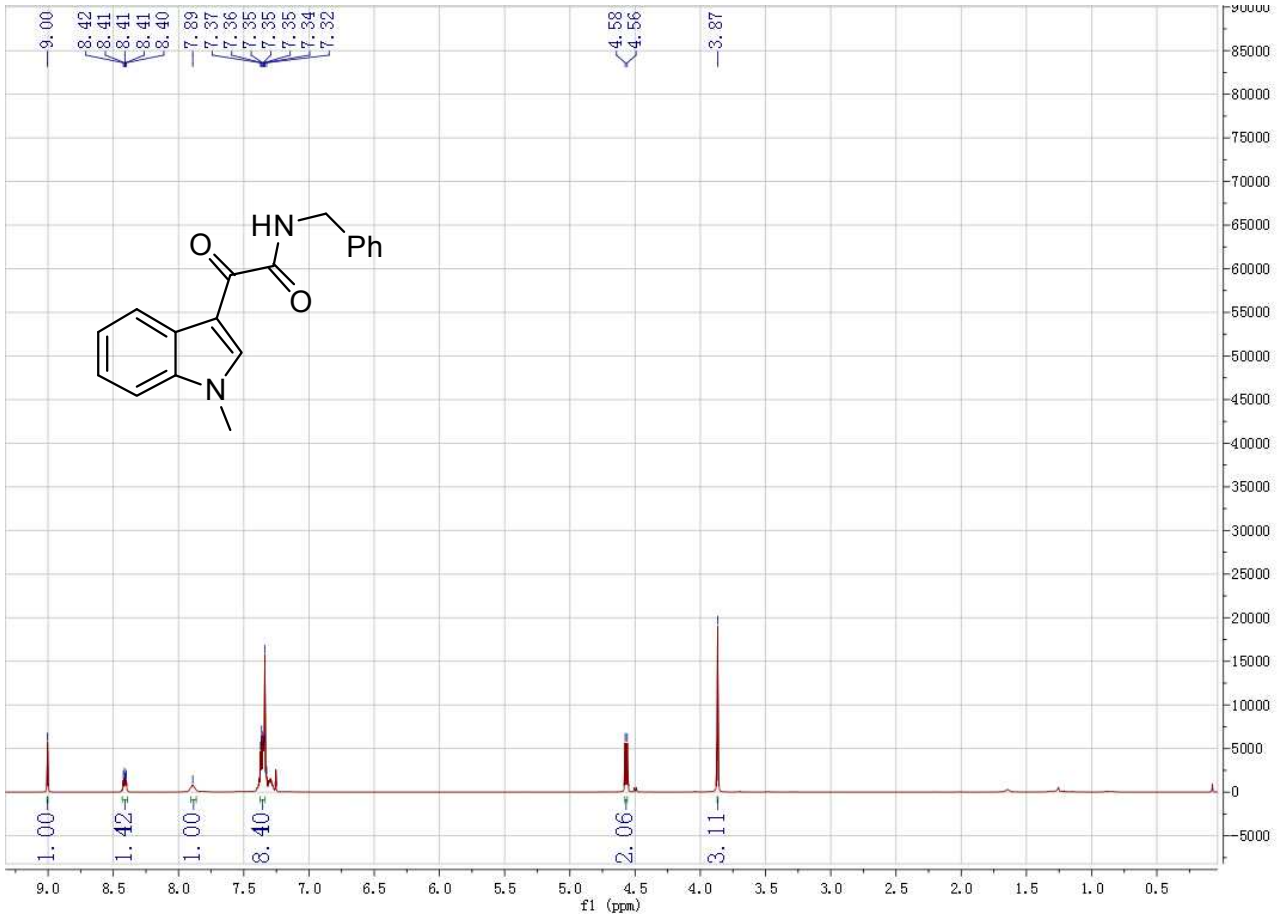

179.77
162.51
142.19
137.06
133.34
127.67
123.91
123.47
122.63
116.84
111.90
109.93
41.61
33.77
HN
O
O
N
f1 (ppm)

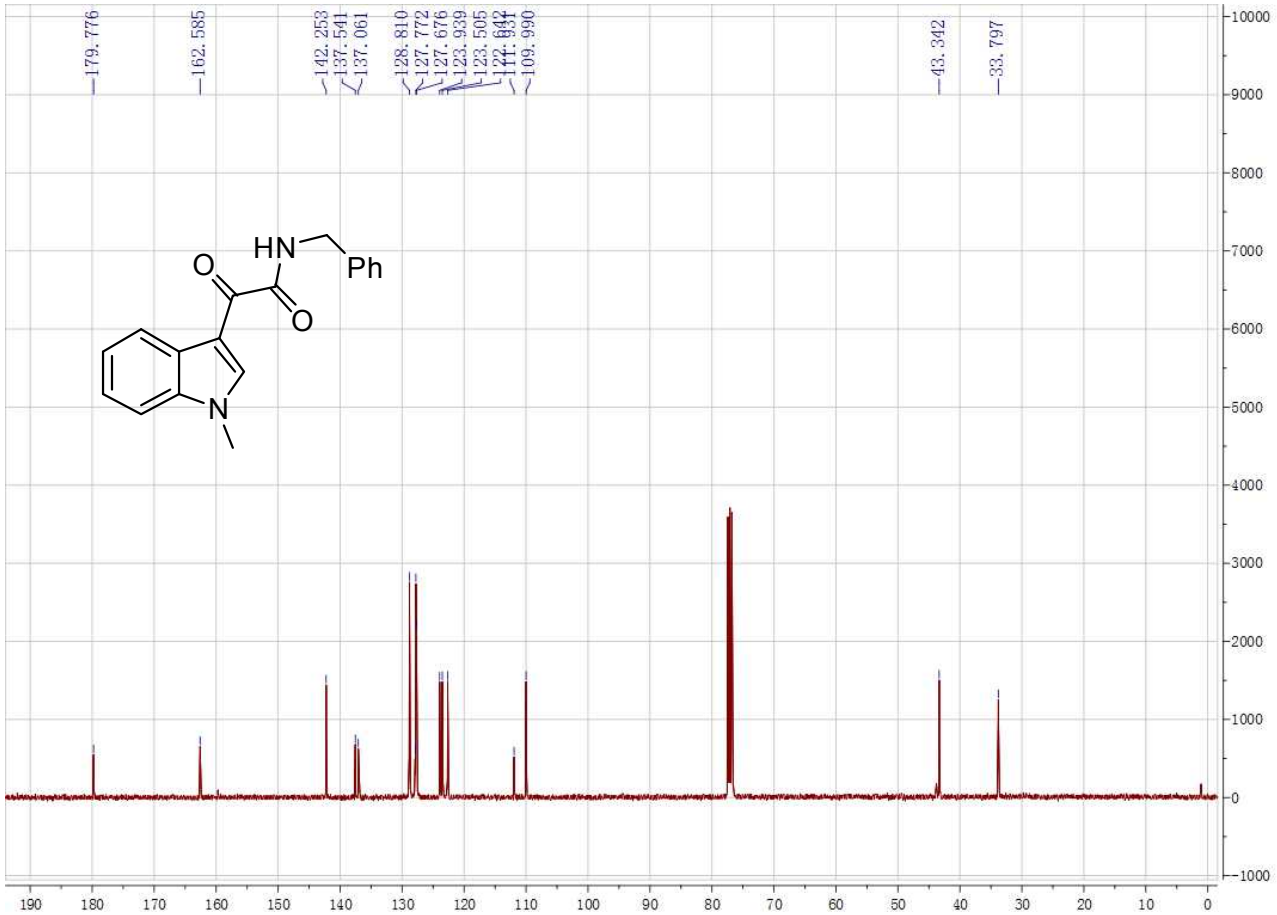
3s


8.980
8.430
8.428
8.419
8.408
7.392
7.386
7.377
7.369
7.362
7.352
7.349
7.344
7.339
7.263
5.537
3.864
3.480
3.463
3.447
3.430
2.252
2.235
2.218
2.021
2.017
2.013
1.997
1.988
1.972
1.657
1.648
1.643
1.634
1.629
1.577
1.572
1.563
1.557
1.549
HN
O
O
N
1.00
1.04
1.07
3.05
1.05
3.20
2.17
2.18
4.14
4.11

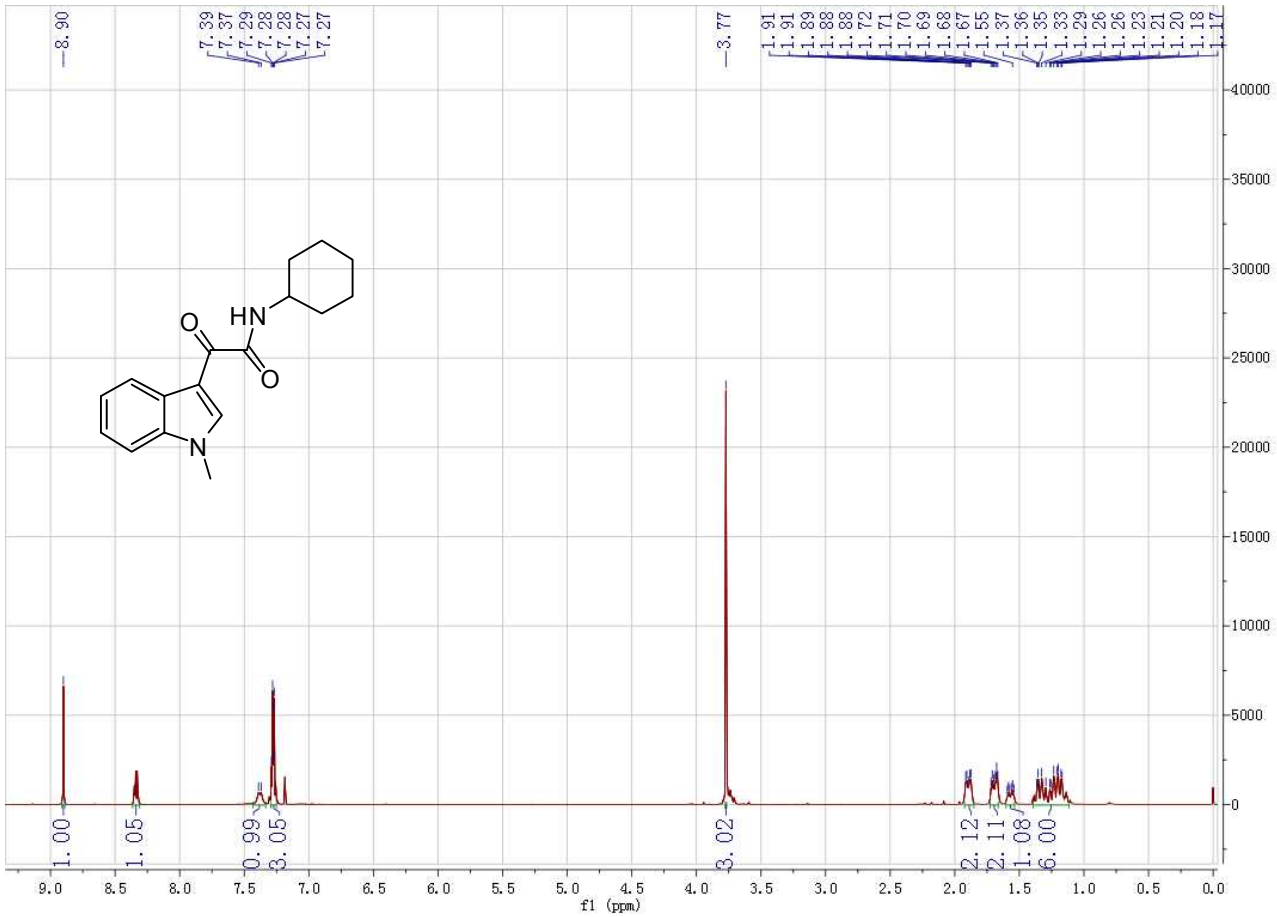

180.120
162.544
142.171
137.028
134.187
127.664
123.887
123.849
123.411
122.592
111.919
109.924
37.435
37.166
33.764
28.016
25.248
22.857
22.341
HN
O
O
N

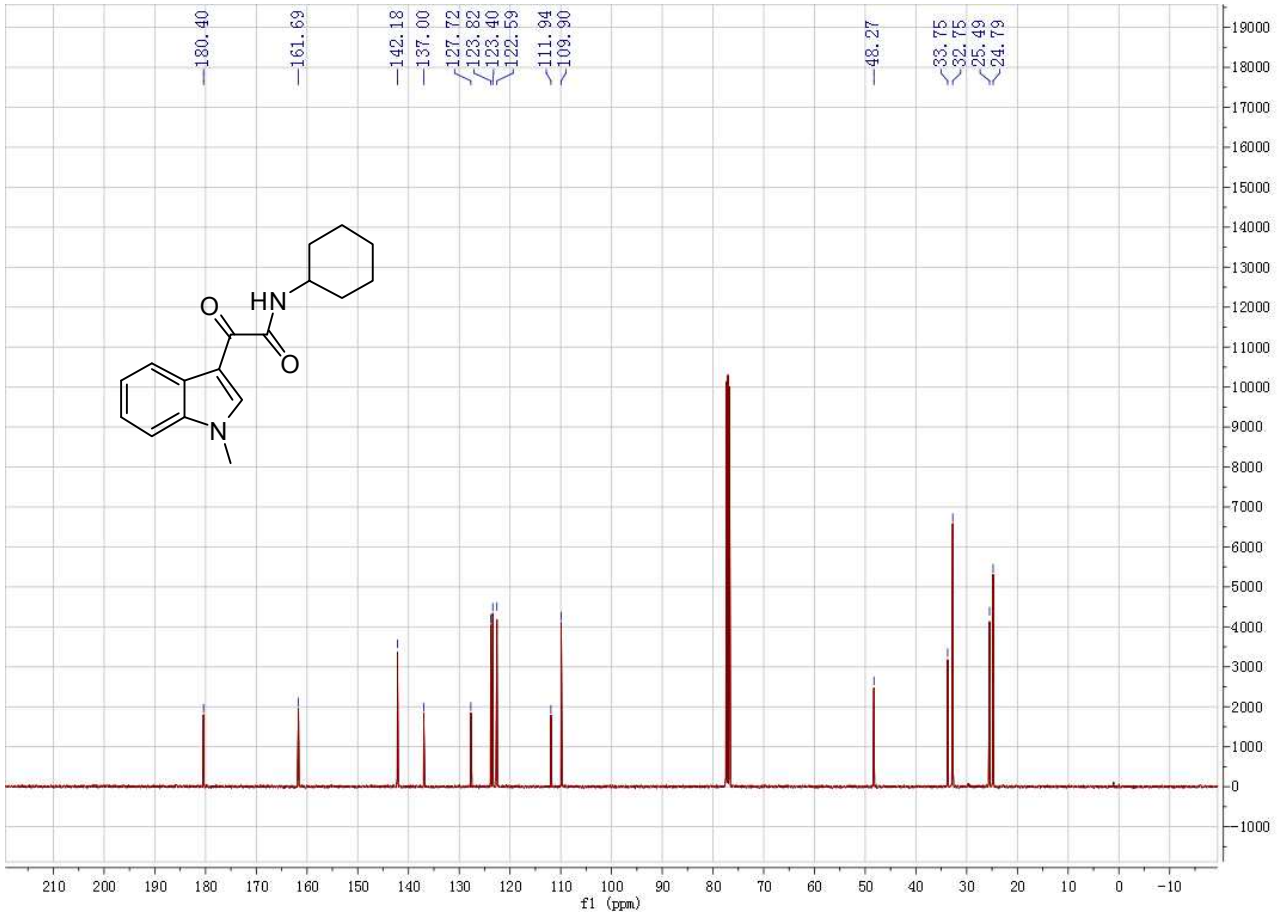
3t


9.00
8.42
8.41
8.41
8.41
8.40
7.89
7.37
7.36
7.35
7.35
7.35
7.34
7.32
4.58
4.56
3.87
HN
Ph
O
O
N
1.00
1.42
1.00
8.40
2.06
3.11
f1 (ppm)

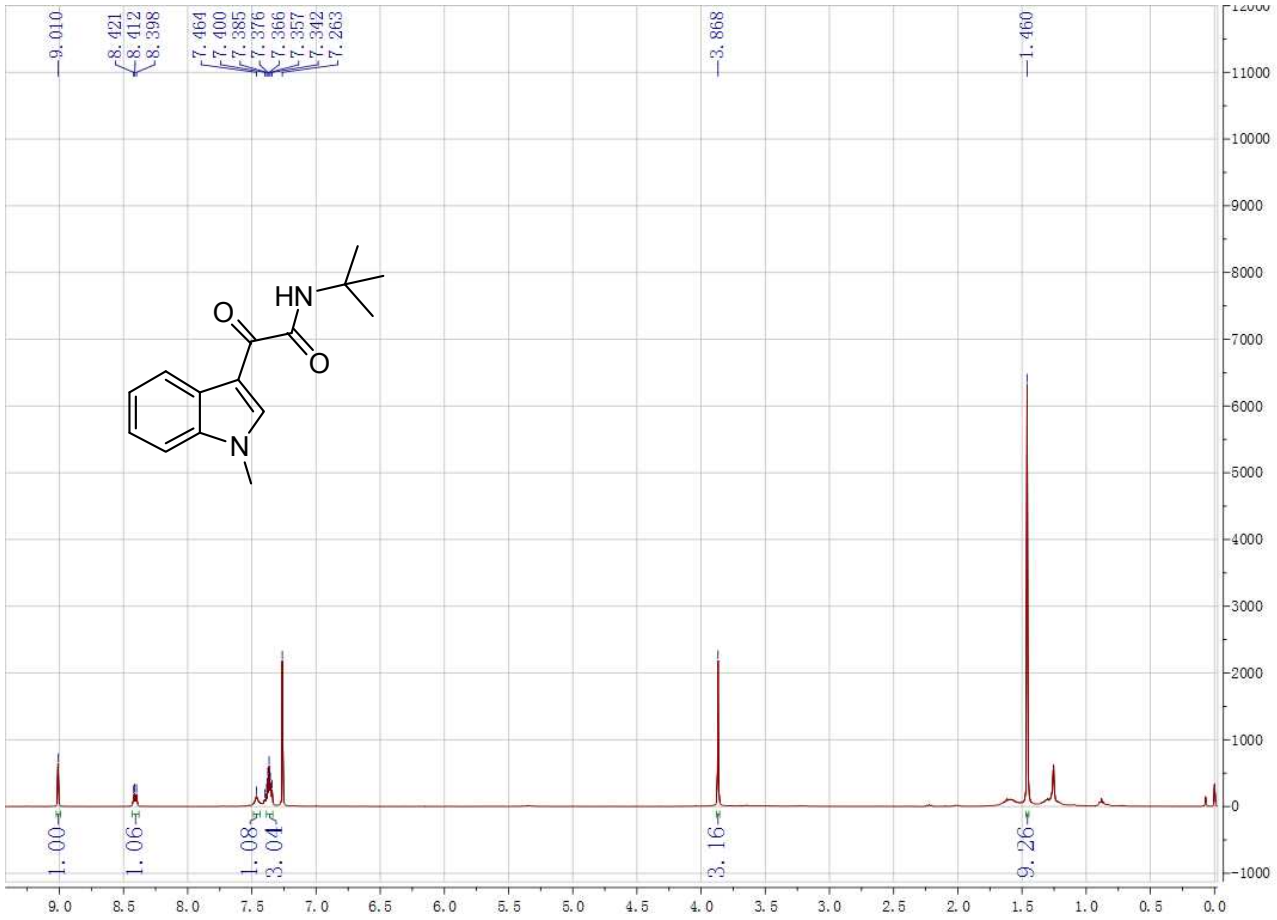

179.776
162.585
142.253
137.541
137.061
128.810
127.772
127.676
123.939
123.505
122.642
111.931
109.990
43.342
33.797
HN
Ph
O
O
N

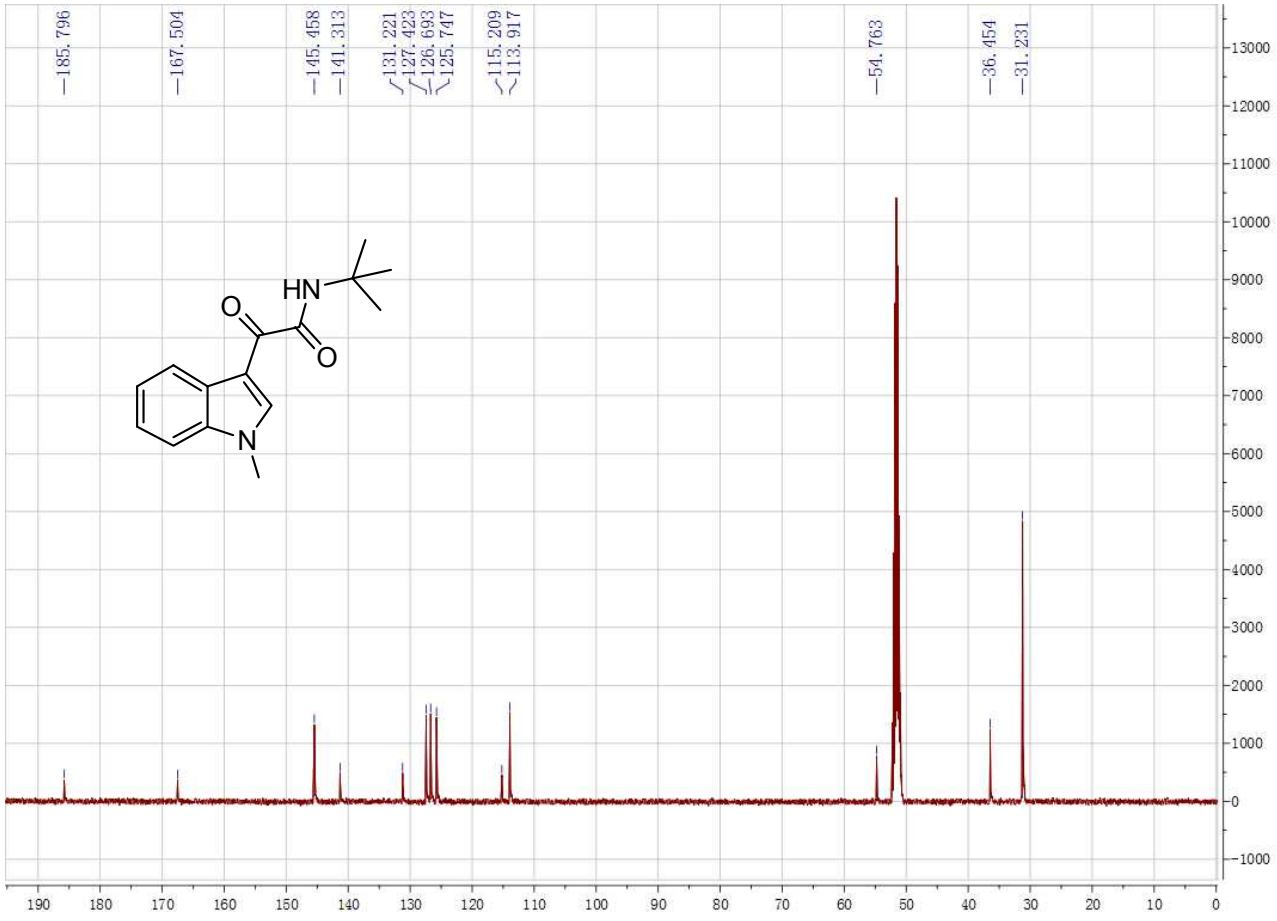
3u


8.90
7.39
7.37
7.29
7.28
7.28
7.27
7.27
3.77
1.91
1.91
1.89
1.88
1.88
1.72
1.71
1.70
1.69
1.68
1.67
1.55
1.37
1.36
1.35
1.33
1.29
1.26
1.26
1.23
1.21
1.20
1.18
1.17
HN
O
O
N
1.00
1.05
0.99
3.05
3.02
2.12
2.11
1.08
6.00
f1 (ppm)


180.40
161.69
142.18
137.00
127.72
123.82
123.40
122.59
111.94
109.90
48.27
33.75
32.75
25.49
24.79
HN
O
O
N
f1 (ppm)

