Supportting Information

Carbene and Photocatalyst Catalyzed 3-acylation of Indoles for Facile Access to Indole-3-yl Aryl Ketones

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Table of Contents

I. General information

All compounds were fully characterized by spectroscopic data. The NMR spectra were recorded on a DRX400 (^{1}H: 400 MHz, ^{13}C: 100 MHz), chemical shifts (δ) are expressed in ppm, and J values are given in Hz, and deuterated $CDCl_3$-*d* and DMSO-d_6 were used as solvent.

All chemicals and solvents were used as received without further purification unless otherwise stated. Column chromatography was performed on silica gel (200 - 300 mesh). Alcohol, acid chlorides, imidazole, photocatalyst and solvents were purchased from Energy Chemical and Adamas beta®. Commercially available materials purchased from Energy Chemical were used as received. NMR spectra were recorded on a Brüker ASCEND 400 (400 MHz) spectrometer (^{1}H: 400 MHz, ^{13}C: 100 MHz). Chemical shifts (δ) for ^{1}H and ^{13}C NMR spectra are given in ppm relative to TMS. The residual solvent signals were used as references for ^{1}H and ^{13}C NMR spectra and the chemical shifts converted to the TMS scale ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.0 ppm). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad, and etc. All first order splitting patterns were assigned on the base of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). High resolution mass spectrometer analysis (HRMS) was performed on Thermo Fisher Q Exactive Mass Spectrometer. Analytical thin layer chromatography (TLC) was carried out on pre coated silica gel plate (0.2 mm thickness).

II. Representative bioactive molecules

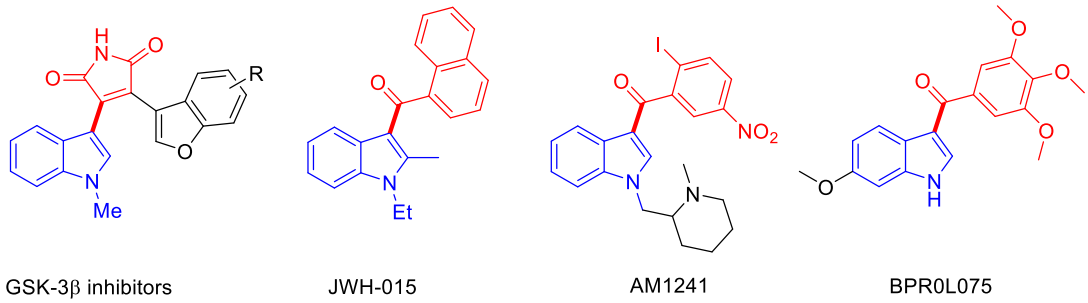


Figure S1. Representative bioactive molecules bearing 3-acyl indole moiety

III. The discussion of the regio-selectivity

our work exhibits different regio-selectivity with Ohmiya's work (*Nat. Synth.*, **2023**, *2*, 1037–1045), whose acylation occurs at 7-positions for indole substrate. This was attributed to the electronic effect of the N-protecting group and the steric effect of the substituents on the phenyl ring. Detailed discussion were listed as below:

The indole substrate used in Ohmiya's work (ref. 13) is protected by Boc, which decreases the electron density of the pyrrole ring of the indole, resulting in the acylation occurring at the electron-rich phenyl ring (C7). In contrast, our substrates (for **3aa** and **3z**) are protected by methyl group, which makes the pyrrole ring more electron-rich, enabling the acylation to occur at the pyrrole ring (C3).

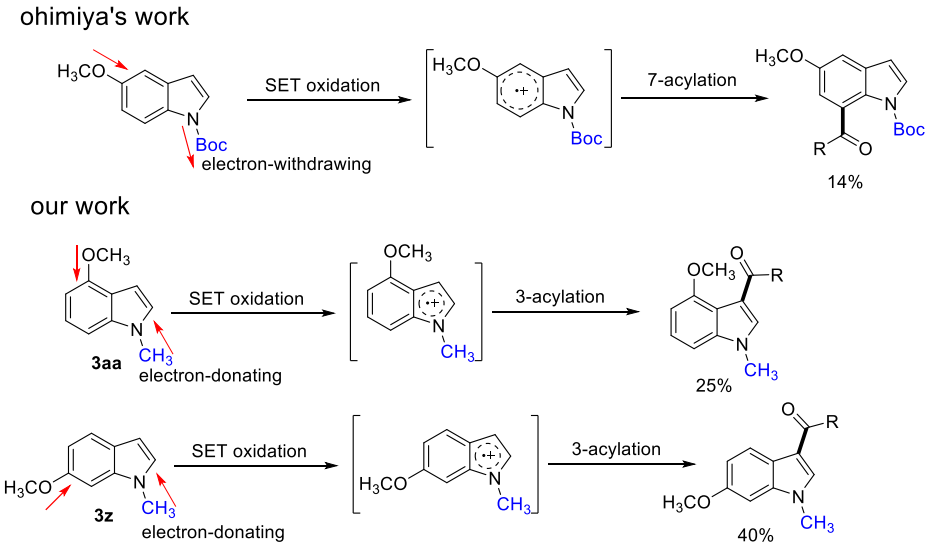


Figure S2. Electronic effect-induced site-selectivity

In terms of **3ag**, the steric effect of the methoxyl group at the 6-position may frustrate the acylation at the 7-position (Figure S3a). To provide further evidence to support the above hypothesis, indole substrate whose methoxyl group is far away from C7 was subjected to our standard conditions (Figure S3b). As expected, a small amount of 7-acylated indole (1%) was

obtained along with the target 3-acylated product (9%). Actually, such an indole compound is not a good substrate for Ohmiya's work too, with only 14% yield obtained.

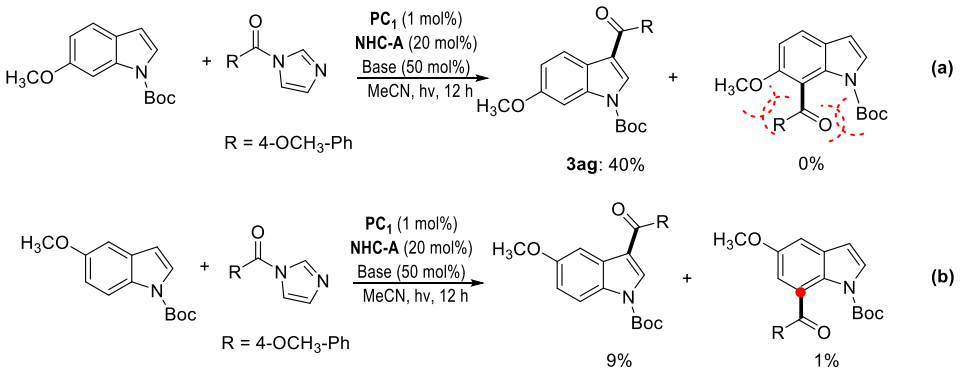
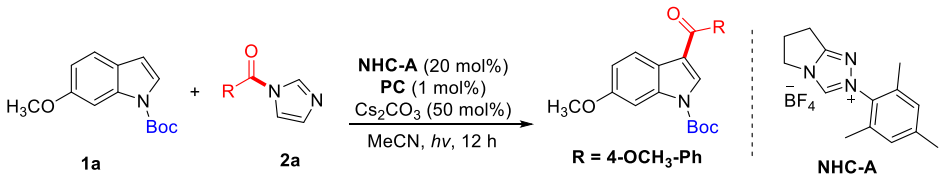


Figure S3. Steric effect-induced site-selectivity

IV. Optimization of tert-butyl 6-methoxy-1H-indole-1-carboxylate condition

We tried substantial additional experiments to improve the yield of **3ag**, including screening of the photocatalyst and reaction solvent. However, no better result was obtained at the current stage.



entry	Variation from standard conditions	Yield/%
1	none	40
2	**PC-1** instead of **PC-2**	42
3	**PC-3** instead of **PC-2**	33
4	**PC-4** instead of **PC-2**	29
5	**PC-5** instead of **PC-2**	15
6	**PC-6** instead of **PC-2**	NR
7	**PC-7** instead of **PC-2**	8
8	**PC-8** instead of **PC-2**	3
9	**PC-9** instead of **PC-2**	27
10	**PC-10** instead of **PC-2**	6
11	**PC-11** instead of **PC-2**	45
12	**PC-12** instead of **PC-2**	NR
13	1,4-Dioxane instead of MeCN	NR
14	DCM, DMF, EA, DMAC, or THF instead of MeCN	18, 21, 11, 27, 15
19	DMAP instead of Cs_2CO_3	NR
20	KOH instead of Cs_2CO_3	28
21	Na_2CO_3instead of Cs_2CO_3	20

[a]The reactions were performed with **1a** (0.1 mmol), **2a** (0.2 mmol), NHC (0.02 mmol), **PC** (0.001 mmol), Base (0.05 mmol, 0.5 equiv.), and solvent (2.0 mL), under irradiation with a blue LED for 12 h;

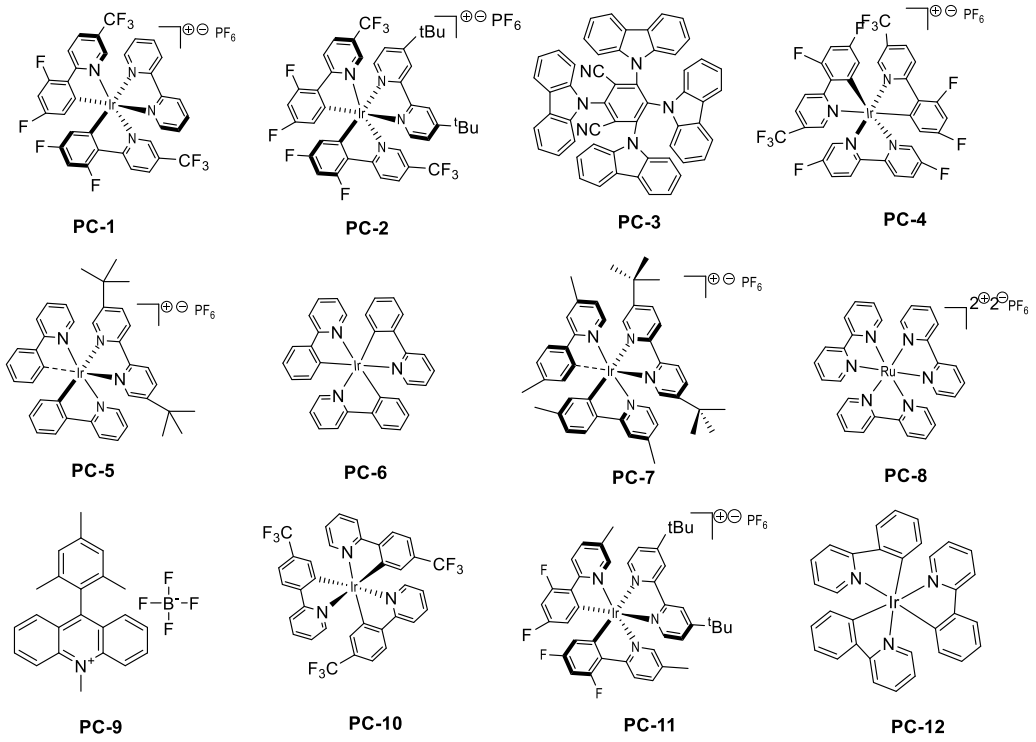


Figure S4. Tested photocatalysts

V. Acylations with other acyl precursors

In addition to acyl imidazole (**2**), we also tried the generality of the current method for other acyl sources including acyl benzyl chloride, 4-nitrophenyl benzoate, benzoyl fluoride, and benzoic anhydride. However, it was found that all the newly tested NHC ketyl radical precursors failed to give the desired acylation product. It's worth noting that a small amount of side product generated via acylation of the *N*-methyl was observed when benzoyl fluoride and benzoic anhydride were used.

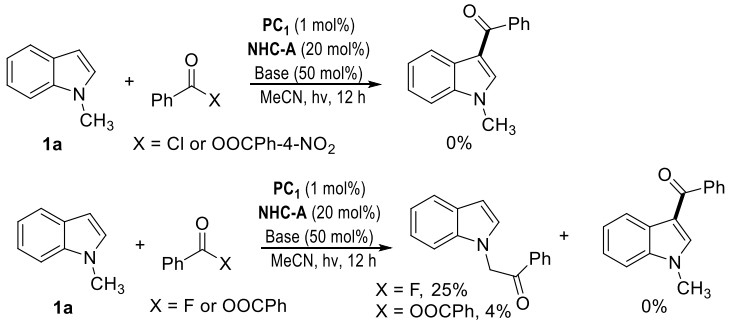
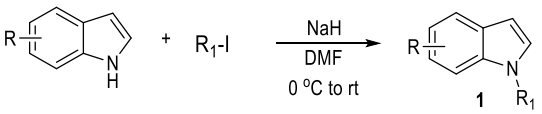


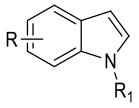
Figure S5. Acylations with other acyl precursors

VI. Preparation of substrates

1. Preparation of substrates 1

Method 1: General Procedure for the Preparation of Indole derivatives[1]

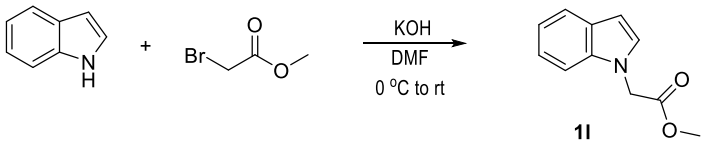




1a, R = 4-OCH_3, R_1 = CH_3
1b, R = 6-OCH_3, R_1 = CH_3
1c, R = 5-Cl, R_1 = CH_3
1d, R = 5-F, R_1 = CH_3
1e, R = 6-CF_3, R_1 = CH_3
1k, R = 5-Cl, 6-F
1f, R = 6-F,7-Cl, R_1 = CH_3
1g, R = 4-CH3, R_1 = CH_3
1h, R = 5-CH3, R_1 = CH_3
1i, R = 6-CH3, R_1 = CH_3
1j, R = 7-CH3, R_1 = CH_3

To a stirred solution of 1H-Indole substrates (10 mmol) in dry DMF (50 ml), NaH (12 mmol, 60% suspension in mineral oil) were added dropwise at 0°C. The mixture was allowed to warm up to room temperature and stirred for 30 min. After cooling down to 0 °C, iodomethane (12 mmol.) was added dropwise. The reaction mixture was stirred at room temperature for another 6 h and then it was quenched by the addition of water and was extracted with ethyl acetate (10 mL, 3 times). The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to give the corresponding compounds **1**.

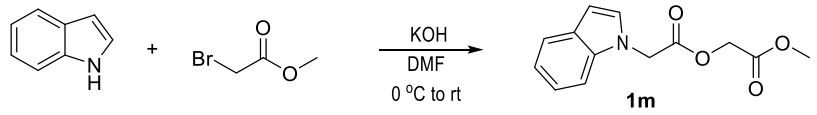
Method 2: General Procedure for the Preparation of ethyl 2-(1*H*-indol-1-yl)acetate (**1l**)[2]



Nethyl 2-bromoacetate (10 mmol) was added to a stirred solution of 1H-Indole (15mmol) and KOH (15 mmol) in DMF (40 mL) at room temperature. The reaction mixture was stirred for 3 h. The reaction mixture was diluted with EtOAc and washed with H_2O (3 × 30 mL). The aqueous phase was extracted with EtOAc (3 × 30 mL), and the combined organic phases were dried over Na_2SO_4. After filtration and evaporation of the solvents in vacuo, the crude product was purified by column chromatography on silica gel (petroleum ether: ethyl acetate = 20:1) to give ethyl 2-(1*H*-indol-1-yl)acetate

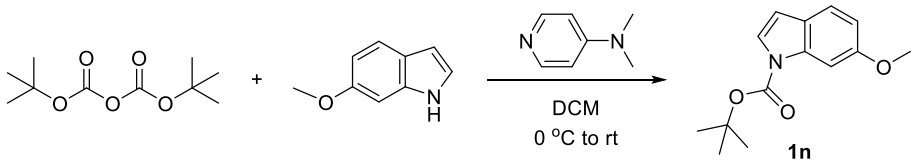
(**1l**).

Method 3: General Procedure for the Preparation of 2-methoxy-2-oxoethyl 2-(1*H*-indol-1-yl)acetate (**1m**)[2]



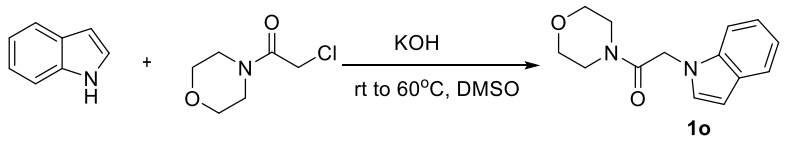
Methyl 2-bromoacetate (14 mmol) was added to a stirred solution of 1H-Indole (10 mmol) and KOH (12 mmol) in DMF (40 mL) at room temperature. The reaction mixture was stirred for 3 h, it was quenched by the addition of Saturated NH_4Cl(40ml) solution and was extracted with ethyl acetate with H_2O (3 × 30 mL). Combined organic phases were dried over Na_2SO_4. After filtration and evaporation of the solvents in vacuo, the crude product was purified by column chromatography on silica gel (petroleum ether: ethyl acetate = 10:1) to give 2-methoxy-2-oxoethyl 2-(1*H*-indol-1-yl)acetated (**1m**).

Method 4: General Procedure for the Preparation of tert-butyl 6-methoxy-1H-indole-1-carboxylate (**1n**)[3]



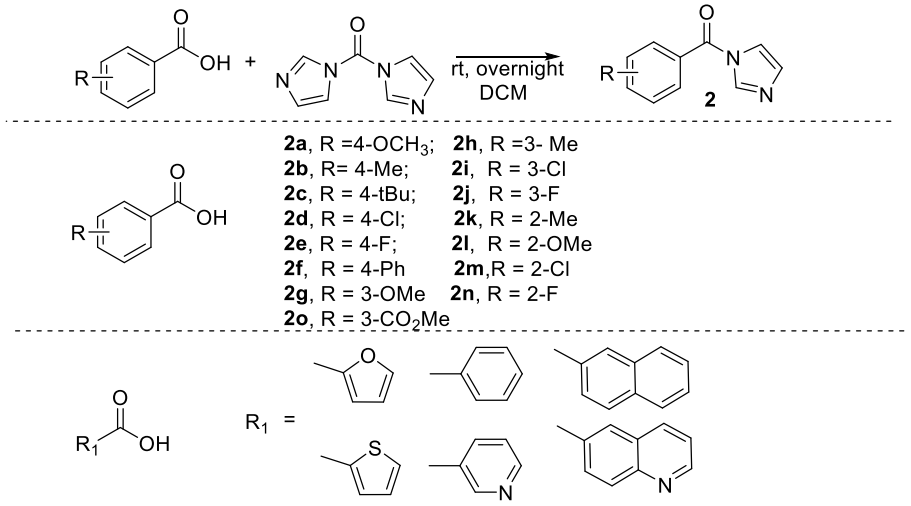
To a solution of 6-methoxy-1H-indole (10 mmol), di-(tert-butyl)dicarbonate (13 mmol) in CH_2Cl_2 (40 mL) was added DMAP (0.2 mmol) at 0° C. The resulting mixture was stirred at room temperature for 16 h, concentrated and partitioned between EtOAc and water. The organic layer was washed with water, brine, dried, concentrated and purified on silica gel (EtOAc/hexane 5%) to tert-butyl 6-methoxy-1*H*-indole-1-carboxylate **1n** as a solid.

Method 5: General Procedure for the Preparation of 2-(1*H*-indol-1-yl)-1-morpholinoethan-1-one (**1o**)[4]



The 1*H*-Indole (10mmol) and KOH (10 mmol) were stirred for 1 hour in DMSO (40 mL) from 0 ℃ to room temperature,then 4-(Chloroacetyl) (12 mmol)morpholine was added to a stirred solution of indole and KOH in DMSO ,the reaction mixture was stirred for 6 h at 60 ℃, and then it was quenched by the addition of Saturated NH_4Cl (40ml) solution and was extracted with ethyl acetate (20 mL, 3 times). Dried over anhydrous Na_2SO_4 and concentrated under reduced pressure,the residue was purified by column chromatography on silica gel to give the 2-(1*H*-indol-1-yl)-1-morpholinoethan-1-one **1o**.

2. Preparation of substrates 2[5]



Charge a round-bottomed flask equipped with a stir bar with acid (10 mmol) and DCM (0.4 M based on carboxylic acid). Add *N*, *N*'-carbonyldiimidazole (20 mmol) slowly to the mixture at room temperature. Stir the resulting mixture at room temperature overnight. Add water to the mixture. Wash the separated organic layer with water twice and brine once. Dry the organic phase over Na_2SO_4. Filter the organic phase. Concentrate the organic phase under reduced pressure.

References:

1 Q-Q. Xia, & G. Liang, *Eur. J. Med. Chem*., 2018, **160**, 120-132.
2 Y-Q. Zou, & J-K. Shen, *Molecules* 2013,**18**,5706-5722.
3 H. Matsuyama, & T-N. Jin, *Org. Lett.*, 2023, **25**,800-804.
4 P. V. R. Chowdary, *Int. J. Res. Pharm. Chem.*, 2013, **3**, 859-862.
5 J-M. Zhuo, & C. Li, *ACS Catal.*, 2020, **10**, 3895-3903.

VII. General procedure for the 3-acylation of indoles

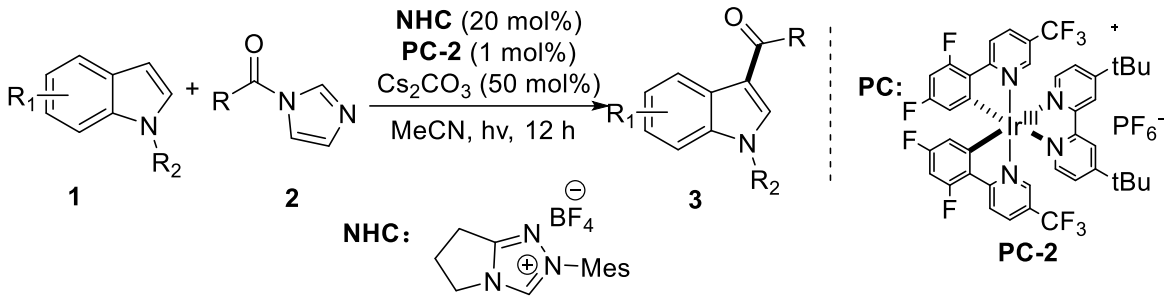


Figure S6. reaction setup with photoreactor

General procedure:

In gloves box, to a 10 mL anaerobic tube equipped with a stir bar added **1** (0.10 mmol), **2** (0.20 mmol), photocatalyst **PC-2** (0.001mmol), pre **NHC** (0.02 mmol), Cs_2CO_3 (0.05 mmol), and dry MeCN (2.0 mL). The reaction mixture was sealed and taken out from the gloves box. The reaction mixture was stirred and irradiated with a photoreactor (λ= 445-450 nm, P = 10 w, reaction set-up see **Figure S6**) at 25 ℃ for 12 h. Then the reaction mixture was monitored by TLC, concentrated under reduced pressure, and the residue was purified via column chromatography on silica gel with PE/EtOAc.

VIII. Stern-Volmer quenching experiments and proposed possible reaction pathway

To support the proposed reductive quenching of photocatalyst **PC-2**) by 1-methyl-1*H*-indole (**1a**), we conducted Stern-Volmer quenching experiments by using the substrate of 1-methyl-1*H*-indole as a quenching agent. It was found that 1-methyl1*H*-indole could effectively quench the emission of **PC-2**.

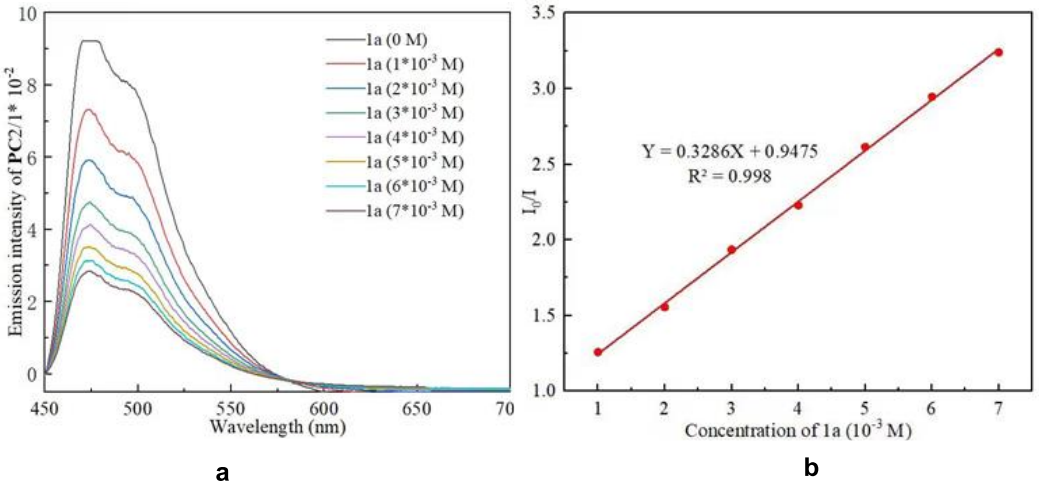


Figure S7:a. Spectra of Stern-Volmer quenching experiments; **b**. Fit line of I0/I at 400 nm.

Experimental protocol: The emission spectra of a solution of **PC-2** (10^{-2} M in DMSO, 2.0 mL) was recorded. Then, a solution of 1-methyl-1*H*-indole in DMSO (1 x 10^{-3} M, 20 μL) was added to the solution of **PC-2**, and another emission spectra was recorded. The addition and the recordation were repeated five consecutive times.

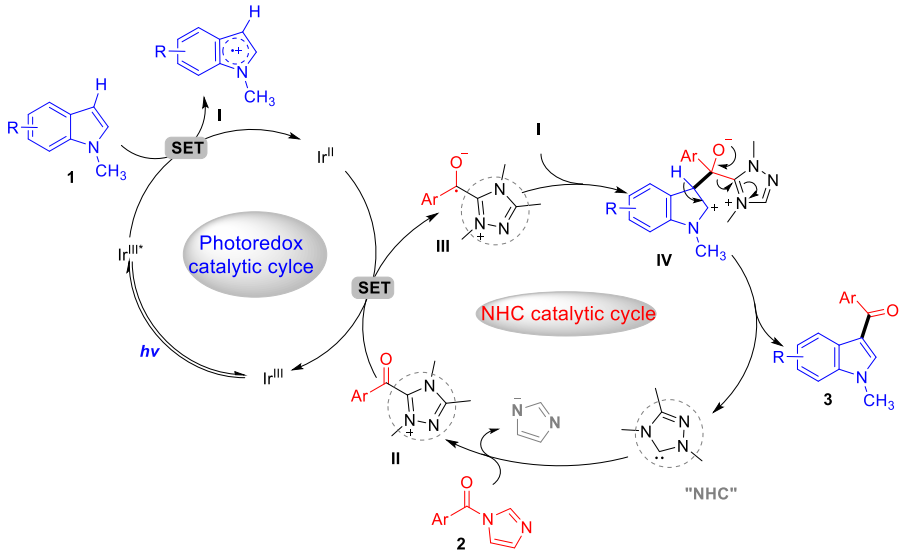


Figure S8. Proposed possible reaction pathway

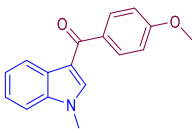
IX. Experimental data of antibacterial activity of target compound

Table 1 Experimental data of antibacterial activity of target compound

Compound	*Xac* inhibition rate (%) [a]		*Xoo* inhibition rate (%) [a]	
	100 (μg/mL)	50 (μg/mL)	100 (μg/mL)	50 (μg/mL)
3i	77.58±3.87	62.26±3.44	40.15±2.06	11.96±0.98
3j	70.7±1.61	59.25±3.22	33.1±1.33	8.6±2.02
3c	70.61±3.46	62.26±1.82	39.51±6.23	9.35±3.97
3d	67.58±2.18	59.67±5.7	26.57±2.4	14.14±4.28
3g	78.82±1.47	57.44±8.57	35.9±1.4	16.14±2.19
3m	69.83±3.04	65.83±2.76	38±9.55	20.25±1.82
3v	73.82±6.6	62.54±5.32	-12.35±1.05	9.47±0.21
3l	58.28 ±3.20	47.43±2.26	37.88±0.57	28.91±3.33
3u	71.39±7.6	54.89±3.62	63.23±1.34	35.02±3.08
3ae	58.18 ±1.18	39.64±5.99	22.44±1.15	8.22±1.68
3aa	62.40 ±1.52	53.82 ±0.78	22.9±1.23	7.48±1.01
BT[b]	55.20 ± 1.46	51.32 ±0.52	93.18±0.36	41.62±0.42
TC[c]	85.74 ±2.25	60.41 ±1.21	84.03±2.55	48.29±2.83

X. Characterizations of products

(4-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3a)**

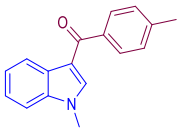


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 – 8.36 (m, 1H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.54 (s, 1H), 7.38 – 7.30 (m, 3H), 6.98 (d, *J* = 8.4 Hz, 2H), 3.88 (s, 3H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.7, 162.2, 137.5, 137.0, 133.5, 130.9, 127.4, 123.5, 122.7, 122.5, 115.8, 113.5, 109.6, 55.4, 33.5.

HRMS (ESI-TOF, m/z): Mass calcd. for $C17H16NO2^{+}$ $[M+H]^{+}$, 266.1176; found: 266.1185.

(1-methyl-1*H*-indol-3-yl)(p-tolyl)methanone **(3b)**

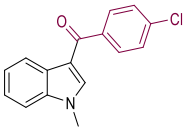


1H NMR (400 MHz, Chloroform-d) δ 8.44 – 8.39 (m, 1H), 7.75 – 7.72 (m, 2H), 7.53 (s, 1H), 7.38 – 7.32 (m, 3H), 7.28 (d, *J* = 7.8 Hz, 2H), 3.83 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.7, 141.5, 138.2, 137.6, 128.94, 128.88, 127.3, 123.6, 122.7,122.6, 115.8, 109.6, 33.5, 21.5.

HRMS (ESI-TOF, m/z): Mass calcd. for $C17H16NO^{+}$ $[M+H]^{+}$, 250.1226; found: 250.1227.

(4-chlorophenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3c)**

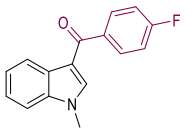


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 – 8.35 (m, 1H), 7.76 – 7.73 (m, 2H), 7.49 (s, 1H), 7.46 – 7.43 (m, 2H), 7.38 – 7.33(m, 3H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.5, 139.2, 137.7, 137.6, 137.3, 130.1, 128.6, 127.1, 123.8, 122.9, 122.7, 115.4, 109.7, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C16H13ClNO^{+}$ $[M+H]^{+}$, 270.0680; found: 270.0674.

(4-fluorophenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3d)**



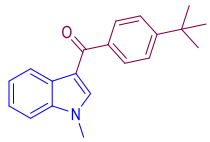
^{1}H NMR (400 MHz, Chloroform-d) δ 8.40 – 8.37 (m, 1H), 7.85 – 7.81 (m, 2H), 7.50 (s, 1H), 7.39 – 7.32 (m, 3H), 7.18 – 7.12 (m, 2H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.33, 164.59 (d, *J* = 251.1 Hz), 137.56, 137.07, 131.03, 127.15, 123.74, 122.69 (d, *J* = 15.0 Hz), 115.31 (d, *J* = 21.5 Hz), 109.70, 33.58.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -108.60.

HRMS (ESI-TOF, m/z): Mass calcd. for $C16H13FNO^{+}$ $[M+H]^{+}$, 254.0976; found: 254.0977.

(4-(tert-butyl)phenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3e)**

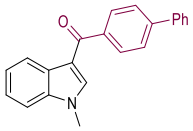


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.47 – 8.42 (m, 1H), 7.79 – 7.76 (m, 2H), 7.57 (s, 1H), 7.52 – 7.48 (m, 2H), 7.40 – 7.32 (m, 3H), 3.85 (s, 3H), 1.38 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.7, 154.6, 138.2, 137.7, 137.6, 128. 7, 127.3, 125.2, 123.6, 122.8, 122.6, 115.8, 109.5, 35.0, 33.5, 31.3.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{20}H_{22}NO^{+}$ $[M+H]^{+}$, 292.1696; found: 292.1691.

[1,1'-biphenyl]-4-yl(1-methyl-1*H*-indol-3-yl)methanone **(3f)**

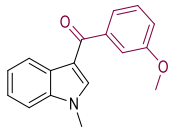


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 – 8.44 (m, 1H), 7.91 (d, *J* = 8.2 Hz, 2H), 7.69 (dd, *J* = 19.5, 7.6 Hz, 4H), 7.60 (s, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.44 – 7.35 (m, 4H), 3.87 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.5, 143.9, 140.3, 139.7, 137.8, 137.6, 129.3, 120.0, 127.9, 127.3, 127.0, 123.7, 122.8, 122.8, 115.7, 109.7, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{22}H_{18}NO^{+}$ $[M+H]^{+}$, 312.1383; found: 312.1376.

(3-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3g)**

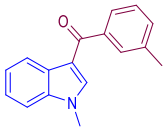


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 – 8.41 (m, 1H), 7.56 (s, 1H), 7.40 – 7.33 (m, 6H), 7.11 – 7.07 (m, 1H), 3.87 (s, 3H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.5, 159.6, 142.3, 137.9, 137.6, 129.2, 127.2, 123.7, 122.8, 122.8, 121.2, 117.2, 115.6, 113.5, 109.6, 55.5, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{17}H_{16}NO2^{+}$ $[M+H]^{+}$, 266.1176; found: 266.1179.

(1-methyl-1*H*-indol-3-yl)(m-tolyl)methanone **(3h)**

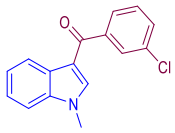


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 – 8.41 (m, 1H), 7.63 – 7.58 (m, 2H), 7.53 (s, 1H), 7.38 – 7.32 (m, 5H), 3.84 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.1, 141.0, 138.1, 137.8, 137.6, 131.8, 129.2, 128.1, 127.3, 125.9, 123.6, 122.8, 122.7, 115.8, 109.6, 33.5, 21.4.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{17}H_{16}NO^{+}$ $[M+H]^{+}$, 250.1226; found: 250.1231.

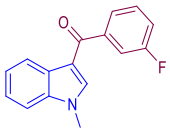
(3-chlorophenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3i)**



^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 – 8.39 (m, 1H), 7.78 (t, *J* = 1.9 Hz, 1H), 7.68 – 7.66 (m, 1H), 7.52 – 7.49 (m, 2H), 7.43 – 7.34 (m, 4H), 3.85 (s, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.0, 142.6, 137.9, 137.7, 134.4, 131.0, 129.7, 128.6, 127.1, 126.8, 123.9, 122.9, 122.7, 115.3, 109.7, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{16}H_{13}ClNO^+$ $[M+H]^+$, 270.0680; found: 270.0682.

(3-fluorophenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3j)**

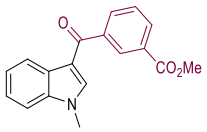


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 – 8.39 (m, 1H), 7.60 – 7.57 (m, 1H), 7.52 – 7.42 (m, 3H), 7.39 – 7.37 (m, 3H), 7.26 – 7.21 (m, 1H), 3.85 (s, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.1 (d, *J* = 2.1 Hz), 162.6 (d, *J* = 247.7 Hz), 143.0 (d, *J* = 6.0 Hz), 137.9, 137.6, 130.0 (d, *J* = 7.9 Hz), 127.1, 124.4 (d, *J* = 3.0 Hz), 123.9, 122.9, 122.7, 118.0 (d, *J* = 21.6 Hz), 115.6 (d, *J* = 22.0 Hz), 115.2, 109.7, 3.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -112.39.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{16}H_{13}FNO^+$ $[M+H]^+$, 254.0976; found: 254.0971

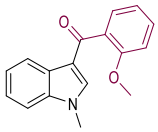
methyl 3-(1-methyl-1*H*-indole-3-carbonyl)benzoate **(3k)**



^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (t, *J* = 1.8 Hz, 1H), 8.43 – 8.41 (m, 1H), 8.21 (dt, *J* = 7.8, 1.6 Hz, 1H), 8.00 (dt, *J* = 7.8, 1.6 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.51 (s, 1H), 7.39 – 7.35 (m, 3H), 3.94 (s, 3H), 3.85 (s, 3H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.6, 166.6, 141.2, 137.9, 137.7, 132.9, 132.0, 130.3, 129.6, 128.6, 127.2, 123.9, 122.9, 122.7, 115.4, 109.7, 52.3, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{18}H_{16}NO_3^+$ $[M+H]^+$, 294.1125; found: 294.1129.

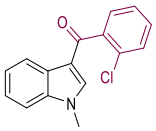
(2-methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3l)**



^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 – 8.37 (m, 1H), 7.44 – 7.29 (m, 6H), 7.01 (t, *J* = 8.0 Hz, 2H), 3.78 (d, *J* = 4.0 Hz, 6H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.10, 156.80, 138.65, 137.74, 130.69, 128.81, 126.68, 123.49, 122.76, 120.22, 117.28, 111.66, 109.62, 55.84, 33.50.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{17}H_{16}NO_2^+$ $[M+H]^+$, 266.1176; found: 266.1168

(2-chlorophenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3m)**

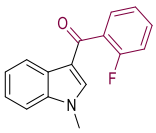


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 – 8.35 (m, 1H), 7.47 – 7.33 (m, 7H), 7.28 (s, 1H), 3.78 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 188.8, 140.6, 138.8, 137.8, 131.0, 130.34, 130.1, 128.7, 126.5, 123.9, 123.1, 122.7, 116.4, 109.8, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{16}H_{13}ClNO^+$ $[M+H]^+$, 270.0680; found: 270.0673

(2-fluorophenyl)(1-methyl-1*H*-indol-3-yl)methanone **(3n)**



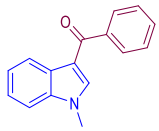
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 –8.40 (m, 1H), 7.58 – 7.54 (m, 1H), 7.50 – 7.43 (m, 2H), 7.37 – 7.34 (m, 3H), 7.26 – 7.22 (m, 1H), 7.19 – 7.15 (m, 1H), 3.82 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 186.6, 159.4 (d, *J* = 249.9 Hz), 138.6 (d, *J* = 2.9 Hz), 137.7, 131.6 (d, *J* = 8.0 Hz), 130.0 (d, *J* = 3.6 Hz), 129.5 (d, *J* = 16.6 Hz), 126.6, 124.1 (d, *J* = 3.6 Hz), 123.8, 123.0, 122.7, 116.8, 116.2 (d, *J* = 21.9 Hz), 109.7, 33.6.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -113.97.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{16}H_{13}FNO^+$ $[M+H]^+$, 254.0976; found: 254.0973

(1-methyl-1*H*-indol-3-yl)(phenyl)methanone **(3o)**



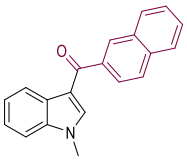
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 – 8.41 (m, 1H), 7.83 – 7.80 (m, 2H), 7.57 – 7.46 (m, 4H), 7.39 – 7.32 (m, 3H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.9, 141.0, 137.9, 137.6, 131.1, 128.7, 128.3, 127.3, 123.7, 122.8, 122.7, 115.7, 109.6, 33.5.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -113.97.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{16}H_{14}NO^+$ $[M+H]^+$, 236.1070; found: 236.1061

(1-methyl-1*H*-indol-3-yl)(naphthalen-2-yl)methanone **(3p)**

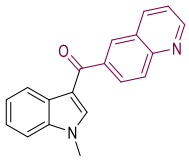


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 – 8.43 (m, 1H), 8.29 (s, 1H), 7.95 – 7.90 (m, 4H), 7.60 – 7.53 (m, 3H), 7.40 – 7.34 (m, 3H), 3.84 (s, 3H)

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.9, 138.2, 137.9, 137.6, 134.7, 132.6, 129.2, 129.1, 128.3, 127.9, 127.5, 127.3, 126.6, 125.6, 123.7, 122.8, 115.9, 109.7, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{20}H_{16}NO^+$ $[M+H]^+$, 286.1226; found: 286.1235

(1-methyl-1*H*-indol-3-yl)(quinolin-6-yl)methanone **(3q)**

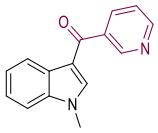


^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.02 (dd, *J* = 4.4, 1.8 Hz, 1H), 8.45 – 8.41 (m, 1H), 8.29 – 8.27 (m, 2H), 8.24 – 8.19 (m, 1H), 8.17 – 8.15 (m, 1H), 7.59 (s, 1H), 7.50 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.44 – 7.35 (m, 3H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.0, 151.8, 149.3, 138.9, 138.0, 137.7, 137.2, 129.7, 129.3, 128.9, 127.6, 127.2, 123.9, 123.0, 122.8, 121.8, 115.8, 109.8, 33.7.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{19}H_{15}N_2O^+$ $[M+H]^+$, 287.1179; found: 287.1174

(1-methyl-1*H*-indol-3-yl)(pyridin-3-yl)methanone **(3r)**

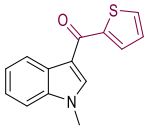


^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.04 (s, 1H), 8.78 (s, 1H), 8.44 – 8.41 (m, 1H), 8.14 – 8.11 (m, 1H), 7.54 (s, 1H), 7.47– 7.44 (m, 1H), 7.41 – 7.35 (m, 3H), 3.87 (s, 3H)

^{13}C NMR (101 MHz, Chloroform-*d*) δ 186.9, 150.4, 148.1, 136.6, 136.2, 134.98, 134.8, 125.6, 122.7, 122.2, 121.7, 121.3, 114.2, 108.4, 32.3.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{15}H_{13}N_2O^+$ $[M+H]^+$, 237.1022; found: 237.1025.

(1-methyl-1*H*-indol-3-yl)(thiophen-2-yl)methanone **(3s)**

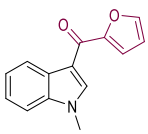


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 – 8.40 (m, 1H), 7.82 (s, 1H), 7.75 (dd, *J* = 3.7, 1.2 Hz, 1H), 7.61 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.40 – 7.31 (m, 3H), 7.16 (dd, *J* = 5.0, 3.7 Hz, 1H), 3.89 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.4, 145.4, 137.5, 136.1, 131.3, 131.0, 127.5, 127.3, 123.8, 122.7, 122.7, 115.6, 109.7, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{14}H_{12}NOS^+$ $[M+H]^+$, 242.0634; found: 242.0630.

furan-2-yl(1-methyl-1*H*-indol-3-yl)methanone **(3t)**

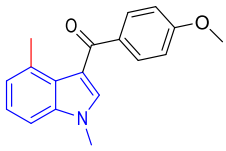


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.56 – 8.53 (m, 1H), 8.25 (s, 1H), 7.60 (d, *J* = 1.8 Hz, 1H), 7.36 – 7.30 (m, 4H), 6.57 (dd, *J* = 3.6, 1.8 Hz, 1H), 3.87 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.1, 154.7, 144.6, 137.2, 137.1, 127.7, 123.6, 123.0, 122.7, 116.1, 114.1, 112.0, 109.6, 33.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{14}H_{12}NO_2^+$ $[M+H]^+$, 226.0863; found: 226.0848

(1,4-dimethyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3u)**

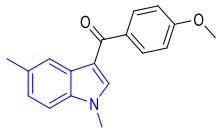


^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 – 7.87 (m, 2H), 7.36 (s, 1H), 7.26 – 7.18 (m, 2H), 7.07 (d, *J* = 7.4 Hz, 1H), 6.99 – 6.94 (m, 2H), 3.90 (d, *J* = 4.6 Hz, 3H), 3.81 (d, *J* = 2.8 Hz, 3H), 2.67 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.1, 162.4, 156.0, 153.6zzz, 138.1, 133.8, 132.8, 126.5, 117.5, 117.3, 115.6, 113.6, 111.0, 109.2, 109.0, 55.4, 33.8. 33.9.

HRMS (ESI-TOF, m/z): Mass calcd. for $C18H18NO2^{+}$ $[M+H]^{+}$, 280.1332; found: 280.1333.

(1,5-dimethyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3v)**

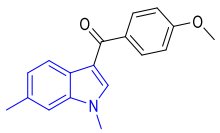


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 – 8.20 (m, 1H), 7.84 – 7.80 (m, 2H), 7.47 (s, 1H), 7.25 – 7.23 (m, 1H), 7.16 (dd, *J* = 8.4, 1.7 Hz, 1H), 6.98 – 6.95 (m, 2H), 3.87 (s, 3H), 3.80 (s, 3H), 2.50 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.8, 162.1, 137.2, 135.9, 133.7, 132.2, 130.8, 127.6, 125.1, 122.4, 115.3, 113.5, 109.2, 55.4, 33.5, 21.5.

HRMS (ESI-TOF, m/z): Mass calcd. for $C18H18NO2^{+}$ $[M+H]^{+}$, 280.1332; found: 280.1335.

(1,6-dimethyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3w)**

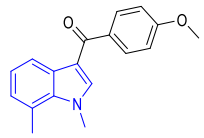


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (d, *J* = 8.6 Hz, 1H), 7.85 – 7.81 (m, 2H), 7.46 (s, 1H), 7.17 – 7.14 (m, 2H), 6.99 – 6.95 (m, 2H), 3.88 (s, 3H), 3.80 (s, 3H), 2.52 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.7, 162.2, 137.9, 136.7, 133.6, 133.5, 130.9, 125.1, 124.2, 122.3, 115.7, 113.5, 109.6, 55.4, 33.4, 21.9.

HRMS (ESI-TOF, m/z): Mass calcd. for $C18H18NO2^{+}$ $[M+H]^{+}$, 280.1332; found: 280.1331.

(1,7-dimethyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3x)**

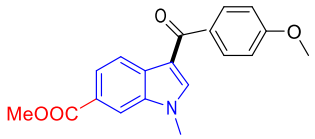


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 8.0 Hz, 1H), 7.84 – 7.81 (m, 2H), 7.42 (s, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.04 – 7.02 (m, 1H), 7.00 – 6.94 (m, 2H), 4.10 (s, 3H), 3.89 (s, 3H), 2.79 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.7, 162.2, 138.7, 136.2, 133.6, 130.9, 128.5, 126.3, 122.7, 121.4, 120.8, 115.3, 113.5, 55.4, 37.7, 19.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C18H18NO2^{+}$ $[M+H]^{+}$, 280.1332; found: 280.1325.

methyl 3-(4-methoxybenzoyl)-1-methyl-1*H*-indole-6-carboxylate **(3y)**

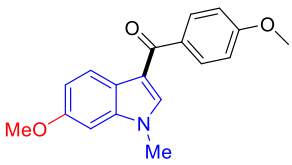


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 – 8.35 (m, 1H), 8.15 – 8.12 (m, 1H), 7.99 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.85 – 7.82 (m, 2H), 7.68 (s, 1H), 7.01 – 6.97 (m, 2H), 3.97 (s, 3H), 3.92 (s, 3H), 3.89 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.26, 162.33, 137.56, 136.09, 133.01, 130.81, 128.84, 126.46, 125.25, 116.19, 115.13, 113.58, 110.99, 55.44, 33.67.

HRMS (ESI-TOF, m/z): Mass calcd. for C19H17NO4Na $^+$ [M+Na]$^+$, 346.1050; found: 346.1045.

(6-methoxy-1-methyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3z)**

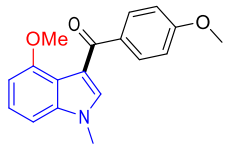


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 8.7 Hz, 1H), 7.85 – 7.81 (m, 2H), 7.44 (s, 1H), 6.99 – 6.96 (m, 3H), 6.81 (d, *J* = 2.2 Hz, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 3.79 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ189.2, 162.5, 156.0, 153.6, 138.2, 133.8, 132.8, 130.8, 126.5, 126.4, 117.6, 115.7, 113.7, 111.1, 109.2, 55.5, 33.9.

HRMS (ESI-TOF, m/z): Mass calcd. for C18H14F3NO2Na $^+$ [M+Na]$^+$, 356.0869; found: 356.0867

(4-methoxy-1-methyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3aa)**

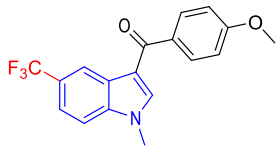


^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.83 (m, 2H), 7.39 (s, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 6.99 (d, *J* = 8.7 Hz, 1H), 6.92 – 6.89 (m, 2H), 6.64 (dd, *J* = 7.9, 0.7 Hz, 1H), 3.87 (s, 3H), 3.82 (s, 3H), 3.71 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.0, 162.5, 154.3, 139.0, 134.1, 133.5, 131.9, 124.0, 116.6, 112.9, 102.72, 102.2, 55.4, 55.3, 33.5.

HRMS (ESI-TOF, m/z): Mass calcd. for C18H17NO3Na $^+$ [M+Na]$^+$, 318.1101; found: 318.1094

(4-methoxyphenyl)(1-methyl-5-(trifluoromethyl)-1H-indol-3-yl)methanone **(3ab)**



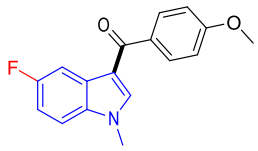
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.75 – 8.69 (m, 1H), 7.86 – 7.82 (m, 2H), 7.62 (s, 1H), 7.57 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.44 (d, *J* = 8.6 Hz, 1H), 7.01 – 6.97 (m, 2H), 3.89 (s, 6H)

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.1, 162.4, 154.8 (d, *J* = 241.2 Hz), 138.1, 133.8, 132.8, 130.8, 126.4 (d, *J* = 9.8 Hz), 117.4 (d, *J* = 21.7 Hz), 115.6 (d, *J* = 4.4 Hz), 111.0, 109.2, 109.0, 55.4, 33.8.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -60.55.

HRMS (ESI-TOF, m/z): Mass calcd. for C18H14F3NO2Na$^+$ [M+Na]$^+$, 356.0869; found: 356.0867

(5-fluoro-1-methyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3ac)**



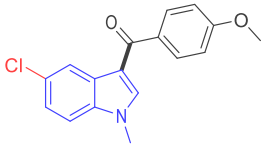
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 – 8.04 (m, 1H), 7.84 – 7.81 (m, 2H), 7.57 (s, 1H), 7.28 (dd, *J* = 9.0, 4.2 Hz, 1H), 7.07 (s, 1H), 7.00 – 6.97 (m, 2H), 3.89 (s, 3H), 3.85 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.46, 162.31, 159.75 (d, *J* = 237.7 Hz), 138.1, 134.0, 133.2, 130.8, 128.1 (d, *J* = 10.9 Hz), 115.6 (d, *J* = 4.8 Hz), 113.6, 111.9 (d, *J* = 26.8 Hz), 110.4 (d, *J* = 9.6 Hz), 108.0 (d, *J* = 24.8 Hz), 55.5, 33.8.

^{19}F NMR (377 MHz, Chloroform-*d*) δ-121.14.

HRMS (ESI-TOF, m/z): Mass calcd. for C17H14FNO2Na^{+} [M+Na]$^{+}$, 306.0901; found: 306.0895

(5-chloro-1-methyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3ad)**

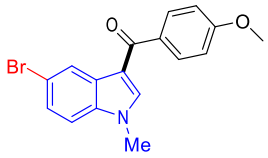


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (dd, *J* = 1.7, 0.8 Hz, 1H), 7.83 – 7.80 (m, 2H), 7.55 (s, 1H), 7.31 – 7.27 (m, 2H), 7.00 – 6.97 (m, 2H), 3.89 (s, 3H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.3, 162.3, 137.7, 135.8, 133.0, 130.8, 128.5, 128.3, 123.9, 122.2, 115.2, 113.6, 110.6, 55.3, 33.7

HRMS (ESI-TOF, m/z): Mass calcd. for C17H14ClNO2Na^{+} [M+Na]$^{+}$, 322.0605; found: 322.0602

(5-bromo-1-methyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3ae)**

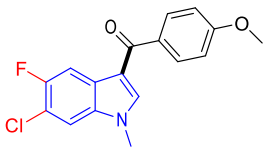


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.54 (d, *J* = 1.8 Hz, 1H), 7.86 – 7.74 (m, 2H), 7.52 (s, 1H), 7.41 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.22 (d, *J* = 8.6 Hz, 1H), 7.01 – 6.94 (m, 2H), 3.89 (s, 3H), 3.83 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.3, 162.3, 137.6, 136.1, 133.0, 130.8, 128.8, 126.5, 125.3, 116.2, 115.1, 113.6, 111.0, 55.4, 33.7.

HRMS (ESI-TOF, m/z): Mass calcd. for C17H14BrNO2Na^{+} [M+Na]$^{+}$, 366.0100; found: 366.0092.

(6-chloro-5-fluoro-1-methyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone **(3af)**



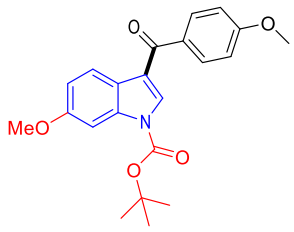
^{1}H NMR (400 MHz, Chloroform-*d*) δ8.14 (d, J = 9.8 Hz, 1H), 7.83 – 7.76 (m, 2H), 7.56 (s, 1H), 7.37 (d, J = 5.9 Hz, 1H), 7.03 – 6.93 (m, 2H), 3.89 (s, 3H), 3.82 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.1, 162.4, 154.8 (d, *J* = 241.1 Hz), 138.1, 133.8, 132.8, 130.8, 126.4 (d, *J* = 9.9 Hz), 117.3, 115.6 (d, *J* = 4.5 Hz), 113.6, 111.0, 109.1 (d, *J* = 24.8 Hz), 55.4, 33.8.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -123.18.

HRMS(ESI-TOF,m/z):Mass calcd. for C17H13ClFNO2Na + [M+Na]+, 340.0511; found: 340.0503.

tert-butyl 6-methoxy-3-(4-methoxybenzoyl)-1*H*-indole-1-carboxylate **(3ag)**

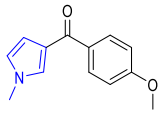


^{1}H NMR (400 MHz, Chloroform-*d*)δ 8.12 (d, *J* = 8.7 Hz, 1H), 7.97 – 7.84 (m, 3H), 7.72 (d, *J* = 2.4 Hz, 1H), 6.99 (dd, *J* = 8.7, 1.9 Hz, 3H), 3.90 (d, *J* = 1.3 Hz, 6H), 1.69 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*)δ 190.0, 162.9, 158.5, 149.4, 136.6, 132.2, 131.7, 131.3, 123.0, 122.2, 119.7, 113.7, 113.3, 99.1, 85.1, 55.6, 55.5, 29.7, 28.1.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{22}H_{23}NO_5Na^+$ $[M+Na]^+$, 404.1468; found: 404.1458.

(4-methoxyphenyl)(1-methyl-1H-pyrrol-3-yl)methanone **(3ah)**

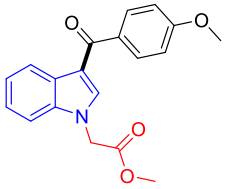


^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 – 7.84 (m, 2H), 7.19 (t, *J* = 1.8 Hz, 1H), 6.97 – 6.93 (m, 2H), 6.66 (dd, *J* = 2.8, 1.8 Hz, 1H), 6.63 (dd, *J* = 2.8, 2.0 Hz, 1H), 3.87 (s, 3H), 3.71 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.4, 162.3, 132.7, 131.1, 128.3, 124.8, 123.0, 113.4, 111.2, 55.4, 36.6.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{13}H_{14}NO_2^+$ $[M+H]^+$, 216.1019; found: 216.1013.

methyl 2-(3-(4-methoxybenzoyl)-1*H*-indol-1-yl)acetate **(4)**

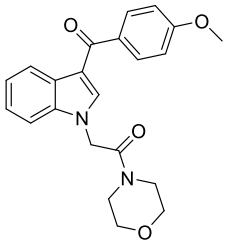


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 – 8.35 (m, 1H), 7.89 – 7.84 (m, 2H), 7.59 (s, 1H), 7.35 – 7.26 (m, 3H), 7.00 – 6.96 (m, 2H), 4.90 (s, 2H), 3.88 (s, 3H), 3.77 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.8, 168.0, 162.3, 137.1, 136., 133.13, 131.0, 127.2, 123.9, 122.8, 122.7, 116.8, 113.5, 109.2, 55.4, 52.8, 47.9.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{19}H_{17}NO_4Na^+$ $[M+Na]^+$, 346.1050; found: 346.1045.

2-(3-(4-methoxybenzoyl)-1*H*-indol-1-yl)-1-morpholinoethan-1-one **(5)**

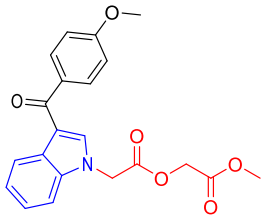


^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 – 8.36 (m, 1H), 7.87 – 7.80 (m, 2H), 7.56 (s, 1H), 7.31 (dt, *J* = 7.1, 3.6 Hz, 2H), 7.24 (dd, *J* = 6.3, 3.0 Hz, 1H), 7.01 – 6.92 (m, 2H), 4.90 (s, 2H), 3.88 (s, 3H), 3.76 – 3.26 (m, 8H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.1, 162.4, 156.0, 153.6, 138.1, 133.8, 132.8, 130.8, 126.5, 126.4, 117.5, 117.3, 115.6, 115.6, 113.6, 111.01, 109.2, 109.0, 55.4, 33.8.

HRMS (ESI-TOF, m/z): Mass calcd. for $C_{22}H_{22}N_2O_4Na^+$ $[M+Na]^+$, 401.1472; found: 401.1463.