3v


9.010
8.421
8.412
8.398
7.464
7.400
7.385
7.376
7.366
7.357
7.342
7.263
3.868
1.460
HN
O
O
N
1.00
1.06
1.08
3.04
3.16
9.26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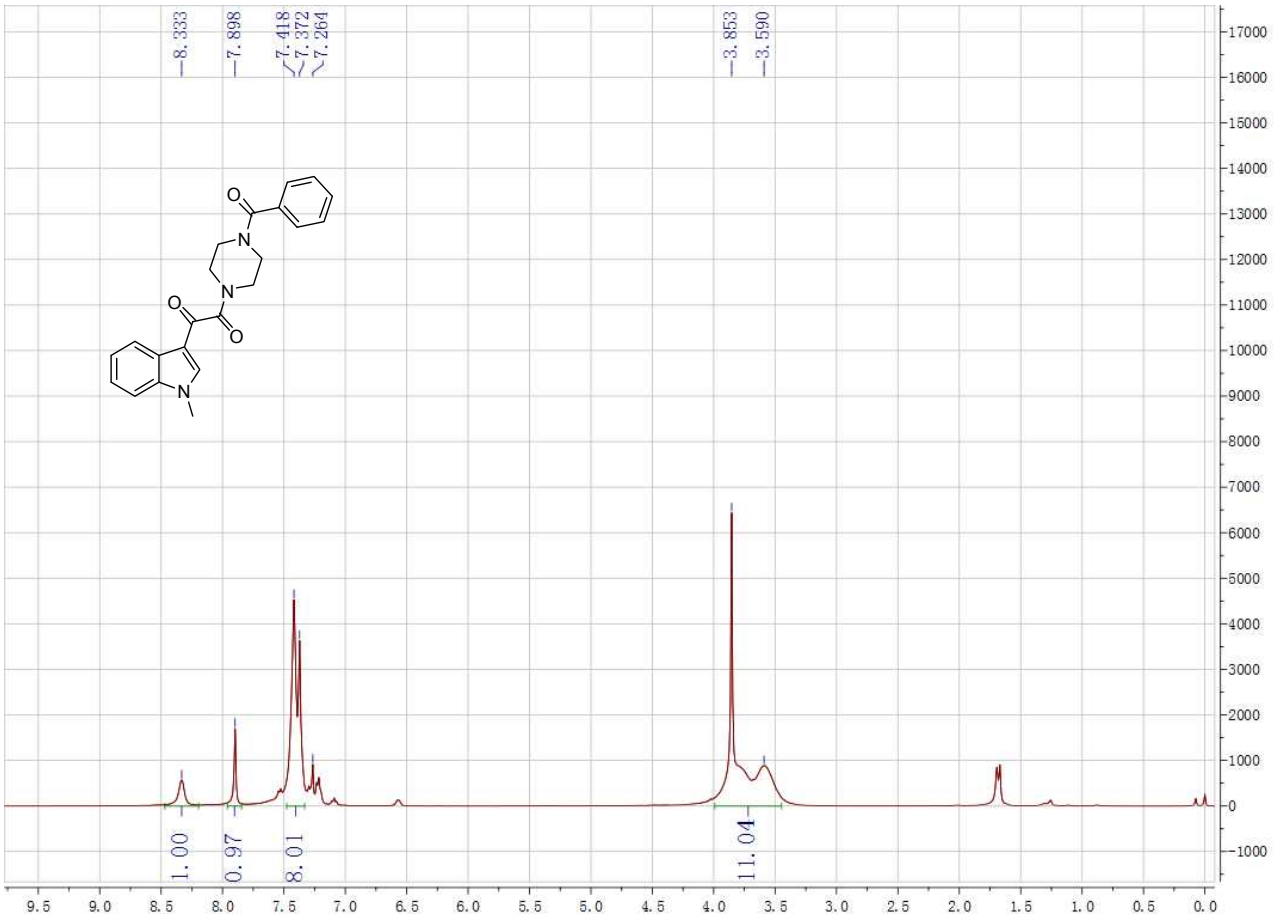
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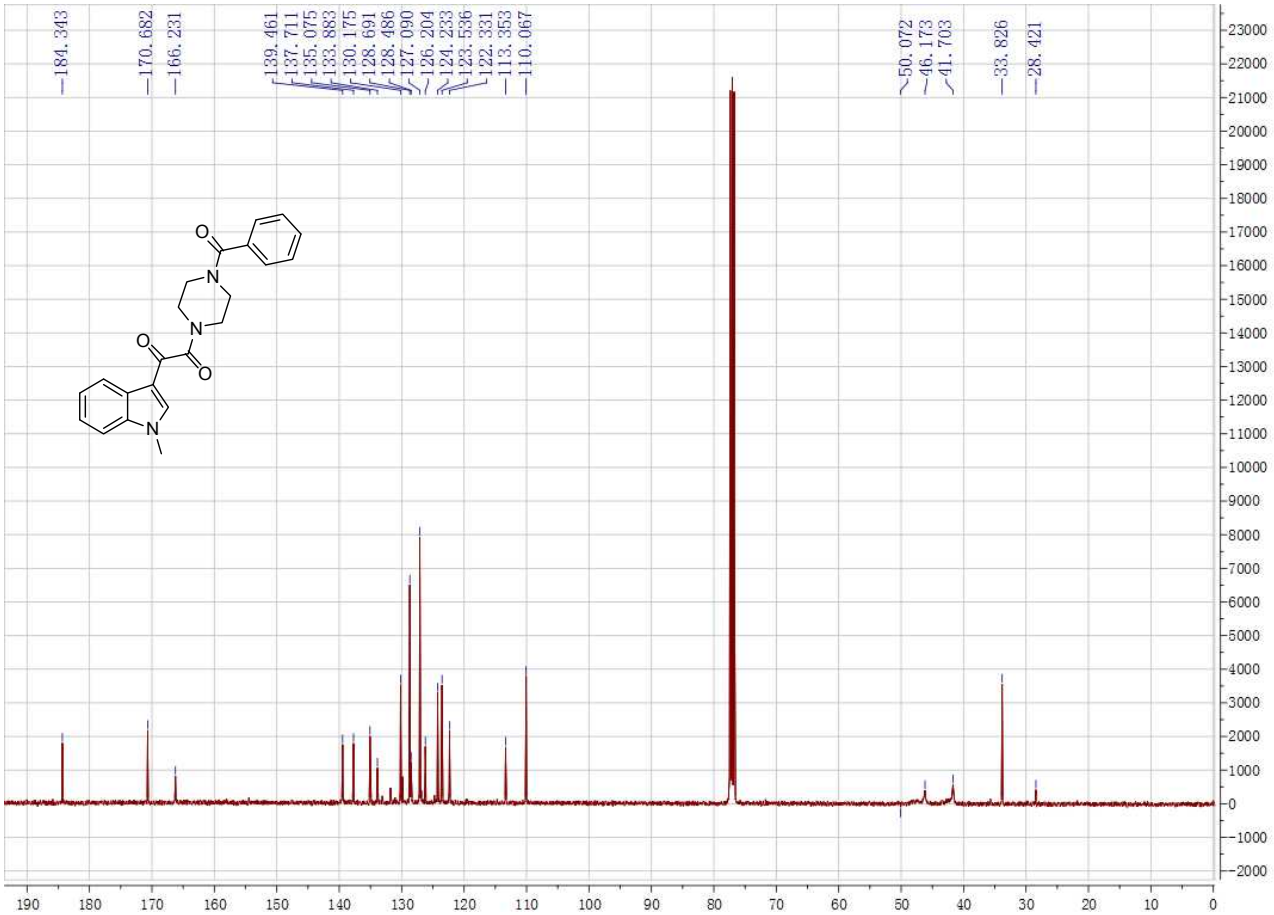
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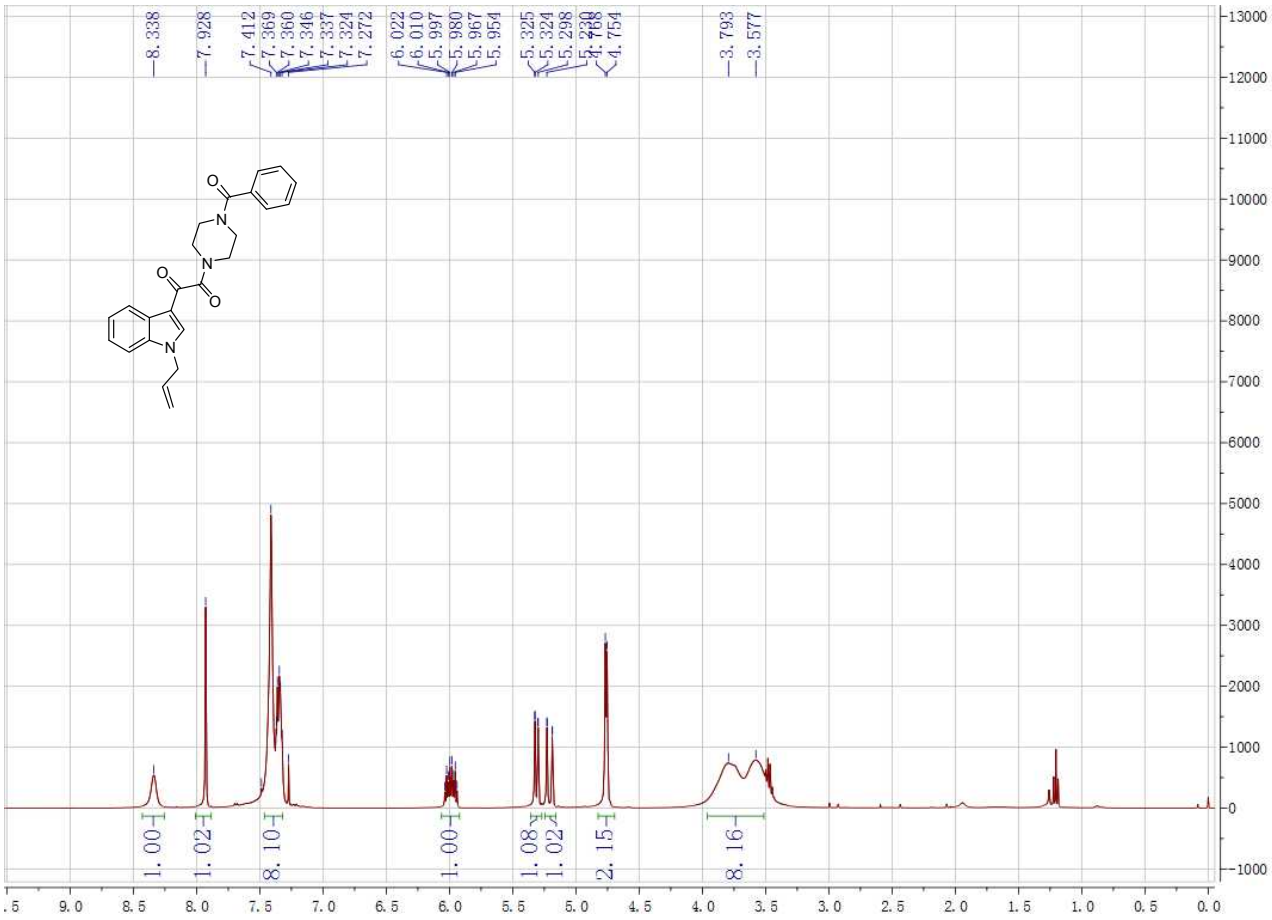
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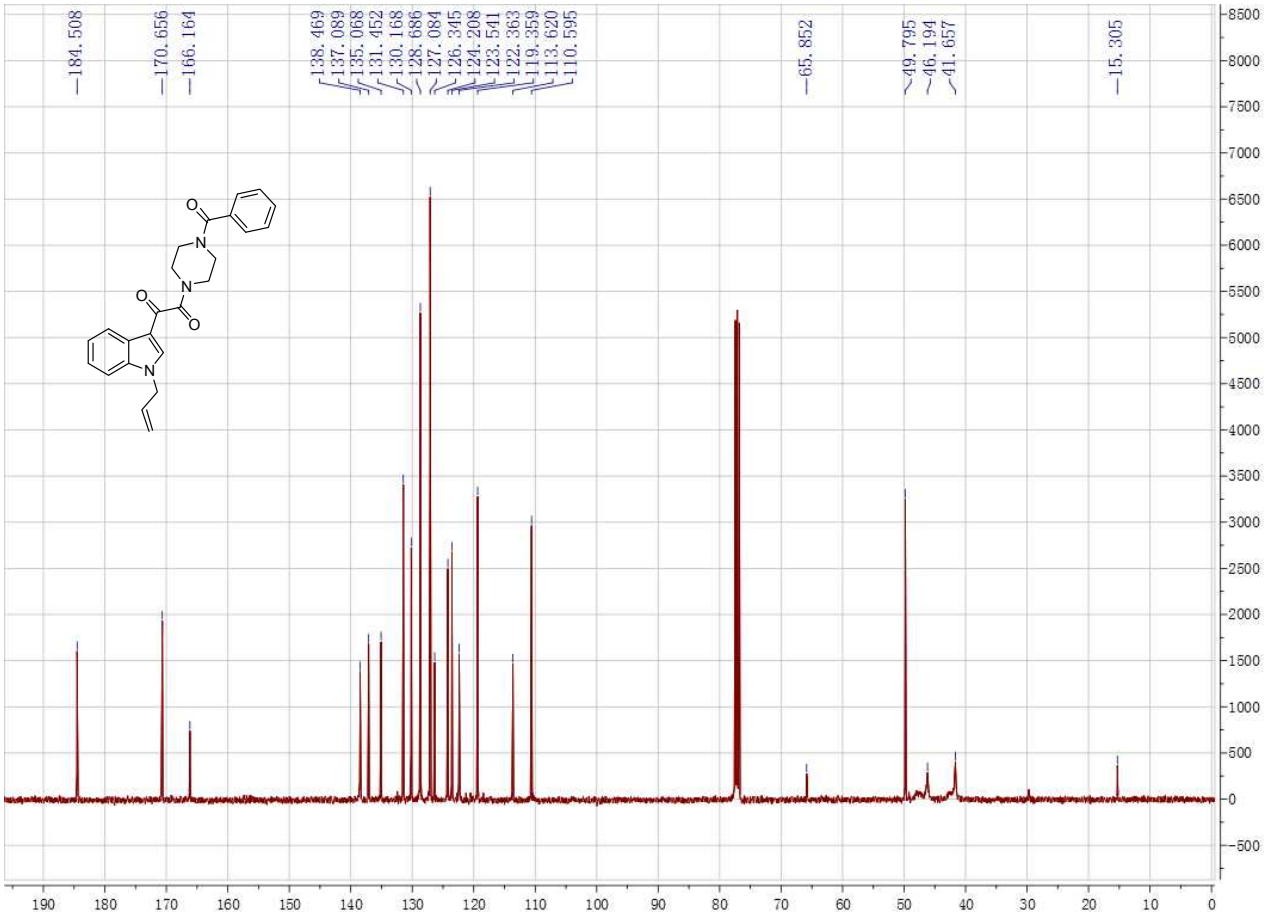
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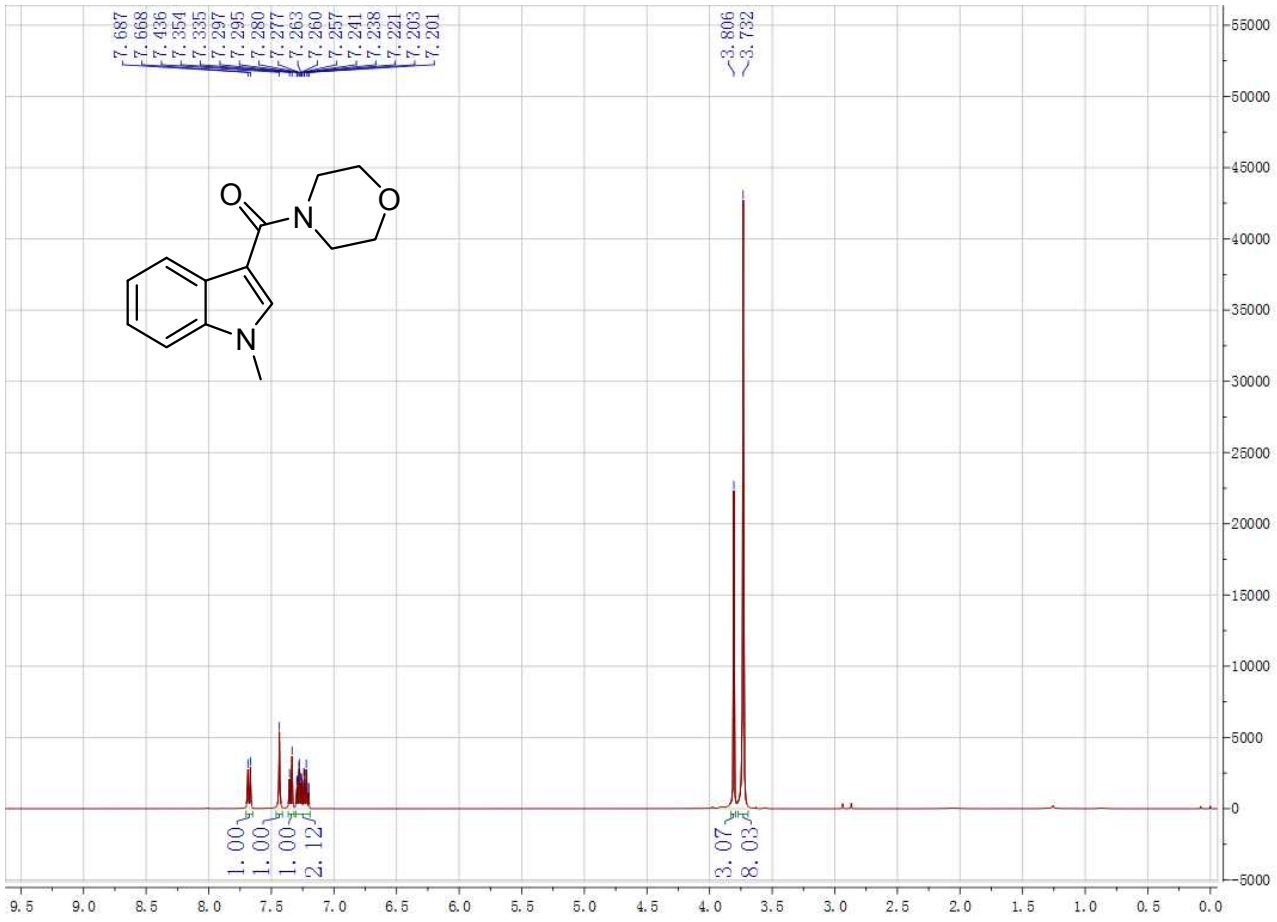
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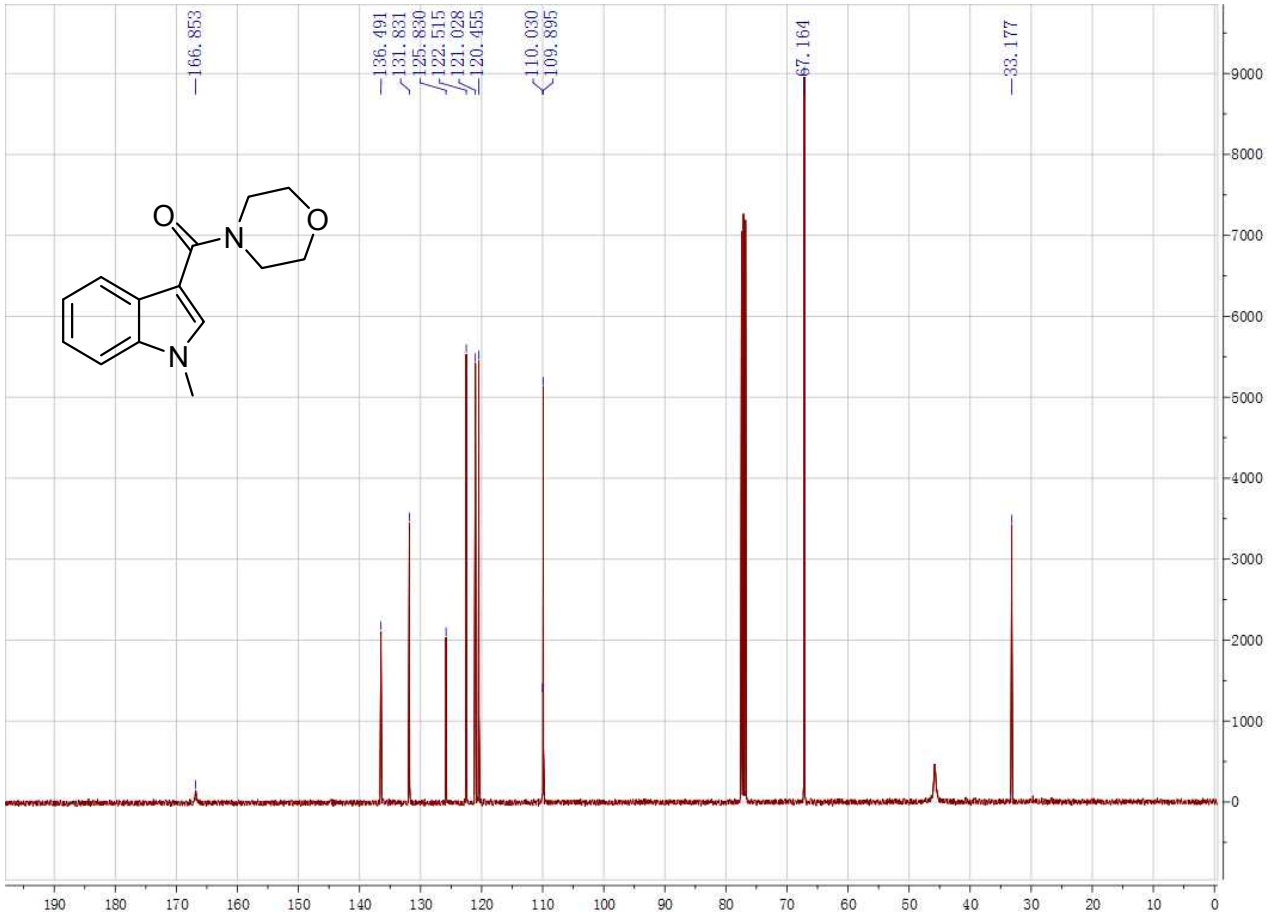
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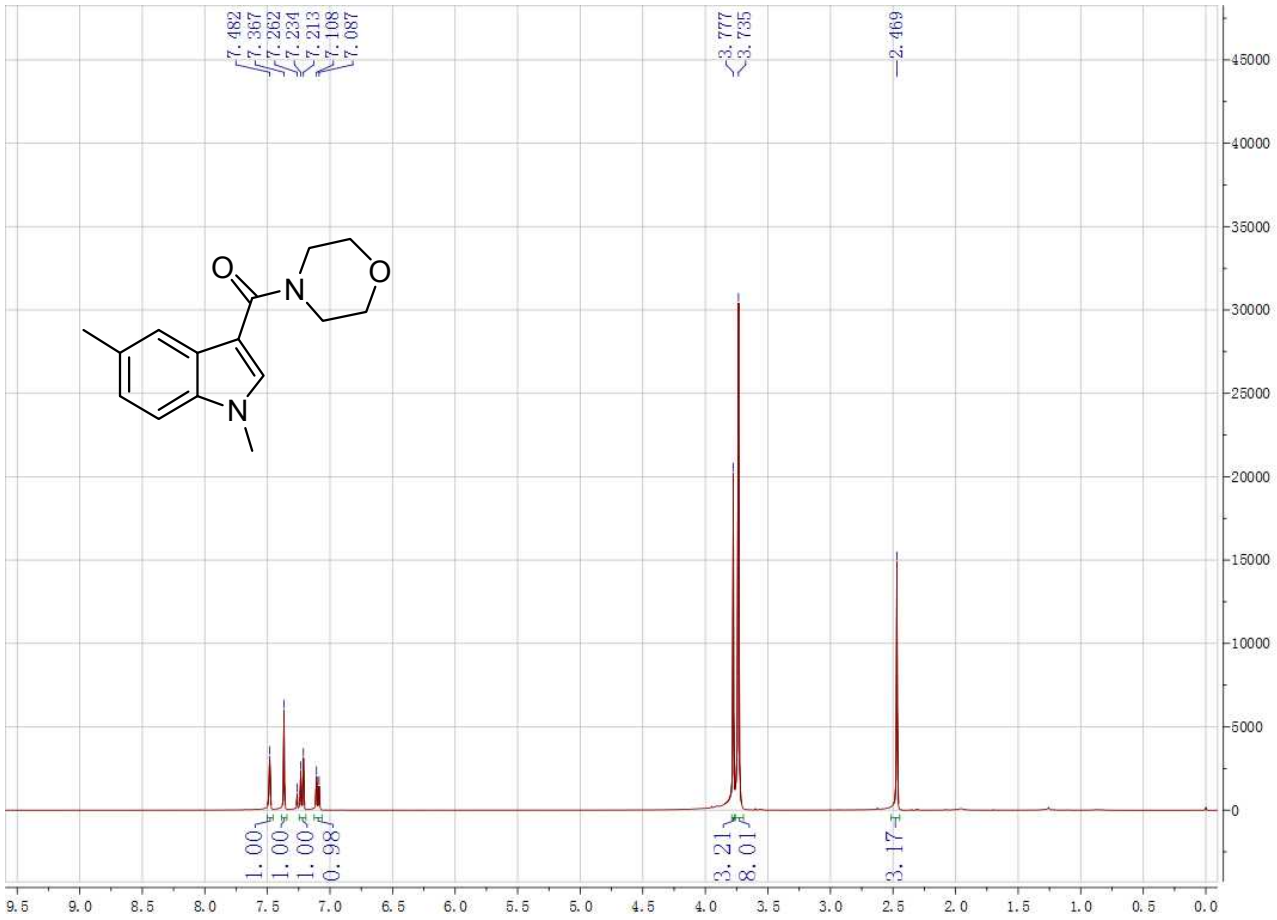
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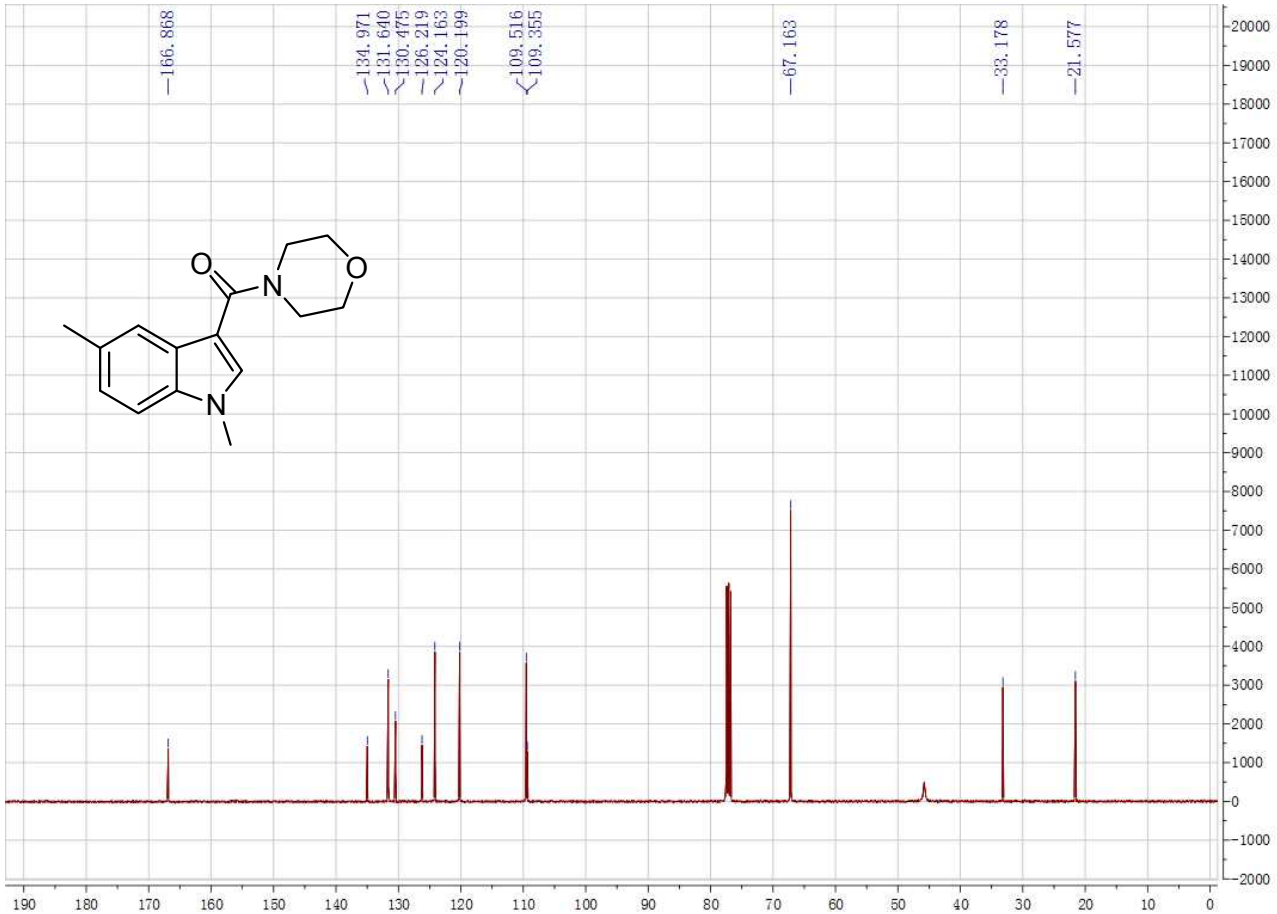
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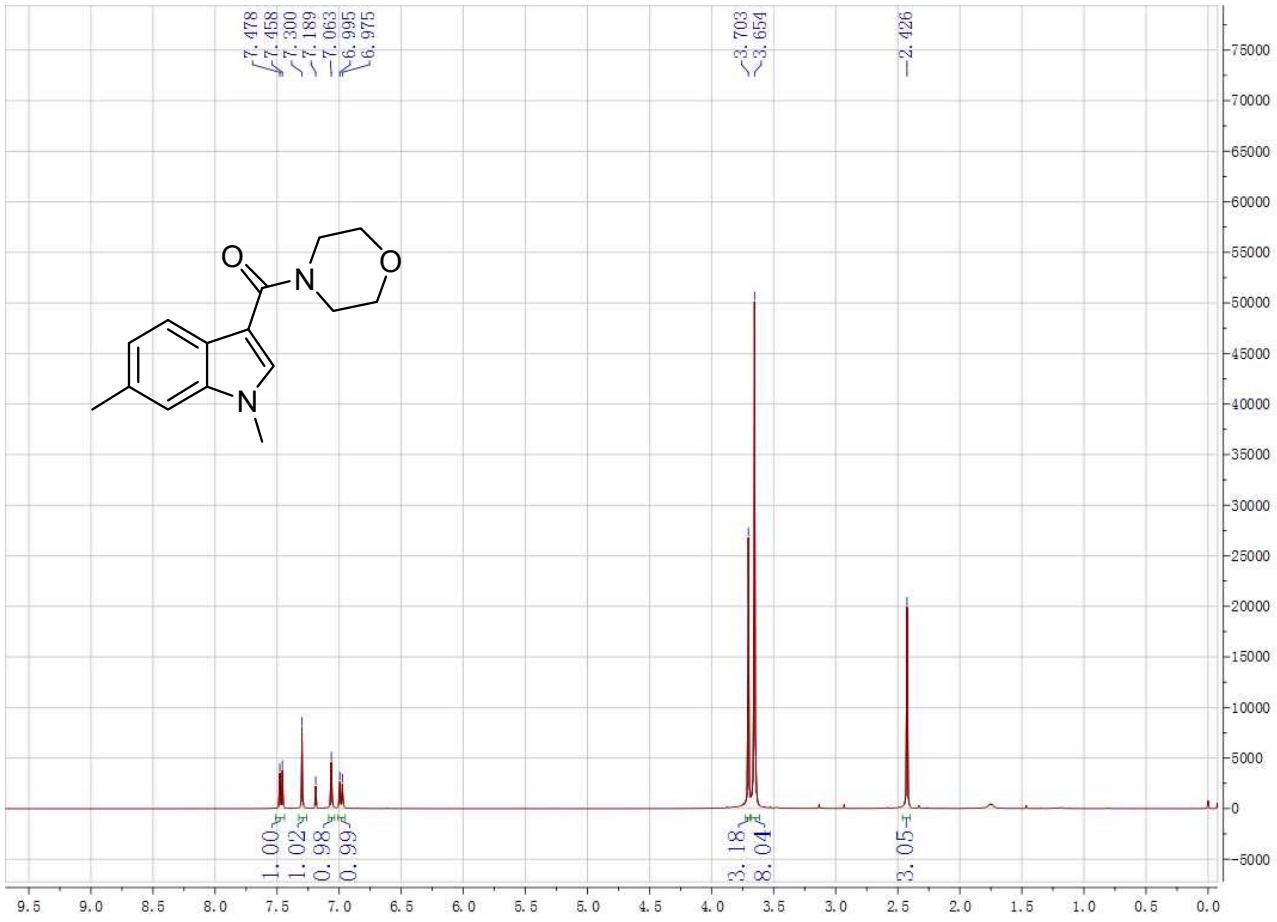
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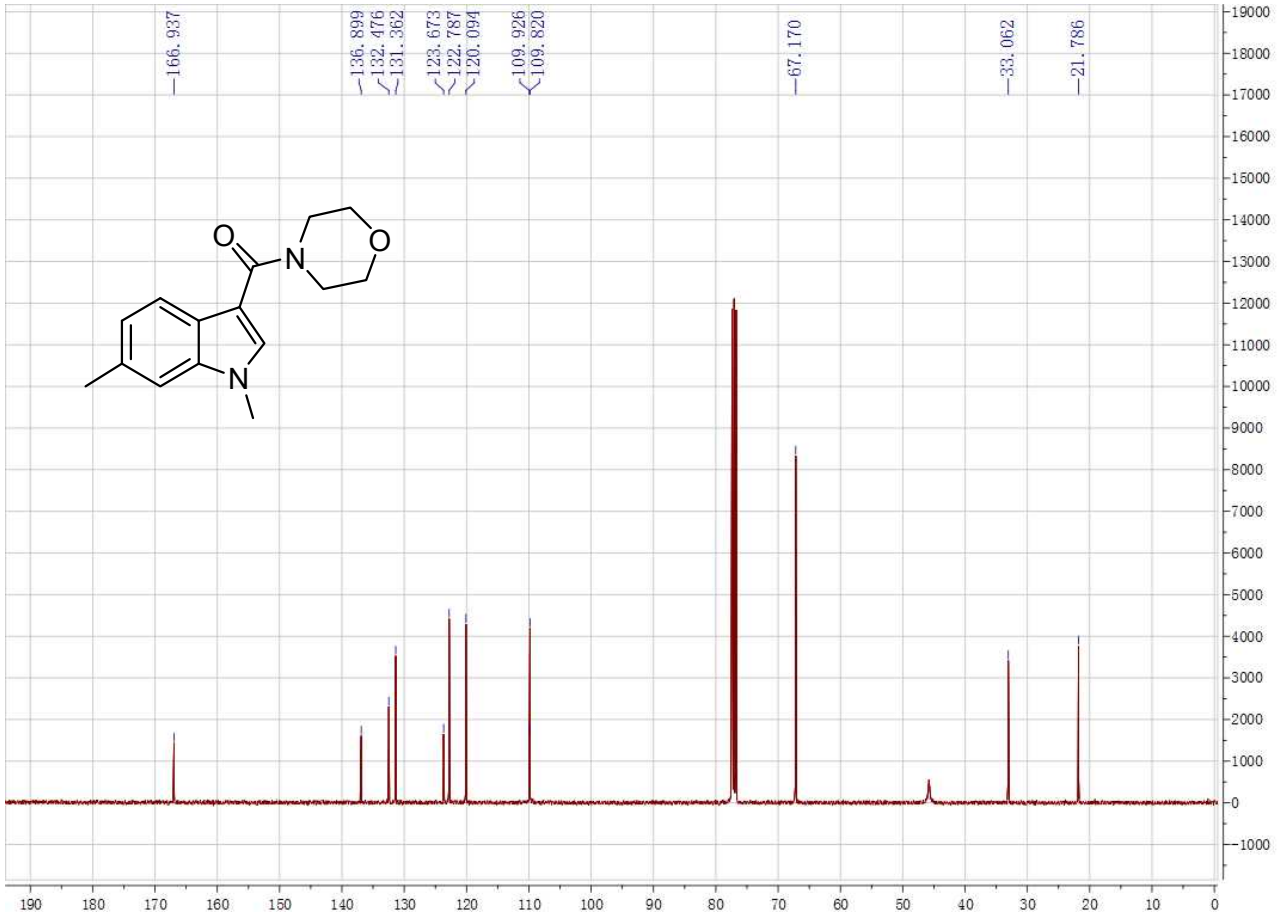