2-methoxy-2-oxoethyl 2-(3-(argiocarbonyl)-1*H*-indol-1-yl)acetate **(6)**



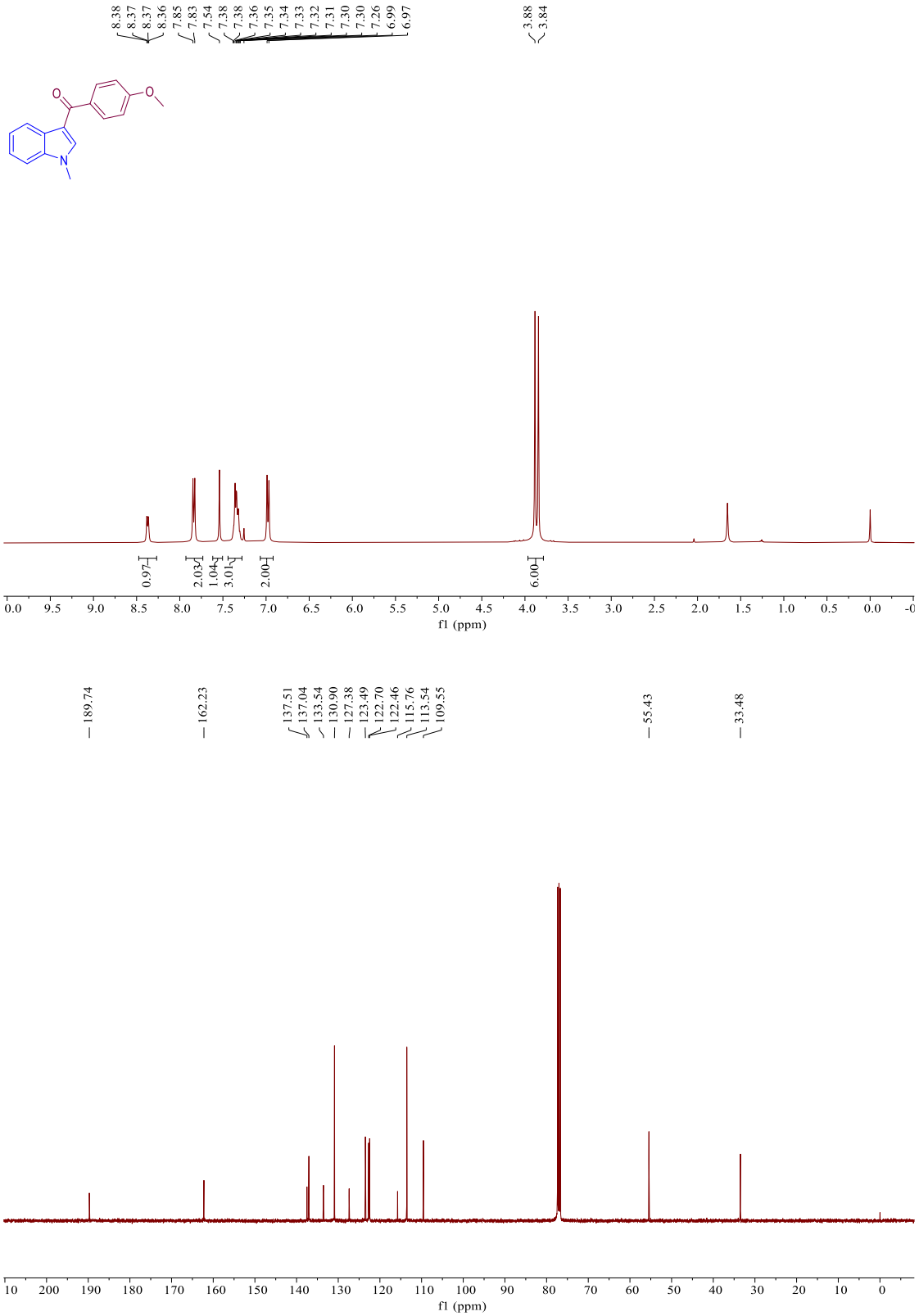
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 – 8.36 (m, 1H), 7.89 – 7.85 (m, 2H), 7.62 (s, 1H), 7.37 – 7.31 (m, 3H), 7.01 – 6.97 (m, 2H), 5.03 (s, 2H), 4.70 (s, 2H), 3.89 (s, 3H), 3.76 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.1, 162.4, 156.0, 153.6, 138.1, 133.8, 132.8, 130.8, 126.5, 126.4, 117.5, 117.3, 115.6, 115.6, 113.6, 111.0, 109.2, 109.0, 55.4, 33.8.

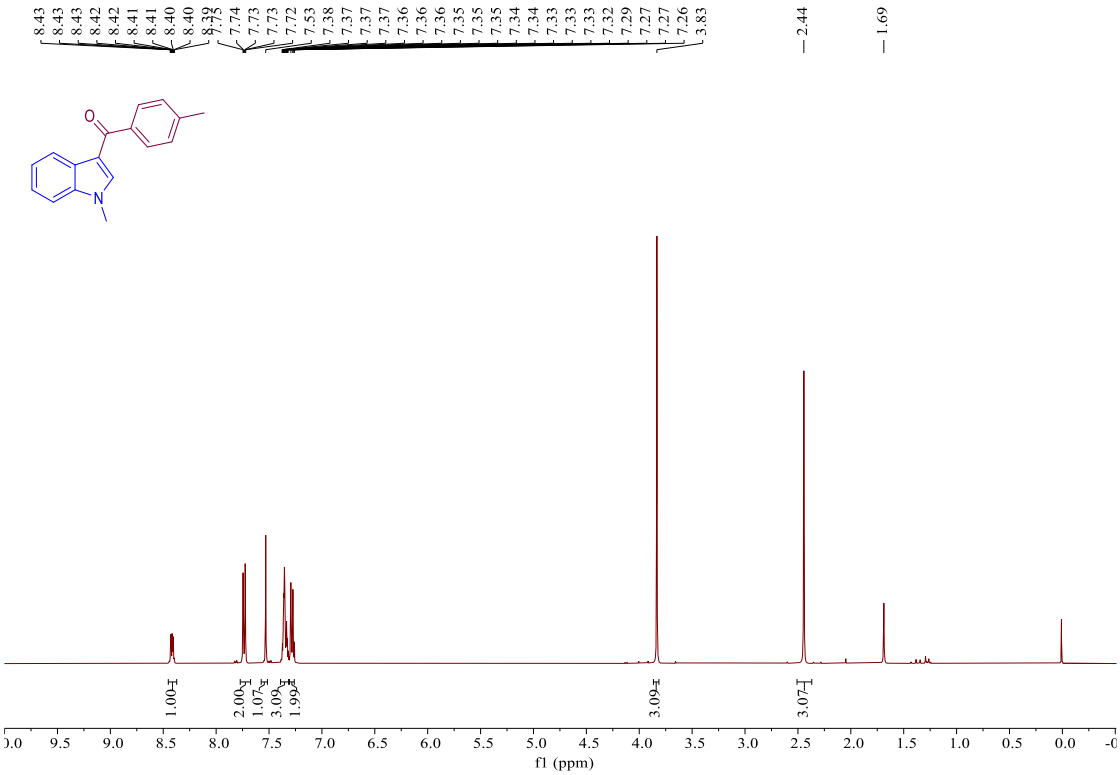
HRMS (ESI-TOF, m/z): Mass calcd. for $C_{21}H_{19}NO_6Na^+$ $[M+Na]^+$, 404.1105; found: 404.1099.

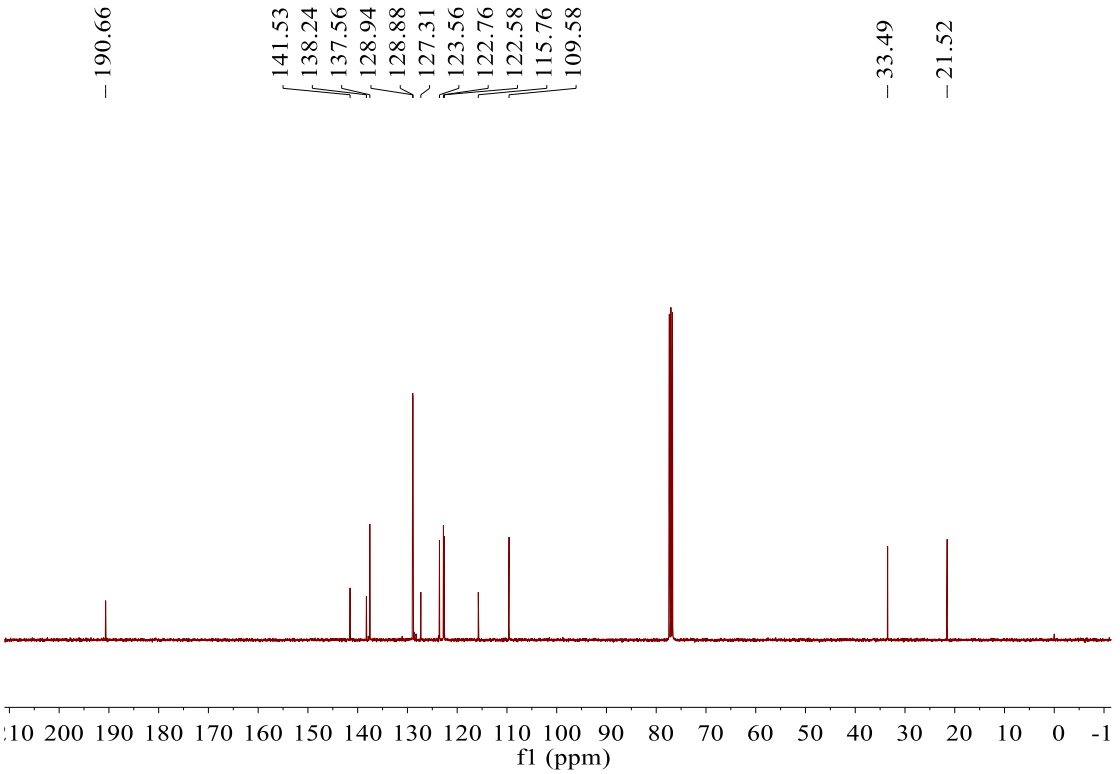
XI. NMR spectra

(4-methoxyphenyl)(1-methyl-1H-indol-3-yl)methanone **（3a）**

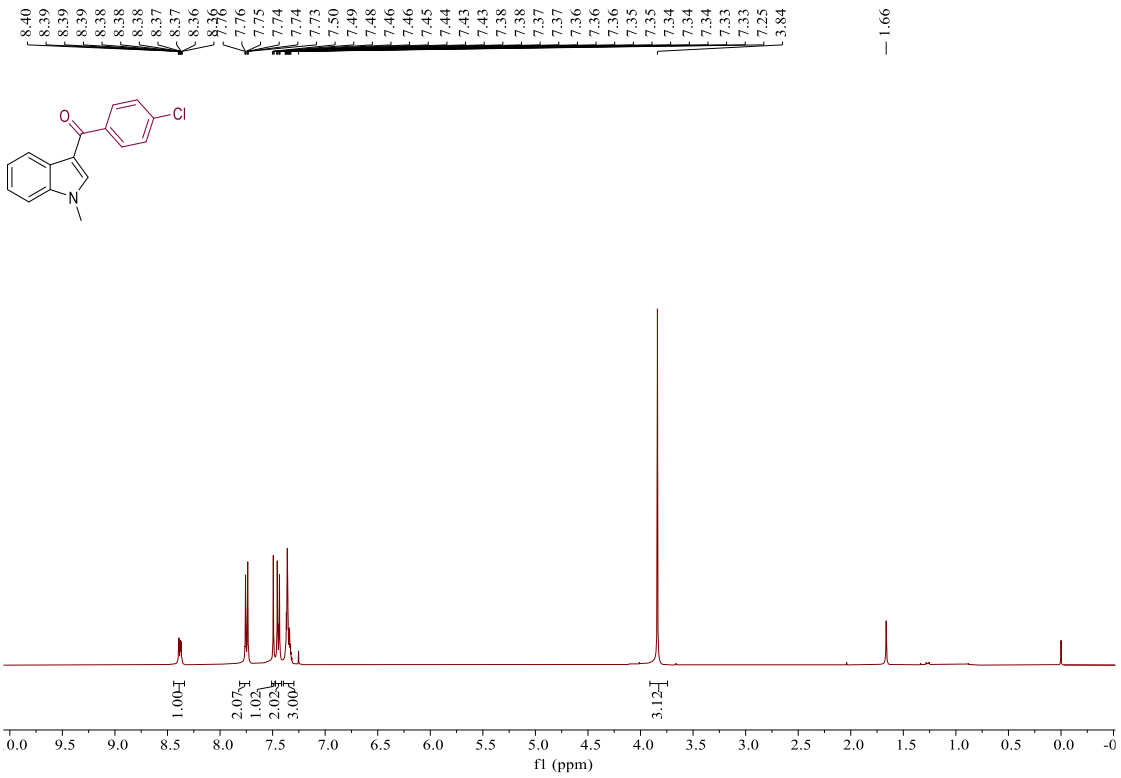


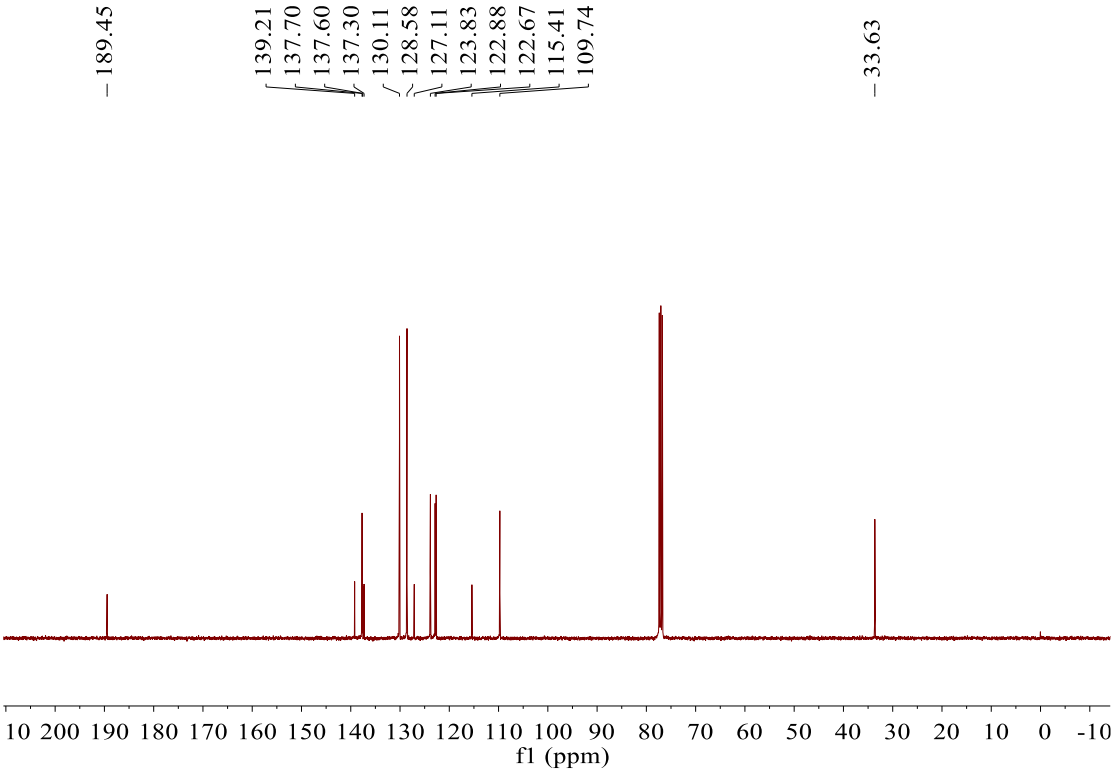
(1-methyl-1H-indol-3-yl)(p-tolyl)methanone **(3b)**



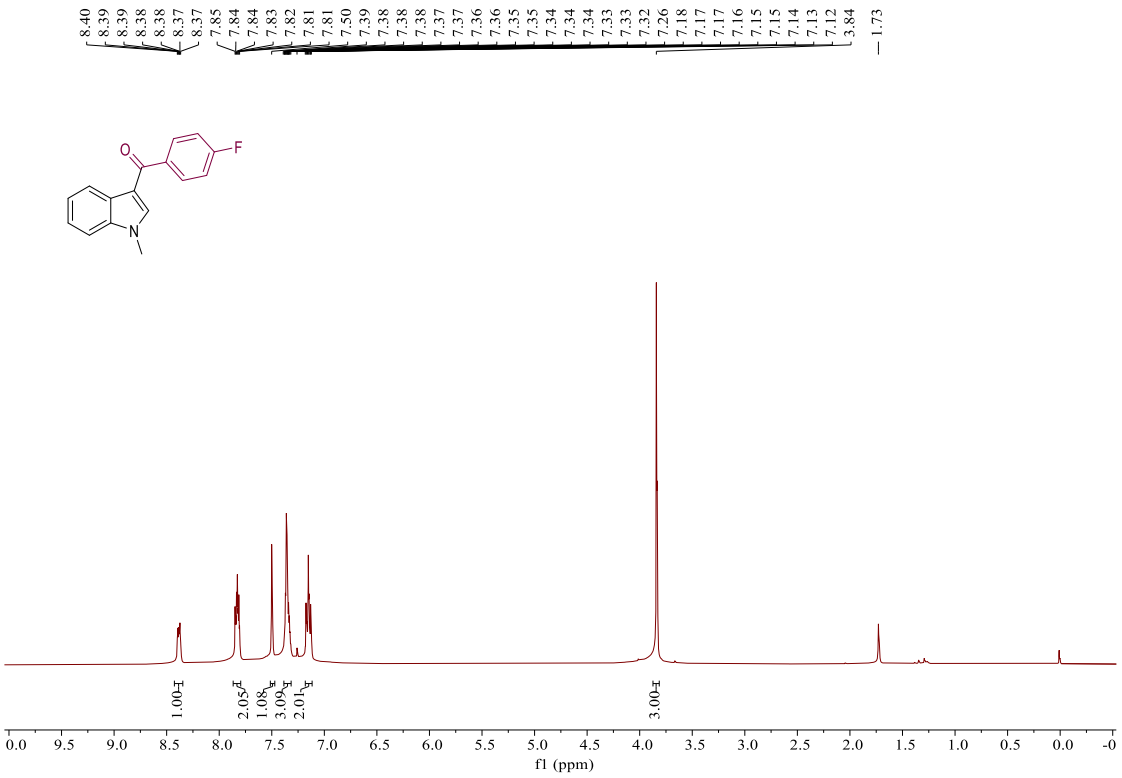


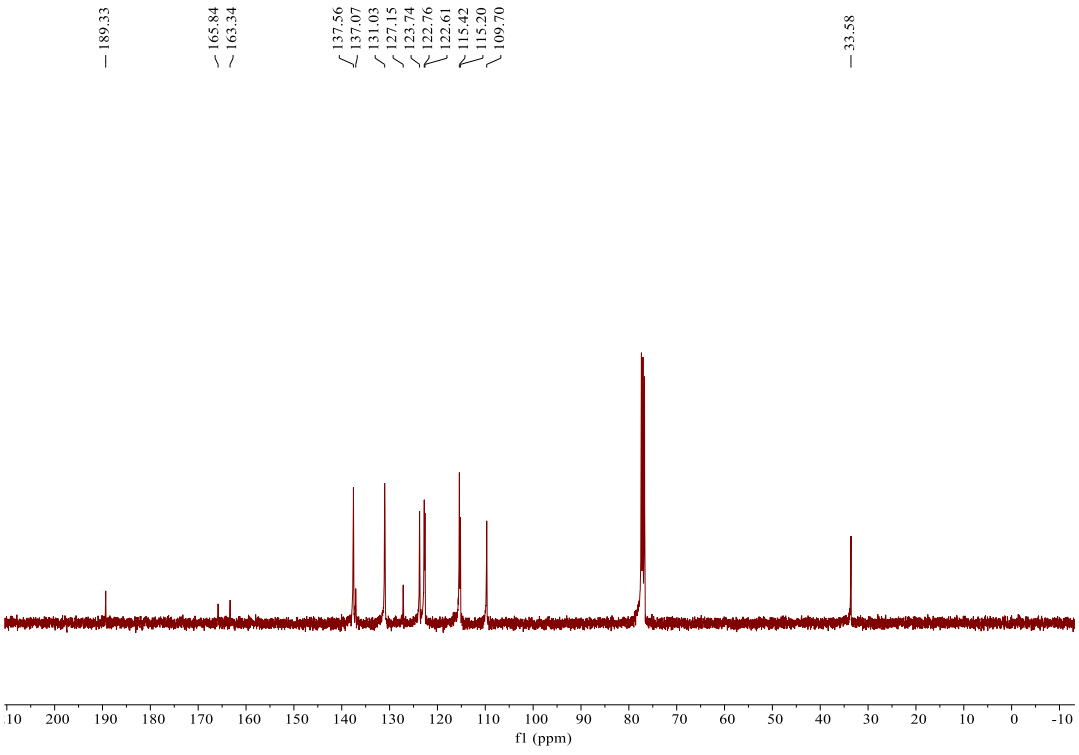
(4-chlorophenyl)(1-methyl-1H-indol-3-yl)methanone **(3c)**

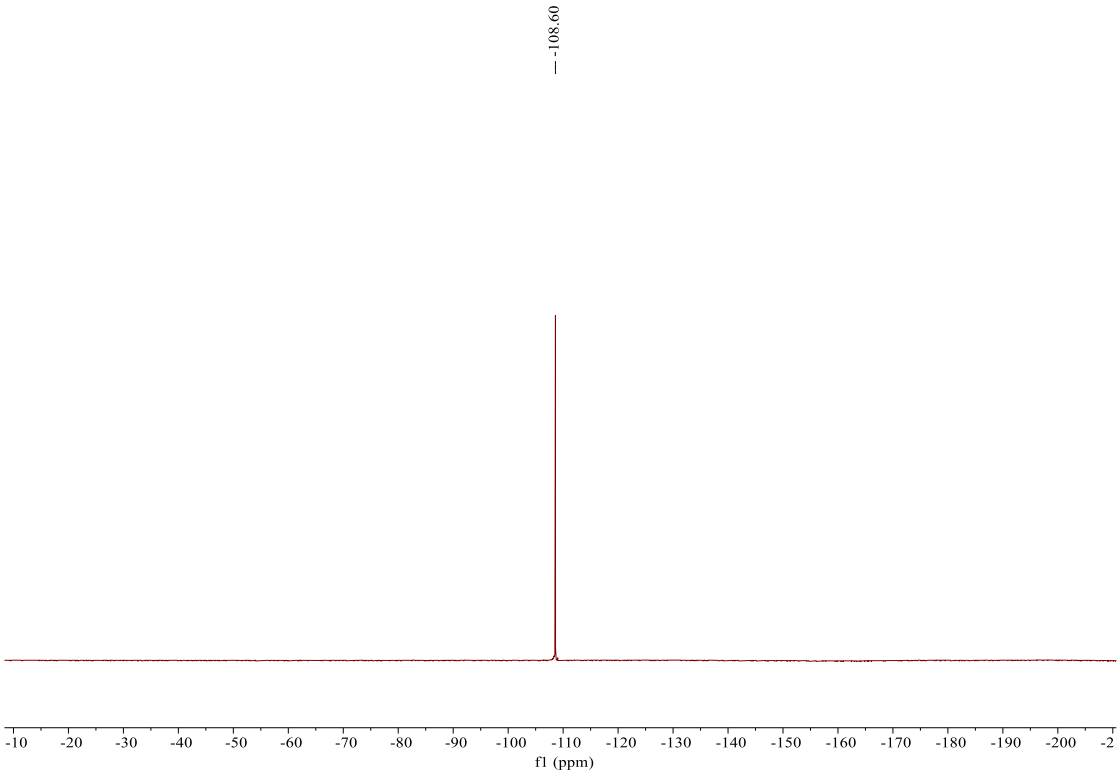




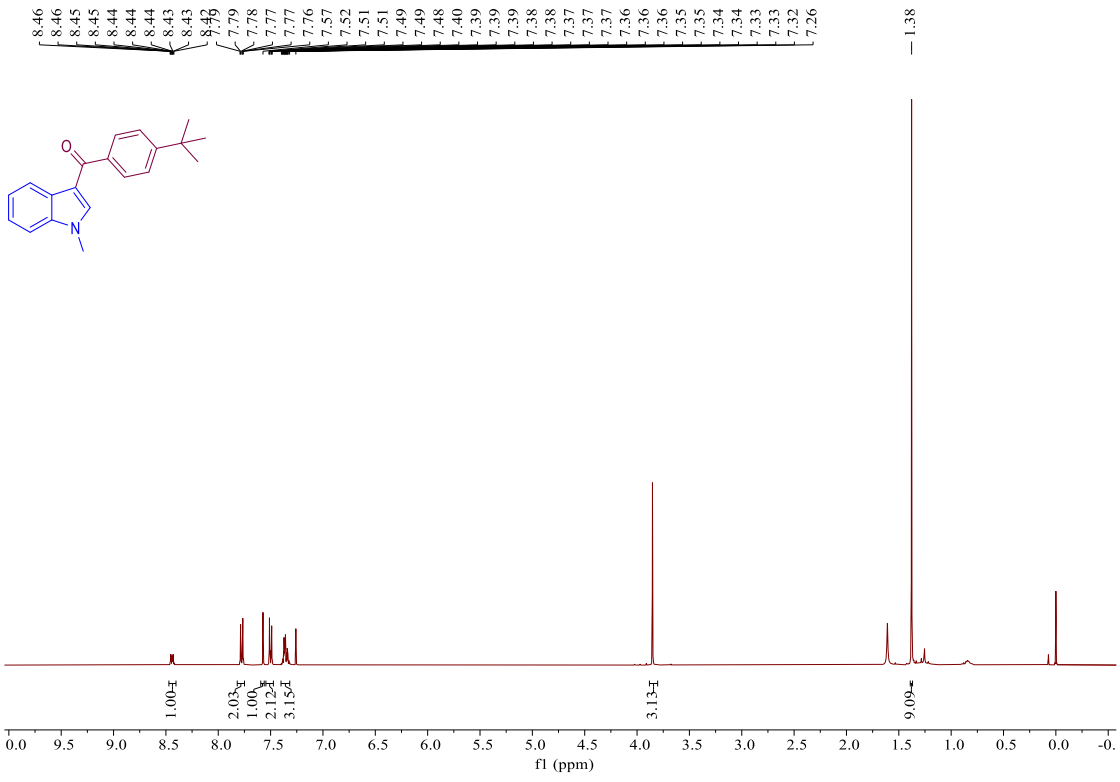
(4-fluorophenyl)(1-methyl-1H-indol-3-yl)methanone **(3d)**