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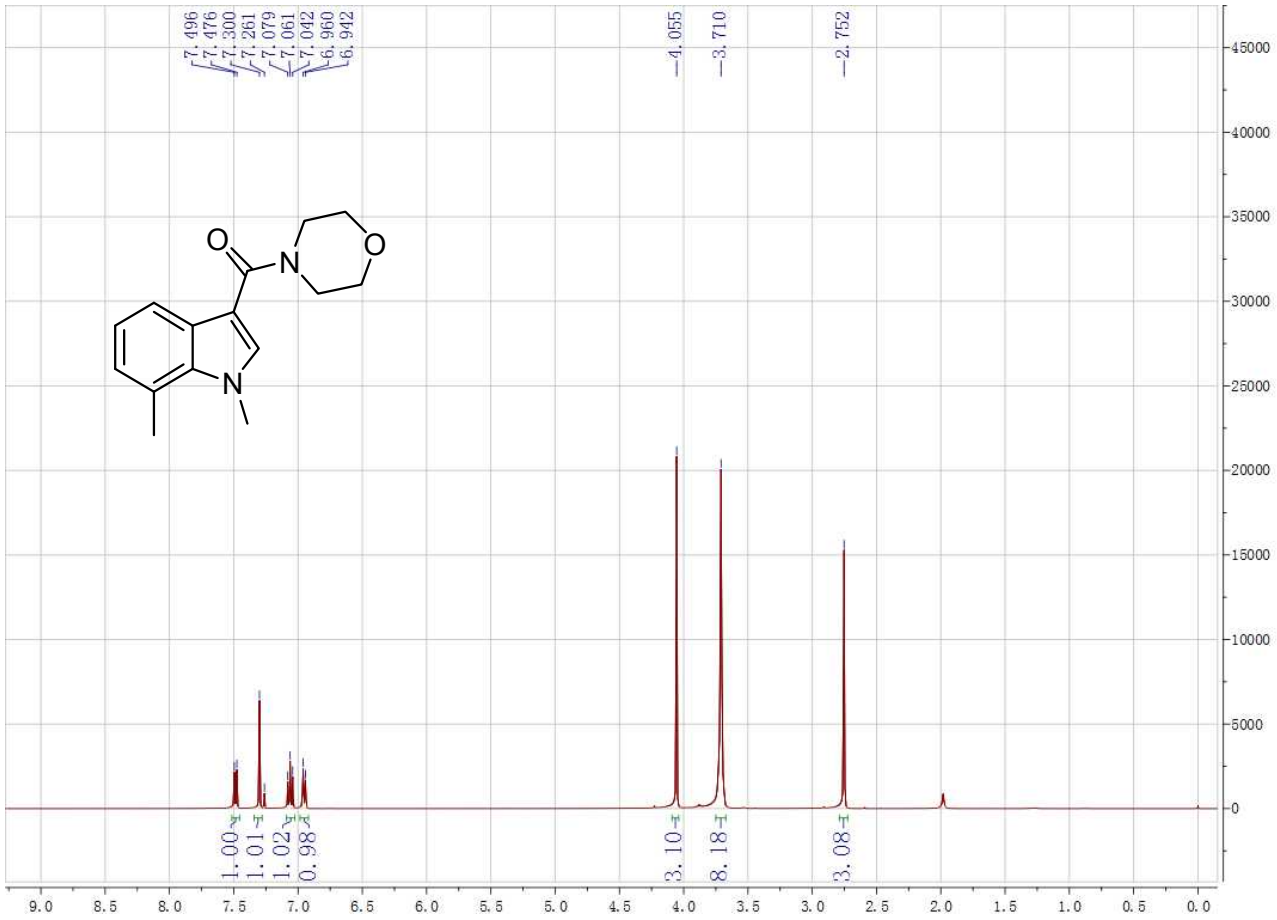
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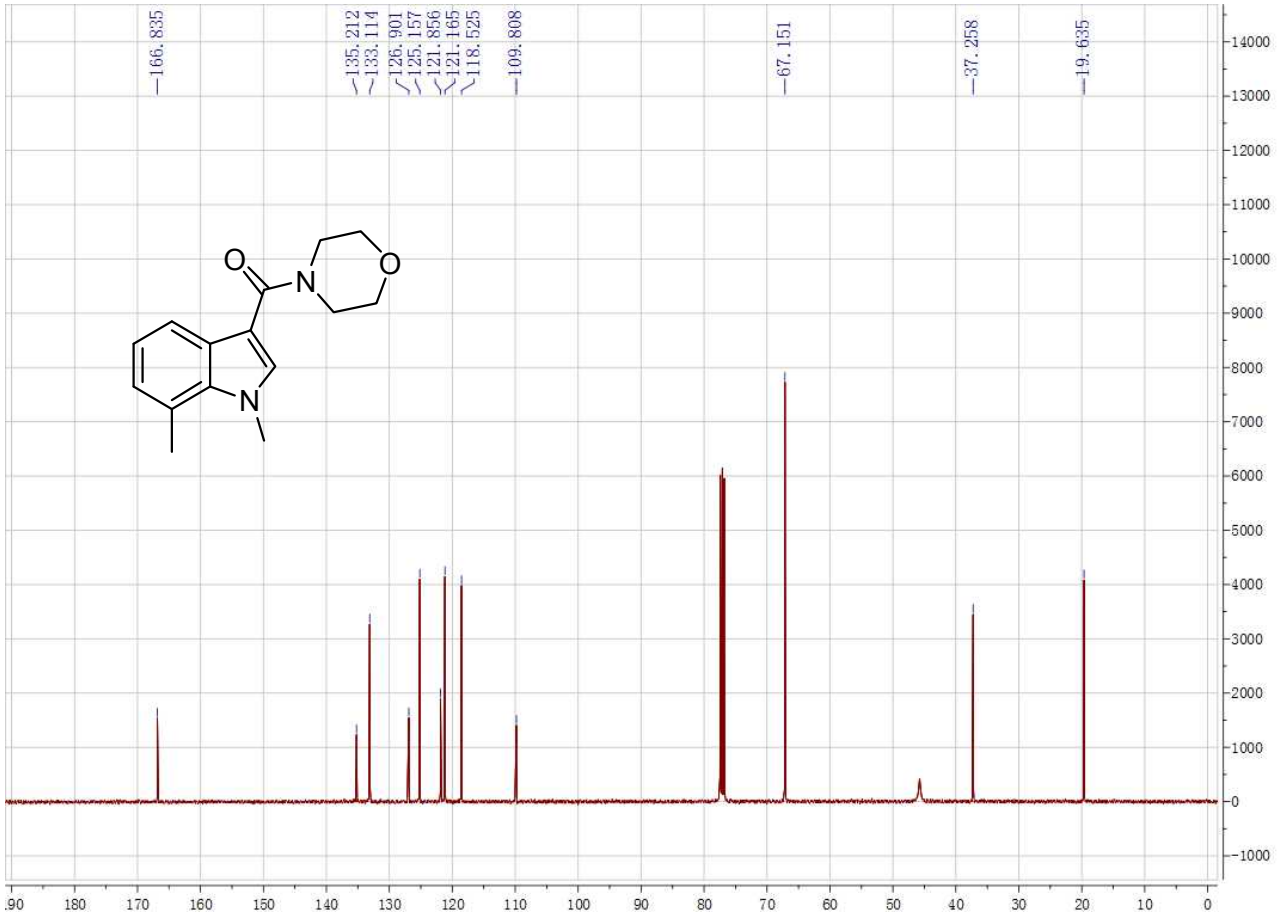
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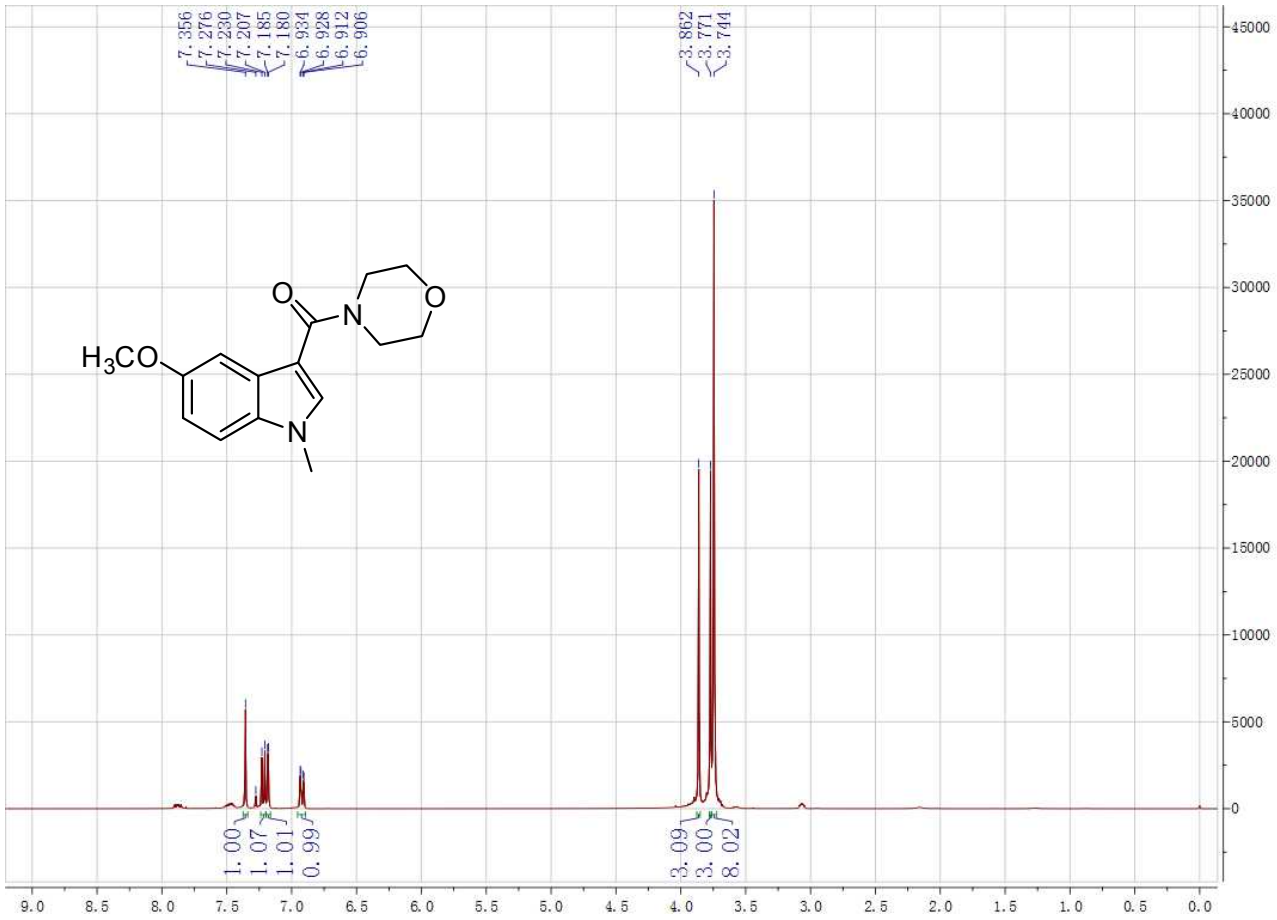
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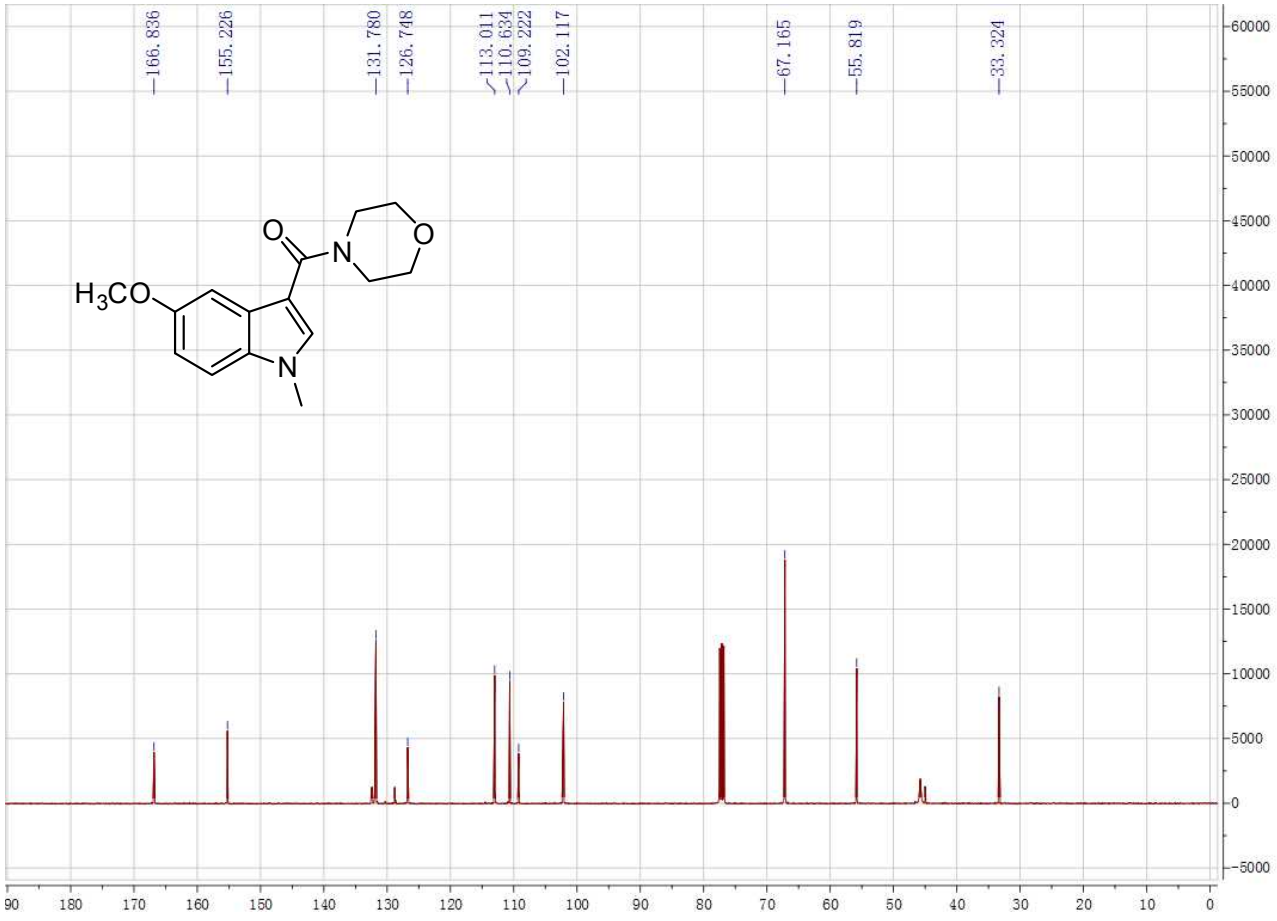
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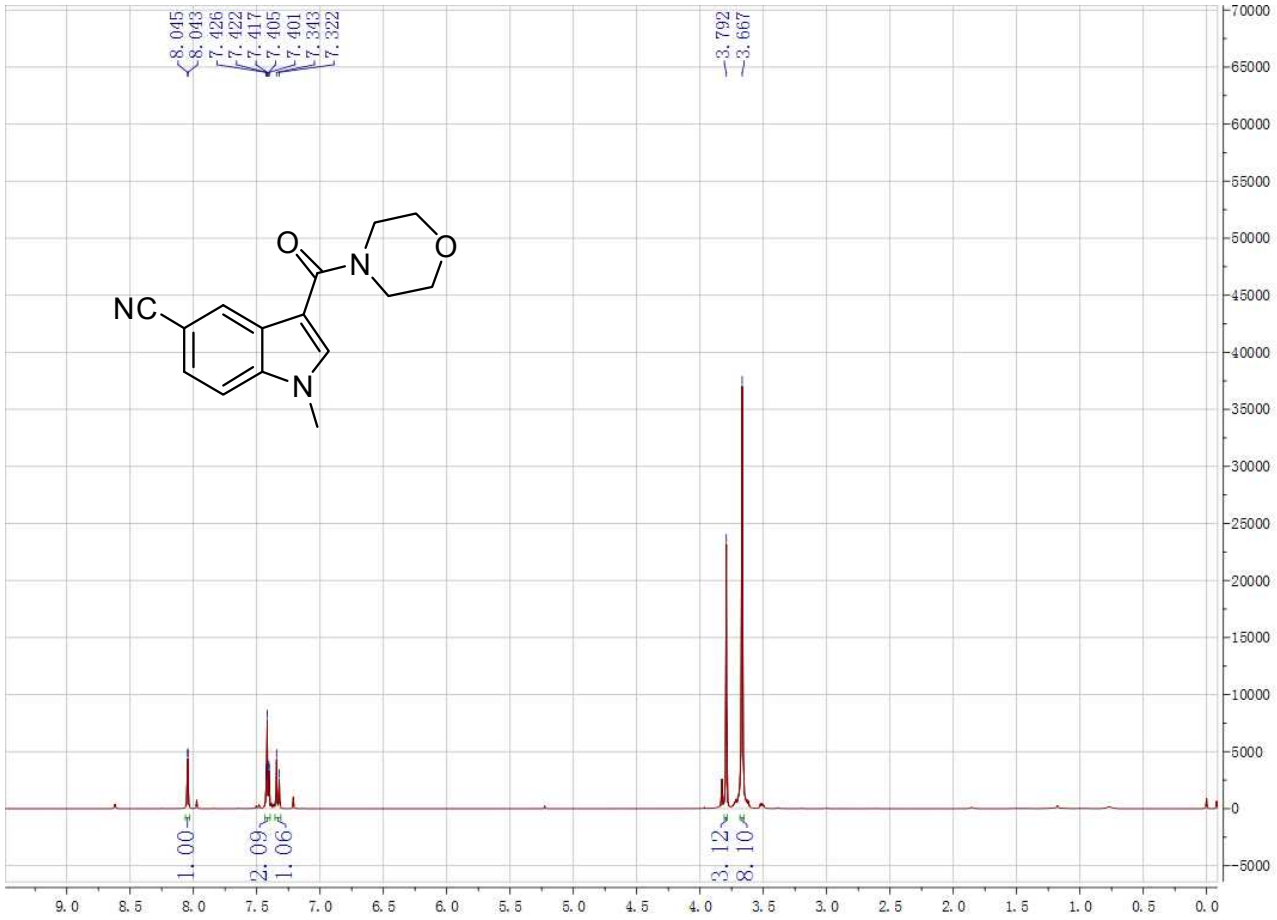
4f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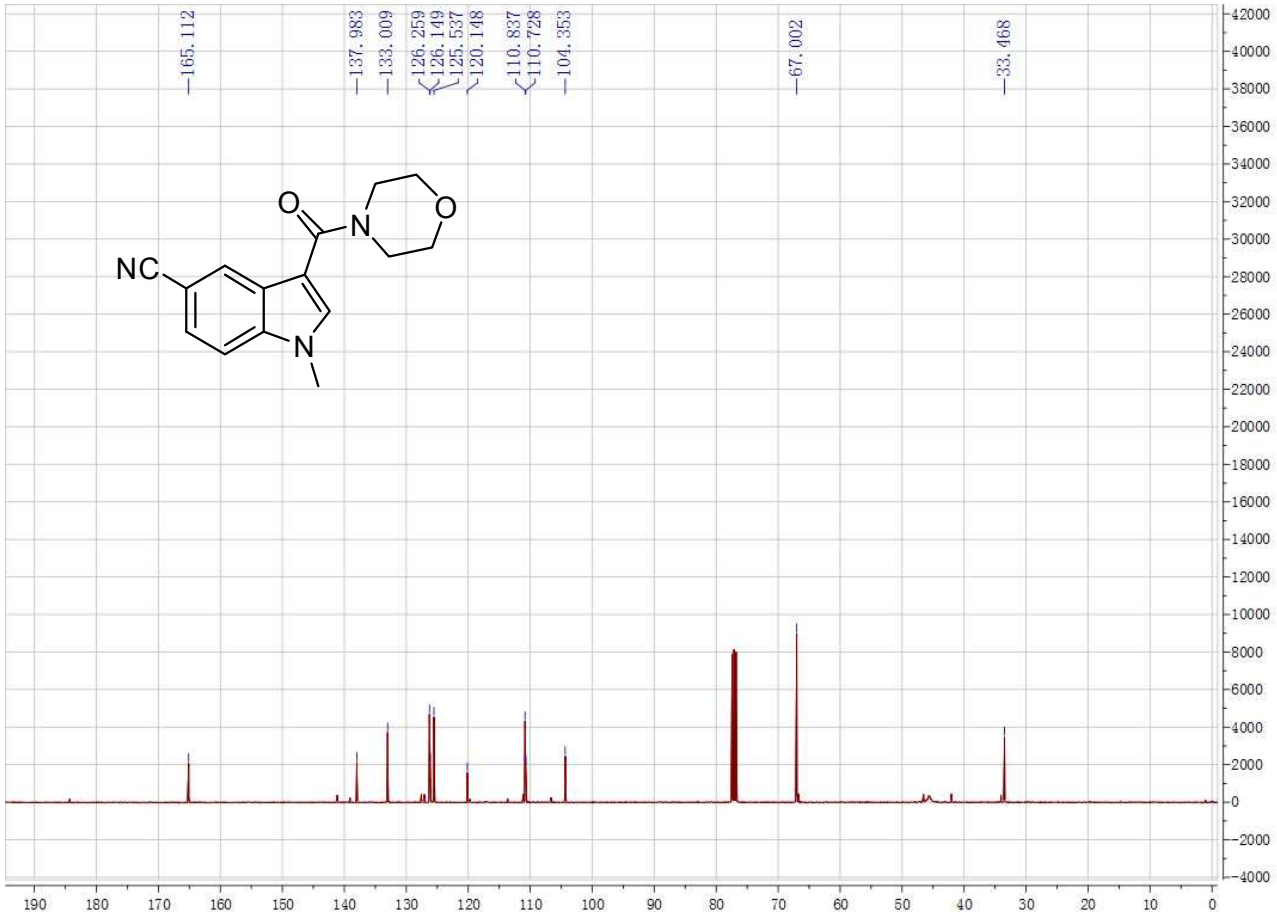
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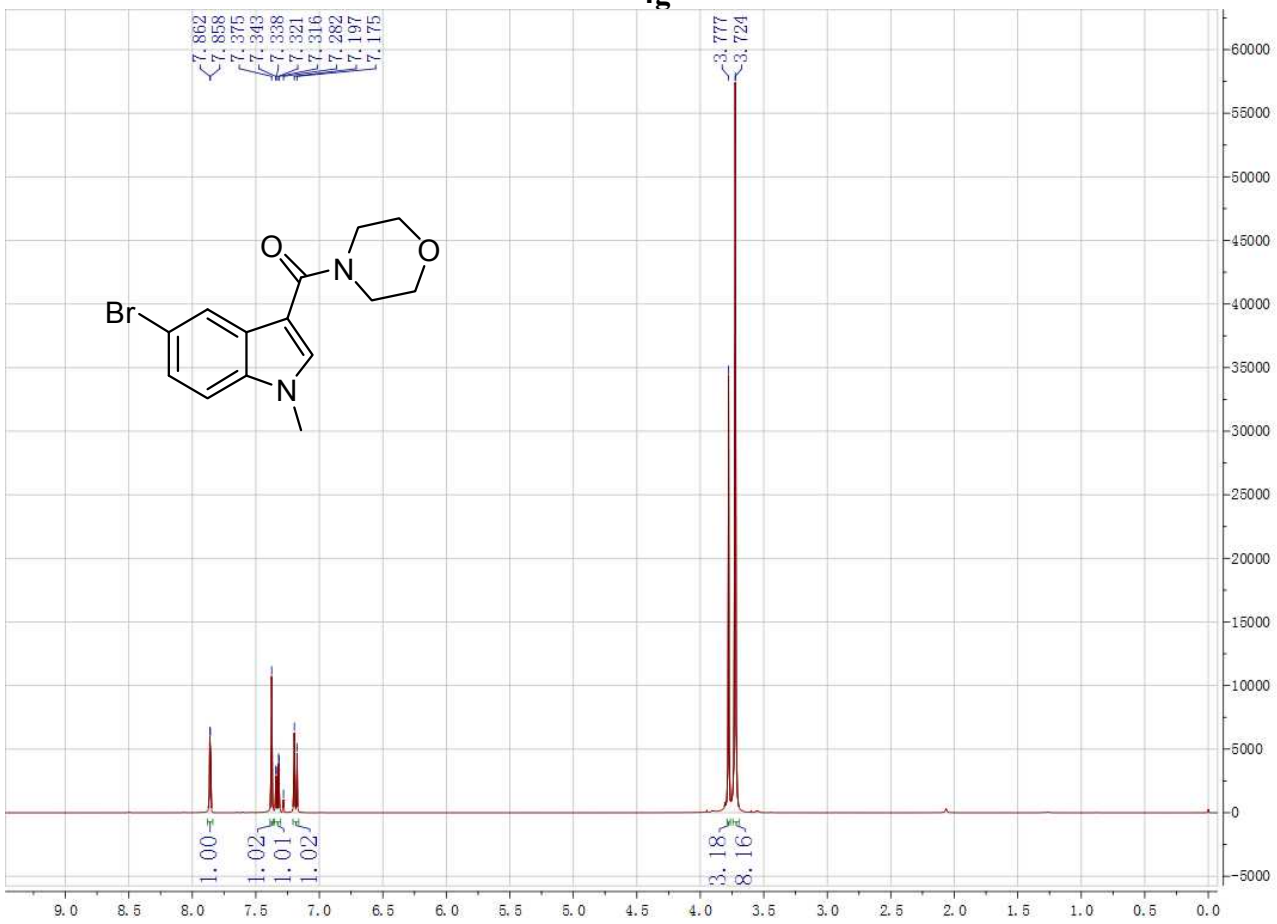
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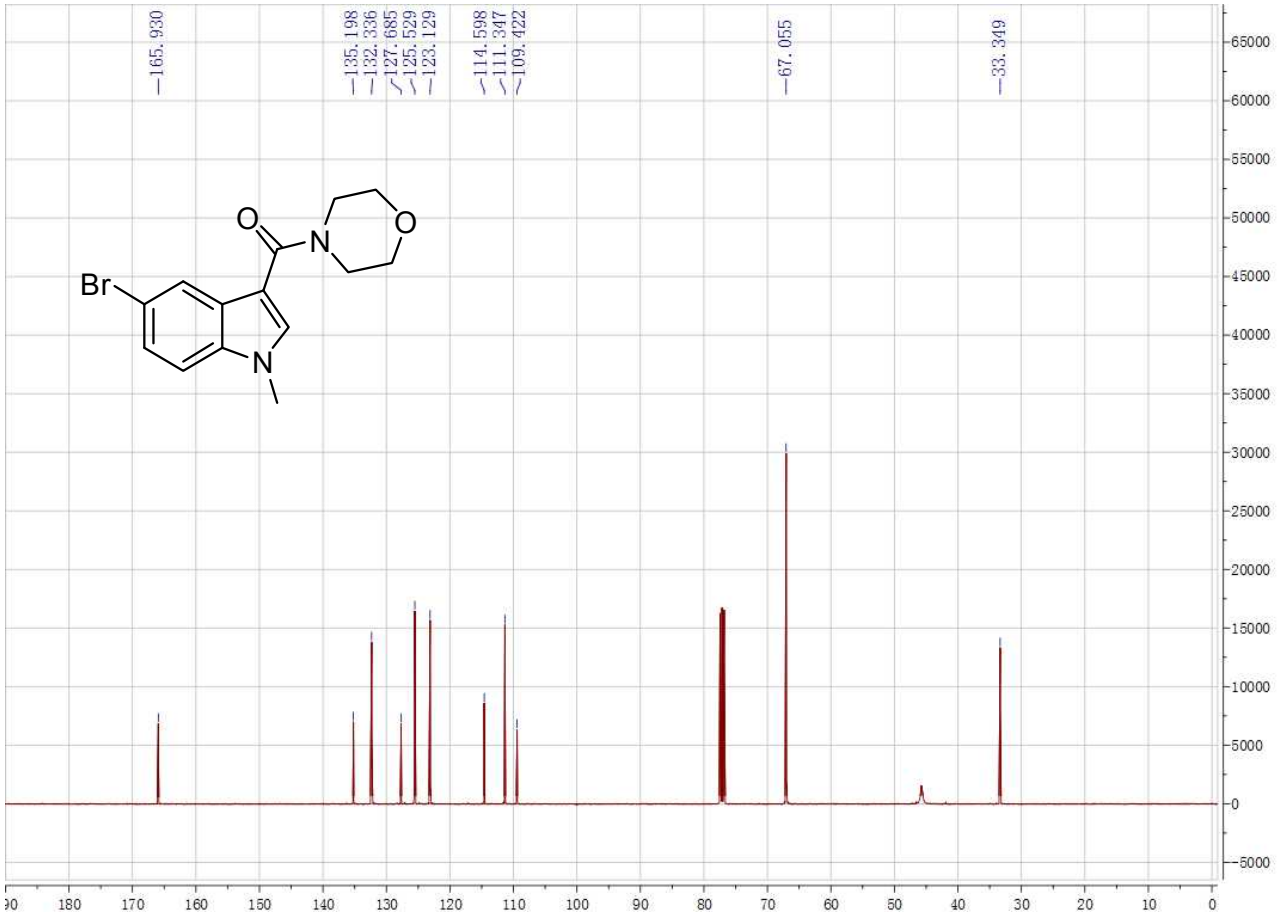
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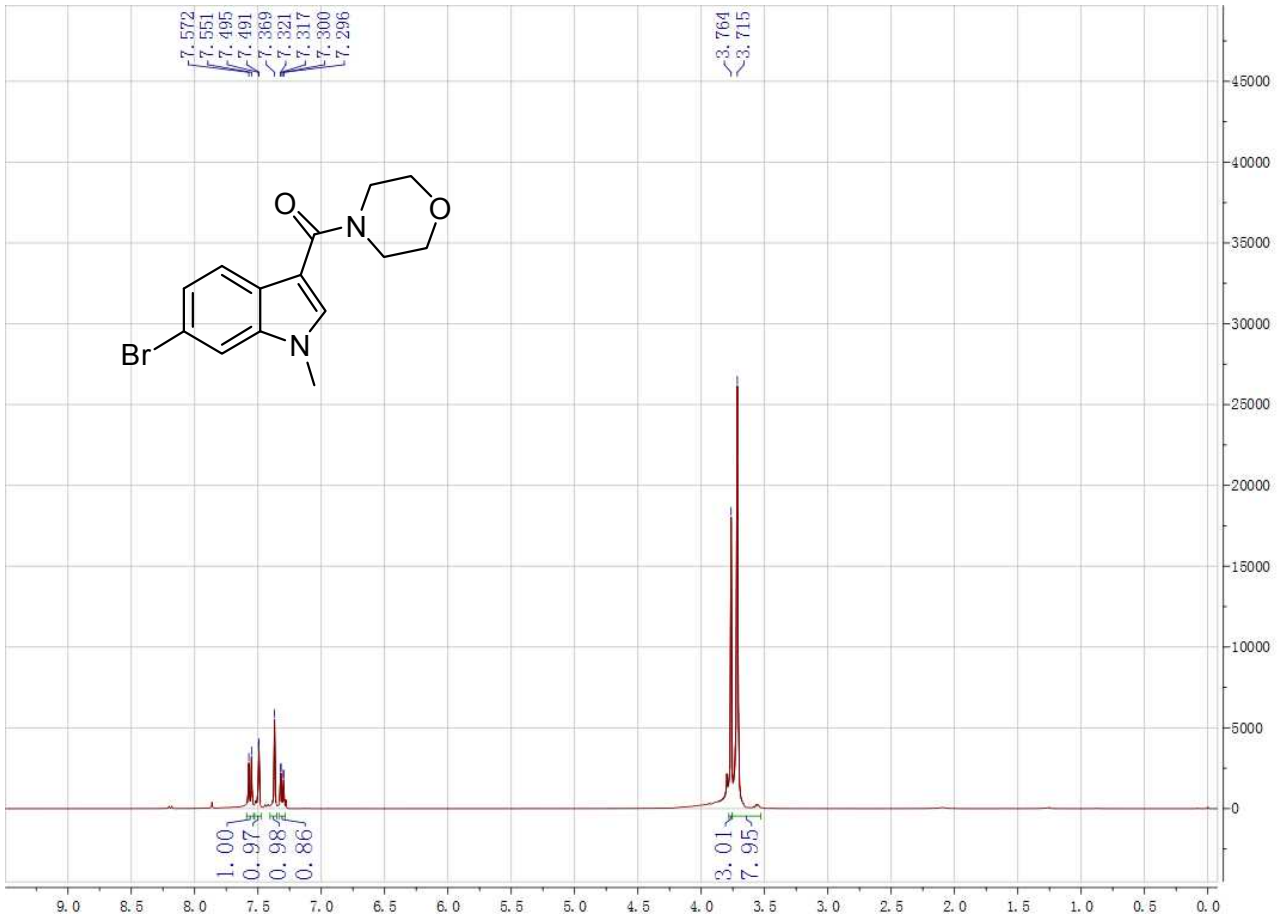
4h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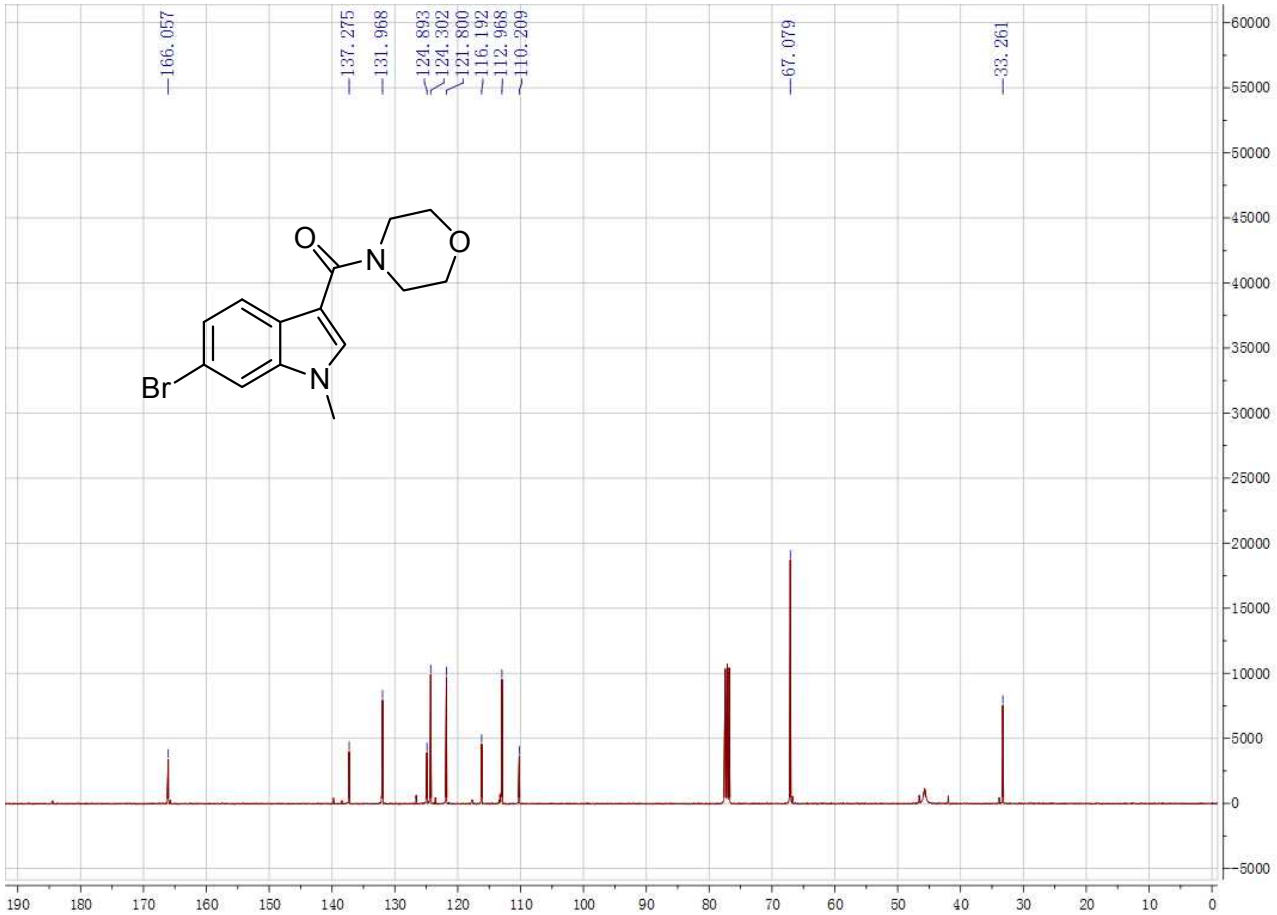
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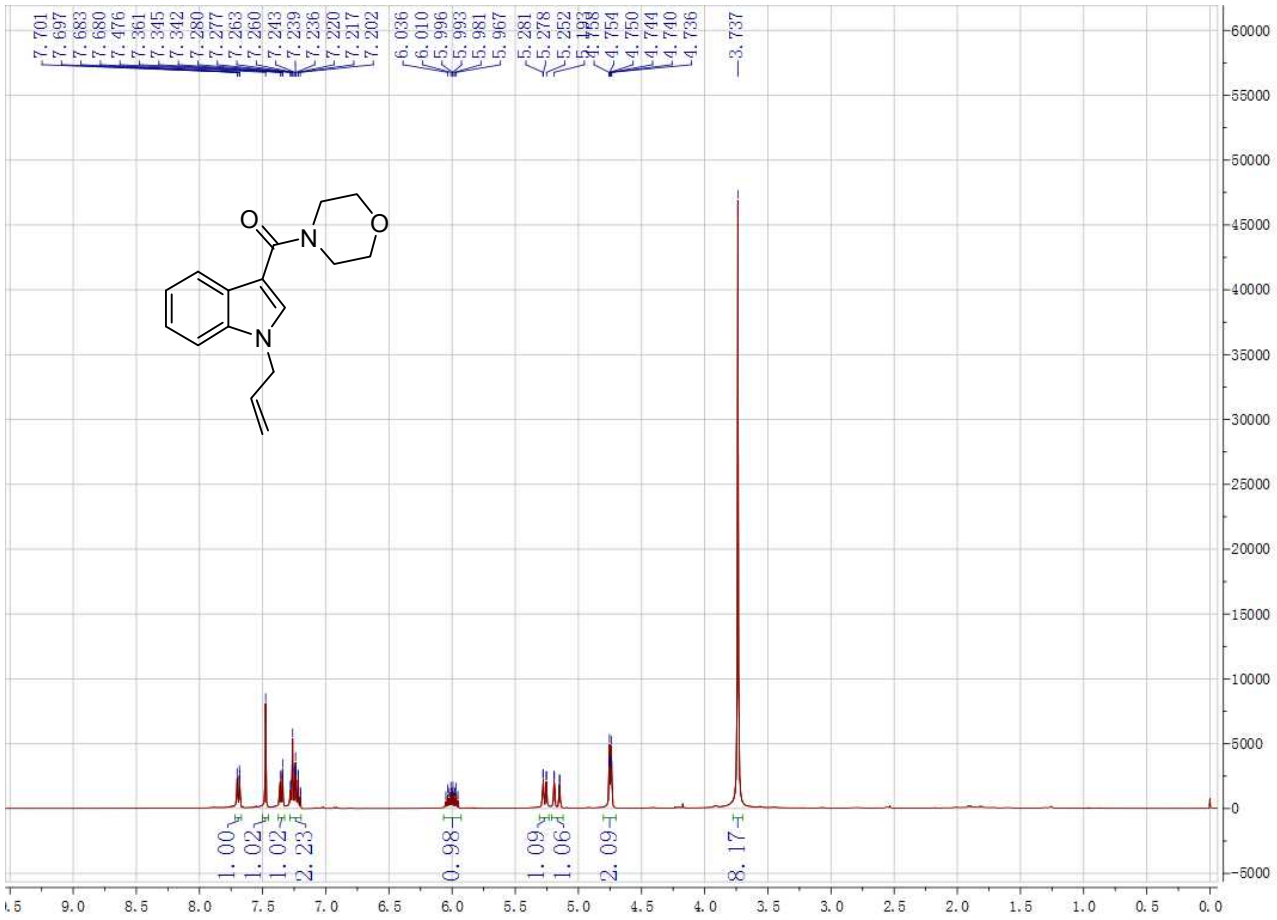
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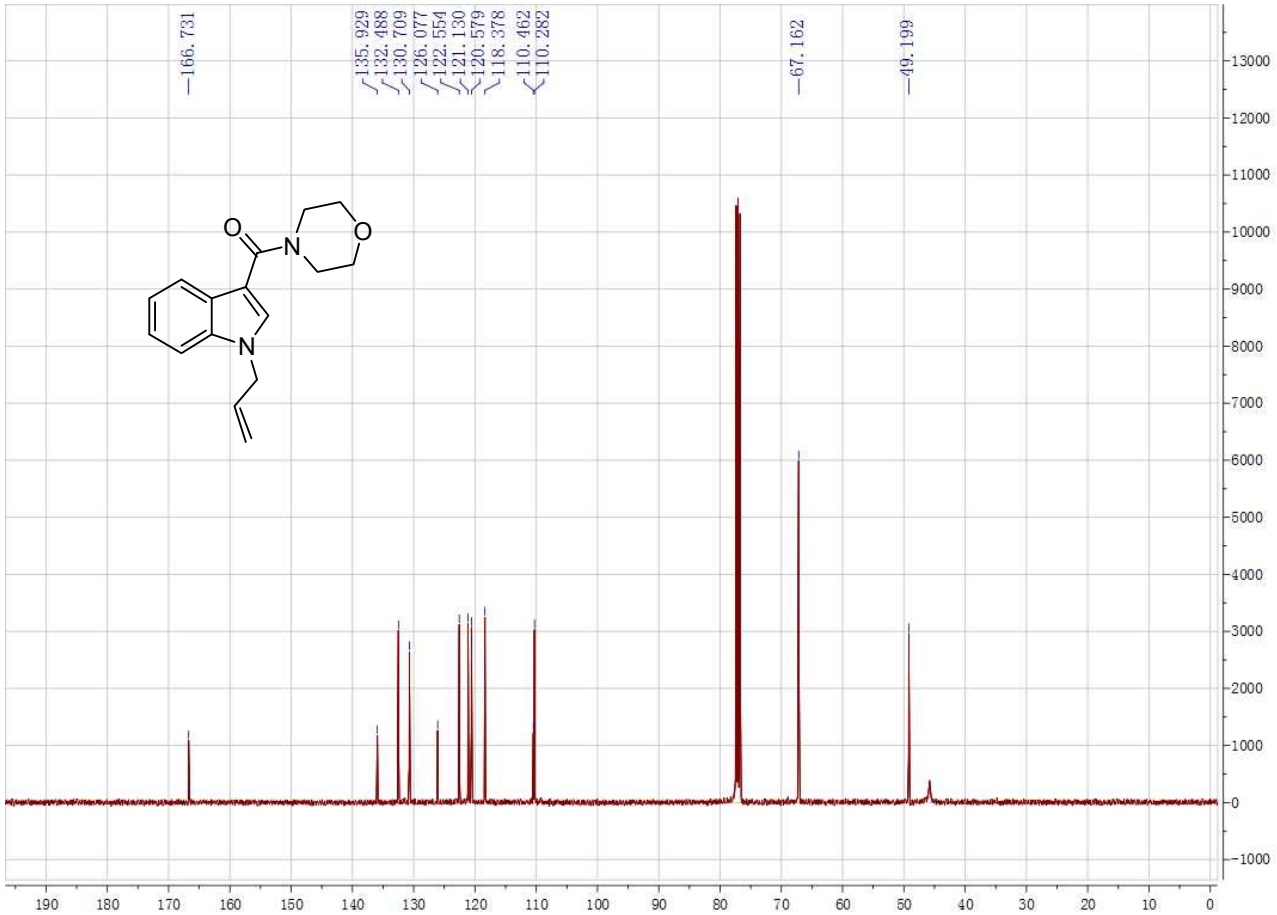