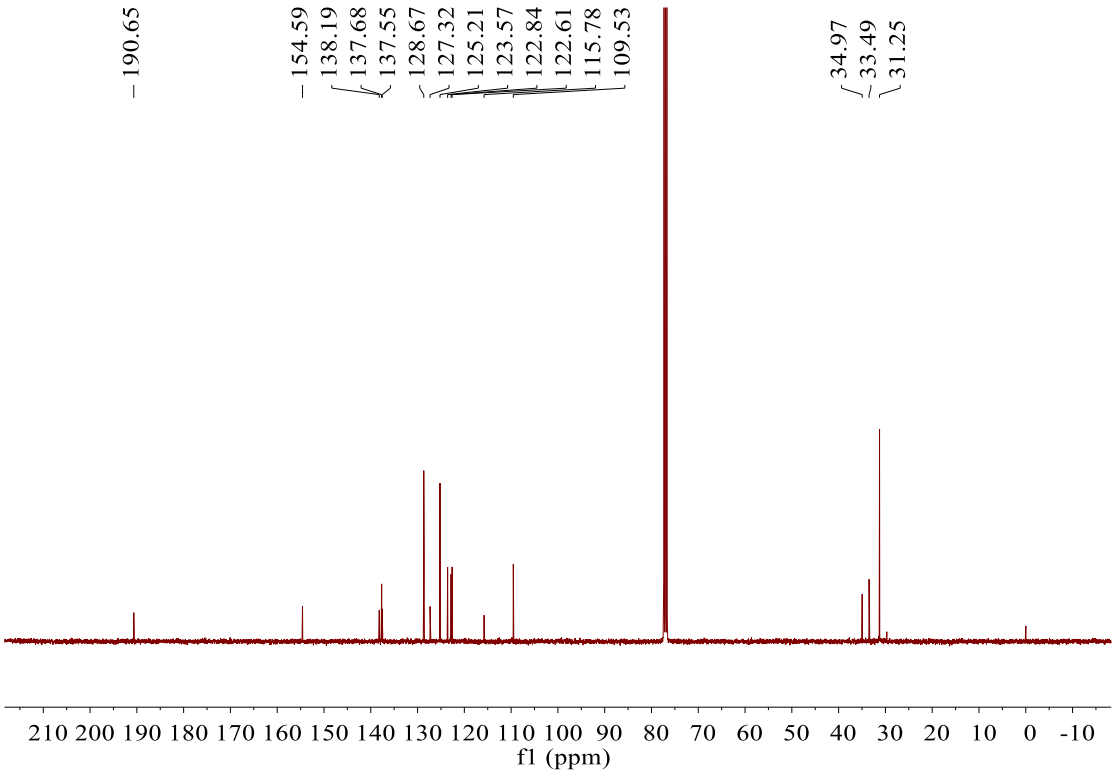




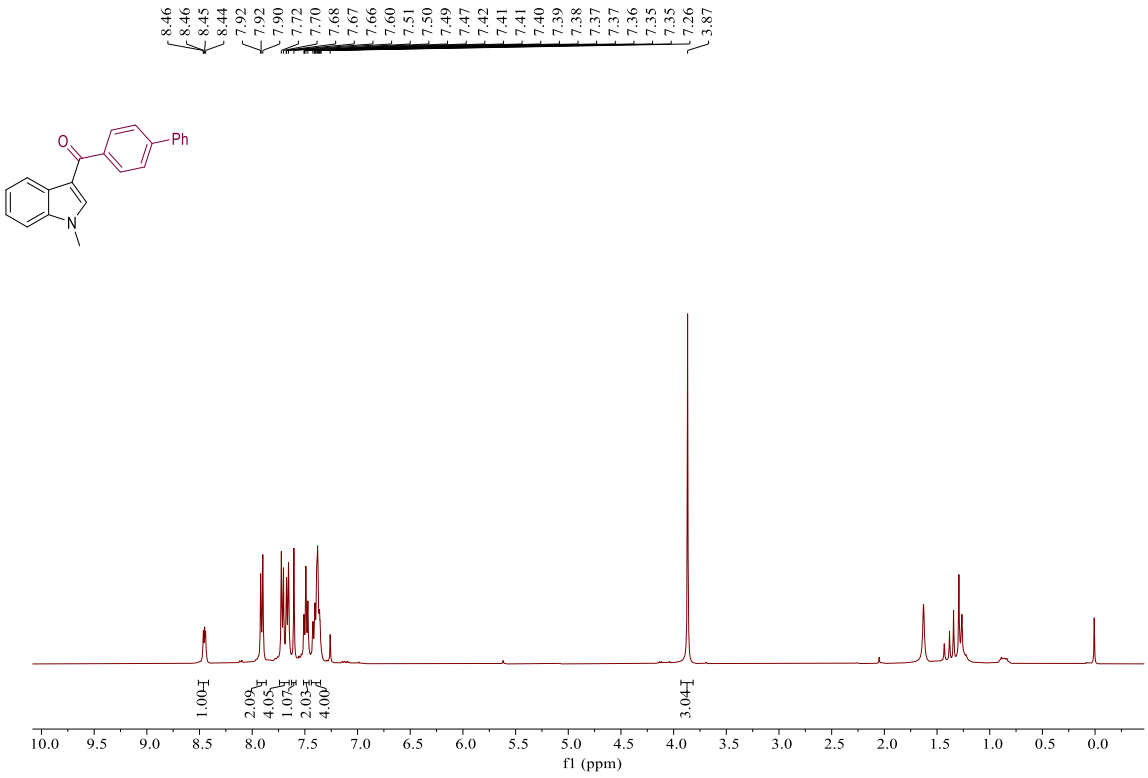


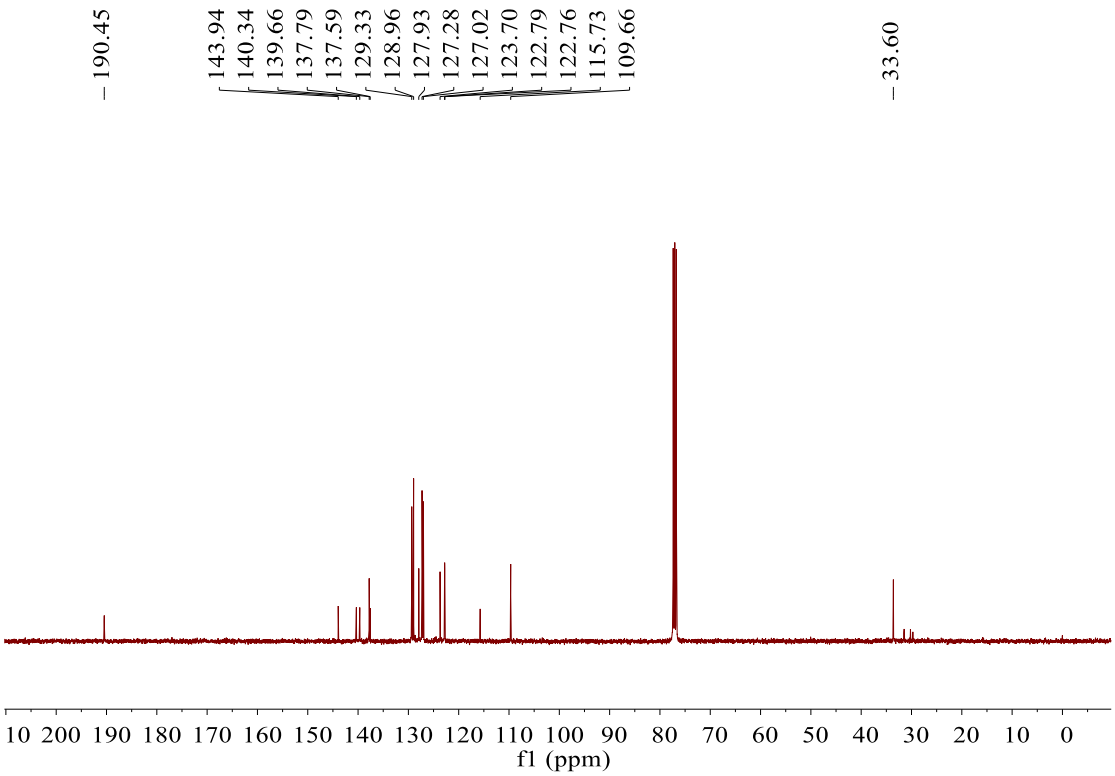
(4-(tert-butyl)phenyl)(1-methyl-1H-indol-3-yl)methanone **(3e)**



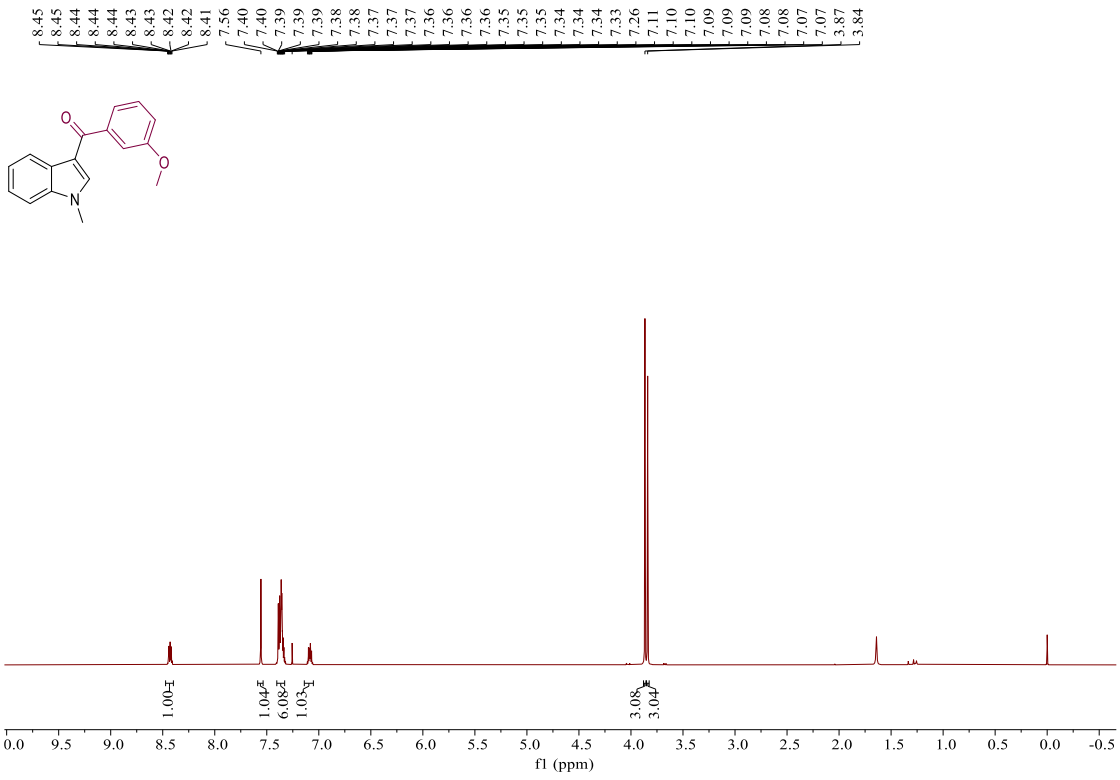


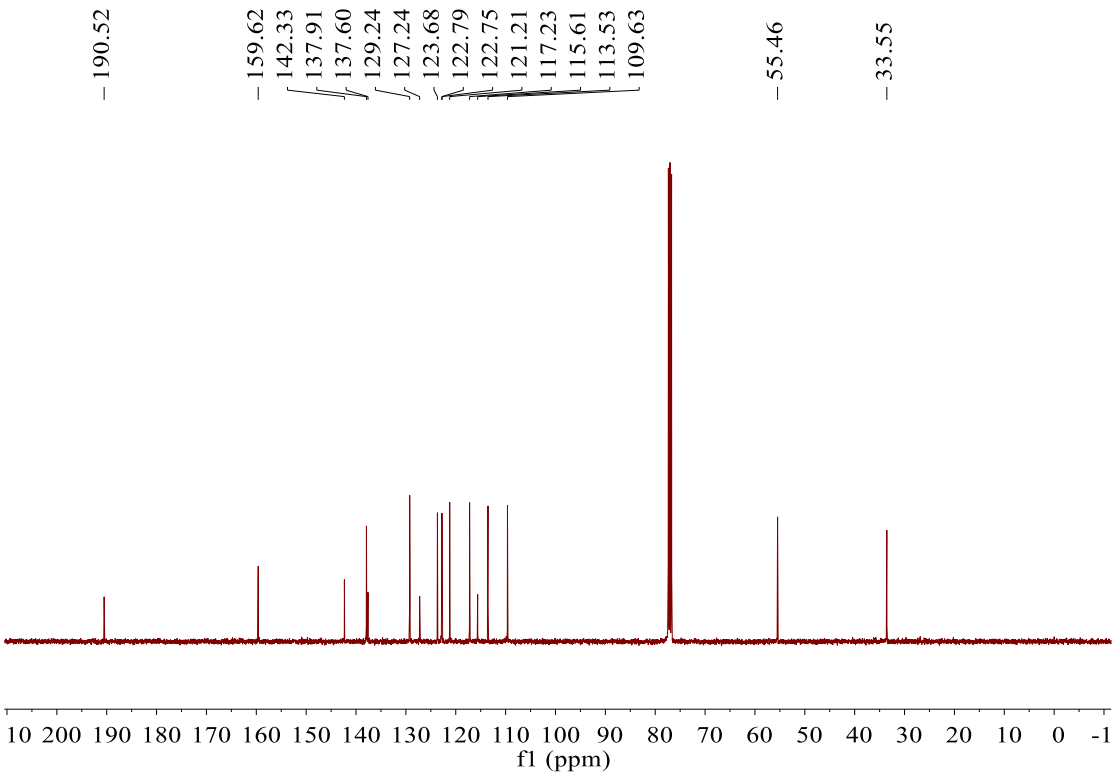
[1,1'-biphenyl]-4-yl(1-methyl-1H-indol-3-yl)methanone **(3f)**



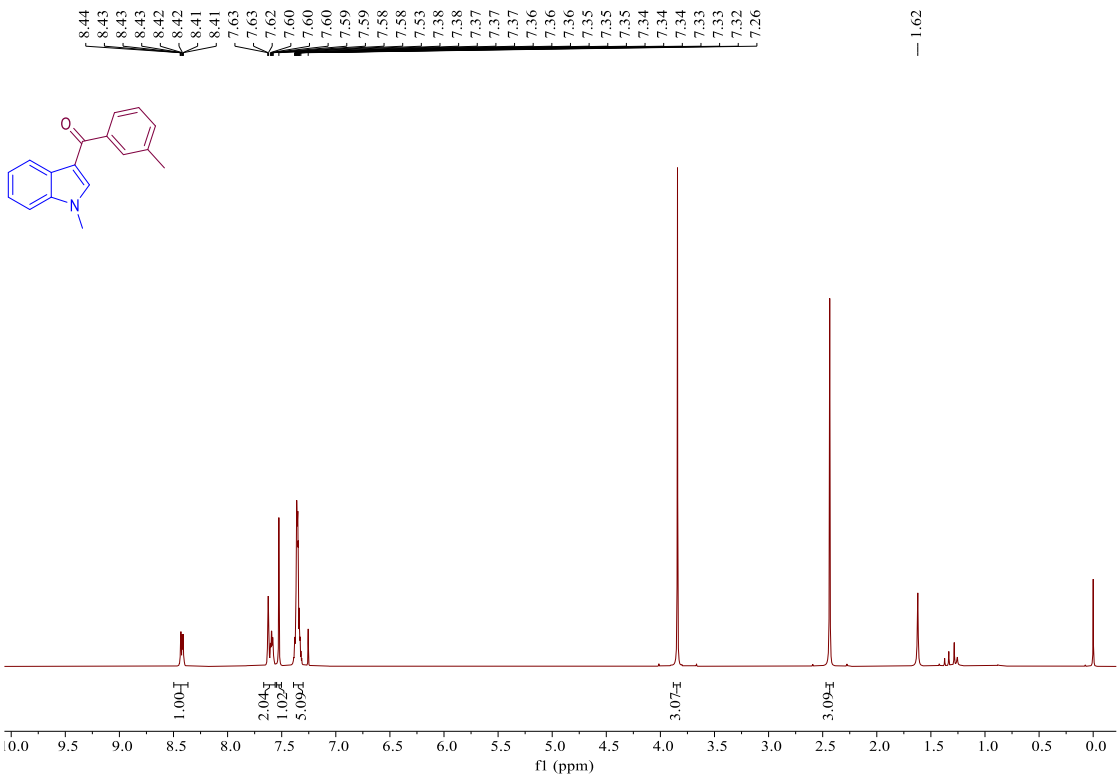


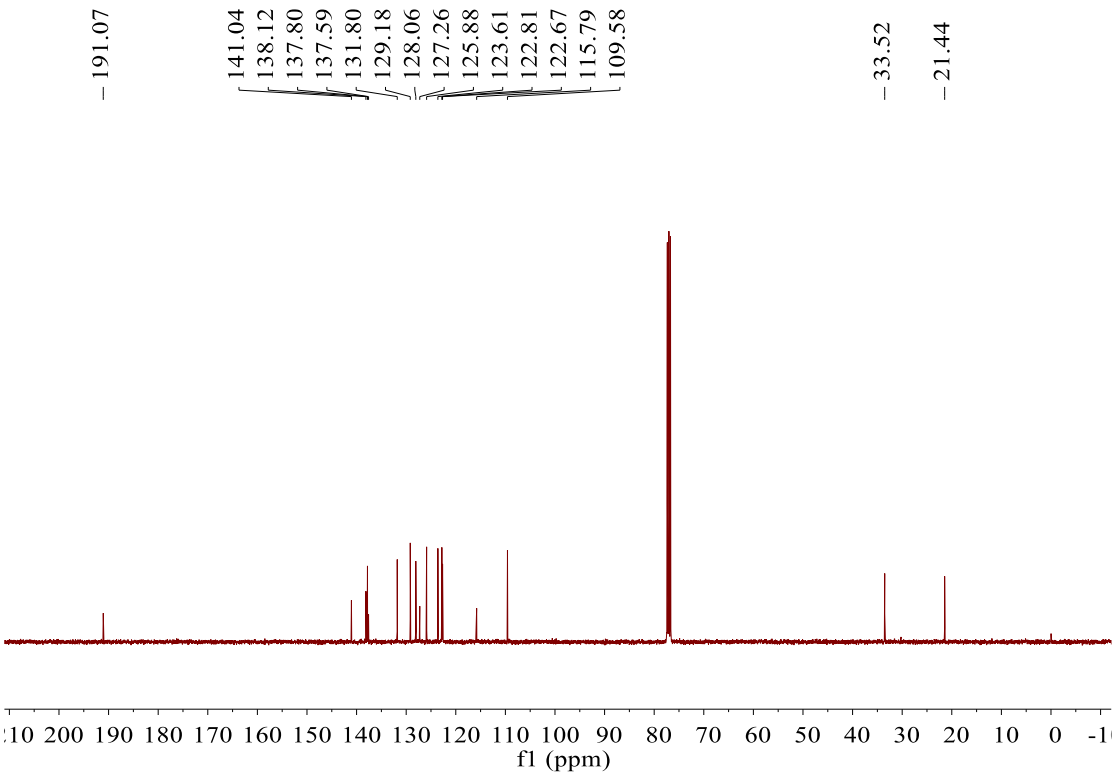
(3-methoxyphenyl)(1-methyl-1H-indol-3-yl)methanone **(3g)**



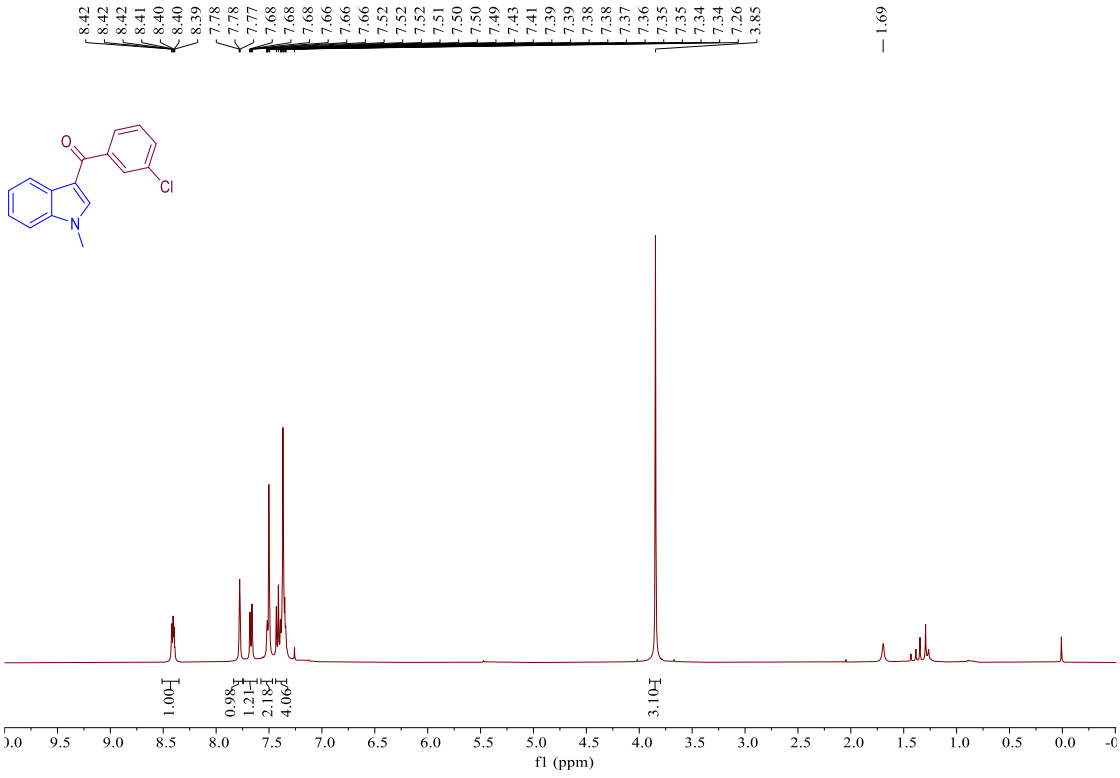


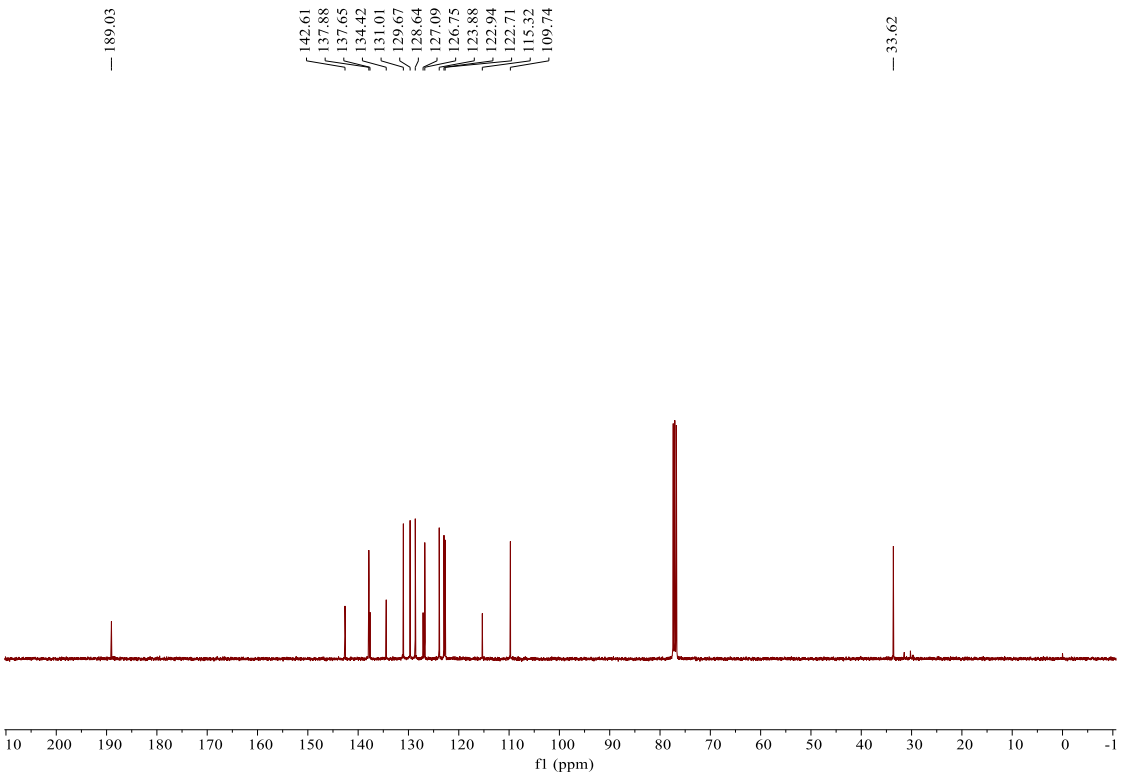
(1-methyl-1H-indol-3-yl)(m-tolyl)methanone **(3h)**



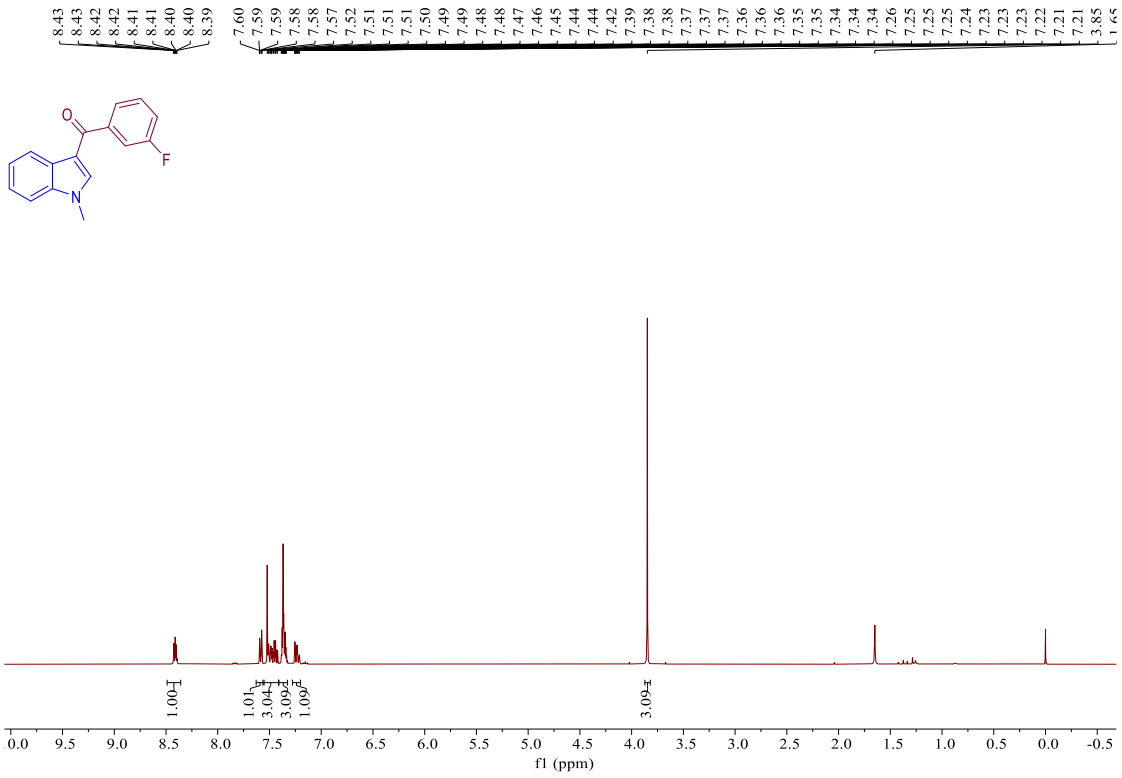


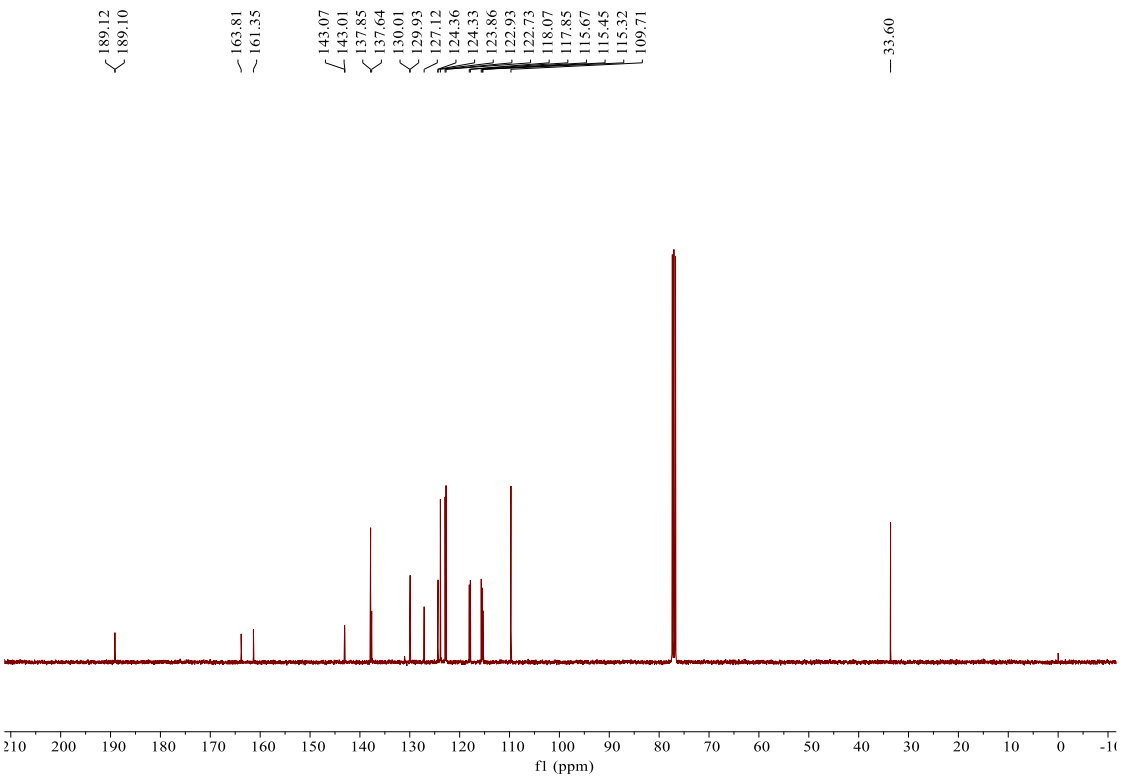
(3-chlorophenyl)(1-methyl-1H-indol-3-yl)methanone **(3i)**

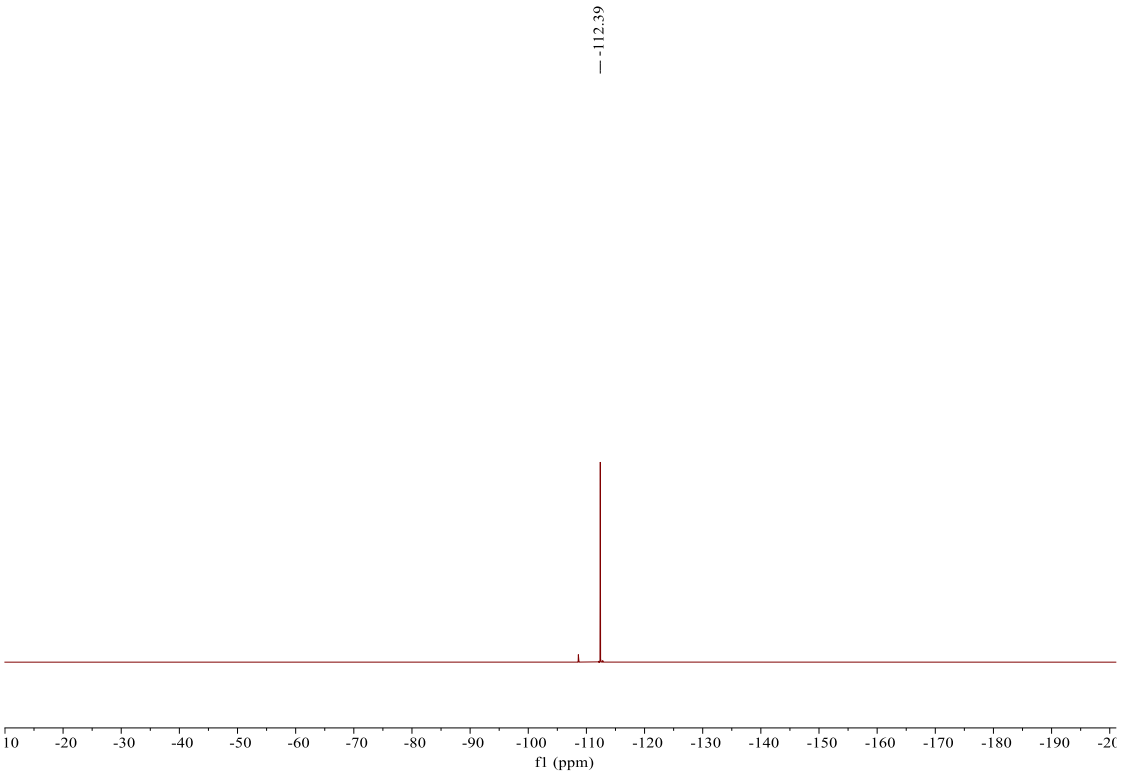




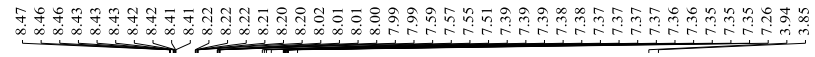
(3-fluorophenyl)(1-methyl-1H-indol-3-yl)methanone **(3j)**