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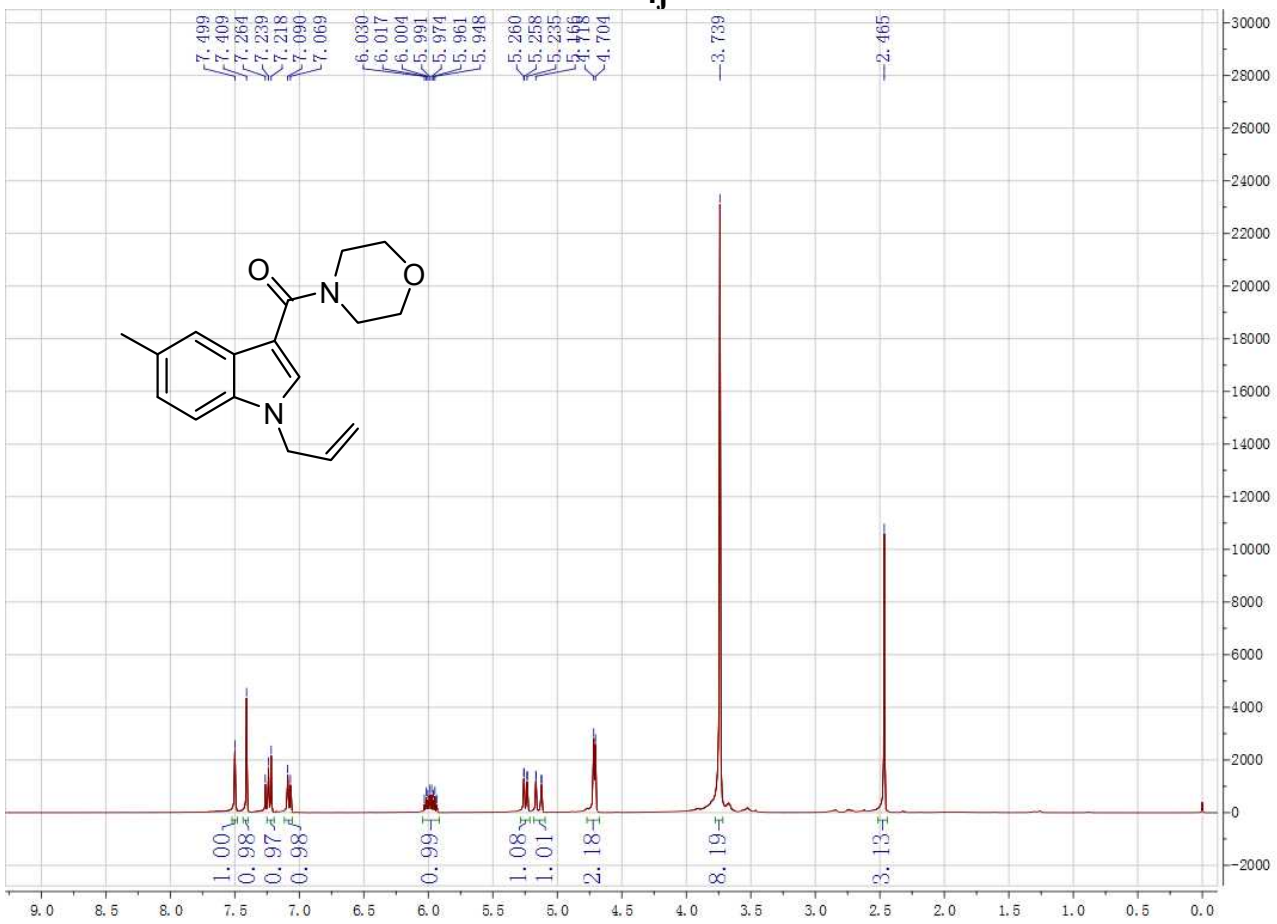
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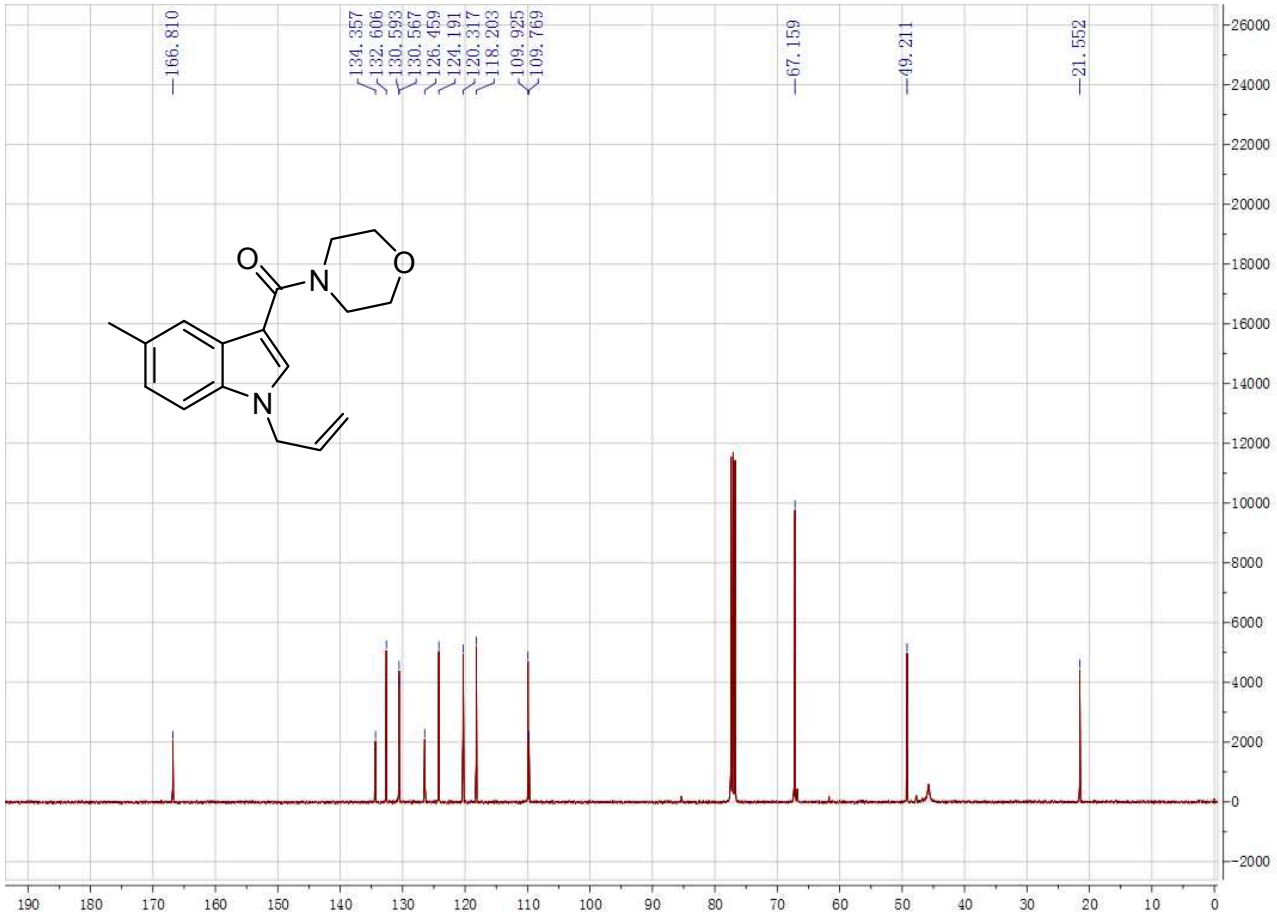
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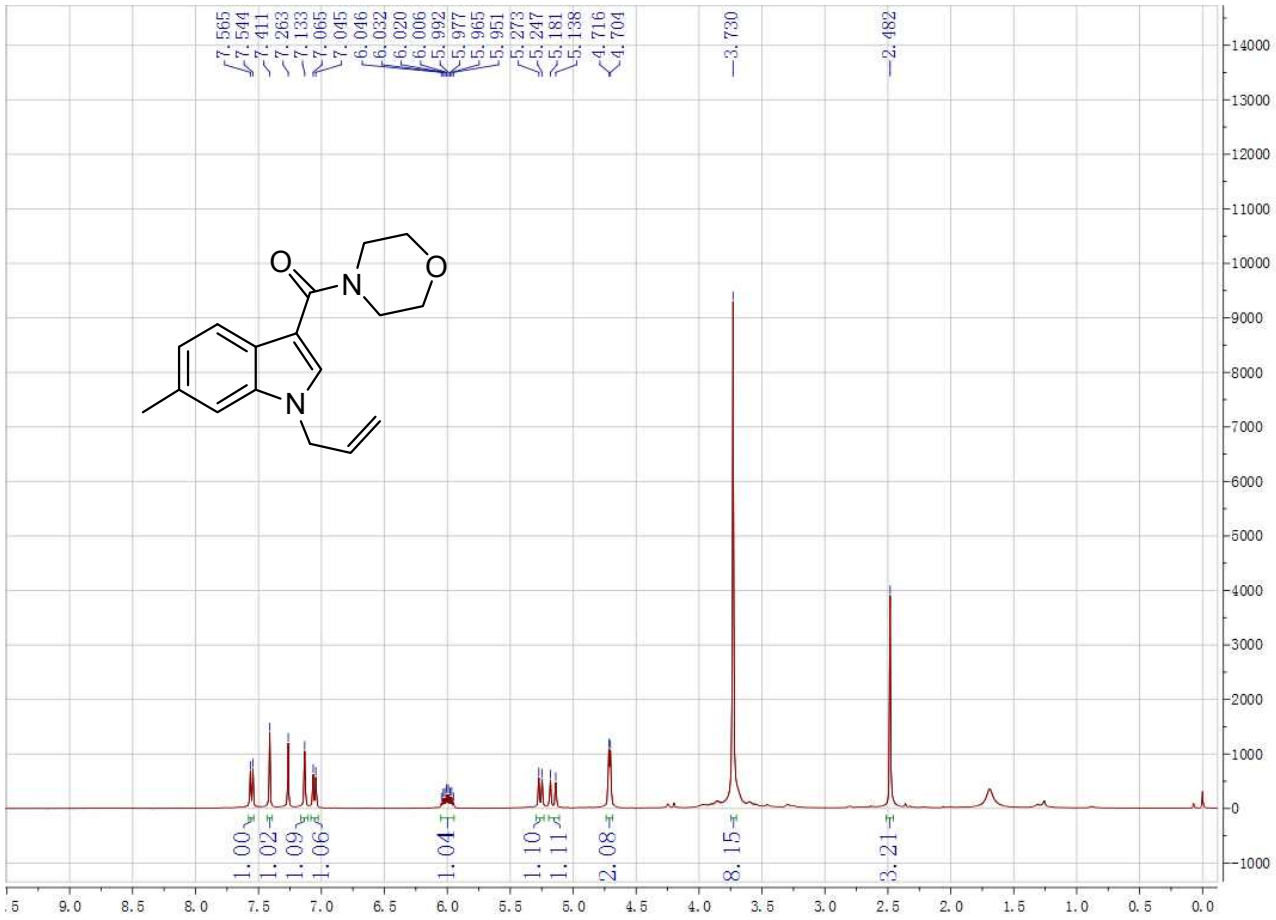
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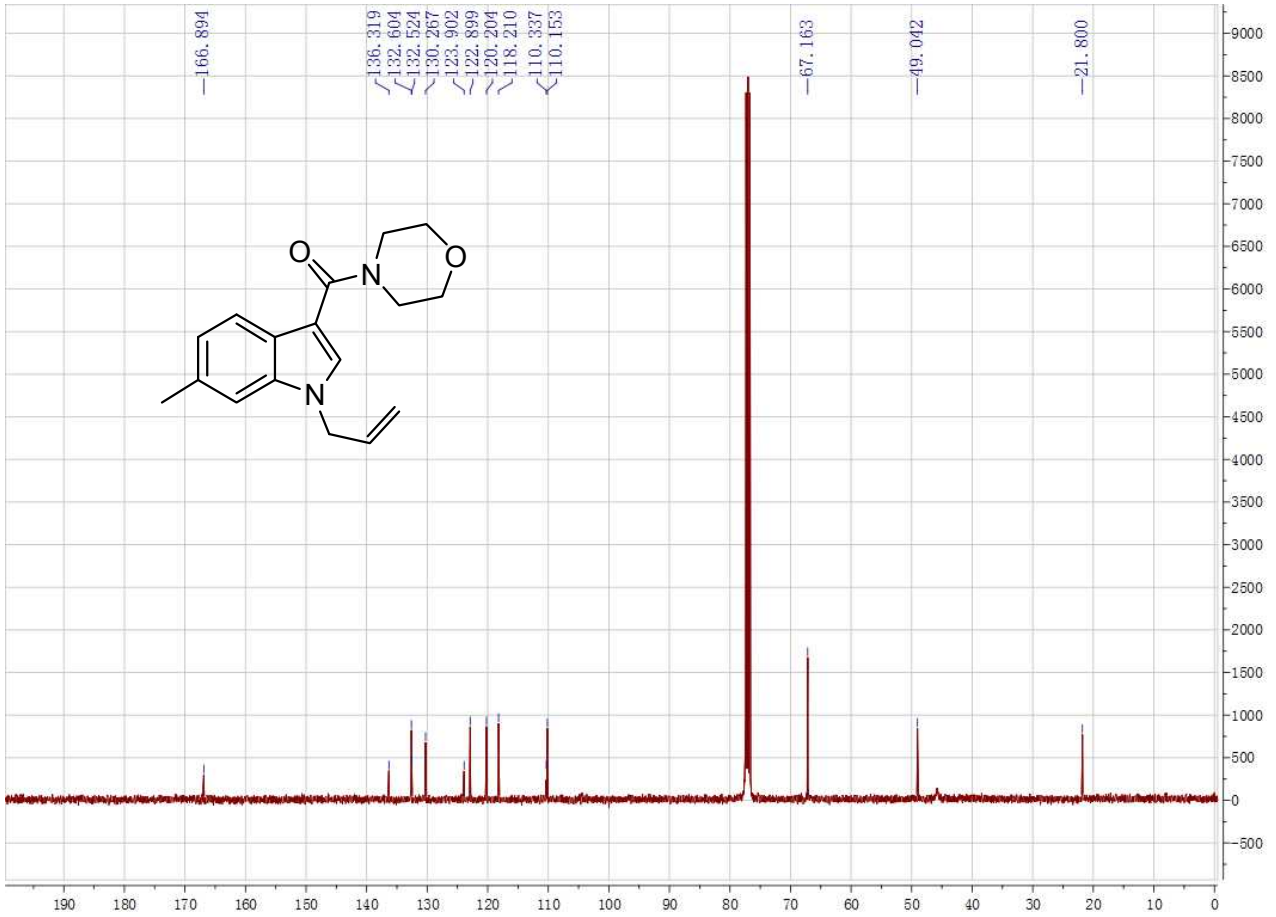
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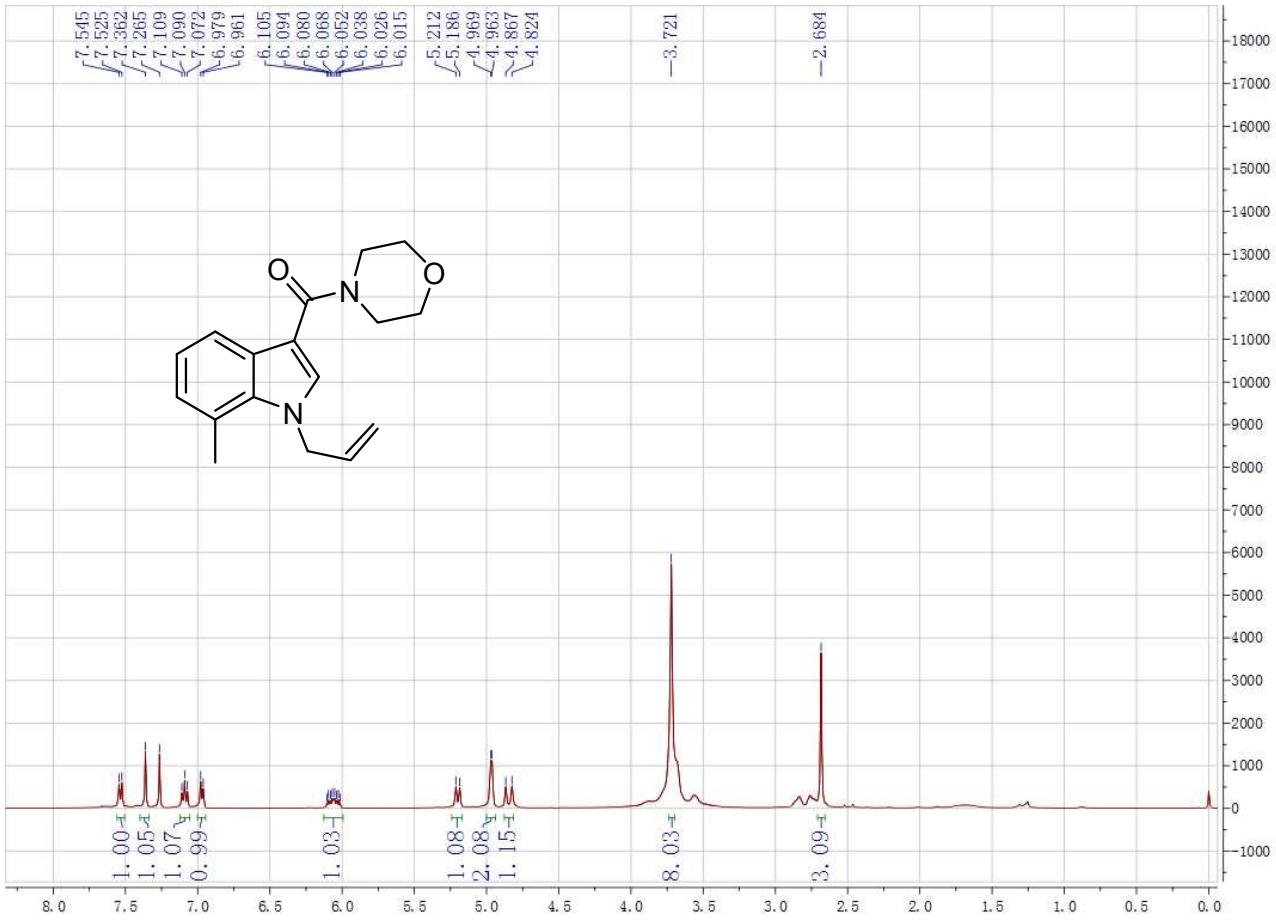
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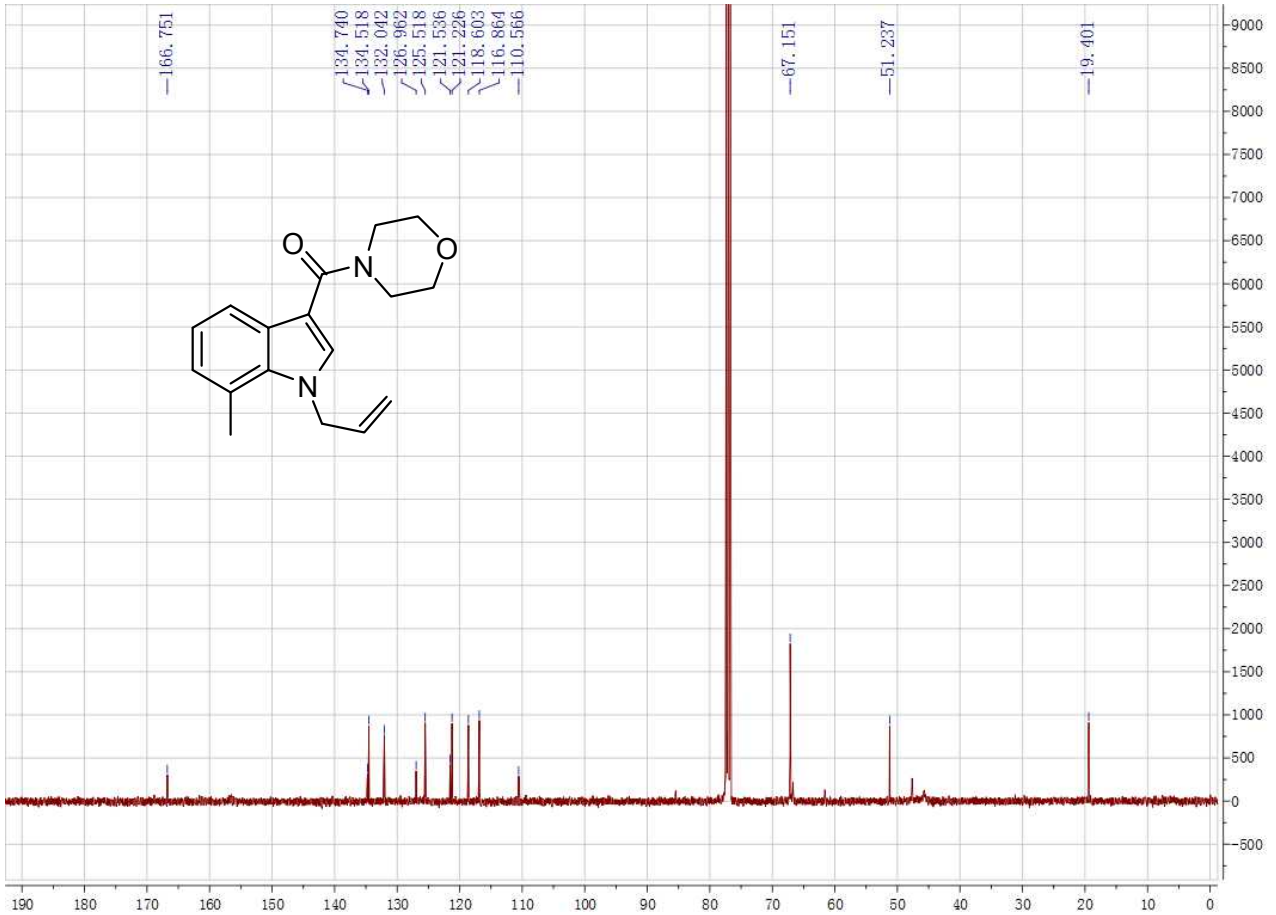
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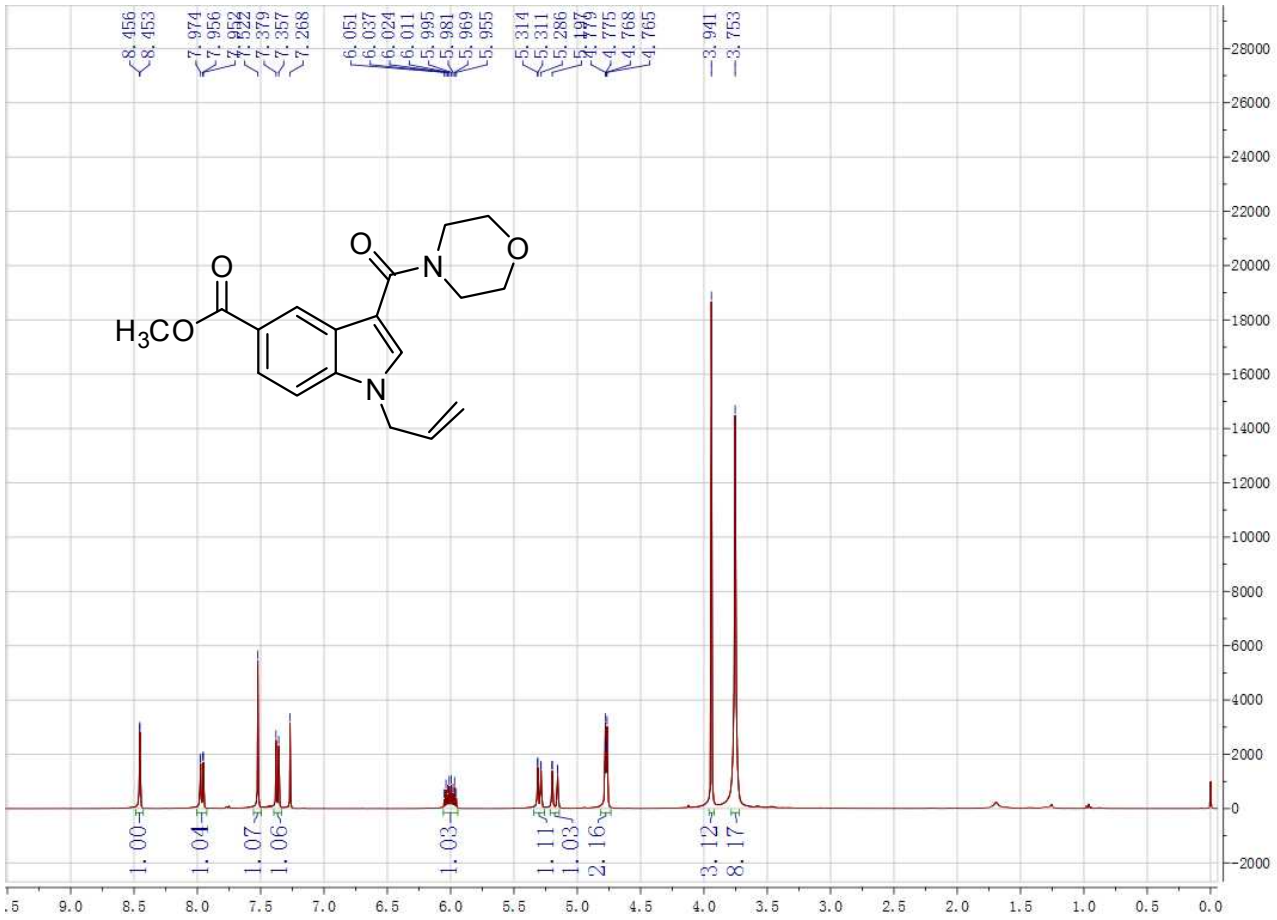
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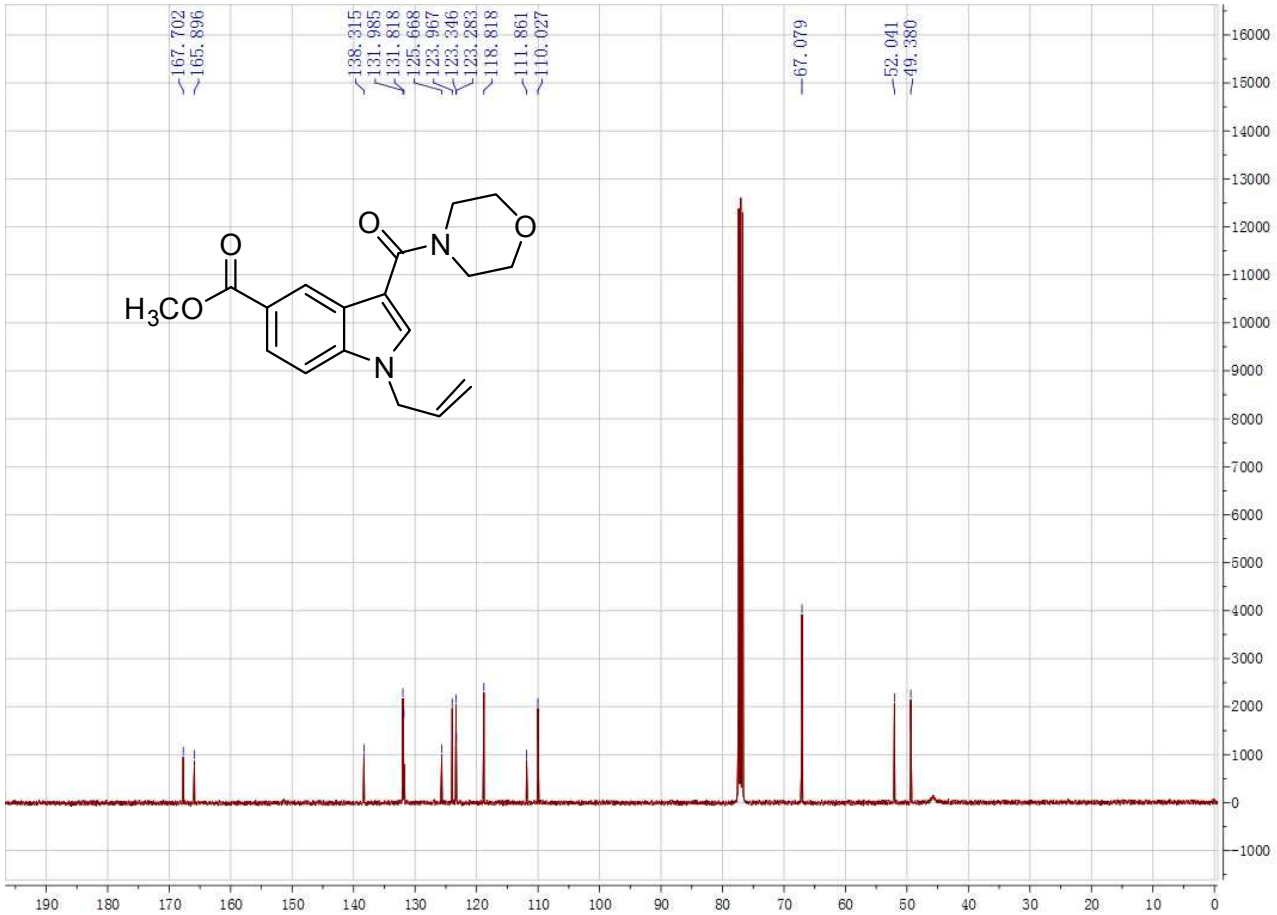
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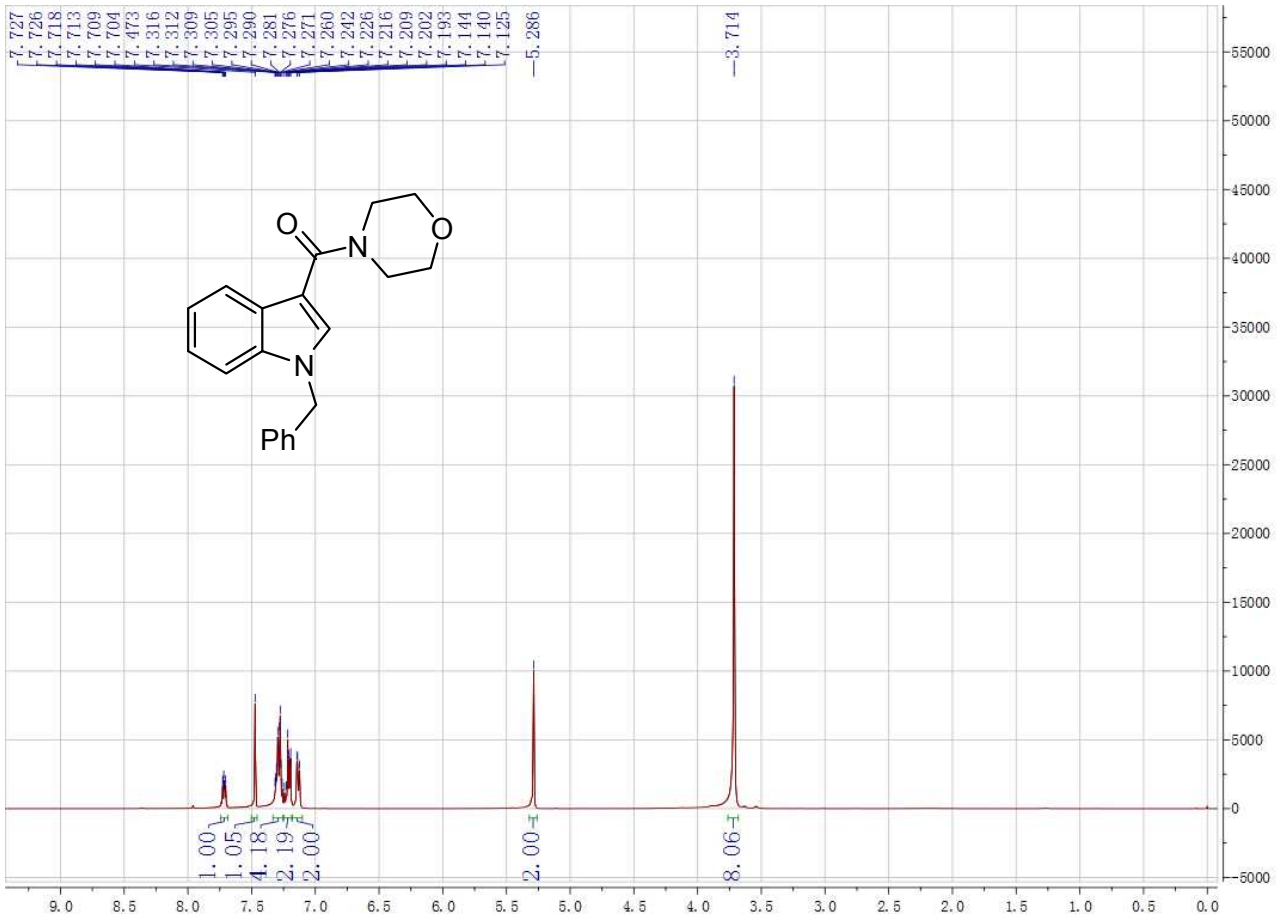
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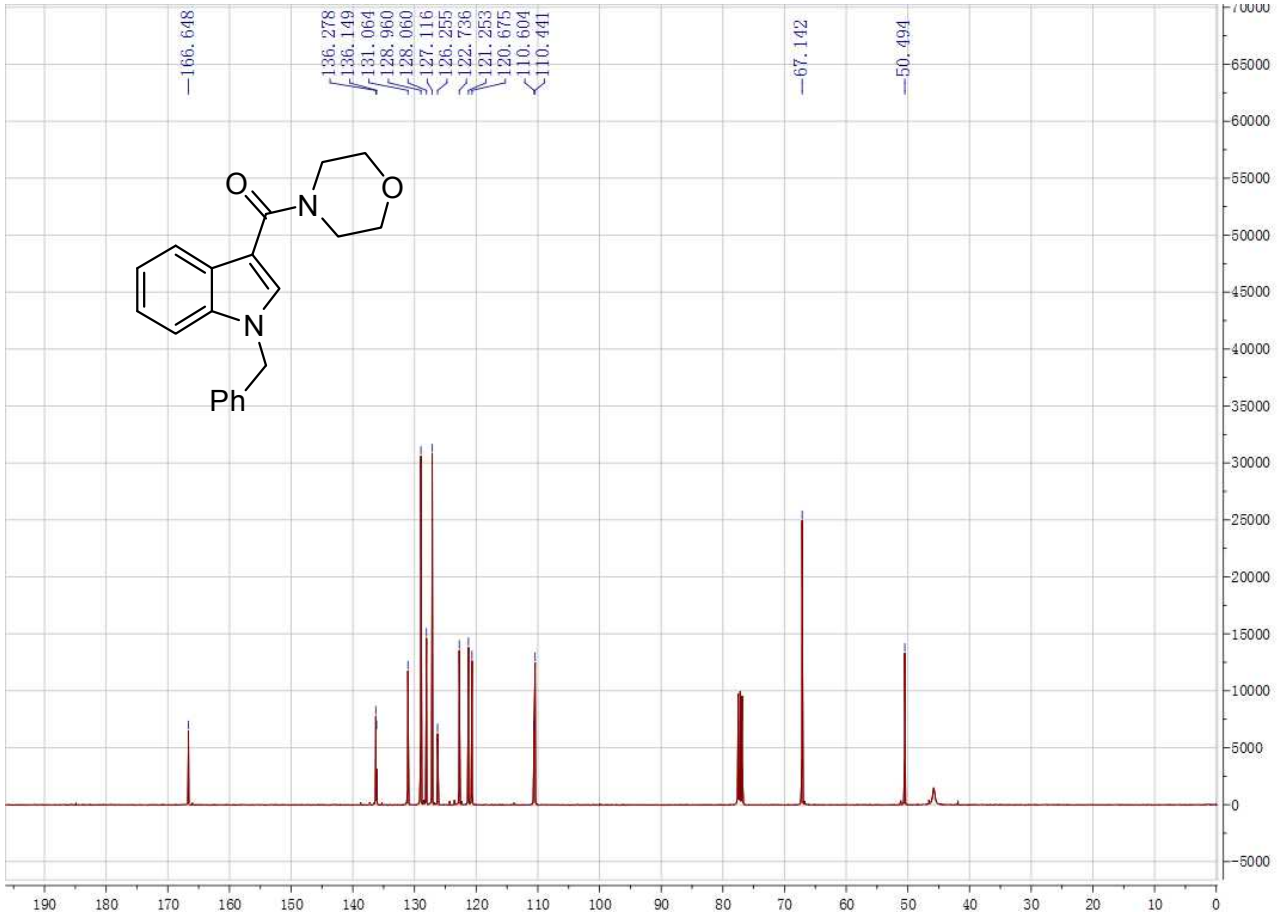
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O
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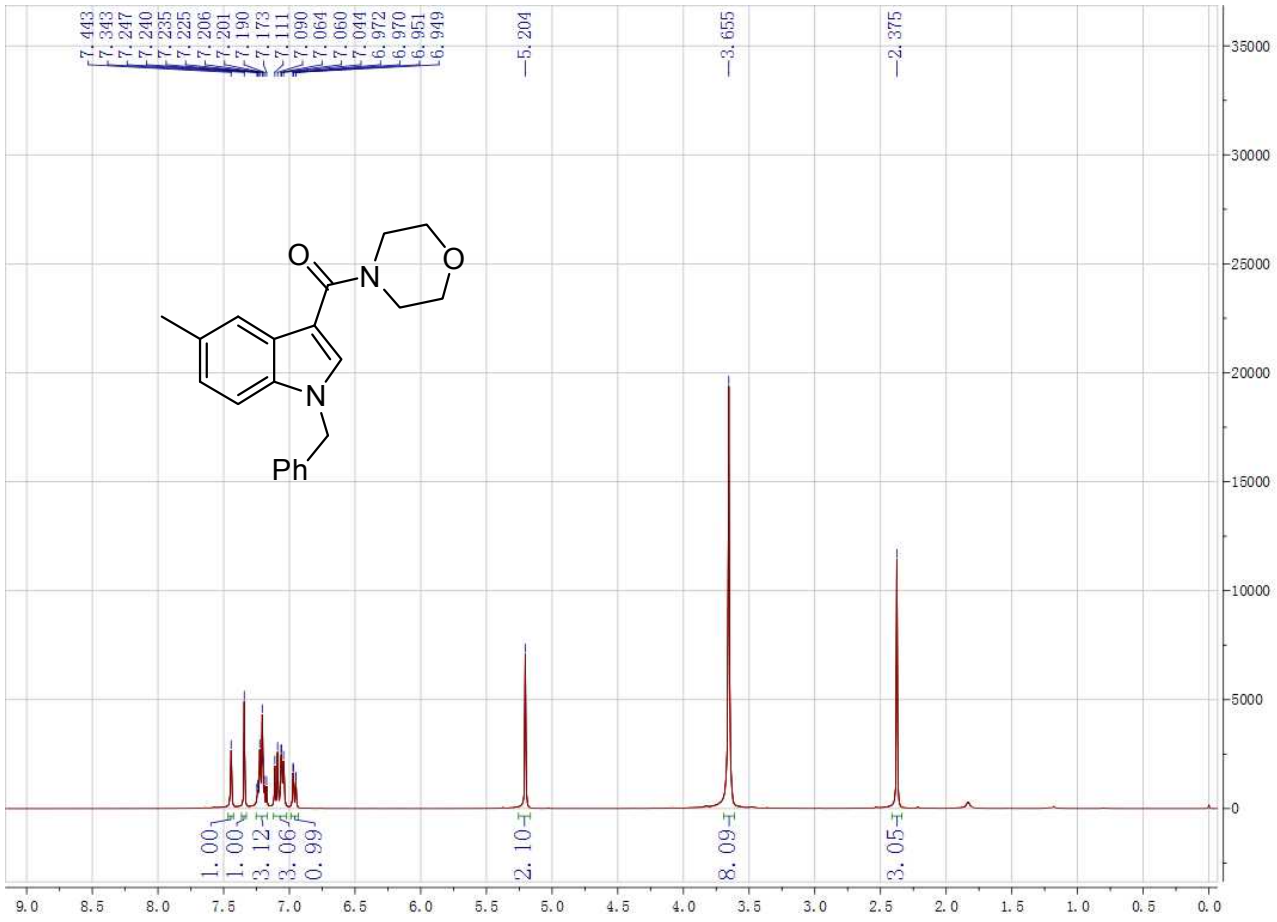
Ph