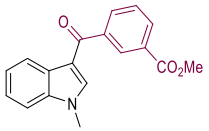


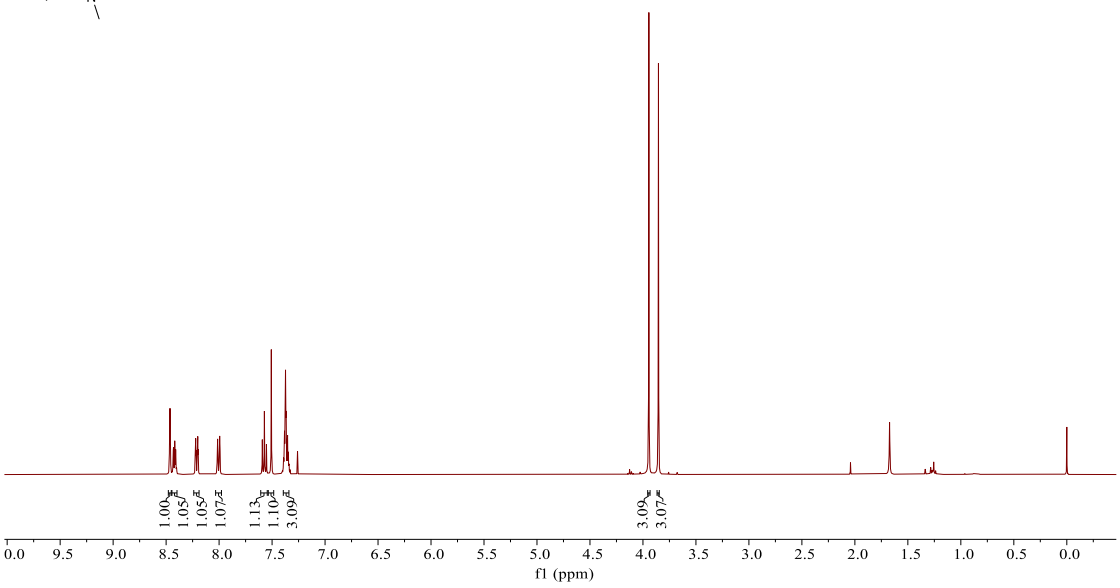

189.12
189.10
163.81
161.35
143.07
143.01
137.85
137.64
130.01
129.93
127.12
124.36
124.33
123.86
122.93
122.73
118.07
117.85
115.67
115.45
115.32
109.71
33.60
f1 (ppm)

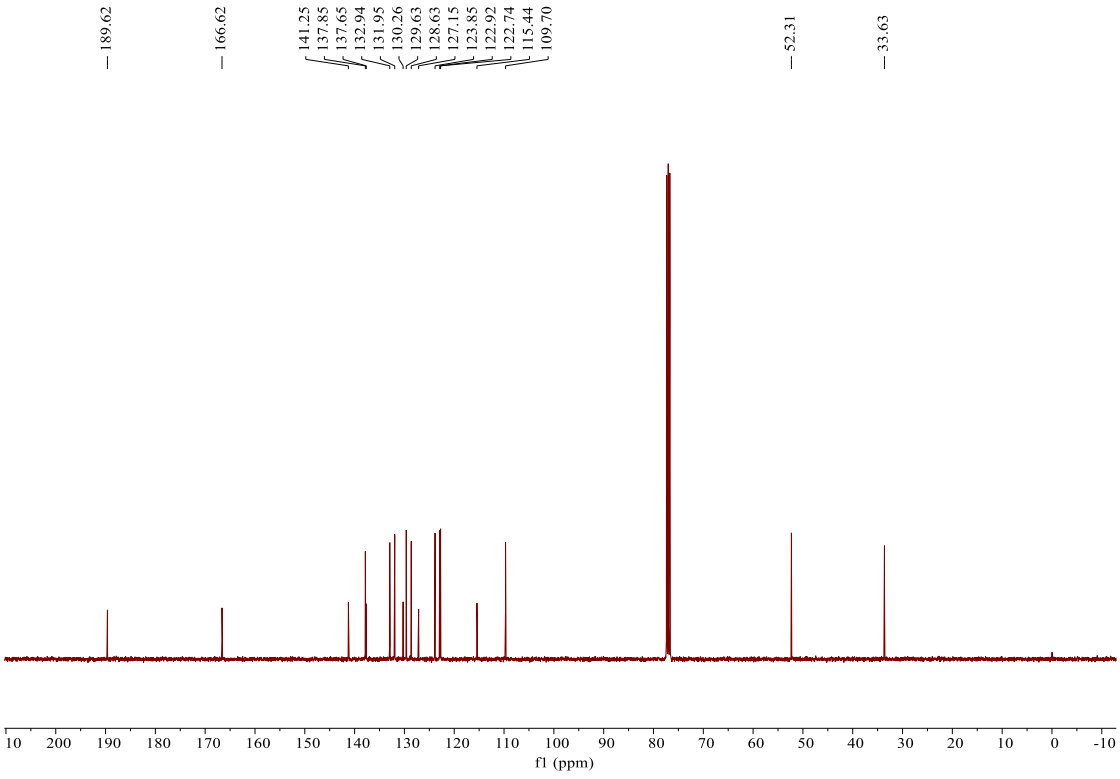

-112.39
f1 (ppm)

methyl 3-(1-methyl-1H-indole-3-carbonyl)benzoate **(3k)**

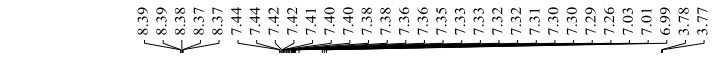


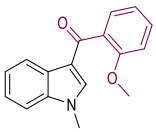


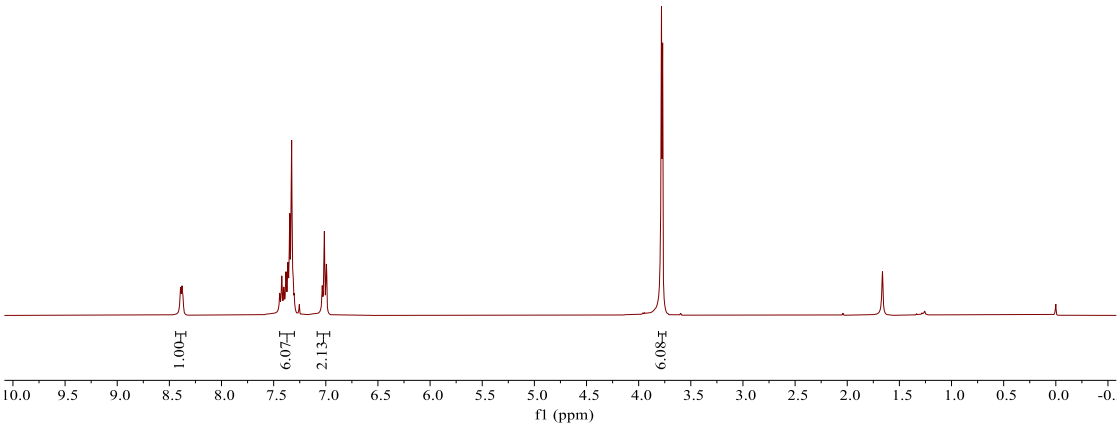


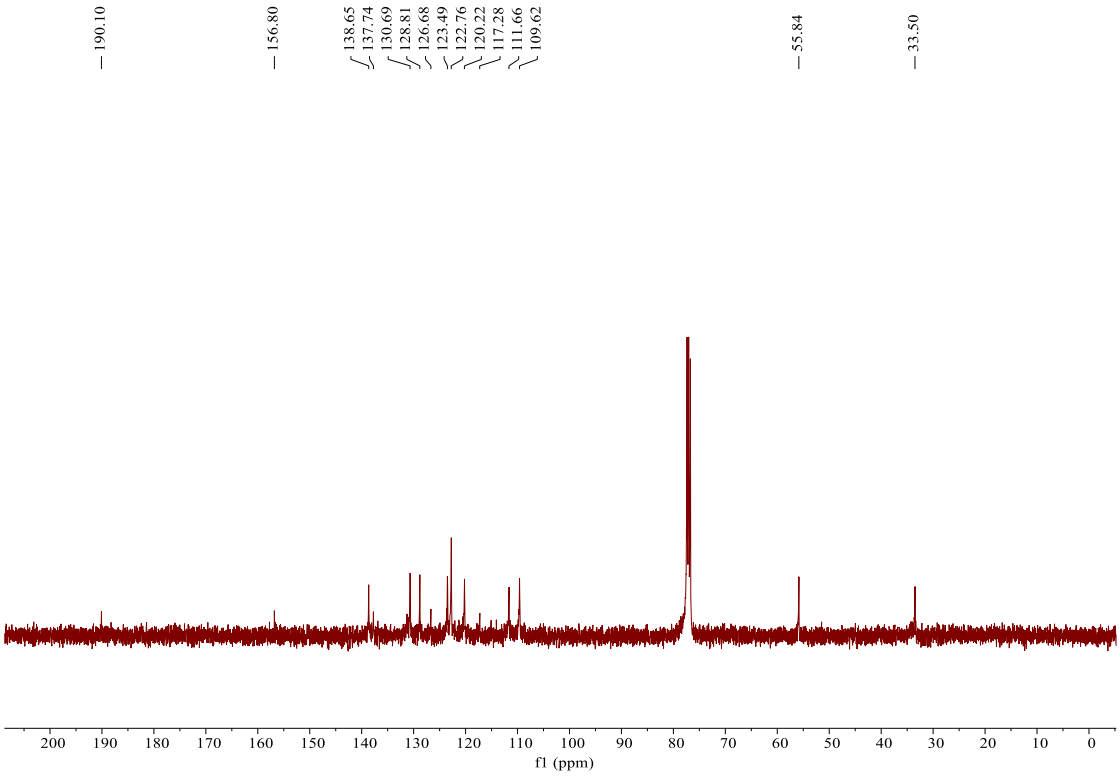


(2-methoxyphenyl)(1-methyl-1H-indol-3-yl)methanone **(3l)**

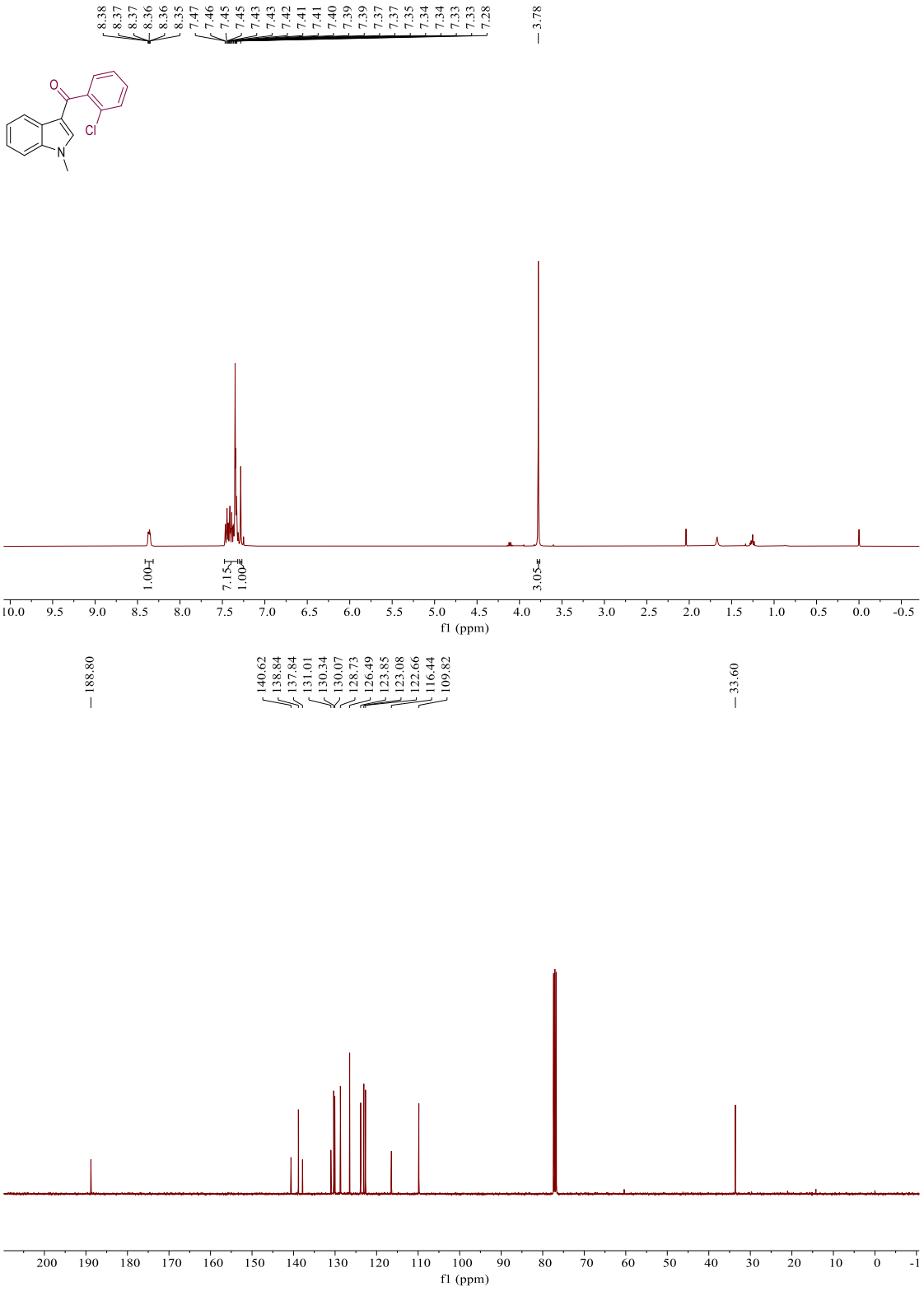




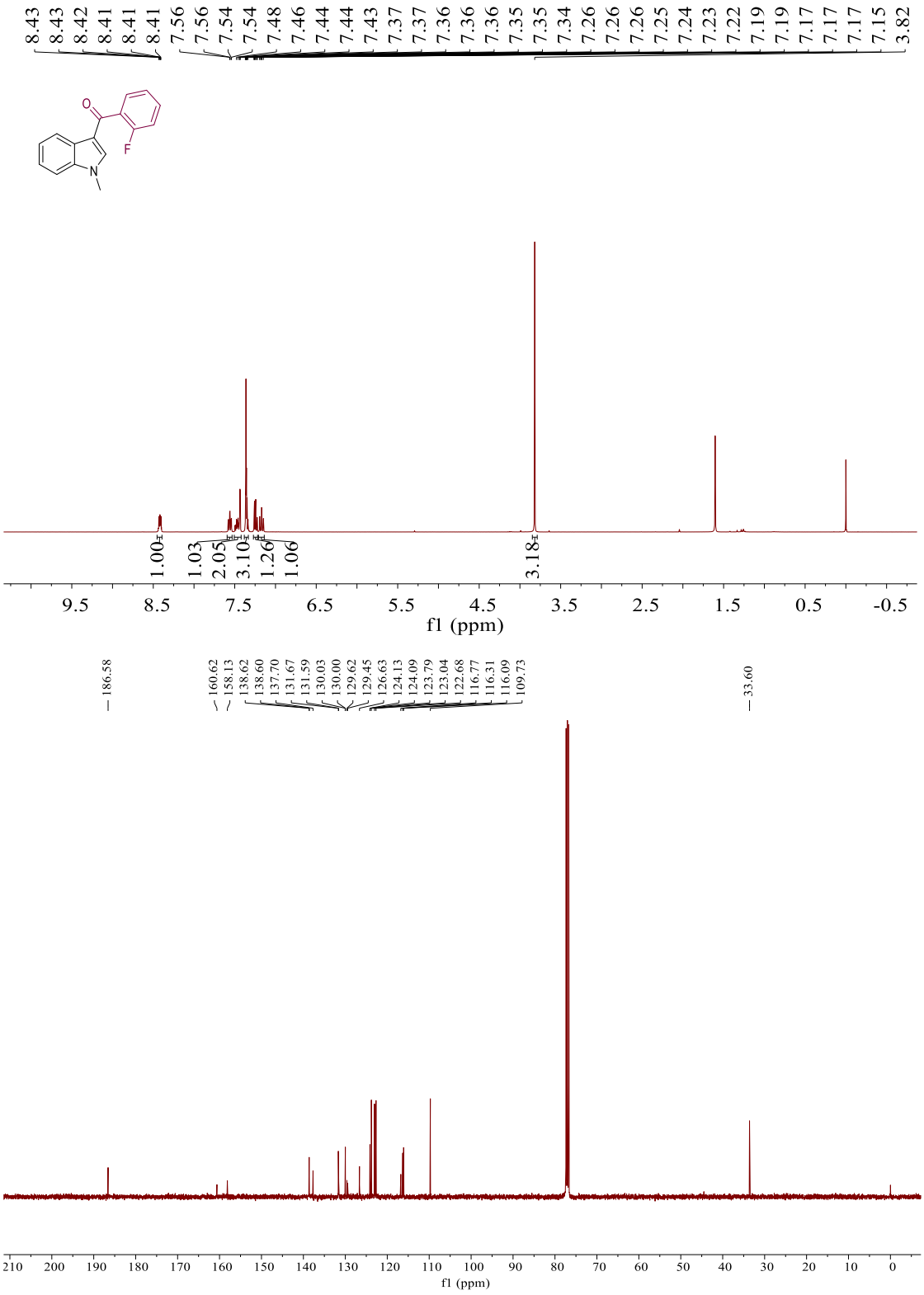


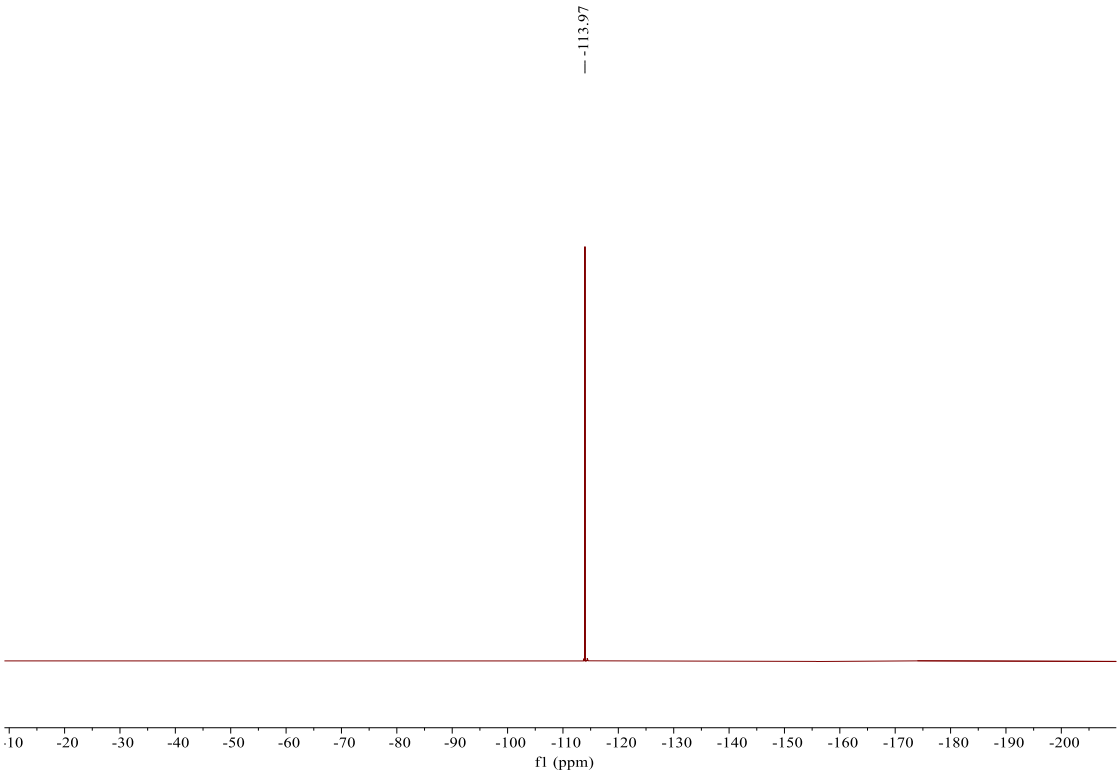


(2-chlorophenyl)(1-methyl-1H-indol-3-yl)methanone **(3m)**

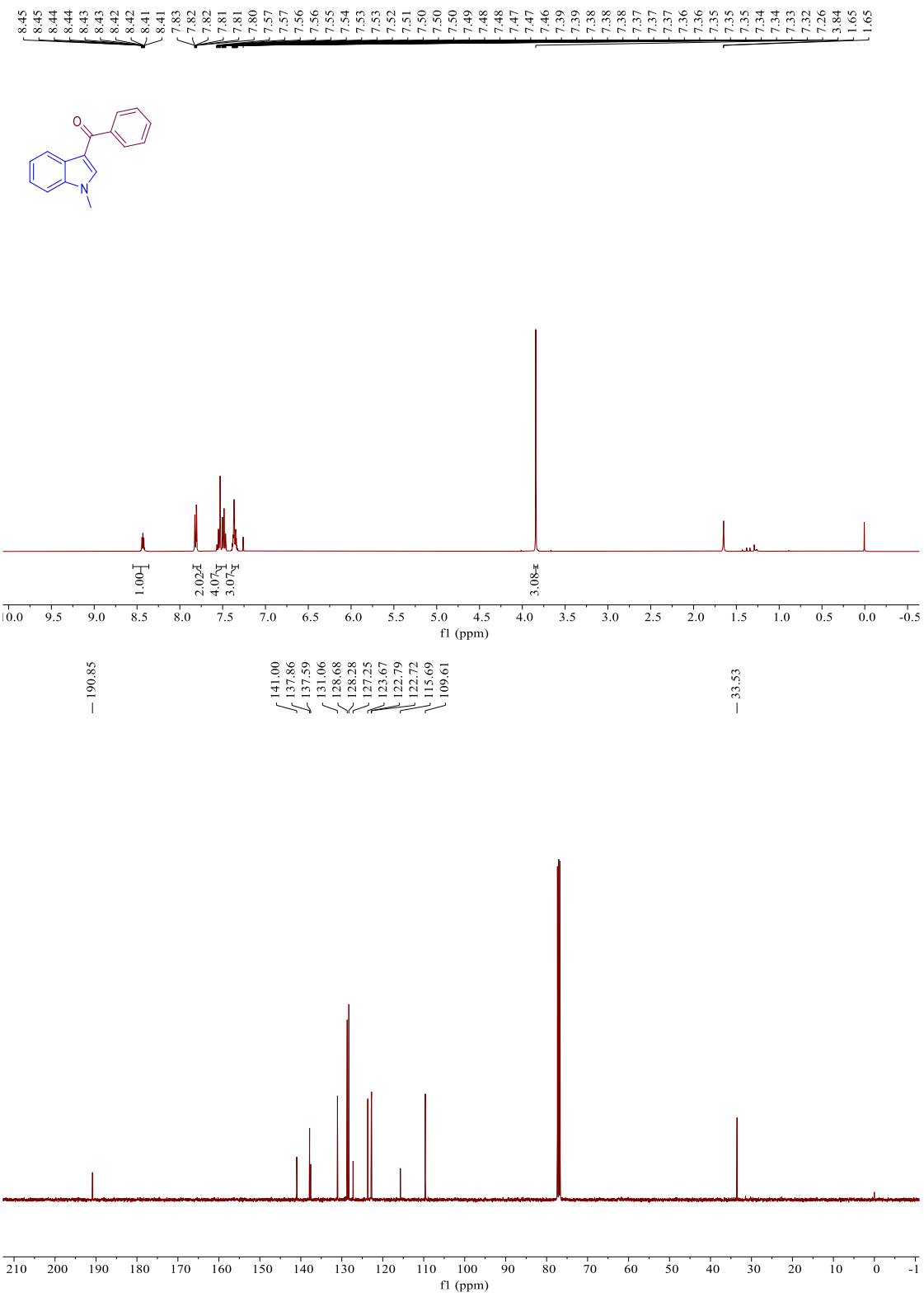


(2-fluorophenyl)(1-methyl-1H-indol-3-yl)methanone **(3n)**

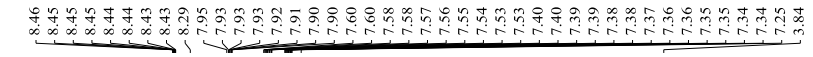


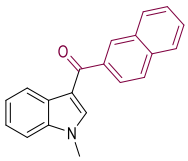

-113.97
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

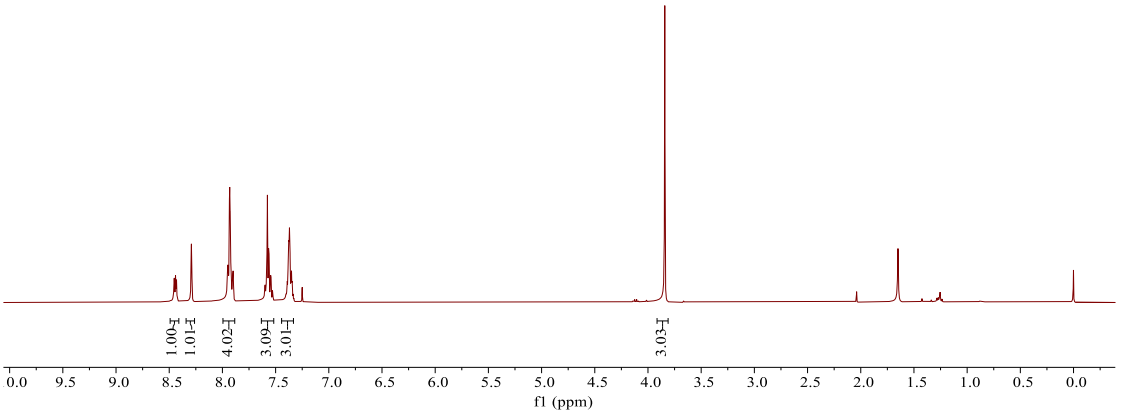
(1-methyl-1H-indol-3-yl)(phenyl)methanone **(3o)**

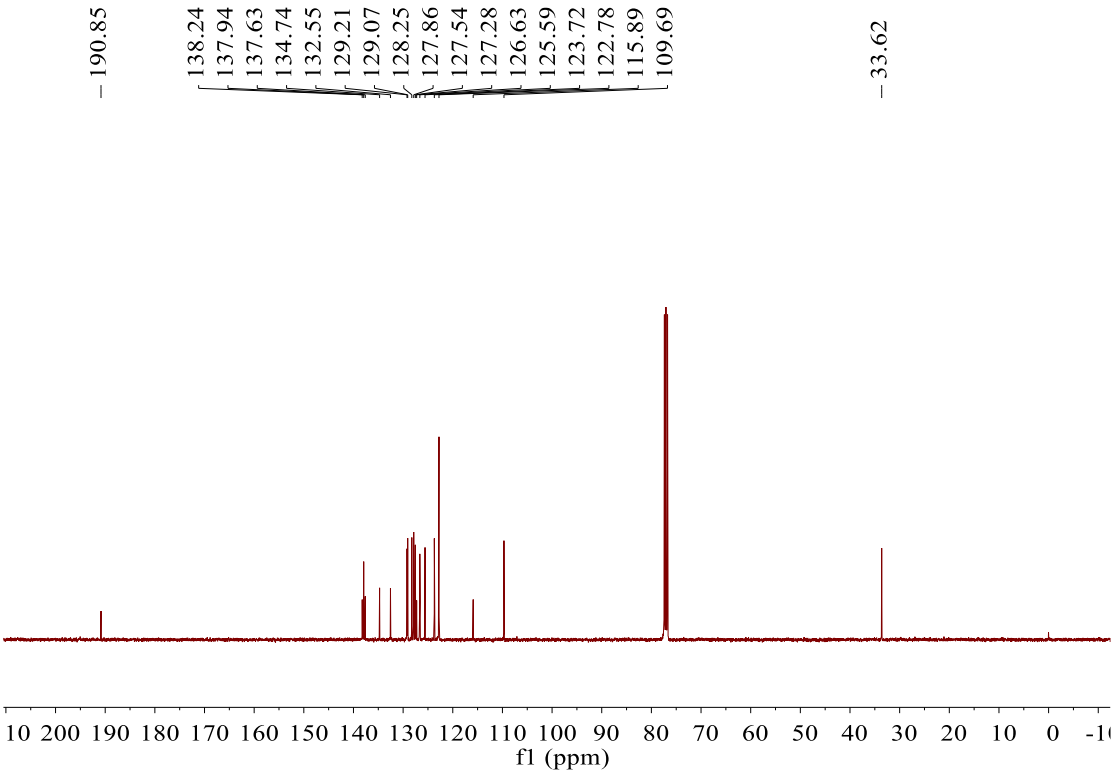


(1-methyl-1H-indol-3-yl)(naphthalen-2-yl)methanone **(3p)**

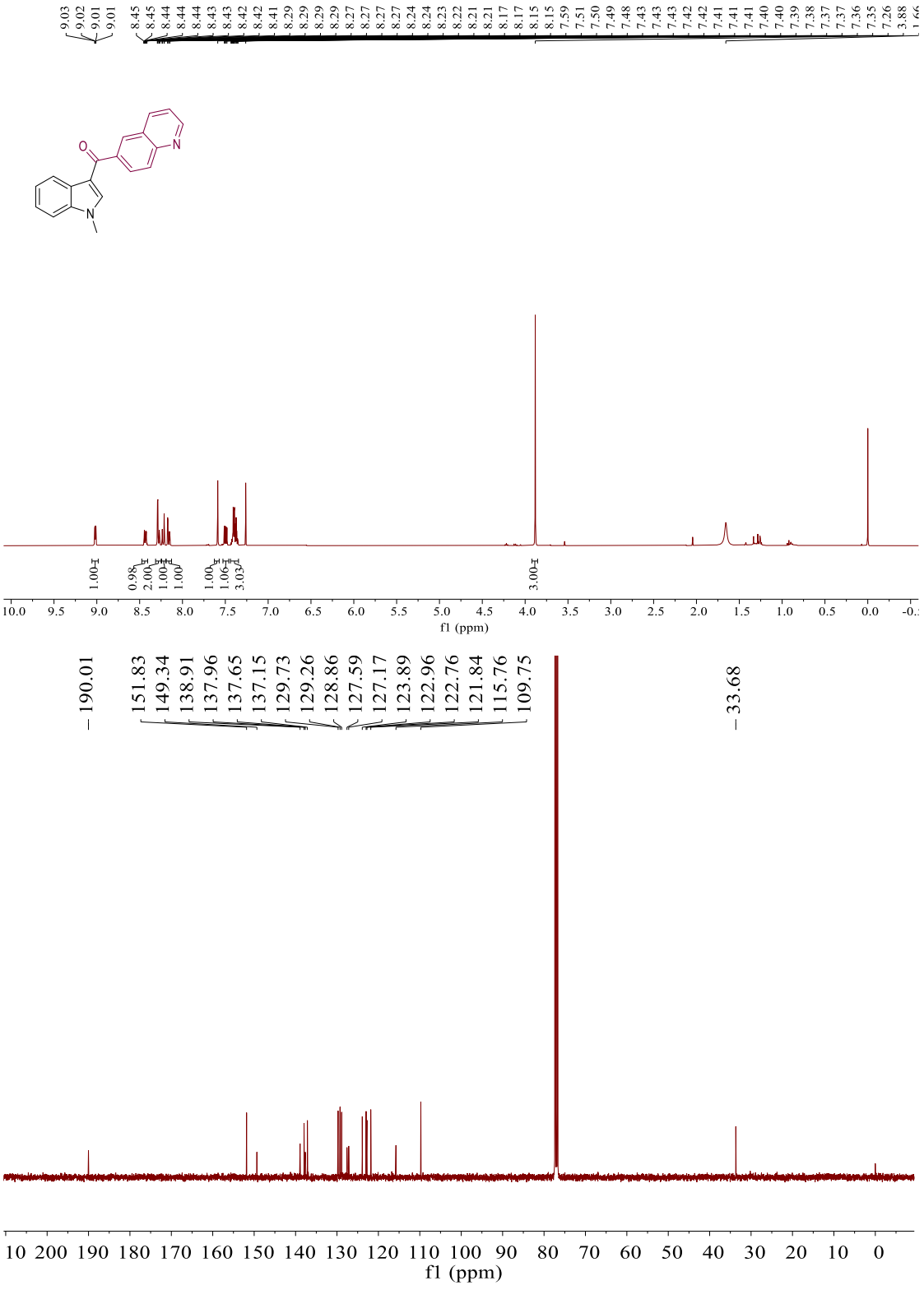




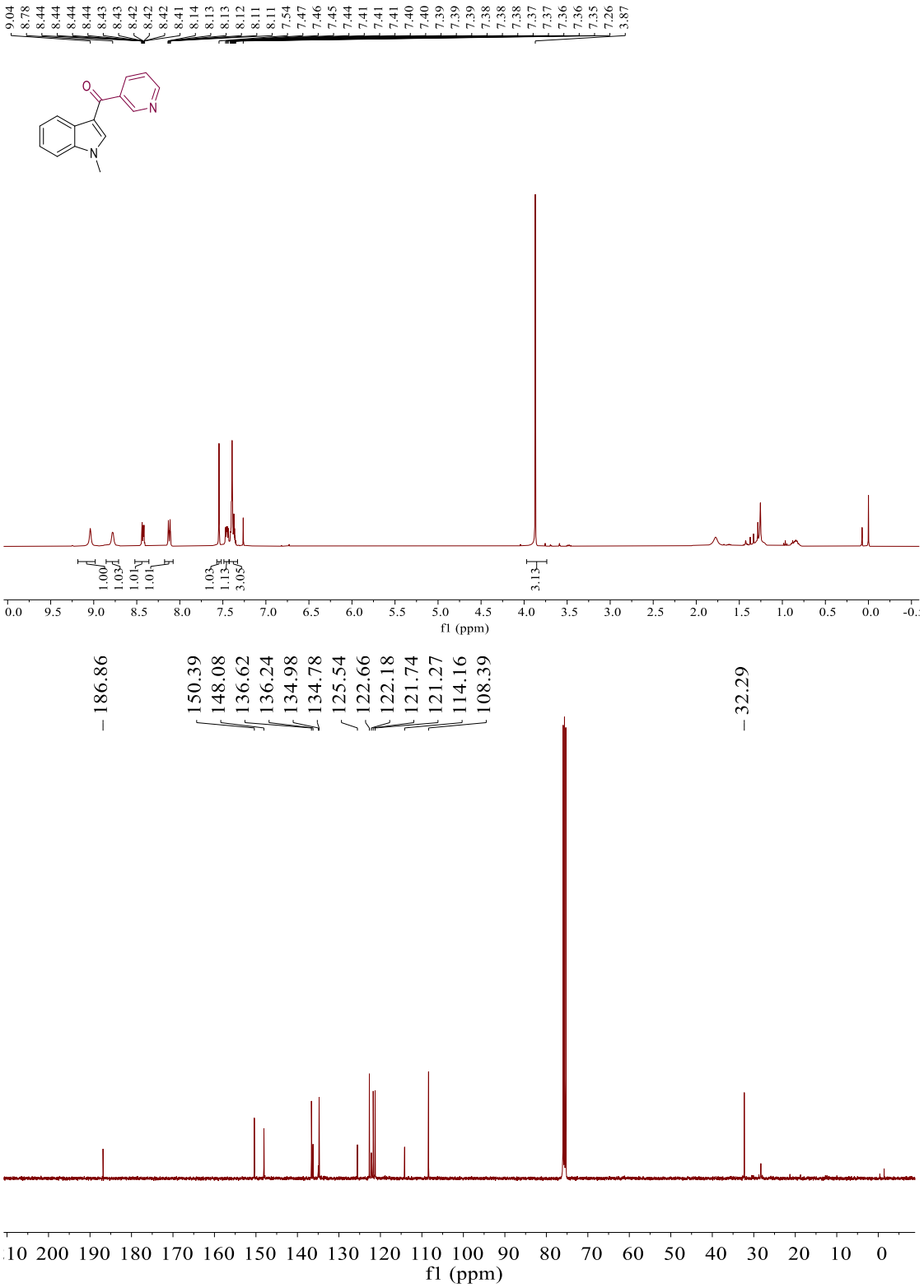




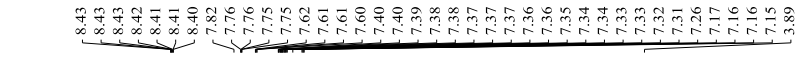
(1-methyl-1H-indol-3-yl)(quinolin-6-yl)methanone **(3q)**

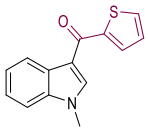


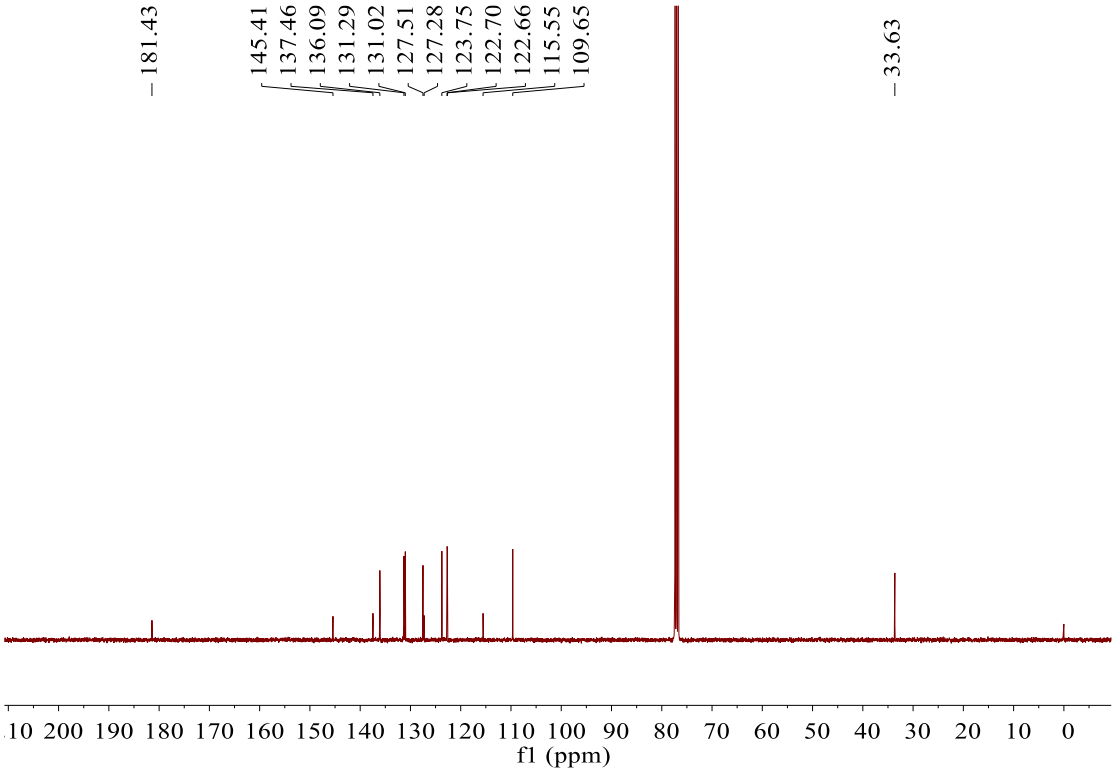
(1-methyl-1H-indol-3-yl)(pyridin-3-yl)methanone **(3r)**



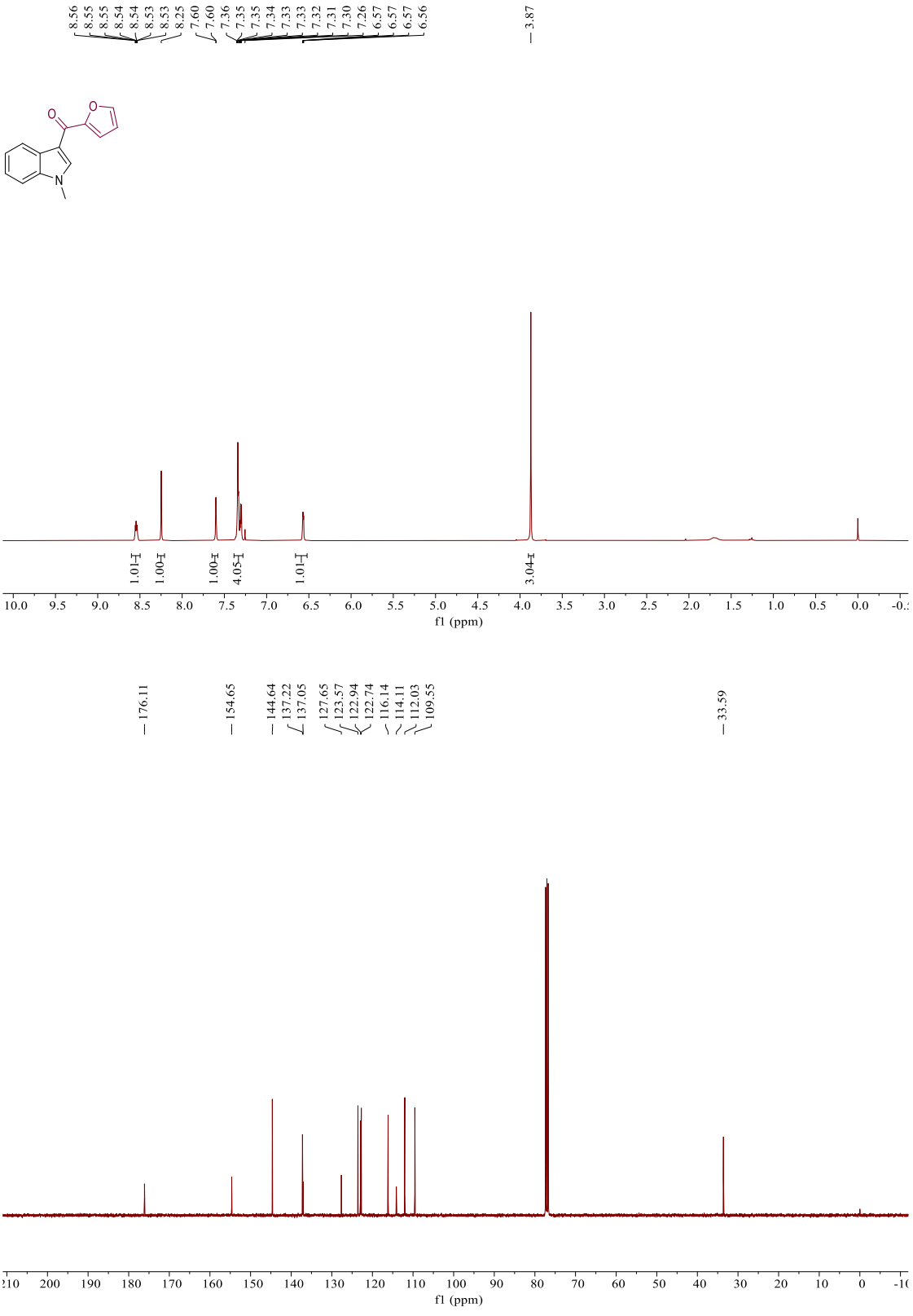
(1-methyl-1H-indol-3-yl)(thiophen-2-yl)methanone **(3s)**



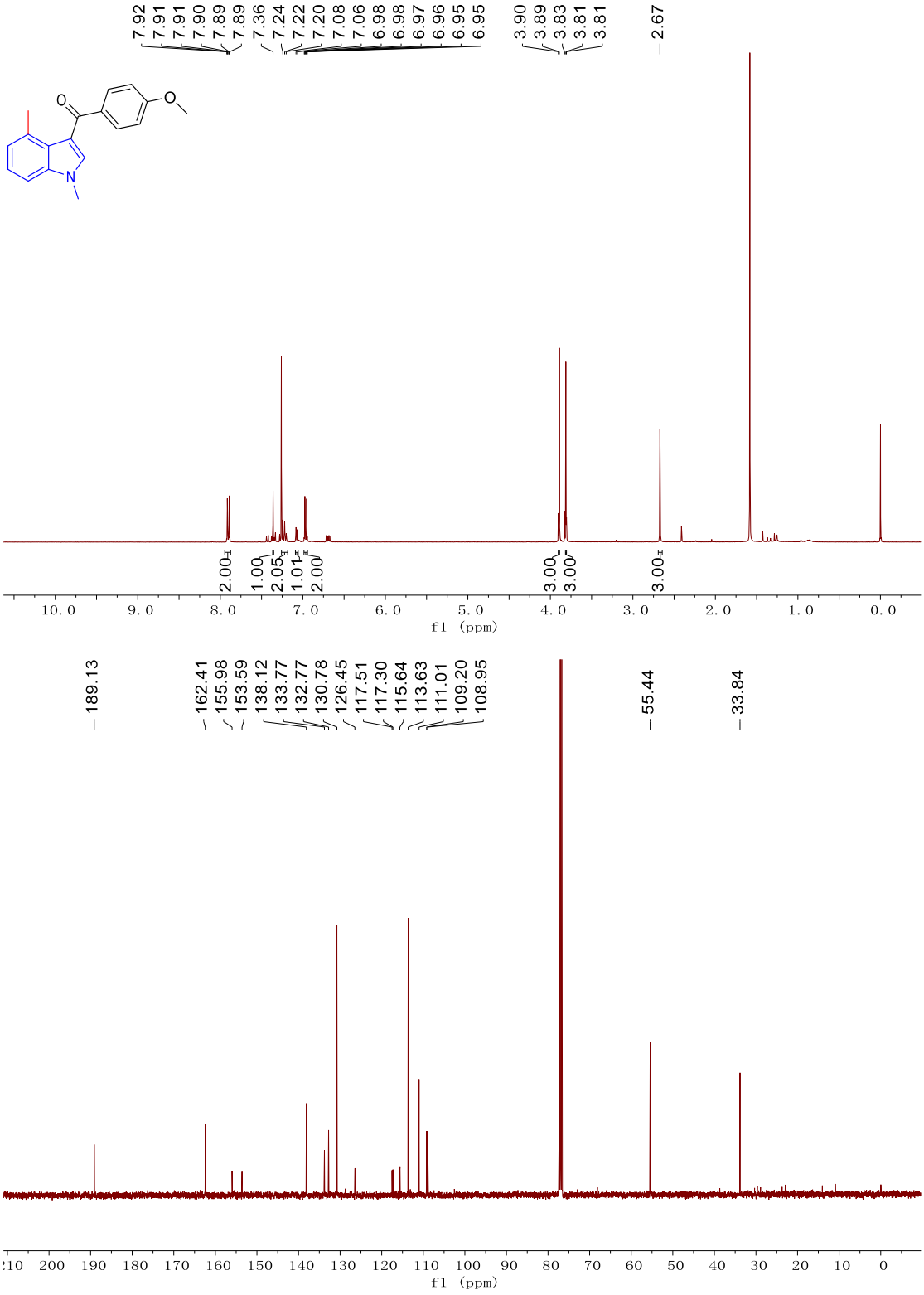




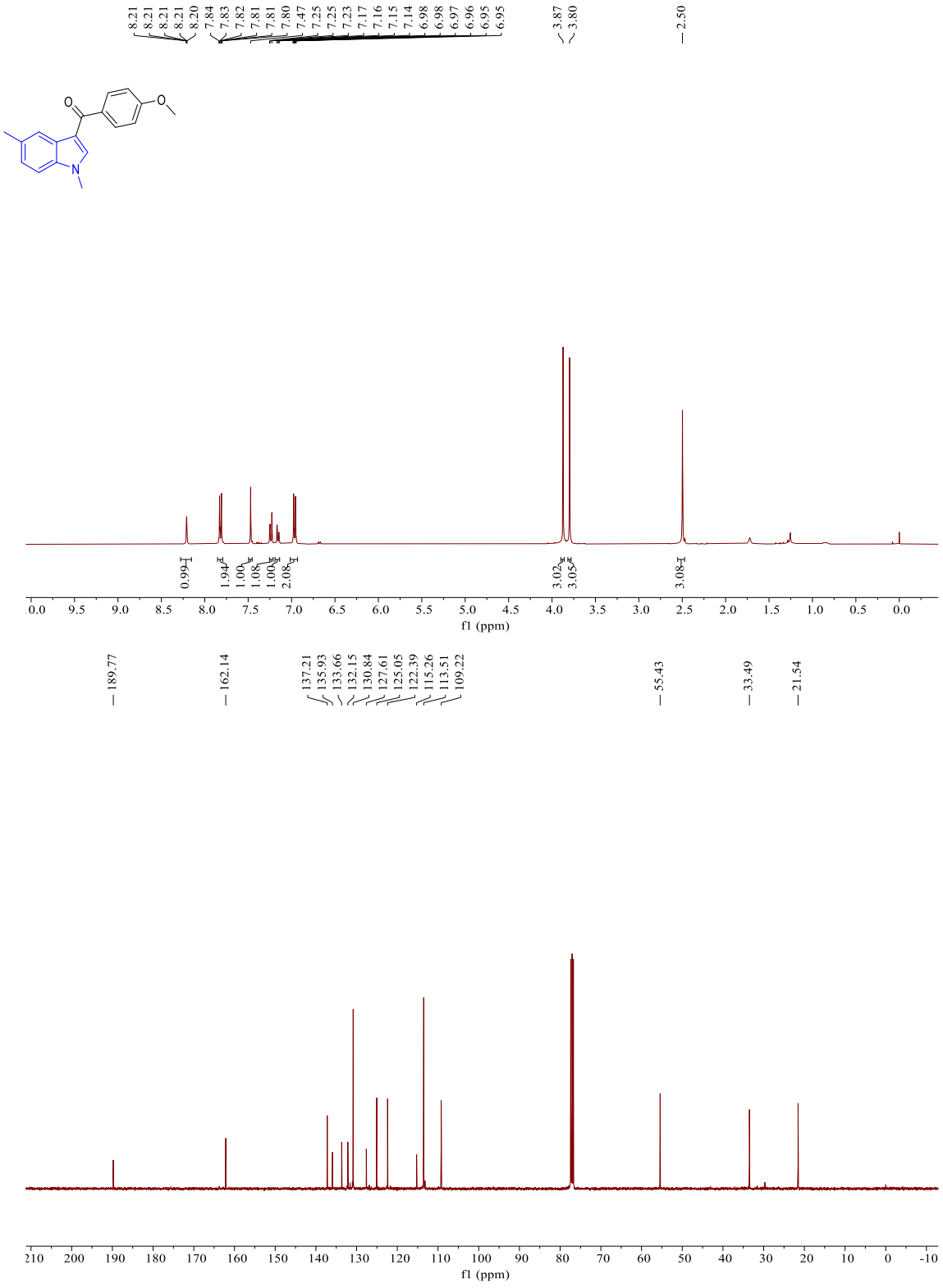
furan-2-yl(1-methyl-1H-indol-3-yl)methanone **(3t)**



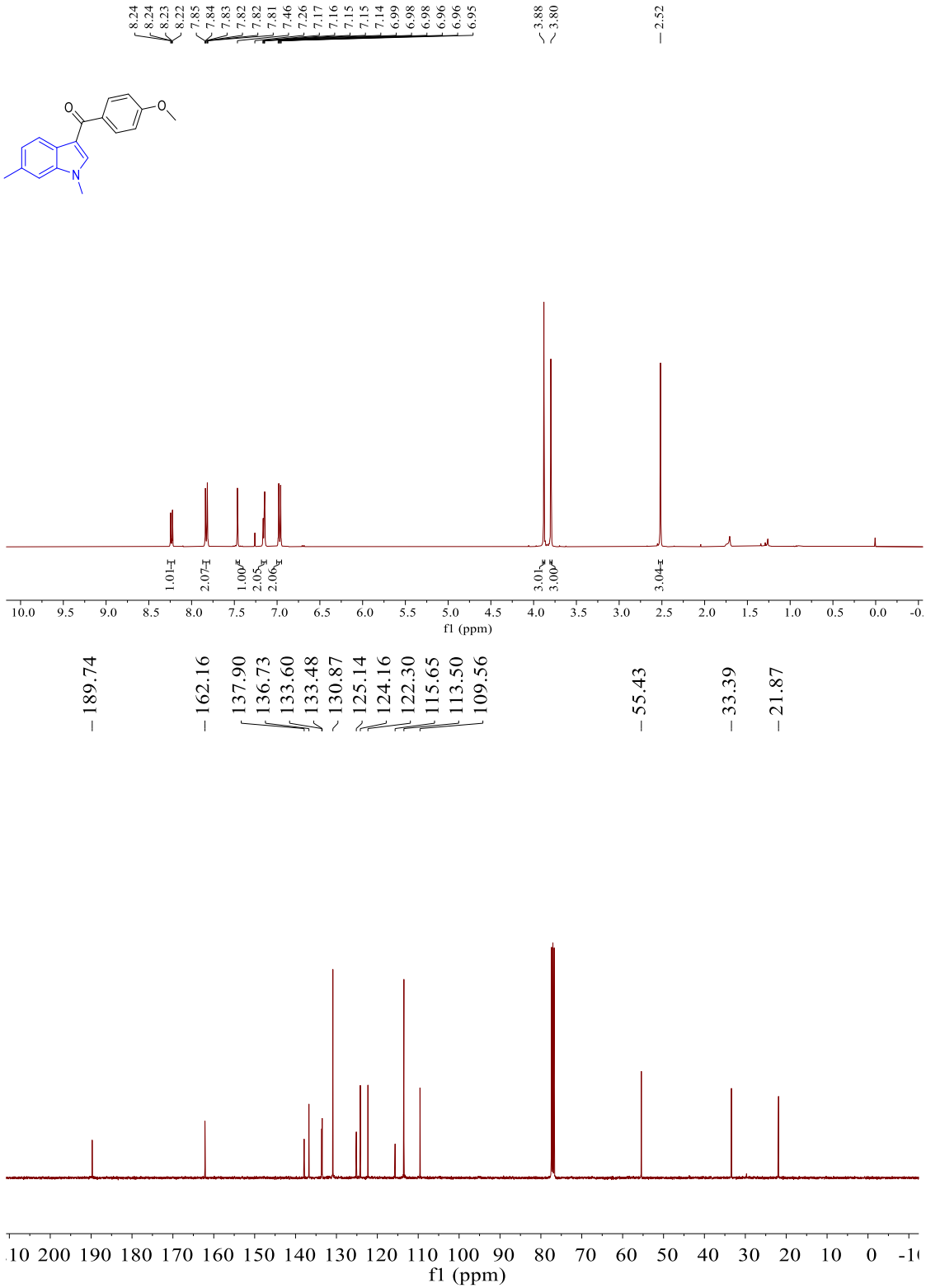
(1,4-dimethyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3u)**



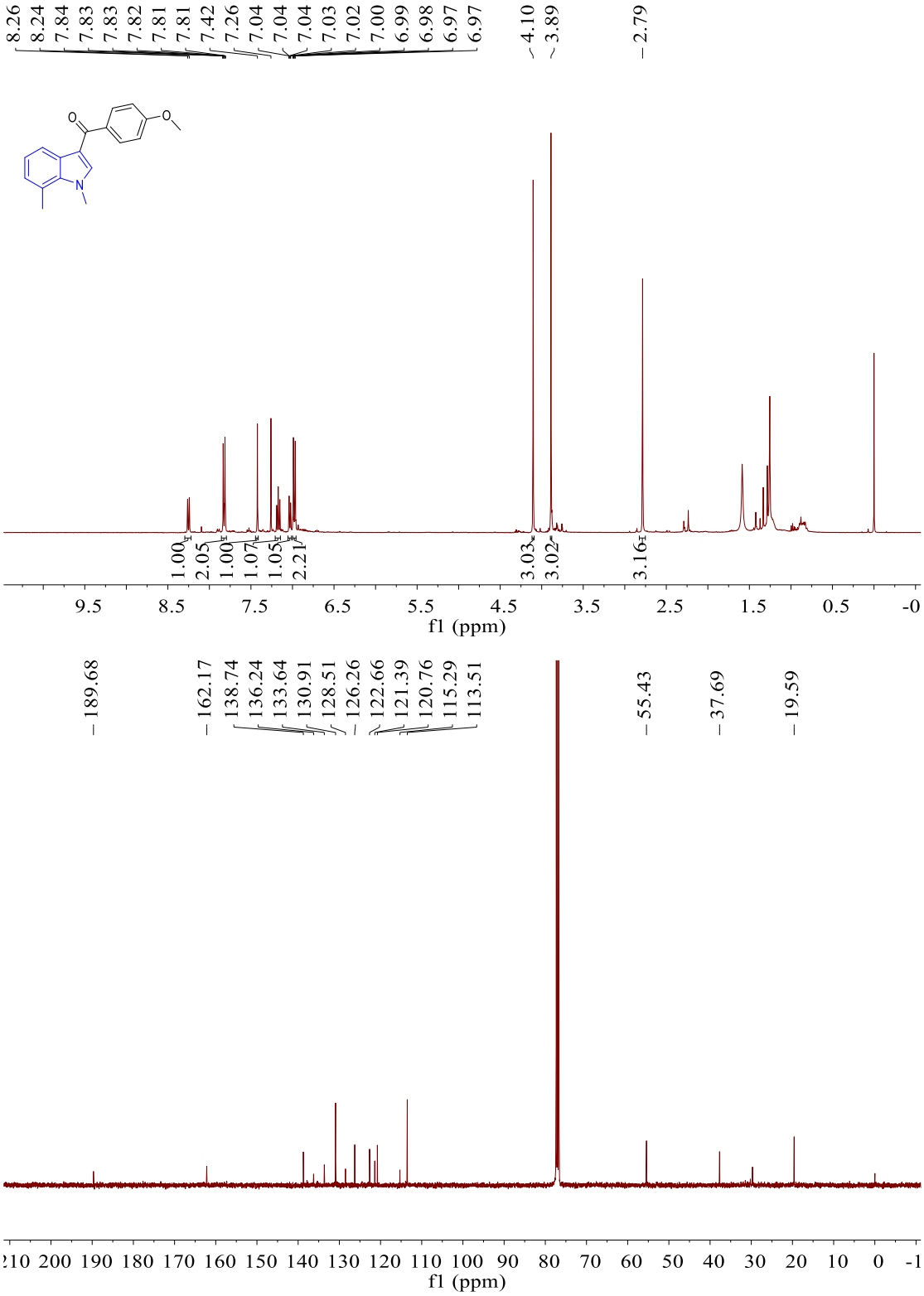
(1,5-dimethyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3v)**