4o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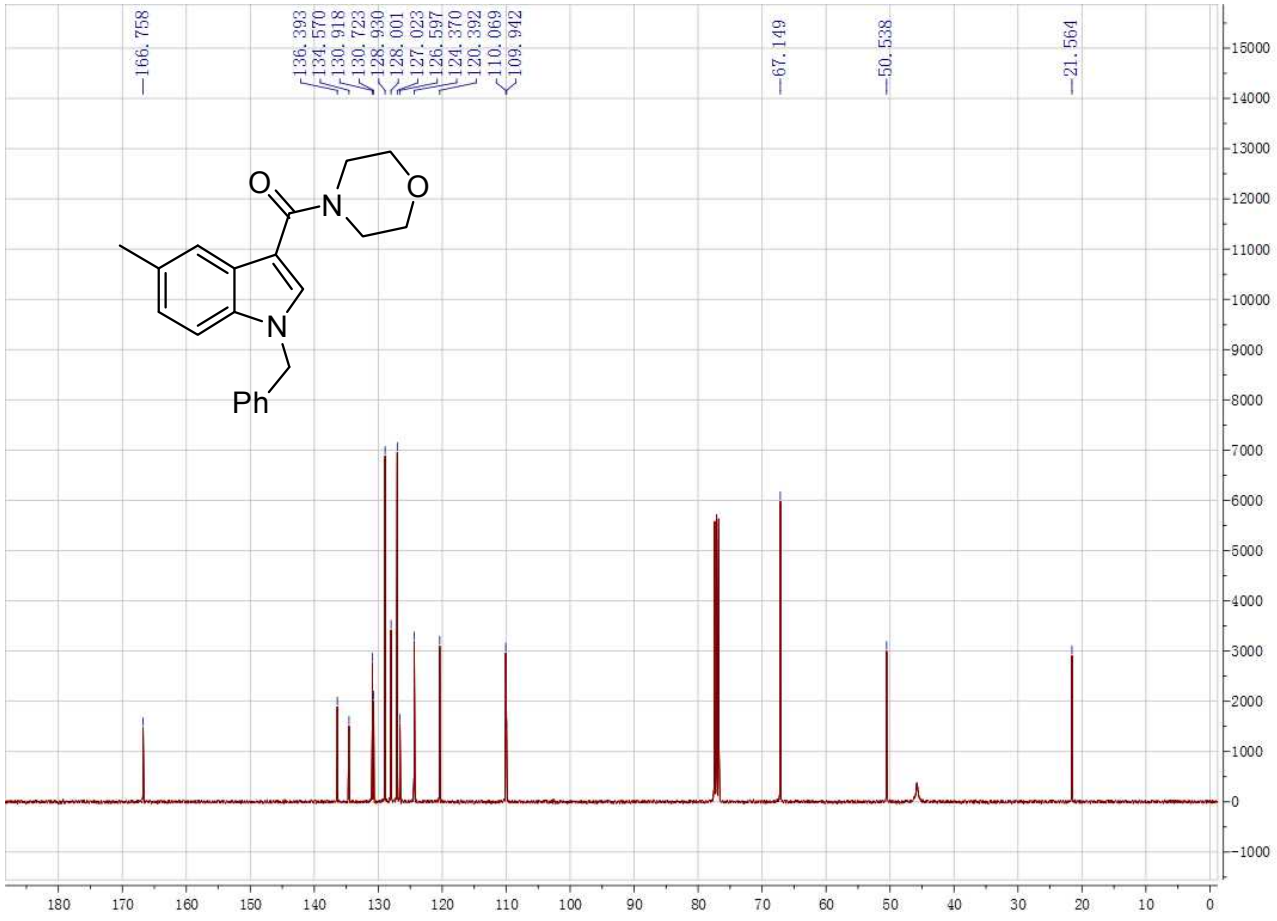
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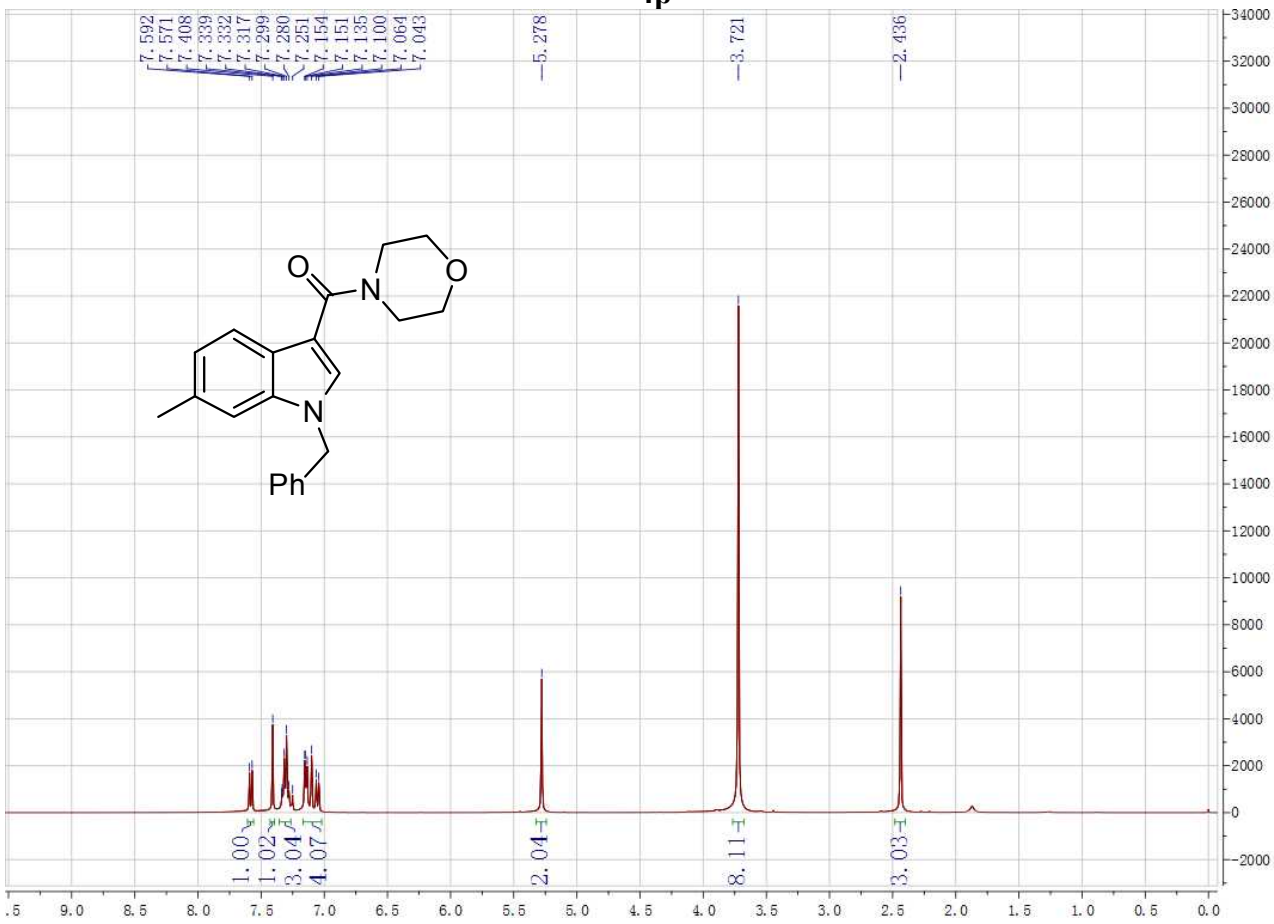
4p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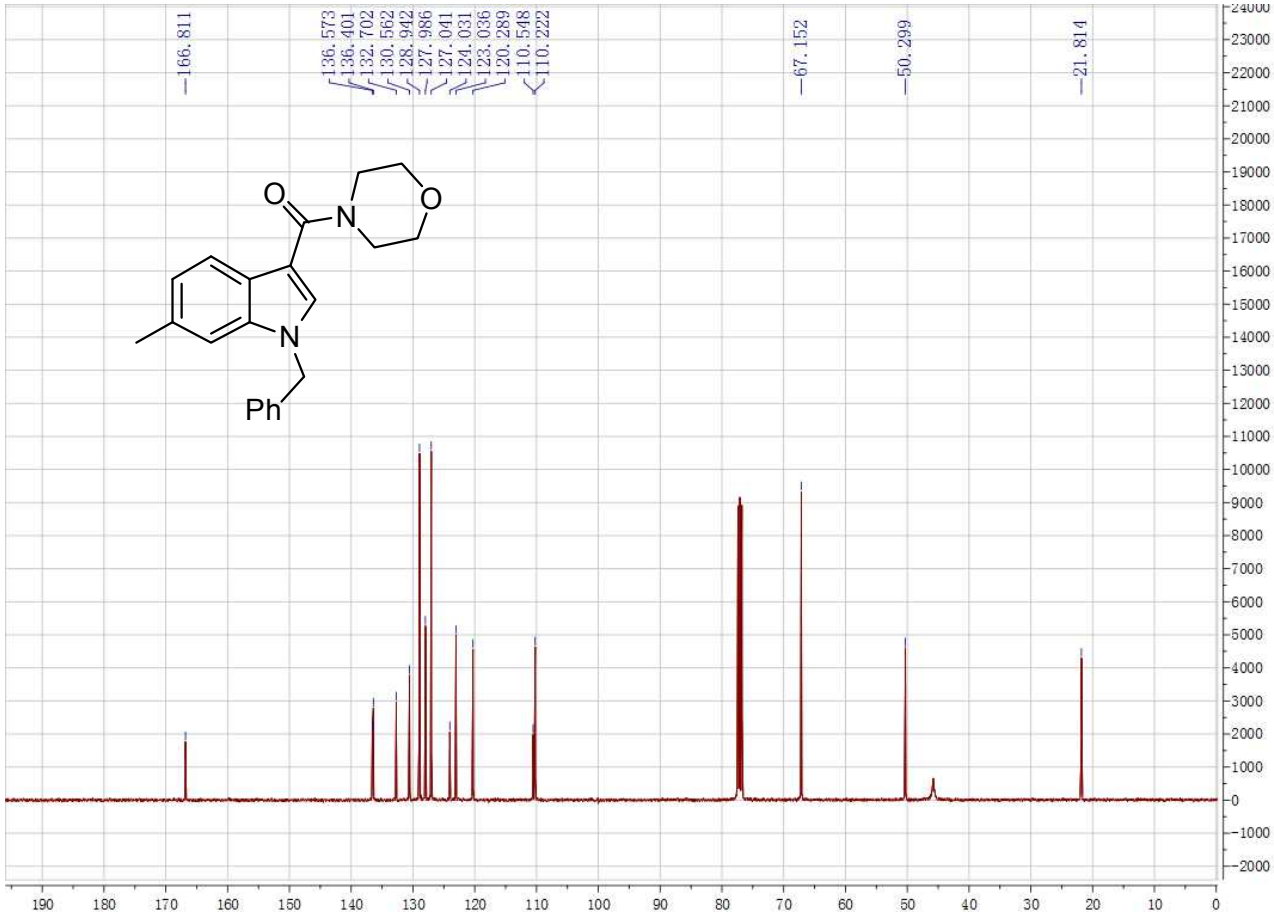
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Ph