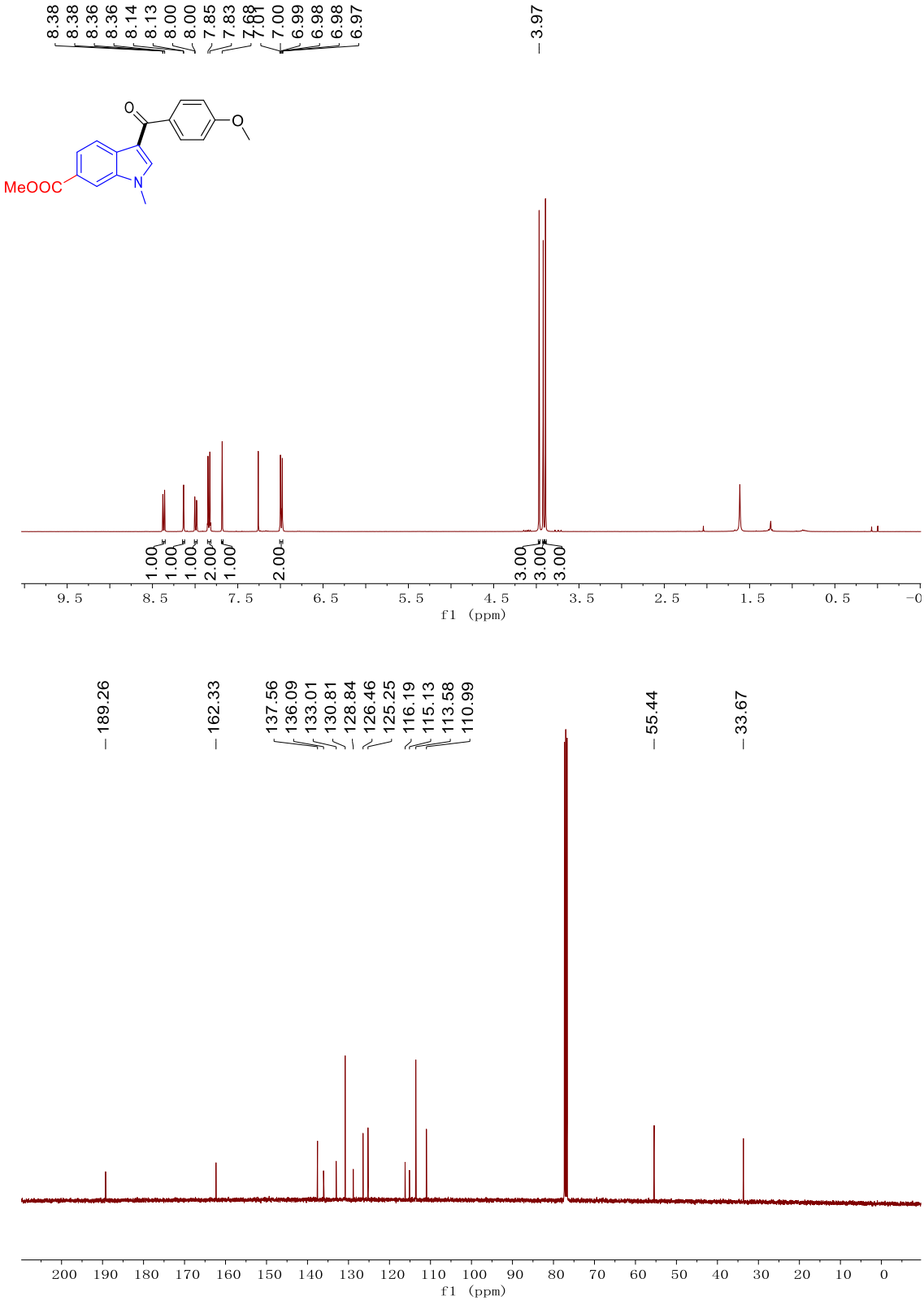
(1,6-dimethyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3w)**



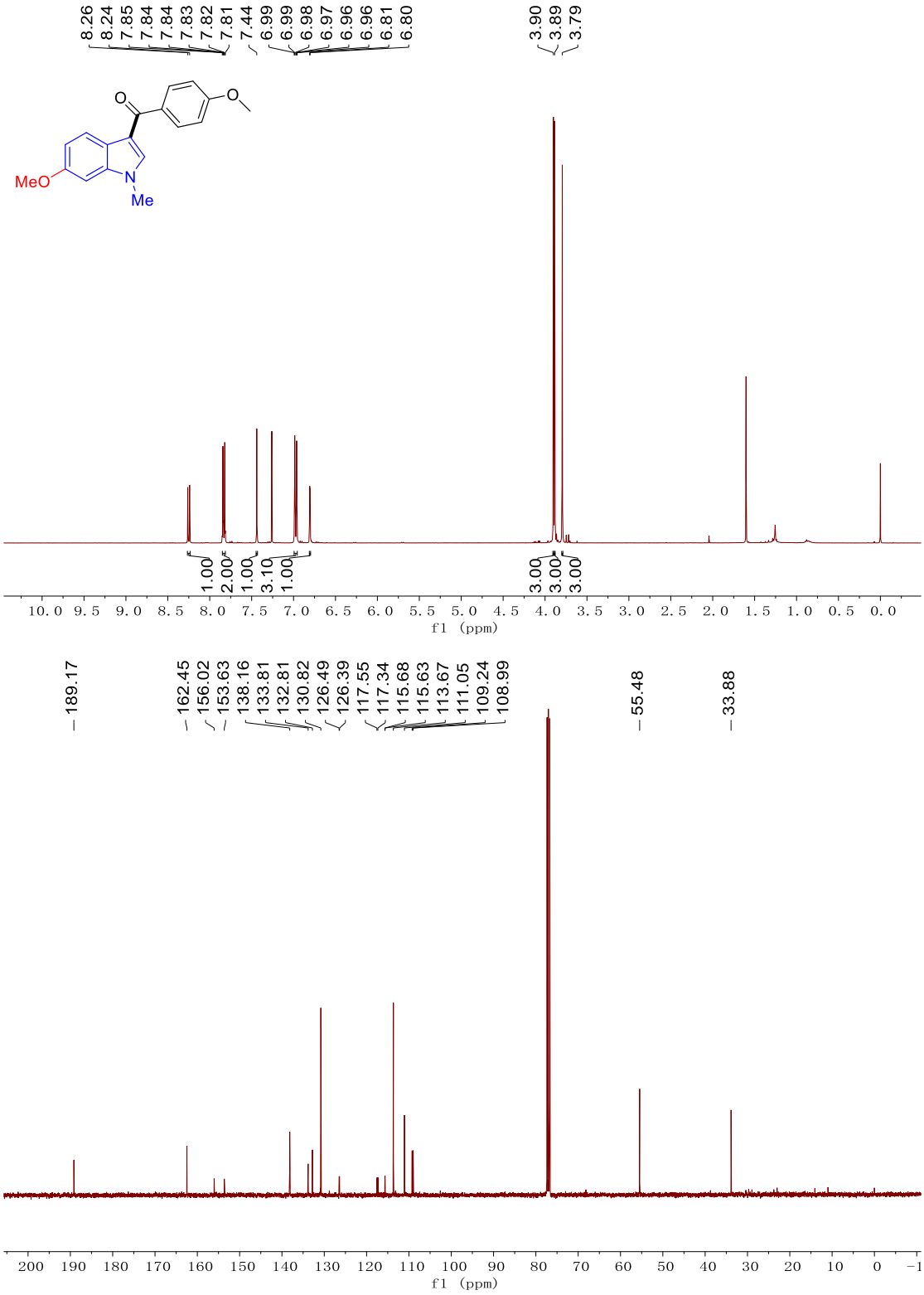
(1,7-dimethyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3x)**



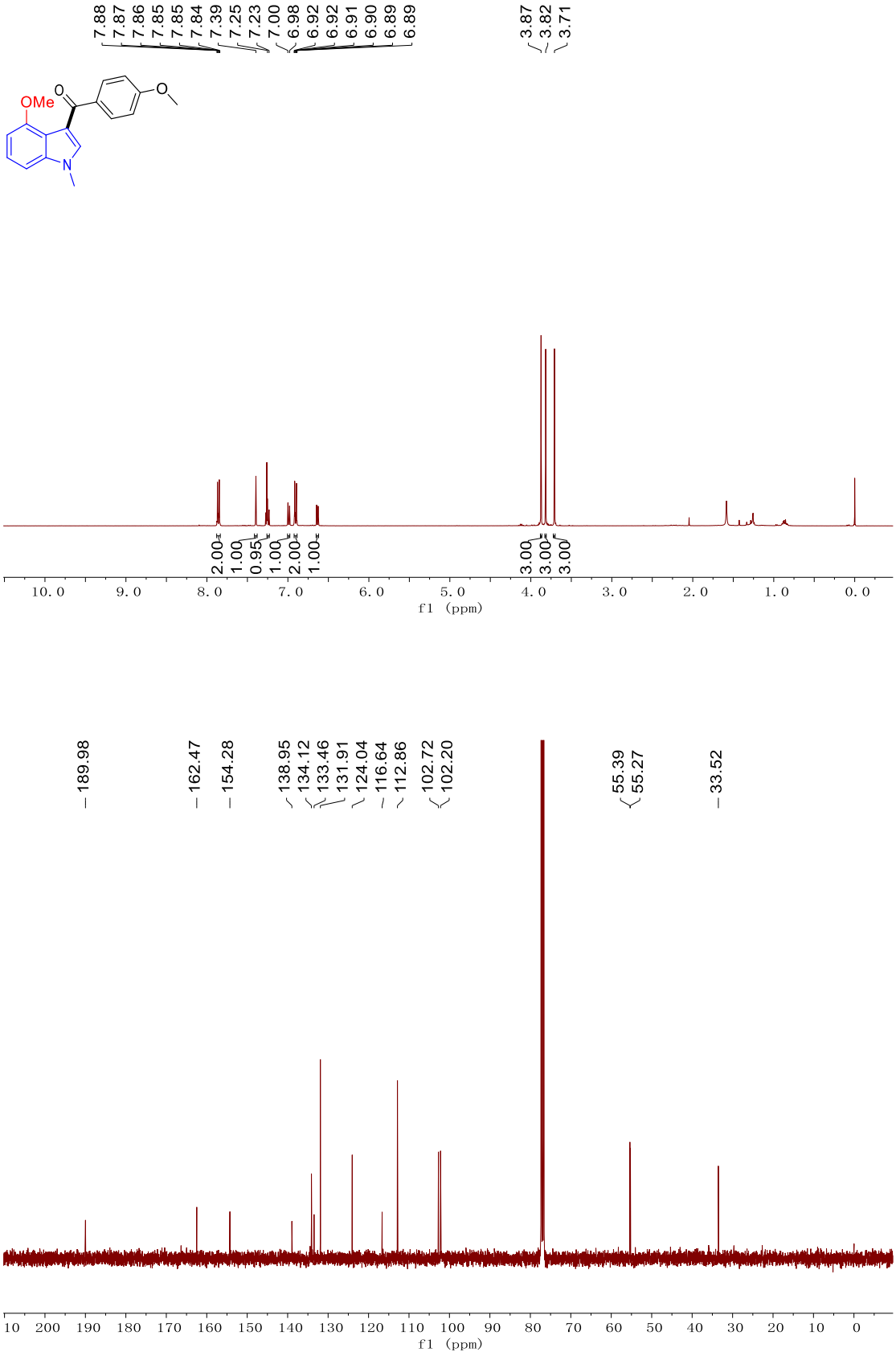
methyl 3-(4-methoxybenzoyl)-1-methyl-1H-indole-6-carboxylate **(3y)**



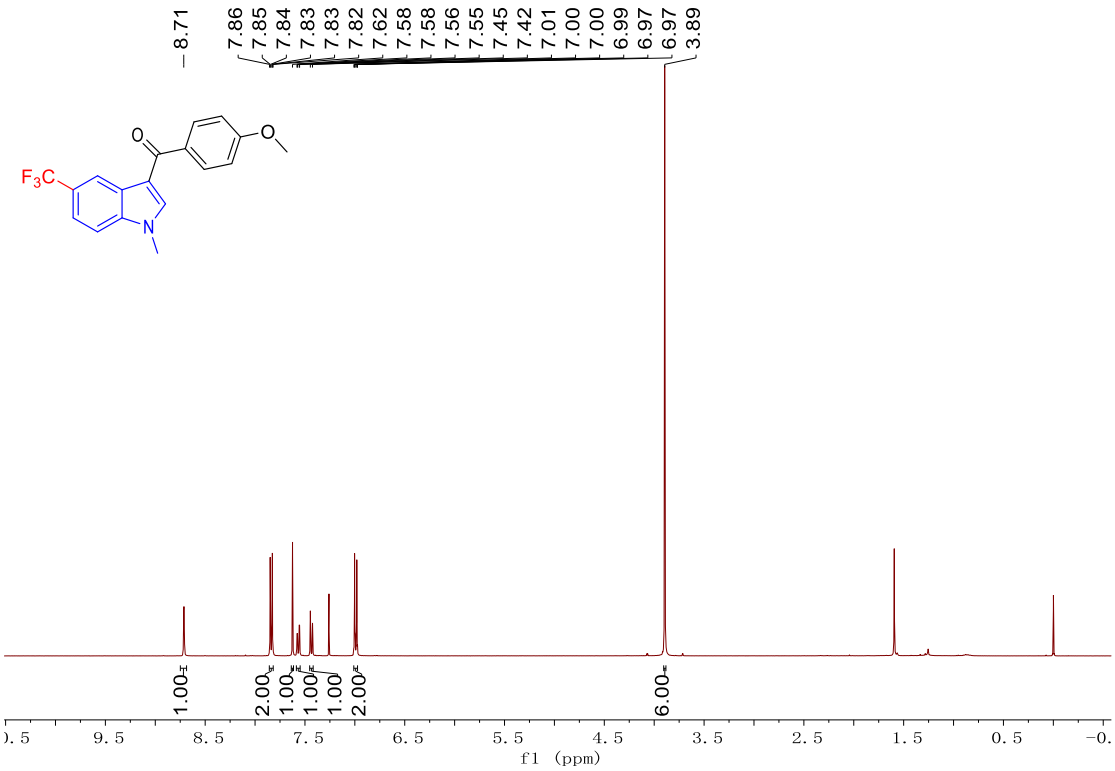
(6-methoxy-1-methyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3z)**

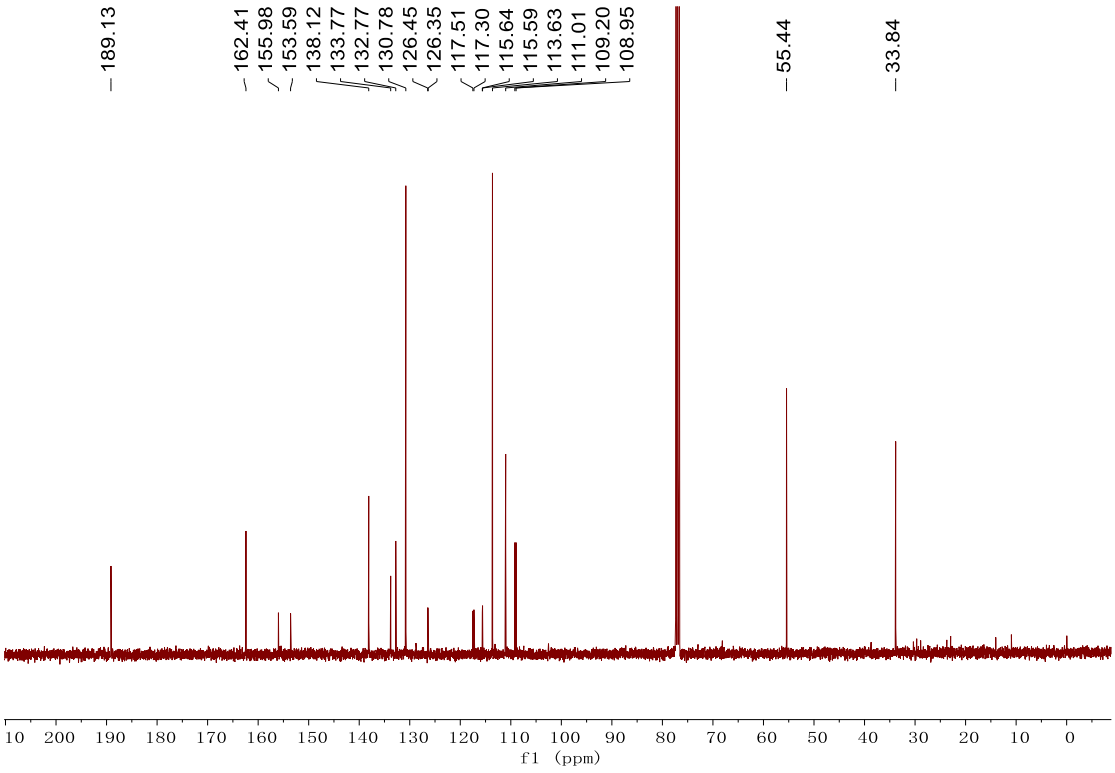


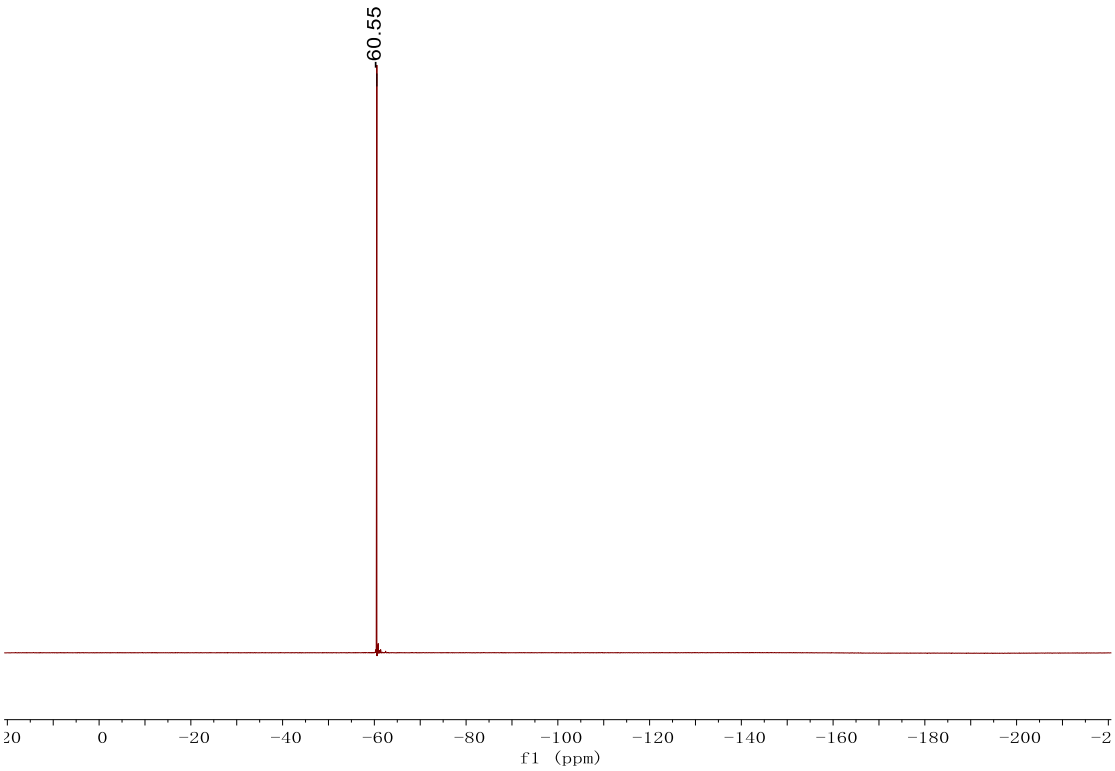
(4-methoxy-1-methyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3aa)**



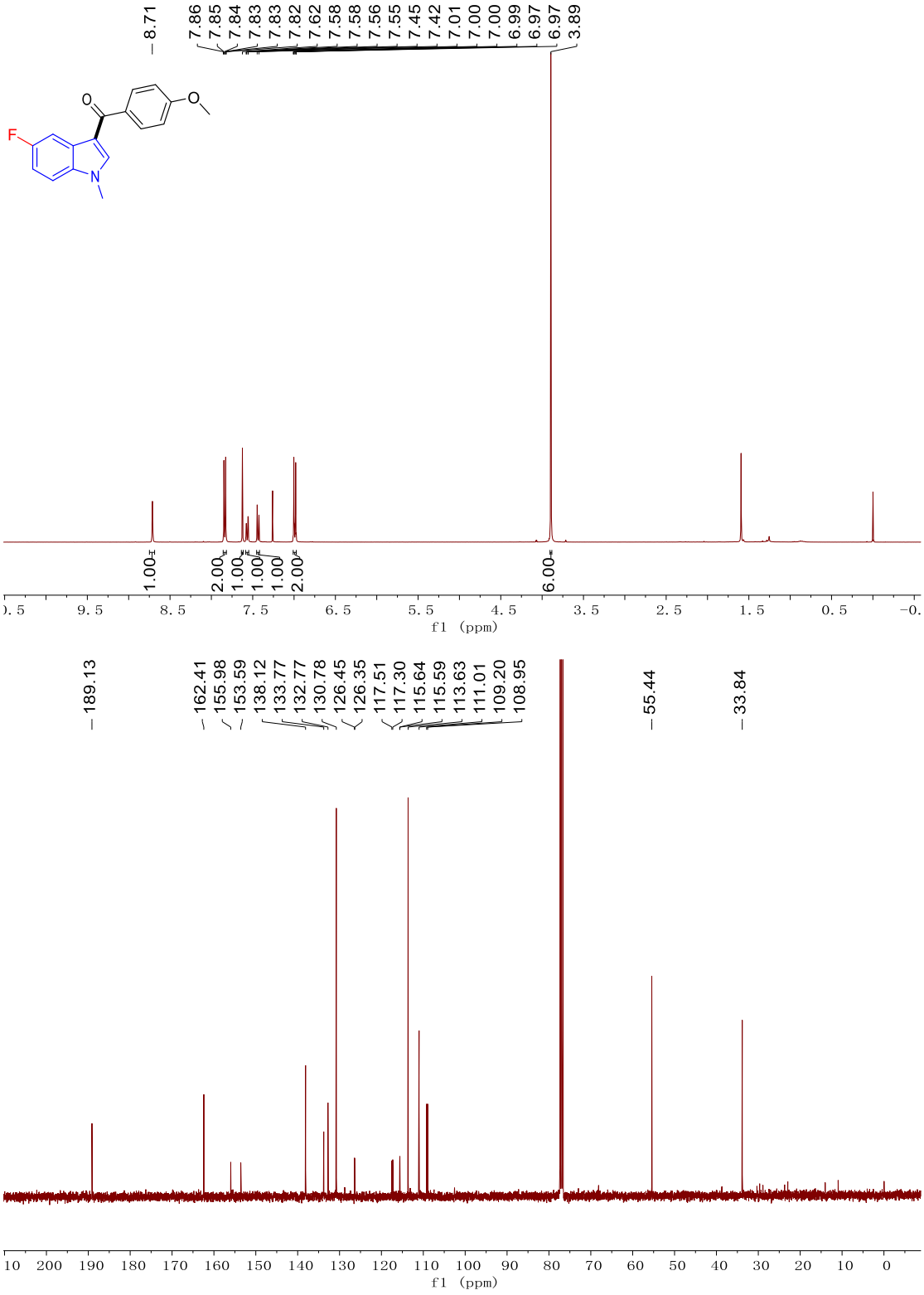
(4-methoxyphenyl)(1-methyl-5-(trifluoromethyl)-1H-indol-3-yl)methanone (3ab)

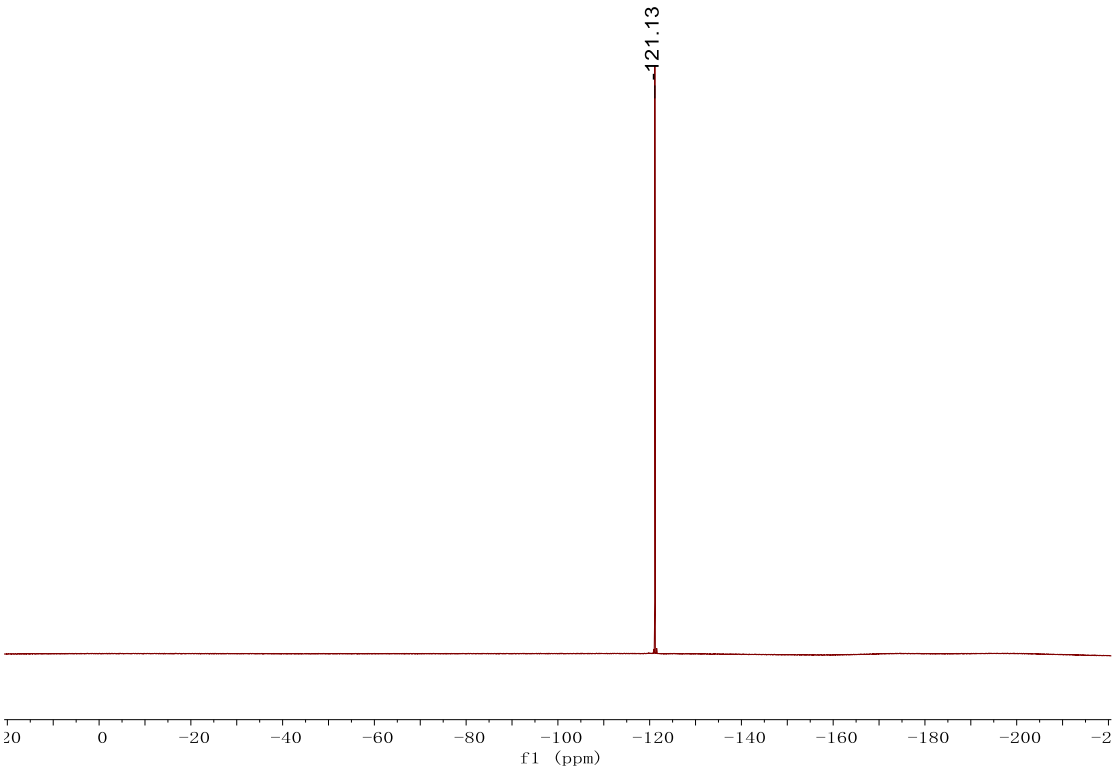




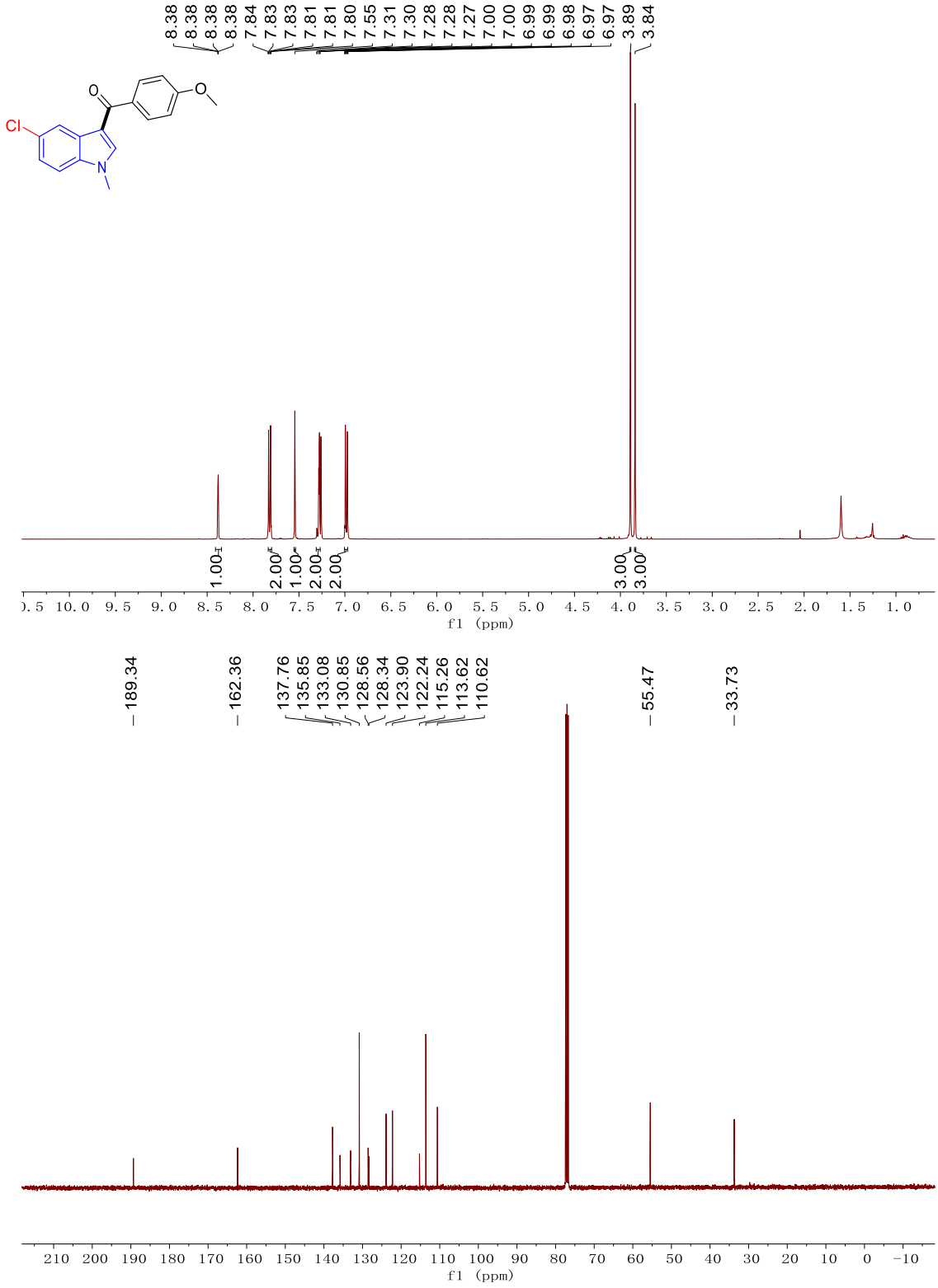

-60.55
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-2
f1 (ppm)