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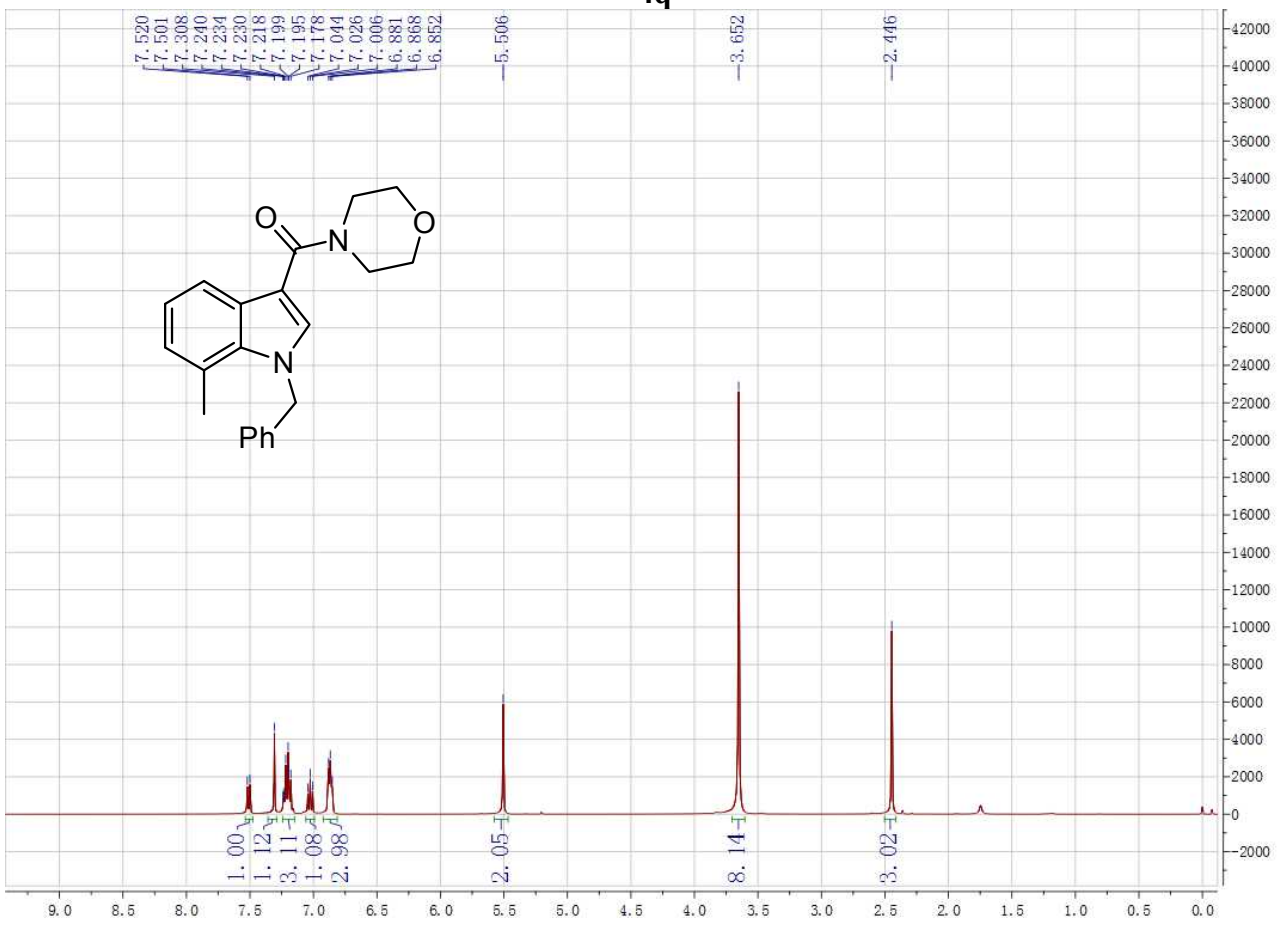
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7.006
6.881
6.868
6.852
5.506
3.652
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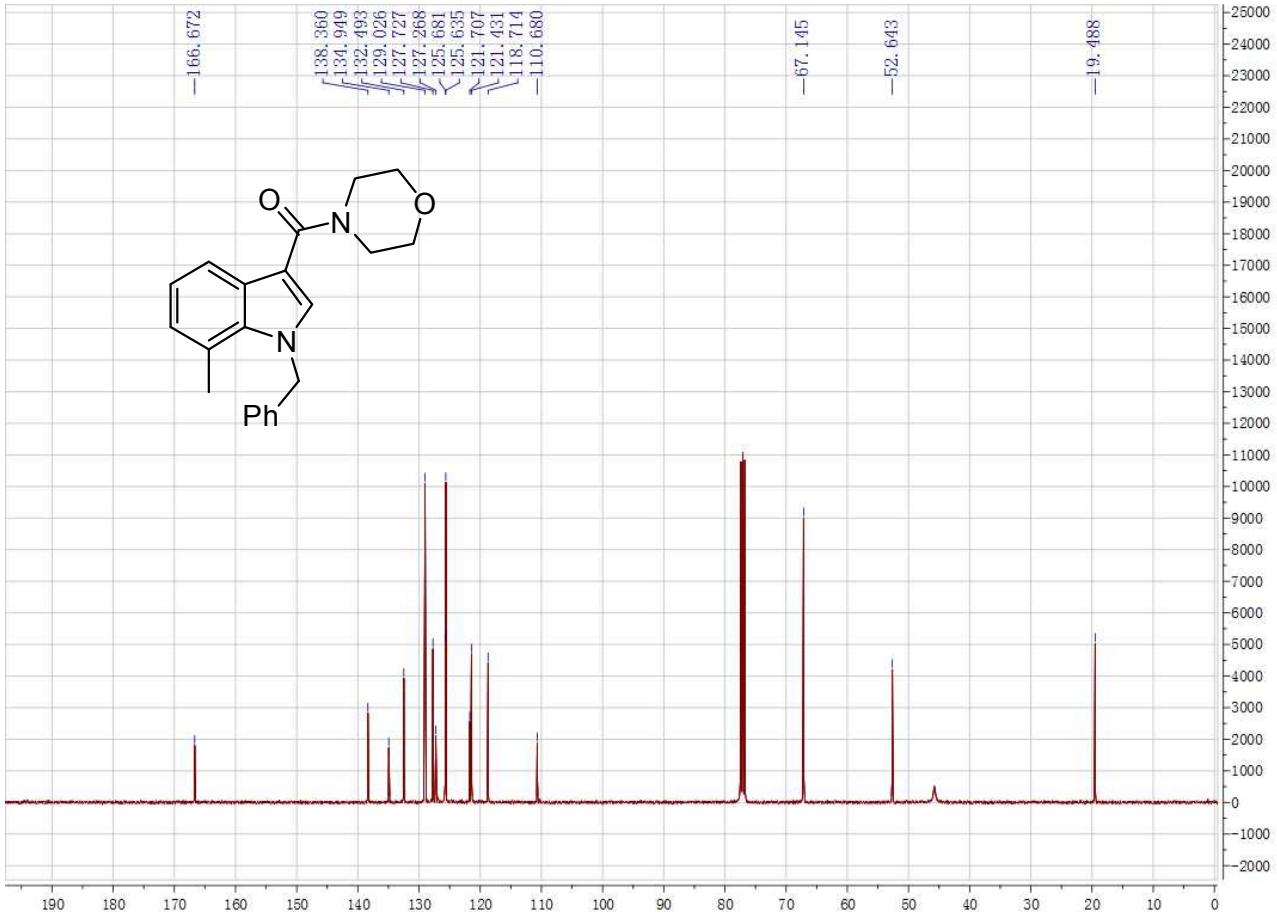
3.02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19.488
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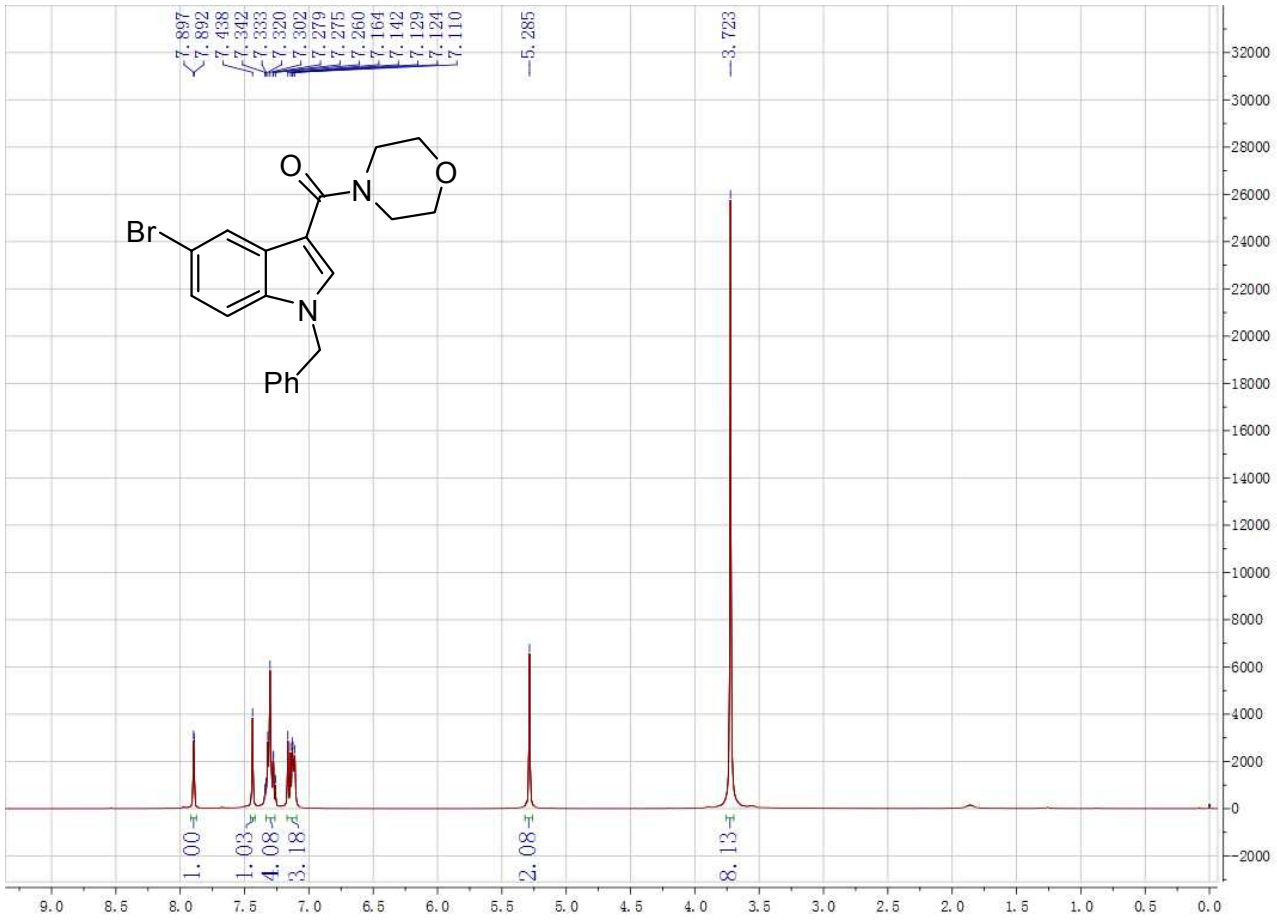
O
N
Ph

4r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7.129
7.124
7.110
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Ph
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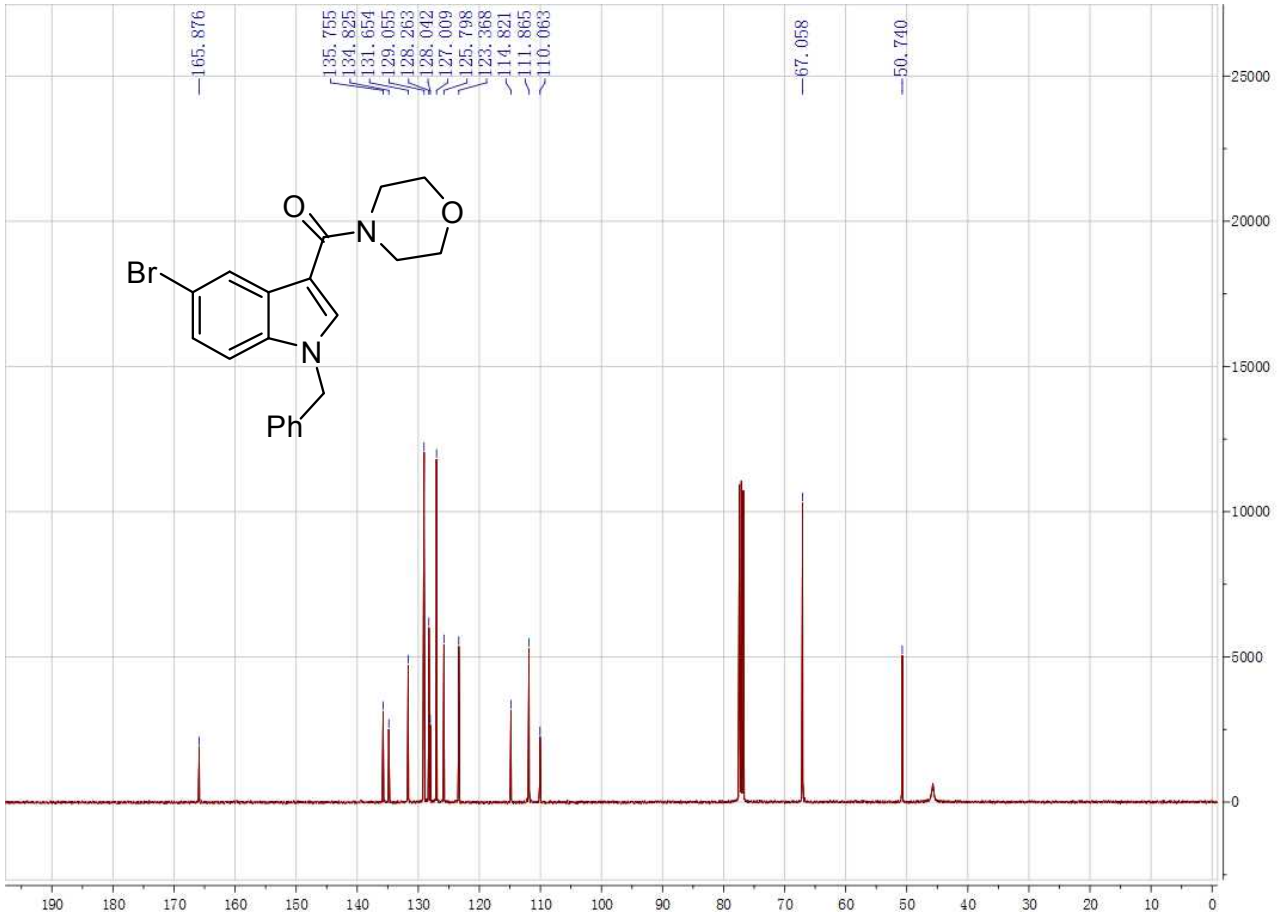
1.03
4.08
3.18
2.08
8.13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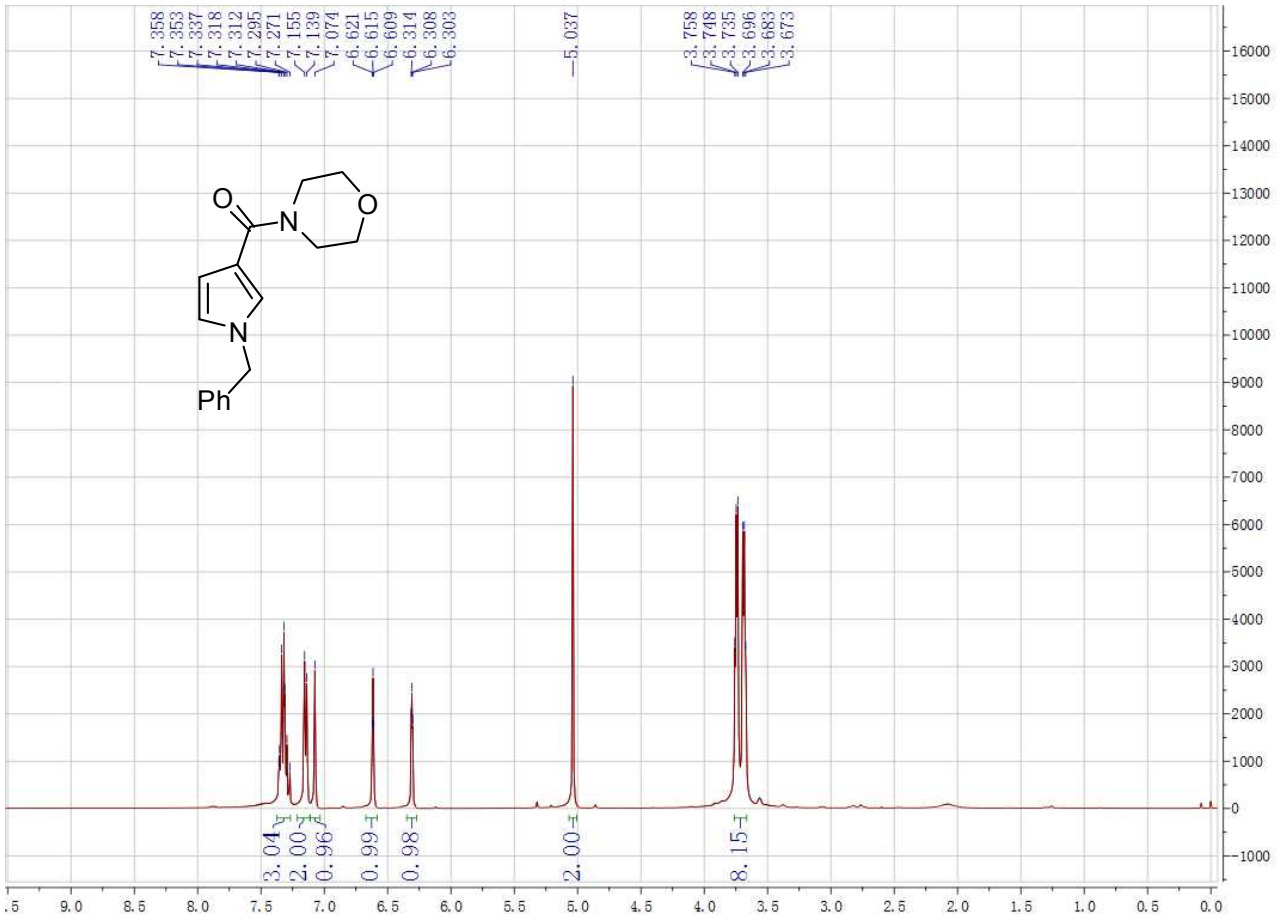
O
Br
N
Ph

4s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3.735
3.696
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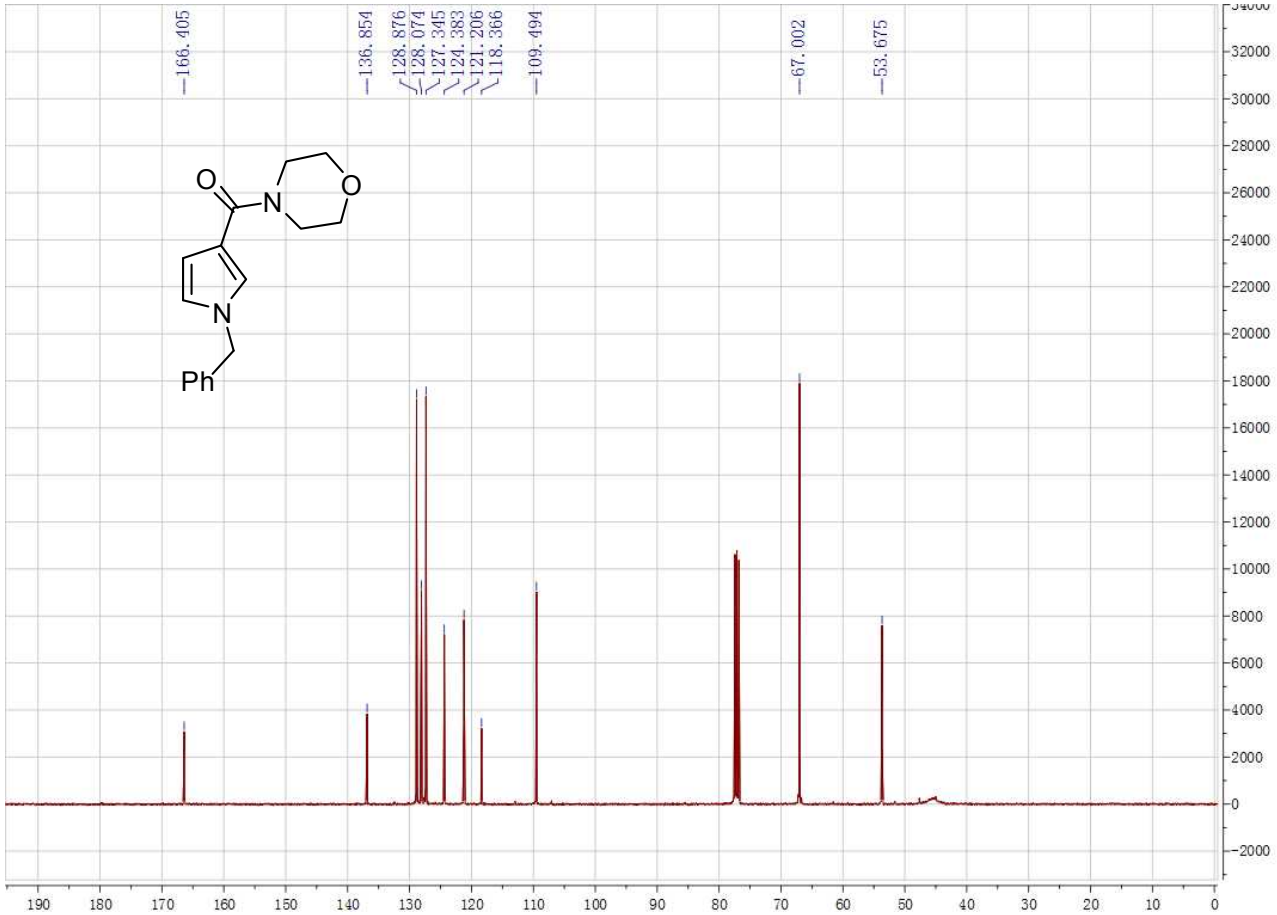
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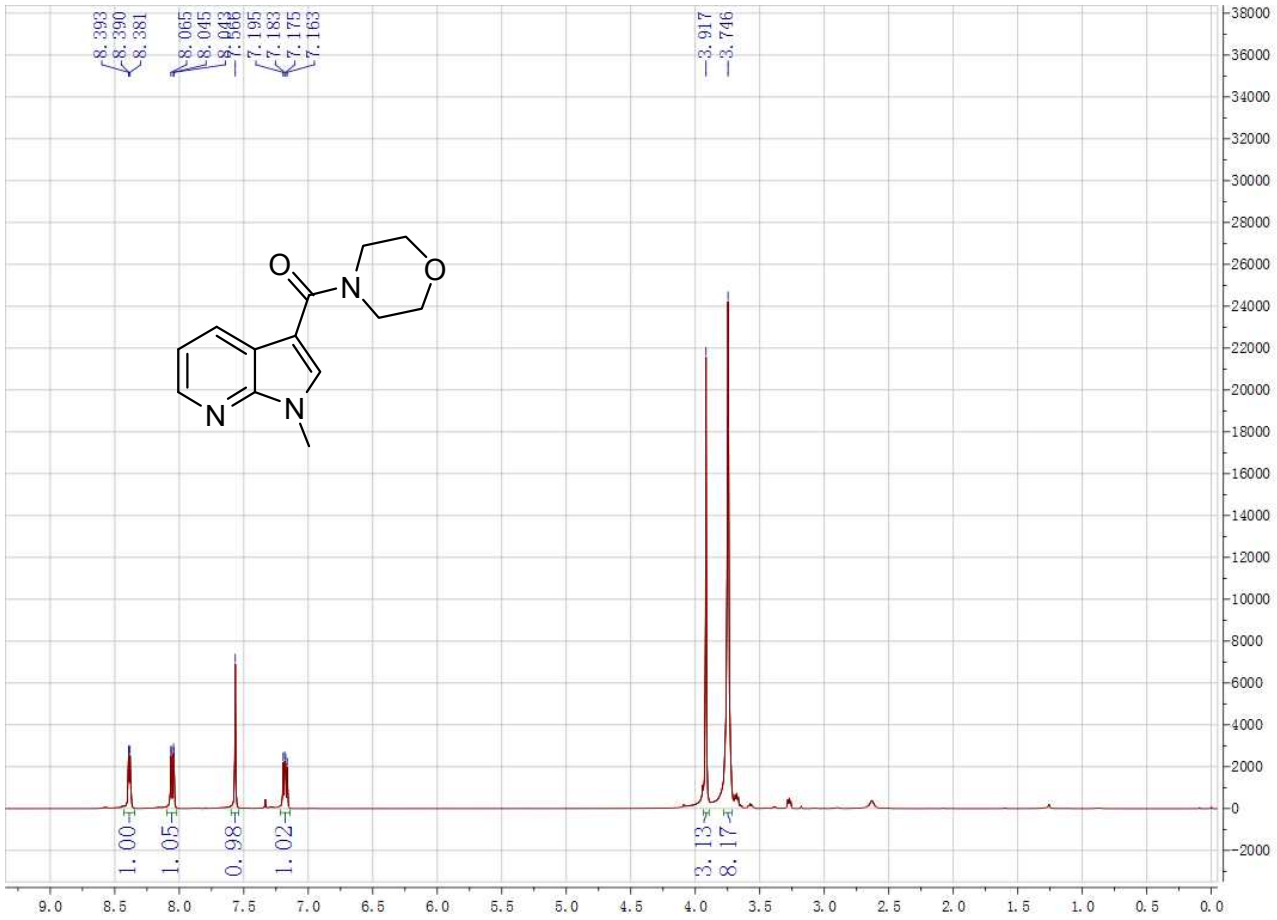
Ph

4t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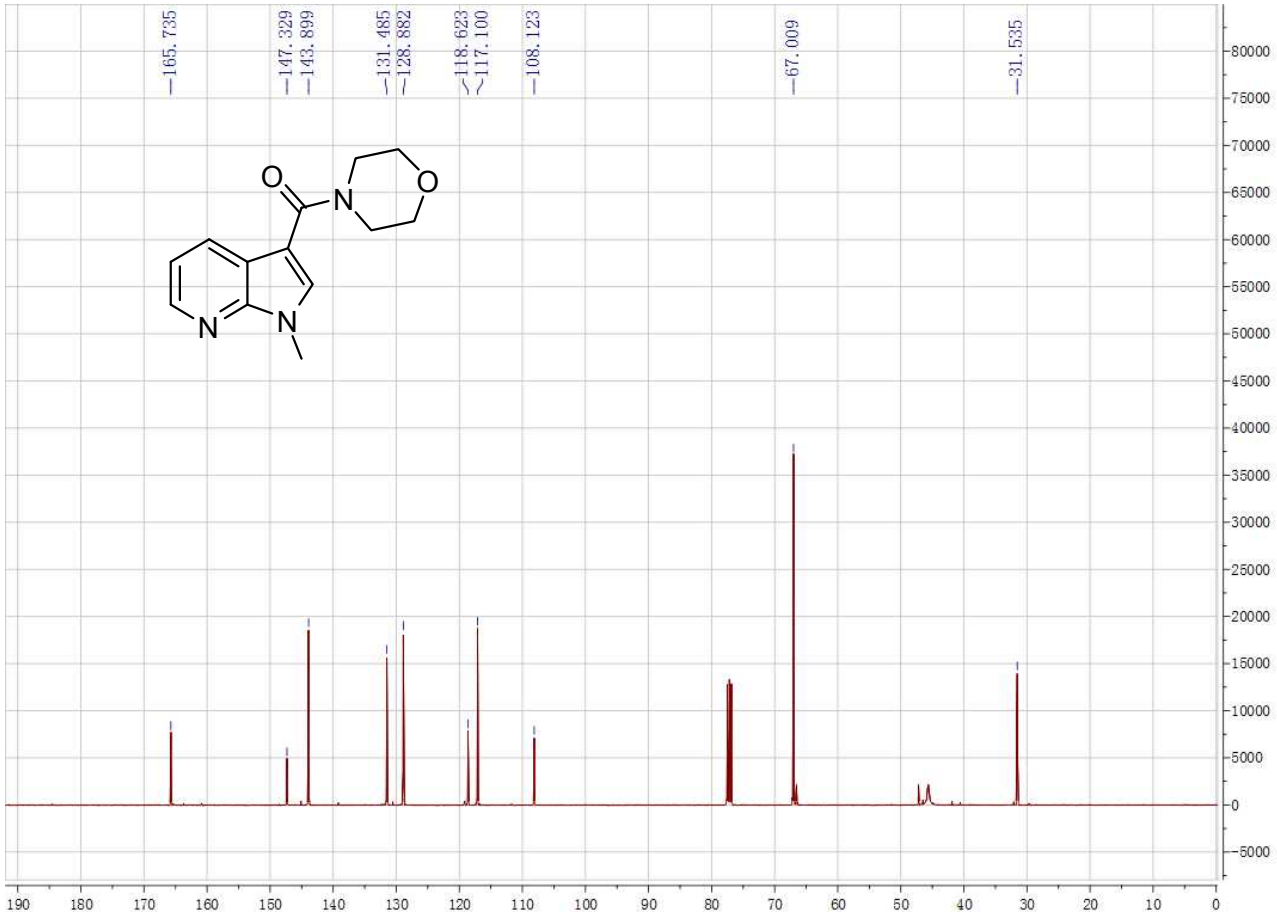
8.17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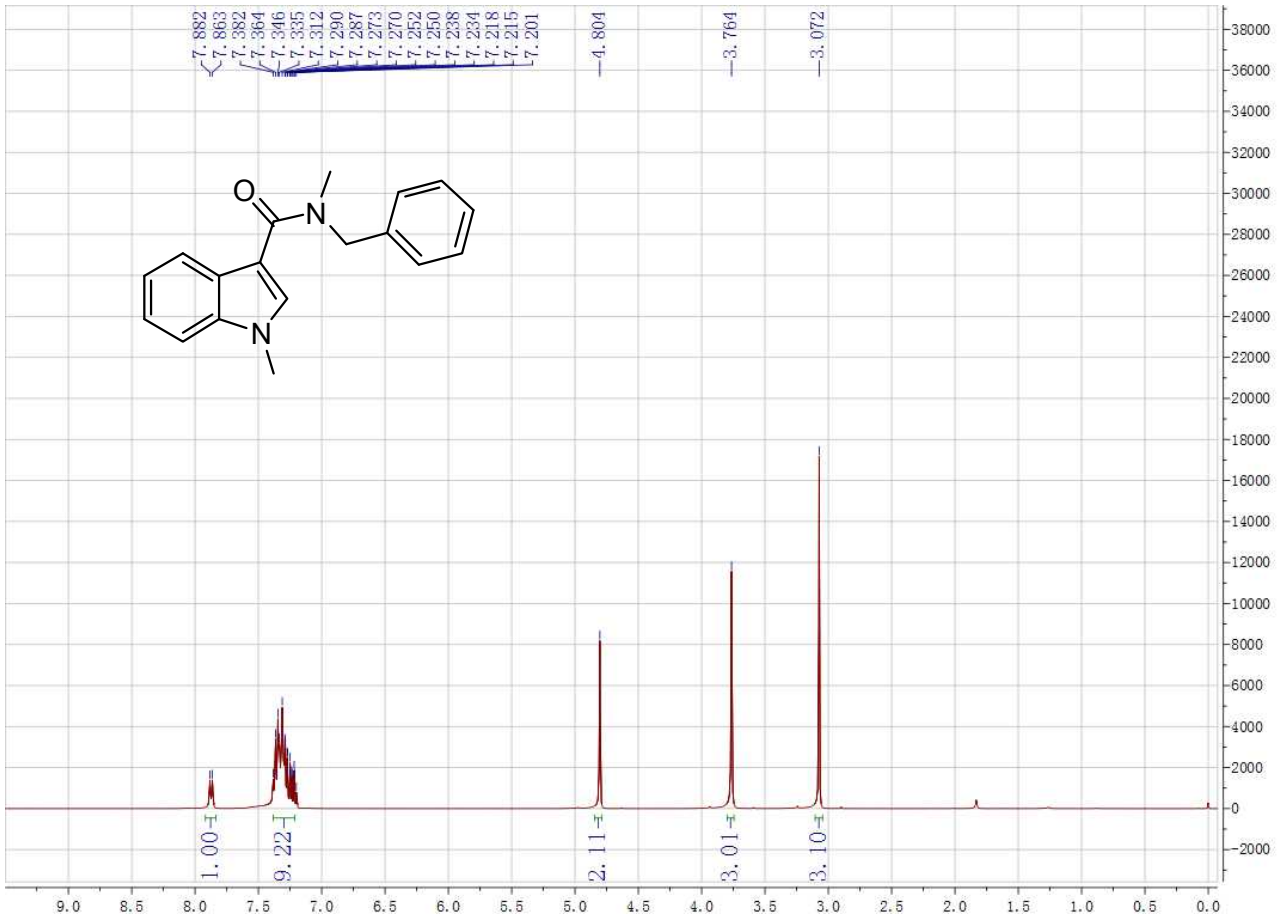
4u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7.250
7.238
7.234
7.218
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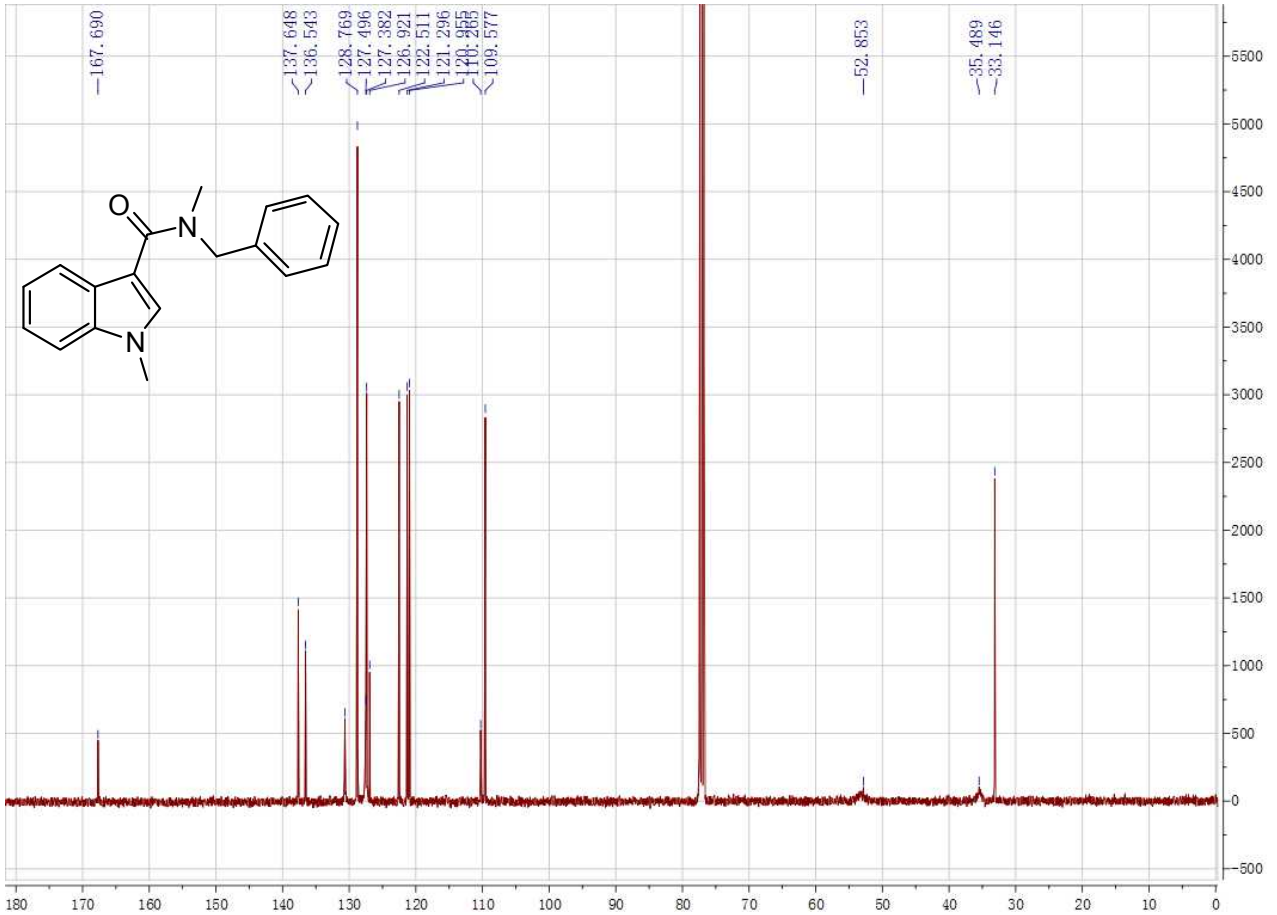
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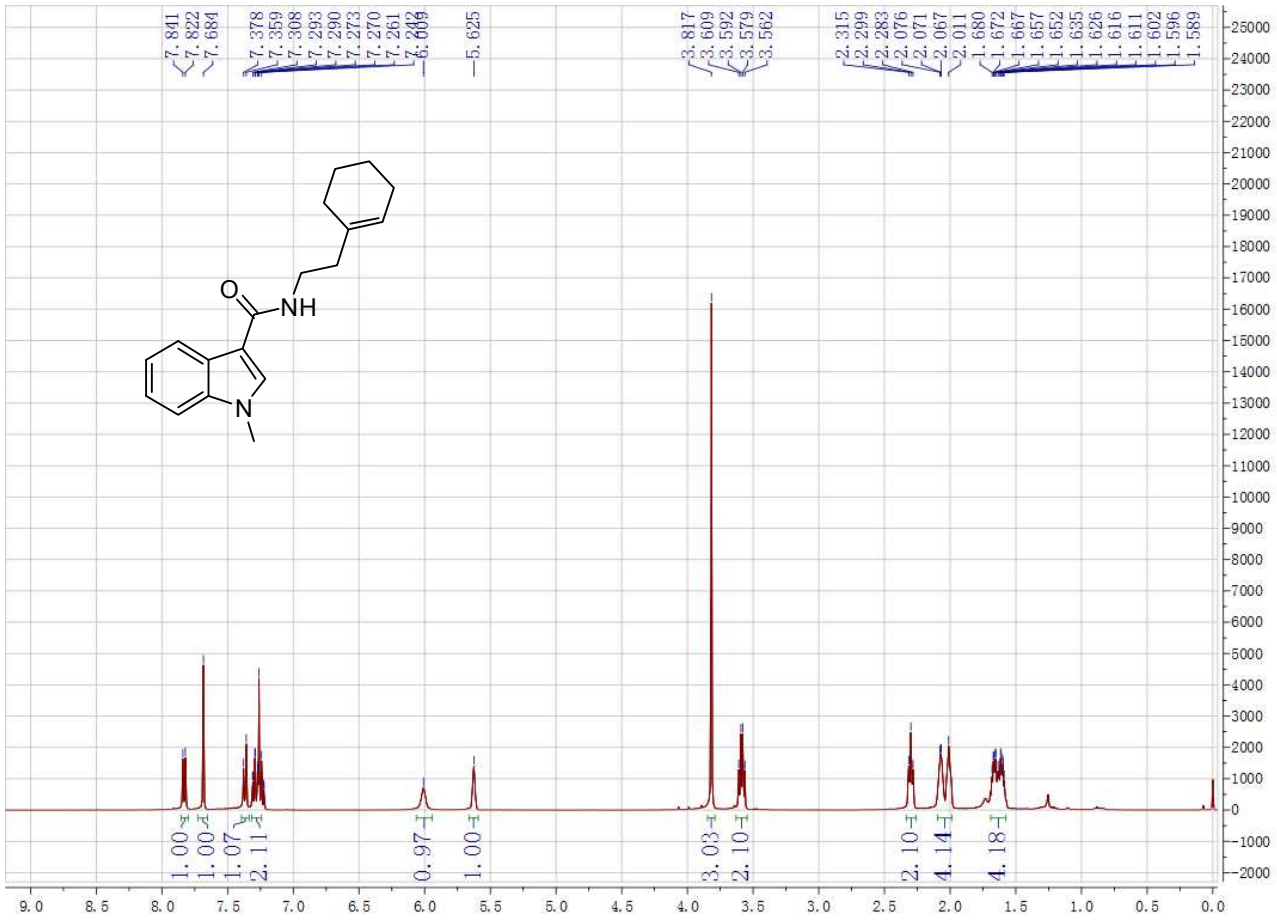
N