(5-fluoro-1-methyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3ac)**

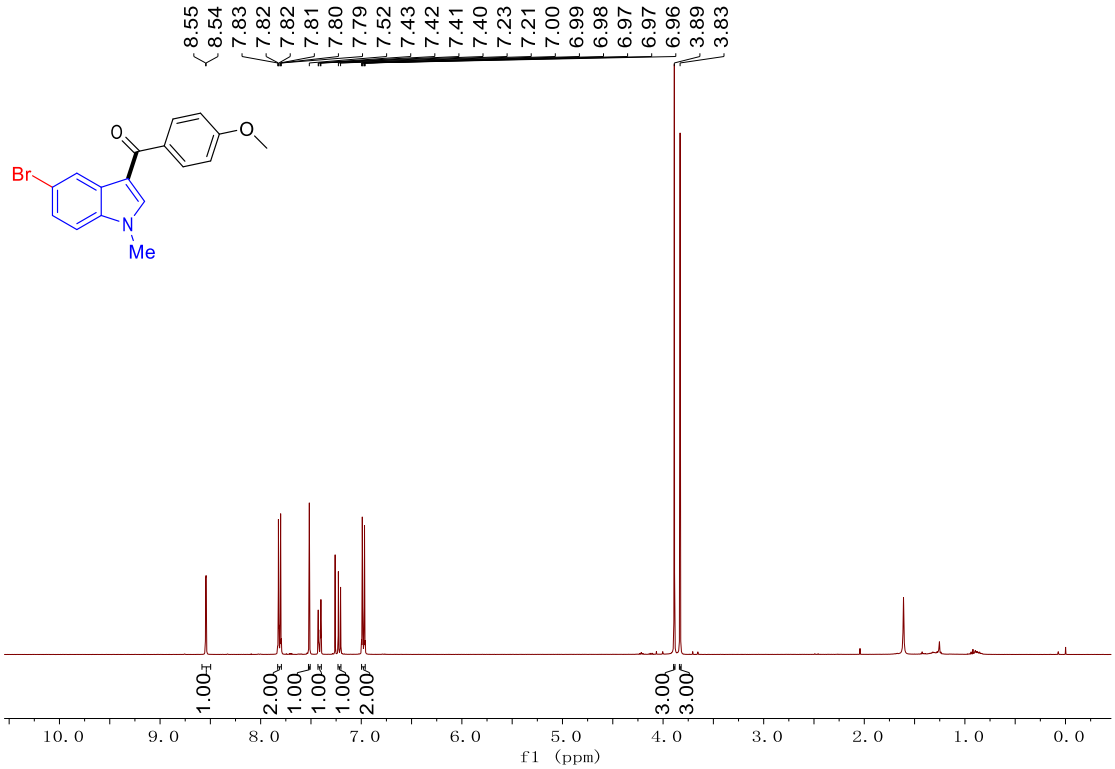


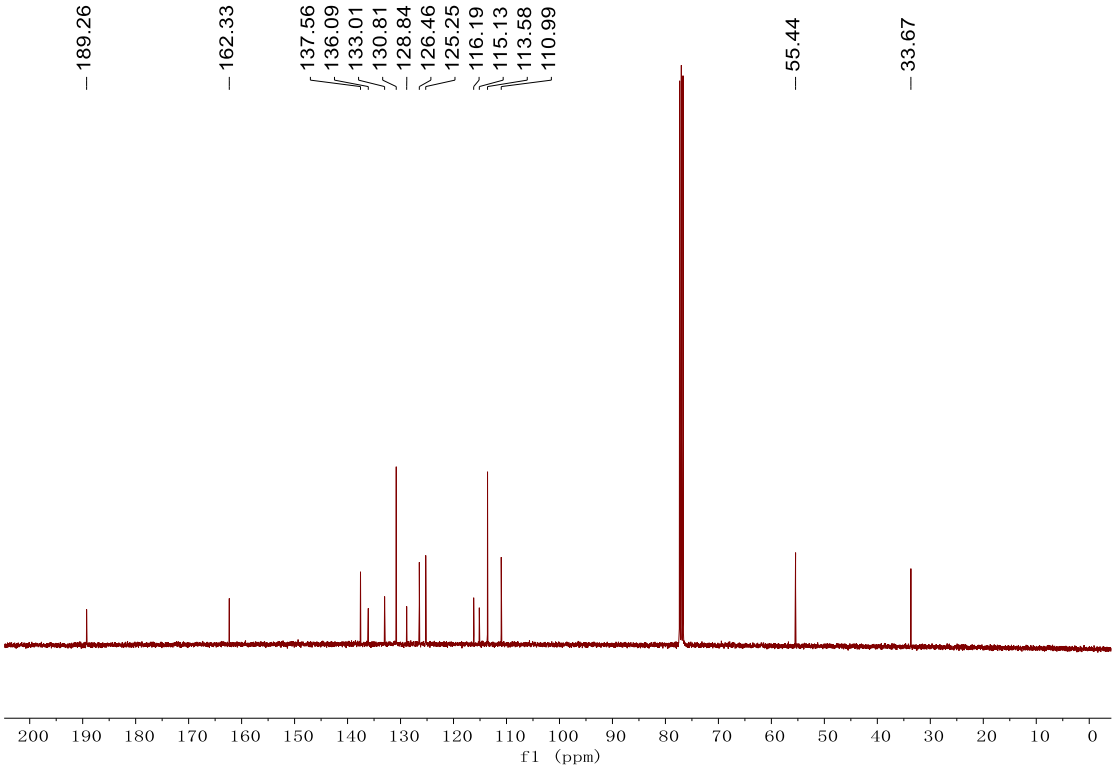

-121.13
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-2
f1 (ppm)

(5-chloro-1-methyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3ad)**

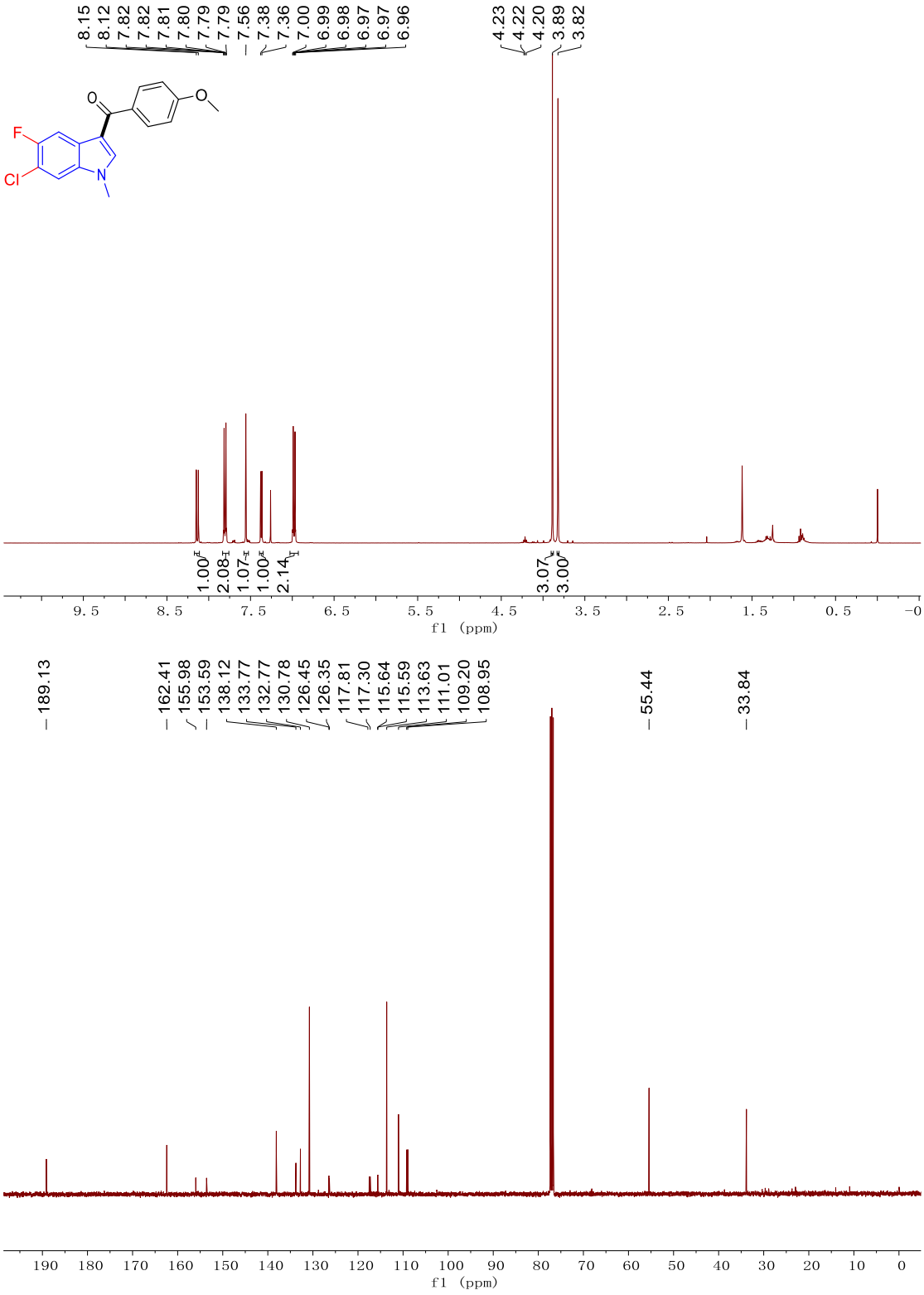


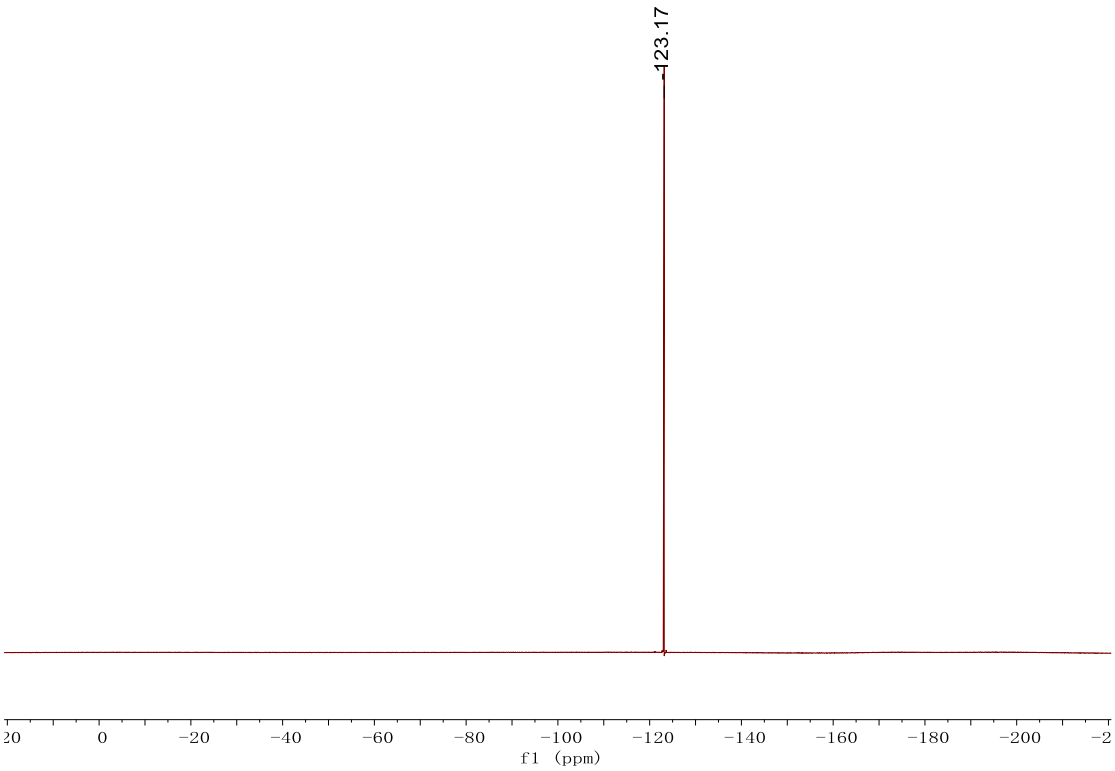
(5-bromo-1-methyl-1H-indol-3-yl)(4-methoxyphenyl)methanone **(3ae)**



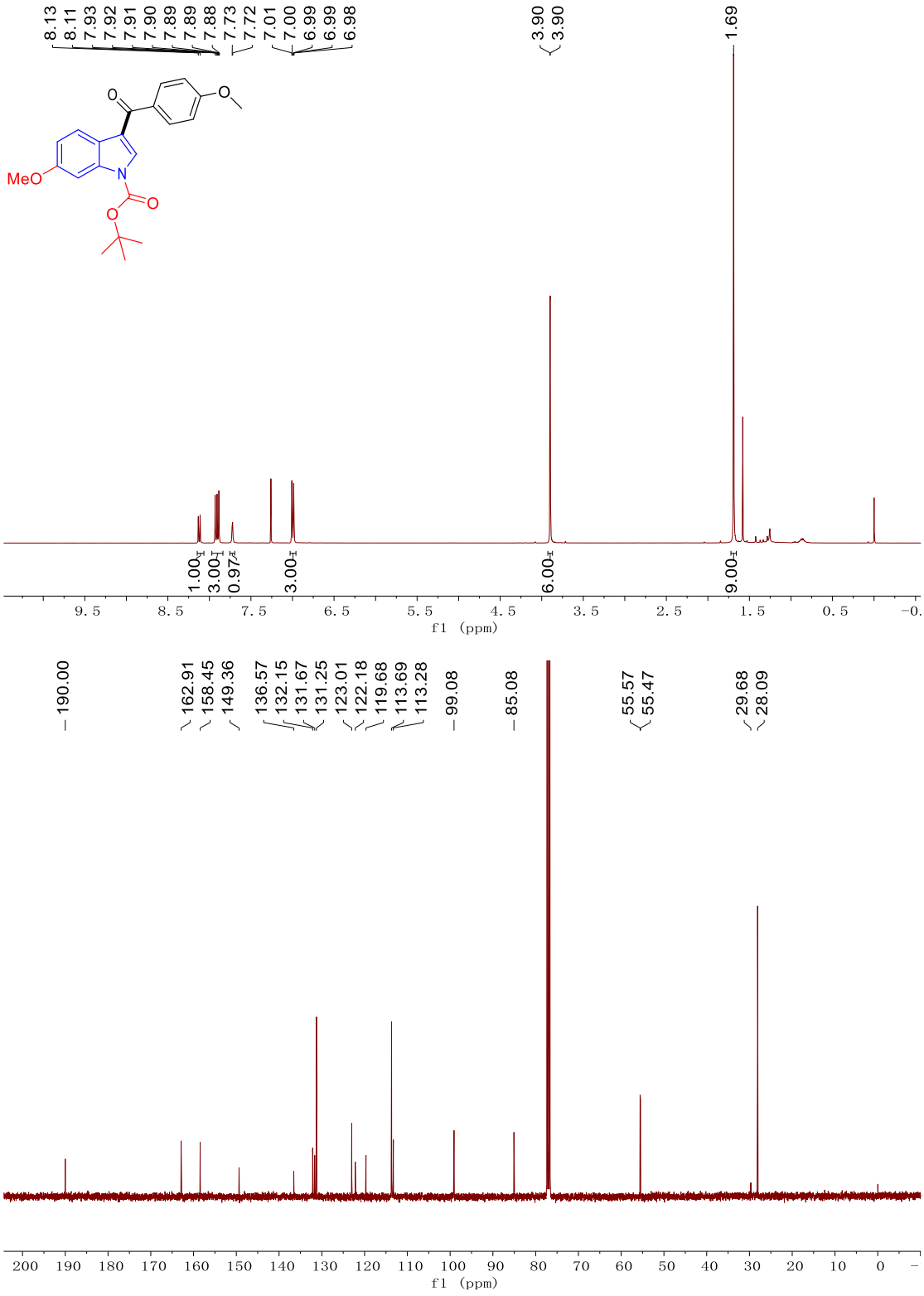


(6-chloro-5-fluoro-1-methyl-1H-indol-3-yl)(4-methoxyphenyl)methanone (3af)

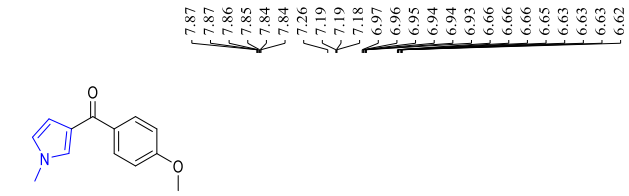


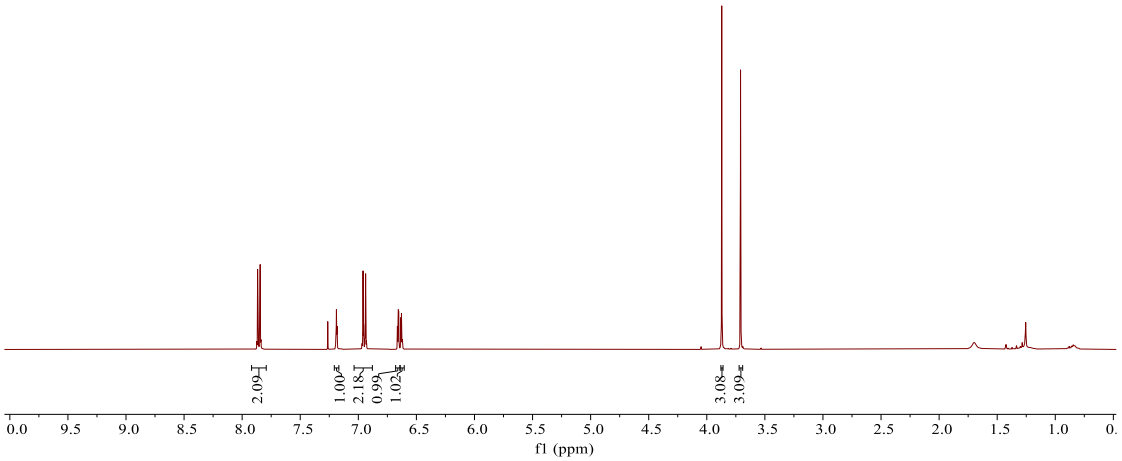

-123.17
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-2
f1 (ppm)

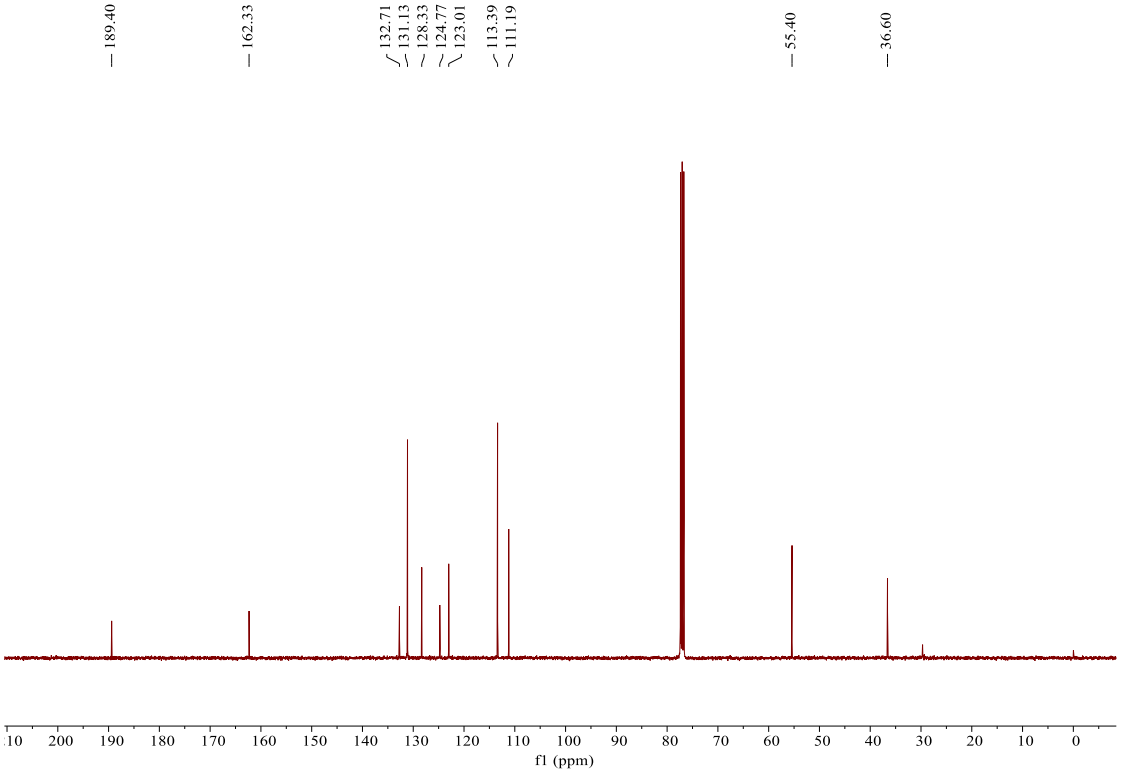
tert-butyl 6-methoxy-3-(4-methoxybenzoyl)-1H-indole-1-carboxylate **(3ag)**



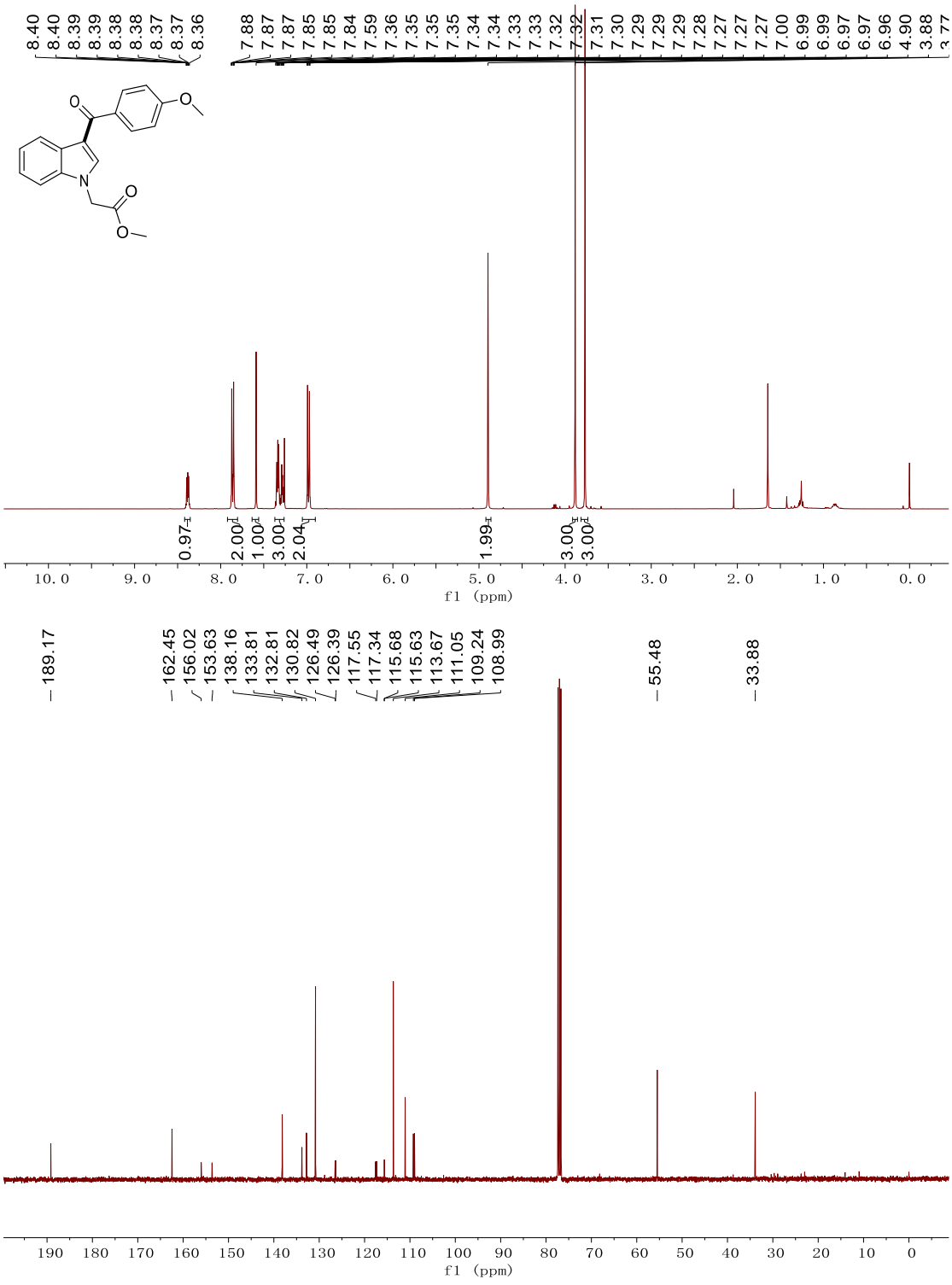
(4-methoxyphenyl)(1-methyl-1H-pyrrol-3-yl)methanone **(3ah)**



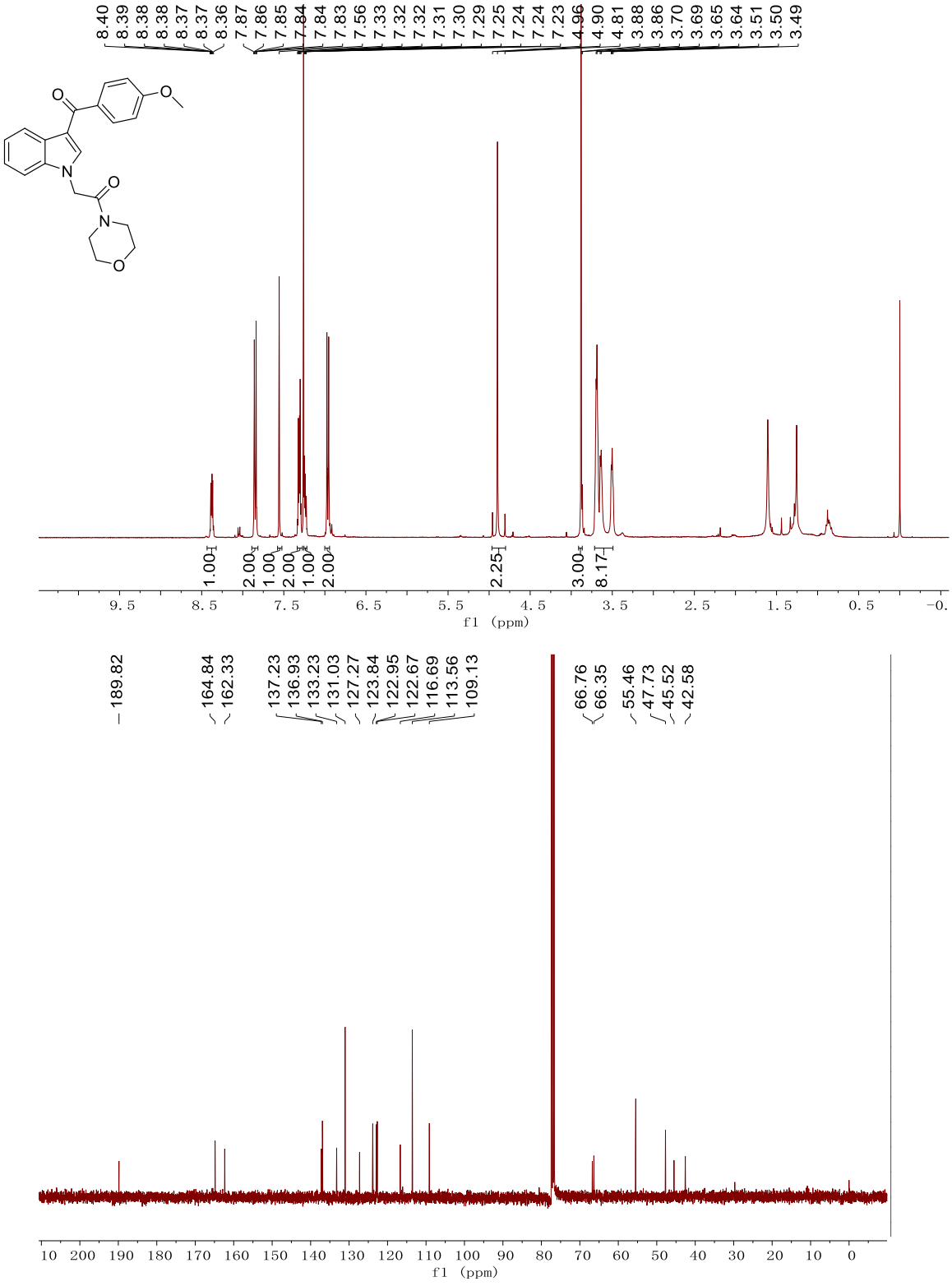




methyl 2-(3-(4-methoxybenzoyl)-1H-indol-1-yl)acetate **(4)**



2-(3-(4-methoxybenzoyl)-1H-indol-1-yl)-1-morpholinoethan-1-one **(5)**



2-methoxy-2-oxoethyl 2-(3-(argiocarbonyl)-1H-indol-1-yl)acetate **(6)**