4v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3.609
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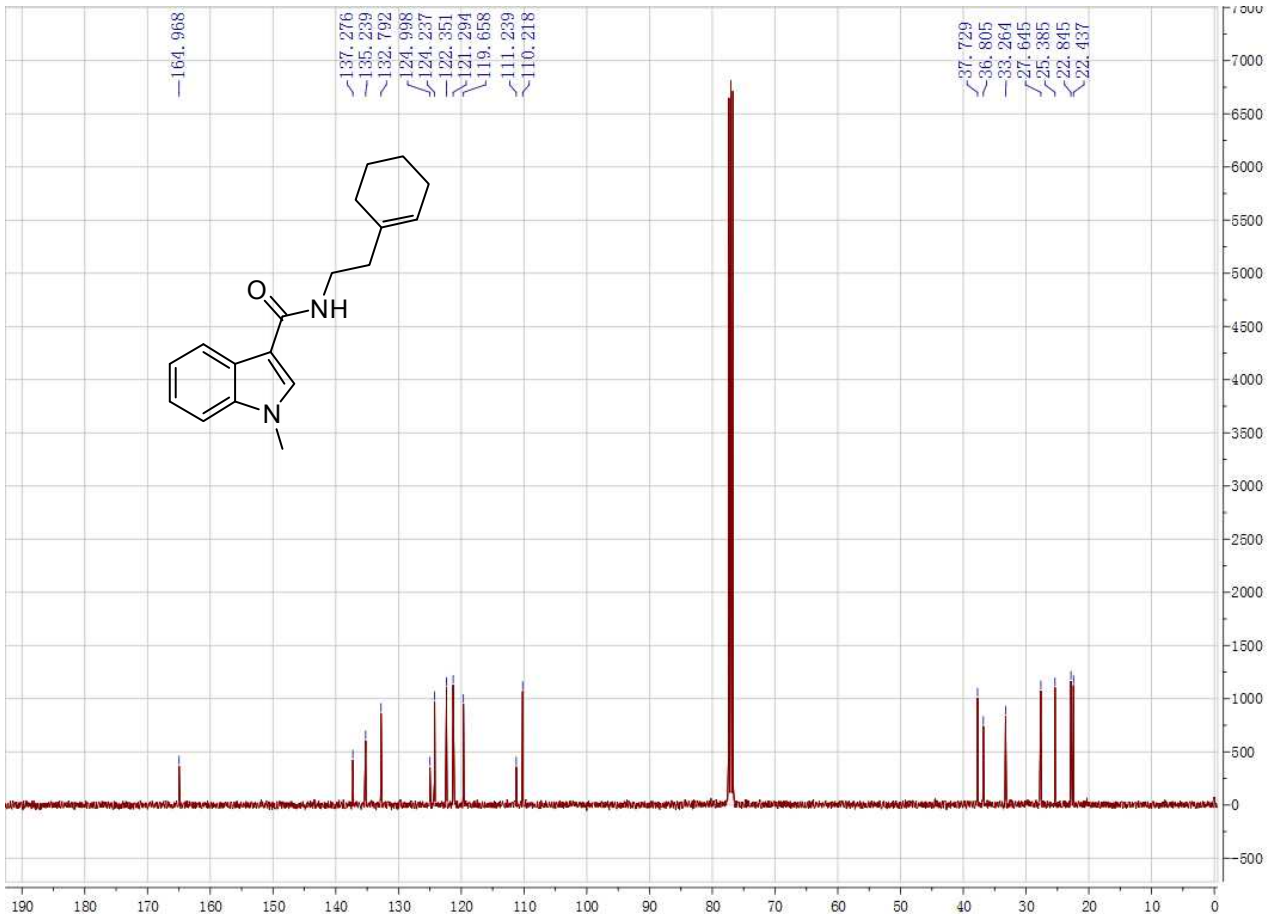
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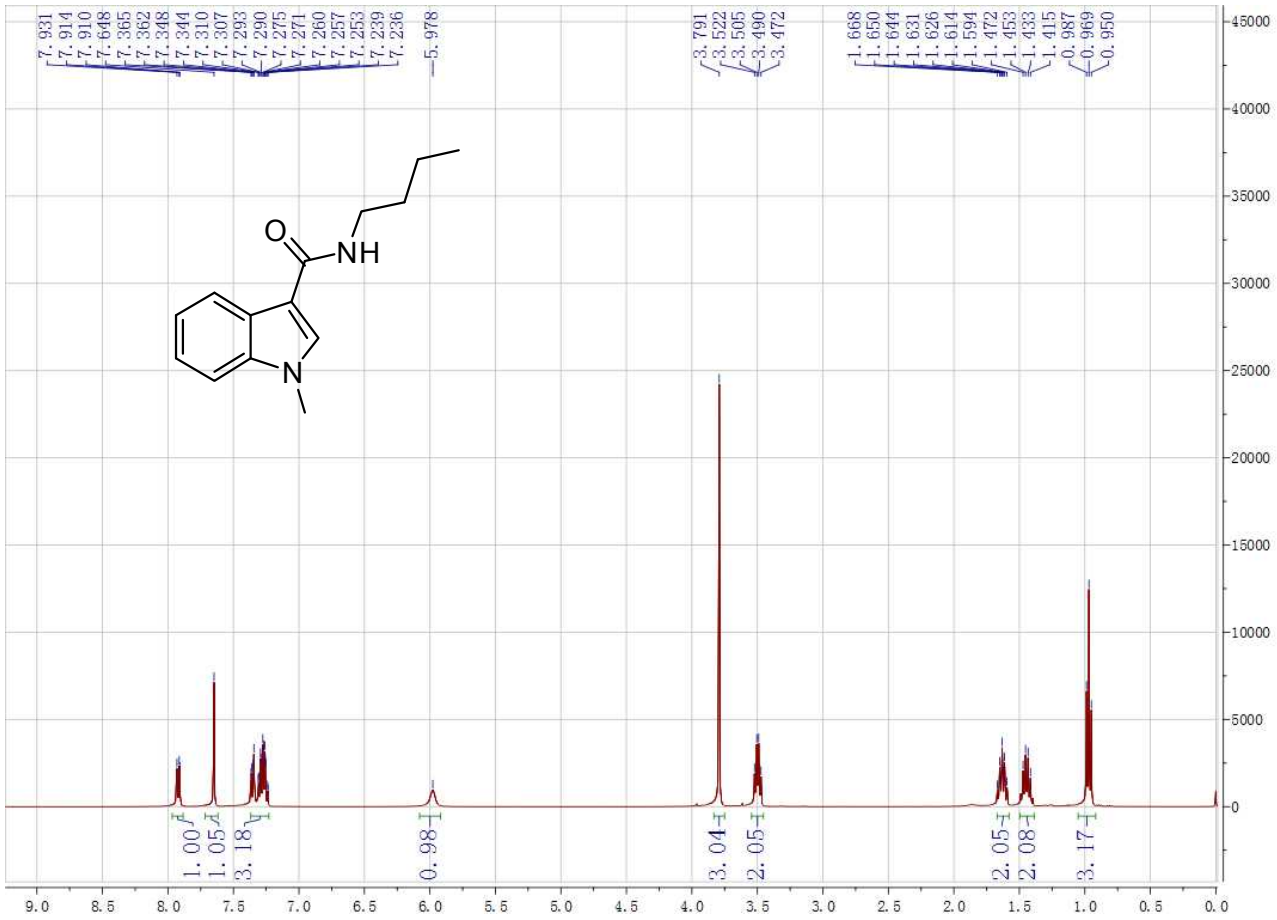
N

4w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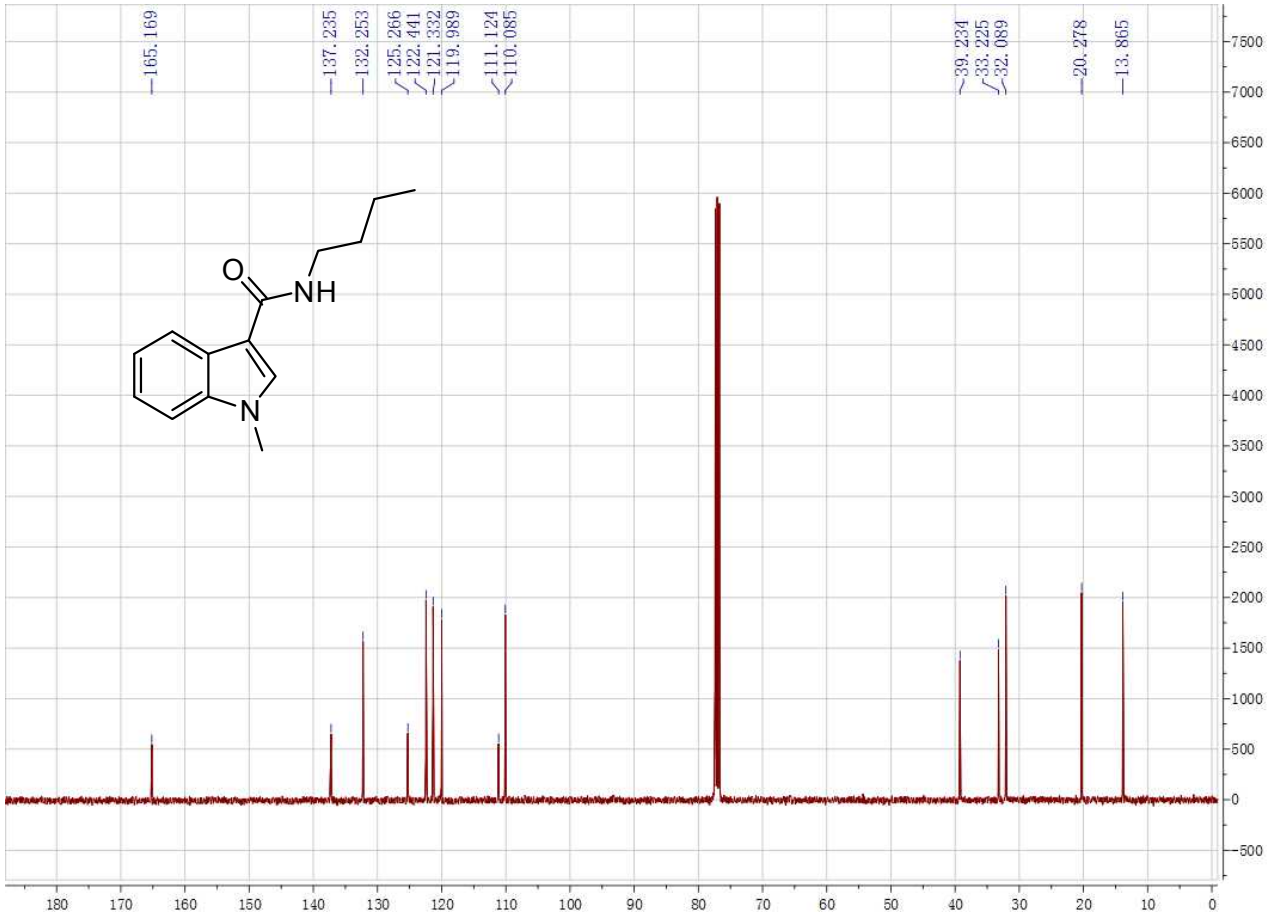
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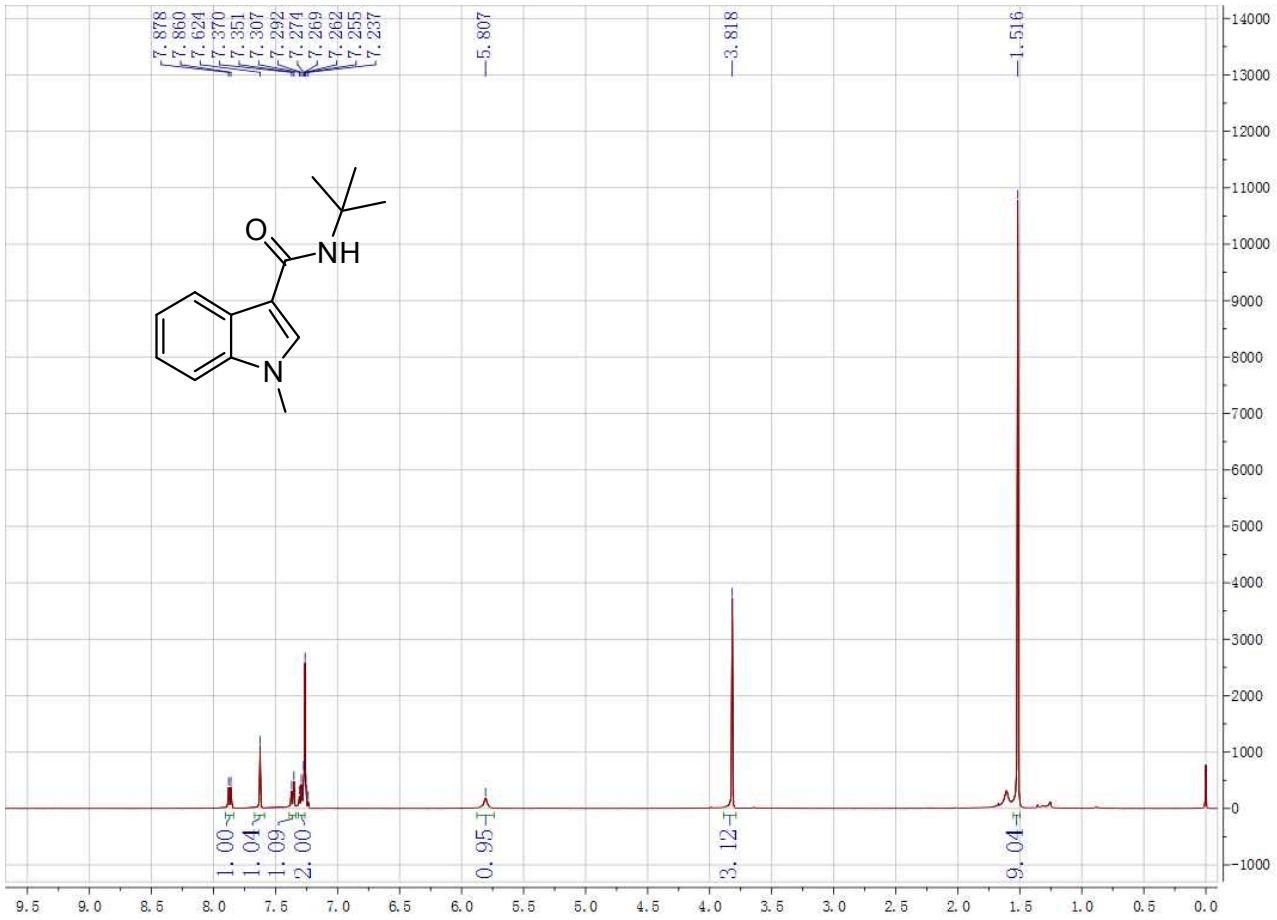
4x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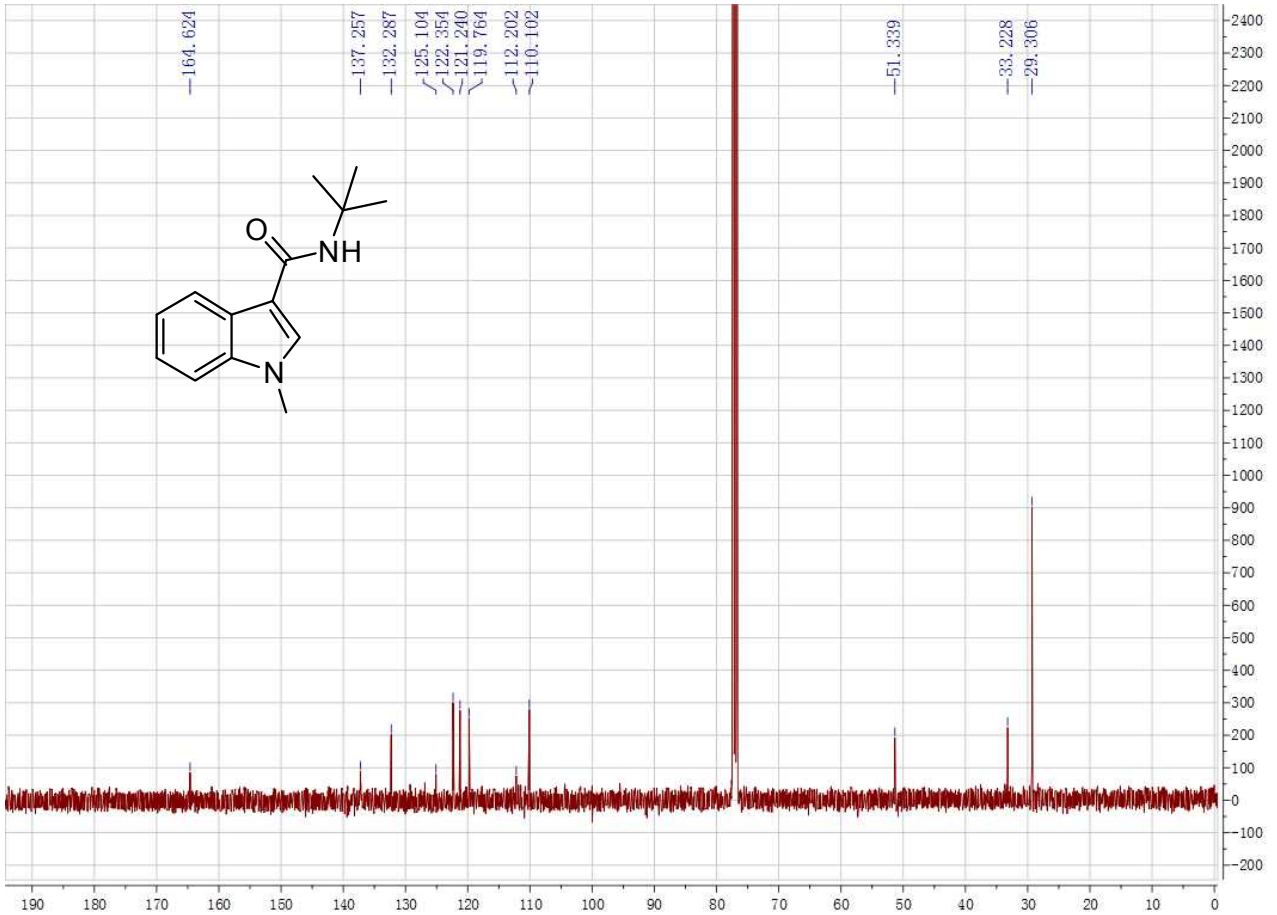
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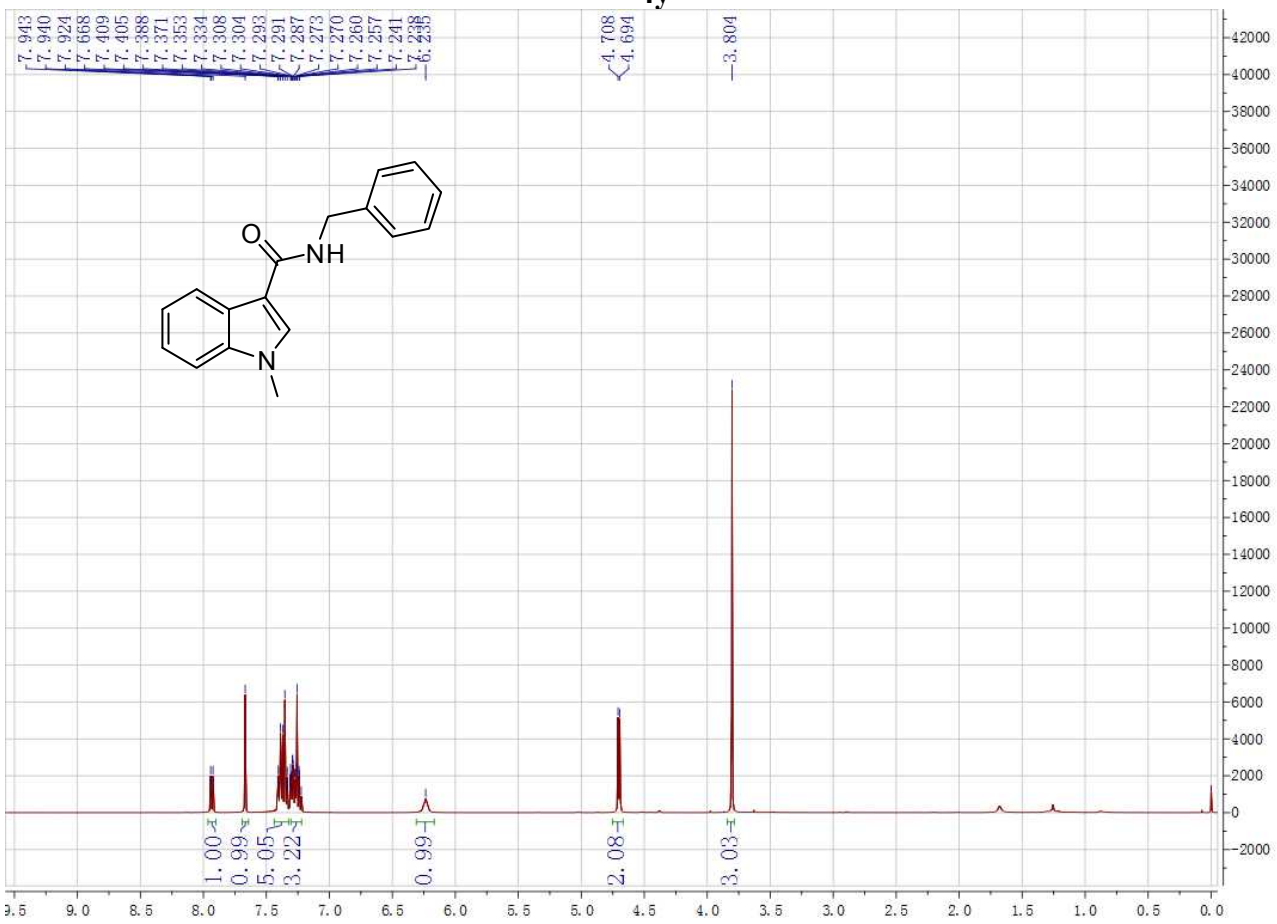
4y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7.241
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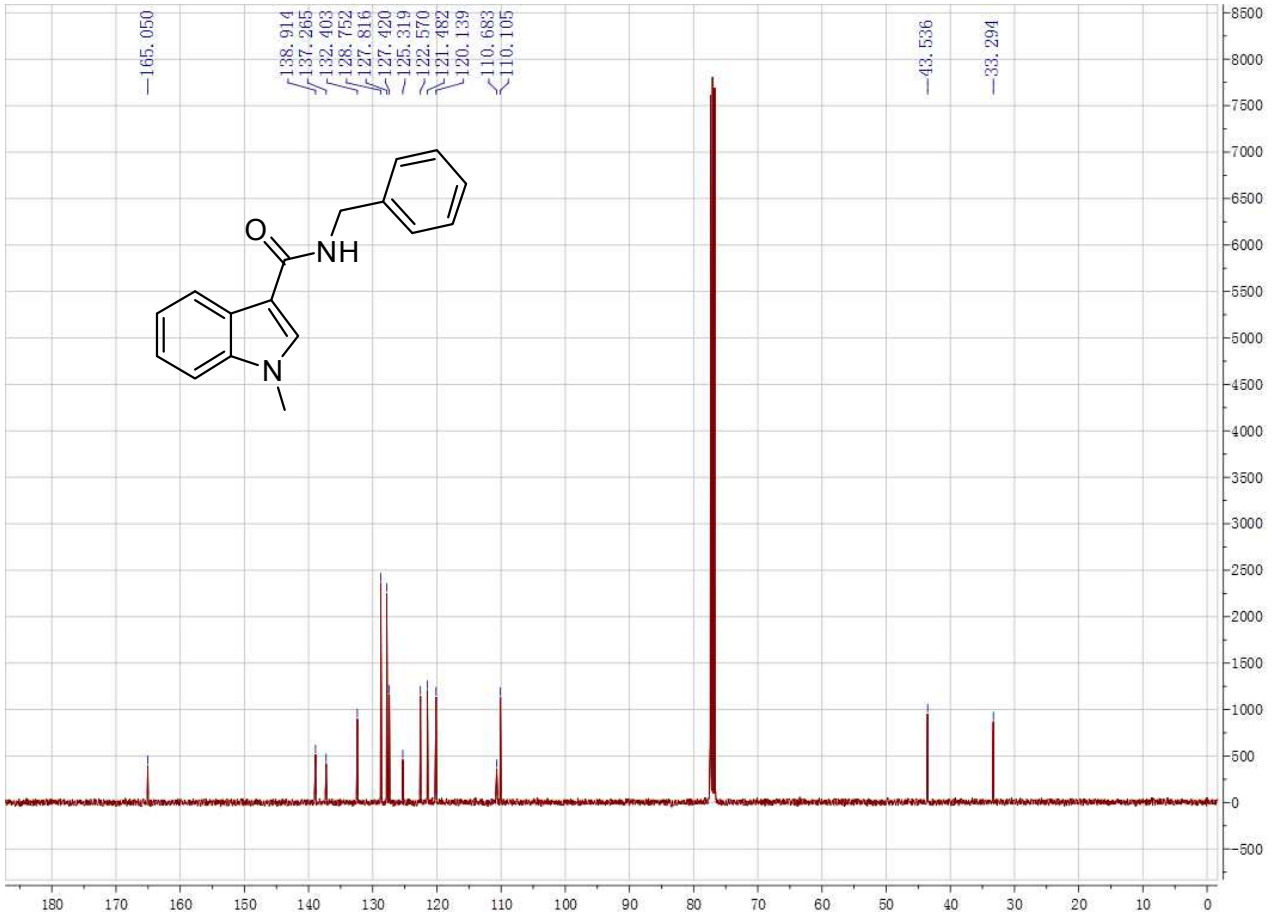
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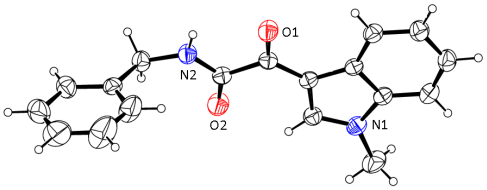
33.294
O
NH
N

6) The Crystal Structure of 3t and 4v

Compound: **3t**

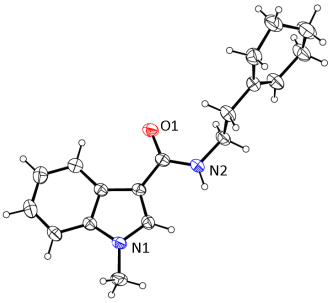
CCDC number: 895174



Scheme S1 The crystal structure of **3t**.

Compound: **4v**

CCDC number: 895173



Scheme S2 The crystal structure of **4v**.

7) References

1 Y. Naruse, Y. Ito, S. Inagaki, *J. Org. Chem.* 1991, **56**, 2256.

2 F. Gagosz, S. Z. Zard, *Org. Lett.* 2002, **4**, 4345.

3 H. Heaney, S. V. Ley, A. Brossi, E. E. Garcia, R. P. Schwartz, *Org. Synth., Coll.* 1988, **6**, 104; 1974, 54, 58.

4 Y. Huang, H. Miao, Q. Zhang, C. Chen, J. Xu, *Catal. Lett.* 2008, **122**, 344.